Supporting Information

Catalyst-Controlled and Tunable, Chemoselective Silver-Catalyzed Intermolecular Nitrene Transfer: Experimental and Computational Studies

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I. Materials and Methods.

All glassware was either oven-dried overnight at 130 °C or flame-dried under a stream of dry nitrogen prior to use. Unless otherwise specified, reagents were used as obtained from the vendor without further purification. Tetrahydrofuran and diethyl ether were freshly distilled from purple Na/benzophenone ketyl. Dichloromethane, acetonitrile and toluene were dried over CaH_2 and freshly distilled prior to use. All other solvents were purified in accordance with "Purification of Laboratory Chemicals".[1] Air- and moisture-sensitive reactions were performed using standard Schlenk techniques under an atmosphere of nitrogen. Analytical thin layer chromatography (TLC) was performed utilizing pre-coated silica gel 60 F_{254} plates containing a fluorescent indicator, while preparative chromatography was performed *via* Still's method[2] using SilicaFlash P60 silica gel (230-400 mesh) or, when specified, Davisil grade 635 silica gel (60-100 mesh). Unless otherwise stated, the mobile phases for column chromatography were mixtures of hexanes/ethyl acetate. Columns were typically run using a gradient method, beginning with 100% hexanes and gradually increasing the polarity using ethyl acetate. Various stains were used to visualize reaction products, including *p*-anisaldehyde, $KMnO_4$, ceric ammonium molybdate (CAM stain) and iodine powder. When specified, column chromatography was performed on a CombiFlash Rf-200 system equipped with an ELSD detector with Redisep Gold normal phase silica columns (Teledyne ISOC Inc., Lincoln, NE).

^{1}H NMR and ^{13}C NMR spectra were obtained using Bruker-300, Varian-300, Varian Inova-500, or Varian Unity-500 spectrometers. For ^{1}H NMR, chemical shifts are reported relative to residual protiated solvent peaks (δ 7.26, 2.49, 7.15 and 7.09 ppm for $CDCl_3$, $(CD_3)_2SO$, C_6D_6 and $CD_3C_6D_5$ respectively). ^{13}C NMR spectra were measured at either 125 MHz or 75 MHz on the same instruments noted above for recording ^{1}H NMR spectra. Chemical shifts were again

reported relative to residual protiated solvent peaks (δ 77.2, 39.5, 128.0 and 137.9 ppm for $CDCl_3$, $(CD_3)_2SO$, C_6D_6, and $CD_3C_6D_5$, respectively). High-pressure liquid chromatography (HPLC) analyses were performed at 215 and 225 nm using a Shimadzu HPLC, Model LC-20AB. Further details are given in Section VII. Accurate mass measurements were acquired at the University of Wisconsin, Madison using a Micromass LCT (electrospray ionization, time-of-flight analyzer or electron impact methods). The NMR and Mass Spectrometry facilities are funded by the NSF (CHE-9974839, CHE-9304546, CHE-9208463, CHE-9629688) and the University of Wisconsin, as well as the NIH (RR08389-01).

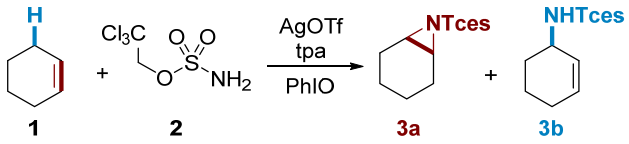
II. Synthesis of Sulfamate Substrates.

General procedure for the synthesis of sulfamates. Formic acid (0.49 mL, 13 mmol, 2.5 equiv) was added dropwise to chlorosulfonyl isocyanate (3.0 equiv) in an ice bath with vigorous stirring. Gas was evolved and the reaction mixture solidified within 5 min. To the solid was added 10.4 mL of CH_3CN and the resulting clear solution was stirred in an ice bath for 30 min, allowed to warm to rt and stirred for an additional 4 h. The flask was placed in an ice bath and to the cold solution was added 5.2 mmol of the alcohol substrate dissolved in 8.7 mL of dimethylacetamide. The solution was warmed to rt and the mixture was stirred for 1 h. The reaction was quenched by the addition of 10 mL of H_2O. The aqueous layer was extracted with 3 x 50 mL of Et_2O, the combined organic layers washed with 5 x 20 ml H_2O, 1 x 25 mL saturated aqueous sodium chloride, dried over $MgSO_4$, filtered and concentrated under reduced pressure. The crude products were purified by silica gel column chromatography using a hexane/EtOAc gradient.

III. Reaction Optimization: Oxidant Loading and Counteranion Effects.

Using the general procedure described above, the PhIO loading was optimized.

Table S1. Optimization of PhIO loading.

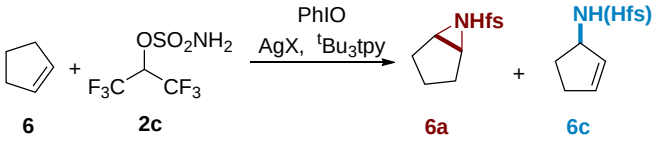


1 **2** **3a** **3b**

Entry	PhIO (equiv)	3a	3b	3a:3b
1	3.5	34%	45%	1:1.3
2	2.0	26%	48%	1:1.8
3	1.2	14%	46%	1:3.3

[a]Total NMR yield; 1,1,1,2-tetrachloroethane as the internal standard. Average of two runs. Conditions: 5 equiv **1**, 1 equiv **2**, 10 mol% AgOTf, 12 mol% tpa, 4 Å MS, CH_2Cl_2 (0.06 M), rt.

Table S2. Optimization of the counteranion for the Ag(I) salt in aziridination.

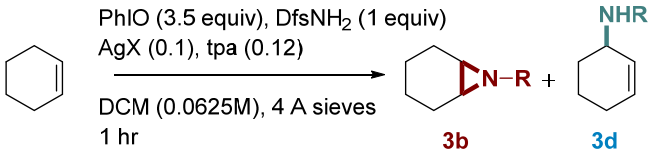


6 **2c** **6a** **6c**

Entry	X =	Yield (%)[a]	6a:6b
1	NO_3	75	4.0 : 1
2	BF_4	42	3.5 : 1
3	TFA	89	4.0 : 1
4	OTs	75	4.7 : 1
5	SbF_6[b]	>99	4.3 : 1
6	OTf	85	4.2 : 1

[a]Total NMR yield; 1,3,5-mesitylene as the internal standard. [b]Run under N_2. Conditions: 5 equiv **1**, 1 equiv **2**, 10 mol% AgX, 12 mol% $^tBu_3tpy$, 4 Å MS, CH_2Cl_2 (0.06 M), rt, absence of light.

Table S3. Optimization of the counteranion for the Ag(I) salt in amination.



entry	X =	3b yield (%)[a]	3d Am:Az
1	OTf	50	6.5 : 1
2	OTs	32	4.6 : 1
3	TFA	20	2.0 : 1
4	NO_3	26	3.5 : 1
5	SbF_6	68	5.3 : 1
6	BF_4	35	5.1 : 1
7	OAc	14	3.4 : 1

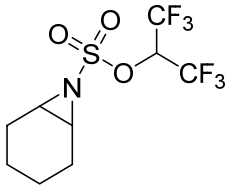
[a]Total NMR yield; 1,3,5-mesitylene as the internal standard. Conditions: 5 equiv **1**, 1 equiv **2**, 10 mol% AgX, 12 mol% tpa, 4 Å MS, CH_2Cl_2 (0.06 M), rt, absence of light, N_2 atmosphere.

IV. Synthesis of Amination Products.

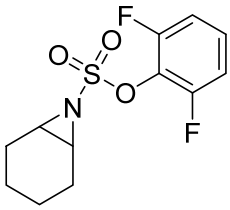
For best results, the silver to ligand ratio needs to be exact. Both silver triflate and $^tBu_3$tpy are highly hydroscopic and will not give good, reproducible results if they are not completely dry. Silver reagents should be stored in a dry box and the ligands in a standard dessicator. Alternatively, the reaction can be carried out in a glove box, although this is not necessary as long as the quality of the reagents is properly maintained.

General procedure for Ag-catalyzed amination. A pre-dried reaction flask was charged with silver triflate (6.4 mg, 0.025 mmol, 0.1 equiv) and ligand (12.0 mg $^tBu_3$tpy or 8.7 mg tpa, 0.03 mmol, 0.12 equiv). Dichloromethane (4 mL) was added to the flask and the mixture was stirred vigorously for 20 min. The substrate (1.25 mmol, 5 equiv), nitrene precursor (0.25 mmol, 1 equiv) and 4 Å molecular sieves (1 mmol substrate/g of sieves) was then added to the reaction flask. Iodosobenzene (193 mg for aziridination, 0.88 mmol, 3.5 equiv or 66 mg for C—H

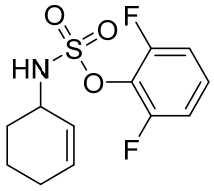
insertion, 0.30 mmol, 1.2 equiv) was added in one portion and the reaction mixture was allowed to stir at rt for 4 h (aziridination) or 1 h (C—H insertion). The reaction mixture was filtered through a glass frit and the filtrate concentrated under reduced pressure. The crude products were purified by silica gel column chromatography. Products formed in sufficient amounts and isolated in sufficient purities were characterized and the data was reported; those forming in trace amounts were compared to analogous compounds to infer identity due to similar key chemical shifts and *J*-couplings for aziridine products, as well as similar key values shared by allylic C-H insertion products.



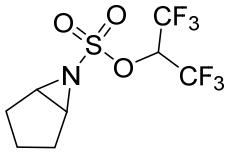
Compound 3a. The product was purified by column chromatography using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in 84% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.21 (hept, *J* = 5.6 Hz, 1H), 3.11 – 3.06 (m, 2H), 1.96 – 1.87 (m, 2H), 1.86 – 1.78 (m, 2H), 1.43 – 1.32 (m, 2H), 1.29 – 1.17 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 118.9 (q, *J* = 285.5 Hz), 72.56 (hept, *J* = 35.3 Hz), 42.1, 21.4, 18.0. HRMS (ESI) m/z calculated for $C_9H_{11}F_6NO_3S$ $[M + NH_4]^+$ 345.0703, found 345.0705.



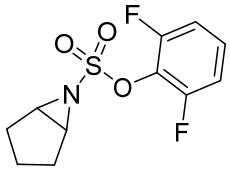
Compound 3b. The product was purified by column chromatography with Davisil silica using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in 10% yield as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (tt, *J* = 8.6, 5.9 Hz, 1H), 7.02 (dd, *J* = 8.6, 7.6 Hz, 2H), 3.23 – 3.15 (m, 2H), 2.06 (dt, *J* = 15.1, 6.7 Hz, 2H), 1.93 – 1.83 (m, 2H), 1.51 – 1.42 (m, 2H), 1.35 – 1.23 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.9 (d, *J* = 2.6 Hz), 154.9 (d, *J* = 2.7 Hz), 127.6 (t, *J* = 9.1 Hz), 112.5 (dd, *J* = 18.4, 3.9 Hz), 42.7, 22.6, 19.2. HRMS (ESI) m/z calculated for $C_{12}H_{13}F_2NO_3S$ $[M + H]^+$ 290.0657, found 290.0654.



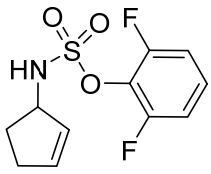
Compound 3d. The product was purified by column chromatography with Davisil silica using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in 42% yield as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21 (tt, *J* = 8.6, 5.9 Hz, 1H), 7.01 (dd, *J* = 8.6, 7.6 Hz, 2H), 5.95 (dtd, *J* = 9.5, 3.7, 1.7 Hz, 1H), 5.78 (ddt, *J* = 10.0, 4.0, 2.3 Hz, 1H), 4.72 (d, *J* = 7.5 Hz, 1H), 4.27 – 4.19 (m, 1H), 2.11 – 1.95 (m, 3H), 1.88 – 1.79 (m, 1H), 1.74 – 1.65 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1 (d, *J* = 3.2 Hz), 155.1 (d, *J* = 3.2 Hz), 132.8, 127.2 (t, *J* = 9.0 Hz), 126.0, 112.5 (dd, *J* = 18.3, 4.0 Hz), 50.9, 29.7, 24.6, 19.0. HRMS (ESI) *m/z* calculated for $C_{12}H_{13}F_2NO_3S$ $[M + NH_4]^+$ 307.0923, found 307.0917.



Compound 6a. The product was purified by column chromatography using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in 61% yield as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.25 (hept, *J* = 5.6 Hz, 1H), 3.49 (d, *J* = 1.5 Hz, 2H), 2.11 (dd, *J* = 13.6, 8.0 Hz, 2H), 1.76 – 1.62 (m, 3H), 1.48 – 1.33 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 119.9 (q, *J* = 283.8 Hz), 73.6 (hept, *J* = 35.4 Hz), 49.7, 26.8, 19.0. HRMS (ESI) m/z calculated for $C_8H_9F_6NO_3S$ $[M + NH_4]^+$ 331.0546, found 331.0542.

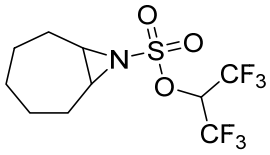


Compound 6b. The product was purified by column chromatography using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in 13% yield as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (tt, *J* = 8.5, 5.1 Hz, 1H), 7.01 (t, *J* = 8.3 Hz, 1H), 3.53 (s, 1H), 2.16 (dd, *J* = 13.6, 7.8 Hz, 2H), 1.76 – 1.60 (m, 2H), 1.52 – 1.35 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.9 (d, *J* = 3.1 Hz), 154.9 (d, *J* = 3.1 Hz), 127.7 (t, *J* = 9.2 Hz), 112.5 (dd, *J* = 18.3, 4.1 Hz), 49.2, 26.9, 19.1. HRMS (ESI) m/z calculated for $C_{11}H_{11}F_2NO_3S$ $[M + NH_4]^+$ 293.0766, found 293.0767.

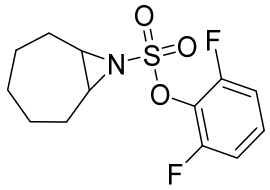


Compound 6d. The product was purified by column chromatography using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in 35% yield as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21 (tt, *J* = 8.6, 5.9 Hz, 1H), 7.01 (dd, *J* = 8.6, 7.7 Hz, 2H), 6.05 (dt, *J* =

5.9, 2.1 Hz, 1H), 5.84 (dt, *J* = 5.6, 2.3 Hz, 1H), 4.77 (dddt, *J* = 8.3, 6.4, 4.3, 2.1 Hz, 1H), 4.71 (d, *J* = 8.5 Hz, 1H), 2.50 (dddt, *J* = 16.0, 9.2, 4.6, 2.3 Hz, 1H), 2.42 (dtd, *J* = 12.4, 7.9, 4.2 Hz, 1H), 2.35 (dddd, *J* = 18.2, 8.5, 4.4, 2.2 Hz, 1H), 1.89 (ddt, *J* = 12.7, 8.4, 4.3 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1 (d, *J* = 3.2 Hz), 155.1 (d, *J* = 3.2 Hz), 136.4, 129.7, 127.3 (t, *J* = 9.2 Hz), 112.5 (dd, *J* = 18.4, 4.0 Hz), 61.7, 31.3, 30.9. HRMS (ESI) m/z calculated for $C_{11}H_{11}F_2NO_3S$ $[M + NH_4]^+$ 293.0766, found 293.0762.

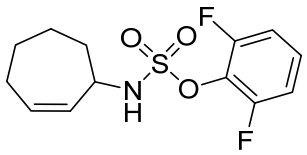


Compound 7a. The product was purified by column chromatography using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in 59% yield as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.29 (hept, *J* = 5.5 Hz, 1H), 3.17 – 3.12 (m, 2H), 2.06 – 1.93 (m, 4H), 1.69 – 1.47 (m, 5H), 1.28 (tdd, *J* = 8.5, 6.8, 3.4 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 119.9 (q, *J* = 283.5 Hz), 73.5 (hept, *J* = 35.5 Hz), 47.7, 30.8, 27.8, 24.9. HRMS (ESI) *m/z* calculated for $C_{10}H_{13}F_6NO_3S$ $[M + NH_4]^+$ 359.0859, found 359.0856.

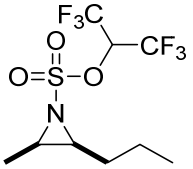


Compound 7b. The product was purified by column chromatography with Davisil silica using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in 20% yield as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (tt, *J* = 8.6, 5.9 Hz, 1H), 7.01 (t, *J* = 8.1 Hz, 2H), 3.19 – 3.13 (m, 2H), 2.09 – 1.89 (m, 2H), 1.67 – 1.45 (m, 5H), 1.33 – 1.22 (m, 2H). ^{13}C

NMR (126 MHz, $CDCl_3$) δ 156.9 (d, *J* = 2.7 Hz), 154.9 (d, *J* = 2.8 Hz), 127.6 (t, *J* = 9.1 Hz), 112.5 (dd, *J* = 18.3, 3.8 Hz), 47.1, 31.0, 28.0, 25.0. HRMS (ESI) *m/z* calculated for $C_{13}H_{15}F_2NO_3S$ $[M + H]^+$ 304.0814, found 304.0814.

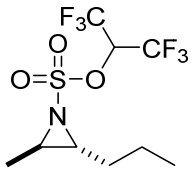


Compound 7d. The product was purified by column chromatography with Davisil silica using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in 24% yield as a white solid. ^1H NMR (500 MHz, $CDCl_3$) δ 7.21 (tt, *J* = 8.5, 5.9 Hz, 1H), 7.00 (t, *J* = 8.2 Hz, 2H), 5.89 (dddd, *J* = 11.9, 7.1, 5.3, 2.0 Hz, 1H), 5.80 – 5.74 (m, 1H), 4.81 (d, *J* = 7.8 Hz, 1H), 4.43 – 4.36 (m, 1H), 2.26 – 2.09 (m, 1H), 2.06 (ddd, *J* = 10.0, 7.0, 3.5 Hz, 1H), 1.96 (dtt, *J* = 11.3, 8.3, 3.9 Hz, 1H), 1.83 – 1.64 (m, 3H), 1.50 – 1.39 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1 (d, *J* = 3.2 Hz), 155.0 (d, *J* = 3.1 Hz), 133.4, 133.0, 127.2 (t, *J* = 9.1 Hz), 112.5 (dd, *J* = 18.3, 3.9 Hz), 56.4, 34.1, 28.3, 26.9, 26.5. HRMS (ESI) *m/z* calculated for $C_{13}H_{15}F_2NO_3S$ $[M + NH_4]^+$ 321.1079, found 321.1084.

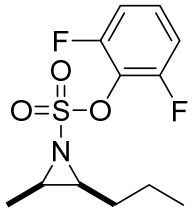


Compound *syn*-8a. The product was purified by column chromatography using a 0→5% gradient of EtOAc in hexanes with 1% increments and obtained as a clear, colorless oil. ^1H NMR (400 MHz, $CDCl_3$) δ 5.25 (hept, *J* = 5.6 Hz, 1H), 3.04 (dq, *J* = 7.5, 5.9 Hz, 1H), 2.97 – 2.90 (m, 1H), 1.63 – 1.44 (m, 4H), 1.31 (d, *J* = 5.9 Hz, 3H), 0.99 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz,

$CDCl_3$) δ 119.9 (q, *J* = 283.4 Hz), 73.4 (hept, *J* = 35.3 Hz), 47.8, 43.6, 28.1, 20.1, 13.7, 11.6. HRMS (ESI) *m/z* calculated for $C_9H_{13}F_6NO_3S$ $[M + NH_4]^+$ 347.0859, found 347.0860.

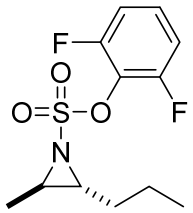


Compound *anti*-8a. The product was purified by column chromatography using a 0→5% gradient of EtOAc in hexanes with 1% increments and obtained as a clear, colorless oil. ^1H NMR (500 MHz, $CDCl_3$) δ 5.26 (hept, *J* = 5.6 Hz, 1H), 2.84 – 2.78 (m, 1H), 2.78 – 2.73 (m, 1H), 1.84 – 1.74 (m, 1H), 1.61 – 1.53 (m, 2H), 1.51 (d, *J* = 5.9 Hz, 3H), 1.50 – 1.42 (m, 1H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 119.9 (q, *J* = 282.7 Hz), 73.4 (hept, *J* = 35.4 Hz), 51.7, 46.8, 31.7, 19.9, 14.6, 13.6. HRMS (ESI) *m/z* calculated for $C_9H_{13}F_6NO_3S$ $[M + NH_4]^+$ 347.0859, found 347.0863.

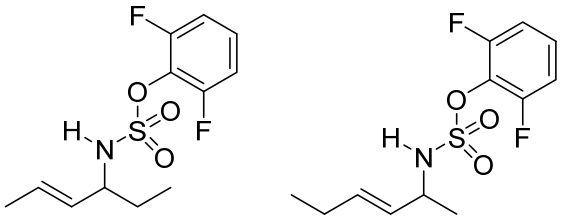


Compound *syn*-8b. The product was purified by column chromatography using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained as a clear, colorless oil. ^1H NMR (500 MHz, $CDCl_3$) δ 7.23 (tt, *J* = 8.5, 5.7 Hz, 1H), 7.01 (t, *J* = 8.1 Hz, 2H), 3.13 – 3.07 (m, 1H), 3.01 – 2.96 (m, 1H), 1.67 – 1.46 (m, 4H), 1.35 (d, *J* = 5.9 Hz, 3H), 0.99 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.9 (d, *J* = 3.1 Hz), 154.9 (d, *J* = 3.2 Hz), 127.6 (t, *J* = 9.2 Hz),

112.5 (dd, J = 18.2, 4.1 Hz), 47.3, 43.2, 28.3, 20.2, 13.7, 11.8. HRMS (ESI) *m/z* calculated for $C_9H_{13}F_6NO_3S$ $[M + NH_4]^+$ 309.1079, found 309.1069.



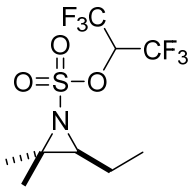
Compound *anti*-8b. The product was purified by column chromatography using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (tt, J = 8.6, 5.9 Hz, 1H), 7.01 (t, J = 8.2 Hz, 2H), 2.85 – 2.75 (m, 2H), 1.92 – 1.81 (m, 1H), 1.63 – 1.56 (m, 2H), 1.55 (d, J = 5.7 Hz, 3H), 1.52 – 1.44 (m, 1H), 0.97 (t, J = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0, 155.0, 127.5 (t, J = 9.1 Hz), 112.5 (dd, J = 18.5, 3.8 Hz), 51.3, 46.4, 31.7, 20.0, 14.7, 13.7. HRMS (ESI) *m/z* calculated for $C_{12}H_{19}F_2N_2O_3S$ $[M + NH_4]^+$ 309.1079, found 347.1077.



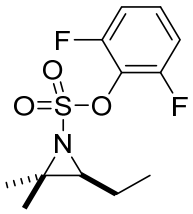
8d **8e**

Compound 8d and e. The products were purified by column chromatography using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained as a clear, colorless oil in a 1.7:1 ratio. Assignments were made for isolable signals with the aid of HSQC data. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 – 7.17 (m, 2H; 1H each product), 7.03 – 6.97 (m, 4H; 2H each product), 5.83 – 5.71 (m, 2H; vinyl 1H each product), 5.49 (ddt, J = 15.4, 6.4, 1.7 Hz, 0.6H; 1H **8e**), 5.40

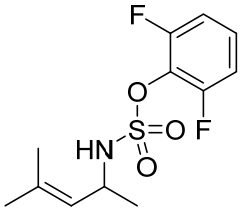
(ddq, J = 15.3, 7.6, 1.7 Hz, 1H, **8d**), 4.71 – 4.63 (m, 1.6H; 1H each product), 4.26 (h, J = 6.8, 6.2 Hz, 0.6H; 1H **8e**), 4.01 (p, J = 7.3 Hz, 1H **8d**), 2.11 – 2.00 (m, 1.6H; 1 H each product), 1.80 – 1.69 (m, 4H; includes vinyl CH_3 for **8d**), 1.68 – 1.60 (m, 2H), 1.41 (d, J = 6.7 Hz, 2H; methyl peak for **8e**), 0.99 (t, J = 7.5 Hz, 2H; methyl for **8e**), 0.96 (t, J = 7.4 Hz, 3H; methyl **8d**). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.06 (dd, J = 253.2, 3.6 Hz; both products), 134.72 (**8e**), 129.43 (**8d**), 129.19 (**8d**), 128.76 (**8e**), 127.82 – 126.67 (m; both products), 113.26 – 111.67 (m; both products), 113.26 – 111.67 (m; both products), 59.31 (**8d**), 53.27 (**8e**), 28.41 (**8d**), 25.18 (**8e**), 21.31 (**8e**), 17.76 (**8d**), 13.25 (**8e**), 9.89 (**8d**). HRMS (ESI) *m/z* calculated for $C_{12}H_{19}F_2N_2O_3S$ [M + NH_4]$^+$ 309.1079, found 309.1074.



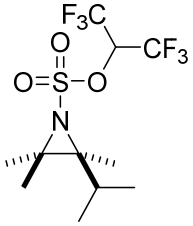
Compound 9a. The product was purified by column chromatography using a 0→5% gradient of EtOAc in hexanes with 1% increments and obtained as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.23 (hept, J = 5.6 Hz, 1H), 2.87 (t, J = 6.8 Hz, 1H), 1.65 (s, 3H), 1.63 – 1.51 (m, 2H), 1.35 (s, 3H), 1.05 (t, J = 7.5 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 120.0 (q, J = 281.6 Hz), 73.2 (hept, J = 35.2 Hz), 57.1, 53.2, 21.3, 20.9, 20.1, 10.8. HRMS (ESI) *m/z* calculated for $C_9H_{13}F_6NO_3S$ [M + H]$^+$ 330.0594, found 330.0605.



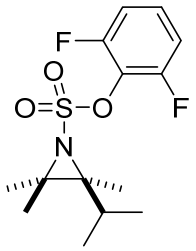
Compound 9b. The product was purified by column chromatography using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 (tt, *J* = 8.6, 5.8 Hz, 1H), 7.00 (t, *J* = 8.1 Hz, 2H), 2.92 (t, *J* = 6.8 Hz, 1H), 1.72 (dp, *J* = 15.1, 7.6 Hz, 1H), 1.66 (s, 3H), 1.57 (dp, *J* = 13.7, 7.3 Hz, 1H), 1.32 (s, 3H), 1.07 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1, 155.0, 127.4 (t, *J* = 9.1 Hz), 112.5 (dd, *J* = 18.5, 3.8 Hz), 56.6, 52.5, 21.3, 21.2, 20.3, 11.0. HRMS (ESI) *m/z* calculated for $C_{12}H_{15}F_2NO_3S$ $[M + H]^+$ 292.0814, found 292.0818.



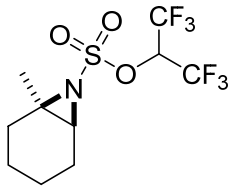
Compound 9d. Characterized as **23c** (*vide infra*).



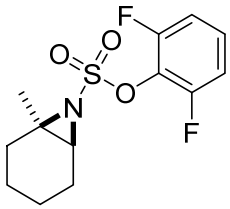
Compound 10a. The product was purified by column chromatography using a 0→5% gradient of EtOAc in hexanes with 1% increments and obtained as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.20 (hept, *J* = 5.7 Hz, 1H), 1.97 (hept, *J* = 6.9 Hz, 1H), 1.59 (s, 3H), 1.47 (s, 3H), 1.45 (s, 3H), 1.12 (d, *J* = 6.7 Hz, 3H), 0.95 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 120.1 (q, *J* = 282.8 Hz), 73.0 (hept, *J* = 35.0 Hz), 62.5, 56.9, 31.9, 20.5, 19.1, 18.2, 18.1, 9.8. HRMS (ESI) *m/z* calculated for $C_{11}H_{17}F_6NO_3S$ $[M + NH_4]^+$ 375.1172, found 375.1175.



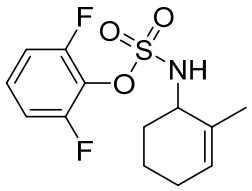
Compound 10b. The product was purified by column chromatography using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 (tt, *J* = 8.6, 5.8 Hz, 1H), 6.99 (dd, *J* = 8.6, 7.5 Hz, 2H), 1.92 (hept, *J* = 6.9 Hz, 1H), 1.57 (s, 3H), 1.46 (s, 3H), 1.44 (s, 3H), 1.03 (d, *J* = 6.7 Hz, 3H), 0.90 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.2 (d, *J* = 3.0 Hz), 155.2 (d, *J* = 3.1 Hz), 127.2 (t, *J* = 9.0 Hz), 112.4 (dd, *J* = 18.5, 3.9 Hz), 61.5, 56.3, 32.0, 20.7, 19.2, 18.2, 9.9. HRMS (ESI) *m/z* calculated for $C_{14}H_{19}F_2NO_3S$ $[M + H]^+$ 320.1127, found 320.1117.



Compound 11a. The product was purified by column chromatography with Davisil silica using a 0→5% gradient of EtOAc in hexanes with 1% increments and obtained in 73% yield as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.25 (hept, *J* = 5.6 Hz, 1H), 3.15 (dd, *J* = 5.0, 1.5 Hz, 1H), 2.07 (dt, *J* = 15.0, 5.4 Hz, 1H), 1.97 – 1.84 (m, 2H), 1.65 (s, 3H), 1.64 – 1.58 (m, 1H), 1.51 – 1.31 (m, 3H), 1.24 – 1.15 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 120.0 (q, *J* = 283.1 Hz), 73.3 (hept, *J* = 35.0 Hz), 52.6, 50.9, 31.4, 22.4, 20.4, 19.3, 19.3. HRMS (ESI) *m/z* calculated for $C_{10}H_{13}F_6NO_3S$ $[M + NH_4]^+$ 359.0859, found 359.0855.

