Electronic Supplementary Material (ESI) for Chemical Communications.

Bimolecular Vinylation of Arenes by Vinyl Cation

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Note added after first publication: This Supplementary Information file replaces that originally published on 05 May 2020. The reaction time in pentane in the scheme on page 2 was incorrectly stated as 1 h in error. This has been corrected to 24 h in this updated version.

Supporting Information

CONTENTS

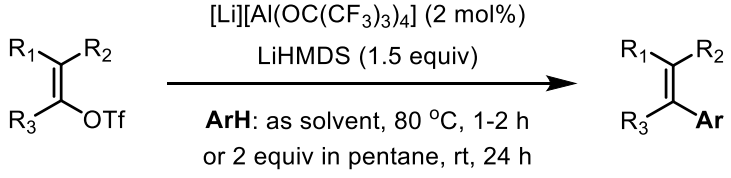
1 General Information

All reactions were performed in a glovebox under argon atmosphere with O_2 and H_2O < 0.5 ppm. All the glassware and stir bars were dried in a 120 °C oven for at least 24 h before use. Reactions were monitored using thin-layer chromatography (TLC) on silica gel plates (0.25 mm). The spots were visualized with ultraviolet light and/or *p*-anisaldehyde stain with heat as developing agent. Products were purified by flash chromatography on silica gel.

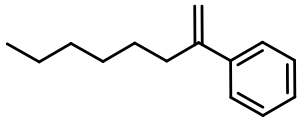
NMR characterization data was collected at 296 K on AM 250, AV 300, AV 360 or DRX 400 Bruker spectrometers operating at 250, 300, 360 or 400 MHz for ^{1}H NMR, ^{13}C NMR and ^{19}F NMR. ^{1}H NMR chemical shifts are reported in ppm using residual solvent peak as reference ($CHCl_3$: δ = 7.26 ppm). Data for ^{1}H NMR are presented as follows: chemical shift δ (ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad), coupling constant *J* (Hz) and integration; ^{13}C NMR spectra were recorded at 63, 75, 91 or 100 MHz using broadband proton decoupling and chemical shifts are reported in ppm using residual solvent peaks as reference ($CHCl_3$: δ = 77.16 ppm). MS were recorded on DSQ Thermo Fisher instrument by electronic impact. HRMS was performed on a MicrOTOFq Bruker spectrometer.

Materials. Reagents were purchased from commercially suppliers (Alfa Aesar, Sigma Aldrich or Strem). All the solvents were distilled, degassed (freeze-pump-thaw technique) and then stored inside the glove box over 4 Å molecular sieves. The liquid substrates were passed through a glass pipette filled with aluminum oxide before use to remove traces of water. The catalyst $[Li][Al(OC(CF_3)_3)_4]$ was synthesized according to a reported protocol.[1] The starting vinyl triflates were synthesized according to described methods.[2,3]

2 General Procedures for the alkenylation of aromatics



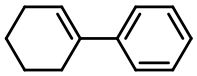
In a glovebox, a dram vial was charged with a magnetic stir bar, [Li][Al(OC(CF_3)$_3$)$_4$] (0.02 equiv, 1.95 mg, 0.002 mmol) and LiHMDS (1.5 equiv, 25.10 mg, 0.15 mmol). These salts were suspended in the indicated aromatic compound (0.5 mL) or in 0.5 mL of pentane in which 2 equiv of aromatic compound were added. The heterogeneous mixture was stirred for 5 min to improve dispersion of the lithium salts. The vinyl triflate (1 equiv, 0.1 mmol) was added to the reaction mixture, which was stirred at 80 °C for 1-2 h (arene as solvent) or at rt for 24 h (pentane as solvent). After completion (TLC monitoring), the reaction mixture was cooled to room temperature and brought outside of the glovebox. It was quenched by addition of technical diethyl ether, passed through a short plug of silica and concentrated. The crude was purified by flash chromatography on silica gel.



Oct-1-en-2-ylbenzene (**2b**).[4] Following the general procedure, using benzene as solvent at 80 °C for 1 h, product **2b** was obtained as a colorless oil in 62% yield after purification.

^{1}H NMR (360 MHz, $CDCl_3$) δ 7.48 – 7.20 (m, 5H), 5.29 (d, *J* = 1.6 Hz, 1H), 5.08 (d, *J* = 1.6 Hz, 1H), 2.53 (td, *J* = 7.4, 1.3 Hz, 2H), 1.53 – 1.41 (m, 2H), 1.41 – 1.25 (m, 7H), 0.90 (t, *J* = 6.7 Hz, 3H).

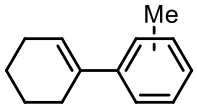
^{13}C NMR (91 MHz, $CDCl_3$) δ 148.81, 141.50, 128.23, 127.23, 126.13, 112.00, 35.38, 31.69, 29.05, 28.25, 22.65, 14.10.



2,3,4,5-Tetrahydro-1,1'-biphenyl (**2d**).[5] Following the general procedure, using benzene as solvent at 80 °C for 2 h, product **2d** was obtained as a colorless oil in 63% yield after purification.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 – 7.21 (m, 5H), 6.16 (dt, *J* = 4.0, 2.2 Hz, 1H), 2.49 – 2.41 (m, 2H), 2.29 – 2.20 (m, 2H), 1.87 – 1.77 (m, 2H), 1.76 – 1.65 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 142.69, 136.57, 128.19, 126.51, 124.93, 124.79, 27.40, 25.90, 23.08, 22.18.



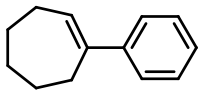
o:*m*:*p* = 3:2:1

Methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (**2e**).[6] Following the general procedure, using toluene as solvent at 80 °C for 2 h, the mixture of *o*,*m*,*p*-product **2e** (ratio = 3:2:1) was obtained as a colorless oil in 73% yield after purification.

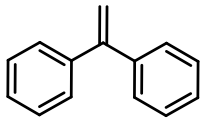
^{1}H NMR (360 MHz, $CDCl_3$) δ 7.33 – 7.08 (m, 8H), 6.17 – 6.09 (m, 1H), 5.61 – 5.56 (m, 1H), 2.46 – 2.40 (m, 2H), 2.39 (s, 1H, *o*-methyl product), 2.37 (s, 2H, *m*-methyl product), 2.32 (s, 3H, *p*-methyl product), 2.26 – 2.17 (m, 6H), 1.85 – 1.66 (m, 8H).

^{13}C NMR (91 MHz, $CDCl_3$) δ 144.68, 142.77, 139.87, 138.86, 137.64, 136.71, 136.39, 136.11, 135.02, 129.96, 128.89, 128.30, 128.10, 127.28, 126.39, 125.81, 125.65, 125.48, 124.82,

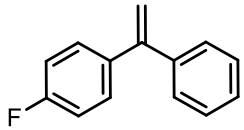
124.63, 123.94, 122.10, 30.12, 27.51, 27.44, 25.88, 25.42, 23.14, 23.11, 22.23, 21.57, 21.06, 19.79.



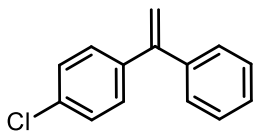
1-Phenylcyclohept-1-ene (**2g**).[5] Following the general procedure, using benzene as solvent at 80 °C for 2 h, product **2g** was obtained as a colorless oil in 82% yield after purification.
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 – 7.20 (m, 5H), 6.15 (t, *J* = 6.8 Hz, 1H), 2.73 – 2.61 (m, 2H), 2.38 – 2.29 (m, 2H), 1.93 – 1.85 (m, 2H), 1.74 – 1.66 (m, 2H), 1.65 – 1.56 (m, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 145.01, 145.00, 130.47, 128.14, 126.27, 125.68, 32.86, 32.82, 28.92, 26.97, 26.84.



Ethene-1,1-diyldibenzene (**2i**).[7] Following the general procedure, using benzene as solvent at 80 °C for 0.5 h or pentane as solvent with 2 equiv of benzene at rt for 24 h, product **2i** was obtained as a colorless oil in 83% yield after purification.
^{1}H NMR (360 MHz, $CDCl_3$) δ 7.43 – 7.34 (m, 10H), 5.52 (s, 2H).
^{13}C NMR (91 MHz, $CDCl_3$) δ 150.20, 141.62, 128.40, 128.29, 127.83, 114.42.

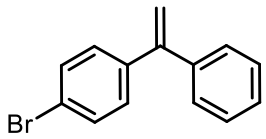


1-Fluoro-4-(1-phenylvinyl)benzene (**2j**).[8] Following the general procedure, using pentane as solvent with 2 equiv of benzene at rt for 24 h, product **2j** was obtained as a colorless oil in 68% yield after purification.
^{1}H NMR (360 MHz, $CDCl_3$) δ 7.39 – 7.29 (m, 4H), 7.09 – 7.02 (m, 2H), 5.47 (d, *J* = 1.2 Hz, 1H), 5.45 (d, *J* = 1.2 Hz, 1H).
^{13}C NMR (91 MHz, $CDCl_3$) δ 162.53 (d, *J* = 246.7 Hz), 149.07, 141.33, 137.56 (d, *J* = 3.3 Hz), 129.90 (d, *J* = 8.0 Hz), 128.26, 128.21, 127.89, 115.05 (d, *J* = 21.3 Hz), 114.24.
^{19}F NMR (235 MHz, $CDCl_3$) δ -114.69.



1-Chloro-4-(1-phenylvinyl)benzene (**2k**).[7] Following the general procedure, using pentane as solvent with 2 equiv of benzene at rt for 24 h, product **2k** was obtained as a colorless oil in 68% yield after purification.
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 – 7.28 (m, 9H), 5.50 (d, *J* = 1.1 Hz, 1H), 5.48 (d, *J* = 1.1 Hz, 1H).

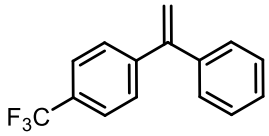
^{13}C NMR (91 MHz, $CDCl_3$) δ 149.00, 141.04, 139.97, 133.62, 129.59, 128.37, 128.30, 128.22, 127.95, 114.72.



1-Bromo-4-(1-phenylvinyl)benzene (**2l**).[8] Following the general procedure, using pentane as solvent with 2 equiv of benzene at rt for 24 h, product **2l** was obtained as a white solid in 69% yield after purification.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 – 7.46 (m, 2H), 7.41 – 7.32 (m, 5H), 7.29 – 7.22 (m, 2H), 5.51 (d, *J* = 1.1 Hz, 1H), 5.49 (d, *J* = 1.1 Hz, 1H).

^{13}C NMR (91 MHz, $CDCl_3$) δ 149.05, 140.95, 140.44, 131.34, 129.93, 128.31, 128.22, 127.98, 121.81, 114.78.

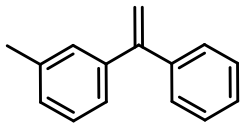


1-(1-Phenylvinyl)-4-(trifluoromethyl)benzene (**2m**).[7] Following the general procedure, using pentane as solvent with 2 equiv of benzene at rt for 24 h, product **2m** was obtained as a white solid in 58% yield after purification.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.2 Hz, 2H), 7.48 (d, *J* = 8.1 Hz, 2H), 7.41 – 7.31 (m, 5H), 5.59 (d, *J* = 1.0 Hz, 1H), 5.54 (d, *J* = 1.0 Hz, 1H).

^{13}C NMR (91 MHz, $CDCl_3$) δ 149.10, 145.23, 140.77, 129.69 (q, *J* = 32.4 Hz), 128.69, 128.50, 128.29, 128.22, 125.30 (q, *J* = 3.8 Hz), 124.34 (d, *J* = 271.8 Hz), 116.04.

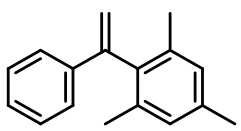
^{19}F NMR (235 MHz, $CDCl_3$) δ -62.43.



1-Methyl-3-(1-phenylvinyl)benzene (**2n**).[8] Following the general procedure, using pentane as solvent with 2 equiv of benzene for 24 h, product **2n** was obtained as a colorless oil in 41% yield after purification.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 (d, *J* = 1.2 Hz, 5H), 7.29 – 7.23 (m, 1H), 7.22 – 7.14 (m, 3H), 5.48 (s, 2H), 2.38 (s, 3H).

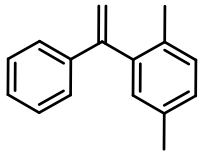
^{13}C NMR (91 MHz, $CDCl_3$) δ 150.16, 141.62, 141.49, 137.74, 128.96, 128.48, 128.28, 128.14, 128.06, 127.66, 125.46, 114.17, 21.45.



1,3,5-Trimethyl-2-(1-phenylvinyl)benzene (**2o**).[9] Following the general procedure, using pentane as solvent with 2 equiv of mesitylene for 24 h, product **2o** was obtained as a colorless oil in 63% yield after purification.

^{1}H NMR (360 MHz, $CDCl_3$) δ 7.26 – 7.13 (m, 5H), 6.90 – 6.80 (m, 2H), 5.88 (d, *J* = 1.4 Hz, 1H), 5.02 (d, *J* = 1.4 Hz, 1H), 2.25 (s, 3H), 2.04 (s, 6H).

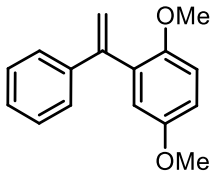
^{13}C NMR (91 MHz, $CDCl_3$) δ 146.84, 139.56, 138.17, 136.45, 136.15, 128.42, 128.10, 127.54, 125.83, 114.56, 21.06, 20.10.



1,4-Dimethyl-2-(1-phenylvinyl)benzene (**2p**).[7] Following the general procedure, using pentane as solvent with 2 equiv of *p*-xylene for 24 h, product **2p** was obtained as a colorless oil in 62% yield after purification.

^{1}H NMR (360 MHz, $CDCl_3$) δ 7.35 – 7.26 (m, 5H), 7.14 – 7.05 (m, 3H), 5.78 (d, *J* = 2.0 Hz, 1H), 5.22 (d, *J* = 2.0 Hz, 1H), 2.37 (s, 3H), 2.04 (s, 3H).

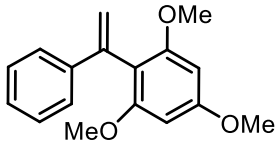
^{13}C NMR (91 MHz, $CDCl_3$) δ 149.57, 141.48, 140.68, 135.07, 132.96, 130.69, 129.98, 128.32, 128.20, 127.53, 126.52, 114.69, 20.94, 19.63.



1,4-Dimethoxy-2-(1-phenylvinyl)benzene (**2q**).[10] Following the general procedure, using pentane as solvent with 2 equiv of 1,4-dimethoxybenzene for 24 h, product **2q** was obtained as a colorless oil in 65% yield after purification.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 – 7.23 (m, 5H), 6.91 – 6.77 (m, 3H), 5.76 (d, *J* = 1.4 Hz, 1H), 5.35 (d, *J* = 1.4 Hz, 1H), 3.81 (s, 3H), 3.60 (s, 3H).

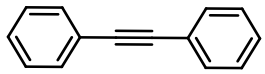
^{13}C NMR (91 MHz, $CDCl_3$) δ 153.59, 151.37, 146.86, 140.81, 132.22, 128.09, 128.05, 127.98, 127.37, 126.38, 126.34, 117.10, 115.47, 113.39, 112.78, 56.48, 55.75.



1,3,5-Trimethoxy-2-(1-phenylvinyl)benzene (**2r**).[11] Following the general procedure, using pentane as solvent with 2 equiv of 1,3,5-trimethoxybenzene for 24 h, product **2r** was obtained as a white solid in 55% yield after purification.

^{1}H NMR (360 MHz, $CDCl_3$) δ 7.37 – 7.32 (m, 2H), 7.28 – 7.20 (m, 3H), 6.22 (s, 2H), 5.96 (d, *J* = 1.5 Hz, 1H), 5.22 (d, *J* = 1.5 Hz, 1H), 3.88 (s, 3H), 3.71 (s, 6H).

^{13}C NMR (91 MHz, $CDCl_3$) δ 160.62, 158.72, 141.12, 140.77, 128.02, 127.98, 127.09, 125.82, 116.26, 112.37, 90.92, 56.03, 55.36.

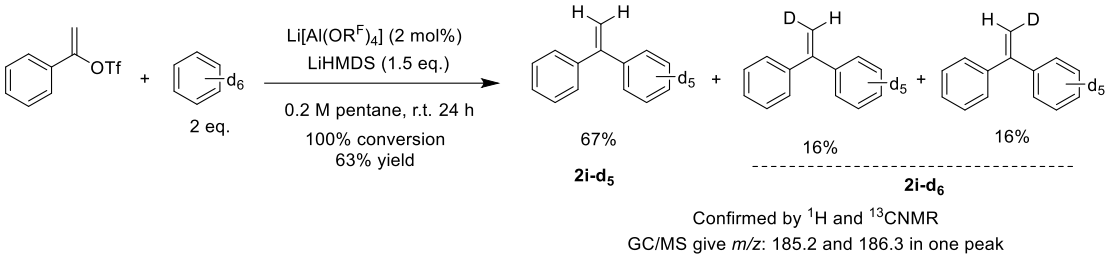


1,2-Diphenylethyne.[12] Following the general procedure, the product was obtained as a white solid in 71% yield.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 – 7.50 (m, 4H), 7.45 – 7.31 (m, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 131.64, 128.36, 128.27, 123.32, 89.40.

3 Deuterium labeling experiment



Following the general procedure, using 2 equiv of d^6-benzene as the nucleophile in 0.2M pentane, compounds **2i-d$_5$**[13] and **2i-d$_6$**[14] (1:1 mixture of *Z*/*E* isomer) were obtained in total 63% isolated yield. The percentage of **2i-d$_5$** is 67%, *E*-**2i-d$_6$** is 16%, *Z*-**2i-d$_6$** is 16%, which has been determined by ^{1}H NMR and ^{13}C NMR.

