Supporting Information

Arylation of aryllithiums with *S*-arylphenothiazinium ions for biaryl synthesis

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1. General

Phenyllithium (**1a**) in cyclohexane-Et_2O (1.09 M), *N*-methylphenothiazine, phenoxathiin, thianthrene, diphenyliodonium hexafluorophosphate, bis(4-chlorophenyl)iodonium hexafluorophosphate, bis(4-*tert*-butylphenyl)iodonium hexafluorophosphate, bis(4-methylphenyl)iodonium hexafluorophosphate, 1,4-dibromobenzene, 3,3'-dibromobiphenyl, 2,2'-dibromobiphenyl, 2,7-dibromonaphthalene, 1,4-diiodobenzene, 1,3-dibromobenzene, 1,3-diiodobenzene, 1-bromo-3-chlorobenzene, 1-bromo-4-chlorobenzene, 4-bromoanisole, 4-bromothioanisole, 2-bromotoluene, 3-bromotoluene, 1-bromonaphthalene, 2-bromonaphthalene, 2-bromodibenzofuran, and 2-bromo-9,9-dimethylfluorene were commercially available. Bis(4-methoxyphenyl) iodonium hexafluorophosphate, bis(4-bromolphenyl)iodonium hexafluorophosphate, and (4-iodolphenyl)iodonium hexafluorophosphate were synthesized according to the reported literature.[1] Super dehydrated THF was purchased from Kanto Chemical Co. and used for solvent without further purification. All materials were obtained from commercial suppliers and used without further purification. Flash chromatography was carried out on a silica gel (Kanto Chem. Co., Silica Gel N, spherical, neutral, 40-100 μm). Preparative gel permeation chromatography (GPC) was carried out on Japan Analytical Industry LC-918 equipped with JAIGEL-1H and 2H using $CHCl_3$ as an eluent. All NMR spectra were measured on Resonance ECZ 400S (JEOL, 400 MHz for ^{1}H, 100 MHz for ^{13}C) or AVANCE III HD Nano Bay (Bruker Co., 400 MHz for ^{1}H, 100 MHz for ^{13}C) at 22 ºC using $CDCl_3$ as a solvent unless otherwise noted. Tetramethylsilane (TMS) ($\delta = 0$), $CHCl_3$ ($\delta = 7.26$), or CHD_2CN ($\delta = 1.94$) served as an internal standard for ^{1}H NMR spectra, and $CDCl_3$ ($\delta = 77.16$) or CD_3CN ($\delta = 1.32$) was used as an internal standard for ^{13}C NMR spectra. X-ray crystallographic analysis was performed on Smart APEX II (Bruker Co.).

2. Synthesis of sulfonium salts

All sulfonium salts were synthesized by a modified method of the reported procedure.[2] A 300 mL round-bottom flask equipped with a magnetic stirring bar and a septum, was dried under vacuum with heating. After cooling the flask to 23 °C, it was purged with argon gas. Cyclic diaryl sulfide (1.2 equiv), chlorobenzene (0.1 M), and diaryliodonium salt (1 equiv) was added to the flask, and mixture was stirred at 120 °C for 16 hours. The resulting mixture was then cooled to 23 °C and opened to air. Ether (20 mL/1 mmol of diaryliodonium) was added, and then, precipitate was formed. The precipitate was collected with filtration and washed with Et_2O. The resulting solid was dissolved in CH_2Cl_2 (33 mL/1 mmol of diaryliodonium). Et_3N (10 equiv) and KPF_6 *sat.* (10 mL/1 mmol of diaryliodonium) was added to the solution. The organic compounds were extracted with CH_2Cl_2 (3×30 mL). Evaporation of the solvents gave a crude material, which was purified by flash chromatography ($MeOH/CH_2Cl_2$ = 2/98) to give the title compounds.

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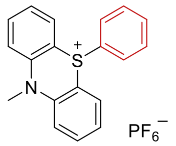
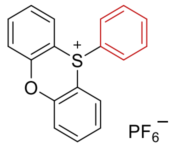
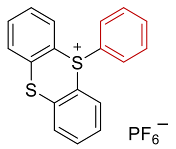
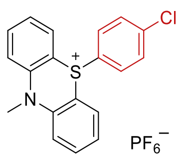
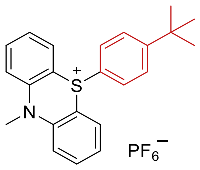
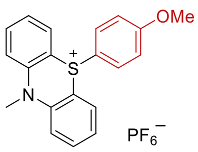
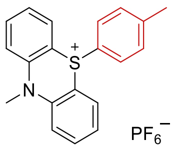
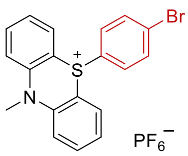
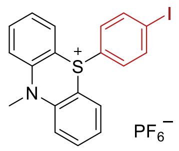
[1] N. Miralles, R. M. Romero, E. Fernández, K. Muñiz, *Chem.Commun.*, 2015, **51**, 14068.
[2] L. Racicot, T. Kasahara, M. A. Ciufolini, *Org. Lett.*, 2014, **16**, 6382.

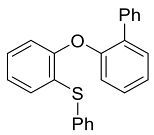
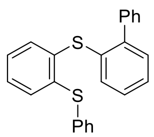
 **2a**	**10-methyl-5-phenylphenotiazinium hexafluorophosphate (2a)** Reaction of *N*-methylphenothiazine (0.78 g, 3.7 mmol) with diphenyliodonium hexafluorophosphate (1.3 g, 3.0 mmol) gave the title compound (1.0 g, 80%, light blue solid). ^{1}H NMR (400 MHz, CD_3CN): δ 8.10 (d, *J* = 7.6 Hz, 2H), 7.88 (t, *J* = 7.6 Hz, 2H), 7.61-7.54 (m, 3H), 7.51-7.45 (m, 4H), 7.19 (d, *J* = 8.0 Hz, 2H), 3.60 (s, 3H); ^{13}C NMR (100 MHz, CD_3CN): δ 144.3, 136.9, 134.1, 133.1, 131.8, 130.3, 127.9, 125.3, 118.9, 105.8, 36.6; HRMS (ESI) *m/z* calcd for $C_{19}H_{16}NS$ $[M–PF_6]^+$: 290.0998, found: 290.1002; m.p.: 231-235 ℃.
 **5**	**10-phenylphenoxathiinium hexafluorophosphate (5)** Reaction of phenoxathiin (0.25 g, 1.2 mmol) with diphenyliodonium hexafluorophosphate (0.42 g, 1.0 mmol) gave the title compound (0.25 g, 58%, white solid). ^{1}H NMR (400 MHz, CD_3CN): δ 8.02 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.91 (t, *J* = 7.8 Hz, 2H), 7.69-7.64 (m, 3H), 7.60-7.53 (m, 6H); ^{13}C NMR (100 MHz, CD_3CN): δ 152.4, 138.0, 135.5, 132.5, 132.4, 132.3, 129.8, 128.4, 121.5, 106.4; HRMS (ESI) *m/z* calcd for $C_{18}H_{13}OS$ $[M–PF_6]^+$: 277.0682, found: 277.0681; m.p.: 196-198 °C.
 **8**	**5-phenylthianthrenium hexafluorophosphate (8)** Reaction of thianthrene (0.26 g, 1.2 mmol) with diphenyliodonium hexafluorophosphate (0.44 g, 1.0 mmol) gave the title compound (0.33 g, 76%, white solid). ^{1}H NMR (400 MHz, CD_3CN): δ 8.38 (d, *J* = 7.6 Hz, 2H), 7.95 (d, *J* = 7.2 Hz, 2H), 7.90 (t, *J* = 7.2 Hz, 2H), 7.83 (t, *J* = 7.2 Hz, 2H), 7.61 (t, *J* = 6.8 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.11 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, CD_3CN): δ 137.7, 136.2, 136.1, 134.0, 131.7, 131.6, 130.9, 128.9, 124.9, 119.5; HRMS (ESI) *m/z* calcd for $C_{18}H_{13}S_2$ $[M–PF_6]^+$: 293.0453, found: 293.0451; m.p.: 263-265 °C.
 **2b**	**5-(4-chlorophenyl)-10-methylphenotiazinium hexafluorophosphate (2b)** Reaction of *N*-methylphenothiazine (1.3 g, 6.0 mmol) with bis(4-chlorophenyl)iodonium hexafluorophosphate (2.5 g, 5.1 mmol) gave the title compound (1.5 g, 65%, light blue solid). ^{1}H NMR (400 MHz, CD_3CN): δ 8.11 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.87 (t, *J* = 7.8 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.51-7.40 (m, 4H), 7.13 (d, *J* = 8.8 Hz, 2H), 3.59 (s, 3H); ^{13}C NMR (100 MHz, CD_3CN): δ 144.3, 140.0, 137.0, 133.1, 131.8, 129.7, 128.9, 125.4, 119.0, 105.5, 36.7; HRMS (ESI) *m/z* calcd for $C_{19}H_{15}ClNS$ $[M–PF_6]^+$: 324.0608, found: 324.0620; m.p.: 221-224 °C.

 **2c**	**10-methyl-5-(4-*tert*-butylphenyl)phenothiazinium hexafluorophosphate (2c)** Reaction of *N*-methylphenothiazine (0.97 g, 4.5 mmol) with bis(4-*tert*-butylphenyl)iodonium hexafluorophosphate (1.8 g, 3.4 mmol) gave the title compound (0.93 g, 57%, light blue solid). ^{1}H NMR (400 MHz, CD_3CN): δ 8.08 (d, J = 7.6 Hz, 2H), 7.88 (t, J = 7.6 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.53-7.44 (m, 4H), 7.18 (d, J = 8.4 Hz, 2H), 3.64 (s, 3H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, CD_3CN): δ 158.3, 144.2, 136.8, 132.9, 129.1, 128.0, 127.1, 125.3, 118.9, 106.0, 36.6, 35.8, 31.0; HRMS (ESI) *m/z* calcd for $C_{23}H_{24}NS$ $[M–PF_6]^+$: 346.1624, found: 346.1623; m.p.: 217-219 °C.
 **2d**	**10-methyl-5-(4-methoxyphenyl)phenothiazinium hexafluorophosphate (2d)** Reaction of *N*-methylphenothiazine (1.3 g, 6.0 mmol) with bis(4-methoxyphenyl)iodonium hexafluorophosphate (2.4 g, 5.0 mmol) gave the title compound (2.1 g, 91%, light blue solid). ^{1}H NMR (400 MHz, CD_3CN): δ 7.90 (dd, J = 7.6, 1.2 Hz, 2H), 7.81 (t, J = 8.0 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 7.40 (t, J = 7.6 Hz, 2H), 7.24 (d, J = 8.8 Hz, 2H), 6.93 (d, J = 9.2, 2H), 3.71(s, 3H), 3.62(s, 3H); ^{13}C NMR (100 MHz, CD_3CN): δ 164.6, 144.1, 136.6, 132.7, 130.5, 125.2, 120.5, 118.9, 117.4, 106.7, 56.7, 36.6; HRMS (ESI) *m/z* calcd for $C_{20}H_{18}NOS$ $[M–PF_6]^+$: 320.1104, found: 320.1094; m.p.: 171-174 °C.
 **2e**	**10-methyl-5-(4-methylphenyl)phenothiazinium hexafluorophosphate (2e)** Reaction of *N*-methylphenothiazine (0.51 g, 2.4 mmol) with bis(4-methylphenyl)iodonium hexafluorophosphate (0.69 g, 1.5 mmol) gave the title compound (0.50 g, 74%, light blue solid). ^{1}H NMR (400 MHz, CD_3CN): δ 8.07 (dd, J = 7.6, 0.8, 2H), 7.85 (dt, J = 7.8, 1.2 Hz, 2H), 7.55 (d, J = 8.4 Hz, 2H), 7.45 (t, J = 7.4 Hz, 2H), 7.27 (d, J = 8.4 Hz, 2H), 7.11 (d, J = 8.4 Hz, 2H), 3.60 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, CD_3CN): δ145.7, 144.1, 136.8, 132.9, 132.4, 128.0, 127.0, 125.3, 118.9, 106.1, 36.6, 21.3; HRMS (ESI) *m/z* calcd for $C_{20}H_{18}NS$ $[M–PF_6]^+$: 304.1155, found: 304.1159; m.p.: 217-220 °C.
 **2f**	**5-(4-bromophenyl)-10-methylphenotiazinium hexafluorophosphate (2f)** Reaction of *N*-methylphenothiazine (2.1 g, 10 mmol) with bis(4-bromophenyl)iodonium hexafluorophosphate (4.6 g, 7.8 mmol) gave the title compound (1.8 g, 46%, light blue solid) ^{1}H NMR (400 MHz, CD_3CN): δ 8.10 (d, J = 7.6 Hz, 2H), 7.88 (t, J = 7.4 Hz, 2H), 7.58 (t, J = 8.4 Hz, 4H), 7.49 (t, J = 7.4 Hz, 2H), 7.05 (d, J = 8.4 Hz, 2H), 3.60 (s, 3H); ^{13}C NMR (100 MHz, CD_3CN): δ 144.3, 137.0, 134.7, 133.1, 129.7, 129.6, 128.4, 125.4, 119.0, 105.4, 36.7; HRMS (ESI) *m/z* calcd for $C_{19}H_{15}{}^{81}BrNS$ $[M–PF_6]^+$: 370.0083, found: 370.0083; m.p.: 230-235 °C.

 **2g**	**10-(4-iodophenyl)-5-methylphenotiazinium hexafluorophosphate (2g)** Reaction of *N*-methylphenothiazine (0.73 g, 3.4 mmol) with bis(4-iodophenyl)iodonium hexafluorophosphate (1.8 g, 2.6 mmol) gave the title compound (0.52 g, 35%, light blue solid). ^{1}H NMR (400 MHz, CD_3CN): δ 8.08 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.89 (t, *J* = 8.0 Hz, 2H), 7.80 (d, *J* = 8.8 Hz, 2H), 7.58 (d, *J* = 8.8 Hz, 2H), 7.48 (t, *J* = 7.6 Hz, 2H), 6.89 (d, *J* = 8.8 Hz, 2H), 3.60 (s, 3H); ^{13}C NMR (100 MHz, CD_3CN): δ 144.3, 140.7, 137.0, 133.1, 130.4, 129.4, 125.4, 119.0, 105.3, 100.8, 36.7; HRMS (ESI) *m/z* calcd for $C_{19}H_{15}INS$ $[M–PF_6]^+$: 415.9964, found: 415.9976; m.p.: 259-263 °C.

3. Reaction of phenyllithium (1a) with sulfonium salts

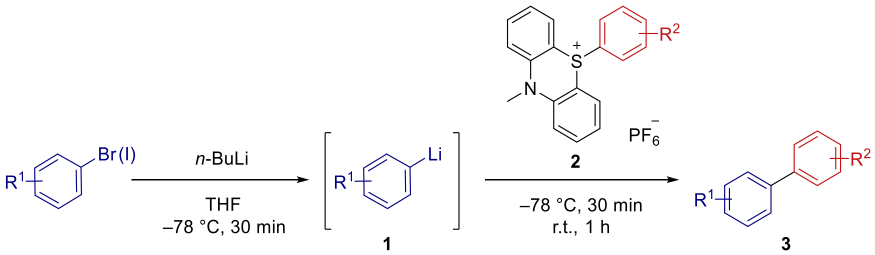
A 30 mL round-bottom flask equipped with a magnetic stirring bar and a septum, was dried under vacuum with heating. After cooling the flask to 23 °C, it was purged with argon gas. Sulfonium salt (0.20 mmol) and THF (5 mL) were added to the flask, and the mixture was cooled to –78 °C. PhLi in cyclohexane-Et_2O (1.09 M, 0.55 mL, 0.60 mmol) was added dropwise at –78 °C. The reaction mixture was stirred at –78 °C for 30 min and at 23 °C for 1 h. The reaction was quenched by ethanol (0.20 mL). Evaporation of the solvents gave a crude material. For entries 1 and 2, yields of **3a** and *N*-methylphenothiazine (**4**) were determined by ^{1}H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard. For entry 3, the crude product was purified with column chromatography (hexane/EtOAc = 100/0 to 80/20). Yields of **3a** and phenoxathiin (**6**) were determined by ^{1}H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard, and ring opening product **7a** was isolated (44 mg, 62%, colorless oil). For entry 4, the crude product was purified with column chromatography (hexane/EtOAc = 100/0 to 80/20). Yield of **3a** was determined by ^{1}H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard. Dibenzothiophene (**9**) (20 mg, 55%), diphenyl sulfide (**10**) (19 mg, 51%), and ring opening product **7b** (23 mg, 31%) were isolated.

 **7a**	^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (d, *J* = 7.2 Hz, 2H), 7.44 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.34-7.22 (m, 9H), 7.21-7.13 (m, 2H), 7.10 (dt, *J* = 7.8, 1.2 Hz, 1H), 6.94 (dt, *J* = 7.6, 1.2 Hz, 1H), 6.86 (dd, *J* = 8.0, 0.8 Hz, 1H), 6.76 (dt, *J* = 8.4, 0.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.5, 153.7, 137.7, 134.8, 133.1, 132.6, 131.7, 131.4, 129.5, 129.3, 128.8, 128.5, 128.2, 127.3, 127.23, 127.16, 124.0, 123.9, 119.0, 118.7; HRMS (ESI) *m/z* calcd for $C_{24}H_{18}OSNa^+$ $[M+Na]^+$: 377.0971, found: 377.0985
 **7b**	^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41 (d, *J* = 7.2 Hz, 2H), 7.37-7.28 (m, 5H), 7.27-7.21 (m, 6H), 7.20-7.18 (m, 1H), 7.09-6.80 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.8, 140.6, 138.8, 136.7, 134.5, 133.7, 132.5, 132.3, 131.7, 131.1, 130.9, 129.45, 129.43, 128.3, 128.1, 127.8, 127.7, 127.5, 127.39, 127.38; HRMS (ESI) *m/z* calcd for $C_{24}H_{18}S_2Na^+$ $[M+Na]^+$: 393.0742, found: 393.0742

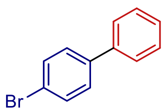
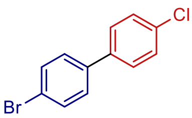
4. Procedure of the arylation of aryllithiums with *S*-arylphenothiazinium ions

General procedure

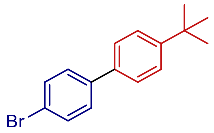
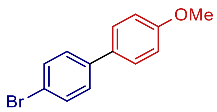
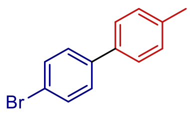
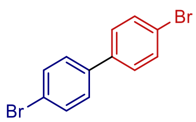
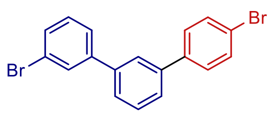
A 30 mL round-bottom flask equipped with a magnetic stirring bar and a septum, was dried under vacuum with heating. After cooling the flask to 23 °C, it was purged with argon gas. Bromo- or iodoarene (0.6 mmol) and THF (5 mL) were added to the flask, and the mixture was cooled to –78 °C. *n*-BuLi in hexane (1.57 M, 0.40 mL, 0.62 mmol) was added dropwise at –78 °C. After stirring at –78 °C for 30 min, *S*-arylphenothiazinium salt **2** was added one portion as a solid. The reaction mixture was stirred at –78 °C for 30 min and at 23 °C for 1 h unless otherwise noted. The reaction was quenched by ethanol (0.20 mL). Evaporation of the solvents gave a crude material, which was purified by flash chromatography or GPC to give desired product **3**.



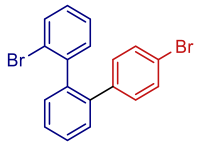
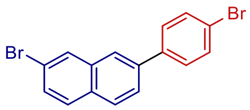
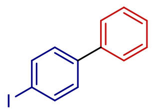
Scheme S1.