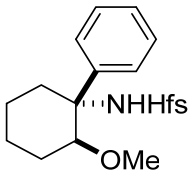


Compound 11b. The product was purified by column chromatography with Davisil silica using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 (tt, *J* = 8.5, 5.8 Hz, 1H), 7.01 (dd, *J* = 8.6, 7.5 Hz, 2H), 3.18 (dd, *J* = 5.4, 1.1 Hz, 1H), 2.02 (ddd, *J* = 15.4, 10.2, 5.6 Hz, 2H), 1.92 (ddt, *J* = 15.9, 11.5, 5.3 Hz, 1H), 1.65 (s, 3H), 1.60 – 1.50 (m, 1H), 1.54 – 1.45 (m, 1H), 1.46 – 1.35 (m, 1H), 1.34 – 1.25 (m, 1H), 1.25 – 1.14 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1 (d, *J* = 2.8 Hz), 155.0 (d, *J* = 3.0 Hz), 127.4 (t, *J* = 9.2 Hz), 112.5 (dd, *J* = 18.4, 4.1 Hz), 51.7, 50.4, 31.4, 22.5, 20.5, 19.6, 19.4. HRMS (ESI) *m/z* calculated for $C_{13}H_{15}F_2NO_3S$ $[M + H]^+$ 304.0814, found 304.0817.

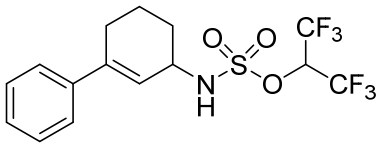


Compound 11d. The product was purified by column chromatography with Davisil silica using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 (tt, *J* = 8.6, 5.9 Hz, 1H), 7.00 (dd, *J* = 8.6, 7.5 Hz, 2H), 5.68 (td, *J* = 3.1, 1.6 Hz, 1H), 4.73 (d, *J* = 8.7 Hz, 1H), 4.07 (dt, *J* = 8.8, 4.2 Hz, 1H), 2.09 (ddd, *J* = 13.0, 6.0, 3.1 Hz, 1H), 2.06 – 1.92 (m, 2H), 1.89 – 1.78 (m, 1H), 1.82 (q, *J* = 2.0 Hz, 3H), 1.73 – 1.64 (m, 1H), 1.62 – 1.53 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0 (d, *J* = 3.4 Hz), 155.0 (d, *J* = 3.4 Hz), 131.5, 128.1, 127.1 (t, *J* = 9.2 Hz), 112.5 (dd, *J* = 18.3, 4.4 Hz), 54.2, 29.6,

24.9, 20.9, 17.6. HRMS (ESI) *m/z* calculated for $C_{13}H_{15}F_2NO_3S$ $[M + NH_4]^+$ 321.1079, found 321.1080.

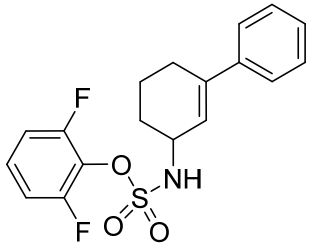


Compound 12a (ring-opened). The product was purified by column chromatography with Davisil silica using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in 43% yield as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.29 (m, 5H), 4.84 (hept, *J* = 5.7 Hz, 1H), 4.61 (s, 1H), 3.72 (s, 1H), 2.94 (s, 3H), 2.25 – 2.11 (m, 2H), 1.94 – 1.76 (m, 2H), 1.71 – 1.56 (m, 3H), 1.45 – 1.34 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.6, 128.6, 128.3, 127.0, 119.9 (q, *J* = 282.1 Hz), 78.3, 72.5 (hept, *J* = 35.0 Hz), 59.8, 49.6, 26.0, 24.9, 20.2, 19.2. HRMS (ESI) *m/z* calculated for $C_{16}H_{19}F_6NO_4S$ $[M + NH_4]^+$ 453.1278, found 453.1276.

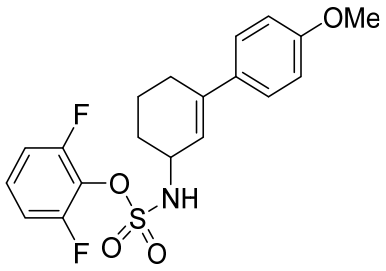


Compound 12c. The product was purified by column chromatography with Davisil silica using a 0→5% gradient of Et_2O in hexanes with 1% increments. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.27 (m, 5H with baseline noise integration error), 6.02 (m, 1H), 5.19 (hept, *J* = 5.7 Hz, 1H), 4.83 (d, *J* = 8.5 Hz, 1H), 4.29 (m, 1H), 2.55 – 2.45 (m, 1H), 2.41 (m, 1H), 2.06 (m, 1H), 1.82 (m, 3H), 1.56 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.9, 140.5, 128.5, 128.5, 128.0, 125.3, 121.8, 73.0 (hept, *J* = 35.2 Hz), 51.9, 29.2, 27.1, 19.6. The CF_3 multiplet was not separable from

the baseline. HRMS (ASAP) *m/z* calculated for $C_{15}H_{16}F_6NO_3S$ $[M + H]^+$ 404.0750, found 404.0745.

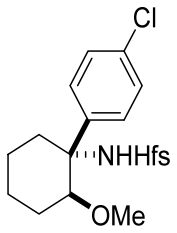


Compound 12d. The product was purified by column chromatography with Davisil silica using a 0→20% gradient of Et_2O in hexanes with 4% increments and obtained as a mixture with **23d** $\mathbf{H_b}$ in 63% yield (**5.6:1**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.28 (m, 5H), 7.21 (tt, *J* = 8.5, 6.0 Hz, 1H), 7.01 (t, *J* = 8.1 Hz, 2H), 6.14 (dd, *J* = 4.1, 2.1 Hz, 1H), 4.82 (d, *J* = 8.3 Hz, 1H), 4.49 – 4.38 (m, 1H), 2.60 – 2.34 (m, 2H), 2.20 – 2.02 (m, 1H), 1.98 – 1.78 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1 (d, *J* = 3.2 Hz), 155.1 (d, *J* = 3.1 Hz), 142.4, 140.8, 128.4, 127.9, 127.3 (t, *J* = 9.2 Hz), 125.4, 122.5, 112.5 (dd, *J* = 18.3, 4.0 Hz), 51.8, 29.4, 27.2, 19.6. HRMS (ESI) *m/z* calculated for $C_{19}H_{19}F_2NO_4S$ $[M + NH_4]^+$ 413.1342, found 413.1345.

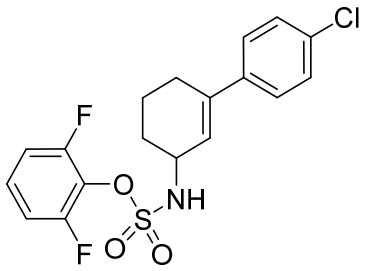


Compound 13d $\mathbf{H_a}$**.** The product was purified by column chromatography with Davisil silica using a 0→20% gradient of EtOAc in hexanes with 4% increments and obtained as a mixture with **24d** $\mathbf{H_b}$ in 65% yield (**6.4:1**). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.8 Hz, 2H), 7.21 (tt, *J* = 8.6, 5.9 Hz, 1H), 7.01 (dd, *J* = 8.6, 7.6 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 6.06 (dt, *J* = 3.6, 1.7 Hz, 1H), 4.46 – 4.40 (m, 1H), 3.82 (s, 3H), 2.51 – 2.42 (m, 1H), 2.41 – 2.34 (m, 1H), 2.12 –

2.03 (m, 1H), 1.94 – 1.79 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.4, 157.1 (d, *J* = 3.5 Hz), 155.1 (d, *J* = 3.6 Hz), 141.6, 133.2, 127.2 (t, *J* = 9.1 Hz), 126.5, 120.9, 113.8, 112.5 (dd, *J* = 18.1, 4.3 Hz), 55.3, 51.9, 29.4, 27.1, 19.6. HRMS (ESI) *m/z* calculated for $C_{19}H_{19}F_2NO_4S$ $[M + NH_4]^+$ 413.1342, found 383.1238.

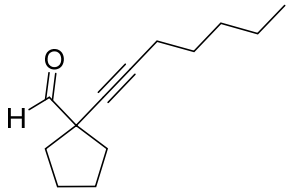


Compound 14a (ring-opened). The product was purified by column chromatography using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in 57% yield as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.7 Hz, 1H), 7.30 (d, *J* = 8.6 Hz, 1H), 4.92 (hept, *J* = 5.7 Hz, 1H), 4.73 (s, 1H), 3.72 – 3.64 (m, 0H), 2.93 (s, 2H), 2.21 (tt, *J* = 14.1, 3.8 Hz, 1H), 2.11 (d, *J* = 14.6 Hz, 0H), 1.85 (d, *J* = 13.7 Hz, 0H), 1.75 (ddd, *J* = 14.5, 12.9, 3.6 Hz, 1H), 1.70 – 1.65 (m, 1H), 1.59 (tdd, *J* = 12.9, 10.1, 3.3 Hz, 0H), 1.34 (tdd, *J* = 13.4, 8.4, 3.5 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.3, 134.2, 128.7, 128.5, 119.9 (q, *J* = 282.3 Hz), 78.1, 72.6 (hept, *J* = 35.3 Hz), 59.6, 49.6, 26.1, 24.9, 20.0, 19.1. HRMS (ESI) *m/z* calculated for $C_{16}H_{18}ClF_6NO_4S$ $[M + NH_4]^+$ 487.0888, found 487.0894.

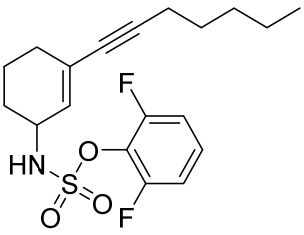


Compound 14d H_a. The product was purified by column chromatography with Davisil silica using a 0→20% gradient of EtOAc in hexanes with 4% increments and obtained as a mixture

with **25d H_b** in 51% yield (5.9:1 ratio) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.31 (m, 4H), 7.24 (tt, *J* = 8.6, 5.9 Hz, 1H), 7.04 (t, *J* = 8.1 Hz, 2H), 6.16 (dd, *J* = 3.9, 1.9 Hz, 1H), 4.85 (d, *J* = 8.2 Hz, 1H), 4.50 – 4.41 (m, 1H), 2.52 – 2.36 (m, 2H), 2.12 (tt, *J* = 13.1, 5.7 Hz, 1H), 1.95 – 1.82 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1 (d, *J* = 3.2 Hz), 155.0 (d, *J* = 3.1 Hz), 141.1, 139.2, 133.7, 128.6, 127.3 (t, *J* = 9.2 Hz), 126.7, 123.1, 112.6 (dd, *J* = 18.3, 4.0 Hz), 51.7, 29.3, 27.1, 19.6. HRMS (ESI) *m/z* calculated for $C_{18}H_{16}ClF_2NO_3S$ $[M + NH_4]^+$ 417.0846, found 417.0840.

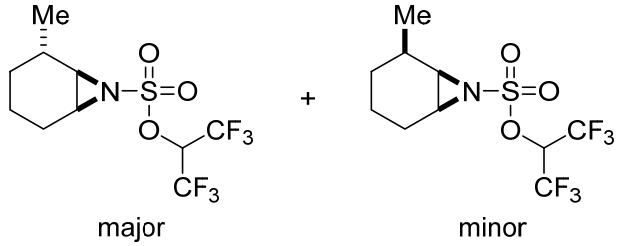


Compound 15a. The product was purified by column chromatography using a 0→4% gradient of Et_2O in hexanes with 1% increments and obtained in 52% yield as a clear, colorless oil corresponding to the ring contraction/hydrolysis product of the initial aziridine. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.40 (s, 1H), 2.12 (t, *J* = 7.1 Hz, 2H), 2.06 – 1.97 (m, 2H), 1.77 – 1.68 (m, 4H), 1.60 – 1.50 (m, 2H), 1.43 (p, *J* = 7.1 Hz, 2H), 1.32 – 1.20 (m, 4H), 0.83 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 197.3, 84.4, 79.2, 52.3, 34.2, 30.0, 27.5, 23.9, 21.1, 17.8, 13.0. HRMS (ESI) *m/z* calculated for $C_{13}H_{20}O$ $[M + H]^+$ 193.1587, found 193.1590.

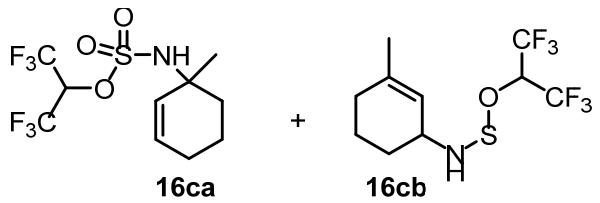


Compound 15d. The product was purified by column chromatography using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in 62% yield as a clear, colorless oil. ^{1}H

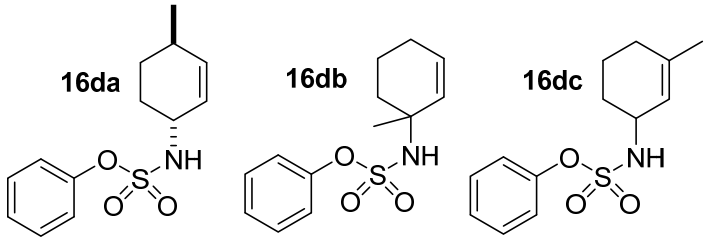
NMR (500 MHz, $CDCl_3$) δ 7.21 (tt, *J* = 8.6, 5.9 Hz, 1H), 7.01 (t, *J* = 8.1 Hz, 2H), 6.01 (dt, *J* = 3.8, 1.9 Hz, 1H), 4.76 (d, *J* = 8.3 Hz, 1H), 4.33 – 4.24 (m, 1H), 2.30 (t, *J* = 7.2 Hz, 2H), 2.21 – 2.06 (m, 2H), 2.03 – 1.95 (m, 1H), 1.83 – 1.75 (m, 1H), 1.75 – 1.64 (m, 2H), 1.53 (p, *J* = 7.2 Hz, 2H), 1.41 – 1.28 (m, 4H), 0.91 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0 (d, *J* = 3.4 Hz), 155.0 (d, *J* = 3.5 Hz), 129.9, 127.3 (t, *J* = 9.2 Hz), 126.9, 112.5 (dd, *J* = 18.2, 4.3 Hz), 91.1, 80.6, 51.1, 31.1, 29.4, 28.9, 28.4, 22.2, 19.3, 19.1, 14.0. HRMS (ESI) *m/z* calculated for $C_{19}H_{23}F_2NO_3S$ $[M + NH_4]^+$ 401.1705, found 401.1705.



Compound 16a. The product was purified by column chromatography using a 0→5% gradient of EtOAc in hexanes with 1% increments and obtained as a mixture of *syn* and *anti* diastereomers (1:4.8 ratio) as a clear, colorless oil. ^1H NMR (400 MHz, $CDCl_3$) δ 5.20 (hept, *J* = 5.6 Hz, 2H), 3.13 (t, *J* = 6.5 Hz, 1H, minor), 3.09 (ddd, *J* = 7.1, 3.9, 1.4 Hz, 1H, major), 3.02 (dd, *J* = 7.1, 3.4 Hz, 1H, minor), 2.76 (d, *J* = 7.1 Hz, 1H, major), 1.98 (dt, *J* = 14.4, 5.0 Hz, 2H, major), 1.92 – 1.86 (m, 2H, minor), 1.71 – 1.53 (m, 4H), 1.41 – 1.33 (m, 2H), 1.26 (dddd, *J* = 12.8, 10.3, 4.9, 2.6 Hz, 1H), 1.06 (d, *J* = 7.4 Hz, 3H, major), 1.04 (s, 3H, minor), 1.04 – 0.86 (m, 1H), 0.80 (dtd, *J* = 13.8, 11.5, 10.7, 3.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 119.9 (q, *J* = 285.4 Hz), 73.6 (hept, *J* = 35.2 Hz), 48.8 (minor), 47.9 (major), 44.5 (minor), 43.9 (major), 28.8 (major), 28.5 (minor), 27.8 (major), 26.6 (minor), 22.7 (major), 21.5 (minor), 20.0 (major), 20.0 (minor), 18.7 (minor), 16.9 (major). HRMS (ESI) *m/z* calculated for $C_{10}H_{13}F_6NO_3S$ $[M + NH_4]^+$ 359.0859, found 359.0860.

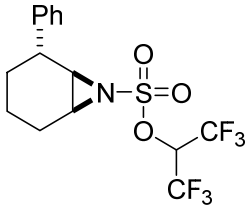


Compound 16ca and 16cb. The products were purified by column chromatography on Davisil silica using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained as a mixture of isomers (1:1.7 ratio) along with other trace side products as a clear, colorless oil. Assignments to specific products were made where possible with 2D HSQC and HMBC data. ^{1}H NMR integrations were made relative to **16cb** as the major product. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.88 (ddd, *J* = 10.0, 4.2, 3.3 Hz, 0.6H; 1H **16ca**), 5.66 – 5.61 (m, 0.8H; 1H **16ca**), 5.42 – 5.38 (m, 1H; **16cb**), 5.21 – 5.10 (m, 2H, **16ca** and **16cb**), 4.79 – 4.70 (m, 2H, NH of both products), 4.11 – 4.01 (m, 1H, **16cb**), 2.20 – 2.11 (m, 1.1H), 2.06 (m, 0.74H, 1H **16ca**), 1.99 (m, 0.7H; 1H), 1.93 (m, 2.3H), 1.90 – 1.84 (m, 1.5H), 1.76 – 1.62 (m, 8H; includes methyl of **16cb**), 1.50 (s, 1.7H; 3H methyl of **16ca**). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.5 (**16cb**), 131.4 (**16ca**), 130.1 (**16ca**), 120.2 (q, CF_3 of both products) 119.6 (**16cb**), 72.9 (m, both products), 57.4 (**16ca**), 51.51 (**16cb**), 35.5, 29.5, 29.1, 26.9 (**16ca**), 24.5, 23.7 (**16cb**), 19.0, 18.4. HRMS (ESI) *m/z* calculated for $C_{10}H_{14}F_6NO_3S$ $[M + H]^+$ 340.0437, found 340.0431.



Compound 16da, 16db, 16dc. The products was purified by column chromatography with Davisil silica using a 0→10% gradient of EtOAc in hexanes with 2% increments and obtained in a 1:1:2 ratio as a clear, colorless oil. Assignments were made to specific compounds where

possible with the aid of HSQC and HMBC data. ^{1}H signals are integrated relative to **16dc** as the major product. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25 – 7.16 (m, 2H; 1H from each product), 7.06 – 6.96 (m, 4H; 2H from each product), 5.95 – 5.84 (m, 0.4H; 1H **16db**), 5.85 – 5.80 (m, 0.5H, 1H **16da**), 5.78 – 5.68 (m, 1H; 1H **16da** and 1H **16db**), 5.52 – 5.48 (m, 1H, 1H **16dc**), 4.92 – 4.71 (m, 2H; 1H from each product), 4.26 – 4.13 (m, 2H; 1H **16da** and 1H **16dc**), 2.30 – 2.22 (m, 0.4H; 1H **16db**), 2.17 (dddq, *J* = 9.3, 7.0, 4.5, 2.2 Hz, 0.4H, 1H **16da**), 2.12 – 1.88 (m, 4H), 1.88 – 1.75 (m, 2H), 1.74 – 1.63 (m, 5H; includes methyl singlet of **16dc**), 1.59 (s, 1.8H; methyl singlet **16db**), 1.02 (d, *J* = 7.1 Hz, 1.5H; methyl doublet **16da**). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.1 (dd, J = 253.3, 3.5 Hz, all products),140.9 (**16dc**), 139.3 (**16da**), 130.8 (**16db**), 130.7 (**16db**), 127.9-126.7 (m, all products) 124.5 (**16da**), 120.3 (**16dc**), 112.5 (ddd, J = 18.3, 4.2, 2.1 Hz, all products) 51.4 (**16dc**), 50.0 (**16da**), 35.6 (**16db**), 30.0, 29.6, 29.3, 28.1, 26.8, 26.4 (**16db**), 24.6, 23.7 (**16dc**), 20.9 (**16da**), 19.1, 18.6. HRMS (ESI) *m/z* calculated for $C_{15}H_{15}F_6NO_3S$ [M + NH_4]$^{+}$ 321.1079, found 321.1074.

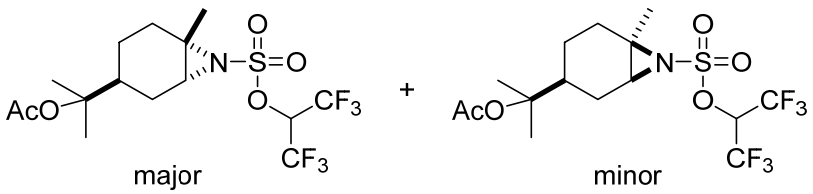


Compound 17a. The product was purified by column chromatography with Davisil silica using a 0→5% gradient of EtOAc in hexanes with 1% increments and obtained in 22% yield as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.32 (m, 5H), 5.24 (hept, *J* = 5.6 Hz, 1H), 3.34 (dd, *J* = 7.2, 2.6 Hz, 1H), 3.22 (t, *J* = 6.8 Hz, 1H), 3.04 (ddd, *J* = 10.7, 5.5, 2.6 Hz, 1H), 2.17 – 2.10 (m, 1H), 1.92 (ddd, *J* = 15.1, 11.8, 6.8 Hz, 1H), 1.75 (dddd, *J* = 13.5, 6.6, 4.4, 1.6 Hz, 1H), 1.70 – 1.63 (m, 2H), 1.47 – 1.34 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.4, 128.9,

127.4, 127.0, 119.9 (q, J = 284.1 Hz), 73.7 (hept, J = 35.7 Hz), 47.0, 43.8, 39.7, 29.6, 22.7, 17.0. HRMS (ESI) *m/z* calculated for $C_{15}H_{15}F_6NO_3S$ $[M + NH_4]^+$ 421.1016, found 421.1019.

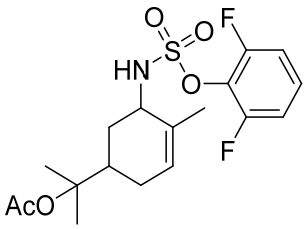
Compound 17c. Complete rearrangement was observed to give an amination product identical to **12c**.

Compound 17d. Due to rearrangement, the C-H insertion product was identical to **12d** and was characterized as noted above.

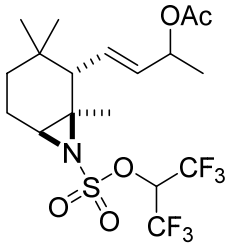


Compound 18a. The product was purified by column chromatography using a 0→80% gradient of CH_2Cl_2 in hexanes with 10% increments and obtained as a mixture of *syn* and *anti* diastereomers (1:11 ratio) as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.27 (h, J = 5.8 Hz, 1H, minor), 5.20 (hept, J = 5.7 Hz, 1H, major), 3.28 (t, J = 2.4 Hz, 1H, major), 3.20 (d, J = 6.7 Hz, 1H, minor), 2.48 – 2.41 (m, 1H, minor), 2.42 – 2.34 (m, 1H, major), 2.21 (dt, J = 14.6, 3.6 Hz, 1H, minor), 2.14 (dd, J = 13.5, 3.4 Hz, 1H, major), 2.06 – 2.02 (m, 1H, minor), 1.99 (s, 4H, minor), 1.98 (s, 3H, major), 1.92 – 1.86 (m, 1H, major), 1.81 (dt, J = 14.1, 3.0 Hz, 1H, minor), 1.69 (s, 3H, major), 1.67 (s, 3H, minor), 1.62 (dd, J = 4.6, 2.1 Hz, 2H, major), 1.58 (s, 3H, minor), 1.56 (s, 3H, major), 1.48 – 1.39 (m, 8H), 1.30 – 1.21 (m, 1H, minor). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.5, 120.0 (q, J = 280.1 Hz), 83.9, 73.4 (hept, J = 36.7 Hz), 52.7, 50.5, 40.8,

35.5, 32.2, 25.4, 23.3, 23.0, 22.3, 19.5. HRMS (ESI) *m/z* calculated for $C_{15}H_{21}F_6NO_5S$ [M + NH_4]$^+$ 459.1383, found 459.1373.

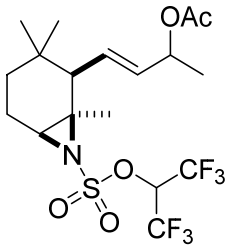


Compound 18d. The product was purified by column chromatography using a 0→20% gradient of EtOAc in hexanes with 2% increments and obtained as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 (tt, *J* = 8.8, 5.9 Hz, 1H), 7.02 (dd, *J* = 8.6, 7.6 Hz, 2H), 5.69 (dt, *J* = 5.6, 1.6 Hz, 1H), 5.07 (dd, *J* = 8.5, 5.0 Hz, 1H), 4.15 (ddt, *J* = 9.7, 5.3, 2.4 Hz, 1H), 2.32 (dq, *J* = 13.7, 2.2 Hz, 1H), 2.25 (dddd, *J* = 15.8, 11.6, 5.0, 2.4 Hz, 1H), 2.10 (dtt, *J* = 17.6, 4.9, 1.4 Hz, 1H), 1.94 (s, 3H), 1.84 (dt, *J* = 2.5, 1.3 Hz, 3H), 1.60 – 1.51 (m, 2H), 1.46 (s, 3H), 1.45 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.6, 157.0 (d, *J* = 3.2 Hz), 155.0 (d, *J* = 3.0 Hz), 131.1, 127.1 (t, *J* = 9.2 Hz), 112.5 (dd, *J* = 18.3, 4.0 Hz), 83.8, 54.7, 36.8, 30.1, 26.4, 23.5, 23.2, 22.3, 20.5. HRMS (ESI) *m/z* calculated for $C_{18}H_{23}F_2NO_5S$ [M + NH_4]$^+$ 421.1603, found 421.1594.

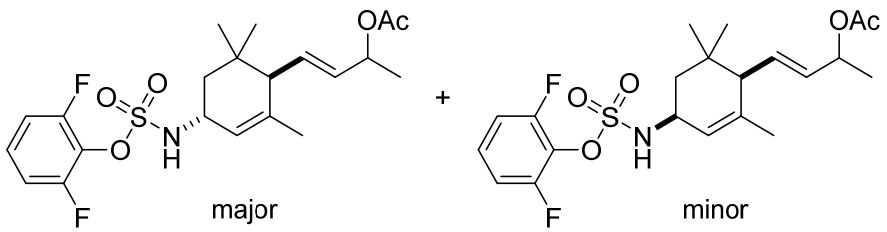


Compound *anti*-19a. The crude material was purified using the CombiFlash system (gradient elution, 100% hexanes to 10% ethyl acetate/hexanes) to yield the product as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.61 – 5.53 (m, 2H), 5.40 – 5.30 (m, 1H), 5.24 (hept, *J* = 5.5 Hz,

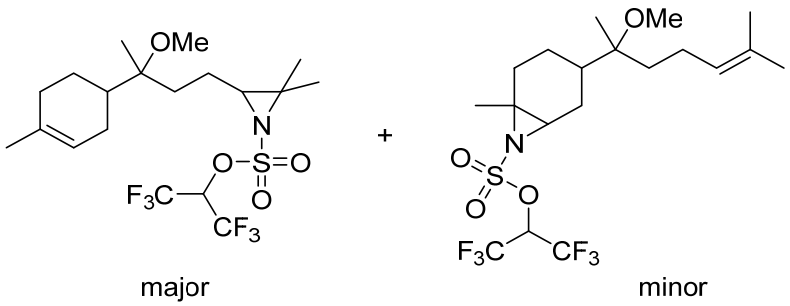
1H), 3.17 (d, *J* = 3.4 Hz, 1H), 2.28 – 2.19 (m, 1H), 2.05 (s, 3H), 2.00 – 1.95 (m, 1H), 1.95 – 1.83 (m, 1H), 1.50 (s, 3H), 1.34 (d, *J* = 6.5 Hz, 3H), 1.29 – 1.19 (m, 2H), 0.80 (s, 3H), 0.79 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.3, 135.4, 128.8, 119.9 (q, *J* = 283.3 Hz), 73.3 (hept, *J* = 35.9 Hz), 70.6, 54.5, 53.6, 51.7, 33.0, 31.4, 29.4, 21.3, 20.6, 20.2, 19.7. HRMS (ESI) *m/z* calculated for $C_{18}H_{25}F_6NO_5S$ $[M + NH_4]^+$ 499.1696, found 499.1696.



Compound *syn*-19a. The crude material was purified using the CombiFlash system (gradient elution, 100% hexanes to 10% ethyl acetate/hexanes) to yield the product as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.61 – 5.53 (m, 2H), 5.40 – 5.31 (m, 1H), 5.24 (hept, *J* = 5.6 Hz, 1H), 3.23 (t, *J* = 2.7 Hz, 1H), 2.04 (s, 3H), 2.04 – 2.01 (m, 1H), 1.91 (ddd, *J* = 13.1, 6.2, 3.3 Hz, 3H), 1.60 (s, 3H), 1.34 (d, *J* = 6.5 Hz, 3H), 1.03 (dt, *J* = 14.7, 5.5 Hz, 1H), 0.87 (s, 3H), 0.75 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.4, 133.1, 129.6, 120.0 (q, *J* = 281.8 Hz), 73.4 (hept, *J* = 35.1 Hz), 54.5, 52.8, 50.8, 30.9, 28.5, 28.0, 26.5, 21.3, 20.4, 20.1. HRMS (ESI) *m/z* calculated for $C_{18}H_{25}F_6NO_5S$ $[M + NH_4]^+$ 499.1696, found 499.1697.