^{1}H NMR (360 MHz, $CDCl_3$) δ 7.33 – 7.20 (m, 5H), 5.39 (s, 1.33H, **2i-d$_5$**), 5.38 (s, 0.16H, **2i-d$_6$**), 5.37 (s, 0.16H, **2i-d$_6$**).

^{13}C NMR (91 MHz, $CDCl_3$) δ 150.03, 149.95, 141.52, 141.32, 128.30, 128.19, 127.73, 114.30 (**2i-d$_5$**), 114.01 (**2i-d$_6$**), 113.74(**2i-d$_6$**).

GC-MS: **2i-d$_5$** *m/z*: 185.2 and **2i-d$_6$** *m/z*: 186.3.

4 DFT calculations

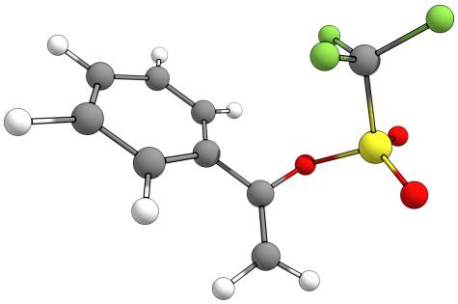
Calculations were performed with the Gaussian 16 software package.[15] Minima and transition states were optimized using the ωB97-XD functional[16] and the 6-311+G(d,p) basis set, with an ultrafine grid. Solvation energy was obtained using the SMD model.[17] This level of theory was recently used by Lavallo, Houk, Nelson and co-workers to study CH-insertion at vinyl carbocations deriving from vinyl triflates.[18] Due to the size of the system, the structure of the **Int-a**/[$Al(OC(CF_3)_3)_4$] adduct was optimized at the ωB97-XD/6-31G(d,p) level.

Table S1. Geometries (selected distances in Å), imaginary frequencies (cm^{-1}), energies (optimized structure and SMD single point, Hartree) and coordinates (x,y,z) of the computed species.

Li^+

E(RwB97XD) = -7.29270972418

E(RwB97XD) = -7.35818344695



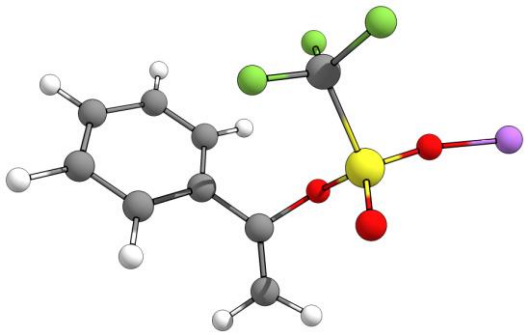
1i

E(RwB97XD) = -1270.43665299

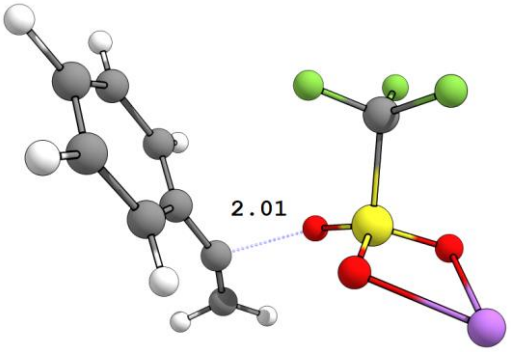
E(RwB97XD) = -1270.44653387

Li	0	0	0

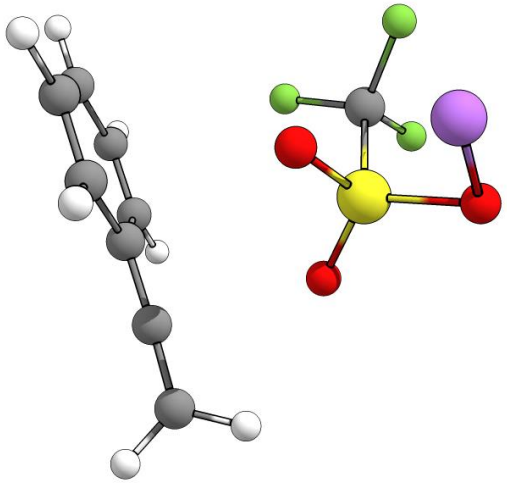
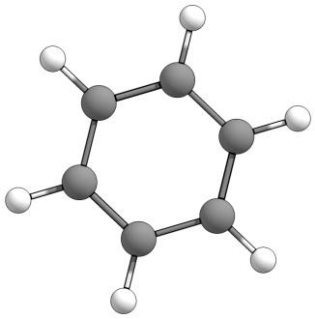
C	0.466848	1.527179	-0.243797
C	0.341221	2.770791	0.194083
H	-0.588612	3.313246	0.09465
O	-2.256873	1.272963	0.910779
S	-1.961389	0.452721	-0.228435
O	-2.891221	0.212445	-1.287718
O	-0.606417	0.931877	-0.948432
C	-1.436739	-1.219814	0.429335
F	-0.493385	-1.07156	1.345416
F	-0.980709	-1.971576	-0.557663
F	-2.494872	-1.797943	0.974063
H	1.180589	3.263754	0.665373
C	1.655645	0.656718	-0.17445
C	2.566449	0.78592	0.875989
C	1.883367	-0.304144	-1.161063
C	3.694438	-0.019846	0.927596
C	3.011577	-1.110712	-1.103753
C	3.920776	-0.969891	-0.062409
H	2.377864	1.500502	1.669032
H	1.17727	-0.415714	-1.974481
H	4.390857	0.083858	1.751682
H	3.180435	-1.851476	-1.876764
H	4.799104	-1.603478	-0.017088



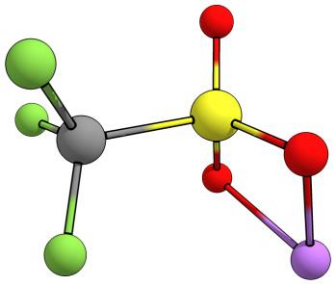
Int-a



TS_{ab}

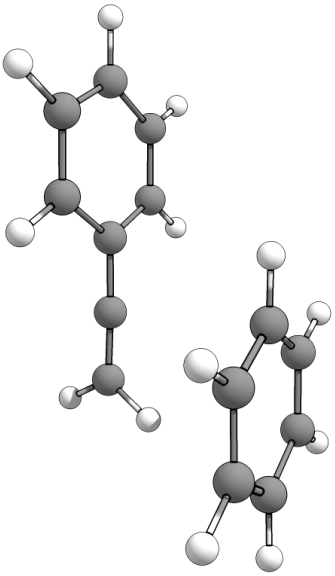
	E(RwB97XD) = -1277.79313653 E(RwB97XD) = -1277.84319326				Frequency -219.7992 E(RwB97XD) = -1277.77231825 E(RwB97XD) = -1277.81838845		
O	-0.676193	1.088084	-0.831958	O	-0.741497	1.225672	-0.780852
C	0.528161	1.67585	-0.270063	C	1.093834	1.93359	-0.367507
C	0.460354	2.949107	0.072531	C	0.898602	3.19151	-0.579348
C	1.660906	0.742565	-0.223191	C	1.859286	0.798418	-0.082303
H	-0.460877	3.512774	0.013836	H	-0.054273	3.616967	-0.859414
H	1.355428	3.453061	0.41268	H	1.769387	3.835522	-0.474326
S	-1.754131	0.42152	0.097991	S	-1.640962	0.482233	0.121602
O	-1.901575	1.057417	1.366247	O	-1.292923	0.541504	1.557892
O	-2.920671	0.284892	-0.780158	O	-3.073413	0.785987	-0.025818
C	-1.175473	-1.356055	0.353867	C	-1.444305	-1.304943	-0.378467
Li	-4.482653	0.409189	-1.650908	Li	-3.274606	0.873638	1.953625
F	-0.154015	-1.369018	1.169628	F	-0.187691	-1.673159	-0.188341
F	-0.858836	-1.875209	-0.813036	F	-1.768898	-1.45262	-1.643739
F	-2.197215	-2.007191	0.877314	F	-2.241749	-2.037666	0.384998
C	2.528683	0.766573	0.870095	C	2.005564	0.365361	1.250887
C	1.884734	-0.157621	-1.267842	C	2.491105	0.108811	-1.137531
C	3.614374	-0.096852	0.912262	C	2.796691	-0.733913	1.519311
H	2.340286	1.445604	1.693981	H	1.493964	0.896441	2.043691
C	2.968715	-1.021068	-1.217281	C	3.276245	-0.989571	-0.851152
H	1.221942	-0.170133	-2.125349	H	2.356521	0.451502	-2.156449
C	3.834056	-0.991738	-0.128486	C	3.425547	-1.406424	0.47187
H	4.283039	-0.078221	1.76442	H	2.927454	-1.073657	2.53897
H	3.145217	-1.71214	-2.032861	H	3.774543	-1.524899	-1.649504
H	4.68006	-1.667781	-0.091396	H	4.043909	-2.269852	0.689931
 **Int-b** E(RwB97XD) = -1277.77682505 E(RwB97XD) = -1277.82401455				 **C_6H_6** E(RwB97XD) = -232.220948799 E(RwB97XD) = -232.228861910			
O	-0.845012	1.438548	-0.633321	C	0.32214	1.352859	0.000036
C	1.778495	2.027541	-0.338009	C	1.332913	0.397381	-0.000069

C	1.472329	3.234183	-0.629993	C	-1.01059	0.955532	0.000026
C	2.165856	0.76065	-0.033351	C	1.010707	-0.955423	-0.000032
H	0.458954	3.458991	-0.95504	C	-1.332907	-0.397521	-0.000024
H	2.213613	4.026201	-0.554049	C	-0.322267	-1.352836	0.000022
S	-1.680013	0.586622	0.186814	H	2.372006	0.707599	-0.000049
O	-1.243508	0.397854	1.598816	H	-1.798525	1.700581	-0.000118
O	-3.13119	0.869187	0.214732	H	1.798375	-1.700722	0.000172
C	-1.54092	-1.110422	-0.565853	H	-2.372078	-0.707368	-0.000106
Li	-3.163458	0.61901	2.14723	H	-0.573152	-2.407804	0.00015
F	-0.264346	-1.494195	-0.55577	H	0.573397	2.407765	0.000197
F	-1.981257	-1.100355	-1.807008				
F	-2.252081	-1.969822	0.154679				
C	1.994105	0.266018	1.290647				
C	2.73052	-0.063862	-1.048412				
C	2.393516	-1.016516	1.581874				
H	1.533862	0.900405	2.037108				
C	3.126042	-1.340631	-0.731459				
H	2.838452	0.33031	-2.051616				
C	2.957355	-1.808027	0.576682				
H	2.268854	-1.415155	2.580267				
H	3.560213	-1.984016	-1.485821				
H	3.269685	-2.818682	0.816747				



LiOTf

E(RwB97XD) = -969.057215322

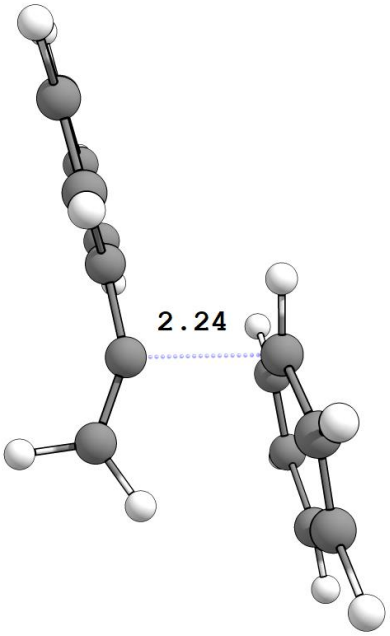
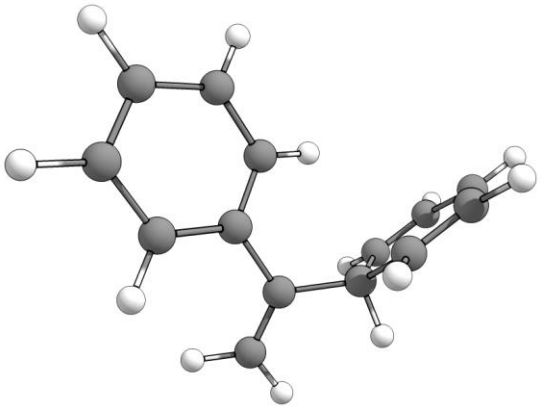


Int-c

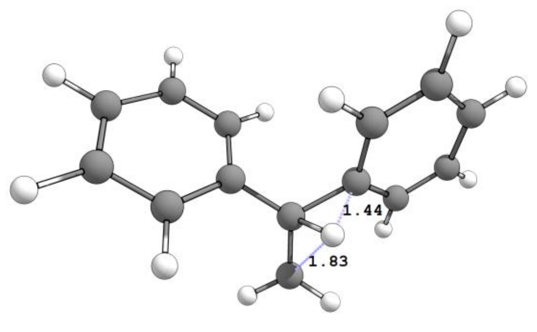
E(RwB97XD) = -540.929527094

E(RwB97XD) = -540.978584690

O	-1.287752	-0.45046	1.189796	C	-1.296276	-0.006476	-1.306931
S	-0.777609	0.290212	-0.000025	C	0.294261	-0.026853	1.449308
O	-1.288251	-0.448944	-1.190443	C	-0.759397	-0.040162	2.168711
O	-0.891127	1.721016	0.000877	C	1.450977	-0.013152	0.728804
C	1.04443	-0.094265	-0.000225	H	-0.688456	-0.055638	3.254541

F	1.622733	0.407086	1.080588	H	-1.748814	-0.03604	1.699772
F	1.623365	0.408817	-1.079564	H	-0.382379	-0.018961	-1.89172
F	1.215637	-1.421008	-0.001088	C	-1.914558	-1.205785	-0.959364
Li	-2.081134	-1.734915	0.00016	C	-1.869943	1.209553	-0.940813
				C	-3.104057	-1.189229	-0.239005
				H	-1.481624	-2.150727	-1.268213
				C	-3.059626	1.226349	-0.220838
				H	-1.402355	2.142428	-1.23569
				C	-3.675213	0.026827	0.132977
				H	-3.5953	-2.11982	0.02064
				H	-3.51625	2.170467	0.052732
				H	-4.611467	0.039908	0.679327
				C	2.051535	-1.241712	0.334279
				C	2.043831	1.229739	0.369036
				C	3.214894	-1.215745	-0.398035
				H	1.580667	-2.175845	0.616101
				C	3.207208	1.231617	-0.363685
				H	1.567151	2.15261	0.676959
				C	3.784824	0.014814	-0.742851
				H	3.689585	-2.138385	-0.706599
				H	3.676096	2.165492	-0.64624
				H	4.702387	0.025803	-1.321166
							
TS_{cd}				**Int-d**			
Frequency -259.7577				E(RwB97XD) = -540.942431730			
E(RwB97XD) = -540.922077870				E(RwB97XD) = -540.994534562			
E(RwB97XD) = -540.969422942							
C	-1.220942	-0.435027	-0.937163	C	-0.073496	1.460269	0.059076
C	-0.009422	-0.126092	0.916909	H	-1.236263	3.168322	0.456664

C	-0.794003	-0.154737	1.944371	C	-0.254628	2.767381	0.235567
C	1.312738	-0.058064	0.414758	H	1.946507	1.791348	-0.486308
H	-0.321097	-0.173787	2.924582	H	0.561301	3.479806	0.180098
H	-1.877918	-0.163979	1.893907	C	1.338735	0.906877	-0.165853
H	-0.349612	-0.789338	-1.471695	C	2.071096	0.500067	1.042304
C	-2.250559	-1.347394	-0.619835	C	1.494897	0.025052	-1.329377
C	-1.458699	0.951996	-0.832973	C	2.947486	-0.548314	1.028391
C	-3.446526	-0.879417	-0.128602	C	2.375946	-1.019427	-1.323442
H	-2.088443	-2.408933	-0.762111	C	3.096327	-1.296192	-0.151169
C	-2.679563	1.417428	-0.353534	H	1.924865	1.10002	1.935012
H	-0.691954	1.650021	-1.149047	H	0.913925	0.262211	-2.214954
C	-3.658198	0.505783	0.007226	H	3.51121	-0.815205	1.913263
H	-4.239961	-1.569933	0.130868	H	2.510532	-1.639726	-2.200275
H	-2.863193	2.481213	-0.270925	H	3.793496	-2.128813	-0.153711
H	-4.611863	0.861929	0.380465	C	-1.161032	0.452346	0.077179
C	2.013876	-1.241855	0.11819	C	-2.432265	0.777023	-0.404343
C	1.934515	1.194076	0.258767	C	-0.938555	-0.836228	0.569727
C	3.326747	-1.167153	-0.305625	C	-3.456845	-0.158323	-0.371532
H	1.522942	-2.200886	0.237808	C	-1.964006	-1.771404	0.603624
C	3.248644	1.253917	-0.167645	C	-3.22712	-1.432844	0.133828
H	1.38535	2.099205	0.49125	H	-2.615239	1.758542	-0.826529
C	3.939566	0.077362	-0.450996	H	0.033818	-1.117147	0.966685
H	3.878721	-2.073134	-0.522703	H	-4.43601	0.106382	-0.752453
H	3.739519	2.212814	-0.277836	H	-1.779105	-2.761662	1.002613
H	4.968473	0.129872	-0.787644	H	-4.028277	-2.161785	0.156012

