Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Lithium diisobutyl-*tert*-butoxyaluminum hydride (LDBBA) catalyzed hydroboration of alkynes and imines with pinacolborane

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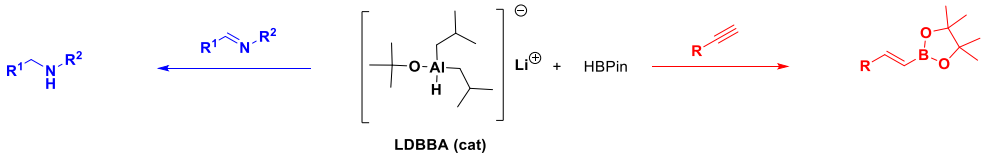

LDBBA (cat)

1. Copies of NMR spectra.

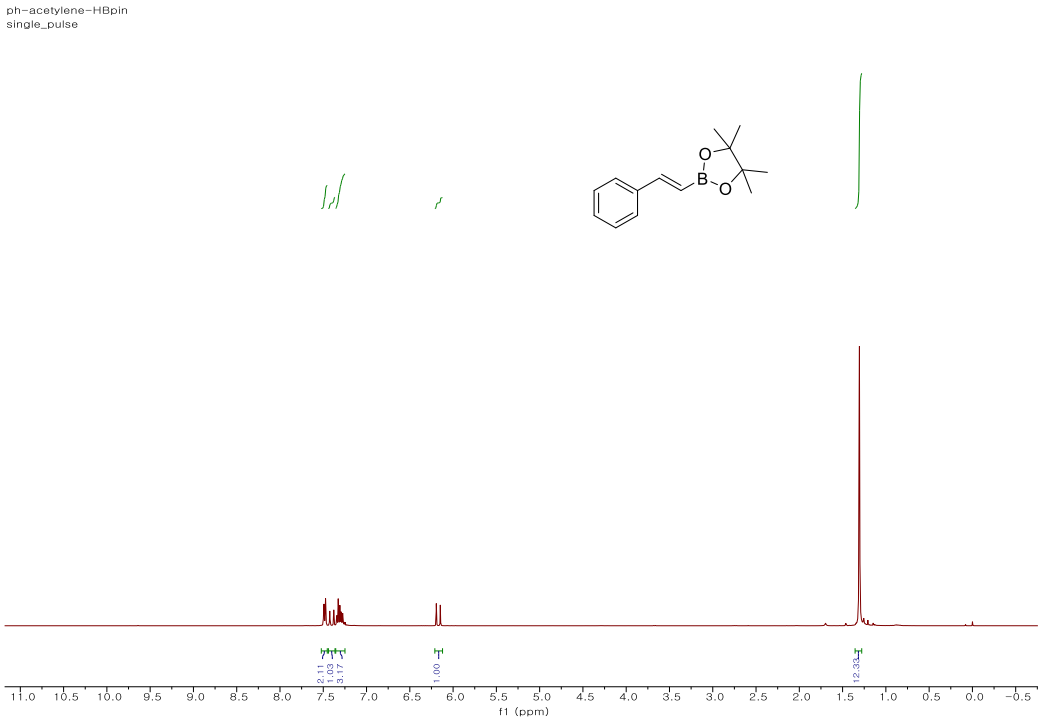

Figure S1: ^{1}H NMR of (*E*)-4,4,5,5-tetramethyl-2-styryl-1,3,2-dioxaborolane (**2a**)

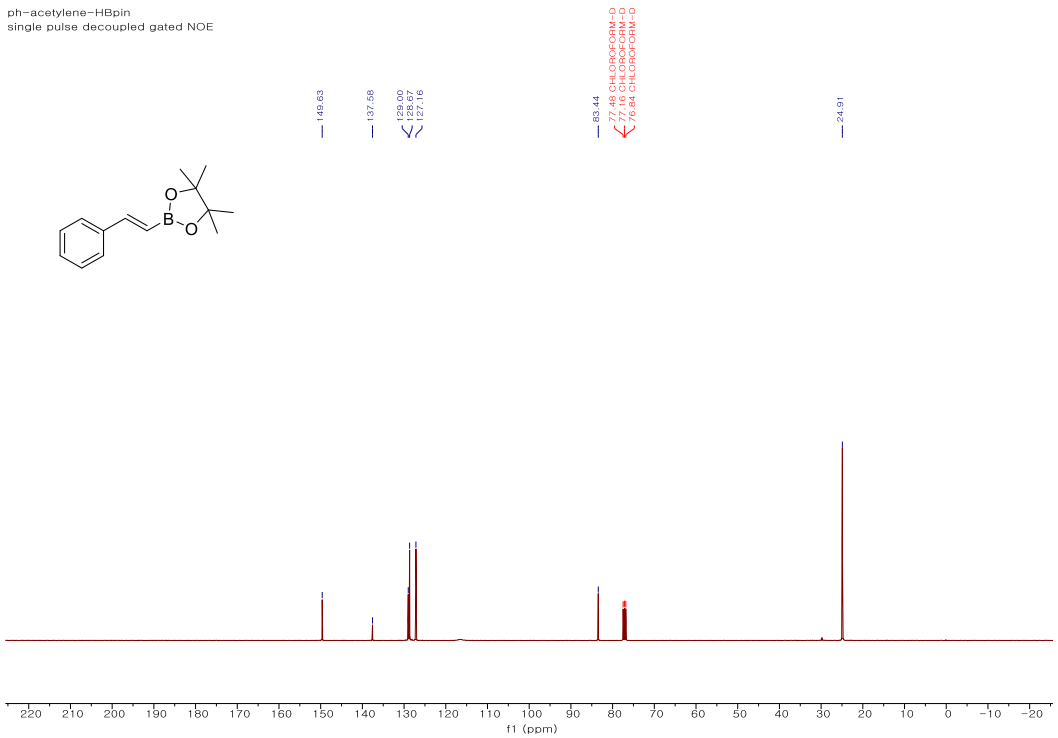

Figure S2: ^{13}C NMR of (*E*)-4,4,5,5-tetramethyl-2-styryl-1,3,2-dioxaborolane (**2a**).

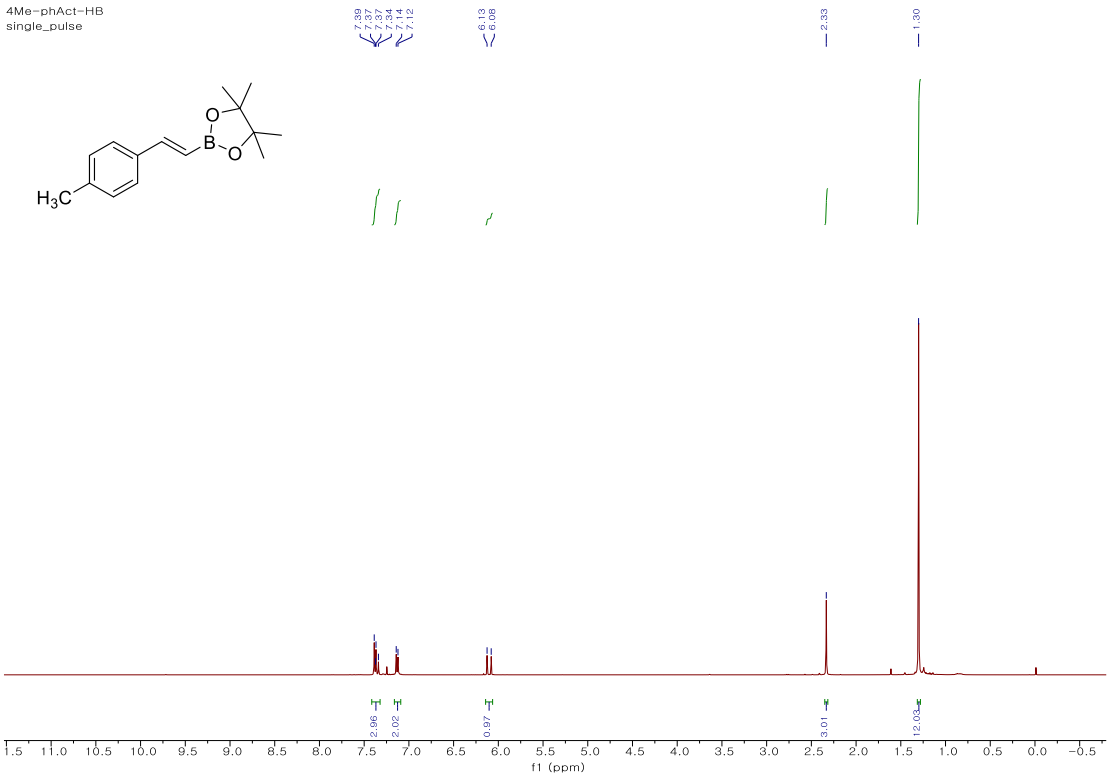

Figure S3: ^{1}H NMR of (*E*)-4,4,5,5-tetramethyl-2-(4-methylstyryl)-1,3,2-dioxaborolane (**2b**)

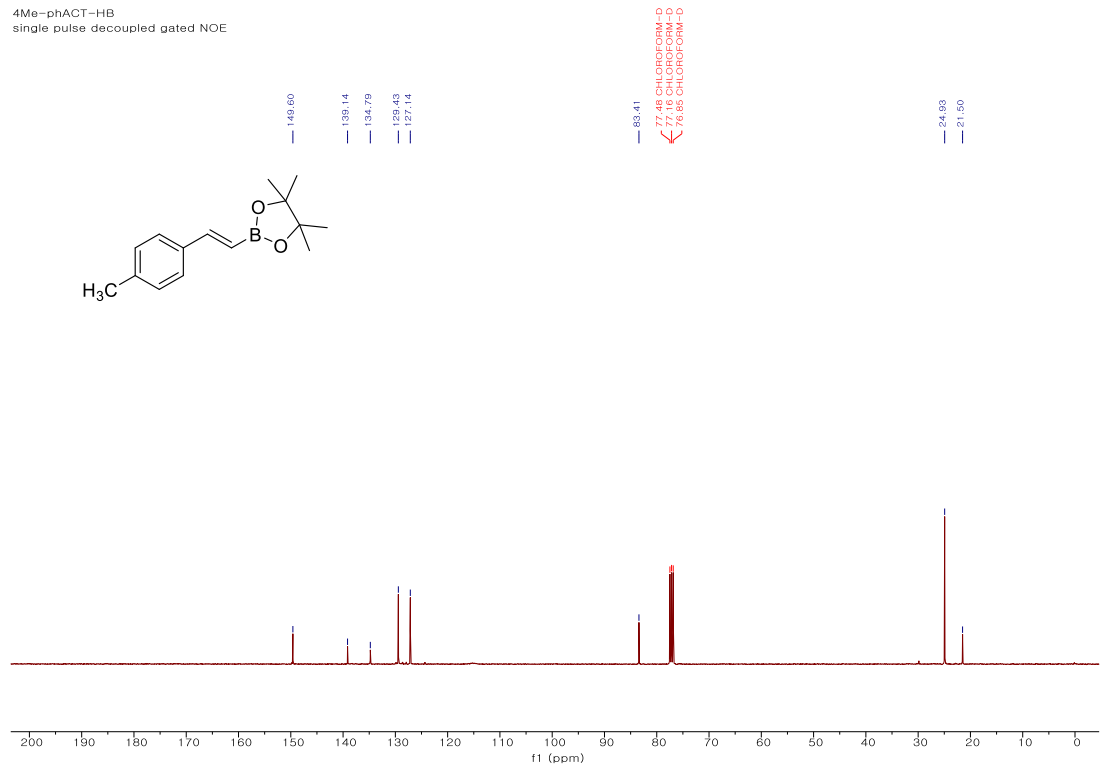

Figure S4: ^{13}C NMR of (*E*)-4,4,5,5-tetramethyl-2-(4-methylstyryl)-1,3,2-dioxaborolane (**2b**)

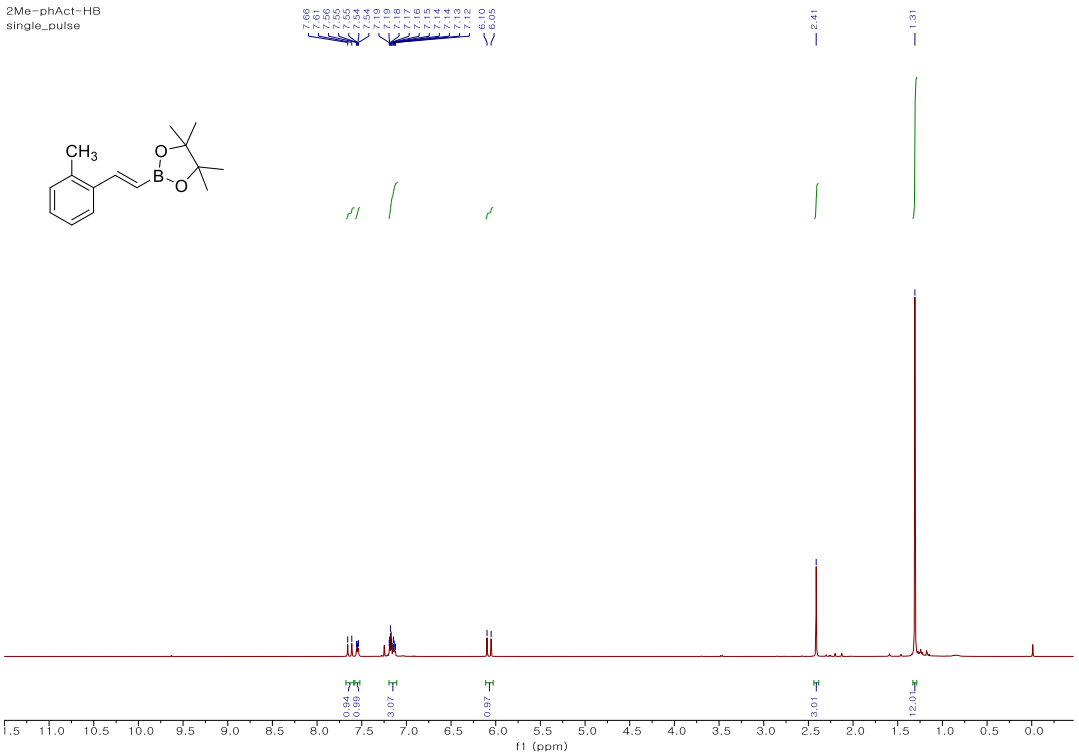

Figure S5: ^{1}H NMR of **(***E*)-4,4,5,5-tetramethyl-2-(2-methylstyryl)-1,3,2-dioxaborolane (**2c**)

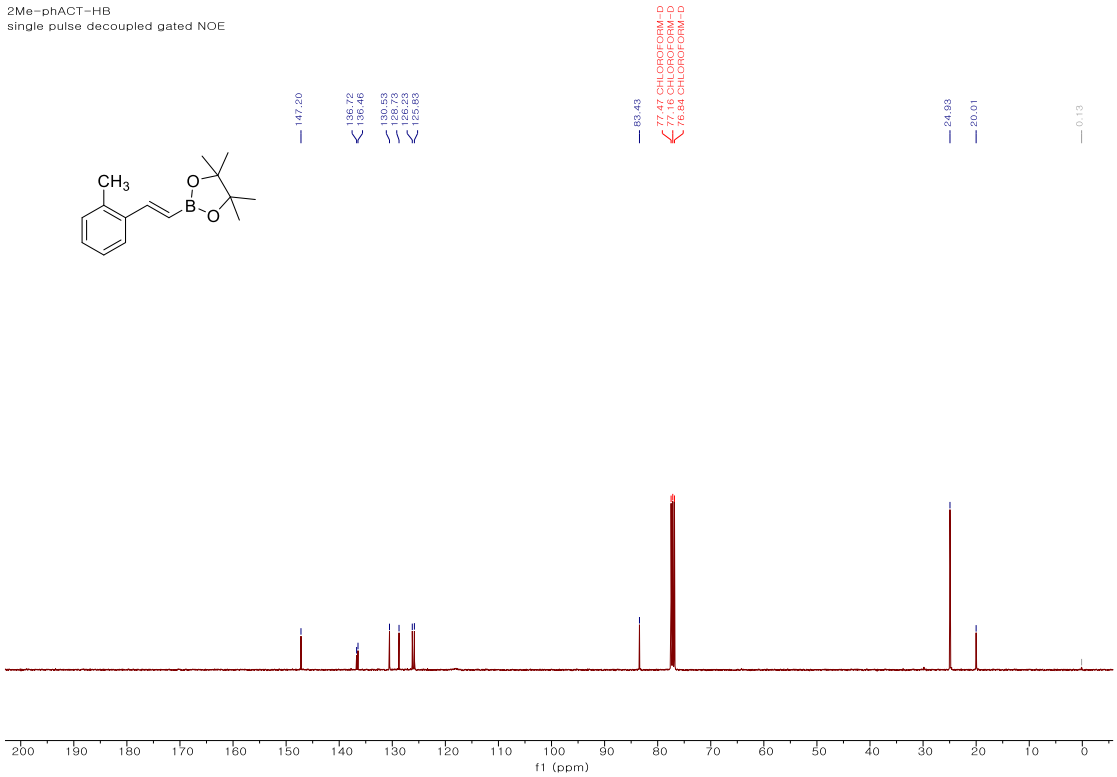

Figure S6: ^{13}C NMR of **(***E*)-4,4,5,5-tetramethyl-2-(2-methylstyryl)-1,3,2-dioxaborolane (**2c**)

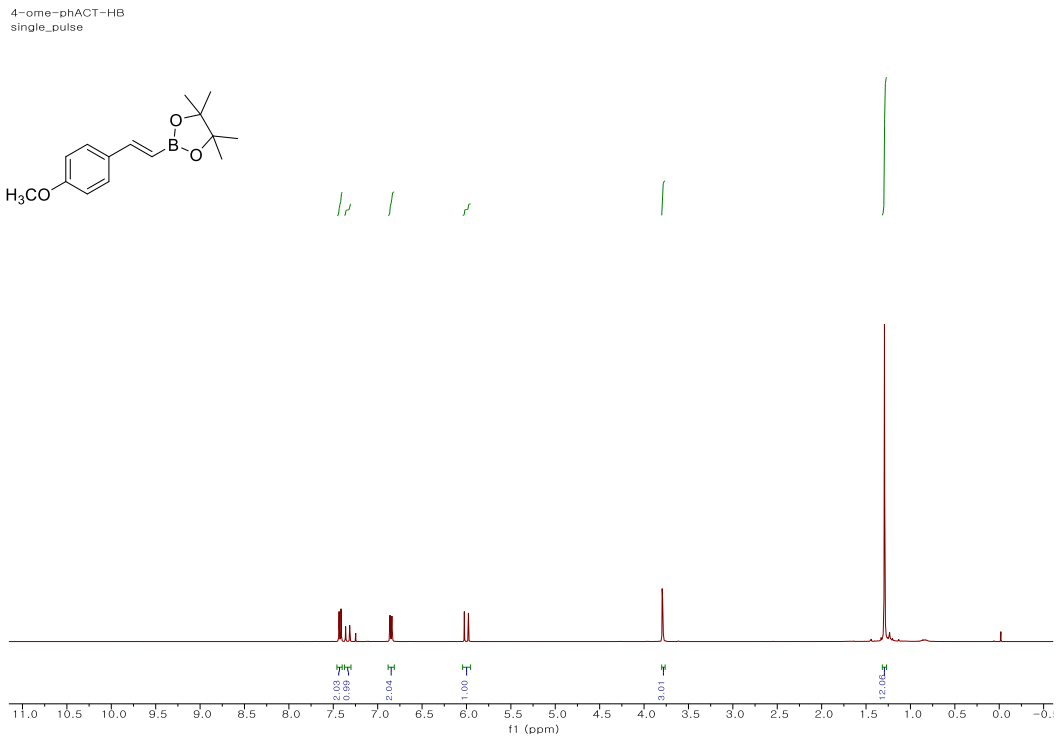

Figure S7: ^{1}H NMR of (*E*)-2-(4-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2d**)

