Electronic Supplementary Information (ESI)

Isomerisation versus carbonylative pathways in the hydroxy-carbonylation, methoxy-carbonylation, and amino-carbonylation of *N*-tosyl 3-pyrroline.

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1. General Information.

All manipulations were carried out under an inert nitrogen atmosphere using standard Schlenk techniques. Dry toluene was obtained from an Innovative Technologies Puresolve 400 solvent still. Other solvents were bought and used as received without further purification. Solvents were degassed prior to use. Carbon monoxide was obtained from BOC. Other reagents were purchased commercially and used as received. [$PdCl_2$(*S*)-Xyl-phanephos] **8m** and [Pd_2Cl_4(*S*)-Xyl-phanephos] **8d** were prepared according to the literature.[1] Solvents were removed by rotary evaporation on a Heidolph labrota 4000. Flash column chromatography was performed on Davisil silica gel Fluorochem 60 Å, particle size 35-70 μm. HPLC analysis was determined on a Varian Prostar operated by Galaxie workstation software. NMR spectra were recorded on Bruker Avance 300, 400 and 500 instruments. Proton chemical shifts are referenced to internal residual solvent protons. Proton signal multiplicities are given as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), br (broad) or a combination of the above. Where appropriate, coupling constants (*J*) are quoted in Hz and are reported to the nearest 0.1 Hz. All spectra were recorded at room temperature and the solvent for a particular spectrum is given in parentheses. Carbon chemical shifts are referenced to the carbon signal of the deuterated solvents. Chemical ionisation mass spectroscopy and electron ionisation mass spectroscopy were performed on a Micromass GCT spectrometer. Electrospray

mass spectroscopy was performed on a Micromass LCT spectrometer. All were operated by Mrs Caroline Horsburgh at St Andrews University. Only major peaks are reported, and intensities are quoted as percentages of the base peaks. Optical rotations were measured on a Perkin elmer 341 polarimeter using a 1 ml cell with a 1 dm path length at 20 ºC using the sodium D-line.

2. Hydroxycarbonylation, methoxycarbonylation, and aminocarbonylation of *N*-tosyl 3-pyrroline. General procedures.

2.1. Hydroxycarbonylation using Pd/Xyl-Phanephos, General method.

Lithium chloride (2.1 mg, 0.05 mmol), *p*TSA (9.5 mg, 0.05 mmol) and the requisite palladium complex (0.005 mmol) were weighed into a Biotage 5 ml microwave vial. A stirring bar was added and the vial was sealed with a crimp cap and put under an argon atmosphere. 1-(4-Toluenesulfonyl)pyrrolidine (112 mg, 0.5 mmol) and internal standard (approximately 25 µl of 1-methylnaphtalene) were added to a Sclenck tube and dissolved in the corresponding solvent (1.5 mL). The resultant solution was added using a syringe to the vial containing the catalyst and additives and a small amount of the alkene solution saved for a t_0 NMR. The required amount of degassed water (i.e.: 2.5 mmol, 5 equiv, 46 µl) was then added using a microsyringe. An autoclave was purged under vacuum and then back filled with argon three times. The cap on the microwave vial was pierced with two needles and placed in the autoclave under a flow of argon before being quickly sealed. The autoclave was purged three times with CO and then pressurised to the required level and heated in a preheated oil bath for 72 h. Upon cooling to rt, the pressure was released slowly. The mixture was stirred before taking another NMR sample (for t_1 NMR approximately 20 µl of solution were taken for calculating conversion). The solvent was carefully removed from the reaction mixture and the residue was dissolved in toluene. The toluene solution was extracted three times with saturated aqueous $NaHCO_3$ solution and the combined extracts were acidified carefully with conc. HCl. The acidic solution was extracted three times with dichloromethane and the combined organic layers were dried over $MgSO_4$, filtered and concentrated *in vacuo* to give the hydroxycarbonylation product without further purification.

2.2. Methoxycarbonylation using Pd/Ligand systems, General methods.

2.2.1. Methanol used as reaction solvent.

The requisite palladium complex (0.005 mmol) (1 mol% of $[Pd(dba)_2]$ used as Pd precursor with 1.1 mol% of the corresponding ligand: 1,2-bis(di-*tert*-butylphosphinoxylene or 4,12-bis(bis(3,5-di-*tert*-butyl-4-methoxyphenyl)phosphino)-[2.2]-*para*-cyclophane. 1,1′-Bis(di-isopropylphosphino)

ferrocene and 1,2-bis(di-tert-butylphosphino)propane were used as their corresponding [(L)$PdCl_2$] complexes) and [4,12-bis(bis(3,5-trifluoromethylphenyl)phosphino)-[2,2]-*para*-cyclophane)] as a dipalladium catalyst: [(L)Pd_2Cl_4]), lithium chloride (4 mg, 0.1 mmol), *p*TSA (9.6 mg, 0.05 mmol) and 1-(4-toluenesulfonyl)pyrrolidine (112 mg, 0.5 mmol) were weighed into a Biotage 5 ml microwave vial. A stirring bar was added and the vial was sealed with a crimp cap and put under an argon or nitrogen atmosphere. Degassed MeOH (1.5 ml) was added using a syringe (*N*-tosyl 3-pyrroline has low solubility in MeOH at r.t.). An autoclave was purged under vacuum and then back filled with argon three times. The cap on the microwave vial was pierced with two needles and placed in the autoclave under a flow of inert gas before being quickly sealed. The autoclave was purged three times with CO and then pressurised to the required level and heated in a preheated oil bath for the required time. Upon cooling to rt, the pressure was released slowly, the autoclave opened and a sample was taken for NMR analysis. The solvent was removed from the reaction mixture and the desired methyl ester and the *N*,*O* acetal were purified on SiO_2 using hexane/EtOAc 2:1 as eluent.

2.2.2. Methoxycarbonylation in toluene as reaction solvent.

Lithium chloride (2.1 mg, 0.05 mmol), *p*TSA (4.8 mg, 0.025 mmol) and the requisite palladium complex, **(*S*)-8m** (1 mol%, 2.2 mg, 0.0025 mmol) were weighed into a Biotage 5 ml microwave vial. A stirring bar was added and the vial was sealed with a crimp cap and put under an argon or nitrogen atmosphere. 1-(4-Toluenesulfonyl)pyrrolidine (56 mg, 0.25 mmol) and internal standard (approximately 25 µl of 1-methylnaphtalene) were added to a Sclenck tube and dissolved in toluene (1.5 mL). The resultant solution was added using a syringe to the vial containing the catalyst and additives and a small amount of the alkene solution saved for a t_0 NMR. The required amount of degassed MeOH (0.5 mmol, 21 µl) was then added using a microsyringe. An autoclave was purged under vacuum and then back filled with argon three times. The cap on the microwave vial was pierced with two needles and placed in the autoclave under a flow of inert gas before being quickly sealed. The autoclave was purged three times with CO and then pressurised to 70 bar and heated in a preheated oil bath at 70 °C for 68h. Upon cooling to rt, the pressure was released slowly, the autoclave opened and a sample was taken for NMR analysis. The solvent was removed from the reaction mixture and the crude was purified on SiO_2 using hexane/EtOAc 2:1 as eluent to afford the corresponding methyl ester (45 mg, 64%, ee 80%).

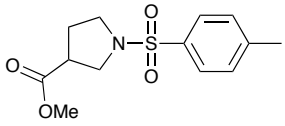
2.3. Aminocarbonylation using Pd/Xyl-Phanephos.

*p*TSA (2.4 mg, 0.0125 mmol) and [Pd_2Cl_4-(*S*)-Xyl-Phanephos] (1 mol% relative to the amine, 2.61 mg, 0.0025 mmol) were weighed into a Biotage 5 ml microwave vial. A stirring bar was

added and the vial was sealed with a crimp cap and put under an argon or nitrogen atmosphere. 1-(4-Toluenesulfonyl)pyrrolidine (112 mg, 0.5 mmol), aniline (23.2 mg, 0.25 mmol) and internal standard (approximately 25 µl of 1-methylnaphtalene) were added to a Sclenck tube and dissolved in toluene (2 mL). The resultant solution was added using a syringe to the vial containing the catalyst and additives and a small amount of the amine and alkene solution saved for a t_0 NMR. An autoclave was purged under vacuum and then back filled with argon three times. The cap on the microwave vial was pierced with two needles and placed in the autoclave under a flow of inert gas before being quickly sealed. The autoclave was purged three times with CO, pressurised to 40 bar and heated in a preheated oil bath for 70h. Upon cooling to rt, the pressure was released slowly, the autoclave opened and a sample was taken for NMR analysis. The solvent was removed from the reaction mixture and the crude was purified on SiO_2 using hexane/EtOAc 2:1 as eluent to afford the corresponding amide (18 mg, 21%).

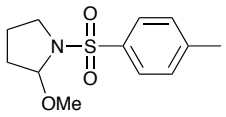
3. Analytical data of selected compounds.

Methyl 1-tosylpyrrolidine-3-carboxylate, **A**



$[\alpha]_D^{20}$ +2.9 (*c* 0.35, $CHCl_3$, ee 84%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.9 Hz, 2H, ArC*H*), 7.32 (d, *J* = 7.9 Hz, 2H, ArC*H*), 3.61 (3H, s, OCH_3), 3.55 (dd, *J* = 10.3, 8.1 Hz, 1H, NCH_2CH), 3.36 (dd, *J* = 10.3, 7.1 Hz, 1H, NCH_2CH), 3.35-3.26 (2H, m, CH_2CH_2N), 2.98-2.92 (1H, m, C*H*), 2.43 (3H, s, CH_3), 2.09-1.98 (2H, m, CHCH_2CH_2); ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.9, 143.8, 133.4, 129.8, 127.8, 52.3, 50.0, 47.5, 42.7, 28.5, 21.7; HRMS (ES)$^+$: 306.0766 $[M+Na]^+$, $C_{13}H_{17}NO_4SNa$ requires 306.0770. The enantiomeric excess was determined by HPLC on a Chiralpak AD-H, 250 x 4.6 mm, 90:10 *n*-hexane: 2-propanol, 0.5 ml/min, 254 nm, t_R = 52.7 (–)-(minor), 56.5 min (+)-(major).

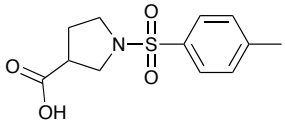
2-Methoxy-1-tosylpyrrolidine, **B**[2]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.2 Hz, 2H, ArCH), 7.30 (d, *J* = 8.2 Hz, 2H, ArCH), 5.10 (d, *J* = 5.1 Hz, 1H, NC*H*(OMe)), 3.43-3.38 (4H, m, NCH_2CH_2 and OCH_3), 3.12 (td, *J* = 9.7, 7.6 Hz, 1H, NCH_2CH_2), 2.41 (3H, s, CH_3), 2.01 (ttd, *J* = 12.2, 9.0, 6.8 Hz, 1H, $CH_2CH_2CH_2$), 1.87-1.83 (m, 1H, CH_2CH(OMe)), 1.75 (dtt, *J* = 11.9, 7.6, 2.1 Hz, 1H, $CH_2CH_2CH_2$), 1.36 (tdd, *J*

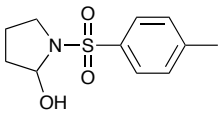
= 12.7, 7.8, 5.2 Hz, 1H, CH_2CH(OMe)); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.6, 135.8, 129.8, 127.5, 91.8, 55.4, 47.4, 32.7, 23.3, 21.6; HRMS (ES)$^+$: 278.0817 $[M+Na]^+$, $C_{12}H_{17}NO_3SNa$ requires 278.0821. The enantiomeric excess was determined by HPLC on a Chiralpak AD-H, 250 x 4.6 mm, 90:10 *n*-hexane: 2-propanol, 0.5 ml/min, 254 nm, t_R = 19.3, 23.5 min.

1-tosylpyrrolidine-3-carboxylic acid, **C**[3]



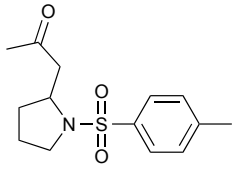
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.1 Hz, 2H, ArC*H*), 7.32 (d, *J* = 8.1 Hz, 2H, ArC*H*), 3.53 (dd, *J* = 10.4, 8.0 Hz, 1H, NCH_2CH), 3.43 (dd, *J* = 10.4, 6.5 Hz, 1H, NCH_2CH), 3.31 (2H, t, *J* = 7.0 Hz, CH_2CH_2N), 3.02-2.95 (1H, m, C*H*), 2.43 (3H, s, CH_3), 2.13-2.00 (2H, m, $CHCH_2CH_2$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.2, 143.9, 133.4, 129.9, 127.8, 49.8, 47.4, 42.6, 28.4, 21.7; MS (CI): 268 [M-H]. The enantiomeric excess was determined by HPLC, using Chirapak OD-H and Chiracel AD-H columns in series, 0.5 ml/min, 90:10:0.1 hexane : *i*-PrOH: trifluoroacetic acid. t_R= 78 (*S*)-(major), (*R*)-(minor), 84 min.

1-tosylpyrrolidine-2-ol, **F**[4]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.3 Hz, 2H, ArCH), 7.32 (d, *J* = 7.9 Hz, 2H, ArCH), 5.44-5.41 (m, 1H, NC*H*(OH)), 3.59-3.54 (1H, m, NCH_2CH_2), 3.09-3.02 (m, 2H, NCH_2CH_2 and O*H*), 2.43 (3H, s, CH_3), 2.16-2.03 (m, 1H, $CH_2CH_2CH_2$), 1.94-1.88 (m, 1H, CH_2CH(OH)), 1.80-1.69 (m, 2H, $CH_2CH_2CH_2$ and CH_2CH(OH)); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 135.7, 129.9, 127.3, 84.1, 47.7, 33.9, 23.1, 21.7; HRMS (ES)$^+$: 264.0654 $[M+Na]^+$, $C_{11}H_{15}NO_3SNa$ requires 264.0665.

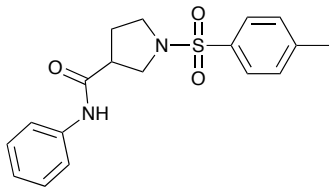
1-(1-tosylpyrrolidin-2-yl)propan-2-one, **G**[5]



Purification of ketone **G** *via* column chromatography on silica gel (eluent petrol:EtOAc 80:20 to 70:30) afforded an analytically pure sample; IR (ATR) 2954, 2854, 1717, 1596, 1457, 1377, 1154, 1090, 1047. ^{1}H NMR δ (500 MHz, CDCl3) 1.47-1.56 (2H, m), 1.70-1.84 (2H, m), 2.19 (3H, s), 2.42 (3H, s), 2.65-2.71 (1H, dd, *J* 17.8, 9.8), 3.05-3.10 (1H, m), 3.24-3.28 (1H, dd, *J* 17.8, 3.3), 3.42-3.46 (1H, m), 3.89-3.94 (1H, m), 7.30-7.34 (2H, m), 7.69-7.73 (2H, m); ^{13}C NMR δ

(125 MHz, CDCl3) 21.8, 24.1, 30.9, 32.4, 49.4, 51.0, 56.2, 127.9, 130.0, 134.1, 143.9, 207.5. HRMS $(ESI)^+$ ($[M+Na]^+$) requires 304.0983; found 304.0967. The enantiomeric excess was determined by HPLC on a Chirapak OD-H 250 x 4.6 mm, 80:20 *n*-hexane: 2-propanol, 0.5 ml/min, 210 nm, t_R = 23.3, 38.3 min.

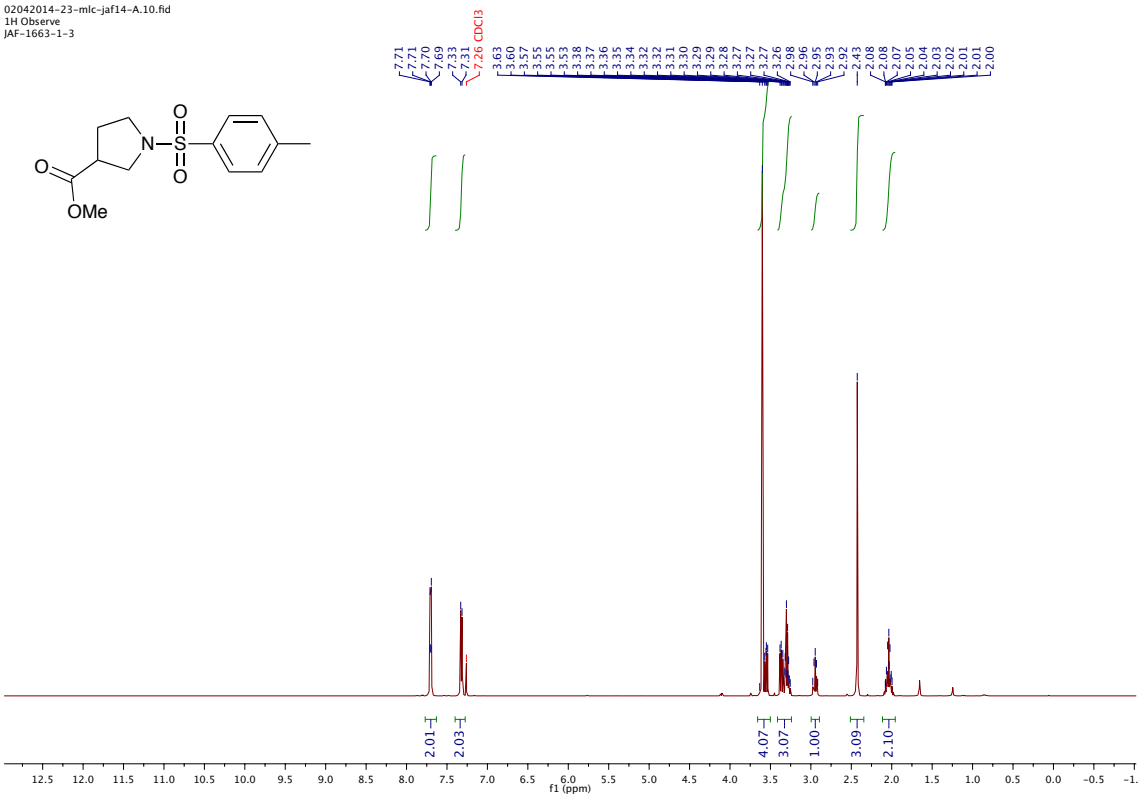
N-Phenyl-1-tosylpyrrolidine-3-carboxamide, **H**

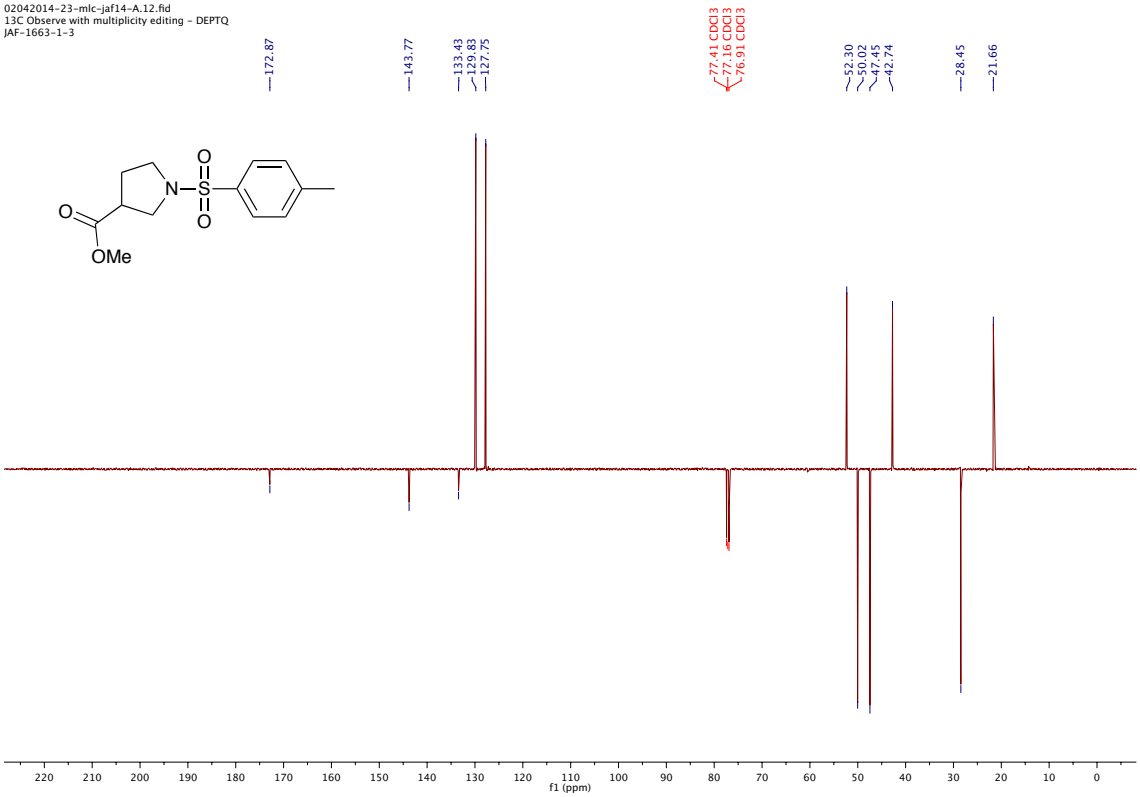


$[\alpha]_D^{20}$ –17.1 (*c* 0.7, $CHCl_3$, ee 52%); ^1H NMR (500 MHz, $CDCl_3$) δ 7.89 (s, 1H, NH), 7.75 (d, *J* = 8.1 Hz, 2H, ArC*H*), 7.51-7.49 (m, 2H, ArC*H*), 7.35 (d, *J* = 8.1 Hz, 2H, ArC*H*), 7.31-7.28 (m, 2H, ArC*H*), 7.12-7.09 (m, 1H, ArC*H*), 3.75-3.71 (m, 1H, NCH_2CH), 3.45-3.40 (m, 1H, CH_2CH_2N), 3.33-3.29 (2H, m, NCH_2CH and CH_2CH_2N), 3.12-3.06 (1H, m, C*H*), 2.45 (3H, s, CH_3), 2.19-2.11 (2H, m, CHCH_2CH_2); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.0, 144.2, 137.8, 132.8, 130.0, 129.1, 127.8, 124.6, 120.0, 51.2, 47.6, 45.3, 29.0, 21.7; HRMS $(ES)^+$: 367.1081 $[M+Na]^+$, $C_{18}H_{20}N_2O_3SNa$ requires 367.1087. The enantiomeric excess was determined by HPLC on a Chiralpak AD-H, 250 x 4.6 mm, 80:20 *n*-hexane: 2-propanol, 0.5 ml/min, 210 nm, t_R = 24.0 min (–)-(major), 35.2 min (+)-(minor).