 **3b**	**4-bromobiphenyl (3b)**[3] Reaction of *p*-dibromobenzene (144 mg, 0.61 mmol) with 10-methyl-5-phenylphenothiazinium hexafluorophosphate **(2a)** (88 mg, 0.20 mmol) gave the title compound (44 mg, 94%, white solid). Purification method: flash chromatography (hexane/EtOAc = 100/0 to 80/20). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59-7.54 (m, 4H), 7.48-7.43 (m, 4H), 7.37 (t, J = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.3, 140.1, 132.0, 129.0, 128.9, 127.8, 127.1, 121.7.
 **3c**	**4-bromo-4'-chlorobiphenyl (3c)**[4] Reaction of *p*-dibromobenzene (149 mg, 0.63 mmol) with 5-(4-chlorophenyl)-10-methylphenothiazinium hexafluorophosphate (**2b**) (95 mg, 0.20 mmol) gave the title compound (56 mg, 98%, white solid). Purification method: flash chromatography (hexane/EtOAc = 100/0 to 80/20). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, J = 8.4 Hz, 2H), 7.48 (d, J = 8.4 Hz, 2H), 7.43-7.38 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.0, 138.6, 133.9, 132.1, 129.2, 128.7, 128.3, 122.0.

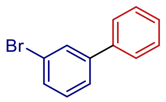
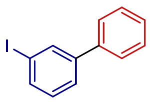
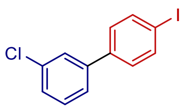
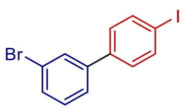
[3] C. Song, X. Dong, Z. Wang, K. Liu, C.-W. Chiang, A. Lei, *Angew. Chem. Int. Ed.*, 2019, **58**, 12206.
[4] Y. Ding, L. Mao, D. Xu, H. Xie, L. Yang, H. Xu, W. Geng, Y. Gao, C. Xia, X. Zhang, Q. Meng, D. Wu, J. Zhao, W. Hu, *Bioorg. Med. Chem. Lett.*, 2015, **25**, 2744.

 **3d**	**4-bromo-4'-*tert*-butylbiphenyl (3d)**[3] Reaction of *p*-dibromobenzene (146 mg, 0.62 mmol) with 10-methyl-5-(4-*tert*-butylphenyl)phenothiazinium hexafluorophosphate (**2c**) (101 mg, 0.21 mmol) gave the title compound (40 mg, 69%, white solid). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56-7.43 (m, 8H), 1.37 (s, 9H); ^{13}C NMR: δ 150.9, 140.1, 137.2, 131.9, 128.7, 126.7, 126.0, 121.3, 34.7, 31.5.
 **3e**	**4-bromo-4'-methoxybiphenyl (3e)**[5] Reaction of *p*-dibromobenzene (142 mg, 0.60 mmol) with 10-methyl-5-(4-methoxyphenyl)phenothiazinium hexafluorophosphate (**2d**) (94 mg, 0.20 mmol) gave the title compound (38 mg, 71%, white solid). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54-7.46 (m, 4H), 7.41 (d, J = 8.4 Hz, 2H), 6.97 (d, J = 8.4 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.5, 139.9, 132.6, 131.9, 128.4, 128.1, 120.9, 114.5, 55.5.
 **3f**	**4-bromo-4'-methylbiphenyl (3f)**[6] Reaction of *p*-dibromobenzene (145 mg, 0.61 mmol) with 10-methyl-5-(4-methylphenyl)phenothiazinium hexafluorophosphate (**2e**) (92 mg, 0.20 mmol) gave the title compound (40 mg, 80%, white solid). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (d, J = 8.4 Hz, 2H), 7.45-7.41 (m, 4H), 7.23 (d, J = 7.6 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.2, 137.7, 137.2, 131.9, 129.8, 128.7, 126.9, 121.3, 21.3.
 **3g**	**4,4'-dibromobiphenyl (3g)**[7] Reaction of *p*-dibromobenzene (144 mg, 0.61 mmol) with 5-(4-bromophenyl)-10-methylphenothiazinium hexafluorophosphate (**2f**) (103 mg, 0.20 mmol) gave the title compound (53 mg, 85%, white solid). Purification method: flash chromatography (hexane/EtOAc = 100/0 to 80/20). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, J = 8.4 Hz, 4H), 7.41 (d, J = 8.8 Hz, 4H).; ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.0, 132.2, 128.6, 122.1.
 **3h**	**3,4'''-dibromo-*m*-terphenyl (3h)** Reaction of 3,3'-dibromobiphenyl (190 mg, 0.61 mmol) with 5-(4-bromophenyl)-10-methylphenothiazinium hexafluorophosphate (**2f**) (103 mg, 0.20 mmol) gave the title compound (35 mg, 45%, white solid). Purification method: flash chromatography (hexane/EtOAc = 100/0 to 80/20).

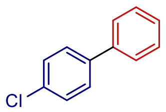
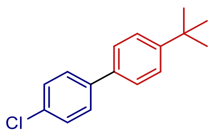
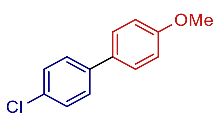
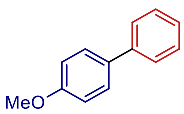
[5] C.-L. Ciana, R. J. Phipps, J. R. Brandt, F.-M. Meyer, M. J. Gaunt, *Angew. Chem. Int. Ed.*, 2011, **50**, 458.
[6] L. Wang, W. Lu, *Org. Lett.*, 2009, **11**, 1079.
[7] Y. Nishii, M. Ikeda, Y. Hayashi, S. Kawauchi, M. Miura, *J. Am. Chem. Soc.*, 2020, **142**, 1621.

	^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (s, 1H), 7.71 (s, 1H) , 7.61-7.49 (m, 9H), 7.33 (t, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.2, 140.9, 140.6, 139.9, 132.1, 130.6, 130.5, 130.4, 129.6, 129.0, 126.60, 126.57, 126.0, 125.9, 123.1, 122.0; HRMS (EI) *m/z* calcd for $C_{18}H_{12}Br_2$ $[M]^{•+}$: 385.9300, found: 385.9304; m.p. 67-68 ℃.
 **3i**	**2,4'''-dibromo-*o*-terphenyl (3i)** Reaction of 2,2'-dibromobiphenyl (181 mg, 0.58 mmol) with 5-(4-bromophenyl)-10-methylphenothiazinium hexafluorophosphate (**2f**) (103 mg, 0.20 mmol) gave the title compound (44 mg, 57%, colorless oil). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (dd, *J* =8.0, 1.2 Hz, 1H), 7.49-7.39 (m, 3H), 7.34-7.29 (m, 3H), 7.19 (dt, *J* = 7.2, 1.6 Hz, 1H), 7.11 (dd, *J* = 7.6, 2.0 Hz, 1H), 7.08 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.01 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.1, 140.1, 140.0, 139.7, 132.8, 132.1, 131.2, 131.01, 130.99, 129.9, 128.8, 128.4, 127.4, 127.1, 123.9, 121.1; HRMS (EI) *m/z* calcd for $C_{18}H_{12}Br_2$ $[M]^{•+}$: 385.9300, found: 385.9301.
 **3j**	**2-bromo-7-(4-bromophenyl)naphthalene (3j)[8]** Reaction of 2,7-dibromonaphthalene (173 mg, 0.61 mmol) with 5-(4-bromophenyl)-10-methylphenothiazinium hexafluorophosphate (**2f**) (103 mg, 0.20 mmol) gave the title compound (37 mg, 51%, white solid). Purification method: GPC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05 (s, 1H), 7.90-7.87 (m, 2H), 7.75-7.68 (m, 2H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.58-7.54 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.6, 138.5, 134.8, 132.2, 131.2, 130.3, 129.7, 129.5, 129.1, 128.7, 125.7, 124.9, 122.1, 120.6.
 **3k**	**4-iodobiphenyl (3k)[9]** Reaction of 3-diiodobenzene (197 mg, 0.60 mmol) with 10-methyl-5-phenylphenothiazinium hexafluorophosphate **(2a)** (87 mg, 0.20 mmol) gave the title compound (23 mg, 40%, white solid). The reaction were stirred at −78 °C for 6 h and quenched at −78 °C. Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 7.6 Hz, 2H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.45 (t, *J* = 7.2 Hz, 2H), 7.39-7.31 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.9, 140.2, 138.0, 129.2, 129.0, 127.8, 127.0, 93.2.

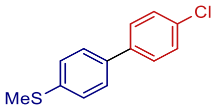
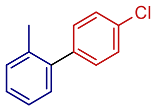
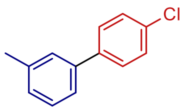
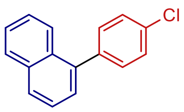
[8] R. Mudududdla, R. Sharma, S. Abbat, P. V. Bharatam, R. A. Vishwakarma, S. B. Bharate, *Chem. Commun.*, 2014, **50**, 12076.
[9] F.-X. Felpin, E. Fouquet, *Adv. Synth. Catal.*, 2008, **350**, 863.

 **3l**	**3-bromobiphenyl (3l)**[10] Reaction of *m*-dibromobenzene (142 mg, 0.60 mmol) with 10-methyl-5-phenylphenothiazinium hexafluorophosphate **(2a)** (87 mg, 0.20 mmol) gave the title compound (33 mg, 71%, colorless oil). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (t, J = 1.8 Hz, 1H), 7.58-7.54 (m, 2H), 7.53-7.43 (m, 4H), 7.38 (t, J = 7.2 Hz, 1H), 7.31 (t, J = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.5, 139.8, 130.40, 130.35, 130.31, 129.0, 128.0, 127.3, 125.9, 123.0.
 **3m**	**3-iodobiphenyl (3m)**[11] Reaction of *m*-diiodobenzene (201 mg, 0.61 mmol) with 10-methyl-5-phenylphenothiazinium hexafluorophosphate **(2a)** (88 mg, 0.20 mmol) gave the title compound (43 mg, 77%, white solid). The reaction were stirred at −78 °C for 6 h and quenched at −78 °C. Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (s, 1H), 7.67 (d, J = 7.6 Hz, 1H), 7.54 (d, J = 7.6 Hz, 3H), 7.44 (t, J = 7.8 Hz, 2H), 7.36 (t, J = 7.2 Hz, 1H), 7.17 (t, J = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.6, 139.7, 136.29, 136.26, 130.5, 129.0, 128.0, 127.2, 126.5, 94.9.
 **3n**	**3-chloro-4'-iodobiphenyl (3n)** Reaction of 1-bromo-3-chlorobenzene (143 mg, 0.75 mmol) with 10-(4-iodophenyl)-5-methylphenothiazinium hexafluorophosphate (**2g**) (113 mg, 0.20 mmol) gave the title compound (39 mg, 61%, white solid). The reaction were stirred at −78 °C for 6 h and quenched at −78 °C. Purification method: flash chromatography (hexane/EtOAc = 100/0 to 80/20). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, J = 8.4 Hz, 2H), 7.53 (s, 1H), 7.44-7.27 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.0, 139.4, 138.1, 134.9, 130.2, 129.0, 127.8, 127.1, 125.1, 93.9; HRMS (EI) *m/z* calcd for $C_{12}H_8ClI$ $[M]^{\bullet+}$: 313.9354, found: 313.9355; m.p. 40-41 °C.
 **3o**	**3-bromo-4'-iodobiphenyl (3o)** Reaction of 1,3-dibromobenzene (142 mg, 0.60 mmol) with 10-(4-iodophenyl)-5-methylphenothiazinium hexafluorophosphate (**2g**) (111 mg, 0.20 mmol) gave the title compound (46 mg, 65%, white solid). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ7.77 (d, J = 8.4 Hz, 2H), 7.69 (s, 1H), 7.48 (t, J = 8.8 Hz, 2H), 7.33-7.26 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ142.3, 139.3, 138.1, 130.8,

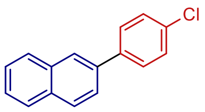
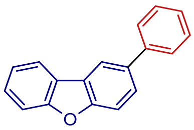
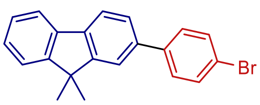
[10] J. Wen, J. Zhang, S.-Y. Chen, J. Li, X.-Q. Yu, *Angew. Chem. Int. Ed.*, 2008, **47**, 8897.
[11] L. K. Rasmussen, M. Begtrup, T. Ruhland, *J. Org. Chem.*, 2006, **71**, 1230.

	130.6, 130.1, 129.1, 125.6, 123.2, 93.9; HRMS (EI) *m/z* calcd for $C_{12}H_8BrI$ $[M]^{•+}$: 357.8849, found: 357.8850; m.p. 44-45 ℃.
 **3p**	**4-chlorobiphenyl (3p)**[12] Reaction of 1-bromo-4-chlorobenzene (114 mg, 0.60 mmol) with 10-methyl-5-phenylphenothiazinium hexafluorophosphate **(2a)** (86 mg, 0.20 mmol) gave the title compound (37 mg, 99%, white solid). Purification method: flash chromatography (hexane/EtOAc = 100/0 to 80/20). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59-7.51 (m, 4H), 7.49-7.36 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.1, 139.8, 133.5, 129.02, 129.00, 128.5, 127.7, 127.1.
 **3q**	**4-*tert*-butyl-4'-chlorobiphenyl (3q)**[3] Reaction of 1-bromo-4-chlorobenzene (116 mg, 0.61 mmol) with 10-methyl-5-(4-*tert*-butylphenyl)phenothiazinium hexafluorophosphate (**2c**) (98 mg, 0.20 mmol) gave the title compound (38 mg, 78%, white solid). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53-7.46 (m, 6H), 7.39 (d, J = 8.8 Hz, 2H), 1.36 (s, 9H); ^{13}C NMR: δ 150.8, 139.6, 137.2, 133.2 129.0, 128.4, 126.8, 126.0, 34.7, 31.5.
 **3r**	**4-chloro-4'-methoxybiphenyl (3r)**[13] Reaction of 1-bromo-4-chlorobenzene (117 mg, 0.61 mmol) with 10-methyl-5-(4-methoxyphenyl)phenothiazinium hexafluorophosphate (**2d**) (96 mg, 0.21 mmol) gave the title compound (34 mg, 77%, white solid). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50-7.45 (m, 4H), 7.38 (d, J = 8.8 Hz 2H), 6.98 (d, J = 8.4 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.5, 139.4, 132.8, 132.6, 129.0, 128.2, 128.1, 114.4, 55.5.
 **3s**	**4-methoxybiphenyl (3s)**[14] 4-Methoxyphenyllithium was synthesized from 4-bromoanisole and isolated according to the literature.[15] Reaction of 4-methoxyphenyllithium (72 mg, 0.63 mmol) with 10-methyl-5-phenylphenothiazinium hexafluorophosphate **(2a)** (84 mg, 0.19 mmol) gave the title compound (24 mg, 67%, white solid). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58-7.52 (m, 4H), 7.43 (t, J = 7.4 Hz, 2H), 7.31 (t, J = 7.6 Hz, 1H), 6.99 (d, J = 9.2 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.3, 141.0, 133.9, 128.9, 128.3, 126.9, 126.8, 114.3, 55.5.

[12] M. Čolović, M. Vukićević, D. Šegan, D. Manojlović, N. Sojic, L. Somsák, R. D. Vukićević, *Adv. Synth. Catal.*, 2008, **350** , 29.
[13] M. L. N. Rao, D. N. Jadhav, D. Banerjee, *Tetrahedron*, 2008, **64**, 5762.
[14] L. Bai, J.-X. Wang, *Adv. Synth. Catal.*, 2008, **350**, 315.
[15] S. Harder, J. Boersma, L. Brandsma, J. A. Kanters, A. J. M. Duisenberg, J. H. Van Lenthe, *Organometallics*, 1990, **9**, 511.

 **3t**	**4-chloro-4'-methylthiobiphenyl (3t)**[16] Reaction of 4-bromothioanisole (122 mg, 0.60 mmol) with 5-(4-chlorophenyl)-10-methylphenothiazinium hexafluorophosphate (**2b**) (95 mg, 0.20 mmol) gave the title compound (27 mg, 57%, white solid). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51-7.47 (m, 4H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.8 Hz, 2H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.1, 138.2, 136.8, 133.4, 129.1, 128.2, 127.4, 127.0, 15.9.
 **3u**	**4-chloro-2'-methylbiphenyl (3u)**[16] Reaction of 2-bromotoluene (118 mg, 0.68 mmol) with 5-(4-chlorophenyl)-10-methylphenothiazinium hexafluorophosphate (**2b**) (95 mg, 0.20 mmol) gave the title compound (34 mg, 85%, colorless oil). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (d, *J* = 8.8 Hz, 2H), 7.28-7.18 (m, 6H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ140.8, 140.5, 135.4, 133.0, 130.7, 130.6, 129.8, 128.4, 127.7, 126.0, 20.6.
 **3v**	**4-chloro-3'-methylbiphenyl (3v)**[17] Reaction of 3-bromotoluene (131 mg, 0.77 mmol) with 5-(4-chlorophenyl)-10-methylphenothiazinium hexafluorophosphate (**2b**) (94 mg, 0.20 mmol) gave the title compound (28 mg, 68%, colorless oil). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 (d, *J* = 8.0 Hz, 2H), 7.42-7.32 (m, 5H) 7.19 (d, *J* = 6.4 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.1, 139.9, 138.7, 133.4, 129.0, 128.9, 128.53, 128.47, 127.9, 124.2, 21.7.
 **3w**	**1-(4-chlorophenyl)naphthalene (3w)**[18] Reaction of 1-bromonaphthalene (127 mg, 0.61 mmol) with 5-(4-chlorophenyl)-10-methylphenothiazinium hexafluorophosphate (**2b**) (94 mg, 0.20 mmol) gave the title compound (43 mg, 90%, white solid). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93-7.83 (m, 3H), 7.55-7.38 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.3, 139.1, 133.9, 133.5, 131.6, 131.5, 128.6, 128.5, 128.1, 127.1, 126.4, 126.0, 125.8, 125.5.

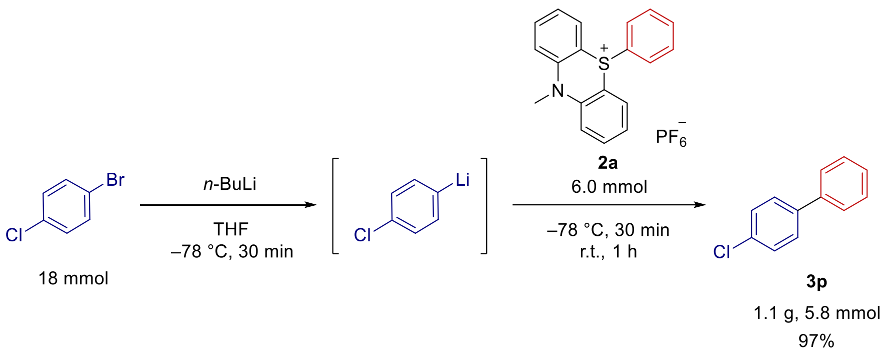
[16] S. E. Denmark, R. C. Smith, W.-T. T. Chang, J. M. Muhuhi, *J. Am. Chem. Soc.*, 2009, **131**, 3104.
[17] T. Narender, S. Sarkar, K. Rajendar, S. Tiwari, *Org. Lett.*, 2011, **13**, 6140.
[18] Z. Zhou, G. Cao, N. Liu, *Chem. Lett.*, 2019, **48**, 547.

 **3x**	**2-(4-chlorophenyl)naphthalene (3x)**[19] Reaction of 2-bromonaphthalene (129 mg, 0.62 mmol) with 5-(4-chlorophenyl)-10-methylphenothiazinium hexafluorophosphate (**2b**) (96 mg, 0.20 mmol) gave the title compound (35 mg, 73%, white solid). Purification method: flash chromatography (hexane/EtOAc = 100/0 to 80/20). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (s,1H), 7.94-7.85 (m, 3H), 7.70 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.53-7.42 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.7, 137.4, 133.7, 133.6, 132.8, 129.1, 128.8, 128.7, 128.3, 127.8, 126.6, 126.3, 125.9, 125.3.
 **3y**	**2-phenyldibenzofuran (3y)**[20] Reaction of 2-bromodibenzofuran (148 mg, 0.60 mmol) with 10-methyl-5-phenylphenothiazinium hexafluorophosphate **(2a)** (88 mg, 0.20 mmol) gave the title compound (46 mg, 95%, white solid). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (d, *J* = 1.2 Hz, 1H), 8.01 (d, *J* = 7.6 Hz, 1H), 7.71-7.58 (m, 5H), 7.51-7.44 (m, 3H), 7.42-7.34 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.8, 155.9, 141.4, 136.5, 129.0, 127.6, 127.4, 127.2, 126.8, 124.8, 124.4, 122.9, 120.8, 119.3, 111.9 (one peak is missing due to overlapping).
 **3z**	**2-(4-bromophenyl)-9,9-dimethylfluorene (3z)**[21] Reaction of 2-bromo-9,9-dimethylfluorene (164 mg, 0.60 mmol) with 5-(4-bromophenyl)-10-methylphenothiazinium hexafluorophosphate (**2f**) (103 mg, 0.20 mmol) gave the title compound (52 mg, 74%, white solid). Purification method: GPC ($CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80-7.74 (m, 2H), 7.62-7.58 (m, 3H), 7.55-7.51 (m, 3H), 7.48-7.45 (m, 1H), 7.40-7.31 (m, 2H), 1.54 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.5, 154.0, 140.6, 139.2, 139.0, 138.8, 132.0, 128.9, 127.6, 127.2, 126.1, 122.8, 121.5, 121.3, 120.5, 120.3, 47.1, 27.4.