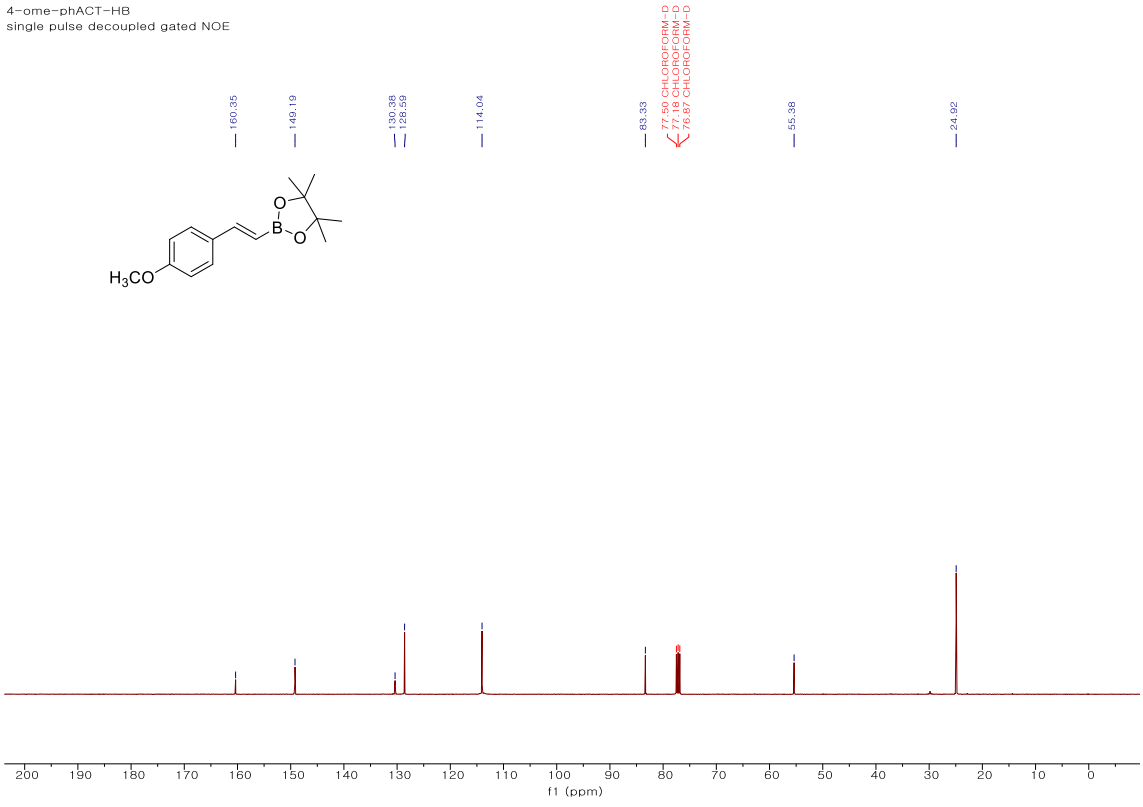

Figure S8: ^{13}C NMR of (*E*)-2-(4-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2d**)

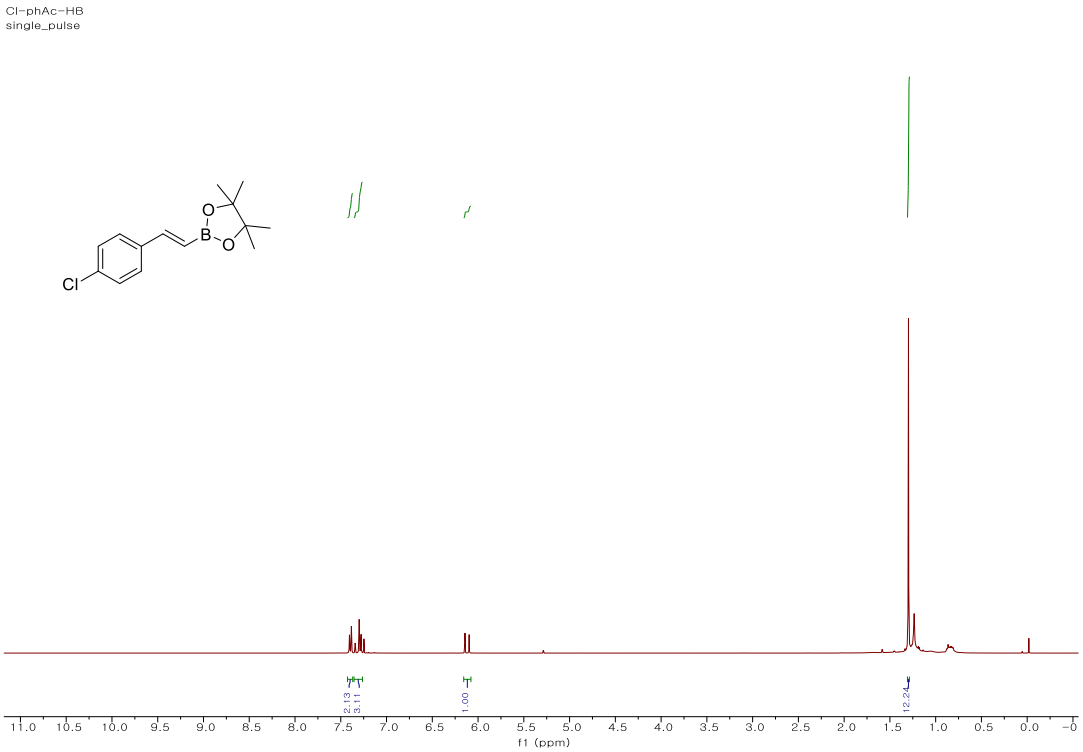

Figure S9: ^{1}H NMR of (*E*)-2-(4-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2e**)

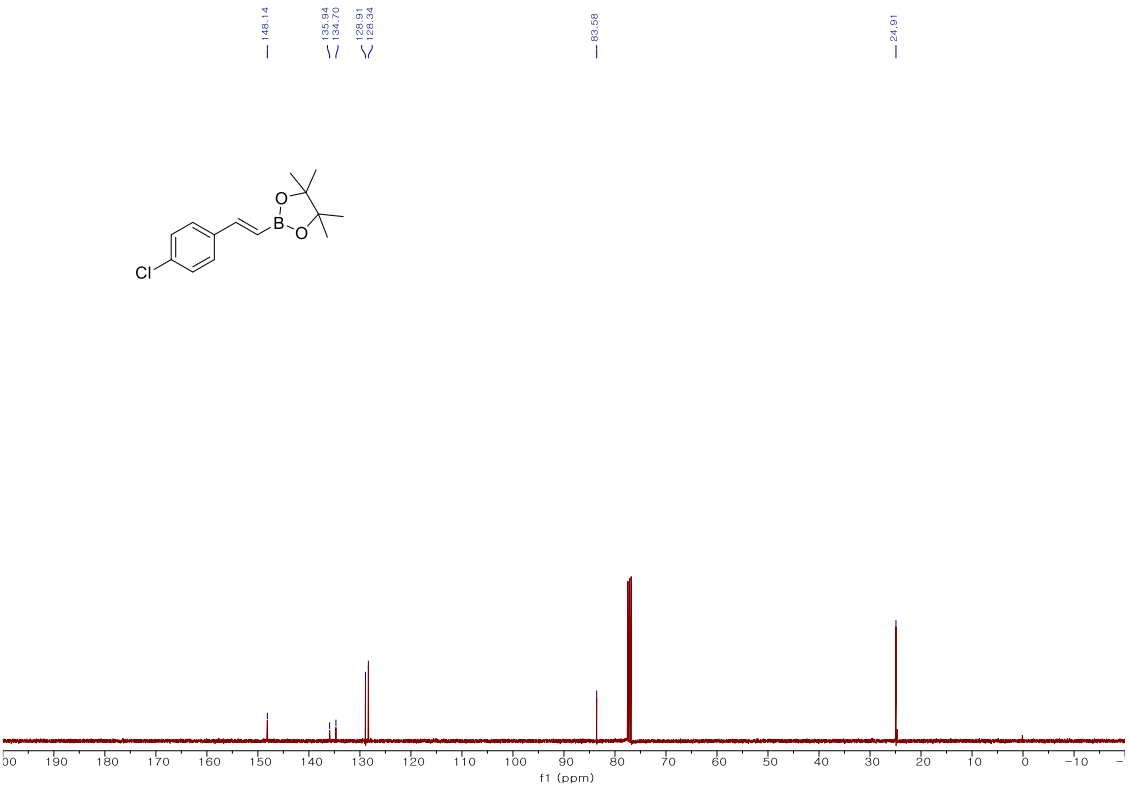

Figure S10: ^{13}C NMR of (*E*)-2-(4-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2e**)

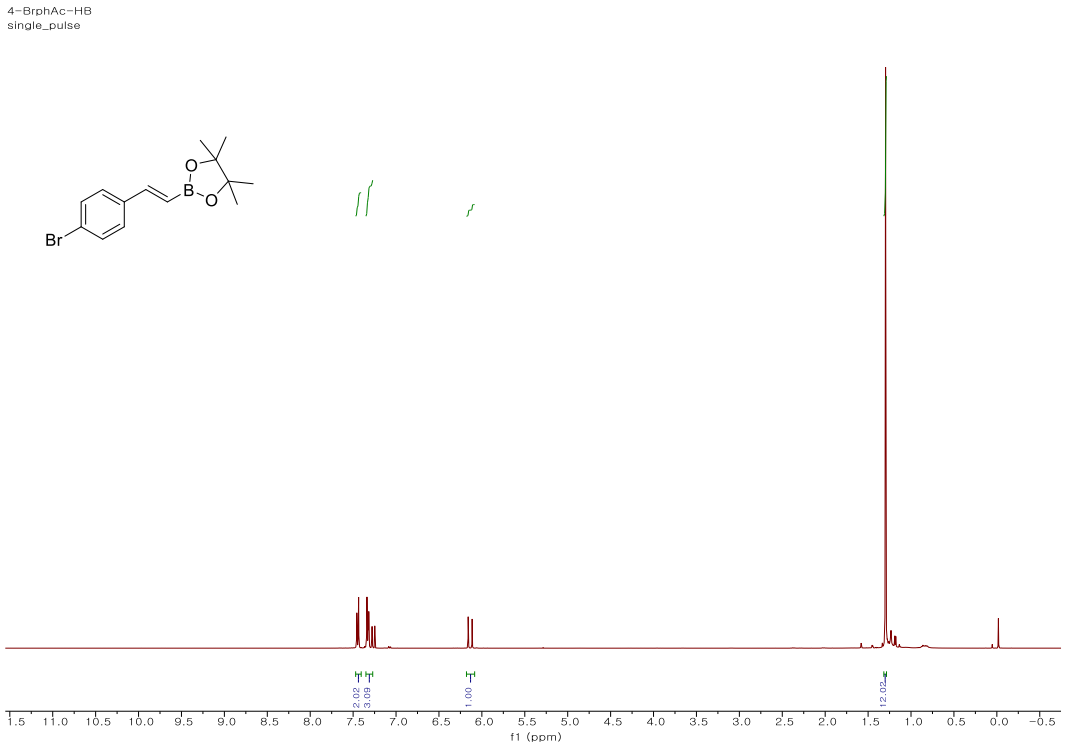

Figure S11: ^{1}H NMR of (*E*)-2-(4-bromostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2f**)

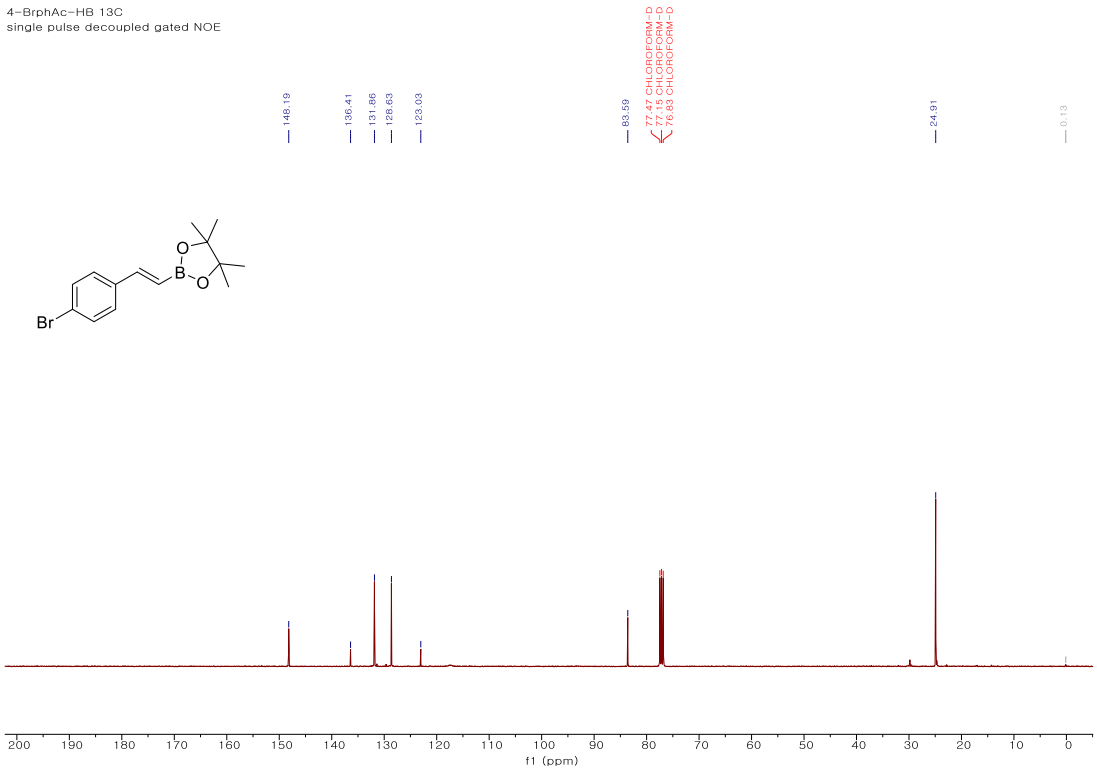

Figure S12: 13C NMR of (*E*)-2-(4-bromostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2f**)

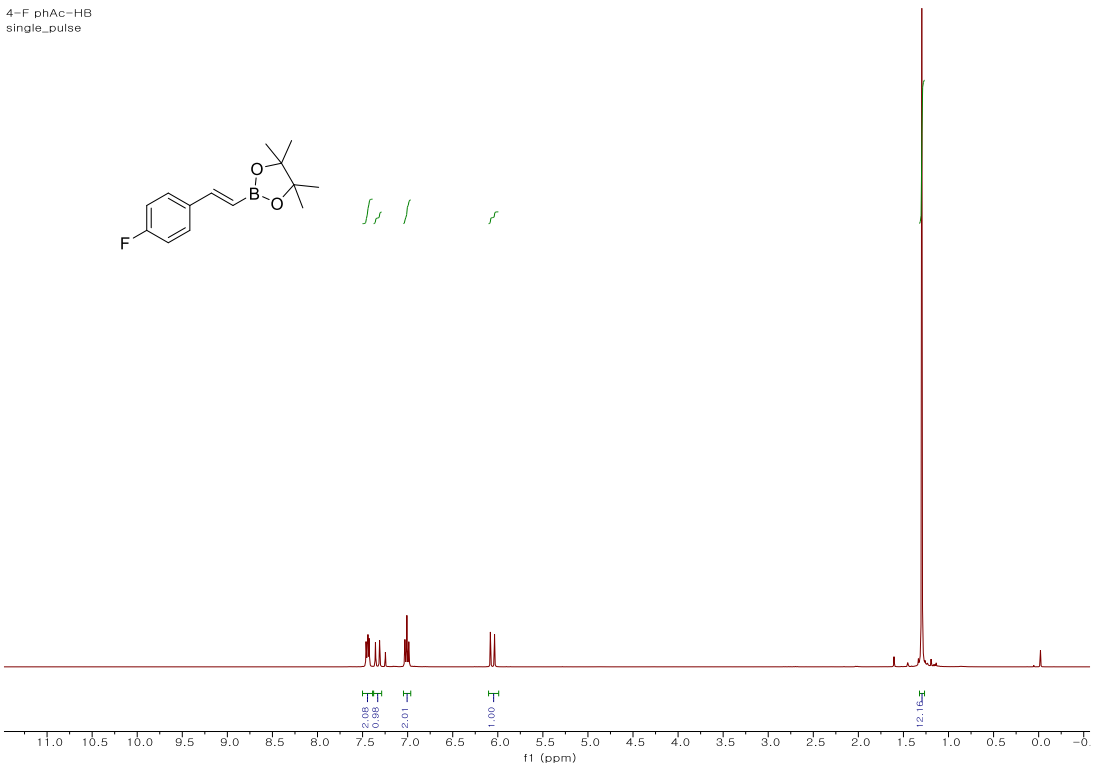

Figure S13: ^{1}H NMR of (*E*)-2-(4-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2g**)

