

Supplementary Materials

Synthesis and Catalytic Application of Knölker-Type Iron Complexes with a Novel Asymmetric Cyclopentadienone Ligand Design

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1. NMR analysis

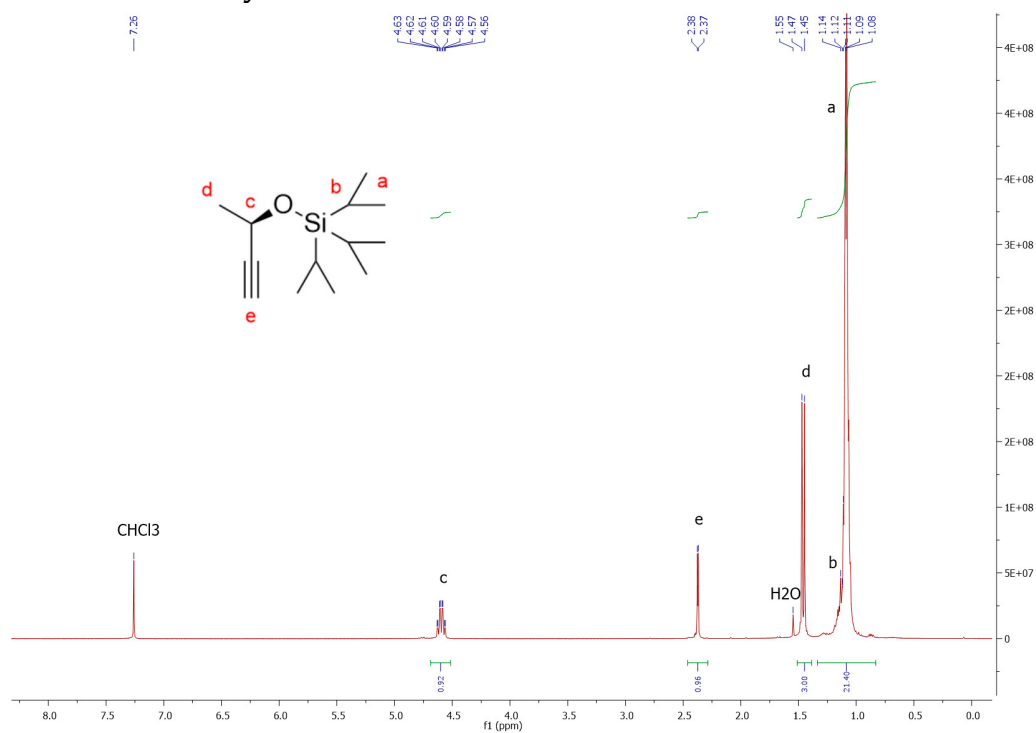


Figure S1.1: ¹H-NMR spectrum of compound **12a** in CDCl₃.

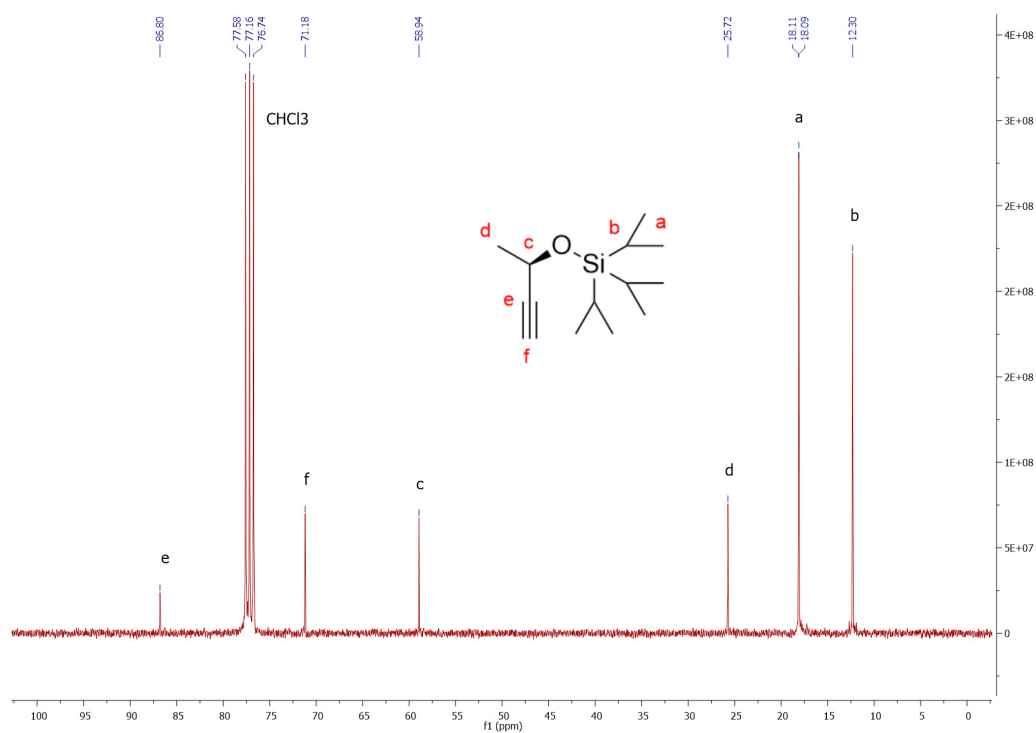


Figure S1.2: ¹³C-NMR spectrum of compound **12a** in CDCl₃.

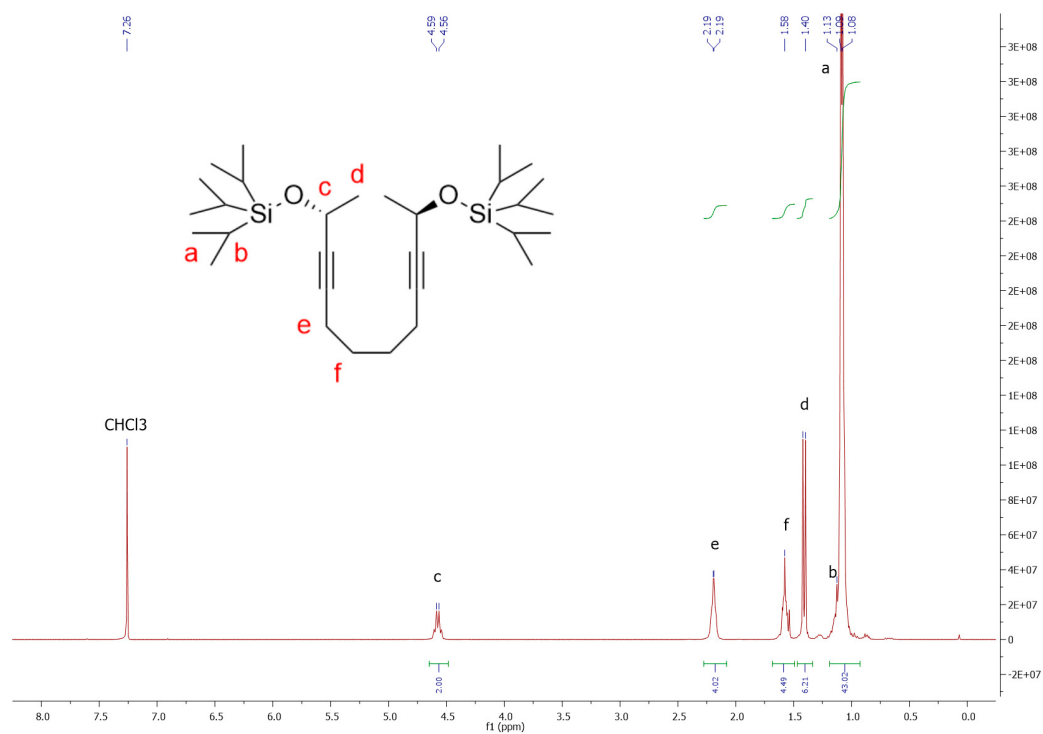


Figure S1.3: ¹H-NMR spectrum of compound **12a** in CDCl₃.

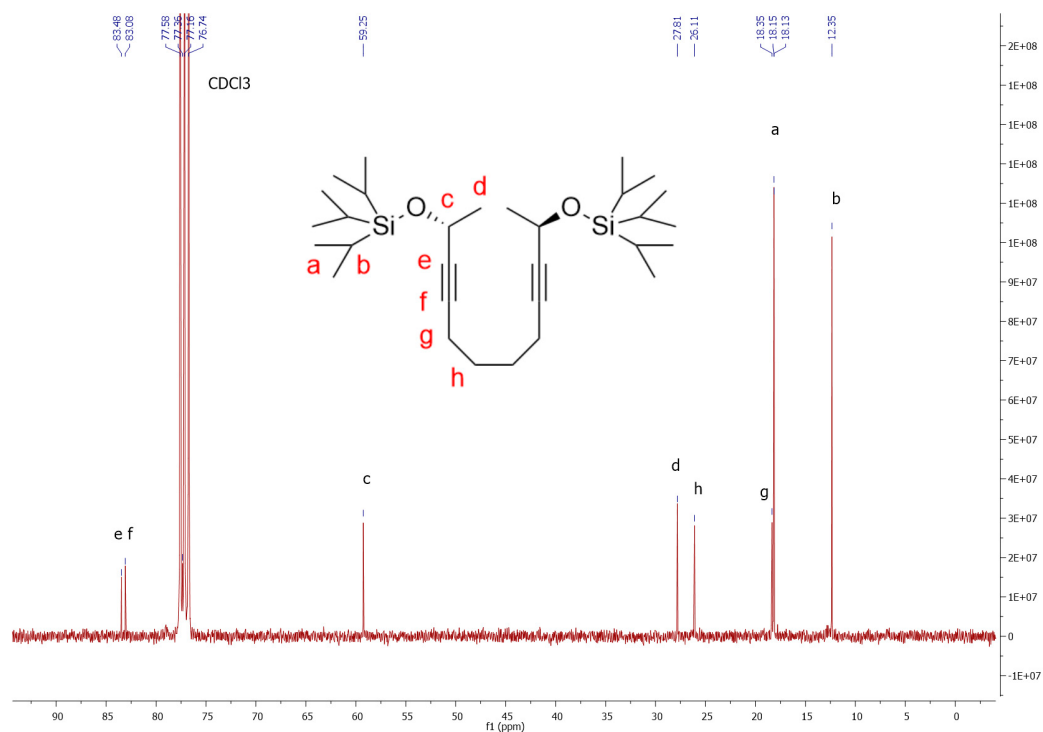


Figure S1.4: ¹³C-NMR spectrum of compound **13a** in CDCl₃.

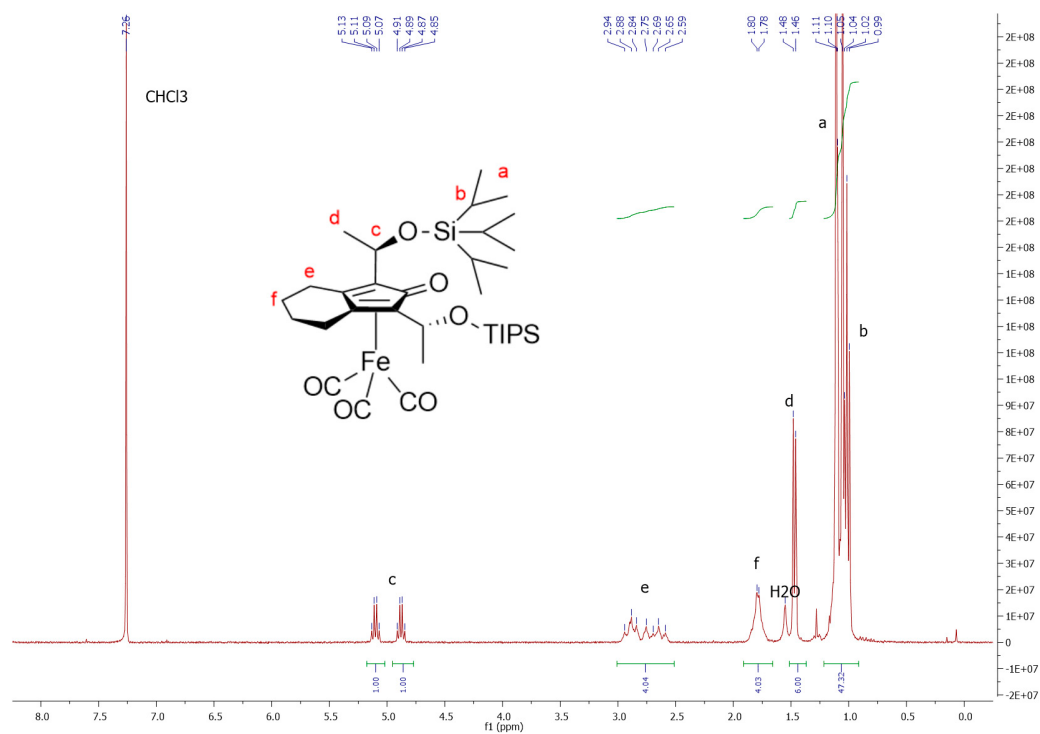


Figure S1.5: ¹H-NMR spectrum of compound **14a** in CDCl₃.

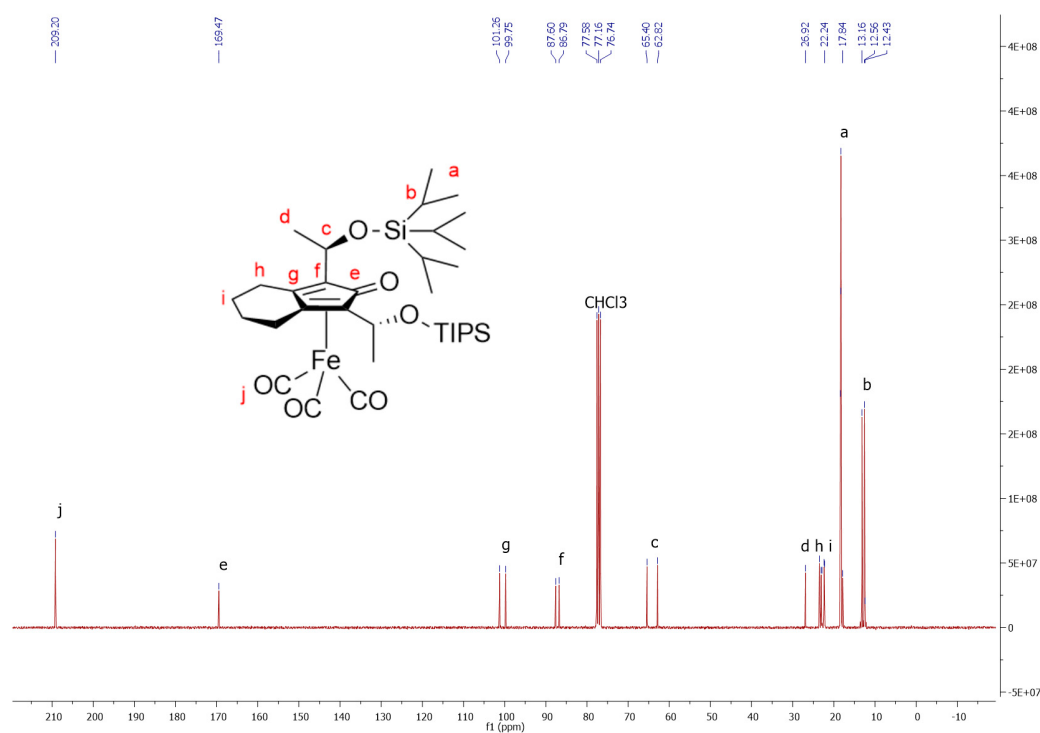
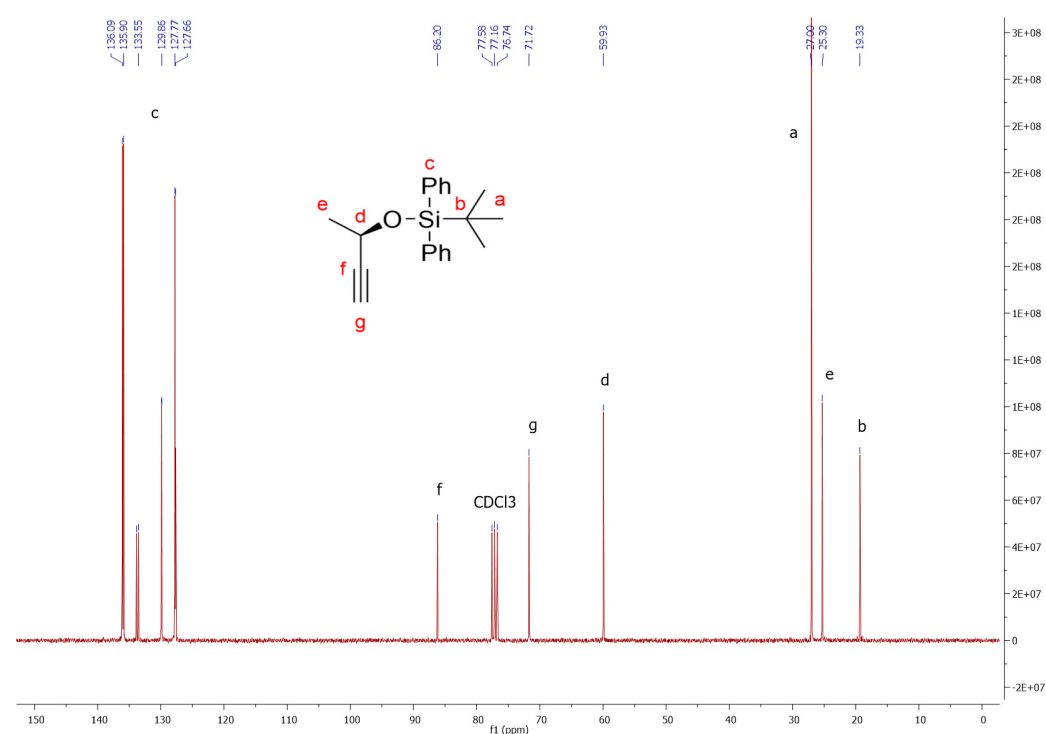
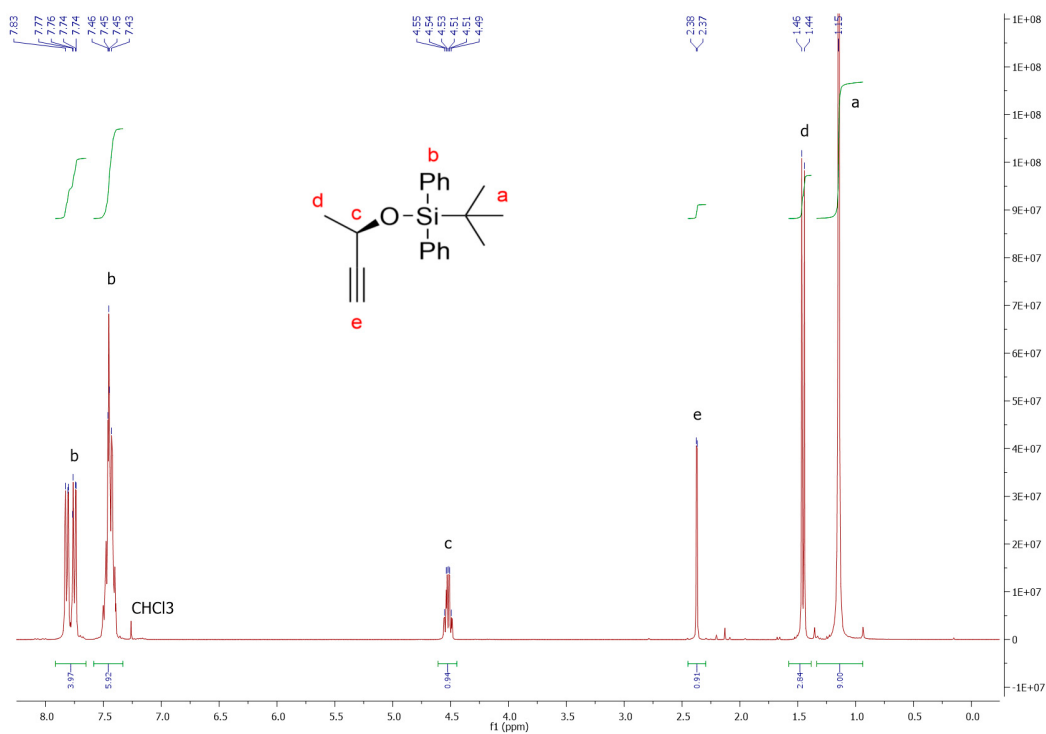


Figure S1.6: ¹³C-NMR spectrum of compound **14a** in CDCl₃.



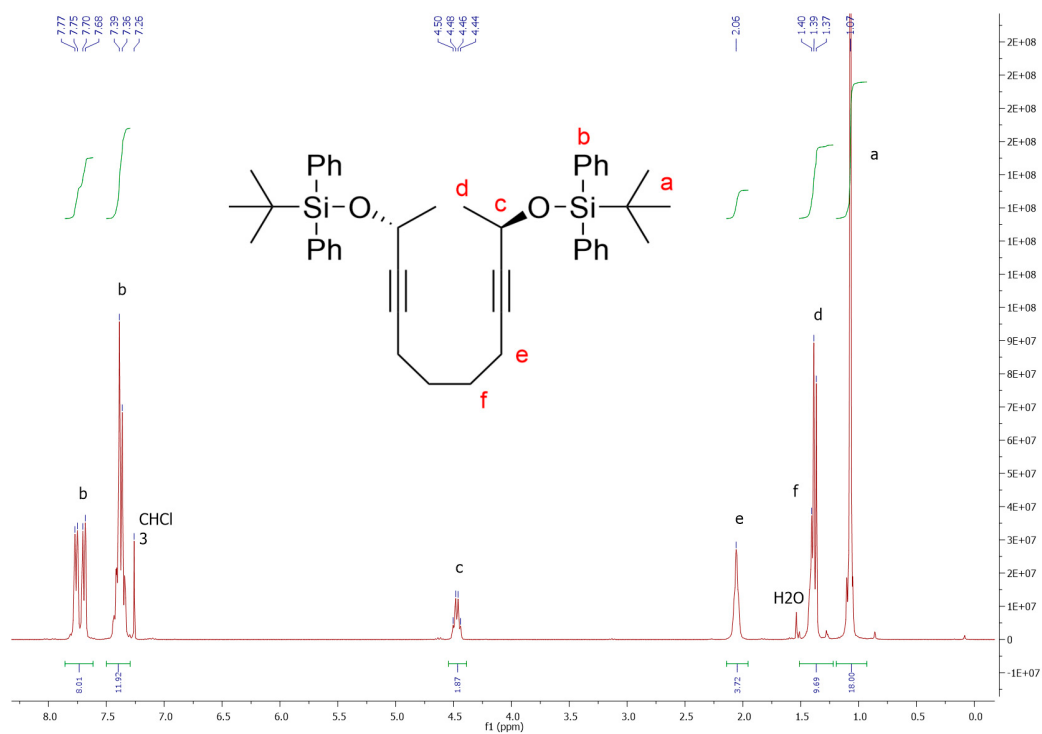


Figure S1.9: ¹H-NMR spectrum of compound **13b** in CDCl₃.

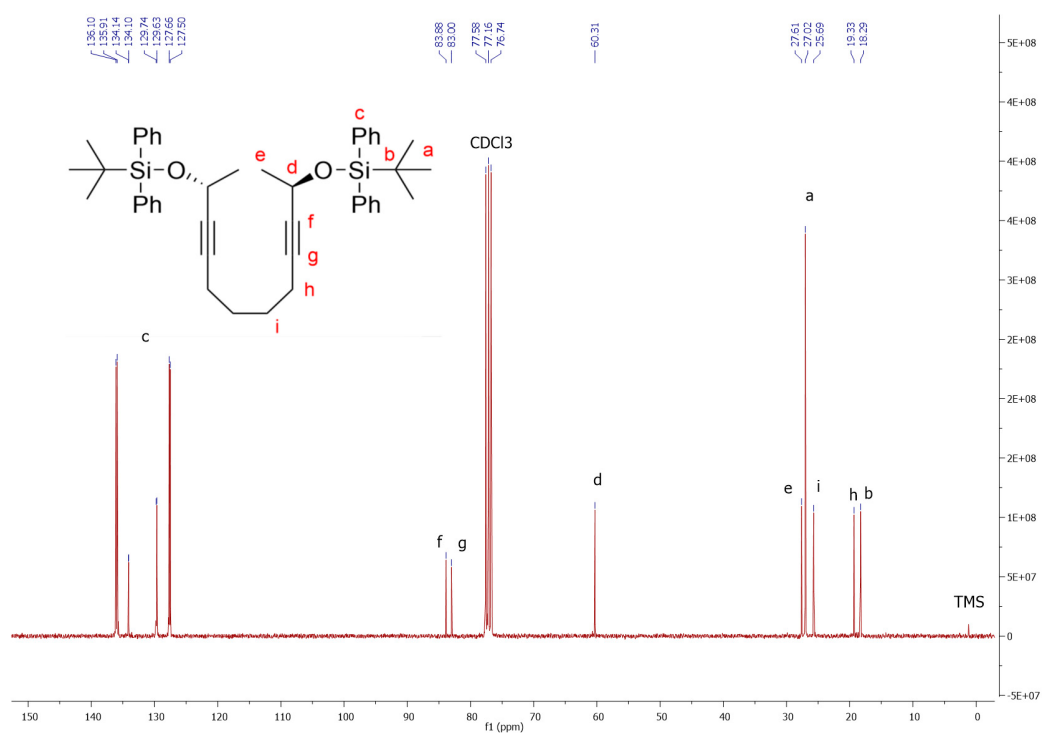


Figure S1.10: ¹³C-NMR spectrum of compound **13b** in CDCl₃.

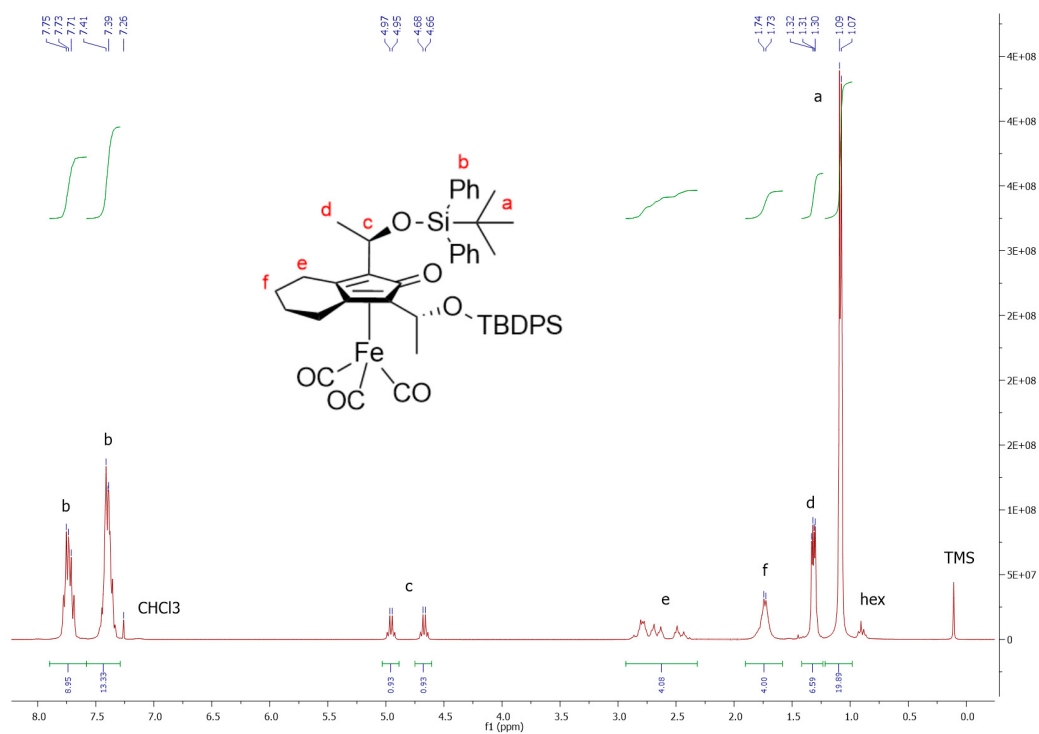


Figure S1.11: ¹H-NMR spectrum of compound **14b** in CDCl₃.

