Selective C–H Halogenation over Hydroxylation by Non-heme iron(IV)-oxo

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1. Experimental Section:

1.1. General Information:

NMR spectra were recorded either on a Bruker 400/500/750MHz. All ^{1}H NMR spectra were reported in units of parts per million (ppm) and measured relative to the signals for residual chloroform (7.26 ppm) in $CDCl_3$/ and for residual CH_3CN in CD_3CN at 1.96 ppm, unless otherwise stated. All ^{13}C NMR spectra were reported in ppm relative to $CDCl_3$ (77.23 ppm), unless otherwise stated and were obtained with ^{1}H decoupling. ESI-MS spectra were recorded in Bruker QTOF ESI-MS instrument. EPR spectra were recorded on JES - FA200 ESR Spectrometer with X and Q band (Standard Frequency (X band) - 8.75-9.65 GHz) at 77 K. UV-vis kinetics studies were performed in Agilent 8453 diode array based UV-vis Spectrophotometer. Synthesis of complex **1** and iron(IV)-oxo complexes **2**were done inside the glove box. Acetonitrile, CD_3CN, $Fe^{II}Cl_2$, $Fe^{II}Br_2$, trimethylsillyltriflate (TMSOTf) were bought from Sigma Aldrich. Diethyl ether was bought from Spectrochem chemicals.Ethylbenzene,was bought from TCI chemical company. $H_2{}^{18}O$ was bought from Sigma Aldrich.2-(chloromethyl)quinoline hydrochloride was purchased from TCI chemical companyand di(2-pyridyl)ketone were bought from alfa aeser. Single crystal of complex **1** was diffracted in Rigaku X-ray single crystal diffractometer. All the kinetics data are carried out under N_2atmosphere. The kinetics of the reactions does not vary from $N_2$to air atmosphere. First order rate constant (k_1) were calculated based on non-linear exponential fit in OriginPro8 software. All the kinetics were carried out in pseudo-first-order conditions (substrate >10 equiv. were used).The rate constant (k_1) was calculated based on the decay pattern of iron(IV)-oxo complex at 770 nm by nonlinear curve fitting, [$y = y_0 + A*\exp(R_0{}^{*}x)$], (where x is time, t and R_0 is rate constant, k_1, y is absorbance) and showed good fit in rate constant value within 10% error. Resulting k_1 values corroborated linearly with substrate concentration to give second-order rate constant k_2.All the products were analyzed by GC/GC-MS analysis. GC-MS was performed on a Thermo Scientific ISQ QD Mass Spectrometer attached with Thermo Scientific TRACE 1300 gas chromatograph using an HP-5ms capillary column (30 m×0.25 mm×0.25 μm, J&W Scientific) with helium as the carrier gas. The product yields were calculated from the GC-trace obtained from the Thermo Scientific GC-MS instrument by comparing with the standard product. Some of the GC-MS analyses were carried out by Agilent 7890A GC system connected with 5975C inert XL EI/CI

MSD (with triple axis detector). Yields of the different products were calculated with respect to area% of the standard products. During bromination-chlorination reactions formation of trace or minor amount of C-H oxidation products cannot be ruled out as sometimes the minor oxidation products might be beyond the detection limit of the GC-MS instrument. Unless otherwise stated all the yields mentioned in the main manuscript are ±5% range of error. Some of the benzyl bromide derivatives and benzyl chloride derivatives by reacting corresponding toluene derivatives with NBS/NCS in presence of benzoyl peroxide under reflux condition.

1.2. Computational Details:[1,2,3,4]

Full geometry optimization was performed by using the density functional theory method at (U) B3LYP levels.Except iron all other elements were assigned the 6-31G* basis set. The LANL2DZ basis set with effective core potential was employed for the iron atom. The vibrational frequency calculation was done to ensure that the optimized geometries represent the local minima and there are only positive eigen values. All calculations were performed with Gaussian 09 program package. Optimized structure was visualized with *ChemCraft*.

1.3. Synthesis and characterization of 2PyN2Q ligand:[5,6,7]

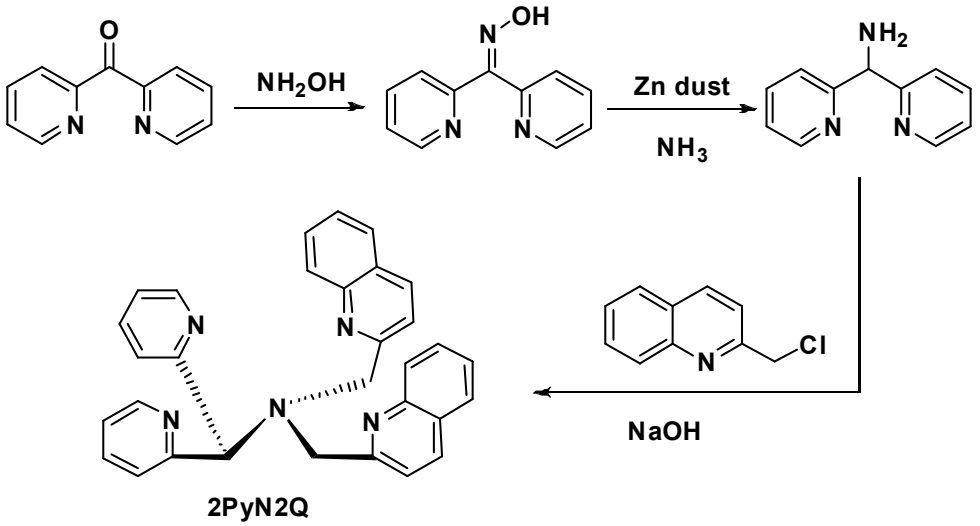


Figure S1. Synthesis of modified ligand **2PyN2Q**

The di(pyridin-2-yl)methanamine was synthesized from di(2-pyridyl)ketone following the previous literature procedure.[5] Subsequently it was reacted with2-(chloromethyl)quinolinehydrochloride in 5 M of NaOH solution as mentioned in the literature.[6,7] The yellowish-brown solid ligand was obtained after work up with perchloric acid.The

synthesized ligand was thoroughly characterized by ^{1}H, ^{13}C NMR and ESI-MS analysis. The obtained NMR data for ligand, N2QuPy:

^{1}H NMR data: **^{1}H NMR (500 MHz, $CDCl_3$, δ)**:4.208 (s, 4H), 5.452 (s, 1H), 7.07-8.54 (m, 20H, Qu, Py). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 58.40, 72.69, 121.51, 122.40, 124.51, 126.20, 127.36, 127.55, 129.06, 129.44, 136.33, 136.57, 147.60, 149.44, 160.54, 160.02.

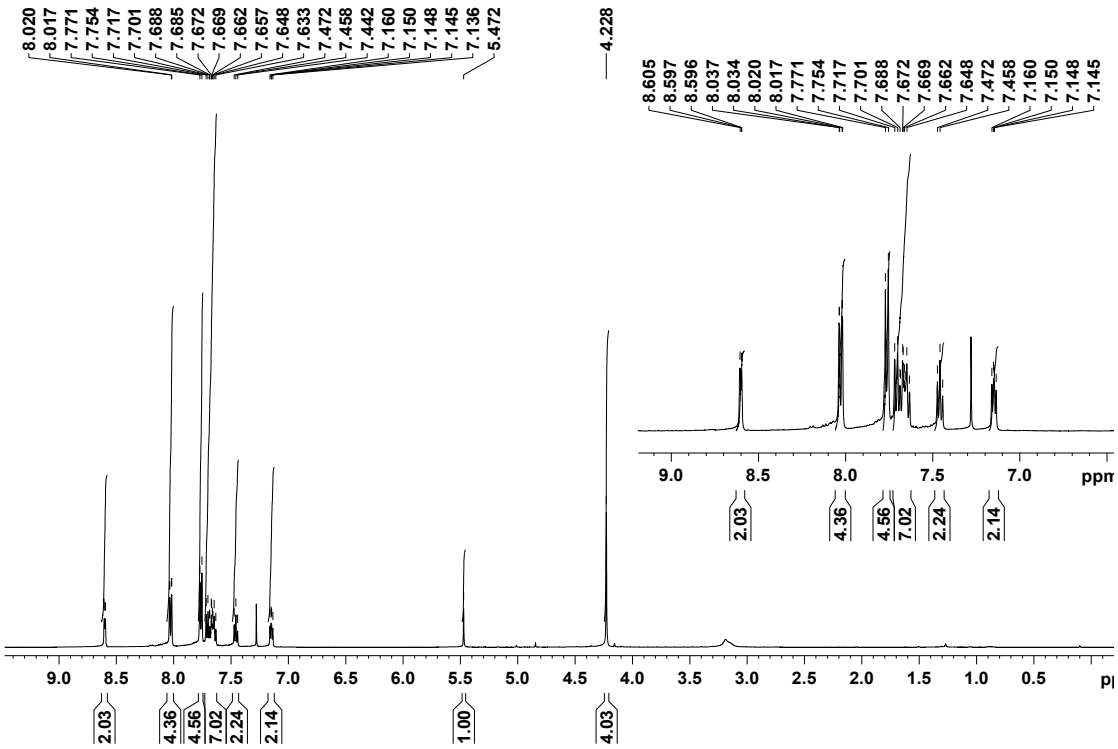


Figure S2. ^{1}H NMR Spectra of **2PyN2Q** ligand

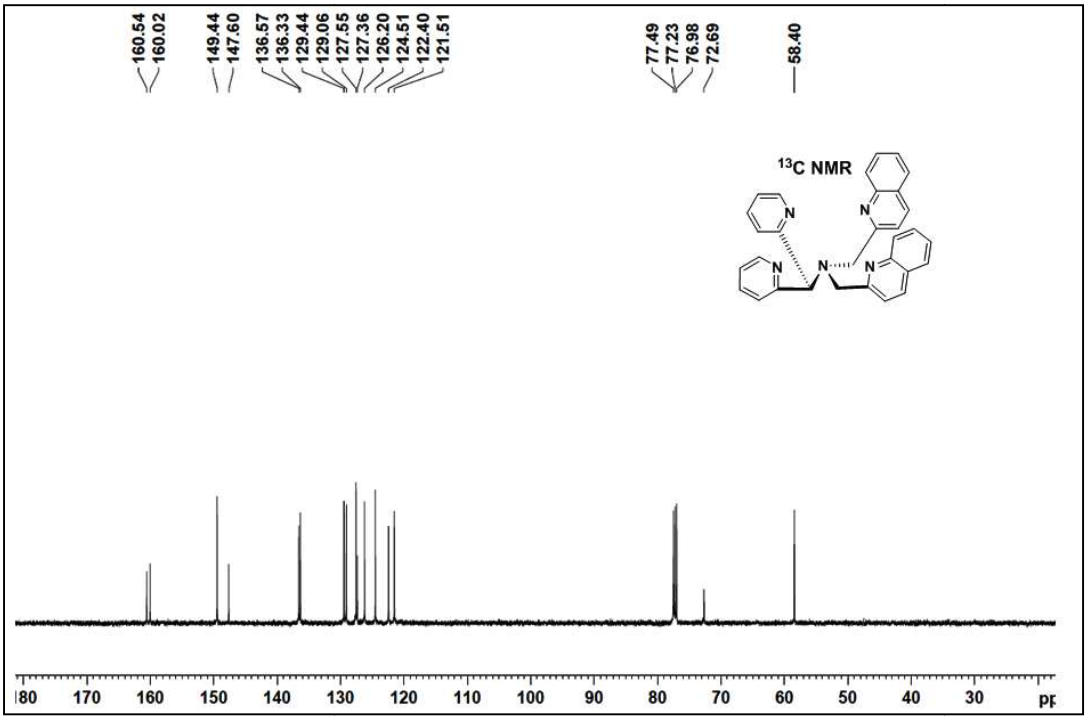


Figure S3. ^{13}C NMR of **2PyN2Q** ligand

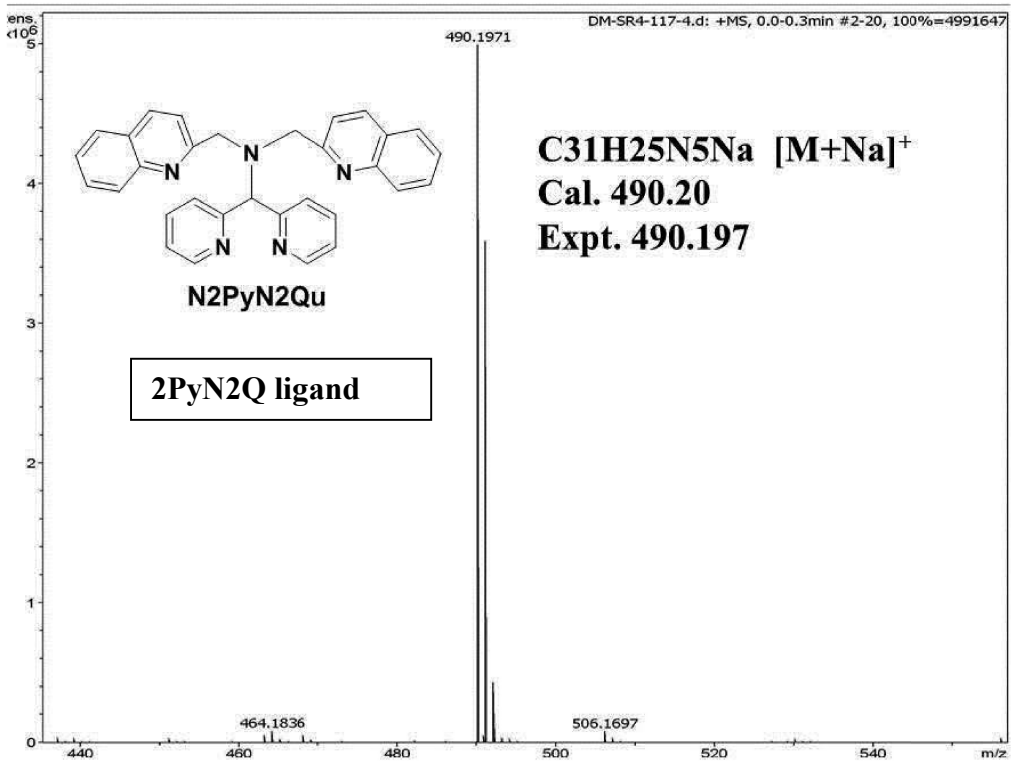


Figure S4. ESI-MS spectra of **2PyN2Q** ligand

1.4. Synthesis and characterization of iron(II)-complex $[Fe^{II}(2PyN2Q)](OTf)_2$:

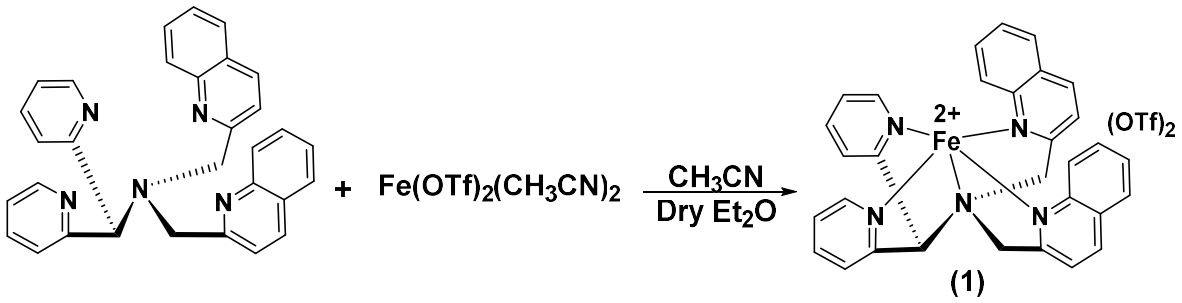


Figure S5. Synthesis of complex **1**

The ligand 2PyN2Q (1.2 mmol) and iron(II)-precursor complex $Fe(OTf)_2.2CH_3CN$ (1.0 mmol) were reacted for overnight in excess amount of acetonitrile (40 mL) inside the glove box. Subsequently the reaction mixture was concentrated by applying vacuum. Then excess dry diethyl ether was added to the reaction mixture and the schlenk was shaken vigorously to get precipitate of complex. Then the mixture was allowed to settle down the precipitate of complex get settled at the bottom of the schlenk flask. The clear solution part above the precipitate was decanted off. Then the precipitate was dried properly by applying vacuum and kept under N_2 atmosphere of glove box. The corresponding triflate anion coordinated single crystal was grown from acetonitrile-toluene or acetonitrile-diethylether solvent combination. The resultant complex was recrystallized from dichloromethane and diethyl ether mixture. The obtained complex was characterized by UV-vis, ESI-Ms, ^1H NMR and X-ray crystallographically.

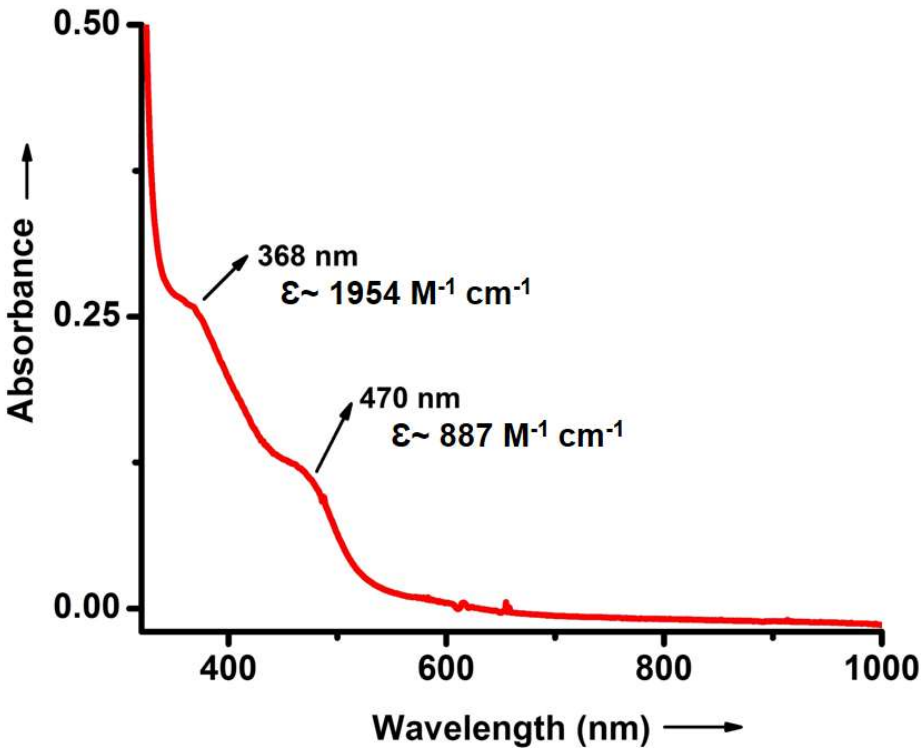


Figure S6. UV-vis of complex **1**, $[Fe^{II}(2PyN2Q)](OTf)_2$

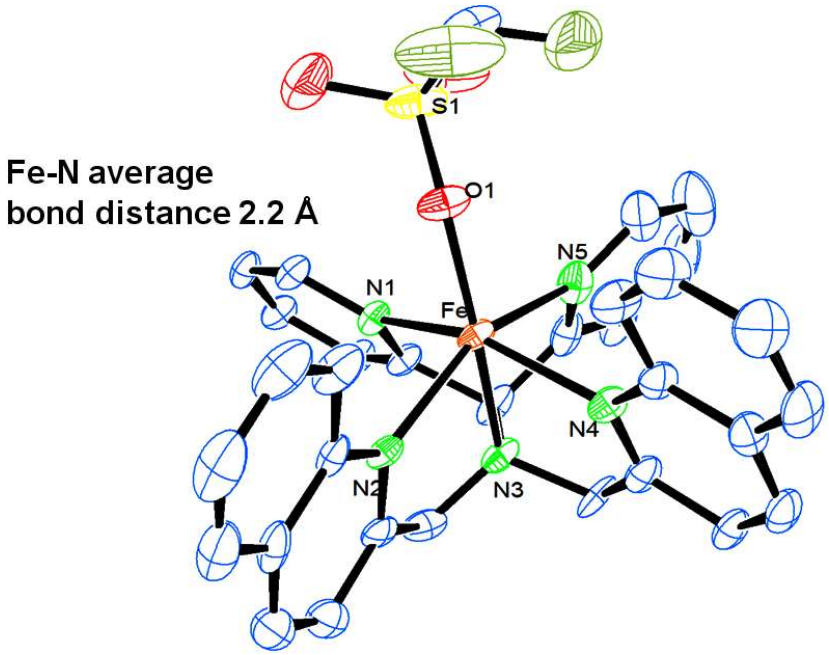


Figure S7. ORTEP diagram of **1**, $[Fe^{II}(2PyN2Q)](OTf)_2$, (cationic part, triflate anion and hydrogen atoms are omitted for pictured clarity)

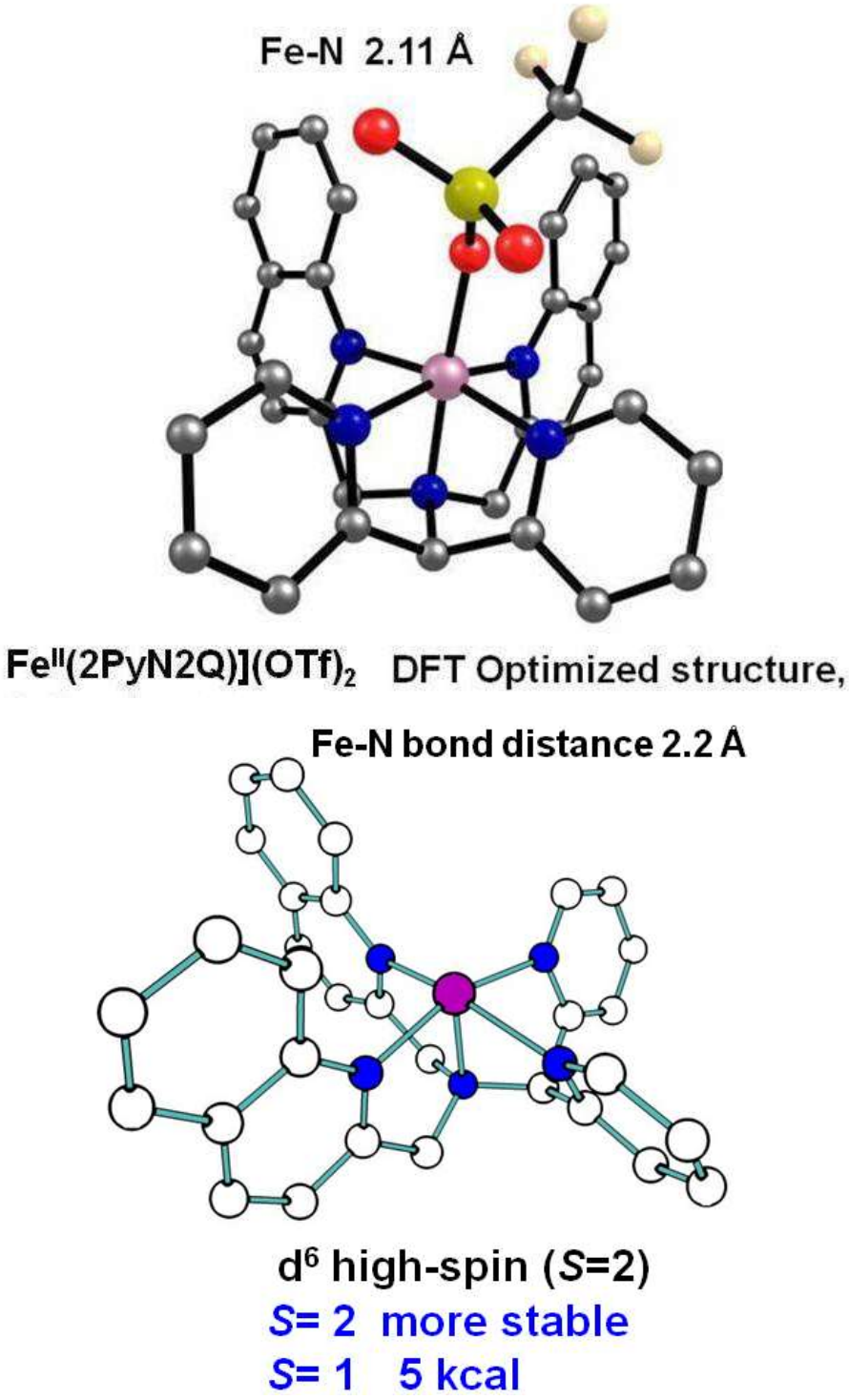


Figure S8. DFT optimized structure of complex **1**, $[Fe^{II}(2PyN2Q)](OTf)_2$

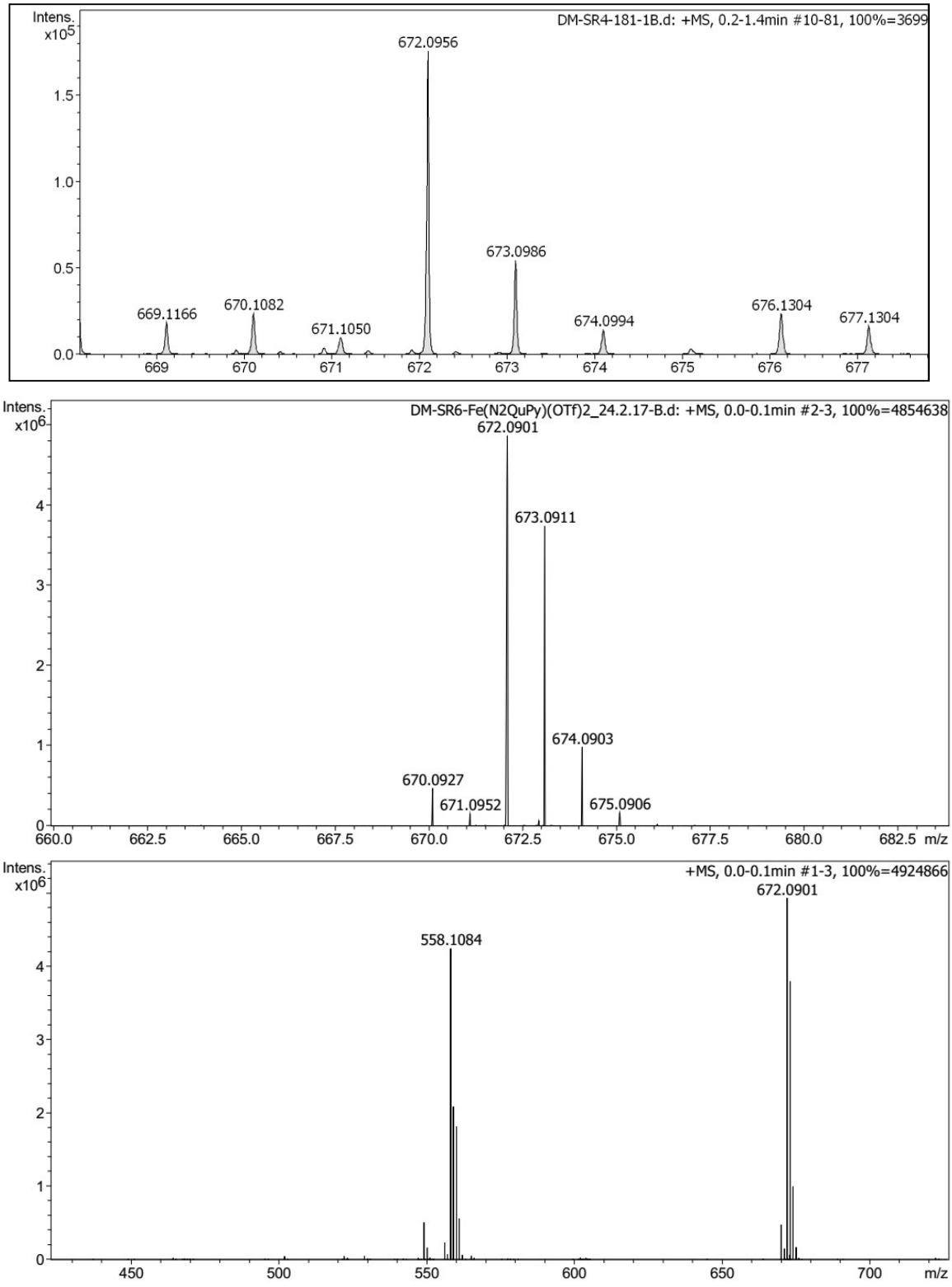


Figure S9.ESI-MS spectra (below) ofcomplex **1**, $[Fe^{II}(2PyN2Q)](OTf)_2$

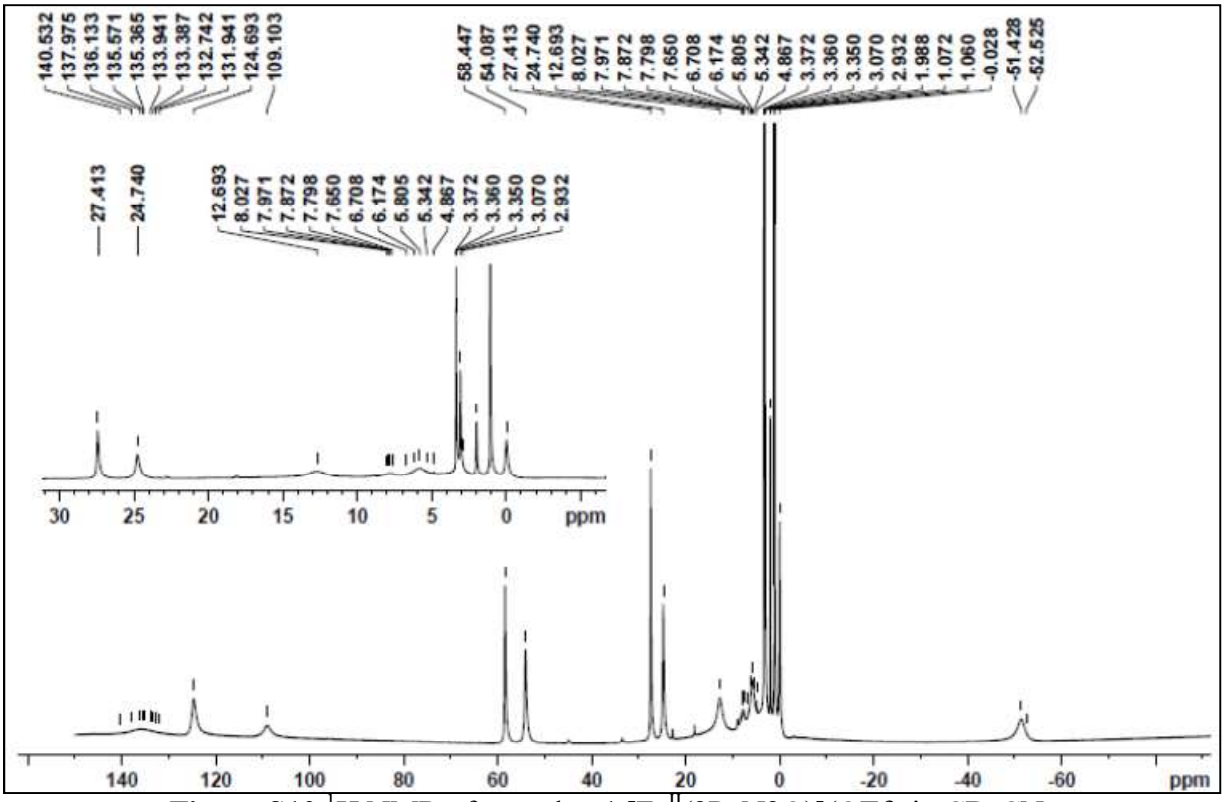


Figure S10. ^{1}H NMR of complex **1**,[Fe^{II}(2PyN2Q)](OTf)$_2$in CD_3CN,

1.5. Synthesis and characterization of iron(IV)-oxo-complex, 2, [Fe^{IV}(2PyN2Q)(O)]$^{2+}$:

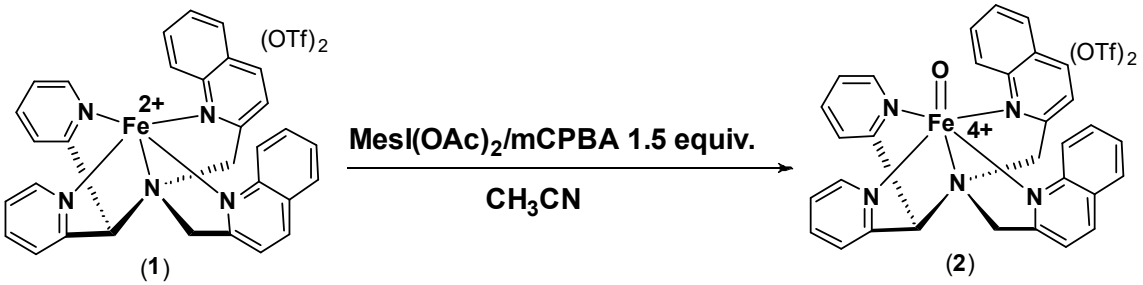


Figure S11. Synthesis of complex **2**

The complex **1** (1.21 mM solution in acetonitrile) was reacted with 1.5 equiv. of MesI(OAc)$_2$ or mCPBA in acetonitrile. The resulting solution forms iron(IV)-oxo complex **2**, within 1-2 mintutes of addition of the oxidants. The formation of the iron(IV)-oxo complex **2** was monitored by UV-vis. The resultant iron(IV)-oxo complex showed the half-life around ~30 minutes.The corresponding iron(IV)-oxo complex showed UV-vis band at 770 nm (d-d transition) with a molar extinction coefficient, ϵ~250 $Lmol^{-1}cm^{-1}$. The iron(IV)-oxo species **2**

was characterized by ESI-MS study. It showed the high abundant peak at 688.090 of $[Fe^{IV}(2PyN2Q)(O)(OTf)]^{+}$ with expected isotopic pattern.

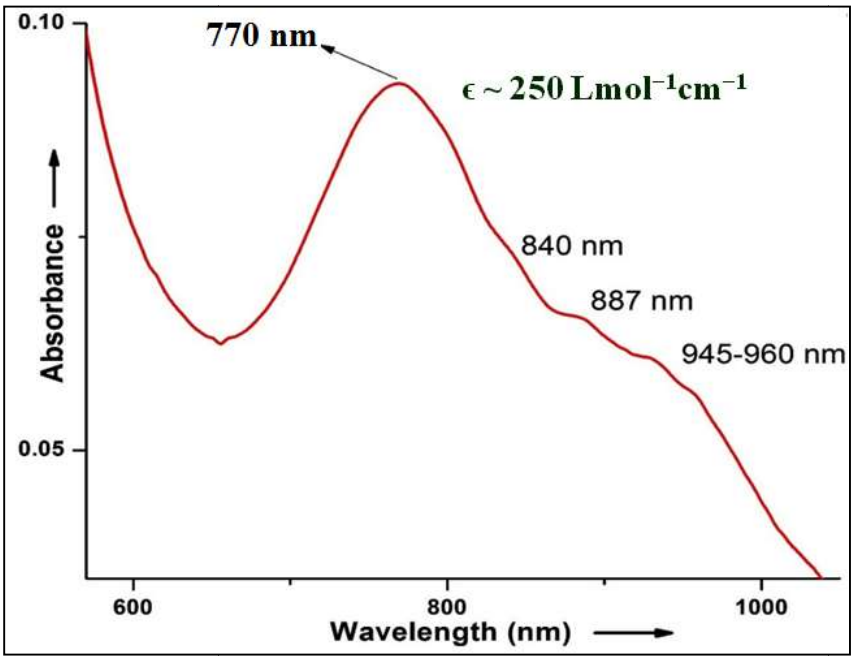
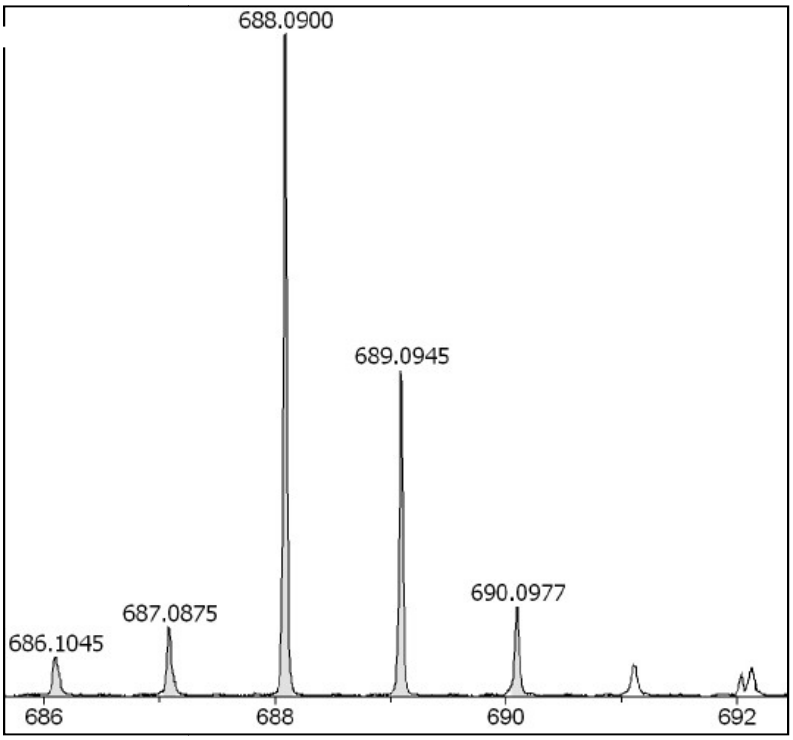
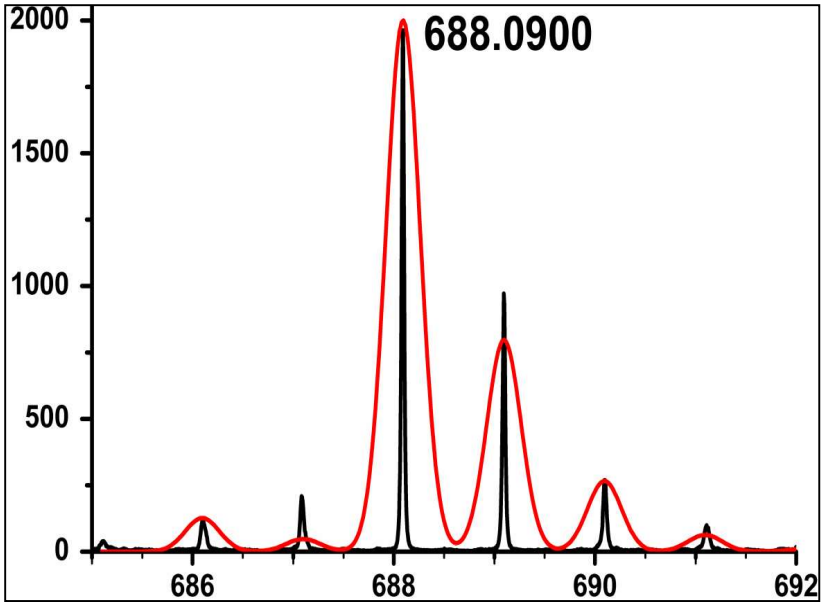
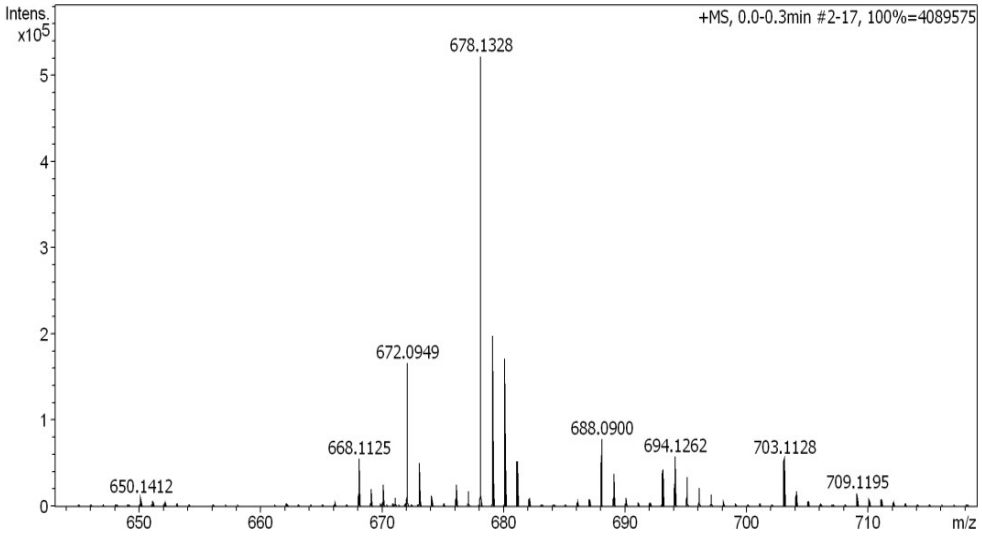


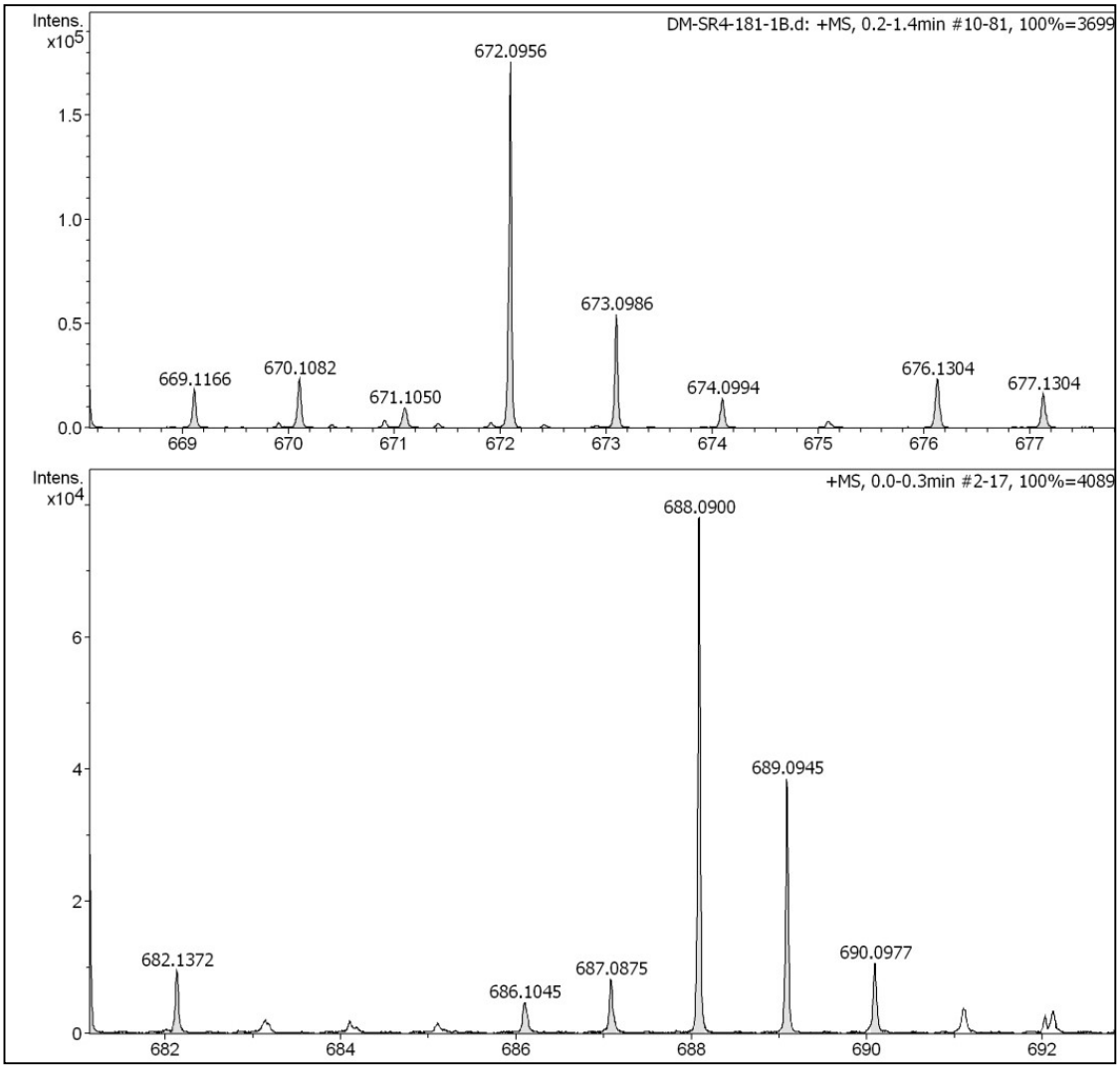
Figure S12. UV-vis of complex **2,** $[Fe^{II}(2PyN2Q)(O)]^{2+}$

1.6. ESI-MS spectra of $[Fe^{IV}(2PyN2Q)(O)(OTf)]^{+}$(2)




688.0900
2000
1500
1000
500
0
686
688
690
692


Intens.
x10^5
+MS, 0.0-0.3min #2-17, 100%=4089575
678.1328
672.0949
668.1125
688.0900
694.1262
703.1128
650.1412
709.1195
m/z


Intens.
x10^5
DM-SR4-181-1B.d: +MS, 0.2-1.4min #10-81, 100%=3699
672.0956
673.0986
669.1166
670.1082
671.1050
674.0994
676.1304
677.1304
Intens.
x10^4
+MS, 0.0-0.3min #2-17, 100%=4089
688.0900
689.0945
682.1372
686.1045
687.0875
690.0977

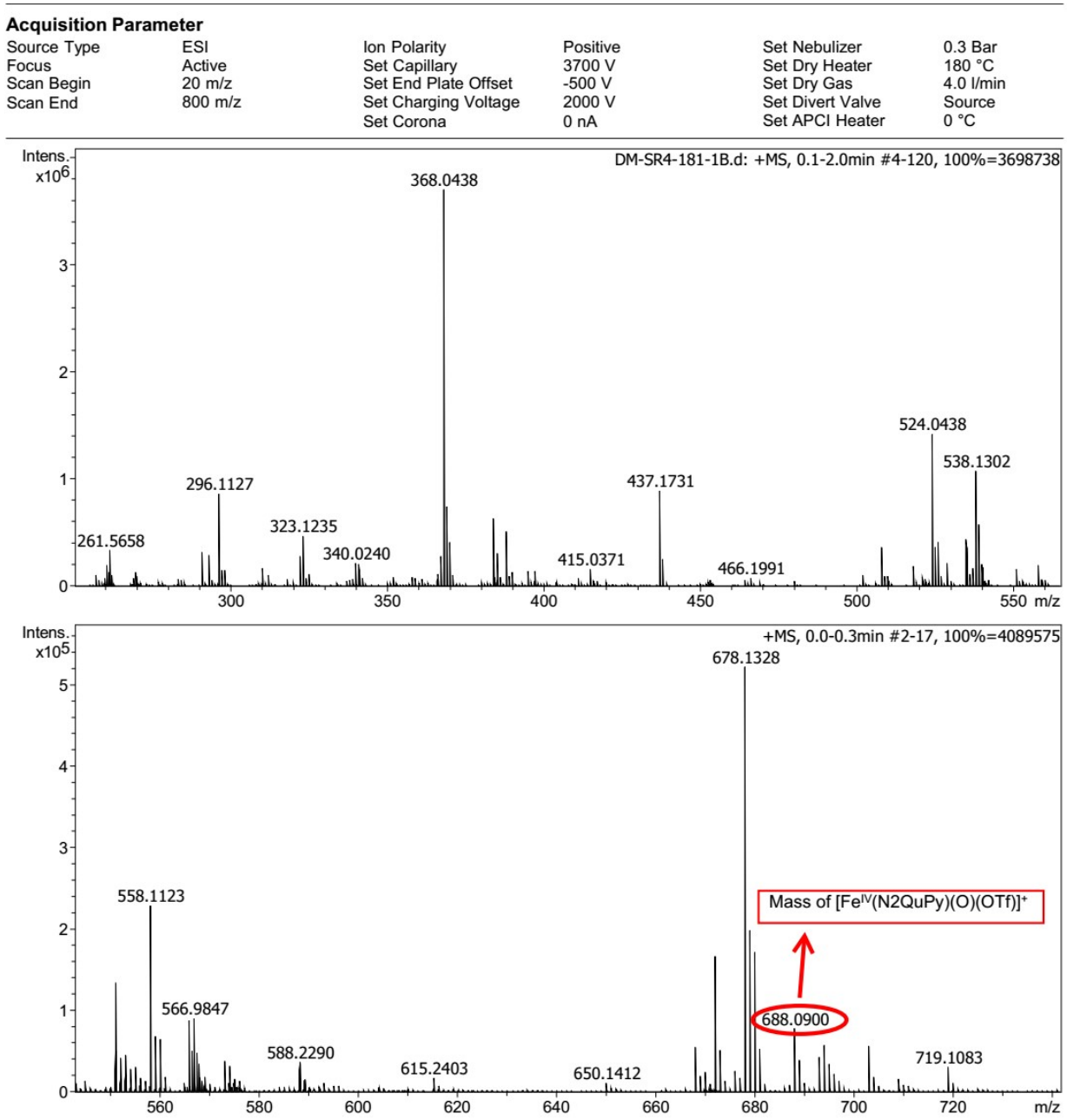


Figure S13. ESI-MS spectra of iron(IV)-oxo, **2**, $[Fe^{IV}(2PyN2Q)(O)(OTf)]^+$ (m/z calculated, 688.093, observed m/z 688.090) with simulated spectra (red color simulated, black experimental), The ESI-MS of complex **2** was tried for several times, but good abundant spectra for complex **2** was not obtained

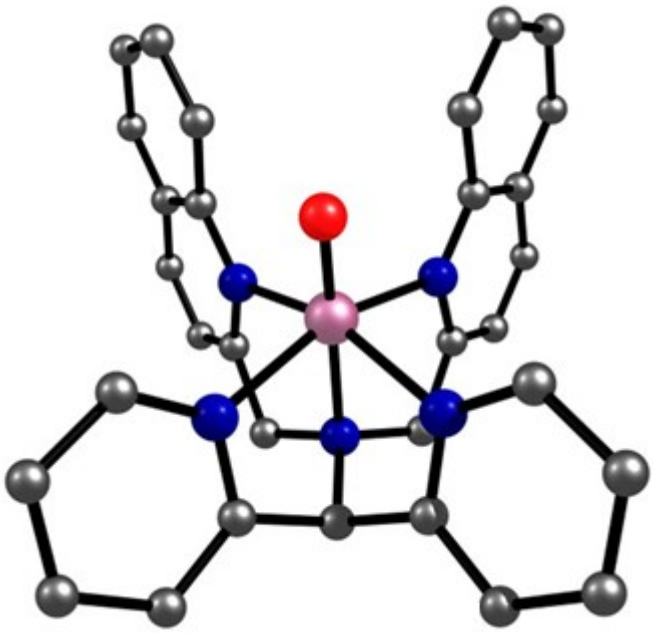
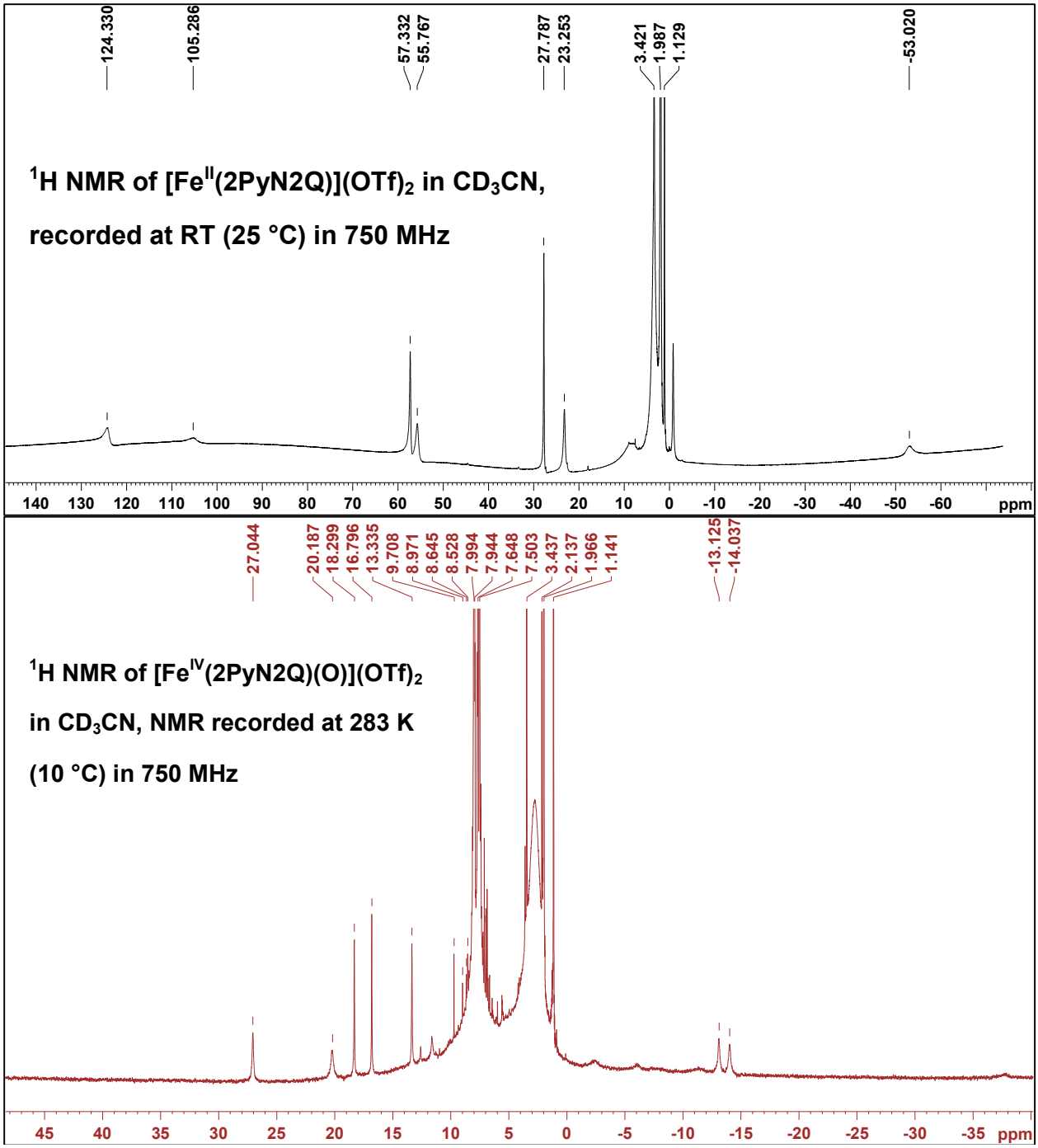
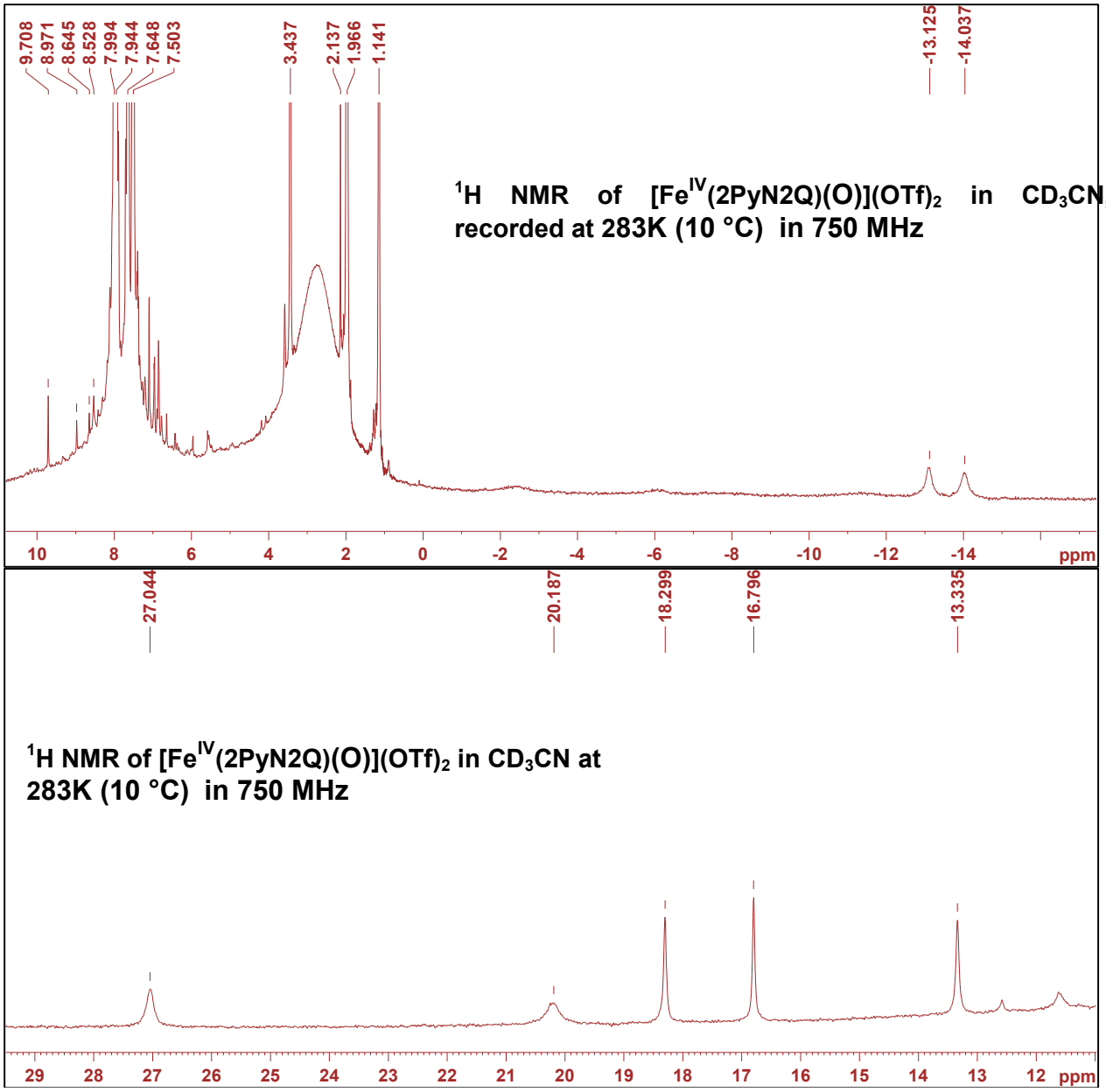


Figure S14. DFT optimized geometry of complex **2**, $[Fe^{IV}(2PyN2Q)(O)](OTf)_2$

1.7. NMR characterization of$[Fe^{IV}(2PyN2Q)(O)(OTf)]^+$ (2), in (NMR of the complexes recorded at 750 MHz Bruker Instrument)

We have carried out the **^{1}H NMR** study of *iron(IV)-oxo complex* in comparison with *iron(II)-complex*in CD_3CN at 283 K. The iron(IV)-oxo NMR samples is prepared at room temperature by reacting iron(II)-triflate,$[Fe^{II}(N2QuPy)](OTf)_2$ with 2 equiv. of mCPBA in CD_3CN. The ^{1}H NMR spectra was recorded at 283 K (10 °C). The **^{1}H NMR** of iron(IV)-oxo complex showed shift: -15 to 30 ppmwhereas native iron(II)-complex showed paramagnetic shift: -55 to 125 ppm. We have also recorded the **^{1}H NMR** of decay product, *iron(III)-complex* (-1 to 58 ppm) obtained from iron(IV)-oxo decay. Similar **^{1}H NMR** shift of iron(IV)-oxo complexes have been previously reported by Que group and Goldberg group.[8]


124.330
105.286
57.332
55.767
27.787
23.253
3.421
1.987
1.129
-53.020
^{1}H NMR of [Fe^{II}(2PyN2Q)](OTf)$_2$ in CD$_3$CN,
recorded at RT (25 °C) in 750 MHz
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 ppm
27.044
20.187
18.299
16.796
13.335
9.708
8.971
8.645
8.528
7.994
7.944
7.648
7.503
3.437
2.137
1.966
1.141
-13.125
-14.037
^{1}H NMR of [Fe^{IV}(2PyN2Q)(O)](OTf)$_2$
in CD$_3$CN, NMR recorded at 283 K
(10 °C) in 750 MHz
45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 ppm



^{1}H NMR of [Fe^{IV}(2PyN2Q)(O)](OTf)$_2$ in CD_3CN, recorded at 283K (10 °C) in 750 MHz

^{1}H NMR of [Fe^{IV}(2PyN2Q)(O)](OTf)$_2$ in CD_3CN at 283K (10 °C) in 750 MHz

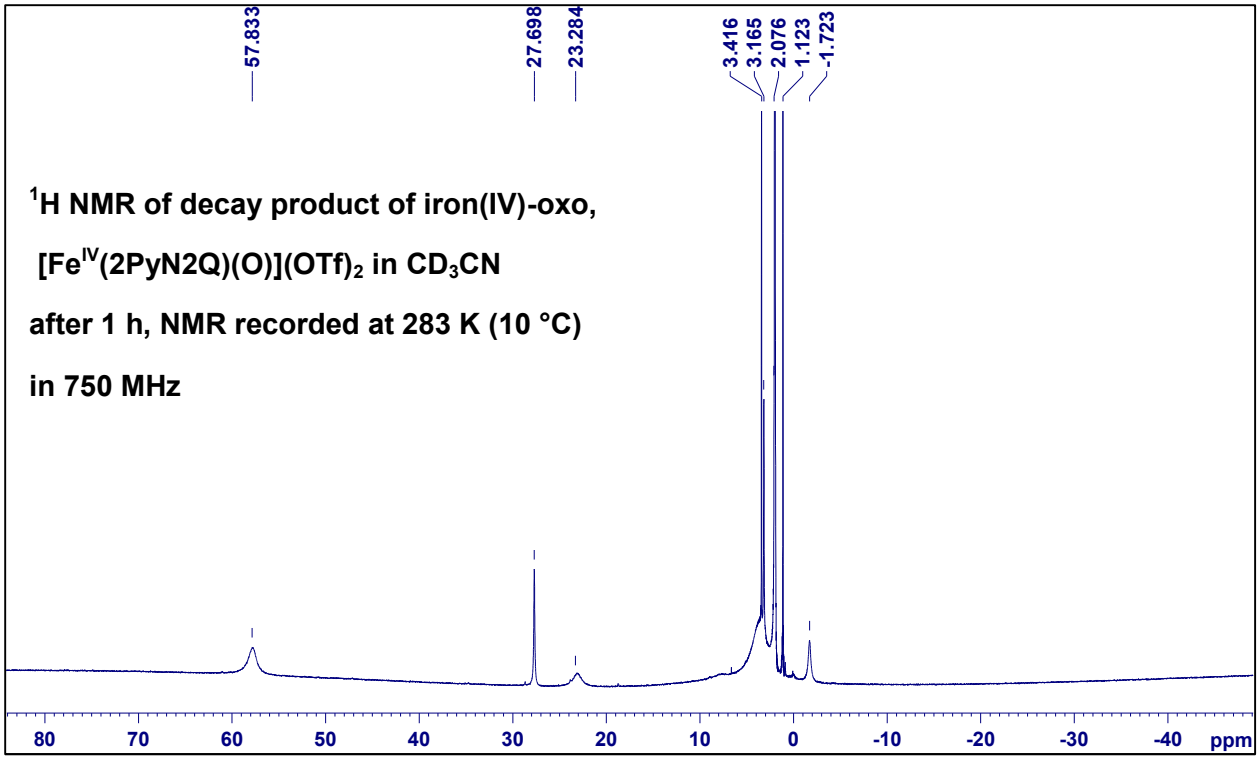


Figure S15: ^{1}**H NMR** spectra of iron(II)-complex**1**, iron(IV)-oxo complex **2**and decay spectra of iron(IV)-oxo complex

1.8. Mössbauer Study of complex 2

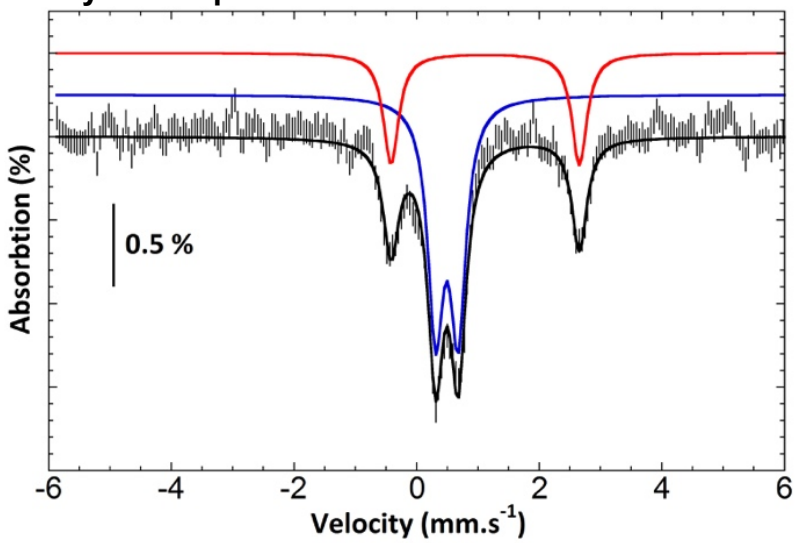
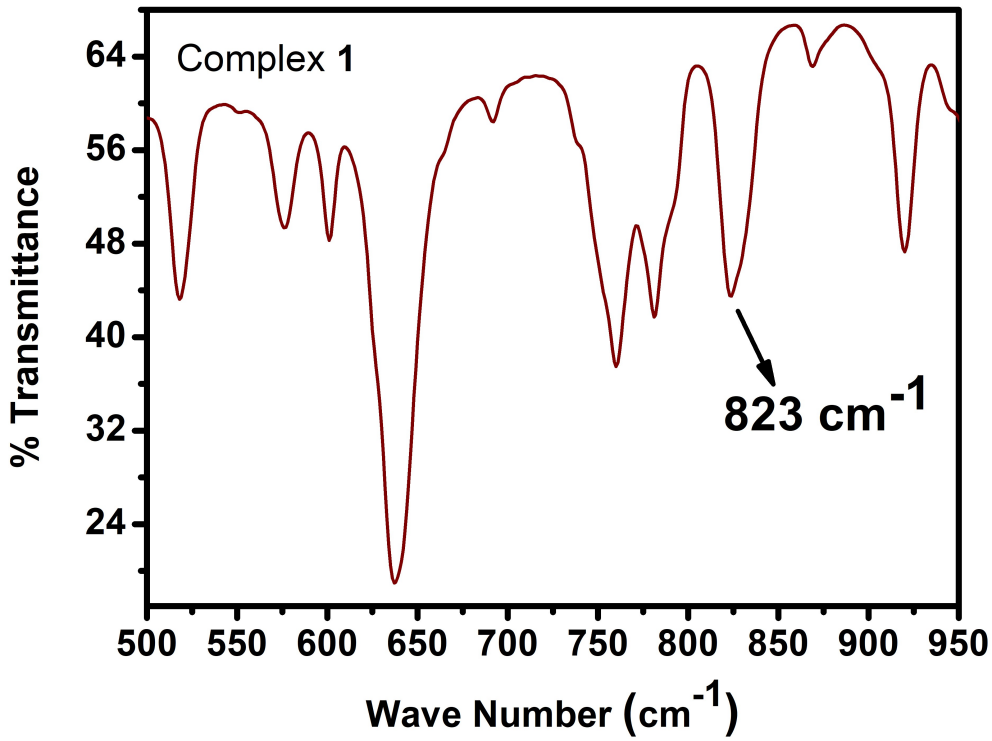


Figure S16.Mössbauer spectrum of **2** recorded at 80 K showing the experimental spectrum (hatched bars), its simulation (black solid line) and deconvolution in low-spin Fe(II) (blue solid line) and high-spin Fe(II) (red solid line) components. See Table S1 for parameters.

