Organic superbase *t*-Bu-P4 catalyzed demethylations of methoxyarenes

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Supporting Information

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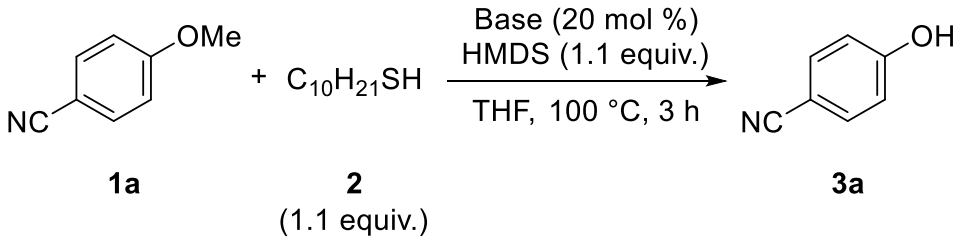
General methods. All reactions were carried out under N_2 or Ar atmosphere. Flash column chromatography was performed with Kanto silica gel 60 N (spherical, neutral, 40–50 μm). Preparative thin-layer chromatography was performed with silica gel (Wakogel® B-5F). Melting points (Mp) were determined with a Yazawa micro melting point apparatus without correction. Infrared (IR) data were recorded on a SHIMADZU SensIR ATR (Attenuated Total Reflectance) FT-IR or JASCO FT/IR-400 spectrophotometer, and absorbance frequencies are reported in reciprocal centimeters (cm^{-1}). NMR data were recorded on a JEOL AL400 spectrometer (395.75 MHz for ^1H, 99.50 MHz for ^{13}C), a Varian Mercury (399.17 MHz for ^1H, 100.38 MHz for ^{13}C), or a JEOL ECA600 spectrometer (597.17 MHz for ^1H, 150.91 MHz for ^{13}C). Chemical shifts are expressed in δ (parts per million, ppm) values, and coupling constants are expressed in herts (Hz). ^1H NMR spectra were referenced to tetramethylsilane as an internal standard or to a solvent signal ($CDCl_3$: 7.26 ppm, DMSO-d_6: 2.49 ppm). ^{13}C NMR spectra were referenced to a solvent signal ($CDCl_3$: 77.0 ppm, DMSO-d_6: 39.5 ppm). Low and high resolution mass spectra (LRMS and HRMS) were obtained from Mass Spectrometry Resource, Graduate School of Pharmaceutical Sciences, Tohoku University, on a JEOL JMS-DX 303 and JMS-700/JMS-T 100 GC spectrometer, respectively.

Table S1. Effects of organic or inorganic bases.[a]

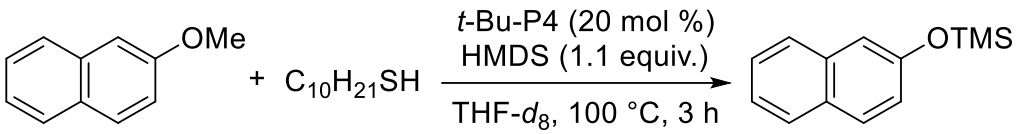


1a **2** (1.1 equiv.) **3a**

Entry	Base	**3a** (%)[b]
1	NEt_3	0
2	*i*-Pr_2NEt	0
3	Pyridine	0
4	Proton sponge[c]	0
5	DBU[d]	0
6	TBD[e]	0
7	*t*-Bu-P2[f]	(67)[g]
8	NaO-*t*-Bu	0
9	KO-*t*-Bu	0
10	NaH	0
11	$LiN(TMS)_2$	(3)[g]
12	$NaN(TMS)_2$	0
13	$KN(TMS)_2$	0

[a]Reaction conditions: Unless otherwise noted, the reactions were conducted with **1a** (0.20 mmol), **2** (0.22 mmol), base (0.04 mmol), HMDS (0.22 mmol), and THF (0.3 mL) at 100 °C for 3 h. The reactions were quenched with K_2CO_3 (1.0 mmol) and MeOH (1 mL). [b]The yields were determined by ^{1}H-NMR using 1,1,2-trichloroethane as an internal standard. [c]Proton sponge: 1,8-bis-(dimethylamino)naphthalene. [d]DBU: 1,8-diazabicyclo[5.4.0]-7-undecene. [e]TBD: 1,5,7-triazabicyclo-[4.4.0]dec-5-ene. [f]*t*-Bu-P2: 1-(*tert*-butylimino)-1,1,3,3,3-pentakis(dimethylamino)-1λ5, 3λ5-diphosphazene. [g]Yield in parentheses denotes the isolated yield of **3a**.

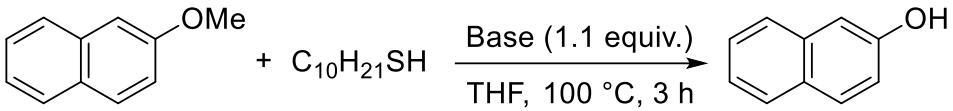
Scheme S1. Reaction of **4a** conducted in THF-d_8[a]



4a **2** (1.1 equiv.) **7a**, quant.[b]

[a]Reaction was conducted on a 0.2 mmol scale. [b]The yield was determined by ^{1}H-NMR using 1,1,2-trichloroethane as an internal standard.

Scheme S2. Reactions of **4a** with a stoichiometric amount of *t*-Bu-P4 or TBD in the absence of HMDS[a]



4a **2** (1.1 equiv.) **5a**

Base:	Yield (%):
t-Bu-P4	80[b]
TBD	0[c]

[a]Reactions were conducted on a 0.2 mmol scale. [b]Isolated yield. [c]The yield was determined by ^{1}H-NMR using 1,1,2-trichloroethane as an internal standard.

Figure S1. Transition states for the TBD-mediated demethylation reaction of anisole with methanethiol calculated at the CPCM(toluene)/ONIOM(B97D/6-311+G(2d,p):B97D/6-311G(d,p)) level of theory. (a) **TS-2a** involves the hydrogen bonding between $[TBD]^+H$ and the anisole oxygen atom. (b) **TS-2b** involves the hydrogen bonding between $[TBD]^+H$ and the methanethiolate sulfur atom.

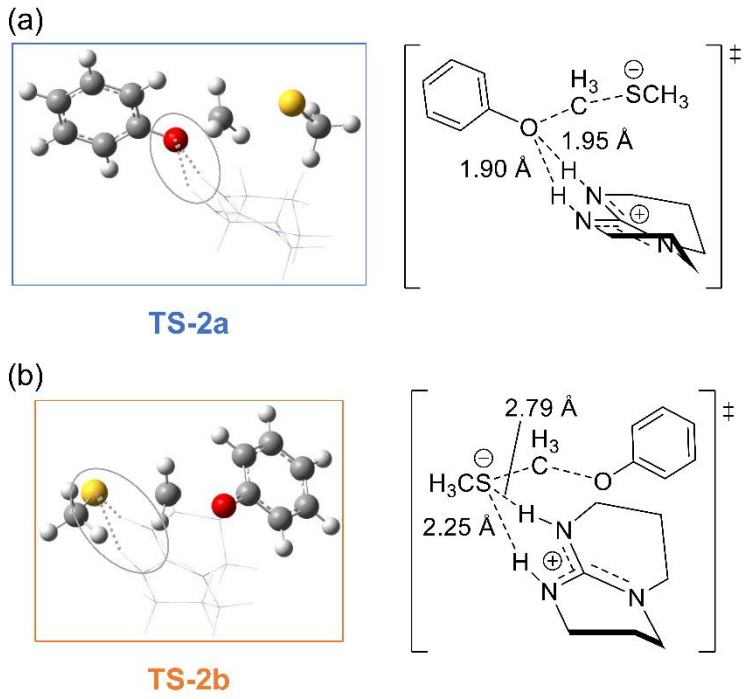


Figure S2. Energy profile of the TBD-mediated demethylation reaction of anisole with methanethiol calculated at the CPCM(toluene)/ONIOM(B97D/6-311+G(2d,p):B97D/6-311G(d,p)) level of theory. Energies are reported in kcal/mol.

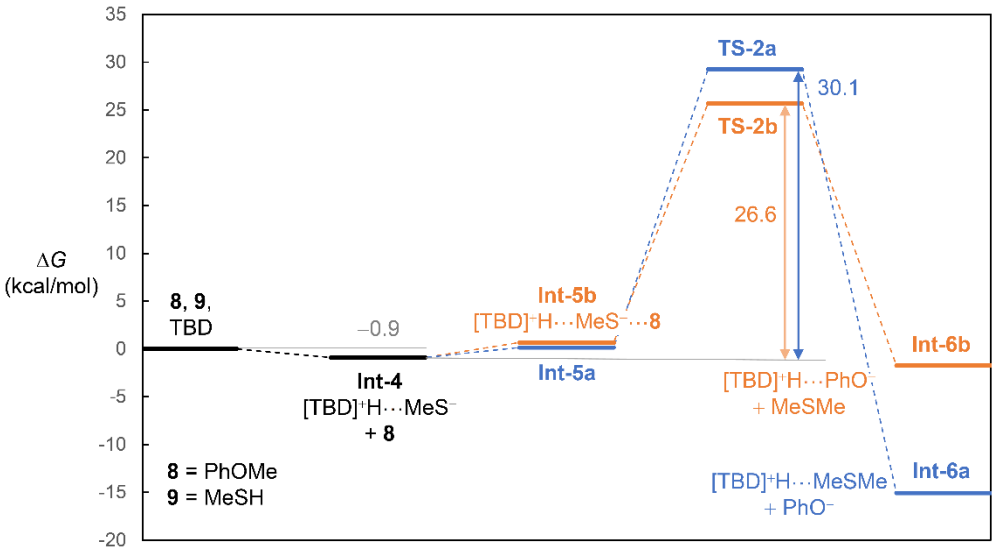


Figure S3. Noncovalent interaction analysis of the transition states (a) **TS-1a** and (b) **TS-1b**. A red surface indicates strong repulsive interactions, while green and blue surfaces show weak and strong attractive interactions, respectively.

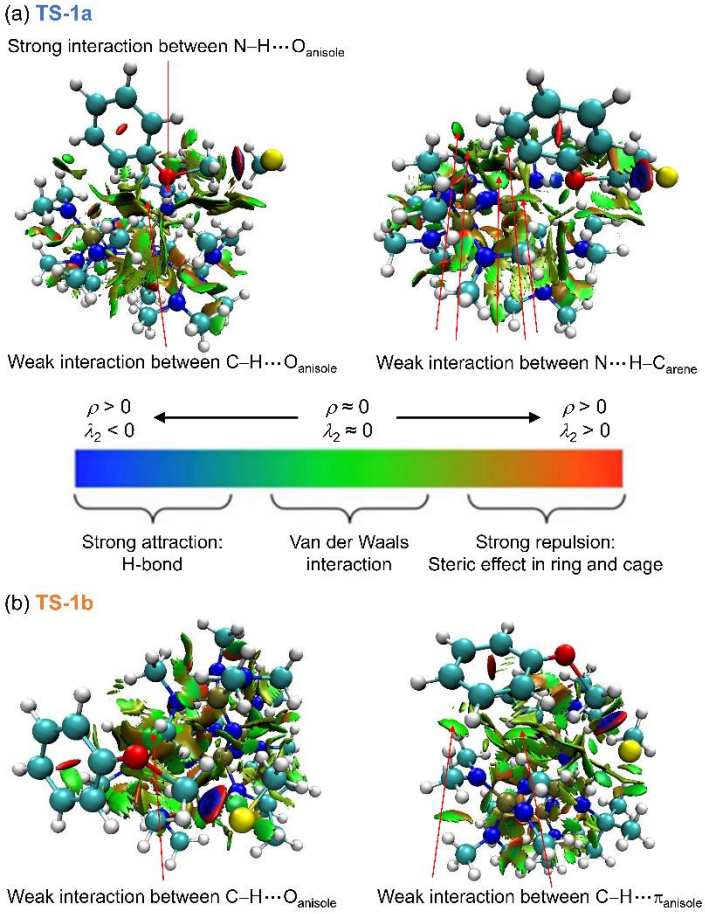


Figure S4. Noncovalent interaction analysis of the transition states (a) **TS-2a** and (b) **TS-2b**. A red surface indicates strong repulsive interactions, while green and blue surfaces show weak and strong attractive interactions, respectively.

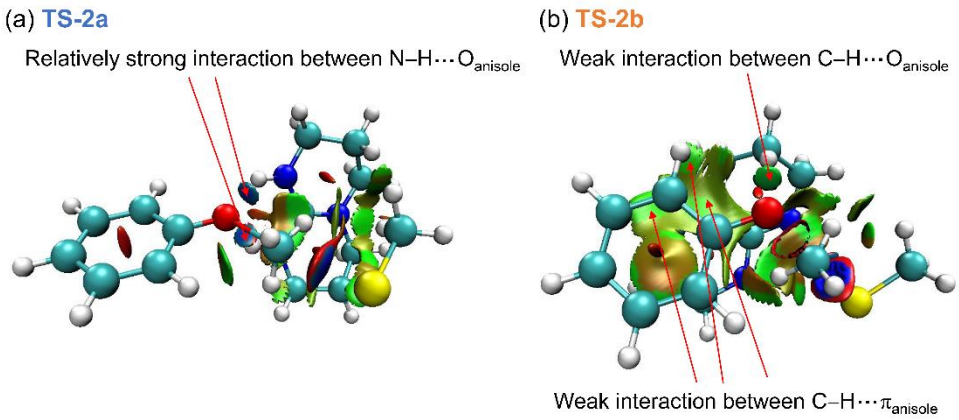


Figure S5. Molecular states of (a) **Int-2a**, (b) **Int-5b**, and (c) **8** calculated at the CPCM(toluene)/ONIOM(B97D/6-311+G(2d,p):B97D/6-311G(d,p)) level of theory. (a) **Int-2a** involves the hydrogen bonding between [*t*-Bu-P4]$^{+}$H and the anisole oxygen atom. (b) **Int-5b** involves the hydrogen bonding between [TBD]$^{+}$H and the methanethiolate sulfur atom. The natural charges of the methoxy methyl carbons calculated at the B97D/6-311+G(2d,p) level of theory are included. The σ^*_{O-C} orbitals (**Int-2a**: LUMO+24; **Int-5b**: LUMO+11; **8**: LUMO+5) and their energies are also noted.

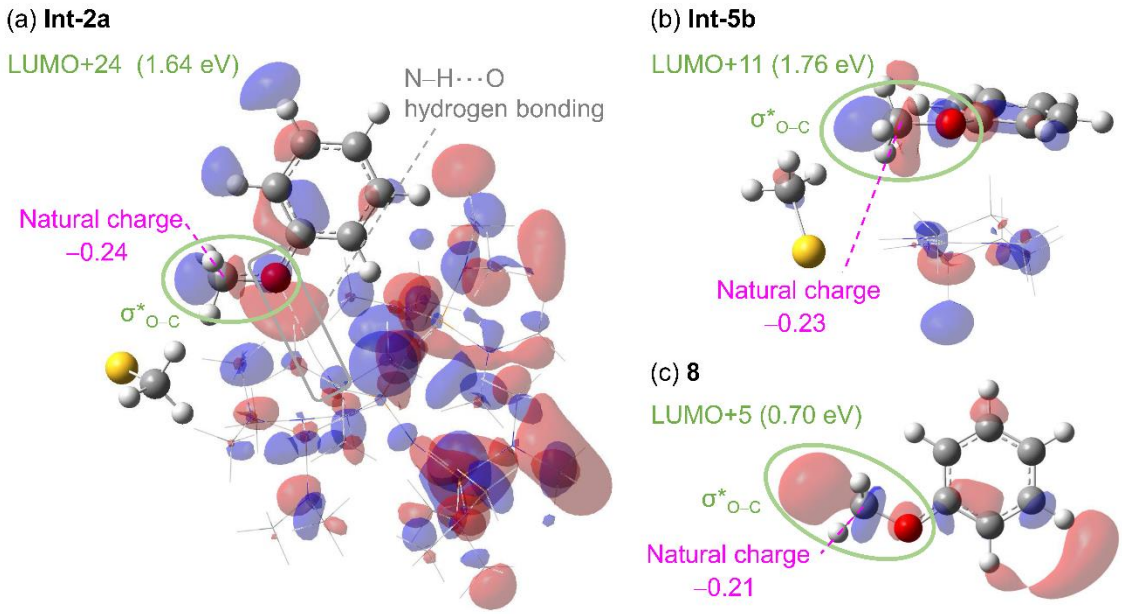
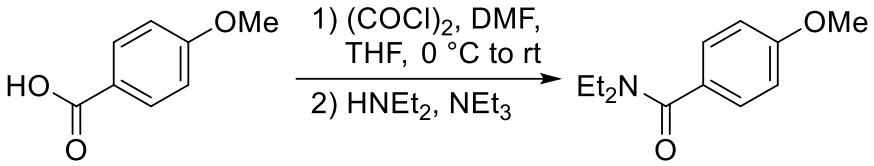


Table S2. NEDA results for **Int-1** ([*t*-Bu-P4]$^{+}$H···MeS^{-}) and **Int-4** ([TBD]$^{+}$H···MeS^{-}) (kcal/mol)

	Int-1	**Int-4**
Electrical (ES+POL+SE)	–108.079	–122.200
Charge Transfer (CT)	–54.918	–83.678
Core (XC+DEF-SE)	81.966	97.469
Total Interaction (E)	–81.031	–108.408

Materials. Unless otherwise noted, materials were purchased from Tokyo Kasei Co., Aldrich Inc. and other commercial suppliers and were used as received. **1g**,[1] **1o**,[2] **4d**,[3] **4e**,[4] **4f**,[5] **4i**,[6] **4j**,[7] **4k**,[8] **4l**,[9] **4o**,[10] **4q**,[11] **4s,**[12] and **4t**[13] were prepared according to the literature procedures. **1k** and **1m** were prepared according to the following Schemes S3 and S4, respectively.

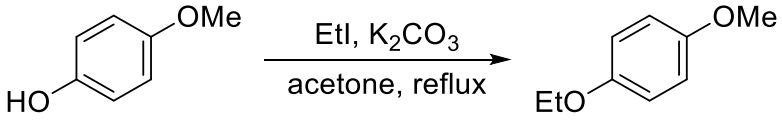
Scheme S3. Preparation of **1k**



S1 **1k**

***N*,*N*-Diethyl-4-methoxybenzamide (1k)**. To a solution of **S1** (304.2 mg, 2.00 mmol) and DMF (1 drop) in THF (4 mL) was added $(COCl)_2$ (317.3 mg, 2.50 mmol) at 0 °C. After stirring at room temperature for 4 h, the mixture was evaporated under reduced pressure. To the residue were added THF (4 mL), triethylamine (607.1 mg, 6.00 mmol), and diethylamine (143.3 mg, 1.96 mmol) at 0 °C. After stirring at room temperature overnight, the mixture was evaporated under reduced pressure. To the residue was added H_2O, and the organic materials were extracted with AcOEt. The combined organic layer was washed with brine, dried over Na_2SO_4, and concentrated. The residue was purified by column chromatography on silica gel (hexane:AcOEt =1:1) to give **1k** (402.4 mg, 1.94 mmol, 97%) as a white solid: Mp 37 °C (Hexane) (lit. 40–40.5 °C[14]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.35 (d, 2H, J = 8.8 Hz), 6.90 (d, 2H, J = 8.8 Hz), 3.83 (s, 3H), 3.41 (br s, 4H), 1.18 (br s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.9, 160.0, 129.2, 127.9, 113.3, 55.0, 43.1, 39.1, 13.6, 12.8. LRMS (EI) *m/z*: 207 (M^+). HRMS m/z: (M^+) Calcd. for $C_{12}H_{17}NO_2$: 207.1259, found: 207.1268. IR (KBr): 2988, 1608, 1468, 1428, 1284, 1248, 1092, 1022, 842, 763 cm^{-1}. The spectra data matched those reported in the literature.[15]

Scheme S4. Preparation of **4m**

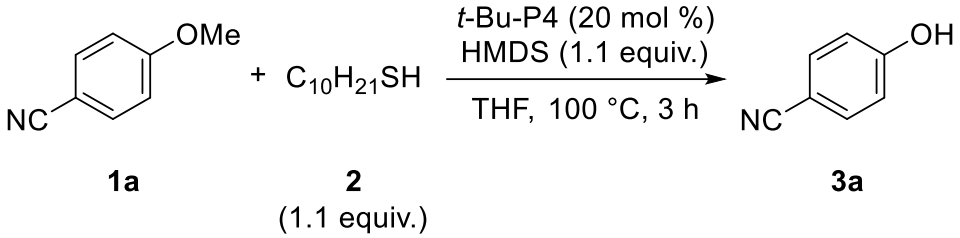


S2 **4m**

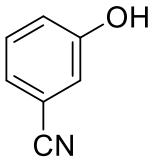
1-Ethoxy-4-methoxybenzene (4m). To a solution of **S2** (499.9 mg, 4.03 mmol) and K_2CO_3 (967.1 mg, 7.00 mmol) in acetone (14 mL) was added iodoethane (0.83 mL, 10.3 mmol). The resulting mixture was refluxed for 24 h. The mixture was cooled to room temperature, and the solvent was removed in vacuo. To the residue was added H_2O, and the organic materials were extracted with AcOEt. The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated. The residue was purified by column chromatography on silica gel (hexane:AcOEt = 20:1) to give **4m**

(455.6mg, 2.99 mmol, 74%) as a white solid: Mp 34 °C (H_2O/MeOH) (lit. 36–38 °C[16]): ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 6.83 (s, 4H), 3.98 (q, 2H, J = 7.0 Hz), 3.77 (s, 3H), 1.39 (t, 3H, J = 7.1 Hz). ^{13}C NMR (100 MHz, $CDCl_3$/TMS) δ 153.7, 153.1, 115.4, 114.6, 64.0, 55.7, 14.9. LRMS (EI) *m/z*: 152 (M^+). HRMS Calcd. for $C_9H_{12}O_2$: 152.0837, found: 152.0826. IR (neat): 2983, 2927, 2853, 1507, 1289, 1231, 1116, 1047, 822, 730 cm^{-1}. The spectra data matched those reported in the literature.[16]

General procedure of *t*-Bu-P4-catalyzed demethylations of methoxyarenes (Table 1, Entry 8).

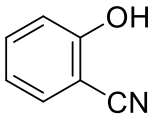


4-Hydroxybenzonitrile (3a). In a glove box under an Ar atmosphere, to a solution of **1a** (26.8 mg, 0.201 mmol) in THF (0.3 mL) were added *t*-Bu-P4 solution (50 μL, 0.8 M in hexane, 0.04 mmol) and HMDS (36.6 mg, 0.227 mmol) in an oven-dried vial equipped with a stirrer bar. The vial was sealed with a cap containing an inner Teflon film, and taken outside the glove box. **2** (45.7 μL, 0.220 mmol) was added to the mixture under a nitrogen atmosphere. The resulting mixture was stirred at 100 °C in a heat block for 3 h. K_2CO_3 (138.5 mg, 1.00 mmol) and MeOH were added to the mixture at 0 °C. After stirring at room temperature for 30 minutes, saturated NH_4Cl aqueous solution (1 mL) was added at 0 °C. The mixture was extracted with AcOEt (10 mL x 3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, and concentrated. The crude material was purified by column chromatography on silica gel (hexane:AcOEt = 3:1) to afford **3a** (21.8 mg, 0.183 mmol, 91%) as a white solid: Mp 109 °C (hexane/CH_2Cl_2) (lit. 109–111 °C[17]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.56 (d, 2H, J = 8.8 Hz), 6.90 (d, 2H, J = 8.8 Hz), 5.35 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 134.3, 119.2, 116.5, 103.1. LRMS (EI) *m/z*: 119 (M^+). HRMS Calcd. for C_7H_5NO: 119.0371, found: 119.0372. IR (neat): 3275, 2233, 1611, 1587, 1509, 1440, 1283, 1221, 1166 cm^{-1}. The spectra data matched those reported in the literature.[17]

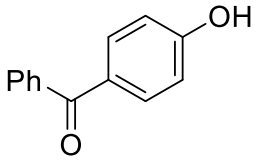


3-Hydroxybenzonitrile (3b). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by preparative thin-layer chromatography of silica gel (toluene:AcOEt = 3:1), **3b** (20.8 mg, 0.175 mmol, 87%) was obtained from **1b** (26.6 mg, 0.200 mmol) as a white solid: Mp 76 °C (hexane/CH_2Cl_2) (lit. 74.8–77.2 °C[18]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.35 (t, 1H, J = 8.1 Hz), 7.26-7.22 (m, 1H), 7.14-7.06 (m, 2H), 5.43 (s, 1H). ^{13}C NMR (100 MHz,

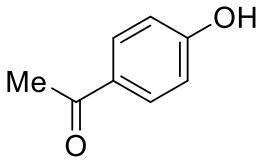
$CDCl_3$) δ 156.2, 130.6, 124.5, 120.8, 118.8, 118.6, 112.8. LRMS (EI) *m/z*: 119 (M^+). HRMS Calcd. for C_7H_5NO: 119.0371, found: 119.0372. IR (neat): 3294, 2245, 1583, 1479, 1289, 1233, 1135, 936, 868, 782 cm^{-1}. The spectra data matched those reported in the literature.[18]



2-Hydroxybenzonitrile (3c). According to the general procedure analogous to that described for **3a**, **3c** (17.7 mg, 0.149 mmol, 74%) was obtained from **1c** (26.9 mg, 0.202 mmol) as a white solid: Mp 94 °C (hexane/CH_2Cl_2) (lit. 93–95 °C[19]). ^1H NMR (400 MHz, $CDCl_3$/TMS) δ 7.53-7.45 (m, 2H), 7.03-6.96 (m, 2H), 5.81 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 134.8, 132.9, 120.9, 116.6, 116.4, 99.4. LRMS (EI) *m/z*: 119 (M^+). HRMS Calcd. for C_7H_5NO: 119.0371, found: 119.0372. IR (neat): 3276, 2230, 1605, 1456, 1351, 1307, 1234, 1160, 849, 747 cm^{-1}. The spectra data matched those reported in the literature.[19]

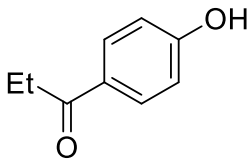


(4-Hydroxyphenyl)(phenyl)methanone (3d). According to the general procedure analogous to that described for **3a**, **3d** (33.4 mg, 0.168 mmol, 86%) was obtained from **1d** (41.6 mg, 0.196 mmol) as a white solid: Mp 136 °C (hexane/CH_2Cl_2) (lit. 132–135 °C[20]). ^1H NMR (400 MHz, $CDCl_3$/TMS) δ 7.82-7.73 (m, 4H), 7.57 (t, 1H, J = 7.3 Hz), 7.47 (t, 2H, J = 7.6 Hz), 6.91 (d, 2H, J = 8.8 Hz), 5.37 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 160.7, 138.1, 133.1, 132.2, 129.8, 129.6, 128.2, 115.4. LRMS (EI) *m/z*: 198 (M^+). HRMS Calcd. for $C_{13}H_{10}O_2$: 198.0681, found: 198.0675. IR (neat): 3127, 1599, 1553, 1313, 1286, 1232, 1148, 924, 849, 740 cm^{-1}. The spectra data matched those reported in the literature.[20]

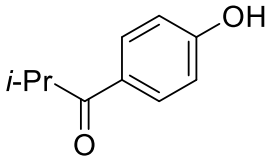


1-(4-Hydroxyphenyl)ethan-1-one (3e). According to the general procedure analogous to that described for **3a**, **3e** (21.9 mg, 0.161 mmol, 81%) was obtained from **1e** (29.8 mg, 0.198 mmol) as a white solid: Mp 108 °C (hexane/CH_2Cl_2) (lit. 107.2–108.5 °C[18]). ^1H NMR (400 MHz, $CDCl_3$/TMS) δ 7.91 (d, 2H, J = 8.8 Hz), 6.88 (d, 2H, J = 8.8 Hz), 5.22 (s, 1H), 2.56 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 161.2, 131.2, 129.8, 115.5, 26.3. LRMS (EI) *m/z*: 136 (M^+). HRMS Calcd. for $C_8H_8O_2$: 136.0524, found: 136.0531. IR (neat): 3308, 1660, 1572, 1355, 1277, 1165, 1107, 962, 847,

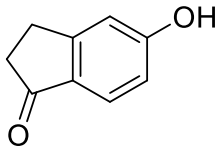
816 cm^{-1}. The spectra data matched those reported in the literature.[18]



1-(4-Hydroxyphenyl)propan-1-one (3f). According to the general procedure analogous to that described for **3a**, **3f** (28.3 mg, 0.188 mmol, 93%) was obtained from **1f** (33.2 mg, 0.202 mmol) as a white solid: Mp 153 °C (hexane/CH_2Cl_2) (lit. 147–148.6 °C[21]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.92 (d, 2H, J = 8.8 Hz), 6.87 (d, 2H, J = 8.8 Hz), 5.25 (s, 1H), 2.95 (q, 2H, J = 7.15 Hz), 1.21 (t, 3H, J = 7.3 Hz). ^{13}C NMR (100 MHz, DMSO-d_6) δ 198.6, 161.8, 130.3, 128.2, 115.1, 30.6, 8.4. LRMS (EI) *m/z*: 150 (M^+). HRMS Calcd. for $C_9H_{10}O_2$: 150.0681, found: 150.0679. IR (neat): 3173, 1660, 1568, 1357, 1287, 1225, 1171, 954, 859, 800 cm^{-1}. The spectra data matched those reported in the literature.[21]

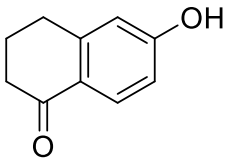


1-(4-Hydroxyphenyl)-2-methylpropan-1-one (3g). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 5:1), **3g** (28.9 mg, 0.176 mmol, 85%) was obtained from **1g** (36.8 mg, 0.206 mmol) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.92 (d, 2H, J = 8.3 Hz), 6.89 (d, 2H, J = 8.8 Hz), 5.59 (s, 1H), 3.52 (sext, 1H, J = 6.8 Hz), 1.21 (d, 6H, J = 6.8 Hz). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.9, 161.1, 131.1, 128.3, 115.6, 35.0, 19.4. LRMS (EI) *m/z*: 164 (M^+). HRMS Calcd. for $C_{10}H_{12}O_2$: 164.0837, found: 164.0854. IR (neat): 3277, 2973, 1653, 1600, 1577, 1384, 1222, 1156, 982, 846 cm^{-1}. The spectra data matched those reported in the literature.[22]

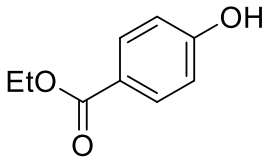


5-Hydroxy-2,3-dihydro-1*H*-inden-1-one (3h). According to the general procedure analogous to that described for **3a**, except that the reaction was conducted with HMDS (66.0 mg, 0.409 mmol), and the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 1:1), **3h** (19.4 mg, 0.131 mmol, 67%) was obtained from **1h** (31.6 mg, 0.195 mmol) as a brown solid: Mp 189 °C (hexane/AcOEt) (lit. 182–185 °C[23]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.68 (d, 1H, J = 8.3 Hz), 6.87 (s, 1H), 6.83 (dd, 1H, J = 8.6, 2.2 Hz), 5.54 (s, 1H), 3.08 (t, 2H, J = 5.8 Hz), 2.70-2.65 (m, 2H).

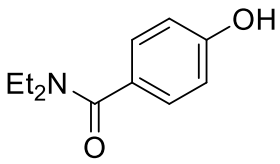
^{13}C NMR (100 MHz, DMSO-d_6) δ 204.0, 163.6, 158.3, 128.6, 124.9, 115.7, 112.0, 35.9, 25.2. LRMS (EI) *m/z*: 148 (M^+). HRMS Calcd. for $C_9H_8O_2$: 148.0524, found: 148.0550. IR (neat): 3096, 2923, 2857, 1728, 1661, 1583, 1468, 1271, 1099, 841 cm^{-1}. The spectra data matched those reported in the literature.[24,25]



6-Hydroxy-3,4-dihydronaphthalen-1(2*H*)-one (3i). According to the general procedure analogous to that described for **3a**, **3i** (27.4 mg, 0.169 mmol, 86%) was obtained from **1i** (34.7 mg, 0.197 mmol) as a brown solid: Mp 159 °C (hexane/AcOEt) (lit. 154–157 °C[26]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.98 (d, 1H, J = 8.8 Hz), 6.75 (dd, 1H, J = 8.3, 2.4 Hz), 6.67 (d, 1H, 3.0 Hz), 5.30 (s, 1H), 2.90 (t, 2H, J = 6.1 Hz), 2.61 (t, 2H, J = 6.6 Hz), 2.11 (quint, 2H, J = 6.5 Hz). ^{13}C NMR (100 MHz, DMSO-d_6) δ 195.8, 162.0, 147.1, 128.9, 124.6, 114.23, 114.16, 38.3, 29.2, 22.9. LRMS (EI) *m/z*: 162 (M^+). HRMS Calcd. for $C_{10}H_{10}O_2$: 162.0681, found: 162.0694. IR (neat): 3042, 2953, 2827, 1643, 1563, 1346, 1285, 1248, 1116, 833 cm^{-1}. The spectra data matched those reported in the literature.[26,27]

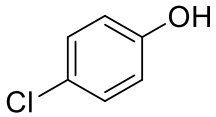


Ethyl 4-hydroxybenzoate (3j). According to the general procedure analogous to that described for **3a**, except that the reaction was conducted at 80°C in a heat block and the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 5:1), **3j** (27.8 mg, 0.167 mmol, 83%) was obtained from **1j** (36.4 mg, 0.202 mmol) as a white solid: Mp 116 °C (hexane/CH_2Cl_2) (lit. 116.6–117.7 °C[21]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.97 (d, 2H, J = 8.8 Hz), 6.85 (d, 2H, J = 8.8 Hz), 5.21 (s, 1H), 4.35 (q, 2H, J = 7.3 Hz), 1.38 (t, 3H, J = 7.3 Hz). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 160.3, 131.9, 122.6, 115.2, 61.0, 14.3. LRMS (EI) *m/z*: 166 (M^+). HRMS Calcd. for $C_9H_{10}O_3$: 166.0630, found: 166.0647. IR (neat): 3191, 1666, 1588, 1443, 1280, 1235, 1164, 1015, 849, 770 cm^{-1}. The spectra data matched those reported in the literature.[21]

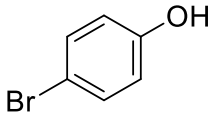


***N*,*N*-Diethyl-4-hydroxybenzamide (3k).** According to the general procedure analogous to that described for **3a**, except that the crude material was purified by column chromatography on silica gel

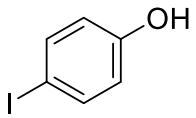
(hexane:AcOEt = 1:1), **3k** (35.7 mg, 0.185 mmol, 91%) was obtained from **1k** (41.9 mg, 0.202 mmol) as a wite solid: Mp 124 °C (hexane/CH_2Cl_2) (lit. 121−123 °C[28]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.22 (d, 2H, J = 8.3 Hz), 6.79 (s, 1H), 6.73 (d, 2H, J = 8.3 Hz), 3.48 (br, 4H), 1.19 (br, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 158.5, 128.0, 126.8, 115.4, 43.7, 39.8, 14.1, 12.8. LRMS (EI) *m/z*: 192 ($M\text{-}H^+$). HRMS Calcd. for $C_{11}H_{14}NO_2$: 192.1025, found: 192.1021. IR (neat): 3091, 2989, 1563, 1446, 1275, 1243, 1170, 1099, 855, 765 cm^{-1}. The spectra data matched those reported in the literature.[29]



4-Chlorophenol (3l). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by preparative thin-layer chromatography of silica gel (toluene:AcOEt = 4:1), **3l** (21.7 mg, 0.169 mmol, 85%) was obtained from **1l** (28.2 mg, 0.198 mmol) as a brown oil. ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.19 (d, 2H, J = 8.8 Hz), 6.77 (d, 2H, J = 8.7 Hz), 4.73 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 129.5, 125.6, 116.7. LRMS (EI) *m/z*: 128 (M^+). HRMS Calcd. for C_6H_5ClO: 128.0029, found: 128.0044. IR (neat): 3328, 1590, 1492, 1433, 1356, 1228, 1166, 1092, 1010, 823 cm^{-1}. The spectra data matched those reported in the literature.[30]

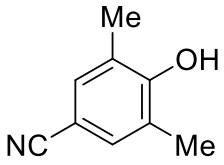


4-Bromophenol (3m). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 5:1), **3m** (29.9 mg, 0.173 mmol, 84%) was obtained from **1m** (38.3 mg, 0.205 mmol) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.34 (d, 2H, J = 8.8 Hz), 6.72 (d, 2H, J = 8.8 Hz), 4.70 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 132.4, 117.2, 112.8. LRMS (EI) *m/z*: 171 (M^+). HRMS Calcd. for C_6H_5BrO: 171.9524, found: 171.9536. IR (neat): 3335, 1587, 1488, 1431, 1355, 1239, 1168, 1070, 1007, 820 cm^{-1}. The spectra data matched those reported in the literature.[31]

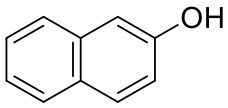


4-Iodophenol (3n). According to the general procedure analogous to that described for **3a**, except that the reaction was conducted with $N(TMS)_3$ (53.4 mg, 0.229 mmol) instead of HMDS and the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 5:1), **3n** (25.6 mg, 0.116 mmol, 57%) was obtained from **1n** (47.5 mg, 0.203 mmol) as a white solid: Mp 63 °C (hexane/CH_2Cl_2) (lit. 66 °C[32]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.52 (d, 2H, J = 8.8 Hz), 6.62 (d, 2H, J = 8.8 Hz), 4.68 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.4, 138.4, 117.8, 82.7. LRMS (EI)

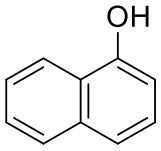
m/z: 219 (M^+). HRMS Calcd. for C_6H_5IO: 219.9385, found: 219.9398. IR (neat): 3296, 1579, 1484, 1422, 1210, 1170, 1094, 1056, 1000, 818 cm^{-1}. The spectra data matched those reported in the literature.[32]



4-Hydroxy-3,5-dimethylbenzonitrile (3o). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 5:1), **3o** (27.3 mg, 0.185 mmol, 94%) was obtained from **1o** (31.9 mg, 0.198 mmol) as a white solid: Mp 125 °C (hexane/CH_2Cl_2) (lit. 125 °C[33]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.29 (s, 2H), 5.10 (s, 1H), 2.26 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.4, 132.6, 124.4, 119.5, 103.1, 15.7. LRMS (EI) *m/z*: 147 (M^+). HRMS Calcd. for C_9H_9NO: 147.0684, found: 147.0688. IR (neat): 3354, 2978, 2919, 2229, 1592, 1479, 1316, 1193, 1142, 945 cm^{-1}. The spectra data matched those reported in the literature.[34]

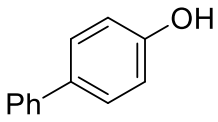


Naphthalen-2-ol (5a). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 10:1), **5a** (26.8 mg, 0.186 mmol, 95%) was obtained from **4a** (31.1 mg, 0.197 mmol) as a white solid: Mp 121 °C (hexane/CH_2Cl_2) (lit. 121–123 °C[19]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.79-7.72 (m, 2H), 7.68 (d, 1H, J = 8.3 Hz), 7.43 (t, 1H, J = 7.6 Hz), 7.32 (t, 1H, J = 7.6 Hz), 7.15 (d, 1H, J = 2.4 Hz), 7.10 (dd, 1H, J = 8.8, 2.4 Hz), 5.01 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 134.6, 129.8, 129.0, 127.8, 126.5, 126.4, 123.6, 117.7, 109.5. LRMS (EI) *m/z*: 144 (M^+). HRMS Calcd. for $C_{10}H_8O$: 144.0575, found: 144.0572. IR (neat): 3238, 1584, 1504, 1456, 1273, 1213, 1170, 958, 842, 811 cm^{-1}. The spectra data matched those reported in the literature.[19]

