Supporting information for

Synthesis, characterization, and catalytic application in aldehyde hydrosilylation of half-sandwich nickel complexes bearing (κ^1-*C*)- and hemilabile (κ^2-*C,S*)-thioether-functionalised NHC ligands

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Figure S1. ^{1}H NMR spectrum of [NiBrCp{Mes-NHC-$(CH_2)_2S^tBu$}] (**1a**)

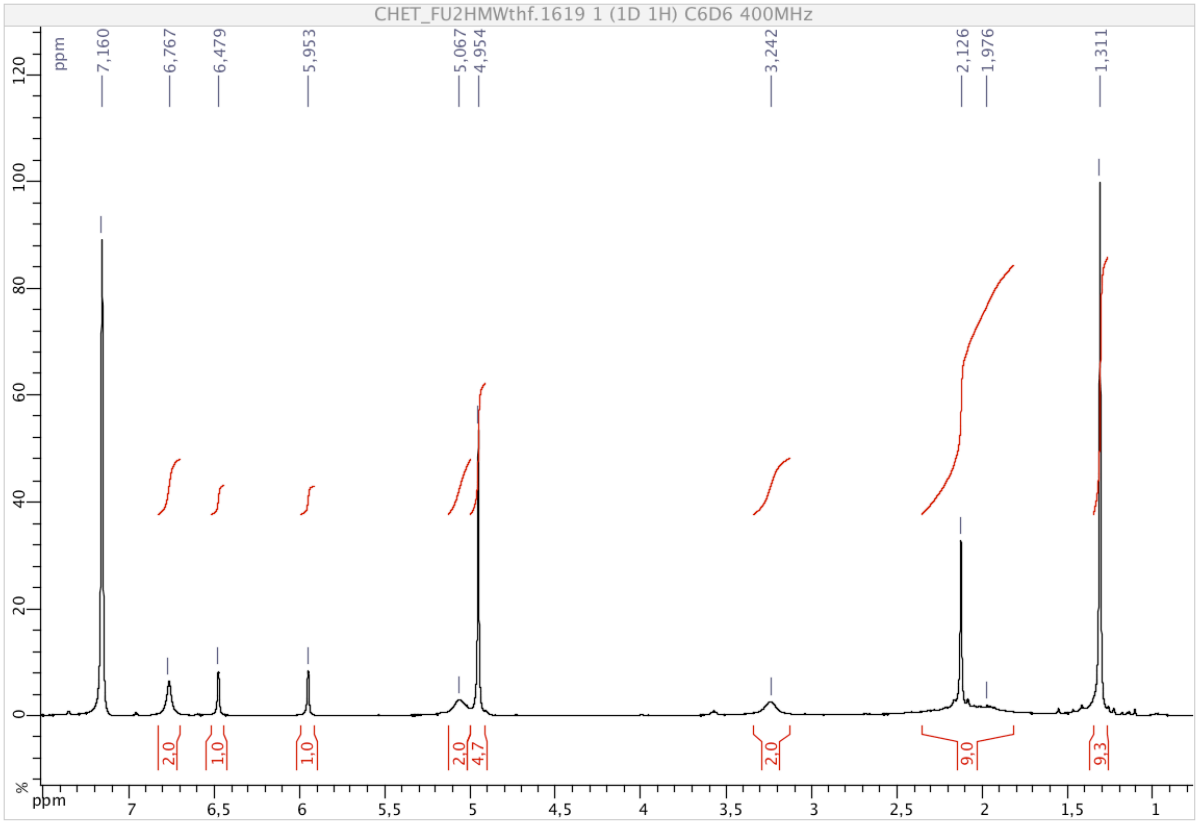


Figure S2. ^{13}C{^{1}H} NMR spectrum of [NiBrCp{Mes-NHC-$(CH_2)_2S^tBu$}] (**1a**)

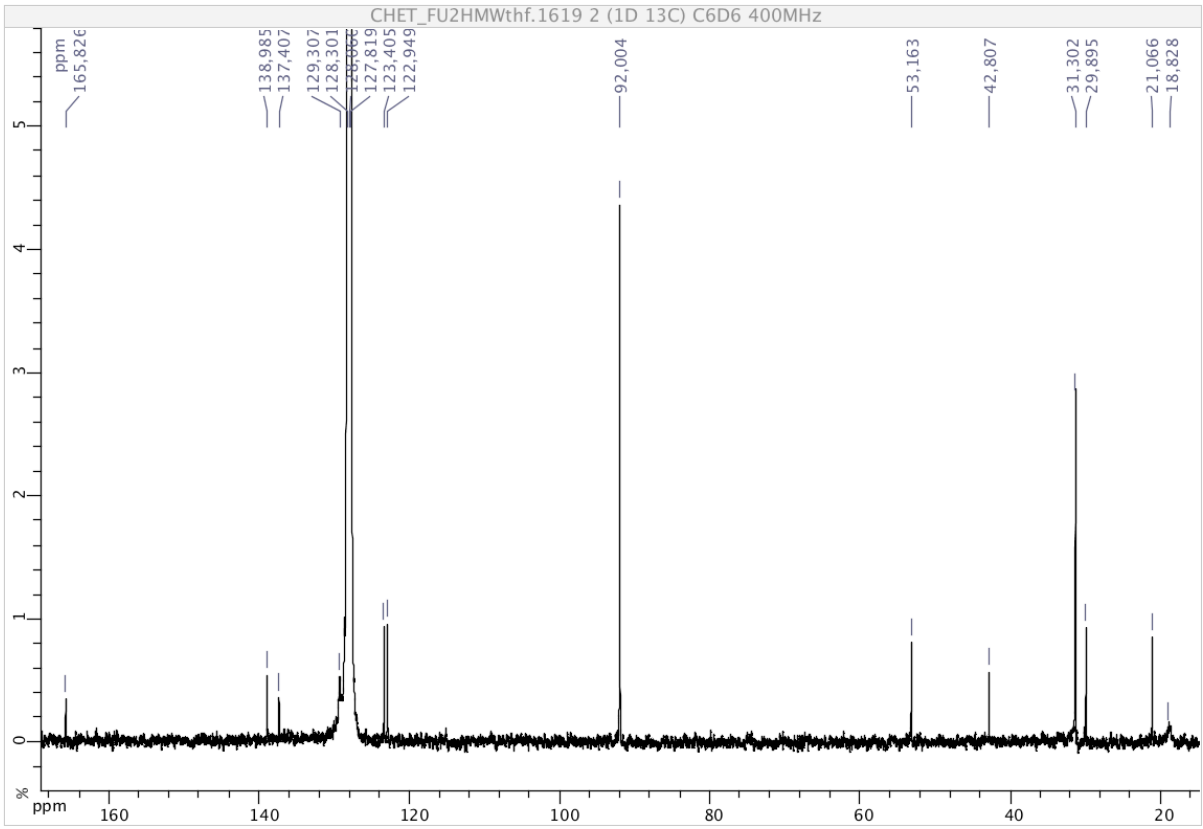


Figure S3. ^{1}H NMR spectrum of [NiBrCp{Mes-NHC-$(CH_2)_2$SPh}] (**1b**)

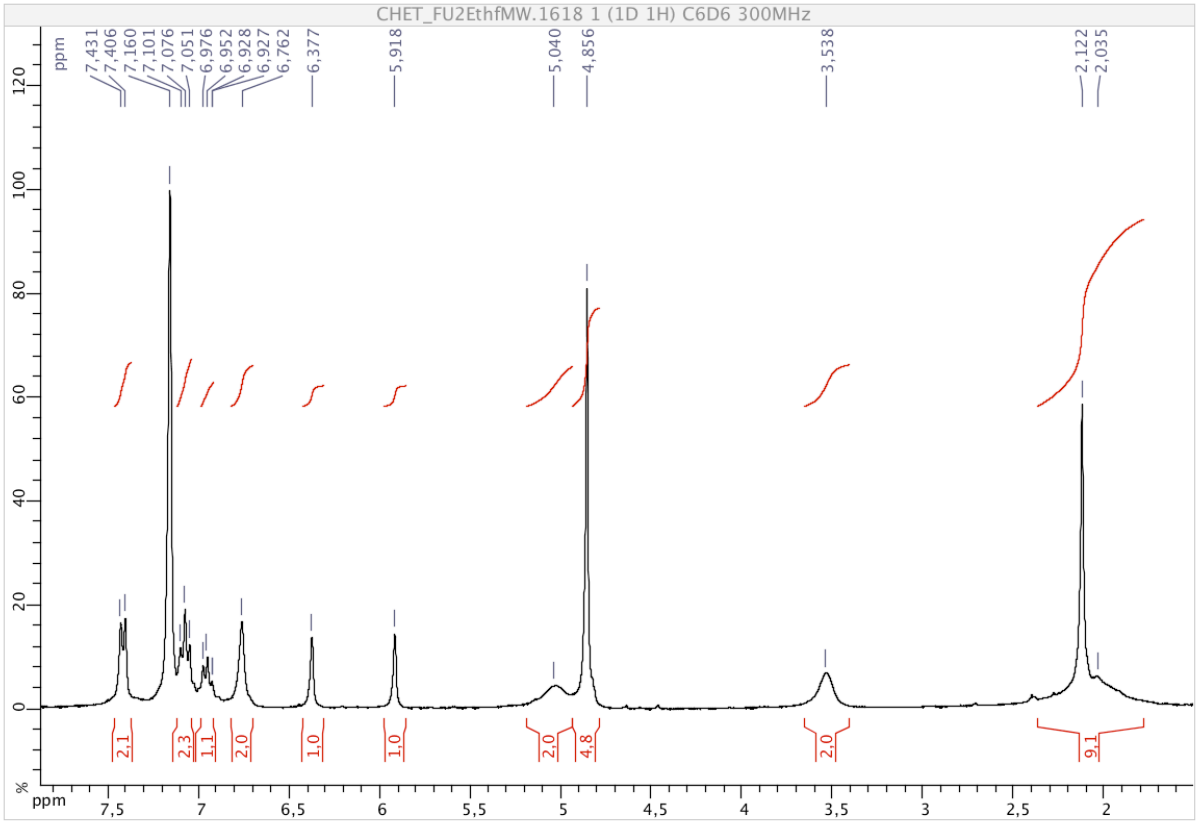


Figure S4. ^{13}C {^{1}H} NMR spectrum of [NiBrCp{Mes-NHC-$(CH_2)_2$SPh}] (**1b**)

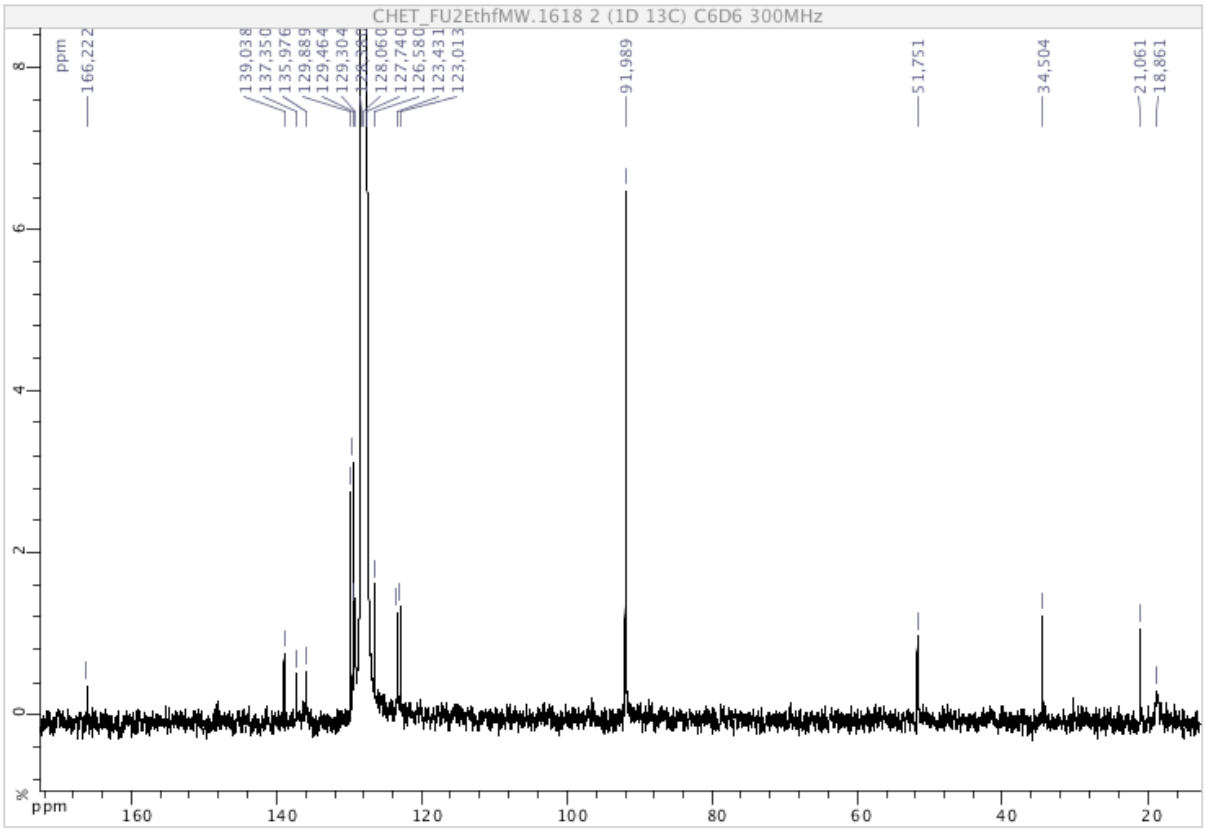


Figure S5. ^{1}H NMR spectrum of [NiBrCp{Bn-NHC-$(CH_2)_2S^tBu$}] (**1c**)

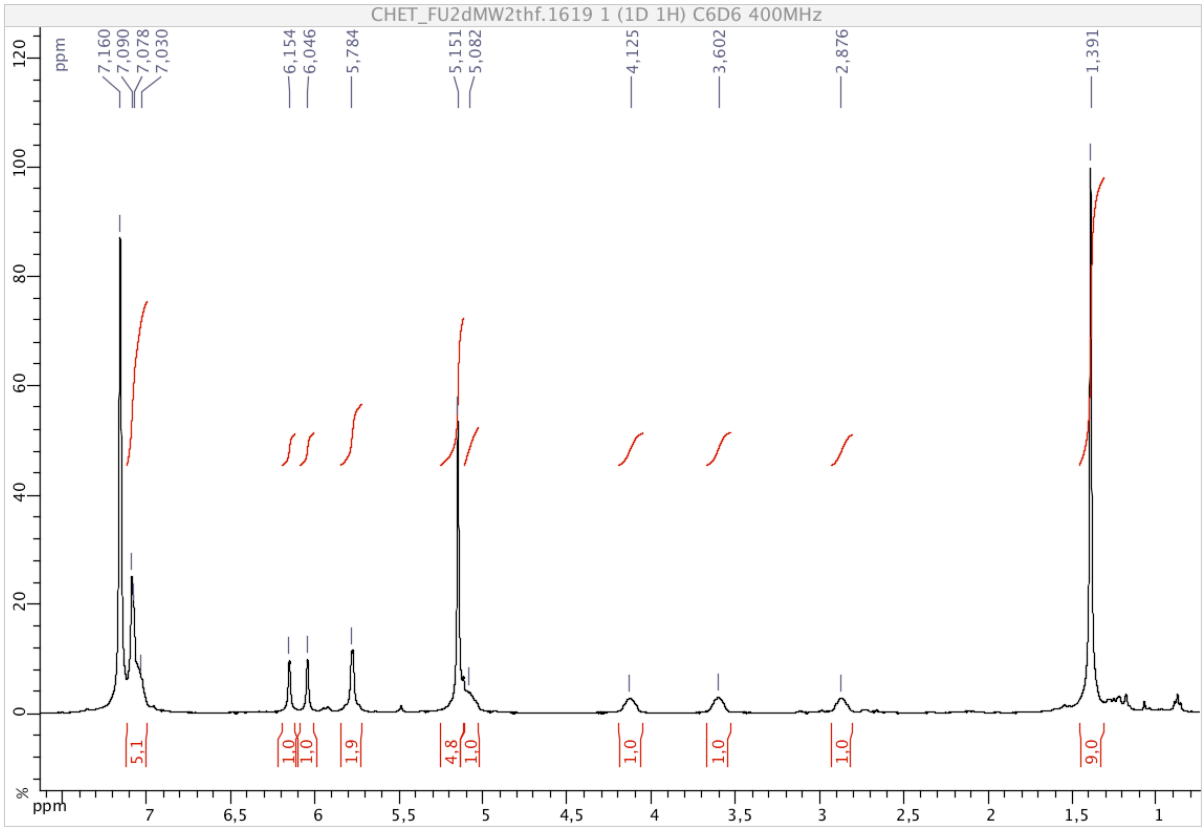


Figure S6. ^{13}C {^{1}H} NMR spectrum of [NiBrCp{Bn-NHC-$(CH_2)_2S^tBu$}] (**1c**)