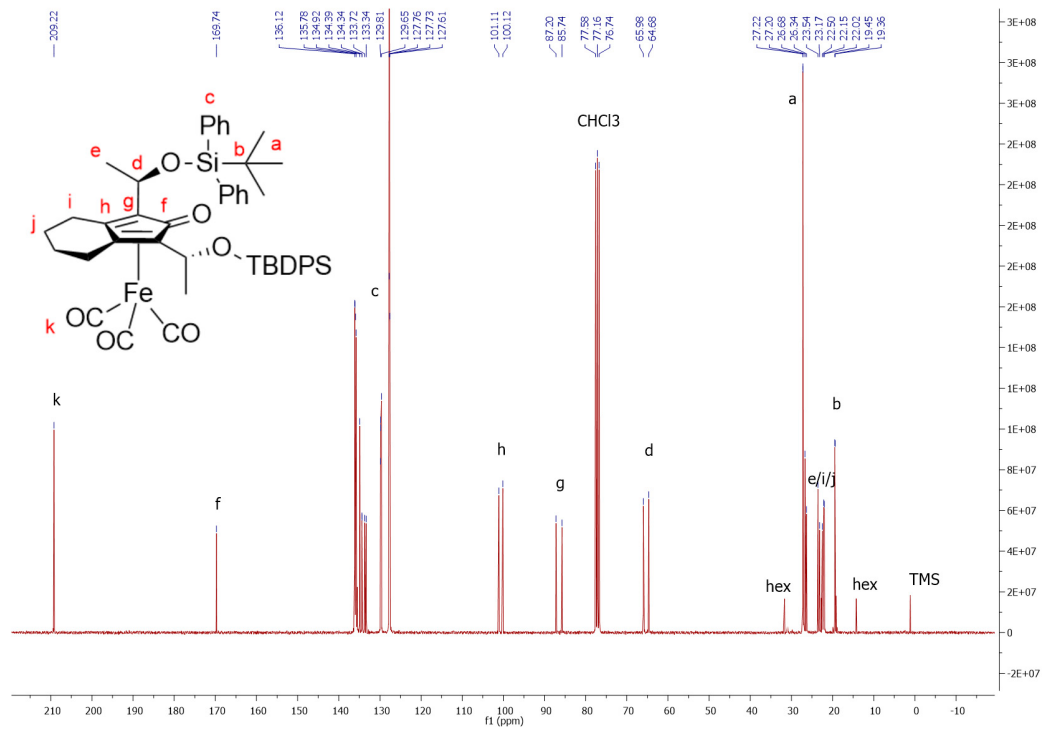
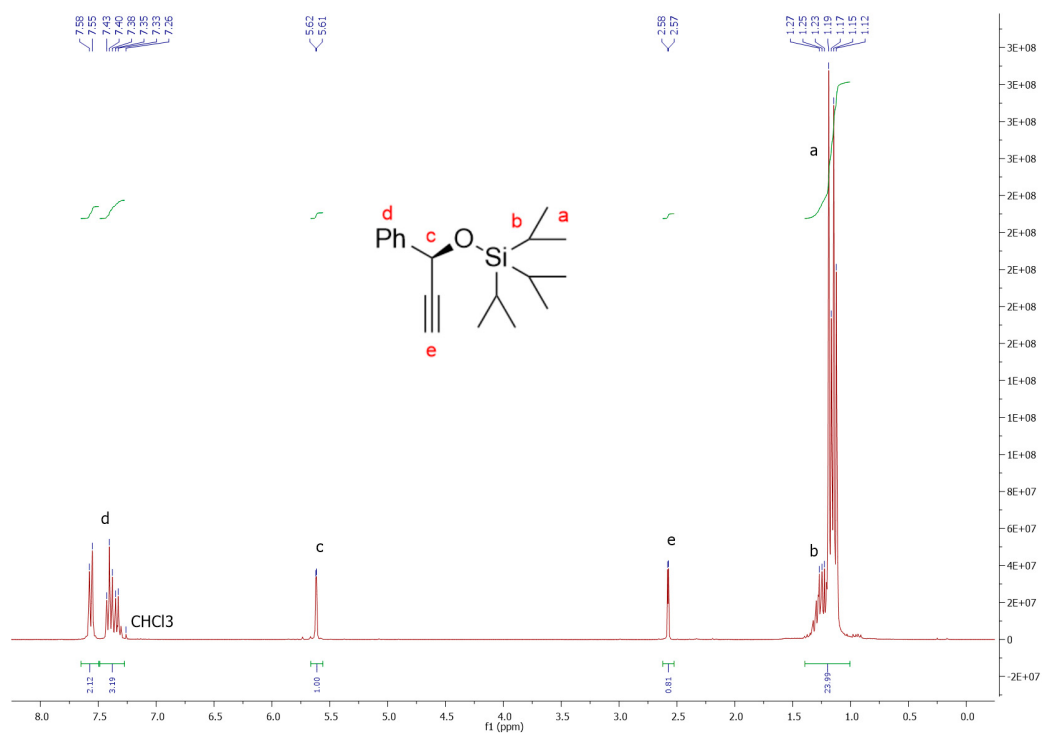


Figure S1.12: ¹³C-NMR spectrum of compound **14b** in CDCl₃.



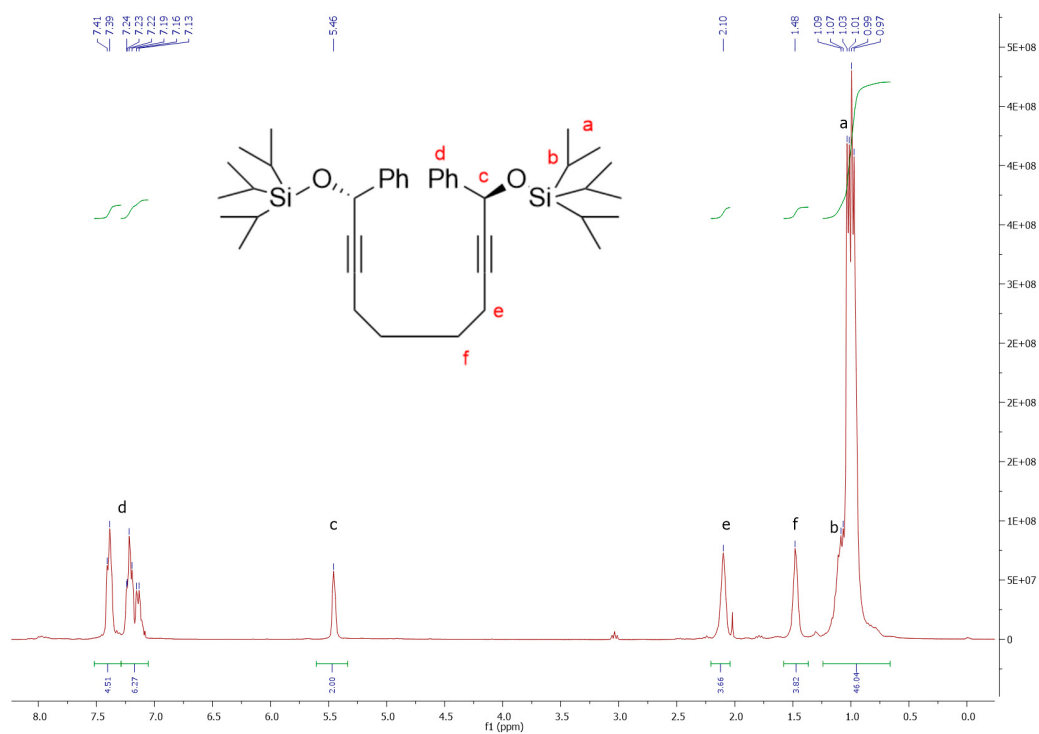


Figure S1.15: ^1H -NMR spectrum of compound **13c** in CDCl_3 .

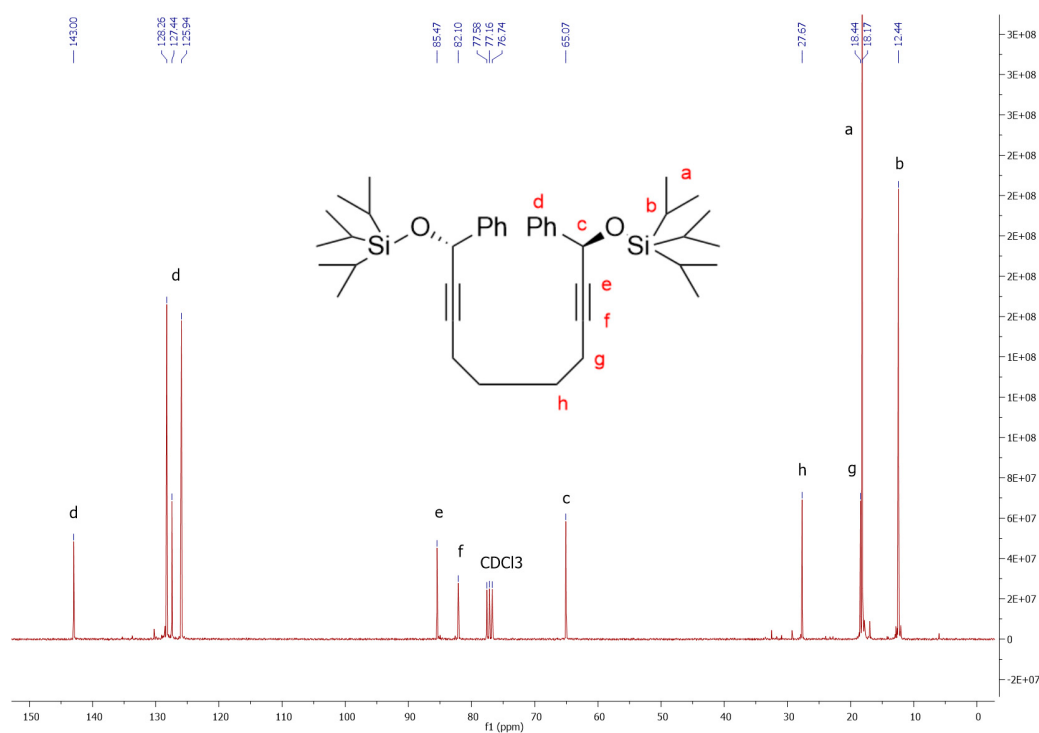


Figure S1.16: ^{13}C -NMR spectrum of compound **13c** in CDCl_3 .

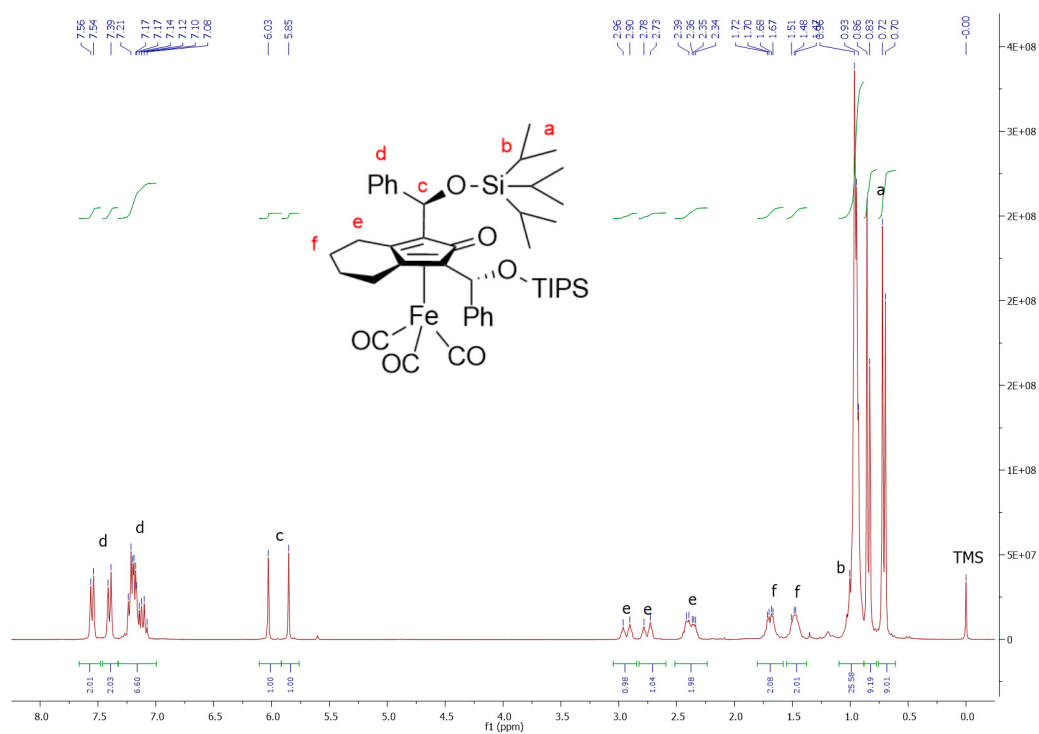


Figure S1.17: ¹H-NMR spectrum of compound **14c** in CDCl₃.

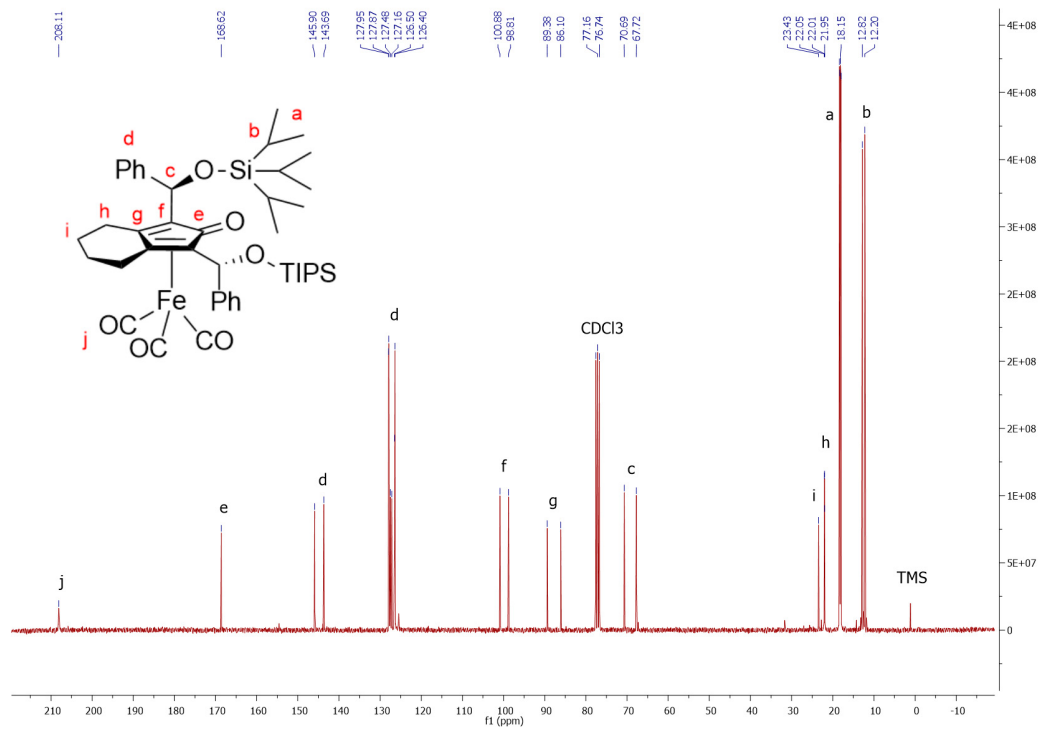


Figure S1.18: ¹³C-NMR spectrum of compound **14c** in CDCl₃.

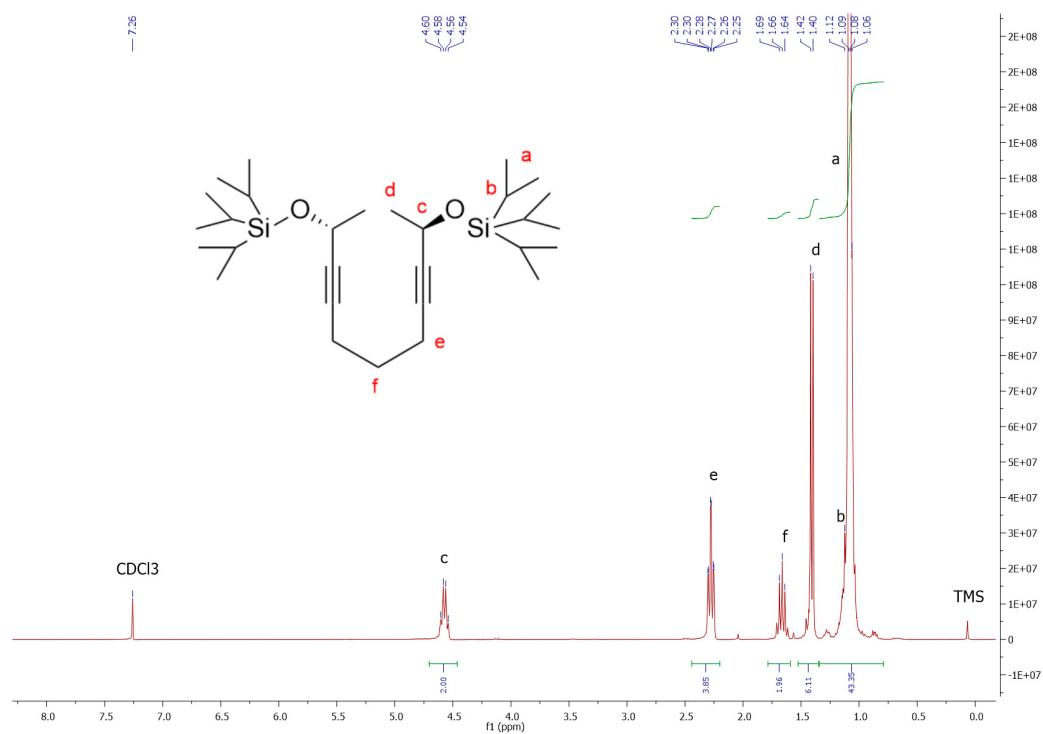


Figure S1.19: ¹H-NMR spectrum of compound **13d** in CDCl₃.

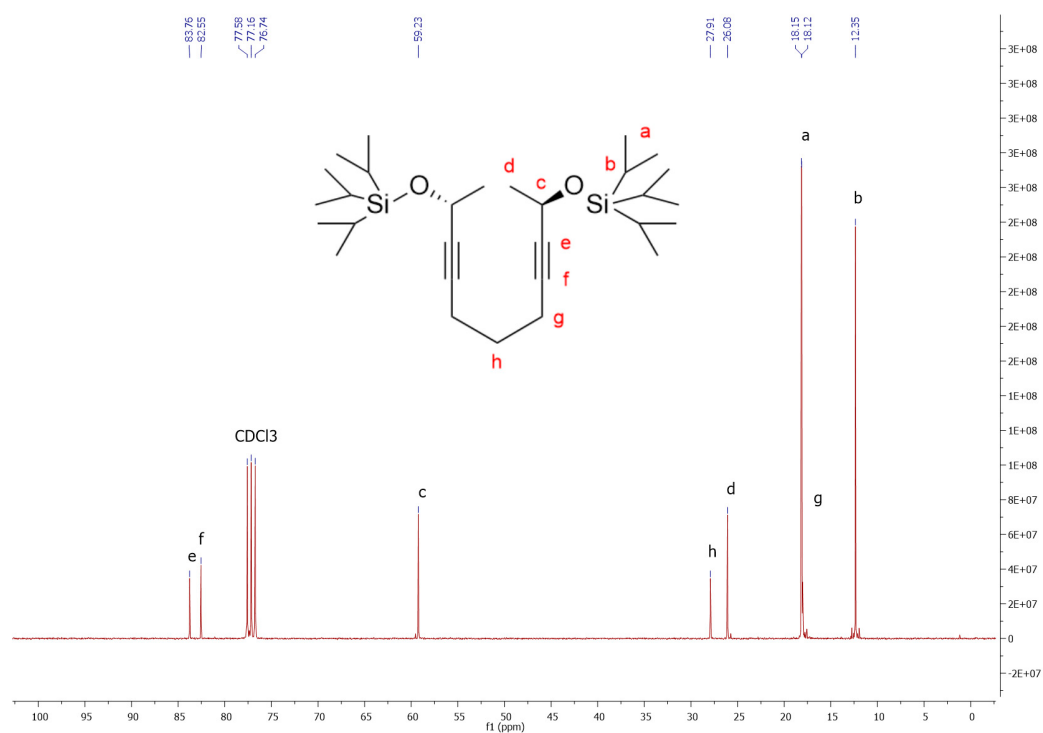


Figure S1.20: ¹³C-NMR spectrum of compound **13d** in CDCl₃.

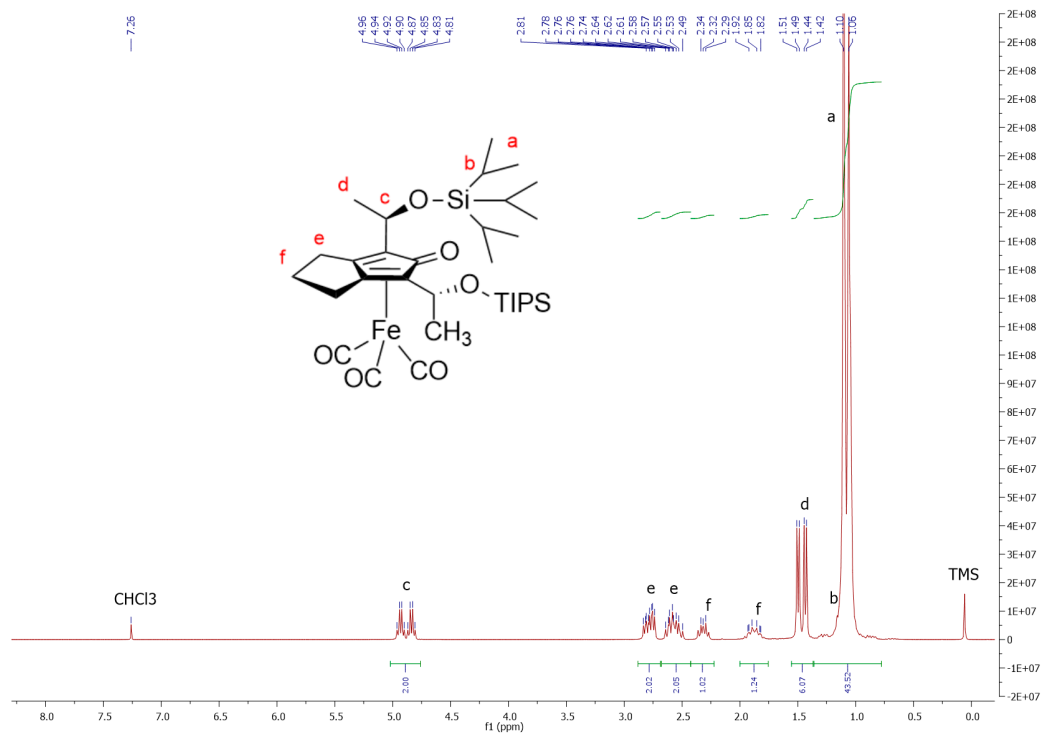


Figure S1.21: ^1H -NMR spectrum of compound **14d** in CDCl_3 .

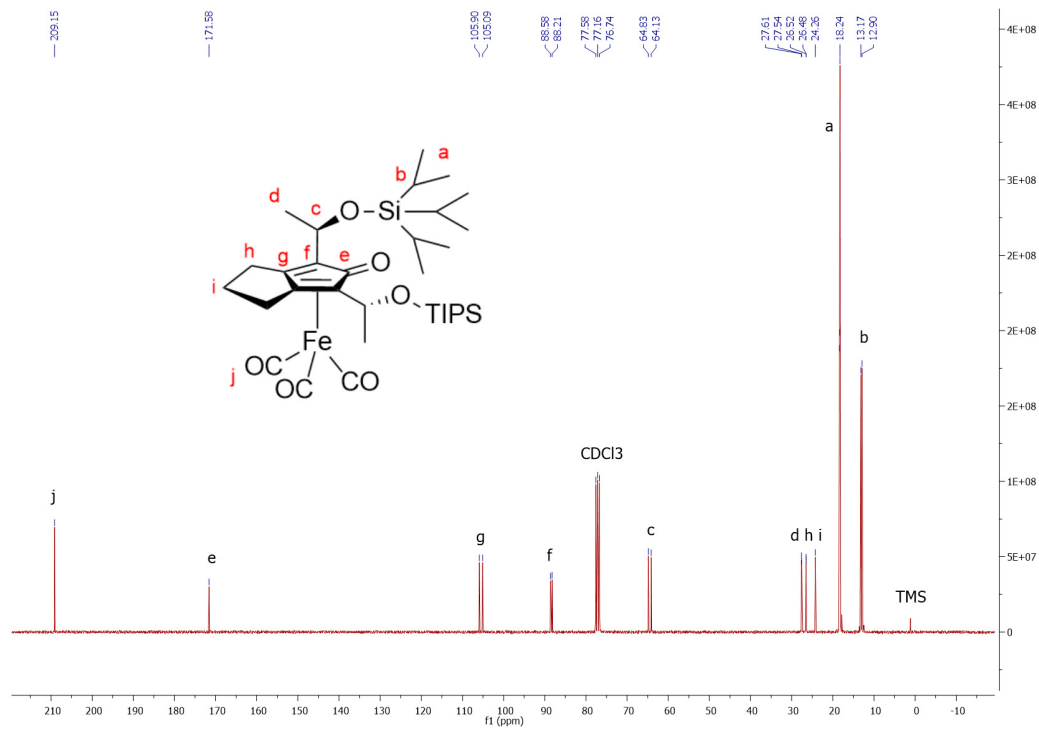


Figure S1.22: ^{13}C -NMR spectrum of compound **14d** in CDCl_3 .

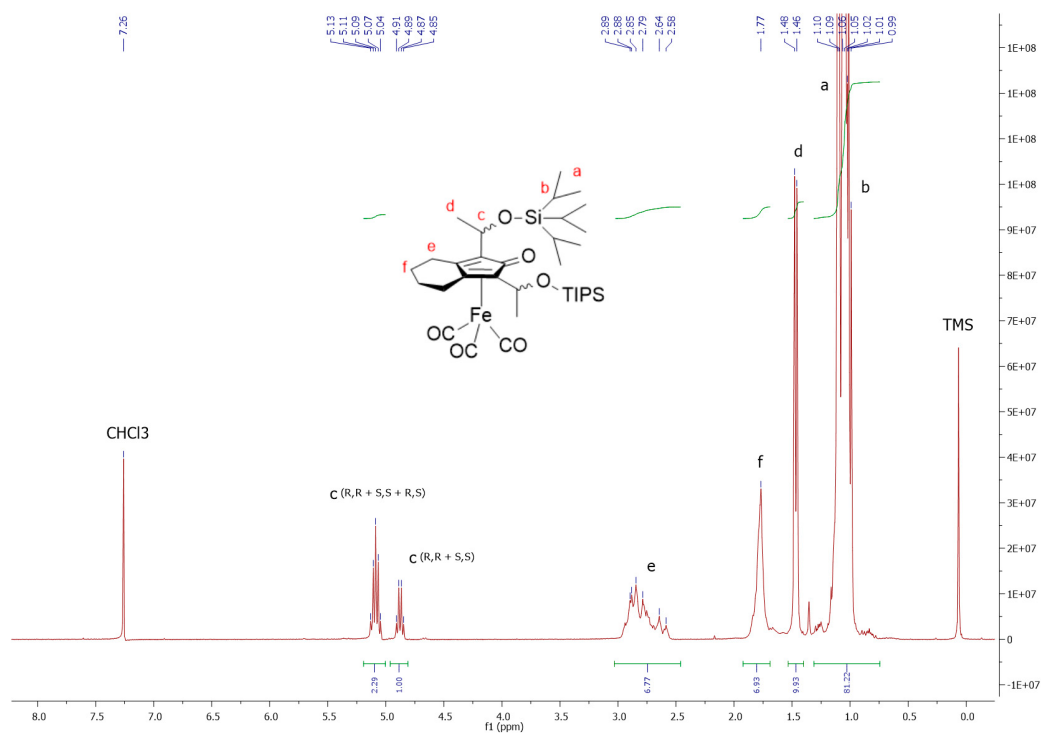


Figure S1.23: ¹H-NMR spectrum of compound **14e** in CDCl₃.

