



Effect of solvent on radical cyclisation pathways: S_{RN}1 vs. aryl-aryl bond forming mechanisms

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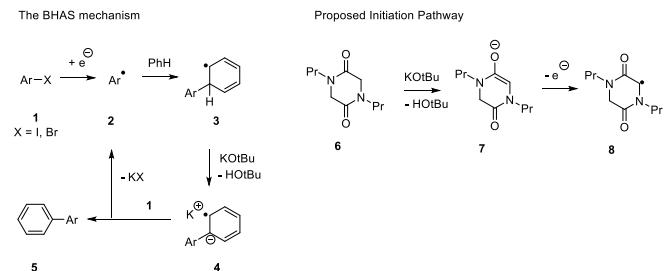
A recent paper identified a series of alternative cyclisation pathways of aryl radicals that resulted from electron transfer to various tethered haloarene–acetylene substrates, in either benzene or DMSO as solvent. The electron transfer occurred from one of two enolates that were formed in the presence of KOtBu: either the enolate of the acetylene, within the haloarene–acetylene substrate, or the enolate **7** of the *N,N'*-dipropyl diketopiperazine (DKP) additive **6**. This paper uses contemporary computational methods to determine the reaction pathways involved; depending on the substrate, the aryl radical underwent (i) S_{RN}1 onto the enolate anion of the acetylene, (ii) aryl-aryl bond formation, (iii) tandem hydrogen atom abstraction followed by S_{RN}1 cyclisation and even (iv) ArC-N cleavage. The influence of the solvent was investigated. In this paper it is shown that the solvent influences which reactive species are present in the reaction mixture, and whether each species acts as an electron donor or an electron acceptor in the radical initiation or propagation steps. The main initiation step is a single electron transfer from the enolate anion **7** of the DKP additive in benzene, but in DMSO the initiation can occur from the enolate anion of the substrate itself. Using computational techniques a deeper understanding of the radical pathways involved has been obtained, which shows how we can use solvent to preferentially access products arising from either S_{RN}1 or aryl-aryl bond formation pathways.

Introduction

The reaction conditions (temperature, pH, solvent, etc.) have a significant effect on both the viability and products of reactions. The choice of solvent affects the chemical reactivity by influencing many factors, such as the rate of reaction (stabilisation of the transition state relative to the starting materials) and the equilibrium (relative stability of the reactants and products), such that changing the solvent may change the preference for competing pathways.¹⁻⁵

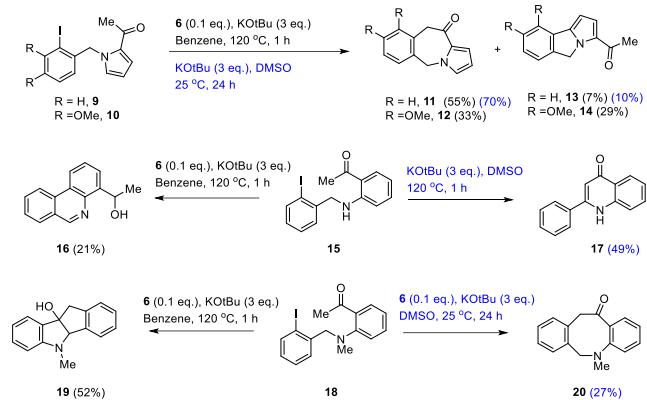
There has been a recent resurgence in the use of radical chemistry within organic synthesis.⁶⁻¹² As part of the resurgence, the transition metal-free formation of biaryl compounds has received increased attention. Typically, these processes involve a haloarene that couples to an aromatic ring, commonly benzene, in the presence of KOtBu and an additive such as *N,N'*-dipropyl diketopiperazine (DKP), **6**.¹³⁻¹⁸ Benzene and pyridine are the most common solvents used in these reactions as they are the coupling partner for the aryl halide in the reactions, and high temperatures are employed to achieve efficient coupling.^{13,15-21} The mechanism by which these coupling reactions occur involves initiation of the reaction *via* a single electron transfer (SET) to the haloarene **1** to form an aryl radical **2**. This aryl radical **2** then attacks a benzene ring in a

base-promoted homolytic aromatic substitution (BHAS) mechanism to form **4** upon deprotonation (Scheme 1).¹⁴ This radical anion **4** propagates the radical chain to yield the product **5** and a new aryl radical **2**. The SET is proposed to occur from an electron donor, such as the enolate anion **7**, which is formed *in situ* from the reaction of KOtBu and an organic additive such as DKP **6**. Alternative partners than benzene have also been shown to couple to the aryl radical **2**, such as alkenes, and carbon monoxide, while enolate anions can undergo coupling to aryl radicals through an S_{RN}1 reaction.²⁰⁻³⁰ Most of these couplings were performed in benzene,¹³⁻²² however it has also been shown that S_{RN}1 coupling to enolate anions can be achieved efficiently in DMSO at room temperature.^{26,30}



Scheme 1. In the BHAS mechanism, the rate determining step is the SET from an electron donor **7**, formed *in situ*, to the haloarene **1**.

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Scheme 2. The products from SET to **9**, **10**, **15** and **18** in benzene (black) or DMSO (blue)

Recent studies in the Murphy laboratory have demonstrated the influence that solvent can have on the cyclisation of an aryl radical onto complex enolate anions, initiated in the ground-state by an additive, DKP **6**.³¹ (This followed a similar study by Rossi *et al.* who used photoactivation to initiate these cyclisations.)³² It was observed that on changing the solvent from benzene to DMSO, the radical cyclisation could be performed at lower temperatures, and in some instances the favoured reaction pathway was changed, resulting in a different product distribution (Scheme 2). The observed strong solvent dependence of these results suggests that these systems represent an excellent case study to probe the various competitive reaction mechanisms and identify what effect the solvent had on these radical cyclisations, as well as specifying the initiation and propagation steps. Through this process, we identify several approaches to tune the reactivity and manipulate the product outcomes by controlling the reaction environment.

Results and Discussion

Methods

The calculations were run using the M06-2X functional³³⁻³⁴ with the 6-311++G(d,p) basis set³⁵⁻³⁹ on all atoms, except for the iodine. Iodine was modelled with the MWB46 relativistic pseudo potential and associated basis set.⁴⁰ All calculations were carried out using the C-PCM implicit solvent model⁴¹⁻⁴² with the dielectric constant for benzene ($\epsilon=2.2706$) or DMSO ($\epsilon=46.826$) as appropriate. All calculations were performed in Gaussian09.⁴³ After optimisation, all equilibrium structures were subjected to a frequency calculation to characterize the optimized structures as minima or transition states, where the transition states were found to each have a single imaginary frequency. In addition, the vibrational frequencies were used to obtain temperature corrected (298.15 K) energies, enthalpies, entropies, and free energies

The Initiation Step

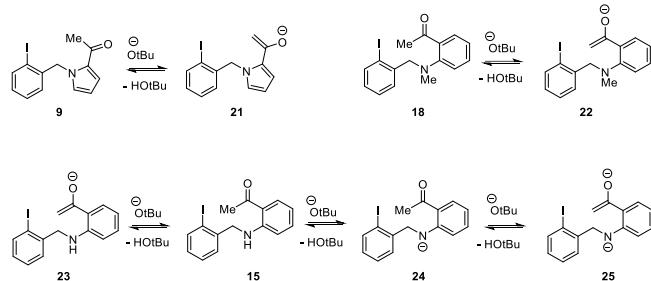
In the presence of KOtBu the substrates **9**, **15** and **18** are present in equilibrium with their deprotonated forms (Scheme 3).

However, the position of this equilibrium will depend upon the reaction environment and, in particular, on the choice of solvent. The energetic barrier, ΔG^* , and the relative energies between the starting material and products, ΔG_{rxn} , for the deprotonation of the substrates **9**, **15** and **18** by KOtBu, in both DMSO and benzene, are displayed in Table 1.

The results show that under the basic reaction conditions, the substrates **9** and **18** will predominantly exist as their respective enolate anions **21** and **22**, in both benzene and DMSO. It should be noted that the deprotonation of **10** was not modeled since it has a very similar structure to **9**. In the deprotonation of substrate **15**, the solvent is playing a key role in differentiating the major species present in the reaction mixture. That is, **15** can potentially form three deprotonated species that may all be present in equilibrium, which are the enolate anion **23**, the N-deprotonated species **24** and the doubly deprotonated enolate anionic species **25**. In benzene, the major species present in the reaction mixture will be **24**, whereas in DMSO the major species will be **25**, as displayed in Scheme 3.

There are different possible ways that these substrates, represented by a generic molecule **26**, could form the cyclized products under the ground-state conditions in the presence of a base (Scheme 4):

1. The benzyne formation pathway.⁴⁴ The base would react with



Scheme 3. The various deprotonation states of the substrates **9**, **15** and **18**

Table 1. The energetics for the deprotonation of substrates **9**, **15** and **18** in the presence of the butoxide anion (OtBu), in both benzene and DMSO

Equilibrium [a]	Benzene ΔG^* (kcal/mol)	Benzene ΔG_{rxn} (kcal/mol)	DMSO ΔG^* (kcal/mol)	DMSO ΔG_{rxn} (kcal/mol)
9 – 21 [21 – 9]	+ 2.5 [+ 8.0]	- 5.5	+ 2.2 [+ 10.8]	- 8.6
15 – 23 [23 – 15]	+ 1.8 [+ 9.9]	- 8.1	+ 1.5 [+ 11.8]	- 10.3
15 – 24 [24 – 15]	0.0 [+ 9.0]	- 9.0	0.0 [+ 10.4]	- 10.4
24 – 25 [25 – 24]	+ 4.5 [+ 1.0]	+ 3.5	+ 4.7 [+ 9.8]	- 5.1
18 – 22 [22 – 18]	+ 1.0 [+ 11.0]	- 10.0	+ 1.2 [+ 10.7]	- 9.5

[a] The equilibrium was also calculated using KOtBu (Supporting Information, Figure S1).

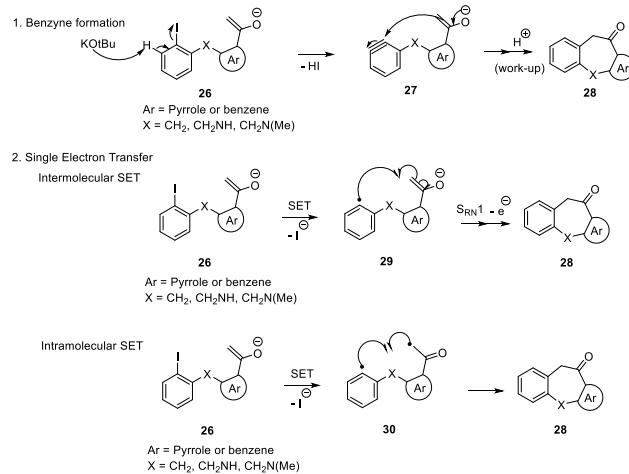
substrate **26**, to deprotonate the proton *ortho* to the iodine and therefore eliminate HI and form a benzyne intermediate **27**. Cyclisation of the enolate onto the benzyne yields **28** upon protonation during work-up.

2. Intermolecular SET to the haloaryl moiety of **26** would yield the aryl radical **29** upon loss of the iodide anion (initiation). The aryl radical would cyclise onto the enolate *via* an $S_{RN}1$ mechanism to yield **28** upon loss of an electron (propagation).

3. Another possibility is intramolecular SET, from the enolate anion to the haloaryl moiety, which will form intermediate **30**. Radical recombination will lead to the product **28**.^{45,32} Experimentally it was shown that substrate **10**, which can only be activated by SET and is incapable of undergoing benzyne formation, was able to cyclise to form **12** and **14**, albeit with lower product yields than the cyclisation of **9**.^{31,46} Therefore SET is implicated in the conversion of substrates **9**, **15** and **18** to form the aryl radical, like **29**. However, in view of the lower yield from substrate **10**, we did not immediately rule out the benzyne mechanism contributing to these results in appropriate substrates. Therefore we modelled the benzyne formation pathway from **21** in DMSO (Supporting Information, Scheme S1.3). The formation of the benzyne intermediate from **21** was calculated to be unfavourable, with a Gibbs free energy, $\Delta G_{rxn} = 18.4$ kcal/mol. Although this benzyne formation is an endergonic reaction pathway, the calculated ΔG_{rxn} would be accessible at room temperature in DMSO (Supporting Information, Scheme S1.3). Furthermore the cyclisation of the enolate anion onto the benzyne intermediate to form the product **11** was calculated to be barrierless and exergonic, $\Delta G_{rxn} = -53.9$ kcal/mol. This suggests that the benzyne pathway may contribute to the formation in **11** in DMSO, albeit as a minor pathway.

The reactive species that are susceptible to an initiation by SET were identified by analysis of the LUMOs of the neutral substrates and their respective deprotonated species (Supporting Information, Table S1.3). For **21**, **23**, **24**, **22** and the enolate anion of **10**, the LUMOs reside on the C-I σ^* in both benzene and DMSO. Therefore SET to these species will give cleavage of the C-I bond and the formation of the aryl radical, analogous to **29** or **30** (depending on whether the SET was intermolecular or intramolecular). For the neutral species **9** the LUMO is delocalized over the molecule, partly residing on both the C-I σ^* and the haloaryl π^* orbitals.⁴⁷⁻⁴⁹ Interestingly the LUMO of the doubly-deprotonated species **25** was different in the two solvents. In DMSO the LUMO resided on the C-I σ^* orbital, whereas in benzene the LUMO did not reside on the C-I σ^* , and it was actually the LUMO+2 orbital that did. Murphy *et al.* proposed that the electron donor is the enolate anion of the DKP additive, **7**, or, in some cases, the enolate anion of the substrates themselves, such as **21**, **22** or **25**. Therefore, the HOMOs of the enolate anion of DKP **7** and the enolate anions of the substrates were analysed and, as expected, they reside on the electron-rich enolate anion moieties (Supporting Information, Table S1.3).^{16,31}

To determine whether the enolate anion of DKP **7** is the electron donor, or whether the enolate anions present in the substrates themselves donate an electron, the energetics for the single



Scheme 4. Possible initiation pathways for the cyclisation of the substrates (applicable to substrates **9**, **15** and **18**)

electron transfer were calculated.^{50,51-53} We investigated the Gibbs free energy profile, both the barrier, ΔG^* , and the relative energy, ΔG_{rxn} , for SET using Marcus Hush theory⁵⁴ in our model systems considering the different polarising ability of the benzene and DMSO solvent *via* the C-PCM implicit solvent model.

In benzene, SET from **7** to **21**, (the enolate of **9**) has an energetic barrier of 34.3 kcal/mol, whereas in DMSO the barrier for SET is much lower, 22.7 kcal/mol (Table 2 and Supporting Information, Table S1.6). Therefore by changing the solvent from benzene to DMSO, a lower energetic barrier is obtained, which is accessible at room temperature. Experimentally it was shown that the reaction can proceed at room temperature with DKP additive in DMSO (forms **11** in 76%) but not in benzene.³¹ It was then investigated whether the enolate anion **21** could act as an electron donor to another molecule of **21**.

Table 2. The ΔG^* and ΔG_{rxn} for SET to the substrates **9**, **10**, **15** and **18**, from either **7** or the enolate anions **21**, **23**, **22** and the enolate anion of **10**, in both benzene and DMSO

Electron Acceptor	Electron Donor	Benzene $\Delta G^*/\Delta G_{rxn}$ (kcal/mol)	DMSO $\Delta G^*/\Delta G_{rxn}$ (kcal/mol)
21 [a]	7	34.3 / 24.7	22.7 / 10.4
21 [a]	21	45.8 / 42.5	33.0 / 27.8
24	7	38.7 / 34.3	23.3 / 11.4
24	25	18.4 / 6.2	20.7 / 10.1
22	7	31.7 / 23.1	22.3 / 10.8
22	22	43.3 / 40.1	31.0 / 26.5
Enolate Anion of 10 [a]	7	33.9 / 25.3	22.6 / 9.8
Enolate Anion of 10 [a]	Enolate Anion of 10	45.0 / 41.3	32.0 / 25.6

[a] SET to the neutral species was also calculated using **7** (Supporting Information Table S1.6). [b] The energetics were not calculated.

In DMSO SET from **21** to **21** has an energetic barrier of 33.0 kcal/mol, which is feasible at high temperatures, however in benzene the barrier is 45.8 kcal/mol which is not accessible. This trend was also observed experimentally.^{55,56} Therefore by changing the solvent from benzene to DMSO the reaction can proceed efficiently in the absence of DKP.⁵⁷ The substrates **18** and **10** show a similar pattern to **9**. This has demonstrated that the solvent has a large influence on the initiation step in the formation of the aryl radical, and that changing the reaction solvent to DMSO enables the initiation step to proceed under milder reaction conditions.⁵⁸ It also shows that by changing solvents, from benzene to DMSO, it increases the strength of the electron donation from the enolate anions of the substrates themselves, and thus in DMSO the reaction will proceed by SET from the enolate anions of the substrates, without the need for the DKP additive **6**.

The energetic barriers, ΔG^* , and the relative energies, ΔG_{rxn} , for the SET to the anions **23**, **24**, **25**, derived from **15**, were determined and the reactivities were dramatically different when comparing the two solvents. In benzene, the major species present was determined to be **24**, however in DMSO the major species formed is **25**, *via* **24**. Therefore, in DMSO there are two possible electron-rich species present in the reaction mixture, **25** and **7**, which may both act as electron donors. The barriers for SET to **24** from both **7** and **25** were calculated in both benzene and DMSO. The barriers for the intermolecular SET are lower in both solvents when the electron donor is **25**, $\Delta G^* = 20.7$ kcal/mol in DMSO, and $\Delta G^* = 18.4$ kcal/mol in benzene. Interestingly in benzene the barrier for the SET from **25** would be accessible at RT, however it is important to note that the species **25** is not present in any significant quantity in the reaction mixture. Experimentally it was shown that the cyclisation of **15** proceeds in DMSO with similar efficiency in the absence of DKP, which suggests that the **25** is the electron donor in this reaction.³¹

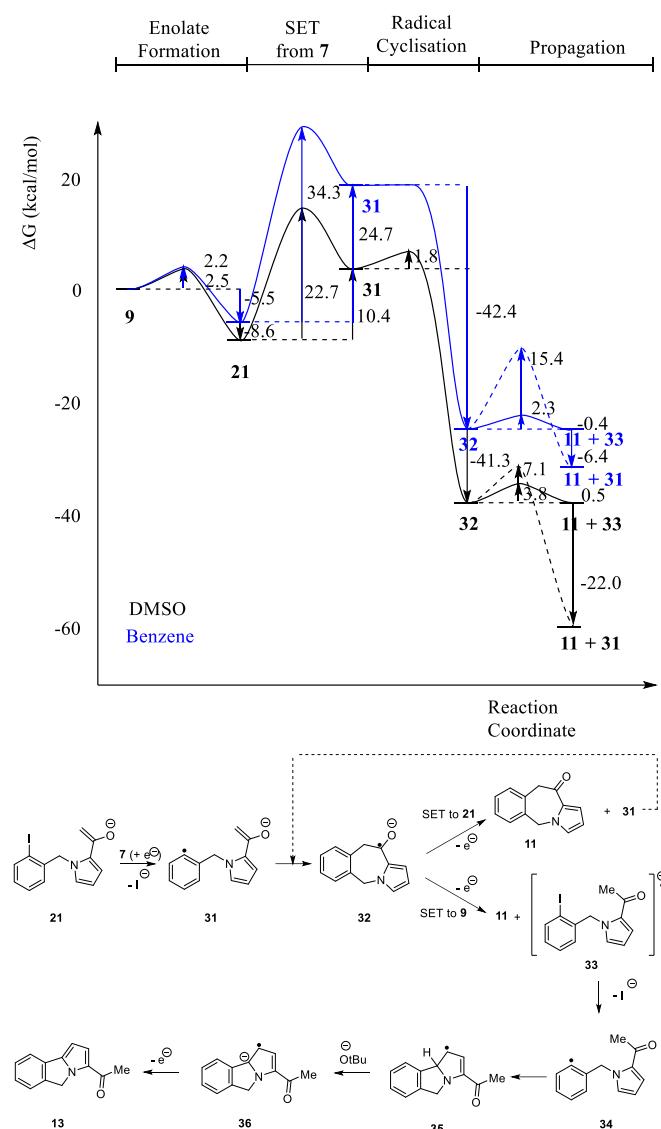
An alternative process for the initiation pathway was an intramolecular SET (Scheme 4). The intramolecular SET for **21** was approximated through a number of approaches (Supporting Information, Section 1.5) which suggest that the intramolecular SET is energetically unfavourable. The HOMO and LUMO for **21** show a lack of orbital overlap in the optimized geometry of the molecule. This suggests that in the optimized geometry **21** has unfavourable energetics for intramolecular SET, and for the rest of the paper we will assume that the process occurs *via* intermolecular SET.

The Cyclisation Mechanisms.

Cyclisation of 1-(1-(2-iodobenzyl)-1*H*-pyrrol-2-yl)ethan-1-one **9**

It has been determined that for these cyclisations, the solvent influences the equilibrium for the deprotonation of the substrates, as well as the energetic reaction profile for the SET step. The substrate **9** is predominantly present in the enolate anionic species **21** in the presence of KOtBu. SET from **7** (or from another molecule of **21**) to **21** leads to the formation of the aryl radical **31** upon the loss of iodide anion (Scheme 5). The radical intermediate **31** is capable of either undergoing an $S_{RN}1$

cyclisation, of the aryl radical onto the enolate anion, or an aryl-aryl bond formation, of the aryl radical onto the pyrrole ring. If the aryl radical **31** underwent an intramolecular cyclisation onto its enolate anion *via* an $S_{RN}1$ pathway, the ketyl radical **32** would be generated (Scheme 5). The $S_{RN}1$ cyclisation of intermediate **31**, in both benzene and DMSO, gave comparable Gibbs free energy profiles, with a barrierless cyclisation on the free energy surface and exergonic overall relative energies in the formation of **32**, $\Delta G_{rxn} = -42.4$ and -41.3 kcal/mol respectively. The aryl-aryl bond formation of the radical **31** had a barrier of $\Delta G^* = 9.1$ kcal/mol in DMSO and $\Delta G^* = 6.4$ kcal/mol in benzene, which is greater than the barrierless $S_{RN}1$ cyclisation of the aryl radical onto the enolate anion (Supporting Information S2.1 and S2.2). Therefore in both solvents the cyclisation of **31** will proceed *via* the $S_{RN}1$ pathway to form **32**. The radical intermediate **32** will donate an electron, to a molecule of either **9** or **21**, to form the product **11** and in doing so propagate the radical chain reaction.



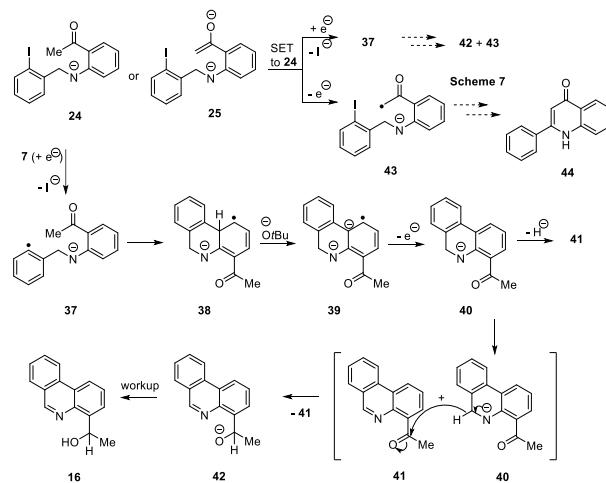
Scheme 5. The energy profile for the radical mechanism in the cyclisation of **9**

Due to the equilibrium for deprotonation of **9** it is most likely that the propagation will occur to **21**, since there is a greater proportion of this species present in the reaction mixture. This will lead to formation of **11** via the pathway described above. This was determined to be the most thermodynamically favoured propagation pathway. However an electron could be donated to **9** in the propagation step, and it was shown that this propagation step has a lower activation barrier and would be the kinetic propagation pathway. If the electron is donated to **9** the radical anion **33** is formed and aryl radical **34** forms on loss of iodide anion. Since there is no enolate anion in **34** the aryl radical will attack the pyrrole ring in the formation of an aryl-aryl bond, through the BHAS mechanism, to yield **13** upon deprotonation and propagation (Supporting Information, Scheme S2.1 and S2.2).

Therefore the major pathway will lead to product **11** and the product **13** will form as a minor product, only when propagation occurs to the neutral starting material **9**, which is only present in minor amounts in the basic reaction mixture. This revision of the previously proposed mechanism agrees with the experimental product selectivities observed.³¹⁻³²

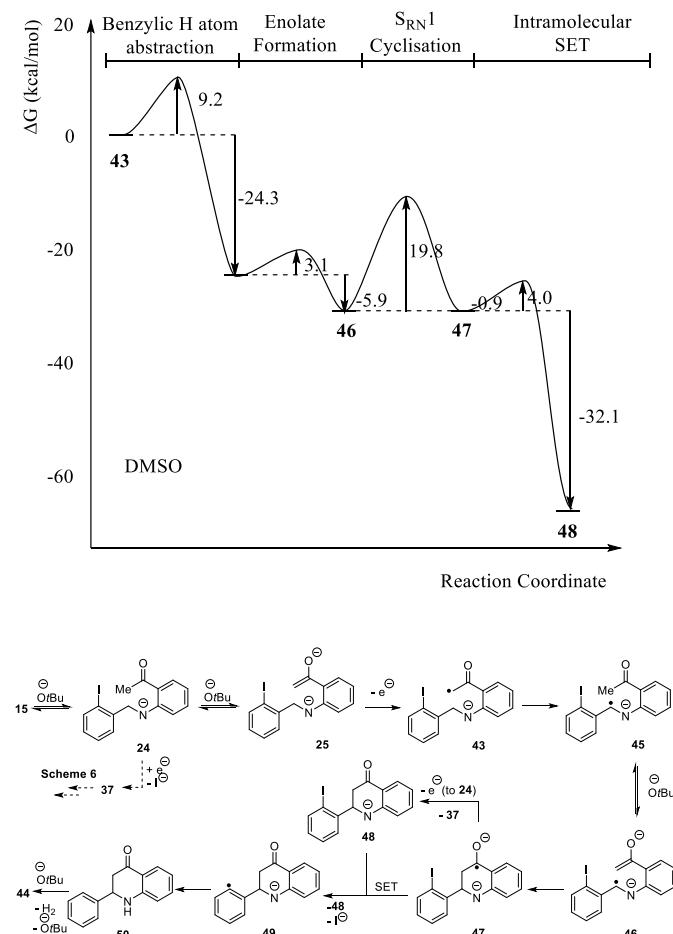
Cyclisation of 1-(2-((2-iodobenzyl)amino)phenyl)ethan-1-one **15**

In DMSO the major deprotonated species derived from **15** will be **25**, whereas in benzene the major species is **24** (Table 1 and Table 2). Another difference between the two solvents is the energetic profile for the intermolecular SET initiation steps to these reactive species. Activation of **24** by SET, from **7** or **25**, forms the radical anion **37**, which will cyclise onto the aromatic system to yield **38** (Scheme 6). Upon deprotonation, **39** is achieved, which is capable of donating an electron to the reactive species, to propagate the cycle. The pathway for this aryl-aryl bond formation has been calculated in both benzene and DMSO, and it has been determined that both pathways have similar energy profiles for the cyclisation. Upon formation, **40** could undergo a hydride elimination to form **41**, which is driven by a gain in aromatic stabilization. If **41** is formation, **40** could undergo a hydride elimination to form **41**, which is driven



Scheme 6. Proposed mechanism in the cyclisation of the anionic species **24** and **25** arising from deprotonations of substrate **15**

by a gain in aromatic stabilization. If **41** is present in the reaction mixture it will form a complex with a molecule of **40**, possibly through π -stacking. Elimination of a hydride anion from **40** to **41** would yield a new molecule of **41** and the reduced product **16**, upon workup of intermediate **42** (Supporting Information, Scheme S3.1). In benzene the hydride transfer step from **40** to **41** is endergonic, $\Delta G_{rxn} = 5.0$ kcal/mol, and it has an overall barrier of $\Delta G^* = 25.1$ kcal/mol.⁵⁹ In DMSO the barrier for this reduction of **41** is similar to that in benzene, $\Delta G^* = 25.1$ kcal/mol and $\Delta G_{rxn} = -1.0$ kcal/mol. This barrier will be achievable at high temperatures however if the reaction is performed at room temperature, the reduction is unlikely to occur, which was observed experimentally.³¹ Although the overall Gibbs free energy profile is similar in both the solvents, the relative energies are different, in DMSO the reduction is exergonic whereas in benzene the reduction is endergonic. Therefore in DMSO all of **41** is expected to be converted to **16**, whereas in benzene an incomplete conversion of **16** is predicted, which agrees with the experimental observations.⁶⁰ The major product present in the reaction mixture, with DMSO as a solvent, is **25**, which will undergo SET to **24**, in the initiation step, to form the radical anion **43** (Scheme 7).⁶¹

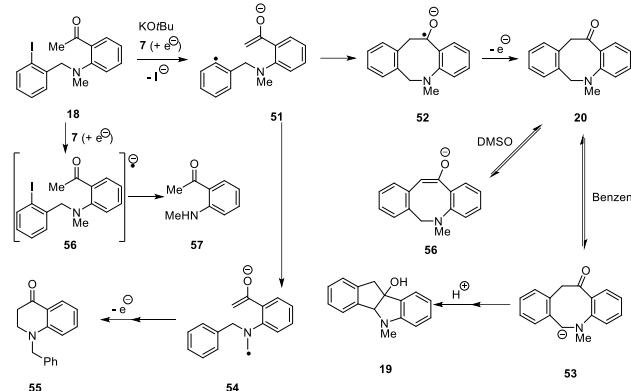


Scheme 7. The proposed mechanism in the cyclisation of **15**

The intermediate **43** could intramolecularly abstract a hydrogen atom from the benzylic position to yield the more stable radical anionic intermediate **45**. The energetics for this hydrogen atom abstraction were exergonic, $\Delta G^* = 9.2$ kcal/mol and $\Delta G_{rxn} = -24.3$ kcal/mol. In the basic reaction mixture an equilibrium will be established between **45** and the enolate anion **46**. In DMSO this equilibrium will largely favour the enolate anion $\Delta G^* = 3.1$ kcal/mol and $\Delta G_{rxn} = -5.9$ kcal/mol. If the enolate anion **46** forms, the benzylic radical will undergo an $S_{RN}1$ cyclisation onto the enolate anion to form **47**. This pathway in DMSO has a barrier for cyclisation of $\Delta G^* = 19.8$ kcal/mol and a relative energy of $\Delta G_{rxn} = -0.9$ kcal/mol. This means that in DMSO the cyclized product **47** is going to be present in high proportions, and will therefore proceed along the reaction pathway to form the **49** upon SET. It was proposed that in DMSO **47** could undergo an intramolecular SET in the formation of the intermediate **49** (Supporting Information, Section 3.3), however it was determined that intermolecular SET was the most favoured energetically. SET from **47** (to **24**) will yield an anionic intermediate **48**. This intermediate can receive an electron (from **47**) into the C-I σ^* orbital, to cleave the C-I bond and form an aryl radical intermediate **49**. The aryl radical within **49** is very reactive and will be quenched in the reaction mixture to form **50**. Molecule **50** can form **44** in two steps (i) a butoxide anion will form the enolate anion of **50** and (ii) this enolate anion will undergo a hydride elimination to a molecule of butanol, to form **44** and hydrogen, and regenerate the butoxide anion (Supporting Information, Scheme S3.5). The energetic profile for the hydride elimination in the formation of **44** from **50** is exergonic, $\Delta G_{rxn} = -7.0$ kcal/mol, with a barrier of $\Delta G^* = 21.6$ kcal/mol. This energetic barrier is the RDS in the reaction pathway and it suggests that lowering the reaction temperature may lead to the isolation of the intermediate **50**, which was shown experimentally.⁶ The influence of solvent in the cyclisation of **15** is to control which reactive species (**24** and **25**) is present in the reaction mixture, and because these reactive intermediates undergo different pathways the selectivity of the reaction can be controlled by changing the solvents. In DMSO the reaction will selectively form **44** from the intermediate **25**, however in benzene the reaction will selectively favour the formation of **41**. It has also been shown that the temperature can be altered to dictate product formation, at low temperatures **41** will be the major product formed in benzene, however increasing that temperature will lead to the formation of **16**. Similarly in DMSO, lowering the reaction temperature could reduce the formation of **44** and the intermediate **50** can be isolated.

Cyclisation of 1-(2-((2-iodobenzyl)(methyl)amino)phenyl)ethan-1-one **18**

The cyclisation of **18** involves the SET initiation to the enolate anion **22**, which could occur at RT in DMSO, however higher temperatures should be used for the reaction in benzene. The solvent influence on the SET to **18** shows similar trends as **9**. Upon SET, the aryl radical intermediate **51** could undergo either an $S_{RN}1$ cyclisation onto the enolate anion to form **52**, or H atom



Scheme 8. The proposed mechanism in the cyclisation of **18**

abstraction from the methyl group, to form radical **54** (Scheme 8) (Supporting Information, Scheme S4.1). The $S_{RN}1$ cyclisation of **51** onto the enolate anion is calculated to be the most favoured pathway in both benzene and DMSO. Cyclisation of **51** ultimately forms **20** which in the presence of a base **20** could be deprotonated either to form the enolate anion **56** or to form the benzylic anion **53**. In both solvents the favoured deprotonation is the enolate formation to form **56**. In DMSO the benzylic deprotonation to form **52** was endergonic, $\Delta G_{rxn} = 4.9$ kcal/mol, however in benzene the deprotonation of the benzylic position to form **52** has similar energetics to this enolate anion formation (Supporting Information, Scheme S4.1). Therefore in benzene the deprotonation equilibrium would form intermediate **52** and this benzylic attack can ionically attack the carbonyl group to form **19** upon workup. Therefore if the reaction is performed in DMSO, the product **20** is formed through this reaction pathway and the reaction can be performed at RT, and in benzene the product formed will be **19**, however because the reaction is performed in benzene the reaction must be performed at high temperatures to overcome the energetic barrier for the SET initiation step.

In both solvents the minor pathway of **51** is the hydrogen atom abstraction to form **54** and ultimately **55** (Supporting Information, Scheme S4.2). In benzene, **51** will cyclise to form **52** with a barrierless transition, whereas in DMSO the transition has a barrier of $\Delta G^* = 2.7$ kcal/mol. Therefore in benzene it is predicted that the $S_{RN}1$ pathway will be the major pathway whereas in DMSO there will be less selectivity for this $S_{RN}1$ cyclisation, and this is seen experimentally.⁶

An interesting observation during this study is that in the propagation step, SET from **52** can occur either to the enolate anion **22** or to the neutral species **18** (Supporting Information, Scheme S4.3). It was found that in both solvents, the lowest barrier is SET to the neutral species, not the enolate anionic species. If this occurs then the radical anion **56** forms, which can undergo fragmentation to form **57** upon workup. However, this pathway will be a minor pathway due to the low population of **18** that will be present in the reaction mixture.

Conclusions

This paper has thoroughly investigated the mechanistic pathways through which various C-C bonds are formed under ground-state thermal activation. The experimental results have been shown to support the proposed pathways and these mechanisms are different from those previously reported, and the rate determining steps for the radical steps in these mechanisms is shown to be the initiation SET step.³¹⁻³² With increased knowledge of these pathways, we could fine tune the reaction conditions to lead to efficient C-C bond formations. Solvent was also shown to affect various reaction pathways because of its more commonly accepted role in the stabilization of intermediates in ionic pathways. Changing the polarity of the solvent was a useful mechanism to influence the product outcomes of radical pathways. The deprotonation energetics were largely influenced by the solvent and this resulted in different reactive species being present prior to the SET step. The largest influence of the choice of solvent on these reaction pathways is on the SET steps, such as the initiation and the propagation steps. The SET step is often the rate determining step in both solvents, and so using DMSO as the solvent instead of benzene allowed milder reaction conditions to be employed for efficient cyclisation. However in some circumstances the rate determining step in DMSO was not the SET and so using milder reaction conditions led to formation of new products, which are intermediates in the reaction pathway. In the cyclisation of substrate **15** the choice of solvent influenced the stability of radical intermediates within the cyclisation pathway and thus changed the product outcomes of the cyclisation. The species that could act as the electron donor in the SET step was also changed when changing solvents from benzene to DMSO. The additive DKP was not required when DMSO was the solvent since the enolate anions of the species themselves were capable of performing the SET step.

Acknowledgements

We thank the EPSRC and University of Strathclyde for the funding. Grant Number: EP/L505080/1.

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Staroverov; R. Kobayashi; J. Normand; K. Raghavachari; A. P. Rendell; J. C. Burant; S. S. Iyengar; J. Tomasi; M. Cossi; N. Rega; N. J. Millam; M. Klene; J. E. Knox; J. B. Cross; V. Bakken; C. Adamo; J. Jaramillo; R. Gomperts; R. E. Stratmann; O. Yazyev; A. J. Austin; R. Cammi; C. Pomelli; J. W. Ochterski; R. L. Martin; K. Morokuma; V. G. Zakrzewski; G. A. Voth; P. Salvador; J. J. Dannenberg; S. Dapprich; A. D. Daniels; Ö. Farkas; J. B. Foresman; J. V. Ortiz; J. Cioslowski; D. J. Fox *Gaussian 09*, Gaussian, Inc.: Wallingford, CT, USA, 2009.

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45. Substrate **9** undergoes cyclisation to **11** and **13** in the presence of KOtBu, FeCl₂ and pinacolone. It can also undergo cyclisation under photoactivation in presence of KOtBu.

46. **10** was shown to cyclise in the presence of additive DKP **6** (31% benzene at 120 °C; 62% DMSO at 120 °C; 54% DMSO at RT).

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50. It must be noted that it has been proposed within the literature that the dimsyl anion is capable of donating an electron to initiate the transition metal free reaction conditions (reference 51 - 53). The KOtBu deprotonation of DMSO was determined to be endogonic, $\Delta G^* = 5.6$ kcal/mol and $\Delta G_{rxn} = 5.4$ kcal/mol, and the SET from the dimsyl anion to **21** was determined to be $\Delta G^* = 29.5$ kcal/mol and $\Delta G_{rxn} = 20.8$ kcal/mol. This gave an overall value of $\Delta G^* = 34.9$ kcal/mol and $\Delta G_{rxn} = 26.2$ kcal/mol for SET from a dimsyl anion. This is less favourable than the SET from **7** or **21** and therefore we conclude the dimsyl anion is not initiating the reaction in this situation.

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55. Experimentally at 120 °C in benzene without the **7** only 23% of **11** was observed in benzene. Since none of **13** was observed we can propose that the small amount of **11** formed through the benzyne pathway.

56. At room temperature in DMSO the reaction efficiently yielded product **11** and **13**. In benzene however only traces of **11** were observed, and starting material was returned.

57. Murphy *et al.* (reference 31) reported that when the reaction was performed in benzene in the absence of the DKP additive **6**, the starting material, **9**, was recovered with 73%.

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59. When the reaction was performed in DMSO at room temperature only the product **16** was observed. No **42** was observed.

60. In DMSO the reduced product **42** was isolated at 120 °C, whereas in benzene both **42** and **16** were isolated. At room temperature the reduction of **16** is not observed in DMSO and only **16** was isolated.

61. Experimentally the substrate **15** will undergo cyclisation in the absence of the DKP additive in both benzene and DMSO, with similar yields to when DKP additive was used (reference 31). This suggests that a deprotonated species of **15** is capable of acting as the electron donor.

Effect of solvent on radical cyclisation pathways: S_{RN1} vs. aryl-aryl bond forming mechanisms

Katie J. Emery, John A. Murphy, and Tell Tuttle

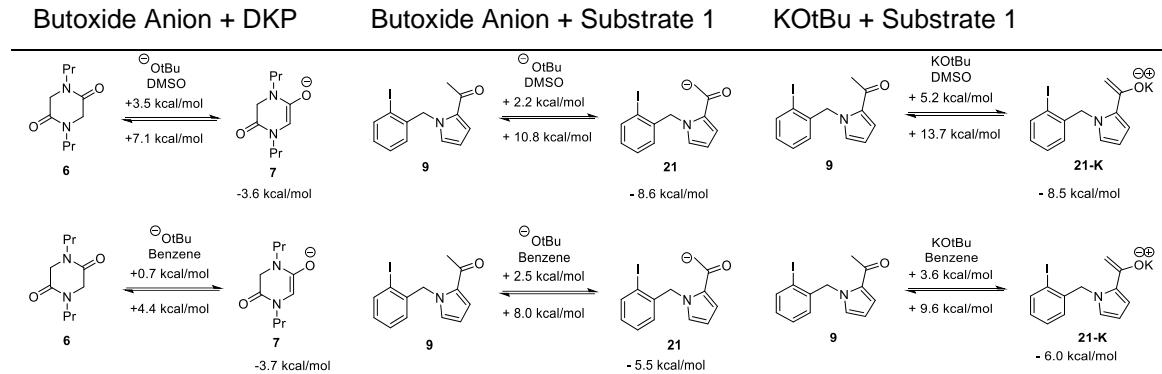
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1. Initiation Calculations

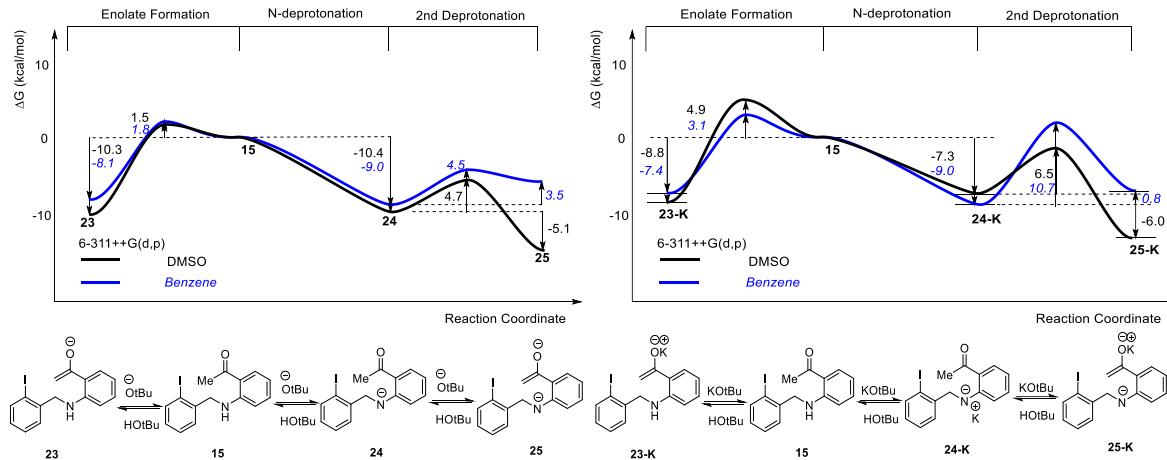
1.1 Enolate Formation

Table S1.1. The deprotonation energetics for DKP and substrate **9** in both DMSO and benzene



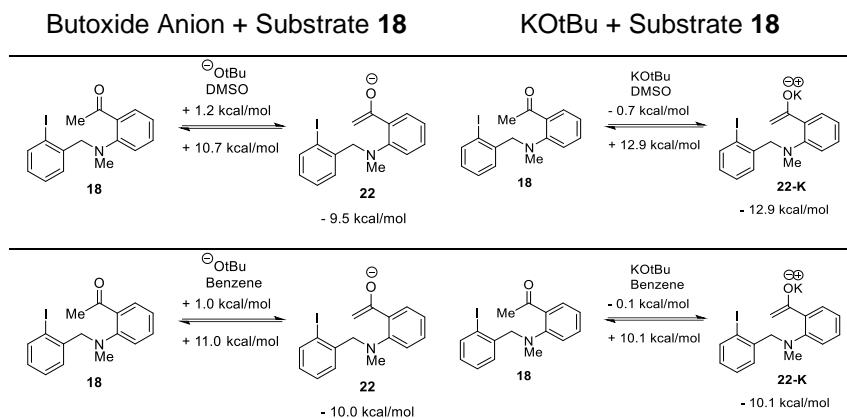
In the basic reaction mixture, the diketopiperazine (DKP) additive **6** will exist predominantly as the enolate anion **7**. The substrate **9** will be in equilibrium with its enolate anion **21** in the presence of base, and the enolate anion **21** will be the major species in both benzene and DMSO. The energetics for the deprotonation of **9** using the tertiary butyl anion or the KOTBu as the base are similar.

Scheme S1.1. The deprotonation energetics for substrate **15** with either a molecule of tertiary butoxide anion or with KOTBu in both DMSO and benzene



In the basic reaction mixture the substrate **15** will be in equilibrium with its various possible deprotonation states. In benzene the most stable species will be **24** and in DMSO the most stable species present will be **25**.

Table S1.2. The deprotonation energetics for substrate **18** with either a molecule of tertiary butoxide anion or with KOtBu in both DMSO and benzene

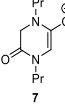
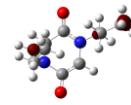
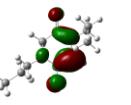
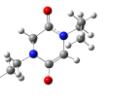
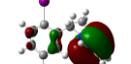
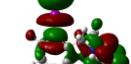
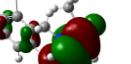
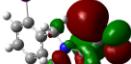
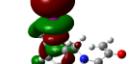
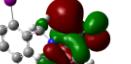
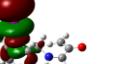
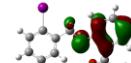
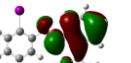
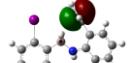
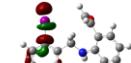
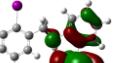
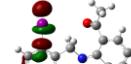
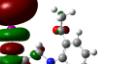
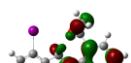
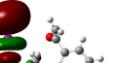
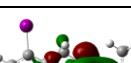
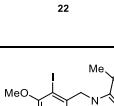
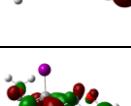
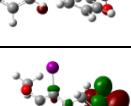
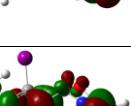
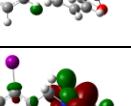


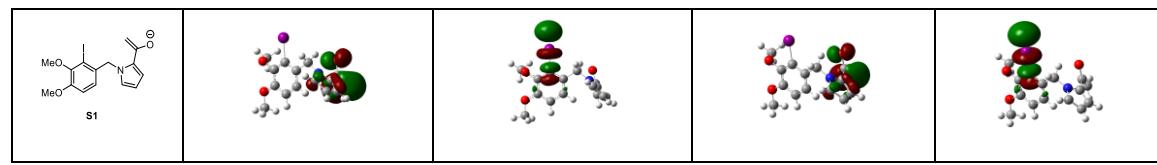
In the basic reaction mixture the substrate **18** will be in equilibrium with its enolate anion **22**. The equilibrium will strongly reside towards the enolate anion **22** in both the solvents.

In the modelling of the reactions from this point throughout the paper, the calculations for the deprotonations will use the butoxide anion for the deprotonations for computational cost and because the results are similar for the equilibrium.

1.2 HOMO-LUMO Diagrams

Table S1.3. The HOMO and LUMO diagrams of reactive species

	Benzene as Solvent		DMSO as Solvent	
	HOMO	LUMO	HOMO	LUMO
				
				
				
				
				
				
				
				
				
				



* LUMO+2 orbital

Table S1.4. Spin density diagrams of the substrates after accepting an electron by SET

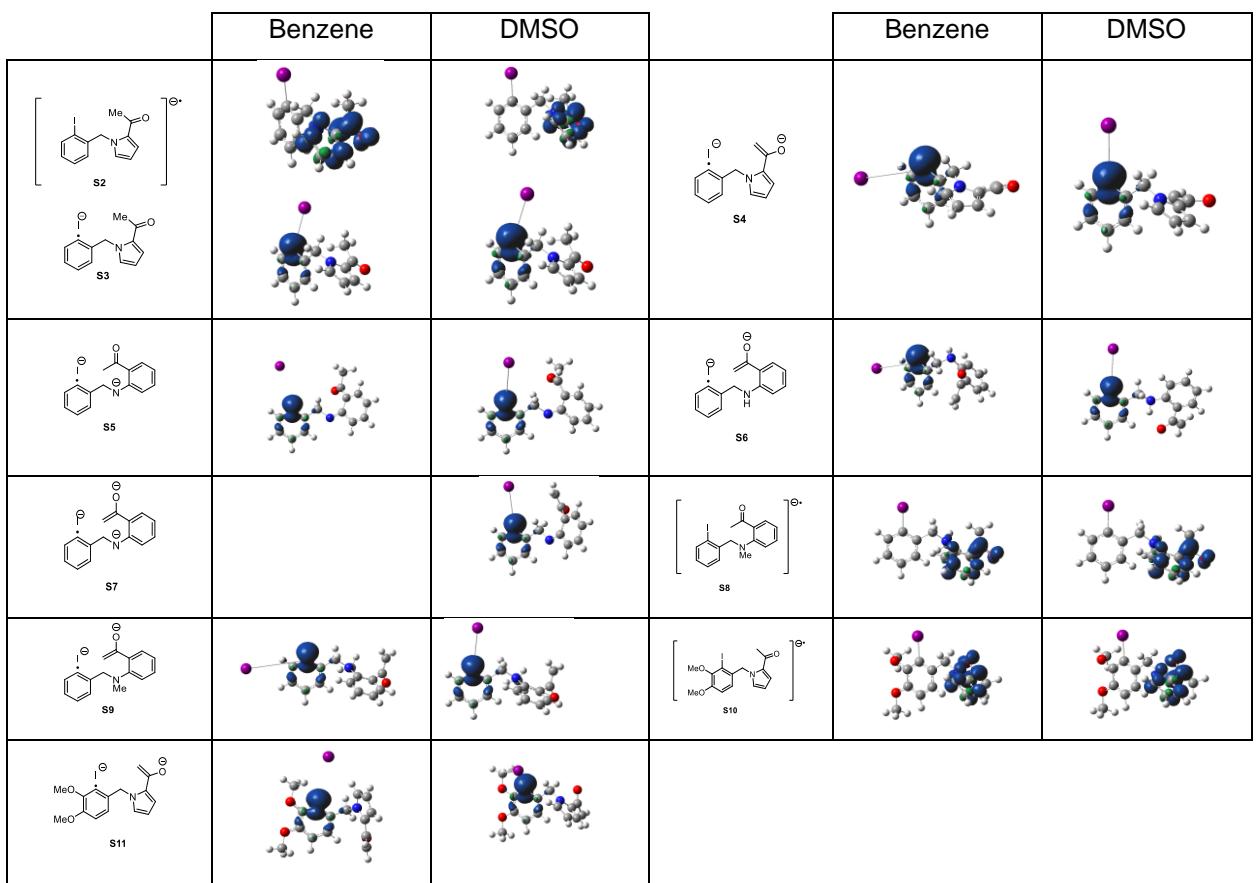
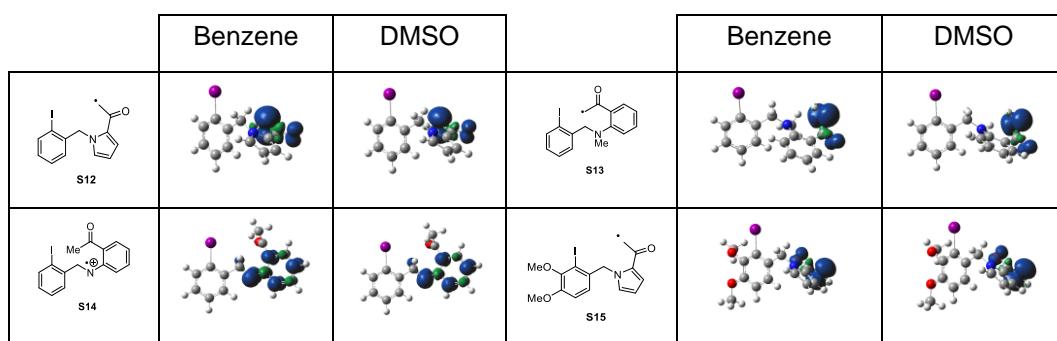
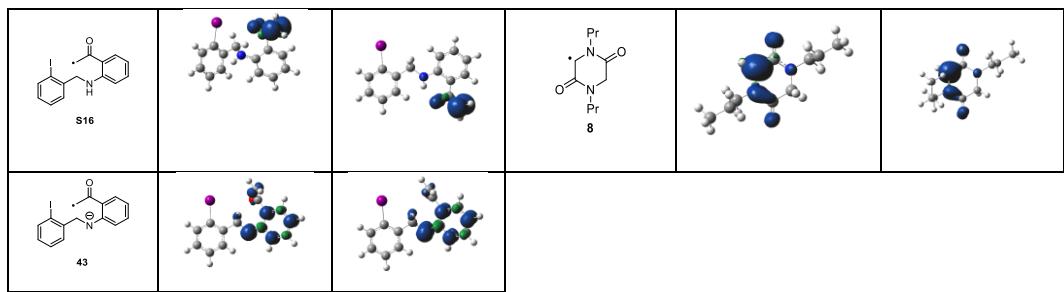


Table S1.5. Spin density diagrams of the substrates after donating a single electron





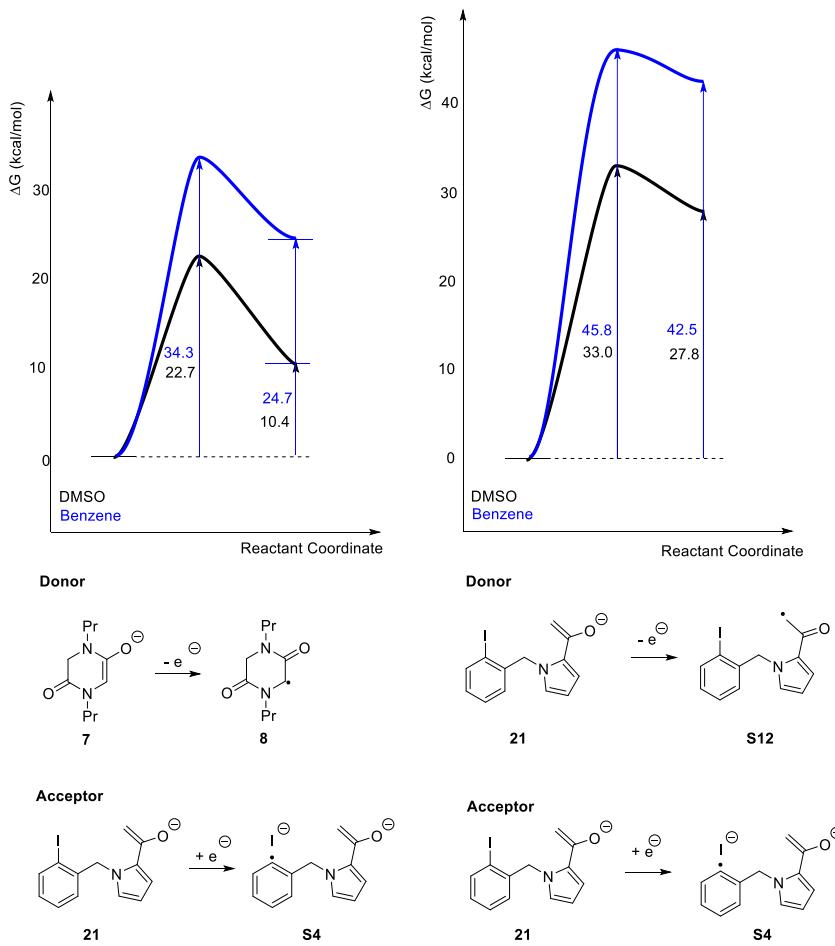
1.3 Energetics of SET – Marcus Hush Theory

Table S1.6. The energetics for the SET initiation to either the neutral or anionic species of substrates **9**, **10**, **15** or **18**, from either the in situ electron donor **7** or the respective anionic species of the substrates **21**, **23**, **24**, **25**, **22** or **S1** in both benzene and DMSO

Electron Acceptor	Electron Donor	Benzene ΔG^*	Benzene ΔG_{rxn}	DMSO ΔG^*	DMSO ΔG_{rxn}
9	7	31.9	30.7	36.0	32.8
9^a	7	18.1	5.7	20.1	8.9
21	7	34.3	24.7	22.7	10.4
9	21	69.2	48.5	74.1	50.2
9^a	21	27.9	23.5	30.5	26.3
21	21	45.8	42.5	33.0	27.8
23	7	30.9	21.9	21.3	8.4
24	7	38.7	34.3	23.3	11.4
25	7	--	--	22.3	13.1
23	23	42.8	39.6	31.2	25.3
23	24	45.4	43.4	30.6	24.5
23	25	13.3	-6.1	18.7	7.1
24	25	18.4	6.2	20.7	10.1
25	25	--	--	19.8	11.8
18^b	7	27.8	27.6	32.3	31.1
22	7	31.7	23.1	22.3	10.8
22	22	43.3	40.1	31.0	26.5
10^b	7	34.9	31.7	37.5	34.4
S1	7	33.9	25.3	22.6	9.8
S1	S1	45.0	41.6	32.0	25.6

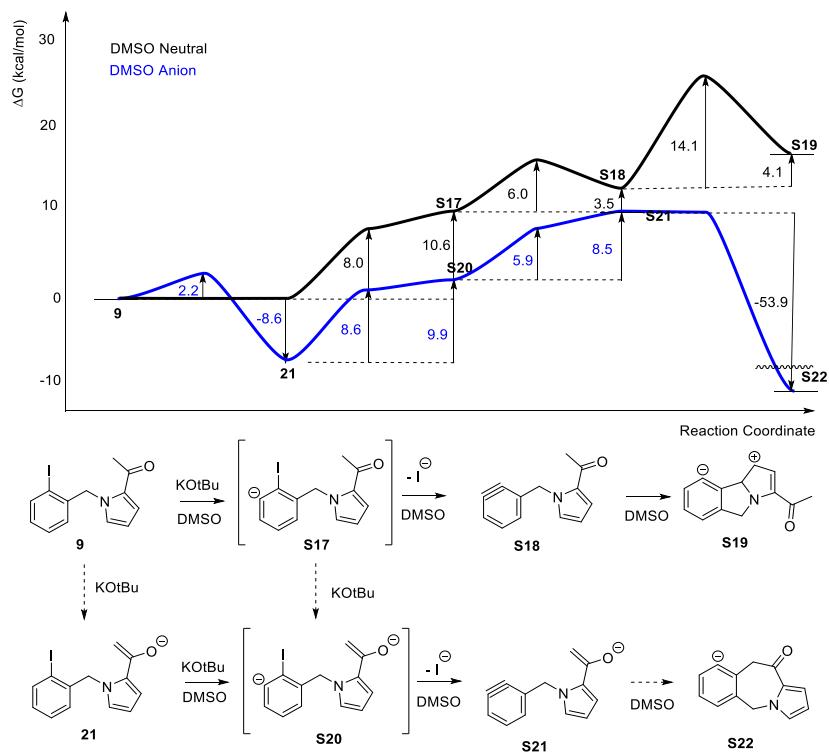
^a Encouraged C-I dissociation. ^b Did not give C-I dissociation.

Scheme S1.2. The energetics for the possible intermolecular SET between **7** or **21** to **9** in both DMSO and benzene.



1.4 Benzyne Pathway

Scheme S1.3. The energetics for possible benzyne formation in DMSO from **9** and **21**

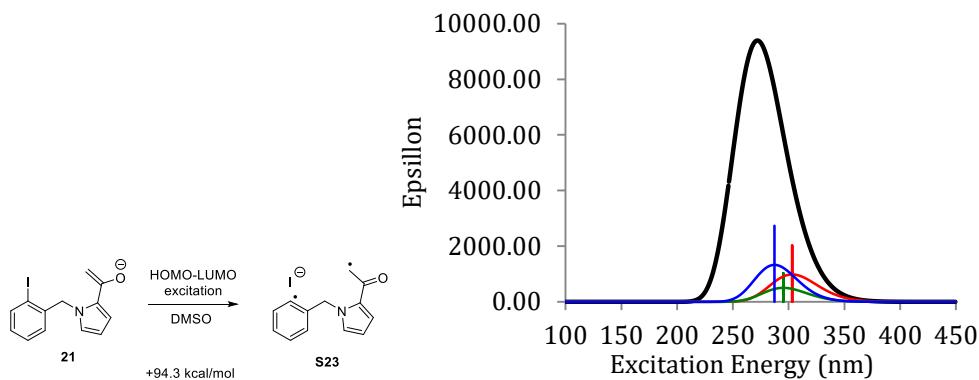


The benzyne formation is accessible at RT in DMSO however it is very endergonic. The formation of the neutral benzyne **S18** is $\Delta G_{rxn} = 14.1$ kcal/mol, and to form **S21** the reaction is endergonic by $\Delta G_{rxn} = 18.4$ kcal/mol. The cyclisation to form **S19** has an overall $\Delta G^* = 28.2$ kcal/mol and $\Delta G_{rxn} = 18.2$ kcal/mol. This is very unfavourable and the product **13** would not form if the reaction proceeded through the benzyne mechanism. The cyclisation of **S21** to **S22** is barrierless and very exothermic, suggesting that if any benzyne forms, then the cyclisation to form **11** will occur. Therefore it is possible that partial amount of the formation of **11** may occur via this pathway.

1.5 Intramolecular Analysis of 21

1.5.1 TD DFT

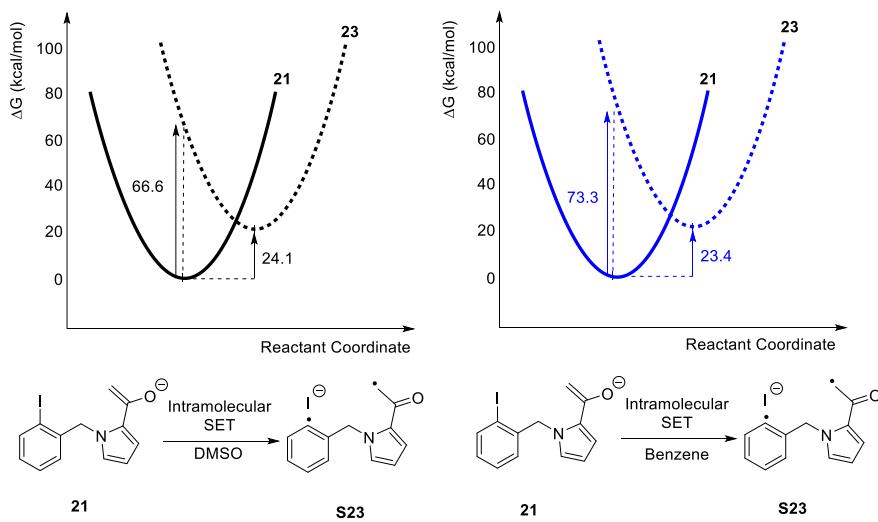
Scheme S1.4: The TDDFT calculations were performed on **21**. The Gaussian curve was generated using the default Gaussian parameters. Black lines = Overall predicted UV-Vis trace. Red Blue and Green vertical transitions correspond to HOMO – LUMO excitations.



The TDDFT results suggest that the intramolecular SET is not possible for **21** in DMSO.

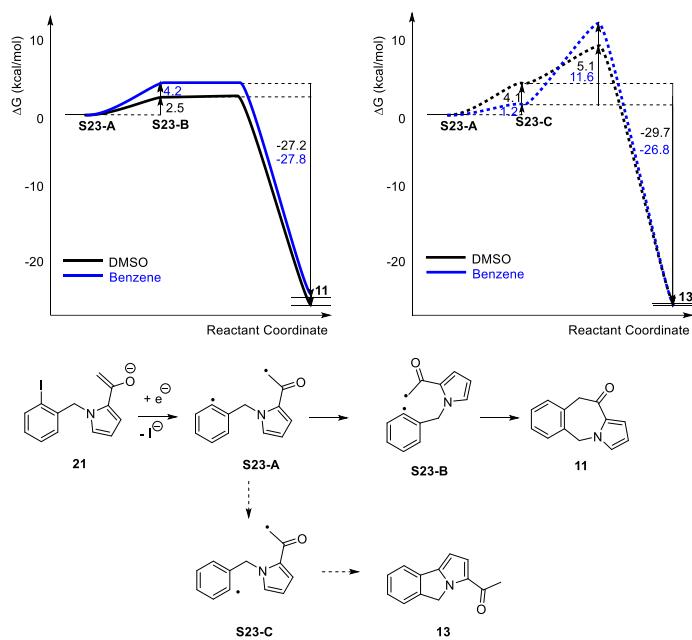
1.5.2 Franck-Condon

Scheme S1.5. The energetics intramolecular SET for **21** in both DMSO and Benzene, calculated using the Frank-Condon principle



The Frank-Condon principle states that the electron transfer step occurs first prior to reorganization of substrates and solvent. Therefore the energetics for intramolecular SET were determined by optimizing the anionic species, and performing a single point energy calculation, on this optimized geometry, using the triplet anion charge and multiplicity. It showed that the intramolecular SET of **21** is not likely to occur in either of the two solvents.

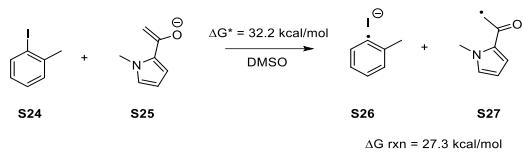
Scheme S1.6. The energetics radical recombination



The results suggest that if the molecule **21** was able to undergo an intramolecular SET initiation pathway then the resulting diradical **S23-A** would easily cyclise to form either **11** or **13** through radical recombination.

1.5.3 SET between the isolated HOMO-LUMO fragments of 21

Scheme S1.7. The energetics for an intermolecular SET between the isolated HOMO and LUMO fragments of substrate 21. The table displays the HOMO/LUMO of the fragments

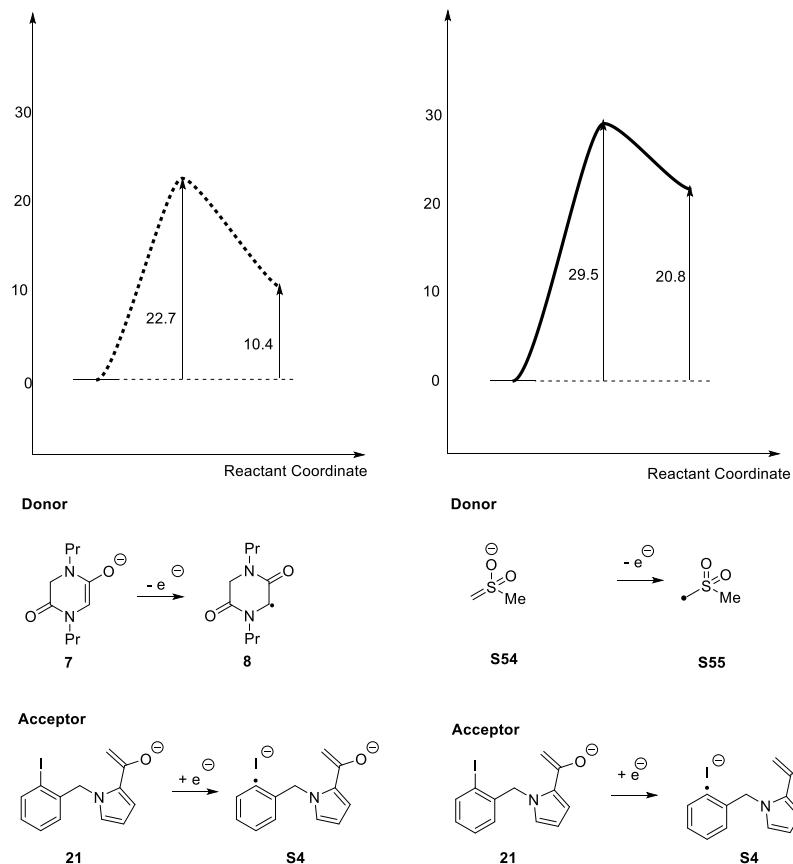


	HOMO	LUMO

The results for the SET between the two fragments yields similar results as the intermolecular SET between two molecules of **21**. The analysis of the HOMO and LUMO for the fragments **S24** and **S25** and for the molecules of **21** are very similar, emphasising that the HOMO and LUMO orbitals of **21** do not overlap in the optimized geometry. This lack of orbital overlap between the HOMO and LUMO of **21** provides a possible explanation for the high energetics calculated for intramolecular SET.

1.6 Possible SET from the dimsyl anion

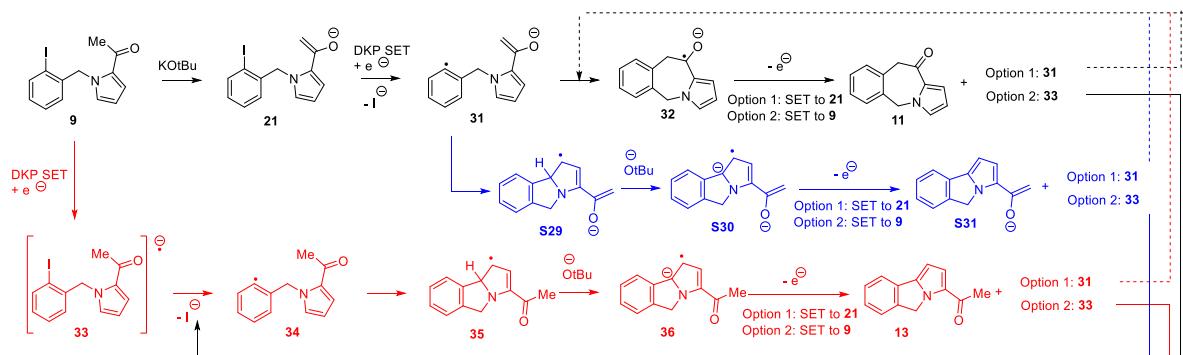
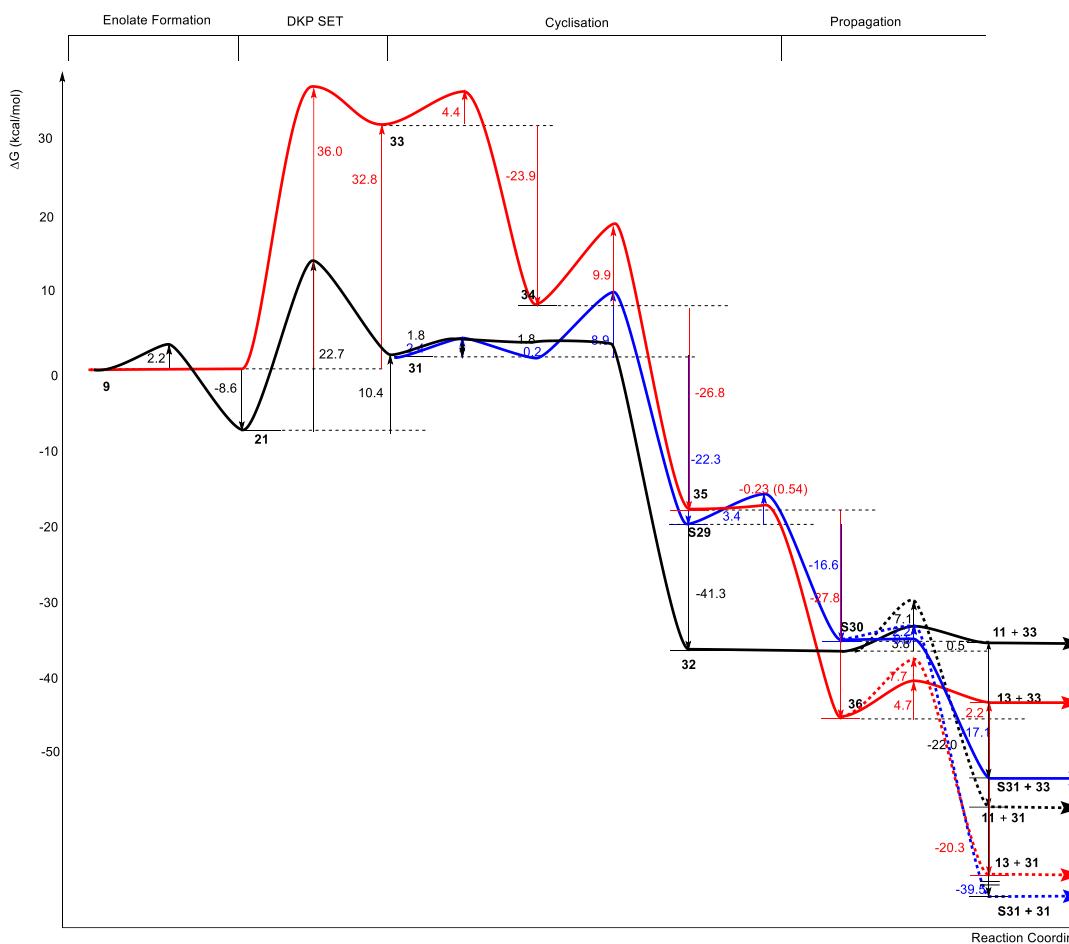
Scheme S1.8. The energetics for an SET from either **7** or a dimsyl anion **S54**, to the enolate anion **21** od substrate **9**



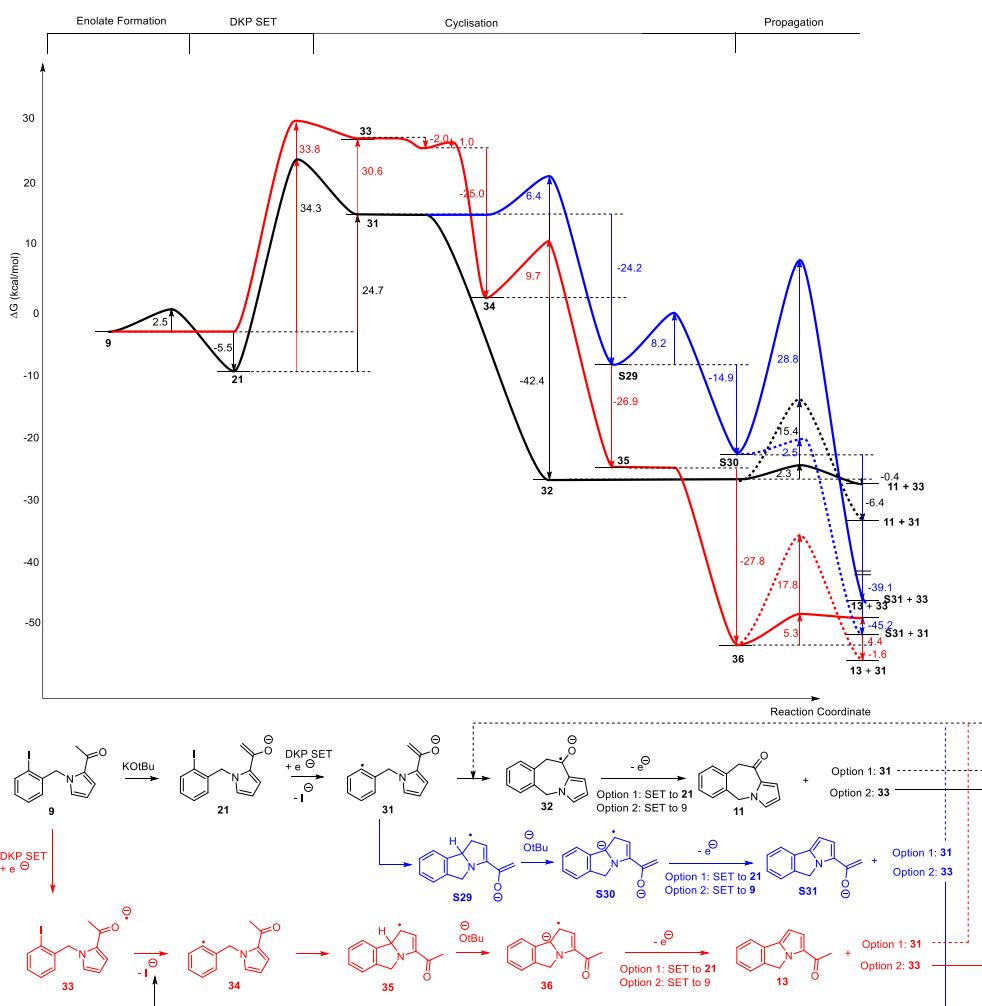
Within the literature it was proposed that the dimsyl anion (formed from the deprotonation of DMSO) was able to donate a single electron to the iodobenzene to form an aryl radical. Therefore the energetics for the SET from the dimsyl anion to the substrate **21** was calculated. This ΔG^* was compared with the barrier for the SET from the enolate anion of DKP **7**. It was shown that the dimsyl anion could donate an electron to **21** at elevated temperatures in DMSO, however the favoured pathway will be SET from the enolate anion of **21**, which has a lower reaction barrier, ΔG^* .

2. Radical Cyclisation of 9 in DMSO and Benzene

Scheme S2.1. The energetics for the formation of 11 and 13 in DMSO from 9



Scheme S2.2. The energetics for the formation of **11 and **13** in benzene from **21****



3. Radical Cyclisation of 15

3.1 The formation of products 16 and 42 from 15

Scheme S3.1. The energetics for the cyclisation of 15 in both benzene and DMSO

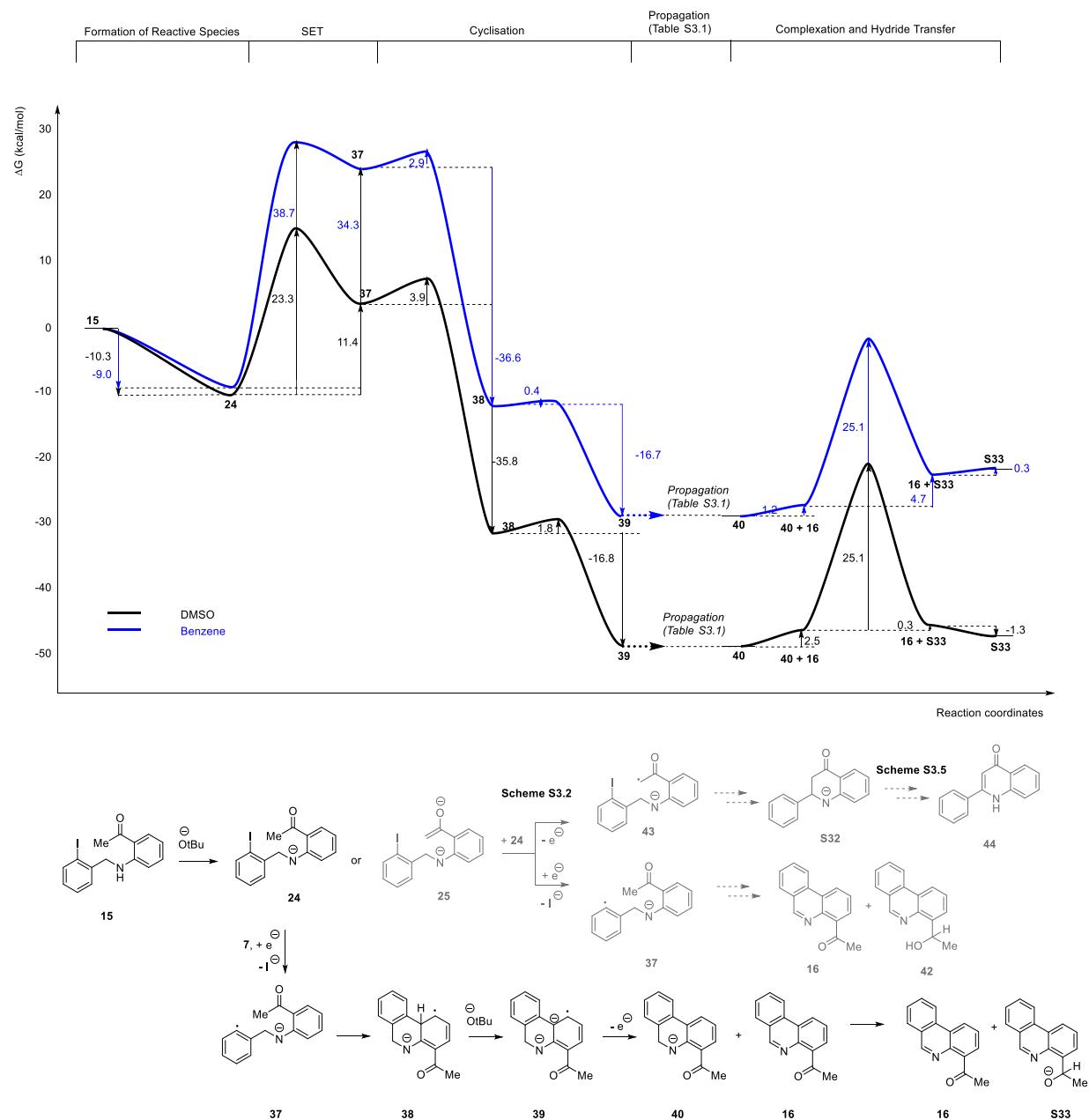
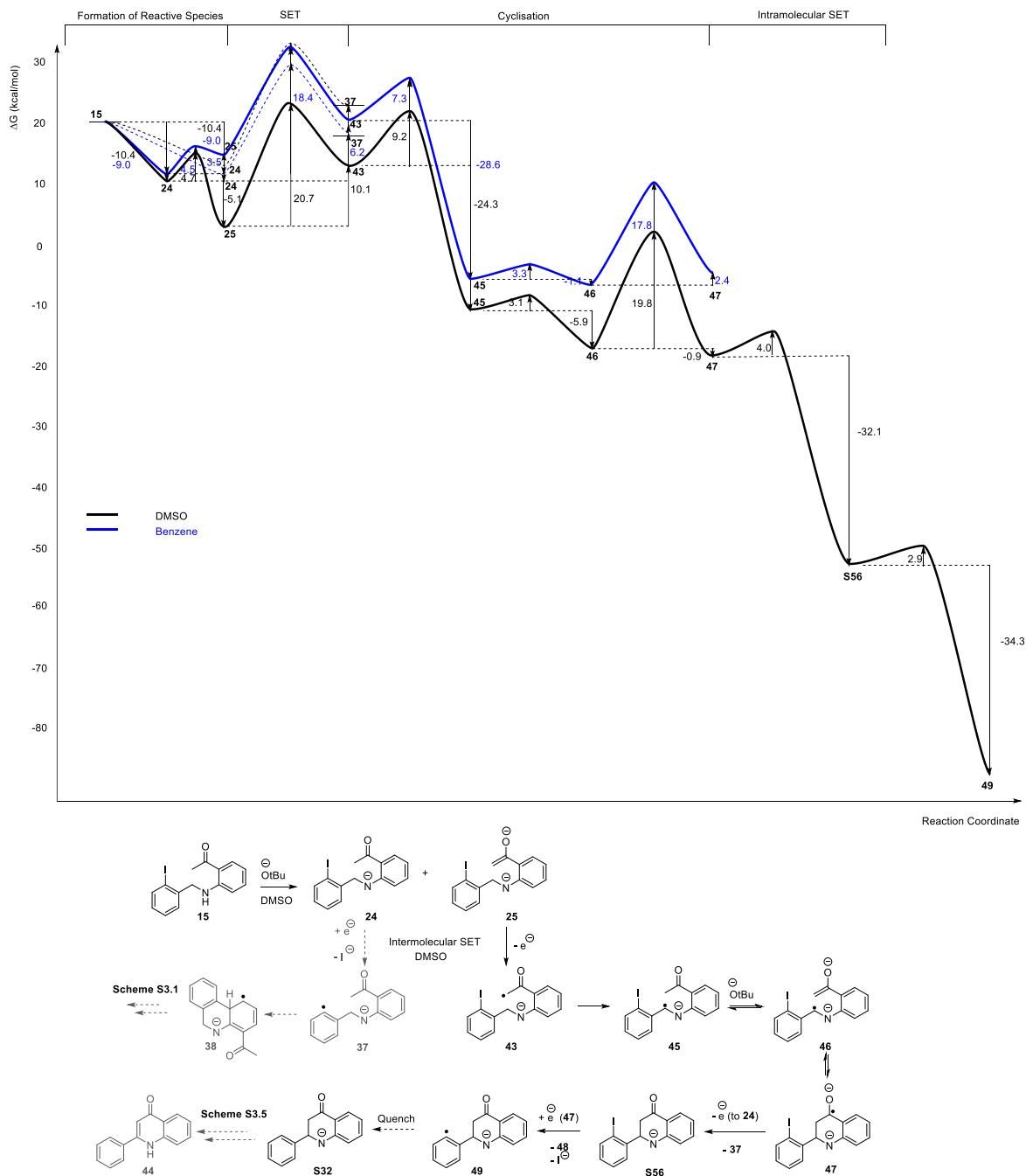


Table S3.1. The energetics for the propagation in the formation of **42**

Propagation	DMSO	Benzene
39 To 25	$\Delta G^* = 3.4$ $\Delta G_{rxn} = -27.9$	--
39 To 24	$\Delta G^* = 4.5$ $\Delta G_{rxn} = -29.6$	$\Delta G^* = 3.4$ $\Delta G_{rxn} = -33.3$

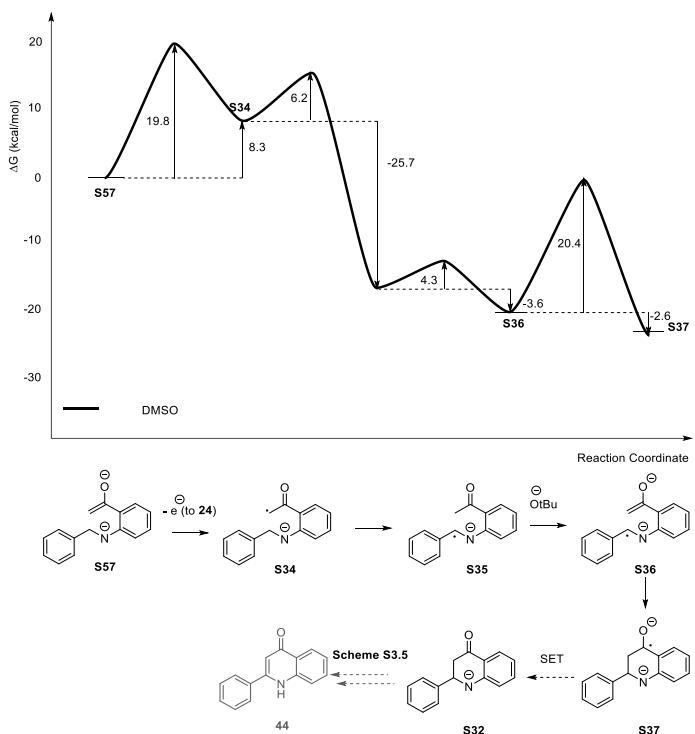
3.2 The formation of product **44** from **15**

Scheme S3.2. The possible reaction pathway in the formation of **44**

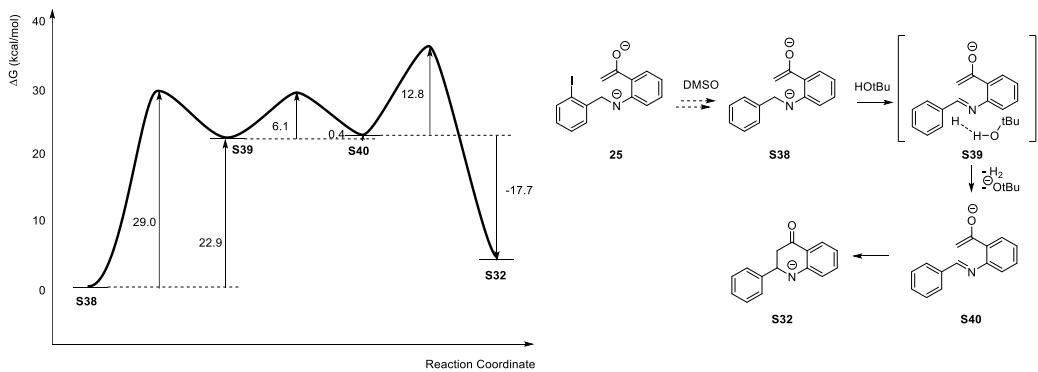


The formation of **44** occurs through tandem hydrogen atom transfer and S_{RN1} cyclisation from **25** to form **S32** as an intermediate. If **25** was efficiently formed in benzene then products **44** may be formed.