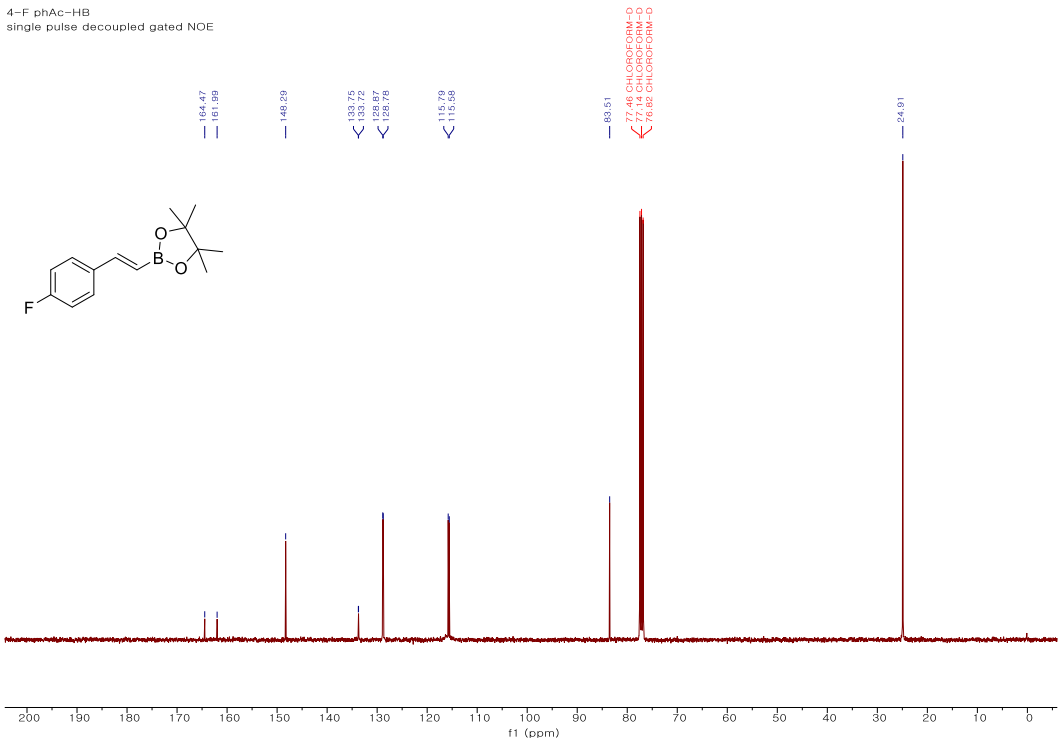

Figure S14: ^{13}C NMR of **(***E*)-2-(4-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2g**)

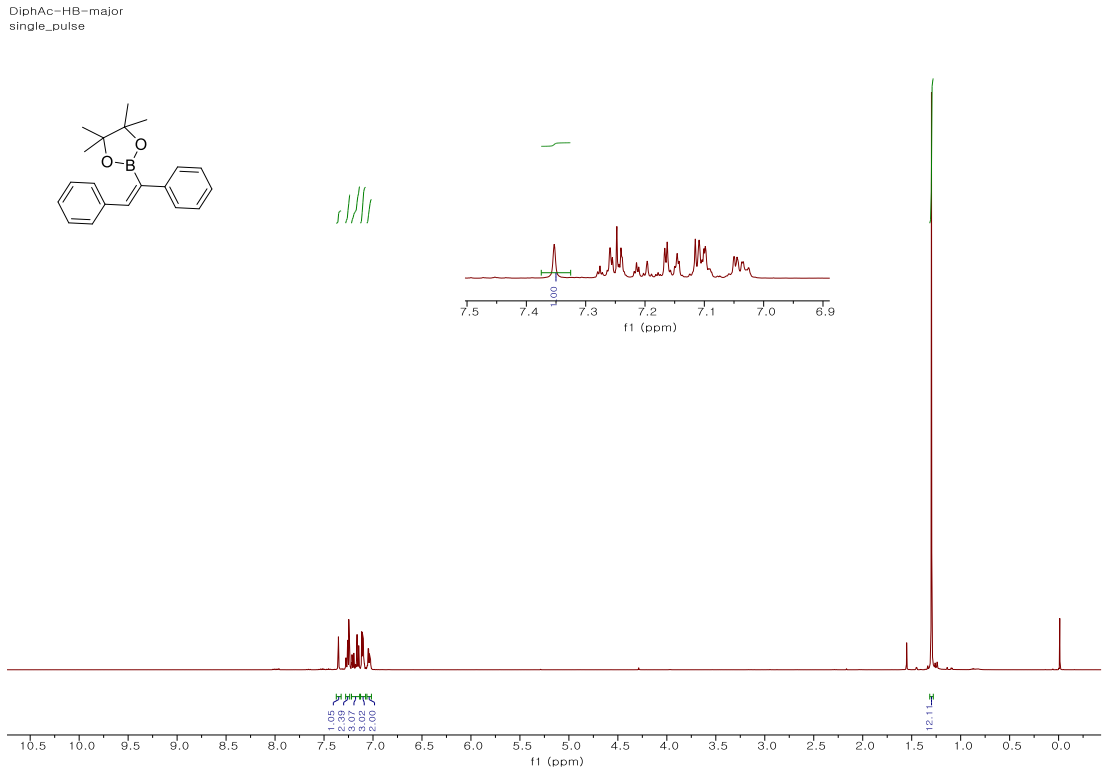

Figure S15: ^{1}H NMR of (*E*)-2-(1,2-diphenylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2h**)

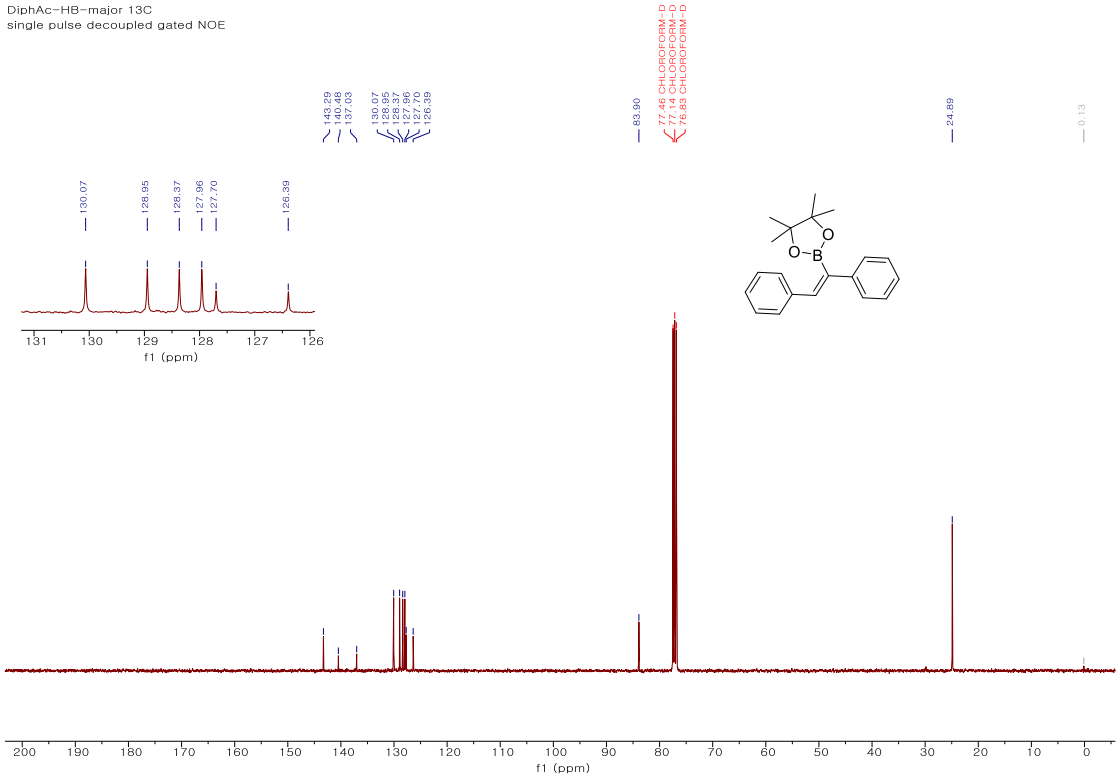

Figure S16: ^{13}C NMR of (*E*)-2-(1,2-diphenylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2h**)

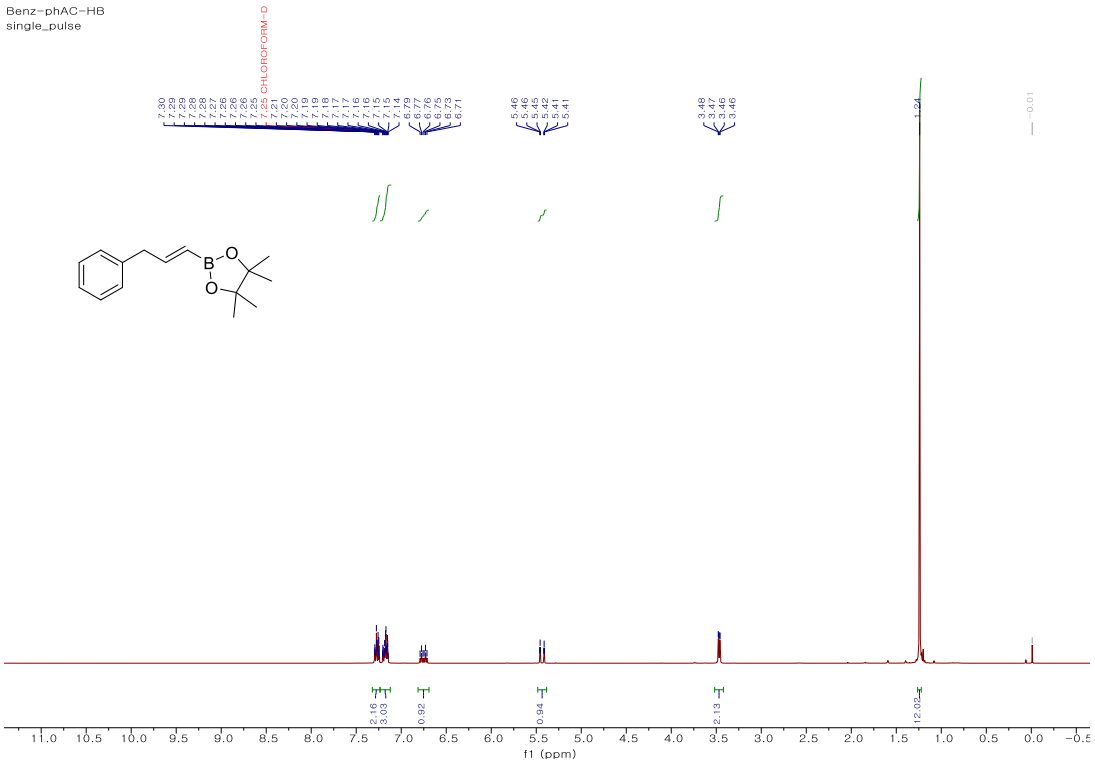

Figure S17: ^{1}H NMR of (*E*)-4,4,5,5-tetramethyl-2-(3-phenylprop-1-en-1-yl)-1,3,2-dioxaborolane (**2i**)

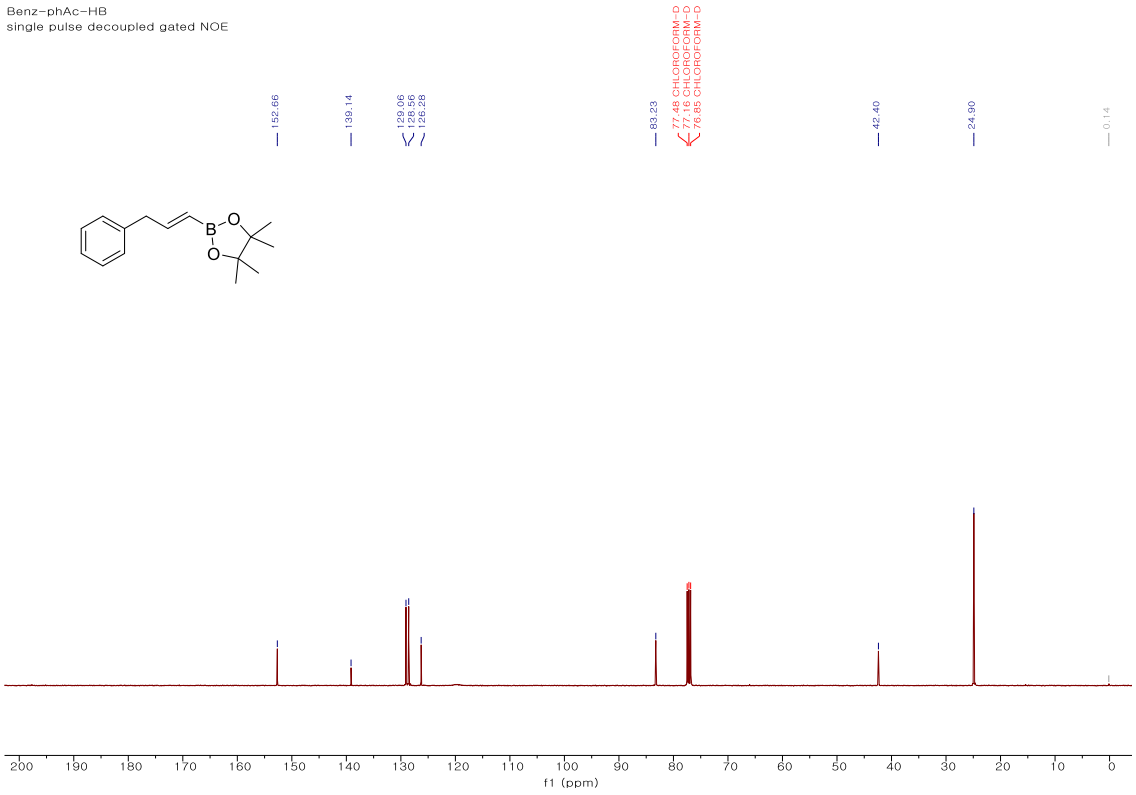

Figure S18: ^{13}C NMR of (*E*)-4,4,5,5-tetramethyl-2-(3-phenylprop-1-en-1-yl)-1,3,2-dioxaborolane (**2i**)

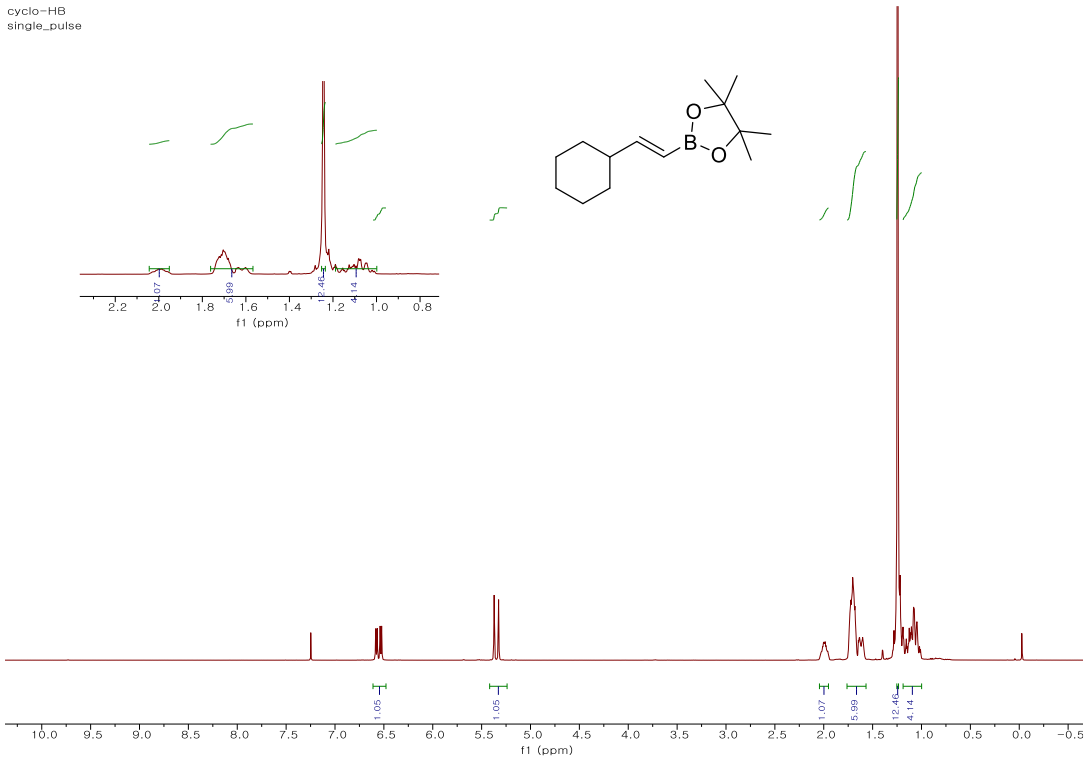

Figure S19: ^{1}H NMR of (*E*)-2-(2-cyclohexylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2j**)

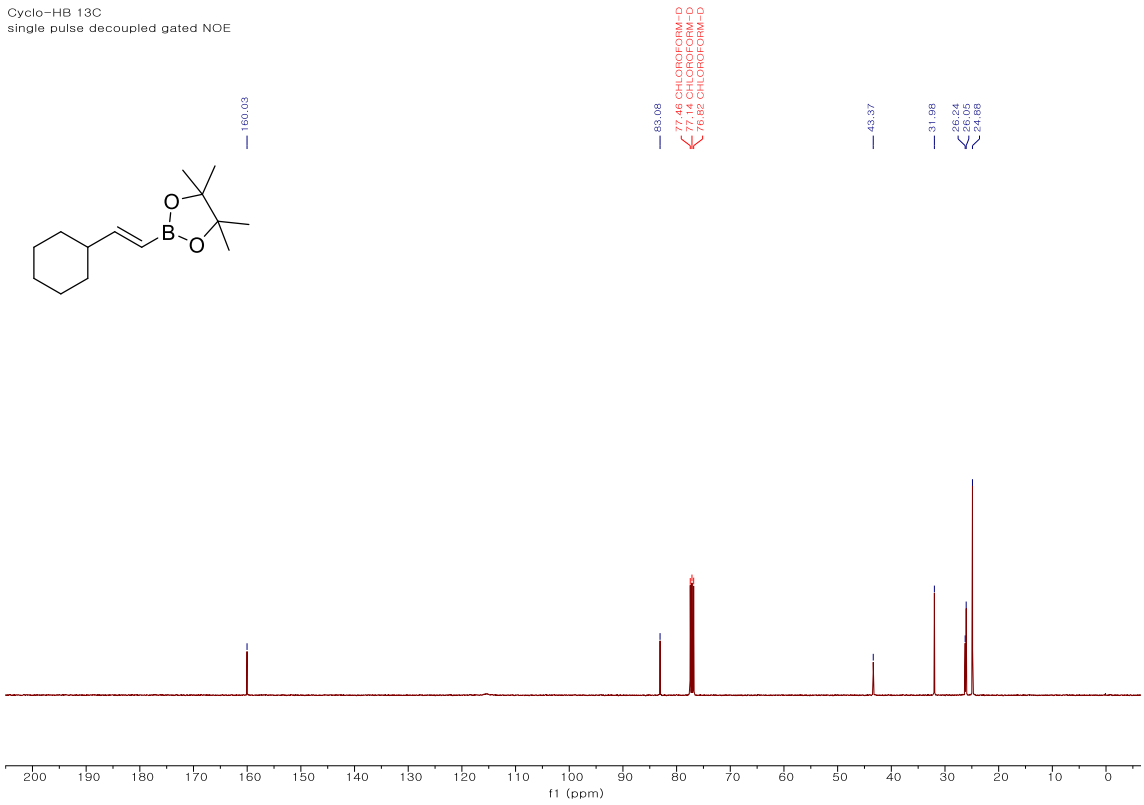

Figure S20: ^{13}C NMR of (*E*)-2-(2-cyclohexylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2j**)