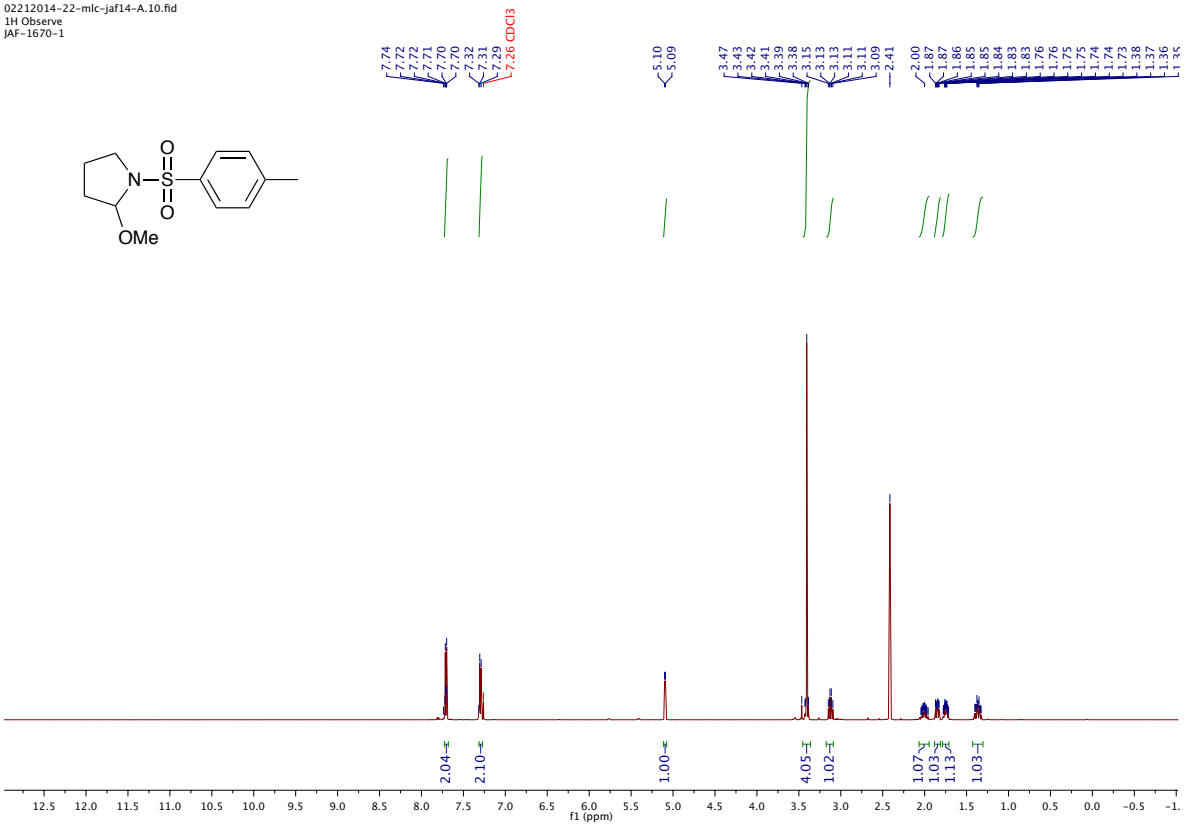
4. NMR spectra of carbonylation reaction products

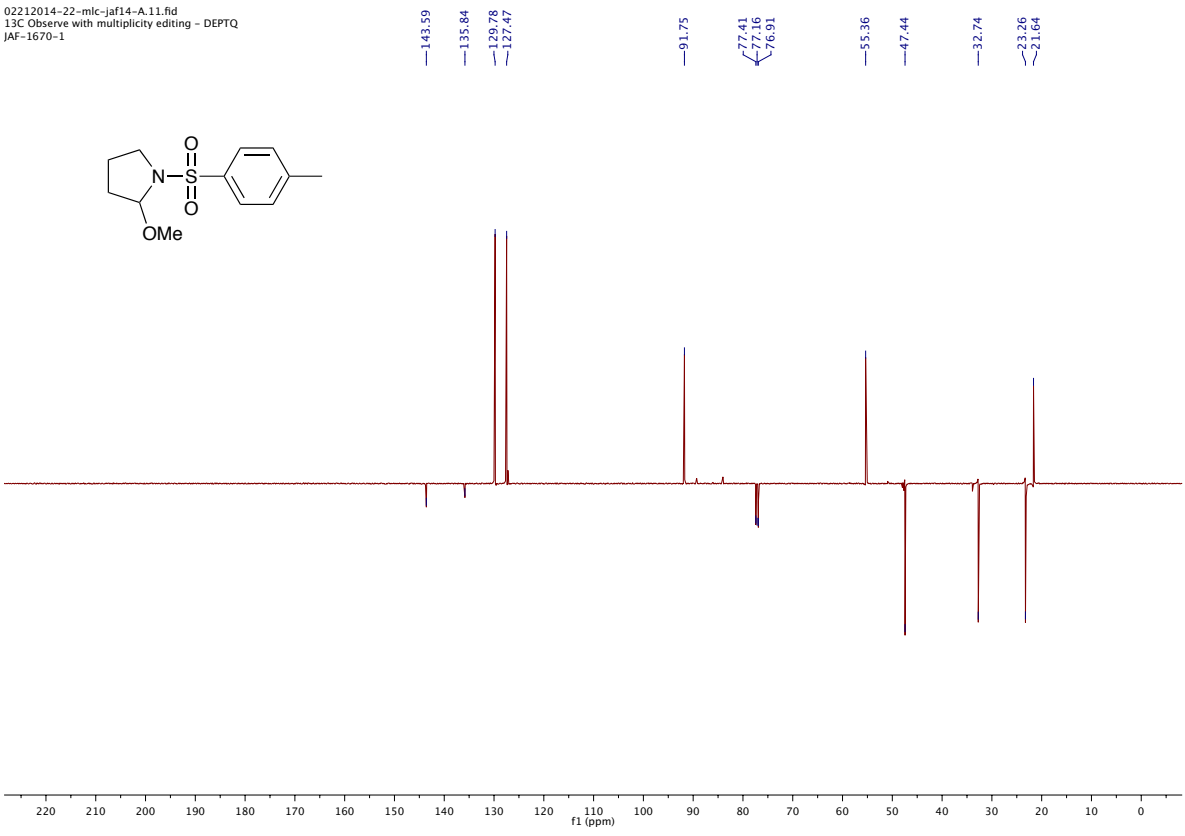
Methyl 1-tosylpyrrolidine-3-carboxylate, **A**



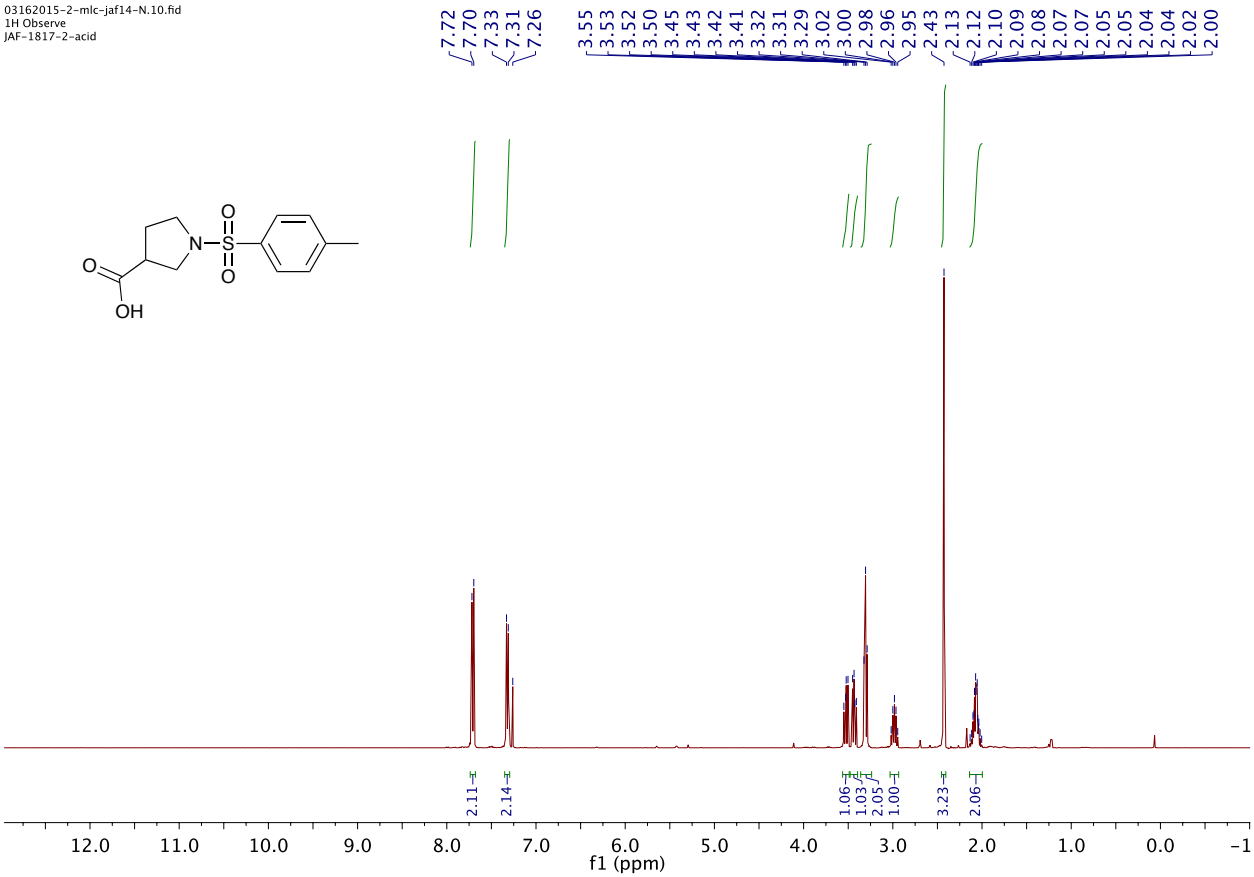


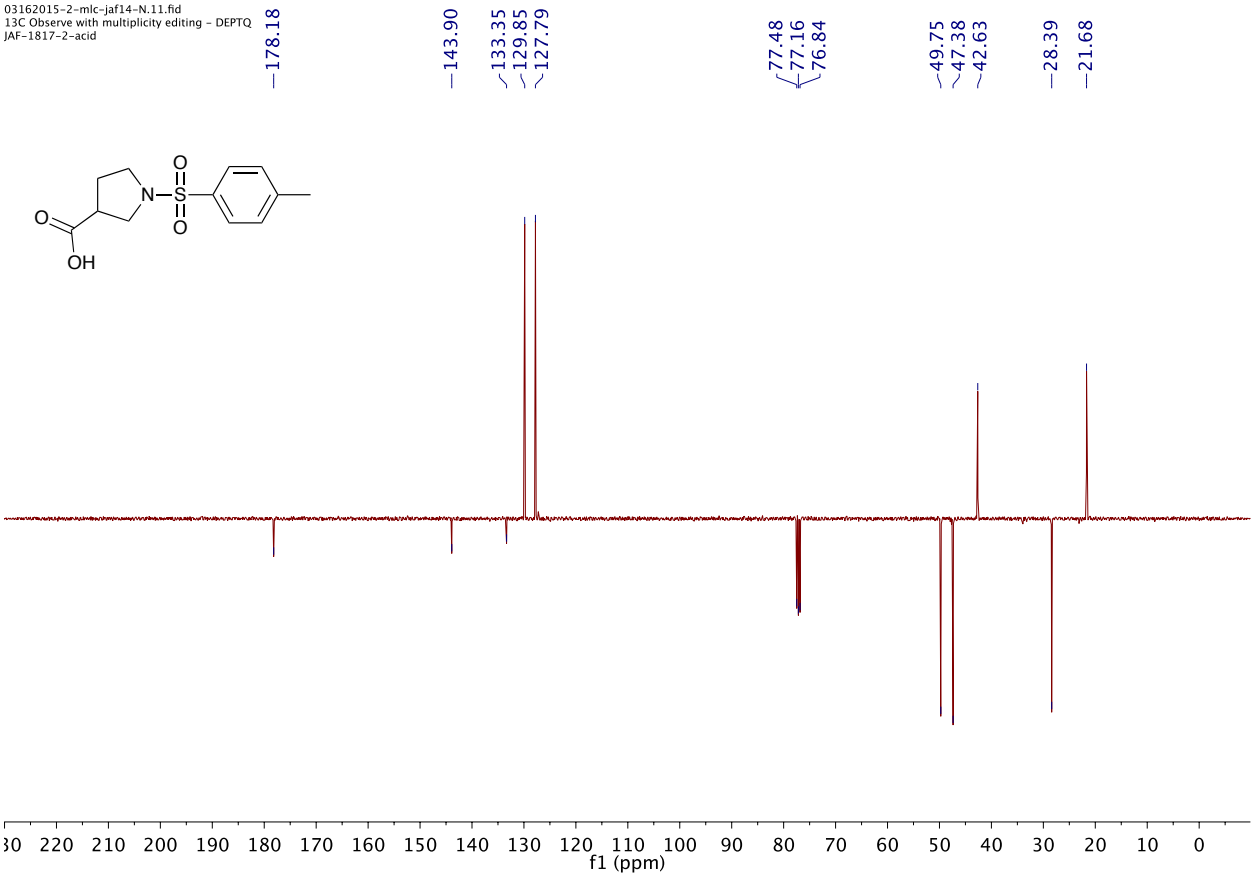
2-Methoxy-1-tosylpyrrolidine, **B**



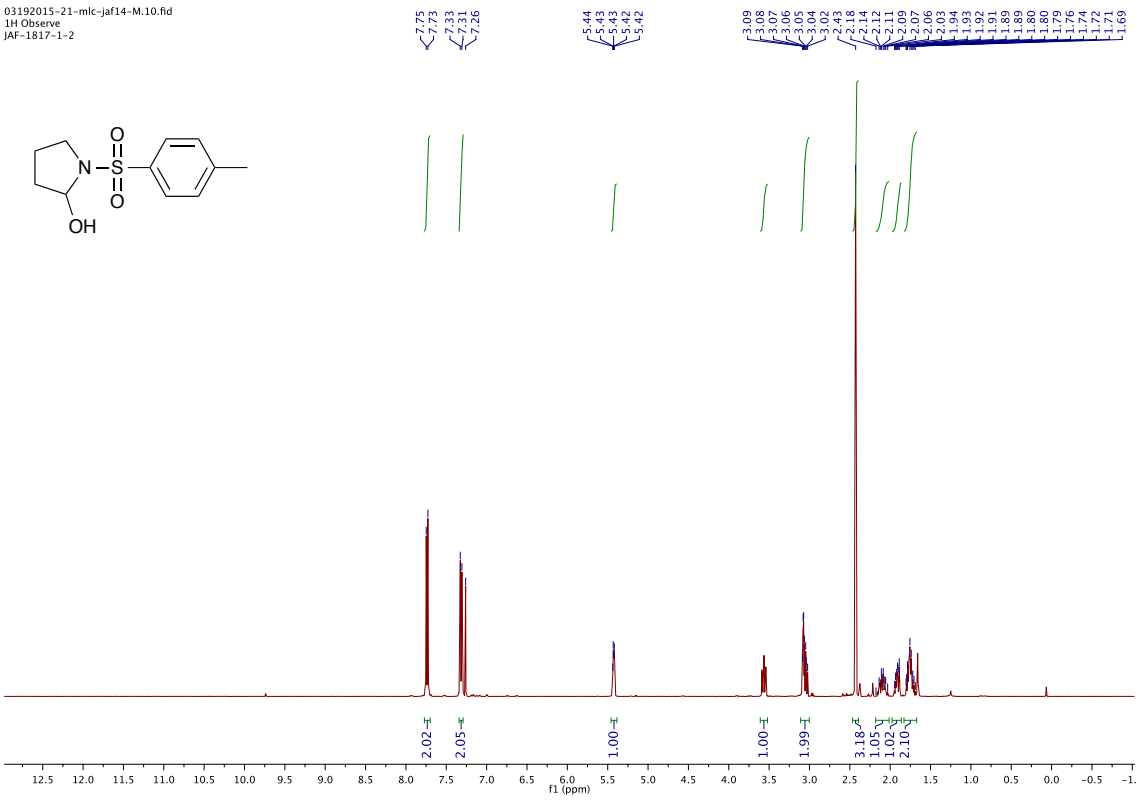


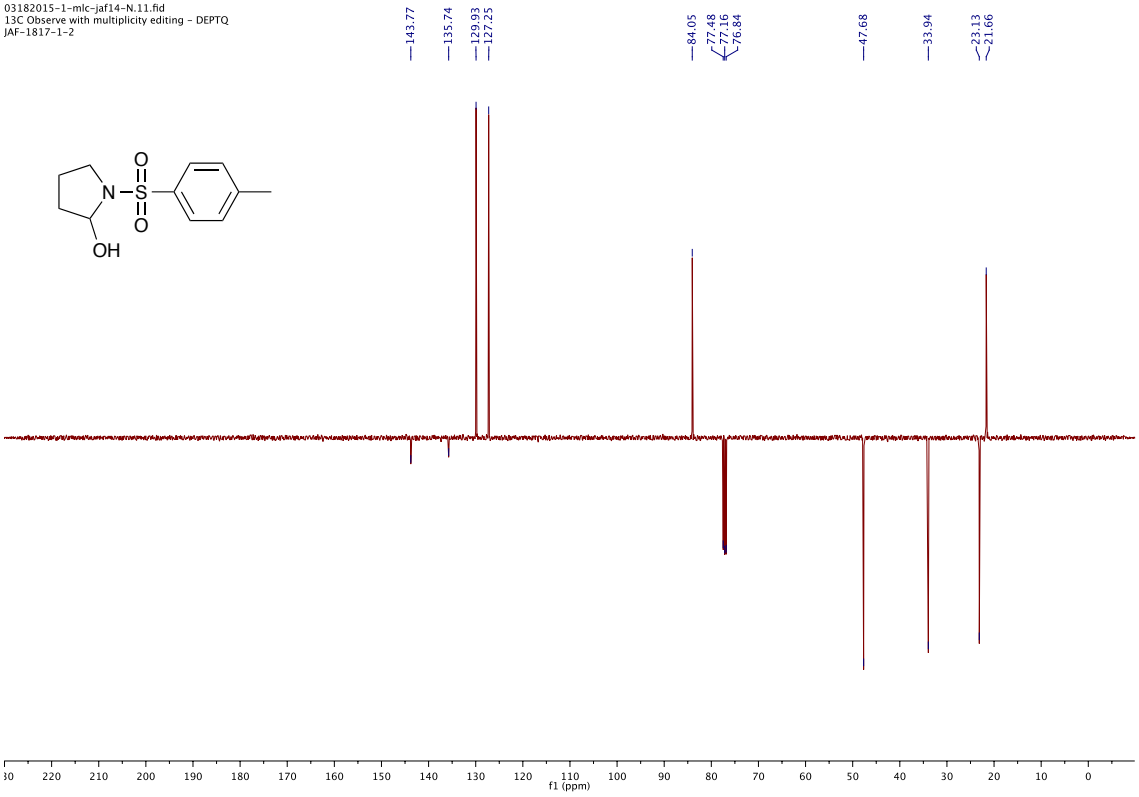
1-tosylpyrrolidine-3-carboxylic acid, **C**