Scheme S3.3: The energetics for the radical cyclisation of the non-halogenated analogues of **43-47 in DMSO solvent**



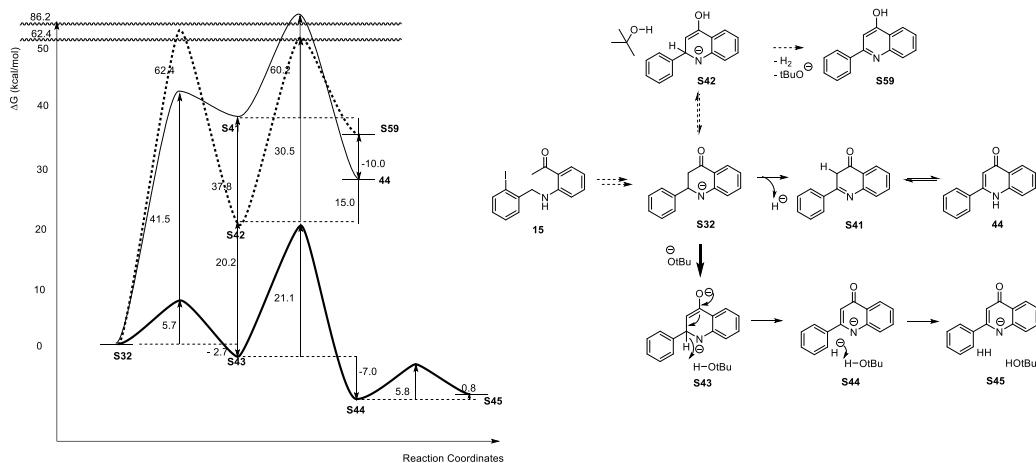
Scheme S3.4: The energetics for a possible ionic pathway to form **S32 and ultimately **44** in DMSO**



The formation of **44** could also occur ionically; the deprotonated species **25** could undergo a hydride elimination to form an imine structure, analogous to **S40**. For simplicity in the computational calculation, the hydride elimination pathway was modelled using the nonhalogenated dianionic species **S38** instead of the iodinated analogue **25**. It was determined that the energetics for this hydride elimination and the ultimate cyclisation for form **S32** would be possible at high temperatures, such as 120 °C. Therefore at the high temperature used in the reaction this pathway may be a minor pathway in the formation of **44**. However experimental results show that **44** is formed from **15** in

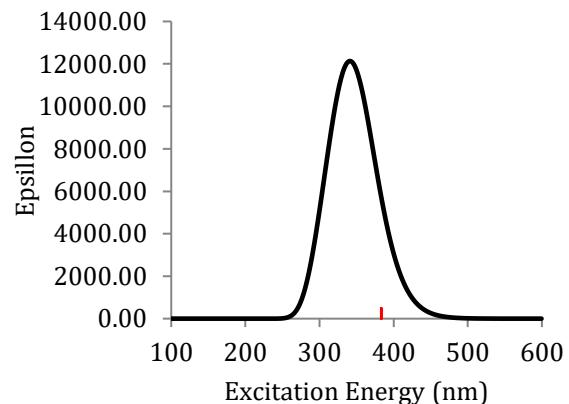
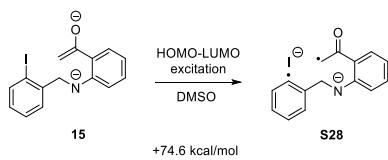
DMSO at room temperature, and therefore it is proposed that the major pathway is indeed a radical initiation followed by the reaction pathway modelled in Scheme S3.2.

Scheme S3.5: The energetics for the formation of **44 from **S32****



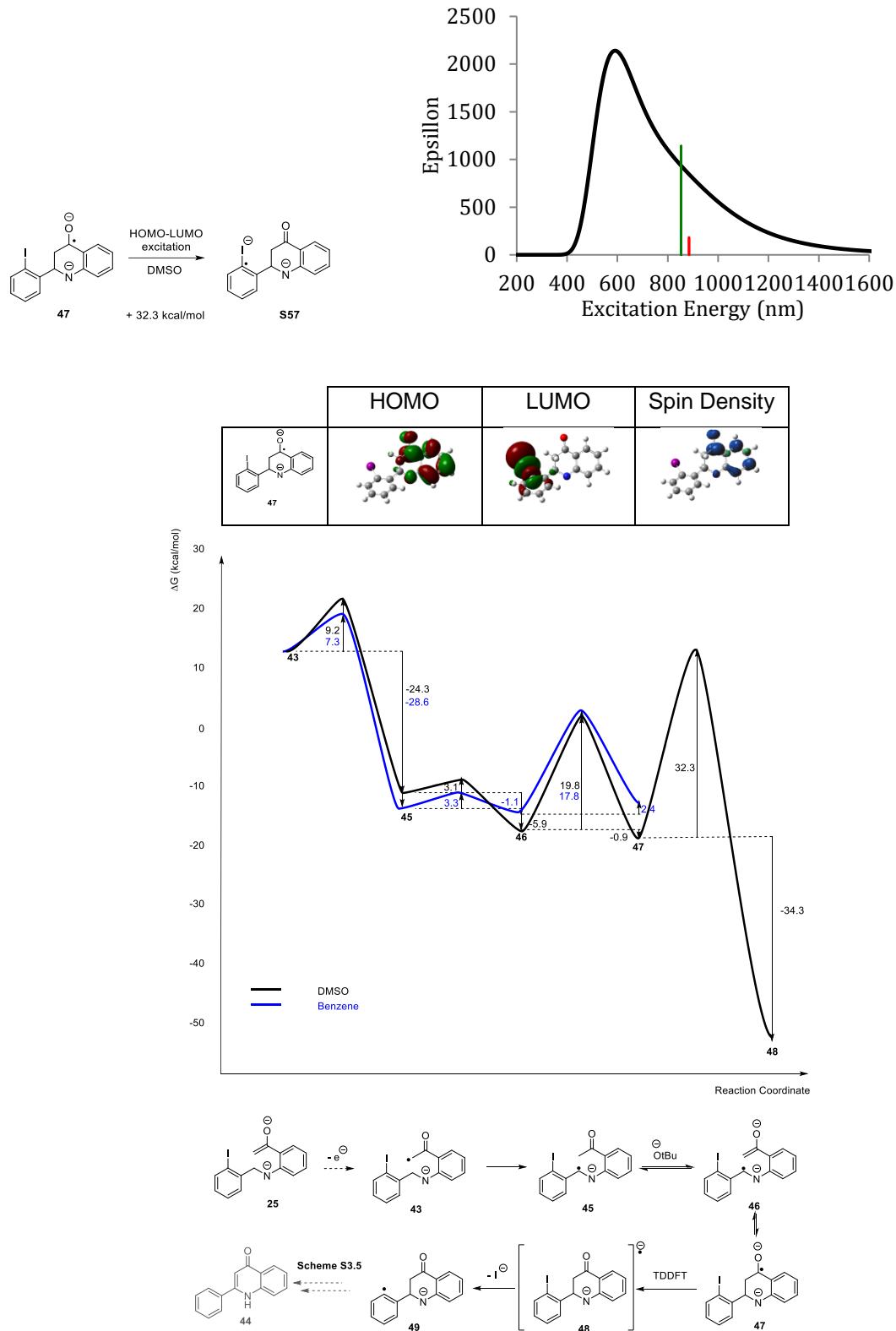
3.3 Intramolecular Analysis of **15**

Scheme S3.6. The TDDFT calculations were performed on **15**. The Gaussian curve was generated using the default Gaussian parameters. Black lines = Overall predicted UV-vis trace. Red vertical transitions corresponds to HOMO – LUMO excitation.



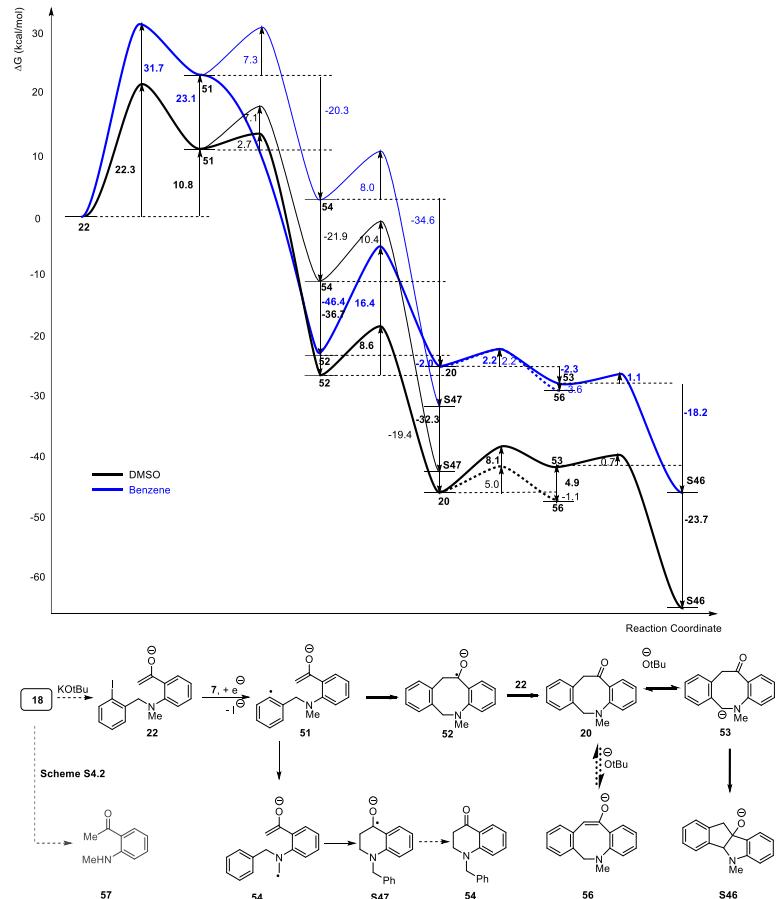
The TDDFT calculations suggests that intramolecular SET is not possible for **15** in DMSO.

Scheme S3.7: The TDDFT calculations were performed on intermediate **47**. The Gaussian curve was generated using the default Gaussian parameters. Black lines = Overall predicted UV-Vis trace. Red and Green vertical transitions correspond to HOMO – LUMO excitations.



4. Radical Cyclisation of 18

Scheme S4.1. Cyclisation reactions of **18** in both solvents



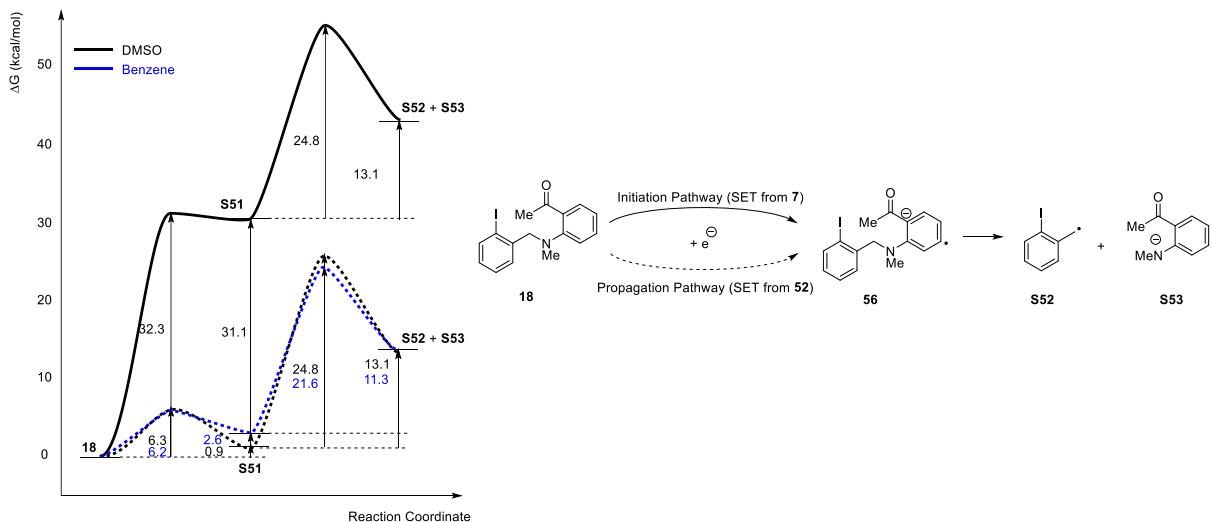
The energetics for the propagation in the formation of **20**

Propagation	DMSO	Benzene
52 To 22	$\Delta G^* = 8.6$ $\Delta G_{rxn} = -19.4$	$\Delta G^* = 16.4$ $\Delta G_{rxn} = -2.0$
52 To 18	$\Delta G^* = 6.3$ $\Delta G_{rxn} = 0.9$	$\Delta G^* = 6.2$ $\Delta G_{rxn} = 2.6$

The energetics for cyclisation from **51** in DMSO are very low barriers to either cyclise and form **52** or undergo hydrogen atom abstraction to form **54**. The formation of **54** is more favourable and thus we expect the major product to form via intermediate **52** (e.g. product **20**) and the minor product to **55**. The energetics for the cyclisation of **51** are more defined than in DMSO. The major product will form via intermediate **52**. There may be trace amounts of **55** forming depending on the conformation of **51** upon accepting the electron, however the energetic suggest that **19** or **20** will be the predominant products. The predominant product will be predicted as **19** in benzene because the equilibrium

between **56**, **20** and **53** is evenly distributed in benzene, however in DMSO the equilibrium strongly favours the enolate product **56** which is inactive to forming **19** and hence we would expect to see some of product **20** and maybe some **19**. Experimentally we only see **20** in DMSO at room temperature, and in benzene we only see **19** when the reaction is heated.¹

Scheme S4.2. Energetics for C-N cleavage of **18 in both solvents**



The LUMO for the neutral species **18** resided on the acetophenone moiety. **18** is present in the basic reaction mixture in low amounts because of the equilibrium to form **22**. If SET occurs to this species the acetophenone moiety may result in cleavage of the C-N bond to form **S53**. The species will be only occur through the chain propagation as the energetics for the initial SET to **18** is too high and endergonic. In the propagation the DMSO solvent is more favourable for the C-N cleavage as the intermediate **S51** is more stable in DMSO than in benzene.

1. K. J. Emery; T. Tuttle; A. R. Kennedy; J. A. Murphy, *Tetrahedron* 2016, **72**, 7875.

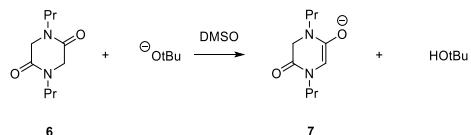
Effect of solvent on radical cyclisation pathways: S_{RN1} vs. aryl-aryl bond forming mechanisms

Katie J. Emery, John A. Murphy, and Tell Tuttle

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1. Enolate Formation



SM: 6 + tert-butoxide anion in DMSO

46

-884.9356036

C	-1.36374	-0.79822	-0.05487
C	-0.09272	-0.05446	0.28824
C	-1.11425	2.07147	-0.36904
C	-2.44057	1.39005	-0.08628
H	0.75743	-0.62637	-0.11841
H	-2.70782	1.59702	0.95824
H	-3.18663	1.86852	-0.72031
N	-0.02520	1.29665	-0.25986
N	-2.43981	-0.03982	-0.36031
O	-1.08861	3.26245	-0.67126
O	-1.38720	-2.02482	-0.04216
C	1.30419	1.88034	-0.44844
H	1.96759	1.06261	-0.74770
H	1.23498	2.60439	-1.26300
C	1.82201	2.56699	0.81368
H	1.07879	3.29453	1.15303
H	1.93685	1.82225	1.60746
C	3.15517	3.26223	0.55111
H	3.54831	3.72302	1.45897
H	3.90058	2.55208	0.18378
H	3.04047	4.04551	-0.20296
C	-3.73030	-0.68246	-0.59575
H	-4.30059	-0.04580	-1.27767
H	-3.53927	-1.63155	-1.09763
C	-4.51247	-0.91900	0.69444
H	-4.68095	0.03770	1.19845
H	-3.90142	-1.53409	1.36132
C	-5.84790	-1.60262	0.41523
H	-6.40277	-1.77410	1.33888
H	-6.46988	-0.98996	-0.24250
H	-5.69571	-2.56978	-0.07064
H	-0.01199	-0.03565	1.38443
O	2.39950	-1.31171	-1.09539
C	3.27185	-1.78200	-0.14304
C	4.63482	-2.15855	-0.76476
H	5.06976	-1.27906	-1.25024
H	5.34989	-2.53395	-0.02339
H	4.48951	-2.93105	-1.52685
C	2.70922	-3.03820	0.56209
H	1.75369	-2.79344	1.03705
H	2.53016	-3.82578	-0.17693
H	3.38613	-3.43163	1.32941
C	3.53125	-0.71644	0.94931
H	3.93310	0.19257	0.49048
H	2.58925	-0.45771	1.44271
H	4.23692	-1.06021	1.71435

TS: 6 + tert-butoxide anion in DMSO

46

-884.9266175

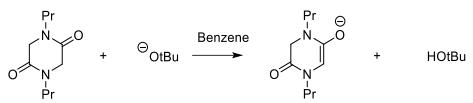
C	1.23006	-0.66572	-0.29670
C	-0.06711	0.01566	-0.38903
C	0.91891	2.07679	0.58258
C	2.27370	1.41055	0.46208
H	-0.94805	-0.74574	0.26462
H	2.77028	1.83917	-0.41974
H	2.85148	1.71419	1.33721
N	-0.13690	1.35665	0.19703
N	2.23191	-0.04056	0.40169
O	0.85738	3.23008	1.02475
O	1.39190	-1.80257	-0.75824
C	-1.47495	1.92986	0.31939
H	-2.13978	1.11927	0.62533
H	-1.45153	2.68310	1.10831
C	-1.96077	2.56031	-0.98390
H	-1.28238	3.37410	-1.25815
H	-1.91255	1.81876	-1.78762
C	-3.38882	3.08008	-0.84426
H	-3.73634	3.54224	-1.76993
H	-4.07300	2.26404	-0.59666
H	-3.45615	3.82709	-0.04872
C	3.50841	-0.72514	0.57338
H	3.97855	-0.32422	1.47739
H	3.29668	-1.78111	0.74482
C	4.45489	-0.57713	-0.61750
H	4.68217	0.48083	-0.78016
H	3.94440	-0.94176	-1.51305
C	5.74963	-1.35282	-0.39015
H	6.43184	-1.24523	-1.23508
H	6.26539	-0.99608	0.50549
H	5.54530	-2.41829	-0.25570
H	-0.39322	0.03501	-1.43401
O	-1.80671	-1.39696	0.99301
C	-2.85744	-1.94263	0.25097
C	-3.79594	-2.70398	1.19560
H	-4.18882	-2.02238	1.95553
H	-4.63994	-3.15026	0.65929
H	-3.24555	-3.50199	1.70224
C	-2.32417	-2.91742	-0.81328
H	-1.65424	-2.39042	-1.49858
H	-1.75431	-3.71618	-0.32921
H	-3.13394	-3.37030	-1.39430
C	-3.66310	-0.83640	-0.45592
H	-4.07598	-0.14524	0.28534
H	-3.01488	-0.26745	-1.13043
H	-4.49083	-1.25020	-1.04081

Prod: 7 + tert-butanol in DMSO

46

-884.9401085

C	1.14689	-0.41369	-0.63019
C	0.02355	0.38278	-0.79957
C	0.76359	2.09557	0.75506
C	2.12425	1.46907	0.51647
H	-1.00391	-0.95525	0.45807
H	2.55324	1.92962	-0.39122
H	2.76245	1.72874	1.36193
N	-0.22071	1.51767	0.05307
N	2.02432	0.02301	0.40394
O	0.61653	3.04921	1.53398
O	1.41488	-1.47135	-1.27037
C	-1.60273	1.95637	0.21921
H	-2.19976	1.08593	0.50837
H	-1.62283	2.67453	1.03920
C	-2.18547	2.59151	-1.04083
H	-1.58617	3.46745	-1.30788
H	-2.11666	1.89020	-1.87756
C	-3.64338	2.98825	-0.82374
H	-4.06918	3.44069	-1.72084
H	-4.24755	2.11317	-0.56835
H	-3.73514	3.70835	-0.00639
C	3.28586	-0.68931	0.55563
H	3.66495	-0.48733	1.56442
H	3.07240	-1.75700	0.49036
C	4.35838	-0.32384	-0.47323
H	4.64226	0.72689	-0.35614
H	3.93005	-0.43589	-1.47329
C	5.59373	-1.20720	-0.32029
H	6.37197	-0.93698	-1.03659
H	6.01698	-1.11448	0.68403
H	5.34065	-2.25896	-0.47916
H	-0.63047	0.26594	-1.64971
O	-1.55898	-1.46684	1.08139
C	-2.51896	-2.19660	0.31008
C	-3.27532	-3.07360	1.29873
H	-3.77278	-2.45513	2.04981
H	-4.03160	-3.66829	0.78132
H	-2.58456	-3.75127	1.80582
C	-1.79079	-3.04940	-0.72779
H	-1.16386	-2.41538	-1.36186
H	-1.14303	-3.77457	-0.22839
H	-2.50266	-3.59085	-1.35599
C	-3.47881	-1.22386	-0.37907
H	-3.97383	-0.59276	0.36384
H	-2.93594	-0.57939	-1.07697
H	-4.24443	-1.76722	-0.93866

**SM: 6 + tert-butoxide anion in Benzene**

46

C	-1.39618	-0.79264	-0.11444
C	-0.13049	-0.03769	0.21737
C	-1.20083	2.10288	-0.30656
C	-2.50669	1.38004	-0.01783
H	0.74825	-0.56438	-0.19831
H	-2.74108	1.52394	1.04624
H	-3.28000	1.88558	-0.59651
N	-0.10268	1.33560	-0.28116
N	-2.49228	-0.02874	-0.37690
O	-1.21463	3.30820	-0.54112
O	-1.42552	-2.01376	-0.12304
C	1.21796	1.92645	-0.51275
H	1.84290	1.15049	-0.96639
H	1.08461	2.77144	-1.19000
C	1.86860	2.38342	0.79069
H	1.21575	3.10350	1.29540
H	1.97959	1.51231	1.44470
C	3.24063	2.99575	0.52403
H	3.73371	3.29395	1.45188
H	3.88349	2.27399	0.01364
H	3.15541	3.88096	-0.11289
C	-3.77427	-0.68456	-0.59507
H	-4.37597	-0.04033	-1.24393
H	-3.57872	-1.61646	-1.12704
C	-4.52281	-0.97723	0.70435
H	-4.69956	-0.04045	1.24278
H	-3.88277	-1.60034	1.33533
C	-5.84992	-1.68081	0.43457
H	-6.38586	-1.88805	1.36246
H	-6.49687	-1.06612	-0.19749
H	-5.68593	-2.63182	-0.07849
H	-0.02987	-0.05267	1.31270
O	2.61202	-0.79913	-0.85451
C	3.37217	-1.65499	-0.11138
C	4.77097	-1.85500	-0.74207
H	5.27232	-0.88494	-0.82074
H	5.40936	-2.53489	-0.16357
H	4.65333	-2.25778	-1.75283
C	2.69914	-3.04446	0.00384
H	1.70911	-2.92993	0.45651
H	2.56263	-3.46137	-0.99867
H	3.28128	-3.75494	0.60446
C	3.57453	-1.11114	1.32604
H	4.05753	-0.12954	1.27470
H	2.59594	-0.98162	1.80090
H	4.18427	-1.77092	1.95623

TS: 6 + *tert*-butoxide anion in Benzene

46

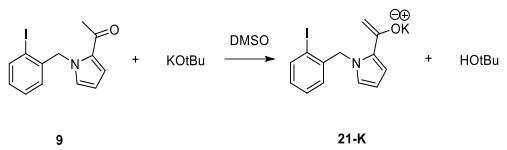
-884.8883013

C	1.22521	-0.65288	-0.28132
C	-0.08105	0.01670	-0.36513
C	0.89037	2.10184	0.57550
C	2.25095	1.43772	0.48029
H	-0.93544	-0.70658	0.29578
H	2.76196	1.87196	-0.39152
H	2.80656	1.75090	1.36702
N	-0.15883	1.36540	0.20052
N	2.22196	-0.01214	0.42225
O	0.82418	3.26265	0.98886
O	1.40595	-1.77596	-0.75255
C	-1.50267	1.92196	0.32519
H	-2.15563	1.10086	0.63238
H	-1.48448	2.67684	1.11318
C	-1.99198	2.54802	-0.97933
H	-1.32529	3.37366	-1.24719
H	-1.92777	1.80747	-1.78309
C	-3.42989	3.04209	-0.84751
H	-3.78358	3.49787	-1.77474
H	-4.09848	2.21278	-0.60163
H	-3.51391	3.78766	-0.05191
C	3.49929	-0.69049	0.58130
H	3.99101	-0.26993	1.46571
H	3.28983	-1.74276	0.77918
C	4.41967	-0.57634	-0.63452
H	4.63464	0.47731	-0.83981
H	3.88837	-0.97848	-1.50090
C	5.72485	-1.33555	-0.41087
H	6.38520	-1.26231	-1.27722
H	6.26317	-0.94157	0.45604
H	5.52776	-2.39512	-0.22739
H	-0.41152	0.02039	-1.40933
O	-1.86816	-1.31424	1.04334
C	-2.80641	-1.96183	0.25373
C	-3.76147	-2.76322	1.15209
H	-4.25230	-2.08765	1.85865
H	-4.53052	-3.28837	0.57368
H	-3.18982	-3.49827	1.72532
C	-2.12251	-2.93133	-0.73038
H	-1.41784	-2.38824	-1.36632
H	-1.55024	-3.67512	-0.16882
H	-2.84772	-3.45082	-1.36720
C	-3.63813	-0.94180	-0.55412
H	-4.14304	-0.25787	0.13553
H	-2.98134	-0.34971	-1.20018
H	-4.39451	-1.42668	-1.18135

Prod: 7 + *tert*-butanol in Benzene

46

C	1.13092	-0.42327	-0.57318
C	-0.01873	0.34347	-0.73148
C	0.76417	2.15701	0.69671
C	2.12179	1.51482	0.47058
H	-1.06328	-0.92885	0.58418
H	2.53997	1.93654	-0.46145
H	2.76556	1.81760	1.29789
N	-0.23746	1.52525	0.06489
N	2.02453	0.06660	0.42709
O	0.63498	3.16361	1.40370
O	1.41159	-1.48347	-1.19009
C	-1.61148	1.97116	0.24906
H	-2.21135	1.10156	0.53725
H	-1.61910	2.68790	1.07168
C	-2.19735	2.61597	-1.00546
H	-1.59376	3.49044	-1.26770
H	-2.12864	1.91674	-1.84432
C	-3.65342	3.01803	-0.78650
H	-4.08041	3.47946	-1.67922
H	-4.26116	2.14403	-0.53546
H	-3.74079	3.73208	0.03703
C	3.28122	-0.64507	0.58501
H	3.69494	-0.38537	1.56768
H	3.05353	-1.71215	0.58958
C	4.32336	-0.36289	-0.50106
H	4.62083	0.69078	-0.46765
H	3.85512	-0.54364	-1.47216
C	5.55340	-1.25003	-0.32907
H	6.30928	-1.04780	-1.09123
H	6.01562	-1.09424	0.65068
H	5.27729	-2.30565	-0.40140
H	-0.63130	0.23869	-1.61453
O	-1.69559	-1.42037	1.15078
C	-2.48851	-2.23700	0.29412
C	-3.34335	-3.10220	1.21267
H	-3.96805	-2.47144	1.85030
H	-3.99062	-3.76182	0.62850
H	-2.70257	-3.71375	1.85203
C	-1.57795	-3.10283	-0.57624
H	-0.89223	-2.47698	-1.15578
H	-0.97083	-3.75437	0.05771
H	-2.16609	-3.72500	-1.25758
C	-3.38549	-1.35412	-0.58003
H	-4.00992	-0.71596	0.05150
H	-2.77539	-0.71418	-1.22283
H	-4.03540	-1.96402	-1.21430



SM: 9 + KOtBu in DMSO

43

-1476.8805597

C	2.99260	3.09117	0.30629
C	1.77409	2.60178	-0.14970
C	1.56689	1.23348	-0.34423
C	2.63292	0.37619	-0.06828
C	3.85940	0.84823	0.38589
C	4.03708	2.21470	0.57661
H	3.12341	4.15670	0.45115
H	0.96311	3.29269	-0.35462
H	4.66819	0.15894	0.59302
H	4.98965	2.58491	0.93600
C	0.23890	0.70540	-0.84491
H	0.33094	0.43854	-1.90144
H	-0.09460	-0.19914	-0.33171
N	-0.83132	1.69123	-0.75556
C	-1.26080	2.40364	-1.83278
C	-1.48578	2.15428	0.37703
C	-2.21575	3.31691	-1.42423
H	-0.85219	2.20398	-2.81191
C	-2.35107	3.16182	-0.03176
H	-3.00830	3.70254	0.63079
H	-2.74314	4.00733	-2.06272
C	-1.35501	1.68906	1.77753
C	-0.48007	0.52331	2.13665
H	0.56807	0.73940	1.91492
H	-0.58994	0.32750	3.20222
O	-2.01063	2.26729	2.63021
I	2.42185	-1.73049	-0.33134
H	-0.79997	-0.34535	1.54695
K	-3.58614	0.31131	-1.01592
O	-1.92862	-1.30645	-0.07269
C	-2.23009	-2.59811	0.31063
C	-3.75891	-2.81164	0.35887
H	-4.20851	-2.08983	1.04930
H	-4.18860	-2.65414	-0.63695
H	-4.03514	-3.81902	0.68810
C	-1.66135	-2.90621	1.71170
H	-1.88061	-3.92989	2.03437
H	-0.57472	-2.76981	1.70470
H	-2.08506	-2.21380	2.44617
C	-1.63862	-3.62260	-0.67942
H	-2.03503	-3.43610	-1.68247
H	-0.55057	-3.51118	-0.71615
H	-1.87172	-4.65690	-0.40237

TS: 9 + KOtBu in DMSO

43

-1476.8690869

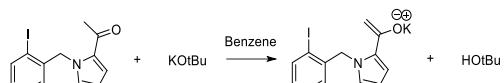
C	-2.56786	-3.30761	0.64319
C	-1.43416	-2.70114	0.11504
C	-1.41646	-1.33832	-0.19343
C	-2.58472	-0.61141	0.03769
C	-3.72697	-1.20108	0.56700
C	-3.71504	-2.55778	0.87375
H	-2.55210	-4.36566	0.87481
H	-0.54191	-3.29266	-0.05930
H	-4.61791	-0.61087	0.73992
H	-4.60256	-3.01904	1.28954
C	-0.17753	-0.68224	-0.77153
H	-0.36203	-0.41327	-1.81512
N	0.98402	-1.55991	-0.75946
C	1.36485	-2.25926	-1.87126
C	1.76433	-1.96354	0.31720
C	2.40782	-3.09838	-1.53987
H	0.85784	-2.10104	-2.81099
C	2.65457	-2.91203	-0.16164
H	3.40776	-3.39048	0.44376
H	2.92442	-3.76064	-2.21627
C	1.76942	-1.44287	1.72276
C	0.94129	-0.31644	2.08699
H	-0.08975	-0.34776	1.74287
H	1.01257	-0.09266	3.15020
O	2.62799	-1.92995	2.46977
I	-2.67849	1.46645	-0.43685
H	1.53772	0.60828	1.34878
K	3.56041	0.02389	-1.22165
O	2.20259	1.34032	0.47780
C	1.91231	2.71184	0.45752
C	3.19678	3.51193	0.71354
H	3.60581	3.25321	1.69419
H	3.94485	3.26542	-0.04629
H	3.01723	4.59124	0.68464
C	0.87718	3.05980	1.53812
H	0.63803	4.12722	1.52874
H	-0.04566	2.49633	1.37117
H	1.26244	2.79856	2.52804
C	1.34811	3.09551	-0.91869
H	2.08344	2.87689	-1.69973
H	0.44386	2.51545	-1.12516
H	1.09774	4.15975	-0.97469
H	0.07425	0.24035	-0.24774

Prod: 21-K + HOtBu in DMSO

43

-1476.8930435

C	-2.96084	-3.04404	1.01082
C	-1.82388	-2.55495	0.37817
C	-1.74772	-1.22894	-0.05459
C	-2.85587	-0.41336	0.17515
C	-4.00170	-0.88480	0.80515
C	-4.05229	-2.21006	1.22475
H	-2.99171	-4.07676	1.33658
H	-0.97265	-3.20798	0.21855
H	-4.84623	-0.22730	0.96808
H	-4.94346	-2.58151	1.71597
C	-0.50634	-0.70158	-0.75056
H	-0.76781	-0.38266	-1.76306
H	-0.12085	0.17582	-0.22809
N	0.54980	-1.68797	-0.86278
C	0.63560	-2.53610	-1.93682
C	1.55299	-1.99056	0.04217
C	1.69962	-3.38535	-1.74582
H	-0.06681	-2.44928	-2.75184
C	2.28327	-3.03367	-0.50270
H	3.14005	-3.48588	-0.02761
H	2.02176	-4.15842	-2.42582
C	1.87572	-1.31029	1.34398
C	0.91766	-0.62637	2.05174
H	-0.13251	-0.65781	1.80157
H	1.20400	-0.16017	2.98821
O	3.11608	-1.40284	1.67868
I	-2.83969	1.63040	-0.44238
H	1.92967	0.79065	0.64135
K	4.43165	-0.56019	-0.39826
O	2.45681	1.24655	-0.04132
C	2.38755	2.65734	0.21428
C	3.00747	2.94510	1.58049
H	2.45581	2.41873	2.36509
H	4.04652	2.60723	1.59987
H	2.98312	4.01488	1.80119
C	0.92466	3.09248	0.17971
H	0.83246	4.16707	0.35525
H	0.48343	2.85569	-0.79181
H	0.35366	2.56846	0.95306
C	3.18335	3.32648	-0.89657
H	4.21826	2.97560	-0.88525
H	2.74469	3.09392	-1.86960
H	3.18348	4.41039	-0.76395



SM: 9 + KOtBu in Benzene

43

-1476.8655305

C	-2.77192	-3.27213	0.02960
C	-1.57793	-2.66482	-0.33941
C	-1.46042	-1.27384	-0.41514
C	-2.59263	-0.51631	-0.10978
C	-3.79514	-1.10849	0.25949
C	-3.88315	-2.49414	0.33132
H	-2.83066	-4.35244	0.08318
H	-0.71493	-3.28075	-0.56966
H	-4.65540	-0.49441	0.49425
H	-4.81782	-2.95659	0.62465
C	-0.15708	-0.62125	-0.82804
H	-0.22578	-0.29066	-1.86841
H	0.10301	0.26892	-0.25227
N	0.97121	-1.54298	-0.75424
C	1.47945	-2.16983	-1.85020
C	1.58582	-2.05126	0.37742
C	2.44465	-3.07682	-1.44929
H	1.10537	-1.92832	-2.83352
C	2.50361	-3.00549	-0.04286
H	3.13761	-3.56704	0.62545
H	3.01910	-3.71740	-2.09967
C	1.39350	-1.65692	1.79984
C	0.48931	-0.52046	2.17933
H	-0.54673	-0.73506	1.90480
H	0.55523	-0.37834	3.25663
O	2.03495	-2.26410	2.63704
I	-2.52796	1.61153	-0.19130
H	0.82217	0.37827	1.64458
K	3.75418	-0.19431	-0.67866
O	1.99216	1.31562	-0.01090
C	2.01282	2.68596	0.14769
C	3.46592	3.20069	0.24050
H	3.97266	2.71532	1.08160
H	4.00533	2.95382	-0.68186
H	3.52579	4.28500	0.38276
C	1.27197	3.09813	1.43493
H	1.26724	4.18259	1.58832
H	0.23542	2.75010	1.38445
H	1.74741	2.62696	2.30110
C	1.33279	3.37988	-1.04911
H	1.86337	3.12233	-1.97161
H	0.30410	3.01914	-1.13754
H	1.31547	4.47099	-0.95096

TS: 9 + KOtBu in Benzene

43

-1476.8560457

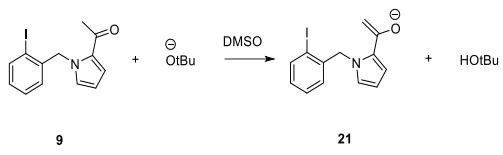
C	2.09652	2.65334	2.21905
C	1.16452	2.35845	1.23231
C	1.34008	1.27858	0.36248
C	2.49812	0.51426	0.51355
C	3.44225	0.79754	1.49453
C	3.23667	1.87033	2.35398
H	1.93020	3.49537	2.87981
H	0.27731	2.97418	1.12699
H	4.33358	0.18972	1.58326
H	3.97176	2.09084	3.11864
C	0.30186	0.95900	-0.69711
H	0.80100	0.75475	-1.64634
N	-0.63445	2.04739	-0.92813
C	-0.33958	3.07903	-1.77214
C	-1.91987	2.21980	-0.44443
C	-1.42009	3.93100	-1.83697
H	0.61582	3.11157	-2.27373
C	-2.42153	3.38031	-1.00763
H	-3.40606	3.77201	-0.80678
H	-1.47597	4.83515	-2.42203
C	-2.64113	1.38280	0.54537
C	-1.93812	0.49991	1.44806
H	-0.90806	0.76060	1.67508
H	-2.52193	0.30907	2.34891
O	-3.88529	1.43002	0.50991
I	2.92323	-1.11913	-0.79373
H	-1.98229	-0.63519	0.80826
K	-4.64268	-1.03584	0.08312
O	-2.26875	-1.75391	0.12468
C	-1.35067	-2.80312	0.24772
C	-2.09168	-4.07991	0.66902
H	-2.57736	-3.92449	1.63686
H	-2.86105	-4.31958	-0.07132
H	-1.41614	-4.93683	0.75369
C	-0.29140	-2.47064	1.31223
H	0.43486	-3.28152	1.41907
H	0.25680	-1.56135	1.04750
H	-0.77267	-2.30287	2.28041
C	-0.66438	-3.04461	-1.10348
H	-1.41321	-3.31860	-1.85217
H	-0.16685	-2.13049	-1.43682
H	0.08323	-3.84246	-1.04654
H	-0.25885	0.05800	-0.43341

Prod: 21-K + KOtBu in Benzene

43

-1476.8753977

C	-2.87504	-3.03826	1.12095
C	-1.75486	-2.54210	0.46570
C	-1.71551	-1.22900	-0.00862
C	-2.84131	-0.43438	0.20409
C	-3.97104	-0.91357	0.85594
C	-3.98510	-2.22553	1.31682
H	-2.87655	-4.05988	1.48087
H	-0.88679	-3.17673	0.32361
H	-4.82994	-0.27151	1.00408
H	-4.86300	-2.60327	1.82688
C	-0.48928	-0.69187	-0.72335
H	-0.77124	-0.35504	-1.72456
H	-0.09034	0.17344	-0.19050
N	0.56189	-1.67755	-0.87244
C	0.61490	-2.52508	-1.94976
C	1.58319	-1.98757	0.00772
C	1.67817	-3.38030	-1.78634
H	-0.11034	-2.43596	-2.74419
C	2.29396	-3.03436	-0.55673
H	3.14464	-3.50407	-0.08737
C	1.97291	-4.15970	-2.47136
C	1.94701	-1.31355	1.30454
C	1.02088	-0.61204	2.03611
H	-0.03846	-0.64375	1.82811
H	1.34100	-0.18301	2.97914
O	3.19423	-1.42168	1.59894
I	-2.88343	1.58853	-0.47933
H	2.11297	0.83061	0.77011
K	4.40094	-0.57347	-0.42901
O	2.65529	1.32088	0.11914
C	2.36211	2.71845	0.24929
C	2.82161	3.19758	1.62502
H	2.29364	2.64980	2.41046
H	3.89377	3.02629	1.74589
C	2.62024	4.26392	1.75272
C	0.85960	2.92887	0.08068
H	0.60326	3.98883	0.15283
H	0.53015	2.55493	-0.89224
H	0.31134	2.39128	0.86076
C	3.13773	3.41573	-0.85911
H	4.20869	3.22755	-0.74786
H	2.81445	3.04690	-1.83535
H	2.97178	4.49441	-0.82191



SM: 9 + *tert*-butoxide anion in DMSO

42

-876.9881769

C	3.51999	1.86939	0.74825
C	2.28579	1.87535	0.10880
C	1.61787	0.68651	-0.20105
C	2.25041	-0.50898	0.14465
C	3.48496	-0.53420	0.78385
C	4.12095	0.66408	1.09066
H	4.00980	2.80795	0.97760
H	1.82594	2.82225	-0.15280
H	3.94827	-1.47810	1.04199
H	5.08048	0.64728	1.59307
C	0.27021	0.70267	-0.89719
H	0.38892	0.31795	-1.91410
H	-0.47729	0.06019	-0.41962
N	-0.27630	2.04806	-1.02282
C	-0.12070	2.78828	-2.15166
C	-0.85751	2.84309	-0.04548
C	-0.61279	4.06230	-1.93643
H	0.32904	2.34807	-3.02880
C	-1.07502	4.09408	-0.60863
H	-1.53512	4.92050	-0.09011
H	-0.63938	4.86051	-2.66096
C	-1.20193	2.48612	1.34540
C	-0.97248	1.10061	1.87641
H	0.08644	0.83353	1.82704
H	-1.30447	1.07164	2.91350
O	-1.70633	3.34934	2.05120
I	1.34734	-2.38779	-0.31158
H	-1.54320	0.38371	1.26423
O	-2.52358	-0.55540	-0.34453
C	-3.39011	-1.54086	0.06698
C	-4.86302	-1.11899	-0.13705
H	-5.06636	-0.20359	0.42777
H	-5.04187	-0.91213	-1.19698
H	-5.57180	-1.88928	0.18824
C	-3.19405	-1.85761	1.56806
H	-3.85972	-2.65376	1.92043
H	-2.15779	-2.16696	1.74411
H	-3.38538	-0.95952	2.16423
C	-3.16634	-2.85061	-0.72203
H	-3.30423	-2.66091	-1.79131
H	-2.14127	-3.20239	-0.56831
H	-3.85413	-3.64912	-0.42051

TS: 9 + *tert*-butoxide anion in DMSO

42

-876.9818173

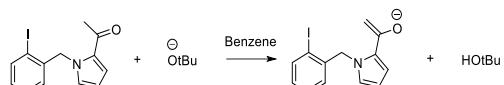
C	0.34025	-2.76997	2.42937
C	0.89692	-2.10487	1.34366
C	0.09849	-1.47341	0.38609
C	-1.28486	-1.55056	0.55469
C	-1.85981	-2.21014	1.63589
C	-1.04076	-2.81938	2.58046
H	0.98673	-3.24798	3.15534
H	1.97545	-2.06658	1.23046
H	-2.93655	-2.25428	1.73918
H	-1.48767	-3.33298	3.42307
C	0.71744	-0.72736	-0.78031
H	0.25990	-1.07244	-1.71030
N	2.15121	-0.94864	-0.90542
C	2.64809	-2.02992	-1.57524
C	3.20867	-0.18589	-0.43812
C	4.02497	-1.98523	-1.54662
H	1.97408	-2.73893	-2.03224
C	4.37627	-0.81598	-0.83569
H	5.36675	-0.45428	-0.60871
H	4.69081	-2.70722	-1.99276
C	3.16155	1.04445	0.40365
C	1.97069	1.36582	1.16993
H	1.43272	0.49770	1.54940
H	2.19943	2.07877	1.96293
O	4.16774	1.76387	0.38606
I	-2.61648	-0.70614	-0.88686
H	1.15486	1.95563	0.38802
O	0.22746	2.53640	-0.46108
C	-0.64879	3.36417	0.23885
C	0.07228	4.64889	0.68691
H	0.92735	4.38976	1.31862
H	0.44607	5.18675	-0.18958
H	-0.58570	5.31812	1.25123
C	-1.20152	2.64989	1.48907
H	-1.92067	3.27555	2.02789
H	-1.70247	1.72207	1.19456
H	-0.38750	2.39620	2.17379
C	-1.82885	3.74489	-0.66618
H	-1.45868	4.24667	-1.56491
H	-2.36376	2.84114	-0.97298
H	-2.53430	4.41293	-0.16043
H	0.51035	0.34467	-0.69942

Prod: 21 + HOtBu in DMSO

42

-877.0023769

C	2.69497	2.61842	1.45047
C	1.59535	2.33744	0.64847
C	1.41930	1.07633	0.07229
C	2.39166	0.11060	0.33257
C	3.49981	0.37377	1.13030
C	3.64944	1.63700	1.69304
H	2.80501	3.60450	1.88555
H	0.84981	3.10397	0.46534
H	4.24035	-0.39542	1.30995
H	4.51112	1.84716	2.31512
C	0.21502	0.78234	-0.80575
H	0.55934	0.45459	-1.78995
H	-0.37621	-0.03330	-0.38554
N	-0.63594	1.93814	-1.00747
C	-0.39087	2.82675	-2.02396
C	-1.68676	2.40442	-0.23216
C	-1.28454	3.86642	-1.92658
H	0.39765	2.63214	-2.73522
C	-2.10494	3.59358	-0.80267
H	-2.92691	4.18288	-0.42954
H	-1.34532	4.71180	-2.59444
C	-2.31103	1.77948	0.98861
C	-1.61702	0.86227	1.75074
H	-0.56973	0.64252	1.60834
H	-2.09552	0.47112	2.64256
O	-3.50431	2.17508	1.22630
I	2.22546	-1.84586	-0.50579
H	-2.71992	-0.43731	0.36791
O	-3.21196	-1.01027	-0.25067
C	-3.05535	-2.36573	0.17901
C	-3.64270	-2.52860	1.58092
H	-3.10929	-1.88889	2.28944
H	-4.69790	-2.24458	1.58163
H	-3.55911	-3.56420	1.92003
C	-1.57124	-2.72763	0.17605
H	-1.41789	-3.76683	0.47909
H	-1.15260	-2.59031	-0.82435
H	-1.02244	-2.08268	0.86975
C	-3.81920	-3.21680	-0.82625
H	-4.87298	-2.92810	-0.84094
H	-3.40554	-3.07936	-1.82814
H	-3.75087	-4.27472	-0.56298



SM: 9 + tert-butoxide anion in Benzene

42

-876.9509341			
C	-1.10231	-3.82205	0.25083
C	-0.21375	-2.82173	-0.12513
C	-0.61524	-1.48569	-0.22747
C	-1.95551	-1.20299	0.04581
C	-2.85869	-2.19145	0.41947
C	-2.42781	-3.50900	0.52824
H	-0.75518	-4.84565	0.32661
H	0.81922	-3.07502	-0.33994
H	-3.89053	-1.93537	0.62482
H	-3.12840	-4.28026	0.82533
C	0.35273	-0.39263	-0.62649
H	0.00096	0.06424	-1.55600
H	0.42373	0.44398	0.09649
N	1.69184	-0.89818	-0.89973
C	2.09640	-1.21187	-2.15915
C	2.70092	-1.23565	-0.01233
C	3.37032	-1.74510	-2.11316
H	1.44354	-1.01967	-2.99701
C	3.74782	-1.75987	-0.75754
H	4.67743	-2.10006	-0.32963
H	3.95210	-2.06650	-2.96257
C	2.71881	-1.12470	1.46642
C	1.54130	-0.59176	2.22758
H	0.63217	-1.14890	1.98868
H	1.75754	-0.68551	3.29094
O	3.73328	-1.47895	2.04677
I	-2.69706	0.78751	-0.13478
H	1.38278	0.46280	1.95147
O	1.07975	2.07440	0.91107
C	1.20306	3.19338	0.13683
C	2.62908	3.78259	0.23958
H	2.84379	4.02112	1.28573
H	3.35235	3.03068	-0.09146
H	2.76209	4.68954	-0.36355
C	0.20025	4.28569	0.57656
H	0.26969	5.20041	-0.02545
H	-0.81698	3.88878	0.49796
H	0.38451	4.53956	1.62497
C	0.93022	2.87568	-1.35499
H	1.62096	2.09302	-1.68938
H	-0.09290	2.50061	-1.46484
H	1.05236	3.75091	-2.00471

TS: 9 + *tert*-butoxide anion in Benzene

42

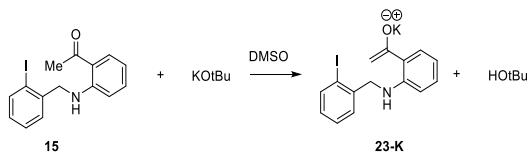
-876.9444239

C	0.37815	-2.71351	2.43847
C	0.92199	-2.04338	1.35019
C	0.11263	-1.42732	0.39103
C	-1.26830	-1.53039	0.56158
C	-1.83088	-2.19587	1.64548
C	-1.00151	-2.78669	2.59196
H	1.03468	-3.17467	3.16663
H	1.99938	-1.98414	1.23427
H	-2.90695	-2.25509	1.74856
H	-1.43836	-3.30248	3.43878
C	0.71976	-0.67128	-0.77407
H	0.25063	-1.00774	-1.70177
N	2.14971	-0.90348	-0.91506
C	2.62663	-1.99403	-1.58675
C	3.22024	-0.16172	-0.44676
C	4.00348	-1.97282	-1.55974
H	1.93843	-2.69069	-2.04140
C	4.37519	-0.81062	-0.84582
H	5.36872	-0.45554	-0.62293
H	4.65619	-2.70314	-2.01187
C	3.20220	1.07744	0.39526
C	2.01609	1.41632	1.16510
H	1.49449	0.55196	1.57785
H	2.25704	2.14717	1.93777
O	4.22458	1.76406	0.37494
I	-2.61304	-0.71389	-0.88148
H	1.15950	1.96098	0.38952
O	0.16129	2.43707	-0.43774
C	-0.70095	3.28670	0.23773
C	0.03174	4.57926	0.64833
H	0.88339	4.33101	1.28834
H	0.41598	5.07784	-0.24604
H	-0.62095	5.27519	1.18757
C	-1.25724	2.60891	1.50806
H	-1.96461	3.25304	2.04266
H	-1.76861	1.68132	1.23176
H	-0.43840	2.35651	2.18820
C	-1.87873	3.65279	-0.67871
H	-1.49635	4.11994	-1.59066
H	-2.41672	2.74317	-0.96041
H	-2.58010	4.34298	-0.19540
H	0.50556	0.40098	-0.68318

Prod: 21 + HOtBu in Benzene

42

C	-2.03379	-2.92336	1.78231
C	-1.04666	-2.58914	0.86355
C	-1.10570	-1.39774	0.13564
C	-2.19105	-0.55575	0.37328
C	-3.18914	-0.87298	1.28728
C	-3.10823	-2.06698	1.99517
H	-1.95862	-3.85176	2.33574
H	-0.20019	-3.24948	0.70726
H	-4.01766	-0.19495	1.44804
H	-3.88202	-2.31763	2.71110
C	-0.02566	-1.03867	-0.86766
H	-0.48026	-0.94134	-1.85823
N	0.40791	-0.06894	-0.62127
N	1.02404	-2.02983	-0.96392
C	0.91957	-3.10630	-1.81107
C	2.21235	-2.11285	-0.25679
C	2.03976	-3.88889	-1.66305
H	0.05850	-3.20748	-2.45431
C	2.85619	-3.25547	-0.69134
H	3.82397	-3.56540	-0.33113
H	2.24996	-4.79821	-2.20503
C	2.75937	-1.16867	0.79123
C	1.88534	-0.41997	1.56469
H	0.81808	-0.59305	1.57344
H	2.30729	0.16562	2.37514
O	4.02199	-1.16099	0.88040
I	-2.37679	1.29402	-0.67959
H	1.92454	1.12316	0.18165
O	1.80123	1.86799	-0.44849
C	2.08156	3.07913	0.24302
C	3.52418	3.05371	0.75056
H	3.66834	2.20857	1.42930
H	4.21246	2.93453	-0.08935
H	3.77054	3.97743	1.28195
C	1.10683	3.24715	1.41182
H	1.28293	4.19197	1.93431
H	0.07815	3.23372	1.04297
H	1.22657	2.42660	2.12371
C	1.88533	4.19736	-0.77356
H	2.56896	4.06158	-1.61481
H	0.86026	4.17844	-1.15252
H	2.07474	5.17295	-0.31827



SM: 15 + KOtBu in DMSO

47

-1554.2949997

C	3.91388	3.35180	0.50774
C	2.97954	2.61965	1.23172
C	2.72040	1.27894	0.93921
C	3.43083	0.69585	-0.11408
C	4.36763	1.41256	-0.84878
C	4.60691	2.74733	-0.53407
H	4.09731	4.39004	0.75591
H	2.43455	3.08937	2.04340
H	4.90807	0.93877	-1.65815
H	5.33712	3.30654	-1.10644
C	1.68158	0.52145	1.72613
H	2.09591	-0.44068	2.04789
H	1.41601	1.08735	2.62229
C	-0.31583	-0.78594	1.07688
C	-1.15982	-1.28451	0.04281
C	-0.34266	-1.42944	2.32987
C	-1.96098	-2.40757	0.30421
C	-1.15743	-2.52469	2.55164
H	0.27045	-1.05155	3.13739
C	-1.97366	-3.03000	1.53792
H	-2.59516	-2.79534	-0.48273
H	-1.15694	-2.99118	3.53023
H	-2.60744	-3.88926	1.71410
N	0.50398	0.30294	0.88701
O	-0.68897	0.43881	-1.50734
C	-1.21885	-0.64798	-1.29175
C	-1.95132	-1.34511	-2.41048
H	-3.02067	-1.38970	-2.18984
H	-1.80094	-0.77898	-3.32700
H	-1.59132	-2.36718	-2.53973
I	3.12844	-1.35401	-0.63877
O	-3.96974	1.29283	-0.14272
C	-5.24583	0.81507	-0.34103
C	-6.27438	1.64004	0.46209
H	-6.22797	2.68850	0.15093
H	-7.30028	1.28204	0.32211
H	-6.03410	1.58993	1.52876
C	-5.36141	-0.65607	0.11055
H	-4.67106	-1.27599	-0.46993
H	-5.08255	-0.73967	1.16588
H	-6.37296	-1.05756	-0.01497
C	-5.63703	0.88842	-1.83169
H	-6.64792	0.50963	-2.01925
H	-5.58704	1.92677	-2.17362
H	-4.93217	0.29955	-2.42723
K	-1.80057	2.19550	0.40117
H	0.60482	0.58424	-0.07974

TS: 15 + KOtBu in DMSO

47

-1554.2868368

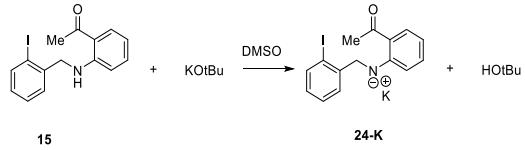
C	-2.02918	3.29105	-1.27630
C	-1.33430	2.15277	-1.66722
C	-1.70160	0.87993	-1.21723
C	-2.79567	0.79248	-0.35338
C	-3.50440	1.92086	0.04729
C	-3.11579	3.17353	-0.41623
H	-1.72281	4.26352	-1.64168
H	-0.48319	2.23971	-2.33474
H	-4.35032	1.82768	0.71600
H	-3.66818	4.05173	-0.10432
C	-0.86424	-0.30993	-1.61542
H	-1.50036	-1.16040	-1.89490
H	-0.26917	-0.03903	-2.49047
C	0.98695	-1.63477	-0.64946
C	1.83599	-1.95162	0.44161
C	1.17825	-2.30569	-1.86631
C	2.79590	-2.95148	0.28952
C	2.15137	-3.29090	-1.99041
H	0.55451	-2.07270	-2.71941
C	2.95577	-3.63629	-0.90992
H	3.42960	-3.19962	1.13308
H	2.26814	-3.79902	-2.94096
H	3.70140	-4.41592	-1.00226
N	0.03720	-0.62734	-0.51802
O	0.64944	-0.76324	2.11678
C	1.75814	-1.16720	1.71860
C	2.99646	-0.73413	2.32158
H	3.11645	0.35986	1.66441
H	2.89173	-0.45635	3.36948
H	3.87802	-1.33225	2.11029
I	-3.44912	-1.09565	0.40319
O	3.03161	1.58917	1.02367
C	3.66261	1.72263	-0.21718
C	2.60411	1.97613	-1.30519
H	2.05083	2.89535	-1.08106
H	3.05002	2.08480	-2.29907
H	1.89661	1.13948	-1.32814
C	4.44581	0.45016	-0.58300
H	5.18689	0.22918	0.19136
H	3.76777	-0.40480	-0.66233
H	4.96783	0.56874	-1.53733
C	4.63578	2.91033	-0.17934
H	5.12998	3.06526	-1.14392
H	4.09388	3.82324	0.08384
H	5.40367	2.73653	0.58006
K	0.53243	1.91320	1.40163
H	-0.38662	-0.62945	0.40253

Prod: 23-K + HOtBu in DMSO

47

-1554.3089965

C	4.29776	3.05512	0.63285
C	3.38922	2.31982	1.38589
C	2.93936	1.06537	0.96785
C	3.43458	0.57324	-0.24383
C	4.34357	1.29305	-1.00994
C	4.77410	2.54108	-0.56718
H	4.63082	4.02472	0.98243
H	3.01399	2.71851	2.32240
H	4.71738	0.88889	-1.94214
H	5.48229	3.10288	-1.16423
C	1.93567	0.31017	1.80240
H	2.28451	-0.71992	1.95098
H	1.87084	0.77645	2.78988
C	-0.24099	-0.74843	1.31156
C	-1.16979	-1.11459	0.30026
C	-0.23044	-1.46191	2.52373
C	-2.06879	-2.14751	0.58391
C	-1.12421	-2.49721	2.75719
H	0.47480	-1.18250	3.29728
C	-2.05963	-2.84313	1.78698
H	-2.80541	-2.40707	-0.16622
H	-1.09591	-3.02231	3.70533
H	-2.77629	-3.63572	1.96475
N	0.63761	0.31316	1.13725
O	-0.76811	0.81175	-1.06755
C	-1.20188	-0.40975	-1.04295
C	-1.72727	-1.05786	-2.13021
H	-3.28447	0.41748	-1.21294
H	-1.74690	-0.54425	-3.08489
H	-2.04046	-2.09154	-2.09917
I	2.83385	-1.34513	-0.96702
O	-3.76279	1.08088	-0.68527
C	-5.16055	0.75762	-0.68549
C	-5.81260	1.74890	0.26806
H	-5.63428	2.77191	-0.07156
H	-6.89029	1.58030	0.31589
H	-5.39798	1.63525	1.27284
C	-5.34883	-0.67579	-0.19443
H	-4.86748	-1.37773	-0.88215
H	-4.90227	-0.79898	0.79542
H	-6.41063	-0.92696	-0.13664
C	-5.71151	0.91714	-2.10071
H	-6.77892	0.68521	-2.12890
H	-5.56609	1.94186	-2.44968
H	-5.19478	0.23894	-2.78618
K	-1.87620	2.07629	0.93561
H	0.60854	0.68182	0.18896

**SM: 15 + KOtBu in DMSO**

47

-1554.2992212

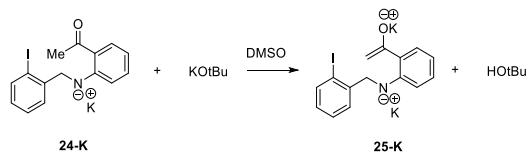
C	-2.35842	3.31462	-0.94803
C	-1.47120	2.40986	-1.51980
C	-1.49637	1.05162	-1.19611
C	-2.45525	0.63180	-0.26815
C	-3.35693	1.51797	0.30833
C	-3.30295	2.86723	-0.03208
H	-2.31189	4.36329	-1.21607
H	-0.73190	2.75059	-2.23592
H	-4.10046	1.16613	1.01211
H	-4.00248	3.55980	0.42061
C	-0.50984	0.11051	-1.84636
H	-1.04992	-0.77094	-2.19457
H	-0.07035	0.59816	-2.72492
C	1.04946	-1.51602	-0.80106
C	1.78907	-1.96398	0.33879
C	0.93381	-2.41472	-1.89466
C	2.41191	-3.22417	0.29735
C	1.53558	-3.65994	-1.87962
H	0.40080	-2.11478	-2.78552
C	2.29976	-4.07657	-0.78680
H	2.98405	-3.55164	1.15646
H	1.42064	-4.30678	-2.74297
H	2.78626	-5.04354	-0.78227
N	0.49475	-0.27324	-0.87275
O	1.03395	-0.27656	1.78746
C	1.79259	-1.21504	1.61768
C	2.72256	-1.63696	2.73401
H	3.74647	-1.74494	2.37149
H	2.68373	-0.87852	3.51343
H	2.41288	-2.59505	3.15625
I	-2.60254	-1.42457	0.28767
O	1.64282	2.14846	0.14657
C	2.84258	2.24525	-0.53080
C	3.83412	1.15458	-0.07063
H	3.41499	0.16098	-0.25988
H	4.79639	1.22165	-0.59112
H	4.01690	1.25119	1.00407
C	3.49805	3.61838	-0.27400
H	2.82802	4.41371	-0.61482
H	3.66297	3.74930	0.80047
H	4.45866	3.73394	-0.78829
C	2.65296	2.10301	-2.05485
H	3.59870	2.19757	-2.60067
H	2.21924	1.12662	-2.28847
H	1.97158	2.88014	-2.41538
K	0.13962	2.20468	2.06791
H	0.79982	0.47952	-0.25357

Prod: 24-K + HOtBu in DMSO

47

-1554.3150774

C	-2.38203	3.25098	-0.71370
C	-1.45383	2.34733	-1.22003
C	-1.58176	0.96837	-1.02258
C	-2.68969	0.53173	-0.29061
C	-3.63442	1.41789	0.21995
C	-3.47518	2.78485	0.00881
H	-2.25083	4.31305	-0.88139
H	-0.59622	2.70865	-1.77683
H	-4.48442	1.05001	0.78035
H	-4.20717	3.47541	0.40955
C	-0.50363	0.03558	-1.52001
H	-0.98710	-0.85163	-1.95050
H	0.02937	0.53229	-2.34622
C	1.28738	-1.25054	-0.65810
C	2.24825	-1.67387	0.34960
C	1.42729	-1.88938	-1.94529
C	3.24618	-2.61009	0.00780
C	2.41122	-2.80970	-2.21670
H	0.74774	-1.62311	-2.74287
C	3.34912	-3.18665	-1.24076
H	3.96138	-2.90812	0.76419
H	2.46388	-3.24428	-3.21029
H	4.12496	-3.90915	-1.45842
N	0.38319	-0.29911	-0.41573
O	1.29328	-0.55403	2.22418
C	2.22327	-1.19319	1.73421
C	3.40382	-1.50364	2.64424
H	4.35306	-1.22704	2.18238
H	3.27104	-0.94420	3.56802
H	3.44452	-2.56900	2.88289
I	-2.98888	-1.54583	0.10885
O	1.70880	1.96947	0.39344
C	2.85447	2.33716	-0.37635
C	4.07233	1.56642	0.13729
H	3.92094	0.49146	0.00166
H	4.97732	1.86071	-0.40069
H	4.21836	1.76557	1.20213
C	3.04563	3.83563	-0.17674
H	2.16683	4.37769	-0.53458
H	3.18471	4.05886	0.88392
H	3.92238	4.18938	-0.72392
C	2.61437	2.01545	-1.85159
H	3.48089	2.30253	-2.45218
H	2.44241	0.94250	-1.98589
H	1.74206	2.55900	-2.22335
K	-0.43918	1.28436	1.83829
H	1.35294	1.09960	0.06788

**SM: 24-K + KOtBu in DMSO**

46

-1553.7986697

C	-1.90090	-3.10103	1.75851
C	-1.32907	-1.86459	2.03750
C	-1.69608	-0.70591	1.34406
C	-2.67104	-0.84413	0.35351
C	-3.26125	-2.07056	0.06012
C	-2.86972	-3.20457	0.76601
H	-1.58886	-3.97909	2.31092
H	-0.56534	-1.78348	2.80406
H	-4.01450	-2.14550	-0.71379
H	-3.32471	-4.16030	0.53579
C	-0.96959	0.58773	1.62705
H	-1.70363	1.40804	1.65297
H	-0.54829	0.51823	2.64161
C	0.80656	1.86861	0.76543
C	1.91186	2.18669	-0.13909
C	0.62497	2.81476	1.85301
C	2.75392	3.28190	0.15016
C	1.46398	3.87844	2.06629
H	-0.20198	2.67633	2.53589
C	2.56488	4.12695	1.22318
H	3.58357	3.48739	-0.51516
H	1.27065	4.53978	2.90598
H	3.22911	4.96311	1.39951
N	0.05662	0.78905	0.61768
O	1.40827	0.61489	-1.85553
C	2.18202	1.43864	-1.36343
C	3.49145	1.67974	-2.10741
H	4.35457	1.58441	-1.44559
H	3.56289	0.94168	-2.90400
H	3.51666	2.67775	-2.55116
I	-3.30430	0.83763	-0.80214
O	2.08681	-2.63846	0.15913
C	3.43968	-2.41210	0.04039
C	4.25555	-3.60753	0.57669
H	3.98486	-4.51251	0.02346
H	5.33711	-3.45621	0.48588
H	4.01627	-3.77046	1.63250
C	3.86085	-1.15223	0.82956
H	3.31967	-0.27963	0.44753
H	3.59947	-1.27825	1.88547
H	4.93609	-0.94997	0.76026
C	3.82453	-2.19090	-1.43987
H	4.89368	-1.98998	-1.57547
H	3.56299	-3.08045	-2.02275
H	3.25838	-1.34145	-1.83563
K	0.17877	-1.47673	-1.00567

TS: 24-K + KOtBu in DMSO

46

-1553.7834681

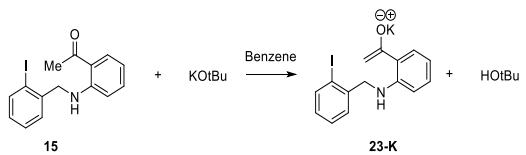
C	2.01200	3.34716	1.25476
C	1.30254	2.23252	1.69032
C	1.58965	0.94397	1.22731
C	2.63754	0.82427	0.31100
C	3.36252	1.92361	-0.13846
C	3.04129	3.19361	0.33292
H	1.75854	4.33096	1.63147
H	0.49388	2.35428	2.40305
H	4.16840	1.79566	-0.85014
H	3.60102	4.05208	-0.01872
C	0.72048	-0.22199	1.64087
H	1.37342	-1.06159	1.93806
H	0.17028	0.06902	2.55346
C	-0.94333	-1.61227	0.71857
C	-1.89185	-2.00449	-0.30719
C	-0.97837	-2.41792	1.91022
C	-2.78179	-3.04819	-0.09375
C	-1.86457	-3.47388	2.06967
H	-0.29907	-2.19097	2.72258
C	-2.78534	-3.81163	1.07841
H	-3.48860	-3.28723	-0.88377
H	-1.83895	-4.04218	2.99561
H	-3.47946	-4.63253	1.20764
N	-0.15529	-0.55159	0.54004
O	-0.91416	-1.13411	-2.30320
C	-1.95082	-1.30305	-1.63307
C	-3.21891	-0.73702	-2.03910
H	-3.09260	0.47301	-1.53161
H	-3.30888	-0.59344	-3.11689
H	-4.10293	-1.17216	-1.57937
I	3.22212	-1.09073	-0.43651
O	-2.84329	1.72199	-1.12512
C	-3.36095	2.07335	0.12794
C	-2.20998	2.47910	1.06287
H	-1.63454	3.29595	0.61272
H	-2.57282	2.81645	2.03959
H	-1.54365	1.62345	1.21442
C	-4.11196	0.89268	0.76983
H	-4.96008	0.59466	0.14606
H	-3.44401	0.03048	0.86971
H	-4.49055	1.16245	1.76059
C	-4.32754	3.25687	-0.02225
H	-4.74368	3.56997	0.94102
H	-3.80435	4.10882	-0.46651
H	-5.15394	2.97991	-0.68324
K	-0.24616	1.34049	-1.41526

Prod: 25-K + HOtBu in DMSO

46

-1553.8064365

C		-1.53869	3.50990	-0.75777
C		-0.87616	2.39790	-1.26554
C		-1.34920	1.09574	-1.06748
C		-2.52960	0.96129	-0.33448
C		-3.21482	2.05878	0.18004
C		-2.71190	3.33947	-0.03023
H		-1.13922	4.50298	-0.92690
H		0.04335	2.52492	-1.82814
H		-4.13089	1.91983	0.74043
H		-3.24103	4.19432	0.37347
C		-0.51664	-0.07341	-1.53971
H		-1.17975	-0.83002	-1.99812
H		0.13195	0.28643	-2.35915
C		1.05948	-1.59468	-0.67700
C		1.82967	-2.16874	0.40309
C		1.26077	-2.19304	-1.96159
C		2.69038	-3.22575	0.17830
C		2.14799	-3.25155	-2.15306
H		0.71457	-1.81655	-2.81852
C		2.87635	-3.78829	-1.09814
H		3.24348	-3.62702	1.02438
H		2.26441	-3.66301	-3.15234
H		3.56211	-4.61343	-1.24811
N		0.22732	-0.57857	-0.41289
O		2.36724	-0.46520	2.00329
C		1.71810	-1.57564	1.78460
C		0.94492	-2.20483	2.71665
H		2.57552	0.92929	1.14238
H		0.85600	-1.80068	3.72122
H		0.41867	-3.12025	2.47727
I		-3.37734	-0.96710	0.03410
O		2.51662	1.88062	0.86238
C		3.41816	2.10255	-0.21978
C		3.14798	3.51291	-0.72892
H		3.31310	4.24198	0.06840
H		3.80860	3.75571	-1.56460
H		2.11261	3.59927	-1.06770
C		3.16662	1.07117	-1.31976
H		3.28682	0.05861	-0.92347
H		2.14268	1.15339	-1.69180
H		3.86369	1.21523	-2.14991
C		4.85705	1.98852	0.28919
H		5.57348	2.17065	-0.51611
H		5.03315	2.71699	1.08459
H		5.03698	0.98682	0.68967
K		0.09283	0.91702	1.82580



SM: 15 + KOtBu in Benzene

47

-1554.2794231

C	4.22831	3.14552	0.53793
C	3.24955	2.47523	1.26202
C	2.86445	1.17351	0.93615
C	3.49527	0.56271	-0.15215
C	4.47592	1.21825	-0.88678
C	4.84137	2.51499	-0.53775
H	4.51068	4.15413	0.81388
H	2.76953	2.96309	2.10365
H	4.95571	0.72388	-1.72183
H	5.60776	3.02453	-1.10929
C	1.79061	0.48230	1.73633
H	2.12994	-0.52449	2.00675
H	1.61821	1.03397	2.66444
C	-0.33618	-0.63248	1.16920
C	-1.24043	-1.07236	0.16421
C	-0.38350	-1.25198	2.43139
C	-2.14253	-2.09927	0.47073
C	-1.28904	-2.26497	2.69632
H	0.28567	-0.92101	3.21500
C	-2.17956	-2.69927	1.71595
H	-2.84686	-2.41716	-0.28620
H	-1.30325	-2.71558	3.68226
H	-2.89508	-3.48391	1.92513
N	0.55901	0.40301	0.95051
O	-0.61940	0.54424	-1.44685
C	-1.26852	-0.46688	-1.19179
C	-2.11536	-1.09274	-2.26304
H	-3.15537	-0.87787	-2.00230
H	-1.87716	-0.61586	-3.21150
H	-1.96493	-2.17062	-2.33268
I	2.99766	-1.43326	-0.72066
O	-3.76678	0.96203	-0.37343
C	-5.11698	0.71673	-0.44393
C	-5.88860	1.62583	0.53757
H	-5.68154	2.67414	0.29918
H	-6.97247	1.46933	0.50043
H	-5.54568	1.43180	1.55900
C	-5.43921	-0.74937	-0.08114
H	-4.97874	-1.42689	-0.80742
H	-5.02770	-0.97926	0.90642
H	-6.51649	-0.94902	-0.06970
C	-5.64973	0.98842	-1.86688
H	-6.72496	0.79879	-1.95976
H	-5.45456	2.03116	-2.13477
H	-5.12283	0.35176	-2.58449
K	-1.87094	2.18067	0.38270
H	0.66313	0.63887	-0.02958

TS: 15 + KOtBu in Benzene

47

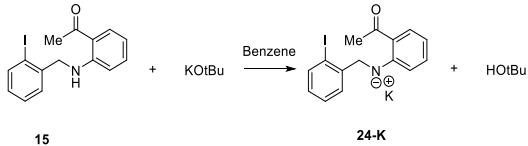
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C	4.95770	-2.15027	-1.65735	
C	4.18278	-1.07006	-2.06384	
C	3.46427	-0.29950	-1.14752	
C	3.54455	-0.65720	0.20173	
C	4.31576	-1.73290	0.62575	
C	5.02357	-2.48160	-0.30993	
H	5.50564	-2.72932	-2.39067	
H	4.12721	-0.80911	-3.11526	
H	4.36734	-1.98600	1.67708	
H	5.62430	-3.32018	0.02147	
C	2.62494	0.85654	-1.63316	
H	2.87541	1.75489	-1.05546	
H	2.87306	1.06103	-2.67986	
C	0.29198	1.53170	-1.19293	
C	-0.88498	1.26590	-0.44156	
C	0.51542	2.84721	-1.64233	
C	-1.79983	2.30310	-0.22957	
C	-0.40752	3.85197	-1.40497	
H	1.40987	3.06787	-2.21201	
C	-1.58484	3.58603	-0.70797	
H	-2.71021	2.08548	0.31532	
H	-0.21140	4.84993	-1.78098	
H	-2.31751	4.36500	-0.53948	
N	1.21256	0.55030	-1.47354	
O	-0.63612	-1.08943	-0.38970	
C	-1.14996	-0.08068	0.14526	
C	-2.07540	-0.22120	1.24806	
H	-3.18616	-0.52999	0.64680	
H	-1.85338	-1.11343	1.83365	
H	-2.21293	0.65846	1.87054	
I	2.50447	0.45558	1.69593	
O	-4.21715	-1.04503	-0.07996	
C	-5.46187	-0.56841	0.33781	
C	-6.53643	-1.04509	-0.64659	
H	-6.53871	-2.13818	-0.68915	
H	-7.53537	-0.70791	-0.35295	
H	-6.31913	-0.66042	-1.64689	
C	-5.45877	0.96834	0.37540	
H	-4.73946	1.32384	1.11932	
H	-5.16546	1.35979	-0.60274	
H	-6.44286	1.37028	0.63475	
C	-5.78341	-1.10466	1.74178	
H	-6.75054	-0.74475	2.10666	
H	-5.80206	-2.19800	1.72476	
H	-5.00775	-0.78664	2.44461	
K	-2.63305	-2.60659	-1.13767	
H	0.97130	-0.36504	-1.11474	

Prod: 23-K + HOtBu in Benzene

47

-1554.2916430

C	4.43272	2.91107	0.74058
C	3.52967	2.15784	1.48174
C	3.00967	0.95528	0.99824
C	3.42638	0.53174	-0.26776
C	4.33001	1.27185	-1.02107
C	4.83287	2.46600	-0.51327
H	4.82086	3.84001	1.14071
H	3.21469	2.50099	2.46152
H	4.64169	0.92229	-1.99692
H	5.53607	3.04174	-1.10302
C	2.01547	0.17862	1.82427
H	2.32163	-0.87443	1.87070
H	2.02434	0.56657	2.84720
C	-0.21498	-0.77059	1.38081
C	-1.15303	-1.08727	0.36405
C	-0.20767	-1.52127	2.56817
C	-2.07178	-2.10953	0.62145
C	-1.11895	-2.54713	2.77578
H	0.51515	-1.28508	3.34048
C	-2.06783	-2.84131	1.80244
H	-2.81509	-2.33124	-0.13441
H	-1.09225	-3.10633	3.70413
H	-2.79685	-3.62696	1.95975
N	0.68152	0.29203	1.23674
O	-0.75335	0.88997	-0.92386
C	-1.17968	-0.33495	-0.95445
C	-1.70138	-0.94160	-2.06304
H	-3.20049	0.55085	-1.07477
H	-1.69997	-0.39788	-3.00043
H	-1.99705	-1.98098	-2.07091
I	2.69893	-1.28974	-1.10325
O	-3.74455	1.11974	-0.49928
C	-5.12431	0.80324	-0.72591
C	-5.91500	1.67693	0.23735
H	-5.71162	2.73273	0.04274
H	-6.98654	1.50250	0.12020
H	-5.63823	1.44823	1.26974
C	-5.35673	-0.67828	-0.43736
H	-4.75811	-1.29066	-1.11803
H	-5.06424	-0.91521	0.58864
H	-6.40927	-0.93817	-0.57445
C	-5.47631	1.12940	-2.17577
H	-6.52840	0.91490	-2.37846
H	-5.28600	2.18494	-2.38168
H	-4.86463	0.52748	-2.85391
K	-1.82312	2.00414	1.07549
H	0.64826	0.66924	0.28950



SM: 15 + KOtBu in Benzene

47

-1554.2875083

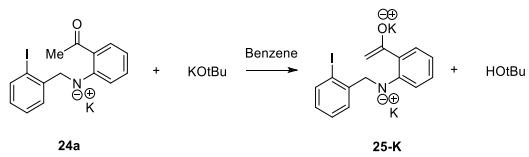
C	0.47626	-3.96565	-0.78078
C	0.09221	-2.78397	-1.39375
C	0.75918	-1.57628	-1.15254
C	1.82531	-1.60367	-0.25014
C	2.24091	-2.78496	0.36246
C	1.55982	-3.96755	0.09548
H	-0.06084	-4.88364	-0.98213
H	-0.74894	-2.77043	-2.07732
H	3.08825	-2.78063	1.03709
H	1.87873	-4.88627	0.57378
C	0.30858	-0.30494	-1.84114
H	1.20187	0.23171	-2.16676
H	-0.26854	-0.55685	-2.74035
C	-0.25495	1.86090	-0.80867
C	-0.64490	2.60350	0.34247
C	0.32236	2.58185	-1.87753
C	-0.54192	4.00204	0.32953
C	0.44287	3.95492	-1.83924
H	0.63635	2.05326	-2.76895
C	-0.00869	4.69289	-0.73987
H	-0.86765	4.55882	1.20031
H	0.87798	4.46121	-2.69312
H	0.06463	5.77187	-0.72015
N	-0.44312	0.52376	-0.92160
O	-0.83360	0.72991	1.76363
C	-1.02573	1.92171	1.60141
C	-1.63971	2.73583	2.71896
H	-2.50521	3.29382	2.35547
H	-1.94720	2.05319	3.50837
H	-0.92196	3.45298	3.12287
I	2.88913	0.18466	0.22879
O	-2.39640	-1.35736	0.14943
C	-3.54574	-0.93927	-0.48373
C	-3.88154	0.51767	-0.10255
H	-3.08511	1.19213	-0.43263
H	-4.81891	0.85623	-0.55968
H	-3.97452	0.59980	0.98499
C	-4.73441	-1.83001	-0.06627
H	-4.51949	-2.86993	-0.33082
H	-4.87147	-1.77688	1.01820
H	-5.67333	-1.53548	-0.54925
C	-3.39939	-1.01598	-2.01481
H	-4.32752	-0.72675	-2.52071
H	-2.60222	-0.35095	-2.35295
H	-3.15182	-2.03972	-2.31094
K	-0.87580	-1.91387	1.90105
H	-1.04800	-0.01190	-0.29046