Table S1.Mössbauer parameters deduced from the simulations.

Cpd	S	D cm^{-1}	E/D	δ ($mm\ s^{-1}$)	ΔE_Q ($mm\ s^{-1}$)	Γ ($mm\ s^{-1}$)	η	A_x (T)	A_y (T)	A_z (T)	%
2	0			0.48	0.34	0.28					67
	2			1.14	2.94	0.27					33
4	1	25.9	0	0.04	0.57	0.30	0.03	-23.9	-23.9	-0.01	35
	0			0.50	1.50	0.50	0				12
	5/2			0.56	0.72	0.48	0	-20.7	-20.7	-20.7	53

1.9. IR Characterization of complex 1 and 2



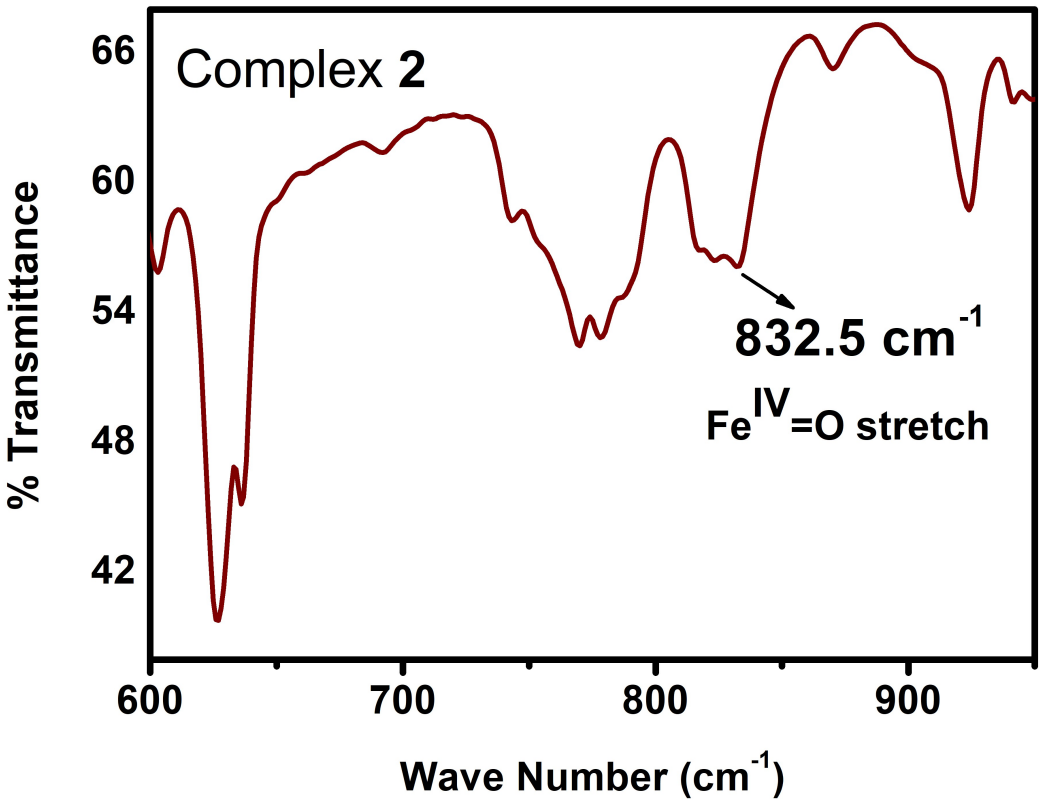


Figure S17. FT-IR spectra of complex **1** and **2**

1.10. Synthesis and characterization of iron(II)-complex [Fe^{II}(2PyN2Q)(Cl)]Cl:

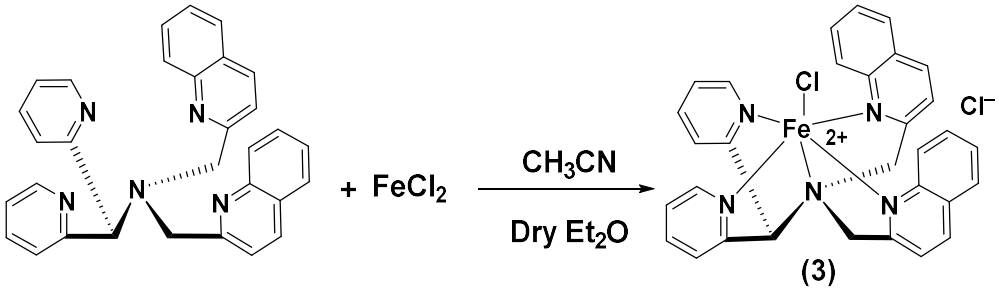


Figure S18. Synthesis of complex **3**

The ligand 2PyN2Q (1 mmol) and iron(II)-chloride, $FeCl_2$ (1.2 mmol) were reacted for overnight in excess amount of tetrahydrofuran (THF) and acetonitrile (40 mL) inside the glove box. Subsequently the reaction mixture was concentrated by applying vacuum. Then excess dry hexane was added to the reaction mixture and shaken to get precipitate of complex. Then the mixture was allowed to settle down the precipitate of complex get settled at the bottom of the

schlenk flask. The clear solution part above the precipitate was decanted off. Then the precipitate was dried properly by applying vacuum and kept under N_2 atmosphere of glove box. The single crystal of the corresponding chloro complex was obtained from acetonitrile.

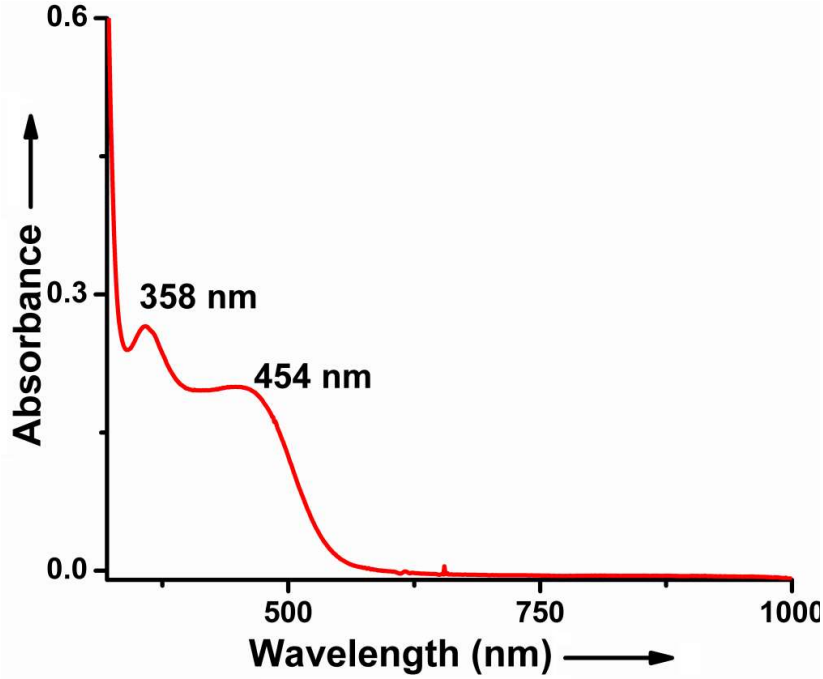


Figure S19. UV-vis spectra of complex **3**, [Fe^{II}(2PyN2Q)(Cl)](Cl) in MeCN

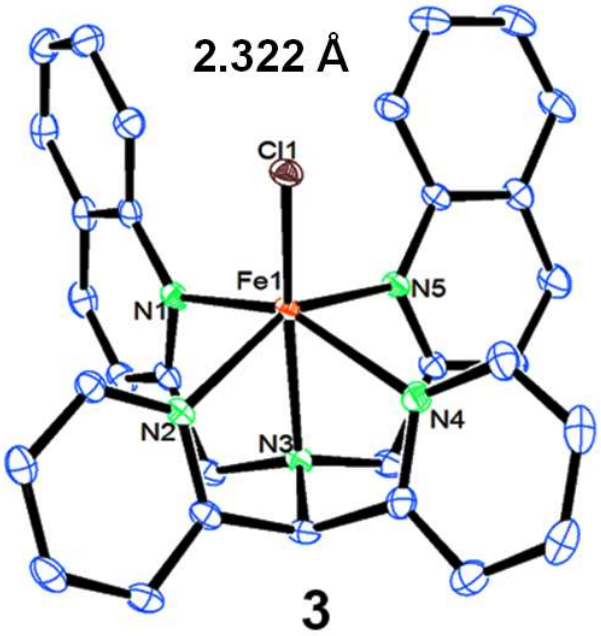


Figure S20. ORTEP diagram of **3**, [Fe^{II}(2PyN2Q)(Cl)](Cl) in MeCN (anion and hydrogens are omitted)

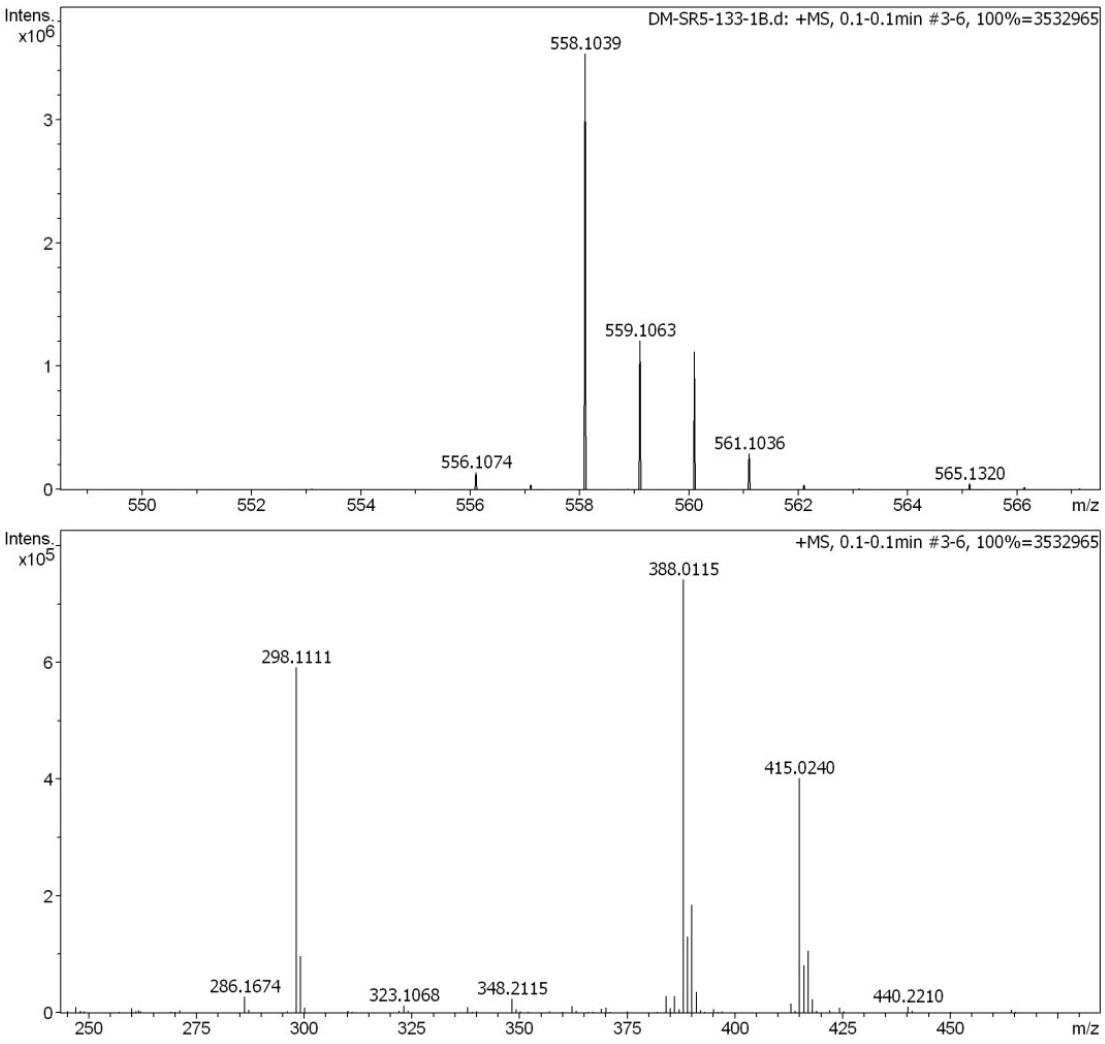


Figure S21. ESI-MS spectra of complex **3**,[Fe^{II}(2PyN2Q)(Cl)](Cl), Calculated m/z-558.115, obtained m/z-558.10

1.11. Synthesis and characterization of iron(II)-complex [Fe^{II}(2PyN2Q)(Br)]Br:

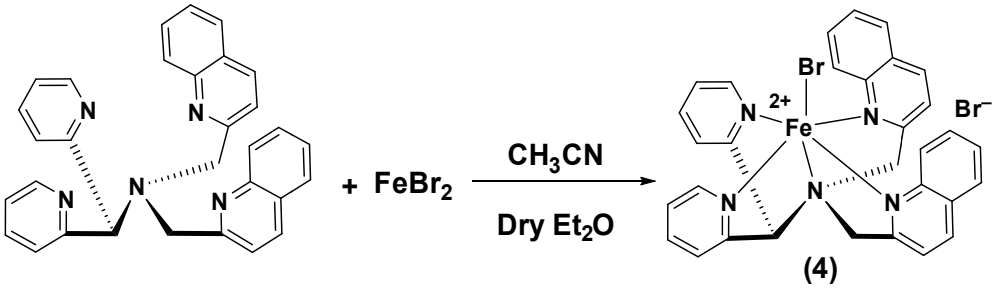


Figure S22. Synthesis of complex **4**, [Fe^{II}(2PyN2Q)(Br)]Br

The ligand 2PyN2Q (1.2 mmol) and iron(II)-bromide, $FeBr_2$ (1.0 mmol) were reacted for overnight in excess amount of tetrahydrofuran (40 mL) and acetonitrile inside the glove box. Subsequently the reaction mixture was concentrated by applying vacuum. Then excess dry hexane was added to the reaction mixture and shaken to get precipitate of complex. Then the mixture was allowed to settle down the precipitate of complex get settled at the bottom of the schlenk flask. The clear solution part above the precipitate was decanted off. Then the precipitate was dried properly by applying vacuum and kept under N_2 atmosphere of glove box.

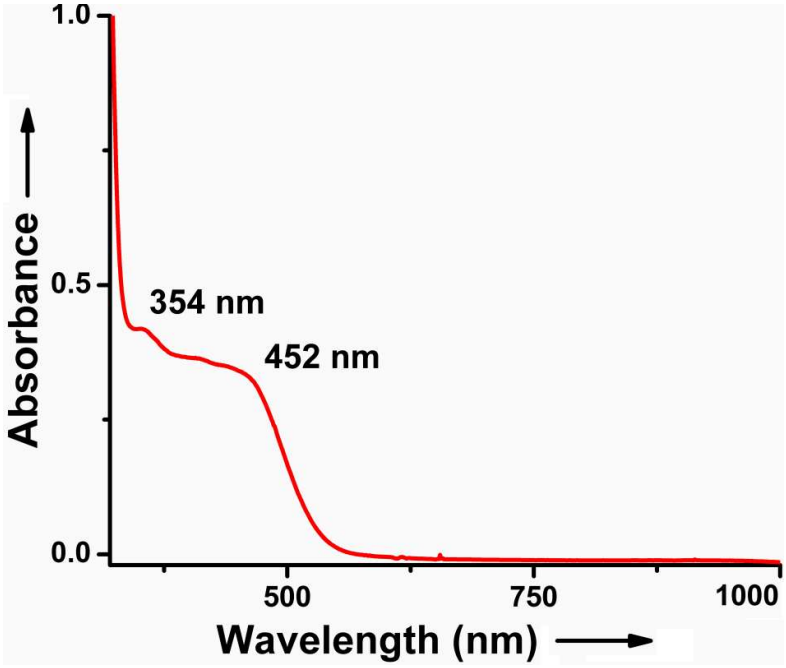


Figure S23. UV-vis of complex **4,** [Fe^{II}(2PyN2Q)(Br)]Br

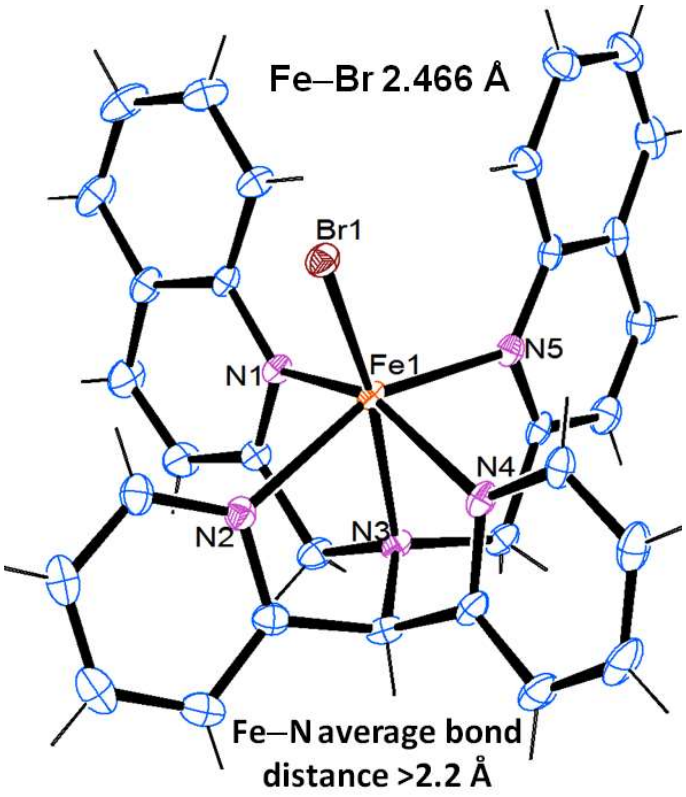


Figure S24. ORTEPdiagram of complex **4,** $[Fe^{II}(2PyN2Q)(Br)]^{+}$ (cationic part of the complex, anion omitted for picture clarity)

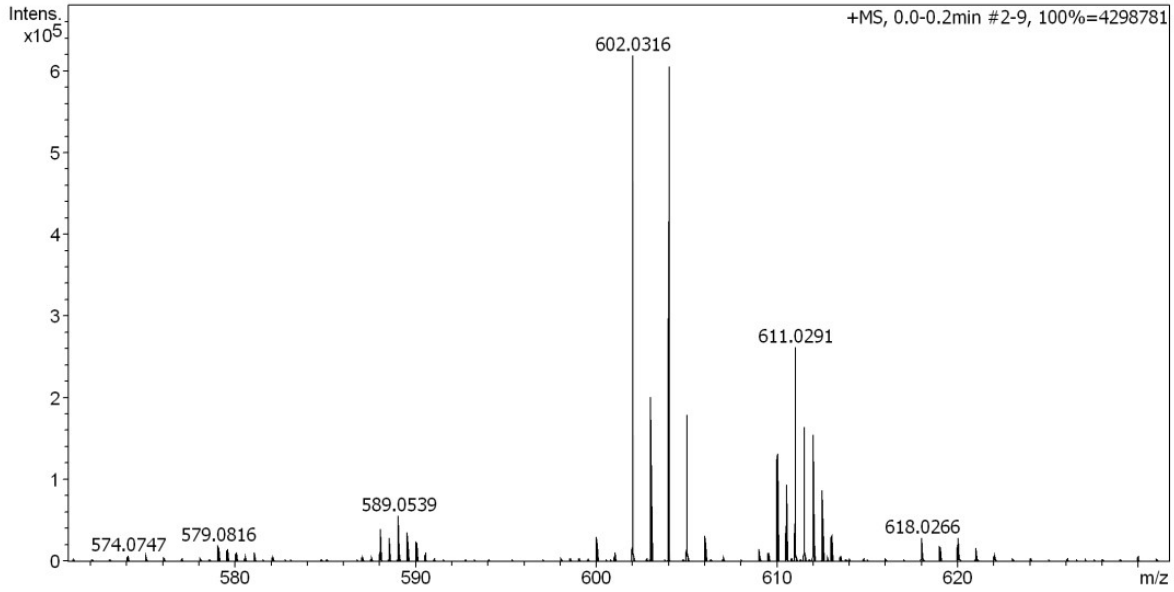
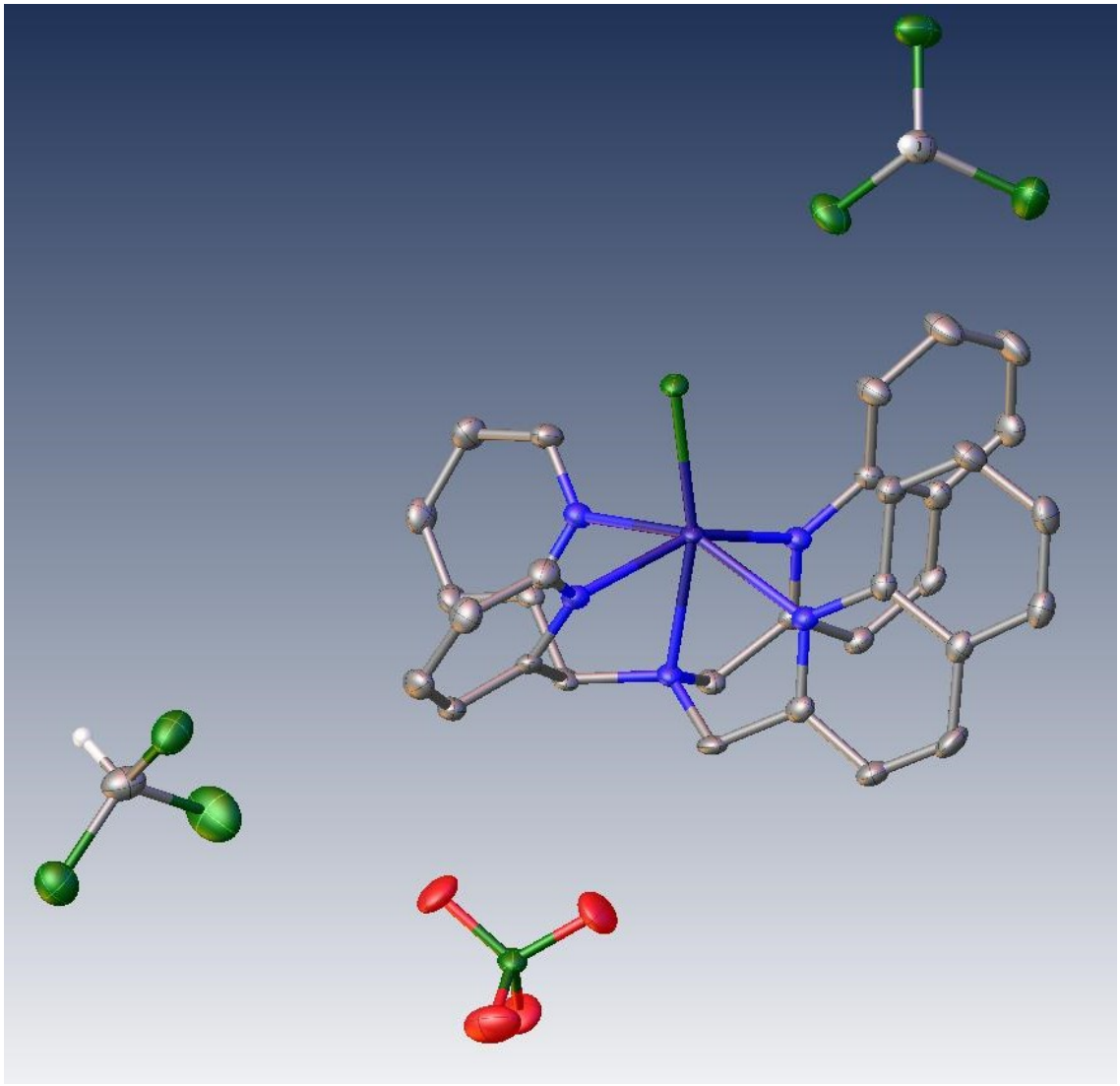


Figure S25. ORTEPdiagram of complex **4,** $[Fe^{II}(2PyN2Q)(Br)]^{+}$ (cationic part of the complex, anion omitted for picture clarity)

2. Synthesis and characterization of iron(II)-complex [Fe^{II}(2PyN2Q)(X)](ClO_4) (5 and **6):**[9]

The above synthesized complexes **3** and **4** were reacted with 2.5 equiv. $NaClO_4$of in MeOH-MeCN solvent and the resulting solution was stirred for 4 hours. This process was repeated for second time. Subsequently the complex solution was dried to get orange powder complex. Then the residue was dissolved in dichloromethane (DCM) to get complex in the solution. The remaining white residue remained at the bottom of the round bottom flask. The solution was kept unstirred for 1 hour to settle down the white precipitate. Then the clear red solution was decanted off and filtered through Whatman filter paper fitted in sintered funnel. The filtrate was dried to get orange powdered [Fe^{II}(2PyN2Q)(X)](ClO_4). The complexes were crystallized from chloroform/hexane and used for halogenations reactions. The anion exchange was carried out for both the complexes **3** and **4**. The obtained perchlorate anion containing complexes **5** and **6** showed the same UV-vis like complexes **3** and **4**. Further the complexes were characterized by X-ray crystallographic study.



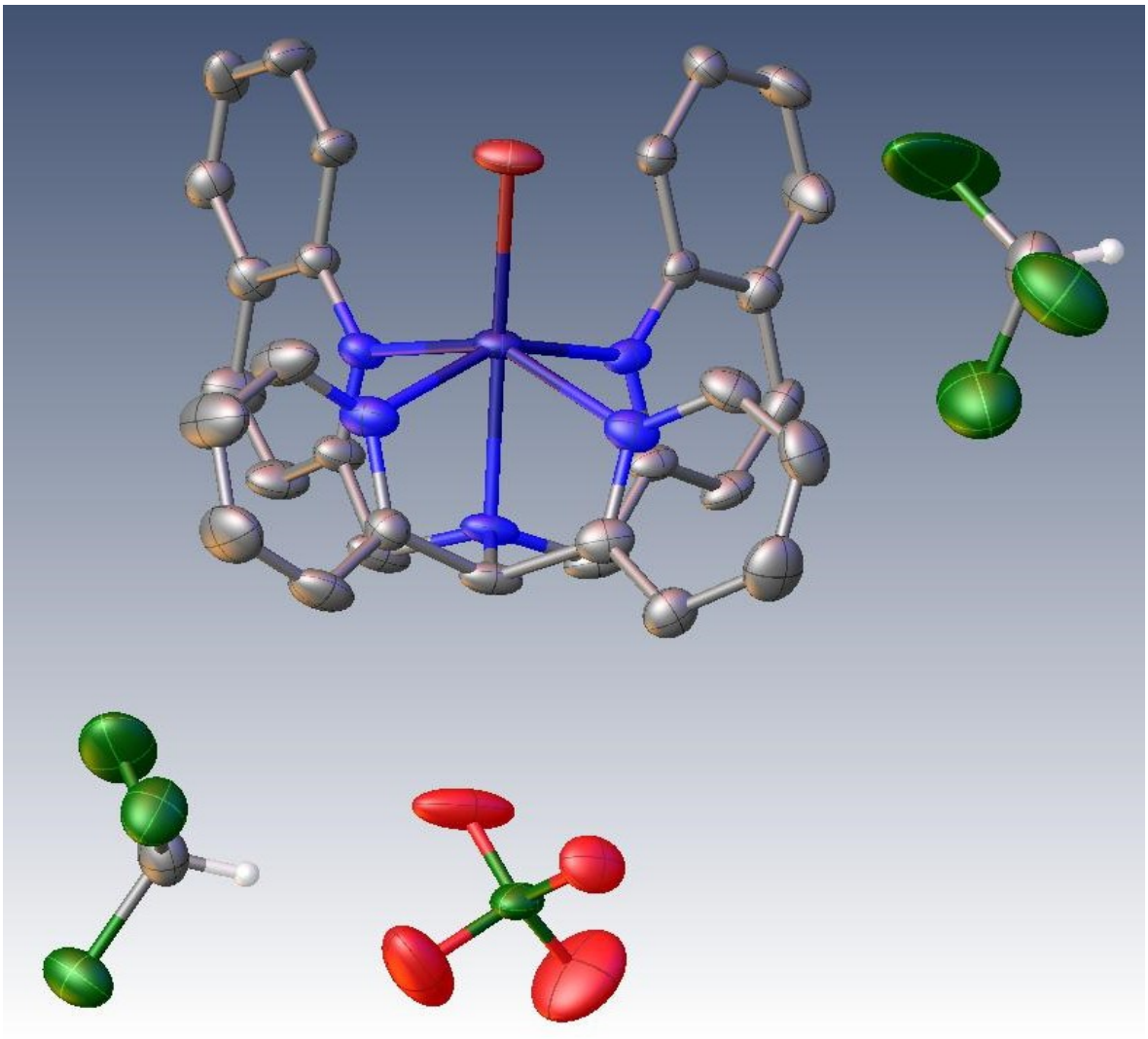


Figure S26. ORTEPdiagram of complex**5**(1516453)and**6** (1516421)**,** [Fe^{II}(2PyN2Q)(X)](ClO_4) (perchlorate anion, solvent $CHCl_3$ in crystal, X= Cl, **5**, Br, **6**)

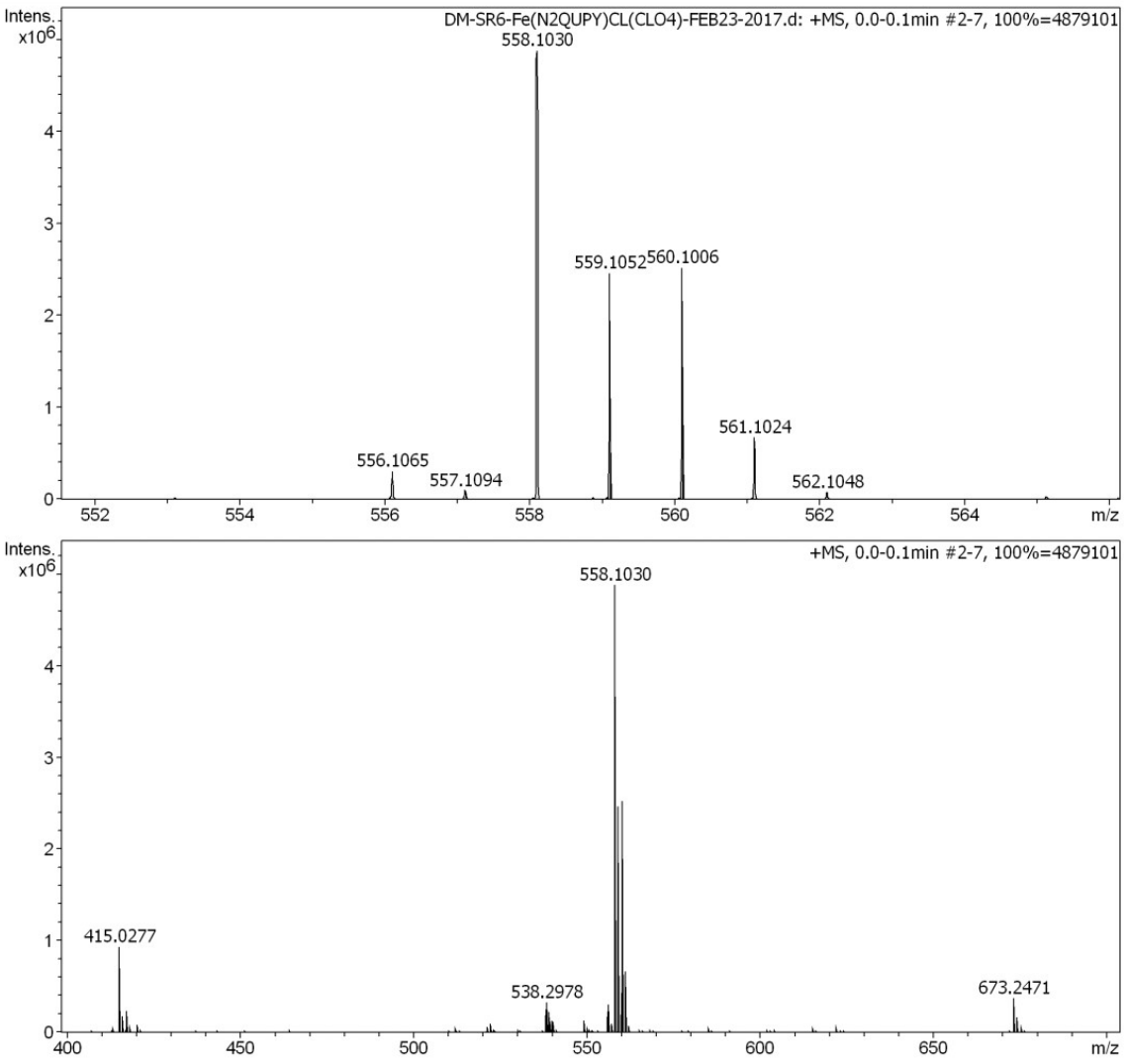


Figure S27. ESI-MS spectra of complex **5**,[Fe^{II}(2PyN2Q)(Cl)](ClO_4), Calculated m/z-558.115, obtained m/z-558.10

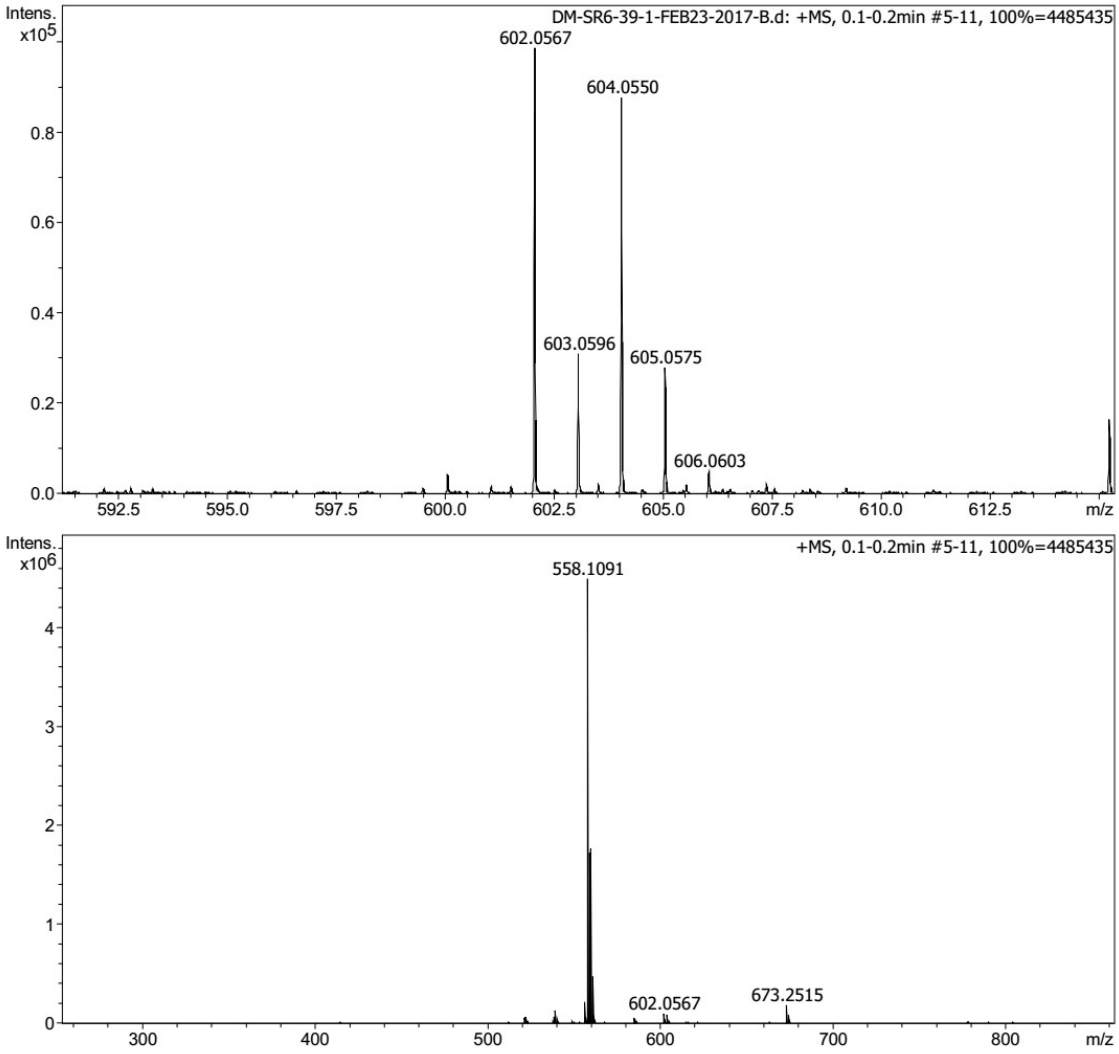


Figure S28. ESI-MS spectra of complex **5**,[Fe^{II}(2PyN2Q)(Cl)](ClO_4), Calculated m/z-558.115, obtained m/z-558.10

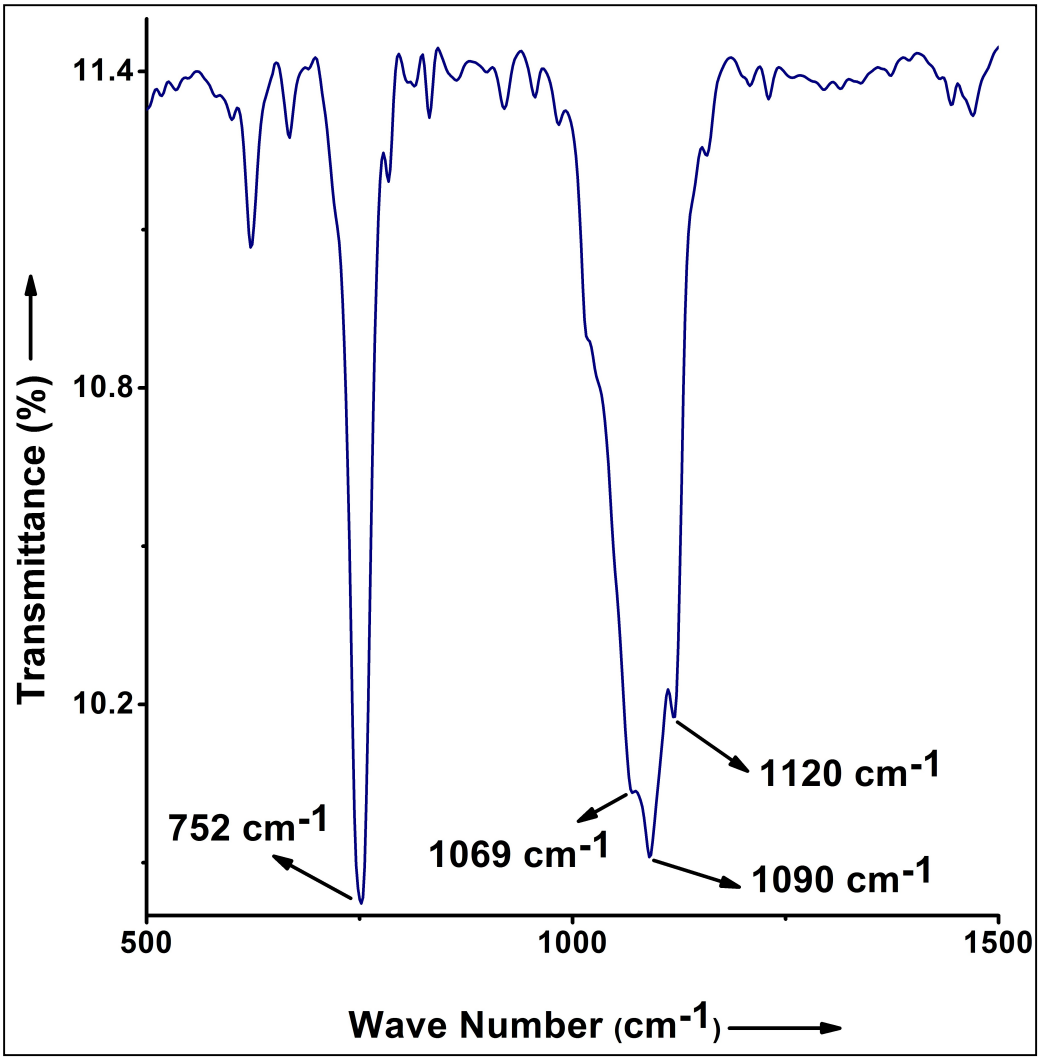


Figure S29. IR spectrum of complex**6,** [Fe^{II}(2PyN2Q)(Br)](ClO_4), [stretching and bending frequencies of ClO_4^- counter anion]

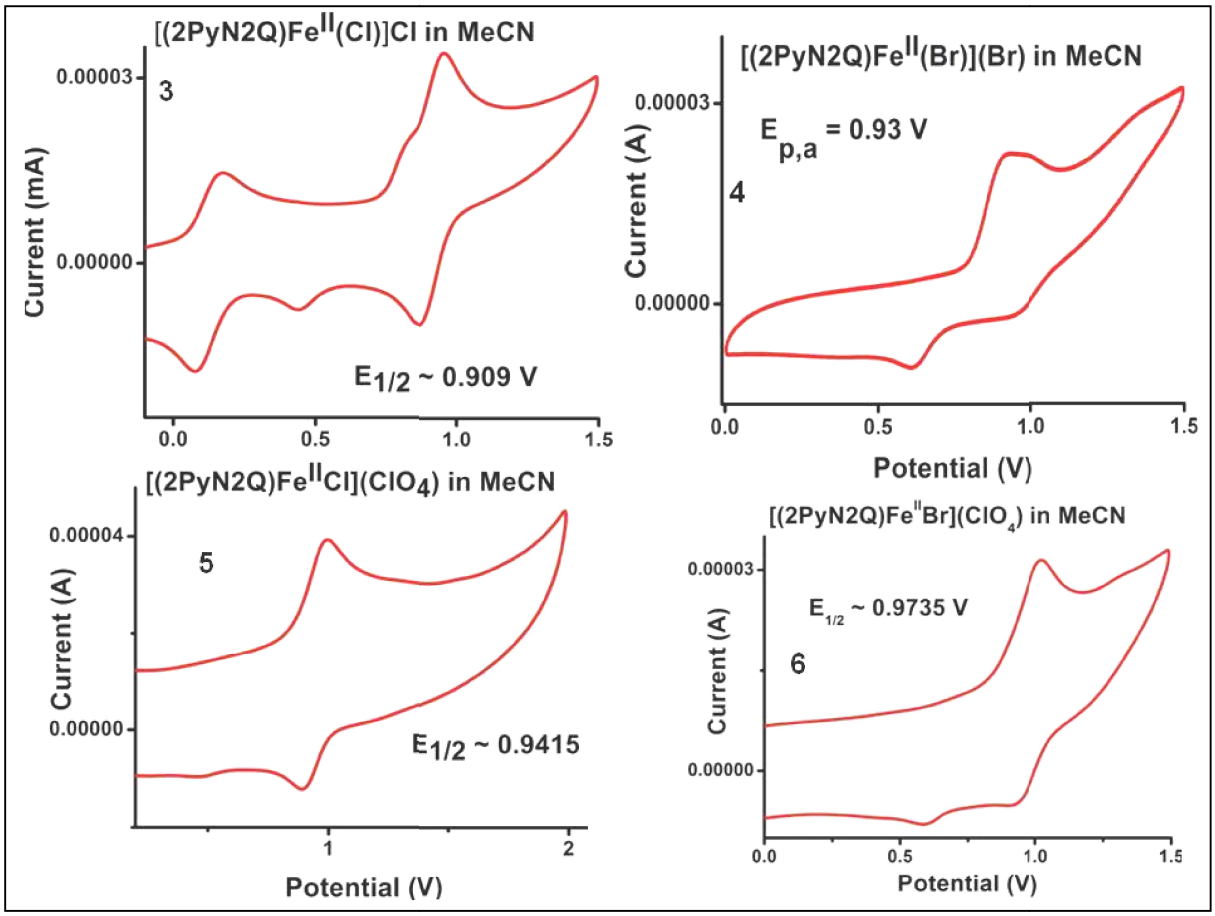


Figure S30. Cyclic Voltametry diagram of complex **3**, **4**, **5** and **6**

2.1. K{Luukkonen, 2017 #612}inetics study

A stock solution of complex 1 (1.21 mM) was prepared in dry acetonitrile inside the glove-box. The kinetics were carried out by taking 2 mL of stock solution of complex **1** and reacting with 1.5 equiv. MesI(OAc)$_2$ or mCPBA. The 2 mL solution was taken in a 3 mL cuvette and subsequently MesI(OAc)$_2$ was added. After addition of oxidant, MesI(OAc)$_2$,within 1-2 minutes of reaction duration the formation of iron(IV)-oxo**2** species gets completed. The complex **2** showed the half-life around 30 min as monitored by UV-vis study. We carried out the kinetics study under pseudo-first order reaction condition (substrates were used >10 equiv. compared to complex concentration). Every kinetics was finished within 10 minutes. The rate constant were determined by following the exponential decay pattern of 770 nm band iron(IV)-oxo.

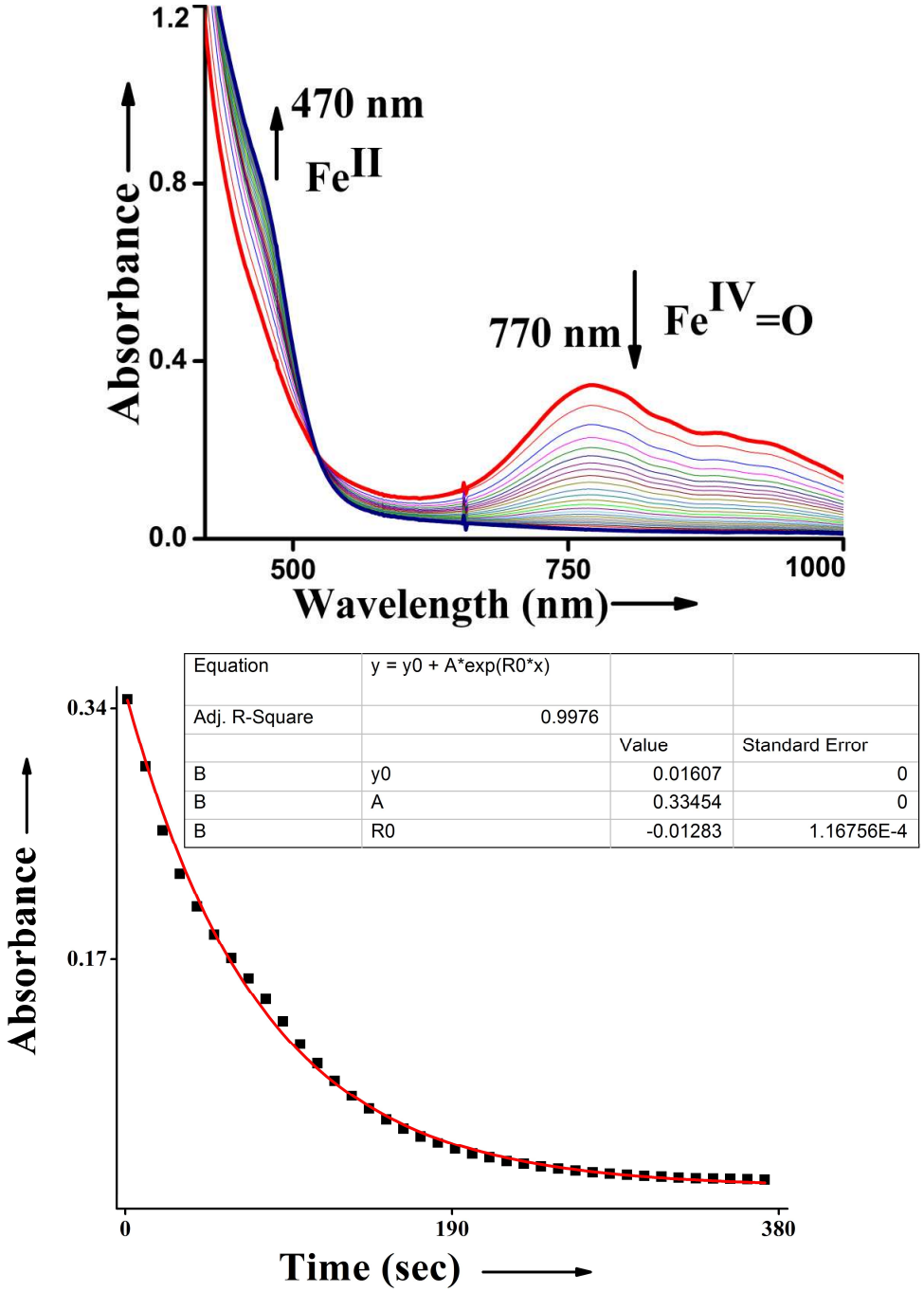
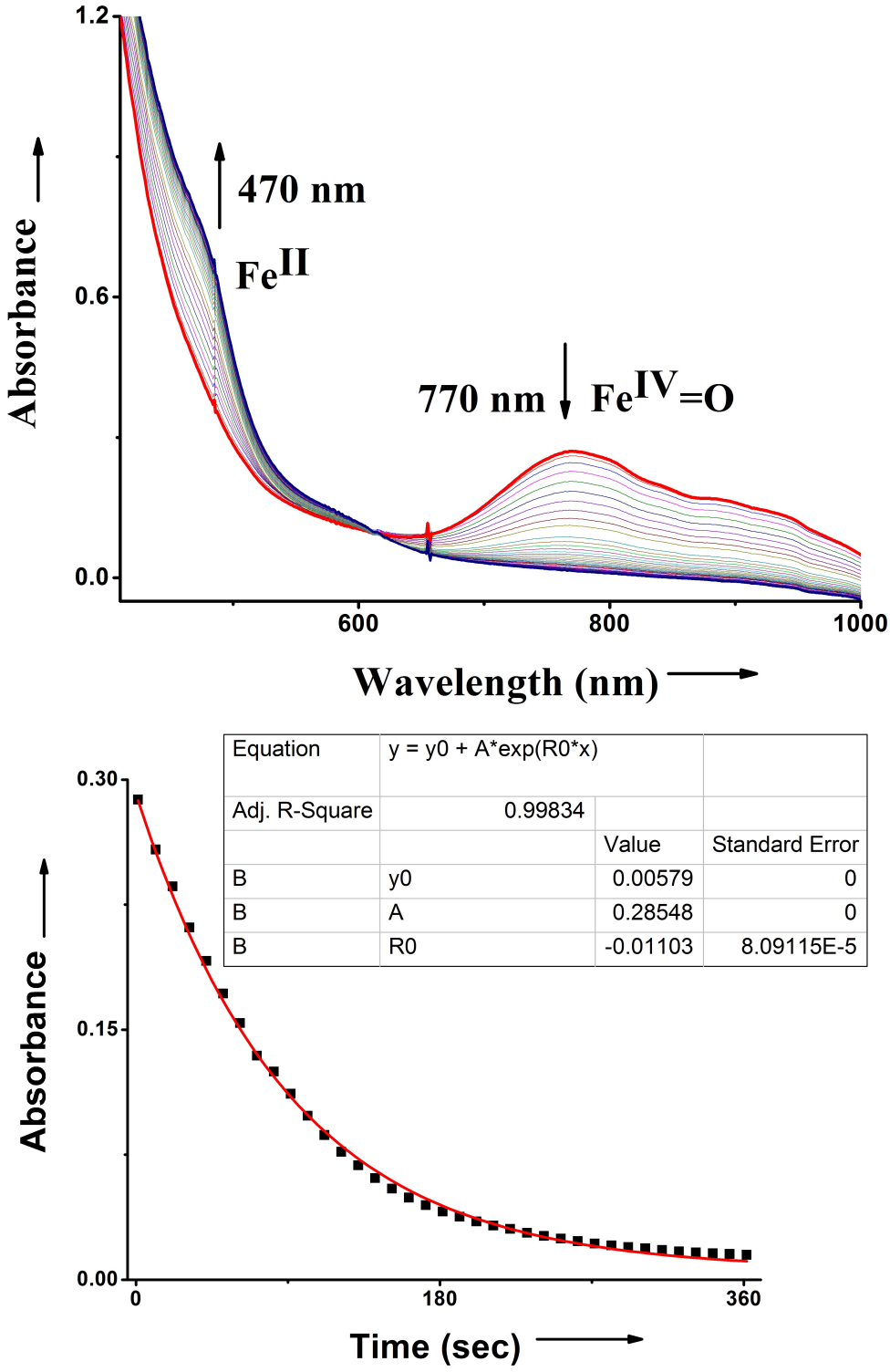


Figure S31. UV-vis change plot during C-H oxidation reaction with triphenylmethane and decay plot at 770 nm band fitted well with exponential curve fitting.



Equation	y = y0 + A*exp(R0*x)		
Adj. R-Square	0.99834		
		Value	Standard Error
B	y0	0.00579	0
B	A	0.28548	0
B	R0	-0.01103	8.09115E-5

Figure S32. UV-vis change plot during C–H oxidation reaction with ethyl benzene and decay plot at 770 nm band fitted well with exponential curve fitting.

2.2. Kinetic study of halide Oxidation by (2PyN2Q)Fe^{IV}=O:

We have carried out kinetics study for halide oxidation by **2** and measured the second order rate constant value for Cl^- and Br^- oxidation by **2**. We found that second order rate constant, k_2 for Cl^- and Br^- oxidation are 221 and 938 M^{-1} s^{-1} respectively. That is complex **2** oxidizes Br^- faster than Cl^- and in turn halide oxidation is much faster process compared to hydrogen atom abstraction (for C–H oxidation of toluene and cyclohexane the second order rate constants are k_2 0.0242 and 0.011 $M^{-1}s^{-1}$ respectively).

Noteworthy, before proceeding for second order kinetics study with lower concentration of halide ions, we have verified that the reaction between **2** and halide ion (at lower conc. of halide ions) is first order *w.r.t* both complex **2** and halide ion. After verifying it we did the second order kinetics study by varying halide ions concentration and keeping constant the concentration of **2**.