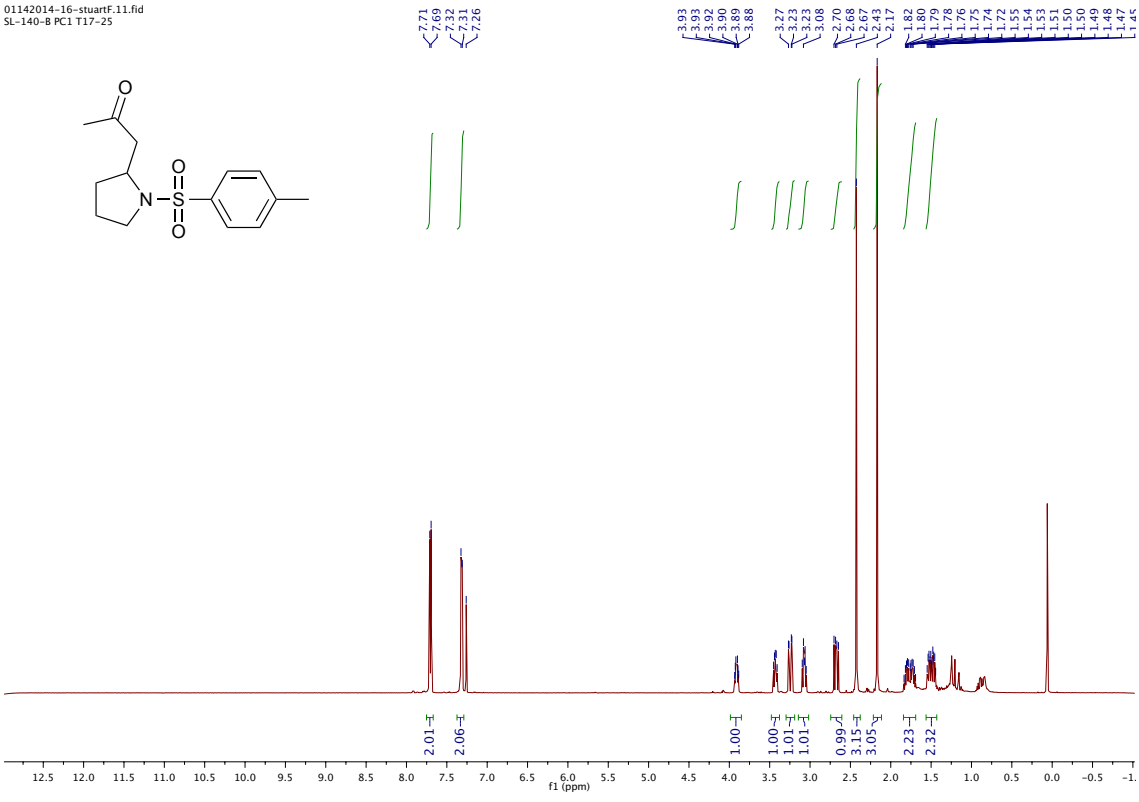


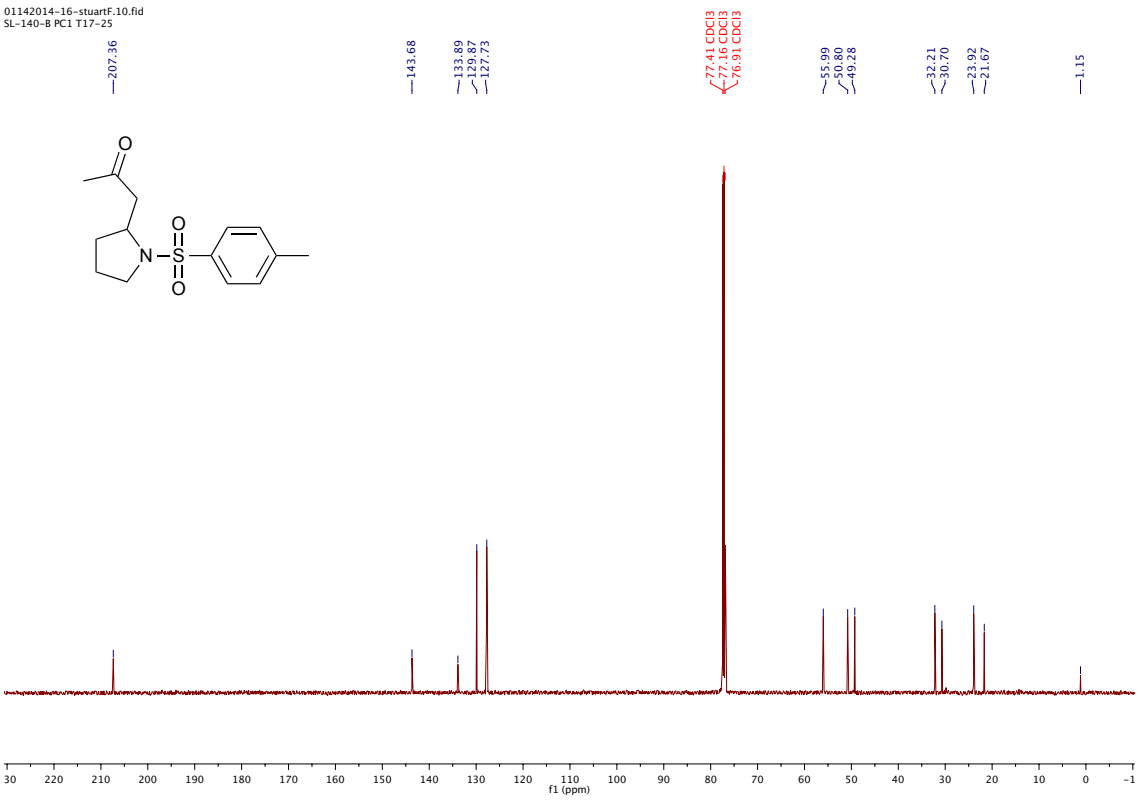
1-tosylpyrrolidin-2-ol, **F**



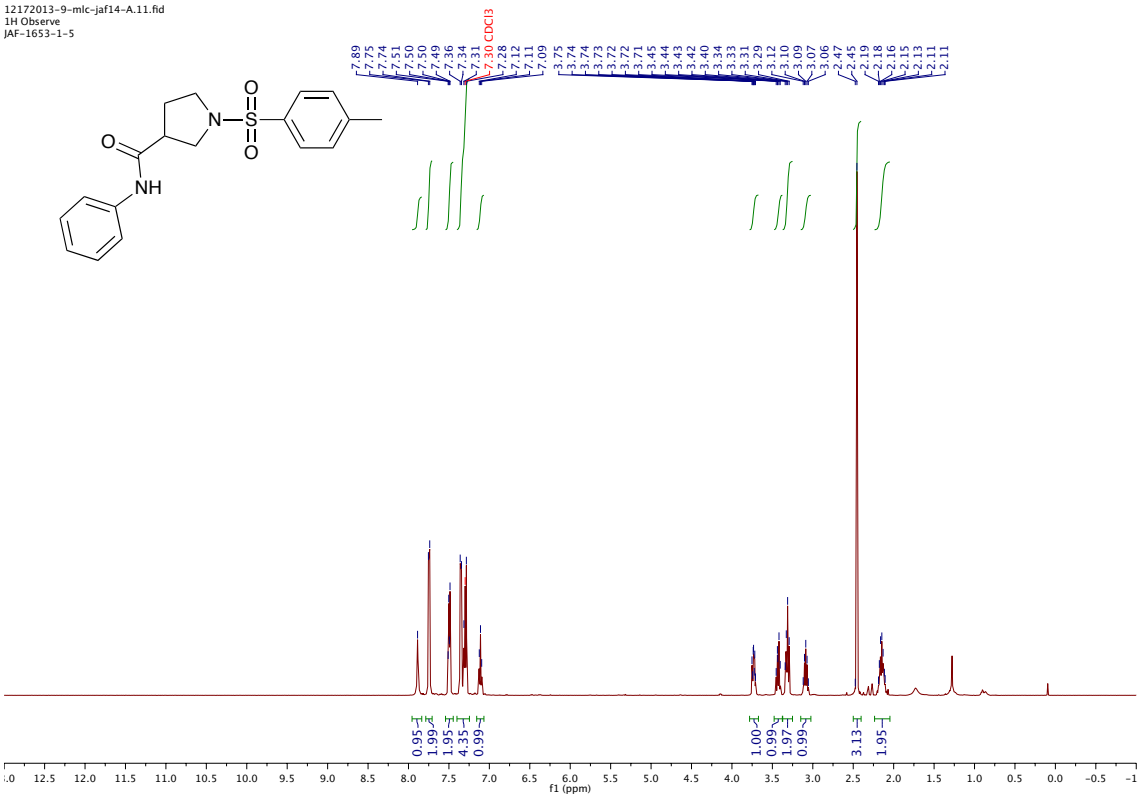


1-(1-tosylpyrrolidin-2-yl)propan-2-one, **G**



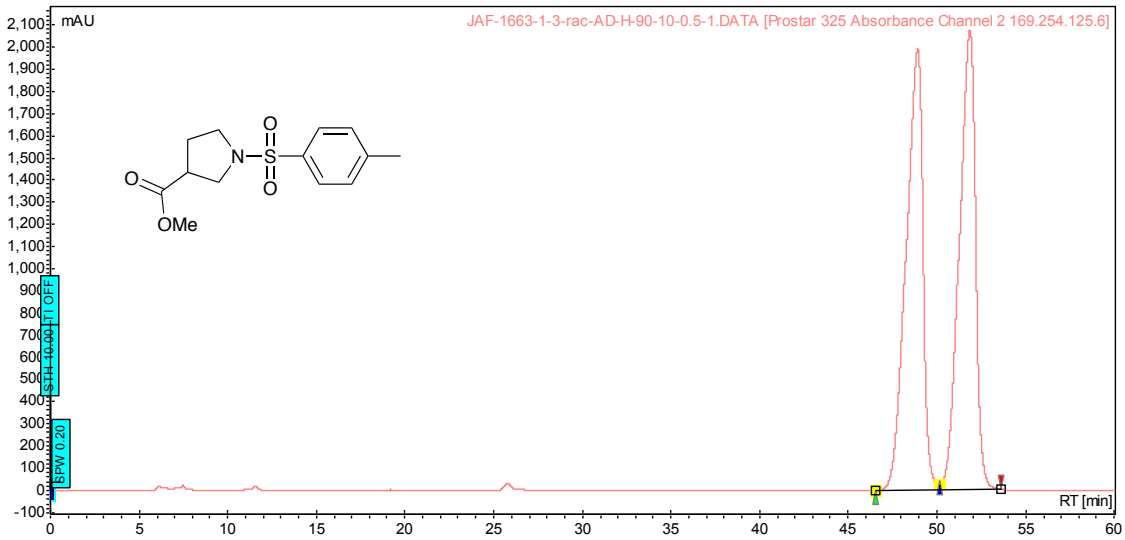


N-Phenyl-1-tosylpyrrolidine-3-carboxamide, **H**

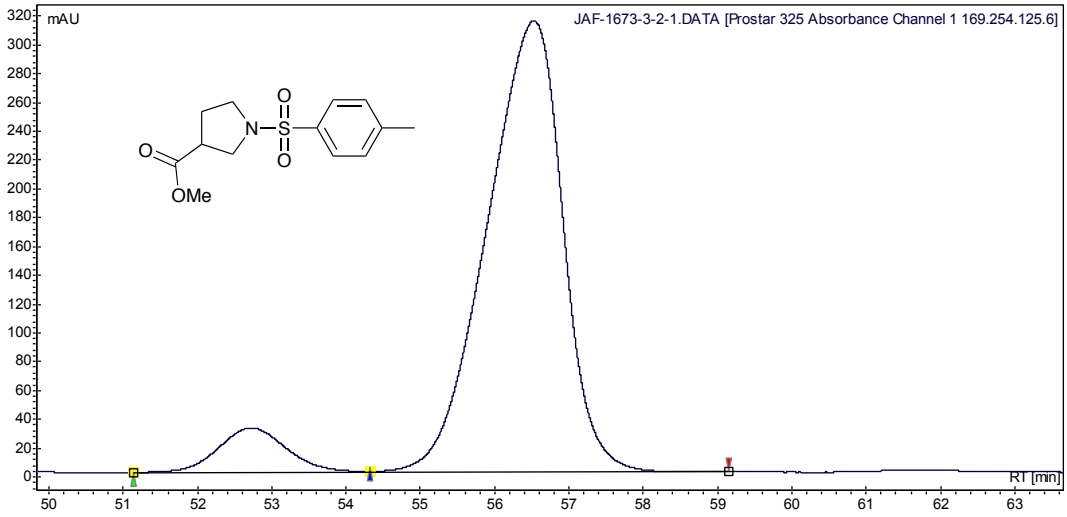


5. HPLC chromatograms for catalysis products.

Methyl 1-tosylpyrrolidine-3-carboxylate, **A**

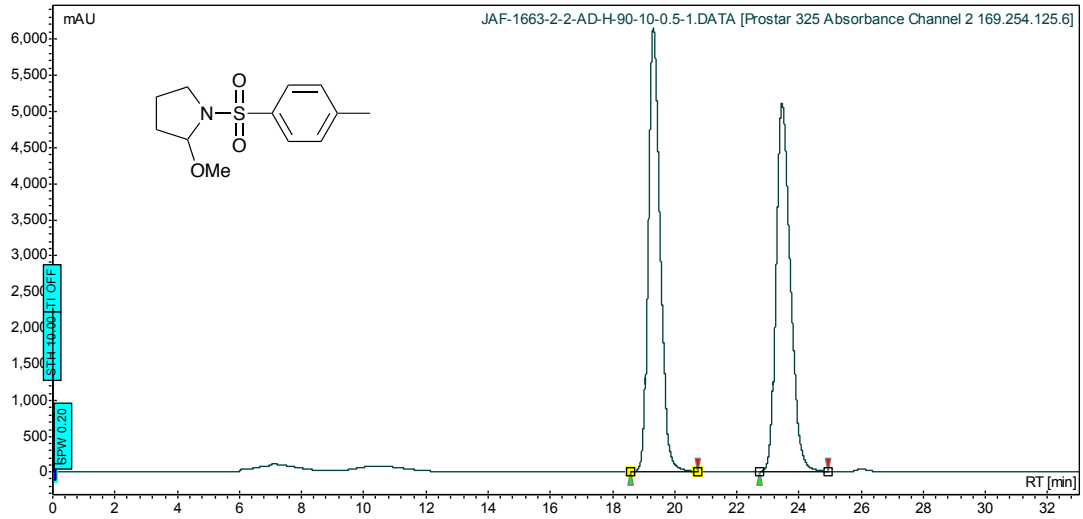


#	Name	Time [Min]	Quantity [% Area]		Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	48.91	50.00		1991.7	2201.4	50.003
2	UNKNOWN	51.86	50.00		2076.0	2201.1	49.997
	Total		100.00		4067.7	4402.4	100.000



#	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	52.73	8.16	30.8	32.9	8.161
2	UNKNOWN	56.53	91.84	313.1	370.1	91.839
	Total		100.00	344.0	403.0	100.000

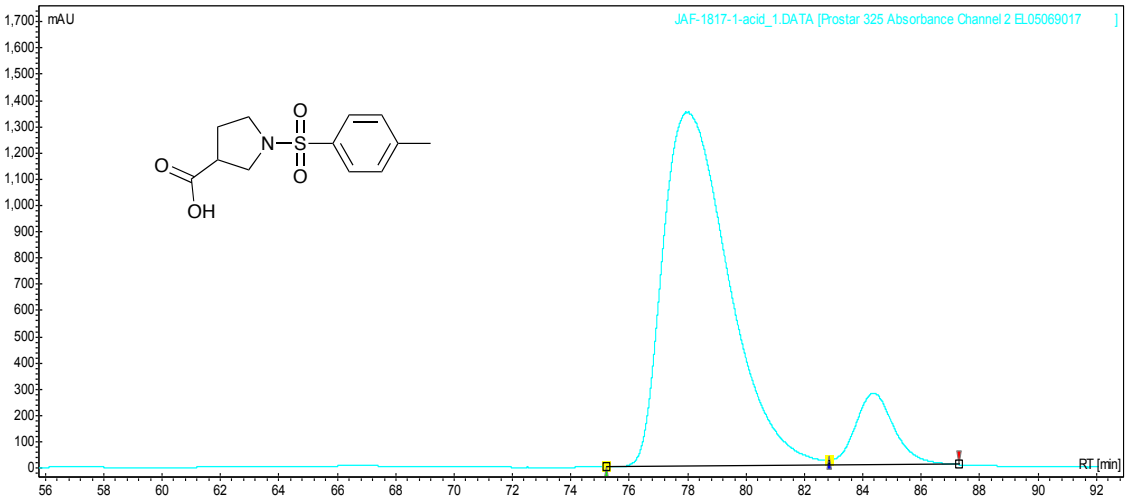
2-Methoxy-1-tosylpyrrolidine, **B**



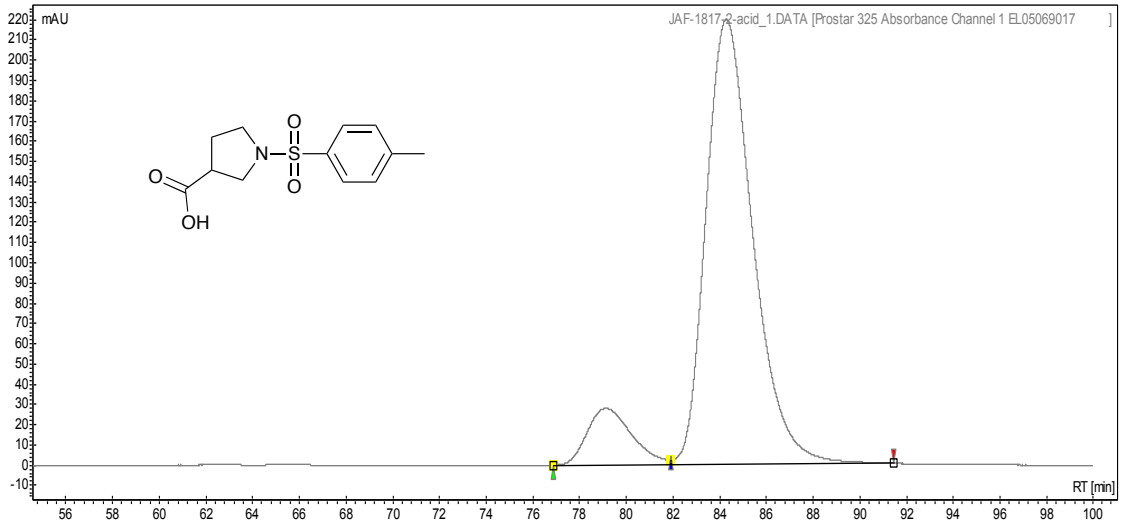
#	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	19.31	49.86	6159.6	2702.8	49.861
2	UNKNOWN	23.46	50.14	5112.6	2717.9	50.139
Total			100.00	11272.1	5420.7	100.000

1-Tosylpyrrolidine-3-carboxylic acid, **C**

Chromatograms showing both major enantiomers of the product, Table 2, entry 3 (bottom) and entry 4 (next page, top).