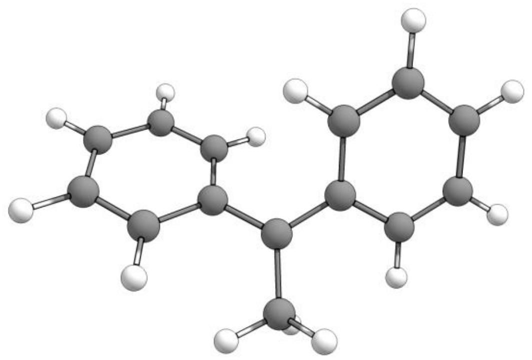


TS$_{de}$

Frequency -922.2303

E(RwB97XD) = -540.912206131

E(RwB97XD) = -540.963235437



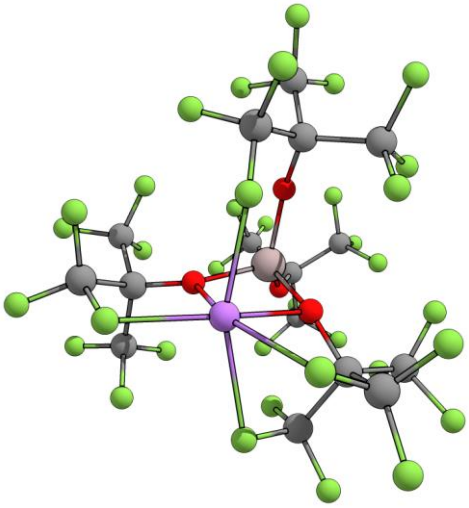
Int-e

E(RwB97XD) = -540.999304895

E(RwB97XD) = -541.047818388

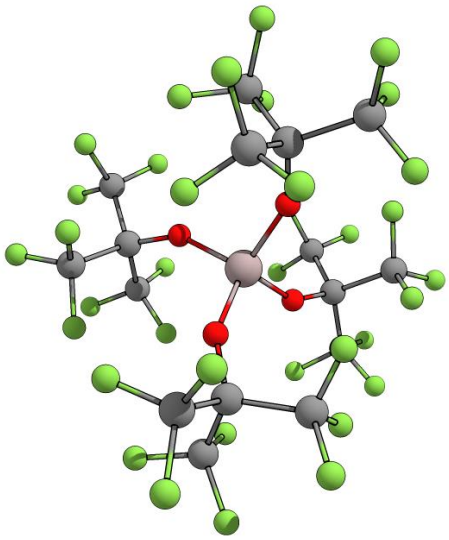
C	-0.031431	1.168073	0.026662	C	-0.004967	1.047341	0.002898
H	-0.933872	3.073748	0.316307	H	-0.821684	2.963582	0.549427
C	-0.015017	2.529166	0.128234	C	-0.02234	2.533338	-0.052826
H	0.63961	1.240327	-1.007962	H	-0.202177	2.815374	-1.099965
H	0.89416	3.105191	-0.013093	H	0.93477	2.97634	0.21288
C	1.314021	0.386959	-0.064582	C	1.248318	0.35053	-0.026389
C	2.471337	0.877728	0.568656	C	2.405967	0.900903	0.571444

C	1.34474	-0.834613	-0.758947	C	1.35651	-0.890524	-0.699049
C	3.632465	0.131901	0.519357	C	3.602489	0.21556	0.53547
C	2.518741	-1.567554	-0.797007	C	2.570093	-1.54669	-0.765891
C	3.658253	-1.085526	-0.162537	C	3.68806	-1.002391	-0.139224
H	2.442511	1.799025	1.136669	H	2.348903	1.832982	1.119215
H	0.453281	-1.195111	-1.259105	H	0.498819	-1.291396	-1.22446
H	4.519148	0.487096	1.029649	H	4.475214	0.625893	1.027837
H	2.545758	-2.511256	-1.326964	H	2.651616	-2.477767	-1.312656
H	4.574807	-1.66284	-0.191793	H	4.636626	-1.525121	-0.183529
C	-1.295185	0.38602	0.043188	C	-1.246843	0.335351	0.036738
C	-2.372294	0.777122	-0.753074	C	-2.430247	0.92315	-0.470131
C	-1.42108	-0.706983	0.902513	C	-1.325983	-0.946653	0.631118
C	-3.569792	0.077501	-0.689055	C	-3.622629	0.233661	-0.432292
C	-2.624262	-1.392495	0.97245	C	-2.53351	-1.615478	0.693889
C	-3.696463	-1.003296	0.175282	C	-3.675894	-1.033654	0.152242
H	-2.272679	1.615345	-1.435372	H	-2.397817	1.901248	-0.934069
H	-0.58627	-1.012545	1.524085	H	-0.44843	-1.376403	1.097419
H	-4.401514	0.375164	-1.315802	H	-4.517939	0.675733	-0.851148
H	-2.726742	-2.231466	1.649883	H	-2.591345	-2.583818	1.174888
H	-4.632397	-1.546694	0.226668	H	-4.620696	-1.563311	0.196182
Al	0.09767	0.007393	0.048726	Al	0.005108	0.015461	-0.022266
O	-0.963034	1.233462	-0.739843	O	0.780448	1.350813	0.804844
C	-1.131168	2.541976	-1.075503	C	0.641188	2.500854	1.475994
C	-2.675697	2.778954	-1.207394	C	2.066271	2.95513	1.954365
F	-3.253713	2.895227	-0.02234	F	2.762416	3.483613	0.94339
F	-2.997762	3.818018	-1.952297	F	2.00909	3.880203	2.926812
F	-3.23785	1.674122	-1.794533	F	2.755103	1.921032	2.421343



[Li][Al(OC(CF$_3$)$_3$)$_4$]

E(RwB97XD) = -4755.41036464



[Al(OC(CF$_3$)$_3$)$_4$]$^-$

E(RwB97XD) = -4747.92059108

E(RwB97XD) = -4747.93722274

C	-0.434146	2.808104	-2.453464	C	-0.284297	2.304554	2.728599
F	-1.11899	2.191514	-3.427526	F	0.357917	1.643999	3.694817
F	-0.370275	4.103946	-2.746221	F	-0.710468	3.46569	3.246776
F	0.792238	2.30867	-2.447564	F	-1.356419	1.590634	2.396022
C	-0.556613	3.512436	0.013045	C	0.029634	3.615651	0.551639
F	-0.796613	3.024544	1.223599	F	0.549053	3.542665	-0.667757
F	0.758454	3.646303	-0.125059	F	-1.292333	3.469788	0.441279
F	-1.111578	4.722349	-0.07734	F	0.258428	4.853145	1.021796
O	-0.392657	-0.20452	1.687146	O	1.246677	-0.815344	-0.93282
O	-0.685691	-1.299735	-0.903476	O	-0.718892	-1.14526	1.067253
O	1.775815	0.249879	-0.166033	O	-1.265277	0.683532	-1.025217
C	-1.308279	-0.598429	2.587999	C	2.372165	-0.755521	-1.653908
C	3.020506	0.293345	0.361709	C	-2.395658	0.480217	-1.713333
C	-0.541993	-2.246761	-1.866454	C	-0.607386	-2.209149	1.870872
C	-2.742934	-0.116311	2.174064	C	3.559335	-0.182547	-0.796232
F	-3.717522	-0.739	2.819185	F	4.760443	-0.502632	-1.305182
F	-2.883486	1.189786	2.344843	F	3.497734	1.148969	-0.728542
F	-2.944382	-0.351315	0.842748	F	3.505692	-0.654729	0.443017
C	-0.930258	0.044347	3.971389	C	2.172934	0.150283	-2.921071
F	0.10659	-0.591821	4.511079	F	1.458947	-0.485008	-3.854081
F	-0.590561	1.316396	3.80596	F	1.511172	1.255832	-2.592648
F	-1.948054	-0.006831	4.837787	F	3.334155	0.516505	-3.483309
C	-1.30194	-2.163826	2.712219	C	2.721306	-2.215879	-2.111987
F	-1.897449	-2.588106	3.826721	F	3.62474	-2.239934	-3.105826
F	-1.945456	-2.710455	1.670898	F	3.224144	-2.924157	-1.096668
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F	3.427575	2.639627	0.147039	F	-3.271596	2.712638	-1.647516
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C	3.218406	-0.852732	1.416887	C	-2.210831	-0.678802	-2.75593
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C	4.039366	0.114061	-0.81661	C	-3.580916	0.117981	-0.746563
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F	3.655148	0.827934	-1.868982	F	-3.522207	0.855969	0.355009
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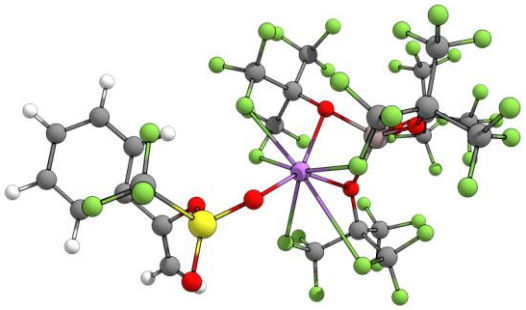

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C	6.04611	-1.391573	-0.465818
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H	6.050329	-1.106258	-3.255936
S	4.172027	1.683385	-0.587147
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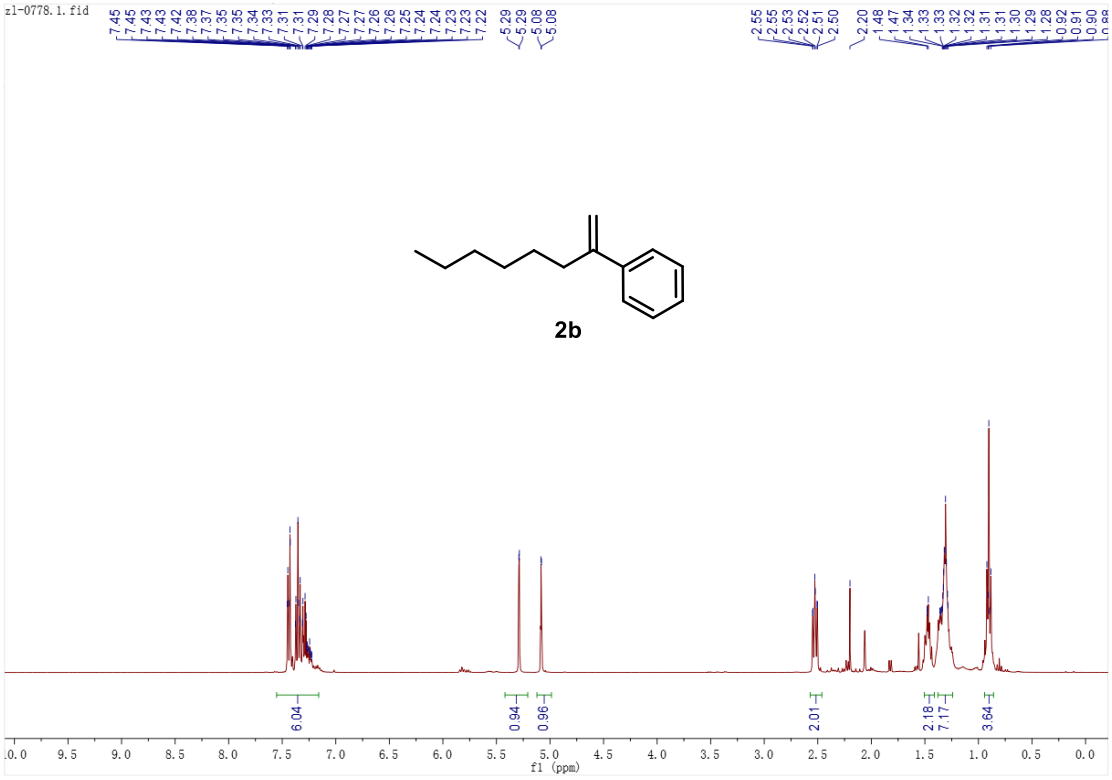
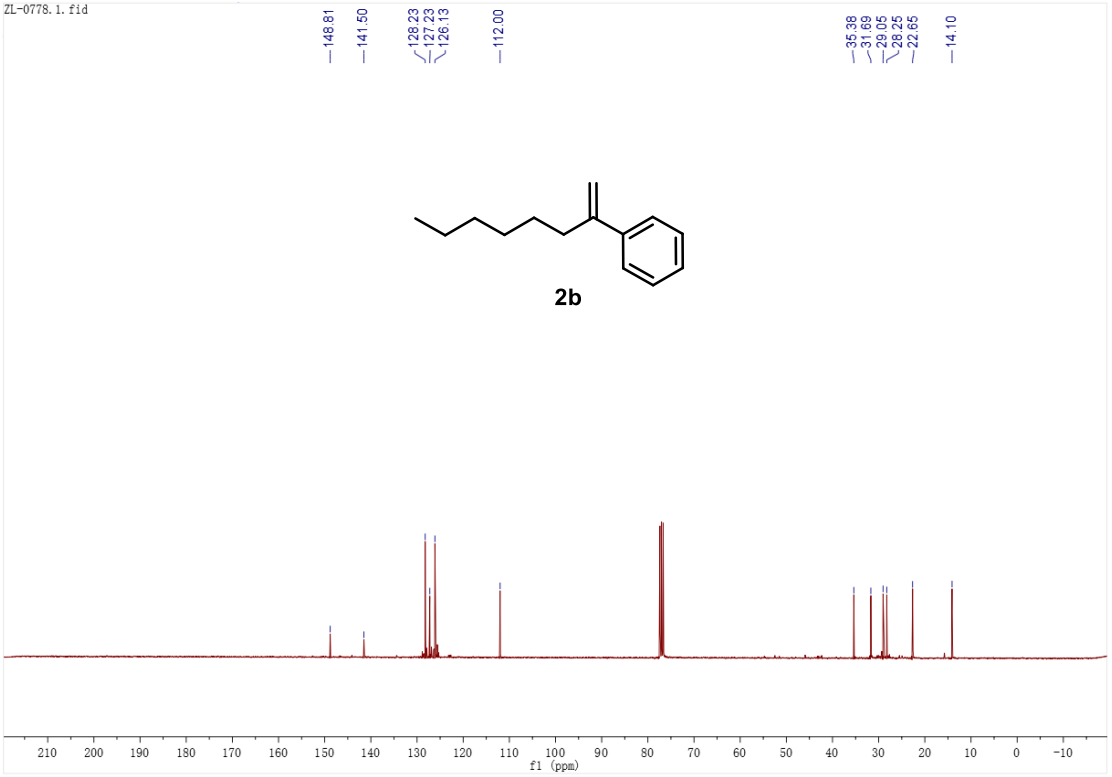
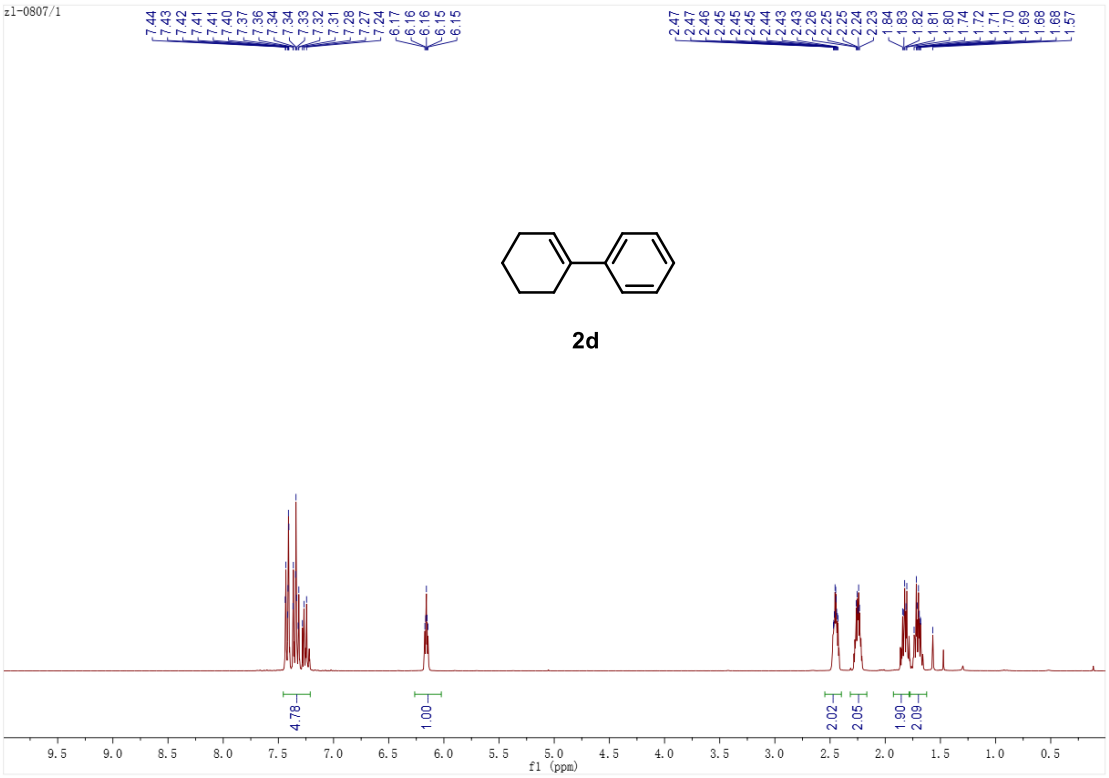
6 ^{1}H, ^{13}C, ^{19}F NMR spectral data