[19] H. Minami, T. Saito, C. Wang, M. Uchiyama. *Angew. Chem. Int. Ed.*, 2015, **54**, 4665.
[20] A K. K. Asahara, T. Okita, A. N. Saito, K. Muto, Y. Nakao, J. Yamaguchi, *Org. Lett.*, 2019, **21**, 4721.
[21] M.-W. Lee, S.-B. Cha, S. W. Park, K. Kim, N.-G. Park, D.-H. Lee, *Bull. Korean Chem. Soc.*, 2009, **30**, 2269.

5. Procedure of gram scale reaction

A 300 mL round-bottom flask equipped with a magnetic stirring bar and a septum, was dried under vacuum with heating. After cooling the flask to 23 °C, it was purged with argon gas. 1-Bromo-4-chlorobenzene (3.4 g, 18 mmol) and THF (150 mL) were added to the flask, and the mixture was cooled to –78 °C. *n*-BuLi in hexane (1.57 M, 12 mL, 19 mmol) was added dropwise at –78 °C. After stirring at –78 °C for 30 min, 10-methyl-5-phenylphenothiazinium hexafluorophosphate **(2a)** (2.6 g, 6.0 mmol) was added one portion. The reaction mixture was stirred at –78 °C for 30 min and at 23 °C for 1 h. The reaction was quenched by ethanol (6 mL). Evaporation of the solvents gave a crude material, which was purified by flash chromatography (hexane/EtOAc = 100/0 to 80/20) to give desired product **3p** (1.1 g, 97%, white solid).



Scheme S2.

6. Mechanistic study based on DFT calculations

All density functional theory (DFT) calculations were conducted with the Gaussian 09 program.[22] Fine grid and Berny algorithm were used as DFT settings. Energetically minimum conformers were optimized from realistic and plausible initial structures in consideration of relatively rigid structures. All structure of intermediates and transition states were calculated at the B3LYP/6-311+G(d,p) level with the polarized continuum model (PCM, THF). Frequency calculation were carried out to characterize the stationary points and to estimate Gibbs free energies at 195.15 K and 1 atm.

6-1. Reaction of phenyllithium (1a) with *S*-phenylphenothiazinium (2a)

Reaction of phenyllithium (**1a**) with *S*-phenylphenothiazinium (**2a**) via corresponding sulfurane was investigated. Relative free energy profiles of formation of biphenyl (**path A**), ring opening reaction (**path B**), and formation of diphenyl sulfide (**path C**) were summarized in Figure S1. Three types of sulfurane intermediates (**IM A**, **IM B**, or **IM C**) afford the corresponding transition states (**TS A**, **TS B**, **TS C**). **TS A** is energetically more stable than **TS B** and **TS C** in good agreement with the experimental results as described in Table 1.

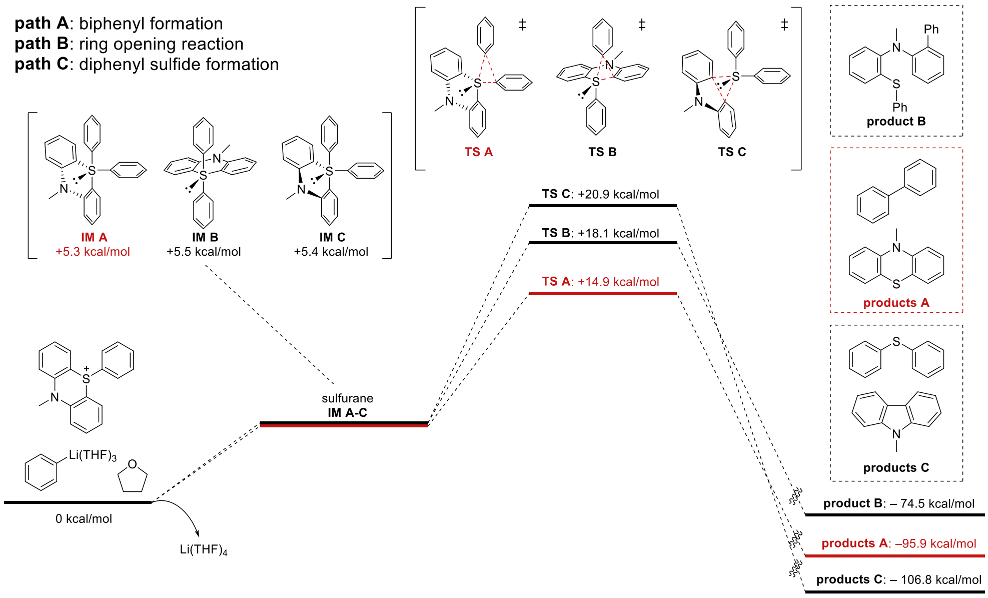


Figure S1.

6-2. Reaction of phenyllithium (1a) with *S*-phenylphenoxathiinium (5)

Reaction of phenyllithium (**1a**) with *S*-phenylphenoxathiinium (**5**) via corresponding sulfurane was investigated. Relative free energy profiles of formation of biphenyl (**path D**), ring opening reaction (**path E**), and formation of diphenyl sulfide (**path F**) were summarized in Figure S2. Three types of sulfurane intermediates (**IM D**, **IM E**,

[22] Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

or **IM F**) afford the corresponding transition states (**TS D**, **TS E**, **TS F**). **TS D** and **TS E** are energetically more stable than **TS F** in good agreement with the experimental results as described in Table 1.

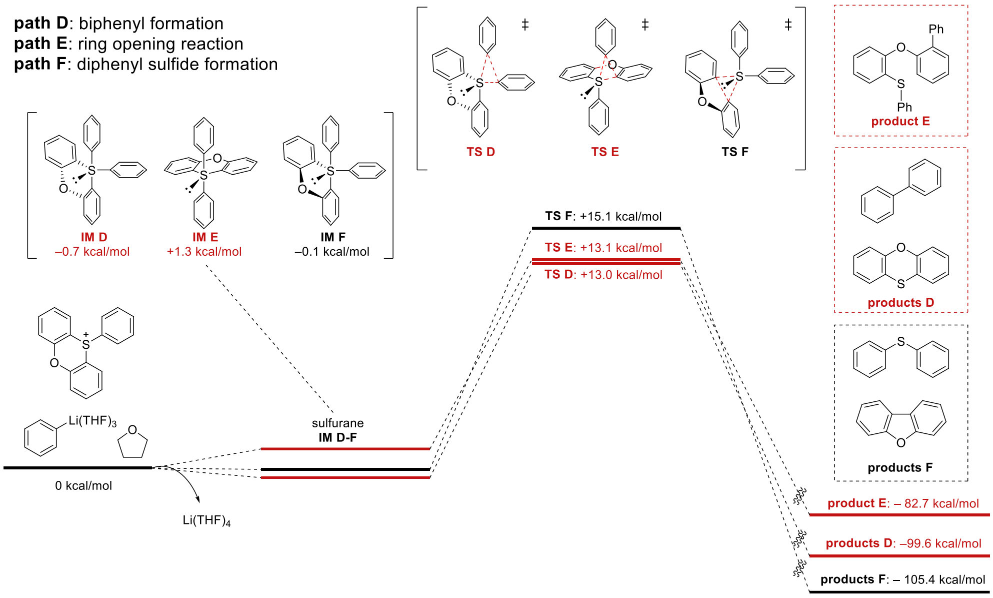


Figure S2.

6-3. Reaction of phenyllithium (1a) with *S*-phenylthianthrenium (8)

Reaction of phenyllithium (**1a**) with *S*-phenylthianthrenium (**8**) via corresponding sulfurane was investigated. Relative free energy profiles of formation of biphenyl (**path G**), ring opening reaction (**path H**), and formation of diphenyl sulfide (**path I**) were summarized in Figure 3. Three types of sulfurane intermediates (**IM G**, **IM H**, or **IM I**) afford the corresponding transition states (**TS G**, **TS H**, **TS I**). **TS I** is energetically more stable than **TS G** and **TS H** in good agreement with the experimental results as described in Table 1.

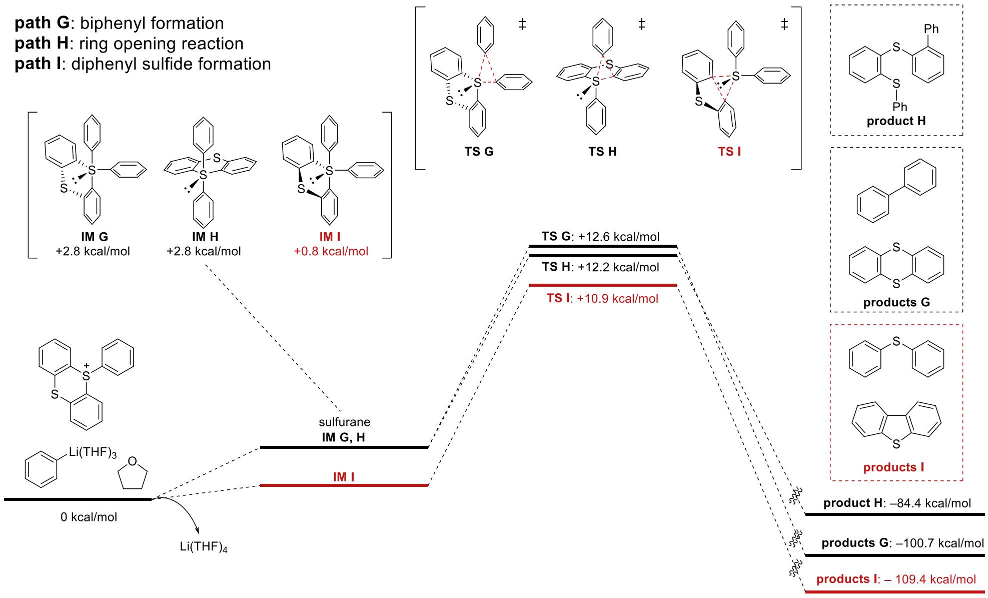


Figure S3.

6-4. Reaction of phenyllithium (1a) with *S*-phenyldibenzothiophenium (11)

Reaction of phenyllithium (**1a**) with *S*-phenyldibenzothiophenium (**11**) via corresponding sulfurane was investigated. Relative free energy profiles of formation of biphenyl (**path J**) and ring opening reaction (**path K**) were summarized in Figure S4. **TS K** is energetically more stable than **TS J** in good agreement with the experimental results reported in the literature.

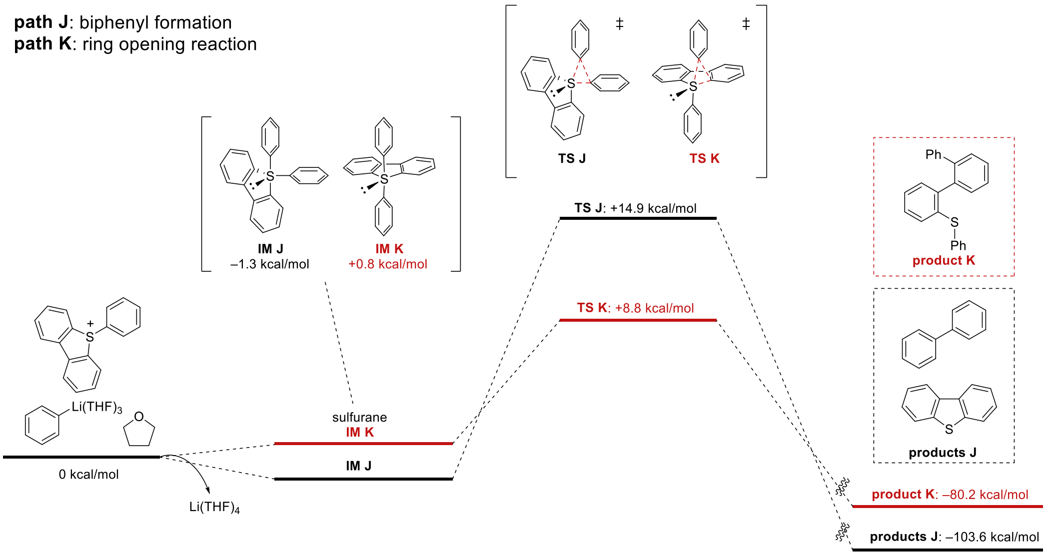


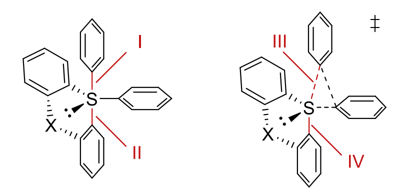
Figure S4.

6-5. Comparison of structures of sulfuranes and transition states

Bond lengths (Å) of apical bonds of sulfuranes and transition states were summarized in Table S1.

Table S1.

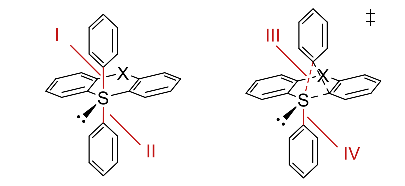
a)



IM A (X = NMe)	**TS A** (X = NMe)
IM D (X = O)	**TS D** (X = O)
IM G (X = S)	**TS G** (X = S)
IM J (X = none)	**TS J** (X = none)

X	I	II	III	IV
NMe	2.20	1.97	2.65	1.81
O	2.11	2.04	2.63	1.82
S	2.13	2.04	2.63	1.83
none	2.09	1.99	2.67	1.83

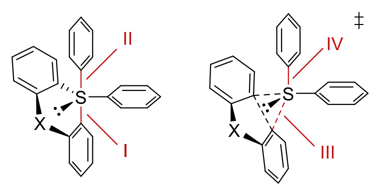
b)



IM B (X = NMe)	**TS B** (X = NMe)
IM E (X = O)	**TS E** (X = O)
IM H (X = S)	**TS H** (X = S)
IM K (X = none)	**TS K** (X = none)

X	I	II	III	IV
NMe	2.12	2.11	2.68	1.84
O	2.14	2.08	2.65	1.84
S	2.12	2.08	2.64	1.85
none	2.12	2.12	2.56	1.87

c)



IM C (X = NMe)	**TS C** (X = NMe)
IM F (X = O)	**TS F** (X = O)
IM I (X = S)	**TS I** (X = S)

X	I	II	III	IV
NMe	2.04	2.12	2.63	1.83
O	2.13	2.04	2.71	1.82
S	2.18	2.03	2.71	1.82

6-6. Verifying the model energetics with higher level of theory

To verify the model energetics with another functional, reaction of phenyllithium (**1a**) with *S*-phenylphenothiazinium (**2a**) via corresponding sulfurane was investigated by DFT calculation at the mPW1PW91/6-311+G(d,p) level with the polarized continuum model (PCM, THF). Relative free energies of sulfuranes (**IM A-C**), transition states (**TS A-C**), and products (**products A-C**) to free energy of starting materials were summarized in Table S2. There was almost no difference in the relative relationship of free energies of **IMs** and **TSs** between these two calculation levels.

Table S2.

	IM (kcal/mol)		**TS** (kcal/mol)		**products** (kcal/mol)	
B3LYP/ 6-311+G(d,p)	**IM A**	+5.3	**TS A**	+14.9	**products A**	–95.9
	IM B	+5.4	**TS B**	+18.1	**product B**	–74.5
	IM C	+5.5	**TS C**	+20.9	**products C**	–106.8
mPW1PW91/ 6-311+G(d,p)	**IM A**	+1.2	**TS A**	+11.5	**products A**	–96.0
	IM B	+1.9	**TS B**	+15.1	**product B**	–76.8
	IM C	+1.3	**TS C**	+17.7	**products C**	–106.9

Cartesian Coordinates:

PhLi(THF)$_3$

O	0.35008500	1.99055500	-0.73119200
C	-0.57855800	2.65168000	-1.60829400
C	1.32485500	2.97599900	-0.34458800
C	-0.78622100	4.03036000	-0.97708300
H	-0.13682600	2.73187000	-2.61052500
H	-1.47402600	2.03404200	-1.65660500
C	0.57249800	4.32382500	-0.28796800
H	1.74232300	2.66055000	0.61073100
H	2.12570600	3.00032800	-1.09341100
H	-1.58924500	3.98476400	-0.23877700
H	-1.05359100	4.78419800	-1.71938000
H	0.42775500	4.65555300	0.74108400
H	1.13359600	5.10046200	-0.81064300
O	1.52547700	-0.94404600	-1.08904600
C	1.67407000	-2.37130400	-0.88532000
C	1.86000500	-0.60118700	-2.45826600
C	1.80414200	-2.97859000	-2.28058900
H	2.57513600	-2.54604800	-0.28684800
H	0.80513700	-2.72605200	-0.32925300
C	2.50290000	-1.85202100	-3.05645500
H	0.93779400	-0.33137500	-2.98250400
H	2.52228600	0.26613000	-2.44088200
H	0.81573000	-3.17782800	-2.70370300
H	2.36884300	-3.91232000	-2.27395100
H	2.35361500	-1.91514400	-4.13548100
H	3.57871300	-1.86297000	-2.85889900
O	1.00921200	0.16500300	1.78181100
C	2.38382700	-0.05771700	2.13535000
C	0.26230800	0.07355300	3.00961600
C	2.35297800	-1.16751400	3.19791300
H	2.91858800	-0.32076500	1.22373600
H	2.80499500	0.87011900	2.54400300
C	0.92725300	-1.06135100	3.80746800
H	0.33509100	1.03013900	3.54226200
H	-0.77641000	-0.11266700	2.74110500
H	3.13820800	-1.02762100	3.94273900

H	2.50134400	-2.14503700	2.73610000
H	0.94767700	-0.83394400	4.87454200
H	0.38053900	-1.99637200	3.67643900
Li	0.12348400	0.10730800	-0.04692300
C	-1.90851100	-0.58256700	-0.06461000
C	-2.96613800	0.23766500	0.40435700
C	-2.35394700	-1.85414700	-0.50599200
C	-4.31314700	-0.14814600	0.43606700
H	-2.73980800	1.24248400	0.76989600
C	-3.69123500	-2.27438300	-0.48930800
H	-1.62506100	-2.57145000	-0.89084000
C	-4.68525100	-1.41665600	-0.01423500
H	-5.07265500	0.53585100	0.81001700
H	-3.95991000	-3.26711400	-0.84527600
H	-5.72517300	-1.72881000	0.00414400

E = –936.84283841 a.u.

THF

O	0.00015200	-1.25518400	-0.00051600
C	1.17381500	-0.42608200	-0.13076800
C	-1.17349700	-0.42647500	0.13142000
C	0.73365100	0.99518400	0.22606500
H	1.94972100	-0.81944200	0.53028900
H	1.53527900	-0.48276100	-1.16477900
C	-0.73414800	0.99474900	-0.22635300
H	-1.95022900	-0.82025300	-0.52840100
H	-1.53346600	-0.48286300	1.16599000
H	1.33917300	1.75559500	-0.27027500
H	0.79932000	1.15648300	1.30606400
H	-0.79996100	1.15523200	-1.30646700
H	-1.33997800	1.75522300	0.26952500

E = –232.52231616 a.u.