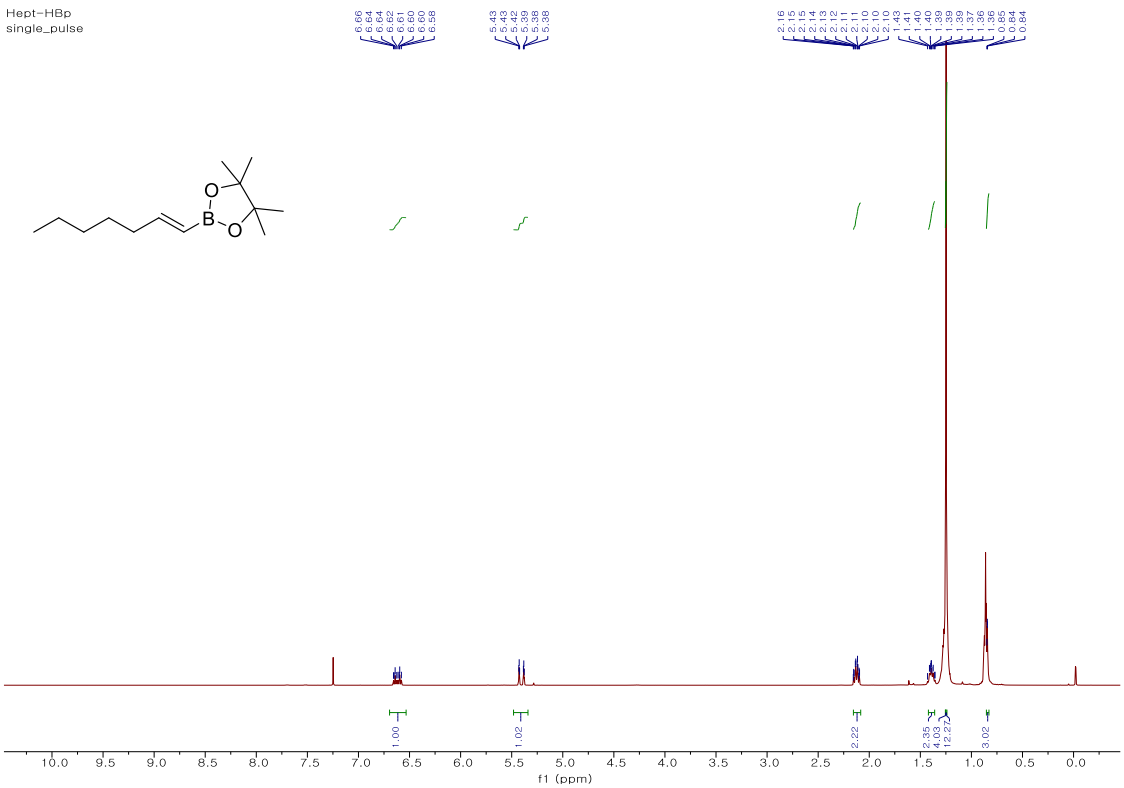

Figure S21: ^{1}H NMR of (*E*)-2-(hept-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2k**)

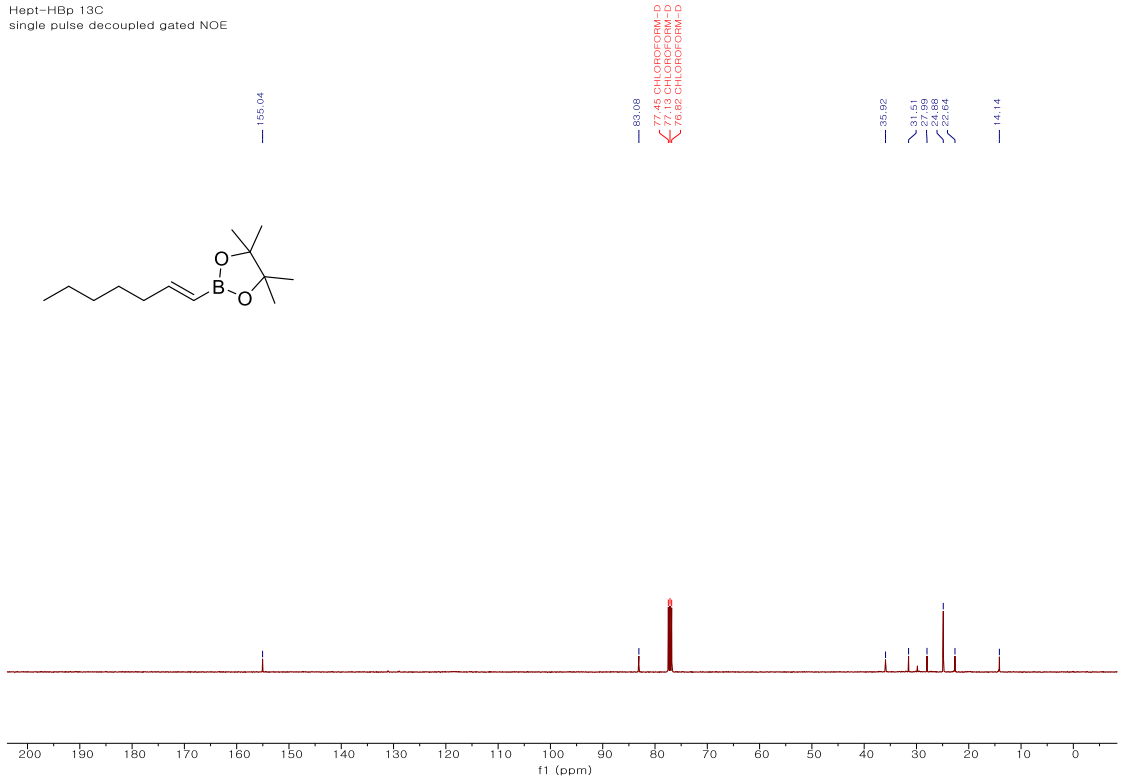

Figure S22: ^{13}C NMR of (*E*)-2-(hept-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**2k**)

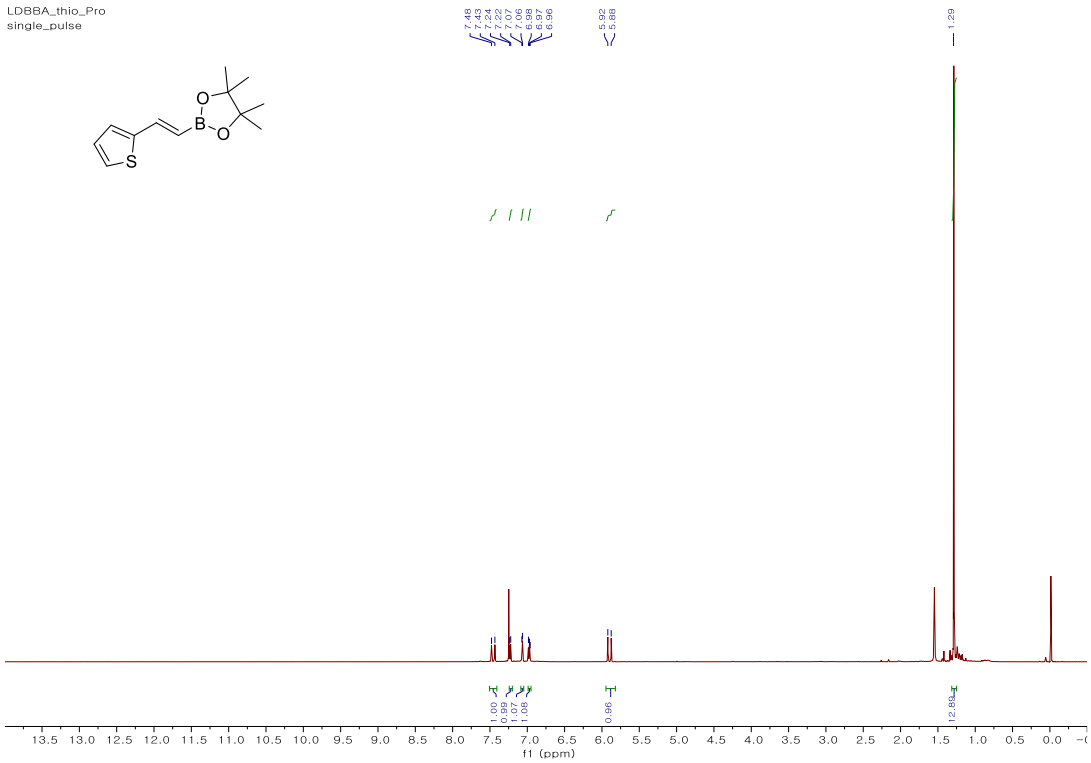

Figure S23: ^{1}H NMR of (E)-4,4,5,5-tetramethyl-2-(2-(thiophen-2-yl)vinyl)-1,3,2-dioxaborolane (**2l**)

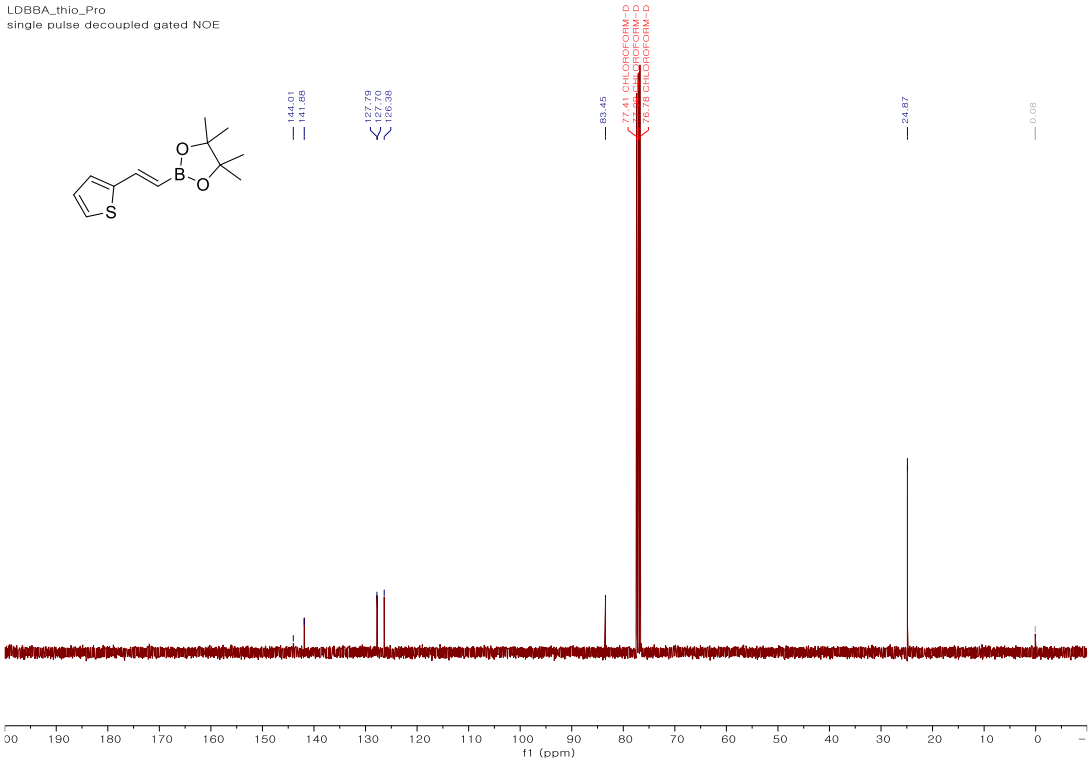

Figure S24: ^{13}C NMR of (E)-4,4,5,5-tetramethyl-2-(2-(thiophen-2-yl)vinyl)-1,3,2-dioxaborolane (**2l**)

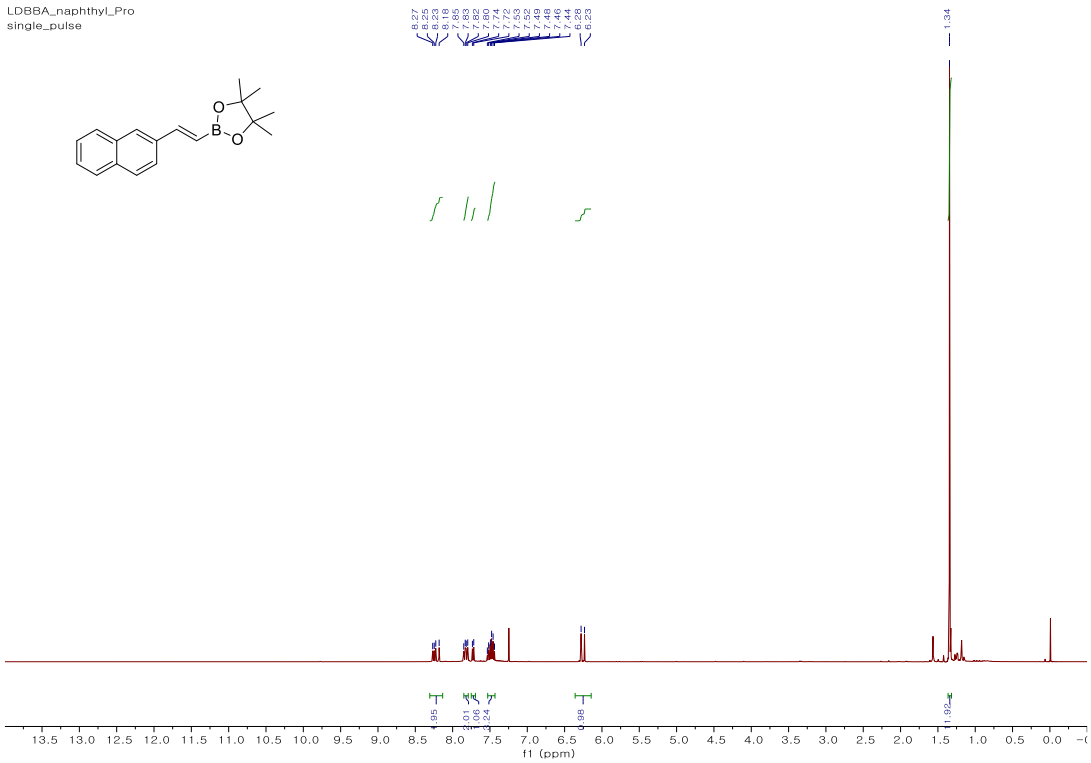

Figure S25: ^{1}H NMR of (E)-4,4,5,5-tetramethyl-2-(2-(naphthalen-2-yl)vinyl)-1,3,2-dioxaborolane (**2m**)

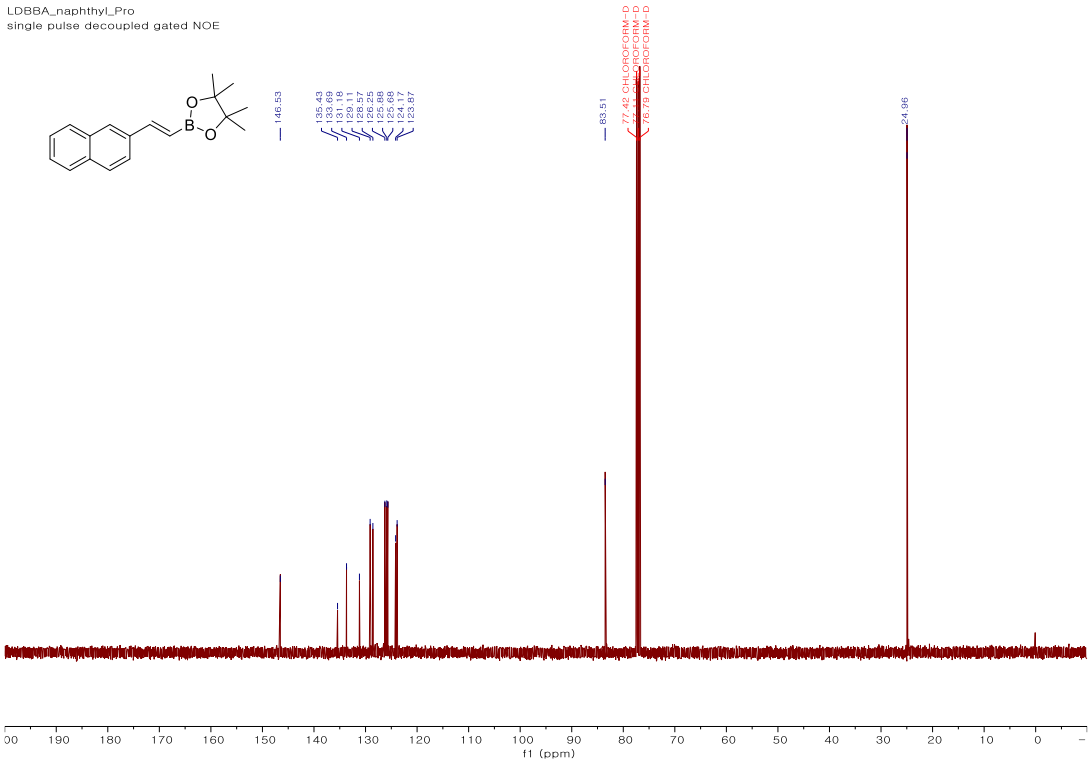

Figure S26: ^{13}C NMR of (E)-4,4,5,5-tetramethyl-2-(2-(naphthalen-2-yl)vinyl)-1,3,2-dioxaborolane (**2m**)