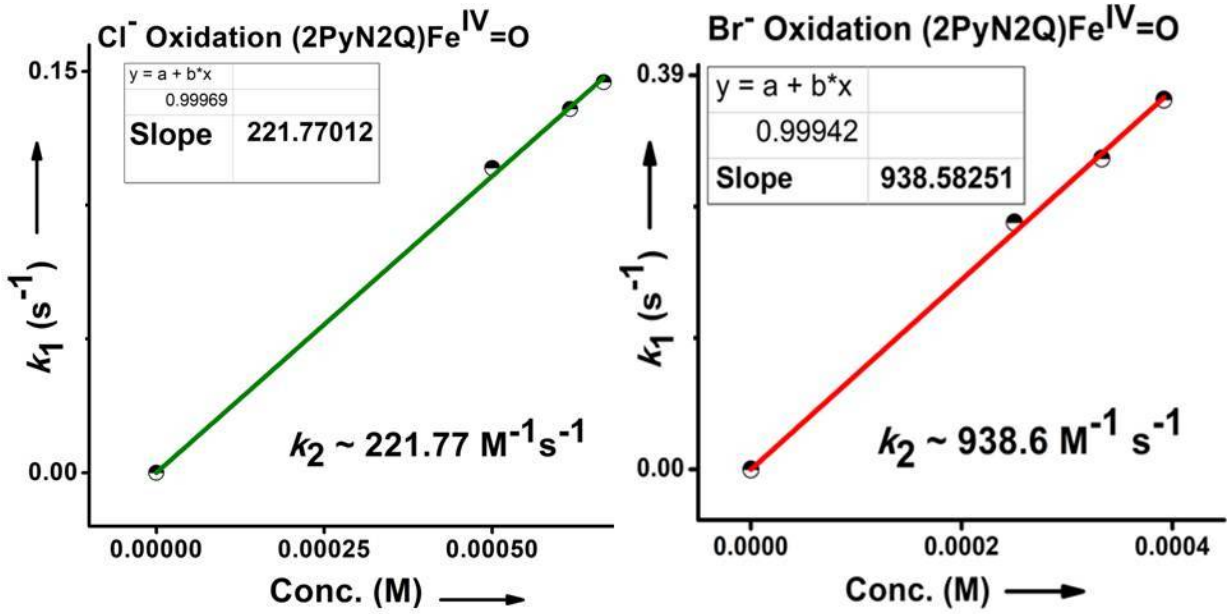
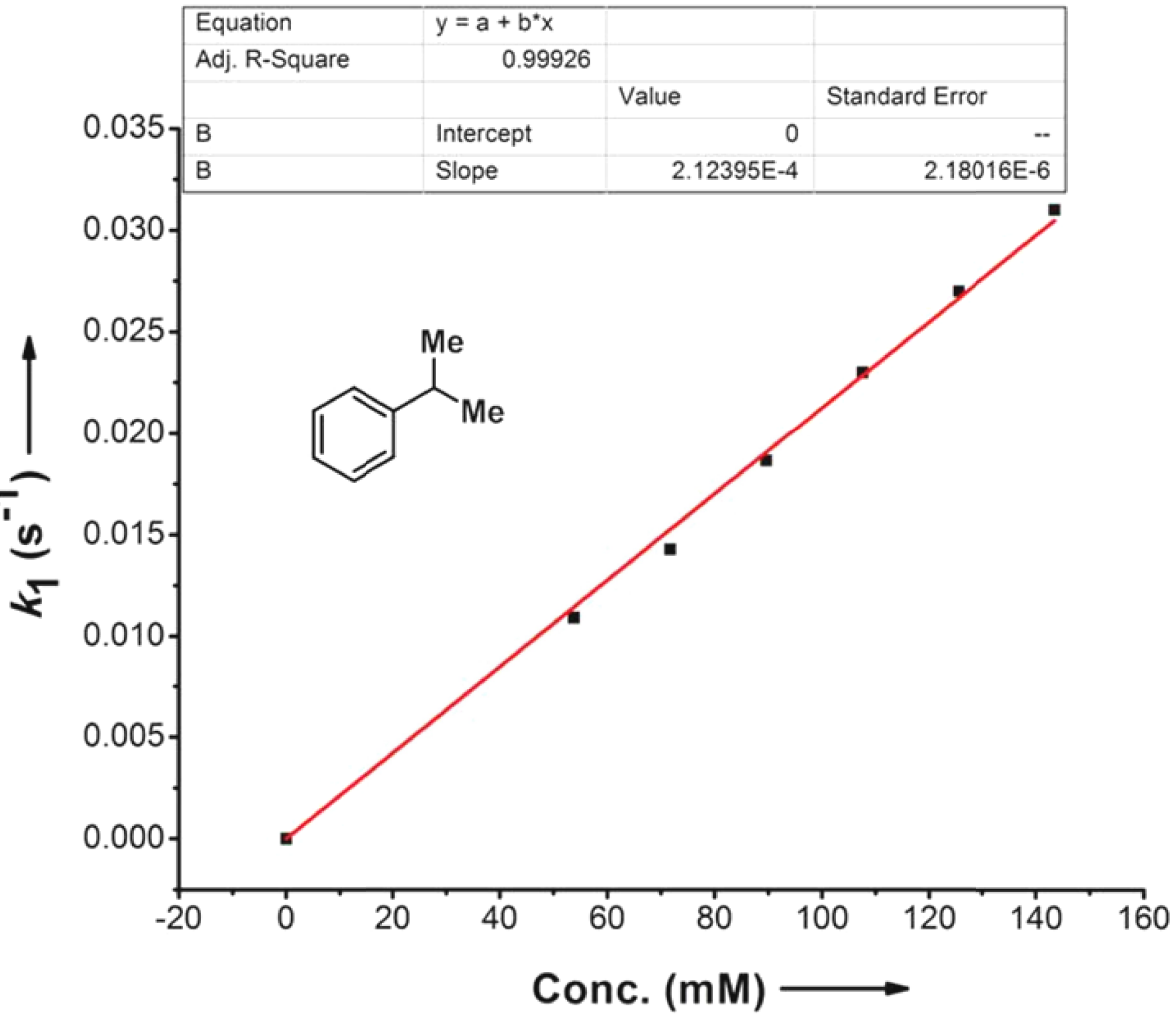


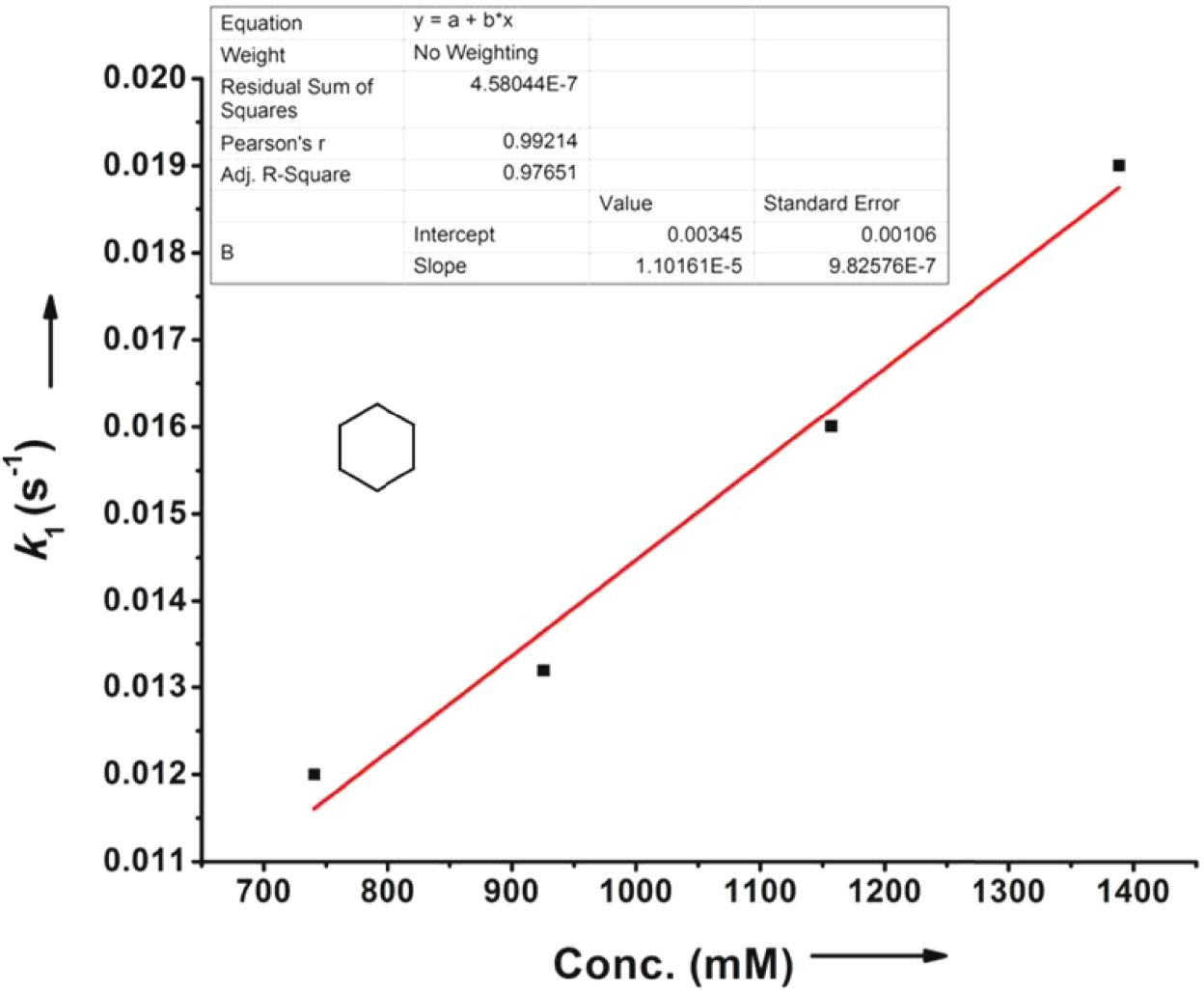
Figure S33. Halide oxidation kinetics plot by **2**

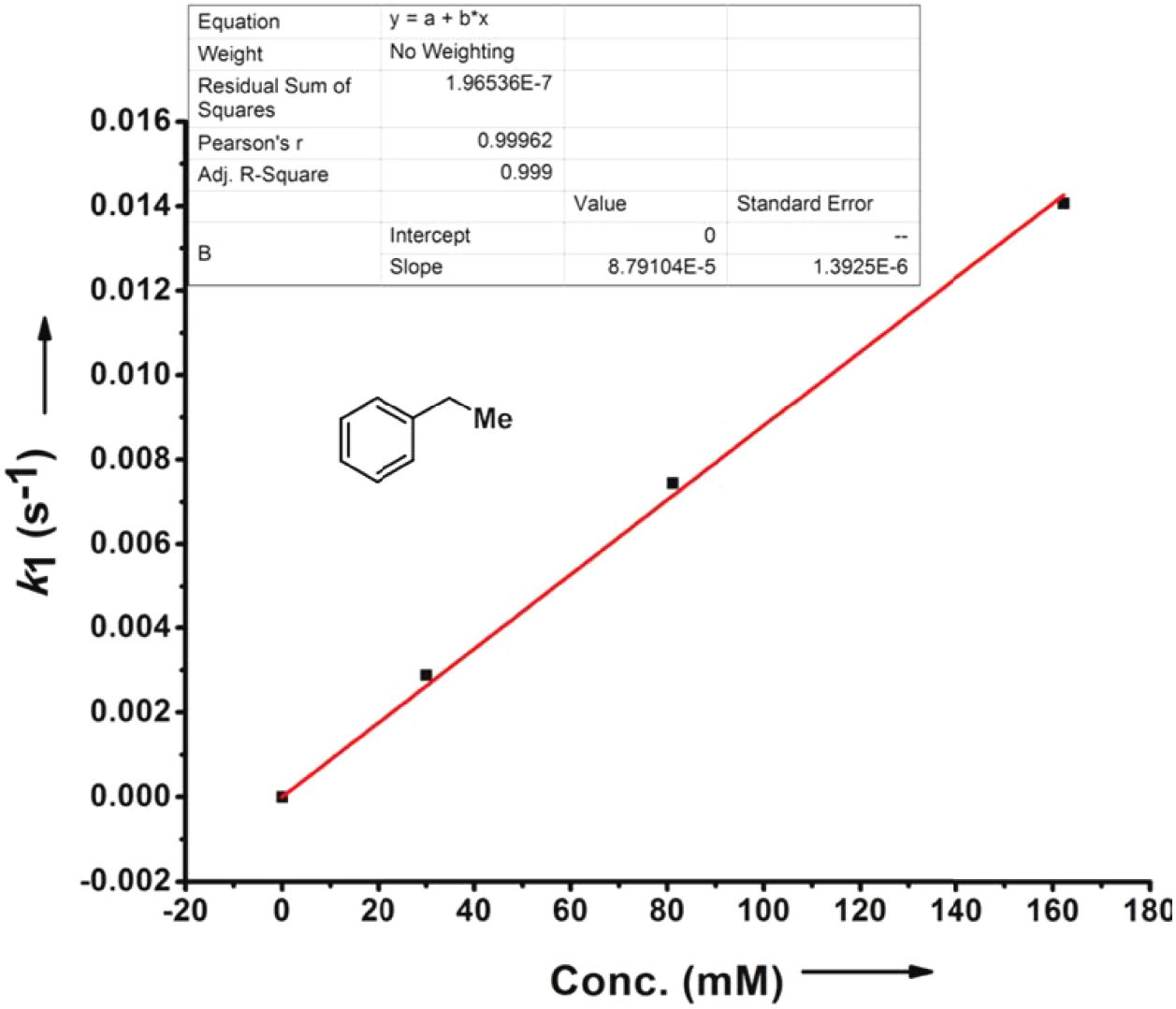
2.3. Correlation diagram: BDE vs logk'2 (Bell-Evans-Polayni plot):

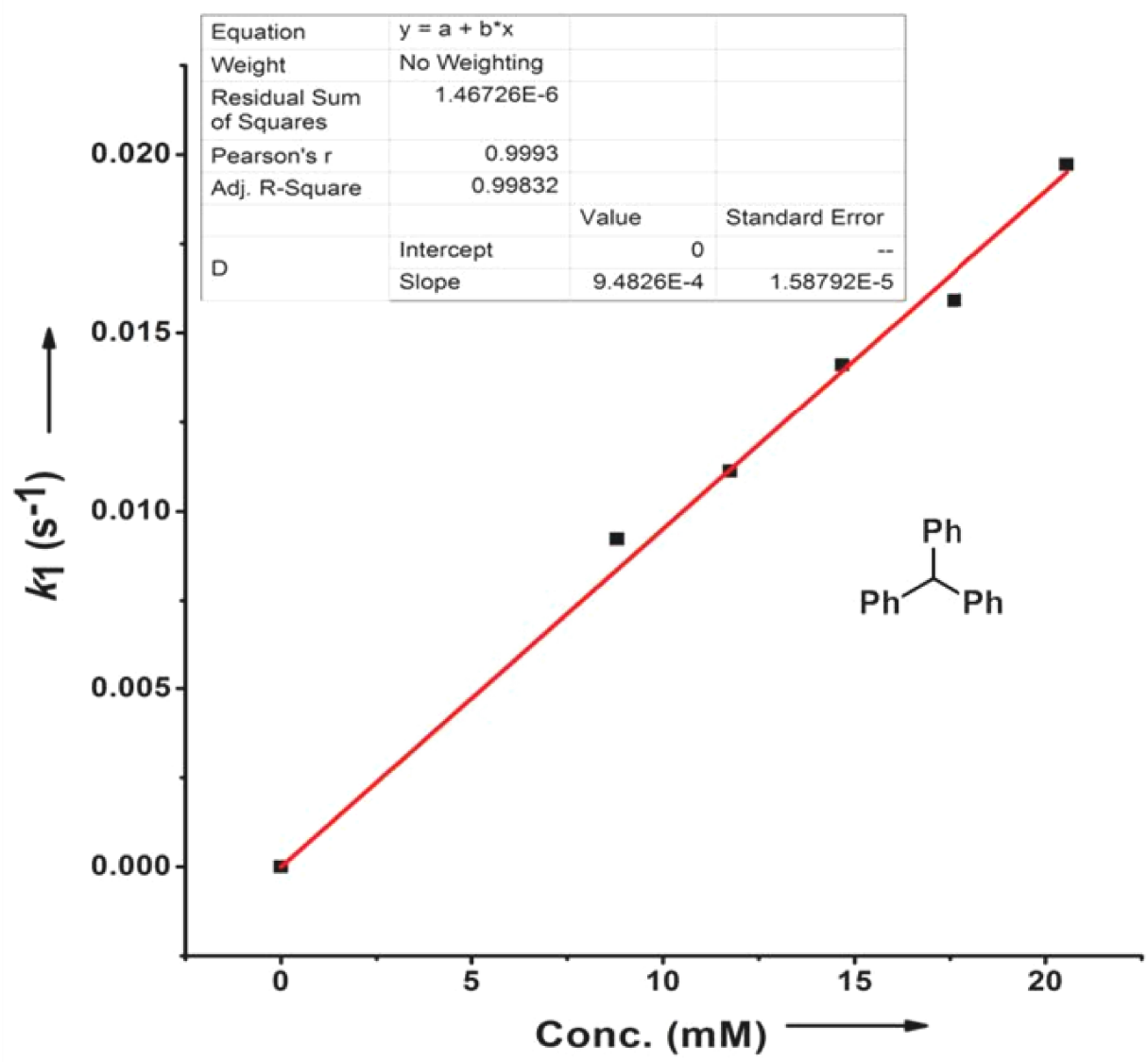
Table S2.

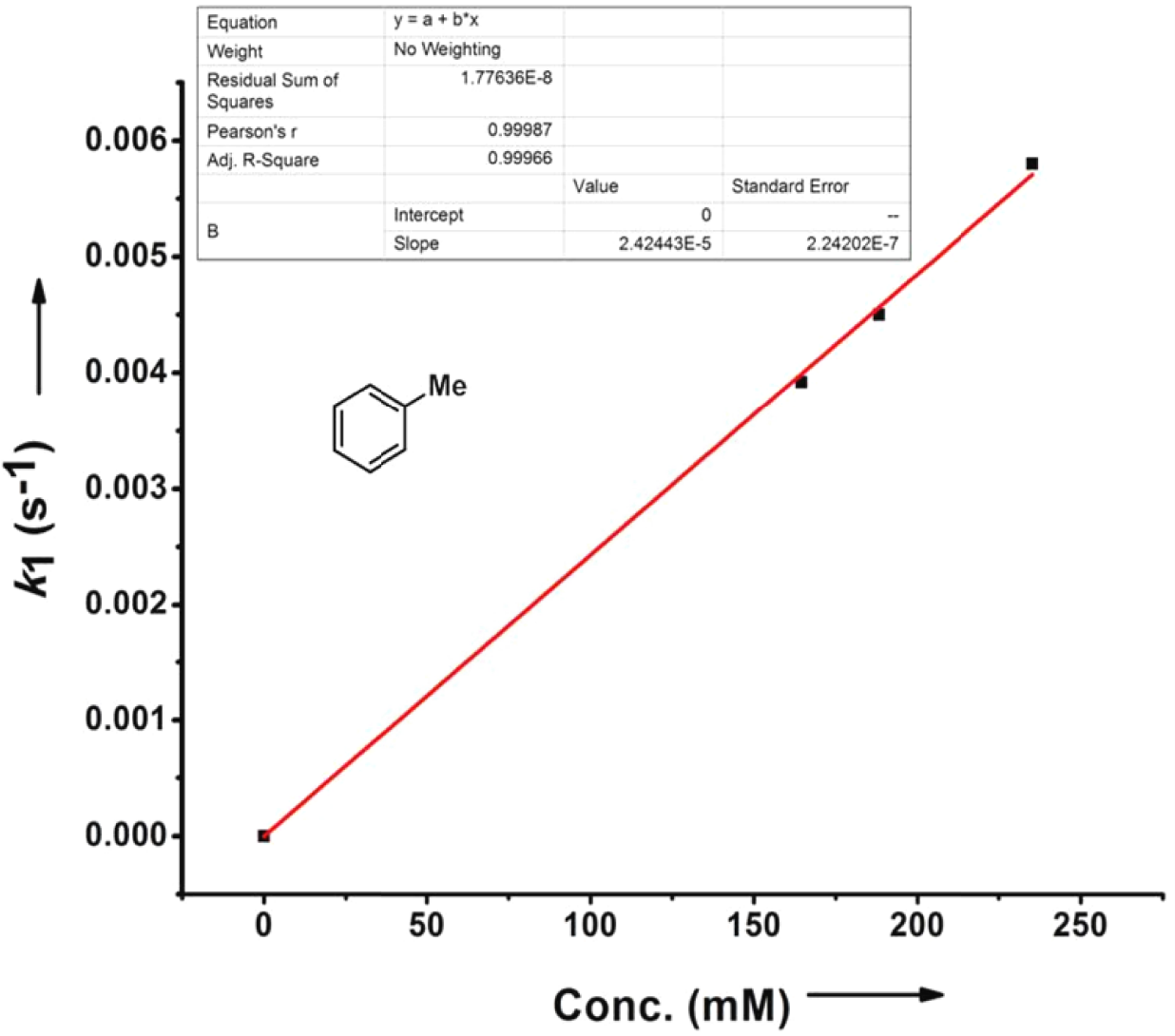
BDE (kcal/mol)	**k_2 ($M^{-1}s^{-1}$)**	**logk'_2**	**Substrate**
81.5	0.948	-0.0232	TPM
85	0.212	-0.673	Cumene
87	0.088	-1.35	Ethylbenzene
90	0.0242	-2.1	Toluene
99.5	0.011	-3.03	Cyclohexane


Equation y = a + b*x
Adj. R-Square 0.99926
Value Standard Error
B Intercept 0 --
B Slope 2.12395E-4 2.18016E-6
Me
Me
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
k_1 (s^{-1})
-20 0 20 40 60 80 100 120 140 160
Conc. (mM)


Equation
y = a + b*x
Weight
No Weighting
Residual Sum of Squares
4.58044E-7
Pearson's r
0.99214
Adj. R-Square
0.97651
Value
Standard Error
B
Intercept
0.00345
0.00106
Slope
1.10161E-5
9.82576E-7
0.020
0.019
0.018
0.017
0.016
0.015
0.014
0.013
0.012
0.011
k_1 (s^{-1})
700
800
900
1000
1100
1200
1300
1400
Conc. (mM)


Equation
y = a + b*x
Weight
No Weighting
Residual Sum of Squares
1.96536E-7
Pearson's r
0.99962
Adj. R-Square
0.999
Value
Standard Error
B
Intercept
0
--
Slope
8.79104E-5
1.3925E-6
Me
k1 (s-1)
Conc. (mM)
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
-0.002
-20
0
20
40
60
80
100
120
140
160
180


Equation
y = a + b*x
Weight
No Weighting
Residual Sum of Squares
1.46726E-6
Pearson's r
0.9993
Adj. R-Square
0.99832
Value
Standard Error
D
Intercept
0
--
Slope
9.4826E-4
1.58792E-5
0.020
0.015
0.010
0.005
0.000
k1 (s-1)
0
5
10
15
20
Conc. (mM)
Ph
Ph
Ph


Equation
y = a + b*x
Weight
No Weighting
Residual Sum of Squares
1.77636E-8
Pearson's r
0.99987
Adj. R-Square
0.99966
Value
Standard Error
B
Intercept
0
--
Slope
2.42443E-5
2.24202E-7
Me
0.006
0.005
0.004
0.003
0.002
0.001
0.000
k1 (s-1)
0
50
100
150
200
250
Conc. (mM)

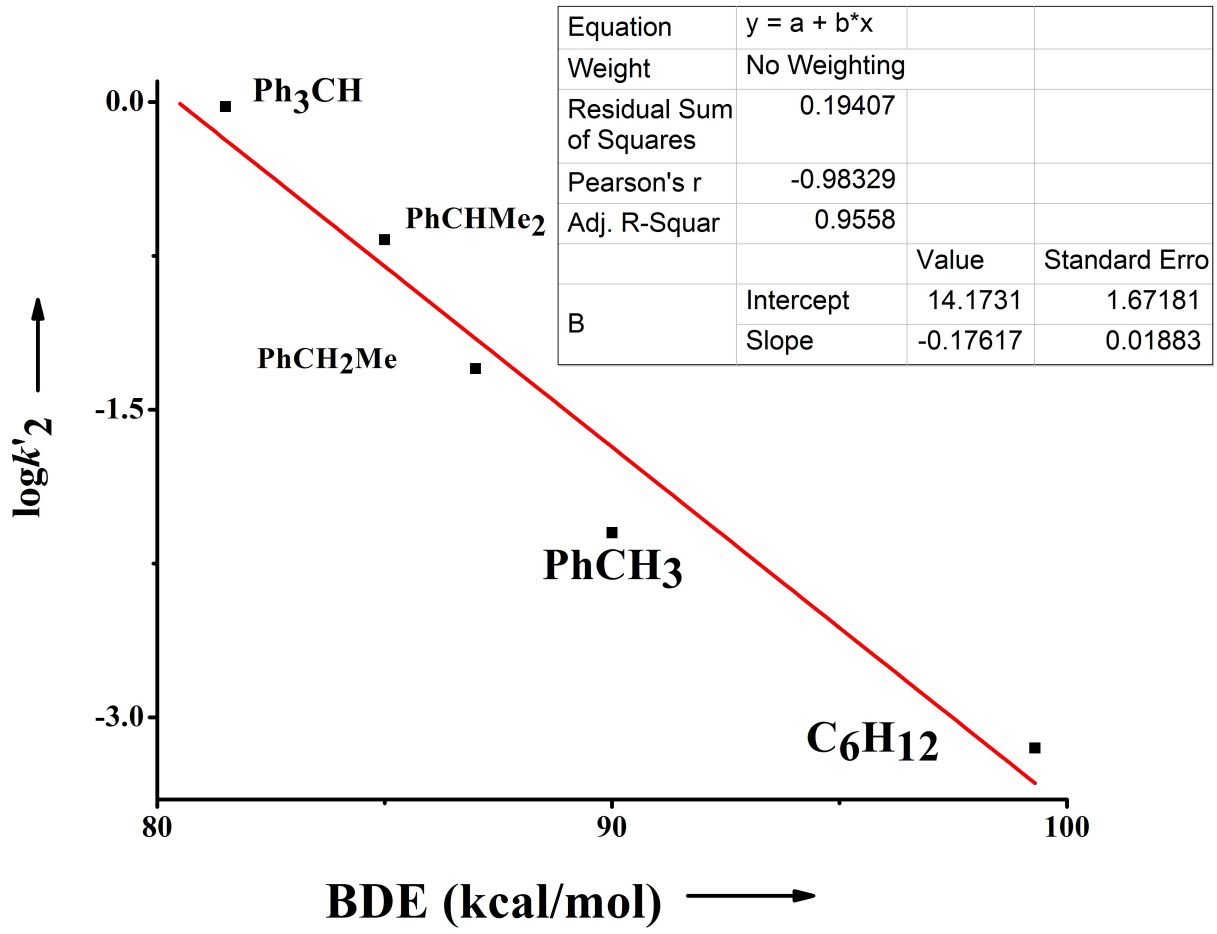


Figure S34. Second order kinetics plot of cumene, cyclohexane, ethylbenzene, triphenylmethane and toluene, for constructing Bells-Evans-Polayni plot[9]

2.4. Kinetic Isotope Effect Study between toluene and toluene-d_8 during C–H oxidation and C–H halogenations:

A stock solution of complex 1 (1.21 mM) was prepared in dry acetonitrile inside the glove-box. The kinetics were carried out by taking 2 mL of stock solution of complex **1** and reacting with 1.5 equiv. MesI(OAc)$_2$ or mCPBA. The 2 mL solution was taken in a 3 mL cuvette and subsequently MesI(OAc)$_2$ was added. After addition of oxidant, MesI(OAc)$_2$,within 1-2 minutes of reaction times the formation of iron(IV)-oxo**2** species gets completed. The complex **2** showed the half-life around 30 min as monitored by UV-vis study. We carried out the kinetics study under pseudo-first order reaction condition (substrates were used >10 equiv. compared to

complex concentration). All the kinetics were finished within 10 minutes. The rate constant were determined by following the exponential decay pattern of 770 nm band iron(IV)-oxo.

During KIE study for C-H halogenations reactions, after generating the complex **2** in cuvette, a solution of complex **4**, [Fe(N2QuPy)(Br)](Br) was added (40 mol% w.r.t. complex **2**) and subsequently substrates were added (toluene and toluene-d_8). The kinetics were monitored by UV-vis study.

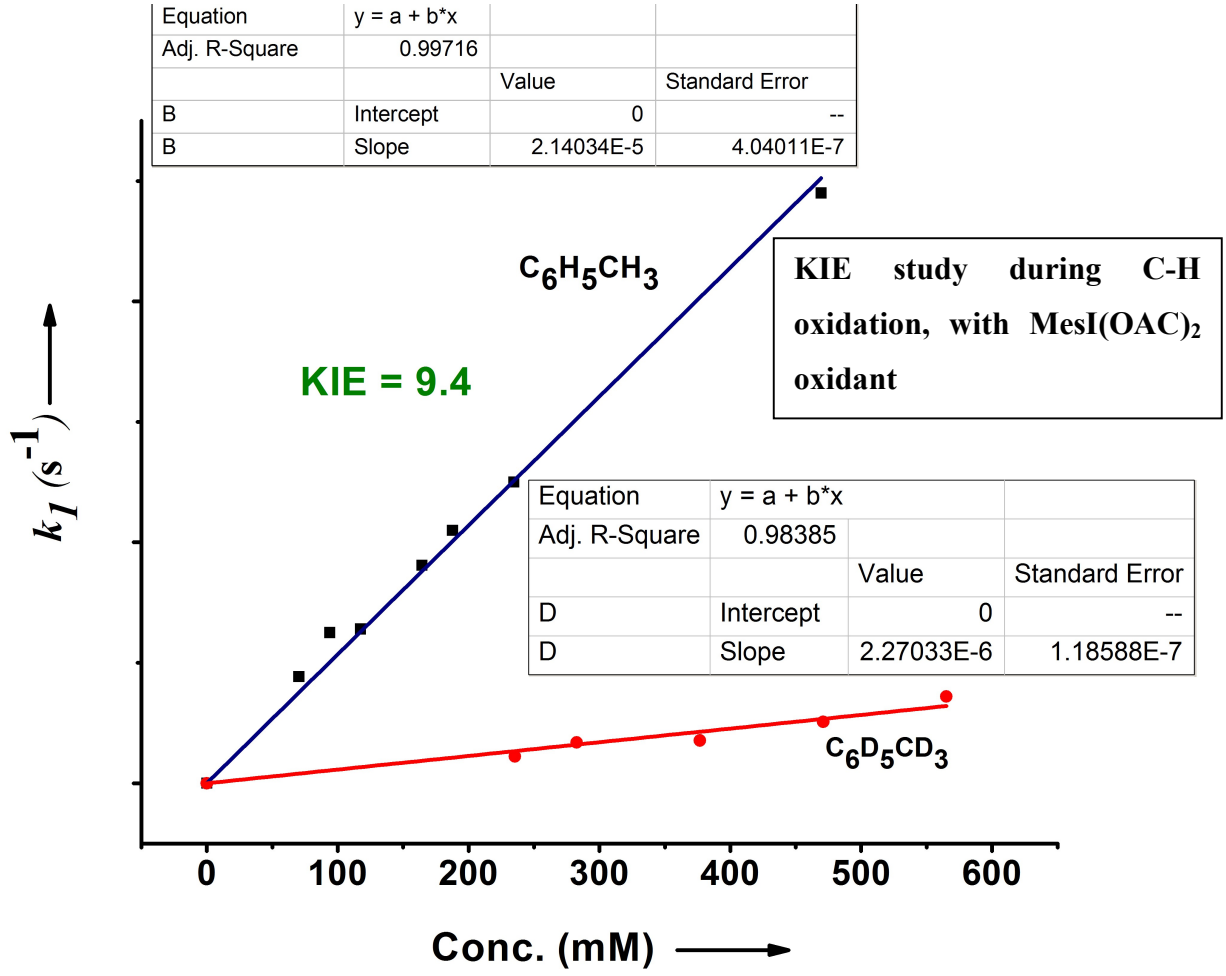
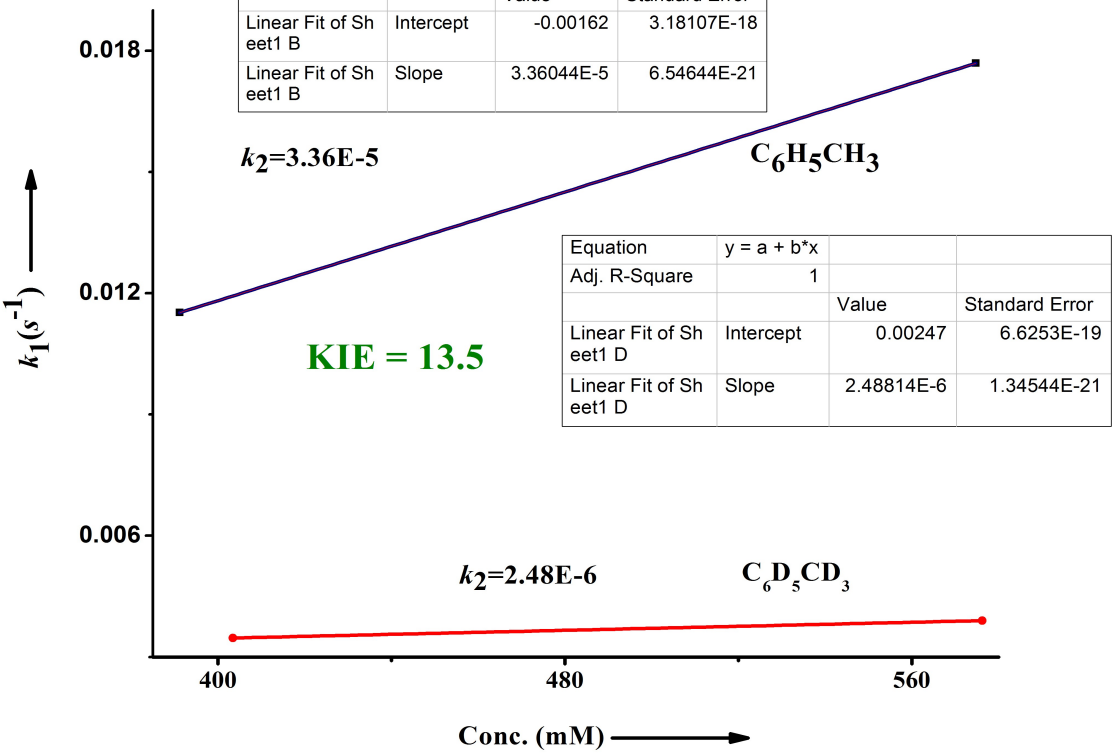


Figure S35. Kinetic isotope effect (KIE) study plot during C–H oxidations

KIE study during C-H bromination, with $MesI(OAC)_2$

Adj. R-Square	1		
		Value	Standard Error
Linear Fit of Sheet1 B	Intercept	-0.00162	3.18107E-18
Linear Fit of Sheet1 B	Slope	3.36044E-5	6.54644E-21



Equation	y = a + b*x		
Adj. R-Square	1		
		Value	Standard Error
Linear Fit of Sheet1 D	Intercept	0.00247	6.6253E-19
Linear Fit of Sheet1 D	Slope	2.48814E-6	1.34544E-21

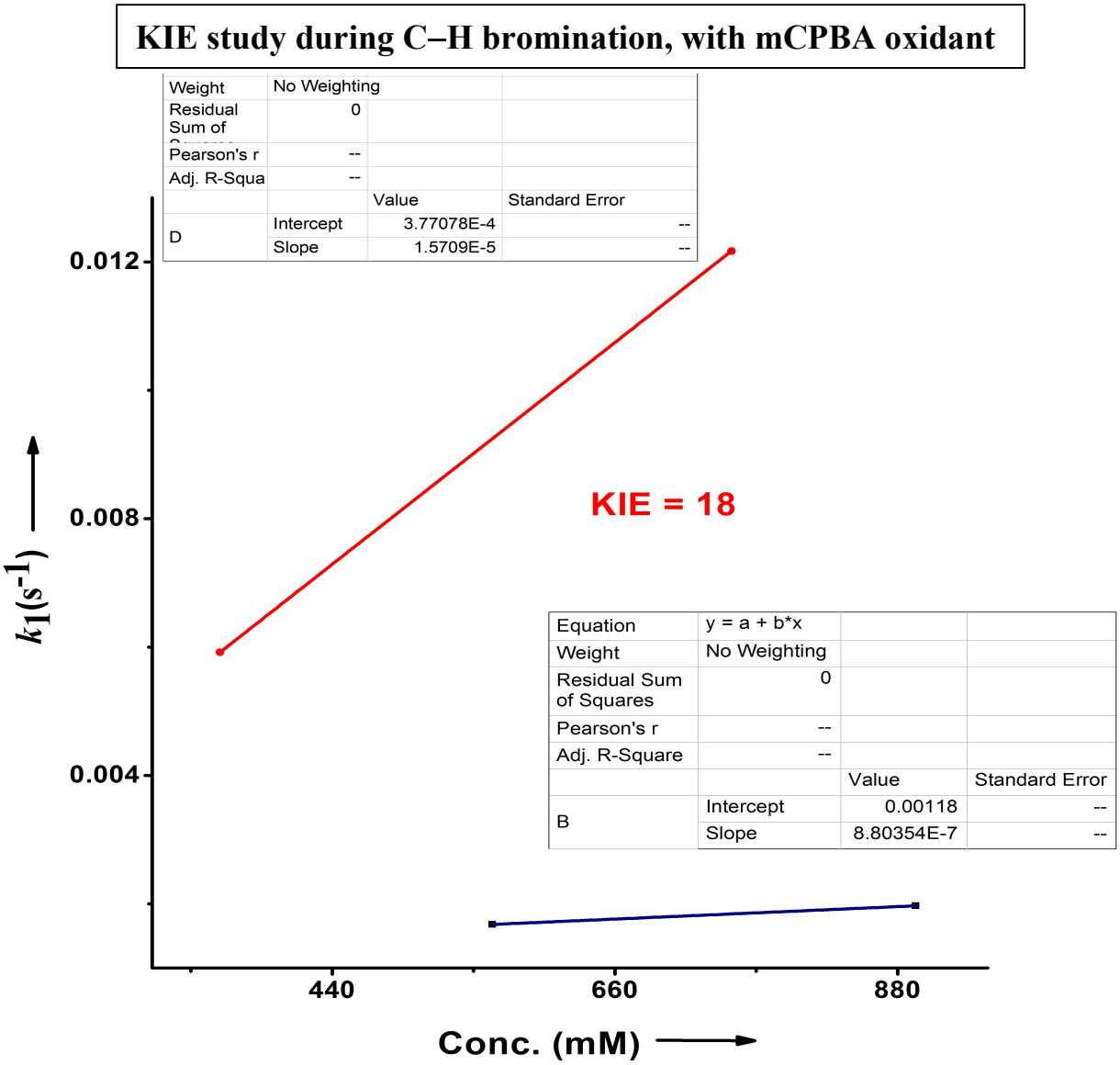
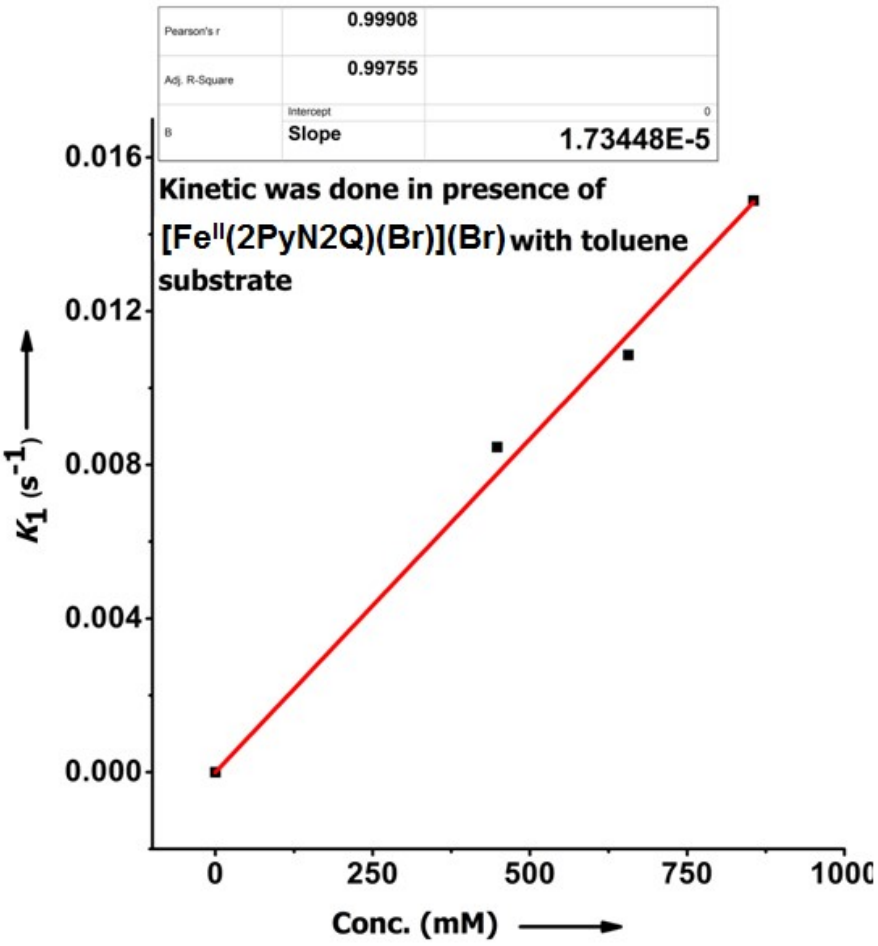


Figure S36. Kinetic isotope effect (KIE) study plot during sp^3 C–H bromination

2.5. Relative kinetics study during reaction with toluene with iron(IV)-oxo complex 2 without iron(II)-bromide complex and with iron(II)-bromide complex

We have carried out the relative kinetics study between iron(IV)-oxo with substrate and iron(IV)-oxo in presence of iron(II)-halide complex with substrate. We have determined second order rate constant of the reaction between iron(IV)-oxo with toluene and the reaction of iron(IV)-oxo with toluene in presence of iron(II)-halide complex. Under both the conditions we have obtained the similar rate constant, k_2 (Figure S34).


Pearson's r
0.99908
Adj. R-Square
0.99755
Intercept
0
B
Slope
1.73448E-5
Kinetic was done in presence of
[Fe^II(2PyN2Q)(Br)](Br) with toluene
substrate
0.016
0.012
0.008
0.004
0.000
K1 (s-1)
0
250
500
750
1000
Conc. (mM)

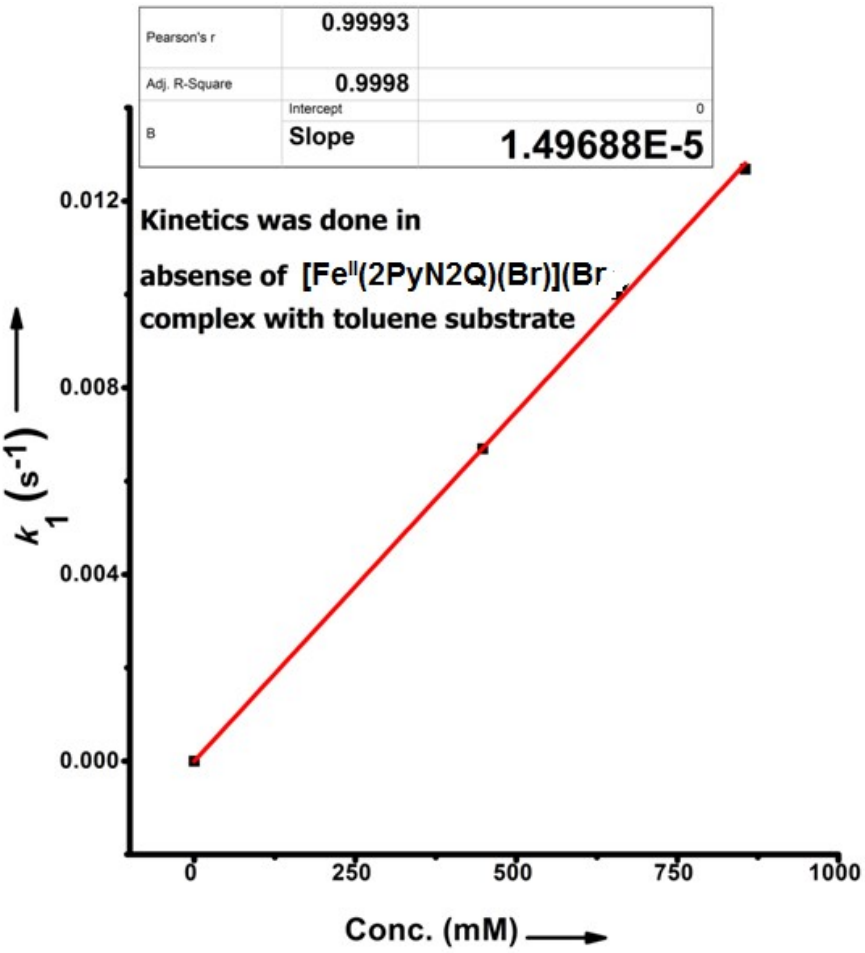
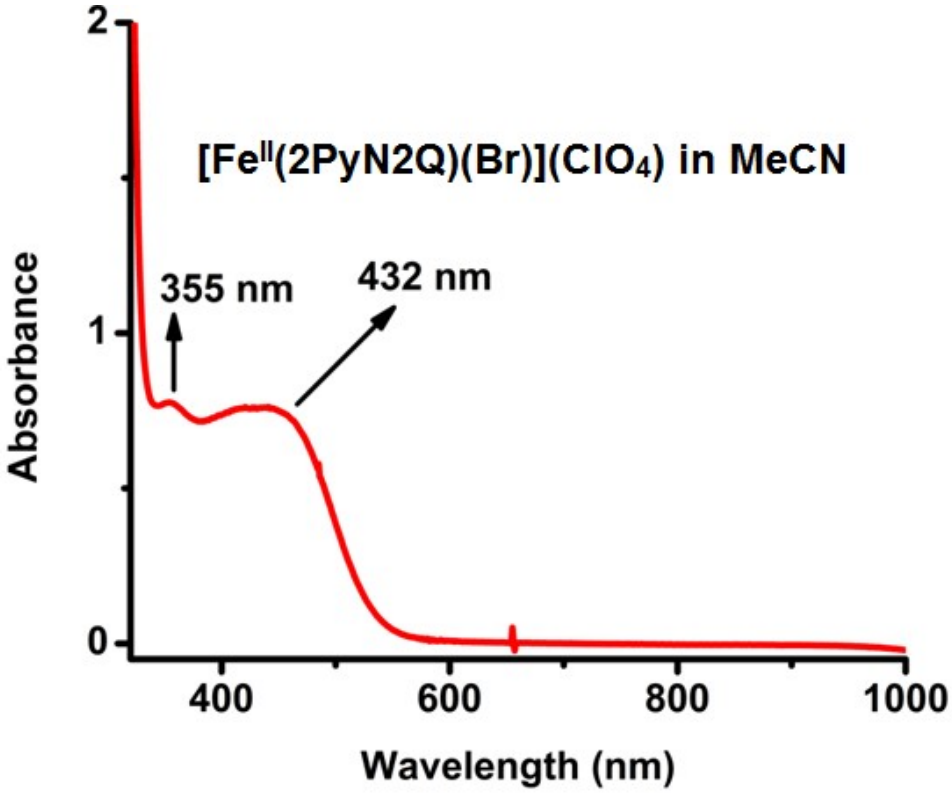
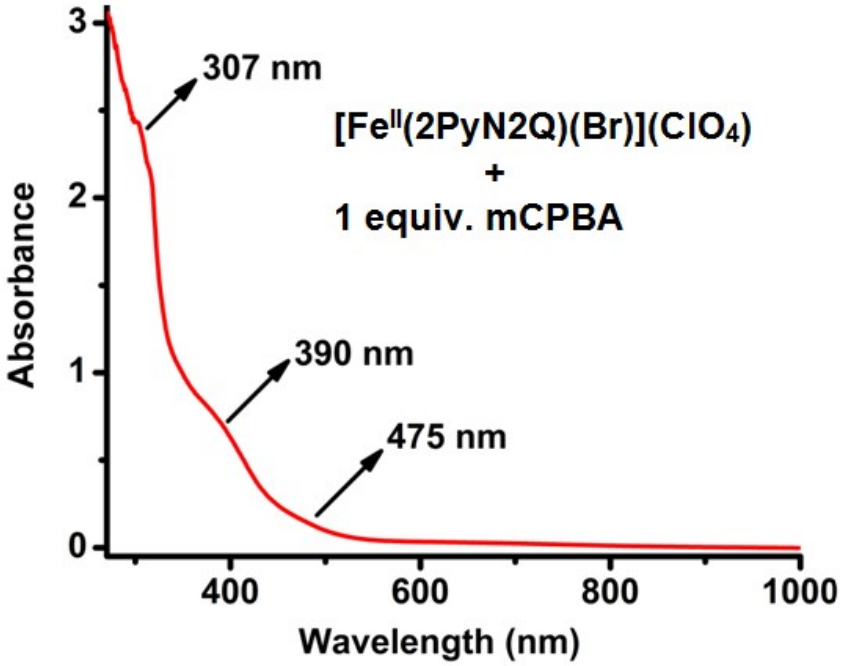


Figure S37. Relative kinetics study during C–H oxidation of toluene with and without iron(II)-bromide complex

2.6. Oxidation of iron(II)-halide complexes with 0.5 or 1 equiv. mCPBA by UV-vis and EPR study





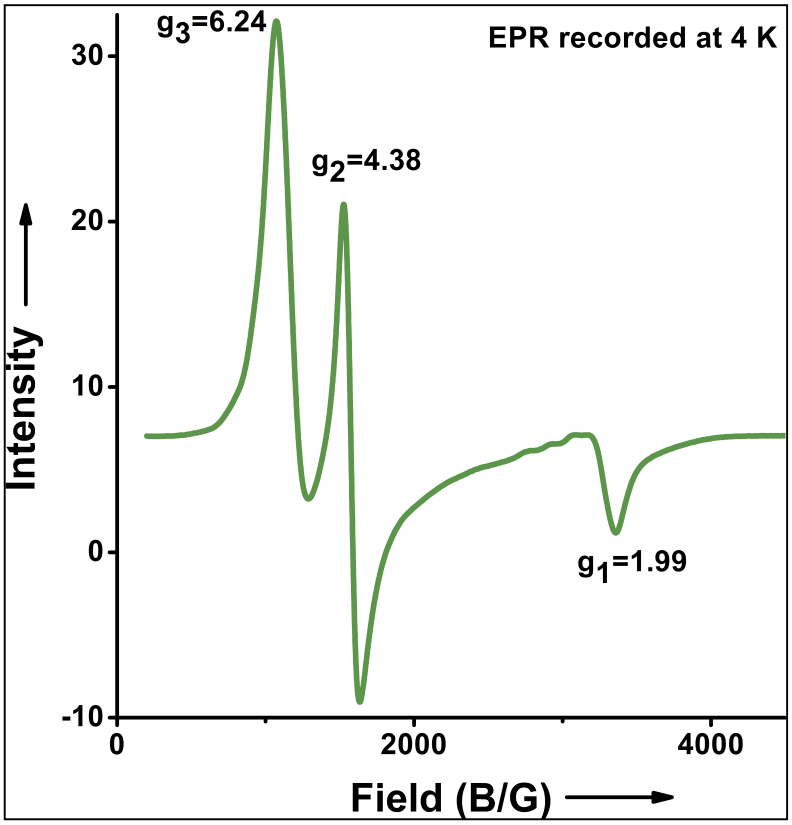


Figure S38. UV-vis change plot of [Fe^{II}(2PyN2Q)(Br)](ClO_4), **6** and then upon addition of 1 equiv. of mCPBA to a solution of (**6**), EPR spectrum showing one electron oxidation of **6** using 0.5 of mCPBA (Temperature 4 k, X-band frequency 9.376 GHz, Modulation Amplitude 4G, Modulation Frequency 100 KHz, Attenuation 22 dB).

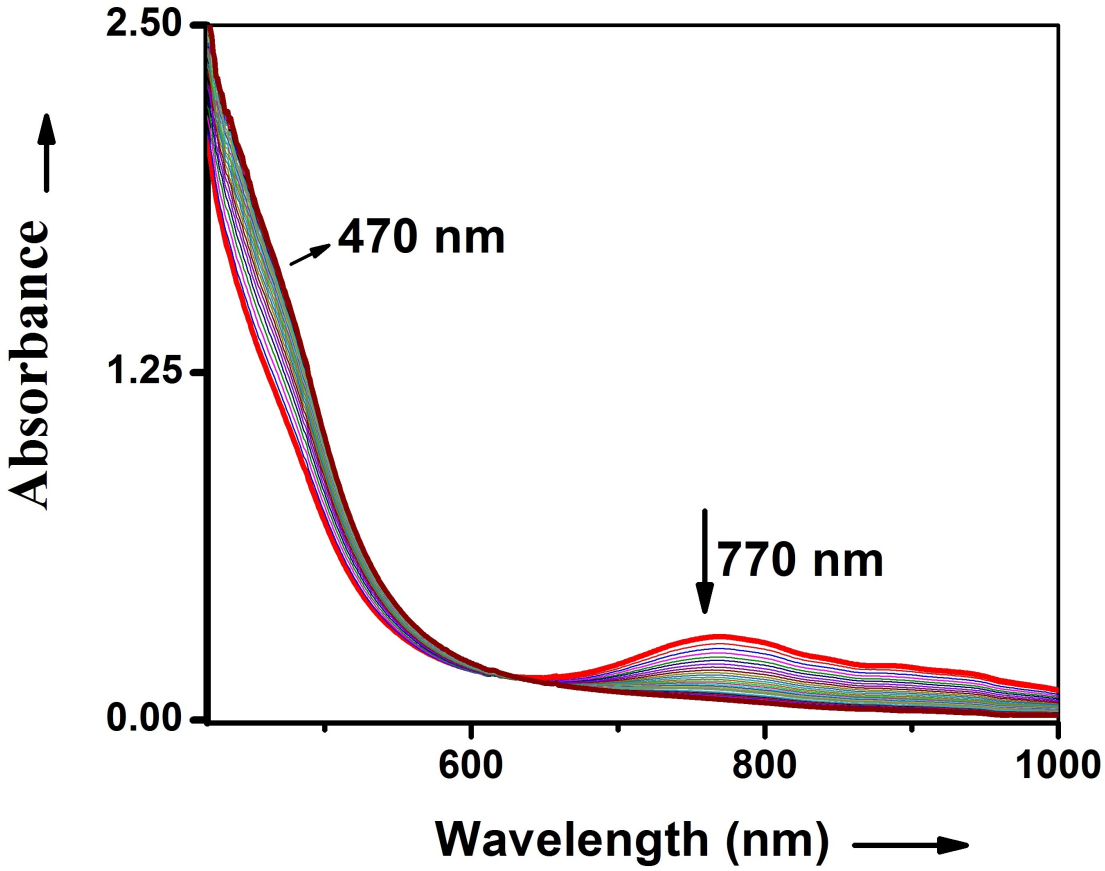


Figure S39. UV-vis change plot of reaction between Toluene and $[FeIV(N2QuPy)O]^{2+}$ in presence of [FeII(N2QuPy)Br](Br)

2.7. Table S3. Comparative rate constant values during C–H oxidation with complex 2, $[Fe^{IV}(2PyN2Q)(O)]^{2+}$

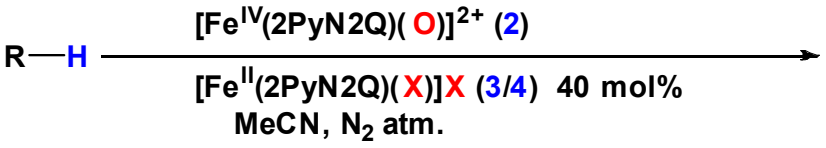
Substrates	K'_2 ($M^{-1}s^{-1}$) ($\times 10^3$) $[Fe(2PyN2Q)(O)]^{2+}$ **2**	K'_2 ($M^{-1}s^{-1}$) ($\times 10^3$) $[Fe(N4Py^{OMe,Me})(O)]^{2+}$	K'_2 ($M^{-1}s^{-1}$) ($\times 10^3$) $[Fe(N4Py)(O)]^{2+}$
Ph_3CH	948.2	nd	37
$PhCH(CH_3)_2$	212.4	10	2
$PhCH_2CH_3$	50.1765	1.15	4
$PhCH_3$	7.44	nd	0.63
$PhCH_2OH$	484.4	22.55	15.1
$Me_2CHCHMe_2$ (2,3-dimethylbutane)	19	nd	0.06
C_6H_{12} (Cyclohexane)	1	nd	0.00416

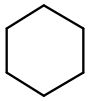
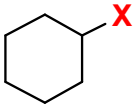
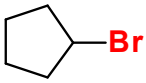
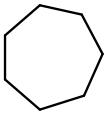
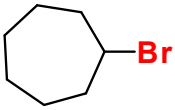
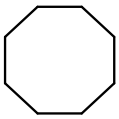
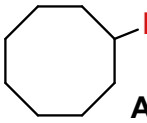
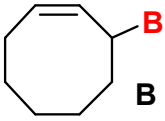
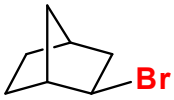
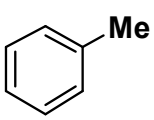
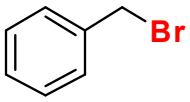
2.8. General procedure for *sp3* C–H halogenations reactions:

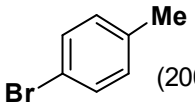
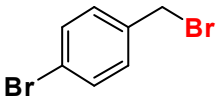
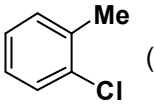
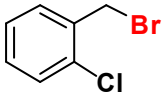
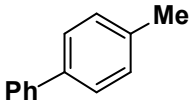
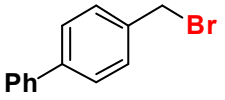
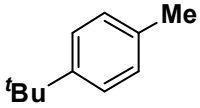
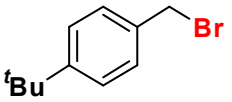
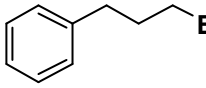
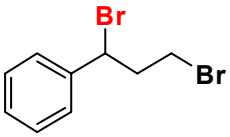
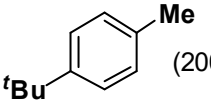
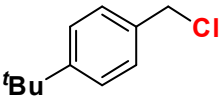
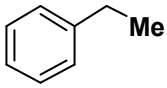
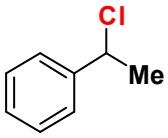
From stock solution of complex **1**, (4mM solution in acetonitrile), 1 mL of solution was taken in a 20 mL vial with a stir bar. Subsequently 2 equiv. of *m*CPBA was added under stirring condition. Immediately a solution of halide complexes **3**,[Fe(2PyN2Q)(Cl)](Cl) or **4**, [Fe(2PyN2Q)(Br)](Br) was added to it (40 mol% *w.r.t.* complex **2** concentration). After that excess amount (>100 equiv.) substrate was added to the reaction mixture and the reaction was stirred for 30 min. Finally the reactions mixtures were analyzed by both GC/GC-Ms. Yield of the

halogenated products were calculated based on calculated area of the standard products.The GC trace and mass spectra are provided in the following section3.

Table S4. Substrate scope for sp^3 C-H halogenations reactions



Entry	Substrate (s)	Product (s)		
1 & 2	 (290 equiv.)		X= Br 90% X= Cl 52%, 10% Cy-OH	*Selective*
3	 (300 equiv.)		52%[a]	*Selective*
4	 (300 equiv.)		60%	*Selective*
5	 (300 equiv.)	 + 	A : B 2.27 : 1 65%	*Selective*
6	 (200 equiv.)		50%[a]	*Selective*
7	(220 equiv.) 		97%	*Selective*

8	 (200 equiv.)		60% *Selective*
9	 (200 equiv.)		54%[a]
10	 (50 equiv.)		50% *Selective*
11	 (200 equiv.)		60% *Selective*
12	 (50 equiv.)		42% *Selective*
13	 (200 equiv.)		56% *Selective*
14	 (50 equiv.)		54%[a]

[a]~5% hydroxylation product *w.r.t.* **3** and **4** were detected:Yields are calculated *w.r.t.* used mol% of complex **3** and **4**, Equivalent amount of substrate used,w.r.t. complex **1** in the reaction is given in the parenthesis

2.9. General procedure for*sp3*C–H oxidation reactions:

From stock solution of complex **1**, (2.43mM solution acetonitrile solution), 1.5 mL of solution was taken in a 20 mL vial with stir bar. Subsequently 1.5 equiv. of $MesI(OAc)_2$ was added under stirring condition. After 1 minutes excess amount (>100 equiv.) substrate was added to the reaction mixture and the reaction was stirred for 30 min. Finally the reactions mixtures were analyzed by GC/GC-Ms. Yield of the hydroxylation products were calculated based on calculated area of the standard products. The GC-Ms spectra are provided in the following section 3. During C-H oxidation reaction of ethyl benzene, it was passed through the activated alumina column. Further ethylbenzene during C–H oxidation reaction using $MesI(OAc)_2$ as

oxidant provided 1-phenylethanol and 1-phenylethyl acetate. During the C-H oxidation reactions of ethyl benzene using $MesI(OAc)_2$ as an oxidant, we had detected 1-phenyl ethanol (34%) and 1-phenylethyl acetate (26%) and 5% acetophenone. We presumed that 1-phenyl ethylacetate might be coming from the reaction between 1-phenyl ethanol and $MesI(OAc)_2$. Further we have carried out control reaction between 1-phenylethanol and $MesI(OAc)_2$ and reaction of 1-phenylethanol with iron(IV)-oxo. None of these cases we did not detect the formation of 1-phenyl ethyl acetate. The formation of 1-phenylethylacetate during the reaction with ethyl benzene could occur *via* reaction between cage escaped radical and acetoxy radical ($^{\bullet}$OAc) generated from $MesI(OAc)_2$ during the reaction. This observation suggests the dissociation of the radical from the solvent cage.

2.10. General procedure for ^{18}O labeling study for *sp3* C–H oxidation reactions:

To solution of 3mM of complex 1.5 equiv. of $MesI(OAc)_2$ was added to generate the iron(IV)-oxo complex **2**inside glove box. Subsequently 50 μL of $H_2{}^{18}O$ was added to this solution. The resulting solution was kept at -35 °C freeze inside the glove box for 30-40 minutes sothat all the iron(IV)-oxo complex **2** gets labeled with ^{18}O. Subsequently the solution was taken out from the freeze and substrates like ethylbenzene, cumene were added in the different sets of reactions. After completion of the reactions the reactions mixture were analyzed by GC-MS in order to detect the percentage of ^{18}O labeled in the products. Interestingly labeling experiment with ethylbenzene provided 86% ^{18}O enriched 1-phenylethanol. The high percentage of ^{18}O labeling in the product occurred due to radical rebound pathway.

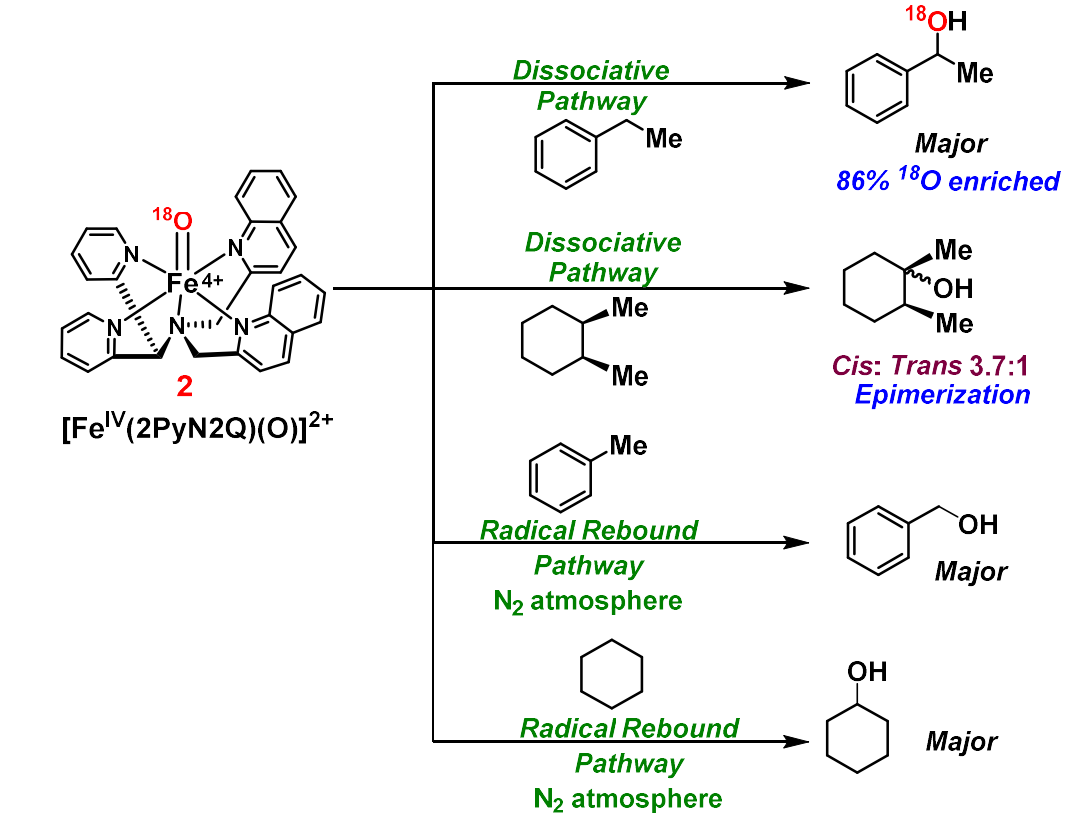


Figure S40. C–H oxidations reactions by complex **2**

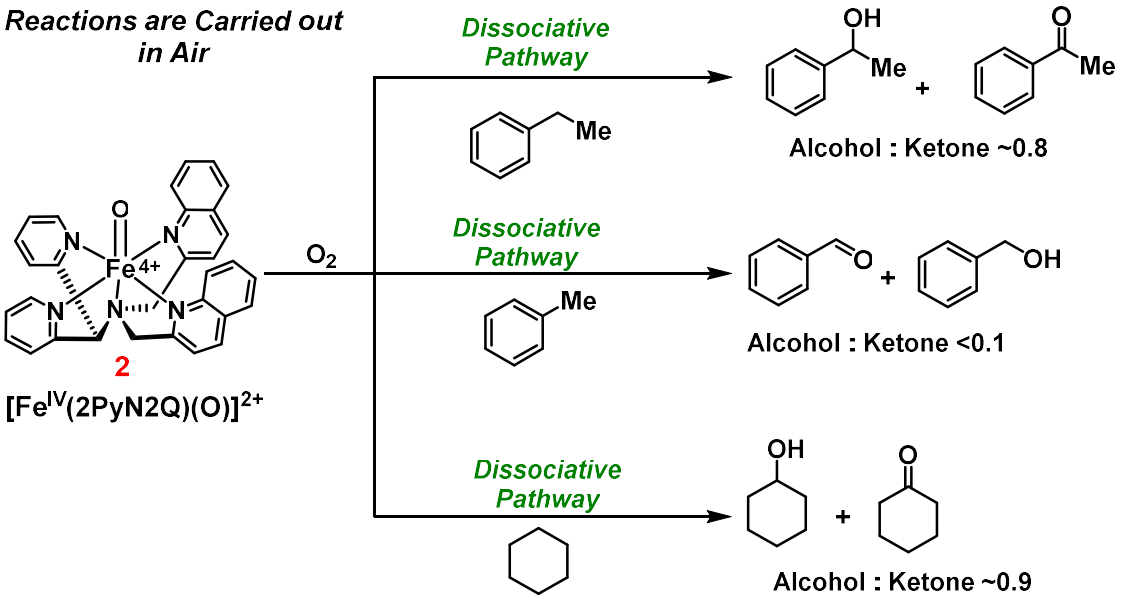


Figure S41. C–H oxidation reaction by complex **2** in air atmosphere

2.11. Radical trapreactions using CCl_3Br:

From stock solution of complex **1**, (2.43 mM solution acetonitrile solution), 1.5 mL of solution was taken in a 20 mL vial with stir bar. Subsequently 1.5 equiv. of $MesI(OAc)_2$/*m*CPBA was added under stirring condition. After 1 minutes excess amount CCl_3Br (>700 equiv.) (250 μL and subsequently substrate (100 equiv.) was added to the reaction mixture and the reaction was stirred for 30 min. Finally the reactions mixtures were analyzed by GC/GC-Ms.