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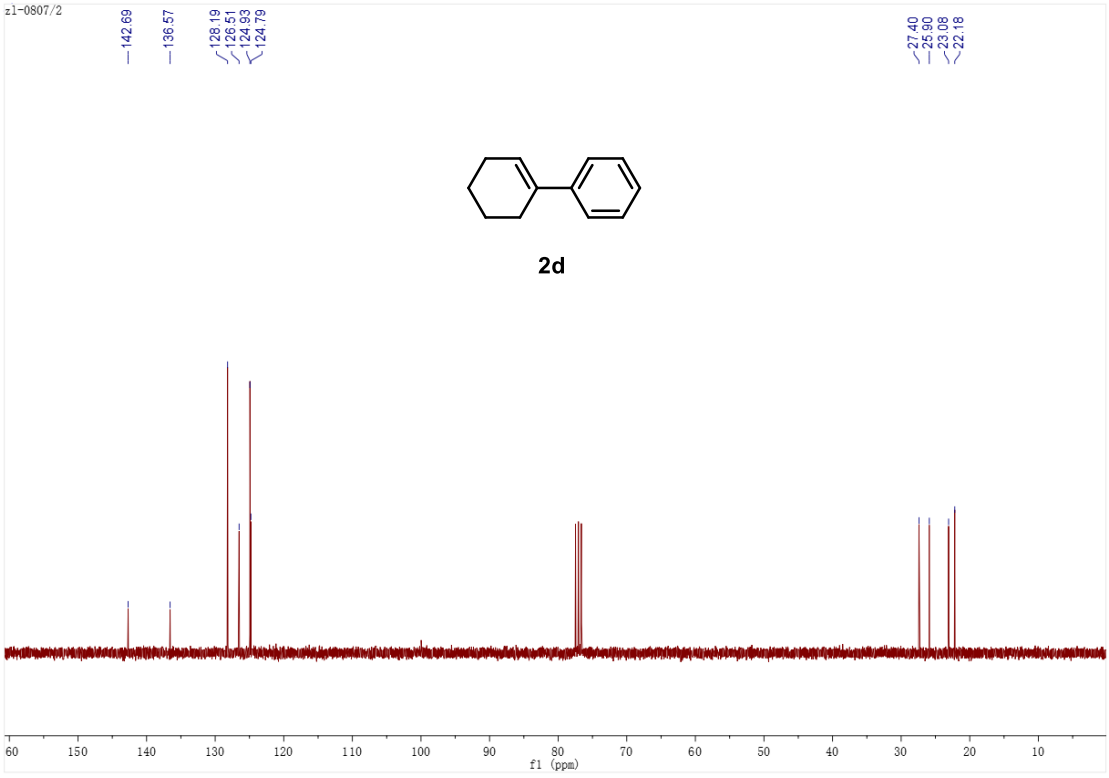
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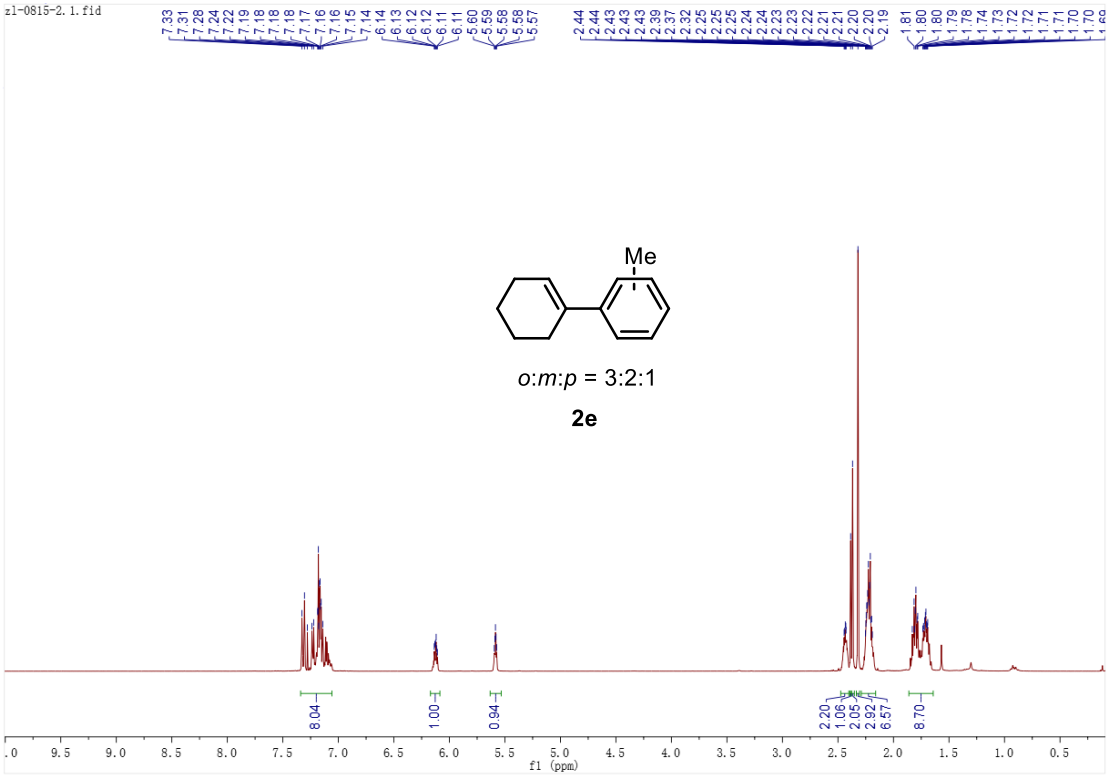
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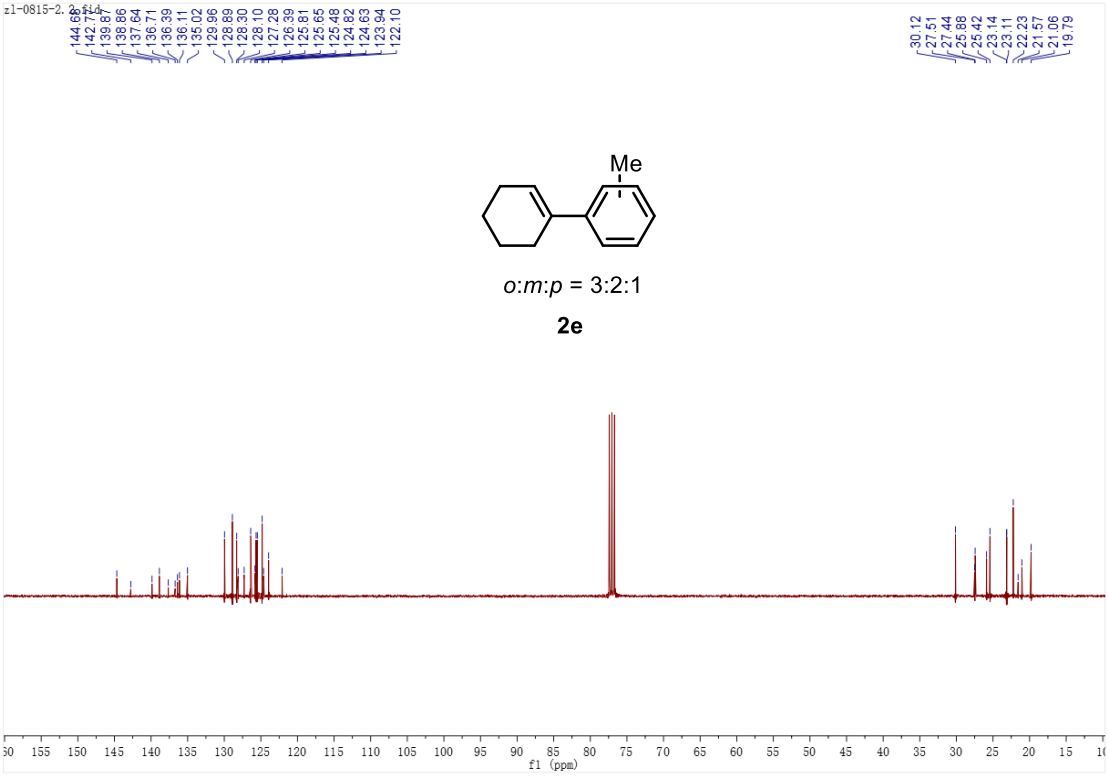
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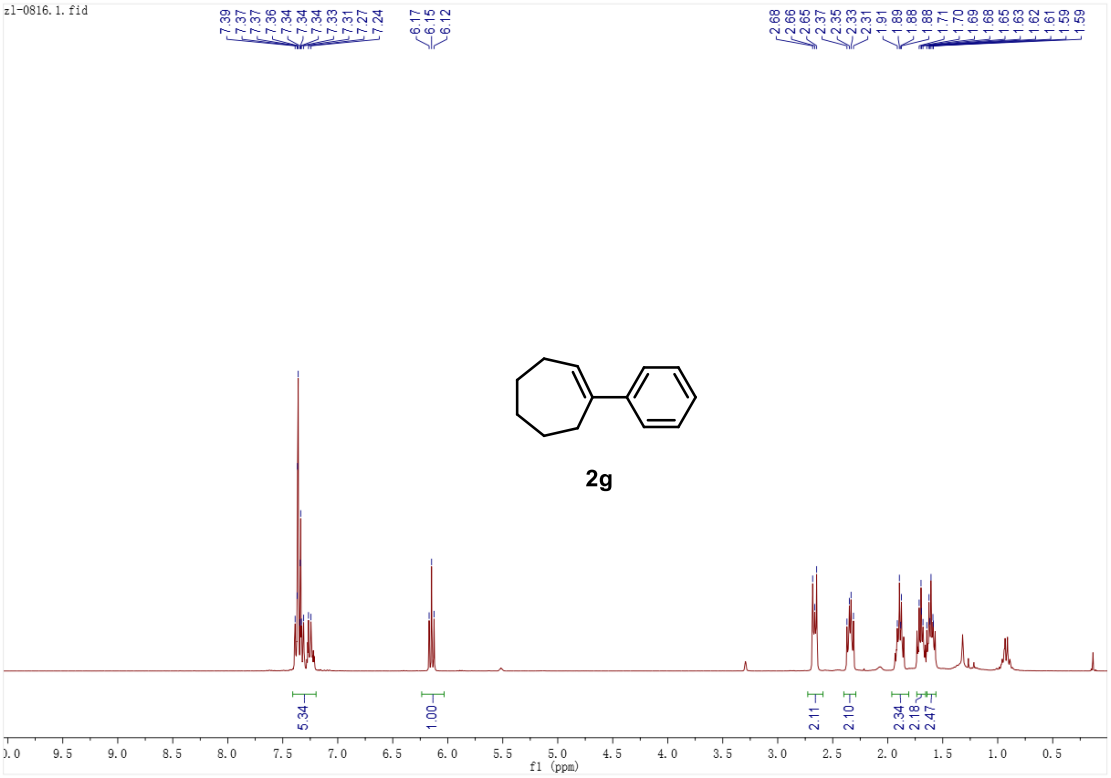
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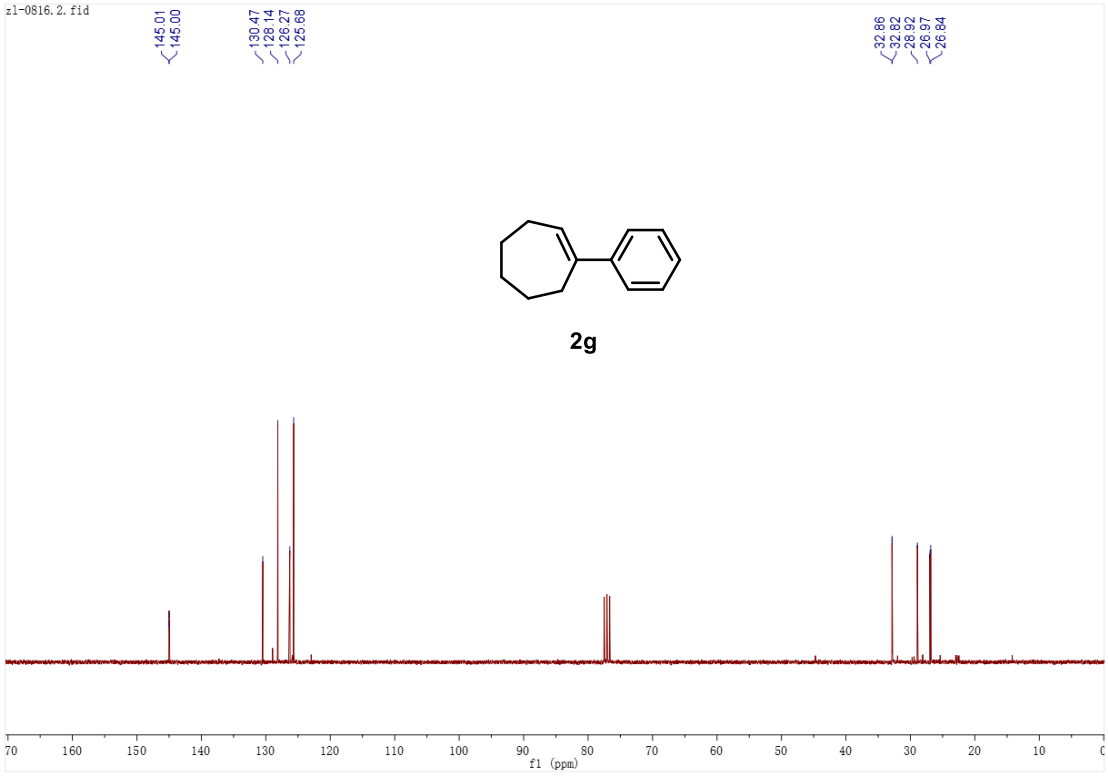
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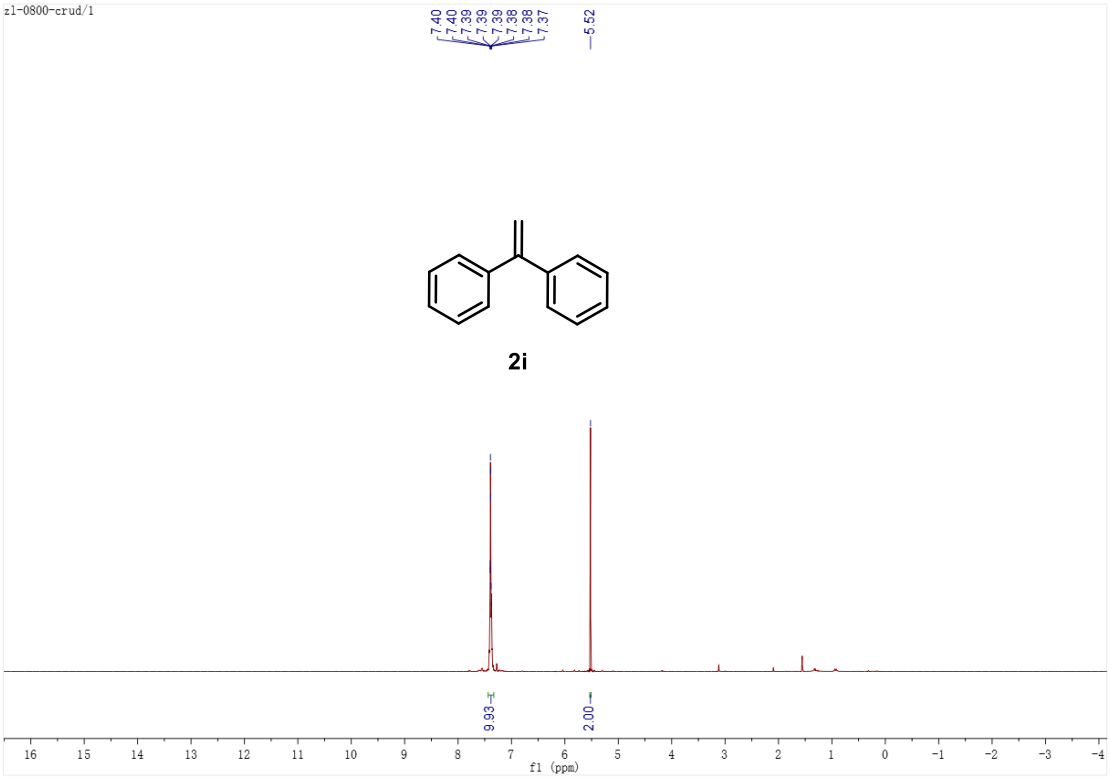
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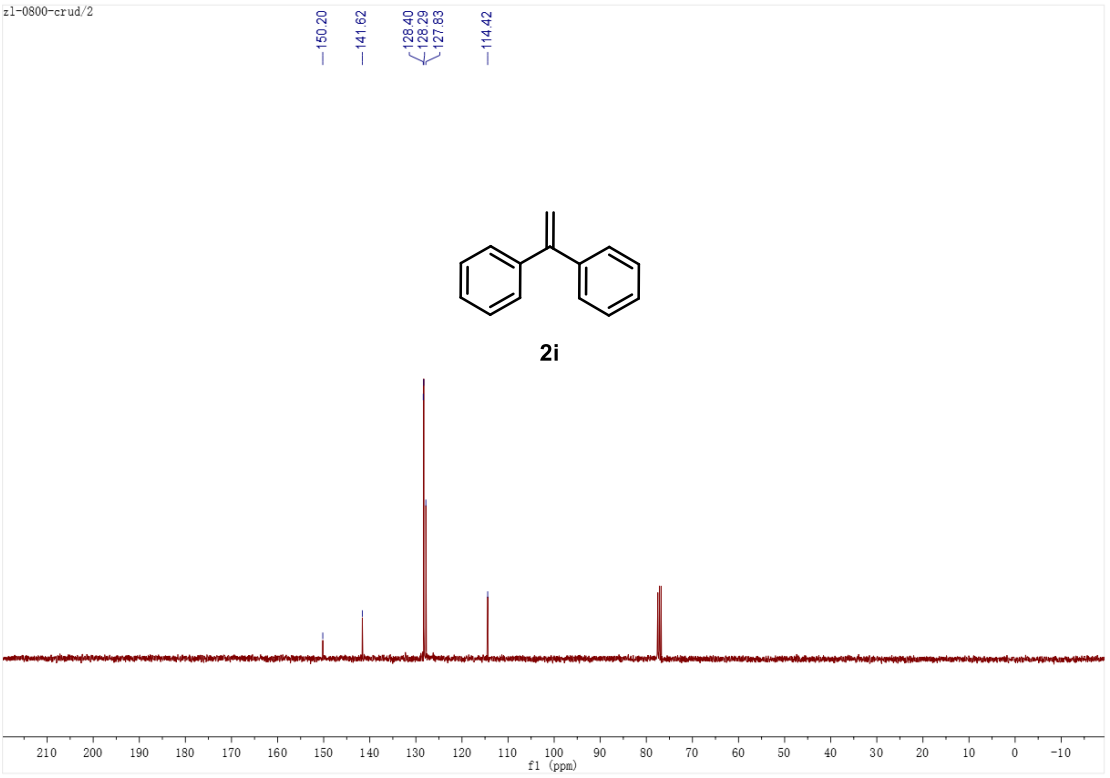
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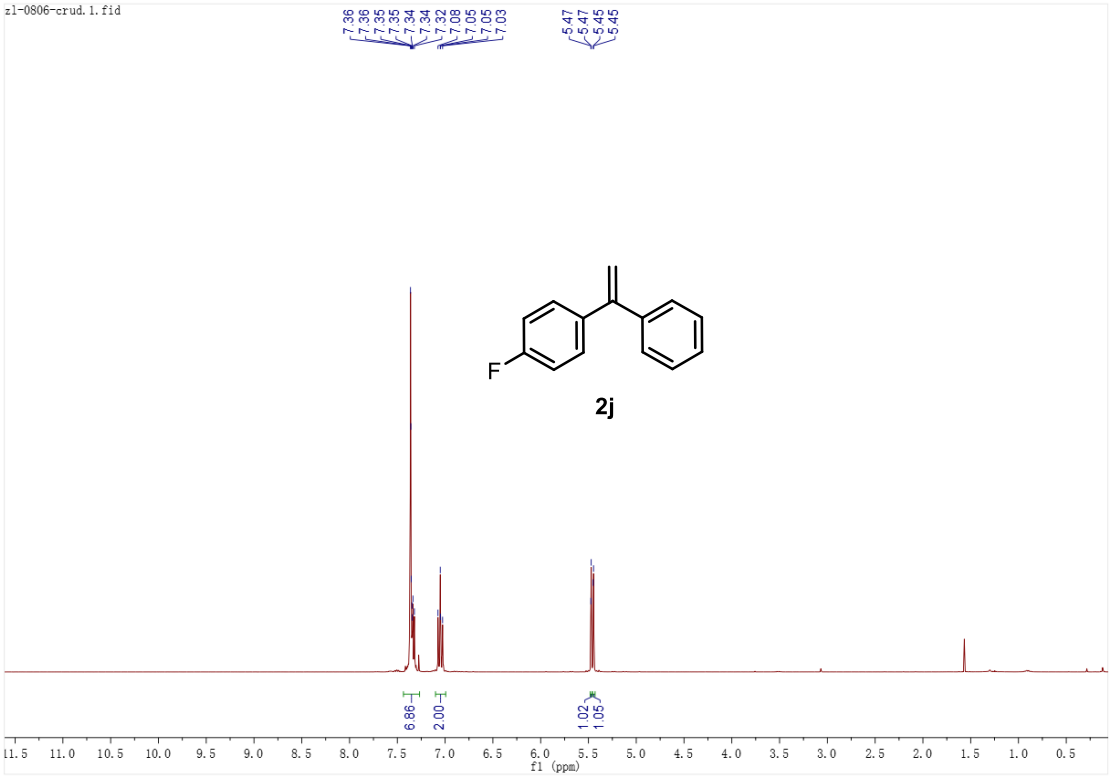