Prod: 24-K + HOtBu in Benzene

47

-1554.3041079

C	-2.49721	3.21857	-0.66858
C	-1.53408	2.37104	-1.20586
C	-1.59001	0.98514	-1.02804
C	-2.66002	0.48078	-0.28252
C	-3.63779	1.31132	0.25928
C	-3.55170	2.68756	0.06636
H	-2.42281	4.28845	-0.82210
H	-0.69956	2.78257	-1.76304
H	-4.45929	0.89030	0.82558
H	-4.31133	3.33532	0.48741
C	-0.47696	0.10879	-1.55298
H	-0.93126	-0.77394	-2.02351
H	0.04790	0.65639	-2.35227
C	1.30811	-1.19811	-0.70561
C	2.22941	-1.68829	0.30772
C	1.46523	-1.78811	-2.01247
C	3.19210	-2.65924	-0.04303
C	2.41815	-2.73595	-2.29403
H	0.82458	-1.46126	-2.81922
C	3.30664	-3.19264	-1.30728
H	3.87522	-3.01369	0.71796
H	2.48516	-3.12993	-3.30346
H	4.05797	-3.93879	-1.53033
N	0.40559	-0.24485	-0.45077
O	1.37227	-0.46036	2.16105
C	2.20458	-1.24088	1.69999
C	3.26635	-1.75330	2.66478
H	4.27167	-1.51715	2.30960
H	3.10150	-1.27127	3.62606
H	3.20119	-2.83573	2.79256
I	-2.83116	-1.61094	0.10312
O	1.46904	2.15535	0.27408
C	2.72697	2.49764	-0.30495
C	3.83391	1.67954	0.36119
H	3.67608	0.61303	0.17561
H	4.81535	1.95721	-0.03237
H	3.82642	1.84995	1.44073
C	2.92597	3.98563	-0.04793
H	2.11901	4.55771	-0.51245
H	2.91947	4.18435	1.02652
H	3.87898	4.32660	-0.45905
C	2.68601	2.20570	-1.80590
H	3.63078	2.47915	-2.28237
H	2.50951	1.13896	-1.98043
H	1.88078	2.77453	-2.27891
K	-0.45994	1.19800	1.80905
H	1.22957	1.22809	-0.00611



SM: 24-K + KOtBu in Benzene

46

C	2.51904	-1.59834	1.98410
C	1.23925	-1.12616	2.25128
C	0.16149	-1.38724	1.39905
C	0.42507	-2.15468	0.26251
C	1.69665	-2.64244	-0.02243
C	2.74845	-2.35726	0.84301
H	3.33837	-1.35395	2.64889
H	1.05915	-0.51806	3.13191
H	1.87010	-3.22884	-0.91590
H	3.74356	-2.71783	0.61233
C	-1.18785	-0.77143	1.68231
H	-1.95609	-1.54973	1.54910
H	-1.21228	-0.48947	2.74692
C	-2.58953	0.92155	0.85523
C	-2.99213	2.02138	-0.02286
C	-3.62031	0.48564	1.78376
C	-4.28620	2.57049	0.09971
C	-4.85961	1.06496	1.85579
H	-3.39983	-0.32179	2.46781
C	-5.22206	2.13156	1.01102
C	-4.56493	3.38859	-0.55300
H	-5.57268	0.69004	2.58492
H	-6.20048	2.59034	1.07353
N	-1.39238	0.36482	0.80179
O	-0.94280	2.26224	-1.21237
C	-2.12007	2.57841	-1.05120
C	-2.67883	3.62775	-2.01280
H	-2.93085	4.55071	-1.48541
H	-1.90470	3.84169	-2.74719
H	-3.57709	3.27618	-2.52319
I	-1.12945	-2.59800	-1.13320
O	3.47060	1.49576	-0.26396
C	4.81078	1.69359	-0.08933
C	5.38436	0.70262	0.95046
H	5.19683	-0.32138	0.61123
H	6.46156	0.82950	1.11346
C	4.86535	0.84331	1.90412
C	5.09595	3.12809	0.41141
H	4.70562	3.84619	-0.31614
H	4.57383	3.28887	1.35963
H	6.16453	3.32432	0.56125
C	5.57829	1.48974	-1.41553
H	6.65931	1.64239	-1.31069
H	5.40141	0.47382	-1.78241
H	5.19594	2.19142	-2.16316
K	1.09748	0.97530	-0.36649

TS: 24-K + KOtBu in Benzene

46

-1553.7444203

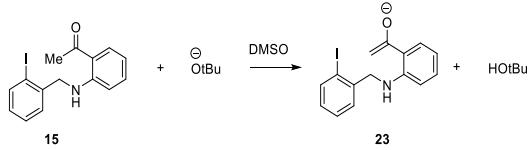
C	1.59155	3.19336	1.43313
C	1.02320	1.97240	1.77692
C	1.50806	0.75842	1.27530
C	2.59334	0.82983	0.40031
C	3.18522	2.04065	0.04714
C	2.67813	3.22844	0.56506
H	1.18253	4.11320	1.83491
H	0.16360	1.94195	2.43894
H	4.03167	2.05779	-0.62808
H	3.13412	4.17137	0.28725
C	0.75997	-0.51680	1.58866
H	1.48566	-1.33151	1.76256
H	0.23560	-0.36797	2.55059
C	-0.98777	-1.79230	0.66593
C	-2.03075	-2.04992	-0.30402
C	-0.99550	-2.66099	1.80821
C	-2.98442	-3.03140	-0.07717
C	-1.94784	-3.65576	1.98060
H	-0.23088	-2.54508	2.56679
C	-2.96421	-3.85930	1.04980
H	-3.76186	-3.16928	-0.82373
H	-1.89637	-4.28200	2.86748
H	-3.71179	-4.63054	1.18911
N	-0.14312	-0.76961	0.49513
O	-1.11473	-1.17498	-2.32139
C	-2.11769	-1.28668	-1.59386
C	-3.35534	-0.59925	-1.89737
H	-3.04733	0.60404	-1.44525
H	-3.51783	-0.44476	-2.96486
H	-4.23674	-0.94753	-1.36324
I	3.40348	-0.93778	-0.48173
O	-2.60050	1.81204	-1.08236
C	-3.20809	2.23694	0.09964
C	-2.51063	3.51685	0.58171
H	-2.58032	4.28807	-0.19120
H	-2.95417	3.90368	1.50605
H	-1.45163	3.30922	0.76664
C	-3.08430	1.15991	1.19365
H	-3.60369	0.24597	0.89053
H	-2.03063	0.89742	1.33301
H	-3.50518	1.50172	2.14585
C	-4.69598	2.53761	-0.14855
H	-5.20448	2.87604	0.76083
H	-4.79395	3.31171	-0.91534
H	-5.19507	1.63403	-0.51025
K	-0.15334	1.09072	-1.44386

Prod: 25-K + HOtBu in Benzene

46

-1553.7645147

C	-1.51650	3.49812	-0.81323
C	-0.87376	2.38029	-1.33272
C	-1.34918	1.08184	-1.11855
C	-2.50852	0.95590	-0.35115
C	-3.17548	2.06067	0.17312
C	-2.67289	3.33804	-0.05682
H	-1.11219	4.48770	-0.99233
H	0.03712	2.49620	-1.91104
H	-4.07734	1.92660	0.75762
H	-3.18727	4.19803	0.35566
C	-0.52790	-0.09517	-1.59136
H	-1.19931	-0.85389	-2.03669
H	0.11442	0.25583	-2.42184
C	1.05569	-1.59865	-0.70758
C	1.83203	-2.14493	0.37892
C	1.25950	-2.20941	-1.98206
C	2.70247	-3.19589	0.16782
C	2.15628	-3.26177	-2.16097
H	0.70420	-1.85293	-2.84186
C	2.89090	-3.77385	-1.09997
H	3.25901	-3.57633	1.02056
H	2.27473	-3.68650	-3.15458
H	3.58552	-4.59364	-1.23933
N	0.21470	-0.57974	-0.46050
O	2.35079	-0.42562	1.97667
C	1.71574	-1.54325	1.75736
C	0.93745	-2.16889	2.68708
H	2.53006	0.96734	1.20203
H	0.86844	-1.77283	3.69676
H	0.41928	-3.08880	2.44963
I	-3.32959	-0.96883	0.07564
O	2.44414	1.91864	0.90529
C	3.35036	2.13359	-0.16839
C	3.06301	3.53050	-0.70687
H	3.20236	4.27432	0.08207
H	3.72927	3.77236	-1.53903
H	2.02940	3.58944	-1.05728
C	3.13076	1.07639	-1.25131
H	3.29129	0.07515	-0.84080
H	2.09934	1.11162	-1.61011
H	3.81485	1.23188	-2.09078
C	4.78426	2.05125	0.36244
H	5.51216	2.21398	-0.43754
H	4.93956	2.80385	1.13990
H	4.95944	1.06353	0.79716
K	0.06771	0.82791	1.77454



SM: 15 + *tert*-butoxide anion in DMSO

46

-954.4014472

C	4.52224	2.80138	1.45063
C	3.54106	1.94592	1.93789
C	3.12581	0.82513	1.21543
C	3.72679	0.59444	-0.02491
C	4.71225	1.43700	-0.52690
C	5.10861	2.54501	0.21702
H	4.82530	3.66349	2.03217
H	3.07972	2.14180	2.89980
H	5.17035	1.23624	-1.48715
H	5.87569	3.20216	-0.17456
C	2.04303	-0.06100	1.77519
H	2.34030	-1.11206	1.67816
H	1.92182	0.14892	2.84282
C	-0.26778	-0.66219	1.13127
C	-1.38472	-0.53180	0.25119
C	-0.30163	-1.68664	2.10506
C	-2.47146	-1.40631	0.40396
C	-1.39202	-2.52905	2.21664
H	0.52803	-1.80122	2.78997
C	-2.49479	-2.39633	1.36943
H	-3.32701	-1.29052	-0.24944
H	-1.38506	-3.29779	2.98163
H	-3.35084	-3.05190	1.46508
N	0.80331	0.17262	1.05786
O	-0.51852	1.31102	-0.95857
C	-1.42410	0.49117	-0.81992
C	-2.61273	0.53448	-1.74166
H	-3.52046	0.81033	-1.17297
H	-2.41872	1.27845	-2.51306
H	-2.78448	-0.43751	-2.20963
I	3.16978	-1.09114	-1.21131
O	-5.12217	1.47224	0.00289
C	-6.32253	0.84854	-0.23280
C	-7.28882	1.01814	0.96111
H	-7.47031	2.08352	1.13574
H	-8.25440	0.52425	0.80132
H	-6.83088	0.59936	1.86295
C	-6.12618	-0.66805	-0.46713
H	-5.44553	-0.82196	-1.31137
H	-5.67544	-1.12112	0.42214
H	-7.06608	-1.18964	-0.68150
C	-7.01831	1.42963	-1.48619
H	-7.98089	0.94989	-1.69814
H	-7.19008	2.50141	-1.34403
H	-6.36909	1.30192	-2.35858
H	0.78390	0.86132	0.31692

TS: 15 + *tert*-butoxide anion in DMSO

46

-954.3958219

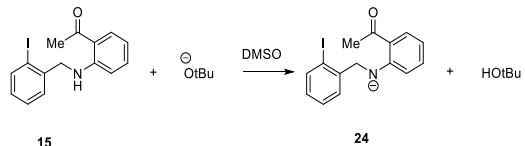
C	-5.09263	-0.62233	2.41772
C	-4.17077	0.40122	2.22939
C	-3.36273	0.45692	1.09170
C	-3.50811	-0.56204	0.14544
C	-4.42479	-1.59277	0.31573
C	-5.21902	-1.62054	1.45927
H	-5.70751	-0.63895	3.30933
H	-4.06717	1.18072	2.97643
H	-4.52509	-2.36713	-0.43418
H	-5.93451	-2.42317	1.59143
C	-2.36919	1.58056	0.93436
H	-2.48876	2.03539	-0.05676
H	-2.58742	2.35562	1.67605
C	0.05529	1.66613	0.46641
C	1.24463	0.94336	0.16912
C	-0.01008	3.02875	0.10839
C	2.31860	1.62756	-0.41203
C	1.07040	3.66832	-0.47684
H	-0.90735	3.59378	0.32848
C	2.25351	2.97609	-0.73177
C	3.23420	1.07968	-0.60045
H	0.99088	4.72149	-0.72292
H	3.10606	3.47810	-1.17194
N	-1.01511	1.07354	1.08579
O	0.59977	-1.06567	1.25336
C	1.36567	-0.52799	0.43501
C	2.43213	-1.26618	-0.22496
H	3.50604	-1.01221	0.42306
H	2.25801	-2.34016	-0.16251
H	2.63175	-0.94566	-1.24724
I	-2.33910	-0.56655	-1.64222
O	4.65203	-0.74385	1.15411
C	5.81478	-0.93029	0.41175
C	7.03927	-0.70301	1.31056
H	7.01637	-1.40412	2.14984
H	7.98004	-0.84180	0.76716
H	7.01785	0.31373	1.71376
C	5.87686	0.06240	-0.76509
H	5.03586	-0.10812	-1.44437
H	5.81149	1.08746	-0.38706
H	6.80443	-0.03798	-1.33823
C	5.87550	-2.36271	-0.15327
H	6.78736	-2.53724	-0.73389
C	5.84445	-3.08484	0.66832
H	5.01291	-2.54541	-0.80104
H	-0.89188	0.08871	1.28871

Prod: 23 + HOtBu in DMSO

46

-954.4188824

C	-4.82281	-1.38921	2.33045
C	-3.96066	-0.29889	2.37377
C	-3.23401	0.10405	1.25096
C	-3.40109	-0.63475	0.07666
C	-4.25903	-1.72647	0.01279
C	-4.97091	-2.10433	1.14834
H	-5.37437	-1.67796	3.21697
H	-3.84111	0.25973	3.29584
H	-4.37548	-2.27929	-0.91082
H	-5.63841	-2.95629	1.10008
C	-2.29149	1.27864	1.34605
H	-2.48350	1.96639	0.51242
H	-2.50285	1.82754	2.27055
C	0.09705	1.58555	0.77268
C	1.25944	0.97785	0.22306
C	-0.00726	2.98806	0.76567
C	2.28217	1.80750	-0.23581
C	1.02152	3.78186	0.27224
H	-0.89295	3.45723	1.17797
C	2.18301	3.19772	-0.22118
H	3.18391	1.34457	-0.62139
H	0.91539	4.86101	0.29085
H	2.99937	3.80938	-0.58587
N	-0.91737	0.81727	1.29914
O	0.82910	-1.22901	1.04832
C	1.37329	-0.53045	0.11405
C	2.05475	-1.05080	-0.96287
H	3.72277	-0.93581	0.40147
H	2.12584	-2.12777	-1.07311
H	2.42125	-0.42634	-1.76638
I	-2.35730	-0.09787	-1.70722
O	4.48840	-0.90300	1.00754
C	5.67783	-1.10314	0.23926
C	6.83169	-1.03491	1.23072
H	6.71696	-1.80792	1.99438
H	7.78603	-1.18619	0.72142
H	6.84968	-0.05929	1.72248
C	5.80541	0.00105	-0.81080
H	4.96557	-0.04284	-1.51038
H	5.80698	0.98134	-0.32722
H	6.73227	-0.10930	-1.37944
C	5.62684	-2.47412	-0.43554
H	6.54054	-2.66191	-1.00512
H	5.51638	-3.25873	0.31695
H	4.77528	-2.52566	-1.11969
H	-0.72582	-0.18079	1.27692

**SM: 15 + *tert*-butoxide anion in DMSO**

46

-954.405613787

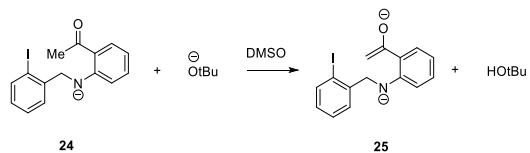
C	-2.50846	3.42287	-0.56243
C	-1.59702	2.53472	-1.12373
C	-1.66590	1.16035	-0.88208
C	-2.69999	0.70658	-0.05893
C	-3.62233	1.57743	0.51013
C	-3.51998	2.94330	0.26025
H	-2.42706	4.48319	-0.76860
H	-0.81114	2.90826	-1.77066
H	-4.41731	1.19966	1.14056
H	-4.23742	3.62260	0.70498
C	-0.62841	0.23909	-1.47724
H	-1.13152	-0.62133	-1.92871
H	-0.09305	0.76388	-2.28164
C	1.21270	-1.17775	-0.69643
C	2.17368	-1.49731	0.30100
C	1.30065	-1.83478	-1.93664
C	3.19628	-2.39504	0.00334
C	2.31138	-2.75698	-2.18978
H	0.59081	-1.60698	-2.72133
C	3.27736	-3.03641	-1.23083
H	3.93747	-2.61993	0.76227
H	2.34959	-3.24454	-3.15782
H	4.07387	-3.74170	-1.43183
N	0.25992	-0.22369	-0.43090
O	0.97279	-0.90175	2.26088
C	2.05476	-1.00189	1.71237
C	3.32736	-0.82740	2.50612
H	4.12647	-0.41121	1.89736
H	3.11960	-0.17346	3.35087
H	3.64417	-1.80135	2.89390
I	-2.96149	-1.37666	0.33025
O	2.09261	1.56443	0.95833
C	2.90794	2.23538	0.07490
C	4.34585	1.67421	0.11236
H	4.32311	0.61068	-0.14738
H	5.01554	2.19037	-0.58518
H	4.75584	1.77285	1.12247
C	2.97206	3.73991	0.41724
H	1.96383	4.16579	0.37776
H	3.35536	3.86704	1.43484
H	3.61453	4.30471	-0.26831
C	2.40097	2.10255	-1.37898
H	3.03398	2.64238	-2.09228
H	2.37184	1.04656	-1.66692
H	1.38515	2.50314	-1.44936
H	0.63904	0.51390	0.18020

Prod: 24 + HOtBu in DMSO

46

-954.4191446

C	2.66186	3.27068	0.49524
C	1.66997	2.45757	1.03144
C	1.65086	1.07552	0.82190
C	2.68476	0.54277	0.05015
C	3.68942	1.33394	-0.49710
C	3.67365	2.70793	-0.27473
H	2.64432	4.33863	0.67751
H	0.87573	2.89603	1.62576
H	4.47987	0.88726	-1.08725
H	4.45461	3.32739	-0.69940
C	0.53703	0.23859	1.40630
H	0.99488	-0.62696	1.91073
H	0.04690	0.82988	2.19810
C	-1.31764	-1.04252	0.71243
C	-2.29364	-1.54235	-0.24805
C	-1.48457	-1.53689	2.06230
C	-3.33619	-2.37825	0.18673
C	-2.51249	-2.37632	2.42601
H	-0.79040	-1.21930	2.82870
C	-3.46952	-2.81013	1.49433
H	-4.06192	-2.72535	-0.53949
H	-2.58400	-2.70070	3.46030
H	-4.27984	-3.46624	1.78489
N	-0.38639	-0.16457	0.36463
O	-1.22142	-0.81695	-2.25199
C	-2.22471	-1.23322	-1.68632
C	-3.46983	-1.46315	-2.53818
H	-4.37014	-1.06706	-2.06602
H	-3.31421	-0.97527	-3.49900
H	-3.62469	-2.53077	-2.71493
I	2.81377	-1.56335	-0.30150
O	-1.29585	2.20501	-0.78097
C	-2.49617	2.62012	-0.14014
C	-3.67774	1.79490	-0.65514
H	-3.55529	0.74622	-0.37123
H	-4.62104	2.15816	-0.23730
H	-3.73161	1.85757	-1.74556
C	-2.68224	4.08983	-0.50166
H	-1.82947	4.67431	-0.14678
H	-2.75314	4.20354	-1.58659
H	-3.59321	4.48998	-0.05023
C	-2.37388	2.45849	1.37721
H	-3.28295	2.80504	1.87637
H	-2.21345	1.40759	1.63515
H	-1.52932	3.04258	1.75214
H	-1.02193	1.30768	-0.45128



SM: 24 + *tert*-butoxide anion in DMSO

45

C	4.11576	3.27706	1.03038
C	3.11773	2.43281	1.50374
C	2.95414	1.13248	1.01580
C	3.84355	0.71702	0.02392
C	4.85141	1.54119	-0.46579
C	4.98561	2.83036	0.04171
H	4.21447	4.27831	1.43274
H	2.43761	2.78083	2.27456
H	5.52749	1.18560	-1.23316
H	5.76992	3.47518	-0.33629
C	1.82875	0.27229	1.53963
H	2.22051	-0.74467	1.70053
H	1.55038	0.65316	2.53579
C	-0.29735	-0.49134	0.88249
C	-1.47883	-0.57924	0.01908
C	-0.34090	-1.34889	2.05783
C	-2.51715	-1.47029	0.35895
C	-1.38702	-2.19275	2.33237
H	0.48457	-1.31965	2.75627
C	-2.50405	-2.27699	1.47888
H	-3.38359	-1.52542	-0.28803
H	-1.34935	-2.80358	3.23030
H	-3.32921	-2.94329	1.69633
N	0.71922	0.30394	0.60867
O	-0.83158	1.04712	-1.60411
C	-1.64781	0.22196	-1.19742
C	-2.92280	0.04388	-2.02111
H	-3.80972	0.30614	-1.43603
H	-2.85404	0.70476	-2.88393
H	-3.03982	-0.98462	-2.37046
I	3.71707	-1.25439	-0.80014
O	-5.48699	1.27436	0.44631
C	-6.61095	0.74010	-0.13240
C	-7.87402	1.03605	0.71090
H	-7.99421	2.11855	0.82259
H	-8.78901	0.63097	0.26306
H	-7.75854	0.60235	1.70955
C	-6.49599	-0.79625	-0.27592
H	-5.64242	-1.04268	-0.91546
H	-6.32324	-1.24317	0.70883
H	-7.39401	-1.25083	-0.71042
C	-6.84591	1.32308	-1.54616
H	-7.73533	0.90777	-2.03417
H	-6.96364	2.40970	-1.47976
H	-5.97485	1.11285	-2.17501

TS: 24 + *tert*-butoxide anion in DMSO

45

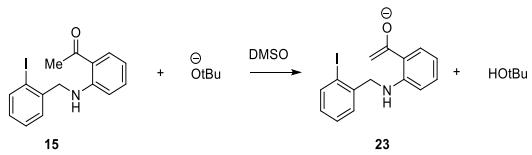
-953.8762757

C	-1.93307	3.62466	-0.85019
C	-1.24174	2.50552	-1.30053
C	-1.63397	1.20582	-0.96316
C	-2.75613	1.08205	-0.14378
C	-3.46680	2.18480	0.31890
C	-3.04992	3.46417	-0.03762
H	-1.60102	4.61680	-1.13230
H	-0.36720	2.62742	-1.93203
H	-4.33515	2.05320	0.95222
H	-3.60124	4.32550	0.32049
C	-0.81163	0.03173	-1.43692
H	-1.50141	-0.75504	-1.79353
H	-0.24706	0.35654	-2.33021
C	0.82258	-1.46132	-0.66089
C	1.76804	-1.96280	0.31714
C	0.84661	-2.14980	-1.92466
C	2.64325	-2.98971	0.00720
C	1.72100	-3.19801	-2.18668
H	0.16745	-1.84207	-2.71006
C	2.63759	-3.64001	-1.23549
H	3.35129	-3.30866	0.76857
H	1.68525	-3.67533	-3.16258
H	3.32165	-4.45344	-1.44331
N	0.04797	-0.41649	-0.36972
O	0.85315	-1.43946	2.45464
C	1.83696	-1.37912	1.70473
C	3.07707	-0.71813	2.07533
H	3.02058	0.48835	1.57914
H	3.19950	-0.61566	3.15592
H	3.96006	-1.13572	1.59125
I	-3.46627	-0.84633	0.45506
O	3.01671	1.76772	1.12220
C	3.99301	1.95673	0.14519
C	3.87738	3.37623	-0.42946
H	4.01076	4.11464	0.36667
H	4.62719	3.56344	-1.20583
H	2.88388	3.51750	-0.86557
C	3.82059	0.94706	-1.00737
H	3.87045	-0.07637	-0.62403
H	2.83761	1.08012	-1.47124
H	4.58909	1.07462	-1.77730
C	5.40031	1.78256	0.74859
H	6.18880	1.93553	0.00422
H	5.54429	2.50288	1.55958
H	5.50620	0.77614	1.16315

Prod: 25 + HotBu in DMSO

45

C	-953.8958041	-1.63245	3.64037	-0.44529
C	-0.95311	2.52965	-0.93191	
C	-1.44371	1.22899	-0.77160	
C	-2.65498	1.09692	-0.09317	
C	-3.35778	2.19148	0.40113	
C	-2.84040	3.47118	0.22356	
H	-1.22162	4.63306	-0.58810	
H	-0.00899	2.65773	-1.45243	
H	-4.29904	2.05221	0.91800	
H	-3.38499	4.32621	0.60610	
C	-0.62922	0.06243	-1.27419	
H	-1.31899	-0.67183	-1.72935	
H	-0.00020	0.42832	-2.10865	
C	0.92690	-1.52172	-0.52620	
C	1.83585	-2.09439	0.44908	
C	0.97260	-2.12721	-1.82847	
C	2.67344	-3.13868	0.10139	
C	1.82374	-3.18806	-2.13267	
H	0.32926	-1.75041	-2.61405	
C	2.68908	-3.71561	-1.18209	
H	3.34794	-3.52286	0.86295	
H	1.80521	-3.60213	-3.13768	
H	3.35345	-4.53905	-1.41592	
N	0.15218	-0.48307	-0.19396	
O	0.89071	-1.77523	2.63067	
C	1.89677	-1.56668	1.86823	
C	3.06349	-0.92011	2.23873	
H	2.93693	1.06649	1.43705	
H	3.20553	-0.58831	3.26427	
H	3.91413	-0.89599	1.56800	
I	-3.52743	-0.83272	0.22228	
O	2.94076	1.99510	1.12835	
C	3.76656	2.08958	-0.03594	
C	3.59019	3.51030	-0.55689	
H	3.89751	4.23295	0.20319	
H	4.19465	3.66944	-1.45291	
H	2.54187	3.69211	-0.80599	
C	3.31295	1.07219	-1.08362	
H	3.37434	0.05437	-0.68559	
H	2.26943	1.25028	-1.35814	
H	3.93504	1.14048	-1.98022	
C	5.22602	1.84299	0.35076	
H	5.88088	1.94027	-0.51907	
H	5.54185	2.56507	1.10787	
H	5.34671	0.83660	0.76025	



SM: 15 + *tert*-butoxide anion in Benzene

46

-954.3624541

C	-5.11516	-0.37059	2.42726
C	-4.09437	0.56235	2.28366
C	-3.28074	0.58724	1.14946
C	-3.52497	-0.36618	0.15617
C	-4.54078	-1.30611	0.28338
C	-5.33654	-1.30735	1.42561
H	-5.72945	-0.36794	3.31966
H	-3.91314	1.29178	3.06581
H	-4.71206	-2.03386	-0.49976
H	-6.12511	-2.04369	1.52555
C	-2.17071	1.60458	1.04067
H	-2.24828	2.11596	0.07363
H	-2.30299	2.36172	1.82162
C	0.22091	1.39375	0.45271
C	1.28491	0.51612	0.09517
C	0.31247	2.74559	0.07426
C	2.40499	1.02791	-0.57559
C	1.42765	3.22054	-0.59915
H	-0.48153	3.43035	0.34562
C	2.48488	2.37153	-0.91670
H	3.25946	0.37967	-0.79473
H	1.47397	4.27206	-0.86337
H	3.36720	2.74752	-1.42010
N	-0.88066	0.94940	1.14289
O	0.39611	-1.40090	1.17250
C	1.21212	-0.94182	0.37713
C	2.12616	-1.86253	-0.38047
H	3.18304	-1.54757	-0.35190
H	1.99964	-2.87252	0.00740
H	1.83771	-1.84105	-1.43731
I	-2.35872	-0.40239	-1.62841
O	4.99999	-0.66947	-0.78205
C	5.75437	-0.66325	0.35493
C	7.11358	0.03939	0.12398
H	6.93336	1.06844	-0.20266
H	7.74521	0.06028	1.02132
H	7.65386	-0.47904	-0.67438
C	6.04415	-2.10668	0.83763
H	5.09599	-2.61966	1.02907
H	6.56814	-2.64938	0.04463
H	6.65150	-2.14218	1.75096
C	5.02948	0.08002	1.50685
H	5.60723	0.08898	2.43947
H	4.83218	1.11427	1.20642
H	4.06376	-0.40014	1.70115
H	-0.86615	-0.03720	1.37203

TS: 15 + *tert*-butoxide anion in Benzene

46

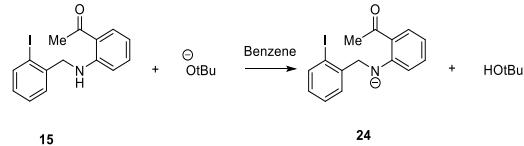
C	-5.37903	-0.33224	1.92442
C	-4.50559	0.71612	1.65847
C	-3.49329	0.60119	0.70410
C	-3.38125	-0.61447	0.02271
C	-4.24689	-1.67228	0.27444
C	-5.24813	-1.52874	1.23088
H	-6.15272	-0.21506	2.67372
H	-4.59757	1.64997	2.20262
H	-4.14143	-2.60383	-0.26698
H	-5.91867	-2.35638	1.42943
C	-2.54873	1.75442	0.46815
H	-2.49008	1.95886	-0.60822
C	-2.95857	2.65072	0.94769
C	-0.08396	1.87160	0.34948
C	1.11339	1.11033	0.37950
C	-0.08779	3.09333	-0.34626
C	2.26636	1.63476	-0.20932
C	1.06816	3.57741	-0.94280
H	-0.99768	3.68115	-0.38318
C	2.26000	2.86237	-0.86144
H	3.18866	1.06774	-0.12430
H	1.03746	4.53136	-1.45847
H	3.17063	3.25207	-1.30022
N	-1.22954	1.42991	0.97623
O	0.36491	-0.55693	1.89208
C	1.15434	-0.26695	0.98317
C	2.16464	-1.18598	0.47669
H	3.31670	-0.81217	0.86869
H	1.97844	-2.20079	0.82748
H	2.26091	-1.14071	-0.61049
I	-1.87617	-0.89605	-1.45968
O	4.59653	-0.37603	1.21117
C	5.58033	-0.88382	0.38292
C	6.96425	-0.56608	0.97451
H	7.04997	-1.02006	1.96586
H	7.78088	-0.93762	0.34419
H	7.07121	0.51664	1.08693
C	5.49495	-0.25243	-1.02383
H	4.51845	-0.46688	-1.46954
H	5.59930	0.83426	-0.94119
H	6.27264	-0.62825	-1.69840
C	5.45022	-2.41558	0.23883
H	6.24006	-2.83989	-0.39143
H	5.50410	-2.87820	1.22873
H	4.48171	-2.66957	-0.20172
H	-1.11437	0.55389	1.47418

Prod: 23 + HOtBu in Benzene

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-954.3766453

C	-5.01236	-1.27271	2.15978
C	-4.18708	-0.15400	2.19364
C	-3.35978	0.17880	1.11969
C	-3.38523	-0.65988	0.00144
C	-4.20413	-1.78143	-0.05068
C	-5.01872	-2.08883	1.03559
H	-5.64010	-1.50893	3.01071
H	-4.17131	0.48082	3.07325
H	-4.20587	-2.41417	-0.92939
H	-5.65185	-2.96745	0.99685
C	-2.45649	1.38659	1.20821
H	-2.59512	2.00175	0.30982
H	-2.76861	1.99653	2.06626
C	-0.04195	1.67383	0.73455
C	1.16132	1.00425	0.37782
C	-0.15544	3.05330	0.49017
C	2.21045	1.76650	-0.12893
C	0.90227	3.77415	-0.05346
H	-1.06978	3.56912	0.76030
C	2.10087	3.13884	-0.35361
H	3.14439	1.26383	-0.35457
H	0.78887	4.84009	-0.22082
H	2.94054	3.69718	-0.75042
N	-1.07815	0.97175	1.30499
O	0.63602	-1.05023	1.48370
C	1.27880	-0.50436	0.52187
C	2.06328	-1.17549	-0.39529
H	3.85222	-0.85777	0.73023
H	2.10544	-2.25807	-0.34658
H	2.45419	-0.68257	-1.27574
I	-2.17679	-0.23229	-1.70024
O	4.72679	-0.73644	1.15618
C	5.74652	-1.04378	0.21461
C	7.06132	-0.94089	0.97958
H	7.06511	-1.64925	1.81123
H	7.90904	-1.16030	0.32535
H	7.17983	0.06698	1.38440
C	5.72197	-0.03177	-0.93358
H	4.77521	-0.09855	-1.47572
H	5.82406	0.98158	-0.53688
H	6.53701	-0.21778	-1.63885
C	5.55356	-2.46240	-0.32530
H	6.35590	-2.72789	-1.01964
H	5.55141	-3.17737	0.50098
H	4.59760	-2.53882	-0.84925
H	-0.83879	-0.00093	1.51053

**SM: 15 + *tert*-butoxide anion in Benzene**

46

-954.3636946

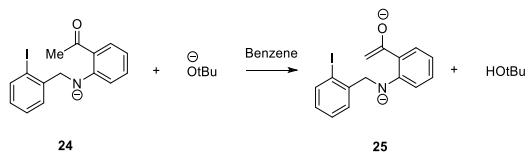
C	-1.88415	3.56066	0.70822
C	-1.02074	2.71512	0.02208
C	-1.39266	1.40052	-0.28477
C	-2.64155	0.96532	0.15352
C	-3.52140	1.79867	0.83542
C	-3.13834	3.10842	1.10571
H	-1.57250	4.57203	0.94259
H	-0.00651	3.01307	-0.24768
H	-4.48681	1.43191	1.16002
H	-3.81855	3.76220	1.63964
C	-0.40264	0.52459	-1.02077
H	-0.94260	-0.20303	-1.62004
H	0.20106	1.15764	-1.67772
C	1.02396	-1.35419	-0.23921
C	2.05756	-1.82805	0.63011
C	0.61893	-2.22123	-1.28502
C	2.64992	-3.07231	0.38435
C	1.20921	-3.45629	-1.47477
H	-0.16285	-1.91645	-1.96572
C	2.24299	-3.89991	-0.64889
H	3.44249	-3.41091	1.04090
H	0.86399	-4.08019	-2.29249
H	2.71213	-4.86264	-0.80652
N	0.47000	-0.12651	-0.05626
O	1.76944	-0.25529	2.38777
C	2.47834	-1.07964	1.84757
C	3.83600	-1.39836	2.45321
H	4.60762	-1.49374	1.68810
H	4.09004	-0.59312	3.13986
H	3.78826	-2.33579	3.01408
I	-3.26442	-1.06141	-0.15029
O	1.93448	2.27260	-0.12724
C	3.13544	2.18121	-0.77334
C	4.13118	1.28701	0.00397
H	3.74983	0.26101	0.02540
H	5.13125	1.26890	-0.44699
H	4.21081	1.64589	1.03479
C	3.77848	3.57709	-0.94099
H	3.09271	4.22263	-1.49874
H	3.93339	4.02130	0.04717
H	4.73992	3.54570	-1.46868
C	2.96212	1.55850	-2.18123
H	3.91017	1.45351	-2.72339
H	2.50880	0.56561	-2.07966
H	2.28819	2.18396	-2.77626
H	1.07615	0.58962	0.37553

Prod: 24 + HOtBu in Benzene

46

-954.3791836

C	2.50784	3.18917	0.85635
C	1.57952	2.27682	1.34616
C	1.61672	0.92287	1.00204
C	2.64207	0.51828	0.14607
C	3.58525	1.41058	-0.35216
C	3.51312	2.75468	0.00129
H	2.44231	4.23362	1.13868
H	0.79176	2.61406	2.01251
H	4.36892	1.06284	-1.01333
H	4.24391	3.45176	-0.39212
C	0.54765	-0.01138	1.51626
H	1.03283	-0.92096	1.90953
H	0.06786	0.47129	2.38767
C	-1.38905	-1.12014	0.77482
C	-2.39942	-1.44694	-0.21255
C	-1.61872	-1.66518	2.08513
C	-3.55684	-2.12643	0.15945
C	-2.76652	-2.37012	2.39955
H	-0.87954	-1.50917	2.86062
C	-3.76918	-2.59861	1.45324
H	-4.30202	-2.33953	-0.60130
H	-2.88804	-2.74774	3.41118
H	-4.66879	-3.14511	1.70663
N	-0.38551	-0.30642	0.45772
O	-1.13009	-1.37644	-2.22285
C	-2.19239	-1.18563	-1.66333
C	-3.36509	-0.68710	-2.49403
H	-4.32115	-0.70872	-1.97446
H	-3.12588	0.35260	-2.73192
H	-3.42284	-1.25314	-3.42545
I	2.84183	-1.52681	-0.42316
O	-1.58034	1.61592	-1.06092
C	-2.31062	2.53786	-0.27103
C	-3.66615	2.72646	-0.95298
H	-4.21820	1.78318	-0.94388
H	-4.26188	3.49059	-0.44540
H	-3.51773	3.02976	-1.99303
C	-1.55497	3.87012	-0.23540
H	-0.56870	3.72521	0.21255
H	-1.41427	4.24220	-1.25353
H	-2.09901	4.62373	0.34242
C	-2.52273	2.01600	1.15200
H	-3.13828	2.71698	1.72317
H	-3.01946	1.04215	1.13115
H	-1.56654	1.89289	1.66692
H	-1.05336	0.97385	-0.49999

**SM: 24 + *tert*-butoxide anion in Benzene**

45

C	-5.10006	-2.03338	-1.42362
C	-4.01896	-2.20136	-0.56712
C	-3.35481	-1.11680	0.01487
C	-3.82831	0.15283	-0.31237
C	-4.91012	0.34992	-1.16485
C	-5.54932	-0.75189	-1.72402
H	-5.58463	-2.89864	-1.86129
H	-3.65398	-3.19814	-0.34215
H	-5.24877	1.35226	-1.39558
H	-6.38836	-0.60187	-2.39361
C	-2.14837	-1.36450	0.88954
H	-2.19727	-0.67738	1.75512
H	-2.25086	-2.38158	1.31312
C	0.18691	-1.30928	0.75898
C	1.46714	-1.11501	0.08852
C	0.28719	-1.57773	2.17572
C	2.66098	-1.10278	0.81331
C	1.49664	-1.59049	2.84639
H	-0.61448	-1.78062	2.73995
C	2.70260	-1.34078	2.18694
H	3.60531	-0.93922	0.29414
H	1.49933	-1.80053	3.91396
H	3.64884	-1.34888	2.71429
N	-0.95889	-1.20229	0.09835
O	0.82868	-1.50844	-2.17878
C	1.57034	-0.95168	-1.38411
C	2.66990	-0.04233	-1.90621
H	3.67505	-0.37964	-1.61693
H	2.59261	0.00805	-2.99293
H	2.54487	0.95868	-1.48126
I	-2.90087	1.90034	0.49750
O	5.73447	-0.64638	-0.70927
C	6.22914	0.59445	-0.46331
C	7.69676	0.53071	0.03791
H	8.31006	0.03057	-0.71905
H	8.12784	1.51946	0.24589
H	7.73263	-0.06926	0.95297
C	5.39737	1.33206	0.61862
H	4.35972	1.41662	0.28112
H	5.39752	0.73831	1.53865
H	5.77874	2.33673	0.84551
C	6.21380	1.47532	-1.74207
H	6.61530	2.48427	-1.57748
H	6.80636	0.98298	-2.52024
H	5.18473	1.56108	-2.10464

TS: 24 + tert-butoxide anion in Benzene

45

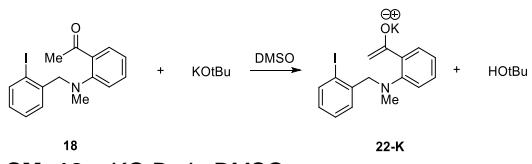
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C	1.09079	-2.93380	1.21116
C	0.58676	-1.66583	0.95068
C	1.40870	-0.62680	0.49783
C	2.75540	-0.93525	0.32096
C	3.28859	-2.19391	0.57587
C	2.44389	-3.20348	1.02709
H	0.42182	-3.71405	1.55734
H	-0.46217	-1.42328	1.07828
H	4.34316	-2.38503	0.42282
H	2.84776	-4.18962	1.22721
C	0.81436	0.74153	0.21969
H	1.42070	1.47761	0.78724
H	1.03149	0.97233	-0.84485
C	-1.20644	1.91251	0.25286
C	-2.64239	2.02058	0.45968
C	-0.58383	3.08893	-0.30440
C	-3.31761	3.17465	0.09795
C	-1.30128	4.23147	-0.62900
H	0.48673	3.08894	-0.47233
C	-2.67974	4.30263	-0.44037
H	-4.39098	3.20825	0.26369
H	-0.76822	5.08521	-1.04201
H	-3.24218	5.19282	-0.69658
N	-0.57417	0.78224	0.53420
O	-3.07131	0.49258	2.23446
C	-3.44396	0.93420	1.14322
C	-4.65119	0.45282	0.47676
H	-4.43002	-0.60060	-0.27499
H	-5.38357	0.08009	1.19758
H	-5.08779	1.16382	-0.22491
I	4.12299	0.56341	-0.39008
O	-4.46470	-1.69330	-1.06689
C	-3.30805	-2.44883	-0.95859
C	-3.01243	-2.78978	0.51718
H	-3.84829	-3.36364	0.93188
H	-2.09402	-3.38068	0.62308
H	-2.90812	-1.86988	1.10024
C	-2.10168	-1.68782	-1.54155
H	-2.31549	-1.42483	-2.58292
H	-1.92020	-0.76923	-0.97429
H	-1.18202	-2.28629	-1.51116
C	-3.48883	-3.76351	-1.73796
H	-2.59651	-4.39956	-1.68639
H	-4.34078	-4.31717	-1.33073
H	-3.69856	-3.53761	-2.78816

Prod: 25 + HOtBu in Benzene

45

C		-1.58567	3.61594	-0.40165
C		-0.91583	2.50388	-0.89588
C		-1.42496	1.20754	-0.76394
C		-2.64286	1.08209	-0.09876
C		-3.33875	2.17835	0.40148
C		-2.80523	3.45399	0.24793
H		-1.15305	4.60369	-0.51479
H		0.04385	2.62223	-1.38857
H		-4.28360	2.03902	0.91195
H		-3.34053	4.31030	0.64204
C		-0.61406	0.03829	-1.26873
H		-1.30872	-0.69705	-1.71969
H		0.00845	0.40363	-2.11348
C		0.93734	-1.52937	-0.50522
C		1.85857	-2.07374	0.47656
C		0.98318	-2.15520	-1.79905
C		2.69576	-3.11948	0.14282
C		1.83675	-3.21900	-2.08757
H		0.33389	-1.79510	-2.58838
C		2.70642	-3.72504	-1.13073
H		3.37774	-3.48068	0.90919
H		1.81627	-3.65148	-3.08602
H		3.37359	-4.55103	-1.35129
N		0.16659	-0.48740	-0.18836
O		0.96449	-1.71307	2.66912
C		1.93902	-1.50913	1.88822
C		3.11523	-0.83128	2.20421
H		2.86431	1.13136	1.45257
H		3.28137	-0.48715	3.22223
H		3.95641	-0.84781	1.52070
I		-3.51805	-0.84444	0.20738
O		2.95132	2.06527	1.15202
C		3.67424	2.09626	-0.06994
C		3.48810	3.50597	-0.62490
H		3.85496	4.24391	0.09400
H		4.03147	3.62907	-1.56596
H		2.42665	3.69557	-0.80224
C		3.12567	1.06050	-1.05225
H		3.24627	0.04794	-0.65773
H		2.05384	1.21135	-1.20130
H		3.64318	1.13136	-2.01438
C		5.16007	1.83413	0.20170
H		5.74395	1.88407	-0.72271
H		5.54729	2.57610	0.90571
H		5.28836	0.84200	0.64072



SM: 18 + KOtBu in DMSO

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-1593.5746123

C	-2.62969	3.45668	-0.10318
C	-1.85846	2.36100	-0.45808
C	-2.37847	1.06219	-0.48742
C	-3.72443	0.90971	-0.15381
C	-4.51848	1.99882	0.20272
C	-3.96800	3.27336	0.23109
H	-2.19230	4.44736	-0.09232
H	-0.81994	2.50482	-0.73050
H	-5.55967	1.85231	0.45891
H	-4.58739	4.11702	0.51073
C	-1.44392	-0.06443	-0.87231
H	-2.00871	-0.97800	-1.08607
H	-0.92962	0.23030	-1.78987
C	0.63819	-1.12612	-0.15509
C	1.71045	-1.34037	0.75756
C	0.69420	-1.80167	-1.39023
C	2.69446	-2.29075	0.45745
C	1.72110	-2.68805	-1.68292
H	-0.09042	-1.67037	-2.12147
C	2.71849	-2.96385	-0.75279
H	3.48578	-2.46953	1.17563
H	1.71776	-3.19274	-2.64228
H	3.50428	-3.67532	-0.97107
N	-0.43314	-0.29909	0.16457
O	1.64017	0.70589	1.94285
C	1.96322	-0.47060	1.94381
C	2.70419	-1.04748	3.12588
H	3.78066	-0.98740	2.93917
H	2.47911	-0.44242	4.00237
H	2.44447	-2.09067	3.30409
I	-4.69208	-0.99755	-0.15498
O	4.45689	1.15103	-0.56506
C	5.74338	0.66582	-0.50247
C	6.77052	1.80019	-0.70117
H	6.63310	2.55983	0.07478
H	7.80517	1.44268	-0.65599
H	6.61066	2.27432	-1.67459
C	5.98254	-0.39762	-1.59459
H	5.27208	-1.22012	-1.46308
H	5.81337	0.04589	-2.58091
H	6.99854	-0.80680	-1.56787
C	6.01119	0.01087	0.86842
H	7.03131	-0.37751	0.96207
H	5.84205	0.74308	1.66455
H	5.31184	-0.81866	1.01152
K	2.13468	1.76926	-0.52172
C	-0.96839	-0.33482	1.52989
H	-0.44023	-1.08075	2.12261
H	-0.87635	0.63366	2.02420
H	-2.02103	-0.62571	1.50141

TS: 18 + KOtBu in DMSO

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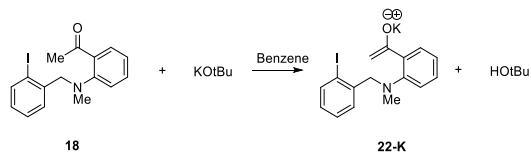
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C	0.95590	-3.15627	-0.23896	
C	0.51235	-1.87228	-0.52073	
C	1.37618	-0.76885	-0.50436	
C	2.71657	-1.01292	-0.20508	
C	3.18157	-2.29717	0.07643	
C	2.29921	-3.36932	0.06096	
H	0.25822	-3.98595	-0.25749	
H	-0.54105	-1.69865	-0.73179	
H	4.22639	-2.45975	0.30722	
H	2.66561	-4.36496	0.28026	
C	0.77643	0.58088	-0.83078	
H	1.56926	1.29444	-1.08164	
H	0.14402	0.46448	-1.71321	
C	-1.00769	2.08124	-0.15738	
C	-2.28553	2.16734	0.42585	
C	-0.67907	2.97663	-1.17961	
C	-3.18688	3.13104	-0.03052	
C	-1.58224	3.94041	-1.61591	
H	0.29640	2.92446	-1.64709	
C	-2.84223	4.02524	-1.03704	
C	-4.17416	3.17724	0.41624	
H	-1.29631	4.62046	-2.40970	
C	-3.55342	4.77078	-1.37148	
N	-0.07330	1.07257	0.26811	
O	-2.04295	1.12114	2.54245	
C	-2.73612	1.23848	1.52507	
C	-3.90782	0.43138	1.26825	
H	-3.38664	-0.59828	0.72138	
H	-4.39136	0.07605	2.17818	
H	-4.60315	0.83977	0.53796	
I	4.17699	0.54999	-0.15087	
O	-2.76116	-1.74831	0.21635	
C	-3.38657	-2.11611	-0.97883	
C	-2.77525	-3.42069	-1.50931	
H	-2.88027	-4.21045	-0.75989	
H	-3.26822	-3.74826	-2.43018	
H	-1.71098	-3.28776	-1.72236	
C	-3.19996	-1.00910	-2.03310	
H	-3.62317	-0.06843	-1.66727	
H	-2.13290	-0.84994	-2.22048	
H	-3.68215	-1.26196	-2.98262	
C	-4.89137	-2.34181	-0.74830	
H	-5.40106	-2.64750	-1.66723	
C	-5.03427	-3.12281	0.00422	
H	-5.36086	-1.42456	-0.38265	
K	-1.05640	-1.34895	2.03987	
C	0.76101	1.55173	1.38251	
H	1.40725	2.38303	1.06614	
H	0.11915	1.87373	2.19861	
H	1.40005	0.73545	1.73123	

Prod: 22-K + HOtBu in DMSO

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-1593.5939433

C	-2.27080	3.49962	-0.73167
C	-1.64921	2.28662	-0.98846
C	-2.24798	1.06095	-0.67673
C	-3.51797	1.10670	-0.09948
C	-4.16290	2.31421	0.16190
C	-3.53492	3.51292	-0.15133
H	-1.77525	4.42734	-0.99001
H	-0.67166	2.27937	-1.45542
H	-5.14941	2.32087	0.60737
H	-4.03903	4.44972	0.05308
C	-1.48532	-0.20790	-0.98905
H	-2.16640	-1.06678	-0.96372
H	-1.10417	-0.12462	-2.00988
C	0.51475	-1.48764	-0.42133
C	1.72032	-1.72374	0.29658
C	0.19965	-2.34233	-1.48968
C	2.51995	-2.80433	-0.08494
C	1.02884	-3.39884	-1.85482
H	-0.71567	-2.20687	-2.04691
C	2.19413	-3.64393	-1.14596
H	3.44157	-2.96810	0.46211
H	0.74582	-4.02960	-2.68965
H	2.84747	-4.46492	-1.41550
N	-0.34343	-0.40249	-0.08534
O	2.26612	0.45388	1.12894
C	2.24438	-0.81949	1.39751
C	2.66719	-1.39401	2.55485
H	3.62454	1.33034	0.70595
H	3.06485	-0.77484	3.35123
H	2.60517	-2.46299	2.70894
I	-4.59472	-0.66257	0.43742
O	4.28746	1.84002	0.17721
C	5.53470	1.14356	0.26039
C	6.57337	2.03257	-0.40862
H	6.64465	2.98922	0.11437
H	7.55478	1.55307	-0.39494
H	6.29424	2.22350	-1.44783
C	5.41411	-0.19504	-0.47050
H	4.62905	-0.80239	-0.00963
H	5.16649	-0.03164	-1.52344
H	6.35232	-0.75362	-0.42282
C	5.88079	0.90740	1.72987
H	6.83872	0.39032	1.82591
H	5.94324	1.86061	2.26056
H	5.10631	0.29228	2.19902
K	2.09576	1.03017	-1.38118
C	-0.77263	-0.39234	1.31956
H	-1.49177	-1.20095	1.51114
H	0.07776	-0.51070	1.98239
H	-1.25027	0.56119	1.54643



SM: 18 + KOtBu in Benzene

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C	-2.54974	3.40318	-0.15063
C	-1.80531	2.26837	-0.42755
C	-2.37556	0.99104	-0.45652
C	-3.74095	0.89827	-0.19202
C	-4.50897	2.02866	0.08518
C	-3.91221	3.28110	0.10647
H	-2.07364	4.37583	-0.13499
H	-0.74233	2.35568	-0.62126
H	-5.56733	1.92875	0.28764
H	-4.51226	4.15564	0.32710
C	-1.46582	-0.18031	-0.76168
H	-2.04916	-1.10132	-0.86902
H	-0.97655	0.01461	-1.71969
C	0.64344	-1.16317	-0.00872
C	1.76834	-1.23789	0.86201
C	0.65300	-1.97117	-1.16010
C	2.77711	-2.17114	0.59605
C	1.69638	-2.84960	-1.41812
H	-0.18215	-1.95176	-1.84569
C	2.75797	-2.97612	-0.53046
H	3.62637	-2.22877	1.26421
H	1.65998	-3.45972	-2.31347
H	3.56538	-3.67045	-0.72268
N	-0.43405	-0.31916	0.26513
O	1.54648	0.87692	1.90758
C	2.03859	-0.23843	1.93967
C	3.00658	-0.59585	3.04061
H	4.02615	-0.47985	2.66086
H	2.86345	0.10491	3.86062
H	2.87909	-1.62187	3.38636
I	-4.78036	-0.96922	-0.16727
O	4.40796	0.96307	-0.55328
C	5.73205	0.60414	-0.59992
C	6.62255	1.83675	-0.86152
H	6.47144	2.57126	-0.06473
H	7.68825	1.58606	-0.90786
H	6.33191	2.29856	-1.80991
C	5.98036	-0.42105	-1.72610
H	5.35998	-1.30597	-1.55251
C	5.68893	0.01596	-2.68603
H	7.02869	-0.73416	-1.78900
C	6.17414	-0.03293	0.73418
H	7.23559	-0.30496	0.74349
H	5.98698	0.67147	1.55104
H	5.58573	-0.93878	0.91447
K	2.16406	1.60730	-0.62799
C	-0.97459	-0.30612	1.62998
H	-0.36857	-0.93277	2.28081
H	-0.99513	0.70454	2.03950
H	-1.99027	-0.71539	1.62267

TS: 18 + KOtBu in Benzene

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-1593.5552182

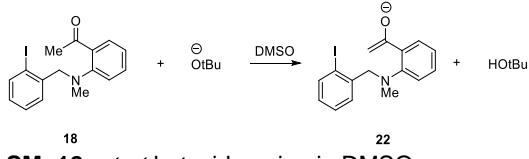
C	-1.65606	2.60591	-1.07301
C	-1.43338	1.57154	-0.17305
C	-2.44757	0.66658	0.15546
C	-3.68923	0.84563	-0.45182
C	-3.92832	1.87265	-1.35876
C	-2.90204	2.75591	-1.67227
H	-0.85281	3.29300	-1.31131
H	-0.45850	1.44433	0.28949
H	-4.90366	1.98239	-1.81554
H	-3.08213	3.55452	-2.38193
C	-2.17852	-0.44037	1.16297
H	-2.62355	-0.15062	2.11855
H	-2.69939	-1.35368	0.85695
C	0.01054	-1.18241	0.35825
C	1.42300	-1.08470	0.37302
C	-0.58743	-1.81778	-0.74902
C	2.17414	-1.72812	-0.61354
C	0.18176	-2.41207	-1.73827
H	-1.66508	-1.86310	-0.83577
C	1.57173	-2.39865	-1.66891
H	3.25403	-1.63429	-0.57485
H	-0.31772	-2.90014	-2.56772
H	2.17236	-2.86989	-2.43688
N	-0.77197	-0.68529	1.38764
O	1.74565	1.02219	1.38151
C	2.16974	-0.14311	1.27464
C	3.44096	-0.56102	1.81865
H	4.27012	-0.16632	0.89209
H	3.72439	0.01185	2.70173
H	3.55952	-1.63478	1.94588
I	-5.33155	-0.44475	0.00859
O	5.01080	0.46748	-0.04300
C	6.07983	-0.23746	-0.60547
C	7.35383	0.61404	-0.51141
H	7.57831	0.82830	0.53724
H	8.21684	0.10982	-0.95729
H	7.20175	1.56393	-1.03242
C	5.78396	-0.53568	-2.08254
H	4.87603	-1.13917	-2.16955
H	5.62053	0.40155	-2.62192
H	6.60651	-1.07456	-2.56301
C	6.31061	-1.56107	0.14120
H	7.16307	-2.10635	-0.27357
H	6.50407	-1.36518	1.19983
H	5.42735	-2.20287	0.07169
K	3.70736	2.50122	0.45961
C	-0.28186	-0.53790	2.74678
H	0.61682	-1.14101	2.88485
H	-0.03944	0.49960	2.99559
H	-1.03893	-0.91032	3.44114

Prod: 22-K + HOtBu in Benzene

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-1593.5770718

C	-2.26058	3.49055	-0.76041
C	-1.64600	2.27391	-1.01378
C	-2.24464	1.05193	-0.69046
C	-3.51175	1.10290	-0.10772
C	-4.14960	2.31470	0.15060
C	-3.52022	3.50970	-0.17138
H	-1.76426	4.41593	-1.02551
H	-0.67176	2.25959	-1.48928
H	-5.13309	2.32563	0.60246
H	-4.01938	4.44909	0.03301
C	-1.48322	-0.21905	-0.99574
H	-2.16397	-1.07830	-0.96849
H	-1.10455	-0.13933	-2.01874
C	0.52077	-1.49416	-0.43249
C	1.72021	-1.73779	0.29389
C	0.21869	-2.33122	-1.51831
C	2.53267	-2.80106	-0.10692
C	1.05896	-3.37409	-1.89834
H	-0.69893	-2.19955	-2.07285
C	2.22221	-3.62059	-1.18811
H	3.44949	-2.96738	0.44700
H	0.78429	-3.99415	-2.74394
H	2.88415	-4.43081	-1.46882
N	-0.34032	-0.40878	-0.09356
O	2.26130	0.42054	1.17270
C	2.22909	-0.85756	1.42188
C	2.63170	-1.45647	2.57043
H	3.63838	1.26062	0.69995
H	3.01475	-0.85260	3.38476
H	2.55708	-2.52725	2.70358
I	-4.58982	-0.65876	0.43955
O	4.25099	1.72653	0.07608
C	5.55229	1.15651	0.22768
C	6.45496	1.87800	-0.76336
H	6.46935	2.94881	-0.54793
H	7.47624	1.49507	-0.70421
H	6.08796	1.73334	-1.78275
C	5.48728	-0.34054	-0.08088
H	4.81433	-0.84068	0.62250
H	5.11540	-0.50220	-1.09743
H	6.47604	-0.79993	0.00008
C	6.03069	1.37779	1.66199
H	7.02950	0.95956	1.81047
H	6.05905	2.44623	1.88738
H	5.34560	0.89202	2.36307
K	2.00501	1.03643	-1.25044
C	-0.76828	-0.39148	1.31385
H	0.08301	-0.49975	1.97652
H	-1.24735	0.56287	1.53283
H	-1.48357	-1.20192	1.50857



SM: 18 + *tert*-butoxide anion in DMSO

49

-993.6862317

C	2.33914	2.46998	1.85356
C	1.75622	1.83461	0.76374
C	2.41549	0.80401	0.08575
C	3.68118	0.44171	0.54461
C	4.27956	1.06421	1.63495
C	3.60078	2.08374	2.29375
H	1.80655	3.26609	2.36027
H	0.76943	2.12979	0.41966
H	5.26366	0.75989	1.96750
H	4.06233	2.56945	3.14507
C	1.76844	0.14749	-1.12315
H	2.25046	0.53688	-2.02291
H	1.97198	-0.92830	-1.11678
C	-0.51814	-0.13389	-0.30583
C	-1.86457	0.30242	-0.18135
C	-0.09063	-1.17236	0.54900
C	-2.76077	-0.40320	0.63216
C	-0.98333	-1.81973	1.38952
H	0.94206	-1.49462	0.54710
C	-2.33026	-1.46685	1.41539
H	-3.80202	-0.07838	0.69354
H	-0.61785	-2.62100	2.02237
H	-3.02546	-1.98788	2.06241
N	0.34910	0.40655	-1.23496
O	-1.60913	2.61075	-0.58995
C	-2.32974	1.63169	-0.69042
C	-3.71104	1.72466	-1.27256
H	-4.47482	1.35272	-0.57114
H	-3.91743	2.75680	-1.55426
H	-3.76312	1.08159	-2.15723
I	4.80154	-1.09634	-0.43297
O	-5.91168	0.51514	0.76085
C	-6.56818	-0.57783	0.24576
C	-8.09575	-0.35044	0.20463
H	-8.31780	0.53306	-0.40271
H	-8.63964	-1.20478	-0.21523
H	-8.46839	-0.16862	1.21782
C	-6.30100	-1.84097	1.09636
H	-5.22722	-2.05227	1.10621
H	-6.62401	-1.66386	2.12730
H	-6.82277	-2.72714	0.71670
C	-6.09948	-0.88432	-1.19708
H	-6.60267	-1.75935	-1.62411
H	-6.29779	-0.02206	-1.84203
H	-5.01999	-1.06760	-1.20239
C	-0.10719	1.05054	-2.45534
H	-1.13234	0.74784	-2.67594
H	-0.07583	2.14188	-2.39148
H	0.51962	0.72013	-3.28549

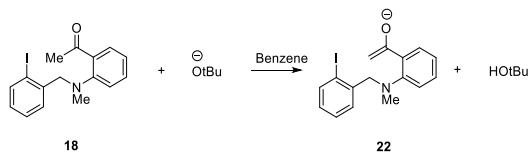
TS: 18 + *tert*-butoxide anion in DMSO

49

C	-1.91139	2.79450	-1.14290
C	-1.46672	1.79217	-0.28820
C	-2.30829	0.74415	0.09873
C	-3.60986	0.74908	-0.40142
C	-4.07205	1.74226	-1.25763
C	-3.21285	2.76987	-1.63266
H	-1.23911	3.59520	-1.42759
H	-0.45040	1.81041	0.09589
H	-5.08920	1.71773	-1.62711
H	-3.56691	3.54445	-2.30234
C	-1.80988	-0.32774	1.05669
H	-2.28362	-0.16673	2.02815
H	-2.15523	-1.31069	0.72064
C	0.46551	-0.68227	0.21932
C	1.83985	-0.33557	0.20550
C	-0.02635	-1.43609	-0.86647
C	2.68019	-0.86470	-0.77652
C	0.82309	-1.91598	-1.85427
H	-1.08048	-1.66873	-0.93743
C	2.19062	-1.66200	-1.80509
H	3.72822	-0.57883	-0.75377
H	0.40480	-2.50324	-2.66431
H	2.85573	-2.04444	-2.56997
N	-0.37889	-0.31640	1.25535
O	1.83633	1.83584	1.11535
C	2.42427	0.74999	1.07955
C	3.70560	0.49194	1.70893
H	4.61122	0.66966	0.80870
H	3.91808	1.19979	2.51063
H	3.83257	-0.54586	2.01772
I	-4.99780	-0.78062	0.15849
O	5.55377	0.92030	-0.14672
C	6.59466	0.00496	-0.28875
C	7.93952	0.68125	0.02786
H	7.93408	1.04985	1.05788
H	8.78473	-0.00510	-0.09058
H	8.08940	1.53441	-0.64034
C	6.63692	-0.51903	-1.73483
H	5.69433	-1.01903	-1.97820
H	6.76743	0.31831	-2.42661
H	7.45483	-1.23005	-1.89201
C	6.42009	-1.19675	0.66036
H	7.23712	-1.91576	0.54600
H	6.39956	-0.85815	1.70070
H	5.47634	-1.71161	0.45543
C	0.09941	-0.00191	2.59069
H	1.09046	-0.43188	2.74106
H	0.15992	1.07488	2.77524
H	-0.57322	-0.45479	3.32231

Prod: 22 + HOtBu in DMSO

49	-993.7021697	C	-1.38499	2.87009	-0.26495
		C	-1.14969	1.63088	0.31897
		C	-2.15447	0.65805	0.37884
		C	-3.39483	0.98249	-0.16699
		C	-3.64715	2.21673	-0.75833
		C	-2.63164	3.16530	-0.80786
		H	-0.59037	3.60647	-0.29927
		H	-0.17189	1.39514	0.73643
		H	-4.62233	2.43693	-1.17433
		H	-2.82051	4.12729	-1.26950
		C	-1.87105	-0.67656	1.05336
		H	-2.31562	-0.65687	2.05238
		H	-2.38870	-1.47832	0.51795
		C	0.33199	-1.13604	0.07769
		C	1.73413	-0.91384	0.08669
		C	-0.26557	-1.54343	-1.13258
		C	2.46950	-1.21946	-1.06035
		C	0.49253	-1.81141	-2.26535
		H	-1.33877	-1.67317	-1.19081
		C	1.87573	-1.67810	-2.23319
		H	3.53913	-1.04144	-1.03638
		H	-0.00843	-2.13275	-3.17197
		H	2.47674	-1.89119	-3.10927
		N	-0.46319	-0.96164	1.20478
		O	1.95511	0.96015	1.51799
		C	2.44855	-0.17778	1.21040
		C	3.58174	-0.75236	1.74175
		H	4.68669	0.48310	0.41186
		H	4.11537	-0.25252	2.54439
		H	3.89921	-1.74435	1.44489
		I	-5.02220	-0.40798	-0.09598
		O	5.22379	1.07525	-0.15207
		C	6.52089	0.49361	-0.30644
		C	7.17671	0.32686	1.06473
		H	6.58155	-0.34555	1.68852
		H	8.18163	-0.09152	0.96594
		H	7.24860	1.29473	1.56694
		C	7.31767	1.46551	-1.16651
		H	6.82934	1.60095	-2.13449
		H	7.38776	2.43725	-0.67195
		H	8.32821	1.08679	-1.33586
		C	6.39781	-0.86225	-1.00298
		H	7.38270	-1.30975	-1.15906
		H	5.80109	-1.54749	-0.39378
		H	5.91057	-0.74346	-1.97437
		C	0.04328	-1.06591	2.56145
		H	0.99553	-1.59267	2.56120
		H	0.19806	-0.08656	3.02502
		H	-0.66482	-1.64424	3.16121



SM: 18 + *tert*-butoxide anion in Benzene

49	-993.6470894	C	2.18800	2.36083	1.94923
		C	1.65847	1.75276	0.81794
		C	2.37702	0.77880	0.11645
		C	3.64347	0.44982	0.59492
		C	4.18968	1.04551	1.72601
		C	3.45187	2.00614	2.40834
		H	1.60754	3.10948	2.47492
		H	0.66921	2.02475	0.46012
		H	5.17622	0.76374	2.07090
		H	3.86901	2.47010	3.29418
		C	1.78564	0.14380	-1.13272
		H	2.28527	0.57802	-2.00273
		H	2.02765	-0.92517	-1.15214
		C	-0.51497	-0.20981	-0.37613
		C	-1.85589	0.23421	-0.24802
		C	-0.09769	-1.27669	0.44150
		C	-2.76263	-0.48030	0.54383
		C	-0.99956	-1.93744	1.26494
		H	0.93235	-1.60819	0.42927
		C	-2.33981	-1.56896	1.29853
		H	-3.80539	-0.14561	0.61359
		H	-0.64395	-2.75985	1.87656
		H	-3.04460	-2.09511	1.93109
		N	0.36780	0.36592	-1.28042
		O	-1.55933	2.54035	-0.64558
		C	-2.30639	1.58020	-0.73550
		C	-3.69871	1.70454	-1.27887
		H	-4.45898	1.37912	-0.54258
		H	-3.87400	2.73477	-1.58715
		H	-3.80655	1.03155	-2.13626
		I	4.85163	-1.00145	-0.41567
		O	-5.73468	0.47561	0.74287
		C	-6.54559	-0.52027	0.28036
		C	-8.03912	-0.14840	0.43825
		H	-8.24215	0.77216	-0.11780
		H	-8.71716	-0.93290	0.07887
		H	-8.25037	0.04203	1.49513
		C	-6.30509	-1.84157	1.05299
		H	-5.26539	-2.15575	0.91684
		H	-6.47106	-1.66548	2.12026
		H	-6.96011	-2.65802	0.72371
		C	-6.28363	-0.80426	-1.22117
		H	-6.91911	-1.60321	-1.62287
		H	-6.46198	0.10925	-1.79814
		H	-5.23477	-1.08988	-1.35782
		C	-0.07531	0.99447	-2.51151
		H	-1.09970	0.69195	-2.73434
		H	-0.04638	2.08682	-2.45912
		H	0.55673	0.65290	-3.33549

TS: 18 + *tert*-butoxide anion in Benzene

49

-993.6422758

C	-1.87745	2.72660	-1.21736
C	-1.43370	1.73532	-0.34971
C	-2.28543	0.70512	0.06303
C	-3.59238	0.72330	-0.42039
C	-4.05411	1.70475	-1.28876
C	-3.18374	2.71132	-1.69337
H	-1.19514	3.51094	-1.52270
H	-0.41213	1.75690	0.02263
H	-5.07667	1.68646	-1.64333
H	-3.53380	3.47800	-2.37453
C	-1.79127	-0.36733	1.02418
H	-2.27780	-0.21136	1.99081
H	-2.13772	-1.34681	0.67902
C	0.49759	-0.70784	0.20492
C	1.84125	-0.26812	0.16017
C	0.04402	-1.53499	-0.84012
C	2.70173	-0.75447	-0.82640
C	0.90800	-1.97787	-1.83291
H	-0.98998	-1.85203	-0.87688
C	2.25001	-1.61350	-1.82231
H	3.72589	-0.38559	-0.83347
H	0.52141	-2.62111	-2.61602
H	2.92628	-1.96130	-2.59415
N	-0.36627	-0.36046	1.24104
O	1.71462	1.91789	1.01831
C	2.36417	0.87171	1.00948
C	3.65093	0.68480	1.65908
H	4.56238	0.77581	0.77411
H	3.83989	1.45091	2.41142
H	3.77913	-0.32786	2.04553
I	-5.00187	-0.76816	0.19916
O	5.53294	0.88164	-0.21132
C	6.56579	-0.03805	-0.23345
C	7.89754	0.65002	0.12291
H	7.82399	1.08406	1.12432
H	8.74755	-0.04204	0.10033
H	8.08513	1.46166	-0.58580
C	6.69001	-0.64723	-1.64374
H	5.75810	-1.15772	-1.90623
H	6.85417	0.15340	-2.37033
H	7.51423	-1.36615	-1.71830
C	6.32962	-1.18737	0.77000
H	7.13917	-1.92430	0.73501
H	6.26444	-0.79039	1.78751
H	5.38614	-1.69523	0.54509
C	0.09656	0.04478	2.55570
H	1.10921	-0.32431	2.72090
H	0.10414	1.13116	2.68954
H	-0.55052	-0.40925	3.31128

Prod: 22 + HOtBu in Benzene

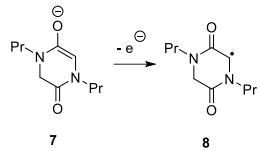
49

-993.6649597

C	-1.72628	2.64279	-1.24787
C	-1.33905	1.59043	-0.42457
C	-2.26940	0.64153	0.00996
C	-3.58993	0.80253	-0.40575
C	-3.99607	1.84603	-1.22794
C	-3.04925	2.77222	-1.65476
H	-0.98301	3.36320	-1.56935
H	-0.30039	1.51366	-0.10249
H	-5.03179	1.93757	-1.52974
H	-3.35387	3.58960	-2.29801
C	-1.84070	-0.51074	0.91102
H	-2.36085	-0.41144	1.86885
H	-2.21250	-1.44281	0.48095
C	0.46330	-1.00555	0.18623
C	1.78422	-0.50948	0.05475
C	0.03967	-1.99920	-0.71786
C	2.61516	-1.05973	-0.92416
C	0.88278	-2.51169	-1.69395
H	-0.96096	-2.40409	-0.64547
C	2.19045	-2.05376	-1.79892
H	3.61515	-0.65081	-1.02237
H	0.51017	-3.27759	-2.36559
H	2.85959	-2.44185	-2.55799
N	-0.42644	-0.58560	1.18678
O	1.66255	1.78222	0.62714
C	2.31533	0.70793	0.80440
C	3.46377	0.53806	1.55139
H	4.93060	0.88836	0.06923
H	3.86120	1.36975	2.12434
H	3.86626	-0.45384	1.71999
I	-5.10557	-0.57011	0.24615
O	5.69049	0.99802	-0.54066
C	6.76176	0.17395	-0.09677
C	7.10240	0.49249	1.36086
H	6.25095	0.26700	2.00755
H	7.96104	-0.09612	1.69627
H	7.34159	1.55379	1.46352
C	7.94228	0.50839	-1.00157
H	7.68390	0.30469	-2.04348
H	8.19438	1.56737	-0.90889
H	8.81793	-0.08800	-0.73281
C	6.38429	-1.30248	-0.24350
H	7.21636	-1.94897	0.04992
H	5.52135	-1.54098	0.38349
H	6.12230	-1.51787	-1.28281
C	0.00590	0.10212	2.39289
H	1.02395	-0.19229	2.63987
H	-0.01090	1.19266	2.29345
H	-0.65019	-0.20280	3.21334

2. Marcus Theory

2.1 Electron Donors



SM (Before SET): 7 in DMSO

31

-651.2914030

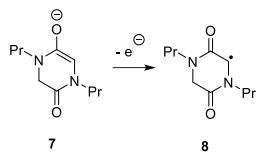
C	-0.56308	1.32020	-0.08500
C	0.94857	1.38523	-0.15358
C	0.68653	-0.85826	-1.02052
C	-0.53159	-1.07745	-0.40237
H	-0.95487	1.54542	-1.09451
H	-0.90990	2.09445	0.60019
H	1.20260	-1.64595	-1.54611
O	-1.22857	-2.13762	-0.46120
O	1.59237	2.38782	0.20409
N	1.49463	0.27481	-0.65443
N	-0.99909	0.01554	0.38634
C	-2.38427	-0.03585	0.83385
H	-2.56466	-1.03220	1.23938
H	-2.49823	0.68362	1.65295
C	-3.41885	0.26076	-0.25427
H	-3.23822	-0.41746	-1.09321
H	-3.28584	1.28187	-0.62565
C	-4.84129	0.08958	0.27265
H	-5.58392	0.30339	-0.49849
H	-5.00491	-0.93344	0.62248
H	-5.02903	0.76281	1.11391
C	2.94718	0.18121	-0.77356
H	3.16093	-0.58781	-1.51969
H	3.31963	1.13584	-1.14936
C	3.62809	-0.15765	0.55220
H	4.70842	-0.18723	0.37822
H	3.43912	0.65910	1.25412
C	3.15542	-1.48089	1.14836
H	3.67449	-1.69466	2.08508
H	2.08166	-1.45355	1.34828
H	3.34336	-2.30950	0.45945

Prod (After SET): 8 in DMSO

31

-651.1622504

C	-0.57919	1.33192	0.04489
C	0.92606	1.35880	-0.10831
C	0.76440	-0.92631	-0.81097
C	-0.58241	-1.08563	-0.31195
H	-0.99785	1.77704	-0.86947
H	-0.82906	1.98945	0.87778
H	1.25190	-1.76322	-1.28656
O	-1.16876	-2.17091	-0.39191
O	1.57458	2.36039	0.12621
N	1.50312	0.20889	-0.59576
N	-1.12745	0.01041	0.29637
C	-2.50434	-0.05456	0.77456
H	-2.65660	-1.04504	1.20502
H	-2.60914	0.68186	1.57636
C	-3.53705	0.20341	-0.32197
H	-3.39189	-0.53448	-1.11595
H	-3.36823	1.19176	-0.76067
C	-4.95687	0.11801	0.23111
H	-5.69665	0.28986	-0.55218
H	-5.14633	-0.86785	0.66361
H	-5.11557	0.86422	1.01395
C	2.95473	0.19775	-0.83939
H	3.14456	-0.58718	-1.57309
H	3.22041	1.15778	-1.27998
C	3.74916	-0.05130	0.44050
H	4.80882	-0.01602	0.17286
H	3.56746	0.77240	1.13528
C	3.42021	-1.38725	1.10105
H	4.05101	-1.54966	1.97649
H	2.37909	-1.42298	1.43192
H	3.58352	-2.21796	0.40879



SM (Before SET): 7 in Benzene

31

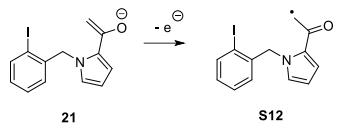
-651.2494131

C	1.09766	-1.31030	-1.01114
C	-0.25598	-1.54171	-0.85917
C	-0.39270	-0.68684	1.41033
C	1.06343	-1.12076	1.42370
H	-0.85494	-1.98727	-1.63940
H	1.56546	-0.62359	2.25541
H	1.07917	-2.20401	1.60368
N	-0.99541	-1.01576	0.26032
N	1.76928	-0.85118	0.18249
O	-0.93836	-0.08052	2.34605
O	1.79364	-1.46834	-2.05196
C	-2.35834	-0.56934	0.02229
H	-2.83142	-1.28472	-0.65784
H	-2.89450	-0.59066	0.97303
C	-2.40342	0.83585	-0.57339
H	-1.93962	1.52310	0.14088
H	-1.79068	0.84585	-1.47992
C	-3.83166	1.27220	-0.88615
H	-3.85914	2.28033	-1.30489
H	-4.29547	0.59608	-1.61023
H	-4.44853	1.26754	0.01701
C	2.40137	0.45497	0.06179
H	3.11381	0.57947	0.88715
H	2.97722	0.44055	-0.86702
C	1.42443	1.63540	0.04331
H	0.86835	1.66706	0.98711
H	0.68986	1.46070	-0.75085
C	2.14639	2.96162	-0.18039
H	1.45195	3.80468	-0.18617
H	2.88324	3.14111	0.60845
H	2.67871	2.95665	-1.13573

Prod (After SET): 8 in Benzene

31

C	0.82862	1.18260	-0.36753
C	-0.61407	1.21798	-0.28654
C	-0.84757	-1.17041	-0.37225
C	0.64396	-1.24926	-0.12831
H	-1.11187	2.17357	-0.22355
H	0.76806	-1.48490	0.93938
H	1.01085	-2.10663	-0.69508
N	-1.39088	0.09556	-0.42397
N	1.38802	-0.06302	-0.50808
O	-1.52852	-2.17137	-0.45516
O	1.49443	2.21741	-0.36392
C	-2.85157	0.22859	-0.49793
H	-3.06657	1.17187	-1.00344
H	-3.22301	-0.58789	-1.11716
C	-3.49171	0.18724	0.88566
H	-3.23177	-0.76214	1.36156
H	-3.06628	0.98764	1.49874
C	-5.00726	0.33700	0.79433
H	-5.46295	0.30522	1.78483
H	-5.28051	1.28724	0.32856
H	-5.44285	-0.46843	0.19810
C	2.84221	-0.17387	-0.52473
H	3.09811	-1.08768	-1.06986
H	3.22702	0.67608	-1.08959
C	3.46396	-0.19278	0.87104
H	3.07282	-1.04347	1.43815
C	3.16029	0.71724	1.39592
C	4.98569	-0.27907	0.79488
H	5.43083	-0.29916	1.79079
H	5.30070	-1.18380	0.26798
H	5.39616	0.58097	0.26001



SM (Before SET): 21 in DMSO

27

-643.3534550

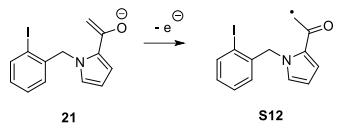
C	-0.19425	3.13096	0.61929
C	0.48823	2.02604	0.12417
C	-0.17065	0.82197	-0.13440
C	-1.54035	0.77040	0.12501
C	-2.24063	1.86417	0.62054
C	-1.56008	3.05215	0.86780
H	0.34214	4.05208	0.81267
H	1.55519	2.08559	-0.06185
H	-3.30395	1.79408	0.81225
H	-2.10092	3.90756	1.25428
C	0.57985	-0.38393	-0.66900
H	0.45527	-1.22759	0.01110
H	0.15768	-0.67123	-1.63589
N	1.99662	-0.15003	-0.85390
C	3.03294	-0.41830	0.02340
C	2.50025	0.40213	-2.00579
C	4.20111	-0.03457	-0.61027
C	3.86647	0.49223	-1.88521
H	1.83713	0.67086	-2.81415
H	5.18521	-0.13959	-0.18118
H	4.54178	0.88030	-2.63237
C	2.94054	-1.03489	1.39655
C	1.83748	-0.79698	2.18125
H	1.03721	-0.13556	1.88257
H	1.79595	-1.22761	3.17605
O	3.96816	-1.72501	1.73723
I	-2.63528	-1.02805	-0.23517

Prod (After SET): S12 in DMSO

27

-643.1944220

C	-0.10861	3.13401	0.50121
C	0.54436	2.00662	0.01592
C	-0.14303	0.81040	-0.19996
C	-1.50863	0.78545	0.08904
C	-2.17613	1.90321	0.57491
C	-1.46909	3.08363	0.78068
H	0.44724	4.04970	0.66111
H	1.60722	2.05029	-0.19666
H	-3.23601	1.85761	0.79129
H	-1.98626	3.95649	1.16013
C	0.56974	-0.42150	-0.72668
H	0.39279	-1.27847	-0.07344
H	0.16320	-0.69001	-1.70463
N	2.00124	-0.23735	-0.88326
C	3.00542	-0.45767	0.04395
C	2.56253	0.21339	-2.04034
C	4.20920	-0.14145	-0.56504
C	3.93018	0.29294	-1.87671
H	1.94042	0.43291	-2.89489
H	5.17277	-0.21842	-0.08626
H	4.63648	0.61868	-2.62346
C	2.86543	-0.94594	1.43005
C	1.65439	-0.76044	2.18891
H	0.82670	-0.14877	1.86062
H	1.62121	-1.20054	3.17677
O	3.84119	-1.47815	1.97467
I	-2.64035	-0.99922	-0.20719



SM (Before SET): 21 in Benzene

27

-643.3105041

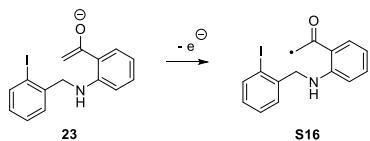
C	-0.18927	3.12100	0.58735
C	0.49230	1.99629	0.14022
C	-0.17445	0.79333	-0.10569
C	-1.54954	0.76710	0.12079
C	-2.25060	1.88075	0.56826
C	-1.56227	3.06648	0.80074
H	0.35526	4.03859	0.77510
H	1.56565	2.03159	-0.01283
H	-3.31885	1.82497	0.73552
H	-2.10197	3.93845	1.15088
C	0.58125	-0.43302	-0.58425
H	0.50250	-1.22551	0.16299
H	0.12667	-0.79352	-1.51161
N	1.98102	-0.18229	-0.83945
C	3.05754	-0.40393	0.00198
C	2.42373	0.34838	-2.02815
C	4.18879	-0.01507	-0.68964
C	3.79149	0.46851	-1.96399
H	1.72174	0.57987	-2.81500
H	5.18798	-0.09880	-0.29290
H	4.42795	0.84543	-2.75009
C	3.03648	-0.99100	1.39692
C	1.96210	-0.72292	2.21838
H	1.16782	-0.04471	1.94020
H	1.96845	-1.11297	3.22993
O	4.07214	-1.66778	1.69508
I	-2.65835	-1.03058	-0.20895

Prod (After SET): S12 in Benzene

27

-643.1887007

C	-0.09337	3.12752	0.49972
C	0.55397	1.99733	0.01438
C	-0.14001	0.80482	-0.20077
C	-1.50532	0.78642	0.08861
C	-2.16682	1.90760	0.57447
C	-1.45380	3.08400	0.77967
H	0.46716	4.04032	0.65978
H	1.61718	2.03354	-0.19857
H	-3.22682	1.86604	0.79088
H	-1.96607	3.95962	1.15949
C	0.56888	-0.43025	-0.72579
H	0.39088	-1.28381	-0.06806
H	0.15659	-0.70224	-1.70070
N	1.99832	-0.24989	-0.88728
C	3.00322	-0.45798	0.04199
C	2.55850	0.20163	-2.04631
C	4.20409	-0.13679	-0.56590
C	3.92404	0.29032	-1.88051
H	1.93564	0.41484	-2.90183
H	5.16599	-0.21339	-0.08417
H	4.63009	0.61443	-2.62800
C	2.86689	-0.94690	1.43095
C	1.65192	-0.77387	2.18989
H	0.82103	-0.16275	1.86775
H	1.62766	-1.21747	3.17643
O	3.84490	-1.46475	1.97641
I	-2.64528	-0.99255	-0.20520

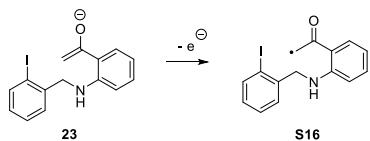


SM (Before SET): 23 in DMSO

31	-720.7677744	C	-1.73558	3.23433	-0.82407
		C	-0.74747	2.25875	-0.73798
		C	-1.04778	0.94259	-0.37419
		C	-2.38964	0.64910	-0.11347
		C	-3.39027	1.60939	-0.19452
		C	-3.05868	2.91335	-0.55025
		H	-1.46657	4.24485	-1.10742
		H	0.27787	2.52227	-0.96792
		H	-4.41934	1.34660	0.01546
		H	-3.83591	3.66528	-0.61419
		I	-2.98852	-1.33445	0.41192
		C	0.02392	-0.12112	-0.28236
		H	-0.08088	-0.64926	0.67715
		H	-0.18166	-0.86304	-1.06129
		N	1.35137	0.42235	-0.44889
		C	2.46684	-0.40524	-0.43250
		C	2.40792	-1.71100	-0.94701
		C	3.69749	0.07171	0.09416
		C	3.54359	-2.51029	-1.00989
		H	1.46993	-2.10088	-1.32247
		C	4.82172	-0.74858	-0.00825
		C	4.76634	-2.02824	-0.55555
		H	3.46706	-3.50859	-1.42643
		H	5.76736	-0.36774	0.36155
		H	5.66056	-2.63672	-0.61833
		C	3.78254	1.42270	0.78244
		C	4.60663	1.53105	1.87219
		H	4.69386	2.48324	2.38419
		H	5.16596	0.68856	2.25480
		O	3.04645	2.37249	0.30271
		H	1.55686	1.31427	0.00096