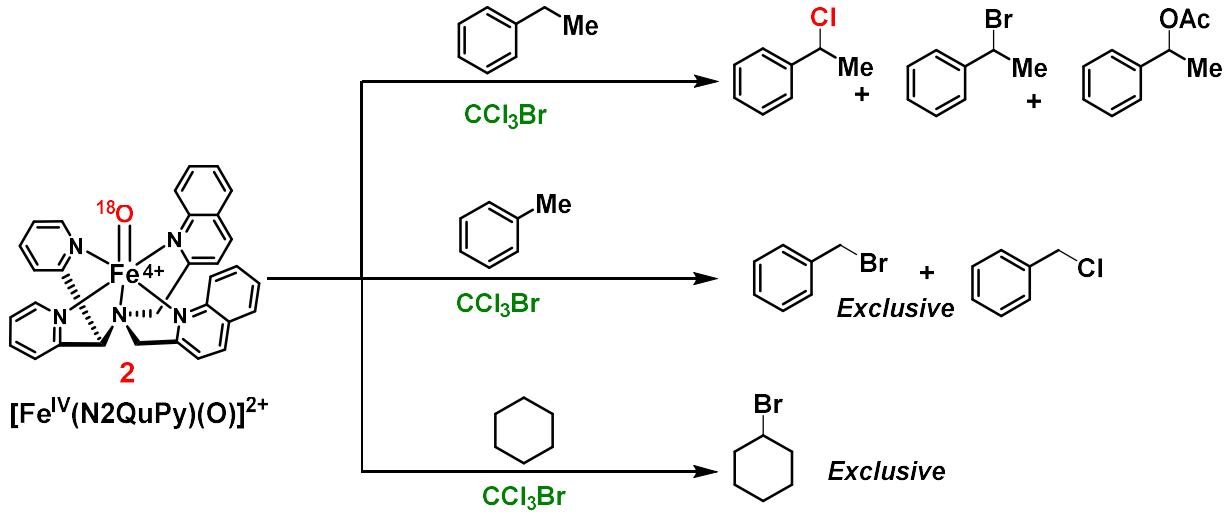
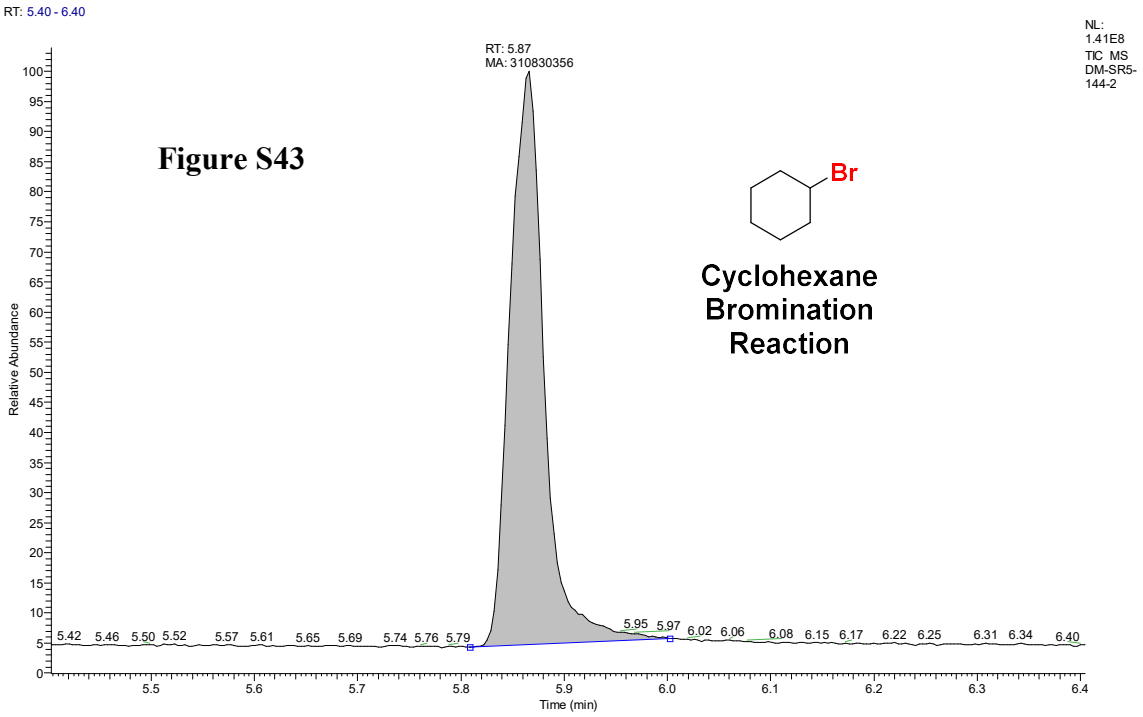
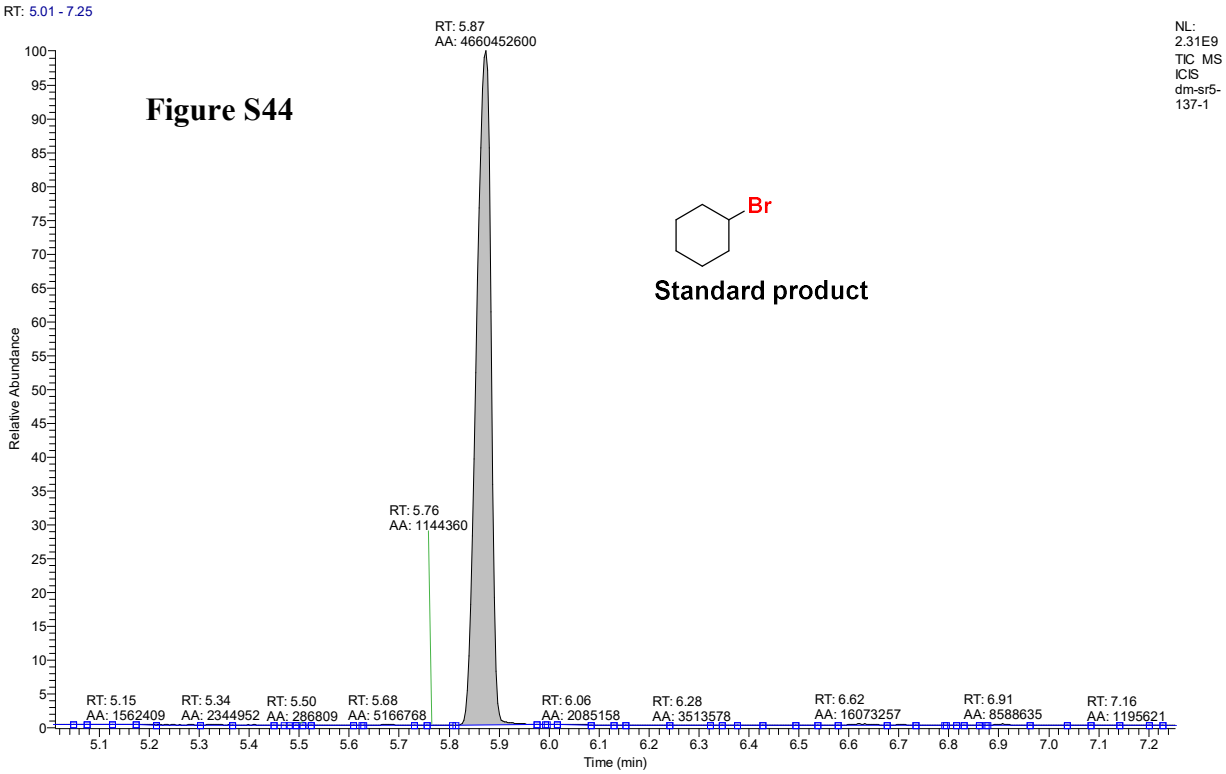


Figure S42. Radical trap experiment during C–H oxidations reactions using CCl_3Br

3. GC/GC-Ms data of the products:



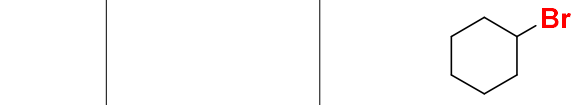


DM-SR5-144-2 #1019 RT: 5.86 AV: 1 NL: 9.66E4
T: + c EI Full ms [20.00-1000.00]

Figure S45

dm-sr5-137-1 #1021 RT: 5.87 AV: 1 NL: 8.48E8
T: + c EI Full ms [20.00-1000.00]

Figure S46



DM-SR5-144-1 #1079 RT: 6.67 AV: 1 NL: 5.62E6
T: + c EI Full ms [50.00-500.00]

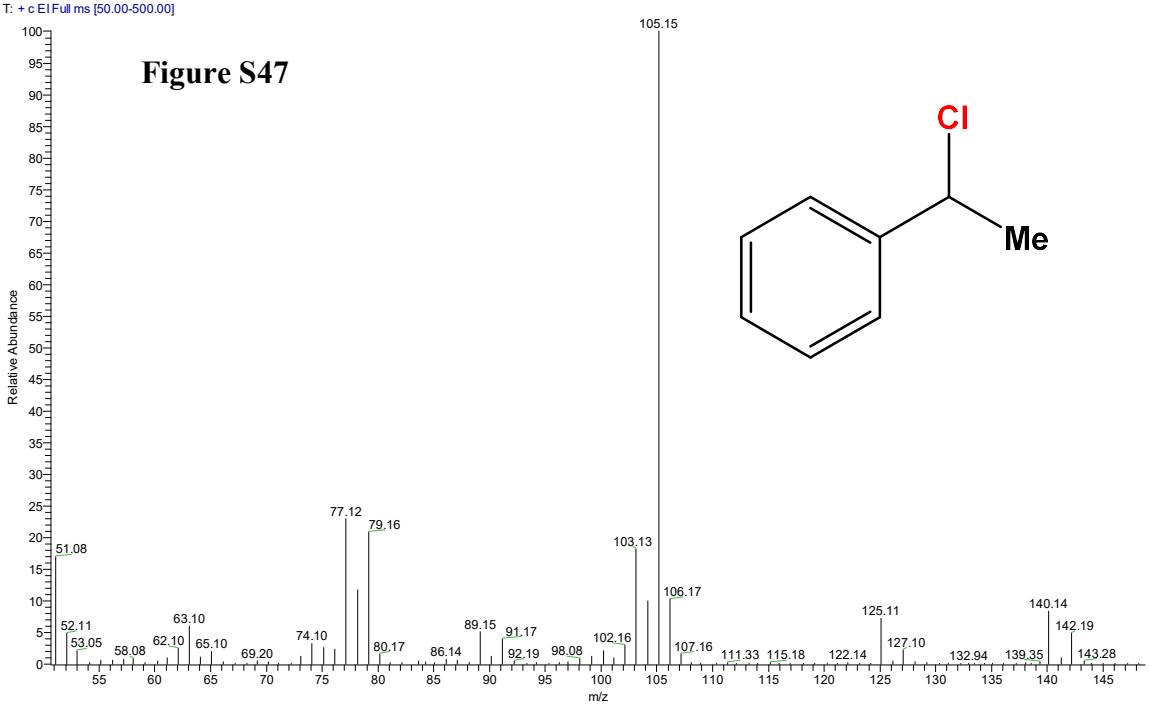


Figure S47

DM-SR5-146-1 #3250 RT: 13.45 AV: 1 NL: 9.31E6
T: + c EI Full ms [20.00-1000.00]

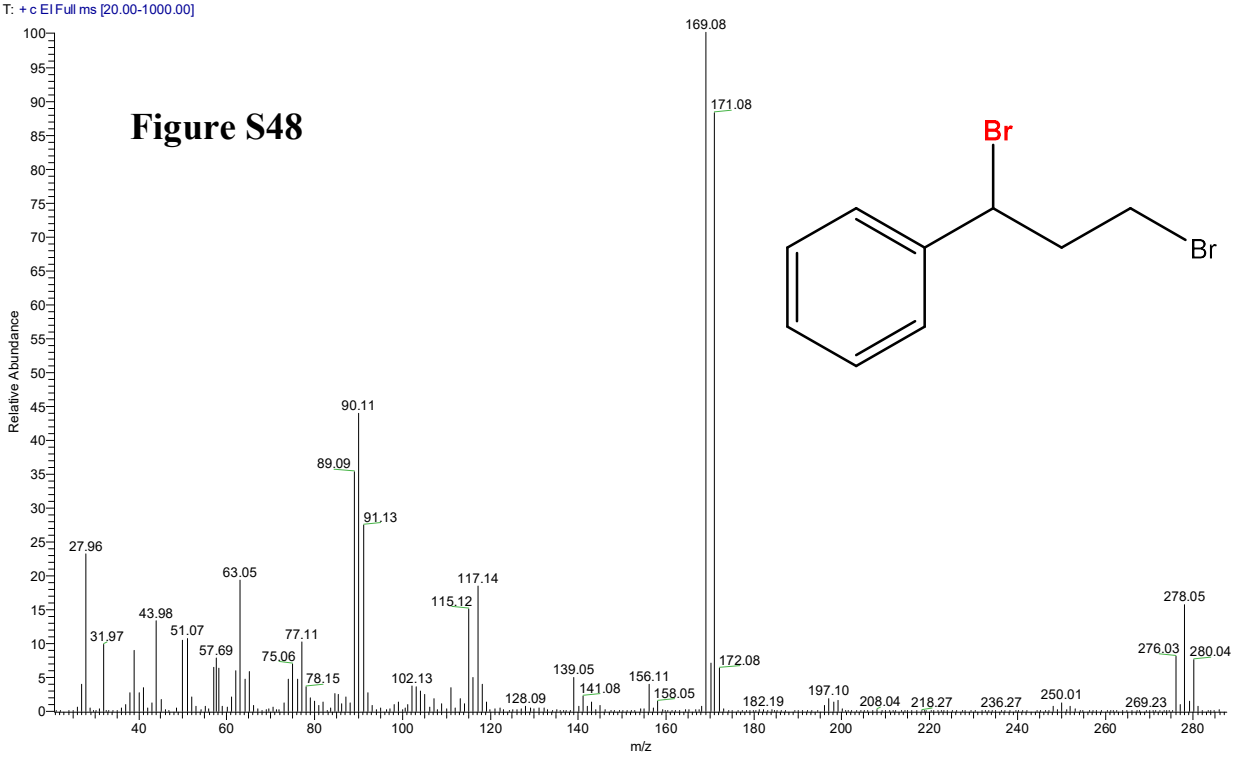


Figure S48

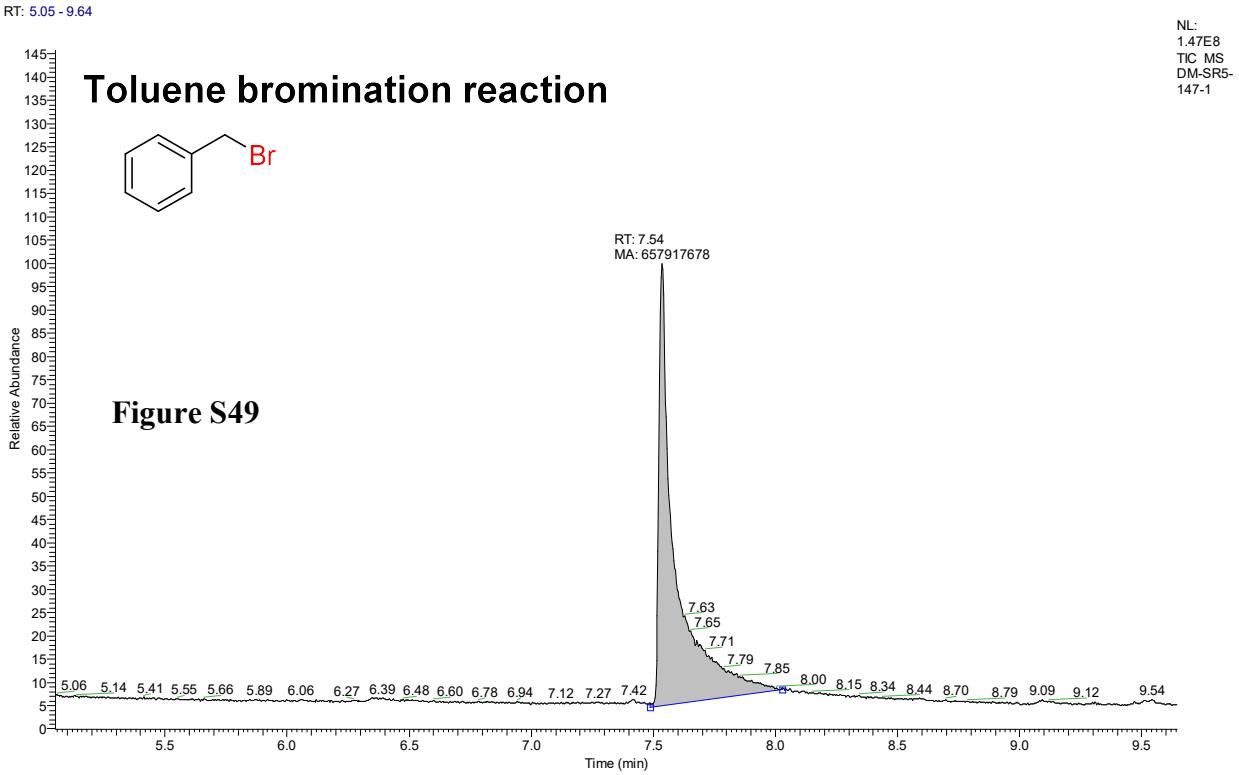


Figure S49

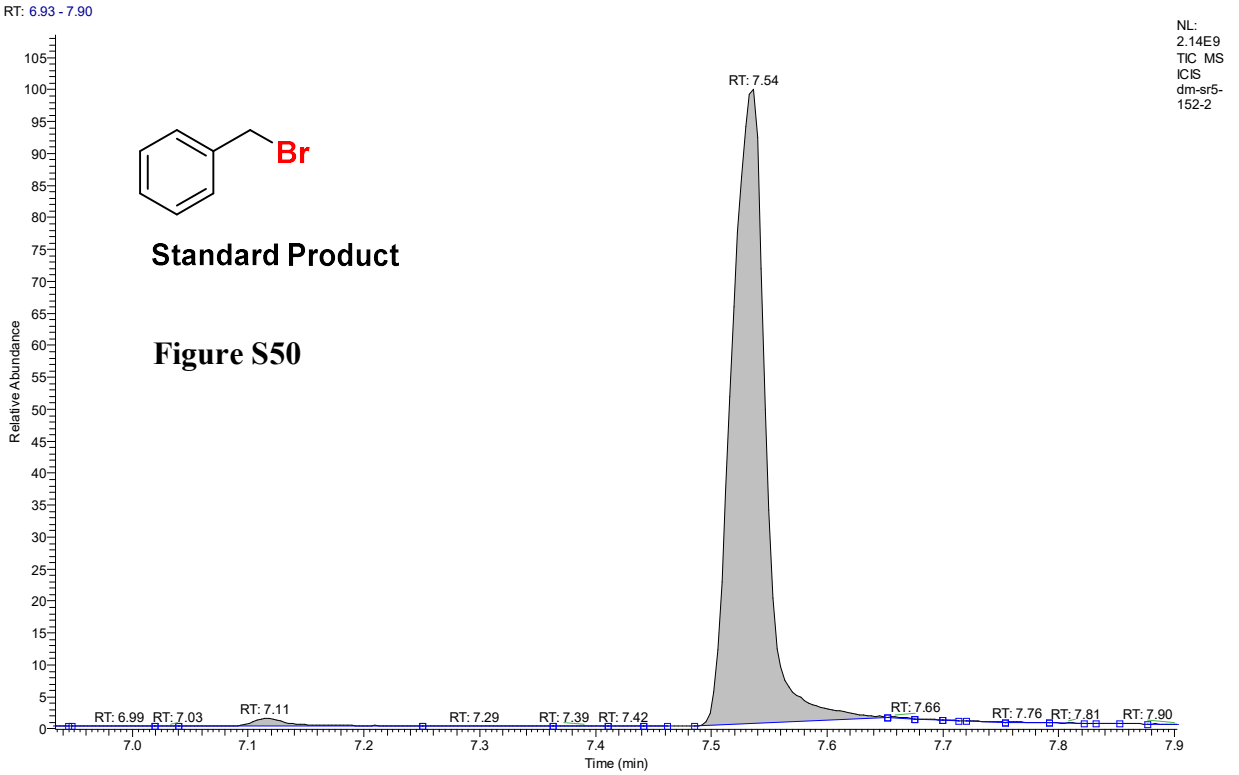


Figure S50

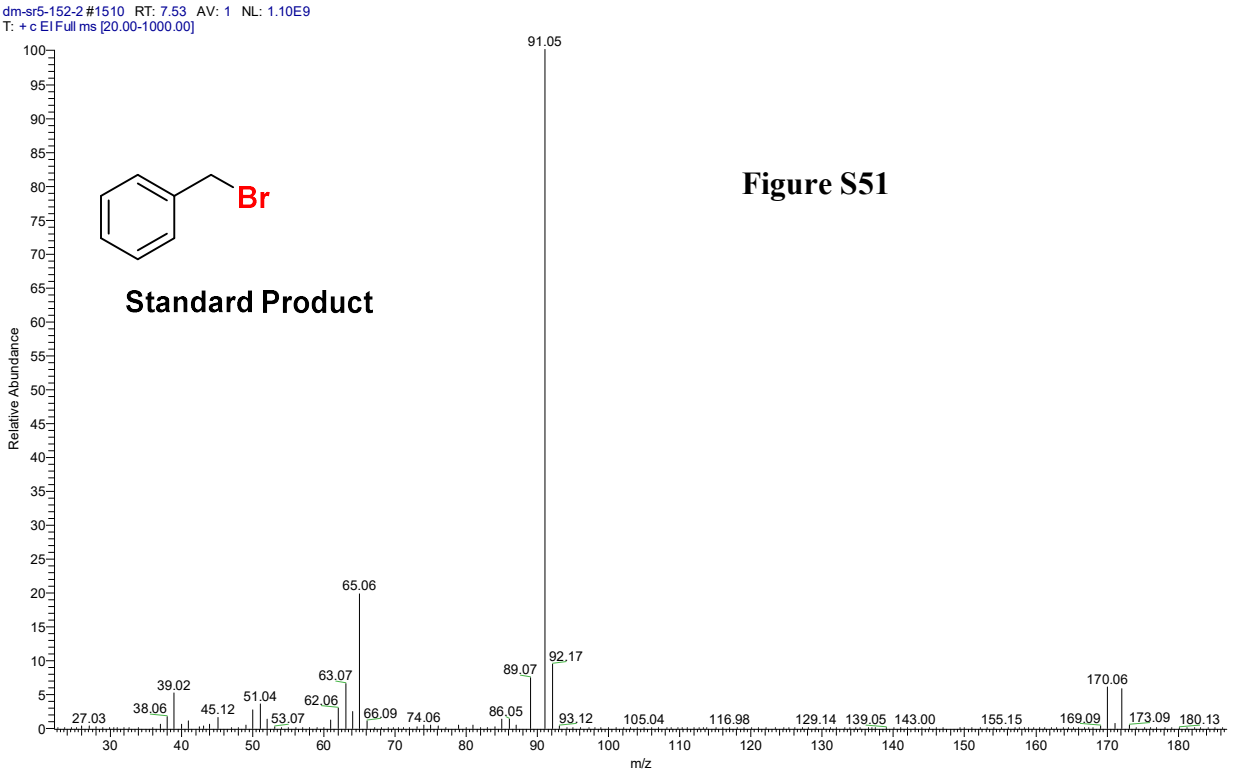


Figure S51

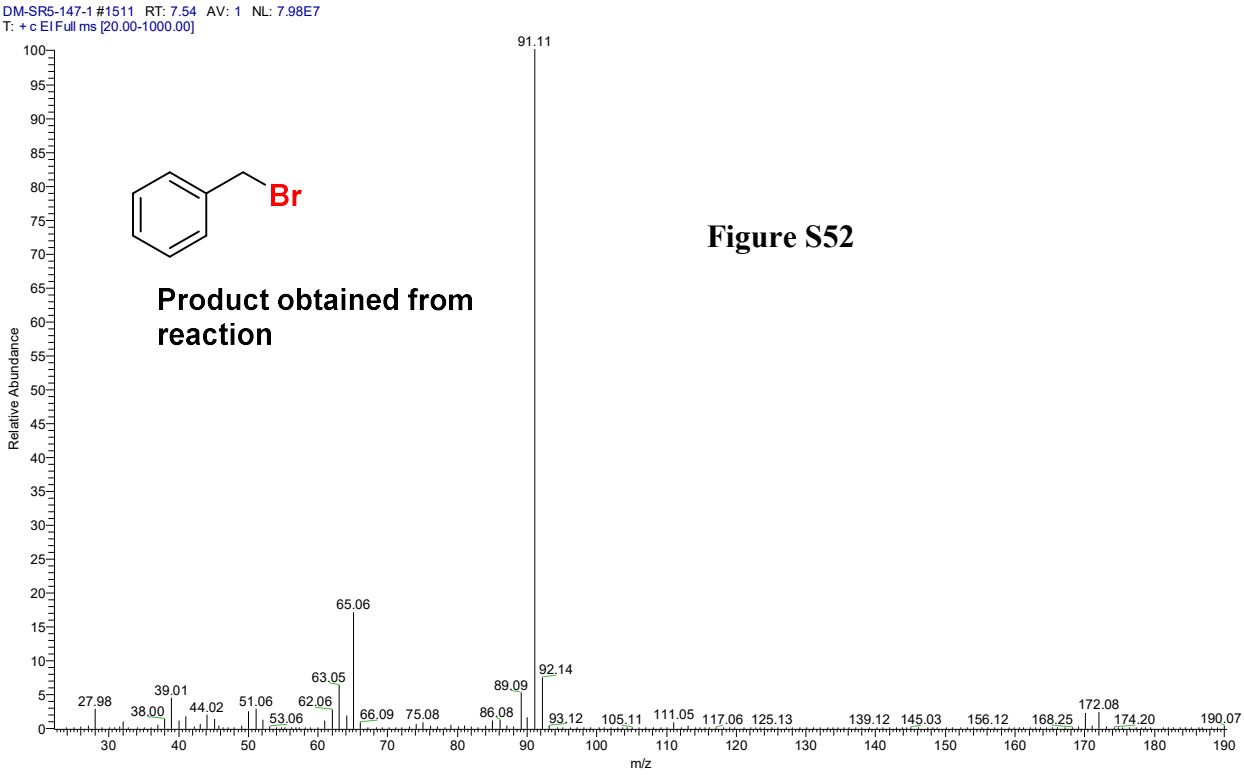


Figure S52

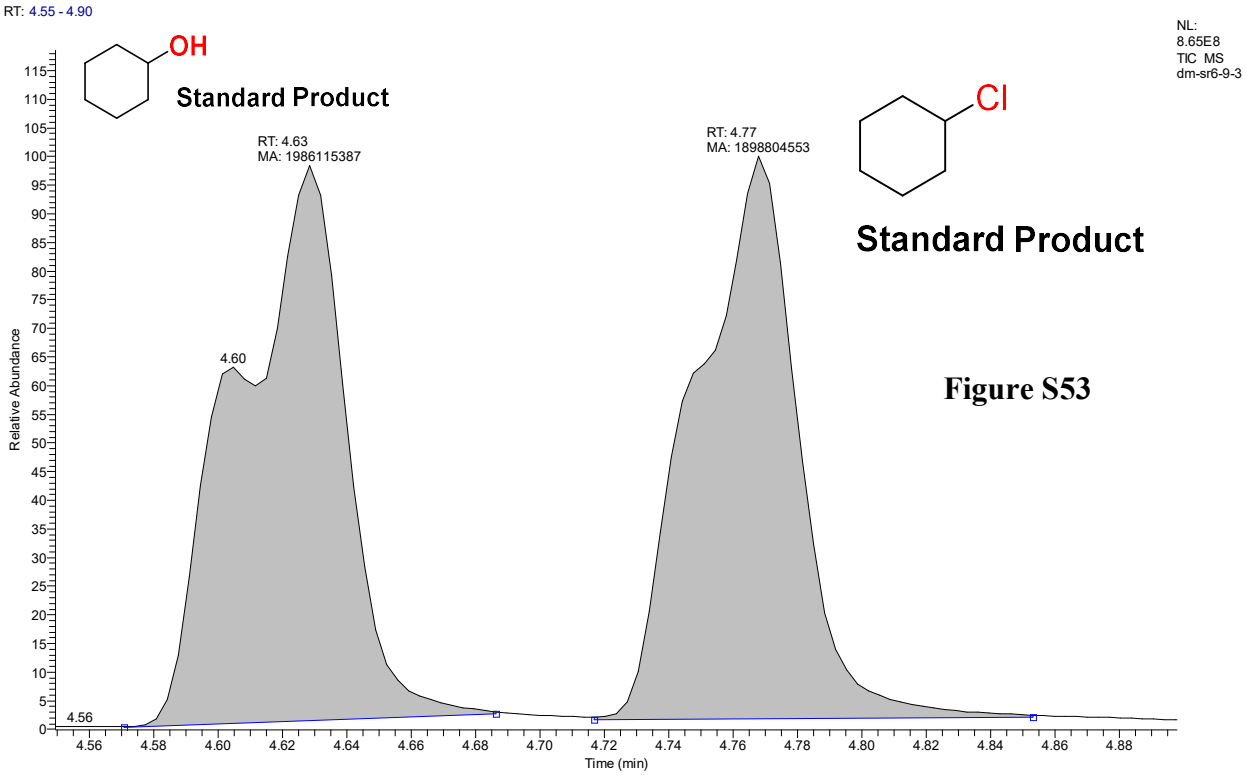


Figure S53

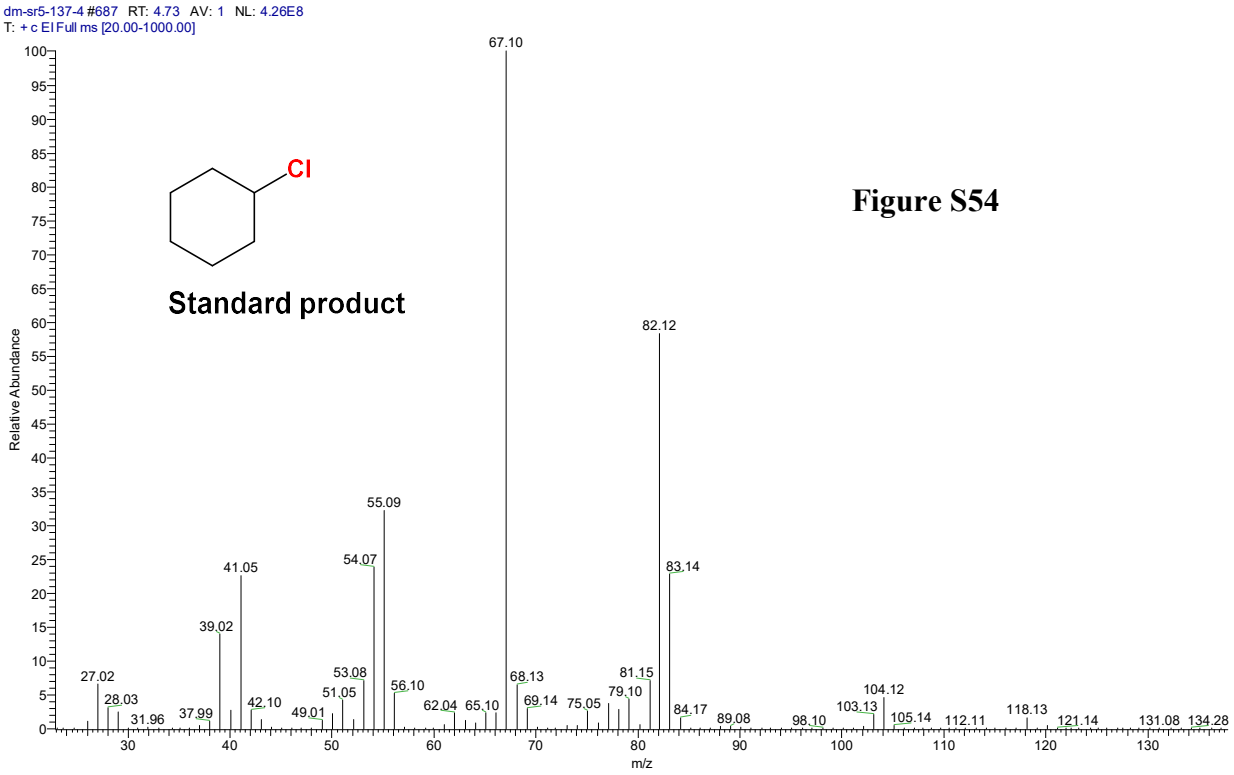


Figure S54

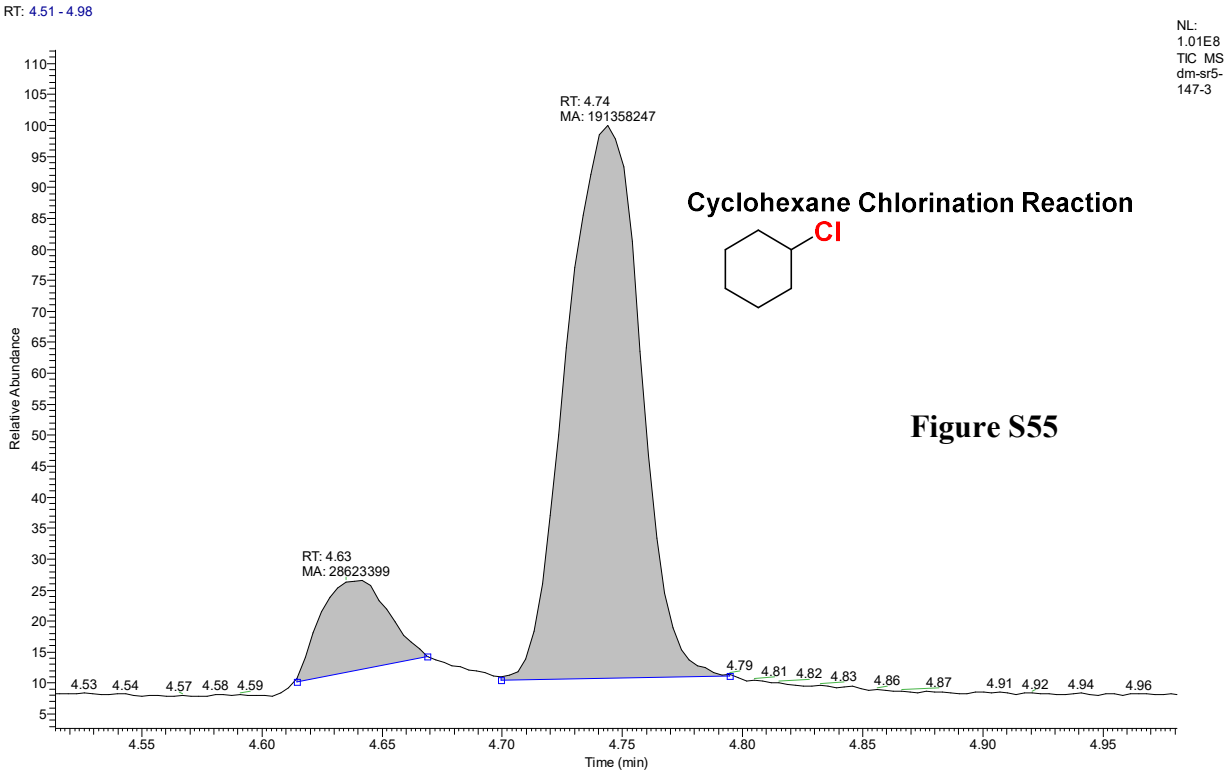


Figure S55

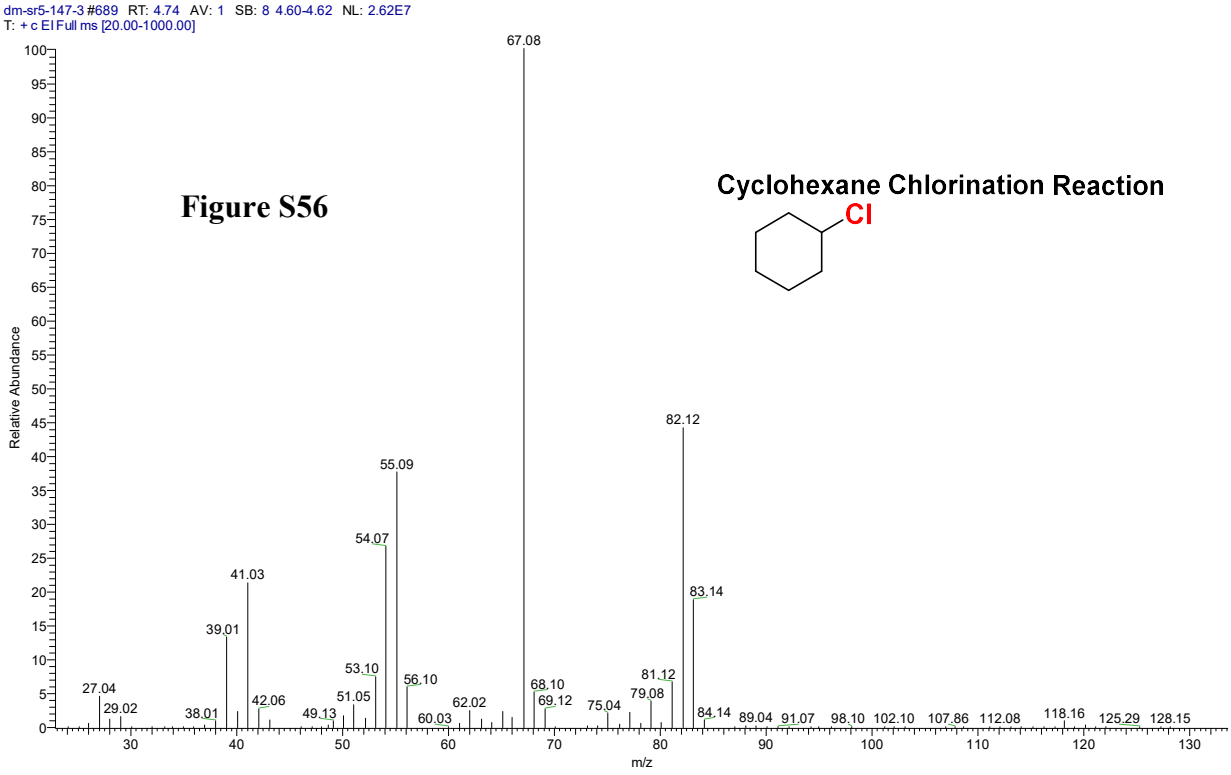


Figure S56

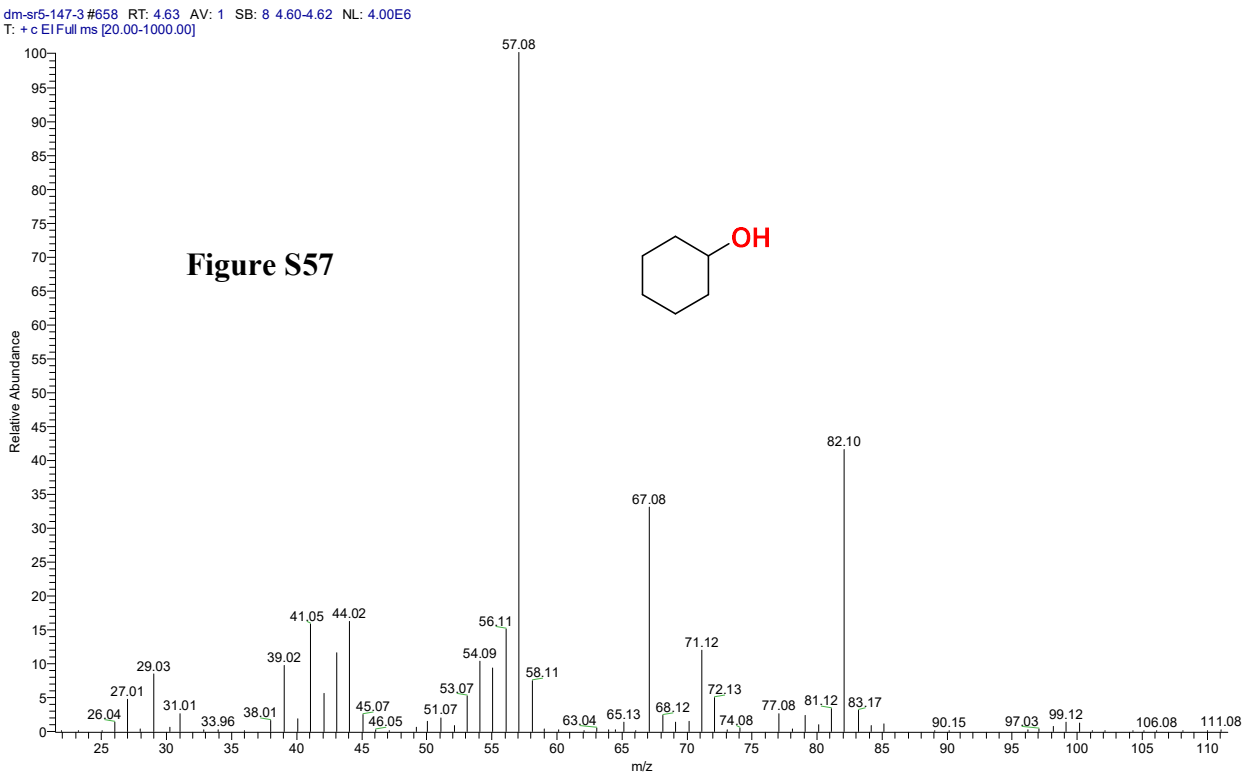


Figure S57

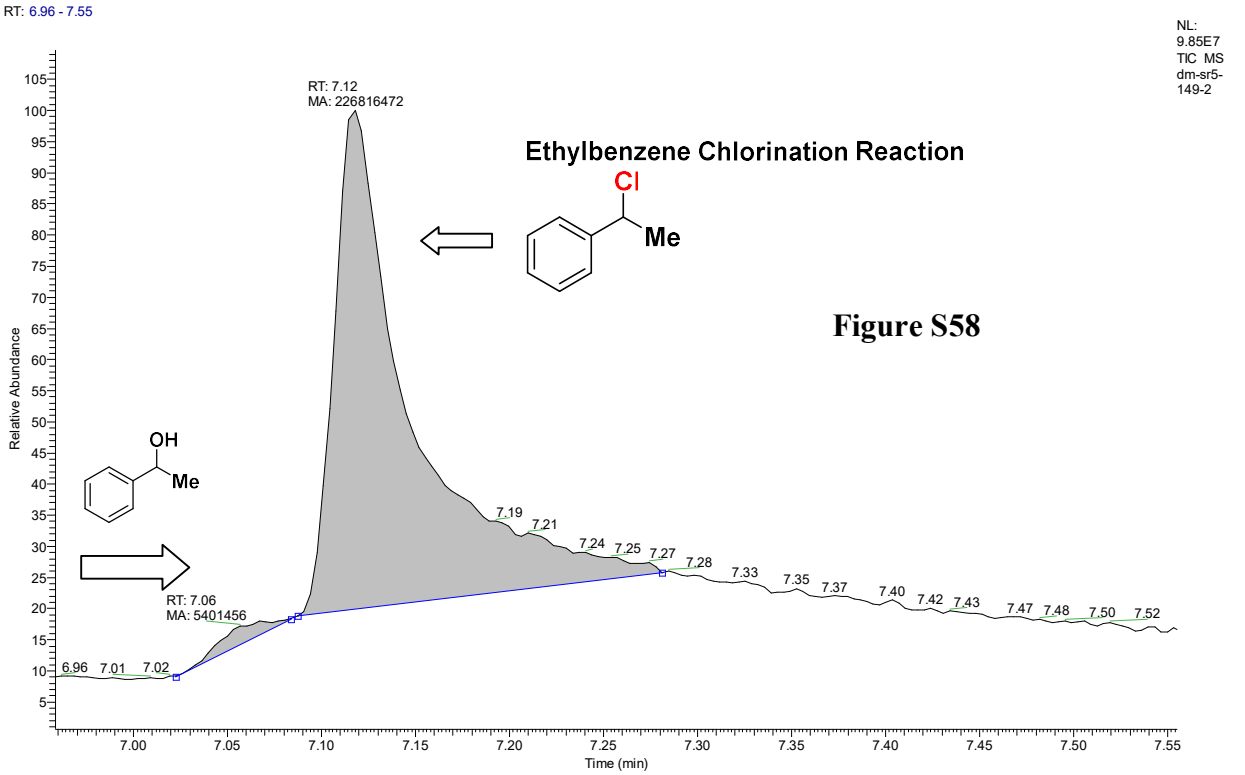


Figure S58

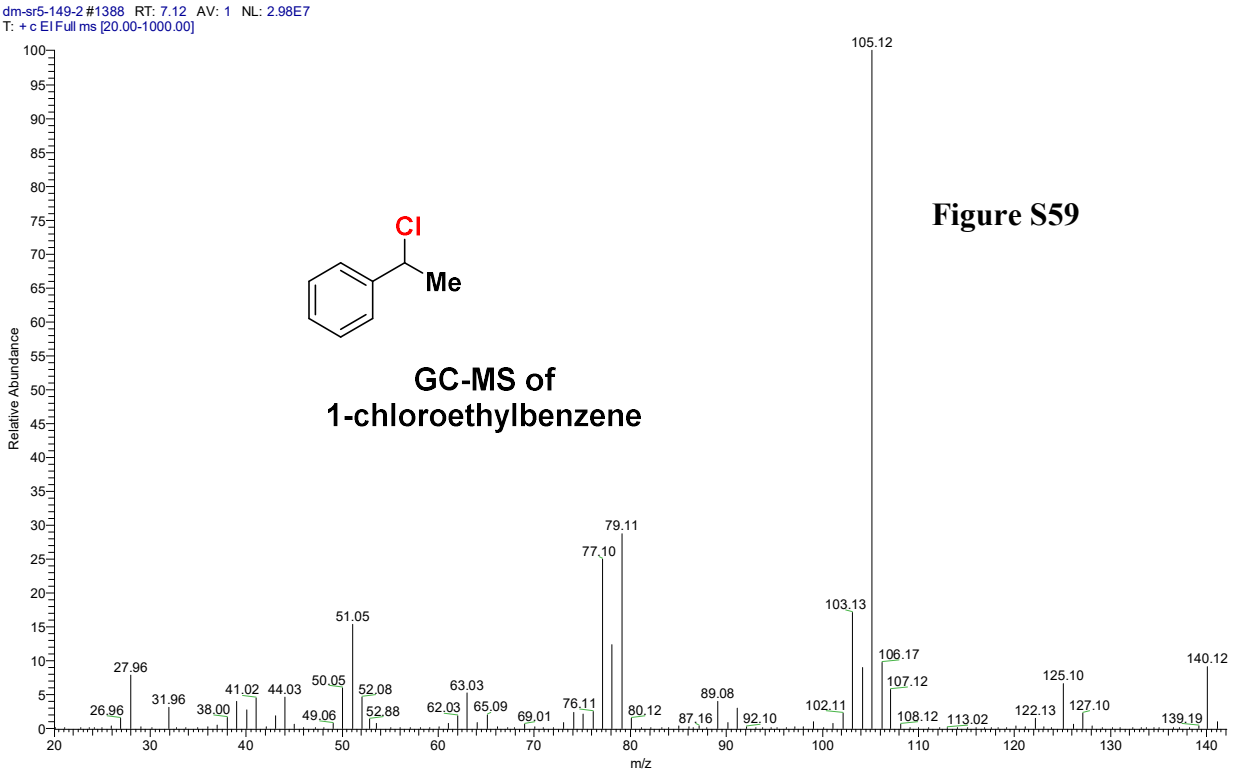


Figure S59

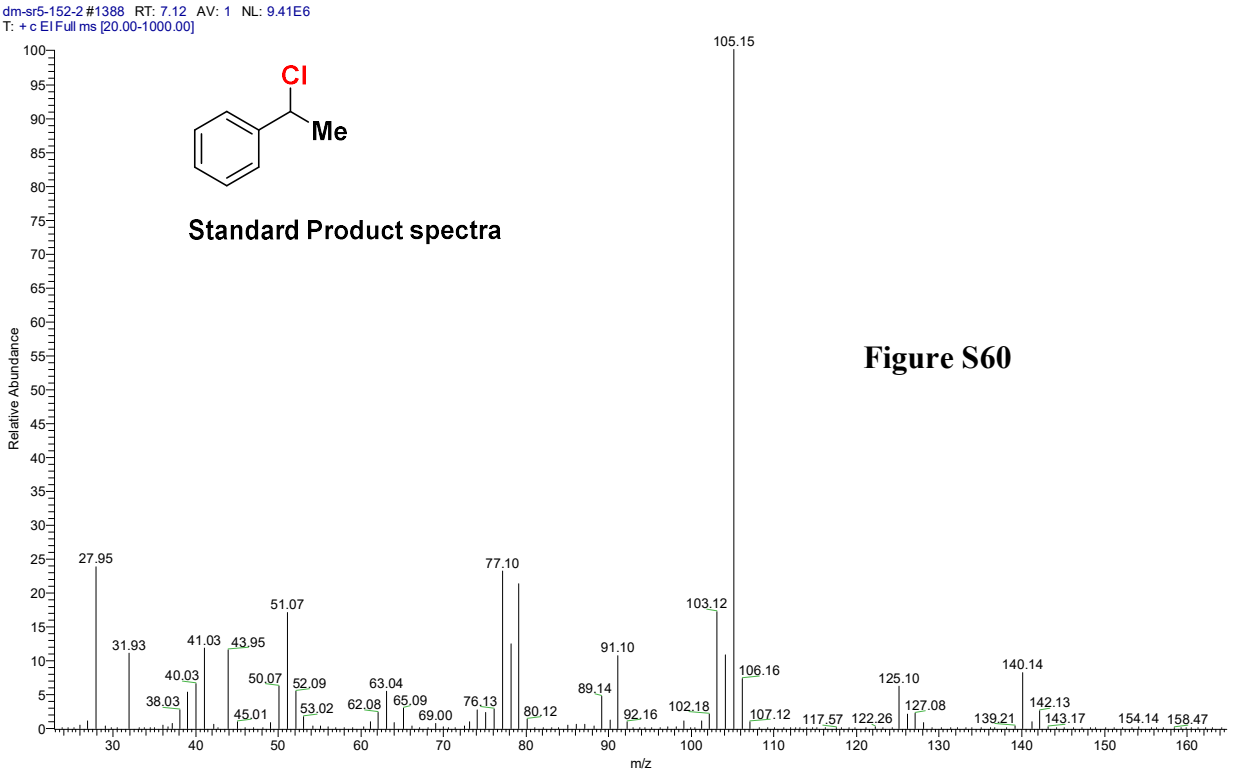


Figure S60

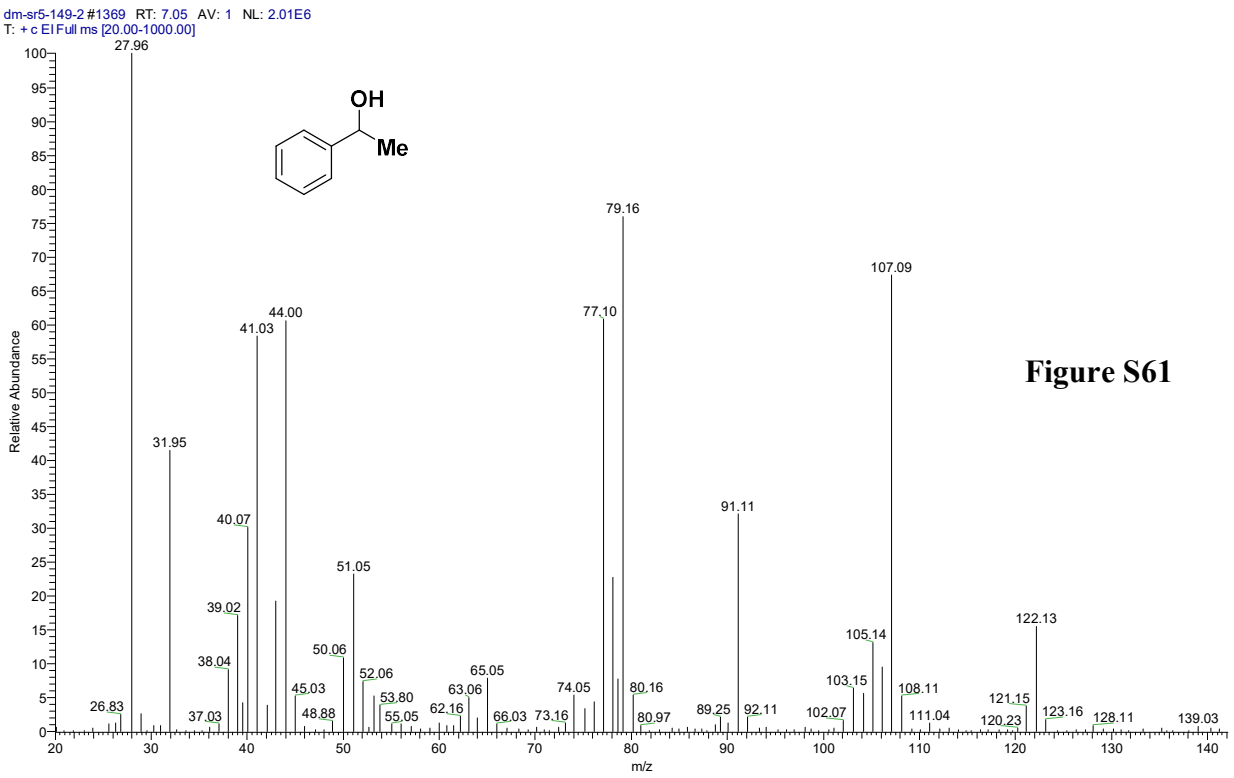

dm-sr5-149-2 #1369 RT: 7.05 AV: 1 NL: 2.01E6
T: + c EI Full ms [20.00-1000.00]
OH
Me
Relative Abundance
m/z
27.96
79.16
107.09
44.00
41.03
77.10
31.95
91.11
40.07
51.05
39.02
122.13
105.14
50.06
38.04
65.05
52.06
103.15
108.11
45.03
63.06
74.05
80.16
53.80
121.15
26.83
48.88
62.16
89.25
92.11
123.16
37.03
55.05
66.03
73.16
102.07
111.04
120.23
128.11
139.03

