

Supporting Information

Iridium-catalysed ortho-Directed Deuterium Labelling of Aromatic Esters – an Experimental and Theoretical Study on Directing Group Chemoselectivity

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Structural Coordinates of Binding Conformers (Gas Phase) – from Scheme 7

Substrate 12 – position 15 (nitro bound reactant)

1 1

C	2.16765800	4.40849900	-0.75910500
C	3.35316300	3.76210000	-0.80718400
N	1.20097100	3.44246900	-0.51859600
N	3.08613700	2.41740300	-0.59687100
C	4.11151500	1.41332600	-0.52887900
C	4.65065100	1.09391600	0.72403200
C	4.51642200	0.78393500	-1.70818500
C	5.61891700	0.09560900	0.77096900
C	5.49110800	-0.20914300	-1.60647500
C	6.04935900	-0.56789600	-0.38031800
H	6.05061900	-0.17493700	1.73619000
H	5.82360700	-0.71535900	-2.51476200
C	-0.19500600	3.72541500	-0.36258700
C	-0.66469800	4.08462700	0.90740700
C	-1.03921400	3.58950000	-1.46932200
C	-2.04027800	4.24795100	1.06215900
C	-2.40497000	3.78432800	-1.26524100
C	-2.92435900	4.09201400	-0.00740600
H	-2.43257200	4.49540100	2.05063500
H	-3.08619500	3.66562900	-2.11006100
C	-0.50622900	3.17973000	-2.80958500
H	0.36584600	3.77681100	-3.10824300
H	-0.17697900	2.12771500	-2.80665100
H	-1.27218300	3.28838300	-3.58536700
C	0.27448700	4.26121800	2.06215400
H	0.91953500	3.38176500	2.20084500
H	0.93794000	5.12410100	1.91178200
H	-0.27737900	4.42288500	2.99464000
C	-4.40123200	4.25037900	0.19141100
H	-4.71177700	3.90484000	1.18559300
H	-4.70478800	5.30298600	0.10679300
H	-4.96861700	3.68734700	-0.55998800
C	7.09242300	-1.63970500	-0.28368400
H	6.78171700	-2.42945300	0.41480000
H	7.28770800	-2.10505700	-1.25746300
H	8.04416700	-1.23913900	0.09005400
C	3.90449600	1.13958100	-3.02881000
H	2.83126000	0.89572500	-3.04821100
H	3.98910100	2.21258900	-3.24885900
H	4.38826100	0.59263100	-3.84540100
C	4.17318600	1.77306000	1.97161100
H	4.17035600	2.86751800	1.87340700
H	3.14378800	1.47334200	2.22001900
H	4.80812400	1.51327900	2.82560600
H	4.36313200	4.11669400	-0.96680500
H	1.90703600	5.45296800	-0.87027700

C	1.75364700	2.20118500	-0.41249600
Ir	0.87719400	0.34545500	-0.09338900
H	2.34297400	-0.10723500	0.12286000
H	1.29984300	-0.00684600	-1.56666800
P	0.34125500	-1.94654700	0.11301500
C	1.83806200	-2.97290900	0.34890800
C	2.91143900	-2.77093000	-0.52676600
C	1.93112900	-3.96163400	1.33090500
C	4.05991100	-3.54364500	-0.41673000
H	2.84812900	-2.00369100	-1.30053600
C	3.08875500	-4.72755100	1.44385500
H	1.10062300	-4.13532800	2.01511500
C	4.15305700	-4.51931500	0.57323900
H	4.88767200	-3.37484600	-1.10503200
H	3.15626800	-5.49206000	2.21557600
H	5.05604900	-5.12103900	0.66200000
C	-0.48979600	-2.73307100	-1.30963000
C	-1.02175500	-1.94941000	-2.33554200
C	-0.62764600	-4.12506100	-1.36858600
C	-1.71339400	-2.53991800	-3.38906900
H	-0.87785300	-0.86885200	-2.31138000
C	-1.31133400	-4.71488500	-2.42415700
H	-0.19723500	-4.74912100	-0.58399300
C	-1.86128500	-3.92208100	-3.42979600
H	-2.13328900	-1.91997200	-4.17880300
H	-1.41385300	-5.79752100	-2.46546500
H	-2.39852900	-4.38739700	-4.25402300
C	-0.72249300	-2.32059900	1.55441200
C	-1.98137900	-2.91406900	1.43921800
C	-0.28156600	-1.89162600	2.81462300
C	-2.78280700	-3.07991000	2.56677700
H	-2.34398900	-3.24462300	0.46616000
C	-1.08363400	-2.05741800	3.93737300
H	0.69752100	-1.41861300	2.91482000
C	-2.33847800	-2.65196400	3.81336400
H	-3.76135500	-3.54702500	2.46609600
H	-0.72972800	-1.71711200	4.90884200
H	-2.96722700	-2.78405300	4.69204600
C	-3.28053700	0.34106900	2.02300200
C	-4.29419600	-0.06305800	1.16765500
C	-4.09091500	-0.05163000	-0.21524800
C	-2.87628300	0.38462200	-0.74238800
C	-1.84571800	0.77008900	0.09995300
C	-2.06150500	0.72867500	1.47609100
H	-3.40245900	0.32688200	3.10251500
H	-5.24706000	-0.39843300	1.56838600
H	-2.76515200	0.43336200	-1.82419200
H	-0.98332300	1.30559500	-0.33956000
N	-0.99569000	1.09521600	2.39374100
O	0.18554100	1.02602200	2.00056900
O	-1.28369000	1.45016300	3.51576200
C	-5.13877400	-0.47771000	-1.19060900
O	-4.95743800	-0.49905700	-2.38671100
O	-6.27525900	-0.82147000	-0.58792200

C	-7.34845100	-1.23161200	-1.46166500
H	-7.00356000	-2.08991600	-2.05190000
H	-7.55193400	-0.41283500	-2.16304900
C	-8.53277500	-1.56091600	-0.59525600
H	-8.84183400	-0.69021100	-0.00548700
H	-9.37953500	-1.86845500	-1.21882700
H	-8.30086000	-2.38096300	0.09401600

Substrate 12 – position 16 (nitro bound transition state)

1 1

C	0.40622500	-4.66648000	-0.57798800
C	-0.93637900	-4.59029300	-0.72229500
N	0.85607300	-3.37497100	-0.34559300
N	-1.28210900	-3.25733300	-0.56975200
C	-2.62824700	-2.75654900	-0.62190300
C	-3.35785300	-2.70224600	0.57038600
C	-3.11332000	-2.25644800	-1.83195600
C	-4.61169100	-2.09874400	0.52761400
C	-4.36972700	-1.65322600	-1.81887100
C	-5.12993100	-1.56350600	-0.65336300
H	-5.20086000	-2.04076500	1.44460200
H	-4.76548100	-1.24194900	-2.74945300
C	2.23608800	-3.03131900	-0.13466400
C	2.76080300	-3.17306800	1.15579000
C	2.99877100	-2.57173000	-1.21393800
C	4.08405600	-2.78571600	1.35768100
C	4.31658800	-2.19792800	-0.95616200
C	4.87264100	-2.28653400	0.32021400
H	4.50741400	-2.86914800	2.36015900
H	4.92780700	-1.82433300	-1.78051400
C	2.43800100	-2.45514200	-2.60040700
H	2.02154100	-1.45108000	-2.78477700
H	3.22178900	-2.61340700	-3.35028200
H	1.63388200	-3.17675400	-2.79352100
C	1.93609700	-3.72880200	2.27768600
H	0.97916000	-3.19881000	2.38295600
H	1.70295900	-4.79082500	2.11733400
H	2.46994800	-3.64786300	3.23047100
C	6.29252000	-1.87350600	0.56152100
H	6.49081600	-1.71361300	1.62798800
H	6.99447300	-2.64183000	0.20965000
H	6.53627500	-0.94696600	0.02553300
C	-6.49022300	-0.93617500	-0.67216700
H	-7.27651900	-1.69992900	-0.74907200
H	-6.68378700	-0.36617700	0.24550500
H	-6.60704100	-0.25918700	-1.52697900
C	-2.31408400	-2.34738700	-3.09692100
H	-1.38107300	-1.76635200	-3.03776300
H	-2.02721100	-3.38290200	-3.32712000
H	-2.88876100	-1.96610400	-3.94852800
C	-2.78672200	-3.22241200	1.85437700
H	-2.49127300	-4.27810700	1.78077600
H	-1.88570800	-2.66169400	2.15008600
H	-3.51497500	-3.13666600	2.66828600
H	-1.68638900	-5.34656500	-0.91315600
H	1.09232600	-5.50229300	-0.61737800
C	-0.17959900	-2.50014100	-0.33181700
Ir	-0.12913500	-0.43195500	-0.05756200
H	-1.65637800	-0.75322000	0.46600500