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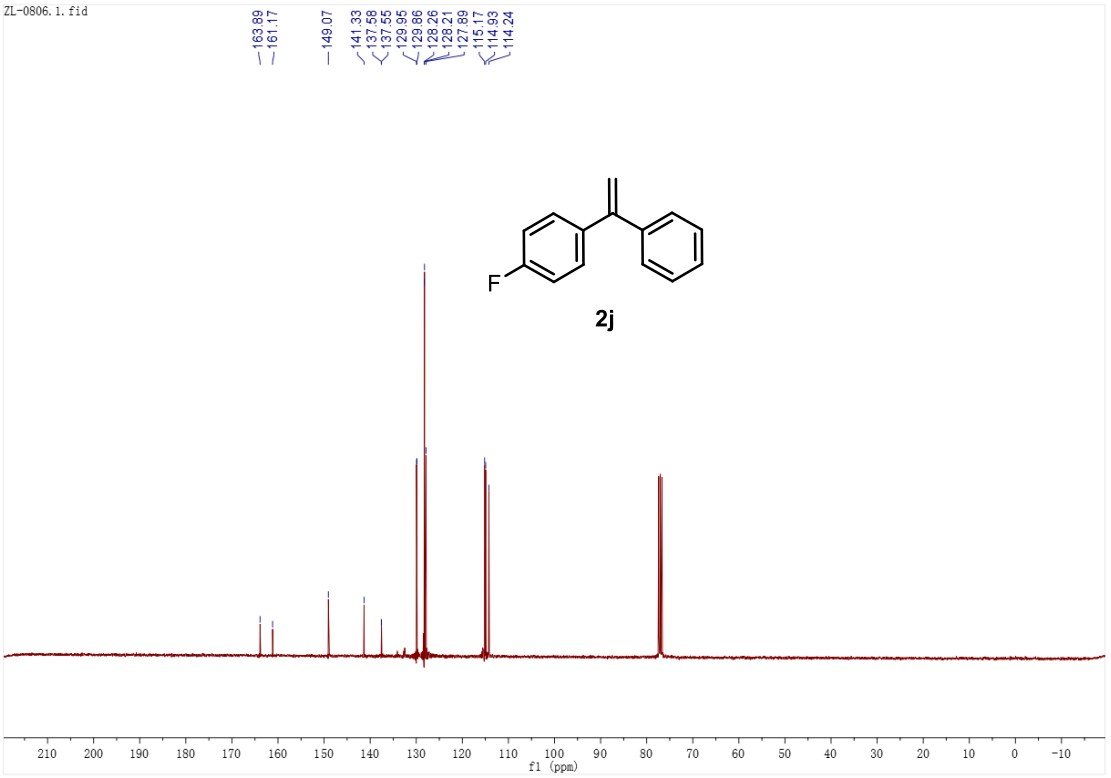
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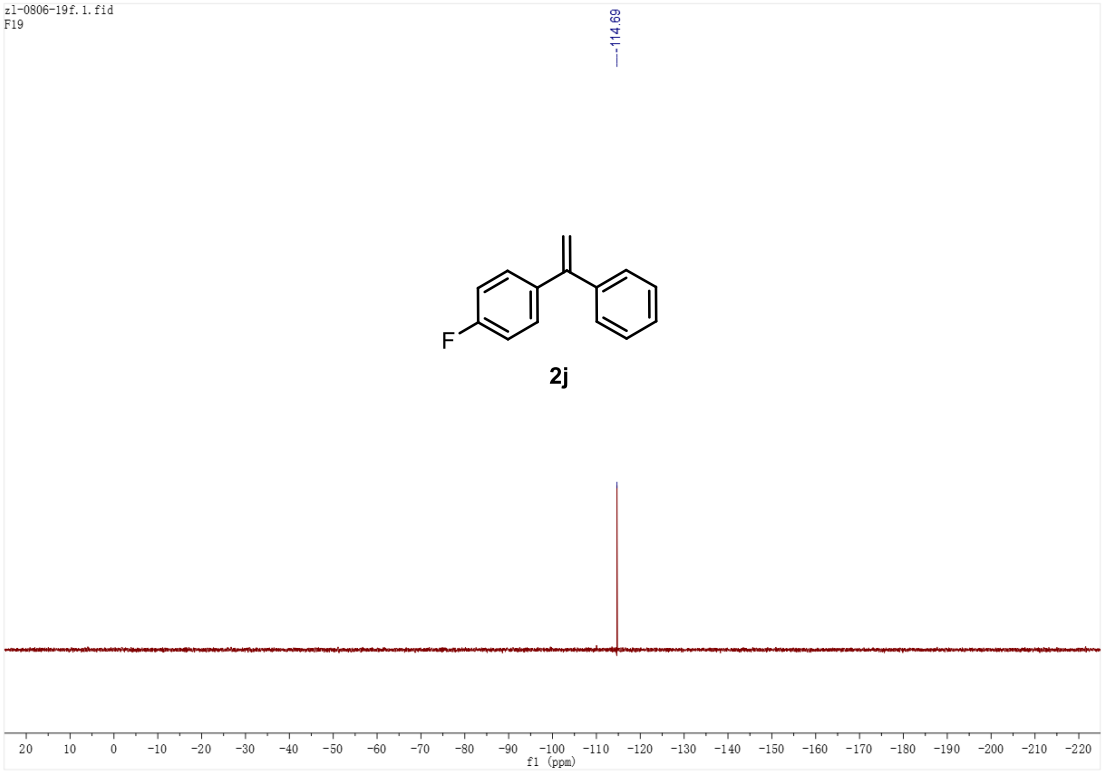
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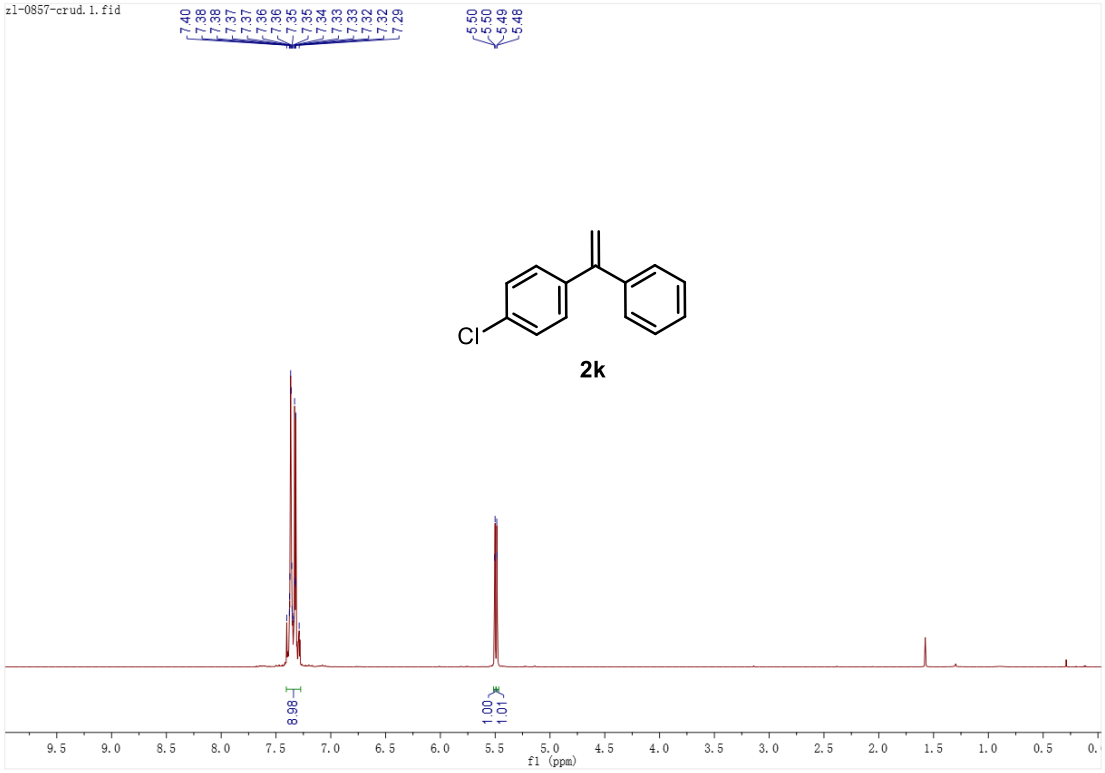
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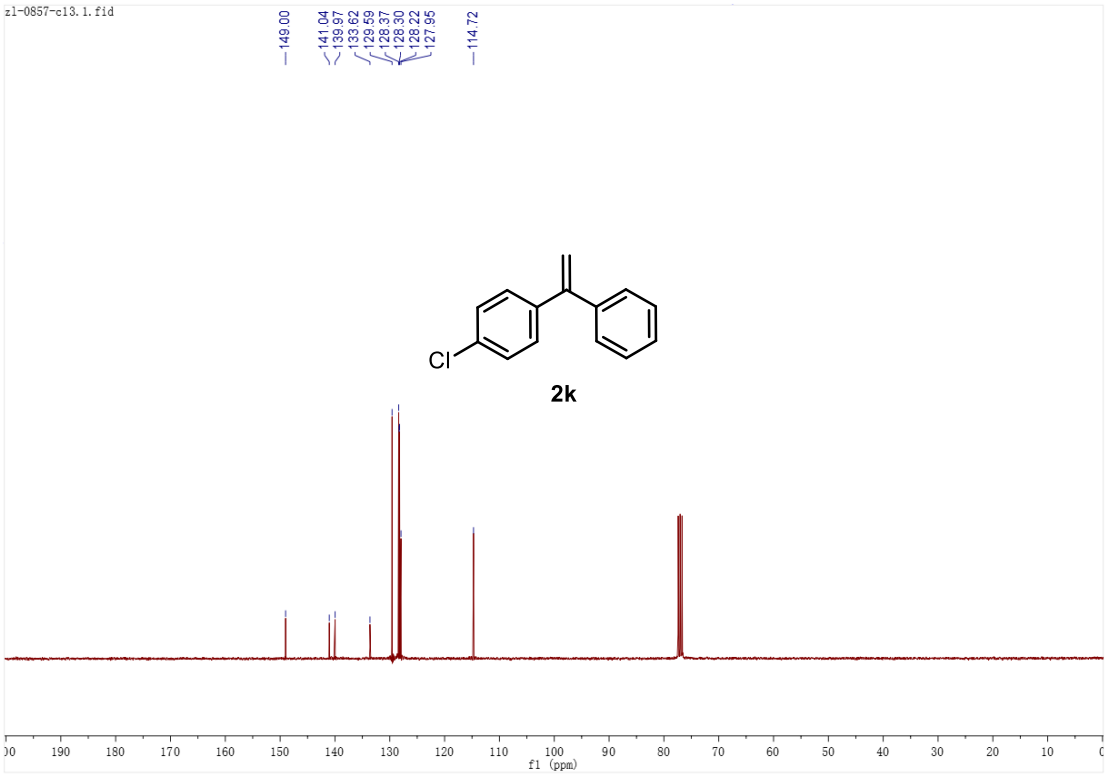
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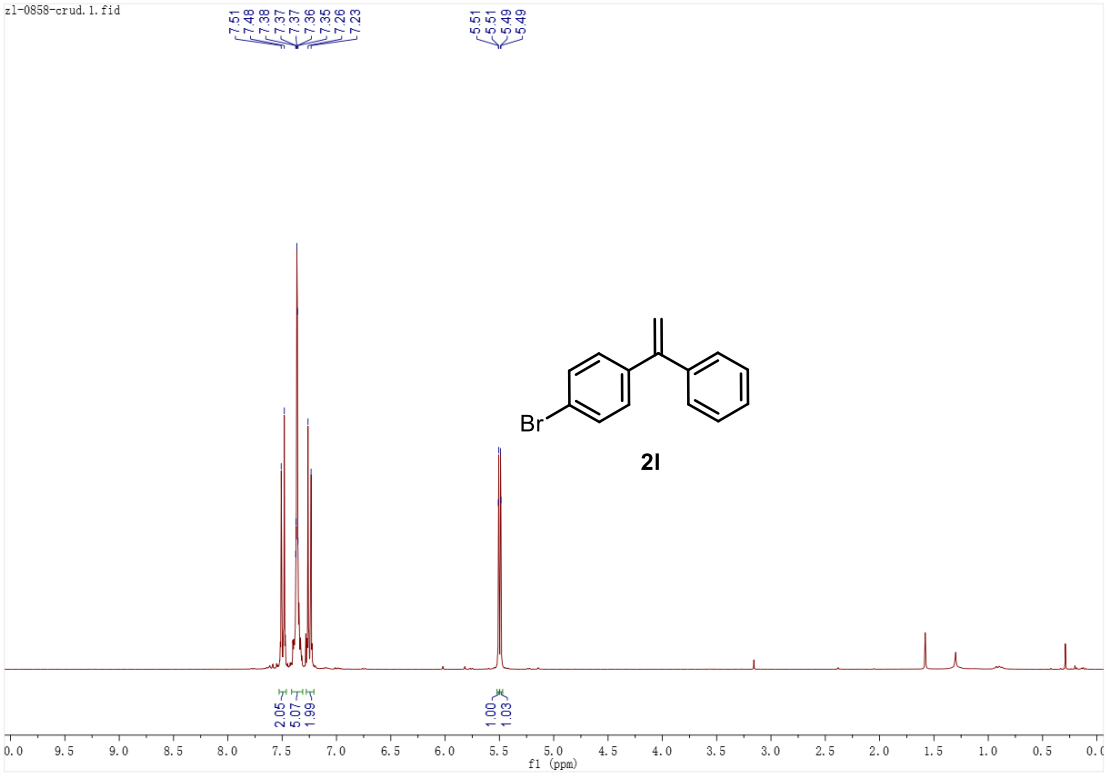
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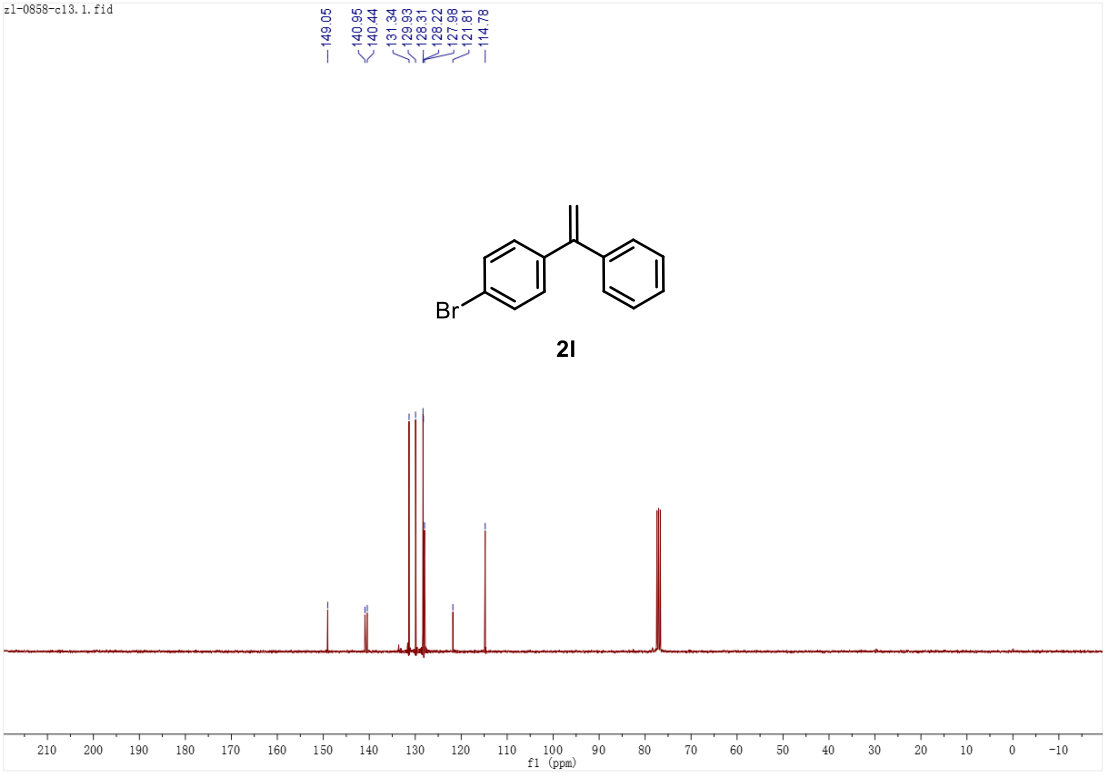
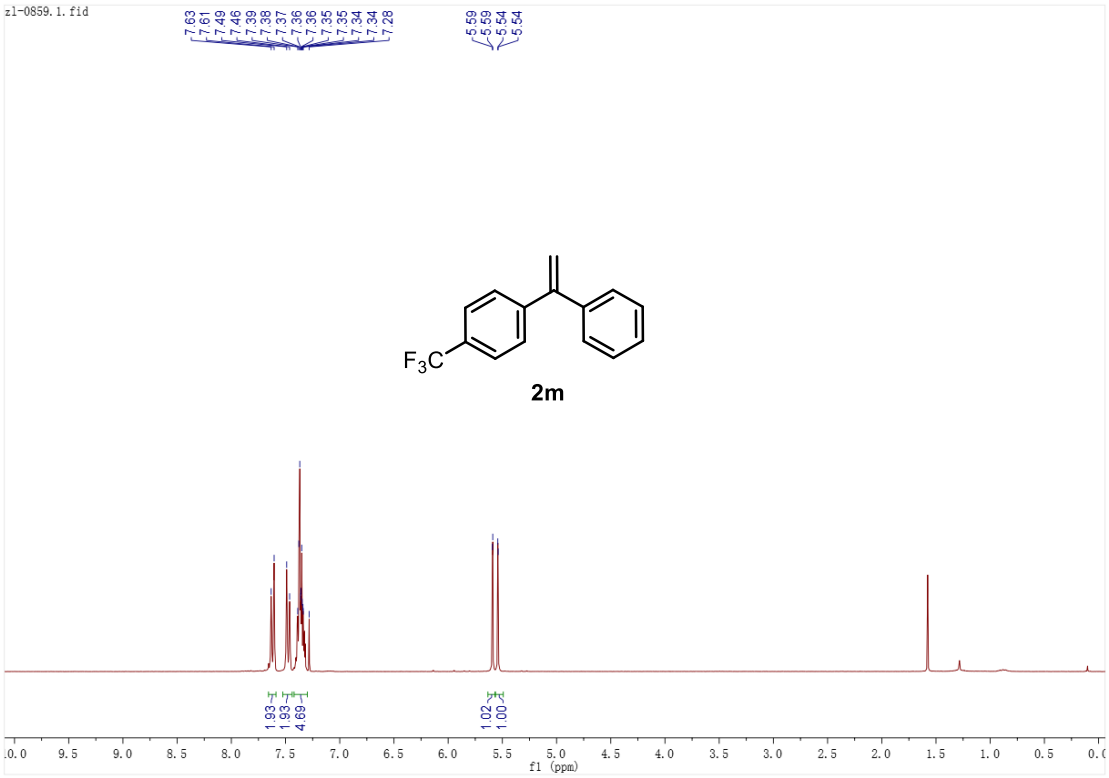
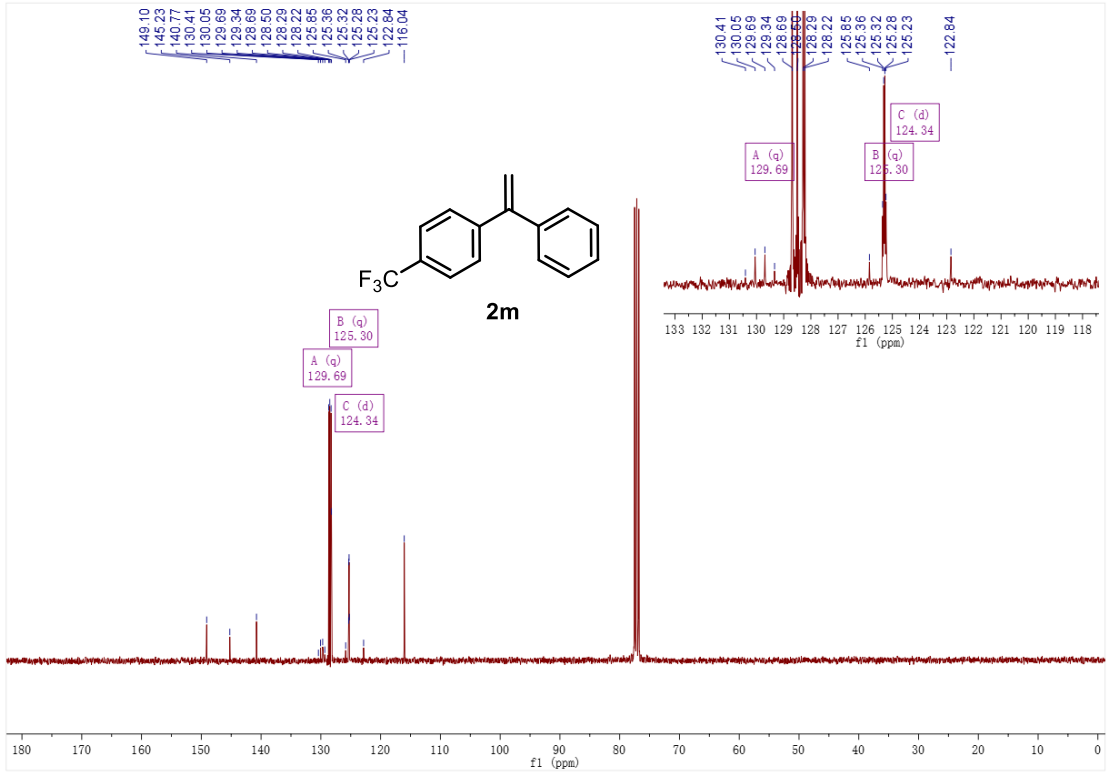
7.51
7.48
7.38
7.37
7.37
7.36
7.35
7.26
7.23
5.51
5.51
5.49
5.49
Br
2.05
5.07
1.99
1.00
1.03
f1 (ppm)