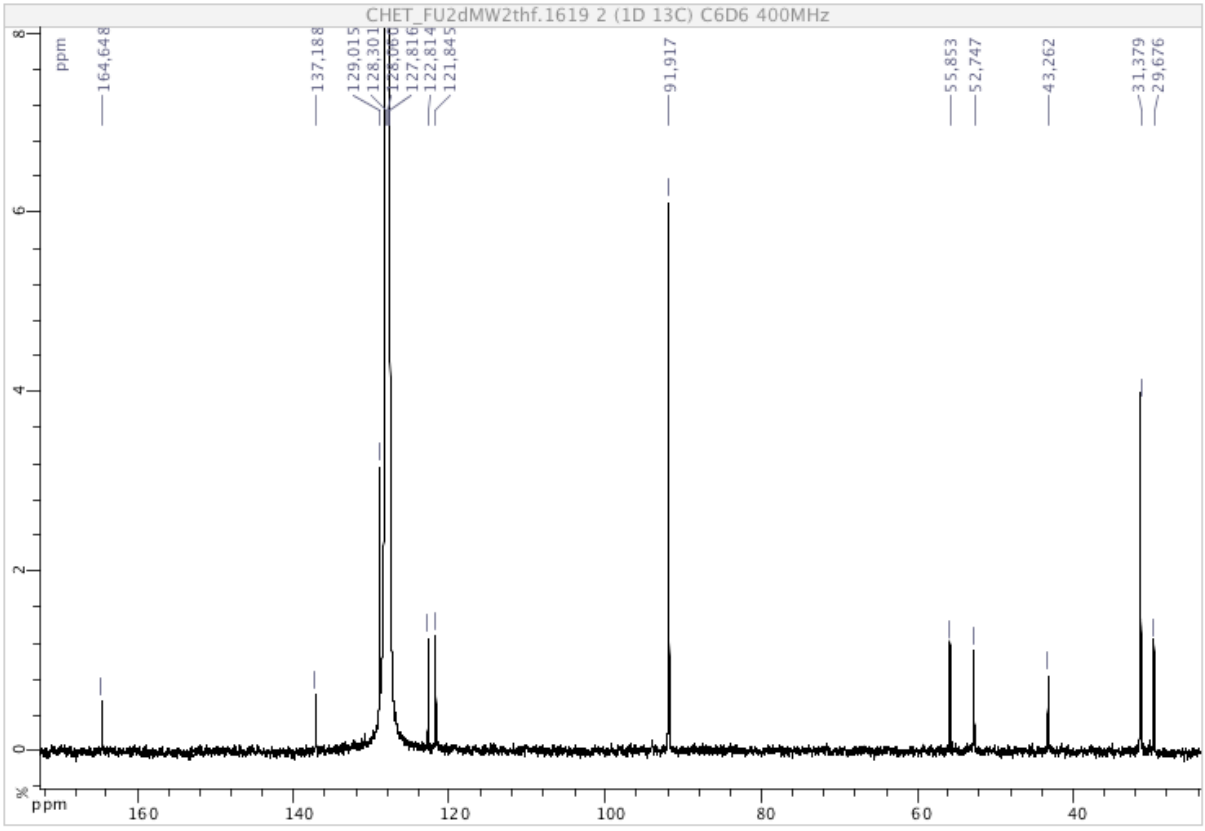


Figure S7. ^{1}H NMR spectrum of [NiBrCp{Bn-NHC-$(CH_2)_2$SPh}] (**1d**)

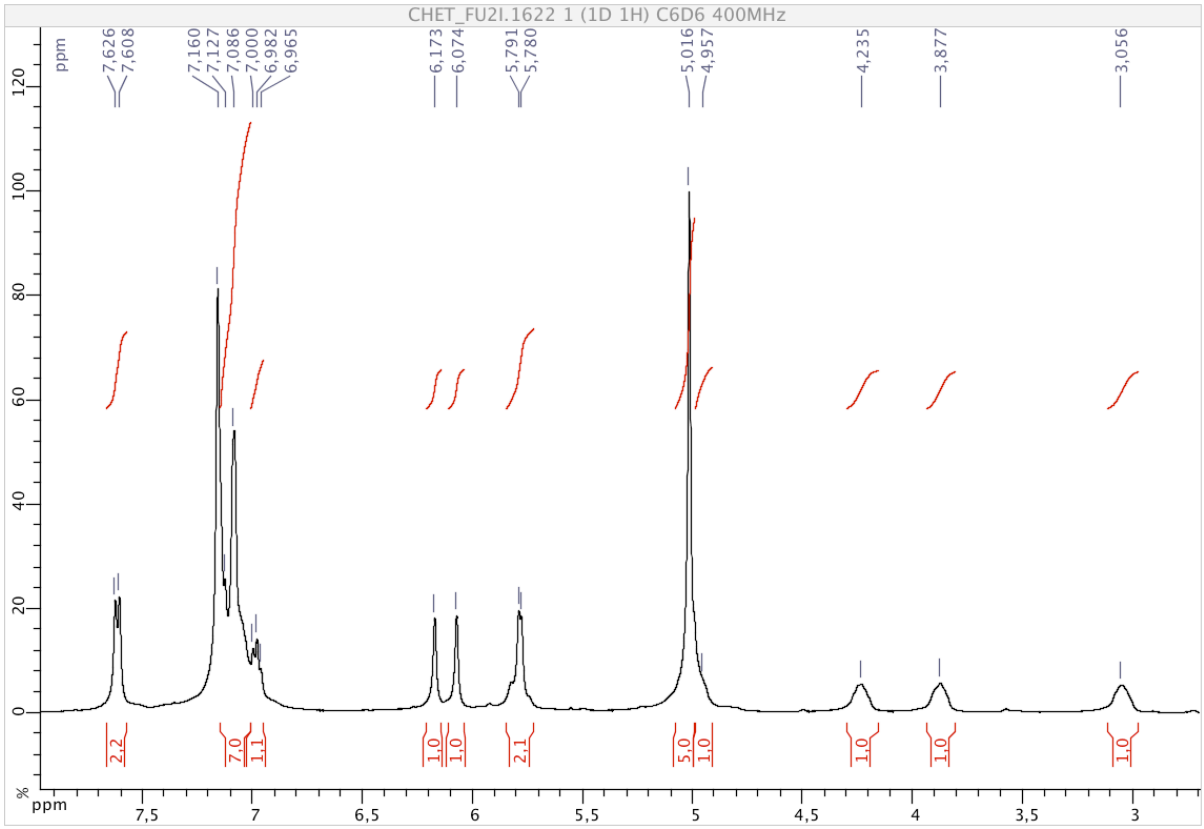


Figure S8. ^{13}C {^{1}H} NMR spectrum of [NiBrCp{Bn-NHC-$(CH_2)_2$SPh}] (**1d**)

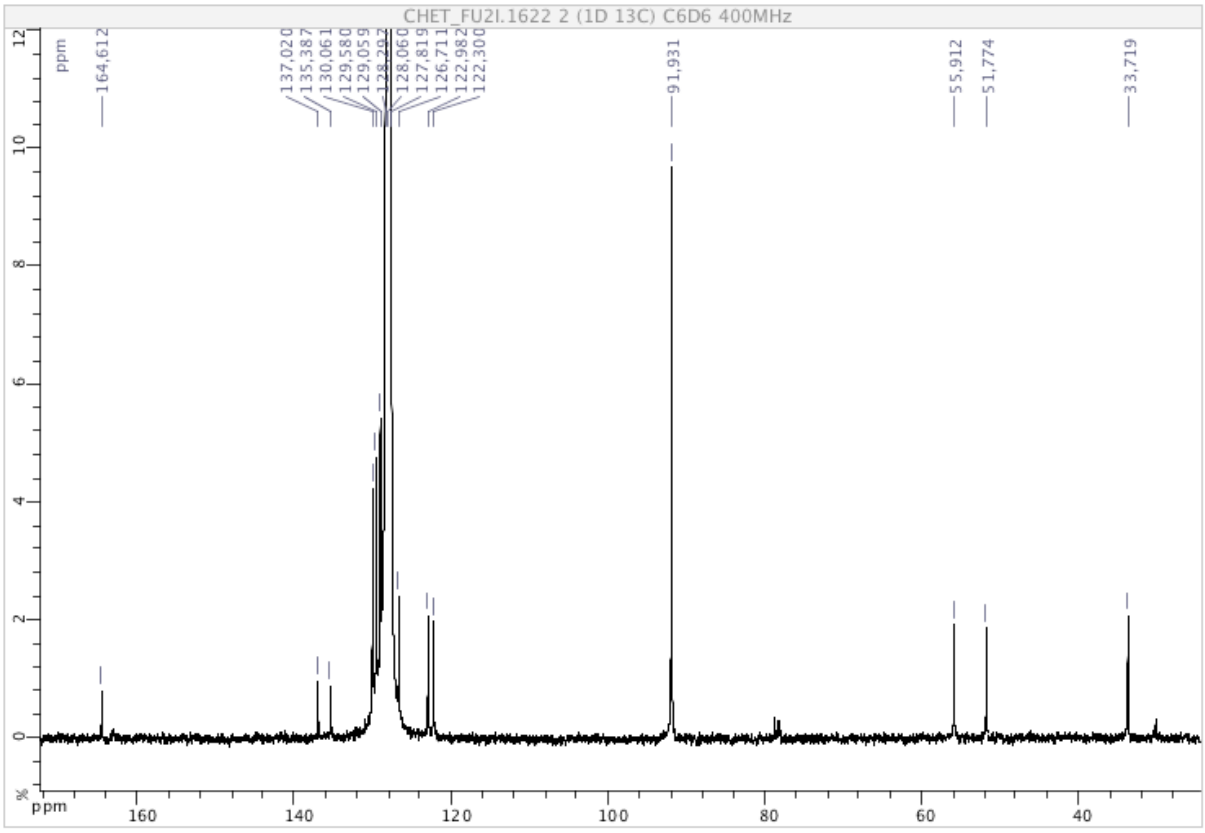


Table S1. X-ray crystallographic data and data collection parameters for **1a** and **1d**

Complex	**1a**	**1d**
Empirical formula	$C_{23}H_{31}BrN_2NiS$	$C_{23}H_{23}BrN_2NiS$
Formula weight	506.18	498.11
Crystal system	Triclinic	Monoclinic
Space group	$P\bar{1}$	$P2_1/c$
Temperature (K)	173(2)	173(2)
a (Å)	9.5279(3)	9.561(4)
b (Å)	12.2430(4)	15.486(6)
c (Å)	12.4761(4)	16.237(5)
α (°)	105.140(1)	90
β (°)	111.771(1)	113.976(17)
γ (°)	105.415(1)	90
V (Å^3)	1193.08(7)	2196.6(13)
Z	2	4
D_{calcd} (Mg.m^{-3})	1.409	1.506
Absorp coeff (mm^{-1})	2.586	2.808
Crystal form, colour	Prism, red	Prism, red
Crystal size (mm)	0.40 × 0.35 × 0.30	0.45 × 0.30 × 0.20
h, *k*, l_{max}	14, 18, 18	13, 21, 19
T_{min}, T_{max}	0.672, 0.746	0.573, 0.746
Measured reflns	38832	30977
Independent reflns, R_{int}	8196, 0.0200	6301, 0.0245
Reflns with I > 2σ(I)	6747	4277
R [$F^2 > 2\sigma(F^2)$]	0.0350	0.0409
wR(F^2)	0.0937	0.1096
GOF on F^2	1.026	1.020

Figure S9. ^{1}H NMR spectra of [NiCp{Mes-NHC-$(CH_2)_2S^tBu$}](PF_6) (**2a**)

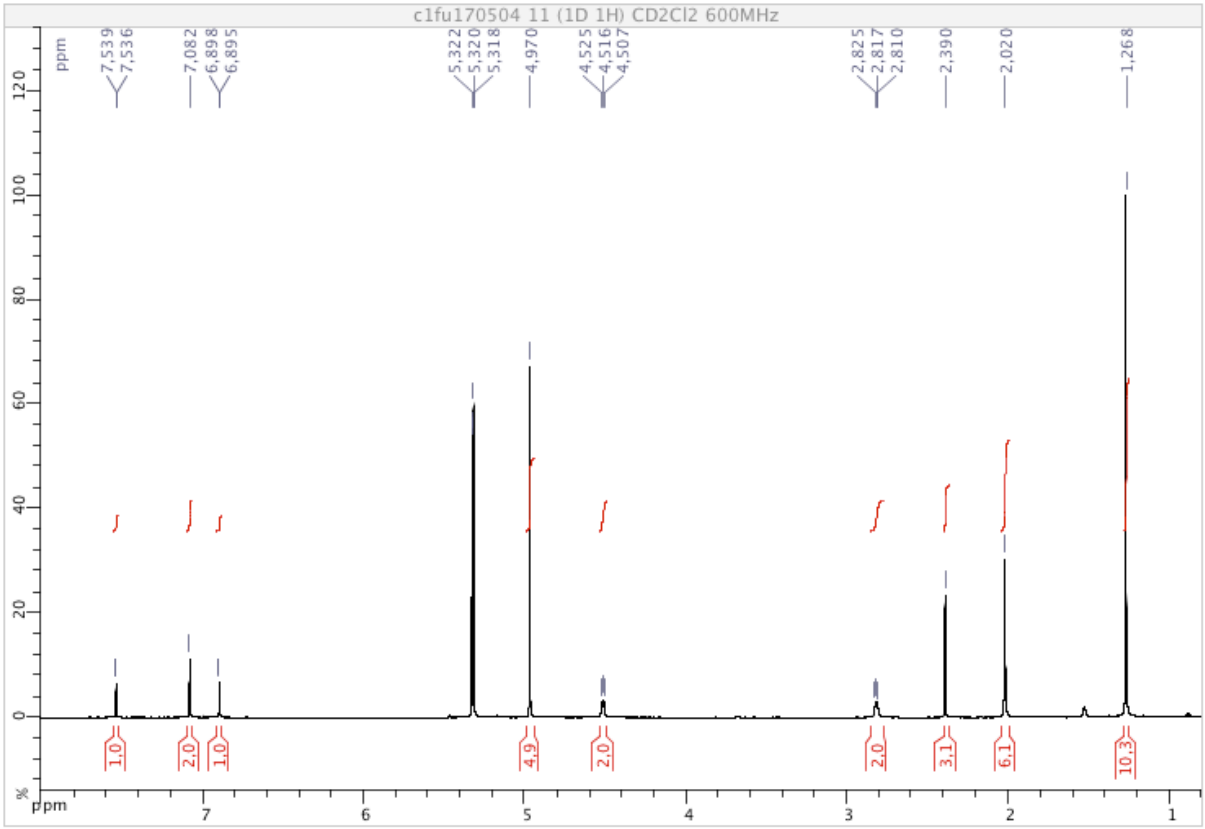


Figure S10. ^{13}C {^{1}H} NMR spectra of [NiCp{Mes-NHC-$(CH_2)_2S^tBu$}](PF_6) (**2a**)

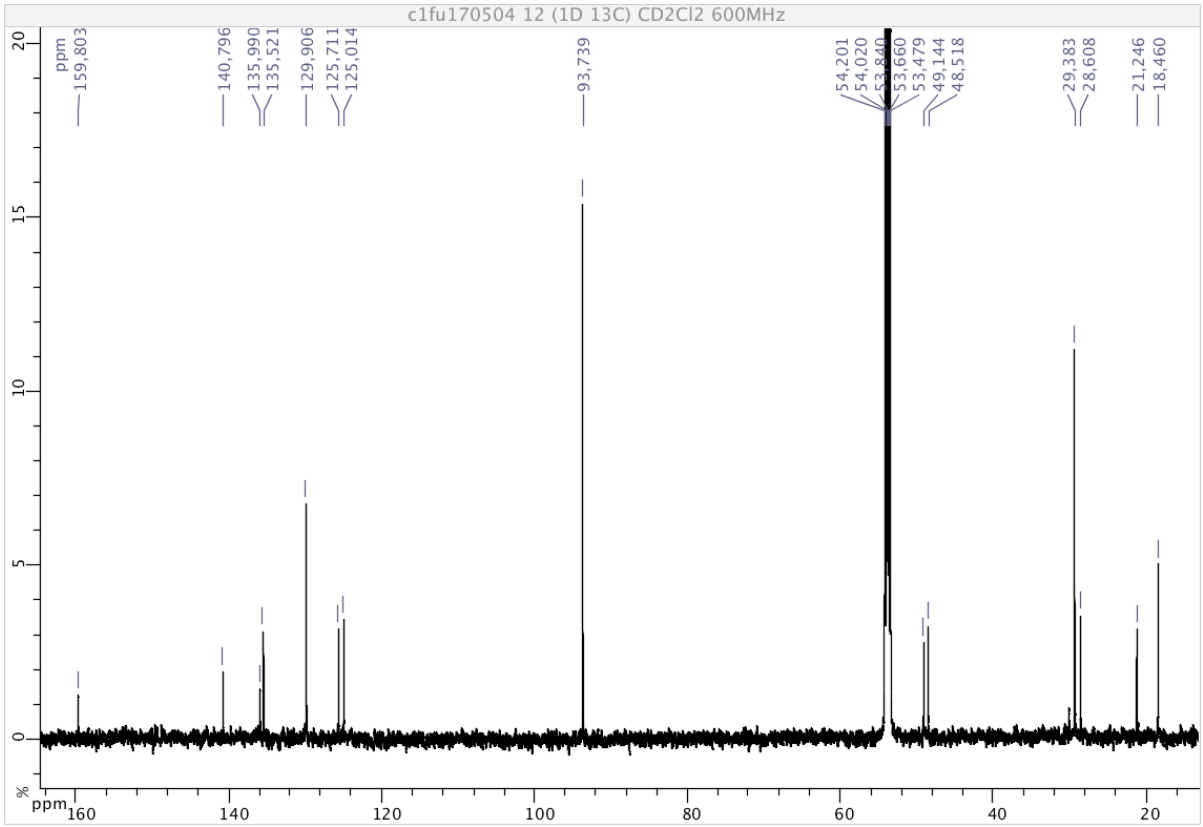


Figure S11. ^{1}H NMR spectra of [NiCp{Mes-NHC-$(CH_2)_2$SPh}](PF_6) (**2b**)