H	-0.94639500	-0.28016700	-1.39384400
P	-1.07864200	1.75566200	0.29609900
C	-1.72619300	2.05877300	1.97211300
C	-2.04034300	0.99687200	2.82473200
C	-1.98968000	3.37278600	2.38248700
C	-2.60493300	1.24580400	4.07223200
H	-1.84053400	-0.02803600	2.51470500
C	-2.55614800	3.61516600	3.62730700
H	-1.75570100	4.20948300	1.72417600
C	-2.86216900	2.55190200	4.47369700
H	-2.83847500	0.41379400	4.73347500
H	-2.75844700	4.63809300	3.93834400
H	-3.30116500	2.74389100	5.45088300
C	-2.51861500	1.93295600	-0.82019600
C	-2.34973300	1.74704900	-2.19898700
C	-3.79579100	2.19144900	-0.32039500
C	-3.43329800	1.84366700	-3.06159900
H	-1.35999500	1.52589700	-2.60434100
C	-4.88302400	2.27726000	-1.18781000
H	-3.94887800	2.32961200	0.74920000
C	-4.70479700	2.10818800	-2.55524900
H	-3.28667400	1.70932300	-4.13193400
H	-5.87441300	2.47982500	-0.78598000
H	-5.55568600	2.18126700	-3.23044100
C	0.01621000	3.18548600	-0.01301200
C	-0.04889300	3.95555200	-1.17551100
C	1.02366400	3.44558700	0.92504500
C	0.89061200	4.96055200	-1.40148500
H	-0.84073300	3.78988000	-1.90481100
C	1.95786400	4.44640700	0.69648900
H	1.07696500	2.86017500	1.84505500
C	1.89813400	5.20179100	-0.47343400
H	0.82572200	5.56412900	-2.30542700
H	2.73929200	4.63311000	1.43096100
H	2.63392000	5.98288800	-0.65507900
C	2.50977500	0.35722500	1.06752100
C	1.78115900	0.47320000	-0.12197000
C	2.38748700	1.23296000	-1.13146100
C	3.63988700	1.81402000	-0.95674700
C	4.34440300	1.63605700	0.24753700
C	3.77957500	0.91110600	1.27192100
H	0.83691700	-0.70800000	-1.29690900
H	1.84930700	1.37931700	-2.06957900
H	5.32335900	2.09905500	0.34838400
H	4.27793500	0.76704100	2.22827800
C	4.28196000	2.67083400	-2.01278000
O	5.36737000	3.17141900	-1.79966700
C	3.54615100	2.89575900	-3.30485700
H	3.33560400	1.94664600	-3.81594700
H	2.58219800	3.39178100	-3.12019900
H	4.15898100	3.52606000	-3.95430500
N	1.88858600	-0.33203000	2.15834400
O	2.45292100	-0.49059500	3.21732000
O	0.70914600	-0.75443400	1.97658500

Substrate 12 – position 17 (nitro bound C-H activated product)

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C	1.30272400	-3.84165600	-2.25084700
C	0.13664500	-3.62764000	-2.89789900
N	1.31450200	-2.99243200	-1.15329700
N	-0.53905000	-2.65396400	-2.18227600
C	-1.83606400	-2.15839600	-2.54312300
C	-2.96312000	-2.80211800	-2.01967900
C	-1.92299100	-1.01938700	-3.34901900
C	-4.20770500	-2.23061500	-2.27593800
C	-3.19183600	-0.48800400	-3.57641300
C	-4.34042800	-1.06538500	-3.03509100
H	-5.10211700	-2.71244200	-1.87656500
H	-3.28421700	0.40636200	-4.19533700
C	2.40559400	-2.97650000	-0.21791900
C	2.29036600	-3.72187100	0.96072800
C	3.56327700	-2.26822700	-0.55530400
C	3.36996700	-3.70356600	1.83902800
C	4.61401000	-2.28047300	0.36093900
C	4.53028700	-2.97731000	1.56538200
H	3.29976700	-4.26494100	2.77193800
H	5.52235400	-1.72253100	0.12548500
C	3.68432400	-1.53816300	-1.85881800
H	3.81520300	-2.23349900	-2.70025700
H	2.79141100	-0.93558400	-2.07880300
H	4.55082300	-0.86718900	-1.85088400
C	1.04817300	-4.49487200	1.28302800
H	0.25062600	-3.82800100	1.64251300
H	0.65728000	-5.03551800	0.40981100
H	1.24008900	-5.22752700	2.07450400
C	5.64002900	-2.91314500	2.56766500
H	5.43288100	-2.13226300	3.31352700
H	5.75114800	-3.85878900	3.11168100
H	6.60088700	-2.67435000	2.09695700
C	-5.68890200	-0.44930500	-3.25504100
H	-6.46423600	-1.21329900	-3.38997400
H	-5.98690700	0.16441700	-2.39326400
H	-5.69691500	0.20198000	-4.13652300
C	-0.70388800	-0.39197600	-3.95561400
H	0.15146700	-0.38678200	-3.26658500
H	-0.38186100	-0.94064400	-4.85257900
H	-0.89938700	0.64335200	-4.26197400
C	-2.84204100	-4.07128700	-1.22847500
H	-2.52971000	-4.91096600	-1.86531900
H	-2.09627300	-3.99978200	-0.42367400
H	-3.80203700	-4.34383400	-0.77625300
H	-0.28639700	-4.06544900	-3.79261400
H	2.12848800	-4.51263400	-2.44806800
C	0.17973400	-2.24818500	-1.09414300
Ir	-0.47617000	-0.74009900	0.22304400
H	-1.69767500	-1.94170000	0.96838800

H	-2.09080700	-1.65900800	0.30011900
P	-1.47102800	1.10281600	1.37295900
C	-2.96809400	0.65058600	2.32588500
C	-4.00626800	0.03709300	1.61317400
C	-3.13988000	0.92894900	3.68260600
C	-5.18769400	-0.31069800	2.25303000
H	-3.89523500	-0.15160700	0.54193200
C	-4.32537400	0.57349900	4.32212400
H	-2.35260300	1.43003600	4.24450400
C	-5.34513900	-0.04966700	3.61307400
H	-5.98995100	-0.78499500	1.69067700
H	-4.45048500	0.79054000	5.38119600
H	-6.26891100	-0.32614100	4.11742700
C	-2.10216300	2.45871300	0.31850000
C	-1.99058900	2.45178600	-1.07242800
C	-2.75216900	3.53126400	0.94486300
C	-2.50060300	3.50599400	-1.82591600
H	-1.51108300	1.61610300	-1.57850500
C	-3.25997900	4.58116600	0.19252600
H	-2.85962100	3.54422600	2.03028600
C	-3.13168300	4.57102700	-1.19529000
H	-2.39667900	3.49139000	-2.90950500
H	-3.76157000	5.40912900	0.68966000
H	-3.52928700	5.39554500	-1.78388700
C	-0.30633300	1.89911000	2.52638200
C	0.27302900	3.13627800	2.22712200
C	0.14039100	1.18487300	3.64617200
C	1.27052700	3.65638100	3.04570700
H	-0.05080000	3.69396400	1.34880900
C	1.13109700	1.71321200	4.46537400
H	-0.27331300	0.20030300	3.86860100
C	1.69769800	2.94939700	4.16516400
H	1.71347900	4.62156000	2.80742100
H	1.46860800	1.15022900	5.33327800
H	2.47639400	3.35977300	4.80511500
C	3.33340500	1.12029000	0.75525500
C	3.48859000	2.01674300	-0.28339200
C	2.48071600	2.11880300	-1.25393400
C	1.33319100	1.33406200	-1.18228800
C	1.12824100	0.42295500	-0.14206200
C	2.16805500	0.35205300	0.80129400
H	4.08511100	0.99967900	1.53137700
H	4.37515500	2.64009700	-0.35546500
H	0.58798500	1.46925700	-1.96326700
H	-1.29001900	-0.23409600	-1.02073700
N	1.99336000	-0.55937800	1.89961600
O	0.92423500	-1.22595800	1.92879100
O	2.83332000	-0.67842400	2.76344700
C	2.57744300	3.06062400	-2.40922500
O	1.73466500	3.14447000	-3.27478600
O	3.69332000	3.79005700	-2.37242300
C	3.86493100	4.72700200	-3.45372400
H	2.99675400	5.39788400	-3.47049800
H	3.86469800	4.16845200	-4.39845000