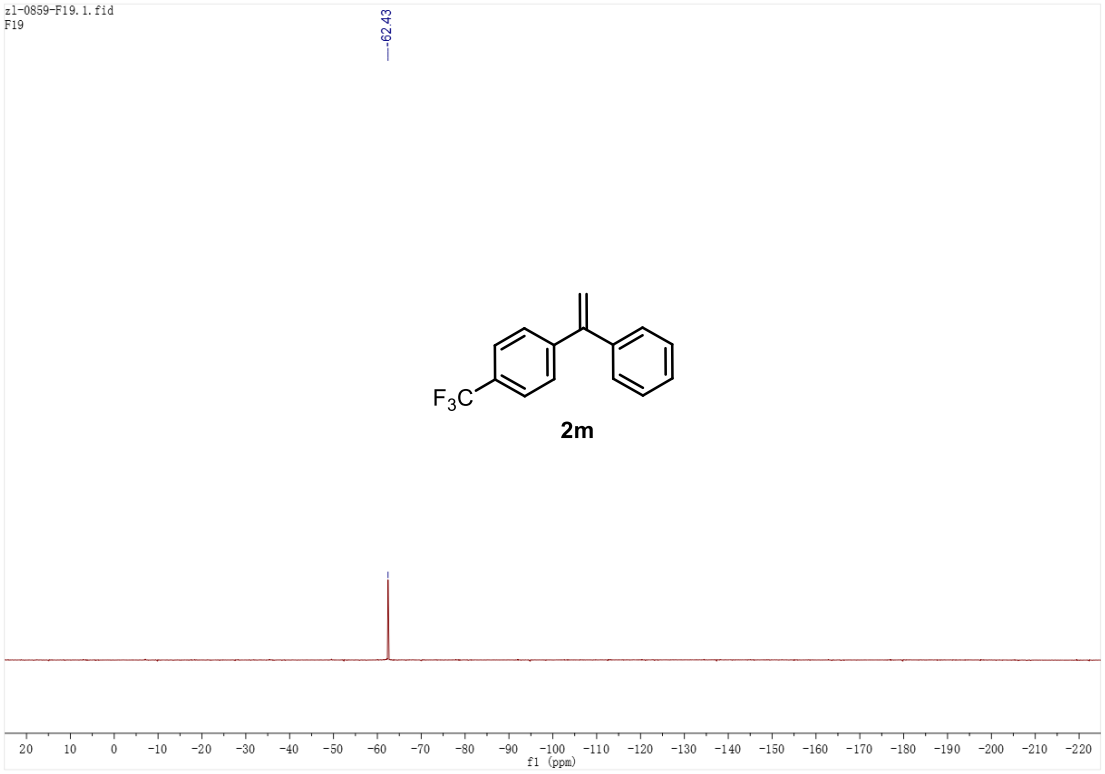
2l

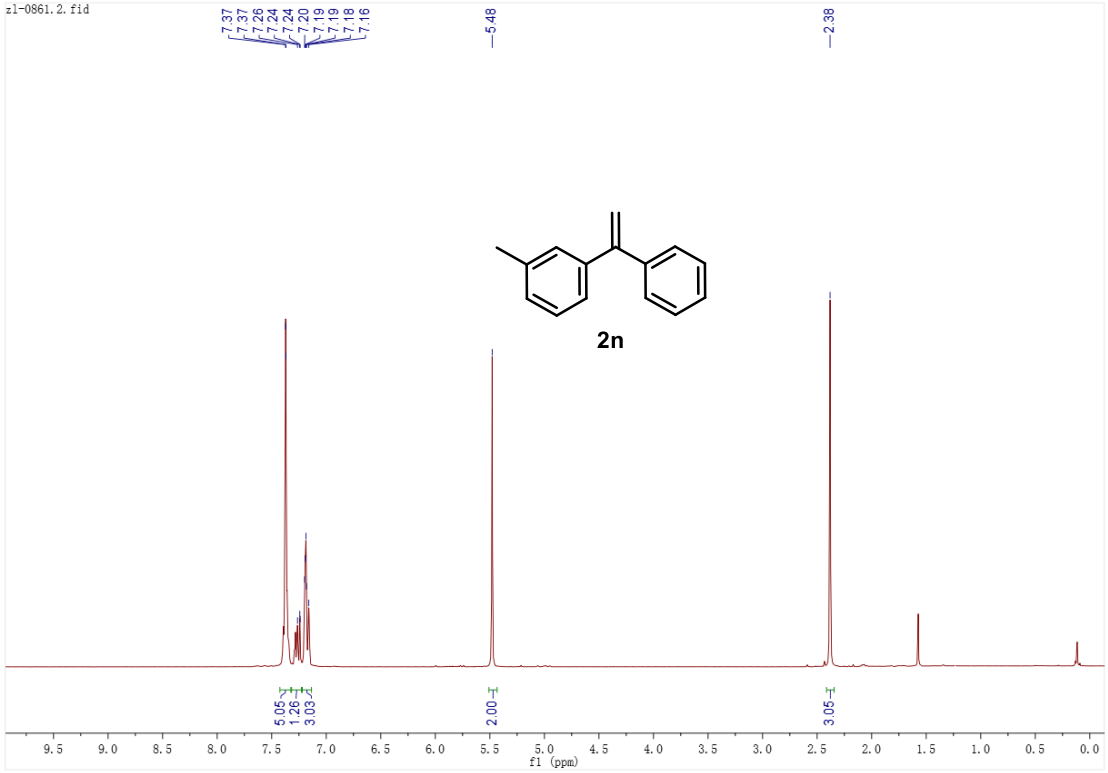

zl-0858-c13.1.fid
149.05
140.95
140.44
131.34
129.93
128.31
128.22
127.98
121.81
114.78
Br
f1 (ppm)

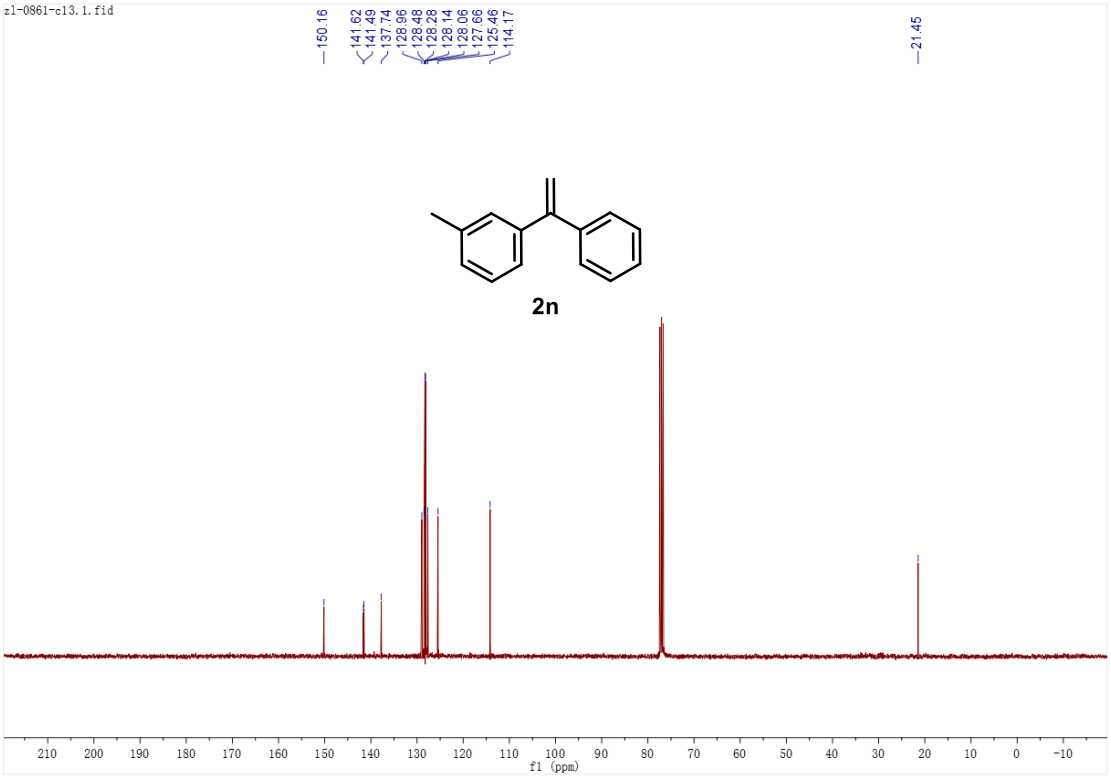
2l

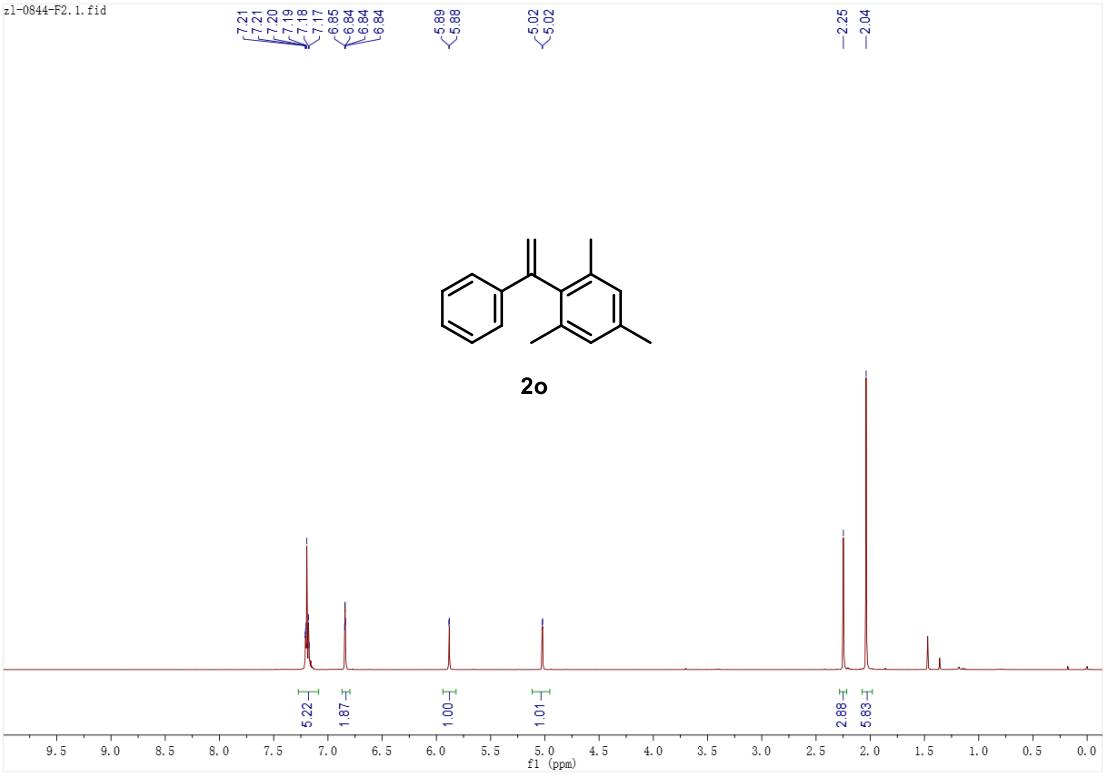

zl-0859.1.fid
7.63
7.61
7.49
7.46
7.39
7.38
7.37
7.36
7.36
7.35
7.35
7.34
7.34
7.28
5.59
5.59
5.54
5.54
F3C
2m
1.93
1.93
4.69
1.02
1.00
f1 (ppm)