Prod (After SET): S16 in DMSO

31	-720.6100231	C	-1.54319	3.33997	-0.42698
		C	-0.61671	2.30467	-0.35827
		C	-1.01433	0.97862	-0.16525
		C	-2.38776	0.73624	-0.06456
		C	-3.32712	1.75720	-0.13411
		C	-2.90004	3.06967	-0.31095
		H	-1.19868	4.35617	-0.57513
		H	0.43509	2.53670	-0.47352
		H	-4.38358	1.53506	-0.05376
		H	-3.63020	3.86810	-0.36324
		I	-3.13409	-1.25303	0.16645
		C	-0.01705	-0.15693	-0.09442
		C	-0.26159	-0.79600	0.76483
		H	-0.14527	-0.77561	-0.99000
		N	1.34620	0.31306	-0.02654
		C	2.41531	-0.54215	-0.08086
		C	2.23525	-1.91507	-0.34713
		C	3.74595	-0.05835	0.08961
		C	3.31720	-2.77410	-0.43069
		H	1.23755	-2.31424	-0.46981
		C	4.81336	-0.96320	0.00908
		C	4.61966	-2.30944	-0.24706
		H	3.13888	-3.82503	-0.62868
		H	5.82238	-0.60628	0.17352
		H	5.46266	-2.98617	-0.29492
		C	4.01330	1.37602	0.36520
		C	5.32500	1.92227	0.12086
		H	5.48583	2.95793	0.38775
		H	6.12050	1.37516	-0.36111
		O	3.12490	2.14193	0.77685
		H	1.52757	1.16565	0.48647

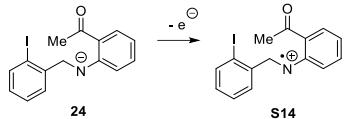


SM (Before SET): 23 in Benzene

	31	-720.7166835	C	1.95348	3.49162	0.32429
C	0.84685	2.68145	C	0.84685	2.68145	0.09345
C	0.96490	1.29622	C	0.96490	1.29622	-0.05250
C	2.25147	0.76030	C	2.25147	0.76030	0.06157
C	3.36928	1.55177	C	3.36928	1.55177	0.29358
C	3.22016	2.92943	C	3.22016	2.92943	0.42086
H	1.82198	4.56218	H	1.82198	4.56218	0.43195
H	-0.14350	3.11596	H	-0.14350	3.11596	0.03528
H	4.34895	1.09873	H	4.34895	1.09873	0.37888
H	4.09062	3.54936	H	4.09062	3.54936	0.60037
I	2.55873	-1.34935	I	2.55873	-1.34935	-0.08140
C	-0.23534	0.40943	C	-0.23534	0.40943	-0.30932
H	-0.01426	-0.28845	H	-0.01426	-0.28845	-1.12271
H	-0.39570	-0.21943	H	-0.39570	-0.21943	0.57205
N	-1.43803	1.17381	N	-1.43803	1.17381	-0.55074
C	-2.74099	0.72080	C	-2.74099	0.72080	-0.27870
C	-3.75412	1.68935	C	-3.75412	1.68935	-0.37674
C	-3.08357	-0.58863	C	-3.08357	-0.58863	0.11585
C	-5.07693	1.39464	C	-5.07693	1.39464	-0.08291
H	-3.47482	2.69722	H	-3.47482	2.69722	-0.66998
C	-4.41787	-0.84662	C	-4.41787	-0.84662	0.44621
C	-5.41660	0.11700	C	-5.41660	0.11700	0.35311
H	-5.83315	2.16641	H	-5.83315	2.16641	-0.17796
H	-4.66773	-1.85817	H	-4.66773	-1.85817	0.74845
H	-6.44308	-0.12992	H	-6.44308	-0.12992	0.59916
C	-2.11843	-1.76731	C	-2.11843	-1.76731	0.04919
C	-1.89246	-2.45649	C	-1.89246	-2.45649	1.21635
H	-1.24235	-3.32494	H	-1.24235	-3.32494	1.21665
H	-2.36416	-2.15346	H	-2.36416	-2.15346	2.14264
O	-1.63191	-1.99588	O	-1.63191	-1.99588	-1.10655
H	-1.39316	1.75253	H	-1.39316	1.75253	-1.37867

Prod (After SET): S16 in Benzene

	31	-720.5944183	C	1.53569	3.47701	0.44173
C	0.55526	2.54071	C	0.55526	2.54071	0.13636
C	0.86297	1.19184	C	0.86297	1.19184	-0.06249
C	2.20012	0.81645	C	2.20012	0.81645	0.09089
C	3.19431	1.73921	C	3.19431	1.73921	0.39416
C	2.86055	3.07886	C	2.86055	3.07886	0.56221
H	1.26120	4.51461	H	1.26120	4.51461	0.58813
H	-0.47822	2.86060	H	-0.47822	2.86060	0.06733
H	4.22217	1.41639	H	4.22217	1.41639	0.49929
H	3.63628	3.79911	H	3.63628	3.79911	0.79223
I	2.79632	-1.22816	I	2.79632	-1.22816	-0.07752
C	-0.21737	0.17561	C	-0.21737	0.17561	-0.38039
H	0.17795	-0.59634	H	0.17795	-0.59634	-1.04432
H	-0.48123	-0.33210	H	-0.48123	-0.33210	0.55363
N	-1.40781	0.77387	N	-1.40781	0.77387	-0.93953
C	-2.69314	0.57644	C	-2.69314	0.57644	-0.49081
C	-3.61927	1.62904	C	-3.61927	1.62904	-0.63213
C	-3.13364	-0.62384	C	-3.13364	-0.62384	0.11133
C	-4.91058	1.52049	C	-4.91058	1.52049	-0.15416
H	-3.29171	2.54819	H	-3.29171	2.54819	-1.10742
C	-4.43715	-0.69001	C	-4.43715	-0.69001	0.62419
C	-5.32919	0.36035	C	-5.32919	0.36035	0.50130
H	-5.59401	2.35300	H	-5.59401	2.35300	-0.27541
H	-4.76976	-1.61602	H	-4.76976	-1.61602	1.08136
H	-6.33634	0.27450	H	-6.33634	0.27450	0.88790
C	-2.34417	-1.89381	C	-2.34417	-1.89381	0.05853
C	-2.40854	-2.79162	C	-2.40854	-2.79162	1.18598
H	-1.89026	-3.73820	H	-1.89026	-3.73820	1.11064
H	-2.91311	-2.52846	H	-2.91311	-2.52846	2.10512
O	-1.66537	-2.19084	O	-1.66537	-2.19084	-0.92545
H	-1.26532	1.60653	H	-1.26532	1.60653	-1.48976

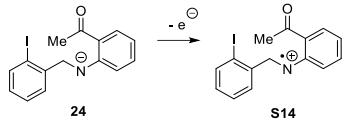


SM (Before SET): 24 in DMSO

31	-720.7637628	C	-2.20085	3.46156	-0.07705
		C	-1.04200	2.72823	0.15431
		C	-1.04319	1.33020	0.16128
		C	-2.26927	0.70695	-0.08198
		C	-3.44070	1.41662	-0.31935
		C	-3.40477	2.80811	-0.31529
		H	-2.16245	4.54474	-0.07323
		H	-0.09563	3.22109	0.33673
		H	-4.37106	0.89531	-0.50637
		H	-4.31436	3.36731	-0.49935
		I	-2.41008	-1.43248	-0.10797
		C	0.22554	0.53757	0.41749
		H	0.03072	-0.15127	1.25273
		H	0.38086	-0.13623	-0.44661
		N	1.36147	1.37618	0.64572
		C	2.56248	0.92364	0.35296
		C	3.64247	1.89392	0.33478
		C	2.94688	-0.42694	-0.04956
		C	4.83261	1.64901	-0.28618
		H	3.43313	2.86716	0.76734
		C	4.16815	-0.60837	-0.75104
		C	5.09689	0.39343	-0.89877
		H	5.58578	2.43047	-0.32256
		H	4.40734	-1.59716	-1.12881
		H	6.03183	0.21465	-1.41465
		C	2.27380	-1.61825	0.44272
		C	2.47154	-2.93961	-0.28996
		H	1.63342	-3.59039	-0.04261
		H	2.53681	-2.81815	-1.37121
O	1.60020	O	1.60020	-1.63374	1.47875
H	3.38859	H	3.38859	-3.42573	0.05498

Prod (After SET): S14 in DMSO

31	-720.6061935	C	-2.12941	3.49306	-0.16946
		C	-0.97564	2.74940	0.05397
		C	-1.01066	1.35511	0.11108
		C	-2.24997	0.73664	-0.06832
		C	-3.41335	1.46196	-0.29368
		C	-3.34983	2.85151	-0.34378
		H	-2.07248	4.57432	-0.20851
		H	-0.02134	3.24133	0.19129
		H	-4.35959	0.95403	-0.42997
		H	-4.25450	3.42069	-0.52035
		I	-2.41311	-1.39580	-0.00652
		C	0.24103	0.53614	0.34971
		H	0.08737	-0.07883	1.24738
		H	0.35016	-0.17320	-0.48333
		N	1.40637	1.35223	0.53191
		C	2.62791	0.86578	0.27866
		C	3.66250	1.85038	0.24158
		C	3.00168	-0.49235	-0.03143
		C	4.94752	1.54813	-0.15437
		H	3.37825	2.86423	0.49672
		C	4.29514	-0.76123	-0.45133
		C	5.26813	0.23989	-0.52133
		H	5.70128	2.32501	-0.19115
		H	4.57921	-1.78048	-0.68675
		H	6.27192	-0.01047	-0.84102
		C	2.12566	-1.67966	0.25960
		C	1.89694	-2.67467	-0.84549
		H	1.27444	-3.49045	-0.48359
		H	1.40960	-2.17338	-1.68642
		O	1.65432	-1.82173	1.36781
		H	2.84555	-3.06760	-1.21715

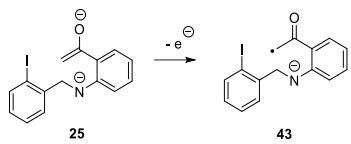


SM (Before SET): 24 in Benzene

31	-720.7285731	C	-2.18980	3.45870	-0.05112
		C	-1.03485	2.71818	0.17078
		C	-1.04312	1.31980	0.16445
		C	-2.27245	0.70673	-0.08112
		C	-3.44121	1.42377	-0.30962
		C	-3.39835	2.81440	-0.29330
		H	-2.14542	4.54188	-0.03705
		H	-0.08056	3.19532	0.35661
		H	-4.37315	0.90612	-0.49875
		H	-4.30555	3.38028	-0.47054
		I	-2.42166	-1.43147	-0.11951
		C	0.22662	0.52742	0.41330
		H	0.04317	-0.15339	1.25819
		H	0.37258	-0.15199	-0.44832
		N	1.35739	1.37496	0.62057
		C	2.55791	0.92505	0.33874
		C	3.62996	1.90546	0.30819
		C	2.95605	-0.42924	-0.04229
		C	4.82307	1.66330	-0.30466
		H	3.40487	2.88034	0.72814
		C	4.18203	-0.60738	-0.73388
		C	5.10250	0.39995	-0.89545
		H	5.56891	2.45178	-0.35078
		H	4.43348	-1.59961	-1.09484
		H	6.04137	0.22084	-1.40455
		C	2.28816	-1.61958	0.46027
		C	2.51571	-2.95171	-0.25343
		H	1.68206	-3.60654	-0.00168
		H	2.58820	-2.84432	-1.33619
O	1.59583	O	1.59583	-1.63596	1.47951
H	3.43603	H	3.43603	-3.41900	0.10860

Prod (After SET): S14 in Benzene

31	-720.6004909	C	-2.16239	3.48716	-0.12517
		C	-1.00117	2.75456	0.09261
		C	-1.02045	1.35961	0.12702
		C	-2.25072	0.72902	-0.06733
		C	-3.42124	1.44377	-0.28761
		C	-3.37380	2.83404	-0.31626
		H	-2.11864	4.56948	-0.14594
		H	-0.05248	3.25302	0.24388
		H	-4.35994	0.92545	-0.43572
		H	-4.28422	3.39538	-0.48851
		I	-2.38905	-1.40529	-0.03086
		C	0.23917	0.55315	0.36408
		H	0.10787	-0.03901	1.28102
		H	0.33676	-0.17782	-0.45130
		N	1.40362	1.37842	0.49932
		C	2.62337	0.88238	0.25263
		C	3.65652	1.86478	0.17514
		C	2.99473	-0.48425	-0.01455
		C	4.94002	1.54965	-0.21513
		H	3.37086	2.88532	0.39965
		C	4.28738	-0.76714	-0.42861
		C	5.26038	0.22943	-0.53607
		H	5.69339	2.32505	-0.28180
		H	4.56845	-1.79478	-0.63001
		H	6.26362	-0.03178	-0.84912
		C	2.11738	-1.66435	0.30940
		C	1.86939	-2.67499	-0.78078
		H	1.25510	-3.48532	-0.39342
		H	1.36128	-2.18547	-1.61648
		O	1.66130	-1.78971	1.42247
		H	2.81039	-3.07126	-1.16804

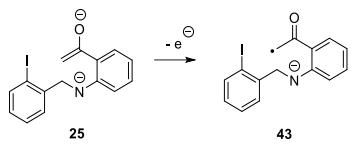


SM (Before SET): 25 in DMSO

30	-720.2417849	C	-2.13089	3.48667	-0.12209
		C	-0.97347	2.73231	0.04084
		C	-0.99777	1.33398	0.07945
		C	-2.25369	0.73645	-0.05454
		C	-3.42555	1.46515	-0.22085
		C	-3.36283	2.85581	-0.25400
		H	-2.07005	4.56888	-0.14653
		H	-0.00328	3.20129	0.14433
		H	-4.37746	0.95970	-0.32513
		H	-4.27271	3.42997	-0.38273
		I	-2.44726	-1.40102	-0.02193
		C	0.27881	0.53079	0.25413
		H	0.11289	-0.16544	1.09151
		H	0.36219	-0.13072	-0.62542
		N	1.43073	1.36730	0.42583
		C	2.64890	0.85584	0.21220
		C	3.74308	1.79505	0.21477
		C	3.03607	-0.51994	-0.05388
		C	5.03922	1.46447	-0.12249
		H	3.49560	2.82383	0.46250
		C	4.35689	-0.80503	-0.41034
		C	5.37358	0.14917	-0.47220
		H	5.80204	2.23874	-0.11717
		H	4.59688	-1.84559	-0.61364
		H	6.38640	-0.12705	-0.74045
O	1.71046	C	2.14051	-1.72034	0.19779
O	1.91602	C	1.91602	-2.60199	-0.83717
O	1.34690	H	1.34690	-3.51182	-0.66687
O	2.29324	H	2.29324	-2.40793	-1.83337
O	1.71046	O	1.71046	-1.86263	1.40308

Prod (After SET): 43 in DMSO

30	-720.1128365	C	-2.15076	3.48302	-0.05636
		C	-0.98080	2.73576	0.02377
		C	-1.00108	1.33810	0.03484
		C	-2.25489	0.72718	-0.04190
		C	-3.43696	1.45410	-0.12376
		C	-3.38318	2.84458	-0.12967
		H	-2.09768	4.56537	-0.06114
		H	-0.01740	3.22522	0.08266
		H	-4.39053	0.94485	-0.18241
		H	-4.30176	3.41570	-0.19153
		I	-2.42678	-1.40719	-0.03936
		C	0.27620	0.52989	0.12722
		H	0.22201	-0.15568	0.98640
		H	0.34337	-0.14560	-0.74046
		N	1.43766	1.35966	0.23231
		C	2.67008	0.83590	0.12843
		C	3.71419	1.81694	0.09168
		C	3.05169	-0.54910	-0.00725
		C	5.03058	1.48485	-0.12970
		H	3.41283	2.85084	0.21586
		C	4.39091	-0.84291	-0.25004
		C	5.37603	0.14142	-0.32070
		H	5.79022	2.25679	-0.16538
		H	4.67088	-1.88520	-0.35732
		H	6.40717	-0.13723	-0.50405
		C	2.11159	-1.71290	0.23056
		C	1.91664	-2.57833	-0.81433
		H	1.25185	-3.42858	-0.70184
		H	2.41462	-2.42862	-1.76366
		O	1.60858	-1.78321	1.40823

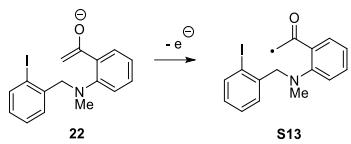


SM (Before SET): 25 in Benzene

30	-720.1214667	C	-2.13006	3.48326	-0.08063
		C	-0.97212	2.72390	0.04319
		C	-1.00023	1.32366	0.06367
		C	-2.26109	0.73416	-0.04657
		C	-3.43479	1.46873	-0.17377
		C	-3.36913	2.85950	-0.19023
		H	-2.06542	4.56626	-0.09175
		H	0.01026	3.17310	0.12987
		H	-4.38871	0.96334	-0.26029
		H	-4.28020	3.43938	-0.28789
		I	-2.44519	-1.40246	-0.03073
		C	0.28209	0.52787	0.20261
		H	0.15756	-0.15014	1.06378
		H	0.32968	-0.15607	-0.66379
		N	1.42583	1.38279	0.30647
		C	2.64735	0.86391	0.15422
		C	3.73661	1.80906	0.13105
		C	3.04676	-0.52384	-0.02686
		C	5.04706	1.46495	-0.13021
		H	3.46986	2.84834	0.30339
		C	4.37986	-0.82164	-0.30280
		C	5.40102	0.13229	-0.37588
		H	5.80649	2.24427	-0.14565
		H	4.62515	-1.87234	-0.43678
		H	6.42636	-0.15667	-0.57852
		C	2.12954	-1.71806	0.21024
		C	1.92439	-2.59215	-0.84132
		H	1.32158	-3.48404	-0.69331
		H	2.32572	-2.38895	-1.82669
O	1.66406	O	1.84866	1.39381	

Prod (After SET): 43 in Benzene

30	-720.0741434	C	-2.14754	3.48074	-0.06301
		C	-0.97917	2.73399	0.03141
		C	-0.99835	1.33603	0.04211
		C	-2.25085	0.72442	-0.04808
		C	-3.43154	1.45203	-0.14507
		C	-3.37923	2.84217	-0.15177
		H	-2.09459	4.56345	-0.06660
		H	-0.01300	3.21684	0.10326
		H	-4.38288	0.93982	-0.21424
		H	-4.29741	3.41316	-0.22533
		I	-2.41074	-1.40783	-0.03724
		C	0.27860	0.53260	0.15251
		C	0.22917	-0.13937	1.02595
		H	0.34475	-0.17006	-0.69600
		N	1.43500	1.36645	0.23497
		C	2.66359	0.83819	0.13695
		C	3.71468	1.81308	0.09678
		C	3.03761	-0.54889	-0.00061
		C	5.02646	1.47353	-0.13159
		H	3.41696	2.84739	0.22672
		C	4.37481	-0.84916	-0.25811
		C	5.36404	0.12707	-0.33086
		H	5.79124	2.24119	-0.16718
		H	4.64253	-1.89444	-0.36874
		H	6.39327	-0.15638	-0.52000
		C	2.08785	-1.70411	0.23953
		C	1.91254	-2.57634	-0.81073
		H	1.22067	-3.40579	-0.71399
		H	2.45058	-2.44700	-1.74098
O	1.54777	O	1.75137	1.39115	



SM (Before SET): 22 in DMSO

34

-760.0540185

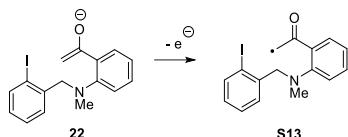
C	1.10317	2.95839	-1.21223
C	0.34944	1.81571	-0.97215
C	0.93793	0.63535	-0.51100
C	2.31536	0.65403	-0.29513
C	3.08908	1.78556	-0.52685
C	2.47607	2.94464	-0.99176
H	0.61775	3.85860	-1.56958
H	-0.72282	1.82904	-1.13443
H	4.15660	1.76629	-0.34843
H	3.07381	3.82903	-1.17678
I	3.32002	-1.08871	0.43335
C	0.09410	-0.61069	-0.25803
H	0.50511	-1.42861	-0.86055
H	0.20993	-0.91637	0.78614
N	-1.30606	-0.48919	-0.57416
C	-2.20050	0.03460	0.35991
C	-1.71345	0.76590	1.46304
C	-3.59808	-0.15726	0.24979
C	-2.57206	1.31749	2.40536
H	-0.64908	0.93206	1.57414
C	-4.43539	0.44762	1.18760
C	-3.94905	1.17864	2.26694
H	-2.15581	1.87252	3.23881
H	-5.50547	0.29998	1.07479
H	-4.62828	1.61458	2.98990
C	-4.27713	-1.02947	-0.79815
C	-4.09119	-2.38033	-0.67816
H	-4.55271	-3.06408	-1.38395
H	-3.44126	-2.78461	0.08817
O	-4.99815	-0.41656	-1.66733
C	-1.62969	-0.60499	-1.98951
H	-1.73882	-1.64958	-2.29449
H	-2.56231	-0.08776	-2.21003
H	-0.83169	-0.14374	-2.58152

Prod (After SET): S13 in DMSO

34

-759.8998739

C	1.14248	2.91624	-1.33950
C	0.37108	1.79676	-1.05007
C	0.94193	0.62936	-0.53697
C	2.31969	0.63613	-0.31735
C	3.10918	1.74492	-0.59940
C	2.51446	2.89074	-1.11775
H	0.67062	3.80654	-1.73701
H	-0.70004	1.82583	-1.21700
H	4.17574	1.71829	-0.41714
H	3.12592	3.75638	-1.34224
I	3.29432	-1.07795	0.50739
C	0.08912	-0.59604	-0.23048
H	0.49649	-1.44893	-0.78369
H	0.18184	-0.85065	0.82884
N	-1.31177	-0.48171	-0.57214
C	-2.20587	0.08958	0.32519
C	-1.74493	0.89855	1.38264
C	-3.60192	-0.10969	0.21100
C	-2.63144	1.53140	2.23983
H	-0.68358	1.06756	1.51155
C	-4.47650	0.58344	1.05404
C	-4.00901	1.40304	2.06846
H	-2.23850	2.15218	3.03689
H	-5.54048	0.42057	0.92381
H	-4.69959	1.91338	2.72760
C	-4.23343	-1.14224	-0.67004
C	-3.62101	-2.44292	-0.74477
H	-4.11075	-3.20857	-1.33188
H	-2.71028	-2.66973	-0.20795
O	-5.31294	-0.92671	-1.22815
C	-1.60609	-0.60859	-1.99643
H	-1.70570	-1.65413	-2.30413
H	-2.52581	-0.07771	-2.24332
H	-0.79525	-0.15825	-2.57631



SM (Before SET): 22 in Benzene

34

-760.0128981

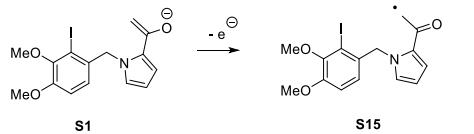
C	1.09738	2.96578	-1.17597
C	0.34622	1.82122	-0.94106
C	0.93858	0.63743	-0.49306
C	2.31605	0.65793	-0.28593
C	3.08877	1.79103	-0.51229
C	2.47170	2.95270	-0.96380
H	0.60754	3.86807	-1.52217
H	-0.72761	1.82968	-1.09364
H	4.15725	1.76895	-0.33986
H	3.06700	3.83978	-1.14501
I	3.32796	-1.09211	0.41862
C	0.08851	-0.60794	-0.24737
H	0.50220	-1.42409	-0.85135
H	0.20165	-0.91531	0.79705
N	-1.30407	-0.47543	-0.57001
C	-2.20638	0.03111	0.36981
C	-1.72297	0.74641	1.48373
C	-3.60158	-0.16744	0.25163
C	-2.58537	1.26945	2.44004
H	-0.65982	0.92174	1.59618
C	-4.44071	0.40528	1.20492
C	-3.95935	1.11579	2.30127
H	-2.17301	1.81163	3.28422
H	-5.50859	0.25093	1.08361
H	-4.64240	1.52780	3.03511
C	-4.27742	-0.98861	-0.84479
C	-4.21461	-2.35012	-0.69650
H	-4.68783	-3.00029	-1.42517
H	-3.69416	-2.79474	0.14299
O	-4.85424	-0.31951	-1.76686
C	-1.62784	-0.61240	-1.98389
H	-1.74306	-1.66224	-2.26946
H	-2.55995	-0.09832	-2.21427
H	-0.82479	-0.16359	-2.58072

Prod (After SET): S13 in Benzene

34

-759.8943754

C	1.13804	2.91243	-1.34061
C	0.36775	1.79513	-1.04180
C	0.94150	0.62904	-0.52940
C	2.32040	0.63509	-0.31856
C	3.10845	1.74210	-0.61043
C	2.51130	2.88599	-1.12893
H	0.66403	3.80217	-1.73673
H	-0.70504	1.82461	-1.19770
H	4.17599	1.71396	-0.43463
H	3.12179	3.75036	-1.36091
I	3.29821	-1.07456	0.50904
C	0.08954	-0.59501	-0.21379
H	0.50383	-1.45180	-0.75635
H	0.18008	-0.83852	0.84853
N	-1.31003	-0.49021	-0.56056
C	-2.21040	0.09260	0.32888
C	-1.75636	0.91692	1.37527
C	-3.60326	-0.11538	0.21037
C	-2.64979	1.55444	2.22248
H	-0.69633	1.09535	1.50299
C	-4.48477	0.58336	1.03958
C	-4.02467	1.41644	2.04662
H	-2.26352	2.18732	3.01320
H	-5.54699	0.41711	0.90039
H	-4.72064	1.93232	2.69562
C	-4.22785	-1.15680	-0.66855
C	-3.61306	-2.45926	-0.72668
H	-4.10337	-3.22849	-1.30861
H	-2.70661	-2.68161	-0.18067
O	-5.29920	-0.94824	-1.23700
C	-1.59747	-0.61240	-1.98605
H	-1.69112	-1.65786	-2.29746
H	-2.52141	-0.08926	-2.23391
H	-0.78824	-0.15478	-2.56325

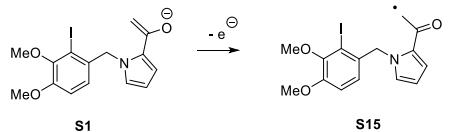


SM (Before SET): S1 in DMSO

	35	-872.3786917	C	-1.91698	0.82802	-0.18954
C	-0.95730	-0.16843	C	-0.95730	-0.16843	-0.32191
C	0.39208	0.12040	C	0.39208	0.12040	-0.55173
C	0.74493	1.46228	C	0.74493	1.46228	-0.64512
C	-0.19235	2.48490	C	-0.19235	2.48490	-0.51601
C	-1.52772	2.17678	C	-1.52772	2.17678	-0.28699
H	0.13290	3.51309	H	0.13290	3.51309	-0.59590
C	1.42824	-0.97997	C	1.42824	-0.97997	-0.69660
H	1.34273	-1.67609	H	1.34273	-1.67609	0.13535
H	1.26609	-1.52389	H	1.26609	-1.52389	-1.63125
N	2.78564	-0.46726	N	2.78564	-0.46726	-0.71240
C	3.46846	-0.15929	C	3.46846	-0.15929	-1.86233
C	3.46148	0.03806	C	3.46148	0.03806	0.37796
C	4.61472	0.51854	C	4.61472	0.51854	-1.51768
H	3.07869	-0.45706	H	3.07869	-0.45706	-2.82389
C	4.60953	0.64274	C	4.60953	0.64274	-0.10068
H	5.37018	1.09744	H	5.37018	1.09744	0.51568
H	5.37494	0.86331	H	5.37494	0.86331	-2.20182
C	2.95968	-0.12347	C	2.95968	-0.12347	1.78702
C	3.18411	0.93112	C	3.18411	0.93112	2.63689
H	3.64783	1.84399	H	3.64783	1.84399	2.28747
H	2.89139	0.85871	H	2.89139	0.85871	3.67891
O	2.37921	-1.23468	O	2.37921	-1.23468	2.07293
H	1.78371	1.72167	H	1.78371	1.72167	-0.81818
O	-3.23265	0.52799	O	-3.23265	0.52799	0.00496
O	-2.52328	3.08368	O	-2.52328	3.08368	-0.14482
C	-2.16929	4.45827	C	-2.16929	4.45827	-0.21474
H	-3.09328	5.01183	H	-3.09328	5.01183	-0.06891
H	-1.45670	4.71718	H	-1.45670	4.71718	0.57258
H	-1.74520	4.70241	H	-1.74520	4.70241	-1.19213
C	-3.64465	0.64846	C	-3.64465	0.64846	1.37072
H	-3.06946	-0.04008	H	-3.06946	-0.04008	1.99596
H	-3.51057	1.67441	H	-3.51057	1.67441	1.71876
H	-4.69868	0.38005	H	-4.69868	0.38005	1.40153
I	-1.63264	-2.18307	I	-1.63264	-2.18307	-0.17108

Prod (After SET): S15 in DMSO

	35	-872.2228704	C	-1.93018	0.81139	-0.18564
C	-0.96610	-0.17708	C	-0.96610	-0.17708	-0.33980
C	0.37079	0.12706	C	0.37079	0.12706	-0.61791
C	0.70494	1.46967	C	0.70494	1.46967	-0.74703
C	-0.23861	2.48387	C	-0.23861	2.48387	-0.59757
C	-1.56025	2.16363	C	-1.56025	2.16363	-0.31373
H	0.07134	3.51401	H	0.07134	3.51401	-0.70596
C	1.41300	-0.96015	C	1.41300	-0.96015	-0.78857
H	1.29834	-1.71350	H	1.29834	-1.71350	-0.01380
H	1.29479	-1.44857	H	1.29479	-1.44857	-1.75904
N	2.77122	-0.43701	N	2.77122	-0.43701	-0.73964
C	3.52343	-0.20168	C	3.52343	-0.20168	-1.84651
C	3.43985	0.04631	C	3.43985	0.04631	0.36956
C	4.69961	0.42006	C	4.69961	0.42006	-1.47116
H	3.16321	-0.49672	H	3.16321	-0.49672	-2.82030
C	4.64719	0.57751	C	4.64719	0.57751	-0.07389
H	5.41045	1.01841	H	5.41045	1.01841	0.54746
H	5.49847	0.71520	H	5.49847	0.71520	-2.13206
C	2.90260	-0.02749	C	2.90260	-0.02749	1.73340
C	3.69435	0.55396	C	3.69435	0.55396	2.78919
H	4.64833	1.02873	H	4.64833	1.02873	2.61413
H	3.30386	0.50207	H	3.30386	0.50207	3.79623
O	1.81561	-0.56111	O	1.81561	-0.56111	1.98890
H	1.73116	1.74311	H	1.73116	1.74311	-0.96701
O	-3.23403	0.49956	O	-3.23403	0.49956	0.05698
O	-2.55983	3.05966	O	-2.55983	3.05966	-0.14595
C	-2.22702	4.43800	C	-2.22702	4.43800	-0.24849
H	-3.15214	4.98148	H	-3.15214	4.98148	-0.07513
H	-1.48876	4.71703	H	-1.48876	4.71703	0.50768
H	-1.84376	4.67292	H	-1.84376	4.67292	-1.24470
C	-3.60446	0.63597	C	-3.60446	0.63597	1.43357
H	-3.00591	-0.04093	H	-3.00591	-0.04093	2.04936
H	-3.46650	1.66728	H	-3.46650	1.66728	1.76350
H	-4.65518	0.36160	H	-4.65518	0.36160	1.49977
I	-1.61500	-2.19461	I	-1.61500	-2.19461	-0.14443



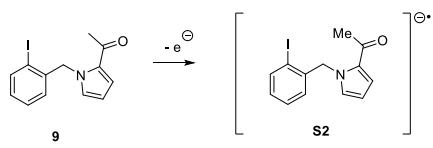
SM (Before SET): S1 in Benzene

	35	-872.3354944	C	-1.94488	0.84280	-0.19539
C	-0.99372	-0.16696	C	-0.26785		
C	0.37014	0.09720	C	-0.42698		
C	0.74922	1.43234	C	-0.50621		
C	-0.17846	2.46843	C	-0.42933		
C	-1.52805	2.18264	C	-0.27283		
H	0.16959	3.49066	H	-0.48625		
C	1.39519	-1.02021	C	-0.48772		
H	1.38430	-1.57867	H	0.44930		
H	1.15657	-1.69539	C	-1.31416		
N	2.74413	-0.53057	H	-0.69210		
C	3.28580	-0.31500	C	-1.93487		
C	3.56030	0.01740	C	0.27489		
C	4.48057	0.34770	C	-1.77566		
H	2.77368	-0.65922	H	-2.82051		
C	4.65393	0.55489	C	-0.37954		
H	5.49516	1.01775	H	0.11279	O	
H	5.15896	0.62460	H	-2.56826	H	
C	3.22070	-0.04045	C	1.74449	O	
C	3.62733	1.03658	C	2.49537	O	
H	4.11390	1.88880	H	2.03972	C	
H	3.45416	1.03984	H	3.56546	H	
O	2.59592	-1.08077	H	2.14812	H	
H	1.80078	1.67308	H	-0.61590	H	
O	-3.27549	0.56453	C	-0.07377	C	
O	-2.51772	3.11109	H	-0.18109	H	
C	-2.13042	4.47174	H	-0.21882	H	
H	-3.04791	5.04767	H	-0.12022	H	
H	-1.45523	4.71151	H	0.60782	I	
H	-1.64612	4.71706	H	-1.16856		
C	-3.75468	0.68712	C	1.26515		
H	-3.21720	-0.00298	C	1.92210		
H	-3.63401	1.71283	C	1.62066		
H	-4.81088	0.42407	C	1.24176		
I	-1.70197	-2.17045	C	-0.11463		

Prod (After SET): S15 in Benzene

	35	-872.2154318	C	-1.96077	0.81044	-0.17571
C	-0.99395	-0.17981	C	0.35392	0.11937	-0.51312
C	0.35392	0.11937	C	0.69962	1.45903	-0.62957
C	0.69962	1.45903	C	-0.24648	2.47591	-0.51659
C	-0.24648	2.47591	C	-1.57906	2.16079	-0.28718
H	0.07121	3.50508	H	1.38922	-0.98002	-0.63614
C	1.38922	-0.98002	H	1.32405	-1.65050	0.21792
H	1.32405	-1.65050	H	1.20965	-1.56503	-1.54178
N	1.20965	-1.56503	N	2.74741	-0.46217	-0.72764
C	2.74741	-0.46217	C	3.39502	-0.27588	-1.90786
C	3.39502	-0.27588	C	3.52494	0.04372	0.29588
C	3.52494	0.04372	C	4.60821	0.33906	-1.66698
H	4.60821	0.33906	H	2.94208	-0.59918	-2.83267
H	2.94208	-0.59918	C	4.69114	0.53993	-0.27621
H	4.69114	0.53993	H	5.51305	0.99409	0.25405
H	5.51305	0.99409	H	5.34413	0.60022	-2.40997
C	5.34413	0.60022	C	3.10476	0.03983	1.70479
C	3.10476	0.03983	C	4.03623	0.56248	2.67602
H	4.03623	0.56248	H	5.01639	0.93034	2.41120
H	5.01639	0.93034	H	3.72505	0.56914	3.71155
H	3.72505	0.56914	O	2.00487	-0.38722	2.06520
H	2.00487	-0.38722	H	1.73462	1.72795	-0.80922
C	1.73462	1.72795	O	-3.27309	0.50086	0.00523
C	-3.27309	0.50086	O	-2.58183	3.06166	-0.15800
C	-2.58183	3.06166	C	-2.24533	4.43391	-0.27240
H	-2.24533	4.43391	H	-3.17624	4.98097	-0.14569
H	-3.17624	4.98097	H	-1.53632	4.72971	0.50604
H	-1.53632	4.72971	H	-1.82343	4.65223	-1.25745
C	-1.82343	4.65223	C	-3.71426	0.64957	1.35677
C	-3.71426	0.64957	H	-3.13632	-0.00709	2.01338
H	-3.13632	-0.00709	H	-3.61351	1.68813	1.67803
H	-3.61351	1.68813	H	-4.76182	0.35564	1.37227
H	-4.76182	0.35564	I	-1.65365	-2.19375	-0.11221

2.2 Electron Acceptors



SM (Before SET): 9 in DMSO

28

-643.8557281

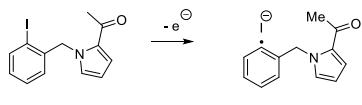
C	0.18047	3.09141	0.31026
C	0.72224	1.91757	-0.19970
C	-0.05597	0.76760	-0.35478
C	-1.39882	0.84048	0.01795
C	-1.95619	2.00733	0.52890
C	-1.15932	3.13741	0.67688
H	0.80720	3.96787	0.42030
H	1.76920	1.88943	-0.48304
H	-3.00081	2.03568	0.81181
H	-1.59042	4.04645	1.07837
C	0.54449	-0.50397	-0.92371
H	0.20556	-1.37489	-0.36709
H	0.20320	-0.64297	-1.95219
N	1.99817	-0.47976	-0.95516
C	2.88474	-0.52587	0.11295
C	2.69008	-0.16022	-2.08201
C	4.14855	-0.24928	-0.38953
C	4.02902	-0.02123	-1.77226
H	2.17213	-0.05099	-3.02279
H	5.04855	-0.24225	0.20522
H	4.81811	0.20689	-2.47062
C	2.60125	-0.83247	1.52534
C	1.24508	-1.32147	1.97376
H	0.96176	-2.22832	1.43507
H	1.29789	-1.53773	3.03880
O	3.50071	-0.70624	2.34069
I	-2.67955	-0.85625	-0.17130
H	0.47694	-0.56326	1.80143

Prod (After SET): S2 in DMSO

28

-643.9298114

C	0.35162	3.00643	0.41367
C	0.82908	1.82249	-0.13577
C	-0.00778	0.71702	-0.32040
C	-1.33922	0.85266	0.06812
C	-1.83643	2.02848	0.62075
C	-0.98173	3.11123	0.79566
H	1.02324	3.84641	0.54479
H	1.87063	1.73919	-0.42789
H	-2.87646	2.10015	0.91227
H	-1.36305	4.02904	1.22705
C	0.53234	-0.56336	-0.93703
H	0.14328	-1.42124	-0.39304
H	0.15238	-0.65202	-1.95944
N	1.97555	-0.61415	-1.00096
C	2.85130	-0.57844	0.10601
C	2.64599	-0.13962	-2.12744
C	4.08697	-0.10265	-0.39035
C	3.94013	0.15508	-1.77581
H	2.13137	-0.07204	-3.07366
H	4.98362	-0.00315	0.20012
H	4.70606	0.50323	-2.45405
C	2.55608	-0.95218	1.44758
C	1.26588	-1.66110	1.82320
H	0.38139	-1.01000	1.80816
H	1.05017	-2.51875	1.17578
O	3.43339	-0.75799	2.37637
I	-2.72160	-0.76076	-0.18746
H	1.38065	-2.03399	2.84198

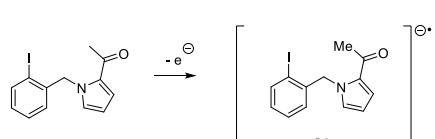


Prod (After SET): S3 in DMSO

28

-643.9665259

C	1.61061	3.28725	0.44105
C	1.75340	2.03697	-0.15938
C	0.62506	1.28615	-0.50875
C	-0.60015	1.85200	-0.22662
C	-0.79512	3.07634	0.36547
C	0.34718	3.81050	0.70463
H	2.49453	3.85420	0.70800
H	2.74541	1.63763	-0.35100
H	-1.78794	3.46249	0.56816
H	0.24504	4.78188	1.17520
C	0.71973	-0.07087	-1.17583
H	-0.08498	-0.71316	-0.82199
H	0.58542	0.03802	-2.25394
N	2.02036	-0.70250	-0.98138
C	2.59246	-1.15269	0.20008
C	2.97907	-0.68168	-1.94603
C	3.92543	-1.43478	-0.06557
C	4.17052	-1.14312	-1.41973
H	2.73951	-0.32978	-2.93794
H	4.61727	-1.83654	0.65829
H	5.09643	-1.26054	-1.95958
C	1.93832	-1.36633	1.50217
C	0.43726	-1.34483	1.63081
H	0.03630	-0.34848	1.42834
H	-0.02447	-2.03378	0.92000
O	2.63630	-1.60308	2.47626
I	-3.21306	-0.69439	-0.16554
H	0.17380	-1.63667	2.64578



SM (Before SET): 9 in Benzene

28

-643.8502505

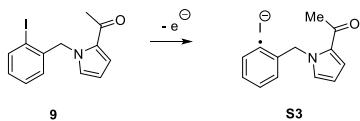
C	0.18553	3.08508	0.30906
C	0.72554	1.90756	-0.19354
C	-0.05735	0.76107	-0.34803
C	-1.40133	0.84038	0.01797
C	-1.95672	2.01128	0.52064
C	-1.15580	3.13829	0.66758
H	0.81598	3.95857	0.42101
H	1.77445	1.87195	-0.46882
H	-3.00268	2.04373	0.79786
H	-1.58485	4.05078	1.06349
C	0.54055	-0.51605	-0.90721
H	0.20671	-1.37893	-0.33488
H	0.18626	-0.66938	-1.92965
N	1.99215	-0.49121	-0.95504
C	2.88893	-0.52629	0.10465
C	2.67241	-0.16776	-2.09006
C	4.14440	-0.24168	-0.40849
C	4.01111	-0.01726	-1.79172
H	2.14529	-0.06563	-3.02648
H	5.04645	-0.22608	0.18266
H	4.79300	0.21415	-2.49688
C	2.62205	-0.82680	1.52550
C	1.26975	-1.31788	1.99055
H	0.98426	-2.23013	1.46178
H	1.33850	-1.52641	3.05622
O	3.52730	-0.69384	2.32685
I	-2.68486	-0.85414	-0.16717
H	0.49659	-0.56373	1.82254

Prod (After SET): S2 in Benzene

28

-643.8897792

C	0.38728	2.98132	0.27210
C	0.84948	1.75579	-0.19225
C	-0.00954	0.65831	-0.31550
C	-1.34192	0.85102	0.03804
C	-1.82666	2.06910	0.50071
C	-0.94924	3.14059	0.62256
H	1.07741	3.81134	0.36522
H	1.89347	1.63156	-0.45993
H	-2.87079	2.17962	0.76357
H	-1.31524	4.09221	0.99012
C	0.51077	-0.67957	-0.82227
H	0.14731	-1.47099	-0.16846
H	0.07595	-0.87241	-1.80845
N	1.94480	-0.74285	-0.95719
C	2.87539	-0.56856	0.09778
C	2.54218	-0.33592	-2.15586
C	4.06149	-0.08629	-0.50208
C	3.83727	0.04137	-1.89170
H	1.98523	-0.37843	-3.07915
H	4.97332	0.10509	0.03998
H	4.55555	0.35761	-2.63507
C	2.66489	-0.82043	1.48203
C	1.41465	-1.53022	1.98023
H	0.51532	-0.89871	1.96559
H	1.18968	-2.43921	1.40976
O	3.56047	-0.50583	2.34030
I	-2.75512	-0.75310	-0.13405
H	1.60070	-1.81605	3.01655

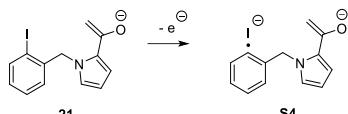


Prod (After SET): S3 in Benzene

28

-643.9288407

C	1.26617	3.30715	0.52518
C	1.52459	2.08200	-0.08792
C	0.46754	1.25222	-0.47816
C	-0.81080	1.70704	-0.22854
C	-1.11079	2.90370	0.37787
C	-0.04264	3.72196	0.75930
H	2.09477	3.93655	0.82826
H	2.55015	1.76249	-0.25237
H	-2.13815	3.19708	0.56385
H	-0.23351	4.67305	1.24450
C	0.68077	-0.08546	-1.15550
H	-0.05604	-0.80113	-0.79415
H	0.51371	0.01391	-2.23011
N	2.03961	-0.59232	-0.98916
C	2.66147	-1.02701	0.17030
C	2.98190	-0.45412	-1.96024
C	4.01074	-1.17910	-0.11282
C	4.21582	-0.82113	-1.45825
H	2.69862	-0.09610	-2.93816
H	4.73801	-1.53727	0.59864
H	5.14281	-0.83548	-2.00888
C	2.04779	-1.33503	1.47953
C	0.55202	-1.40383	1.64309
H	0.08087	-0.43394	1.46402
H	0.11003	-2.10911	0.93530
O	2.78585	-1.56912	2.42114
I	-3.07672	-0.78031	-0.17658
H	0.33345	-1.72506	2.65966



SM (Before SET): 21 in DMSO

27

-643.3534550

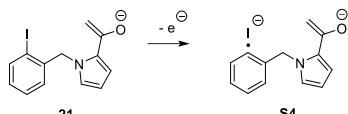
C	-0.19425	3.13096	0.61929
C	0.48823	2.02604	0.12417
C	-0.17065	0.82197	-0.13440
C	-1.54035	0.77040	0.12501
C	-2.24063	1.86417	0.62054
C	-1.56008	3.05215	0.86780
H	0.34214	4.05208	0.81267
H	1.55519	2.08559	-0.06185
H	-3.30395	1.79408	0.81225
H	-2.10092	3.90756	1.25428
C	0.57985	-0.38393	-0.66900
H	0.45527	-1.22759	0.01110
H	0.15768	-0.67123	-1.63589
N	1.99662	-0.15003	-0.85390
C	3.03294	-0.41830	0.02340
C	2.50025	0.40213	-2.00579
C	4.20111	-0.03457	-0.61027
C	3.86647	0.49223	-1.88521
H	1.83713	0.67086	-2.81415
H	5.18521	-0.13959	-0.18118
H	4.54178	0.88030	-2.63237
C	2.94054	-1.03489	1.39655
C	1.83748	-0.79698	2.18125
H	1.03721	-0.13556	1.88257
H	1.79595	-1.22761	3.17605
O	3.96816	-1.72501	1.73723
I	-2.63528	-1.02805	-0.23517

Prod (After SET): S4 in DMSO

27

-643.4599916

C	1.08996	3.43497	0.40198
C	1.44914	2.15214	-0.01206
C	0.47511	1.16324	-0.18882
C	-0.82665	1.53919	0.06836
C	-1.23423	2.78496	0.47838
C	-0.24179	3.75810	0.64773
H	1.85916	4.18665	0.53549
H	2.49200	1.90906	-0.19347
H	-2.27831	3.01125	0.66585
H	-0.51257	4.75720	0.96992
C	0.80446	-0.25182	-0.62616
H	0.45846	-0.96029	0.12658
H	0.27681	-0.47112	-1.55755
N	2.22107	-0.46648	-0.85392
C	3.17217	-0.95319	0.02476
C	2.81692	-0.16150	-2.05184
C	4.37810	-0.96160	-0.65432
C	4.15772	-0.45302	-1.96104
H	2.22595	0.22647	-2.86773
H	5.30861	-1.30924	-0.23302
H	4.88649	-0.32488	-2.74688
C	2.96378	-1.41266	1.44531
C	2.01637	-0.80003	2.22917
H	1.43201	0.04278	1.89019
H	1.89377	-1.12593	3.25654
O	3.75758	-2.34956	1.82339
I	-3.58070	-0.88515	-0.13706



SM (Before SET): 21 in Benzene

27

-643.3105041

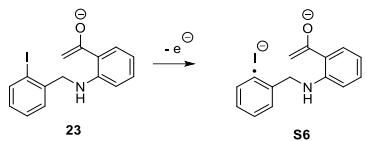
C	-0.18927	3.12100	0.58735
C	0.49230	1.99629	0.14022
C	-0.17445	0.79333	-0.10569
C	-1.54954	0.76710	0.12079
C	-2.25060	1.88075	0.56826
C	-1.56227	3.06648	0.80074
H	0.35526	4.03859	0.77510
H	1.56565	2.03159	-0.01283
H	-3.31885	1.82497	0.73552
H	-2.10197	3.93845	1.15088
C	0.58125	-0.43302	-0.58425
H	0.50250	-1.22551	0.16299
H	0.12667	-0.79352	-1.51161
N	1.98102	-0.18229	-0.83945
C	3.05754	-0.40393	0.00198
C	2.42373	0.34838	-2.02815
C	4.18879	-0.01507	-0.68964
C	3.79149	0.46851	-1.96399
H	1.72174	0.57987	-2.81500
H	5.18798	-0.09880	-0.29290
H	4.42795	0.84543	-2.75009
C	3.03648	-0.99100	1.39692
C	1.96210	-0.72292	2.21838
H	1.16782	-0.04471	1.94020
H	1.96845	-1.11297	3.22993
O	4.07214	-1.66778	1.69508
I	-2.65835	-1.03058	-0.20895

Prod (After SET): S4 in Benzene

27

-643.3576895

C	-0.05400	-0.27796	1.58633
C	1.17450	-0.18181	0.93511
C	1.23681	-0.15230	-0.46374
C	0.02585	-0.22406	-1.11735
C	-1.21307	-0.31423	-0.53243
C	-1.24527	-0.34148	0.86592
H	-0.08071	-0.29470	2.66974
H	2.09884	-0.11374	1.50196
H	-2.13847	-0.35037	-1.09815
H	-2.20625	-0.40137	1.36627
C	2.54622	-0.05390	-1.21916
H	2.93107	-1.05034	-1.44017
H	2.37170	0.46377	-2.16619
N	3.57327	0.65683	-0.47574
C	4.78016	0.17099	-0.00853
C	3.50839	2.01194	-0.26265
C	5.47988	1.25044	0.49589
C	4.67503	2.41127	0.34585
H	2.63594	2.56902	-0.56975
H	6.46446	1.17594	0.93009
H	4.91534	3.42032	0.64560
C	5.25247	-1.26546	-0.02163
C	4.32882	-2.25325	0.24150
H	3.30255	-2.02865	0.50305
H	4.65231	-3.28794	0.27083
O	6.50058	-1.41824	-0.23247
I	-5.37621	0.03708	-0.04705

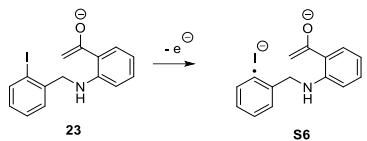


SM (Before SET): 23 in DMSO

31	-720.7677742	C	-1.73521	3.23425	-0.82395
		C	-0.74727	2.25840	-0.73862
		C	-1.04762	0.94227	-0.37487
		C	-2.38944	0.64904	-0.11343
		C	-3.38986	1.60958	-0.19368
		C	-3.05818	2.91355	-0.54936
		H	-1.46607	4.24474	-1.10728
		H	0.27796	2.52175	-0.96924
		H	-4.41887	1.34701	0.01688
		H	-3.83530	3.66566	-0.61261
		I	-2.98859	-1.33448	0.41185
		C	0.02394	-0.12163	-0.28393
		H	-0.08108	-0.65083	0.67493
		H	-0.18166	-0.86267	-1.06371
		N	1.35143	0.42203	-0.44956
		H	1.55653	1.31405	0.00029
		C	2.46702	-0.40533	-0.43267
		C	2.40860	-1.71112	-0.94711
		C	3.69740	0.07189	0.09438
		C	3.54448	-2.51021	-1.00943
		H	1.47090	-2.10121	-1.32304
		C	4.82180	-0.74816	-0.00737
		C	4.76692	-2.02791	-0.55458
		H	3.46825	-3.50854	-1.42596
		H	5.76719	-0.36705	0.36287
		H	5.66131	-2.63620	-0.61686
O	3.04644	O	2.37270	0.30152	

Prod (After SET): S6 in DMSO

31	-720.8779936	C	-0.29112	4.12372	-0.61728
		C	0.31451	2.87992	-0.77439
		C	-0.38679	1.69917	-0.48625
		C	-1.68333	1.86308	-0.05377
		C	-2.33425	3.06337	0.11437
		C	-1.61009	4.22314	-0.17488
		H	0.26851	5.02313	-0.84530
		H	1.34207	2.82051	-1.12369
		H	-3.36100	3.11473	0.45925
		H	-2.07462	5.19552	-0.05557
		I	-3.85375	-1.38368	0.27772
		C	0.24523	0.33809	-0.65952
		H	-0.44703	-0.41948	-0.28130
		H	0.38419	0.14130	-1.73451
		N	1.51346	0.27503	0.04836
		H	2.02962	1.15368	0.11044
		C	2.39091	-0.77057	-0.20320
		C	1.95480	-1.97628	-0.77269
		C	3.75368	-0.63279	0.17082
		C	2.84155	-3.03180	-0.97337
		H	0.91548	-2.09605	-1.05332
		C	4.61453	-1.70319	-0.05398
		C	4.17793	-2.90354	-0.61767
		H	2.47836	-3.95268	-1.41638
		H	5.65947	-1.58456	0.21187
		H	4.87559	-3.71593	-0.78227
		C	4.25431	0.66634	0.77392
		C	5.13118	0.58570	1.82225
		H	5.52006	1.49193	2.27420
		H	5.45251	-0.36795	2.21937
O	3.79664	O	1.75748	0.24915	

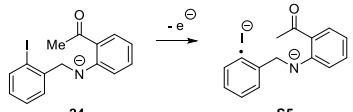


SM (Before SET): 23 in Benzene

31	-720.7166835	C	1.95348	3.49162	0.32429
		C	0.84685	2.68145	0.09345
		C	0.96490	1.29622	-0.05250
		C	2.25147	0.76030	0.06157
		C	3.36928	1.55177	0.29358
		C	3.22016	2.92943	0.42086
		H	1.82198	4.56218	0.43195
		H	-0.14350	3.11596	0.03528
		H	4.34895	1.09873	0.37888
		H	4.09062	3.54936	0.60037
		I	2.55873	-1.34935	-0.08140
		C	-0.23534	0.40943	-0.30932
		H	-0.01426	-0.28845	-1.12271
		H	-0.39570	-0.21943	0.57205
		N	-1.43803	1.17381	-0.55074
		C	-2.74099	0.72080	-0.27870
		C	-3.75412	1.68935	-0.37674
		C	-3.08357	-0.58863	0.11585
		C	-5.07693	1.39464	-0.08291
		H	-3.47482	2.69722	-0.66998
		C	-4.41787	-0.84662	0.44621
		C	-5.41660	0.11700	0.35311
		H	-5.83315	2.16641	-0.17796
		H	-4.66773	-1.85817	0.74845
		H	-6.44308	-0.12992	0.59916
		C	-2.11843	-1.76731	0.04919
		C	-1.89246	-2.45649	1.21635
		H	-1.24235	-3.32494	1.21665
		H	-2.36416	-2.15346	2.14264
		O	-1.63191	-1.99588	-1.10655
		H	-1.39316	1.75253	-1.37867

Prod (After SET): S6 in Benzene

31	-720.7688898	C	0.22378	-0.62542	1.56039
		C	-0.93782	-0.96737	0.86825
		C	-0.92013	-1.11163	-0.52647
		C	0.29861	-0.88846	-1.13192
		C	1.47568	-0.55705	-0.50636
		C	1.42608	-0.42157	0.88610
		H	0.19064	-0.52254	2.63925
		H	-1.87466	-1.13961	1.39288
		H	2.41227	-0.40547	-1.03320
		H	2.33569	-0.16509	1.41939
		I	5.61979	0.21417	0.03942
		C	-2.17727	-1.42426	-1.31363
		H	-1.91548	-2.00323	-2.20158
		H	-2.86901	-2.01933	-0.72136
		N	-2.86556	-0.21610	-1.77958
		C	-3.46755	0.65558	-0.85649
		C	-3.21249	2.02863	-0.99772
		C	-4.33631	0.22473	0.17291
		C	-3.79911	2.97425	-0.16748
		H	-2.52609	2.35105	-1.77561
		C	-4.89400	1.19756	1.00673
		C	-4.64509	2.55900	0.85437
		H	-3.57910	4.02631	-0.31291
		H	-5.56474	0.85644	1.78785
		H	-5.10736	3.27960	1.51947
		C	-4.76805	-1.22544	0.36450
		C	-4.60962	-1.74209	1.63093
		H	-4.90737	-2.76420	1.83934
		H	-4.19063	-1.14704	2.43272
		O	-5.23534	-1.81857	-0.66104
		H	-2.25173	0.30477	-2.39479



SM (Before SET): 24 in DMSO

31

-720.7637628

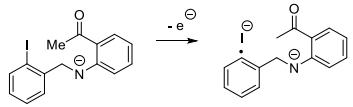
C	-2.20085	3.46156	-0.07705
C	-1.04200	2.72823	0.15431
C	-1.04319	1.33020	0.16128
C	-2.26927	0.70695	-0.08198
C	-3.44070	1.41662	-0.31935
C	-3.40477	2.80811	-0.31529
H	-2.16245	4.54474	-0.07323
H	-0.09563	3.22109	0.33673
H	-4.37106	0.89531	-0.50637
H	-4.31436	3.36731	-0.49935
I	-2.41008	-1.43248	-0.10797
C	0.22554	0.53757	0.41749
H	0.03072	-0.15127	1.25273
H	0.38086	-0.13623	-0.44661
N	1.36147	1.37618	0.64572
C	2.56248	0.92364	0.35296
C	3.64247	1.89392	0.33478
C	2.94688	-0.42694	-0.04956
C	4.83261	1.64901	-0.28618
H	3.43313	2.86716	0.76734
C	4.16815	-0.60837	-0.75104
C	5.09689	0.39343	-0.89877
H	5.58578	2.43047	-0.32256
H	4.40734	-1.59716	-1.12881
H	6.03183	0.21465	-1.41465
C	2.27380	-1.61825	0.44272
C	2.47154	-2.93961	-0.28996
H	1.63342	-3.59039	-0.04261
H	2.53681	-2.81815	-1.37121
O	1.60020	-1.63374	1.47875
H	3.38859	-3.42573	0.05498

Prod (After SET): S5 in DMSO

31

-720.8694189

C	-0.12726	4.73811	-0.29030
C	0.59354	3.56886	-0.03737
C	-0.06068	2.35267	0.19168
C	-1.43972	2.41520	0.14479
C	-2.20452	3.52685	-0.10270
C	-1.51850	4.72849	-0.32542
H	0.40607	5.66608	-0.46306
H	1.67650	3.57633	-0.01065
H	-3.28796	3.48719	-0.12616
H	-2.07094	5.63989	-0.52472
I	-3.16960	-1.52326	-0.16550
C	0.66061	1.04467	0.46486
H	0.20811	0.58976	1.35745
H	0.40462	0.34224	-0.35134
N	2.07679	1.22118	0.58362
C	2.88005	0.21915	0.29758
C	4.29244	0.52887	0.15888
C	2.52811	-1.17000	0.01044
C	5.16694	-0.31217	-0.46550
H	4.61529	1.50592	0.50409
C	3.45646	-1.97711	-0.69851
C	4.74396	-1.57602	-0.96158
H	6.20124	-0.00669	-0.59257
H	3.15763	-2.97981	-0.98607
H	5.43604	-2.22797	-1.47949
C	1.39745	-1.84287	0.63018
C	0.87579	-3.13832	0.02083
H	-0.17265	-3.23881	0.30071
H	0.96538	-3.16478	-1.06511
O	0.87752	-1.45648	1.68292
H	1.42365	-3.99111	0.43250



SM (Before SET): 24 in Benzene

31

-720.7285731

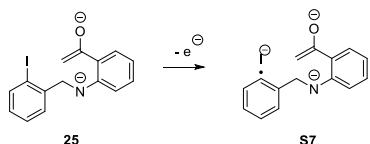
C	-2.18980	3.45870	-0.05112
C	-1.03485	2.71818	0.17078
C	-1.04312	1.31980	0.16445
C	-2.27245	0.70673	-0.08112
C	-3.44121	1.42377	-0.30962
C	-3.39835	2.81440	-0.29330
H	-2.14542	4.54188	-0.03705
H	-0.08056	3.19532	0.35661
H	-4.37315	0.90612	-0.49875
H	-4.30555	3.38028	-0.47054
I	-2.42166	-1.43147	-0.11951
C	0.22662	0.52742	0.41330
H	0.04317	-0.15339	1.25819
H	0.37258	-0.15199	-0.44832
N	1.35739	1.37496	0.62057
C	2.55791	0.92505	0.33874
C	3.62996	1.90546	0.30819
C	2.95605	-0.42924	-0.04229
C	4.82307	1.66330	-0.30466
H	3.40487	2.88034	0.72814
C	4.18203	-0.60738	-0.73388
C	5.10250	0.39995	-0.89545
H	5.56891	2.45178	-0.35078
H	4.43348	-1.59961	-1.09484
H	6.04137	0.22084	-1.40455
C	2.28816	-1.61958	0.46027
C	2.51571	-2.95171	-0.25343
H	1.68206	-3.60654	-0.00168
H	2.58820	-2.84432	-1.33619
O	1.59583	-1.63596	1.47951
H	3.43603	-3.41900	0.10860

Prod (After SET): S5 in Benzene

31

-720.7602330

C	-0.01608	4.58619	0.09895
C	0.77667	3.45780	0.30054
C	0.22023	2.17253	0.27831
C	-1.13855	2.12368	0.03455
C	-1.97289	3.19610	-0.18130
C	-1.38205	4.46482	-0.13940
H	0.43818	5.57096	0.12420
H	1.84390	3.54053	0.46829
H	-3.03180	3.06234	-0.37175
H	-1.98982	5.34934	-0.30106
I	-4.08618	-1.28295	-0.25067
C	1.04633	0.92658	0.54448
H	0.81618	0.58873	1.56452
H	0.67294	0.11511	-0.10418
N	2.44737	1.17976	0.35099
C	3.28475	0.19962	0.06265
C	4.60367	0.59925	-0.40900
C	3.05956	-1.25257	0.06143
C	5.42367	-0.24806	-1.09274
H	4.86884	1.64267	-0.27111
C	3.90981	-2.07001	-0.72305
C	5.05781	-1.60390	-1.31921
H	6.36941	0.12243	-1.47929
H	3.67669	-3.12735	-0.80592
H	5.69738	-2.26436	-1.89189
C	2.17480	-1.92161	1.00288
C	1.73663	-3.35500	0.70955
H	0.86960	-3.57069	1.33208
H	1.48100	-3.50458	-0.34033
O	1.81047	-1.42289	2.07009
H	2.53366	-4.05661	0.97234

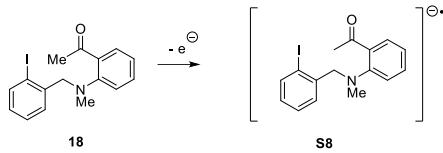


SM (Before SET): 25 in DMSO

30	-720.2417849	C	-2.13089	3.48667	-0.12209
		C	-0.97347	2.73231	0.04084
		C	-0.99777	1.33398	0.07945
		C	-2.25369	0.73645	-0.05454
		C	-3.42555	1.46515	-0.22085
		C	-3.36283	2.85581	-0.25400
		H	-2.07005	4.56888	-0.14653
		H	-0.00328	3.20129	0.14433
		H	-4.37746	0.95970	-0.32513
		H	-4.27271	3.42997	-0.38273
		I	-2.44726	-1.40102	-0.02193
		C	0.27881	0.53079	0.25413
		H	0.11289	-0.16544	1.09151
		H	0.36219	-0.13072	-0.62542
		N	1.43073	1.36730	0.42583
		C	2.64890	0.85584	0.21220
		C	3.74308	1.79505	0.21477
		C	3.03607	-0.51994	-0.05388
		C	5.03922	1.46447	-0.12249
		H	3.49560	2.82383	0.46250
		C	4.35689	-0.80503	-0.41034
		C	5.37358	0.14917	-0.47220
		H	5.80204	2.23874	-0.11717
		H	4.59688	-1.84559	-0.61364
		H	6.38640	-0.12705	-0.74045
		C	2.14051	-1.72034	0.19779
		C	1.91602	-2.60199	-0.83717
		H	1.34690	-3.51182	-0.66687
		H	2.29324	-2.40793	-1.83337
		O	1.71046	-1.86263	1.40308

Prod (After SET): S7 in DMSO

30	-720.3443286	C	-0.57977	4.53469	-0.00855
		C	0.31687	3.46577	0.07255
		C	-0.13711	2.14321	0.15123
		C	-1.51198	2.00012	0.14122
		C	-2.44244	3.00519	0.05829
		C	-1.95449	4.31761	-0.01640
		H	-0.19722	5.54765	-0.06890
		H	1.38770	3.62885	0.07119
		H	-3.50786	2.80136	0.04814
		H	-2.64486	5.15122	-0.08282
		I	-3.41021	-1.54257	-0.24121
		C	0.78877	0.94584	0.25871
		H	0.56355	0.44944	1.21651
		H	0.46588	0.21852	-0.50715
		N	2.16839	1.31608	0.10750
		C	3.08345	0.35217	-0.04701
		C	4.39701	0.77627	-0.46230
		C	2.93760	-1.08529	0.11904
		C	5.41167	-0.09413	-0.80333
		H	4.55343	1.84831	-0.54447
		C	3.98533	-1.92995	-0.25723
		C	5.21760	-1.48072	-0.73527
		H	6.36654	0.30701	-1.13324
		H	3.82722	-2.99753	-0.12737
		H	6.00296	-2.17726	-1.00337
		C	1.78899	-1.73937	0.86806
		C	1.06583	-2.72735	0.23909
		H	0.29276	-3.26830	0.77778
		H	1.24134	-2.97837	-0.79969
		O	1.62589	-1.36143	2.08955



SM (Before SET): 18 in DMSO

35

-760.5580475

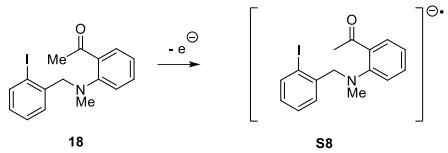
C	1.17159	2.91478	-1.35050
C	0.39692	1.79919	-1.05438
C	0.96541	0.63198	-0.53866
C	2.34386	0.63423	-0.32314
C	3.13636	1.73911	-0.61173
C	2.54405	2.88513	-1.13258
H	0.70187	3.80519	-1.75025
H	-0.67450	1.83050	-1.21893
H	4.20336	1.70937	-0.43265
H	3.15798	3.74771	-1.36207
I	3.31460	-1.08076	0.50404
C	0.10841	-0.58845	-0.22601
H	0.50454	-1.44412	-0.78291
H	0.20766	-0.84492	0.83225
N	-1.29351	-0.46107	-0.55722
C	-2.17786	0.11159	0.34451
C	-1.70761	0.90016	1.41330
C	-3.57716	-0.05282	0.21581
C	-2.58790	1.53872	2.27296
H	-0.64412	1.04926	1.54950
C	-4.44414	0.64770	1.06088
C	-3.96658	1.44078	2.09212
H	-2.18769	2.14153	3.08020
H	-5.51064	0.51279	0.91895
H	-4.65090	1.95635	2.75365
C	-4.22614	-1.05657	-0.68456
C	-3.69737	-2.47242	-0.67154
H	-3.77441	-2.90892	-1.66778
H	-2.67948	-2.54373	-0.29411
O	-5.23879	-0.78360	-1.29844
C	-1.60837	-0.61690	-1.97276
H	-1.71214	-1.66758	-2.25759
H	-2.52963	-0.08735	-2.21793
H	-0.80659	-0.17886	-2.57418
H	-4.35511	-3.03815	-0.00457

Prod (After SET): 56 in DMSO

35

-760.6360878

C	-1.28159	2.92099	1.34846
C	-0.47075	1.84238	1.01702
C	-1.00016	0.65891	0.49258
C	-2.38104	0.61684	0.30140
C	-3.21250	1.68403	0.62430
C	-2.65691	2.84220	1.15687
H	-0.83876	3.82322	1.75305
H	0.60273	1.91189	1.14984
H	-4.28031	1.61524	0.46125
H	-3.29946	3.67589	1.41326
I	-3.30856	-1.11024	-0.55715
C	-0.09955	-0.52611	0.14646
H	-0.53105	-1.41513	0.62346
H	-0.14663	-0.70099	-0.93346
N	1.28045	-0.44230	0.54767
C	2.23469	0.18996	-0.28266
C	1.82818	1.13168	-1.22130
C	3.64485	-0.14034	-0.16981
C	2.74029	1.86313	-2.00335
H	0.77153	1.35258	-1.32292
C	4.54328	0.74744	-0.85358
C	4.10843	1.69586	-1.75970
H	2.37932	2.58421	-2.72683
H	5.60317	0.58080	-0.70649
H	4.83536	2.29727	-2.29701
C	4.22621	-1.27000	0.49627
C	3.43661	-2.52164	0.83636
H	3.43290	-2.70287	1.91769
H	2.40862	-2.50622	0.47984
O	5.48414	-1.33347	0.71672
C	1.49760	-0.53977	1.98416
H	1.22014	-1.53661	2.34180
H	2.54962	-0.37562	2.20910
H	0.90599	0.19667	2.54148
H	3.95840	-3.36711	0.37692



SM (Before SET): 18 in Benzene

35

-760.5528685

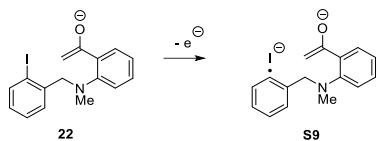
C	1.17064	2.91392	-1.34787
C	0.39581	1.80080	-1.04477
C	0.96569	0.63368	-0.53082
C	2.34506	0.63355	-0.32293
C	3.13734	1.73630	-0.61900
C	2.54411	2.88176	-1.13880
H	0.69997	3.80483	-1.74537
H	-0.67708	1.83368	-1.19925
H	4.20513	1.70376	-0.44559
H	3.15806	3.74280	-1.37400
I	3.31647	-1.07943	0.50486
C	0.10797	-0.58486	-0.21153
H	0.50997	-1.44434	-0.75892
H	0.20403	-0.83227	0.84937
N	-1.29224	-0.46377	-0.54826
C	-2.18307	0.11612	0.34770
C	-1.72013	0.91778	1.40785
C	-3.57909	-0.05876	0.21437
C	-2.60789	1.55806	2.25910
H	-0.65789	1.07681	1.54337
C	-4.45357	0.64475	1.04718
C	-3.98403	1.44955	2.07324
H	-2.21503	2.17159	3.06177
H	-5.51823	0.50633	0.89566
H	-4.67402	1.96898	2.72573
C	-4.21838	-1.07102	-0.68716
C	-3.68598	-2.48741	-0.65231
H	-3.77642	-2.94187	-1.63928
H	-2.66346	-2.54903	-0.28505
O	-5.21979	-0.80533	-1.31608
C	-1.60157	-0.61381	-1.96492
H	-1.70887	-1.66372	-2.25367
H	-2.52182	-0.08306	-2.21159
H	-0.79677	-0.17651	-2.56355
H	-4.33416	-3.04155	0.03328

Prod (After SET): 56 in Benzene

35

-760.5987172

C	-1.27974	2.92331	1.33531
C	-0.46954	1.84840	0.99360
C	-1.00141	0.66291	0.47487
C	-2.38346	0.61916	0.30102
C	-3.21568	1.68247	0.63392
C	-2.65734	2.84122	1.16087
H	-0.83349	3.82712	1.73281
H	0.60618	1.91911	1.10698
H	-4.28473	1.60863	0.48135
H	-3.29889	3.67354	1.42498
I	-3.31652	-1.10828	-0.55460
C	-0.09505	-0.51724	0.12097
H	-0.53540	-1.41169	0.58148
H	-0.13149	-0.67393	-0.96243
N	1.27689	-0.43700	0.53460
C	2.24630	0.19544	-0.28947
C	1.85441	1.15446	-1.21444
C	3.64908	-0.15210	-0.16559
C	2.77914	1.88368	-1.98363
H	0.80025	1.38804	-1.31995
C	4.56255	0.73286	-0.83299
C	4.14505	1.69403	-1.72959
H	2.43246	2.61605	-2.70267
H	5.61783	0.55002	-0.67239
H	4.88392	2.29181	-2.25510
C	4.21975	-1.29083	0.49928
C	3.41095	-2.53918	0.82168
H	3.39799	-2.72612	1.90222
H	2.38714	-2.51298	0.45224
O	5.46387	-1.36608	0.73638
C	1.48624	-0.53031	1.97019
H	1.18120	-1.51848	2.33234
H	2.54354	-0.39708	2.19225
H	0.91705	0.22543	2.52787
H	3.93566	-3.38245	0.36247

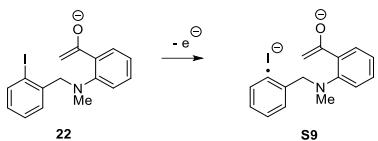


SM (Before SET): 22 in DMSO

34
-760.0540185
C 1.10317 2.95839 -1.21223
C 0.34944 1.81571 -0.97215
C 0.93793 0.63535 -0.51100
C 2.31536 0.65403 -0.29513
C 3.08908 1.78556 -0.52685
C 2.47607 2.94464 -0.99176
H 0.61775 3.85860 -1.56958
H -0.72282 1.82904 -1.13443
H 4.15660 1.76629 -0.34843
H 3.07381 3.82903 -1.17678
I 3.32002 -1.08871 0.43335
C 0.09410 -0.61069 -0.25803
H 0.50511 -1.42861 -0.86055
H 0.20993 -0.91637 0.78614
N -1.30606 -0.48919 -0.57416
C -2.20050 0.03460 0.35991
C -1.71345 0.76590 1.46304
C -3.59808 -0.15726 0.24979
C -2.57206 1.31749 2.40536
H -0.64908 0.93206 1.57414
C -4.43539 0.44762 1.18760
C -3.94905 1.17864 2.26694
H -2.15581 1.87252 3.23881
H -5.50547 0.29998 1.07479
H -4.62828 1.61458 2.98990
C -4.27713 -1.02947 -0.79815
C -4.09119 -2.38033 -0.67816
H -4.55271 -3.06408 -1.38395
H -3.44126 -2.78461 0.08817
O -4.99815 -0.41656 -1.66733
C -1.62969 -0.60499 -1.98951
H -1.73882 -1.64958 -2.29449
H -2.56231 -0.08776 -2.21003
H -0.83169 -0.14374 -2.58152

Prod (After SET): S9 in DMSO

34
-760.1608524
C -0.08793 3.88895 -0.46274
C -0.51017 2.56010 -0.50459
C 0.41306 1.51192 -0.41907
C 1.73347 1.88821 -0.29312
C 2.20806 3.17555 -0.24215
C 1.26180 4.20397 -0.33187
H -0.82136 4.68372 -0.53236
H -1.56625 2.32683 -0.60049
H 3.26496 3.39481 -0.13841
H 1.58291 5.23899 -0.29935
I 4.06952 -1.34618 0.20229
C 0.00211 0.04343 -0.46170
H 0.57196 -0.44550 -1.25831
H 0.30973 -0.44240 0.46822
N -1.40012 -0.20127 -0.70118
C -2.31284 -0.19776 0.35285
C -1.95134 0.36198 1.59611
C -3.60717 -0.75748 0.22363
C -2.84376 0.40830 2.65914
H -0.96769 0.79613 1.72584
C -4.49556 -0.64979 1.29393
C -4.13807 -0.08057 2.51199
H -2.52575 0.84918 3.59757
H -5.48959 -1.06749 1.16352
H -4.84656 -0.03427 3.33042
C -4.10417 -1.54433 -0.98245
C -3.47595 -2.73512 -1.23176
H -3.78464 -3.35557 -2.06743
H -2.62370 -3.04630 -0.64004
O -5.10289 -1.04414 -1.61810
C -1.82033 -0.04486 -2.08653
H -1.67056 -0.96348 -2.66083
H -2.87676 0.21640 -2.13601
H -1.24481 0.76353 -2.55067

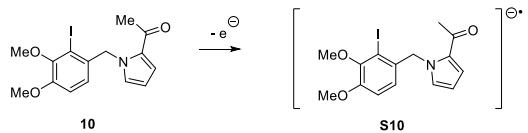


SM (Before SET): 22 in Benzene

	34	-760.0128981	C	1.09738	2.96578	-1.17597
C	0.34622	1.82122	C	0.34622	1.82122	-0.94106
C	0.93858	0.63743	C	0.93858	0.63743	-0.49306
C	2.31605	0.65793	C	2.31605	0.65793	-0.28593
C	3.08877	1.79103	C	3.08877	1.79103	-0.51229
C	2.47170	2.95270	C	2.47170	2.95270	-0.96380
H	0.60754	3.86807	H	0.60754	3.86807	-1.52217
H	-0.72761	1.82968	H	-0.72761	1.82968	-1.09364
H	4.15725	1.76895	H	4.15725	1.76895	-0.33986
H	3.06700	3.83978	H	3.06700	3.83978	-1.14501
I	3.32796	-1.09211	I	3.32796	-1.09211	0.41862
C	0.08851	-0.60794	C	0.08851	-0.60794	-0.24737
H	0.50220	-1.42409	H	0.50220	-1.42409	-0.85135
H	0.20165	-0.91531	H	0.20165	-0.91531	0.79705
N	-1.30407	-0.47543	N	-1.30407	-0.47543	-0.57001
C	-2.20638	0.03111	C	-2.20638	0.03111	0.36981
C	-1.72297	0.74641	C	-1.72297	0.74641	1.48373
C	-3.60158	-0.16744	C	-3.60158	-0.16744	0.25163
C	-2.58537	1.26945	C	-2.58537	1.26945	2.44004
H	-0.65982	0.92174	H	-0.65982	0.92174	1.59618
C	-4.44071	0.40528	C	-4.44071	0.40528	1.20492
C	-3.95935	1.11579	C	-3.95935	1.11579	2.30127
H	-2.17301	1.81163	H	-2.17301	1.81163	3.28422
H	-5.50859	0.25093	H	-5.50859	0.25093	1.08361
H	-4.64240	1.52780	H	-4.64240	1.52780	3.03511
C	-4.27742	-0.98861	C	-4.27742	-0.98861	-0.84479
C	-4.21461	-2.35012	C	-4.21461	-2.35012	-0.69650
H	-4.68783	-3.00029	H	-4.68783	-3.00029	-1.42517
H	-3.69416	-2.79474	H	-3.69416	-2.79474	0.14299
O	-4.85424	-0.31951	O	-4.85424	-0.31951	-1.76686
C	-1.62784	-0.61240	C	-1.62784	-0.61240	-1.98389
H	-1.74306	-1.66224	H	-1.74306	-1.66224	-2.26946
H	-2.55995	-0.09832	H	-2.55995	-0.09832	-2.21427
H	-0.82479	-0.16359	H	-0.82479	-0.16359	-2.58072

Prod (After SET): S9 in Benzene

	34	-760.0619544	C	-0.86869	0.38184	1.54492
C	0.32970	0.07187	C	0.32970	0.07187	0.90057
C	0.32681	-0.45906	C	0.32681	-0.45906	-0.39382
C	-0.91809	-0.64967	C	-0.91809	-0.64967	-0.95517
C	-2.12851	-0.36316	C	-2.12851	-0.36316	-0.37665
C	-2.09366	0.17177	C	-2.09366	0.17177	0.91697
H	-0.84187	0.79127	H	-0.84187	0.79127	2.54825
H	1.28364	0.23667	H	1.28364	0.23667	1.39379
H	-3.08269	-0.53119	H	-3.08269	-0.53119	-0.86614
H	-3.03037	0.41252	H	-3.03037	0.41252	1.40874
I	-6.24127	0.04238	I	-6.24127	0.04238	-0.05047
C	1.60859	-0.79982	C	1.60859	-0.79982	-1.14733
C	1.48547	-1.79534	C	1.48547	-1.79534	-1.59014
H	1.72572	-0.10370	H	1.72572	-0.10370	-1.98266
N	2.81324	-0.80106	N	2.81324	-0.80106	-0.35876
C	3.62290	0.33097	C	3.62290	0.33097	-0.27381
C	3.06359	1.60435	C	3.06359	1.60435	-0.50383
C	5.00123	0.24471	C	5.00123	0.24471	0.03115
C	3.82937	2.75937	C	3.82937	2.75937	-0.40825
H	2.00624	1.69193	H	2.00624	1.69193	-0.72653
C	5.72994	1.42472	C	5.72994	1.42472	0.16718
C	5.17210	2.68091	C	5.17210	2.68091	-0.05339
H	3.36234	3.72167	H	3.36234	3.72167	-0.58969
H	6.78144	1.33329	H	6.78144	1.33329	0.42209
H	5.77515	3.57721	H	5.77515	3.57721	0.03707
C	5.78312	-1.05826	C	5.78312	-1.05826	0.18873
C	6.00580	-1.76452	C	6.00580	-1.76452	-0.96666
H	6.56924	-2.69176	H	6.56924	-2.69176	-0.93897
H	5.60057	-1.42374	H	5.60057	-1.42374	-1.91181
O	6.18349	-1.33379	O	6.18349	-1.33379	1.36947
C	3.00733	-1.97024	C	3.00733	-1.97024	0.48072
C	3.36365	-2.82830	C	3.36365	-2.82830	-0.09903
H	3.74304	-1.76336	H	3.74304	-1.76336	1.25663
H	2.05582	-2.23022	H	2.05582	-2.23022	0.96071

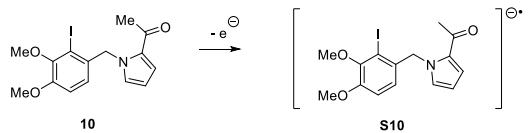


SM (Before SET): 10 in DMSO

36	-872.8836869			
C	-1.96544	0.81152	-0.17338	
C	-1.00435	-0.17946	-0.33007	
C	0.33089	0.12059	-0.62009	
C	0.66733	1.46174	-0.75635	
C	-0.27305	2.47850	-0.60402	
C	-1.59346	2.16234	-0.30995	
H	0.03828	3.50754	-0.71864	
C	1.36737	-0.97159	-0.79597	
H	1.27409	-1.70711	-0.00059	
H	1.21870	-1.48297	-1.75027	
N	2.72664	-0.45207	-0.79760	
C	3.44646	-0.22705	-1.92574	
C	3.43660	0.02575	0.28984	
C	4.64092	0.38430	-1.58873	
H	3.05544	-0.52207	-2.88778	
C	4.63367	0.54343	-0.19054	
H	5.41378	0.97917	0.41478	
H	5.42041	0.67067	-2.27614	
C	2.95885	-0.02559	1.67194	
C	3.87716	0.55722	2.71998	
H	4.03580	1.62139	2.53234	
H	3.42584	0.42273	3.70073	
O	1.87773	-0.50606	1.97463	
H	1.69264	1.73165	-0.98453	
O	-3.26846	0.50309	0.07751	
O	-2.59016	3.06123	-0.14013	
C	-2.25604	4.43827	-0.25500	
H	-3.17922	4.98437	-0.07952	
H	-1.51242	4.72195	0.49416	
H	-1.87907	4.66522	-1.25545	
C	-3.63262	0.64740	1.45495	
H	-3.03436	-0.02908	2.07147	
H	-3.48919	1.67966	1.77950	
H	-4.68415	0.37763	1.52667	
I	-1.65459	-2.19532	-0.12249	
H	4.85148	0.06562	2.69135	