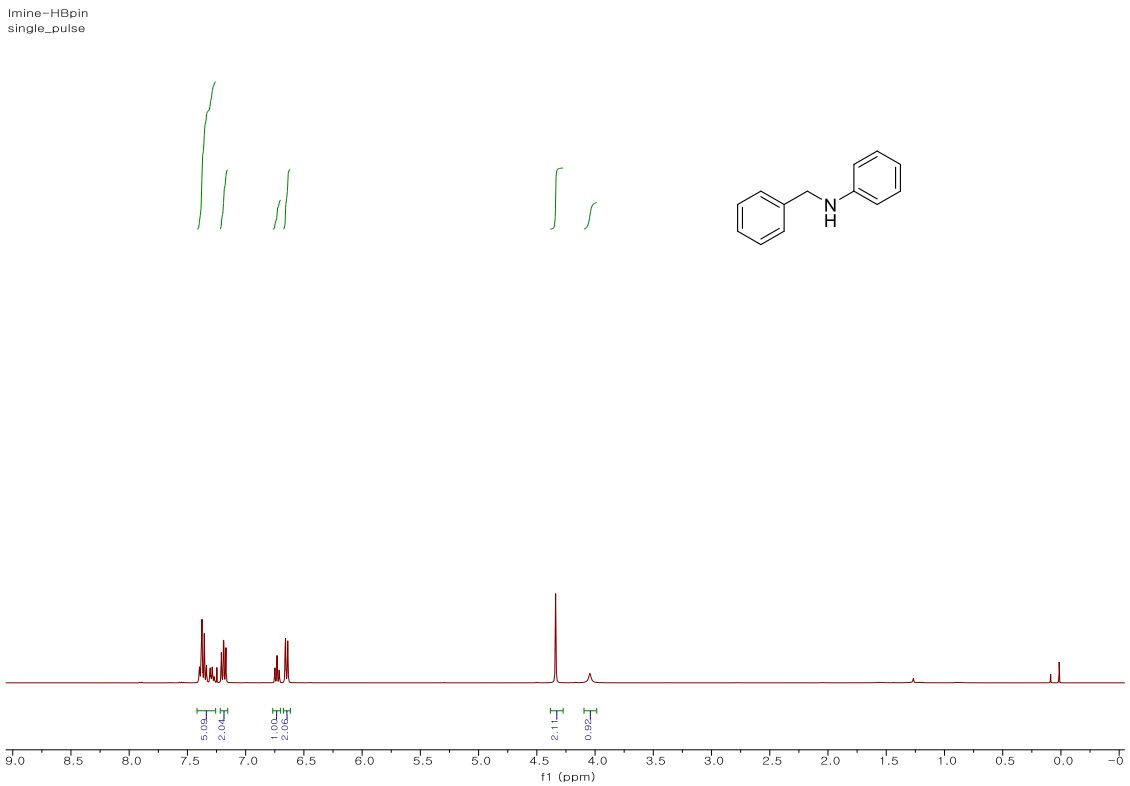

Figure S27: ^{1}H NMR of *N*-Benzylaniline (**4a**)

Figure S28: ^{13}C NMR of *N*-Benzylaniline (**4a**)

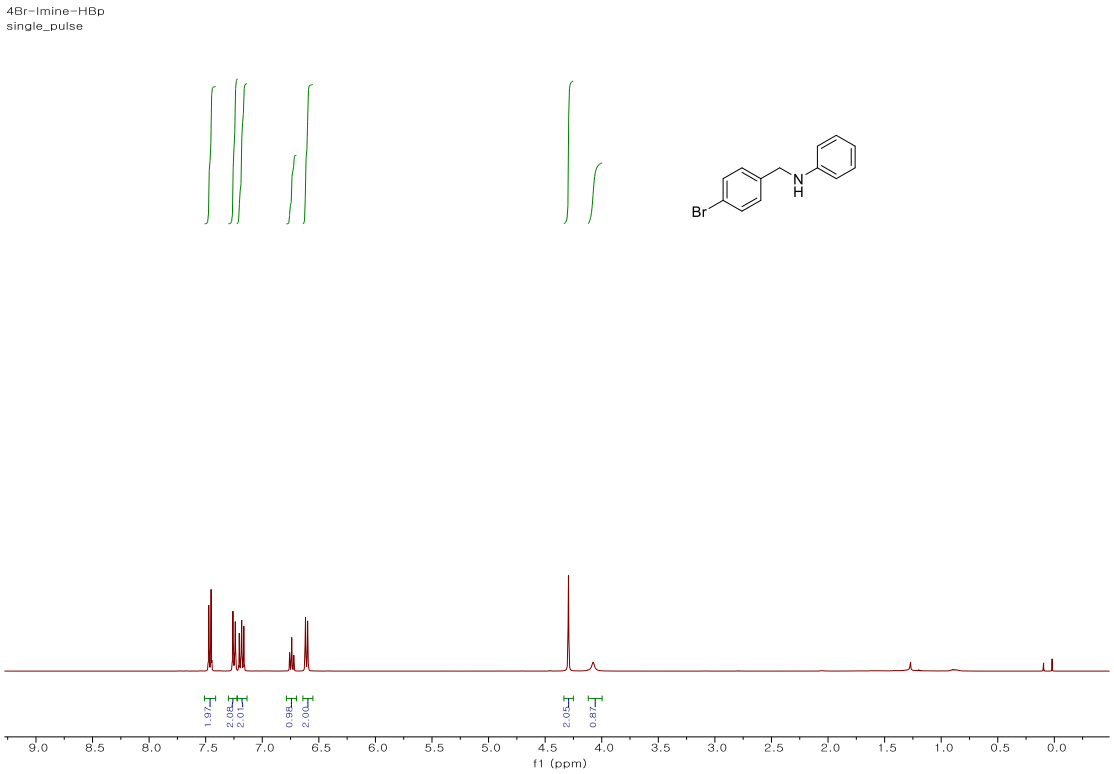

Figure S29: ^{1}H NMR of *N*-(4-bromobenzyl)aniline (**4b**)

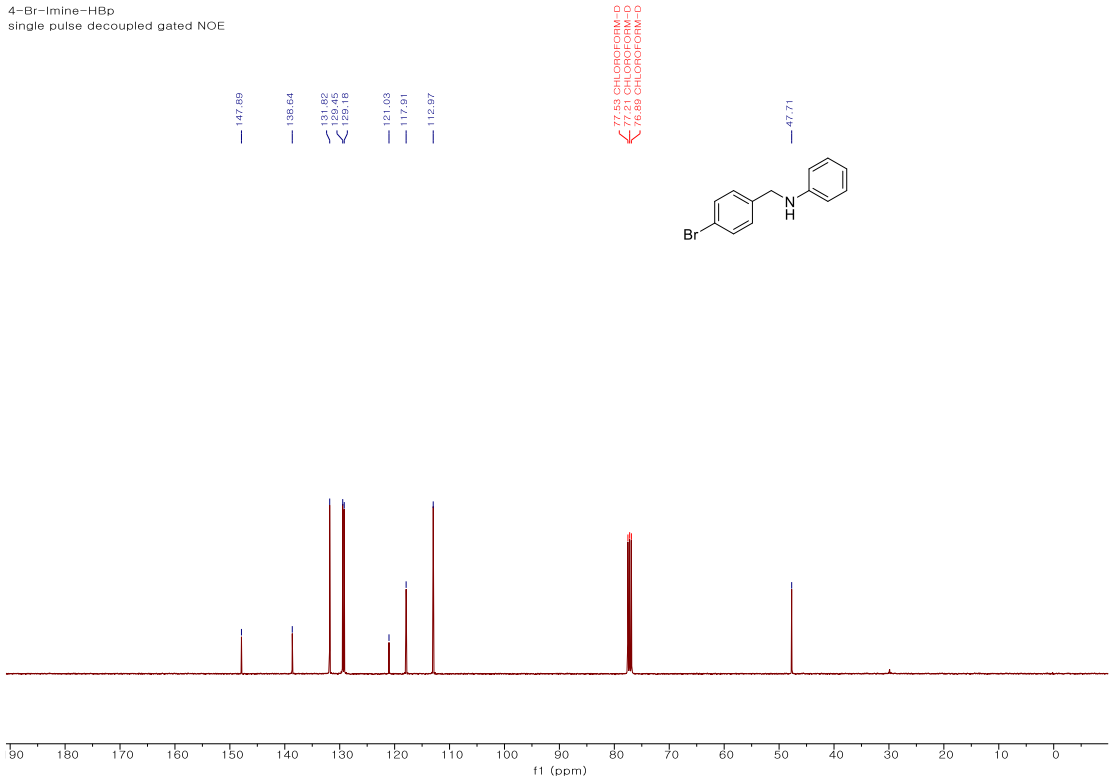

Figure S30: ^{13}C NMR of *N*-(4-bromobenzyl)aniline (**4b**)

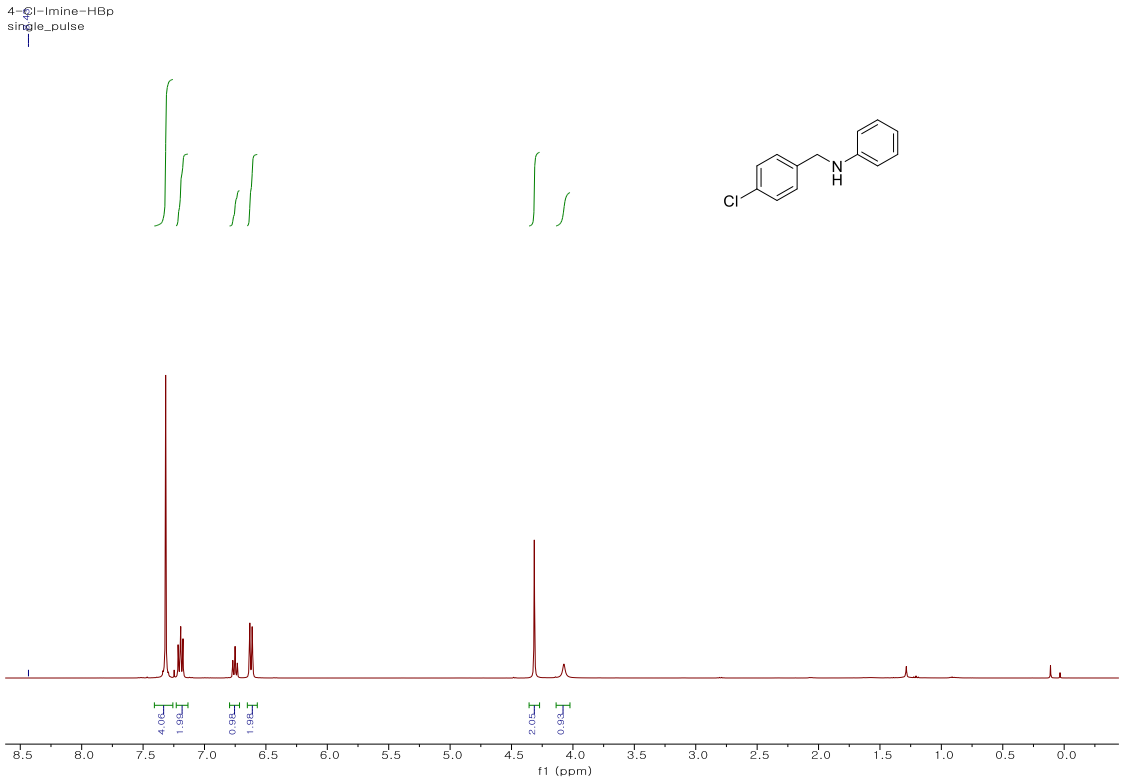

Figure S31: ^{1}H NMR of *N*-(4-bromobenzyl)aniline **(4c)**

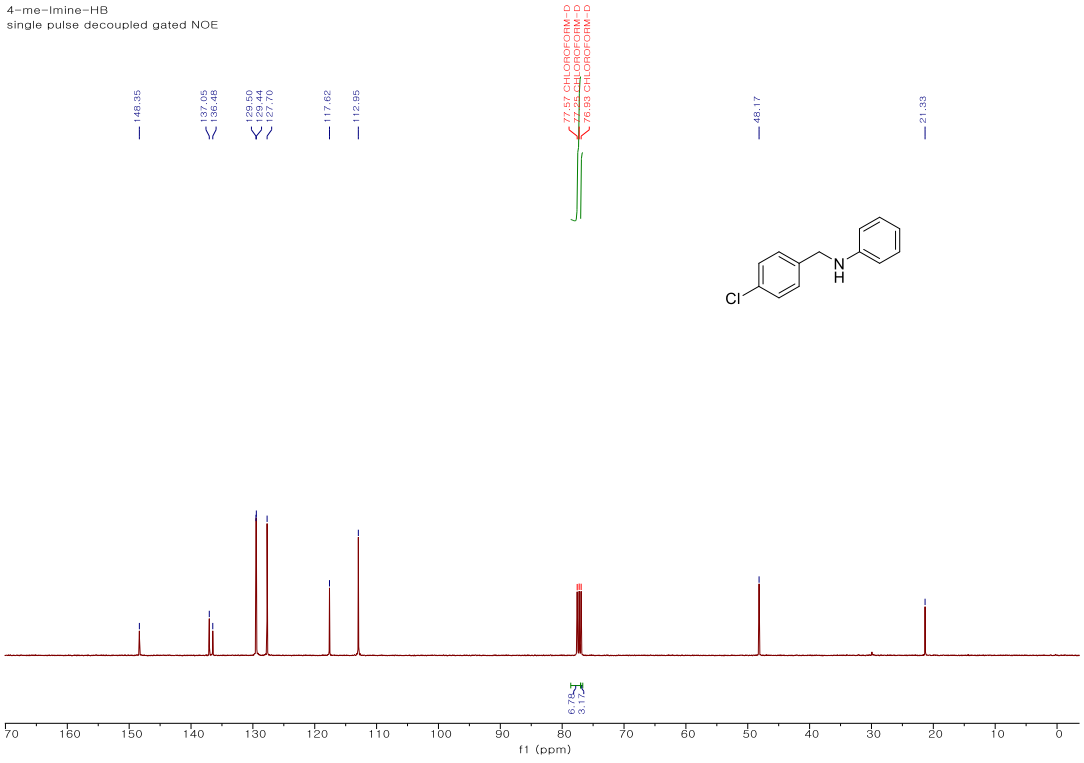

Figure S32: ^{13}C NMR of *N*-(4-bromobenzyl)aniline **(4c)**

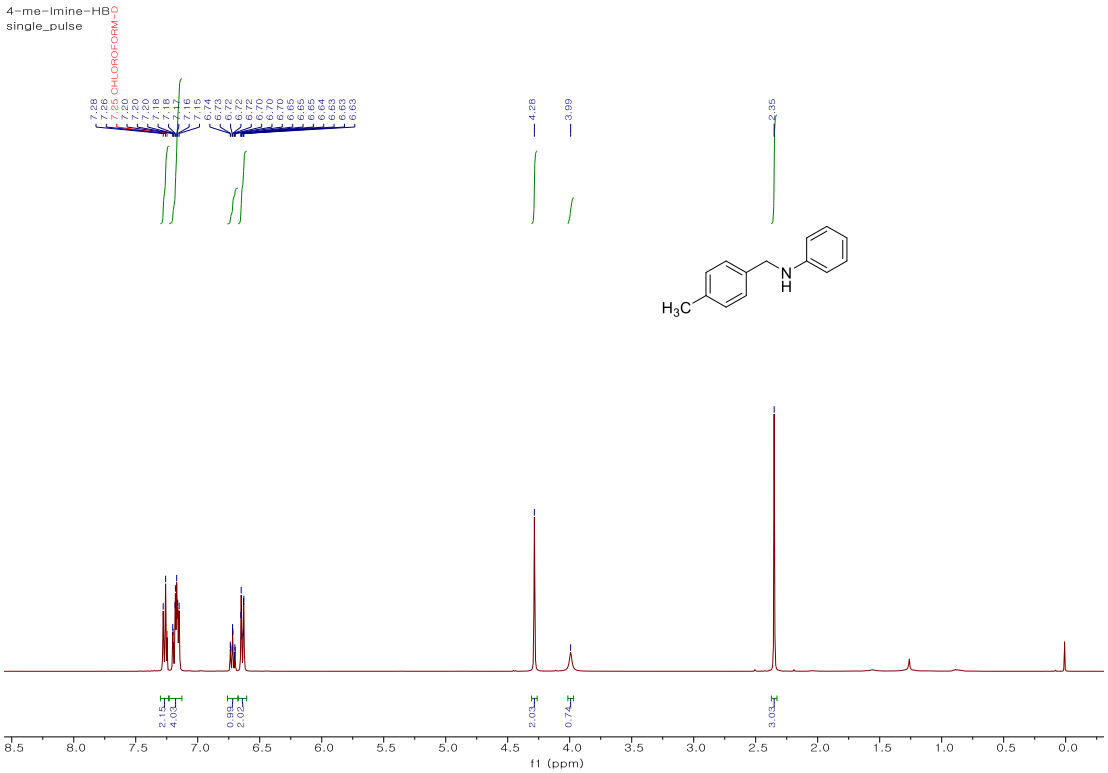

Figure S33: ^{1}H NMR of *N*-(4-methylbenzyl)aniline (**4d**)

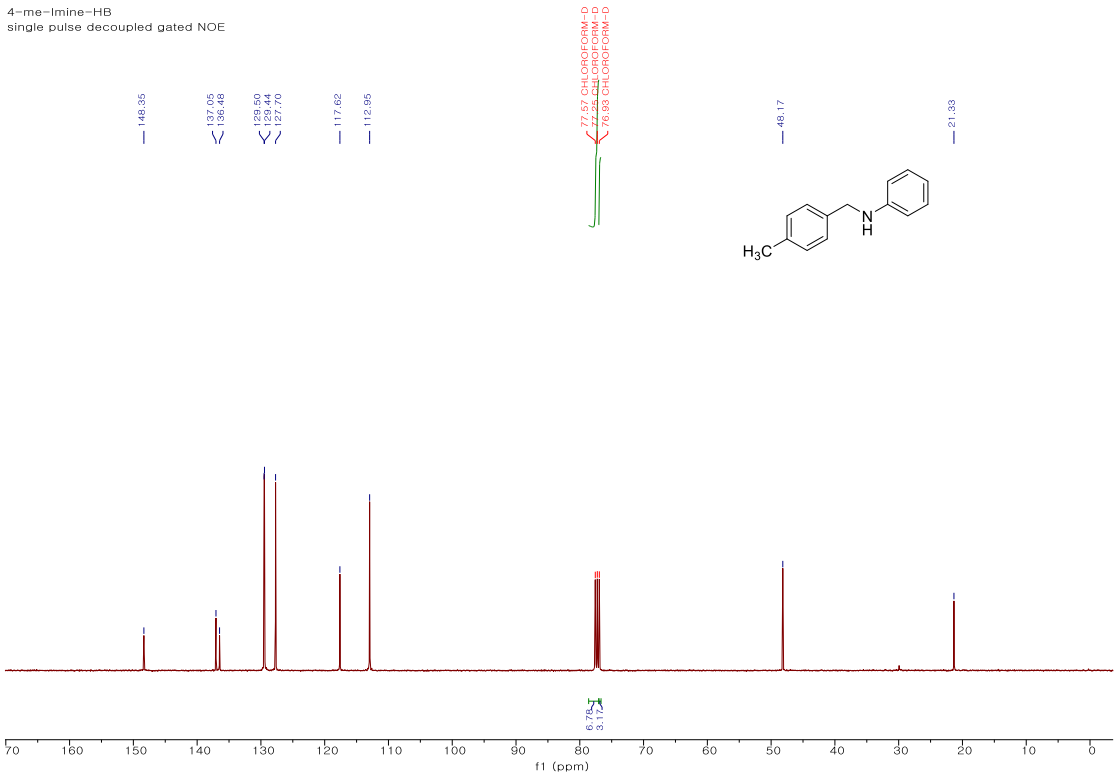

Figure S34: ^{13}C NMR of *N*-(4-methylbenzyl)aniline (**4d**)