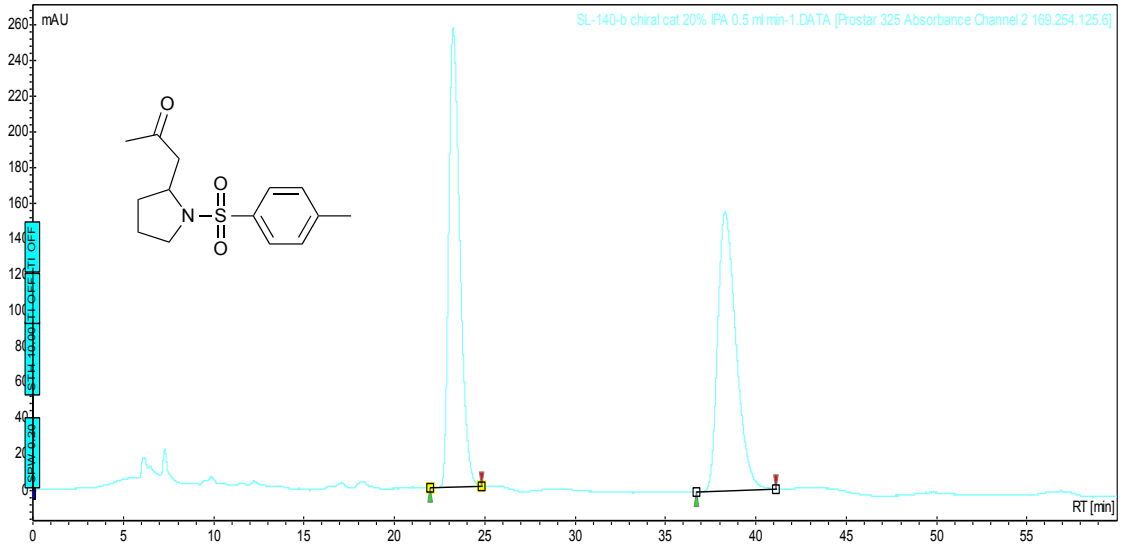


#	Name	Time [Min]	Quantity [% Area]		Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	78.03	89.21		1350.3	3536.7	89.207
2	UNKNOWN	84.35	10.79		275.2	427.9	10.793
	Total		100.00		1625.5	3964.6	100.000



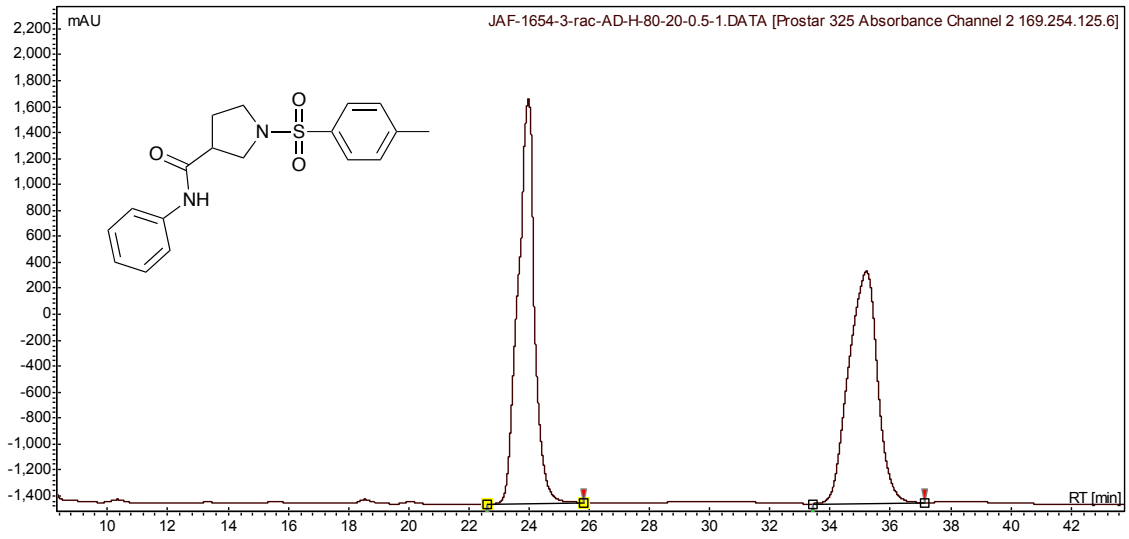
#	Name	Time [Min]	Quantity [% Area]		Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	79.12	10.77		27.9	61.6	10.766
2	UNKNOWN	84.28	89.23		219.7	510.5	89.234
	Total		100.00		247.6	572.1	100.000

1-(1-tosylpyrrolidin-2-yl)propan-2-one, **G**

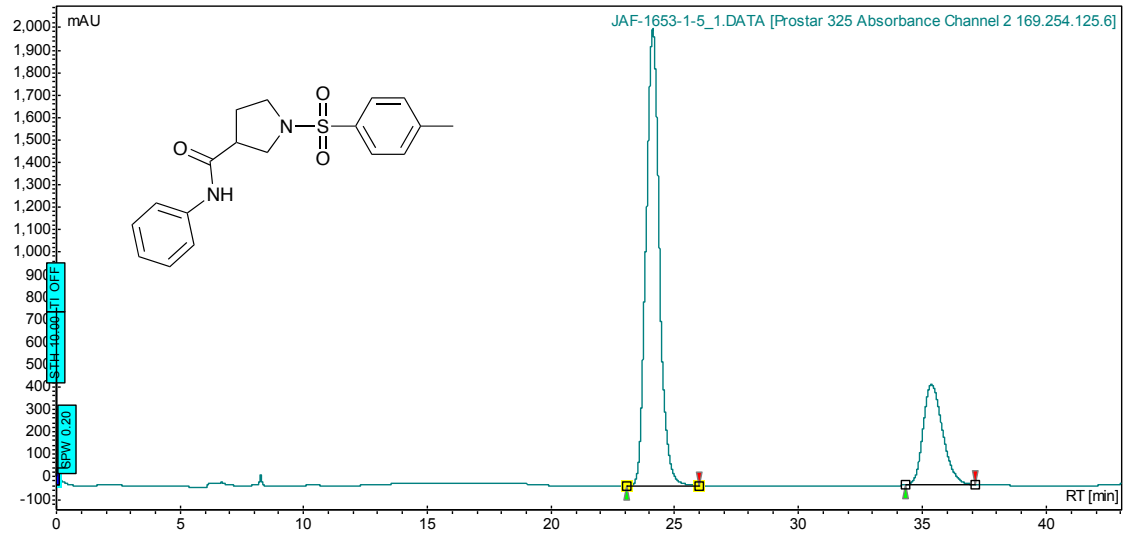


#	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	23.26	50.08	256.8	183.7	50.081
2	UNKNOWN	38.30	49.92	156.3	183.1	49.919
Total			100.00	413.1	366.9	100.000

N-Phenyl-1-tosylpyrrolidine-3-carboxamide, **H**



#	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	23.98	50.03	3114.8	1990.9	50.026
2	UNKNOWN	35.21	49.97	1788.4	1988.8	49.974
Total			100.00	4903.2	3979.7	100.000



#	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	24.11	75.77	2035.3	1282.1	75.768
3	UNKNOWN	35.38	24.23	448.4	410.0	24.232
Total			100.00	2483.7	1692.1	100.000

6. Computational details.

6.1. Figure 1: TS1-5 showing concerted hydrometallation leading to complex 5.

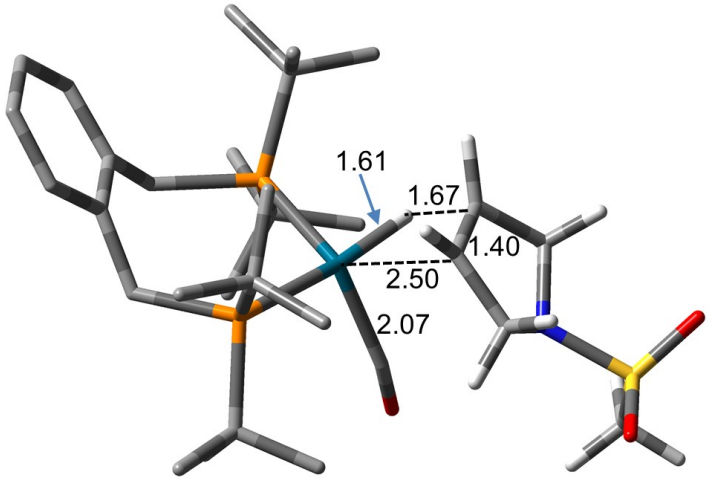


Figure 1: **TS1-5** showing concerted hydrometallation leading to complex **5**. Distances in Å. Hydrogens of the DTBPX ligand have been removed for clarity.

6.2. Figure 2 showing geometries for **2**, **4**, **TS4-6**, **6**, **TS6-7** and **7**.

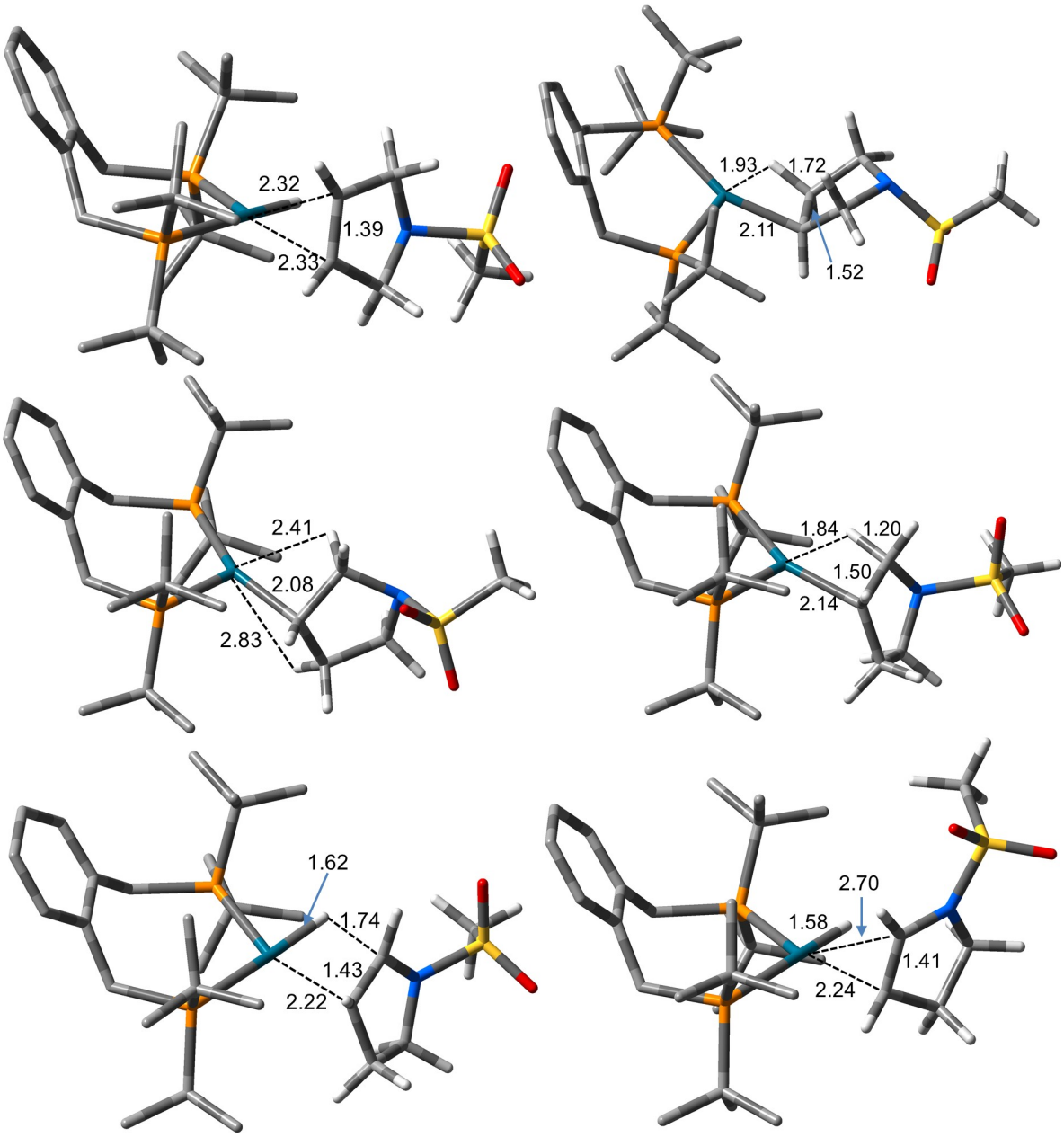


Figure 2: Complex **2** (top left), **4** (top right), **TS4-6** (centre left), **6** (centre right), **TS6-7** (bottom left) and **7** (bottom right). All distances are in Å.

6.3. BP86/ECP1 optimised structure of all complexes of this study (Cartesian coordinates in Å, xyz format).

Complex 1

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Complex1

Pd	0.037782	-1.486069	-0.568648
P	-1.863478	-0.058246	0.305046
P	1.992847	-0.373822	0.102355
C	-2.841830	-1.167728	1.557267
C	-1.924519	-1.416871	2.781931
H	-1.835529	-0.532485	3.435810
H	-0.910779	-1.740182	2.481019
H	-2.362690	-2.225774	3.396817
C	-4.177915	-0.568134	2.048348
H	-4.055800	0.439428	2.482905
H	-4.590244	-1.216147	2.845563
H	-4.936804	-0.514050	1.249905
C	-3.103708	-2.539692	0.892166
H	-2.154162	-3.015040	0.579713
H	-3.762082	-2.465476	0.012007
H	-3.592793	-3.213970	1.620916
C	-3.039550	0.703162	-1.024055
C	-3.912529	-0.390936	-1.681155
H	-3.307578	-1.226382	-2.066283
H	-4.444369	0.060383	-2.540664
H	-4.684754	-0.778802	-0.994940
C	-3.971592	1.811748	-0.485631
H	-4.608787	1.473734	0.346985
H	-4.644473	2.129705	-1.304853
H	-3.416861	2.705636	-0.165545
C	-2.103102	1.303609	-2.104281
H	-1.477349	0.524482	-2.574605
H	-1.438596	2.083535	-1.694521
H	-2.718901	1.769501	-2.897591
C	-1.407878	1.395100	1.432417
H	-2.348103	1.815607	1.831912
H	-0.894973	0.919061	2.287027
C	-0.548091	2.515860	0.882984
C	-1.143726	3.775069	0.644419
H	-2.212806	3.901295	0.847241
C	-0.405797	4.880080	0.201859
H	-0.905475	5.839106	0.029480
C	0.978152	4.751542	0.021064
H	1.582587	5.606429	-0.299770
C	1.592244	3.524914	0.301530
H	2.682939	3.452350	0.222947
C	0.858756	2.389703	0.718376
C	1.639990	1.166434	1.164805
H	1.184364	0.740933	2.078328
H	2.643957	1.512433	1.463963
C	3.001922	0.268446	-1.419470
C	4.226847	1.113738	-0.997110
H	5.027423	0.490070	-0.564154

H	3.989957	1.920465	-0.285084
H	4.646244	1.592704	-1.901999
C	2.020762	1.120433	-2.265024
H	1.152035	0.522629	-2.595692
H	2.552676	1.464210	-3.172596
H	1.648605	2.009999	-1.734971
C	3.499841	-0.883909	-2.323153
H	2.673884	-1.495683	-2.713884
H	4.224055	-1.546601	-1.825619
H	4.018920	-0.428525	-3.188188
C	3.103147	-1.335920	1.376328
C	2.138961	-1.988537	2.398819
H	1.573941	-1.235455	2.976712
H	2.729727	-2.577811	3.125583
H	1.408420	-2.663966	1.922858
C	4.087445	-0.436589	2.169996
H	3.575931	0.243427	2.871234
H	4.751691	0.157482	1.522157
H	4.732978	-1.096188	2.780389
C	3.935959	-2.426936	0.661510
H	4.818753	-1.997549	0.158540
H	3.366044	-2.996742	-0.089423
H	4.310065	-3.144349	1.416172
H	1.191444	-2.407008	-1.131974
C	-1.366211	-2.220679	-1.837527
O	-1.960837	-2.759961	-2.611937

TS1-1A

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TS1-1A

Pd	0.2070050584	-0.5618122103	-0.3491212353
P	0.2314696698	1.797250474	-0.8047170052
P	-2.2558779391	-1.1035887812	-0.0420024236
C	-1.4532514791	2.5751684406	-1.1897075002
H	-1.2201348381	3.599155387	-1.5341099881
H	-1.7892751354	2.0220261704	-2.084243507
C	-2.5997834056	2.650199866	-0.1982625617
C	-2.8708516744	3.8921153515	0.4194029851
H	-2.1944866178	4.7340858151	0.2369246654
C	-4.0106109148	4.1066795846	1.2049394141
H	-4.1828229716	5.0852138663	1.665141337
C	-4.9480439468	3.0747097842	1.3431282707
H	-5.872022765	3.2298101834	1.9098862472
C	-4.7101714548	1.8463439911	0.7130680742
H	-5.4803433651	1.0692819155	0.7698728468
C	-3.5348015583	1.5900723396	-0.0291823309
C	-3.4064038194	0.2475260768	-0.7267842659
H	-3.0502765745	0.3914663078	-1.762973719
H	-4.4113828329	-0.2043069344	-0.8085919838
H	1.7070343328	-0.1170797163	-0.4336305515
C	0.70631706	-1.7721352445	-1.870865483
O	1.3165717339	-2.2180803062	-2.7550212483
C	1.229680338	-1.3756825983	1.9327406888
H	0.38172949	-1.1525295385	2.582348825

C	1.303372217	-2.4175082614	1.0398893541
H	0.5302378952	-3.1670582159	0.8573778294
C	1.0383238609	2.8849460855	0.5674600272
C	1.105718421	2.084298628	-2.5272325483
C	-2.8385545503	-1.4011551862	1.7839833725
C	-2.7890425236	-2.595780493	-1.1789201657
C	0.7966547569	4.4048826278	0.4030504523
H	1.3192891407	4.9244707835	1.2282157507
H	1.1913603951	4.8122142901	-0.5393637114
H	-0.2681164488	4.6699183905	0.4838571315
C	0.396465381	2.4311498934	1.8999598788
H	0.6069024406	1.3680498039	2.1033108532
H	0.8201741233	3.0318543492	2.7270263596
H	-0.697575596	2.5753350662	1.9026149009
C	2.5622732142	2.6298961253	0.6177014474
H	2.9609593576	3.0420371875	1.5637582463
H	2.8225630929	1.5569588702	0.5882190987
H	3.0944357079	3.1375691028	-0.2046294005
C	1.331776396	3.5814095863	-2.8511442728
H	2.1207859747	4.0290104607	-2.2249408998
H	1.667836108	3.662701773	-3.9019586361
H	0.417933716	4.1935110154	-2.7611928923
C	0.1962292987	1.4751910746	-3.6271909529
H	0.7794721835	1.3925956472	-4.5629889393
H	-0.1577167892	0.4613001045	-3.3683967582
H	-0.6798587249	2.1078136382	-3.8504666976
C	2.4756656394	1.3686201563	-2.5848512581
H	2.9364175682	1.5803327368	-3.5682678879
H	3.1761136003	1.719505678	-1.8111341694
H	2.3779956451	0.2755434297	-2.4967352664
C	-4.370363089	-1.4969048266	1.9780164583
H	-4.5758189249	-1.5400329446	3.0647592877
H	-4.9034339161	-0.6184854931	1.5877594058
H	-4.8067673055	-2.4004577881	1.5292599447
C	-2.3272816297	-0.1930417941	2.6085676503
H	-2.5129081845	-0.3861611428	3.6823448391
H	-1.2479363919	-0.0168337291	2.4725132118
H	-2.8516311629	0.7377234125	2.3385735832
C	-2.2102257905	-2.7031256983	2.3364680378
H	-2.3990186236	-2.7522653326	3.4256575476
H	-2.6628289244	-3.6051961034	1.8913268469
H	-1.1189030812	-2.7566647731	2.1917276148
C	-4.2391151807	-3.080998398	-0.9419371005
H	-4.5127608467	-3.7758043755	-1.7583408244
H	-4.3409884407	-3.6391527039	0.0027697311
H	-4.9832886544	-2.2662818087	-0.9501221307
C	-2.6699695104	-2.1241219372	-2.6511523899
H	-1.6959350163	-1.6517653562	-2.8709491734
H	-2.765238583	-3.0036457586	-3.3150199395
H	-3.4713299114	-1.4192914892	-2.9313222344
C	-1.841825101	-3.8013939154	-0.9690527743
H	-1.8856641033	-4.2030034331	0.0562619724
H	-2.1459197919	-4.616345228	-1.6527962947
H	-0.7923879775	-3.5556204703	-1.2020548106
C	2.6107991498	-0.8305691219	2.2047174286

H	2.9658179138	-1.2476409063	3.1737850826
H	2.6909601497	0.2637225463	2.2704851221
C	2.7453857439	-2.6346887955	0.6294314448
H	3.1604572489	-3.4994546857	1.1926373927
H	2.8951510087	-2.8241592876	-0.4470431172
N	3.3838663211	-1.3490401064	1.034859492
S	5.0975680882	-1.440014319	1.3785845896
O	5.4089530669	-0.1755144615	2.0774118987
O	5.4293540472	-2.7554913683	1.9751915285
C	5.7832848044	-1.3828722628	-0.2949058388
H	6.8758600429	-1.4344104772	-0.1763243883
H	5.4292530971	-2.2514384335	-0.8686297214
H	5.486429087	-0.4376040056	-0.76775399