C	5.15771900	5.45782000	-3.21418900
H	6.00539100	4.76310200	-3.19849800
H	5.32960800	6.18904900	-4.01190600
H	5.13364300	5.99441200	-2.25863000

Substrate 12 – position 15 (ester bound reactant)

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C	-0.40952000	-4.63890100	-0.28308100
C	0.93416900	-4.66810400	-0.14591900
N	-0.76833200	-3.30345300	-0.41873400
N	1.36735200	-3.35246400	-0.20206500
C	2.73394800	-2.93904000	-0.05201900
C	3.52145600	-2.79842900	-1.19820800
C	3.19449600	-2.60147800	1.22659200
C	4.80332700	-2.27200200	-1.03925900
C	4.48398200	-2.09139500	1.33208100
C	5.29650600	-1.90252500	0.21137300
H	5.43246100	-2.14232300	-1.92130700
H	4.86730300	-1.81848500	2.31737700
C	-2.13382900	-2.88365600	-0.54982700
C	-2.65468400	-2.67255300	-1.83247100
C	-2.91189800	-2.75649000	0.60650200
C	-3.99908600	-2.32073800	-1.93343100
C	-4.25186200	-2.40421900	0.45122500
C	-4.81394100	-2.18862700	-0.80571800
H	-4.42675200	-2.14561100	-2.92247700
H	-4.87137800	-2.28314800	1.34249700
C	-2.34262500	-3.00116500	1.97294900
H	-2.37685100	-4.06767100	2.23843400
H	-1.29063400	-2.69223000	2.04654600
H	-2.91816600	-2.46087400	2.73624600
C	-1.79169300	-2.81401000	-3.04991900
H	-0.96341700	-2.09022700	-3.04296400
H	-1.33819200	-3.81335000	-3.11300700
H	-2.37371800	-2.65326200	-3.96380000
C	-6.26174300	-1.82809200	-0.94637800
H	-6.43698100	-1.18928800	-1.82092900
H	-6.88106400	-2.72646800	-1.07460600
H	-6.63756600	-1.30688200	-0.05549600
C	6.66485900	-1.31245300	0.36605000
H	7.16048100	-1.17856300	-0.60196700
H	6.61478700	-0.33112700	0.85757100
H	7.30801300	-1.95023500	0.98699900
C	2.30878500	-2.71573100	2.43088600
H	1.47674800	-1.99502100	2.37870600
H	1.86020200	-3.71415000	2.52815000
H	2.87368300	-2.51133600	3.34847000
C	2.98091500	-3.13083200	-2.55514800
H	2.56168300	-4.14498700	-2.59909300
H	2.17011000	-2.43994800	-2.83442600
H	3.76333700	-3.05636500	-3.31827800
H	1.63015100	-5.48669500	-0.01671800
H	-1.15197100	-5.42600000	-0.30345900
C	0.32292800	-2.49073900	-0.37133600
Ir	0.54312800	-0.43410500	-0.44280400
H	0.81387700	-0.54236700	-1.98376800

H	2.05956600	-0.72969600	-0.54809600
P	1.23120800	1.82232900	-0.47607300
C	1.93652800	2.44118100	-2.04402300
C	2.78502700	1.58608000	-2.75731600
C	1.72582900	3.74193800	-2.51000500
C	3.40562400	2.02565200	-3.91987500
H	2.96419500	0.57146600	-2.39608100
C	2.34140000	4.17439400	-3.68090700
H	1.07795800	4.42335200	-1.95865100
C	3.17928800	3.31787700	-4.38688900
H	4.06379800	1.35486400	-4.46891400
H	2.16583600	5.18651700	-4.04043600
H	3.65844000	3.65784300	-5.30295900
C	2.57112600	2.12549800	0.73772100
C	2.82442600	1.19458000	1.74923000
C	3.32259600	3.30483400	0.69049800
C	3.80875600	1.44216800	2.70263400
H	2.24797100	0.26995200	1.78664500
C	4.30674400	3.54802500	1.64079500
H	3.14001700	4.03700900	-0.09692600
C	4.55026900	2.61759200	2.64906500
H	3.99737000	0.70862800	3.48624100
H	4.88842100	4.46668100	1.59476800
H	5.32201000	2.81010800	3.39216700
C	-0.06682000	3.01875900	0.00369100
C	-0.11232500	3.57254400	1.28697100
C	-1.12150100	3.26805500	-0.88319700
C	-1.19271700	4.36322500	1.67220400
H	0.70439000	3.39513200	1.98805100
C	-2.19118100	4.06786500	-0.50056200
H	-1.10451400	2.83075700	-1.88401400
C	-2.23026600	4.61446500	0.78082500
H	-1.21524700	4.79526400	2.67118200
H	-3.00024300	4.26071000	-1.20379600
H	-3.07056200	5.23779900	1.08100100
C	-4.69431700	1.45381700	1.21303500
C	-3.58130200	1.12520000	1.97238300
C	-2.43384000	0.60698800	1.35873100
C	-2.41758800	0.43141000	-0.02692600
C	-3.51625000	0.76470800	-0.80119600
C	-4.63975700	1.26358400	-0.16064300
H	-5.59977300	1.84908000	1.66442500
H	-3.59657300	1.26883900	3.04902500
H	-1.56063600	0.00096500	-0.56152300
H	-3.51536600	0.63005700	-1.87906400
N	-5.82976700	1.58119700	-0.97156100
O	-5.74904000	1.39379300	-2.17399500
O	-6.81117100	1.99456400	-0.38260700
C	-1.25916300	0.22386200	2.17422400
O	-0.20832200	-0.23369400	1.72500400
O	-1.43240400	0.39290600	3.46949200
C	-0.32831700	0.02664600	4.33078500
H	0.56318300	0.57740700	3.99933900
H	-0.13495400	-1.04596700	4.19004900

C	-0.73082000	0.36152000	5.73989300
H	-1.62709700	-0.19461500	6.03652300
H	0.07842400	0.09757400	6.42950400
H	-0.93464100	1.43278400	5.84669400

Substrate 12 – position 16 (ester bound transition state)

1 1

C	1.04591000	-4.04666400	-1.79856100
C	-0.25835000	-4.33674400	-1.60820500
N	1.22559200	-2.73310900	-1.38673300
N	-0.84969600	-3.19631900	-1.08755400
C	-2.25054600	-3.13266200	-0.77073800
C	-2.65737400	-3.42780000	0.53444500
C	-3.15014300	-2.76589500	-1.77740400
C	-4.01446200	-3.31223000	0.82952600
C	-4.49631500	-2.66681700	-1.43170400
C	-4.94649100	-2.93386500	-0.13718200
H	-4.35282600	-3.52806600	1.84423200
H	-5.21653400	-2.37803100	-2.19913900
C	2.50602700	-2.08810100	-1.44098800
C	3.44471700	-2.38090200	-0.44570400
C	2.78938500	-1.24242700	-2.52018000
C	4.67316200	-1.72286900	-0.50618100
C	4.03602900	-0.61976700	-2.53853700
C	4.97929600	-0.82721800	-1.52976700
H	5.41278400	-1.91766500	0.27272700
H	4.28497100	0.03801800	-3.37532700
C	1.79384600	-1.01510400	-3.61721800
H	1.35752700	-1.95770100	-3.97550300
H	0.96107600	-0.38208000	-3.27779800
H	2.26604700	-0.51814400	-4.47296800
C	3.16832100	-3.38156600	0.63696600
H	2.14340300	-3.31237700	1.02668200
H	3.30194900	-4.41010600	0.27191300
H	3.85866100	-3.24766600	1.47845000
C	6.27672500	-0.07866000	-1.53741500
H	7.04921000	-0.59239900	-0.95371300
H	6.65884000	0.06232000	-2.55628100
H	6.14750000	0.92295300	-1.09967200
C	-6.40572100	-2.85053000	0.19613800
H	-6.56669900	-2.69537200	1.27030300
H	-6.90132100	-2.03707400	-0.34951800
H	-6.92652800	-3.77898200	-0.07615000
C	-2.68496500	-2.47835000	-3.17207600
H	-3.52615200	-2.19190300	-3.81249100
H	-1.95245100	-1.65801200	-3.18865800
H	-2.20033900	-3.35142400	-3.63110700
C	-1.66614900	-3.82135300	1.58632000
H	-1.02402100	-4.65134200	1.26103300
H	-0.99718500	-2.98355100	1.83387600
H	-2.17104400	-4.12736700	2.50869700
H	-0.83351000	-5.23542100	-1.78905100
H	1.87037900	-4.63203600	-2.18393000
C	0.06014000	-2.18880500	-0.94239300
Ir	-0.42974300	-0.26016600	-0.26141100
H	-1.70857400	-1.02497300	0.23260400