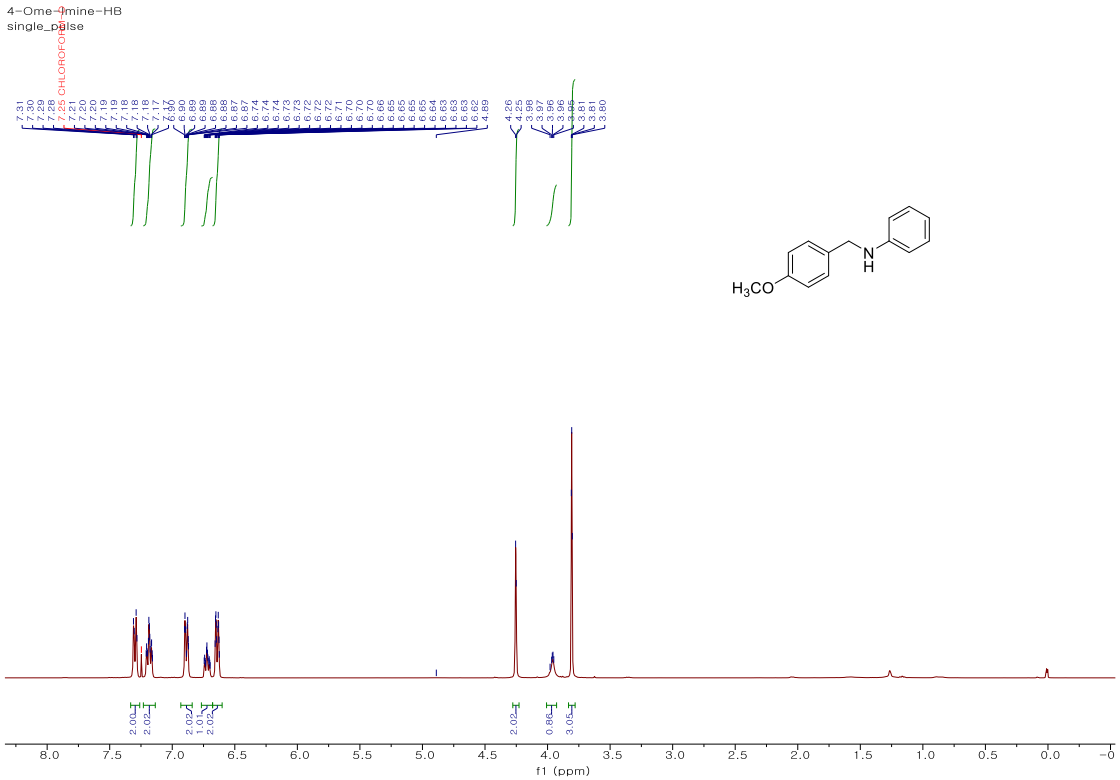

Figure S35: ^{1}H NMR of *N*-(4-methoxybenzyl)aniline (**4e**)

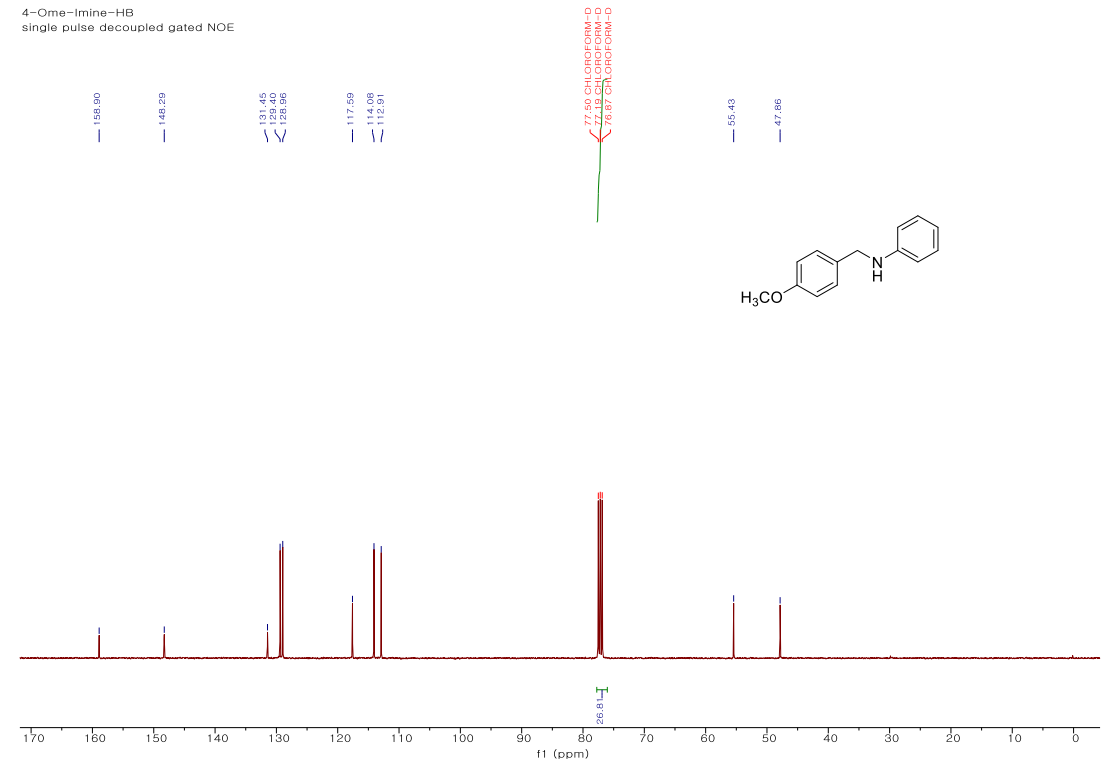

Figure S36: ^{13}C NMR of *N*-(4-methoxybenzyl)aniline (**4e**)

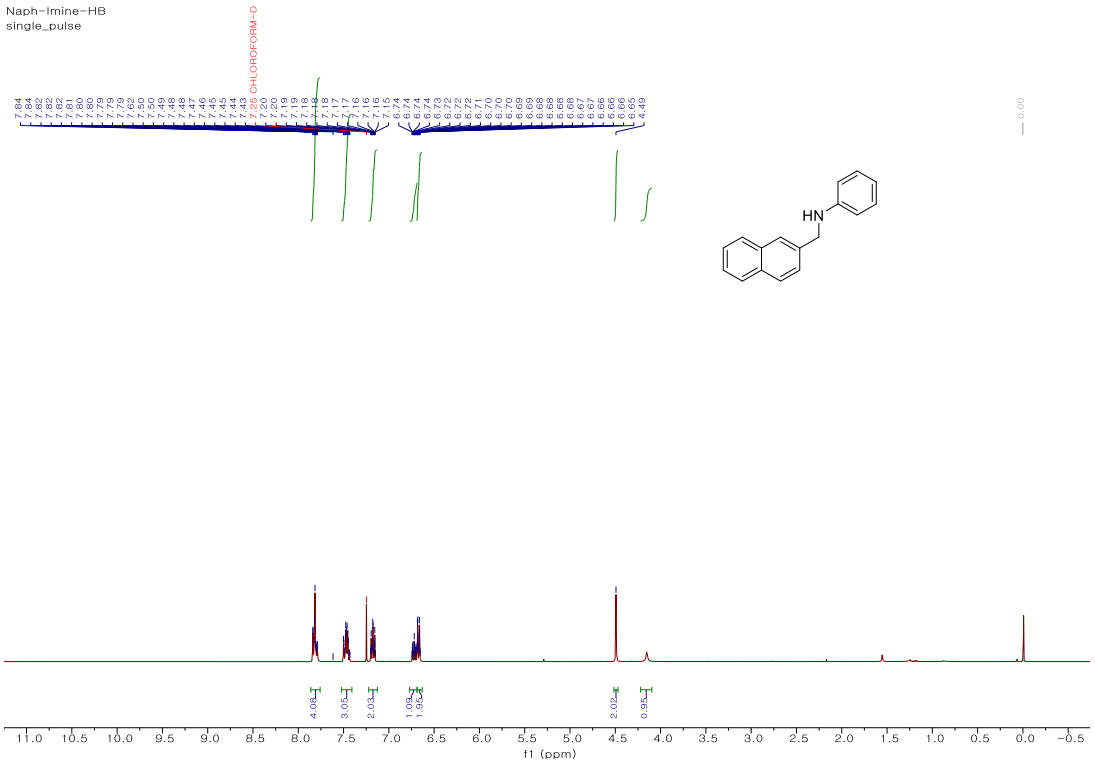

Figure S37: ^{1}H NMR of *N*-(naphthalen-2-ylmethyl)aniline (**4f**)

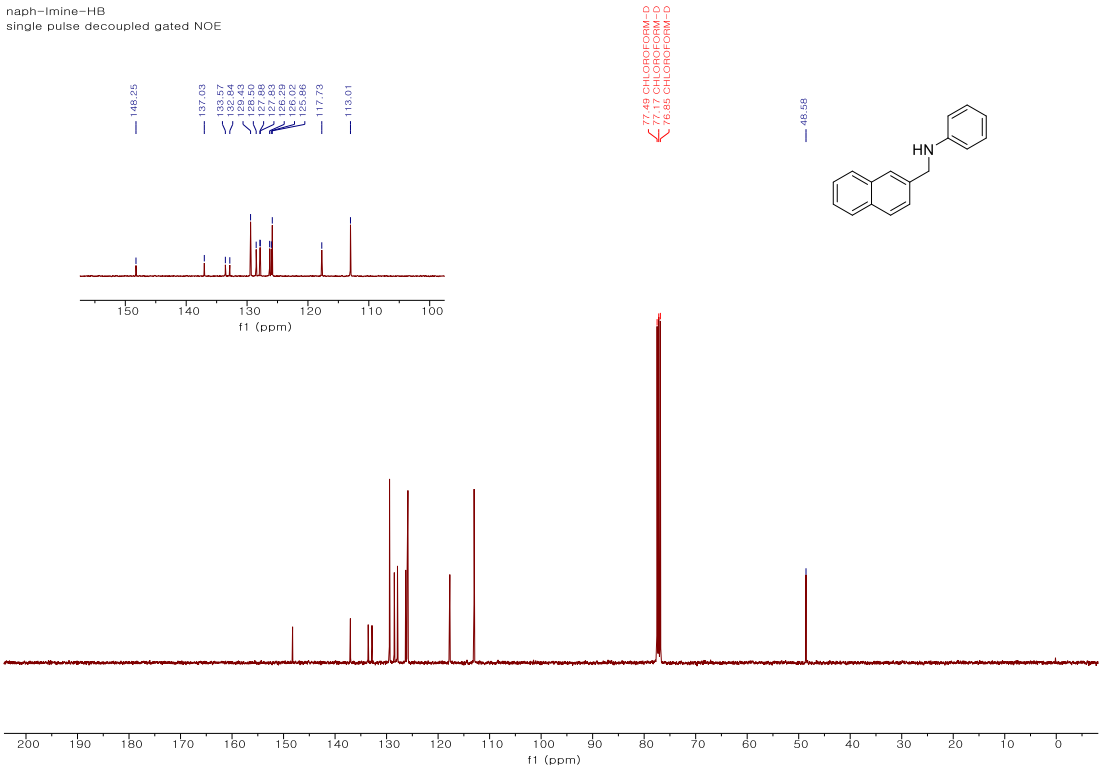

Figure S38: ^{13}C NMR of *N*-(naphthalen-2-ylmethyl)aniline (**4f**)

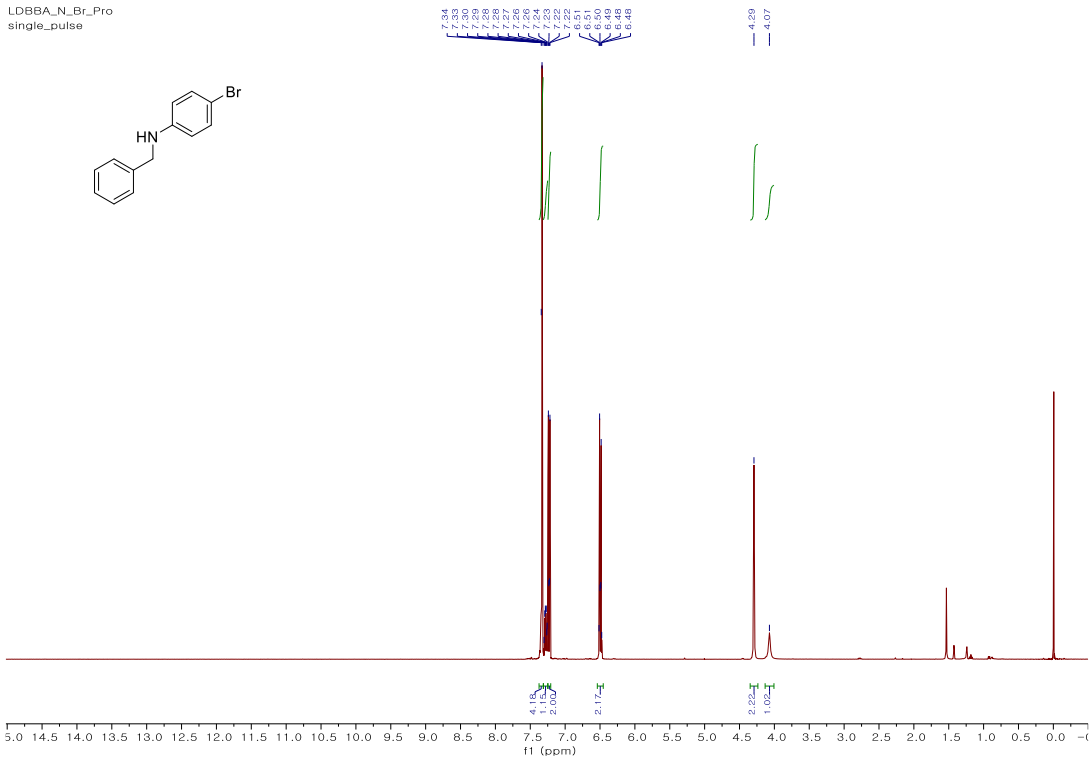

Figure S39: ^{1}H NMR of N-benzyl-4-bromoaniline (**4g**)

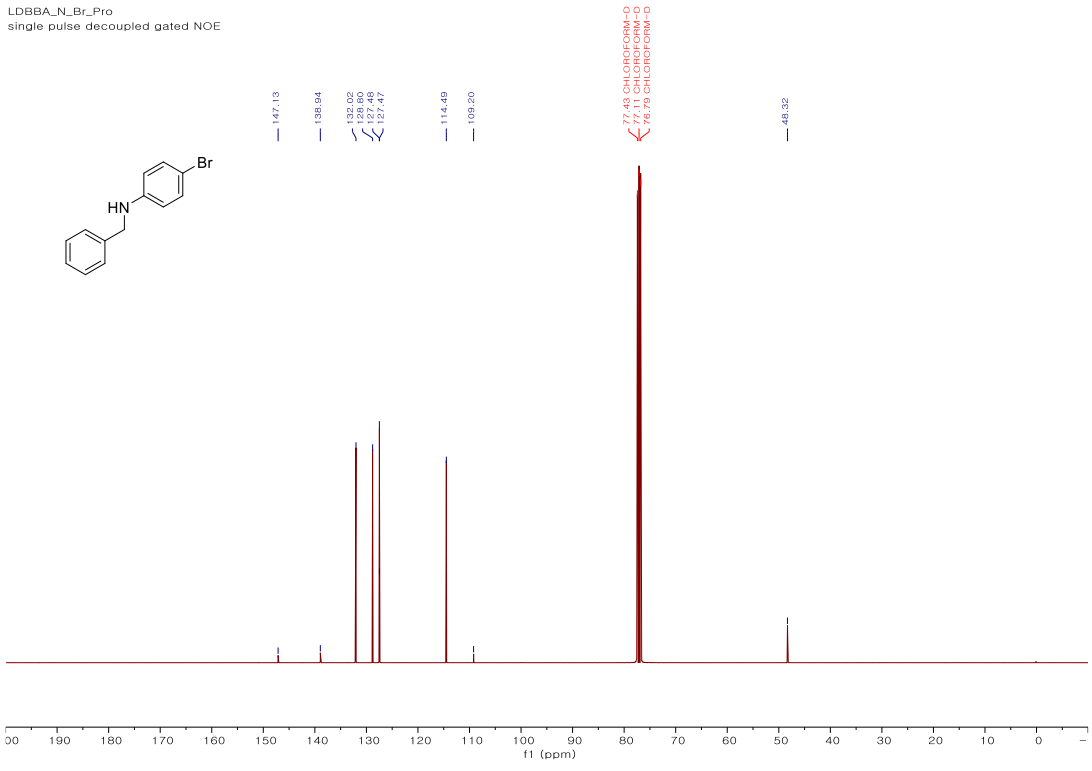

Figure S40: ^{13}C NMR of N-benzyl-4-bromoaniline (**4g**)

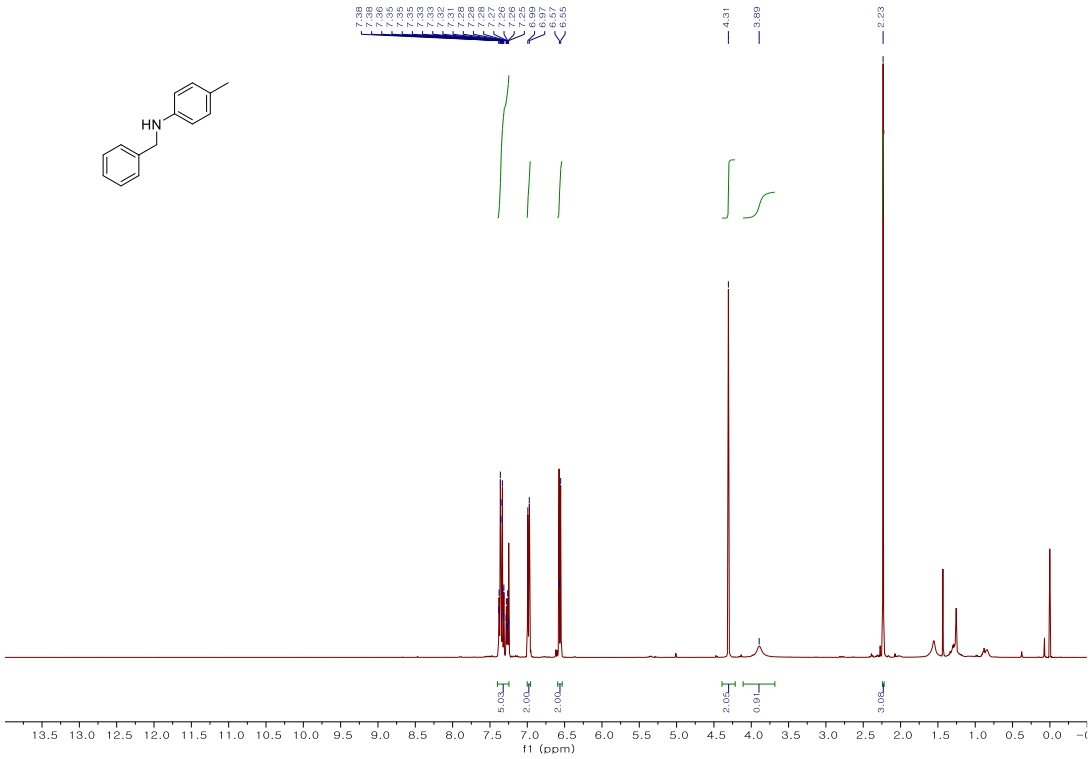

Figure S41: ^{1}H NMR of N-benzyl-4-methylaniline (**4h**)