149.10
145.23
140.77
130.41
130.05
129.69
129.34
128.69
128.50
128.29
128.22
125.85
125.36
125.32
125.28
125.23
122.84
116.04
F3C
2m
B (q)
125.30
A (q)
129.69
C (d)
124.34
f1 (ppm)

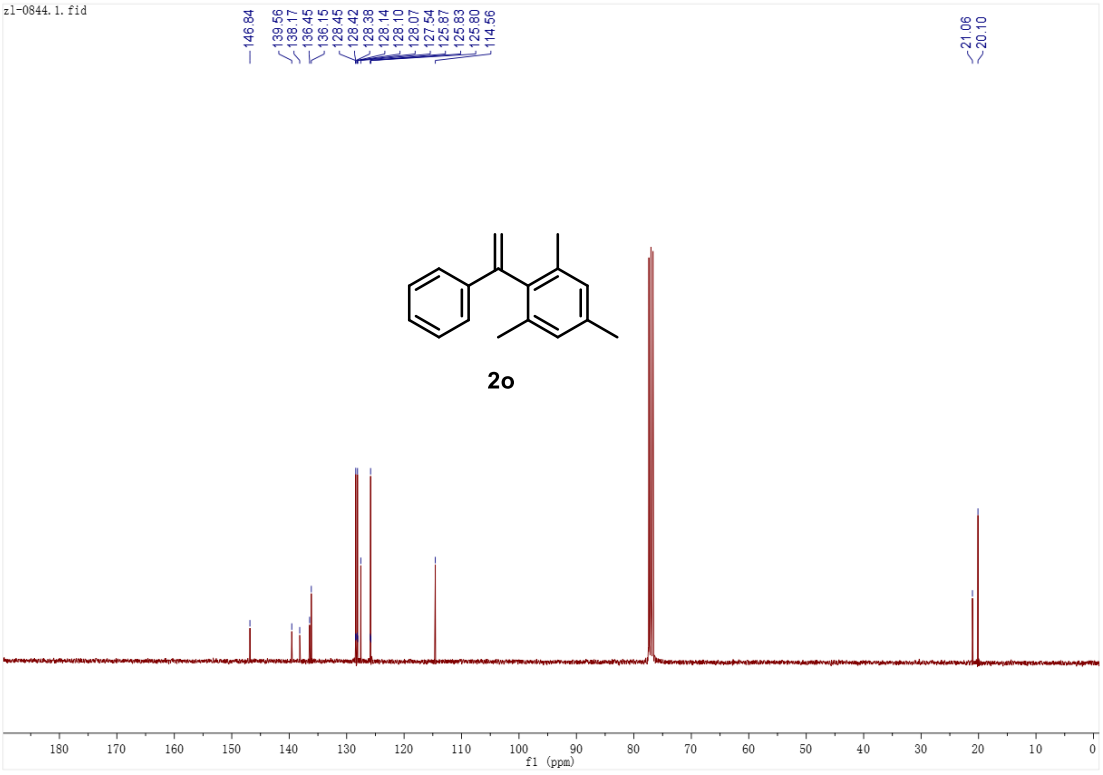

z1-0859-F19.1.fid
F19
-62.43
F3C
2m
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)


zl-0861.2.fid
7.37
7.37
7.26
7.24
7.24
7.20
7.19
7.19
7.18
7.16
5.48
2.38
2n
5.05
1.26
3.03
2.00
3.05
f1 (ppm)

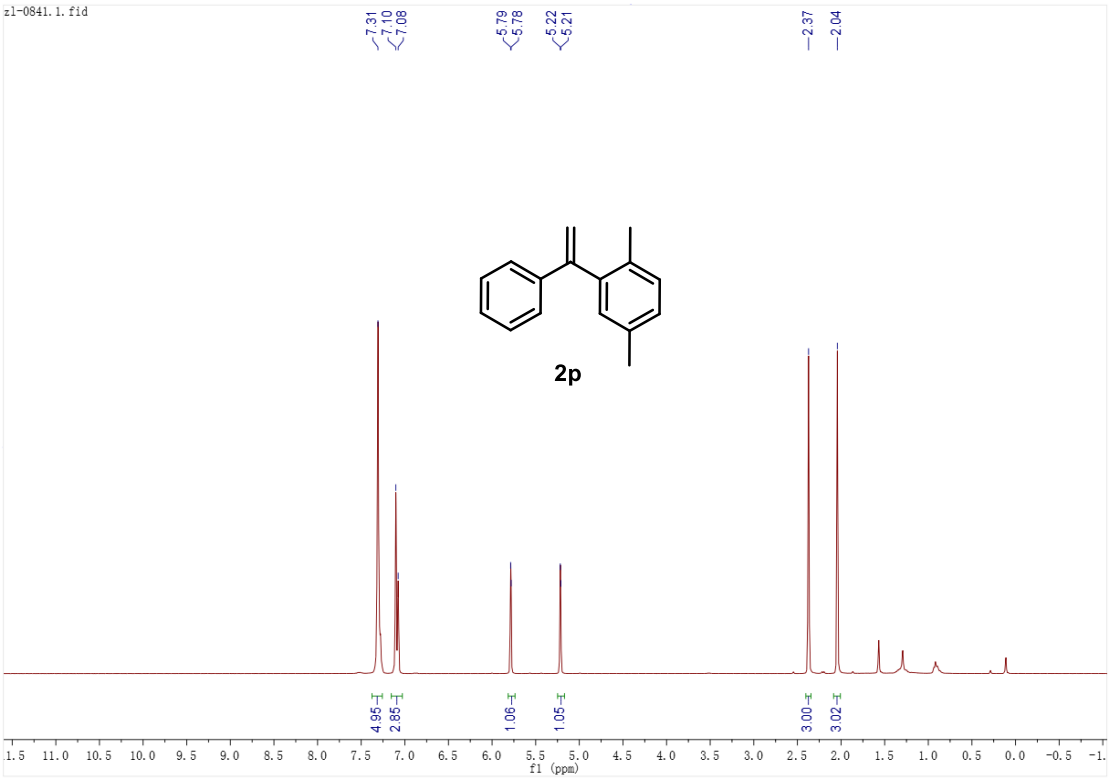

zl-0861-c13.1.fid
150.16
141.62
141.49
137.74
128.96
128.48
128.28
128.14
128.06
127.66
125.46
114.17
21.45
2n
f1 (ppm)

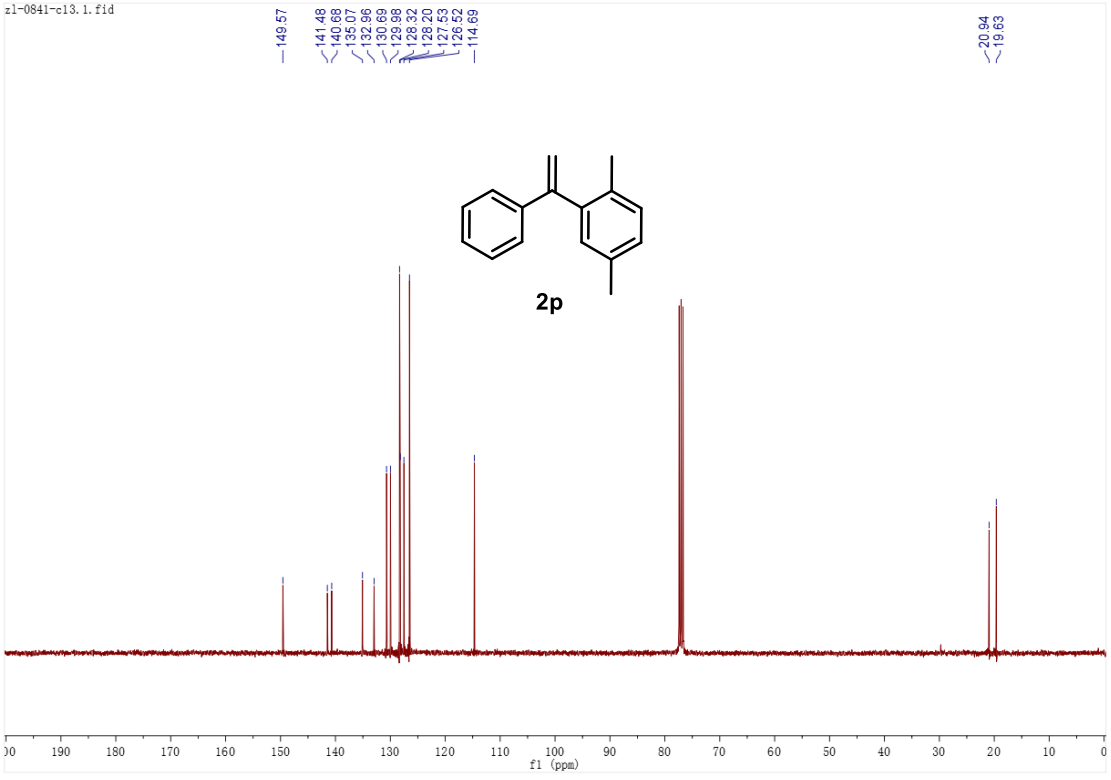

zl-0844-F2.1.fid
7.21
7.21
7.20
7.19
7.18
7.17
6.85
6.84
6.84
6.84
5.89
5.88
5.02
5.02
2.25
2.04
5.22
1.87
1.00
1.01
2.88
5.83
f1 (ppm)

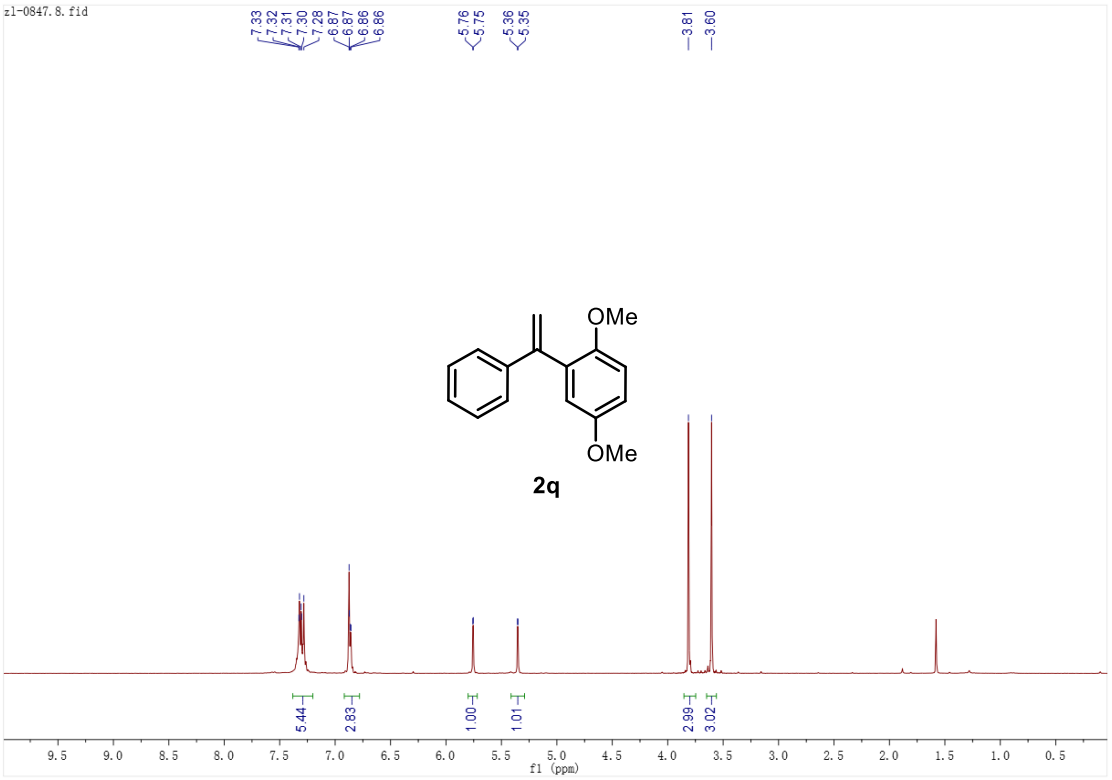
2o

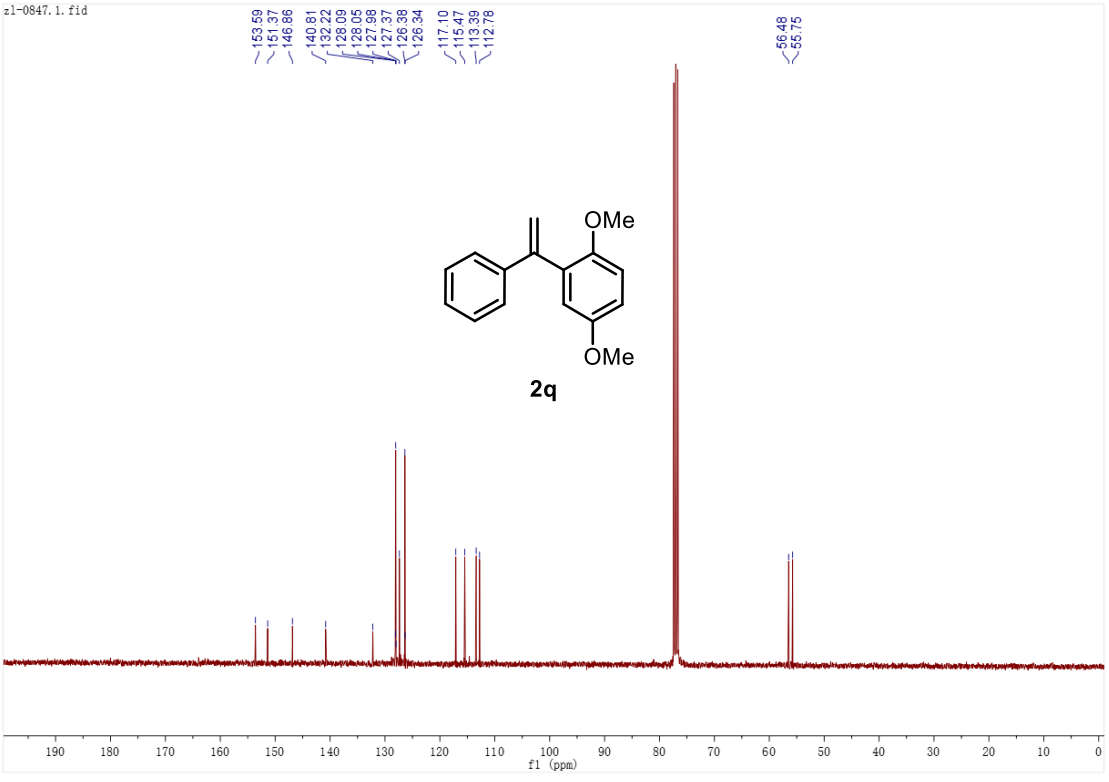

zl-0844.1.fid
146.84
139.56
138.17
136.45
136.15
128.45
128.42
128.38
128.14
128.10
128.07
127.54
125.87
125.83
125.80
114.56
21.06
20.10
f1 (ppm)