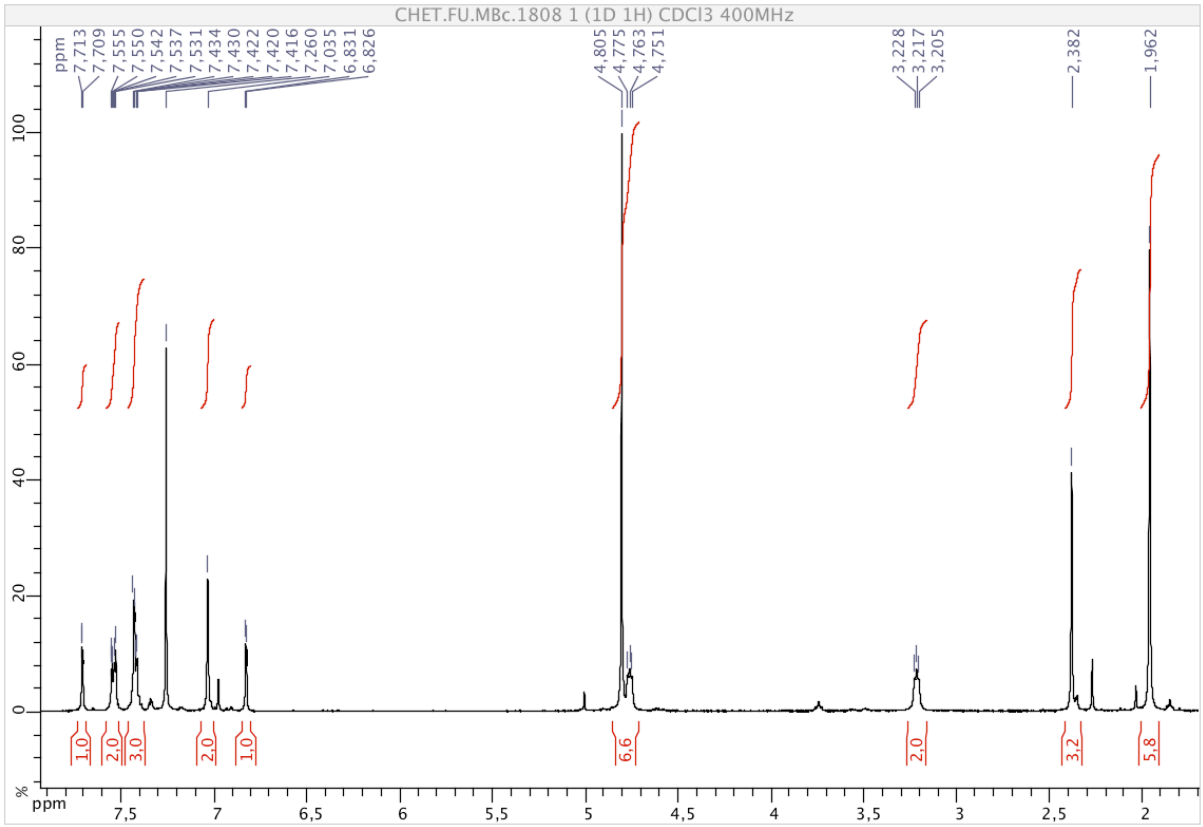


Figure S12. ^{13}C {^{1}H} NMR spectrum of [NiCp{Mes-NHC-$(CH_2)_2$SPh}](PF_6) (**2b**)

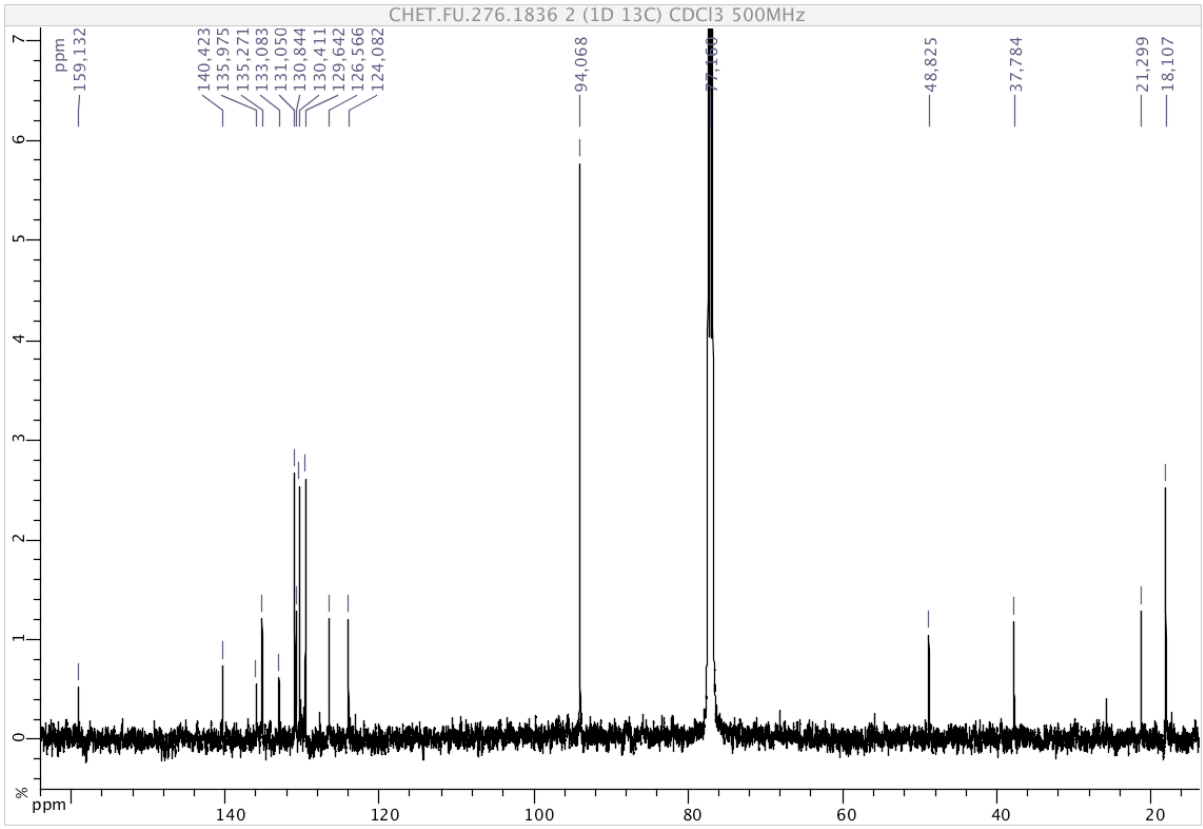


Figure S13. ^{1}H NMR spectra of [NiCp{Bn-NHC-$(CH_2)_2S^tBu$}](PF_6) (**2c**)

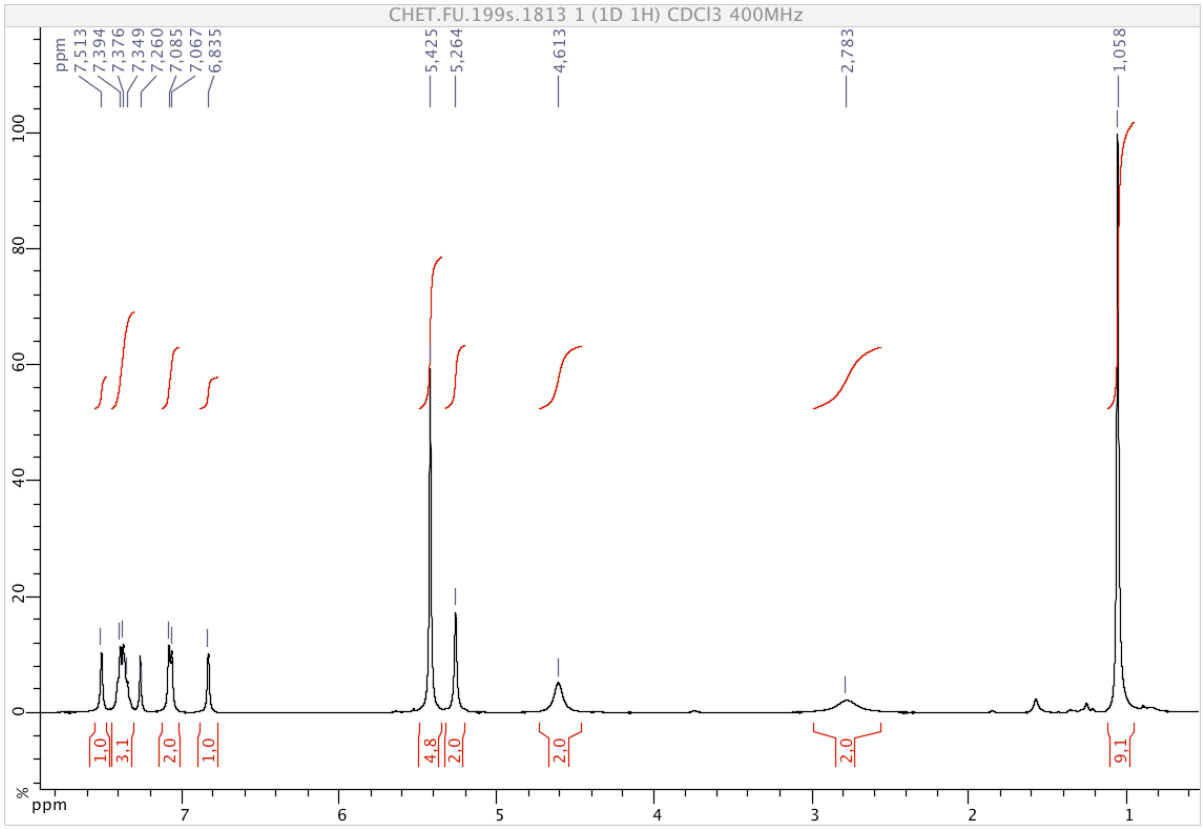


Figure S14. ^{13}C {^{1}H} NMR spectrum of [NiCp{Bn-NHC-$(CH_2)_2S^tBu$}](PF_6) (**2c**)

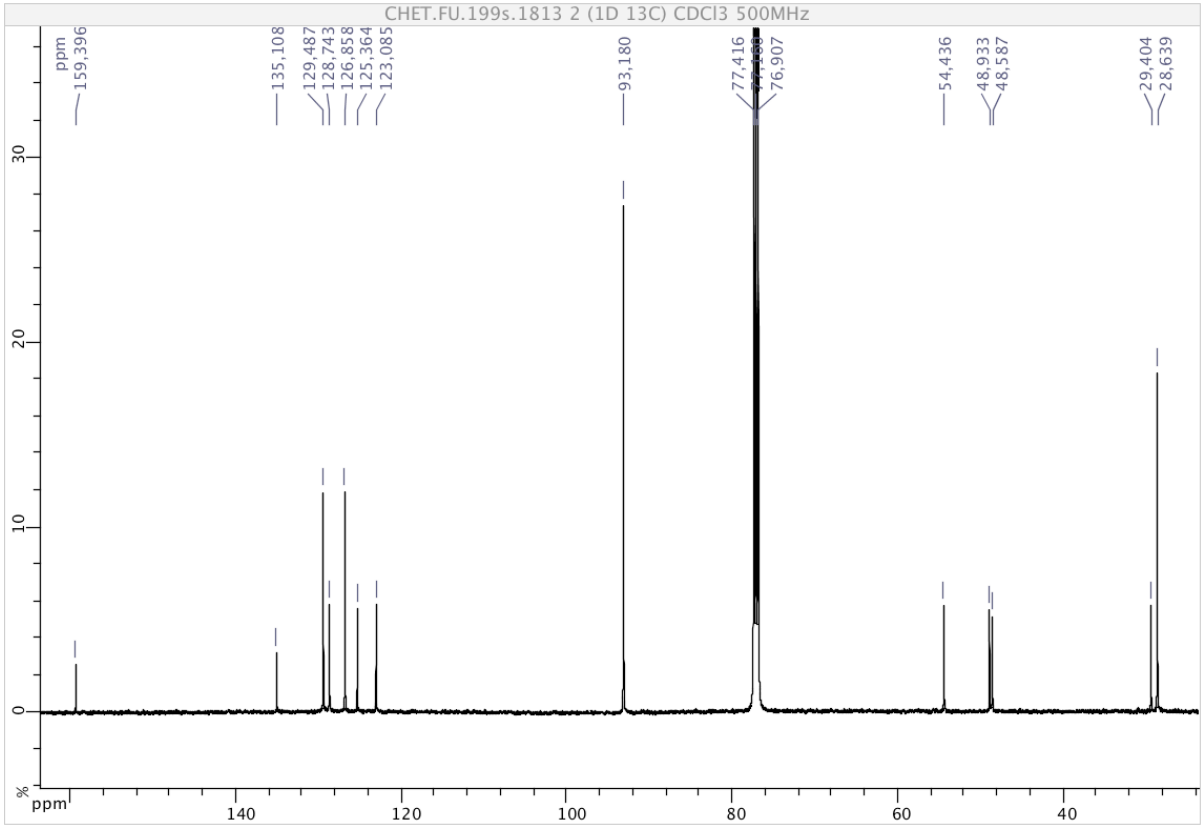


Table S2. X-ray crystallographic data and data collection parameters for **2a** and **2c**

Complex	**2a**	**2c**
Empirical formula	$C_{23}H_{31}N_2NiS{\cdot}F_6P$	$C_{21}H_{27}N_2NiS{\cdot}F_6P$
Formula weight	571.24	543.18
Crystal system	Orthorhombic	Monoclinic
Space group	*Pbca*	$P2_1/c$
Temperature (K)	173(2)	173(2)
a (Å)	12.2564(3)	9.2425(2)
b (Å)	15.4610(4)	15.5464(4)
c (Å)	27.1428(7)	16.5839(5)
α (°)	90	90
β (°)	90	95.409(1)
γ (°)	90	90
V (Å^3)	5143.5(2)	2372.29(11)
Z	8	4
D_{calcd} (Mg.m^{-3})	1.475	1.521
Absorp coeff (mm^{-1})	0.956	3.178
Crystal form, colour	Prism, green	Block, green
Crystal size (mm)	0.25 × 0.20 × 0.18	0.18 × 0.12 × 0.08
h, *k*, l_{max}	17, 21, 38	10, 16, 18
T_{min}, T_{max}	0.651, 0.746	0.649, 0.753
Measured reflns	50260	23312
Independent reflns, R_{int}	7498, 0.0370	4166, 0.0330
Reflns with I > 2σ(I)	5579	3634
R [$F^2 > 2\sigma(F^2)$]	0.0377	0.0563
wR(F^2)	0.0924	0.1510
GOF on F^2	1.082	1.049

Solvent *vs.* Gas Phase calculations

The addition of solvent effects is key for the discrimination of solvent coordination over sulfur inversion. This effect is highlighted when the combination of charged species and solvent coordination are present. Transitions states are stabilized by at least 13 kcal/mol and the reaction becomes exothermic. Tables **S3**, **S4** and **S5** show the differences computed.