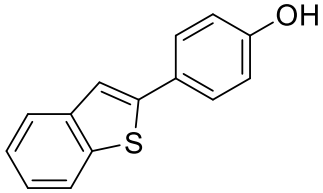


Naphthalen-1-ol (5b). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 10:1), **5b** (24.6 mg, 0.171 mmol, 86%) was obtained from **4b** (31.3 mg, 0.198 mmol) as a white solid: Mp 93 °C (hexane/CH_2Cl_2) (lit. 91–93 °C[35]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 8.22-8.14 (m, 1H), 7.84-

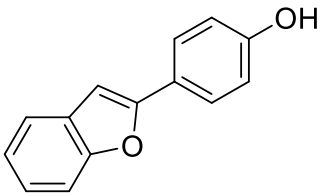
7.79 (m, 1H), 7.52-7.46 (m, 2H), 7.44 (d, 2H, J = 7.8 Hz), 7.31 (t, 1H, J = 7.8 Hz), 6.82 (d, 2H, J = 7.3 Hz), 5.26 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.3, 134.8, 127.7, 126.4, 125.8, 125.2, 124.4, 121.5, 120.7, 108.6. LRMS (EI) *m/z*: 144 (M^+). HRMS Calcd. for $C_{10}H_8O$: 144.0575, found: 144.0593. IR (neat): 3296, 1581, 1385, 1296, 1148, 1083, 1016, 876, 789, 763 cm^{-1}. The spectra data matched those reported in the literature.[35]



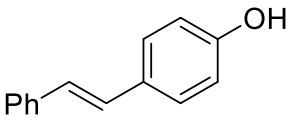
[1,1'-Biphenyl]-4-ol (5c). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 4:1), **5c** (32.0 mg, 0.188 mmol, 95%) was obtained from **4c** (36.6 mg, 0.199 mmol) as a white solid: Mp 168 °C (hexane/AcOEt) (lit. 166–168 °C[36]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.56-7.52 (m, 2H), 7.48 (d, 2H, J = 8.8 Hz), 7.41 (t, 2H, J = 7.6 Hz), 7.30 (t, 1H, J = 7.6 Hz), 6.91 (d, 2H, J = 8.8 Hz), 4.73 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 157.5, 140.6, 131.3, 129.2, 128.1, 126.8, 126.4, 116.1. LRMS (EI) *m/z*: 170 (M^+). HRMS Calcd. for $C_{12}H_{10}O$: 170.0732, found: 170.0741. IR (neat): 3393, 1603, 1462, 1335, 1257, 1169, 1114, 1004, 832, 755 cm^{-1}. The spectra data matched those reported in the literature.[37]



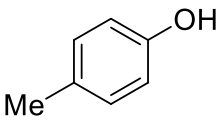
4-(Benzo[*b*]thiophen-2-yl)phenol (5d). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 5:1), **5d** (37.5 mg, 0.166 mmol, 84%) was obtained from **4d** (47.6 mg, 0.198 mmol) as a white solid: Mp 243 °C (hexane/AcOEt). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.80 (d, 1H, J = 7.8 Hz), 7.74 (d, 1H, J = 7.8 Hz), 7.60 (d, 2H, J = 8.3 Hz), 7.42 (s, 1H), 7.34 (t, 1H, J = 7.6 Hz), 7.29 (d, 1H, J = 7.8 Hz), 6.89 (d, 2H, J = 8.8 Hz), 4.85 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.0, 143.8, 140.7, 138.0, 127.5, 124.6, 124.5, 124.0, 123.2, 122.2, 117.7, 115.9. LRMS (EI) *m/z*: 226 (M^+). HRMS Calcd. for $C_{14}H_{10}OS$: 226.0452, found: 226.0472. IR (neat): 3238, 1609, 1499, 1428, 1256, 1177, 1107, 945, 817, 726 cm^{-1}. The spectra data matched those reported in the literature.[38]



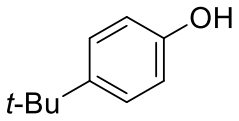
4-(Benzofuran-2-yl)phenol (5e). According to the general procedure analogous to that described for **3a**, **5e** (37.1 mg, 0.176 mmol, 89%) was obtained from **4e** (44.4 mg, 0.198 mmol) as a white solid: Mp 200 °C (hexane/AcOEt) (lit. 194–195 °C[39]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.78-7.74 (m, 2H), 7.57-7.53 (m, 1H), 7.49 (d, 1H, J = 7.8 Hz), 7.26-7.18 (m, 2H), 6.94-6.87 (m, 3H), 4.86 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.3, 155.9, 153.9, 129.2, 126.4, 123.7, 123.0, 120.9, 120.6, 115.9, 110.8, 99.3. LRMS (EI) *m/z*: 210 (M^+). HRMS Calcd. for $C_{14}H_{10}O_2$: 210.0681, found: 210.0686. IR (neat): 3439, 1612, 1505, 1432, 1254, 1168, 1106, 1031, 802, 741 cm^{-1}. The spectra data matched those reported in the literature.[39,40]



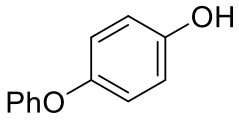
(*E*)-4-styrylphenol (5f). According to the general procedure analogous to that described for **3a**, **5f** (34.8 mg, 0.177 mmol, 90%) was obtained from **4f** (41.6 mg, 0.198 mmol) as a white solid: Mp 197 °C (hexane/AcOEt) (lit. 195–196 °C[41]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.48 (d, 2H, J = 8.3 Hz), 7.41 (d, 2H, J = 8.8 Hz), 7.34 (t, 2H, J = 7.8 Hz), 7.26-7.23 (m, 1H), 7.05 (d, 1H, J = 16.6 Hz), 6.96 (d, 1H, J = 16.6 Hz), 6.83 (d, 2H, J = 8.3 Hz), 4.74 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 157.3, 137.5, 128.6, 128.4, 128.1, 127.8, 126.9, 126.0, 125.1, 115.5. LRMS (EI) *m/z*: 196 (M^+). HRMS Calcd. for $C_{14}H_{12}O$: 196.0888, found: 196.0888. IR (neat): 3420, 3031, 1591, 1511, 1451, 1355, 1246, 1105, 960, 818 cm^{-1}. The spectra data matched those reported in the literature.[42,43]



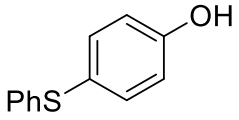
***p*-Cresol (5g).** According to the general procedure analogous to that described for **3a**, except that the reaction was conducted in toluene at 140 °C in a heat block and the crude material was purified by preparative thin-layer chromatography of silica gel (toluene:AcOEt = 3:1), **5g** (17.3 mg, 0.160 mmol, 80%) was obtained from **4g** (24.5 mg, 0.201 mmol) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.03 (d, 2H, J = 8.8 Hz), 6.73 (d, 2H, J = 8.8 Hz), 4.56 (s, 1H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 130.1, 130.0, 115.1, 20.4. LRMS (EI) *m/z*: 108 (M^+). HRMS Calcd. for C_7H_8O: 108.0575, found: 108.0594. IR (neat): 3332, 3022, 2922, 1600, 1512, 1435, 1360, 1235, 1104, 813 cm^{-1}. The spectra data matched those reported in the literature.[44]



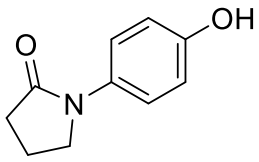
4-(*tert*-Butyl)phenol (5h). According to the general procedure analogous to that described for **3a**, except that the reaction was conducted in toluene at 140 °C in a heat block and the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 10:1), **5h** (27.8 mg, 0.185 mmol, 90%) was obtained from **4h** (33.7 mg, 0.205 mmol) as a white solid: Mp 99 °C (hexane) (lit. 97–99 °C[45]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.26 (d, 2H, J = 8.6 Hz), 6.77 (d, 2H, J = 8.6 Hz), 4.59 (s, 1H), 1.30 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 143.6, 126.4, 114.8, 34.0, 31.5. LRMS (EI) *m/z*: 150 (M^+). HRMS Calcd. for $C_{10}H_{14}O$: 150.1045, found: 150.1046. IR (neat): 3227, 2959, 1599, 1512, 1444, 1236, 1183, 1113, 1015, 812 cm^{-1}. The spectra data matched those reported in the literature.[45]



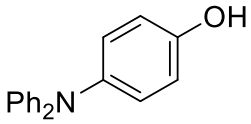
4-Phenoxyphenol (5i). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 4:1), **5i** (33.0 mg, 0.177 mmol, 90%) was obtained from **4i** (39.4 mg, 0.197 mmol) as a white solid: Mp 80 °C (hexane/CH_2Cl_2) (lit. 82–83 °C[46]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.32-7.27 (m, 2H), 7.04 (t, 1H, J = 7.3 Hz), 6.96-6.91 (m, 4H), 6.81 (d, 2H, J = 9.2 Hz), 4.64 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 151.7, 150.1, 129.6, 122.5, 120.9, 117.6, 116.4. LRMS (EI) *m/z*: 186 (M^+). HRMS Calcd. for $C_{12}H_{10}O_2$: 186.0681, found: 186.0670. IR (neat): 3238, 1601, 1504, 1485, 1439, 1195, 1095, 850, 812, 749 cm^{-1}. The spectra data matched those reported in the literature.[47]



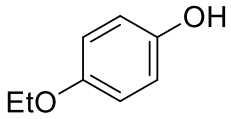
4-(Phenylthio)phenol (5j). According to the general procedure analogous to that described for **3a**, except that the reaction was conducted at 80°C in a heat block and the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 5:1), **5j** (38.6 mg, 0.191 mmol, 95%) was obtained from **4j** (43.6 mg, 0.202 mmol) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.37 (d, 2H, J = 8.3 Hz), 7.23 (d, 2H, J = 7.3 Hz), 7.20-7.12 (m, 3H), 6.83 (d, 2H, J = 8.8 Hz), 4.81 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.9, 138.3, 135.4, 128.9, 128.4, 125.9, 124.6, 116.5. LRMS (EI) *m/z*: 202 (M^+). HRMS Calcd. for $C_{12}H_{10}OS$: 202.0452, found: 202.0444. IR (neat): 3350, 1599, 1583, 1493, 1478, 1259, 1169, 1024, 828, 738 cm^{-1}. The spectra data matched those reported in the literature.[48]



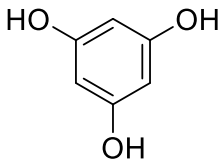
1-(4-Hydroxyphenyl)pyrrolidin-2-one (5k). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 1:2), **5k** (28.5 mg, 0.161 mmol, 81%) was obtained from **4k** (37.8 mg, 0.198 mmol) as a white solid: Mp 168 °C (hexane/AcOEt) (lit. 168 °C[49]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.39 (d, 2H, J = 9.0 Hz), 6.80 (d, 2H, J = 9.0 Hz), 5.31 (s, 1H), 3.82 (t, 2H, J = 7.0 Hz), 2.60 (t, 2H, J = 8.2 Hz), 2.16 (quint, 2H, J = 7.6 Hz). ^{13}C NMR (100 MHz, DMSO-d_6) δ 173.0, 153.9, 131.4, 121.5, 115.0, 48.5, 32.0, 17.4. LRMS (EI) *m/z*: 177 (M^+). HRMS Calcd. for $C_{10}H_{11}NO_2$: 177.0790, found: 177.0797. IR (neat): 3116, 2935, 1640, 1633, 1412, 1271, 1230, 1180, 1122, 826 cm^{-1}. The spectra data matched those reported in the literature.[49]



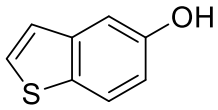
4-(Diphenylamino)phenol (5l). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 10:1), **5l** (47.3 mg, 0.181 mmol, 91%) was obtained from **4l** (55.0 mg, 0.200 mmol) as a blue solid: Mp 132 °C (hexane/CH_2Cl_2) (lit. 121 °C[50]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.26-7.15 (m, 4H), 7.15-6.88 (m, 8H), 6.88-6.68 (m, 2H), 4.58 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.9, 148.2, 141.0, 129.1, 127.5, 122.9, 121.9, 116.3. LRMS (EI) *m/z*: 261 (M^+). HRMS Calcd. for $C_{18}H_{15}NO$: 261.1154, found: 261.1164. IR (neat): 3536, 3427, 3036, 1585, 1506, 1487, 1282, 1229, 837, 751 cm^{-1}. The spectra data matched those reported in the literature.[50]



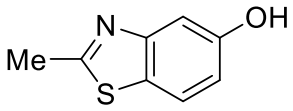
4-Ethoxyphenol (5m). According to the general procedure analogous to that described for **3a**, except that the reaction was conducted in toluene at 140 °C in a heat block and the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 10:1), **5m** (23.4 mg, 0.169 mmol, 86%) was obtained from **4m** (30.1 mg, 0.198 mmol) as a white solid: Mp 61 °C (hexane/CH_2Cl_2) (lit. 64–66 °C[51]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 6.82-6.72 (m, 4H), 4.42 (s, 1H), 3.97 (q, 2H, J = 7.0 Hz), 1.38 (t, 3H, J = 7.1 Hz). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 149.5, 116.1, 115.8, 64.2, 14.9. LRMS (EI) *m/z*: 138 (M^+). HRMS Calcd. for $C_8H_{10}O_2$: 138.0681, found: 138.0690. IR (neat): 3375, 2975, 2926, 1510, 1206, 1116, 1046, 922, 827, 753 cm^{-1}. The spectra data matched those reported in the literature.[51]



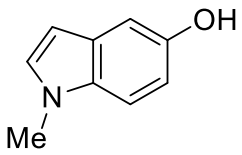
Benzene-1,3,5-triol (5n). According to the general procedure analogous to that described for **3a**, except that the reaction was conducted with HMDS (106.1 mg, 0.657 mmol) and 1-decanthiol (137.0 μL, 0.660 mmol) and the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 1:3), **5n** (18.0 mg, 0.143 mmol, 73%) was obtained from **4n** (33.0 mg, 196 mmol) as a white solid: Mp 220 °C (lit. 220.1 °C[52]). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.91 (s, 3H), 5.64 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.9, 94.0. LRMS (EI) *m/z*: 126 (M^+). HRMS Calcd. for $C_6H_6O_3$: 126.0317, found: 126.0304. IR (neat): 3211, 1619, 1503, 1418, 1297, 1155, 1008, 998, 814, 800 cm^{-1}. The spectra data matched those reported in the literature.[53]



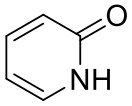
Benzo[*b*]thiophen-5-ol (5o). According to the general procedure analogous to that described for **3a**, except that the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 10:1), **5o** (27.4 mg, 0.182 mmol, 93%) was obtained from **4o** (32.3 mg, 0.197 mmol) as a white solid: Mp 102 °C (hexane/CH_2Cl_2) (lit. 102–104 °C[54]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.71 (d, 1H, J = 8.8 Hz), 7.44 (d, 1H, J = 5.8 Hz), 7.24 (d, 1H, J = 2.4 Hz), 7.21 (s, 1H, J = 5.4 Hz), 6.92 (dd, 1H, J = 8.8, 2.4 Hz), 4.72 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 140.8, 132.3, 127.9, 123.3, 123.2, 114.3, 108.5. LRMS (EI) *m/z*: 150 (M^+). HRMS Calcd. for C_8H_6OS: 150.0139, found: 150.0133. IR (neat): 3212, 1600, 1563, 1423, 1267, 1139, 1088, 944, 889, 829 cm^{-1}. The spectra data matched those reported in the literature.[55]



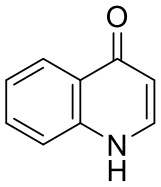
2-Methylbenzo[*d*]thiazol-5-ol (5p). According to the general procedure analogous to that described for **3a**, **5p** (26.4 mg, 0.160 mmol, 79%) was obtained from **4p** (36.1 mg, 0.201 mmol) as a yellow solid: Mp 201 °C (hexane/AcOEt) (lit. 187–189 °C[46]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.64 (d, 1H, J = 8.8 Hz), 7.41 (s, 1H), 6.94 (dd, 1H, J = 8.3, 1.4 Hz), 5.57 (s, 1H), 2.81 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 167.5, 156.3, 154.4, 125.2, 122.0, 114.5, 107.3, 19.7. LRMS (EI) *m/z*: 165 (M^+). HRMS Calcd. for C_8H_7NOS: 165.0248, found: 165.0254. IR (neat): 3054, 2901, 2787, 1598, 1460, 1354, 1316, 1211, 1165, 953, 855 cm^{-1}. The spectra data matched those reported in the literature.[46]



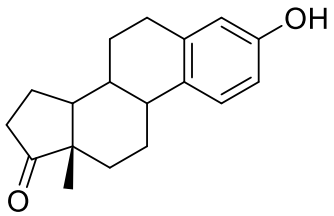
1-Methyl-1*H*-indol-5-ol (5q). According to the general procedure analogous to that described for **3a**, except that the reaction was conducted in toluene at 140 °C in a heat block and the crude material was purified by column chromatography on silica gel (hexane:AcOEt = 2:1), **5q** (19.0 mg, 0.129 mmol, 66%) was obtained from **4q** (31.4 mg, 0.195 mmol) as a pink solid: Mp 134 °C (hexane/AcOEt) (lit. 130–132 °C[56]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.17 (d, 1H, J = 8.8 Hz), 7.03-7.01 (m, 2H), 6.80 (dd, 1H, J = 8.8, 2.4 Hz), 6.35 (d, 1H, J = 2.9 Hz), 4.43 (s, 1H), 3.76 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 150.6, 131.2, 129.6, 128.7, 111.2, 109.8, 104.2, 99.1, 32.4. LRMS (EI) *m/z*: 147 (M^+). HRMS Calcd. for C_9H_9NO: 147.0684, found: 147.0706. IR (neat): 3177, 2939, 1620, 1489, 1424, 1234, 1145, 950, 839, 796 cm^{-1}. The spectra data matched those reported in the literature.[57]



Pyridin-2(1*H*)-one (5r). In a glove box under an Ar atmosphere, to a solution of **4r** (21.4 mg, 0.196 mmol) in THF (0.3 mL) were added *t*-Bu-P4 solution (50 μL, 0.8 M in hexane, 0.04 mmol) and HMDS (38.2 mg, 0.237 mmol) in an oven-dried vial equipped with a stirrer bar. The vial was sealed with a cap containing an inner Teflon film, and taken outside the glove box. **2** (45.7 μL, 0.220 mmol) was added to the mixture under a nitrogen atmosphere. The resulting mixture was stirred at 100 °C in a heat block for 3 h. MeOH was added to the mixture at 0 °C. After stirring at room temperature for 30 minutes, the mixture was concentrated. 4 M HCl in 1,4-dioxane (10 μL) and THF (1 mL) were added to the crude material. After stirring at room temperature for 5 minutes, the mixture was concentrated. The resulting material was purified by column chromatography on silica gel (CH_2Cl_2:MeOH = 10:1) and GPC (THF) to afford **5r** (14.8 mg, 0.156 mmol, 79%) as a white solid: Mp 107 °C (hexane/CH_2Cl_2) (lit. 106–108 °C[58]). ^{1}H NMR (600 MHz, $CDCl_3$/TMS) δ 13.00 (br, 1H), 7.50-7.45 (m, 1H), 7.37 (d, 1H, J = 6.5 Hz), 6.60 (d, 1H, J = 9.5 Hz), 6.29 (t, 1H, J = 6.5 Hz). ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.6, 141.8, 134.8, 120.3, 107.0. LRMS (EI) *m/z*: 95 (M^+). HRMS Calcd. for C_5H_5NO: 95.0371, found: 95.0371. IR (neat): 3122, 2978, 2801, 2720, 1645, 1615, 1544, 1471, 987, 769 cm^{-1}. The spectra data matched those reported in the literature.[58]



Quinolin-4(1*H*)-one (5s). In a glove box under an Ar atmosphere, to a solution of **4s** (31.3 mg, 0.197 mmol) in toluene (0.3 mL) were added *t*-Bu-P4 solution (50 μL, 0.8 M in hexane, 0.04 mmol) and HMDS (38.2 mg, 0.227 mmol) in an oven-dried vial equipped with a stirrer bar. The vial was sealed with a cap containing an inner Teflon film, and taken outside the glove box. **2** (45.7 μL, 0.220 mmol) was added to the mixture under a nitrogen atmosphere. The resulting mixture was stirred at 140 °C in a heat block for 3 h. MeOH was added to the mixture at 0 °C. After stirring at room temperature for 30 minutes, the mixture was concentrated. The crude material was purified by preparative thin-layer chromatography of sílica gel (CH_2Cl_2:MeOH = 10:1) and by recrystallization from AcOEt to afford **5s** (17.6 mg, 0.121 mmol, 62%) as a white solid: Mp 211 °C (AcOEt) (lit. 199–200 °C[59]). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.70 (br, 1H), 8.04 (d, 1H, J = 8.0 Hz), 7.86 (dd, 1H, J = 7.3, 6.1 Hz), 7.60 (t, 1H, J = 7.7 Hz), 7.49 (d, 1H, J = 8.0 Hz), 7.27 (t, 1H, J = 7.5 Hz), 5.99 (d, 1H, J = 7.4 Hz). ^{13}C NMR (150 MHz, DMSO-d_6) δ 176.9, 140.0, 139.3, 131.6, 125.8, 124.9, 123.0, 118.2, 108.7. LRMS (EI) *m/z*: 145 (M^+). HRMS Calcd. for C_9H_7NO: 145.0528, found: 145.0520. IR (neat): 3237, 3070, 2980, 2784, 1635, 1504, 1474, 1362, 1201, 753 cm^{-1}. The spectra data matched those reported in the literature.[60]



(13*S*)-3-hydroxy-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta[*a*]phenanthren-17-one (5t). According to the general procedure analogous to that described for **3a**, except that the reaction was conducted with HMDS (97.4 mg, 0.604 mmol), **5t** (32.1 mg, 0.119 mmol, 60%) was obtained from **4t** (56.6 mg, 0.199 mmol) as a white solid: Mp 259 °C (hexane/AcOEt) (lit. 254–256 °C[61]). ^{1}H NMR (400 MHz, $CDCl_3$/TMS) δ 7.16 (d, 1H, J = 7.8 Hz), 6.64 (dd, 1H, J = 8.5, 2.7 Hz), 6.59 (s, 1H), 4.52 (s, 1H), 2.91-2.84 (m, 2H), 2.55-2.45 (m, 1H), 2.42-2.35 (m, 1H), 2.30-1.93 (m, 5H), 1.70-1.38 (m, 6H), 0.91 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 219.6, 155.0, 137.1, 129.9, 126.0, 114.9, 112.8, 49.6, 47.3, 43.4, 38.0, 35.3, 31.3, 29.0, 26.1, 25.5, 21.1, 13.5. LRMS (EI) *m/z*: 270 (M^+). HRMS Calcd. for $C_{18}H_{22}O_2$: 270.1620, found: 270.1640. IR (neat): 3329, 2933, 2863, 1712, 1581, 1501, 1287, 1248, 1055, 920 cm^{-1}. The spectra data matched those reported in the literature. [61]

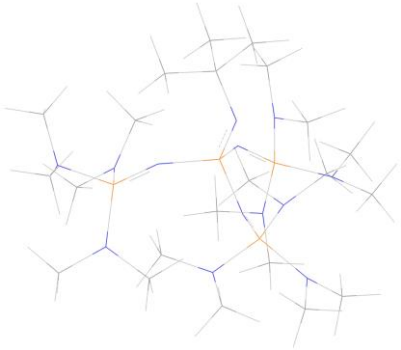
Computational section.

Calculation methods.

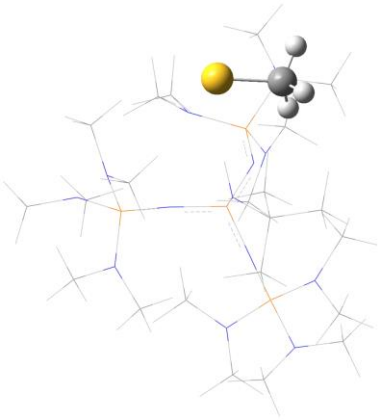
All calculations were performed with the Gaussian 16 (revision C.01) program.[62] Geometries were fully optimized and characterized by frequency calculation using ONIOM method,[63] combining B97D[64] density functional theory (DFT) with 6-311g(d,p) basis set[65] in the low level layer and same DFT with 6-311+g(2d,p) basis set in the high level layer, with the SCRF method based on CPCM (toluene).[66] The distribution of atoms in these two layers is shown in Figure 2 and Figure S2, and below, where the atoms in the high level layer are represented by a "ball & bond type" model and the atoms in the low level layer by a "wireframe" model. The intrinsic reaction coordinate (IRC) calculations[67] were performed at same level of theory. The calculations of the natural atomic charges[68] and the natural energy decomposition analysis[69] in the optimized structures were performed by using NBO7 (version 7.0.10) program at the B97D/6-311+g(2d,p). The calculations of the non-covalent interaction (NCI) analysis[70] were performed by using Multiwfn (version 3.6) program with PROAIMS wavefunction files written at the B97D/6-311+g(2d,p),[71] and the graphics were depicted by using VMD (version 1.9.4a53) program.[72]

Figures of optimized structures.

t-Bu-P4



Int-1



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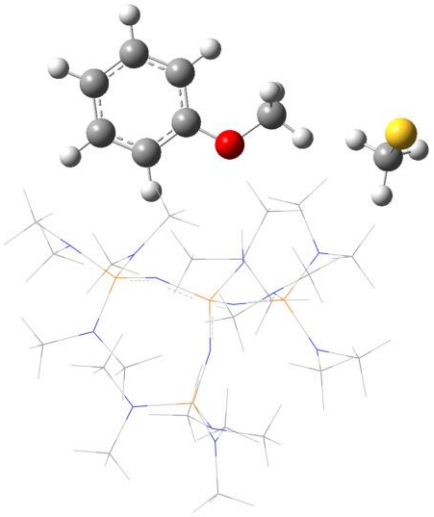
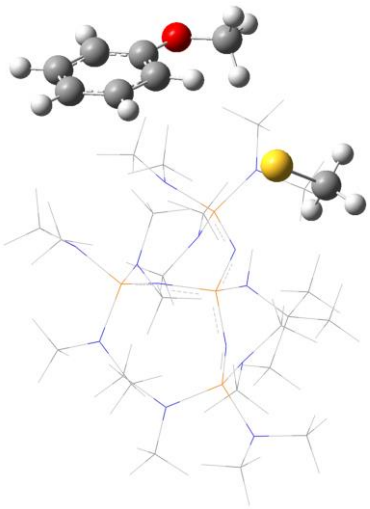
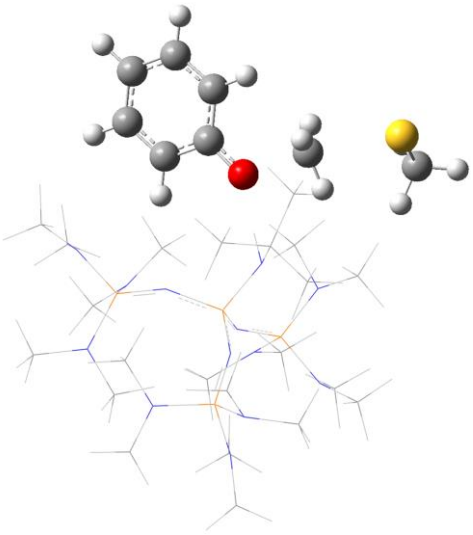


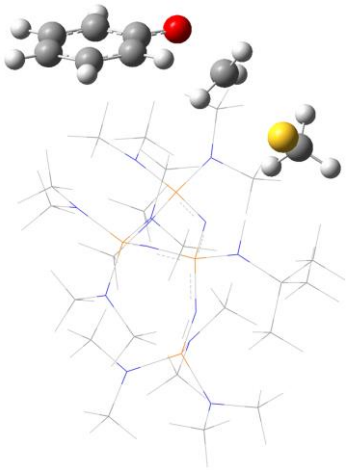
Int-2b



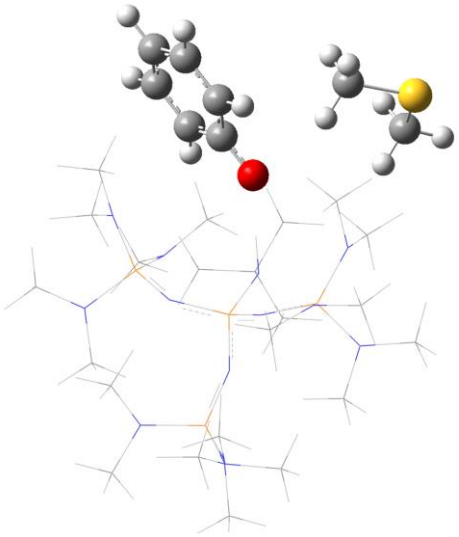
TS-1a



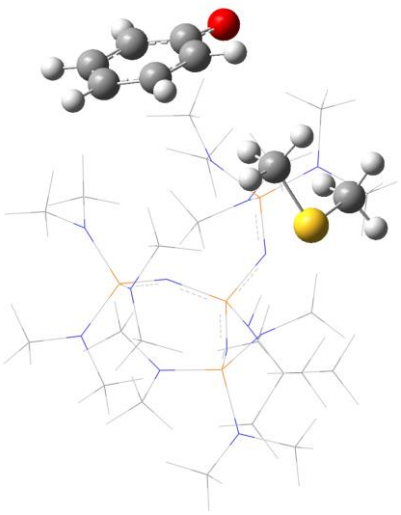
TS-1b



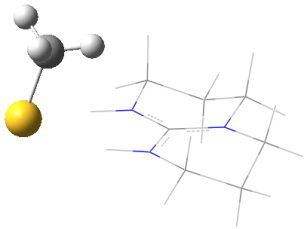
Int-3a



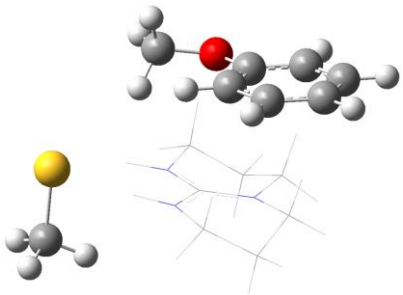
Int-3b



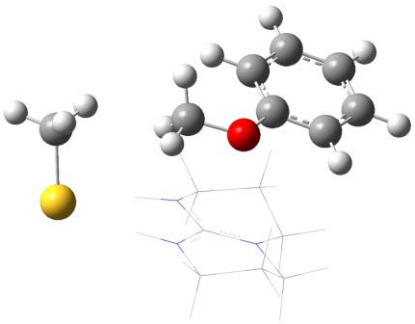
Int-4



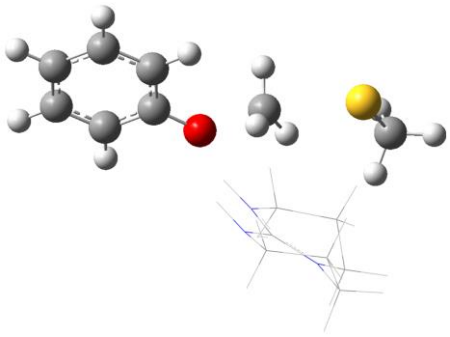
Int-5a



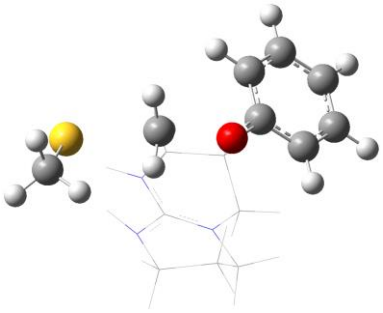
Int-5b



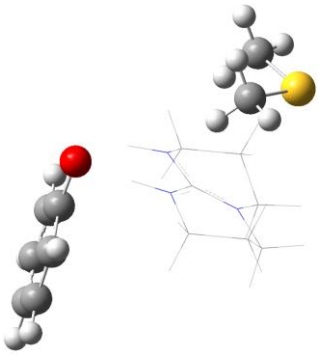
TS-2a



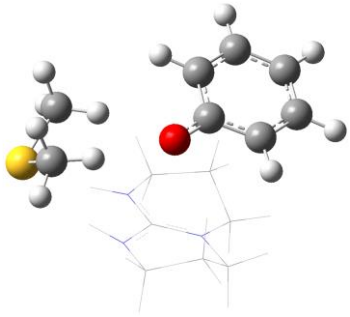
TS-2b



Int-6a



Int-6b



Cartesian coordinates.

t-Bu-P4
Sum of electronic and thermal Free Energies = -2952.137423 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.139306	-0.072739	0.766116
2	7	0	0.884962	-1.362055	0.468105
3	7	0	-1.272880	0.015624	-0.448955
4	7	0	0.835758	1.269631	0.596129
5	15	0	-2.761088	-0.503321	-0.525626
6	15	0	0.919848	2.635039	-0.143782
7	15	0	2.011052	-1.932999	-0.444954
8	7	0	1.379126	2.738633	-1.790358
9	7	0	2.212097	3.499772	0.564492
10	7	0	-0.540111	3.501292	-0.162931
11	7	0	-2.818435	-2.046645	-1.239679
12	7	0	-3.635270	0.552413	-1.521760
13	7	0	-3.781861	-0.584107	0.825502
14	6	0	-0.261792	-0.557061	3.441605
15	6	0	-1.269305	-0.182622	4.553862
16	1	0	-0.884594	-0.462701	5.547484
17	1	0	-1.458509	0.900788	4.536804
18	1	0	-2.223509	-0.701087	4.383925
19	6	0	1.068689	0.184057	3.737019
20	1	0	0.908424	1.269783	3.700721
21	1	0	1.454894	-0.086117	4.733280
22	1	0	1.824130	-0.077193	2.984455
23	6	0	0.004386	-2.085006	3.523294
24	1	0	0.416344	-2.367237	4.506799
25	1	0	-0.937652	-2.630950	3.365765
26	1	0	0.707311	-2.375728	2.734074
27	6	0	-3.958232	0.654050	1.608582
28	1	0	-4.890726	0.565775	2.188257
29	1	0	-3.099634	0.800065	2.280451
30	1	0	-4.045715	1.510980	0.931260
31	6	0	-3.696342	-1.772545	1.689911
32	1	0	-2.821026	-1.703530	2.352517
33	1	0	-4.619381	-1.827143	2.288041
34	1	0	-3.626523	-2.681361	1.082883
35	6	0	-4.095108	-2.621171	-1.662908
36	1	0	-4.588220	-3.192600	-0.853930
37	1	0	-4.778032	-1.836219	-2.000711
38	1	0	-3.915358	-3.307741	-2.505072
39	6	0	-1.792613	-3.049204	-0.941327
40	1	0	-0.869971	-2.562671	-0.617249
41	1	0	-2.122062	-3.748751	-0.150096
42	1	0	-1.587144	-3.634056	-1.852375
43	6	0	-2.996653	1.070402	-2.731162
44	1	0	-3.334031	0.518456	-3.628446
45	1	0	-3.260225	2.132932	-2.861452
46	1	0	-1.911658	0.988673	-2.640072
47	6	0	-5.092917	0.665717	-1.548076
48	1	0	-5.377634	1.731147	-1.557032
49	1	0	-5.516683	0.195875	-2.455711
50	1	0	-5.525688	0.188542	-0.664690
51	6	0	2.503289	4.861927	0.109590
52	1	0	3.558652	5.090442	0.325439
53	1	0	2.341592	4.939973	-0.970503
54	1	0	1.879128	5.617891	0.622123
55	6	0	2.489834	3.307254	1.991009
56	1	0	1.866447	3.964637	2.627451
57	1	0	2.301779	2.266557	2.265383
58	1	0	3.547032	3.552236	2.179853
59	6	0	-1.533281	3.280689	0.892713
60	1	0	-1.465724	4.063752	1.671420
61	1	0	-2.540280	3.322841	0.448487
62	1	0	-1.401610	2.298778	1.357633
63	6	0	-0.681680	4.800026	-0.824240
64	1	0	-1.682931	4.866924	-1.281467
65	1	0	-0.576668	5.635706	-0.108783
66	1	0	0.070372	4.909648	-1.611510
67	6	0	2.718422	2.217260	-2.122100
68	1	0	2.749239	1.114755	-2.092734
69	1	0	2.980723	2.559890	-3.134118
70	1	0	3.453804	2.607587	-1.411972
71	6	0	0.388294	2.351437	-2.805058
72	1	0	0.282724	1.257333	-2.877502
73	1	0	-0.587411	2.779513	-2.564489
74	1	0	0.720189	2.739040	-3.780314
75	6	0	2.144208	-3.427581	-2.819309
76	1	0	2.708864	-2.984693	-3.660818
77	1	0	2.823693	-4.031822	-2.211629
78	1	0	1.362567	-4.079689	-3.244282
79	6	0	3.763411	-0.024088	0.490509
80	1	0	2.885148	0.257058	1.074443
81	1	0	4.527379	-0.493033	1.138202
82	1	0	4.188011	0.894606	0.060227
83	6	0	1.580963	-4.457318	0.363683
84	1	0	0.968902	-4.234396	1.254777
85	1	0	0.921178	-4.518403	-0.508820
86	1	0	2.078236	-5.428749	0.502150
87	6	0	0.655375	-1.484041	-2.754250
88	1	0	-0.074952	-2.077335	-3.327118
89	1	0	0.094074	-0.830064	-2.077133
90	1	0	1.241457	-0.873703	-3.465690
91	7	0	1.517444	-2.392264	-1.996656
92	6	0	4.459274	-1.273816	-1.499580
93	1	0	4.084383	-1.813139	-2.374424
94	1	0	4.951767	-0.352653	-1.847958
95	1	0	5.218608	-1.901044	-0.995331
96	7	0	3.358906	-0.909753	-0.607209
97	6	0	3.547298	-3.337217	1.268843
98	1	0	3.976244	-4.334002	1.445106
99	1	0	4.364416	-2.649122	1.028893
100	1	0	3.053845	-2.999909	2.198778
101	7	0	2.612171	-3.428339	0.137856
102	7	0	-0.883150	-0.191621	2.170375

PhOMe **8**
Sum of electronic and thermal Free Energies = -346.527941 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.860299	-0.998039	0.000017
2	6	0	2.286998	0.338836	-0.000003
3	6	0	1.331992	1.358073	-0.000030
4	6	0	-0.038928	1.062735	-0.000038
5	6	0	-0.456057	-0.278580	-0.000015
6	6	0	0.501417	-1.309454	0.000012
7	1	0	2.591874	-1.804558	0.000039
8	1	0	1.646391	2.400681	-0.000048
9	1	0	-0.761915	1.872850	-0.000064
10	1	0	0.160668	-2.342928	0.000029
11	1	0	3.348337	0.578218	0.000003
12	8	0	-1.765677	-0.685043	-0.000029
13	6	0	-2.775385	0.333732	0.000062
14	1	0	-3.731659	-0.196623	0.000122
15	1	0	-2.695083	0.964425	0.897830
16	1	0	-2.695217	0.964456	-0.897698

MeOH **9**
Sum of electronic and thermal Free Energies = -438.695792 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.048307	1.172228	0.000000
2	1	0	1.101385	1.472383	0.000000
3	1	0	-0.437951	1.561507	0.900067
4	1	0	-0.437951	1.561507	-0.900067
5	16	0	0.048307	-0.674164	0.000000
6	1	0	-1.288231	-0.842143	0.000000

