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

Supporting Information

Quantitative catalytic hydroboration of imines using NaH as catalyst

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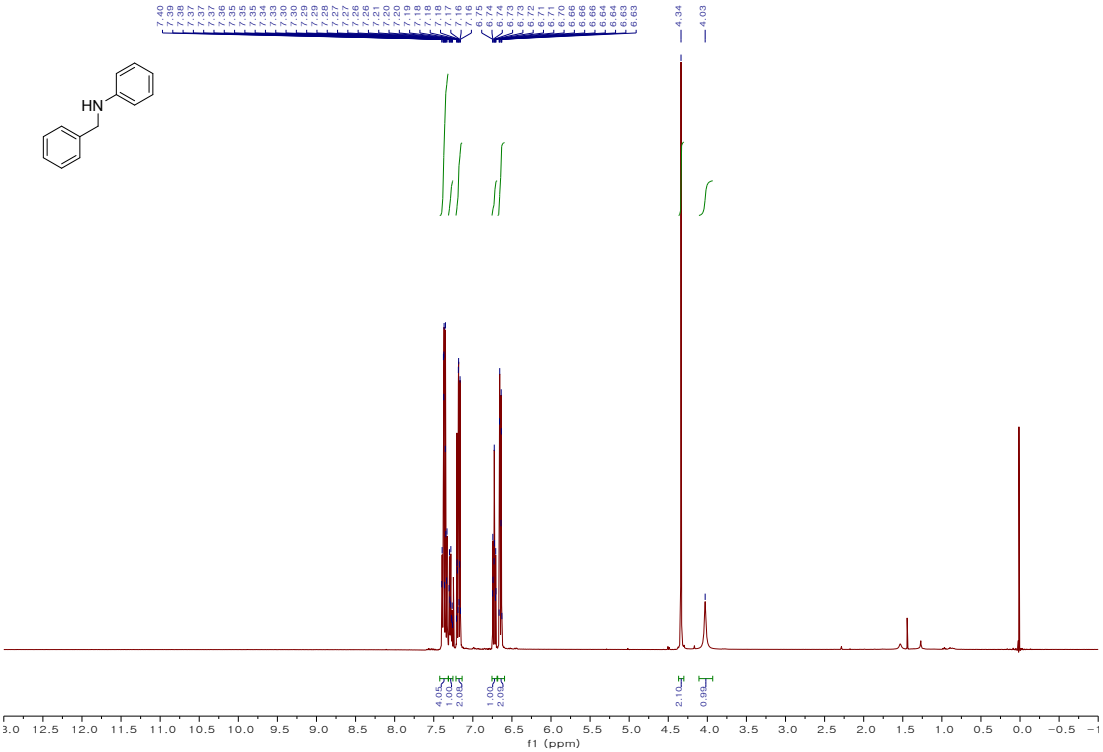


Figure S1: ^{1}H NMR of *N*-Benzylaniline (**2a**)

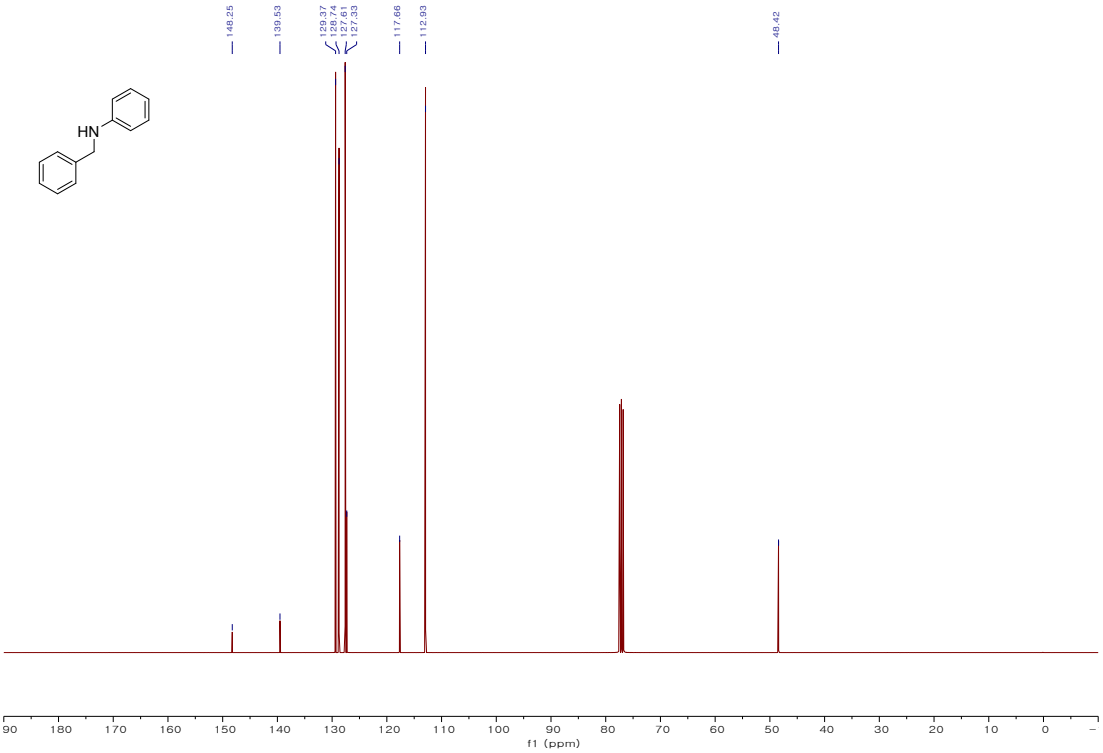


Figure S2: ^{13}C NMR of *N*-Benzylaniline (**2a**)

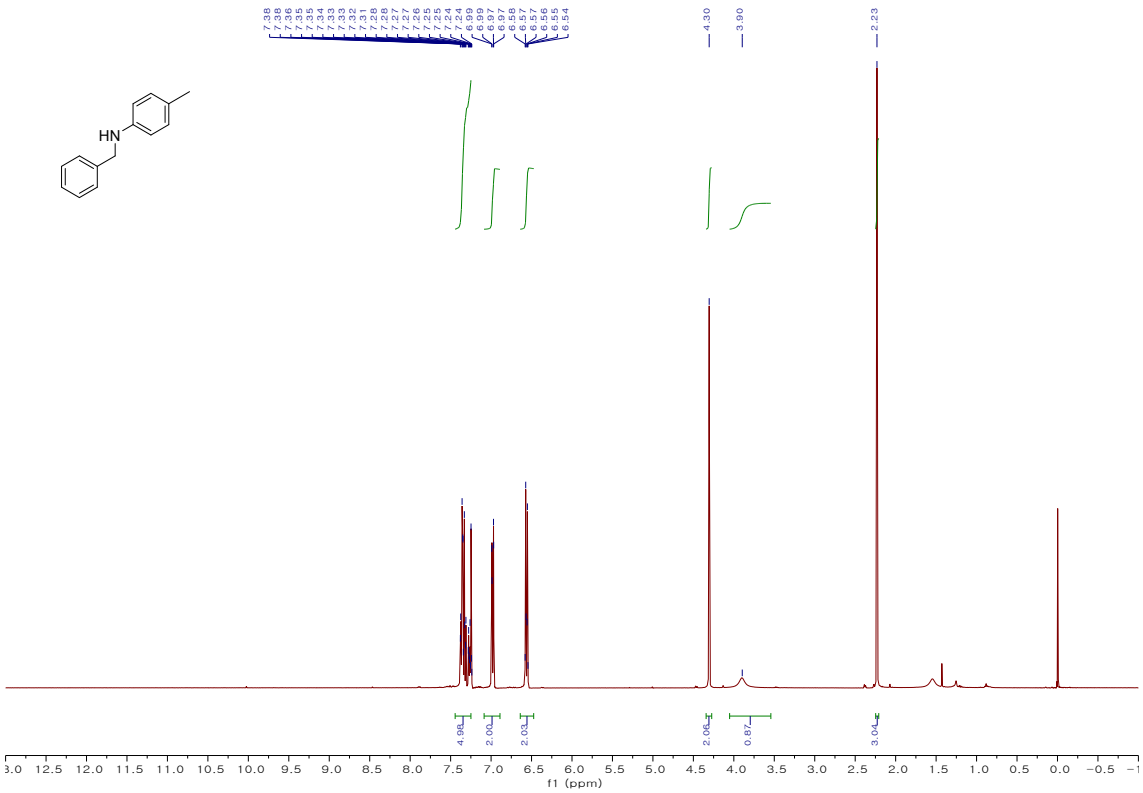


Figure S3: ^{1}H NMR of N-benzyl-4-methylaniline (**2b**)

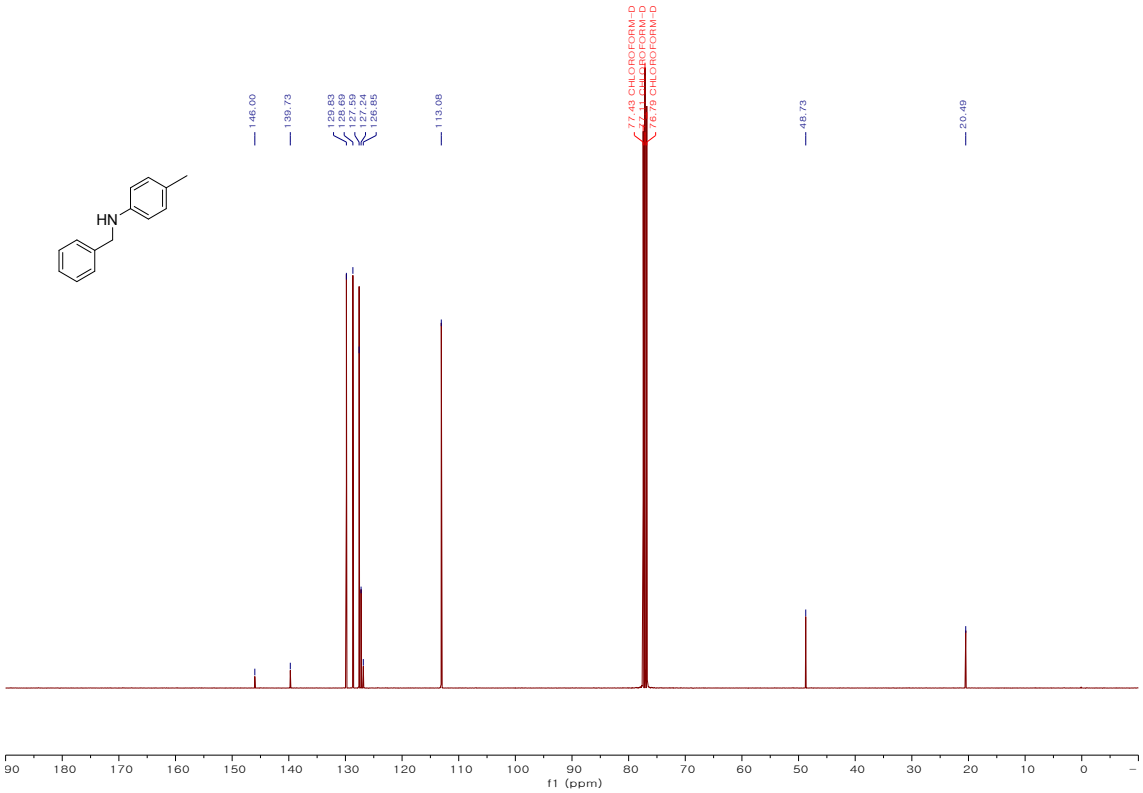


Figure S4: ^{13}C NMR of N-benzyl-4-methylaniline (**2b**)

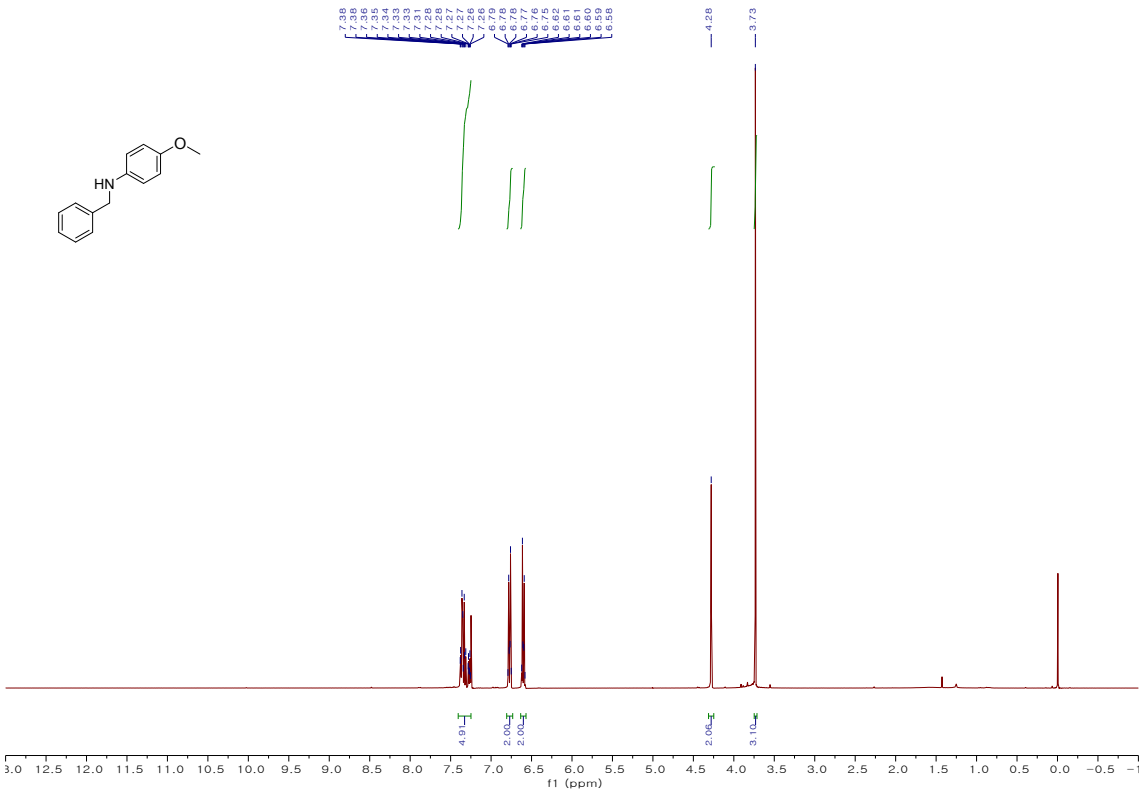


Figure S5: [1]H NMR of N-benzyl-4-methoxyaniline (**2c**)

