

# Supplementary Materials

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

Substrate 12—Position 15 (nitro Bound Reactant)

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|   |             |             |             |
|---|-------------|-------------|-------------|
| 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)

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|   |             |             |             |
|---|-------------|-------------|-------------|
| 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)

1 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| 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 |