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Sum of electronic and thermal Free Energies = -3390.844002 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.021516	-0.089848	0.468009
2	7	0	1.632319	-0.307739	0.440861
3	7	0	-0.681789	-0.883340	-0.770393
4	7	0	-0.364093	1.494753	0.396288
5	15	0	-1.486170	-2.237728	-0.905815
6	15	0	-0.948329	2.560595	-0.610399
7	15	0	3.078578	-0.131709	-0.104055
8	7	0	0.261151	3.296664	-1.532861
9	7	0	-1.631885	3.888326	0.179525
10	7	0	-2.087087	1.933078	-1.675684
11	7	0	-0.499997	-3.588082	-0.625426
12	7	0	-2.148430	-2.182324	-2.468600
13	7	0	-2.824011	-2.625104	0.027009
14	6	0	0.259720	-0.897004	3.188637
15	6	0	-0.751816	-1.323188	4.270165
16	1	0	-0.231094	-1.426275	5.232536
17	1	0	-1.558537	-0.587159	4.363896
18	1	0	-1.202919	-2.288834	4.006058
19	6	0	0.955689	0.412297	3.622013
20	1	0	0.211111	1.206379	3.753398
21	1	0	1.486604	0.260495	4.574082
22	1	0	1.679680	0.725496	2.860898
23	6	0	1.302406	-2.021124	3.033961
24	1	0	1.804166	-2.194472	3.997749
25	1	0	0.805120	-2.949302	2.720296
26	1	0	2.045966	-1.748728	2.283226
27	6	0	-4.147848	-2.026692	-0.216324
28	1	0	-4.914505	-2.775296	0.037611
29	1	0	-4.292490	-1.136654	0.414573
30	1	0	-4.253082	-1.753928	-1.269527
31	6	0	-2.674541	-3.078558	1.423777
32	1	0	-2.914430	-2.254944	2.112182
33	1	0	-3.367415	-3.918755	1.595829
34	1	0	-1.649452	-3.406593	1.610230
35	6	0	-1.009491	-4.962209	-0.651966
36	1	0	-0.537433	-5.538026	0.160254
37	1	0	-2.092288	-4.970890	-0.499840
38	1	0	-0.775878	-5.460055	-1.609752
39	6	0	0.953299	-3.512541	-0.784677
40	1	0	1.302012	-2.488554	-0.649062
41	1	0	1.427463	-4.142920	-0.015730
42	1	0	1.272153	-3.881050	-1.777205
43	6	0	-1.595357	-1.286959	-3.490488
44	1	0	-0.738768	-1.741362	-4.022926
45	1	0	-2.385398	-1.077035	-4.228280
46	1	0	-1.277674	-0.350463	-3.023498
47	6	0	-2.753947	-3.398219	-3.017102
48	1	0	-3.515049	-3.113973	-3.759076
49	1	0	-2.010385	-4.047705	-3.514440
50	1	0	-3.245075	-3.966977	-2.220459
51	6	0	-3.087915	3.871630	0.424589
52	1	0	-3.374408	4.863480	0.800660
53	1	0	-3.618075	3.697668	-0.518496
54	1	0	-3.393126	3.103075	1.151425
55	6	0	-0.840400	4.495335	1.262245
56	1	0	-0.931431	3.933917	2.204960
57	1	0	0.216139	4.531457	0.970189
58	1	0	-1.196194	5.524267	1.420060
59	6	0	-3.158291	1.047086	-1.196197
60	1	0	-4.126639	1.576101	-1.207739
61	1	0	-3.217328	0.168113	-1.849948
62	1	0	-2.968694	0.720533	-0.167554
63	6	0	-2.399642	2.604240	-2.937216
64	1	0	-2.710846	1.844328	-3.669721
65	1	0	-3.223222	3.334087	-2.827742
66	1	0	-1.518666	3.120610	-3.330685
67	6	0	0.213202	4.665523	-2.048764
68	1	0	1.191858	5.147287	-1.889808
69	1	0	-0.002411	4.682099	-3.133097
70	1	0	-0.558836	5.234895	-1.524218
71	6	0	1.196906	2.430823	-2.243941
72	1	0	2.201413	2.878252	-2.230459
73	1	0	1.258926	1.462939	-1.745350
74	1	0	0.889530	2.276700	-3.294814
75	6	0	4.618255	-1.116391	-2.208580
76	1	0	4.869342	-0.355037	-2.968532
77	1	0	5.392483	-1.121607	-1.436038
78	1	0	4.603292	-2.100548	-2.703364
79	6	0	2.853254	2.510504	0.669541
80	1	0	1.843242	2.183563	0.925871
81	1	0	3.423533	2.728181	1.591493
82	1	0	2.771338	3.437298	0.081635
83	6	0	4.378168	-2.364604	0.825301
84	1	0	3.787461	-2.786332	1.654606
85	1	0	4.011585	-2.783253	-0.116606
86	1	0	5.430367	-2.658130	0.960579
87	6	0	2.223641	-0.844295	-2.606193
88	1	0	2.241996	-1.796032	-3.159183
89	1	0	1.247320	-0.752875	-2.120979
90	1	0	2.355966	-0.020653	-3.329075
91	7	0	3.302619	-0.861116	-1.612485
92	6	0	4.858914	1.899466	-0.599545
93	1	0	5.286887	1.157185	-1.278072
94	1	0	4.779444	2.855841	-1.139593
95	1	0	5.553604	2.039011	0.248897
96	7	0	3.527327	1.496125	-0.146795
97	6	0	4.696223	-0.280751	2.066205
98	1	0	5.725455	-0.589669	2.301032
99	1	0	4.670538	0.811064	1.988700
100	1	0	4.036645	-0.592748	2.893172
101	7	0	4.297465	-0.895376	0.792140
102	7	0	-0.514331	-0.737793	1.921952
103	1	0	-1.500058	-0.446571	2.093504
104	16	0	-3.582549	0.498594	2.578829
105	6	0	-2.479317	1.806327	3.290155
106	1	0	-1.596176	1.931600	2.649691
107	1	0	-2.999269	2.772551	3.360272
108	1	0	-2.140014	1.537072	4.301640

TS-1a

Sum of electronic and thermal Free Energies = -3737.343520 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.313367	4.003401	-1.208977
2	6	0	4.680746	4.306237	-1.296124
3	6	0	5.611451	3.285560	-1.064343
4	6	0	5.194506	1.988452	-0.746329
5	6	0	3.815485	1.678487	-0.654381
6	6	0	2.877041	2.713433	-0.900070
7	1	0	2.575839	4.783863	-1.393556
8	1	0	6.678536	3.498235	-1.128784
9	1	0	5.932381	1.211614	-0.562915
10	1	0	1.816534	2.486456	-0.827502
11	1	0	5.012135	5.313261	-1.543040
12	15	0	-0.452014	-0.114110	-0.323418
13	7	0	-1.803192	-0.558155	-1.115201
14	7	0	-0.304284	-0.841806	1.117343
15	7	0	-0.370767	1.501351	-0.121539
16	15	0	0.185970	-2.143026	1.862008
17	15	0	-0.570130	2.560929	1.025203
18	15	0	-3.360294	-0.540041	-1.260868
19	7	0	-2.182872	2.810436	1.458576
20	7	0	-0.007313	4.032538	0.444021
21	7	0	0.231233	2.177701	2.444894
22	7	0	-0.800615	-3.473594	1.484589
23	7	0	0.100312	-1.814903	3.509366
24	7	0	1.771728	-2.685055	1.690900
25	6	0	0.845162	-0.472952	-2.813809
26	6	0	2.317896	-0.590719	-3.247676
27	1	0	2.374752	-0.560964	-4.344335
28	1	0	2.909443	0.235261	-2.836193
29	1	0	2.748636	-1.536697	-2.898570
30	6	0	0.287259	0.879257	-3.310768
31	1	0	0.838272	1.707128	-2.847789
32	1	0	0.394822	0.944070	-4.403605
33	1	0	-0.774696	0.974853	-3.056755

34	6	0	0.049848	-1.635405	-3.433413
35	1	0	0.104971	-1.579859	-4.530630
36	1	0	0.473156	-2.594809	-3.105448
37	1	0	-0.995101	-1.582982	-3.119589
38	6	0	2.858653	-1.791193	2.151223
39	1	0	3.799725	-2.351753	2.092269
40	1	0	2.945554	-0.884840	1.540134
41	1	0	2.679022	-1.505786	3.193247
42	6	0	2.060694	-3.432269	0.443422
43	1	0	1.830498	-2.840299	-0.456552
44	1	0	3.128758	-3.688506	0.433301
45	1	0	1.474714	-4.358624	0.420135
46	6	0	-0.658517	-4.716945	2.250207
47	1	0	0.153954	-5.357984	1.862966
48	1	0	-0.467067	-4.505248	3.305105
49	1	0	-1.602651	-5.277607	2.180544
50	6	0	-1.277410	-3.704337	0.115161
51	1	0	-1.371061	-2.762108	-0.427492
52	1	0	-0.603131	-4.376723	-0.443254
53	1	0	-2.272290	-4.173316	0.167248
54	6	0	-0.911958	-0.889893	4.026228
55	1	0	-1.844675	-1.411923	4.306255
56	1	0	-0.507776	-0.401846	4.925835
57	1	0	-1.124789	-0.121191	3.279223
58	6	0	0.715437	-2.657384	4.538997
59	1	0	1.237606	-2.015814	5.266638
60	1	0	-0.043111	-3.246229	5.084160
61	1	0	1.440269	-3.339310	4.084894
62	6	0	0.623122	5.037983	1.296457
63	1	0	-0.073072	5.853973	1.564912
64	1	0	0.995588	4.576236	2.215633
65	1	0	1.480626	5.469748	0.759794
66	6	0	-0.416815	4.504385	-0.880036
67	1	0	0.420892	5.045710	-1.341887
68	1	0	-0.666835	3.648455	-1.514077
69	1	0	-1.284919	5.186823	-0.826022
70	6	0	1.566580	1.567685	2.415099
71	1	0	2.333518	2.293710	2.735189
72	1	0	1.577042	0.703229	3.093255
73	1	0	1.811054	1.218484	1.409276
74	6	0	-0.167664	2.687240	3.755715
75	1	0	-0.124468	1.868140	4.489108
76	1	0	0.504208	3.493309	4.100337
77	1	0	-1.191473	3.073599	3.724830
78	6	0	-2.776037	4.115584	1.728520
79	1	0	-3.770662	4.170251	1.256091
80	1	0	-2.902928	4.293342	2.812762
81	1	0	-2.151005	4.912232	1.314678
82	6	0	-2.968425	1.672667	1.933071
83	1	0	-3.945122	1.656607	1.428849
84	1	0	-2.451285	0.738664	1.697710
85	1	0	-3.122075	1.721187	3.026518
86	6	0	-5.512766	-2.054696	-0.329173
87	1	0	-6.220285	-1.572961	0.368352
88	1	0	-5.855104	-1.893986	-1.355077
89	1	0	-5.508424	-3.136517	-0.118056
90	6	0	-3.218156	2.187367	-1.652844
91	1	0	-2.150618	1.962343	-1.627321
92	1	0	-3.517027	2.482987	-2.675210
93	1	0	-3.401344	3.030564	-0.972339
94	6	0	-3.675938	-2.624497	-2.991661
95	1	0	-2.695791	-2.788735	-3.467794
96	1	0	-3.714233	-3.196278	-2.059175
97	1	0	-4.461220	-2.994579	-3.667604
98	6	0	-3.658566	-1.658472	1.217805
99	1	0	-3.734151	-2.712862	1.522423
100	1	0	-2.606528	-1.372588	1.273911
101	1	0	-4.247893	-1.045233	1.921406
102	7	0	-4.159158	-1.520168	-0.151260
103	6	0	-5.430806	1.247551	-1.173002
104	1	0	-5.945116	0.430468	-0.659210
105	1	0	-5.642655	2.180849	-0.629477
106	1	0	-5.842481	1.340759	-2.194583
107	7	0	-3.983307	1.028732	-1.179765
108	6	0	-3.818822	-0.366861	-3.927425
109	1	0	-4.497541	-0.774292	-4.690240
110	1	0	-4.125201	0.660930	-3.708791
111	1	0	-2.794552	-0.356553	-4.338497
112	7	0	-3.921674	-1.197816	-2.720055
113	7	0	0.827489	-0.599888	-1.316110
114	1	0	1.700751	-0.209589	-0.923547
115	8	0	3.361994	0.460941	-0.334777
116	6	0	4.499079	-0.993353	-0.584819
117	1	0	3.666597	-1.674074	-0.571957
118	1	0	4.922651	-0.697628	-1.535104
119	1	0	5.088540	-0.865976	0.311267
120	16	0	5.739757	-3.241823	-0.905835
121	6	0	4.601083	-3.680176	-2.291318
122	1	0	4.740705	-3.006295	-3.148835
123	1	0	4.789112	-4.708528	-2.629503
124	1	0	3.548226	-3.613314	-1.974976

TS-1b

Sum of electronic and thermal Free Energies = -3737.339672 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.247465	0.177505	-2.332823
2	6	0	6.240879	1.511238	-1.889587
3	6	0	6.022605	1.763908	-0.528335
4	6	0	5.802542	0.719122	0.373881
5	6	0	5.784019	-0.635789	-0.060298
6	6	0	6.022810	-0.874157	-1.444432
7	1	0	6.424646	-0.042420	-3.386301
8	1	0	6.023443	2.790610	-0.160985
9	1	0	5.642649	0.937315	1.427356
10	1	0	6.013921	-1.904909	-1.797580
11	1	0	6.416225	2.329464	-2.585814
12	15	0	-0.942699	0.046144	0.560369
13	7	0	-2.535022	0.213120	0.296495
14	7	0	-0.085354	1.024902	-0.405946
15	7	0	-0.424149	-1.493072	0.374082
16	15	0	0.618611	2.437695	-0.397168
17	15	0	0.207840	-2.358111	-0.795584
18	15	0	-3.853244	0.072964	-0.524456
19	7	0	-0.847683	-2.689862	-2.067812
20	7	0	0.617161	-3.898444	-0.233301
21	7	0	1.549362	-1.632634	-1.487532
22	7	0	-0.521261	3.662220	-0.687970
23	7	0	1.763404	2.418773	-1.622472
24	7	0	1.526030	2.945790	0.927560
25	6	0	-1.698964	0.364007	3.292657
26	6	0	-0.941344	0.666936	4.598688
27	1	0	-1.636355	0.585434	5.445862
28	1	0	-0.105870	-0.029446	4.742069
29	1	0	-0.534074	1.687399	4.574387
30	6	0	-2.298622	-1.056702	3.367345
31	1	0	-1.496351	-1.795708	3.485364
32	1	0	-2.982434	-1.133027	4.225915
33	1	0	-2.856194	-1.283069	2.451281
34	6	0	-2.816385	1.410980	3.133632
35	1	0	-3.487535	1.360733	4.003517
36	1	0	-2.380167	2.417815	3.081465
37	1	0	-3.389111	1.226682	2.224431
38	6	0	2.691498	2.133962	1.329824
39	1	0	3.394434	2.784751	1.870400
40	1	0	2.400405	1.301231	1.990733
41	1	0	3.201806	1.739394	0.447226
42	6	0	0.836938	3.565148	2.071267
43	1	0	0.359403	2.807953	2.711279
44	1	0	1.582061	4.122185	2.657134
45	1	0	0.077015	4.271114	1.721229
46	6	0	-0.067967	5.023108	-0.990167
47	1	0	0.089989	5.623968	-0.075767
48	1	0	0.864207	5.001722	-1.561491
49	1	0	-0.834780	5.522143	-1.601780
50	6	0	-1.860671	3.616655	-0.091269
51	1	0	-2.153914	2.585725	0.117708
52	1	0	-1.913506	4.199243	0.845892
53	1	0	-2.579808	4.047543	-0.805182
54	6	0	1.541342	1.613541	-2.828942
55	1	0	1.063701	2.204697	-3.630666
56	1	0	2.518077	1.261204	-3.192128
57	1	0	0.926061	0.742081	-2.586396
58	6	0	2.842487	3.404225	-1.757908
59	1	0	3.788510	2.875680	-1.947932
60	1	0	2.646750	4.095487	-2.596972
61	1	0	2.942722	3.981306	-0.834069

62	6	0	2.007731	-4.172768	0.163523
63	1	0	2.172834	-5.258538	0.110037
64	1	0	2.708046	-3.683201	-0.518904
65	1	0	2.217348	-3.835186	1.190220
66	6	0	-0.374418	-4.585907	0.608758
67	1	0	-0.339706	-4.229300	1.651228
68	1	0	-1.382640	-4.419786	0.213044
69	1	0	-0.163120	-5.665154	0.589034
70	6	0	2.520167	-0.910749	-0.653169
71	1	0	3.389310	-1.540325	-0.427073
72	1	0	2.860073	-0.015392	-1.186211
73	1	0	2.044320	-0.599107	0.278519
74	6	0	2.112618	-2.128609	-2.745583
75	1	0	2.546547	-1.280244	-3.294082
76	1	0	2.912998	-2.870200	-2.575325
77	1	0	1.330828	-2.584246	-3.362414
78	6	0	-0.965335	-3.962616	-2.775414
79	1	0	-2.031596	-4.210739	-2.909054
80	1	0	-0.499233	-3.905729	-3.776558
81	1	0	-0.478230	-4.757698	-2.204877
82	6	0	-1.367185	-1.544648	-2.815383
83	1	0	-2.447688	-1.658954	-2.976680
84	1	0	-1.201458	-0.621060	-2.255801
85	1	0	-0.856555	-1.451754	-3.791193
86	6	0	-5.150977	1.421662	-2.587618
87	1	0	-5.160302	0.933744	-3.577850
88	1	0	-6.029266	1.101220	-2.020191
89	1	0	-5.207209	2.511385	-2.742603
90	6	0	-3.567790	-2.653618	-0.217757
91	1	0	-2.690225	-2.333901	0.347540
92	1	0	-4.323800	-3.075142	0.470472
93	1	0	-3.253154	-3.439775	-0.918948
94	6	0	-5.521556	1.942988	0.607567
95	1	0	-5.172577	2.199251	1.620831
96	1	0	-5.012969	2.589550	-0.113995
97	1	0	-6.604649	2.132155	0.552537
98	6	0	-2.707930	1.537747	-2.550602
99	1	0	-2.801884	2.608818	-2.786467
100	1	0	-1.828062	1.407588	-1.916325
101	1	0	-2.568220	0.984242	-3.494600
102	7	0	-3.921726	1.101177	-1.855284
103	6	0	-5.268682	-1.892443	-1.809621
104	1	0	-5.535570	-1.080362	-2.491144
105	1	0	-5.010770	-2.774629	-2.414802
106	1	0	-6.151377	-2.141393	-1.192697
107	7	0	-4.109668	-1.531301	-0.991317
108	6	0	-5.830894	-0.387169	1.288098
109	1	0	-6.908686	-0.188935	1.382971
110	1	0	-5.698245	-1.426558	0.972322
111	1	0	-5.360430	-0.252882	2.276842
112	7	0	-5.268380	0.529181	0.288302
113	7	0	-0.702360	0.498844	2.177558
114	1	0	0.226087	0.185239	2.490360
115	8	0	5.527940	-1.655471	0.745956
116	6	0	4.237621	-1.274943	2.125157
117	1	0	3.799971	-2.256436	2.014983
118	1	0	4.943486	-1.099810	2.924927
119	1	0	3.817829	-0.434912	1.599726
120	16	0	2.322248	-0.862503	3.742561
121	6	0	1.374528	-2.404704	3.380135
122	1	0	2.043451	-3.277640	3.377581
123	1	0	0.617348	-2.567362	4.160238
124	1	0	0.862441	-2.336024	2.411852

Int-2a

Sum of electronic and thermal Free Energies= -3737.359905 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.023009	4.201577	-0.905362
2	6	0	4.289512	4.800853	-0.965535
3	6	0	5.424373	3.986330	-0.986336
4	6	0	5.308077	2.590206	-0.946257
5	6	0	4.032480	2.004027	-0.884706
6	6	0	2.883611	2.814646	-0.868438
7	1	0	2.129819	4.818214	-0.885275
8	1	0	6.417087	4.431427	-1.033953
9	1	0	6.202609	1.975931	-0.963131
10	1	0	1.898007	2.356756	-0.814390
11	1	0	4.386916	5.884356	-0.996114
12	15	0	-0.491473	-0.137418	-0.307250
13	7	0	-1.885231	-0.555391	-1.027094
14	7	0	-0.285857	-0.844550	1.135594
15	7	0	-0.327509	1.483908	-0.155233
16	15	0	0.324900	-2.181209	1.741144
17	15	0	-0.583190	2.523537	1.008292
18	15	0	-3.447771	-0.537374	-1.103449
19	7	0	-2.171845	2.656323	1.552737
20	7	0	-0.153707	4.035429	0.397731
21	7	0	0.310554	2.189220	2.383909
22	7	0	-0.749626	-3.477711	1.537585
23	7	0	0.547107	-1.894395	3.382583
24	7	0	1.837127	-2.709806	1.253822
25	6	0	0.700014	-0.606589	-2.855480
26	6	0	2.146039	-0.850415	-3.323946
27	1	0	2.176448	-0.861427	-4.421629
28	1	0	2.808328	-0.056995	-2.957760
29	1	0	2.517302	-1.813788	-2.951492
30	6	0	0.222770	0.772290	-3.359232
31	1	0	0.853672	1.568289	-2.943662
32	1	0	0.280061	0.807018	-4.457016
33	1	0	-0.815335	0.952591	-3.054869
34	6	0	-0.200687	-1.719481	-3.418163
35	1	0	-0.162428	-1.702516	-4.516969
36	1	0	0.149611	-2.698928	-3.065911
37	1	0	-1.231363	-1.572047	-3.089223
38	6	0	2.963848	-1.766381	1.411014
39	1	0	3.884971	-2.292981	1.123242
40	1	0	2.852786	-0.877797	0.774178
41	1	0	3.031680	-1.440180	2.455730
42	6	0	1.926512	-3.587359	0.062940
43	1	0	1.636031	-3.054459	-0.854656
44	1	0	2.971091	-3.921373	-0.020435
45	1	0	1.281410	-4.462191	0.198523
46	6	0	-0.563080	-4.699300	2.329204
47	1	0	0.171375	-5.387561	1.874397
48	1	0	-0.236552	-4.453555	3.343558
49	1	0	-1.529901	-5.220102	2.396473
50	6	0	-1.390756	-3.728507	0.239980
51	1	0	-1.497649	-2.799221	-0.323523
52	1	0	-0.818828	-4.451044	-0.365988
53	1	0	-2.394813	-4.142182	0.420152
54	6	0	-0.386135	-1.042486	4.122452
55	1	0	-1.185423	-1.632378	4.605831
56	1	0	0.171920	-0.510358	4.908077
57	1	0	-0.826908	-0.302796	3.449318
58	6	0	1.412587	-2.711423	4.239498
59	1	0	2.051835	-2.048802	4.844192
60	1	0	0.818006	-3.336992	4.928040
61	1	0	2.048776	-3.356788	3.627274
62	6	0	0.243601	5.127731	1.287906
63	1	0	-0.603472	5.776795	1.574349
64	1	0	0.703170	4.724948	2.195693
65	1	0	0.992803	5.746674	0.774049
66	6	0	-0.623482	4.451068	-0.928003
67	1	0	0.102093	5.155080	-1.359099
68	1	0	-0.690856	3.575730	-1.580315
69	1	0	-1.605972	4.955702	-0.889241
70	6	0	1.635268	1.560756	2.305183
71	1	0	2.418223	2.268123	2.625004
72	1	0	1.653060	0.671228	2.950071
73	1	0	1.843229	1.243726	1.281947
74	6	0	-0.044345	2.669782	3.719102
75	1	0	-0.019928	1.829499	4.429456
76	1	0	0.667918	3.437533	4.067955
77	1	0	-1.051385	3.099442	3.717582
78	6	0	-2.939381	3.890983	1.656055
79	1	0	-3.935888	3.743046	1.207982
80	1	0	-3.079873	4.191497	2.710472
81	1	0	-2.441862	4.705290	1.124432
82	6	0	-2.823303	1.487245	2.141472
83	1	0	-3.772107	1.292134	1.621393
84	1	0	-2.184191	0.606714	2.030362
85	1	0	-3.018665	1.645305	3.216988
86	6	0	-5.575820	-1.997954	-0.051468
87	1	0	-6.234369	-1.506146	0.685315
88	1	0	-5.969963	-1.826589	-1.056781
89	1	0	-5.580252	-3.080624	0.154506

90	6	0	-3.290770	2.172234	-1.570305
91	1	0	-2.224206	1.941234	-1.562279
92	1	0	-3.610709	2.425874	-2.597424
93	1	0	-3.456906	3.047697	-0.928310
94	6	0	-3.870480	-2.651904	-2.775785
95	1	0	-2.918498	-2.843901	-3.296049
96	1	0	-3.872123	-3.203301	-1.830453
97	1	0	-4.695223	-3.021077	-3.403283
98	6	0	-3.626645	-1.668803	1.390566
99	1	0	-3.723879	-2.725310	1.680946
100	1	0	-2.564090	-1.419454	1.388308
101	1	0	-4.152445	-1.050482	2.137413
102	7	0	-4.203875	-1.489864	0.056397
103	6	0	-5.496192	1.273188	-0.982252
104	1	0	-5.997383	0.486830	-0.410723
105	1	0	-5.683029	2.233430	-0.479032
106	1	0	-5.942020	1.318598	-1.992544
107	7	0	-4.050214	1.041539	-1.025007
108	6	0	-4.031216	-0.411165	-3.752147
109	1	0	-4.749372	-0.831221	-4.470595
110	1	0	-4.322136	0.622528	-3.541737
111	1	0	-3.029257	-0.415794	-4.214831
112	7	0	-4.077489	-1.215176	-2.523509
113	7	0	0.722478	-0.694145	-1.355249
114	1	0	1.625967	-0.377732	-1.003421
115	8	0	3.813251	0.651869	-0.831489
116	6	0	4.969113	-0.217473	-0.878551
117	1	0	4.608046	-1.245336	-0.816023
118	1	0	5.517887	-0.064340	-1.817186
119	1	0	5.628405	-0.013920	-0.024702
120	16	0	5.580896	-3.849624	-0.608001
121	6	0	4.727965	-3.646793	-2.243568
122	1	0	4.876527	-2.635716	-2.654518
123	1	0	5.111675	-4.365535	-2.982479
124	1	0	3.640830	-3.809288	-2.156206

Int-2b

Sum of electronic and thermal Free Energies = -3737.369217 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.245028	1.248505	-1.776511
2	6	0	6.056956	2.181478	-0.745022
3	6	0	5.779491	1.721374	0.545171
4	6	0	5.679774	0.351546	0.820621
5	6	0	5.877461	-0.573957	-0.216990
6	6	0	6.159991	-0.119228	-1.518354
7	1	0	6.461905	1.588595	-2.788257
8	1	0	5.622456	2.431394	1.354871
9	1	0	5.422071	0.019967	1.821953
10	1	0	6.301955	-0.850849	-2.311525
11	1	0	6.126762	3.248400	-0.946840
12	15	0	-0.976093	0.060321	0.543982
13	7	0	-2.602925	0.155369	0.449595
14	7	0	-0.288474	1.064658	-0.536794
15	7	0	-0.429737	-1.456719	0.309726
16	15	0	0.359090	2.502987	-0.567295
17	15	0	0.317657	-2.292276	-0.804110
18	15	0	-3.916641	-0.147936	-0.342527
19	7	0	-0.696594	-2.797212	-2.056682
20	7	0	0.901204	-3.759182	-0.194631
21	7	0	1.585881	-1.458414	-1.515257
22	7	0	-0.841632	3.662417	-0.885090
23	7	0	1.489635	2.512415	-1.811386
24	7	0	1.258374	3.104923	0.723035
25	6	0	-1.476096	0.570446	3.307422
26	6	0	-0.578857	0.857897	4.527115
27	1	0	-1.197786	0.870481	5.435312
28	1	0	0.205693	0.097798	4.623341
29	1	0	-0.089566	1.835931	4.421812
30	6	0	-2.213356	-0.769099	3.531259
31	1	0	-1.485486	-1.581459	3.643063
32	1	0	-2.825237	-0.712630	4.444328
33	1	0	-2.867125	-0.988614	2.680217
34	6	0	-2.492103	1.720024	3.167153
35	1	0	-3.131990	1.755698	4.061326
36	1	0	-1.965204	2.678798	3.074301
37	1	0	-3.114644	1.572032	2.282567
38	6	0	2.465443	2.368041	1.147417
39	1	0	3.126867	3.073487	1.671372
40	1	0	2.221547	1.530933	1.820207
41	1	0	2.997647	1.981395	0.275388
42	6	0	0.561140	3.738644	1.851473
43	1	0	0.176961	2.983113	2.551204
44	1	0	1.276394	4.391108	2.373830
45	1	0	-0.269656	4.354583	1.493680
46	6	0	-0.461889	5.034485	-1.230027
47	1	0	-0.331900	5.670662	-0.335055
48	1	0	0.468581	5.043995	-1.804953
49	1	0	-1.255366	5.475247	-1.852626
50	6	0	-2.171805	3.561961	-0.274650
51	1	0	-2.400402	2.523584	-0.024126
52	1	0	-2.250771	4.174545	0.641514
53	1	0	-2.921523	3.923641	-0.995609
54	6	0	1.287335	1.669749	-2.994567
55	1	0	0.777846	2.221003	-3.805227
56	1	0	2.272850	1.345579	-3.361694
57	1	0	0.711507	0.780621	-2.721356
58	6	0	2.525104	3.535275	-1.979600
59	1	0	3.494453	3.043191	-2.155829
60	1	0	2.303330	4.191049	-2.840488
61	1	0	2.602652	4.145126	-1.074933
62	6	0	2.284263	-3.754634	0.329353
63	1	0	2.555327	-4.793641	0.562664
64	1	0	2.972337	-3.386054	-0.438874
65	1	0	2.398532	-3.133466	1.231478
66	6	0	-0.038694	-4.547309	0.620661
67	1	0	-0.147856	-4.136026	1.636551
68	1	0	-1.022847	-4.565308	0.137795
69	1	0	0.338243	-5.578355	0.687245
70	6	0	2.505198	-0.657788	-0.691099
71	1	0	3.462663	-1.181616	-0.589267
72	1	0	2.670954	0.313192	-1.172801
73	1	0	2.099337	-0.504783	0.313738
74	6	0	2.184246	-1.931368	-2.764280
75	1	0	2.584588	-1.064739	-3.310486
76	1	0	3.015899	-2.636471	-2.583431
77	1	0	1.432853	-2.420864	-3.392515
78	6	0	-0.595764	-4.067041	-2.774358
79	1	0	-1.602883	-4.499526	-2.896163
80	1	0	-0.161854	-3.925151	-3.781704
81	1	0	0.032453	-4.764862	-2.214364
82	6	0	-1.411725	-1.756372	-2.793072
83	1	0	-2.447691	-2.071854	-2.979656
84	1	0	-1.437779	-0.833389	-2.210467
85	1	0	-0.917195	-1.545928	-3.759452
86	6	0	-5.460000	1.121309	-2.294846
87	1	0	-5.524265	0.640793	-3.287187
88	1	0	-6.269329	0.746695	-1.662299
89	1	0	-5.586412	2.207448	-2.433775
90	6	0	-3.387905	-2.841301	-0.047196
91	1	0	-2.592436	-2.443780	0.585983
92	1	0	-4.136893	-3.369251	0.571091
93	1	0	-2.932168	-3.558341	-0.744943
94	6	0	-5.633457	1.527555	0.964159
95	1	0	-5.209665	1.741779	1.958726
96	1	0	-5.223908	2.243456	0.244021
97	1	0	-6.725252	1.658972	1.012840
98	6	0	-3.028741	1.281284	-2.504134
99	1	0	-3.172414	2.333939	-2.791258
100	1	0	-2.088214	1.209421	-1.950645
101	1	0	-2.965977	0.674973	-3.424376
102	7	0	-4.158805	0.861262	-1.670439
103	6	0	-5.074055	-2.216904	-1.712738
104	1	0	-5.387780	-1.416256	-2.388325
105	1	0	-4.695951	-3.051231	-2.323565
106	1	0	-5.956141	-2.572997	-1.149436
107	7	0	-4.002809	-1.761749	-0.827260
108	6	0	-5.769975	-0.850038	1.515814
109	1	0	-6.838419	-0.696579	1.726111
110	1	0	-5.640461	-1.859519	1.113369
111	1	0	-5.210719	-0.768067	2.464102
112	7	0	-5.338991	0.152031	0.533022
113	7	0	-0.573353	0.534269	2.113164
114	1	0	0.366225	0.164699	2.357490
115	8	0	5.778043	-1.931619	-0.070886
116	6	0	5.505341	-2.435382	1.256831
117	1	0	5.455954	-3.522583	1.147481

118	1	0	6.324179	-2.162858	1.938358
119	1	0	4.553133	-2.042762	1.645972
120	16	0	2.395546	-0.927056	3.085912
121	6	0	1.175722	-2.274911	3.445075
122	1	0	1.666684	-3.258923	3.472900
123	1	0	0.680980	-2.119837	4.415477
124	1	0	0.405205	-2.293264	2.662070

Int-3a

Sum of electronic and thermal Free Energies = -3737.403433 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.288106	3.354156	-1.954489
2	6	0	5.168621	3.763254	-0.939555
3	6	0	5.244254	2.987268	0.229132
4	6	0	4.458081	1.844981	0.387785
5	6	0	3.549372	1.407722	-0.628264
6	6	0	3.497238	2.212082	-1.809822
7	1	0	4.213855	3.939482	-2.872425
8	1	0	5.924358	3.282265	1.029776
9	1	0	4.529167	1.252961	1.299371
10	1	0	2.816397	1.920096	-2.607861
11	1	0	5.782449	4.654092	-1.059125
12	15	0	-0.814040	-0.153893	-0.379667
13	7	0	-2.220416	-0.649859	-1.054794
14	7	0	-0.526037	-0.855485	1.061006
15	7	0	-0.906673	1.457078	-0.167269
16	15	0	0.222257	-2.130922	1.612893
17	15	0	-0.402923	2.590597	0.800295
18	15	0	-3.770633	-0.470879	-0.900276
19	7	0	-1.730874	3.589625	1.132387
20	7	0	0.751784	3.548689	0.056067
21	7	0	0.240794	2.103835	2.276823
22	7	0	-0.515524	-3.569075	1.087065
23	7	0	0.209576	-1.941314	3.299793
24	7	0	1.833469	-2.478136	1.309322
25	6	0	0.357573	-0.635862	-2.930528
26	6	0	1.789926	-0.981209	-3.390042
27	1	0	1.844933	-0.946593	-4.487092
28	1	0	2.512292	-0.276929	-2.961414
29	1	0	2.056222	-1.992323	-3.053824
30	6	0	-0.043187	0.742743	-3.498168
31	1	0	0.634537	1.518160	-3.120246
32	1	0	0.003585	0.733348	-4.597678
33	1	0	-1.066546	0.993240	-3.193646
34	6	0	-0.597146	-1.720916	-3.464624
35	1	0	-0.511423	-1.774633	-4.560334
36	1	0	-0.325097	-2.696896	-3.038842
37	1	0	-1.631561	-1.498297	-3.190108
38	6	0	2.928685	-1.779790	2.009866
39	1	0	3.768557	-2.484497	2.110785
40	1	0	3.249152	-0.906912	1.424117
41	1	0	2.601589	-1.468125	3.005549
42	6	0	2.253328	-2.944637	-0.026663
43	1	0	2.598392	-2.093985	-0.626379
44	1	0	3.079643	-3.660615	0.099274
45	1	0	1.419500	-3.430709	-0.539956
46	6	0	0.019438	-4.894584	1.416932
47	1	0	-0.161241	-5.574016	0.568966
48	1	0	1.096504	-4.836663	1.596464
49	1	0	-0.472819	-5.319866	2.309967
50	6	0	-1.958169	-3.589355	0.831973
51	1	0	-2.303691	-2.608423	0.505281
52	1	0	-2.165516	-4.314391	0.029357
53	1	0	-2.525492	-3.900014	1.729848
54	6	0	-0.710773	-1.010431	3.957629
55	1	0	-1.683133	-1.483201	4.190468
56	1	0	-0.254140	-0.682200	4.904933
57	1	0	-0.873682	-0.141311	3.314364
58	6	0	0.607701	-3.072390	4.140377
59	1	0	1.041220	-2.688373	5.076453
60	1	0	-0.249031	-3.722107	4.397114
61	1	0	1.368024	-3.672925	3.630135
62	6	0	1.794886	4.290235	0.768278
63	1	0	1.580037	5.375662	0.768953
64	1	0	1.863390	3.950642	1.805730
65	1	0	2.760958	4.114699	0.277297
66	6	0	0.547822	3.980140	-1.329117
67	1	0	1.516612	3.968605	-1.845744
68	1	0	-0.129573	3.285487	-1.836381
69	1	0	0.125250	5.001686	-1.371088
70	6	0	1.476862	1.310565	2.315156
71	1	0	2.327730	1.936452	2.634939
72	1	0	1.350036	0.482742	3.024769
73	1	0	1.716083	0.893077	1.331618
74	6	0	-0.076502	2.762954	3.542049
75	1	0	-0.065981	2.007750	4.342575
76	1	0	0.662336	3.545193	3.799487
77	1	0	-1.072237	3.214466	3.510802
78	6	0	-1.565063	4.995458	1.499166
79	1	0	-2.392640	5.578096	1.065004
80	1	0	-1.573644	5.152333	2.593593
81	1	0	-0.622749	5.382623	1.099573
82	6	0	-3.011820	3.004602	1.526690
83	1	0	-3.826452	3.650706	1.163040
84	1	0	-3.122845	2.020107	1.064187
85	1	0	-3.111999	2.914119	2.625332
86	6	0	-5.769703	-1.676229	0.650495
87	1	0	-6.427519	-0.991267	1.215637
88	1	0	-6.206568	-1.853581	-0.335691
89	1	0	-5.717085	-2.628779	1.201886
90	6	0	-3.554822	2.128769	-1.811614
91	1	0	-2.502498	1.851254	-1.883017
92	1	0	-3.998904	2.234490	-2.817776
93	1	0	-3.607935	3.099108	-1.297019
94	6	0	-4.301986	-2.783382	-2.173019
95	1	0	-3.327037	-2.962076	-2.656327
96	1	0	-4.280744	-3.218499	-1.168264
97	1	0	-5.090167	-3.279362	-2.757676
98	6	0	-3.831642	-0.718503	1.799839
99	1	0	-3.877384	-1.571815	2.493235
100	1	0	-2.777877	-0.448253	1.681489
101	1	0	-4.385808	0.126069	2.246575
102	7	0	-4.419343	-1.120640	0.517076
103	6	0	-5.672591	1.487064	-0.750086
104	1	0	-6.119618	0.797621	-0.027814
105	1	0	-5.710265	2.502361	-0.327656
106	1	0	-6.277991	1.473142	-1.674690
107	7	0	-4.273866	1.136842	-1.004059
108	6	0	-4.702204	-0.715525	-3.417431
109	1	0	-5.449700	-1.261361	-4.009884
110	1	0	-5.029553	0.324888	-3.322132
111	1	0	-3.739347	-0.741738	-3.958240
112	7	0	-4.615707	-1.344880	-2.090317
113	7	0	0.395621	-0.643779	-1.439263
114	1	0	1.308055	-0.258356	-1.102339
115	8	0	2.825674	0.332347	-0.471771
116	6	0	5.871491	-1.301888	-0.455275
117	1	0	4.812892	-1.026690	-0.403815
118	1	0	6.374015	-0.712006	-1.231428
119	1	0	6.350398	-1.108576	0.511131
120	16	0	6.061749	-3.095306	-0.795469
121	6	0	5.101889	-3.201007	-2.352864
122	1	0	5.529474	-2.532705	-3.110427
123	1	0	5.165314	-4.237255	-2.704436
124	1	0	4.053603	-2.936136	-2.174999