H	-1.42298600	-0.20972600	-1.56525900
P	-1.43317600	1.82811900	0.27795300
C	-2.97051300	1.66871000	1.24435100
C	-3.89297200	0.68815800	0.86002900
C	-3.27997000	2.52700900	2.30351300
C	-5.10230700	0.56527200	1.53274700
H	-3.66761900	0.01933400	0.02770100
C	-4.49121600	2.39689800	2.97626600
H	-2.57218200	3.29797500	2.60839100
C	-5.40121800	1.41670900	2.59305000
H	-5.80968100	-0.20494500	1.22663000
H	-4.72351200	3.06491600	3.80329900
H	-6.34690200	1.31655600	3.12231300
C	-1.87854600	2.89688900	-1.13495200
C	-1.35084100	2.66992800	-2.40929700
C	-2.72424600	3.99257900	-0.92506200
C	-1.66636300	3.52864600	-3.45812800
H	-0.69080000	1.82141300	-2.58170200
C	-3.03850800	4.84498900	-1.97603000
H	-3.14805300	4.17618800	0.06267600
C	-2.50982800	4.61366100	-3.24328900
H	-1.25677900	3.34367500	-4.44959600
H	-3.70256300	5.69007500	-1.80602200
H	-2.76095200	5.27959000	-4.06670400
C	-0.28332100	2.83625800	1.27677700
C	0.43260600	3.88854700	0.69947300
C	0.03303100	2.43021800	2.58057200
C	1.44985300	4.52070200	1.41155300
H	0.18970500	4.22035700	-0.31069100
C	1.04168900	3.06756200	3.29075300
H	-0.51308500	1.60737700	3.04583300
C	1.75684600	4.11081800	2.70377000
H	1.99729200	5.34275200	0.95339100
H	1.27368700	2.74865100	4.30535000
H	2.54972800	4.60776600	3.25950900
C	3.61471400	0.11350200	2.69801600
C	3.40573700	0.84826800	1.54164700
C	2.24952700	0.65319800	0.78294000
C	1.23326000	-0.25453900	1.17152600
C	1.48145100	-1.01165100	2.31753200
C	2.65375700	-0.82738200	3.03806000
H	4.50138800	0.23217700	3.31327100
H	4.15039000	1.56455700	1.20026800
H	-0.38484300	-0.36795300	1.34097000
H	0.77156500	-1.75416600	2.67849100
N	2.89396600	-1.69021300	4.21187200
O	2.15344700	-2.64775100	4.35832100
O	3.82244600	-1.39273900	4.94075600
C	2.09621300	1.29523300	-0.52255300
O	1.13730400	1.02818900	-1.26295600
O	3.04148900	2.12975300	-0.89070500
C	2.88516300	2.75791800	-2.18394900
H	2.01555200	3.42888800	-2.12828500
H	2.66006500	1.97539900	-2.91998100

C	4.16765800	3.48054300	-2.48522700
H	5.00394300	2.77289200	-2.54420900
H	4.08942400	3.99739700	-3.44801100
H	4.39520900	4.22430900	-1.71331100

Substrate 12 – position 17 (ester bound C-H activated product)

1 1

C	1.17639400	-4.30903200	-0.93467400
C	-0.14610400	-4.55419900	-0.82445800
N	1.33974300	-2.93456300	-0.82722000
N	-0.76435700	-3.32594200	-0.65197200
C	-2.18855600	-3.18579700	-0.53029600
C	-2.77836400	-3.15928400	0.73525700
C	-2.93846600	-3.07448100	-1.71175000
C	-4.16177400	-2.96959500	0.79726600
C	-4.30909100	-2.87197000	-1.59372000
C	-4.93851700	-2.80554500	-0.34612500
H	-4.64111500	-2.94934300	1.77868000
H	-4.90917100	-2.77746700	-2.50031300
C	2.63096700	-2.31618100	-0.93458300
C	3.51930200	-2.42560400	0.14240300
C	2.97975600	-1.69969600	-2.14122900
C	4.76509300	-1.81545500	0.01097300
C	4.23843900	-1.10530900	-2.21855700
C	5.13433200	-1.13434500	-1.14876800
H	5.46689000	-1.87090200	0.84528700
H	4.53609700	-0.61901000	-3.15058400
C	2.04333300	-1.67656800	-3.31170800
H	1.55474300	-2.64879300	-3.46578700
H	1.25213500	-0.92549800	-3.16906500
H	2.58146600	-1.42220500	-4.23237800
C	3.17031200	-3.19002700	1.38470800
H	2.14339800	-2.99732900	1.72440100
H	3.25532900	-4.27458800	1.22571700
H	3.85081500	-2.93187300	2.20484400
C	6.45267300	-0.42839700	-1.23365800
H	7.23827800	-0.96345900	-0.68684900
H	6.78343200	-0.30773500	-2.27230300
H	6.38166000	0.57727500	-0.79338900
C	-6.41292200	-2.55514700	-0.25237700
H	-6.97062700	-3.15184000	-0.98470200
H	-6.80162600	-2.79352700	0.74459000
H	-6.64597800	-1.50022500	-0.45595700
C	-2.28545100	-3.17230300	-3.05838300
H	-1.46523900	-2.44862100	-3.17760200
H	-1.84791800	-4.16641400	-3.22580100
H	-3.01178800	-2.99250200	-3.85825600
C	-1.99223500	-3.29020700	2.00504500
H	-0.96605000	-3.63973100	1.83898200
H	-1.93321200	-2.32272300	2.52715000
H	-2.47990100	-3.99027500	2.69443500
H	-0.71707300	-5.47318200	-0.84465400
H	2.02335800	-4.96572900	-1.08335600
C	0.14517000	-2.30549200	-0.65607000
Ir	-0.39453800	-0.29956000	-0.37314000
H	-1.94192500	-0.64419800	-1.37302800

H	-1.41360200	-0.38582600	-1.94959600
P	-1.34347100	1.84133200	0.11744400
C	-2.74421000	1.77834100	1.28739200
C	-3.58332500	0.65857500	1.28561300
C	-3.05823000	2.86362700	2.11338100
C	-4.70494600	0.61811600	2.10558900
H	-3.36434300	-0.19303900	0.64004700
C	-4.18089400	2.81914200	2.93358800
H	-2.42470900	3.75068200	2.11541300
C	-5.00339200	1.69633600	2.93304600
H	-5.34315200	-0.26508100	2.09799100
H	-4.41402400	3.66673800	3.57499000
H	-5.87921200	1.66407100	3.57821500
C	-2.02365200	2.67882200	-1.36349900
C	-1.35426200	2.55811400	-2.58934000
C	-3.18807300	3.44950800	-1.29460100
C	-1.84225300	3.20379300	-3.72038300
H	-0.44021300	1.96601100	-2.65448100
C	-3.67477000	4.08781100	-2.43090300
H	-3.72556000	3.54776100	-0.35217200
C	-3.00424400	3.96655000	-3.64319900
H	-1.31623600	3.10531200	-4.66842800
H	-4.58454300	4.68155000	-2.36725200
H	-3.38880700	4.46480600	-4.53103500
C	-0.14864800	3.02044000	0.83258200
C	0.51057200	3.95388700	0.02829000
C	0.22967400	2.88343000	2.17401000
C	1.54211800	4.72804500	0.55385300
H	0.20841900	4.08827500	-1.01085800
C	1.24712900	3.66945000	2.69858200
H	-0.27414700	2.15736300	2.81298600
C	1.91299900	4.58576100	1.88632800
H	2.04659700	5.45543400	-0.08027400
H	1.52749200	3.56088000	3.74488200
H	2.71435300	5.19628100	2.29797300
C	3.24070000	0.47793400	2.75213200
C	3.24586900	0.98635900	1.46358900
C	2.17789000	0.71023000	0.60556500
C	1.05458600	-0.04890900	1.00768100
C	1.06878800	-0.56100900	2.30695500
C	2.15263700	-0.30043500	3.13314200
H	4.05246500	0.65300600	3.45121300
H	4.08127900	1.58710400	1.10827100
H	-1.35747000	-0.93001300	0.68709500
H	0.25597700	-1.17783400	2.68332600
N	2.17454400	-0.92743200	4.47016100
O	1.33151700	-1.77830300	4.70141100
O	3.04162900	-0.56467200	5.24479300
C	2.15866100	1.16428100	-0.78279300
O	1.23304700	0.85172500	-1.55151300
O	3.16666500	1.91399000	-1.17380700
C	3.13372700	2.40547700	-2.52949000
H	2.22697500	3.01558800	-2.64752000
H	3.05167200	1.54691000	-3.20988900