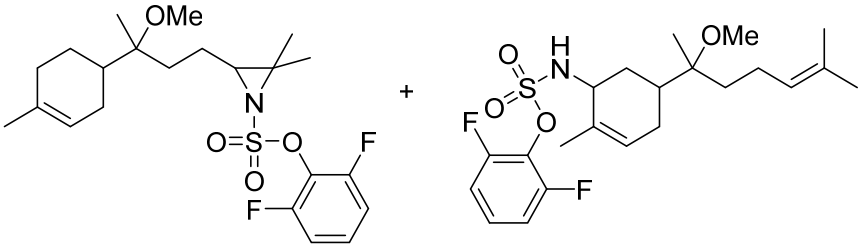


Compound 19d. The crude material was purified using the CombiFlash system (gradient elution, 100% hexanes to 10% ethyl acetate/hexanes) to yield the product as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21 (tt, *J* = 8.5, 5.9 Hz, 2H), 7.01 (t, *J* = 8.1 Hz, 4H), 5.58 – 5.39 (m, 6H), 5.37 – 5.29 (m, 2H), 4.86 (dd, *J* = 8.6, 4.3 Hz, 1H, minor), 4.82 (d, *J* = 8.5 Hz, 1H, major), 4.28 – 4.17 (m, 2H), 2.33 (d, *J* = 9.8 Hz, 1H, major), 2.11 (d, *J* = 8.1 Hz, 1H, minor), 2.04 (d, *J* = 1.3 Hz, 6H), 2.02 – 1.96 (m, 1H, major), 1.85 – 1.79 (m, 1H, minor), 1.64 (d, *J* = 1.7 Hz, 3H, minor), 1.64 – 1.58 (m, 3H, major), 1.44 (dd, *J* = 13.2, 8.2 Hz, 1H, major), 1.41 – 1.36 (m, 1H, minor), 1.33 – 1.30 (m, 6H), 0.97 (s, 3H, minor), 0.96 (s, 3H, major), 0.87 (s, 3H, minor), 0.86 (s, 3H, major). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.4 (minor), 170.3 (major), 157.1 (d, *J* = 3.7 Hz), 155.1 (d, *J* = 3.7 Hz), 139.4 (minor), 139.2 (major), 133.6 (minor), 133.5 (major), 131.0 (major), 130.9 (minor), 127.2 (t, *J* = 9.1 Hz), 121.2 (major), 121.1 (minor), 112.5 (dd, *J* = 18.2, 4.2 Hz), 70.8 (minor), 70.7 (major), 53.5 (major), 53.4 (minor), 51.7 (minor), 51.1 (major), 42.6 (major), 42.5 (major), 38.2 (minor), 38.2 (minor), 33.9 (minor), 33.5 (major), 29.0 (major), 28.6 (major), 26.5 (minor), 22.9, (minor), 22.7 (major), 22.6 (minor), 21.4, 20.5 (major), 20.5 (minor). HRMS (ESI) *m/z* calculated for $C_{21}H_{27}F_2NO_5S$ $[M + NH_4]^+$ 461.1917, found 461.1920.



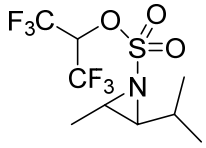
Compound 20aa and 20ab. The crude material was purified using the CombiFlash system (gradient elution, 100% hexanes to 10% ethyl acetate/hexanes) to yield a mixture (1.4:1 ratio) as

a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.39 – 5.35 (m, 1H, major), 5.31 – 5.20 (m, 2H), 5.11 – 5.06 (m, 1H, minor), 3.17 (dd, *J* = 12.6, 5.6 Hz, 1H, major), 3.14 (s, 3H, major), 3.12 (s, 3H, minor), 2.93 – 2.87 (m, 1H, minor), 2.25 – 2.17 (m, 1H, major), 2.04 – 1.88 (m, 9H), 1.87 – 1.71 (m, 6H), 1.69 (s, 3H, major), 1.67 – 1.60 (m, 9H), 1.54 – 1.38 (m, 7H), 1.35 (s, 3H, major), 1.32 – 1.19 (m, 2H), 1.05 (s, 3H, major), 0.96 (s, 3H, minor). ^{13}C NMR (126 MHz, $CDCl_3$) δ 134.3 (major), 131.7 (minor), 124.1 (minor), 120.4 (major), 120.0 (q, *J* = 280.1 Hz), 77.7 (major), 77.5 (minor), 73.1 (hept, *J* = 35.2 Hz), 56.4 (major), 53.4 (major), 53.0 (minor), 50.7 (minor), 48.5 (major), 48.5 (minor), 39.8 (major), 38.9 (minor), 34.3 (minor), 32.3 (minor), 31.3 (major), 31.0 (major), 26.8 (major), 25.7 (minor), 23.8 (minor), 23.3 (major), 21.3 (minor), 21.2 (major), 21.2 (major), 20.4 (major), 19.6 (minor), 18.9 (major), 18.8 (minor), 18.6 (major), 18.3 (minor), 17.6 (minor). HRMS (ESI) *m/z* calculated for $C_{19}H_{29}F_6NO_4S$ $[M + H]^+$ 482.1795, found 482.1796.

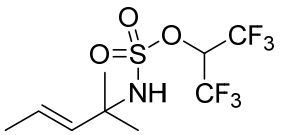


Compound 20b and 20d. The crude material was purified using the CombiFlash system (gradient elution, 100% hexanes to 10% ethyl acetate/hexanes) to yield the product mixture as a clear, colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25 – 7.14 (m, 2H), 7.00 (dd, *J* = 8.7, 7.4 Hz, 4H), 5.67 (d, *J* = 4.7 Hz, 1H, minor), 5.39 – 5.35 (m, 1H, major), 5.08 (tt, *J* = 7.2, 1.5 Hz, 1H, minor), 4.95 (d, *J* = 8.1 Hz, 1H, minor), 4.15 – 4.09 (m, 1H, minor), 3.15 (s, 3H, major), 3.14 (s, 3H, minor), 2.95 (q, *J* = 6.2 Hz, 1H, major), 2.32 (dt, *J* = 13.6, 2.1 Hz, 1H, minor), 2.04 – 1.91 (m, 6H), 1.87 (ddd, *J* = 7.8, 4.5, 2.5 Hz, 3H), 1.83 (s, 3H, major), 1.81 – 1.71 (m, 4H), 1.68 –

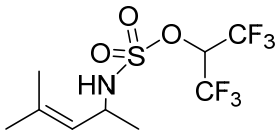
1.64 (m, 9H), 1.64 – 1.59 (m, 3H, major), 1.55 – 1.38 (m, 5H), 1.33 (d, *J* = 1.4 Hz, 3H, major), 1.29 – 1.23 (m, 1H, major), 1.06 (s, 3H, major), 1.05 (s, 3H, minor). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0 (d, *J* = 2.2 Hz), 155.0 (d, *J* = 2.6 Hz), 134.3, 131.5, 131.2 (minor), 127.9 (minor), 127.5 (t, *J* = 9.0 Hz, major), 127.1 (t, *J* = 8.5 Hz, minor), 124.43 (minor), 120.5 (major), 112.6 – 112.4 (m), 77.8 (minor), 77.2 (major), 55.8 (major), 54.8 (minor), 52.7 (major), 48.6 (minor), 48.5 (major), 40.0, 39.8, 34.9 (minor), 34.2 (minor), 31.5 (major), 31.4, 31.0 (major), 31.0, 29.7 (minor), 27.0, 26.9 (major), 26.7 (minor), 25.7 (minor), 23.4 (major), 23.3 (major), 21.6 (minor), 21.4 (major), 21.3 (major), 20.6 (minor), 20.5 (minor), 18.9 (major), 18.8 (minor), 17.7 (minor). HRMS (ESI) *m/z* calculated for $C_{22}H_{31}F_2NO_4S$ $[M + NH_4]^+$ 444.2015, found 444.2003.



Compound 23a. The compound was isolated from column chromatography on Davisil silica with a 0→5% gradient of EtOAc in hexanes with 2% increments. The compound was isolated in 16% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.27 (hept, *J* = 5.6 Hz, 1H), 2.82 (qd, *J* = 6.0, 5.0 Hz, 1H), 2.64 (dd, *J* = 7.7, 4.9 Hz, 1H), 1.74 – 1.66 (m, 1H), 1.57 (d, *J* = 6.0 Hz, 3H), 1.06 (d, *J* = 6.7 Hz, 3H), 1.00 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 119.9 (q, *J* = 281.1 Hz, CF_3), 73.3 (p, J = 35.2 Hz), 57.6, 45.7, 29.5, 19.3, 19.0, 14.1. HRMS (ESI) *m/z* calculated for $C_9H_{14}F_6NO_3S$ $[M+H]^+$ 330.0593, found 330.0586.

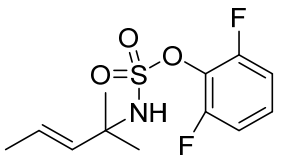


23b

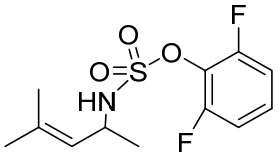


23c

Compounds 23b and 23c. The compounds were isolated from column chromatograpy on Davisil silica with a 0→5% gradient of EtOAc in hexanes with 2% increments. The isolated amounts were 6% and 5%, respectively and co-eluted as an approximately 1:1 mixture. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.70 (dq, *J* = 15.6, 6.4 Hz, 1H; **23b**), 5.59 (dq, *J* = 15.6, 1.5 Hz, 1H; **23b**), 5.16 – 5.08 (m, 2H; CF_3 for both products), 5.07 – 5.01 (m, 1H; **23c**), 4.78 (s, 1H; **23b**), 4.65 (d, *J* = 6.8 Hz, 1H; **23c**), 4.39 (dp, *J* = 9.1, 6.6 Hz, 1H; **23c**), 1.71 (m, 9H; vinyl Me groups of both products), 1.47 (s, 6H, **23b**), 1.31 (d, *J* = 6.6 Hz, 3H; **23c**). ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.0 (**23c**), 135.0 (**23b**), 125.7 (**23b**), 124.5 (**23c**), 120.2 (q, *J* = 281.0 Hz, CF_3 both products), 72.7 (hept, *J* = 34.7 Hz), 72.5 (hept, *J* = 35.1 Hz), 59.0 (**23b**), 50.3 (**23c**), 27.5 (**23b**), 25.5 (**23c**), 22.0 (**23b**), 18.0 (**23c**), 17.6 (**23c**). HRMS (ASAP-MS) *m/z* calculated for $C_9H_{12}F_6NO_3S$ $[M-H]^+$ 328.0437, found 328.0429.



24a



24b

Compounds 24a and 24b. The compounds were isolated from column chromatograpy on Davisil silica with a 0→5% gradient of EtOAc in hexanes with 2% increments. The isolated amounts were 15% and 19%, respectively and co-eluted during purification as an approximately 1:1 mixture. Specific NMR assignments were made where unambiguous. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 (tt, *J* = 8.5, 5.8 Hz, 2H; 1H each product), 7.04 – 6.95 (m, 4H; 2H each product),

5.79 – 5.65 (m, 2H; **23a**), 1.54 – 1.53 (m, 1H; **23b**), 5.10 (ddd, *J* = 9.1, 2.8, 1.5 Hz, 1H; **23b**), 4.72 (s, 1H; **23a**), 4.60 (d, *J* = 6.3 Hz, 1H; **23b**), 4.52 (dp, *J* = 8.9, 6.5 Hz, 1H; **23b**), 1.73 m, 6H, both products), 1.55 (d, *J* = 6.3 Hz, 9H overlap with water; both products), 1.36 (d, *J* = 6.5 Hz, 3H; **23b**). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.2 (dd, *J* = 253.4, 3.7 Hz), 156.1 (dd, *J* = 253.2, 3.6 Hz), 136.3 (**24a**), 135.7 (**24b**), 127.4 – 126.9 (m), 125.0, 125.0, 112.6 (t, *J* = 3.8 Hz), 112.4 (t, *J* = 3.9, 3.3 Hz), 58.6, 50.2, 29.7, 27.5, 25.6, 22.2, 18.1, 17.7. HRMS (ESI) *m/z* calculated for $C_{12}H_{19}F_2N_2O_3S$ $[M+NH_4]^+$ 309.1079, found 309.1070.

V. Computational Methods.

All calculations were performed using the Orca 3.0.3 program packages.[3] For computational convenience, all the *tert*-butyl groups on ^{t}Bu$_3$tpy were replaced with H atoms (tpy). Unless specified, the resolution of identity (RI) approximation and the chain-of-sphere approximation (COSX), with the corresponding auxiliary basis sets, were applied to the Coulomb integrals on the DFT portion and exchange integrals on the Hartree-Fock (HF) portion, respectively. Molecular graphics and analyses were performed with the UCSF Chimera package.[4]

Density functional benchmark against crystal structure of catalyst ***A*****.** Initial structures for geometry optimization were obtained by reported crystal structures.[5a] Geometry optimization was performed using functionals BP86,[6] BLYP,[7] PBE,[8] TPSS,[9] B3LYP[10], PBE0[8] and TPSSh[9] with the dispersion correction (D3BJ) from Grimme, et al. in 2010.[11] The zeroth-order regular approximation with model potential as described by van Wuellen[12] and the one-center approximation were applied to the integrals to account for relativistic effects. The segmented all-electron relativistically recontracted (SARC) version of the def2-TZVPP basis set was used.[13] The Ahlrichs (2df,2pd) polarization functions were obtained from the TurboMole basis set

library at ftp.chemie.uni-karlsruhe.de/pub/basen and were used on the metal atoms, while the def2-SVP basis set[13] was used on the rest of the atoms. Frequency calculations were performed on optimized geometries using the same method and no imaginary frequencies were found, indicating that the geometries were indeed local minima. B3LYP was found to be one of the most robust functionals (Table S1-4), therefore, it was the functional used for further computational studies.

Ground state geometry optimizations. Initial geometries for geometry optimization were obtained by modifying reported crystal structures.[5] Geometry optimization was performed using the unrestricted hybrid-GGA B3LYP[6] with the dispersion correction (D3BJ) from Grimme, et al. in 2010.[11] The same basis sets and corrections for relativity as described above were applied. Frequency calculations were performed on optimized geometries using the same method as above and no imaginary frequencies were found, indicating that the geometries were indeed local minima.

For OS singlet calculations, the wavefunctions were converged to broken symmetry solutions by first converging to the triplet state, followed by flipping the spin of one of the two unpaired electrons.

Transition state geometry optimizations. The same methods as for the ground state geometry optimization were employed for transition state geometry optimizations as those employed for ground state geometry optimizations. Relaxed surface scans along bonds that led to intermediates were performed on optimized ground state geometries. Transition state optimizations were performed starting with the geometries of the highest energy point on the relaxed surface scans. Frequency calculations were performed on optimized transition state

geometries and one imaginary frequency was found, which was verified as the vibration leading reactants to intermediates or products in each case.

Single point energy calculations on optimized ground and transition state geometries. Single-point energy calculations on optimized geometries were performed using range-separated hybrid meta-GGA wB97X[14] with the dispersion correction of Grimme, et al. (wB97X-D3).[11] This functional has been shown to give reaction[14] and non-covalent interaction energies[15] that are close to those calculated by canonical CCSD theory. The zeroth-order regular approximation with model potential of van Wuellen[12] and *without* the one-center approximation was applied to the integrals to account for relativistic effects. The same basis sets were applied as for geometry optimization. The RI approximation was applied to the Coulomb integral on the DFT portion and the exchange integrals on the HF portion were solved exactly. Numerical grid was increased to "grid 4" in Orca notation, which equals to 302 Lebedev points. Solvent effects were modeled by the conductor-like screening model (COSMO) with ε = 9.08 and refractive index = 1.424 for CH_2Cl_2. For broken symmetry wavefunctions, procedures proposed by Houk and coworkers[16] for correcting for spin contamination from the first triplet excited state were employed.

Complete active space self-consistent field (CASSCF) calculations. Single point energy calculations using the CASSCF method on the optimized geometry of triplet and OS singlet Ag-nitrene complexes were performed using the same basis sets as for geometry optimization. An active space of 8 electrons in 5 orbitals (8,5) was selected to includeone N 2s and three N 2p orbitals and the Ag d_{z2} orbital. This choice of active space allows the inclusion of all possible electron configurations pointed out in the literature: namely Ag(I)-^{3}nitrene, Ag(I)-^{OS1}nitrene, Ag(I)-^{CS1}nitrene, ^{OS1}{Ag(II)-nitrene$^{\bullet-}$}, and ^{3}{Ag(II)-nitrene$^{\bullet-}$}.

VI. Keywords and Energies for Computations. *Keywords:* 0bs = OS singlet

Functional benchmark

Table S4. Analysis of the difference between experimental and calculated geometries for several DFT functionals

	BP86	BLYP	PBE	TPSS	B3LYP	PBE0	TPSSh
STDEV[a]	0.086	0.085	0.086	0.083	0.081	0.081	0.081
MAX[a]	0.168	0.166	0.168	0.161	0.160	0.160	0.159
MIN[a]	-0.060	-0.008	-0.029	-0.086	-0.018	-0.024	-0.071
MAD[a]	0.054	0.052	0.052	0.053	0.049	0.048	0.050

[a]STDEV = standard deviation, $\sqrt{\frac{\sum_i (d_{xtl}-d_i)^2}{n-1}}$. MAX = maximum deviation. MIN = maximum negative deviation. MAD = mean absolute deviation, $\frac{\sum_i |d_{xtl}-d_i|}{n}$.

Structures

Isomers

The nitrene complex **B(N)** can also exist with the nitrene ligand binding axial (trans to the tertiary amine), **B(N_{ax})**. The structure of **B(N_{ax})** is depicted in Figure S1. Howver, the **B(N_{ax})** isomer is thermodynamically unfavored ($\Delta G_{eq\text{-}ax}^{CH_2Cl_2}$ = 3.43 kcal·mol^{-1}); in addition, the formation of **B(N_{ax})** requires a reorganization of the OTf^- ligand. This reorganization will make the formation of **B(N_{ax})** kinetically unfavorable. Dissociation of the OTf ligand before ($K_{eq}^{CH_2Cl_2} = 2.45 \times 10^8$; eq. 1) or after ($K_{eq}^{CH_2Cl_2} = 6.28 \times 10^8$; eq. 2) the formation of the nitrene complex, respectively, is also found to be thermodynamically unfavorable.

The nitrene complex of **A'** can also exist with the nitrene group attached to Ag_O. However, this coordination isomer was found to be less stable than the structure with the nitrene attached to Ag_N ($\Delta G_{Ag_N\text{-}Ag_O}^{CH_2Cl_2}$ = –2.66 kcal·mol^{-1}; eq. 3), which renders the nitrene N atom sterically inaccessible (Figure S2).

$$[(tpa)Ag]^+ + OTf^- \rightleftharpoons (tpa)Ag(OTf) \quad (1)$$

$$[(tpa)Ag(NSO_3R)]^+ + OTf^- \rightleftharpoons (tpa)Ag(OTf)(NSO_3R) \quad (2)$$

$$\{(tpy)_2[Ag_NAg_O(OTf)(NSO_3R)]\}^+ \ (A'(N_O)) \rightleftharpoons \{(tpy)_2[(TfO)Ag_OAg_N(NSO_3R)]\}^+ \ (A'(N)) \quad (3)$$

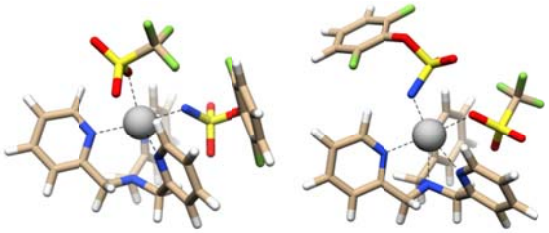


Figure S1. The optimized structures of the axial isomers of **B(N)**, **B(N_{ax})**.

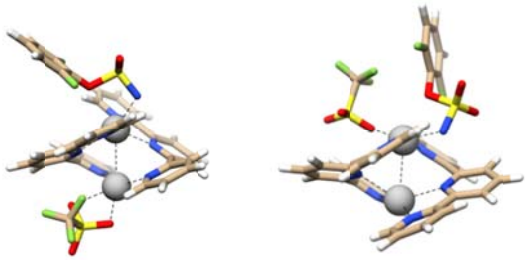


Figure S2. The optimized structures of the Ag_O isomers of $[(tpy)Ag]_2(OTf)(NSO_3dFPh)$.

Effect of truncation on A and A(N)

The structures of **A** and **A(N)** were optimized *without* truncating the peripheral ^{t}Bu groups on the para-positions of tpy ligands. The overlays of the truncated and untruncated structures are shown in Figure S1-3 and S1-4.

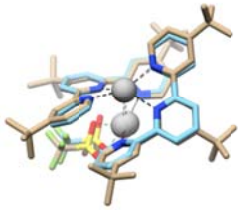


Figure S3. Overlay of the optimized structure of **A** (in beige) and **A'** (in cyan). Hydrogen atoms are omitted for clarity.

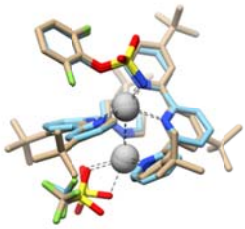


Figure S4. Overlay of the optimized structure of **A(N)** (in beige) and **A'(N)** (in cyan). Hydrogen atoms are omitted for clarity.

Electronic structure

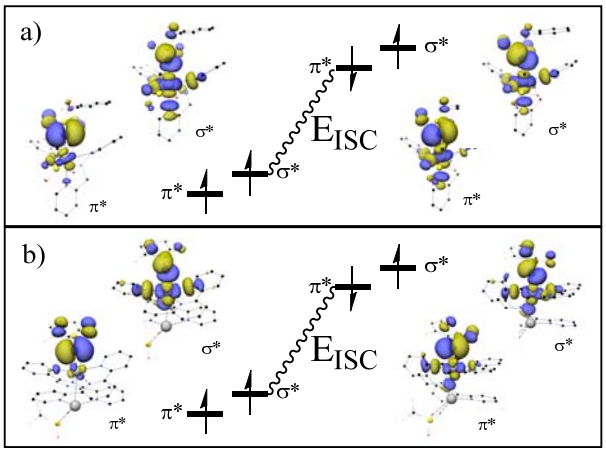


Figure S5. Frontier unrestricted natural orbitals of the silver-nitrene complexes. a) Orbitals of the triplet ground state and OS singlet excited state of **B(N)** and b) orbitals of the triplet ground state and OS singlet excited state of **A'(N).**

Energies

Table S5. Absolute energies, Zero-point vibrational energy, entropy, and solvent energies of two isomers of **B(N)** at the triplet spin state. Energy unit is Eh.

Complex	S	E	ZPVE+Thermo[a]	S[b]	Solv[c]
B(N)	1	-8368.161	0.492	0.106	-0.042
B(N_{ax})	1	-8368.156	0.492	0.107	-0.041

[a]ZPVE+Thermo = zero-point vibrational energy + thermal population of translation, rotational, and vibrational states at 295 K. [b]entropy at 295 K. [c]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424).

Table S6. Relative (to **B(N)**) energies, enthalpy, enthalpy in solvent, entropy, Gibbs free energy, and Gibbs free energy in solvent of two isomers of **B(N)** at the triplet spin state. Energy unit is kcal·mol^{-1}.

Complex	S	ΔE	ΔH	ΔH_{solv}[a]	ΔS[b]	ΔG[b]	ΔG_{solv}[a,b]
B(N)	1	0.000	0.000	0.000	0.000	0.000	0.000
B(N_{ax})	1	3.18	3.24	3.90	6.53	2.78	3.43

[a]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424). [b]entropy at 295 K.

Table S7. Absolute energies, Zero-point vibrational energy, entropy, and solvent energies of OTf^-, $[(tpa)Ag]^+$, triplet $[(tpa)Ag(NSO_3R)]^+$, and triplet **B(N_{ax})**.

Complex	S	E	ZPVE+Thermo[a]	S[b]	Solv[c]

OTf^-	0	-962.740	0.035	0.040	-0.081
$[(tpa)Ag]^+$	0	-6295.417	0.351	0.064	-0.054
$[(tpa)Ag(NSO_3R)]^+$	1	-7405.271	0.455	0.087	-0.069
$B(N_{ax})$	1	-8368.149	0.492	0.100	-0.050

[a]ZPVE+Thermo = zero-point vibrational energy + thermal population of translation, rotational, and vibrational states at 295 K. [b]entropy at 295 K. [c]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424).

Table S8. Absolute energies, Zero-point vibrational energy, entropy, and solvent energies of isomers of **A'(N)** at the triplet state spin.

Complex	S	E	ZPVE+Thermo[a]	S[b]	Solv[c]
$A'(N_O)$	1	-14317.12	0.63	0.12	-0.08
A'(N)	1	-14317.11	0.63	0.13	-0.09

[a]ZPVE+Thermo = zero-point vibrational energy + thermal population of translation, rotational, and vibrational states at 295 K. [b]entropy at 295 K. [c]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424).

Table S9. Reaction energies, enthalpy, enthalpy in solvent, entropy, Gibbs free energy, and Gibbs free energy in solvent of **eq. 1**, **2**, and **3** at the triplet spin state. Energy unit is kcal·mol^{-1}.

Rxn	S	ΔE	ΔH	ΔH_{solv}[a]	ΔS[b]	ΔG[b]	ΔG_{solv}[a,b]	K_{eq}
Eq. 1	1	-91.21	-92.05	-28.21	-235.31	-75.28	-11.44	2.45×10^8
Eq. 2	1	-94.07	-92.65	-24.81	-179.69	-79.85	-12.00	6.28×10^8
Eq. 3	1	8.26	8.69	-0.34	2.31	6.38	-2.66	88.89

[a]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424). [b]entropy at 295 K.

Table S10. Absolute energies, Zero-point vibrational energy, entropy, and solvent energies of **B(N)** at singlet, OS singlet, and triplet spin state.

Complex	S	E	ZPVE+Thermo[a]	S[b]	Solv[c]
B(N)	0	-8368.149	0.492	0.100	-0.050
B(N)	0bs	-8368.154	0.491	0.104	-0.044
B(N)	1	-8368.161	0.492	0.106	-0.042

[a]ZPVE+Thermo = zero-point vibrational energy + thermal population of translation, rotational, and vibrational states at 295 K. [b]entropy at 295 K. [c]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424).

Table S11. Relative (to ^{3}**B(N)**) energies, enthalpy, enthalpy in solvent, entropy, Gibbs free energy, and Gibbs free energy in solvent of **1N** at singlet, OS singlet, and triplet spin state. Energy unit is kcal·mol^{-1}.

Complex	S	ΔE	ΔH	ΔH_{solv}[a]	ΔS[b]	ΔG[b]	ΔG_{solv}[a,b]
B(N)	0	7.644	7.661	3.069	-4.163	11.823	7.232
B(N)	0bs	4.109	3.568	2.598	-1.536	5.104	4.133
B(N)	1	0.000	0.000	0.000	0.000	0.000	0.000

[a]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424). [b]entropy at 295 K.

Table S12. Absolute energies, Zero-point vibrational energy, entropy, and solvent energies of **2'N** at singlet, OS singlet, and triplet spin state.

Complex	S	E	ZPVE+Thermo[a]	S[b]	Solv[c]
A'(N)	0	-14317.096	0.629	0.123	-0.092
A'(N)	0bs	-14317.103	0.628	0.122	-0.091
A'(N)	1	-14317.111	0.630	0.128	-0.091

[a]ZPVE+Thermo = zero-point vibrational energy + thermal population of translation, rotational, and vibrational states at 295 K. [b]entropy at 295 K. [c]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424).

Table S13. Relative (to ^{3}**A'(N)**) energies, enthalpy, enthalpy in solvent, entropy, Gibbs free energy, and Gibbs free energy in solvent of **A'(N)** at singlet, OS singlet, and triplet spin state. Energy unit is kcal·mol^{-1}.

Complex	S	ΔE	ΔH	ΔH_{solv}[a]	ΔS[b]	ΔG[b]	ΔG_{solv}[a,b]
A'(N)	0	9.739	9.418	8.697	-3.395	12.814	12.092
A'(N)	0bs	5.498	4.311	4.382	-3.885	8.196	8.267
A'(N)	1	0.000	0.000	0.000	0.000	0.000	0.000

[a]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424). [b]entropy at 295 K.

Table S14. Absolute energies, Zero-point vibrational energy, entropy, and solvent energies of **B(N)** + sub **1** along the reaction coordinates **R**, $\mathbf{TS_I}$, $\mathbf{Int_I}$, $\mathbf{PC_I}$, $\mathbf{TS_A}$, $\mathbf{Int_A}$, and $\mathbf{PC_A}$ on either the triplet or OS singlet PES.

Complex	S	E	ZPVE+Thermo[a]	S[b]	Solv[c]
$\mathbf{R_{tpa,1}}$	0bs	-8602.74	0.643	0.138	-0.046
	1	-8602.752	0.644	0.140	-0.045
$\mathbf{TS_{tpa,I,1}}$	0bs	-8602.762	0.643	0.117	-0.040
	1	-8602.762	0.640	0.117	-0.038
$\mathbf{Int_{tpa,I,1}}$	0bs	-8602.809	0.644	0.117	-0.041

	1	-8602.813	0.644	0.116	-0.040
$PC_{tpa,I,1}$	0	-8602.909	0.648	0.115	-0.030
$TS_{tpa,A,1}$	1	-8602.768	0.645	0.116	-0.037
$Int_{tpa,A,1}$	0bs	-8602.803	0.647	0.116	-0.036
	1	-8602.803	0.647	0.116	-0.036
$PC_{tpa,A,1}$	0	-8602.884	0.649	0.114	-0.033

[a]ZPVE+Thermo = zero-point vibrational energy + thermal population of translation, rotational, and vibrational states at 295 K. [b]entropy at 295 K. [c]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424).

Table S15. Relative (to ^{3}**R**) energies, enthalpy, enthalpy in solvent, entropy, Gibbs free energy, and Gibbs free energy in solvent of **B(N)** + sub **1** along the reaction coordinates **R**, TS_I, Int_I, PC_I, TS_A, Int_A, and PC_A on either the triplet or OS singlet PES.