Int-3b

Sum of electronic and thermal Free Energies = -3737.391090 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.515105	0.935371	-2.318905
2	6	0	5.782036	1.680392	-1.155905
3	6	0	6.007341	0.979144	0.042992
4	6	0	5.936702	-0.411866	0.090688
5	6	0	5.592784	-1.202237	-1.062521
6	6	0	5.433548	-0.457217	-2.285575
7	1	0	5.365058	1.455571	-3.267353
8	1	0	6.237119	1.533598	0.955076
9	1	0	6.095194	-0.936344	1.033477

10	1	0	5.208402	-1.010591	-3.197319
11	1	0	5.848113	2.766533	-1.189904
12	15	0	-1.012367	0.167040	0.572718
13	7	0	-2.618984	0.145737	0.305123
14	7	0	-0.247241	1.071483	-0.533356
15	7	0	-0.337206	-1.307090	0.668428
16	15	0	0.345746	2.525067	-0.705532
17	15	0	0.512848	-2.237558	-0.299921
18	15	0	-3.799332	-0.383230	-0.580710
19	7	0	-0.394439	-2.931018	-1.543502
20	7	0	1.104961	-3.493491	0.647049
21	7	0	1.775618	-1.451340	-1.041887
22	7	0	-0.870319	3.568364	-1.265024
23	7	0	1.594038	2.441009	-1.812674
24	7	0	1.086179	3.318092	0.588192
25	6	0	-1.839702	0.917613	3.213240
26	6	0	-1.099894	1.418929	4.468068
27	1	0	-1.810000	1.502668	5.301672
28	1	0	-0.301108	0.723433	4.756168
29	1	0	-0.652883	2.405353	4.284329
30	6	0	-2.427603	-0.480719	3.504270
31	1	0	-1.620027	-1.185858	3.744207
32	1	0	-3.117064	-0.430074	4.360080
33	1	0	-2.973534	-0.852499	2.630724
34	6	0	-2.960132	1.916749	2.873047
35	1	0	-3.685671	1.953918	3.698604
36	1	0	-2.535460	2.919436	2.729206
37	1	0	-3.468622	1.613651	1.955607
38	6	0	2.271967	2.696820	1.202979
39	1	0	2.866555	3.485790	1.686928
40	1	0	1.989012	1.952027	1.963348
41	1	0	2.888766	2.213799	0.439123
42	6	0	0.263506	4.063657	1.550527
43	1	0	-0.191531	3.390844	2.293114
44	1	0	0.908011	4.793523	2.062246
45	1	0	-0.529226	4.610650	1.030859
46	6	0	-0.520596	4.898676	-1.770226
47	1	0	-0.495698	5.658448	-0.967321
48	1	0	0.454467	4.878026	-2.265002
49	1	0	-1.275353	5.205056	-2.510149
50	6	0	-2.245342	3.475660	-0.762320
51	1	0	-2.457105	2.463817	-0.408455
52	1	0	-2.431750	4.188199	0.061574
53	1	0	-2.938645	3.712839	-1.584261
54	6	0	1.609468	1.406738	-2.854566
55	1	0	1.204886	1.790671	-3.807982
56	1	0	2.651941	1.095487	-3.010468
57	1	0	1.036025	0.537483	-2.521896
58	6	0	2.589904	3.499940	-2.019012
59	1	0	3.592590	3.049172	-2.001848
60	1	0	2.437461	3.998575	-2.992503
61	1	0	2.521954	4.244819	-1.220652
62	6	0	2.383914	-4.152020	0.349497
63	1	0	2.258560	-5.035782	-0.301428
64	1	0	3.094119	-3.460675	-0.117351
65	1	0	2.821449	-4.487086	1.301471
66	6	0	0.223997	-4.221733	1.561465
67	1	0	0.778726	-4.454574	2.483071
68	1	0	-0.636722	-3.596214	1.819254
69	1	0	-0.133992	-5.171049	1.122602
70	6	0	2.621552	-0.574157	-0.215309
71	1	0	3.409274	-1.150058	0.284611
72	1	0	3.107143	0.165759	-0.859621
73	1	0	1.999272	-0.057064	0.518271
74	6	0	2.440749	-1.995045	-2.243663
75	1	0	2.609682	-1.172192	-2.950107
76	1	0	3.415873	-2.436914	-1.987467
77	1	0	1.799303	-2.743256	-2.721223
78	6	0	-0.296420	-4.331308	-1.943122
79	1	0	-1.301928	-4.711744	-2.186717
80	1	0	0.344794	-4.460442	-2.834536
81	1	0	0.114318	-4.934193	-1.128184
82	6	0	-0.942286	-2.043821	-2.569661
83	1	0	-1.982747	-2.321790	-2.787716
84	1	0	-0.929196	-1.009810	-2.214128
85	1	0	-0.344973	-2.095980	-3.497659
86	6	0	-5.158837	0.425052	-2.876096
87	1	0	-5.040459	-0.170244	-3.797995
88	1	0	-6.005939	0.037277	-2.303741
89	1	0	-5.370267	1.467027	-3.166806
90	6	0	-3.170448	-2.942586	0.236341
91	1	0	-2.484068	-2.388749	0.879476
92	1	0	-3.971376	-3.402060	0.843990
93	1	0	-2.597179	-3.737705	-0.258558
94	6	0	-5.757857	1.336266	0.228351
95	1	0	-5.455164	1.746745	1.205751
96	1	0	-5.322057	1.953289	-0.564171
97	1	0	-6.854639	1.385114	0.152996
98	6	0	-2.751666	0.859421	-2.795976
99	1	0	-2.962871	1.860654	-3.201650
100	1	0	-1.889639	0.939997	-2.128824
101	1	0	-2.506974	0.187445	-3.635601
102	7	0	-3.933637	0.384455	-2.070376
103	6	0	-4.632590	-2.726963	-1.721003
104	1	0	-4.864956	-2.082933	-2.573978
105	1	0	-4.140090	-3.633744	-2.102653
106	1	0	-5.577548	-3.025488	-1.231320
107	7	0	-3.719156	-2.054554	-0.795783
108	6	0	-5.820388	-0.927336	1.152468
109	1	0	-6.911503	-0.813834	1.225893
110	1	0	-5.598835	-1.975966	0.931990
111	1	0	-5.374822	-0.663621	2.127815
112	7	0	-5.333277	-0.063636	0.070005
113	7	0	-0.832254	0.898521	2.104921
114	1	0	0.087971	0.642936	2.468291
115	8	0	5.381268	-2.477204	-0.988636
116	6	0	3.977633	0.164600	3.146696
117	1	0	4.720662	-0.494405	3.611062
118	1	0	4.245073	1.208632	3.343522
119	1	0	3.952066	-0.006703	2.067211
120	16	0	2.332737	-0.113297	3.904025
121	6	0	2.080623	-1.884072	3.505319
122	1	0	2.912427	-2.478135	3.902758
123	1	0	1.150111	-2.185601	3.999170
124	1	0	1.975479	-2.033704	2.427020

TBD

Sum of electronic and thermal Free Energies = -438.462286 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.413520	-0.766463	0.209243
2	6	0	-0.064045	-0.730118	-0.043862
3	6	0	1.200107	1.402034	0.228412
4	6	0	2.447341	0.680543	-0.285760
5	1	0	2.508021	-0.778087	1.312893
6	1	0	3.247584	-1.345676	-0.207164
7	1	0	1.121086	2.406661	-0.211282
8	1	0	1.271325	1.526807	1.327597
9	1	0	2.454246	0.689821	-1.384296
10	1	0	3.347524	1.191980	0.079312
11	6	0	-1.262951	1.383961	0.190284
12	1	0	-1.188329	2.386036	-0.256262
13	1	0	-1.372910	1.512835	1.284945
14	6	0	-2.458777	0.612701	-0.370476
15	1	0	-2.380190	0.583609	-1.466997
16	1	0	-3.395979	1.121463	-0.104906
17	6	0	-2.426400	-0.819362	0.191237
18	1	0	-2.736796	-0.797447	1.252398
19	1	0	-3.167655	-1.442925	-0.332685
20	7	0	-0.022402	0.667760	-0.123471
21	7	0	1.160820	-1.379060	-0.244723
22	7	0	-1.119320	-1.469839	0.086710
23	1	0	1.065616	-2.366870	-0.037635

TS-2a

Sum of electronic and thermal Free Energies = -1223.639416 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.020796	0.927277	0.083002
2	6	0	-5.684859	-0.292523	0.253897

3	6	0	-4.947997	-1.482990	0.169484
4	6	0	-3.574536	-1.455615	-0.079772
5	6	0	-2.899414	-0.224961	-0.253292
6	6	0	-3.644023	0.971226	-0.167944
7	1	0	-5.576443	1.862360	0.144258
8	1	0	-5.447213	-2.442937	0.298195
9	1	0	-3.006138	-2.382781	-0.146045
10	1	0	-3.149175	1.929683	-0.297065
11	1	0	-6.755285	-0.317318	0.447600
12	8	0	-1.568313	-0.249983	-0.486561
13	6	0	-0.638173	1.336863	-0.631015
14	1	0	0.275204	0.825261	-0.883941
15	1	0	-1.181666	1.823642	-1.430600
16	1	0	-0.794747	1.684627	0.379419
17	16	0	1.143398	3.289605	-0.652037
18	6	0	2.412945	2.188826	-1.419700
19	1	0	2.064466	1.794776	-2.386987
20	1	0	3.343345	2.745075	-1.597650
21	1	0	2.651807	1.332202	-0.769324
22	6	0	1.606812	-2.259061	-1.755596
23	6	0	1.363803	-1.139357	0.449802
24	6	0	3.612254	-1.620726	-0.408447
25	6	0	2.978657	-1.582321	-1.802443
26	1	0	1.720871	-3.347536	-1.637895
27	1	0	1.042672	-2.072191	-2.675899
28	1	0	4.535309	-1.030860	-0.390270
29	1	0	3.858249	-2.654287	-0.118303
30	1	0	2.867117	-0.537853	-2.117904
31	1	0	3.629699	-2.100900	-2.515790
32	6	0	3.269479	-0.339092	1.765319
33	1	0	4.237068	0.071896	1.456507
34	1	0	3.444818	-1.065546	2.574624
35	6	0	2.329172	0.779497	2.223011
36	1	0	2.237236	1.544232	1.438248
37	1	0	2.731731	1.250508	3.127241
38	6	0	0.950716	0.186037	2.514463
39	1	0	0.969026	-0.411749	3.437758
40	1	0	0.202813	0.978246	2.631066
41	7	0	2.700459	-1.029188	0.589518
42	7	0	0.818475	-1.724641	-0.637339
43	7	0	0.522705	-0.669050	1.393592
44	1	0	-0.177235	-1.518013	-0.779185
45	1	0	-0.447102	-0.592680	1.072004

TS-2b

Sum of electronic and thermal Free Energies = -1223.645102 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.666278	-0.432618	-0.899982
2	6	0	3.983929	-1.281431	0.172070
3	6	0	3.022342	-2.204914	0.607235
4	6	0	1.767877	-2.280746	-0.005185
5	6	0	1.431595	-1.434922	-1.100078
6	6	0	2.417145	-0.497336	-1.520899
7	1	0	4.402417	0.289034	-1.255775
8	1	0	3.251176	-2.874916	1.436198
9	1	0	1.035969	-3.010188	0.336229
10	1	0	2.183501	0.157372	-2.359624
11	1	0	4.958434	-1.226780	0.653198
12	8	0	0.263210	-1.496819	-1.720177
13	6	0	-1.257251	-1.674511	-0.512645
14	1	0	-1.836278	-1.078604	-1.200139
15	1	0	-1.345228	-2.751427	-0.547919
16	1	0	-0.704411	-1.221374	0.295521
17	16	0	-3.245506	-1.433662	0.980616
18	6	0	-4.517625	-1.477695	-0.357082
19	1	0	-4.852698	-2.507546	-0.531304
20	1	0	-5.385565	-0.868210	-0.075610
21	1	0	-4.106115	-1.084755	-1.298651
22	6	0	0.497380	0.818723	2.726552
23	6	0	-0.736790	1.405915	0.635542
24	6	0	1.590088	2.133239	0.899101
25	6	0	1.749669	0.954903	1.860536
26	1	0	0.445611	1.629379	3.470184
27	1	0	0.494225	-0.139410	3.258951
28	1	0	2.427162	2.151238	0.193806
29	1	0	1.560383	3.093260	1.439126
30	1	0	1.903685	0.042645	1.276111
31	1	0	2.626587	1.114343	2.498383
32	6	0	0.342631	2.491945	-1.282269
33	1	0	1.352092	2.347812	-1.683198
34	1	0	0.121512	3.571381	-1.270905
35	6	0	-0.678471	1.725776	-2.125437
36	1	0	-0.352224	0.681686	-2.222734
37	1	0	-0.745322	2.182130	-3.120432
38	6	0	-2.040328	1.778077	-1.428845
39	1	0	-2.457219	2.796065	-1.463606
40	1	0	-2.757908	1.102664	-1.907940
41	7	0	0.358514	1.977993	0.100911
42	7	0	-0.696308	0.861393	1.871823
43	7	0	-1.908849	1.352688	-0.026073
44	1	0	-1.551459	0.420619	2.193522
45	1	0	-2.550226	0.605778	0.319850

Int-4

Sum of electronic and thermal Free Energies = -877.159517 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-3.246227	0.000238	-0.536927
2	6	0	-3.147248	-0.000195	1.316691
3	1	0	-3.639445	0.889081	1.732563
4	1	0	-3.639412	-0.889687	1.732141
5	1	0	-2.098984	-0.000254	1.655945
6	6	0	0.271853	-2.469155	-0.081838
7	6	0	0.368849	0.000021	-0.172151
8	6	0	2.388383	-1.257205	0.453758
9	6	0	1.782421	-2.427489	-0.327057
10	1	0	0.064977	-2.774322	0.957232
11	1	0	-0.217877	-3.188265	-0.748944
12	1	0	3.446402	-1.124065	0.195047
13	1	0	2.324427	-1.443949	1.539100
14	1	0	1.979259	-2.291231	-1.398795
15	1	0	2.247050	-3.366130	-0.002236
16	6	0	2.388422	1.256963	0.454012
17	1	0	3.446495	1.123728	0.195578
18	1	0	2.324191	1.443688	1.539342
19	6	0	1.782761	2.427305	-0.326951
20	1	0	1.979720	2.290923	-1.398651
21	1	0	2.247501	3.365899	-0.002152
22	6	0	0.272174	2.469265	-0.081904
23	1	0	0.065234	2.774765	0.957052
24	1	0	-0.217365	3.188271	-0.749267
25	7	0	1.698102	-0.000074	0.121459
26	7	0	-0.302303	-1.150707	-0.345409
27	7	0	-0.302204	1.150838	-0.345114
28	1	0	-1.336739	-1.038292	-0.518652
29	1	0	-1.336657	1.038560	-0.518374

Int-5a

Sum of electronic and thermal Free Energies = -1223.685779 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.693670	2.079402	-0.355577
2	6	0	-3.817256	1.259870	-0.496935
3	6	0	-3.923266	0.105136	0.292856
4	6	0	-2.920614	-0.223785	1.204963
5	6	0	-1.791252	0.603974	1.340528
6	6	0	-1.676291	1.761770	0.554624
7	1	0	-2.598370	2.982009	-0.956894
8	1	0	-4.793869	-0.541919	0.200840
9	1	0	-3.002591	-1.108934	1.832311
10	1	0	-0.809025	2.408371	0.641700
11	1	0	-4.601619	1.517280	-1.205167

12	8	0	-0.858461	0.196009	2.253866
13	6	0	0.205084	1.116558	2.576740
14	1	0	0.792780	0.623220	3.354816
15	1	0	0.842347	1.312896	1.705859
16	1	0	-0.214714	2.058011	2.956898
17	16	0	3.468479	1.630402	0.500014
18	6	0	4.490669	0.682380	-0.727369
19	1	0	4.799461	1.329542	-1.559041
20	1	0	5.393908	0.281359	-0.249236
21	1	0	3.918516	-0.162442	-1.141976
22	6	0	0.228238	0.992919	-2.318711
23	6	0	0.790723	-0.637598	-0.535267
24	6	0	-1.184657	-1.029228	-1.931493
25	6	0	-0.479539	-0.183321	-2.996163
26	1	0	-0.516014	1.719957	-1.962240
27	1	0	0.903948	1.502722	-3.016542
28	1	0	-1.610143	-1.937168	-2.376965
29	1	0	-1.997253	-0.460489	-1.458946
30	1	0	0.252807	-0.803658	-3.530433
31	1	0	-1.216038	0.188622	-3.718514
32	6	0	-0.566869	-2.642136	-0.097214
33	1	0	-1.002764	-3.384906	-0.777573
34	1	0	-1.332664	-2.362202	0.641728
35	6	0	0.672975	-3.208389	0.601777
36	1	0	1.359994	-3.625199	-0.147025
37	1	0	0.371253	-4.011207	1.285302
38	6	0	1.371701	-2.086883	1.374708
39	1	0	0.739565	-1.758973	2.213540
40	1	0	2.337936	-2.419920	1.771013
41	7	0	-0.218781	-1.463480	-0.907471
42	7	0	1.026691	0.509999	-1.192694
43	7	0	1.624627	-0.966897	0.468911
44	1	0	1.777514	1.115718	-0.772571
45	1	0	2.313434	-0.218568	0.731936

Int-5b

Sum of electronic and thermal Free Energies = -1223.684945 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.787568	-0.242649	-0.370072
2	6	0	3.894537	-1.497283	0.249559
3	6	0	2.843092	-2.409464	0.124826
4	6	0	1.689425	-2.086192	-0.602787
5	6	0	1.594672	-0.830311	-1.224745
6	6	0	2.649237	0.092489	-1.101692
7	1	0	4.597052	0.480207	-0.281952
8	1	0	2.908195	-3.385484	0.602683
9	1	0	0.880539	-2.806095	-0.677162
10	1	0	2.561912	1.061337	-1.588400
11	1	0	4.783810	-1.755985	0.819997
12	8	0	0.524602	-0.415014	-1.966225
13	6	0	-0.622582	-1.282103	-2.023745
14	1	0	-1.374855	-0.740608	-2.601488
15	1	0	-0.367262	-2.226879	-2.523934
16	1	0	-1.001541	-1.480127	-1.015433
17	16	0	-3.917155	-1.014890	0.556349
18	6	0	-3.418110	-2.581022	-0.307160
19	1	0	-2.418665	-2.913155	0.010571
20	1	0	-4.130381	-3.381518	-0.069099
21	1	0	-3.406193	-2.448340	-1.397935
22	6	0	-0.122786	-0.341630	2.552962
23	6	0	-0.812832	0.976295	0.585942
24	6	0	1.234181	1.622065	1.793684
25	6	0	1.291917	0.174757	2.286643
26	1	0	-0.559228	0.159759	3.432936
27	1	0	-0.114298	-1.420560	2.747351
28	1	0	2.218548	1.932017	1.421381
29	1	0	0.943248	2.305086	2.609652
30	1	0	1.771475	-0.445616	1.524829
31	1	0	1.890642	0.128501	3.204495
32	6	0	0.403376	2.979607	-0.146353
33	1	0	1.474899	3.160279	-0.300254
34	1	0	-0.011076	3.842742	0.401525
35	6	0	-0.309622	2.797232	-1.489452
36	1	0	0.208948	2.028171	-2.071582
37	1	0	-0.293752	3.743483	-2.043501
38	6	0	-1.754198	2.354081	-1.242621
39	1	0	-2.345043	3.185893	-0.825631
40	1	0	-2.232357	2.036811	-2.177413
41	7	0	0.285972	1.766041	0.676476
42	7	0	-0.957396	-0.108810	1.372669
43	7	0	-1.770239	1.218088	-0.322904
44	1	0	-1.908945	-0.554291	1.314641
45	1	0	-2.593609	0.570260	-0.281671

Int-6a

Sum of electronic and thermal Free Energies = -1223.710046 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.405840	-1.323054	0.253727
2	6	0	5.006420	-0.086180	0.530811
3	6	0	4.495868	1.064112	-0.088191
4	6	0	3.403557	0.987077	-0.957986
5	6	0	2.779621	-0.257306	-1.248598
6	6	0	3.312904	-1.412637	-0.613959
7	1	0	4.792652	-2.229516	0.719871
8	1	0	4.953517	2.033811	0.108948
9	1	0	3.022364	1.887646	-1.439361
10	1	0	2.860137	-2.381057	-0.826680
11	1	0	5.857528	-0.021555	1.205923
12	8	0	1.706129	-0.329794	-2.033701
13	6	0	-3.470914	-1.677635	-1.381716
14	1	0	-2.378381	-1.613662	-1.315299
15	1	0	-3.786858	-1.726002	-2.430806
16	1	0	-3.821462	-2.573986	-0.857281
17	16	0	-4.238247	-0.233509	-0.552233
18	6	0	-3.519416	1.106365	-1.577218
19	1	0	-3.831234	0.991816	-2.622521
20	1	0	-3.910419	2.052938	-1.186711
21	1	0	-2.425359	1.100736	-1.505581
22	6	0	0.038996	2.532091	-0.117398
23	6	0	-0.311794	0.127238	0.245965
24	6	0	-0.995922	1.713569	2.002826
25	6	0	-1.095017	2.754785	0.885271
26	1	0	1.014371	2.749898	0.347723
27	1	0	-0.073947	3.183339	-0.991934
28	1	0	-1.896539	1.732703	2.629830
29	1	0	-0.126650	1.921026	2.648284
30	1	0	-2.061135	2.654720	0.375636
31	1	0	-1.030676	3.759764	1.318906
32	6	0	-1.120477	-0.753342	2.399804
33	1	0	-2.008823	-0.486456	2.986453
34	1	0	-0.265389	-0.833594	3.091027
35	6	0	-1.343908	-2.074300	1.660405
36	1	0	-2.301961	-2.031224	1.129424
37	1	0	-1.378554	-2.895853	2.385686
38	6	0	-0.209451	-2.295281	0.658073
39	1	0	0.744962	-2.463006	1.183327
40	1	0	-0.407626	-3.168465	0.025360
41	7	0	-0.876848	0.350949	1.455379
42	7	0	0.002927	1.144852	-0.583538
43	7	0	-0.104319	-1.124406	-0.214339
44	1	0	0.653927	0.835638	-1.354867
45	1	0	0.558298	-1.137946	-1.033433

Int-6b

Sum of electronic and thermal Free Energies = -1223.688775 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.464813	-0.579416	-1.161728
2	6	0	3.714101	-1.784761	-0.482697
3	6	0	2.623142	-2.628455	-0.208748
4	6	0	1.323249	-2.274308	-0.574430

5	6	0	1.024981	−1.037363	−1.252472
6	6	0	2.171841	−0.211835	−1.537296
7	1	0	4.298116	0.082911	−1.404932
8	1	0	2.792377	−3.578311	0.301806
9	1	0	0.494796	−2.949039	−0.359025
10	1	0	2.014846	0.719824	−2.080184
11	1	0	4.725121	−2.065749	−0.193893
12	8	0	−0.182485	−0.695415	−1.565359
13	6	0	−2.294066	−2.307929	0.650772
14	1	0	−1.398571	−1.896941	0.169648
15	1	0	−2.565573	−3.266357	0.193372
16	1	0	−2.135045	−2.457239	1.725592
17	16	0	−3.675747	−1.111358	0.453384
18	6	0	−3.606341	−0.927071	−1.376124
19	1	0	−3.962225	−1.846599	−1.854700
20	1	0	−4.269018	−0.096882	−1.645689
21	1	0	−2.571459	−0.720555	−1.672190
22	6	0	0.633760	−0.053564	2.683319
23	6	0	−0.446120	1.241165	0.842262
24	6	0	1.915878	1.653104	1.363297
25	6	0	1.943882	0.243600	1.955312
26	1	0	0.575157	0.500252	3.634394
27	1	0	0.550780	−1.125148	2.899400
28	1	0	2.774661	1.783384	0.696495
29	1	0	1.956808	2.423582	2.150960
30	1	0	2.086605	−0.476368	1.146224
31	1	0	2.782057	0.161174	2.657417
32	6	0	0.774342	2.827328	−0.566193
33	1	0	1.781959	2.746714	−0.989564
34	1	0	0.641552	3.849119	−0.173503
35	6	0	−0.274898	2.494229	−1.627469
36	1	0	−0.051359	1.505105	−2.047293
37	1	0	−0.264542	3.263179	−2.409507
38	6	0	−1.653902	2.422359	−0.972650
39	1	0	−2.005519	3.422400	−0.674293
40	1	0	−2.387619	1.988891	−1.660878
41	7	0	0.706101	1.861300	0.545462
42	7	0	−0.498342	0.319829	1.827774
43	7	0	−1.598301	1.554955	0.215118
44	1	0	−1.398497	−0.105086	1.999995
45	1	0	−2.347745	0.867709	0.329679

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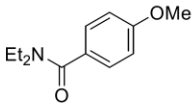
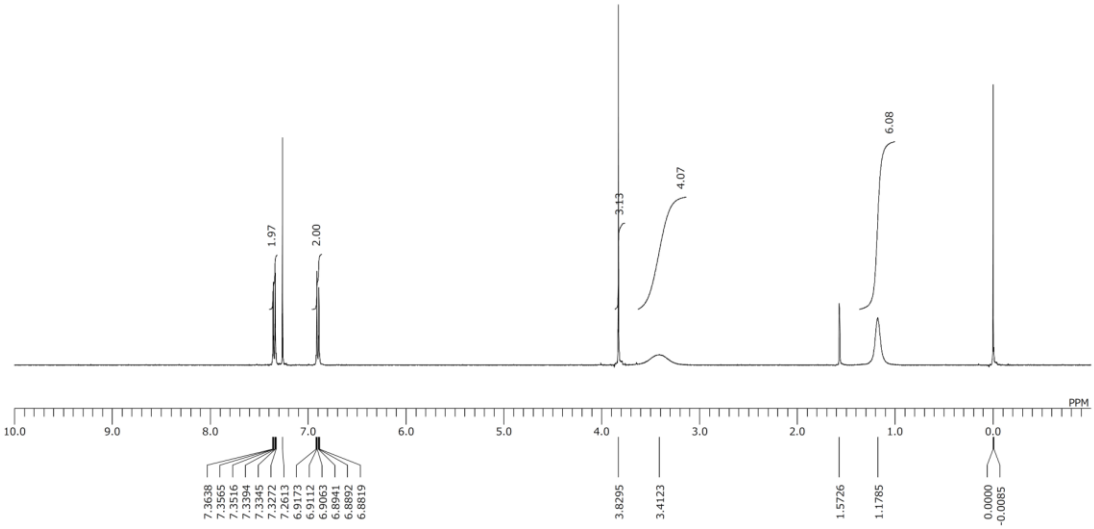
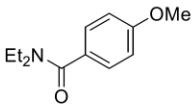
^{1}H NMR spectra of **1k** ($CDCl_3$, 400 MHz)



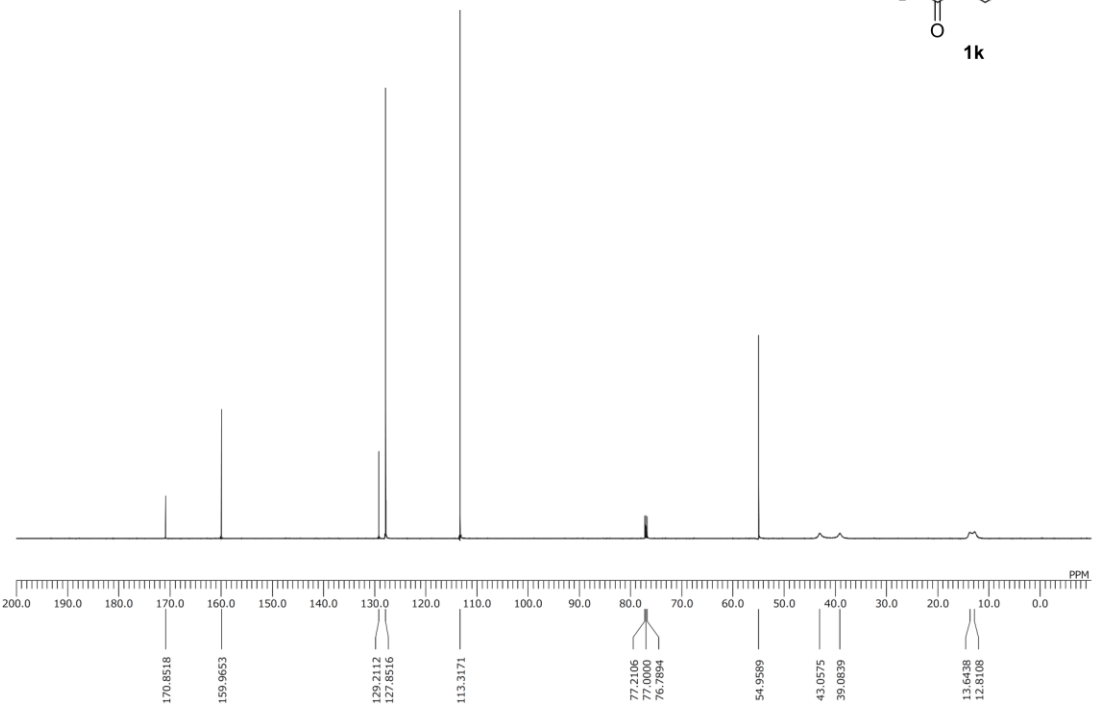
1k



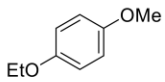
^{13}C NMR spectra of **1k** ($CDCl_3$, 150 MHz)



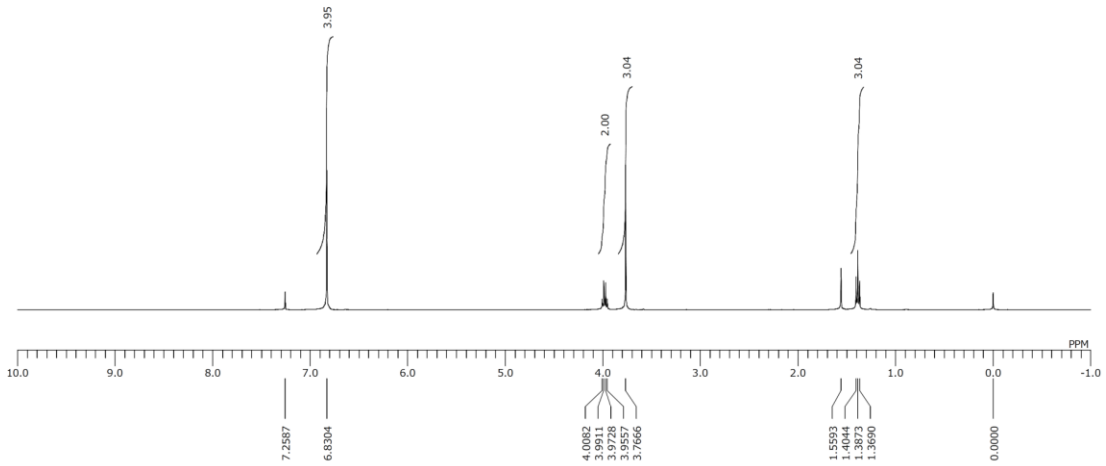
1k



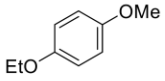
^{1}H NMR spectra of **4m** ($CDCl_3$, 400 MHz)



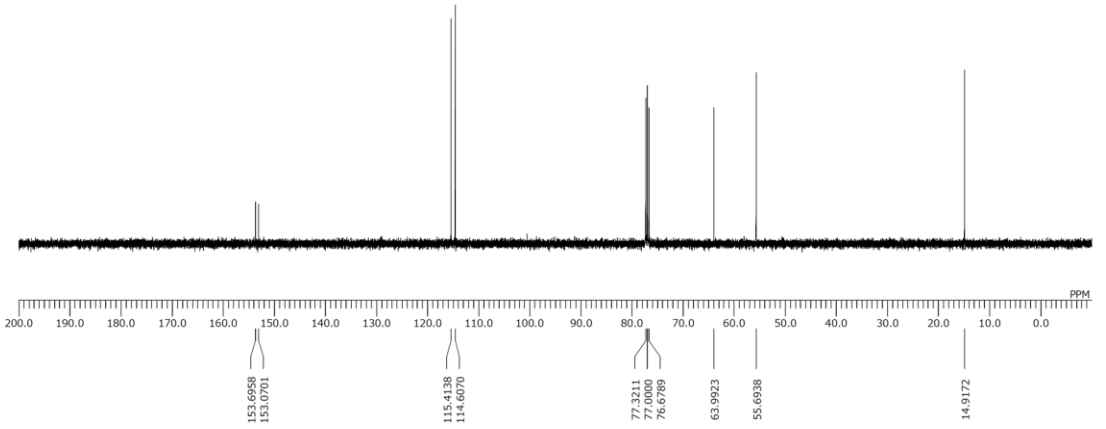
4m



^{13}C NMR spectra of **4m** ($CDCl_3$, 100 MHz)



4m



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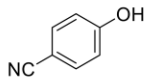
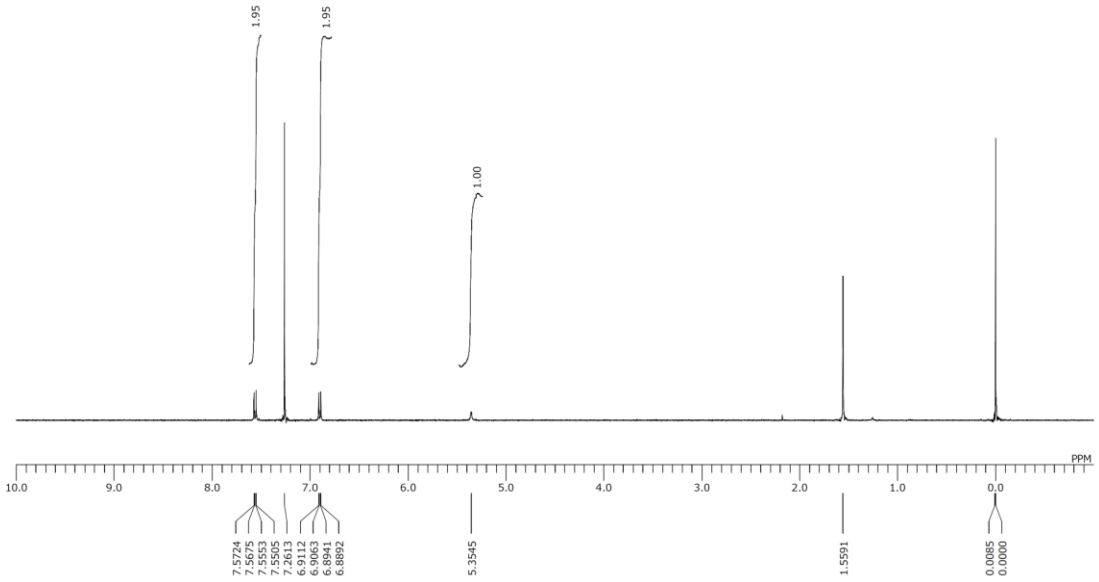
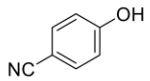


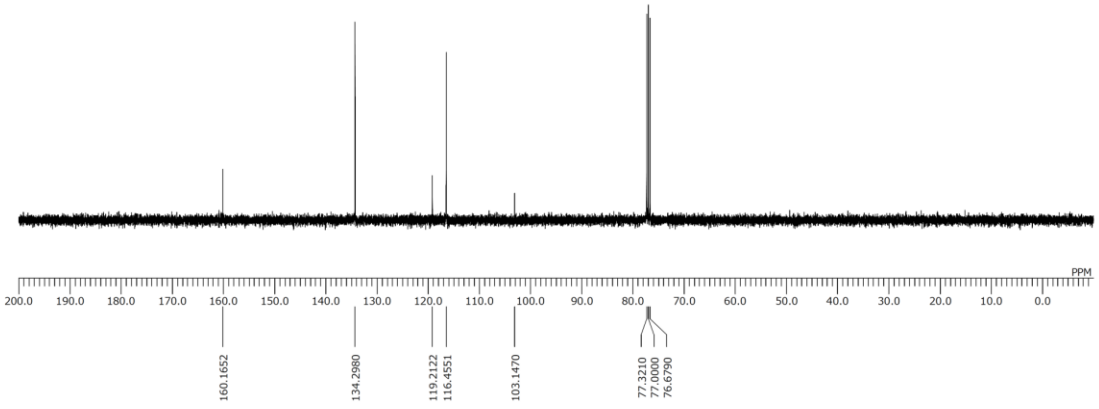
3a



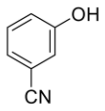
^{13}C NMR spectra of **3a** ($CDCl_3$, 100 MHz)



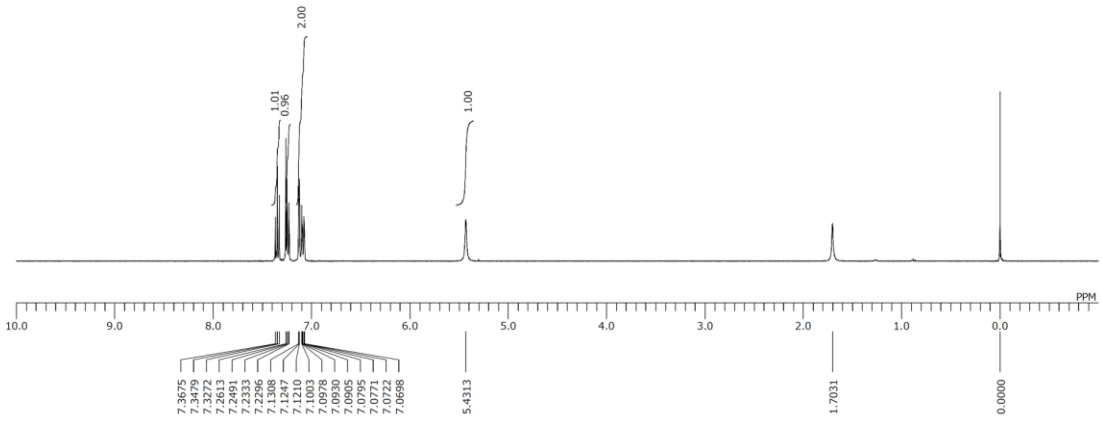
3a



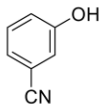
^{1}H NMR spectra of **3b** ($CDCl_3$, 400 MHz)