Prod (After SET): S10 in DMSO

36	-872.9563131			
C	-1.95406	0.87453	-0.12500	
C	-1.02696	-0.14850	-0.28420	
C	0.32967	0.09728	-0.51639	
C	0.72813	1.42881	-0.57729	
C	-0.17443	2.47871	-0.41780	
C	-1.51931	2.21108	-0.19171	
H	0.18427	3.49743	-0.47383	
C	1.33257	-1.03389	-0.68542	
H	1.27313	-1.68969	0.18064	
H	1.08008	-1.61098	-1.58079	
N	2.69648	-0.57467	-0.82232	
C	3.19566	-0.14150	-2.04615	
C	3.47685	-0.03921	0.21881	
C	4.31444	0.62370	-1.81418	
H	2.70733	-0.43077	-2.96425	
C	4.50727	0.70451	-0.41376	
H	5.32220	1.19944	0.09157	
H	4.94194	1.06173	-2.57701	
C	3.23826	-0.28433	1.59693	
C	4.13014	0.41778	2.59869	
H	4.57589	1.33454	2.20687	
H	3.54231	0.67184	3.48558	
O	2.36114	-1.12313	2.04097	
H	1.77479	1.65306	-0.75118	
O	-3.27987	0.61410	0.06435	
O	-2.48420	3.14854	-0.02552	
C	-2.08386	4.51101	-0.06516	
H	-2.98760	5.09263	0.09827	
H	-1.35949	4.72788	0.72423	
H	-1.65553	4.76385	-1.03858	
C	-3.68539	0.71142	1.43328	
H	-3.13363	-0.01328	2.03849	
H	-3.51597	1.72229	1.80917	
H	-4.74801	0.47844	1.45977	
I	-1.76334	-2.14690	-0.16581	
H	4.94927	-0.23445	2.93288	



SM (Before SET): 10 in Benzene

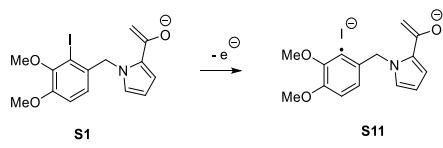
36

-872.8766886

C	-1.97292	0.81331	-0.17019
C	-1.01345	-0.18100	-0.30894
C	0.32712	0.11309	-0.57992
C	0.67237	1.45094	-0.71710
C	-0.26657	2.47152	-0.58061
C	-1.59146	2.16168	-0.30368
H	0.05029	3.49907	-0.69334
C	1.35773	-0.98771	-0.73094
H	1.27974	-1.68663	0.09886
H	1.18542	-1.54055	-1.65799
N	2.71858	-0.47425	-0.78687
C	3.40334	-0.27792	-1.94234
C	3.46552	0.02108	0.26576
C	4.61093	0.33207	-1.65726
H	2.98012	-0.59108	-2.88473
C	4.64932	0.51981	-0.26261
H	5.45092	0.96310	0.30804
H	5.37031	0.59729	-2.37481
C	3.02296	0.00583	1.66335
C	3.98161	0.59203	2.67507
H	4.15495	1.64925	2.46239
H	3.55103	0.48444	3.66832
O	1.94423	-0.44538	2.00314
H	1.70223	1.71478	-0.93136
O	-3.27929	0.50959	0.05750
O	-2.58672	3.06626	-0.14654
C	-2.25187	4.43645	-0.28717
H	-3.17660	4.98700	-0.13324
H	-1.51516	4.73909	0.46247
H	-1.86460	4.64344	-1.28876
C	-3.67247	0.66506	1.42302
H	-3.07928	0.00351	2.06081
H	-3.55023	1.70307	1.73865
H	-4.72185	0.38216	1.47477
I	-1.67454	-2.19187	-0.10688
H	4.94485	0.07987	2.63161

Prod (After SET): S10 in Benzene

36				
-872.9164480				
C	-1.93883	0.89430	-0.14198	
C	-1.02837	-0.14634	-0.28076	
C	0.33373	0.06848	-0.50136	
C	0.75808	1.39113	-0.58105	
C	-0.12685	2.45799	-0.44273	
C	-1.47697	2.21870	-0.21967	
H	0.25337	3.46842	-0.50706	
C	1.32330	-1.08089	-0.62540	
H	1.26605	-1.68677	0.27811	
H	1.05299	-1.69825	-1.48861	
N	2.68731	-0.64301	-0.79768	
C	3.17898	-0.25843	-2.04234	
C	3.47775	-0.07041	0.21705	
C	4.30457	0.50794	-1.84552	
H	2.68593	-0.58313	-2.94574	
C	4.50844	0.64248	-0.45195	
H	5.33087	1.14826	0.02955	
H	4.93075	0.91012	-2.62907	
C	3.23167	-0.25176	1.60295	
C	4.14171	0.48209	2.56841	
H	4.54468	1.40949	2.15262	
H	3.57350	0.71958	3.47174	
O	2.33613	-1.03716	2.08028	
H	1.81102	1.59229	-0.74511	
O	-3.27208	0.66262	0.04544	
O	-2.42640	3.18179	-0.06121	
C	-1.99417	4.52748	-0.11686	
H	-2.88289	5.13545	0.03837	
H	-1.26303	4.73984	0.66893	
H	-1.55776	4.76109	-1.09262	
C	-3.66875	0.76280	1.41204	
H	-3.12420	0.03181	2.01696	
H	-3.48575	1.77169	1.78928	
H	-4.73470	0.54312	1.44322	
I	-1.80096	-2.13112	-0.14322	
H	4.99224	-0.14409	2.87303	

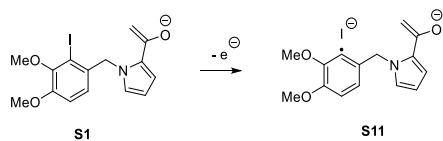


SM (Before SET): S1 in DMSO

	35	-872.3786917	C	-1.91698	0.82802	-0.18954
			C	-0.95730	-0.16843	-0.32191
			C	0.39208	0.12040	-0.55173
			C	0.74493	1.46228	-0.64512
			C	-0.19235	2.48490	-0.51601
			C	-1.52772	2.17678	-0.28699
			H	0.13290	3.51309	-0.59590
			C	1.42824	-0.97997	-0.69660
			H	1.34273	-1.67609	0.13535
			H	1.26609	-1.52389	-1.63125
			N	2.78564	-0.46726	-0.71240
			C	3.46846	-0.15929	-1.86233
			C	3.46148	0.03806	0.37796
			C	4.61472	0.51854	-1.51768
			H	3.07869	-0.45706	-2.82389
			C	4.60953	0.64274	-0.10068
			H	5.37018	1.09744	0.51568
			H	5.37494	0.86331	-2.20182
			C	2.95968	-0.12347	1.78702
			C	3.18411	0.93112	2.63689
			H	3.64783	1.84399	2.28747
			H	2.89139	0.85871	3.67891
			O	2.37921	-1.23468	2.07293
			H	1.78371	1.72167	-0.81818
			O	-3.23265	0.52799	0.00496
			O	-2.52328	3.08368	-0.14482
			C	-2.16929	4.45827	-0.21474
			H	-3.09328	5.01183	-0.06891
			H	-1.45670	4.71718	0.57258
			H	-1.74520	4.70241	-1.19213
			C	-3.64465	0.64846	1.37072
			H	-3.06946	-0.04008	1.99596
			H	-3.51057	1.67441	1.71876
			H	-4.69868	0.38005	1.40153
			I	-1.63264	-2.18307	-0.17108

Prod (After SET): S11 in DMSO

	35	-872.4892911	C	-1.08704	2.26190	0.48439
			C	-0.59231	1.01688	0.77266
			C	0.57883	0.46276	0.29322
			C	1.32010	1.27631	-0.55819
			C	0.88003	2.56415	-0.88929
			C	-0.30999	3.07006	-0.37948
			H	1.48286	3.16636	-1.55556
			C	1.00076	-0.93632	0.69742
			H	1.34685	-0.94295	1.73038
			H	0.14309	-1.60658	0.60349
			N	2.07512	-1.45586	-0.13124
			C	1.85342	-2.02077	-1.36116
			C	3.42374	-1.22689	0.03762
			C	3.06687	-2.19378	-1.98578
			H	0.84626	-2.24836	-1.67841
			C	4.06025	-1.69210	-1.09948
			H	5.12896	-1.69250	-1.25149
			H	3.22154	-2.64817	-2.95272
			C	3.99995	-0.61683	1.28684
			C	5.06190	0.23620	1.11274
			H	5.42040	0.49084	0.12417
			H	5.55810	0.66690	1.97583
			O	3.46246	-0.95858	2.40414
			H	2.25171	0.90642	-0.97486
			O	-2.25114	2.76706	0.95720
			O	-0.81554	4.30073	-0.64774
			C	-0.06587	5.13610	-1.51674
			H	-0.62683	6.06369	-1.59953
			H	0.92458	5.34212	-1.10195
			H	0.03792	4.67983	-2.50488
			C	-2.98887	1.89200	1.80588
			H	-3.26059	0.97670	1.27288
			H	-2.40129	1.63295	2.69137
			H	-3.88254	2.43726	2.09982
			I	-2.92630	-2.09972	-0.18627



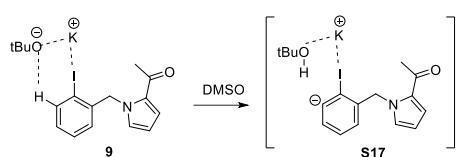
SM (Before SET): S1 in Benzene

	35	-872.3354944	C	-1.94488	0.84280	-0.19539
C	-0.99372	-0.16696	C	-0.26785		
C	0.37014	0.09720	C	-0.42698		
C	0.74922	1.43234	C	-0.50621		
C	-0.17846	2.46843	C	-0.42933		
C	-1.52805	2.18264	C	-0.27283		
H	0.16959	3.49066	H	-0.48625		
C	1.39519	-1.02021	C	-0.48772		
H	1.38430	-1.57867	C	0.44930		
H	1.15657	-1.69539	C	-1.31416		
N	2.74413	-0.53057	C	-0.69210		
C	3.28580	-0.31500	C	-1.93487		
C	3.56030	0.01740	C	0.27489		
C	4.48057	0.34770	C	-1.77566		
H	2.77368	-0.65922	C	-2.82051		
C	4.65393	0.55489	C	-0.37954		
H	5.49516	1.01775	C	0.11279		
H	5.15896	0.62460	C	-2.56826		
C	3.22070	-0.04045	C	1.74449		
C	3.62733	1.03658	C	2.49537		
H	4.11390	1.88880	C	2.03972		
H	3.45416	1.03984	C	3.56546		
O	2.59592	-1.08077	C	2.14812		
H	1.80078	1.67308	C	-0.61590		
O	-3.27549	0.56453	C	-0.07377		
O	-2.51772	3.11109	C	-0.18109		
C	-2.13042	4.47174	C	-0.21882		
H	-3.04791	5.04767	C	-0.12022		
H	-1.45523	4.71151	C	0.60782		
H	-1.64612	4.71706	C	-1.16856		
C	-3.75468	0.68712	C	1.26515		
H	-3.21720	-0.00298	C	1.92210		
H	-3.63401	1.71283	C	1.62066		
H	-4.81088	0.42407	C	1.24176		
I	-1.70197	-2.17045	C	-0.11463		

Prod (After SET): S11 in Benzene

	35	-872.3823971	C	-0.66226	2.34181	0.15912
C	-0.29479	1.08633	C	-0.25676	-0.25676	
C	-1.11607	0.13163	C	-0.81844	-0.81844	
C	-2.45258	0.49501	C	-0.97132	-0.97132	
C	-2.89642	1.75859	C	-0.56768	-0.56768	
C	-2.02207	2.68372	C	-0.00536	-0.00536	
H	-3.94198	2.00612	C	-0.69165	-0.69165	
C	-0.61422	-1.24545	C	-1.19209	-1.19209	
H	-1.19921	-1.64088	C	-2.01953	-2.01953	
H	0.44457	-1.19685	C	-1.45339	-1.45339	
N	-0.73706	-2.17794	C	-0.07427	-0.07427	
C	0.27922	-2.40499	C	0.81608	0.81608	
C	-1.89377	-2.78561	C	0.36429	0.36429	
C	-0.20798	-3.19900	C	1.83032	1.83032	
H	1.25711	-1.97364	C	0.64788	0.64788	
C	-1.57900	-3.44112	C	1.54236	1.54236	
H	-2.26957	-4.04914	C	2.10688	2.10688	
H	0.36415	-3.57297	C	2.66585	2.66585	
C	-3.19876	-2.71626	C	-0.38875	-0.38875	
C	-4.34173	-2.72148	C	0.37811	0.37811	
H	-4.29572	-2.71453	C	1.45893	1.45893	
H	-5.31119	-2.72091	C	-0.10827	-0.10827	
O	-3.13496	-2.65714	C	-1.66642	-1.66642	
H	-3.14517	-0.22981	C	-1.38944	-1.38944	
O	0.17372	3.25558	C	0.70842	0.70842	
O	-2.37362	3.93256	C	0.41790	0.41790	
C	-3.73681	4.28309	C	0.31466	0.31466	
H	-3.82144	5.29088	C	0.71705	0.71705	
H	-4.07091	4.27749	C	-0.72784	-0.72784	
H	-4.36556	3.60287	C	0.89792	0.89792	
C	1.52033	2.80974	C	0.85166	0.85166	
H	1.56930	1.91590	C	1.47928	1.47928	
H	1.95979	2.56674	C	-0.11891	-0.11891	
H	2.06331	3.62882	C	1.31886	1.31886	
I	3.99816	-0.16318	C	-0.23170	-0.23170	

3. Benzyne Pathway



SM: 9 + KOtBu in DMSO

43

-1476.8731516

C	-0.67449	2.75628	-0.42616
C	-1.68164	1.81817	-0.62197
C	-1.39262	0.45361	-0.70260
C	-0.05554	0.07237	-0.58163
C	0.96975	0.98965	-0.38285
C	0.64685	2.34278	-0.30475
H	-0.92600	3.80848	-0.36862
H	-2.71107	2.14809	-0.71349
H	2.00837	0.65795	-0.28937
H	1.43645	3.07000	-0.15135
C	-2.49906	-0.55905	-0.93123
H	-2.47909	-0.89888	-1.96957
H	-2.34912	-1.44269	-0.31481
N	-3.82555	-0.01266	-0.68849
C	-4.62598	0.41655	-1.70131
C	-4.38399	0.38682	0.51857
C	-5.72180	1.07063	-1.17247
H	-4.34972	0.22617	-2.72739
C	-5.56523	1.05376	0.22518
H	-6.23590	1.45524	0.96863
H	-6.53550	1.49708	-1.73682
C	-3.88226	0.14553	1.88227
C	-2.72383	-0.78564	2.14624
H	-1.80096	-0.39684	1.70817
H	-2.59613	-0.87129	3.22352
O	-4.44374	0.69664	2.81558
I	0.49833	-1.99167	-0.70851
H	-2.91543	-1.77471	1.72470
O	3.97600	-0.00846	0.09901
C	4.78869	1.06840	-0.18692
C	4.61798	2.16699	0.88532
H	5.22619	3.05600	0.68518
H	3.56646	2.46944	0.93286
H	4.90153	1.77030	1.86619
C	4.44064	1.67882	-1.56113
H	3.40146	2.02203	-1.56734
H	5.08365	2.52809	-1.81720
H	4.55037	0.91541	-2.33766
C	6.27323	0.65075	-0.21287
H	6.94185	1.49140	-0.42952
H	6.55258	0.22707	0.75697
H	6.42503	-0.11759	-0.97736
K	2.93316	-0.84513	2.17672

TS: 9 + KOtBu in DMSO

43

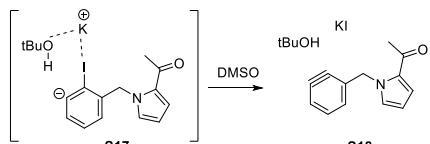
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C	-0.52224	2.72389	-0.54108
C	-1.53972	1.79061	-0.72195
C	-1.25405	0.42414	-0.72744
C	0.08793	0.07162	-0.54975
C	1.14740	0.93524	-0.36031
C	0.78910	2.29653	-0.36000
H	-0.76292	3.78184	-0.53931
H	-2.56392	2.12282	-0.85666
H	2.51379	0.52719	-0.19922
H	1.56277	3.04834	-0.21566
C	-2.35862	-0.59586	-0.92768
H	-2.31732	-0.99635	-1.94345
H	-2.22836	-1.44249	-0.25805
N	-3.69120	-0.03583	-0.74796
C	-4.46948	0.33113	-1.80031
C	-4.28216	0.42043	0.42199
C	-5.58392	1.00248	-1.33364
H	-4.16682	0.08811	-2.80766
C	-5.46182	1.06037	0.06609
H	-6.15325	1.49401	0.77160
H	-6.38694	1.38972	-1.93995
C	-3.80946	0.25797	1.80710
C	-2.64847	-0.64533	2.14670
H	-1.72169	-0.27882	1.69754
H	-2.53798	-0.66362	3.22909
O	-4.39732	0.85143	2.69792
I	0.57181	-2.07649	-0.56551
H	-2.82785	-1.65986	1.78409
O	3.60719	0.11525	0.03548
C	4.61365	1.06354	-0.23121
C	4.58927	2.16580	0.83757
H	5.35015	2.92960	0.65160
H	3.60936	2.65208	0.85409
H	4.77406	1.73249	1.82533
C	4.40404	1.68981	-1.61688
H	3.44552	2.21420	-1.65906
H	5.19889	2.40309	-1.85310
H	4.40028	0.90774	-2.38134
C	5.96659	0.35026	-0.19466
H	6.78972	1.04655	-0.38075
H	6.11734	-0.11223	0.78469
H	5.99549	-0.43468	-0.95512
K	2.40816	-0.53864	2.22339

Prod: S17 + K⁺ + HOtBu in DMSO

43

-1476.8579160
 C -0.50431 2.73422 -0.08616
 C -1.52135 1.84009 -0.41436
 C -1.24270 0.47995 -0.55945
 C 0.09188 0.11051 -0.36154
 C 1.15585 0.91444 -0.03740
 C 0.79612 2.27379 0.09865
 H -0.73729 3.78859 0.02362
 H -2.53614 2.19747 -0.55568
 H 2.84821 0.41511 -0.14661
 H 1.56262 3.00514 0.35296
 C -2.33688 -0.50437 -0.92366
 H -2.20800 -0.83940 -1.95567
 H -2.27851 -1.39632 -0.30394
 N -3.67492 0.06446 -0.83006
 C -4.33462 0.53573 -1.92056
 C -4.39160 0.41133 0.30688
 C -5.49456 1.16994 -1.51645
 H -3.92396 0.38612 -2.90779
 C -5.52697 1.09203 -0.11321
 H -6.28985 1.46580 0.55147
 H -6.22642 1.62117 -2.16711
 C -4.06782 0.12770 1.71493
 C -2.90834 -0.75888 2.09970
 H -1.96154 -0.35267 1.73580
 H -2.87951 -0.82785 3.18527
 O -4.77681 0.61019 2.58451
 I 0.54823 -2.06175 -0.61945
 H -3.03573 -1.75924 1.67916
 O 3.80621 0.04365 -0.11275
 C 4.73168 1.11415 -0.28104
 C 4.69866 2.01978 0.95350
 H 5.38799 2.86088 0.84307
 H 3.69049 2.41705 1.10262
 H 4.98771 1.45519 1.84455
 C 4.36954 1.91915 -1.53118
 H 3.37695 2.36456 -1.42114
 H 5.09349 2.72069 -1.69890
 H 4.36164 1.26697 -2.40819
 C 6.11080 0.48418 -0.43720
 H 6.87741 1.25411 -0.55519
 H 6.35293 -0.11597 0.44356
 H 6.12977 -0.16466 -1.31618
 K 2.53097 -0.73445 2.13646



TS (Cl bond cleavage): S17 in DMSO

43

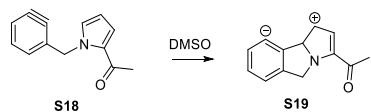
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 C 1.32378 -0.61631 -0.82083
 C -0.03715 -0.48877 -0.64475
 C -1.00144 -1.30853 -0.51639
 C -0.67053 -2.67785 -0.54749
 H 0.99433 -4.02208 -0.75115
 H 2.69412 -2.25932 -0.98211
 H -2.90698 -0.48009 -0.42882
 H -1.40677 -3.46828 -0.44441
 C 2.33776 0.48939 -0.97154
 H 2.30495 0.88310 -1.98951
 H 2.08855 1.31720 -0.31312
 N 3.69712 0.02810 -0.73161
 C 4.55034 -0.26881 -1.74853
 C 4.25690 -0.41066 0.46044
 C 5.68139 -0.87312 -1.23443
 C 4.28330 -0.02947 -2.76681
 C 5.49222 -0.96526 0.15640
 H 6.17570 -1.36363 0.88991
 H 6.53935 -1.19356 -1.80357
 C 3.70880 -0.29035 1.82195
 C 2.50766 0.57634 2.11400
 H 1.60802 0.17592 1.63908
 H 2.35939 0.59973 3.19178
 O 4.26904 -0.88144 2.73146
 I -0.66366 2.37522 -0.51458
 H 2.66250 1.59263 1.74526
 O -3.72955 -0.12639 -0.04063
 C -4.73027 -1.15655 -0.12646
 C -4.41771 -2.24989 0.89422
 H -5.14509 -3.06220 0.82533
 H -3.42108 -2.66363 0.71566
 H -4.45208 -1.84529 1.90913
 C -4.73453 -1.72829 -1.54180
 H -3.76897 -2.19222 -1.76736
 H -5.51178 -2.48805 -1.64933
 H -4.91771 -0.93434 -2.26933
 C -6.05433 -0.47897 0.19460
 H -6.86821 -1.20690 0.17673
 H -6.01391 -0.02620 1.18811
 H -6.26593 0.30236 -0.53848
 K -2.06962 0.46462 2.04148

Prod (Cl bond cleavage): **S18** + KI + H₂OtBu in DMSO

43

-1476.8508356

C	1.95681	1.64693	2.74714
C	2.34921	0.67198	1.81448
C	1.49113	-0.35613	1.37667
C	0.26539	-0.20509	1.99851
C	-0.11765	0.63909	2.82883
C	0.67559	1.67264	3.31746
H	2.67497	2.40664	3.03695
H	3.35941	0.70659	1.41525
H	-1.64835	0.82110	0.52838
H	0.37825	2.42450	4.03705
C	1.90704	-1.45420	0.43048
H	2.18902	-2.33964	1.00431
H	1.06901	-1.74501	-0.19890
N	3.06686	-1.07626	-0.36658
C	4.33036	-1.45848	-0.03111
C	3.14780	-0.06716	-1.31459
C	5.23943	-0.73623	-0.77870
H	4.48443	-2.21166	0.72689
C	4.49165	0.14580	-1.58244
H	4.86262	0.84557	-2.31524
H	6.31144	-0.84808	-0.74908
C	2.03504	0.60894	-2.00082
C	0.65102	0.00968	-1.99786
H	0.18049	0.10610	-1.01451
H	0.04385	0.54951	-2.72372
O	2.26053	1.63812	-2.61732
I	-1.86645	-2.31136	0.38187
H	0.68193	-1.05162	-2.25433
O	-2.07256	1.32339	-0.18223
C	-1.75013	2.72198	-0.05807
C	-0.23848	2.90823	-0.16790
H	0.02674	3.95742	-0.01574
H	0.28109	2.31282	0.58941
H	0.11449	2.60354	-1.15559
C	-2.27466	3.24316	1.27706
H	-1.78323	2.73118	2.10843
H	-2.08049	4.31395	1.37213
H	-3.35148	3.07460	1.34934
C	-2.46157	3.40051	-1.22038
H	-2.26638	4.47458	-1.20795
H	-2.10383	2.99615	-2.17100
H	-3.54078	3.24316	-1.15067
K	-3.37479	-0.17776	-1.91160



SM: S18 in DMSO

26	-631.7536745			
C	-3.01287	-1.27646	-0.51769	
C	-1.85308	-1.13014	0.26223	
C	-1.37796	0.11691	0.70491	
C	-2.21787	1.13823	0.26880	
C	-3.23298	0.97641	-0.42418	
C	-3.79910	-0.18186	-0.91685	
H	-3.31741	-2.27149	-0.82319	
H	-1.30519	-2.02401	0.54265	
H	-4.69391	-0.28250	-1.51428	
C	-0.12786	0.29048	1.52861	
H	-0.30079	1.00745	2.33102	
H	0.16472	-0.65277	1.98126	
N	0.96869	0.81642	0.71169	
C	1.06354	2.15168	0.45138	
C	1.71814	0.13084	-0.23404	
C	1.90419	2.34983	-0.62395	
H	0.50515	2.85940	1.04563	
C	2.31083	1.07228	-1.06023	
H	3.00823	0.83645	-1.84914	
H	2.20151	3.30468	-1.02709	
C	2.01950	-1.30928	-0.26887	
C	1.91824	-2.14882	0.98423	
H	0.91164	-2.56216	1.08422	
H	2.61058	-2.98354	0.88577	
O	2.42566	-1.80643	-1.30577	
H	2.15301	-1.57574	1.88144	

TS: S18 in DMSO

26

-631.7310143

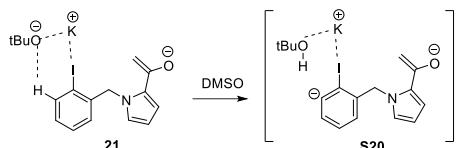
C	-3.51929	-1.07893	-0.61996
C	-2.35453	-1.61168	-0.04649
C	-1.34671	-0.75188	0.37484
C	-1.62566	0.59220	0.16395
C	-2.66950	1.16721	-0.33876
C	-3.69214	0.30019	-0.77411
H	-4.29982	-1.75685	-0.95086
H	-2.23820	-2.68446	0.06542
H	-4.61227	0.66726	-1.21986
C	-0.01640	-1.06931	1.01909
H	-0.12167	-1.30425	2.08064
H	0.49908	-1.88785	0.52409
N	0.72969	0.18819	0.86528
C	-0.03795	1.35344	1.01324
C	1.71981	0.43397	-0.02912
C	0.62150	2.36790	0.28215
H	-0.56613	1.50387	1.94721
C	1.69337	1.79030	-0.38068
H	2.40791	2.26471	-1.03444
H	0.32257	3.40500	0.26071
C	2.73885	-0.54281	-0.49987
C	3.02939	-1.78066	0.31007
H	2.52398	-2.63653	-0.14582
H	4.10166	-1.96839	0.26587
O	3.36522	-0.28125	-1.50540
H	2.70892	-1.68938	1.34713

Prod: S19 in DMSO

26

-631.7485995

C	-3.66122	-0.98075	-0.55156
C	-2.47591	-1.63265	-0.20195
C	-1.41511	-0.83381	0.19083
C	-1.56600	0.56068	0.22648
C	-2.71139	1.28523	-0.09927
C	-3.75646	0.41513	-0.50187
H	-4.51535	-1.57149	-0.87014
H	-2.38882	-2.71264	-0.24388
H	-4.71613	0.84028	-0.79659
C	-0.02704	-1.27683	0.61276
H	0.00453	-1.70057	1.61956
H	0.44684	-1.96145	-0.08741
N	0.67351	0.02484	0.60782
C	-0.25746	1.14055	0.77759
C	1.77477	0.43365	0.05036
C	0.48856	2.27750	0.19235
H	-0.36794	1.32911	1.85877
C	1.71593	1.85951	-0.18393
H	2.52673	2.42944	-0.60952
H	0.10216	3.28605	0.16309
C	2.94532	-0.44429	-0.35214
C	3.13576	-1.77356	0.31330
H	2.64342	-2.54486	-0.28609
H	4.20092	-1.99700	0.34013
O	3.68678	0.00498	-1.18741
H	2.71636	-1.79277	1.31883



SM: 21 + KOtBu in DMSO

42

-1476.3702982

C	0.68359	-2.62655	-0.97128
C	1.70437	-1.68371	-0.97059
C	1.43337	-0.31930	-0.83165
C	0.09609	0.05300	-0.69931
C	-0.94507	-0.86901	-0.68538
C	-0.63831	-2.22067	-0.82392
H	0.92304	-3.67753	-1.08137
H	2.73666	-2.00311	-1.07055
H	-1.98133	-0.54777	-0.55257
H	-1.43982	-2.95108	-0.81554
C	2.56298	0.69262	-0.84567
H	2.63537	1.15305	-1.83497
H	2.35528	1.48250	-0.12998
N	3.85231	0.09288	-0.54985
C	4.76621	-0.22625	-1.52606
C	4.21082	-0.52117	0.63439
C	5.73829	-1.02215	-0.96843
H	4.63828	0.14041	-2.53301
C	5.38079	-1.21451	0.39431
H	5.92300	-1.77898	1.13743
H	6.60662	-1.41004	-1.47845
C	3.44274	-0.44173	1.92999
C	2.97081	0.78527	2.32836
H	2.43121	0.87857	3.26489
O	3.33158	-1.54788	2.57103
I	-0.43935	2.12085	-0.51434
H	3.18785	1.68696	1.77094
O	-3.93315	0.01263	0.18001
C	-4.74781	-1.03392	-0.19771
C	-4.46074	-2.27700	0.67273
H	-5.06771	-3.14442	0.39067
H	-3.40387	-2.54915	0.58248
H	-4.66161	-2.04383	1.72388
C	-4.51571	-1.41899	-1.67481
H	-3.47603	-1.72574	-1.82531
H	-5.16525	-2.23940	-1.99909
H	-4.70885	-0.55132	-2.31362
C	-6.23648	-0.66607	-0.03225
H	-6.90501	-1.48625	-0.31683
H	-6.43608	-0.40387	1.01148
H	-6.47186	0.20365	-0.65359
K	-2.59283	0.53974	2.18040

TS: 21 + KOtBu in DMSO

42

-1476.3517258

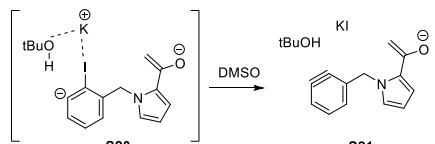
C	0.55168	-2.65323	-0.71792
C	1.56919	-1.70605	-0.79970
C	1.27995	-0.34296	-0.71019
C	-0.06974	-0.01448	-0.54975
C	-1.13193	-0.88881	-0.45076
C	-0.76687	-2.24569	-0.53944
H	0.79725	-3.70800	-0.78777
H	2.60068	-2.01958	-0.92370
H	-2.51040	-0.49049	-0.25878
H	-1.53983	-3.00906	-0.46790
C	2.38330	0.69356	-0.80107
H	2.33513	1.20361	-1.76734
H	2.24009	1.44440	-0.02964
N	3.71402	0.12199	-0.68029
C	4.48643	-0.18510	-1.77433
C	4.25535	-0.46911	0.44405
C	5.54995	-0.95026	-1.35742
H	4.20376	0.16524	-2.75520
C	5.39710	-1.13583	0.04389
H	6.05176	-1.68099	0.70671
H	6.34520	-1.32147	-1.98547
C	3.68276	-0.40183	1.83750
C	3.24454	0.81446	2.30163
H	2.84262	0.89768	3.30576
O	3.69667	-1.50793	2.48898
I	-0.56783	2.13476	-0.44844
H	3.35130	1.71857	1.71697
O	-3.59238	-0.10225	0.02022
C	-4.59252	-1.05037	-0.27263
C	-4.52512	-2.20784	0.73420
H	-5.28184	-2.97063	0.52834
H	-3.53937	-2.68066	0.69586
H	-4.68707	-1.83040	1.74848
C	-4.40884	-1.59786	-1.69465
H	-3.44363	-2.10303	-1.78792
H	-5.19851	-2.31070	-1.94904
H	-4.43647	-0.77622	-2.41587
C	-5.95300	-0.35953	-0.16448
H	-6.77136	-1.05695	-0.36680
H	-6.08521	0.04905	0.84110
H	-6.01178	0.46377	-0.88135
K	-2.30070	0.37402	2.21663

Prod: S20 + K⁺ + HOtBu in DMSO

42

-1476.3532145

C	-0.51262	2.70532	-0.21595
C	-1.53955	1.78997	-0.44011
C	-1.26108	0.42484	-0.53063
C	0.08612	0.07854	-0.38538
C	1.16093	0.89925	-0.15651
C	0.79967	2.26287	-0.07426
H	-0.74703	3.76339	-0.15080
H	-2.56534	2.12942	-0.54199
H	2.83792	0.40189	-0.19328
H	1.57276	3.01039	0.10169
C	-2.36511	-0.58666	-0.77601
H	-2.22059	-1.06521	-1.74821
H	-2.31566	-1.36437	-0.01818
N	-3.69362	0.00253	-0.77410
C	-4.27323	0.49701	-1.91780
C	-4.39175	0.45907	0.32673
C	-5.36838	1.24850	-1.56402
H	-3.84527	0.27525	-2.88363
C	-5.43688	1.23008	-0.14382
H	-6.17849	1.70383	0.48114
H	-6.04437	1.74043	-2.24658
C	-4.06604	0.15794	1.76787
C	-3.75863	-1.13701	2.10673
H	-3.54320	-1.38866	3.13982
O	-4.15302	1.15691	2.56943
I	0.54516	-2.10920	-0.57079
H	-3.79208	-1.93775	1.37954
O	3.80017	0.03678	-0.09466
C	4.72921	1.10397	-0.25684
C	4.63103	2.05819	0.93732
H	5.31689	2.90189	0.82473
H	3.61341	2.44949	1.02510
H	4.88522	1.53337	1.86273
C	4.43037	1.85757	-1.55497
H	3.43146	2.30056	-1.51490
H	5.15903	2.65608	-1.71682
H	4.47077	1.17091	-2.40433
C	6.11770	0.47753	-0.31575
H	6.88609	1.24717	-0.42450
H	6.31567	-0.08459	0.60041
H	6.18584	-0.20644	-1.16511
K	2.44586	-0.64099	2.13820



TS (Cl bond cleavage): S20 in DMSO

42

-1476.3437007

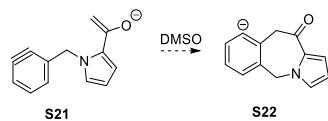
C	0.68858	-2.87018	-0.73413
C	1.66660	-1.87105	-0.81957
C	1.34422	-0.50676	-0.73441
C	-0.01851	-0.37650	-0.57039
C	-1.00517	-1.19029	-0.47857
C	-0.65957	-2.55723	-0.55930
H	0.99428	-3.90887	-0.80368
H	2.71125	-2.14191	-0.94469
H	-2.87983	-0.46875	-0.39995
H	-1.39961	-3.34921	-0.49049
C	2.36860	0.59646	-0.82866
H	2.29673	1.08048	-1.80582
H	2.15047	1.34758	-0.07630
N	3.72610	0.10223	-0.67983
C	4.53300	-0.16739	-1.75967
C	4.27403	-0.46333	0.45544
C	5.62355	-0.88022	-1.32208
H	4.25249	0.16997	-2.74564
C	5.45343	-1.07393	0.07628
H	6.12230	-1.58611	0.75105
H	6.44840	-1.21128	-1.93427
C	3.67382	-0.42072	1.83806
C	3.15088	0.76905	2.28244
H	2.72904	0.83562	3.27953
O	3.74648	-1.51800	2.50019
I	-0.64425	2.39373	-0.43926
H	3.20926	1.67300	1.69076
O	-3.74228	-0.13029	-0.07759
C	-4.70014	-1.19353	-0.20824
C	-4.42053	-2.25839	0.85206
H	-5.12057	-3.09208	0.75851
H	-3.40424	-2.64720	0.74071
H	-4.52649	-1.83383	1.85387
C	-4.59327	-1.79257	-1.60896
H	-3.60047	-2.22756	-1.76105
H	-5.33818	-2.57902	-1.75000
H	-4.75350	-1.01893	-2.36346
C	-6.06641	-0.55964	0.01030
H	-6.85162	-1.31611	-0.05493
H	-6.11329	-0.09356	0.99739
H	-6.25273	0.20506	-0.74699
K	-2.13279	0.45596	2.05898

Prod (Cl bond cleavage): **S21** + KI + HOtBu in DMSO

42

-1476.3410468

C	-1.31533	3.15966	-1.08685
C	-2.08264	1.98407	-1.09054
C	-1.51779	0.69785	-0.97151
C	-0.15252	0.84781	-0.85559
C	0.58659	1.85261	-0.85553
C	0.08280	3.14927	-0.95546
H	-1.82643	4.11227	-1.18034
H	-3.16459	2.05631	-1.16956
H	2.65914	0.29967	-0.39226
H	0.66777	4.06065	-0.94821
C	-2.32659	-0.57271	-0.96589
H	-2.40483	-0.96310	-1.98351
H	-1.81176	-1.31835	-0.36838
N	-3.68451	-0.34628	-0.49075
C	-4.75456	-0.25123	-1.34911
C	-4.05062	0.13501	0.75170
C	-5.82678	0.25807	-0.65697
H	-4.65279	-0.55142	-2.38074
C	-5.37612	0.51296	0.66750
H	-5.95389	0.90552	1.49037
H	-6.81653	0.41988	-1.05566
C	-3.16469	0.21046	1.96847
C	-2.33032	-0.84763	2.23344
H	-1.70034	-0.82803	3.11682
O	-3.31269	1.26334	2.68784
I	1.07399	-2.34724	-0.74223
H	-2.32218	-1.73727	1.61820
O	3.40997	0.28277	0.21855
C	4.23240	1.44818	0.02346
C	3.64926	2.61707	0.81392
H	4.25161	3.51669	0.66733
H	2.62702	2.82301	0.48999
H	3.63195	2.37865	1.88039
C	4.29692	1.77372	-1.46572
H	3.30117	2.02075	-1.84709
H	4.95227	2.62939	-1.64128
H	4.68286	0.91748	-2.02388
C	5.60722	1.07167	0.56025
H	6.28803	1.92282	0.49182
H	5.53120	0.77200	1.60825
H	6.02381	0.24059	-0.01255
K	2.14658	-0.92103	2.24050



SM: S21 in DMSO

25

C	3.32120	-0.97214	-0.60505
C	2.18469	-1.44545	0.07174
C	1.20448	-0.57879	0.59012
C	1.58129	0.71539	0.31525
C	2.55163	1.22889	-0.28925
C	3.54856	0.39469	-0.81340
H	4.03949	-1.69206	-0.98328
H	2.04995	-2.51493	0.20367
H	4.42771	0.73969	-1.34526
C	-0.03663	-1.04047	1.29924
H	0.04744	-2.10396	1.52074
H	-0.14510	-0.50902	2.24273
N	-1.23637	-0.87408	0.47916
C	-1.95587	-1.94860	0.01793
C	-1.70911	0.28119	-0.11494
C	-2.91062	-1.49417	-0.86102
H	-1.71456	-2.94720	0.34797
C	-2.74564	-0.08723	-0.95155
H	-3.32446	0.60434	-1.54403
H	-3.63756	-2.10432	-1.37444
C	-1.20868	1.68149	0.11585
C	-0.79957	2.03543	1.38811
H	-0.44727	3.04416	1.57094
O	-1.23241	2.45014	-0.90092
H	-0.93594	1.37936	2.23601

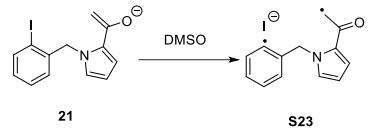
Prod: S22 in DMSO

25

-631.3484140
C 3.23835 -1.07105 -0.69639
C 2.09876 -1.58257 -0.08121
C 1.16739 -0.69727 0.45654
C 1.39006 0.68878 0.37501
C 2.52023 1.26777 -0.24261
C 3.42291 0.31240 -0.76558
H 3.97358 -1.75100 -1.11856
H 1.93088 -2.65360 -0.01922
H 4.33254 0.65638 -1.26032
C -0.07880 -1.22839 1.12099
H -0.05025 -2.31626 1.17857
H -0.17689 -0.84396 2.14044
N -1.29650 -0.88355 0.37603
C -2.22725 -1.79045 -0.00959
C -1.67566 0.36705 -0.07775
C -3.22802 -1.14234 -0.71593
H -2.10783 -2.83368 0.23969
C -2.87714 0.21831 -0.75988
H -3.42016 1.02586 -1.22583
H -4.09962 -1.60987 -1.14567
C -0.94095 1.61902 0.14497
C 0.32176 1.59748 0.97667
H 0.69892 2.61716 1.02257
O -1.35597 2.65785 -0.34837
H 0.05216 1.27856 1.99160

4. Intramolecular Analysis of 9

4.1 Franck-Condon



SM: Singlet **21** in DMSO

27

-643.3534550

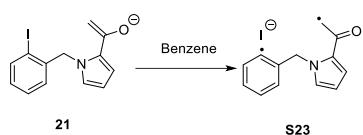
C	-0.19425	3.13096	0.61929
C	0.48823	2.02604	0.12417
C	-0.17065	0.82197	-0.13440
C	-1.54035	0.77040	0.12501
C	-2.24063	1.86417	0.62054
C	-1.56008	3.05215	0.86780
H	0.34214	4.05208	0.81267
H	1.55519	2.08559	-0.06185
H	-3.30395	1.79408	0.81225
H	-2.10092	3.90756	1.25428
C	0.57985	-0.38393	-0.66900
H	0.45527	-1.22759	0.01110
H	0.15768	-0.67123	-1.63589
N	1.99662	-0.15003	-0.85390
C	3.03294	-0.41830	0.02340
C	2.50025	0.40213	-2.00579
C	4.20111	-0.03457	-0.61027
C	3.86647	0.49223	-1.88521
H	1.83713	0.67086	-2.81415
H	5.18521	-0.13959	-0.18118
H	4.54178	0.88030	-2.63237
C	2.94054	-1.03489	1.39655
C	1.83748	-0.79698	2.18125
H	1.03721	-0.13556	1.88257
H	1.79595	-1.22761	3.17605
O	3.96816	-1.72501	1.73723
I	-2.63528	-1.02805	-0.23517

Prod: Triplet **S23** in DMSO

27

-643.3070148

C	2.42454	3.05870	0.83435
C	2.28273	1.82170	0.20566
C	1.09848	1.50018	-0.46580
C	0.11395	2.46484	-0.45441
C	0.19652	3.69455	0.14834
C	1.39428	3.99435	0.80913
H	3.34805	3.29000	1.35130
H	3.08975	1.09637	0.24306
H	-0.62220	4.40440	0.12339
H	1.51234	4.95172	1.30327
C	0.86947	0.17649	-1.16622
H	-0.13084	-0.19307	-0.93372
H	0.91288	0.32288	-2.24735
N	1.85465	-0.83846	-0.82632
C	1.81153	-1.76805	0.19707
C	2.99442	-1.03203	-1.54831
C	2.95086	-2.55063	0.09671
C	3.70442	-2.07991	-0.99891
H	3.20115	-0.41299	-2.40814
H	3.19419	-3.36141	0.76529
H	4.64872	-2.45882	-1.35611
C	0.77051	-1.92585	1.23569
C	-0.03840	-0.82219	1.67093
H	0.11150	0.19425	1.34130
H	-0.77012	-1.01916	2.44174
O	0.65136	-3.02987	1.78868
I	-3.02129	-0.29998	-0.23650



SM: Singlet **21** in Benzene

27

-643.3105041

C	-0.18927	3.12100	0.58735
C	0.49230	1.99629	0.14022
C	-0.17445	0.79333	-0.10569
C	-1.54954	0.76710	0.12079
C	-2.25060	1.88075	0.56826
C	-1.56227	3.06648	0.80074
H	0.35526	4.03859	0.77510
H	1.56565	2.03159	-0.01283
H	-3.31885	1.82497	0.73552
H	-2.10197	3.93845	1.15088
C	0.58125	-0.43302	-0.58425
H	0.50250	-1.22551	0.16299
H	0.12667	-0.79352	-1.51161
N	1.98102	-0.18229	-0.83945
C	3.05754	-0.40393	0.00198
C	2.42373	0.34838	-2.02815
C	4.18879	-0.01507	-0.68964
C	3.79149	0.46851	-1.96399
H	1.72174	0.57987	-2.81500
H	5.18798	-0.09880	-0.29290
H	4.42795	0.84543	-2.75009
C	3.03648	-0.99100	1.39692
C	1.96210	-0.72292	2.21838
H	1.16782	-0.04471	1.94020
H	1.96845	-1.11297	3.22993
O	4.07214	-1.66778	1.69508
I	-2.65835	-1.03058	-0.20895

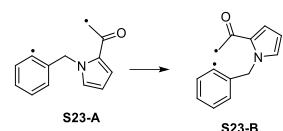
Prod: Triplet **S23** in Benzene

27

-643.2687235

C	1.16950	3.39675	0.96605
C	1.49399	2.21879	0.29350
C	0.51780	1.52400	-0.42800
C	-0.75127	2.06461	-0.42530
C	-1.12255	3.21392	0.22743
C	-0.12885	3.89809	0.93617
H	1.93723	3.91958	1.52432
H	2.50661	1.82870	0.33847
H	-2.14585	3.57132	0.20720
H	-0.37480	4.80916	1.47031
C	0.79712	0.23558	-1.17405
H	0.00713	-0.48841	-0.96209
H	0.77184	0.42170	-2.24994
N	2.09867	-0.33602	-0.86314
C	2.42866	-1.21794	0.14759
C	3.22520	-0.03229	-1.56775
C	3.78735	-1.46826	0.05576
C	4.29489	-0.71168	-1.02191
H	3.16950	0.63931	-2.41090
H	4.32589	-2.13246	0.71290
H	5.31414	-0.67026	-1.37181
C	1.52467	-1.82127	1.15748
C	0.31158	-1.17485	1.57164
H	0.03914	-0.16864	1.29267
H	-0.31597	-1.70551	2.27409
O	1.87706	-2.87869	1.69687
I	-2.83454	-0.85652	-0.24132

4.2 Radical Recombination



SM S23-A in DMSO

26

-631.7419276

C	2.63794	-0.35321	1.49596
C	1.44942	-0.50963	0.78324
C	1.39954	-0.21781	-0.58419
C	2.57647	0.22132	-1.15098
C	3.77193	0.39365	-0.50229
C	3.79484	0.09465	0.86587
H	2.65614	-0.58261	2.55458
H	0.55314	-0.85447	1.29044
H	4.66066	0.74444	-1.01418
H	4.71390	0.21431	1.42768
C	0.14046	-0.35826	-1.41807
H	-0.07040	0.57031	-1.95145
H	0.28810	-1.12866	-2.17665
N	-1.02330	-0.73812	-0.63367
C	-1.92889	0.07468	0.02671
C	-1.36750	-2.03939	-0.42277
C	-2.85348	-0.75100	0.64668
C	-2.49392	-2.08603	0.37302
H	-0.78581	-2.83204	-0.86872
H	-3.68540	-0.39946	1.23658
H	-2.99570	-2.98108	0.70418
C	-1.94755	1.54934	0.08499
C	-0.75294	2.33544	-0.08943
H	0.23908	1.91207	-0.14312
H	-0.86723	3.41120	-0.08715
O	-3.01266	2.12131	0.35139

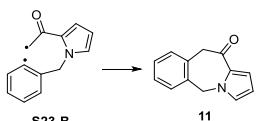
S23-B in DMSO in conformation for S_{RN1}

cyclisation

26

-631.7389322

C	-3.47356	-0.93170	-0.39313
C	-2.26951	-1.12262	0.27746
C	-1.45112	-0.03136	0.60469
C	-1.93545	1.20339	0.24110
C	-3.11377	1.45834	-0.41771
C	-3.89913	0.34919	-0.74330
H	-4.08972	-1.78843	-0.63769
H	-1.96586	-2.12517	0.56101
H	-3.42576	2.46382	-0.67459
H	-4.84052	0.48926	-1.26183
C	-0.13488	-0.21899	1.33272
H	0.20276	0.71604	1.77539
H	-0.26873	-0.93384	2.14591
N	0.92708	-0.74540	0.47005
C	1.99612	-0.07831	-0.10508
C	1.04623	-2.07459	0.19302
C	2.78013	-1.02132	-0.75043
C	2.17504	-2.28107	-0.57304
H	0.33403	-2.78197	0.58885
H	3.68144	-0.79076	-1.29639
H	2.51913	-3.23286	-0.94544
C	2.30239	1.36468	-0.06518
C	1.27096	2.35914	0.07191
H	0.21526	2.12864	0.03027
H	1.58218	3.39302	0.14097
O	3.47569	1.72893	-0.21938

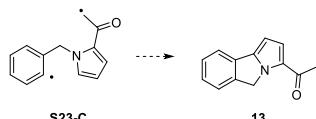


Product 11 in DMSO

26

-631.7856371

C	-3.23615	-1.12117	-0.67279
C	-2.09499	-1.59048	-0.02810
C	-1.15827	-0.70098	0.49233
C	-1.35577	0.68255	0.36496
C	-2.49832	1.14099	-0.28951
C	-3.43592	0.24868	-0.80370
H	-3.96141	-1.82149	-1.06974
H	-1.93038	-2.65803	0.07443
H	-2.65768	2.20917	-0.39218
H	-4.32099	0.62525	-1.30297
C	0.08912	-1.20899	1.17255
H	0.19255	-0.78663	2.17698
H	0.05270	-2.29280	1.27360
N	1.28654	-0.88838	0.39764
C	1.66300	0.35259	-0.03596
C	2.24301	-1.83320	-0.03459
C	2.94172	0.16858	-0.78111
C	3.24731	-1.16696	-0.75292
H	2.12097	-2.87836	0.20123
H	3.47684	0.97999	-1.24505
H	4.10198	-1.65136	-1.19835
C	0.99843	1.58374	0.16748
C	-0.33150	1.65203	0.90782
H	-0.69490	2.67410	0.79989
H	-0.17849	1.47868	1.97980
O	1.54538	2.63698	-0.28999



SM S23-C in DMSO

26

-631.7377405

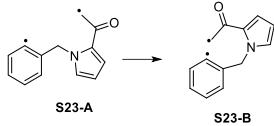
C	3.29759	-1.32007	-0.38802
C	2.03205	-1.25568	0.19333
C	1.46931	-0.02281	0.54411
C	2.26643	1.08082	0.32630
C	3.51284	1.08348	-0.24533
C	4.03521	-0.16188	-0.61463
H	3.71267	-2.28412	-0.65555
H	1.49061	-2.17308	0.40128
H	4.07619	1.99650	-0.39869
H	5.01870	-0.22096	-1.06645
C	0.12653	0.09997	1.23012
H	-0.21995	-0.87849	1.56123
H	0.22056	0.73097	2.11485
N	-0.90624	0.69410	0.36977
C	-2.09268	0.13322	-0.06628
C	-0.94687	2.03619	0.12273
C	-2.86915	1.14366	-0.60463
C	-2.13859	2.34740	-0.49687
H	-0.13293	2.67124	0.44020
H	-3.83577	0.99549	-1.06122
H	-2.44123	3.32790	-0.82834
C	-2.42586	-1.30296	-0.07703
C	-1.38607	-2.26264	-0.34339
H	-0.41125	-1.94906	-0.68838
H	-1.62526	-3.31647	-0.29242
O	-3.59913	-1.66884	0.05033

TS S23-C in DMSO

26

-631.7281116

C	3.36451	-1.25743	-0.49701
C	2.20395	-1.59006	0.20146
C	1.28891	-0.58978	0.52929
C	1.57324	0.70398	0.14036
C	2.70717	1.07445	-0.54724
C	3.61772	0.06126	-0.87104
H	4.07388	-2.03450	-0.75573
H	2.01245	-2.62081	0.48387
H	2.89737	2.10270	-0.83563
H	4.52161	0.30560	-1.41805
C	-0.00584	-0.80582	1.28808
H	-0.48310	-1.74386	1.00946
H	0.16850	-0.81903	2.36679
N	-0.87310	0.33033	0.96269
C	-1.75076	0.34934	-0.11202
C	-0.29222	1.58507	1.05036
C	-1.81915	1.64317	-0.60548
C	-0.93338	2.43380	0.14277
H	0.30024	1.84514	1.91541
H	-2.49012	1.96686	-1.38630
H	-0.76606	3.49545	0.05202
C	-2.59248	-0.78315	-0.52837
C	-2.93385	-1.81134	0.42176
H	-2.69672	-1.72267	1.47298
H	-3.50264	-2.66204	0.07162
O	-3.06132	-0.81325	-1.67409

**SM S23-A in Benzene**

26

-631.7362148

C	2.63201	-0.35421	1.49600
C	1.44510	-0.51108	0.78155
C	1.39852	-0.21908	-0.58580
C	2.57577	0.22065	-1.15065
C	3.76964	0.39321	-0.49945
C	3.78969	0.09408	0.86818
H	2.64832	-0.58327	2.55467
H	0.54644	-0.85512	1.28519
H	4.65887	0.74435	-1.01005
H	4.70743	0.21394	1.43211
C	0.13881	-0.35863	-1.41931
H	-0.07104	0.57208	-1.94992
H	0.28786	-1.12697	-2.18029
N	-1.02420	-0.73909	-0.63795
C	-1.92570	0.07387	0.02796
C	-1.36876	-2.04154	-0.42478
C	-2.84720	-0.74962	0.65099
C	-2.49047	-2.08580	0.37538
H	-0.78929	-2.83467	-0.87251
H	-3.67803	-0.39304	1.23897
H	-2.99385	-2.97959	0.70698
C	-1.94560	1.55115	0.08442
C	-0.75022	2.33864	-0.09344
H	0.24407	1.91843	-0.13588
H	-0.87109	3.41368	-0.09305
O	-3.00622	2.12175	0.35289

Prod 13 cyclisation in DMSO

XYZ_Diradical_RadicalRecom_Prod.log

26

-631.7863794

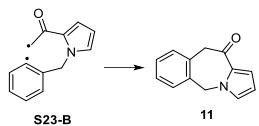
C	3.55933	-1.03398	-0.64531
C	2.35228	-1.65443	-0.32719
C	1.31253	-0.87514	0.16359
C	1.47603	0.49478	0.33945
C	2.67690	1.11855	0.02907
C	3.72037	0.34090	-0.46945
H	4.37996	-1.62453	-1.03511
H	2.22881	-2.72281	-0.46571
H	2.80231	2.18689	0.16744
H	4.66436	0.80813	-0.72374
C	-0.07582	-1.30121	0.57955
H	-0.58101	-1.87619	-0.19874
H	-0.05531	-1.90020	1.49435
N	-0.77018	-0.01490	0.80877
C	-1.81108	0.39039	-0.01260
C	0.20591	1.10081	0.89605
C	-1.61196	1.74914	-0.40959
C	-0.44455	2.19966	0.10249
H	0.35804	1.40411	1.94076
H	-2.32137	2.30471	-1.00540
H	-0.02888	3.19319	0.01617
C	-2.97313	-0.41545	-0.30525
C	-3.21451	-1.65576	0.40361
H	-2.61569	-1.96190	1.25024
H	-4.05595	-2.26073	0.09633
O	-3.80223	-0.02449	-1.15807

S23-B in DMSO in conformation for S_{RN1} cyclisation

26

-631.7324459

C	-3.50592	-0.91638	-0.34556
C	-2.29777	-1.10732	0.31684
C	-1.45611	-0.02245	0.60032
C	-1.92149	1.20852	0.20164
C	-3.10263	1.46345	-0.45132
C	-3.91193	0.35994	-0.73170
H	-4.14009	-1.76872	-0.55687
H	-2.00641	-2.10598	0.62619
H	-3.39899	2.46583	-0.73690
H	-4.85661	0.50057	-1.24405
C	-0.13352	-0.21236	1.31596
H	0.20995	0.72499	1.74980
H	-0.26475	-0.92115	2.13567
N	0.91950	-0.74453	0.44968
C	2.00669	-0.08881	-0.10397
C	1.02420	-2.07428	0.16222
C	2.78595	-1.03541	-0.74493
C	2.16051	-2.28872	-0.58759
H	0.29623	-2.77437	0.54153
H	3.69909	-0.80964	-1.27237
H	2.49783	-3.24137	-0.96343
C	2.32766	1.35265	-0.05121
C	1.29783	2.35500	0.05855
H	0.24239	2.13210	-0.02275
H	1.61781	3.38550	0.13720
O	3.50327	1.70764	-0.17217

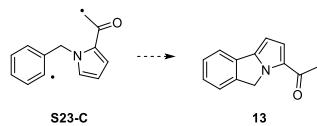


Product 11 in Benzene

26

-631.7777499

C	-3.24319	-1.11523	-0.66482
C	-2.10426	-1.58419	-0.01737
C	-1.16297	-0.69582	0.49588
C	-1.35329	0.68781	0.35930
C	-2.49345	1.14503	-0.29943
C	-3.43517	0.25410	-0.80658
H	-3.97183	-1.81483	-1.05663
H	-1.94499	-2.65205	0.09228
H	-2.64551	2.21302	-0.41292
H	-4.31750	0.63140	-1.30995
C	0.08497	-1.20577	1.17377
H	0.19163	-0.77835	2.17675
H	0.04131	-2.28937	1.28189
N	1.28021	-0.89748	0.39577
C	1.66408	0.34953	-0.03524
C	2.23195	-1.84146	-0.04028
C	2.94475	0.16117	-0.77791
C	3.24202	-1.17437	-0.75484
H	2.10392	-2.88857	0.18322
H	3.47952	0.97590	-1.23635
H	4.09443	-1.66077	-1.20257
C	1.00926	1.58183	0.16793
C	-0.32849	1.65935	0.89643
H	-0.68363	2.68225	0.77179
H	-0.18340	1.50086	1.97188
O	1.56717	2.62886	-0.27634



SM S23-C in Benzene

26

-631.7348295

C	-3.51878	0.98611	0.05748
C	-2.31151	0.97903	0.75302
C	-1.40716	-0.07737	0.59670
C	-1.79356	-1.08320	-0.26102
C	-2.96371	-1.12737	-0.97553
C	-3.84770	-0.05675	-0.80447
H	-4.20478	1.81450	0.18566
H	-2.06237	1.80139	1.41782
H	-3.20024	-1.94958	-1.64073
H	-4.78606	-0.04116	-1.34655
C	-0.10867	-0.14370	1.37192
H	0.16326	0.84225	1.75059
H	-0.23425	-0.79584	2.23928
N	0.99722	-0.67771	0.58720
C	1.99529	0.00758	-0.08169
C	1.24268	-2.01572	0.48443
C	2.87173	-0.92812	-0.60127
C	2.39010	-2.20788	-0.25564
H	0.58749	-2.72535	0.96655
H	3.74779	-0.68188	-1.18049
H	2.82666	-3.16111	-0.50656
C	2.10581	1.46904	-0.25777
C	0.92269	2.29159	-0.32802
H	-0.07120	1.87596	-0.41851
H	1.06253	3.36254	-0.39287
O	3.21591	1.98037	-0.42166

TS S23-C in Benzene

26

-631.7173855

C	3.35734	-1.12035	-0.33860
C	2.26878	-1.36982	0.49759
C	1.29950	-0.38321	0.66794
C	1.45039	0.81972	0.00041
C	2.51691	1.10171	-0.82387
C	3.48256	0.10163	-0.99532
H	4.11021	-1.88649	-0.48133
H	2.17720	-2.32480	1.00688
H	2.61385	2.05440	-1.33324
H	4.33077	0.28042	-1.64701
C	0.05665	-0.48911	1.53458
H	-0.37348	-1.48776	1.57577
H	0.27484	-0.18362	2.56164
N	-0.88457	0.46666	0.96712
C	-1.83606	0.24157	-0.00604
C	-0.40954	1.75926	0.81184
C	-2.09389	1.44381	-0.65309
C	-1.21145	2.40292	-0.14162
H	0.17179	2.21150	1.60257
H	-2.84041	1.57239	-1.42142
H	-1.14590	3.44443	-0.41350
C	-2.44965	-1.05662	-0.36688
C	-1.64881	-2.25262	-0.44605
H	-0.56728	-2.21975	-0.45309
H	-2.15792	-3.19067	-0.62271
O	-3.63727	-1.09125	-0.69872

Prod 13 cyclisation in Benzene

26

-631.7808325

C	3.56443	-1.03261	-0.64193
C	2.35577	-1.65236	-0.33105
C	1.31482	-0.87448	0.15846
C	1.47828	0.49413	0.34034
C	2.68102	1.11683	0.03676
C	3.72573	0.34087	-0.46023
H	4.38581	-1.62230	-1.03122
H	2.23216	-2.72002	-0.47550
H	2.80693	2.18476	0.17801
H	4.67086	0.80832	-0.70956
C	-0.07629	-1.29975	0.56570
H	-0.58200	-1.86268	-0.22157
H	-0.05936	-1.91199	1.47247
N	-0.76923	-0.01668	0.80977
C	-1.81343	0.38981	-0.01064
C	0.20645	1.09960	0.89300
C	-1.61320	1.74412	-0.41373
C	-0.44443	2.19601	0.09492
H	0.35688	1.40626	1.93735
H	-2.32483	2.29284	-1.01299
H	-0.02794	3.18853	0.00179
C	-2.97918	-0.41408	-0.30125
C	-3.22169	-1.65171	0.40976
H	-2.62265	-1.95719	1.25673
H	-4.07179	-2.24782	0.10929
O	-3.80614	-0.02252	-1.15173

4.3 The isolated HOMO-LUMO fragments of 21

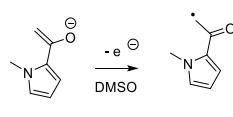


SM (Before SET): S24 in DMSO

15	-282.2764280
C	-3.28995
C	-2.66576
C	-1.27245
C	-0.53375
C	-1.13558
C	-2.52387
H	-4.37155
H	-3.26701
H	-0.53158
H	-2.99575
I	1.60244
C	-0.63745
H	-0.00416
H	-0.00411
H	-1.40259
-0.39200	0.00000
0.84989	0.00001
0.97831	-0.00000
-0.20839	-0.00000
-1.46161	0.00000
-1.55233	-0.00001
-0.45173	-0.00000
1.75271	0.00001
-2.36020	-0.00001
-2.52737	-0.00001
-0.14758	0.00000
2.34153	-0.00001
2.47910	0.88028
2.47908	-0.88025
3.11769	-0.00004

Prod (After SET): S26 in DMSO

15	-282.3841184
C	-4.22541
C	-3.56934
C	-2.17036
C	-1.51482
C	-2.10314
C	-3.50315
H	-5.30871
H	-4.14749
H	-1.51653
H	-4.01711
I	2.44999
C	-1.43599
H	-0.79503
H	-0.79421
H	-2.13704
-0.38262	-0.00069
0.84888	-0.00053
0.92532	0.00026
-0.29045	0.00084
-1.53077	0.00071
-1.57234	-0.00008
-0.40983	-0.00131
1.76788	-0.00101
-2.44281	0.00120
-2.52674	-0.00021
-0.10471	-0.00011
2.24108	0.00046
2.32525	0.88067
2.32506	-0.87918
3.07612	0.00004



SM (Before SET): S25 in DMSO

17	-401.5715769
C	2.10188
C	2.02545
C	0.64382
C	-0.07791
N	0.82936
H	2.95312
H	2.86375
H	0.20974
C	0.51909
H	0.14766
H	-0.24430
H	1.42931
C	-1.56107
C	-2.34576
H	-3.42676
H	-1.90501
O	-1.95825
0.14788	0.04160
-1.21550	-0.13998
-1.54373	-0.19784
-0.37121	-0.05237
0.65230	0.08578
0.80234	0.14949
-1.88998	-0.22522
-2.52117	-0.34576
2.05496	0.32219
2.52866	-0.58430
2.14286	1.09449
2.55117	0.65715
-0.12756	-0.07978
-1.05328	0.56415
-0.96719	0.52981
-1.88126	1.10360
0.91488	-0.71594

Prod (After SET): S27 in DMSO

17	-401.4123853
C	-2.09389
C	-2.03252
C	-0.66827
C	0.06404
N	-0.83168
H	-2.94407
H	-2.87735
H	-0.23530
C	-0.55281
H	0.25372
H	-0.28912
H	-1.45133
C	1.53376
C	2.21796
H	3.29556
H	1.71452
O	2.19318
0.18436	-0.03158
-1.19257	-0.13543
-1.54042	-0.10500
-0.36685	-0.00122
0.68517	0.04159
0.84749	0.01315
-1.85754	-0.21795
-2.52639	-0.17136
2.10277	0.24566
2.22749	0.96677
2.59255	-0.69225
2.56952	0.64365
-0.28221	0.02306
0.90331	-0.42801
0.92481	-0.33586
1.72468	-0.91434
-1.26864	0.37652

5. DMSO Possible Formation



S54

S55

9

-552.6394561

S	0.11620	0.14532	-0.41122
C	1.37804	-0.82514	0.19707
H	2.33634	-0.46410	-0.17547
H	1.34642	-0.92997	1.28568
C	-1.31527	-0.82293	0.13069
H	-1.21349	-0.99446	1.20441
H	-2.21398	-0.24264	-0.07344
H	-1.34041	-1.76910	-0.40571
O	-0.14384	1.49544	0.34718

S54

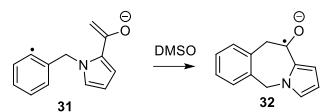
9

-552.4905292

S	-0.10845	-0.14067	-0.41933
C	-0.99298	1.21313	0.23115
H	-0.66455	2.20876	-0.03750
H	-2.01291	1.01551	0.53267
C	1.53727	0.29296	0.20630
H	1.49395	0.31959	1.29417
H	2.21611	-0.48349	-0.14191
H	1.82330	1.26022	-0.20606
O	-0.54830	-1.38830	0.33040

6. Radical Cyclisation of 9

6.1 DMSO (Scheme S2.1)



26

-631.9004297

C	-2.73321	-0.24997	1.46881
C	-1.51740	-0.34745	0.79266
C	-1.43908	-0.06963	-0.57663
C	-2.62254	0.29578	-1.18084
C	-3.84593	0.40838	-0.57080
C	-3.89495	0.12471	0.79976
H	-2.77073	-0.46932	2.52926
H	-0.61652	-0.63782	1.32527
H	-4.73703	0.70032	-1.11485
H	-4.83619	0.19696	1.33251
C	-0.14614	-0.14734	-1.36586
H	-0.29852	-0.78439	-2.24021
H	0.13102	0.84661	-1.71700
N	0.95989	-0.68853	-0.59962
C	1.13717	-2.03963	-0.43162
C	1.97371	-0.00531	0.04656
C	2.26998	-2.24094	0.32095
H	0.44438	-2.73840	-0.87608
C	2.80228	-0.95738	0.61235
H	3.69321	-0.72842	1.17614
H	2.66920	-3.19919	0.61627
C	2.16332	1.48827	0.12080
C	1.06007	2.29996	0.22510
H	0.05565	1.90693	0.29775
H	1.19697	3.37341	0.30032
O	3.38819	1.87454	0.12507

Prod: 32 cyclised in DMSO

26	-631.9716451		
C	3.20248	-1.13436	-0.66836
C	2.07161	-1.58973	0.00598
C	1.14374	-0.69065	0.52606
C	1.33639	0.69138	0.36891
C	2.46994	1.13552	-0.31364
C	3.39892	0.23380	-0.82882
H	3.92186	-1.84193	-1.06397
H	1.90747	-2.65555	0.13099
H	2.62842	2.20195	-0.43921
H	4.27569	0.60051	-1.35047
C	-0.11209	-1.17057	1.20902
H	-0.07093	-2.24938	1.36177
H	-0.22159	-0.70211	2.19351
N	-1.28916	-0.89095	0.40117
C	-2.17400	-1.86261	-0.02910
C	-1.69304	0.36422	-0.06993
C	-3.15891	-1.25065	-0.77192
H	-2.02068	-2.89684	0.23709
C	-2.87789	0.13744	-0.80685
H	-3.44009	0.90587	-1.31317
H	-3.99182	-1.75637	-1.23877
C	-1.02377	1.60374	0.15698
C	0.31089	1.65890	0.90611
H	0.17592	1.49319	1.98467
H	0.68336	2.67795	0.79193
O	-1.52363	2.71259	-0.27614

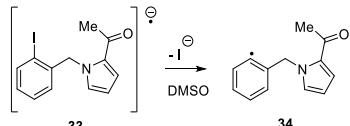


Prod (After SET): 11 in DMSO

26

-631.8980850

C	3.22968	-1.12300	-0.66874
C	2.07908	-1.60447	-0.04937
C	1.13629	-0.72203	0.46962
C	1.34190	0.65928	0.37190
C	2.49217	1.13391	-0.25355
C	3.43476	0.24820	-0.77096
H	3.95928	-1.81671	-1.06914
H	1.91189	-2.67322	0.03168
H	2.65423	2.20354	-0.33074
H	4.32737	0.63173	-1.25073
C	-0.11543	-1.22897	1.13930
H	-0.09034	-2.31386	1.22672
H	-0.21084	-0.81551	2.14727
N	-1.31780	-0.89133	0.37382
C	-2.23824	-1.80310	-0.02365
C	-1.70667	0.36076	-0.07345
C	-3.23937	-1.15891	-0.73265
H	-2.11417	-2.84619	0.22367
C	-2.90235	0.20413	-0.76421
H	-3.44805	1.00927	-1.23105
H	-4.10292	-1.63170	-1.17226
C	-0.98781	1.61730	0.14334
C	0.31507	1.61627	0.92979
H	0.07974	1.35476	1.96833
H	0.69244	2.63778	0.92086
O	-1.43356	2.66291	-0.29821



TS: 33 C-I elongation to give 34 in DMSO

28

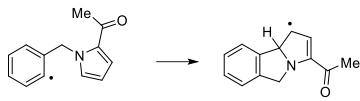
-643.9223676			
C	0.48610	3.05031	0.42108
C	0.93172	1.85744	-0.13740
C	0.06284	0.77512	-0.32724
C	-1.24423	0.97526	0.07610
C	-1.73502	2.14067	0.63405
C	-0.84252	3.19639	0.80844
H	1.18216	3.86946	0.55573
H	1.97009	1.74459	-0.43259
H	-2.77201	2.23162	0.92729
H	-1.19278	4.12390	1.24546
C	0.54580	-0.51976	-0.96062
H	0.10440	-1.36254	-0.43401
H	0.17271	-0.56746	-1.98791
N	1.98448	-0.63619	-1.00994
C	2.84452	-0.63766	0.11086
C	2.68730	-0.16627	-2.11975
C	4.09930	-0.18610	-0.35838
C	3.98248	0.09000	-1.74290
H	2.19062	-0.07141	-3.07317
H	4.98908	-0.12089	0.24740
H	4.76884	0.42441	-2.40439
C	2.51764	-1.03020	1.43920
C	1.21051	-1.72888	1.77244
H	0.34005	-1.05893	1.78323
H	0.98295	-2.54820	1.08137
O	3.37686	-0.86603	2.38843
I	-2.79681	-0.75524	-0.18895
H	1.30956	-2.15286	2.77284

Prod: 34 + Iodide anion in DMSO

28

-643.9665259

C	1.61061	3.28725	0.44105
C	1.75340	2.03697	-0.15938
C	0.62506	1.28615	-0.50875
C	-0.60015	1.85200	-0.22662
C	-0.79512	3.07634	0.36547
C	0.34718	3.81050	0.70463
H	2.49453	3.85420	0.70800
H	2.74541	1.63763	-0.35100
H	-1.78794	3.46249	0.56816
H	0.24504	4.78188	1.17520
C	0.71973	-0.07087	-1.17583
H	-0.08498	-0.71316	-0.82199
H	0.58542	0.03802	-2.25394
N	2.02036	-0.70250	-0.98138
C	2.59246	-1.15269	0.20008
C	2.97907	-0.68168	-1.94603
C	3.92543	-1.43478	-0.06557
C	4.17052	-1.14312	-1.41973
H	2.73951	-0.32978	-2.93794
H	4.61727	-1.83654	0.65829
H	5.09643	-1.26054	-1.95958
C	1.93832	-1.36633	1.50217
C	0.43726	-1.34483	1.63081
H	0.03630	-0.34848	1.42834
H	-0.02447	-2.03378	0.92000
O	2.63630	-1.60308	2.47626
I	-3.21306	-0.69439	-0.16554
H	0.17380	-1.63667	2.64578



SM: 34 cyclisation to 35 in DMSO

27

-632.4034071			
C	-2.25369	-0.20247	1.70411
C	-1.21388	-0.46653	0.84509
C	-1.28560	-0.47851	-0.52875
C	-2.54046	-0.19943	-1.08451
C	-3.63157	0.06905	-0.26337
C	-3.49602	0.07024	1.12447
H	-2.12458	-0.20319	2.78022
H	-4.59502	0.28355	-0.70984
H	-4.34989	0.28617	1.75621
C	-0.09207	-0.77758	-1.41044
H	-0.21815	-1.75321	-1.88277
H	-0.01683	-0.04561	-2.21401
N	1.15349	-0.83631	-0.65611
C	1.72816	-2.02126	-0.31429
C	1.77755	0.17835	0.05605
C	2.74824	-1.79332	0.58858
H	1.35848	-2.94360	-0.73610
C	2.77384	-0.40669	0.82457
H	3.45220	0.14315	1.45794
H	3.39692	-2.54374	1.01124
C	1.51280	1.62506	-0.00086
C	0.65557	2.21983	-1.09078
H	-0.38742	1.91795	-0.96808
H	0.72046	3.30404	-1.02382
O	2.03157	2.35060	0.83278
H	-2.65589	-0.18906	-2.16420
H	0.99543	1.89255	-2.07519

TS: 34 cyclisation to **35** in DMSO

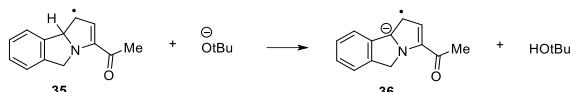
27

-632.3878362
 C -2.74967 1.07494 -0.54232
 C -1.61746 0.70058 0.14464
 C -1.32200 -0.59506 0.51610
 C -2.22651 -1.59766 0.16726
 C -3.38554 -1.26376 -0.53338
 C -3.64861 0.05837 -0.88790
 H -2.94691 2.10619 -0.81436
 H -4.08620 -2.04272 -0.80944
 H -4.55098 0.30325 -1.43708
 C -0.02968 -0.80909 1.28069
 H -0.21149 -0.81917 2.35831
 H 0.45062 -1.74459 1.01004
 N 0.83291 0.33286 0.96354
 C 0.24381 1.57775 1.07941
 C 1.71916 0.38362 -0.10557
 C 0.87980 2.45738 0.19511
 H -0.35865 1.81025 1.94561
 C 1.77636 1.69653 -0.56232
 H 2.45290 2.04539 -1.32730
 H 0.70268 3.51942 0.13248
 C 2.60285 -0.69863 -0.55389
 C 2.85016 -1.89756 0.33200
 H 2.19547 -2.71845 0.02596
 H 3.87906 -2.22193 0.18007
 O 3.17941 -0.59733 -1.62623
 H -2.02802 -2.63088 0.43528
 H 2.67989 -1.68267 1.38644

Prod: 35 in DMSO

27

-632.4493559
 C -2.71868 1.11644 0.02551
 C -1.51273 0.49955 0.32838
 C -1.34430 -0.87105 0.16069
 C -2.38510 -1.65833 -0.31409
 C -3.59750 -1.04483 -0.62559
 C -3.76285 0.33051 -0.45860
 H -2.84779 2.18492 0.15862
 H -4.41920 -1.64168 -1.00328
 H -4.71102 0.79182 -0.70792
 C 0.05215 -1.28849 0.56082
 H 0.05061 -1.88389 1.47785
 H 0.55191 -1.85898 -0.22248
 N 0.73547 0.00368 0.77148
 C -0.24261 1.11058 0.87721
 C 1.79415 0.42252 -0.00631
 C 0.40706 2.22384 0.10652
 H -0.38711 1.40091 1.92724
 C 1.58623 1.79857 -0.38405
 H 2.30336 2.36919 -0.95532
 H -0.01639 3.21531 0.03136
 C 2.96123 -0.35378 -0.32023
 C 3.16882 -1.69687 0.34439
 H 2.84032 -2.50092 -0.32009
 H 4.23634 -1.82837 0.52208
 O 3.80584 0.08803 -1.11463
 H -2.25837 -2.72711 -0.44603
 H 2.62704 -1.78297 1.28659



TS: 35 + *tert*-butoxide anion in DMSO

41				
-865.5785755				
C	-0.91934	2.39230	0.99531	
C	-0.03961	1.51988	0.36417	
C	0.92844	2.00905	-0.51540	
C	1.03104	3.36687	-0.78154	
C	0.15310	4.24443	-0.14451	
C	-0.81167	3.75896	0.73828	
H	-1.67458	2.01964	1.67829	
H	0.22313	5.30897	-0.33422	
H	-1.48552	4.45164	1.22934	
C	1.76063	0.87430	-1.07094	
H	1.61285	0.75466	-2.14907	
H	2.82821	1.01297	-0.88593	
N	1.25808	-0.28973	-0.32682	
C	0.02793	0.02477	0.41572	
C	2.02922	-1.16648	0.40310	
C	0.19606	-0.71963	1.68447	
H	-0.91268	-0.41637	-0.19747	
H	1.34022	-1.44091	1.64015	
N	1.22872	-0.45901	-0.40216	
C	1.70448	-2.14083	2.37817	
C	0.03174	0.01147	0.33506	
C	1.93099	-1.33750	0.39134	
C	0.13455	-0.70904	1.64244	
H	-0.90467	-0.26952	-0.21372	
C	1.22592	-1.49932	1.64089	
H	1.54767	-2.17729	2.41771	
H	-0.61375	-0.63777	2.42011	
C	3.11927	-2.04367	0.01421	
C	3.62013	-1.95970	-1.41180	
H	4.40837	-1.20591	-1.49428	
H	4.05396	-2.92376	-1.67866	
O	3.72688	-2.74239	0.84627	
H	2.31670	3.48853	-1.46328	
H	2.82766	-1.70885	-2.11750	
O	-2.46892	-0.56656	-1.27368	
C	-3.43304	-1.02483	-0.40421	
C	-4.79051	-1.20816	-1.11624	
H	-4.68301	-1.93016	-1.93183	
H	-5.57561	-1.56549	-0.43983	
H	-5.11165	-0.25377	-1.54573	
C	-3.64443	-0.03325	0.76429	
H	-2.70570	0.09760	1.31175	
H	-3.94428	0.94276	0.36910	
H	-4.40925	-0.37153	1.47257	
C	-3.02469	-2.38715	0.20158	
H	-2.90086	-3.12173	-0.60055	
H	-2.06452	-2.28416	0.71793	
H	-3.76218	-2.77375	0.91440	

SM: 35 + *tert*-butoxide anion in DMSO

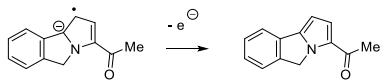
41				
-865.5794437				
C	-0.56013	2.48129	0.96682	
C	0.18440	1.51200	0.30678	
C	1.21127	1.87118	-0.56259	
C	1.51636	3.20692	-0.78786	
C	0.77719	4.18370	-0.12118	
C	-0.25134	3.82359	0.74961	
H	-1.36383	2.20286	1.63963	
H	1.00524	5.23125	-0.27907	
H	-0.81494	4.59465	1.26185	
C	1.85861	0.64032	-1.15687	
H	1.65229	0.55135	-2.22750	
H	2.93990	0.63218	-1.01235	
N	1.22872	-0.45901	-0.40216	
C	0.03174	0.01147	0.33506	
C	1.93099	-1.33750	0.39134	
C	0.13455	-0.70904	1.64244	
H	-0.90467	-0.26952	-0.21372	
C	1.22592	-1.49932	1.64089	
H	1.54767	-2.17729	2.41771	
H	-0.61375	-0.63777	2.42011	
C	3.11927	-2.04367	0.01421	
C	3.62013	-1.95970	-1.41180	
H	4.40837	-1.20591	-1.49428	
H	4.05396	-2.92376	-1.67866	
O	3.72688	-2.74239	0.84627	
H	2.31670	3.48853	-1.46328	
H	2.82766	-1.70885	-2.11750	
O	-2.46892	-0.56656	-1.27368	
C	-3.43304	-1.02483	-0.40421	
C	-4.79051	-1.20816	-1.11624	
H	-4.68301	-1.93016	-1.93183	
H	-5.57561	-1.56549	-0.43983	
H	-5.11165	-0.25377	-1.54573	
C	-3.64443	-0.03325	0.76429	
H	-2.70570	0.09760	1.31175	
H	-3.94428	0.94276	0.36910	
H	-4.40925	-0.37153	1.47257	
C	-3.02469	-2.38715	0.20158	
H	-2.90086	-3.12173	-0.60055	
H	-2.06452	-2.28416	0.71793	
H	-3.76218	-2.77375	0.91440	

Prod: 36 + *tert*-butanol in DMSO

41

-865.6231594

C	2.82167	-0.62636	1.29333
C	1.58573	-0.95655	0.72539
C	1.53381	-1.47941	-0.58724
C	2.68826	-1.68087	-1.32011
C	3.92335	-1.35190	-0.74853
C	3.97814	-0.82831	0.54667
H	2.87773	-0.21718	2.29606
H	4.83734	-1.50245	-1.31011
H	4.94043	-0.57563	0.97828
C	0.09404	-1.72900	-0.98764
H	-0.22197	-1.09386	-1.82533
H	-0.07130	-2.77399	-1.26671
N	-0.62123	-1.36368	0.23115
C	0.23900	-0.84271	1.20313
C	-1.94653	-1.02438	0.53062
C	-0.53663	-0.21253	2.17067
H	-0.82768	1.04344	-0.04327
C	-1.87708	-0.32101	1.77039
H	-2.74093	0.04755	2.30118
H	-0.16267	0.28197	3.05563
C	-3.11728	-1.30433	-0.21901
C	-3.08842	-2.16675	-1.46386
H	-3.84388	-2.95313	-1.36146
H	-3.36334	-1.57593	-2.34501
O	-4.25628	-0.84909	0.15056
H	2.64058	-2.08048	-2.32801
H	-2.13006	-2.64452	-1.65631
O	-0.66352	1.58100	-0.83054
C	-0.05613	2.81164	-0.41513
C	0.05607	3.65805	-1.67556
H	-0.93344	3.82353	-2.10815
H	0.50410	4.62726	-1.44664
H	0.68063	3.15185	-2.41548
C	1.32555	2.53025	0.17314
H	1.23758	1.92330	1.07821
H	1.93704	1.97869	-0.54627
H	1.83385	3.46447	0.42582
C	-0.95067	3.49060	0.62035
H	-1.93969	3.68218	0.19693
H	-1.06590	2.84485	1.49639
H	-0.51860	4.43997	0.94624



SM (Before SET): 36 in DMSO

26

-631.9734622			
C	-2.81274	1.23120	-0.00306
C	-1.57030	0.58300	-0.00898
C	-1.52182	-0.83264	-0.00126
C	-2.67864	-1.58706	0.01092
C	-3.91864	-0.93519	0.01658
C	-3.97235	0.46187	0.00967
H	-2.87069	2.31386	-0.00842
H	-4.83466	-1.51320	0.02634
H	-4.93694	0.95763	0.01429
C	-0.07948	-1.29990	-0.01034
H	0.16786	-1.89476	0.87690
H	0.14706	-1.90473	-0.89616
N	0.63819	-0.03275	-0.02423
C	-0.22174	1.06473	-0.01946
C	1.96950	0.38842	-0.00513
C	0.55773	2.21821	-0.00383
C	1.89838	1.81445	0.00483
H	2.76555	2.45638	0.01579
H	0.18547	3.23226	0.00206
C	3.15281	-0.39387	0.00367
C	3.13156	-1.90793	-0.01216
H	3.75343	-2.26585	-0.83992
H	3.58188	-2.29346	0.91006
O	4.30702	0.16634	0.03493
H	-2.63111	-2.67130	0.01680
H	2.14308	-2.35012	-0.11626

Prod (After SET): 13 in DMSO

26

-631.8971159

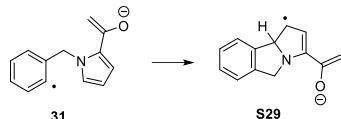
C	2.77758	1.23734	0.00042
C	1.55750	0.57055	0.00004
C	1.50265	-0.83030	-0.00034
C	2.66276	-1.58587	-0.00039
C	3.88905	-0.91886	-0.00008
C	3.94406	0.47569	0.00033
H	2.81968	2.32001	0.00075
H	4.80888	-1.49117	-0.00014
H	4.90687	0.97253	0.00064
C	0.06398	-1.29471	-0.00031
H	-0.17817	-1.88003	-0.88923
H	-0.17774	-1.88068	0.88831
N	-0.65337	-0.01546	0.00028
C	0.18581	1.05952	0.00028
C	-1.96169	0.42255	-0.00032
C	-0.56971	2.22445	-0.00015
C	-1.91551	1.81635	-0.00054
H	-2.78963	2.44927	-0.00085
H	-0.18919	3.23321	-0.00021
C	-3.16157	-0.41459	0.00011
C	-3.00852	-1.91493	0.00044
H	-3.99602	-2.37149	0.00011
H	-2.45653	-2.24442	-0.88283
O	-4.26746	0.10390	0.00014
H	2.62413	-2.66916	-0.00070
H	-2.45724	-2.24411	0.88425