C	4.39362400	3.19537100	-2.74892200
H	5.28037700	2.55962800	-2.63903800
H	4.40070100	3.61751100	-3.75983700
H	4.46860700	4.02005300	-2.03074100

Substrate 14 – position 15 (ketone bound reactant)

1 1

C	-0.33391300	-4.60848000	0.08449600
C	0.97572000	-4.62509000	-0.24579000
N	-0.68618800	-3.27482800	0.24389000
N	1.39378800	-3.30528800	-0.28622300
C	2.74683500	-2.91795900	-0.57230400
C	3.10953100	-2.66285600	-1.89618900
C	3.64095200	-2.78097100	0.49659100
C	4.41504000	-2.23074800	-2.13510600
C	4.93140700	-2.34750900	0.20537400
C	5.33474400	-2.06093200	-1.10135800
H	4.72082000	-2.02691000	-3.16292300
H	5.64710100	-2.23250200	1.02136600
C	-2.01316000	-2.87592100	0.61242500
C	-2.98440800	-2.77335800	-0.38948800
C	-2.30089100	-2.66206400	1.96492400
C	-4.27695700	-2.41688700	-0.00646400
C	-3.60757700	-2.30593500	2.29480200
C	-4.60625100	-2.17589600	1.32676300
H	-5.04423300	-2.31140800	-0.77634000
H	-3.85747500	-2.14060300	3.34554800
C	-1.24312000	-2.78970700	3.01856600
H	-0.71357000	-3.75024000	2.95251100
H	-0.48639000	-1.99682700	2.91998400
H	-1.67970800	-2.71386700	4.02105500
C	-2.65098000	-3.04672300	-1.82510300
H	-1.72729800	-2.53841000	-2.13859200
H	-2.49077900	-4.11944000	-2.00322300
H	-3.46353400	-2.72253000	-2.48555900
C	-6.00388300	-1.80103600	1.71738600
H	-6.51452600	-1.25370000	0.91500400
H	-6.60775700	-2.69245700	1.93589800
H	-6.01810500	-1.17751800	2.62116200
C	6.72751300	-1.57807300	-1.37299400
H	6.93658000	-1.52753000	-2.44793000
H	6.88778600	-0.57544900	-0.95232800
H	7.47623500	-2.23786100	-0.91631600
C	3.21837100	-3.06604200	1.90691000
H	2.41018500	-2.39152500	2.22995100
H	2.84215900	-4.09164800	2.02599100
H	4.05740000	-2.93724200	2.59920200
C	2.12616800	-2.81490100	-3.01667000
H	1.63914500	-3.79953700	-3.00775400
H	1.32548800	-2.06317200	-2.94662600
H	2.61604000	-2.69062700	-3.98849300
H	1.65767300	-5.43887700	-0.45556000
H	-1.05560600	-5.40201500	0.22866900
C	0.37399900	-2.44759100	0.01771800
Ir	0.58989600	-0.38635600	0.09987000
H	1.40553000	-0.55933700	-1.22068100

H	2.05940400	-0.68753700	0.49449500
P	1.25323700	1.87369500	0.15553200
C	2.42522600	2.38094700	-1.15109700
C	3.41003700	1.46776200	-1.54676400
C	2.40696900	3.65657900	-1.72406400
C	4.35119700	1.82271200	-2.50537700
H	3.44266000	0.46891800	-1.10841100
C	3.34825400	4.00533600	-2.68776400
H	1.64958200	4.38178400	-1.42570000
C	4.31863100	3.08953300	-3.08160100
H	5.10588000	1.09904400	-2.81053800
H	3.32021300	4.99774900	-3.13362300
H	5.04984600	3.36382000	-3.83950400
C	2.07996000	2.34426400	1.71707500
C	2.03140900	1.48420300	2.81856800
C	2.73037800	3.57737500	1.83688000
C	2.62055700	1.85591100	4.02424500
H	1.53267800	0.51768100	2.72914400
C	3.31617400	3.94558500	3.04124000
H	2.78242000	4.25279500	0.98232600
C	3.26047500	3.08535800	4.13599400
H	2.58326600	1.18024500	4.87683000
H	3.82050600	4.90620500	3.12676100
H	3.72255100	3.37517400	5.07784600
C	-0.16683900	3.02223600	0.03789300
C	-0.71181200	3.61201100	1.18236500
C	-0.82680500	3.17418500	-1.18772800
C	-1.89232600	4.34804700	1.09910900
H	-0.20766100	3.50189600	2.14391700
C	-1.99861000	3.91641800	-1.26935100
H	-0.42065600	2.70818900	-2.08784400
C	-2.53861600	4.49814400	-0.12377200
H	-2.30091100	4.81505400	1.99448300
H	-2.49571100	4.03805200	-2.23067400
H	-3.45627700	5.08006100	-0.18871600
C	-4.47981400	0.99126500	-1.75851000
C	-4.99921500	1.41157000	-0.54238400
C	-4.20054600	1.30729900	0.58665200
C	-2.89988000	0.79331200	0.50218100
C	-2.40778300	0.40445700	-0.74845000
C	-3.19026800	0.49640900	-1.88765600
H	-6.01119100	1.80328500	-0.49563700
H	-4.60460300	1.62570000	1.54517600
H	-1.38663300	0.01974700	-0.87000200
H	-2.82403100	0.18956900	-2.86377500
C	-2.08057900	0.61553100	1.72349400
O	-0.95361100	0.11497200	1.68347200
C	-2.63100900	1.02374900	3.05456800
H	-2.89852400	2.08862400	3.05934700
H	-3.53844000	0.45101000	3.29070100
H	-1.87766000	0.83766100	3.82550100
N	-5.32947700	1.07243600	-2.96281200
O	-4.86422700	0.63066900	-3.99823400
O	-6.43254600	1.56999600	-2.83204800

Substrate 14 – position 16 (ketone bound transition state)

1 1

C	1.80535000	-3.91934300	-1.20978800
C	0.58290000	-4.37979700	-0.87297200
N	1.76551000	-2.53935400	-1.06152900
N	-0.18184600	-3.27508500	-0.53167000
C	-1.57704400	-3.39924100	-0.20476500
C	-1.96655600	-3.51781800	1.13122800
C	-2.49585800	-3.42076100	-1.26387000
C	-3.33208000	-3.64728700	1.39544700
C	-3.84358700	-3.54900500	-0.94621800
C	-4.28142300	-3.66722200	0.37627400
H	-3.65754600	-3.74443400	2.43285400
H	-4.57650700	-3.56818700	-1.75467700
C	2.88866300	-1.70637800	-1.38096100
C	3.98537700	-1.68865100	-0.50883500
C	2.87301200	-0.99715600	-2.58562100
C	5.05601300	-0.86150200	-0.83917200
C	3.96786400	-0.17894600	-2.86472600
C	5.06053400	-0.09001900	-2.00244700
H	5.91562000	-0.82129900	-0.16688200
H	3.97234500	0.39228300	-3.79546200
C	1.73449700	-1.11563200	-3.55302500
H	1.44856200	-2.16456000	-3.71527700
H	0.83998200	-0.58814300	-3.19251800
H	2.00599500	-0.68655800	-4.52403400
C	4.03164200	-2.54335100	0.72278000
H	3.08352500	-2.53543000	1.27837500
H	4.24564000	-3.59297500	0.47589300
H	4.82756600	-2.20991600	1.39948900
C	6.22671700	0.79701600	-2.31958000
H	7.11336700	0.20879400	-2.59189900
H	6.00975800	1.46888400	-3.15884900
H	6.51014200	1.41088000	-1.45343700
C	-5.74042800	-3.83530500	0.67656400
H	-6.34363600	-3.06313500	0.18073600
H	-6.10977200	-4.80498100	0.31647400
H	-5.94139900	-3.78666900	1.75347100
C	-2.04331000	-3.28883400	-2.68587100
H	-1.58903300	-2.30246100	-2.86465000
H	-1.28785200	-4.04150700	-2.95102900
H	-2.88530100	-3.40141800	-3.37720800
C	-0.97897100	-3.45768100	2.25647900
H	-0.01252600	-3.90941100	1.99758800
H	-0.78262500	-2.41303900	2.54433300
H	-1.36470600	-3.96874200	3.14552600
H	0.17030400	-5.37956300	-0.83863300
H	2.70178100	-4.42424800	-1.54469900
C	0.53816700	-2.12167100	-0.64534400
Ir	-0.25695600	-0.21115500	-0.27217900
H	-1.33183100	-1.10705400	0.43765700
H	-1.29487200	-0.57401300	-1.49236200