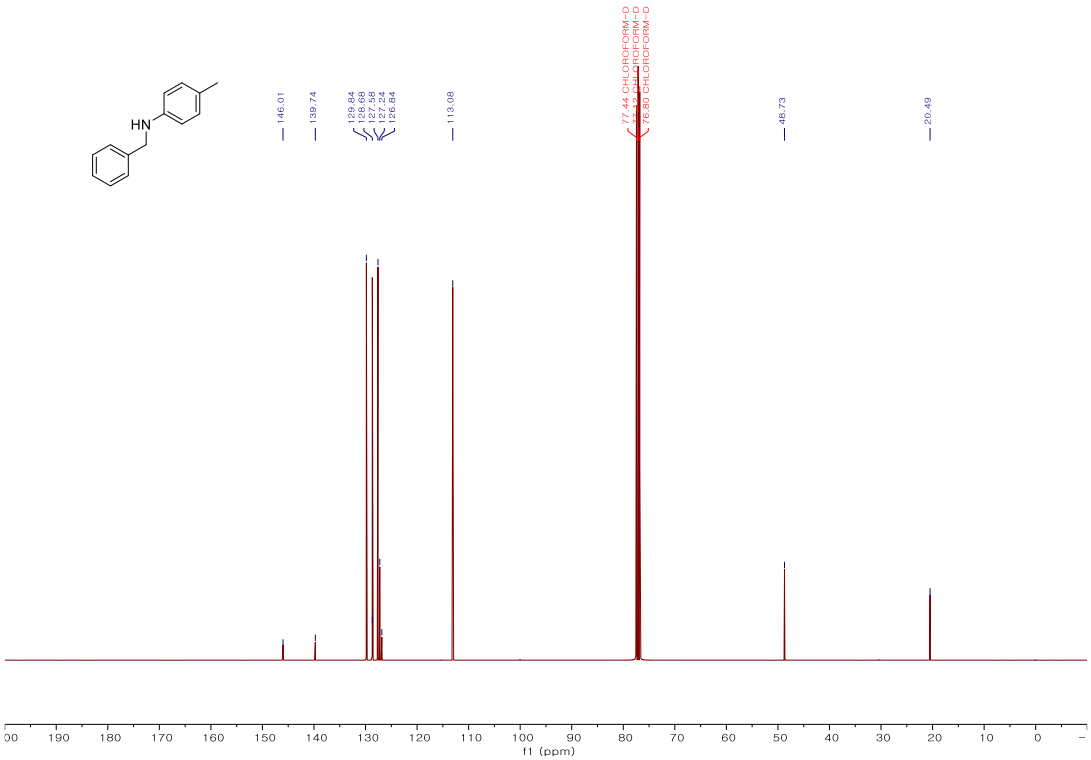

Figure S42: ^{13}C NMR of N-benzyl-4-methylaniline (**4h**)

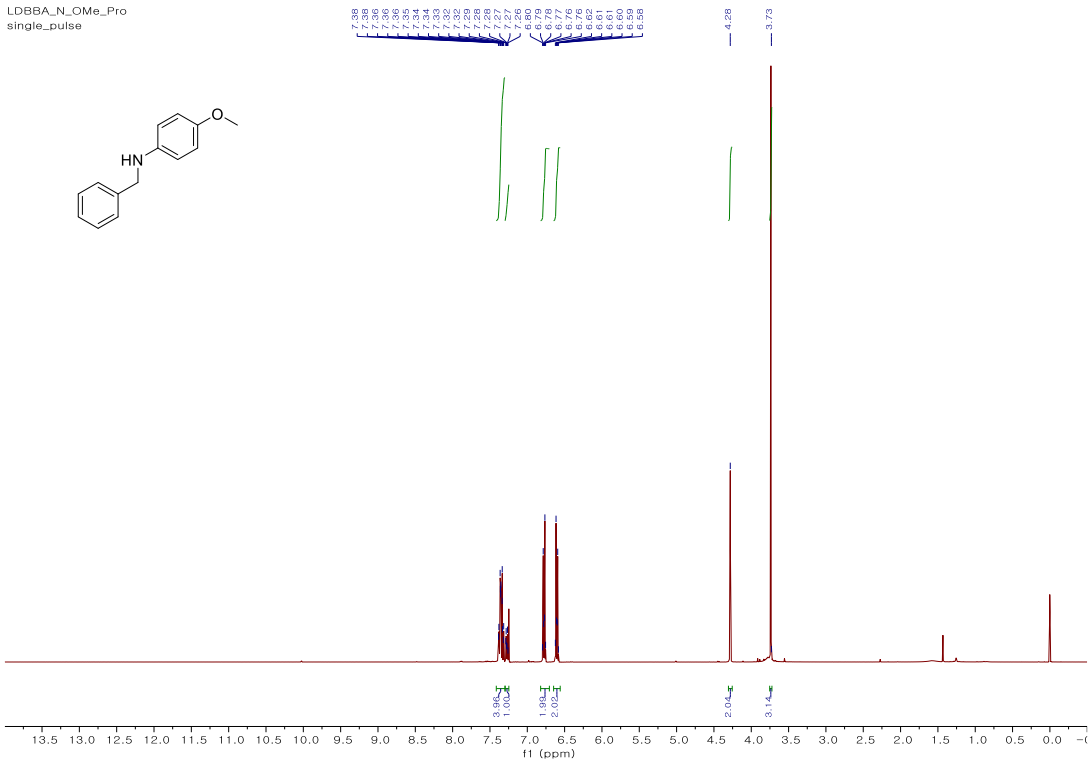

Figure S43: ^{1}H NMR of N-benzyl-4-methoxyaniline (**4i**)

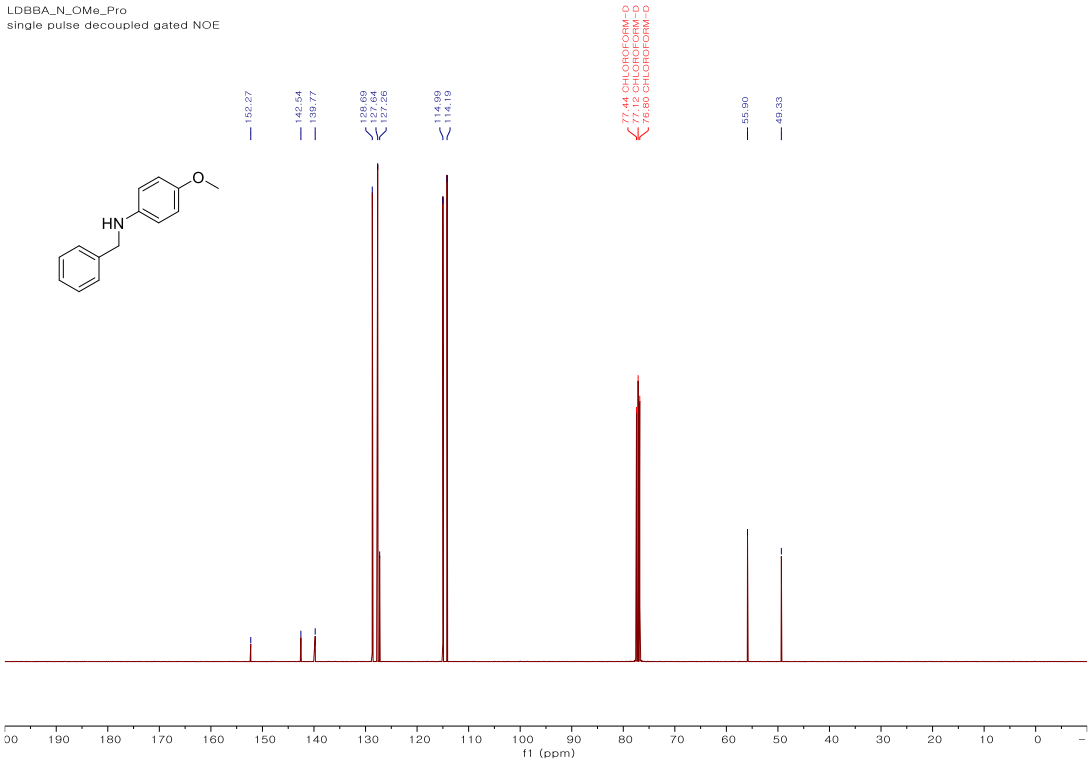

Figure S44: ^{13}C NMR of N-benzyl-4-methoxyaniline (**4i**)

2. Computational Section

Geometry optimizations and energy calculations for all the compounds were conducted in the gas phase at the M06-2X/6-31G(d,p) level of theory. Frequency calculations at the same level of theory were performed to confirm the optimized geometries with no imaginary frequency and transition states with one imaginary frequency and to evaluate the thermodynamic free energies. Intrinsic reaction coordinate (IRC) calculations were also employed to validate the transition states. Natural bond orbital (NBO) calculations were also carried out to obtain NBO atomic charges at the M06-2X/6-31G(d,p) level of theory. All calculations were carried out using the Gaussian 16 [S1] and NBO 7 [S2] programs.

LDBBA

Atom	x	y	z
Li	-0.703336	-0.740896	-2.450763
Al	0.378717	0.160275	-0.330901
O	-0.891065	-1.130648	-0.736583
C	-1.539093	-2.047410	0.136166
C	-1.586117	-1.465344	1.549384
H	-0.570862	-1.298652	1.929515
H	-2.117460	-0.509154	1.547334
H	-2.094241	-2.148709	2.235855
C	-2.958480	-2.267484	-0.386406
H	-3.508390	-1.321767	-0.395482
H	-2.927625	-2.667162	-1.407119
H	-3.504892	-2.981435	0.236658
C	-0.759836	-3.362843	0.130756
H	-0.714765	-3.770921	-0.884555
H	0.262281	-3.195965	0.480538
H	-1.234430	-4.105664	0.779062
C	-0.324840	1.798406	0.545215
H	0.549041	2.446665	0.717616
C	-1.393147	2.602893	-0.211912
H	-1.031922	2.781670	-1.236532
C	-1.651788	3.966479	0.433971
H	-2.404713	4.543685	-0.114711
H	-2.012101	3.833192	1.460907
H	-0.733735	4.559748	0.478819

C	-2.704933	1.820999	-0.311022
H	-3.461544	2.364859	-0.886586
H	-2.549802	0.839397	-0.772742
H	-3.114294	1.646066	0.692553
C	2.060266	-0.616277	0.391324
H	2.145110	-0.374052	1.463938
C	3.339189	-0.118067	-0.307051
H	3.294491	-0.419568	-1.364495
C	3.431134	1.409070	-0.267440
H	2.601394	1.878452	-0.808806
H	3.395871	1.764122	0.769754
H	4.363869	1.768717	-0.714045
C	4.599429	-0.735533	0.303654
H	4.557087	-1.828667	0.272468
H	5.507029	-0.413807	-0.219208
H	4.693097	-0.436519	1.354360
H	-0.706940	1.573818	1.554717
H	2.040278	-1.714973	0.342016
H	0.522672	0.461593	-2.005008

SDBBA

Atom	x	y	z
Na	1.196562	-0.422967	2.508409
Al	-0.438280	0.144474	0.225232
O	0.918765	-1.070388	0.504381
C	1.491301	-1.966223	-0.430067
C	1.426468	-1.377829	-1.841834
H	0.384298	-1.212520	-2.140367
H	1.950626	-0.418204	-1.876799
H	1.881986	-2.055042	-2.570611
C	2.952940	-2.183720	-0.030189
H	3.495993	-1.233375	-0.057495
H	3.005460	-2.593813	0.986488
H	3.455291	-2.887713	-0.700203
C	0.732539	-3.294113	-0.379423
H	0.756739	-3.700195	0.637154
H	-0.312148	-3.140447	-0.661901
H	1.173124	-4.031044	-1.058347

C	0.165714	1.805039	-0.707202
H	-0.732740	2.426491	-0.847109
C	1.227258	2.643437	0.022437
H	0.900193	2.783259	1.065833
C	1.401358	4.033467	-0.595167
H	2.153525	4.629150	-0.064662
H	1.719549	3.942005	-1.640352
H	0.457862	4.586762	-0.582893
C	2.578220	1.922439	0.048882
H	3.328100	2.473953	0.627231
H	2.483099	0.907454	0.453649
H	2.963816	1.812741	-0.972883
C	-2.137273	-0.685651	-0.401525
H	-2.261286	-0.507738	-1.483220
C	-3.401276	-0.168432	0.309248
H	-3.314329	-0.404943	1.380449
C	-3.526800	1.351395	0.182524
H	-2.687799	1.866537	0.663777
H	-3.535172	1.643841	-0.874709
H	-4.451230	1.719331	0.640101
C	-4.669418	-0.844286	-0.218299
H	-4.604355	-1.932602	-0.122435
H	-5.565492	-0.507322	0.315168
H	-4.804360	-0.612113	-1.281422
H	0.526350	1.600092	-1.728388
H	-2.100488	-1.779294	-0.289405
H	-0.527459	0.549201	1.871489

PDBBA

Atom	x	y	z
K	-1.548528	0.498030	2.285512
Al	0.243974	-0.782247	-0.026893
O	-0.084106	0.986510	0.324595
C	0.163180	2.096311	-0.510472
C	-0.204351	1.780474	-1.964925
H	0.406585	0.953124	-2.341258
H	-1.256234	1.488028	-2.040671
H	-0.035139	2.647749	-2.611051

C	-0.706786	3.252674	-0.003419
H	-1.768186	2.982902	-0.065228
H	-0.454878	3.477381	1.040323
H	-0.556779	4.164692	-0.588926
C	1.641028	2.487806	-0.420303
H	1.911137	2.679803	0.622923
H	2.268739	1.671682	-0.789524
H	1.854188	3.385633	-1.009732
C	-1.289112	-1.605148	-1.034797
H	-1.037038	-2.672668	-1.137148
C	-2.663981	-1.500277	-0.355508
H	-2.537318	-1.728058	0.720583
C	-3.679356	-2.511033	-0.896135
H	-4.656285	-2.420628	-0.405425
H	-3.824763	-2.352179	-1.970695
H	-3.319994	-3.534346	-0.756783
C	-3.237825	-0.084054	-0.486882
H	-4.153881	0.052661	0.102996
H	-2.496625	0.676413	-0.213998
H	-3.496928	0.112513	-1.534072
C	2.069216	-1.112518	-0.751819
H	2.147954	-2.146425	-1.124720
C	3.237721	-0.865116	0.220337
H	3.069634	0.086658	0.749468
C	3.307709	-1.970705	1.275341
H	2.359973	-2.062145	1.813898
H	3.513333	-2.934329	0.793641
H	4.105661	-1.783774	2.002166
C	4.577887	-0.753836	-0.511158
H	4.565833	0.069956	-1.232678
H	5.411263	-0.587545	0.181236
H	4.779134	-1.677604	-1.066624
H	-1.385458	-1.232733	-2.067224
H	2.211130	-0.487474	-1.648516
H	0.006171	-1.302186	1.543601

LDBBA w/o Li^+

Atom	x	y	z
Al	0.117181	-0.471816	-0.532690
H	0.056269	-1.311576	-1.945821
O	-1.366412	-0.766193	0.443188
C	-2.683545	-0.873640	0.011268
C	-3.590559	-0.682498	1.234533
H	-3.334013	-1.426551	1.994847
H	-3.421362	0.311578	1.661056
H	-4.652798	-0.784070	0.980829
C	-3.020725	0.198512	-1.037471
H	-2.826015	1.192553	-0.622065
H	-2.386759	0.070440	-1.921740
H	-4.071009	0.143118	-1.349540
C	-2.920356	-2.266876	-0.592753
H	-2.246368	-2.409889	-1.442512
H	-2.690300	-3.030113	0.157475
H	-3.956541	-2.400964	-0.928287
C	0.335250	1.503934	-0.944086
H	1.162667	1.619390	-1.664278
H	-0.551182	1.905082	-1.465967
C	1.624749	-1.139424	0.636145
H	1.888590	-0.383432	1.397221
H	1.244378	-1.999222	1.209342
C	2.915895	-1.556146	-0.078919
H	2.674096	-2.366582	-0.783327
C	0.617024	2.404266	0.267232
H	1.478996	1.988929	0.813066
C	3.487894	-0.396696	-0.897711
H	2.791036	-0.096279	-1.685670
H	3.650390	0.475916	-0.251165
H	4.447119	-0.655032	-1.364563
C	3.981426	-2.083599	0.889342
H	3.593716	-2.922709	1.476769
H	4.890684	-2.418367	0.371764
H	4.269217	-1.293406	1.594627
C	0.975872	3.840441	-0.130807
H	1.186931	4.476145	0.739942

H	1.853485	3.857690	-0.786203
H	0.142375	4.293889	-0.682666
C	-0.575444	2.413026	1.227356
H	-0.369886	3.001555	2.130646
H	-1.445681	2.863286	0.729263
H	-0.854976	1.393972	1.511650

Phenyl acetylene

Atom	x	y	z
C	-1.509285	-1.205996	-0.000002
C	-0.119805	-1.210153	0.000003
C	0.586337	-0.000021	0.000003
C	-0.119788	1.210144	0.000002
C	-1.509252	1.206017	-0.000001
C	-2.206580	0.000011	-0.000005
H	-2.049799	-2.146837	-0.000003
H	0.431939	-2.143963	0.000005
H	0.432000	2.143928	0.000004
H	-2.049766	2.146858	-0.000003
H	-3.291697	0.000033	-0.000009
C	2.022017	-0.000012	0.000011
C	3.228461	0.000003	0.000007
H	4.294698	0.000019	-0.000096