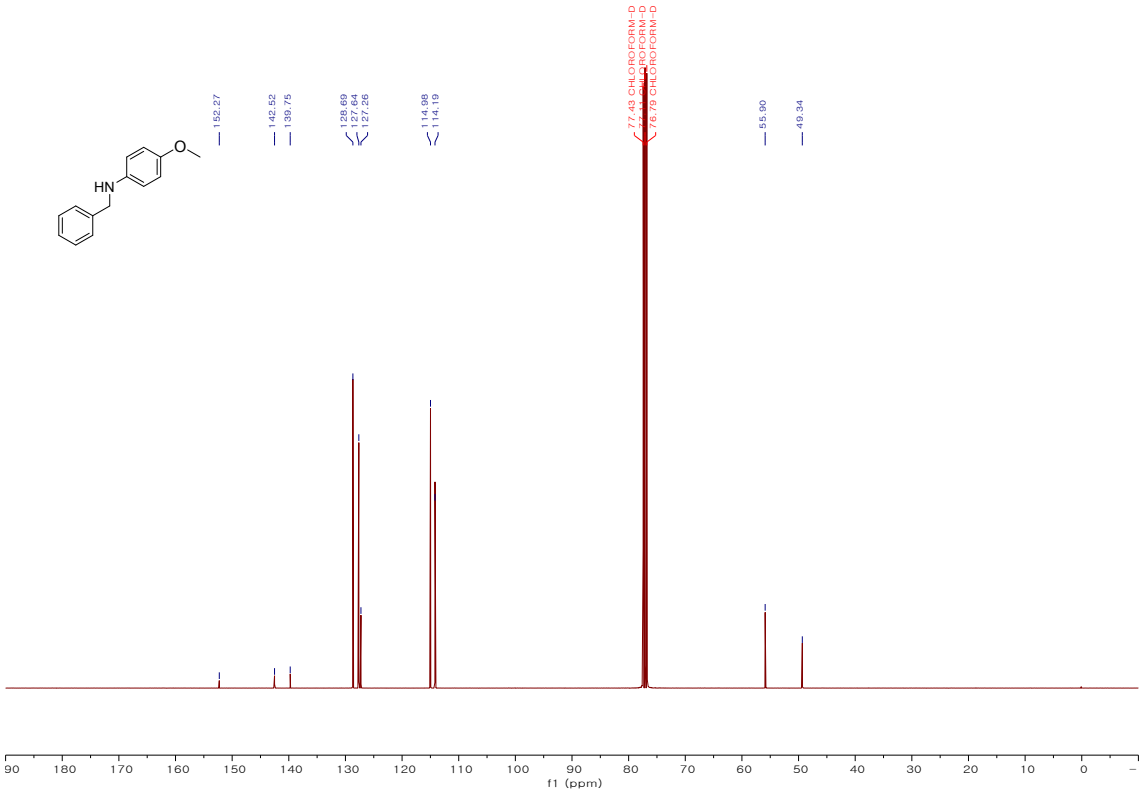


Figure S6: [13]C NMR of N-benzyl-4-methoxyaniline (**2c**)

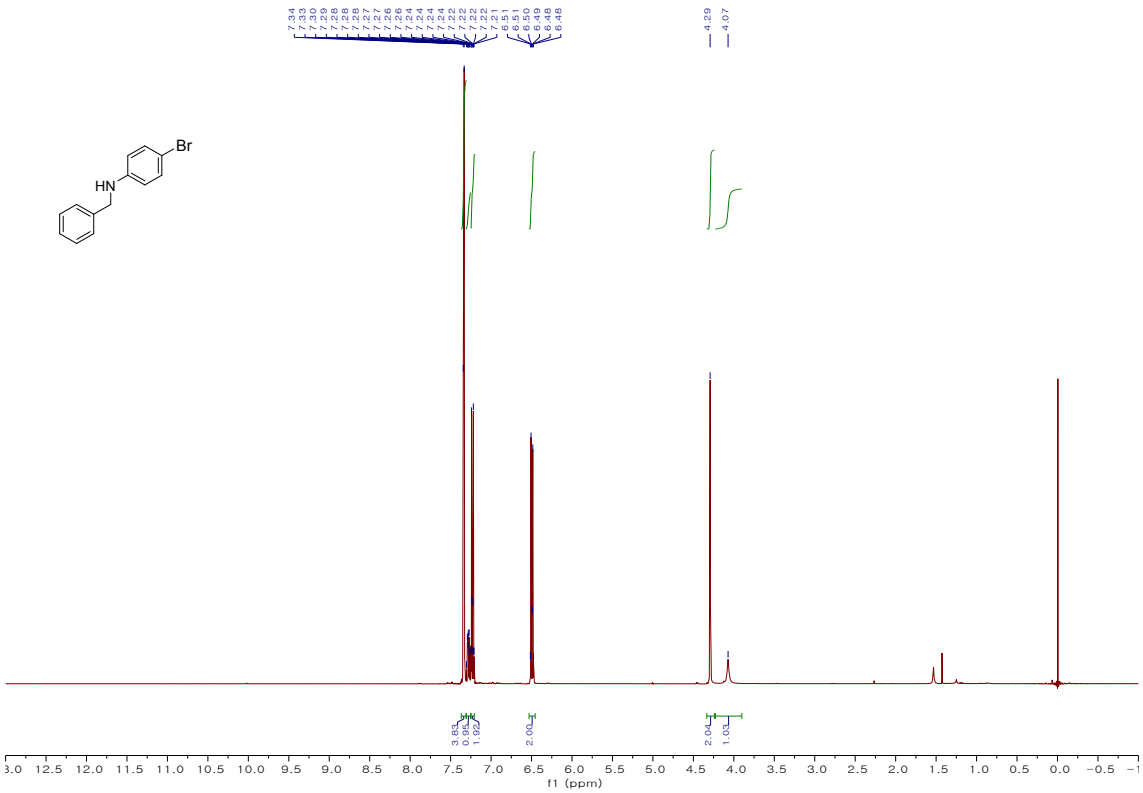


Figure S7: ^{1}H NMR of N-benzyl-4-bromoaniline (**2d**)

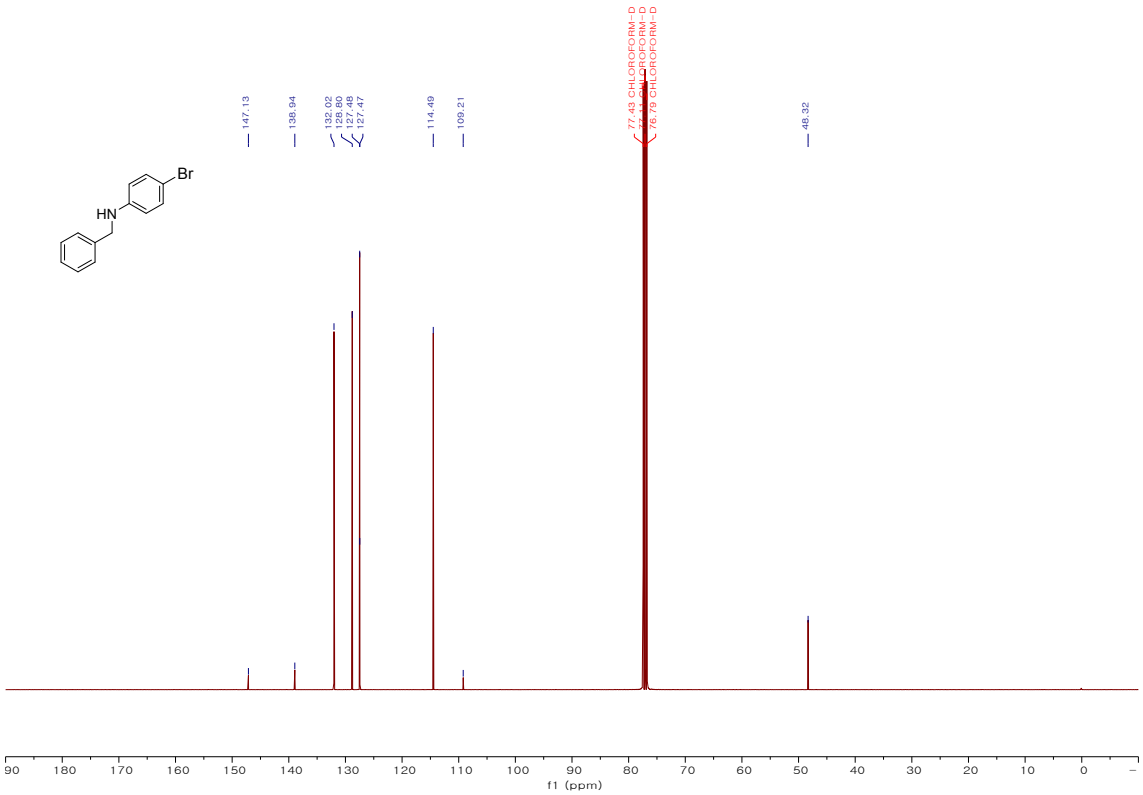


Figure S8: ^{13}C NMR of N-benzyl-4-bromoaniline (**2d**)

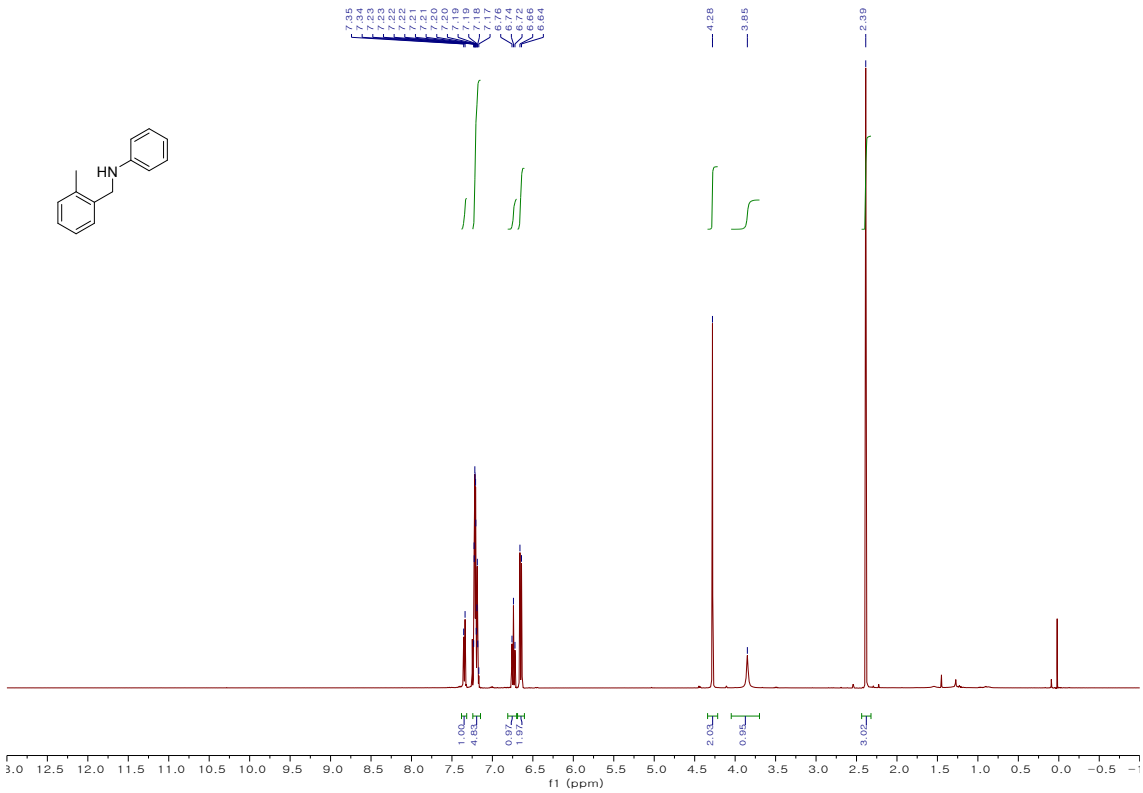


Figure S9: ^{1}H NMR of *N*-(2-methylbenzyl)aniline (**2e**)

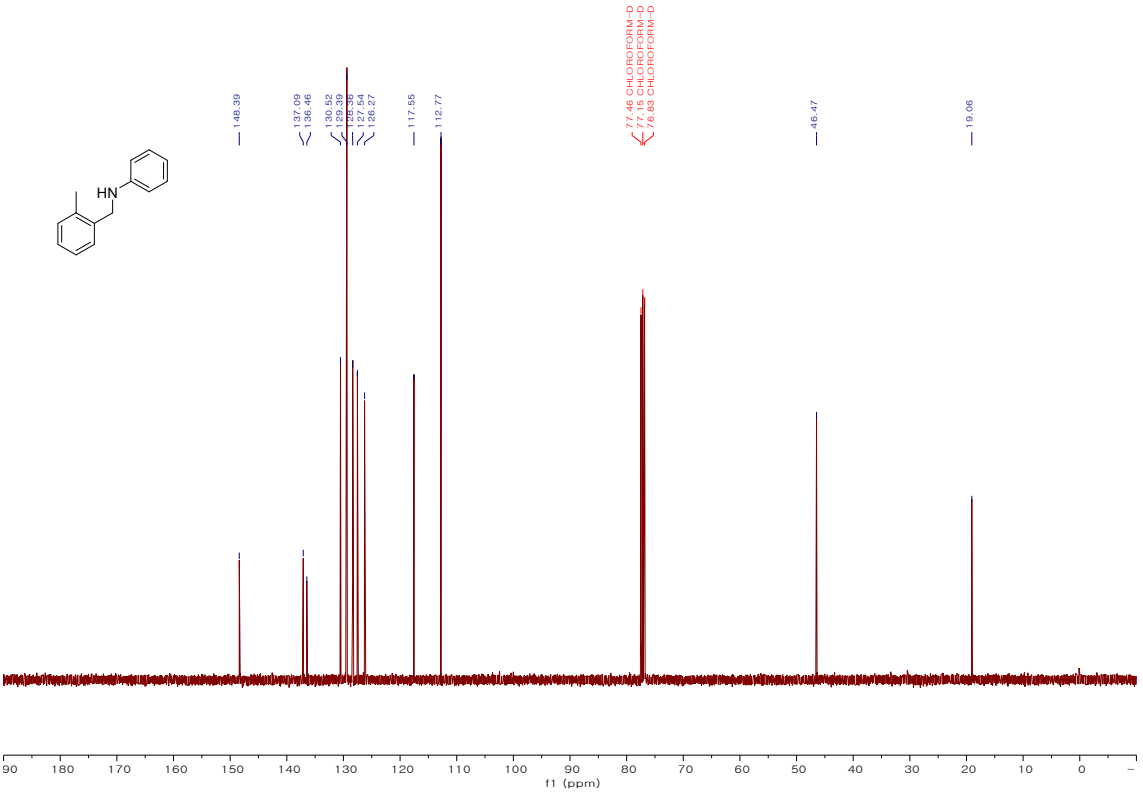


Figure S10: ^{13}C NMR of *N*-(2-methylbenzyl)aniline (**2e**)

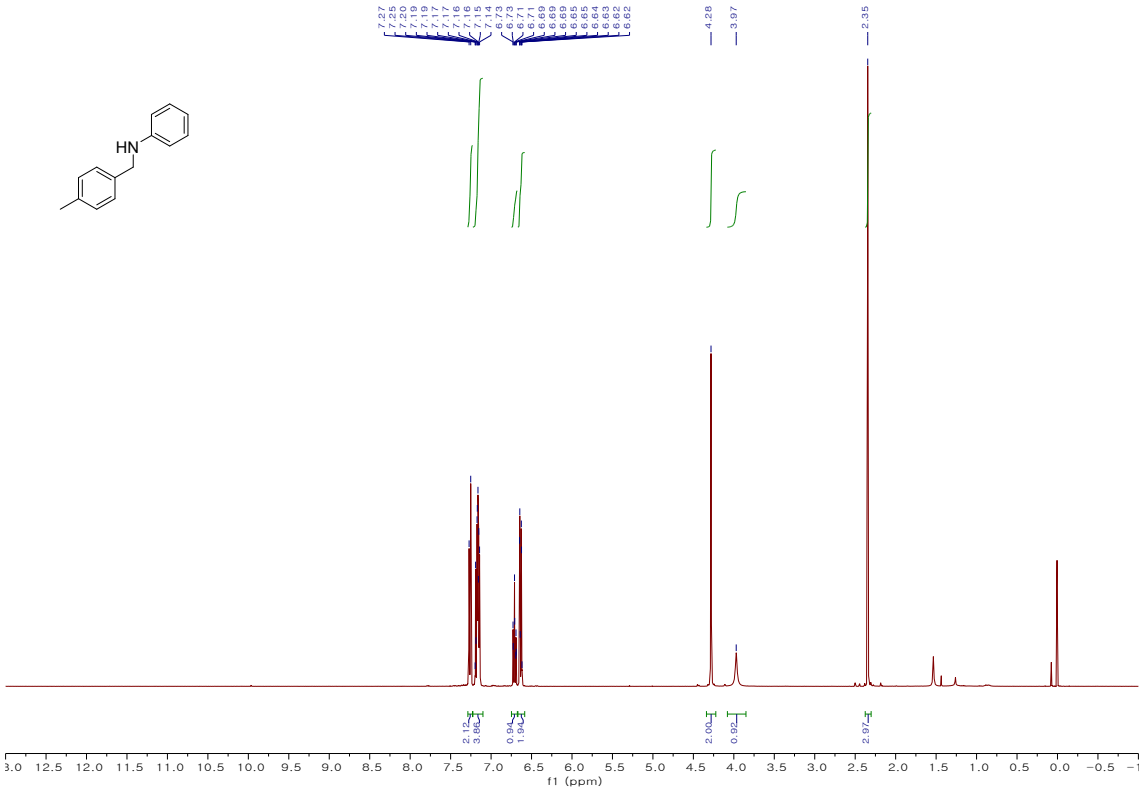


Figure S11: ^{1}H NMR of *N*-(4-methylbenzyl)aniline (**2f**)