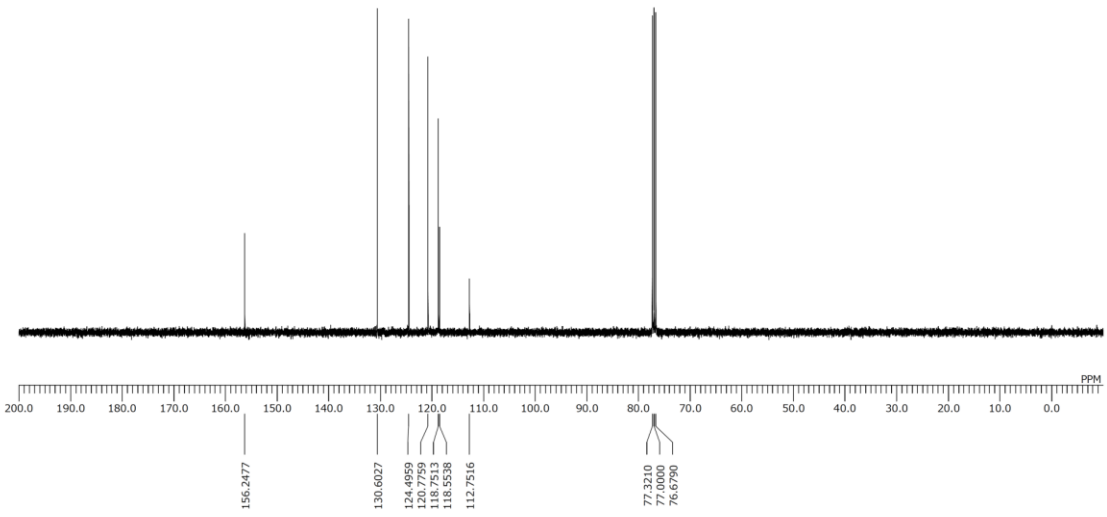
3b



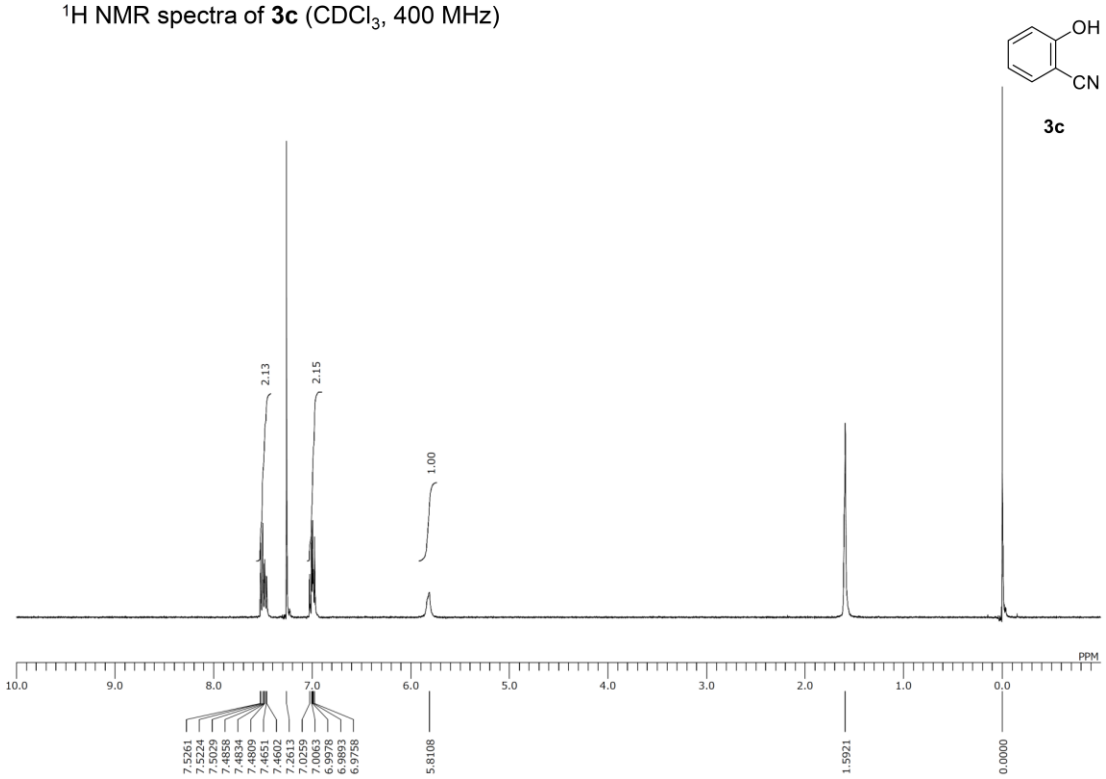
^{13}C NMR spectra of **3b** ($CDCl_3$, 100 MHz)



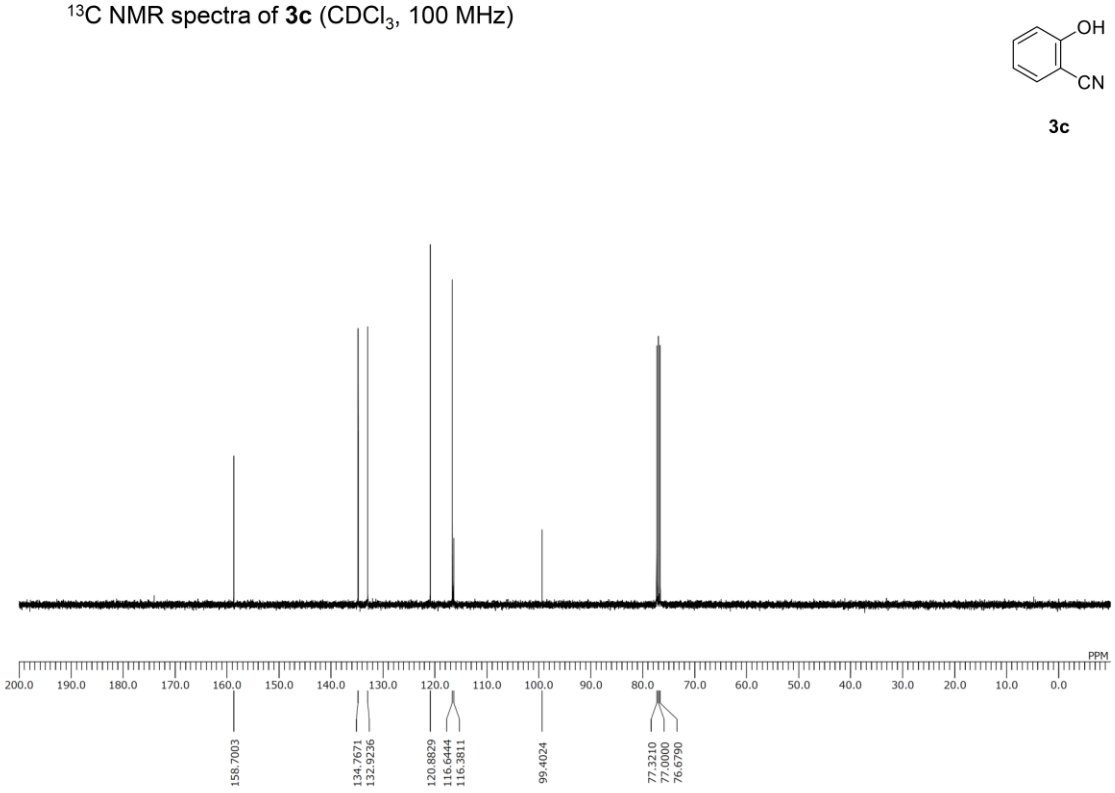
3b



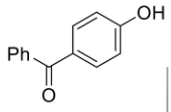
^{1}H NMR spectra of **3c** ($CDCl_3$, 400 MHz)



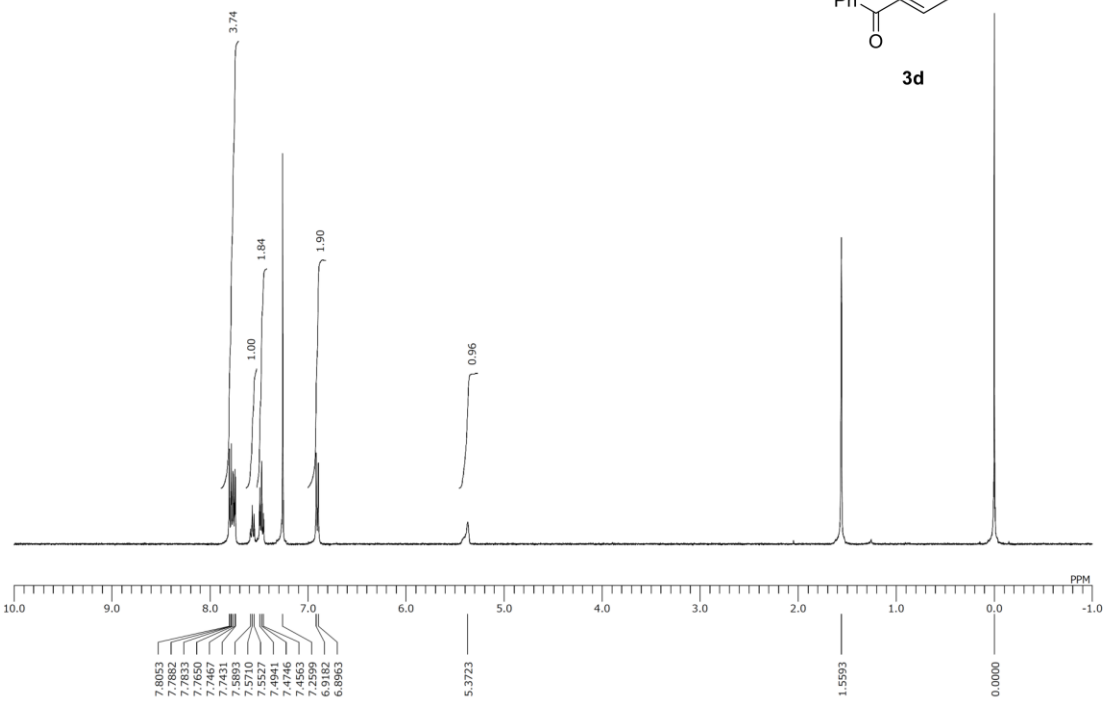
^{13}C NMR spectra of **3c** ($CDCl_3$, 100 MHz)



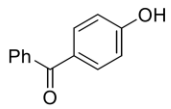
^{1}H NMR spectra of **3d** ($CDCl_3$, 400 MHz)



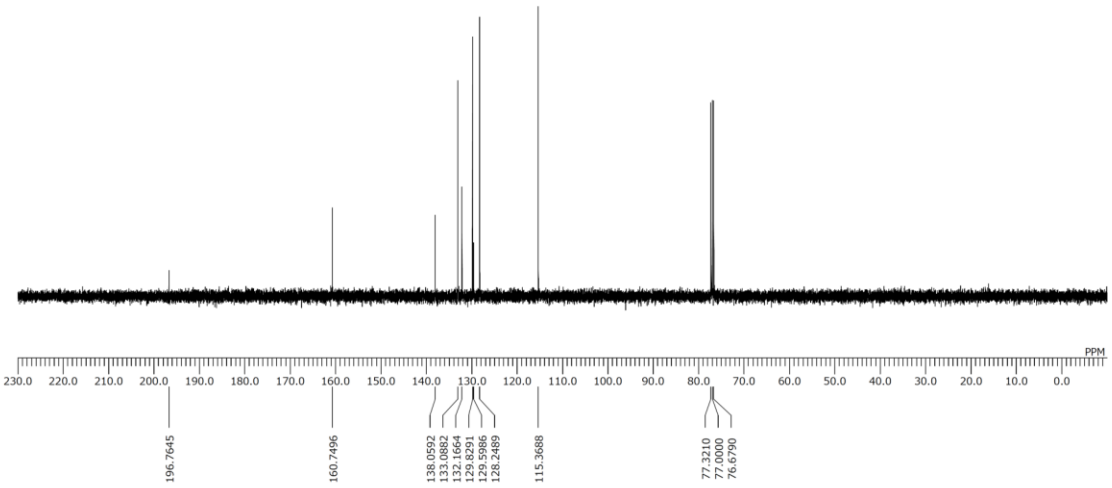
3d



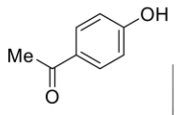
^{13}C NMR spectra of **3d** ($CDCl_3$, 100 MHz)



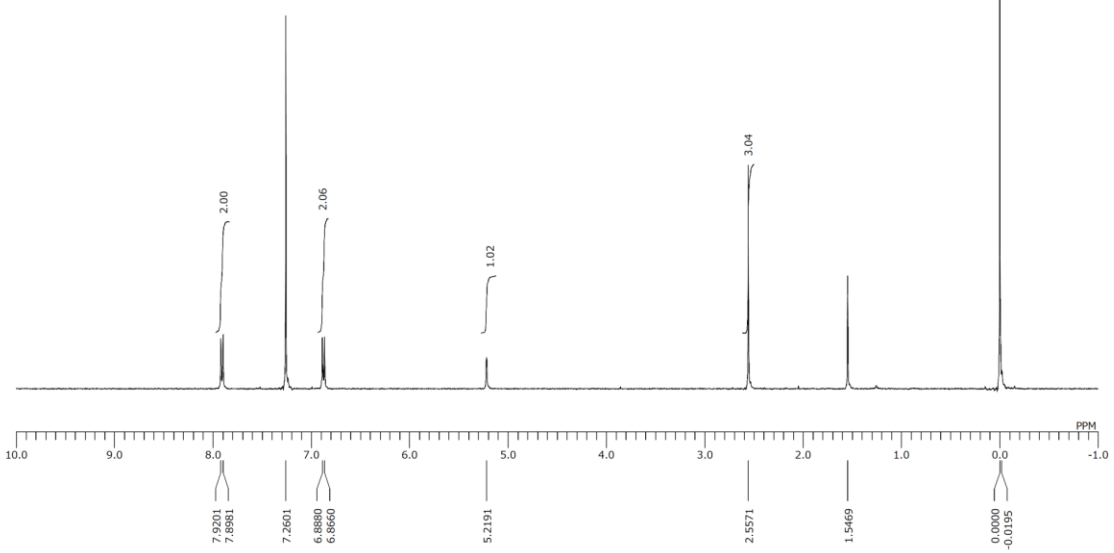
3d



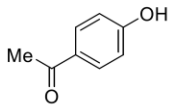
^{1}H NMR spectra of **3e** ($CDCl_3$, 400 MHz)



3e

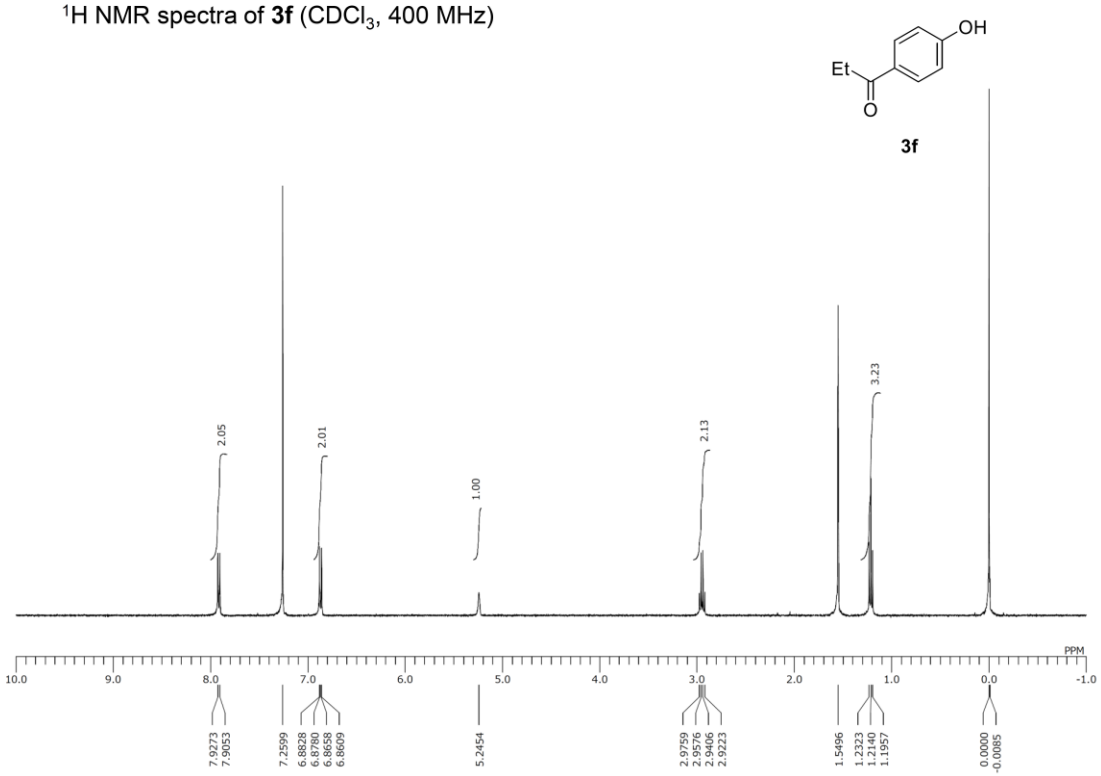


^{13}C NMR spectra of **3e** ($CDCl_3$, 100 MHz)

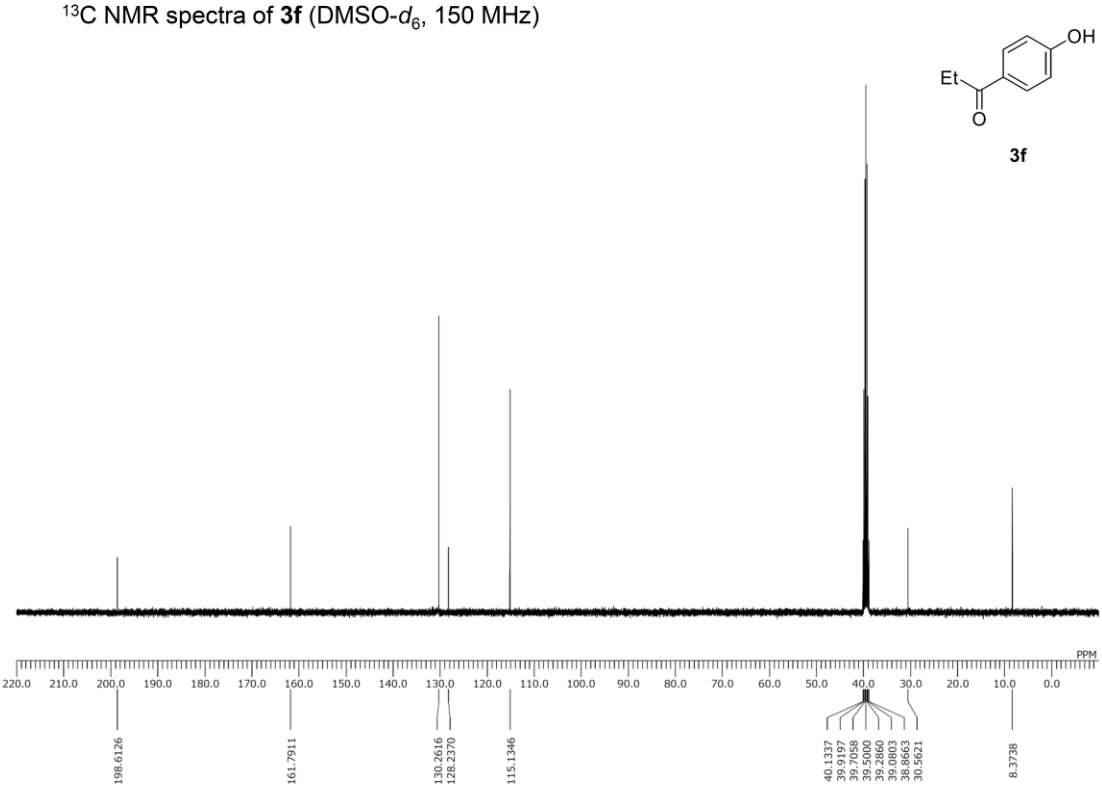


3e

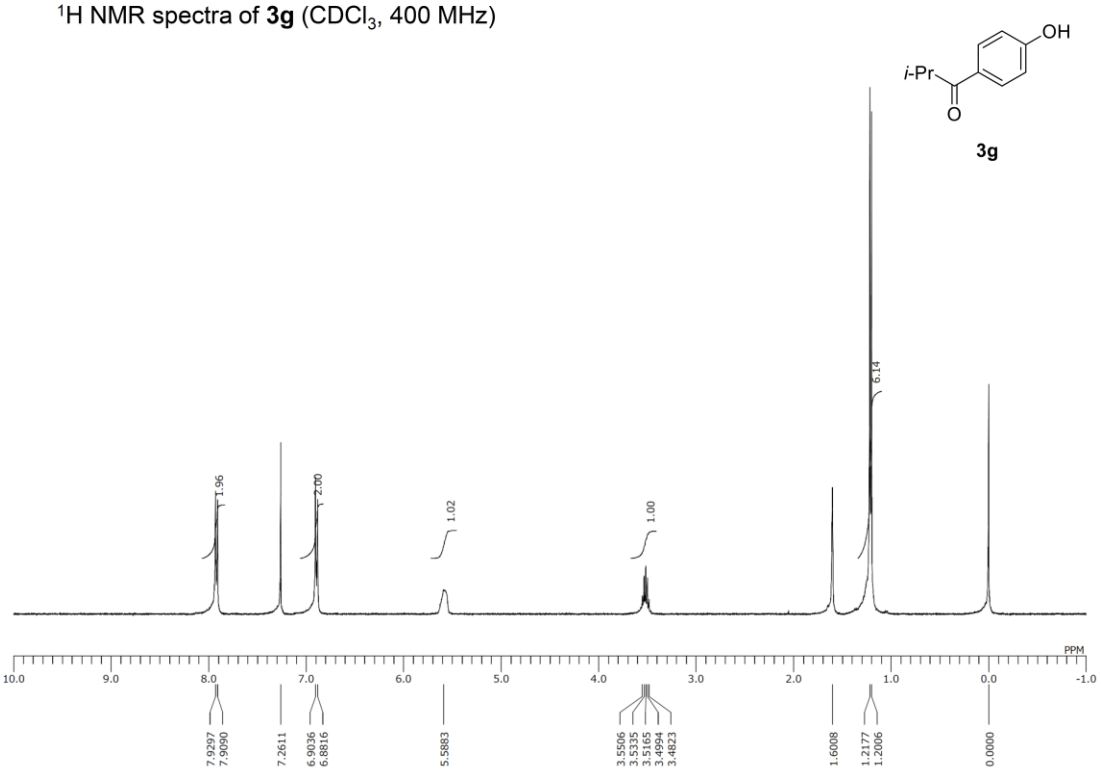
^{1}H NMR spectra of **3f** ($CDCl_3$, 400 MHz)



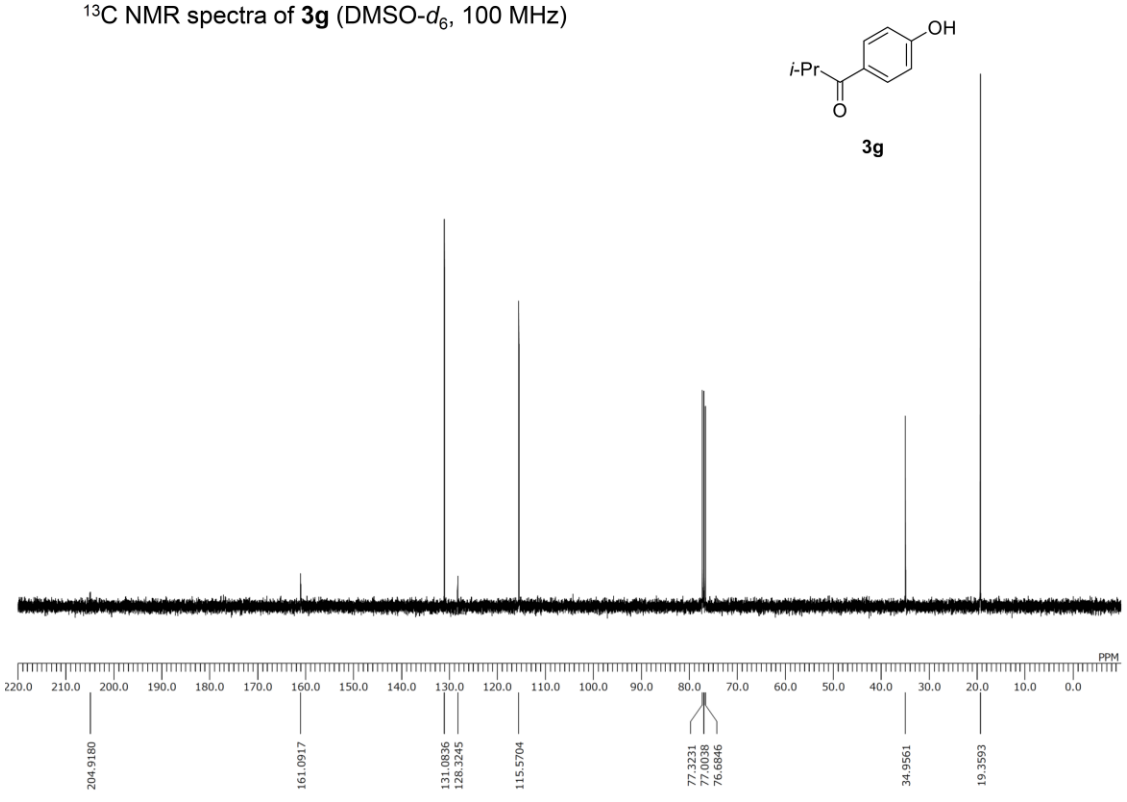
^{13}C NMR spectra of **3f** (DMSO-d_6, 150 MHz)



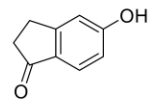
^{1}H NMR spectra of **3g** ($CDCl_3$, 400 MHz)



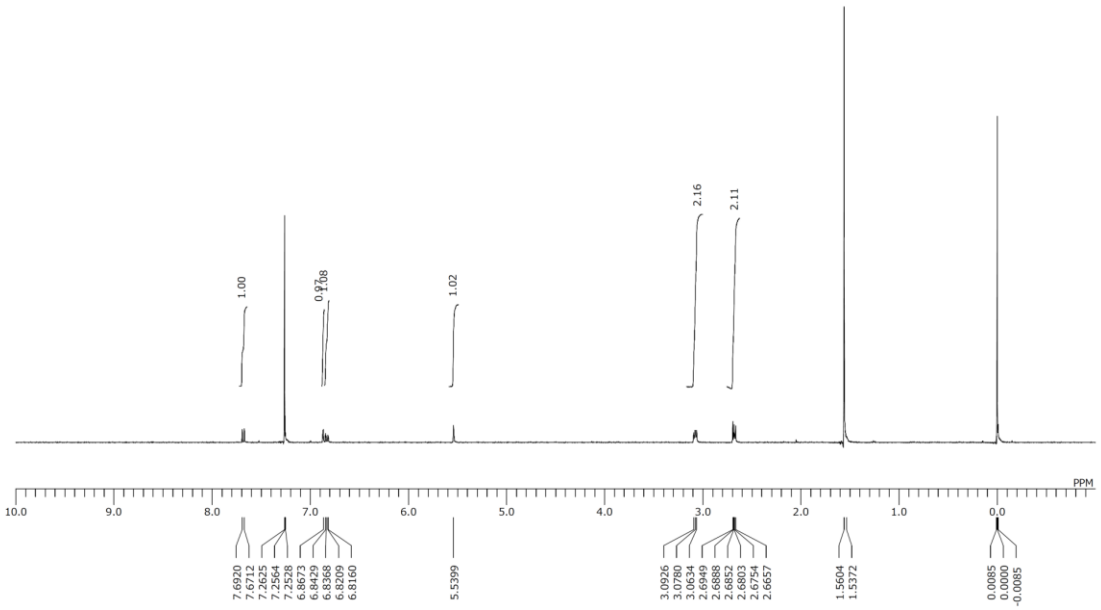
^{13}C NMR spectra of **3g** (DMSO-d_6, 100 MHz)



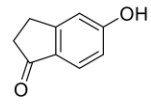
^{1}H NMR spectra of **3h** ($CDCl_3$, 400 MHz)



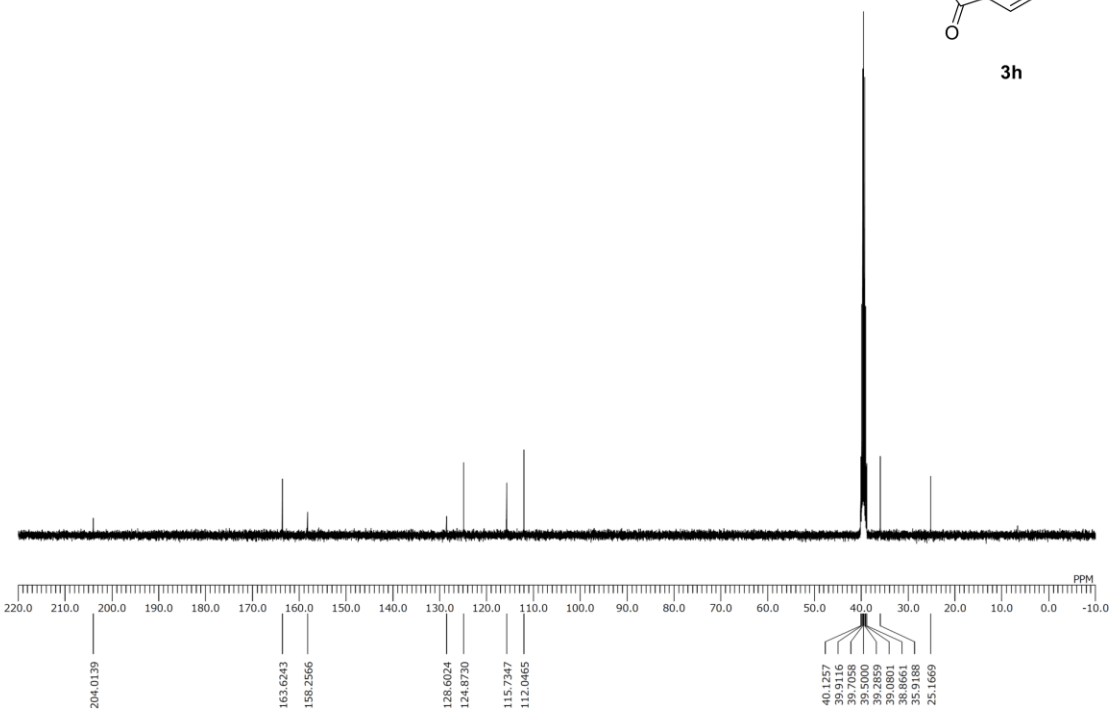
3h



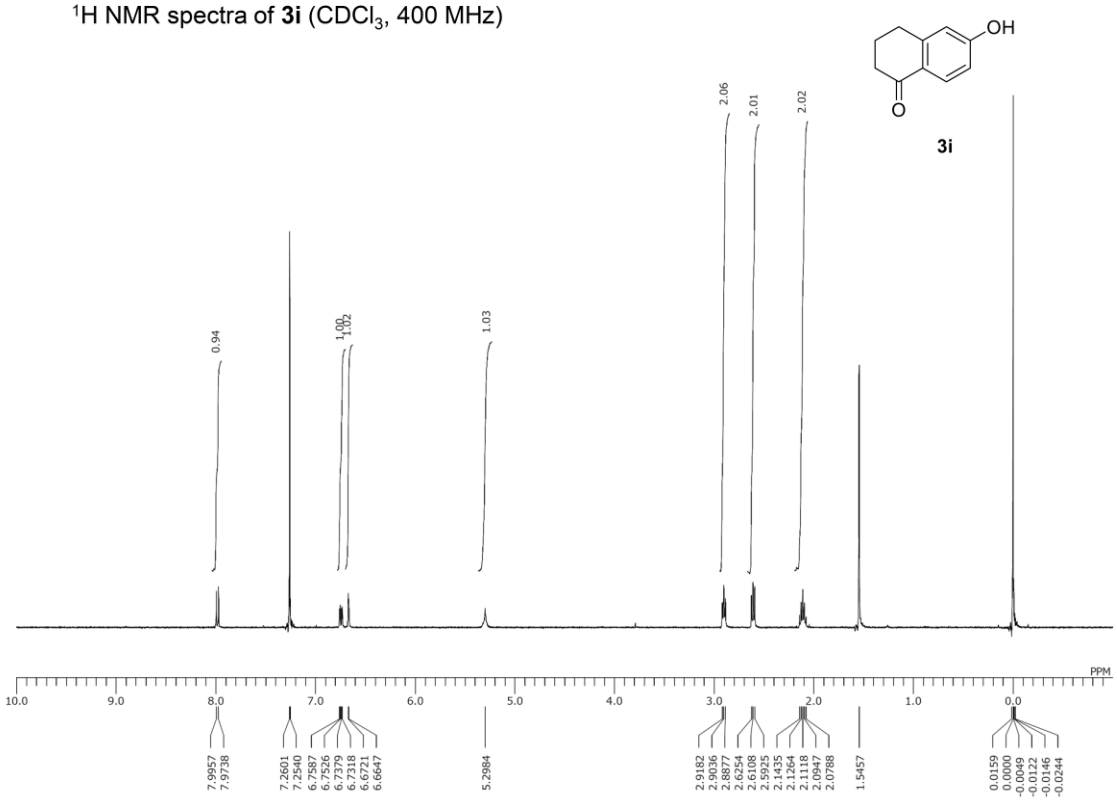
^{13}C NMR spectra of **3h** (DMSO-d_6, 100 MHz)



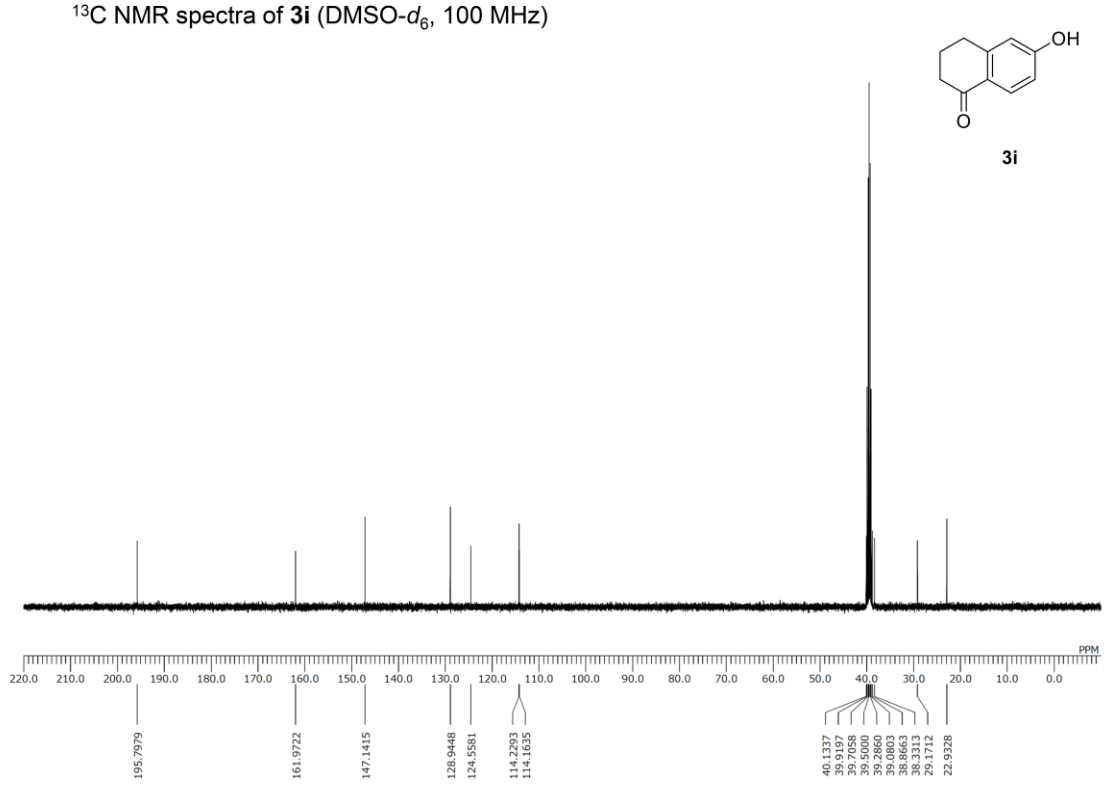
3h



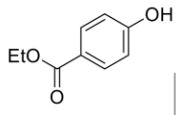
^{1}H NMR spectra of **3i** ($CDCl_3$, 400 MHz)



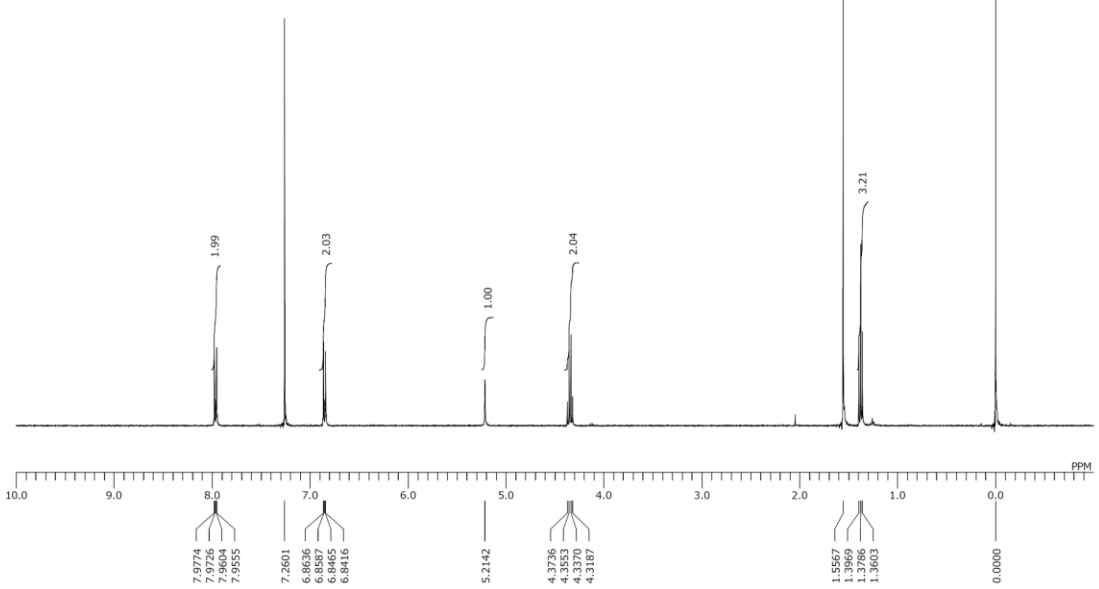
^{13}C NMR spectra of **3i** (DMSO-d_6, 100 MHz)



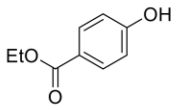
^{1}H NMR spectra of **3j** ($CDCl_3$, 400 MHz)



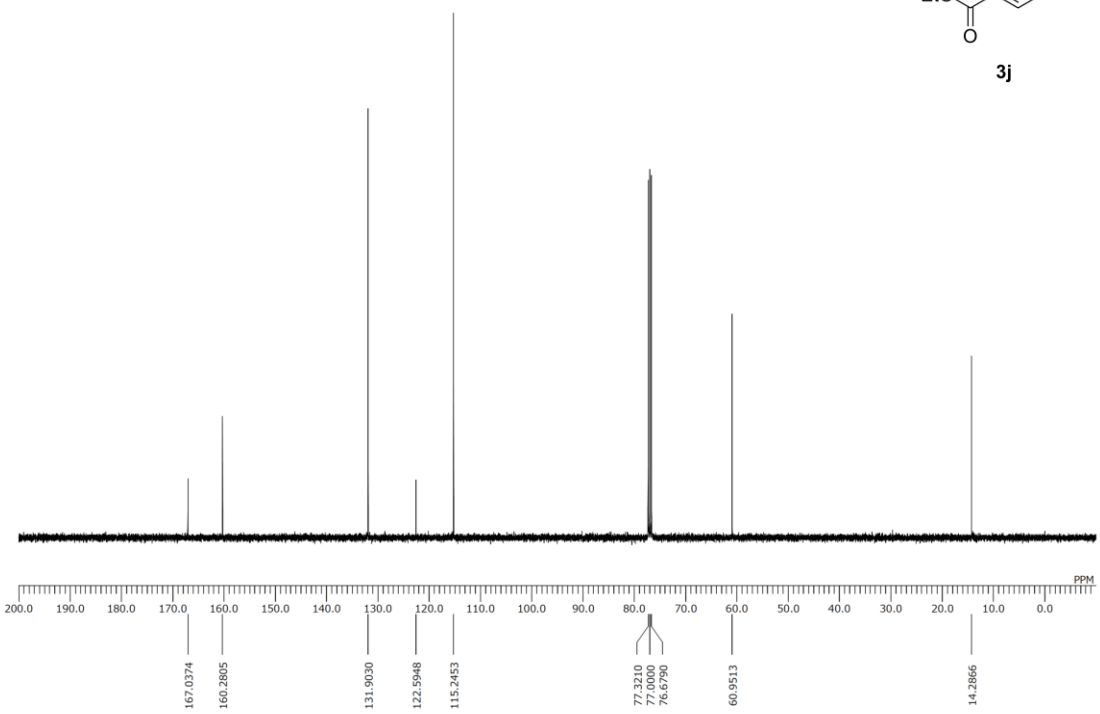
3j



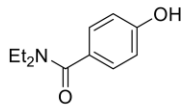
^{13}C NMR spectra of **3j** ($CDCl_3$, 100 MHz)