Table S3. ΔG energies, in kcal/mol, in gas phase and single point solvent (benzene) for the monodentate to bidentate process of **1d**

	1d	**TS- (Ni-S)-coord**	**1d^{+}Br^{-}**
ΔG (gas phase)	0.0	+23.9	+19.0
ΔG (solvent)	0.0	+22.6	+13.5

Table S4. ΔG energies, in kcal/mol, in gas phase and single point solvent for the sulphur inversion process of **(*R*)-2a** and **(*R*)-2c**

	(*R*)-2a	**TS- inversion**	**(*S*)-2a**
ΔG (gas phase)	0.0	+7.8	+0.5
ΔG (solvent = THF)	0.0	+9.1	+0.8
ΔG (solvent = DCM)	0.0	+9.0	+0.7
	(*R*)-2c	**TS- inversion**	**(*S*)-2c**
ΔG (gas phase)	0.0	+11.3	+4.1
ΔG (solvent = THF)	0.0	+13.3	+5.4
ΔG (solvent = DCM)	0.0	+13.2	+5.4

Table S5. ΔG energies, in kcal/mol, in gas phase and single point solvent (THF) for the solvent coordination process of **2a** and **2c**

	2a + THF	**TS- (2a-THF)-coord**	**2a-THF**
ΔG (gas phase)	0.0	+24.0	+11.7
ΔG (solvent)	0.0	+11.1	-6.2
	2c + THF	**TS- (2c-THF)-coord**	**2c-THF**
ΔG (gas phase)	0.0	+27.4	+10.7
ΔG (solvent)	0.0	+11.5	-7.6

Atomic coordinates of the optimized species

1d			**TS-(Ni-S)-coord**		
E (SCF) = -1194.09914458 E (SCF; solvent = benzene) = -5480.6631 Zero-point correction = 0.407827 Thermal correction to Enthalpy = 0.435682 Thermal correction to Gibbs Free Energy = 0.344133			E (SCF) = -1194.06428906 E (SCF; solvent = benzene) = -5480.63034 Zero-point correction = 0.407570 Thermal correction to Enthalpy = 0.434640 Thermal correction to Gibbs Free Energy = 0.34745		
C	0.631039	0.718591	0.243872	C	-0.112439	4.878496	9.063168
C	2.662001	0.023252	0.953787	C	2.101340	4.572143	9.460652
H	3.511812	-0.635285	1.038952	H	3.036628	4.035157	9.475528
C	2.448661	1.253935	1.478161	C	1.798857	5.837681	9.827382
H	3.070803	1.876831	2.100985	H	2.414394	6.631930	10.218528
C	1.384595	-1.490364	-0.601715	C	0.878979	2.656104	8.438809
H	2.115429	-1.453271	-1.419031	H	1.906221	2.279313	8.418187
H	0.390924	-1.421725	-1.049418	H	0.516087	2.748395	7.407487
C	1.570088	-2.782584	0.187737	C	0.010449	1.713628	9.252316
H	2.559123	-2.815783	0.655449	H	0.295992	1.723752	10.308939
H	1.513512	-3.639924	-0.488219	H	0.102402	0.691952	8.877018
C	-0.797066	-4.203750	0.861387	C	-2.419848	0.952778	8.022007
C	0.597754	2.952114	1.354047	C	-0.213451	7.280618	9.828224
C	-2.376747	0.527579	0.756137	C	-3.385836	5.697077	9.632926
H	-2.118156	0.439674	1.804294	H	-3.210895	6.116155	10.617039
C	-2.793566	1.723813	0.092873	C	-3.111643	6.365652	8.359866
H	-2.860027	2.713107	0.525057	H	-2.700826	7.359230	8.235913
C	-2.986172	1.380889	-1.256719	C	-3.536236	5.528340	7.333426
H	-3.210877	2.064467	-2.064965	H	-3.417636	5.699463	6.273850
C	-2.848049	-0.050820	-1.400180	C	-3.957420	4.302838	7.940738
H	-2.942717	-0.591009	-2.332868	H	-4.312092	3.433102	7.401156
C	-2.510936	-0.585259	-0.155022	C	-4.000602	4.477921	9.362878
N	1.536810	-0.293402	0.211456	N	0.930706	3.998877	9.004277
N	1.202273	1.659241	1.038320	N	0.447009	6.003920	9.592289
S	0.374845	-3.047720	1.553132	S	-1.775271	2.160361	9.192175
Ni	-0.965461	0.848009	-0.726213	Ni	-1.868270	4.497173	8.442308
Br	0.176449	1.386972	-2.697724	Br	-0.725970	4.351392	5.902620
C	1.473353	4.119229	0.964606	C	0.123489	8.332496	8.793724
H	-0.350284	2.966459	0.807719	H	-1.282521	7.076339	9.848790
H	0.373781	2.983827	2.426242	H	0.072983	7.627801	10.826628
C	1.937540	5.010650	1.934804	C	0.404582	9.639296	9.202216
C	2.732799	6.099120	1.574912	C	0.673244	10.632717	8.261733
C	3.072086	6.298878	0.239022	C	0.670323	10.322379	6.903178
C	2.611754	5.410458	-0.734751	C	0.395273	9.018325	6.491010
C	1.815120	4.326187	-0.378083	C	0.120108	8.024141	7.427836
H	1.671070	4.857334	2.978805	H	0.412842	9.883407	10.262930
H	3.086137	6.787116	2.338102	H	0.891492	11.644763	8.591720
H	3.691762	7.145103	-0.044911	H	0.884509	11.093299	6.168009
H	2.870072	5.565067	-1.778700	H	0.392205	8.767130	5.434158
H	1.454224	3.636138	-1.138814	H	-0.091828	7.010563	7.089817
H	-2.315230	-1.621568	0.083665	H	-4.302704	3.735873	10.089850
C	-1.419286	-5.078536	1.762124	C	-3.114066	-0.145519	8.542104
C	-2.384043	-5.976058	1.313148	C	-3.652463	-1.093906	7.673910

C	-2.726859	-6.027756	-0.037762	C	-3.498811	-0.944635	6.295708
C	-2.104675	-5.162815	-0.935122	C	-2.812933	0.157100	5.785096
C	-1.153432	-4.244265	-0.491758	C	-2.273784	1.116750	6.641759
H	-1.134974	-5.061518	2.810724	H	-3.230600	-0.251298	9.617064
H	-2.857230	-6.649401	2.022612	H	-4.191910	-1.947138	8.075809
H	-3.472244	-6.735877	-0.387284	H	-3.919766	-1.684289	5.620117
H	-2.367477	-5.187666	-1.989157	H	-2.701269	0.282718	4.711712
H	-0.705320	-3.558812	-1.204149	H	-1.764014	1.995506	6.247201

$1d^{+}Br^{-}$			**2a**		
E (SCF) = -1194.07556059 E (SCF; solvent = benzene) = -5480.64829 Zero-point correction = 0.409272 Thermal correction to Enthalpy = 0.436316 Thermal correction to Gibbs Free Energy = 0.350775			E (SCF) = -1106.718457 E (SCF; solvent = THF) = -3143.767957 Zero-point correction = 0.440418 Thermal correction to Enthalpy = 0.466361 Thermal correction to Gibbs Free Energy = 0.384129		
C	1.014939	0.262670	1.232243	C	0.013567	0.034963	0.008206
C	3.268833	0.013777	1.222311	C	0.029159	0.039299	2.270209
H	4.202693	-0.504172	1.073105	H	0.461479	0.036477	3.258787
C	3.007585	1.289663	1.583902	C	-1.265324	0.065567	1.867307
H	3.663910	2.113998	1.812294	H	-2.182973	0.075631	2.433283
C	1.915200	-1.957845	0.532629	C	2.244395	-0.063930	1.057694
H	2.922831	-2.376180	0.454978	H	2.634017	0.036878	2.074429
H	1.498255	-1.898557	-0.483653	H	2.626739	0.775239	0.468669
C	1.093982	-2.805679	1.483573	C	2.703293	-1.395183	0.473241
H	1.444940	-2.700352	2.515028	H	2.265279	-2.222704	1.034984
H	1.130441	-3.861115	1.204265	H	3.791918	-1.469954	0.532736
C	-1.292001	-3.346204	0.132910	C	0.992571	0.199909	-3.831472
C	1.010037	2.703320	1.892843	H	1.311663	-0.594294	-4.494124
C	-2.252542	1.426369	1.583186	C	-0.337323	0.518501	-3.496080
H	-2.152863	2.105042	2.420385	H	-1.232242	0.018001	-3.839229
C	-1.647491	1.582819	0.267379	C	-0.265673	1.593039	-2.556683
H	-1.044821	2.419517	-0.059932	H	-1.110006	2.083186	-2.090199
C	-2.096428	0.534700	-0.574849	C	1.104899	2.044183	-2.455600
H	-1.787185	0.377439	-1.599999	H	1.453467	2.877296	-1.860475
C	-2.809571	-0.355044	0.255826	C	1.877145	1.169966	-3.217190
H	-3.242546	-1.297697	-0.054067	H	2.954727	1.179519	-3.319011
C	-2.954768	0.230520	1.576159	N	0.794852	0.024272	1.118781
N	2.049292	-0.597513	1.025621	N	-1.256479	0.056233	0.483910
N	1.632243	1.422689	1.598140	S	2.248565	-1.572372	-1.304404
S	-0.686248	-2.346242	1.512166	Ni	0.759486	0.019103	-1.715285
Ni	-0.825464	-0.191052	0.994515	C	1.522593	-3.318370	-1.412037
Br	1.035905	-0.204802	-2.420212	C	1.185539	-3.490674	-2.894042
C	1.234786	3.738159	0.808431	C	2.623979	-4.294725	-0.995602
H	-0.050516	2.508882	2.051928	C	0.274981	-3.460888	-0.549450
H	1.412881	3.064875	2.845742	H	2.260024	-5.318113	-1.137398
C	1.279916	5.091434	1.159787	H	3.524115	-4.170723	-1.604377
C	1.438880	6.070467	0.181656	H	2.898957	-4.194542	0.058507
C	1.562821	5.703342	-1.158133	H	0.806367	-4.505282	-3.054323
C	1.526659	4.355731	-1.511728	H	0.412040	-2.787585	-3.216405
C	1.364068	3.371642	-0.536546	H	2.068317	-3.361373	-3.527701
H	1.191881	5.382554	2.205049	H	-0.126258	-4.473519	-0.669935
H	1.473865	7.118318	0.467397	H	0.478481	-3.320349	0.516203

H	1.691661	6.465354	-1.921876	H	-0.494408	-2.746951	-0.853544
H	1.625237	4.054197	-2.550469	C	-2.472229	0.115761	-0.347440
H	1.341583	2.325175	-0.842902	H	-2.206145	-0.335622	-1.306370
H	-3.473746	-0.222121	2.411386	C	-3.652697	-0.578781	0.282765
C	-1.996836	-4.506883	0.467544	H	-2.713359	1.168698	-0.525845
C	-2.472981	-5.332940	-0.549651	C	-4.683151	0.171765	0.857558
C	-2.240923	-4.999326	-1.883858	C	-5.779117	-0.462417	1.442007
C	-1.538695	-3.837278	-2.203361	C	-5.852032	-1.853519	1.456169
C	-1.062789	-2.994412	-1.199193	C	-4.829758	-2.610132	0.881473
H	-2.171726	-4.757708	1.510308	C	-3.737384	-1.976116	0.296928
H	-3.024405	-6.234161	-0.296818	H	-4.634376	1.258391	0.840607
H	-2.611762	-5.644921	-2.675178	H	-6.576056	0.130701	1.880389
H	-1.354700	-3.569397	-3.239770	H	-6.706492	-2.348891	1.907496
H	-0.523275	-2.082167	-1.470853	H	-4.889638	-3.694512	0.882345
				H	-2.948836	-2.570496	-0.158298

TS-(2a-THF)-coord			**2a-THF**		
E (SCF) = -1339.06456879 E (SCF; solvent = THF) = -3143.755709 Zero-point correction = 0.558638 Thermal correction to Enthalpy = 0.590731 Thermal correction to Gibbs Free Energy = 0.494113			E (SCF) = -1339.08711648 E (SCF; solvent = THF) = -3143.78042 Zero-point correction = 0.558934 Thermal correction to Enthalpy = 0.591920 Thermal correction to Gibbs Free Energy = 0.489986		
C	-0.310682	-0.678296	-0.973858	C	0.381485	-0.159702	-0.691068
C	-0.673095	-2.494967	-2.290125	C	-0.726324	-1.930856	-1.546914
H	-1.138536	-3.069499	-3.075829	H	-1.522864	-2.451576	-2.054436
C	0.326531	-2.808905	-1.437279	C	0.415623	-2.399056	-0.988333
H	0.901470	-3.713621	-1.317143	H	0.803160	-3.401840	-0.900601
C	-2.071912	-0.509835	-2.791061	C	-1.821292	0.317850	-1.773538
H	-2.227186	-1.115695	-3.687553	H	-1.874542	0.306007	-2.868343
H	-1.676285	0.459049	-3.103718	H	-1.542376	1.325519	-1.455564
C	-3.400204	-0.343709	-2.064020	C	-3.182227	-0.073765	-1.203161
H	-3.636949	-1.250363	-1.500465	H	-3.460517	-1.079788	-1.532397
H	-4.190620	-0.172773	-2.799844	H	-3.919302	0.626423	-1.607385
C	-0.983966	1.663109	1.833901	C	-0.446827	2.603622	1.061600
H	-1.862342	1.333247	2.368621	H	-1.524041	2.516960	1.015120
C	0.226212	0.949389	1.696827	C	0.444565	1.632267	1.665247
H	0.457373	0.017656	2.196890	H	0.122122	0.743415	2.191488
C	1.180963	1.791821	0.970840	C	1.784907	2.136670	1.617206
H	2.221692	1.557756	0.786820	H	2.662804	1.679910	2.053158
C	0.512942	2.936791	0.582278	C	1.739523	3.289082	0.820228
H	0.910996	3.749634	-0.010131	H	2.590987	3.886747	0.517388
C	-0.859686	2.810800	1.021512	C	0.356114	3.597791	0.509940
H	-1.636242	3.546065	0.847549	H	0.019032	4.458242	-0.054231
N	-1.047514	-1.194308	-2.004085	N	-0.734281	-0.561892	-1.351119
N	0.542377	-1.692851	-0.652076	N	1.078582	-1.303415	-0.468402
S	-3.309928	1.093493	-0.939552	S	-3.165608	0.009391	0.624822
Ni	-0.596241	1.059811	-0.226845	Ni	0.917124	1.620050	-0.308528
C	-4.691781	0.759129	0.287382	C	-4.916946	-0.444155	1.102673
C	-4.788069	2.044346	1.114056	C	-4.888247	-0.387691	2.633717
C	-5.998456	0.534490	-0.476297	C	-5.911178	0.577488	0.550848
C	-4.355854	-0.440669	1.171350	C	-5.253645	-1.858104	0.629768
H	-6.820788	0.435588	0.241591	H	-6.919776	0.337499	0.907406

H	-6.225761	1.375887	-1.137151	H	-5.665085	1.590351	0.881472
H	-5.978771	-0.382878	-1.071703	H	-5.948020	0.568182	-0.543064
H	-5.583862	1.935896	1.858622	H	-5.880111	-0.638582	3.024810
H	-3.860100	2.258102	1.650979	H	-4.172180	-1.104509	3.047780
H	-5.031869	2.905590	0.484739	H	-4.628813	0.612719	2.994355
H	-5.151791	-0.585308	1.911006	H	-6.245276	-2.142471	1.000644
H	-4.280951	-1.367998	0.595024	H	-5.288618	-1.928796	-0.461838
H	-3.413819	-0.293849	1.705050	H	-4.527610	-2.585511	1.003761
O	-0.526239	2.127745	-2.231322	O	1.662839	1.953959	-2.103312
C	0.761727	2.049758	-2.886540	C	2.946071	1.397549	-2.486698
C	0.709622	3.085695	-3.998196	C	3.175519	1.912045	-3.897060
C	-0.140581	4.185781	-3.357373	C	2.547719	3.308113	-3.834085
C	-1.170268	3.386787	-2.566038	C	1.326319	3.091811	-2.948996
H	1.544601	2.277817	-2.152992	H	3.708614	1.756039	-1.784966
H	0.896831	1.022145	-3.234985	H	2.864203	0.311356	-2.411822
H	0.211588	2.677790	-4.884531	H	2.652834	1.282295	-4.624415
H	1.704246	3.426907	-4.295368	H	4.235245	1.932645	-4.161326
H	-0.608215	4.851859	-4.086305	H	2.275696	3.700318	-4.816608
H	0.472114	4.798593	-2.687428	H	3.239439	4.016723	-3.367227
H	-2.063204	3.160162	-3.159216	H	0.433963	2.819028	-3.521606
H	-1.485304	3.871117	-1.639523	H	1.094505	3.941811	-2.304520
C	1.624047	-1.674332	0.327230	C	2.364602	-1.386487	0.222386
H	1.783671	-0.632447	0.600178	H	2.594079	-0.363686	0.539724
C	1.371513	-2.542424	1.541379	C	2.358356	-2.341111	1.394445
H	2.533630	-2.006585	-0.184019	H	3.131870	-1.687726	-0.499439
C	2.463648	-3.109142	2.206663	C	3.485610	-3.129598	1.641523
C	2.271751	-3.874477	3.354280	C	3.528108	-3.974337	2.749392
C	0.984071	-4.089858	3.844041	C	2.438345	-4.045649	3.614746
C	-0.109059	-3.534668	3.181838	C	1.306469	-3.268863	3.368426
C	0.082398	-2.762347	2.036708	C	1.266432	-2.418820	2.265776
H	3.470564	-2.953761	1.825230	H	4.336820	-3.084038	0.965561
H	3.127788	-4.310816	3.860336	H	4.409475	-4.582516	2.930010
H	0.833660	-4.693105	4.734277	H	2.467930	-4.708164	4.474589
H	-1.114941	-3.705174	3.554682	H	0.451832	-3.325436	4.036340
H	-0.775790	-2.339665	1.520757	H	0.374909	-1.826917	2.074382