Complex	**S**	**ΔE**	**ΔH**	**$ΔH_{solv}$[a]**	**$ΔS^b$**	**$ΔG^b$**	**$ΔG_{solv}$[a,b]**
$R_{tpa,1}$	0bs	4.109	3.568	2.598	-21.553	5.104	4.133
	1	0.000	0.000	0.000	0.000	0.000	0.000
$TS_{tpa,I,1}$	0bs	-6.493	-7.065	-4.301	-201.988	7.328	10.092
	1	-6.314	-8.397	-4.530	-207.118	6.363	10.229
$Int_{tpa,I,1}$	0bs	-36.178	-35.815	-33.729	-203.188	-21.336	-19.250
	1	-38.253	-37.724	-34.695	-210.181	-22.746	-19.717
$PC_{tpa,I,1}$	0	-98.966	-96.178	-87.080	-220.721	-80.449	-71.351
$TS_{tpa,A,1}$	1	-10.441	-9.485	-4.748	-216.175	5.920	10.657
$Int_{tpa,A,1}$	0bs	-31.962	-29.963	-24.679	-215.873	-14.580	-9.296
	1	-32.224	-30.225	-24.915	-215.873	-14.842	-9.532
$PC_{tpa,A,1}$	0	-83.165	-79.978	-72.711	-230.138	-63.579	-56.311

[a]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424). [b]entropy at 295 K.

Table S16. Absolute energies, Zero-point vibrational energy, entropy, and solvent energies of **A'(N)** + sub **1** along the reaction coordinates **R**, TS_I, Int_I, PC_I, TS_A, Int_A, and PC_A on either the triplet or OS singlet PES.

Complex	**S**	**E**	**ZPVE+Thermo[a]**	**S^b**	**Solv[c]**
$R_{tpy,1}$	0bs	-14551.69	0.78	0.16	-0.09
	1	-14551.70	0.78	0.16	-0.09
$TS_{tpy,I,1}$	0bs	-14551.70	0.78	0.14	-0.09
	1	-14551.70	0.78	0.14	-0.09
$Int_{tpy,I,1}$	1	-14551.75	0.78	0.14	-0.09
$PC_{tpy,I,1}$	0	-14551.87	0.79	0.14	-0.09
$TS_{tpy,A,1}$	0bs	-14551.70	0.78	0.13	-0.09

	1	-14551.71	0.78	0.14	-0.09
$Int_{tpy,A,1}$	1	-14551.74	0.78	0.14	-0.09
$PC_{tpy,A,1}$	0	-14551.84	0.79	0.14	-0.08

[a]ZPVE+Thermo = zero-point vibrational energy + thermal population of translation, rotational, and vibrational states at 295 K. [b]entropy at 295 K. [c]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424).

Table S17. Relative (to ^{3}**R**) energies, enthalpy, enthalpy in solvent, entropy, Gibbs free energy, and Gibbs free energy in solvent of **A'(N)** + sub **1** along the reaction coordinates **R**, TS_I, Int_I, PC_I, TS_A, Int_A, and PC_A on either the triplet or OS singlet PES.

Complex	S	ΔE	ΔH	ΔH_{solv}[a]	ΔS[b]	ΔG[b]	ΔG_{solv}[a,b]
$R_{tpy,1}$	0bs	5.50	4.31	4.38	-54.52	8.20	8.27
	1	0.00	0.00	0.00	0.00	0.00	0.00
$TS_{tpy,I,1}$	0bs	3.82	1.90	1.25	-214.69	19.20	16.55
	1	-1.18	-3.44	-3.00	-202.22	10.97	11.41
$Int_{tpy,I,1}$	0	-29.75	-29.02	-29.38	-187.74	-15.64	-16.00
$PC_{tpy,I,1}$	0	-102.70	-98.47	-95.55	-194.29	-84.63	-81.71
$TS_{tpy,A,1}$	0bs	-1.27	-1.91	-1.55	-260.18	16.63	17.00
	1	-7.87	-7.25	-5.58	-210.02	7.71	9.38
$Int_{tpy,A,1}$	0	-25.74	-24.25	-23.00	-206.06	-9.57	-8.32
$PC_{tpy,A,1}$	0	-87.59	-84.62	-79.66	-240.06	-67.51	-62.55

[a]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424). [b]entropy at 295 K.

Table S18. Absolute energies, Zero-point vibrational energy, entropy, and solvent energies of **B(N)** + sub **21** along the reaction coordinates **R**, TS_I, Int_I, Int_I^{iso}, PC_I, TS_A, Int_A, Int_A^{iso}, and PC_A on either the triplet or OS singlet PES.

Complex	S	E	ZPVE+Thermo[a]	S[b]	Solv[c]
$R_{tpa,21}$	0bs	-8603.945	0.663	0.142	-0.046
	1	-8603.951	0.664	0.145	-0.045
$TS_{tpa,I,21}$	0bs	-8603.959	0.664	0.117	-0.045
	1	-8603.957	0.663	0.122	-0.039
$Int_{tpa,I,21}$	0bs	-8603.994	0.666	0.122	-0.041
	1	-8604.005	0.666	0.122	-0.039
$Int^{iso}_{tpa,I,21}$	1	-8604.014	0.667	0.125	-0.039
$TS_{tpa,A,21}$	1	-8603.968	0.666	0.119	-0.037
$Int_{tpa,A,21}$	1	-8604.007	0.665	0.114	-0.037
$Int^{iso}_{tpa,A,21}$	1	-8604.009	0.668	0.121	-0.035

[a]ZPVE+Thermo = zero-point vibrational energy + thermal population of translation, rotational, and vibrational states at 295 K. [b]entropy at 295 K. [c]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424).

Table S19. Relative (to ^{3}**R**) energies, enthalpy, enthalpy in solvent, entropy, Gibbs free energy, and Gibbs free energy in solvent of **B(N)** + sub **21** along the reaction coordinates **R**, $\mathbf{TS_I}$, $\mathbf{Int_I}$, $\mathbf{Int_I^{iso}}$, $\mathbf{PC_I}$, $\mathbf{TS_A}$, $\mathbf{Int_A}$, $\mathbf{Int_A^{iso}}$, and $\mathbf{PC_A}$ on either the triplet or OS singlet PES.

Complex	S	ΔE	ΔH	ΔH_{solv}[a]	ΔS[b]	ΔG[b]	ΔG_{solv}[a,b]
$\mathbf{R_{tpa,21}}$	0bs	4.109	3.568	2.598	-21.553	5.104	4.133
	1	0.000	0.000	0.000	0.000	0.000	0.000
$\mathbf{TS_{tpa,I,21}}$	0bs	-5.069	-4.974	-4.887	-238.598	12.028	12.115
	1	-3.216	-4.143	-0.514	-198.817	10.025	13.654
$\mathbf{Int_{tpa,I,21}}$	0bs	-26.552	-25.460	-23.110	-195.804	-11.507	-9.158
	1	-33.364	-32.148	-28.733	-195.414	-18.222	-14.808
$\mathbf{Int^{iso}_{tpa,I,21}}$	1	-39.561	-38.013	-34.397	-176.356	-25.446	-21.830
$\mathbf{TS_{tpa,A,21}}$	1	-10.461	-9.583	-4.693	-223.327	6.331	11.221
$\mathbf{Int_{tpa,A,21}}$	1	-34.665	-33.829	-29.034	-269.140	-14.650	-9.856
$\mathbf{Int^{iso}_{tpa,A,21}}$	1	-36.408	-34.057	-28.048	-205.366	-19.423	-13.414

[a]Solvent = CH_2Cl_2 (ε = 9.08 and refract = 1.424). [b]entropy at 295 K.

VII. Molecular Parameters for Computations. The molecular parameters for the computational studies are shown in the following tables.

Table S20. Selected bond lengths of catalyst **A'** optimized by different functionals, in unit Å.

Functional	Ag-Ag	Ag-$N_{pyr,mid}$	Ag-$N_{pyr,ter}$	Ag-O
BP86	2.837	2.386 (Ag_N)	2.238	2.305
BLYP	2.899	2.445 (Ag_N)	2.273	2.335
PBE	2.869	2.394 (Ag_N)	2.256	2.311
TPSS	2.810	2.400 (Ag_N)	2.240	2.286
B3LYP	2.922	2.432 (Ag_N)	2.295	2.360
PBE0	2.896	2.397 (Ag_N)	2.282	2.357
TPSSh	2.826	2.395 (Ag_N)	2.255	2.306
B3LYP[b]	3.080	2.376 (Ag_N)	2.292	2.466
–[a]	2.897	2.438 (Ag_N) 2.522 (Ag_N)	2.215	2.517

[a]optimized structure of the untruncated catalyst (**A**). [b]bond lengths from the crystal structure.

Table S21. Selected bond lengths of triplet **B(N_{ax})**, triplet $[(tpa)Ag(NSO_3R)]^+$, CS and OS singlet **B(N)**, and triplet **B(N)** in unit Å.

Complex	S	Ag-$N_{nitrene}$	Ag-$N_{pyr,cis}$	Ag-$N_{pyr,trans}$	Ag-$N_{tertiary}$	Ag-O
B(N_{ax})	1	2.117	2.563	2.276	2.511	2.207
$[(tpa)Ag(NSO_3R)]^+$	1	2.090	2.327	–	2.339	–
B(N)	0	1.997	2.216	2.248	2.613	2.462
B(N)	0bs	2.097	2.390	2.240	2.675	2.352
B(N)	1	2.117	2.402	2.255	2.672	2.341

Table S22. Selected bond lengths of triplet **A(N_O)** and CS and OS singlet **A'(N)**, triplet **A'(N)** ,and triplet **A(N)** in unit Å.

Complex	S	Ag_N-$N_{nitrene}$	Ag-Ag	Ag_N-$N_{pyr,eq}$	Ag_N-$N_{pyr,ax}$	Ag_O-$N_{pyr,}$	Ag-O
A'(N_O)	1	2.166	3.056	2.260	2.424	2.278	2.238
A'(N)	0	2.030	3.226	2.214	2.455	2.307	2.308
A'(N)	0bs	2.135	3.178	2.243	2.510	2.276	2.437
A'(N)	1	2.182	3.139	2.263	2.501	2.274	2.436
A(N)	1	2.186	3.447	2.236	2.478	2.242	2.340

Table S23. Selected bond lengths around the silver-nitrene complex in **B(N)** + sub **1** along the reaction coordinates $\mathbf{TS_I}$, $\mathbf{Int_I}$, and $\mathbf{PC_I}$ on either the triplet or OS singlet PES in unit Å.

Complex	S	Ag-$N_{nitrene}$	Ag-N_{pyr}[a]	Ag-$N_{tertiary}$	Ag-O
$\mathbf{TS_{tpa,I,1}}$	0bs	2.087	2.447 (cis)	2.679	2.385
	1	2.131	2.507 (cis)	2.693	2.325
$\mathbf{Int_{tpa,I,1}}$	0bs	2.157	2.530 (cis)	2.701	2.419
	1	2.125	2.442 (cis)	2.697	2.348
$\mathbf{PC_{tpa,I,1}}$	0	–	2.541 (cis)	2.622	2.400

[a]The longest Ag-N_{pyr} distance among the three Ag-N_{pyr} bonds and its relative position to $N_{nitrene}$.

Table S24. Selected bond lengths around the substrate in **B(N)** + sub **1** along the reaction coordinates sub **1**, $\mathbf{TS_I}$, $\mathbf{Int_I}$, and $\mathbf{PC_I}$ on either the triplet or OS singlet PES. Bonds are in units of Å and angles are in units of °.

Complex	S	$N_{nitrene}$-H	H-C	C=C	C3-(C=C)	ω(HC3C2H)
Sub 1	0	–	1.100	1.340	1.509	43.1
$\mathbf{TS_{tpa,I,1}}$	0bs	1.642	1.155	1.348	1.482	57.0

	1	1.465	1.232	1.353	1.469	59.4
$Int_{tpa,I,1}$	0bs	1.022	2.273	1.390	1.395	74.4
	1	1.024	2.375	1.394	1.393	77.4
$PC_{tpa,I,1}$	0	1.033	–	1.338	1.512	–

Table S25. Selected bond lengths around the silver-nitrene complex in **B(N)** + sub **1** along the reaction coordinates **TS_A**, **Int_A**, and **PC_A** on either the triplet or OS singlet PES in unit Å.

Complex	S	Ag-$N_{nitrene}$	Ag-N_{pyr}[a]	Ag-$N_{tertiary}$	Ag-O
$TS_{tpa,A,1}$	1	2.152	2.460 (cis)	2.667	2.357
$Int_{tpa,A,1}$	1	2.173	2.469 (cis)	2.672	2.329
$PC_{tpa,A,1}$	0	–	2.458 (trans)	2.633	2.447

[a]The longest Ag-N_{pyr} distance among the three Ag-N_{pyr} bonds and its relative position to $N_{nitrene}$.

Table S26. Selected bond lengths around the substrate in **B(N)** + sub **1** along the reaction coordinates sub **1**, **TS_A**, **Int_A**, and **PC_A** on either the triplet or OS singlet PES. Bonds are in units of Å and angles are in units of °.

Complex	S	$N_{nitrene}$-C	C=C	<NC1C2	ω(NC1C2H)	ω(HC1C2H)
Sub 1	0	–	1.340	–	–	1.24
$TS_{tpa,A,1}$	1	2.165	1.384	101.4	74.4	12.8
$Int_{tpa,A,1}$	1	1.504	1.499	113.6	78.7	31.9
$PC_{tpa,A,1}$	0	1.466	1.504	59.1	99.6	0.0

Table S27. Selected bond lengths and angles around the silver-nitrene complex in **A'(N)** + sub **1** along the reaction coordinates **TS_I**, **Int_I**, and **PC_I** on either the triplet or OS singlet PES. Bonds are in units of Å and angles are in units of °.

Complex	S	Ag-$N_{nitrene}$	Ag-Ag	Ag-O	Ag-Ag-$N_{nitrene}$
$TS_{tpy,I,1}$	0bs	2.212	2.955	2.328	168.45
	1	2.235	2.967	2.331	168.55
$Int_{tpy,I,1}$	1	2.212	2.947	2.316	169.39
$PC_{tpy,I,1}$	0	–	2.913	2.380	–

[a]The longest Ag-N_{pyr} distance among the three Ag-N_{pyr} bonds and its relative position to $N_{nitrene}$.

Table S28. Selected bond lengths and angles around the substrate in **A'(N)** + sub **1** along the reaction coordinates Sub **1**, $\mathbf{TS_A}$, $\mathbf{Int_A}$, and $\mathbf{PC_A}$ on either the triplet or OS singlet PES. Bonds are in units of Å and angles are in units of °.

Complex	S	$N_{nitrene}$-H	H-C	C=C	C3-(C=C)	ω(HC3C2H)
Sub 1	0	–	1.100	1.340	1.509	43.1
$\mathbf{TS_{tpa,I,1}}$	0bs	1.495	1.198	1.351	1.475	60.58
	1	1.444	1.224	1.353	1.469	63.72
$\mathbf{Int_{tpy,I,1}}$	1	1.023	2.371	1.394	1.394	0.76
$\mathbf{PC_{tpa,I,1}}$	0	1.016	–	1.339	1.510	–

Table S29. Selected bond lengths and angles around the silver-nitrene complex in **A'(N)** + sub **1** along the reaction coordinates $\mathbf{TS_A}$, $\mathbf{Int_A}$, and $\mathbf{PC_A}$ on either the triplet or OS singlet PES. Bonds are in units of Å and angles are in units of °.

Complex	S	Ag-$N_{nitrene}$	Ag-Ag	Ag-O	Ag-Ag-$N_{nitrene}$
$\mathbf{TS_{tpy,A,1}}$	0bs	2.197	2.913	2.326	168.95
	1	2.241	2.943	2.333	168.12
$\mathbf{Int_{tpy,A,1}}$	1	2.251	2.929	2.326	169.35
$\mathbf{PC_{tpy,A,1}}$	0	–	2.955	2.352	–

Table S30. Selected bond lengths and angles around the substrate in **A'(N)** + sub **1** along the reaction coordinates sub **1**, $\mathbf{TS_A}$, $\mathbf{Int_A}$, and $\mathbf{PC_A}$ on either the triplet or OS singlet PES. Bonds are in units of Å and angles are in units of °.

Complex	S	$N_{nitrene}$-C	C=C	<NC1C2	ω(NC1C2H)	ω(HC1C2H)
Sub 1	0	–	1.340	–	–	1.24
$\mathbf{TS_{tpa,A,1}}$	0bs	2.196	1.377	101.92	78.32	10.22
	1	2.061	1.392	106.26	78.52	15.52
$\mathbf{Int_{tpy,A,1}}$	1	1.493	1.496	115.71	64.03	49.24
$\mathbf{PC_{tpa,A,1}}$	0	1.468	1.504	58.85	99.33	1.18

Table S31. Selected bond lengths around the silver-nitrene complex in **B(N)** + sub 2**1** along the reaction coordinates $\mathbf{TS_I}$, $\mathbf{Int_I}$, and $\mathbf{PC_I}$ on either the triplet or OS singlet PES in unit Å

Complex	S	Ag-$N_{nitrene}$	Ag-N_{pyr}[a]	Ag-$N_{tertiary}$	Ag-O
$\mathbf{TS_{tpa,I,21}}$	0bs	2.071	2.328	2.667	2.399
	1	2.119	2.485	2.684	2.330
$\mathbf{Int_{tpa,I,21}}$	0bs	2.144	2.590	2.688	2.420
	1	2.116	2.458	2.694	2.350
$\mathbf{Int^{iso}_{tpa,I,21}}$	1	2.121	2.425	2.669	2.346

[a]The longest Ag-N_{pyr} distance among the three Ag-N_{pyr} bonds and its relative position to $N_{nitrene}$.

Table S32. Selected bond lengths around the substrate in **B(N)** + sub 2**1** along the reaction coordinates sub **21**, $\mathbf{TS_I}$, $\mathbf{Int_I}$, and $\mathbf{PC_I}$ on either the triplet or OS singlet PES. Bonds are in units of Å and angles are in units of °.

Complex	S	$N_{nitrene}$-H	H-C	C=C	C4-(C=C)	ω(HC4C3H)
Sub 21	0	–	1.098	1.341	1.504	164.87
$\mathbf{TS_{tpa,I,21}}$	0bs	1.744	1.149	1.349	1.482	77.35
	1	1.531	1.201	1.354	1.476	93.32
$\mathbf{Int_{tpa,I,21}}$	0bs	1.023	2.157	1.390	1.394	80.62
	1	1.025	2.319	1.394	1.393	78.79
$\mathbf{Int^{iso}_{tpa,I,21}}$	1	1.024	2.399	1.391	1.393	65.18

Table S33. Selected bond lengths around the silver-nitrene complex in **A'(N)** + sub **1** along the reaction coordinates $\mathbf{TS_A}$, $\mathbf{Int_A}$, and $\mathbf{PC_A}$ on either the triplet or OS singlet PES in unit Å.

Complex	S	Ag-$N_{nitrene}$	Ag-N_{pyr}[a]	Ag-$N_{tertiary}$	Ag-O
$\mathbf{TS_{tpa,A,21}}$	1	2.143	2.474	2.666	2.344
$\mathbf{Int_{tpa,A,21}}$	1	2.154	2.494	2.669	2.323
$\mathbf{Int^{iso}_{tpa,A,21}}$	1	2.149	2.504	2.647	2.362

[a]The longest Ag-N_{pyr} distance among the three Ag-N_{pyr} bonds and its relative position to $N_{nitrene}$.

Table S34. Selected bond lengths around the substrate in **A'(N)** + sub **1** along the reaction coordinates sub **21**, $\mathbf{TS_A}$, $\mathbf{Int_A}$, and $\mathbf{PC_A}$ on either the triplet or OS singlet PES. Bonds are in units of Å and angles are in units of °.

Complex	S	$N_{nitrene}$-C	C=C	<NC2C3	ω(NC2C3H)	ω(HC2C3H)
Sub 1	0	–	1.341	–	–	0.83
$\mathbf{TS_{tpa,A,21}}$	1	2.264	1.376	101.06	77.48	8.34
$\mathbf{Int_{tpa,A,21}}$	1	1.502	1.503	112.09	88.09	23.23
$\mathbf{Int^{iso}_{tpa,A,21}}$	1	1.500	1.499	112.06	87.00	160.98

VIII. Spin Populations.

Table S35. Group spin populations in triplet **B(N_{ax})**, triplet $[(tpa)Ag(NSO_3R)]^+$, CS and OS singlet **B(N)**, and triplet **B(N)** in unit Å.

Complex	S	ρ(Ag)	ρ($N_{nitrene}$)	ρ(SO_3R)	ρ(L)	ρ(OTf^-)
B(N_{ax})	1	0.458	1.172	0.113	0.190	0.067
$[(tpa)Ag(NSO_3R)]^+$	1	0.416	1.183	0.106	0.294	–
B(N)	0	–	–	–	–	–
B(N)	0bs	0.496	-0.720	-0.056	0.245	0.034
B(N)	1	0.463	1.145	0.116	0.242	0.034

Table S36. Group spin populations in triplet $\{(tpy)_2[Ag_NAg_O(OTf)(NSO_3R)]\}^+$ and CS and OS singlet **A'(N)**, and triplet **A'(N)** in unit Å.

Complex	S	ρ(Ag_N)	ρ(Ag_O)	ρ($N_{nitrene}$)	ρ(SO_3R)	ρ(L)	ρ(OTf^-)
$\{(tpy)_2[Ag_NAg_O(OTf)(NSO_3R)$	1	0.00	0.40	1.33	0.00	0.25	0.02
A'(N)	0	–	–	–	–	–	–
A'(N)	0bs	0.44	0.00	-0.74	0.00	0.30	0.00
A'(N)	1	0.41	0.00	1.28	0.00	0.31	0.00

Table S37. Group spin populations around the silver nitrene complexes in **B(N)** + sub **1** along the reaction coordinates TS_I and Int_I on either the triplet or OS singlet PES.

Complex	S	ρ(Ag)	ρ($N_{nitrene}$)	ρ(SO_3R)	ρ(L)	ρ(OTf^-)
$TS_{tpa,I,1}$	0bs	0.484	-0.544	-0.035	0.230	0.032
	1	0.469	0.804	0.085	0.212	0.040
$Int_{tpa,I,1}$	0bs	0.511	0.166	0.025	0.240	0.033
	1	0.520	0.177	0.027	0.256	0.036

Table S38. Group spin populations around the substrate in **B(N)** + sub **1** along the reaction coordinates TS_I and Int_I on either the triplet or OS singlet PES.

Complex	S	ρ(C1)	ρ(C2)	ρ(C3)
$TS_{tpa,I,1}$	0bs	-0.078	0.052	-0.179
	1	0.220	-0.137	0.361
$Int_{tpa,I,1}$	0bs	-0.676	0.313	-0.669
	1	0.693	-0.319	0.673

Table S39. Group spin populations around the silver nitrene complexes in **B(N)** + sub **1** along the reaction coordinates $\mathbf{TS_A}$ and $\mathbf{Int_A}$ on either the triplet or OS singlet PES.

Complex	S	ρ(Ag)	$\rho(N_{nitrene})$	$\rho(SO_3R)$	ρ(L)	$\rho(OTf^-)$
$\mathbf{TS_{tpa,A,1}}$	1	0.442	0.791	0.090	0.207	0.024
$\mathbf{Int_{tpa,A,1}}$	0bs	0.500	0.136	0.020	0.240	0.033
	1	0.499	0.234	0.033	0.251	0.035

Table S40. Group spin populations around the silver nitrene complexes in **A'(N)** + sub **1** along the reaction coordinates $\mathbf{TS_I}$ and $\mathbf{Int_I}$ on either the triplet or OS singlet PES.

Complex	S	ρ(C1)	ρ(C2)	ρ(C3)
$\mathbf{TS_{tpa,A,1}}$	1	0.011	-0.123	0.570
$\mathbf{Int_{tpa,A,1}}$	0bs	0.004	0.052	-1.015
	1	0.015	-0.061	1.016

Table S41. Group spin populations around the silver nitrene complexes in **A'(N)** + sub **1** along the reaction coordinates $\mathbf{TS_I}$ and $\mathbf{Int_I}$ on either the triplet or OS singlet PES.

Complex	S	$\rho(Ag_N)$	$\rho(Ag_O)$	$\rho(N_{nitrene})$	$\rho(SO_3R)$	ρ(L)	$\rho(OTf^-)$
$\mathbf{TS_{tpy,I,1}}$	0bs	-0.432	-0.015	0.396	0.023	-0.300	-0.001
	1	0.357	0.012	0.903	0.077	0.246	0.001
$\mathbf{Int_{tpy,I,1}}$	1	0.427	0.014	0.241	0.029	0.297	0.001

Table S42. Group spin populations around the substrate in **A'(N)** + sub **1** along the reaction coordinates $\mathbf{TS_I}$ and $\mathbf{Int_I}$ on either the triplet or OS singlet PES.

Complex	S	ρ(C1)	ρ(C2)	ρ(C3)
$\mathbf{TS_{tpy,I,1}}$	0bs	0.178	-0.108	0.303
	1	0.230	-0.136	0.356
$\mathbf{Int_{tpy,I,1}}$	1	0.694	-0.319	0.676

Table S43. Group spin populations around the silver nitrene complexes in **A'(N)** + sub **1** along the reaction coordinates $\mathbf{TS_A}$ and $\mathbf{Int_A}$ on either the triplet or OS singlet PES.

Complex	S	$\rho(Ag_N)$	$\rho(Ag_O)$	$\rho(N_{nitrene})$	$\rho(SO_3R)$	ρ(L)	$\rho(OTf^-)$
$\mathbf{TS_{tpy,A,1}}$	0bs	-0.375	-0.016	0.215	0.001	-0.234	-0.001
	1	0.279	0.009	0.953	0.074	0.171	0.001
$\mathbf{Int_{tpy,A,1}}$	1	0.342	0.013	0.425	0.035	0.222	0.001

Table S44. Group spin populations around the substrate in **A'(N**)+ sub **1** along the reaction coordinates $\mathbf{TS_A}$ and $\mathbf{Int_A}$ on either the triplet or OS singlet PES.

Complex	S	ρ(C1)	ρ(C2)	ρ(C3)
$\mathbf{TS_{tpy,A,1}}$	0bs	-0.037	0.495	-0.079
	1	-0.120	0.632	-0.047
$\mathbf{Int_{tpy,A,1}}$	1	-0.079	1.012	-0.072

Table S45. Group spin populations around the silver nitrene complexes in **B(N)** + sub **21** along the reaction coordinates $\mathbf{TS_I}$, $\mathbf{Int_I}$, and $\mathbf{Int_I^{iso}}$ on either the triplet or OS singlet PES.

Complex	S	ρ(Ag)	ρ($\mathbf{N_{nitrene}}$)	ρ($\mathbf{SO_3R}$)	ρ(L)	ρ($\mathbf{OTf^-}$)
$\mathbf{TS_{tpa,I,21}}$	0bs	0.436	-0.530	-0.035	0.244	0.015
	1	0.468	0.856	0.090	0.216	0.038
$\mathbf{Int_{tpa,I,21}}$	0bs	0.519	0.151	0.021	0.245	0.037
	1	0.520	0.184	0.027	0.245	0.038
$\mathbf{Int^{iso}_{tpa,I,21}}$	1	0.511	0.186	0.029	0.250	0.034

Table S46. Group spin populations around the substrate in **B(N)** + sub **21** along the reaction coordinates $\mathbf{TS_I}$, $\mathbf{Int_I}$, and $\mathbf{Int_I^{iso}}$ on either the triplet or OS singlet PES.

Complex	S	ρ(C2)	ρ(C3)	ρ(C4)
$\mathbf{TS_{tpa,I,21}}$	0bs	-0.087	0.053	-0.125
	1	0.205	-0.122	0.304
$\mathbf{Int_{tpa,I,21}}$	0bs	-0.694	0.328	-0.660
	1	0.709	-0.333	0.669
$\mathbf{Int_{tpa,I,21}}$	1	0.694	-0.330	0.683

Table S47. Group spin populations around the silver nitrene complexes in **B(N)** + sub **21** along the reaction coordinates $\mathbf{TS_A}$, $\mathbf{Int_A}$, and $\mathbf{Int^{iso}_{tpa,A,21}}$ on either the triplet or OS singlet PES.

Complex	S	ρ(Ag)	ρ($\mathbf{N_{nitrene}}$)	ρ($\mathbf{SO_3R}$)	ρ(L)	ρ($\mathbf{OTf^-}$)
$\mathbf{TS_{tpa,A,21}}$	1	0.441	0.878	0.099	0.205	0.027
$\mathbf{Int_{tpa,A,21}}$	1	0.510	0.216	0.032	0.260	0.035
$\mathbf{Int^{iso}_{tpa,A,21}}$	1	0.501	0.225	0.030	0.251	0.038

Table S48. Group spin populations around the substrate complexes in **B(N)** + sub **21** along the reaction coordinates $\mathbf{TS_A}$, $\mathbf{Int_A}$, and $\mathbf{Int^{iso}_{tpa,A,21}}$ on either the triplet or OS singlet PES.