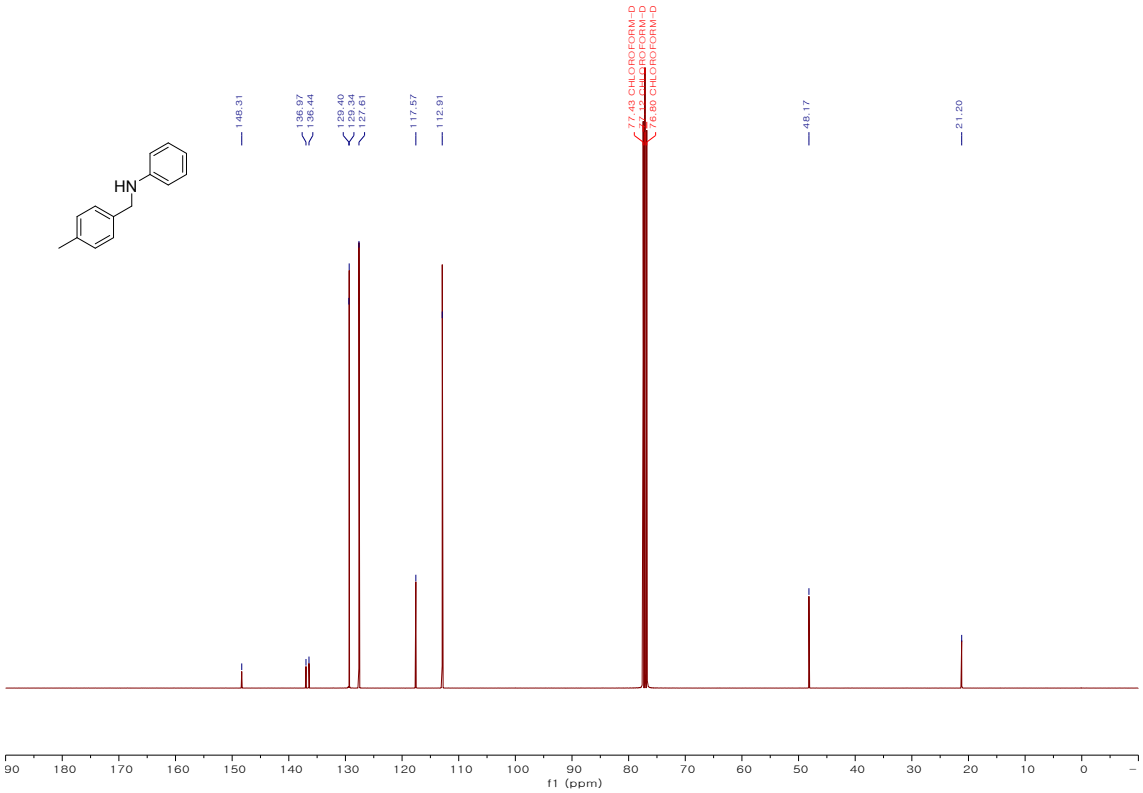


Figure S12: ^{13}C NMR of *N*-(4-methylbenzyl)aniline (**2f**)

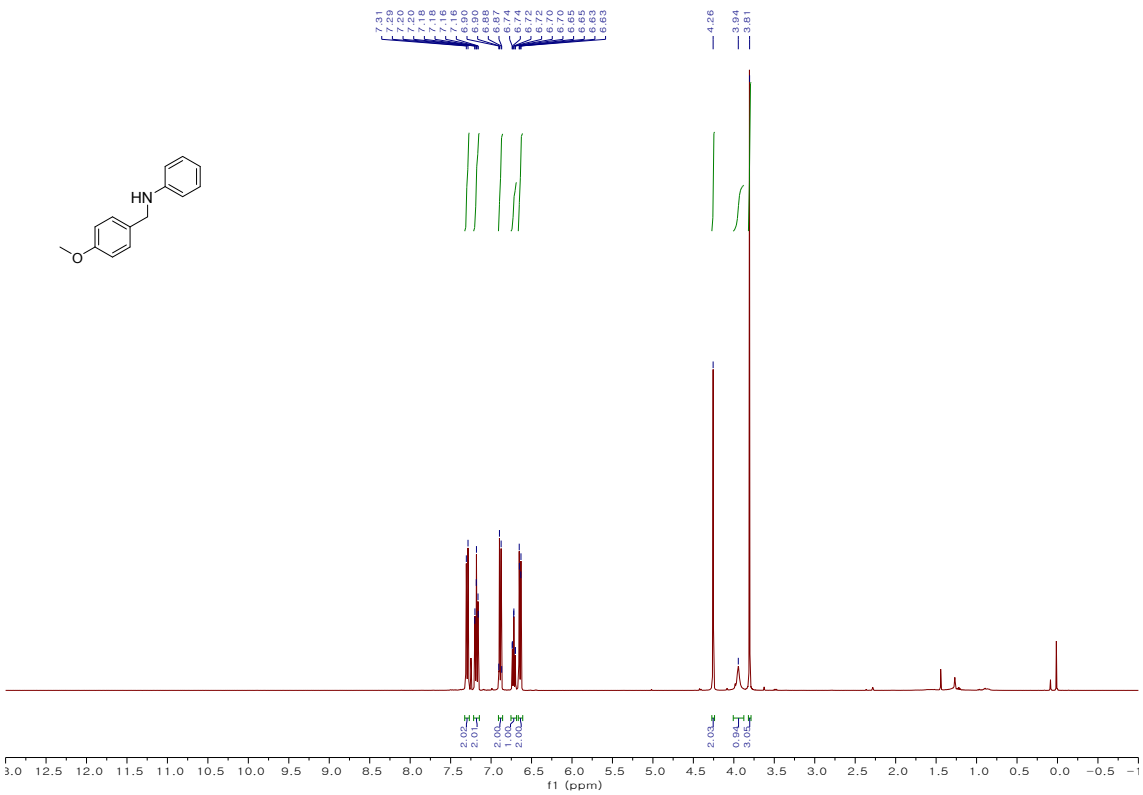


Figure S13: ^{1}H NMR of *N*-(4-methoxybenzyl)aniline (**2g**)

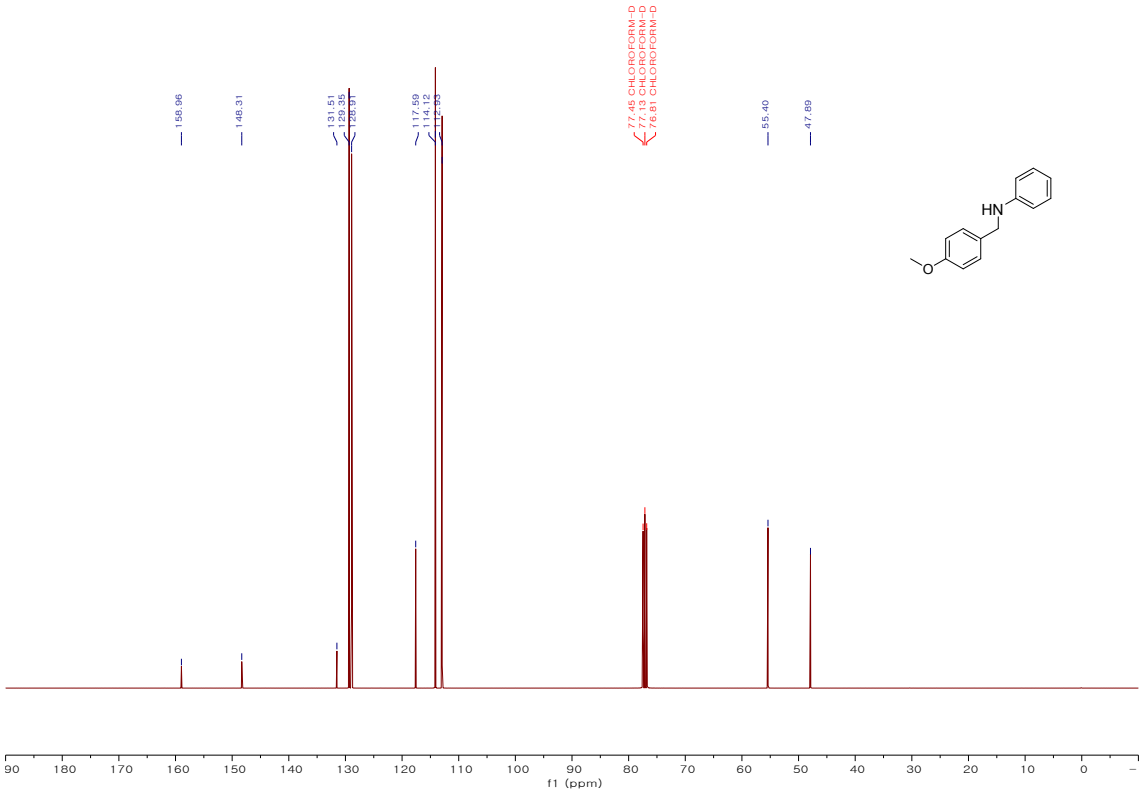


Figure S14: ^{13}C NMR of *N*-(4-methoxybenzyl)aniline (**2g**)

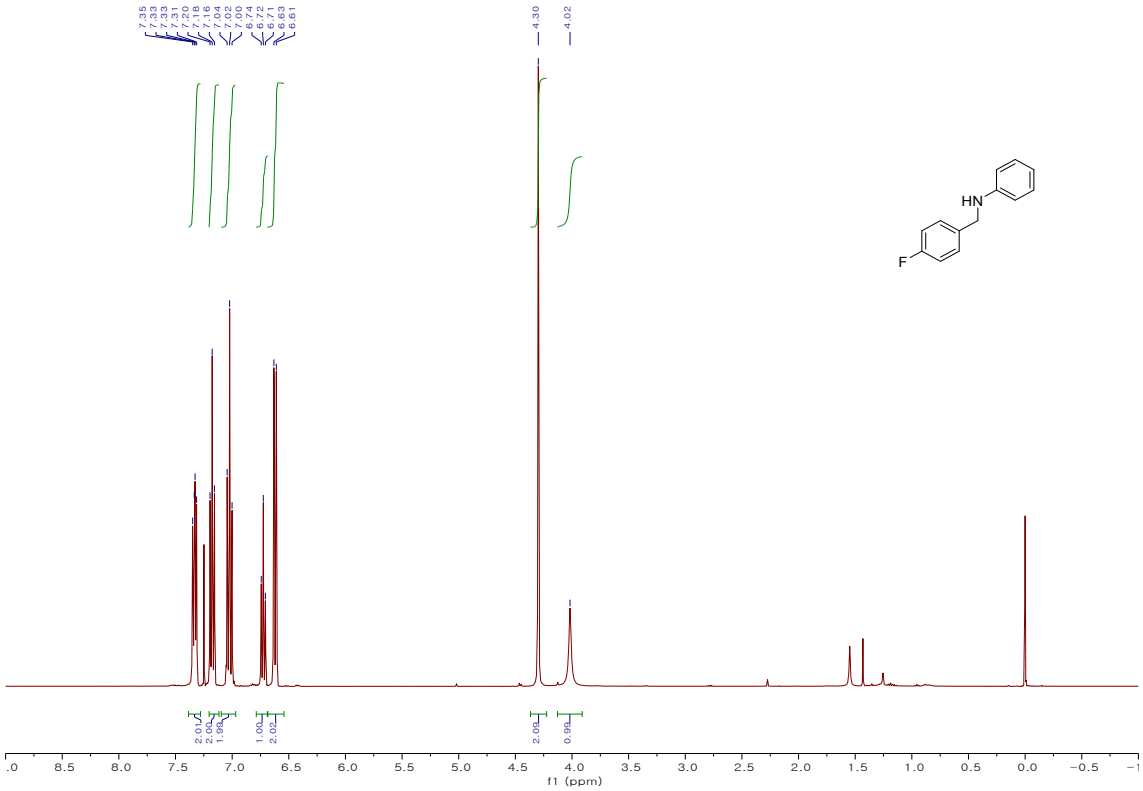


Figure S15: ^{1}H NMR of *N*-(4-fluorobenzyl)aniline (**2h**)

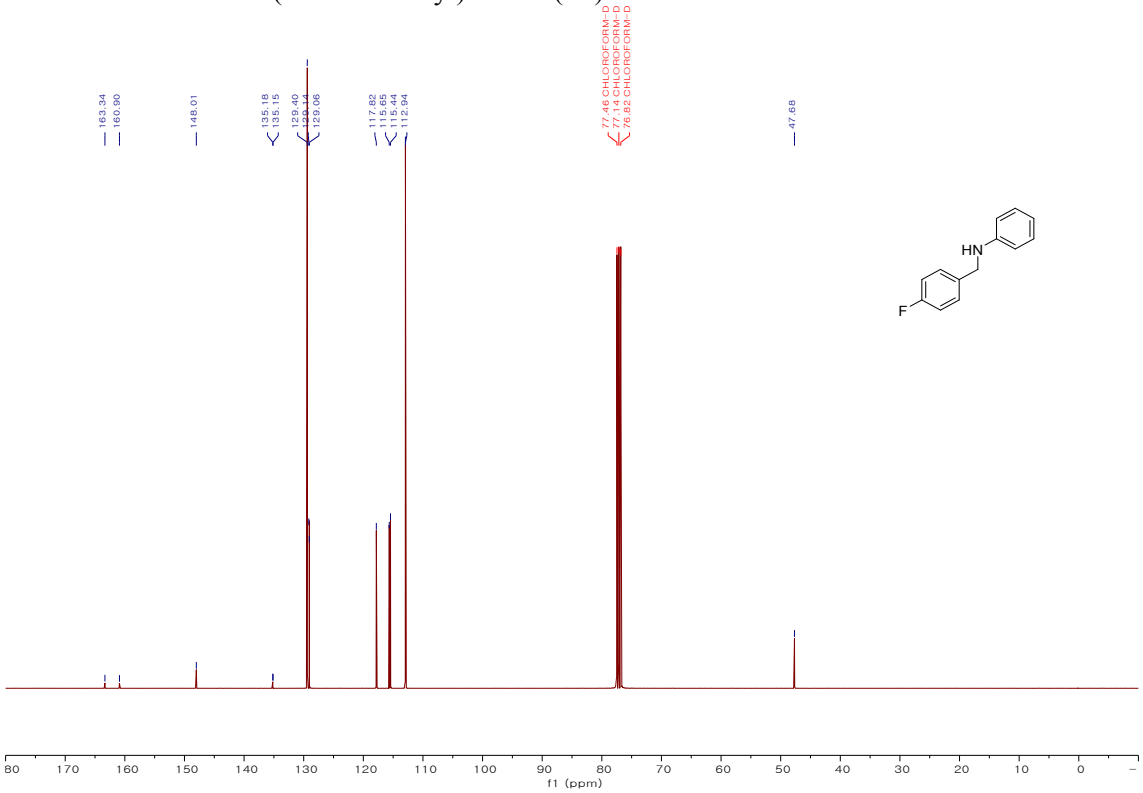


Figure S16: ^{13}C NMR of *N* -(4-fluorobenzyl)aniline (**2h**)