TS: 31 cyclisation to form S29 in DMSO

26

-631.8883080

C	2.72254	1.06651	0.58404
C	1.57975	0.73495	-0.11500
C	1.30112	-0.54739	-0.55007
C	2.21671	-1.56087	-0.26378
C	3.37980	-1.26029	0.44583
C	3.63411	0.04254	0.87047
H	2.91989	2.08188	0.91313
H	4.08861	-2.04836	0.67206
H	4.53886	0.26518	1.42602
C	0.00239	-0.75238	-1.30916
H	0.17841	-0.73528	-2.38878
H	-0.47891	-1.69366	-1.05367
N	-0.87826	0.35711	-0.94990
C	-0.32417	1.63025	-1.01003
C	-1.78869	0.32265	0.09352
C	-1.00684	2.44000	-0.10199
H	0.26876	1.92094	-1.86452
C	-1.89236	1.60598	0.60962
H	-2.57539	1.89488	1.39336
H	-0.86892	3.50415	0.01521
C	-2.59390	-0.87409	0.51180
C	-2.95890	-1.76918	-0.46443
H	-2.69341	-1.61564	-1.50220
H	-3.56939	-2.62835	-0.20889
O	-2.91425	-0.91728	1.75385
H	2.02390	-2.57947	-0.58804

**SM: 31 cyclisation to form S29 in DMSO**

26

-631.9002517

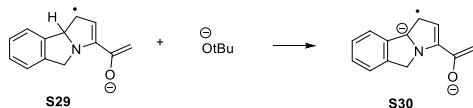
C	2.79905	-0.94212	-1.21862
C	1.64483	-0.88465	-0.47479
C	1.41100	-0.04832	0.59319
C	2.45850	0.81601	0.93481
C	3.65316	0.80191	0.21883
C	3.82960	-0.07003	-0.85450
H	2.91357	-1.62825	-2.05002
H	4.45043	1.48113	0.49604
H	4.76029	-0.07251	-1.41012
C	0.11410	-0.05963	1.37513
H	0.24800	-0.64684	2.28790
H	-0.15433	0.95661	1.66141
N	-0.98909	-0.64177	0.63177
C	-1.19529	-1.99708	0.56976
C	-1.97525	0.00916	-0.08416
C	-2.32234	-2.23322	-0.18305
H	-0.52997	-2.67246	1.08612
C	-2.81909	-0.96576	-0.58567
H	-3.69436	-0.76165	-1.18275
H	-2.74027	-3.20307	-0.40580
C	-2.11464	1.49400	-0.29380
C	-0.98146	2.25365	-0.45588
H	0.00783	1.81835	-0.47803
H	-1.07650	3.31931	-0.63549
O	-3.32524	1.91869	-0.35002
H	2.32792	1.50875	1.76100

Prod: S29 cyclised in DMSO

26

-631.9403183

C	-2.66979	1.11985	0.01693
C	-1.47624	0.49287	0.35042
C	-1.31460	-0.87755	0.17675
C	-2.34952	-1.65169	-0.33409
C	-3.54937	-1.02799	-0.67491
C	-3.70842	0.34758	-0.50136
H	-2.79295	2.18945	0.15131
H	-4.36455	-1.61541	-1.08122
H	-4.64567	0.81878	-0.77377
C	0.06615	-1.30018	0.62038
H	0.02062	-1.89715	1.53734
H	0.59490	-1.88525	-0.13274
N	0.77067	-0.02375	0.85557
C	-0.20955	1.09431	0.92641
C	1.80879	0.36653	-0.00791
C	0.44430	2.19180	0.13282
H	-0.38964	1.39414	1.96897
C	1.60536	1.70362	-0.40407
H	2.31101	2.24443	-1.01798
H	0.03938	3.18952	0.04578
C	3.00379	-0.44954	-0.32210
C	3.24492	-1.56927	0.44734
H	2.59917	-1.84348	1.27097
H	4.12585	-2.17248	0.25592
O	3.74507	-0.02217	-1.28775
H	-2.22831	-2.72094	-0.47122



TS: S29 + tert-butoxide anion in DMSO

40	-865.0544641			
C	-0.97476	2.33664	0.99465	
C	-0.07487	1.48834	0.34934	
C	0.87305	2.02601	-0.53162	
C	0.92694	3.38856	-0.78428	
C	0.02167	4.23632	-0.14028	
C	-0.91820	3.70842	0.74562	
H	-1.71000	1.93691	1.68510	
H	0.05228	5.30380	-0.32502	
H	-1.61272	4.37321	1.24777	
C	1.74105	0.92231	-1.09381	
H	1.61957	0.83517	-2.18037	
H	2.80541	1.08121	-0.89775	
N	1.26453	-0.28283	-0.39848	
C	0.04009	0.00878	0.38816	
C	2.11033	-1.10121	0.36419	
C	0.25251	-0.72705	1.65108	
H	-0.99487	-0.47468	-0.28785	
H	1.46248	-1.38496	1.58359	
H	1.87126	-2.06113	2.32219	
H	-0.47106	-0.78670	2.45316	
C	3.37196	-1.69723	-0.11471	
C	3.69316	-1.58809	-1.45781	
H	3.03268	-1.10398	-2.16482	
C	4.09676	-2.30451	0.77035	
H	1.66540	3.79587	-1.46810	
H	-1.93436	-0.93631	-1.09227	
C	-3.03030	-1.43068	-0.38231	
C	-4.20294	-1.64936	-1.34783	
H	-3.91179	-2.35495	-2.13121	
O	-5.08498	-2.04577	-0.83380	
H	-4.47483	-0.70224	-1.82274	
H	-3.46735	-0.43528	0.70835	
O	-2.66005	-0.29225	1.43227	
C	-3.69525	0.53459	0.25592	
C	-4.35388	-0.78644	1.24618	
H	-2.67637	-2.77033	0.28700	
H	-2.38360	-3.49813	-0.47578	
H	-1.83166	-2.62777	0.96764	
C	-3.51791	-3.18201	0.85425	
H	4.61430	-2.02550	-1.82836	
H	3.85657	-2.18753	1.36933	
H	4.36695	-0.51250	1.67443	
C	3.15827	0.62389	-0.51718	
H	3.07038	0.84380	-1.58697	
H	2.20091	0.86297	-0.04295	
H	3.92976	1.27719	-0.09269	

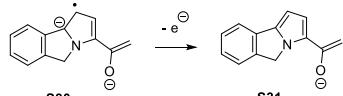
SM: S29 + tert-butoxide anion in DMSO

40	-865.0661243			
C	-1.66618	-2.45343	0.95276	
C	-1.37281	-1.26848	0.29004	
C	-2.20263	-0.79195	-0.72048	
C	-3.34559	-1.49336	-1.08628	
C	-3.64871	-2.68051	-0.41925	
C	-2.81530	-3.15716	0.59339	
H	-1.01645	-2.82362	1.73899	
H	-4.53960	-3.23641	-0.68798	
H	-3.06393	-4.08032	1.10406	
C	-1.64984	0.49779	-1.28284	
H	-1.29223	0.35746	-2.30880	
H	-2.38167	1.30711	-1.29470	
N	-0.53592	0.83173	-0.37506	
C	-0.19229	-0.34176	0.47853	
C	-0.60908	1.96615	0.44564	
C	0.00221	0.26353	1.84086	
H	0.72721	-0.83339	0.11083	
C	-0.25552	1.60702	1.76314	
H	-0.17656	2.32633	2.56592	
H	0.33526	-0.29582	2.70349	
C	-0.87825	3.34052	-0.03528	
C	-0.80508	3.57285	-1.39426	
H	-0.97755	4.57078	-1.78228	
O	-1.14063	4.22454	0.86857	
H	-3.99527	-1.12617	-1.87374	
H	-0.53906	2.78684	-2.08859	
O	2.51284	-1.67724	-0.88328	
C	3.48134	-0.87811	-0.32388	
C	4.86594	-1.14433	-0.95837	
H	4.81856	-0.94779	-2.03442	
H	5.65687	-0.51946	-0.52706	
H	5.13909	-2.19513	-0.81621	
C	3.60260	-1.13642	1.19624	
H	2.63998	-0.93235	1.67578	
H	3.85657	-2.18753	1.36933	
H	4.36695	-0.51250	1.67443	
C	3.15827	0.62389	-0.51718	
H	3.07038	0.84380	-1.58697	
H	2.20091	0.86297	-0.04295	
H	3.92976	1.27719	-0.09269	

Prod: S30 + *tert*-butanol in DMSO

40

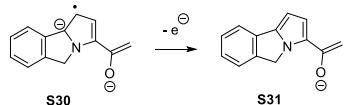
-865.0879020			
C	2.91802	-0.09566	1.26263
C	1.72101	-0.65361	0.70176
C	1.80837	-1.32326	-0.56759
C	2.99342	-1.45832	-1.23810
C	4.19169	-0.91232	-0.66919
C	4.10790	-0.23978	0.56808
H	2.89452	0.43226	2.21060
H	5.14019	-1.00970	-1.18224
H	5.01414	0.18253	0.99544
C	0.42051	-1.79466	-0.97476
H	0.05728	-1.29849	-1.88294
H	0.38076	-2.87484	-1.14416
N	-0.38458	-1.40381	0.18173
C	0.37015	-0.69783	1.12212
C	-1.74582	-1.32603	0.48821
C	-0.52353	-0.21128	2.08946
H	-0.96266	0.90487	-0.17437
C	-1.82447	-0.60931	1.67456
H	-2.75450	-0.40589	2.18414
H	-0.26710	0.37893	2.95666
C	-2.88297	-1.91247	-0.27096
C	-2.64472	-2.67903	-1.39580
H	-3.48883	-3.09794	-1.93325
H	-1.65354	-2.89909	-1.76021
O	-4.05696	-1.65028	0.19479
H	3.02883	-1.96820	-2.19730
O	-0.98855	1.52027	-0.92156
C	-0.63886	2.82377	-0.43899
C	-0.75905	3.75264	-1.63927
H	-1.78146	3.74394	-2.02440
H	-0.50116	4.77584	-1.35731
H	-0.08324	3.42972	-2.43481
C	0.79350	2.80445	0.09163
H	0.88213	2.08727	0.91199
H	1.48355	2.49993	-0.70000
H	1.08597	3.79491	0.45015
C	-1.61361	3.23264	0.66422
H	-2.63752	3.23022	0.28211
H	-1.54905	2.52711	1.49760
H	-1.38149	4.23379	1.03613



SM (Before SET): S30 in DMSO

25

-631.4374431			
C	-2.79124	1.26514	-0.03428
C	-1.52033	0.59767	-0.01463
C	-1.50643	-0.84003	0.03415
C	-2.65735	-1.57863	0.06318
C	-3.92635	-0.90930	0.05628
C	-3.94576	0.50111	0.00413
H	-2.85017	2.34808	-0.07328
H	-4.84929	-1.47497	0.07621
H	-4.90616	1.01074	-0.00693
C	-0.06235	-1.31783	0.05460
H	0.20737	-1.80693	0.99987
H	0.15109	-2.02042	-0.75538
N	0.67435	-0.06519	-0.10493
C	-0.17549	1.04143	-0.07918
C	2.00643	0.34087	0.00070
C	0.63440	2.18704	-0.04995
C	1.97854	1.72837	0.01005
H	2.86933	2.33883	0.03823
H	0.29246	3.21106	-0.03223
C	3.21748	-0.52175	0.01397
C	3.10427	-1.88389	-0.19345
H	2.16240	-2.37461	-0.38345
H	4.00222	-2.49267	-0.18194
O	4.33494	0.09001	0.21968
H	-2.61412	-2.66400	0.10238



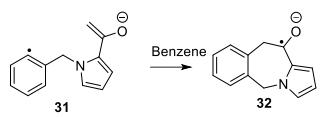
Prod (After SET): S31 in DMSO

25

-631.3942397

C	2.74636	1.25209	0.01558
C	1.53102	0.57328	0.01894
C	1.49907	-0.83073	-0.01366
C	2.67026	-1.56790	-0.04680
C	3.89022	-0.88731	-0.05001
C	3.92389	0.50736	-0.01907
H	2.77656	2.33524	0.03913
H	4.81741	-1.44709	-0.07678
H	4.87920	1.01919	-0.02248
C	0.06721	-1.31760	0.00484
H	-0.19168	-1.90664	-0.87862
H	-0.14328	-1.91596	0.89487
N	-0.67293	-0.05751	0.03138
C	0.15578	1.04304	0.04473
C	-1.98882	0.33877	0.01475
C	-0.62745	2.17983	0.04665
C	-1.97294	1.72961	0.02603
H	-2.86385	2.33760	0.01929
H	-0.27532	3.19978	0.05542
C	-3.20803	-0.53368	-0.02024
C	-3.07542	-1.89403	0.13286
H	-2.12949	-2.38357	0.30019
H	-3.96596	-2.51251	0.11165
O	-4.31315	0.09649	-0.18993
H	2.64520	-2.65177	-0.07051

6.2 Benzene (Scheme S2.2)



26

-631.8573282

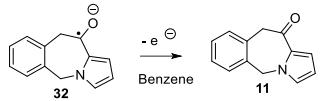
C	2.73158	0.13430	1.48264
C	1.51391	0.22203	0.81044
C	1.44844	0.03122	-0.57467
C	2.64705	-0.24167	-1.19640
C	3.87385	-0.34112	-0.58997
C	3.90960	-0.14513	0.79548
H	2.75716	0.28290	2.55568
H	0.59713	0.43491	1.35254
H	4.77653	-0.56119	-1.14864
H	4.85231	-0.21272	1.32688
C	0.14597	0.09761	-1.34899
H	0.29848	0.69261	-2.25338
H	-0.15469	-0.90869	-1.64472
N	-0.93582	0.68359	-0.58618
C	-1.05561	2.04109	-0.40674
C	-1.98223	0.03644	0.04562
C	-2.18600	2.27948	0.33887
H	-0.32832	2.71378	-0.83597
C	-2.77379	1.01631	0.61300
H	-3.68112	0.80927	1.15791
H	-2.54812	3.25084	0.64002
C	-2.24024	-1.45337	0.10031
C	-1.16059	-2.30278	0.21461
H	-0.14894	-1.94008	0.33726
H	-1.33609	-3.36978	0.29306
O	-3.47065	-1.77794	0.07717

Prod: 32 cyclised in Benzene

26

-631.9298533

C	3.17523	-1.14539	-0.68892
C	2.04985	-1.59794	-0.00470
C	1.13565	-0.69948	0.53888
C	1.33234	0.68461	0.39034
C	2.45978	1.12538	-0.30600
C	3.37675	0.22414	-0.83958
H	3.88429	-1.85406	-1.10153
H	1.87573	-2.66405	0.10669
H	2.61632	2.19211	-0.43076
H	4.24772	0.59087	-1.37156
C	-0.12269	-1.17707	1.21786
H	-0.08572	-2.25818	1.36138
H	-0.22953	-0.71662	2.20770
N	-1.29339	-0.88635	0.41181
C	-2.18576	-1.85133	-0.02542
C	-1.67855	0.37235	-0.07086
C	-3.15314	-1.22641	-0.78276
H	-2.04792	-2.88648	0.24501
C	-2.85485	0.15462	-0.82131
H	-3.39497	0.93413	-1.33395
H	-3.98684	-1.72317	-1.25813
C	-1.00606	1.61084	0.15835
C	0.31526	1.65038	0.93878
H	0.16249	1.46830	2.01243
H	0.68821	2.67067	0.84013
O	-1.46737	2.71285	-0.29852

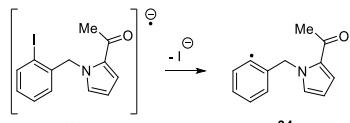


Prod (After SET): 11 in Benzene

26

-631.8918340

C	3.23064	-1.12431	-0.66784
C	2.07944	-1.60437	-0.04983
C	1.13720	-0.72204	0.46933
C	1.34376	0.65916	0.37379
C	2.49472	1.13187	-0.25118
C	3.43646	0.24634	-0.76882
H	3.95927	-1.81827	-1.06944
H	1.91070	-2.67324	0.02802
H	2.65582	2.20143	-0.33029
H	4.32873	0.62958	-1.24932
C	-0.11679	-1.22885	1.13511
H	-0.09030	-2.31437	1.22071
H	-0.21068	-0.81847	2.14516
N	-1.31867	-0.89163	0.37258
C	-2.24278	-1.80317	-0.02372
C	-1.70806	0.36025	-0.07390
C	-3.24285	-1.15749	-0.72921
H	-2.11959	-2.84656	0.22241
C	-2.90341	0.20585	-0.76111
H	-3.44475	1.01490	-1.22572
H	-4.10790	-1.62805	-1.16783
C	-0.98776	1.61979	0.14001
C	0.31687	1.61667	0.92852
H	0.08042	1.35749	1.96755
H	0.69213	2.63896	0.91719
O	-1.43097	2.66248	-0.29917



TS: 33 C-I elongation to give 34 in Benzene

28

-643.8878222

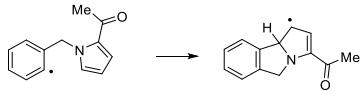
C	0.45728	2.99938	0.30352
C	0.90343	1.77418	-0.17821
C	0.07523	0.69032	-0.31691
C	-1.29197	0.91209	0.04184
C	-1.77325	2.12042	0.52019
C	-0.87703	3.17629	0.65589
H	1.19856	3.81734	0.40937
H	1.94275	1.63856	-0.44631
H	-2.81633	2.23819	0.78252
H	-1.22733	4.12906	1.03573
C	0.51819	-0.65123	-0.84581
H	0.12785	-1.44320	-0.20897
H	0.08527	-0.81232	-1.83820
N	1.95058	-0.74485	-0.97010
C	2.87093	-0.59906	0.09810
C	2.56768	-0.32506	-2.15406
C	4.06814	-0.11644	-0.47768
C	3.86290	0.03537	-1.86775
H	2.02123	-0.34487	-3.08433
H	4.97636	0.05317	0.07748
H	4.59382	0.35627	-2.59660
C	2.63912	-0.87845	1.47426
C	1.38307	-1.60322	1.93405
H	0.48767	-0.96600	1.94220
H	1.15688	-2.48337	1.32090
O	3.51747	-0.57895	2.35256
I	-2.79249	-0.74732	-0.14162
H	1.56055	-1.93659	2.95759

Prod: 34 + Iodide anion in Benzene

28

-643.9288407

C	1.26617	3.30715	0.52518
C	1.52459	2.08200	-0.08792
C	0.46754	1.25222	-0.47816
C	-0.81080	1.70704	-0.22854
C	-1.11079	2.90370	0.37787
C	-0.04264	3.72196	0.75930
H	2.09477	3.93655	0.82826
H	2.55015	1.76249	-0.25237
H	-2.13815	3.19708	0.56385
H	-0.23351	4.67305	1.24450
C	0.68077	-0.08546	-1.15550
H	-0.05604	-0.80113	-0.79415
H	0.51371	0.01391	-2.23011
N	2.03961	-0.59232	-0.98916
C	2.66147	-1.02701	0.17030
C	2.98190	-0.45412	-1.96024
C	4.01074	-1.17910	-0.11282
C	4.21582	-0.82113	-1.45825
H	2.69862	-0.09610	-2.93816
H	4.73801	-1.53727	0.59864
H	5.14281	-0.83548	-2.00888
C	2.04779	-1.33503	1.47953
C	0.55202	-1.40383	1.64309
H	0.08087	-0.43394	1.46402
H	0.11003	-2.10911	0.93530
O	2.78585	-1.56912	2.42114
I	-3.07672	-0.78031	-0.17658
H	0.33345	-1.72506	2.65966



SM: 34 cyclisation to 35 in Benzene

27

-632.3967710			
C	-2.25152	-0.19440	1.70366
C	-1.21279	-0.46335	0.84550
C	-1.28790	-0.48055	-0.52763
C	-2.54304	-0.20373	-1.08291
C	-3.63284	0.06860	-0.26188
C	-3.49424	0.07599	1.12534
H	-2.11853	-0.18867	2.77913
H	-4.59701	0.28184	-0.70738
H	-4.34691	0.29609	1.75723
C	-0.09308	-0.77975	-1.40788
H	-0.22027	-1.75524	-1.88131
H	-0.01968	-0.04592	-2.21073
N	1.15246	-0.83891	-0.65787
C	1.72528	-2.02565	-0.31099
C	1.77839	0.17584	0.05326
C	2.74338	-1.79637	0.59086
H	1.35351	-2.94864	-0.72930
C	2.77163	-0.40825	0.82241
H	3.44581	0.14609	1.45600
H	3.38946	-2.54629	1.01790
C	1.51834	1.62660	-0.00269
C	0.64750	2.22247	-1.08483
H	-0.39396	1.91917	-0.95340
H	0.71376	3.30622	-1.01198
O	2.04891	2.34991	0.81898
H	-2.66073	-0.19720	-2.16269
H	0.98135	1.90101	-2.07358

TS: 34 cyclisation to 35 in Benzene

27

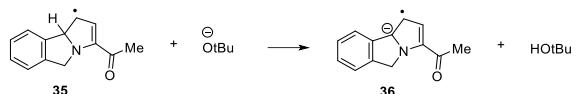
-632.3816047

C	-2.75247	1.07209	-0.54556
C	-1.62043	0.70381	0.14435
C	-1.32387	-0.59048	0.51787
C	-2.22573	-1.59567	0.17117
C	-3.38469	-1.26664	-0.53064
C	-3.64909	0.05371	-0.88880
H	-2.94935	2.10168	-0.82354
H	-4.08309	-2.04766	-0.80626
H	-4.55070	0.29508	-1.44073
C	-0.03047	-0.80146	1.28157
H	-0.21248	-0.81269	2.35982
H	0.45063	-1.73693	1.01080
N	0.83435	0.33746	0.96646
C	0.24645	1.58477	1.07730
C	1.72017	0.38448	-0.10395
C	0.88292	2.45844	0.18988
H	-0.35579	1.82128	1.94242
C	1.77881	1.69295	-0.56548
H	2.45314	2.03208	-1.33641
H	0.70660	3.52016	0.12177
C	2.60300	-0.70166	-0.55504
C	2.84567	-1.90392	0.33228
H	2.18534	-2.72113	0.02875
H	3.87180	-2.23349	0.17382
O	3.18060	-0.60101	-1.62166
H	-2.02516	-2.62843	0.44028
H	2.68213	-1.68651	1.38763

Prod: 35 in Benzene

27

C	-2.72298	1.11329	0.03468
C	-1.51483	0.49814	0.33099
C	-1.34520	-0.87083	0.15554
C	-2.38629	-1.65687	-0.31986
C	-3.60054	-1.04472	-0.62430
C	-3.76743	0.32891	-0.44974
H	-2.85362	2.18112	0.17199
H	-4.42220	-1.64094	-1.00286
H	-4.71694	0.78997	-0.69416
C	0.05380	-1.28653	0.54820
H	0.05541	-1.89660	1.45621
H	0.55472	-1.84421	-0.24425
N	0.73556	0.00242	0.77614
C	-0.24368	1.10951	0.87699
C	1.79361	0.42296	-0.00804
C	0.40456	2.22056	0.09991
H	-0.38844	1.40323	1.92644
C	1.58355	1.79278	-0.39181
H	2.30145	2.35589	-0.96953
H	-0.01944	3.21127	0.01883
C	2.96830	-0.35047	-0.31893
C	3.17877	-1.69093	0.35436
H	2.84637	-2.49839	-0.30395
H	4.24772	-1.82030	0.52310
O	3.80647	0.09015	-1.11064
H	-2.25862	-2.72476	-0.45884
H	2.64309	-1.76929	1.30107



SM: 35 + *tert*-butoxide anion in Benzene

41

-865.5414505

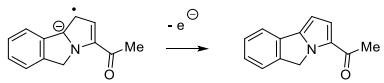
C	-1.44550	2.14282	1.20218
C	-0.46990	1.40486	0.54401
C	-0.05056	1.76949	-0.73533
C	-0.58781	2.87960	-1.37119
C	-1.55437	3.63362	-0.70512
C	-1.97912	3.26528	0.57140
H	-1.79146	1.84179	2.18479
H	-1.98229	4.50669	-1.18410
H	-2.73815	3.85348	1.07459
C	0.97265	0.78170	-1.25232
H	0.58828	0.22957	-2.11715
H	1.91159	1.26342	-1.53727
N	1.18418	-0.10652	-0.10207
C	0.19817	0.13377	0.96416
C	2.41720	-0.36217	0.46075
C	1.00953	0.04775	2.20293
H	-0.63274	-0.70828	1.00024
C	2.28358	-0.28485	1.89227
H	3.09466	-0.50253	2.57146
H	0.58449	0.12832	3.19393
C	3.59978	-0.72149	-0.25442
C	3.50356	-1.00206	-1.74351
H	2.49861	-1.30275	-2.04379
H	3.78981	-0.11813	-2.32134
O	4.69868	-0.83155	0.32233
H	-0.26541	3.15921	-2.36884
O	-1.80194	-1.73305	1.05373
C	-2.44472	-2.05176	-0.11914
C	-2.50310	-3.58342	-0.29855
H	-3.01634	-4.02722	0.55951
H	-3.02601	-3.88167	-1.21532
H	-1.48485	-3.98242	-0.32812
C	-1.71273	-1.45246	-1.34242
H	-1.71620	-0.35899	-1.27261
H	-0.67186	-1.79358	-1.34786
H	-2.18439	-1.73951	-2.28923
C	-3.88773	-1.50449	-0.11299
H	-4.43372	-1.93383	0.73232
H	-3.85722	-0.41807	0.01799
H	-4.43337	-1.73226	-1.03670
H	4.20995	-1.79790	-1.98271

Prod: 36 + *tert*-butanol in Benzene

41

-865.5881066

C	3.07456	-0.36323	1.22371
C	1.85844	-0.68374	0.59286
C	1.84017	-0.87216	-0.81774
C	2.98008	-0.71865	-1.57566
C	4.18879	-0.38626	-0.94197
C	4.21823	-0.22044	0.44757
H	3.11643	-0.21896	2.29762
H	5.09294	-0.25910	-1.52455
H	5.15610	0.03204	0.93151
C	0.44895	-1.29671	-1.24516
H	0.08808	-0.76056	-2.12604
H	0.40518	-2.37710	-1.45591
N	-0.33467	-0.98648	-0.04337
C	0.53109	-0.85633	1.06974
C	-1.57286	-1.50257	0.40823
C	-0.20612	-1.15018	2.22274
H	-0.71292	0.84944	-0.68056
C	-1.48175	-1.54714	1.82277
H	-2.30731	-1.82404	2.46116
H	0.16502	-1.09603	3.23589
C	-2.70802	-1.75413	-0.40275
C	-2.63486	-1.39762	-1.88173
H	-2.00273	-2.09357	-2.44238
H	-3.64407	-1.44668	-2.29056
O	-3.77635	-2.22873	0.06309
H	2.94962	-0.86359	-2.65130
H	-2.23607	-0.38908	-2.03103
O	-0.87087	1.72001	-1.08495
C	-0.89221	2.67683	-0.02434
C	-1.38153	3.97789	-0.64681
H	-2.37949	3.83916	-1.06910
H	-1.42391	4.77121	0.10356
H	-0.70582	4.28859	-1.44749
C	0.52001	2.84334	0.53855
H	0.87325	1.89420	0.95166
H	1.20477	3.15091	-0.25586
H	0.53828	3.59697	1.33119
C	-1.84882	2.19590	1.06581
H	-2.85024	2.05609	0.65053
H	-1.50777	1.23755	1.47095
H	-1.90372	2.91893	1.88444



SM (Before SET): 36 in Benzene

26

-631.9360589

C	-2.81716	1.23354	-0.00400
C	-1.56492	0.58968	-0.01302
C	-1.52384	-0.83500	-0.00138
C	-2.67900	-1.58470	0.01539
C	-3.92532	-0.93635	0.02282
C	-3.97310	0.46364	0.01357
H	-2.87836	2.31612	-0.01101
H	-4.84121	-1.51430	0.03593
H	-4.93751	0.96133	0.02032
C	-0.08030	-1.30179	-0.01060
H	0.17357	-1.89055	0.88109
H	0.14713	-1.91489	-0.89238
N	0.63616	-0.03755	-0.03630
C	-0.22577	1.06055	-0.02863
C	1.96818	0.38507	-0.00609
C	0.56699	2.21633	-0.00723
C	1.89738	1.80923	0.00670
H	2.77318	2.43951	0.02263
H	0.19959	3.23197	-0.00018
C	3.16051	-0.38584	0.00781
C	3.13624	-1.90398	-0.02166
H	3.76880	-2.24570	-0.84704
H	3.58245	-2.28871	0.90182
O	4.30021	0.16506	0.05184
H	-2.63010	-2.66970	0.02409
H	2.14828	-2.34511	-0.13811

Prod (After SET): 13 in Benzene

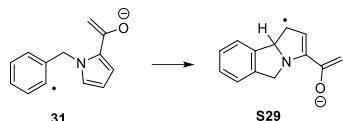
26

-631.8907121			
C	2.77921	1.23558	0.00029
C	1.55803	0.57164	0.00007
C	1.50400	-0.82922	-0.00020
C	2.66317	-1.58516	-0.00033
C	3.89027	-0.92015	-0.00014
C	3.94510	0.47362	0.00018
H	2.82243	2.31812	0.00051
H	4.80969	-1.49297	-0.00026
H	4.90800	0.97024	0.00040
C	0.06407	-1.29229	0.00005
H	-0.17777	-1.87927	-0.88840
H	-0.17702	-1.87899	0.88894
N	-0.65279	-0.01517	0.00024
C	0.18717	1.06168	0.00026
C	-1.96101	0.42310	-0.00024
C	-0.56941	2.22384	-0.00014
C	-1.91580	1.81474	-0.00048
H	-2.79342	2.44246	-0.00085
H	-0.19102	3.23321	-0.00026
C	-3.16535	-0.41269	0.00009
C	-3.01199	-1.91596	0.00008
H	-4.00145	-2.36822	-0.00002
H	-2.46162	-2.24595	-0.88417
O	-4.26696	0.10372	0.00021
H	2.62436	-2.66863	-0.00064
H	-2.46169	-2.24597	0.88436

TS: 31 cyclisation to form S29 in Benzene

26

-631.8456646			
C	2.76532	1.07428	0.58402
C	1.60796	0.75090	-0.09553
C	1.32297	-0.53103	-0.52810
C	2.24428	-1.54477	-0.26118
C	3.42106	-1.24936	0.42617
C	3.68331	0.05166	0.85026
H	2.96615	2.08787	0.91724
H	4.13140	-2.03997	0.63962
H	4.59704	0.27168	1.39273
C	0.01265	-0.75382	-1.26267
H	0.17690	-0.77011	-2.34524
H	-0.46431	-1.68820	-0.97196
N	-0.87425	0.35290	-0.92476
C	-0.34858	1.63546	-0.99750
C	-1.81789	0.31439	0.08642
C	-1.06551	2.44093	-0.11320
H	0.26159	1.92510	-1.83945
C	-1.95610	1.60211	0.58347
H	-2.65997	1.87446	1.35398
H	-0.94857	3.50891	-0.00648
C	-2.61506	-0.89302	0.50763
C	-2.93240	-1.80414	-0.47773
H	-2.65999	-1.63756	-1.51216
H	-3.55102	-2.66049	-0.23469
O	-2.96269	-0.91751	1.73076
H	2.03989	-2.56350	-0.57872



SM: 31 cyclisation to form S29 in Benzene

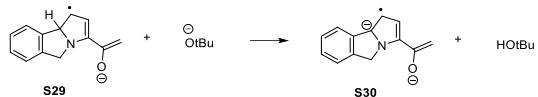
26

-631.8555478			
C	3.01738	-1.11400	-0.91319
C	1.82597	-1.04667	-0.23348
C	1.41994	-0.01870	0.58835
C	2.32281	1.04128	0.72970
C	3.55026	1.02566	0.07101
C	3.90264	-0.04365	-0.74917
H	3.26628	-1.95393	-1.55184
H	4.23032	1.86133	0.18692
H	4.85500	-0.04520	-1.26738
C	0.09421	-0.02971	1.31940
H	0.20854	-0.58354	2.25671
H	-0.20300	0.99247	1.55125
N	-0.97306	-0.65175	0.56011
C	-1.14079	-2.01394	0.49373
C	-2.00423	-0.02259	-0.11016
C	-2.28719	-2.27222	-0.22227
H	-0.43923	-2.67447	0.98042
C	-2.83561	-1.01590	-0.59110
H	-3.73692	-0.82389	-1.15153
H	-2.68288	-3.25175	-0.44442
C	-2.18813	1.46733	-0.28650
C	-1.06305	2.22908	-0.52280
H	-0.08925	1.77869	-0.66496
H	-1.17122	3.29281	-0.70364
O	-3.39436	1.87020	-0.23716
H	2.04335	1.89223	1.34394

Prod: S29 cyclised in Benzene

26

-631.8968615			
C	-2.67329	1.11582	0.01557
C	-1.47728	0.49519	0.34985
C	-1.31232	-0.87553	0.17852
C	-2.34628	-1.65183	-0.32996
C	-3.54903	-1.03383	-0.67061
C	-3.71156	0.34102	-0.49950
H	-2.79662	2.18639	0.14370
H	-4.36197	-1.62451	-1.07736
H	-4.64973	0.80987	-0.77392
C	0.07203	-1.29124	0.61779
H	0.02941	-1.89564	1.53103
H	0.60784	-1.86838	-0.13709
N	0.76859	-0.01557	0.85912
C	-0.20996	1.10137	0.92144
C	1.81538	0.37177	0.00084
C	0.44701	2.19580	0.12408
H	-0.39496	1.40439	1.96373
C	1.61371	1.70079	-0.40373
H	2.32825	2.22451	-1.02201
H	0.04373	3.19367	0.03092
C	3.00786	-0.45417	-0.32755
C	3.23978	-1.56800	0.45897
H	2.60931	-1.80509	1.30617
H	4.11839	-2.17609	0.27588
O	3.72622	-0.03784	-1.30002
H	-2.21986	-2.72046	-0.46897



SM: S29 + tert-butoxide anion in Benzene

40

-864.9549963

C	0.85455	1.06787	-0.06983
C	-0.47646	0.81097	0.24507
C	-1.44999	1.80054	0.14536
C	-1.11651	3.07752	-0.29001
C	0.21150	3.34534	-0.62276
C	1.18393	2.35052	-0.50972
H	1.64902	0.32560	0.02139
H	0.49035	4.33499	-0.96895
H	2.21730	2.56471	-0.75955
C	-2.79363	1.26870	0.58462
H	-3.12815	1.75720	1.50748
H	-3.57628	1.40855	-0.16348
N	-2.55906	-0.17142	0.80055
C	-1.10184	-0.47177	0.75327
C	-3.22539	-1.10379	-0.01773
C	-1.01915	-1.68885	-0.12898
H	-0.71359	-0.68567	1.76122
C	-2.28526	-2.00733	-0.54735
H	-2.57679	-2.83681	-1.17571
H	-0.09333	-2.20394	-0.34030
C	-4.69759	-1.17848	-0.20120
C	-5.48330	-0.44367	0.67071
H	-5.04795	0.13087	1.47794
H	-6.56341	-0.49387	0.58772
O	-5.11535	-1.94031	-1.14293
H	-1.87306	3.85173	-0.37252
O	3.66166	-0.21646	0.13167
C	4.91207	-0.73971	0.05415
C	5.43281	-1.16975	1.45087
H	5.43538	-0.29758	2.11256
H	4.74787	-1.91178	1.87298
H	6.44430	-1.59635	1.42409
C	5.92020	0.29002	-0.52166
H	5.92636	1.17797	0.11854
H	6.94416	-0.09985	-0.59510
H	5.58743	0.59461	-1.51896
C	4.94628	-1.98885	-0.86457
H	4.25878	-2.74238	-0.46781
H	4.59541	-1.70502	-1.86170
H	5.94577	-2.43452	-0.95488

TS: S29 + tert-butoxide anion in Benzene

40

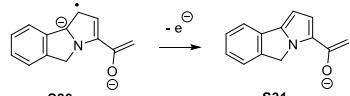
	-864.9392848			
C	-1.99798	-2.10920	1.01013	
C	-1.49756	-0.97287	0.37432	
C	-2.24758	-0.36596	-0.64397	
C	-3.47698	-0.87451	-1.02944	
C	-3.97801	-2.01336	-0.39010	
C	-3.23742	-2.62025	0.62453	
H	-1.42512	-2.59194	1.79555	
H	-4.93974	-2.42181	-0.68052	
H	-3.63075	-3.50279	1.11901	
C	-1.50126	0.83499	-1.18125	
H	-1.21188	0.67910	-2.22895	
H	-2.08396	1.75936	-1.13776	
N	-0.32615	0.93066	-0.31076	
C	-0.20345	-0.27201	0.54793	
C	-0.03518	2.07037	0.45070	
C	0.21698	0.27911	1.85690	
H	0.71139	-1.10566	0.09016	
C	0.32483	1.65177	1.74301	
H	0.67022	2.34410	2.49862	
H	0.48060	-0.32604	2.71396	
C	0.02682	3.45987	-0.06817	
C	-0.00388	3.64390	-1.44353	
H	-0.00124	2.80613	-2.12907	
H	0.06647	4.64863	-1.84685	
O	0.11626	4.39581	0.80779	
H	-4.05087	-0.39171	-1.81543	
O	1.58865	-1.98765	-0.37859	
C	2.88387	-1.49131	-0.33698	
C	2.93206	-0.01598	-0.77986	
H	2.50884	0.07950	-1.78431	
H	2.33177	0.60661	-0.11024	
H	3.95864	0.36845	-0.79215	
C	3.76980	-2.32147	-1.28193	
H	3.38254	-2.24572	-2.30213	
H	4.81266	-1.98178	-1.27480	
H	3.73952	-3.37366	-0.98203	
C	3.45460	-1.59357	1.09185	
H	2.83010	-1.00349	1.76862	
H	3.43072	-2.63800	1.41939	
H	4.48583	-1.22626	1.15578	

Prod: S30 + *tert*-butanol in Benzene

40

-864.9792918

C	1.85336	-1.64040	1.41101
C	0.61634	-1.34843	0.73276
C	0.51133	-1.65961	-0.66167
C	1.54468	-2.21504	-1.36879
C	2.78265	-2.51012	-0.68871
C	2.88752	-2.20717	0.68321
H	1.97785	-1.41382	2.46467
H	3.62181	-2.93307	-1.22654
H	3.82539	-2.41733	1.19270
C	-0.87248	-1.25756	-1.15132
H	-0.83630	-0.51542	-1.95608
H	-1.44855	-2.11732	-1.51007
N	-1.47349	-0.69148	0.05250
C	-0.60826	-0.74429	1.13942
C	-2.64179	-0.01127	0.38461
C	-1.24423	-0.10852	2.20801
H	2.34709	0.16200	-0.47327
C	-2.50515	0.34244	1.71614
H	-3.27096	0.87552	2.25909
H	-0.84054	0.02579	3.20069
C	-3.82106	0.27846	-0.49153
C	-3.84374	-0.20410	-1.78968
H	-3.05378	-0.80607	-2.21048
H	-4.70770	0.01444	-2.40856
O	-4.74914	0.97433	0.04908
H	1.43910	-2.42182	-2.43013
O	2.76675	0.98802	-0.75860
C	2.00604	2.09308	-0.26900
C	0.58667	2.05101	-0.83415
H	0.61954	1.99629	-1.92566
H	0.04784	1.18179	-0.44997
H	0.02510	2.94349	-0.54386
C	2.74485	3.33156	-0.76400
H	2.78707	3.33003	-1.85617
H	2.23551	4.23999	-0.43330
H	3.76717	3.33858	-0.37704
C	1.96609	2.06123	1.25842
H	1.45438	1.15634	1.59596
H	2.98313	2.06694	1.66023
H	1.42360	2.92764	1.64789



SM (Before SET): S30 in Benzene

25

C	-2.79616	1.26861	0.00015
C	-1.52389	0.59435	0.00004
C	-1.51194	-0.83559	-0.00005
C	-2.66046	-1.58186	-0.00015
C	-3.93709	-0.90684	-0.00020
C	-3.95083	0.50225	0.00006
H	-2.85190	2.35223	0.00036
H	-4.86243	-1.47021	-0.00020
H	-4.91169	1.01378	0.00010
C	-0.06641	-1.31351	-0.00001
H	0.17602	-1.91101	0.88519
H	0.17614	-1.91105	-0.88515
N	0.67585	-0.05781	-0.00000
C	-0.17135	1.04350	0.00005
C	2.00992	0.34145	-0.00004
C	0.63535	2.18530	0.00006
C	1.98545	1.72613	0.00002
H	2.88326	2.32595	-0.00012
H	0.29084	3.20876	0.00017
C	3.23170	-0.52363	-0.00003
C	3.09615	-1.90294	0.00040
H	2.14214	-2.40623	0.00069
H	3.99521	-2.51046	0.00041
O	4.35035	0.09968	-0.00038
H	-2.61396	-2.66783	-0.00023

Prod (After SET): S31 in Benzene

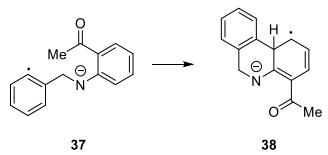
25

-631.3512135

C	2.74842	1.25041	0.01241
C	1.52881	0.57753	0.01708
C	1.49794	-0.82908	-0.01138
C	2.66811	-1.56564	-0.04115
C	3.89161	-0.88963	-0.04531
C	3.92515	0.50439	-0.01881
H	2.78056	2.33361	0.03254
H	4.81784	-1.45138	-0.06942
H	4.88094	1.01613	-0.02303
C	0.06475	-1.31299	0.00664
H	-0.19781	-1.90316	-0.87556
H	-0.15083	-1.91007	0.89694
N	-0.67205	-0.05547	0.03047
C	0.15787	1.04719	0.04134
C	-1.98701	0.33549	0.01570
C	-0.63175	2.18072	0.04132
C	-1.97404	1.72659	0.02375
H	-2.87361	2.32114	0.01379
H	-0.28332	3.20213	0.04710
C	-3.21504	-0.53492	-0.01937
C	-3.06975	-1.90053	0.11270
H	-2.12065	-2.38667	0.27177
H	-3.95880	-2.52041	0.09539
O	-4.30755	0.09998	-0.16883
H	2.64008	-2.64990	-0.06167

7. Radical Cyclisation of 15

7.1 DMSO (Scheme S3.1)



SM: 37 cyclisation to 38

30
-709.3095148

C	4.58104	-0.24887	0.06626
C	3.57387	-0.58111	-0.83645
C	2.21899	-0.46079	-0.49229
C	1.97671	-0.00355	0.78379
C	2.92485	0.34277	1.71871
C	4.26559	0.21217	1.34390
C	1.12087	-0.82697	-1.48381
C	-0.36685	1.42481	-0.78481
C	-0.87213	0.07126	-0.58955
C	-2.21732	0.00434	-0.00811
C	-2.91854	1.20227	0.25562
C	-2.40637	2.45979	0.01924
C	-1.09916	2.54725	-0.50411
H	1.42590	-1.77035	-1.94943
H	5.61919	-0.35412	-0.22673
H	3.83453	-0.94338	-1.82747
H	2.65394	0.70083	2.70582
H	5.05238	0.46664	2.04502
H	-3.91559	1.13775	0.67350
H	-2.98186	3.34884	0.24365
H	-0.65535	3.52326	-0.68079
C	-2.88338	-1.25560	0.32630
C	-4.30753	-1.20848	0.88485
H	-4.34957	-0.67120	1.83468
H	-4.99809	-0.71910	0.19502
H	-4.63309	-2.23448	1.04560
O	-2.37893	-2.37015	0.19849
N	-0.19231	-1.01092	-0.91213
H	1.14369	-0.07879	-2.29519
H	0.63770	1.55601	-1.16388

TS: 37 cyclisation to 38

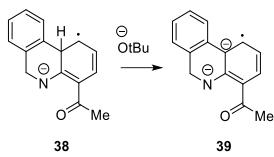
30 -709.3041328	C	4.19763	-0.64349	0.80006
	C	3.28584	-1.32197	-0.01074
	C	2.08972	-0.71053	-0.40197
	C	1.85085	0.57069	0.05780
	C	2.73377	1.27836	0.84772
	C	3.92834	0.65315	1.23043
	C	1.07338	-1.42647	-1.28808
	C	-0.15018	1.04407	-1.18393
	C	-0.80525	-0.16226	-0.66975
	C	-2.07616	0.07380	0.02016
	C	-2.48675	1.39350	0.27573
	C	-1.80537	2.51034	-0.18632
	C	-0.66445	2.31340	-0.97363
	H	1.36561	-2.47703	-1.36303
	H	5.11942	-1.13110	1.09659
	H	3.50648	-2.33328	-0.34241
	H	2.51917	2.29144	1.17643
	H	4.63912	1.17743	1.86072
	H	-3.40477	1.55566	0.82781
	H	-2.18289	3.50581	0.01157
	H	-0.16276	3.16419	-1.42482
	C	-2.95718	-1.01591	0.44702
	C	-4.08621	-0.70102	1.42614
	H	-3.74539	-0.10841	2.27601
	H	-4.88427	-0.14404	0.92813
	H	-4.49551	-1.64545	1.78081
	O	-2.86259	-2.17473	0.05055
	N	-0.27409	-1.35800	-0.76213
	H	1.15689	-1.01177	-2.30684
	H	0.62029	0.92654	-1.93432

Prod: 38 cyclised

30

-709.3701967

C	-4.04103	-0.48513	-0.88523
C	-3.20372	-1.37654	-0.21558
C	-2.01500	-0.92168	0.34469
C	-1.64738	0.42052	0.22750
C	-2.47464	1.30641	-0.45674
C	-3.67380	0.85225	-1.00717
C	-1.01094	-1.79428	1.04544
C	-0.32055	0.77450	0.87742
C	0.70707	-0.30969	0.46468
C	2.02482	0.11977	-0.00425
C	2.30288	1.51852	-0.06575
C	1.36657	2.50738	0.28221
C	0.10672	2.19800	0.71406
H	-1.25009	-2.85015	0.90623
H	-4.97119	-0.83548	-1.31794
H	-3.47397	-2.42462	-0.13281
H	-2.18644	2.34541	-0.56756
H	-4.31801	1.54417	-1.53775
H	3.27374	1.84982	-0.40641
H	1.66225	3.54939	0.20267
H	-0.59269	2.97435	1.00371
C	3.04320	-0.81538	-0.41563
C	4.39085	-0.24886	-0.86807
H	4.28464	0.39822	-1.74255
H	4.86650	0.34129	-0.08070
H	5.03830	-1.08591	-1.12429
O	2.92731	-2.05396	-0.44084
N	0.35208	-1.54778	0.57353
H	-1.06452	-1.59373	2.12848
H	-0.48168	0.57862	1.95550

**SM: 38 + *tet*-butoxide anion**

44

-942.4969340			
C	4.69901	0.32158	-0.38556
C	3.67732	0.35918	-1.33412
C	2.35082	0.25457	-0.92980
C	2.02994	0.09139	0.42039
C	3.05361	0.03561	1.36370
C	4.38427	0.15843	0.96050
C	1.17144	0.24851	-1.86030
C	0.54593	-0.01987	0.71906
C	-0.08318	-0.98282	-0.31339
C	-1.03731	-1.99217	0.15806
C	-1.30147	-2.07116	1.56049
C	-0.68016	-1.24265	2.51166
C	0.22052	-0.27837	2.15461
H	1.49604	0.16106	-2.89935
H	5.73365	0.40984	-0.69686
H	3.91222	0.46924	-2.38848
H	2.82137	-0.11033	2.41226
H	5.17601	0.11745	1.70025
H	-2.00004	-2.81104	1.92638
H	-0.93436	-1.37734	3.55927
H	0.65675	0.37856	2.89972
C	-1.71032	-2.90058	-0.73337
C	-2.70071	-3.89547	-0.12096
H	-2.21240	-4.56772	0.58961
H	-3.50828	-3.38814	0.41333
H	-3.12782	-4.48670	-0.92957
O	-1.56445	-2.95953	-1.97113
N	0.23757	-0.83775	-1.55699
H	0.64372	1.20995	-1.75478
H	0.12352	0.97684	0.44612
O	-0.65130	3.01185	0.28832
C	-1.96551	2.80430	-0.05644
C	-2.74466	4.13726	-0.13675
H	-2.28113	4.78974	-0.88409
H	-3.79796	3.99592	-0.40670
H	-2.70216	4.64670	0.83135
C	-2.67956	1.90035	0.97654
H	-2.15790	0.93975	1.04496
H	-2.64616	2.37421	1.96390
H	-3.72908	1.71246	0.72000
C	-2.08186	2.10647	-1.43154
H	-1.58265	2.71270	-2.19520
H	-1.58542	1.13207	-1.38907
H	-3.12360	1.95308	-1.73837

TS: 38 + tert-butoxide anion

44

-942.4919052

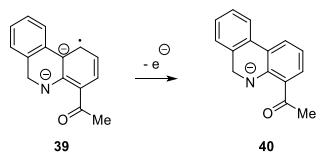
C	4.64152	-0.75862	-0.39032
C	3.63516	-0.60535	-1.34555
C	2.31639	-0.41182	-0.95126
C	1.96251	-0.40438	0.40566
C	2.97568	-0.58029	1.35611
C	4.30354	-0.74321	0.96001
C	1.17312	-0.20353	-1.90120
C	0.51175	-0.19761	0.71550
C	-0.36560	-0.92246	-0.29114
C	-1.62453	-1.52882	0.18652
C	-1.88430	-1.52253	1.59535
C	-1.01495	-0.94285	2.53233
C	0.14949	-0.33222	2.14371
H	1.46905	-0.45790	-2.92273
H	5.67252	-0.89271	-0.69711
H	3.87943	-0.62467	-2.40404
H	2.73458	-0.60015	2.41236
H	5.07436	-0.87070	1.71273
H	-2.79218	-1.97597	1.96923
H	-1.28570	-0.97162	3.58456
H	0.78166	0.15150	2.88148
C	-2.61164	-2.08008	-0.69549
C	-3.88888	-2.64827	-0.06437
H	-3.67604	-3.46828	0.62728
H	-4.43968	-1.88756	0.49619
H	-4.52316	-3.02163	-0.86719
O	-2.55295	-2.13896	-1.94734
N	-0.01742	-0.97140	-1.54021
H	0.91183	0.86601	-1.88275
H	0.34817	1.02165	0.44051
O	0.28188	2.45418	0.21862
C	-1.00262	2.88846	-0.08606
C	-1.05724	4.42466	-0.04095
H	-0.34840	4.84193	-0.76294
H	-2.05660	4.80915	-0.27380
H	-0.77468	4.77454	0.95657
C	-2.02578	2.33050	0.92326
H	-1.99784	1.23641	0.91893
H	-1.77342	2.67232	1.93255
H	-3.04541	2.65892	0.69237
C	-1.41708	2.42293	-1.49565
H	-0.71784	2.82253	-2.23739
H	-1.38216	1.33040	-1.54637
H	-2.42715	2.75673	-1.75801

Prod: 39 + tert-butanol

44

-942.5251437

C	4.76189	-0.43530	-0.35936
C	3.73286	-0.43840	-1.30991
C	2.40407	-0.38475	-0.91929
C	2.03944	-0.38239	0.44847
C	3.08992	-0.38838	1.39751
C	4.42146	-0.40058	0.99373
C	1.24697	-0.24310	-1.86327
C	0.63131	-0.46252	0.78013
C	-0.24673	-1.03204	-0.24466
C	-1.54282	-1.59081	0.21639
C	-1.89770	-1.39166	1.59892
C	-1.06448	-0.76210	2.51696
C	0.19474	-0.31727	2.13227
H	1.56026	-0.45880	-2.89028
H	5.80061	-0.45149	-0.66870
H	3.97209	-0.45111	-2.37050
H	2.86243	-0.40707	2.45730
H	5.20434	-0.40009	1.74592
H	-2.85767	-1.74486	1.95177
H	-1.40414	-0.62200	3.53940
H	0.84960	0.15292	2.85890
C	-2.46449	-2.28297	-0.62847
C	-3.81792	-2.68201	-0.02528
H	-3.70818	-3.41439	0.78194
H	-4.36144	-1.82825	0.39112
H	-4.41830	-3.13006	-0.81681
O	-2.29195	-2.63301	-1.83369
N	0.10102	-1.07316	-1.51971
H	0.93940	0.82202	-1.84088
H	0.16303	1.67579	0.37362
O	0.03903	2.63386	0.24718
C	-1.30670	2.85768	-0.19104
C	-1.46584	4.36916	-0.28665
H	-0.74435	4.78180	-0.99626
H	-2.47220	4.62569	-0.62539
H	-1.29885	4.83077	0.68971
C	-2.27835	2.26912	0.82951
H	-2.11632	1.19072	0.92658
H	-2.12360	2.73201	1.80828
H	-3.31305	2.44366	0.52143
C	-1.52101	2.20390	-1.55621
H	-0.81909	2.61619	-2.28619
H	-1.35890	1.12348	-1.48801
H	-2.53916	2.38496	-1.91161



SM (Before SET): 39

29

-708.8734067

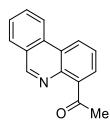
C	-4.25019	-0.50109	-0.57560
C	-3.28984	-1.37406	-0.04735
C	-2.03226	-0.91300	0.30985
C	-1.65769	0.43701	0.10194
C	-2.63749	1.30690	-0.43517
C	-3.90896	0.84192	-0.75336
C	-0.98802	-1.72824	1.01218
C	-0.28641	0.80680	0.36872
C	0.69342	-0.27642	0.30560
C	2.09655	0.10945	0.01646
C	2.43155	1.50319	0.17155
C	1.47564	2.49599	0.37116
C	0.12235	2.16991	0.41137
H	-1.24941	-2.79133	0.99673
H	-5.24052	-0.85829	-0.83280
H	-3.53739	-2.41967	0.11863
H	-2.39061	2.34569	-0.62618
H	-4.63995	1.53288	-1.16227
H	3.46815	1.80687	0.09985
H	1.79236	3.52991	0.47533
H	-0.62479	2.95048	0.51771
C	3.11218	-0.80830	-0.38136
C	4.53502	-0.26116	-0.54886
H	4.59473	0.50848	-1.32579
H	4.92091	0.18794	0.37245
H	5.18400	-1.08997	-0.83124
O	2.97164	-2.04346	-0.64101
N	0.34951	-1.54255	0.46931
H	-0.99236	-1.41083	2.07774

Prod (After SET): 40

29

-708.8121885

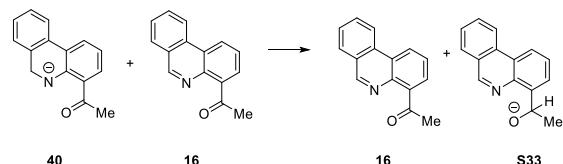
C	-4.27740	-0.48206	-0.48141
C	-3.31826	-1.35696	0.02321
C	-2.03386	-0.90577	0.31439
C	-1.67921	0.42860	0.07110
C	-2.64292	1.29580	-0.46384
C	-3.93422	0.84900	-0.71907
C	-0.97064	-1.76748	0.93928
C	-0.27772	0.80783	0.30006
C	0.70708	-0.28460	0.25128
C	2.08607	0.14186	-0.00175
C	2.41437	1.50193	0.14408
C	1.47759	2.48844	0.39558
C	0.12092	2.12167	0.41638
H	-1.22844	-2.82367	0.82168
H	-5.28018	-0.83416	-0.69400
H	-3.57213	-2.39644	0.20886
H	-2.37869	2.32029	-0.70195
H	-4.66917	1.53461	-1.12577
H	3.45019	1.80277	0.04156
H	1.77601	3.52202	0.51334
H	-0.63507	2.89690	0.50715
C	3.14571	-0.79127	-0.38291
C	4.58982	-0.29318	-0.40224
H	4.73897	0.45334	-1.18596
H	4.87817	0.15992	0.54785
H	5.23437	-1.14623	-0.60642
O	2.94975	-1.95810	-0.71670
N	0.37398	-1.54002	0.42222
H	-0.97391	-1.56715	2.02691



Prod: 16
28

-708.1155762

C	3.25938	-0.63601	-0.06414
O	4.24665	-0.34068	-0.70712
C	2.09626	0.31820	-0.03538
C	0.74366	-0.10641	-0.03377
C	2.39464	1.66699	0.00542
C	-0.28957	0.85812	0.03705
C	1.37277	2.62190	0.08735
H	3.43308	1.97619	-0.01018
C	-1.66469	0.39133	0.01802
C	0.05468	2.22283	0.10721
C	-0.73377	-1.86157	-0.17069
H	1.62086	3.67501	0.13614
C	-1.87838	-0.99705	-0.08649
C	-2.79075	1.23667	0.09302
H	-0.72183	2.97435	0.17003
H	-0.90814	-2.93257	-0.26350
C	-3.18383	-1.52491	-0.11479
C	-4.06322	0.70617	0.06606
H	-2.66944	2.30884	0.17371
C	-4.26810	-0.68165	-0.03855
H	-3.31751	-2.59820	-0.19716
H	-4.91838	1.36904	0.12506
H	-5.27526	-1.07911	-0.05924
C	3.22756	-1.89618	0.76159
H	2.56791	-1.80042	1.62290
H	2.84347	-2.70938	0.14365
H	4.24583	-2.12973	1.07199
N	0.49520	-1.46273	-0.14969



SM: Hydride transfer between 40 and 16

57

C	4.09971	0.25057	-2.25134
C	3.53712	1.22362	-1.43258
C	2.16249	1.26594	-1.20146
C	1.31106	0.34678	-1.83123
C	1.89111	-0.62327	-2.66530
C	3.26374	-0.68169	-2.86323
C	1.57702	2.27570	-0.24522
C	-0.14378	0.49252	-1.63953
C	-0.61656	1.68015	-0.91795
C	-2.06549	1.82659	-0.82784
C	-2.91246	0.92820	-1.49894
C	-2.43408	-0.16577	-2.18628
C	-1.04273	-0.36735	-2.23166
H	2.17075	3.19652	-0.29248
H	5.17049	0.22398	-2.41738
H	4.17392	1.97029	-0.96591
H	1.26734	-1.34511	-3.17795
H	3.68035	-1.44839	-3.50701
H	-3.98148	1.08693	-1.40527
H	-3.10907	-0.88226	-2.63750
H	-0.67466	-1.24261	-2.75783
C	-2.73418	2.80244	0.03771
C	-2.00088	3.46876	1.18292
H	-2.74020	3.72141	1.94559
H	-1.20646	2.83894	1.57834
H	-1.52536	4.38670	0.83015
O	-3.93949	3.05488	-0.08810
N	0.17659	2.59847	-0.41586
H	1.72458	1.89194	0.78304
C	2.58689	0.21800	2.62530
O	2.07597	0.42942	3.70393
C	1.99088	-0.75100	1.64583
C	0.58422	-0.87884	1.46711
C	2.85033	-1.58543	0.95543
C	0.08560	-1.92897	0.65910
C	2.35309	-2.60442	0.13283
H	3.92224	-1.46716	1.06391
C	-1.35264	-2.07338	0.52686
C	0.99481	-2.78174	0.00340
C	-1.51646	-0.03836	1.86080
H	3.03969	-3.25162	-0.39883
C	-2.16080	-1.10215	1.14316
C	-1.98399	-3.12321	-0.17224
H	0.62755	-3.57590	-0.63455
H	-2.14949	0.73368	2.29763
C	-3.56401	-1.17299	1.05598
C	-3.35944	-3.19145	-0.23519
H	-1.39742	-3.89332	-0.65668
C	-4.16067	-2.21162	0.37887
H	-4.16054	-0.39909	1.52982
H	-3.83029	-4.01085	-0.76626
H	-5.24012	-2.27570	0.31198
C	3.90612	0.86331	2.25857
H	4.72183	0.19117	2.54145
H	3.98283	1.05425	1.18839
H	4.01569	1.78684	2.82498
N	-0.24085	0.06858	2.04336

TS: Hydride transfer between **40** and **16**

57

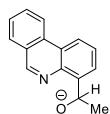
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C	-4.00974	-0.45497	2.21452
C	-3.61584	0.63311	1.45657
C	-2.25917	0.87423	1.20634
C	-1.27416	0.04718	1.77078
C	-1.69193	-1.05978	2.53163
C	-3.03627	-1.31525	2.73600
C	-1.82956	1.98574	0.34058
C	0.12643	0.43817	1.59910
C	0.39237	1.67847	0.93673
C	1.75077	2.11455	0.88006
C	2.76291	1.36967	1.47640
C	2.49238	0.15111	2.09249
C	1.18179	-0.30267	2.13741
H	-2.60113	2.73371	0.14106
H	-5.06039	-0.63931	2.40514
H	-4.35640	1.31534	1.05209
H	-0.96239	-1.72495	2.97634
H	-3.33418	-2.17675	3.32288
H	3.78081	1.73788	1.41030
H	3.29345	-0.44568	2.51088
H	0.97981	-1.25502	2.61417
C	2.18168	3.32583	0.12274
C	1.51980	3.67309	-1.18863
H	2.28329	4.07907	-1.85435
H	1.01915	2.81088	-1.62694
H	0.76147	4.43816	-1.01279
O	3.13066	3.98765	0.51431
N	-0.57262	2.47636	0.40942
H	-2.00543	1.38984	-0.94535
C	-2.33224	0.77681	-2.09406
O	-1.79839	1.36041	-3.10458
C	-1.79248	-0.57556	-1.62923
C	-0.39190	-0.80255	-1.46889
C	-2.66522	-1.58833	-1.27110
C	0.07053	-2.03139	-0.93009
C	-2.20674	-2.81595	-0.77022
H	-3.73265	-1.44264	-1.37569
C	1.49552	-2.19896	-0.70567
C	-0.86096	-3.03392	-0.59534
C	1.74347	0.05020	-1.60526
H	-2.92076	-3.58859	-0.50866
C	2.34255	-1.13338	-1.05890
C	2.07959	-3.34874	-0.13037
H	-0.52353	-3.97945	-0.19081
H	2.40477	0.87605	-1.87129
C	3.73227	-1.21361	-0.84906
C	3.44175	-3.41445	0.07355
H	1.46595	-4.19090	0.16234
C	4.28080	-2.34361	-0.28833
H	4.35484	-0.36852	-1.12491
H	3.87219	-4.30405	0.51865
H	5.34855	-2.41174	-0.11855
C	-3.85627	0.93515	-1.99638
H	-4.32972	0.36694	-2.80455
H	-4.28203	0.60963	-1.04822
H	-4.08729	1.99100	-2.14691
N	0.47840	0.21985	-1.79842

Prod: Hydride transfer results in **16** and **S33**

57

C	2.25520	-2.85565	-2.41522
C	2.22552	-1.47987	-2.43298
C	1.05134	-0.79594	-2.06654
C	-0.10567	-1.50413	-1.68867
C	-0.04911	-2.91244	-1.66131
C	1.11054	-3.56944	-2.01812
C	1.00074	0.63925	-2.07397
C	-1.28305	-0.72865	-1.34617
C	-1.19263	0.68340	-1.39061
C	-2.33816	1.46459	-1.08320
C	-3.52766	0.83883	-0.75743
C	-3.61119	-0.55768	-0.69737
C	-2.50543	-1.32637	-0.98110
H	1.90182	1.18020	-2.35861
H	3.15590	-3.38991	-2.69239
H	3.10162	-0.90620	-2.71744
H	-0.91260	-3.49280	-1.36196
H	1.13866	-4.65267	-1.99251
H	-4.39473	1.44833	-0.53170
H	-4.54258	-1.03162	-0.41212
H	-2.58265	-2.40435	-0.91943
C	-2.34907	2.96986	-1.07957
C	-1.15676	3.74524	-0.58762
H	-1.50799	4.69904	-0.19335
H	-0.58905	3.18726	0.15748
H	-0.48562	3.92552	-1.42969
O	-3.36334	3.54824	-1.42175
N	-0.03949	1.34448	-1.77110
H	2.50360	2.79620	1.98635
C	3.11098	2.34371	1.17588
O	4.45201	2.47566	1.38855
C	2.64390	0.87381	1.11157
C	1.30664	0.47302	1.39242
C	3.56484	-0.10710	0.80193
C	0.95259	-0.90080	1.39635
C	3.21126	-1.46534	0.76133
H	4.58451	0.20919	0.61442
C	-0.40402	-1.26650	1.75958
C	1.92874	-1.86137	1.06324
C	-0.82334	1.12577	1.99951
H	3.95462	-2.20982	0.49639
C	-1.29866	-0.22813	2.08331
C	-0.87984	-2.59435	1.81211
H	1.67410	-2.91309	1.03634
H	-1.53107	1.92734	2.21675
C	-2.62038	-0.51172	2.47696
C	-2.17807	-2.85769	2.19707
H	-0.22887	-3.42034	1.55549
C	-3.05724	-1.81518	2.54135
H	-3.28526	0.31149	2.71827
H	-2.52548	-3.88391	2.23558
H	-4.07340	-2.04087	2.84183
C	2.65660	3.03878	-0.12833
H	3.24457	2.63467	-0.96036
H	1.59532	2.89105	-0.34250
H	2.86655	4.11045	-0.05494
N	0.38193	1.46785	1.68357



S33

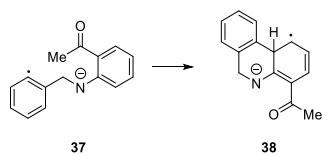
Prod: S33

29

-708.8113747

H	2.84092	-1.57502	-0.97048
C	3.20989	-0.80983	-0.25665
O	4.39887	-0.26364	-0.63469
C	2.06554	0.21834	-0.15296
C	0.69323	-0.15777	-0.12722
C	2.37601	1.56079	-0.06838
C	-0.32181	0.82525	-0.00289
C	1.37779	2.53996	0.06337
H	3.42461	1.83068	-0.11543
C	-1.70773	0.39013	0.01215
C	0.04839	2.18200	0.09796
C	-0.84045	-1.88065	-0.22892
H	1.65321	3.58664	0.13466
C	-1.96217	-0.99054	-0.10160
C	-2.81256	1.26077	0.13112
H	-0.70802	2.94979	0.19891
H	-1.04510	-2.94675	-0.32568
C	-3.28169	-1.48422	-0.09817
C	-4.09892	0.76469	0.13416
H	-2.66174	2.32849	0.22040
C	-4.34291	-0.61650	0.01892
H	-3.44426	-2.55308	-0.18959
H	-4.93421	1.44910	0.22578
H	-5.35996	-0.98899	0.02230
C	3.30292	-1.52324	1.11544
H	3.62206	-0.79827	1.87223
H	2.35366	-1.96776	1.42648
H	4.06065	-2.31021	1.05697
N	0.39629	-1.51008	-0.24243

7.2 Benzene (Scheme S3.1)



SM: 37 cyclisation to 38

30
-709.2689329

C	4.58455	-0.41627	0.14332
C	3.56161	-0.80707	-0.71828
C	2.22382	-0.47117	-0.46553
C	2.01126	0.25740	0.68414
C	2.97600	0.67465	1.57053
C	4.30037	0.32359	1.28946
C	1.11199	-0.90267	-1.41676
C	-0.39707	1.38724	-0.87493
C	-0.87900	0.04138	-0.58251
C	-2.22095	-0.00483	0.00959
C	-2.92019	1.19687	0.23461
C	-2.42144	2.44844	-0.06902
C	-1.13195	2.51736	-0.63361
H	1.41531	-1.87429	-1.82198
H	5.60840	-0.69720	-0.07698
H	3.79663	-1.39249	-1.60361
H	2.72610	1.25144	2.45441
H	5.09723	0.62295	1.96143
H	-3.91043	1.14571	0.67111
H	-2.99826	3.34343	0.12757
H	-0.70257	3.48588	-0.87702
C	-2.88404	-1.26087	0.37652
C	-4.29203	-1.19064	0.98660
H	-4.30397	-0.61369	1.91393
H	-5.00744	-0.73463	0.29827
H	-4.60277	-2.21232	1.19796
O	-2.40566	-2.37855	0.23483
N	-0.19018	-1.05099	-0.82292
H	1.12686	-0.20591	-2.27501
H	0.59392	1.50600	-1.29302

TS: 37 cyclisation to 38

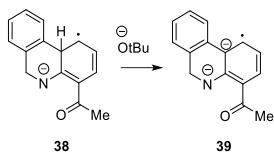
30 -709.2652784			
C	4.20852	-0.67887	0.78337
C	3.27799	-1.33006	-0.02784
C	2.09422	-0.69166	-0.41190
C	1.88435	0.59254	0.05417
C	2.78669	1.27162	0.84717
C	3.96899	0.62008	1.22272
C	1.06265	-1.39224	-1.29540
C	-0.17527	1.07814	-1.17429
C	-0.81141	-0.13959	-0.66575
C	-2.08668	0.07612	0.02413
C	-2.51205	1.38190	0.29336
C	-1.84170	2.51531	-0.15523
C	-0.69986	2.33903	-0.94294
H	1.35119	-2.44318	-1.38533
H	5.11921	-1.19047	1.07499
H	3.47163	-2.34582	-0.36364
H	2.59213	2.28563	1.18593
H	4.69210	1.12390	1.85648
H	-3.43344	1.52618	0.84597
H	-2.22944	3.50434	0.05571
H	-0.20496	3.20121	-1.38084
C	-2.95550	-1.03668	0.43076
C	-4.06144	-0.75443	1.45233
H	-3.70018	-0.17767	2.30504
H	-4.87970	-0.19652	0.98889
H	-4.44718	-1.71405	1.79271
O	-2.87367	-2.17453	-0.00710
N	-0.27459	-1.32839	-0.75702
H	1.13913	-0.96345	-2.31009
H	0.60399	0.97767	-1.91777

Prod: 38 cyclised

30

-709.3311818

C	-4.04792	-0.48957	-0.87668
C	-3.19979	-1.38281	-0.22408
C	-2.01073	-0.92929	0.33589
C	-1.65113	0.41672	0.23258
C	-2.48824	1.30384	-0.43724
C	-3.68888	0.85095	-0.98447
C	-0.99613	-1.80686	1.01487
C	-0.32289	0.77351	0.87574
C	0.70914	-0.30652	0.45345
C	2.02426	0.12978	-0.00725
C	2.29648	1.52499	-0.07389
C	1.35860	2.51071	0.27767
C	0.09998	2.19913	0.71482
H	-1.22917	-2.86192	0.85538
H	-4.97790	-0.84106	-1.30966
H	-3.45921	-2.43504	-0.15708
H	-2.19908	2.34309	-0.54273
H	-4.33921	1.54564	-1.50454
H	3.26694	1.85920	-0.41356
H	1.65150	3.55400	0.19953
H	-0.59714	2.97446	1.01400
C	3.04967	-0.81401	-0.40137
C	4.38633	-0.24137	-0.89102
H	4.25489	0.40623	-1.76171
H	4.87935	0.34753	-0.11274
H	5.02421	-1.08152	-1.16130
O	2.95153	-2.04557	-0.38037
N	0.36110	-1.54596	0.54670
H	-1.04978	-1.62772	2.10264
H	-0.47780	0.56827	1.95363

**SM: 38 + *tert*-butoxide anion**

44

	-942.3803722		
C	-1.63032	3.69975	0.22487
C	-1.16058	3.01134	-0.89485
C	-0.53728	1.77850	-0.74466
C	-0.36563	1.22824	0.53007
C	-0.81278	1.92482	1.64726
C	-1.45191	3.15671	1.49414
C	0.02095	0.94355	-1.86244
C	0.29995	-0.13326	0.53638
C	1.53640	-0.04344	-0.39139
C	2.82389	-0.55963	0.09624
C	2.86751	-1.13819	1.39757
C	1.74835	-1.21432	2.24926
C	0.52183	-0.72948	1.88823
H	0.04156	1.50708	-2.79840
H	-2.12500	4.65814	0.10637
H	-1.28292	3.43389	-1.88811
H	-0.66849	1.50411	2.63661
H	-1.80771	3.69213	2.36832
H	3.80239	-1.53488	1.77070
H	1.87344	-1.68000	3.22395
H	-0.33414	-0.83005	2.54826
C	4.03035	-0.49074	-0.68711
C	5.30529	-1.09253	-0.07248
H	5.58709	-0.58418	0.85428
H	5.18221	-2.15429	0.15908
H	6.10615	-0.97476	-0.80171
O	4.15650	0.01257	-1.81584
N	1.37732	0.47702	-1.55791
H	-0.65690	0.08069	-1.98073
H	-0.42640	-0.76195	-0.02805
O	-2.19314	-1.44093	-1.21230
C	-3.24612	-1.72356	-0.40280
C	-3.08700	-3.11459	0.26757
H	-3.00405	-3.87942	-0.51163
H	-2.15989	-3.12331	0.84982
H	-3.92355	-3.37435	0.93044
C	-3.38764	-0.67575	0.73238
H	-2.47569	-0.67196	1.33734
H	-3.49325	0.32155	0.29231
H	-4.24622	-0.86876	1.39005
C	-4.58175	-1.73782	-1.19350
H	-4.51207	-2.48171	-1.99388
H	-5.45409	-1.97149	-0.56811
H	-4.73167	-0.75635	-1.65486

TS: 38 + tert-butoxide anion

44

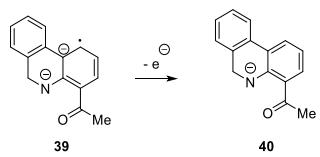
-942.3748136

C	-2.30341	3.61536	0.28038
C	-1.58450	3.13522	-0.81723
C	-0.82797	1.97538	-0.71222
C	-0.73958	1.28428	0.50777
C	-1.44220	1.78590	1.60902
C	-2.22744	2.93286	1.49149
C	-0.04487	1.36062	-1.83673
C	0.09909	0.05309	0.50249
C	1.36294	0.28730	-0.31885
C	2.63707	-0.27307	0.17728
C	2.61106	-1.02571	1.39175
C	1.45429	-1.18907	2.17130
C	0.25563	-0.63312	1.80231
H	0.03488	2.05766	-2.67658
H	-2.90800	4.51185	0.19197
H	-1.62158	3.66269	-1.76689
H	-1.36913	1.28352	2.56713
H	-2.77218	3.30045	2.35577
H	3.52411	-1.47767	1.75615
H	1.52066	-1.76821	3.08948
H	-0.62666	-0.79097	2.41567
C	3.88674	-0.09352	-0.50704
C	5.12760	-0.76579	0.10989
H	5.33854	-0.38736	1.11504
H	5.00953	-1.85098	0.18768
H	5.97506	-0.54416	-0.53842
O	4.09340	0.55653	-1.55190
N	1.29693	0.94966	-1.42763
H	-0.59923	0.47086	-2.17437
H	-0.58822	-0.72805	-0.23267
O	-1.36866	-1.54707	-1.10831
C	-2.40775	-2.22437	-0.50704
C	-1.88003	-3.40598	0.33502
H	-1.33967	-4.10047	-0.31574
H	-1.17735	-3.02668	1.08262
H	-2.68439	-3.95192	0.84424
C	-3.22153	-1.29028	0.41549
H	-2.58476	-0.91332	1.22019
H	-3.57268	-0.42736	-0.15939
H	-4.08620	-1.79712	0.86152
C	-3.35605	-2.78072	-1.58746
H	-2.79253	-3.43514	-2.25920
H	-4.19102	-3.34861	-1.15745
H	-3.76011	-1.95260	-2.17741

Prod: 39 + tert-butanol

44

C	3.06303	-3.28308	0.12012
C	2.14454	-2.96762	-0.89875
C	1.16474	-2.01177	-0.70661
C	1.00840	-1.35495	0.54373
C	1.94229	-1.68279	1.56444
C	2.94872	-2.61720	1.34207
C	0.25918	-1.49734	-1.78788
C	-0.09941	-0.45674	0.70468
C	-1.23984	-0.65016	-0.21621
C	-2.54817	-0.12280	0.23283
C	-2.55221	0.77440	1.35688
C	-1.42734	1.02382	2.13246
C	-0.22197	0.37751	1.85291
H	0.26618	-2.17472	-2.64942
H	3.84598	-4.01536	-0.04361
H	2.22131	-3.45391	-1.86911
H	1.85407	-1.22250	2.54252
H	3.64653	-2.84313	2.14434
H	-3.47625	1.26455	1.63669
H	-1.49508	1.71222	2.97112
H	0.64023	0.53829	2.49385
C	-3.78629	-0.43675	-0.41311
C	-5.04588	0.29536	0.08745
H	-5.27541	0.04661	1.12930
H	-4.94348	1.38393	0.02922
H	-5.87883	-0.01917	-0.54159
O	-3.97866	-1.26372	-1.33471
N	-1.11318	-1.26744	-1.36564
H	0.68782	-0.53360	-2.13403
H	0.30296	1.41135	-0.53450
O	0.58900	2.15492	-1.09528
C	1.73916	2.75579	-0.51201
C	1.32589	3.57937	0.71027
H	0.61875	4.35769	0.41123
H	0.83607	2.93040	1.44075
H	2.19571	4.05182	1.17747
C	2.75249	1.68175	-0.11444
H	2.33645	1.02903	0.65695
H	2.99898	1.05999	-0.97992
H	3.67087	2.13939	0.26593
C	2.31922	3.66317	-1.59220
H	1.56943	4.39299	-1.90837
H	3.19633	4.19800	-1.21782
H	2.61144	3.06879	-2.46134



SM (Before SET): 39

29

-708.7533311

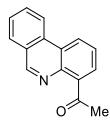
C	-4.27121	-0.50667	-0.55120
C	-3.28326	-1.38655	-0.06941
C	-2.02582	-0.92901	0.27578
C	-1.65900	0.43470	0.10360
C	-2.66776	1.31311	-0.38461
C	-3.93947	0.84473	-0.69081
C	-0.97241	-1.76012	0.94704
C	-0.29770	0.80613	0.35497
C	0.69892	-0.27876	0.28799
C	2.09658	0.12158	0.00568
C	2.42286	1.51739	0.13445
C	1.46387	2.50229	0.34206
C	0.11049	2.16711	0.40238
H	-1.21997	-2.82588	0.87870
H	-5.26398	-0.86517	-0.79965
H	-3.51463	-2.44071	0.07006
H	-2.43286	2.35857	-0.55248
H	-4.68389	1.54357	-1.06466
H	3.45603	1.82980	0.04696
H	1.77354	3.54026	0.43556
H	-0.63771	2.94575	0.51983
C	3.12520	-0.80376	-0.35655
C	4.55154	-0.24224	-0.51535
H	4.61285	0.50736	-1.31186
H	4.91518	0.23176	0.40289
H	5.20442	-1.07852	-0.76665
O	3.00884	-2.03318	-0.58460
N	0.37095	-1.54101	0.43933
H	-0.99329	-1.49379	2.02679

Prod (After SET): 40

29

-708.7732472

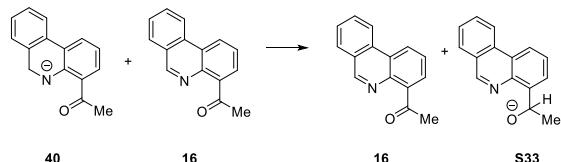
C	-4.27535	-0.49062	-0.47992
C	-3.30930	-1.36115	0.01972
C	-2.02763	-0.90668	0.31340
C	-1.67818	0.43101	0.07256
C	-2.64829	1.29291	-0.45973
C	-3.93828	0.84229	-0.71327
C	-0.96266	-1.76717	0.93874
C	-0.28045	0.81345	0.29878
C	0.70482	-0.28096	0.25684
C	2.08414	0.14626	-0.00217
C	2.41126	1.50188	0.13800
C	1.47401	2.49405	0.38683
C	0.11911	2.12804	0.40951
H	-1.21429	-2.82427	0.81091
H	-5.27651	-0.84781	-0.69316
H	-3.55544	-2.40375	0.19972
H	-2.38580	2.31746	-0.69974
H	-4.67638	1.52616	-1.11831
H	3.44734	1.80228	0.03189
H	1.77464	3.52759	0.50094
H	-0.63772	2.90302	0.50106
C	3.13947	-0.79572	-0.38585
C	4.59010	-0.30030	-0.38915
H	4.74988	0.44431	-1.17300
H	4.86991	0.15124	0.56459
H	5.22859	-1.15961	-0.58713
O	2.94472	-1.95290	-0.73157
N	0.38253	-1.53195	0.43725
H	-0.97623	-1.57345	2.02822



Prod: 16
28

-708.1103926

C	3.26851	-0.63245	-0.06342
O	4.26867	-0.30225	-0.66285
C	2.09594	0.31516	-0.03000
C	0.74288	-0.10817	-0.02801
C	2.39238	1.66419	0.00818
C	-0.29078	0.85706	0.03846
C	1.37129	2.61944	0.08655
H	3.43164	1.96982	-0.01395
C	-1.66599	0.39150	0.01836
C	0.05330	2.22131	0.10556
C	-0.73684	-1.86158	-0.15963
H	1.61994	3.67269	0.13152
C	-1.88158	-0.99640	-0.08218
C	-2.79216	1.23734	0.08808
H	-0.72357	2.97274	0.16441
H	-0.91091	-2.93331	-0.24816
C	-3.18752	-1.52199	-0.11173
C	-4.06498	0.70922	0.05965
H	-2.66928	2.30956	0.16537
C	-4.27133	-0.67834	-0.04101
H	-3.32200	-2.59552	-0.19090
H	-4.91943	1.37348	0.11425
H	-5.27881	-1.07499	-0.06302
C	3.22484	-1.92829	0.70632
H	2.57701	-1.85983	1.57963
H	2.81625	-2.70632	0.06008
H	4.24369	-2.18906	0.99131
N	0.49121	-1.46417	-0.13700



SM: Hydride transfer between 40 and 16

57

C	4.40909	1.35674	-1.49923
C	3.76213	1.63235	-0.29955
C	2.37217	1.58684	-0.19783
C	1.59103	1.30597	-1.32826
C	2.25616	1.06341	-2.54218
C	3.64138	1.06735	-2.62545
C	1.69213	1.79715	1.13196
C	0.12511	1.33007	-1.19322
C	-0.43269	1.82950	0.07492
C	-1.89272	1.93133	0.11956
C	-2.65428	1.60694	-1.01388
C	-2.09638	1.13974	-2.18461
C	-0.69952	1.00260	-2.24588
H	2.26061	2.53910	1.70688
H	5.49122	1.38184	-1.56127
H	4.34466	1.89209	0.58071
H	1.68723	0.87099	-3.44321
H	4.12247	0.86213	-3.57579
H	-3.73053	1.70069	-0.92266
H	-2.71390	0.86867	-3.03199
H	-0.26375	0.61981	-3.16376
C	-2.67361	2.25174	1.32372
C	-2.00174	2.60845	2.62977
H	-2.77841	2.74187	3.38356
H	-1.28848	1.83440	2.91779
H	-1.40097	3.51235	2.51659
O	-3.91016	2.21940	1.30981
N	0.30220	2.18321	1.10125
H	1.77792	0.85796	1.71311
C	2.46361	-1.62500	2.29208
O	1.96397	-2.13205	3.27209
C	1.80851	-1.69478	0.94282
C	0.39784	-1.58741	0.78970
C	2.60353	-1.93672	-0.16090
C	-0.17932	-1.86986	-0.46985
C	2.03048	-2.16240	-1.42025
H	3.68182	-1.96817	-0.05463
C	-1.62351	-1.81191	-0.59023
C	0.66252	-2.15295	-1.56331
C	-1.61498	-0.99147	1.70911
H	2.66758	-2.33897	-2.27832
C	-2.34503	-1.34671	0.52312
C	-2.34121	-2.19504	-1.74159
H	0.23053	-2.33202	-2.54021
H	-2.17690	-0.57759	2.54628
C	-3.74604	-1.22380	0.46944
C	-3.71565	-2.10202	-1.77063
H	-1.81845	-2.57771	-2.60909
C	-4.42658	-1.60031	-0.66594
H	-4.27143	-0.82169	1.32916
H	-4.25385	-2.40647	-2.66112
H	-5.50523	-1.50812	-0.71332
C	3.83424	-0.98112	2.37535
H	4.59076	-1.75209	2.19659
H	3.96789	-0.19018	1.63853
H	3.97587	-0.60009	3.38583
N	-0.34038	-1.13747	1.86626