Figure S61

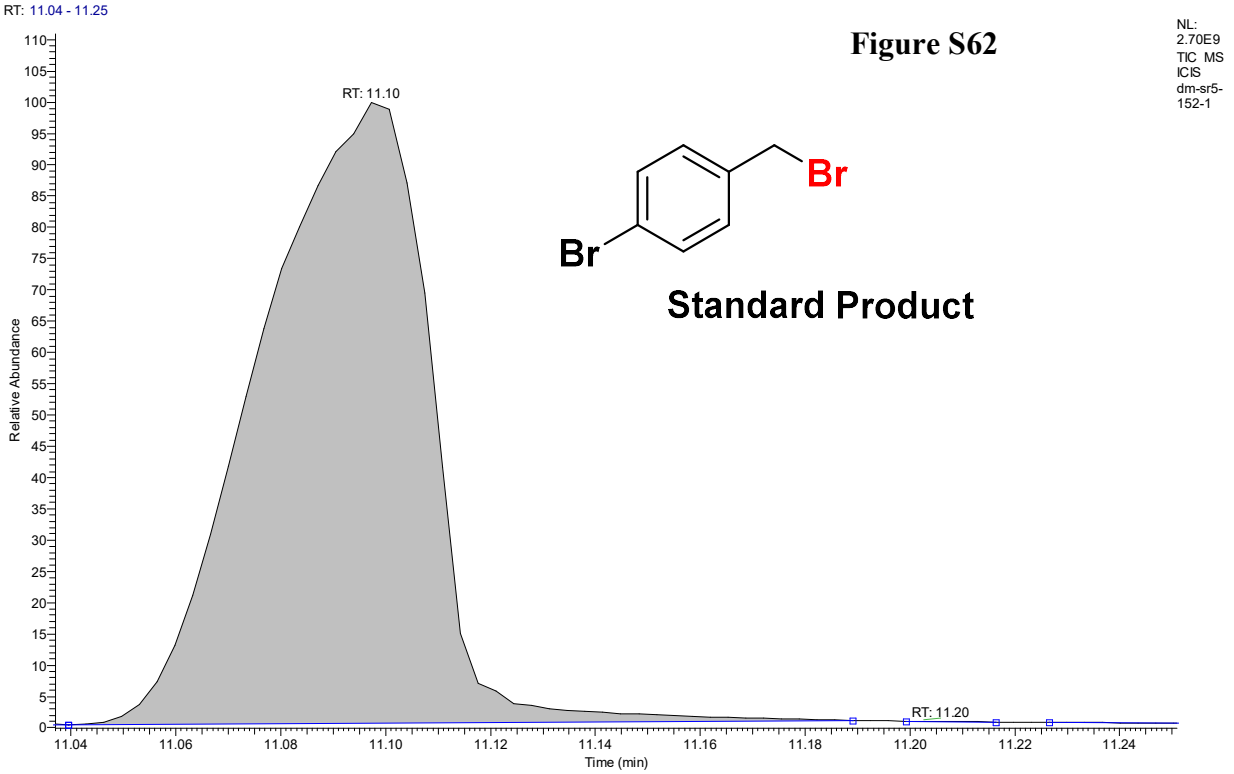


Figure S62

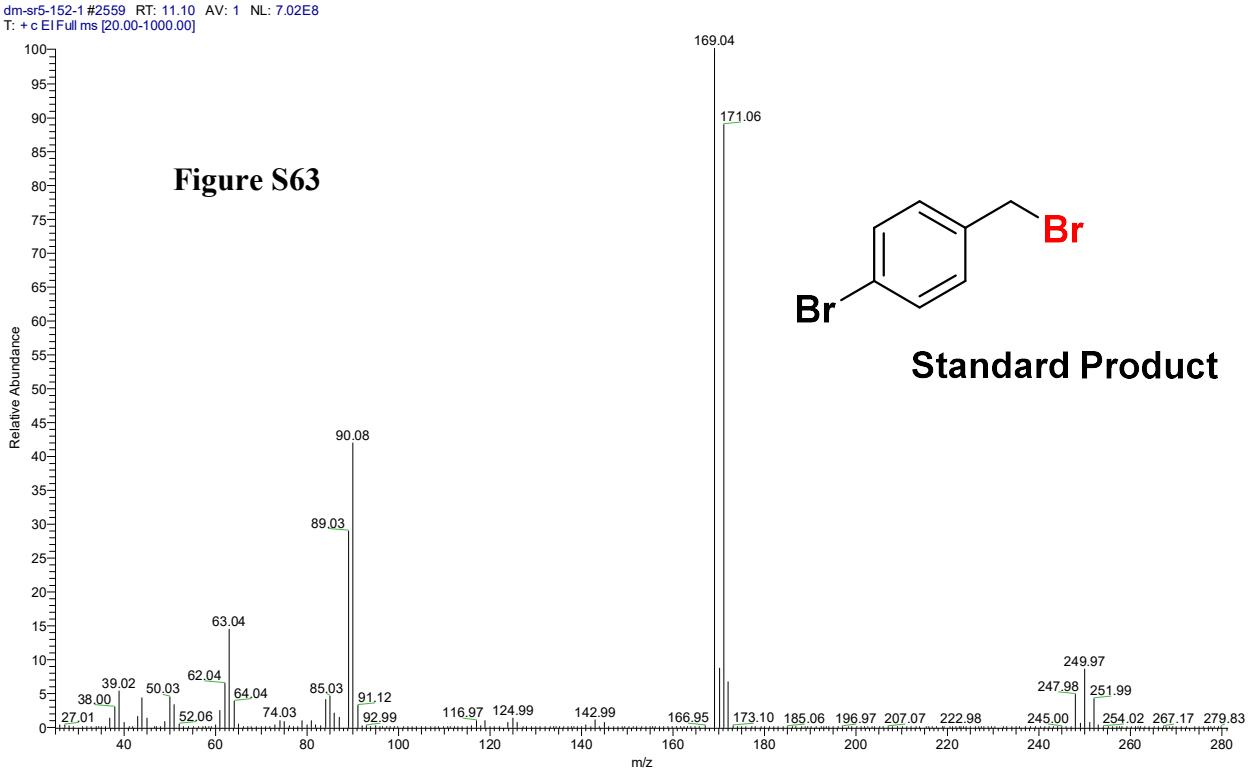


Figure S63

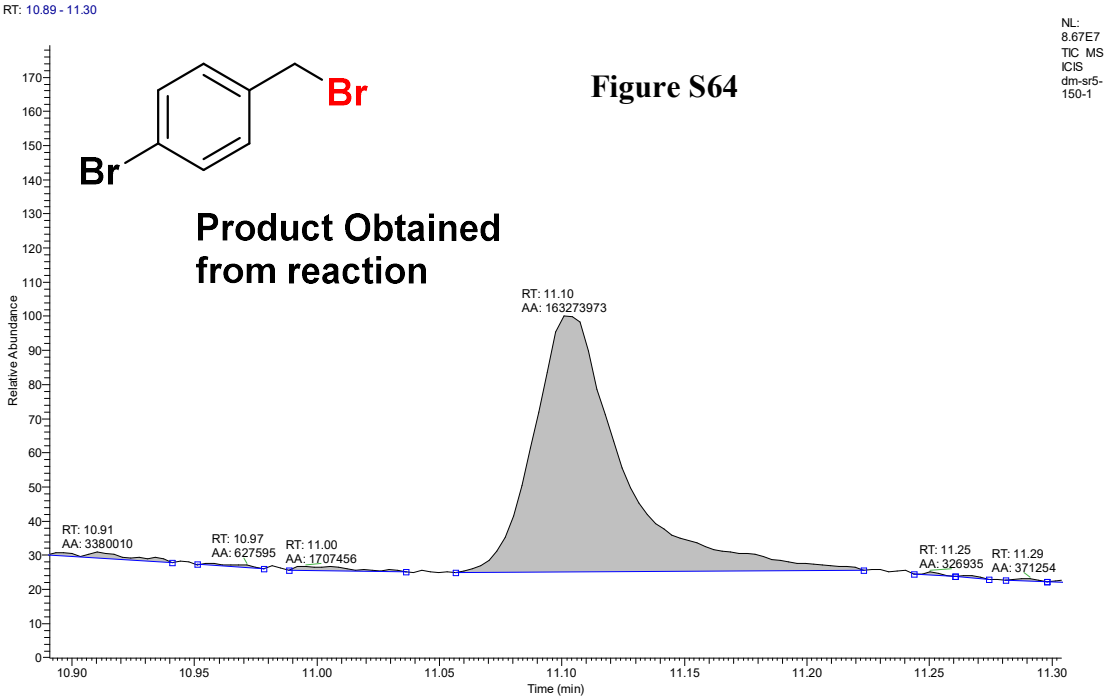


Figure S64

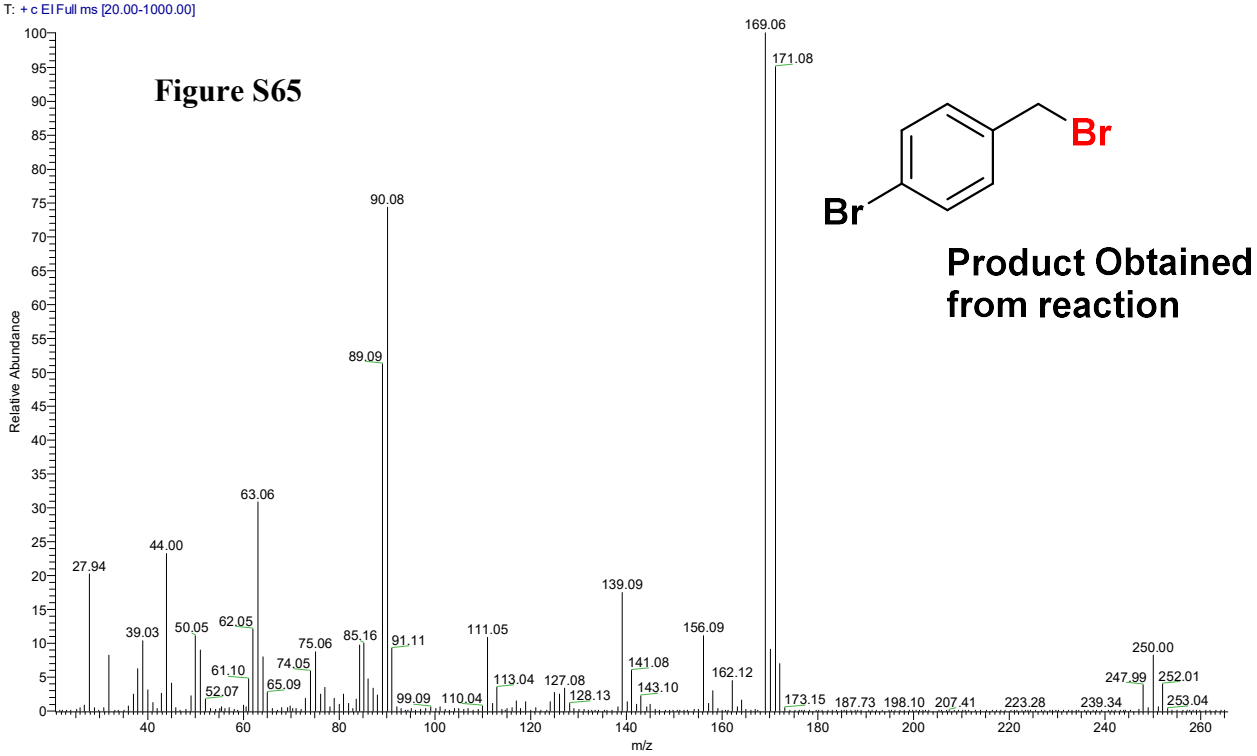


Figure S65

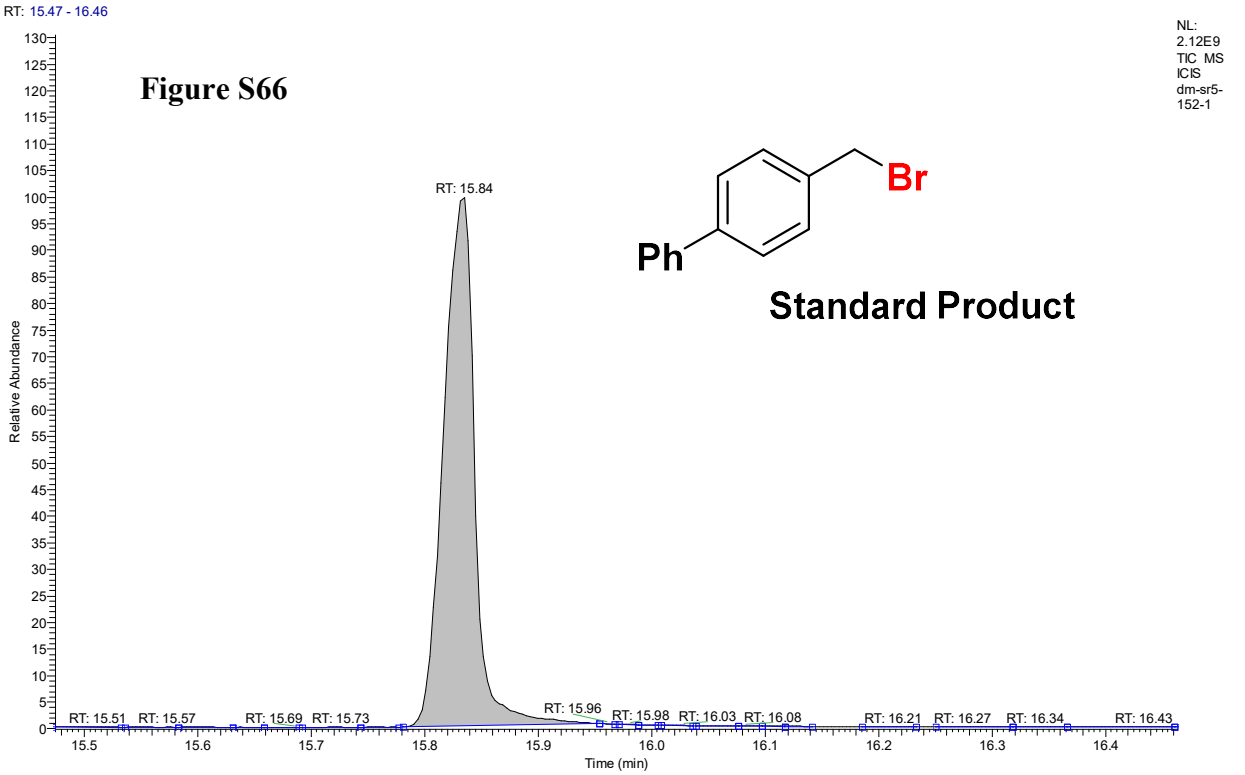


Figure S66

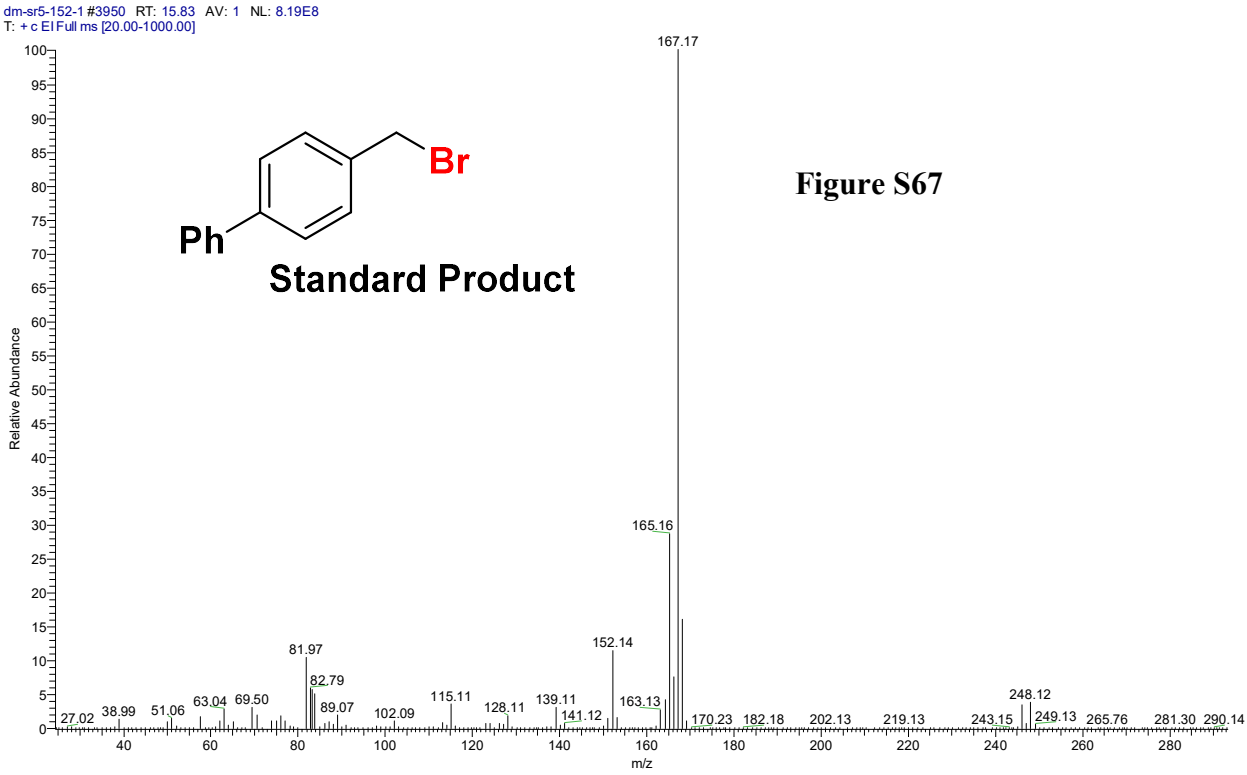
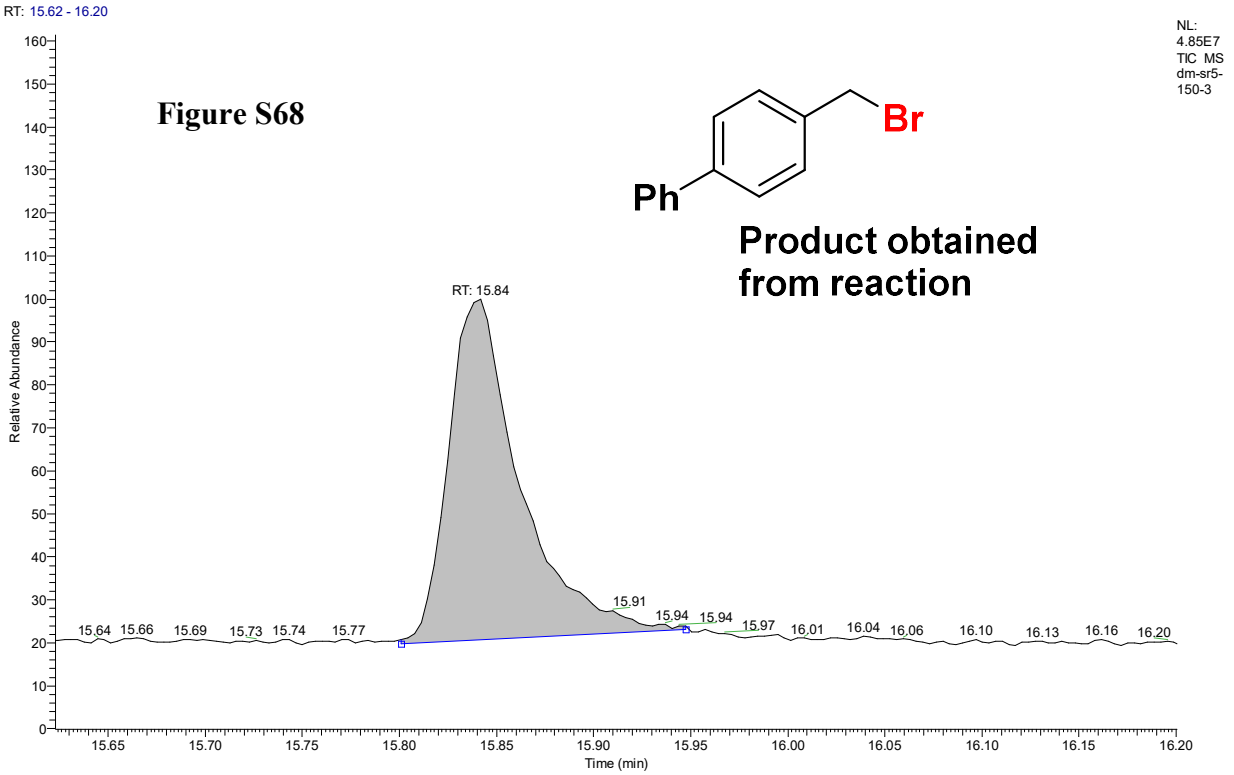
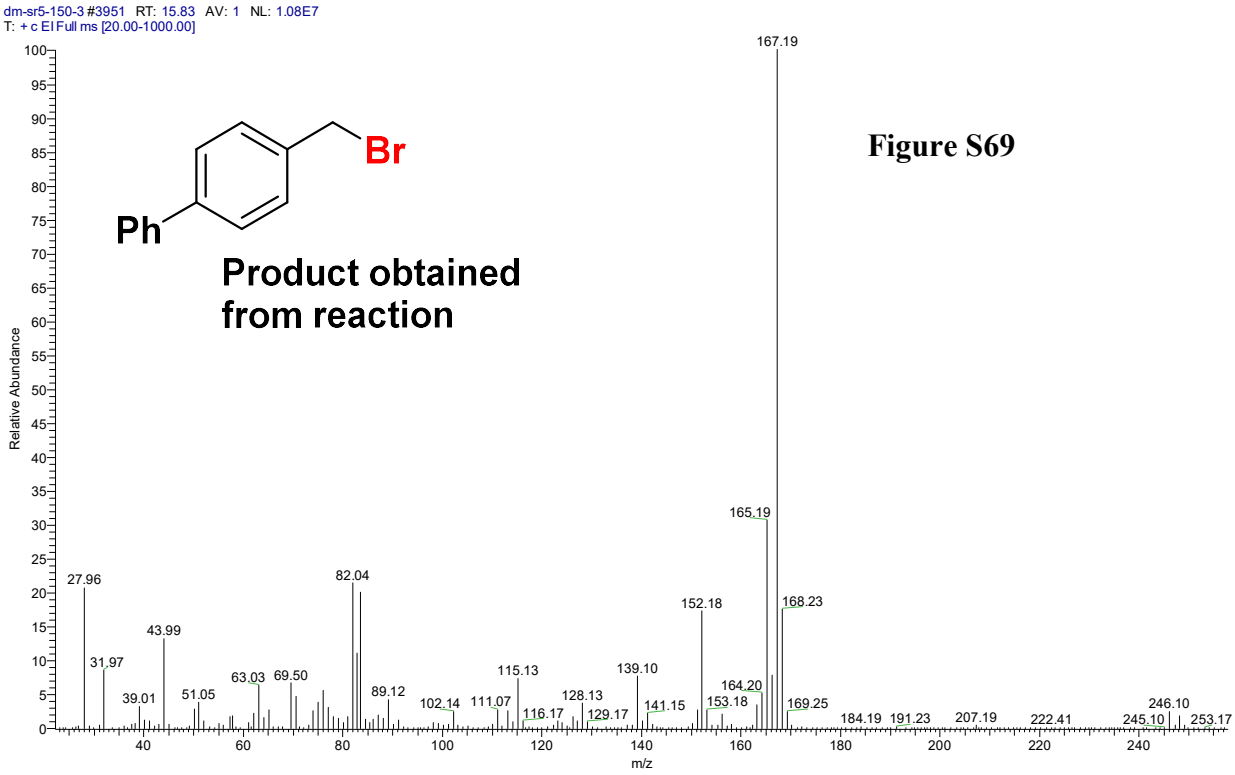


Figure S67


RT: 15.62 - 16.20
NL:
4.85E7
TIC MS
dm-sr5-
150-3
Figure S68
Br
Ph
Product obtained
from reaction
RT: 15.84
Relative Abundance
Time (min)


dm-sr5-150-3 #3951 RT: 15.83 AV: 1 NL: 1.08E7
T: + c EI Full ms [20.00-1000.00]
Figure S69
Br
Ph
Product obtained
from reaction
Relative Abundance
m/z

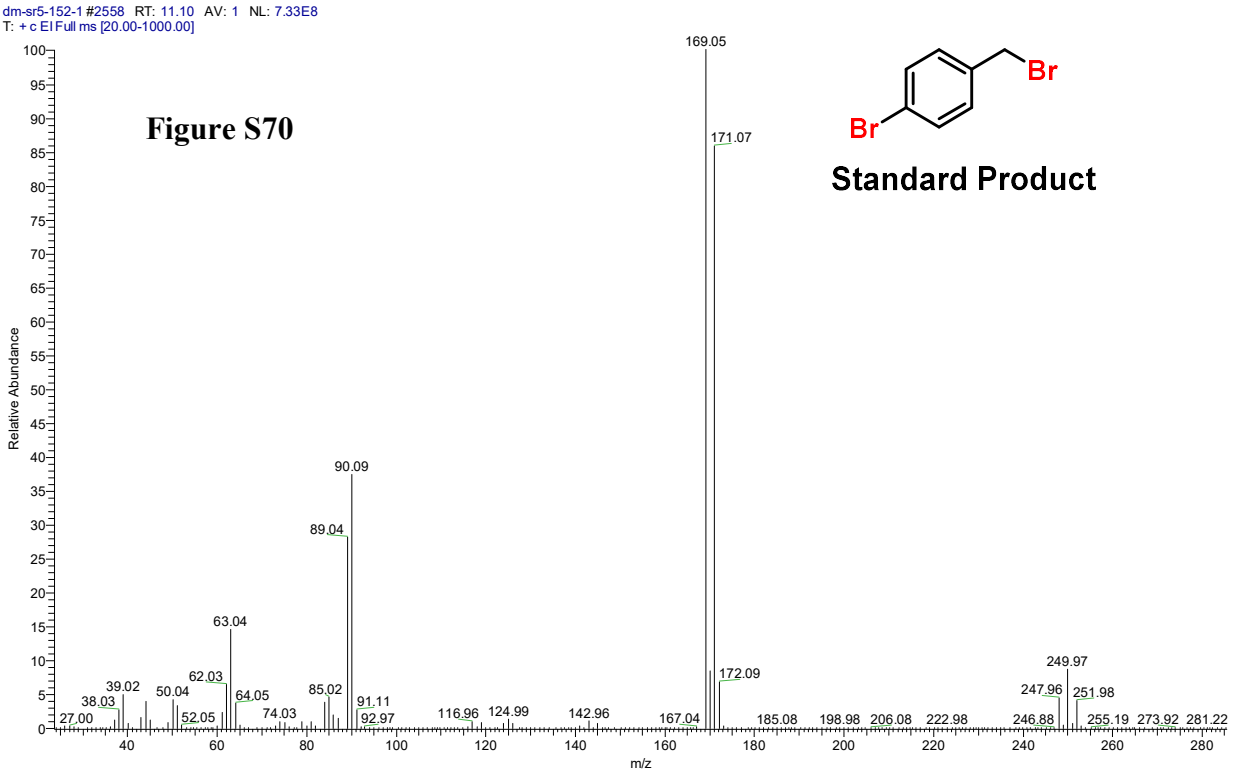
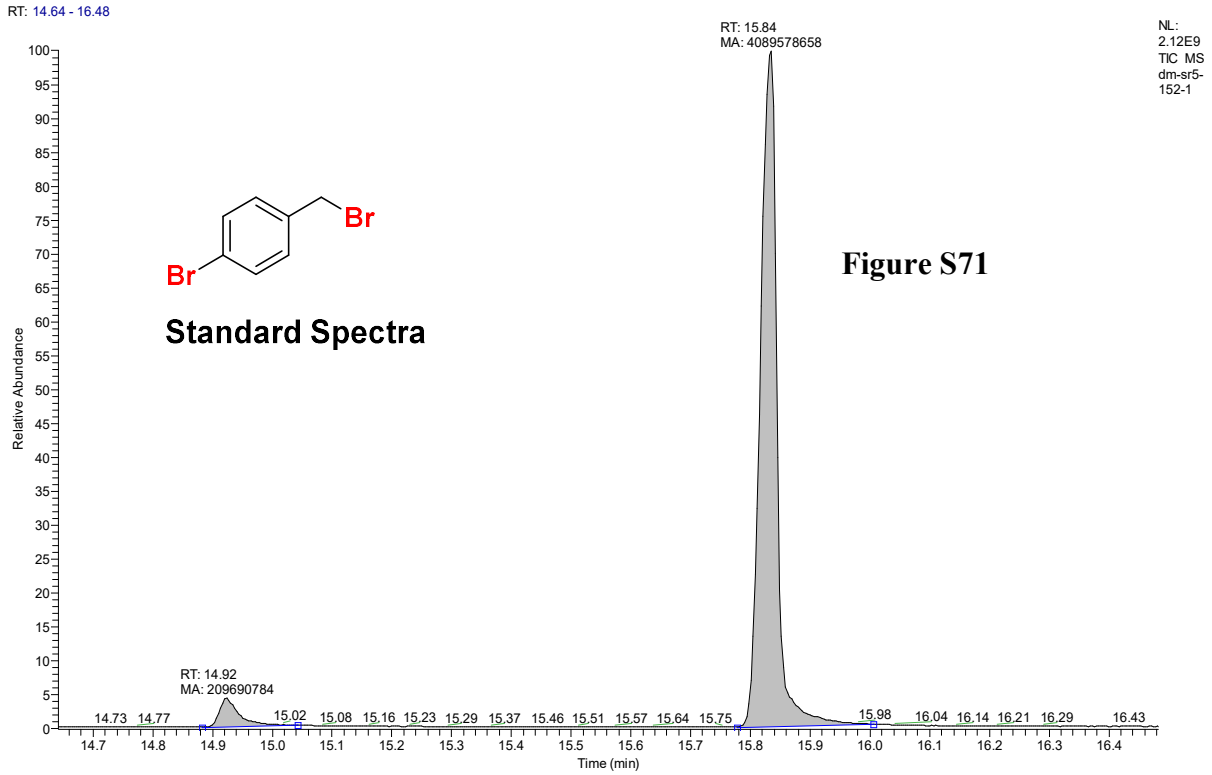


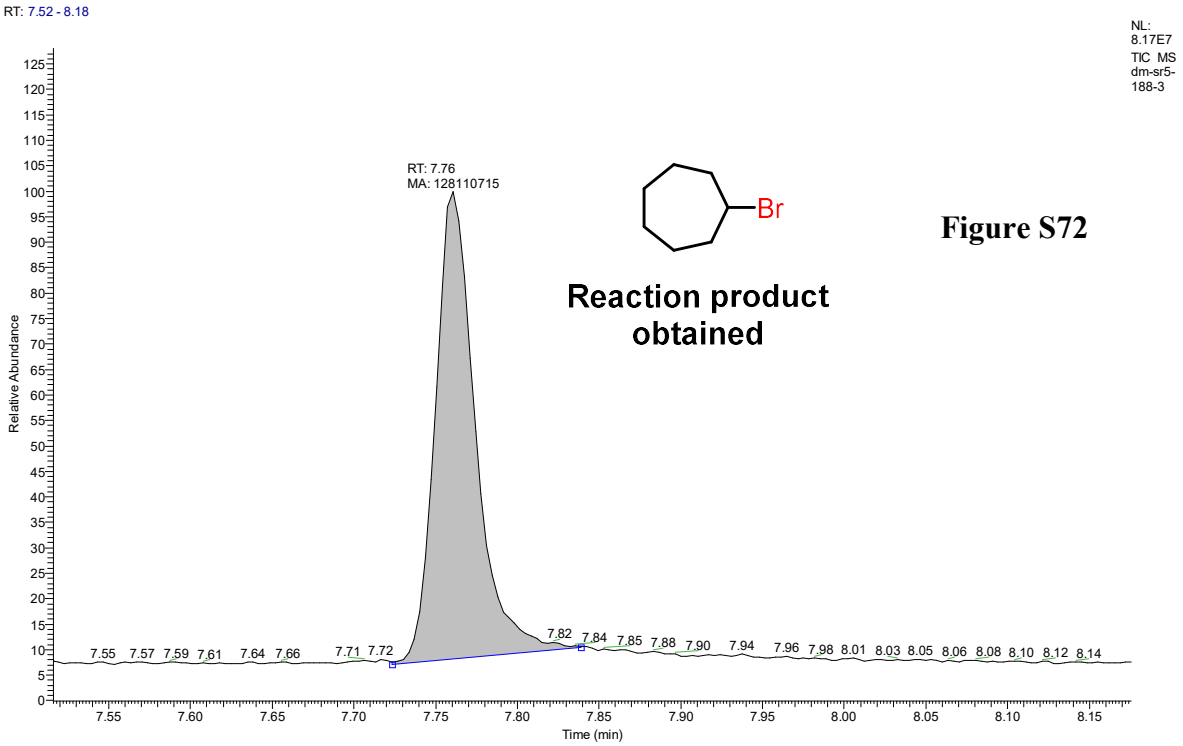
Figure S70

Standard Product



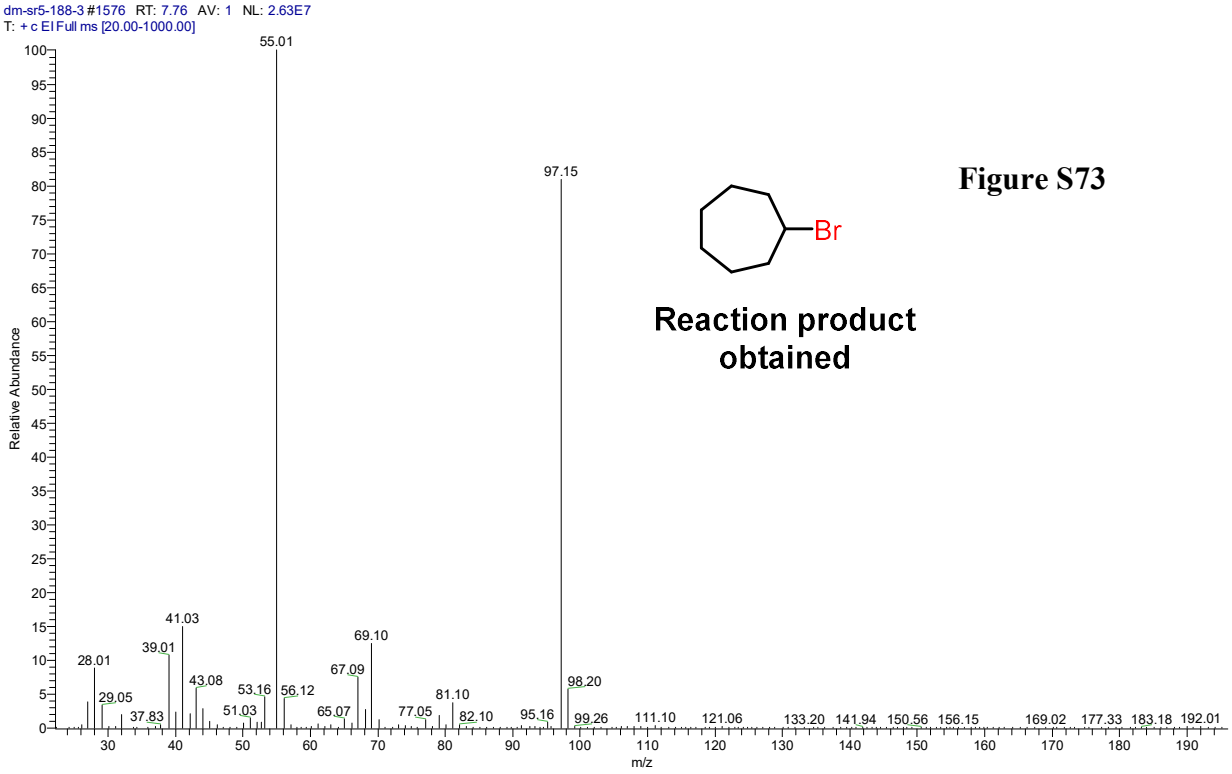
Standard Spectra

Figure S71



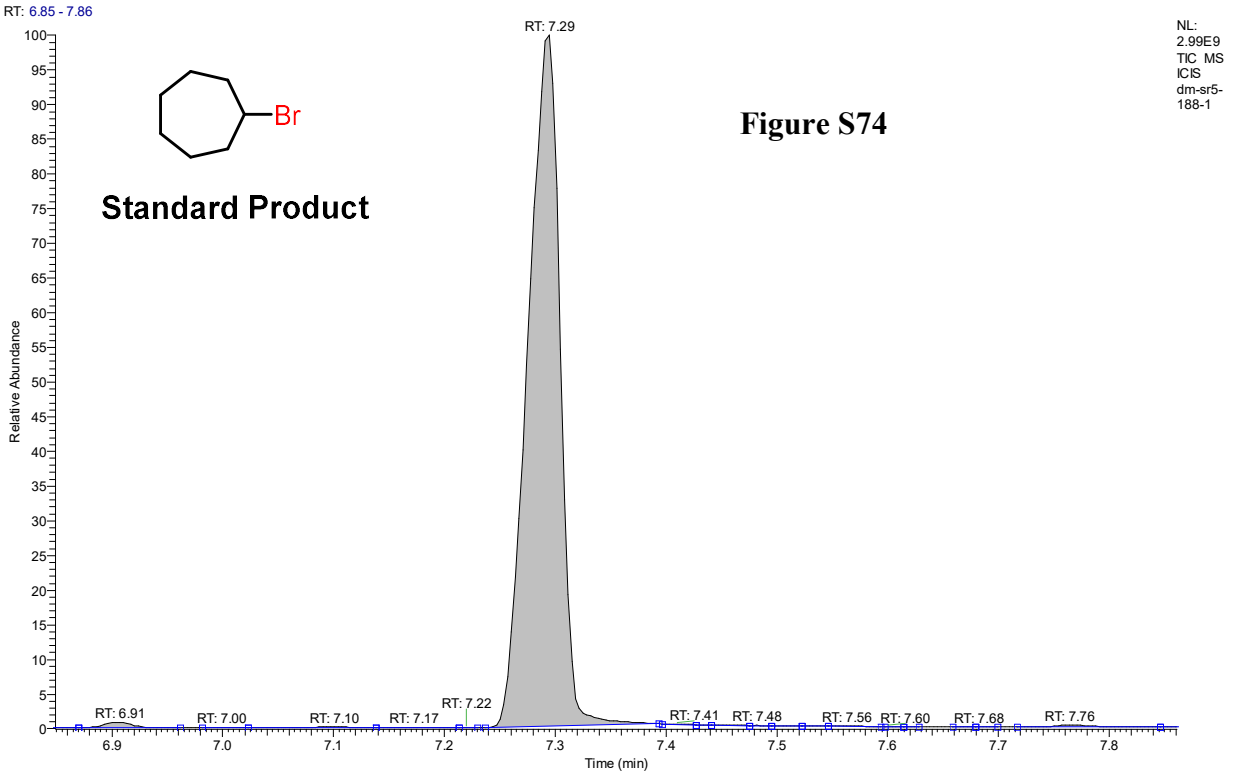
Reaction product obtained

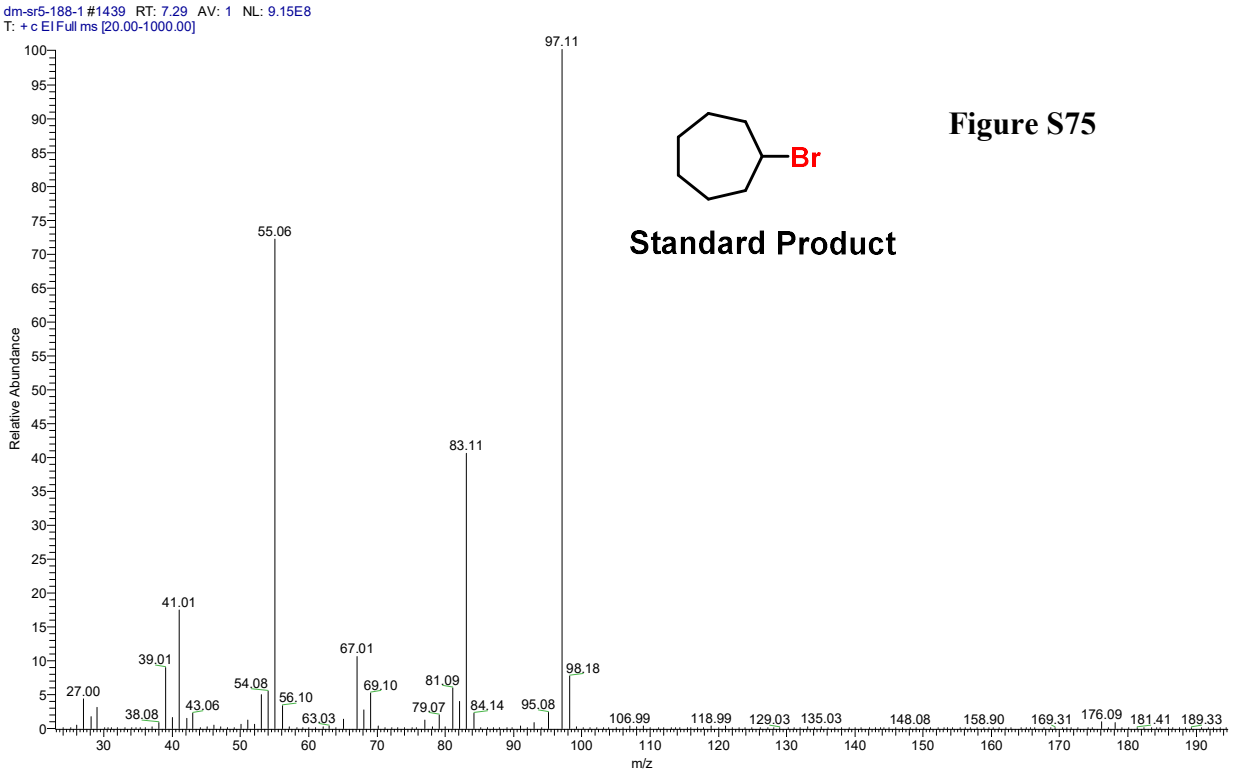
Figure S72



Reaction product obtained

Figure S73


RT: 6.85 - 7.86
NL:
2.99E9
TIC MS
ICIS
dm-sr5-
188-1
Br
Standard Product
Figure S74
RT: 7.29
RT: 6.91
RT: 7.00
RT: 7.10
RT: 7.17
RT: 7.22
RT: 7.41
RT: 7.48
RT: 7.56
RT: 7.60
RT: 7.68
RT: 7.76
Relative Abundance
Time (min)


dm-sr5-188-1 #1439 RT: 7.29 AV: 1 NL: 9.15E8
T: + c EI Full ms [20.00-1000.00]
Br
Standard Product
Figure S75
97.11
55.06
83.11
41.01
39.01
67.01
27.00
54.08
69.10
81.09
98.18
38.08
43.06
56.10
63.03
79.07
84.14
95.08
106.99
118.99
129.03
135.03
148.08
158.90
169.31
176.09
181.41
189.33
Relative Abundance
m/z

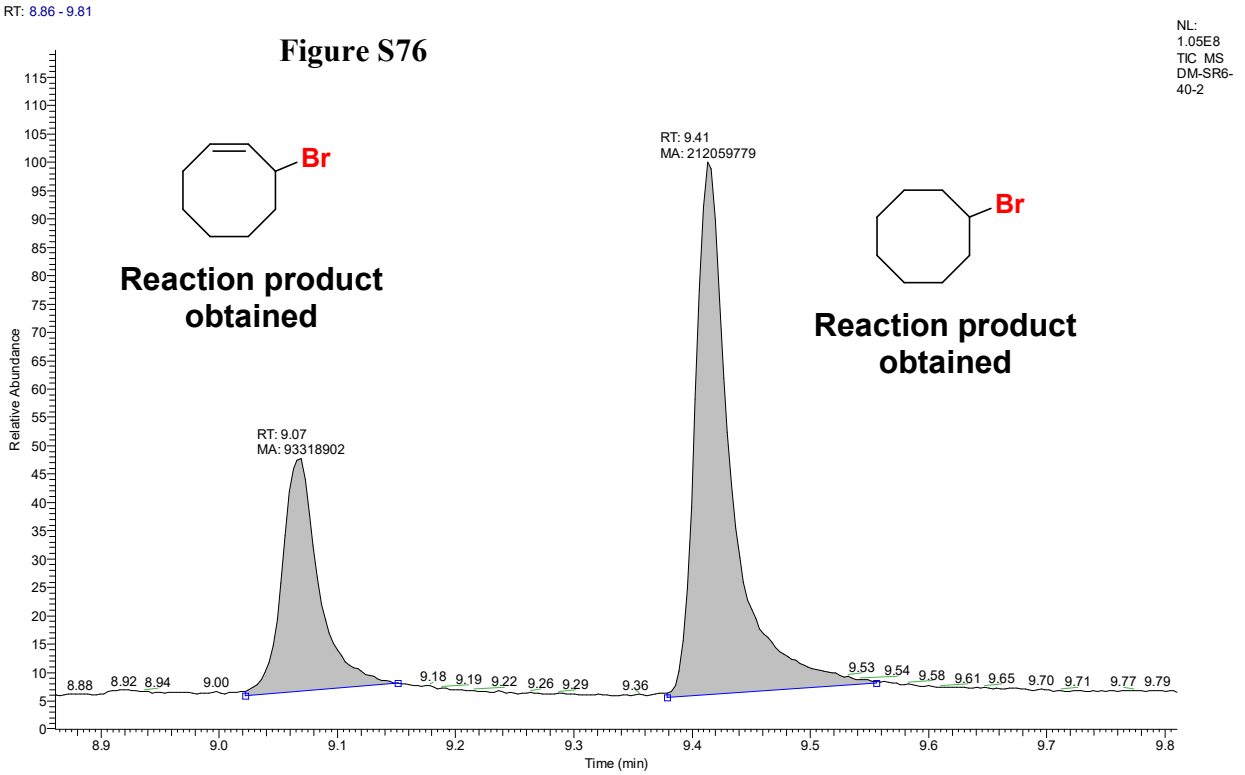


Figure S76

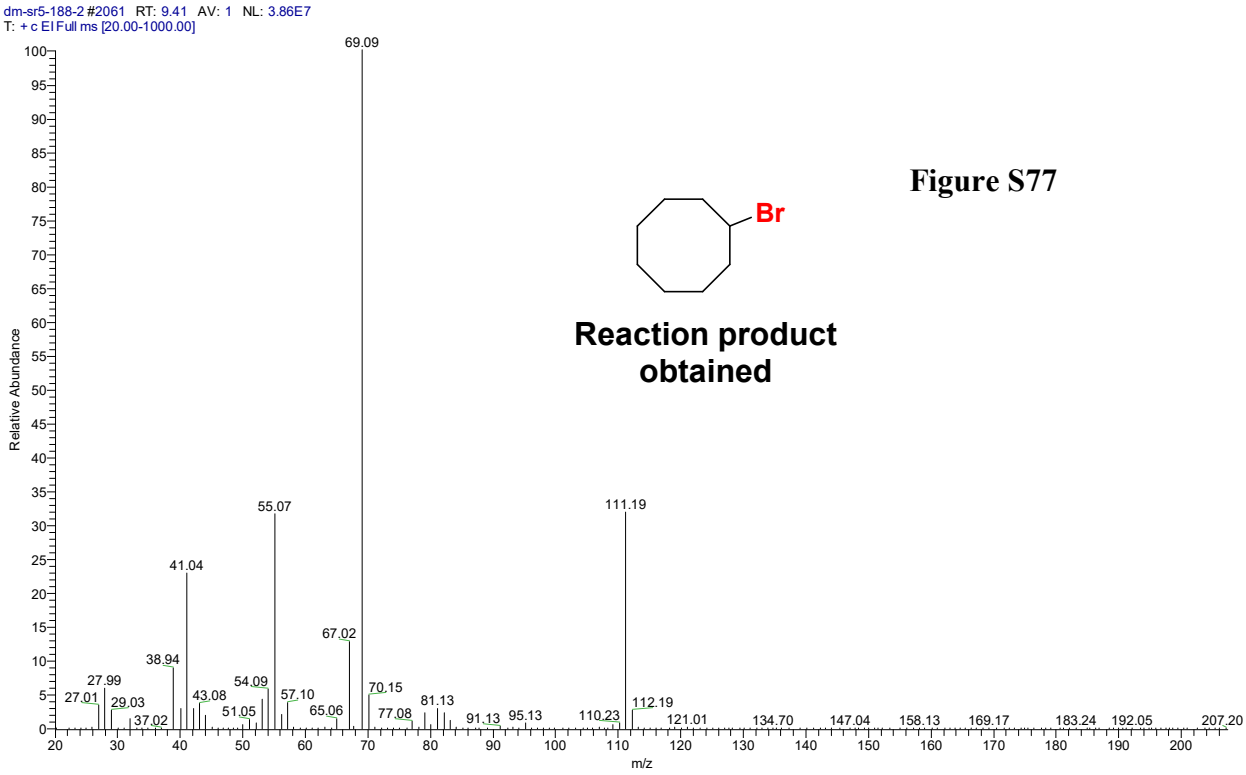


Figure S77

Reaction product obtained

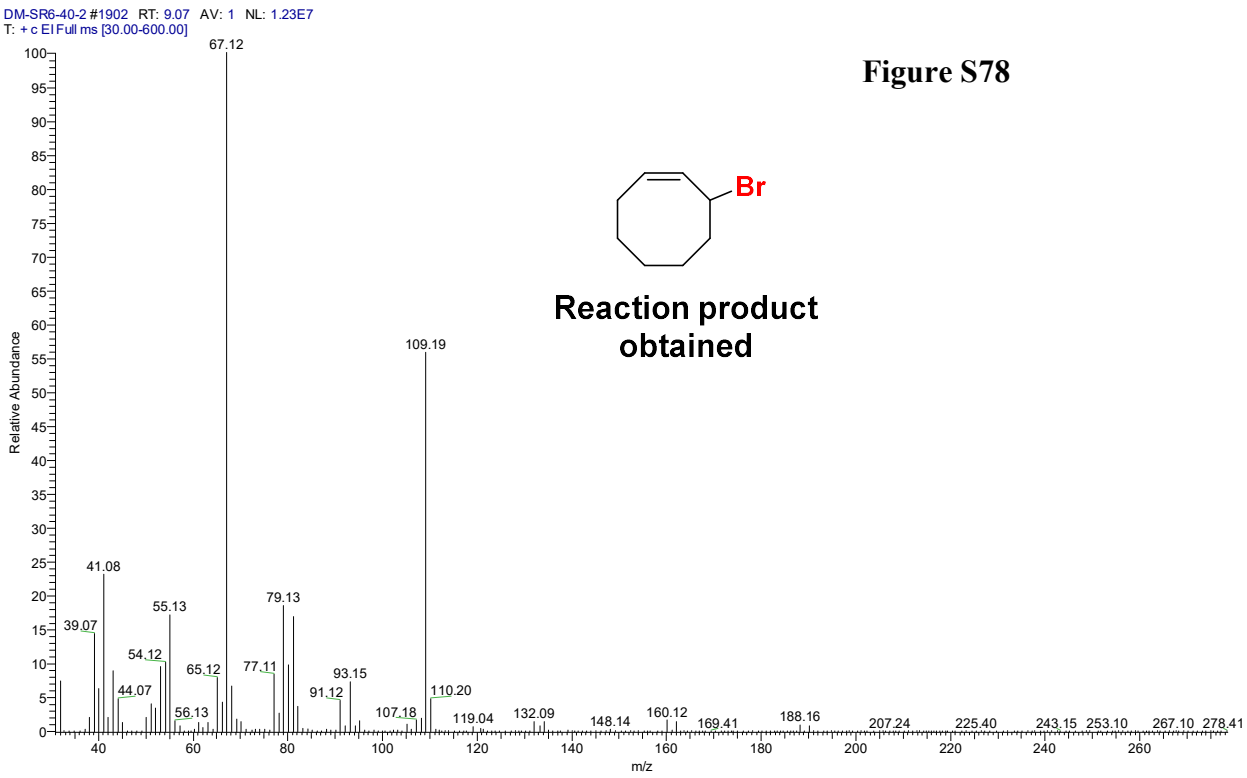

DM-SR6-40-2 #1902 RT: 9.07 AV: 1 NL: 1.23E7
T: + c EI Full ms [30.00-600.00]
Relative Abundance
m/z
67.12
109.19
41.08
79.13
55.13
39.07
54.12
65.12
77.11
93.15
44.07
91.12
110.20
56.13
107.18
119.04
132.09
148.14
160.12
169.41
188.16
207.24
225.40
243.15
253.10
267.10
278.41
Br
Reaction product obtained

Figure S78

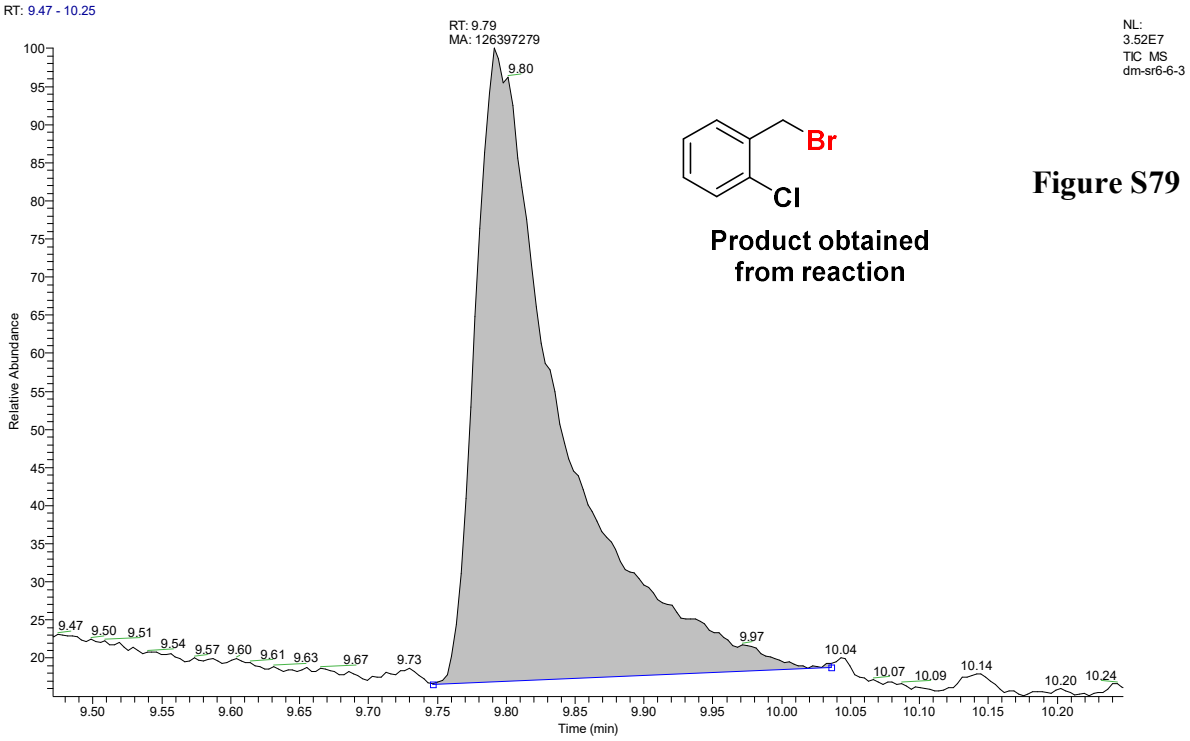


Figure S79

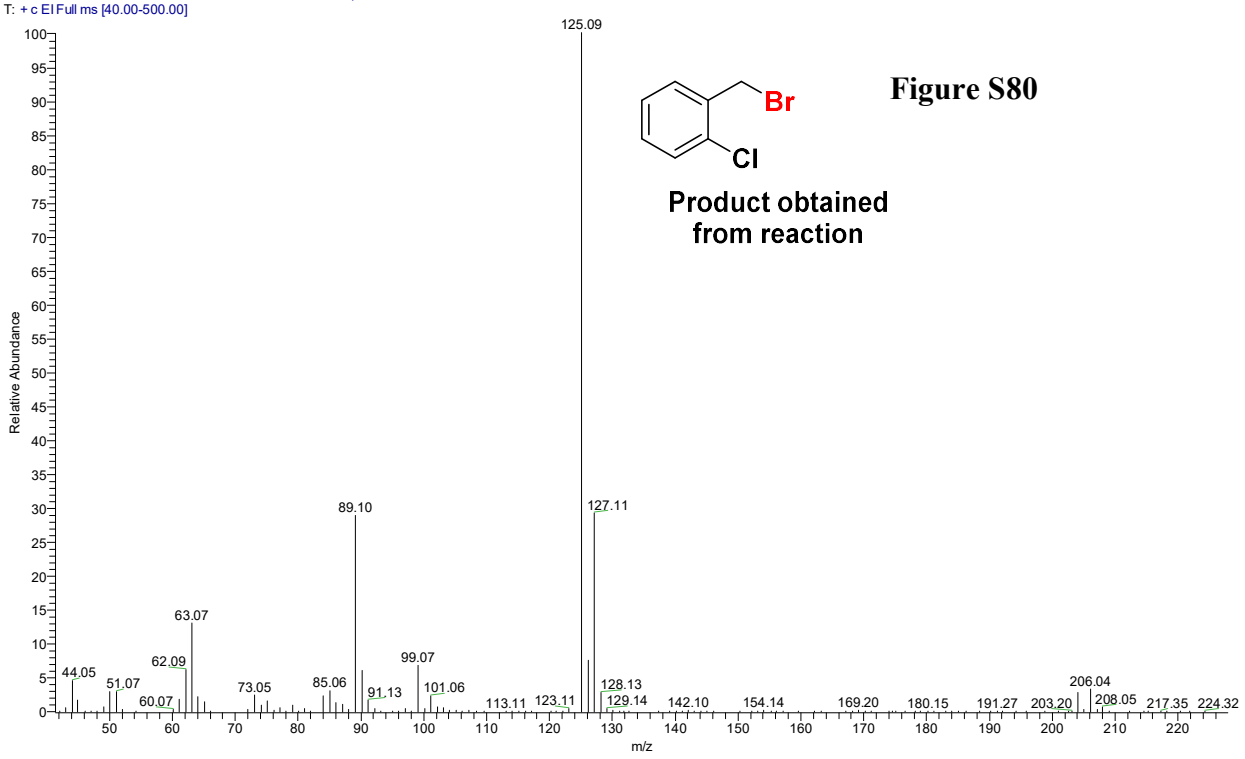


Figure S80

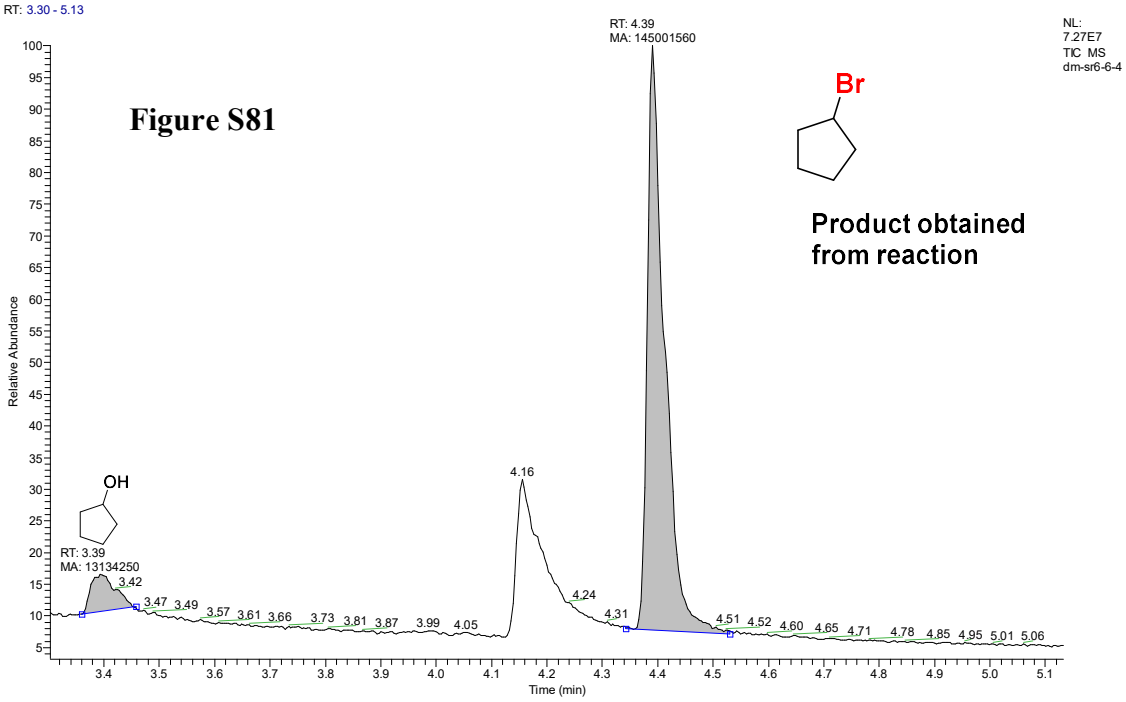


Figure S81

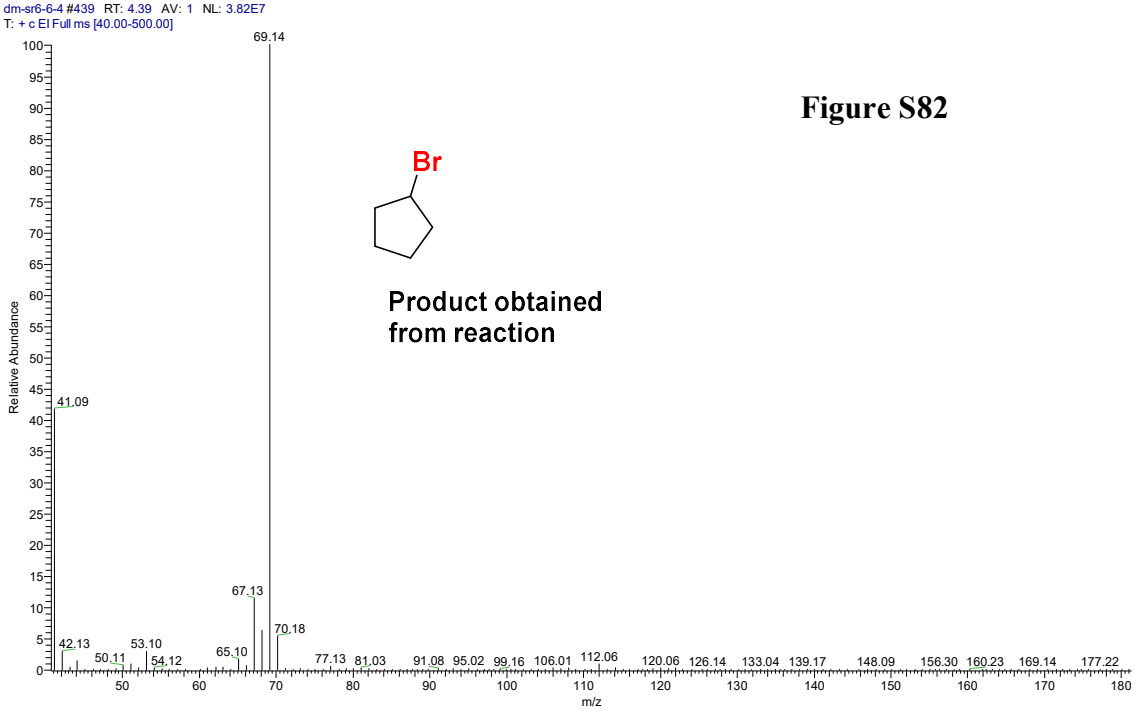
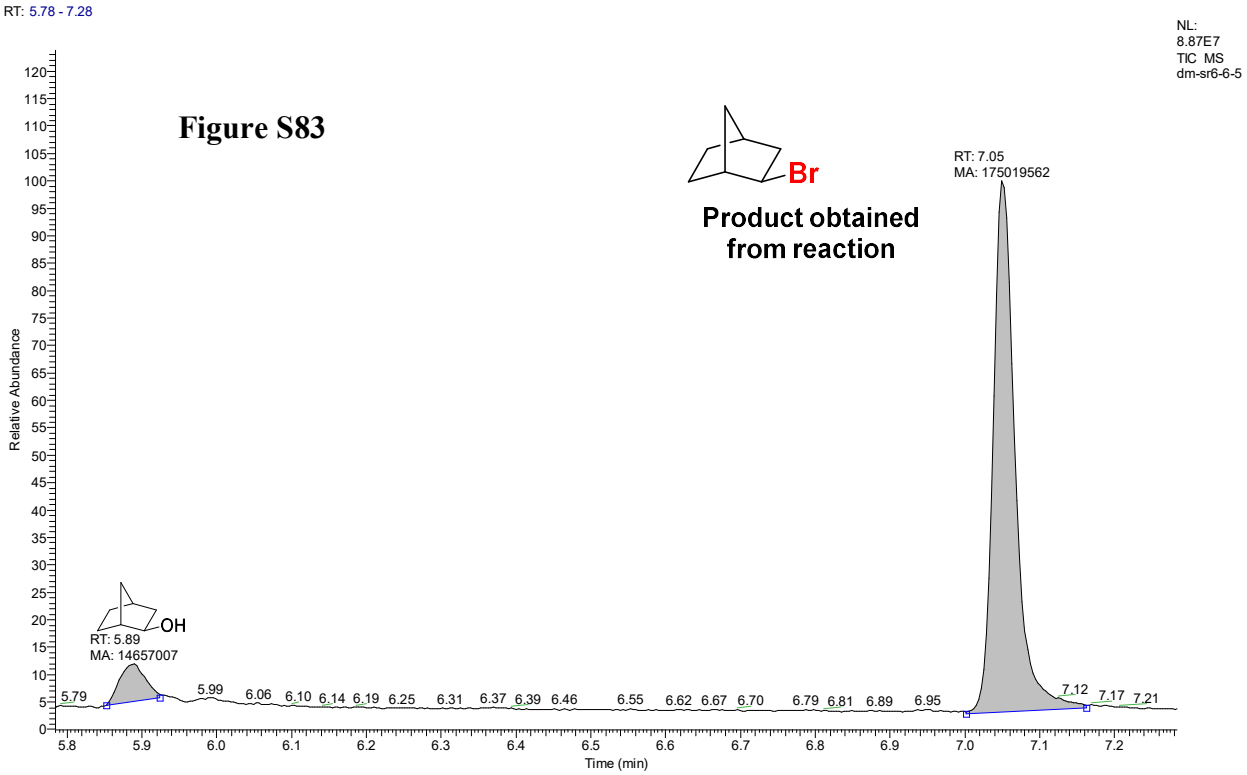


Figure S82


RT: 5.78 - 7.28
NL:
8.87E7
TIC MS
dm-sr6-6-5
Figure S83
Br
Product obtained
from reaction
RT: 7.05
MA: 175019562
OH
RT: 5.89
MA: 14657007
Relative Abundance
Time (min)
5.79
5.99
6.06
6.10
6.14
6.19
6.25
6.31
6.37
6.39
6.46
6.55
6.62
6.67
6.70
6.79
6.81
6.89
6.95
7.12
7.17
7.21