2c	**TS-(2c-THF)-coord**
E (SCF) = -1185.333063 E (SCF; solvent = THF) = -3065.10851 Zero-point correction = 0.494422 Thermal correction to Enthalpy = 0.524308 Thermal correction to Gibbs Free Energy = 0.43503	E (SCF) = -1417.683377 E (SCF; solvent = THF) = -3065.096269 Zero-point correction = 0.612064 Thermal correction to Enthalpy = 0.648291 Thermal correction to Gibbs Free Energy = 0.54360

C	0.129145	-1.031380	-0.293900	C	-0.195405	-0.503549	-0.759140
C	0.201165	-2.648422	-1.888290	C	-0.486119	-2.431076	-1.932082
H	-0.071282	-3.142155	-2.808151	H	-0.916719	-3.074791	-2.683364
C	1.100395	-2.979428	-0.932870	C	0.483164	-2.659108	-1.019056
H	1.768186	-3.821553	-0.844693	H	1.074239	-3.536085	-0.807672
C	-1.397137	-0.753501	-2.242409	C	-1.934437	-0.536492	-2.606281
H	-1.578625	-1.323580	-3.157097	H	-2.055448	-1.210926	-3.458102
H	-1.018203	0.230952	-2.536869	H	-1.584144	0.425964	-2.983907
C	-2.696089	-0.632754	-1.460862	C	-3.274376	-0.380987	-1.895556
H	-2.955710	-1.595944	-1.014222	H	-3.475208	-1.257620	-1.273433

H	-3.501008	-0.316271	-2.128393
C	1.919137	-2.004177	1.178415
C	-0.132849	1.624906	2.465242
H	-0.677076	1.451093	3.383466
C	1.051465	1.004898	2.067524
H	1.610275	0.261228	2.617147
C	1.426628	1.551559	0.769572
H	2.317194	1.281908	0.219128
C	0.497923	2.547455	0.411208
H	0.505540	3.153425	-0.484050
C	-0.520802	2.517266	1.402101
H	-1.412469	3.132138	1.396494
N	-0.375447	-1.458372	-1.483333
N	1.049757	-1.986037	0.031544
S	-2.527006	0.645505	-0.159874
Ni	-0.416913	0.572116	0.559532
C	3.245498	-1.575457	1.024978
C	4.068576	-1.601105	2.154742
C	3.614228	-2.057749	3.394087
C	2.291994	-2.506164	3.490481
C	1.427116	-2.499609	2.395716
C	3.801191	-1.129402	-0.302206
H	5.096357	-1.258867	2.058583
C	4.532267	-2.104463	4.584900
H	1.925223	-2.879384	4.443792
C	0.020828	-3.016505	2.519940
H	4.634115	-0.436178	-0.159773
H	4.190005	-1.982658	-0.870855
H	3.050487	-0.642651	-0.930282
H	3.985610	-1.953965	5.519740
H	5.028445	-3.079990	4.651104
H	5.314777	-1.344104	4.519169
H	-0.710404	-2.253936	2.235927
H	-0.145020	-3.881768	1.868064
H	-0.189217	-3.327340	3.545523
C	-3.877709	0.168157	1.081116
C	-3.954677	1.352791	2.045056
C	-5.187254	0.038500	0.300590
C	-3.527229	-1.116093	1.821951
H	-6.006497	-0.095630	1.015108
H	-5.401812	0.936825	-0.286078
H	-5.196481	-0.829535	-0.364074
H	-4.749443	1.162620	2.773967
H	-3.022831	1.484902	2.600135
H	-4.194312	2.284581	1.524182
H	-4.338248	-1.359960	2.517445
H	-3.410080	-1.970998	1.149141
H	-2.608608	-0.997248	2.401961

H	-4.066502	-0.298316	-2.644928
C	1.640527	-1.401293	0.731090
C	-0.834566	2.083875	1.790201
H	-1.683398	1.780573	2.385682
C	0.394365	1.392327	1.662724
H	0.690726	0.517046	2.221158
C	1.294570	2.189275	0.829848
H	2.327826	1.946952	0.624672
C	0.576119	3.275251	0.368191
H	0.922194	4.041224	-0.313173
C	-0.775293	3.156356	0.878097
H	-1.581345	3.849255	0.667695
N	-0.886834	-1.117129	-1.767513
N	0.651762	-1.480239	-0.312025
S	-3.256958	1.131070	-0.869745
Ni	-0.490869	1.301942	-0.209346
C	2.926472	-0.941989	0.414628
C	3.878512	-0.923912	1.437046
C	3.585421	-1.360914	2.731729
C	2.298911	-1.843645	2.991961
C	1.309673	-1.882662	2.007247
C	3.286466	-0.506060	-0.980116
H	4.881388	-0.569760	1.210118
C	4.621804	-1.301225	3.820471
H	2.058196	-2.206010	3.988597
C	-0.065151	-2.412203	2.315494
H	4.325591	-0.172695	-1.025155
H	3.168401	-1.324748	-1.698807
H	2.649346	0.316246	-1.321295
H	4.557461	-0.351953	4.365626
H	4.484955	-2.104638	4.549301
H	5.634243	-1.376738	3.415201
H	-0.843366	-1.690968	2.043757
H	-0.277492	-3.334398	1.763000
H	-0.163885	-2.635271	3.379948
C	-4.586646	0.799922	0.410389
C	-4.756619	2.139373	1.132924
C	-5.889852	0.418136	-0.293777
C	-4.141353	-0.293272	1.380760
H	-6.686942	0.319701	0.452103
H	-6.193568	1.182606	-1.014729
H	-5.813967	-0.541453	-0.813538
H	-5.515735	2.034668	1.915362
H	-3.829371	2.466764	1.611555
H	-5.087280	2.923289	0.444990
H	-4.910877	-0.441153	2.147359
H	-3.998559	-1.255018	0.878290
H	-3.206035	-0.026417	1.879160
O	-0.564974	2.200853	-2.291575
C	0.679354	2.121404	-3.022256
C	0.473656	2.993038	-4.249890
C	-0.384342	4.125792	-3.680564
C	-1.291901	3.394262	-2.695654
H	1.490081	2.499561	-2.386916
H	0.867687	1.067123	-3.242630

	H -0.072120 2.444140 -5.025127 H 1.416945 3.339755 -4.678819 H -0.953742 4.662316 -4.443183 H 0.246353 4.853736 -3.159234 H -2.231991 3.071385 -3.155284 H -1.527611 3.975949 -1.802094

2c-THF	***R*-2a**
E (SCF) = -1417.70021881 E (SCF; solvent = THF) = -3065.122691 Zero-point correction = 0.612609 Thermal correction to Enthalpy = 0.649653 Thermal correction to Gibbs Free Energy = 0.54080	E (SCF) = -1185.33304904 E (SCF; solvent = THF) = -2832.614903 E (SCF; solvent = DCM) = -2911.277611 Zero-point correction = 0.494694 Thermal correction to Enthalpy = 0.524452 Thermal correction to Gibbs Free Energy = 0.43595
C 0.291340 -0.452091 -0.450909 C -0.662984 -2.336025 -1.268492 H -1.371410 -2.924472 -1.830220 C 0.398150 -2.712317 -0.516699 H 0.801725 -3.686957 -0.292188 C -1.785030 -0.164306 -1.819875 H -1.762482 -0.327276 -2.903645 H -1.544364 0.882549 -1.627718 C -3.176553 -0.507560 -1.295110 H -3.401243 -1.563903 -1.472531 H -3.894732 0.088626 -1.865785 C 2.069938 -1.582713 0.911537 C -0.397845 2.370174 1.425256 H -1.468547 2.306535 1.559332 C 0.567448 1.377165 1.820070 H 0.343190 0.482209 2.382847 C 1.895996 1.862528 1.527608 H 2.821248 1.354942 1.761417 C 1.733692 3.038681 0.798767 H 2.523414 3.634951 0.358503 C 0.313702 3.348838 0.731315 H -0.110603 4.217259 0.243087 N -0.717700 -0.955360 -1.211225 N 0.970262 -1.553236 -0.018591 S -3.315580 -0.121917 0.487990 Ni 0.658760 1.392385 -0.196697 C 3.371205 -1.318652 0.459466 C 4.410815 -1.391792 1.388429 C 4.188353 -1.722863 2.728387 C 2.879838 -2.001415 3.129548 C 1.803045 -1.949071 2.240873 C 3.658810 -0.961572 -0.972041 H 5.425974 -1.195866 1.050855 C 5.326001 -1.767473 3.711835 H 2.687823 -2.278220 4.163614 C 0.419240 -2.312925 2.713871 H 4.724390 -1.065021 -1.189102 H 3.107329 -1.597498 -1.671504	C -0.238940 -0.910178 -0.825808 C -0.737829 -3.025680 -1.486549 H -1.289805 -3.795942 -2.002507 C 0.356453 -3.094678 -0.693482 H 0.951002 -3.935309 -0.372782 C -2.208676 -1.178558 -2.324693 H -2.672432 -2.028406 -2.831903 H -1.842758 -0.492604 -3.096034 C -3.238048 -0.502907 -1.432121 H -3.450629 -1.129032 -0.561951 H -4.162054 -0.338556 -1.991389 C -3.610126 1.465508 0.686907 C -5.089606 1.269588 0.349497 H -5.339985 0.224249 0.149667 H -5.395758 1.877274 -0.507375 H -5.687809 1.584421 1.211325 C -3.161510 0.555353 1.823186 H -3.766470 0.767710 2.711988 H -2.113530 0.731478 2.077605 H -3.292475 -0.505440 1.588893 C -3.334372 2.932676 1.017053 H -3.902441 3.205440 1.912560 H -3.647890 3.596598 0.206019 H -2.277161 3.107351 1.230542 C 1.802728 -1.503570 0.514336 C 0.446777 2.677919 0.395777 H 0.142812 3.035546 1.370186 C 1.433765 1.731519 0.126579 H 2.049597 1.211574 0.846125 C 1.502036 1.562059 -1.318904 H 2.193825 0.908983 -1.832232 C 0.604346 2.464574 -1.926809 H 0.435646 2.600840 -2.985874 C -0.122308 3.072522 -0.870351 H -0.930356 3.782775 -0.996811 N -1.081726 -1.687903 -1.558230 N 0.652618 -1.799766 -0.299022 S -2.622195 1.136962 -0.897361

H	3.375459	0.077132	-1.175129
H	5.481113	-0.784730	4.172869
H	5.130869	-2.478478	4.518953
H	6.263780	-2.051169	3.226554
H	-0.364644	-1.735592	2.215175
H	0.203725	-3.371403	2.524811
H	0.328710	-2.156366	3.791671
C	-5.083850	-0.583254	0.891835
C	-5.203928	-0.249452	2.382617
C	-6.063357	0.262885	0.078279
C	-5.317573	-2.076505	0.662659
H	-7.090120	0.036693	0.388909
H	-5.888129	1.331191	0.232823
H	-5.999317	0.051419	-0.993787
H	-6.215375	-0.489251	2.727816
H	-4.497415	-0.831565	2.982685
H	-5.028333	0.814300	2.571269
H	-6.328660	-2.344825	0.990671
H	-5.242903	-2.348011	-0.395114
H	-4.603537	-2.681283	1.228653
O	0.741051	1.878931	-2.129463
C	1.479820	1.166996	-3.150454
C	0.965942	1.760886	-4.448003
C	0.827809	3.243514	-4.083563
C	0.420510	3.217192	-2.608044
H	2.552996	1.349934	-3.015896
H	1.275204	0.104070	-3.016438
H	-0.005396	1.327264	-4.707400
H	1.649889	1.591392	-5.282835
H	0.093005	3.765903	-4.700085
H	1.787862	3.754058	-4.205100
H	-0.652465	3.359872	-2.451229
H	0.969336	3.944553	-2.005313
Ni	-0.405713	0.975102	-0.702128
C	3.063015	-1.449138	-0.098713
C	4.165285	-1.159615	0.711056
C	4.041960	-0.954912	2.086985
C	2.768416	-1.052936	2.659439
C	1.634511	-1.336270	1.897570
C	3.257696	-1.725501	-1.566662
H	5.148798	-1.099826	0.250912
C	5.249349	-0.676029	2.939840
H	2.655164	-0.913526	3.732050
C	0.283639	-1.465981	2.544176
H	4.160785	-1.233904	-1.936988
H	3.380346	-2.799674	-1.749419
H	2.411089	-1.393869	-2.173666
H	6.060468	-0.233487	2.356113
H	5.011048	0.002198	3.763869
H	5.631530	-1.603431	3.382544
H	-0.429951	-0.752792	2.121240
H	-0.135366	-2.467860	2.396997
H	0.349582	-1.287130	3.619448

TS-inversion (2a)			***S*-2a**		
E (SCF) = -1185.31751426 E (SCF; solvent = THF) = -2832.593135 E (SCF; solvent = DCM) = -2911.260047 Zero-point correction = 0.493104 Thermal correction to Enthalpy = 0.522787 Thermal correction to Gibbs Free Energy = 0.43280			E (SCF) = -1185.33105615 E (SCF; solvent = THF) = -2832.60782 E (SCF; solvent = DCM) = -2911.275188 Zero-point correction = 0.494106 Thermal correction to Enthalpy = 0.524107 Thermal correction to Gibbs Free Energy = 0.43473		
C	4.705647	8.784785	3.103937	C	-0.141000	-1.022679	-0.687323
C	4.194102	6.663613	2.491696	C	-0.561208	-3.111895	-1.457086
H	3.623670	5.880838	2.016112	H	-1.113744	-3.887858	-1.963879
C	5.339868	6.616563	3.212723	C	0.635670	-3.140467	-0.821228
H	5.966726	5.786957	3.498694	H	1.332128	-3.946858	-0.654885
C	2.624941	8.500709	1.777554	C	-2.294868	-1.305230	-1.835214
H	2.206677	7.690909	1.174196	H	-2.750116	-2.067084	-2.474371
H	2.911802	9.313419	1.103776	H	-2.116601	-0.409743	-2.437354
C	1.576050	8.981694	2.775189	C	-3.222223	-0.990998	-0.670203
H	1.282700	8.173002	3.449748	H	-3.448331	-1.894492	-0.098584
H	0.699145	9.331728	2.224097	H	-4.158415	-0.581120	-1.053075