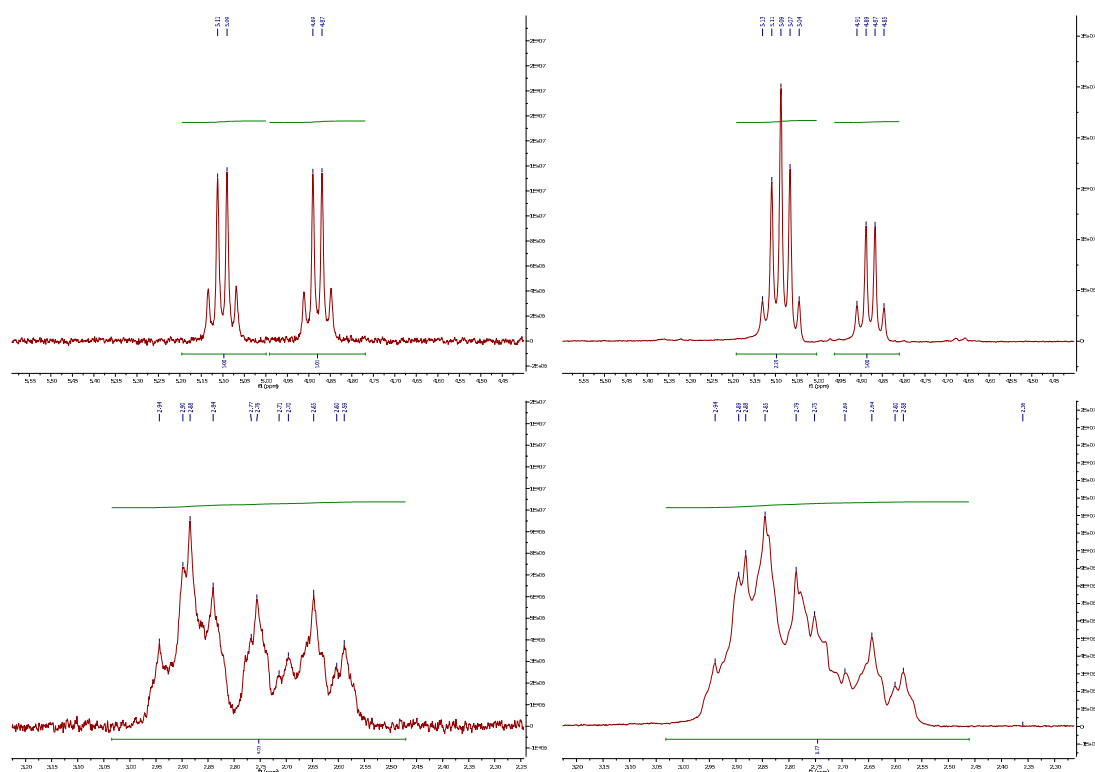


Figure S1.24: ¹H-NMR spectrum zooms of diastereo-pure compound **14a** (left), and corresponding racemic compound **14e** (right) in CDCl₃. The pentet signal in the top-right zoom is actually two overlapping quartets.

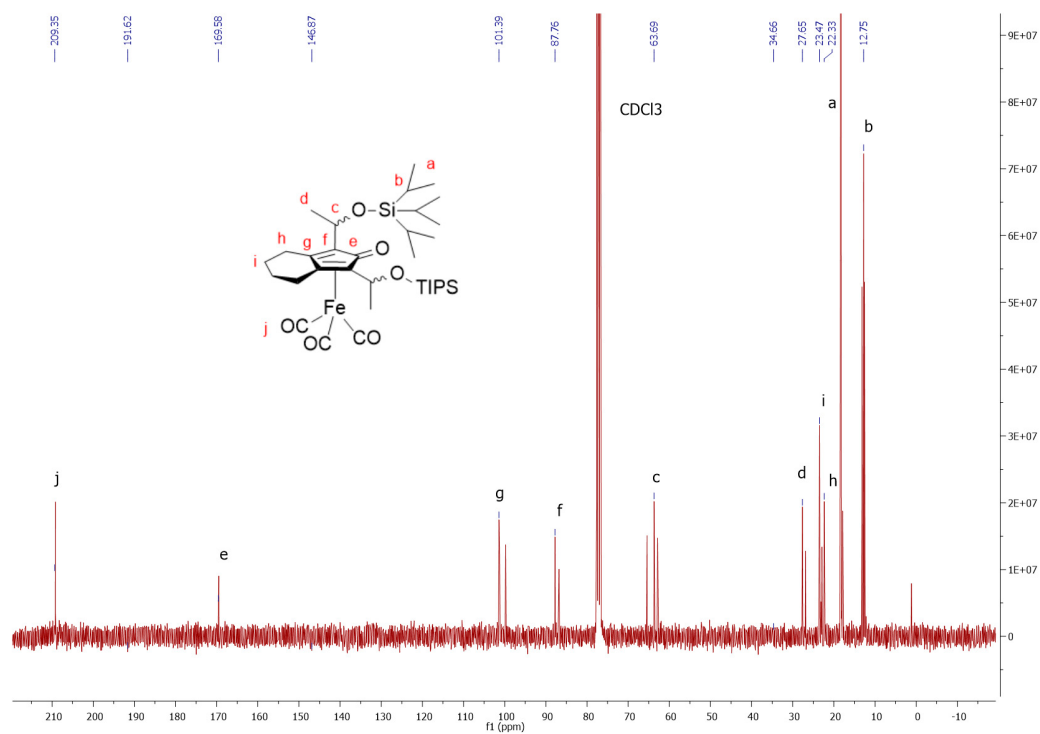
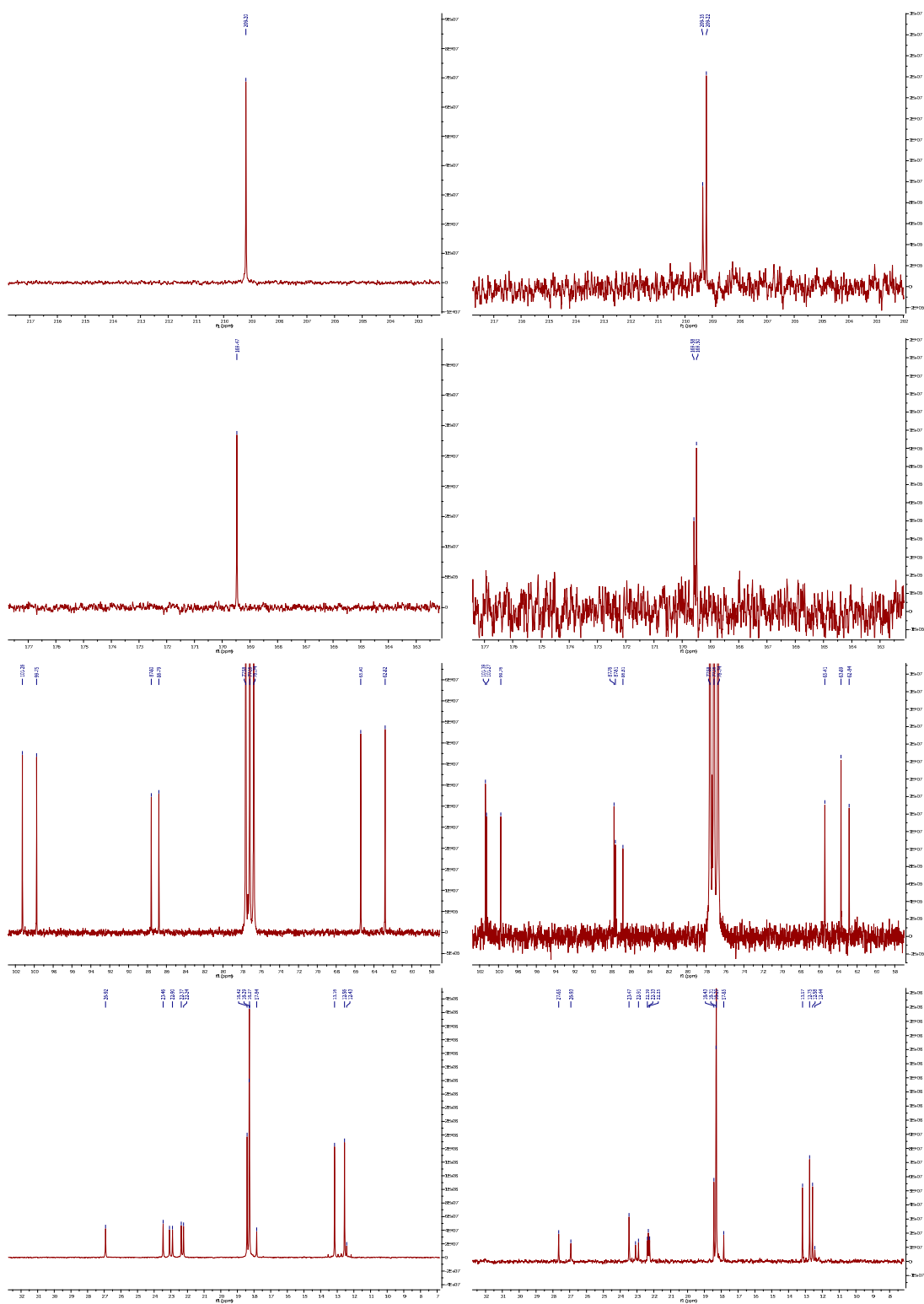


Figure S1.25: ^{13}C -NMR spectrum of compound **14e** in CDCl_3 .



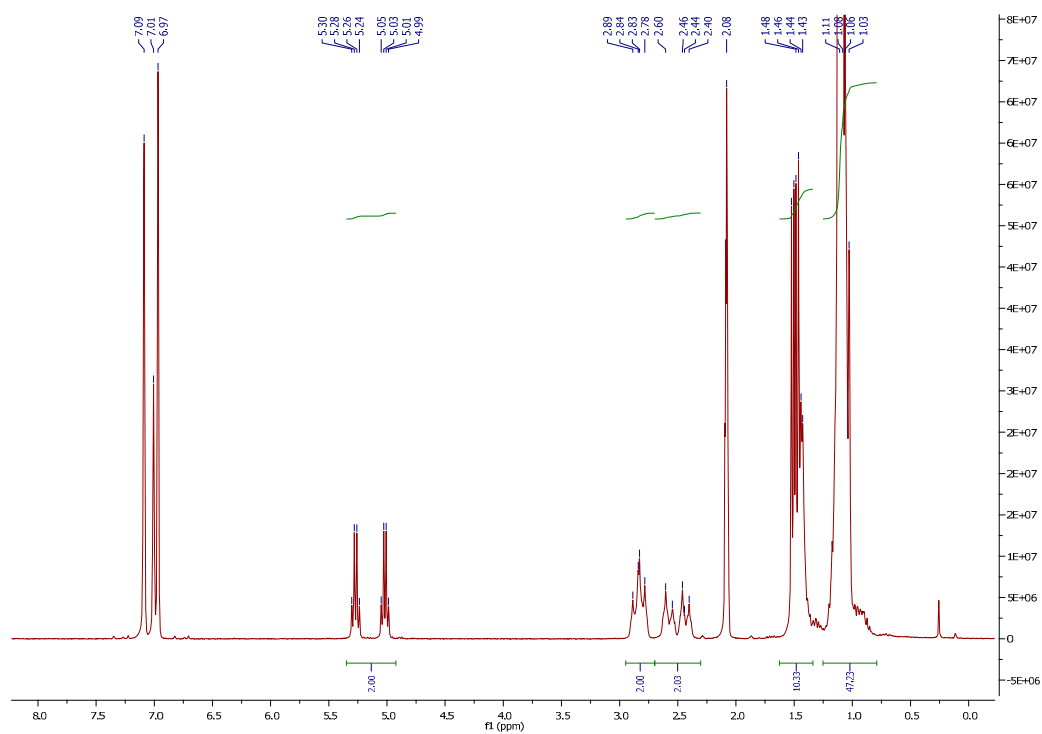


Figure S1.27: ¹H-NMR spectrum of compound **14a** in toluene-d₈.

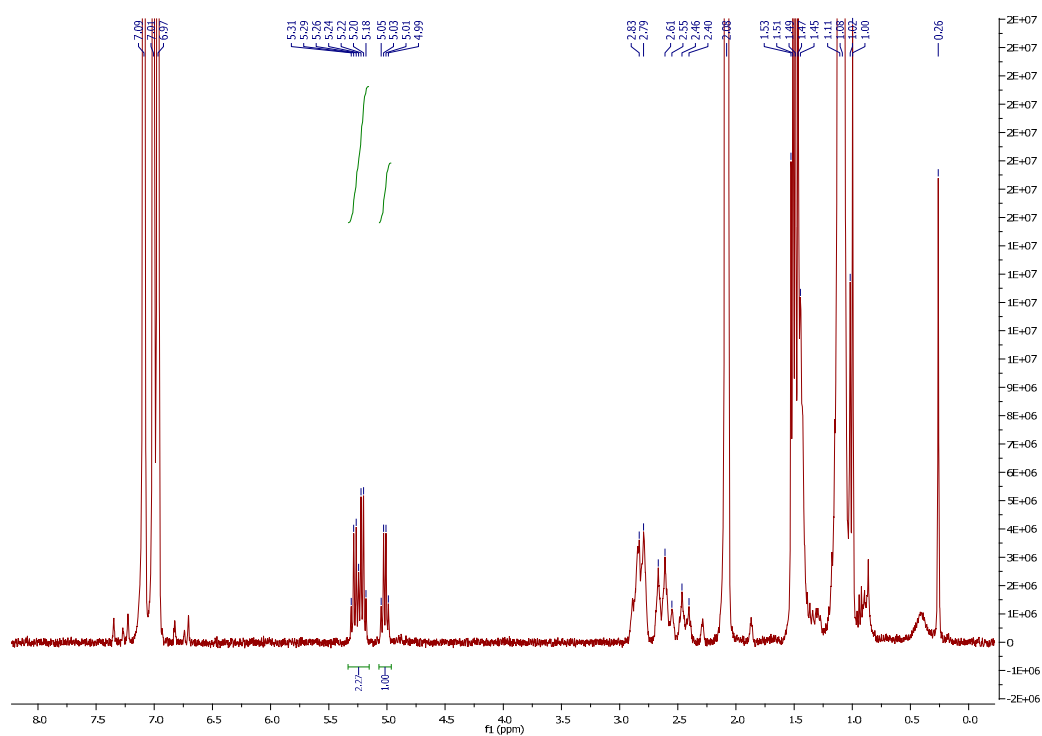


Figure S1.28: ¹H-NMR spectrum of compound **14e** in toluene-d₈.

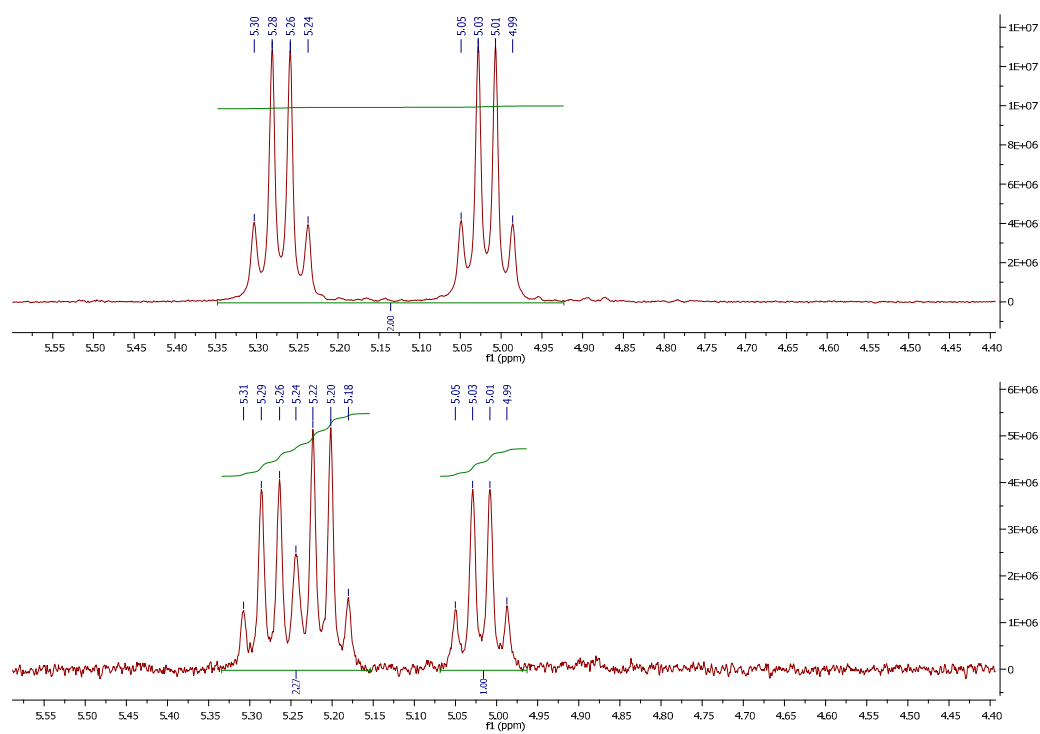


Figure S1.30: ^1H -NMR spectrum zooms of diastereo-pure compound **14a** (top), the corresponding racemic compound **14e** (bottom) in toluene- d_8 .

2. FT-IR spectra

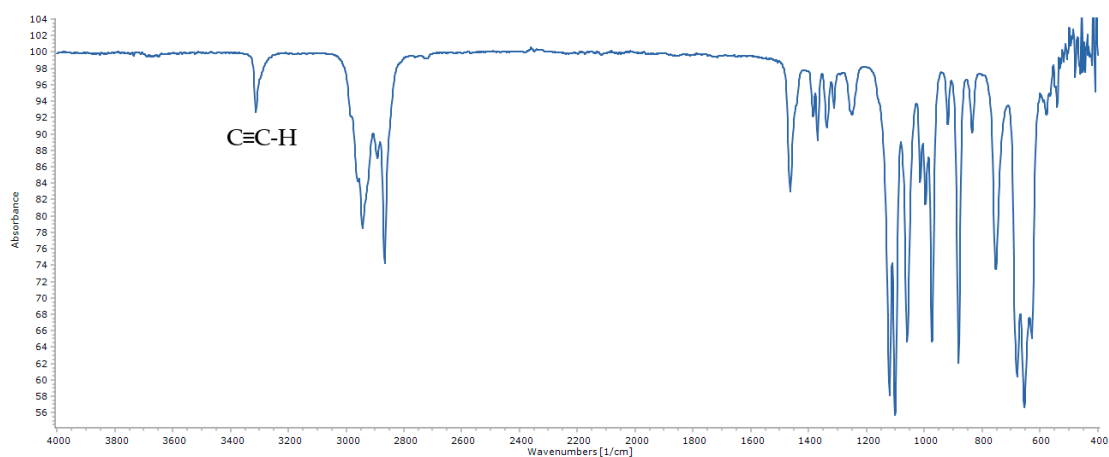


Figure S2.1: FT-IR (ATR) spectrum of compound **12a**.

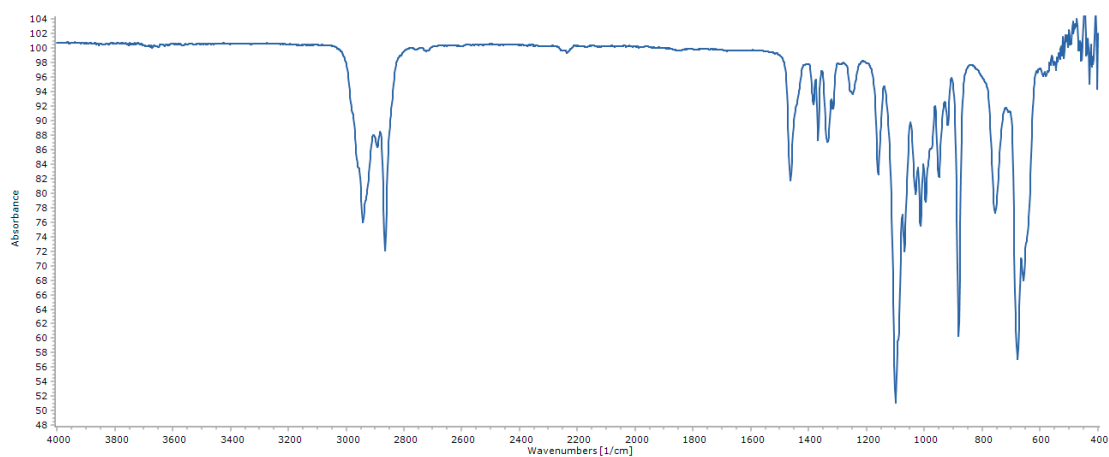


Figure S2.2: FT-IR (ATR) spectrum of compound **13a**.

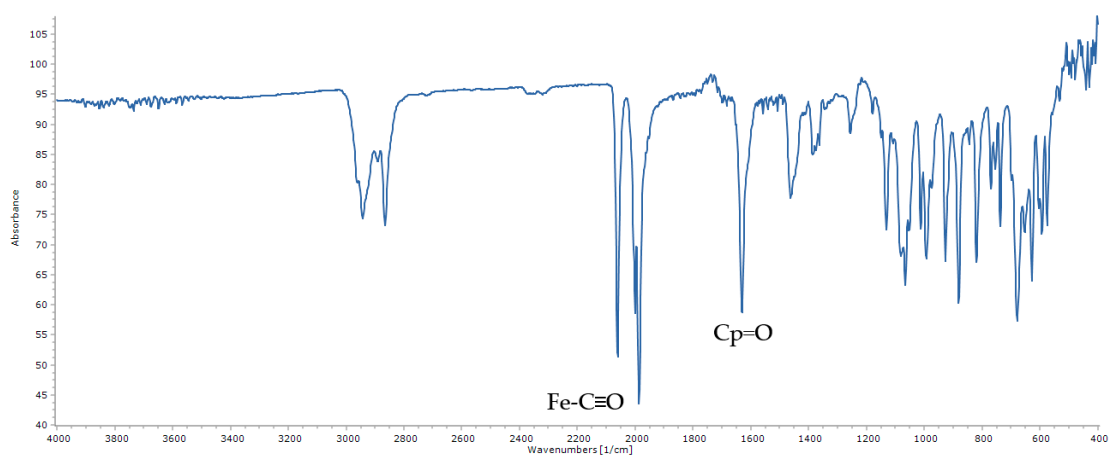


Figure S2.3: FT-IR (ATR) spectrum of compound **14a**.

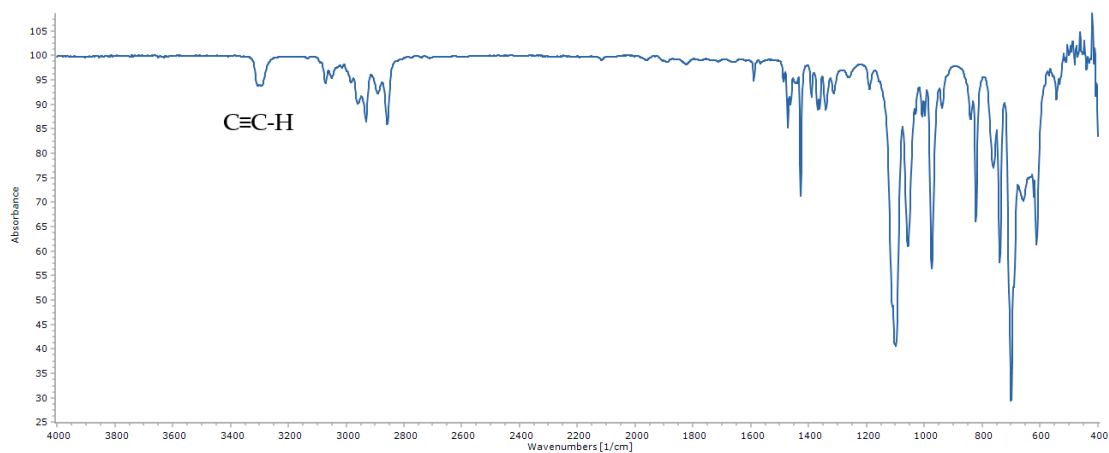


Figure S2.4: FT-IR (ATR) spectrum of compound **12b**.

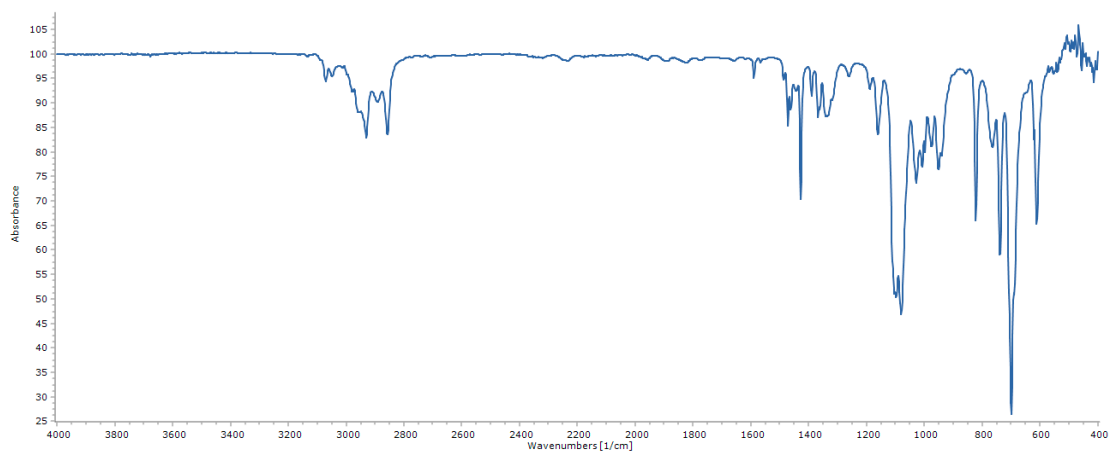


Figure S2.5: FT-IR (ATR) spectrum of compound **13b**.

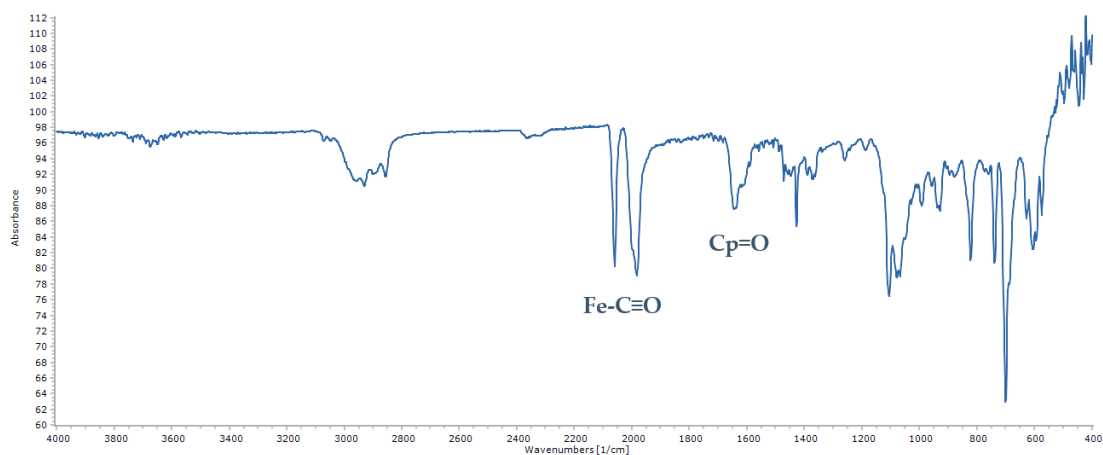


Figure S2.6: FT-IR (ATR) spectrum of compound **14b**.

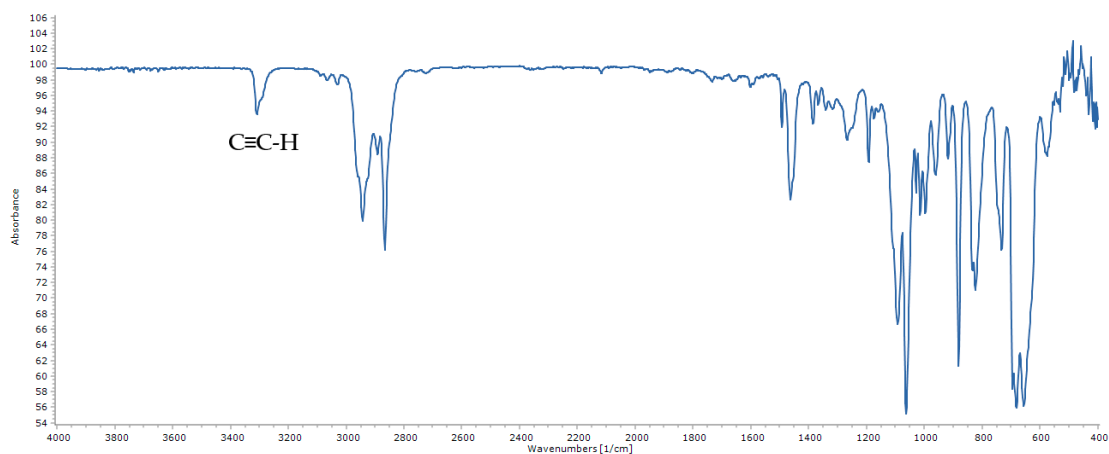


Figure S2.7: FT-IR (ATR) spectrum of compound **12c**.