Complex	S	ρ(C2)	ρ(C3)	ρ(C4)
$\mathbf{TS_{tpa,A,21}}$	1	-0.119	0.472	-0.036

$\mathbf{Int_{tpa,A,21}}$	1	-0.061	1.022	-0.079
$\mathbf{Int^{iso}_{tpa,A,21}}$	1	-0.062	1.022	-0.083

IX. Coordinates.

Coordinates
L = tpa

^{3}B(N_{ax})

S	6.58560	3.35020	3.32017
N	5.06333	-0.34224	2.12087
O	6.53544	3.53568	4.77171
N	4.19593	1.07791	4.30161
O	5.19394	3.39666	2.68218
N	6.11053	1.49596	0.09366
C	3.70835	1.83503	5.29043
C	6.82602	2.52234	-0.36513
C	2.79387	-0.84698	1.28505
C	3.86312	-1.17185	2.29843
H	3.45424	-0.95279	3.29158
H	4.10796	-2.24654	2.26383
O	7.41799	2.24798	2.79655
C	5.81142	-0.74705	0.91238
H	5.07470	-0.97501	0.13228
H	6.38075	-1.67061	1.10741
C	1.71250	0.85421	0.09929
C	8.20669	2.42761	-0.57462
N	2.66491	0.44474	0.93733
C	0.91918	-1.39938	-0.12405
H	0.23415	-2.13301	-0.54594
C	0.80782	-0.04916	-0.45983
C	6.71997	0.34157	0.38980
C	5.32801	0.39772	4.49394
C	8.84721	1.22741	-0.27923
H	9.92287	1.12362	-0.41323
C	1.92471	-1.80521	0.75925
H	2.03774	-2.85020	1.04070
C	4.31910	1.92213	6.53888
C	6.00455	0.41578	5.71951
H	6.93416	-0.13779	5.84022
C	8.09097	0.15877	0.21495
H	8.55926	-0.78866	0.47661
C	5.92110	-0.34181	3.31090
H	6.84544	0.18668	3.04729
H	6.18175	-1.37633	3.60000
C	5.48931	1.19044	6.75533
H	6.00762	1.24508	7.71097
H	2.80665	2.40446	5.06371
H	3.90201	2.56379	7.31144
H	1.69926	1.92716	-0.10065
H	0.04474	0.31234	-1.14488
H	6.27931	3.44982	-0.53280
H	8.75998	3.29167	-0.93479
Ag	4.13673	1.84116	1.71227
N	2.96978	3.29620	0.95076
S	3.58661	4.79103	0.87953
O	4.84578	4.90500	0.12336
O	3.37421	5.67939	2.01126
O	2.30482	5.27917	-0.21772
C	7.33787	4.91836	2.64496
F	8.45580	5.16122	3.32037
F	7.63734	4.76301	1.36158
F	6.50395	5.92497	2.79172
C	2.51655	5.12223	-1.54441
C	2.89418	4.81758	-4.31102
C	3.37642	5.98286	-2.25271
C	1.83913	4.12480	-2.26345
C	2.02114	3.96229	-3.63241
C	3.56729	5.83039	-3.62434
H	1.47431	3.17423	-4.14566
H	4.23907	6.51813	-4.13344
H	3.04347	4.69878	-5.38233
F	3.97786	6.96434	-1.60856
F	0.99574	3.32271	-1.61183

^{1}B(N)

S	2.16256	4.18508	1.51443
N	6.29754	0.21795	1.81731
O	0.79611	4.27466	0.98535

N	5.25078	2.07461	3.72984
O	3.18893	3.81808	0.46980
N	5.63278	1.94769	-0.45972
C	4.59144	2.81244	4.63306
C	5.19851	2.68071	-1.49194
C	3.99963	-0.61767	1.27494
C	5.31362	-0.83180	1.99559
H	5.07261	-0.89151	3.06620
H	5.71618	-1.82182	1.71361
O	2.34238	3.37694	2.75272
C	7.04903	0.17633	0.57580
H	7.26067	-0.86351	0.27133
H	8.00913	0.67483	0.74750
C	2.31468	0.84130	0.61717
C	5.58123	2.38382	-2.79826
N	3.51903	0.63262	1.16997
C	2.00873	-1.50913	0.24405
H	1.42379	-2.35151	-0.12142
C	1.52071	-0.20623	0.15230
C	6.45058	0.90352	-0.62765
C	6.21877	1.21926	4.09642
C	6.42014	1.28684	-3.01092
H	6.73340	1.01734	-4.01840
C	3.26864	-1.71396	0.80696
H	3.68923	-2.71421	0.89251
C	4.87496	2.71033	5.99395
C	6.52667	1.04735	5.44802
H	7.31783	0.35759	5.73237
C	6.85385	0.53737	-1.91768
H	7.51246	-0.31908	-2.05285
C	7.04592	0.52428	3.02672
H	7.85586	1.21547	2.77028
H	7.50774	-0.37378	3.47510
C	5.85609	1.80911	6.40595
H	6.10839	1.71080	7.45983
H	3.82499	3.47489	4.23419
H	4.34001	3.33467	6.70454
H	1.98791	1.87044	0.52463
H	0.54775	0.01352	-0.28001
H	4.52225	3.49721	-1.23915
H	5.22083	2.99527	-3.62196
Ag	4.86361	2.38906	1.57282
N	5.92758	4.07422	1.69289
S	7.49517	3.99515	1.81501
O	8.03039	5.34949	1.68947
O	8.15456	2.87558	1.12081
O	7.93005	3.48610	3.43289
C	2.62888	5.91412	2.03088
F	1.60954	6.46505	2.67974
F	3.68013	5.87103	2.84023
F	2.91921	6.64903	0.96901
C	7.75679	4.16168	4.59058
C	7.49241	5.25928	7.18120
C	6.93067	5.27465	4.82299
C	8.43715	3.62032	5.69820
C	8.31685	4.14851	6.97643
C	6.80862	5.81889	6.10305
H	8.86893	3.68017	7.78862
H	6.15799	6.68283	6.22221
H	7.39048	5.68944	8.17512
F	6.24447	5.82213	3.83308
F	9.18832	2.53851	5.49346

^{OS1}B(N)

S	2.07063	3.96915	2.14930
N	5.90736	-0.14061	1.66856
O	0.68294	4.21053	1.74140
N	5.41976	1.66264	3.72581
O	3.00556	3.76942	0.96859
N	5.86056	1.79384	-0.51045
C	4.95996	2.38037	4.76031
C	6.02816	2.81637	-1.35222
C	3.51167	-0.68514	1.41970
C	4.81426	-0.97727	2.13009
H	4.65350	-0.77038	3.19574
H	5.04071	-2.05683	2.05001
O	2.30124	2.95841	3.21278
C	6.37594	-0.45206	0.32919
H	5.57325	-0.99819	-0.18594
H	7.24634	-1.13100	0.34519
C	2.05738	0.91402	0.55782
C	7.05368	2.84261	-2.29898
N	3.22342	0.59565	1.13590
C	1.38806	-1.38930	0.51762
H	0.67209	-2.17289	0.27522
C	1.10580	-0.05317	0.23552
C	6.69881	0.74962	-0.54606
C	6.47485	0.85297	3.86233
C	7.94929	1.77611	-2.33074
H	8.78437	1.77307	-3.02972
C	2.61023	-1.70840	1.11205

H	2.87030	-2.74003	1.34190
C	5.55943	2.31079	6.01512
C	7.13168	0.73760	5.09323
H	7.99036	0.07532	5.18893
C	7.77109	0.71298	-1.44061
H	8.45407	-0.13506	-1.43758
C	6.95216	0.07113	2.65199
H	7.74617	0.66345	2.18383
H	7.39791	-0.88140	2.99854
C	6.67098	1.48102	6.17844
H	7.17380	1.41338	7.14176
H	4.09472	3.00756	4.55514
H	5.17081	2.90865	6.83445
H	1.89455	1.97010	0.35499
H	0.16910	0.24957	-0.22612
H	5.33363	3.64904	-1.24721
H	7.16399	3.70035	-2.95773
Ag	4.68366	2.23681	1.57537
N	5.84448	3.93869	1.96455
S	7.41154	3.97385	1.60124
O	7.68381	4.54702	0.28698
O	8.08333	2.72683	2.00093
O	8.03215	5.17246	2.62696
C	2.66443	5.57515	2.91351
F	1.65494	6.17218	3.53287
F	3.61537	5.31209	3.81383
F	3.15360	6.38216	1.98986
C	7.57587	5.23373	3.91324
C	6.72693	5.53875	6.55796
C	6.48190	6.05783	4.21943
C	8.21798	4.54010	4.94739
C	7.81194	4.70731	6.26978
C	6.05116	6.20871	5.53533
H	8.34752	4.17237	7.05077
H	5.19324	6.84624	5.73359
H	6.40369	5.66439	7.58961
F	5.88479	6.70756	3.24000
F	9.22928	3.73514	4.65984

^{3}B(N)

S	2.10396	3.98050	2.11456
N	5.89359	-0.15944	1.65675
O	0.72551	4.22714	1.67819
N	5.38948	1.57935	3.75315
O	3.06518	3.79895	0.95206
N	5.86722	1.79899	-0.50052
C	4.95424	2.31247	4.78750
C	6.02731	2.81760	-1.34901
C	3.49332	-0.70304	1.39120
C	4.79509	-0.99750	2.10543
H	4.62838	-0.79545	3.17078
H	5.02241	-2.07656	2.02011
O	2.31036	2.95628	3.16958
C	6.36759	-0.46091	0.31758
H	5.56742	-1.00364	-0.20516
H	7.23816	-1.13986	0.33127
C	2.03652	0.90049	0.54398
C	7.03621	2.83369	-2.31340
N	3.20445	0.57811	1.11404
C	1.36733	-1.40222	0.49185
H	0.65045	-2.18432	0.24717
C	1.08277	-0.06417	0.21970
C	6.69318	0.74539	-0.55130
C	6.47598	0.81102	3.86448
C	7.92476	1.76148	-2.35565
H	8.74853	1.75079	-3.06790
C	2.59146	-1.72550	1.08043
H	2.85094	-2.75872	1.30411
C	5.61148	2.29988	6.01511
C	7.18935	0.74556	5.06803
H	8.07505	0.11689	5.14205
C	7.75183	0.70059	-1.46201
H	8.42671	-0.15387	-1.47040
C	6.93915	0.03508	2.64405
H	7.73865	0.62599	2.18196
H	7.38092	-0.92438	2.97743
C	6.75353	1.50589	6.15163
H	7.30082	1.48249	7.09259
H	4.06594	2.91384	4.59979
H	5.24437	2.91178	6.83421
H	1.87065	1.95767	0.34821
H	0.14340	0.24049	-0.23532
H	5.33797	3.65360	-1.23724
H	7.13962	3.68719	-2.97891
Ag	4.68273	2.22030	1.56275
N	5.86792	3.88799	2.10569
S	7.44072	3.94145	1.68862
O	7.63273	4.45923	0.33891
O	8.16041	2.73561	2.11935
O	8.02654	5.19360	2.65520
C	2.67892	5.57433	2.91586

F	1.65928	6.15486	3.53458
F	3.62054	5.29935	3.82191
F	3.17398	6.40254	2.01332
C	7.57011	5.28151	3.94524
C	6.69871	5.61237	6.57760
C	6.46631	6.09931	4.23077
C	8.21713	4.61358	4.99313
C	7.79716	4.79191	6.30968
C	6.02465	6.26275	5.54152
H	8.33306	4.27456	7.10221
H	5.15763	6.89229	5.72496
H	6.36422	5.74588	7.60468
F	5.86928	6.72876	3.23865
F	9.24287	3.82158	4.72438

L = tpa and substrate = **1**

Sub **1**

C	-0.01520	-0.01361	0.01880
C	0.81446	-1.27240	0.07428
C	2.14935	-1.27266	0.19089
C	2.97955	-0.01421	0.24589
C	2.18038	1.22410	-0.18492
C	0.78448	1.22449	0.44924
H	0.23823	2.14003	0.18522
H	0.88894	1.22370	1.54502
H	2.07593	1.22303	-1.28069
H	2.72702	2.13949	0.07883
H	3.36514	0.12326	1.27068
H	3.87109	-0.13152	-0.38804
H	2.68119	-2.22457	0.24793
H	0.28222	-2.22410	0.01762
H	-0.40065	0.12369	-1.00607
H	-0.90684	-0.13031	0.65270

$^{OS1}TS_{tpa,I,1}$

S	0.17346	-0.03006	0.21379
O	-1.18414	0.15410	-0.31214
O	1.22819	-0.07563	-0.87413
Ag	2.88135	-1.76576	-0.55691
N	3.49088	-2.32415	1.67267
C	3.10285	-1.52477	2.67324
C	3.62252	-1.65637	3.95939
C	4.58132	-2.64337	4.19361
C	4.97219	-3.47193	3.14257
C	4.40246	-3.28049	1.87852
C	4.81658	-4.14527	0.70387
N	3.76958	-4.27910	-0.29080
C	2.56697	-4.94182	0.17586
C	1.33763	-4.52879	-0.60382
N	1.24162	-3.24669	-0.99094
C	0.14388	-2.81697	-1.62792
C	-0.92597	-3.66362	-1.91426
C	-0.84039	-5.00085	-1.52796
H	-1.65368	-5.69397	-1.73678
C	0.30958	-5.43861	-0.86871
H	0.41565	-6.47493	-0.55366
H	-1.80229	-3.26752	-2.42139
H	0.12111	-1.76267	-1.89180
H	2.39934	-4.65017	1.22042
H	2.65413	-6.04465	0.16583
C	4.22223	-4.71673	-1.59675
H	3.34827	-5.09885	-2.14233
H	4.93590	-5.55797	-1.52926
C	4.82583	-3.62288	-2.46029
N	4.19550	-2.43988	-2.50784
C	4.62331	-1.49104	-3.34392
C	5.71586	-1.67983	-4.19301
C	6.39785	-2.89201	-4.13506
H	7.27641	-3.06763	-4.75395
C	5.94572	-3.87936	-3.25425
H	6.45453	-4.83876	-3.17914
H	6.03655	-0.87154	-4.84508
H	4.09958	-0.53682	-3.31988
H	5.67378	-3.65000	0.23176
H	5.16016	-5.12678	1.08458
H	5.70937	-4.25912	3.29115
H	5.01643	-2.76953	5.18377
H	3.28635	-0.99036	4.74838
H	2.34790	-0.78406	2.42842
N	4.14306	-0.12576	-0.28238
S	5.73983	-0.26424	-0.40781
O	6.33373	0.14434	-1.68093
O	6.17815	-1.53492	0.19351
O	6.31443	0.98260	0.60514
C	5.83859	1.06238	1.88056
C	4.74994	1.89543	2.17974
C	4.31183	2.06307	3.49081
C	4.97828	1.39993	4.52350
C	6.06083	0.56109	4.24760

C	6.47591	0.38319	2.92961
F	7.49842	-0.41012	2.65746
H	6.59150	0.03218	5.03610
H	4.64979	1.53675	5.55205
H	3.45773	2.70972	3.67565
F	4.15938	2.55715	1.19733
O	0.37387	-1.07898	1.23949
C	0.57715	1.55084	1.11375
F	-0.38611	1.83673	1.97778
F	1.72336	1.40723	1.78767
F	0.71002	2.56205	0.26260
C	3.49071	2.20690	-1.67217
C	2.89161	1.69456	-2.92701
C	3.39412	1.96349	-4.14864
C	4.56520	2.88931	-4.35783
C	4.74654	3.83473	-3.16161
C	4.75926	3.04456	-1.84630
H	4.88632	3.70843	-0.98389
H	5.62873	2.37506	-1.85506
H	3.91943	4.56104	-3.15437
H	5.67697	4.40923	-3.26687
H	5.48570	2.29697	-4.50224
H	4.42652	3.46037	-5.28748
H	2.91928	1.53119	-5.03205
H	2.00731	1.06758	-2.80988
H	2.72721	2.67426	-1.03755
H	3.73650	1.27822	-1.03088

$^3TS_{tpa,I,1}$

S	0.18182	-0.01668	0.25637
O	-1.15342	0.26102	-0.28382
O	1.25009	-0.04662	-0.82455
Ag	2.86787	-1.70828	-0.66599
N	3.42016	-2.43646	1.66860
C	3.09819	-1.63249	2.68846
C	3.77059	-1.68105	3.90783
C	4.80737	-2.60530	4.06038
C	5.12290	-3.45017	2.99861
C	4.40759	-3.32404	1.80149
C	4.77254	-4.16642	0.59513
N	3.70702	-4.25155	-0.38630
C	2.49381	-4.89335	0.08174
C	1.26681	-4.45651	-0.68869
N	1.19777	-3.17886	-1.09369
C	0.09523	-2.72676	-1.70642
C	-1.00404	-3.54585	-1.95728
C	-0.94433	-4.88088	-1.55726
H	-1.78101	-5.55397	-1.73762
C	0.20793	-5.34133	-0.91884
H	0.29178	-6.37567	-0.59080
H	-1.88296	-3.13199	-2.44544
H	0.08982	-1.67335	-1.97512
H	2.33407	-4.59916	1.12594
H	2.56217	-5.99763	0.06570
C	4.13543	-4.69011	-1.69743
H	3.24117	-4.99413	-2.25924
H	4.78911	-5.58091	-1.64966
C	4.82111	-3.61629	-2.52075
N	4.28869	-2.38457	-2.51580
C	4.79392	-1.44255	-3.31828
C	5.86625	-1.68575	-4.17850
C	6.44603	-2.95131	-4.17349
H	7.30329	-3.17497	-4.80663
C	5.91457	-3.93175	-3.33075
H	6.33951	-4.93332	-3.29769
H	6.24763	-0.88262	-4.80384
H	4.33616	-0.45859	-3.26991
H	5.63369	-3.67548	0.12289
H	5.10671	-5.16673	0.93492
H	5.92441	-4.18259	3.08042
H	5.36254	-2.66582	4.99521
H	3.49217	-1.00193	4.70848
H	2.27834	-0.94360	2.50874
N	4.15286	-0.09199	-0.13821
S	5.75761	-0.26168	-0.21407
O	6.40718	0.02123	-1.49538
O	6.17408	-1.46104	0.52566
O	6.26414	1.08184	0.70499
C	5.78958	1.20921	1.97918
C	4.67193	2.01503	2.24031
C	4.21571	2.21162	3.54071
C	4.88876	1.59981	4.60045
C	6.00441	0.79348	4.36275
C	6.44276	0.59145	3.05590
F	7.49890	-0.16850	2.82212
H	6.54402	0.30824	5.17300
H	4.54194	1.75486	5.62031
H	3.33829	2.83368	3.69735
F	4.06595	2.62162	1.22956
O	0.32075	-1.12663	1.22113
C	0.64591	1.49892	1.23943

F	-0.32903	1.80552	2.08235
F	1.75649	1.25946	1.94163
F	0.86726	2.53665	0.43832
C	3.50564	2.02390	-1.67788
C	2.87042	1.55334	-2.91571
C	3.36169	1.82699	-4.14582
C	4.55595	2.71961	-4.35775
C	4.76487	3.65408	-3.15745
C	4.77478	2.85549	-1.84597
H	4.90431	3.51047	-0.97826
H	5.64439	2.18595	-1.85955
H	3.95110	4.39462	-3.13959
H	5.70505	4.21144	-3.26501
H	5.46047	2.10346	-4.50817
H	4.42950	3.29663	-5.28513
H	2.85630	1.42512	-5.02618
H	1.96382	0.96119	-2.79663
H	2.77664	2.41436	-0.96030
H	3.79258	1.02625	-1.01394

^{3}TS$_{tpa,A,1}$

S	-0.38416	-0.32886	-0.53353
O	-1.58134	-0.60627	-1.33846
O	0.86880	-0.16793	-1.37513
Ag	2.70700	-1.55315	-0.86694
N	2.93470	-1.75316	1.57386
C	2.39918	-0.81845	2.36619
C	2.76654	-0.68685	3.70392
C	3.73043	-1.55776	4.21758
C	4.28292	-2.52674	3.38225
C	3.85938	-2.59169	2.04857
C	4.46304	-3.61046	1.09980
N	3.60518	-3.92086	-0.02912
C	2.35180	-4.56032	0.33648
C	1.29502	-4.41092	-0.73331
N	1.21160	-3.22515	-1.35479
C	0.26547	-3.01471	-2.27657
C	-0.66144	-3.99690	-2.62635
C	-0.58628	-5.23745	-1.99468
H	-1.29149	-6.03016	-2.23958
C	0.40977	-5.44870	-1.03868
H	0.50212	-6.40399	-0.52553
H	-1.42693	-3.77556	-3.36595
H	0.23134	-2.02166	-2.71597
H	1.96845	-4.06420	1.23696
H	2.47698	-5.63108	0.58579
C	4.28448	-4.53347	-1.15510
H	3.55933	-5.16591	-1.68670
H	5.09180	-5.21077	-0.82734
C	4.84784	-3.57882	-2.19858
N	4.15054	-2.47979	-2.51822
C	4.56113	-1.69846	-3.52165
C	5.70588	-1.97234	-4.26800
C	6.45684	-3.09665	-3.93030
H	7.37542	-3.33261	-4.46495
C	6.01997	-3.91074	-2.88400
H	6.58372	-4.79501	-2.59247
H	6.00989	-1.29790	-5.06428
H	3.96471	-0.81119	-3.72024
H	5.38715	-3.17093	0.70731
H	4.73323	-4.51832	1.67434
H	5.03685	-3.22123	3.74851
H	4.04874	-1.48335	5.25573
H	2.30797	0.08246	4.32095
H	1.64496	-0.18160	1.91348
N	3.98365	0.12569	-0.43733
S	5.54824	-0.08836	-0.73229
O	6.07694	0.37666	-2.01810
O	6.00833	-1.40311	-0.24552
O	6.25841	1.05488	0.34668
C	6.45815	0.68677	1.64019
C	5.58954	1.11211	2.65544
C	5.86104	0.84420	3.99457
C	6.98815	0.09185	4.32946
C	7.84977	-0.37414	3.33307
C	7.58747	-0.06893	1.99971
F	8.42232	-0.46401	1.05482
H	8.73871	-0.95507	3.56918
H	7.20018	-0.12863	5.37389
H	5.17468	1.21866	4.74963
F	4.50379	1.80593	2.33406
O	-0.17029	-1.14777	0.67598
C	-0.60911	1.39449	0.12732
F	-1.68047	1.45414	0.90259
F	0.46650	1.72808	0.86114
F	-0.72788	2.26990	-0.85941
C	3.94686	3.05913	-0.74292
C	3.11320	1.92382	-1.27157
C	3.08279	1.61367	-2.62045
C	4.05290	2.18907	-3.60332
C	4.60692	3.54820	-3.14149

C	5.08106	3.48742	-1.68398
H	5.46856	4.46553	-1.36815
H	5.90820	2.77434	-1.60247
H	3.81755	4.30975	-3.24172
H	5.42997	3.85741	-3.79946
H	4.89287	1.48197	-3.70950
H	3.57849	2.27052	-4.59201
H	2.32369	0.90439	-2.94961
H	2.26523	1.61853	-0.67170
H	3.24611	3.89905	-0.59070
H	4.32646	2.80279	0.24991

$^{OS1}Int_{tpa,I,1}$

S	-0.05364	0.04919	-0.09074
O	-1.42494	0.27932	-0.55918
O	0.95721	-0.02637	-1.21672
O	0.15224	-1.00218	0.93157
C	0.44228	1.61485	0.78818
F	-0.48468	1.97045	1.66444
F	1.59324	1.42277	1.43875
F	0.61348	2.60857	-0.08533
Ag	2.61875	-1.73285	-0.79140
N	3.29888	-2.31936	1.43346
C	2.85066	-1.60634	2.47197
C	3.36338	-1.77994	3.75683
C	4.38624	-2.71107	3.94539
C	4.84637	-3.44514	2.85259
C	4.26841	-3.22566	1.59633
C	4.71498	-4.01316	0.38036
N	3.63648	-4.22535	-0.56902
C	2.49640	-4.95892	-0.05822
C	1.20049	-4.59381	-0.75497
N	1.02369	-3.31961	-1.13498
C	-0.13450	-2.93824	-1.68904
C	-1.18877	-3.82745	-1.89302
C	-1.01957	-5.15909	-1.51280
H	-1.81723	-5.88574	-1.65949
C	0.19358	-5.54711	-0.94238
H	0.36513	-6.57766	-0.63637
H	-2.11569	-3.47088	-2.33574
H	-0.21676	-1.88921	-1.96414
H	2.37160	-4.70687	1.00216
H	2.63656	-6.05587	-0.10421
C	4.06434	-4.65358	-1.88616
H	3.17935	-5.03103	-2.41678
H	4.78190	-5.49437	-1.83778
C	4.64918	-3.54772	-2.74358
N	3.95645	-2.40366	-2.83136
C	4.38247	-1.43733	-3.64300
C	5.53169	-1.56068	-4.42745
C	6.27120	-2.73691	-4.33108
H	7.19022	-2.86508	-4.90075
C	5.82307	-3.74656	-3.47468
H	6.37778	-4.67699	-3.36706
H	5.84784	-0.73731	-5.06255
H	3.80256	-0.51538	-3.64557
H	5.49391	-3.42137	-0.11721
H	5.17205	-4.96475	0.71594
H	5.63480	-4.18736	2.96568
H	4.81839	-2.86757	4.93269
H	2.97420	-1.18804	4.58059
H	2.05194	-0.90058	2.25595
N	3.86980	0.01555	-0.61355
S	5.44748	-0.03653	-0.79895
O	5.97736	0.55429	-2.03407
O	5.96123	-1.33667	-0.35808
O	6.05756	1.11634	0.33120
C	5.58025	1.11262	1.60333
C	4.54123	1.98299	1.96234
C	4.09770	2.08270	3.27709
C	4.71187	1.30484	4.26135
C	5.74253	0.42337	3.92756
C	6.15814	0.31407	2.60241
F	7.12414	-0.53016	2.27961
H	6.22879	-0.19750	4.67622
H	4.38184	1.38366	5.29531
H	3.28335	2.76594	3.50545
F	4.00612	2.75254	1.02135
C	3.23854	2.94700	-1.86147
C	2.59844	2.20478	-2.85457
C	3.23149	1.92741	-4.06058
C	4.61853	2.41544	-4.34455
C	4.94582	3.69021	-3.54920
C	4.59954	3.53029	-2.06129
H	4.67331	4.49017	-1.53115
H	5.33504	2.86777	-1.57621
H	4.36547	4.52692	-3.96573
H	6.00693	3.94318	-3.66491
H	5.32719	1.62376	-4.04595
H	4.75691	2.57761	-5.42271
H	2.71935	1.31878	-4.80643

H	1.61601	1.78605	-2.64164
H	2.73565	3.10029	-0.91209
H	3.46932	0.81468	-1.10970

$^3Int_{tpa,I,1}$

S	-0.03937	-0.01176	-0.09590
O	-1.38501	0.20733	-0.63597
O	1.02779	-0.06731	-1.17756
Ag	2.60372	-1.76879	-0.81379
N	1.02381	-3.29875	-1.20084
C	1.16796	-4.58142	-0.83102
C	2.43714	-4.97484	-0.10725
N	3.60188	-4.26454	-0.59798
C	4.66914	-4.09833	0.37044
C	4.25488	-3.25700	1.56221
N	3.24868	-2.39174	1.40721
C	2.84754	-1.62253	2.42710
C	3.45211	-1.69240	3.67941
C	4.51474	-2.58135	3.85744
C	4.91871	-3.37946	2.78921
H	5.73863	-4.08788	2.89451
H	5.02143	-2.65257	4.81851
H	3.10531	-1.05227	4.48532
H	2.01762	-0.95218	2.21960
H	5.49436	-3.56697	-0.11900
H	5.05852	-5.06944	0.73381
C	4.03484	-4.67356	-1.91943
H	3.16395	-5.09392	-2.44177
H	4.78864	-5.48081	-1.87968
C	4.55942	-3.54768	-2.79346
N	3.88089	-2.39149	-2.80025
C	4.23934	-1.41519	-3.63845
C	5.30314	-1.54851	-4.53239
C	6.03229	-2.73494	-4.51980
H	6.89015	-2.86865	-5.17700
C	5.65555	-3.74968	-3.63535
H	6.20430	-4.68894	-3.59432
H	5.56559	-0.72042	-5.18542
H	3.67741	-0.48516	-3.57955
H	2.29752	-4.71594	0.94957
H	2.55561	-6.07395	-0.14988
C	0.15096	-5.51232	-1.06566
C	-1.03386	-5.09642	-1.67474
C	-1.16553	-3.75867	-2.04730
C	-0.10595	-2.88959	-1.79478
H	-0.16137	-1.83687	-2.06052
H	-2.06841	-3.38003	-2.51998
H	-1.83820	-5.80699	-1.85810
H	0.29409	-6.54896	-0.76667
N	3.87733	-0.09030	-0.54074
S	5.46324	-0.18899	-0.71805
O	6.01555	0.28865	-1.98629
O	5.93846	-1.46442	-0.17359
O	6.04808	1.03215	0.33264
C	5.57997	1.09753	1.60901
C	4.49896	1.93607	1.91754
C	4.06622	2.10405	3.22960
C	4.73228	1.43189	4.25706
C	5.80655	0.58552	3.97254
C	6.21261	0.40515	2.65189
F	7.22049	-0.40459	2.37312
H	6.33578	0.04916	4.75689
H	4.41047	1.56820	5.28776
H	3.21918	2.75800	3.42145
F	3.91386	2.60417	0.93421
O	0.13118	-1.08140	0.91359
C	0.39588	1.54483	0.82867
F	-0.57067	1.85051	1.68073
F	1.52590	1.35415	1.51473
F	0.57159	2.55829	-0.01224
C	3.19682	2.88168	-1.97293
C	2.62984	2.16534	-3.02420
C	3.33370	1.89830	-4.19801
C	4.75713	2.35562	-4.35718
C	5.03516	3.61897	-3.52389
C	4.58894	3.43891	-2.06447
H	4.64645	4.39392	-1.52256
H	5.28866	2.76452	-1.54608
H	4.48466	4.46301	-3.96568
H	6.10282	3.87148	-3.56504
H	5.43597	1.55747	-4.01144
H	4.99055	2.53318	-5.41697
H	2.85831	1.33643	-5.00247
H	1.61889	1.77842	-2.89794
H	2.62713	3.03211	-1.06135
H	3.50273	0.71437	-1.05157