P	-1.66048700	1.68613200	0.03830900
C	-2.99763700	1.37310600	1.24078100
C	-3.66689900	0.14394200	1.19096600
C	-3.40055000	2.33510800	2.17246500
C	-4.70843000	-0.12106600	2.07089300
H	-3.37577100	-0.61246600	0.45989600
C	-4.44480500	2.06385300	3.05148900
H	-2.89515200	3.30002200	2.21810400
C	-5.09647400	0.83567100	3.00503700
H	-5.21086300	-1.08659100	2.02756500
H	-4.74789000	2.81639800	3.77675200
H	-5.90807900	0.62422200	3.69844900
C	-2.49085500	2.33524200	-1.44847500
C	-1.99802100	2.04829300	-2.72447200
C	-3.59586700	3.18261900	-1.30821400
C	-2.60516200	2.60502600	-3.84583900
H	-1.13659500	1.39226300	-2.83965500
C	-4.20133100	3.73150100	-2.43183300
H	-3.99031300	3.40904300	-0.31740300
C	-3.70585400	3.44343500	-3.70082500
H	-2.21878700	2.37781300	-4.83762300
H	-5.06410300	4.38443500	-2.31657900
H	-4.18208500	3.87317600	-4.58006600
C	-0.70270100	3.09809600	0.69477600
C	-0.38119100	4.18724100	-0.11912100
C	-0.14940100	3.01888600	1.98059400
C	0.47304300	5.18451200	0.34850800
H	-0.80058600	4.26034800	-1.12295700
C	0.69985700	4.01457000	2.44448900
H	-0.38750600	2.17335200	2.62829600
C	1.01738500	5.09748800	1.62525000
H	0.70715300	6.03579200	-0.28872300
H	1.11654500	3.94576900	3.44779000
H	1.68264700	5.87802300	1.98961300
C	3.11096600	0.16029100	2.71270800
C	3.89022900	1.16751300	2.16107700
C	3.46593500	1.71636000	0.96248800
C	2.28094700	1.28345500	0.35373100
C	1.46669100	0.28202100	0.94997000
C	1.92557600	-0.28019000	2.14297000
H	4.80543500	1.47949400	2.65503100
H	4.07927100	2.47545400	0.47919800
H	-0.11518800	0.01282200	1.31475800
H	1.37177800	-1.06884100	2.64968400
C	1.89524000	1.76534200	-0.96975500
O	0.94240700	1.21394800	-1.55159700
C	2.61017100	2.88686600	-1.64604700
H	2.58743200	3.78609400	-1.01482700
H	3.66298300	2.62885400	-1.82520400
H	2.12806400	3.10169100	-2.60399300
N	3.57913800	-0.49653200	3.95127500
O	2.94925700	-1.46454900	4.34055200
O	4.56882500	-0.03190600	4.48637200

Substrate 14 – position 17 (ketone bound C-H activated product)

1 1

C	1.61237600	-4.27065600	-0.44674200
C	0.33713200	-4.60393800	-0.15722300
N	1.65065100	-2.88755300	-0.54907700
N	-0.37564400	-3.41705700	-0.08341300
C	-1.77547200	-3.37411100	0.23317500
C	-2.16347600	-3.20737500	1.56532900
C	-2.70053000	-3.50875400	-0.81050400
C	-3.53049000	-3.11279400	1.82988300
C	-4.05149000	-3.39166300	-0.49560200
C	-4.48512200	-3.17908700	0.81623600
H	-3.85605100	-2.98915400	2.86439800
H	-4.79028000	-3.48375400	-1.29362300
C	2.88169000	-2.18468900	-0.76852600
C	3.72357900	-1.97716500	0.33070000
C	3.21703100	-1.79339900	-2.06672600
C	4.91403100	-1.29037400	0.10565300
C	4.42261000	-1.11279900	-2.23680700
C	5.27490800	-0.84218800	-1.16587000
H	5.57603800	-1.09208800	0.95100100
H	4.70704700	-0.79188700	-3.24131600
C	2.31803300	-2.08851700	-3.22877300
H	2.10834600	-3.16377400	-3.31648300
H	1.35210800	-1.57243000	-3.12910600
H	2.77622000	-1.76010700	-4.16887500
C	3.36938600	-2.48705200	1.69601100
H	2.31189800	-2.31915100	1.94459700
H	3.54868600	-3.56900400	1.77636100
H	3.97670800	-2.00121200	2.46870900
C	6.55729000	-0.09398400	-1.37029600
H	6.69941500	0.67378000	-0.59766300
H	7.42512400	-0.76491100	-1.31332100
H	6.58944100	0.39668600	-2.35086600
C	-5.94483600	-3.02770400	1.11942900
H	-6.14361300	-3.09601000	2.19535500
H	-6.32074100	-2.05477100	0.77255400
H	-6.54280100	-3.79760300	0.61599500
C	-2.25270900	-3.77446700	-2.21634800
H	-1.48445300	-3.06265900	-2.55356500
H	-1.80862800	-4.77501200	-2.31375400
H	-3.09541000	-3.71800300	-2.91376200
C	-1.16030900	-3.11617700	2.67459000
H	-0.34202800	-3.83855000	2.55455900
H	-0.70126000	-2.11721100	2.71807500
H	-1.63383700	-3.29850600	3.64547600
H	-0.14202400	-5.55960000	0.01141700
H	2.50360300	-4.86739900	-0.59046400
C	0.42629600	-2.33778100	-0.33188400
Ir	-0.27866500	-0.36046500	-0.36050000
H	-1.91548200	-1.06203300	-0.93205600
H	-1.53308700	-0.89962800	-1.64392900

P	-1.42702100	1.73458100	-0.19146100
C	-2.61694500	1.82689600	1.19004000
C	-3.33634300	0.67993000	1.54636200
C	-2.91903900	3.04294500	1.81307400
C	-4.33073700	0.74956400	2.51548800
H	-3.12596500	-0.27812800	1.06664900
C	-3.90692200	3.10505100	2.79040100
H	-2.38302500	3.94911900	1.53197000
C	-4.61302400	1.95940500	3.14305600
H	-4.88649000	-0.14772800	2.78403500
H	-4.12660100	4.05440800	3.27480700
H	-5.38637600	2.01115100	3.90690500
C	-2.44263600	2.09740200	-1.67218800
C	-1.95893600	1.74108600	-2.93816600
C	-3.68183500	2.73646100	-1.56790500
C	-2.70227700	2.02767800	-4.07806400
H	-0.99017000	1.24882600	-3.03283900
C	-4.42359500	3.01463800	-2.71142400
H	-4.07615100	3.01276600	-0.59081000
C	-3.93650700	2.66142400	-3.96557900
H	-2.31746600	1.74953800	-5.05752300
H	-5.38909400	3.50827700	-2.61886800
H	-4.52009700	2.88074400	-4.85759700
C	-0.32082600	3.17465100	-0.00251200
C	0.05926600	3.93086400	-1.11368800
C	0.26714700	3.44119000	1.24074200
C	1.01652200	4.93533100	-0.98433100
H	-0.40039100	3.74601400	-2.08499000
C	1.21924900	4.44451400	1.36625900
H	-0.02401300	2.86393900	2.11884600
C	1.60108800	5.18908500	0.25171600
H	1.29359100	5.53018400	-1.85354800
H	1.66818500	4.64257300	2.33821600
H	2.34621400	5.97598400	0.35258300
C	2.71630400	0.99394500	2.46736600
C	3.59270300	1.73871600	1.68524100
C	3.34361700	1.79463500	0.32539000
C	2.23550700	1.13160800	-0.21999800
C	1.32082700	0.40841600	0.59307500
C	1.59894500	0.34637100	1.96142600
H	4.43995400	2.23772500	2.14558200
H	4.01505100	2.36199200	-0.31837800
H	-0.96186400	-0.78495100	0.99319300
H	0.95655000	-0.19847600	2.64915500
C	1.95217300	1.13902000	-1.64855900
O	0.95459600	0.51387400	-2.06652900
C	2.79014200	1.89219100	-2.62753100
H	2.65001500	2.97200600	-2.47367300
H	3.85643100	1.67458100	-2.49441600
H	2.48903600	1.63327400	-3.64704200
N	3.00190800	0.86809300	3.91157700
O	2.35062000	0.05114200	4.54039700
O	3.87591500	1.58033500	4.37268800