$Li(THF)_4$

O	-1.05091500	1.06301900	-1.25383300
C	-2.41611100	0.71604700	-1.60845500
C	-0.63820000	2.25882800	-1.97105400
C	-2.74237300	1.55020800	-2.84426100

H	-2.45998900	-0.36051600	-1.77952000
H	-3.06941100	0.96912200	-0.76715500
C	-1.90917300	2.81845600	-2.60670700
H	-0.16888100	2.93769600	-1.25769800
H	0.09889400	1.96881100	-2.72639300
H	-3.81099200	1.74886300	-2.93587300
H	-2.40959800	1.03737500	-3.75085400
H	-2.42283300	3.48797100	-1.91135300
H	-1.70007900	3.37290000	-3.52249200
O	-1.11482800	-0.51224400	1.51648300
C	-1.49385500	-1.89449500	1.76558300
C	-1.92441000	0.37761300	2.33038700
C	-2.45410100	-1.85525000	2.95374400
H	-1.97659500	-2.28330500	0.86416900
H	-0.58725600	-2.46963000	1.95868800
C	-3.09822200	-0.46800300	2.81320000
H	-1.31675900	0.73570700	3.16779600
H	-2.21453400	1.22849300	1.71207300
H	-1.90212300	-1.92487600	3.89500600
H	-3.17764100	-2.67086700	2.92218100
H	-3.51954200	-0.09321800	3.74697400
H	-3.89145400	-0.48709200	2.06074900
O	0.79895700	-1.55333800	-0.78885600
C	1.86611300	-2.36631500	-0.23174700
C	0.30783100	-2.15333400	-2.01910200
C	1.81276000	-3.68998000	-0.98943500
H	2.81770300	-1.84953400	-0.39281000
H	1.69528300	-2.46511500	0.84136800
C	1.30983900	-3.25003400	-2.37238500
H	-0.68851400	-2.56426200	-1.82722000
H	0.23006700	-1.36772500	-2.77189800
H	1.09769300	-4.37167600	-0.52080100
H	2.78487600	-4.18362800	-1.02236800
H	0.84893500	-4.05951400	-2.93991800
H	2.13231600	-2.84137500	-2.96573500
O	1.56128700	1.17944300	0.67149300
C	2.72576700	1.49150100	-0.13947600
C	1.71883800	1.74255300	2.00381500

C	3.79998500	1.93644800	0.84734400
H	2.98790200	0.59945300	-0.70961500
H	2.46218300	2.29416900	-0.83599500
C	2.96583900	2.62369800	1.93846900
H	0.81074400	2.29391600	2.25291200
H	1.84056100	0.91658400	2.71063200
H	4.53339200	2.59935200	0.38629700
H	4.32796500	1.07003800	1.25518900
H	2.70161700	3.63914100	1.63135100
H	3.47768800	2.68029400	2.89995400
Li	0.05609300	0.07529400	0.04525900

E = –937.60011385 a.u.

***N*-methyl-*S*-phenylphenothiazinium ion**

C	0.44852900	2.60798700	-1.31897500
C	0.65463700	1.41691100	-0.61931900
C	1.52070400	1.32609900	0.48661500
C	2.15388000	2.51797100	0.88649300
C	1.92958600	3.70919600	0.20917700
C	1.08403100	3.76683600	-0.90030600
H	-0.21685300	2.62064200	-2.17391000
H	2.84762400	2.50987200	1.71442500
H	2.44118500	4.60354100	0.54442600
H	0.92497900	4.69725100	-1.42958800
C	0.79040500	-2.50330200	-1.34460400
C	1.57293400	-3.57197900	-0.93539400
C	2.40204500	-3.41403400	0.17688700
C	2.46705500	-2.20997700	0.86522400
C	1.68345400	-1.10755500	0.47458300
C	0.83679900	-1.30186000	-0.63368900
H	0.13303400	-2.59600600	-2.20098100
H	1.53856400	-4.51023900	-1.47349200
H	3.02648300	-4.23627900	0.50540700
H	3.15303800	-2.11892000	1.69465400
C	-4.12164000	-0.26874700	1.26028000
C	-2.90698200	-0.27319100	1.95037200
C	-1.70336400	-0.19637000	1.25710600
C	-1.74339300	-0.11478300	-0.13560800

C	-2.94567600	-0.11156800	-0.84197500
C	-4.14228800	-0.18867100	-0.12982500
H	-5.05278800	-0.32993700	1.81073800
H	-2.89549300	-0.33702800	3.03164500
H	-0.76482600	-0.20113500	1.79396800
H	-2.95242700	-0.05233600	-1.92359400
H	-5.08381700	-0.18789100	-0.66506900
S	-0.25814600	-0.00743300	-1.17087200
N	1.75907800	0.11641600	1.14980700
C	2.41145500	0.15593200	2.46447800
H	3.50016700	0.23769000	2.39081600
H	2.02536200	1.00469200	3.02527400
H	2.15567000	-0.74739900	3.01403100

E = −1186.61999478 a.u.

IM A

C	-0.83868800	2.51907500	-0.65132100
C	0.06916700	1.52063800	-0.29100700
C	1.21164600	1.82908400	0.48571300
C	1.32311700	3.15042300	0.96705000
C	0.39782800	4.12633800	0.62746000
C	-0.67570400	3.82495200	-0.21144200
H	-1.69356400	2.25197700	-1.25678300
H	2.17217100	3.42435200	1.57740600
H	0.53260900	5.13481700	1.00183200
H	-1.38594300	4.58907700	-0.50236900
C	2.03247300	-1.19752400	-2.26753500
C	3.36129300	-1.58898600	-2.44585000
C	4.31269200	-1.19444500	-1.50573100
C	3.95913500	-0.38996900	-0.42215800
C	2.62485300	0.02106700	-0.26696900
C	1.66023900	-0.41838700	-1.17999200
H	1.27017400	-1.52477200	-2.97156400
H	3.64781200	-2.20013600	-3.29436600
H	5.34748900	-1.49834700	-1.61978700
H	4.72710200	-0.07306000	0.27168900
C	-0.29805600	-3.21325600	2.54172000
C	-0.31580000	-1.85302900	2.84719900

C	-0.29811100	-0.90028100	1.82872500
C	-0.25257800	-1.32313800	0.50413900
C	-0.22263700	-2.67995900	0.18417900
C	-0.25590900	-3.62360800	1.20954600
H	-0.31689200	-3.94941900	3.33697000
H	-0.34739500	-1.52686400	3.88061000
H	-0.33018300	0.15340200	2.07045500
H	-0.17671900	-3.00300500	-0.84869000
H	-0.24438900	-4.67909400	0.96302900
C	-4.50252300	-0.60238700	-1.67540800
C	-5.25024300	-0.16495700	-0.58304800
C	-4.59256700	0.36606500	0.53051300
C	-3.19805600	0.45480600	0.54561300
C	-2.42983200	0.01759000	-0.54092100
C	-3.10581700	-0.50679900	-1.64313400
H	-5.00347000	-1.01335800	-2.54723800
H	-6.33280000	-0.23440200	-0.59653700
H	-5.16893000	0.70917900	1.38518000
H	-2.71753400	0.87768400	1.42492900
H	-2.53584700	-0.85373000	-2.50620700
S	-0.26633400	-0.15251500	-0.89406300
N	2.21990800	0.89489100	0.76303900
C	3.14268400	1.15465300	1.86417200
H	3.58922700	0.21143300	2.17716000
H	3.94699800	1.85181900	1.59833300
H	2.59043500	1.56065600	2.71058300

E = −1418.39480930 a.u.

IM B

C	-0.65279300	-2.59545100	0.06720900
C	-0.10801500	-1.34477900	0.33823300
C	0.53661600	-1.06272600	1.55387800
C	0.61766000	-2.11198400	2.48970600
C	0.10294100	-3.37203400	2.20599800
C	-0.53632600	-3.62618300	0.99386700
H	-1.16248500	-2.76012000	-0.87438000
H	1.07274900	-1.93804500	3.45443700
H	0.19059500	-4.15538400	2.95012200

H	-0.94256400	-4.60557500	0.77368600
C	-0.61458400	2.58679100	-0.47614800
C	-0.48557000	3.78519600	0.21813700
C	0.14398300	3.77694200	1.46162200
C	0.63981300	2.59601500	2.00251000
C	0.54589500	1.37686500	1.30295000
C	-0.09554300	1.41043800	0.05374200
H	-1.11419400	2.56089700	-1.43716000
H	-0.87421700	4.70405900	-0.20291100
H	0.24095400	4.69567400	2.02871600
H	1.09205100	2.62064300	2.98397500
C	4.49244500	-0.31113000	-2.24575400
C	3.97412600	0.91944400	-1.84284700
C	2.67735800	1.00092900	-1.32315700
C	1.87965200	-0.13973100	-1.19367100
C	2.40652100	-1.36327500	-1.61864900
C	3.70193500	-1.45649200	-2.13331000
H	5.49822900	-0.37716900	-2.64636000
H	4.57892300	1.81719300	-1.93013000
H	2.29998900	1.97273800	-1.01845700
H	1.80679700	-2.26843900	-1.55100900
H	4.09378700	-2.41946600	-2.44670100
C	-4.51089300	0.07304600	0.26596200
C	-5.13187400	-0.09192800	-0.97604700
C	-4.35331600	-0.24053800	-2.12294700
C	-2.95697200	-0.22355800	-2.02120800
C	-2.32780600	-0.06090900	-0.78886800
C	-3.11738400	0.08805000	0.35426700
H	-5.11494800	0.18910700	1.16097200
H	-6.21426000	-0.10396500	-1.04583300
H	-4.82975600	-0.36866900	-3.09021600
H	-2.35587300	-0.34059500	-2.92251300
H	-2.65247700	0.21725100	1.32910000
S	-0.21631900	-0.08285400	-0.93472200
N	1.08033300	0.19789900	1.84298300
C	2.05668900	0.30481400	2.92664900
H	1.59335000	0.40504100	3.91531400
H	2.69044900	-0.58053300	2.92379500

H	2.69432500	1.16886800	2.74746700

E = –1418.39342417 a.u.

IM C

C	0.62142200	-1.33701500	1.78172800
C	-0.26238800	-1.06244400	0.74017300
C	-1.45979600	-1.79513700	0.58943400
C	-1.69101500	-2.84771600	1.49279700
C	-0.79495300	-3.13099200	2.51742700
C	0.35712300	-2.36514400	2.68131600
H	1.53186400	-0.76284600	1.87491700
H	-2.59447100	-3.43520500	1.40425600
H	-1.01097300	-3.94573000	3.19917900
H	1.05293900	-2.57294700	3.48495900
C	-2.11305200	2.18920800	-0.62262500
C	-3.40562500	2.55764800	-1.00958000
C	-4.36548200	1.56791100	-1.20241900
C	-4.04246800	0.22510200	-1.00552800
C	-2.74006100	-0.13507800	-0.62353600
C	-1.76524100	0.85522800	-0.42450400
H	-1.36681300	2.96595900	-0.49018000
H	-3.65439000	3.60271100	-1.16013900
H	-5.37465200	1.83249100	-1.49879300
H	-4.81291700	-0.52353300	-1.13681800
C	1.76621000	4.05549900	1.27489500
C	0.96629800	3.22629900	2.05993400
C	0.47236600	2.02879100	1.54149000
C	0.80403200	1.66541000	0.24019500
C	1.60905700	2.48092200	-0.55305300
C	2.08208200	3.68430600	-0.03224100
H	2.14098700	4.98876300	1.67908300
H	0.71623200	3.51137300	3.07529000
H	-0.17321600	1.39911500	2.13993600
H	1.86560100	2.18429800	-1.56261100
H	2.69744100	4.32837000	-0.64956300
C	3.28826000	-2.25164800	-2.14253600
C	4.49793800	-1.89784300	-1.54365100
C	4.51264000	-0.91372700	-0.55370500

C	3.32252100	-0.29142200	-0.16351500
C	2.10300000	-0.64420300	-0.74838700
C	2.10623800	-1.62060100	-1.74554800
H	3.26748300	-3.01035200	-2.91885800
H	5.42069100	-2.37938900	-1.84870100
H	5.45066000	-0.62998500	-0.08590100
H	3.36460300	0.47539100	0.60521200
H	1.17028500	-1.89749600	-2.22989300
C	-3.32893400	-2.53078300	-0.82650000
H	-3.68907300	-2.30925100	-1.83103800
H	-2.81623000	-3.49121700	-0.85719600
H	-4.19491300	-2.61389700	-0.15684800
N	-2.38304100	-1.49483900	-0.42414700
S	0.15306900	0.15449000	-0.52497700

E = –1418.39503022 a.u.

TS A

C	-0.61403000	2.43478200	-0.88337100
C	0.31739400	1.48329900	-0.46306900
C	1.41453100	1.83188400	0.35374400
C	1.48813000	3.16978300	0.78848300
C	0.53747400	4.10325800	0.39773000
C	-0.51087200	3.75039900	-0.45284600
H	-1.43011100	2.12372000	-1.52056900
H	2.31254800	3.48914700	1.40993300
H	0.63330000	5.12536500	0.74582200
H	-1.24010200	4.48537400	-0.76935900
C	2.21152700	-1.59727300	-2.03110800
C	3.50791000	-2.09829800	-2.04835200
C	4.42827300	-1.61806400	-1.11568300
C	4.07523100	-0.63856100	-0.19390000
C	2.76999800	-0.11385900	-0.17207000
C	1.84581200	-0.62568700	-1.09935800
H	1.46986000	-1.96759000	-2.73067300
H	3.79346100	-2.85435100	-2.76908900
H	5.44324900	-1.99860600	-1.11176900
H	4.82620200	-0.26577500	0.48835200
C	-0.93462100	-2.86114800	2.63150400

C	-0.65736000	-1.50702100	2.83366700
C	-0.47444900	-0.63370000	1.76692500
C	-0.65164500	-1.09788100	0.44150000
C	-0.79212200	-2.49710000	0.23269000
C	-0.98305900	-3.34064900	1.31592000
H	-1.06886900	-3.53202800	3.47121800
H	-0.56887800	-1.11788400	3.84342700
H	-0.26739500	0.41138800	1.95653400
H	-0.82121600	-2.89609700	-0.77501200
H	-1.15241800	-4.39658100	1.12990200
C	-4.51291300	-0.44520300	-1.73806700
C	-5.28529600	0.14550900	-0.73579500
C	-4.66578200	0.58592000	0.43688000
C	-3.28421600	0.43358300	0.59587800
C	-2.49406600	-0.13387400	-0.40310200
C	-3.12953300	-0.57846400	-1.56591400
H	-4.98671400	-0.79549100	-2.65151400
H	-6.35741700	0.25340900	-0.86271000
H	-5.26110400	1.03826500	1.22584600
H	-2.82536000	0.75350100	1.53201700
H	-2.55158400	-1.03980300	-2.36779100
S	0.08573500	-0.20231400	-1.00109900
N	2.40354100	0.90886300	0.71051300
C	3.28527200	1.21621500	1.83741400
H	3.67034400	0.28491600	2.24903300
H	4.12800200	1.85703300	1.55525700
H	2.70812900	1.70997200	2.61694600

E = – 1418.37793292 a.u.

TS B

C	-0.22803800	-2.56288900	0.09698100
C	-0.25478600	-1.15877200	0.27999600
C	-0.21609300	-0.64501400	1.61199400
C	-0.50432800	-1.52469500	2.65536200
C	-0.65903000	-2.90191400	2.44470000
C	-0.48254700	-3.41655200	1.16241200
H	-0.08945900	-2.96150400	-0.90110500
H	-0.60369900	-1.14451500	3.66269500

H	-0.86662100	-3.55272300	3.28505700
H	-0.52356900	-4.48598000	0.98634000
C	0.14048900	2.46761700	-1.44374000
C	-0.11476300	3.78597700	-1.07488300
C	-0.35262700	4.06695100	0.26823100
C	-0.33095100	3.06203900	1.23095900
C	-0.04101500	1.72439600	0.89071400
C	0.18986300	1.47020300	-0.47663100
H	0.30445800	2.21030800	-2.48374900
H	-0.14161300	4.56791200	-1.82298200
H	-0.57727900	5.08124900	0.57826300
H	-0.55941000	3.31725100	2.25593700
C	5.09595900	-0.72362100	-0.77140100
C	4.44490400	-0.06072300	0.27138300
C	3.06836000	0.14364900	0.22412600
C	2.35078500	-0.31944300	-0.88059100
C	2.99117500	-0.98863800	-1.92402800
C	4.37095100	-1.18690000	-1.86731300
H	6.16784000	-0.87771500	-0.72726600
H	5.01002900	0.29748300	1.12408300
H	2.56679900	0.65878200	1.03308800
H	2.42274700	-1.34655300	-2.77519500
H	4.87401300	-1.69976900	-2.67865100
C	-4.44769300	0.12386400	-0.25004600
C	-4.86531200	-0.52958600	-1.41139500
C	-3.91556000	-1.14753000	-2.22842000
C	-2.56136400	-1.10543100	-1.87812200
C	-2.12466500	-0.44143600	-0.72888900
C	-3.08779500	0.16338700	0.08061600
H	-5.18057900	0.60052000	0.39586000
H	-5.91767600	-0.56273200	-1.67328800
H	-4.23079000	-1.65978500	-3.13385100
H	-1.84533500	-1.61233100	-2.52666400
H	-2.79379500	0.67568900	0.99631200
S	0.52637500	-0.18574100	-1.04192000
N	0.05023300	0.73052000	1.86259500
C	0.24546700	1.14112200	3.25125400
H	-0.69835100	1.28729500	3.79001000

H	0.82734800	0.37954000	3.76950700
H	0.81297600	2.06943500	3.27853000

E = −1418.37079329 a.u.

TS C

C	0.21631100	-0.71671200	2.12364300
C	-0.47023600	-0.67113400	0.89248800
C	-1.29429200	-1.78478800	0.53578100
C	-1.41108800	-2.86373500	1.40321900
C	-0.72951300	-2.89148100	2.62819400
C	0.05406900	-1.80092900	2.98921800
H	0.89093000	0.07892900	2.40887200
H	-2.07312500	-3.68101900	1.14242800
H	-0.82841600	-3.74788300	3.28423800
H	0.58162400	-1.79381600	3.93724600
C	-2.65163600	1.94671400	0.11253400
C	-3.87656100	2.19942900	-0.52653600
C	-4.49605200	1.17647900	-1.24094700
C	-3.92121500	-0.09653800	-1.30487300
C	-2.70401800	-0.33052500	-0.64815400
C	-2.05129700	0.69593900	0.04388100
H	-2.16997900	2.76343800	0.64614400
H	-4.32982900	3.18480000	-0.47548500
H	-5.44150200	1.35608600	-1.74213000
H	-4.43862100	-0.88267200	-1.84221800
C	1.75569200	4.37018900	0.57881300
C	0.89723100	3.68088400	1.43319500
C	0.47980700	2.38573300	1.12702100
C	0.94253100	1.78243900	-0.03966200
C	1.78693000	2.47063500	-0.91497200
C	2.19459200	3.76407600	-0.59764200
H	2.07392500	5.37680600	0.82332500
H	0.54245000	4.14849600	2.34422600
H	-0.20664100	1.86761400	1.77918100
H	2.12723100	2.00795700	-1.83333600
H	2.85073400	4.29617900	-1.27631700
C	3.34989400	-2.36714000	-1.90251400
C	4.41208500	-2.16714100	-1.02229300

C	4.30329700	-1.22816300	0.00530200
C	3.13594600	-0.48391500	0.15682600
C	2.07853800	-0.68491200	-0.73337000
C	2.17571400	-1.62911700	-1.75745900
H	3.43300600	-3.09226800	-2.70362500
H	5.32464800	-2.74079500	-1.13560900
H	5.12861100	-1.07449900	0.69090500
H	3.06057300	0.25033700	0.94849700
H	1.34644100	-1.78149200	-2.43912200
S	0.44358100	0.12094800	-0.56948100
N	-2.08112900	-1.61191700	-0.61823000
C	-2.77205400	-2.75704300	-1.18700500
H	-3.04401800	-2.54317500	-2.22125800
H	-2.10005200	-3.61499600	-1.18804500
H	-3.68543400	-3.02524600	-0.63674600

E = –1418.36820417 a.u.

biphenyl

C	1.46482200	-1.13415200	0.40456200
C	0.74324400	-0.00001600	-0.00001300
C	1.46480500	1.13414000	-0.40455100
C	2.85802200	1.13441900	-0.40478000
C	3.56144400	0.00000900	0.00000300
C	2.85803600	-1.13440800	0.40480000
H	0.93180400	-2.01570300	0.74219900
H	0.93177700	2.01569300	-0.74216900
H	3.39418600	2.01930600	-0.72943200
H	4.64551900	0.00001700	0.00001100
H	3.39421600	-2.01928000	0.72946700
C	-0.74324400	-0.00001600	-0.00000100
C	-1.46480300	1.13413900	0.40455300
C	-1.46482400	-1.13415100	-0.40456500
C	-2.85801700	1.13442200	0.40478200
H	-0.93176800	2.01568800	0.74217000
C	-2.85804100	-1.13440700	-0.40479300
H	-0.93181200	-2.01570600	-0.74220200
C	-3.56144400	0.00001100	-0.00000100
H	-3.39418300	2.01930700	0.72943700

H	-3.39422000	-2.01928100	-0.72945600
H	-4.64551900	0.00002500	-0.00000100

E = –463.42642893 a.u.