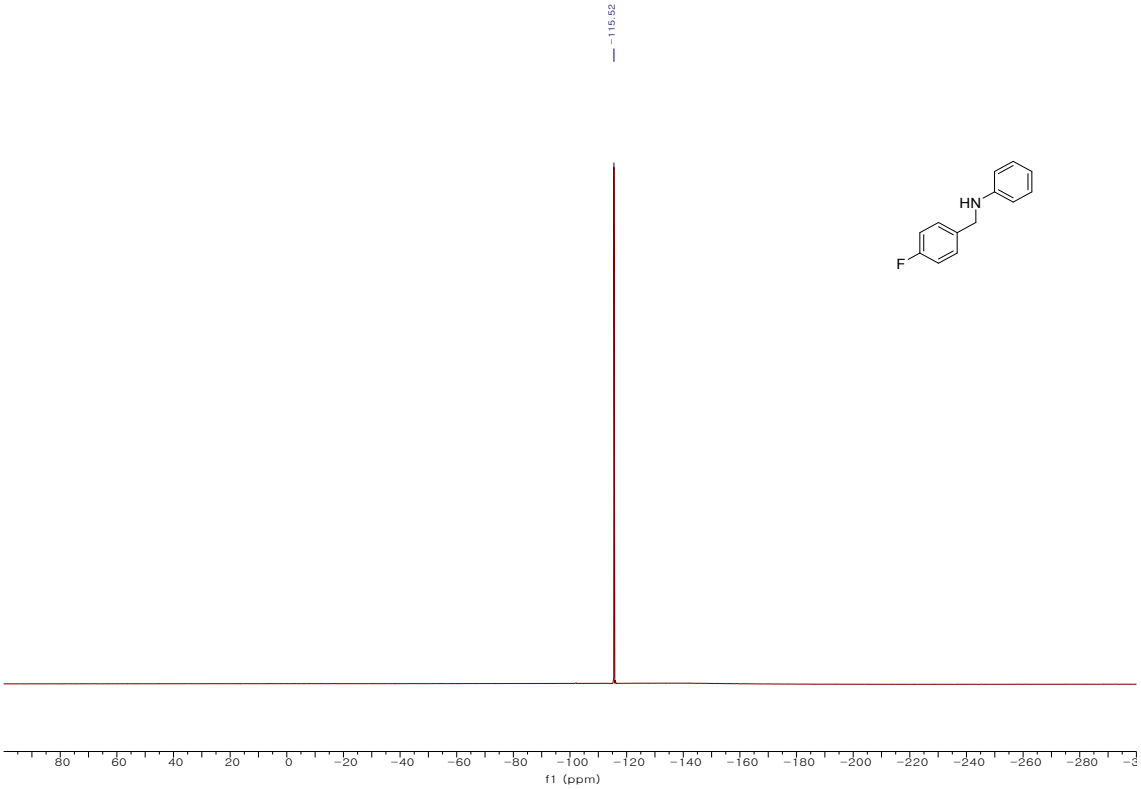


Figure S17: ^{19}F NMR of *N* -(4-fluorobenzyl)aniline (**2h**)

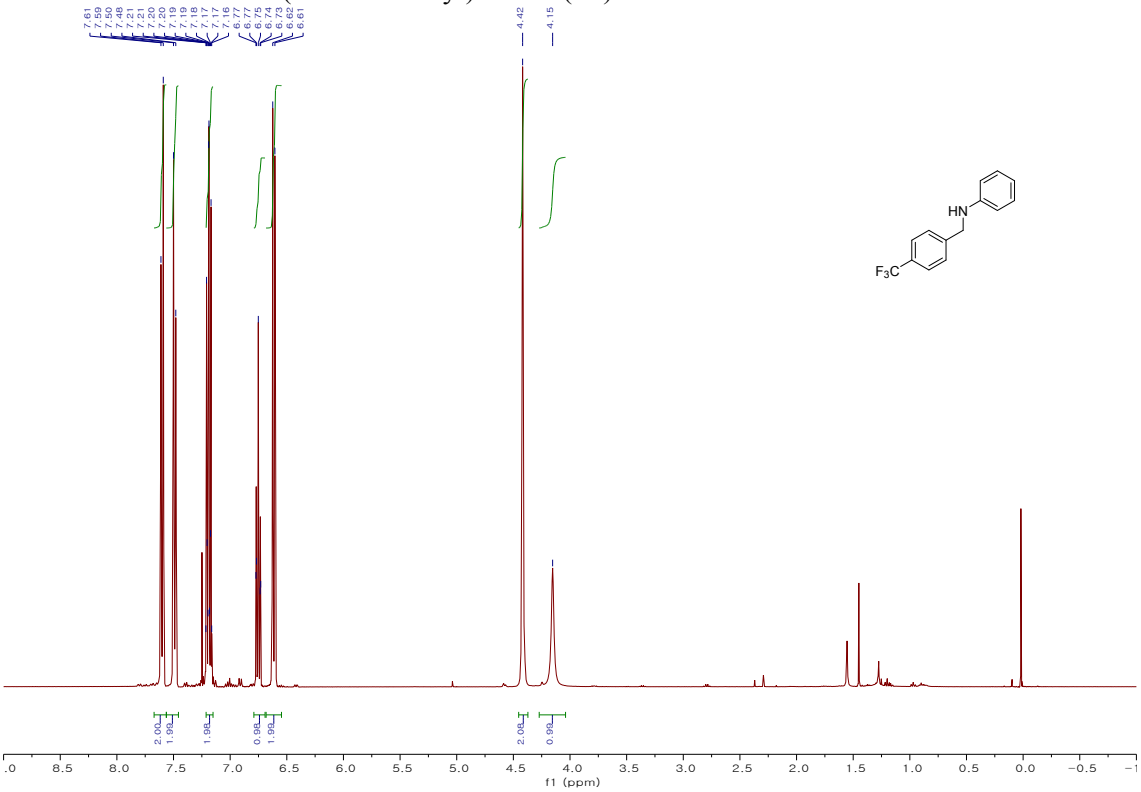


Figure S18: ^{1}H NMR of *N* -(4-(trifluoromethyl)benzyl)aniline (**2i**)

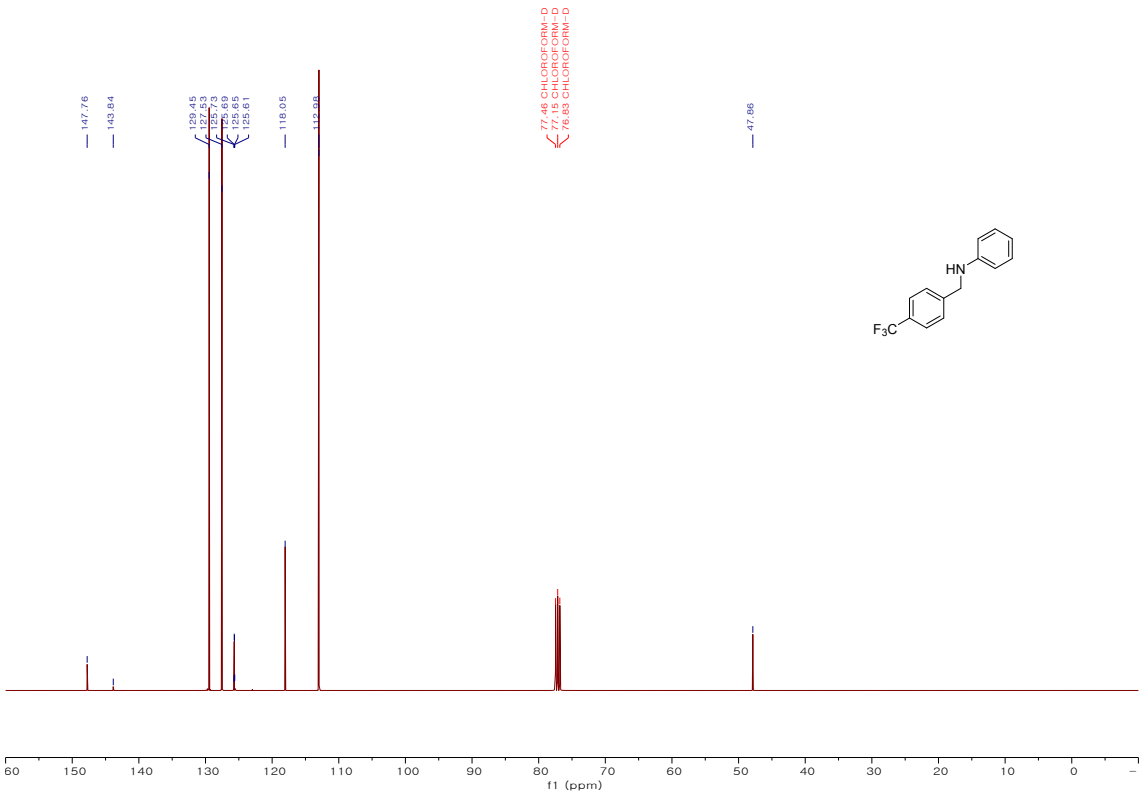


Figure S19: ^{13}C NMR of *N* -(4-(trifluoromethyl)benzyl)aniline (**2i**)

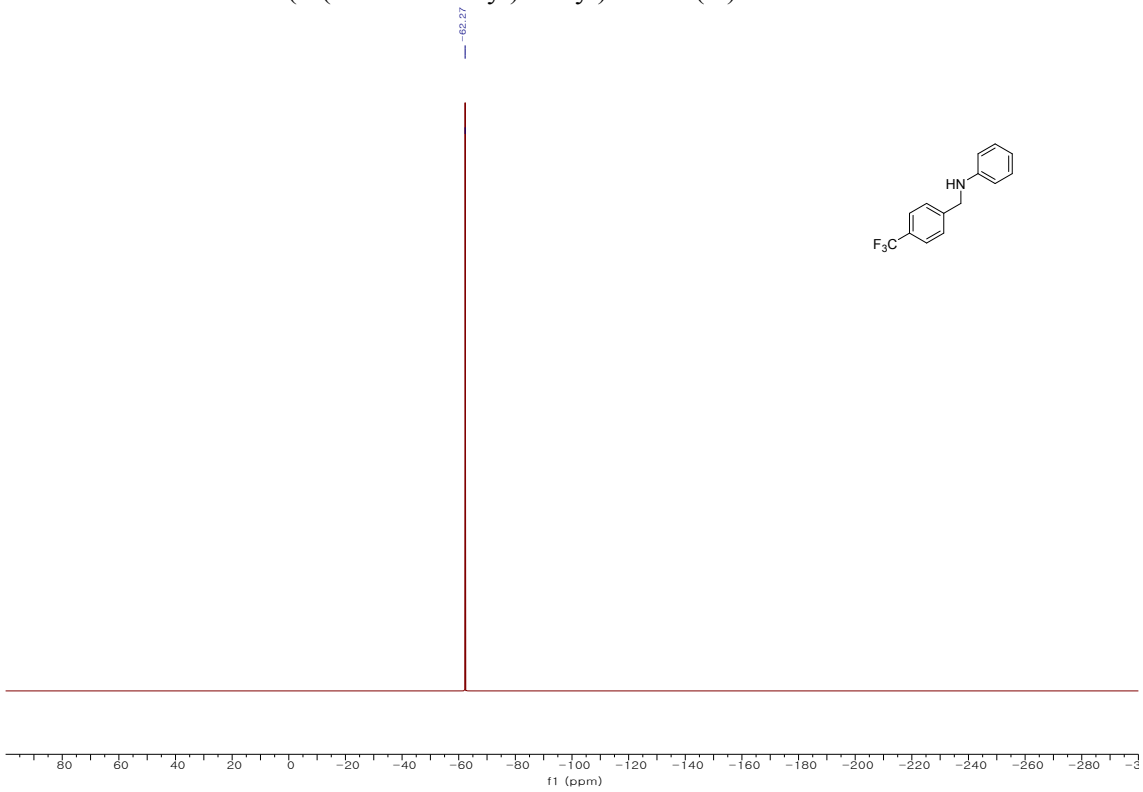


Figure S20: ^{19}F NMR of *N* -(4-(trifluoromethyl)benzyl)aniline (**2i**)

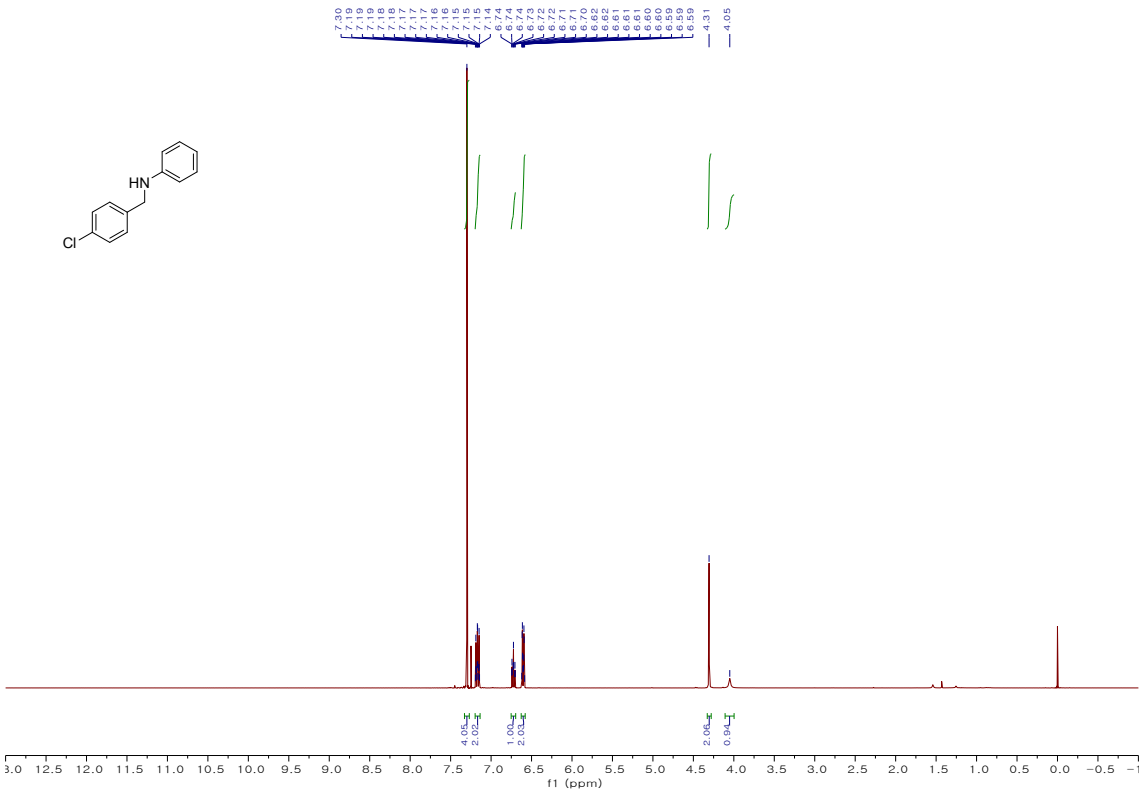


Figure S21: ^{1}H NMR of *N*-(4-chlorobenzyl)aniline (**2j**)