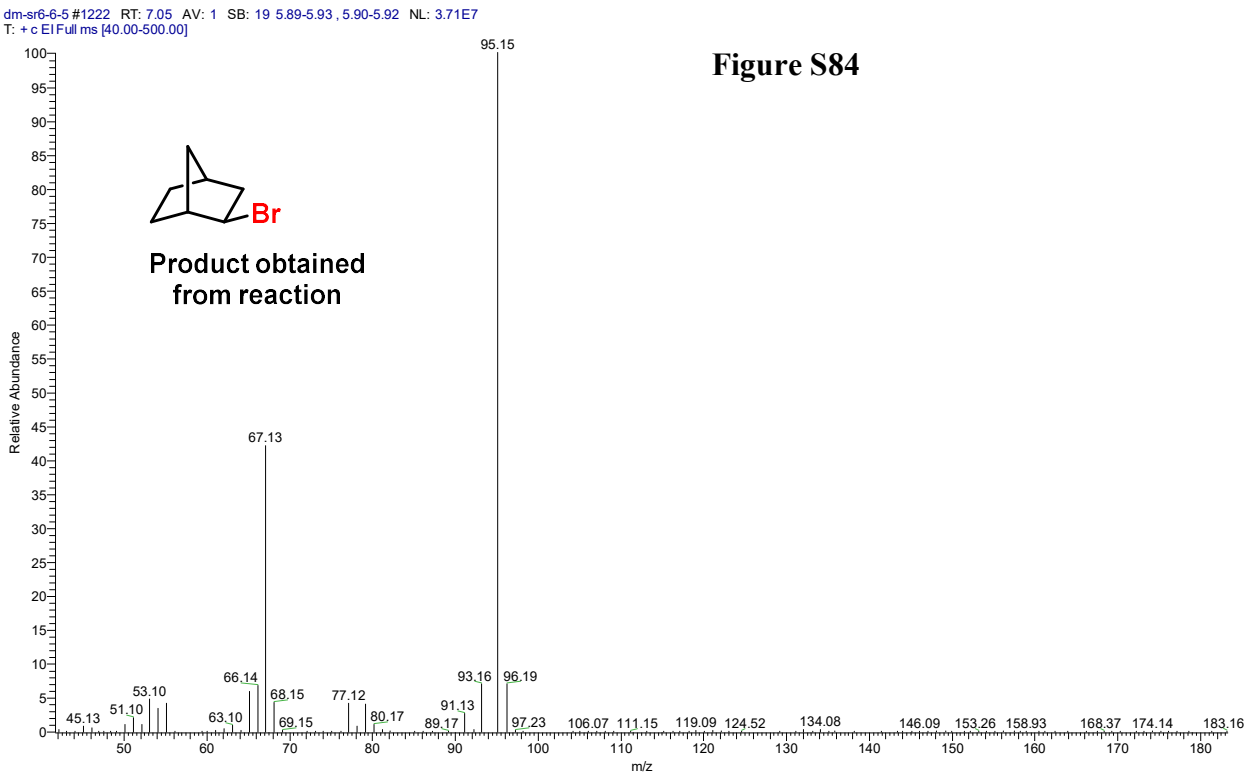
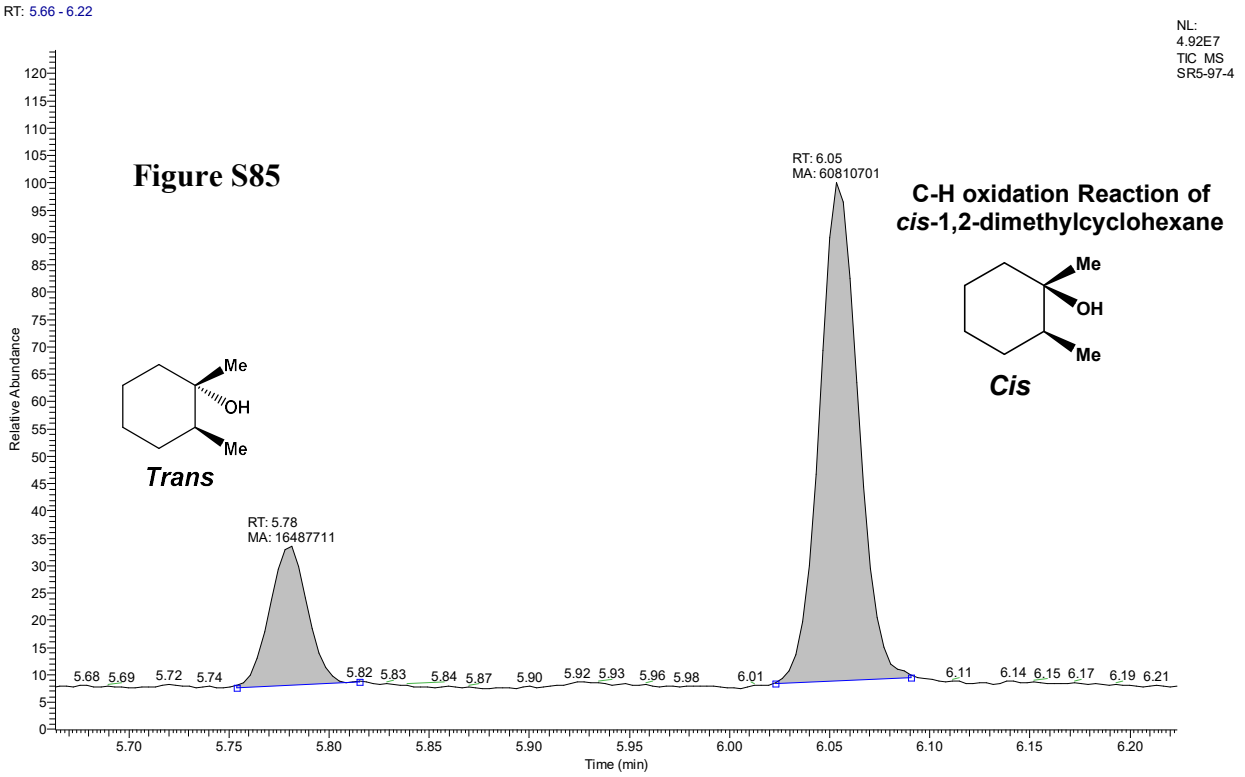
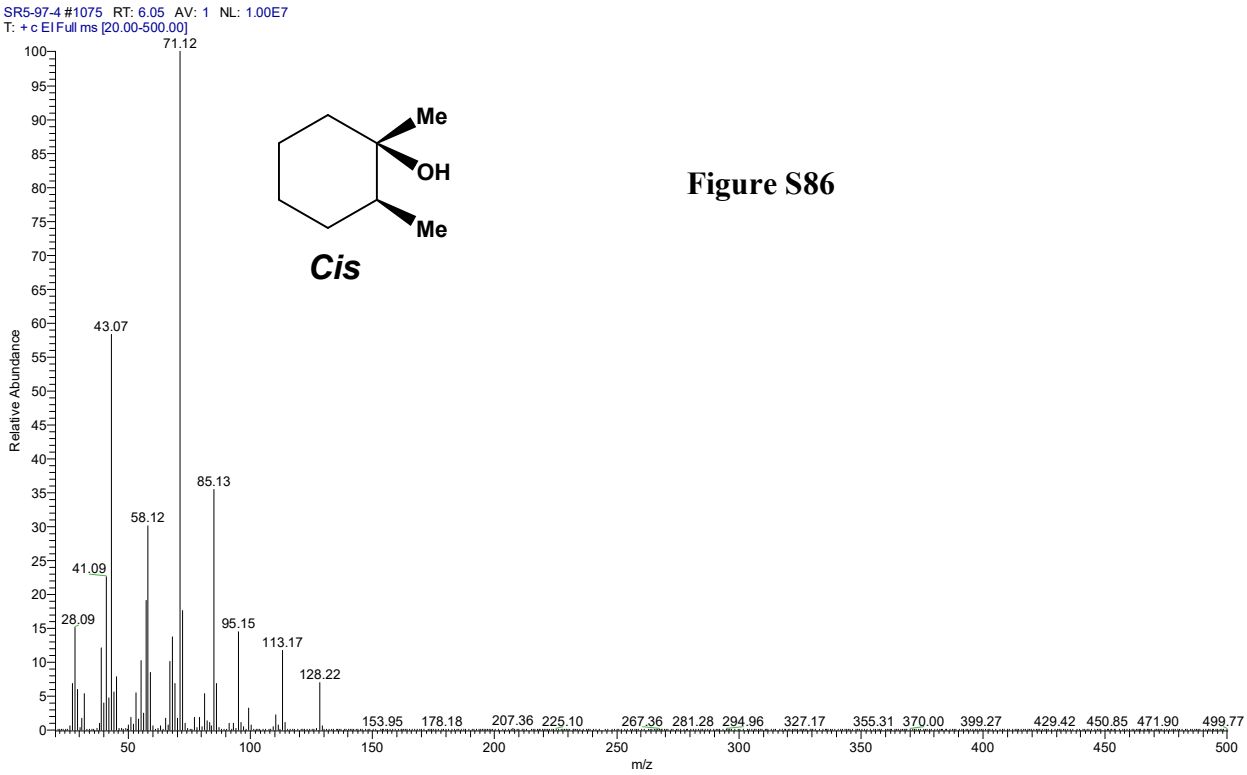

dm-sr6-6-5 #1222 RT: 7.05 AV: 1 SB: 19 5.89-5.93 , 5.90-5.92 NL: 3.71E7
T: + c EI Full ms [40.00-500.00]
Br
Product obtained from reaction
Relative Abundance
m/z
95.15
67.13
66.14
93.16
96.19
53.10
68.15
77.12
91.13
51.10
45.13
63.10
69.15
80.17
89.17
97.23
106.07
111.15
119.09
124.52
134.08
146.09
153.26
158.93
168.37
174.14
183.16

Figure S84


RT: 5.66 - 6.22
NL:
4.92E7
TIC MS
SR5-97-4
Figure S85
C-H oxidation Reaction of
cis-1,2-dimethylcyclohexane
RT: 6.05
MA: 60810701
Me
OH
Me
Cis
Me
OH
Me
Trans
RT: 5.78
MA: 16487711
Relative Abundance
Time (min)


SR5-97-4 #1075 RT: 6.05 AV: 1 NL: 1.00E7
T: + c EI Full ms [20.00-500.00]
Figure S86
Me
OH
Me
Cis
Relative Abundance
m/z

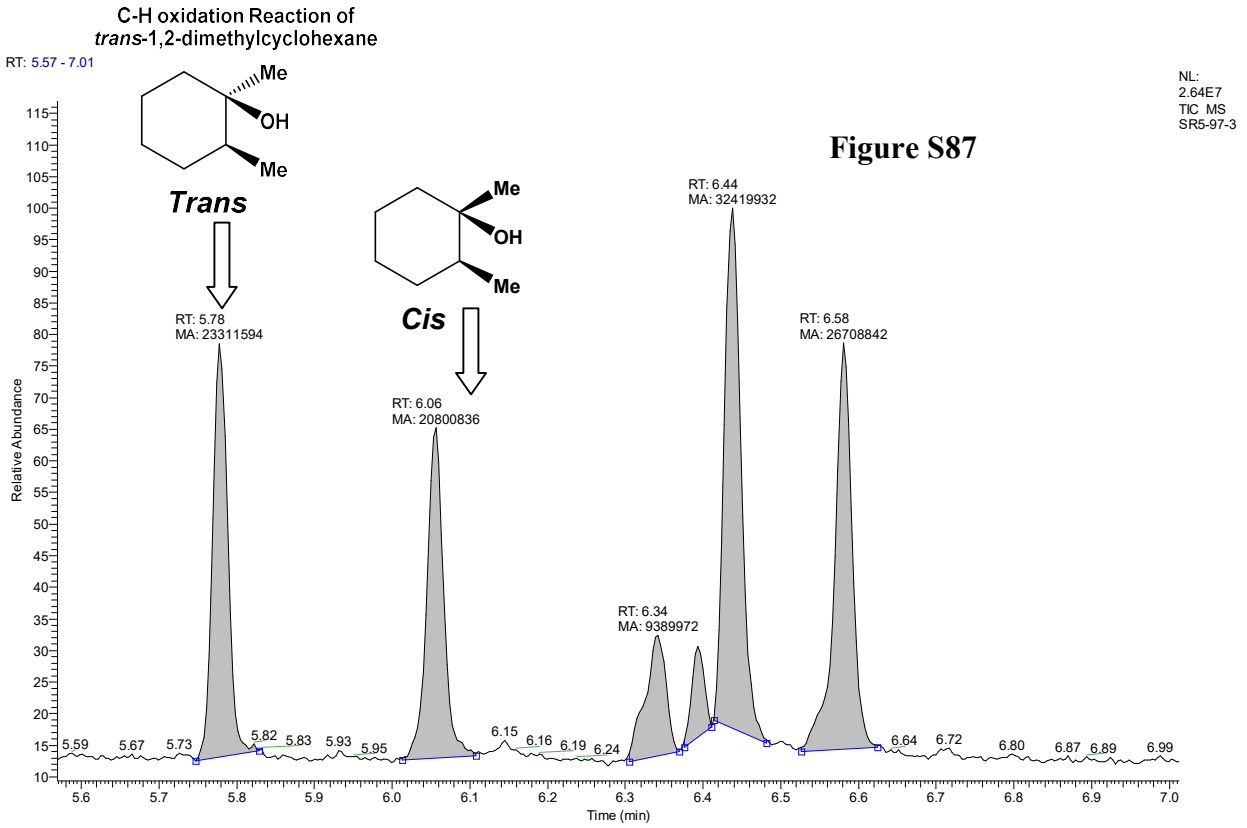


Figure S87

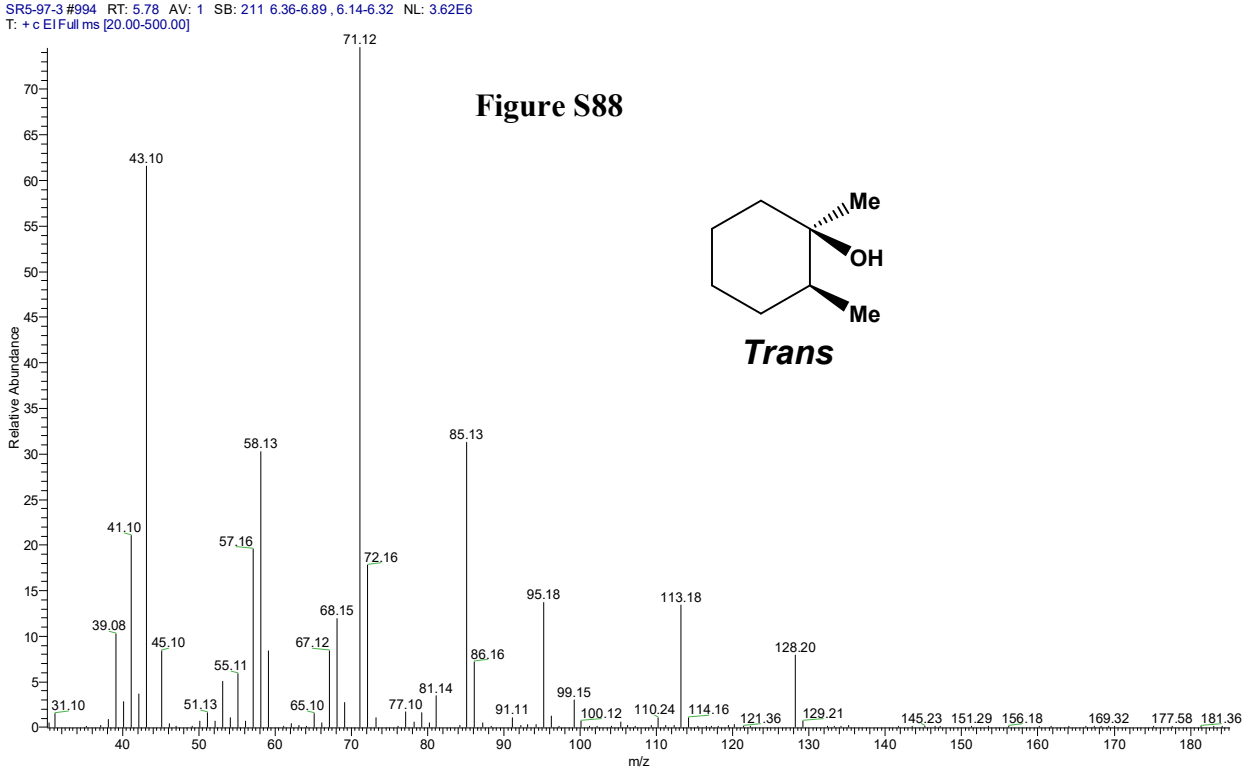
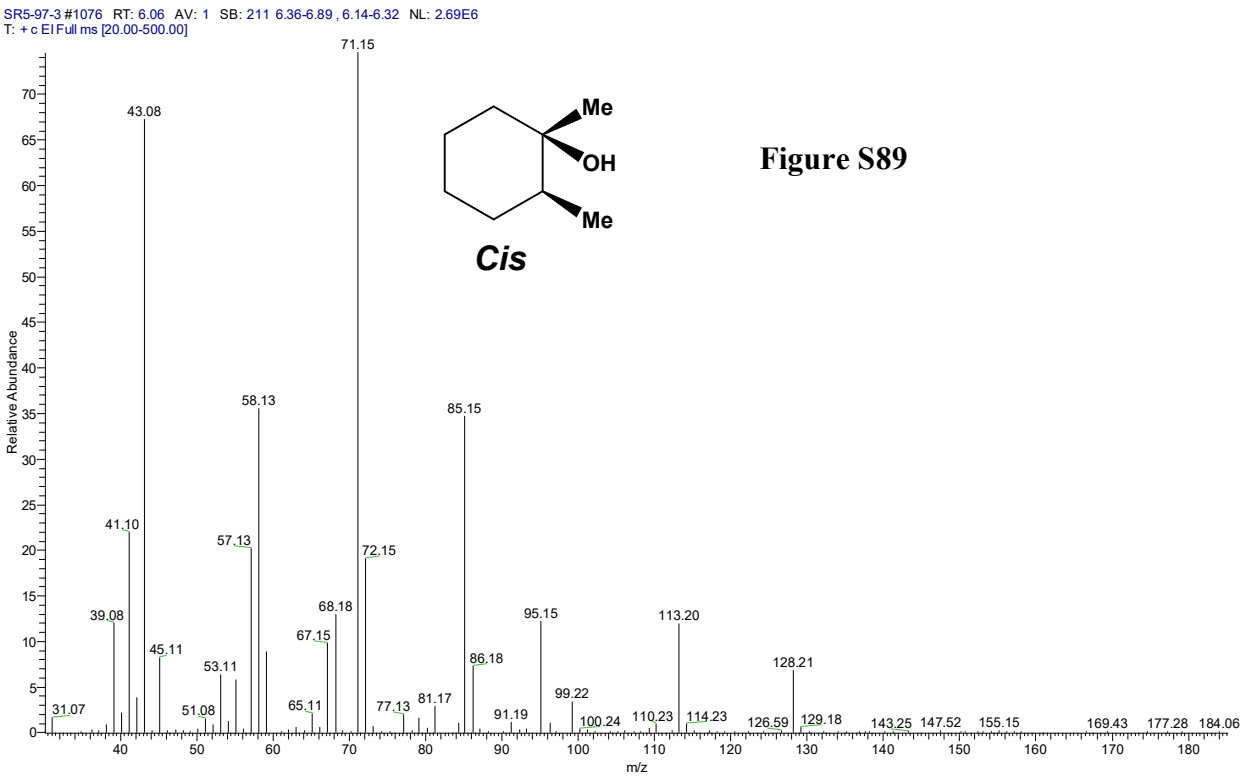


Figure S88



Cis

Figure S89

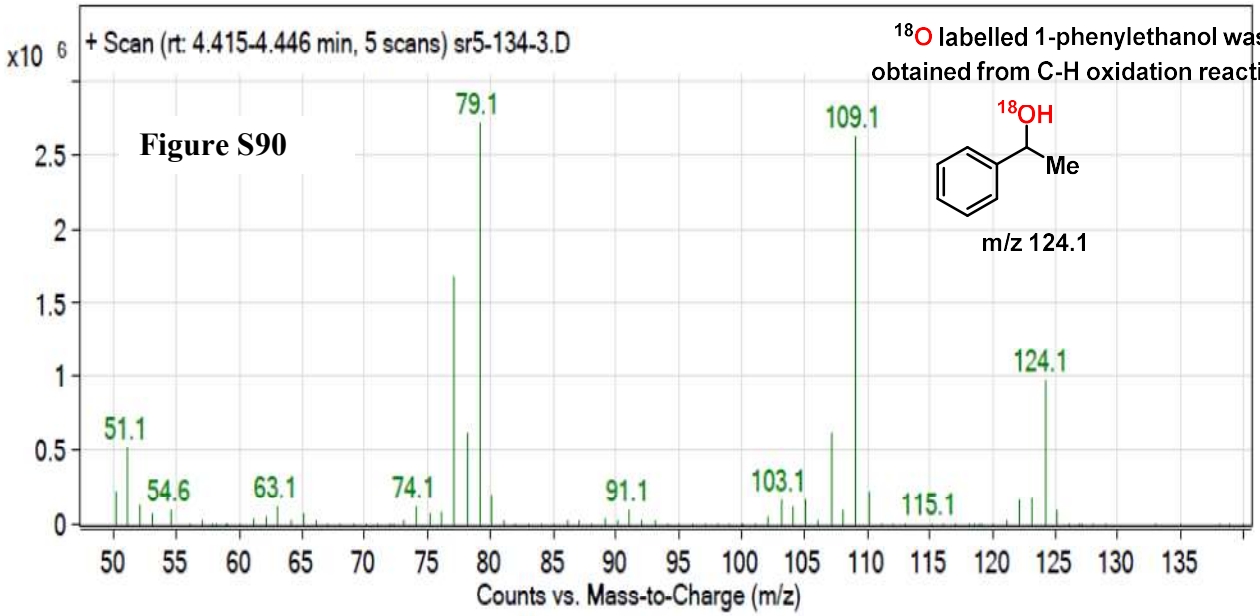
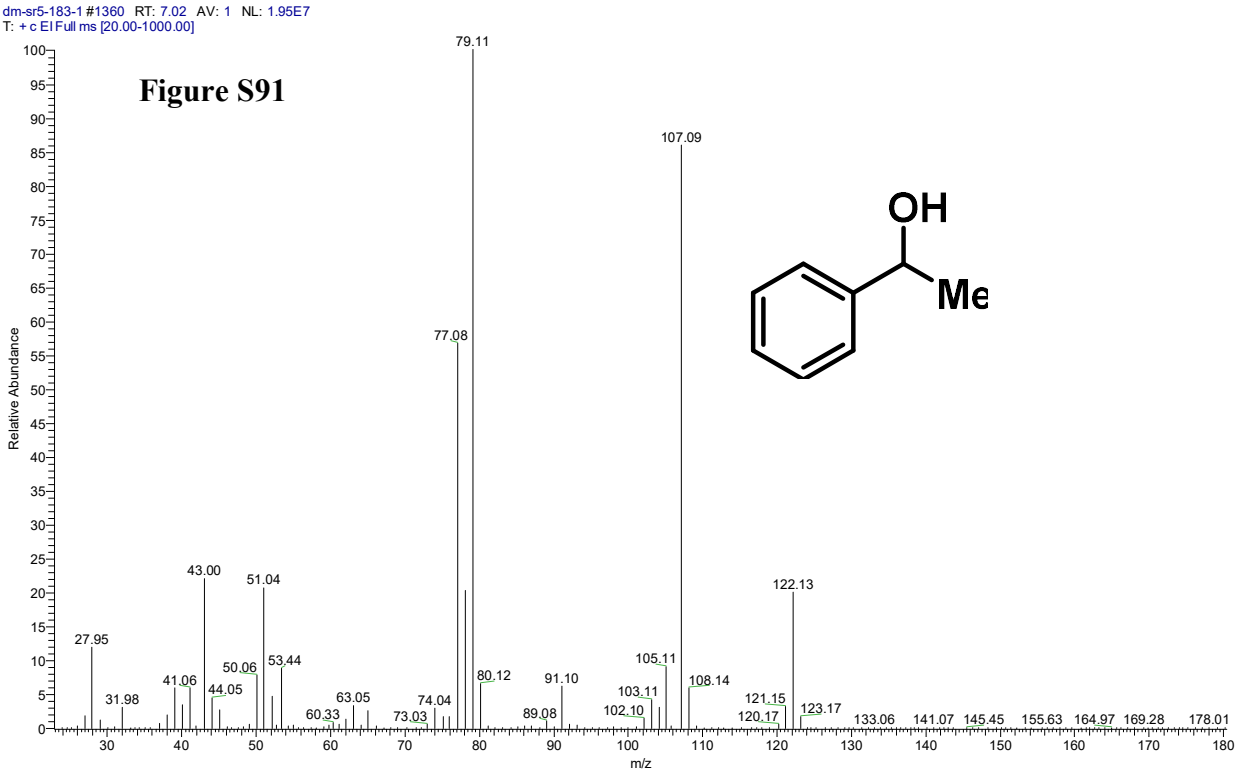
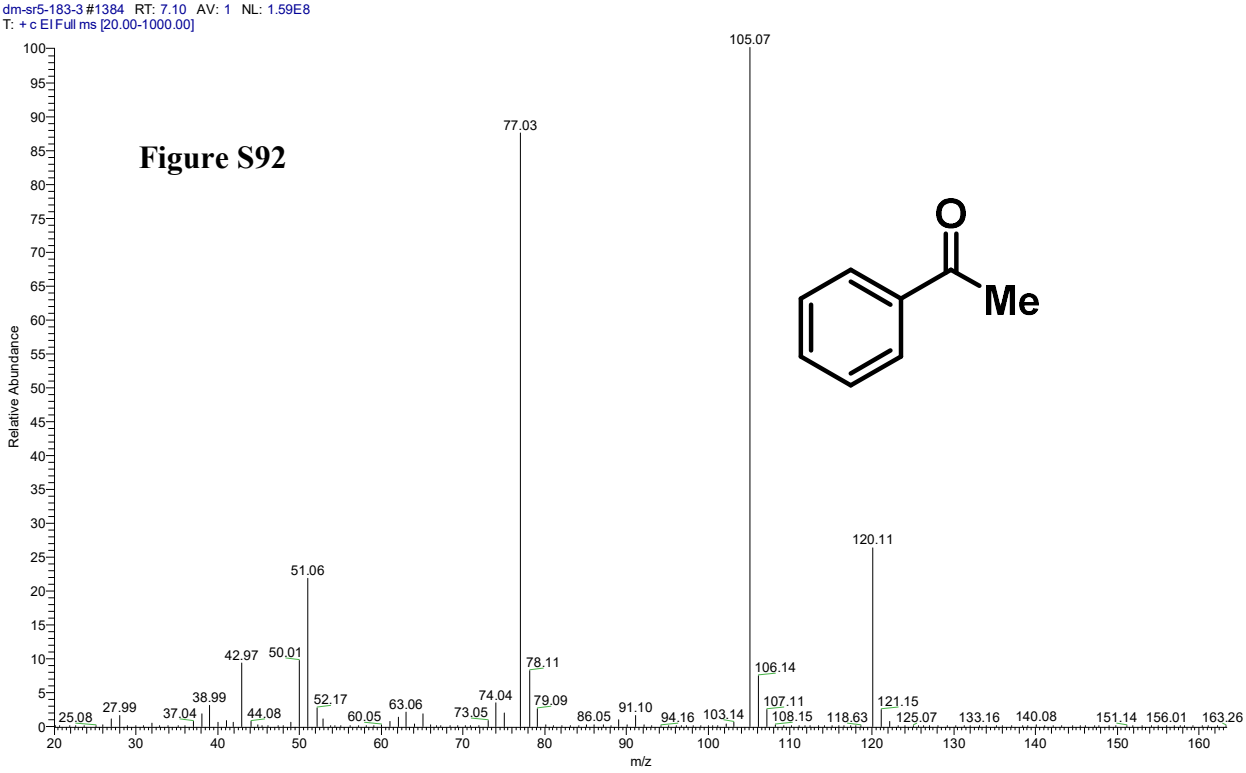


Figure S90

^{18}O labelled 1-phenylethanol was obtained from C-H oxidation reaction

m/z 124.1


dm-sr5-183-1 #1360 RT: 7.02 AV: 1 NL: 1.95E7
T: + c EI Full ms [20.00-1000.00]
Figure S91
Relative Abundance
m/z
OH
Me


dm-sr5-183-3 #1384 RT: 7.10 AV: 1 NL: 1.59E8
T: + c EI Full ms [20.00-1000.00]
Figure S92
Relative Abundance
m/z
O
Me

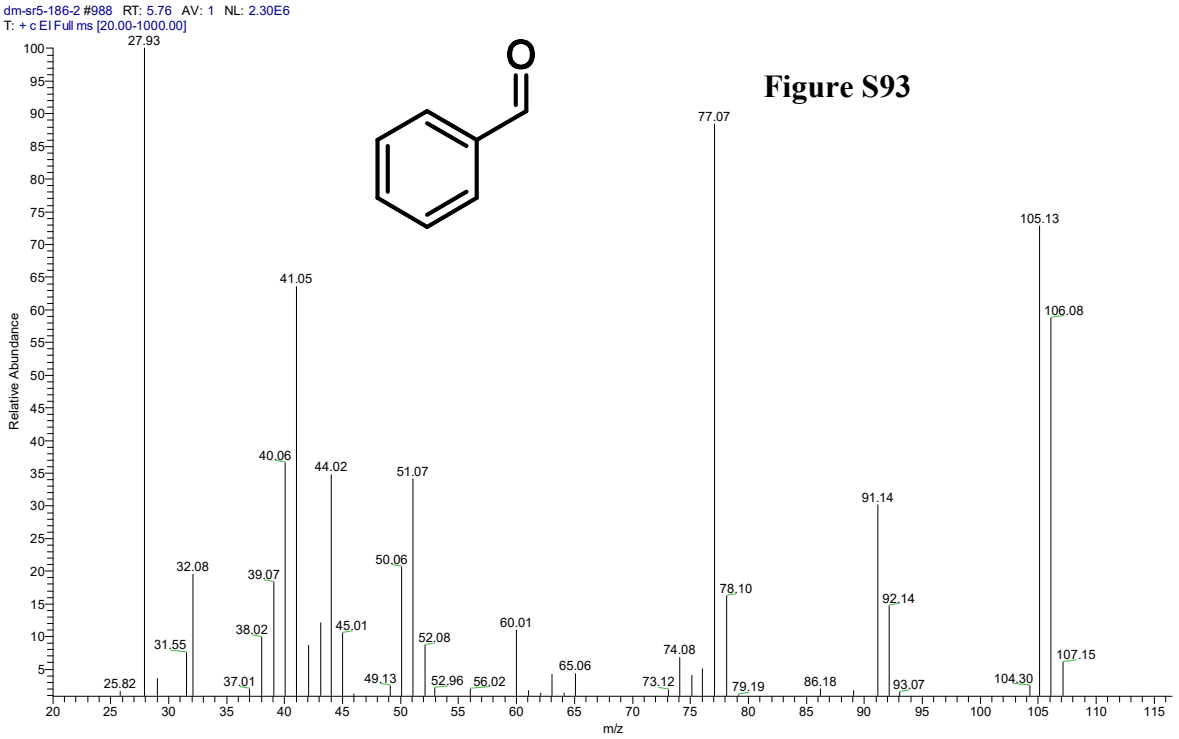


Figure S93

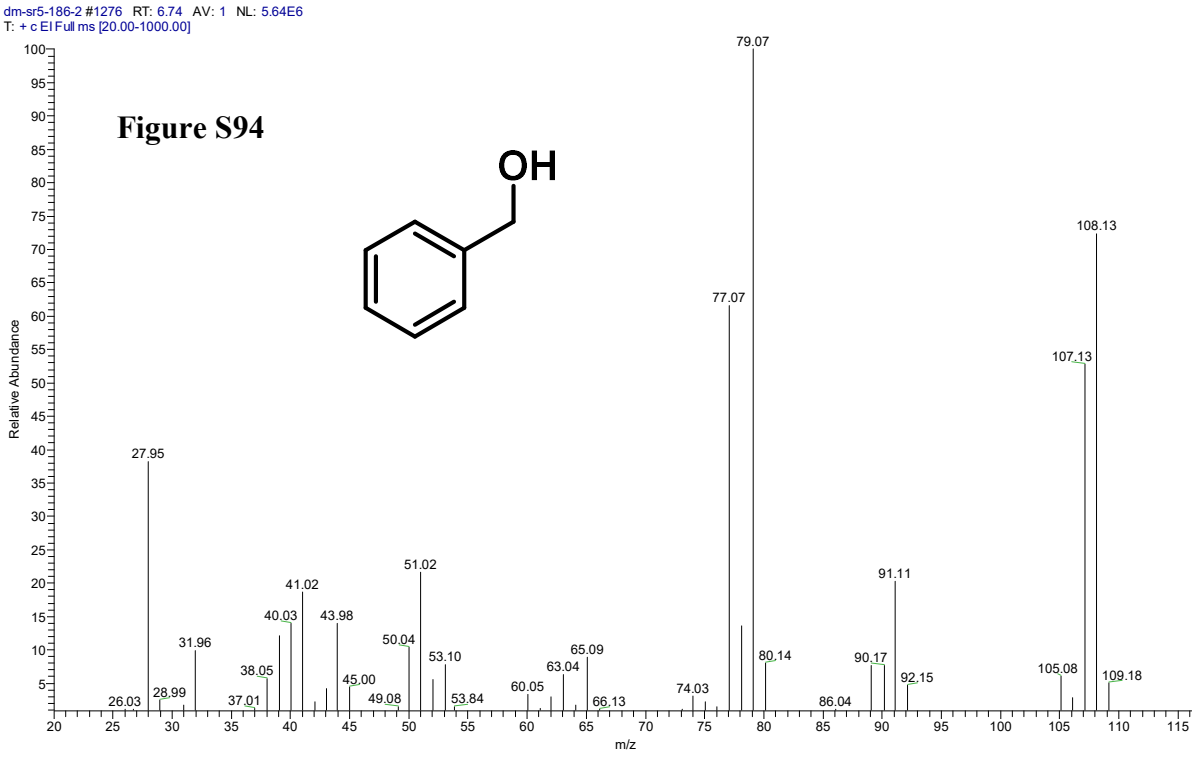


Figure S94

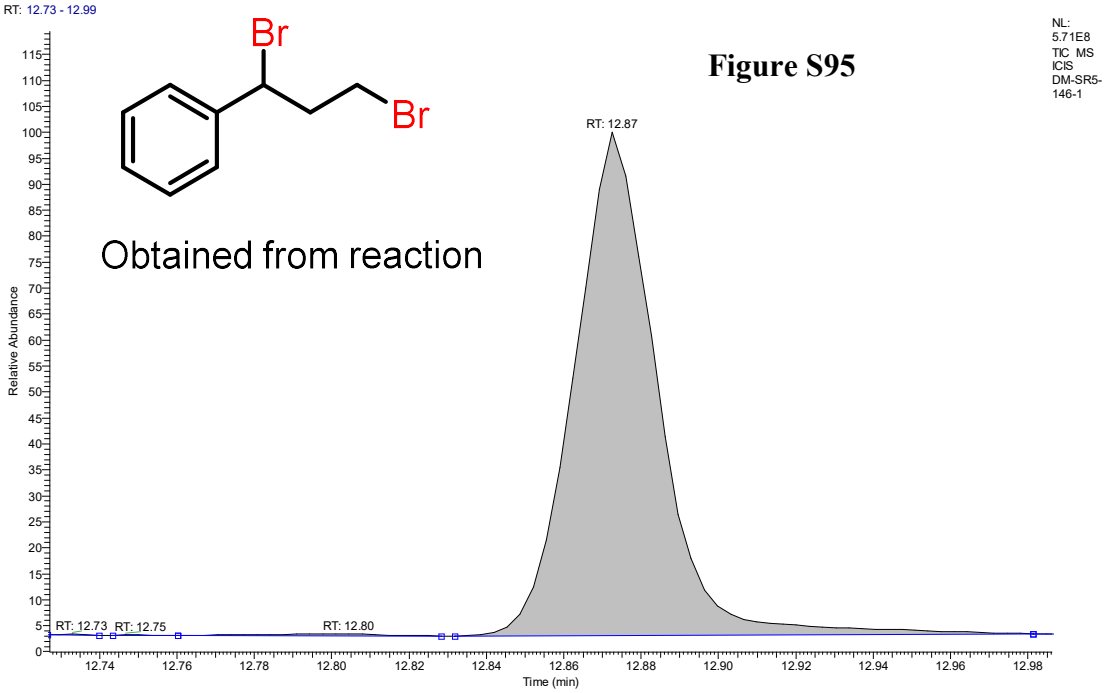


Figure S95

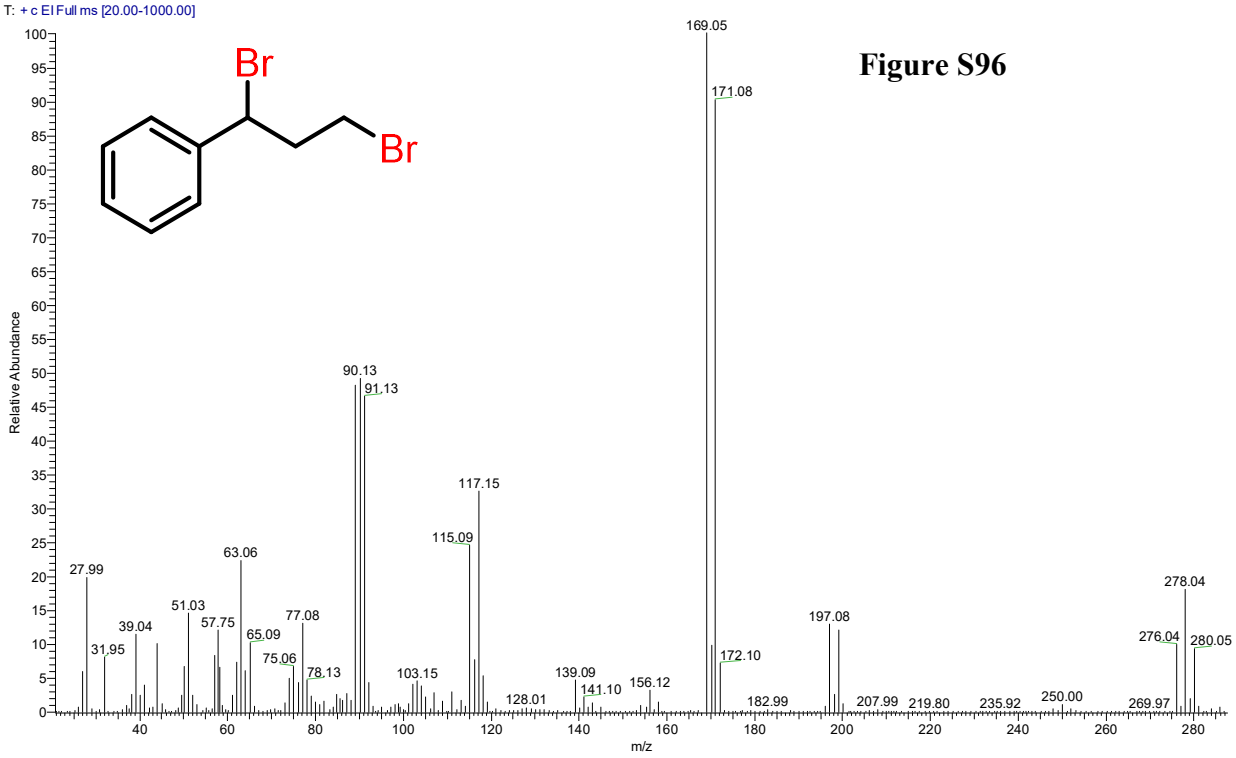


Figure S96

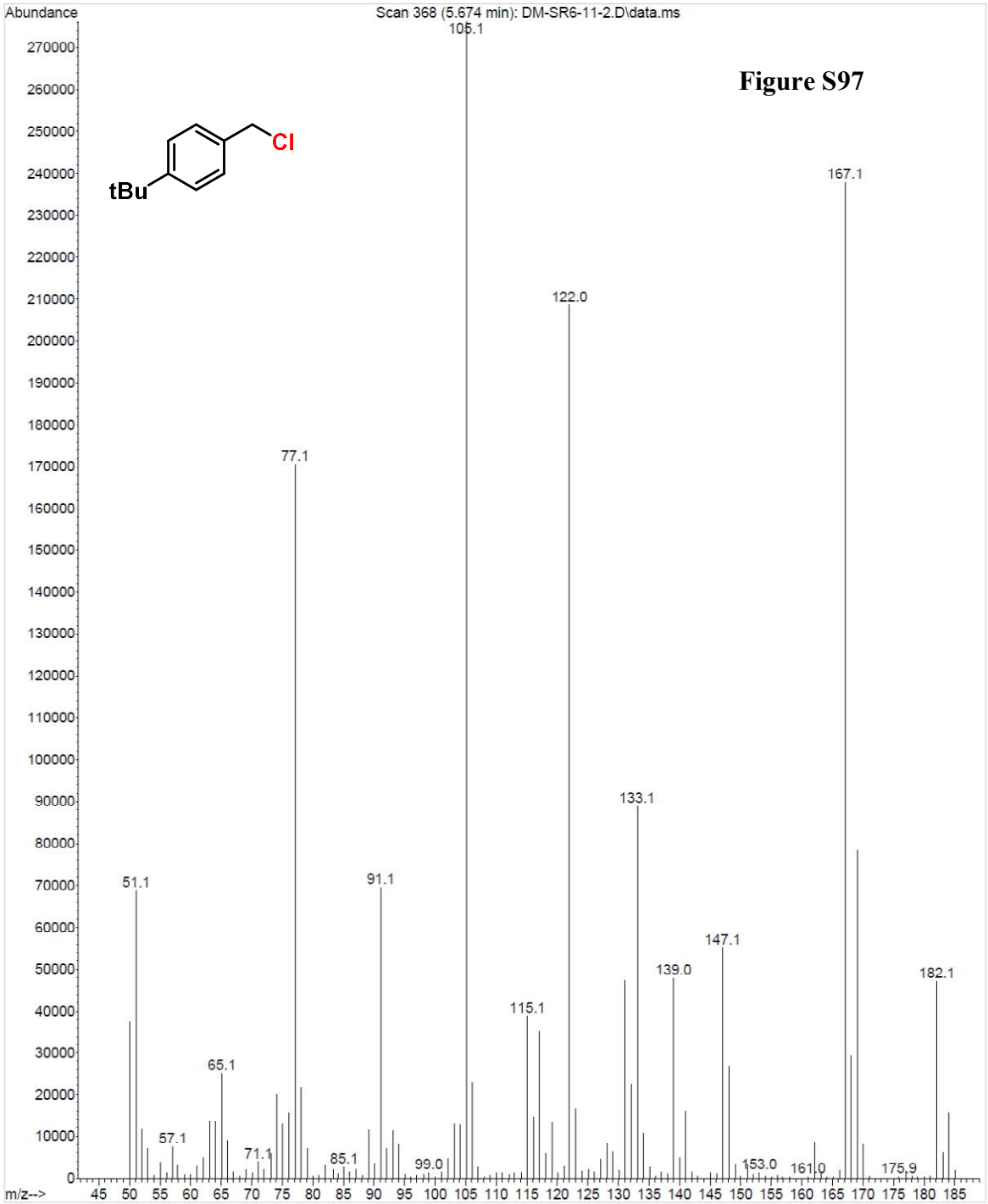

Abundance
Scan 368 (5.674 min): DM-SR6-11-2.D\data.ms
105.1
167.1
122.0
77.1
133.1
51.1
91.1
147.1
139.0
182.1
115.1
65.1
57.1
71.1
85.1
99.0
153.0
161.0
175.9
m/z-->
Cl
tBu

Figure S97

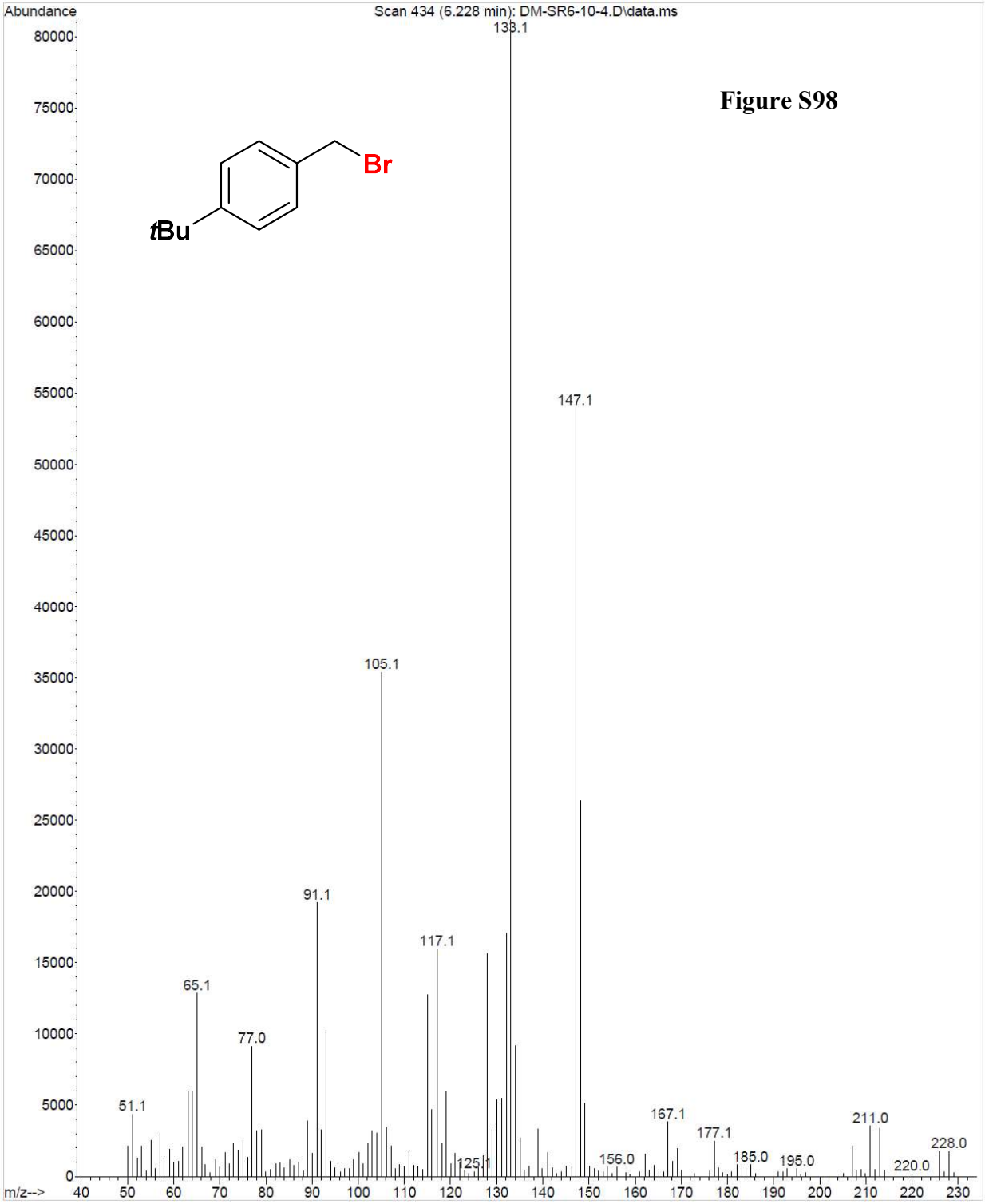

Abundance
Scan 434 (6.228 min): DM-SR6-10-4.D\data.ms
138.1
147.1
105.1
91.1
117.1
65.1
77.0
51.1
125.1
156.0
167.1
177.1
185.0
195.0
211.0
220.0
228.0
Br
tBu
m/z-->

Figure S98

4. Computational details:

4.1. Table S5: Selected structural parameters of transition states and intermediates. All the bond lengths are in Angstrom.

	Fe-O	O-H	Fe-N	Fe-N1	Fe-N2	Fe-N3	Fe-N4	Fe-Cl	C-H	C-Cl	O-C
^{5}R+CH	1.619		2.103	2.132	2.132	2.142	2.142				
^{3}R+CH	1.626		2.086	2.000	2.000	2.036	2.036				
^{1}R+CH	1.631		2.084	2.016	2.016	2.008	2.007				
^{5}ts1	1.693	1.432	2.240	2.174	2.182	2.172	2.162		1.194		
^{3}ts1	1.737	1.237	2.070	2.010	2.018	2.036	2.061		1.315		
^{1}ts1	1.710	1.385	2.067	2.032	2.054	2.021	2.015		1.195		
^{7}Int1$_{hs}$	1.796	0.991	2.272	2.211	2.204	2.174	2.151				3.002
^{5}Int1$_{hs}$	1.792	1.002	2.285	2.216	2.201	2.184	2.164				2.880
^{5}Int1$_{is}$	1.811	0.984	2.244	2.211	2.232	2.198	2.194				3.080
^{3}Int1$_{is}$	1.761	0.991	2.100	2.004	2.261	2.065	2.242				2.990
^{3}Int1$_{ls}$	1.784	0.987	2.054	1.986	1.986	2.059	2.059				3.073
^{1}Int1$_{ls}$	1.787	0.982	2.051	1.989	1.985	2.061	2.056				3.118
^{6}Int2	1.812	0.971	2.263	2.203	2.202	2.151	2.152				
^{4}Int2	1.851	0.970	2.279	2.066	2.067	2.051	2.051				
^{2}Int2	1.780	0.971	2.050	1.994	1.994	2.076	2.076				
^{7}ts2	1.896	0.973	2.256	2.206	2.195	2.189	2.060				2.094
^{5}ts2	1.920	0.970	2.334	2.262	2.306	2.284	2.250				3.268
^{3}ts2	1.810	0.972	2.082	1.996	2.001	2.064	2.060				2.687

^{6}Int3			2.248	2.195		2.167		2.263			
^{4}Int3			2.260	2.069		2.072		2.332			
^{2}Int3			2.012	2.012	2.012	2.055	2.055	2.288			
^{7}Int4			2.248	2.205	2.193	2.170	2.163	2.249		3.442	
^{5}Int4			2.274	2.223	2.236	2.260	2.239	2.439		3.06	
^{3}Int4			2.220	2.010	2.162	2.060	2.134	2.549		3.010	
^{7}ts3			2.249	2.235	2.212	2.097	2.228	2.435		2.536	
^{5}ts3			2.218	2.021	2.076	1.983	2.024	2.602		2.368	
^{3}ts3			2.233	2.023	2.078	2.056	2.078	2.764		2.575	
^{5}P+P_{OH}	2.104	0.974	2.246	2.294	2.192	2.361	2.201				1.473
^{3}P+P_{OH}	2.127	0.973	2.264	2.255	2.255	2.129	2.202				1.478
^{1}P+P_{OH}											
^{5}P+P_{Cl}			2.228	2.204	2.221	2.172	2.199	2.762		1.948	
^{3}P+P_{Cl}			2.210	2.026	2.018	2.024	2.023	3.237		1.900	
^{1}P+P_{Cl}			1.978	2.000	2.003	2.013	2.013	3.141		1.911	

4.2. Table S6 : Computed spin density values for the intermediates and transition states.

	Fe	O	H	N	N1	N2	N3	N4	Cl	C
^{5}**R+CH**	2.933	0.723		-0.034	0.074	0.074	0.079	0.079		
^{3}**R+CH**	1.198	0.854		-0.019	-0.007	-0.007	-0.002	-0.002		
^{5}**ts1**	3.775	1.693	-0.035	0.032	0.063	0.065	0.063	0.059		
^{3}**ts1**	0.952	0.603	0.020	-0.018	-0.016	-0.006	-0.002	-0.017		
^{7}**Int1$_{hs}$**	4.183	0.338	0.008	0.082	0.084	0.083	0.071	0.071		0.998
^{5}**Int1$_{hs}$**	4.162	0.096	0.069	-0.037	0.026	0.020	0.031	0.027		-0.865
^{5}**Int1$_{is}$**	3.785	0.016	0.003	0.051	0.026	0.024	0.027	0.022		0.912
^{3}**Int1$_{is}$**	0.939	0.129	-3.030	-0.014	-0.019	-0.015	-0.014	-0.010		-1.000
^{3}**Int1$_{ls}$**	0.935	0.168	0.017	-0.015	-0.017	-0.017	-0.013	-0.013		0.999
^{5}**ts2**	3.777	0.100	0.008	0.028	0.021	0.020	0.019	0.026		0.008
^{3}**ts2**	1.052	0.084	-0.002	-0.008	-0.020	-0.018	-0.016	-0.015		0.986
^{6}**Int2**	4.189	0.325	0.010	0.075	0.083	0.083	0.087	0.087		
^{4}**Int2**	2.726	0.292	0.010	0.079	-0.015	-0.015	-0.032	-0.032		
^{2}**Int2**	0.937	0.148	-0.005	-0.016	-0.017	-0.017	-0.013	-0.013		
^{6}**Int3**	3.987			0.131	0.123	0.123	0.112	0.112	0.333	
^{4}**Int3**	2.763			0.111	-0.018			-0.040	0.267	
^{2}**Int3**	1.048			-0.022	-0.021		-0.022		0.033	
^{7}**Int4**	4.182			0.118	0.091	0.098	0.076	0.076	0.265	1.044
^{5}**Int4**	3.782			0.047	0.025	0.024	0.013	0.022	0.049	0.007
^{3}**Int4**	1.993			0.047	0.035	0.015	-0.028	0.001	0.026	0.006
^{7}**ts3**	4.207			0.129	0.084	0.089	0.077	0.073	0.237	0.962
^{5}**ts3**	3.780			0.054	0.023	0.020	0.019	0.015	0.006	0.003
^{3}**ts3**	2.016			0.056	-0.031	-0.006	-0.030	-0.012	-0.002	0.031
^{5}**P+P$_{OH}$**	3.789	0.020		0.039	0.014	0.025	0.004	0.015		0.006
^{3}**P+P$_{OH}$**	3.785	0.020		0.051	0.026	0.024	0.027	0.022		0.010

^{5}P+P_{Cl}	3.767			0.052	0.024	0.020	0.023	0.012	0.008	0.010
^{3}P+P_{Cl}	2.027			0.051	-0.025	-0.026	-0.028	-0.029	0.007	0.004

5. Optimized Cartesian coordinates using B3LYP density functional for all the species involved in the reaction pathway and their corresponding energies:

Solvation energies = E and {Solvation energy + Gibbs free energy} =G

^{5}R ;

S= -3045.441827 ,**G**=-3044.856438

Fe	0.564952000	0.000204000	-0.507102000
O	0.196225000	-0.000052000	-2.083889000
N	1.335549000	0.000141000	1.449370000
N	2.149827000	1.420039000	-0.643393000
N	-0.760756000	1.445991000	0.350624000
N	-0.760787000	-1.446043000	0.351306000
N	2.148924000	-1.420335000	-0.643267000
C	-0.486197000	1.679113000	1.639463000
C	3.098480000	1.221586000	0.297607000
C	3.386183000	3.263280000	-1.512379000
H	3.471501000	4.057307000	-2.246380000
C	-2.246737000	1.724572000	-1.553162000
H	-1.541157000	1.199593000	-2.182400000
C	4.222366000	2.028980000	0.390670000
H	4.967716000	1.853010000	1.159798000
C	2.281684000	2.409813000	-1.536166000

H	1.488764000	2.500343000	-2.271265000
C	-1.357352000	-2.369293000	2.500137000
H	-1.080327000	-2.521297000	3.538127000
C	0.864755000	1.235605000	2.147074000
H	0.843284000	1.074296000	3.230283000
H	1.583807000	2.038181000	1.954421000
C	-0.486727000	-1.678108000	1.640384000
C	-1.939569000	1.920555000	-0.187254000
C	0.864354000	-1.234768000	2.147790000
H	0.842971000	-1.072820000	3.230905000
H	1.583147000	-2.037685000	1.955574000
C	-2.873748000	2.637205000	0.637529000
C	-2.552074000	-2.841677000	1.997160000
H	-3.251376000	-3.374360000	2.635963000
C	-2.874420000	-2.635974000	0.638632000
C	2.817461000	-0.000266000	1.160118000
H	3.415039000	-0.000409000	2.078159000
C	-1.939583000	-1.920633000	-0.186524000
C	-2.246015000	-1.726067000	-1.552804000
H	-1.539876000	-1.202140000	-2.182305000
C	-1.356229000	2.371529000	2.498792000
H	-1.078839000	2.524339000	3.536565000
C	3.097707000	-1.222387000	0.297719000

C	-3.428265000	-2.215205000	-2.071606000
H	-3.647490000	-2.068610000	-3.125087000
C	4.364566000	3.071486000	-0.535658000
H	5.231933000	3.723126000	-0.491638000
C	-2.550848000	2.844095000	1.995725000
H	-3.249662000	3.377760000	2.634241000
C	-3.428998000	2.213678000	-2.071973000
H	-3.648785000	2.065946000	-3.125178000
C	-4.084759000	3.116665000	0.072149000
H	-4.780003000	3.654654000	0.710212000
C	4.221040000	-2.030536000	0.390875000
H	4.966510000	-1.854986000	1.159983000
C	3.384021000	-3.264517000	-1.512014000
H	3.468806000	-4.058684000	-2.245923000
C	-4.085425000	-3.115453000	0.073263000
H	-4.781217000	-3.652405000	0.711604000
C	-4.359533000	-2.908625000	-1.259459000
H	-5.282166000	-3.280292000	-1.693653000
C	2.280097000	-2.410306000	-1.535911000
H	1.487107000	-2.500378000	-2.270988000
C	-4.359563000	2.908486000	-1.260209000
H	-5.282214000	3.280097000	-1.694412000
C	4.362532000	-3.073258000	-0.535318000

H	5.229453000	-3.725484000	-0.491208000

^{3}R;

S= -3045.450963, **G**= -3044.86126

Fe	0.565881000	-0.000109000	-0.395985000
O	0.185323000	-0.000360000	-1.976666000
N	1.394225000	0.000384000	1.518837000
N	1.999660000	1.374198000	-0.631830000
N	-0.689776000	1.392106000	0.398771000
N	-0.689785000	-1.391933000	0.399424000
N	1.999486000	-1.374714000	-0.631256000
C	-0.397362000	1.692748000	1.670876000
C	3.030399000	1.218392000	0.229143000
C	3.076424000	3.265851000	-1.595042000
H	3.065484000	4.060305000	-2.333327000
C	-2.175254000	1.670349000	-1.519703000
H	-1.491571000	1.106392000	-2.136764000
C	4.121263000	2.073989000	0.228876000
H	4.932289000	1.932711000	0.936062000
C	2.010432000	2.367579000	-1.530542000
H	1.156263000	2.414746000	-2.196345000
C	-1.236691000	-2.460240000	2.497443000
H	-0.941357000	-2.656041000	3.522966000
C	0.935576000	1.234442000	2.211812000
H	0.883084000	1.073790000	3.293971000

H	1.669137000	2.029814000	2.042813000
C	-0.398014000	-1.691110000	1.672046000
C	-1.852003000	1.894374000	-0.161915000
C	0.935142000	-1.233042000	2.212641000
H	0.882913000	-1.071787000	3.294724000
H	1.668295000	-2.028864000	2.043927000
C	-2.752766000	2.682829000	0.635797000
C	-2.418532000	-2.943759000	1.982414000
H	-3.096163000	-3.530495000	2.596510000
C	-2.753398000	-2.681471000	0.637153000
C	2.845715000	0.000074000	1.118574000
H	3.528549000	0.000216000	1.974695000
C	-1.851797000	-1.894642000	-0.161214000
C	-2.173956000	-1.672802000	-1.519638000
H	-1.489586000	-1.110115000	-2.137134000
C	-1.235253000	2.463455000	2.495632000
H	-0.939342000	2.660435000	3.520763000
C	3.030187000	-1.218708000	0.229726000
C	-3.338109000	-2.190348000	-2.051828000
H	-3.562664000	-2.019448000	-3.100525000
C	4.141508000	3.118593000	-0.705168000
H	4.980605000	3.806944000	-0.733630000
C	-2.417033000	2.946954000	1.980497000

H	-3.094039000	3.534951000	2.594078000
C	-3.339630000	2.187404000	-2.051915000
H	-3.565060000	2.014701000	-3.100128000
C	-3.948559000	3.185589000	0.058744000
H	-4.616201000	3.774260000	0.681295000
C	4.120865000	-2.074548000	0.229981000
H	4.931836000	-1.933125000	0.937203000
C	3.075947000	-3.267059000	-1.593461000
H	3.064911000	-4.061852000	-2.331378000
C	-3.949028000	-3.184652000	0.060096000
H	-4.617352000	-3.772006000	0.683162000
C	-4.241107000	-2.942419000	-1.262316000
H	-5.151773000	-3.333231000	-1.704807000
C	2.010139000	-2.368531000	-1.529483000
H	1.156016000	-2.415848000	-2.195330000
C	-4.241709000	2.941232000	-1.263064000
H	-5.152544000	3.331672000	-1.705543000
C	4.140972000	-3.119614000	-0.703553000
H	4.979912000	-3.808172000	-0.731601000

^{1}R;

S= -3045.405489, **G**=-3044.815087

Fe	-0.529773000	-0.000085000	-0.372447000
O	-0.246481000	-0.000223000	-1.978229000

N	-1.399530000	-0.000115000	1.521013000
N	-1.964330000	-1.395390000	-0.618256000
N	0.682055000	-1.392282000	0.417111000
N	0.681869000	1.392128000	0.417276000
N	-1.964324000	1.395209000	-0.618374000
C	0.382548000	-1.703859000	1.684305000
C	-3.015063000	-1.223481000	0.213818000
C	-3.026190000	-3.286034000	-1.595323000
H	-3.001379000	-4.087408000	-2.325797000
C	2.149536000	-1.665363000	-1.512627000
H	1.452522000	-1.107063000	-2.123284000
C	-4.111604000	-2.071809000	0.191050000
H	-4.941366000	-1.919128000	0.873748000
C	-1.957484000	-2.391972000	-1.511516000
H	-1.088004000	-2.438752000	-2.157555000
C	1.216181000	2.489783000	2.498876000
H	0.920463000	2.698170000	3.521790000
C	-0.948722000	-1.234993000	2.221080000
H	-0.897464000	-1.070281000	3.302688000
H	-1.685734000	-2.027594000	2.054404000
C	0.382322000	1.703789000	1.684434000
C	1.837141000	-1.895492000	-0.153554000
C	-0.948831000	1.234689000	2.221247000

H	-0.897488000	1.069806000	3.302827000
H	-1.685953000	2.027240000	2.054754000
C	2.735374000	-2.694735000	0.634787000
C	2.397087000	2.970541000	1.977432000
H	3.072355000	3.566461000	2.585286000
C	2.734894000	2.695069000	0.634724000
C	-2.844973000	-0.000066000	1.100983000
H	-3.539360000	-0.000025000	1.947836000
C	1.836817000	1.895532000	-0.153498000
C	2.149228000	1.665332000	-1.512554000
H	1.452340000	1.106776000	-2.123133000
C	1.216560000	-2.489567000	2.498872000
H	0.920849000	-2.697907000	3.521795000
C	-3.014985000	1.223379000	0.213816000
C	3.306488000	2.185832000	-2.056277000
H	3.524208000	2.013150000	-3.106087000
C	-4.112858000	-3.124519000	-0.734515000
H	-4.955183000	-3.808085000	-0.778997000
C	2.397593000	-2.970117000	1.977524000
H	3.072988000	-3.565801000	2.585470000
C	3.306940000	-2.185646000	-2.056256000
H	3.524659000	-2.013019000	-3.106075000
C	3.925964000	-3.197401000	0.047321000

H	4.594675000	-3.794493000	0.660630000
C	-4.111498000	2.071747000	0.191137000
H	-4.941195000	1.919118000	0.873928000
C	-3.026241000	3.285849000	-1.595408000
H	-3.001479000	4.087183000	-2.325928000
C	3.925354000	3.197943000	0.047165000
H	4.593950000	3.795239000	0.660401000
C	4.211351000	2.944967000	-1.275003000
H	5.118456000	3.335358000	-1.725127000
C	-1.957564000	2.391742000	-1.511683000
H	-1.088163000	2.438461000	-2.157834000
C	4.211949000	-2.944494000	-1.274874000
H	5.119160000	-3.334728000	-1.724922000
C	-4.112812000	3.124428000	-0.734466000
H	-4.955107000	3.808035000	-0.778875000

CH (cyclohexane);
S=-235.9808645, **G**=-235.8383585

C	1.068748000	-0.999793000	0.235082000
C	-0.331774000	-1.425134000	-0.235083000
C	-1.400597000	-0.425315000	0.235119000
C	-1.068748000	0.999785000	-0.235092000
C	0.331766000	1.425138000	0.235078000
C	1.400601000	0.425319000	-0.235103000

H	-2.391743000	-0.726161000	-0.128858000
H	-0.341689000	-1.467848000	-1.334747000
H	-0.566906000	-2.434084000	0.128357000
H	1.101065000	-1.029938000	1.334778000
H	1.825016000	-1.707765000	-0.128494000
H	-1.101049000	1.029905000	-1.334791000
H	-1.825022000	1.707767000	0.128450000
H	0.566900000	2.434082000	-0.128378000
H	0.341675000	1.467871000	1.334741000
H	1.443317000	0.438260000	-1.334730000
H	2.391734000	0.726161000	0.128915000
H	-1.443280000	-0.438247000	1.334750000

^{5}ts1;

S= -3045.434165, **G**=-3044.834821

Fe	-0.233553000	-0.260660000	0.011901000
O	-0.610157000	1.389190000	0.041764000
N	-0.177421000	-2.499175000	-0.027128000
N	-1.783660000	-0.848706000	-1.406378000
N	1.316054000	-0.619028000	-1.466866000
N	1.339567000	-0.647179000	1.444279000
N	-1.721655000	-0.886918000	1.467536000
C	1.539081000	-1.908714000	-1.730656000
C	-2.270113000	-2.089219000	-1.199148000
C	-3.295543000	-0.557586000	-3.230486000

H	-3.678872000	0.077355000	-4.021926000
C	1.977494000	1.705700000	-1.688146000
H	1.105953000	2.001294000	-1.119716000
C	-3.277146000	-2.628058000	-1.988412000
H	-3.644549000	-3.632322000	-1.802235000
C	-2.280843000	-0.092362000	-2.393044000
H	-1.856560000	0.900380000	-2.493227000
C	2.742362000	-2.406772000	2.308065000
H	2.898995000	-3.473974000	2.426902000
C	0.502642000	-2.915440000	-1.277669000
H	0.962135000	-3.904295000	-1.157898000
H	-0.244822000	-3.007962000	-2.072564000
C	1.595122000	-1.944336000	1.635998000
C	2.196440000	0.330874000	-1.940824000
C	0.559131000	-2.950225000	1.179054000
H	1.030547000	-3.924670000	1.002382000
H	-0.155129000	-3.088636000	1.997716000
C	3.348073000	-0.059067000	-2.703945000
C	3.644823000	-1.489353000	2.801948000
H	4.543042000	-1.815735000	3.319280000
C	3.403034000	-0.107604000	2.637481000
C	-1.644675000	-2.787813000	0.001496000
H	-1.866713000	-3.861778000	-0.007702000