TS: Hydride transfer between **40** and **16**

57

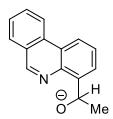
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C	-4.00972	-0.55095	2.16211
C	-3.61331	0.57575	1.46569
C	-2.25549	0.84034	1.24728
C	-1.27193	-0.00671	1.78582
C	-1.69295	-1.15270	2.48455
C	-3.03713	-1.42823	2.65615
C	-1.82435	1.99409	0.44644
C	0.12744	0.39208	1.63832
C	0.39447	1.64736	1.00727
C	1.75516	2.07173	0.92723
C	2.76701	1.30977	1.49760
C	2.49453	0.08643	2.10578
C	1.18371	-0.36342	2.15496
H	-2.59352	2.74532	0.25574
H	-5.06191	-0.75357	2.32486
H	-4.35172	1.26979	1.07766
H	-0.96304	-1.83582	2.90061
H	-3.33666	-2.32116	3.19341
H	3.78578	1.67278	1.41794
H	3.29695	-0.52161	2.50541
H	0.98211	-1.32552	2.61214
C	2.18873	3.27762	0.15453
C	1.43908	3.68772	-1.08979
H	2.15008	4.16048	-1.76909
H	0.92459	2.84616	-1.55668
H	0.66718	4.40803	-0.81364
O	3.20121	3.87550	0.48009
N	-0.57107	2.46519	0.51546
H	-2.02269	1.43659	-0.92627
C	-2.32497	0.86023	-2.06329
O	-1.78487	1.44784	-3.06296
C	-1.79526	-0.51263	-1.62661
C	-0.39546	-0.74522	-1.47348
C	-2.66505	-1.53646	-1.29566
C	0.07027	-1.98964	-0.97449
C	-2.20498	-2.77816	-0.83186
H	-3.73267	-1.38633	-1.39264
C	1.49558	-2.15847	-0.75696
C	-0.85899	-3.00293	-0.66793
C	1.73508	0.11678	-1.59382
H	-2.91899	-3.55759	-0.58931
C	2.33965	-1.08314	-1.08643
C	2.08410	-3.31771	-0.20558
H	-0.52007	-3.96038	-0.29319
H	2.39187	0.95459	-1.83374
C	3.72852	-1.16518	-0.87617
C	3.44570	-3.38516	-0.00091
H	1.47031	-4.16561	0.07046
C	4.28142	-2.30456	-0.33920
H	4.34686	-0.30985	-1.12964
H	3.87761	-4.28255	0.42761
H	5.34925	-2.37085	-0.16780
C	-3.85870	0.99990	-1.99361
H	-4.30690	0.43947	-2.82149
H	-4.30419	0.66028	-1.05800
H	-4.08931	2.05635	-2.13979
N	0.47041	0.28953	-1.76965

Prod: Hydride transfer results in **16** and **S33**

57

C	2.37325	-2.72111	-2.41218
C	2.29733	-1.34716	-2.39372
C	1.09152	-0.71261	-2.04508
C	-0.04887	-1.46795	-1.71345
C	0.05442	-2.87371	-1.72319
C	1.24311	-3.48283	-2.06848
C	0.99190	0.72101	-2.02487
C	-1.25756	-0.74082	-1.37356
C	-1.21487	0.67449	-1.38825
C	-2.38772	1.41105	-1.07366
C	-3.55770	0.73770	-0.77468
C	-3.59558	-0.66141	-0.74720
H	1.88019	1.29983	-2.27039
H	3.30065	-3.21632	-2.67342
H	3.16255	-0.73636	-2.62954
H	-0.79698	-3.48785	-1.45824
H	1.30693	-4.56515	-2.07127
H	-4.44505	1.31688	-0.54799
H	-4.51311	-1.17276	-0.48165
H	-2.50142	-2.46749	-0.99321
C	-2.45426	2.91828	-1.02492
C	-1.27372	3.72682	-0.55950
H	-1.64272	4.67979	-0.18036
H	-0.68507	3.19667	0.19072
H	-0.60764	3.90109	-1.40648
O	-3.50491	3.46027	-1.30669
N	-0.08003	1.38108	-1.73560
H	2.53972	2.80053	2.04525
C	3.10717	2.37019	1.18901
O	4.44547	2.47544	1.31653
C	2.62440	0.89823	1.11758
C	1.29241	0.47579	1.38605
C	3.56842	-0.07040	0.83645
C	0.96007	-0.90550	1.39200
C	3.23738	-1.43294	0.79640
H	4.58249	0.28454	0.68429
C	-0.39279	-1.29219	1.74260
C	1.95563	-1.85085	1.07560
C	-0.85248	1.09269	1.98056
H	3.99870	-2.16799	0.55445
C	-1.30729	-0.26972	2.06165
C	-0.84994	-2.62775	1.78973
H	1.71944	-2.90710	1.05091
H	-1.57508	1.88312	2.19250
C	-2.62624	-0.57768	2.44442
C	-2.14560	-2.91486	2.16494
H	-0.18083	-3.44095	1.53845
C	-3.04417	-1.88767	2.50467
H	-3.30575	0.23503	2.68162
H	-2.47502	-3.94752	2.20169
H	-4.05870	-2.12935	2.79917
C	2.58200	3.10469	-0.07216
H	3.13864	2.72985	-0.93881
H	1.51047	2.97278	-0.24436
H	2.80808	4.16982	0.03203
N	0.34653	1.45320	1.66887



S33

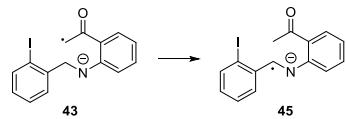
Prod: S33

29

-708.7642915

H	2.90016	-1.53626	-1.02537
C	3.23607	-0.79724	-0.26243
O	4.41349	-0.21043	-0.55373
C	2.06507	0.20995	-0.15585
C	0.69283	-0.16123	-0.13494
C	2.37702	1.55290	-0.07347
C	-0.32240	0.82427	-0.00740
C	1.38132	2.53239	0.05705
H	3.43188	1.80073	-0.12635
C	-1.70733	0.39097	0.01112
C	0.04963	2.17948	0.09379
C	-0.84584	-1.87945	-0.24616
H	1.65888	3.57933	0.12565
C	-1.96678	-0.98841	-0.10789
C	-2.81220	1.26157	0.14080
H	-0.70519	2.94924	0.19472
H	-1.05200	-2.94524	-0.35080
C	-3.28781	-1.47663	-0.09810
C	-4.09989	0.77074	0.15001
H	-2.65571	2.32818	0.23466
C	-4.34806	-0.60926	0.03011
H	-3.45220	-2.54526	-0.19320
H	-4.93244	1.45772	0.25069
H	-5.36578	-0.98066	0.03893
C	3.28402	-1.57414	1.08267
H	3.53567	-0.87047	1.88336
H	2.34439	-2.07965	1.32450
H	4.08645	-2.31435	1.01774
N	0.38915	-1.51077	-0.26008

7.3 DMSO (Scheme S3.2)



SM: **43** abstracting H atom from benzylic position to form **45**

30

-720.1128365

C	-2.15076	3.48302	-0.05636
C	-0.98080	2.73576	0.02377
C	-1.00108	1.33810	0.03484
C	-2.25489	0.72718	-0.04190
C	-3.43696	1.45410	-0.12376
C	-3.38318	2.84458	-0.12967
H	-2.09768	4.56537	-0.06114
H	-0.01740	3.22522	0.08266
H	-4.39053	0.94485	-0.18241
H	-4.30176	3.41570	-0.19153
I	-2.42678	-1.40719	-0.03936
C	0.27620	0.52989	0.12722
H	0.22201	-0.15568	0.98640
H	0.34337	-0.14560	-0.74046
N	1.43766	1.35966	0.23231
C	2.67008	0.83590	0.12843
C	3.71419	1.81694	0.09168
C	3.05169	-0.54910	-0.00725
C	5.03058	1.48485	-0.12970
H	3.41283	2.85084	0.21586
C	4.39091	-0.84291	-0.25004
C	5.37603	0.14142	-0.32070
H	5.79022	2.25679	-0.16538
H	4.67088	-1.88520	-0.35732
H	6.40717	-0.13723	-0.50405
C	2.11159	-1.71290	0.23056
C	1.91664	-2.57833	-0.81433
H	1.25185	-3.42858	-0.70184
H	2.41462	-2.42862	-1.76366
O	1.60858	-1.78321	1.40823

30			
-720.0955497			
C	2.33489	3.38090	0.34782
C	1.11275	2.72770	0.26375
C	1.02803	1.34363	0.05858
C	2.23805	0.65036	-0.04463
C	3.47225	1.28582	0.03397
C	3.52114	2.66208	0.23193
H	2.36188	4.45323	0.50264
H	0.18268	3.27583	0.34837
H	4.38884	0.71602	-0.05373
H	4.48083	3.16072	0.29588
I	2.26154	-1.47207	-0.33030
C	-0.30219	0.66172	0.00329
H	-0.32318	-0.15041	-0.74278
H	-0.41585	-0.07214	0.98565
N	-1.40325	1.49114	-0.00257
C	-2.63689	0.90641	-0.10047
C	-3.68948	1.75940	-0.52765
C	-2.97921	-0.45438	0.18412
C	-4.97858	1.30520	-0.72755
H	-3.43403	2.79458	-0.72630
C	-4.28800	-0.88675	-0.03609
C	-5.28970	-0.03729	-0.49256
H	-5.74422	1.99195	-1.07099
H	-4.51794	-1.92559	0.17979
H	-6.29502	-0.40958	-0.64860
C	-2.04686	-1.47746	0.80687
C	-1.33265	-1.08840	1.95321
H	-0.66803	-1.80560	2.42207
H	-1.67766	-0.24483	2.54078
O	-1.91980	-2.57952	0.22045

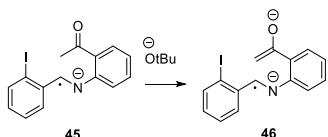
TS: **43** abstracting H atom from benzylic position to form **45**

Prod: 45 after H atom abstraction from
benzylic position

30

-720.1524777

C	2.44456	3.28542	0.45865
C	1.19789	2.73232	0.24976
C	1.01754	1.34617	-0.05010
C	2.21776	0.58239	-0.08479
C	3.46864	1.13109	0.12671
C	3.60067	2.49745	0.39652
H	2.52610	4.34495	0.67676
H	0.30667	3.34584	0.30108
H	4.35021	0.50224	0.08904
H	4.58173	2.92530	0.55978
I	2.14751	-1.53236	-0.44900
C	-0.28051	0.81407	-0.26682
H	-0.36059	-0.25068	-0.48948
H	-0.12544	-0.63452	2.09108
N	-1.38505	1.56286	-0.23343
C	-2.59991	0.95088	-0.22801
C	-3.69767	1.66898	-0.78175
C	-2.87353	-0.37384	0.24520
C	-4.92955	1.08640	-0.97476
H	-3.51326	2.69039	-1.09653
C	-4.13068	-0.95491	-0.00243
C	-5.15536	-0.25367	-0.60782
H	-5.72990	1.66516	-1.42358
H	-4.29505	-1.96824	0.34834
H	-6.12280	-0.71452	-0.76454
C	-1.97384	-1.15062	1.13288
C	-1.19233	-0.43302	2.21580
H	-1.50881	-0.85956	3.17081
H	-1.35417	0.64313	2.21496
O	-1.94495	-2.37363	1.09739



SM: 45 + *tert*-butoxide anion

44	-953.2772133	C	-3.48496	3.03921	-1.47257
		C	-2.37228	2.62827	-0.76778
		C	-2.26266	1.31680	-0.20688
		C	-3.37862	0.46897	-0.45603
		C	-4.49483	0.87551	-1.16183
		C	-4.56653	2.17383	-1.67933
		H	-3.51838	4.04751	-1.87166
		H	-1.53896	3.30198	-0.60983
		H	-5.31625	0.18679	-1.31863
		H	-5.44227	2.48896	-2.23238
		I	-3.37969	-1.55779	0.25486
		C	-1.10704	0.93570	0.52443
		H	-1.08117	-0.07484	0.93309
		H	0.06821	-1.23361	-1.66188
		N	-0.09237	1.77203	0.75566
		C	1.05797	1.28493	1.30227
		C	1.85883	2.18888	2.05344
		C	1.51832	-0.06930	1.23282
		C	2.95212	1.76956	2.78100
		H	1.54781	3.22800	2.07346
		C	2.60661	-0.47632	2.01944
		C	3.32501	0.41524	2.79715
		H	3.52005	2.49356	3.35586
		H	2.91115	-1.51615	1.96059
		H	4.17872	0.08236	3.37477
		C	1.02958	-1.07492	0.24788
		C	0.85292	-0.64343	-1.18511
		H	1.82715	-0.84708	-1.66020
		H	0.64060	0.41914	-1.28044
		O	0.93984	-2.25810	0.54652
		O	3.97145	-0.94344	-2.07496
		C	5.09637	-0.37871	-1.52559
		C	6.19112	-0.15419	-2.59419
		H	5.80708	0.50917	-3.37582
		H	7.10387	0.29099	-2.18125
		H	6.45317	-1.11079	-3.05799
		C	5.69402	-1.28349	-0.42310
		H	5.95374	-2.25815	-0.84940
		H	6.59292	-0.85612	0.03682
		H	4.94628	-1.44115	0.36070
		C	4.77849	0.99309	-0.88307
		H	4.37541	1.66847	-1.64550
		H	4.02226	0.86842	-0.09998
		H	5.66212	1.46586	-0.43738

TS: 45 + tert-butoxide anion

44

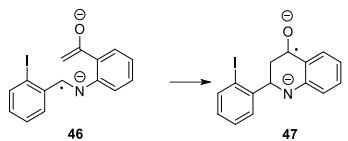
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C	-2.84406	2.63231	2.32412
C	-1.84831	1.69189	2.16351
C	-1.92147	0.65453	1.17725
C	-3.09393	0.69312	0.36715
C	-4.09266	1.63484	0.52171
C	-3.98521	2.62236	1.51005
H	-2.73598	3.39335	3.09021
H	-0.96639	1.70922	2.79185
H	-4.96228	1.61430	-0.12473
H	-4.76964	3.35875	1.62987
I	-3.37052	-0.75143	-1.19714
C	-0.87475	-0.29501	1.05180
H	-0.96361	-1.04223	0.26338
H	0.56342	0.87815	-1.95839
N	0.18012	-0.31031	1.86688
C	1.24140	-1.12641	1.56615
C	2.01465	-1.60675	2.65456
C	1.63837	-1.54621	0.26062
C	3.05630	-2.49924	2.48461
H	1.73834	-1.26729	3.64726
C	2.67424	-2.47555	0.11949
C	3.38754	-2.96436	1.20629
H	3.61012	-2.84620	3.35087
H	2.94244	-2.78348	-0.88652
H	4.19651	-3.67064	1.06378
C	1.12977	-0.94695	-1.02836
C	1.20671	0.49341	-1.16450
H	2.43987	0.71300	-1.52176
H	1.08170	1.03134	-0.22658
O	0.84632	-1.70574	-1.96705
O	3.71339	0.97042	-1.91751
C	4.39157	1.71795	-0.95551
C	5.83995	1.94755	-1.41123
H	5.84924	2.48263	-2.36551
H	6.41040	2.53136	-0.68080
H	6.34084	0.98530	-1.55327
C	4.41063	0.97830	0.39602
H	4.90044	0.00649	0.27665
H	4.94456	1.54615	1.16551
H	3.38871	0.79339	0.74096
C	3.71465	3.08826	-0.75916
H	3.69600	3.62958	-1.70986
H	2.68285	2.95062	-0.42399
H	4.23934	3.70254	-0.01991

Prod: 46 + tert-butanol

44

C	-3.03547	3.44386	0.67746
C	-1.97240	2.60221	0.92547
C	-2.00857	1.19986	0.61657
C	-3.22283	0.76809	0.00369
C	-4.28942	1.60702	-0.24785
C	-4.21747	2.96603	0.09194
H	-2.95214	4.49388	0.93971
H	-1.06377	2.98025	1.37824
H	-5.18630	1.21602	-0.71313
H	-5.05605	3.62154	-0.10508
I	-3.45596	-1.28108	-0.60472
C	-0.90348	0.36380	0.91804
H	-0.98456	-0.69128	0.66096
H	0.67944	-0.42880	-2.46042
N	0.19246	0.81978	1.51501
C	1.26241	-0.03750	1.68696
C	2.04463	0.17271	2.84931
C	1.65730	-1.09512	0.81568
C	3.10717	-0.64468	3.19161
H	1.75960	0.99843	3.49344
C	2.71597	-1.92290	1.20346
C	3.44482	-1.72438	2.37117
H	3.66611	-0.44896	4.10096
H	2.98428	-2.73266	0.53198
H	4.26864	-2.38105	2.62631
C	1.11363	-1.35428	-0.58293
C	1.05884	-0.28649	-1.45282
H	3.16453	-0.37334	-1.66286
H	1.17593	0.72544	-1.08503
O	0.85297	-2.57411	-0.87582
O	4.13423	-0.37030	-1.80909
C	4.64775	0.90588	-1.42020
C	6.16489	0.78690	-1.49347
H	6.47325	0.50327	-2.50283
H	6.63771	1.73861	-1.24001
H	6.51810	0.02483	-0.79441
C	4.20341	1.23978	0.00436
H	4.47027	0.42978	0.68835
H	4.67506	2.16600	0.34464
H	3.11872	1.36447	0.05019
C	4.14761	1.97460	-2.39429
H	4.47065	1.73963	-3.41157
H	3.05498	2.01456	-2.37643
H	4.53383	2.96101	-2.12395



SM: 46 cyclisation from the benzylic

29

-719.6364475

C	2.41851	3.31312	0.49110
C	1.18132	2.73280	0.31111
C	1.01506	1.33434	0.02563
C	2.24113	0.60558	-0.03850
C	3.48233	1.18070	0.14420
C	3.59528	2.55316	0.41063
H	2.47870	4.37624	0.70177
H	0.27944	3.32885	0.37797
H	4.37585	0.57016	0.08425
H	4.57002	3.00221	0.55291
I	2.22457	-1.50799	-0.43230
C	-0.27922	0.78251	-0.16129
H	-0.35243	-0.28822	-0.34838
N	-1.37866	1.53048	-0.13435
C	-2.61322	0.91403	-0.21199
C	-3.63984	1.65192	-0.85422
C	-2.95884	-0.37221	0.29795
C	-4.91335	1.14622	-1.05089
H	-3.38352	2.64169	-1.21810
C	-4.24517	-0.86647	0.06173
C	-5.22777	-0.13897	-0.60228
H	-5.65909	1.74816	-1.55970
H	-4.47718	-1.85620	0.44460
H	-6.21730	-0.55543	-0.75168
C	-2.07514	-1.26093	1.16431
C	-1.66291	-0.75766	2.37158
H	-1.04350	-1.35804	3.03128
H	-1.86720	0.27127	2.64208
O	-1.85805	-2.44742	0.71759

TS: 46 cyclisation from the benzylic

29

-719.6065580

C	2.13213	3.33574	0.49459
C	0.94696	2.67314	0.23573
C	0.89485	1.27778	-0.05881
C	2.15685	0.62736	-0.03989
C	3.34920	1.27914	0.21509
C	3.35502	2.65351	0.48723
H	2.11100	4.40055	0.70398
H	0.00261	3.20357	0.23761
H	4.28182	0.72742	0.20483
H	4.28815	3.16316	0.69152
I	2.28613	-1.48355	-0.42771
C	-0.37356	0.62165	-0.23308
H	-0.31917	-0.37026	-0.69080
N	-1.48497	1.39677	-0.53297
C	-2.68739	0.80472	-0.36783
C	-3.83903	1.39578	-0.97504
C	-2.92973	-0.41083	0.38415
C	-5.08779	0.80585	-0.94033
H	-3.69254	2.32927	-1.51158
C	-4.19869	-0.99960	0.36198
C	-5.28544	-0.42452	-0.28712
H	-5.92116	1.29589	-1.43572
H	-4.32135	-1.93120	0.90827
H	-6.25957	-0.89905	-0.27383
C	-1.85278	-1.02034	1.20949
C	-0.84015	-0.12878	1.64275
H	0.01661	-0.56174	2.15525
H	-1.10344	0.88490	1.92743
O	-1.78700	-2.29194	1.33863

Prod: 47 cyclised

29

-719.6427170

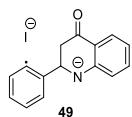
C	1.99970	3.32703	0.59693
C	0.84976	2.57504	0.39414
C	0.89358	1.20646	0.09781
C	2.16443	0.63669	0.00725
C	3.33322	1.36881	0.19996
C	3.24991	2.72406	0.50021
H	1.92148	4.38364	0.82647
H	-0.13274	3.02809	0.44841
H	4.30044	0.88997	0.11321
H	4.15796	3.29592	0.65049
I	2.43357	-1.44364	-0.46376
C	-0.40898	0.43502	-0.03970
H	-0.22620	-0.37294	-0.77201
N	-1.47728	1.28848	-0.50511
C	-2.70574	0.74632	-0.43084
C	-3.79422	1.36120	-1.10177
C	-3.01006	-0.47613	0.32937
C	-5.09384	0.81793	-1.11209
H	-3.58432	2.27464	-1.65286
C	-4.33399	-1.01725	0.26055
C	-5.35778	-0.38381	-0.44475
H	-5.88406	1.32705	-1.65639
H	-4.53259	-1.92839	0.81559
H	-6.35424	-0.81551	-0.46682
C	-2.03526	-1.01886	1.19862
C	-0.72411	-0.26584	1.29314
H	0.07473	-0.96220	1.57228
H	-0.77637	0.49885	2.08570
O	-2.22028	-2.04319	1.95724

**Product S56**

29

-719.5859468

C	2.01189	3.33512	0.56672
C	0.85506	2.58962	0.37861
C	0.89470	1.22002	0.09290
C	2.15923	0.63518	-0.00006
C	3.33172	1.36397	0.17864
C	3.25638	2.72246	0.46617
H	1.94215	4.39372	0.78799
H	-0.12105	3.05479	0.43957
H	4.29617	0.87993	0.09128
H	4.16853	3.29042	0.60492
I	2.40019	-1.44823	-0.44527
C	-0.40626	0.45148	-0.03700
H	-0.25381	-0.34681	-0.78492
N	-1.48630	1.30283	-0.49702
C	-2.68299	0.75904	-0.39067
C	-3.81592	1.42251	-1.00356
C	-2.98773	-0.49000	0.28008
C	-5.05855	0.85865	-1.02614
H	-3.63255	2.38044	-1.47941
C	-4.29029	-1.03935	0.22670
C	-5.31971	-0.40515	-0.42064
H	-5.86952	1.38579	-1.52009
H	-4.45706	-1.98122	0.74029
H	-6.31323	-0.83411	-0.45528
C	-1.99126	-1.07086	1.15069
C	-0.72521	-0.24675	1.29071
H	0.09066	-0.88660	1.63200
H	-0.90624	0.51734	2.06010
O	-2.14206	-2.10661	1.80536



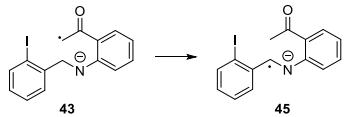
Product 49

29

-719.6931479

C	0.53756	4.49515	0.22893
C	-0.33505	3.41199	0.10845
C	0.15365	2.10818	-0.03499
C	1.52922	1.99037	-0.04976
C	2.43620	3.01471	0.05966
C	1.91685	4.30794	0.20519
H	0.13379	5.49525	0.33863
H	-1.40863	3.55810	0.11390
H	3.50616	2.83952	0.03402
H	2.58882	5.15414	0.29464
I	3.11042	-1.73631	-0.29779
C	-0.75268	0.89666	-0.11977
H	-0.32176	0.22660	-0.88977
N	-2.10020	1.25415	-0.51360
C	-2.97896	0.28071	-0.37064
C	-4.31072	0.44502	-0.91796
C	-2.73326	-0.99135	0.28248
C	-5.23050	-0.56332	-0.89908
H	-4.54292	1.39929	-1.37957
C	-3.71563	-2.00854	0.27467
C	-4.94294	-1.82934	-0.31137
H	-6.20709	-0.39704	-1.34443
H	-3.47309	-2.94131	0.77442
H	-5.68763	-2.61537	-0.31032
C	-1.54401	-1.13888	1.09244
C	-0.69620	0.11307	1.19567
H	0.32799	-0.16096	1.45676
H	-1.10800	0.73133	2.00660
O	-1.24493	-2.15477	1.72750

7.4 Benzene (Scheme S3.2)



SM: 43 abstracting H atom from benzylic position to form 45

30

-720.0741434

C	-2.14754	3.48074	-0.06301
C	-0.97917	2.73399	0.03141
C	-0.99835	1.33603	0.04211
C	-2.25085	0.72442	-0.04808
C	-3.43154	1.45203	-0.14507
C	-3.37923	2.84217	-0.15177
H	-2.09459	4.56345	-0.06660
H	-0.01300	3.21684	0.10326
H	-4.38288	0.93982	-0.21424
H	-4.29741	3.41316	-0.22533
I	-2.41074	-1.40783	-0.03724
C	0.27860	0.53260	0.15251
H	0.22917	-0.13937	1.02595
H	0.34475	-0.17006	-0.69600
N	1.43500	1.36645	0.23497
C	2.66359	0.83819	0.13695
C	3.71468	1.81308	0.09678
C	3.03761	-0.54889	-0.00061
C	5.02646	1.47353	-0.13159
H	3.41696	2.84739	0.22672
C	4.37481	-0.84916	-0.25811
C	5.36404	0.12707	-0.33086
H	5.79124	2.24119	-0.16718
H	4.64253	-1.89444	-0.36874
H	6.39327	-0.15638	-0.52000
C	2.08785	-1.70411	0.23953
C	1.91254	-2.57634	-0.81073
H	1.22067	-3.40579	-0.71399
H	2.45058	-2.44700	-1.74098
O	1.54777	-1.75137	1.39115

TS: 43 abstracting H atom from benzylic position to form 45

30

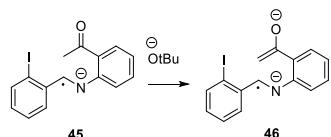
	-720.0604115		
C	2.29903	3.40675	0.28462
C	1.08521	2.73797	0.20822
C	1.01823	1.34913	0.03398
C	2.23608	0.66790	-0.04606
C	3.46231	1.31945	0.02436
C	3.49466	2.70013	0.19110
H	2.31261	4.48277	0.41641
H	0.14401	3.26960	0.27598
H	4.38423	0.75559	-0.04483
H	4.44820	3.21185	0.24897
I	2.26943	-1.45905	-0.27190
C	-0.30553	0.65076	-0.01850
H	-0.32346	-0.12906	-0.80005
H	-0.39314	-0.10445	0.92572
N	-1.40973	1.48302	0.00389
C	-2.63963	0.90086	-0.07654
C	-3.71254	1.77489	-0.40663
C	-2.97179	-0.47578	0.14224
C	-5.00863	1.33103	-0.57279
H	-3.46116	2.81951	-0.55360
C	-4.28762	-0.89658	-0.04513
C	-5.30956	-0.02422	-0.40378
H	-5.78957	2.03537	-0.83876
H	-4.50305	-1.94905	0.11139
H	-6.32081	-0.38967	-0.53812
C	-2.01104	-1.53911	0.65217
C	-1.30741	-1.24981	1.83619
H	-0.60515	-1.98190	2.21822
H	-1.67199	-0.47747	2.50373
O	-1.86037	-2.56432	-0.04529

Prod: 45 after H atom abstraction from
benzylic position

30

-720.1210729

C	2.43364	3.28932	0.47541
C	1.19204	2.72387	0.27932
C	1.02306	1.33695	-0.02438
C	2.23112	0.58880	-0.07913
C	3.47825	1.14971	0.11943
C	3.59911	2.51540	0.39571
H	2.50509	4.34926	0.69640
H	0.29124	3.32238	0.33937
H	4.36462	0.52875	0.06681
H	4.57728	2.95370	0.54970
I	2.17767	-1.52488	-0.45209
C	-0.27442	0.79790	-0.23047
H	-0.35383	-0.26271	-0.47356
H	-0.15348	-0.73236	2.01148
N	-1.37377	1.54629	-0.17214
C	-2.59369	0.95036	-0.19653
C	-3.67097	1.71090	-0.73596
C	-2.90007	-0.38529	0.22690
C	-4.90666	1.15906	-0.97783
H	-3.45722	2.74015	-1.00266
C	-4.16102	-0.93247	-0.07240
C	-5.16019	-0.19267	-0.67266
H	-5.68844	1.76999	-1.41739
H	-4.34404	-1.95714	0.23322
H	-6.13024	-0.63258	-0.86974
C	-2.04557	-1.20950	1.11738
C	-1.21312	-0.53329	2.19162
H	-1.48777	-0.99559	3.14231
H	-1.36473	0.54406	2.23304
O	-2.09346	-2.43098	1.09478



SM: 45 + *tert*-butoxide anion

44			
-953.1685996			
C	3.18881	-0.68751	3.36762
C	2.29844	0.12395	2.69976
C	2.19968	0.14465	1.27027
C	3.08210	-0.75482	0.60629
C	3.97454	-1.57194	1.27096
C	4.04713	-1.54991	2.66962
H	3.21943	-0.65968	4.45234
H	1.63354	0.78529	3.24149
H	4.61778	-2.23668	0.70671
H	4.74619	-2.19354	3.18874
I	3.05321	-0.90499	-1.53541
C	1.27735	1.00840	0.62623
H	1.24340	0.98973	-0.46370
H	-0.59509	-1.17011	-0.59277
N	0.50946	1.85658	1.30568
C	-0.45878	2.56426	0.65368
C	-0.82741	3.81500	1.21842
C	-1.11861	2.19161	-0.55858
C	-1.70478	4.67586	0.59309
H	-0.35549	4.08579	2.15662
C	-1.97899	3.09762	-1.18899
C	-2.28166	4.33383	-0.63836
H	-1.94233	5.62724	1.05874
H	-2.44521	2.78208	-2.11673
H	-2.97155	5.00518	-1.13534
C	-1.05966	0.82760	-1.17878
C	-1.28466	-0.37486	-0.29991
H	-2.31630	-0.73151	-0.46932
H	-1.15572	-0.14417	0.75666
O	-0.96118	0.70833	-2.38844
O	-4.31494	-1.64377	-0.63494
C	-5.21375	-2.14202	0.24948
C	-5.83251	-3.47350	-0.25715
H	-5.03039	-4.20177	-0.41392
H	-6.56793	-3.90200	0.43728
H	-6.32020	-3.29471	-1.22100
C	-6.38453	-1.15159	0.49330
H	-6.88320	-0.94712	-0.45961
H	-7.12867	-1.52876	1.20782
H	-5.97875	-0.20842	0.87232
C	-4.55808	-2.43016	1.62670
H	-3.74174	-3.14658	1.49043
H	-4.13005	-1.50268	2.01989
H	-5.26292	-2.83447	2.36566

TS: 45 + tert-butoxide anion

44

-953.1630718

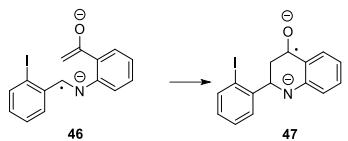
C	-2.92502	2.68552	2.23663
C	-1.89950	1.78018	2.08322
C	-1.94659	0.71371	1.12304
C	-3.13418	0.69149	0.33380
C	-4.16441	1.59775	0.48141
C	-4.08188	2.61542	1.44332
H	-2.83022	3.46969	2.98189
H	-1.00604	1.83919	2.69254
H	-5.03991	1.52580	-0.15354
H	-4.89053	3.32668	1.55630
I	-3.37948	-0.80475	-1.18629
C	-0.86908	-0.20260	1.01926
H	-0.93892	-0.98404	0.26199
H	0.64269	0.61607	-2.16150
N	0.17924	-0.14493	1.83286
C	1.25358	-0.97328	1.61843
C	2.00734	-1.33592	2.76423
C	1.68684	-1.50509	0.36793
C	3.07121	-2.21633	2.70364
H	1.69581	-0.90718	3.71093
C	2.74642	-2.41425	0.33842
C	3.44534	-2.78410	1.48163
H	3.61160	-2.46781	3.61124
H	3.04181	-2.80253	-0.63115
H	4.27822	-3.47504	1.41983
C	1.18338	-1.07082	-0.99507
C	1.25449	0.34364	-1.29970
H	2.50891	0.54841	-1.62711
H	1.07500	0.98732	-0.43899
O	0.91173	-1.94682	-1.82351
O	3.78798	0.79854	-1.97628
C	4.40066	1.63943	-1.06263
C	5.89495	1.76293	-1.40932
H	6.00303	2.14506	-2.42898
H	6.42497	2.43390	-0.72206
H	6.36085	0.77399	-1.36418
C	4.27565	1.09458	0.37565
H	4.69481	0.08494	0.42359
H	4.79839	1.73064	1.10009
H	3.22426	1.02619	0.66801
C	3.76762	3.04643	-1.11245
H	3.87151	3.45546	-2.12226
H	2.70088	2.97398	-0.88308
H	4.23204	3.73948	-0.40073

Prod: 46 + tert-butanol

44

-953.1764289

C	-2.47178	3.45492	0.95624
C	-1.50844	2.47631	1.04055
C	-1.75349	1.11061	0.66107
C	-3.07386	0.87360	0.17291
C	-4.04362	1.84977	0.08577
C	-3.76332	3.16806	0.48133
H	-2.22344	4.46823	1.25826
H	-0.51231	2.70314	1.40143
H	-5.02760	1.59881	-0.29342
H	-4.52544	3.93391	0.40900
I	-3.64299	-1.09682	-0.47470
C	-0.72682	0.14083	0.78505
H	-0.92982	-0.87047	0.43220
H	0.61858	-0.21617	-2.73971
N	0.45020	0.43507	1.31634
C	1.44055	-0.52731	1.32441
C	2.26983	-0.54038	2.47185
C	1.71378	-1.48481	0.30212
C	3.24264	-1.50322	2.67882
H	2.08281	0.22593	3.21711
C	2.67309	-2.47012	0.55988
C	3.43424	-2.50585	1.72443
H	3.84014	-1.48081	3.58532
H	2.82627	-3.20657	-0.22142
H	4.17988	-3.27971	1.87206
C	1.16504	-1.48568	-1.12742
C	0.98953	-0.25530	-1.72016
H	2.98429	0.36347	-1.99273
H	0.93756	0.64667	-1.12414
O	1.04607	-2.61886	-1.69168
O	3.83382	0.79946	-2.19275
C	4.34518	1.36367	-0.99668
C	5.46870	2.29881	-1.43578
H	5.06956	3.08307	-2.08397
H	5.94641	2.76495	-0.56977
H	6.22317	1.73891	-1.99461
C	4.89354	0.25502	-0.09418
H	5.64211	-0.32875	-0.63655
H	5.35602	0.67431	0.80503
H	4.08329	-0.41544	0.21530
C	3.26163	2.14824	-0.25546
H	2.81859	2.89576	-0.91907
H	2.46974	1.48071	0.09853
H	3.68973	2.65853	0.61302



SM: 46 cyclisation from the benzylic

29

-719.5213947

C	2.44423	3.31253	0.48016
C	1.20554	2.72930	0.34339
C	1.03268	1.32898	0.05916
C	2.25982	0.60516	-0.04183
C	3.50361	1.18235	0.09757
C	3.62503	2.55810	0.35824
H	2.50635	4.37660	0.69024
H	0.29913	3.31471	0.44013
H	4.39374	0.56967	0.01082
H	4.60296	3.01027	0.46880
I	2.22254	-1.51151	-0.42084
C	-0.26555	0.77938	-0.09803
H	-0.34557	-0.28669	-0.30665
H	-1.00354	-1.54681	2.89207
N	-1.35377	1.52962	-0.02308
C	-2.59751	0.93560	-0.14056
C	-3.59848	1.74271	-0.73619
C	-2.97449	-0.37854	0.27139
C	-4.87804	1.28201	-0.99420
H	-3.30782	2.74980	-1.01795
C	-4.26228	-0.82563	-0.03508
C	-5.22013	-0.02976	-0.65695
H	-5.60332	1.93828	-1.46621
H	-4.50541	-1.84293	0.25644
H	-6.21259	-0.41777	-0.86040
C	-2.13729	-1.35985	1.09542
C	-1.59752	-0.88702	2.26729
H	-1.63236	0.16906	2.50555
O	-2.09347	-2.56038	0.65429

TS: 46 cyclisation from the benzylic

29

-719.4950127

C	2.04347	3.35333	0.50594
C	0.88718	2.66654	0.20647
C	0.86924	1.26048	-0.07684
C	2.15308	0.64651	-0.01345
C	3.31905	1.32281	0.27754
C	3.28965	2.70107	0.55201
H	1.98799	4.41998	0.70520
H	-0.07038	3.17186	0.16045
H	4.26123	0.78744	0.29477
H	4.20195	3.23019	0.79829
I	2.35037	-1.45933	-0.43194
C	-0.38012	0.58137	-0.25810
H	-0.30828	-0.41298	-0.70875
H	0.00075	-0.59963	2.14377
N	-1.49765	1.34226	-0.57438
C	-2.69678	0.76539	-0.39695
C	-3.84959	1.36095	-1.00432
C	-2.95209	-0.43489	0.37325
C	-5.10580	0.79146	-0.93680
H	-3.69085	2.28113	-1.55947
C	-4.22600	-0.99832	0.39050
C	-5.31812	-0.41776	-0.25202
H	-5.93840	1.28582	-1.43200
H	-4.34587	-1.91784	0.95801
H	-6.30090	-0.87372	-0.21056
C	-1.86831	-1.05935	1.19450
C	-0.85500	-0.16539	1.63217
H	-1.12311	0.84941	1.90620
O	-1.82740	-2.31477	1.33675

Prod: 47 cyclised

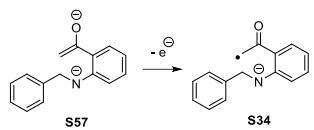
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29

-719.5231012

C	1.99969	3.32703	0.59693
C	0.84975	2.57504	0.39413
C	0.89357	1.20645	0.09780
C	2.16443	0.63669	0.00724
C	3.33322	1.36880	0.19995
C	3.24990	2.72406	0.50020
H	1.92147	4.38364	0.82646
H	-0.13274	3.02808	0.44841
H	4.30043	0.88997	0.11321
H	4.15795	3.29592	0.65049
I	2.43357	-1.44364	-0.46375
C	-0.40897	0.43502	-0.03969
H	-0.22619	-0.37293	-0.77200
N	-1.47727	1.28847	-0.50510
C	-2.70573	0.74631	-0.43083
C	-3.79421	1.36120	-1.10177
C	-3.01005	-0.47612	0.32937
C	-5.09384	0.81793	-1.11209
H	-3.58432	2.27464	-1.65286
C	-4.33399	-1.01725	0.26054
C	-5.35778	-0.38381	-0.44474
H	-5.88406	1.32704	-1.65638
H	-4.53258	-1.92839	0.81558
H	-6.35424	-0.81550	-0.46682
C	-2.03526	-1.01886	1.19862
C	-0.72411	-0.26583	1.29314
H	0.07473	-0.96219	1.57228
H	-0.77636	0.49884	2.08570
O	-2.22027	-2.04318	1.95723

7.5 DMSO (Scheme S3.3)

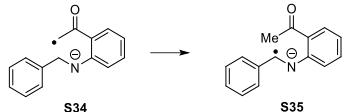


SM (Before SET): S57

30
 -709.4712098
 C 4.07685 -1.49832 -0.11775
 C 2.70729 -1.26871 0.02669
 C 2.19690 0.02885 0.04213
 C 3.09822 1.09360 -0.08435
 C 4.46234 0.87155 -0.23158
 C 4.96037 -0.43219 -0.24910
 H 4.45349 -2.51567 -0.12719
 H 2.00980 -2.09029 0.12954
 H 5.14024 1.71235 -0.33022
 H 6.02366 -0.61033 -0.36224
 C 0.71593 0.32901 0.17890
 H 0.60744 1.08895 0.96904
 H 0.41052 0.85645 -0.74138
 N -0.07496 -0.84854 0.40560
 C -1.39642 -0.78917 0.21184
 C -2.10642 -2.04433 0.24371
 C -2.23275 0.36957 -0.06366
 C -3.43983 -2.18029 -0.08287
 H -1.52200 -2.92314 0.50232
 C -3.57384 0.18183 -0.40837
 C -4.20475 -1.06290 -0.44655
 H -3.89356 -3.16768 -0.05827
 H -4.15643 1.07460 -0.62108
 H -5.25232 -1.15298 -0.70798
 C -1.80197 1.80577 0.17957
 C -1.89884 2.70981 -0.85573
 H -1.67967 3.76057 -0.68877
 H -2.19646 2.39641 -1.84861
 O -1.43939 2.08934 1.38204
 H 2.71669 2.11128 -0.06807

Product (After SET): S34

30
 -709.3399758
 C -3.85414 -1.31968 0.65750
 C -2.55253 -1.42403 0.17173
 C -1.96847 -0.36179 -0.51832
 C -2.70868 0.80422 -0.71378
 C -4.01073 0.90966 -0.23367
 C -4.58827 -0.15390 0.45575
 H -4.29623 -2.15160 1.19426
 H -1.98063 -2.33011 0.33427
 H -4.57040 1.82475 -0.39061
 H -5.60000 -0.07308 0.83575
 C -0.57150 -0.45759 -1.09246
 C 1.58147 -0.82852 -0.06485
 C 1.99417 0.53564 0.05563
 C 2.57624 -1.84165 0.04798
 C 3.35950 0.81742 0.08707
 C 3.91845 -1.52990 0.10854
 H 2.24327 -2.87283 0.01479
 C 4.31933 -0.18781 0.10235
 C 3.65984 1.85822 0.14686
 H 4.65794 -2.32092 0.15311
 H 5.37217 0.06620 0.14480
 N 0.32036 -1.27836 -0.30067
 O 1.19497 2.73081 -0.42986
 C 1.04286 1.68748 0.29982
 C 0.16537 1.51718 1.34006
 H 0.10714 0.57882 1.87640
 H -0.51589 2.31570 1.61469
 H -2.25336 1.64155 -1.23372
 H -0.65168 -0.97944 -2.06039
 H -0.19287 0.54434 -1.30670



TS S34 to S35

30

-709.3271991

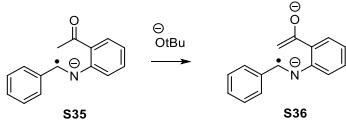
C	-4.08760	-1.26008	0.63897
C	-2.70604	-1.10686	0.57605
C	-2.13750	-0.06522	-0.16362
C	-2.98894	0.82257	-0.82991
C	-4.37068	0.67215	-0.76586
C	-4.92730	-0.37192	-0.03030
H	-4.51248	-2.07600	1.21327
H	-2.05076	-1.79662	1.09445
H	-5.01331	1.36760	-1.29390
H	-6.00310	-0.49303	0.01925
C	-0.65994	0.14687	-0.20844
C	1.48480	-0.80446	-0.00668
C	2.22963	0.41757	0.03489
C	2.23107	-2.00711	-0.13334
C	3.61599	0.37676	-0.12358
C	3.60509	-2.01764	-0.27654
H	1.66937	-2.93485	-0.14514
C	4.31553	-0.81364	-0.28562
H	4.15405	1.31929	-0.09814
H	4.12711	-2.96179	-0.38601
H	5.39251	-0.80627	-0.40246
N	0.12621	-0.95364	0.06685
O	1.89031	2.71291	-0.47437
C	1.64336	1.78443	0.33354
C	0.79893	1.89048	1.45176
H	0.84863	1.13844	2.23142
H	0.37481	2.85799	1.69686
H	-2.56055	1.63574	-1.40848
H	-0.35599	0.73889	-1.08969
H	-0.35468	0.99940	0.62781

Prod S35

30

-709.3821569

C	-4.10915	-1.18041	0.67171
C	-2.73061	-1.15880	0.53141
C	-2.09467	-0.18625	-0.28689
C	-2.93248	0.75568	-0.94133
C	-4.30731	0.72427	-0.79016
C	-4.91785	-0.24490	0.01781
H	-4.56651	-1.93455	1.30433
H	-2.11445	-1.88382	1.04935
H	-4.91716	1.45969	-1.30438
H	-5.99434	-0.26649	0.13589
C	-0.67946	-0.12563	-0.44157
C	1.48975	-0.83536	0.05442
C	2.17167	0.42790	-0.04311
C	2.31221	-2.00304	0.06623
C	3.55388	0.44439	-0.32910
C	3.66450	-1.94770	-0.16637
H	1.81439	-2.95632	0.20969
C	4.30329	-0.70971	-0.40368
H	4.03105	1.41322	-0.43267
H	4.24393	-2.86489	-0.17764
H	5.36807	-0.66675	-0.59657
N	0.14879	-1.02980	0.08080
O	2.00656	2.78436	-0.14552
C	1.57999	1.72951	0.31881
C	0.52799	1.79512	1.40932
H	0.34794	0.83181	1.88370
H	0.87883	2.52026	2.14679
H	-2.47580	1.51364	-1.57143
H	-0.28557	0.69581	-1.04961
H	-0.41498	2.16161	0.99602



S35 + tert-butoxide anion

44

-942.5061170

C	-5.15623	-1.18328	-1.36036
C	-4.06199	-0.36016	-1.14870
C	-3.39764	-0.33493	0.10957
C	-3.90605	-1.19330	1.12373
C	-4.99773	-2.01059	0.89715
C	-5.64250	-2.01909	-0.34875
H	-5.64210	-1.18070	-2.33113
H	-3.69221	0.27803	-1.94224
H	-5.35730	-2.65310	1.69427
H	-6.49660	-2.66147	-0.52492
C	-2.26584	0.48802	0.36250
C	-0.60649	1.99691	-0.28620
C	0.45146	1.52814	0.56455
C	-0.40854	3.27159	-0.89565
C	1.51193	2.39010	0.89590
C	0.66542	4.07407	-0.58644
H	-1.17355	3.61515	-1.58394
C	1.63426	3.65191	0.34554
H	2.27697	2.01054	1.56559
H	0.75904	5.04666	-1.05856
H	2.47527	4.28613	0.59710
N	-1.78969	1.37267	-0.51865
O	1.09695	-0.15269	2.09856
C	0.60623	0.12105	1.00972
C	0.32421	-0.98734	0.02231
H	-0.24142	-0.64684	-0.84243
H	1.30051	-1.36718	-0.31389
H	-3.41830	-1.20040	2.09447
H	-1.80525	0.39293	1.35180
H	-0.21160	-1.79953	0.51884
O	3.32340	-2.09638	-1.46702
C	4.22133	-1.72206	-0.49771
C	5.66618	-2.12068	-0.87875
H	6.39947	-1.83589	-0.11498
H	5.72024	-3.20463	-1.02255
H	5.94488	-1.63782	-1.82103
C	4.19784	-0.19117	-0.27924
H	4.44723	0.31666	-1.21674
H	3.19134	0.11910	0.01738
H	4.90182	0.14143	0.49312
C	3.89404	-2.39040	0.85870
H	2.88912	-2.09720	1.17719
H	3.91695	-3.47930	0.74450
H	4.60114	-2.11144	1.64909

S35 TS to S36

44

-942.4970965

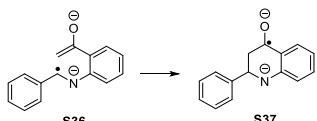
C	-5.16113	-0.93974	-1.39973
C	-3.99840	-0.21918	-1.18319
C	-3.37233	-0.19867	0.09879
C	-3.99728	-0.96272	1.12722
C	-5.15642	-1.67768	0.89434
C	-5.76268	-1.67851	-0.37327
H	-5.61208	-0.93220	-2.38757
H	-3.54245	0.34310	-1.98929
H	-5.60347	-2.24540	1.70437
H	-6.67207	-2.23872	-0.55279
C	-2.18666	0.53858	0.35698
C	-0.40328	1.91135	-0.27307
C	0.61060	1.37855	0.58531
C	-0.12515	3.16603	-0.88143
C	1.73664	2.15250	0.88671
C	1.01428	3.89202	-0.59504
H	-0.87031	3.56119	-1.56429
C	1.95648	3.40178	0.32000
H	2.47554	1.72481	1.55688
H	1.17062	4.85318	-1.07420
H	2.84718	3.96956	0.56077
N	-1.61927	1.34656	-0.54181
O	0.99064	-0.25873	2.25753
C	0.65982	-0.04592	1.08099
C	0.52760	-1.09471	0.09048
H	-0.14983	-0.84379	-0.72454
H	1.69836	-1.17350	-0.49070
H	-3.54637	-0.97420	2.11578
H	-1.76577	0.45095	1.36398
H	0.30930	-2.06878	0.53220
O	2.82548	-1.26123	-1.23381
C	3.92992	-1.66502	-0.48601
C	5.15256	-1.79065	-1.40659
H	6.04636	-2.10615	-0.85763
H	4.95227	-2.52393	-2.19346
H	5.35975	-0.82696	-1.88129
C	4.24232	-0.63718	0.61665
C	4.42884	0.34155	0.16363
H	3.38480	-0.54279	1.28956
H	5.12075	-0.92156	1.20612
C	3.66646	-3.03071	0.17650
H	2.79768	-2.96058	0.83748
H	3.45253	-3.78053	-0.59139
H	4.52415	-3.37217	0.76547

S36 Product

44

-942.5143115

C	5.94162	-0.33798	0.33024
C	4.68996	0.25018	0.24766
C	3.53632	-0.51415	-0.10542
C	3.74857	-1.90260	-0.35482
C	5.00217	-2.47533	-0.26567
C	6.12662	-1.70343	0.07775
H	6.79710	0.27498	0.59958
H	4.56722	1.30742	0.44936
H	5.11860	-3.53632	-0.46405
H	7.10940	-2.15342	0.14791
C	2.23145	0.04274	-0.21553
C	0.73863	1.89309	-0.05478
C	-0.53414	1.23982	0.05877
C	0.70683	3.31403	-0.14665
C	-1.69815	2.01220	0.07495
C	-0.46317	4.05106	-0.14318
H	1.66559	3.81719	-0.22200
C	-1.69554	3.40275	-0.03026
H	-2.64631	1.49205	0.18116
H	-0.41638	5.13263	-0.22226
H	-2.62448	3.96065	-0.01658
N	1.99880	1.34568	-0.03146
O	-0.73895	-0.92452	-0.93619
C	-0.73915	-0.26433	0.16023
C	-0.97019	-0.77628	1.41852
H	-0.92014	-0.14046	2.29431
H	-3.07616	-0.65068	1.13743
H	2.89372	-2.51759	-0.62403
H	1.43815	-0.64254	-0.50714
H	-1.09632	-1.84582	1.56072
O	-4.05410	-0.67620	1.15913
C	-4.52189	-1.33563	-0.02219
C	-6.01802	-1.53833	0.17797
H	-6.45976	-2.02214	-0.69616
H	-6.20253	-2.16514	1.05389
H	-6.51159	-0.57482	0.32829
C	-4.25352	-0.45380	-1.24173
H	-4.74461	0.51582	-1.12102
H	-3.17647	-0.29876	-1.35516
H	-4.63567	-0.92592	-2.15118
C	-3.80362	-2.67545	-0.17918
H	-2.73194	-2.50315	-0.31723
H	-3.95825	-3.29242	0.71007
H	-4.18498	-3.21687	-1.04917



29

-708.8652412

C	-4.13028	-1.34456	0.53952
C	-2.75309	-1.28125	0.40870
C	-2.11781	-0.14793	-0.18829
C	-2.97957	0.90026	-0.63240
C	-4.35084	0.82324	-0.49114
C	-4.95640	-0.30236	0.09772
H	-4.57775	-2.22208	0.99741
H	-2.13221	-2.09696	0.75946
H	-4.96879	1.64535	-0.83898
H	-6.03240	-0.36023	0.20786
C	-0.70952	-0.03588	-0.33703
C	1.49554	-0.80771	-0.02869
C	2.20222	0.43452	0.03782
C	2.28794	-1.98411	-0.12522
C	3.59544	0.42907	-0.05381
C	3.66925	-1.95835	-0.20633
H	1.75921	-2.93182	-0.14844
C	4.34747	-0.73718	-0.18219
H	4.10699	1.38714	-0.00001
H	4.21932	-2.89028	-0.28931
H	5.42863	-0.69547	-0.24366
N	0.13426	-1.00279	0.03135
O	1.38528	2.51352	-0.81705
C	1.56324	1.80212	0.23972
C	1.29043	2.17300	1.53176
H	0.84284	3.13960	1.74422
H	1.48319	1.49794	2.35675
H	-2.53377	1.78027	-1.08862
H	-0.34142	0.88046	-0.80056

TS of S36 to S37

29

-708.8343256

C	-3.91162	-1.23563	0.77608
C	-2.54367	-1.14762	0.55276
C	-2.00248	-0.15769	-0.30737
C	-2.92261	0.73724	-0.91211
C	-4.28404	0.64302	-0.68258
C	-4.80305	-0.34786	0.16621
H	-4.29355	-2.00847	1.43664
H	-1.86159	-1.84279	1.02809
H	-4.95754	1.34247	-1.16805
H	-5.86902	-0.42081	0.34526
C	-0.58025	-0.00211	-0.48905
C	1.57194	-0.81587	-0.11758
C	2.14843	0.49572	0.11707
C	2.50521	-1.89300	-0.22274
C	3.53934	0.65424	0.08151
C	3.87424	-1.70312	-0.20599
H	2.09645	-2.89110	-0.35747
C	4.41805	-0.41116	-0.07888
H	3.92543	1.66086	0.22063
H	4.53291	-2.56109	-0.30544
H	5.49046	-0.25428	-0.08573
N	0.25197	-1.08092	-0.24390
O	1.61213	2.83512	0.01451
C	1.28113	1.66216	0.42420
C	0.02131	1.35046	0.98818
H	-0.67917	2.17157	1.12954
H	-0.06771	0.52745	1.69038
H	-2.53980	1.51203	-1.57136
H	-0.30913	0.67697	-1.30961

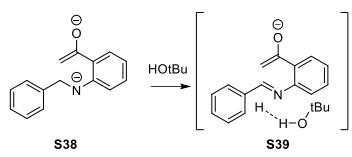
Product S37

29

-708.8746445

C	3.88159	-1.29060	-0.78141
C	2.51427	-1.11552	-0.56942
C	2.04077	-0.07758	0.23413
C	2.97638	0.77620	0.82860
C	4.34174	0.60590	0.62262
C	4.80174	-0.43121	-0.18786
H	4.22894	-2.10439	-1.40906
H	1.79095	-1.78814	-1.01426
H	5.04839	1.27891	1.09587
H	5.86472	-0.56939	-0.34952
C	0.55583	0.17263	0.42826
C	-1.55658	-0.81629	0.11964
C	-2.17462	0.51353	-0.01231
C	-2.44309	-1.92360	0.16453
C	-3.60369	0.61298	0.01617
C	-3.84531	-1.78586	0.14808
H	-1.99806	-2.91262	0.24353
C	-4.42443	-0.51300	0.09338
H	-4.04246	1.60225	-0.06514
H	-4.47242	-2.67133	0.19875
H	-5.50486	-0.40081	0.10121
N	-0.22811	-1.01434	0.18688
O	-1.80205	2.83178	-0.48147
C	-1.36053	1.63803	-0.28142
C	0.12518	1.37877	-0.42319
H	0.67949	2.27713	-0.12532
H	0.38118	1.17958	-1.47731
H	2.62575	1.58496	1.46407
H	0.43609	0.50368	1.48207

7.6 DMSO (Scheme S3.4)



45

-943.1293587

C	-5.23735	-0.27394	-0.59614
C	-3.96667	-0.47743	-1.13464
C	-2.85164	0.17476	-0.60948
C	-3.03607	1.03916	0.47325
C	-4.30002	1.24833	1.01547
C	-5.40740	0.59037	0.48082
H	-6.09253	-0.78941	-1.01892
H	-3.83857	-1.15349	-1.97462
H	-4.42485	1.92637	1.85246
H	-6.39354	0.75200	0.90100
C	-1.46609	-0.06119	-1.16278
H	-1.56862	-0.48060	-2.18116
C	0.55913	-1.13162	-0.65825
C	1.44179	-1.92094	0.18160
C	1.16364	-0.61023	-1.85408
C	2.75875	-2.12377	-0.17749
C	2.50109	-0.84983	-2.18412
H	0.56126	-0.03935	-2.55133
C	3.32412	-1.59898	-1.35760
H	3.38248	-2.71272	0.49117
H	2.89449	-0.43235	-3.10792
H	4.36333	-1.77896	-1.60608
N	-0.70524	-0.91594	-0.28080
O	0.24402	-3.64201	1.33505
C	0.93253	-2.56167	1.45785
C	1.28368	-1.95994	2.64456
H	1.88426	-1.05791	2.65444
H	0.95847	-2.37902	3.59316
H	-2.17290	1.54908	0.89029
O	2.09105	2.38109	-1.07642
C	2.10343	2.49480	0.35317
C	0.70113	2.21858	0.89353
H	0.38264	1.20444	0.62785
H	0.68035	2.31388	1.98299
H	-0.01074	2.93251	0.46902
C	2.53080	3.92489	0.65178
H	2.57061	4.09315	1.73025
H	3.52076	4.11875	0.23176
H	1.82084	4.63181	0.21547
C	3.10195	1.49242	0.92888
H	4.10307	1.69105	0.53671
H	3.13435	1.56177	2.01971
H	2.81195	0.47286	0.65411
H	1.84930	1.46629	-1.29206
H	-0.98122	0.92627	-1.29984

TS of S38 to S39

45

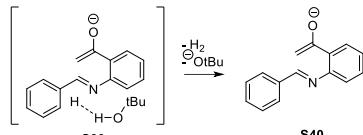
C	-2.96816	-2.69682	-1.45585
C	-1.78774	-1.99552	-1.68319
C	-0.97821	-1.60934	-0.61276
C	-1.36355	-1.93096	0.69300
C	-2.53893	-2.63228	0.91887
C	-3.34469	-3.01525	-0.15468
H	-3.59260	-2.99035	-2.29138
H	-1.49326	-1.73731	-2.69552
H	-2.83628	-2.87698	1.93203
H	-4.26556	-3.55746	0.02615
C	0.25058	-0.84433	-0.88645
H	0.42934	-0.58526	-1.93748
C	-1.60185	1.64143	-2.19435
C	2.14615	0.33568	-0.32007
C	3.43253	0.04241	0.16686
C	1.92286	1.49924	-1.06347
C	4.46960	0.92222	-0.14080
C	2.97328	2.36577	-1.35331
H	0.91156	1.73217	-1.38291
C	4.25294	2.07562	-0.89448
H	5.46610	0.69192	0.22074
H	2.78506	3.26676	-1.92592
H	5.07795	2.74332	-1.11458
N	1.05953	-0.49581	0.02920
O	3.48487	-2.32897	0.31745
C	3.70203	-1.23181	0.94435
C	4.16426	-1.07967	2.22742
H	4.31413	-0.09577	2.65340
H	4.38874	-1.95000	2.83592
H	-0.73541	-1.61692	1.51830
H	-2.10082	2.09023	-1.53161
O	-2.80929	2.80234	-0.65617
C	-3.09870	2.10073	0.51502
C	-3.89236	0.81836	0.20020
H	-3.29862	0.15219	-0.43247
H	-4.16069	0.27088	1.11000
H	-4.81234	1.07661	-0.33378
C	-3.94222	2.98667	1.44291
H	-4.19636	2.47193	2.37575
H	-3.38984	3.89834	1.68896
H	-4.87075	3.27328	0.94034
C	-1.80244	1.71116	1.24967
H	-1.23382	2.61307	1.49782
C	-2.00712	1.16289	2.17604
H	-1.18239	1.07749	0.61042

Intermediate S39

45

-943.0842956

C	-2.94408	-2.67901	-1.46906
C	-1.76638	-1.97331	-1.69657
C	-0.95756	-1.58562	-0.62589
C	-1.34051	-1.91086	0.67980
C	-2.51243	-2.61825	0.90544
C	-3.31803	-3.00159	-0.16798
H	-3.56833	-2.97307	-2.30453
H	-1.47384	-1.71194	-2.70854
H	-2.80759	-2.86635	1.91840
H	-4.23663	-3.54770	0.01259
C	0.27176	-0.82056	-0.89928
H	0.45165	-0.56197	-1.95060
H	-1.85358	1.61560	-2.64167
C	2.17225	0.35198	-0.32387
C	3.45212	0.05099	0.17583
C	1.96483	1.51615	-1.07055
C	4.49807	0.92317	-0.12285
C	3.02352	2.37543	-1.35128
H	0.95953	1.75867	-1.40088
C	4.29657	2.07711	-0.87978
H	5.48938	0.68633	0.24852
H	2.84658	3.27700	-1.92641
H	5.12799	2.73916	-1.09262
N	1.07909	-0.47330	0.01842
O	3.48587	-2.32020	0.32869
C	3.70520	-1.22439	0.95698
C	4.15710	-1.07436	2.24392
H	4.30994	-0.09123	2.67059
H	4.36978	-1.94578	2.85506
H	-0.71191	-1.59756	1.50510
H	-2.62543	2.31243	-1.34486
O	-3.10956	2.81318	-0.64358
C	-3.15993	2.03563	0.55201
C	-3.88567	0.71488	0.28819
H	-3.33081	0.10678	-0.43211
H	-3.98401	0.13567	1.21045
H	-4.88419	0.91069	-0.11175
C	-3.93413	2.87117	1.56458
H	-4.00608	2.34789	2.52105
H	-3.43112	3.82750	1.72721
H	-4.94460	3.06722	1.19735
C	-1.74045	1.76790	1.05643
H	-1.22264	2.71278	1.24270
H	-1.75789	1.18852	1.98418
H	-1.17374	1.19989	0.31446

**TS of S39 to S40**

45

-943.0712537

C	-2.96849	-2.69734	-1.45564
C	-1.78799	-1.99622	-1.68312
C	-0.97847	-1.60983	-0.61277
C	-1.36388	-1.93109	0.69307
C	-2.53933	-2.63225	0.91907
C	-3.34510	-3.01540	-0.15440
H	-3.59293	-2.99102	-2.29112
H	-1.49345	-1.73830	-2.69551
H	-2.83672	-2.87668	1.93228
H	-4.26602	-3.55748	0.02654
C	0.25032	-0.84486	-0.88659
H	0.42923	-0.58628	-1.93770
H	-1.60184	1.64056	-2.19466
C	2.14583	0.33542	-0.32023
C	3.43215	0.04226	0.16694
C	1.92268	1.49874	-1.06403
C	4.46932	0.92186	-0.14096
C	2.97319	2.36511	-1.35406
H	0.91143	1.73161	-1.38368
C	4.25280	2.07502	-0.89505
H	5.46577	0.69161	0.22072
H	2.78507	3.26592	-1.92699
H	5.07787	2.74260	-1.11531
N	1.05919	-0.49596	0.02913
O	3.48456	-2.32906	0.31811
C	3.70149	-1.23175	0.94483
C	4.16338	-1.07930	2.22797
H	4.31307	-0.09530	2.65378
H	4.38772	-1.94950	2.83673
H	-0.73576	-1.61689	1.51831
H	-2.10032	2.08961	-1.53188
O	-2.80733	2.80300	-0.65600
C	-3.09768	2.10155	0.51501
C	-3.89171	0.81950	0.19980
H	-3.29791	0.15295	-0.43241
H	-4.16086	0.27225	1.10950
H	-4.81123	1.07815	-0.33480
C	-3.94136	2.98783	1.44243
H	-4.19587	2.47336	2.37533
H	-3.38894	3.89948	1.68843
H	-4.86970	3.27443	0.93950
C	-1.80193	1.71156	1.25033
H	-1.23321	2.61332	1.49880
H	-2.00717	1.16331	2.17659
H	-1.18171	1.07779	0.61133

Prod S40

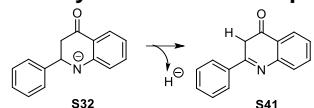
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-943.0786893

C	3.07899	-3.99769	-0.72763
C	2.23204	-2.91419	-0.94389
C	2.38035	-1.74282	-0.19844
C	3.39198	-1.66337	0.76521
C	4.23763	-2.74229	0.97739
C	4.08160	-3.91276	0.23308
H	2.95635	-4.90485	-1.30716
H	1.44885	-2.97688	-1.69299
H	5.02102	-2.67529	1.72323
H	4.74312	-4.75410	0.40318
C	1.46123	-0.61553	-0.43995
H	0.72928	-0.75630	-1.24565
H	-0.78823	-2.44165	0.20896
C	0.54388	1.46020	-0.00928
C	0.94756	2.80630	-0.06828
C	-0.81251	1.12976	-0.08742
C	-0.03413	3.78262	-0.23488
C	-1.77626	2.12112	-0.24717
H	-1.11183	0.09244	0.01680
C	-1.38667	3.45336	-0.32552
H	0.27551	4.82078	-0.29311
H	-2.82328	1.84436	-0.29693
H	-2.12862	4.23391	-0.44917
N	1.51100	0.46024	0.23347
O	3.13925	2.73131	-0.98313
C	2.41697	3.17994	-0.02335
C	2.81702	3.96732	1.02675
H	2.11126	4.29059	1.78132
H	3.85283	4.27876	1.11568
H	3.50179	-0.74927	1.33634
H	-1.52296	-2.34885	0.29592
O	-4.27389	-2.61632	0.32458
C	-4.68032	-1.31566	0.17176
C	-4.15006	-0.42483	1.31945
H	-3.05622	-0.46794	1.33857
H	-4.45448	0.62413	1.22217
H	-4.52143	-0.80380	2.27730
C	-6.22326	-1.20331	0.16751
H	-6.57518	-0.17075	0.05870
H	-6.63154	-1.79594	-0.65763
H	-6.61993	-1.60728	1.10464
C	-4.16338	-0.72052	-1.15897
H	-4.52160	-1.33103	-1.99436
H	-4.49219	0.31288	-1.32166
H	-3.06844	-0.74151	-1.16837

7.7 DMSO (Scheme S3.5)

1. Hydride Elimination pathway



SM S32

29

-708.8185638

C

C 2.9

C	4.33215	0.59416	0.64822
C	2.96723	0.77402	0.84986
C	2.03292	-0.06256	0.23323
C	2.49720	-1.08991	-0.58829
C	3.86349	-1.27256	-0.79468
C	4.78598	-0.43179	-0.17847
H	5.04198	1.25096	1.13835
H	2.61949	1.57372	1.49776
H	4.20775	-2.07661	-1.43574
H	5.84850	-0.57664	-0.33621
C	0.55090	0.19523	0.41572
C	-1.53530	-0.79846	0.13176
C	-2.17683	0.49738	0.01256
C	-2.43743	-1.93308	0.15084
C	-3.58717	0.60838	0.02064
C	-3.79342	-1.77981	0.15206
H	-1.99105	-2.92119	0.19861
C	-4.40243	-0.49152	0.10411
H	-4.01112	1.60426	-0.06573
H	-4.42535	-2.66226	0.19037
H	-5.48081	-0.39403	0.10860
N	-0.23858	-1.00815	0.24035
O	-1.79151	2.79616	-0.45597
C	-1.36108	1.64988	-0.29353
C	0.10892	1.34040	-0.50367
H	1.77470	-1.74966	-1.05350
H	0.69918	2.24416	-0.33899
H	0.23987	1.03357	-1.55156
H	0.40831	0.56277	1.45105

TS of S32 to S41

29

-708.7451341

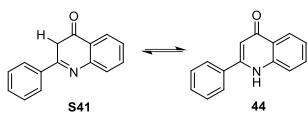
C	3.93692	-1.44068	0.53080
C	2.56527	-1.23457	0.50288
C	2.03273	-0.03996	0.00437
C	2.90731	0.93933	-0.47275
C	4.28478	0.72895	-0.45271
C	4.80403	-0.45761	0.05160
H	4.33514	-2.36645	0.93008
H	1.88458	-1.98884	0.87826
H	4.94985	1.49530	-0.83330
H	5.87545	-0.61837	0.07303
C	0.55519	0.14745	-0.03861
C	-1.55266	-0.76893	-0.17483
C	-2.20432	0.45497	0.09072
C	-2.34393	-1.92184	-0.33320
C	-3.59955	0.50766	0.19625
C	-3.72173	-1.85401	-0.23827
H	-1.84285	-2.86477	-0.51962
C	-4.36069	-0.63492	0.03148
H	-4.06540	1.46686	0.39268
H	-4.31203	-2.75424	-0.36663
H	-5.44057	-0.59049	0.10343
N	-0.17480	-0.91877	-0.18756
O	-1.87225	2.78068	0.43657
C	-1.40132	1.69128	0.15815
C	0.01939	1.53063	-0.30984
H	0.63591	2.31231	0.12463
H	-0.00053	1.67379	-1.40521
H	2.52452	1.86810	-0.87846
H	0.12903	0.66632	2.04534

Product S41

29

-708.7506846

C	3.95531	-1.48963	0.36020
C	2.58193	-1.29730	0.31379
C	2.05053	-0.05496	-0.05336
C	2.92554	0.98875	-0.36989
C	4.30265	0.79137	-0.33187
C	4.82081	-0.44596	0.03445
H	4.35393	-2.45322	0.65481
H	1.90318	-2.10111	0.56906
H	4.96816	1.60694	-0.58789
H	5.89316	-0.59761	0.06968
C	0.57643	0.13321	-0.09738
C	-1.56587	-0.76926	-0.10948
C	-2.23052	0.46350	0.00646
C	-2.32656	-1.94004	-0.18989
C	-3.62463	0.51462	0.04531
C	-3.71241	-1.87967	-0.16193
H	-1.80858	-2.88816	-0.27061
C	-4.36855	-0.65158	-0.04403
H	-4.10572	1.48107	0.14164
H	-4.28920	-2.79481	-0.22755
H	-5.45051	-0.61270	-0.02152
N	-0.16850	-0.90888	-0.11302
O	-1.91833	2.79115	0.30296
C	-1.42915	1.69903	0.09506
C	0.05178	1.54517	-0.14428
H	0.58801	2.18818	0.55594
H	0.24339	1.95066	-1.14810
H	2.54460	1.96019	-0.66053
H	-0.35810	0.65009	3.17342

**SM S41**

28

-708.1012114

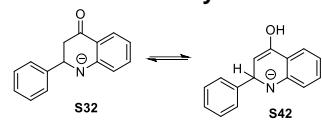
C	3.95977	-1.52775	-0.15676
C	2.58660	-1.33262	-0.14196
C	2.05181	-0.04648	0.01069
C	2.92621	1.03626	0.14891
C	4.30377	0.83792	0.13830
C	4.82384	-0.44225	-0.01577
H	4.36054	-2.52703	-0.27924
H	1.90869	-2.16935	-0.25118
H	4.96859	1.68602	0.24905
H	5.89640	-0.59583	-0.02710
C	0.57603	0.14331	0.02290
C	-1.56868	-0.76376	0.03068
C	-2.24065	0.46937	-0.01245
C	-2.32177	-1.94157	0.06858
C	-3.63592	0.51470	-0.01929
C	-3.70798	-1.88757	0.06721
H	-1.79724	-2.88893	0.09837
C	-4.37203	-0.65883	0.02378
H	-4.12382	1.48171	-0.05652
H	-4.27940	-2.80781	0.09825
H	-5.45431	-0.62511	0.02275
N	-0.17035	-0.89738	0.02606
O	-1.94966	2.81167	-0.17204
C	-1.44788	1.71099	-0.06388
C	0.05021	1.55618	0.04058
H	0.35413	2.03817	0.97790
H	2.54757	2.04339	0.27094
H	0.50858	2.14570	-0.75840

TS of S41 tautomerising to 44

28

-708.0005752			
C	3.86113	-1.38761	-0.69882
C	2.49592	-1.17757	-0.53033
C	2.04481	-0.02565	0.11091
C	2.96297	0.90638	0.59485
C	4.32620	0.68968	0.43049
C	4.77756	-0.45661	-0.21882
H	4.20745	-2.28011	-1.20619
H	1.77850	-1.89998	-0.89936
H	5.03512	1.41305	0.81513
H	5.84019	-0.62453	-0.34765
C	0.56726	0.21581	0.25921
C	-1.55725	-0.75968	0.20483
C	-2.17040	0.49305	-0.08162
C	-2.37574	-1.92045	0.33606
C	-3.56660	0.55023	-0.24695
C	-3.72820	-1.83406	0.15607
H	-1.88729	-2.86009	0.56390
C	-4.33112	-0.58655	-0.13592
H	-4.01511	1.51286	-0.45899
H	-4.34563	-2.71994	0.24137
H	-5.40540	-0.53283	-0.26619
N	-0.22670	-0.93408	0.34912
O	-1.87898	2.83299	-0.39911
C	-1.37443	1.72045	-0.17366
C	0.02964	1.50366	-0.02390
H	0.70371	2.34734	-0.11042
H	2.61746	1.79442	1.11303
H	0.31934	0.13792	1.41003

2. Enol Pathway



SM S32

29

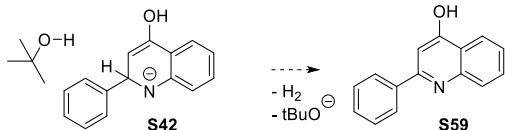
-708.8185638			
C	4.33215	0.59416	0.64822
C	2.96723	0.77402	0.84986
C	2.03292	-0.06256	0.23323
C	2.49720	-1.08991	-0.58829
C	3.86349	-1.27256	-0.79468
C	4.78598	-0.43179	-0.17847
H	5.04198	1.25096	1.13835
H	2.61949	1.57372	1.49776
H	4.20775	-2.07661	-1.43574
H	5.84850	-0.57664	-0.33621
C	0.55090	0.19523	0.41572
C	-1.53530	-0.79846	0.13176
C	-2.17683	0.49738	0.01256
C	-2.43743	-1.93308	0.15084
C	-3.58717	0.60838	0.02064
C	-3.79342	-1.77981	0.15206
H	-1.99105	-2.92119	0.19861
C	-4.40243	-0.49152	0.10411
H	-4.01112	1.60426	-0.06573
H	-4.42535	-2.66226	0.19037
H	-5.48081	-0.39403	0.10860
N	-0.23858	-1.00815	0.24035
O	-1.79151	2.79616	-0.45597
C	-1.36108	1.64988	-0.29353
C	0.10892	1.34040	-0.50367
H	1.77470	-1.74966	-1.05350
H	0.69918	2.24416	-0.33899
H	0.23987	1.03357	-1.55156
H	0.40831	0.56277	1.45105

TS of S32 to S42

29

-708.7131734

C	4.33989	0.56196	0.66081
C	2.97782	0.74989	0.86950
C	2.03342	-0.07040	0.24504
C	2.48666	-1.08849	-0.59327
C	3.85160	-1.27929	-0.80770
C	4.78308	-0.45601	-0.18279
H	5.05693	1.20641	1.15697
H	2.63489	1.54517	1.52494
H	4.18685	-2.07662	-1.46192
H	5.84385	-0.60708	-0.34652
C	0.55962	0.20581	0.44412
C	-1.54052	-0.80475	0.11195
C	-2.19775	0.50464	0.02308
C	-2.44670	-1.94304	0.08236
C	-3.61739	0.62313	0.09232
C	-3.79561	-1.78070	0.12289
H	-2.00524	-2.93400	0.07083
C	-4.41206	-0.48241	0.15168
H	-4.04845	1.61951	0.07375
H	-4.43292	-2.65962	0.13649
H	-5.49049	-0.39805	0.19951
N	-0.25445	-1.00053	0.22108
O	-1.60482	2.80844	-0.55478
C	-1.33981	1.54916	-0.30643
C	0.09850	1.37935	-0.41038
H	1.75886	-1.73581	-1.06759
H	0.42230	0.48822	1.50395
H	-0.36335	2.81260	-0.44964
H	0.37210	1.26233	-1.46911



SM S42 and *tert*-butanol

44

-942.4470121

C	-1.63293	3.82120	0.24331
C	-1.02626	2.94510	-0.65326
C	-0.39779	1.78091	-0.20781
C	-0.38360	1.51120	1.16174
C	-0.98614	2.38563	2.06345
C	-1.61507	3.54285	1.60813
H	-2.12576	4.71521	-0.12265
H	-1.05118	3.16091	-1.71813
H	-0.97202	2.16061	3.12450
H	-2.08798	4.21981	2.31024
C	0.27381	0.83825	-1.21509
C	1.31682	-1.03705	-0.15481
C	2.59982	-0.38634	-0.10236
C	1.24667	-2.31450	0.49027
C	3.67595	-0.95637	0.58177
C	2.32437	-2.84920	1.16596
H	0.30218	-2.84718	0.44678
C	3.55698	-2.17621	1.23698
H	4.62291	-0.42620	0.58705
H	2.21291	-3.81303	1.65445
H	4.39457	-2.60412	1.77362
N	0.24542	-0.54855	-0.78032
O	4.01135	1.28570	-1.04960
C	2.72980	0.81380	-0.91378
C	1.66554	1.36010	-1.51928
H	0.08545	0.59944	1.51491
H	-1.11297	-1.48592	-1.03262
H	1.77148	2.22451	-2.16924
H	-0.32807	0.91705	-2.13105
O	-1.91132	-2.07816	-1.22843
C	-2.95546	-1.74400	-0.32430
C	-3.44834	-0.32081	-0.60421
H	-4.27094	-0.04996	0.06430
H	-2.63285	0.39258	-0.45914
H	-3.80109	-0.24431	-1.63667
C	-2.44484	-1.84427	1.11674
H	-2.11006	-2.86398	1.32708
H	-1.59770	-1.16589	1.25201
H	-3.23029	-1.58093	1.83107
C	-4.08174	-2.74480	-0.55913
H	-4.92713	-2.54172	0.10349
H	-4.42843	-2.68418	-1.59407
H	-3.72697	-3.76140	-0.37075
H	3.99019	2.10537	-1.55437

Product S42

29

-708.7875514

C	-4.39623	0.43940	-0.55700
C	-3.07001	0.60165	-0.94755
C	-2.04281	-0.10296	-0.31531
C	-2.37312	-0.98091	0.71561
C	-3.69937	-1.15052	1.10875
C	-4.71604	-0.43999	0.47554
H	-5.18081	0.99229	-1.06166
H	-2.82545	1.28222	-1.75857
H	-3.94025	-1.84075	1.90995
H	-5.74786	-0.57350	0.77942
C	-0.59454	0.13700	-0.72576
C	1.52989	-0.81783	-0.25750
C	2.13926	0.47284	-0.02183
C	2.44210	-1.92936	-0.22260
C	3.51679	0.60981	0.15853
C	3.79983	-1.76138	-0.05580
H	2.02456	-2.92246	-0.35787
C	4.37075	-0.48673	0.12438
H	3.91594	1.60288	0.34011
H	4.44231	-2.63747	-0.06419
H	5.43950	-0.36628	0.24985
N	0.23460	-1.02604	-0.45390
O	1.75998	2.72211	0.67951
C	1.20874	1.57069	0.17379
C	-0.10061	1.41793	-0.07335
H	-1.57502	-1.53561	1.19489
H	-0.63335	0.30671	-1.82314
H	1.07660	3.39889	0.72775
H	-0.80593	2.22068	0.12527

TS of S42 to S59

44

-942.3906873

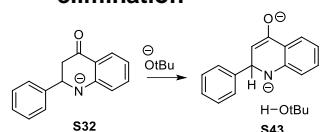
C	-4.76810	1.30737	0.55190
C	-3.41060	1.05594	0.70017
C	-2.77616	0.06541	-0.05727
C	-3.53969	-0.66416	-0.96869
C	-4.90060	-0.40520	-1.12923
C	-5.52215	0.57746	-0.36832
H	-5.23925	2.08230	1.14599
H	-2.82878	1.66026	1.38721
H	-5.47518	-0.98109	-1.84602
H	-6.58040	0.77793	-0.48883
C	-1.31776	-0.26368	0.12839
C	0.44689	-1.60678	-0.51956
C	1.12973	-1.43857	0.71558
C	1.11216	-2.34284	-1.53554
C	2.42367	-1.95726	0.89892
C	2.38181	-2.83882	-1.34178
H	0.59535	-2.48624	-2.47805
C	3.05417	-2.64386	-0.11900
H	2.91724	-1.80732	1.85225
H	2.87274	-3.38304	-2.14140
H	4.05453	-3.03557	0.02043
N	-0.79342	-1.11443	-0.76620
O	1.01089	-0.70959	2.96970
C	0.40736	-0.75704	1.75179
C	-0.80053	-0.21032	1.48330
H	-3.05307	-1.43685	-1.54966
H	0.74921	1.73625	0.15283
H	-1.34608	0.32218	2.25369
H	-0.78727	1.40716	-0.41334
O	1.63023	1.91502	0.55792
C	2.56817	2.21827	-0.47416
C	2.20248	3.55067	-1.13097
H	2.92820	3.81795	-1.90392
H	1.21432	3.48334	-1.59461
H	2.18064	4.34615	-0.38181
C	2.58655	1.09888	-1.51613
H	2.80141	0.14044	-1.03639
H	1.61460	1.01882	-2.01113
H	3.34720	1.29535	-2.27725
C	3.92414	2.31713	0.21465
H	4.70559	2.57680	-0.50344
H	3.89585	3.08402	0.99282
H	4.17741	1.35968	0.67765
H	0.47130	-0.19651	3.58109

Product S59 + H₂ + tert-butoxide anion

44

C	-942.4159297	4.73228	1.24277	-0.95152
C	C	3.56486	0.49031	-1.03603
C	C	2.86939	0.12988	0.12159
C	C	3.35933	0.54262	1.36433
C	C	4.53017	1.28629	1.44825
C	C	5.22062	1.63825	0.29011
H	H	5.25701	1.52374	-1.85697
H	H	3.18424	0.20580	-2.01040
H	H	4.90593	1.59138	2.41787
H	H	6.13255	2.22011	0.35489
C	C	1.61667	-0.67126	0.04763
C	C	-0.44523	-1.17796	0.92790
C	C	-0.73226	-2.10832	-0.10228
C	C	-1.42357	-0.96544	1.93371
C	C	-1.97375	-2.78619	-0.12564
C	C	-2.62182	-1.63156	1.89432
H	H	-1.19561	-0.25932	2.72380
C	C	-2.90386	-2.54827	0.85428
H	H	-2.17414	-3.48909	-0.92461
H	H	-3.36305	-1.45605	2.66544
H	H	-3.85627	-3.06394	0.83637
N	N	0.71732	-0.46931	0.98809
O	O	0.00941	-3.21699	-2.04710
C	C	0.27693	-2.31434	-1.08377
C	C	1.44821	-1.60798	-1.00449
H	H	2.81658	0.26642	2.25996
H	H	-1.88007	1.20288	-1.67256
H	H	2.23512	-1.76760	-1.73152
H	H	-0.45746	1.15059	-2.49842
O	O	-2.75025	1.13906	-1.20629
C	C	-2.96652	2.31603	-0.43029
C	C	-3.18518	3.51044	-1.36136
H	H	-3.38180	4.42194	-0.79048
H	H	-2.29769	3.67422	-1.97885
H	H	-4.03594	3.32068	-2.02049
C	C	-1.77027	2.57237	0.48830
H	H	-1.58401	1.69395	1.11077
H	H	-0.87060	2.77597	-0.09831
H	H	-1.96093	3.43115	1.13764
C	C	-4.21703	2.04895	0.39904
H	H	-4.46988	2.91955	1.00904
H	H	-5.06261	1.82523	-0.25622
H	H	-4.05208	1.19374	1.06012
H	H	0.74241	-3.27230	-2.67103