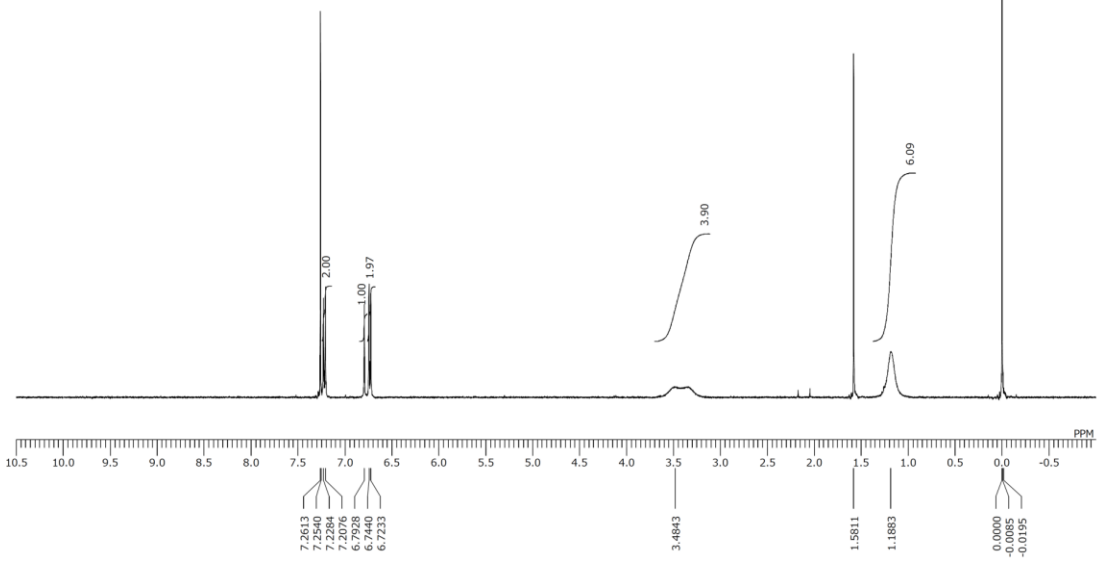
3j



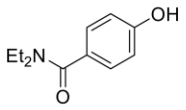
^{1}H NMR spectra of **3k** ($CDCl_3$, 400 MHz)



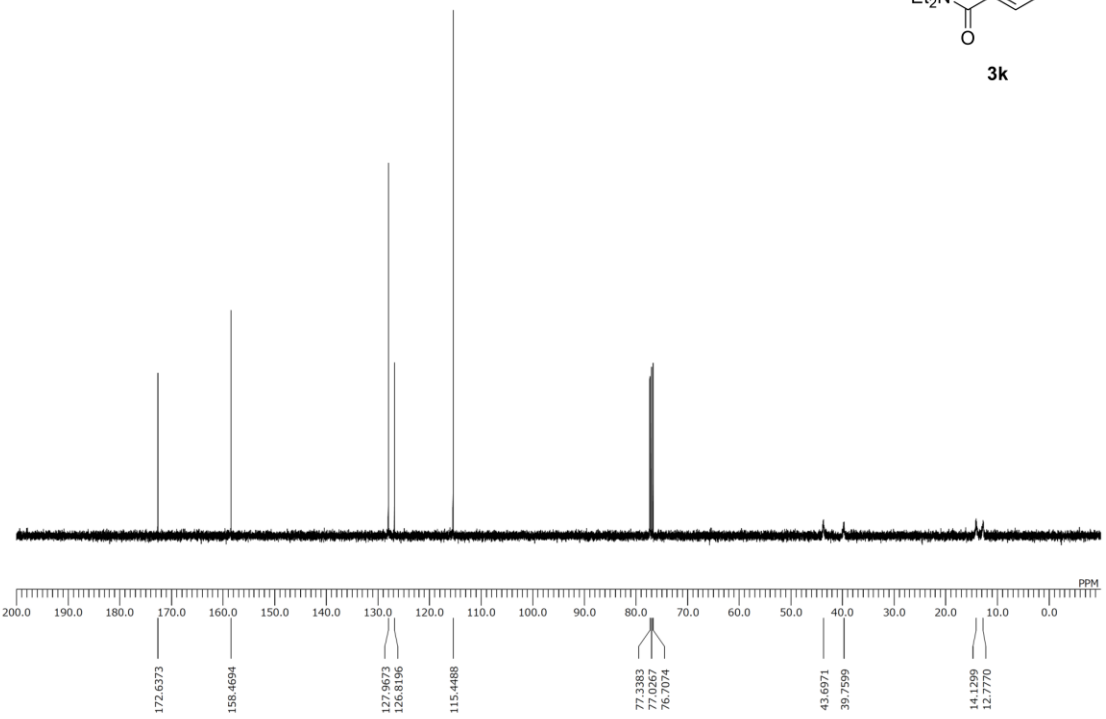
3k



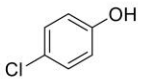
^{13}C NMR spectra of **3k** ($CDCl_3$, 100 MHz)



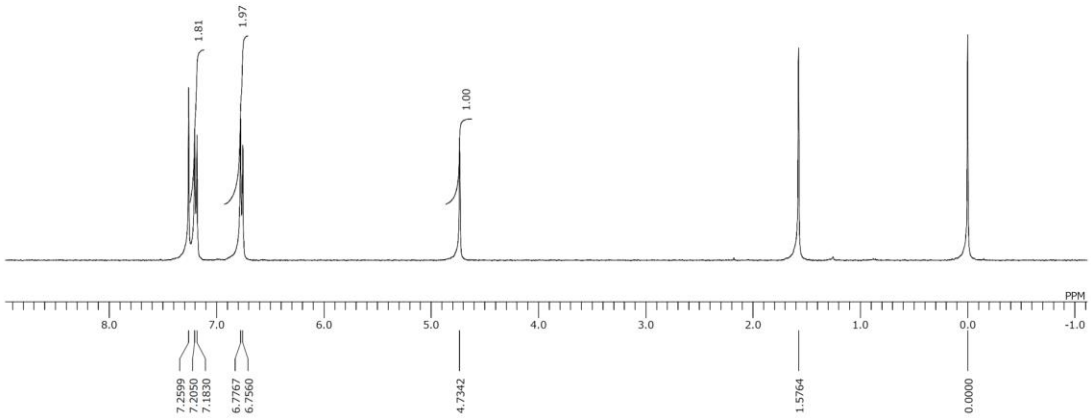
3k



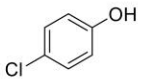
^{1}H NMR spectra of **3l** ($CDCl_3$, 400 MHz)



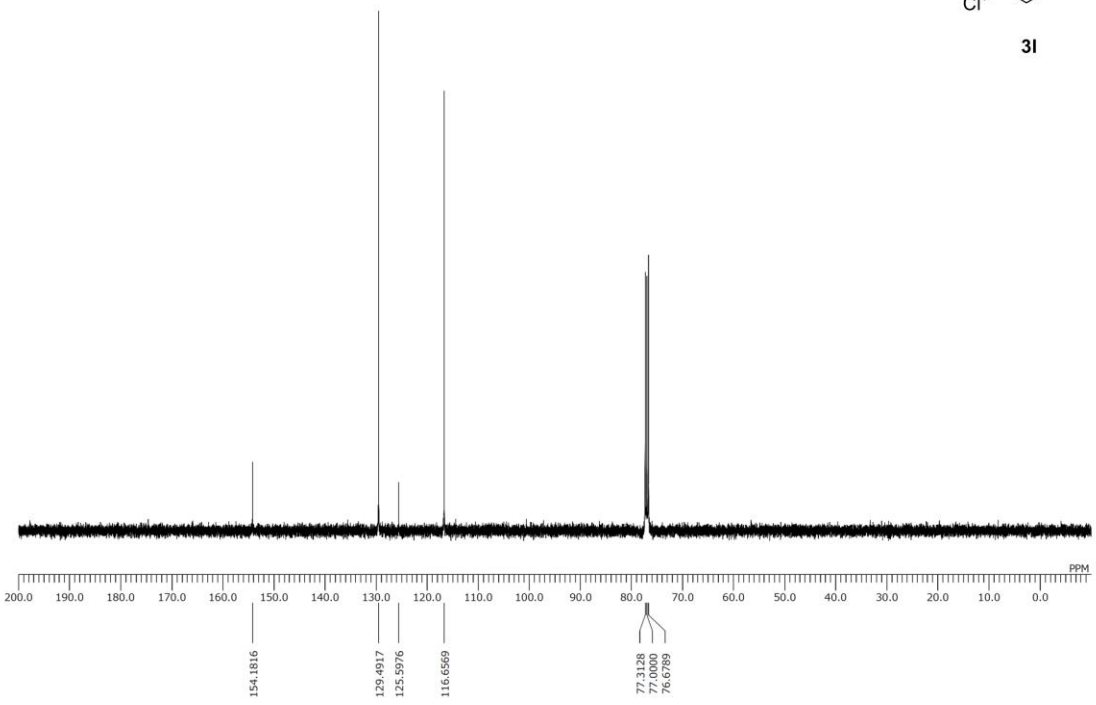
3l



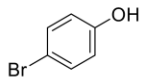
^{13}C NMR spectra of **3l** ($CDCl_3$, 100 MHz)



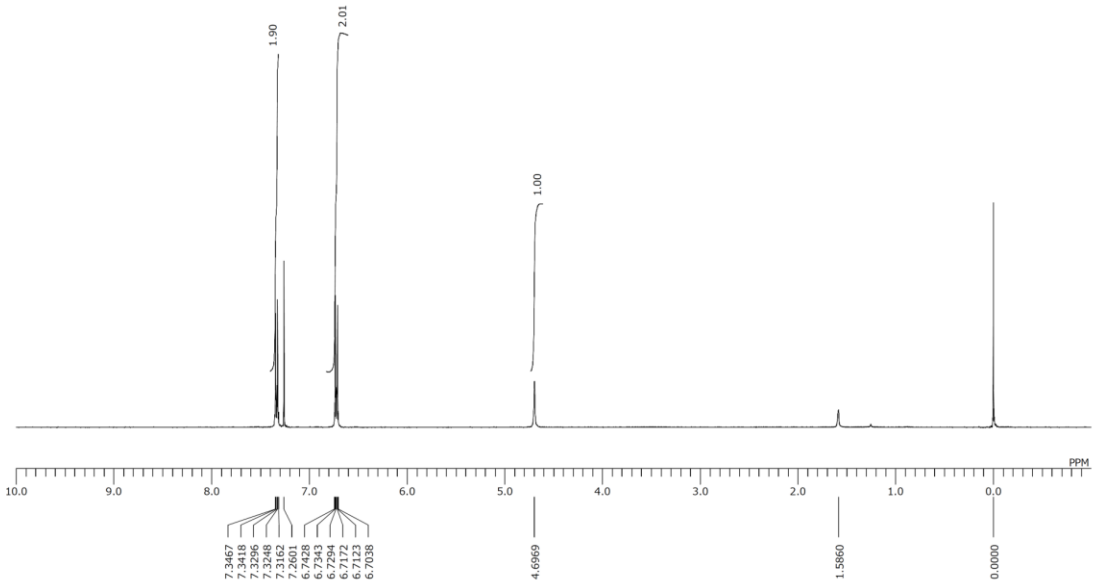
3l



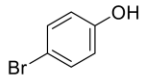
^{1}H NMR spectra of **3m** ($CDCl_3$, 400 MHz)



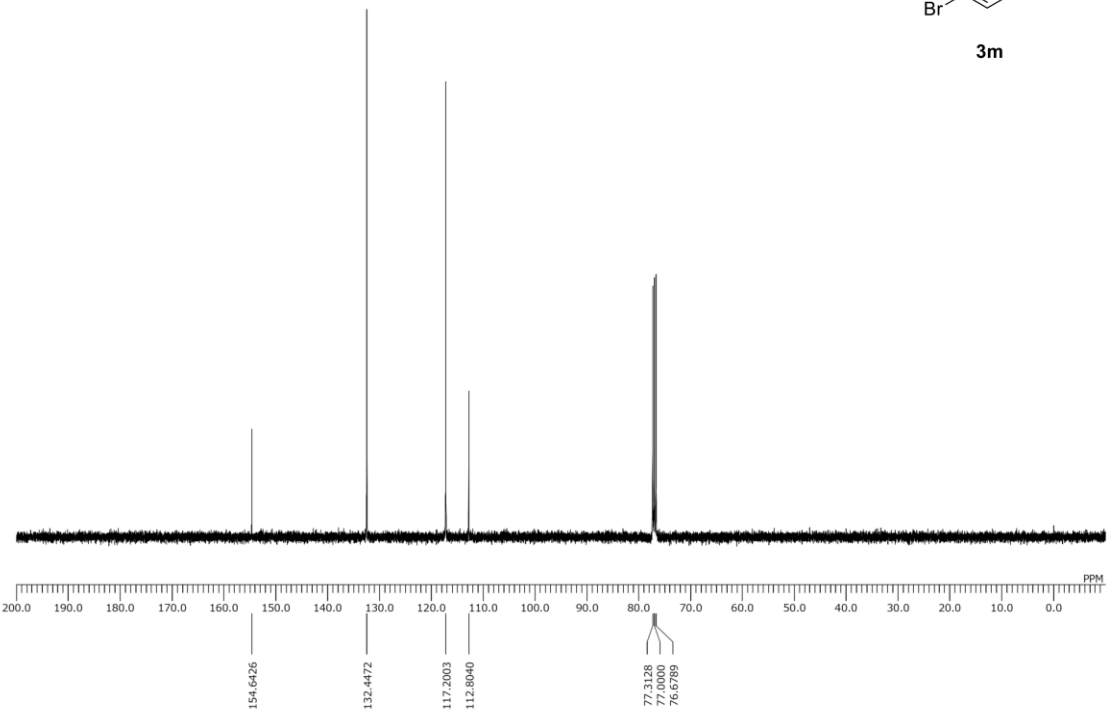
3m



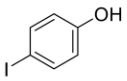
^{13}C NMR spectra of **3m** ($CDCl_3$, 100 MHz)



3m



^{1}H NMR spectra of **3n** ($CDCl_3$, 400 MHz)



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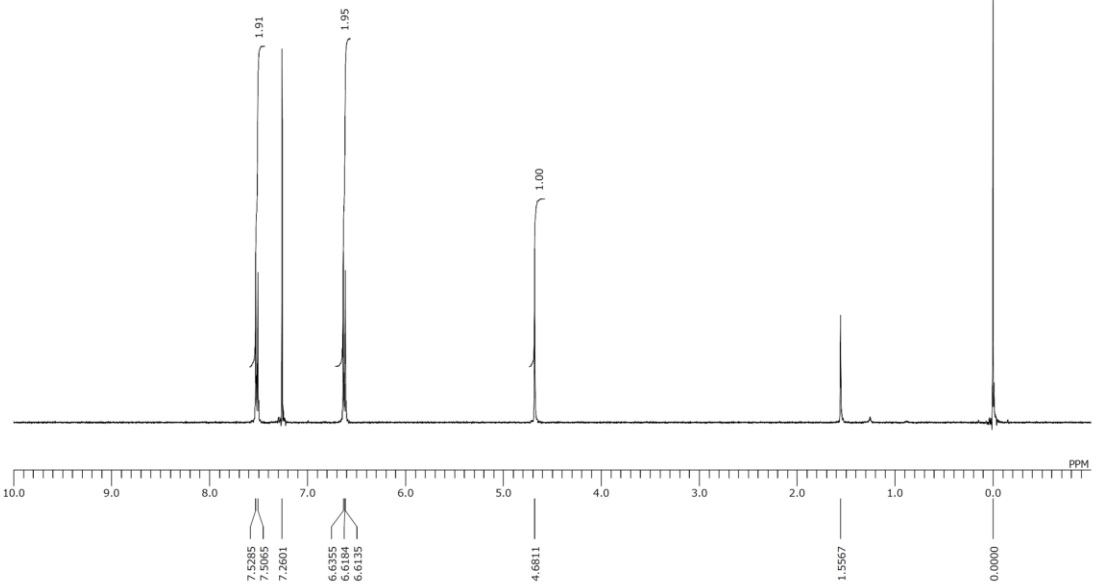
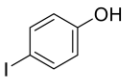
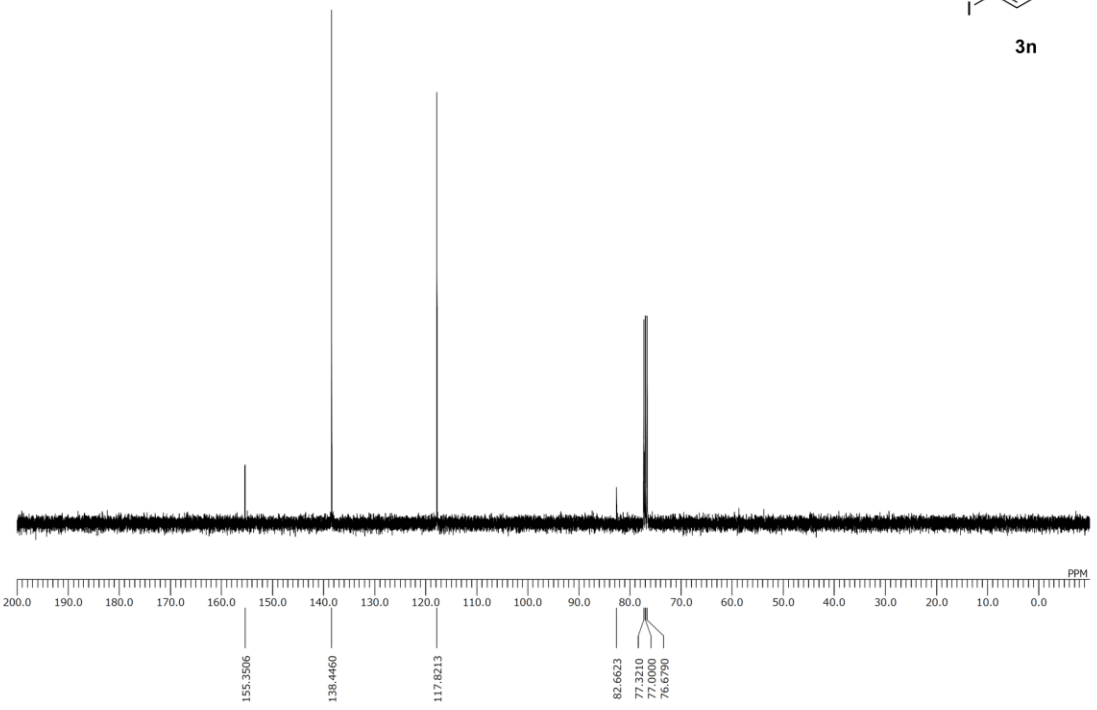


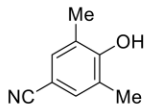
^{13}C NMR spectra of **3n** ($CDCl_3$, 100 MHz)



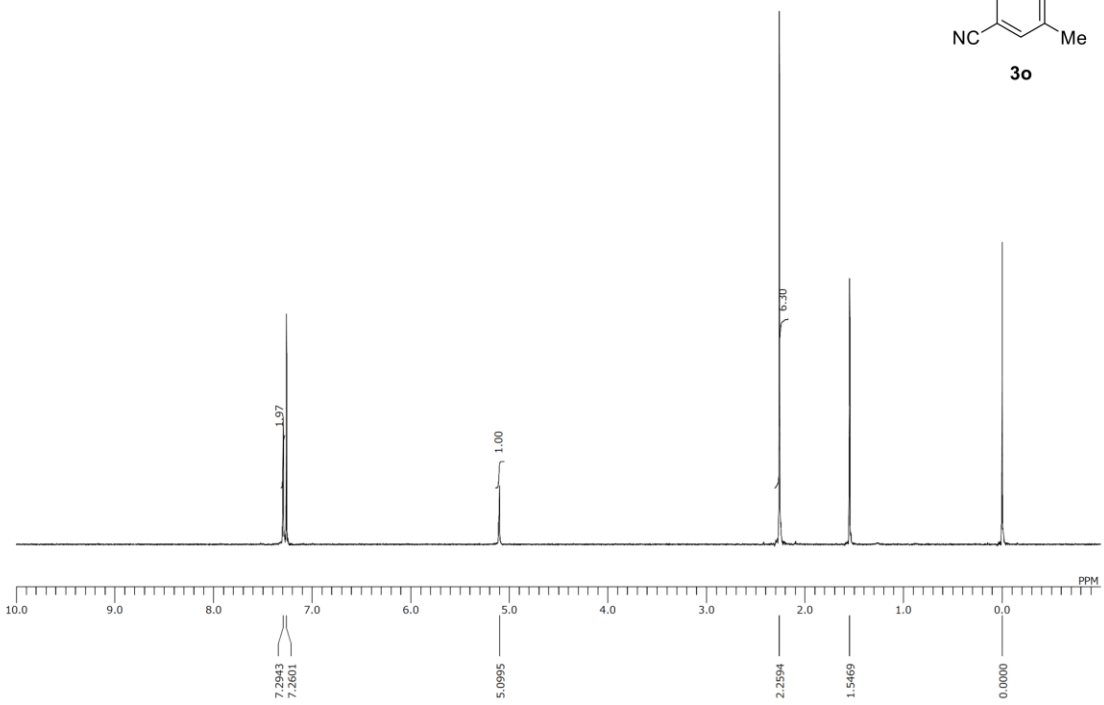
3n



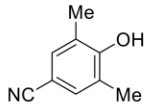
^{1}H NMR spectra of **3o** ($CDCl_3$, 400 MHz)



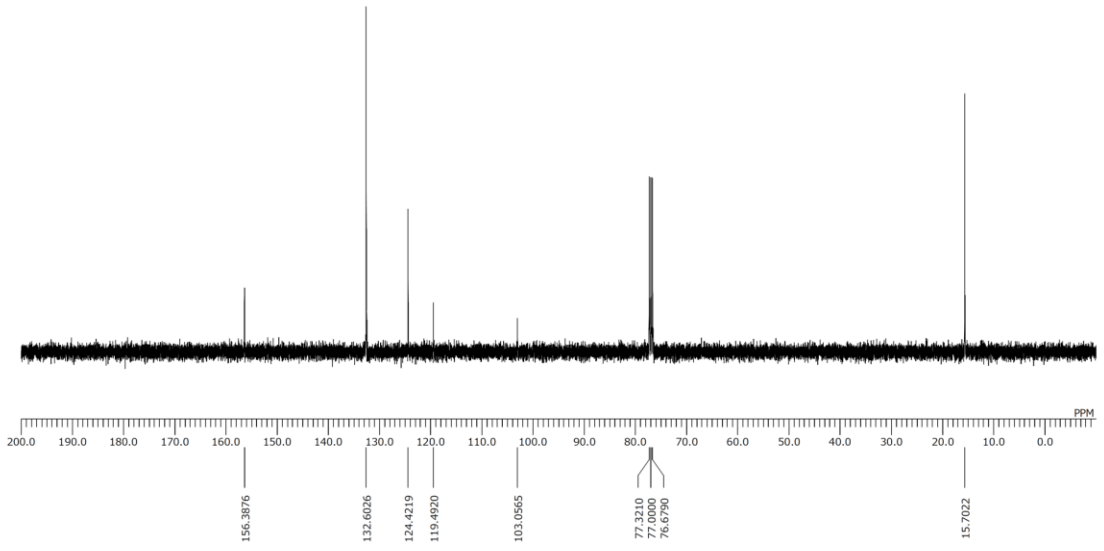
3o



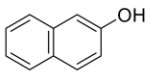
^{13}C NMR spectra of **3o** ($CDCl_3$, 100 MHz)



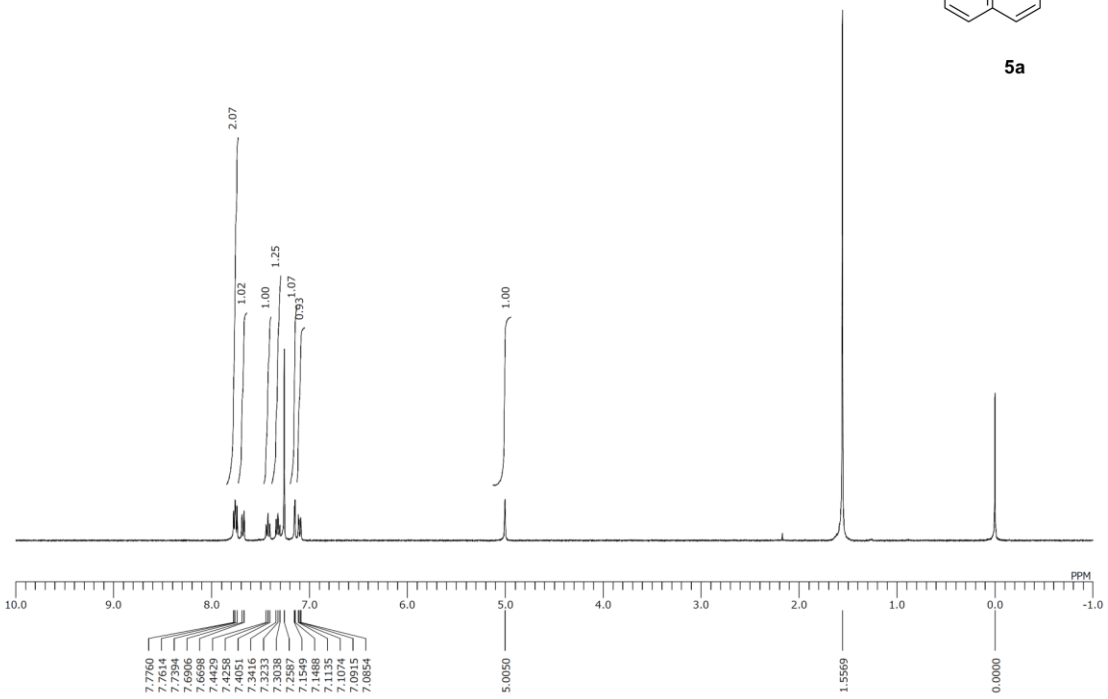
3o



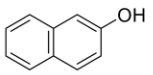
^{1}H NMR spectra of **5a** ($CDCl_3$, 400 MHz)



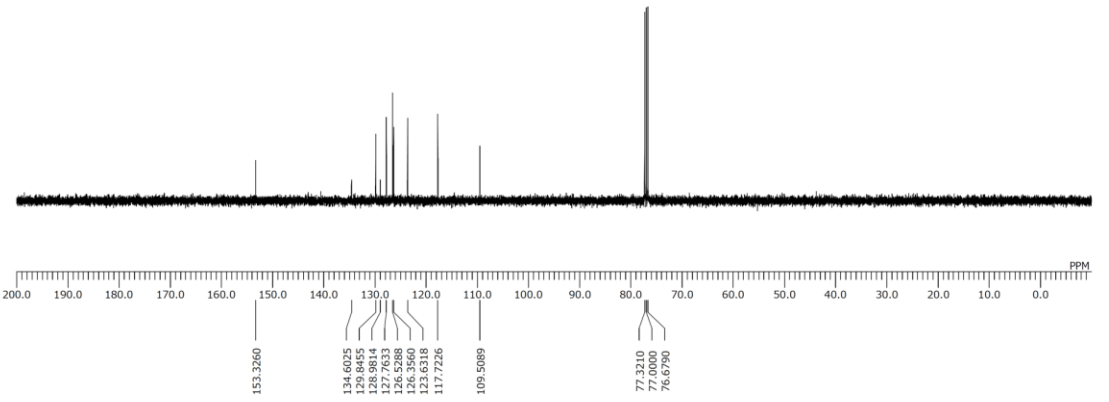
5a



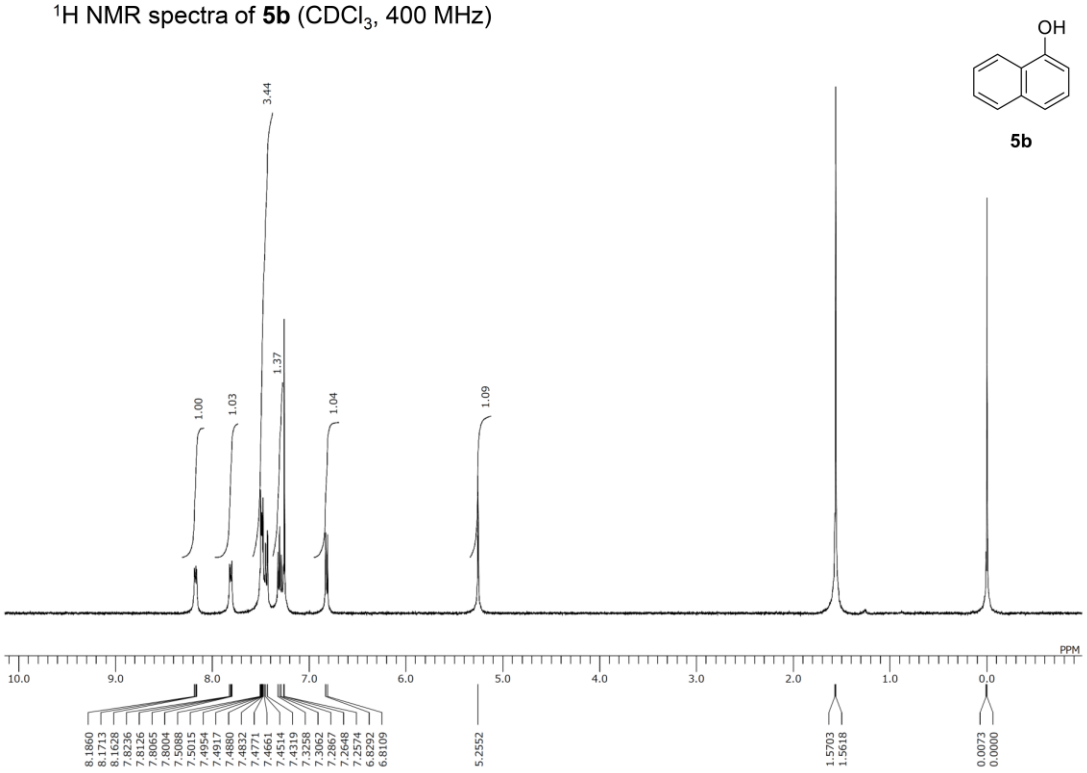
^{13}C NMR spectra of **5a** ($CDCl_3$, 100 MHz)



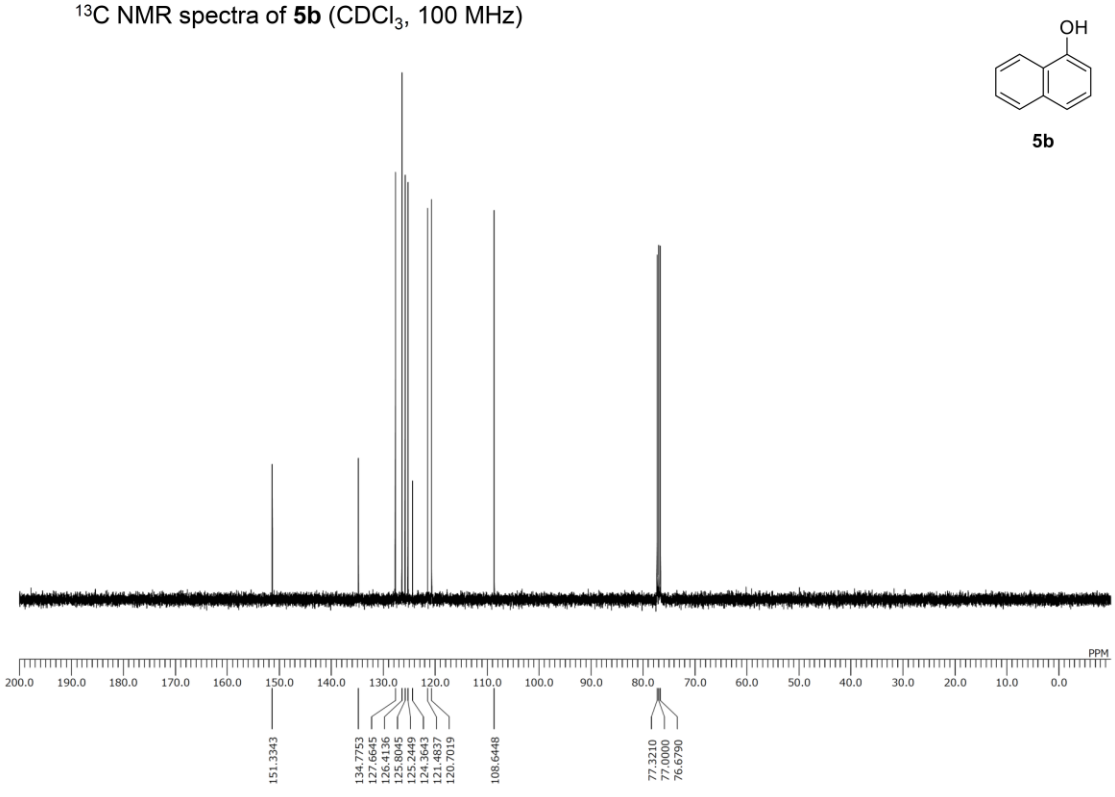
5a



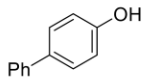
^{1}H NMR spectra of **5b** ($CDCl_3$, 400 MHz)



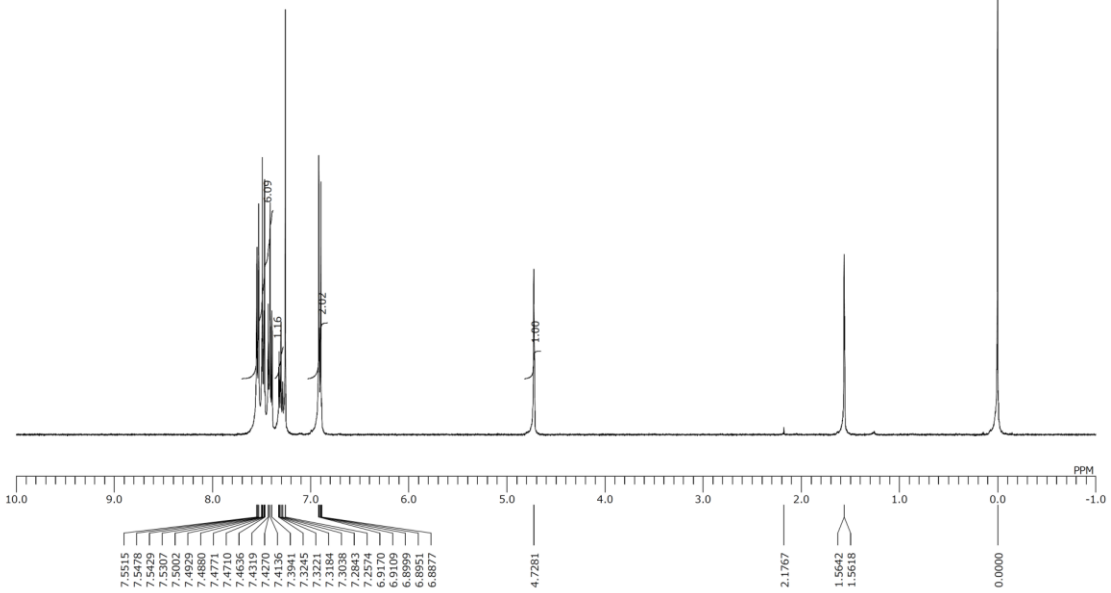
^{13}C NMR spectra of **5b** ($CDCl_3$, 100 MHz)



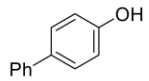
^{1}H NMR spectra of **5c** ($CDCl_3$, 400 MHz)



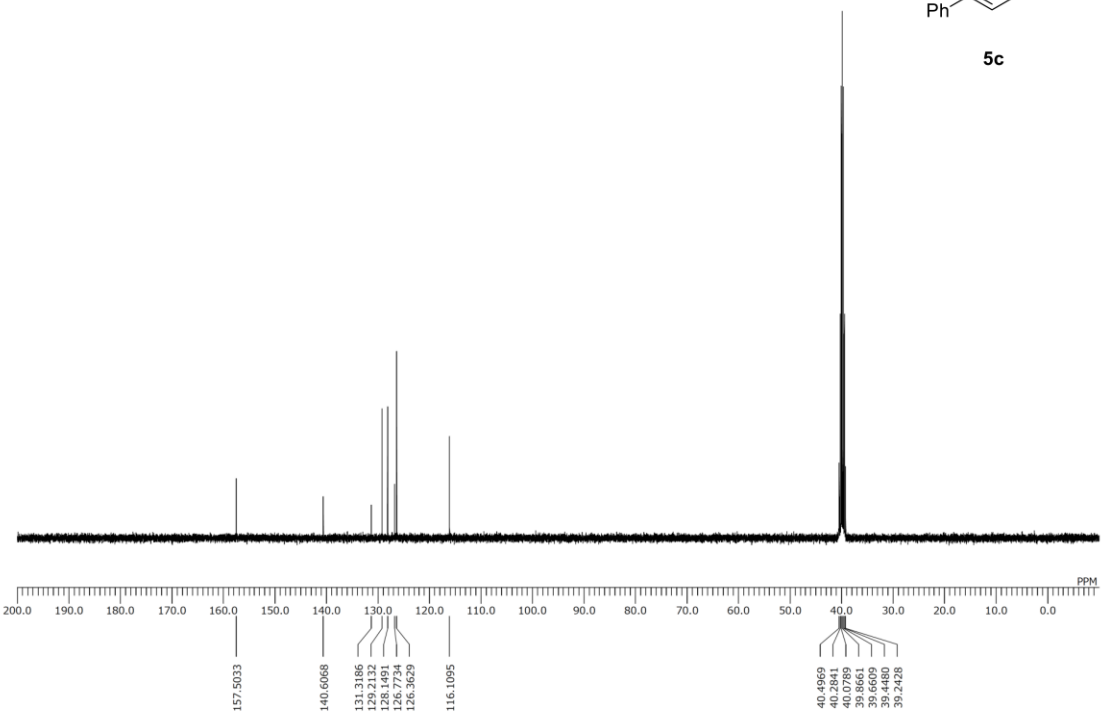
5c



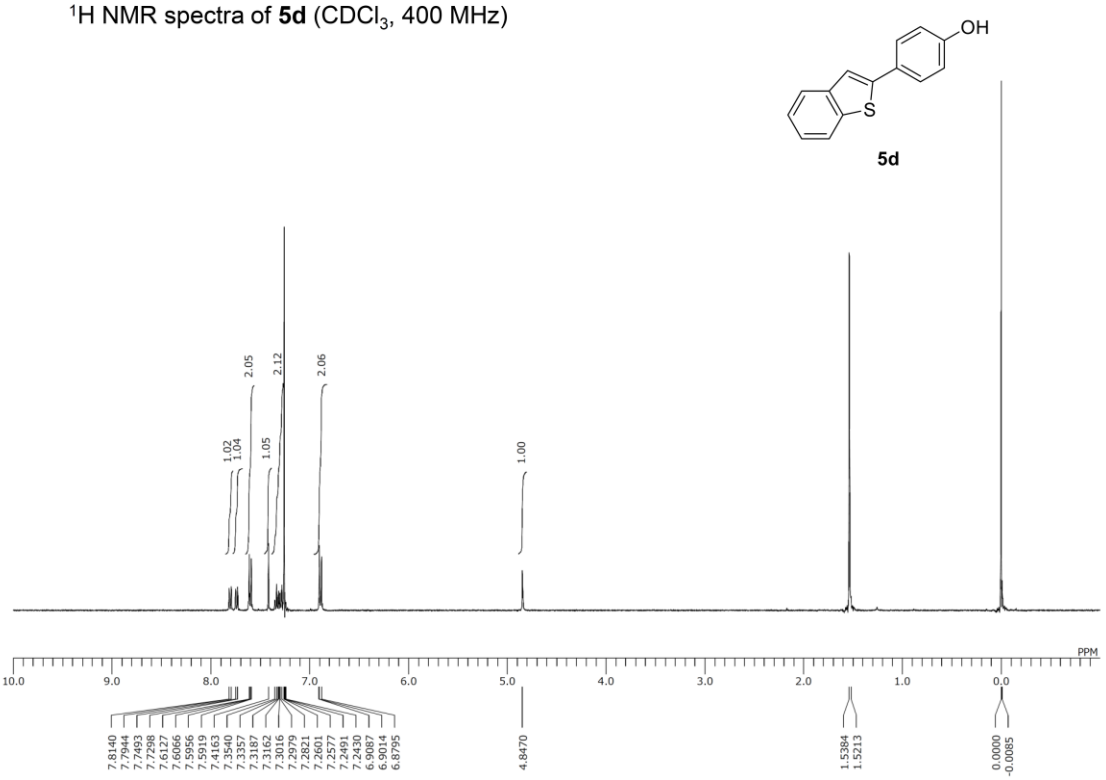
^{13}C NMR spectra of **5c** (DMSO-d_6, 100 MHz)