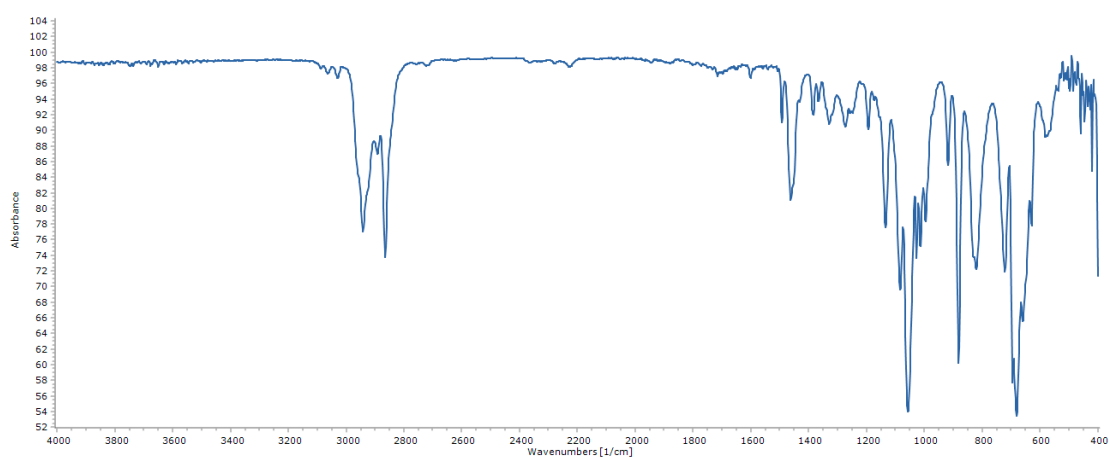


Figure S2.8: FT-IR (ATR) spectrum of compound **13c**.

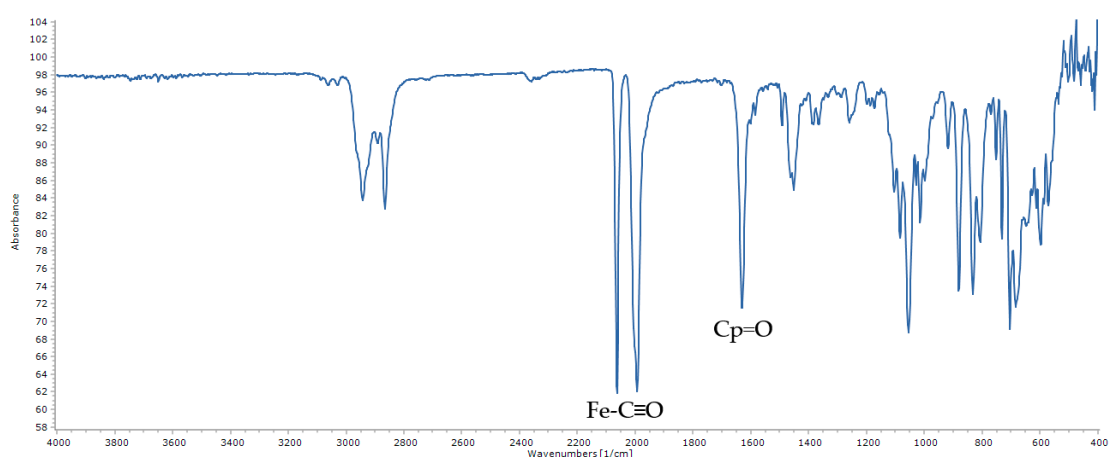


Figure S2.9: FT-IR (ATR) spectrum of compound **14c**.

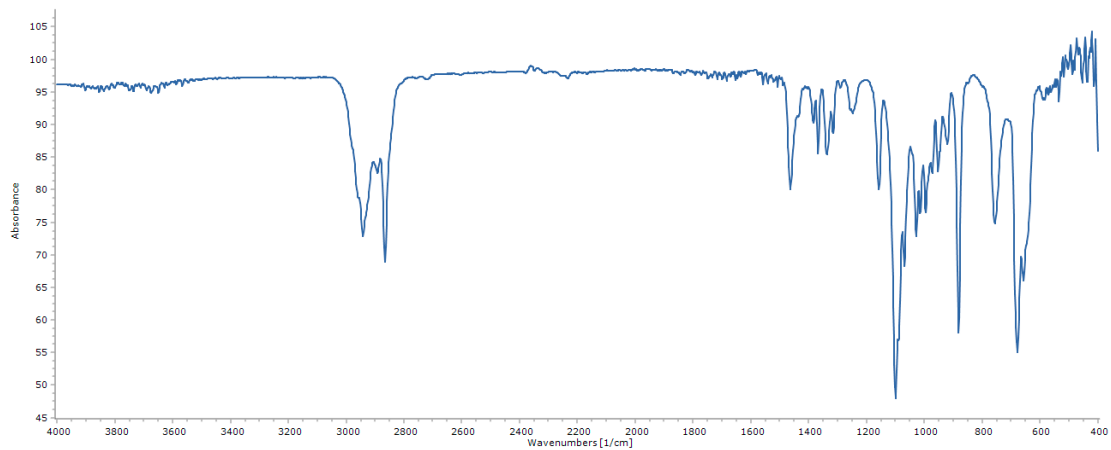


Figure S2.10: FT-IR (ATR) spectrum of compound **13d**.

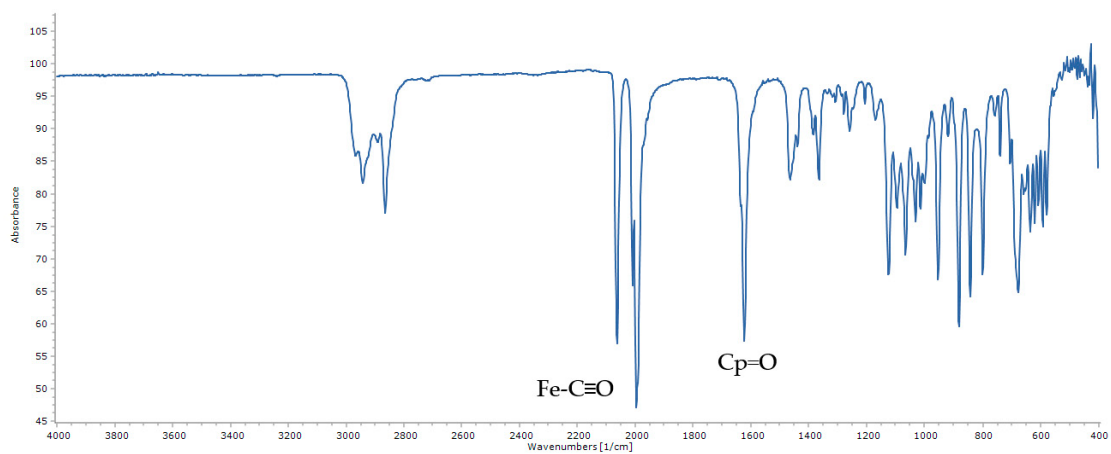


Figure S2.11: FT-IR (ATR) spectrum of compound **14d**.

3. ESI-MS spectra

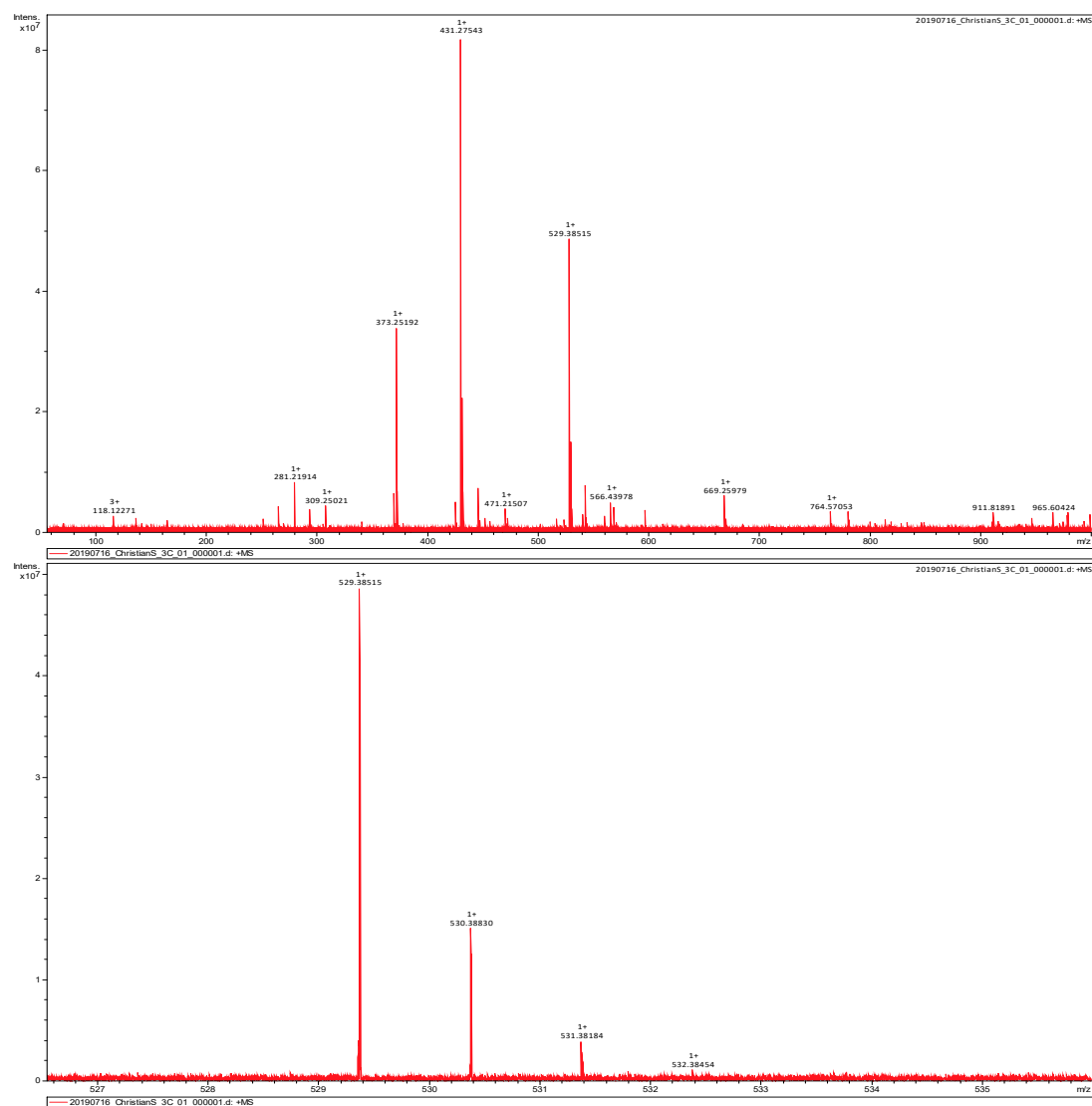


Figure S3.1: HR-MS analysis in ESI+ mode of compound **13a**; full spectrum (top) and zoom of $[13a + Na]^+$ (bottom).

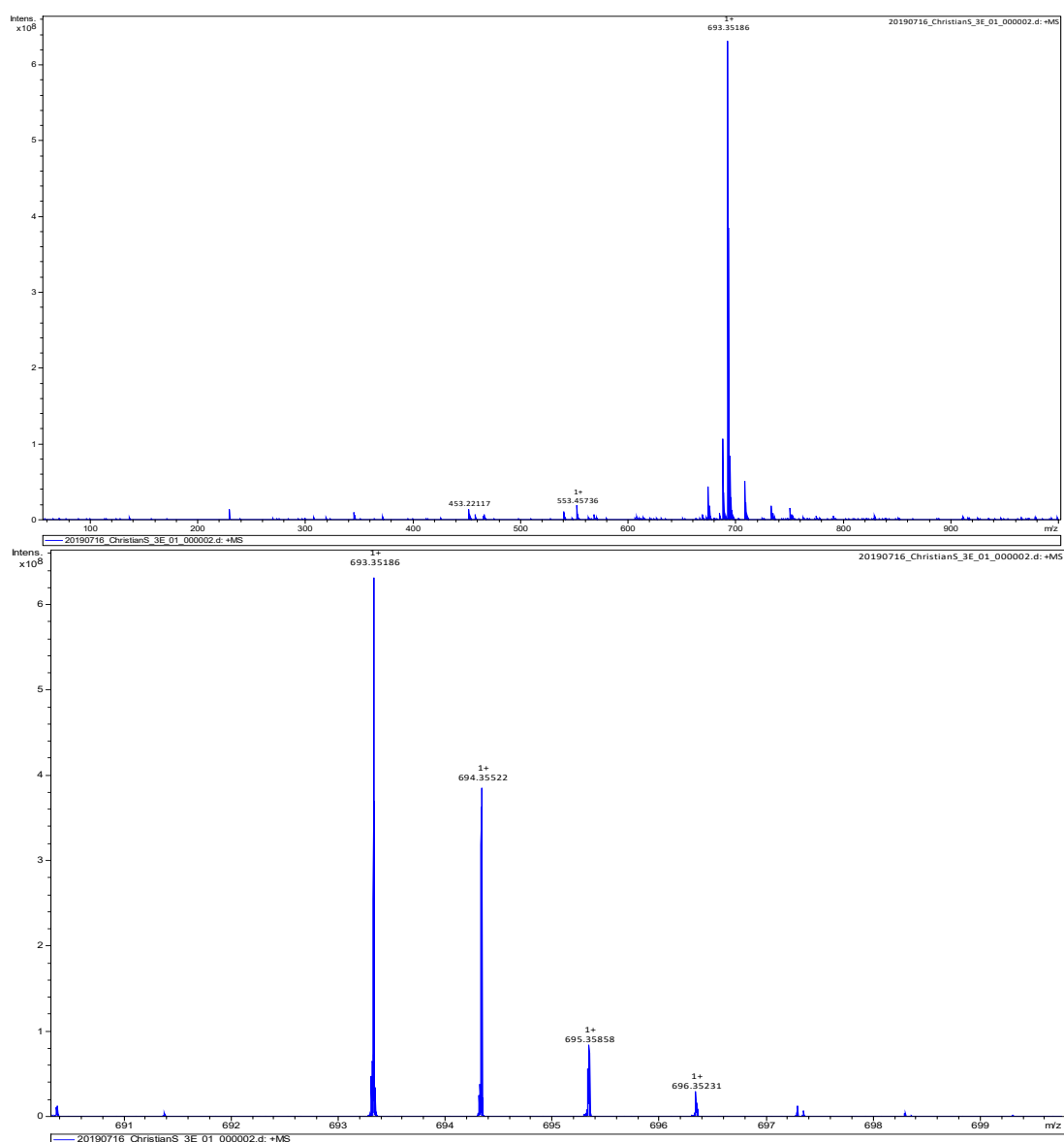


Figure S3.2: HR-MS analysis in ESI+ mode of compound **13b**; full spectrum (top) and zoom of $[13b + Na]^+$ (bottom).

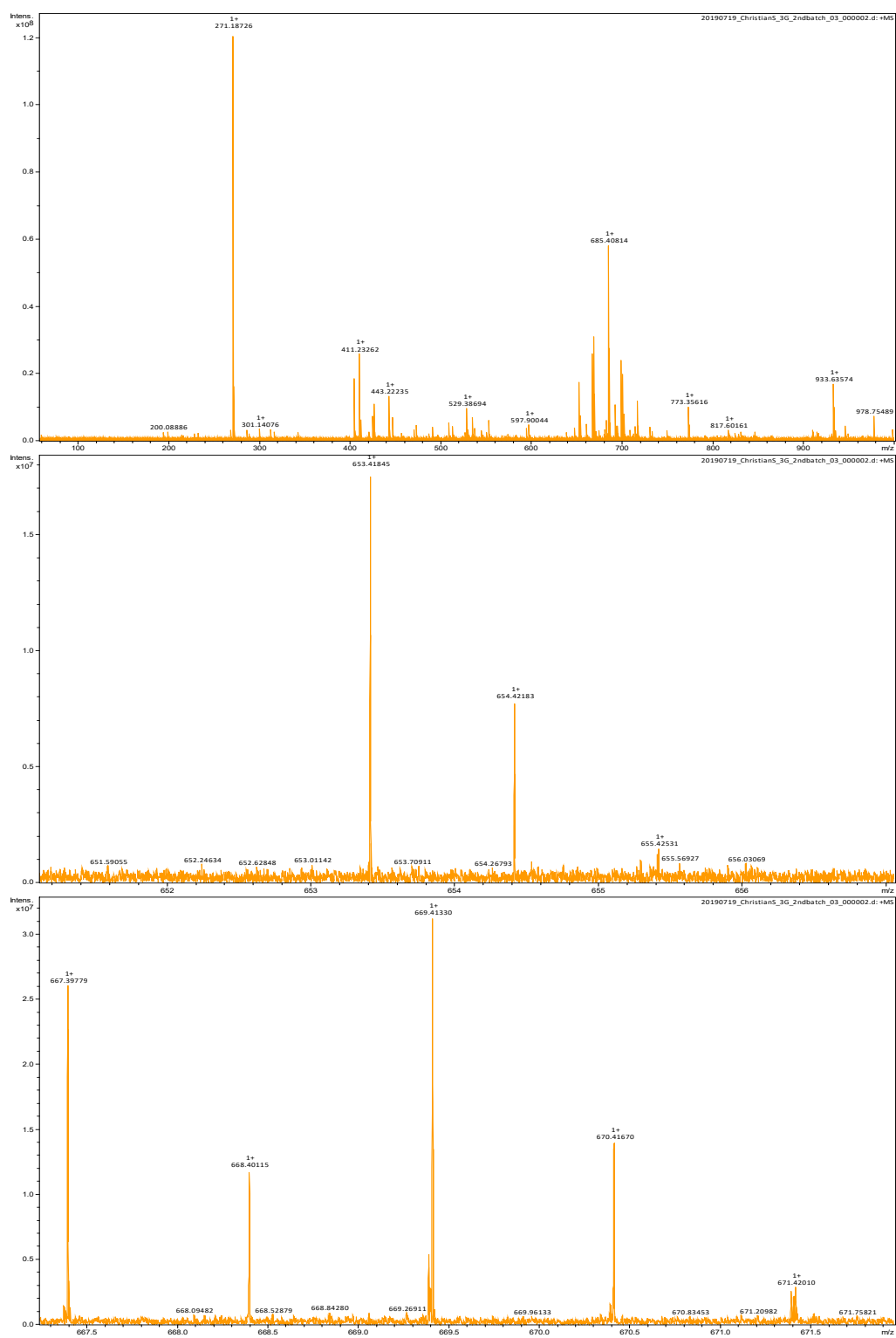


Figure S3.3: HR-MS analysis in ESI⁺ mode of compound 6c; full spectrum (top), zoom of [13c + Na]⁺ (middle), and zoom of [13c + K]⁺ (bottom).

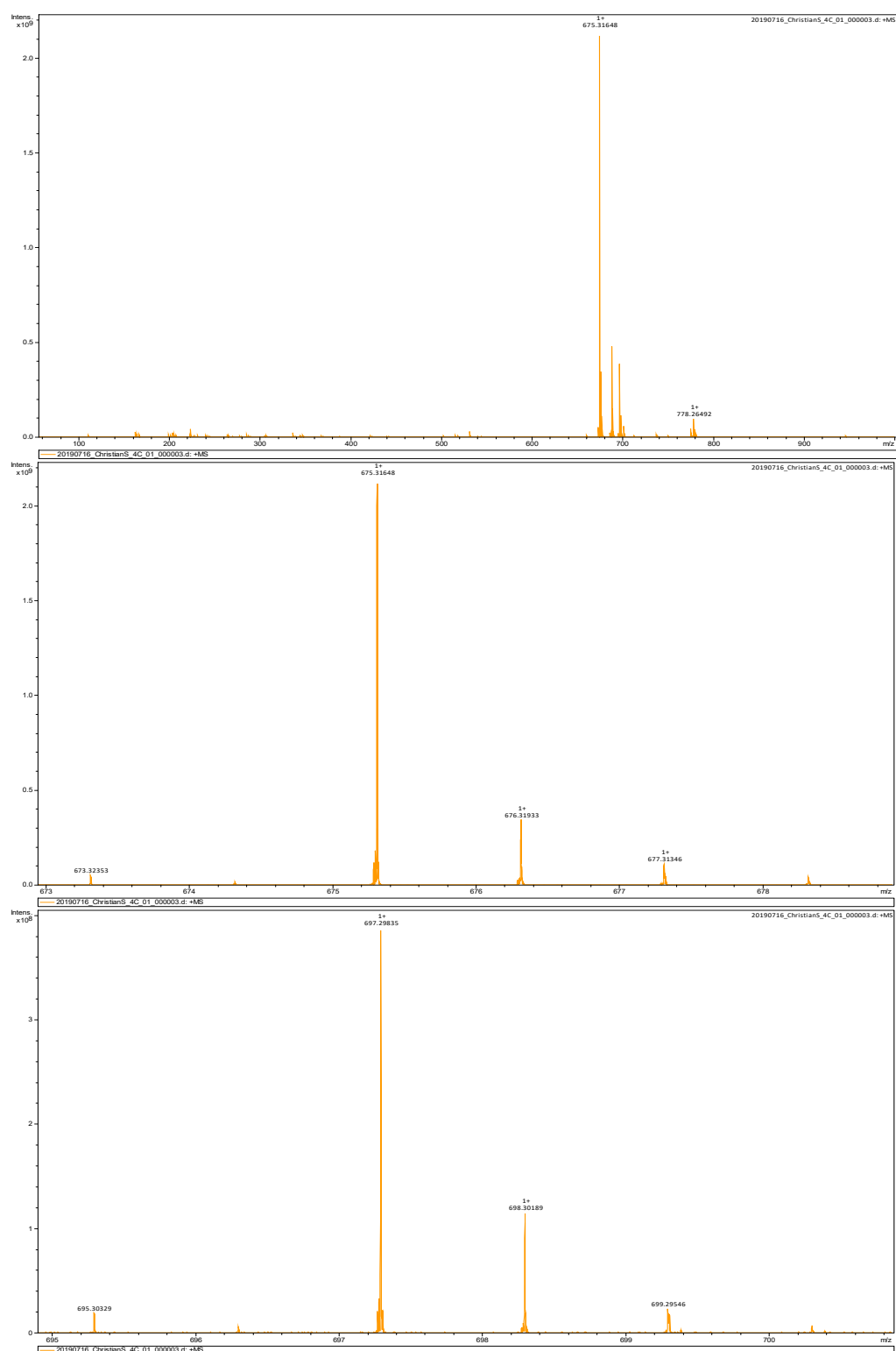


Figure S3.4: HR-MS analysis in ESI+ mode of compound **14a**; full spectrum (top), zoom of [**14a** + H]⁺ (middle), and zoom of [**14a** + Na]⁺ (bottom).

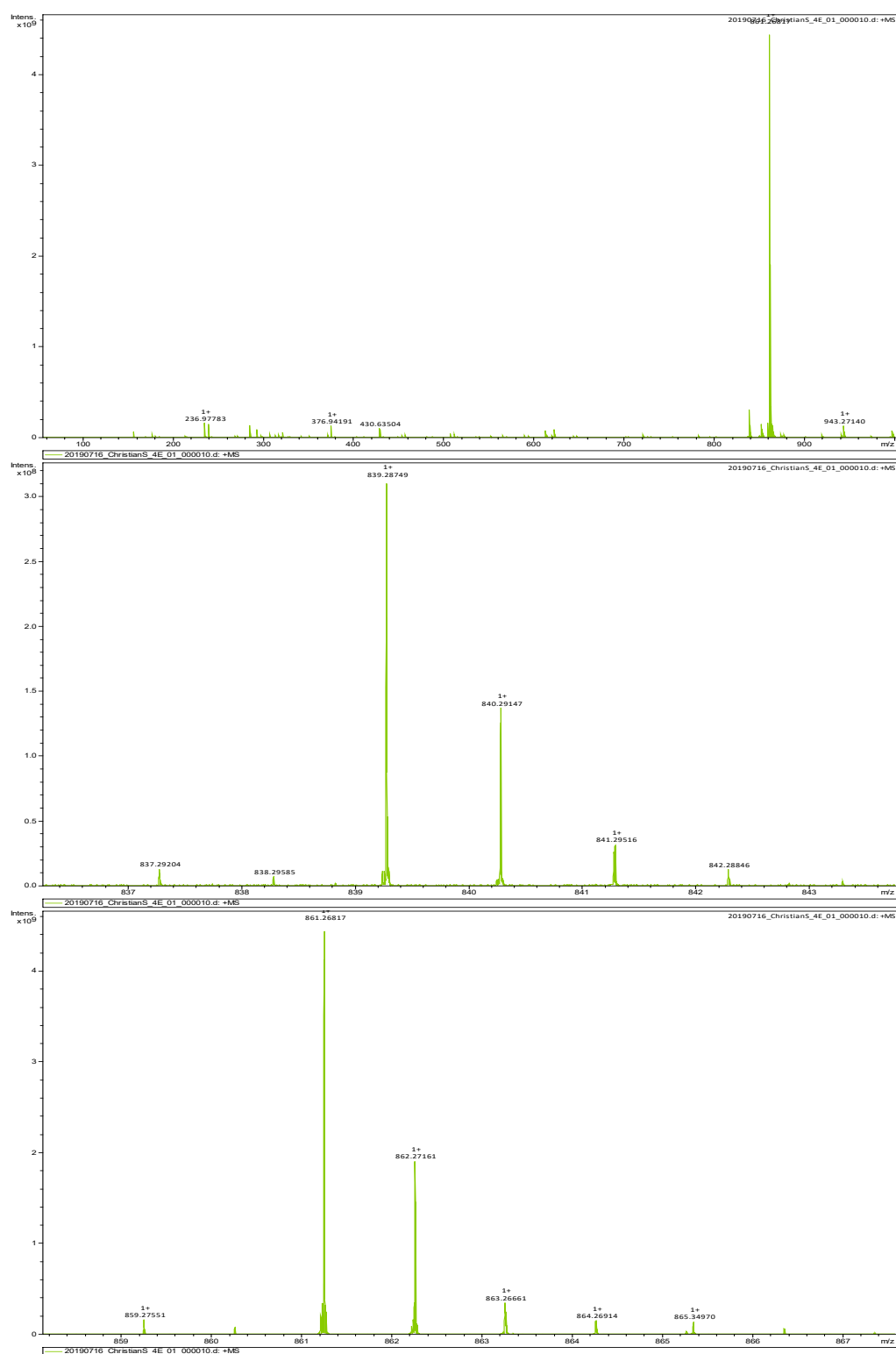


Figure S3.5: HR-MS analysis in ESI+ mode of compound **14b**; full spectrum (top), zoom of $[14b + H]^+$ (middle), and zoom of $[14b + Na]^+$ (bottom).