***N*-methylphenothiazine**

C	2.53672600	-1.44133800	-0.24931400
C	1.34920300	-0.82915700	0.14346900
C	1.21632500	0.57201300	0.12219900
C	2.31840700	1.33368000	-0.29219400
C	3.51808900	0.71722100	-0.64825600
C	3.63412100	-0.66961300	-0.63143100
H	2.60548900	-2.52316000	-0.23682300
H	2.24718200	2.41185600	-0.33812200
H	4.35789700	1.33167000	-0.95186800
H	4.56215300	-1.15063400	-0.91628300
C	-2.53678500	-1.44132100	-0.24920900
C	-3.63414200	-0.66957500	-0.63136500
C	-3.51805300	0.71725900	-0.64833400
C	-2.31835400	1.33369700	-0.29230800
C	-1.21633900	0.57199800	0.12219400
C	-1.34923000	-0.82914500	0.14352700
H	-2.60558500	-2.52313800	-0.23666100
H	-4.56220600	-1.15057000	-0.91616200
H	-4.35784100	1.33169400	-0.95202800
H	-2.24706100	2.41186200	-0.33836200
S	-0.00000500	-1.81432900	0.76845900
N	0.00001900	1.16912600	0.52522200
C	0.00001300	2.60009200	0.81097000
H	0.00009400	3.22465400	-0.09194200
H	-0.88155400	2.84314600	1.40326400
H	0.88150600	2.84313000	1.40339300

E = –955.11774354 a.u.

product B

C	-2.32859100	-2.31866400	-1.36585000
C	-2.07584000	-1.28509800	-0.45385900
C	-1.39238700	-1.59261200	0.75181000
C	-1.08412000	-2.93995600	1.01972600

C	-1.38621400	-3.95063400	0.11453100
C	-1.99281900	-3.64325700	-1.10088400
H	-2.84797200	-2.07281900	-2.28574500
H	-0.56502500	-3.19637600	1.93324000
H	-1.12629300	-4.97567100	0.35543400
H	-2.22105000	-4.42025800	-1.82104200
C	1.24654200	1.97883000	0.18614100
C	0.68674100	3.14386200	0.69804100
C	-0.43817800	3.07141900	1.51931000
C	-1.00044500	1.83234100	1.79750600
C	-0.45169800	0.64475700	1.29644000
C	0.70966300	0.72338000	0.49913900
H	2.12505700	2.04091200	-0.44330900
H	1.12867800	4.10291100	0.45267300
H	-0.88520300	3.97259500	1.92266700
H	-1.89197400	1.76307500	2.40949200
C	5.88100800	0.28478400	-0.79972600
C	5.37289200	0.24852100	0.50065800
C	4.03188700	-0.05508000	0.72110800
C	3.18506400	-0.30600600	-0.36482700
C	3.69309400	-0.26989500	-1.66608500
C	5.04172300	0.02069700	-1.88008200
H	6.92703000	0.51453900	-0.96738300
H	6.02390600	0.44619000	1.34478500
H	3.64123900	-0.09791800	1.73081400
H	3.03628000	-0.46572500	-2.50518500
H	5.43071300	0.04564600	-2.89168500
C	-4.22883800	1.83563700	-0.31693500
C	-3.84917600	2.49888100	-1.48479600
C	-2.86312100	1.94426600	-2.29918300
C	-2.26321500	0.73451800	-1.94915300
C	-2.63218100	0.06249700	-0.77687900
C	-3.62447200	0.63127700	0.03415200
H	-5.00076500	2.25518000	0.31915500
H	-4.31950900	3.43699100	-1.75764500
H	-2.55943200	2.45156200	-3.20837800
H	-1.49675700	0.30843700	-2.58725000
H	-3.92977900	0.11853200	0.93929700

S	1.47297800	-0.79281500	-0.10284800
N	-1.05501800	-0.59277600	1.68873700
C	-0.80479700	-0.98689100	3.07748900
H	-1.56737300	-1.69526200	3.40591600
H	0.18511200	-1.44114700	3.22100400
H	-0.86453200	-0.10236000	3.71079300

E = –1418.52128351 a.u.

diphenyl sulfide

C	-3.71469700	-1.07227800	-0.19926200
C	-3.66553900	0.01596000	0.66967600
C	-2.51450800	0.80081300	0.74964700
C	-1.41224400	0.50822300	-0.05885800
C	-1.46517400	-0.57593700	-0.94230900
C	-2.60933500	-1.36744100	-1.00001400
H	-4.60563600	-1.68711000	-0.25355500
H	-4.51666300	0.25068600	1.29888000
H	-2.47082200	1.63424600	1.44107000
H	-0.61770200	-0.80011000	-1.57883500
H	-2.64153600	-2.20989200	-1.68187700
S	-0.00013300	1.61839300	-0.00002400
C	1.41219200	0.50849100	0.05882900
C	2.51362700	0.79994400	-0.75119700
C	1.46604700	-0.57435900	0.94384100
C	3.66478200	0.01525900	-0.67120300
H	2.46920900	1.63236600	-1.44378600
C	2.61029000	-1.36573000	1.00158900
H	0.61920600	-0.79759300	1.58153700
C	3.71484000	-1.07168200	0.19929800
H	4.51528100	0.24908900	-1.30158100
H	2.64322400	-2.20716300	1.68467200
H	4.60586900	-1.68638100	0.25363100

E = –861.63357469 a.u.

***N*-methylcarbazole**

C	-3.42247100	-0.08155100	0.00820600
C	-3.03884600	-1.43333800	0.00583600
C	-1.69302600	-1.78741400	0.00001400

C	-0.72347800	-0.77956300	-0.00561900
C	-1.12728700	0.58269700	-0.01103000
C	-2.47825000	0.94180200	0.00171100
H	-4.47640400	0.17295400	0.01795000
H	-3.80001400	-2.20486400	0.01169100
H	-1.40047500	-2.83181700	0.00229100
H	-2.79059600	1.97902700	0.01078100
C	0.72338800	-0.77961900	-0.00561800
C	1.12727600	0.58260700	-0.01103800
C	1.69289500	-1.78750800	0.00001500
C	2.47824100	0.94168400	0.00170400
C	3.03873100	-1.43347500	0.00583900
H	1.40031400	-2.83190300	0.00229600
C	3.42242300	-0.08170600	0.00820700
H	2.79058100	1.97891100	0.01077500
H	3.79986700	-2.20503300	0.01169700
H	4.47636900	0.17274400	0.01795100
N	0.00003700	1.39163800	-0.03312800
C	0.00027200	2.84246600	0.01705800
H	0.88072000	3.22676500	-0.49810400
H	-0.88207300	3.22684800	-0.49472400
H	0.00225000	3.21241000	1.04756300

E = –556.92445868 a.u.

***S*-phenylphenoxathiinium ion**

C	0.39520200	2.64229900	-1.20037100
C	0.61774600	1.40651900	-0.58516500
C	1.48656700	1.28907400	0.50132800
C	2.10875300	2.43078400	1.00403300
C	1.86970400	3.66254500	0.40893100
C	1.02253000	3.77302900	-0.69796300
H	-0.26927300	2.71121500	-2.05321000
H	2.77967600	2.32794800	1.84754400
H	2.35977000	4.54421800	0.80339300
H	0.85292300	4.73447600	-1.16508500
C	0.72582900	-2.56630500	-1.22406600
C	1.49754300	-3.61062100	-0.73610100
C	2.33033000	-3.40145100	0.36756900

C	2.41081300	-2.15489700	0.97399600
C	1.64216600	-1.09882800	0.48625300
C	0.79036400	-1.31737900	-0.59830300
H	0.07136600	-2.71322500	-2.07473000
H	1.45074600	-4.58173200	-1.21157500
H	2.93333800	-4.21557600	0.75053700
H	3.06711100	-1.97381800	1.81584400
C	-4.19712900	-0.25477200	1.11085200
C	-3.00098300	-0.26516000	1.83293400
C	-1.78015500	-0.19608700	1.17049900
C	-1.78733800	-0.11716700	-0.22229700
C	-2.96854400	-0.10742400	-0.96222100
C	-4.18272000	-0.17657500	-0.27945000
H	-5.14229500	-0.30944800	1.63745600
H	-3.01737100	-0.32731300	2.91408500
H	-0.85692500	-0.20609200	1.73480800
H	-2.94709100	-0.04865800	-2.04355000
H	-5.11050400	-0.17055700	-0.83794800
S	-0.26716400	-0.01479400	-1.20279700
O	1.77738500	0.10497000	1.12805500

E = –1167.16224726 a.u.

IM D

C	-0.90339900	2.55378100	-0.32246100
C	0.06817200	1.57797900	-0.06592400
C	1.18378200	1.91955600	0.72042100
C	1.25082900	3.18791200	1.30753500
C	0.26514800	4.13310800	1.06841800
C	-0.80470400	3.82488500	0.22597000
H	-1.75067900	2.30103800	-0.94358900
H	2.11015200	3.41244600	1.92758700
H	0.34226200	5.11495500	1.52055000
H	-1.56558100	4.56401600	0.00721600
C	2.41752600	-0.92706600	-2.04954600
C	3.78967000	-1.18136900	-2.11550300
C	4.63281300	-0.69608900	-1.11218100
C	4.11539000	0.06378000	-0.06320700
C	2.74481900	0.31024700	-0.04196700

C	1.87947500	-0.18982600	-0.99736500
H	1.75845300	-1.32532000	-2.81881500
H	4.20031600	-1.75848800	-2.93690100
H	5.69747000	-0.89693000	-1.15174800
H	4.75576000	0.46827500	0.71269100
C	-0.05773600	-3.44803900	2.27762100
C	-0.01349600	-2.12774000	2.72008900
C	-0.03147400	-1.07433300	1.80503400
C	-0.08999900	-1.35993500	0.44476200
C	-0.13229100	-2.67684300	-0.01348900
C	-0.11844500	-3.71933100	0.91042200
H	-0.04439300	-4.26202800	2.99298200
H	0.03371900	-1.90901800	3.78069500
H	-0.00349100	-0.05291500	2.15997400
H	-0.17696800	-2.89207300	-1.07420500
H	-0.15380200	-4.74371700	0.55797100
C	-4.26689300	-0.41807000	-1.89653700
C	-5.04324700	-0.28270700	-0.74717100
C	-4.42190600	-0.02836000	0.47905300
C	-3.03244600	0.08906200	0.55040800
C	-2.24238000	-0.04244400	-0.59661000
C	-2.87468100	-0.29834500	-1.81242800
H	-4.74095900	-0.61460700	-2.85323800
H	-6.12256500	-0.37444400	-0.80238100
H	-5.02199800	0.07571300	1.37801000
H	-2.57397100	0.28649500	1.51527200
H	-2.27733000	-0.40596900	-2.71697200
S	-0.14636200	-0.05752900	-0.82879000
O	2.24852800	1.09926900	0.99418600

E = –1398.94483027 a.u.

IM E

C	-0.29742600	-2.62969500	0.27086400
C	0.00313100	-1.29029600	0.51520900
C	0.37835200	-0.87472700	1.79039500
C	0.48152300	-1.81216000	2.81913200
C	0.21086400	-3.15169700	2.56764100
C	-0.18395000	-3.56487300	1.29351900

H	-0.61447700	-2.93594700	-0.71870100
H	0.77426000	-1.46920800	3.80401200
H	0.29945400	-3.87299500	3.37126000
H	-0.40441200	-4.60682600	1.09714200
C	-0.43235900	2.60815000	-0.64326000
C	-0.39598800	3.83618500	0.00721700
C	-0.02014600	3.89544700	1.35119300
C	0.31806800	2.73630000	2.03812000
C	0.29431100	1.50406100	1.38100900
C	-0.07935000	1.44620700	0.04127500
H	-0.73279500	2.54710200	-1.68249800
H	-0.66142600	4.73845000	-0.52964900
H	0.00604000	4.84744900	1.86782900
H	0.60727400	2.76072500	3.08166200
C	4.78208500	-0.34004000	-1.62304600
C	4.36339000	0.63248800	-0.71482500
C	3.01026200	0.74347300	-0.37479600
C	2.05634800	-0.11239300	-0.93354300
C	2.49087200	-1.06834600	-1.85478800
C	3.83922500	-1.19505900	-2.19642400
H	5.83065500	-0.42696800	-1.88647200
H	5.08939000	1.30666500	-0.27015700
H	2.71883300	1.51369200	0.33303200
H	1.76634300	-1.73325400	-2.32564400
H	4.15328100	-1.95088000	-2.90986400
C	-4.40147200	-0.05698600	0.08521700
C	-4.93475800	-0.32801400	-1.17822600
C	-4.08042500	-0.52131900	-2.26254700
C	-2.69541600	-0.44311900	-2.07791400
C	-2.15537300	-0.17370600	-0.82237700
C	-3.01844000	0.01945200	0.25901300
H	-5.06453100	0.09353000	0.93151600
H	-6.00923900	-0.38666600	-1.31340100
H	-4.48892600	-0.73099100	-3.24609500
H	-2.03325000	-0.59507500	-2.92901100
H	-2.62412600	0.23201400	1.24943500
S	-0.08070700	-0.11615300	-0.83913000
O	0.68487400	0.42145300	2.13416500

E = −1398.94234066 a.u.

IM F

C	0.77289200	-1.51679900	1.62409400
C	-0.13377600	-1.29115200	0.58516600
C	-1.20610000	-2.18000500	0.39828800
C	-1.31831400	-3.30351100	1.21911200
C	-0.39947600	-3.53055200	2.23685500
C	0.63898200	-2.62520300	2.45329700
H	1.59483900	-0.83252100	1.77616300
H	-2.14533300	-3.98061800	1.04319000
H	-0.50264400	-4.40625400	2.86681600
H	1.35081500	-2.78395800	3.25418500
C	-2.66215000	1.59334700	-0.70312500
C	-3.99217800	1.64687800	-1.13176300
C	-4.69584800	0.46393200	-1.36752500
C	-4.07195000	-0.76684300	-1.16634700
C	-2.74606700	-0.77582400	-0.74127100
C	-2.01098000	0.37339900	-0.50055700
H	-2.12843700	2.52530100	-0.53767500
H	-4.47622100	2.60608200	-1.28385400
H	-5.72733800	0.49595800	-1.70000300
H	-4.59782400	-1.70158400	-1.32755400
C	0.66118700	4.09938600	1.54428900
C	0.06265300	3.04612600	2.23519900
C	-0.11004300	1.80754600	1.61748700
C	0.34035800	1.63405500	0.31338400
C	0.94410600	2.67506700	-0.38877600
C	1.09539500	3.91466300	0.23217200
H	0.78610300	5.06218800	2.02603800
H	-0.27977100	3.18642200	3.25385200
H	-0.60151800	0.99788300	2.14124700
H	1.29318900	2.52718000	-1.40343500
H	1.55319200	4.73200000	-0.31260100
C	3.66843000	-1.47875800	-2.17283600
C	4.73756100	-0.91612700	-1.47525900
C	4.48723100	-0.02847400	-0.42799700
C	3.17293500	0.29259800	-0.07677700

C	2.09778200	-0.27504500	-0.76405100
C	2.35812300	-1.15058100	-1.81849600
H	3.85394000	-2.16408000	-2.99343200
H	5.75758500	-1.16252800	-1.74866700
H	5.31465200	0.41576700	0.11607100
H	3.00318100	0.98952300	0.73775800
H	1.53067800	-1.58484500	-2.37631600
S	0.09540200	0.07206400	-0.57911800
O	-2.15625600	-2.04046100	-0.57666000

E = –1398.94641097 a.u.

TS D

C	-0.59623200	2.50913800	-0.59632600
C	0.38810400	1.57113300	-0.26795700
C	1.46038700	1.94080100	0.55384400
C	1.50356200	3.22512600	1.09851800
C	0.50237000	4.13882300	0.79803200
C	-0.54108300	3.79000100	-0.06289600
H	-1.40794100	2.21485900	-1.24625700
H	2.33631500	3.48578300	1.73981100
H	0.54681000	5.13462400	1.22286500
H	-1.30995100	4.50997200	-0.31356500
C	2.53842900	-1.39809900	-1.81793000
C	3.86272100	-1.81391500	-1.73823800
C	4.70281100	-1.26523900	-0.76529900
C	4.23401900	-0.29136800	0.10988700
C	2.90848800	0.12821400	0.01562500
C	2.05687700	-0.42795100	-0.93514300
H	1.87098400	-1.82878600	-2.55634000
H	4.23662300	-2.56478800	-2.42326600
H	5.73382200	-1.59075600	-0.69405400
H	4.87837700	0.15857500	0.85526900
C	-0.76866700	-2.98878700	2.50397900
C	-0.56212300	-1.63836800	2.78944500
C	-0.38683600	-0.69808400	1.77819500
C	-0.49962300	-1.09613400	0.42575600
C	-0.57353000	-2.48522300	0.13437100
C	-0.75627700	-3.39526300	1.16294400

H	-0.89580100	-3.71154100	3.30052000
H	-0.52215500	-1.30269800	3.82100600
H	-0.23076600	0.34216600	2.03292500
H	-0.55526500	-2.82779600	-0.89397600
H	-0.87026000	-4.44543600	0.91367200
C	-4.25141200	-0.49979600	-1.92564100
C	-5.10280900	-0.01798000	-0.92941100
C	-4.56676900	0.37886600	0.29863300
C	-3.18852300	0.29126300	0.51942800
C	-2.32279000	-0.16942900	-0.47135000
C	-2.87267200	-0.57059600	-1.69173500
H	-4.65995900	-0.81400800	-2.88245500
H	-6.17195500	0.03971800	-1.10426600
H	-5.22392800	0.74624500	1.08233700
H	-2.79319800	0.57421500	1.49512300
H	-2.23158900	-0.94650900	-2.48960500
S	0.26364000	-0.08780100	-0.92776200
O	2.50513300	1.11602300	0.88300800

E = –1398.92374449 a.u.

TS E

C	-0.22179400	-2.49736500	0.21991500
C	-0.30466700	-1.09289500	0.39718000
C	-0.31001000	-0.61787600	1.72838600
C	-0.45924300	-1.48214200	2.79824900
C	-0.51524800	-2.86436400	2.59728800
C	-0.38245600	-3.35792900	1.29753500
H	-0.08851700	-2.89741500	-0.77830200
H	-0.52852400	-1.05461200	3.79235500
H	-0.62423500	-3.53374000	3.44097800
H	-0.37493800	-4.42754400	1.11865200
C	0.43711900	2.64619200	-1.04429100
C	0.30945300	3.93824100	-0.54893100
C	-0.01423800	4.12422600	0.79706800
C	-0.21308500	3.03528600	1.63509800
C	-0.08189300	1.73008800	1.14571600
C	0.25555000	1.55061300	-0.19907100
H	0.67822100	2.48066600	-2.08793000

H	0.45343900	4.78672000	-1.20564300
H	-0.11932700	5.12599300	1.19673000
H	-0.47138800	3.16648900	2.67876800
C	5.01461600	-0.82480300	-0.73683600
C	4.41321900	-0.17032200	0.34036200
C	3.04863600	0.10663500	0.32095600
C	2.29302700	-0.27936900	-0.78767700
C	2.88316200	-0.94144200	-1.86475300
C	4.25192100	-1.20883200	-1.83810600
H	6.07783700	-1.03374200	-0.71577500
H	5.00761000	0.12736500	1.19631000
H	2.59181200	0.62560500	1.15415800
H	2.28470100	-1.24066600	-2.71827000
H	4.71738400	-1.71434400	-2.67603200
C	-4.49284200	0.31669700	-0.33018400
C	-4.87878400	-0.42232600	-1.44995600
C	-3.91282500	-1.12764400	-2.17162900
C	-2.57439600	-1.08626800	-1.76687700
C	-2.16751300	-0.34059300	-0.65848800
C	-3.14731600	0.35400300	0.05656000
H	-5.23851200	0.86365100	0.24072300
H	-5.91983600	-0.45304800	-1.75374800
H	-4.20331500	-1.70684100	-3.04417500
H	-1.84446100	-1.66032900	-2.33996200
H	-2.88270000	0.93760900	0.93655200
S	0.46615300	-0.07689800	-0.90323800
O	-0.29450700	0.73896100	2.04891500

E = –1398.92175935 a.u.