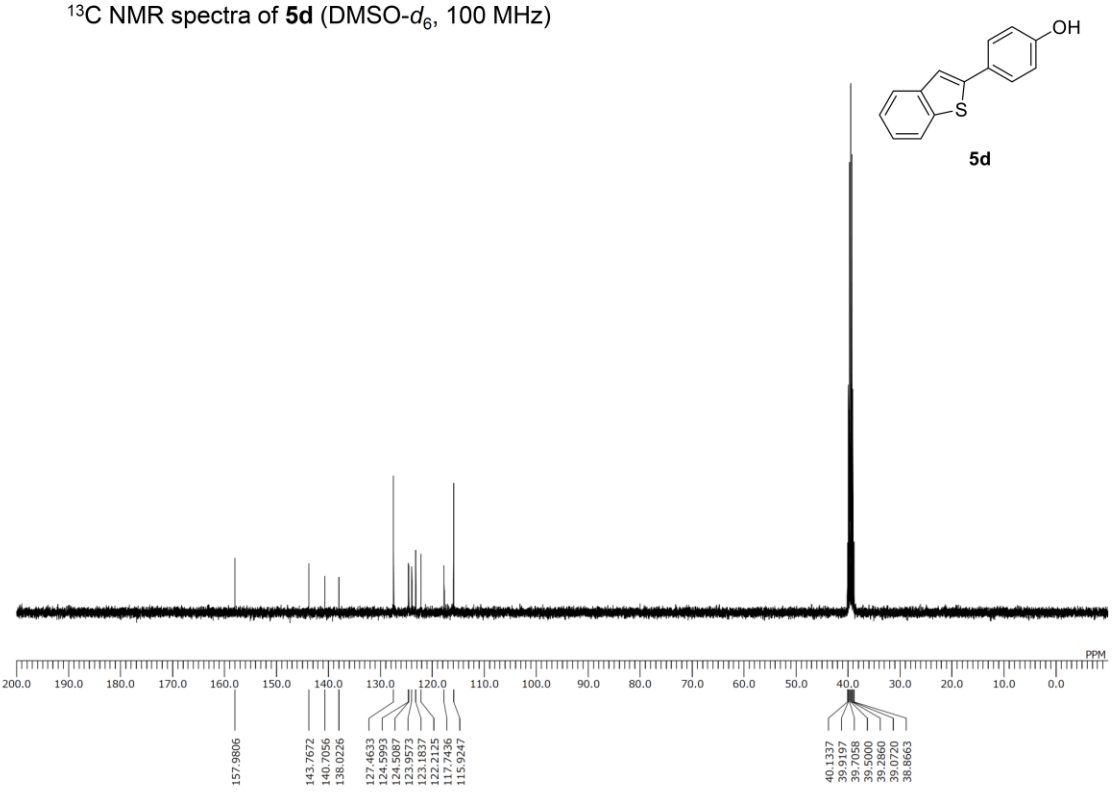
5c



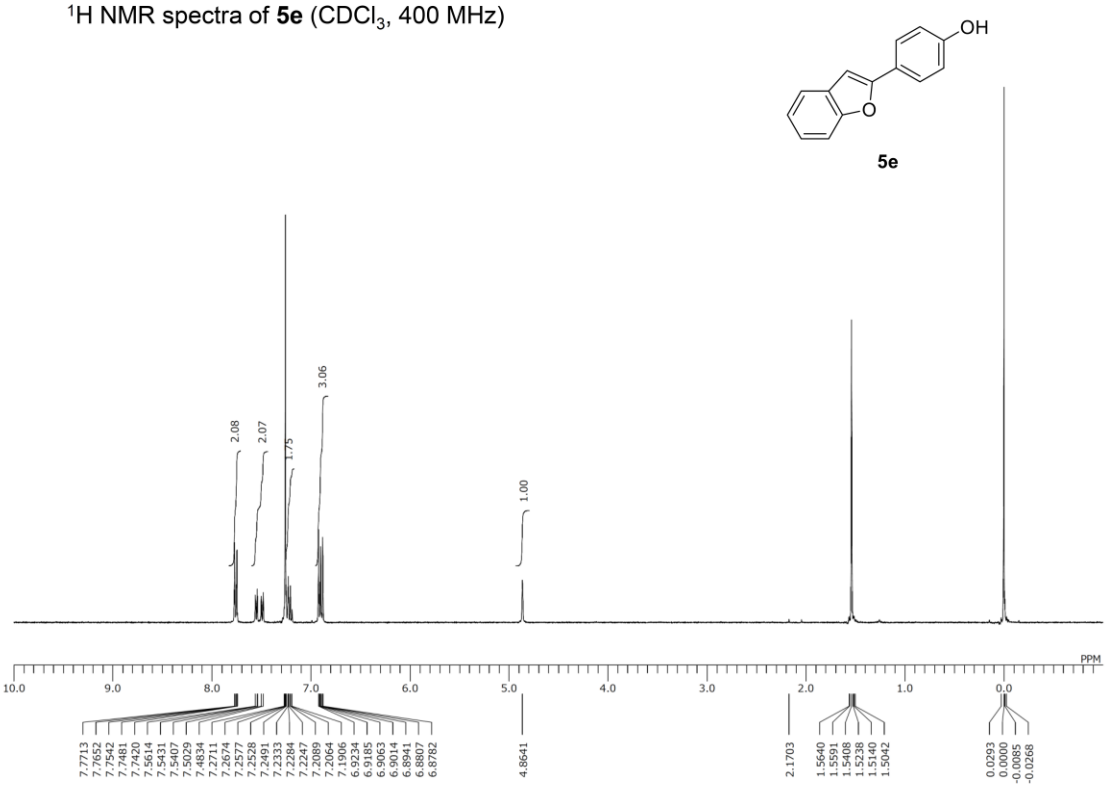
^{1}H NMR spectra of **5d** ($CDCl_3$, 400 MHz)



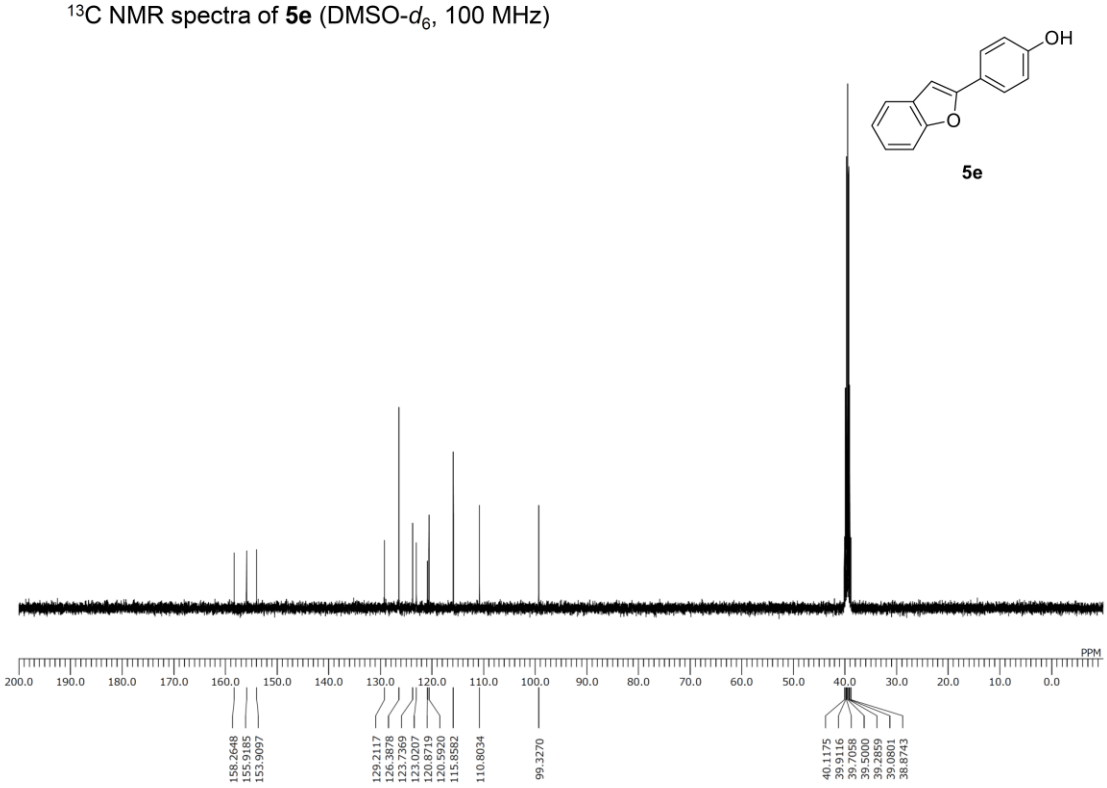
^{13}C NMR spectra of **5d** ($DMSO$-d_6, 100 MHz)



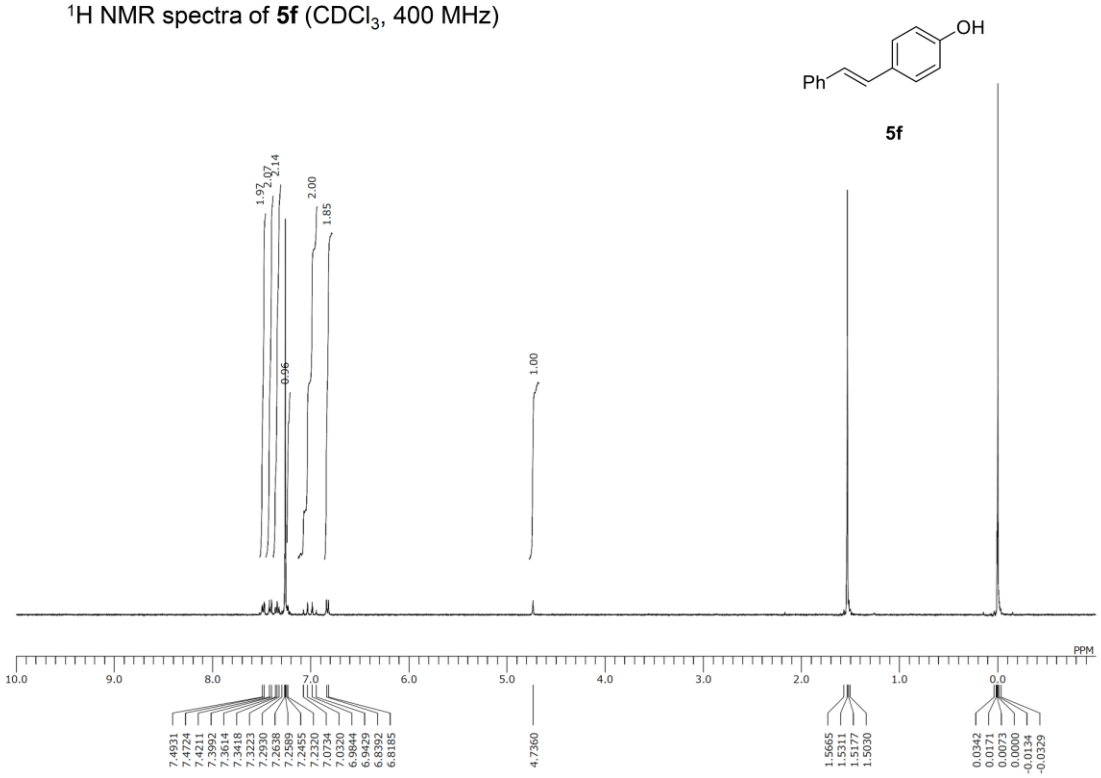
^{1}H NMR spectra of **5e** ($CDCl_3$, 400 MHz)



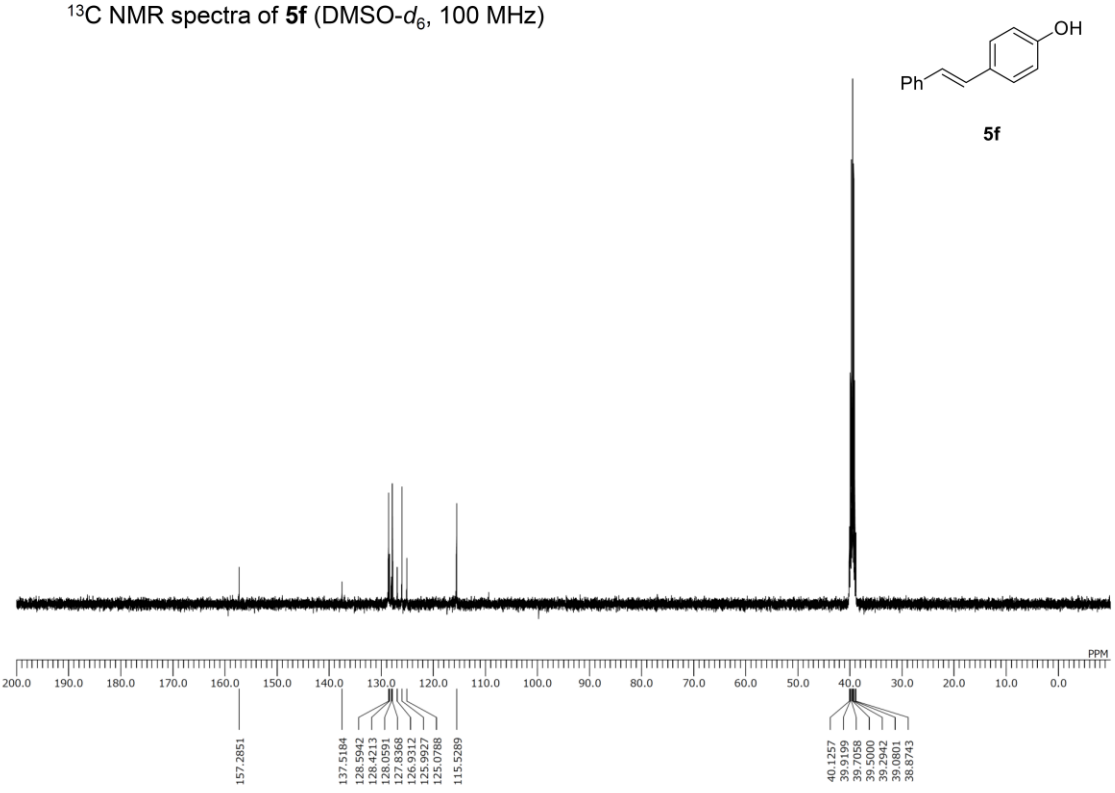
^{13}C NMR spectra of **5e** (DMSO-d_6, 100 MHz)



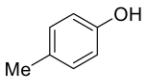
^{1}H NMR spectra of **5f** ($CDCl_3$, 400 MHz)



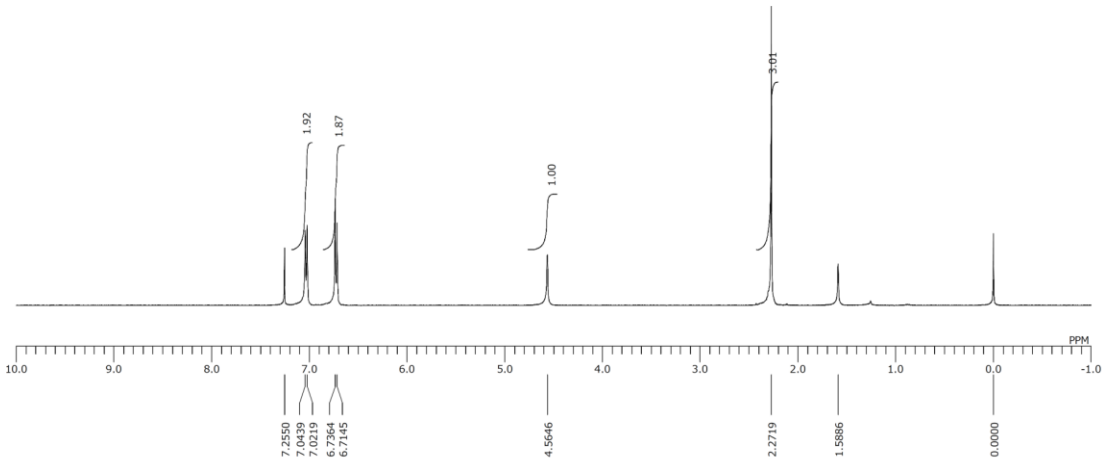
^{13}C NMR spectra of **5f** (DMSO-d_6, 100 MHz)



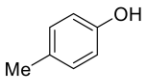
^{1}H NMR spectra of **5g** ($CDCl_3$, 400 MHz)



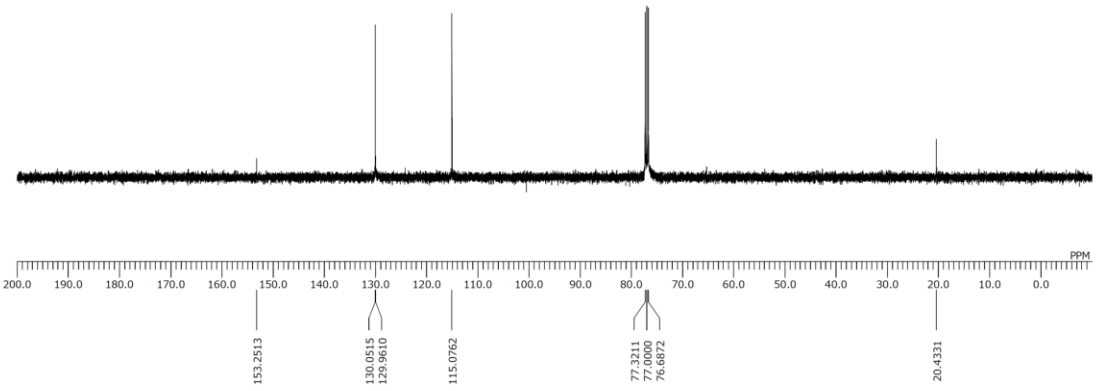
5g



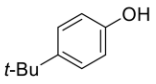
^{13}C NMR spectra of **5g** ($CDCl_3$, 100 MHz)



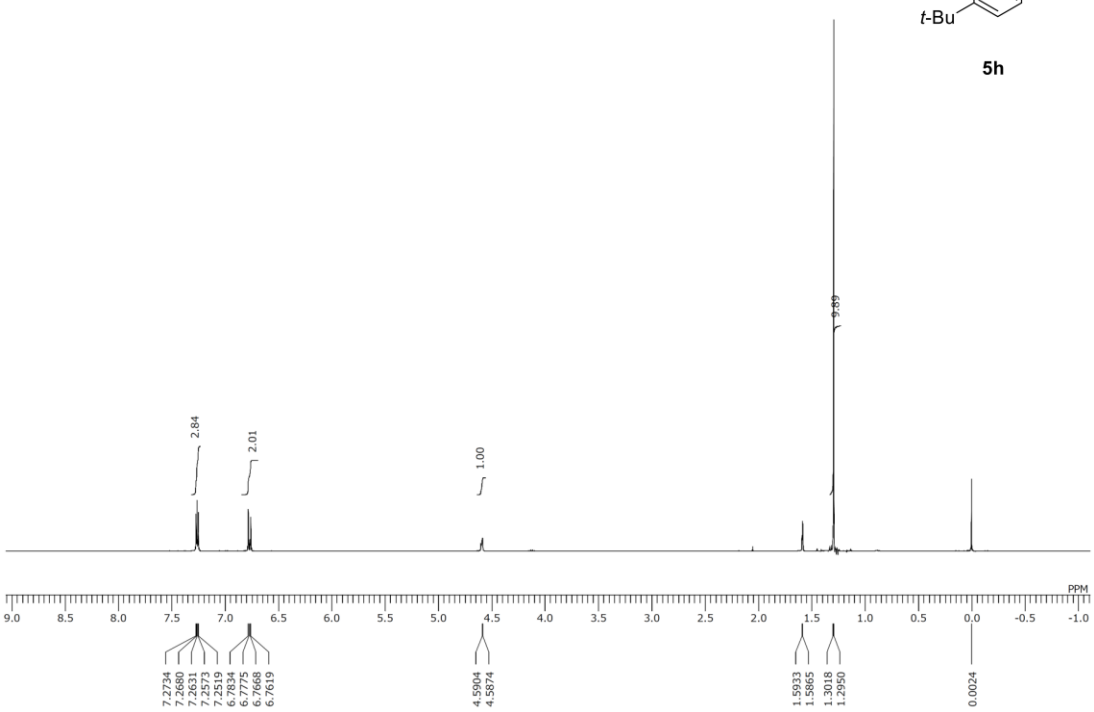
5g



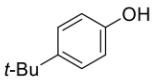
^{1}H NMR spectra of **5h** ($CDCl_3$, 400 MHz)



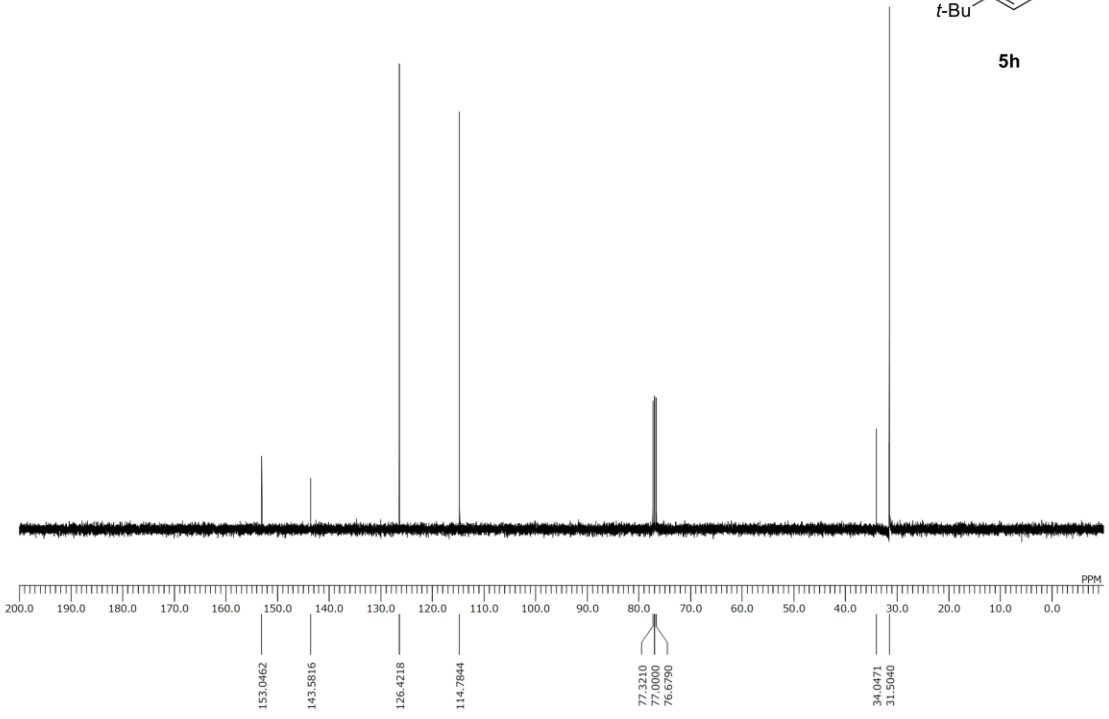
5h



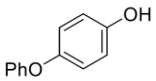
^{13}C NMR spectra of **5h** ($CDCl_3$, 100 MHz)



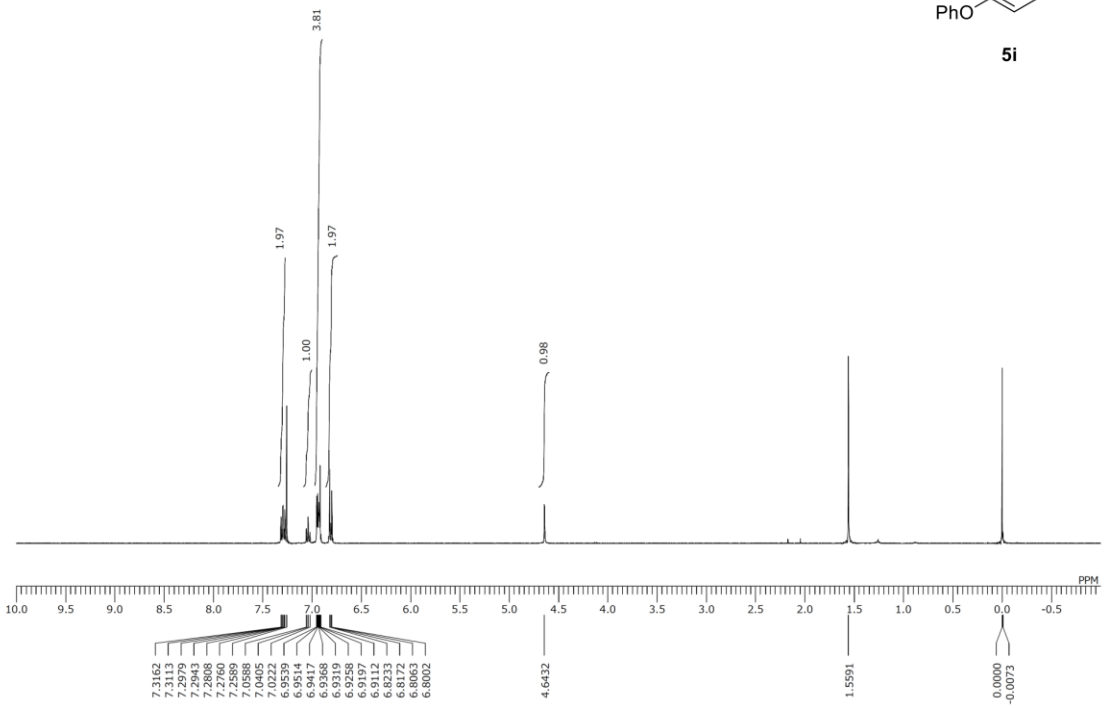
5h



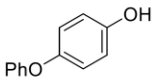
^{1}H NMR spectra of **5i** ($CDCl_3$, 400 MHz)



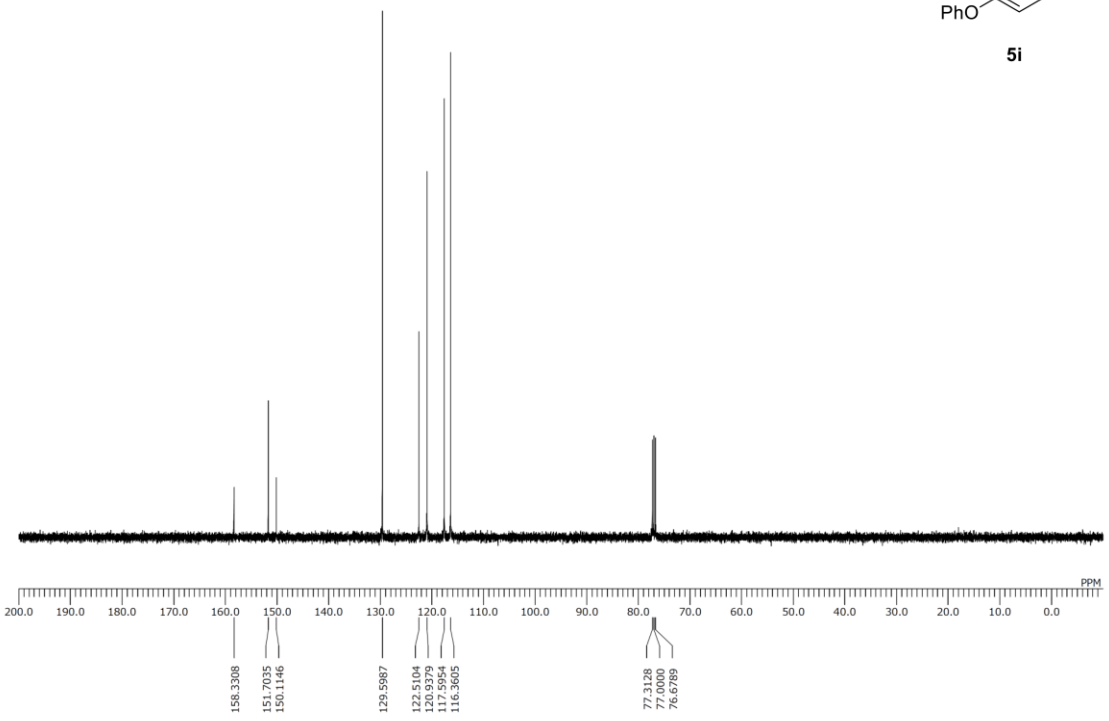
5i



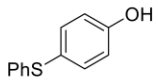
^{13}C NMR spectra of **5i** ($CDCl_3$, 100 MHz)



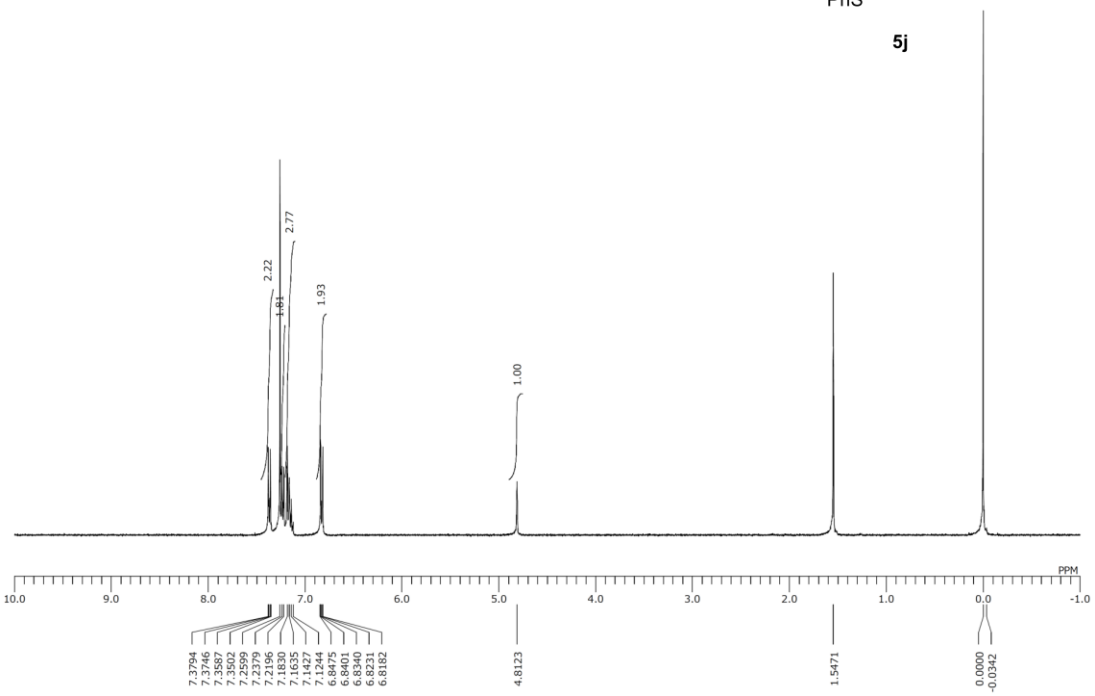
5i



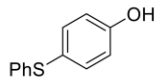
^{1}H NMR spectra of **5j** ($CDCl_3$, 400 MHz)



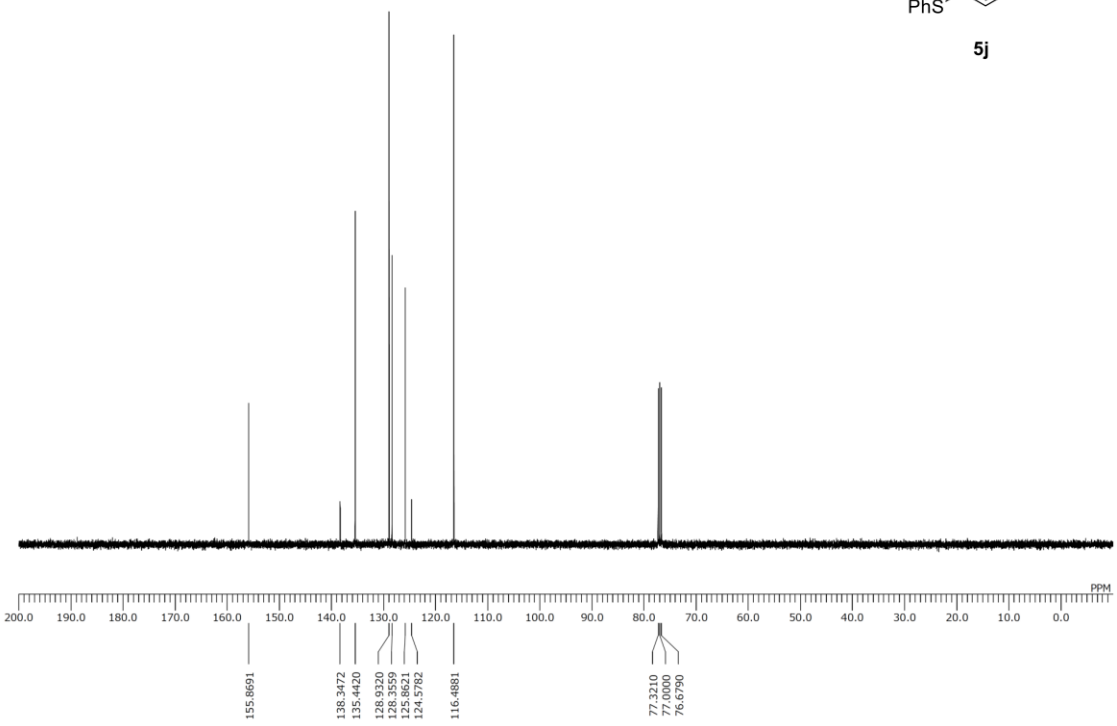
5j



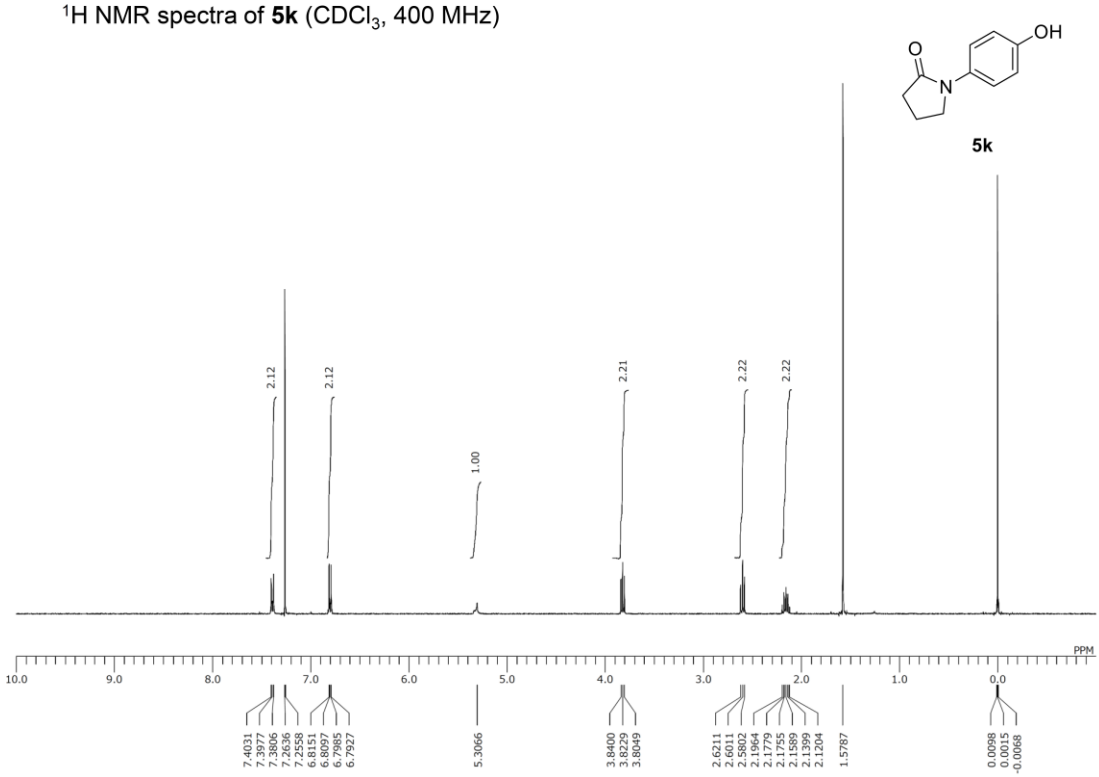
^{13}C NMR spectra of **5j** ($CDCl_3$, 100 MHz)