TS1

Atom	x	y	z
Al	-1.645412	-0.012541	-0.523426
C	1.203277	0.330058	-1.219555
C	2.390335	0.336824	-0.875675
C	3.756891	0.294719	-0.459161
C	4.634371	1.369681	-0.694078
C	4.272876	-0.835567	0.204159
C	5.961782	1.315601	-0.286007
C	5.600002	-0.884835	0.611441
C	6.455733	0.189233	0.369570
H	4.248227	2.247130	-1.202815
H	3.603574	-1.670334	0.390553
H	6.617369	2.160586	-0.480113

H	5.971490	-1.769154	1.122541
H	7.493035	0.148859	0.688499
H	-1.153508	0.380022	-2.347163
H	-0.384875	0.376885	-2.050710
O	-1.431240	-1.731627	-0.373066
C	-0.512374	-2.605927	0.227842
C	-1.317437	-3.789978	0.775979
H	-2.019141	-3.441906	1.541216
H	-1.894300	-4.247281	-0.033564
H	-0.663441	-4.549396	1.219133
C	0.480622	-3.093740	-0.831477
H	-0.064470	-3.578649	-1.647910
H	1.032804	-2.237772	-1.229733
H	1.190146	-3.814825	-0.407434
C	0.242302	-1.917543	1.369993
H	0.841239	-1.091750	0.973340
H	-0.470612	-1.520418	2.102060
H	0.907145	-2.623661	1.881719
C	-3.499918	0.387198	-1.145873
H	-3.515125	1.398891	-1.584376
H	-3.815415	-0.291490	-1.954166
C	-4.543628	0.324790	-0.018063
H	-4.186126	0.943811	0.820776
C	-1.101364	1.252185	0.902928
H	-1.612505	0.934064	1.828424
H	-0.024953	1.166989	1.098120
C	-1.445183	2.725427	0.635085
H	-2.531159	2.811253	0.468041
C	-1.087339	3.616264	1.828763
H	-0.007501	3.573764	2.013935
H	-1.359580	4.665208	1.656478
H	-1.594007	3.276706	2.738329
C	-0.736091	3.230680	-0.624086
H	0.340531	3.041253	-0.554213
H	-1.092676	2.707127	-1.518113
H	-0.900059	4.304413	-0.776243
C	-5.904270	0.879474	-0.450780
H	-6.296005	0.293104	-1.291257

H	-6.643655	0.841917	0.359371
H	-5.815727	1.918735	-0.784027
C	-4.704134	-1.107685	0.497119
H	-3.744492	-1.528117	0.812844
H	-5.410627	-1.160910	1.333897
H	-5.084053	-1.750160	-0.307118

H_2

Atom	x	y	z
H	0.000000	0.000000	0.368564
H	0.000000	0.000000	-0.368564

INT1

Atom	x	y	z
Al	1.085440	0.167301	-0.563417
C	-0.925346	0.094555	-0.599713
C	-2.148021	0.015958	-0.568146
C	-3.573927	-0.088847	-0.504726
C	-4.197792	-0.683670	0.605484
C	-4.386581	0.395702	-1.543285
C	-5.581645	-0.788426	0.671579
C	-5.770332	0.287956	-1.472267
C	-6.376478	-0.304011	-0.365906
H	-3.572808	-1.058954	1.409719
H	-3.909761	0.856338	-2.402077
H	-6.043941	-1.251277	1.538864
H	-6.380758	0.669112	-2.286122
H	-7.457808	-0.386907	-0.312431
C	1.820937	-1.267744	-1.767247
H	1.127229	-2.121254	-1.823208
H	1.900367	-0.888365	-2.801159
C	3.205182	-1.785928	-1.346024
H	3.114653	-2.230216	-0.343289
C	3.735981	-2.868292	-2.291917
H	4.704130	-3.270126	-1.965018
H	3.028808	-3.701019	-2.369311
H	3.868493	-2.453710	-3.299431
C	4.219145	-0.645367	-1.230755

H	4.283229	-0.095797	-2.178839
H	3.919242	0.060870	-0.450005
H	5.222181	-1.018731	-0.989037
C	1.709724	2.019434	-1.023971
H	2.641192	1.962605	-1.609557
H	0.980718	2.517709	-1.685623
C	1.947092	2.924635	0.193906
H	2.659099	2.418690	0.862088
C	0.652239	3.122623	0.983495
H	0.799450	3.783915	1.846845
H	-0.118796	3.569418	0.342732
H	0.275851	2.161655	1.344963
C	2.537975	4.283964	-0.195000
H	2.731624	4.919432	0.679349
H	3.479059	4.161676	-0.742164
H	1.841878	4.821573	-0.851706
O	1.614425	-0.130625	1.113919
C	1.135561	-1.017491	2.077435
C	0.574445	-2.302650	1.447047
H	1.339210	-2.781632	0.826947
H	0.253365	-3.014704	2.216906
H	-0.285718	-2.066507	0.812109
C	2.308861	-1.374393	2.998346
H	2.722042	-0.457943	3.430495
H	2.005738	-2.046283	3.810106
H	3.096728	-1.858510	2.412046
C	0.026984	-0.331017	2.889325
H	-0.791554	-0.055271	2.215991
H	-0.364895	-0.980681	3.681819
H	0.421604	0.583038	3.345099

HBpin

Atom	x	y	z
C	0.779683	-0.185969	-0.054546
O	1.062091	1.183268	-0.421467
C	-0.779682	-0.185972	0.054543
B	-0.000003	1.933384	-0.000002
O	-1.062096	1.183265	0.421459
H	-0.000007	3.119237	-0.000009
C	-1.467848	-0.432554	-1.286578
H	-1.357745	-1.471788	-1.608018
H	-2.531828	-0.208870	-1.181123
H	-1.055583	0.220082	-2.061465
C	-1.347307	-1.109990	1.119729
H	-0.984071	-0.842748	2.112990
H	-2.437450	-1.035897	1.122617
H	-1.073940	-2.148954	0.909820
C	1.347319	-1.109993	-1.119722
H	2.437463	-1.035908	-1.122592
H	1.073940	-2.148955	-0.909816
H	0.984102	-0.842749	-2.112989
C	1.467842	-0.432539	1.286580
H	1.055579	0.220109	2.061458
H	1.357731	-1.471769	1.608033
H	2.531824	-0.208863	1.181125

TS2

Atom	x	y	z
Al	-0.804317	1.090183	0.001936
C	0.154853	-0.704967	-0.013546
C	0.063231	-1.953991	0.135451
C	-0.655408	-3.215463	0.243898
C	-0.052862	-4.454491	0.464980
C	-2.050915	-3.143323	0.113939
C	-0.831247	-5.603860	0.557066
C	-2.820887	-4.294884	0.206539
C	-2.215312	-5.531007	0.428415
H	1.026914	-4.505828	0.562267
H	-2.510372	-2.174497	-0.061307

H	-0.350963	-6.562325	0.729704
H	-3.899449	-4.226257	0.103487
H	-2.818999	-6.430614	0.499324
H	1.590203	-2.607862	0.273652
B	1.758143	-1.357387	0.094363
O	2.562637	-1.213194	-1.102287
O	2.459004	-0.755507	1.207016
C	3.596973	-0.297333	-0.783561
C	3.777563	-0.502768	0.759304
C	4.637184	-1.733881	1.071796
H	5.694103	-1.576596	0.831012
H	4.548441	-1.955659	2.139006
H	4.272808	-2.598500	0.507960
C	4.310903	0.719028	1.496881
H	5.283172	1.030955	1.097514
H	3.601651	1.545056	1.412471
H	4.433940	0.481978	2.558159
C	3.123802	1.117812	-1.121722
H	2.805530	1.128378	-2.169457
H	2.268834	1.403531	-0.500412
H	3.923476	1.858473	-0.995164
C	4.828632	-0.648064	-1.612487
H	4.619099	-0.460115	-2.669693
H	5.688167	-0.034311	-1.318693
H	5.089826	-1.702513	-1.500515
C	-2.042701	0.784776	1.559603
H	-2.579511	-0.169279	1.405874
H	-1.375402	0.588548	2.414015
C	-3.077932	1.837402	1.977217
H	-2.562331	2.795806	2.135115
C	-3.775669	1.470840	3.292015
H	-4.502640	2.232229	3.603335
H	-4.312084	0.520353	3.178413
H	-3.046859	1.343481	4.098663
C	-4.127528	2.051661	0.884591
H	-4.869986	2.805660	1.172830
H	-3.664219	2.364401	-0.056218
H	-4.662405	1.112906	0.688526

C	-1.746046	1.330466	-1.760212
H	-2.215742	2.328849	-1.752913
H	-1.042474	1.357874	-2.607241
C	-2.829046	0.274608	-2.056654
H	-3.285069	-0.049995	-1.105657
C	-3.961545	0.826481	-2.927506
H	-4.717072	0.063518	-3.154866
H	-4.463017	1.664661	-2.431478
H	-3.555789	1.195392	-3.877770
C	-2.215370	-0.957755	-2.725009
H	-1.362430	-1.335277	-2.154258
H	-2.946086	-1.767940	-2.837311
H	-1.849829	-0.692333	-3.724883
O	0.411207	2.335974	0.340316
C	0.488001	3.694313	0.036216
C	1.720238	4.255272	0.756733
H	2.618903	3.746971	0.392794
H	1.833618	5.333061	0.591918
H	1.632055	4.064975	1.830318
C	-0.768851	4.424188	0.530248
H	-1.661185	3.999023	0.054350
H	-0.866440	4.295512	1.612639
H	-0.734813	5.496303	0.303617
C	0.646808	3.906815	-1.476704
H	1.519968	3.352651	-1.834112
H	-0.234155	3.536536	-2.008427
H	0.780034	4.967949	-1.718882

INT2

Atom	x	y	z
Al	1.056746	-0.640153	0.217481
C	-0.099480	1.046434	0.039582
C	0.315509	2.330952	-0.051362
C	1.688962	2.854853	0.115316
C	2.059213	4.040795	-0.534454
C	2.636851	2.234512	0.939266
C	3.339626	4.567042	-0.405593
C	3.917935	2.759049	1.071673

C	4.278837	3.923857	0.397642
H	1.325075	4.543333	-1.160209
H	2.357446	1.341690	1.490498
H	3.605826	5.480238	-0.931048
H	4.637249	2.255237	1.710929
H	5.280202	4.331023	0.503686
H	-0.400050	3.132033	-0.283421
B	-1.639751	0.966650	-0.068188
O	-2.415819	1.749113	-0.920406
O	-2.454973	0.175695	0.732668
C	-3.783054	1.349011	-0.785321
C	-3.793247	0.668250	0.621011
C	-3.989396	1.672213	1.759256
H	-5.012289	2.060366	1.790339
H	-3.770898	1.169170	2.704261
H	-3.294319	2.510386	1.652868
C	-4.770642	-0.488534	0.769165
H	-5.801911	-0.139711	0.644496
H	-4.571640	-1.274349	0.038687
H	-4.668143	-0.920737	1.768080
C	-4.092359	0.373569	-1.921305
H	-3.846447	0.857861	-2.870028
H	-3.485545	-0.531860	-1.835907
H	-5.149914	0.090788	-1.932307
C	-4.672165	2.580042	-0.902384
H	-4.600906	2.984791	-1.915561
H	-5.718928	2.322601	-0.706868
H	-4.362218	3.357849	-0.202580
C	2.720176	-0.429719	-0.924531
H	3.547430	-0.087263	-0.278702
H	2.595039	0.377594	-1.664532
C	3.205947	-1.695350	-1.644693
H	2.441781	-1.995224	-2.377783
C	4.508359	-1.462519	-2.418788
H	5.310758	-1.183009	-1.724455
H	4.834168	-2.357305	-2.965865
H	4.395799	-0.643648	-3.137193
C	3.379657	-2.856964	-0.663185

H	4.103408	-2.582315	0.115390
H	2.427645	-3.092450	-0.176579
H	3.749533	-3.762366	-1.161890
C	1.522018	-1.077600	2.139100
H	2.605402	-1.281604	2.195450
H	1.355208	-0.223637	2.819066
C	0.765745	-2.282972	2.719513
H	0.863407	-3.122366	2.015959
C	1.328246	-2.725386	4.074800
H	1.236928	-1.910071	4.804296
H	0.797524	-3.597275	4.480027
H	2.390848	-2.980217	3.996771
C	-0.727116	-1.976081	2.846125
H	-1.279462	-2.826068	3.268063
H	-0.881523	-1.114098	3.509529
H	-1.154041	-1.731934	1.870412
O	0.118907	-2.071729	-0.299846
C	-0.601991	-2.489437	-1.409405
C	-2.034397	-2.804781	-0.951756
H	-2.010666	-3.622035	-0.223272
H	-2.440103	-1.924539	-0.446103
H	-2.687666	-3.091932	-1.786142
C	0.032848	-3.773162	-1.966167
H	1.046564	-3.573145	-2.324835
H	0.098187	-4.514065	-1.163214
H	-0.555966	-4.193904	-2.790350
C	-0.628358	-1.414909	-2.507440
H	-1.161011	-1.761318	-3.401448
H	-1.118251	-0.502239	-2.150182
H	0.396271	-1.149166	-2.790383

TS3

Atom	x	y	z
Al	-0.189618	0.626239	1.047028
C	-0.769733	0.187435	-1.118730
C	-0.684424	1.326301	-1.851715
C	0.505098	2.168549	-2.063746
C	1.790861	1.614407	-2.120817

C	0.351927	3.548388	-2.255030
C	2.895649	2.431808	-2.338049
C	1.458602	4.365605	-2.454224
C	2.735137	3.807277	-2.496263
H	1.914926	0.541453	-1.989400
H	-0.647501	3.976139	-2.224952
H	3.886471	1.988315	-2.374096
H	1.327232	5.436316	-2.579267
H	3.601523	4.442477	-2.655926
H	-1.584034	1.707515	-2.349575
B	-2.138248	-0.544471	-1.229965
O	-2.429775	-1.786290	-0.720183
O	-3.235707	-0.002922	-1.891107
C	-3.855764	-1.926848	-0.731986
C	-4.263131	-1.003455	-1.923622
C	-4.163501	-1.708995	-3.275656
H	-4.961286	-2.446749	-3.405455
H	-4.243586	-0.960830	-4.068398
H	-3.197258	-2.211569	-3.373404
C	-5.615729	-0.324211	-1.772358
H	-6.414718	-1.068447	-1.684640
H	-5.630137	0.320018	-0.891388
H	-5.815717	0.294090	-2.651823
C	-4.367314	-1.407100	0.612426
H	-3.857079	-1.947145	1.413073
H	-4.128569	-0.345819	0.733091
H	-5.448562	-1.546339	0.713246
C	-4.210923	-3.395146	-0.907597
H	-3.887263	-3.953994	-0.025718
H	-5.293823	-3.519547	-1.018029
H	-3.712484	-3.819945	-1.780486
H	0.236381	-0.600333	-0.882372
C	1.410921	-1.578592	-0.836455
C	2.613201	-1.848179	-0.809626
C	4.024996	-2.075866	-0.753770
C	4.877294	-1.073109	-0.253489
C	4.606155	-3.276608	-1.195982
C	6.251836	-1.267497	-0.201405

C	5.982424	-3.465818	-1.140863
C	6.814408	-2.464014	-0.644865
H	4.429107	-0.147035	0.096958
H	3.955888	-4.054894	-1.582166
H	6.889643	-0.479845	0.190530
H	6.409825	-4.402771	-1.488018
H	7.889113	-2.614297	-0.602590
O	-0.974547	-0.708827	1.862008
C	-0.618096	-1.896287	2.519060
C	-0.908010	-3.101539	1.619609
H	-0.355427	-2.995776	0.681404
H	-0.610364	-4.033263	2.115750
H	-1.973387	-3.151989	1.379742
C	-1.469940	-1.971422	3.792167
H	-1.238551	-1.122245	4.443490
H	-2.531019	-1.916302	3.528010
H	-1.290910	-2.900773	4.344683
C	0.867781	-1.914135	2.892990
H	1.479442	-1.930367	1.985401
H	1.123921	-1.023052	3.477260
H	1.104236	-2.802173	3.490494
C	-1.210828	2.288773	1.495293
H	-0.698618	2.648374	2.403626
H	-1.042130	3.086776	0.752667
C	1.779462	0.941114	1.187036
H	2.293795	0.071964	1.618534
H	2.186632	1.022835	0.174113
C	-2.714984	2.191857	1.804998
H	-2.923765	1.192039	2.215472
C	-3.550950	2.372818	0.537458
H	-4.623225	2.242272	0.736686
H	-3.409104	3.386725	0.140100
H	-3.262328	1.671050	-0.248531
C	-3.153956	3.223386	2.849697
H	-2.937830	4.237395	2.489899
H	-4.229015	3.162675	3.062561
H	-2.612632	3.083161	3.790832
C	2.171181	2.196516	1.981903

H	1.547494	3.041956	1.652918
C	1.935723	1.988760	3.479497
H	0.899783	1.698178	3.687180
H	2.582027	1.181298	3.846561
H	2.160144	2.890974	4.060778
C	3.633324	2.583008	1.736144
H	3.805760	2.774257	0.671515
H	3.927613	3.478617	2.298578
H	4.293709	1.761095	2.041632

PD

Atom	x	y	z
C	0.591574	-0.741496	-0.097992
C	1.507512	0.229837	0.040217
C	2.972863	0.095190	0.023074
C	3.757883	1.245978	0.161683
C	3.620892	-1.138835	-0.127071
C	5.146810	1.173345	0.149566
C	5.006888	-1.213948	-0.139293
C	5.775952	-0.058414	-0.001395
H	3.265801	2.207740	0.279659
H	3.035028	-2.046199	-0.233469
H	5.736869	2.077684	0.258072
H	5.492687	-2.177453	-0.256162
H	6.859310	-0.120822	-0.011212
H	1.144753	1.248755	0.182485
B	-0.918245	-0.406801	-0.049295
O	-1.918990	-1.325999	-0.247450
O	-1.401402	0.858814	0.196035
C	-3.160631	-0.679934	0.100786
C	-2.813241	0.831529	-0.094827
C	-2.979344	1.292607	-1.541959
H	-4.033898	1.364442	-1.822078
H	-2.520145	2.277840	-1.650762
H	-2.479527	0.603587	-2.228868
C	-3.532753	1.779994	0.850283
H	-4.616515	1.708599	0.713424
H	-3.292599	1.560047	1.891407

H	-3.227809	2.807736	0.638429
C	-3.452286	-1.034174	1.557998
H	-3.472249	-2.121879	1.657142
H	-2.670750	-0.643774	2.216111
H	-4.417012	-0.634636	1.882588
C	-4.263568	-1.204547	-0.804087
H	-4.434135	-2.263521	-0.595462
H	-5.198017	-0.664002	-0.622375
H	-3.995183	-1.102747	-1.856533
H	0.906458	-1.772715	-0.246487

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