TS F

C	0.25723300	-1.06057200	1.95258400
C	-0.42441100	-0.98366300	0.71811000
C	-1.02514300	-2.17523000	0.23065800
C	-0.97789500	-3.35480000	0.94791200
C	-0.29690500	-3.41736300	2.17079100
C	0.28736500	-2.25691800	2.67148300
H	0.77086100	-0.19758100	2.35421200
H	-1.51284900	-4.21316300	0.55624700

H	-0.24460500	-4.34911500	2.72018800
H	0.80503200	-2.27477700	3.62473900
C	-3.12768600	1.19178000	0.13354600
C	-4.35065900	1.21638000	-0.55289700
C	-4.70602800	0.15029900	-1.38280200
C	-3.85933500	-0.95310900	-1.51140100
C	-2.66782600	-0.94353800	-0.79294200
C	-2.26231900	0.10540100	0.00857800
H	-2.85910900	2.04833500	0.74817500
H	-5.01520600	2.06904000	-0.45130400
H	-5.64718200	0.16913100	-1.92150900
H	-4.12466000	-1.80003200	-2.13590600
C	0.64412000	4.44841000	0.87818900
C	0.01325800	3.50068700	1.68200800
C	-0.09128600	2.17369300	1.26547500
C	0.45198200	1.80790900	0.03677600
C	1.06788400	2.75143400	-0.78880400
C	1.16701300	4.07242300	-0.35845700
H	0.72012000	5.47733200	1.20953200
H	-0.40550800	3.78860000	2.63908600
H	-0.60434800	1.45022800	1.88131100
H	1.46769100	2.46473600	-1.75403500
H	1.64667600	4.80523100	-0.99638400
C	3.78333600	-1.62405200	-1.90354100
C	4.74188100	-1.23172500	-0.97071200
C	4.39217600	-0.37998100	0.07881900
C	3.08506600	0.08358100	0.20218200
C	2.13275000	-0.31000900	-0.74064000
C	2.47158300	-1.16604400	-1.79098800
H	4.05306400	-2.28189500	-2.72122900
H	5.76170500	-1.58728300	-1.06057800
H	5.13778600	-0.07593600	0.80414300
H	2.82031000	0.75178000	1.01155100
H	1.72337500	-1.46648600	-2.51548600
S	0.37117900	0.12413900	-0.62735700
O	-1.83361700	-2.07929100	-0.88232700

E = –1398.91978625 a.u.

phenoxathiin

C	-2.58822100	1.16239900	-0.31460100
C	-1.35080300	0.66026200	0.09371100
C	-1.19182600	-0.71754200	0.25865100
C	-2.25424300	-1.58604800	0.03024500
C	-3.49384300	-1.07560600	-0.35003200
C	-3.66105100	0.29807500	-0.52407800
H	-2.70973400	2.23002900	-0.45713400
H	-2.09724500	-2.64969500	0.16325800
H	-4.32298400	-1.75274400	-0.51701800
H	-4.62056200	0.69871400	-0.82834000
C	2.58824000	1.16240200	-0.31457600
C	3.66106600	0.29806700	-0.52404200
C	3.49384400	-1.07561600	-0.35002700
C	2.25423100	-1.58604400	0.03022800
C	1.19183000	-0.71752000	0.25865500
C	1.35082200	0.66027900	0.09372500
H	2.70977400	2.23002900	-0.45710800
H	4.62058600	0.69871000	-0.82826800
H	4.32297600	-1.75276000	-0.51702900
H	2.09720700	-2.64968900	0.16322200
S	-0.00001800	1.76484500	0.46436400
O	-0.00000100	-1.27359500	0.69018100

E = –935.66606644 a.u.

product E

C	-1.38048200	-3.05732400	-0.29181300
C	-1.41019300	-1.74092200	0.19538600
C	-0.29443400	-1.30555400	0.92859400
C	0.75562800	-2.16975100	1.23128600
C	0.74370500	-3.47761500	0.76043200
C	-0.32247000	-3.91979500	-0.02202600
H	-2.22939500	-3.41243200	-0.86528600
H	1.58498500	-1.79091000	1.81579400
H	1.56745400	-4.14190600	0.99485000
H	-0.34097600	-4.93419000	-0.40308000
C	0.07520800	2.69651900	-1.01843000
C	-0.63313200	3.68958700	-0.35307300

C	-1.17596500	3.41441500	0.90195200
C	-1.03072600	2.15155500	1.46024700
C	-0.33964600	1.14189500	0.78366800
C	0.25228300	1.42001700	-0.46300200
H	0.52404800	2.90190700	-1.98281700
H	-0.74924300	4.66789300	-0.80366600
H	-1.72143700	4.17873500	1.44334000
H	-1.45593800	1.91619300	2.42792300
C	5.43285800	0.21530300	0.39112500
C	4.49953400	1.12823000	0.87871900
C	3.20309600	1.16613900	0.36383900
C	2.83141000	0.27666500	-0.64726800
C	3.76608900	-0.64511500	-1.13784300
C	5.05872100	-0.66957000	-0.62160600
H	6.43858300	0.19205300	0.79412800
H	4.77650800	1.82193800	1.66494400
H	2.49237100	1.88607000	0.74914200
H	3.48345400	-1.34115400	-1.92025600
H	5.77333600	-1.38623800	-1.01094000
C	-4.52853800	0.34048600	0.77991600
C	-4.97748500	0.54921000	-0.52426800
C	-4.24959800	0.02949600	-1.59396800
C	-3.08140400	-0.69436500	-1.36029800
C	-2.61783700	-0.90474500	-0.05446100
C	-3.35823200	-0.37813700	1.01285500
H	-5.09259900	0.73436800	1.61816100
H	-5.88728900	1.11059600	-0.70466800
H	-4.58906900	0.18798500	-2.61154600
H	-2.51836800	-1.09292200	-2.19693700
H	-3.02179000	-0.54465900	2.02973100
S	1.20650800	0.23606900	-1.40983900
O	-0.20613700	-0.03377300	1.48985400

E = –1399.07711099 a.u.

dibenzofuran

C	3.39893500	-0.25312500	0.00014200
C	3.05628900	1.10827100	-0.00000600
C	1.72418400	1.51417300	-0.00011000

C	0.72626000	0.53411800	-0.00000700
C	1.10135600	-0.82057700	0.00024200
C	2.42011500	-1.24712300	0.00025400
H	4.44402500	-0.54000600	-0.00001600
H	3.84302800	1.85352800	-0.00001000
H	1.46914700	2.56754700	-0.00017500
H	2.67295300	-2.29998800	-0.00001600
C	-0.72626000	0.53411800	-0.00001400
C	-1.10135600	-0.82057700	0.00023500
C	-1.72418400	1.51417300	-0.00010500
C	-2.42011400	-1.24712300	0.00024700
C	-3.05629000	1.10827100	0.00000000
H	-1.46914700	2.56754700	-0.00017300
C	-3.39893500	-0.25312500	0.00014200
H	-2.67295200	-2.29998800	-0.00002700
H	-3.84302800	1.85352800	0.00000200
H	-4.44402500	-0.54000700	-0.00001400
O	0.00000000	-1.64887700	-0.00071100

E = –537.46658457 a.u.

***S*-phenylthianthrenium**

C	0.52390300	2.35463000	-1.75747400
C	0.51812600	1.36897900	-0.76852200
C	1.10159400	1.57540200	0.48782500
C	1.65690700	2.82938100	0.75913000
C	1.62923400	3.83128900	-0.20714200
C	1.07871000	3.59619300	-1.46732600
H	0.08919600	2.15585300	-2.72941500
H	2.12512100	3.01042400	1.71890700
H	2.06407500	4.79693800	0.02071200
H	1.07986600	4.37349300	-2.22068700
C	1.06118000	-2.55410000	-1.16116100
C	1.86886200	-3.53957300	-0.60439200
C	2.43353800	-3.34158800	0.65596000
C	2.22015900	-2.15792600	1.35716700
C	1.40891500	-1.15608900	0.81607200
C	0.82183100	-1.38637600	-0.43460400
H	0.61146600	-2.69218000	-2.13678300

H	2.05500800	-4.45457400	-1.15198400
H	3.06631500	-4.10582200	1.09061600
H	2.69670100	-1.99978000	2.31687300
C	-4.11675800	-0.29434500	1.34950300
C	-3.35460200	-1.45148600	1.19920200
C	-2.16157900	-1.42100000	0.47849400
C	-1.75407800	-0.21086600	-0.07351800
C	-2.50293700	0.95555100	0.05198900
C	-3.69168500	0.90395000	0.77771500
H	-5.04203700	-0.32626600	1.91193700
H	-3.68111600	-2.38361700	1.64395200
H	-1.57009100	-2.32056000	0.36762300
H	-2.17595300	1.88858000	-0.38869800
H	-4.28126100	1.80517700	0.89352500
S	-0.27956600	-0.18231800	-1.16148400
S	1.16332700	0.33182500	1.75927300

E = −1490.13753131 a.u.

IM G

C	-0.88058300	2.53828200	-0.65484400
C	-0.02181100	1.57089600	-0.12330900
C	0.93941700	1.93727200	0.83348200
C	0.93798600	3.25553700	1.31486000
C	0.05263800	4.20099700	0.81415300
C	-0.83877700	3.85003200	-0.19989500
H	-1.59988700	2.25121200	-1.41002400
H	1.67103600	3.53926600	2.06065200
H	0.08191100	5.21629600	1.19202400
H	-1.50706200	4.58818300	-0.62667100
C	2.26768500	-0.76821000	-2.22418100
C	3.62450900	-1.02373000	-2.43637200
C	4.54796800	-0.73734400	-1.42926100
C	4.12250100	-0.16762300	-0.22952200
C	2.75965900	0.08321800	-0.04100700
C	1.82033400	-0.23736800	-1.01597800
H	1.54636000	-1.00564800	-3.00379600
H	3.96048200	-1.44614300	-3.37732100
H	5.60294700	-0.93406900	-1.58384000

H	4.84255700	0.09576000	0.53809700
C	-0.20682900	-3.49837900	2.27668800
C	-0.59784000	-2.22022000	2.67327100
C	-0.58889500	-1.16636200	1.76097800
C	-0.16926200	-1.40041100	0.45555300
C	0.23875000	-2.66973800	0.04922800
C	0.20599800	-3.72170700	0.96388000
H	-0.22331700	-4.31645100	2.98750500
H	-0.91440000	-2.03825400	3.69376200
H	-0.90682300	-0.18081600	2.07114300
H	0.57709900	-2.84337600	-0.96420400
H	0.50780000	-4.71306800	0.64634200
C	-4.27800000	-0.95378900	-1.76567500
C	-5.11458800	-0.38561300	-0.80619500
C	-4.55669700	0.34837200	0.24372000
C	-3.17150400	0.50704700	0.33205900
C	-2.31962400	-0.06526200	-0.61887100
C	-2.89249900	-0.78689400	-1.66529600
H	-4.70097500	-1.51956500	-2.59015500
H	-6.19006600	-0.50744100	-0.87608100
H	-5.20213800	0.79811500	0.99232800
H	-2.76904100	1.09380100	1.15313800
H	-2.25084200	-1.23243800	-2.42529800
S	-0.20169600	-0.09909100	-0.82413200
S	2.21364200	0.86288000	1.47898100

E = –1721.91721198 a.u.

IM H

C	-0.62736400	-2.62222200	-0.29920600
C	-0.07639500	-1.44526100	0.20949600
C	0.48156100	-1.41316300	1.48751500
C	0.48930300	-2.59172200	2.24907800
C	-0.02424700	-3.77283500	1.72866100
C	-0.58616800	-3.79164700	0.45095200
H	-1.08184300	-2.61915900	-1.28229800
H	0.90007400	-2.57317500	3.25202100
H	0.00130700	-4.67559700	2.32747900
H	-0.99571800	-4.70779900	0.04328700

C	-0.62648100	2.62252100	-0.29944300
C	-0.58479100	3.79202900	0.45055300
C	-0.02278900	3.77317700	1.72823100
C	0.49034600	2.59194200	2.24877600
C	0.48210200	1.41329200	1.48736200
C	-0.07593200	1.44541200	0.20938600
H	-1.08102900	2.61949600	-1.28250300
H	-0.99401800	4.70828600	0.04280000
H	0.00316800	4.67601900	2.32691100
H	0.90118300	2.57337100	3.25169200
C	4.65000400	-0.00080300	-1.91595600
C	3.98182200	1.20334500	-1.69241500
C	2.65856100	1.19914500	-1.24279400
C	1.98283300	-0.00029600	-0.99834000
C	2.65802000	-1.19998600	-1.24305100
C	3.98128900	-1.20469800	-1.69265200
H	5.67737400	-0.00098800	-2.26327800
H	4.49037000	2.14676100	-1.86569700
H	2.16237400	2.15179400	-1.08153400
H	2.16141200	-2.15245400	-1.08200100
H	4.48940400	-2.14831200	-1.86611300
C	-4.43532100	0.00029400	0.16908800
C	-5.00919000	0.00031500	-1.10602300
C	-4.18803500	0.00034000	-2.23263900
C	-2.79652500	0.00032100	-2.07803800
C	-2.21501500	0.00030300	-0.81206700
C	-3.04617700	0.00029500	0.31083500
H	-5.07237600	0.00028600	1.04851600
H	-6.08814300	0.00031000	-1.21707300
H	-4.62733600	0.00037800	-3.22554500
H	-2.16250100	0.00033800	-2.96394100
H	-2.61944500	0.00031100	1.31127500
S	-0.09583600	0.00003900	-0.87138000
S	1.26379000	-0.00006700	2.23526400

E = –1721.91636127 a.u.

IM I

C	0.80015300	-1.19338500	1.87676600

C	-0.03858100	-1.16659500	0.76223400
C	-0.98873100	-2.18110500	0.56475600
C	-1.06653800	-3.22292100	1.49532200
C	-0.22404500	-3.25328800	2.60243600
C	0.70248600	-2.23124100	2.79933300
H	1.54124600	-0.42007400	2.02024900
H	-1.80129200	-4.00483300	1.34560800
H	-0.29944200	-4.06819900	3.31276300
H	1.35850800	-2.24262500	3.66153900
C	-2.59136700	1.77168600	-0.37009500
C	-3.92071000	1.94965100	-0.76618000
C	-4.68243200	0.85282000	-1.17122000
C	-4.11318100	-0.41943500	-1.17126000
C	-2.77812100	-0.56372200	-0.78029700
C	-1.99022200	0.50746300	-0.37174500
H	-2.02247100	2.64529100	-0.06711800
H	-4.36071500	2.94195000	-0.75716000
H	-5.71551100	0.98185200	-1.47459000
H	-4.70082400	-1.28444100	-1.46186700
C	0.96864400	4.26651100	1.22466800
C	0.35445100	3.30833800	2.02973900
C	0.10310500	2.02847000	1.53447700
C	0.49219100	1.71545600	0.23619700
C	1.10765100	2.66336600	-0.57981700
C	1.33694900	3.94481900	-0.08156800
H	1.15587700	5.26139000	1.61166600
H	0.05886700	3.55445300	3.04296300
H	-0.40723100	1.29810600	2.14813400
H	1.40744100	2.41064300	-1.58954700
H	1.80553700	4.68782500	-0.71619000
C	3.57861800	-1.65128000	-2.18862700
C	4.69242000	-1.13209700	-1.52942400
C	4.51628300	-0.20352200	-0.50215600
C	3.23129700	0.20196800	-0.13296100
C	2.11184500	-0.32285000	-0.78231600
C	2.29634400	-1.24165800	-1.81534500
H	3.70680700	-2.36679200	-2.99415200
H	5.69067100	-1.44293600	-1.81701400

H	5.37951100	0.20752300	0.01136200
H	3.12013800	0.93304900	0.66125500
H	1.43270900	-1.64345700	-2.34042700
S	0.14687800	0.10158400	-0.51694600
S	-2.06818400	-2.22742200	-0.85149100

E = –1721.92070782 a.u.

TS G

C	-0.67781100	2.44280000	-0.83780000
C	0.27086500	1.56198400	-0.30950400
C	1.24925600	2.02043700	0.58572200
C	1.21089700	3.36140900	0.99178500
C	0.23573100	4.22207100	0.50232500
C	-0.70067600	3.77016700	-0.42737100
H	-1.40673900	2.07363100	-1.54555800
H	1.96437600	3.72789100	1.67879500
H	0.22561400	5.25516000	0.82921300
H	-1.44617100	4.44440000	-0.83029700
C	2.35129200	-1.38037800	-2.01427300
C	3.65630400	-1.85529000	-2.09683300
C	4.59343500	-1.46424000	-1.13982000
C	4.23783300	-0.58583900	-0.12083300
C	2.92595900	-0.10641600	-0.03348700
C	1.98234400	-0.51903700	-0.97758700
H	1.61129800	-1.68556100	-2.74612400
H	3.93834200	-2.52661800	-2.89870600
H	5.61215400	-1.82956700	-1.19496500
H	4.97944600	-0.25790700	0.59836500
C	-0.91479600	-2.97996600	2.58174400
C	-0.74403100	-1.61935400	2.85020100
C	-0.54027500	-0.69508800	1.83201200
C	-0.58680600	-1.11986000	0.48320300
C	-0.62064600	-2.51462400	0.21510400
C	-0.83585400	-3.41012500	1.25187200
H	-1.06522500	-3.68963000	3.38600300
H	-0.75600900	-1.26462700	3.87611300
H	-0.41523000	0.35193200	2.07218500
H	-0.55050000	-2.87532200	-0.80477900

H	-0.92158100	-4.46632900	1.01699800
C	-4.30809000	-0.60486900	-1.93491600
C	-5.17625500	-0.07623500	-0.97743900
C	-4.66196100	0.36983100	0.24295700
C	-3.28871700	0.28425400	0.49503600
C	-2.40622200	-0.22194300	-0.45785500
C	-2.93475000	-0.67172000	-1.67024800
H	-4.69968400	-0.95890400	-2.88498600
H	-6.24145000	-0.02067400	-1.17573200
H	-5.33226000	0.77440400	0.99677400
H	-2.91241400	0.60643800	1.46614500
H	-2.27941800	-1.08446500	-2.43820700
S	0.19188000	-0.13717500	-0.88575000
S	2.54520000	1.02329600	1.28542500

E = –1721.89552552 a.u.

TS H

C	-0.31310600	-2.58159500	-0.28897700
C	-0.28462400	-1.24385900	0.19662200
C	-0.28708900	-1.06066500	1.60265500
C	-0.60892700	-2.12962900	2.43880100
C	-0.79036800	-3.41596900	1.93424600
C	-0.60738500	-3.63117900	0.56213100
H	-0.17238900	-2.76245800	-1.34818400
H	-0.68862300	-1.95304700	3.50692600
H	-1.02351700	-4.23573400	2.60187300
H	-0.67956400	-4.63314000	0.15326200
C	0.19896500	2.62065200	-1.07563700
C	-0.00484100	3.91566600	-0.60834700
C	-0.21429700	4.12685700	0.75311100
C	-0.22347100	3.05445900	1.64005000
C	0.00621300	1.74790500	1.18932100
C	0.22310600	1.55294600	-0.17923800
H	0.33869700	2.43696900	-2.13429400
H	-0.01245500	4.74538500	-1.30406600
H	-0.38714200	5.12834400	1.12910400
H	-0.40961400	3.22524600	2.69405600
C	5.10308200	-0.63104600	-0.82168100

C	4.48178200	-0.13530700	0.32661900
C	3.10464200	0.07162000	0.34894400
C	2.35672300	-0.22040200	-0.79273200
C	2.96764800	-0.72007600	-1.94354900
C	4.34776700	-0.92317300	-1.95544500
H	6.17535100	-0.78861500	-0.83038200
H	5.07032200	0.09035600	1.20841100
H	2.62798600	0.45318400	1.24317200
H	2.37615700	-0.94309800	-2.82472500
H	4.82724300	-1.30571600	-2.84885700
C	-4.42447500	0.17078100	-0.15195100
C	-4.82904900	-0.13832200	-1.45250400
C	-3.87290600	-0.52698500	-2.39319600
C	-2.52315300	-0.59694900	-2.02865000
C	-2.10148800	-0.27737000	-0.73510900
C	-3.07109700	0.09493700	0.19680300
H	-5.16306900	0.46546900	0.58879500
H	-5.87715700	-0.08409000	-1.72740900
H	-4.17826500	-0.77235500	-3.40701300
H	-1.80131300	-0.91032600	-2.78352100
H	-2.78575700	0.32199300	1.22311000
S	0.52056100	-0.05707800	-0.91161400
S	0.10201400	0.48094300	2.42949000

E = −1721.89508626 a.u.