C	0.897027	11.180063	4.722979	C	-3.868062	1.536499	0.641956
C	-0.098518	11.820216	3.758298	C	-4.173702	2.179195	-0.706789
H	-0.587954	11.080425	3.117920	H	-4.607240	1.470365	-1.418602
H	0.382700	12.568432	3.123700	H	-3.282754	2.618463	-1.159892
H	-0.886177	12.315829	4.337207	H	-4.912106	2.975879	-0.563311
C	0.237441	10.114886	5.596369	C	-5.097930	0.831119	1.221346
H	-0.549859	10.587749	6.194360	H	-5.883239	1.577374	1.384275
H	0.954823	9.653337	6.279905	H	-4.876610	0.359761	2.183012
H	-0.238123	9.329817	5.001239	H	-5.510878	0.073964	0.548978
C	1.599284	12.234387	5.575209	C	-3.340174	2.556246	1.651773
H	0.847631	12.738768	6.191654	H	-4.123879	3.295742	1.846460
H	2.087198	12.995151	4.959746	H	-2.464144	3.090026	1.280531
H	2.339346	11.786923	6.244486	H	-3.084799	2.082899	2.604760
C	6.797968	8.259560	4.363844	C	2.063077	-1.507452	0.387354
C	5.207271	12.503171	4.220820	C	0.266024	2.641427	0.596051
H	4.887769	12.920404	5.166354	H	0.016621	3.005606	1.583944
C	6.262940	11.618843	4.017071	C	1.326689	1.805084	0.265297
H	6.929436	11.207004	4.761569	H	2.060832	1.382459	0.936797
C	6.268657	11.291364	2.601746	C	1.232256	1.540537	-1.157762
H	6.980402	10.631323	2.124705	H	1.926591	0.932570	-1.721300
C	5.306529	12.105299	1.927854	C	0.185420	2.333415	-1.712723
H	5.108733	12.124104	0.865383	H	-0.092196	2.399272	-2.755465
C	4.591800	12.772097	2.932259	C	-0.468855	2.932631	-0.621271
H	3.732137	13.412146	2.777599	H	-1.328443	3.586737	-0.685161
N	3.825882	7.995748	2.431244	N	-1.013244	-1.808287	-1.367845
N	5.640239	7.919348	3.579427	N	0.880443	-1.857374	-0.355393
S	2.282178	10.368412	3.727444	S	-2.499549	0.229933	0.514535
Ni	4.475770	10.646013	3.329688	Ni	-0.498846	0.797296	-0.349191
C	8.050204	8.303056	3.734073	C	3.273003	-1.346766	-0.303128
C	9.159004	8.627584	4.520479	C	4.404275	-1.005772	0.444015
C	9.048300	8.881116	5.889579	C	4.357273	-0.847266	1.830613
C	7.780651	8.805037	6.477513	C	3.132187	-1.041996	2.478451
C	6.639076	8.489343	5.739352	C	1.970936	-1.380460	1.782843
C	8.225290	7.984894	2.272057	C	3.388368	-1.557288	-1.790461
H	10.137215	8.676075	4.047879	H	5.349146	-0.865675	-0.075869
C	10.264702	9.189653	6.719208	C	5.597697	-0.514635	2.614053
H	7.677781	8.987583	7.544691	H	3.080299	-0.937016	3.559654
C	5.292539	8.396765	6.403754	C	0.675047	-1.600679	2.514596
H	9.142351	8.435791	1.885324	H	4.214249	-0.970759	-2.200669
H	8.306011	6.903469	2.109861	H	3.595869	-2.608329	-2.024005
H	7.387243	8.335256	1.662679	H	2.474863	-1.286287	-2.326843
H	11.056217	9.644985	6.118407	H	6.336123	0.003782	1.997097
H	10.027881	9.867398	7.543908	H	5.370338	0.115718	3.478201
H	10.674095	8.272533	7.159120	H	6.070788	-1.428018	2.993653
H	4.605791	9.162130	6.025126	H	-0.053589	-0.814872	2.286669
H	4.822064	7.423858	6.223815	H	0.215669	-2.556920	2.242426
H	5.386591	8.527898	7.483914	H	0.839204	-1.603890	3.594286

***R*-2c**	**TS-inversion (2c)**
E (SCF) = -1106.718383 E (SCF; solvent = THF) = -2911.271506 E (SCF; solvent = DCM) = -2832.621163 Zero-point correction = 0.440080 Thermal correction to Enthalpy = 0.466167 Thermal correction to Gibbs Free Energy = 0.38337	E (SCF) = -1106.69985154 E (SCF; solvent = THF) = -2911.253798 E (SCF; solvent = DCM) = -2832.599463 Zero-point correction = 0.439672 Thermal correction to Enthalpy = 0.465270 Thermal correction to Gibbs Free Energy = 0.38282
C -0.155083 -0.420676 -0.999062 C -0.838470 -2.529324 -1.450028 H -1.486518 -3.299636 -1.838478 C 0.348229 -2.611638 -0.799251 H 0.931486 -3.466269 -0.496051 C -2.335561 -0.613459 -2.138413 H -2.906109 -1.424338 -2.599404 H -2.058176 0.091750 -2.927802 C -3.192627 0.065108 -1.076444 H -3.394810 -0.628932 -0.257938 H -4.143374 0.381472 -1.512445 C -2.647319 1.415898 1.474562 C -4.156396 1.392164 1.721543 H -4.635242 0.494819 1.319009 H -4.648595 2.271357 1.296024 H -4.336645 1.395959 2.801940 C -1.953325 0.180608 2.035401 H -2.108817 0.148279 3.119675 H -0.878023 0.216470 1.842486 H -2.350255 -0.752772 1.625444 C -2.029687 2.692141 2.047902 H -2.188616 2.705568 3.131162 H -2.495349 3.590611 1.631536 H -0.952085 2.732567 1.865215 C 2.015875 -0.968958 0.140587 H 1.862548 0.015787 0.588327 H 2.790964 -0.873177 -0.626796 C 2.439030 -1.985023 1.170691 C 1.815095 -2.037696 2.422818 H 1.020821 -1.334445 2.661567 C 2.212355 -2.978068 3.368848 H 1.726895 -3.007393 4.339909 C 3.240110 -3.875196 3.074438 H 3.552685 -4.605032 3.815265 C 3.869976 -3.827277 1.832782 H 4.675742 -4.517596 1.601993 C 3.470250 -2.885424 0.885180 H 3.971290 -2.844646 -0.079600 C 0.331029 3.508634 -0.801722 H -0.092859 4.219370 -0.104068 C 1.457603 2.696795 -0.579669 H 2.063057 2.655245 0.315325 C 1.610100 1.891853 -1.753489 H 2.383064 1.152432 -1.916981	C 4.834299 8.941745 2.451749 C 4.160995 6.847643 1.928927 H 3.487758 6.081560 1.576613 C 5.433618 6.768332 2.388896 H 6.083439 5.919932 2.533259 C 2.496637 8.728263 1.661773 H 1.921021 7.949954 1.154143 H 2.620023 9.566102 0.969288 C 1.746221 9.179035 2.912963 H 1.602576 8.342587 3.601867 H 0.772287 9.576253 2.615395 C 1.675035 11.246128 5.117055 C 0.408729 11.859359 4.524739 H -0.239575 11.107938 4.064708 H 0.642637 12.625528 3.781363 H -0.166522 12.328853 5.330929 C 1.357041 10.145437 6.126784 H 0.784304 10.579250 6.954446 H 2.268003 9.701470 6.536309 H 0.743039 9.351032 5.692183 C 2.573684 12.317225 5.729633 H 2.052017 12.761957 6.583616 H 2.786688 13.117743 5.016436 H 3.517385 11.899774 6.092686 C 7.148445 8.389981 3.257885 H 7.064308 9.412442 3.631607 H 7.876231 8.383048 2.439726 C 7.579034 7.442094 4.349097 C 6.931310 7.451038 5.590485 H 6.113656 8.146440 5.767702 C 7.331882 6.578638 6.597683 H 6.827973 6.594256 7.559678 C 8.385980 5.690434 6.376045 H 8.700427 5.013216 7.164544 C 9.037783 5.678493 5.145282 H 9.862143 4.993721 4.970210 C 8.634129 6.551276 4.134697 H 9.150918 6.544824 3.177385 C 5.262627 12.852149 3.029472 H 4.981419 13.458374 3.880720 C 6.413870 12.052145 2.934940 H 7.175211 11.917821 3.690867 C 6.334525 11.392561 1.665813 H 7.062310 10.695856 1.269369

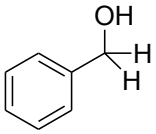
C	0.677731	2.341455	-2.760836
H	0.599358	1.955916	-3.768163
C	-0.128964	3.307730	-2.161755
H	-0.973336	3.813799	-2.612000
N	-1.126346	-1.181720	-1.565458
N	0.748182	-1.315724	-0.526492
S	-2.384100	1.574871	-0.393464
Ni	-0.251509	1.454651	-0.994572

C	5.232042	11.954609	0.908055
H	4.964625	11.691069	-0.106092
C	4.561290	12.822061	1.757846
H	3.644729	13.355621	1.541953
N	3.812774	8.185280	1.971016
N	5.825802	8.055927	2.707398
S	2.714231	10.497716	3.727111
Ni	4.696986	10.804811	2.720745

***S*-2c**			**THF**		
E (SCF) = -1106.71340015 E (SCF; solvent = THF) = -2911.268974 E (SCF; solvent = DCM) = -2832.614094 Zero-point correction = 0.440623 Thermal correction to Enthalpy = 0.466514 Thermal correction to Gibbs Free Energy = 0.38490			E (SCF) = -232.373176 Zero-point correction = 0.117293 Thermal correction to Enthalpy = 0.123171 Thermal correction to Gibbs Free Energy = 0.08881		
C	0.026531	-0.661074	-0.925435	O	0.867132	2.649561	-3.224959
C	-0.589515	-2.756663	-1.505354	C	2.004885	2.362944	-4.035264
H	-1.246510	-3.535589	-1.860030	C	1.942368	3.312949	-5.232848
C	0.706772	-2.799932	-1.105987	C	1.187777	4.506696	-4.641936
H	1.395762	-3.625865	-1.027627	C	0.194365	3.800058	-3.723405
C	-2.318810	-0.892572	-1.595742	H	2.918992	2.528658	-3.445271
H	-2.929938	-1.649244	-2.095281	H	1.982302	1.306123	-4.328653
H	-2.233128	-0.027382	-2.258825	H	1.361710	2.865818	-6.047937
C	-2.979559	-0.486825	-0.280501	H	2.931483	3.567654	-5.624288
H	-3.254032	-1.364923	0.308791	H	0.703587	5.135722	-5.394595
H	-3.882796	0.087112	-0.499556	H	1.867357	5.136667	-4.056278
C	-3.032192	1.816187	1.539995	H	-0.706383	3.498979	-4.282877
C	-3.604767	2.772489	0.501233	H	-0.126804	4.412837	-2.873422
H	-4.191126	2.255972	-0.264982				
H	-2.821637	3.350041	0.007362				
H	-4.278891	3.477255	1.000707				
C	-4.139917	1.038153	2.256047				
H	-4.755720	1.749138	2.817544				
H	-3.733186	0.313657	2.967375				
H	-4.804947	0.515706	1.562594				
C	-2.161318	2.545626	2.565145				
H	-2.767420	3.305758	3.068750				
H	-1.311535	3.049884	2.099176				
H	-1.780145	1.859738	3.327346				
C	2.392265	-1.136807	-0.239325				
H	2.272766	-0.142718	0.198023				
H	3.077648	-1.055718	-1.089502				
C	2.924342	-2.123277	0.769547				
C	2.347351	-2.216932	2.041982				
H	1.513762	-1.569966	2.306635				
C	2.839097	-3.129653	2.970144				
H	2.389227	-3.193891	3.956560				
C	3.914886	-3.955020	2.637776				
H	4.300436	-4.663626	3.364757				
C	4.497438	-3.863794	1.376001				
H	5.338720	-4.499059	1.115561				

C	4.002274	-2.951122	0.444497
H	4.464634	-2.876854	-0.537431
C	0.023602	3.292574	-0.499264
H	-0.365189	3.943645	0.272788
C	1.297045	2.680120	-0.490072
H	2.036020	2.735164	0.297329
C	1.370030	1.906306	-1.678956
H	2.207703	1.296007	-1.990476
C	0.207593	2.193717	-2.502846
H	0.023268	1.789338	-3.489226
C	-0.616947	3.042780	-1.774527
H	-1.579604	3.428117	-2.082699
N	-0.985571	-1.437757	-1.388953
N	1.062893	-1.511568	-0.748624
S	-1.861277	0.539679	0.777895
Ni	-0.236017	1.179558	-0.615981

Figure S15. ^{1}H NMR spectrum of benzyl alcohol



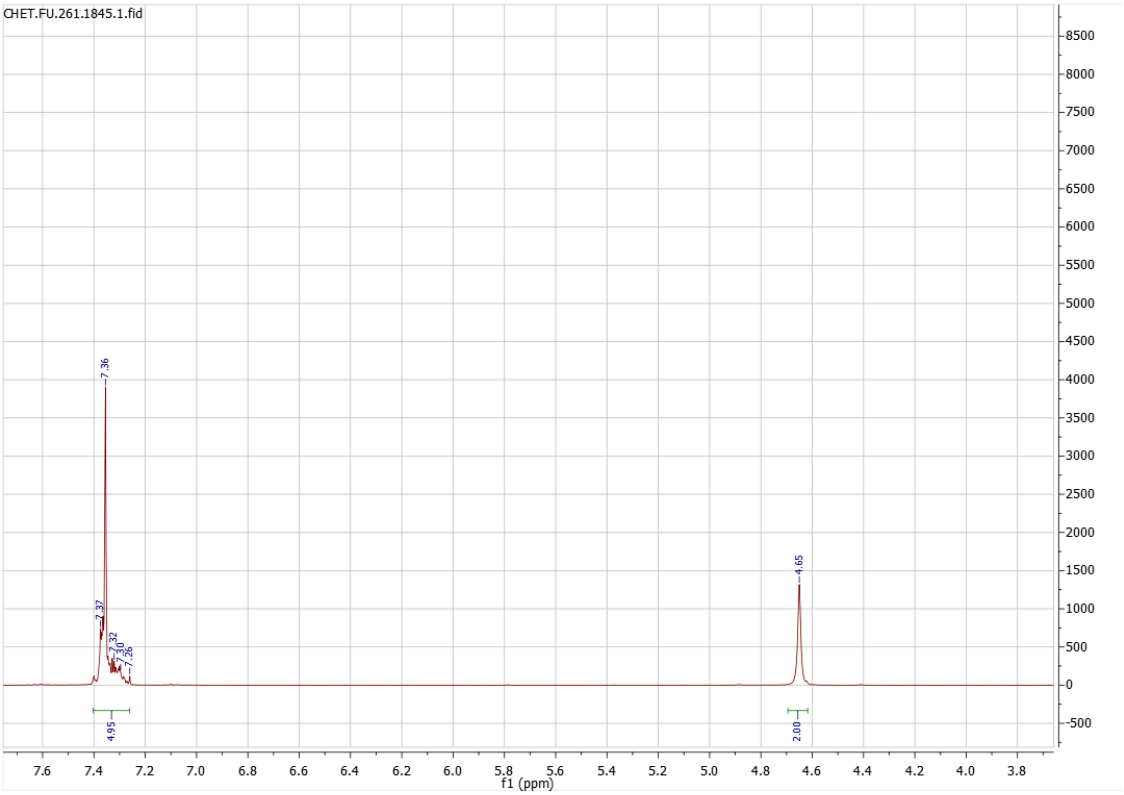


Figure S16. ^{13}C {^{1}H} NMR spectrum of benzyl alcohol

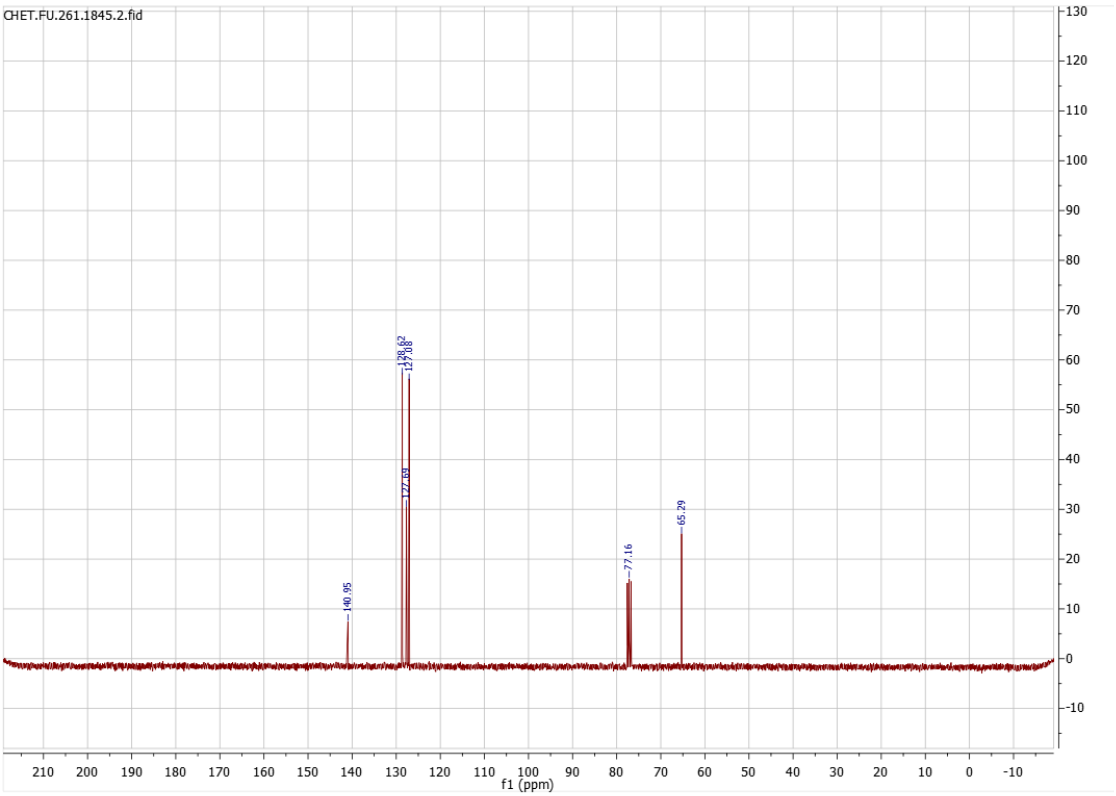
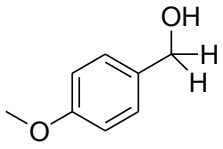