C	2.214319000	0.296551000	1.941359000
C	1.949829000	1.677506000	1.784775000
H	1.045179000	1.982495000	1.274907000
C	2.650635000	-2.358939000	-2.468409000
H	2.780649000	-3.421647000	-2.645548000
C	-2.217049000	-2.121629000	1.246491000
C	2.832368000	2.609861000	2.291882000
H	2.616470000	3.667855000	2.174438000
C	-3.798322000	-1.843177000	-3.025009000
H	-4.585391000	-2.234933000	-3.662178000
C	3.551842000	-1.434854000	-2.951578000
H	4.421886000	-1.751054000	-3.520797000
C	2.865282000	2.645372000	-2.171820000
H	2.685868000	3.698855000	-1.977424000
C	4.242840000	0.934306000	-3.181246000
H	5.109315000	0.621793000	-3.757021000
C	-3.189060000	-2.682757000	2.064026000
H	-3.564244000	-3.681957000	1.866413000
C	-3.150779000	-0.648638000	3.364565000
H	-3.497373000	-0.037596000	4.191022000
C	4.292707000	0.878975000	3.137937000
H	5.188342000	0.555714000	3.660705000
C	4.013880000	2.216078000	2.967652000

H	4.691009000	2.970780000	3.354826000
C	-2.172005000	-0.159592000	2.498582000
H	-1.735516000	0.826408000	2.612984000
C	4.006816000	2.265026000	-2.919942000
H	4.688651000	3.025123000	-3.287816000
C	-3.664380000	-1.927602000	3.143501000
H	-4.423489000	-2.337417000	3.802856000
H	-1.017142000	2.734682000	-0.231926000
C	-1.452239000	3.813009000	-0.501954000
C	-1.923913000	4.400042000	0.820647000
C	-2.566664000	3.540681000	-1.501920000
H	-0.595992000	4.343909000	-0.936878000
C	-3.076905000	3.583561000	1.426495000
H	-1.087670000	4.488655000	1.524973000
H	-2.273598000	5.426219000	0.617302000
C	-3.702969000	2.718160000	-0.872356000
H	-2.164498000	3.057103000	-2.402507000
H	-2.964723000	4.515151000	-1.830189000
C	-4.216155000	3.385156000	0.414340000
H	-2.688711000	2.598081000	1.723473000
H	-3.447618000	4.076295000	2.332349000
H	-3.321868000	1.715655000	-0.627829000
H	-4.520062000	2.593684000	-1.593001000

H	-5.017154000	2.782228000	0.858625000
H	-4.652668000	4.362216000	0.165208000

^{3}ts1;

S= -3045.428614, **G**=-3044.824687

Fe	0.433753000	-0.408739000	-0.029875000
O	0.339230000	1.294650000	-0.354827000
N	0.930572000	-2.409565000	0.152257000
N	1.925112000	-0.296060000	1.325113000
N	-0.873216000	-0.823416000	1.475626000
N	-0.993727000	-1.111718000	-1.340001000
N	1.831484000	-0.551002000	-1.467662000
C	-0.720833000	-2.055745000	1.971520000
C	2.809485000	-1.311267000	1.189095000
C	3.198538000	0.552299000	3.157830000
H	3.314209000	1.304359000	3.930768000
C	-2.123940000	1.262864000	1.436040000
H	-1.485180000	1.622280000	0.647361000
C	3.922550000	-1.439195000	2.006832000
H	4.607633000	-2.270592000	1.875158000
C	2.101963000	0.608413000	2.296896000
H	1.345624000	1.377054000	2.374516000
C	-1.962783000	-3.209034000	-2.056648000
H	-1.862131000	-4.288430000	-2.103305000
C	0.435546000	-2.890537000	1.471930000

H	0.143602000	-3.944758000	1.410005000
H	1.248661000	-2.833837000	2.203155000
C	-0.946329000	-2.444453000	-1.455667000
C	-1.903404000	-0.033455000	1.952736000
C	0.308512000	-3.141475000	-0.982954000
H	0.100315000	-4.180966000	-0.707604000
H	1.018365000	-3.166493000	-1.816494000
C	-2.771999000	-0.518623000	2.988577000
C	-3.067582000	-2.565691000	-2.567932000
H	-3.879792000	-3.126156000	-3.022773000
C	-3.139331000	-1.157157000	-2.515926000
C	2.428096000	-2.262729000	0.066323000
H	2.954449000	-3.220324000	0.142138000
C	-2.060766000	-0.433256000	-1.900035000
C	-2.101385000	0.980726000	-1.913753000
H	-1.268748000	1.524031000	-1.490727000
C	-1.551116000	-2.595935000	2.972672000
H	-1.373555000	-3.607458000	3.323631000
C	2.710627000	-1.550645000	-1.244269000
C	-3.172191000	1.638849000	-2.483378000
H	-3.179044000	2.725012000	-2.499242000
C	4.125466000	-0.478996000	3.005851000
H	4.987148000	-0.547880000	3.662678000

C	-2.568078000	-1.824852000	3.485970000
H	-3.223414000	-2.209642000	4.262521000
C	-3.147794000	2.043612000	1.932800000
H	-3.302983000	3.037783000	1.523516000
C	-3.814473000	0.311689000	3.476755000
H	-4.459312000	-0.072680000	4.261816000
C	3.753879000	-1.824627000	-2.116391000
H	4.441801000	-2.639622000	-1.915294000
C	2.977163000	0.014985000	-3.475771000
H	3.055740000	0.655656000	-4.347416000
C	-4.235184000	-0.446680000	-3.073361000
H	-5.043920000	-1.013202000	-3.526096000
C	-4.256257000	0.928968000	-3.055109000
H	-5.090030000	1.470932000	-3.490027000
C	1.952497000	0.225092000	-2.551788000
H	1.219354000	1.017678000	-2.645123000
C	-4.000202000	1.574524000	2.961045000
H	-4.797698000	2.208368000	3.335446000
C	3.886395000	-1.021199000	-3.256494000
H	4.689798000	-1.206638000	-3.962799000
H	0.509898000	2.222407000	0.446056000
C	0.603859000	3.399418000	1.025569000
C	-0.380552000	4.252631000	0.245942000

C	2.061377000	3.781402000	0.847788000
H	0.292004000	3.207284000	2.060044000
C	0.019726000	4.400297000	-1.233196000
H	-1.397645000	3.851637000	0.341581000
H	-0.394370000	5.250568000	0.715867000
C	2.435724000	3.899731000	-0.640016000
H	2.720741000	3.070465000	1.361825000
H	2.212753000	4.759280000	1.336154000
C	1.480979000	4.855991000	-1.372485000
H	-0.104045000	3.430509000	-1.733532000
H	-0.651360000	5.113298000	-1.725689000
H	2.375479000	2.901083000	-1.096731000
H	3.471415000	4.245246000	-0.734260000
H	1.753753000	4.925856000	-2.432114000
H	1.588393000	5.864576000	-0.948977000

^{1}ts1;

S= -3045.402097, **G**=-3044.794539

Fe	0.469167000	-0.378676000	0.032295000
O	0.423425000	1.282187000	-0.372699000
N	1.319954000	-2.208248000	0.483193000
N	2.027478000	0.168174000	1.253984000
N	-0.662518000	-0.796257000	1.654350000
N	-0.797395000	-1.455383000	-1.107218000

N	1.826031000	-0.521170000	-1.473788000
C	-0.214753000	-1.818513000	2.386614000
C	3.060397000	-0.697469000	1.184034000
C	3.281702000	1.552105000	2.731709000
H	3.336099000	2.453059000	3.333177000
C	-2.369795000	0.869527000	1.257954000
H	-1.920675000	1.076741000	0.303915000
C	4.244982000	-0.491392000	1.876698000
H	5.058429000	-1.206521000	1.805787000
C	2.125513000	1.272517000	2.001302000
H	1.264155000	1.929465000	1.981507000
C	-1.507230000	-3.733549000	-1.461977000
H	-1.289171000	-4.788137000	-1.328706000
C	1.018155000	-2.539503000	1.906569000
H	0.898063000	-3.621713000	2.030456000
H	1.866210000	-2.247227000	2.533688000
C	-0.587942000	-2.771746000	-1.001688000
C	-1.803705000	-0.137186000	2.065028000
C	0.751727000	-3.214518000	-0.458558000
H	0.678649000	-4.197409000	0.018331000
H	1.434191000	-3.322747000	-1.309061000
C	-2.441240000	-0.473786000	3.304250000
C	-2.670021000	-3.311200000	-2.069600000

H	-3.411407000	-4.027613000	-2.412684000
C	-2.885791000	-1.930603000	-2.280811000
C	2.767406000	-1.863059000	0.249694000
H	3.438808000	-2.711347000	0.421841000
C	-1.897216000	-1.007847000	-1.805255000
C	-2.035722000	0.364775000	-2.109399000
H	-1.245911000	1.036251000	-1.811015000
C	-0.813405000	-2.226457000	3.595481000
H	-0.395837000	-3.068216000	4.138734000
C	2.856844000	-1.337022000	-1.171162000
C	-3.137320000	0.810981000	-2.809417000
H	-3.223108000	1.866271000	-3.053212000
C	4.353636000	0.660494000	2.666628000
H	5.264958000	0.854017000	3.224140000
C	-1.908690000	-1.539289000	4.065550000
H	-2.382043000	-1.816504000	5.003449000
C	-3.497252000	1.545823000	1.676310000
H	-3.924915000	2.315521000	1.040301000
C	-3.593453000	0.247252000	3.712696000
H	-4.061464000	-0.012586000	4.657843000
C	3.881462000	-1.594755000	-2.071113000
H	4.696139000	-2.260060000	-1.803540000
C	2.765082000	-0.120538000	-3.624407000

H	2.700211000	0.380963000	-4.583956000
C	-4.020971000	-1.434749000	-2.975752000
H	-4.770498000	-2.141815000	-3.319469000
C	-4.150127000	-0.087205000	-3.229564000
H	-5.013074000	0.287006000	-3.771040000
C	1.773128000	0.085553000	-2.664843000
H	0.927968000	0.746494000	-2.816460000
C	-4.110074000	1.246368000	2.917332000
H	-4.992685000	1.794481000	3.231053000
C	3.829652000	-0.972182000	-3.324585000
H	4.612839000	-1.151851000	-4.054696000
H	-0.498212000	2.314880000	-0.419686000
C	-1.125819000	3.308209000	-0.635674000
C	-0.638453000	3.807319000	-1.986378000
C	-0.805192000	4.219646000	0.538003000
H	-2.170294000	2.975965000	-0.653925000
C	0.843649000	4.215506000	-1.943609000
H	-0.821759000	3.052643000	-2.763435000
H	-1.250500000	4.684999000	-2.252638000
C	0.675823000	4.634289000	0.550289000
H	-1.099784000	3.740025000	1.480319000
H	-1.432341000	5.120903000	0.433195000
C	1.103727000	5.215940000	-0.806358000

H	1.452280000	3.315376000	-1.780906000
H	1.136720000	4.646388000	-2.907699000
H	1.291001000	3.749120000	0.763643000
H	0.849954000	5.359747000	1.353164000
H	2.164728000	5.489980000	-0.780454000
H	0.539411000	6.139287000	-0.999639000

^{7}Int1;

S=-3045.452615, **G**=-3044.850865

Fe	0.115685000	-0.104615000	-0.048576000
O	0.540802000	0.844035000	1.416375000
N	0.106082000	-1.453217000	-1.877351000
N	1.604757000	-1.684639000	0.330859000
N	-1.507939000	-1.478538000	0.403739000
N	-1.348237000	0.880190000	-1.279634000
N	1.684985000	0.660384000	-1.405283000
C	-1.712137000	-2.439965000	-0.499053000
C	2.122565000	-2.244408000	-0.780764000
C	2.955535000	-3.116962000	1.682392000
H	3.258130000	-3.438372000	2.673229000
C	-2.242409000	-0.270325000	2.377067000
H	-1.341738000	0.329964000	2.345014000
C	3.076450000	-3.251567000	-0.724558000
H	3.471793000	-3.686359000	-1.637198000
C	2.005729000	-2.104985000	1.537337000

H	1.555688000	-1.607443000	2.389867000
C	-2.695582000	0.612746000	-3.256313000
H	-2.842846000	0.096491000	-4.199407000
C	-0.628845000	-2.690468000	-1.526183000
H	-1.058249000	-3.153843000	-2.423021000
H	0.075574000	-3.413927000	-1.102897000
C	-1.585341000	0.290261000	-2.453559000
C	-2.439939000	-1.275305000	1.400967000
C	-0.565439000	-0.705049000	-2.968677000
H	-1.038839000	-1.396650000	-3.675979000
H	0.189514000	-0.145237000	-3.530492000
C	-3.624227000	-2.084190000	1.465011000
C	-3.576778000	1.581432000	-2.823081000
H	-4.447679000	1.844728000	-3.417378000
C	-3.348971000	2.243805000	-1.596438000
C	1.575241000	-1.645797000	-2.069198000
H	1.810106000	-2.287034000	-2.927536000
C	-2.196761000	1.868750000	-0.828233000
C	-1.934737000	2.533646000	0.392655000
H	-1.054111000	2.269106000	0.965976000
C	-2.851221000	-3.267204000	-0.493351000
H	-2.962768000	-4.029953000	-1.257188000
C	2.198249000	-0.267614000	-2.236957000

C	-2.792289000	3.523104000	0.831295000
H	-2.580905000	4.036203000	1.764897000
C	3.500776000	-3.694024000	0.534736000
H	4.241494000	-4.483918000	0.614285000
C	-3.803783000	-3.086687000	0.486355000
H	-4.696955000	-3.705110000	0.514283000
C	-3.185504000	-0.079626000	3.367441000
H	-3.022341000	0.689395000	4.116849000
C	-4.573850000	-1.856524000	2.495061000
H	-5.464354000	-2.477612000	2.529959000
C	3.217236000	0.024525000	-3.133821000
H	3.605248000	-0.744766000	-3.794042000
C	3.175508000	2.292355000	-2.312553000
H	3.532937000	3.316336000	-2.315617000
C	-4.213076000	3.259142000	-1.109160000
H	-5.082938000	3.532361000	-1.699600000
C	-3.940708000	3.887493000	0.085300000
H	-4.597987000	4.667918000	0.455313000
C	2.154153000	1.914847000	-1.440513000
H	1.703059000	2.616411000	-0.748441000
C	-4.359948000	-0.869569000	3.430544000
H	-5.084003000	-0.697166000	4.220499000
C	3.717645000	1.331696000	-3.167249000

H	4.513138000	1.594083000	-3.858078000
H	1.325353000	0.864865000	2.020945000
H	3.897025000	-0.664536000	2.720608000
C	3.975546000	0.428661000	2.721854000
C	4.176390000	0.971917000	1.291835000
C	2.793489000	1.067949000	3.387789000
H	4.882025000	0.668272000	3.308716000
C	4.222753000	2.509065000	1.295475000
H	3.342683000	0.629302000	0.662573000
H	5.100212000	0.563755000	0.864225000
C	2.704547000	2.566159000	3.343303000
H	2.298720000	0.542063000	4.204396000
C	2.959417000	3.119570000	1.924035000
H	4.355713000	2.884760000	0.272850000
H	5.102296000	2.836067000	1.866850000
H	1.741100000	2.918680000	3.730515000
H	3.477748000	2.977327000	4.019320000
H	2.084880000	2.879566000	1.304198000
H	3.041418000	4.211597000	1.962415000

^{5}Int1$_{hs}$

S=-3045.454266, **G**= -3044.853354

Fe	0.115685000	-0.104615000	-0.048576000
O	0.540802000	0.844035000	1.416375000

N	0.106082000	-1.453217000	-1.877351000
N	1.604757000	-1.684639000	0.330859000
N	-1.507939000	-1.478538000	0.403739000
N	-1.348237000	0.880190000	-1.279634000
N	1.684985000	0.660384000	-1.405283000
C	-1.712137000	-2.439965000	-0.499053000
C	2.122565000	-2.244408000	-0.780764000
C	2.955535000	-3.116962000	1.682392000
H	3.258130000	-3.438372000	2.673229000
C	-2.242409000	-0.270325000	2.377067000
H	-1.341738000	0.329964000	2.345014000
C	3.076450000	-3.251567000	-0.724558000
H	3.471793000	-3.686359000	-1.637198000
C	2.005729000	-2.104985000	1.537337000
H	1.555688000	-1.607443000	2.389867000
C	-2.695582000	0.612746000	-3.256313000
H	-2.842846000	0.096491000	-4.199407000
C	-0.628845000	-2.690468000	-1.526183000
H	-1.058249000	-3.153843000	-2.423021000
H	0.075574000	-3.413927000	-1.102897000
C	-1.585341000	0.290261000	-2.453559000
C	-2.439939000	-1.275305000	1.400967000
C	-0.565439000	-0.705049000	-2.968677000

H	-1.038839000	-1.396650000	-3.675979000
H	0.189514000	-0.145237000	-3.530492000
C	-3.624227000	-2.084190000	1.465011000
C	-3.576778000	1.581432000	-2.823081000
H	-4.447679000	1.844728000	-3.417378000
C	-3.348971000	2.243805000	-1.596438000
C	1.575241000	-1.645797000	-2.069198000
H	1.810106000	-2.287034000	-2.927536000
C	-2.196761000	1.868750000	-0.828233000
C	-1.934737000	2.533646000	0.392655000
H	-1.054111000	2.269106000	0.965976000
C	-2.851221000	-3.267204000	-0.493351000
H	-2.962768000	-4.029953000	-1.257188000
C	2.198249000	-0.267614000	-2.236957000
C	-2.792289000	3.523104000	0.831295000
H	-2.580905000	4.036203000	1.764897000
C	3.500776000	-3.694024000	0.534736000
H	4.241494000	-4.483918000	0.614285000
C	-3.803783000	-3.086687000	0.486355000
H	-4.696955000	-3.705110000	0.514283000
C	-3.185504000	-0.079626000	3.367441000
H	-3.022341000	0.689395000	4.116849000
C	-4.573850000	-1.856524000	2.495061000

H	-5.464354000	-2.477612000	2.529959000
C	3.217236000	0.024525000	-3.133821000
H	3.605248000	-0.744766000	-3.794042000
C	3.175508000	2.292355000	-2.312553000
H	3.532937000	3.316336000	-2.315617000
C	-4.213076000	3.259142000	-1.109160000
H	-5.082938000	3.532361000	-1.699600000
C	-3.940708000	3.887493000	0.085300000
H	-4.597987000	4.667918000	0.455313000
C	2.154153000	1.914847000	-1.440513000
H	1.703059000	2.616411000	-0.748441000
C	-4.359948000	-0.869569000	3.430544000
H	-5.084003000	-0.697166000	4.220499000
C	3.717645000	1.331696000	-3.167249000
H	4.513138000	1.594083000	-3.858078000
H	1.325353000	0.864865000	2.020945000
H	3.897025000	-0.664536000	2.720608000
C	3.975546000	0.428661000	2.721854000
C	4.176390000	0.971917000	1.291835000
C	2.793489000	1.067949000	3.387789000
H	4.882025000	0.668272000	3.308716000
C	4.222753000	2.509065000	1.295475000
H	3.342683000	0.629302000	0.662573000

H	5.100212000	0.563755000	0.864225000
C	2.704547000	2.566159000	3.343303000
H	2.298720000	0.542063000	4.204396000
C	2.959417000	3.119570000	1.924035000
H	4.355713000	2.884760000	0.272850000
H	5.102296000	2.836067000	1.866850000
H	1.741100000	2.918680000	3.730515000
H	3.477748000	2.977327000	4.019320000
H	2.084880000	2.879566000	1.304198000
H	3.041418000	4.211597000	1.962415000

^{5}Int1$_{is}$;

S=-3045.44526, **G**=-3044.83771

Fe	0.165598000	-0.105823000	-0.020232000
O	0.562830000	0.958122000	1.389884000
N	0.146390000	-1.536516000	-1.748923000
N	1.647630000	-1.700929000	0.468941000
N	-1.501973000	-1.438430000	0.504114000
N	-1.366588000	0.785812000	-1.312183000
N	1.705383000	0.622528000	-1.430513000
C	-1.695832000	-2.443992000	-0.349019000
C	2.178221000	-2.276580000	-0.627951000
C	2.945773000	-3.153952000	1.854927000
H	3.211139000	-3.488859000	2.852196000
C	-2.251696000	-0.124584000	2.391269000

H	-1.330380000	0.443711000	2.346673000
C	3.126015000	-3.290162000	-0.547713000
H	3.532081000	-3.736836000	-1.449921000
C	2.008070000	-2.134640000	1.682949000
H	1.523539000	-1.648114000	2.524188000
C	-2.713555000	0.347208000	-3.259105000
H	-2.847024000	-0.233887000	-4.165885000
C	-0.584366000	-2.759020000	-1.329070000
H	-0.984122000	-3.289071000	-2.202658000
H	0.116320000	-3.441132000	-0.838465000
C	-1.588071000	0.117127000	-2.442458000
C	-2.454483000	-1.171241000	1.460574000
C	-0.531923000	-0.873367000	-2.892739000
H	-0.971213000	-1.621149000	-3.564316000
H	0.214629000	-0.324061000	-3.475158000
C	-3.657292000	-1.949694000	1.533293000
C	-3.625390000	1.310518000	-2.883270000
H	-4.506862000	1.507841000	-3.487532000
C	-3.412071000	2.059315000	-1.703259000
C	1.619412000	-1.730416000	-1.937067000
H	1.847083000	-2.411188000	-2.766635000
C	-2.243695000	1.770544000	-0.923892000
C	-1.987457000	2.523540000	0.247042000

H	-1.090567000	2.318011000	0.820409000
C	-2.850373000	-3.252135000	-0.333507000
H	-2.953993000	-4.053524000	-1.057917000
C	2.232594000	-0.358000000	-2.190114000
C	-2.870857000	3.511615000	0.631146000
H	-2.669541000	4.091187000	1.527435000
C	3.521241000	-3.730646000	0.720771000
H	4.256151000	-4.523929000	0.818954000
C	-3.828986000	-3.000169000	0.603505000
H	-4.734285000	-3.600357000	0.638498000
C	-3.215502000	0.142202000	3.342325000
H	-3.055117000	0.945817000	4.055248000
C	-4.628288000	-1.643610000	2.522320000
H	-5.535549000	-2.239540000	2.565881000
C	3.241089000	-0.116574000	-3.115611000
H	3.642378000	-0.927016000	-3.716117000
C	3.140252000	2.211945000	-2.492490000
H	3.464267000	3.242239000	-2.594040000
C	-4.303169000	3.076842000	-1.272356000
H	-5.186957000	3.285257000	-1.868691000
C	-4.038232000	3.789105000	-0.124182000
H	-4.716434000	4.571462000	0.201670000
C	2.135683000	1.881588000	-1.582585000

H	1.662048000	2.626938000	-0.952692000
C	-4.412800000	-0.613521000	3.410035000
H	-5.153951000	-0.381614000	4.168411000
C	3.707283000	1.194857000	-3.262678000
H	4.491943000	1.418247000	-3.979209000
H	1.373020000	0.998137000	1.947052000
H	3.827594000	-0.479971000	2.695098000
C	3.977540000	0.603549000	2.645964000
C	4.179828000	1.096586000	1.193357000
C	2.899420000	1.331617000	3.361492000
H	4.917231000	0.804338000	3.201700000
C	4.233421000	2.630084000	1.127493000
H	3.347207000	0.727961000	0.580762000
H	5.103062000	0.660205000	0.796966000
C	2.739240000	2.798036000	3.188088000
H	2.315245000	0.816799000	4.122885000
C	2.972884000	3.264451000	1.732262000
H	4.342191000	2.949020000	0.083711000
H	5.123291000	2.987328000	1.662967000
H	1.774687000	3.141367000	3.576924000
H	3.510067000	3.267653000	3.834483000
H	2.096087000	2.968326000	1.142626000
H	3.037097000	4.357032000	1.712911000

^{3}Int1$_{is}$;

S=-3045.454266, **G**=-3044.853354

Fe	-0.046760000	0.115165000	-0.092038000
O	-0.399463000	-0.167175000	1.609613000
N	-0.042212000	0.615012000	-2.131893000
N	-1.620571000	1.727901000	-0.278776000
N	1.505256000	1.475192000	-0.006695000
N	1.555515000	-1.249639000	-0.864444000
N	-1.427283000	-1.169176000	-0.771327000
C	1.689822000	2.103688000	-1.177249000
C	-2.159941000	1.690004000	-1.509721000
C	-3.065702000	3.539919000	0.289772000
H	-3.396578000	4.263373000	1.027212000
C	2.255291000	1.024919000	2.260429000
H	1.374246000	0.423922000	2.429921000
C	-3.173867000	2.549623000	-1.910741000
H	-3.585186000	2.497926000	-2.914136000
C	-2.053918000	2.629484000	0.606659000
H	-1.581473000	2.604632000	1.583639000
C	2.927185000	-1.577053000	-2.816567000
H	3.059209000	-1.410985000	-3.880991000
C	0.629364000	1.944588000	-2.242322000
H	1.063446000	2.071001000	-3.240116000
H	-0.117562000	2.732556000	-2.113760000

C	1.777975000	-1.089513000	-2.163194000
C	2.428813000	1.651910000	1.005384000
C	0.671545000	-0.418137000	-2.946519000
H	1.054026000	0.032009000	-3.868997000
H	-0.052817000	-1.185449000	-3.239164000
C	3.580189000	2.486768000	0.799109000
C	3.864994000	-2.263769000	-2.073018000
H	4.767595000	-2.649853000	-2.539066000
C	3.654761000	-2.473588000	-0.690082000
C	-1.533306000	0.614428000	-2.384818000
H	-1.765733000	0.775512000	-3.443349000
C	2.459588000	-1.941166000	-0.101381000
C	2.210205000	-2.146529000	1.276881000
H	1.301408000	-1.743442000	1.708967000
C	2.794015000	2.933777000	-1.437743000
H	2.888938000	3.407909000	-2.409081000
C	-2.023412000	-0.747495000	-1.914294000
C	3.120751000	-2.849928000	2.038153000
H	2.926458000	-3.011990000	3.094408000
C	-3.635380000	3.493612000	-0.982865000
H	-4.423797000	4.187319000	-1.258618000
C	3.737899000	3.121547000	-0.451069000
H	4.606987000	3.750325000	-0.624709000

C	3.191948000	1.212729000	3.257507000
H	3.044417000	0.733397000	4.220886000
C	4.525025000	2.650327000	1.845888000
H	5.390013000	3.283827000	1.671483000
C	-2.969873000	-1.524338000	-2.566579000
H	-3.428089000	-1.172128000	-3.485119000
C	-2.674725000	-3.200051000	-0.851921000
H	-2.906871000	-4.160978000	-0.406653000
C	4.573096000	-3.184567000	0.126362000
H	5.476903000	-3.583092000	-0.325735000
C	4.310404000	-3.368800000	1.465710000
H	5.010293000	-3.917300000	2.088206000
C	-1.739799000	-2.363230000	-0.245177000
H	-1.221766000	-2.631913000	0.667880000
C	4.337088000	2.021426000	3.055437000
H	5.056939000	2.149198000	3.857637000
C	-3.299842000	-2.772912000	-2.023599000
H	-4.031334000	-3.404768000	-2.517992000
H	-1.293441000	-0.561902000	1.775670000
H	-2.490135000	0.838458000	3.107375000
C	-3.355737000	0.164598000	3.045864000
C	-4.371259000	0.641143000	1.989156000
C	-2.906753000	-1.251200000	2.825005000

H	-3.842159000	0.215342000	4.038540000
C	-5.502136000	-0.380218000	1.811395000
H	-3.860608000	0.764631000	1.023777000
H	-4.767449000	1.622124000	2.275961000
C	-3.904819000	-2.271634000	2.364485000
H	-2.064621000	-1.609804000	3.419683000
C	-4.920178000	-1.721387000	1.344442000
H	-6.236872000	-0.013012000	1.085362000
H	-6.030851000	-0.516607000	2.764891000
H	-3.401787000	-3.170987000	1.983548000
H	-4.466650000	-2.611103000	3.255394000
H	-4.420047000	-1.564658000	0.378376000
H	-5.714375000	-2.459239000	1.184049000

^{3}Int1$_{ls}$;

S=-3045.455881, **G**=-3044.852709

Fe	0.013825000	0.000003000	-0.198914000
O	0.235041000	-0.000190000	1.570918000
N	0.059967000	0.000304000	-2.252609000
N	1.411174000	-1.381064000	-0.488727000
N	-1.479672000	-1.393158000	-0.457548000
N	-1.479631000	1.393325000	-0.457470000
N	1.411280000	1.381069000	-0.488356000
C	-1.680650000	-1.677965000	-1.749637000

C	2.050818000	-1.232299000	-1.670292000
C	2.573966000	-3.421367000	-0.102160000
H	2.755373000	-4.275846000	0.540486000
C	-2.165367000	-1.664038000	1.862524000
H	-1.290750000	-1.113390000	2.178138000
C	2.987950000	-2.151970000	-2.116600000
H	3.484147000	-2.014673000	-3.071974000
C	1.652410000	-2.448201000	0.283427000
H	1.091398000	-2.493647000	1.209522000
C	-2.777646000	2.421431000	-2.220421000
H	-2.881086000	2.605872000	-3.284737000
C	-0.624462000	-1.232379000	-2.733878000
H	-1.057150000	-1.069637000	-3.726712000
H	0.116979000	-2.031547000	-2.835780000
C	-1.680569000	1.678487000	-1.749477000
C	-2.368850000	-1.884089000	0.480177000
C	-0.624331000	1.233083000	-2.733742000
H	-1.056929000	1.070543000	-3.726650000
H	0.117153000	2.032242000	-2.835416000
C	-3.514151000	-2.647667000	0.062774000
C	-3.698640000	2.896706000	-1.313465000
H	-4.564081000	3.465430000	-1.642514000
C	-3.514126000	2.647680000	0.063153000

C	1.568672000	0.000260000	-2.415939000
H	1.882674000	0.000377000	-3.464798000
C	-2.368824000	1.884006000	0.480374000
C	-2.165341000	1.663608000	1.862662000
H	-1.290705000	1.112920000	2.178160000
C	-2.777751000	-2.420763000	-2.220756000
H	-2.881238000	-2.604890000	-3.285121000
C	2.050862000	1.232636000	-1.669988000
C	-3.066529000	2.165562000	2.780378000
H	-2.894284000	1.996171000	3.839373000
C	3.253946000	-3.267334000	-1.310970000
H	3.977349000	-4.010085000	-1.632842000
C	-3.698710000	-2.896307000	-1.313905000
H	-4.564162000	-3.464937000	-1.643085000
C	-3.066532000	-2.166252000	2.780120000
H	-2.894283000	-1.997127000	3.839157000
C	-4.424507000	-3.137630000	1.035728000
H	-5.285372000	-3.708539000	0.699677000
C	2.987886000	2.152497000	-2.116146000
H	3.484058000	2.015452000	-3.071568000
C	2.573833000	3.421432000	-0.101422000
H	2.755171000	4.275820000	0.541362000
C	-4.424508000	3.137364000	1.036221000

H	-5.285376000	3.708352000	0.700310000
C	-4.207480000	2.899772000	2.373979000
H	-4.900339000	3.279508000	3.118193000
C	1.652433000	2.448064000	0.284031000
H	1.091452000	2.493243000	1.210157000
C	-4.207467000	-2.900389000	2.373544000
H	-4.900305000	-3.280338000	3.117669000
C	3.253778000	3.267724000	-1.310299000
H	3.977062000	4.010641000	-1.632057000
H	1.197742000	-0.000322000	1.790186000
H	3.046478000	-2.137435000	2.626086000
C	3.744572000	-1.291031000	2.682665000
C	4.683259000	-1.254090000	1.460925000
C	3.007686000	-0.000308000	2.895442000
H	4.364150000	-1.484608000	3.578738000
C	5.567335000	-0.000377000	1.486635000
H	4.085858000	-1.234801000	0.538631000
H	5.292986000	-2.164820000	1.435316000
C	3.745126000	1.290250000	2.683639000
H	2.201497000	-0.000401000	3.630769000
C	4.683954000	1.253857000	1.461982000
H	6.253223000	-0.000200000	0.631225000
H	6.184641000	-0.000937000	2.395480000

H	3.047351000	2.136947000	2.627507000
H	4.364601000	1.483005000	3.579959000
H	4.086640000	1.235733000	0.539611000
H	5.294200000	2.164261000	1.437265000

^{1}Int1$_{ls}$;

S=-3045.445527, **G**=-3044.835922

Fe	0.006643000	-0.071070000	-0.208959000
O	0.244520000	0.072829000	1.555876000
N	0.030780000	-0.283916000	-2.248790000
N	1.325582000	-1.545637000	-0.370388000
N	-1.562176000	-1.404041000	-0.311243000
N	-1.412941000	1.363296000	-0.602463000
N	1.481061000	1.194024000	-0.634956000
C	-1.789779000	-1.807224000	-1.566934000
C	1.972426000	-1.540408000	-1.556637000
C	2.442071000	-3.554271000	0.244907000
H	2.601635000	-4.337899000	0.977419000
C	-2.236241000	-1.407310000	2.027050000
H	-1.327722000	-0.881927000	2.283187000
C	2.891554000	-2.522308000	-1.894005000
H	3.394964000	-2.499995000	-2.855165000
C	1.536577000	-2.528529000	0.514560000
H	0.969085000	-2.461402000	1.435190000
C	-2.671896000	2.281514000	-2.452316000

H	-2.777074000	2.363989000	-3.529154000
C	-0.718590000	-1.524276000	-2.594933000
H	-1.148406000	-1.447249000	-3.599239000
H	-0.018999000	-2.366302000	-2.609086000
C	-1.612606000	1.528632000	-1.915266000
C	-2.467220000	-1.750147000	0.674337000
C	-0.595253000	0.925148000	-2.853954000
H	-1.049225000	0.680039000	-3.819980000
H	0.185290000	1.668518000	-3.046703000
C	-3.656918000	-2.486261000	0.340602000
C	-3.555265000	2.894950000	-1.592286000
H	-4.391980000	3.475199000	-1.971622000
C	-3.370024000	2.773573000	-0.198754000
C	1.534163000	-0.372396000	-2.423233000
H	1.833944000	-0.492758000	-3.469337000
C	-2.263910000	1.993254000	0.287108000
C	-2.058885000	1.899302000	1.683119000
H	-1.212289000	1.333138000	2.044765000
C	-2.930203000	-2.532024000	-1.956679000
H	-3.053060000	-2.817668000	-2.996299000
C	2.087093000	0.901923000	-1.807552000
C	-2.922671000	2.536902000	2.551231000
H	-2.749940000	2.462532000	3.621014000

C	3.132095000	-3.546250000	-0.968014000
H	3.842923000	-4.333135000	-1.200776000
C	-3.868030000	-2.860685000	-1.003261000
H	-4.766599000	-3.410164000	-1.270286000
C	-3.153365000	-1.765461000	2.994897000
H	-2.959747000	-1.504147000	4.031246000
C	-4.582499000	-2.825569000	1.362226000
H	-5.477211000	-3.377899000	1.089440000
C	3.064372000	1.720784000	-2.353650000
H	3.529249000	1.467691000	-3.301050000
C	2.775918000	3.184360000	-0.453459000
H	3.024093000	4.078358000	0.107554000
C	-4.242847000	3.405465000	0.725489000
H	-5.075155000	3.986762000	0.339051000
C	-4.026196000	3.288669000	2.079228000
H	-4.690758000	3.776505000	2.785250000
C	1.810781000	2.305110000	0.037432000
H	1.281669000	2.470247000	0.968365000
C	-4.337881000	-2.470236000	2.668754000
H	-5.042487000	-2.735835000	3.450485000
C	3.412365000	2.886683000	-1.658664000
H	4.167451000	3.554938000	-2.060980000
H	1.196805000	0.220733000	1.744709000

H	2.503925000	-1.372400000	2.816566000
C	3.403279000	-0.740395000	2.815478000
C	4.358471000	-1.121965000	1.667175000
C	3.030642000	0.714031000	2.799766000
H	3.916048000	-0.959894000	3.771055000
C	5.545097000	-0.151761000	1.597395000
H	3.817784000	-1.077925000	0.710334000
H	4.702825000	-2.154267000	1.800124000
C	4.084815000	1.729589000	2.471654000
H	2.208183000	1.032473000	3.441931000
C	5.037751000	1.274974000	1.349163000
H	6.236754000	-0.452464000	0.801598000
H	6.105108000	-0.187477000	2.542041000
H	3.632831000	2.703278000	2.238096000
H	4.689882000	1.901692000	3.381871000
H	4.505461000	1.291323000	0.387855000
H	5.874588000	1.978177000	1.269485000

^{7}ts2;

S=-3045.405914, **G**=-3044.804547

Fe	0.348011000	-0.217523000	-0.008496000
N	0.517263000	-2.367354000	-0.670498000
N	1.756085000	-1.186543000	1.369209000
N	-1.359259000	-1.142230000	1.002256000
N	-0.882909000	-0.120925000	-1.657311000

N	2.103092000	-0.293293000	-1.343431000
C	-1.512105000	-2.445181000	0.709369000
C	2.392280000	-2.257698000	0.850937000
C	2.897214000	-1.509373000	3.444322000
H	3.060781000	-1.194768000	4.469449000
C	-2.340058000	0.946400000	1.753284000
H	-1.355865000	1.394013000	1.755710000
C	3.316392000	-2.991461000	1.585318000
H	3.810113000	-3.850959000	1.143050000
C	1.988943000	-0.824289000	2.638050000
H	1.423827000	0.028388000	2.999287000
C	-2.546908000	-1.752219000	-2.317481000
H	-2.770008000	-2.774196000	-2.607142000
C	-0.275027000	-3.191906000	0.275985000
H	-0.543881000	-4.150028000	-0.185596000
H	0.341770000	-3.410052000	1.153041000
C	-1.230350000	-1.393891000	-2.049161000
C	-2.463302000	-0.417565000	1.411400000
C	-0.094096000	-2.378045000	-2.039229000
H	-0.436229000	-3.386927000	-2.296830000
H	0.676174000	-2.079902000	-2.756572000
C	-3.756692000	-1.031456000	1.489619000
C	-3.562035000	-0.810618000	-2.180923000

H	-4.599540000	-1.080574000	-2.350150000
C	-3.231947000	0.539477000	-1.862518000
C	1.995506000	-2.564018000	-0.587277000
H	2.308631000	-3.575435000	-0.872606000
C	-1.853408000	0.873848000	-1.684063000
C	-1.485830000	2.224359000	-1.537717000
H	-0.430908000	2.487800000	-1.558874000
C	-2.742462000	-3.116174000	0.814131000
H	-2.792931000	-4.173493000	0.575169000
C	2.641031000	-1.520828000	-1.483118000
C	-2.459925000	3.216888000	-1.461724000
H	-2.163749000	4.257425000	-1.364267000
C	3.576262000	-2.604682000	2.904581000
H	4.288381000	-3.161375000	3.506170000
C	-3.865162000	-2.410382000	1.187077000
H	-4.834553000	-2.896477000	1.252334000
C	-3.453939000	1.683768000	2.111116000
H	-3.342495000	2.732485000	2.370264000
C	-4.878961000	-0.249469000	1.861073000
H	-5.851793000	-0.730145000	1.914760000
C	3.685108000	-1.774732000	-2.364325000
H	4.092258000	-2.776483000	-2.458541000
C	3.604400000	0.552053000	-2.998249000

H	3.952476000	1.393393000	-3.587744000
C	-4.198753000	1.563778000	-1.760499000
H	-5.247067000	1.303501000	-1.877500000
C	-3.822400000	2.882689000	-1.541563000
H	-4.577032000	3.659765000	-1.474490000
C	2.558846000	0.720046000	-2.091273000
H	2.070902000	1.678458000	-1.948829000
C	-4.735247000	1.089726000	2.157041000
H	-5.597766000	1.684324000	2.440637000
C	4.178907000	-0.714142000	-3.131917000
H	4.990947000	-0.879403000	-3.833399000
H	3.075536000	1.530571000	2.365850000
C	2.950015000	2.549998000	1.988219000
C	3.679454000	2.756797000	0.649328000
C	1.516177000	2.936615000	1.954637000
H	3.404774000	3.213840000	2.749438000
C	3.364199000	4.130999000	0.038876000
H	3.363159000	1.964794000	-0.037124000
H	4.757415000	2.644212000	0.806548000
C	1.122707000	4.175917000	1.226478000
H	0.884766000	2.613096000	2.778040000
C	1.850476000	4.335474000	-0.123320000
H	3.863066000	4.234324000	-0.931474000

H	3.767740000	4.921054000	0.687112000
H	0.031722000	4.242437000	1.123117000
H	1.409511000	5.017650000	1.884518000
H	1.453765000	3.590877000	-0.827912000
H	1.633218000	5.325231000	-0.537367000
O	0.636590000	1.522997000	0.685056000
H	-0.053902000	2.122386000	0.351920000

^{5}ts2;

S=-3045.448271, **G**=-3044.84917

Fe	0.614929000	0.173654000	-0.276219000
O	-0.478007000	1.216108000	-1.461015000
N	1.943492000	-0.674772000	1.445619000
N	2.104731000	1.820023000	0.346414000
N	-0.685439000	0.159938000	1.600941000
N	0.069905000	-2.008336000	-0.214071000
N	2.483293000	-0.633596000	-1.264013000
C	-0.046522000	-0.036343000	2.748553000
C	3.243241000	1.319445000	0.863929000
C	3.056739000	4.020891000	0.475321000
H	2.942011000	5.085959000	0.302878000
C	-2.736330000	0.168248000	0.339485000
H	-2.154779000	0.300810000	-0.566888000
C	4.326752000	2.118537000	1.215846000

H	5.221340000	1.670845000	1.637767000
C	2.019240000	3.143001000	0.158507000
H	1.089250000	3.500502000	-0.266245000
C	0.245943000	-4.051066000	1.049041000
H	0.742583000	-4.585954000	1.852995000
C	1.468672000	-0.051353000	2.696392000
H	1.868269000	-0.572654000	3.578039000
H	1.827295000	0.980646000	2.741368000
C	0.639231000	-2.725822000	0.743174000
C	-2.052615000	0.097318000	1.584276000
C	1.829010000	-2.149744000	1.493673000
H	1.801049000	-2.494153000	2.535641000
H	2.730873000	-2.593246000	1.054421000
C	-2.805510000	-0.100372000	2.785377000
C	-0.757959000	-4.637935000	0.315379000
H	-1.085560000	-5.652258000	0.527499000
C	-1.367648000	-3.915165000	-0.739297000
C	3.272225000	-0.195911000	0.981653000
H	4.084907000	-0.503732000	1.653996000
C	-0.917236000	-2.578142000	-0.980962000
C	-1.489300000	-1.838087000	-2.045883000
H	-1.146949000	-0.821508000	-2.214804000
C	-0.715140000	-0.226132000	3.980791000

H	-0.135980000	-0.371711000	4.887160000
C	3.523031000	-0.753691000	-0.416875000
C	-2.470367000	-2.408831000	-2.831162000
H	-2.897509000	-1.843456000	-3.655053000
C	4.232506000	3.498253000	1.014910000
H	5.059996000	4.150081000	1.278089000
C	-2.091056000	-0.238014000	4.001512000
H	-2.636071000	-0.387282000	4.929753000
C	-4.113273000	0.012582000	0.306874000
H	-4.629016000	0.010972000	-0.650005000
C	-4.220110000	-0.202396000	2.713599000
H	-4.782408000	-0.341694000	3.632883000
C	4.734379000	-1.323674000	-0.795788000
H	5.545810000	-1.411239000	-0.079673000
C	3.795404000	-1.664708000	-2.986336000
H	3.860189000	-2.016644000	-4.010457000
C	-2.386677000	-4.467025000	-1.558385000
H	-2.721233000	-5.482446000	-1.364634000
C	-2.927862000	-3.728244000	-2.587639000
H	-3.699857000	-4.156239000	-3.219630000
C	2.613997000	-1.088580000	-2.516783000
H	1.739286000	-0.994624000	-3.154333000
C	-4.864278000	-0.157477000	1.492940000

H	-5.942999000	-0.267012000	1.440649000
C	4.874267000	-1.782621000	-2.109342000
H	5.806734000	-2.232311000	-2.436844000
H	-0.095347000	1.362626000	-2.339747000
C	-2.062115000	4.509776000	-2.589997000
C	-1.082807000	4.274780000	-1.429824000
C	-1.781783000	3.765331000	-0.158873000
C	-2.993185000	2.975978000	-0.340289000
C	-3.702068000	2.877482000	-1.608697000
C	-2.881952000	3.238117000	-2.853186000
H	-1.112622000	3.214928000	0.522536000
H	-0.372530000	3.499776000	-1.726699000
H	-0.529907000	5.189821000	-1.192214000
H	-2.737583000	5.346193000	-2.361084000
H	-1.502794000	4.791016000	-3.487693000
H	-3.486139000	2.595306000	0.550918000
H	-4.264852000	1.939835000	-1.672006000
H	-4.499373000	3.645864000	-1.446297000
H	-2.210342000	2.397697000	-3.062962000
H	-3.556752000	3.365511000	-3.704496000
H	-2.148007000	4.602692000	0.479289000

^{3}ts2;

S=-3045.429144, **G**=-3044.835614

Fe	-0.534771000	-0.417483000	0.046778000
O	-0.275524000	1.186087000	-0.752578000
N	-1.123403000	-2.228808000	0.886679000
N	-1.964847000	-0.929756000	-1.255361000
N	0.872912000	-1.587523000	-0.906447000
N	0.797683000	-0.397900000	1.618042000
N	-2.017572000	0.244288000	1.208209000
C	0.735464000	-2.884167000	-0.605904000
C	-2.876930000	-1.770364000	-0.718622000
C	-3.078348000	-1.048578000	-3.357647000
H	-3.129574000	-0.743664000	-4.397312000
C	2.151921000	0.168441000	-2.004692000
H	1.366738000	0.874497000	-1.777620000
C	-3.924416000	-2.290341000	-1.464453000
H	-4.638891000	-2.970728000	-1.012196000
C	-2.049543000	-0.572358000	-2.544247000
H	-1.275811000	0.102211000	-2.894342000
C	1.536823000	-1.759930000	3.473315000
H	1.349606000	-2.630031000	4.094192000
C	-0.557244000	-3.318905000	0.049101000
H	-0.406514000	-4.225810000	0.645151000
H	-1.276706000	-3.569297000	-0.737637000
C	0.638410000	-1.442316000	2.437839000

C	1.994707000	-1.179521000	-1.603210000
C	-0.615446000	-2.273805000	2.282980000
H	-0.435764000	-3.308804000	2.594570000
H	-1.383025000	-1.869166000	2.951405000
C	3.018821000	-2.127176000	-1.949574000
C	2.635484000	-0.954957000	3.674314000
H	3.352383000	-1.174609000	4.460754000
C	2.831955000	0.174650000	2.850820000
C	-2.611536000	-2.022979000	0.757119000
H	-3.197520000	-2.862940000	1.145831000
C	1.879028000	0.441320000	1.808314000
C	2.058882000	1.584953000	0.997049000
H	1.330685000	1.795719000	0.228783000
C	1.696015000	-3.861292000	-0.924442000
H	1.521600000	-4.894243000	-0.641394000
C	-2.924151000	-0.721633000	1.482159000
C	3.136738000	2.419288000	1.211573000
H	3.253141000	3.302008000	0.589476000
C	-4.025602000	-1.916673000	-2.811058000
H	-4.832507000	-2.305868000	-3.424391000
C	2.841783000	-3.479323000	-1.585860000
H	3.610596000	-4.205326000	-1.836016000
C	3.282684000	0.554166000	-2.695711000

H	3.387411000	1.590750000	-3.003843000
C	4.173059000	-1.689543000	-2.651285000
H	4.937693000	-2.420140000	-2.899400000
C	-4.010256000	-0.494036000	2.314444000
H	-4.718095000	-1.289143000	2.525981000
C	-3.219035000	1.772426000	2.587401000
H	-3.306153000	2.768846000	3.006836000
C	3.936280000	1.048338000	3.031569000
H	4.648143000	0.828376000	3.822038000
C	4.088332000	2.153979000	2.226227000
H	4.928908000	2.825445000	2.370096000
C	-2.148214000	1.465033000	1.747350000
H	-1.379266000	2.183805000	1.485916000
C	4.307163000	-0.369798000	-3.016475000
H	5.187230000	-0.037013000	-3.557646000
C	-4.159859000	0.781828000	2.873728000
H	-4.998697000	0.993417000	3.529719000
H	-1.126800000	1.625543000	-0.919783000
C	0.041058000	3.349412000	-2.313834000
C	-1.381040000	3.783090000	-2.483889000
C	0.932599000	4.091939000	-1.372846000
H	0.489292000	2.708705000	-3.069063000
C	-2.050132000	4.181668000	-1.149255000

H	-1.968504000	3.015060000	-3.006538000
H	-1.404728000	4.671871000	-3.143231000
C	0.218193000	4.467483000	-0.057290000
H	1.845259000	3.515188000	-1.175158000
H	1.263811000	5.030491000	-1.857134000
C	-1.145941000	5.117940000	-0.333540000
H	-2.260531000	3.278339000	-0.551540000
H	-3.018310000	4.653601000	-1.350388000
H	0.852363000	5.140160000	0.531314000
H	0.073045000	3.555004000	0.537148000
H	-1.635463000	5.392027000	0.609067000
H	-0.996462000	6.049914000	-0.895924000

^{6}Int2;
S=-3045.442159, **G** = -3044.843384

Fe	0.496339000	0.000019000	-0.606741000
O	0.273912000	-0.000236000	-2.405515000
N	1.361911000	-0.000158000	1.483952000
N	2.160436000	1.442573000	-0.632794000
N	-0.761952000	1.447305000	0.368321000
N	-0.761998000	-1.447513000	0.368158000
N	2.160535000	-1.442534000	-0.632864000
C	-0.474639000	1.673369000	1.653069000
C	3.100947000	1.226126000	0.308743000

C	3.392682000	3.325995000	-1.433466000
H	3.474701000	4.146130000	-2.138677000
C	-2.255206000	1.712683000	-1.524143000
H	-1.543369000	1.204186000	-2.163065000
C	4.221607000	2.036720000	0.432375000
H	4.958789000	1.841832000	1.204953000
C	2.295303000	2.465951000	-1.488367000
H	1.503650000	2.584739000	-2.221608000
C	-1.344388000	-2.361944000	2.518178000
H	-1.060270000	-2.513627000	3.554383000
C	0.880198000	1.228750000	2.162553000
H	0.847107000	1.081959000	3.248803000
H	1.591815000	2.039177000	1.973573000
C	-0.474587000	-1.673733000	1.652870000
C	-1.947674000	1.915310000	-0.158695000
C	0.880318000	-1.229265000	2.162291000
H	0.847383000	-1.082758000	3.248584000
H	1.591922000	-2.039617000	1.972986000
C	-2.882557000	2.619943000	0.671606000
C	-2.546880000	-2.827396000	2.027543000
H	-3.243407000	-3.354111000	2.674358000
C	-2.882687000	-2.619972000	0.671546000
C	2.823051000	-0.000033000	1.168319000

H	3.450896000	-0.000036000	2.067540000
C	-1.947809000	-1.915322000	-0.158767000
C	-2.255500000	-1.712468000	-1.524155000
H	-1.543673000	-1.203950000	-2.163069000
C	-1.344470000	2.361563000	2.518373000
H	-1.060429000	2.513094000	3.554622000
C	3.101100000	-1.226045000	0.308594000
C	-3.448775000	-2.183651000	-2.035347000
H	-3.674471000	-2.032186000	-3.086791000
C	4.368370000	3.106696000	-0.459292000
H	5.232276000	3.760635000	-0.388784000
C	-2.546864000	2.827168000	2.027675000
H	-3.243417000	3.353873000	2.674469000
C	-3.448378000	2.184066000	-2.035413000
H	-3.673961000	2.032775000	-3.086906000
C	-4.102344000	3.083667000	0.112874000
H	-4.800857000	3.615046000	0.752905000
C	4.221890000	-2.036489000	0.432056000
H	4.959121000	-1.841543000	1.204573000
C	3.392940000	-3.325744000	-1.433786000
H	3.474990000	-4.145827000	-2.139051000
C	-4.102591000	-3.083492000	0.112885000
H	-4.801079000	-3.614880000	0.752935000

C	-4.382581000	-2.867240000	-1.217743000
H	-5.312891000	-3.225750000	-1.646623000
C	2.295448000	-2.465840000	-1.488523000
H	1.503730000	-2.584693000	-2.221676000
C	-4.382202000	2.867629000	-1.217823000
H	-5.312429000	3.226299000	-1.646749000
C	4.368707000	-3.106379000	-0.459698000
H	5.232705000	-3.760211000	-0.389328000
H	0.957960000	-0.000609000	-3.094367000

^{4}Int2;
S=-3045.399381, **G**= -3044.817218

Fe	0.496339000	0.000019000	-0.606741000
O	0.273912000	-0.000236000	-2.405515000
N	1.361911000	-0.000158000	1.483952000
N	2.160436000	1.442573000	-0.632794000
N	-0.761952000	1.447305000	0.368321000
N	-0.761998000	-1.447513000	0.368158000
N	2.160535000	-1.442534000	-0.632864000
C	-0.474639000	1.673369000	1.653069000
C	3.100947000	1.226126000	0.308743000
C	3.392682000	3.325995000	-1.433466000
H	3.474701000	4.146130000	-2.138677000
C	-2.255206000	1.712683000	-1.524143000

H	-1.543369000	1.204186000	-2.163065000
C	4.221607000	2.036720000	0.432375000
H	4.958789000	1.841832000	1.204953000
C	2.295303000	2.465951000	-1.488367000
H	1.503650000	2.584739000	-2.221608000
C	-1.344388000	-2.361944000	2.518178000
H	-1.060270000	-2.513627000	3.554383000
C	0.880198000	1.228750000	2.162553000
H	0.847107000	1.081959000	3.248803000
H	1.591815000	2.039177000	1.973573000
C	-0.474587000	-1.673733000	1.652870000
C	-1.947674000	1.915310000	-0.158695000
C	0.880318000	-1.229265000	2.162291000
H	0.847383000	-1.082758000	3.248584000
H	1.591922000	-2.039617000	1.972986000
C	-2.882557000	2.619943000	0.671606000
C	-2.546880000	-2.827396000	2.027543000
H	-3.243407000	-3.354111000	2.674358000
C	-2.882687000	-2.619972000	0.671546000
C	2.823051000	-0.000033000	1.168319000
H	3.450896000	-0.000036000	2.067540000
C	-1.947809000	-1.915322000	-0.158767000
C	-2.255500000	-1.712468000	-1.524155000

H	-1.543673000	-1.203950000	-2.163069000
C	-1.344470000	2.361563000	2.518373000
H	-1.060429000	2.513094000	3.554622000
C	3.101100000	-1.226045000	0.308594000
C	-3.448775000	-2.183651000	-2.035347000
H	-3.674471000	-2.032186000	-3.086791000
C	4.368370000	3.106696000	-0.459292000
H	5.232276000	3.760635000	-0.388784000
C	-2.546864000	2.827168000	2.027675000
H	-3.243417000	3.353873000	2.674469000
C	-3.448378000	2.184066000	-2.035413000
H	-3.673961000	2.032775000	-3.086906000
C	-4.102344000	3.083667000	0.112874000
H	-4.800857000	3.615046000	0.752905000
C	4.221890000	-2.036489000	0.432056000
H	4.959121000	-1.841543000	1.204573000
C	3.392940000	-3.325744000	-1.433786000
H	3.474990000	-4.145827000	-2.139051000
C	-4.102591000	-3.083492000	0.112885000
H	-4.801079000	-3.614880000	0.752935000
C	-4.382581000	-2.867240000	-1.217743000
H	-5.312891000	-3.225750000	-1.646623000
C	2.295448000	-2.465840000	-1.488523000

H	1.503730000	-2.584693000	-2.221676000
C	-4.382202000	2.867629000	-1.217823000
H	-5.312429000	3.226299000	-1.646749000
C	4.368707000	-3.106379000	-0.459698000
H	5.232705000	-3.760211000	-0.389328000
H	0.957960000	-0.000609000	-3.094367000
Fe	0.504055000	-0.000008000	-0.498265000
O	0.258990000	0.000181000	-2.332491000
N	1.435093000	-0.000087000	1.582305000
N	2.011194000	1.409313000	-0.617017000
N	-0.695113000	1.388593000	0.419044000
N	-0.695351000	-1.388465000	0.419299000
N	2.010582000	-1.409490000	-0.617150000
C	-0.390698000	1.675842000	1.689018000
C	3.032488000	1.225334000	0.246079000
C	3.094805000	3.333768000	-1.513632000
H	3.086805000	4.154227000	-2.223103000
C	-2.169145000	1.654082000	-1.498796000
H	-1.462520000	1.121735000	-2.122879000
C	4.125937000	2.080028000	0.275018000
H	4.931033000	1.916100000	0.984308000
C	2.029569000	2.433425000	-1.481351000
H	1.176324000	2.503591000	-2.147537000

C	-1.240682000	-2.431851000	2.518286000
H	-0.944011000	-2.626995000	3.543682000
C	0.950031000	1.227507000	2.238140000
H	0.880249000	1.089998000	3.324114000
H	1.669897000	2.036112000	2.070808000
C	-0.391032000	-1.675645000	1.689288000
C	-1.862485000	1.878021000	-0.137011000
C	0.949779000	-1.227465000	2.238349000
H	0.880021000	-1.089756000	3.324300000
H	1.669490000	-2.036240000	2.071159000
C	-2.774715000	2.641854000	0.667578000
C	-2.433587000	-2.899729000	2.013062000
H	-3.116131000	-3.470976000	2.636395000
C	-2.775128000	-2.641414000	0.667817000
C	2.853891000	-0.000316000	1.133110000
H	3.578761000	-0.000515000	1.956237000
C	-1.862749000	-1.877771000	-0.136775000
C	-2.169279000	-1.653882000	-1.498599000
H	-1.462550000	-1.121643000	-2.122666000
C	-1.240207000	2.432244000	2.517975000
H	-0.943460000	2.627431000	3.543341000
C	3.031976000	-1.225942000	0.245946000
C	-3.346700000	-2.147504000	-2.026043000

H	-3.568411000	-1.979661000	-3.075891000
C	4.155967000	3.153193000	-0.624565000
H	4.996974000	3.839910000	-0.625548000
C	-2.433072000	2.900245000	2.012776000
H	-3.115505000	3.471642000	2.636094000
C	-3.346538000	2.147824000	-2.026194000
H	-3.568332000	1.979937000	-3.076018000
C	-3.980175000	3.121741000	0.092356000
H	-4.661210000	3.694375000	0.715382000
C	4.125107000	-2.081047000	0.274737000
H	4.930288000	-1.917482000	0.984013000
C	3.093463000	-3.334239000	-1.514001000
H	3.085140000	-4.154619000	-2.223559000
C	-3.980612000	-3.121181000	0.092549000
H	-4.661775000	-3.693673000	0.715566000
C	-4.265900000	-2.874747000	-1.231445000
H	-5.185003000	-3.247140000	-1.672487000
C	2.028551000	-2.433525000	-1.481594000
H	1.175258000	-2.503295000	-2.147756000
C	-4.265593000	2.875245000	-1.231596000
H	-5.184675000	3.247727000	-1.672603000
C	4.154721000	-3.154132000	-0.624954000
H	4.995482000	-3.841149000	-0.626036000

H	0.987766000	0.000275000	-2.973020000

^{2}Int2;
S=-3045.403836, **G** =-3044.818741

Fe	-0.636299000	-0.000009000	-0.373601000
O	-0.270318000	-0.000020000	-2.115747000
N	-1.352423000	-0.000030000	1.546966000
N	-2.093362000	-1.344134000	-0.590652000
N	0.690578000	-1.414169000	0.368060000
N	0.690579000	1.414119000	0.368075000
N	-2.093328000	1.344148000	-0.590624000
C	0.517960000	-1.580566000	1.686338000
C	-3.061195000	-1.212923000	0.345493000
C	-3.247011000	-3.201608000	-1.531641000
H	-3.295783000	-3.969704000	-2.295849000
C	1.976001000	-2.001501000	-1.619925000
H	1.125888000	-1.784488000	-2.251066000
C	-4.150011000	-2.068714000	0.401924000
H	-4.908581000	-1.946641000	1.168422000
C	-2.176047000	-2.306022000	-1.517911000
H	-1.377906000	-2.323547000	-2.250450000
C	1.501161000	2.109107000	2.539283000
H	1.295724000	2.204672000	3.600173000
C	-0.845435000	-1.223324000	2.227033000
H	-0.825151000	-1.083036000	3.312899000

H	-1.527691000	-2.052286000	2.013514000
C	0.517973000	1.580504000	1.686354000
C	1.841342000	-1.908076000	-0.213543000
C	-0.845408000	1.223234000	2.227069000
H	-0.825096000	1.082902000	3.312929000
H	-1.527669000	2.052207000	2.013604000
C	2.913921000	-2.401169000	0.607182000
C	2.717590000	2.474238000	2.002901000
H	3.518101000	2.846620000	2.636301000
C	2.913891000	2.401193000	0.607165000
C	-2.825708000	-0.000006000	1.232291000
H	-3.457907000	-0.000007000	2.126174000
C	1.841322000	1.908056000	-0.213545000
C	1.975964000	2.001460000	-1.619929000
H	1.125859000	1.784385000	-2.251058000
C	1.501152000	-2.109140000	2.539279000
H	1.295703000	-2.204717000	3.600166000
C	-3.061162000	1.212940000	0.345521000
C	3.148315000	2.471063000	-2.178787000
H	3.224129000	2.559147000	-3.258563000
C	-4.240014000	-3.085822000	-0.558297000
H	-5.079368000	-3.774295000	-0.544581000
C	2.717604000	-2.474222000	2.002914000

H	3.518120000	-2.846575000	2.636325000
C	3.148375000	-2.471064000	-2.178766000
H	3.224200000	-2.559165000	-3.258540000
C	4.117681000	-2.847840000	-0.000909000
H	4.921774000	-3.200542000	0.638702000
C	-4.149956000	2.068757000	0.401973000
H	-4.908528000	1.946686000	1.168469000
C	-3.246930000	3.201673000	-1.531568000
H	-3.295685000	3.969788000	-2.295757000
C	4.117627000	2.847906000	-0.000943000
H	4.921714000	3.200643000	0.638656000
C	4.242339000	2.867056000	-1.371061000
H	5.157103000	3.221192000	-1.835252000
C	-2.175989000	2.306060000	-1.517859000
H	-1.377847000	2.323585000	-2.250397000
C	4.242409000	-2.866998000	-1.371025000
H	5.157192000	-3.221103000	-1.835203000
C	-4.239935000	3.085889000	-0.558224000
H	-5.079272000	3.774382000	-0.544491000
H	0.686028000	-0.000055000	-2.281037000