TS I

C	0.14748000	-0.60137300	2.14222500
C	-0.39957300	-0.76069800	0.84182400
C	-0.88069700	-2.05804900	0.48477800
C	-0.93959100	-3.07168800	1.43638500
C	-0.44797800	-2.88426800	2.72804200
C	0.08464300	-1.63688500	3.06530300
H	0.61159900	0.32934600	2.43609900
H	-1.39144200	-4.01655300	1.15451400
H	-0.48041400	-3.69016700	3.45066600
H	0.48243600	-1.46742800	4.06059000
C	-3.03676200	1.39974200	0.23461100
C	-4.28121900	1.52783500	-0.39635800

C	-4.71663500	0.54325400	-1.28540200
C	-3.92528000	-0.58229300	-1.51996900
C	-2.70369000	-0.69065300	-0.85011900
C	-2.22472900	0.28785900	0.00175100
H	-2.71562300	2.19879600	0.89871400
H	-4.90320600	2.39649400	-0.20183400
H	-5.67604700	0.63931200	-1.78223700
H	-4.26903700	-1.36225400	-2.19299800
C	1.15706400	4.55067600	0.54699100
C	0.28521300	3.79828800	1.33004200
C	0.05039600	2.45392600	1.04016200
C	0.71081000	1.86774600	-0.03651300
C	1.57388500	2.61708600	-0.84158600
C	1.79719900	3.95780400	-0.54096000
H	1.33263800	5.59465300	0.77809900
H	-0.22287500	4.25260700	2.17248800
H	-0.64045000	1.88567000	1.64244200
H	2.07144600	2.16614200	-1.69124300
H	2.46909200	4.53659800	-1.16350800
C	3.62778700	-1.93086800	-1.88016000
C	4.61584100	-1.67230400	-0.93235900
C	4.35440000	-0.81521100	0.13870300
C	3.10636800	-0.21202000	0.26746700
C	2.12445600	-0.47375500	-0.69049200
C	2.37283800	-1.33410000	-1.76095600
H	3.82921000	-2.59333600	-2.71361500
H	5.59062800	-2.13655000	-1.02638000
H	5.12325100	-0.61536000	0.87585900
H	2.91104300	0.45952900	1.09320400
H	1.59892800	-1.53394100	-2.49272500
S	0.41983300	0.15883900	-0.57544000
S	-1.69699200	-2.20408000	-1.07697200

E = –1721.89908576 a.u.

thianthrene

C	2.49734200	-1.39504600	-0.30387500
C	1.38256000	-0.70056200	0.17490800
C	1.38250300	0.70051600	0.17483600

C	2.49718200	1.39509000	-0.30406600
C	3.61988700	0.69746800	-0.74323000
C	3.61997200	-0.69734800	-0.74309400
H	2.48442500	-2.47848000	-0.32324000
H	2.48411100	2.47851600	-0.32357100
H	4.48586800	1.24407000	-1.09754300
H	4.48601600	-1.24392000	-1.09730300
C	-2.49716500	-1.39507300	-0.30409000
C	-3.61988200	-0.69745700	-0.74322000
C	-3.61999300	0.69735400	-0.74308500
C	-2.49734000	1.39505100	-0.30387000
C	-1.38257800	0.70055600	0.17487800
C	-1.38246300	-0.70054000	0.17482200
H	-2.48412600	-2.47850500	-0.32361100
H	-4.48584500	-1.24409400	-1.09752400
H	-4.48604300	1.24392900	-1.09726800
H	-2.48442200	2.47848200	-0.32322300
S	0.00000700	-1.62428300	0.83180900
S	-0.00001600	1.62428000	0.83180300

E = –1258.64374299 a.u.

product H

C	-2.58055800	-2.48150000	-1.15685800
C	-2.32549900	-1.41440000	-0.28147000
C	-1.45176600	-1.64550100	0.80088700
C	-0.91588700	-2.92142400	1.00899400
C	-1.21662500	-3.97422000	0.14988600
C	-2.04048800	-3.74762300	-0.94957800
H	-3.24516600	-2.31362200	-1.99696200
H	-0.24199100	-3.07849800	1.84250900
H	-0.79332400	-4.95571500	0.32989800
H	-2.27170000	-4.55227900	-1.63819600
C	1.53421800	1.98746500	-0.13589500
C	0.87617600	3.21269000	-0.08003500
C	-0.34350100	3.32701400	0.58318900
C	-0.90659400	2.19875900	1.17110300
C	-0.26053300	0.95878200	1.12325100
C	0.99174400	0.85368200	0.48087200

H	2.48489700	1.91672700	-0.64763400
H	1.32365300	4.07740900	-0.55713600
H	-0.85869100	4.27889200	0.63323700
H	-1.86494700	2.26589800	1.67025400
C	6.10457300	0.15638000	-0.94277000
C	5.73655900	0.43465900	0.37460500
C	4.43396500	0.18968100	0.80402100
C	3.48974900	-0.32471900	-0.09124200
C	3.85858700	-0.60643100	-1.40969600
C	5.16660400	-0.36594800	-1.83195800
H	7.12018900	0.34253500	-1.27287100
H	6.46493300	0.83502700	1.07056500
H	4.14850900	0.39434600	1.82897700
H	3.12624900	-1.00981400	-2.09870100
H	5.44923900	-0.58648900	-2.85500200
C	-4.66095900	1.55439200	0.10052400
C	-4.45636000	2.22995900	-1.10327000
C	-3.54014600	1.72841000	-2.02637400
C	-2.83389800	0.55886000	-1.74745100
C	-3.02493900	-0.12166400	-0.53848800
C	-3.94980900	0.38984000	0.38164600
H	-5.37936300	1.93156800	0.82006600
H	-5.00908100	3.13711600	-1.32044800
H	-3.37318000	2.24633800	-2.96430700
H	-2.12166900	0.17468000	-2.46932900
H	-4.11970700	-0.13297100	1.31533600
S	1.83240700	-0.73119500	0.47683700
S	-1.01656500	-0.39593000	2.03606100

E = −1722.05625125 a.u.

dibenzothiophene

C	3.49235700	0.13528800	0.00014100
C	2.98233200	1.44211700	-0.00002300
C	1.61135200	1.66619500	-0.00001200
C	0.72732900	0.57734200	-0.00004000
C	1.25999500	-0.72962800	-0.00004800
C	2.63622200	-0.96118100	0.00027300
H	4.56432500	-0.02492300	0.00030100

H	3.66468200	2.28413300	-0.00018400
H	1.22694300	2.67992200	-0.00032600
H	3.03125600	-1.97018100	0.00031300
C	-0.72732900	0.57734200	-0.00004200
C	-1.25999400	-0.72962900	-0.00005000
C	-1.61135100	1.66619500	-0.00001500
C	-2.63622200	-0.96118100	0.00027200
C	-2.98233200	1.44211800	-0.00002100
H	-1.22694200	2.67992200	-0.00033000
C	-3.49235700	0.13528900	0.00014200
H	-3.03125600	-1.97018000	0.00030500
H	-3.66468200	2.28413400	-0.00018000
H	-4.56432500	-0.02492200	0.00031000
S	-0.00000100	-1.96872000	-0.00023000

E = –860.44848194 a.u.

***S*-phenyldibenzothiophenium ion**

C	0.49859200	2.64688100	-0.70548900
C	0.70728600	1.28636700	-0.55322700
C	1.80238700	0.73375200	0.12624100
C	2.72960200	1.61210700	0.69046900
C	2.53499000	2.98662000	0.56472400
C	1.43375900	3.50335700	-0.12289300
H	-0.35301900	3.03492700	-1.24962200
H	3.59415700	1.23223600	1.22065300
H	3.25432400	3.66635400	1.00501800
H	1.30388500	4.57453400	-0.21288000
C	0.49921900	-2.64701300	-0.70501200
C	1.43468400	-3.50315600	-0.12241300
C	2.53590900	-2.98602100	0.56491700
C	2.73020100	-1.61144000	0.69041300
C	1.80261300	-0.73341300	0.12630500
C	0.70757600	-1.28641700	-0.55296000
H	-0.35238500	-3.03534000	-1.24896300
H	1.30507800	-4.57438300	-0.21219500
H	3.25551400	-3.66550200	1.00516200
H	3.59478700	-1.23128200	1.22034600
C	-4.23532900	-0.00019500	1.11737500

C	-3.02497600	0.00030300	1.81651100
C	-1.81762100	0.00031700	1.12742500
C	-1.85429100	-0.00017600	-0.26652000
C	-3.04755300	-0.00067500	-0.98532700
C	-4.24838500	-0.00068100	-0.27503800
H	-5.17038200	-0.00020800	1.66447400
H	-3.02097000	0.00068400	2.89956900
H	-0.87774300	0.00072000	1.66505600
H	-3.04545700	-0.00105000	-2.06836300
H	-5.18737000	-0.00107100	-0.81443900
S	-0.33952400	-0.00023200	-1.25542700

E = –1091.93700750 a.u.

IM J

C	0.36099800	-2.34497500	0.88121300
C	-0.49196000	-1.42155500	0.28447200
C	-1.89052000	-1.58034800	0.34482200
C	-2.41195600	-2.70625900	0.99256000
C	-1.56270600	-3.63519000	1.58470400
C	-0.18001500	-3.45349300	1.53225900
H	1.43091800	-2.21141600	0.84110500
H	-3.48528000	-2.84743300	1.04171400
H	-1.97784200	-4.49763100	2.09364600
H	0.48368800	-4.17213200	1.99858100
C	-2.40836300	1.60337800	-1.42823100
C	-3.79115200	1.66020800	-1.61603900
C	-4.60982100	0.62174000	-1.15358900
C	-4.05569900	-0.47678800	-0.50163600
C	-2.66842500	-0.51878900	-0.30091400
C	-1.85759000	0.52058100	-0.74994400
H	-1.77956400	2.40923700	-1.79756500
H	-4.23622200	2.51143500	-2.12075900
H	-5.68149900	0.67008400	-1.31104300
H	-4.69706600	-1.28451700	-0.16516100
C	0.93150000	3.87962200	1.71257600
C	0.16840300	2.86757600	2.29413500
C	-0.09988400	1.69570800	1.58639500
C	0.41811100	1.54283800	0.30421500

C	1.19589900	2.53827400	-0.28319300
C	1.43943000	3.71573300	0.42366500
H	1.13084900	4.79250400	2.26189500
H	-0.22430100	2.98819000	3.29724800
H	-0.70860400	0.91679500	2.02961200
H	1.61059300	2.39987700	-1.27427700
H	2.03056700	4.50077100	-0.03376800
C	3.87345200	-1.42201300	-1.94626000
C	4.80407200	-1.14702300	-0.94435800
C	4.38353300	-0.53596200	0.23932100
C	3.03756000	-0.20493700	0.41778200
C	2.09527500	-0.48260000	-0.57708900
C	2.52951600	-1.08427700	-1.75763400
H	4.19315300	-1.89254400	-2.87086700
H	5.84884500	-1.40238200	-1.08442200
H	5.10442600	-0.31674100	1.02110400
H	2.73194800	0.27099900	1.34571800
H	1.81174900	-1.29517000	-2.54910400
S	0.07223200	0.04196100	-0.67244000

E = –1323.72326098 a.u.

IM K

C	0.02314000	-0.41482800	2.60678800
C	0.01186300	0.09181800	1.31725500
C	0.00672300	1.46721900	1.03788100
C	0.01476800	2.36331300	2.11199700
C	0.02675000	1.87261100	3.41510000
C	0.03074900	0.49626300	3.66353200
H	0.02642500	-1.48164900	2.79272900
H	0.01160800	3.43246700	1.93423000
H	0.03295900	2.56654100	4.24747500
H	0.03986800	0.13100200	4.68361200
C	-0.02360000	0.64448800	-2.57937400
C	-0.03400700	1.89675600	-3.19452200
C	-0.03167600	3.06553000	-2.42618800
C	-0.01831900	3.00614300	-1.03513600
C	-0.00723300	1.76062300	-0.39801700
C	-0.01103100	0.60517100	-1.19459900

H	-0.02625200	-0.26432300	-3.16819600
H	-0.04427000	1.96072300	-4.27612000
H	-0.04041300	4.03026700	-2.91977000
H	-0.01676000	3.91991800	-0.45247300
C	4.87467400	-1.51086700	-0.29167400
C	4.43702800	-0.19215100	-0.14172200
C	3.07016500	0.09398100	-0.10118400
C	2.12343400	-0.92929600	-0.20887400
C	2.57251300	-2.24010800	-0.36184900
C	3.93922900	-2.53841500	-0.40198200
H	5.93599000	-1.73239200	-0.32273200
H	5.16200800	0.61181800	-0.05682700
H	2.75600600	1.12723800	0.01636600
H	1.84962900	-3.05056200	-0.45141900
H	4.27060000	-3.56554700	-0.52001300
C	-4.43620600	-0.21394700	-0.02678700
C	-4.87287100	-1.51919400	-0.26942500
C	-3.93667000	-2.53243000	-0.46918200
C	-2.57017900	-2.23352900	-0.42453500
C	-2.12210800	-0.93569500	-0.18336000
C	-3.06962900	0.07307600	0.01509400
H	-5.16182600	0.57868200	0.12941700
H	-5.93399100	-1.74143300	-0.30213400
H	-4.26724100	-3.54909900	-0.65858600
H	-1.84668600	-3.03298900	-0.58205300
H	-2.75621300	1.09578000	0.20482400
S	0.00147100	-0.88097700	-0.19085900

E = –1323.71767508 a.u.

TS J

C	-0.12975300	2.49554700	0.13482900
C	0.73591600	1.44119200	-0.11516600
C	2.10813100	1.50573700	0.18160800
C	2.60690300	2.66448200	0.78135500
C	1.74467100	3.72151900	1.06381600
C	0.38815600	3.64068500	0.74215300
H	-1.17575100	2.41854500	-0.12520600
H	3.66059300	2.74370100	1.02065700

H	2.13439000	4.61934800	1.52907900
H	-0.27108700	4.47347800	0.95545100
C	2.52824500	-1.83403200	-1.35068000
C	3.88912500	-2.10157600	-1.18541800
C	4.72059600	-1.17242200	-0.55412100
C	4.21392000	0.03483200	-0.07486100
C	2.85277900	0.31051000	-0.22472300
C	2.03884200	-0.63093000	-0.86402800
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H	4.87354600	0.74740800	0.40624700
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C	-0.79433100	-1.85888800	2.59814700
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H	-1.07267200	-2.61980900	-1.18792800
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C	-4.23702600	0.42849600	-1.96952800
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C	-4.50247700	0.89598400	0.38173900
C	-3.15238800	0.59145200	0.58490200
C	-2.32080200	0.22099700	-0.47239800
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H	-2.75168800	0.63067100	1.59846800
H	-2.27744400	-0.16297500	-2.60403600
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E = –1323.69677753 a.u.

TS K

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C	-0.67534900	0.51699800	2.87069000
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H	-0.75856800	1.44984300	3.41847400
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H	-5.21943800	0.75952700	-0.28955900

H	-5.81205400	-1.24336900	-1.63527200
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E = –1323.70554716 a.u.

product K

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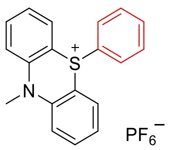
H	-1.13489900	-4.87877600	-1.28681000
H	-0.93669000	-4.40699000	1.14584400
H	-1.50278800	-2.17245400	2.02425900
H	-2.49447800	-0.86326200	-1.94097100
S	0.97606400	0.64473900	0.99560400

E = −1323.84967501 a.u.

7. NMR spectra



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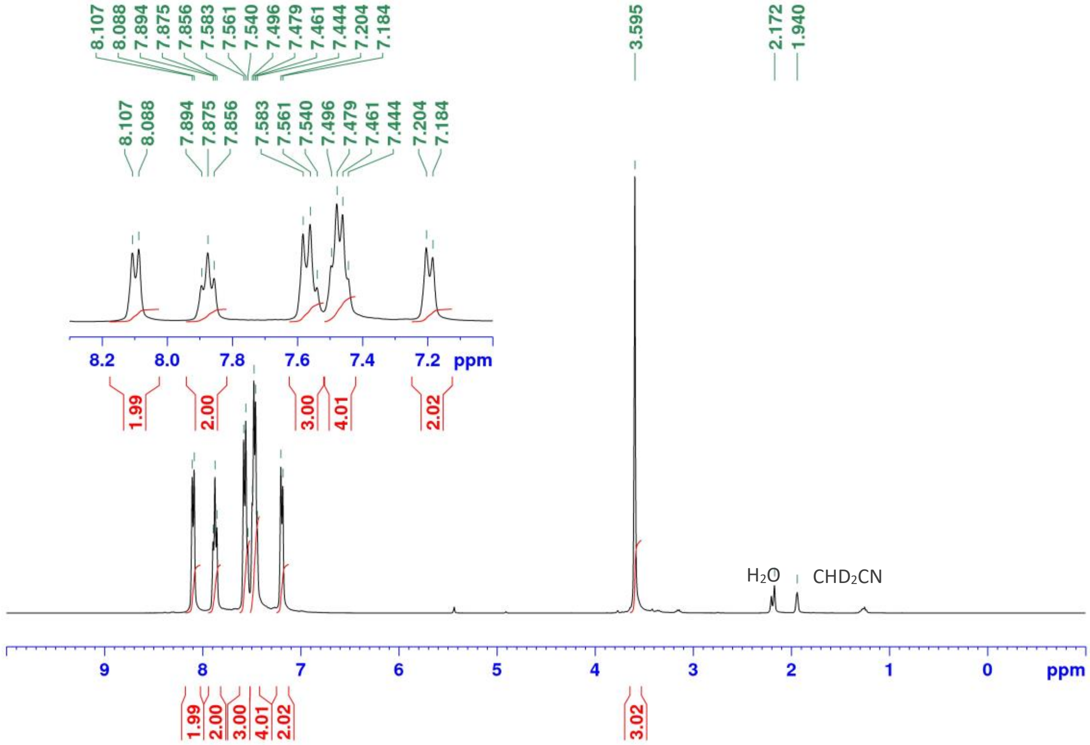
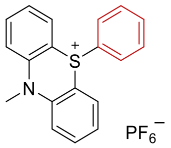


Figure S5. ^{1}H NMR (400 MHz) spectrum of **2a** in CD_3CN.