$^3Int_{tpa,A,1}$

S	0.00045	-0.16594	0.20000
O	-1.16427	-0.52093	-0.62264

O	1.23165	0.16122	-0.62961
Ag	3.14291	-1.14868	-0.39373
N	1.66489	-2.79964	-0.86007
C	1.68739	-3.95975	-0.18737
C	2.71706	-4.10024	0.90742
N	3.99053	-3.50572	0.53622
C	4.84750	-3.18551	1.66431
C	4.23160	-2.15596	2.59219
N	3.42639	-1.23298	2.05744
C	2.87633	-0.29168	2.82765
C	3.09907	-0.23731	4.20331
C	3.93285	-1.19686	4.77918
C	4.50786	-2.17188	3.96453
H	5.16205	-2.93667	4.37903
H	4.13287	-1.18832	5.84945
H	2.62762	0.54027	4.79981
H	2.22469	0.42119	2.33370
H	5.77414	-2.75484	1.26851
H	5.11072	-4.08680	2.25144
C	4.66182	-4.15779	-0.57268
H	3.92319	-4.77546	-1.10267
H	5.44468	-4.85445	-0.22653
C	5.26590	-3.23275	-1.61978
N	4.59080	-2.13223	-1.98224
C	5.04671	-1.36509	-2.97765
C	6.22055	-1.65641	-3.67090
C	6.94547	-2.78454	-3.29298
H	7.88339	-3.03367	-3.78650
C	6.45893	-3.58374	-2.25667
H	7.00293	-4.46916	-1.93291
H	6.56469	-0.98987	-4.45732
H	4.46975	-0.47104	-3.20452
H	2.32899	-3.55889	1.78000
H	2.80729	-5.16395	1.19837
C	0.76914	-4.97232	-0.47495
C	-0.19232	-4.76098	-1.46595
C	-0.20265	-3.54618	-2.14935
C	0.75121	-2.58643	-1.81289
H	0.76144	-1.60760	-2.28413
H	-0.94202	-3.32511	-2.91477
H	-0.92286	-5.53448	-1.69720
H	0.80967	-5.90829	0.07866
N	4.37593	0.62761	-0.17429
S	5.94984	0.36038	-0.30795
O	6.59896	0.80749	-1.54251
O	6.25580	-0.98554	0.19697
O	6.65646	1.43684	0.84064
C	6.85800	0.98979	2.10828
C	6.01450	1.38096	3.15697
C	6.29149	1.02672	4.47488
C	7.39832	0.22250	4.75142
C	8.23554	-0.20922	3.71913
C	7.96771	0.18179	2.40990
F	8.77663	-0.18378	1.43064
H	9.10854	-0.82969	3.90995
H	7.61352	-0.06608	5.77839
H	5.62548	1.37608	5.25920
F	4.94649	2.12478	2.88836
O	0.29751	-1.01761	1.36802
C	-0.39217	1.50208	0.92657
F	-1.37312	1.39380	1.80972
F	0.69302	1.98495	1.54972
F	-0.74367	2.35602	-0.02160
C	4.31948	3.19223	-0.25145
C	3.71476	1.85422	-0.74088
C	3.54630	1.81173	-2.23004
C	4.48293	2.51478	-3.15804
C	4.92366	3.88737	-2.60921
C	5.40759	3.78105	-1.15795
H	5.68182	4.77667	-0.78084
H	6.31385	3.16786	-1.11556
H	4.07211	4.58421	-2.65977
H	5.71460	4.30461	-3.24778
H	5.39324	1.90298	-3.29194
H	4.02439	2.62537	-4.15095
H	2.71925	1.21563	-2.61615
H	2.72032	1.77466	-0.29599
H	3.47884	3.90155	-0.21664
H	4.67515	3.06995	0.77413

$^{1}PC_{tpa,I,1}$

S	0.63161	0.84818	-0.03371
O	-0.64812	0.12542	0.01097
O	1.50043	0.44970	-1.21468
O	1.39161	0.96276	1.22775
C	0.19968	2.60193	-0.47487
F	-0.40334	3.18971	0.54685
F	1.31341	3.28027	-0.76546
F	-0.60047	2.62301	-1.52965
Ag	2.31702	-1.71370	-0.57324
N	3.24060	-2.04596	1.61057

C	2.72202	-1.47888	2.70170
C	3.04533	-1.91773	3.99019
C	3.96539	-2.95439	4.13078
C	4.50650	-3.53849	2.98074
C	4.10120	-3.06868	1.72793
C	4.55639	-3.72689	0.44079
N	3.41866	-4.08698	-0.40121
C	2.41520	-4.94326	0.21343
C	1.00960	-4.67781	-0.30645
N	0.59110	-3.40415	-0.30681
C	-0.65764	-3.10780	-0.67898
C	-1.56303	-4.09204	-1.09109
C	-1.13664	-5.41988	-1.11339
H	-1.80708	-6.21378	-1.43945
C	0.16906	-5.71942	-0.71119
H	0.53325	-6.74574	-0.71037
H	-2.57157	-3.81420	-1.38967
H	-0.93017	-2.05109	-0.63581
H	2.40306	-4.73958	1.29099
H	2.65059	-6.01785	0.10020
C	3.77614	-4.49323	-1.75194
H	2.88763	-4.95461	-2.20150
H	4.57475	-5.25935	-1.75372
C	4.17534	-3.33695	-2.64605
N	3.24326	-2.39274	-2.84023
C	3.51120	-1.37562	-3.66102
C	4.73386	-1.23957	-4.32441
C	5.71805	-2.20014	-4.10068
H	6.69780	-2.10630	-4.56500
C	5.43134	-3.27381	-3.25423
H	6.17317	-4.04515	-3.05357
H	4.92546	-0.37874	-4.95828
H	2.72875	-0.62397	-3.76587
H	5.17174	-3.00861	-0.11864
H	5.19304	-4.59981	0.68262
H	5.21125	-4.36548	3.04978
H	4.25131	-3.31590	5.11773
H	2.58915	-1.44213	4.85569
H	2.03959	-0.64698	2.52483
N	3.95447	1.36519	-1.97222
S	5.31323	0.62905	-1.50324
O	6.36482	0.81017	-2.48810
O	4.95839	-0.67971	-0.95021
O	5.89920	1.53479	-0.19654
C	5.40087	1.29754	1.05645
C	4.30141	2.00663	1.55384
C	3.89760	1.85792	2.87756
C	4.58703	0.97265	3.70525
C	5.65833	0.21872	3.21577
C	6.04789	0.37425	1.89104
F	7.05605	-0.32966	1.39867
H	6.18583	-0.49972	3.83835
H	4.27366	0.84962	4.73940
H	3.02946	2.41434	3.21954
F	3.65979	2.84984	0.75487
C	3.90402	2.63858	-2.71419
C	4.16023	2.43989	-4.19074
C	4.80380	3.32859	-4.95651
C	5.35173	4.63052	-4.43171
C	4.77933	4.97272	-3.04922
C	4.79095	3.74852	-2.13059
H	4.44400	3.99213	-1.12288
H	5.81838	3.37525	-2.03870
H	3.74590	5.33411	-3.16453
H	5.34912	5.79226	-2.59214
H	6.45145	4.56250	-4.37912
H	5.13809	5.43861	-5.14700
H	4.94625	3.11297	-6.01723
H	3.76017	1.52594	-4.62719
H	2.85505	2.94006	-2.58627
H	3.08925	1.05043	-1.50273

$^1PC_{tpa,A,1}$

S	0.01872	0.23878	-1.77514
O	-1.22845	-0.45484	-2.13576
O	1.23741	-0.22940	-2.52242
Ag	2.17080	-1.84734	-0.94170
N	2.69979	-1.46828	1.33290
C	2.05358	-0.55264	2.06266
C	2.20841	-0.46038	3.44803
C	3.06373	-1.36064	4.08288
C	3.72252	-2.32252	3.31400
C	3.51719	-2.34773	1.92984
C	4.20984	-3.36983	1.04964
N	3.30750	-3.98636	0.09030
C	2.21022	-4.74534	0.66484
C	0.99623	-4.82385	-0.24861
N	0.53183	-3.66929	-0.74889
C	-0.56618	-3.66501	-1.51162
C	-1.26079	-4.84011	-1.82128
C	-0.78298	-6.04936	-1.31738

H	-1.29085	-6.98619	-1.54296
C	0.36340	-6.04209	-0.51618
H	0.76402	-6.96634	-0.10234
H	-2.15039	-4.79650	-2.44608
H	-0.90026	-2.69139	-1.87706
H	1.89453	-4.23371	1.58329
H	2.51235	-5.76887	0.96054
C	3.97226	-4.64311	-1.02074
H	3.21427	-5.22642	-1.56115
H	4.74285	-5.36120	-0.68005
C	4.59015	-3.67756	-2.01715
N	3.79924	-2.70195	-2.48128
C	4.26258	-1.85642	-3.40445
C	5.56071	-1.93755	-3.91186
C	6.40047	-2.93700	-3.42072
H	7.42941	-3.01496	-3.76738
C	5.90620	-3.82567	-2.46397
H	6.53461	-4.61412	-2.05317
H	5.90955	-1.21226	-4.64194
H	3.56788	-1.08462	-3.73458
H	4.98937	-2.84145	0.48610
H	4.71373	-4.11715	1.69366
H	4.38434	-3.05336	3.77540
H	3.20546	-1.32612	5.16255
H	1.66204	0.29595	4.00745
H	1.37482	0.09781	1.50986
N	4.33393	0.62259	-1.34822
S	5.87357	0.18860	-1.10534
O	6.66494	0.49687	-2.28793
O	5.93793	-1.14030	-0.50293
O	6.41066	1.23733	0.13623
C	7.01294	0.65556	1.21917
C	6.25952	0.28949	2.33919
C	6.86151	-0.27594	3.45856
C	8.24147	-0.49843	3.44733
C	9.01052	-0.15897	2.33092
C	8.39170	0.40822	1.21915
F	9.09339	0.71967	0.14297
H	10.08423	-0.33060	2.30197
H	8.72243	-0.94131	4.31708
H	6.24229	-0.53952	4.31222
F	4.94714	0.49703	2.31758
O	0.27214	0.42557	-0.32131
C	-0.20104	1.98020	-2.38670
F	-1.24890	2.53941	-1.80079
F	0.88661	2.70488	-2.09262
F	-0.37321	1.99358	-3.70073
C	3.65022	2.64384	0.21156
C	3.33601	1.51652	-0.74993
C	3.70965	1.63572	-2.20141
C	4.46644	2.86306	-2.69352
C	4.23514	4.07912	-1.78812
C	4.57494	3.74262	-0.33489
H	4.47810	4.63302	0.30037
H	5.62130	3.42036	-0.27046
H	3.17988	4.38453	-1.86009
H	4.83991	4.92473	-2.14123
H	5.53704	2.63361	-2.76123
H	4.13080	3.07791	-3.71511
H	3.01897	1.16927	-2.90231
H	2.41822	0.98201	-0.51909
H	2.66591	3.08257	0.43104
H	4.02906	2.23285	1.15180

L = tpa and substrate = **21**

Sub **21**

C	4.15160	3.75953	-0.33729
C	3.47787	2.49136	-0.77917
C	3.65196	1.83535	-1.93617
C	4.54796	2.22471	-3.07997
H	5.11543	1.34074	-3.41211
H	3.05886	0.93081	-2.09604
H	2.76454	2.07143	-0.06525
H	3.40903	4.54890	-0.14866
H	4.69381	3.60848	0.60774
H	4.86411	4.14245	-1.07557
H	5.29503	2.96322	-2.75964
C	3.76773	2.78851	-4.28183
H	3.21111	3.67810	-3.95275
H	3.00835	2.05647	-4.59578
C	4.66686	3.14195	-5.46744
H	5.20167	2.25651	-5.83783
H	5.42183	3.88816	-5.18369
H	4.08761	3.55472	-6.30322

$^{OS1}TS_{tpa,I,21}$

S	0.23533	0.34174	-0.26228
O	-1.09075	0.59923	-0.83405
O	1.25042	-0.10740	-1.29166

Ag	2.93594	-1.62613	-0.51097
N	3.34744	-1.83551	1.77039
C	2.69701	-1.04747	2.63212
C	2.67734	-1.30833	4.00413
C	3.36607	-2.42010	4.48149
C	4.05946	-3.22434	3.57352
C	4.03385	-2.90241	2.21370
C	4.79508	-3.73346	1.19929
N	3.99647	-4.01696	0.01256
C	2.84630	-4.85947	0.28078
C	1.63170	-4.55332	-0.56713
N	1.32710	-3.26493	-0.78745
C	0.21577	-2.95022	-1.46563
C	-0.65866	-3.92261	-1.95296
C	-0.35076	-5.26576	-1.74130
H	-1.00093	-6.05356	-2.11830
C	0.81435	-5.58363	-1.04130
H	1.09413	-6.61935	-0.85716
H	-1.55205	-3.61762	-2.49273
H	0.03847	-1.89236	-1.63691
H	2.54523	-4.70215	1.32553
H	3.09115	-5.93378	0.18423
C	4.73938	-4.36538	-1.18504
H	4.80588	-5.46076	-1.31442
H	5.75986	-3.98438	-1.06958
C	4.24315	-3.76258	-2.49539
N	3.66234	-2.55971	-2.49457
C	3.34394	-1.94025	-3.63487
C	3.59431	-2.51844	-4.87803
C	4.17918	-3.78694	-4.90833
H	4.38235	-4.28001	-5.85774
C	4.50371	-4.41689	-3.70640
H	4.96783	-5.40168	-3.69976
H	3.33324	-1.98713	-5.79014
H	2.87699	-0.96145	-3.53643
H	5.66821	-3.15133	0.88829
H	5.15365	-4.65382	1.69574
H	4.61040	-4.10182	3.90707
H	3.36442	-2.66287	5.54318
H	2.12245	-0.64968	4.66805
H	2.14757	-0.21571	2.20415
N	4.22397	-0.03495	-0.82220
S	5.75786	-0.40284	-1.11537
O	6.29533	0.01845	-2.40528
O	6.04049	-1.78008	-0.66274
O	6.64704	0.60122	-0.03502
C	6.25601	0.53418	1.26956
C	5.33852	1.46570	1.78038
C	4.95480	1.44209	3.11744
C	5.48088	0.46357	3.96348
C	6.38223	-0.48436	3.47566
C	6.76203	-0.44686	2.13551
F	7.61603	-1.35018	1.67229
H	6.80116	-1.25805	4.11473
H	5.18077	0.43399	5.00837
H	4.23919	2.18359	3.46513
F	4.85003	2.39120	0.97360
O	0.29759	-0.46588	0.97822
C	0.89297	2.00218	0.25521
F	0.10358	2.53681	1.17760
F	2.11707	1.86187	0.77189
F	0.95808	2.82176	-0.78796
C	4.37251	2.39255	-2.23294
H	4.06182	1.56345	-1.50083
H	5.46338	2.33133	-2.23533
C	3.89733	3.68989	-1.69794
H	2.83845	3.91184	-1.82082
C	4.65212	4.60157	-1.04967
H	4.15925	5.52417	-0.73135
C	6.10777	4.49550	-0.70629
H	6.26342	4.73087	0.35587
H	6.70156	5.22352	-1.28049
H	6.51532	3.49662	-0.88478
C	3.84429	1.97427	-3.60998
H	4.25946	2.66465	-4.36163
H	4.28200	0.99185	-3.82996
C	2.32065	1.91643	-3.74178
H	1.86606	2.91114	-3.65274
H	1.87259	1.28221	-2.96831
H	2.03182	1.52060	-4.72551

$^{3}TS_{tpa,I,21}$

S	0.08505	0.14895	0.07332
O	-1.18380	0.52387	-0.56310
O	1.21829	0.03193	-0.92927
Ag	2.79442	-1.67463	-0.75017
N	3.22168	-2.39765	1.58900
C	2.84684	-1.58746	2.58684
C	3.47702	-1.60845	3.82826
C	4.53090	-2.50522	4.02489
C	4.90080	-3.35621	2.98605

C	4.21999	-3.26522	1.76527
C	4.62600	-4.13536	0.59085
N	3.61031	-4.21358	-0.44361
C	2.36954	-4.84522	-0.03288
C	1.18278	-4.39890	-0.85906
N	1.11830	-3.10769	-1.22167
C	0.04460	-2.64394	-1.87490
C	-1.02673	-3.46759	-2.21807
C	-0.96863	-4.81666	-1.86838
H	-1.78223	-5.49347	-2.12430
C	0.15167	-5.28713	-1.18121
H	0.23167	-6.33204	-0.88742
H	-1.88260	-3.04770	-2.74093
H	0.04189	-1.58098	-2.10547
H	2.16361	-4.54920	1.00255
H	2.43112	-5.94960	-0.04581
C	4.10037	-4.66936	-1.72839
H	3.23563	-5.00365	-2.31857
H	4.76842	-5.54517	-1.63498
C	4.79514	-3.60066	-2.55096
N	4.22848	-2.38598	-2.60635
C	4.74103	-1.45665	-3.41624
C	5.85352	-1.69091	-4.22562
C	6.46862	-2.93779	-4.15564
H	7.35860	-3.15395	-4.74450
C	5.93050	-3.90753	-3.30500
H	6.38289	-4.89415	-3.22317
H	6.24015	-0.89556	-4.85758
H	4.25540	-0.48586	-3.40688
H	5.52179	-3.67416	0.15617
H	4.91518	-5.13771	0.96428
H	5.71635	-4.06783	3.10406
H	5.05751	-2.53887	4.97716
H	3.15748	-0.92766	4.61190
H	2.01883	-0.91859	2.36875
N	4.13926	-0.12480	-0.22102
S	5.73719	-0.31561	-0.30534
O	6.38004	-0.00436	-1.58151
O	6.14560	-1.53943	0.40206
O	6.26168	0.99509	0.64951
C	5.79721	1.08770	1.92977
C	4.68458	1.88912	2.22605
C	4.24342	2.05196	3.53638
C	4.92854	1.41394	4.57262
C	6.03782	0.60989	4.30053
C	6.45884	0.43928	2.98324
F	7.50927	-0.31818	2.71701
H	6.58733	0.10424	5.09141
H	4.59519	1.54500	5.60030
H	3.36943	2.67259	3.71739
F	4.06926	2.52731	1.24211
O	0.06797	-0.95379	1.05545
C	0.57694	1.63524	1.08431
F	-0.40566	1.96325	1.90990
F	1.66471	1.35647	1.80695
F	0.84523	2.67742	0.29965
C	3.49514	2.07114	-1.68848
H	2.75869	2.36499	-0.93847
H	3.86351	1.06921	-1.13880
C	4.62954	3.01571	-1.67980
H	4.63048	3.70378	-0.83423
C	5.70725	3.09870	-2.49523
H	6.42195	3.89183	-2.26060
C	6.11153	2.22616	-3.64110
H	7.08317	1.76579	-3.41561
H	6.22890	2.81487	-4.56369
H	5.41059	1.41228	-3.82636
C	2.77821	1.69841	-2.98958
H	3.44485	1.80220	-3.85261
H	2.46002	0.65072	-2.93713
C	1.52211	2.55414	-3.19704
H	1.76815	3.62434	-3.20591
H	0.80603	2.36630	-2.38930
H	1.03138	2.31141	-4.14904

^{3}TS$_{tpa,A,21}$

S	-0.33973	-0.35743	-0.38723
O	-1.55174	-0.62102	-1.17464
O	0.89506	-0.17438	-1.25047
Ag	2.76189	-1.54452	-0.88826
N	3.04615	-1.82294	1.55307
C	2.51130	-0.93458	2.39733
C	2.89151	-0.86968	3.73630
C	3.87348	-1.75169	4.19323
C	4.42966	-2.66787	3.30235
C	3.98622	-2.67290	1.97347
C	4.57938	-3.63865	0.96478
N	3.68166	-3.93208	-0.13781
C	2.44586	-4.59051	0.24935
C	1.34629	-4.40246	-0.77166
N	1.25808	-3.20724	-1.37453

C	0.27157	-2.96563	-2.24553
C	-0.69334	-3.92256	-2.55933
C	-0.61357	-5.17241	-1.94680
H	-1.34802	-5.94635	-2.16425
C	0.42482	-5.41734	-1.04569
H	0.52157	-6.38094	-0.54917
H	-1.49100	-3.67435	-3.25497
H	0.23522	-1.96608	-2.66932
H	2.09546	-4.13425	1.18359
H	2.58222	-5.67024	0.44898
C	4.32521	-4.51152	-1.30100
H	3.56414	-5.06849	-1.86527
H	5.09853	-5.24892	-1.02171
C	4.92914	-3.51446	-2.27700
N	4.24223	-2.39754	-2.55604
C	4.69010	-1.55949	-3.49485
C	5.86348	-1.78845	-4.21188
C	6.60051	-2.93322	-3.91666
H	7.53830	-3.13852	-4.43012
C	6.12394	-3.80899	-2.93873
H	6.67545	-4.71124	-2.68110
H	6.19645	-1.06490	-4.95147
H	4.10270	-0.66213	-3.66267
H	5.47376	-3.15828	0.54930
H	4.90032	-4.55799	1.49285
H	5.19766	-3.36933	3.62323
H	4.20417	-1.72438	5.22974
H	2.43024	-0.13983	4.39764
H	1.74769	-0.28168	1.98543
N	4.00409	0.13441	-0.40603
S	5.58019	0.00735	-0.70742
O	6.07336	0.58680	-1.95954
O	6.09729	-1.31445	-0.30579
O	6.24407	1.11090	0.42833
C	6.41790	0.71790	1.71804
C	5.52142	1.12084	2.71830
C	5.77274	0.84987	4.06062
C	6.90631	0.11500	4.41220
C	7.79356	-0.33168	3.42972
C	7.55221	-0.02215	2.09327
F	8.41381	-0.39342	1.16275
H	8.68795	-0.89837	3.67944
H	7.10272	-0.10762	5.45921
H	5.06557	1.20675	4.80498
F	4.43045	1.79664	2.37842
O	-0.10017	-1.20059	0.80017
C	-0.54953	1.35384	0.30773
F	-1.59726	1.40031	1.11567
F	0.54641	1.67926	1.01294
F	-0.70008	2.24233	-0.66334
C	3.09190	2.02004	-1.26624
C	2.94736	1.66433	-2.58748
H	2.10459	1.01122	-2.81854
H	2.28532	1.73949	-0.59890
C	4.05846	3.05097	-0.76827
H	5.01639	3.01359	-1.29579
H	4.24656	2.91702	0.29855
H	3.62406	4.05244	-0.91683
C	3.85567	2.09266	-3.69761
H	4.85297	1.66214	-3.50671
H	4.00922	3.18377	-3.65523
C	3.36418	1.70269	-5.09567
H	2.39897	2.19213	-5.29296
H	3.15756	0.62167	-5.12364
C	4.36311	2.05753	-6.19759
H	5.32128	1.54319	-6.04000
H	4.57066	3.13608	-6.21250
H	3.98965	1.77610	-7.19038

$^{OS1}Int_{tpa,I,21}$

S	-0.11429	0.14498	-0.05806
O	-1.46113	0.41064	-0.57678
O	0.94560	0.11724	-1.14054
Ag	2.52762	-1.68740	-0.82979
N	0.88403	-3.20711	-1.17383
C	1.02801	-4.48876	-0.80499
C	2.30613	-4.88557	-0.09291
N	3.47379	-4.19293	-0.60293
C	4.55854	-4.02222	0.34859
C	4.14595	-3.22139	1.56757
N	3.19802	-2.29182	1.41406
C	2.78379	-1.56475	2.45668
C	3.31274	-1.74369	3.73424
C	4.31438	-2.69974	3.91187
C	4.73617	-3.45241	2.81625
H	5.50561	-4.21552	2.92124
H	4.75818	-2.86192	4.89306
H	2.95107	-1.13877	4.56095
H	1.99846	-0.84147	2.25197
H	5.35910	-3.45903	-0.14843
H	4.97913	-4.99175	0.68071

C	3.89667	-4.65494	-1.91252
H	3.00330	-5.00673	-2.44574
H	4.58391	-5.51898	-1.84324
C	4.52710	-3.57826	-2.77358
N	3.82758	-2.44707	-2.93659
C	4.29461	-1.50173	-3.75145
C	5.49264	-1.63467	-4.45771
C	6.23782	-2.79753	-4.27886
H	7.19234	-2.93002	-4.78542
C	5.74650	-3.78704	-3.42286
H	6.30183	-4.70768	-3.25270
H	5.84038	-0.82900	-5.09898
H	3.70161	-0.59167	-3.82559
H	2.17985	-4.61593	0.96281
H	2.41447	-5.98639	-0.12549
C	0.00225	-5.41682	-1.01506
C	-1.19455	-4.99495	-1.59634
C	-1.33038	-3.65525	-1.96142
C	-0.25898	-2.79253	-1.73412
H	-0.31807	-1.73830	-1.99478
H	-2.24441	-3.27299	-2.40947
H	-2.00609	-5.70188	-1.76199
H	0.14622	-6.45421	-0.71829
N	3.85899	-0.00914	-0.74643
S	5.43451	-0.08816	-0.88109
O	6.02209	0.42748	-2.12211
O	5.90480	-1.38060	-0.37082
O	6.01904	1.10949	0.21877
C	5.57375	1.08071	1.50188
C	4.48251	1.86887	1.89689
C	4.07945	1.93928	3.22710
C	4.77749	1.20674	4.18909
C	5.85532	0.39874	3.81973
C	6.23835	0.32621	2.48245
F	7.25898	-0.43569	2.12699
H	6.40723	-0.18820	4.55030
H	4.47553	1.26139	5.23319
H	3.22413	2.56027	3.48084
F	3.85132	2.59688	0.98027
O	0.04053	-0.95737	0.91685
C	0.34378	1.65831	0.92890
F	-0.62651	1.96476	1.77579
F	1.45897	1.42112	1.62638
F	0.56177	2.70328	0.12943
C	3.06088	2.74740	-2.08613
H	2.41272	2.91126	-1.22602
H	3.47625	0.85738	-1.13238
C	4.36193	3.23247	-1.96491
H	4.60399	3.64116	-0.98586
C	5.41885	3.20178	-2.86759
H	6.37530	3.54907	-2.47644
C	5.43885	2.70227	-4.27174
H	6.26949	3.14724	-4.83213
H	4.50824	2.89832	-4.81398
H	5.60483	1.61339	-4.24882
C	2.40616	2.06414	-3.24209
H	3.14306	1.54292	-3.86164
H	1.71826	1.31258	-2.82960
C	1.59112	3.04191	-4.11446
H	2.23276	3.81304	-4.55990
H	0.82271	3.54750	-3.51702
H	1.08555	2.50157	-4.92459

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S	-0.08164	0.07936	-0.05803
O	-1.40868	0.33616	-0.62712
O	1.01166	0.03800	-1.11395
Ag	2.53654	-1.72089	-0.79514
N	0.92964	-3.21499	-1.19154
C	1.05426	-4.50399	-0.83646
C	2.30820	-4.91965	-0.09943
N	3.49126	-4.23036	-0.57811
C	4.55343	-4.09581	0.40111
C	4.15200	-3.24683	1.59168
N	3.15937	-2.36653	1.43549
C	2.77408	-1.58777	2.45418
C	3.38138	-1.66215	3.70486
C	4.42961	-2.56790	3.88360
C	4.81611	-3.37756	2.81759
H	5.62448	-4.09912	2.92330
H	4.93797	-2.64336	4.84344
H	3.04769	-1.01351	4.50947
H	1.95456	-0.90481	2.24810
H	5.39755	-3.58545	-0.07820
H	4.91212	-5.07885	0.76421
C	3.92879	-4.64773	-1.89574
H	3.05661	-5.05695	-2.42460
H	4.67111	-5.46494	-1.84802
C	4.47483	-3.53135	-2.76857
N	3.79833	-2.37409	-2.80087
C	4.17408	-1.41071	-3.64513

C	5.25167	-1.55642	-4.52007
C	5.98082	-2.74195	-4.47693
H	6.85131	-2.88378	-5.11539
C	5.58695	-3.74447	-3.58645
H	6.13437	-4.68320	-3.52261
H	5.52817	-0.73819	-5.17976
H	3.60958	-0.48209	-3.60532
H	2.16230	-4.65672	0.95547
H	2.40858	-6.02054	-0.14024
C	0.03034	-5.42023	-1.09698
C	-1.14118	-4.98281	-1.71670
C	-1.25387	-3.63839	-2.07086
C	-0.18837	-2.78455	-1.79203
H	-0.23111	-1.72757	-2.04261
H	-2.14641	-3.24323	-2.54960
H	-1.95007	-5.68220	-1.92164
H	0.15800	-6.46226	-0.80998
N	3.85468	-0.08705	-0.53254
S	5.43943	-0.23102	-0.69245
O	6.02063	0.15719	-1.97589
O	5.87303	-1.49250	-0.08165
O	6.01453	1.02911	0.31165
C	5.58428	1.07543	1.60330
C	4.48079	1.86595	1.95882
C	4.08835	2.00227	3.28769
C	4.81033	1.34215	4.28408
C	5.90336	0.53791	3.95293
C	6.27429	0.39383	2.61759
F	7.30562	-0.36847	2.29569
H	6.47711	0.01021	4.71151
H	4.51726	1.45349	5.32633
H	3.22364	2.62123	3.51368
F	3.82773	2.52335	1.01056
O	0.04789	-1.02323	0.92092
C	0.34024	1.59792	0.93634
F	-0.65619	1.87841	1.76215
F	1.44162	1.36986	1.65635
F	0.55480	2.64367	0.14574
C	3.00803	2.70824	-2.15156
H	2.33562	2.86513	-1.30981
H	3.51945	0.75700	-1.00727
C	4.31644	3.15433	-1.98009
H	4.52269	3.56000	-0.99028
C	5.41940	3.13150	-2.83287
H	6.35779	3.48071	-2.40204
C	5.50206	2.58594	-4.22443
H	6.39584	2.95982	-4.73883
H	4.62941	2.84103	-4.83775
H	5.58443	1.48810	-4.18839
C	2.36438	2.09554	-3.36198
H	3.10045	1.56126	-3.97391
H	1.63189	1.35563	-3.01160
C	1.64249	3.13422	-4.24120
H	2.34798	3.87939	-4.63168
H	0.88018	3.67079	-3.66205
H	1.14217	2.65378	-5.09288