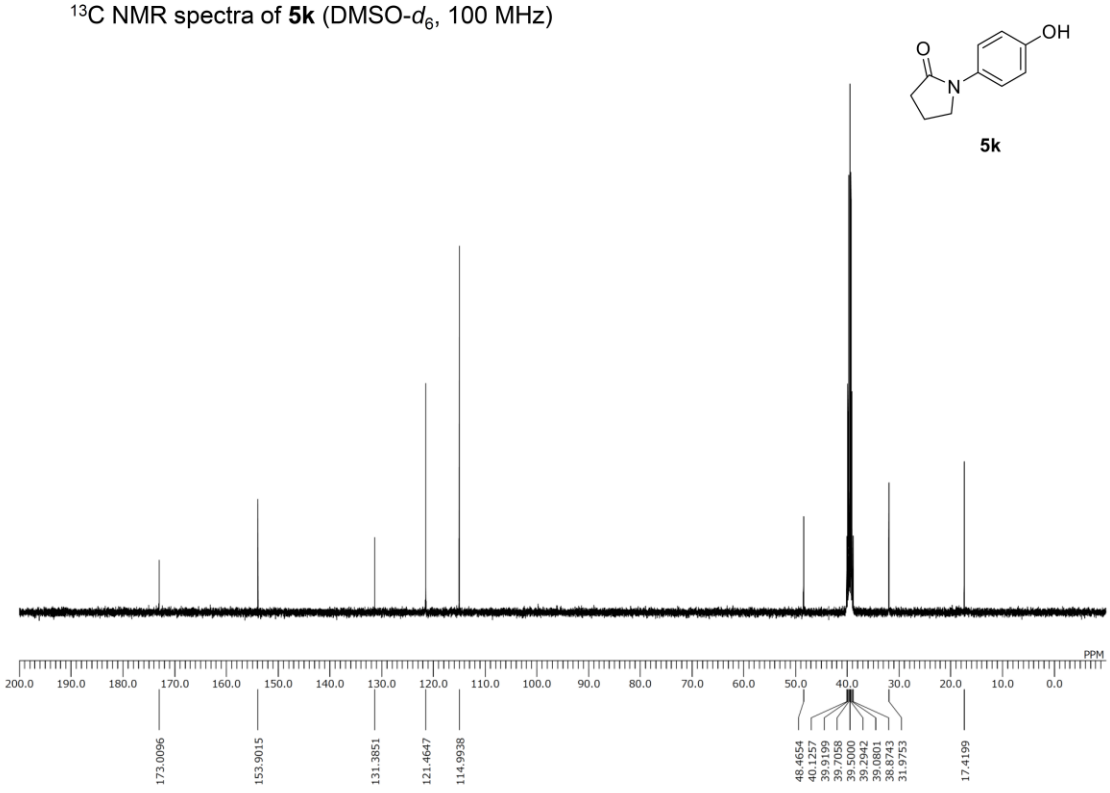
5j



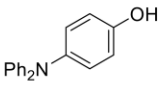
^{1}H NMR spectra of **5k** ($CDCl_3$, 400 MHz)



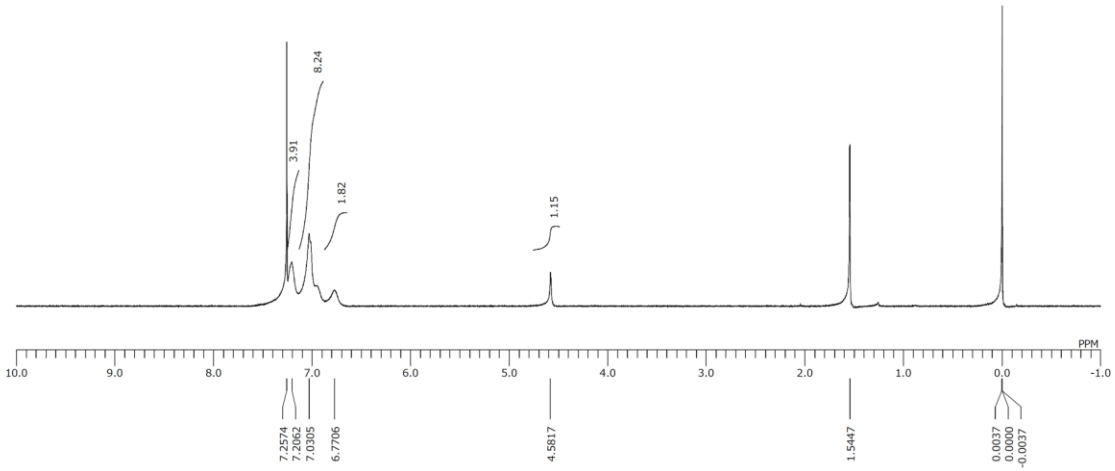
^{13}C NMR spectra of **5k** (DMSO-d_6, 100 MHz)



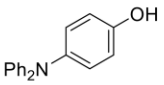
^{1}H NMR spectra of **5l** ($CDCl_3$, 400 MHz)



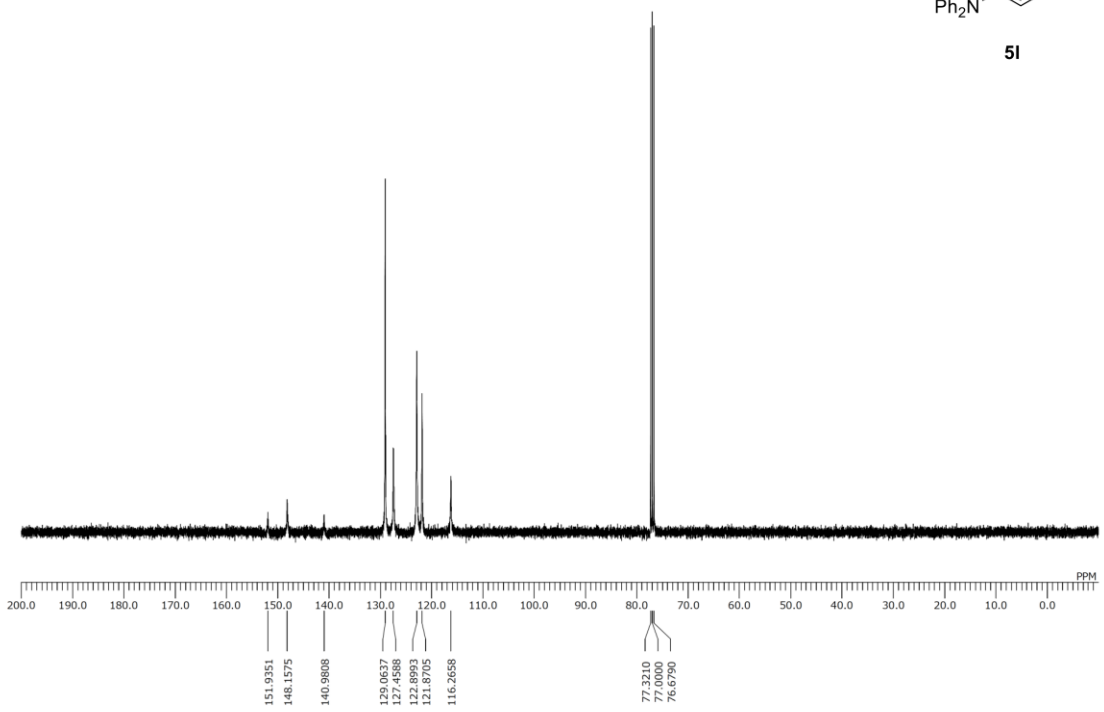
5l



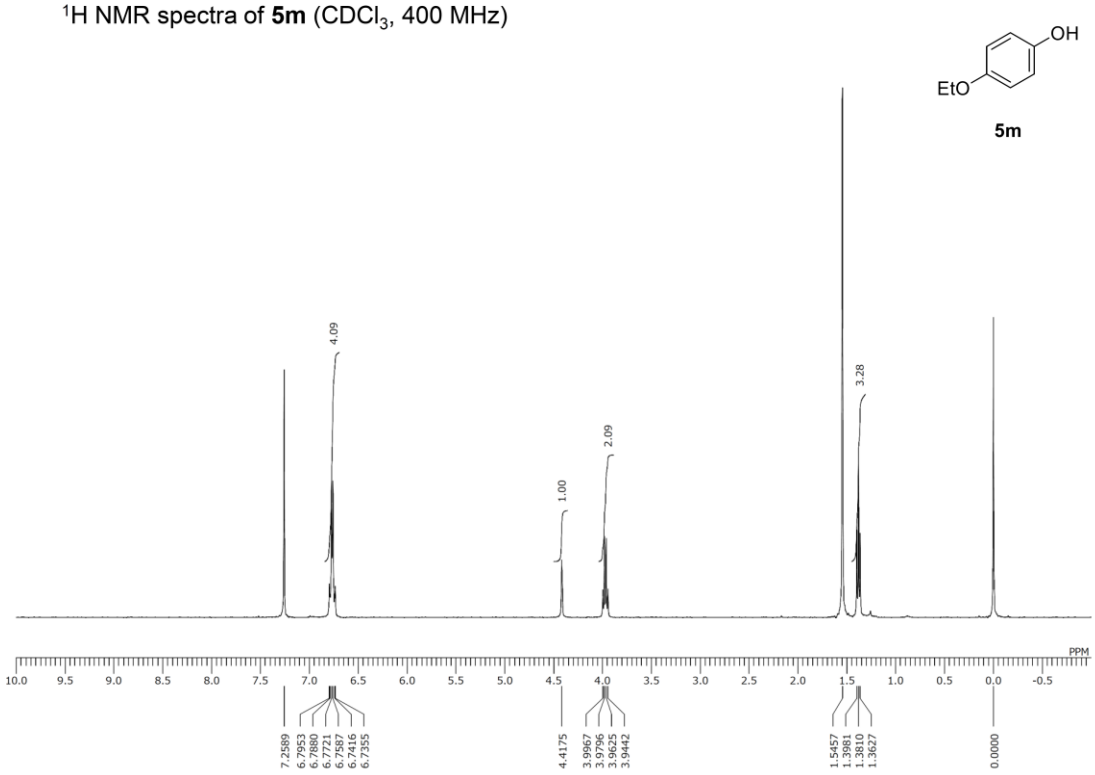
^{13}C NMR spectra of **5l** ($CDCl_3$, 100 MHz)



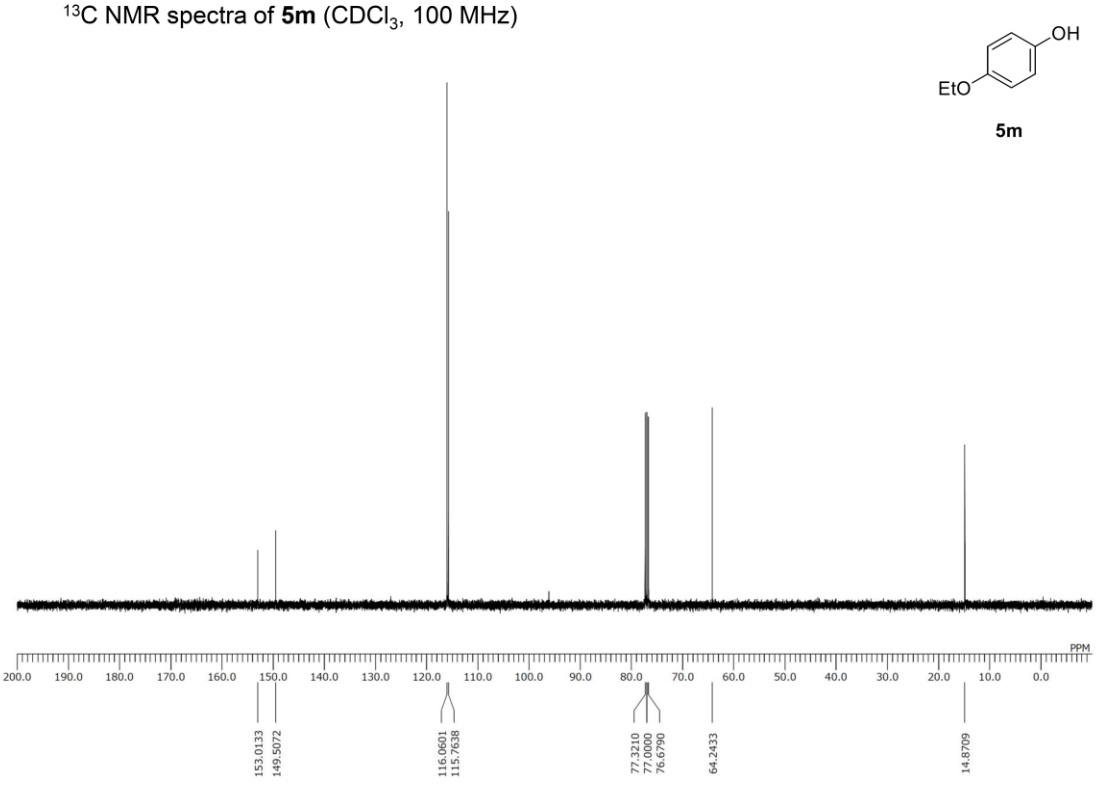
5l



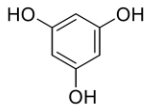
^{1}H NMR spectra of **5m** ($CDCl_3$, 400 MHz)



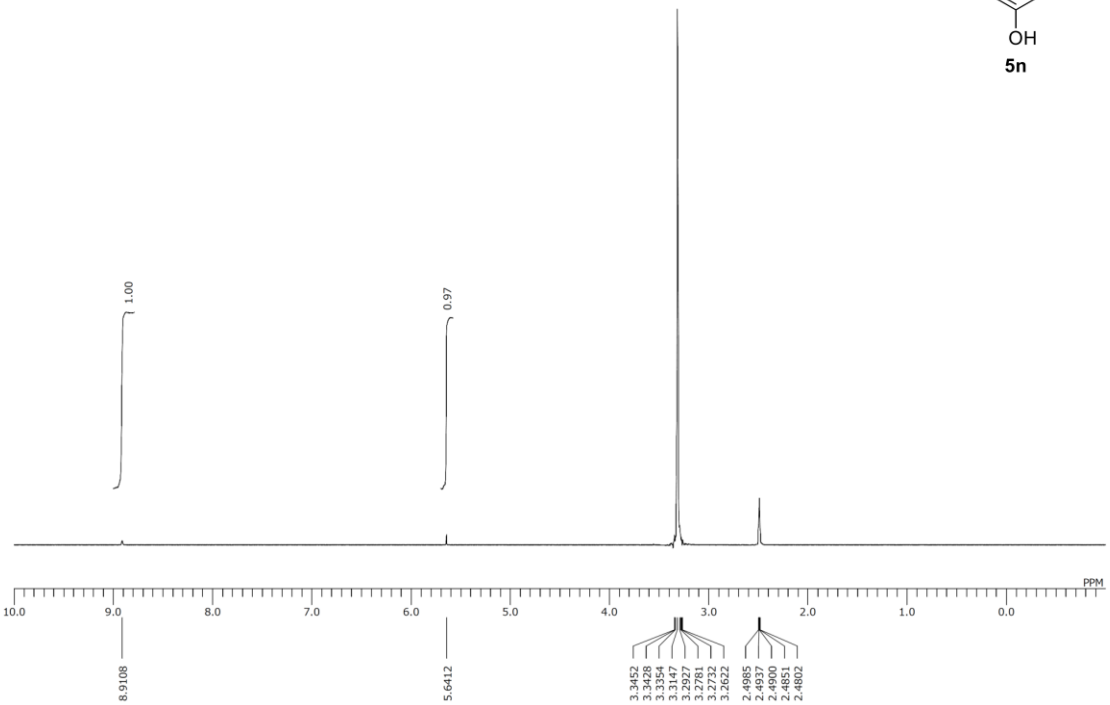
^{13}C NMR spectra of **5m** ($CDCl_3$, 100 MHz)



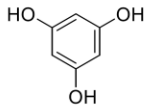
^{1}H NMR spectra of **5n** (DMSO-d_6, 400 MHz)



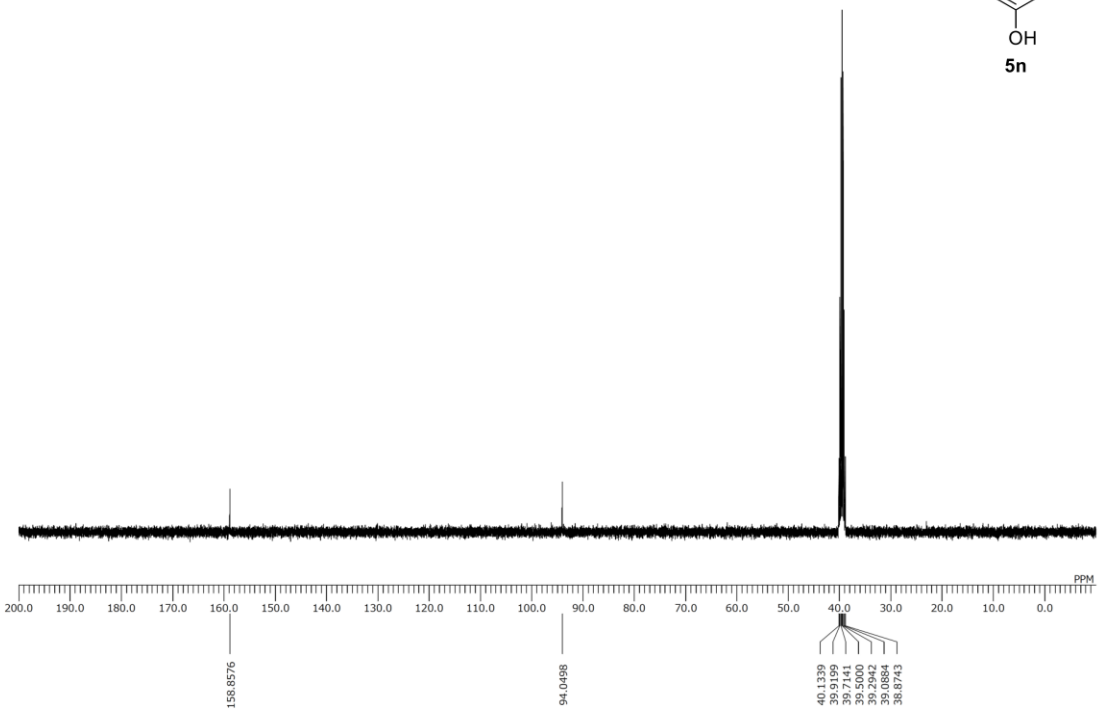
5n



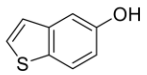
^{13}C NMR spectra of **5n** (DMSO-d_6, 100 MHz)



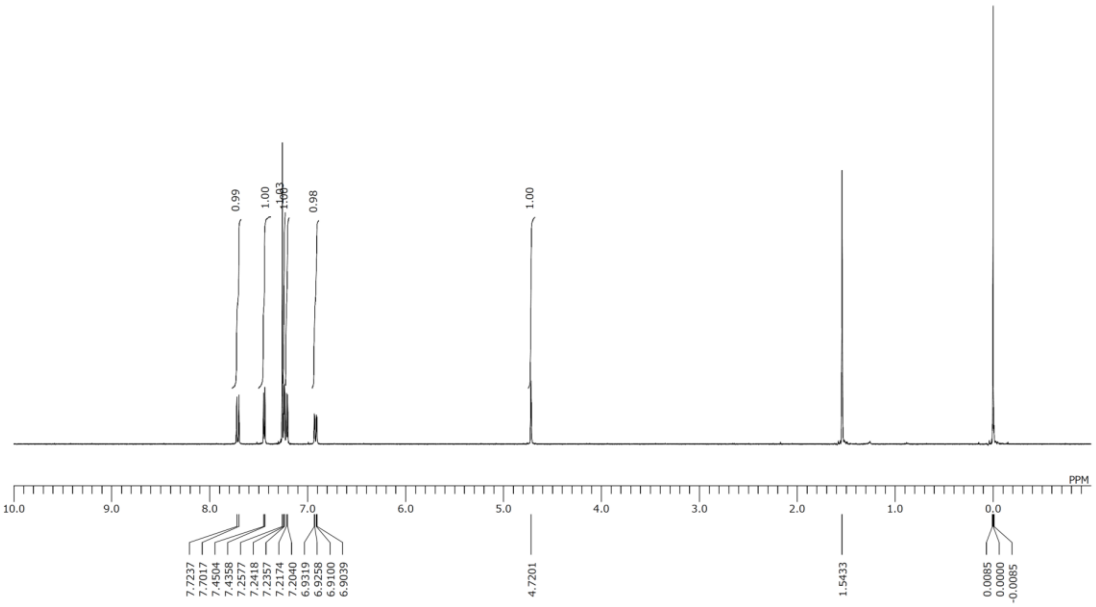
5n



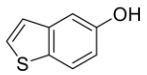
^{1}H NMR spectra of **5o** ($CDCl_3$, 400 MHz)



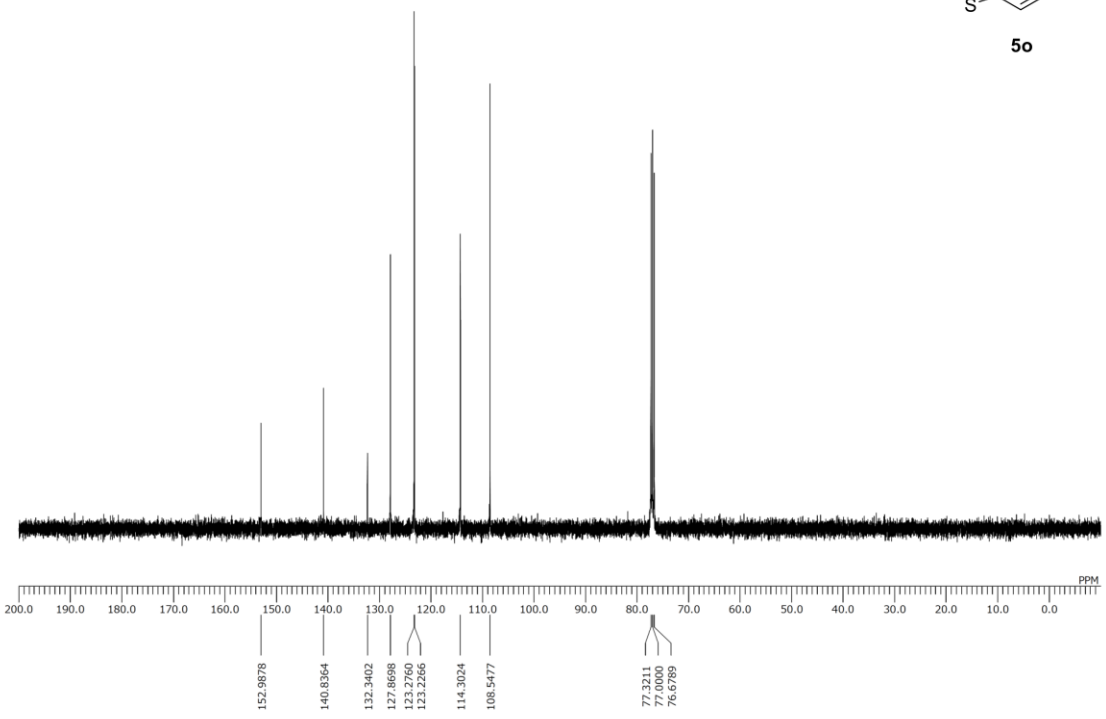
5o



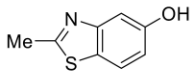
^{13}C NMR spectra of **5o** ($CDCl_3$, 100 MHz)



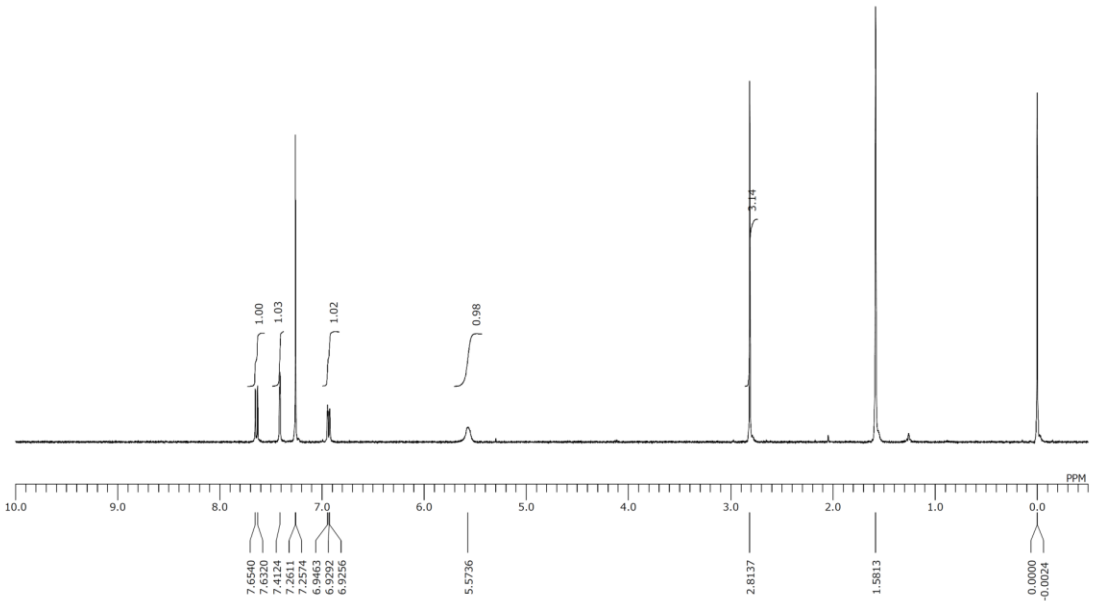
5o



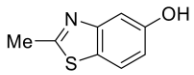
^{1}H NMR spectra of **5p** ($CDCl_3$, 400 MHz)



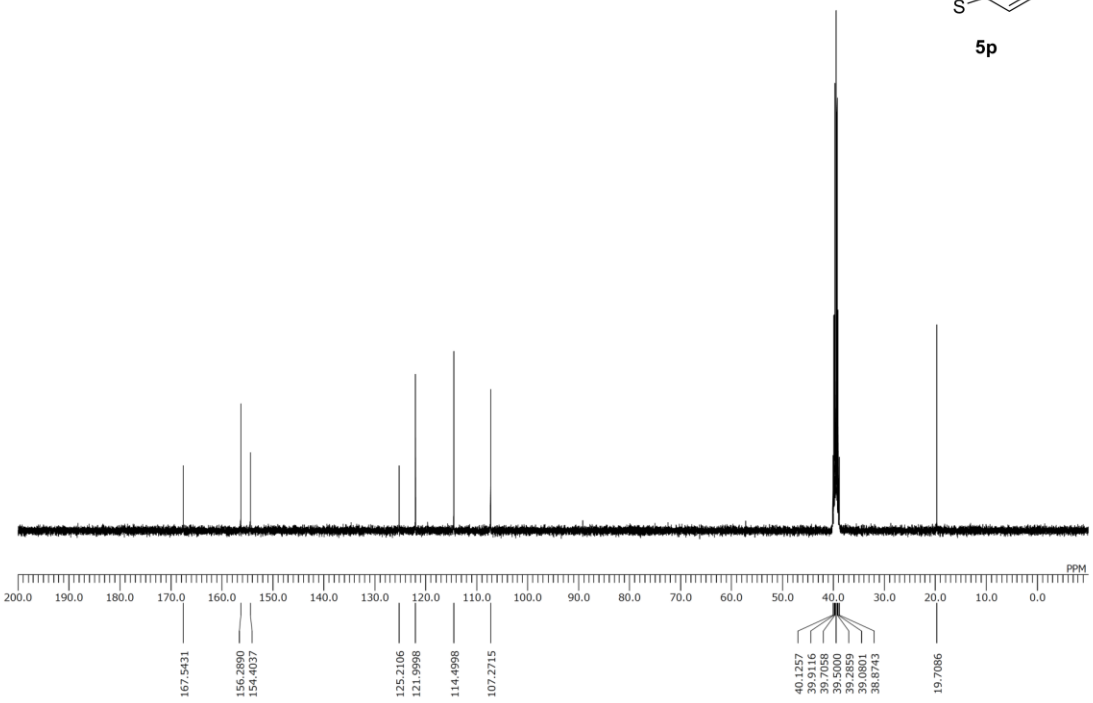
5p



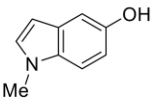
^{13}C NMR spectra of **5p** (DMSO-d_6, 100 MHz)



5p

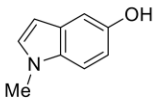


^{1}H NMR spectra of **5q** ($CDCl_3$, 400 MHz)

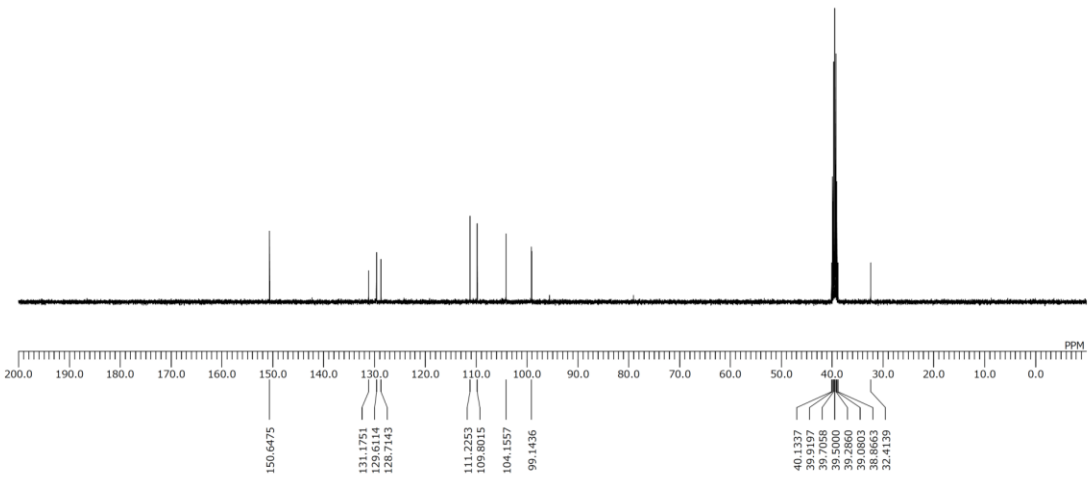


5q

^{13}C NMR spectra of **5q** (DMSO-d_6, 100 MHz)

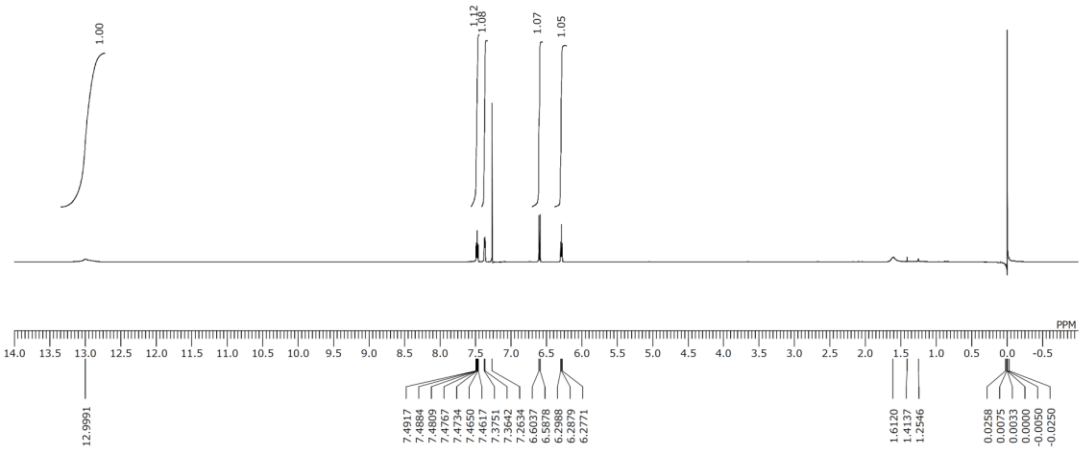


5q



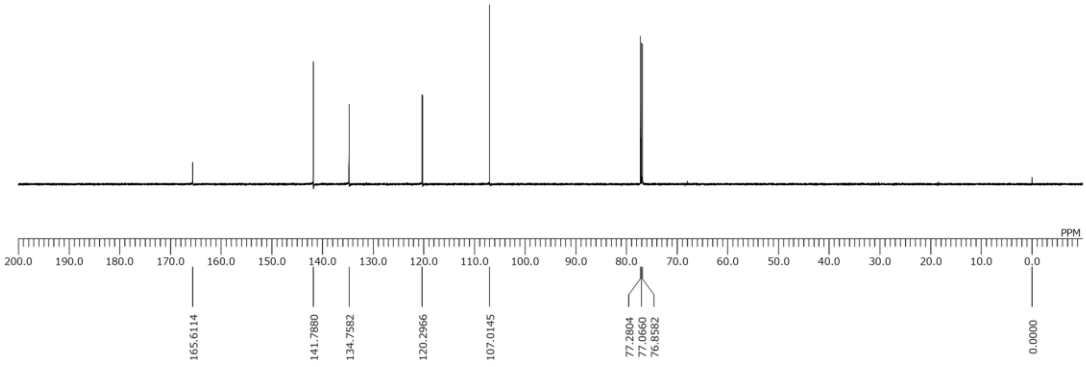
^{1}H NMR spectra of **5r** ($CDCl_3$, 600 MHz)

5r

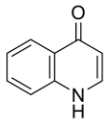


^{13}C NMR spectra of **5r** ($CDCl_3$, 150 MHz)

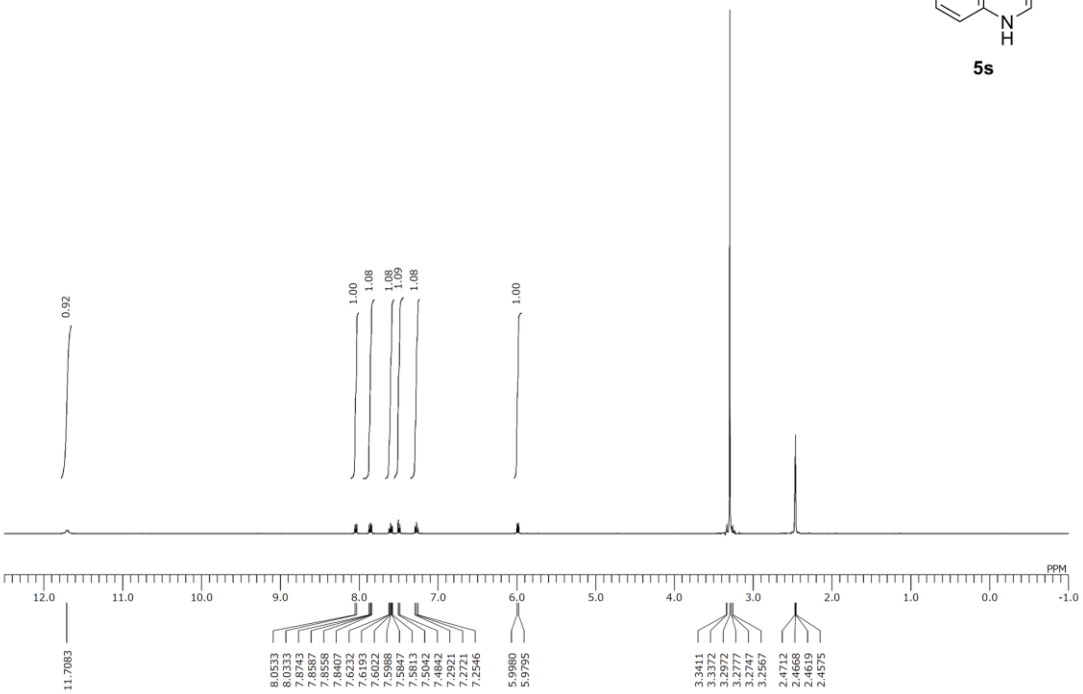
5r



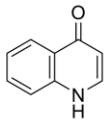
^{1}H NMR spectra of **5s** (DMSO-d_6, 400 MHz)



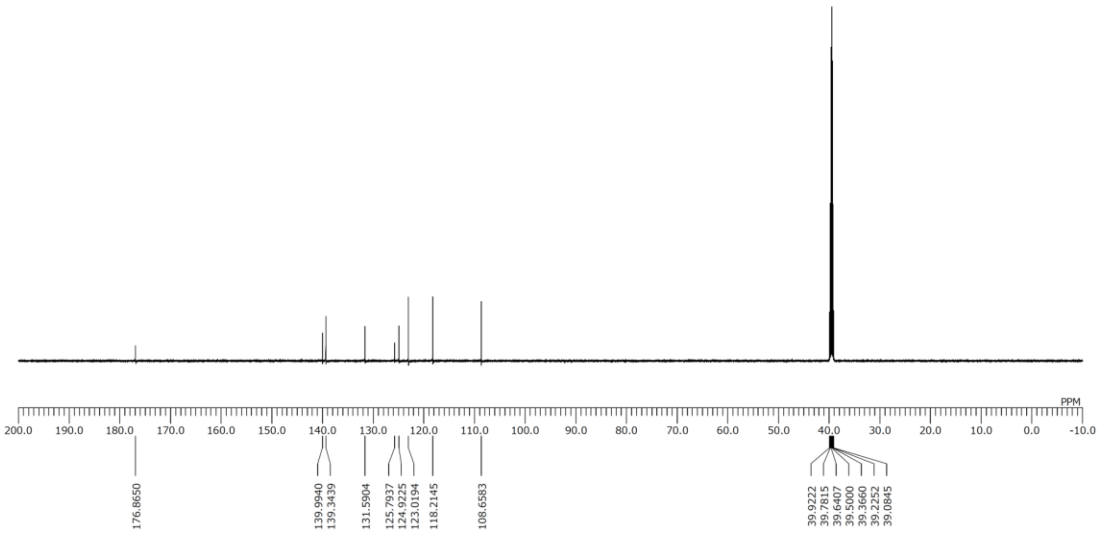
5s



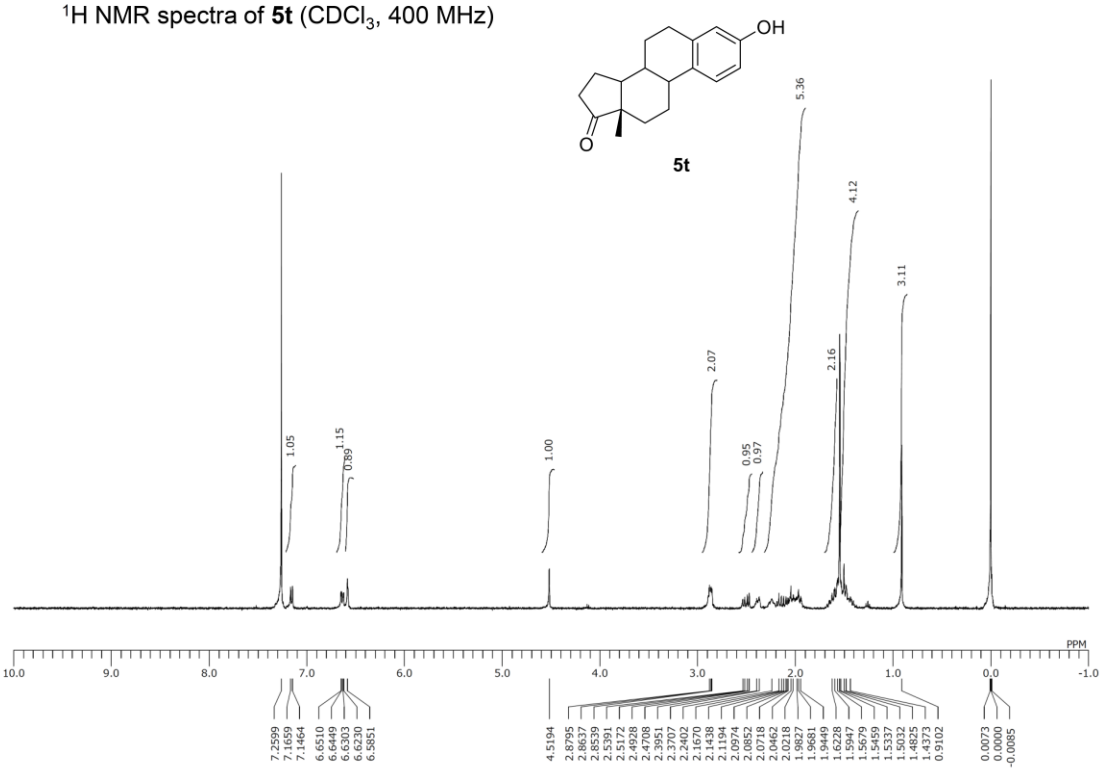
^{13}C NMR spectra of **5s** (DMSO-d_6, 150 MHz)



5s



^{1}H NMR spectra of **5t** ($CDCl_3$, 400 MHz)



^{13}C NMR spectra of **5t** (DMSO-d_6, 100 MHz)