Complex 1A

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Complex 1A

Pd	0.2696711685	-1.2983374449	0.5822133528
P	2.0632147778	0.2043138957	-0.2014049189
P	-1.8623879642	-0.0410106437	-0.1647203332
C	1.5439294263	1.5683860238	-1.4129271466
H	2.4883733055	1.9961083759	-1.7961473182
H	1.0998189324	1.0043775894	-2.2524787846
C	0.6183510405	2.7116023646	-1.0369906523
C	1.1885406058	3.988316445	-0.8281728217
H	2.2776999996	4.095509068	-0.8721406682
C	0.410394569	5.135787741	-0.630291633
H	0.8938690137	6.1053307482	-0.4714131075
C	-0.9852567328	5.0323898018	-0.6932417122
H	-1.6180600825	5.9195853085	-0.586045527
C	-1.5669445003	3.7826073716	-0.9411942514
H	-2.6541620043	3.726124707	-1.0622273353
C	-0.8004689887	2.6034402898	-1.0858611223
C	-1.5240941014	1.3189382976	-1.4510742944
H	-0.9676805143	0.7902128754	-2.2457849729
H	-2.5033533371	1.5816515067	-1.8914784353
H	1.5916755601	-1.9437270828	1.1135318211
C	0.205106247	-2.8847749368	-0.6746582594
O	0.402999363	-3.9839551648	-0.9989101935
C	-0.1209319746	-1.4789631743	2.8770155871
H	-0.698072283	-0.5933470235	3.1494283168
C	-0.6463970363	-2.6084842463	2.2301509118
H	-1.6915908111	-2.7389857073	1.9395725814
C	3.0281445889	1.0672856678	1.2307115452
C	3.2857325998	-0.7889709458	-1.3515569163
C	-2.9012590222	0.8223874073	1.2270413115
C	-3.000955159	-1.2096924744	-1.2344275011
C	3.9507350528	2.2234077574	0.776820032
H	4.4659167991	2.6210211589	1.6716420925
H	4.729375419	1.9119446074	0.0652958928
H	3.3830848892	3.0569688706	0.3382520838
C	1.9573800967	1.6504414602	2.1839114233
H	1.3118627298	0.8588678134	2.5986718019
H	2.4656046878	2.1570402116	3.026349981
H	1.316351991	2.3945818344	1.6808116658

C	3.878838044	0.0230242628	1.9905242376
H	4.205301575	0.4613355509	2.9523906831
H	3.3245688533	-0.9043565494	2.2194078536
H	4.7915724667	-0.250226703	1.4343817901
C	4.5725087874	-0.0012791873	-1.7003125496
H	5.2481946643	0.1008213554	-0.8354470288
H	5.1242371985	-0.5626856905	-2.4777136753
H	4.3730576041	1.0023835	-2.113626011
C	2.5438738029	-1.1138930411	-2.6749252788
H	3.1258309434	-1.8742993183	-3.2282128097
H	1.5346778162	-1.5312059341	-2.5081716522
H	2.4548804732	-0.2341617657	-3.3348034471
C	3.7048130121	-2.1231954365	-0.6896140732
H	4.4092892381	-2.6417999564	-1.3671486599
H	4.2178990623	-1.9797598904	0.2742241174
H	2.8475918737	-2.7952190915	-0.5289848334
C	-4.0534131351	1.7266375461	0.7271712991
H	-4.4445467633	2.2934299691	1.5933905417
H	-3.7253895654	2.4666721089	-0.0168904116
H	-4.8932467627	1.1571731398	0.3054361653
C	-1.9150851463	1.7123716929	2.0269618135
H	-2.4336342381	2.104622136	2.9225020031
H	-1.0195714458	1.165617689	2.3636016806
H	-1.5716394511	2.5749351923	1.4335194476
C	-3.5136787821	-0.2437972224	2.1671484914
H	-3.9660184677	0.2681953263	3.0375096593
H	-4.319200497	-0.8168781621	1.6771429314
H	-2.7709457292	-0.9577572711	2.5582532282
C	-4.3925508522	-0.6173476848	-1.5614434561
H	-4.8696563777	-1.2532377084	-2.3310745316
H	-5.062400894	-0.6158018678	-0.6862763133
H	-4.3468273303	0.4058746778	-1.9719540724
C	-2.2725549092	-1.4849286753	-2.5755326728
H	-1.2164321383	-1.7780600253	-2.4373289722
H	-2.7807532734	-2.3220544503	-3.0896463934
H	-2.3084448419	-0.6174814735	-3.2562712807
C	-3.2096111046	-2.5578236251	-0.5039694531
H	-3.7295561894	-2.4424990356	0.4615854646
H	-3.8372084304	-3.2142508157	-1.1358799464
H	-2.2575690056	-3.0849320012	-0.3283755098
C	1.0708496312	-1.8996139655	3.7093638238
H	0.7132142985	-2.0588165681	4.7517682792
H	1.9136485901	-1.1970237604	3.7493321327
C	0.209847655	-3.8149173475	2.5816032116
H	-0.2867573024	-4.3845831987	3.3973683048
H	0.4057999884	-4.5074121322	1.7463843138
N	1.4729706154	-3.177730357	3.0520514054
S	2.4756252859	-4.1649495512	4.0974568755
O	3.4362851978	-3.2172954736	4.6996655091
O	1.6240112045	-5.0427436838	4.9335498834
C	3.3317790206	-5.1897177966	2.8767399606
H	4.0008742197	-5.8479209095	3.4508149334
H	2.5988608355	-5.7938937468	2.3230589287
H	3.9068875039	-4.537145128	2.2068831371

TS1A-2

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TS1A-2

Pd	0.1773564406	-1.1673398804	0.567443367
P	2.0047836362	0.0796611178	-0.2999976725
P	-1.8869002104	0.0506022895	-0.279202887
C	1.5696697524	1.5445625507	-1.4232808352
H	2.5319275611	1.9226320391	-1.8155962069
H	1.0584491369	1.0603867726	-2.2740798553
C	0.7469007701	2.7225991387	-0.9317091278
C	1.4178555065	3.9340555467	-0.6473035574
H	2.5074171918	3.9739264088	-0.7523508029
C	0.7360868873	5.1040869468	-0.2903064326
H	1.2954663125	6.0212160168	-0.078254224
C	-0.6644609762	5.0938858076	-0.2546368729
H	-1.2248479307	6.0023634219	-0.0102179221
C	-1.3478520926	3.916669564	-0.5854642672
H	-2.4420384117	3.9412629827	-0.6311592079
C	-0.6767883193	2.7156150973	-0.9100039714
C	-1.5017342703	1.536502112	-1.3980525783
H	-0.9988288657	1.0823857703	-2.2702477133
H	-2.4712428698	1.9143036748	-1.7696723806
H	1.4853654498	-1.8828030018	1.0284543948
C	0.1477360682	-3.5809782525	-1.3334531665
O	0.3173189268	-4.7105545256	-1.1914551317
C	-0.4765200662	-1.8215467059	2.6983964338
H	-1.110237465	-0.969884559	2.957163461
C	-0.8429060745	-2.8779663473	1.8778339842
H	-1.8117870465	-2.9937501263	1.3861140912
C	3.0082472603	0.7900173431	1.1900812785
C	3.1360884639	-0.9493339507	-1.495992358
C	-3.0296585489	0.772361838	1.1102646701
C	-2.9308529866	-1.0212734013	-1.5244401723
C	4.0262722022	1.8836944009	0.791559801
H	4.5367136508	2.228141116	1.7106491946
H	4.8049262638	1.5234164569	0.1028587686
H	3.5398106343	2.7631284465	0.3468154613
C	1.9636639143	1.4089265183	2.1524318372
H	1.2502061282	0.6478247736	2.514519739
H	2.4911867918	1.8305999626	3.0292498601
H	1.3899790635	2.2225622501	1.6781530308
C	3.7637079019	-0.3403185117	1.9254574431
H	4.1348388915	0.0561776248	2.8892677461
H	3.1218178569	-1.2111384963	2.1501115036
H	4.6442099096	-0.6897504762	1.3599565778
C	4.4714554611	-0.2407375196	-1.8294223625
H	5.1610896299	-0.2241136519	-0.9695672579
H	4.9732893892	-0.8059019483	-2.6372980723
H	4.3407154662	0.7923023772	-2.1960025366
C	2.3494631544	-1.1692949332	-2.8145463273
H	2.889180642	-1.916906599	-3.4256220198
H	1.332103376	-1.5602022927	-2.6363060503
H	2.276622057	-0.251499491	-3.4224306776
C	3.4571433301	-2.331635545	-0.8841590351
H	4.077125965	-2.9005023004	-1.6027156467

H	4.0215831386	-2.2590249208	0.0584802741
H	2.5433956202	-2.9153421337	-0.6892829625
C	-4.1251907337	1.7527925542	0.6279909556
H	-4.6274695069	2.175087783	1.5193619054
H	-3.7183039137	2.6029661708	0.0602932901
H	-4.9011315954	1.2674563949	0.018241877
C	-2.0969048417	1.5471292275	2.0784993178
H	-2.6781335968	1.8642067592	2.9652666576
H	-1.2408100769	0.9461273729	2.4293324756
H	-1.6860103826	2.4536224735	1.6045846126
C	-3.7317562681	-0.3818852385	1.8653282107
H	-4.2064940324	0.0230423334	2.7791954344
H	-4.5341308614	-0.8388326471	1.2615269347
H	-3.0445294247	-1.1846153129	2.1802892173
C	-4.2922500338	-0.4060355956	-1.9239349418
H	-4.7109119016	-0.9961484236	-2.7614008514
H	-5.0280357527	-0.4464102471	-1.1037780041
H	-4.2124837411	0.6376348103	-2.2739251809
C	-2.0823440499	-1.2053519316	-2.8093112237
H	-1.046392568	-1.5138419601	-2.584484046
H	-2.5385925758	-2.0035632954	-3.4247536649
H	-2.0588227959	-0.2951576826	-3.4325805024
C	-3.187389207	-2.4226454367	-0.9205385524
H	-3.7436472385	-2.3855728478	0.0306897092
H	-3.7944643769	-3.0148012264	-1.6313449891
H	-2.2444727835	-2.9713180192	-0.7587320226
C	0.6527223122	-2.2388275747	3.6089827675
H	0.2165189572	-2.4437393206	4.6123218742
H	1.4547254726	-1.4984447372	3.7446704627
C	0.0334271519	-4.0760268521	2.1907785301
H	-0.5458135349	-4.7821652554	2.8262306101
H	0.3983156863	-4.6322614162	1.3133667556
N	1.172159436	-3.4667983412	2.9379546247
S	1.9785072597	-4.5356921686	4.064041111
O	2.743789301	-3.6407589233	4.9572407719
O	1.0159894539	-5.5270396399	4.6005258634
C	3.1244558743	-5.3955350692	2.9590810311
H	3.6813360212	-6.1038900968	3.5904120232
H	2.5567123087	-5.944268183	2.1938479936
H	3.80178448	-4.6578637528	2.5093469165

Complex 2

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Complex2

Pd	-0.3351328749	-0.2769193744	0.0481770486
P	0.3591078771	1.9282756772	0.5138880952
P	1.698255326	-1.7095530618	0.3042177569
C	-0.4573655305	2.6250357458	2.1274973993
C	0.2349687309	1.9693195927	3.3487508483
H	1.2654095167	2.3308567675	3.5051292799
H	0.2464282368	0.8679492348	3.27553037
H	-0.3385403365	2.2314293225	4.2575166254
C	-0.3249769112	4.1618901809	2.2499408706
H	0.7176178954	4.5133512842	2.1595029491
H	-0.6818942901	4.4651151066	3.2521977852

H	-0.9420135807	4.6978539594	1.5102403158
C	-1.9535010255	2.2348583971	2.1776556499
H	-2.0814225014	1.1393058936	2.2214637992
H	-2.5257743646	2.6109909076	1.3151543237
H	-2.3989854967	2.6685212356	3.0931690216
C	-0.0580610371	3.0187600306	-1.0237180537
C	-1.5832009056	3.2399855361	-1.1389063562
H	-2.1560119044	2.2961961163	-1.0915643578
H	-1.7954119979	3.7052985486	-2.1197623193
H	-1.9695650859	3.9236389811	-0.3642548632
C	0.6413944043	4.3981333216	-1.0088559172
H	0.3396559399	5.028371502	-0.1586128041
H	0.3612716807	4.9382679201	-1.9327197191
H	1.7370543147	4.3087588936	-1.010333534
C	0.4280632499	2.2206809089	-2.2605370973
H	-0.071503743	1.2363852365	-2.3266513381
H	1.5187971518	2.0568489864	-2.250383322
H	0.179659158	2.7933359849	-3.1745447359
C	2.1976068332	2.1848120142	0.8873872707
H	2.3245712785	3.2565725359	1.1297879332
H	2.3428741005	1.6337632456	1.8329289937
C	3.2578806444	1.7690724879	-0.1165387487
C	3.9067453171	2.7756072746	-0.867712331
H	3.6103685759	3.8203358517	-0.7238253213
C	4.9534409749	2.4911999081	-1.7536799184
H	5.4304245594	3.3009382434	-2.315667711
C	5.4041272662	1.1700517521	-1.8788427165
H	6.2375539997	0.9243086556	-2.5452431698
C	4.8068688324	0.1682503895	-1.1034658604
H	5.2080972761	-0.8506341111	-1.1563524437
C	3.7293059241	0.4309919761	-0.226698046
C	3.2592354189	-0.6958996578	0.6763449675
H	3.0635226254	-0.3003296954	1.6914239411
H	4.0893457452	-1.4133779311	0.78985113
C	2.1537465637	-2.7793133623	-1.242074488
C	3.5071789819	-3.5129215644	-1.1111571406
H	3.4868672495	-4.2914201846	-0.3292856556
H	4.3497485877	-2.8333727621	-0.9011356104
H	3.7328895719	-4.0206883168	-2.0682459616
C	2.2023141018	-1.7940237445	-2.4391834345
H	1.2400639621	-1.2674819758	-2.5748320691
H	2.4061969187	-2.3655105278	-3.3648216815
H	2.9885627971	-1.0305174318	-2.3352363752
C	1.0584551448	-3.8304633148	-1.5476663937
H	0.0434026114	-3.4010348806	-1.5604890938
H	1.0636098324	-4.6757236656	-0.8437461404
H	1.247038151	-4.2463176602	-2.555574271
C	1.6591551061	-2.7878135411	1.9294569226
C	0.9118784654	-1.9315974256	2.9802845061
H	1.4163858741	-0.9661511373	3.1618721104
H	0.8866640152	-2.4732957362	3.9453112453
H	-0.1311554133	-1.7226239721	2.6787856862
C	3.0633260679	-3.1350979543	2.4837263168
H	3.6184816814	-2.2479359484	2.8305779089
H	3.6888956161	-3.6754932436	1.7538752471

H	2.9381090566	-3.7981031272	3.3608126672
C	0.8880386554	-4.1142427285	1.7406836688
H	1.4635620556	-4.8516044493	1.1574934189
H	-0.0974537149	-3.9862907013	1.2617856664
H	0.7074088909	-4.5601692613	2.737145958
C	-1.7467139744	-1.4346615458	-1.3904062222
H	-1.0247820293	-1.7426377752	-2.1517735013
C	-1.8891689236	-2.0058014326	-0.1354652033
C	-3.2453614301	-1.6506988231	0.4362095466
H	-3.9092472641	-2.5409778249	0.3840048235
H	-3.2164296755	-1.307074373	1.4853451078
C	-3.0077232804	-0.6976626274	-1.7734597683
H	-3.5633340264	-1.3280583229	-2.5019377194
H	-1.5747014868	0.6716511578	-0.002839824
N	-3.7138325249	-0.5539235702	-0.4630343099
S	-5.4485966946	-0.4532441505	-0.6602746056
O	-5.6497634849	0.3376630139	-1.8923129671
O	-6.0564662414	-1.7951384316	-0.4929655249
C	-5.9006798486	0.5526649513	0.773839976
H	-5.4099243662	1.5310472039	0.6890009942
H	-6.9951668724	0.6594605378	0.7390054309
H	-5.6053514554	0.0301378363	1.6951425035
H	-2.8544857276	0.2860575594	-2.2424659914
H	-1.3225867918	-2.8581455412	0.2417905572

Complex 3

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Complex 3

Pd	0.013555	-1.264614	-0.530437
P	-1.845719	0.111180	0.292536
P	1.925531	-0.285947	0.196626
C	-2.926060	-0.876509	1.563151
C	-2.130609	-0.994978	2.887574
H	-2.090332	-0.045164	3.447773
H	-1.101025	-1.358978	2.723174
H	-2.639224	-1.730033	3.539498
C	-4.294656	-0.229752	1.869945
H	-4.202229	0.816047	2.212522
H	-4.781339	-0.796157	2.687000
H	-4.979265	-0.255153	1.006257
C	-3.132624	-2.309579	1.016737
H	-2.162376	-2.820035	0.877599
H	-3.673512	-2.332093	0.057995
H	-3.719952	-2.894653	1.749716
C	-2.927389	0.783347	-1.154963
C	-3.759151	-0.366303	-1.773289
H	-3.149907	-1.261794	-1.981564
H	-4.191004	-0.014016	-2.729664
H	-4.603535	-0.666438	-1.129512
C	-3.879136	1.936262	-0.763646
H	-4.588978	1.660049	0.031152
H	-4.475348	2.216704	-1.653113
H	-3.332860	2.837915	-0.447694
C	-1.927427	1.302067	-2.220068
H	-1.269848	0.493973	-2.590830

H	-1.286342	2.110782	-1.829903
H	-2.493439	1.703714	-3.082385
C	-1.376341	1.628234	1.322574
H	-2.315663	2.112483	1.646611
H	-0.922523	1.197381	2.233121
C	-0.443829	2.678750	0.744658
C	-0.984948	3.929142	0.369352
H	-2.063444	4.091638	0.473105
C	-0.185359	4.985504	-0.086028
H	-0.645535	5.939108	-0.365369
C	1.205194	4.819049	-0.142252
H	1.854454	5.638087	-0.468819
C	1.763059	3.600394	0.264132
H	2.854287	3.494130	0.271357
C	0.968643	2.513006	0.694155
C	1.682741	1.284998	1.229557
H	1.176591	0.912166	2.140368
H	2.695980	1.585330	1.549371
C	3.047209	0.193413	-1.301373
C	4.331280	0.927263	-0.846956
H	5.027786	0.256559	-0.315799
H	4.130358	1.800946	-0.205848
H	4.859795	1.299059	-1.744442
C	2.191168	1.112856	-2.209181
H	1.281710	0.590461	-2.557587
H	2.789342	1.383142	-3.099999
H	1.883750	2.044937	-1.711477
C	3.457391	-1.034511	-2.146455
H	2.580505	-1.605757	-2.496538
H	4.133599	-1.721853	-1.617093
H	3.993904	-0.665833	-3.040990
C	2.816574	-1.418032	1.492432
C	1.710206	-1.952480	2.434353
H	1.173403	-1.140755	2.956617
H	2.177314	-2.587190	3.211028
H	0.972583	-2.565104	1.885771
C	3.864179	-0.654897	2.342802
H	3.409153	0.113643	2.989789
H	4.652086	-0.181679	1.734033
H	4.361332	-1.383017	3.010625
C	3.506368	-2.623756	0.816007
H	4.438501	-2.335443	0.303601
H	2.846950	-3.138185	0.095263
H	3.779617	-3.354560	1.600280
C	-1.067261	-4.112617	-1.666504
H	-0.001983	-4.357934	-1.815371
H	-1.376774	-4.402737	-0.653019
H	-1.697999	-4.633419	-2.406690
O	-1.293733	-2.673601	-1.767339
H	-1.043652	-2.405213	-2.677502
H	1.208909	-2.187715	-1.031307