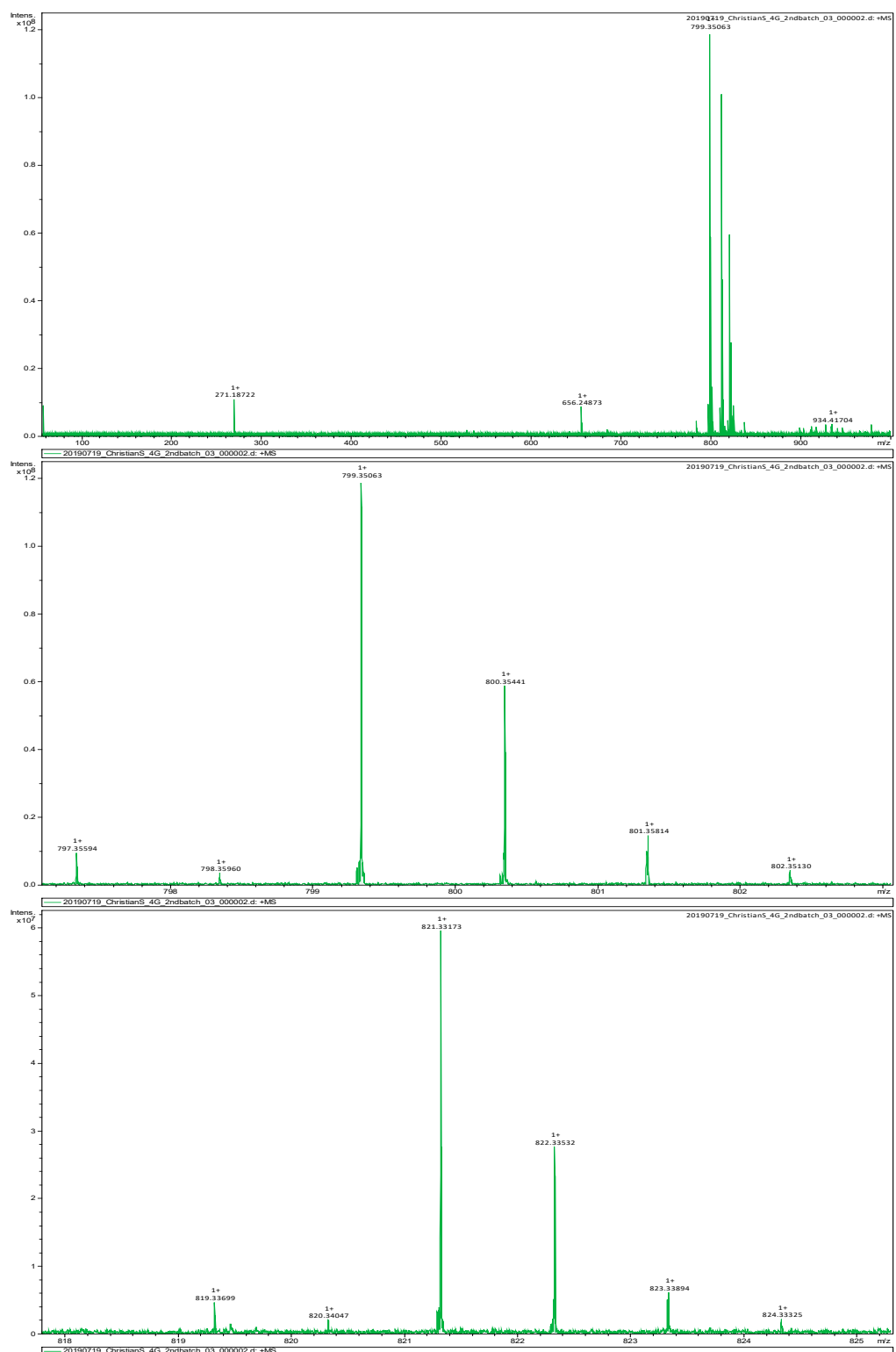


Figure S3.6: HR-MS analysis in ESI⁺ mode of compound **14c**; full spectrum (top), zoom of [14c + H]⁺ (middle), and zoom of [14c + Na]⁺ (bottom).

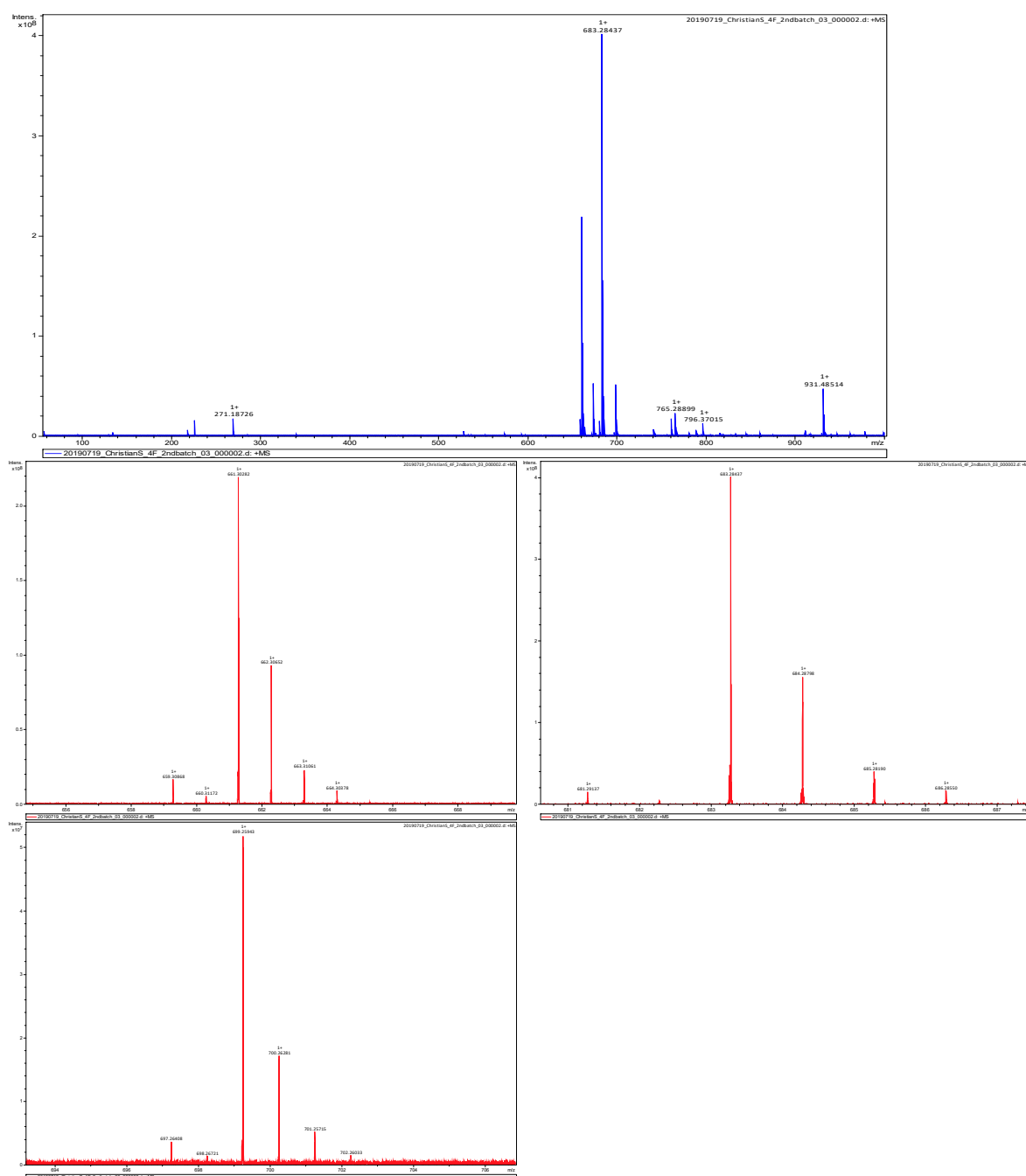


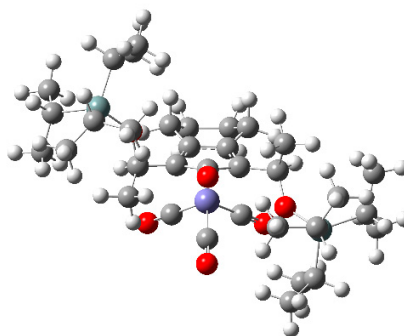
Figure S3.7: HR-MS analysis in ESI+ mode of compound **14d**; full spectrum (top), zoom of **[14d + H]⁺** (middle-left), zoom of **[14d + Na]⁺** (middle-right), and zoom of **[14d + K]⁺** (bottom).

4. DFT calculations

14a: $E_{\text{Gibbs}} = -1912.97019587 \text{ eH}$

C	0.11923100	-0.43429500	-0.10042600
C	-0.91471600	0.41265900	-0.80070300
C	-0.24010200	1.58715300	-1.30553700
C	1.05150900	1.67668300	-0.67830000
C	1.20274700	0.55897200	0.22390300
O	0.04288500	-1.64562500	0.22120400
C	-0.59141500	2.53635000	-2.41929100
H	-0.13788700	2.12764900	-3.33770300
H	-1.67166000	2.57544800	-2.60230400
C	2.02993400	2.72242000	-1.13347300
H	2.83437600	2.87361200	-0.40442700
H	2.51345900	2.33200300	-2.04249000
C	-0.04919300	3.97697400	-2.17803000
C	1.33559000	4.07691900	-1.44723600
H	-0.79238500	4.52470500	-1.58577400
H	0.00438000	4.48523100	-3.14912400
H	1.19046700	4.61009400	-0.49955100
H	2.02503600	4.68902000	-2.04251300
C	-2.23740900	-0.11440800	-1.31969900
H	-2.71888000	0.68072800	-1.91362200
C	2.49106600	0.22846000	0.94944600
H	2.97237300	1.17386100	1.25304200
C	-1.96216600	-1.32429900	-2.24609100
H	-1.48233500	-2.12679100	-1.68110500
H	-2.88804700	-1.69178000	-2.69501700
H	-1.28948200	-1.02497000	-3.06152100
C	2.28664700	-0.64075000	2.20259000
H	1.77256600	-1.56977600	1.94652900
H	3.25030700	-0.86660100	2.67070300
H	1.67801900	-0.10043500	2.93853400
O	3.33623900	-0.39901900	-0.05598900
O	-3.11123500	-0.42280500	-0.20548900
Si	4.87583500	-1.16119300	-0.20024600
Si	-4.64095200	-1.21540100	-0.00912900
C	-5.93024400	-0.75062700	-1.38112000
H	-6.73424500	-1.49502900	-1.22751100
C	-5.32637300	-0.56042700	1.66905300
H	-6.42248600	-0.66880300	1.57177700
C	-4.42070400	-3.12945100	0.09940800
H	-5.25356200	-3.45230200	0.75080800
C	5.20580400	-1.12601700	-2.09925900
H	6.30576500	-1.11068800	-2.20399100
C	4.85516100	-2.98603600	0.42357800
H	5.62607400	-3.47974400	-0.19675700
C	6.26237500	-0.15827400	0.69969400
H	7.11638600	-0.85852400	0.74878600
C	-4.57314000	-3.92193900	-1.22570300
H	-5.53154800	-3.72734500	-1.72480100
H	-3.76556700	-3.69141000	-1.93223400
H	-4.52292100	-5.00141200	-1.02066300
C	-3.09458400	-3.52782700	0.80607900
H	-2.21680700	-3.15788400	0.26535900
H	-3.02942800	-3.12454200	1.82244100
H	-3.01877000	-4.62344400	0.87424200
C	-4.90295500	-1.37401100	2.92182300
H	-5.15937600	-2.43760700	2.84014000
H	-3.82392500	-1.29528500	3.10076100
H	-5.41416000	-0.97918500	3.81256700
C	-5.02192200	0.94135800	1.91578600
H	-3.94622200	1.09086000	2.05104100
H	-5.34200300	1.58744300	1.09172600
H	-5.52706800	1.28538300	2.83069000
C	-6.57264300	0.65191500	-1.19592400
H	-5.82502100	1.45159900	-1.29073800
H	-7.33611200	0.82138400	-1.96977800

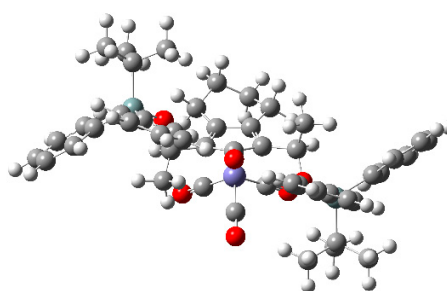
H	-7.06058300	0.76372500	-0.22107700
C	-5.46380800	-0.89015600	-2.85562800
H	-6.30866100	-0.70153200	-3.53449700
H	-4.68554900	-0.15386000	-3.09697400
H	-5.07307000	-1.88675700	-3.08564100
C	4.69259900	-2.36650500	-2.87830500
H	5.10289100	-3.30753000	-2.49130800
H	3.59758000	-2.43247900	-2.83843400
H	4.98098100	-2.29064500	-3.93727700
C	4.64429900	0.15716100	-2.76873000
H	3.55306600	0.18453200	-2.66268500
H	5.04546200	1.07468600	-2.32270000
H	4.88849900	0.16680800	-3.84158100
C	6.74329600	1.09286400	-0.08362600
H	5.93976200	1.83683200	-0.17776800
H	7.57664400	1.57644300	0.44739900
H	7.09275800	0.84607500	-1.09332200
C	5.92172500	0.25837500	2.15705700
H	5.09824400	0.98452600	2.17599800
H	5.63690800	-0.59146000	2.78631500
H	6.79109400	0.74179400	2.62632500
C	3.50564600	-3.70508100	0.14617500
H	2.68213700	-3.24226600	0.70063700
H	3.22846200	-3.68121800	-0.91287000
H	3.57018000	-4.75933300	0.45367400
C	5.27345000	-3.20941800	1.90142600
H	6.25587800	-2.77692300	2.13198400
H	4.53991800	-2.78243200	2.59791300
H	5.32988500	-4.28702300	2.11427200
Fe	-0.48267100	1.78417700	0.80936800
C	0.42851800	2.95486100	1.79081000
C	-1.91094800	2.82895600	0.59973100
C	-1.10721900	0.74719900	2.13114500
O	1.05680000	3.70038400	2.45187600
O	-1.50589800	0.09426400	3.01943000
O	-2.86142400	3.50252000	0.43872500



14b: $E_{\text{Gibbs}} = -2443.98743404 \text{ eH}$

C	0.05925900	-0.22709200	0.11834100
C	-1.04562000	-1.11432700	0.61710900
C	-0.43244200	-2.30643700	1.16774000
C	0.93993400	-2.35236800	0.72661200
C	1.18551600	-1.19580900	-0.10761400
O	0.02006600	1.00443700	-0.13294700
C	-0.99840200	-3.30160700	2.15301200
H	-1.03974400	-2.81070000	3.13896000
H	-2.03005000	-3.57888300	1.90440100
C	1.93592000	-3.38344500	1.21743100
H	2.20471700	-4.08887200	0.42103400
H	2.85982000	-2.86017400	1.49408100
C	-0.10148000	-4.55880300	2.25594600
C	1.38228800	-4.16348200	2.43962400
H	-0.21142400	-5.17030800	1.34843100
H	-0.43435700	-5.17392400	3.10175400
H	1.99533600	-5.05844800	2.60606400
H	1.47359100	-3.54077200	3.34219100
C	-2.43558200	-0.63042100	0.95724600
H	-3.04302300	-1.48987100	1.28447400
C	2.55057400	-0.82603800	-0.64765800
H	3.09698700	-1.75148300	-0.89262600
C	-2.36578200	0.38448300	2.12475300
H	-1.77538300	1.25829700	1.83882900
H	-3.37044200	0.70708200	2.41724400
H	-1.89643800	-0.08518200	2.99972900
C	2.51308800	0.05785800	-1.90727000
H	1.93461600	0.96802200	-1.73607100
H	3.53040600	0.32408700	-2.21366800
H	2.05294400	-0.49729900	-2.73395400
O	3.24124700	-0.20204800	0.48501800
O	-3.05015400	-0.08290600	-0.24453200
Si	4.66159000	0.76516700	0.62089400
Si	-4.51857400	0.81387900	-0.42163800
C	-5.13094100	0.43790400	-2.21088000
C	5.22628200	0.44725000	2.43765900
C	-4.16278200	1.10078800	-3.23112200
H	-4.12520600	2.19000600	-3.10528600
H	-3.14231600	0.71448700	-3.13552700
H	-4.50789000	0.89113500	-4.25535300
C	-5.17887700	-1.09012700	-2.48430500
H	-4.21261600	-1.56603800	-2.27885700
H	-5.94774500	-1.59210500	-1.88281200
H	-5.42552300	-1.26575500	-3.54253500
C	4.07727600	0.88158400	3.39080900
H	3.83986800	1.94758700	3.28194600
H	3.16111400	0.31045200	3.19469400
H	4.37488800	0.70757100	4.43647800
C	5.53150000	-1.05617800	2.67543800
H	4.67260000	-1.68561000	2.40798500
H	6.40377400	-1.39361600	2.10118600
H	5.75271200	-1.22455500	3.74062000
Fe	-0.38209100	-2.40949900	-0.96420500
C	0.65978500	-3.55708300	-1.83943900
C	-1.82531300	-3.45087200	-0.99969000
C	-0.81379900	-1.34209000	-2.33826200
O	1.37428700	-4.30029900	-2.40767200
O	-1.08459000	-0.68295000	-3.26857500
O	-2.79741700	-4.11355600	-0.99630400
C	-6.55474000	1.03107300	-2.41186300
H	-6.56033000	2.12396900	-2.30406100
H	-6.90705600	0.80210300	-3.42898300
H	-7.28228000	0.61058400	-1.70431800
C	6.50094200	1.27444700	2.76225800
H	6.31324500	2.35334500	2.69390200
H	6.82732400	1.06213300	3.79156600
H	7.33558900	1.02514300	2.09197900
C	5.92834400	0.17529000	-0.67102500

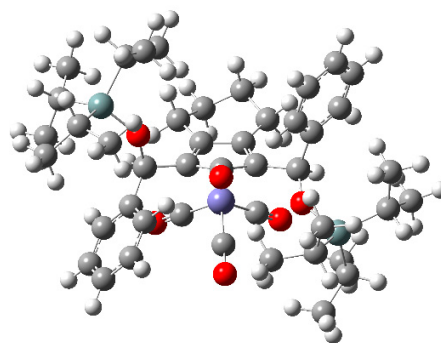
C	6.55853100	1.05901900	-1.58172400
C	6.24077800	-1.20590400	-0.77594000
C	7.47522200	0.58992400	-2.54268500
H	6.32110900	2.11914000	-1.56054400
C	7.15233300	-1.68158300	-1.73590900
H	5.76303100	-1.92239000	-0.11109000
C	7.77797500	-0.78219600	-2.62090100
H	7.94329800	1.29121400	-3.23003200
H	7.37064400	-2.74563900	-1.79537600
H	8.48332800	-1.14647800	-3.36456000
C	4.20868900	2.58993600	0.38438800
C	2.84849500	2.97771600	0.28452800
C	5.19294300	3.61248100	0.36763400
C	2.49006100	4.33438700	0.16481600
H	2.06207700	2.22744700	0.29987300
C	4.83648900	4.96872000	0.24848100
H	6.24873900	3.36149400	0.45597600
C	3.48042200	5.33418000	0.14490900
H	1.43894400	4.60349800	0.08780400
H	5.61105800	5.73263700	0.23790000
H	3.20131600	6.38166800	0.05192200
C	-4.11859900	2.65749300	-0.25191500
C	-5.12700300	3.65363100	-0.19488900
C	-2.76473900	3.08063200	-0.26984000
C	-4.79991400	5.02192800	-0.14335300
H	-6.17917700	3.37282200	-0.19911300
C	-2.43679700	4.44902700	-0.21796300
H	-1.96546000	2.34523800	-0.33119700
C	-3.45037500	5.42377500	-0.15183800
H	-5.59194400	5.76659900	-0.09976800
H	-1.39121100	4.74920900	-0.23454700
H	-3.19392700	6.48048100	-0.11268600
C	-5.74149400	0.21396900	0.91019700
C	-6.05767000	-1.16677800	1.01103800
C	-6.33762500	1.09109900	1.84997700
C	-6.94173800	-1.64745100	1.99459900
H	-5.60874500	-1.87935500	0.32230000
C	-7.22567600	0.61697600	2.83508100
H	-6.09820400	2.15102600	1.82901300
C	-7.53386900	-0.75435200	2.90852200
H	-7.16696100	-2.71051400	2.04685300
H	-7.66965900	1.31395700	3.54263100
H	-8.21963600	-1.12227900	3.66862500



14c: $E_{\text{Gibbs}} = -2296.37946435 \text{ eH}$

C	0.00931000	0.13544000	0.15239100
C	1.08594100	0.44724500	-0.86128900
C	0.42412700	0.84479000	-2.08363800
C	-0.95806700	0.43521200	-1.99990200
C	-1.17084400	-0.20640800	-0.71488900
O	0.10451200	0.10118900	1.40041500
C	0.97084600	1.66796000	-3.23594600
H	1.54824500	2.50387300	-2.82261500
H	1.67029900	1.08294900	-3.84661200
C	-1.97108300	0.79238700	-3.06111000
H	-2.68722500	-0.02120000	-3.22910800
H	-2.55367800	1.64892700	-2.68818800
C	-0.16684900	2.22763300	-4.13080500
C	-1.28024000	1.18774900	-4.38688600
H	0.25973900	2.57111100	-5.08191900
H	-0.61242600	3.10736100	-3.64327500
H	-0.85288200	0.29555200	-4.86741200
H	-2.02740800	1.59981800	-5.07738200
C	2.53186900	0.79514700	-0.51957000
H	3.13195400	0.69518200	-1.44028800
C	-2.55139300	-0.62549200	-0.22509400
H	-3.17590200	-0.77264100	-1.12012800
O	-3.05957000	0.51814700	0.51323800
O	3.01158600	-0.12231000	0.47659400
Si	-4.57096400	1.20595500	0.98955700
Si	4.49971200	-0.62283100	1.21331100
C	5.92008000	0.69097400	1.22721400
H	6.68380100	0.18051500	1.84629500
C	5.19505900	-2.11406300	0.19545600
H	6.29222300	-2.03809600	0.29712900
C	3.99293300	-1.18740900	2.97999500
H	4.74988100	-1.93669600	3.27295400
C	-4.23106300	3.10258600	0.95259200
H	-5.21649200	3.57533300	0.79112000
C	-5.06204200	0.63902400	2.76249200
H	-5.72287300	1.44635200	3.12978900
C	-6.01527000	0.80372400	-0.23350100
H	-6.91665400	1.02899900	0.36629000
C	4.00469700	-0.08227600	4.06881300
H	5.00530500	0.33733400	4.23090900
H	3.32253800	0.73876500	3.81140800
H	3.66445800	-0.50396600	5.02617800
C	2.60343500	-1.88399500	2.97830100
H	1.82451100	-1.18767600	2.64932200
H	2.56838600	-2.75497000	2.31529700
H	2.35926200	-2.22747600	3.99507600
C	4.79252100	-3.52308900	0.70547200
H	5.04034700	-3.67197500	1.76401300
H	3.71723600	-3.70133900	0.58510300
H	5.32188300	-4.29723600	0.12952900
C	4.85053100	-1.99850200	-1.31322700
H	3.76610100	-2.05932000	-1.45841600
H	5.19597600	-1.05638400	-1.75744100
H	5.30911600	-2.82147800	-1.88075600
C	6.56382400	0.93245300	-0.16798100
H	5.85401400	1.41658700	-0.85280000
H	7.42845500	1.60524000	-0.07013300
H	6.91720400	0.00819800	-0.63970700
C	5.64396500	2.06656400	1.89073200
H	5.22638000	1.98075100	2.89697600
H	6.58386200	2.63434100	1.96742500
H	4.94932300	2.66370900	1.29289600
C	-3.65394800	3.69403600	2.26634000
H	-4.29623400	3.49628700	3.13353000
H	-2.65814500	3.28422400	2.47890800
H	-3.54987300	4.78524500	2.17256200
C	-3.30774900	3.50199600	-0.23026000
H	-2.33178300	3.01268600	-0.12669300

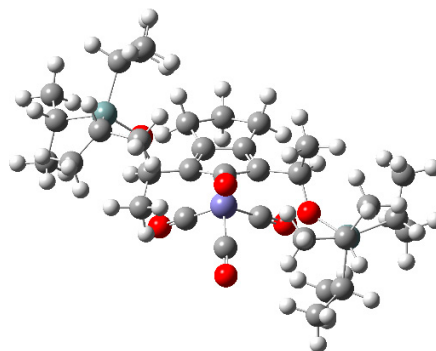
H	-3.72707000	3.21684400	-1.20286900
H	-3.14799900	4.59034400	-0.24071700
C	-6.07874300	1.70762500	-1.49469100
H	-5.20431100	1.54998600	-2.14163700
H	-6.97243300	1.46514300	-2.08882500
H	-6.12583900	2.77483600	-1.24660100
C	-6.12393500	-0.68229000	-0.67659300
H	-5.35401900	-0.92247800	-1.42189400
H	-6.01589800	-1.38891400	0.15182000
H	-7.09878200	-0.86510100	-1.15221500
C	-3.85323900	0.54000400	3.73222900
H	-3.18006700	-0.26608300	3.42492000
H	-3.26399000	1.46120800	3.77554500
H	-4.20484500	0.31553400	4.75033900
C	-5.87556000	-0.68159400	2.82800500
H	-6.80688600	-0.63301700	2.24935100
H	-5.28531500	-1.53038600	2.45836000
H	-6.14710900	-0.90181100	3.87083600
Fe	0.26503100	-1.29361400	-1.88118800
C	-0.92284100	-2.29732400	-2.74284000
C	1.52840500	-1.54555500	-3.10856100
C	0.79482800	-2.50767100	-0.67055600
O	-1.73066500	-2.94611500	-3.30137300
O	1.14450300	-3.34748600	0.06764300
O	2.35603900	-1.68200200	-3.93473300
C	2.61727200	2.25960400	-0.06148900
C	3.29680200	3.21047100	-0.85018700
C	2.01040000	2.67131500	1.14644800
C	3.37041600	4.55794100	-0.44724400
H	3.78660500	2.89782400	-1.77202400
C	2.08651000	4.01497000	1.54998800
H	1.49102900	1.93573300	1.75395500
C	2.76309800	4.96396900	0.75550300
H	3.90432400	5.27980500	-1.06090800
H	1.61889100	4.32385600	2.48204600
H	2.81976200	6.00267100	1.07298200
C	-2.60834600	-1.93373700	0.56652600
C	-3.31771900	-3.02791900	0.02540500
C	-1.97988200	-2.08375000	1.82291100
C	-3.39846600	-4.25163900	0.71619600
H	-3.81004100	-2.93097700	-0.94087200
C	-2.06214300	-3.30480200	2.51433800
H	-1.41201000	-1.25494500	2.23167600
C	-2.77021000	-4.39347200	1.96729500
H	-3.94715300	-5.08382800	0.28109400
H	-1.56561600	-3.40847200	3.47639200
H	-2.82810500	-5.33681700	2.50561000



14d: $E_{\text{Gibbs}} = -1873.6595537 \text{ eH}$

C	0.12591500	-0.37718600	-0.11372500
C	-0.92211000	0.39869100	-0.88691000
C	-0.24812000	1.51985500	-1.48258300
C	1.04397300	1.67042000	-0.87278500
C	1.21798900	0.64432500	0.11893900
O	0.05397500	-1.55332800	0.31578900
C	-0.41215400	2.48509200	-2.63513400
H	-0.25655400	1.93938000	-3.57845800
H	-1.39198300	2.96956400	-2.69672000
C	1.84493100	2.74528500	-1.56848000
H	2.40528700	3.40725800	-0.90040000
H	2.57334200	2.26023300	-2.23360600
C	0.75130800	3.50909400	-2.39237900
H	0.37381400	4.35336100	-1.80259300
H	1.14854400	3.90725900	-3.33179100
C	-2.24929600	-0.16851200	-1.34905300
H	-2.72269800	0.57411700	-2.01411400
C	2.50731900	0.38742300	0.87277000
H	2.98007400	1.36135600	1.08565500
C	-1.98834300	-1.46291700	-2.15692900
H	-1.50245200	-2.20917900	-1.52399300
H	-2.92216600	-1.86842100	-2.55397900
H	-1.32740600	-1.24675600	-3.00742900
C	2.30614800	-0.36683200	2.19892700
H	1.78574200	-1.31169600	2.02743100
H	3.27203400	-0.55872600	2.67750400
H	1.70644800	0.23909100	2.88967700
O	3.35774700	-0.32665800	-0.06727900
O	-3.12084200	-0.36409100	-0.20777400
Si	4.92506400	-1.04195000	-0.13603100
Si	-4.65495100	-1.12379500	0.06924100
C	-5.95093700	-0.76699400	-1.32822500
H	-6.75969700	-1.48863500	-1.10656700
C	-5.31571900	-0.32329100	1.69354000
H	-6.41366800	-0.43293200	1.62146200
C	-4.45470700	-3.02384200	0.33988600
H	-5.28133100	-3.27508400	1.02969300
C	5.25755500	-1.18366500	-2.02965100
H	6.35661300	-1.14665200	-2.13857000
C	4.95663900	-2.80142400	0.65821300
H	5.73271100	-3.33425000	0.07806500
C	6.27239600	0.08783000	0.66418500
H	7.15428600	-0.57139900	0.76410700
C	-4.64144100	-3.92725900	-0.90802800
H	-5.59860400	-3.75128700	-1.41640900
H	-3.83442800	-3.78339400	-1.63805800
H	-4.61818100	-4.98512400	-0.60756800
C	-3.12363500	-3.38175400	1.05840900
H	-2.24956300	-3.07371900	0.47460800
H	-3.03580600	-2.89515700	2.03571800
H	-3.06289700	-4.46873200	1.21803400
C	-4.87638500	-1.03106600	3.00404200
H	-5.13704500	-2.09669200	3.01522200
H	-3.79435000	-0.94242700	3.15927500
H	-5.37254300	-0.56045700	3.86592900
C	-5.00096600	1.19237300	1.80803400
H	-3.92162200	1.34711000	1.90031200
H	-5.34363300	1.77024800	0.94341400
H	-5.47929800	1.61183400	2.70569600
C	-6.57951200	0.65154300	-1.25879800
H	-5.82663800	1.43271500	-1.43286200
H	-7.35179900	0.75988500	-2.03488900
H	-7.05339700	0.85169400	-0.29126000
C	-5.49344300	-1.03620800	-2.78753700
H	-6.33995400	-0.89885800	-3.47650900
H	-4.71023000	-0.32998400	-3.09397100
H	-5.11193800	-2.05217800	-2.93297400
C	4.77716900	-2.51084500	-2.67494400