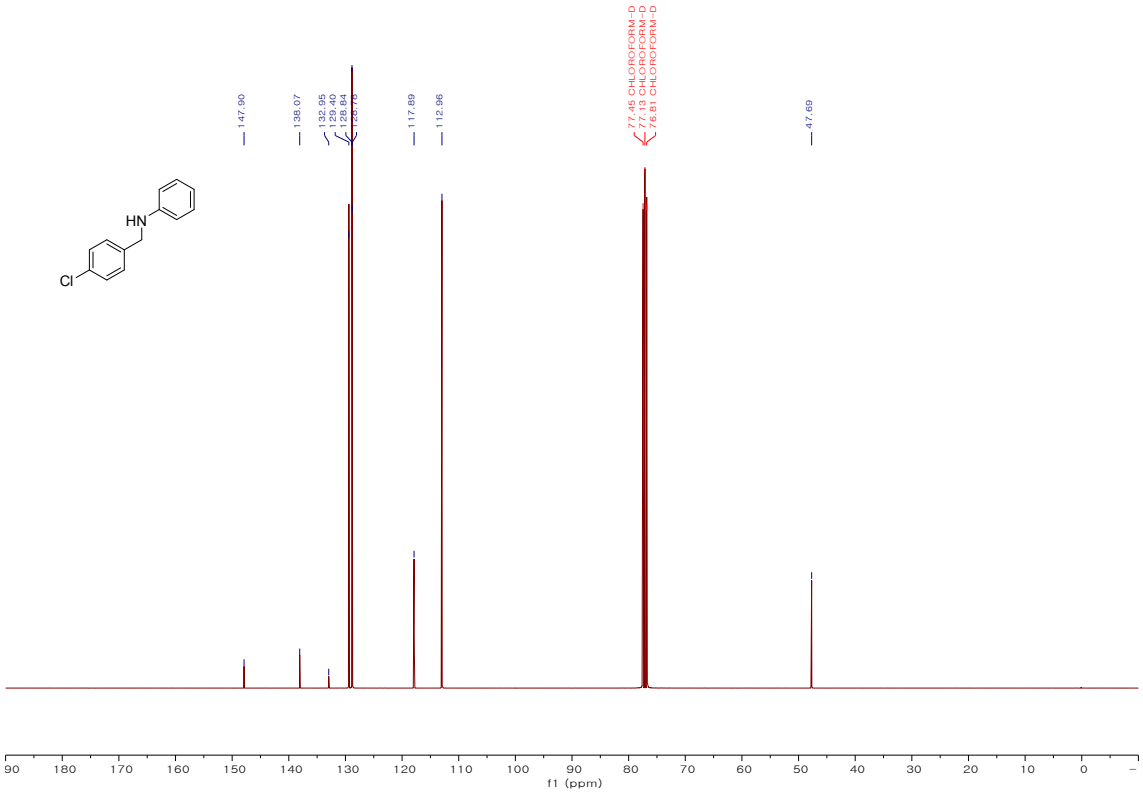


Figure S22: ^{13}C NMR of *N*-(4-chlorobenzyl)aniline (**2j**)

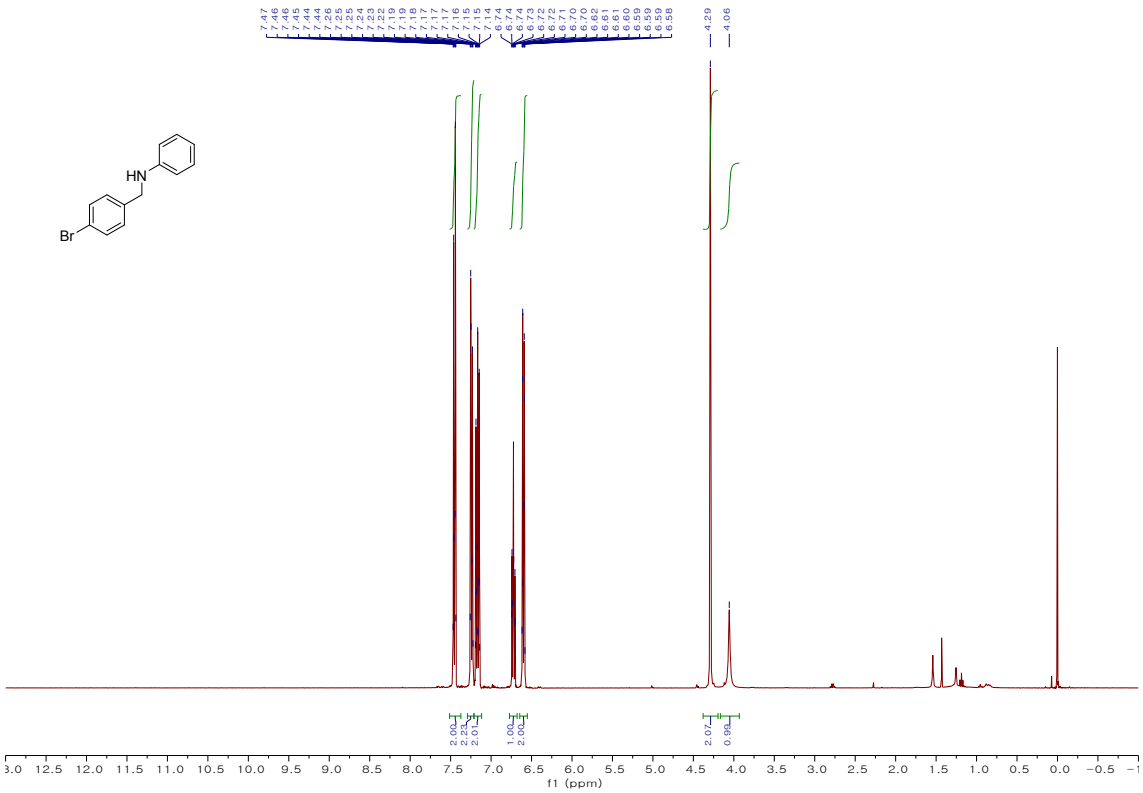


Figure S23: ^{1}H NMR of *N*-(4-bromobenzyl)aniline (**2k**)

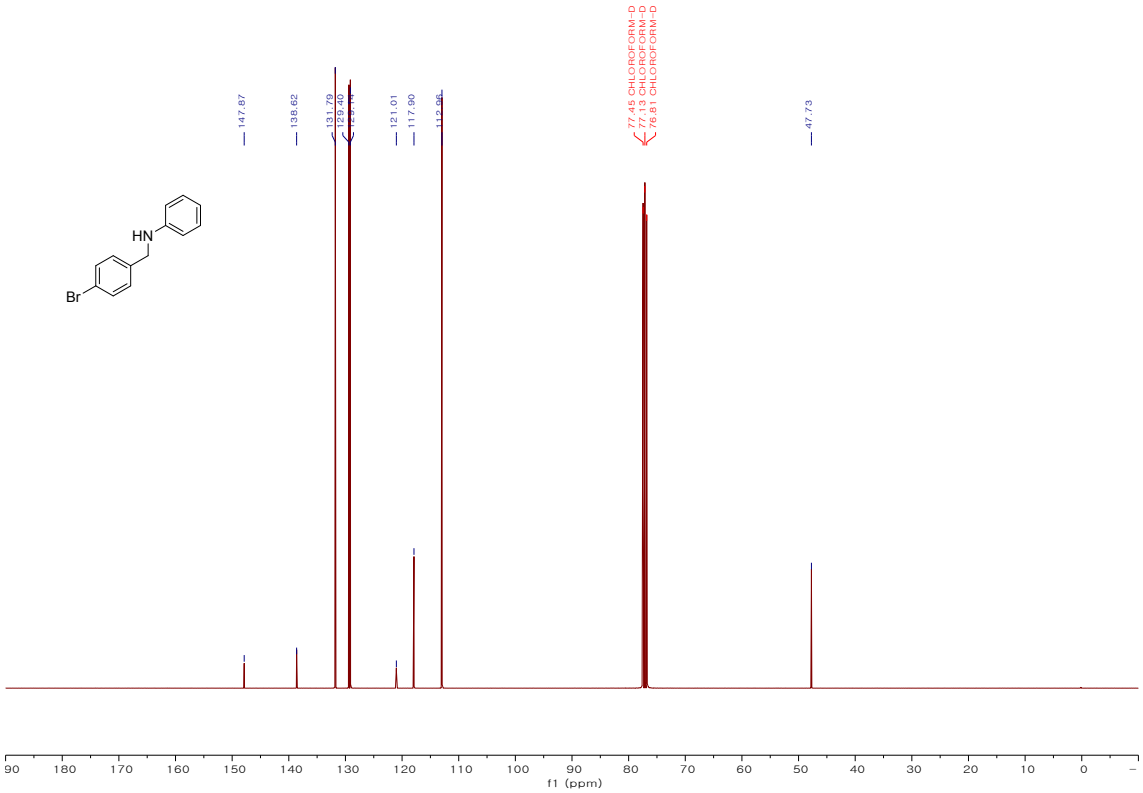


Figure S24: ^{13}C NMR of *N*-(4-bromobenzyl)aniline (**2k**)

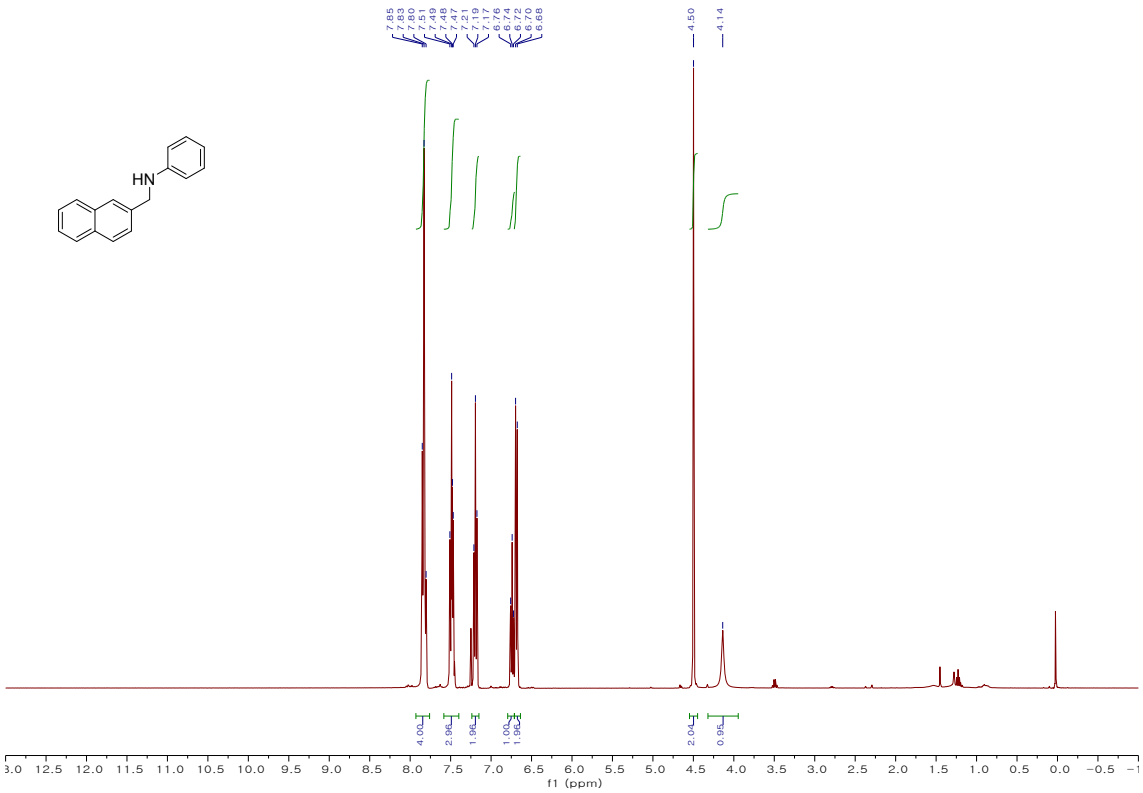


Figure S25: ^{1}H NMR of *N*-(naphthalen-2-ylmethyl)aniline (**2l**)

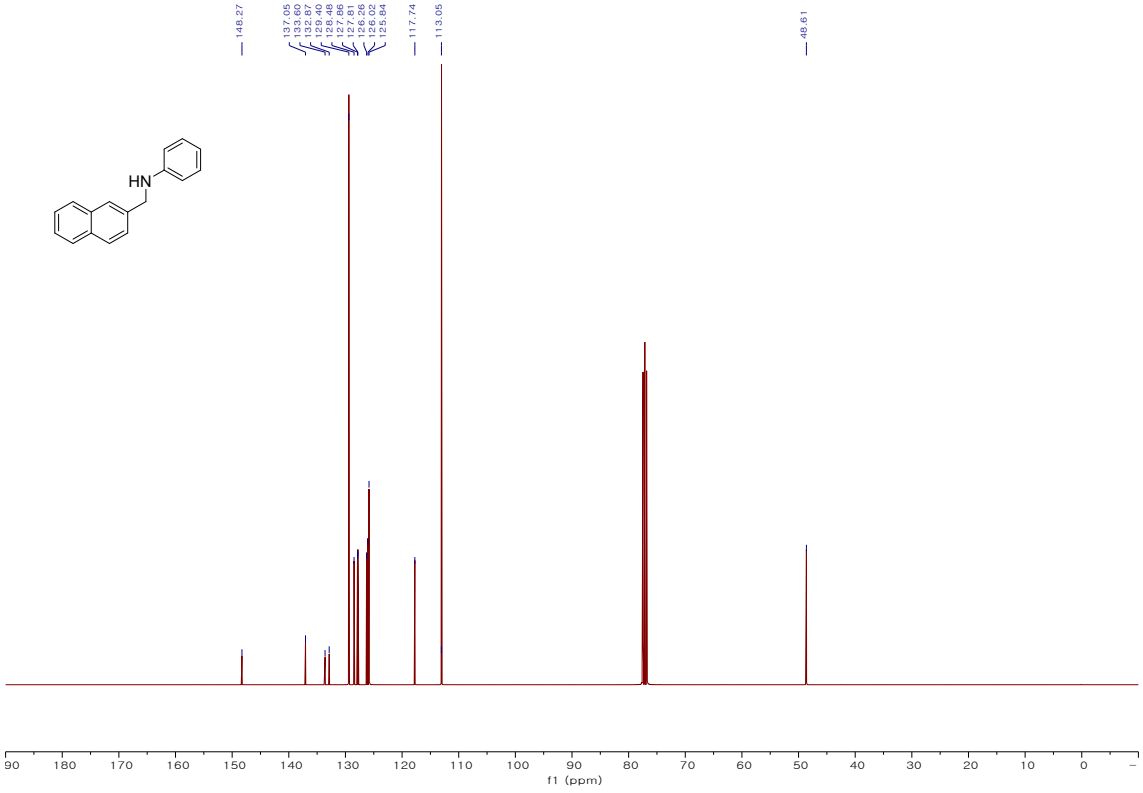


Figure S26: ^{13}C NMR of *N*-(naphthalen-2-ylmethyl)aniline (**2l**)