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S	-0.08164	0.07936	-0.05803
O	-1.40868	0.33616	-0.62712
O	1.01166	0.03800	-1.11395
Ag	2.53654	-1.72089	-0.79514
N	0.92964	-3.21499	-1.19154
C	1.05426	-4.50399	-0.83646
C	2.30820	-4.91965	-0.09943
N	3.49126	-4.23036	-0.57811
C	4.55343	-4.09581	0.40111
C	4.15200	-3.24683	1.59168
N	3.15937	-2.36653	1.43549
C	2.77408	-1.58777	2.45418
C	3.38138	-1.66215	3.70486
C	4.42961	-2.56790	3.88360
C	4.81611	-3.37756	2.81759
H	5.62448	-4.09912	2.92330
H	4.93797	-2.64336	4.84344
H	3.04769	-1.01351	4.50947
H	1.95456	-0.90481	2.24810
H	5.39755	-3.58545	-0.07820
H	4.91212	-5.07885	0.76421
C	3.92879	-4.64773	-1.89574
H	3.05661	-5.05695	-2.42460
H	4.67111	-5.46494	-1.84802
C	4.47483	-3.53135	-2.76857
N	3.79833	-2.37409	-2.80087
C	4.17408	-1.41071	-3.64513
C	5.25167	-1.55642	-4.52007
C	5.98082	-2.74195	-4.47693
H	6.85131	-2.88378	-5.11539
C	5.58695	-3.74447	-3.58645
H	6.13437	-4.68320	-3.52261
H	5.52817	-0.73819	-5.17976

H	3.60958	-0.48209	-3.60532
H	2.16230	-4.65672	0.95547
H	2.40858	-6.02054	-0.14024
C	0.03034	-5.42023	-1.09698
C	-1.14118	-4.98281	-1.71670
C	-1.25387	-3.63839	-2.07086
C	-0.18837	-2.78455	-1.79203
H	-0.23111	-1.72757	-2.04261
H	-2.14641	-3.24323	-2.54960
H	-1.95007	-5.68220	-1.92164
H	0.15800	-6.46226	-0.80998
N	3.85468	-0.08705	-0.53254
S	5.43943	-0.23102	-0.69245
O	6.02063	0.15719	-1.97589
O	5.87303	-1.49250	-0.08165
O	6.01453	1.02911	0.31165
C	5.58428	1.07543	1.60330
C	4.48079	1.86595	1.95882
C	4.08835	2.00227	3.28769
C	4.81033	1.34215	4.28408
C	5.90336	0.53791	3.95293
C	6.27429	0.39383	2.61759
F	7.30562	-0.36847	2.29569
H	6.47711	0.01021	4.71151
H	4.51726	1.45349	5.32633
H	3.22364	2.62123	3.51368
F	3.82773	2.52335	1.01056
O	0.04789	-1.02323	0.92092
C	0.34024	1.59792	0.93634
F	-0.65619	1.87841	1.76215
F	1.44162	1.36986	1.65635
F	0.55480	2.64367	0.14574
C	3.00803	2.70824	-2.15156
H	2.33562	2.86513	-1.30981
H	3.51945	0.75700	-1.00727
C	4.31644	3.15433	-1.98009
H	4.52269	3.56000	-0.99028
C	5.41940	3.13150	-2.83287
H	6.35779	3.48071	-2.40204
C	5.50206	2.58594	-4.22443
H	6.39584	2.95982	-4.73883
H	4.62941	2.84103	-4.83775
H	5.58443	1.48810	-4.18839
C	2.36438	2.09554	-3.36198
H	3.10045	1.56126	-3.97391
H	1.63189	1.35563	-3.01160
C	1.64249	3.13422	-4.24120
H	2.34798	3.87939	-4.63168
H	0.88018	3.67079	-3.66205
H	1.14217	2.65378	-5.09288

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S	0.09591	-0.03446	0.33226
O	-1.04845	-0.36546	-0.52863
O	1.35443	0.28991	-0.45538
Ag	3.26155	-1.03224	-0.35939
N	1.77863	-2.68468	-0.77512
C	1.85260	-3.87279	-0.15642
C	2.90123	-4.02753	0.91967
N	4.14918	-3.37530	0.56003
C	4.98609	-2.99630	1.69271
C	4.24414	-2.08899	2.65257
N	3.53507	-1.08615	2.11904
C	2.85044	-0.25650	2.90633
C	2.81726	-0.40818	4.29467
C	3.53878	-1.45532	4.86531
C	4.27270	-2.30453	4.03416
H	4.84979	-3.13140	4.44339
H	3.53295	-1.61131	5.94323
H	2.22795	0.27615	4.90081
H	2.29334	0.53385	2.41651
H	5.84921	-2.44657	1.29809
H	5.35890	-3.88008	2.24446
C	4.85547	-4.01113	-0.53855
H	4.16146	-4.70459	-1.03460
H	5.69366	-4.63084	-0.17758
C	5.37463	-3.08215	-1.62567
N	4.63785	-2.02237	-1.97979
C	5.03661	-1.23207	-2.98202
C	6.21090	-1.46209	-3.69433
C	6.99407	-2.55861	-3.33470
H	7.93336	-2.76186	-3.84616
C	6.56694	-3.38045	-2.29168
H	7.16142	-4.23588	-1.97620
H	6.50907	-0.77656	-4.48323
H	4.41185	-0.36775	-3.19172
H	2.50495	-3.54295	1.82114
H	3.02770	-5.09939	1.16217
C	0.96364	-4.90226	-0.47463
C	-0.02367	-4.67976	-1.43738
C	-0.08967	-3.43538	-2.06187

C	0.83880	-2.45990	-1.70003
H	0.80883	-1.46279	-2.12991
H	-0.85068	-3.20507	-2.80299
H	-0.73096	-5.46740	-1.69209
H	1.04614	-5.86036	0.03476
N	4.52010	0.71356	-0.26874
S	6.09782	0.50768	-0.39405
O	6.74323	1.13085	-1.55068
O	6.43678	-0.87936	-0.04322
O	6.78270	1.45003	0.87892
C	6.83751	0.89331	2.11611
C	5.90252	1.23291	3.10366
C	6.01439	0.74273	4.40155
C	7.04517	-0.14548	4.71271
C	7.97393	-0.52225	3.73897
C	7.87245	0.00478	2.45361
F	8.77026	-0.31126	1.53631
H	8.79210	-1.20461	3.95958
H	7.12826	-0.54331	5.72198
H	5.28043	1.05167	5.14002
F	4.90643	2.05803	2.79775
O	0.34407	-0.90371	1.49803
C	-0.29209	1.63587	1.05567
F	-1.29847	1.54166	1.91141
F	0.78204	2.10261	1.70925
F	-0.60421	2.49511	0.09851
C	3.84207	1.96721	-0.74426
C	3.46897	1.89128	-2.19824
H	2.49317	1.45908	-2.42391
H	2.90837	1.95713	-0.17473
C	4.60496	3.24003	-0.35178
H	5.56688	3.32060	-0.86702
H	4.78931	3.24593	0.72487
H	3.99271	4.11114	-0.61556
C	4.32996	2.40211	-3.30562
H	5.36516	2.05676	-3.15227
H	4.39871	3.50605	-3.25003
C	3.84624	2.01588	-4.70859
H	2.81763	2.37973	-4.85153
H	3.78602	0.91931	-4.78812
C	4.74821	2.55468	-5.82001
H	5.77744	2.18753	-5.70472
H	4.78976	3.65211	-5.79814
H	4.39326	2.25384	-6.81429

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S	0.00465	-0.20842	0.68241
O	-1.03574	-0.38510	-0.34440
O	1.26912	0.44188	0.14785
Ag	3.15608	-0.86427	-0.40943
N	1.62588	-2.42813	-0.93325
C	1.59082	-3.59756	-0.27542
C	2.63793	-3.82240	0.78865
N	3.92389	-3.26378	0.40170
C	4.84323	-3.00169	1.50088
C	4.22760	-2.07808	2.53117
N	3.50852	-1.05331	2.06272
C	2.91222	-0.20961	2.90201
C	2.99726	-0.35921	4.28782
C	3.74572	-1.42132	4.79450
C	4.37571	-2.29484	3.90466
H	4.96303	-3.13762	4.26433
H	3.83660	-1.57350	5.86916
H	2.47978	0.33941	4.94131
H	2.33752	0.59112	2.44917
H	5.72749	-2.50351	1.08172
H	5.17408	-3.93457	1.99626
C	4.53057	-3.89765	-0.75330
H	3.73763	-4.40930	-1.31562
H	5.25348	-4.68046	-0.46332
C	5.20706	-2.94699	-1.72708
N	4.57844	-1.80858	-2.05877
C	5.11606	-0.99483	-2.97235
C	6.32637	-1.27039	-3.60599
C	6.99788	-2.44143	-3.26316
H	7.95966	-2.68345	-3.71210
C	6.42584	-3.29217	-2.31581
H	6.92570	-4.21162	-2.01710
H	6.73706	-0.55791	-4.31649
H	4.58704	-0.06894	-3.17739
H	2.28305	-3.29696	1.68471
H	2.68977	-4.89907	1.03692
C	0.59718	-4.53943	-0.54577
C	-0.38103	-4.24645	-1.49900
C	-0.33221	-3.02367	-2.16473
C	0.69463	-2.13672	-1.84643
H	0.75093	-1.15587	-2.30974
H	-1.08313	-2.73804	-2.89638
H	-1.17237	-4.96316	-1.71221
H	0.59004	-5.48305	-0.00407
N	4.38152	0.88666	-0.18675

S	5.96288	0.70313	-0.37259
O	6.54102	1.37214	-1.53905
O	6.33161	-0.68721	-0.06963
O	6.66142	1.62686	0.90250
C	6.86022	1.01473	2.09839
C	6.00445	1.25347	3.18170
C	6.26684	0.71212	4.43750
C	7.37343	-0.12200	4.60714
C	8.22549	-0.39804	3.53419
C	7.97107	0.17696	2.29185
F	8.79003	-0.04033	1.27744
H	9.09839	-1.03796	3.64482
H	7.57709	-0.55639	5.58382
H	5.59217	0.94290	5.25690
F	4.94011	2.03022	3.00660
O	0.26812	-1.34789	1.58345
C	-0.65689	1.14313	1.77721
F	-1.77169	0.73454	2.36541
F	0.23452	1.45737	2.72222
F	-0.91118	2.22614	1.05704
C	3.71435	2.14315	-0.66079
C	3.53974	2.16065	-2.14955
H	4.35913	2.54077	-2.76146
H	2.72216	2.06849	-0.20080
C	4.39282	3.40336	-0.10968
H	5.37878	3.55605	-0.56180
H	4.51871	3.32118	0.97310
H	3.76565	4.27355	-0.33793
C	2.42712	1.40083	-2.79144
H	1.46707	1.67154	-2.32126
H	2.52494	0.32107	-2.54764
C	2.33933	1.53567	-4.31351
H	3.31801	1.29471	-4.75726
H	2.14474	2.58694	-4.57086
C	1.26403	0.63666	-4.92657
H	0.27349	0.86193	-4.50814
H	1.47417	-0.42326	-4.72392
H	1.20312	0.75986	-6.01521

L = tpy

^{3}A'(N_O)

Ag	2.51167	0.92914	4.24093
C	3.99694	2.98912	2.28531
H	3.61903	3.69415	3.02450
C	4.52645	3.43724	1.07559
H	4.57546	4.50196	0.85951
C	4.97877	2.48344	0.16231
C	4.90018	1.13261	0.49833
H	5.22546	0.37810	-0.21129
C	4.37223	0.76083	1.74451
C	4.26628	-0.66987	2.15668
C	5.01289	-1.67564	1.52506
H	5.72701	-1.43246	0.74406
C	4.84170	-2.99913	1.92547
C	3.92641	-3.29142	2.93374
H	3.70959	-4.31637	3.21822
C	3.22587	-2.23301	3.52874
C	2.20134	-2.52337	4.57269
C	2.49915	-3.39733	5.62316
H	3.49384	-3.82975	5.69707
C	1.51387	-3.69630	6.56706
C	0.25523	-3.11718	6.43085
H	-0.55083	-3.33385	7.12709
C	0.02413	-2.25769	5.35650
H	-0.94019	-1.78319	5.18672
C	0.98090	0.44090	-0.12575
H	1.01864	-0.64113	-0.23062
C	1.30002	1.27566	-1.19476
H	1.56886	0.84236	-2.15511
C	1.26510	2.65538	-0.99374
C	0.88660	3.14082	0.25625
H	0.85432	4.20977	0.44916
C	0.55337	2.24430	1.28129
C	0.05380	2.74486	2.58809
C	-0.80820	3.85008	2.62991
H	-1.08339	4.36829	1.71599
C	-1.38153	4.20592	3.84641
C	-1.09975	3.44115	4.97622
H	-1.56209	3.66977	5.93154
C	-0.21121	2.36573	4.86052
C	0.09167	1.49745	6.02893
N	1.33319	0.98624	6.13373
C	1.64357	0.21801	7.18903
H	2.66090	-0.16764	7.22835
C	0.72323	-0.08782	8.18836
H	1.02039	-0.70997	9.02928
C	-0.58066	0.40128	8.06479
C	-0.90394	1.20179	6.97129
H	-1.92352	1.53302	6.79211
C	-3.80290	-0.85999	3.18267

F	-3.70881	-1.81354	4.10540
F	-5.05656	-0.46298	3.08142
F	-3.39449	-1.34752	2.01585
N	3.92196	1.69254	2.60494
N	3.41888	-0.96322	3.15337
N	0.97941	-1.96336	4.46760
N	0.36880	2.05764	3.69067
N	0.62754	0.91237	1.07871
O	-1.42783	-0.17493	4.03064
O	-3.33281	1.20204	4.81894
O	-2.54429	1.36457	2.42358
S	-2.70535	0.56835	3.65050
H	-1.34035	0.15048	8.80282
H	1.73118	-4.37562	7.38952
H	5.40168	-3.79678	1.44161
H	1.52391	3.34359	-1.79632
H	5.38447	2.78459	-0.80170
H	-2.07559	5.04136	3.90682
Ag	0.34334	-0.60667	2.73219
N	1.34280	-2.02505	1.43607
S	0.52899	-3.43577	1.31724
O	0.15982	-3.67960	-0.07189
O	1.21684	-4.46427	2.09862
O	-0.88919	-3.03507	2.15771
C	-1.87061	-4.00144	2.22617
C	-3.89964	-5.89397	2.42090
C	-2.84724	-4.08500	1.22621
C	-1.91893	-4.87033	3.32091
C	-2.93144	-5.81811	3.42663
C	-3.86402	-5.03141	1.32200
H	-2.94850	-6.48040	4.28928
H	-4.61326	-5.07759	0.53480
H	-4.69300	-6.63478	2.49583
F	-2.79118	-3.25268	0.20565
F	-0.99093	-4.76271	4.26582

^{1}A'(N)

Ag	-0.47523	-0.75863	2.72385
C	2.16992	4.48529	3.45044
H	1.38442	4.74822	4.15880
C	2.91296	5.46933	2.79509
H	2.72080	6.52317	2.98116
C	3.91877	5.05459	1.92190
C	4.14988	3.68985	1.74153
H	4.94854	3.36700	1.08158
C	3.35772	2.76991	2.44286
C	3.56718	1.29491	2.34734
C	4.54021	0.74854	1.49770
H	5.13274	1.39087	0.85619
C	4.75499	-0.62530	1.49005
C	4.01585	-1.43193	2.35275
H	4.17261	-2.50657	2.39416
C	3.05866	-0.83905	3.18514
C	2.35828	-1.66025	4.21441
C	3.11173	-2.51715	5.02401
H	4.18699	-2.59700	4.88545
C	2.47051	-3.20669	6.05345
C	1.09862	-3.02816	6.23371
H	0.55912	-3.54233	7.02564
C	0.41432	-2.17538	5.36700
H	-0.66123	-2.02597	5.43798
C	1.29252	-0.10843	0.18254
H	1.40023	-1.19052	0.23003
C	1.97702	0.63811	-0.77559
H	2.62498	0.13904	-1.49221
C	1.80442	2.02336	-0.79032
C	0.94725	2.60452	0.14407
H	0.79297	3.68052	0.17171
C	0.29192	1.78461	1.07043
C	-0.70235	2.36539	2.01961
C	-1.79871	3.04983	1.48717
H	-1.89784	3.15261	0.40971
C	-2.77557	3.53551	2.35222
C	-2.61200	3.35186	3.71869
H	-3.36623	3.71596	4.40665
C	-1.47852	2.68184	4.19473
C	-1.23882	2.50460	5.64542
N	-0.08989	1.90078	6.00972
C	0.22290	1.69237	7.28673
H	1.18082	1.20166	7.45908
C	-0.62330	2.10304	8.31593
H	-0.33219	1.93800	9.34972
C	-1.82112	2.73030	7.97683
C	-2.13317	2.93322	6.63213
H	-3.07259	3.40215	6.36258
C	-3.51702	-0.26122	5.40620
F	-4.09312	0.94122	5.45041
F	-4.21759	-1.10707	6.13126
F	-2.28853	-0.14654	5.94599
N	2.38879	3.18876	3.26088
N	2.82664	0.48528	3.12625

N	1.03497	-1.51160	4.38049
N	-0.55149	2.19059	3.34231
N	0.47483	0.45239	1.08444
O	-2.88457	0.39496	2.92994
O	-4.67711	-1.34889	3.27682
O	-2.24454	-1.84581	3.73147
S	-3.36405	-0.82961	3.63534
H	-2.51202	3.06124	8.74963
H	3.03919	-3.85967	6.71295
H	5.50381	-1.06112	0.83137
H	2.32733	2.64244	-1.51689
H	4.53129	5.78406	1.39538
H	-3.65885	4.03828	1.96449
Ag	1.26231	1.35172	4.43728
N	2.55894	0.71655	5.86404
S	3.70669	1.77353	6.17004
O	4.61009	2.15928	5.08230
O	4.26638	1.36509	7.46264
O	2.77513	3.21492	6.47052
C	3.33640	4.13802	7.30458
C	4.44931	6.03044	9.03006
C	4.13090	5.17649	6.80186
C	3.10807	4.06373	8.68556
C	3.65669	5.00342	9.55183
C	4.68538	6.12573	7.65543
H	3.46334	4.91593	10.61860
H	5.29664	6.92116	7.23473
H	4.88663	6.76556	9.70203
F	4.32967	5.25075	5.48958
F	2.33857	3.08367	9.14908

^{OS1}A'(N)

Ag	-0.15392	-0.34374	2.78035
C	2.99976	4.03896	3.03527
H	2.37165	4.49556	3.79440
C	3.81179	4.81640	2.21384
H	3.81869	5.89759	2.32451
C	4.62144	4.16324	1.28508
C	4.60525	2.77037	1.22884
H	5.24562	2.25479	0.52077
C	3.78263	2.04991	2.10625
C	3.79583	0.55763	2.16871
C	4.66489	-0.21811	1.38364
H	5.32499	0.23732	0.65255
C	4.69126	-1.59904	1.57233
C	3.87941	-2.17153	2.55217
H	3.88918	-3.24316	2.73587
C	3.02975	-1.33331	3.28857
C	2.18123	-1.87740	4.38899
C	2.74152	-2.72466	5.35175
H	3.79717	-2.98018	5.30391
C	1.93351	-3.20013	6.38651
C	0.59019	-2.82422	6.42123
H	-0.07942	-3.18020	7.20063
C	0.10335	-1.98371	5.41928
H	-0.94102	-1.68683	5.37672
C	1.25801	0.77956	0.17761
H	1.44111	-0.28952	0.08403
C	1.75636	1.67600	-0.76641
H	2.33313	1.31067	-1.61297
C	1.49467	3.03670	-0.59491
C	0.73188	3.44253	0.49987
H	0.51293	4.49384	0.67001
C	0.26460	2.47731	1.40090
C	-0.60914	2.85845	2.54651
C	-1.75043	3.63014	2.30806
H	-1.96208	3.98587	1.30345
C	-2.63696	3.86161	3.35563
C	-2.36362	3.31669	4.60551
H	-3.05439	3.46928	5.42722
C	-1.19078	2.57644	4.79021
C	-0.83425	1.99303	6.10717
N	0.41137	1.49993	6.23980
C	0.84882	1.00120	7.39533
H	1.88488	0.66383	7.41180
C	0.02593	0.94311	8.51876
H	0.40955	0.54163	9.45323
C	-1.28400	1.41151	8.40413
C	-1.72003	1.94273	7.19031
H	-2.74541	2.27898	7.07955
C	-3.79762	-0.26837	4.83618
F	-4.34868	0.94123	4.94219
F	-4.67127	-1.18039	5.20795
F	-2.75215	-0.30540	5.68985
N	2.98534	2.70489	2.96636
N	2.98180	-0.01862	3.05792
N	0.88677	-1.51862	4.43599
N	-0.32686	2.38393	3.77009
N	0.53628	1.17133	1.23563
O	-2.52915	0.73890	2.75838
O	-4.38247	-0.91177	2.32976

O	-2.15787	-1.63694	3.28333
S	-3.19169	-0.56016	3.09463
H	-1.96480	1.36411	9.25195
H	2.34976	-3.85213	7.15240
H	5.35257	-2.22126	0.97234
H	1.87607	3.77026	-1.30232
H	5.27364	4.72794	0.62138
H	-3.54633	4.43583	3.19294
Ag	1.69666	1.61169	4.46886
N	3.37868	1.07642	5.66984
S	4.18143	2.39419	6.13350
O	5.11936	2.88315	5.12431
O	4.59083	2.23714	7.52694
O	2.88943	3.57047	6.15151
C	3.02888	4.63749	6.99433
C	3.27655	6.82365	8.71140
C	3.53370	5.85663	6.52437
C	2.63880	4.53353	8.33651
C	2.76142	5.61843	9.19837
C	3.65742	6.95225	7.37219
H	2.45737	5.50512	10.23640
H	4.05246	7.88513	6.97634
H	3.37965	7.67377	9.38222
F	3.86747	5.95569	5.23918
F	2.13107	3.38326	8.76315

^{3}A'(N)

Ag	-0.06346	-0.15709	2.82996
C	3.52845	3.75752	2.84822
H	2.97435	4.30921	3.60151
C	4.40806	4.41176	1.98861
H	4.53376	5.48902	2.06368
C	5.12421	3.64344	1.07206
C	4.94736	2.26001	1.05986
H	5.51867	1.65608	0.36281
C	4.05695	1.66360	1.96529
C	3.88901	0.18032	2.05286
C	4.59509	-0.69708	1.21235
H	5.24717	-0.32684	0.42802
C	4.46418	-2.07127	1.40432
C	3.64678	-2.54248	2.43160
H	3.52538	-3.60777	2.61199
C	2.95442	-1.60753	3.21410
C	2.06989	-2.06134	4.32878
C	2.54146	-2.97628	5.27780
H	3.56307	-3.34413	5.21937
C	1.68744	-3.38556	6.30489
C	0.38851	-2.87815	6.34447
H	-0.31541	-3.17870	7.11683
C	-0.00996	-1.97583	5.35690
H	-1.01783	-1.57128	5.31834
C	1.23261	1.15245	0.25026
H	1.39852	0.09316	0.06093
C	1.67765	2.11789	-0.65255
H	2.19656	1.81804	-1.55996
C	1.43457	3.46110	-0.36191
C	0.75061	3.78240	0.81066
H	0.55568	4.81872	1.07615
C	0.33976	2.75366	1.66707
C	-0.39801	3.05530	2.92497
C	-1.47628	3.94616	2.91994
H	-1.76774	4.44571	2.00016
C	-2.20764	4.11424	4.09190
C	-1.84560	3.39781	5.22966
H	-2.41431	3.51361	6.14600
C	-0.74053	2.54057	5.17442
C	-0.28606	1.75984	6.35401
N	0.92012	1.16700	6.27794
C	1.42624	0.48762	7.31068
H	2.42231	0.06973	7.17894
C	0.72129	0.33478	8.50161
H	1.16205	-0.21684	9.32804
C	-0.54665	0.91023	8.59728
C	-1.05517	1.62726	7.51678
H	-2.04983	2.05598	7.56848
C	-3.72041	0.13508	4.87109
F	-4.23475	1.35589	4.99044
F	-4.61620	-0.75816	5.23953
F	-2.67082	0.05693	5.72006
N	3.35786	2.43175	2.82122
N	3.07135	-0.29270	3.00244
N	0.81801	-1.57572	4.38216
N	-0.03460	2.40349	4.03632
N	0.58822	1.46242	1.38113
O	-2.38879	1.10109	2.81856
O	-4.32977	-0.43807	2.35237
O	-2.16019	-1.30358	3.30481
S	-3.12622	-0.16184	3.12831
H	-1.13584	0.80370	9.50603
H	2.03376	-4.09120	7.05799
H	5.00070	-2.76735	0.76254

H	1.77288	4.24653	-1.03482
H	5.82764	4.10855	0.38382
H	-3.06802	4.77965	4.11439
Ag	2.06856	1.49674	4.43364
N	3.90321	1.43534	5.61309
S	4.15271	2.88269	6.31591
O	5.20544	3.59618	5.59897
O	4.14848	2.77408	7.76964
O	2.67132	3.71556	5.91744
C	2.38049	4.83157	6.65570
C	1.77756	7.12096	8.13250
C	2.75569	6.09823	6.19016
C	1.68881	4.72910	7.86990
C	1.38553	5.86708	8.61048
C	2.45656	7.24549	6.91676
H	0.85495	5.75616	9.55326
H	2.76258	8.21386	6.52747
H	1.54895	8.01195	8.71302
F	3.37923	6.18294	5.01773
F	1.30890	3.52949	8.29319

L = tpy and substrate = **1**

$^{OS1}TS_{tpa,I,1}$

C	-0.15520	0.82348	-0.47594
F	-0.62040	2.03072	-0.18664
F	-1.13195	-0.06004	-0.40413
F	0.76140	0.50493	0.46940
S	0.65240	0.81110	-2.16272
O	1.39650	2.09197	-2.19539
O	-0.45110	0.63433	-3.10108
O	1.58368	-0.37868	-2.04417
Ag	3.85150	0.13650	-1.94429
N	4.05693	-1.74725	-0.64538
C	5.16271	-2.48714	-0.45452
C	6.35839	-2.20853	-1.30097
C	7.12544	-3.26724	-1.81265
C	8.23698	-2.96869	-2.59913
C	8.54956	-1.63581	-2.85748
C	7.73040	-0.62928	-2.32016
C	8.02375	0.81469	-2.54109
C	8.90510	1.23973	-3.54352
C	9.16909	2.60123	-3.69918
C	8.53793	3.51084	-2.85526
C	7.66181	3.02294	-1.88516
H	7.15292	3.69843	-1.20703
N	7.41816	1.71649	-1.74131
Ag	6.00459	1.05356	-0.14065
N	4.67345	0.52915	1.53355
C	3.48283	1.14084	1.66939
C	3.16730	2.24377	0.72739
C	2.25220	3.25227	1.04900
C	2.08571	4.31630	0.16546
C	2.81858	4.34028	-1.01601
C	3.67809	3.27012	-1.29337
C	4.38997	3.17000	-2.59368
C	4.83764	4.31666	-3.26337
C	5.47707	4.18162	-4.49407
C	5.66372	2.90248	-5.02183
C	5.21045	1.80996	-4.28383
H	5.34270	0.79416	-4.65329
N	4.59229	1.94130	-3.10456
H	6.15142	2.74832	-5.98119
H	5.83236	5.06055	-5.02857
H	4.72264	5.29179	-2.79957
N	3.85211	2.27224	-0.42334
H	2.67539	5.13441	-1.74252
H	1.38764	5.11694	0.39693
H	1.70633	3.22764	1.98649
C	2.61130	0.75487	2.69710
C	3.00552	-0.23566	3.59305
C	4.26668	-0.82106	3.45540
C	5.07519	-0.40459	2.40134
H	6.07544	-0.80516	2.25236
H	4.62068	-1.58227	4.14590
H	2.33622	-0.54439	4.39379
H	1.62721	1.20478	2.76917
N	7.49911	1.38775	1.45511
S	7.71419	2.98888	1.66119
O	8.79557	3.54086	0.83956
O	7.57600	3.41610	3.04838
O	6.23031	3.51907	0.85919
C	5.56255	4.61455	1.30503
C	5.54903	5.77902	0.52754
C	4.81356	6.89587	0.90549
C	4.07697	6.84854	2.09351
C	4.06015	5.69223	2.87876
C	4.78666	4.57784	2.47166
F	4.72119	3.44487	3.15857
H	3.48102	5.63467	3.79752
H	3.50894	7.72103	2.40839

H	4.83015	7.78241	0.27559
F	6.23146	5.77620	-0.62262
H	8.71097	4.58135	-2.92936
H	9.85593	2.93981	-4.47278
H	9.37207	0.52003	-4.20832
N	6.66813	-0.93350	-1.56104
H	9.42982	-1.39046	-3.44287
H	8.85459	-3.76617	-3.00720
H	6.84183	-4.29782	-1.61632
C	5.19678	-3.51757	0.49487
H	6.11061	-4.08564	0.65077
C	4.05246	-3.78858	1.24655
C	2.90638	-3.02708	1.02278
H	1.98629	-3.20846	1.57297
C	2.95099	-2.01257	0.06474
H	2.08501	-1.39699	-0.16657
H	4.05984	-4.58206	1.99195
C	11.51162	-1.21102	2.45078
C	10.43762	-1.77550	1.56240
C	9.73310	-1.01670	0.69443
C	9.86907	0.44941	0.61369
C	10.82032	1.07601	1.63307
C	12.00454	0.15198	1.94565
H	12.66367	0.62015	2.68728
H	12.60446	0.00046	1.03597
H	10.26347	1.25825	2.56496
H	11.15336	2.05793	1.28119
H	9.99418	0.81921	-0.41387
H	8.78491	0.87867	0.88841
H	9.01441	-1.49641	0.02931
H	10.26010	-2.85194	1.59917
H	11.11861	-1.11250	3.47750
H	12.34376	-1.92552	2.52269