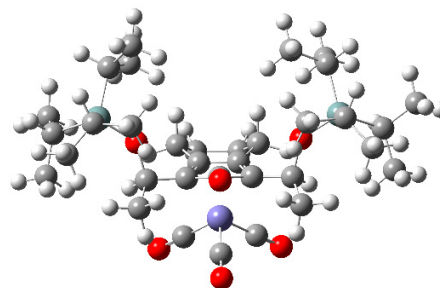
H	5.21185200	-3.39544900	-2.19333700
H	3.68423500	-2.59953800	-2.62245700
H	5.06136300	-2.53810500	-3.73731700
C	4.65729400	0.00798400	-2.82340600
H	3.56537000	0.01098600	-2.71949700
H	5.02932700	0.97786700	-2.47287900
H	4.90286500	-0.08197100	-3.89214400
C	6.70043900	1.28685100	-0.22523800
H	5.86533400	1.98390100	-0.38175300
H	7.51074000	1.84925100	0.26170500
H	7.06308100	0.96934000	-1.21034200
C	5.92688000	0.61284700	2.08546100
H	5.07827300	1.30886200	2.05375100
H	5.67820000	-0.19057100	2.78678400
H	6.78210400	1.16433600	2.50293900
C	3.62179000	-3.57361200	0.46525300
H	2.79399800	-3.07919700	0.98493600
H	3.33252100	-3.65591200	-0.58763200
H	3.71364700	-4.59280500	0.86946700
C	5.39272000	-2.87669800	2.14539900
H	6.36501700	-2.40005600	2.32400200
H	4.65419200	-2.40616300	2.80772000
H	5.47896400	-3.92833800	2.45548700
Fe	-0.47674100	1.91619400	0.59577200
C	0.44200600	3.18223400	1.44148800
C	-1.89823600	2.94341400	0.28205700
C	-1.09045200	1.01012000	2.01725300
O	1.08109700	3.99858200	2.00016000
O	-1.48045100	0.44568000	2.96775100
O	-2.83758600	3.60730700	0.03837300



14f: $E_{\text{Gibbs}} = -1912.97429946 \text{ eH}$

C	0.03322800	-0.26815700	-1.00864000
C	-1.12638600	-0.92535300	-0.30087900
C	-0.64708900	-1.37388700	0.98516700
C	0.79068400	-1.34606900	0.97276600
C	1.22996800	-0.87750100	-0.32056700
O	0.00992500	0.49963800	-1.99970500
C	-1.36951200	-1.67040700	2.26837900
H	-1.37813900	-0.73260100	2.84660400
H	-2.42050500	-1.93064400	2.09857000
C	1.55012300	-1.61223000	2.24138700
H	2.60315500	-1.84655900	2.04690600
H	1.55183000	-0.66730400	2.80611300
C	-0.66621100	-2.78470200	3.09431500
C	0.90245800	-2.73382000	3.10522500
H	-0.98020600	-3.75515500	2.69037100
H	-1.04604500	-2.74191700	4.12292600
H	1.28233900	-3.70100300	2.75275100
H	1.26326900	-2.61981500	4.13534100
C	-2.58963200	-0.70375600	-0.62619800
C	2.67769600	-0.59559100	-0.66863100
H	3.30127600	-1.38111300	-0.20820900
C	2.95657600	-0.57510800	-2.18212500
H	2.31092200	0.14931000	-2.68295700
H	4.00590700	-0.32524400	-2.36819000
H	2.76770800	-1.56535000	-2.61501400
O	2.99249600	0.66638900	-0.01506900
O	-2.94516600	0.54515100	0.03185600
Si	4.33579600	1.74192500	0.13631800
Si	-4.35638100	1.53170300	0.18881400
C	-4.56810700	2.72948900	-1.31092800
H	-5.01153400	3.63761700	-0.86308700
C	-3.97682400	2.55951600	1.76591400
H	-4.82503700	3.25399900	1.89643600
C	-5.89877100	0.43569400	0.56249000
H	-5.62927500	-0.10356600	1.48656800
C	3.89823900	2.78646300	1.69562400
H	4.87027600	3.10928200	2.11095700
C	4.51101800	2.91290500	-1.38811800
H	4.94190600	3.83496100	-0.95610800
C	5.99094200	0.79124900	0.45267100
H	6.77341100	1.55721000	0.29915900
C	-7.14054900	1.31153000	0.89443900
H	-6.94440000	2.01510400	1.71416200
H	-7.46907600	1.89587000	0.02426700
H	-7.98574400	0.67740200	1.19890100
C	-6.26783000	-0.64601700	-0.48681700
H	-6.55538000	-0.20661800	-1.44893700
H	-5.44160400	-1.34365500	-0.67000400
H	-7.12299700	-1.23938900	-0.13004700
C	-3.88960900	1.67497800	3.03762400
H	-4.82317500	1.13328000	3.23925300
H	-3.08396000	0.93571100	2.93740900
H	-3.66927500	2.29267700	3.92056300
C	-2.68700800	3.41333400	1.63460600
H	-1.82527300	2.78267300	1.38117300
H	-2.77958100	4.18581700	0.86138500
H	-2.46896000	3.92332100	2.58469300
C	-3.20708400	3.14206100	-1.94005900
H	-2.69762100	2.28424300	-2.39189900
H	-3.37087000	3.89184300	-2.72824000
H	-2.51553100	3.56965200	-1.20691200
C	-5.53508400	2.26416300	-2.43202600
H	-5.63254000	3.05262500	-3.19263400
H	-5.15904300	1.36833800	-2.94323400
H	-6.54122800	2.04284900	-2.05547200
C	3.07390900	4.07081200	1.41129600
H	3.56671700	4.73958100	0.69491700
H	2.08078100	3.82178200	1.01557300

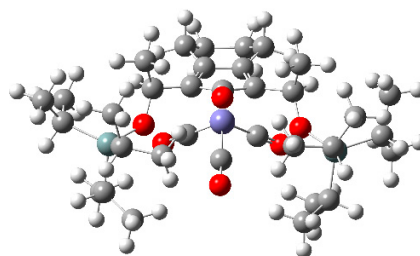
H	2.92601500	4.63591900	2.34341100
C	3.16606500	1.95398700	2.78235600
H	2.20172700	1.60497500	2.39439800
H	3.73741100	1.07414100	3.10061300
H	2.97569300	2.57225400	3.67235600
C	6.14898400	0.26745500	1.90576800
H	5.38735000	-0.48874900	2.14241700
H	7.13309800	-0.20744300	2.03251100
H	6.06918900	1.06882700	2.64981700
C	6.28427100	-0.36989600	-0.53709100
H	5.56351800	-1.18824700	-0.41083100
H	6.25579800	-0.05401300	-1.58514300
H	7.28377700	-0.78673000	-0.34436100
C	3.14048400	3.29127700	-2.01561000
H	2.63792600	2.41460800	-2.43866000
H	2.45274700	3.73093400	-1.28587700
H	3.28462200	4.02140400	-2.82582200
C	5.48898200	2.45381600	-2.50159100
H	6.49123600	2.22973600	-2.11445300
H	5.11699100	1.56310400	-3.02448200
H	5.59606700	3.24772200	-3.25521300
Fe	0.08521100	-2.70428900	-0.52821700
C	1.42085000	-3.83751000	-0.20885600
C	-1.20631900	-3.88651800	-0.20464800
C	0.08059300	-2.81071300	-2.31325600
O	2.32684300	-4.56450100	-0.01709600
O	0.07881800	-2.92742500	-3.48193700
O	-2.08437400	-4.64692300	-0.01260200
C	-2.89106200	-0.69380000	-2.13620500
H	-3.94954200	-0.47270900	-2.30890500
H	-2.27322500	0.04773000	-2.64688900
H	-2.68159200	-1.67911200	-2.57108300
H	-3.17487700	-1.51366100	-0.15633100



14g: E_{Gibbs} = -1912.96587538 eH

C	0.03584200	0.23887700	-1.34785000
C	-1.16182800	1.10019400	-1.04681900
C	-0.72223600	2.47706100	-1.09096200
C	0.71731700	2.49847900	-1.06307300
C	1.19440000	1.13464300	-1.00038500
O	0.06208600	-0.96131900	-1.71926700
C	-1.48289500	3.75520100	-1.32100200
H	-1.48813900	3.93220700	-2.40964400
H	-2.53370500	3.66656700	-1.02111500
C	1.44293400	3.80405000	-1.24897400
H	2.48638300	3.74575500	-0.91763300
H	1.47296600	4.00977000	-2.33224300
C	-0.83736100	4.97990300	-0.60635600
C	0.72868300	4.97772800	-0.52094800
H	-1.23758900	5.02835700	0.41381100
H	-1.18135300	5.88964900	-1.11468800
H	1.01933300	4.94184100	0.53581800
H	1.12322700	5.92180000	-0.91761700
C	-2.59822700	0.64373200	-1.20299600
H	-3.25985100	1.51031500	-1.03354800
C	2.65072400	0.72798800	-1.08211200
C	-2.81179200	0.13671900	-2.65019400
H	-2.15587300	-0.71444500	-2.84793700
H	-3.85258900	-0.15707200	-2.80830100
H	-2.57464100	0.93460200	-3.36741000
O	2.94818400	-0.25946200	-0.06358100
O	-2.90330100	-0.35144400	-0.19683300
Si	4.24168400	-1.39633600	0.17963600
Si	-4.23030700	-1.41402600	0.13997100
C	-5.96447600	-0.58243500	-0.10658600
H	-6.65722200	-1.44451600	-0.07590900
C	-4.04718800	-1.84711600	2.00811700
H	-5.07016300	-2.11834100	2.32862200
C	-4.10626900	-3.03523600	-0.89797200
H	-4.57655100	-3.79557900	-0.24758300
C	4.34927700	-1.64506800	2.08701800
H	5.31413500	-2.16852900	2.22511200
C	5.97477600	-0.61416200	-0.26143300
H	6.57168300	-0.85685600	0.63525900
C	3.78714200	-3.07572600	-0.65826100
H	4.34487800	-3.83039400	-0.07310600
C	-4.88853500	-3.06680300	-2.23833600
H	-5.95188900	-2.82411900	-2.11263000
H	-4.46260500	-2.37138000	-2.97335000
H	-4.83104900	-4.07342500	-2.67822100
C	-2.63389800	-3.47225800	-1.13746200
H	-2.07442500	-2.72180400	-1.70607400
H	-2.08669800	-3.62594900	-0.20135600
H	-2.60885700	-4.41765600	-1.70006200
C	-3.13853700	-3.06803900	2.31614500
H	-3.45694700	-3.97481100	1.78707600
H	-2.09511600	-2.86340000	2.04755600
H	-3.16401200	-3.28814000	3.39379600
C	-3.58476700	-0.64353500	2.87224800
H	-2.57472200	-0.33869700	2.58227500
H	-4.23439900	0.23224900	2.77255600
H	-3.56055100	-0.92688100	3.93506300
C	-6.38079900	0.37069900	1.04721400
H	-5.71097900	1.23926600	1.11390000
H	-7.39777100	0.75226800	0.87159600
H	-6.38005600	-0.12840500	2.02290500
C	-6.20546500	0.14079300	-1.45986000
H	-7.25189300	0.47419800	-1.52419500
H	-5.57622600	1.03655600	-1.54983200
H	-6.01134900	-0.50048400	-2.32610100
C	4.44556200	-0.29184800	2.84174600
H	5.29755100	0.31537400	2.50949800
H	3.53530100	0.30146500	2.69528500

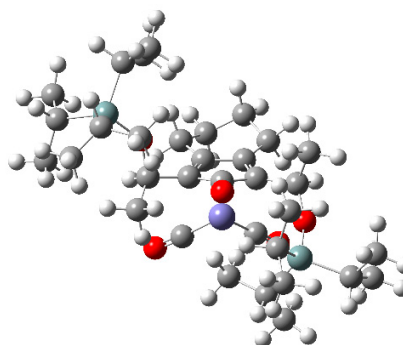
H	4.56500100	-0.46417000	3.92151700
C	3.25968600	-2.53429100	2.73789100
H	2.25708800	-2.11400000	2.59899500
H	3.25938600	-3.55229100	2.32893100
H	3.44037900	-2.61421000	3.82057100
C	2.26629500	-3.37872300	-0.49765000
H	1.65643800	-2.66103800	-1.05698800
H	2.05057600	-4.38597000	-0.88516900
H	1.93064600	-3.34385800	0.54320600
C	4.16916900	-3.28310000	-2.14872400
H	3.68395700	-2.54164300	-2.79496400
H	5.24779500	-3.23836200	-2.32725700
H	3.82077300	-4.27282200	-2.47884800
C	5.95012300	0.93799100	-0.36037300
H	5.50943700	1.26743300	-1.31031000
H	5.38358600	1.40325200	0.45510800
H	6.97610000	1.33329600	-0.32646000
C	6.75773500	-1.19149300	-1.46827000
H	6.94774200	-2.26660500	-1.36238200
H	6.22713400	-1.03635500	-2.41671600
H	7.73450300	-0.69121400	-1.55282200
Fe	-0.02211800	1.59226200	0.71794600
C	1.26249700	2.30684000	1.72137700
C	-1.36526700	2.28606000	1.65889600
C	0.00196400	-0.05633300	1.42986000
O	2.13266300	2.76390700	2.36828000
O	0.02203500	-1.11806000	1.92225700
O	-2.27289900	2.74259400	2.25239700
H	3.26382300	1.61786000	-0.87104000
C	2.97543300	0.23796100	-2.51375800
H	4.03441100	-0.03219900	-2.59998900
H	2.35705700	-0.62845600	-2.76219300
H	2.77148900	1.03400500	-3.24279500



16a: $E_{\text{Gibbs}} = -1799.6331598 \text{ eH}$

C	-0.20975000	-0.18343500	-0.38708600
C	-1.09356300	0.81033300	-1.07917300
C	-0.34832300	2.02378400	-1.25475700
C	0.84261000	1.94196800	-0.43285800
C	0.86956600	0.64511500	0.21021000
O	-0.44433800	-1.41872800	-0.22692600
C	-0.63424300	3.19252800	-2.17743300
H	-0.96078500	2.80523900	-3.15248200
H	-1.46555000	3.80113700	-1.79934400
C	1.90695400	3.00913200	-0.44857300
H	2.32696900	3.17095300	0.55212000
H	2.73487500	2.64450200	-1.07575400
C	0.62217200	4.08453500	-2.36655800
C	1.36265500	4.33441300	-1.03254000
H	0.32226300	5.03793100	-2.82032500
H	1.31469900	3.59773300	-3.06961300
H	0.67701000	4.80528100	-0.31288000
H	2.19494400	5.03243300	-1.19087100
C	-2.39535300	0.46837600	-1.77490500
H	-2.84815900	1.40903600	-2.12314600
C	2.05206100	0.11449900	0.99179800
H	2.54109200	0.96062800	1.50314200
C	-2.14384900	-0.42205600	-3.01232100
H	-1.61661000	-1.33703200	-2.73331100
H	-3.10079100	-0.68452900	-3.47843900
H	-1.53464100	0.11887600	-3.74954800
C	1.66910200	-0.93679400	2.04884100
H	1.15592100	-1.77977700	1.58120700
H	2.55982500	-1.29254500	2.57692300
H	0.99604800	-0.48940300	2.79191700
O	2.98155300	-0.39324300	-0.00838800
O	-3.37749500	-0.09694200	-0.89367400
Si	4.49091400	-1.21406600	-0.12311000
Si	-4.01384700	-1.27827800	0.15865400
C	-5.87675700	-1.32995700	-0.32222400
H	-6.41475400	-1.77658000	0.53242100
C	-3.75548100	-0.63282600	1.96617100
H	-3.93371200	-1.51325800	2.60832300
C	-3.21325900	-3.03107000	0.15034200
H	-2.26508900	-2.91373900	0.69477400
C	5.03299200	-0.88240700	-1.94229500
H	6.13561500	-0.95546900	-1.93803400
C	4.31324800	-3.11535100	0.16238100
H	5.12139200	-3.54879300	-0.45565200
C	5.81592100	-0.47989700	1.07892900
H	6.61562000	-1.24284400	1.09956900
C	-4.10462800	-4.02138500	0.95711500
H	-4.33112800	-3.66248000	1.97097300
H	-5.05983800	-4.21598300	0.45176600
H	-3.58883600	-4.98676000	1.06207200
C	-2.84114400	-3.63653200	-1.22548800
H	-3.69186700	-3.67664800	-1.91714300
H	-2.03606800	-3.06200900	-1.69059000
H	-2.47468700	-4.66576900	-1.09295800
C	-2.28900400	-0.20558800	2.22604900
H	-1.55875800	-0.96376400	1.93398600
H	-2.11458200	0.71548900	1.60794300
H	-2.13224100	0.07734500	3.27528100
C	-4.72363200	0.48255300	2.43171000
H	-4.63981200	1.37528000	1.79796300
H	-5.76873600	0.15171400	2.40650100
H	-4.49695400	0.78472100	3.46566400
C	-6.46604800	0.08290800	-0.58410800
H	-5.92255500	0.57472200	-1.40034000
H	-7.52392200	0.00424900	-0.87651200
H	-6.40960200	0.73826900	0.29109300
C	-6.15255700	-2.21829100	-1.56756800
H	-7.22396400	-2.19846300	-1.81597100

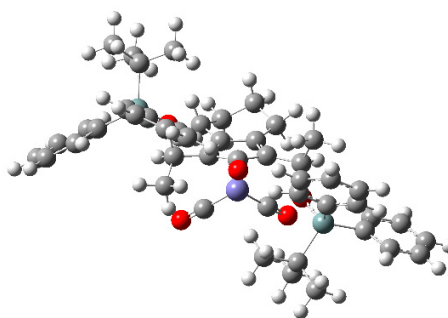
H	-5.60553300	-1.84424100	-2.44451700
H	-5.86703000	-3.26496900	-1.41271900
C	4.51070300	-1.91587600	-2.97583500
H	4.80624200	-2.94385400	-2.73173600
H	3.41542200	-1.88431800	-3.04433800
H	4.91133400	-1.68465300	-3.97402000
C	4.64925100	0.54376500	-2.42179300
H	3.55850100	0.65884900	-2.41394800
H	5.07388000	1.33047200	-1.78743800
H	5.00642100	0.71015400	-3.44918500
C	6.45995400	0.84196400	0.58144700
H	5.71773500	1.65071200	0.52701700
H	7.24734300	1.16601000	1.27814000
H	6.91724700	0.73757300	-0.40978900
C	5.32572900	-0.28376900	2.54004900
H	4.54676300	0.48846000	2.59276400
H	4.92145400	-1.20217000	2.97899300
H	6.15731300	0.05028600	3.17777700
C	2.96715900	-3.68111500	-0.36880400
H	2.11331900	-3.25286200	0.16731800
H	2.81417300	-3.46839100	-1.43180100
H	2.93763300	-4.77298700	-0.23658500
C	4.55393500	-3.61434100	1.61226900
H	5.52593600	-3.29742600	2.01230300
H	3.77114100	-3.26035600	2.29613900
H	4.53063100	-4.71378100	1.63770800
Fe	-0.83991500	1.79220600	0.82386500
C	-0.05996400	2.48370700	2.25879100
C	-2.12165800	3.02190200	0.75096400
O	0.51225400	2.94752800	3.18089400
O	-2.93103600	3.87495000	0.65842200



16b: E_{Gibbs} = -2330.63441584 eH

C	-0.03868800	-0.28865000	0.37060300
C	-1.07896300	-1.10700000	1.07435900
C	-0.48494100	-2.33910700	1.48335400
C	0.81610800	-2.44614500	0.84454000
C	1.05197800	-1.25307600	0.07003800
O	-0.15903300	0.90816000	-0.03499200
C	-1.01210700	-3.37864700	2.45178900
H	-1.45716100	-2.87070400	3.31816600
H	-1.81914500	-3.96486300	1.99330600
C	1.75860600	-3.58658500	1.12792700
H	2.29671900	-3.89304300	0.22237200
H	2.52207500	-3.21883100	1.83228000
C	0.11619200	-4.33246200	2.92700900
C	1.01569700	-4.78984300	1.75577700
H	-0.33246600	-5.20195900	3.42429500
H	0.73933600	-3.81998300	3.67515300
H	0.40002800	-5.28650100	0.99140900
H	1.74845700	-5.52639700	2.10976200
C	-2.46326900	-0.60319800	1.39965200
H	-3.05251800	-1.43264600	1.82295400
C	2.35974100	-0.90986000	-0.60402100
H	2.87261500	-1.84583600	-0.87864300
C	-2.43145600	0.54251300	2.43043500
H	-1.83212900	1.37898600	2.06508100
H	-3.44386500	0.90082300	2.65015900
H	-1.98902200	0.17585200	3.36663400
C	2.21131500	-0.05455600	-1.87620400
H	1.67854900	0.87498600	-1.66691000
H	3.19617100	0.17180600	-2.29961900
H	1.64563700	-0.61315500	-2.63344900
O	3.16450300	-0.26528500	0.43792900
O	-3.07144500	-0.25306900	0.12361400
Si	4.62106400	0.64869600	0.43036300
Si	-4.24837400	0.84864500	-0.47336600
C	-4.00554500	0.75247200	-2.38517600
C	5.35087700	0.31076200	2.18344300
C	-2.62283700	1.32730700	-2.79879900
H	-2.56080300	2.40769700	-2.62008900
H	-1.80062100	0.84960200	-2.25215900
H	-2.46493300	1.15921200	-3.87567700
C	-4.08424100	-0.73022500	-2.84018800
H	-3.26207500	-1.31573000	-2.40989200
H	-5.02935700	-1.20594600	-2.54665000
H	-4.00357200	-0.78763600	-3.93682600
C	4.32376300	0.79684700	3.24459900
H	4.13006400	1.87388700	3.16001800
H	3.36602500	0.27221100	3.13808700
H	4.71280400	0.60303600	4.25624600
C	5.60183200	-1.20738200	2.39148400
H	4.68840800	-1.78983400	2.21203700
H	6.39290500	-1.58554400	1.73133500
H	5.92166800	-1.39084000	3.42879800
Fe	-0.66268100	-2.28333000	-0.66587200
C	0.18230900	-3.19898200	-1.92858900
C	-2.13700500	-3.28292200	-0.71114400
O	0.79079600	-3.82786900	-2.72057100
O	-3.07807800	-3.99082900	-0.65905600
C	-5.12328200	1.56520500	-3.09686100
H	-5.14209200	2.61340900	-2.76689800
H	-4.94516900	1.56425800	-4.18272500
H	-6.11632300	1.13005600	-2.92570800
C	6.68995000	1.07410400	2.37606200
H	6.54878100	2.16137700	2.32713200
H	7.10966500	0.84183000	3.36655600
H	7.43841600	0.78827800	1.62360900
C	5.74286300	0.02635900	-0.97544100
C	6.32729000	0.89703700	-1.92832800
C	5.99193200	-1.36424400	-1.11920100

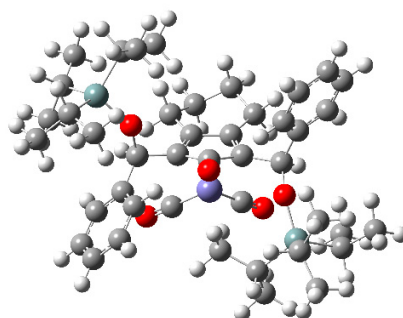
C	7.14011300	0.40562700	-2.96839200
H	6.13444400	1.96523700	-1.87680500
C	6.79934700	-1.86194600	-2.15792200
H	5.54591800	-2.07031600	-0.42180500
C	7.38172200	-0.97585800	-3.08487900
H	7.57518000	1.09728000	-3.68655800
H	6.97049100	-2.93265100	-2.24575200
H	8.00664800	-1.35711500	-3.88947600
C	4.19423300	2.48509600	0.23259800
C	2.83816800	2.89873500	0.24017400
C	5.19238200	3.48922400	0.13631700
C	2.49542100	4.26116500	0.14535900
H	2.04495900	2.16024500	0.32292500
C	4.85252500	4.85195300	0.04301900
H	6.24698900	3.21855700	0.14105600
C	3.49953500	5.24236500	0.04495900
H	1.44670900	4.55032100	0.15012000
H	5.63769600	5.60154200	-0.02965300
H	3.23331900	6.29476000	-0.02841000
C	-3.96902300	2.60753000	0.18970700
C	-5.01110100	3.38165100	0.75687300
C	-2.67541900	3.19044300	0.11584500
C	-4.78284200	4.69457300	1.21405900
H	-6.00651600	2.96036800	0.86688800
C	-2.44525700	4.50063200	0.57263800
H	-1.83702200	2.60992600	-0.26018300
C	-3.49857000	5.26103800	1.11741900
H	-5.60102600	5.26625500	1.64708000
H	-1.44428500	4.92252000	0.51063800
H	-3.31858300	6.27450100	1.47003000
C	-5.95351900	0.16541900	0.01724100
C	-7.16932300	0.84811700	-0.24541900
C	-6.04076600	-1.11120400	0.62768100
C	-8.41376300	0.28859500	0.10020900
H	-7.15766100	1.82029700	-0.73411100
C	-7.28168600	-1.67658400	0.97682700
H	-5.13095200	-1.67601800	0.81575800
C	-8.47420800	-0.97542600	0.71766900
H	-9.32960300	0.83520400	-0.11408900
H	-7.31715200	-2.65971300	1.44127900
H	-9.43506600	-1.40930300	0.98563800