Complex 3i
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Complex 3i

Pd	0.0200754043	-1.2862755989	-0.4847423648
P	-1.9078229313	-0.3214413677	0.2195798485
P	1.8506254872	0.1427768798	0.2529869085
C	-2.8212836993	-1.4765460501	1.4856515905
C	-2.0537855007	-1.4252234143	2.8319220013
H	-2.2051953598	-0.476720557	3.3749435868
H	-0.9703780899	-1.5948186203	2.7001534366
H	-2.4369336736	-2.2328468516	3.4831791524
C	-4.2865533014	-1.0430694155	1.731929385
H	-4.3799920238	0.0120313507	2.0436746751
H	-4.6984198772	-1.6586667174	2.5535915933
H	-4.9268705045	-1.2085833101	0.8498743125
C	-2.8027876241	-2.9422029444	0.9910044228
H	-1.7731087449	-3.3359953354	0.9397069421
H	-3.2688520595	-3.0707635945	0.0009875714
H	-3.3707954571	-3.5612757523	1.7109549285
C	-3.0189826528	0.1270593878	-1.2896409426
C	-3.6176862181	-1.1472137393	-1.926224569
H	-2.8447362123	-1.896822824	-2.1721947339
H	-4.1169598686	-0.8627292217	-2.8715282194
H	-4.378558394	-1.6207512843	-1.2835025694
C	-4.1727788584	1.0938328105	-0.9322752621
H	-4.8701816511	0.6821996503	-0.1866915234
H	-4.7551462942	1.2911126875	-1.8515689739
H	-3.8032446555	2.0649842941	-0.5726367608
C	-2.086109587	0.8132993855	-2.3188388055
H	-1.2867100031	0.1270310729	-2.6529376755
H	-1.6185578138	1.726602871	-1.9123024055
H	-2.6832695911	1.1031421504	-3.2043667981
C	-1.6955549374	1.2489117977	1.2617296744
H	-2.7110812312	1.5076592994	1.6163249959
H	-1.1441934731	0.8848522519	2.1467711484
C	-1.0234860918	2.5036110366	0.730893892
C	-1.8363582453	3.6007580397	0.3644972696
H	-2.9253536491	3.4977191484	0.4238498513
C	-1.2998683168	4.8368562304	-0.0174920918
H	-1.9663916526	5.6611612586	-0.2919442059
C	0.0903798141	5.0149735054	-0.0024035225
H	0.5335986791	5.9800608357	-0.2693761295
C	0.9097318891	3.9522966874	0.3982724971
H	1.993909277	4.1090375252	0.4602901224
C	0.3870071399	2.6879737581	0.7538403761
C	1.3650346057	1.6541837886	1.2818988421
H	0.974926828	1.2048610434	2.2163391407
H	2.2981148041	2.1726432178	1.5650542673
C	2.8878668381	0.8182086572	-1.230824879
C	4.1656780886	1.5675035561	-0.793875183
H	4.9175081061	0.8981273472	-0.342750327
H	3.9482085487	2.3781461307	-0.0770105337
H	4.6331929628	2.0351415752	-1.6813105276
C	1.9856336456	1.7728361955	-2.0536735643
H	1.0232191945	1.301694177	-2.3240118
H	2.5098953888	2.0272752194	-2.9948766188
H	1.766694225	2.7132668602	-1.5282304606
C	3.2675327065	-0.3463637977	-2.1811179267

H	2.358701347	-0.7540310228	-2.6672732732
H	3.8339745627	-1.1547317749	-1.6905269744
H	3.9023160752	0.0480133524	-2.9968154609
C	2.9735008256	-0.7778115209	1.5438800808
C	2.0006674015	-1.5764269972	2.4475103017
H	1.3059254926	-0.9210744087	3.0034327979
H	2.5824659856	-2.1431798839	3.1996200044
H	1.4022435996	-2.296976484	1.8602874205
C	3.8183814029	0.1676305582	2.4297854682
H	3.1981245011	0.8021842431	3.0852624556
H	4.4867561532	0.8206625948	1.8451093312
H	4.4576692697	-0.4473282254	3.0910996751
C	3.9141519137	-1.7872463788	0.8462729497
H	4.7072141704	-1.2887450204	0.263428504
H	3.3655680341	-2.4867595758	0.1923159852
H	4.419425043	-2.3917426959	1.6234367097
C	0.874034579	-4.0982505748	-1.8333447166
H	0.2689769786	-4.5472682456	-1.0354517709
H	0.2402034068	-3.9057050237	-2.7144729729
H	1.7037039059	-4.7756264078	-2.0940129809
O	1.4107922886	-2.8576625543	-1.2887346958
H	2.0292609548	-2.4716763457	-1.9408820873
H	-1.1654481701	-2.1832022446	-1.003796639

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TS2-4

Pd	-0.3302896139	-0.3158014302	0.3190663764
P	0.3383960929	1.9179031098	0.5865736837
P	1.7793607716	-1.6608304446	0.2664405366
C	-0.2967924151	2.6307331482	2.2748454646
C	0.5824897621	2.0475779495	3.4108920397
H	1.5933256445	2.4888355484	3.436795333
H	0.6746423522	0.9484580912	3.3474802718
H	0.1040485417	2.282931386	4.3798704605
C	-0.2236359421	4.1748282426	2.3330993726
H	0.7806718275	4.5675283751	2.0968560561
H	-0.4617071259	4.5001081654	3.3633196833
H	-0.9555852677	4.6554931814	1.6633193153
C	-1.7533857824	2.1798071622	2.5298772044
H	-1.81684881	1.0842234762	2.6463982407
H	-2.4448350353	2.482379732	1.7265996371
H	-2.108383544	2.6435311779	3.4696044107
C	-0.2987680146	2.9359884204	-0.920581742
C	-1.8361779822	3.0915332526	-0.8711316184
H	-2.3560467383	2.1217369904	-0.7623078986
H	-2.1669153178	3.5395013061	-1.8274328819
H	-2.1666177286	3.7666376252	-0.0633164784
C	0.3344780042	4.3423673792	-1.0425251665
H	0.1179516204	4.9919714732	-0.1807290734
H	-0.0890320101	4.8338356318	-1.9383575661
H	1.4234577668	4.2996984834	-1.1879682049
C	0.0774251892	2.1008846956	-2.1714087484
H	-0.4186240736	1.1130228261	-2.157416729
H	1.1661721988	1.9440608493	-2.254764336

H	-0.2594294921	2.6388487934	-3.0780830507
C	2.1934477809	2.2365716772	0.7363496196
H	2.3071774414	3.3155067834	0.95079634
H	2.4633142044	1.7063376671	1.6661852345
C	3.153862519	1.8455416722	-0.3714210019
C	3.6651485245	2.8705326985	-1.1993622967
H	3.3149552675	3.897127879	-1.0475404134
C	4.6483746312	2.6341847704	-2.1679996617
H	5.015574346	3.4572602742	-2.7898218003
C	5.1883176898	1.3476867356	-2.2872816368
H	5.9911166253	1.1409989804	-3.0027391347
C	4.7259607431	0.3307032097	-1.4421166271
H	5.2235000082	-0.6433955764	-1.4820440673
C	3.6918413316	0.5321601858	-0.4989204358
C	3.3577507129	-0.6086661426	0.4529938357
H	3.2884880457	-0.2179064992	1.4852318188
H	4.2052988563	-1.3155575425	0.4534340282
C	2.0769380564	-2.6679866174	-1.3663862706
C	3.5581576826	-3.0400060793	-1.6113306401
H	4.0084893723	-3.5942686769	-0.771728109
H	4.1786027247	-2.1603907671	-1.8272605691
H	3.6115719345	-3.6952055454	-2.5015081922
C	1.5929662153	-1.7405674073	-2.5102287171
H	0.5084406386	-1.539236084	-2.4453172903
H	1.7870451424	-2.231408332	-3.483389159
H	2.1247177363	-0.7733877014	-2.5126299962
C	1.2777858827	-3.99295872	-1.4149104964
H	0.216255576	-3.8988250911	-1.1344142234
H	1.7308898616	-4.7707872938	-0.7781370448
H	1.3012860287	-4.3718425731	-2.4541874377
C	1.9475604047	-2.7950080017	1.8367509372
C	1.7505301553	-1.8705895993	3.0651633002
H	2.5666986267	-1.1373050866	3.1883013162
H	1.7324455398	-2.4874449579	3.9833452084
H	0.7928997377	-1.319768938	3.0108968786
C	3.3067854877	-3.5208501188	1.9579211244
H	4.166888054	-2.8302253698	1.9776300637
H	3.4622486789	-4.253662219	1.1482384084
H	3.3258410343	-4.0839737936	2.9106114211
C	0.8226560559	-3.8584075926	1.8688568009
H	0.9621851609	-4.6518183343	1.1195296622
H	-0.1800379476	-3.4228792979	1.7241699162
H	0.8255015564	-4.3457872378	2.8622844889
C	-1.8004617932	-2.006714772	-0.3277340035
H	-1.110310628	-2.8080428506	-0.5871418436
C	-2.155796823	-1.6505586823	0.962282902
C	-3.5108991055	-0.9821690531	0.9588042729
H	-4.2675426199	-1.7180005545	1.308848939
H	-3.5859242395	-0.0900490098	1.602910241
C	-2.8433565857	-1.5227985274	-1.311051577
H	-3.3972423509	-2.3934189703	-1.7193771473
H	-1.5612263881	0.6406844533	0.2703474124
N	-3.7055462201	-0.6224689715	-0.47459342
S	-5.3787957889	-0.6115011915	-0.9965932416
O	-5.3464549135	-0.9049064208	-2.4451247681

O	-6.1964067244	-1.4150491016	-0.0567381626
C	-5.8091239187	1.1297119626	-0.7598522599
H	-5.1748174311	1.7425568633	-1.4137499612
H	-6.8685400161	1.2266132885	-1.040600468
H	-5.6746482065	1.3944977376	0.2987431236
H	-2.4369052523	-0.96617389	-2.171401043
H	-1.7453199973	-2.0802042441	1.8803402312

Complex 4

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Complex 4

Pd	0.2747762574	-0.2264704624	0.3712397089
P	-1.6252874153	-1.7544516772	0.3463677619
P	-0.6459839107	1.9081380427	0.5357754455
C	-1.6826069954	-2.948600753	1.8747172678
C	-2.2446993512	-2.1537042446	3.0799158027
H	-3.3298169257	-1.9711323487	3.0001244907
H	-1.7277987681	-1.1875803164	3.2162292417
H	-2.0846576817	-2.7459532707	4.0003137775
C	-2.5647586235	-4.1978621545	1.6526827475
H	-3.5938667268	-3.941976042	1.3450274643
H	-2.6418344985	-4.7532721511	2.6068694331
H	-2.1382242022	-4.8906736012	0.9085093231
C	-0.2441224751	-3.3864355925	2.2386550614
H	0.3717740327	-2.521837967	2.5433067951
H	0.2695565798	-3.9132490368	1.4178462679
H	-0.2867511236	-4.0811480206	3.0986352408
C	-1.4861216881	-2.749840481	-1.3045820242
C	-0.304236924	-3.7439178216	-1.2305005559
H	0.6391773169	-3.2532861715	-0.9297103312
H	-0.1402249761	-4.1753195156	-2.2361842021
H	-0.4938132785	-4.584783268	-0.5420883194
C	-2.763152236	-3.5271468296	-1.6988649274
H	-3.0610179105	-4.2805503688	-0.9535619119
H	-2.5670861103	-4.0634954287	-2.6468389685
H	-3.6159020316	-2.8564907304	-1.8824696536
C	-1.1785341145	-1.7033326746	-2.406739994
H	-0.2178711132	-1.1864901913	-2.219760002
H	-1.9682516966	-0.9375977098	-2.4862013609
H	-1.1029814106	-2.2184252428	-3.3837620222
C	-3.3787382449	-1.0503901001	0.3660447654
H	-4.079053453	-1.9046728682	0.3291388826
H	-3.4843283433	-0.6112940688	1.3744777196
C	-3.775182671	-0.0294388299	-0.6833897368
C	-4.6918595849	-0.4198006843	-1.6854235469
H	-5.0655425316	-1.4499117776	-1.6888603716
C	-5.1754879752	0.4772351715	-2.6462976566
H	-5.8865567583	0.1362581815	-3.4060077944
C	-4.7677034394	1.8170589971	-2.5971188551
H	-5.1515854499	2.5453952786	-3.3190811717
C	-3.8933551343	2.2299491946	-1.5835127238
H	-3.6346468144	3.2923287981	-1.515617675
C	-3.3679454297	1.3328410809	-0.6254848887
C	-2.546286251	1.8985222459	0.5207376521
H	-2.8058841878	1.3775402477	1.4607539479

H	-2.8403967682	2.9519735579	0.6710685846
C	-0.1354579962	3.1542131	-0.8492230012
C	-0.942766942	4.4737570294	-0.8109425257
H	-0.7037710289	5.0808958817	0.0782215694
H	-2.0334087415	4.328041128	-0.8489595818
H	-0.6652097182	5.0753897041	-1.696948387
C	-0.3902732162	2.4089389669	-2.1848266822
H	0.1916862634	1.471645247	-2.2397863259
H	-0.0702187303	3.0581901027	-3.0217634381
H	-1.4523007432	2.1597487983	-2.3383292753
C	1.3629195187	3.5219435137	-0.7705917186
H	2.0068631215	2.6442512111	-0.6224923412
H	1.5784907304	4.2482037145	0.0278443637
H	1.6561098293	3.9930177531	-1.7276156092
C	-0.3436663815	2.6022657065	2.329108286
C	-0.5737674146	1.4237056711	3.3057493843
H	-1.6064477409	1.0349794302	3.2642496764
H	-0.4017377592	1.7778765792	4.3399661162
H	0.1233759556	0.5892567337	3.1089946859
C	-1.3123636103	3.7508256985	2.7088942004
H	-2.364830559	3.4253751118	2.7596704139
H	-1.2451446386	4.6154644269	2.0283695102
H	-1.0384041934	4.1109964763	3.7184610878
C	1.1076170246	3.1021378727	2.5140595988
H	1.2916419286	4.0608162492	2.0040712533
H	1.8597047756	2.3727049184	2.1716159225
H	1.2819838154	3.2703751415	3.5933632745
H	1.421435461	-1.7610968567	0.5921563588
C	2.3216013202	0.253312605	0.2512543435
H	2.673410947	0.9653963653	1.0069106706
C	2.4543348456	-1.2089877413	0.6120195416
H	2.8059164694	-1.3858795308	1.6401069865
C	3.3536081219	-1.8433086577	-0.4958192908
H	4.1203201791	-2.5035133048	-0.065234131
H	2.7579404178	-2.4170523735	-1.227927223
C	2.9904779264	0.3990366657	-1.1345120102
H	3.4988033394	1.3621311083	-1.2792248351
H	2.2718688267	0.2509885807	-1.9629446736
N	3.9814335047	-0.7084776402	-1.2132896497
S	5.5720691493	-0.2647858062	-0.5751933857
O	5.584194502	1.2040821533	-0.3698817129
O	5.9177589858	-1.2013101528	0.5223666238
C	6.6188308741	-0.6470238476	-1.9999075298
H	6.2967749534	-0.0271350576	-2.8476562389
H	7.6513860014	-0.4047243601	-1.7075200393
H	6.5224706638	-1.7166377111	-2.2319619504

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TS4-5

Pd	0.0801444319	-0.5335544283	0.1664230942
P	-2.2833512506	-1.3591593872	0.1716755773
P	-0.0216987005	1.7351702262	0.5922861596
C	-2.573647395	-2.6674095409	1.5803588106
C	-2.5968713005	-1.90871621	2.9317180687

H	-3.5272742167	-1.3359681601	3.0844417798
H	-1.7343292926	-1.2255614656	3.0379397763
H	-2.5358507004	-2.6461723736	3.7541333583
C	-3.8838198054	-3.472179195	1.4322359006
H	-4.776723942	-2.826926624	1.3584132757
H	-4.0173174359	-4.1063318662	2.3295701792
H	-3.866053878	-4.144860306	0.558685063
C	-1.3763922327	-3.642600995	1.619724023
H	-0.4278542277	-3.1043706649	1.8034761459
H	-1.2771743458	-4.2287639772	0.6920317487
H	-1.5161666627	-4.3607171718	2.4502338747
C	-2.7708049611	-2.0654325958	-1.5640695371
C	-2.0592955075	-3.4106305431	-1.8277008184
H	-0.9656322114	-3.3279638452	-1.7067348076
H	-2.2496690341	-3.7136422339	-2.8747540271
H	-2.4270490086	-4.2248626165	-1.1800964572
C	-4.288788566	-2.2666455049	-1.7729414846
H	-4.7387943105	-2.9611229913	-1.0462061443
H	-4.4489469688	-2.6968949452	-2.7799468664
H	-4.8411797415	-1.3159705546	-1.7426372376
C	-2.2507406731	-1.0267171128	-2.5907261755
H	-1.1599256527	-0.8709036044	-2.4923643324
H	-2.7500996762	-0.0492423611	-2.4804447143
H	-2.4534221439	-1.3959723729	-3.6144683335
C	-3.6683159268	-0.1377096144	0.5791987547
H	-4.6161106641	-0.7049376276	0.5734219085
H	-3.4861098421	0.141553133	1.6323095138
C	-3.8247398394	1.1146707781	-0.2579044085
C	-4.9602047756	1.2403008647	-1.0896206344
H	-5.6817197288	0.4167596234	-1.1310125872
C	-5.2188736866	2.4027082204	-1.8267504622
H	-6.1100672966	2.4631514278	-2.4601345695
C	-4.3482038339	3.4951984142	-1.7112594342
H	-4.5437861246	4.4257299631	-2.2542984064
C	-3.2427438313	3.4026305892	-0.8566808001
H	-2.606311401	4.2845912563	-0.7242059259
C	-2.9441033937	2.2239099835	-0.1348427843
C	-1.8252303104	2.2667253362	0.8892874547
H	-2.1026632979	1.6730163285	1.7790210787
H	-1.7358980196	3.3095340167	1.237607282
C	0.6454441896	2.9100676002	-0.7966490836
C	0.3895478241	4.3898827804	-0.4175492787
H	1.0279306993	4.7140740188	0.4218238318
H	-0.6587778971	4.613972154	-0.165063564
H	0.654451607	5.0183737904	-1.2882672878
C	-0.1040227297	2.5322876988	-2.0986171392
H	0.0848861962	1.4794042028	-2.3744569449
H	0.2835602898	3.1659303414	-2.9188113201
H	-1.1917563436	2.6857907966	-2.0386502429
C	2.1562499055	2.7549028582	-1.0785108609
H	2.4085949836	1.7728126576	-1.5000291693
H	2.7989736963	2.9387441492	-0.2051154455
H	2.4302247386	3.5047206103	-1.8444988748
C	0.7018256126	2.1719509727	2.3600606364
C	0.4085077567	0.9540347458	3.2687067922

H	-0.6746711317	0.7607262546	3.3696727837
H	0.7988989995	1.161263893	4.2832839567
H	0.8899163114	0.0342216116	2.8943458785
C	0.0303505598	3.419858527	2.9961418982
H	-1.0281980936	3.2561157937	3.2566786262
H	0.1071944643	4.3234959769	2.369275984
H	0.5607693272	3.6380219107	3.9419212479
C	2.2271412694	2.4346358188	2.3364765227
H	2.4810653144	3.3750165438	1.819614542
H	2.8196045117	1.6213359212	1.8902174351
H	2.5680898891	2.5448526559	3.3832479651
H	2.0045391865	-2.0943150621	1.5330721231
C	2.1575347388	-0.3728863272	0.117532763
H	2.5628530841	0.6352417484	0.2663208753
C	2.723437656	-1.3144374959	1.2154555794
H	3.0012019685	-0.7489742292	2.1190417545
C	3.9754437628	-1.9708331982	0.5470954392
H	4.8843890832	-1.809347804	1.1460798811
H	3.847844837	-3.0569119646	0.4018804311
C	2.7618980889	-0.9108037873	-1.2036051394
H	2.8288262647	-0.1731395277	-2.0162304595
H	2.2383623559	-1.8003912811	-1.597313554
N	4.129200597	-1.353561793	-0.8081923595
S	5.2848728203	-0.029641642	-0.8346442124
O	4.8971820963	0.8431749116	-1.9692768165
O	5.4706672046	0.5414750728	0.5267289553
C	6.7870072124	-0.9326362821	-1.2826890449
H	6.6344241773	-1.3896570634	-2.269358854
H	7.6002821187	-0.1923848656	-1.3099197458
H	6.9927421628	-1.6958561962	-0.518682503
C	1.0189655186	-3.5255847749	-0.4855689288
O	1.4821494973	-4.5722209947	-0.5821999519

Complex 5

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Complex 5

Pd	-0.663352994	0.2463600143	0.1272729656
P	0.8064591827	2.222658421	0.6777817644
P	1.0131093672	-1.5581725336	0.1379117075
C	0.1873677262	3.0322402782	2.3336304122
C	0.5540178781	2.0679172695	3.4905666439
H	1.6344775724	2.0536165972	3.712921818
H	0.2158854473	1.0351515593	3.2879505838
H	0.0412289902	2.4079485183	4.4097848941
C	0.8250476372	4.4158036201	2.602196624
H	1.9286218247	4.3948207255	2.5891475878
H	0.5230259224	4.7518086157	3.6121949489
H	0.4801625199	5.1823027932	1.8885678305
C	-1.3517752995	3.1803591193	2.3289003836
H	-1.8509283807	2.1958400002	2.3194842055
H	-1.7323662396	3.7797539719	1.4870142189
H	-1.659050814	3.6910116436	3.2610544648
C	0.8130871614	3.4915091312	-0.7834495659
C	-0.521431039	4.2640737294	-0.8792521596
H	-1.4020391852	3.6088098553	-0.9507524557