3. Enolate formation then hydride elimination



SM S32 + *tert*-butoxide anion

43

-941.9423188

C -2.40412

C	-2.40412	2.63236	1.03236
C	-1.31683	1.78209	1.23161
C	-0.36976	1.58227	0.22737
C	-0.53631	2.25193	-0.98845
C	-1.61898	3.09972	-1.19359
C	-2.55801	3.29494	-0.18044
H	-3.12988	2.77524	1.82539
H	-1.20161	1.26889	2.18160
H	-1.73125	3.61269	-2.14239
H	-3.40074	3.95808	-0.33851
C	0.80288	0.64556	0.42689
C	3.10439	0.51998	0.07980
C	3.05096	-0.93002	0.06089
C	4.43697	1.08732	0.01084
C	4.23887	-1.69614	0.07878
C	5.55780	0.30803	0.02430
H	4.51486	2.16947	-0.02036
C	5.48196	-1.11388	0.07697
H	4.13468	-2.77696	0.06802
H	6.53329	0.78461	-0.00707
H	6.38471	-1.71194	0.08779
N	2.06532	1.32626	0.17353
O	1.61549	-2.79896	-0.24053
C	1.77519	-1.57572	-0.16546
C	0.62393	-0.62414	-0.41188
H	0.20158	2.11230	-1.77169
H	-0.33624	-1.11077	-0.21407
H	0.65204	-0.35545	-1.47916
H	0.78605	0.32298	1.48599
O	-2.49498	-1.87033	-0.18338
C	-3.83718	-1.62297	-0.03429
C	-4.68765	-2.83190	-0.48903
H	-5.76473	-2.65871	-0.38015
H	-4.47723	-3.05186	-1.54069
H	-4.41760	-3.71269	0.10269
C	-4.27016	-0.39743	-0.87279
H	-3.69374	0.47968	-0.55926
H	-4.05657	-0.58728	-1.92996
H	-5.33757	-0.16709	-0.77172
C	-4.18984	-1.32971	1.44254
H	-5.25830	-1.13777	1.59610
H	-3.89885	-2.18367	2.06318
H	-3.62880	-0.45299	1.78226

TS S32 to S43

43

-941.9287739

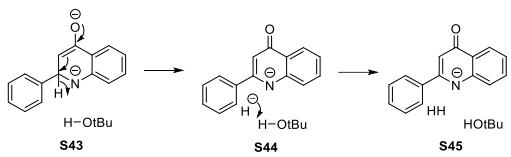
C	4.22704	-2.19490	0.08914	
C	2.84892	-2.12873	-0.09427	
C	2.21044	-0.91742	-0.37897	
C	2.99735	0.23197	-0.48392	
C	4.37725	0.17423	-0.29276	
C	4.99925	-1.03837	-0.00589	
H	4.70035	-3.14782	0.29996	
H	2.25219	-3.03409	-0.01784	
H	4.97002	1.07930	-0.37280	
H	6.07293	-1.08342	0.13615	
C	0.68465	-0.87695	-0.51095	
C	-0.08329	1.34072	-0.78402	
C	-0.15658	1.56123	0.64569	
C	-0.40773	2.49458	-1.59481	
C	-0.46033	2.82702	1.16332	
C	-0.69801	3.71912	-1.04729	
H	-0.39643	2.36263	-2.67270	
C	-0.71882	3.91974	0.35369	
H	-0.50082	2.92309	2.24465	
H	-0.91787	4.55309	-1.70861	
H	-0.94666	4.89212	0.77276	
N	0.24755	0.20860	-1.37835	
O	-0.09932	0.52778	2.78694	
C	-0.02970	0.40182	1.54174	
C	0.03786	-0.88321	0.88006	
H	2.51757	1.17466	-0.72160	
H	-1.23447	-1.29345	0.80920	
H	0.45747	-1.65460	1.53358	
H	0.41126	-1.82266	-1.00177	
O	-2.41164	-1.87291	0.89797	
C	-3.28299	-1.54413	-0.14217	
C	-4.63240	-2.23534	0.09515	
H	-5.35301	-2.00444	-0.69673	
H	-4.49407	-3.31987	0.13178	
H	-5.05187	-1.90997	1.05167	
C	-2.70897	-2.01146	-1.49120	
H	-1.74937	-1.51648	-1.66690	
H	-2.54826	-3.09404	-1.46872	
H	-3.38131	-1.77907	-2.32433	
C	-3.50321	-0.02196	-0.19985	
H	-4.18979	0.26066	-1.00516	
H	-3.92168	0.32592	0.75014	
H	-2.54587	0.48156	-0.35982	

Prod S43 + *tert*-butanol

43

-941.9454129

C	4.52548	-1.98616	0.02516
C	3.14025	-1.99015	-0.13094
C	2.42748	-0.80183	-0.30538
C	3.14315	0.39854	-0.33591
C	4.52635	0.41078	-0.17729
C	5.22527	-0.78233	0.00574
H	5.05821	-2.92203	0.15582
H	2.59921	-2.93288	-0.11580
H	5.06479	1.35238	-0.20102
H	6.30268	-0.77316	0.12473
C	0.89457	-0.81708	-0.39937
C	-0.09825	1.31767	-0.75664
C	-0.35556	1.51750	0.65384
C	-0.46519	2.42169	-1.60458
C	-0.87328	2.72163	1.11838
C	-0.97409	3.60579	-1.10510
H	-0.31725	2.30019	-2.67419
C	-1.17992	3.79003	0.27158
H	-1.05348	2.79719	2.18677
H	-1.21770	4.40746	-1.79785
H	-1.57431	4.72173	0.66003
N	0.40735	0.21583	-1.30083
O	-0.54867	0.48259	2.81209
C	-0.18029	0.36276	1.58092
C	0.31222	-0.78731	1.00181
H	2.59891	1.32446	-0.48990
H	-1.68775	-1.44136	0.91602
H	0.48565	-1.65866	1.63319
H	0.65818	-1.79672	-0.85019
O	-2.55281	-1.90229	0.96478
C	-3.27225	-1.64127	-0.24267
C	-4.58143	-2.41170	-0.12866
H	-5.19757	-2.25185	-1.01667
H	-4.38422	-3.48205	-0.02990
H	-5.14199	-2.07850	0.74839
C	-2.45628	-2.13194	-1.43861
H	-1.51634	-1.57458	-1.49711
H	-2.23660	-3.19751	-1.33025
H	-3.00748	-1.98343	-2.37133
C	-3.53662	-0.14023	-0.36371
H	-4.09822	0.08425	-1.27483
H	-4.11529	0.20834	0.49636
H	-2.58857	0.40520	-0.39288



SM S43 + *tert*-butanol

43

-941.9444083

C	4.29886	-2.23872	-0.02344
C	2.92812	-2.08145	-0.22709
C	2.34902	-0.81331	-0.29392
C	3.18199	0.30177	-0.16548
C	4.55021	0.15350	0.03819
C	5.11612	-1.12015	0.11175
H	4.72882	-3.23358	0.02367
H	2.29436	-2.95821	-0.33460
H	5.18143	1.03057	0.13502
H	6.18260	-1.23725	0.26695
C	0.83054	-0.64719	-0.44611
C	-0.02038	1.56129	-0.77540
C	-0.40837	1.71066	0.61103
C	-0.27011	2.71254	-1.60380
C	-0.93402	2.91038	1.07735
C	-0.79039	3.89145	-1.10219
H	-0.01594	2.63324	-2.65712
C	-1.12661	4.02337	0.25364
H	-1.20507	2.95010	2.12845
H	-0.93967	4.72942	-1.77856
N	0.51131	0.47280	-1.31819
O	-0.71836	0.62809	2.73311
C	-0.29670	0.53005	1.51576
C	0.20232	-0.61467	0.93527
H	2.73759	1.28995	-0.23250
H	-1.95627	-1.00363	1.03865
H	0.31990	-1.50535	1.55263
H	0.50719	-1.57252	-0.95750
O	-2.88739	-1.30076	1.05465
C	-3.19198	-1.83041	-0.23802
C	-2.33237	-3.06863	-0.49469
H	-2.55124	-3.50015	-1.47504
H	-1.27301	-2.79878	-0.46258
H	-2.52289	-3.82512	0.27091
C	-2.92037	-0.76437	-1.29903
H	-3.53259	0.12042	-1.10152
H	-1.86541	-0.46911	-1.27857
H	-3.16329	-1.13923	-2.29728
C	-4.66876	-2.20112	-0.20370
H	-4.98286	-2.61605	-1.16425
H	-4.85387	-2.94576	0.57459
H	-5.27431	-1.31677	0.00920

TS1 of S43 to S44

43

-941.9073462

C	-4.72378	1.36066	0.53814
C	-3.37042	1.08710	0.68388
C	-2.75351	0.07267	-0.05776
C	-3.53542	-0.65705	-0.95302
C	-4.89420	-0.37763	-1.11236
C	-5.49596	0.62871	-0.36709
H	-5.17926	2.15387	1.12087
H	-2.76880	1.68389	1.36108
H	-5.48180	-0.95477	-1.81817
H	-6.55095	0.84646	-0.48773
C	-1.29669	-0.27249	0.14052
C	0.46197	-1.58546	-0.56298
C	1.10739	-1.50747	0.70727
C	1.16772	-2.25179	-1.60688
C	2.40003	-2.02371	0.87189
C	2.43947	-2.74917	-1.41896
H	0.67877	-2.33554	-2.57265
C	3.08074	-2.62956	-0.17131
H	2.85363	-1.93737	1.85394
H	2.95227	-3.23423	-2.24391
H	4.08361	-3.01634	-0.03087
N	-0.76255	-1.07513	-0.82394
O	0.85875	-0.97345	3.02718
C	0.36977	-0.93048	1.84711
C	-0.86610	-0.38004	1.51126
H	-3.06271	-1.44554	-1.52455
H	0.78128	1.66852	0.24454
H	-1.44831	0.09944	2.29144
H	-0.79056	1.29033	-0.32671
O	1.62856	1.95390	0.65470
C	2.57366	2.26927	-0.36758
C	2.16619	3.57013	-1.06243
H	2.88831	3.84345	-1.83681
H	1.18492	3.45381	-1.53093
H	2.10851	4.38406	-0.33526
C	2.66336	1.13023	-1.38410
H	2.86685	0.18205	-0.87950
H	1.72124	1.02390	-1.92837
H	3.45752	1.33003	-2.10952
C	3.90968	2.44393	0.34567
H	4.69306	2.72302	-0.36303
H	3.83153	3.22602	1.10515
H	4.19691	1.51014	0.83593

S44 + Hydride anion + tert-butoxide anion

43

-941.9511334

C	-4.29359	-0.35691	0.75613
C	-2.91868	-0.37921	0.97175
C	-2.07856	-1.15317	0.16410
C	-2.65534	-1.91016	-0.86135
C	-4.02908	-1.89483	-1.07378
C	-4.85523	-1.11458	-0.26747
H	-4.92501	0.26078	1.38472
H	-2.49811	0.23503	1.75888
H	-4.45719	-2.49131	-1.87147
H	-5.92552	-1.09630	-0.43680
C	-0.59357	-1.15539	0.34933
C	1.47608	-1.44893	-0.59541
C	2.14209	-1.12122	0.61272
C	2.27087	-1.75721	-1.73318
C	3.55054	-1.10706	0.65382
C	3.64351	-1.73653	-1.66884
H	1.75773	-2.00465	-2.65620
C	4.29888	-1.40725	-0.46232
H	4.02722	-0.84870	1.59267
H	4.22815	-1.97446	-2.55091
H	5.38172	-1.39197	-0.42078
N	0.12012	-1.46806	-0.73212
O	1.89982	-0.48168	2.89759
C	1.35463	-0.78514	1.80107
C	-0.04687	-0.83660	1.59629
H	-2.00828	-2.50544	-1.49334
H	-0.68879	-0.61964	2.44130
H	-2.33873	1.64316	-2.25097
H	-1.23986	2.80547	-1.71740
O	-0.65182	3.56344	-1.48464
C	0.17630	3.20407	-0.37781
C	1.02173	4.43327	-0.06678
H	1.69325	4.23442	0.77188
H	1.62351	4.70619	-0.93727
H	0.38056	5.27928	0.19293
C	1.07028	2.02249	-0.75513
H	0.46363	1.14487	-0.99531
H	1.68297	2.27698	-1.62482
H	1.73102	1.75333	0.07391
C	-0.69593	2.83628	0.82352
H	-1.31305	1.96609	0.58459
H	-0.07831	2.58524	1.69057
H	-1.35001	3.67236	1.08510

TS2 of S44 to S45

43

-941.9382458

C	-4.51461	0.60183	0.83251
C	-3.21494	0.13101	0.99742
C	-2.55143	-0.51470	-0.05044
C	-3.21848	-0.67422	-1.26896
C	-4.51995	-0.21313	-1.43211
C	-5.17344	0.42822	-0.38129
H	-5.01001	1.11103	1.65137
H	-2.70329	0.28916	1.94007
H	-5.02584	-0.35325	-2.38064
H	-6.18570	0.79358	-0.50924
C	-1.14524	-0.99470	0.10570
C	0.91857	-1.28950	-0.84559
C	1.47860	-1.75395	0.37216
C	1.77100	-1.19137	-1.97926
C	2.84627	-2.09058	0.42856
C	3.10119	-1.52569	-1.89902
H	1.33954	-0.83251	-2.90772
C	3.65346	-1.97938	-0.68119
H	3.24203	-2.43978	1.37589
H	3.73351	-1.43834	-2.77592
H	4.70467	-2.23775	-0.62647
N	-0.38565	-0.91522	-0.98511
O	1.07539	-2.30618	2.65705
C	0.62745	-1.87627	1.55977
C	-0.71460	-1.47046	1.34859
H	-2.70176	-1.16458	-2.08510
H	-1.40851	-1.53732	2.17837
H	-1.20793	2.73899	-1.25177
H	-0.26556	2.75093	-1.15190
O	1.05604	2.75462	-1.12849
C	1.64544	2.77221	0.13789
C	2.97013	1.99487	0.10059
H	3.48607	2.02727	1.06665
H	2.77948	0.94763	-0.15593
H	3.63120	2.42383	-0.65891
C	0.73209	2.11397	1.18884
H	-0.21522	2.65453	1.27130
H	0.51223	1.08168	0.89919
H	1.20833	2.10185	2.17501
C	1.93158	4.22182	0.56846
H	0.99686	4.78955	0.60159
H	2.40449	4.27397	1.55499
H	2.59496	4.69882	-0.15946

Product S45 + H₂ + tert-butoxide anion

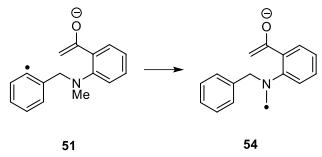
43

-941.9468177

C	4.82143	-1.97082	0.19592
C	3.55797	-1.46360	0.48603
C	3.16329	-0.21133	0.00461
C	4.06314	0.51731	-0.77992
C	5.32871	0.01621	-1.06283
C	5.71334	-1.23139	-0.57585
H	5.10724	-2.94769	0.56876
H	2.86667	-2.05527	1.07530
H	6.01693	0.59982	-1.66374
H	6.69830	-1.62511	-0.79834
C	1.80966	0.34910	0.30253
C	0.04219	1.62887	-0.39654
C	-0.68231	1.38774	0.79858
C	-0.56747	2.43643	-1.39486
C	-1.96381	1.95011	0.96566
C	-1.82016	2.97111	-1.21014
H	-0.01337	2.61576	-2.30996
C	-2.53283	2.72988	-0.01582
H	-2.49044	1.74047	1.89012
H	-2.26563	3.58185	-1.98787
H	-3.52264	3.15087	0.11879
N	1.28584	1.12494	-0.64364
O	-0.68072	0.33864	2.94057
C	-0.08795	0.55681	1.84990
C	1.19383	0.04618	1.52185
H	3.75570	1.48373	-1.16000
H	1.70635	-0.56214	2.25778
H	0.21948	-1.62265	-1.36272
H	-0.51945	-1.52865	-1.29777
O	-2.98781	-1.08576	-1.57410
C	-3.67476	-1.68873	-0.54860
C	-4.76257	-0.75519	0.03361
H	-5.33549	-1.22658	0.84106
H	-4.29339	0.15310	0.42645
H	-5.45936	-0.46535	-0.76000
C	-2.73055	-2.08109	0.61352
H	-1.95765	-2.76212	0.24323
H	-2.23606	-1.18859	1.01304
H	-3.26259	-2.57686	1.43455
C	-4.37634	-2.98069	-1.03109
H	-3.62933	-3.67201	-1.43473
H	-4.92228	-3.49183	-0.22932
H	-5.08452	-2.73987	-1.83043

7. Radical Cyclisation of 18

7.1 DMSO (Scheme S4.1)



SM 51
33
-748.6003293

C	-4.13227	1.19690	0.77983
C	-2.81680	1.04009	0.42253
C	-2.30591	0.05521	-0.39807
C	-3.24156	-0.85698	-0.89875
C	-4.59558	-0.74533	-0.58005
C	-5.04608	0.27272	0.25457
H	-4.46101	1.99584	1.43497
H	-2.90046	-1.66371	-1.54054
H	-5.30040	-1.46484	-0.98008
H	-6.09802	0.35261	0.50405
C	-0.83806	-0.02742	-0.74943
H	-0.62654	-0.98364	-1.24943
H	-0.60023	0.77586	-1.45228
C	1.32874	0.61456	0.13190
C	2.47003	-0.19974	0.00320
C	1.45782	2.00155	-0.00869
C	3.70788	0.42270	-0.20283
C	2.68842	2.59745	-0.25348
H	0.56369	2.60767	0.10042
C	3.82849	1.80176	-0.33338
H	4.58690	-0.20638	-0.29423
H	2.75861	3.67419	-0.35866
H	4.80035	2.24986	-0.50701
N	0.01516	0.13415	0.42444
O	1.57793	-2.18830	-0.92643
C	2.39134	-1.71554	-0.05384
C	3.20463	-2.42287	0.79398
H	3.85361	-1.91802	1.49826
H	3.20768	-3.50773	0.77014
C	-0.11131	-0.97044	1.36681
H	-1.11379	-0.94135	1.80280
H	0.04630	-1.94801	0.89635
H	0.61502	-0.84267	2.16983

TS of 51 to 54

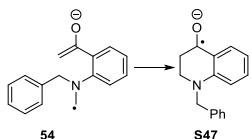
33	-748.5874472			
C	-3.25610	-0.84811	1.51199	
C	-2.21373	-0.97949	0.60979	
C	-2.19194	-0.31976	-0.60589	
C	-3.26499	0.51434	-0.93225	
C	-4.32784	0.66148	-0.04262	
C	-4.32752	-0.01503	1.17570	
H	-3.25278	-1.37273	2.46174	
H	-3.26788	1.05187	-1.87643	
H	-5.15692	1.31086	-0.29912	
H	-5.15583	0.10694	1.86517	
C	-1.01399	-0.53337	-1.55586	
H	-1.20361	-1.43267	-2.15184	
H	-0.91559	0.29945	-2.25220	
C	0.95814	0.37039	-0.37787	
C	2.28286	0.23029	0.10730	
C	0.37999	1.64907	-0.40701	
C	2.95133	1.37523	0.54211	
C	1.08180	2.77363	0.01582	
H	-0.64078	1.77543	-0.74219	
C	2.37539	2.64289	0.50125	
H	3.96807	1.25903	0.90062	
H	0.60308	3.74534	-0.02763	
H	2.93344	3.50994	0.83460	
N	0.23587	-0.74936	-0.84427	
O	3.14215	-1.67934	-1.04177	
C	3.05891	-1.08134	0.08715	
C	3.61041	-1.48385	1.27833	
H	3.47980	-0.90364	2.18263	
H	4.19300	-2.39810	1.32713	
C	0.15854	-1.90893	-0.02109	
H	-0.89872	-1.72802	0.63108	
H	-0.02789	-2.81389	-0.60325	
H	0.98674	-2.01423	0.67248	

Product 54

33

-748.6348906

C	-3.49171	0.45919	1.48549
C	-2.29102	0.09820	0.87707
C	-2.28151	-0.39511	-0.42580
C	-3.49183	-0.52527	-1.11003
C	-4.69100	-0.16438	-0.50551
C	-4.69399	0.33020	0.79711
H	-3.48574	0.84038	2.50016
H	-3.49314	-0.91365	-2.12410
H	-5.62299	-0.27091	-1.04855
H	-5.62700	0.61010	1.27189
C	-0.99511	-0.78043	-1.13790
H	-1.12323	-1.77450	-1.57849
H	-0.81371	-0.09186	-1.96633
C	1.03773	0.30034	-0.22218
C	2.41602	0.18094	0.05991
C	0.49483	1.58048	-0.43951
C	3.17656	1.34753	0.15239
C	1.28454	2.71963	-0.36934
H	-0.56380	1.68749	-0.64389
C	2.63714	2.61220	-0.06034
H	4.23524	1.24421	0.37035
H	0.83419	3.69055	-0.54201
H	3.26245	3.49485	0.00274
N	0.19146	-0.82156	-0.29952
O	3.40832	-1.47166	1.46136
C	3.16629	-1.13190	0.24684
C	3.54799	-1.78173	-0.89536
H	4.10323	-2.71272	-0.83896
H	3.28553	-1.39098	-1.87062
C	0.31586	-1.90774	0.54028
H	1.14378	-1.93634	1.22978
H	-0.23041	-2.79957	0.26701
H	-1.35599	0.19430	1.41801

**TS of 54 cyclising to form S47**

33

-748.6199687

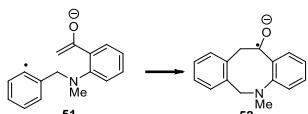
C	-3.33798	0.39382	1.61348
C	-2.18570	0.01891	0.92489
C	-2.25883	-0.38226	-0.40736
C	-3.50257	-0.40145	-1.04156
C	-4.65402	-0.02692	-0.35694
C	-4.57447	0.37203	0.97624
H	-3.26786	0.70398	2.64989
H	-3.56853	-0.71530	-2.07926
H	-5.61290	-0.04815	-0.86202
H	-5.47017	0.66219	1.51287
C	-1.01786	-0.79239	-1.18521
H	-1.17489	-1.79515	-1.59522
H	-0.88716	-0.12584	-2.04234
C	1.03475	0.29856	-0.34941
C	2.40232	0.19374	0.04282
C	0.51017	1.58034	-0.62584
C	3.13384	1.37365	0.21714
C	1.28466	2.72160	-0.49440
H	-0.53123	1.68467	-0.90706
C	2.60738	2.62952	-0.05067
H	4.16317	1.27109	0.54439
H	0.84527	3.68851	-0.71369
H	3.21179	3.52027	0.07332
N	0.20251	-0.81573	-0.40505
O	3.97694	-1.19247	1.18630
C	3.10590	-1.11528	0.24676
C	2.66725	-2.18565	-0.52998
H	3.13298	-3.15617	-0.38427
H	2.15501	-2.01756	-1.46801
C	0.50361	-1.97702	0.31246
H	0.82893	-1.84893	1.34016
H	-0.14655	-2.81721	0.09996
H	-1.22155	0.03628	1.42168

Product S47

33

-748.6938199

C	-3.01829	0.45070	1.68042
C	-1.94970	0.10432	0.85439
C	-2.17258	-0.30007	-0.46083
C	-3.48676	-0.35082	-0.93332
C	-4.55461	-0.00247	-0.11357
C	-4.32299	0.40041	1.20018
H	-2.82757	0.76242	2.70110
H	-3.67289	-0.66946	-1.95491
H	-5.56733	-0.04844	-0.49751
H	-5.15292	0.67049	1.84257
C	-1.04195	-0.69370	-1.40350
H	-1.29591	-1.65951	-1.85091
H	-1.00295	0.01928	-2.23268
C	1.01813	0.33186	-0.51542
C	2.30809	0.15256	0.11682
C	0.57045	1.61073	-0.81546
C	3.06263	1.33316	0.40243
C	1.35117	2.75435	-0.53402
H	-0.40939	1.75099	-1.25608
C	2.59514	2.59816	0.08155
H	4.03239	1.20587	0.86954
H	0.97155	3.73784	-0.78379
H	3.20072	3.46979	0.31058
N	0.27861	-0.81654	-0.82995
O	3.99634	-1.33312	0.89284
C	2.83888	-1.13834	0.39170
C	1.99042	-2.33985	0.02773
H	2.17325	-3.13280	0.75953
H	2.29659	-2.72850	-0.95297
C	0.51007	-1.99524	-0.00033
H	0.15350	-1.83468	1.02821
H	-0.07252	-2.81795	-0.42175
H	-0.93615	0.16073	1.23351



33

-748.6017885

C	-3.58497	1.23402	0.50896
C	-2.32613	0.81357	0.15848
C	-2.01264	-0.38378	-0.45232
C	-3.09389	-1.22640	-0.73056
C	-4.39768	-0.85289	-0.39986
C	-4.64829	0.36862	0.21766
H	-3.75999	2.19156	0.98689
H	-2.90822	-2.18403	-1.20848
H	-5.21983	-1.52255	-0.62291
H	-5.66226	0.65413	0.47462
C	-0.58992	-0.74580	-0.80212
H	-0.58702	-1.66619	-1.40845
H	-0.16748	0.06057	-1.39881
C	1.62403	-0.64130	0.16007
C	2.02873	0.69534	-0.04826
C	2.58420	-1.65779	0.13688
C	3.37077	0.95130	-0.32223
C	3.92673	-1.37370	-0.11083
H	2.28628	-2.68568	0.30375
C	4.32396	-0.06701	-0.35745
H	3.67555	1.98071	-0.48278
H	4.65096	-2.18041	-0.12210
H	5.36329	0.16400	-0.56120
N	0.24853	-0.92203	0.38862
O	0.87422	2.18813	1.38239
C	1.09035	1.87863	0.15598
C	0.62482	2.52339	-0.95945
H	0.88157	2.17483	-1.95246
H	-0.03153	3.38282	-0.86446
C	-0.05506	-2.17199	1.06539
H	-1.10609	-2.16120	1.36204
H	0.10489	-3.05696	0.42935
H	0.55634	-2.26760	1.96350

TS of 51 to form 52

33

-748.5990491

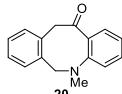
C	-3.40678	1.36530	0.04122
C	-2.17026	0.85432	-0.29235
C	-1.93485	-0.49576	-0.50101
C	-3.02070	-1.36792	-0.37328
C	-4.28611	-0.88516	-0.03424
C	-4.48239	0.47681	0.17531
H	-3.55806	2.42994	0.19469
H	-2.87461	-2.43148	-0.54419
H	-5.11705	-1.57422	0.06324
H	-5.46658	0.85087	0.43725
C	-0.54886	-0.98756	-0.84279
H	-0.60841	-1.97245	-1.33163
H	-0.09797	-0.29111	-1.54688
C	1.65227	-0.63568	0.11220
C	1.89079	0.74724	-0.01647
C	2.72347	-1.52902	0.01236
C	3.18495	1.18215	-0.29586
C	4.01498	-1.07103	-0.24246
H	2.54973	-2.59269	0.12433
C	4.24819	0.28761	-0.41499
H	3.36442	2.24880	-0.39086
H	4.83044	-1.78152	-0.31788
H	5.24737	0.65212	-0.62366
N	0.32101	-1.07787	0.34102
O	0.77148	2.11378	1.54631
C	0.82800	1.78647	0.31183
C	0.04972	2.29664	-0.70312
H	0.19271	1.98481	-1.72999
H	-0.63832	3.10991	-0.50229
C	0.16346	-2.35025	1.02493
H	-0.88180	-2.45737	1.32425
H	0.42167	-3.21579	0.39512
H	0.78210	-2.36996	1.92321

Product 52

33

-748.6670331

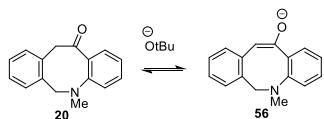
C	2.95787	1.40855	-0.15517
C	1.85409	0.75931	0.39822
C	1.88541	-0.63931	0.52352
C	3.00966	-1.35001	0.11163
C	4.10612	-0.69149	-0.44471
C	4.07410	0.69152	-0.58514
H	2.94683	2.49079	-0.24150
H	3.02545	-2.43011	0.22391
H	4.97574	-1.25488	-0.76305
H	4.92049	1.21516	-1.01513
C	0.63948	-1.34340	0.99464
H	0.87288	-2.37664	1.27923
H	0.21994	-0.86235	1.87900
C	-1.59823	-0.66753	0.07743
C	-1.66647	0.77410	-0.01274
C	-2.77357	-1.41284	0.10614
C	-2.97452	1.32148	-0.19740
C	-4.04357	-0.83264	-0.00230
H	-2.69584	-2.49347	0.16572
C	-4.12393	0.55357	-0.17872
H	-3.04176	2.39391	-0.33613
H	-4.93309	-1.45093	0.01638
H	-5.09030	1.03319	-0.30057
N	-0.35740	-1.34437	-0.08113
O	-0.69001	2.85996	-0.55717
C	-0.56404	1.70821	-0.01184
C	0.66430	1.54150	0.89808
H	0.34790	1.12905	1.86157
H	0.99291	2.56542	1.08946
C	-0.36045	-2.59636	-0.81633
H	0.65895	-2.80423	-1.15510
H	-0.69286	-3.45837	-0.21674
H	-1.00274	-2.51363	-1.69370

**SM 20**

33

-748.5884117

C	3.04806	-1.38735	0.00123
C	1.86468	-0.78877	-0.42655
C	1.79792	0.60921	-0.52760
C	2.92181	1.37327	-0.22202
C	4.10299	0.76875	0.20234
C	4.16347	-0.61483	0.31871
H	3.10054	-2.46822	0.07693
H	2.86968	2.45336	-0.31644
H	4.96882	1.37552	0.44008
H	5.07709	-1.09627	0.64707
C	0.49598	1.26968	-0.90450
H	0.68146	2.29386	-1.24513
H	0.02377	0.74616	-1.73878
C	-1.67024	0.63501	0.05914
C	-1.68171	-0.77066	0.01954
C	-2.89174	1.31199	-0.00656
C	-2.88263	-1.46177	-0.12241
C	-4.08673	0.61359	-0.15087
H	-2.90771	2.39323	0.05231
C	-4.08822	-0.77466	-0.22437
H	-2.87068	-2.54618	-0.13112
H	-5.01973	1.16211	-0.20838
H	-5.01746	-1.31925	-0.33656
N	-0.43937	1.30592	0.23614
O	-0.34289	-2.23742	1.27771
C	-0.43466	-1.58168	0.26482
C	0.66873	-1.64565	-0.78669
H	0.26623	-1.36307	-1.76101
H	0.98028	-2.69052	-0.83399
C	-0.47932	2.60771	0.88600
H	0.53490	2.87156	1.19266
H	-0.85457	3.40450	0.22835
H	-1.10434	2.55818	1.77807



Opt SM 20 + *tert*-butoxide anion
47
-981.7268409

C	0.50269	2.97545	0.01083
C	-0.31472	1.84961	-0.08191
C	-1.69754	2.01813	-0.24993
C	-2.23048	3.30404	-0.30489
C	-1.40891	4.42502	-0.20412
C	-0.03775	4.25891	-0.04787
H	1.57189	2.82496	0.12691
H	-3.30155	3.42953	-0.43058
H	-1.83929	5.41860	-0.24931
H	0.61177	5.12365	0.02602
C	-2.60338	0.81627	-0.42041
H	-3.64603	1.15277	-0.44225
H	-2.41353	0.35002	-1.39121
C	-2.05159	-1.48016	0.27782
C	-0.98240	-1.64840	-0.63183
C	-2.66485	-2.63106	0.79983
C	-0.62395	-2.92374	-1.06928
C	-2.26125	-3.89410	0.38506
H	-3.47963	-2.53915	1.50612
C	-1.25378	-4.05380	-0.56537
H	0.19290	-3.01311	-1.77752
H	-2.75687	-4.76545	0.79804
H	-0.95502	-5.04190	-0.89169
N	-2.46401	-0.20097	0.62196
O	0.30952	-0.40284	-2.17462
C	-0.11924	-0.49968	-1.04015
C	0.30989	0.47706	0.04041
H	0.06639	0.05847	1.02029
H	1.40565	0.57707	-0.04499
C	-3.35617	-0.01627	1.75246
H	-3.34507	1.03934	2.02891
H	-4.39081	-0.30367	1.52068
H	-3.00819	-0.59442	2.60876
O	3.45405	0.84966	-0.17901
C	3.97309	-0.30491	0.35639
C	3.35462	-1.56313	-0.30140
H	2.27411	-1.58480	-0.12589
H	3.52120	-1.53178	-1.38317
H	3.78080	-2.49463	0.08868
C	3.68900	-0.38644	1.87435
H	4.07691	-1.30425	2.33139
H	4.14663	0.47158	2.37728
H	2.60835	-0.34304	2.04380
C	5.50380	-0.37993	0.15835
H	5.73731	-0.35479	-0.91100
H	5.97560	0.48843	0.62923
H	5.94346	-1.28828	0.58677

TS of 20 deprotonation to form 56

47

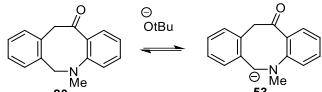
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C	0.55625	2.99815	0.07557	
C	-0.22127	1.84940	-0.08300	
C	-1.61227	1.99847	-0.26448	
C	-2.17661	3.27239	-0.28192	
C	-1.38708	4.41036	-0.12198	
C	-0.01622	4.27003	0.05857	
H	1.62632	2.87433	0.20761	
H	-3.24905	3.37726	-0.41917	
H	-1.84202	5.39409	-0.13610	
H	0.60898	5.14730	0.18346	
C	-2.50376	0.78639	-0.47623	
H	-3.54496	1.12352	-0.53240	
H	-2.28304	0.32978	-1.44423	
C	-1.93628	-1.51245	0.24550	
C	-0.81731	-1.65911	-0.61058	
C	-2.53028	-2.67808	0.75892	
C	-0.38823	-2.92633	-0.99310	
C	-2.05395	-3.93496	0.40063	
H	-3.38473	-2.60759	1.41964	
C	-0.99253	-4.07426	-0.48934	
H	0.45953	-2.99956	-1.66716	
H	-2.53617	-4.81551	0.81036	
H	-0.63711	-5.05616	-0.77625	
N	-2.41637	-0.24549	0.55958	
O	0.19192	-0.27350	-2.24632	
C	-0.05100	-0.44065	-1.05015	
C	0.38817	0.47428	0.00670	
H	0.13751	0.05201	0.98374	
H	1.72317	0.58721	-0.07039	
C	-3.38394	-0.09651	1.62977	
H	-3.43611	0.95910	1.90154	
C	-4.39059	-0.42965	1.33951	
H	-3.06720	-0.65619	2.51074	
O	3.00095	0.79349	-0.13007	
C	3.70060	-0.30631	0.37529	
C	3.24098	-1.60787	-0.30812	
H	2.18537	-1.79683	-0.09298	
H	3.35882	-1.52023	-1.39255	
H	3.81909	-2.47168	0.03574	
C	3.46744	-0.43760	1.89115	
H	4.00522	-1.29107	2.31685	
H	3.80430	0.47234	2.39638	
H	2.39986	-0.56579	2.09155	
C	5.19996	-0.11408	0.11708	
H	5.38531	-0.03277	-0.95789	
H	5.54455	0.80732	0.59542	
H	5.78874	-0.95006	0.50907	

Product 56

47

-981.7275513

C	-1.38218	2.56355	-0.08239
C	-0.28886	1.72115	0.13253
C	0.99252	2.30863	0.28378
C	1.12718	3.69446	0.24659
C	0.02014	4.52053	0.04509
C	-1.23592	3.95062	-0.12698
H	-2.36325	2.11521	-0.20669
H	2.11225	4.13790	0.36383
H	0.14398	5.59703	0.01398
H	-2.10199	4.58235	-0.29214
C	2.22626	1.43984	0.50390
H	3.10374	2.09481	0.54669
H	2.15968	0.95308	1.47882
C	2.39528	-0.94356	-0.23511
C	1.34893	-1.45886	0.57818
C	3.31770	-1.85920	-0.77161
C	1.28833	-2.81713	0.85995
C	3.21436	-3.22241	-0.50384
H	4.13338	-1.51024	-1.39192
C	2.20783	-3.71558	0.31818
H	0.48362	-3.17478	1.49564
H	3.94347	-3.89957	-0.93541
H	2.13545	-4.77560	0.52962
N	2.48340	0.42145	-0.52272
O	0.28386	-0.25293	2.33664
C	0.33395	-0.46749	1.09296
C	-0.35100	0.23642	0.09701
H	-0.18507	-0.15246	-0.90712
H	-2.22025	-0.28485	0.57623
C	3.37945	0.85939	-1.57481
H	3.13064	1.89056	-1.83173
H	4.43873	0.82520	-1.27932
H	3.24686	0.24937	-2.46995
O	-3.16299	-0.50124	0.78211
C	-3.70537	-1.19642	-0.34009
C	-2.90551	-2.47704	-0.58967
H	-1.86492	-2.23167	-0.81960
H	-2.92359	-3.11027	0.30116
H	-3.32507	-3.04069	-1.42726
C	-3.65923	-0.29616	-1.57673
H	-4.09237	-0.80249	-2.44353
H	-4.22161	0.62294	-1.39238
H	-2.62440	-0.02928	-1.80888
C	-5.14733	-1.53021	0.02116
H	-5.17611	-2.15850	0.91487
H	-5.70691	-0.61339	0.22255
H	-5.63627	-2.06441	-0.79701

**SM 20 + tert-butoxide anion**

47

-981.7280946

C	3.91574	-0.11221	-1.10856
C	2.64768	-0.35110	-0.58037
C	2.21140	0.40250	0.52009
C	3.06057	1.36311	1.06702
C	4.32720	1.59433	0.53530
C	4.75579	0.85338	-0.55925
H	4.24953	-0.69226	-1.96264
H	2.72217	1.93935	1.92265
H	4.97230	2.34588	0.97518
H	5.73788	1.02119	-0.98585
C	0.81294	0.23377	1.07273
H	0.73780	0.78812	2.01568
H	0.08730	0.71449	0.39989
C	-0.65711	-1.68425	0.64802
C	-0.76790	-1.47684	-0.74579
C	-1.67631	-2.40325	1.29609
C	-1.93426	-1.84876	-1.41874
C	-2.80578	-2.80506	0.59711
H	-1.60916	-2.60125	2.35792
C	-2.96053	-2.50690	-0.75768
H	-1.99670	-1.65126	-2.48312
H	-3.58883	-3.33843	1.12456
H	-3.85365	-2.80847	-1.29034
N	0.42595	-1.15597	1.32974
O	0.20292	-0.36026	-2.59061
C	0.37498	-0.99158	-1.56544
C	1.78457	-1.43916	-1.18409
H	1.72786	-2.28704	-0.49935
H	2.24297	-1.77343	-2.11723
C	0.70871	-1.61608	2.67767
H	1.72162	-1.30764	2.94122
H	0.01425	-1.19389	3.41693
H	0.66117	-2.70452	2.72514
O	-1.01047	2.52026	-0.36242
C	-2.34304	2.47556	-0.03251
C	-2.82133	3.82551	0.55104
H	-2.24498	4.06193	1.45138
H	-2.64909	4.62108	-0.18120
H	-3.88571	3.82198	0.81411
C	-2.62503	1.37817	1.02136
H	-3.67472	1.35769	1.33806
H	-2.37174	0.39679	0.60770
H	-1.99953	1.54605	1.90487
C	-3.21732	2.16120	-1.26846
H	-3.06702	2.93108	-2.03235
H	-2.91408	1.19658	-1.68945
H	-4.28668	2.11376	-1.03085

TS of 20 to form 53

47

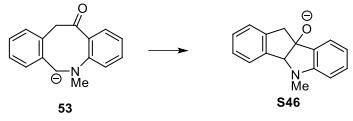
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C	3.92765	-0.82851	-0.65598
C	2.60433	-0.75629	-0.22571
C	2.14085	0.38675	0.45902
C	3.06056	1.42725	0.67559
C	4.37663	1.35310	0.23250
C	4.82346	0.21636	-0.43529
H	4.25958	-1.71793	-1.18341
H	2.72532	2.31290	1.20819
H	5.05557	2.17843	0.41840
H	5.84732	0.14247	-0.78218
C	0.71936	0.57039	0.83659
H	0.66094	1.39300	1.56071
H	-0.04542	1.17705	-0.15021
C	-1.00087	-1.21141	0.82489
C	-0.89723	-1.53363	-0.54903
C	-2.19207	-1.56435	1.49164
C	-1.98614	-2.07742	-1.23309
C	-3.25000	-2.13616	0.79923
H	-2.30536	-1.34803	2.54635
C	-3.16791	-2.38157	-0.57283
H	-1.86865	-2.29873	-2.28848
H	-4.16056	-2.37738	1.33692
H	-4.00144	-2.82203	-1.10566
N	0.04910	-0.58153	1.45869
O	0.46693	-1.22818	-2.45865
C	0.40071	-1.46688	-1.26531
C	1.65958	-1.90022	-0.51620
H	1.37835	-2.41004	0.40646
H	2.15707	-2.61655	-1.17487
C	0.08600	-0.59915	2.91084
H	1.10489	-0.37453	3.22935
H	-0.58393	0.15304	3.35345
H	-0.18667	-1.58316	3.29853
O	-0.67320	1.91135	-0.93586
C	-1.90645	2.37772	-0.46549
C	-2.13548	3.79880	-0.99872
H	-1.34101	4.46240	-0.64515
H	-2.11434	3.79168	-2.09232
H	-3.09860	4.20506	-0.67271
C	-1.94565	2.41502	1.07310
H	-2.90143	2.81077	1.43010
H	-1.81442	1.40843	1.48218
H	-1.14287	3.05008	1.45944
C	-3.04383	1.46915	-0.95778
H	-3.02984	1.42000	-2.05108
H	-2.90395	0.45769	-0.56759
H	-4.02508	1.83699	-0.63891

Product 53 + tert-butanol

47

C	4.06524	-0.63097	-0.62269
C	2.73889	-0.63938	-0.21008
C	2.17221	0.48393	0.45406
C	3.02573	1.60291	0.63063
C	4.34378	1.60425	0.19531
C	4.89013	0.47994	-0.42560
H	4.45759	-1.50627	-1.13386
H	2.62723	2.48175	1.13039
H	4.95684	2.48573	0.35655
H	5.91976	0.47144	-0.76226
C	0.77921	0.54337	0.81448
H	0.54551	1.44459	1.39149
H	-0.45776	1.43762	-0.47184
C	-0.86287	-1.30285	0.81642
C	-0.73698	-1.57530	-0.56675
C	-2.02179	-1.76524	1.47199
C	-1.77622	-2.18488	-1.26862
C	-3.03440	-2.39500	0.75831
H	-2.15349	-1.58875	2.53181
C	-2.93350	-2.59634	-0.61882
H	-1.64129	-2.36687	-2.32968
H	-3.92587	-2.71601	1.28645
H	-3.73199	-3.08263	-1.16554
N	0.14024	-0.60409	1.45135
O	0.61285	-1.03820	-2.43804
C	0.55748	-1.36136	-1.26172
C	1.83444	-1.80080	-0.53797
H	1.56113	-2.35952	0.35932
H	2.34439	-2.47928	-1.22801
C	0.14090	-0.58437	2.90619
H	1.13387	-0.28506	3.24124
H	-0.58754	0.13394	3.31145
H	-0.07951	-1.57294	3.31694
O	-0.98972	2.08899	-0.99877
C	-2.27219	2.29091	-0.40489
C	-2.74861	3.66158	-0.87546
H	-2.06285	4.43874	-0.52932
H	-2.78517	3.69138	-1.96738
H	-3.74740	3.87773	-0.48855
C	-2.17041	2.26034	1.12107
H	-3.14409	2.47471	1.56958
H	-1.84271	1.27375	1.46217
H	-1.45263	3.00642	1.47261
C	-3.23706	1.20350	-0.87922
H	-3.28924	1.19989	-1.97137
H	-2.89326	0.22216	-0.54418
H	-4.24215	1.37434	-0.48274



SM 53

32

-748.0665397

C	3.10061	-0.99463	0.91698
C	1.86670	-0.46060	0.57690
C	1.75868	0.60213	-0.37665
C	2.98496	1.02461	-0.97116
C	4.20567	0.46628	-0.62747
C	4.29199	-0.54226	0.33760
H	3.13149	-1.81316	1.63221
H	2.95038	1.82143	-1.70942
H	5.10885	0.83132	-1.10800
H	5.24447	-0.97927	0.61081
C	0.50763	1.12326	-0.79475
H	0.56111	1.92227	-1.53973
C	-1.74320	0.62787	0.07323
C	-1.65844	-0.76410	-0.16426
C	-3.02497	1.19146	0.22353
C	-2.81161	-1.52158	-0.36011
C	-4.16369	0.41236	0.05111
H	-3.13533	2.24877	0.42579
C	-4.07246	-0.94346	-0.26210
H	-2.70309	-2.58453	-0.54838
H	-5.13806	0.87962	0.14647
H	-4.96614	-1.53877	-0.40205
N	-0.57550	1.35872	0.14155
O	-0.09447	-2.44763	-0.73952
C	-0.35084	-1.46302	-0.06378
C	0.58725	-1.07451	1.08648
H	0.05710	-0.40768	1.76907
H	0.81046	-2.00692	1.61337
C	-0.66447	2.72391	0.64001
H	0.33957	3.05461	0.90311
H	-1.06721	3.41595	-0.11440
H	-1.29218	2.77990	1.53319

TS 53 cyclising to form S46

32

-748.0659566

C	3.10118	-0.99582	1.00100
C	1.86825	-0.52209	0.57842
C	1.77100	0.52389	-0.38099
C	2.98890	1.00403	-0.92032
C	4.21901	0.50521	-0.50551
C	4.29386	-0.48571	0.47392
H	3.13565	-1.80805	1.72243
H	2.95307	1.79213	-1.66755
H	5.13056	0.90377	-0.94034
H	5.25128	-0.87388	0.80049
C	0.47942	0.93435	-0.85708
H	0.52132	1.64244	-1.69369
C	-1.74516	0.64300	0.09035
C	-1.68915	-0.74194	-0.18697
C	-3.00149	1.22296	0.33472
C	-2.85493	-1.48617	-0.31429
C	-4.15948	0.45420	0.22402
H	-3.08607	2.27701	0.56518
C	-4.10303	-0.89441	-0.11734
H	-2.77237	-2.54535	-0.53579
H	-5.12089	0.92854	0.39008
H	-5.01099	-1.47793	-0.20838
N	-0.55141	1.33180	0.08602
O	-0.12445	-2.36596	-0.95089
C	-0.35557	-1.40594	-0.21868
C	0.56773	-1.15122	0.99141
H	0.03408	-0.52553	1.71064
H	0.74450	-2.12877	1.45075
C	-0.58050	2.74221	0.44110
C	0.44542	3.07931	0.58475
H	-1.04033	3.35628	-0.34787
H	-1.13007	2.90580	1.37180

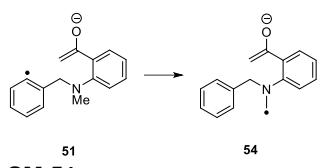
Product S46

32

-748.1071091

C	-3.11162	-1.14171	-1.05056
C	-1.87630	-0.82133	-0.50129
C	-1.75125	0.29425	0.33635
C	-2.85359	1.08051	0.64450
C	-4.09472	0.75847	0.08926
C	-4.21993	-0.34315	-0.75395
H	-3.22136	-2.00817	-1.69483
H	-2.75840	1.92801	1.31619
H	-4.96515	1.36110	0.32268
H	-5.18868	-0.59057	-1.17356
C	-0.32928	0.41932	0.80449
H	-0.23703	0.73939	1.85335
C	1.74961	0.69497	-0.17514
C	1.70254	-0.66105	0.18629
C	2.94351	1.28894	-0.57869
C	2.84572	-1.43210	0.13850
C	4.09243	0.48984	-0.63475
H	2.99571	2.34041	-0.83627
C	4.05399	-0.85520	-0.28233
H	2.80613	-2.47451	0.44020
H	5.03035	0.93714	-0.94554
H	4.95887	-1.45073	-0.32040
N	0.48708	1.28222	-0.06818
O	0.15025	-1.85221	1.66525
C	0.27910	-1.03062	0.60717
C	-0.54859	-1.51862	-0.64992
H	-0.07840	-1.21271	-1.59237
H	-0.62440	-2.60797	-0.64088
C	0.38767	2.71231	0.13429
H	-0.66474	3.00049	0.12680
H	0.83317	3.02517	1.09091
H	0.88663	3.24611	-0.67620

9 Cyclisation of 18 in Benzene Scheme S4.1



SM 51

33

-748.5611009

C	-4.12495	1.20792	0.75190
C	-2.80403	1.03867	0.42030
C	-2.28731	0.04678	-0.38833
C	-3.22410	-0.85696	-0.90232
C	-4.58263	-0.73085	-0.61096
C	-5.03926	0.29364	0.21215
H	-4.45552	2.01119	1.40103
H	-2.87579	-1.67111	-1.53056
H	-5.28635	-1.44613	-1.02110
H	-6.09512	0.38416	0.44193
C	-0.81548	-0.05505	-0.71638
H	-0.58759	-1.03371	-1.16085
H	-0.57215	0.71176	-1.45798
C	1.34103	0.62811	0.14480
C	2.45512	-0.21642	-0.01866
C	1.50005	2.01162	0.01626
C	3.69995	0.37631	-0.26140
C	2.73820	2.57884	-0.25949
H	0.62321	2.63531	0.16005
C	3.85169	1.75314	-0.38497
H	4.55590	-0.27820	-0.38582
H	2.83440	3.65480	-0.35590
H	4.82924	2.17695	-0.58804
N	0.01840	0.17777	0.45936
O	1.46120	-2.18746	-0.87557
C	2.33092	-1.73301	-0.05824
C	3.16613	-2.44363	0.76816
H	3.85816	-1.94058	1.43171
H	3.13481	-3.52768	0.76897
C	-0.10078	-0.89213	1.44561
H	-1.09967	-0.84379	1.88971
H	0.05604	-1.88561	1.01054
H	0.63475	-0.73396	2.23486

TS of 51 to form 54

33

-748.5452234

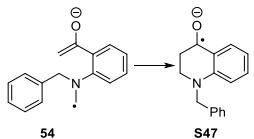
C	3.34033	-0.81390	-1.44741
C	2.25745	-0.96373	-0.59699
C	2.18732	-0.32401	0.62741
C	3.24702	0.49966	1.01633
C	4.34897	0.66105	0.17892
C	4.39903	0.00796	-1.05076
H	3.37554	-1.31747	-2.40817
H	3.20741	1.02079	1.96943
H	5.16714	1.30404	0.48320
H	5.25636	0.14161	-1.70214
C	0.96831	-0.54255	1.52511
H	1.13657	-1.44457	2.12519
H	0.84295	0.29072	2.21776
C	-0.97401	0.37516	0.31064
C	-2.30743	0.22803	-0.12619
C	-0.39229	1.65209	0.31823
C	-2.99124	1.36134	-0.56053
C	-1.10993	2.76979	-0.09377
H	0.63816	1.77779	0.62575
C	-2.41722	2.62931	-0.54314
H	-4.01338	1.23157	-0.90152
H	-0.63469	3.74425	-0.07455
H	-2.98433	3.49326	-0.87067
N	-0.25170	-0.75150	0.77111
O	-3.12909	-1.64034	-1.33230
C	-3.06070	-1.09964	-0.17627
C	-3.59844	-1.53956	1.00365
H	-4.16392	-2.46495	1.03251
H	-3.45926	-0.97973	1.92017
C	-0.15428	-1.88966	-0.07865
H	-0.96707	-1.97348	-0.79635
H	0.01505	-2.80799	0.48923
H	0.92063	-1.70065	-0.68866

Product 54

33

-748.5921792

C	-3.51057	0.40350	1.49075
C	-2.30458	0.04181	0.89484
C	-2.27767	-0.40319	-0.42478
C	-3.47621	-0.48546	-1.13595
C	-4.68115	-0.12426	-0.54354
C	-4.70126	0.32324	0.77536
H	-3.51770	0.74749	2.51877
H	-3.46258	-0.83712	-2.16365
H	-5.60372	-0.19246	-1.10897
H	-5.63833	0.60429	1.24182
C	-0.98027	-0.78307	-1.12126
H	-1.10120	-1.77856	-1.56348
H	-0.79705	-0.09135	-1.94741
C	1.03852	0.30931	-0.20191
C	2.42051	0.18675	0.05332
C	0.48659	1.58838	-0.39726
C	3.17942	1.35300	0.14274
C	1.27618	2.72875	-0.33347
H	-0.57709	1.69346	-0.57800
C	2.63375	2.61870	-0.05063
H	4.24021	1.24407	0.34537
H	0.82167	3.70107	-0.48918
H	3.25920	3.50205	0.00871
N	0.19455	-0.81636	-0.27571
O	3.39920	-1.47790	1.43568
C	3.16812	-1.13353	0.22893
C	3.53589	-1.77005	-0.92789
H	4.08580	-2.70423	-0.88455
H	3.27596	-1.35766	-1.89500
C	0.33146	-1.90985	0.55607
H	1.17212	-1.93704	1.23240
H	-0.16809	-2.81657	0.24179
H	-1.37707	0.09597	1.45396

**TS of 54 cyclising to form S47**

33

-748.5797844

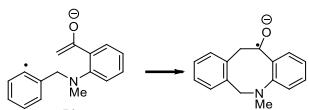
C	-3.39545	0.45421	1.57517
C	-2.22702	0.07908	0.91627
C	-2.27507	-0.37390	-0.40016
C	-3.51025	-0.44636	-1.04619
C	-4.67854	-0.07150	-0.39108
C	-4.62376	0.38085	0.92545
H	-3.34436	0.80497	2.59971
H	-3.55544	-0.80275	-2.07146
H	-5.63090	-0.13406	-0.90564
H	-5.53203	0.67186	1.44038
C	-1.01120	-0.77312	-1.14660
C	-1.15545	-1.77514	-1.56677
H	-0.86600	-0.09875	-1.99601
C	1.04583	0.30716	-0.31931
C	2.41796	0.17737	0.03889
C	0.53640	1.59591	-0.58751
C	3.17516	1.34103	0.18904
C	1.33664	2.72313	-0.48527
H	-0.51254	1.71732	-0.83442
C	2.66708	2.60631	-0.07563
H	4.20651	1.21107	0.49964
H	0.91003	3.69764	-0.69797
H	3.29259	3.48539	0.02769
N	0.18777	-0.79084	-0.34267
O	4.00555	-1.21398	1.14112
C	3.11486	-1.14421	0.23677
C	2.65159	-2.20857	-0.53731
H	3.12074	-3.17928	-0.40988
H	2.10666	-2.02981	-1.45480
C	0.47884	-1.95476	0.38070
H	0.83835	-1.82465	1.39548
H	-0.18868	-2.78531	0.18648
H	-1.26676	0.13362	1.41777

Product S47

33

-748.6544530

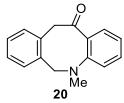
C	-3.00664	0.50616	1.66388
C	-1.94208	0.16355	0.83277
C	-2.17485	-0.28274	-0.46735
C	-3.49420	-0.37992	-0.91604
C	-4.55887	-0.03465	-0.09066
C	-4.31724	0.41064	1.20670
H	-2.80769	0.85286	2.67163
H	-3.68671	-0.73314	-1.92534
H	-5.57592	-0.11665	-0.45755
H	-5.14361	0.67934	1.85458
C	-1.04349	-0.67156	-1.41236
H	-1.30734	-1.62982	-1.87262
H	-0.99768	0.05356	-2.23121
C	1.02815	0.33451	-0.52645
C	2.30933	0.13671	0.11264
C	0.59372	1.61658	-0.82483
C	3.07793	1.30733	0.40205
C	1.38654	2.75191	-0.53926
H	-0.38572	1.76927	-1.26329
C	2.62778	2.57553	0.08009
H	4.04261	1.15935	0.87310
H	1.01988	3.74055	-0.78804
H	3.24467	3.43899	0.31154
N	0.27215	-0.81076	-0.84164
O	3.96309	-1.37010	0.91681
C	2.82485	-1.15929	0.40186
C	1.95737	-2.35003	0.03460
H	2.13138	-3.14163	0.77002
H	2.26162	-2.74116	-0.94558
C	0.48261	-1.98253	0.00121
H	0.12830	-1.80637	1.02889
H	-0.11546	-2.79991	-0.41251
H	-0.92351	0.25757	1.19028

**Product 52 after SRN1 cyclisation**

33

-748.6424854

C	3.12564	-1.10191	0.68063
C	1.86789	-0.54916	0.43315
C	1.79132	0.58175	-0.39931
C	2.95654	1.13288	-0.92694
C	4.20609	0.57349	-0.66600
C	4.28760	-0.55542	0.13873
H	3.19055	-1.98323	1.31098
H	2.88266	2.01231	-1.56041
H	5.10122	1.01435	-1.08993
H	5.24915	-1.01148	0.34727
C	0.44751	1.15388	-0.78801
H	0.59449	2.12370	-1.28312
H	-0.00731	0.48744	-1.52517
C	-1.71329	0.62449	0.18602
C	-1.65549	-0.79872	-0.05164
C	-2.93199	1.28447	0.20093
C	-2.87241	-1.41417	-0.48072
C	-4.13708	0.61028	-0.08064
H	-2.95815	2.35221	0.39024
C	-4.07644	-0.73496	-0.46765
H	-2.82976	-2.46390	-0.74626
H	-5.07960	1.14379	-0.05244
H	-4.98676	-1.25797	-0.74559
N	-0.48195	1.31294	0.33209
O	-0.39383	-2.78151	-0.35361
C	-0.48562	-1.60943	0.12248
C	0.63670	-1.16064	1.06936
H	0.24609	-0.46195	1.81167
H	0.94665	-2.07161	1.58858
C	-0.50282	2.65432	0.86484
H	0.52314	2.95987	1.08718
H	-0.93483	3.39294	0.16750
H	-1.07826	2.67812	1.79235

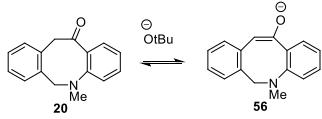


Product 20

33

-748.5933166

C	3.07550	-1.11816	0.84233
C	1.84290	-0.61645	0.42964
C	1.81484	0.49160	-0.42962
C	3.01047	1.07408	-0.84090
C	4.23754	0.56945	-0.41871
C	4.26820	-0.53258	0.42564
H	3.10127	-1.98087	1.49946
H	2.97946	1.93380	-1.50290
H	5.15895	1.03471	-0.74811
H	5.21497	-0.93895	0.76153
C	0.49697	1.02689	-0.94376
H	0.67883	1.94395	-1.51668
H	0.05936	0.30999	-1.64361
C	-1.70057	0.65194	0.08880
C	-1.72729	-0.74107	-0.13886
C	-2.91957	1.32042	0.27856
C	-2.94576	-1.40542	-0.28117
C	-4.12079	0.63008	0.18251
H	-2.93091	2.38613	0.46627
C	-4.14709	-0.73024	-0.11888
H	-2.92738	-2.47151	-0.47764
H	-5.05060	1.16925	0.32386
H	-5.08919	-1.25601	-0.20802
N	-0.47826	1.31310	0.10789
O	-0.35624	-2.54848	-0.80925
C	-0.48541	-1.57112	-0.10513
C	0.56839	-1.24541	0.95474
H	0.13054	-0.59497	1.71492
H	0.81484	-2.20396	1.41616
C	-0.40609	2.66544	0.62788
H	0.64247	2.90783	0.80951
H	-0.81896	3.40660	-0.07083
H	-0.93927	2.73349	1.57651



Opt SM 20 + *tert*-butoxide anion

47

-981.6838637	C	1.39365	2.42079	0.00428
	C	0.22650	1.66292	-0.10495
	C	-1.00293	2.30890	-0.29851
	C	-1.04827	3.69979	-0.36423
	C	0.11598	4.45556	-0.24797
	C	1.33532	3.81179	-0.06653
	H	2.33335	1.88633	0.14327
	H	-2.00436	4.19403	-0.51160
	H	0.06798	5.53754	-0.30044
	C	2.24787	4.39143	0.01897
	C	-2.26945	1.50069	-0.47784
	C	-3.12664	2.18218	-0.54693
	H	-2.23045	0.96000	-1.42718
	C	-2.59567	-0.81699	0.29852
	C	-1.64102	-1.39068	-0.57093
	C	-3.59185	-1.64837	0.83492
	C	-1.75641	-2.72439	-0.95317
	C	-3.66110	-2.98914	0.47517
	H	-4.33133	-1.23982	1.51197
	C	-2.75963	-3.53484	-0.43504
	H	-1.01314	-3.12480	-1.63412
	H	-4.44350	-3.60848	0.89974
	H	-2.82609	-4.57742	-0.71999
	N	-2.52671	0.53766	0.59323
	O	-0.00018	-0.74706	-2.14357
	C	-0.41703	-0.63721	-1.00934
	C	0.32728	0.15969	0.04260
	H	-0.04141	-0.12266	1.03249
	H	1.39843	-0.10321	-0.01313
	C	-3.28306	1.07157	1.70596
	H	-2.88186	2.05690	1.95106
	H	-4.35414	1.17928	1.47782
	H	-3.16977	0.43259	2.58269
	O	3.36979	0.06570	0.36274
	C	3.98735	-1.15099	0.37774
	C	2.96890	-2.29915	0.15497
	H	2.20885	-2.26701	0.94344
	H	2.46614	-2.15565	-0.80759
	H	3.43635	-3.29150	0.16165
	C	4.69241	-1.40454	1.73272
	H	5.19066	-2.38113	1.78283
	H	5.43820	-0.62132	1.90096
	H	3.95264	-1.34552	2.53728
	C	5.05639	-1.24985	-0.73741
	H	4.57651	-1.09237	-1.70824
	H	5.79803	-0.45786	-0.59354
	H	5.57396	-2.21760	-0.75317

TS 20 deprotonation to form **56**

47

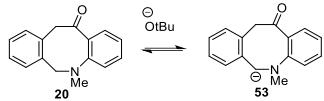
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C	0.86660	2.86018	0.26028
C	-0.03663	1.82231	0.02159
C	-1.36828	2.14932	-0.30589
C	-1.75747	3.48496	-0.38233
C	-0.84636	4.51154	-0.13941
C	0.46825	4.19389	0.18247
H	1.89193	2.59321	0.49728
H	-2.78690	3.72585	-0.63439
H	-1.16370	5.54655	-0.20163
H	1.18818	4.98365	0.36863
C	-2.37784	1.05729	-0.61417
H	-3.35503	1.52234	-0.79497
H	-2.10395	0.55514	-1.54491
C	-2.20090	-1.28234	0.19912
C	-1.01892	-1.59759	-0.51297
C	-2.99536	-2.34237	0.66512
C	-0.70637	-2.92053	-0.79804
C	-2.64018	-3.66286	0.40589
H	-3.90670	-2.13675	1.21242
C	-1.50427	-3.96527	-0.33759
H	0.20157	-3.12130	-1.35787
H	-3.27377	-4.46068	0.77793
H	-1.23865	-4.99476	-0.54537
N	-2.54461	0.04617	0.43200
O	0.29084	-0.39352	-2.07287
C	-0.06645	-0.49363	-0.90341
C	0.37929	0.38526	0.18133
H	-0.01287	0.01987	1.13503
H	1.70162	0.35647	0.26586
C	-3.56010	0.36110	1.41183
H	-3.48010	1.42118	1.66086
H	-4.58123	0.16708	1.04807
H	-3.39839	-0.21211	2.32630
O	2.98431	0.50227	0.44515
C	3.74017	-0.65749	0.33337
C	2.86960	-1.86749	-0.06263
H	2.07527	-2.02296	0.67510
H	2.40057	-1.68891	-1.03469
H	3.46786	-2.78273	-0.12478
C	4.42409	-0.96267	1.67821
H	5.05729	-1.85615	1.63025
H	5.04188	-0.10930	1.97236
H	3.66281	-1.11323	2.44910
C	4.82459	-0.46752	-0.74173
H	4.34828	-0.25593	-1.70300
H	5.45339	0.38724	-0.47631
H	5.46100	-1.35352	-0.84966

Product 56

47

C	-1.02221	2.78710	-0.05615
C	-0.06252	1.79660	0.17277
C	1.29299	2.19589	0.28381
C	1.62986	3.54387	0.19267
C	0.65493	4.51860	-0.02396
C	-0.67410	4.13373	-0.15515
H	-2.06117	2.48330	-0.13982
H	2.67249	3.83895	0.27928
H	0.93537	5.56360	-0.09549
H	-1.44247	4.88071	-0.32516
C	2.39132	1.16322	0.50266
H	3.35555	1.68623	0.52360
H	2.27053	0.70039	1.48344
C	2.19782	-1.22696	-0.23059
C	1.10627	-1.58146	0.60670
C	2.95848	-2.26441	-0.79448
C	0.84700	-2.91552	0.88241
C	2.65514	-3.59923	-0.53271
H	3.80356	-2.03317	-1.43091
C	1.60540	-3.93847	0.31145
H	0.01387	-3.14848	1.53851
H	3.26137	-4.37574	-0.98702
H	1.37683	-4.97732	0.51904
N	2.48124	0.11103	-0.51676
O	0.32874	-0.21794	2.38809
C	0.27231	-0.44594	1.15774
C	-0.35785	0.34195	0.17908
H	-0.29594	-0.07957	-0.82474
H	-2.29723	0.06506	0.64365
C	3.35843	0.42609	-1.62130
H	3.22890	1.48044	-1.87424
H	4.42287	0.25593	-1.39256
H	3.09410	-0.16458	-2.50083
O	-3.27304	-0.05610	0.75636
C	-3.75386	-0.81227	-0.34481
C	-3.01181	-2.14949	-0.42905
H	-1.94608	-1.98223	-0.60454
H	-3.12191	-2.69146	0.51377
H	-3.40922	-2.76781	-1.23945
C	-3.56787	-0.01917	-1.64200
H	-3.95247	-0.57487	-2.50253
H	-4.09942	0.93377	-1.57319
H	-2.50741	0.18940	-1.80403
C	-5.23698	-1.04743	-0.07909
H	-5.36488	-1.60316	0.85291
H	-5.75431	-0.08957	0.01639
H	-5.69380	-1.61489	-0.89440



SM 20 + *tert*-butoxide anion

47

-981.6817071

C	4.13108	-0.45909	-0.59342
C	2.78165	-0.48545	-0.24370
C	2.19546	0.65835	0.31801
C	2.98288	1.79142	0.51834
C	4.32993	1.81075	0.16853
C	4.90827	0.67797	-0.39059
H	4.57752	-1.34336	-1.03668
H	2.52377	2.67626	0.94772
H	4.91957	2.70573	0.33081
H	5.95503	0.67661	-0.67259
C	0.72223	0.71125	0.64422
H	0.52478	1.61595	1.22926
H	0.09601	0.86161	-0.25513
C	-0.74433	-1.25524	0.86587
C	-0.60412	-1.71247	-0.46327
C	-1.88174	-1.65803	1.58756
C	-1.62906	-2.44241	-1.06575
C	-2.86709	-2.42581	0.98310
H	-2.01834	-1.32543	2.60852
C	-2.76214	-2.80761	-0.35347
H	-1.49576	-2.74801	-2.09740
H	-3.74384	-2.70388	1.55789
H	-3.54666	-3.38547	-0.82584
N	0.22988	-0.43747	1.41622
O	0.69600	-1.49564	-2.42928
C	0.67332	-1.58055	-1.22054
C	1.98541	-1.75502	-0.45072
H	1.77924	-2.22010	0.51544
H	2.57871	-2.44560	-1.05404
C	0.25303	-0.23969	2.85196
H	1.22011	0.18852	3.12246
H	-0.53564	0.44732	3.19226
H	0.14454	-1.19365	3.37129
O	-1.27455	2.02148	-1.14155
C	-2.49144	2.18578	-0.55595
C	-3.14081	3.52876	-0.97556
H	-2.48054	4.35303	-0.68736
H	-3.24804	3.54714	-2.06456
H	-4.12704	3.69214	-0.52146
C	-2.38080	2.18530	0.99349
H	-3.34675	2.33247	1.49360
H	-1.96373	1.22706	1.32188
H	-1.69810	2.98278	1.30665
C	-3.46538	1.04595	-0.94636
H	-3.56964	1.02307	-2.03580
H	-3.04230	0.08850	-0.62608
H	-4.46175	1.15797	-0.49831

TS 20 deprotonation to form 53

47

-981.6749539

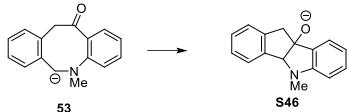
C	3.93132	-0.81603	-0.66124
C	2.60841	-0.74051	-0.23165
C	2.15177	0.40405	0.45211
C	3.07230	1.44148	0.66803
C	4.38816	1.36283	0.22752
C	4.83070	0.22441	-0.43892
H	4.25834	-1.70407	-1.19397
H	2.73404	2.33141	1.19073
H	5.06855	2.18799	0.40939
H	5.85362	0.14796	-0.78866
C	0.73043	0.59008	0.83397
H	0.67109	1.41582	1.55429
H	-0.01916	1.13528	-0.12739
C	-0.98897	-1.19074	0.83474
C	-0.89614	-1.51909	-0.53800
C	-2.17428	-1.53716	1.51327
C	-1.99160	-2.06312	-1.20690
C	-3.23922	-2.11396	0.83498
H	-2.27860	-1.30872	2.56641
C	-3.16833	-2.36487	-0.53485
H	-1.88230	-2.27959	-2.26390
H	-4.14604	-2.34961	1.38188
H	-4.00834	-2.80176	-1.06066
N	0.07030	-0.56574	1.46166
O	0.44666	-1.29970	-2.47471
C	0.39753	-1.47600	-1.27513
C	1.66531	-1.88569	-0.52071
H	1.38787	-2.39214	0.40564
H	2.16775	-2.60114	-1.17627
C	0.11797	-0.57990	2.91053
H	1.13905	-0.35024	3.21965
H	-0.55123	0.17135	3.35824
H	-0.14835	-1.56494	3.30224
O	-0.71895	1.84383	-0.95067
C	-1.92486	2.34286	-0.48105
C	-2.13500	3.76202	-1.03735
H	-1.31536	4.40851	-0.71077
H	-2.12556	3.72746	-2.13034
H	-3.08401	4.19986	-0.70652
C	-1.95498	2.41609	1.06055
H	-2.90264	2.83057	1.42099
H	-1.83122	1.41563	1.48814
H	-1.13844	3.04840	1.42290
C	-3.09382	1.45365	-0.94281
H	-3.07274	1.36706	-2.03319
H	-2.98386	0.45114	-0.52158
H	-4.06649	1.85864	-0.63844

Product 53 + *tert*-butanol

47

-981.6845553

C	4.09018	-0.59050	-0.58003
C	2.75878	-0.60518	-0.18698
C	2.16764	0.53124	0.43141
C	3.00212	1.66835	0.57834
C	4.32515	1.67365	0.16329
C	4.89740	0.53647	-0.40860
H	4.50005	-1.47520	-1.06046
H	2.58014	2.55955	1.03455
H	4.92152	2.57110	0.29809
H	5.93092	0.53233	-0.73368
C	0.77345	0.57972	0.77855
H	0.51331	1.49493	1.32055
H	-0.49476	1.50131	-0.54906
C	-0.83623	-1.29383	0.82717
C	-0.69774	-1.60953	-0.54570
C	-1.99208	-1.75029	1.49158
C	-1.72575	-2.25193	-1.23076
C	-2.99517	-2.41300	0.79349
H	-2.13051	-1.53853	2.54425
C	-2.88440	-2.65422	-0.57510
H	-1.58081	-2.45803	-2.28595
H	-3.88707	-2.72509	1.32681
H	-3.67662	-3.16108	-1.11257
N	0.15260	-0.56131	1.44447
O	0.65295	-1.16566	-2.43852
C	0.60106	-1.41196	-1.24870
C	1.87991	-1.79210	-0.49184
H	1.60581	-2.32822	0.41967
H	2.41475	-2.47930	-1.15365
C	0.16249	-0.51427	2.89617
H	1.15438	-0.19464	3.21611
H	-0.57204	0.20327	3.29467
H	-0.04273	-1.49832	3.32795
O	-1.04709	2.17305	-1.01775
C	-2.33560	2.26551	-0.42802
C	-2.90362	3.60863	-0.87869
H	-2.26603	4.42219	-0.52444
H	-2.93829	3.64850	-1.97017
H	-3.91464	3.75530	-0.48917
C	-2.24025	2.21839	1.09912
H	-3.22586	2.37027	1.54886
H	-1.85793	1.24712	1.42566
H	-1.56409	2.99780	1.46072
C	-3.22406	1.12338	-0.92544
H	-3.26000	1.13058	-2.01777
H	-2.82136	0.16176	-0.60062
H	-4.24276	1.22128	-0.53712



SM 53

32

-748.0309499

C	3.10684	-0.96942	0.92380
C	1.87035	-0.44529	0.58343
C	1.75326	0.60474	-0.38501
C	2.97397	1.00630	-1.00766
C	4.19599	0.45658	-0.66160
C	4.29387	-0.52621	0.32916
H	3.14281	-1.78061	1.64743
H	2.93008	1.78215	-1.76728
H	5.09414	0.80718	-1.16272
H	5.24882	-0.95858	0.60135
C	0.50456	1.12710	-0.78450
H	0.51981	1.87900	-1.57717
C	-1.74189	0.62946	0.07490
C	-1.65468	-0.76256	-0.15976
C	-3.02356	1.19419	0.21422
C	-2.80525	-1.51594	-0.36750
C	-4.16265	0.41730	0.02821
H	-3.13214	2.25210	0.41529
C	-4.06843	-0.93641	-0.28555
H	-2.69067	-2.57767	-0.55887
H	-5.13769	0.88620	0.11218
H	-4.96056	-1.53090	-0.44036
N	-0.57296	1.35702	0.15522
O	-0.11182	-2.47544	-0.69248
C	-0.34765	-1.47236	-0.04480
C	0.59636	-1.06634	1.09782
H	0.06131	-0.40090	1.77924
H	0.83001	-1.99526	1.62639
C	-0.65829	2.71355	0.67031
H	0.34813	3.03504	0.93604
H	-1.05796	3.41824	-0.07568
H	-1.28753	2.76014	1.56459

TS of 53 cyclising to form S46

32

-748.0303177

C	3.10343	-0.97492	1.01492
C	1.86914	-0.51582	0.58441
C	1.76747	0.51554	-0.39083
C	2.98252	0.98655	-0.94384
C	4.21396	0.50143	-0.51980
C	4.29399	-0.46755	0.48069
H	3.14119	-1.77983	1.74457
H	2.94078	1.75652	-1.70933
H	5.12380	0.89324	-0.96498
H	5.25334	-0.84705	0.81240
C	0.47357	0.91207	-0.85982
H	0.48474	1.57412	-1.73321
C	-1.74446	0.64648	0.09179
C	-1.69120	-0.73848	-0.18318
C	-2.99725	1.23215	0.33459
C	-2.85728	-1.47659	-0.31206
C	-4.15914	0.46735	0.22194
H	-3.07605	2.28737	0.56277
C	-4.10567	-0.87966	-0.11901
H	-2.77266	-2.53440	-0.53910
H	-5.11965	0.94548	0.38477
H	-5.01560	-1.45979	-0.21553
N	-0.54505	1.32461	0.08794
O	-0.14122	-2.37845	-0.93540
C	-0.35533	-1.40947	-0.21781
C	0.57151	-1.15169	0.99413
H	0.03395	-0.52975	1.71474
H	0.75275	-2.13047	1.44919
C	-0.55806	2.73135	0.44630
H	0.47301	3.05559	0.58391
H	-1.01641	3.35390	-0.33860
H	-1.10137	2.89796	1.38152

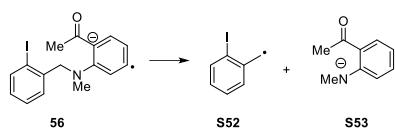
Product S46

32

-748.0629296

C	-3.11022	-1.12742	-1.05971
C	-1.87379	-0.81536	-0.50848
C	-1.74976	0.29071	0.34256
C	-2.85381	1.06977	0.66061
C	-4.09539	0.75642	0.10194
C	-4.21956	-0.33404	-0.75497
H	-3.21896	-1.98844	-1.71161
H	-2.75810	1.90542	1.34730
H	-4.96661	1.35489	0.34478
H	-5.18853	-0.57793	-1.17713
C	-0.33003	0.41292	0.81295
H	-0.23459	0.72302	1.86391
C	1.74671	0.69518	-0.17801
C	1.70354	-0.66111	0.17971
C	2.93830	1.29453	-0.57913
C	2.84990	-1.42478	0.14250
C	4.09141	0.50011	-0.63226
H	2.98736	2.34716	-0.83391
C	4.05717	-0.84327	-0.27607
H	2.80545	-2.46247	0.45876
H	5.02885	0.95146	-0.93997
H	4.96616	-1.43371	-0.30654
N	0.48294	1.27827	-0.06194
O	0.16022	-1.87163	1.64216
C	0.28194	-1.04500	0.60903
C	-0.54986	-1.51438	-0.66283
H	-0.07859	-1.20337	-1.60356
H	-0.62841	-2.60323	-0.64909
C	0.37955	2.70527	0.13166
H	-0.67463	2.98898	0.12762
H	0.82975	3.02895	1.08407
H	0.87196	3.23707	-0.68536

10 Possible CN cleavage in DMSO
Scheme 4.2



TS of CN cleavage of 56

35

-760.5905567

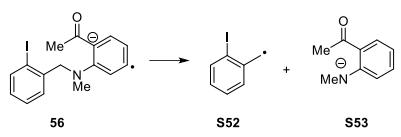
C	-2.69899	3.29057	0.44189
C	-1.56304	2.77252	-0.14371
C	-1.38412	1.37302	-0.38558
C	-2.47975	0.56034	0.02461
C	-3.62596	1.07187	0.60414
C	-3.74944	2.44805	0.83291
H	-2.77710	4.36097	0.60035
H	-4.43691	0.40774	0.87866
H	-4.64537	2.84312	1.29442
C	-0.12108	0.91790	-0.86280
H	-0.01755	-0.12208	-1.15233
H	0.43624	1.62018	-1.47291
C	2.42582	0.83986	0.12344
C	3.32954	-0.28398	0.19932
C	2.95471	2.03232	-0.47079
C	4.70526	-0.07073	-0.05602
C	4.28131	2.17427	-0.78782
H	2.26753	2.86322	-0.59834
C	5.19398	1.12355	-0.53834
H	5.39346	-0.89962	0.07036
H	4.63693	3.11155	-1.20342
H	6.24851	1.24307	-0.75333
N	1.15747	0.92742	0.58405
O	1.79165	-2.05985	-0.08607
C	2.88953	-1.67592	0.31864
C	3.85494	-2.71299	0.87274
H	4.50702	-2.31284	1.64876
H	3.26949	-3.54094	1.27113
C	0.66616	-0.02985	1.55091
H	0.33835	-0.97757	1.11412
H	1.44697	-0.26173	2.28781
H	-0.18385	0.42059	2.07303
H	-0.75451	3.43594	-0.43557
H	4.48273	-3.10521	0.06718
I	-2.46643	-1.54876	-0.36662

Products of CN cleavage S52 and S53

35

-760.6046657			
C	2.03457	3.37251	-0.60934
C	1.57725	2.80456	0.56216
C	1.78436	1.43099	0.86935
C	2.50108	0.67947	-0.09891
C	2.96030	1.24348	-1.27572
C	2.72767	2.59429	-1.53888
H	1.85079	4.42166	-0.80771
H	3.49707	0.64012	-1.99676
H	3.08909	3.02746	-2.46347
C	1.25232	0.90486	2.06237
H	1.36673	-0.13314	2.33622
H	0.70446	1.55399	2.73185
C	-2.94097	0.81897	0.07546
C	-3.43638	-0.52136	-0.24841
C	-3.93621	1.70590	0.66076
C	-4.83975	-0.72302	-0.34456
C	-5.27123	1.43362	0.61647
H	-3.57480	2.64770	1.06213
C	-5.75699	0.22047	0.04926
H	-5.20316	-1.68902	-0.68050
H	-5.97708	2.15728	1.01388
H	-6.82004	0.02336	-0.00887
N	-1.75834	1.33035	-0.17006
O	-1.51175	-1.74982	0.37856
C	-2.58998	-1.69807	-0.22658
C	-3.07670	-2.97630	-0.90157
H	-3.64371	-2.78535	-1.81279
H	-2.20475	-3.58660	-1.13488
C	-0.82249	0.60286	-0.99029
H	-0.24652	-0.14823	-0.43648
H	-1.32659	0.05519	-1.80599
H	-0.11100	1.31076	-1.42664
H	1.02835	3.40442	1.27971
H	-3.71190	-3.54588	-0.21717
I	2.88082	-1.39674	0.19925

11 Possible CN cleavage in Benzene
Scheme 4.2



TS of CN cleavage of 56

35

-760.5585428

C	-2.70397	3.28389	0.45696
C	-1.56839	2.76966	-0.12993
C	-1.39203	1.37263	-0.38743
C	-2.48769	0.55802	0.01905
C	-3.63344	1.06584	0.60031
C	-3.75802	2.44055	0.83709
H	-2.77811	4.35273	0.62861
H	-4.44243	0.39783	0.87083
H	-4.65433	2.83328	1.30014
C	-0.13560	0.92049	-0.87763
H	-0.02719	-0.11876	-1.16754
H	0.42339	1.62569	-1.48216
C	2.42310	0.83942	0.11761
C	3.33298	-0.27965	0.20612
C	2.95034	2.02886	-0.48757
C	4.70720	-0.06250	-0.04623
C	4.27700	2.17378	-0.79739
H	2.25830	2.85425	-0.62234
C	5.19436	1.12996	-0.53467
H	5.39816	-0.88808	0.08844
H	4.63041	3.10974	-1.21862
H	6.24955	1.25250	-0.74551
N	1.15907	0.92685	0.57433
O	1.79293	-2.05891	-0.06010
C	2.89142	-1.67135	0.32687
C	3.86787	-2.71067	0.86854
H	4.51137	-2.31591	1.65517
H	3.28454	-3.54840	1.24894
C	0.66144	-0.02003	1.54608
H	0.33576	-0.97277	1.11770
H	1.43921	-0.24409	2.28922
H	-0.19067	0.43936	2.05709
H	-0.75279	3.43106	-0.40511
H	4.50299	-3.08315	0.05947
I	-2.46046	-1.55048	-0.36831

Products of CN cleavage S52 and S53

35

-760.5719419			
C	-1.59237	3.07639	0.62609
C	-0.82792	1.96219	0.34530
C	-1.42238	0.70236	0.03872
C	-2.84218	0.66987	0.03822
C	-3.60974	1.78629	0.31922
C	-2.98759	2.99908	0.61696
H	-1.10269	4.01573	0.85572
H	-4.69036	1.72067	0.30942
H	-3.59296	3.86976	0.83897
C	-0.58211	-0.39552	-0.22917
H	-0.98177	-1.37424	-0.45222
H	0.49416	-0.27807	-0.18773
C	3.35232	0.79831	-0.06078
C	4.06928	-0.46380	0.13347
C	3.83033	1.60115	-1.17620
C	5.34473	-0.61961	-0.47169
C	5.02889	1.36703	-1.77977
H	3.22386	2.45870	-1.44974
C	5.84850	0.26916	-1.38950
H	5.91933	-1.51305	-0.24812
H	5.36946	2.03408	-2.56662
H	6.81437	0.10685	-1.85196
N	2.40305	1.31967	0.67705
O	2.20835	-1.78994	0.75530
C	3.43191	-1.64362	0.68453
C	4.30311	-2.82194	1.11985
H	5.21723	-2.50714	1.62491
H	3.70800	-3.44555	1.78595
C	2.07189	0.72445	1.94667
H	1.32630	-0.07919	1.87231
H	2.94837	0.27494	2.44224
H	1.66511	1.50403	2.59998
H	0.26002	2.00828	0.35231
H	4.58314	-3.42406	0.25073
I	-3.88962	-1.13888	-0.40621