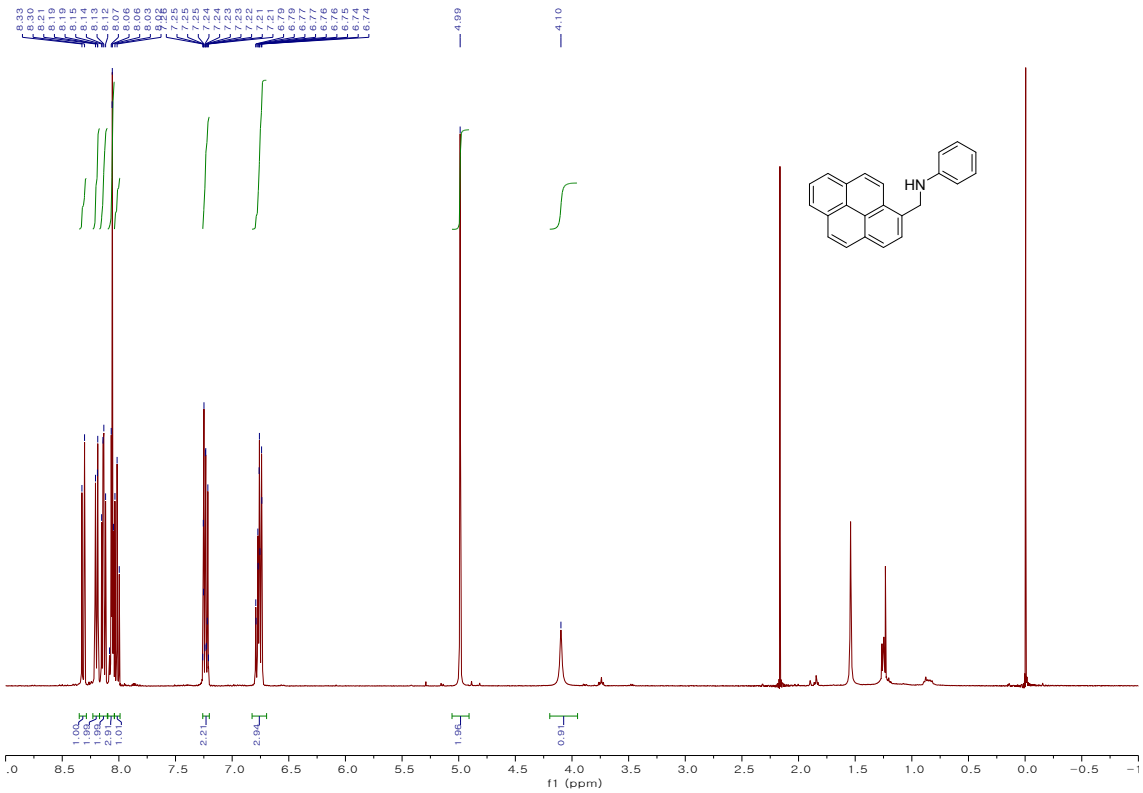


Figure S27: ^{1}H NMR of *N* -(pyren-1-ylmethyl)aniline (**2m**)

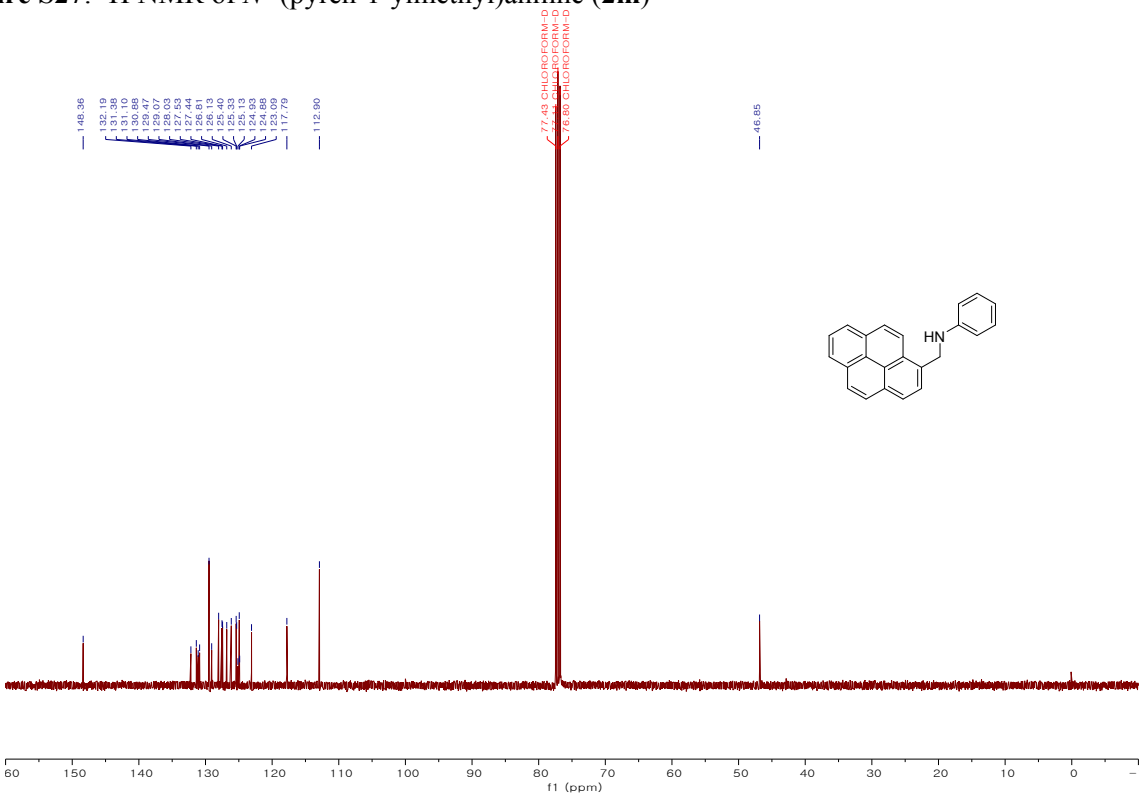


Figure S28: ^{13}C NMR of -(pyren-1-ylmethyl)aniline (**2m**)

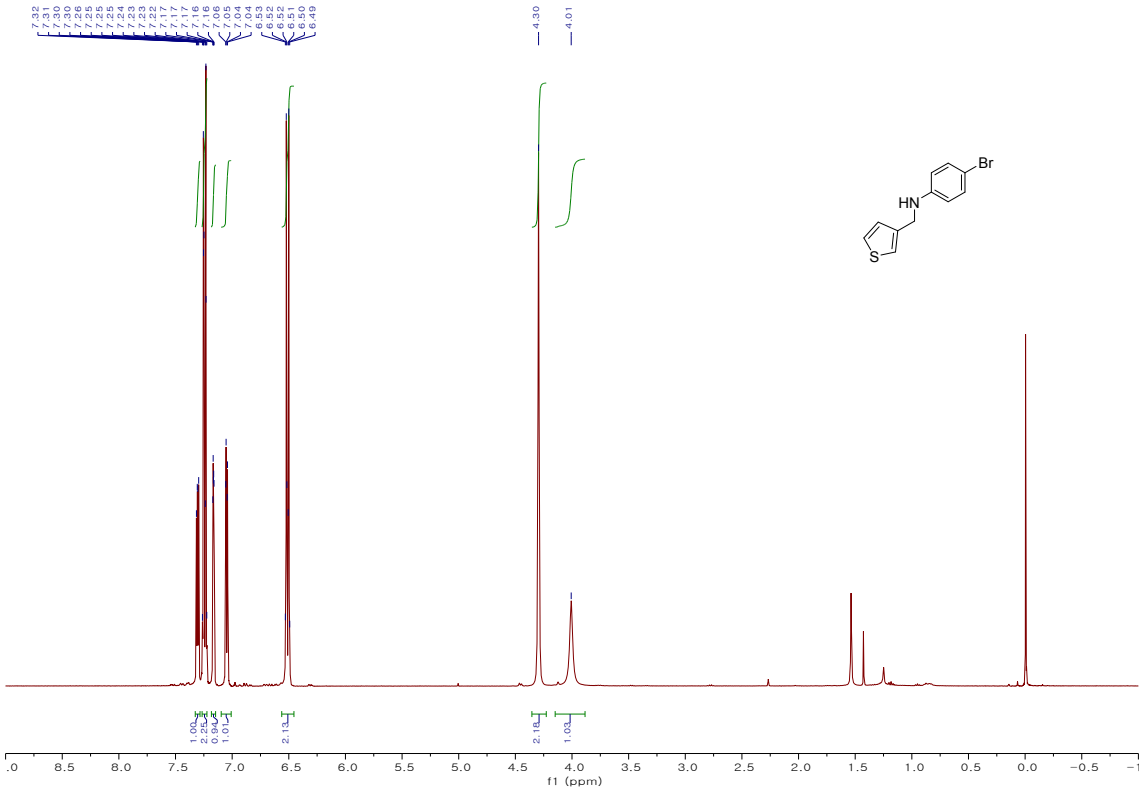


Figure S29: ^{1}H NMR of 4-bromo-*N*-(thiophen-3-ylmethyl)aniline (**2n**)

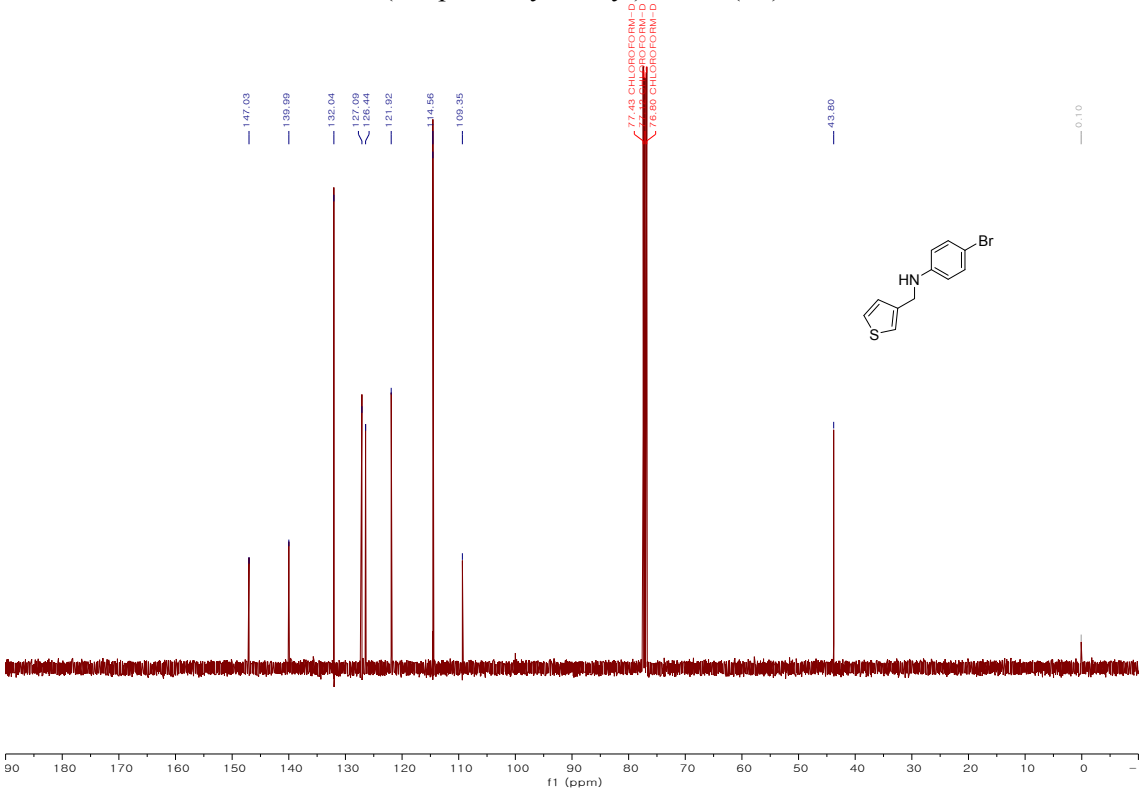
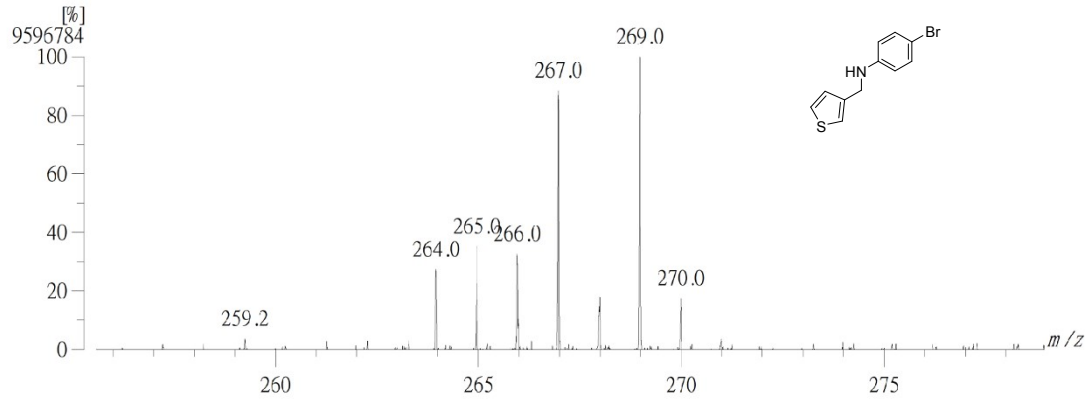


Figure S30: ^{13}C NMR of 4-bromo-*N*-(thiophen-3-ylmethyl)aniline (**2n**)

[Mass Spectrum]
Data : 2n_amine HR_re 2 Date : 24-Apr-2020 14:47
RT : 0.04 min Scan# : 2
Elements : C 11/0, H 23/0, 79Br 1/0, 81Br 1/0, N 1/0, S 1/0
Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 10mmu if m/z > 10
Unsaturation (U.S.) : -0.5 - 20.0



	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	266.9719	88.40	+0.6 / +0.2	8.0	C11 H10 79Br N S

Figure S31: HRMS of 4-bromo-*N*-(thiophen-3-ylmethyl)aniline (**2n**)

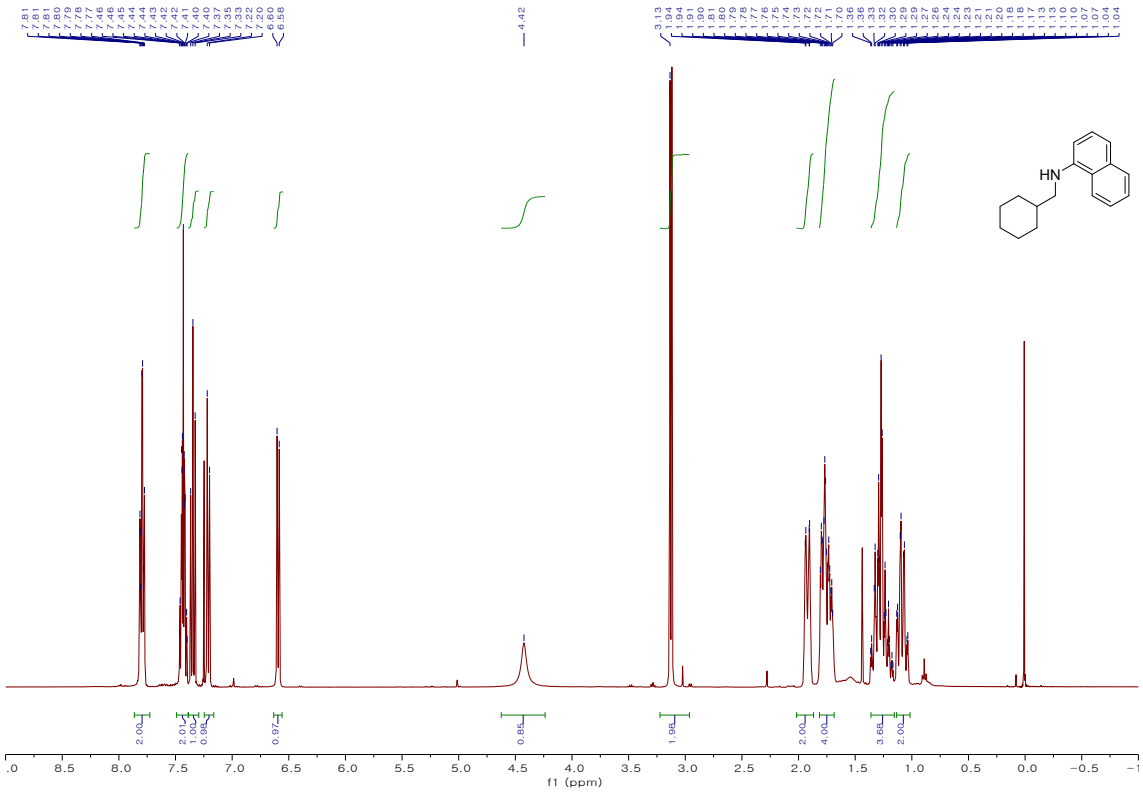


Figure S32: ^{1}H NMR of N-(cyclohexylmethyl)naphthalen-1-amine (**2o**)