H	-0.4992287067	4.8716776102	-1.8034669951
H	-0.6673297928	4.9610362994	-0.0371830608
C	1.9582264906	4.5265536737	-0.6894102551
H	1.9401015198	5.1097024801	0.2448321138
H	1.8463651861	5.242942153	-1.5250060688
H	2.9454604198	4.0571620658	-0.7975306415
C	1.0013874958	2.643939336	-2.0671242596
H	0.1648698776	1.9363417634	-2.2159454115
H	1.9440486271	2.0704753823	-2.0499306086
H	1.0332394814	3.3188738549	-2.9436308462
C	2.6295988719	1.9469010004	1.1157935059
H	3.0142413156	2.9255342547	1.4545775743
H	2.5937516799	1.3010494095	2.0119454728
C	3.5893997156	1.3546756706	0.1037006522
C	4.5850020144	2.180996593	-0.4648707865
H	4.6285762729	3.2374112379	-0.1782498981
C	5.5544802335	1.6808926274	-1.3438392426
H	6.3107660652	2.3521749974	-1.7638073932
C	5.5665491373	0.312147715	-1.6453357077
H	6.32732292	-0.1065624395	-2.3123502643
C	4.6240529975	-0.5298339882	-1.0413166221
H	4.6855899107	-1.6091021063	-1.22335119
C	3.6223021335	-0.0372565096	-0.1740880512
C	2.7788165869	-1.0392136696	0.5896116131
H	2.6827381519	-0.7158233319	1.6433289852
H	3.3401712728	-1.9870021785	0.6205210652
C	1.1827623089	-2.4240318304	-1.5796629501
C	2.2387786306	-3.5526935972	-1.5438390194
H	1.9140612405	-4.4011376661	-0.9181228524
H	3.2298993782	-3.2195255336	-1.1938020103
H	2.3714461583	-3.9391742069	-2.5717479514
C	1.5847757424	-1.3287935666	-2.6005065048
H	0.846889958	-0.5056664789	-2.6153955797
H	1.5942552031	-1.7823181996	-3.6097986324
H	2.5800899813	-0.8983490836	-2.4158127019
C	-0.1578793717	-3.0154834366	-2.0665126709
H	-0.8990478846	-2.2237091381	-2.249427436
H	-0.5992876439	-3.7647612203	-1.3932926472
H	0.0200967542	-3.5176997232	-3.0358406517
C	0.7284652209	-2.8283722975	1.6037879269
C	0.2041637516	-1.9859524963	2.7918292978
H	0.9424413526	-1.2340102765	3.1263487893
H	0.0085216428	-2.653524258	3.6525279996
H	-0.7363903475	-1.462557125	2.5466194571
C	2.0304716193	-3.5426613124	2.0546868009
H	2.7621867759	-2.8627317019	2.5205358939
H	2.5273434292	-4.0945849994	1.2392886629
H	1.753839557	-4.2866329146	2.8250460305
C	-0.2957110742	-3.9344807024	1.2558873506
H	0.085146871	-4.6205901063	0.4813846746
H	-1.2819558309	-3.5688650482	0.93387915
H	-0.4635143545	-4.5412754774	2.1658455393
H	-3.310354913	-0.3083580505	1.6598123836
C	-2.2889937357	-1.2204240218	-0.1152098824
H	-1.7502449997	-2.1694480912	-0.2107156354

C	-3.2139801171	-1.2746823455	1.1342319599
H	-2.8384866821	-2.0037625898	1.8698966215
C	-4.6026876972	-1.7164420734	0.5658402233
H	-5.0071813622	-2.5938799565	1.0920786447
H	-5.343196168	-0.9007175741	0.6283749051
C	-3.2708432303	-1.1555202757	-1.312469072
H	-2.8573265965	-1.5277717625	-2.2611528037
H	-3.7026456019	-0.1570833187	-1.4927526333
N	-4.4035006115	-2.0212824938	-0.8824533004
S	-4.1293351278	-3.7187271895	-1.2071325408
O	-3.3620813291	-3.790289669	-2.4742183045
O	-3.6371247291	-4.4237140829	0.0090997134
C	-5.8266566292	-4.2592125854	-1.5218653514
H	-6.2058417616	-3.7149024527	-2.3968869761
H	-5.7808704214	-5.3408863271	-1.7166066451
H	-6.4411745827	-4.0577696793	-0.6328370463
C	-2.1779845021	1.3639599977	-0.1388596993
O	-3.1587634058	1.949977698	-0.3423902278

TS1-5

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TS1-5

Pd	0.3400112293	-0.1753262025	0.0200579134
P	-1.3108748661	-1.8989260787	0.2839049169
P	-0.9297894412	1.9335134329	0.3452887641
C	-3.0027164617	-1.3452496473	0.9264109811
H	-3.5555980259	-2.2755039559	1.1512739401
H	-2.7626218365	-0.8867153524	1.902493641
C	-3.9131520696	-0.4184930918	0.1426698627
C	-5.0530658263	-0.97168712	-0.4839159654
H	-5.2134972778	-2.0539139851	-0.4329917265
C	-6.0223313182	-0.1798321256	-1.1126741626
H	-6.8901208942	-0.6495745953	-1.5873210552
C	-5.8930125613	1.214255135	-1.0750161486
H	-6.6582046049	1.8597770669	-1.5187107029
C	-4.7961444678	1.7813026322	-0.4134495811
H	-4.7549307274	2.8704198658	-0.3078514971
C	-3.7778629585	0.997833352	0.1764497711
C	-2.7034957975	1.7028335945	0.9856608185
H	-2.5671429212	1.1789193162	1.9488887662
H	-3.0663390464	2.7152286291	1.2384924334
H	1.1172790567	-1.4501545853	-0.5712407515
C	1.777434237	-0.1421897244	1.5050372708
O	2.3182018801	-0.454198533	2.485341939
C	2.0312012605	-0.8215160207	-1.8184994431
H	1.463746008	-1.3817632543	-2.5678894202
C	1.971868637	0.5725381816	-1.7153507221
H	1.3033522342	1.188109061	-2.3182775173
C	-1.646415899	-2.8591022363	-1.3629172517
C	-0.7994440417	-3.1265471413	1.7050271008
C	-1.1088536407	3.0475719947	-1.2270104764
C	-0.1956824302	2.9706176818	1.8255878263
C	3.4047192522	-1.2957449292	-1.3659442039
H	4.0219117112	-1.5258086109	-2.2603115474
H	3.3940877741	-2.1933042319	-0.7230635988

C	3.2655380177	1.1106484148	-1.1540198669
H	3.8482394346	1.5853262096	-1.9736903707
H	3.1519450544	1.8643764014	-0.3599173646
N	3.9145846325	-0.1197478988	-0.6098012543
S	5.6591133448	-0.0021089366	-0.518566678
O	5.9511485032	1.4416264281	-0.3926858074
O	6.2599615157	-0.8304948528	-1.5900751001
C	5.9786917424	-0.8081345322	1.0685660779
H	5.6334711309	-1.8508001052	1.0199971269
H	7.068345155	-0.7778271481	1.2178366926
H	5.4586213741	-0.2504008781	1.8585763871
C	-0.4430512881	-3.7600082442	-1.7243205514
H	-0.5557125093	-4.0958645844	-2.772612902 7
H	0.5279458571	-3.2404830739	-1.6469478869
H	-0.3984362285	-4.6660071792	-1.0966280935
C	-1.829817654	-1.7812217406	-2.4595047403
H	-0.9217343072	-1.1677755699	-2.5910272239
H	-2.0504891297	-2.2808140723	-3.4221393352
H	-2.6688823351	-1.1021123438	-2.2312691847
C	-2.9157312358	-3.7435681043	-1.3338273126
H	-2.9859665308	-4.2789558091	-2.2996529911
H	-2.8983953949	-4.5048021939	-0.5400535167
H	-3.8327522723	-3.1465096249	-1.2327936722
C	-1.706846604	-4.3769185092	1.8019475591
H	-1.5562086328	-5.0717688107	0.9593987234
H	-1.4448211859	-4.9282576034	2.7247360789
H	-2.781081574	-4.1327239713	1.8706208751
C	0.6611361601	-3.6009940408	1.5157796977
H	0.9322367527	-4.2512717913	2.3687757156
H	0.7989247079	-4.1929623596	0.5975399225
H	1.3748549793	-2.7623959964	1.4998966614
C	-0.8906595045	-2.3529794644	3.0468482658
H	-0.3687695348	-1.3808019732	3.0142433053
H	-1.9333855955	-2.182652313	3.3653927308
H	-0.4077017752	-2.9578665255	3.8366330181
C	-1.4981770214	2.1058380809	-2.3940793324
H	-1.6528962492	2.7111821602	-3.3077133677
H	-0.7200061723	1.3560795084	-2.6154211496
H	-2.4368677306	1.5645943672	-2.1860655252
C	0.2274521588	3.7618129544	-1.5458635535
H	0.1879715097	4.1423153281	-2.5841589515
H	0.3884492793	4.6335247109	-0.8890734127
H	1.1106557317	3.1086429797	-1.4617213167
C	-2.2051829375	4.1337439405	-1.1117605034
H	-2.08869072	4.7787958339	-0.2286597714
H	-2.1408133606	4.7848186933	-2.0043776331
H	-3.2147648062	3.7005763069	-1.1056499301
C	1.3195476611	3.2096371355	1.625614794
H	1.536793645	3.8612138901	0.7647066924
H	1.7208724319	3.7115461287	2.5261343718
H	1.8775257527	2.2673858893	1.4993630928
C	-0.8713050431	4.3478416585	2.0365829681
H	-0.4888622518	4.7791722934	2.9810957479
H	-0.6261585554	5.0644666634	1.235339417
H	-1.9690977993	4.2879499933	2.1354548402

C	-0.3945919335	2.1331048508	3.1164652381
H	-1.4438940011	2.1309053438	3.4582225055
H	-0.0618873702	1.0870063268	3.0001603307
H	0.2069285457	2.5824352374	3.9284642905

TS4-6

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TS4-6

Pd	0.267438	-0.250339	0.272876
P	-1.607481	-1.797820	0.293871
P	-0.517590	1.896725	0.451705
C	-1.372093	-2.988006	1.799781
C	-1.691066	-2.180972	3.084544
H	-2.773107	-2.012129	3.220187
H	-1.173091	-1.204002	3.099584
H	-1.341303	-2.755430	3.962919
C	-2.260894	-4.251412	1.769223
H	-3.333937	-4.013190	1.662276
H	-2.142286	-4.794433	2.726173
H	-1.975012	-4.947783	0.963295
C	0.118317	-3.404988	1.866695
H	0.774653	-2.522987	1.997754
H	0.454592	-3.960121	0.976361
H	0.274341	-4.060501	2.744756
C	-1.757587	-2.771136	-1.361190
C	-0.546874	-3.721075	-1.513823
H	0.417180	-3.201009	-1.358161
H	-0.537510	-4.123827	-2.544175
H	-0.594602	-4.582023	-0.826463
C	-3.064081	-3.582785	-1.508167
H	-3.178363	-4.361432	-0.738124
H	-3.055814	-4.090711	-2.491295
H	-3.956496	-2.937678	-1.488778
C	-1.687780	-1.713819	-2.493103
H	-0.739618	-1.146853	-2.458517
H	-2.522198	-0.994043	-2.449887
H	-1.738951	-2.231941	-3.470017
C	-3.314444	-1.068460	0.638034
H	-4.033602	-1.903958	0.717877
H	-3.219958	-0.639493	1.651874
C	-3.856072	-0.019980	-0.313612
C	-4.929291	-0.376739	-1.161388
H	-5.314589	-1.401984	-1.122253
C	-5.542374	0.545391	-2.018522
H	-6.373751	0.230880	-2.658039
C	-5.104132	1.877211	-2.018390
H	-5.584829	2.623867	-2.659038
C	-4.067609	2.255981	-1.156717
H	-3.770338	3.310842	-1.120333
C	-3.412800	1.332264	-0.308481
C	-2.409310	1.884010	0.688668
H	-2.526059	1.380863	1.666965
H	-2.664294	2.944118	0.861544
C	-0.173079	2.994846	-1.102386
C	-0.808365	4.397904	-0.943701

H	-0.287000	5.004716	-0.184295
H	-1.881108	4.366559	-0.690263
H	-0.717146	4.932978	-1.907458
C	-0.780469	2.264740	-2.325998
H	-0.346587	1.256413	-2.446928
H	-0.532673	2.846142	-3.234421
H	-1.874625	2.165609	-2.276820
C	1.337775	3.168036	-1.389151
H	1.813061	2.220277	-1.688412
H	1.906367	3.602902	-0.553347
H	1.439628	3.860246	-2.246316
C	-0.018307	2.774604	2.118201
C	-0.034042	1.681239	3.214395
H	-1.031849	1.224523	3.342419
H	0.238851	2.142102	4.182764
H	0.690726	0.877454	3.001878
C	-1.001261	3.897692	2.543005
H	-1.995612	3.511205	2.821472
H	-1.127550	4.682579	1.779724
H	-0.585346	4.386283	3.444068
C	1.402745	3.378520	2.040446
H	1.448803	4.262296	1.382467
H	2.159872	2.649396	1.710611
H	1.692344	3.715345	3.053655
H	2.219135	-0.631326	2.281584
C	2.258762	0.337566	0.269338
H	2.526879	1.378897	0.071761
C	2.938095	-0.248141	1.531944
H	3.537472	0.528954	2.037880
C	3.843144	-1.401921	0.999574
H	4.844291	-1.403091	1.453221
H	3.378187	-2.389169	1.174823
C	2.658182	-0.601334	-0.878286
H	2.735923	-0.111694	-1.858886
H	1.930379	-1.454012	-0.984391
N	3.950035	-1.225984	-0.475737
S	5.340168	-0.245649	-0.973675
O	4.844824	0.864062	-1.827511
O	6.181550	0.018048	0.217638
C	6.206400	-1.428119	-2.033939
H	5.542318	-1.708623	-2.862863
H	7.105131	-0.916388	-2.409132
H	6.480094	-2.304884	-1.431197

Complex 6

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Complex 6

Pd	-0.365036847	-0.2756043236	-0.0543891472
P	0.5624783053	1.914272904	0.4358089356
P	1.4207081061	-1.7652516642	0.1933172686
C	-0.4106434148	2.6467220118	1.9427623211
C	-0.043524779	1.7956563355	3.1862584062
H	0.9817396449	1.9831678843	3.5488728781
H	-0.1604189874	0.7133400243	2.9919513834
H	-0.7285667123	2.0611592741	4.0134204326

C	-0.0948090186	4.1317921963	2.2310713611
H	0.9835353448	4.3252604138	2.3672250242
H	-0.5969883754	4.4271454229	3.1720132686
H	-0.4724713201	4.7991921801	1.4385112524
C	-1.9321850742	2.4911472085	1.709558429
H	-2.2261663847	1.4367014393	1.5655360832
H	-2.2955631732	3.0653379125	0.8435069389
H	-2.4683622834	2.8650361491	2.6026687836
C	0.4762088999	3.0843044649	-1.1018736251
C	-0.987064238	3.4596453516	-1.4299632322
H	-1.6536669155	2.5808368125	-1.4935593788
H	-1.0088171961	3.9521133076	-2.4204595323
H	-1.4124936886	4.1721781141	-0.7036610749
C	1.2973739365	4.3844426648	-0.9485953377
H	0.9701752642	5.0058319551	-0.0999675396
H	1.1716197324	4.9890888125	-1.8666248193
H	2.374324444	4.1836485677	-0.8419186494
C	1.0471473115	2.2622906659	-2.2846391616
H	0.4449874071	1.3544003806	-2.4716690321
H	2.0932097855	1.9562716431	-2.1147508138
H	1.0210274052	2.8824883403	-3.201063397
C	2.3357321323	2.0472114902	1.0701957358
H	2.5192893959	3.1118891475	1.2993741215
H	2.312149418	1.5234557898	2.0429765201
C	3.4846679502	1.5109339513	0.2375875994
C	4.3784364666	2.4338675703	-0.3511197628
H	4.189500524	3.5062905057	-0.2283306253
C	5.5245879592	2.0252889479	-1.0451228574
H	6.1935362	2.7719681021	-1.4855881788
C	5.8220199768	0.6581968139	-1.1317188578
H	6.7272165822	0.314009289	-1.6427830556
C	4.9661025751	-0.2674779542	-0.5219023555
H	5.2319883995	-1.3308727619	-0.5479104882
C	3.7847637145	0.1240783989	0.1494401187
C	2.9982491146	-0.9505943131	0.8788596741
H	2.6767382841	-0.5824297201	1.8724100219
H	3.6866974964	-1.788872239	1.0785401233
C	1.9400782516	-2.6078855384	-1.4692962761
C	3.1310190311	-3.5747457217	-1.2669383822
H	2.8428695952	-4.4737716026	-0.6954666002
H	3.9938164352	-3.1058047154	-0.7662302443
H	3.4788842623	-3.9179943263	-2.2594727511
C	2.318891204	-1.4778106205	-2.4581654195
H	1.4775242464	-0.776550025	-2.6013103644
H	2.5444756289	-1.9339996972	-3.4408486955
H	3.201090612	-0.9015847288	-2.1432409061
C	0.7750916971	-3.3913678447	-2.1210100916
H	-0.0417896281	-2.7170676639	-2.4240835493
H	0.3623279523	-4.1941300004	-1.4921323642
H	1.1610669959	-3.8631317007	-3.044390433
C	1.1279214091	-3.0632018621	1.6104513054
C	0.3750861048	-2.3001318315	2.7289980329
H	0.9838565761	-1.4794615706	3.1500136899
H	0.1478369454	-2.9966893477	3.5583926821
H	-0.5737911283	-1.8669270468	2.3664151971

C	2.4273169523	-3.6514749023	2.2179909727
H	3.0177196691	-2.9045158585	2.7739488858
H	3.0774503814	-4.1294138088	1.4668818389
H	2.1385992142	-4.4349724259	2.9439328756
C	0.2624552492	-4.2416263227	1.1081288803
H	0.8470160111	-4.9396393338	0.4854526774
H	-0.6173461468	-3.9166415158	0.5321274017
H	-0.1001118777	-4.8147060487	1.9825928885
H	-2.2545504637	-2.8474227128	1.275457988
C	-1.9402874192	-1.6237016899	-0.5703029526
H	-1.6549794869	-2.2323709954	-1.4339919174
C	-2.8088836716	-2.3067079271	0.4937573136
H	-3.4685699651	-3.0395297557	-0.0096278948
C	-3.6522521797	-1.1596337109	1.0907704756
H	-4.6513146096	-1.4854366395	1.4167335985
H	-3.138866281	-0.6906334919	1.9518150862
C	-2.6083375147	-0.3155452701	-0.8740384516
H	-2.8525355457	-0.0985255082	-1.9272944924
H	-1.8732006737	0.6064331099	-0.6320529352
N	-3.7663752049	-0.1346805175	0.014738067
S	-5.2964081477	-0.119245418	-0.8603137241
O	-4.9754978512	0.3664404262	-2.2229946578
O	-6.0127345142	-1.3964859359	-0.638340425
C	-6.1800190372	1.185118082	0.0273650115
H	-5.619957033	2.1235678285	-0.0773101955
H	-7.1718128195	1.2635236259	-0.4424994581
H	-6.2814075938	0.8944310932	1.0826375541

TS6-7
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TS6-7

Pd	-0.2987418278	-0.1802026058	0.8506237132
P	0.7050447662	1.9486676014	0.5577873489
P	1.4692904451	-1.7435674016	0.3351165588
C	0.6372950151	2.8930512138	2.2517493706
C	1.6223718217	2.1905738887	3.2218936542
H	2.6793447665	2.3938959599	2.9793546779
H	1.4666417405	1.0963879787	3.2468280471
H	1.4494017412	2.5756304953	4.2445322222
C	1.0194307186	4.3876607765	2.1382936968
H	2.0053135574	4.5440121045	1.6668276883
H	1.0769765316	4.8196296373	3.1554571218
H	0.2686581893	4.970817674	1.5789905018
C	-0.7774984512	2.7813010769	2.8653990014
H	-1.0587958973	1.7281532661	3.0421839345
H	-1.5499963623	3.2417677525	2.2287495085
H	-0.7845124291	3.3078761108	3.8388564053
C	-0.1666430988	2.9398394715	-0.847235369
C	-1.5875622601	3.3774795174	-0.4259995466
H	-2.1876501959	2.5435252025	-0.0203867222
H	-2.116237989	3.7542758656	-1.321826134
H	-1.5752197378	4.1981945201	0.3118372207
C	0.617660026	4.1890415709	-1.3104953818
H	0.79547407	4.912585192	-0.4995501232
H	0.0241687739	4.7059809416	-2.0878399347