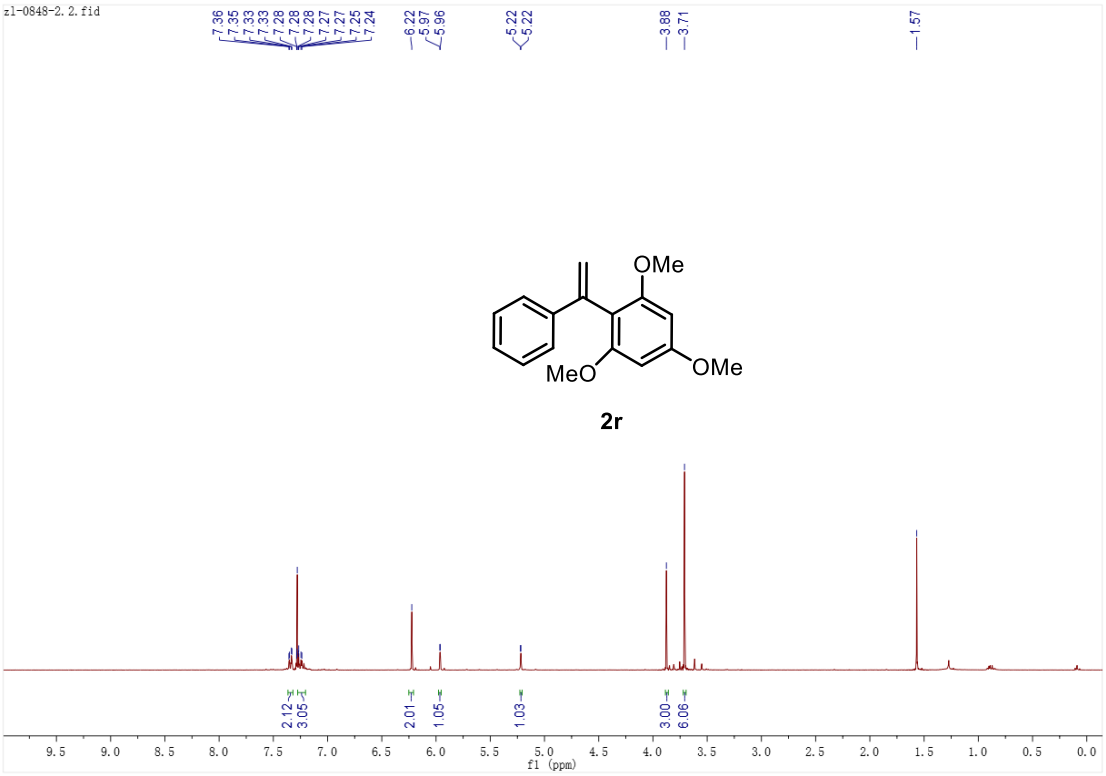
2o

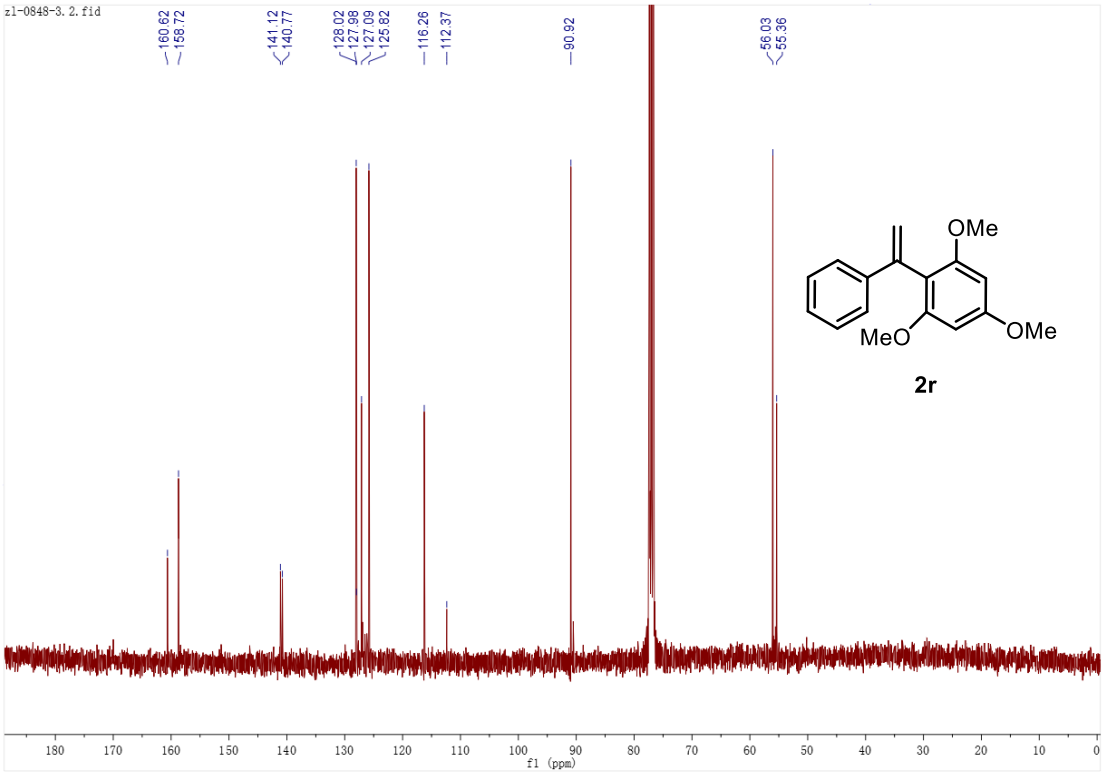

z1-0841.1.fid
7.31
7.10
7.08
5.79
5.78
5.22
5.21
2.37
2.04
2p
4.95
2.85
1.06
1.05
3.00
3.02
f1 (ppm)

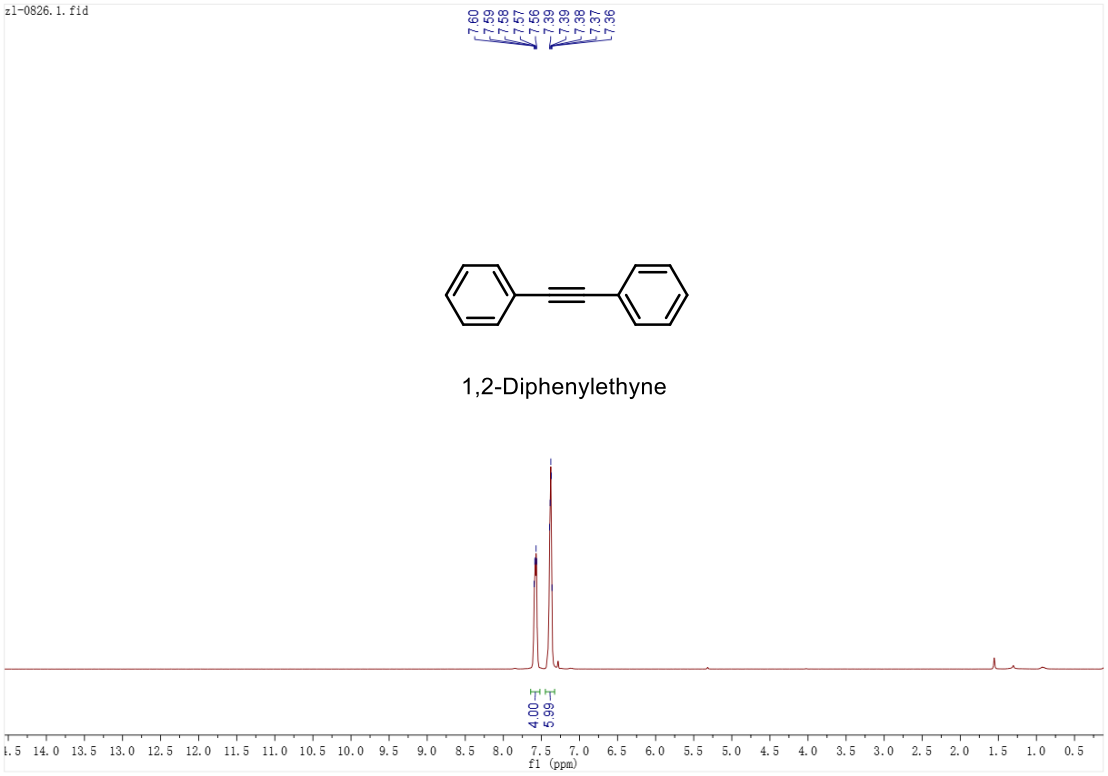

z1-0841-c13.1.fid
149.57
141.48
140.88
135.07
132.96
130.69
129.98
128.32
128.20
127.53
126.52
114.69
20.94
19.63
2p
f1 (ppm)


zl-0847.8.fid
7.33
7.32
7.31
7.30
7.28
6.87
6.87
6.86
6.86
5.76
5.75
5.36
5.35
3.81
3.60
OMe
OMe
2q
5.44
2.83
1.00
1.01
2.99
3.02
f1 (ppm)

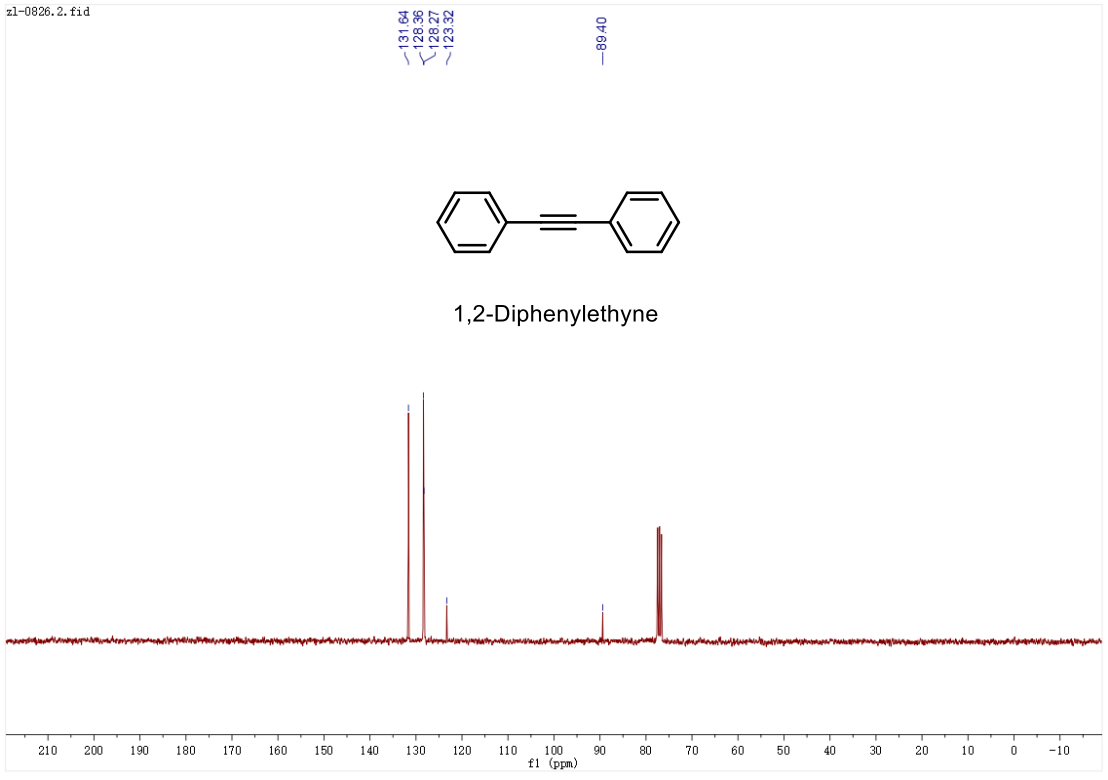

zl-0847.1.fid
153.59
151.37
146.86
140.81
132.22
128.09
128.05
127.98
127.37
126.38
126.34
117.10
115.47
113.39
112.78
56.48
55.75
OMe
OMe
2q
f1 (ppm)


z1-0848-2.2.fid
7.36
7.35
7.33
7.28
7.28
7.28
7.27
7.27
7.25
7.24
6.22
5.97
5.96
5.22
5.22
3.88
3.71
1.57
OMe
MeO
OMe
2r
2.12
3.05
2.01
1.05
1.03
3.00
6.06
f1 (ppm)

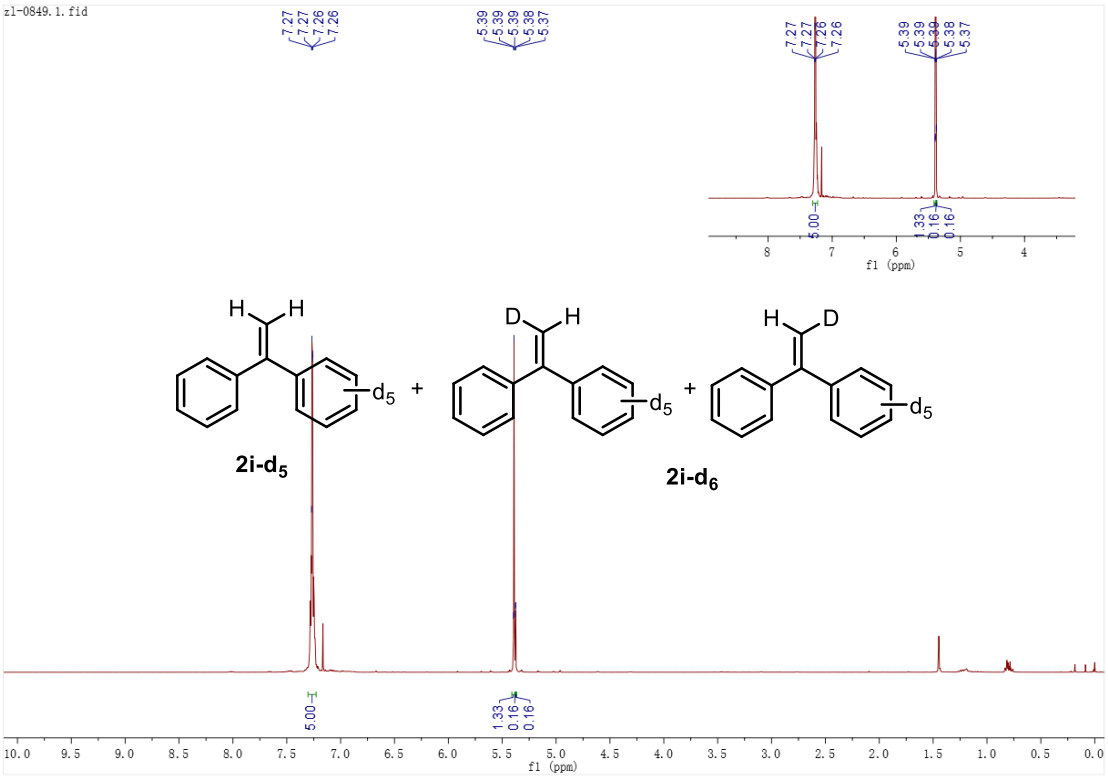

z1-0848-3.2.fid
160.62
158.72
141.12
140.77
128.02
127.98
127.09
125.82
116.26
112.37
90.92
56.03
55.36
OMe
MeO
OMe
2r
f1 (ppm)

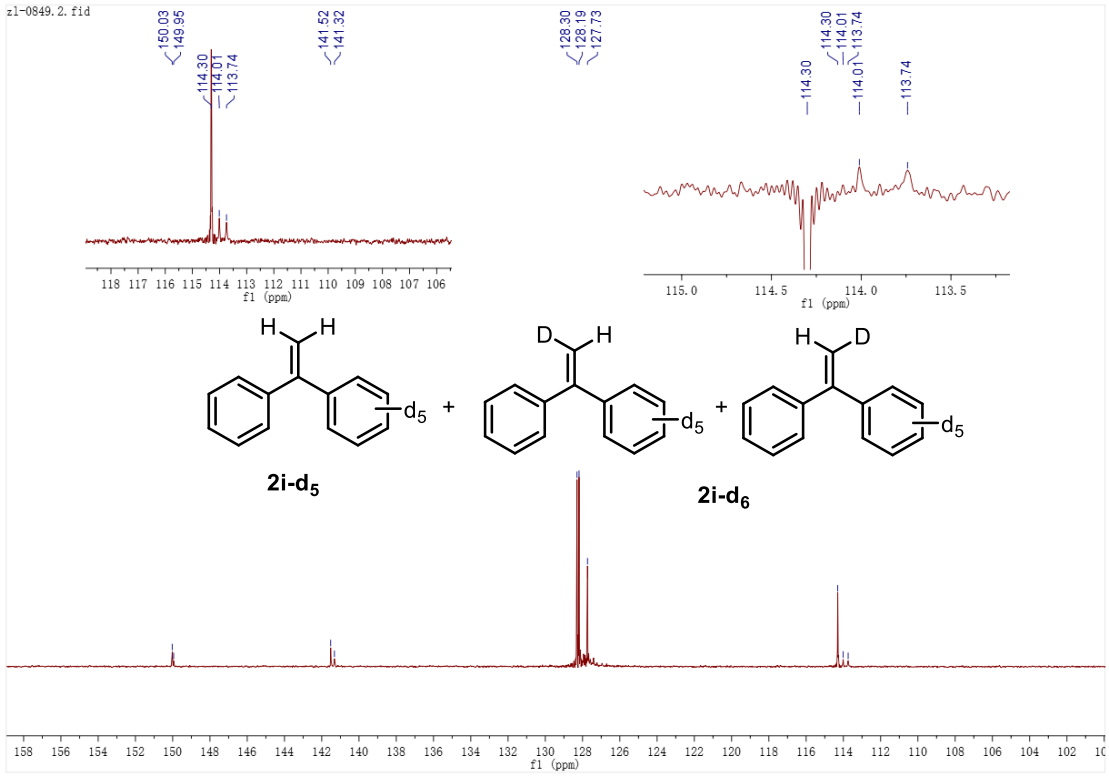


1,2-Diphenylethyne



1,2-Diphenylethyne


zl-0849.1.fid
7.27
7.27
7.26
7.26
5.39
5.39
5.39
5.38
5.37
5.00
1.33
0.16
0.16
f1 (ppm)
H
H
D
H
H
D
d5
d5
d5
+
+
2i-d5
2i-d6


zl-0849.2.fid
150.03
149.95
141.52
141.32
128.30
128.19
127.73
114.30
114.01
113.74
f1 (ppm)
H
H
D
H
H
D
d5
d5
d5
+
+
2i-d5
2i-d6