Substrate 14 – position 15 (nitro bound reactant)

1 1

C	-1.41596500	-4.58130400	-0.59248200
C	-2.66926200	-4.07680900	-0.56490400
N	-0.55527300	-3.50536000	-0.42709700
N	-2.54744900	-2.70740400	-0.38442500
C	-3.67642500	-1.82661200	-0.26939500
C	-4.18140200	-1.55528900	1.00842500
C	-4.22203800	-1.27509300	-1.43108800
C	-5.26846900	-0.69147300	1.09918500
C	-5.31231800	-0.41666600	-1.28502100
C	-5.84680100	-0.11424500	-0.03355000
H	-5.68118200	-0.46483400	2.08382300
H	-5.75970400	0.02274700	-2.17875700
C	0.87168900	-3.61400500	-0.38128000
C	1.48199600	-3.89026100	0.84901100
C	1.59989500	-3.41478000	-1.55938900
C	2.87495800	-3.91863400	0.88267100
C	2.99068000	-3.46918800	-1.47349100
C	3.64358100	-3.69774800	-0.26193400
H	3.37456200	-4.11759300	1.83289600
H	3.58136300	-3.30868000	-2.37730400
C	0.91345200	-3.09951200	-2.85442200
H	0.13242800	-3.83289500	-3.09695900
H	0.41773900	-2.11623000	-2.81569700
H	1.62920000	-3.08319600	-3.68356100
C	0.66831000	-4.14212900	2.08284500
H	-0.08418700	-3.35740400	2.24635700
H	0.12604100	-5.09590500	2.01787500
H	1.30826800	-4.18507900	2.97112000
C	5.13806300	-3.64547700	-0.17635300
H	5.46680100	-2.64378000	0.14036000
H	5.53113600	-4.36034600	0.55638500
H	5.60942600	-3.85208400	-1.14413400
C	-7.01620900	0.81178000	0.10948000
H	-7.84684400	0.32774800	0.63950300
H	-6.74180500	1.70340800	0.69092300
H	-7.39194800	1.14674400	-0.86475100
C	-3.63977800	-1.56685200	-2.78036500
H	-2.62516400	-1.14929600	-2.87236200
H	-3.55553900	-2.64487300	-2.97379100
H	-4.25447200	-1.13101000	-3.57544900
C	-3.55466700	-2.14965700	2.23298600
H	-3.43414500	-3.23863200	2.14977800
H	-2.55262300	-1.73151900	2.41211300
H	-4.16179000	-1.94461000	3.12131600
H	-3.63954000	-4.54780700	-0.65460800
H	-1.04286200	-5.58994600	-0.71360200
C	-1.24049300	-2.33595600	-0.29348000
Ir	-0.55057900	-0.39568400	-0.07574400
H	-2.04752300	-0.08508100	0.16503200
H	-1.03699100	-0.15377900	-1.55152300

P	-0.26003900	1.95203200	-0.02302400
C	-1.86267900	2.80629600	0.22183800
C	-2.93937000	2.41743000	-0.58432400
C	-2.03735300	3.84091200	1.14357700
C	-4.16986600	3.04925600	-0.46354900
H	-2.81636200	1.61483000	-1.31363400
C	-3.27593900	4.46537300	1.26823200
H	-1.20551500	4.16112400	1.77046300
C	-4.34250400	4.07025700	0.46814900
H	-4.99693600	2.73819500	-1.10062200
H	-3.40446100	5.26571900	1.99452900
H	-5.30954300	4.56058800	0.56766300
C	0.40197800	2.72314300	-1.54031500
C	1.02947200	1.93843600	-2.51061300
C	0.30725400	4.10641800	-1.73308600
C	1.57847200	2.52655000	-3.64609000
H	1.07211800	0.85656000	-2.38029700
C	0.84866500	4.69191200	-2.87068300
H	-0.19502200	4.72572200	-0.98864500
C	1.48909200	3.90289400	-3.82430500
H	2.07340100	1.90824900	-4.39227800
H	0.76854300	5.76745300	-3.01611300
H	1.91374600	4.36391200	-4.71403600
C	0.80669500	2.57019400	1.33042200
C	1.94622200	3.34617600	1.10808100
C	0.48431300	2.18439100	2.63934000
C	2.74454400	3.73826600	2.18040700
H	2.21355800	3.64357600	0.09402000
C	1.28284500	2.57684700	3.70650600
H	-0.40750500	1.58149700	2.82235400
C	2.41568600	3.35697800	3.47714900
H	3.62519900	4.35295000	1.99886200
H	1.01927800	2.27626900	4.71891800
H	3.03783100	3.67083100	4.31349800
C	2.43871300	-0.32837900	1.48143300
C	3.56987200	0.30130100	1.98581500
C	4.50057400	0.80566700	1.08759500
C	4.31542900	0.65060800	-0.28983400
C	3.20101700	-0.04677100	-0.76224200
C	2.24505500	-0.52775000	0.11542700
H	3.67999600	0.43198400	3.05887900
H	5.36903300	1.33613600	1.47313300
H	3.11295000	-0.20683000	-1.83555100
H	1.46703100	-1.21546800	-0.26186700
C	5.25960200	1.20901800	-1.31869000
O	5.01716600	1.04836600	-2.49774100
C	6.46924500	1.96365800	-0.84659700
H	6.17829600	2.84150400	-0.25331900
H	7.10593200	1.33623300	-0.20846100
H	7.04465800	2.29258800	-1.71535900
N	1.43054900	-0.77426800	2.42953500
O	0.25370200	-0.89621100	2.03844500
O	1.76144200	-1.00068900	3.57277800

Substrate 14 – position 16 (nitro bound transition state)

1 1

C	-1.45843500	-4.57539500	-0.60701000
C	-2.69215400	-4.08114300	-0.84988700
N	-0.64072600	-3.48850000	-0.33592400
N	-2.60675600	-2.70334200	-0.71736600
C	-3.73286100	-1.83239000	-0.91703800
C	-4.54841000	-1.52957200	0.17618100
C	-3.96676200	-1.33050900	-2.20146600
C	-5.62832500	-0.67607700	-0.04774300
C	-5.06176400	-0.48735600	-2.37270300
C	-5.90363600	-0.15170800	-1.31003400
H	-6.27520400	-0.41648300	0.79201300
H	-5.26717500	-0.08487600	-3.36624000
C	0.76583800	-3.60670700	-0.06589700
C	1.17765700	-3.92169000	1.23648900
C	1.66902900	-3.41875300	-1.11736600
C	2.54831500	-3.97795200	1.47885500
C	3.02942100	-3.48700100	-0.81871900
C	3.48729700	-3.74940700	0.47099600
H	2.89273300	-4.19576600	2.49168600
H	3.75290300	-3.32643300	-1.62048100
C	1.22067300	-3.13885600	-2.52095200
H	0.24623200	-3.59027800	-2.74744400
H	1.12954500	-2.05758000	-2.71331600
H	1.94918200	-3.52555300	-3.24280300
C	0.19061200	-4.19475700	2.33195600
H	-0.64468300	-3.48230600	2.32153400
H	-0.23707600	-5.20361200	2.24275000
H	0.67225100	-4.12602100	3.31372000
C	4.95484400	-3.80622900	0.76943400
H	5.17534500	-3.40399800	1.76664500
H	5.32580100	-4.84011300	0.75026300
H	5.53662200	-3.23560000	0.03521000
C	-7.08777800	0.73981000	-1.53483000
H	-7.51384000	1.09397400	-0.58801100
H	-6.82287200	1.61615300	-2.14123100
H	-7.88623100	0.21070900	-2.07280400
C	-3.06399700	-1.67324100	-3.34779600
H	-2.06392800	-1.23357800	-3.21380100
H	-2.92267700	-2.75787900	-3.45274600
H	-3.46891500	-1.29503200	-4.29272200
C	-4.25825300	-2.07511500	1.54082900
H	-4.17787800	-3.17091700	1.53880300
H	-3.30592300	-1.68549400	1.93239400
H	-5.04771900	-1.79937500	2.24804600
H	-3.62782400	-4.56266800	-1.10225500
H	-1.07078200	-5.58558900	-0.60175400
C	-1.34257400	-2.32702700	-0.39533400
Ir	-0.66342300	-0.38564300	-0.03400100
H	-2.21879900	-0.23123700	0.43509100
H	-1.32841900	0.08122400	-1.39231000