Figure S17. ^{1}H NMR spectrum of 4-methoxybenzyl alcohol



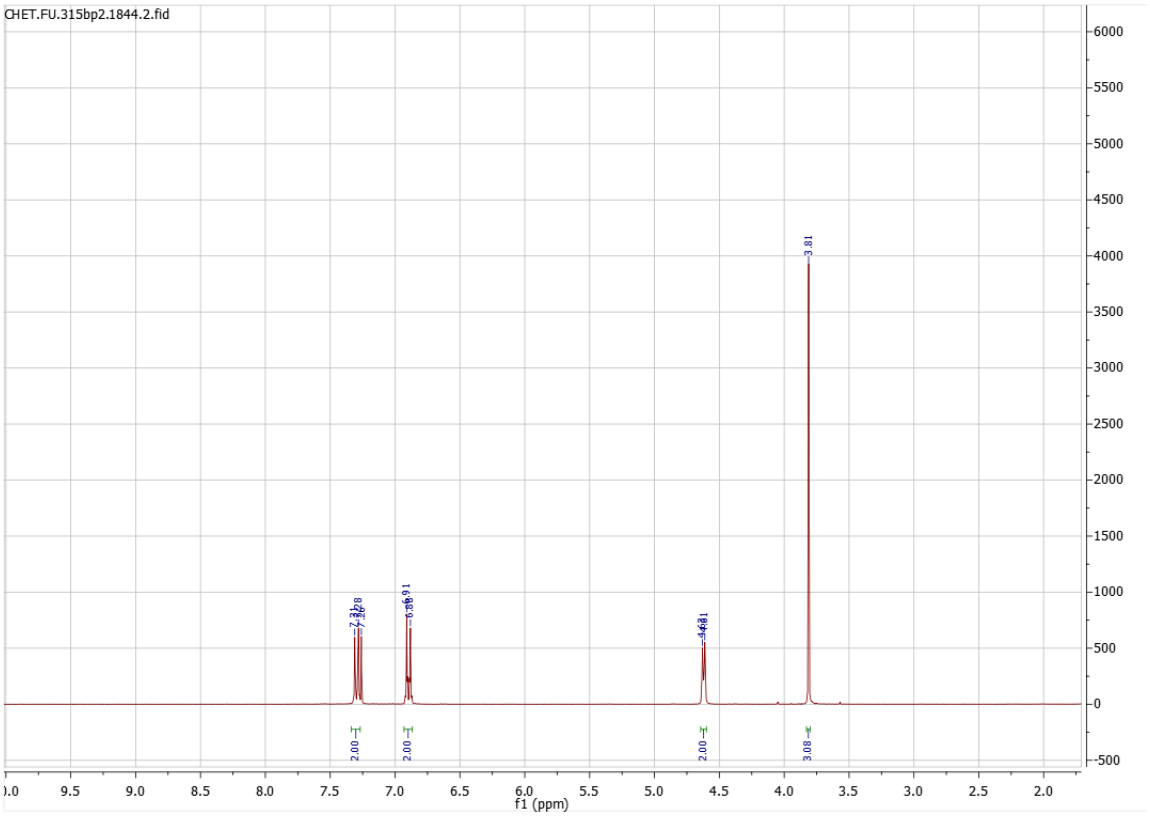


Figure S18. ^{13}C {^{1}H} NMR spectrum of 4-methoxybenzyl alcohol

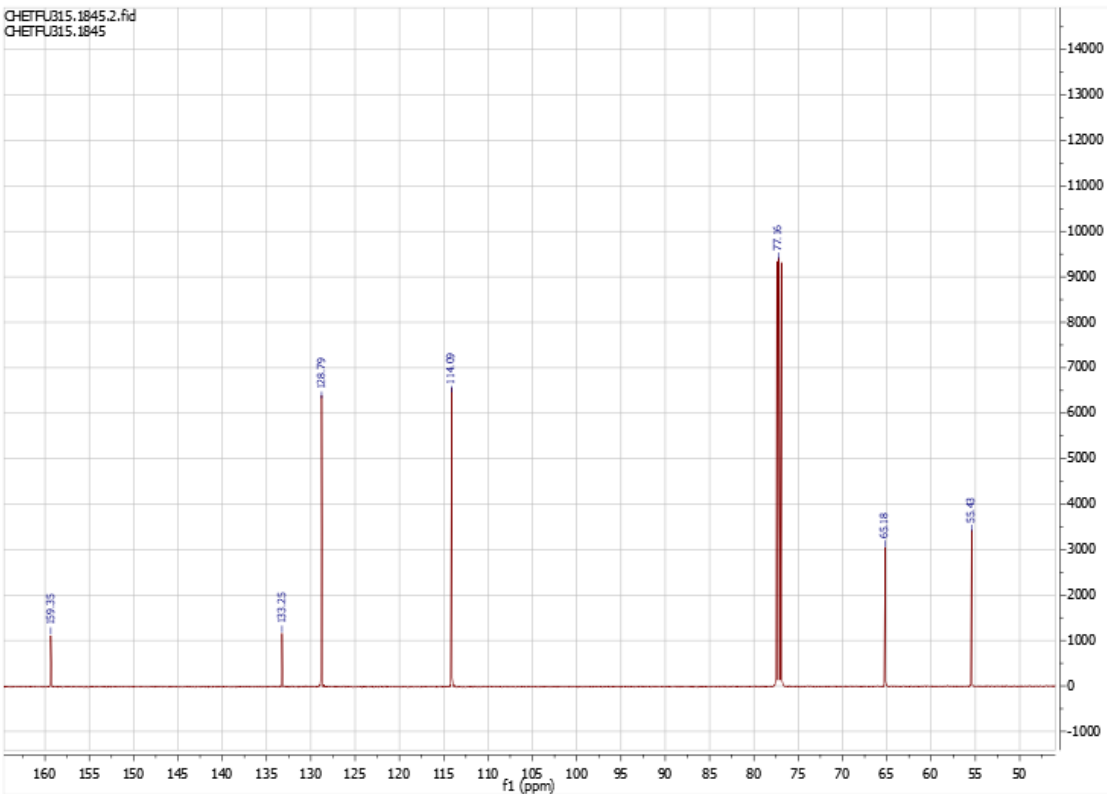


Figure S19. ^{1}H NMR spectrum of 4-cyanobenzyl alcohol

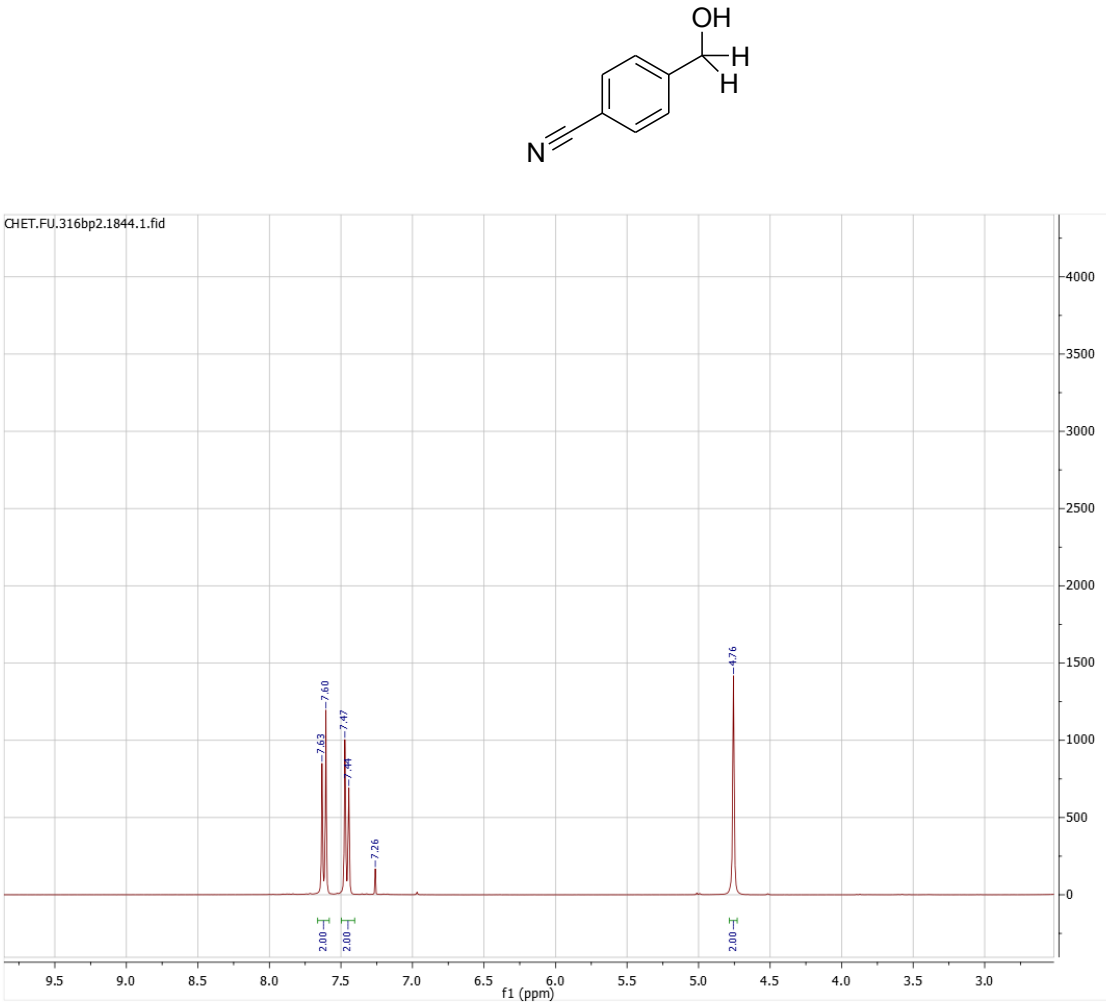


Figure S20. ^{13}C {^{1}H} NMR spectrum of 4-cyanobenzyl alcohol

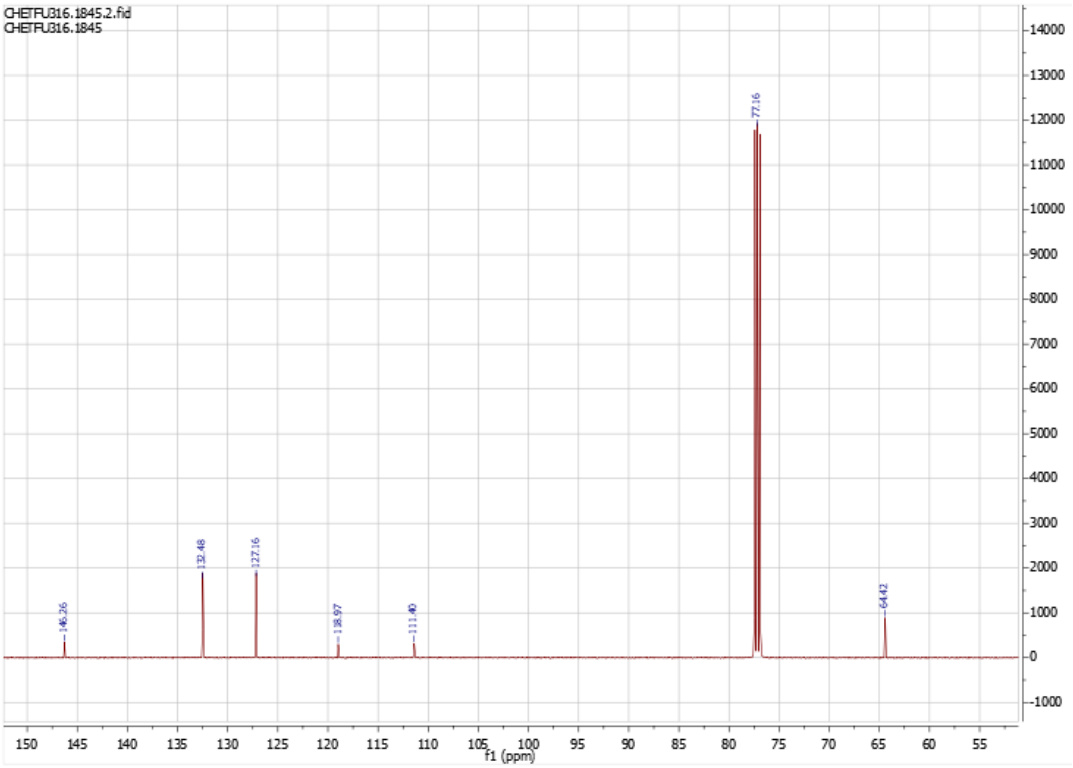
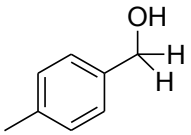


Figure S21. ^{1}H NMR spectrum of 4-methylbenzyl alcohol



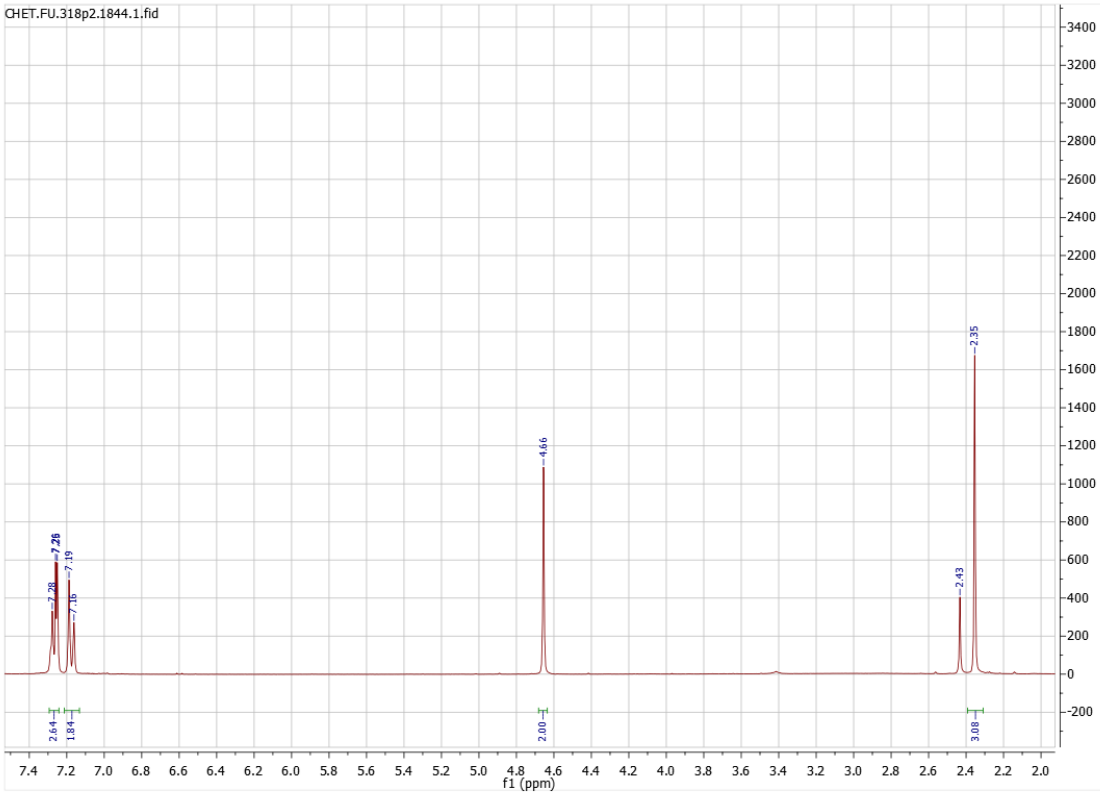


Figure S22. ^{13}C {^{1}H} NMR spectrum of 4-methylbenzyl alcohol

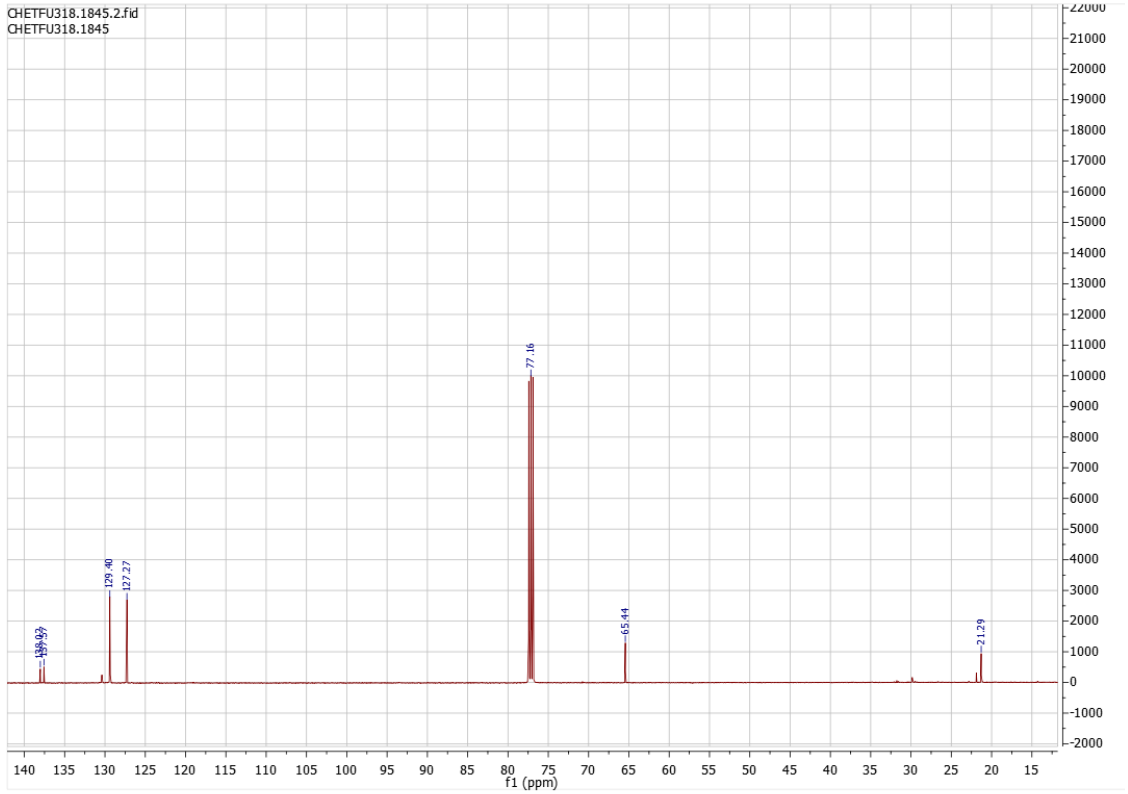
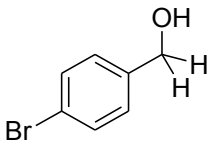