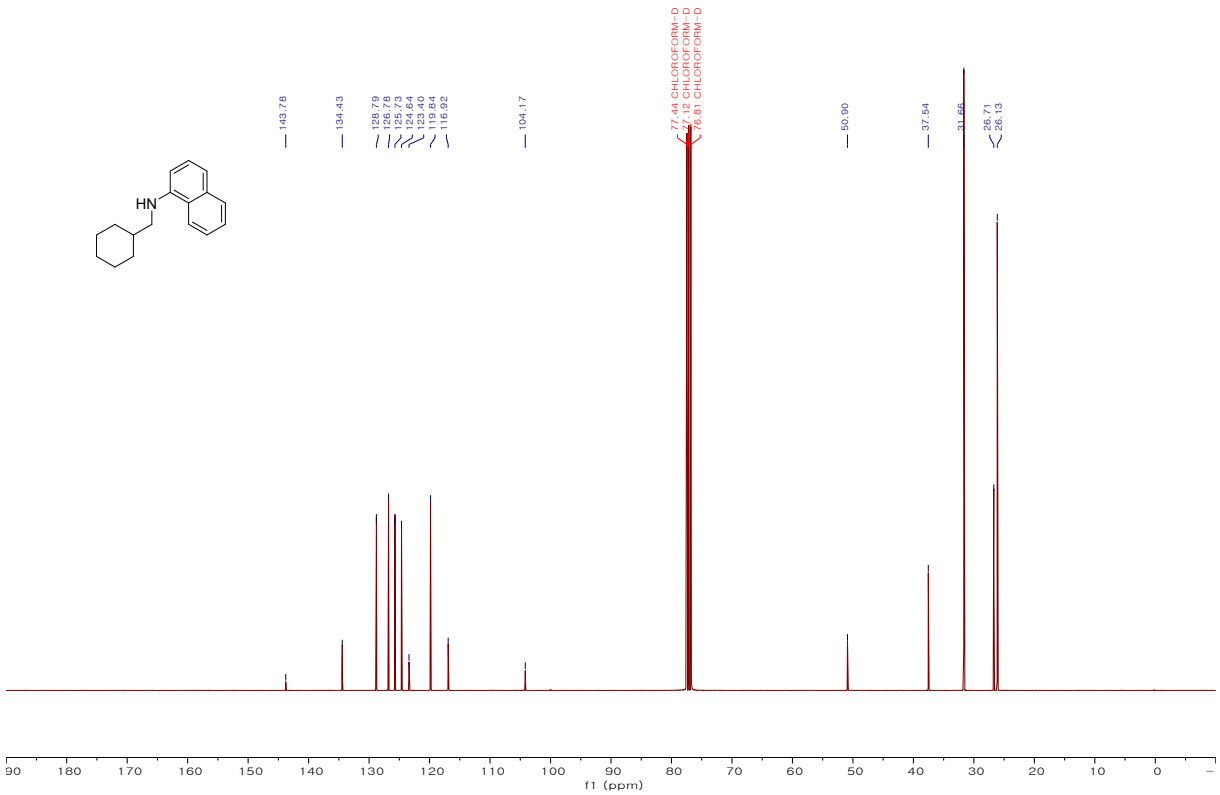


Figure S33: ^{13}C NMR of N-(cyclohexylmethyl)naphthalen-1-amine (**2o**)

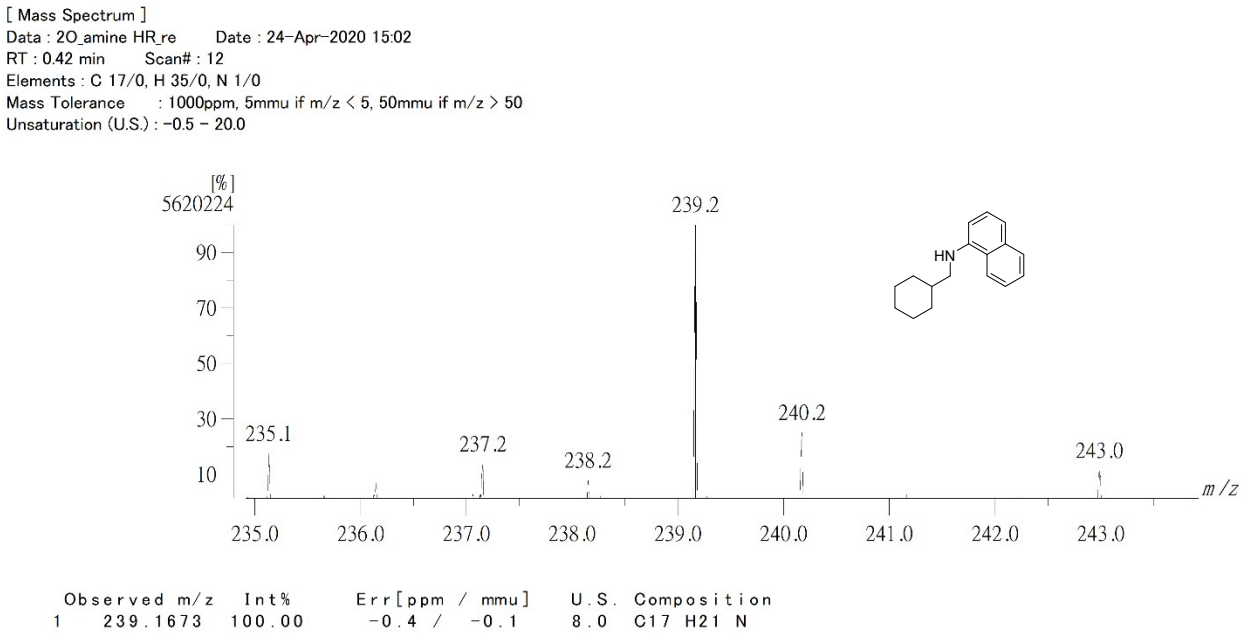


Figure S34: HRMS of N-(cyclohexylmethyl)naphthalen-1-amine (**2o**)

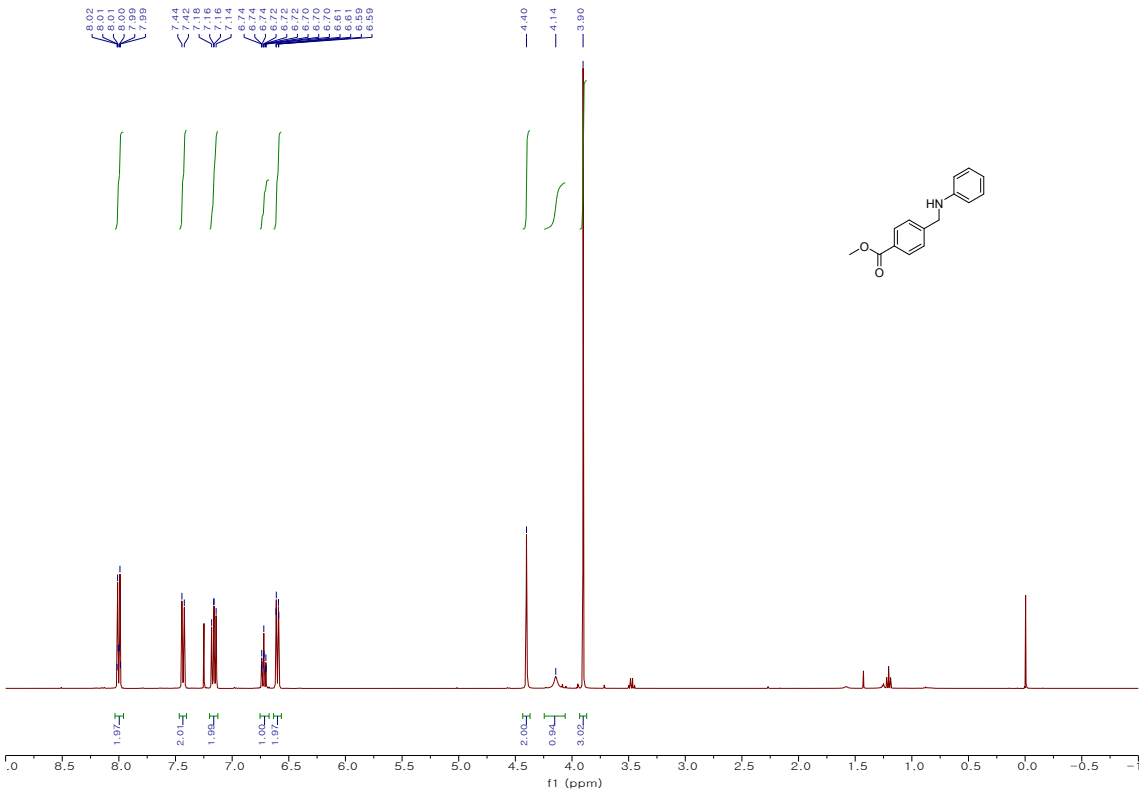


Figure S35: ^{1}H NMR of methyl 4-((phenylamino)methyl)benzoate **(4a)**

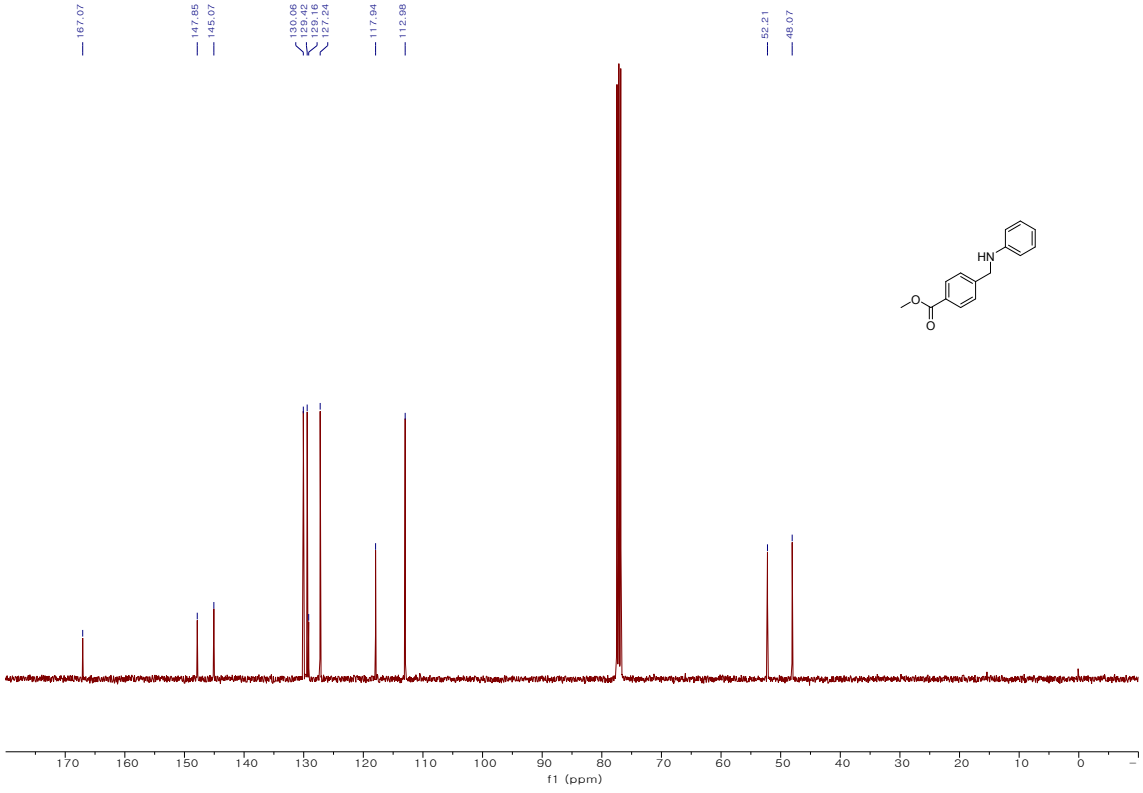


Figure S36: ^{13}C NMR of methyl 4-((phenylamino)methyl)benzoate **(4a)**

2. Computational Section

All calculation results were obtained using the density functional theory (DFT) method as implemented in the Gaussian 16 program.[S1] Geometry optimizations and energy evaluations for all the compounds were conducted 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. Intrinsic reaction coordinate (IRC) calculations were also employed to validate the transition states.

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

NaH

Atom	X	Y	Z
Na	0.000000	0.000000	0.156316
H	0.000000	0.000000	-1.719477

INT1

Atom	X	Y	Z
C	-0.120129	0.756505	-0.056771
C	-1.085577	-0.465124	-0.166154
O	-0.862246	-1.149521	1.095746
O	0.942906	0.220693	0.798288
B	0.375715	-0.812583	1.523169
H	0.944769	-1.335077	2.423631
C	0.477315	1.210392	-1.377189
H	-0.320464	1.531939	-2.054106
H	1.134695	2.070476	-1.211277
H	1.050180	0.415064	-1.861993
C	-0.723418	1.932100	0.705001
H	0.062684	2.659237	0.922199
H	-1.497868	2.425550	0.112459
H	-1.162618	1.604115	1.651393
C	-0.690111	-1.435136	-1.275836
H	-1.252038	-2.362332	-1.142193

H	-0.931133	-1.021610	-2.259040
H	0.381110	-1.666954	-1.255415
C	-2.556896	-0.098911	-0.262816
H	-2.740309	0.504773	-1.156953
H	-3.151415	-1.011939	-0.339500
H	-2.891343	0.455809	0.615133
Na	3.002179	-0.256432	-0.086662
H	3.018823	-1.353719	-1.656579

TS1

Atom	X	Y	Z
C	0.215465	-0.807039	-0.024963
C	1.015191	0.538675	-0.131992
O	0.502982	1.295157	0.978568
O	-1.002516	-0.407278	0.646013
B	-0.750202	0.835987	1.268364
H	-1.394769	1.225520	2.181091
C	-0.144041	-1.432130	-1.364559
H	0.759570	-1.693348	-1.923750
H	-0.716304	-2.351231	-1.203650
H	-0.731613	-0.744336	-1.979170
C	0.888592	-1.836268	0.879773
H	0.197215	-2.665610	1.049773
H	1.803634	-2.230621	0.429810
H	1.134457	-1.392172	1.847785
C	0.712652	1.331464	-1.401706
H	1.211088	2.300648	-1.324504
H	1.084923	0.819239	-2.293854
H	-0.360959	1.520545	-1.492714

C	2.519173	0.382255	0.042480
H	2.934309	-0.255606	-0.744704
H	2.991023	1.364694	-0.029276
H	2.768929	-0.045194	1.014612
Na	-2.993138	0.168388	-0.245450
H	-2.251893	1.950500	-0.164166