P	-0.61397200	1.97314200	0.44798200
C	-2.22633300	2.66505000	0.96333200
C	-3.38431500	2.25585000	0.29342000
C	-2.31329400	3.66605900	1.93587400
C	-4.60817100	2.84097000	0.59403400
H	-3.33545800	1.46819900	-0.46022400
C	-3.54349400	4.24010000	2.24045200
H	-1.42166500	3.99406800	2.46949200
C	-4.69070000	3.83103400	1.56910100
H	-5.50273200	2.51369600	0.06508500
H	-3.60373600	5.01075500	3.00645300
H	-5.65147600	4.28322400	1.80768300
C	-0.11617300	3.05482000	-0.93748100
C	0.10060600	2.54673800	-2.21916800
C	0.01089700	4.43276900	-0.71739100
C	0.46511400	3.39412500	-3.26126100
H	-0.02444900	1.48141000	-2.40671900
C	0.37114800	5.27712400	-1.75880400
H	-0.16962500	4.85001300	0.27354200
C	0.60350700	4.75762800	-3.03064500
H	0.64132000	2.98423700	-4.25361800
H	0.46869200	6.34586200	-1.57856700
H	0.88876800	5.42080100	-3.84489500
C	0.54333500	2.33143600	1.81104500
C	1.80372900	2.89045800	1.58133600
C	0.21962300	1.86955100	3.09433900
C	2.72323300	2.99065700	2.62101900
H	2.07554400	3.23744400	0.58466100
C	1.14167000	1.97175200	4.12840800
H	-0.75603700	1.41981900	3.28606500
C	2.39580700	2.53059600	3.89238700
H	3.70187800	3.42917400	2.43362300
H	0.88178800	1.60733400	5.12021500
H	3.11783400	2.60851700	4.70298100
C	3.39161800	-0.40502700	1.52909500
C	4.24569900	0.09417100	0.56691900
C	3.72332600	0.46482500	-0.68026500
C	2.36832100	0.31441800	-0.96197300
C	1.47017300	-0.19467200	-0.01947900
C	2.03538800	-0.53339600	1.22079700
H	3.73805800	-0.69106100	2.51962900
H	5.30624400	0.21335700	0.76980100
H	2.02955200	0.61197000	-1.95287800
H	0.33458600	-0.89228500	-1.18806300
N	1.16295800	-1.00173600	2.25778500
O	-0.07223400	-1.04261700	1.99727300
O	1.58519000	-1.33315600	3.34271700
C	4.57553800	1.04209400	-1.76390900
O	4.14411600	1.37820100	-2.84338900
O	5.85261100	1.14739400	-1.39464000
C	6.74581800	1.70794000	-2.37751900
H	6.36724300	2.69695800	-2.66470600
H	6.71619900	1.07447100	-3.27325100
C	8.11508300	1.76944100	-1.75783000

H	8.46242000	0.76999600	-1.47144300
H	8.83217200	2.18778700	-2.47291500
H	8.11423700	2.40378700	-0.86382600

Substrate 14 – position 17 (nitro bound C-H activated product)

1 1

C	-1.37648400	-4.40690800	0.21511500
C	-0.07724200	-4.63088000	0.50532500
N	-1.48898300	-3.06268000	-0.10918900
N	0.57679800	-3.41814700	0.35429400
C	1.98334100	-3.24948400	0.58934900
C	2.87108000	-3.49649400	-0.46242800
C	2.40982600	-2.81115000	1.84973800
C	4.22292500	-3.22632400	-0.24435800
C	3.76846900	-2.55693100	2.01528400
C	4.68706000	-2.74557500	0.97895200
H	4.93289500	-3.40172900	-1.05416700
H	4.12478800	-2.20771200	2.98617100
C	-2.76071500	-2.45115200	-0.37624600
C	-3.18897000	-2.32627400	-1.70134200
C	-3.54532000	-2.06329900	0.71629300
C	-4.42265000	-1.71514000	-1.91947100
C	-4.77173500	-1.46344700	0.44102500
C	-5.21898100	-1.26709600	-0.86591400
H	-4.76546500	-1.57744800	-2.94611000
H	-5.39251000	-1.12855000	1.27491900
C	-3.10873700	-2.30709500	2.13019100
H	-3.35115500	-3.33222200	2.44701100
H	-2.02691400	-2.17908700	2.26696400
H	-3.61556000	-1.62721800	2.82508300
C	-2.37033100	-2.84382600	-2.84563800
H	-1.37351700	-2.38559700	-2.88377600
H	-2.22688600	-3.93135200	-2.77239500
H	-2.86463300	-2.63558500	-3.80089200
C	-6.53324400	-0.59654700	-1.12839600
H	-6.53838300	-0.08818200	-2.10035300
H	-7.35819000	-1.32208300	-1.13735400
H	-6.76526200	0.14486300	-0.35271300
C	6.14122900	-2.45644700	1.19724600
H	6.72215600	-2.58260800	0.27634400
H	6.29495900	-1.43157700	1.56107800
H	6.56982400	-3.12831200	1.95279700
C	1.44693800	-2.62185100	2.98281300
H	0.72226400	-1.82052300	2.77629800
H	0.86283400	-3.53185000	3.17846800
H	1.97802900	-2.36144100	3.90485300
C	2.38887100	-4.00593000	-1.78737100
H	1.92015300	-4.99536700	-1.69694000
H	1.63303500	-3.34421900	-2.23722500
H	3.21796300	-4.09568000	-2.49728000
H	0.45572700	-5.52418600	0.80406200
H	-2.24136400	-5.05731600	0.20888000
C	-0.28804700	-2.43239300	-0.03296100
Ir	0.31613800	-0.43964200	-0.35009100
H	1.62923700	-1.04737800	-1.51094000
H	1.97528700	-1.17964100	-0.77501500

P	1.32866700	1.72761600	-0.37607900
C	2.91812800	1.74785500	-1.28583500
C	3.90570100	0.84686400	-0.86395200
C	3.19975100	2.63751000	-2.32310900
C	5.14550600	0.82594100	-1.48790900
H	3.71298900	0.16467900	-0.03065300
C	4.44473800	2.60975400	-2.94834100
H	2.45092500	3.36055900	-2.64416000
C	5.41434500	1.70369800	-2.53642100
H	5.90800900	0.12462100	-1.15267200
H	4.65464400	3.30516600	-3.75859800
H	6.38530400	1.68415700	-3.02739200
C	1.82616100	2.41263800	1.24517800
C	1.56255300	1.76417100	2.45213100
C	2.52146200	3.63014500	1.26145500
C	1.97196800	2.32638500	3.65862900
H	1.03498500	0.81237500	2.45319800
C	2.92628100	4.19043900	2.46488900
H	2.74748800	4.14119700	0.32458400
C	2.64994700	3.53935700	3.66578200
H	1.75370300	1.81376900	4.59340200
H	3.46520200	5.13581200	2.46673700
H	2.97030900	3.97879800	4.60847400
C	0.25264700	2.99542600	-1.12358900
C	-0.35674000	3.98132800	-0.34112500
C	-0.09416500	2.88231700	-2.47694700
C	-1.28598900	4.84805900	-0.90771600
H	-0.10922300	4.07258700	0.71583300
C	-1.02116800	3.75250100	-3.03807600
H	0.34562500	2.09647900	-3.09338500
C	-1.61931600	4.73560400	-2.25355900
H	-1.74998600	5.61642500	-0.29210500
H	-1.28447400	3.65389700	-4.08932400
H	-2.34657900	5.41509700	-2.69378800
C	-2.27031400	0.86626600	-0.60933100
C	-3.43663400	1.58268800	-0.34047900
C	-3.72458800	1.89288800	0.97455800
C	-2.86447200	1.45256200	1.99319600
C	-1.71212800	0.72944700	1.68472200
C	-1.35860900	0.42329700	0.36895100
H	-4.08319800	1.87980400	-1.16326600
H	-4.62220100	2.46131900	1.20956100
H	-1.09420400	0.40630100	2.52115900
H	1.00837200	-0.60195900	1.05227000
C	-3.14616000	1.70192500	3.44890300
O	-2.43616000	1.19921800	4.29782100
C	-4.31937700	2.56850100	3.81427400
H	-4.24176000	3.55999700	3.34889600
H	-5.26131900	2.12171700	3.46809900
H	-4.35606200	2.67858100	4.90088500
N	-1.97975500	0.53685300	-1.97500600
O	-0.90205700	-0.08187600	-2.19924500
O	-2.73151000	0.83225100	-2.87719500