$^{3}TS_{tpa,I,1}$

C	-0.14878	0.83355	-0.45081
F	-0.60201	2.04336	-0.15260
F	-1.13256	-0.04205	-0.37485
F	0.77248	0.50344	0.48544
S	0.64460	0.82120	-2.14428
O	1.39512	2.09838	-2.18019
O	-0.46778	0.65347	-3.07394
O	1.57014	-0.37373	-2.03658
Ag	3.84186	0.14161	-1.96257
N	4.07102	-1.75131	-0.66993
C	5.17748	-2.49014	-0.47769
C	6.37558	-2.21339	-1.32169
C	7.15098	-3.27295	-1.81969
C	8.26936	-2.97651	-2.59723
C	8.57957	-1.64445	-2.86353
C	7.74988	-0.63758	-2.34364
C	8.03320	0.80599	-2.58195
C	8.89248	1.22457	-3.60607
C	9.13881	2.58643	-3.78607
C	8.50966	3.50160	-2.94660
C	7.65777	3.01848	-1.95288
H	7.15195	3.69969	-1.27828
N	7.43469	1.71168	-1.78132
Ag	6.02991	1.04040	-0.17230
N	4.70007	0.51745	1.52526
C	3.51007	1.12767	1.66774
C	3.19130	2.23683	0.73273
C	2.28339	3.24733	1.06978
C	2.10859	4.31478	0.19216
C	2.82744	4.34105	-0.99784
C	3.68206	3.27047	-1.28861
C	4.38135	3.17730	-2.59661
C	4.81627	4.32864	-3.26728
C	5.44238	4.20162	-4.50553
C	5.63061	2.92536	-5.03968
C	5.19140	1.82798	-4.30047
H	5.32542	0.81417	-4.67473
N	4.58474	1.95159	-3.11434
H	6.10922	2.77719	-6.00454
H	5.78696	5.08448	-5.04061
H	4.70151	5.30150	-2.79882
N	3.86301	2.26774	-0.42523
H	2.67714	5.13807	-1.71972
H	1.41514	5.11620	0.43466
H	1.74864	3.22039	2.01362
C	2.63915	0.73826	2.69516
C	3.03317	-0.25765	3.58518
C	4.29336	-0.84354	3.44162
C	5.09976	-0.42139	2.38794
H	6.09863	-0.82457	2.23566
H	4.64725	-1.60982	4.12663
H	2.36455	-0.57035	4.38500
H	1.65548	1.18842	2.77093
N	7.51533	1.41106	1.45645
S	7.75203	3.02805	1.58211
O	8.79839	3.53999	0.69396

O	7.68813	3.48727	2.96343
O	6.25036	3.52627	0.83388
C	5.58107	4.61581	1.29924
C	5.53773	5.78100	0.52544
C	4.80102	6.88874	0.92731
C	4.09566	6.82875	2.13367
C	4.10969	5.66969	2.91501
C	4.83726	4.56461	2.48517
F	4.80667	3.42870	3.16867
H	3.55500	5.60334	3.84809
H	3.52705	7.69425	2.46634
H	4.79199	7.77801	0.30115
F	6.19121	5.78752	-0.64072
H	8.66684	4.57283	-3.04236
H	9.80821	2.92126	-4.57643
H	9.35294	0.49948	-4.26972
N	6.68291	-0.93952	-1.59032
H	9.46481	-1.39908	-3.44160
H	8.89398	-3.77505	-2.99239
H	6.86913	-4.30317	-1.61910
C	5.21243	-3.51876	0.47397
H	6.12670	-4.08571	0.63106
C	4.06898	-3.78952	1.22688
C	2.92263	-3.02891	1.00256
H	2.00303	-3.20906	1.55397
C	2.96623	-2.01630	0.04242
H	2.09935	-1.40172	-0.18902
H	4.07748	-4.58156	1.97380
C	11.39839	-1.20464	2.55788
C	10.36515	-1.76355	1.61962
C	9.71381	-0.99925	0.71285
C	9.86466	0.46029	0.64254
C	10.79977	1.08659	1.67674
C	11.94552	0.13895	2.05627
H	12.58067	0.60364	2.82057
H	12.58207	-0.04066	1.17742
H	10.21964	1.31222	2.58509
H	11.17415	2.04793	1.30957
H	9.97119	0.85082	-0.37807
H	8.75774	0.89599	0.93143
H	9.02684	-1.47306	0.01139
H	10.17551	-2.83797	1.64941
H	10.95084	-1.07922	3.55911
H	12.21083	-1.93301	2.68882

$^{OS1}TS_{tpa,A,1}$

C	-0.02566	0.19746	-0.51009
C	0.66597	-0.96571	0.12118
C	1.50419	-1.81209	-0.57005
C	1.61331	-1.78186	-2.07715
C	0.58550	-0.84193	-2.72764
C	0.45768	0.46731	-1.94129
H	-0.23361	1.15478	-2.44337
H	1.43235	0.97290	-1.90821
H	-0.39542	-1.33960	-2.76348
H	0.87466	-0.64376	-3.76681
H	2.63412	-1.47407	-2.34187
H	1.49440	-2.80628	-2.45863
H	1.86602	-2.70107	-0.05804
H	0.53132	-1.11967	1.19196
H	-1.11212	-0.00519	-0.50254
H	0.11853	1.07980	0.12783
C	10.14773	-3.53632	3.40178
F	10.81154	-2.39547	3.52920
F	11.00116	-4.54034	3.34591
F	9.48472	-3.48890	2.21990
S	8.92005	-3.75366	4.80056
O	8.39048	-2.38371	4.99806
O	9.68386	-4.35365	5.88968
O	7.89811	-4.67227	4.16333
Ag	5.89442	-3.63743	3.59416
N	5.77318	-5.15441	1.88010
C	4.66274	-5.60713	1.27263
C	3.33796	-5.25126	1.85946
C	2.29401	-6.18987	1.88236
C	1.06912	-5.81405	2.43204
C	0.92022	-4.52914	2.95185
C	2.01582	-3.65102	2.91401
C	1.92707	-2.26595	3.46118
C	0.91627	-1.89299	4.35701
C	0.86591	-0.57988	4.82826
C	1.83007	0.33002	4.40104
C	2.81697	-0.11036	3.51815
H	3.58427	0.56602	3.15545
N	2.85574	-1.36981	3.07366
Ag	4.49127	-1.95907	1.67099
N	6.13928	-2.39039	0.24631
C	7.39931	-2.01974	0.53369
C	7.61709	-1.20830	1.75800
C	8.71827	-0.35431	1.88696
C	8.82532	0.43386	3.03064

C	7.84415	0.34516	4.01146
C	6.78764	-0.55636	3.82702
C	5.76829	-0.77155	4.88811
C	5.38814	0.27230	5.74277
C	4.46228	0.02514	6.75450
C	3.92518	-1.25752	6.87960
C	4.33011	-2.23431	5.97067
H	3.92871	-3.24509	6.02343
N	5.22391	-1.99655	5.00460
H	3.20667	-1.50128	7.65847
H	4.16004	0.82294	7.43026
H	5.78909	1.26949	5.58721
N	6.68524	-1.28929	2.71610
H	7.92951	0.91311	4.93258
H	9.66954	1.10767	3.15532
H	9.46193	-0.28299	1.09956
C	8.45153	-2.37688	-0.32147
C	8.17447	-3.08488	-1.48818
C	6.85078	-3.41862	-1.78649
C	5.85929	-3.04876	-0.88181
H	4.80959	-3.26853	-1.06448
H	6.58883	-3.95480	-2.69514
H	8.98272	-3.37138	-2.15835
H	9.47403	-2.13173	-0.05383
N	3.48398	-1.02130	-0.04151
S	3.55136	0.59766	0.11453
O	2.49224	1.21510	0.92211
O	3.96088	1.27453	-1.11624
O	4.95115	0.60812	1.18819
C	5.88414	1.59134	1.10930
C	5.97322	2.54051	2.13485
C	6.96814	3.51124	2.13634
C	7.89428	3.53227	1.08844
C	7.83831	2.58230	0.06411
C	6.84421	1.60905	0.08815
F	6.81281	0.65191	-0.82904
H	8.55953	2.57821	-0.75036
H	8.66965	4.29540	1.07214
H	7.00615	4.23331	2.94906
F	5.09936	2.46374	3.14209
H	1.83026	1.36454	4.73396
H	0.08476	-0.27896	5.52396
H	0.18703	-2.62060	4.69986
N	3.18149	-4.02425	2.36812
H	-0.03594	-4.21562	3.35929
H	0.23843	-6.51670	2.45910
H	2.44745	-7.19494	1.49871
C	4.73638	-6.41531	0.12932
H	3.82648	-6.75060	-0.36241
C	5.98856	-6.76608	-0.37811
C	7.13086	-6.30473	0.27432
H	8.12851	-6.56042	-0.07450
C	6.97800	-5.49924	1.40453
H	7.83058	-5.12469	1.96506
H	6.06626	-7.38940	-1.26721

^{3}TS$_{tpa,A,1}$

C	0.08369	0.31325	-0.74750
C	0.72335	-0.82545	-0.02328
C	1.64594	-1.68354	-0.61479
C	1.80484	-1.74416	-2.12387
C	0.80857	-0.83914	-2.86817
C	0.65089	0.51027	-2.15980
H	-0.00492	1.17547	-2.73428
H	1.62729	1.01003	-2.09906
H	-0.17204	-1.33571	-2.92147
H	1.14530	-0.69876	-3.90239
H	2.83485	-1.46113	-2.37723
H	1.68688	-2.78895	-2.44452
H	1.90538	-2.58387	-0.06035
H	0.50368	-0.94245	1.03767
H	-1.00388	0.12321	-0.79533
H	0.19947	1.22411	-0.14358
C	9.97729	-3.63717	3.66368
F	10.62217	-2.48132	3.76517
F	10.84522	-4.62919	3.70031
F	9.37150	-3.65702	2.45272
S	8.69070	-3.80308	5.01878
O	8.19164	-2.41775	5.18714
O	9.40179	-4.41313	6.13799
O	7.66447	-4.69821	4.35628
Ag	5.67061	-3.63196	3.78130
N	5.50803	-5.18185	2.09390
C	4.39118	-5.60195	1.47497
C	3.07055	-5.16750	2.01712
C	1.98903	-6.06238	2.05475
C	0.76686	-5.61454	2.55428
C	0.65781	-4.30298	3.01363
C	1.78992	-3.47269	2.96898
C	1.74604	-2.06680	3.46628
C	0.74009	-1.63060	4.33904

C	0.73559	-0.30469	4.77490
C	1.74230	0.55341	4.33887
C	2.72071	0.05047	3.48052
H	3.52149	0.68600	3.11746
N	2.71288	-1.21917	3.06296
Ag	4.38022	-1.93787	1.74929
N	6.06396	-2.49875	0.37616
C	7.32844	-2.17449	0.69422
C	7.53934	-1.33134	1.89947
C	8.67125	-0.51999	2.03745
C	8.77603	0.30154	3.15745
C	7.76211	0.28663	4.10806
C	6.67401	-0.57535	3.91779
C	5.61409	-0.71087	4.95241
C	5.25378	0.37677	5.76021
C	4.28484	0.20563	6.74678
C	3.68527	-1.04654	6.89418
C	4.07686	-2.07085	6.03323
H	3.62849	-3.06045	6.10536
N	5.01313	-1.90691	5.09202
H	2.92973	-1.23136	7.65408
H	3.99733	1.03869	7.38548
H	5.70435	1.34967	5.58810
N	6.57381	-1.33946	2.82749
H	7.84370	0.87987	5.01345
H	9.64472	0.94217	3.28857
H	9.44317	-0.50939	1.27445
C	8.39322	-2.60409	-0.11134
C	8.12454	-3.33886	-1.26357
C	6.79822	-3.62626	-1.59639
C	5.79524	-3.18339	-0.73804
H	4.74391	-3.36730	-0.95010
H	6.54361	-4.18286	-2.49489
H	8.94151	-3.68256	-1.89517
H	9.41607	-2.39549	0.18383
N	3.51425	-0.99089	-0.08781
S	3.62878	0.63282	0.07634
O	2.56272	1.29273	0.83573
O	4.09979	1.25423	-1.16017
O	4.97614	0.60172	1.18727
C	5.94138	1.56002	1.14188
C	6.00744	2.52193	2.15637
C	7.02694	3.46633	2.18856
C	8.00084	3.44428	1.18490
C	7.96786	2.47833	0.17468
C	6.94783	1.53192	0.16730
F	6.93040	0.56187	-0.73522
H	8.72676	2.44042	-0.60388
H	8.79665	4.18619	1.19292
H	7.04668	4.20163	2.98994
F	5.08533	2.48544	3.12189
H	1.78295	1.59450	4.64821
H	-0.04126	0.04508	5.45231
H	-0.01980	-2.32032	4.69347
N	2.95239	-3.91380	2.46873
H	-0.29452	-3.93278	3.38082
H	-0.09233	-6.28170	2.58950
H	2.11158	-7.08895	1.71992
C	4.45116	-6.44924	0.35945
H	3.53701	-6.75854	-0.14148
C	5.69617	-6.87281	-0.10850
C	6.84457	-6.44153	0.55366
H	7.83640	-6.75268	0.23475
C	6.70576	-5.59406	1.65472
H	7.56289	-5.24041	2.22326
H	5.76360	-7.52828	-0.97509

^{3}Int$_{tpa,I,1}$

C	0.04924	-0.08365	0.13995
F	-0.39740	1.11995	0.47279
F	-0.93099	-0.96147	0.22344
F	0.99450	-0.42904	1.04628
S	0.79656	-0.06054	-1.57534
O	1.53192	1.22507	-1.61583
O	-0.34017	-0.23004	-2.47418
O	1.74096	-1.24478	-1.51171
Ag	3.99665	-0.72167	-1.52896
N	4.29939	-2.60113	-0.23294
C	5.41840	-3.33284	-0.09649
C	6.57596	-3.03552	-0.98860
C	7.31803	-4.08061	-1.56048
C	8.40005	-3.76031	-2.37951
C	8.71241	-2.42094	-2.60275
C	7.92241	-1.42890	-1.99909
C	8.22465	0.02097	-2.16396
C	9.13846	0.48428	-3.11925
C	9.41659	1.84923	-3.20505
C	8.76581	2.72742	-2.34230
C	7.85319	2.20441	-1.42629
H	7.32753	2.85333	-0.73494
N	7.59772	0.89456	-1.34951

Ag	6.18991	0.17798	0.22223
N	4.93351	-0.33916	1.94867
C	3.74861	0.27259	2.12588
C	3.40155	1.37012	1.18887
C	2.49041	2.37613	1.52997
C	2.30728	3.44419	0.65458
C	3.01838	3.47475	-0.54025
C	3.87252	2.40642	-0.83826
C	4.57012	2.31370	-2.14677
C	5.04076	3.46206	-2.79718
C	5.68697	3.33335	-4.02525
C	5.85373	2.05872	-4.57039
C	5.37154	0.96414	-3.85388
H	5.48590	-0.04815	-4.23864
N	4.74883	1.08898	-2.67617
H	6.34757	1.90961	-5.52744
H	6.06395	4.21299	-4.54349
H	4.93999	4.43180	-2.31861
N	4.06319	1.40479	0.02410
H	2.86376	4.27311	-1.26000
H	1.61213	4.24252	0.90233
H	1.96021	2.34699	2.47614
C	2.92327	-0.09942	3.19540
C	3.36036	-1.07399	4.08911
C	4.61843	-1.65467	3.90908
C	5.37980	-1.25377	2.81424
H	6.37773	-1.64578	2.62926
H	5.00591	-2.39977	4.59920
H	2.72761	-1.37171	4.92306
H	1.94256	0.35032	3.30512
N	7.80105	0.48324	1.70729
S	7.92890	2.05671	2.10961
O	8.94286	2.78459	1.33756
O	7.81540	2.28830	3.54248
O	6.39752	2.53928	1.43236
C	5.76037	3.64637	1.90344
C	5.73182	4.81206	1.12940
C	5.02071	5.93476	1.53551
C	4.31984	5.88821	2.74491
C	4.31456	4.72839	3.52508
C	5.01972	3.60936	3.09288
F	4.96255	2.47402	3.77428
H	3.76134	4.67184	4.45972
H	3.76951	6.76436	3.08050
H	5.02597	6.82383	0.90907
F	6.37522	4.80832	-0.04302
H	8.66429	0.23166	1.21936
H	8.95363	3.79788	-2.35899
H	10.13351	2.21511	-3.93782
H	9.62824	-0.20836	-3.79611
N	6.88172	-1.75476	-1.22015
H	9.57108	-2.16293	-3.21417
H	8.99701	-4.54619	-2.83775
H	7.03905	-5.11594	-1.38321
C	5.50544	-4.36595	0.84651
H	6.43001	-4.92759	0.95582
C	4.40076	-4.64592	1.65262
C	3.24037	-3.89089	1.48753
H	2.35006	-4.07810	2.08290
C	3.23118	-2.87520	0.52997
H	2.35088	-2.26446	0.34462
H	4.44985	-5.44064	2.39514
C	10.24578	-1.18000	3.28237
C	9.60864	-2.12424	2.30484
C	9.79760	-1.96563	0.93301
C	10.56469	-0.92898	0.40399
C	11.30405	0.03248	1.29490
C	11.52346	-0.54669	2.70366
H	11.89894	0.23329	3.37707
H	12.30118	-1.32141	2.64604
H	10.76077	0.99226	1.35775
H	12.27087	0.29003	0.83925
H	10.66336	-0.82583	-0.67605
H	9.31709	-2.66673	0.25081
H	8.97703	-2.93170	2.67543
H	9.51869	-0.39087	3.54415
H	10.47267	-1.69864	4.22374

^{3}Int$_{tpa,A,1}$

C	0.00001	0.04107	0.15279
C	0.87096	-0.94139	0.86273
C	2.00355	-1.69480	0.23996
C	2.00087	-1.69128	-1.32516
C	0.67568	-1.21096	-1.92329
C	0.31697	0.16091	-1.34536
H	-0.53592	0.60430	-1.87353
H	1.16857	0.84140	-1.49202
H	-0.13164	-1.92961	-1.71152
H	0.77685	-1.16182	-3.01539
H	2.79847	-1.02581	-1.67093
H	2.25954	-2.69792	-1.67732

H	1.93784	-2.74213	0.57684
H	0.73255	-1.06702	1.93501
H	-1.05550	-0.26007	0.28187
H	0.08164	1.02450	0.64512
C	9.87447	-3.95075	4.40413
F	10.51689	-2.79311	4.50201
F	10.74519	-4.94029	4.43478
F	9.26074	-3.97175	3.19707
S	8.59761	-4.12033	5.76830
O	8.09266	-2.73736	5.93784
O	9.31776	-4.72608	6.88375
O	7.57054	-5.02044	5.11301
Ag	5.58128	-3.96426	4.53028
N	5.42713	-5.51858	2.85142
C	4.30927	-5.95220	2.24401
C	2.98961	-5.52717	2.79621
C	1.92505	-6.43954	2.86827
C	0.70431	-6.00334	3.38127
C	0.58012	-4.68536	3.81736
C	1.69524	-3.83507	3.73549
C	1.63235	-2.41759	4.19741
C	0.59143	-1.95306	5.01256
C	0.56148	-0.61096	5.39395
C	1.57876	0.23850	4.96452
C	2.59568	-0.29208	4.17074
H	3.40131	0.33675	3.80833
N	2.61108	-1.57765	3.80597
Ag	4.27416	-2.28861	2.51465
N	5.95693	-2.84549	1.14174
C	7.21932	-2.49584	1.44235
C	7.43290	-1.65936	2.65169
C	8.56620	-0.85115	2.79715
C	8.67044	-0.03559	3.92185
C	7.65296	-0.04941	4.86874
C	6.56339	-0.90737	4.67071
C	5.49249	-1.04249	5.69370
C	5.10892	0.04976	6.48389
C	4.11505	-0.11752	7.44623
C	3.51846	-1.37166	7.59007
C	3.94005	-2.40293	6.75191
H	3.49774	-3.39525	6.82395
N	4.89740	-2.24155	5.83179
H	2.74383	-1.55295	8.33137
H	3.80627	0.71992	8.06905
H	5.56147	1.02261	6.31660
N	6.46591	-1.66829	3.57838
H	7.73136	0.54165	5.77593
H	9.54150	0.60069	4.05848
H	9.34137	-0.83865	2.03765
C	8.27922	-2.89633	0.61580
C	8.00811	-3.62896	-0.53720
C	6.68328	-3.94342	-0.85031
C	5.68516	-3.52813	0.02746
H	4.63535	-3.73644	-0.16910
H	6.42593	-4.49941	-1.74839
H	8.82190	-3.94948	-1.18486
H	9.30235	-2.66606	0.89356
N	3.36972	-1.30837	0.70137
S	3.68170	0.30999	0.73886
O	2.78576	1.13704	1.55285
O	4.08744	0.81301	-0.57139
O	5.09208	0.11864	1.68856
C	5.99295	1.14448	1.73424
C	5.97648	2.05571	2.79450
C	6.93566	3.05767	2.89132
C	7.93300	3.13708	1.91397
C	7.98362	2.21815	0.86123
C	7.01829	1.21908	0.78260
F	7.07334	0.29305	-0.16111
H	8.76254	2.26035	0.10300
H	8.68272	3.92309	1.97630
H	6.89329	3.75637	3.72381
F	5.04189	1.92160	3.73916
H	1.59598	1.29318	5.22645
H	-0.24726	-0.23988	6.02073
H	-0.18321	-2.63011	5.35847
N	2.85690	-4.26684	3.22447
H	-0.37251	-4.32762	4.19505
H	-0.14226	-6.68433	3.44479
H	2.06020	-7.46964	2.54936
C	4.36782	-6.80652	1.13388
H	3.45234	-7.12760	0.64278
C	5.61305	-7.22202	0.65899
C	6.76282	-6.77661	1.30949
H	7.75481	-7.08152	0.98502
C	6.62512	-5.92354	2.40617
H	7.48352	-5.55907	2.96545
H	5.67970	-7.88269	-0.20372

$^{1}PC_{tpa,I,1}$

C	0.09794	-0.08918	0.25872

F	-0.38271	1.14542	0.34299	C	4.66395	-0.75877	4.25534
F	-0.84792	-0.95418	0.57108	C	5.41911	-0.48190	3.11719
F	1.08613	-0.20331	1.17662	H	6.40834	-0.91250	2.99182
S	0.78662	-0.41660	-1.44484	H	5.06287	-1.40469	5.03368
O	1.58522	0.80716	-1.72586	H	2.75411	-0.40106	5.21110
O	-0.38416	-0.67077	-2.27775	H	1.93378	1.03926	3.35871
O	1.68788	-1.60387	-1.19743	N	9.84574	1.49996	0.83238
Ag	3.90995	-0.76563	-1.42184	S	9.13667	2.84221	1.42812
N	4.44674	-2.34635	0.20381	O	9.18471	3.89345	0.42672
C	5.61915	-2.96825	0.41325	O	9.52662	3.03878	2.81139
C	6.72216	-2.78051	-0.57448	O	7.49575	2.31004	1.44865
C	7.45945	-3.88905	-1.01775	C	6.58900	3.10078	2.10525
C	8.52175	-3.67926	-1.89589	C	5.85489	4.07008	1.41287
C	8.80698	-2.38269	-2.31750	C	4.88763	4.83067	2.05905
C	8.00286	-1.32535	-1.86193	C	4.64153	4.60676	3.41630
C	8.23727	0.07915	-2.30866	C	5.34875	3.62847	4.12206
C	8.98026	0.37230	-3.46192	C	6.31999	2.88344	3.46193
C	9.17637	1.70492	-3.82796	F	6.98378	1.92740	4.10018
C	8.61354	2.71212	-3.04529	H	5.16418	3.43642	5.17645
C	7.87303	2.34243	-1.92071	H	3.88950	5.20143	3.93035
H	7.42661	3.09094	-1.27343	H	4.33591	5.57546	1.49123
N	7.70262	1.06441	-1.56239	F	6.07279	4.23300	0.10732
Ag	6.09014	0.45980	0.06949	H	8.74389	3.76433	-3.28574
N	4.98598	0.31248	2.13533	H	9.75579	1.94845	-4.71667
C	3.76981	0.88204	2.22479	H	9.38761	-0.42392	-4.07785
C	3.34522	1.78997	1.12325	N	6.99701	-1.54163	-1.00083
C	2.30314	2.71232	1.28517	H	9.65085	-2.19704	-2.97472
C	1.96022	3.53862	0.21861	H	9.12232	-4.51642	-2.24608
C	2.65937	3.42918	-0.97981	H	7.19568	-4.89024	-0.68686
C	3.67624	2.47205	-1.07315	C	5.81815	-3.80345	1.52164
C	4.38210	2.23375	-2.36125	H	6.78286	-4.28010	1.67726
C	4.74394	3.30640	-3.18707	C	4.77111	-3.99813	2.42423
C	5.38551	3.05196	-4.39807	C	3.55567	-3.35856	2.18744
C	5.65966	1.72933	-4.74982	H	2.70591	-3.48656	2.85355
C	5.27906	0.71836	-3.86866	C	3.43551	-2.54059	1.06219
H	5.47440	-0.32687	-4.10369	H	2.50508	-2.03663	0.81577
N	4.65580	0.96227	-2.70992	H	4.90618	-4.63952	3.29344
H	6.15589	1.47990	-5.68440	C	9.82356	-2.65567	1.72685
H	5.67360	3.87301	-5.05177	C	10.82158	-1.93907	0.85624
H	4.54119	4.32524	-2.86700	C	10.98175	-0.60963	0.84805
N	4.00855	1.69801	-0.03640	C	10.14099	0.32827	1.68112
H	2.37744	4.01934	-1.84695	C	8.88667	-0.36576	2.22998
H	1.14194	4.24904	0.31641	C	9.23714	-1.73811	2.80690
H	1.77349	2.79360	2.22827	H	8.35009	-2.20246	3.25871
C	2.93654	0.62800	3.32470	H	9.96839	-1.61536	3.61883
C	3.39064	-0.19593	4.35228	H	8.16945	-0.48181	1.40346

H	8.41184	0.27802	2.97619
H	10.74121	0.71095	2.51904
H	11.75240	-0.14651	0.23068
H	11.46214	-2.55175	0.21995
H	9.02082	-3.05641	1.08862
H	10.30246	-3.53277	2.18475
H	9.53936	1.30267	-0.11577

$^{1}PC_{tpa,A,1}$

C	0.34347	-0.43847	0.22246
C	1.45469	-1.39959	0.59453
C	2.41740	-1.88904	-0.45205
C	2.28921	-1.43879	-1.90221
C	0.93705	-0.77643	-2.21359
C	0.52708	0.23948	-1.14374
H	-0.41626	0.72404	-1.42325
H	1.27107	1.04361	-1.08479
H	0.16003	-1.55278	-2.28473
H	0.98972	-0.29567	-3.19779
H	3.11216	-0.75548	-2.13864
H	2.42471	-2.32455	-2.53445
H	2.84037	-2.88413	-0.30433
H	1.21878	-2.06653	1.42501
H	-0.58058	-1.03431	0.21109
H	0.23331	0.30629	1.02030
C	10.27518	-3.88333	3.35016
F	10.86430	-2.69288	3.41542
F	11.19061	-4.81845	3.18807
F	9.47998	-3.87714	2.25687
S	9.23421	-4.19581	4.87004
O	8.60423	-2.87334	5.12383
O	10.16819	-4.70729	5.86815
O	8.22042	-5.18987	4.34960
Ag	6.17098	-4.02184	4.28415
N	5.70642	-5.33233	2.40515
C	4.49518	-5.75244	2.00522
C	3.32460	-5.40864	2.86791
C	2.55326	-6.43231	3.43340
C	1.50286	-6.08301	4.28245
C	1.24246	-4.73474	4.51771
C	2.03406	-3.76160	3.88550
C	1.77258	-2.30347	4.07388
C	0.53251	-1.83032	4.52888
C	0.34722	-0.45465	4.68699
C	1.40248	0.40730	4.39410
C	2.60293	-0.14666	3.93990
H	3.44508	0.48918	3.68727
N	2.77262	-1.45811	3.77823
Ag	4.57922	-2.38097	2.41983
N	6.27614	-2.43417	0.78922
C	7.49132	-1.96463	1.12126
C	7.64019	-1.28649	2.44045
C	8.73313	-0.45533	2.72450
C	8.77998	0.20482	3.94890
C	7.74832	0.01777	4.86501
C	6.70823	-0.85221	4.52324
C	5.61677	-1.15952	5.48734
C	5.01068	-0.13689	6.22825
C	3.97588	-0.45251	7.10817
C	3.57745	-1.78481	7.22787
C	4.23168	-2.74407	6.45522
H	3.95356	-3.79489	6.51905
N	5.22100	-2.44038	5.60736
H	2.77920	-2.08054	7.90457
H	3.48374	0.32944	7.68337
H	5.32450	0.89248	6.07663
N	6.66498	-1.46766	3.33898
H	7.77259	0.49062	5.84291
H	9.62003	0.85240	4.18960
H	9.52192	-0.29960	1.99664
C	8.57451	-2.08710	0.23658
C	8.37946	-2.67263	-1.01052
C	7.10594	-3.13504	-1.34899
C	6.08946	-3.00028	-0.40560
H	5.08686	-3.36906	-0.61726
H	6.90517	-3.59660	-2.31292
H	9.21185	-2.77507	-1.70433
H	9.56554	-1.76342	0.53563
N	2.85978	-0.99066	0.62929
S	3.42247	0.56366	0.55555
O	2.58965	1.41728	1.39084
O	3.84859	0.99334	-0.76863
O	4.82705	0.22095	1.42867
C	5.84428	1.14414	1.39209
C	6.03798	2.00148	2.48015
C	7.10014	2.89748	2.50452
C	7.98488	2.92898	1.42295
C	7.81968	2.06663	0.33557
C	6.75546	1.17009	0.32731
F	6.60533	0.31591	-0.67118
H	8.50451	2.07468	-0.50951

H	8.81443	3.63287	1.42853	H	2.79931	-7.47292	3.23622
H	7.22187	3.55171	3.36449	C	4.32574	-6.52447	0.85016
F	5.19499	1.92683	3.51062	H	3.33108	-6.85293	0.55618
H	1.30419	1.48589	4.48967	C	5.45054	-6.85614	0.08969
H	-0.61222	-0.06681	5.02485	C	6.70371	-6.41927	0.51765
H	-0.28684	-2.51435	4.73081	H	7.60905	-6.66430	-0.03257
N	3.05733	-4.11438	3.08974	C	6.78897	-5.66266	1.68838
H	0.44604	-4.44437	5.19654	H	7.74134	-5.32125	2.08441
H	0.90373	-6.85201	4.76631	H	5.34637	-7.45215	-0.81533

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