^{6}Int3;
S=-3194.515942, **G** =-3194.076888

Fe	0.515863000	0.000008000	-0.526057000

N	1.323697000	-0.000169000	1.571323000
N	2.161894000	1.452302000	-0.503652000
N	-0.790279000	1.439873000	0.430656000
N	-0.790265000	-1.439989000	0.430460000
N	2.162049000	-1.452147000	-0.503905000
C	-0.517983000	1.660408000	1.721922000
C	3.091092000	1.225038000	0.447735000
C	3.429247000	3.316913000	-1.291379000
H	3.530656000	4.131660000	-2.000191000
C	-2.285746000	1.719469000	-1.462695000
H	-1.568162000	1.235538000	-2.109491000
C	4.220327000	2.020075000	0.583812000
H	4.947006000	1.813238000	1.363123000
C	2.321841000	2.471259000	-1.361868000
H	1.552659000	2.591556000	-2.116629000
C	-1.399561000	-2.330830000	2.587470000
H	-1.121190000	-2.476000000	3.626081000
C	0.832826000	1.228590000	2.242866000
H	0.793693000	1.081591000	3.328616000
H	1.542479000	2.040769000	2.055951000
C	-0.517810000	-1.660946000	1.721620000
C	-1.980676000	1.902602000	-0.096146000
C	0.832993000	-1.229145000	2.242588000

H	0.793909000	-1.082419000	3.328378000
H	1.542713000	-2.041208000	2.055433000
C	-2.928900000	2.587852000	0.737577000
C	-2.605058000	-2.787106000	2.096103000
H	-3.311287000	-3.299389000	2.743913000
C	-2.928773000	-2.588221000	0.737236000
C	2.793442000	-0.000044000	1.296821000
H	3.389637000	-0.000096000	2.216939000
C	-1.980720000	-1.902569000	-0.096350000
C	-2.286037000	-1.718840000	-1.462763000
H	-1.568613000	-1.234540000	-2.109457000
C	-1.399896000	2.329902000	2.587908000
H	-1.121659000	2.474733000	3.626602000
C	3.091242000	-1.224927000	0.447499000
C	-3.480895000	-2.183819000	-1.975962000
H	-3.695002000	-2.045330000	-3.031480000
C	4.390767000	3.087914000	-0.306326000
H	5.263013000	3.729721000	-0.227810000
C	-2.605382000	2.786235000	2.096564000
H	-3.311742000	3.298206000	2.744480000
C	-3.480552000	2.184591000	-1.975887000
H	-3.694465000	2.046571000	-3.031506000
C	-4.151416000	3.046023000	0.179864000

H	-4.856205000	3.562702000	0.824998000
C	4.220585000	-2.019837000	0.583414000
H	4.947254000	-1.813037000	1.362745000
C	3.429632000	-3.316460000	-1.291977000
H	3.531129000	-4.131073000	-2.000930000
C	-4.151341000	-3.046249000	0.179520000
H	-4.855993000	-3.563248000	0.824546000
C	-4.425755000	-2.845817000	-1.154727000
H	-5.357457000	-3.201588000	-1.582681000
C	2.322113000	-2.470939000	-1.362297000
H	1.552935000	-2.591210000	-2.117066000
C	-4.425602000	2.846147000	-1.154512000
H	-5.357260000	3.202035000	-1.582464000
C	4.391146000	-3.087502000	-0.306910000
H	5.263480000	-3.729206000	-0.228524000
Cl	0.493851000	0.000124000	-2.788505000

^{4}Int3;
S=-3194.58262, **G** = -3194.141638

Fe	0.522238000	0.000007000	-0.431498000
N	1.400431000	-0.000071000	1.650469000
N	2.014457000	1.431029000	-0.505192000
N	-0.721165000	1.388072000	0.475169000
N	-0.721070000	-1.388198000	0.475003000
N	2.014697000	-1.430861000	-0.505299000

C	-0.421301000	1.672390000	1.749228000
C	3.028020000	1.226964000	0.364004000
C	3.118993000	3.370830000	-1.344239000
H	3.119589000	4.204954000	-2.037475000
C	-2.222565000	1.648788000	-1.426159000
H	-1.525683000	1.124511000	-2.061987000
C	4.127553000	2.071242000	0.419675000
H	4.923745000	1.884181000	1.133164000
C	2.047429000	2.477929000	-1.343968000
H	1.212667000	2.573343000	-2.028067000
C	-1.272475000	-2.420242000	2.582674000
H	-0.972945000	-2.611173000	3.607972000
C	0.913890000	1.227710000	2.305842000
H	0.837944000	1.086694000	3.390596000
H	1.635652000	2.035321000	2.143750000
C	-0.421074000	-1.672785000	1.748976000
C	-1.898860000	1.870060000	-0.070571000
C	0.914076000	-1.228041000	2.305631000
H	0.838135000	-1.087231000	3.390412000
H	1.635942000	-2.035526000	2.143380000
C	-2.812737000	2.627260000	0.741022000
C	-2.468636000	-2.885752000	2.084057000
H	-3.151518000	-3.452159000	2.711362000

C	-2.812511000	-2.627638000	0.740756000
C	2.831937000	0.000078000	1.237604000
H	3.529444000	0.000103000	2.083571000
C	-1.898801000	-1.870117000	-0.070727000
C	-2.222723000	-1.648431000	-1.426194000
H	-1.525984000	-1.123883000	-2.061950000
C	-1.272858000	2.419542000	2.583040000
H	-0.973439000	2.610257000	3.608410000
C	3.028241000	-1.226690000	0.363890000
C	-3.405594000	-2.135301000	-1.947190000
H	-3.630187000	-1.965543000	-2.995955000
C	4.174555000	3.162538000	-0.456271000
H	5.022354000	3.840598000	-0.438798000
C	-2.469032000	2.885033000	2.084433000
H	-3.152042000	3.451191000	2.711824000
C	-3.405402000	2.135726000	-1.947166000
H	-3.629826000	1.966301000	-2.996022000
C	-4.024886000	3.102455000	0.175749000
H	-4.702477000	3.670764000	0.806415000
C	4.127927000	-2.070773000	0.419480000
H	4.924098000	-1.883624000	1.132971000
C	3.119567000	-3.370402000	-1.344515000
H	3.120298000	-4.204472000	-2.037817000

C	-4.024690000	-3.102772000	0.175497000
H	-4.702145000	-3.671335000	0.806081000
C	-4.321358000	-2.858389000	-1.146264000
H	-5.245026000	-3.228397000	-1.579512000
C	2.047846000	-2.477687000	-1.344159000
H	1.213096000	-2.573193000	-2.028262000
C	-4.321349000	2.858464000	-1.146132000
H	-5.244990000	3.228527000	-1.579389000
C	4.175108000	-3.161994000	-0.456551000
H	5.023029000	-3.839904000	-0.439147000
Cl	0.481229000	-0.000016000	-2.762726000

^{2}Int3;
S=-3194.587868, **G**= -3194.143200

Fe	-0.602631000	-0.000010000	-0.307037000
N	-1.380943000	0.000051000	1.548064000
N	-2.004074000	-1.430826000	-0.503565000
N	0.709684000	-1.394892000	0.438913000
N	0.709675000	1.394931000	0.438833000
N	-2.004106000	1.430775000	-0.503651000
C	0.414725000	-1.687120000	1.714959000
C	-3.050468000	-1.229769000	0.329782000
C	-3.071652000	-3.379172000	-1.365086000
H	-3.045164000	-4.220084000	-2.049492000
C	2.243962000	-1.643909000	-1.441129000

H	1.558114000	-1.112132000	-2.079783000
C	-4.149965000	-2.072570000	0.355039000
H	-4.971671000	-1.886554000	1.039125000
C	-2.001791000	-2.484181000	-1.334362000
H	-1.139088000	-2.581427000	-1.981792000
C	1.256489000	2.428179000	2.560577000
H	0.951772000	2.617139000	3.584639000
C	-0.921037000	-1.236364000	2.247699000
H	-0.874943000	-1.064488000	3.327589000
H	-1.654428000	-2.030949000	2.079541000
C	0.414658000	1.687306000	1.714832000
C	1.898281000	-1.870028000	-0.091515000
C	-0.921092000	1.236544000	2.247594000
H	-0.874998000	1.064759000	3.327499000
H	-1.654515000	2.031086000	2.079367000
C	2.806544000	-2.628779000	0.728199000
C	2.456330000	2.891675000	2.068138000
H	3.137222000	3.457543000	2.698043000
C	2.806491000	2.628912000	0.728064000
C	-2.850506000	0.000013000	1.192575000
H	-3.491464000	0.000034000	2.080216000
C	1.898297000	1.870017000	-0.091594000
C	2.244081000	1.643695000	-1.441147000

H	1.558297000	1.111797000	-2.079766000
C	1.256621000	-2.427856000	2.560760000
H	0.951953000	-2.616702000	3.584858000
C	-3.050499000	1.229736000	0.329703000
C	3.433814000	2.128997000	-1.947754000
H	3.672717000	1.953202000	-2.992423000
C	-4.160389000	-3.168141000	-0.518573000
H	-5.005924000	-3.849110000	-0.528574000
C	2.456460000	-2.891368000	2.068328000
H	3.137402000	-3.457126000	2.698277000
C	3.433672000	-2.129260000	-1.947741000
H	3.672496000	-1.953628000	-2.992456000
C	4.026375000	-3.102351000	0.177851000
H	4.696411000	-3.670439000	0.816731000
C	-4.150020000	2.072508000	0.354907000
H	-4.971725000	1.886506000	1.038999000
C	-3.071728000	3.379053000	-1.365273000
H	-3.045256000	4.219934000	-2.049717000
C	4.026343000	3.102437000	0.177724000
H	4.696322000	3.670638000	0.816563000
C	4.339998000	2.855174000	-1.139171000
H	5.269546000	3.223032000	-1.561644000
C	-2.001843000	2.484094000	-1.334495000

H	-1.139136000	2.581336000	-1.981920000
C	4.339933000	-2.855281000	-1.139103000
H	5.269463000	-3.223179000	-1.561583000
C	-4.160468000	3.168033000	-0.518762000
H	-5.006022000	3.848979000	-0.528802000
Cl	-0.434724000	-0.000090000	-2.589227000

^{7}Int4;
S =-3429.921279, **G** = -3429.331482

Fe	-0.759826000	0.199461000	-0.002883000
N	-2.611774000	-1.074607000	0.041272000
N	-2.141201000	1.082685000	-1.459518000
N	-0.239070000	-1.340509000	-1.439806000
N	-0.203465000	-1.309622000	1.443516000
N	-2.127830000	1.127049000	1.456828000
C	-1.188123000	-2.269021000	-1.608005000
C	-3.443259000	0.825490000	-1.219827000
C	-2.752094000	2.404664000	-3.351667000
H	-2.440450000	3.027817000	-4.182959000
C	2.047287000	-0.600772000	-1.824020000
H	1.837789000	0.363098000	-1.378690000
C	-4.456555000	1.332419000	-2.021360000
H	-5.495200000	1.103100000	-1.804945000
C	-1.793857000	1.857692000	-2.497855000
H	-0.733068000	2.042596000	-2.627189000

C	-0.938874000	-3.365619000	2.468673000
H	-1.763286000	-4.044107000	2.662148000
C	-2.593722000	-1.933516000	-1.167187000
H	-3.167744000	-2.851176000	-0.992996000
H	-3.085535000	-1.400475000	-1.987111000
C	-1.166864000	-2.193182000	1.727089000
C	1.031032000	-1.577320000	-1.930624000
C	-2.577761000	-1.876055000	1.288604000
H	-3.152158000	-2.801709000	1.163764000
H	-3.061970000	-1.307771000	2.089002000
C	1.337706000	-2.825176000	-2.576038000
C	0.332064000	-3.627482000	2.934705000
H	0.540015000	-4.527556000	3.507001000
C	1.379063000	-2.721425000	2.663019000
C	-3.670397000	-0.019221000	0.023474000
H	-4.681997000	-0.441831000	0.035493000
C	1.081111000	-1.542149000	1.897818000
C	2.123943000	-0.629384000	1.625467000
H	1.921899000	0.275414000	1.070695000
C	-0.953067000	-3.503642000	-2.236690000
H	-1.765536000	-4.215722000	-2.337023000
C	-3.432843000	0.871485000	1.231761000
C	3.400308000	-0.875486000	2.091862000

H	4.181096000	-0.152007000	1.885687000
C	-4.100661000	2.139107000	-3.109388000
H	-4.868439000	2.551304000	-3.757073000
C	0.311400000	-3.783506000	-2.710126000
H	0.528393000	-4.734009000	-3.190043000
C	3.308823000	-0.861476000	-2.323593000
H	4.074242000	-0.097688000	-2.244225000
C	2.648442000	-3.062128000	-3.066318000
H	2.859253000	-4.011878000	-3.549471000
C	-4.440171000	1.413288000	2.017778000
H	-5.481042000	1.184091000	1.812111000
C	-2.723826000	2.515566000	3.306509000
H	-2.404472000	3.162910000	4.116105000
C	2.703596000	-2.947071000	3.120517000
H	2.908260000	-3.843446000	3.698899000
C	3.699842000	-2.039563000	2.839520000
H	4.711551000	-2.207862000	3.194445000
C	-1.772389000	1.933426000	2.468320000
H	-0.710243000	2.115491000	2.588920000
C	3.620862000	-2.096761000	-2.940446000
H	4.621927000	-2.271945000	-3.321242000
C	-4.075192000	2.253856000	3.076652000
H	-4.837863000	2.694123000	3.711774000

Cl	0.509210000	2.055881000	-0.009035000
C	3.671523000	2.502066000	-1.294029000
C	3.604459000	3.998778000	-1.293010000
C	4.413784000	1.804471000	-0.193648000
H	3.484725000	1.975361000	-2.228116000
C	3.329533000	4.571079000	0.113478000
H	2.853767000	4.355181000	-2.010014000
H	4.573631000	4.406984000	-1.640081000
C	4.124409000	2.427457000	1.189703000
H	4.186952000	0.728551000	-0.186491000
H	5.504290000	1.881323000	-0.371994000
C	4.277733000	3.955432000	1.152424000
H	2.291742000	4.346513000	0.397891000
H	3.435853000	5.661841000	0.096043000
H	4.798523000	1.997121000	1.941991000
H	3.094817000	2.182936000	1.489498000
H	4.082654000	4.377232000	2.145728000
H	5.316338000	4.207320000	0.893712000

^{5}Int4;
S=-3430.014407,**G** = -3429.424074

Fe	-0.770494000	0.257089000	-0.047000000
N	-2.571491000	-1.130226000	-0.074374000
N	-2.262333000	1.226449000	-1.401262000
N	-0.167097000	-1.404013000	-1.456416000

N	-0.190844000	-1.311284000	1.442480000
N	-2.108278000	1.058813000	1.536939000
C	-1.167023000	-2.201270000	-1.818907000
C	-3.527332000	0.875204000	-1.092892000
C	-3.107727000	2.707875000	-3.083700000
H	-2.899912000	3.432025000	-3.864163000
C	2.195274000	-0.933076000	-1.403179000
H	1.981668000	-0.088921000	-0.759887000
C	-4.631294000	1.402844000	-1.751566000
H	-5.633899000	1.089243000	-1.477768000
C	-2.056733000	2.125898000	-2.372520000
H	-1.020723000	2.385473000	-2.563694000
C	-0.720437000	-3.567970000	2.097012000
H	-1.463802000	-4.358349000	2.125960000
C	-2.569130000	-1.834977000	-1.372221000
H	-3.192689000	-2.738718000	-1.329178000
H	-3.007730000	-1.183086000	-2.133667000
C	-1.052700000	-2.319229000	1.524841000
C	1.108563000	-1.725561000	-1.847490000
C	-2.477255000	-2.073977000	1.061036000
H	-2.959767000	-3.028054000	0.813071000
H	-3.026089000	-1.656969000	1.913194000
C	1.373842000	-2.861948000	-2.676261000

C	0.545436000	-3.757660000	2.603512000
H	0.836366000	-4.710902000	3.036684000
C	1.476757000	-2.691830000	2.575418000
C	-3.641914000	-0.104044000	0.068687000
H	-4.646126000	-0.547542000	0.092159000
C	1.059916000	-1.455531000	1.987354000
C	1.948916000	-0.352117000	1.999731000
H	1.612759000	0.593888000	1.589982000
C	-0.986963000	-3.346669000	-2.628486000
H	-1.846266000	-3.956165000	-2.889888000
C	-3.390486000	0.687336000	1.349977000
C	3.202552000	-0.482880000	2.561434000
H	3.865346000	0.377440000	2.600153000
C	-4.415443000	2.339491000	-2.768131000
H	-5.256299000	2.770482000	-3.303081000
C	0.276443000	-3.666663000	-3.067294000
H	0.447338000	-4.538094000	-3.693623000
C	3.483913000	-1.258407000	-1.773548000
H	4.319594000	-0.666558000	-1.408639000
C	2.710277000	-3.158899000	-3.052423000
H	2.895979000	-4.021545000	-3.686041000
C	-4.405401000	1.043755000	2.230922000
H	-5.425698000	0.718083000	2.053083000

C	-2.751409000	2.219348000	3.530349000
H	-2.459376000	2.828709000	4.378965000
C	2.783267000	-2.799801000	3.121324000
H	3.090481000	-3.745243000	3.559529000
C	3.632752000	-1.715817000	3.114014000
H	4.624542000	-1.796248000	3.547876000
C	-1.794482000	1.808919000	2.600443000
H	-0.749017000	2.086011000	2.694910000
C	3.749478000	-2.371605000	-2.609856000
H	4.771603000	-2.605138000	-2.890618000
C	-4.077013000	1.826816000	3.342957000
H	-4.845943000	2.122282000	4.050388000
Cl	0.692102000	2.198456000	-0.242916000
C	3.571947000	2.277565000	-1.274340000
C	3.502645000	3.683301000	-1.649705000
C	4.182835000	1.822953000	-0.028322000
H	3.284851000	1.521748000	-2.006893000
C	3.446345000	4.674141000	-0.468166000
H	2.736213000	3.845629000	-2.415468000
H	4.472342000	3.808092000	-2.191539000
C	4.117167000	2.832395000	1.135976000
H	3.837250000	0.816118000	0.232831000
H	5.245539000	1.687413000	-0.340254000

C	4.404788000	4.263096000	0.658046000
H	2.413309000	4.682535000	-0.101874000
H	3.680724000	5.677061000	-0.836177000
H	4.828096000	2.527872000	1.910426000
H	3.107680000	2.775147000	1.559967000
H	4.302004000	4.957423000	1.498286000
H	5.444842000	4.336582000	0.310847000

^{3}Int4;
S=-3429.987499, **G** = -3429.393147

Fe	0.808786000	-0.161700000	0.029113000
N	2.792465000	0.828046000	0.142128000
N	2.056522000	-1.326999000	-1.297575000
N	0.516047000	1.282388000	-1.410317000
N	0.372899000	1.358771000	1.461349000
N	1.637227000	-1.269368000	1.486899000
C	1.633472000	1.920083000	-1.772349000
C	3.348510000	-1.286639000	-0.915956000
C	2.653453000	-2.797707000	-3.085643000
H	2.338463000	-3.386044000	-3.940813000
C	-1.898765000	1.119847000	-1.537289000
H	-1.869314000	0.364835000	-0.766462000
C	4.349106000	-1.983180000	-1.580572000
H	5.379297000	-1.919328000	-1.244357000

C	1.711852000	-2.065679000	-2.359262000
H	0.656343000	-2.073417000	-2.606677000
C	1.234482000	3.418871000	2.367895000
H	2.099528000	4.058572000	2.511300000
C	2.958872000	1.531877000	-1.142243000
H	3.572967000	2.433322000	-1.016138000
H	3.497986000	0.889576000	-1.845849000
C	1.387371000	2.187627000	1.693710000
C	-0.678401000	1.686027000	-1.975936000
C	2.783731000	1.734972000	1.302134000
H	3.424567000	2.607578000	1.123324000
H	3.206368000	1.208440000	2.166294000
C	-0.720007000	2.703330000	-2.983671000
C	-0.010138000	3.782441000	2.828023000
H	-0.163750000	4.730186000	3.336856000
C	-1.101369000	2.897765000	2.658028000
C	3.579713000	-0.426176000	0.317188000
H	4.651209000	-0.244662000	0.470343000
C	-0.867692000	1.663389000	1.970944000
C	-1.926490000	0.729730000	1.857478000
H	-1.736533000	-0.223228000	1.377137000
C	1.661091000	2.937614000	-2.752650000
H	2.608414000	3.407069000	-2.998680000

C	2.989495000	-1.184344000	1.499706000
C	-3.165484000	1.023353000	2.389142000
H	-3.961554000	0.286815000	2.328574000
C	3.990292000	-2.757825000	-2.689584000
H	4.745437000	-3.315805000	-3.234831000
C	0.495411000	3.313994000	-3.371827000
H	0.487853000	4.088413000	-4.133911000
C	-3.095279000	1.542464000	-2.080965000
H	-4.029910000	1.126028000	-1.714308000
C	-1.965544000	3.097410000	-3.538482000
H	-1.972896000	3.866224000	-4.305846000
C	3.758513000	-1.788207000	2.485838000
H	4.839587000	-1.693247000	2.466140000
C	1.719416000	-2.602767000	3.472308000
H	1.180172000	-3.157930000	4.232184000
C	-2.396728000	3.180186000	3.166383000
H	-2.562121000	4.124526000	3.677247000
C	-3.412827000	2.260390000	3.034742000
H	-4.397355000	2.471425000	3.440208000
C	1.015598000	-1.964451000	2.451084000
H	-0.064563000	-2.008908000	2.376666000
C	-3.137932000	2.528824000	-3.095663000
H	-4.091134000	2.841168000	-3.510318000

C	3.110864000	-2.512126000	3.492516000
H	3.685805000	-2.993897000	4.277389000
Cl	-0.955111000	-1.971550000	-0.304003000
C	-3.770780000	-1.868829000	-1.363040000
C	-3.880440000	-3.298504000	-1.642000000
C	-4.370874000	-1.260142000	-0.172918000
H	-3.365077000	-1.208377000	-2.129492000
C	-3.923585000	-4.197975000	-0.386414000
H	-3.141447000	-3.609559000	-2.387077000
H	-4.865949000	-3.356196000	-2.161915000
C	-4.390327000	-2.178546000	1.068321000
H	-3.945784000	-0.269893000	0.019834000
H	-5.419445000	-1.077464000	-0.500713000
C	-4.826691000	-3.604039000	0.702670000
H	-2.895544000	-4.287651000	-0.017297000
H	-4.265762000	-5.194976000	-0.678662000
H	-5.058687000	-1.746061000	1.819744000
H	-3.373666000	-2.191202000	1.479168000
H	-4.791523000	-4.238848000	1.594392000
H	-5.870961000	-3.595136000	0.360409000

^{7}ts3;
S=-3429.882872, **G** = -3429.29846

Fe	-0.759600000	0.021757000	-0.134890000
N	-2.256526000	-1.634107000	0.137558000

N	-2.479545000	0.568938000	-1.413524000
N	0.043921000	-1.398164000	-1.452963000
N	0.270566000	-1.295967000	1.337524000
N	-2.167893000	0.711294000	1.457928000
C	-0.651393000	-2.616885000	-1.401862000
C	-3.639308000	-0.007009000	-1.036457000
C	-3.623879000	1.670156000	-3.202309000
H	-3.578194000	2.340388000	-4.053913000
C	2.059604000	-0.215423000	-1.993700000
H	1.507892000	0.710618000	-1.883776000
C	-4.833770000	0.213714000	-1.710608000
H	-5.747052000	-0.271818000	-1.381381000
C	-2.469250000	1.392582000	-2.470196000
H	-1.511644000	1.838354000	-2.716873000
C	0.168652000	-3.542534000	2.206731000
H	-0.449634000	-4.406408000	2.428577000
C	-2.109470000	-2.488070000	-1.072456000
H	-2.564681000	-3.473853000	-0.914408000
H	-2.635362000	-1.999053000	-1.898450000
C	-0.421856000	-2.397182000	1.631772000
C	1.365566000	-1.427536000	-1.820503000
C	-1.913444000	-2.379606000	1.371811000
H	-2.297856000	-3.405895000	1.315690000

H	-2.405272000	-1.895763000	2.221409000
C	2.068712000	-2.666806000	-2.023078000
C	1.521234000	-3.545939000	2.461468000
H	2.006319000	-4.417806000	2.891884000
C	2.292751000	-2.399139000	2.156347000
C	-3.520923000	-0.851317000	0.223256000
H	-4.404749000	-1.488428000	0.351289000
C	1.619916000	-1.266922000	1.594155000
C	2.366132000	-0.100781000	1.299997000
H	1.851452000	0.765635000	0.904269000
C	-0.034652000	-3.826098000	-1.602251000
H	-0.616551000	-4.739605000	-1.528802000
C	-3.376903000	0.117735000	1.390882000
C	3.724145000	-0.066353000	1.546196000
H	4.283184000	0.840341000	1.337195000
C	-4.823539000	1.069709000	-2.816960000
H	-5.738867000	1.261432000	-3.368578000
C	1.345171000	-3.880705000	-1.900827000
H	1.845488000	-4.830447000	-2.057918000
C	3.435809000	-0.198773000	-2.320535000
H	3.943245000	0.750091000	-2.460425000
C	3.437917000	-2.621746000	-2.336774000
H	3.973751000	-3.555941000	-2.479089000

C	-4.400747000	0.405219000	2.284720000
H	-5.359519000	-0.096941000	2.200847000
C	-2.909338000	1.964927000	3.357055000
H	-2.685442000	2.701235000	4.121455000
C	3.691271000	-2.334305000	2.387428000
H	4.190083000	-3.198408000	2.817317000
C	4.396722000	-1.189148000	2.085207000
H	5.464680000	-1.140026000	2.272984000
C	-1.937343000	1.617174000	2.417731000
H	-0.952403000	2.072200000	2.416884000
C	4.121823000	-1.389119000	-2.481675000
H	5.176782000	-1.390293000	-2.736505000
C	-4.159706000	1.349500000	3.288836000
H	-4.936776000	1.596031000	4.005967000
Cl	0.120277000	2.287797000	-0.282183000
C	2.146721000	3.444012000	-1.276691000
C	1.682904000	4.840986000	-1.127403000
C	3.259178000	2.934117000	-0.442183000
H	1.936229000	2.936244000	-2.215463000
C	1.701389000	5.354963000	0.325232000
H	0.715387000	4.986980000	-1.618628000
H	2.416659000	5.422479000	-1.725481000
C	3.246539000	3.464998000	1.004324000

H	3.326341000	1.842625000	-0.498767000
H	4.168036000	3.317293000	-0.951602000
C	3.010411000	4.982606000	1.036564000
H	0.849933000	4.910999000	0.854849000
H	1.557924000	6.439905000	0.320476000
H	4.196196000	3.211568000	1.487663000
H	2.447935000	2.952550000	1.554780000
H	2.982058000	5.331155000	2.074421000
H	3.853377000	5.494336000	0.551238000

^{5}ts3;
S=-3429.927922, **G** = -3429.337081

Fe	-0.794209000	0.017462000	-0.013600000
N	-2.636796000	-1.177203000	0.300627000
N	-2.141951000	0.843274000	-1.360105000
N	-0.319822000	-1.471787000	-1.234446000
N	-0.096032000	-1.244884000	1.406310000
N	-1.713415000	1.085854000	1.434514000
C	-1.295680000	-2.426996000	-1.315035000
C	-3.429938000	0.712597000	-0.960956000
C	-2.873586000	1.936542000	-3.352508000
H	-2.616343000	2.403410000	-4.296927000
C	1.984956000	-0.808866000	-1.618570000
H	1.748295000	0.182045000	-1.262367000
C	-4.486642000	1.208140000	-1.714103000

H	-5.506830000	1.088432000	-1.363653000
C	-1.865660000	1.430239000	-2.537277000
H	-0.818379000	1.501254000	-2.803428000
C	-0.532373000	-3.443351000	2.290174000
H	-1.267602000	-4.204286000	2.531740000
C	-2.691229000	-2.053213000	-0.893088000
H	-3.279594000	-2.954951000	-0.686787000
H	-3.199610000	-1.509319000	-1.697309000
C	-0.965949000	-2.232980000	1.737792000
C	0.966545000	-1.776388000	-1.658451000
C	-2.428783000	-1.934337000	1.554537000
H	-3.019041000	-2.858084000	1.556241000
H	-2.781480000	-1.313294000	2.387921000
C	1.276481000	-3.085409000	-2.155488000
C	0.815474000	-3.648729000	2.520589000
H	1.173886000	-4.589203000	2.928172000
C	1.740776000	-2.607188000	2.253995000
C	-3.573609000	-0.016095000	0.359687000
H	-4.616043000	-0.301104000	0.543636000
C	1.246528000	-1.376029000	1.711149000
C	2.134459000	-0.300140000	1.526087000
H	1.757304000	0.644527000	1.155030000
C	-1.033117000	-3.712214000	-1.800434000

H	-1.845677000	-4.430701000	-1.839916000
C	-3.058801000	0.899119000	1.455788000
C	3.478224000	-0.443539000	1.834196000
H	4.145432000	0.403349000	1.709741000
C	-4.203077000	1.836161000	-2.929957000
H	-5.007924000	2.228718000	-3.543613000
C	0.240251000	-4.052458000	-2.214867000
H	0.459709000	-5.049534000	-2.584323000
C	3.272312000	-1.120763000	-2.032838000
H	4.045096000	-0.358729000	-1.994067000
C	2.598153000	-3.372207000	-2.570910000
H	2.816139000	-4.366600000	-2.949906000
C	-3.863708000	1.527778000	2.398413000
H	-4.936267000	1.361907000	2.390852000
C	-1.872528000	2.514023000	3.340106000
H	-1.370450000	3.135661000	4.073173000
C	3.123658000	-2.727687000	2.534811000
H	3.489801000	-3.665686000	2.942383000
C	3.982571000	-1.665479000	2.324246000
H	5.038076000	-1.762647000	2.557382000
C	-1.127592000	1.863464000	2.363124000
H	-0.051336000	1.962292000	2.293489000
C	3.587415000	-2.407293000	-2.507750000

H	4.597294000	-2.636674000	-2.832152000
C	-3.262805000	2.351688000	3.353175000
H	-3.868546000	2.850260000	4.103490000
Cl	0.532298000	2.209069000	-0.471138000
C	2.605424000	2.775566000	-1.465418000
C	2.458298000	4.251995000	-1.591001000
C	3.624967000	2.235619000	-0.522710000
H	2.376959000	2.173196000	-2.342331000
C	2.549716000	4.998040000	-0.247340000
H	1.555822000	4.509842000	-2.154216000
H	3.315316000	4.548781000	-2.228477000
C	3.699278000	3.001297000	0.809903000
H	3.504294000	1.157731000	-0.380672000
H	4.582878000	2.367184000	-1.063862000
C	3.753096000	4.519268000	0.578341000
H	1.621880000	4.821455000	0.310581000
H	2.617457000	6.073407000	-0.440061000
H	4.579583000	2.666555000	1.369747000
H	2.812847000	2.749747000	1.406888000
H	3.777962000	5.041846000	1.540613000
H	4.684549000	4.773208000	0.053163000

^{3}ts3;
S=-3429.962289, **G** = -3429.363514

Fe	0.833145000	-0.126787000	-0.004069000

N	2.798960000	0.867088000	0.364523000
N	2.023333000	-0.978117000	-1.479599000
N	0.535639000	1.555223000	-1.148328000
N	0.295756000	1.045722000	1.625386000
N	1.675384000	-1.478082000	1.243182000
C	1.609910000	2.345210000	-1.246487000
C	3.329771000	-0.965737000	-1.134791000
C	2.605375000	-1.969320000	-3.576887000
H	2.279073000	-2.356694000	-4.536035000
C	-1.809916000	1.173658000	-1.611252000
H	-1.734769000	0.202552000	-1.142388000
C	4.325258000	-1.448628000	-1.973493000
H	5.364592000	-1.415679000	-1.662310000
C	1.666398000	-1.464467000	-2.676714000
H	0.604641000	-1.456422000	-2.892704000
C	1.074665000	2.811956000	3.068467000
H	1.920595000	3.395447000	3.417700000
C	2.946891000	1.852248000	-0.717251000
H	3.545948000	2.710484000	-0.386037000
H	3.492208000	1.396442000	-1.550811000
C	1.286365000	1.791868000	2.116641000
C	-0.657171000	1.989014000	-1.689899000
C	2.714279000	1.475647000	1.699838000

H	3.326148000	2.385122000	1.756123000
H	3.125327000	0.777358000	2.438293000
C	-0.756220000	3.262978000	-2.339495000
C	-0.198666000	3.047764000	3.533200000
H	-0.393002000	3.834573000	4.256977000
C	-1.267783000	2.244112000	3.074132000
C	3.589517000	-0.389273000	0.250113000
H	4.665640000	-0.246095000	0.412764000
C	-0.980781000	1.224322000	2.110148000
C	-2.025376000	0.374449000	1.677628000
H	-1.802354000	-0.422811000	0.978935000
C	1.579130000	3.610056000	-1.871583000
H	2.487252000	4.203306000	-1.909091000
C	3.025908000	-1.383957000	1.257558000
C	-3.301861000	0.543205000	2.173344000
H	-4.093247000	-0.124849000	1.847988000
C	3.953717000	-1.964962000	-3.219684000
H	4.707469000	-2.349481000	-3.899986000
C	0.402887000	4.067968000	-2.415746000
H	0.349785000	5.040066000	-2.898319000
C	-3.004021000	1.610312000	-2.147393000
H	-3.882632000	0.977939000	-2.075397000
C	-2.000704000	3.682054000	-2.878013000

H	-2.056954000	4.651566000	-3.364679000
C	3.811910000	-2.156721000	2.102378000
H	4.892004000	-2.050253000	2.089284000
C	1.789101000	-3.152068000	2.948261000
H	1.263051000	-3.839627000	3.601693000
C	-2.596855000	2.404301000	3.546431000
H	-2.801722000	3.187092000	4.271188000
C	-3.598258000	1.569395000	3.103991000
H	-4.611813000	1.686807000	3.474218000
C	1.068153000	-2.340733000	2.072426000
H	-0.012979000	-2.377545000	2.008363000
C	-3.108664000	2.871129000	-2.783555000
H	-4.060082000	3.192521000	-3.195432000
C	3.180697000	-3.060339000	2.963780000
H	3.768241000	-3.676473000	3.637499000
Cl	-0.925448000	-2.159754000	-0.646798000
C	-3.062493000	-3.220670000	-1.615364000
C	-3.463582000	-4.066178000	-0.472165000
C	-3.864288000	-2.035611000	-1.989113000
H	-2.427262000	-3.664632000	-2.378053000
C	-4.056991000	-3.280510000	0.710026000
H	-2.651773000	-4.739801000	-0.183098000
H	-4.251457000	-4.713525000	-0.913555000

C	-4.476789000	-1.285737000	-0.793661000
H	-3.305420000	-1.381962000	-2.666231000
H	-4.678684000	-2.479465000	-2.599519000
C	-5.091469000	-2.253031000	0.228987000
H	-3.232719000	-2.769028000	1.222672000
H	-4.506756000	-3.983124000	1.418292000
H	-5.233706000	-0.583919000	-1.159803000
H	-3.682376000	-0.698158000	-0.320265000
H	-5.487005000	-1.691569000	1.083176000
H	-5.946161000	-2.772948000	-0.225044000

^{5}P+P$_{OH}$;
S=-3429.970153, **G**=-3429.379854

Fe	0.412196000	-0.193812000	0.083789000
N	0.425280000	-2.403100000	0.486873000
N	2.024158000	-0.442189000	1.548999000
N	-1.157230000	-0.348948000	1.840235000
N	-1.280176000	-0.912939000	-1.126065000
N	1.952145000	-1.078607000	-1.367371000
C	-1.465508000	-1.645935000	1.867607000
C	2.501715000	-1.703258000	1.571327000
C	3.485125000	0.130044000	3.358416000
H	3.844412000	0.881919000	4.052890000
C	-1.852880000	1.936273000	2.180688000
H	-0.826547000	2.201091000	2.427375000

C	3.481810000	-2.109863000	2.468834000
H	3.837293000	-3.135487000	2.463412000
C	2.497066000	0.452065000	2.427982000
H	2.065148000	1.445006000	2.372836000
C	-2.506555000	-2.887252000	-1.772094000
H	-2.539343000	-3.971879000	-1.793933000
C	-0.288103000	-2.602122000	1.774257000
H	-0.622300000	-3.642592000	1.877762000
H	0.401096000	-2.383261000	2.593216000
C	-1.399062000	-2.239316000	-1.185916000
C	-2.166241000	0.567577000	1.965676000
C	-0.275120000	-3.085692000	-0.620281000
H	-0.672863000	-4.054799000	-0.290193000
H	0.435430000	-3.294311000	-1.426030000
C	-3.542258000	0.175259000	1.922131000
C	-3.530921000	-2.128577000	-2.290528000
H	-4.402013000	-2.598482000	-2.739379000
C	-3.457233000	-0.717781000	-2.226949000
C	1.897609000	-2.621431000	0.518290000
H	2.165552000	-3.664129000	0.733293000
C	-2.290978000	-0.129513000	-1.638397000
C	-2.192437000	1.280236000	-1.581505000
H	-1.299343000	1.724361000	-1.162831000

C	-2.791287000	-2.121933000	1.920064000
H	-2.980153000	-3.190075000	1.946018000
C	2.459814000	-2.217001000	-0.842431000
C	-3.216239000	2.068536000	-2.066047000
H	-3.130620000	3.150249000	-2.018556000
C	3.986790000	-1.172107000	3.376313000
H	4.752262000	-1.459242000	4.090830000
C	-3.827186000	-1.210064000	1.893182000
H	-4.861763000	-1.542470000	1.874577000
C	-2.858028000	2.881552000	2.232543000
H	-2.613845000	3.921979000	2.427007000
C	-4.552785000	1.174166000	1.951047000
H	-5.593771000	0.867370000	1.898574000
C	3.425481000	-2.978767000	-1.491141000
H	3.799893000	-3.888138000	-1.031268000
C	3.346179000	-1.399906000	-3.301003000
H	3.657365000	-1.045382000	-4.277875000
C	-4.492306000	0.120267000	-2.718361000
H	-5.369847000	-0.340563000	-3.163074000
C	-4.377931000	1.489949000	-2.634787000
H	-5.169213000	2.129864000	-3.012113000
C	2.381677000	-0.695241000	-2.579776000
H	1.936871000	0.205298000	-2.984323000

C	-4.216845000	2.503975000	2.079037000
H	-4.991763000	3.263019000	2.113196000
C	3.886099000	-2.557546000	-2.742348000
H	4.638941000	-3.132286000	-3.273234000
C	1.208299000	3.035893000	-0.439262000
C	2.113079000	3.691063000	0.597391000
C	1.984340000	2.510162000	-1.632075000
H	0.450436000	3.751248000	-0.782857000
C	2.912130000	4.838074000	-0.049639000
H	2.811171000	2.930994000	0.973093000
H	1.517681000	4.056035000	1.445491000
C	2.808254000	3.640640000	-2.278170000
H	2.653064000	1.710399000	-1.284727000
H	1.278925000	2.079900000	-2.354567000
C	3.722446000	4.321579000	-1.248332000
H	3.570515000	5.292717000	0.697969000
H	2.217931000	5.621307000	-0.384929000
H	3.395005000	3.235130000	-3.109903000
H	2.121739000	4.385042000	-2.704665000
H	4.265937000	5.147047000	-1.720150000
H	4.473482000	3.600474000	-0.893918000
O	0.474555000	1.907838000	0.160369000
H	-0.267578000	2.255520000	0.686375000

^{3}P+P_{OH};
S=-3430.030707, **G**= -3429.436529

Fe	0.301714000	-0.200949000	-0.058380000
O	1.099400000	1.658856000	-0.714500000
N	0.389228000	-2.423183000	0.365590000
N	1.908178000	-0.432668000	1.507453000
N	-1.196969000	-0.440240000	1.520212000
N	-1.312441000	-0.965215000	-1.346998000
N	1.919969000	-0.989362000	-1.417269000
C	-1.352332000	-1.674121000	1.989130000
C	2.437755000	-1.673977000	1.475207000
C	3.353637000	0.111971000	3.344110000
H	3.682910000	0.845904000	4.071920000
C	-1.923635000	1.846659000	1.386922000
H	-1.062431000	2.061120000	0.765477000
C	3.435959000	-2.081587000	2.353938000
H	3.830536000	-3.091698000	2.302693000
C	2.351373000	0.434910000	2.428431000
H	1.885239000	1.414633000	2.425206000
C	-2.633961000	-2.940604000	-1.736214000
H	-2.708780000	-4.020237000	-1.654673000
C	-0.276896000	-2.692113000	1.661291000
H	-0.700404000	-3.704480000	1.676811000
H	0.470466000	-2.653013000	2.461312000

C	-1.468720000	-2.286160000	-1.283775000
C	-2.102870000	0.529258000	1.865640000
C	-0.302032000	-3.102273000	-0.754658000
H	-0.643809000	-4.101301000	-0.454828000
H	0.408684000	-3.240432000	-1.575516000
C	-3.221194000	0.236783000	2.707773000
C	-3.660024000	-2.190664000	-2.270728000
H	-4.574187000	-2.665275000	-2.617170000
C	-3.522850000	-0.786575000	-2.373760000
C	1.870777000	-2.590910000	0.393617000
H	2.168593000	-3.628269000	0.594739000
C	-2.305961000	-0.199733000	-1.900047000
C	-2.121415000	1.197712000	-2.018657000
H	-1.175951000	1.622292000	-1.702216000
C	-2.430267000	-2.043190000	2.823843000
H	-2.511381000	-3.067855000	3.172478000
C	2.437766000	-2.142726000	-0.947953000
C	-3.112554000	1.983885000	-2.566989000
H	-2.962365000	3.055090000	-2.666255000
C	3.907100000	-1.168113000	3.302898000
H	4.684787000	-1.457582000	4.003163000
C	-3.361152000	-1.091332000	3.177663000
H	-4.204250000	-1.346942000	3.813825000

C	-2.821617000	2.837279000	1.724233000
H	-2.675979000	3.849639000	1.358624000
C	-4.133082000	1.274902000	3.033646000
H	-4.981113000	1.045831000	3.672717000
C	3.420445000	-2.849699000	-1.632254000
H	3.807532000	-3.779709000	-1.227636000
C	3.346511000	-1.150122000	-3.338784000
H	3.674073000	-0.728222000	-4.283003000
C	-4.529354000	0.050296000	-2.924561000
H	-5.451104000	-0.402508000	-3.278739000
C	-4.329645000	1.410030000	-3.015979000
H	-5.097569000	2.047214000	-3.442919000
C	2.358890000	-0.508735000	-2.590045000
H	1.896697000	0.414419000	-2.927994000
C	-3.937683000	2.550543000	2.550538000
H	-4.634169000	3.343038000	2.805039000
C	3.887321000	-2.339759000	-2.848726000
H	4.653231000	-2.869777000	-3.406732000
H	2.061219000	1.518338000	-0.761224000
H	0.871121000	3.123335000	1.508086000
C	1.371293000	3.654905000	0.688009000
C	2.904355000	3.560834000	0.794469000
C	0.869165000	3.117209000	-0.651640000

H	1.069572000	4.708028000	0.757535000
C	3.585145000	4.267776000	-0.388710000
H	3.213446000	2.503398000	0.813414000
H	3.233821000	3.994144000	1.745169000
C	1.564132000	3.776843000	-1.843843000
H	-0.215096000	3.214675000	-0.737460000
C	3.098121000	3.695936000	-1.729603000
H	4.673888000	4.177407000	-0.309333000
H	3.347035000	5.339368000	-0.350182000
H	1.205679000	3.323530000	-2.775972000
H	1.261456000	4.831624000	-1.856010000
H	3.434867000	2.648550000	-1.827312000
H	3.553215000	4.232198000	-2.568636000

1P+POH;
S=-3429.962038, **G** = -3429.364276

Fe	-0.325986000	-0.484582000	0.000094000
N	-0.155715000	-2.487261000	0.000046000
N	-1.685710000	-0.913353000	-1.418216000
N	1.214649000	-0.577731000	-1.444547000
N	1.214559000	-0.577768000	1.444924000
N	-1.685795000	-0.913323000	1.418266000
C	1.614068000	-1.848030000	-1.572286000
C	-2.200776000	-2.151147000	-1.230327000
C	-2.934256000	-0.741234000	-3.453988000

H	-3.184915000	-0.158066000	-4.333600000
C	1.571708000	1.738697000	-2.086117000
H	0.521100000	1.940785000	-1.930610000
C	-3.111587000	-2.727320000	-2.104546000
H	-3.494605000	-3.725560000	-1.917828000
C	-2.022960000	-0.237285000	-2.525814000
H	-1.540791000	0.720620000	-2.660216000
C	2.885828000	-2.226566000	2.042596000
H	3.143784000	-3.278690000	2.102652000
C	0.590323000	-2.901253000	-1.219027000
H	1.055525000	-3.883025000	-1.077887000
H	-0.112466000	-2.987645000	-2.052851000
C	1.614208000	-1.848040000	1.572181000
C	2.042013000	0.409887000	-1.932863000
C	0.590411000	-2.901263000	1.219060000
H	1.055570000	-3.883052000	1.077903000
H	-0.112315000	-2.987591000	2.052943000
C	3.377821000	0.109436000	-2.363519000
C	3.785647000	-1.243069000	2.389604000
H	4.792463000	-1.492869000	2.713092000
C	3.378018000	0.109510000	2.363074000
C	-1.627986000	-2.827617000	0.000076000
H	-1.817452000	-3.906717000	0.000057000

C	2.041919000	0.409850000	1.933227000
C	1.571374000	1.738487000	2.087344000
H	0.520582000	1.940426000	1.932763000
C	2.885417000	-2.226629000	-2.043383000
H	3.143185000	-3.278779000	-2.103797000
C	-2.200762000	-2.151171000	1.230496000
C	2.414474000	2.731723000	2.544878000
H	2.030482000	3.738125000	2.685329000
C	-3.499157000	-1.997694000	-3.234159000
H	-4.210073000	-2.416123000	-3.939906000
C	3.785209000	-1.243200000	-2.390639000
H	4.791813000	-1.493086000	-2.714722000
C	2.414743000	2.731933000	-2.543750000
H	2.030912000	3.738494000	-2.683500000
C	4.229857000	1.160199000	-2.797640000
H	5.243922000	0.914888000	-3.100684000
C	-3.111478000	-2.727345000	2.104812000
H	-3.494427000	-3.725633000	1.918212000
C	-2.934294000	-0.741088000	3.454040000
H	-3.185004000	-0.157849000	4.333592000
C	4.230082000	1.160290000	2.797086000
H	5.244361000	0.915083000	3.099502000
C	3.765189000	2.453835000	2.868871000

H	4.413845000	3.252551000	3.213889000
C	-2.023086000	-0.237142000	2.525777000
H	-1.541037000	0.720846000	2.660010000
C	3.765193000	2.453865000	-2.868697000
H	4.413815000	3.252576000	-3.213793000
C	-3.499056000	-1.997639000	3.234372000
H	-4.209889000	-2.416074000	3.940200000
C	-1.518172000	2.759986000	0.000168000
C	-2.373281000	2.778824000	-1.260148000
C	-2.374180000	2.778942000	1.259883000
H	-0.870938000	3.646284000	0.000365000
C	-3.292638000	4.015283000	-1.263272000
H	-2.985300000	1.868203000	-1.282920000
H	-1.728093000	2.781744000	-2.148469000
C	-3.293586000	4.015366000	1.262207000
H	-2.986134000	1.868267000	1.282378000
H	-1.729612000	2.782045000	2.148649000
C	-4.165336000	4.054103000	-0.000861000
H	-3.913145000	4.005375000	-2.165934000
H	-2.675559000	4.923620000	-1.308309000
H	-3.914775000	4.005507000	2.164400000
H	-2.676559000	4.923718000	1.307647000
H	-4.789139000	4.954339000	-0.001117000

H	-4.844891000	3.189485000	-0.001091000
O	-0.594432000	1.602932000	0.000595000
H	0.307472000	1.956624000	0.000839000

^{5}P+P_{Cl};
S=-3045.549509, **G** = -3044.95921

Fe	-0.029574000	-0.244401000	-0.007032000
N	-0.367874000	-2.442158000	0.132191000
N	1.431800000	-0.883514000	1.537878000
N	-1.607714000	-0.321809000	1.483771000
N	-1.686590000	-0.476260000	-1.433635000
N	1.438442000	-1.101496000	-1.409199000
C	-2.032752000	-1.553397000	1.763813000
C	1.712181000	-2.197456000	1.398606000
C	2.776162000	-0.825537000	3.522383000
H	3.168228000	-0.250449000	4.354516000
C	-1.886402000	2.068147000	1.631338000
H	-0.938001000	2.205028000	1.123421000
C	2.533407000	-2.880613000	2.288606000
H	2.732287000	-3.938585000	2.148083000
C	1.944663000	-0.216850000	2.580861000
H	1.679252000	0.832734000	2.652454000
C	-3.247982000	-2.139039000	-2.216536000
H	-3.491873000	-3.193124000	-2.302126000
C	-1.146023000	-2.717446000	1.361602000

H	-1.750882000	-3.625131000	1.241996000
H	-0.451363000	-2.908963000	2.186664000
C	-2.050557000	-1.751961000	-1.579414000
C	-2.346755000	0.758991000	1.899908000
C	-1.102685000	-2.836600000	-1.091651000
H	-1.658805000	-3.768482000	-0.927421000
H	-0.379914000	-3.035979000	-1.889106000
C	-3.578852000	0.582453000	2.607763000
C	-4.088617000	-1.168147000	-2.716093000
H	-5.020089000	-1.436933000	-3.207122000
C	-3.740584000	0.195133000	-2.583648000
C	1.061495000	-2.871166000	0.190778000
H	1.170033000	-3.960484000	0.270265000
C	-2.506988000	0.511163000	-1.925145000
C	-2.135978000	1.868205000	-1.784680000
H	-1.195414000	2.110796000	-1.306850000
C	-3.230590000	-1.804648000	2.464045000
H	-3.530676000	-2.828768000	2.661334000
C	1.753405000	-2.369998000	-1.070177000
C	-2.953975000	2.867224000	-2.269123000
H	-2.655182000	3.905598000	-2.160744000
C	3.079492000	-2.178611000	3.369099000
H	3.720320000	-2.686234000	4.083728000

C	-4.001853000	-0.739806000	2.878072000
H	-4.935297000	-0.903093000	3.410044000
C	-2.628102000	3.158839000	2.035526000
H	-2.265465000	4.161603000	1.829995000
C	-4.321587000	1.724612000	3.006750000
H	-5.255906000	1.580421000	3.541799000
C	2.635776000	-3.140452000	-1.817329000
H	2.862050000	-4.158986000	-1.517854000
C	2.867202000	-1.272817000	-3.323216000
H	3.277825000	-0.807530000	-4.212948000
C	-4.563321000	1.245396000	-3.069207000
H	-5.495500000	0.991857000	-3.566029000
C	-4.178321000	2.558245000	-2.913735000
H	-4.805953000	3.360567000	-3.288432000
C	1.975296000	-0.566644000	-2.514869000
H	1.680990000	0.452117000	-2.742979000
C	-3.856477000	2.989736000	2.722923000
H	-4.423448000	3.862339000	3.031282000
C	3.207135000	-2.577496000	-2.964452000
H	3.896145000	-3.156080000	-3.572353000
Cl	1.222481000	2.182352000	-0.421839000
C	3.099375000	2.690172000	-0.303643000
C	3.657296000	2.296561000	1.047492000

C	3.854622000	2.085920000	-1.469405000
H	2.988336000	3.771464000	-0.403255000
C	5.125745000	2.781517000	1.118942000
H	3.630822000	1.204668000	1.142415000
H	3.064371000	2.735248000	1.857178000
C	5.323348000	2.569236000	-1.391776000
H	3.827424000	0.992304000	-1.390007000
H	3.400587000	2.380292000	-2.421394000
C	5.953424000	2.207246000	-0.039432000
H	5.545633000	2.486314000	2.086988000
H	5.146534000	3.878781000	1.080702000
H	5.883764000	2.121441000	-2.219871000
H	5.353884000	3.657640000	-1.534307000
H	6.980282000	2.585077000	0.009610000
H	6.005540000	1.112966000	0.057499000

^{3}P+P$_{Cl}$;
S=-3045.610063**,G** = -3045.015885

Fe	0.243095000	-0.260602000	-0.264634000
N	0.527623000	-1.337750000	-2.173489000
N	-1.322352000	0.488886000	-1.293413000
N	1.470349000	1.088879000	-1.142734000
N	1.891247000	-1.302783000	0.274514000
N	-0.910749000	-1.886045000	0.099036000
C	1.835585000	0.776286000	-2.388497000

C	-1.702914000	-0.356431000	-2.279537000
C	-2.965231000	2.066560000	-2.018999000
H	-3.435353000	3.035300000	-1.888519000
C	1.582680000	2.569383000	0.759409000
H	0.781896000	2.013275000	1.233179000
C	-2.729399000	-0.043384000	-3.161288000
H	-3.008583000	-0.742711000	-3.942989000
C	-1.926037000	1.680981000	-1.172827000
H	-1.571156000	2.316571000	-0.369410000
C	3.583561000	-2.803812000	-0.544769000
H	3.911647000	-3.462272000	-1.342729000
C	1.092124000	-0.344699000	-3.104569000
H	1.759627000	-0.825917000	-3.830327000
H	0.279023000	0.109215000	-3.682763000
C	2.345992000	-2.138536000	-0.662717000
C	2.031007000	2.181473000	-0.523490000
C	1.455449000	-2.440245000	-1.861569000
H	2.077168000	-2.684691000	-2.731867000
H	0.876734000	-3.341286000	-1.629029000
C	3.050437000	2.949650000	-1.171730000
C	4.353378000	-2.603968000	0.580311000
H	5.315564000	-3.096593000	0.690719000
C	3.884309000	-1.755928000	1.610153000

C	-0.922353000	-1.668039000	-2.305011000
H	-1.163320000	-2.239358000	-3.210615000
C	2.617303000	-1.114547000	1.427277000
C	2.102106000	-0.295956000	2.457680000
H	1.126657000	0.160472000	2.335491000
C	2.830268000	1.492718000	-3.085368000
H	3.099098000	1.187837000	-4.091681000
C	-1.330673000	-2.447774000	-1.058555000
C	2.824818000	-0.104148000	3.616859000
H	2.416760000	0.517687000	4.407956000
C	-3.377309000	1.189521000	-3.023401000
H	-4.181453000	1.463123000	-3.699618000
C	3.443372000	2.564923000	-2.474633000
H	4.220822000	3.126264000	-2.985660000
C	2.140455000	3.665122000	1.385121000
H	1.783222000	3.962926000	2.366360000
C	3.614779000	4.062963000	-0.495256000
H	4.393118000	4.635770000	-0.991227000
C	-2.068579000	-3.623868000	-1.083131000
H	-2.384835000	-4.049579000	-2.030140000
C	-1.925071000	-3.672808000	1.322348000
H	-2.134300000	-4.130795000	2.283141000
C	4.610366000	-1.527602000	2.808545000

H	5.573741000	-2.013009000	2.935635000
C	4.092197000	-0.714816000	3.792511000
H	4.646433000	-0.546722000	4.710366000
C	-1.190027000	-2.488638000	1.265059000
H	-0.823963000	-1.995344000	2.158539000
C	3.170588000	4.412769000	0.760840000
H	3.599167000	5.268071000	1.273370000
C	-2.375735000	-4.245790000	0.132530000
H	-2.947210000	-5.168850000	0.145798000
Cl	-1.485556000	0.867508000	2.228208000
C	-3.385676000	0.839940000	2.218573000
C	-3.896273000	2.241437000	1.920183000
C	-3.884946000	-0.206607000	1.232150000
H	-3.609696000	0.550873000	3.247651000
C	-5.440103000	2.224994000	1.925319000
H	-3.541255000	2.548198000	0.927874000
H	-3.508986000	2.953599000	2.655510000
C	-5.429554000	-0.203912000	1.235508000
H	-3.520151000	0.039381000	0.227844000
H	-3.501300000	-1.196355000	1.498557000
C	-5.983871000	1.193910000	0.926239000
H	-5.806992000	3.230433000	1.691348000
H	-5.797162000	1.980772000	2.934960000

H	-5.788633000	-0.939375000	0.505984000
H	-5.789243000	-0.528178000	2.221458000
H	-7.078789000	1.179746000	0.954484000
H	-5.689273000	1.484524000	-0.093679000

$^1P+P_{Cl}$;
S=-3045.541394**,G** = -3044.943632

Fe	-0.211369000	-0.283587000	-0.342618000
N	-0.394081000	-1.172425000	-2.100106000
N	0.945418000	-1.870276000	0.053234000
N	-1.839623000	-1.340121000	0.189195000
N	-1.441472000	1.118735000	-1.100221000
N	1.345733000	0.595820000	-1.237229000
C	-2.260755000	-2.138257000	-0.793790000
C	1.465054000	-2.357335000	-1.096692000
C	1.950709000	-3.680878000	1.247240000
H	2.112242000	-4.184503000	2.194322000
C	-2.138074000	-0.436731000	2.405400000
H	-1.157003000	0.016749000	2.346071000
C	2.256197000	-3.496824000	-1.137419000
H	2.651430000	-3.859375000	-2.081085000
C	1.168619000	-2.526108000	1.201762000
H	0.715471000	-2.101018000	2.090001000
C	-2.770087000	1.572840000	-3.062300000

H	-2.996674000	1.313714000	-4.091464000
C	-1.301928000	-2.351042000	-1.944138000
H	-1.837900000	-2.551063000	-2.877721000
H	-0.693429000	-3.234963000	-1.726836000
C	-1.766702000	0.867440000	-2.369709000
C	-2.610330000	-1.206443000	1.318727000
C	-0.942453000	-0.183434000	-3.078898000
H	-1.526279000	-0.691031000	-3.853737000
H	-0.106271000	0.313944000	-3.581282000
C	-3.882556000	-1.857477000	1.422651000
C	-3.447647000	2.579887000	-2.409089000
H	-4.236167000	3.135439000	-2.909224000
C	-3.108177000	2.902992000	-1.074927000
C	1.068243000	-1.519785000	-2.301131000
H	1.252201000	-2.042290000	-3.246175000
C	-2.071202000	2.145830000	-0.439365000
C	-1.679281000	2.478506000	0.876591000
H	-0.865871000	1.934208000	1.338704000
C	-3.494400000	-2.816804000	-0.759835000
H	-3.786327000	-3.443544000	-1.596302000
C	1.824874000	-0.204532000	-2.216930000
C	-2.307436000	3.507561000	1.546699000
H	-1.993428000	3.763716000	2.554146000

C	2.510353000	-4.167577000	0.064855000
H	3.122134000	-5.064434000	0.071942000
C	-4.308820000	-2.663682000	0.341801000
H	-5.272990000	-3.161835000	0.394673000
C	-2.907548000	-0.295935000	3.541259000
H	-2.531840000	0.288193000	4.375970000
C	-4.656941000	-1.681770000	2.599747000
H	-5.623004000	-2.173780000	2.667083000
C	2.888898000	0.163773000	-3.028556000
H	3.245517000	-0.504153000	-3.806229000
C	2.955814000	2.257672000	-1.834373000
H	3.371076000	3.244565000	-1.660618000
C	-3.744043000	3.947617000	-0.353523000
H	-4.533744000	4.512945000	-0.840077000
C	-3.353963000	4.242276000	0.934131000
H	-3.837593000	5.045368000	1.481060000
C	1.884305000	1.810906000	-1.060600000
H	1.447741000	2.414674000	-0.273592000
C	-4.180890000	-0.912102000	3.637988000
H	-4.771947000	-0.784456000	4.539265000
C	3.472275000	1.419858000	-2.824059000
H	4.305263000	1.742577000	-3.441006000
Cl	1.348234000	0.763820000	2.175133000

C	3.258794000	0.761429000	2.226414000
C	3.813488000	-0.223712000	1.208861000
C	3.754135000	2.185305000	2.026033000
H	3.441502000	0.420579000	3.247635000
C	5.356731000	-0.197251000	1.280968000
H	3.491198000	0.070324000	0.204214000
H	3.438336000	-1.231820000	1.406414000
C	5.297190000	2.191231000	2.094468000
H	3.436062000	2.540770000	1.038352000
H	3.325507000	2.849292000	2.783124000
C	5.897764000	1.223089000	1.065505000
H	5.758242000	-0.889349000	0.531466000
H	5.679903000	-0.565698000	2.263983000
H	5.654478000	3.213482000	1.928451000
H	5.617987000	1.899616000	3.103578000
H	6.990849000	1.225386000	1.135641000
H	5.635857000	1.560754000	0.051343000

$ArCO_3^-$;
S=-495.6629823**,G** = -495.5913303

C	-2.075415000	-1.367394000	0.000030000
C	-0.693422000	-1.181698000	0.000213000
C	-0.141831000	0.113420000	0.000269000
C	-1.019494000	1.211264000	0.000113000
C	-2.401982000	1.025215000	-0.000074000

C	-2.940880000	-0.265537000	-0.000116000
H	-2.483009000	-2.377440000	0.000000000
H	-0.019009000	-2.031172000	0.000328000
H	-0.575938000	2.202374000	0.000159000
H	-3.064467000	1.890009000	-0.000184000
H	-4.019583000	-0.412821000	-0.000260000
C	1.338161000	0.393470000	0.000482000
O	1.777060000	1.544846000	-0.000077000
O	2.013575000	-0.742782000	0.000008000
O	3.430763000	-0.657488000	-0.000624000

$ArCO_3H$;
S=-496.1435714**,G** = -496.0594294

C	2.121687000	-1.373121000	-0.000015000
C	0.740261000	-1.184117000	-0.000026000
C	0.213498000	0.116776000	-0.000011000
C	1.079296000	1.220190000	0.000012000
C	2.458779000	1.025317000	0.000027000
C	2.981826000	-0.271210000	0.000013000
H	2.527190000	-2.381132000	-0.000029000
H	0.074216000	-2.040016000	-0.000048000
H	0.649870000	2.216730000	0.000020000
H	3.125831000	1.882923000	0.000047000
H	4.057983000	-0.423269000	0.000025000
C	-1.249948000	0.413503000	-0.000029000

O -1.747483000 1.511564000 -0.000036000

O -1.967141000 -0.756169000 0.000023000

O -3.385679000 -0.451289000 0.000026000

H -3.705061000 -1.372106000 0.000062000

Cl^-;
S=-460.402326**,G** = -460.417349

Cl 0.000000000 0.000000000 0.000000000

H_2O;
S=-76.4682999**,G** = -76.4648039

O 0.000000000 0.000000000 0.119677000

H 0.000000000 0.761819000 -0.478710000

H 0.000000000 -0.761819000 -0.478710000

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