16c: $E_{\text{Gibbs}} = -2183.03729803 \text{ eH}$

C	0.08450300	0.26468900	0.32583800
C	1.14571500	0.86173000	-0.56385900
C	0.51071800	1.31058200	-1.76732800
C	-0.80685600	0.70948600	-1.82952200
C	-1.01964200	-0.06702100	-0.62326600
O	0.17672700	-0.00106700	1.55409600
C	1.01925800	2.30233000	-2.79440900
H	1.46628300	3.15321000	-2.26344300
H	1.81998800	1.86454800	-3.40439500
C	-1.78305600	1.04368400	-2.93018400
H	-2.36709800	0.16544900	-3.23226900
H	-2.50278200	1.77569200	-2.52991700
C	-0.12306800	2.80530600	-3.71631000
C	-1.06342400	1.65946300	-4.15346900
H	0.31266100	3.29711100	-4.59551400
H	-0.71450700	3.56496900	-3.18378300
H	-0.48416100	0.88330600	-4.67438300
H	-1.81113700	2.03639000	-4.86336800
C	2.55361700	1.24235000	-0.13221500
H	3.16943600	1.32791000	-1.04194800
C	-2.36560700	-0.68680000	-0.27779000
H	-2.91518000	-0.78895800	-1.22530800
O	-3.05689000	0.28558500	0.55615300
O	3.10016800	0.24202400	0.73964700
Si	-4.67289000	0.78539600	0.90448700
Si	4.17915900	-1.07640500	0.87790600
C	5.83524700	-0.70898000	-0.02987400
H	6.42357100	-1.64132200	0.03045800
C	3.34372900	-2.72779600	0.28649000
H	3.49989800	-3.40315400	1.14691000
C	4.37332600	-1.28110600	2.77322000
H	3.42001800	-1.73883800	3.09035400
C	-4.49416200	2.67128800	1.25321300
H	-5.49207100	3.10519700	1.06198800
C	-5.35907000	-0.13321300	2.45172500
H	-6.12783400	0.55032700	2.85779600
C	-5.90587000	0.52768200	-0.56835900
H	-6.89123100	0.55736300	-0.06719700
C	5.51062800	-2.27372200	3.13964100
H	5.39939900	-3.24684000	2.63926200
H	6.49695500	-1.87086500	2.87089900
H	5.52003300	-2.46281900	4.22250200
C	4.50818500	0.04722500	3.55802300
H	5.47583000	0.53345700	3.37886700
H	3.72051700	0.75105200	3.27012700
H	4.42876400	-0.13830200	4.63962800
C	1.80866000	-2.59897300	0.13746300
H	1.33150600	-2.07812800	0.97050000
H	1.61032200	-2.01226800	-0.79977200
H	1.33035900	-3.57582100	-0.00966300
C	3.95707600	-3.43707400	-0.94739400
H	3.76768600	-2.87854700	-1.87254100
H	5.04298800	-3.56594600	-0.85394500
H	3.51390900	-4.43610900	-1.07405300
C	5.67255500	-0.35893600	-1.53507600
H	5.15062200	0.59907000	-1.66191700
H	6.66041600	-0.25075600	-2.00617300
H	5.12142000	-1.11968600	-2.09794300
C	6.65498500	0.40941800	0.67030200
H	6.94169100	0.13586800	1.69228900
H	7.57869300	0.61217400	0.10829800
H	6.08483500	1.34689300	0.72341100
C	-4.11439700	3.02947900	2.71495800
H	-4.83691600	2.64109100	3.44364900
H	-3.12318300	2.63421000	2.97145500
H	-4.07676500	4.12234800	2.83539700
C	-3.48153300	3.34686700	0.28861000
H	-2.48773500	2.90034500	0.41359000

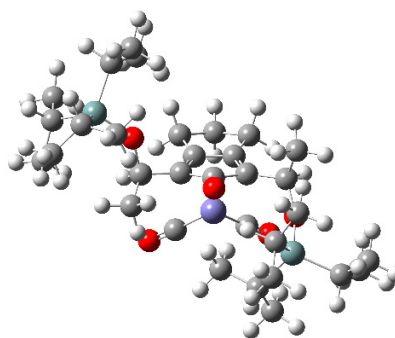
H	-3.76966600	3.24207000	-0.76461500
H	-3.40485500	4.42225000	0.50770700
C	-5.91110100	1.66063500	-1.62880100
H	-4.95907300	1.69927400	-2.17625500
H	-6.70592100	1.48346300	-2.36884500
H	-6.08462900	2.64892800	-1.18653000
C	-5.80786600	-0.84315100	-1.29488700
H	-4.93392200	-0.86884700	-1.95956100
H	-5.72992600	-1.69104000	-0.60698600
H	-6.69468900	-1.00230500	-1.92598000
C	-4.28922700	-0.35454600	3.55506900
H	-3.50782500	-1.03188500	3.19715000
H	-3.80230300	0.57425500	3.86843300
H	-4.75149400	-0.81035400	4.44334300
C	-6.06204600	-1.48453200	2.14936100
H	-6.89808700	-1.37841300	1.44616300
H	-5.35467800	-2.21487900	1.73431200
H	-6.46596200	-1.91281600	3.07854500
Fe	0.61107000	-0.83363500	-1.78557900
C	-0.35858200	-2.01835800	-2.68401500
C	1.91637400	-0.83613000	-2.98243400
O	-1.03794600	-2.75327400	-3.30801100
O	2.74259600	-0.77763900	-3.82588600
C	2.58460500	2.59734400	0.58183200
C	3.28268300	3.68260100	0.01551100
C	1.92377100	2.76793400	1.81915400
C	3.31855900	4.93107300	0.66773300
H	3.81200300	3.55336900	-0.92816600
C	1.96224500	4.01190900	2.47043100
H	1.39630700	1.92420100	2.25618600
C	2.65571000	5.09869800	1.89728800
H	3.86361700	5.76101000	0.22352100
H	1.45250200	4.13654200	3.42313300
H	2.68247200	6.05997000	2.40566600
C	-2.33226800	-2.08039700	0.35448600
C	-2.89373100	-3.16476200	-0.35418900
C	-1.78131000	-2.31644600	1.63416000
C	-2.90224500	-4.46213300	0.19254000
H	-3.32429800	-3.00232300	-1.34083100
C	-1.79222400	-3.61099600	2.18239400
H	-1.33270900	-1.48982800	2.17413100
C	-2.35096300	-4.68962400	1.46700200
H	-3.33730500	-5.28427600	-0.37115200
H	-1.36516100	-3.77794400	3.16902500
H	-2.35782000	-5.68890200	1.89691100



16d: E_{Gibbs} = 1760.31677074 eH

C	0.20717700	-0.25366900	0.46363800
C	1.10104300	0.69866800	1.22033700
C	0.33713300	1.87964000	1.46921700
C	-0.86668700	1.83425200	0.67684200
C	-0.90587100	0.59989700	-0.05780300
O	0.45498600	-1.46730100	0.20284400
C	0.34284900	3.09898300	2.36108500
H	0.07090500	2.78992500	3.38204500
H	1.30401200	3.61962400	2.42380100
C	-1.75986700	3.00802200	0.99351700
H	-2.23364800	3.47007100	0.12090600
H	-2.56427600	2.66902800	1.66222600
C	-0.78801500	3.98935700	1.73607300
H	-0.34473100	4.68157800	1.01012900
H	-1.30582500	4.58541900	2.49481100
C	2.41671100	0.32402800	1.87322500
H	2.81555500	1.22672500	2.36073500
C	-2.08586500	0.12981800	-0.88049900
H	-2.55117400	1.01668100	-1.34135100
C	2.19412700	-0.74505700	2.96615400
H	1.69567200	-1.62641000	2.55434500
H	3.15752300	-1.03520300	3.40160600
H	1.56344800	-0.33304700	3.76562400
C	-1.71096400	-0.86319800	-1.99479700
H	-1.23754400	-1.75076700	-1.56885700
H	-2.60134500	-1.15532500	-2.56298700
H	-1.00533100	-0.39534900	-2.69366800
O	-3.03506300	-0.43550400	0.06993000
O	3.43486000	-0.05126400	0.92711800
Si	-4.66202200	-1.00389300	0.08603300
Si	4.12090800	-1.12802200	-0.21124000
C	6.02018700	-0.99673600	0.09092800
H	6.49618800	-1.18030400	-0.88867000
C	3.72321000	-0.43033000	-1.97553100
H	3.93335000	-1.26476200	-2.66637700
C	3.42618200	-2.92333300	-0.15341900
H	2.35092600	-2.80865900	-0.35362100
C	-5.16482700	-0.84126300	1.93960700
H	-6.26541700	-0.74330500	1.94157800
C	-4.77210200	-2.85245000	-0.45777800
H	-5.62910300	-3.24661400	0.11879400
C	-5.84167200	0.07705000	-1.00019400
H	-6.74721500	-0.54861300	-1.10626800
C	4.03979800	-3.79752300	-1.28611800
H	3.83499300	-3.39864700	-2.28800500
H	5.12978900	-3.89947100	-1.18056600
H	3.61403800	-4.81068300	-1.24781000
C	3.54524800	-3.68343500	1.19515100
H	4.57953100	-3.97714700	1.40931400
H	3.18154500	-3.09480200	2.04179700
H	2.94471400	-4.60406800	1.15301400
C	2.22797900	-0.08015400	-2.16331600
H	1.54950000	-0.88237700	-1.86430000
H	2.03422000	0.81251600	-1.51040300
H	2.01186700	0.22765500	-3.19495700
C	4.60235800	0.76459900	-2.42520200
H	4.46521700	1.63301400	-1.76781300
H	5.66930200	0.51234400	-2.42555800
H	4.33522400	1.07560200	-3.44673400
C	6.43077200	0.42593500	0.56170900
H	5.95407100	0.66211000	1.52066200
H	7.52149300	0.48141500	0.69569100
H	6.13793900	1.20727600	-0.14782800
C	6.59418300	-2.04455000	1.08127200
H	7.67316300	-1.88012200	1.21893800
H	6.12097000	-1.96369300	2.06945200
H	6.45814900	-3.07246900	0.72499700
C	-4.81186400	-2.07411900	2.81409800

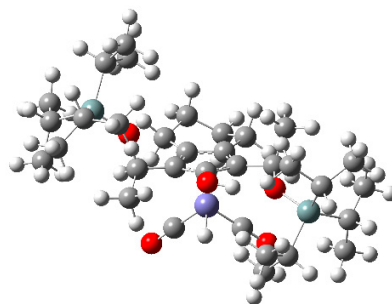
H	-5.24991500	-3.00356300	2.42940100
H	-3.72460600	-2.21236800	2.87764200
H	-5.18724100	-1.93000800	3.83802600
C	-4.56717300	0.43189500	2.59681200
H	-3.47172300	0.38139100	2.57781800
H	-4.86982500	1.35128400	2.08179000
H	-4.89239600	0.51048200	3.64499400
C	-6.28685100	1.40738500	-0.33471200
H	-5.43361000	2.08336700	-0.18331200
H	-7.00798500	1.93036400	-0.98026800
H	-6.76773200	1.24865500	0.63806800
C	-5.32415100	0.37875700	-2.43468100
H	-4.47338900	1.07200100	-2.40890500
H	-5.00882000	-0.52131600	-2.97286100
H	-6.11473900	0.86041200	-3.02867500
C	-3.51765700	-3.67203600	-0.04752800
H	-2.62667800	-3.32128800	-0.58020100
H	-3.29985700	-3.59973900	1.02303200
H	-3.66198500	-4.73478100	-0.29283600
C	-5.09328800	-3.10674800	-1.95430100
H	-6.01100200	-2.60063200	-2.28072200
H	-4.27190900	-2.77634800	-2.60424500
H	-5.23002100	-4.18390800	-2.13021400
Fe	0.80088300	1.81721900	-0.60191300
C	-0.00233000	2.63615900	-1.95484600
C	2.07941600	3.03897300	-0.42671300
O	-0.59126900	3.18410400	-2.81846100
O	2.88689200	3.88159700	-0.25817700



17a: E_{Gibbs} = -1800.85849767 eH

C	0.16120300	-0.05189000	-0.09152600
C	1.04797900	0.75080100	0.70854100
C	0.28862900	1.91338500	1.16683900
C	-1.00608300	1.84887900	0.57302400
C	-1.07272100	0.66241400	-0.28219200
O	0.48413800	-1.28635500	-0.59486000
C	0.69003000	2.97926300	2.15818400
H	0.65243200	2.55516900	3.17525100
H	1.72337700	3.31354800	1.99505800
C	-2.11136800	2.83763800	0.87768900
H	-2.30876900	3.48853700	0.01568200
H	-3.03899900	2.28535800	1.07426400
C	-0.28114300	4.18315800	2.08449800
C	-1.75261800	3.70634600	2.11253600
H	-0.09476200	4.74843200	1.15982100
H	-0.08917800	4.86151700	2.92650100
H	-2.42870400	4.57026700	2.15888200
H	-1.91660800	3.12007400	3.02968700
C	2.39275200	0.27739500	1.21697400
H	3.10447000	1.11304000	1.23023000
C	-2.32480000	0.18216900	-0.97876100
H	-2.91074600	1.06948700	-1.26719600
C	2.26663800	-0.31350900	2.63728100
H	1.56270800	-1.15333800	2.63512900
H	3.23867300	-0.66656400	2.99966300
H	1.89611100	0.44598600	3.33650800
C	-2.05944100	-0.66011700	-2.23777100
H	-1.48607100	-1.55584800	-1.98815600
H	-3.00624200	-0.94766000	-2.70861400
H	-1.47874700	-0.07756000	-2.96265700
O	-3.08566300	-0.55106600	0.02922900
O	2.88666900	-0.75050400	0.29077600
Si	-4.64009400	-1.27267200	0.19650600
Si	4.48595800	-1.33556000	-0.10304500
C	5.89878800	-0.11684600	0.38975000
H	6.79391100	-0.76352700	0.31584400
C	4.45935900	-1.57269400	-2.01134800
H	5.52378800	-1.57806000	-2.30958600
C	4.71717400	-3.04457000	0.76136800
H	5.35293900	-3.61865300	0.06378300
C	-4.93935000	-1.25685700	2.10112200
H	-6.03727100	-1.24374200	2.22668100
C	-4.64330400	-3.09404100	-0.44157100
H	-5.38807000	-3.59926600	0.20033700
C	-6.03779100	-0.25440300	-0.66819900
H	-6.90148800	-0.94491700	-0.67658400
C	5.45605300	-3.02992900	2.12557500
H	6.44454200	-2.55698800	2.06561600
H	4.87326800	-2.50451100	2.89459300
H	5.60463400	-4.05981800	2.48123100
C	3.37560400	-3.81431400	0.90943500
H	2.69701600	-3.28858500	1.59246900
H	2.85170500	-3.93913700	-0.04497100
H	3.55718800	-4.81675400	1.32302800
C	3.84827200	-2.91931800	-2.48812800
H	4.33466900	-3.79185700	-2.03446200
H	2.77409700	-2.97202800	-2.26429500
H	3.95496100	-3.01033100	-3.57850000
C	3.75997300	-0.40497400	-2.75948600
H	2.69761700	-0.34881600	-2.49631700
H	4.20228900	0.57141500	-2.53568200
H	3.82806700	-0.56196900	-3.84582200
C	6.11701600	1.06059600	-0.59997400
H	5.25567400	1.74041800	-0.62827300
H	6.99048500	1.65175600	-0.28801900
H	6.30373200	0.71411300	-1.62310800
C	5.87177900	0.43569000	1.84292300
H	6.82864500	0.92734200	2.06996000

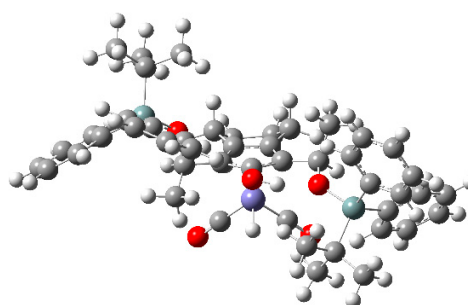
H	5.08872900	1.19382000	1.96743800
H	5.71356000	-0.34231400	2.59662200
C	-4.40885800	-2.50470300	2.85680700
H	-4.82200600	-3.44331300	2.46654900
H	-3.31422500	-2.56472800	2.79729400
H	-4.67840600	-2.44208200	3.92162300
C	-4.36456600	0.01962200	2.77300700
H	-3.27815200	0.06197100	2.63013200
H	-4.79136200	0.94092300	2.35931400
H	-4.57220300	0.00932900	3.85358300
C	-6.47699900	1.01052800	0.11791400
H	-5.66120100	1.74439300	0.18045000
H	-7.31906900	1.50096200	-0.39265900
H	-6.79942900	0.77735600	1.13974800
C	-5.75166500	0.14187200	-2.14340700
H	-4.93744100	0.87537700	-2.20450700
H	-5.48027100	-0.71448800	-2.76921800
H	-6.64219700	0.60952800	-2.58853100
C	-3.27899200	-3.80360800	-0.22004100
H	-2.49166000	-3.33865800	-0.82432200
H	-2.95030400	-3.76323900	0.82390400
H	-3.34974900	-4.86203100	-0.51204600
C	-5.10686800	-3.30830200	-1.90690700
H	-6.10246300	-2.88817800	-2.10030200
H	-4.40307100	-2.86098200	-2.62158200
H	-5.15441500	-4.38430500	-2.13082200
Fe	0.49829600	1.96370000	-0.97976700
C	-0.39550900	2.92340600	-2.13989200
C	2.00235300	2.84077200	-1.11991500
O	-1.00359100	3.54006900	-2.94556700
O	3.05466500	3.37625900	-1.21724600
H	0.98709300	1.21944100	-2.18811200
H	1.46022900	-1.41664000	-0.40177800



17b: $E_{\text{Gibbs}} = -2331.86011936 \text{ eH}$

C	0.03327300	-0.81405400	0.31021200
C	-1.12582100	-1.56217300	0.69826500
C	-0.67479800	-2.92979400	0.96767300
C	0.71984700	-3.01392100	0.67084700
C	1.16011000	-1.71039000	0.18791000
O	0.09291900	0.54216100	0.10684400
C	-1.45651300	-4.07739000	1.56186800
H	-1.61662900	-3.88454900	2.63564100
H	-2.45204700	-4.16353800	1.10814500
C	1.55786700	-4.24906300	0.93217200
H	1.84031500	-4.74386200	-0.00659500
H	2.49922300	-3.95958200	1.42314000
C	-0.68318300	-5.40911900	1.39922600
C	0.79244200	-5.25256000	1.83482800
H	-0.72197800	-5.72923600	0.34777300
H	-1.17046900	-6.19130900	1.99629900
H	1.30098200	-6.22531900	1.80990000
H	0.81906300	-4.90060500	2.87749200
C	-2.49670000	-1.02281000	1.04384800
H	-3.17296100	-1.88588900	1.15030100
C	2.59847800	-1.28710100	-0.05439600
H	3.19665800	-1.61098400	0.81188400
C	-2.45884200	-0.28142000	2.40074600
H	-1.78167600	0.57580000	2.35686100
H	-3.45832100	0.07505500	2.67758300
H	-2.11124700	-0.96592300	3.18574900
C	3.23776900	-1.85291400	-1.33005300
H	2.67536800	-1.52966300	-2.21083700
H	4.27743400	-1.51813200	-1.42329000
H	3.23456100	-2.94887600	-1.30395700
O	2.63854100	0.19516600	-0.07528200
O	-2.99550400	-0.21096400	-0.04301200
Si	4.02334000	1.20691500	0.23217700
Si	-4.07418100	1.10520400	-0.25176700
C	-3.95576800	1.47059200	-2.14032500
C	3.30384300	2.79248100	1.06567700
C	-2.47149200	1.68954400	-2.54374300
H	-2.05537800	2.59584500	-2.08461000
H	-1.84809900	0.83789700	-2.24871000
H	-2.40349400	1.80864100	-3.63652900
C	-4.52119500	0.25975600	-2.93270100
H	-3.97056100	-0.66053400	-2.70854300
H	-5.58166000	0.08406000	-2.70802000
H	-4.43452600	0.45224800	-4.01338800
C	2.40527100	3.54459900	0.04084700
H	2.95422800	3.80765000	-0.87148800
H	1.52411300	2.95861400	-0.25149200
H	2.04061400	4.47913800	0.49308400
C	2.45453400	2.46944300	2.32623300
H	1.64822500	1.75727100	2.11229000
H	3.06753100	2.07093400	3.14399100
H	1.98810100	3.39502900	2.69586700
Fe	-0.39045500	-2.47714000	-1.11799600
C	0.47938800	-3.45653200	-2.27510000
C	-1.96865700	-2.87435200	-1.76619100
O	1.06716200	-4.10541000	-3.07208000
O	-3.03191000	-3.11933000	-2.21786800
C	-4.77636400	2.74135400	-2.49610900
H	-4.42885400	3.62448000	-1.94281300
H	-4.67000000	2.95776500	-3.56996700
H	-5.84837500	2.60672000	-2.29655600
C	4.47905600	3.72653600	1.47500400
H	5.06375100	4.05376400	0.60538700
H	4.07830800	4.62945000	1.95873400
H	5.16070800	3.24290700	2.18774400
C	5.23037900	0.21503900	1.31190100
C	6.47927300	-0.22680600	0.80647600
C	4.89178000	-0.15925800	2.63923000

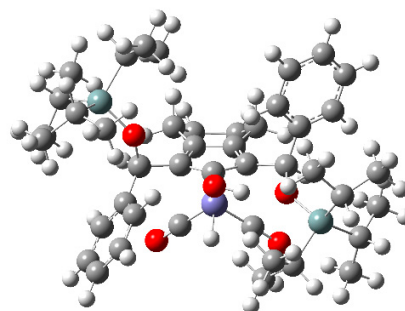
C	7.36101800	-0.98977400	1.59587900
H	6.76787500	0.01488800	-0.21314200
C	5.76825900	-0.92230500	3.43222100
H	3.93497700	0.13384400	3.06333200
C	7.01037300	-1.33640200	2.91379800
H	8.31338200	-1.31305900	1.18194700
H	5.48290900	-1.19218900	4.44646300
H	7.69073600	-1.92454100	3.52545800
C	4.80348600	1.65961700	-1.43214000
C	4.09320100	1.44482800	-2.63911400
C	6.06859100	2.29657200	-1.51321200
C	4.62624400	1.84205800	-3.87971100
H	3.11594200	0.96911200	-2.60955100
C	6.60590400	2.69585400	-2.75124900
H	6.64510300	2.48874600	-0.60980100
C	5.88577100	2.46809700	-3.93967800
H	4.06058700	1.66502200	-4.79146500
H	7.57843500	3.18162200	-2.78699800
H	6.29912200	2.77587100	-4.89747800
C	-3.51868500	2.59532500	0.79383000
C	-4.41436000	3.38787700	1.55241800
C	-2.14529200	2.95521200	0.80559600
C	-3.96572700	4.50886300	2.27873600
H	-5.46798100	3.12704800	1.60053300
C	-1.69385300	4.07399700	1.52939700
H	-1.42282700	2.33735900	0.27906000
C	-2.60319000	4.86016000	2.26360300
H	-4.67547600	5.09922700	2.85469800
H	-0.63549300	4.32664900	1.52342500
H	-2.25453500	5.72642200	2.82235000
C	-5.83164000	0.54310700	0.21133000
C	-6.94781900	1.41890700	0.18837600
C	-6.07690800	-0.81562900	0.53225400
C	-8.24540700	0.96292200	0.48788300
H	-6.81725100	2.46596300	-0.07801200
C	-7.37117700	-1.27875000	0.83500500
H	-5.25289100	-1.52426900	0.52551500
C	-8.46134500	-0.38865100	0.81782900
H	-9.08200100	1.65788200	0.45991800
H	-7.52831000	-2.32826700	1.07475800
H	-9.46328300	-0.74341600	1.04948100
H	-0.38584000	-1.42286400	-2.18683800
H	1.05932700	0.73724500	-0.08575800



17c: $E_{\text{Gibbs}} = -2184.24233969 \text{ eH}$

C	0.08708780	-0.16965711	-0.01636010
C	1.09437144	0.16137952	-0.99186011
C	0.42641396	0.27711822	-2.27949290
C	-0.94137324	-0.06508593	-2.09451589
C	-1.16224986	-0.41647806	-0.68896552
O	0.32913009	-0.21622664	1.33184269
C	0.90763321	0.77906342	-3.61239485
H	0.63602106	1.84399495	-3.69753726
H	2.00020552	0.73234792	-3.70154328
C	-1.90153905	0.08420123	-3.24240982
H	-2.83217744	-0.47394434	-3.08165402
H	-2.18433944	1.14768278	-3.30106838
C	0.25659167	-0.02094864	-4.77730666
C	-1.26695279	-0.35210747	-4.59832775
H	0.80648920	-0.96494956	-4.87713462
H	0.40970818	0.53343462	-5.71265166
H	-1.39593692	-1.43693502	-4.69830035
H	-1.84664339	0.10650022	-5.41042736
C	2.50224901	0.60802681	-0.65116547
H	3.20795963	0.20538712	-1.38698554
C	-2.52756846	-0.67702111	-0.08019017
H	-3.20104506	-0.90304833	-0.91986209
O	-2.94550684	0.57214332	0.54403947
O	2.83166363	0.05117359	0.67238792
Si	-4.40079704	1.48668865	0.71027417
Si	4.32166021	-0.40561776	1.47457684
C	5.73804608	-0.95646186	0.28205916
H	6.62389075	-0.86604269	0.93938038
C	3.81290897	-1.88979649	2.58853973
H	4.76680541	-2.40875199	2.79606922
C	4.92373572	1.06650229	2.56229820
H	5.47855010	0.57921542	3.38525097
C	-3.91364467	3.28551647	0.21181496
H	-4.85834358	3.77879236	-0.08004653
C	-4.97104336	1.43479947	2.54892080
H	-5.54506810	2.36917666	2.69028919
C	-5.84924120	0.88869544	-0.42624790
H	-6.73559181	1.33385662	0.06338481
C	5.90615447	2.04761027	1.86947533
H	6.79635972	1.54247047	1.47397110
H	5.41855823	2.58200384	1.04333354
H	6.24959379	2.80435138	2.58981389
C	3.75658502	1.87164955	3.19621629
H	3.18871766	2.40191394	2.42383151
H	3.05560640	1.23882831	3.75122444
H	4.15196999	2.62341697	3.89490595
C	3.20443277	-1.50518562	3.96483729
C	3.86182429	-0.84945365	4.54936340
H	2.23492285	-1.00201417	3.84931205
H	3.02775935	-2.41353415	4.55853636
C	2.87242582	-2.90181464	1.87730173
H	1.89016243	-2.46039317	1.67444114
H	3.27302151	-3.25717336	0.92250944
H	2.71345661	-3.77913379	2.52100174
C	5.67694532	-2.43740998	-0.18188008
H	4.81792810	-2.62152903	-0.83858673
H	6.58363312	-2.68398382	-0.75380537
H	5.61855135	-3.13811289	0.65913832
C	6.00667947	-0.05382617	-0.95416076
H	6.98943047	-0.29449357	-1.38443092
H	5.26360643	-0.24110974	-1.74032204
H	5.99790169	1.01521512	-0.71930557
C	-3.29221921	4.12946376	1.35621059
H	-3.94950391	4.19913212	2.23182545
H	-2.33463021	3.70293753	1.68343223
H	-3.09659865	5.15387242	1.00548366
C	-2.95981970	3.31153200	-1.01329174
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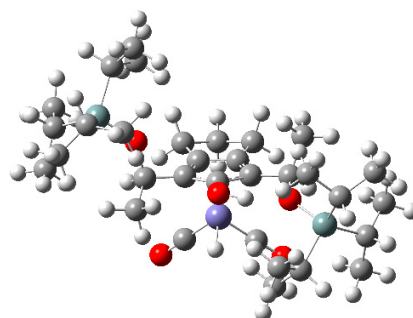
H	-3.40429231	2.84558097	-1.90071386
H	-2.70088961	4.34823941	-1.27546818
C	-5.81744219	1.43891567	-1.87732204
H	-4.95011231	1.05590185	-2.43248576
H	-6.71942201	1.12133752	-2.42120519
H	-5.78002174	2.53445934	-1.90924671
C	-6.08241844	-0.64784209	-0.47223103
H	-5.32765224	-1.14025749	-1.09829971
H	-6.04953256	-1.12029329	0.51411936
H	-7.06339733	-0.86733004	-0.91885237
C	-3.78598251	1.44849658	3.55222588
H	-3.19775875	0.53018811	3.45700926
H	-3.10743258	2.29354790	3.39715331
H	-4.16448534	1.50305782	4.58387810
C	-5.91806800	0.25658040	2.90273082
H	-6.82387080	0.24172917	2.28343395
H	-5.40688442	-0.70849253	2.78667574
H	-6.23725406	0.33382821	3.95259723
Fe	0.29132240	-1.75585555	-1.56791079
C	-0.75405688	-3.04160842	-2.13213300
C	1.76688553	-2.41625777	-2.22355291
O	-1.45804408	-3.92435041	-2.48335836
O	2.80010510	-2.85403330	-2.60501249
C	2.61207567	2.13622748	-0.65328334
C	3.57286711	2.77961502	-1.45843911
C	1.73939058	2.92168701	0.13319279
C	3.67121083	4.18480024	-1.47586179
H	4.24214619	2.18725007	-2.07883643
C	1.83818629	4.32226798	0.12098134
H	0.98505586	2.43986945	0.75005561
C	2.80566634	4.96000423	-0.68318092
H	4.41591406	4.66847839	-2.10360833
H	1.16201125	4.91649140	0.73099198
H	2.87863450	6.04493375	-0.69344691
C	-2.62551313	-1.84961920	0.89659036
C	-3.25392837	-3.04236059	0.48366888
C	-2.12095810	-1.76388211	2.21126860
C	-3.37212785	-4.13721069	1.36027297
H	-3.64946496	-3.12676161	-0.52730890
C	-2.24303457	-2.85309308	3.09035880
H	-1.61672931	-0.85741366	2.52353750
C	-2.86764504	-4.04489084	2.67047603
H	-3.85421720	-5.05146872	1.02182781
H	-1.84678449	-2.77546336	4.10061978
H	-2.95853560	-4.88713817	3.35298967
H	0.56126023	-2.68100028	-0.41942704
H	1.32674211	-0.14600852	1.43352474