H	1.5834789278	3.92630016	-1.7671421422
C	-0.2879122936	1.9504037889	-2.0341622309
H	-0.922750693	1.0847078707	-1.7706219853
H	0.6951983179	1.5738428517	-2.3647361769
H	-0.75778283	2.4698064661	-2.891256979
C	2.5587267252	2.0519531146	0.1915274094
H	2.8194335343	3.1257129621	0.1984362493
H	3.0249653246	1.6154471978	1.0929645926
C	3.1580673896	1.4048189578	-1.0434608735
C	3.603052589	2.2370312525	-2.095713237
H	3.4577492749	3.3200058855	-2.0142354762
C	4.2737804949	1.7306101842	-3.2164211715
H	4.6039762854	2.4092655086	-4.0098118889
C	4.551845402	0.3586117368	-3.2867234973
H	5.1011823921	-0.0577212191	-4.1376454689
C	4.153070858	-0.4741295151	-2.2336385038
H	4.4184690251	-1.5376885561	-2.2685526501
C	3.4413053523	0.0136453488	-1.1134716815
C	3.1697429885	-0.9550373148	0.022118446
H	3.4114076371	-0.4805640274	0.993156066
H	3.87468637	-1.7964616824	-0.0819372221
C	1.1038362016	-2.7938733507	-1.2494946443
C	2.2255815395	-3.8131644908	-1.5529241755
H	2.2670274687	-4.6228566086	-0.804427893
H	3.2238886813	-3.3475996905	-1.6165016415
H	2.0245668166	-4.2850053557	-2.5334924854
C	0.9430157855	-1.8080310955	-2.4334794292
H	0.1713460001	-1.0475400046	-2.2187121845
H	0.6122724554	-2.378836687	-3.3222375636
H	1.8754628311	-1.2879340514	-2.6955980416
C	-0.2431444294	-3.5483407116	-1.130579988
H	-1.0895741554	-2.8421046865	-1.0937608529
H	-0.3051014979	-4.2276737297	-0.2675026715
H	-0.3769300135	-4.1605985986	-2.0425429273
C	1.9642361825	-2.8805173629	1.8355920785
C	1.8756190203	-1.9804238948	3.093863505
H	2.5862987572	-1.1349592291	3.0501223941
H	2.1344531351	-2.5773696999	3.9894566576
H	0.8628957861	-1.563480841	3.2365673423
C	3.3979884437	-3.4627224079	1.7630164329
H	4.1767836166	-2.6909149804	1.8823876811
H	3.5937048973	-4.0165845805	0.8304431291
H	3.5257310643	-4.1762152484	2.5991075981
C	0.9710326411	-4.055303518	1.9792317226
H	1.1325802691	-4.8277867882	1.2084058526
H	-0.0798163765	-3.7295118429	1.9292707726
H	1.1262407005	-4.5403987289	2.961921577
H	-1.1334435125	-2.4649853652	3.3364425572
C	-1.912726346	-1.5988175106	1.4228874148
H	-1.9522657898	-2.3020229712	0.5875861814
C	-2.0669067655	-2.1354113637	2.8574871867
H	-2.7491404685	-3.0064705236	2.838000791
C	-2.6998128446	-0.9557812107	3.6458221249
H	-3.5001596005	-1.2662731926	4.3351603526
H	-1.9339515714	-0.392728169	4.211351284

C	-2.7432548263	-0.4336645318	1.3408615875
H	-3.2906465756	-0.0917762955	0.4575913697
H	-1.5600104441	0.8062356576	1.0285712114
N	-3.2578641057	-0.0785290883	2.5837197092
S	-4.8279846143	0.6692438457	2.6936033666
O	-5.1348174503	1.1064939492	1.3166477997
O	-5.6944738075	-0.2475642007	3.4573234396
C	-4.5050214914	2.1208880774	3.7212799202
H	-3.7824286266	2.7690318223	3.2080774881
H	-5.4715809019	2.6326974289	3.8439168619
H	-4.1280673448	1.7891946642	4.6993842295

Complex 7

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Complex 7

Pd	-0.3955164069	-0.1604841142	0.6242239331
P	0.6431463564	1.955184074	0.6518564299
P	1.4510302401	-1.7767758608	0.2911968892
C	0.4967373172	2.7962565076	2.3935753216
C	1.482646938	2.0840778907	3.3537540959
H	2.5365429278	2.3429964214	3.1546019922
H	1.3699381903	0.9866766653	3.3203372972
H	1.2627583745	2.4079840051	4.3882159976
C	0.8335837361	4.3055931788	2.3672790068
H	1.8202253135	4.5186413597	1.9204242415
H	0.8630656519	4.6781685056	3.4086220526
H	0.0713281333	4.8962193811	1.8328653071
C	-0.9282199268	2.605807773	2.9657441167
H	-1.1643597358	1.5371377877	3.1083367554
H	-1.7104477136	3.0487860221	2.3286597522
H	-0.9800691502	3.1032222588	3.9528367725
C	-0.1345617709	3.0613584875	-0.7278826972
C	-1.5721138515	3.4844127559	-0.3503185575
H	-2.1936621675	2.6216835992	-0.0513020503
H	-2.043018775	3.9530985575	-1.2357032607
H	-1.5951804675	4.2314956843	0.4614366534
C	0.677949694	4.3390501729	-1.0450914325
H	0.7831732953	5.0101528068	-0.1789992557
H	0.1467040369	4.9025540774	-1.8353839464
H	1.6789639867	4.1086595691	-1.4365237688
C	-0.1918297164	2.1732122348	-1.9970886489
H	-0.8169880153	1.2763763895	-1.8305708901
H	0.8087948505	1.8357512854	-2.3165670283
H	-0.6308471226	2.7584011067	-2.8283625122
C	2.5157549196	2.0286782134	0.3741636215
H	2.8144822268	3.0894248436	0.4661484083
H	2.9233849113	1.5146461201	1.2621061009
C	3.1360858573	1.4449030025	-0.8823927023
C	3.5943963519	2.3310963491	-1.8839919842
H	3.4625762936	3.4091288009	-1.7401466498
C	4.260843966	1.8849851552	-3.032359865
H	4.6001347334	2.6058057516	-3.7836540695
C	4.5212575929	0.5163750957	-3.183588217
H	5.0644092856	0.1431931617	-4.0581757207
C	4.1190924263	-0.3701557336	-2.1767590703

H	4.3840585506	-1.4295211898	-2.2701942324
C	3.4160283549	0.0573488628	-1.0269630311
C	3.1520531233	-0.9643170124	0.0646744467
H	3.3537522697	-0.5148019492	1.0559858902
H	3.8813473136	-1.783932099	-0.0474268271
C	1.2387575112	-2.9056877732	-1.2636232199
C	2.4744083246	-3.7748085688	-1.5901971791
H	2.6574626606	-4.5448875904	-0.8210904626
H	3.398144998	-3.1882618037	-1.7189447964
H	2.293868671	-4.3069644068	-2.5436604282
C	0.9442777826	-1.9369108513	-2.4395466395
H	0.0365078702	-1.334897242	-2.2487637381
H	0.7697952866	-2.5296890876	-3.3578453533
H	1.7734519386	-1.2403956904	-2.6405479628
C	0.0213524672	-3.8526375527	-1.124765592
H	-0.8879015469	-3.3384306751	-0.7763731636
H	0.2119708929	-4.700578992	-0.4495247194
H	-0.2061582225	-4.2763378832	-2.121301286
C	1.8435346688	-2.8182437115	1.8951565134
C	1.6811196118	-1.8360380845	3.0810303343
H	2.3911895864	-0.9917757175	3.0239149774
H	1.8880665462	-2.3690705407	4.0288177658
H	0.6568245614	-1.4244216523	3.135787261
C	3.276515201	-3.4046683809	1.9343070397
H	4.0570611547	-2.6271503573	1.9794526623
H	3.4930098585	-4.0684018647	1.0805234842
H	3.3789609392	-4.0130671796	2.8531159871
C	0.850255712	-3.9861987041	2.0916172951
H	1.0338135804	-4.8124403352	1.3864681272
H	-0.2068365516	-3.6825295001	2.0066452823
H	0.9858396021	-4.3946067501	3.1112205297
H	-2.7666169818	-0.7023947199	2.8671477982
C	-2.0527314292	-1.6296090672	0.9674475944
H	-1.4728783715	-2.5383702938	1.1408568883
C	-3.1435724177	-1.2215842241	1.9733431467
H	-3.6849032403	-2.1260022213	2.3104917544
C	-4.0801649985	-0.3057559424	1.13996239
H	-5.1522305159	-0.435057992	1.3481911781
H	-3.8016798453	0.760448481	1.2587838465
C	-2.5991216497	-1.4091414292	-0.3105152388
H	-2.2605259348	-1.7772951643	-1.2815019102
H	-1.5515029902	0.8799546963	0.8826637513
N	-3.7722841495	-0.7211086173	-0.2537362595
S	-4.7945122483	-0.4418380791	-1.6480876
O	-4.1429244013	-1.1892516211	-2.7385765585
O	-6.1663524034	-0.7010137357	-1.1853392701
C	-4.6119203899	1.332808325	-1.9484089529
H	-3.55827784	1.5529945102	-2.1692896554
H	-5.2474674443	1.5611435644	-2.817794032
H	-4.9692952525	1.883747471	-1.0665282535

MeOH

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MeOH

C	0.658550	-0.019425	-0.000024

H	1.085824	0.996709	-0.000639
H	1.043456	-0.547652	-0.898596
H	1.043453	-0.546568	0.899190
O	-0.758465	0.129757	-0.000112
H	-1.138567	-0.767458	0.000154

CO

2

CO

C	1.175031	0.000000	0.000000
O	0.024969	0.000000	0.000000

2-pyrroline

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2-pyrroline

C	-0.961100	-0.925465	0.441557
C	0.560502	-1.082129	0.722110
C	0.904078	0.216344	1.425978
C	-0.108502	1.093995	1.297584
N	-1.194131	0.555675	0.537730
H	-1.568662	-1.441502	1.206116
H	0.773578	-1.984032	1.323025
H	1.872003	0.437052	1.877640
H	-0.185106	2.127682	1.634203
H	-1.258788	-1.290642	-0.554604
H	1.130311	-1.184246	-0.222991
S	-2.792901	1.065122	0.993585
O	-3.515911	-0.036681	1.675802
O	-2.654929	2.400536	1.616987
C	-3.532505	1.272864	-0.647594
H	-4.577332	1.577864	-0.488234
H	-2.974116	2.049212	-1.187651
H	-3.494824	0.312730	-1.182099

3-pyrroline

18

3-pyrroline

C	-0.909592	-1.017116	0.367172
C	0.476387	-1.047647	0.960655
C	0.910489	0.185562	1.265074
C	-0.116671	1.235375	0.923176
N	-1.262369	0.435703	0.390648
H	-1.644616	-1.607667	0.945017
H	1.879484	0.441506	1.701648
H	0.251832	1.942090	0.150966
H	-0.924888	-1.400605	-0.674107
H	1.026562	-1.981424	1.103570
S	-2.825236	0.839594	0.983132
O	-3.536816	-0.409070	1.351304
O	-2.700034	1.967937	1.938255
C	-3.619269	1.488186	-0.511721
H	-4.643601	1.780098	-0.235906
H	-3.049671	2.360165	-0.862462
H	-3.634548	0.696341	-1.273660
H	-0.431807	1.837686	1.795430

DBPX (-PH_2 variant) 1

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Complex1

Pd	-0.1444926258	-0.4816956354	-0.5121128546
P	-1.3005856719	1.4219223653	-1.1815178483
P	-1.9663766973	-2.051023942	-0.3526862795
C	-3.1338193131	1.3688110046	-1.5451493468
H	-3.4187857607	2.3820230125	-1.8814372406
H	-3.2736358467	0.6921838204	-2.4069513106
C	-3.9358716998	0.9585972892	-0.3233273992
C	-4.4441107276	1.9740949079	0.5139646408
H	-4.2591310574	3.0238582493	0.2546064397
C	-5.1985357173	1.6693277212	1.6557537936
H	-5.588053891	2.476596921	2.2841958569
C	-5.4611313109	0.3288058021	1.9750371574
H	-6.0584964939	0.0750551624	2.8566331695
C	-4.9666072417	-0.6906141161	1.1488535153
H	-5.1915833136	-1.736781666	1.3899793878
C	-4.2023925917	-0.400067443	-0.0005081137
C	-3.7036421811	-1.5591093953	-0.8456098326
H	-3.6814487023	-1.330063255	-1.9261768735
H	-4.3497779221	-2.4450081178	-0.7172428906
H	1.0005175786	0.5996437152	-0.6310573408
H	-1.1935086063	2.4688821667	-0.2303717181
H	-0.7301618808	2.0530237009	-2.3201503663
H	-2.1641852407	-2.5593852176	0.9599356548
H	-1.7558787739	-3.279303818	-1.0429256159
C	1.303609521	-1.6703355502	-0.013248077
O	2.2132725281	-2.3149651226	0.2717705927

DBPX (-PH_2 variant) TS1-1A

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TS1-1A

Pd	-0.1391941773	1.1522103358	0.1670052822
P	-0.7694609618	-0.5253362405	1.6504302142
P	-2.3090941403	1.7381080961	-0.7378562668
C	-2.5793455043	-0.7982183009	2.0519359048
H	-2.616368947	-1.5286855919	2.8798649797
H	-2.9715837732	0.1563514148	2.4445702356
C	-3.3508188622	-1.3099598982	0.8493351717
C	-3.4707752684	-2.7056954113	0.6781735636
H	-3.0209871573	-3.3751613483	1.4219710834
C	-4.1713664464	-3.2517999868	-0.4063207193
H	-4.2581713922	-4.3383368487	-0.50937312
C	-4.7721640328	-2.3976765694	-1.3434809141
H	-5.3341747562	-2.808468291	-2.1885488586
C	-4.6651772982	-1.0088580799	-1.1836109301
H	-5.1539201427	-0.3432605523	-1.9056926972
C	-3.9609596454	-0.4443321809	-0.0990958238
C	-3.8951579319	1.068542513	0.0061208535
H	-3.9386985193	1.4305167591	1.0490723744
H	-4.7400346123	1.5329200385	-0.5312450829
H	1.2847672338	0.6194139733	0.6596293544
H	-0.3472623359	-1.8502518177	1.3540469456
H	-0.1739537522	-0.3941668729	2.9357135572

H	-2.4866001556	1.3956686507	-2.1083881208
H	-2.5885283399	3.1319020219	-0.8381754166
C	0.762260217	2.860584899	-0.0658587688
O	1.292990695	3.8869693305	-0.1092169239
C	1.067475872	-0.7256194837	-1.892414315
H	0.1646435497	-1.1250828694	-2.3609368562
C	1.6873202664	0.4377026917	-2.2077112665
H	1.3703396064	1.1582704386	-2.9660908036
C	1.9060393818	-1.5161013135	-0.9168122273
H	2.4715374096	-2.3072202803	-1.4557797889
H	1.3541295758	-2.0072706615	-0.1010691325
C	2.9973396535	0.5522171321	-1.4599677593
H	3.8499476367	0.2831839268	-2.1203838417
H	3.19257279	1.5542613268	-1.0385446765
N	2.8042911623	-0.4482015937	-0.3674554193
S	4.2650964237	-1.1410312292	0.3308443574
O	3.7654852505	-2.2119717817	1.2175082438
O	5.2523670768	-1.4128383211	-0.7378369867
C	4.8598615542	0.2443305277	1.3311371318
H	5.7677037583	-0.1215994402	1.8339641748
H	5.1150177849	1.0912374688	0.6778232393
H	4.0919552542	0.5134014198	2.0689370489

DBPX (-PH_2 variant) 1A

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Complex 1A

Pd	1.5194104356	0.0933673004	0.4940903891
P	0.007154798	1.9515264613	0.3183405728
P	0.3260999742	-1.4546176108	-0.9804654422
C	-1.4873167801	1.9156449948	-0.8200424039
H	-1.9836017347	2.8993738332	-0.747706553
H	-1.1036408477	1.8218322902	-1.8516049745
C	-2.4475915233	0.802763797	-0.4423795409
C	-3.5081056348	1.1056638359	0.4379413531
H	-3.6175753265	2.1335185723	0.805621502
C	-4.4340250817	0.1296746679	0.8328572952
H	-5.2531607005	0.3951534037	1.5091309572
C	-4.3131876164	-1.1787558059	0.3410280714
H	-5.0364298621	-1.9489946447	0.6281813972
C	-3.2685011956	-1.4933392879	-0.5398520338
H	-3.1899172811	-2.5110925691	-0.9419270169
C	-2.3263587561	-0.5229301984	-0.9419711963
C	-1.2264429424	-0.9430518216	-1.9007012404
H	-0.9335232411	-0.139115094	-2.5992815741
H	-1.5505385403	-1.8013582276	-2.5146675593
H	2.2348901082	0.9976867435	1.5891223314
H	-0.6074517956	2.3639899023	1.5349363998
H	0.6083324307	3.1982785015	-0.0226123077
H	-0.1244868953	-2.645458489	-0.3394193822
H	1.0975393782	-2.0657448056	-2.0116488804
C	3.1320537127	0.3571257485	-0.6328529336
O	4.1023325715	0.5648929177	-1.2247654224
C	0.8437486391	-0.8723552772	2.4450375659
H	-0.1362613829	-1.3243375384	2.2710130961
C	2.0771414896	-1.4473941888	2.0790002729

H	2.1966934481	-2.410486073	1.574994976
C	1.0787092105	0.0592036314	3.6233466783
H	0.8660893489	-0.4803406339	4.5702972476
H	0.4819137986	0.9858385672	3.615544224
C	3.1640271252	-0.9023994354	2.9863951932
H	3.3342628531	-1.6323550632	3.8072243856
H	4.1324760337	-0.6922366208	2.5120901015
N	2.5328876204	0.3578743116	3.4855206307
S	3.3247402047	0.9993594305	4.9373755733
O	2.5083022019	0.6395972719	6.1173823335
O	4.7405822715	0.6056416489	4.8066463898
C	3.1726115092	2.7780924185	4.6478702181
H	3.6367244839	3.2673678153	5.5175310985
H	3.7109672191	3.0341048501	3.7254896496
H	2.1083745117	3.0478869097	4.5897779176

DBPX (-PH_2 variant) 2

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Complex 2

Pd	-0.3439264304	-0.2675596406	0.1507373171
P	0.4692506968	1.7685094349	0.8516667647
P	1.707849983	-1.5659491342	0.1268414852
C	2.2740916222	2.0079717527	1.2943897159
H	2.3879658386	3.0548615248	1.628889456
H	2.4817015285	1.3648475186	2.1680782851
C	3.1809602581	1.7179876101	0.1124954726
C	3.5521184121	2.7922262211	-0.7235708144
H	3.1906140901	3.8010098992	-0.488436431
C	4.3892212687	2.6006096806	-1.831462625
H	4.6690564265	3.4530420793	-2.4588472618
C	4.8762940273	1.3162309612	-2.1169291755
H	5.5419743906	1.1523923759	-2.9705660264
C	4.5198131276	0.2402962839	-1.2916696724
H	4.9194836156	-0.7587325356	-1.5050916822
C	3.6735518479	0.4158676589	-0.1766351208
C	3.3329801202	-0.7990405679	0.6683610484
H	3.231977943	-0.5611332012	1.7425732989
H	4.1194579832	-1.568266381	0.5813029654
C	-1.5973430329	-1.6841796058	-1.1704875212
H	-0.8376427273	-2.1166422403	-1.8290329953
C	-1.8193551442	-2.0461416176	0.1530450511
C	-3.2071883992	-1.6206979107	0.571954662
H	-3.8701867526	-2.5134559866	0.5802172395
H	-3.2586735763	-1.1568377852	1.5709408967
C	-2.8199566881	-0.9921395268	-1.7263694467
H	-3.3566945681	-1.7070982248	-2.3872274705
H	-1.6516262591	0.6025578553	0.1632167778
N	-3.5866943797	-0.6490517381	-0.492070079
S	-5.3196438173	-0.4885499481	-0.7620959161
O	-5.4783912026	-0.2555049261	-2.2126837853
O	-6.0084431709	-1.5961052837	-0.061563856
C	-5.6690128346	1.0497906663	0.1216792518
H	-5.0953719545	1.8615591495	-0.3454399021
H	-6.7502639407	1.2265515862	0.0193642821
H	-5.4032494965	0.9239910263	1.1808816741

H	-2.6130525732	-0.090571632	-2.3233864994
H	-1.2623341196	-2.8074597705	0.7081397819
H	0.2571276067	2.8042489541	-0.0967690619
H	-0.2216646032	2.3278107384	1.9633079884
H	2.0784226849	-2.0975263976	-1.1424759051
H	1.7028920395	-2.7957947431	0.8532893432

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