Figure S23. ^{1}H NMR spectrum of 4-bromobenzyl alcohol



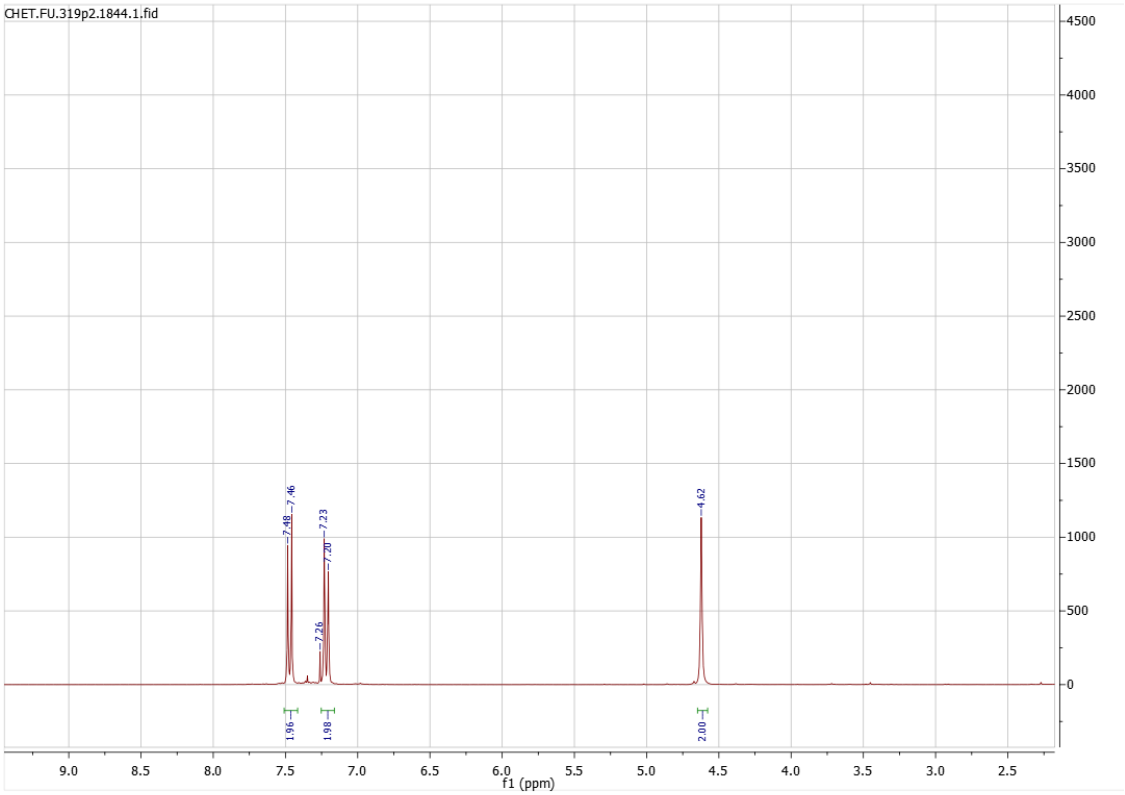


Figure S24. ^{13}C {^{1}H} NMR spectrum of 4-bromobenzylic alcohol

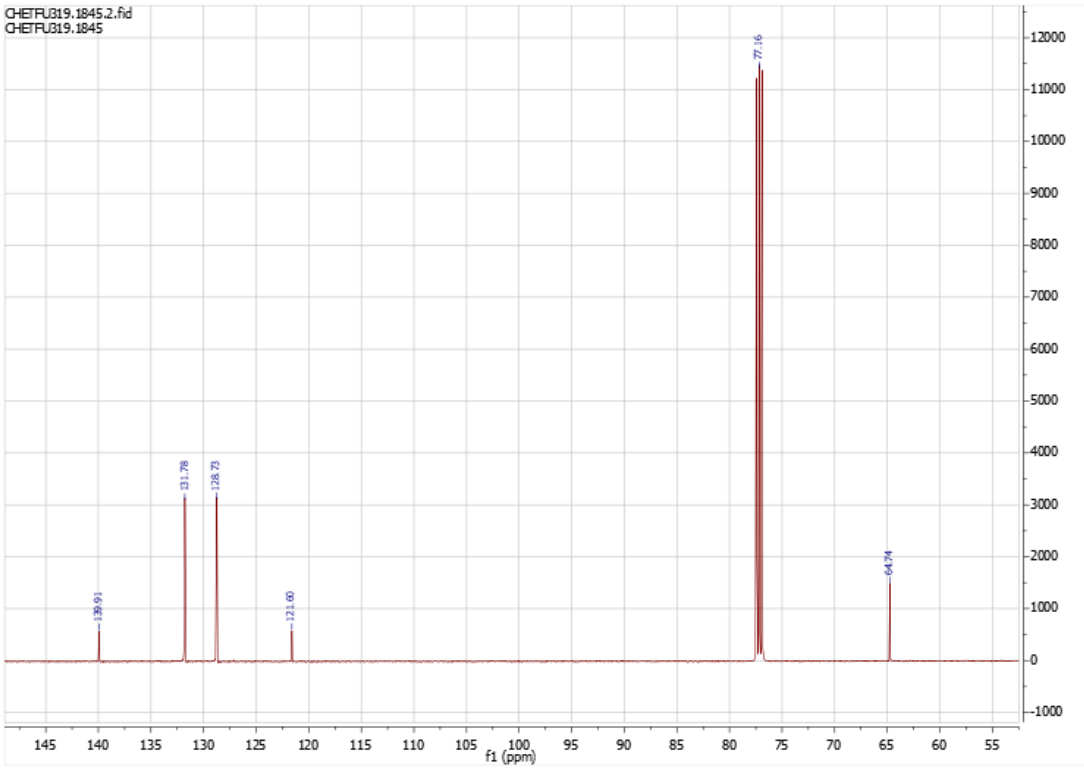
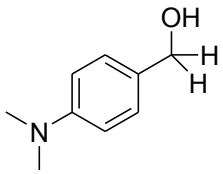


Figure S25. ^{1}H NMR spectra of 4-(*N,N*-dimethylamino)benzyl alcohol



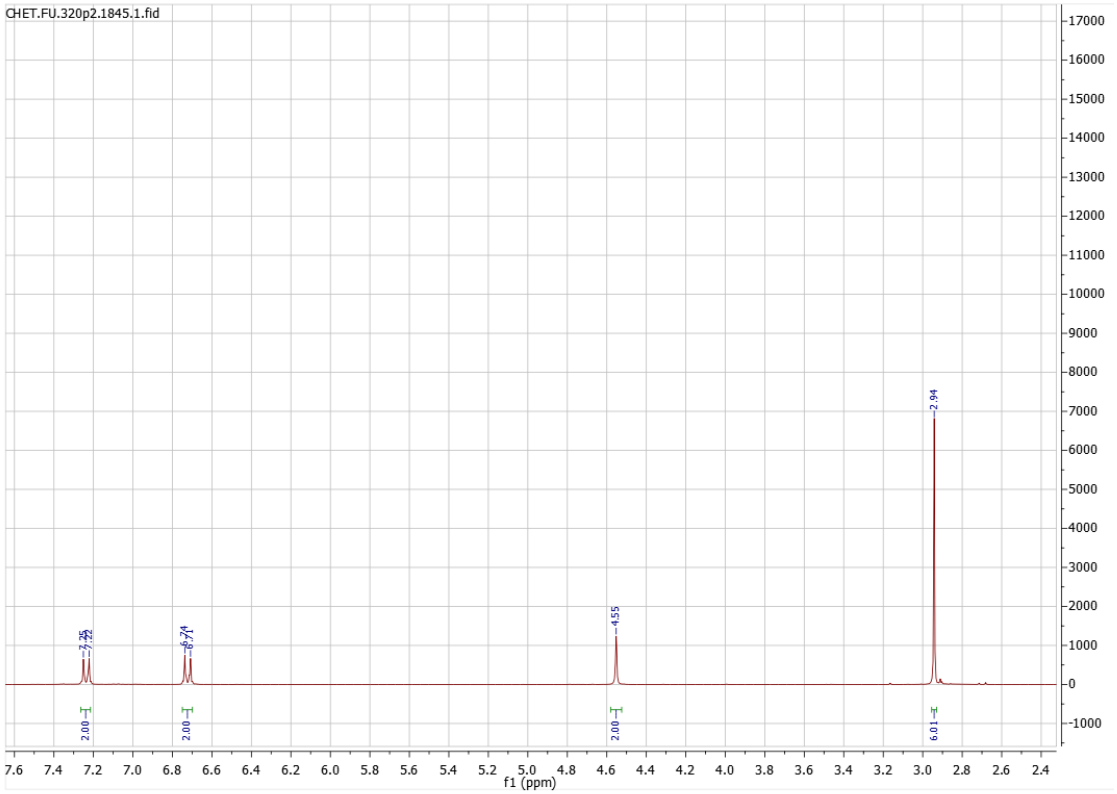


Figure S26. ^{13}C {^{1}H} NMR spectra of 4-(*N,N*-dimethylamino)benzyl alcohol

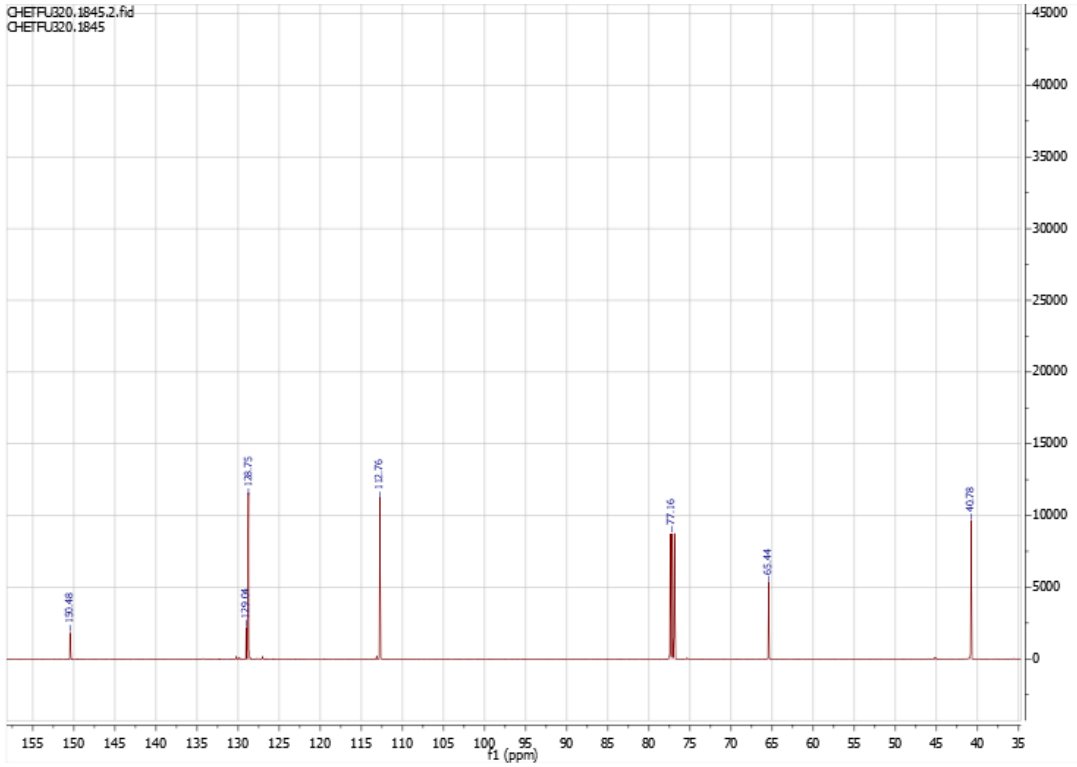


Figure S27. ^{1}H NMR spectra of methyl 4-(hydroxymethyl) benzoate

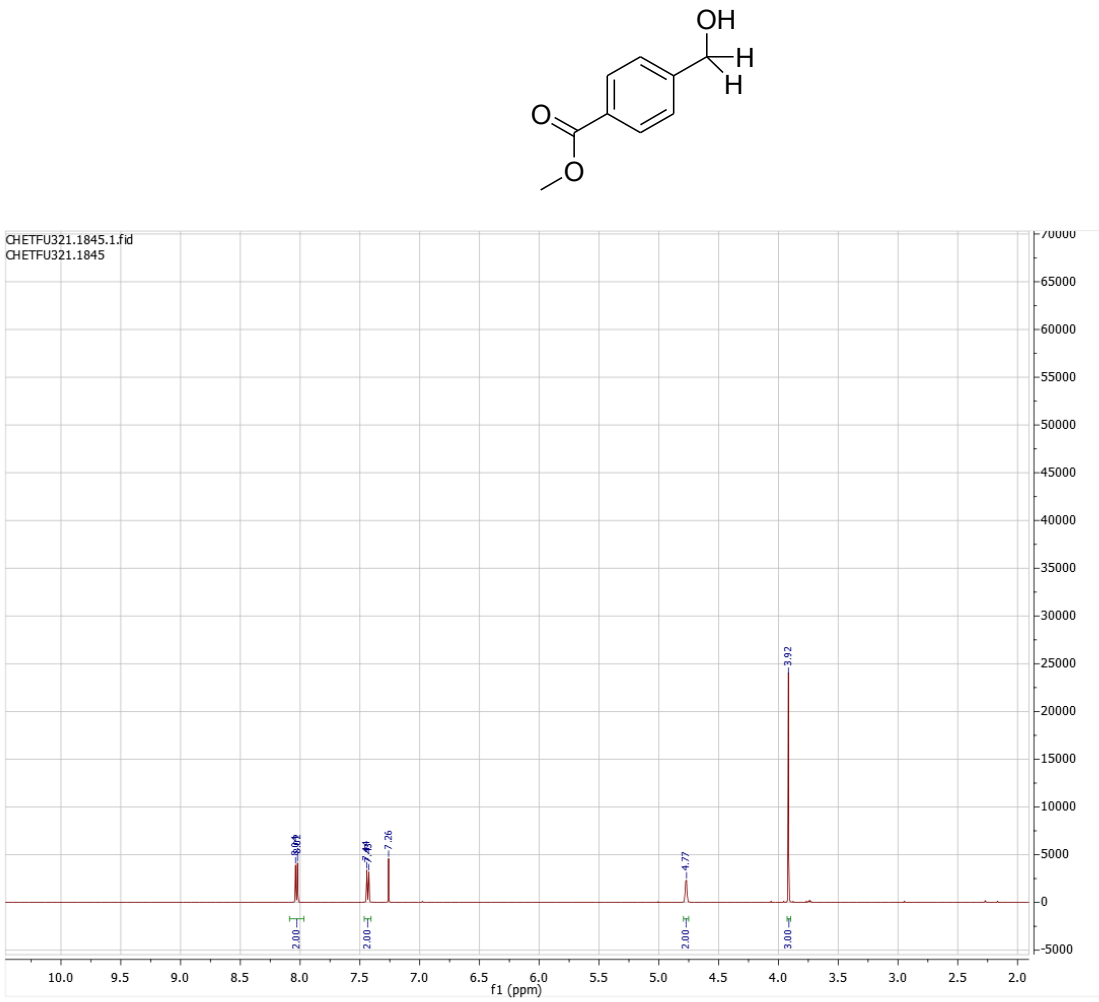


Figure S28. ^{13}C {^{1}H} NMR spectra of methyl 4-(hydroxymethyl) benzoate