17d: $E_{\text{Gibbs}} = -1761.54015169 \text{ eH}$

C	0.14234000	0.04580200	-0.03019000
C	1.04620700	0.75901200	0.84507800
C	0.28787400	1.86582600	1.40462800
C	-1.00382000	1.86376100	0.81415800
C	-1.10024700	0.77488500	-0.14540300
O	0.45906100	-1.13060800	-0.65881500
C	0.39561800	2.91193200	2.49057300
H	0.30409300	2.43777600	3.48044600
H	1.32837600	3.48696800	2.48616800
C	-1.89031800	2.91572500	1.43685500
H	-2.49148500	3.49097200	0.72423700
H	-2.58431800	2.43574000	2.14197200
C	-0.85246200	3.81782900	2.19337400
H	-0.54493700	4.63878900	1.53416500
H	-1.27186500	4.25467400	3.10644800
C	2.39852300	0.24056700	1.28414900
H	3.11703500	1.06852900	1.33213600
C	-2.35394700	0.36849800	-0.88381800
H	-2.94472200	1.28155400	-1.06100300
C	2.30268500	-0.43708000	2.66674300
H	1.59197100	-1.27039800	2.63090500
H	3.28063800	-0.81806100	2.98173900
H	1.95571600	0.28202800	3.41940000
C	-2.09238600	-0.32323000	-2.23245900
H	-1.48912700	-1.22295100	-2.09094600
H	-3.04119100	-0.58885600	-2.71208000
H	-1.54500800	0.35175400	-2.90122400
O	-3.10064700	-0.48316800	0.03495200
O	2.85940300	-0.72537400	0.27864800
Si	-4.67316400	-1.17258400	0.15689100
Si	4.44204900	-1.28869000	-0.20277200
C	5.87682300	-0.09838700	0.29660400
H	6.76366200	-0.74849400	0.17035200
C	4.34131100	-1.42718500	-2.11867200
H	5.39378000	-1.41073100	-2.45606500
C	4.70754400	-3.03716300	0.56775800
H	5.33207400	-3.56862800	-0.17238800
C	-4.94264500	-1.34244900	2.05803600
H	-6.03774700	-1.34171900	2.20515700
C	-4.71750000	-2.92288900	-0.65916700
H	-5.44861700	-3.48688500	-0.05143000
C	-6.05870200	-0.04908100	-0.58826900
H	-6.93287200	-0.72300600	-0.65736100
C	5.47941200	-3.08111200	1.91329800
H	6.45920100	-2.59045700	1.85470100
H	4.90829600	-2.60487500	2.72225300
H	5.65104400	-4.12546000	2.21184900
C	3.37711400	-3.82719700	0.71022300
H	2.70665500	-3.33768500	1.42740500
H	2.83525000	-3.91837600	-0.23781200
H	3.57737100	-4.84376700	1.07830000
C	3.71853200	-2.74984500	-2.64420500
H	4.22471200	-3.64222200	-2.25546200
H	2.65333300	-2.82126300	-2.38576500
H	3.78648300	-2.78200500	-3.74094900
C	3.61175100	-0.22378800	-2.77760100
H	2.55821200	-0.18695100	-2.47762600

H	4.05821400	0.74140400	-2.51624000
H	3.64372000	-0.32102300	-3.87258800
C	6.07716100	1.11621100	-0.65080200
H	5.22672700	1.80926500	-0.61789700
H	6.97067500	1.68107600	-0.34695900
H	6.22123600	0.81059400	-1.69373100
C	5.89665500	0.39473600	1.77119200
H	6.86751900	0.86034400	1.99343500
H	5.13098200	1.16071600	1.94566000
H	5.74305000	-0.41058700	2.49680900
C	-4.39655700	-2.66102700	2.66816700
H	-4.81843600	-3.55365900	2.18969500
H	-3.30366600	-2.71110100	2.57533600
H	-4.64067400	-2.71162000	3.73967500
C	-4.34937600	-0.14105800	2.84265500
H	-3.26396800	-0.09618100	2.69213300
H	-4.77022200	0.81948200	2.52327800
H	-4.54545600	-0.25275400	3.91965900
C	-6.47613200	1.13852400	0.32152400
H	-5.64844700	1.84871300	0.45620300
H	-7.31014900	1.69013300	-0.13696000
H	-6.80281400	0.80966500	1.31543000
C	-5.78094900	0.48660100	-2.02074400
H	-4.95986900	1.21491500	-2.01884300
H	-5.52455700	-0.30691100	-2.73014700
H	-6.67076800	1.00395300	-2.40872000
C	-3.35341100	-3.65909400	-0.55206900
H	-2.57913500	-3.13349100	-1.12263600
H	-2.99651300	-3.73520700	0.48059600
H	-3.43932300	-4.67901800	-0.95641400
C	-5.22193000	-2.98055000	-2.12510400
H	-6.21299600	-2.52554800	-2.24688500
H	-4.52761500	-2.47468000	-2.80940700
H	-5.29546700	-4.02736100	-2.45497900
Fe	0.47704800	2.14451900	-0.71452500
C	-0.42105200	3.25227600	-1.73083400
C	1.99554600	3.00421700	-0.78454800
O	-1.03023700	3.97208700	-2.44464700
O	3.05737600	3.52656700	-0.84077200
H	0.92991200	1.53570300	-2.01278300
H	1.43279700	-1.29008900	-0.47195600



4. GC-fid chromatograms

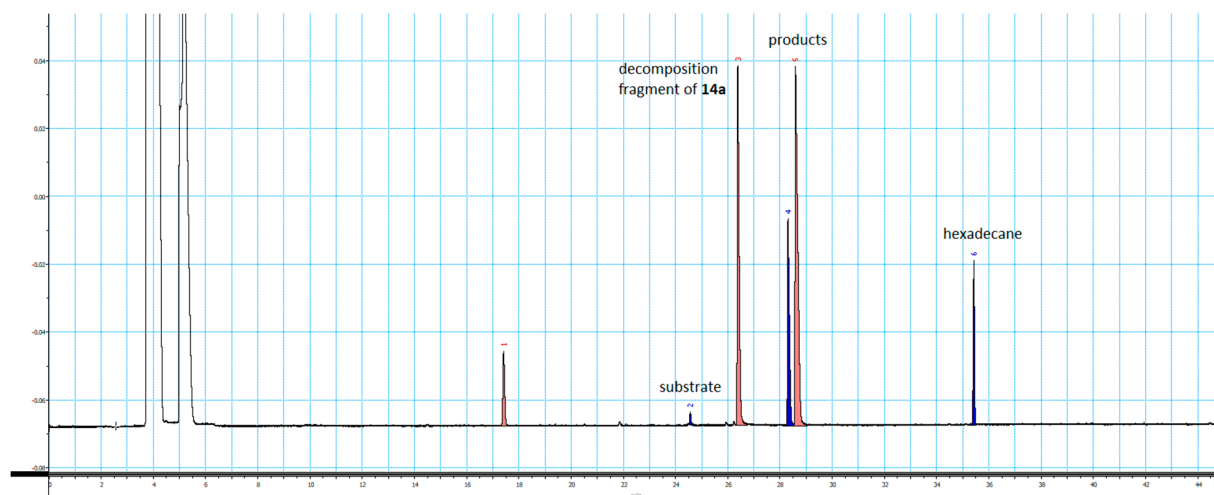


Figure S4.1: Chromatogram of acetophenone hydrogenation catalyzed by 14a.

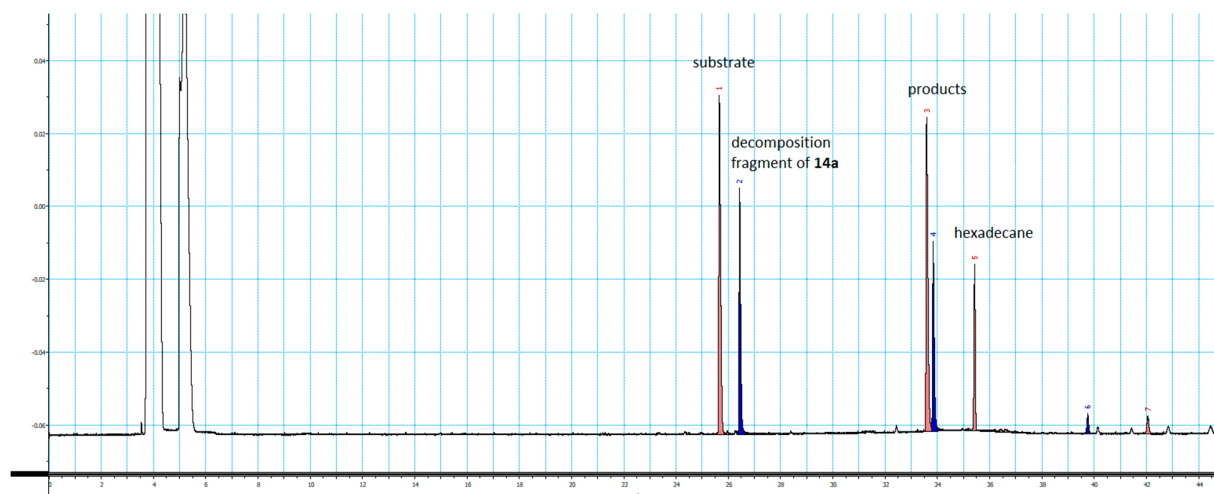


Figure 4.2: Chromatogram of 4-methoxyacetophenone hydrogenation catalyzed by 14a.

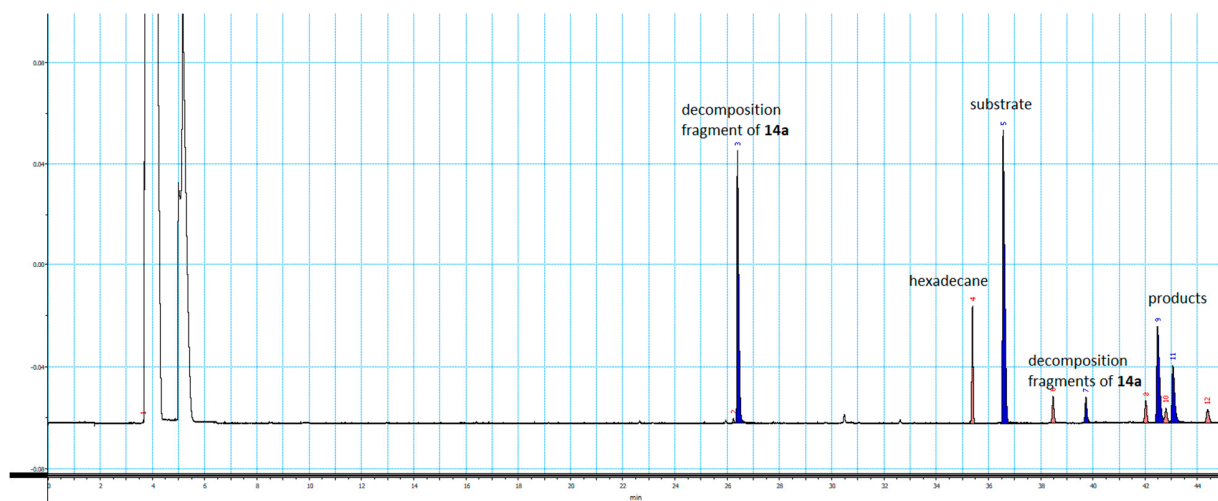


Figure 4.3: Chromatogram of 4-nitroacetophenone hydrogenation catalyzed by **14a**.

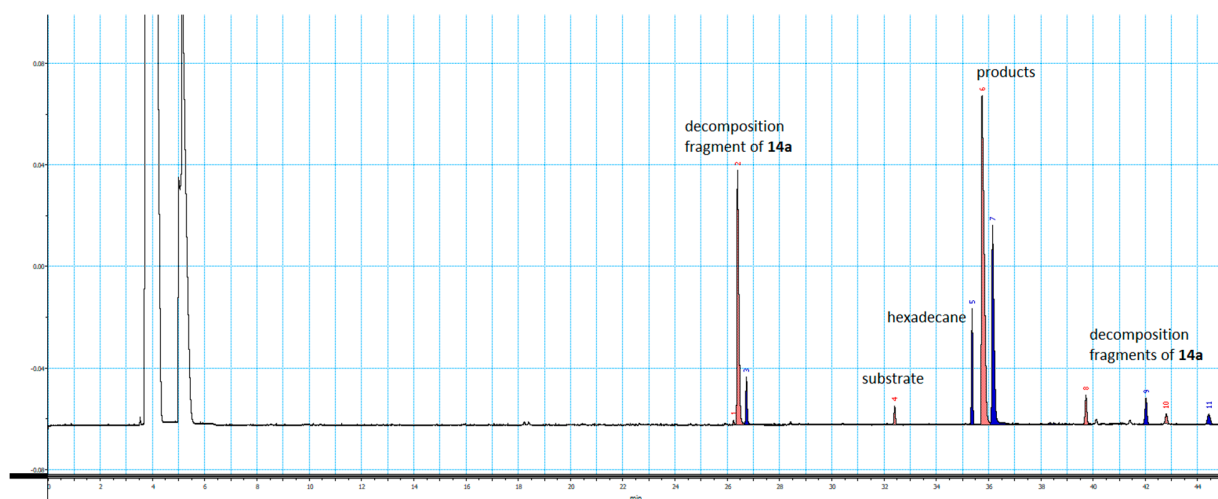


Figure 4.4: Chromatogram of 4-bromoacetophenone hydrogenation catalyzed by **14a**.

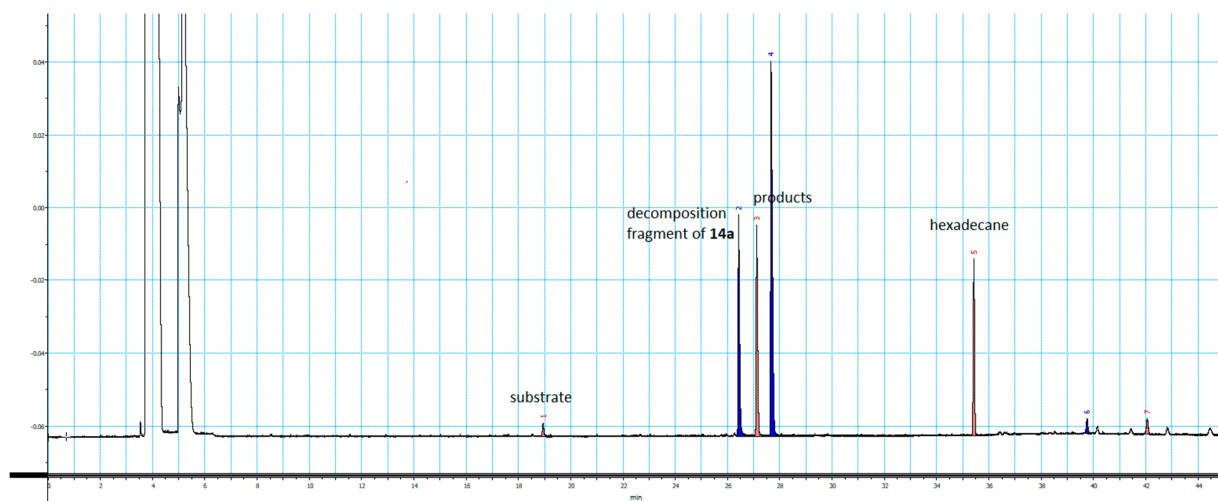


Figure 4.5: Chromatogram of 3,5-bis(trifluoromethyl)acetophenone hydrogenation catalyzed by 14a.

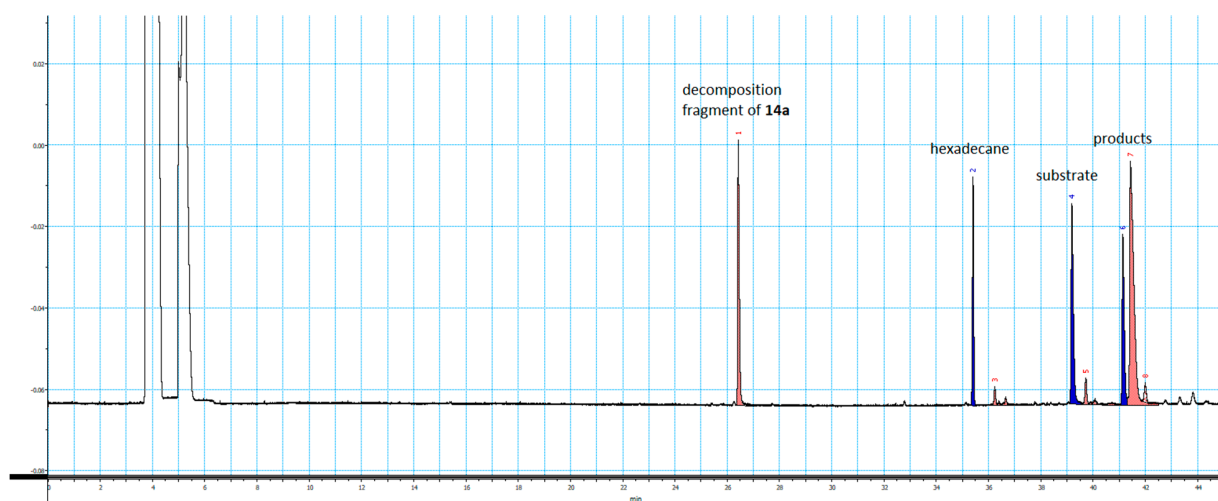


Figure 4.6: Chromatogram of 2,6-bis(hydroxy)bromoacetophenone hydrogenation catalyzed by 14a.

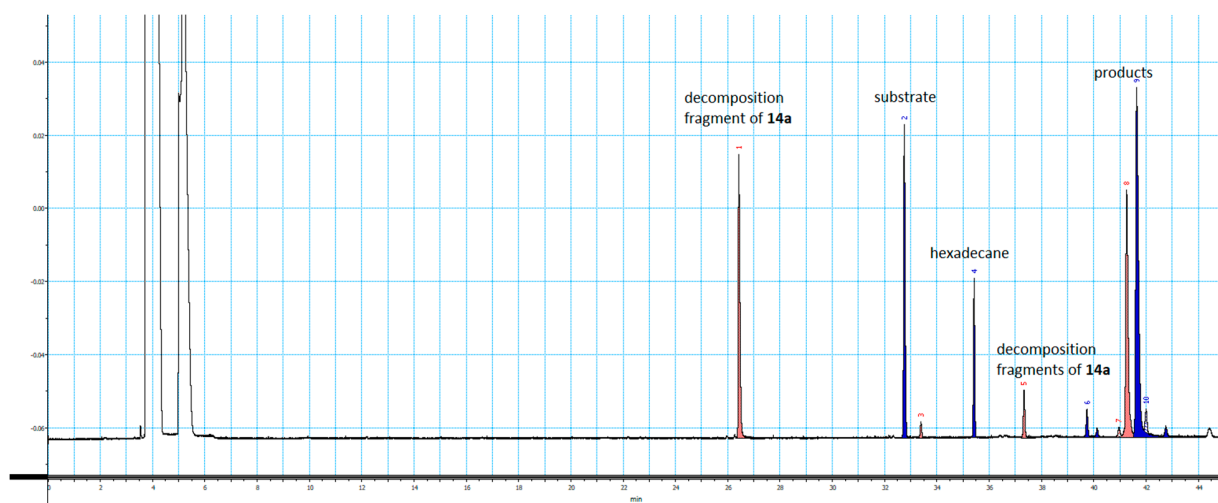


Figure 4.7: Chromatogram of acetophenone hydrogenation catalyzed by 14a.

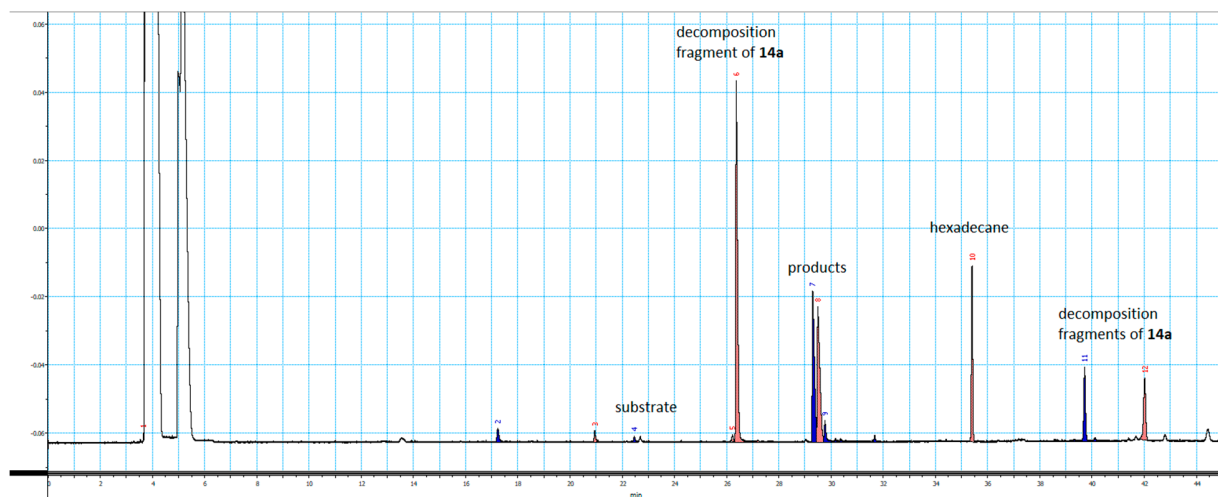


Figure 4.8: Chromatogram of 1-(5-methylfuran-2-yl)ethan-1-one hydrogenation catalyzed by 14a.

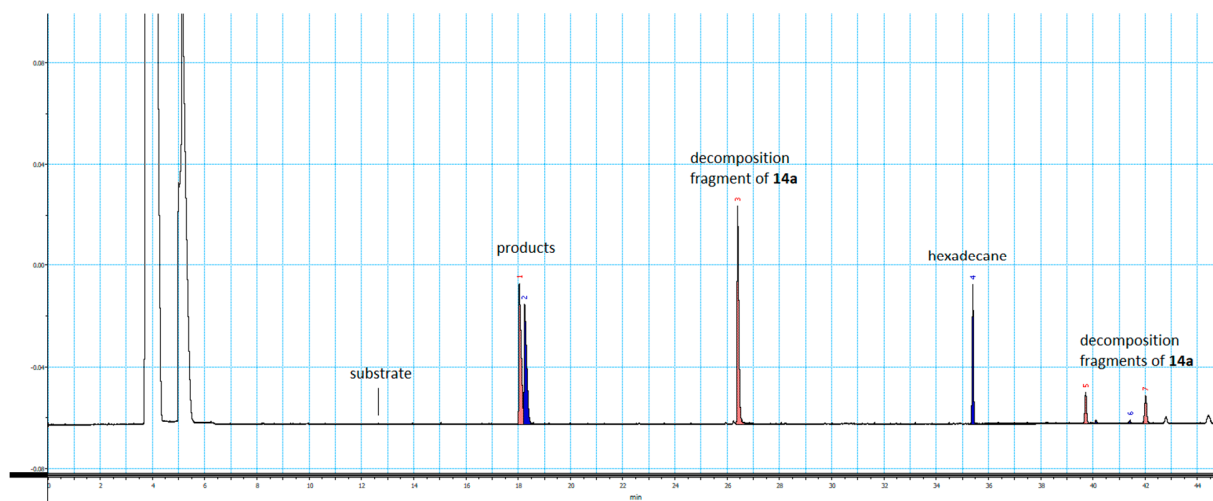


Figure 4.9: Chromatogram of 3,3-dimethylbutan-2-one hydrogenation catalyzed by **14a**.

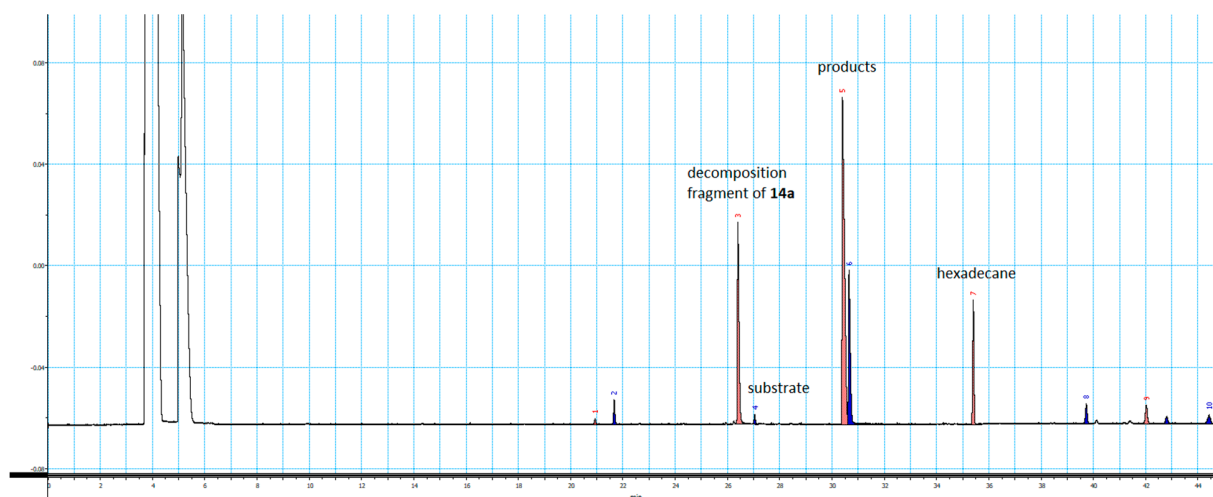


Figure 4.10: Chromatogram of propiophenone hydrogenation catalyzed by **14a**.

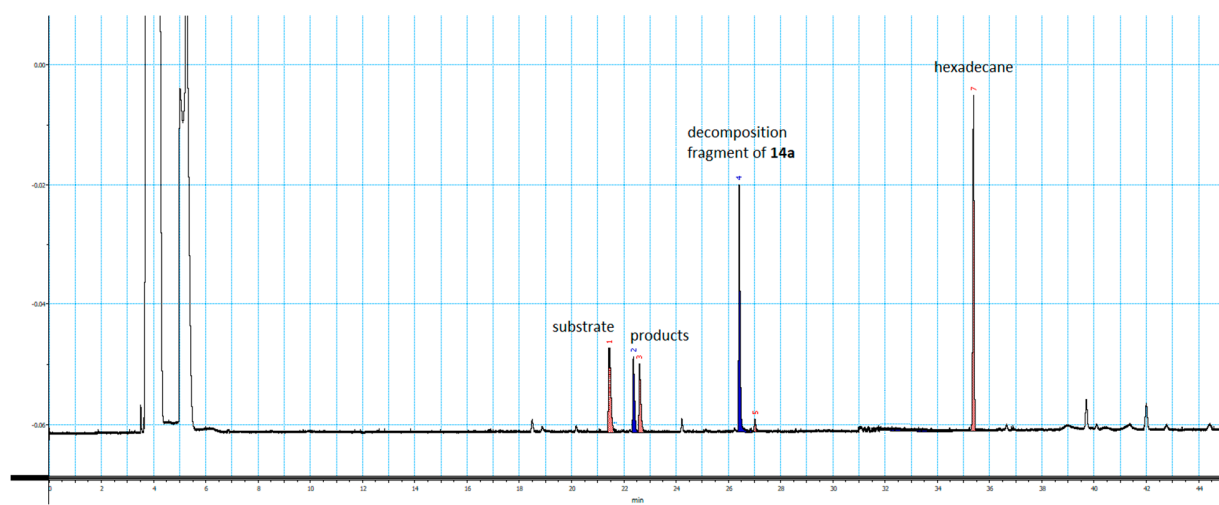


Figure 4.11: Chromatogram of methyl levulinate hydrogenation catalyzed by **14a**.