INT2

Atom	X	Y	Z
C	0.282270	0.816668	0.027985
C	0.891080	-0.619027	0.113711
O	0.354423	-1.254125	-1.021033
O	-1.040549	0.548383	-0.418343
B	-0.966074	-0.713171	-1.297182
H	-1.160307	-0.486859	-2.475258
C	0.227072	1.568170	1.351815
H	1.229757	1.697907	1.771874
H	-0.206793	2.561459	1.199436
H	-0.381024	1.033352	2.088773
C	0.985145	1.665670	-1.032715
H	0.385871	2.560761	-1.220956
H	1.984558	1.975073	-0.712420
H	1.066577	1.100192	-1.964293
C	0.439417	-1.361167	1.380599
H	0.710184	-2.414434	1.276371
H	0.904515	-0.964164	2.288369
H	-0.649926	-1.314475	1.502661
C	2.413018	-0.654753	0.028224
H	2.873065	-0.061202	0.826181

H	2.759863	-1.687240	0.124034
H	2.748690	-0.276015	-0.938329
Na	-2.859956	-0.139156	0.354081
H	-1.914144	-1.475217	-0.878132

Imine

Atom	X	Y	Z
N	-0.449161	0.524211	0.141799
C	0.386538	-0.386676	-0.164149
H	0.060848	-1.376952	-0.516496
C	-1.825557	0.229882	0.083580
C	-2.361463	-0.981079	0.537547
C	-2.684363	1.218143	-0.408922
C	-3.732648	-1.206409	0.468097
H	-1.703502	-1.725912	0.974890
C	-4.049969	0.979947	-0.491091
H	-2.254228	2.160251	-0.731811
C	-4.580101	-0.233276	-0.053749
H	-4.140420	-2.144304	0.831760
H	-4.706201	1.747670	-0.888429
H	-5.648879	-0.412039	-0.105924
C	1.840569	-0.177685	-0.082880
C	2.370049	1.038655	0.364457
C	2.703808	-1.209687	-0.457414
C	3.744798	1.212872	0.432474
H	1.682448	1.827475	0.650769
C	4.082396	-1.033682	-0.387730
H	2.290017	-2.152947	-0.805050
C	4.603281	0.177707	0.057363

H	4.153905	2.156302	0.779240
H	4.748022	-1.839135	-0.679982
H	5.678088	0.317846	0.112940

INT3

Atom	X	Y	Z
B	-0.766819	1.544533	-0.892367
H	-0.047900	0.501992	-0.977420
O	-1.105550	1.697043	0.597339
O	-2.069525	1.378213	-1.531916
C	-3.022924	1.066519	-0.546851
C	-2.511464	1.866249	0.693482
C	-2.993104	1.334385	2.038108
H	-4.085996	1.357305	2.103416
H	-2.666566	0.300662	2.195254
H	-2.592679	1.952198	2.848371
C	-2.826779	3.358487	0.571590
H	-3.890881	3.567203	0.719492
H	-2.255118	3.901680	1.329262
H	-2.524327	3.717958	-0.415163
C	-3.024239	-0.448527	-0.291211
H	-3.180220	-0.955775	-1.247162
H	-2.059625	-0.792206	0.103179
H	-3.812807	-0.758187	0.403019
C	-4.402030	1.494997	-1.037088
H	-4.699479	0.869739	-1.883658
H	-5.157502	1.390752	-0.250089
H	-4.380316	2.531813	-1.376366
C	1.703087	-1.513139	-0.536514

H	2.036991	-1.395579	-1.575061
H	-0.138854	2.491927	-1.337392
C	3.320125	0.017728	0.111771
C	3.163453	0.971583	-0.900386
C	4.479904	0.000092	0.890852
C	4.186660	1.884626	-1.142410
H	2.225988	1.026314	-1.448803
C	5.501238	0.903025	0.625184
H	4.570437	-0.735714	1.683504
C	5.357586	1.847213	-0.391447
H	4.057675	2.633781	-1.916458
H	6.409327	0.876626	1.218579
H	6.151472	2.560456	-0.585909
N	2.280209	-0.896453	0.422776
C	0.529243	-2.372731	-0.305297
C	-0.292893	-2.706042	-1.384728
C	0.199585	-2.818642	0.982692
C	-1.438861	-3.466418	-1.179586
H	-0.046541	-2.340084	-2.377154
C	-0.949532	-3.574426	1.183960
H	0.870792	-2.593849	1.807734
C	-1.770203	-3.896761	0.102770
H	-2.082148	-3.709764	-2.018289
H	-1.199318	-3.925465	2.179824
H	-2.667636	-4.485367	0.261564
Na	0.289576	0.206612	1.147765

TS2

Atom	X	Y	Z
B	0.551380	-1.089421	-1.223157
H	-0.137804	0.053936	-0.872359
O	0.321675	-2.003831	-0.077620
O	1.947657	-0.815008	-1.254484
C	2.524868	-1.255644	-0.033207
C	1.612050	-2.463335	0.346216
C	1.563688	-2.792390	1.831780
H	2.555662	-3.068688	2.202510
H	1.215945	-1.940107	2.425298
H	0.891601	-3.638828	2.003618
C	1.947722	-3.717865	-0.459959
H	2.890211	-4.167492	-0.134495
H	1.146252	-4.449078	-0.326587
H	2.019403	-3.473228	-1.522805
C	2.454804	-0.130923	1.004889
H	2.921604	0.767180	0.592313
H	1.418832	0.136324	1.245018
H	2.968169	-0.403475	1.932432
C	3.979741	-1.625773	-0.289148
H	4.545249	-0.722320	-0.531509
H	4.431293	-2.087372	0.595539
H	4.061789	-2.313687	-1.131948
C	-0.840658	1.422919	-0.605011
H	-1.157686	1.417492	-1.656894
H	0.028282	-1.370359	-2.279615
C	-2.930496	0.626469	0.036367
C	-3.065199	-0.274368	-1.042962

C	-4.018622	0.761741	0.924407
C	-4.256035	-0.978915	-1.229709
H	-2.238375	-0.434425	-1.729241
C	-5.197862	0.062844	0.721167
H	-3.908131	1.450458	1.756704
C	-5.326470	-0.814672	-0.359629
H	-4.336933	-1.664673	-2.067643
H	-6.026811	0.200911	1.408689
H	-6.249176	-1.363416	-0.513799
N	-1.743816	1.291755	0.357584
C	0.390756	2.215267	-0.339022
C	1.387914	2.287956	-1.314648
C	0.560699	2.885649	0.873725
C	2.543778	3.023813	-1.080723
H	1.266037	1.739163	-2.244255
C	1.722776	3.613550	1.110416
H	-0.233565	2.833050	1.610857
C	2.715376	3.684892	0.134781
H	3.315600	3.072949	-1.841880
H	1.850410	4.135592	2.053563
H	3.619082	4.257194	0.319306
Na	-1.106795	-0.836258	1.054393

INT4

Atom	X	Y	Z
C	1.496847	-1.803367	0.249100
C	2.840634	-1.834972	-0.547226
O	3.752149	-1.122676	0.329650
O	1.651692	-0.570358	1.030281
B	3.005113	-0.318650	1.122398
H	3.447066	0.519797	1.836523
C	0.248192	-1.713406	-0.610396
H	0.215073	-2.568561	-1.293473
H	-0.658223	-1.737359	0.002151
H	0.220639	-0.791239	-1.194359
C	1.374235	-2.934380	1.264760
H	0.512664	-2.741435	1.909016
H	1.215202	-3.892070	0.763344
H	2.269889	-3.008023	1.888496
C	2.778393	-1.035970	-1.845833
H	3.790668	-0.930550	-2.242434
H	2.157087	-1.536587	-2.592391
H	2.370952	-0.037010	-1.664112
C	3.392301	-3.227755	-0.798406
H	2.681757	-3.817068	-1.385881
H	4.325036	-3.153007	-1.361947
H	3.597706	-3.750273	0.136747
Na	-0.017880	0.874088	1.400337
N	-1.863173	0.854717	0.205657
C	-1.755335	1.877338	-0.810970
H	-1.733196	1.466264	-1.839445
H	-2.592078	2.602356	-0.794667

C	-2.896419	-0.013464	0.070961
C	-3.033986	-1.069891	1.017488
C	-3.875179	0.020054	-0.958635
C	-4.044902	-2.009531	0.934901
H	-2.315405	-1.113177	1.837428
C	-4.887229	-0.932212	-1.027063
H	-3.845510	0.807589	-1.704177
C	-4.991085	-1.958963	-0.093863
H	-4.103705	-2.793288	1.686422
H	-5.614685	-0.863701	-1.832614
H	-5.785154	-2.694570	-0.157674
C	-0.454144	2.605567	-0.559405
C	-0.355014	3.522569	0.495486
C	0.717607	2.235627	-1.226669
C	0.882048	4.039197	0.883412
H	-1.262443	3.814464	1.018778
C	1.958166	2.750045	-0.845721
H	0.647891	1.529674	-2.051414
C	2.044515	3.645963	0.218444
H	0.939273	4.753718	1.699061
H	2.856907	2.452461	-1.378876
H	3.007304	4.046430	0.518566

TS3

Atom	X	Y	Z
C	-3.072605	-1.066108	-0.033228
C	-2.777875	0.452390	-0.256662
O	-1.685833	0.411792	-1.191289
O	-1.762327	-1.660479	-0.217419
B	-1.023095	-0.766945	-1.022224
H	-0.104197	-1.103574	-1.684284
C	-3.587829	-1.419536	1.353196
H	-4.545092	-0.925603	1.544651
H	-3.749591	-2.499669	1.426450
H	-2.890739	-1.105505	2.135615
C	-3.981799	-1.659320	-1.106124
H	-3.981184	-2.748307	-1.013730
H	-5.008986	-1.300000	-1.001958
H	-3.617808	-1.398610	-2.103347
C	-2.269163	1.148209	1.001791
H	-1.837004	2.111580	0.719109
H	-3.072886	1.312083	1.725936
H	-1.474298	0.558069	1.464989
C	-3.923829	1.235253	-0.876885
H	-4.808067	1.201542	-0.232157
H	-3.622880	2.278885	-0.992528
H	-4.186251	0.844632	-1.861141
Na	-0.307451	-2.321052	1.373479
N	0.892845	-0.556449	0.831624
C	1.167055	0.687499	1.512475
H	0.376736	0.868119	2.254752
H	2.097985	0.637246	2.105216

C	1.975278	-1.190230	0.283579
C	3.309522	-0.692730	0.272053
C	1.807386	-2.469745	-0.331099
C	4.364888	-1.445443	-0.222085
H	3.509658	0.307617	0.638920
C	2.875028	-3.210172	-0.821483
H	0.802170	-2.857438	-0.511335
C	4.176013	-2.719611	-0.757796
H	5.363901	-1.017435	-0.197263
H	2.679514	-4.176867	-1.278819
H	5.010440	-3.295616	-1.140985
C	1.233998	1.937808	0.643533
C	1.268013	1.867315	-0.747872
C	1.245641	3.196948	1.252170
C	1.314726	3.030892	-1.514207
H	1.257266	0.893125	-1.225914
C	1.289285	4.359776	0.491336
H	1.215681	3.261479	2.338544
C	1.323962	4.279061	-0.900158
H	1.341057	2.958700	-2.597196
H	1.294135	5.328981	0.981254
H	1.357074	5.183961	-1.498858

INT5

Atom	X	Y	Z
C	-3.066049	0.100624	0.334306
C	-2.743307	-1.356576	-0.135527
O	-1.359607	-1.268350	-0.443646
B	-1.153127	0.110125	-1.060421
C	-4.520461	0.512214	0.122072
H	-5.205857	-0.150772	0.661853
H	-4.669451	1.531776	0.487621
H	-4.770786	0.496220	-0.939230
C	-2.702557	0.346431	1.806946
H	-2.794190	1.415569	2.014655
H	-3.350868	-0.199903	2.498959
H	-1.661000	0.076194	2.024541
C	-3.507754	-1.734096	-1.407260
H	-3.081879	-2.658531	-1.806520
H	-4.571697	-1.894173	-1.209635
H	-3.398549	-0.953010	-2.162958
C	-2.957210	-2.429562	0.925675
H	-4.002062	-2.458104	1.251154
H	-2.700212	-3.411046	0.516838
H	-2.339474	-2.253813	1.814138
O	-2.235813	0.896558	-0.481422
H	-1.197373	0.077558	-2.280065
N	0.343136	0.506945	-0.642561
C	1.262040	-0.324500	-1.424490
H	0.657218	-1.041982	-1.987604
H	1.796020	0.266941	-2.181445
C	0.768244	1.827433	-0.390811

C	-0.103863	2.760117	0.210211
C	2.079421	2.265053	-0.662683
C	0.319242	4.046962	0.506873
H	-1.124867	2.462945	0.404214
C	2.491435	3.560340	-0.354171
H	2.807794	1.592807	-1.102005
C	1.620761	4.467131	0.232937
H	-0.387399	4.736850	0.959633
H	3.513014	3.851696	-0.580755
H	1.943532	5.474604	0.471896
C	2.264116	-1.124095	-0.599860
C	2.649953	-2.399125	-1.029793
C	2.782448	-0.651334	0.616504
C	3.530042	-3.175670	-0.281194
H	2.245340	-2.785633	-1.961655
C	3.657341	-1.433758	1.373385
H	2.514578	0.347019	0.957209
C	4.034661	-2.697191	0.926482
H	3.813469	-4.161538	-0.635791
H	4.055211	-1.044268	2.305527
H	4.717633	-3.303207	1.512447
Na	0.197079	-1.136497	1.049995

Pd

Atom	X	Y	Z
C	2.862130	0.156750	-0.701024
C	2.881412	-0.878644	0.468215
O	1.488180	-0.949644	0.828221
O	1.768981	1.020434	-0.323079
B	0.921031	0.248456	0.442622
C	4.123863	0.991503	-0.839416
H	4.988780	0.348727	-1.031552
H	4.015846	1.681017	-1.680221
H	4.311900	1.577077	0.061735
C	2.486322	-0.479570	-2.038050
H	2.268385	0.314881	-2.755432
H	3.299251	-1.095734	-2.431863
H	1.593650	-1.104035	-1.931897
C	3.640767	-0.367588	1.691020
H	3.431695	-1.028171	2.535623
H	4.720004	-0.354483	1.515889
H	3.316104	0.643038	1.955406
C	3.361919	-2.267653	0.081837
H	4.387351	-2.226657	-0.299117
H	3.348662	-2.916875	0.960714
H	2.717633	-2.710499	-0.678841
N	-0.416803	0.575872	0.804042
C	-1.183271	-0.468305	1.471352
H	-1.930508	0.001991	2.120922
H	-0.496862	-1.022775	2.117344
C	-1.091287	1.750061	0.396367
C	-0.377240	2.937074	0.177729

C	-2.482477	1.762933	0.232429
C	-1.040794	4.093422	-0.209615
H	0.696870	2.945130	0.314986
C	-3.136649	2.932899	-0.143841
H	-3.057634	0.854851	0.375134
C	-2.424661	4.104485	-0.370953
H	-0.467542	5.000766	-0.373159
H	-4.215143	2.917360	-0.266528
H	-2.937891	5.013093	-0.666845
C	-1.865358	-1.459024	0.540948
C	-2.660035	-2.466906	1.093051
C	-1.710681	-1.405414	-0.842946
C	-3.282572	-3.406775	0.279948
H	-2.787249	-2.515022	2.172324
C	-2.335203	-2.345860	-1.660541
H	-1.113462	-0.611598	-1.283363
C	-3.120135	-3.349538	-1.103240
H	-3.895453	-4.184721	0.724340
H	-2.209499	-2.288916	-2.737265
H	-3.606013	-4.081246	-1.740485

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