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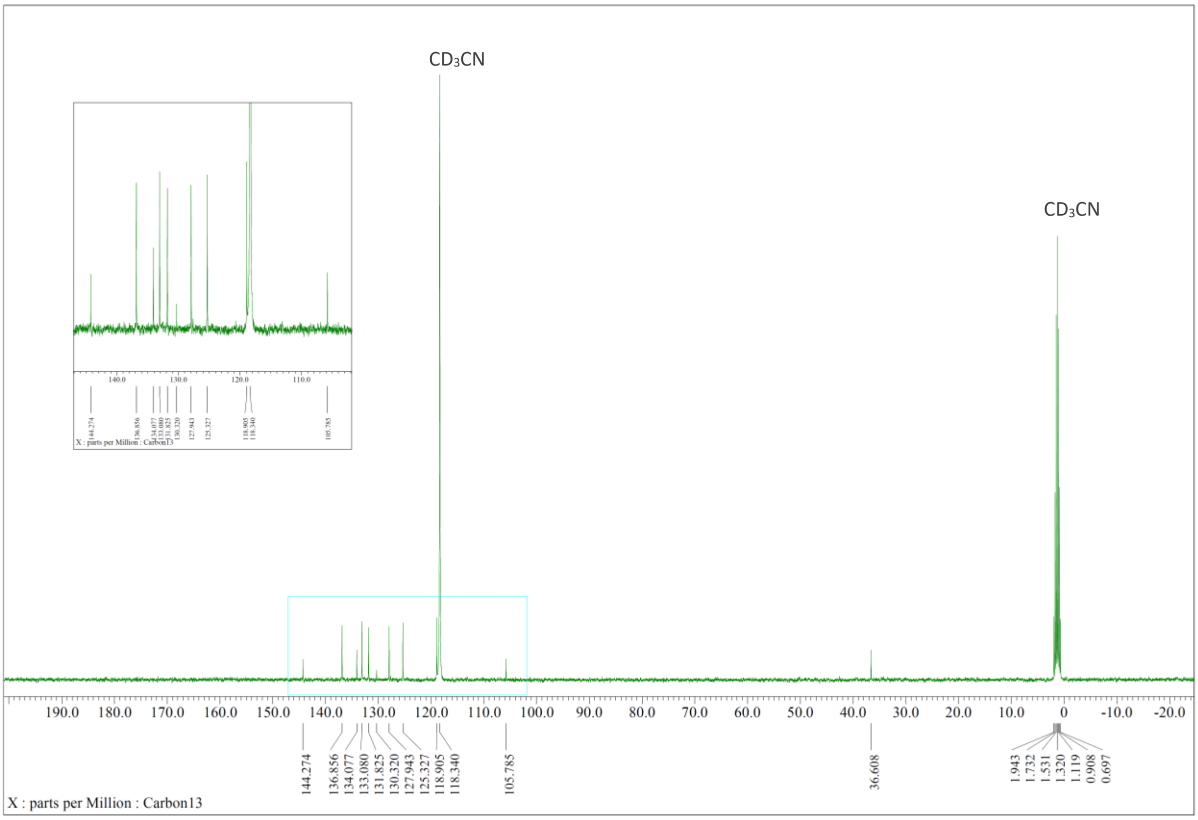
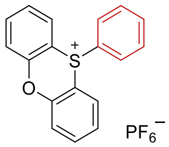


Figure S6. ^{13}C NMR (100 MHz) spectrum of **2a** in CD_3CN.



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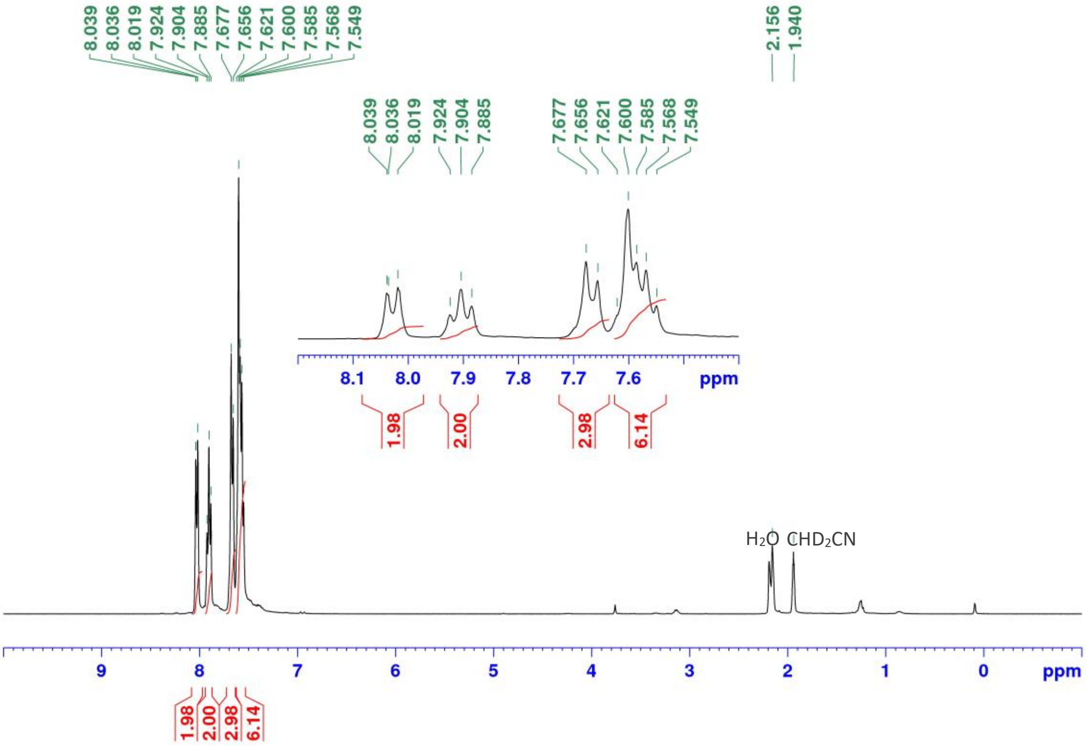
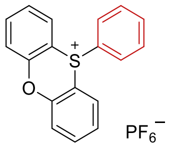


Figure S7. ^{1}H NMR (400 MHz) spectrum of **5** in CD_3CN.



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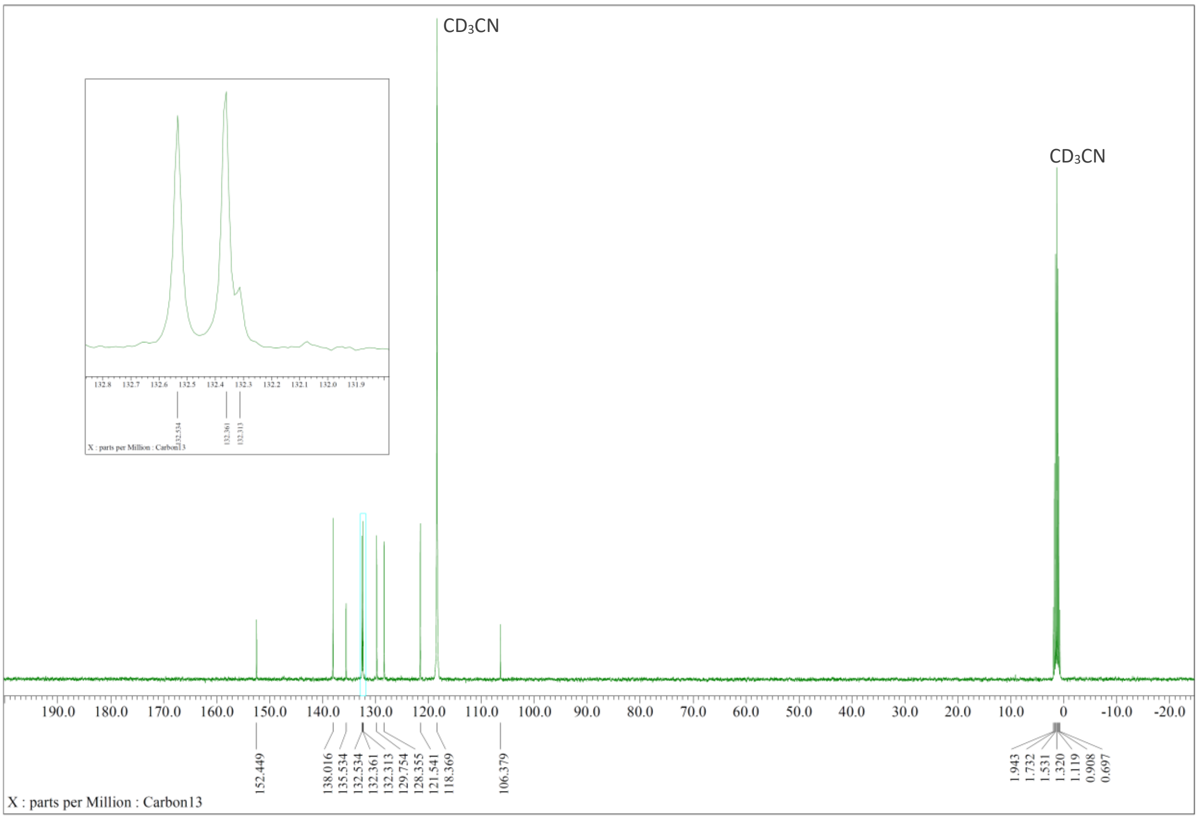
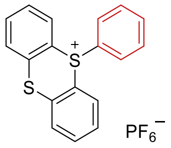


Figure S8. ^{13}C NMR (100 MHz) spectrum of **5** in CD_3CN.



8

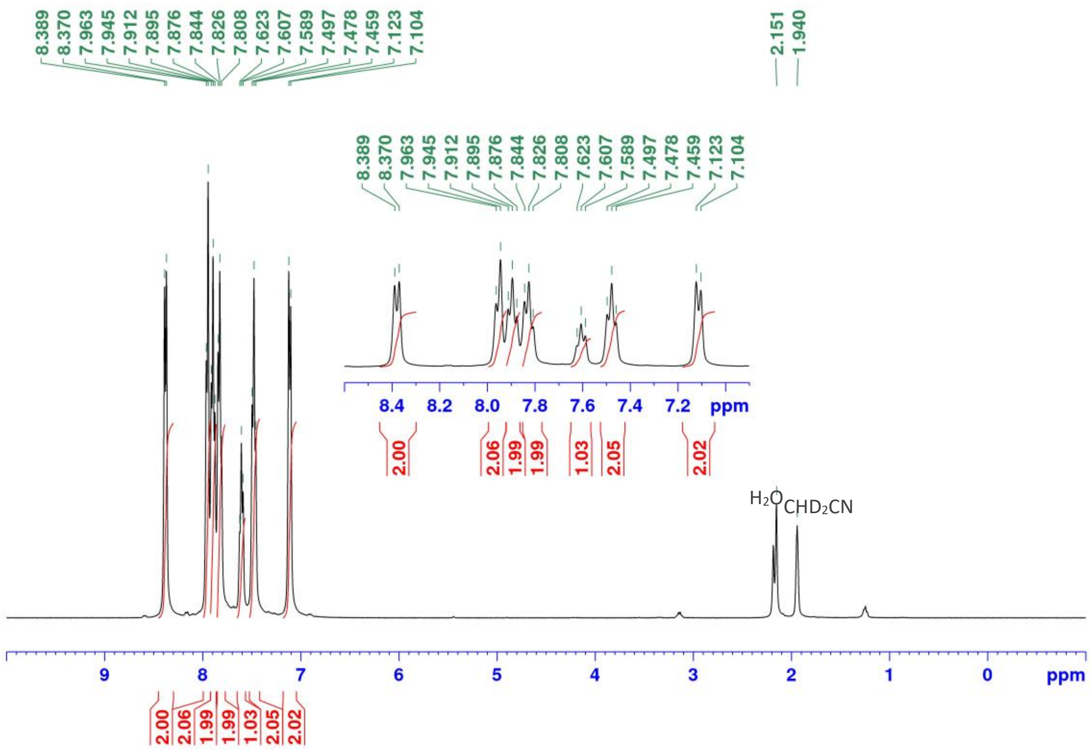
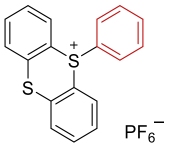


Figure S9. ^{1}H NMR (400 MHz) spectrum of **8** in CD_3CN.



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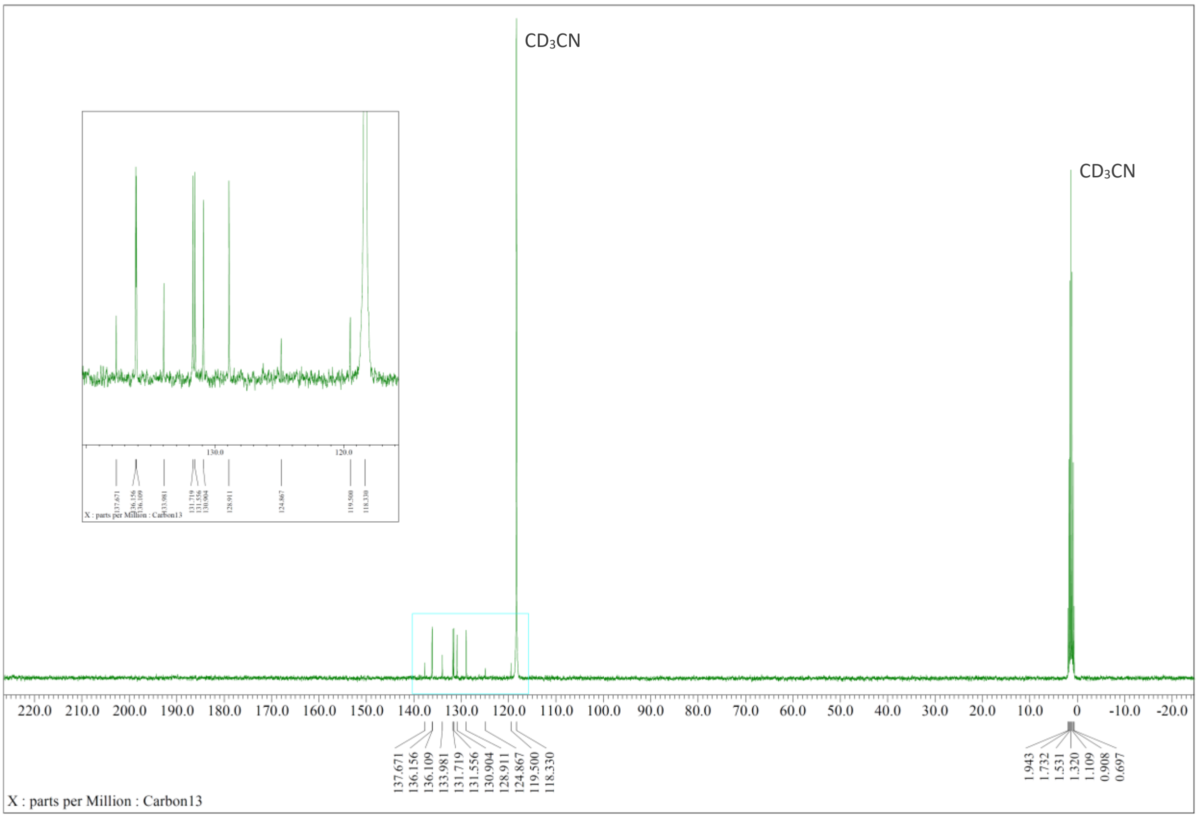
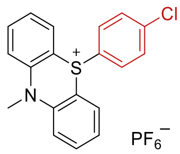


Figure S10. ^{13}C NMR (100 MHz) spectrum of **8** in CD_3CN.



2b

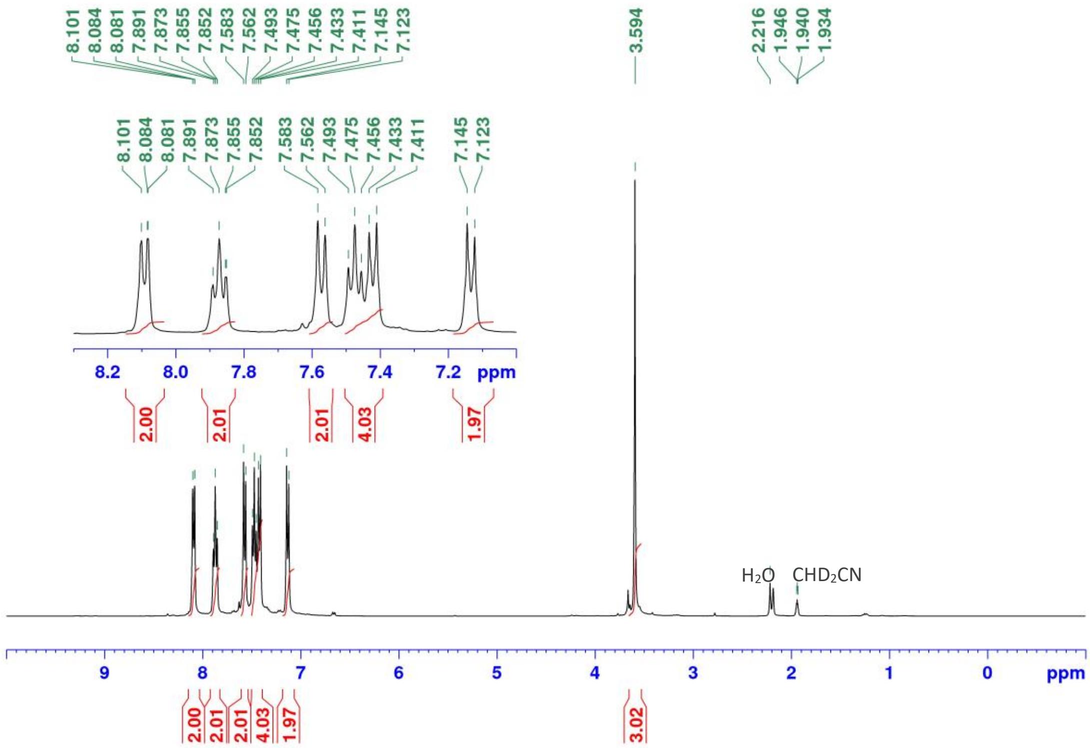
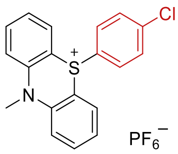


Figure S11. ^{1}H NMR (400 MHz) spectrum of **2b** in CD_3CN.



2b

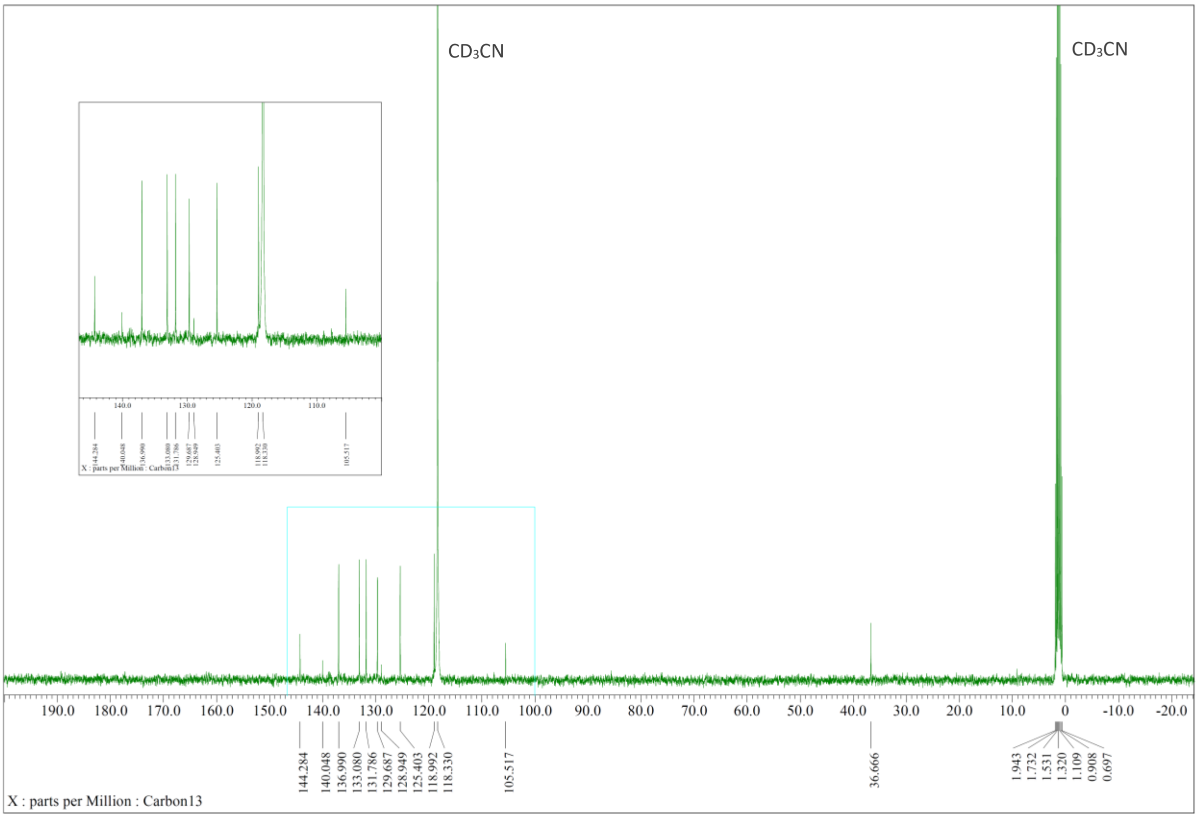
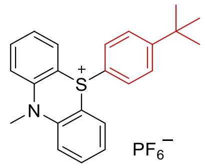


Figure S12. ^{13}C NMR (100 MHz) spectrum of **2b** in CD_3CN



2c

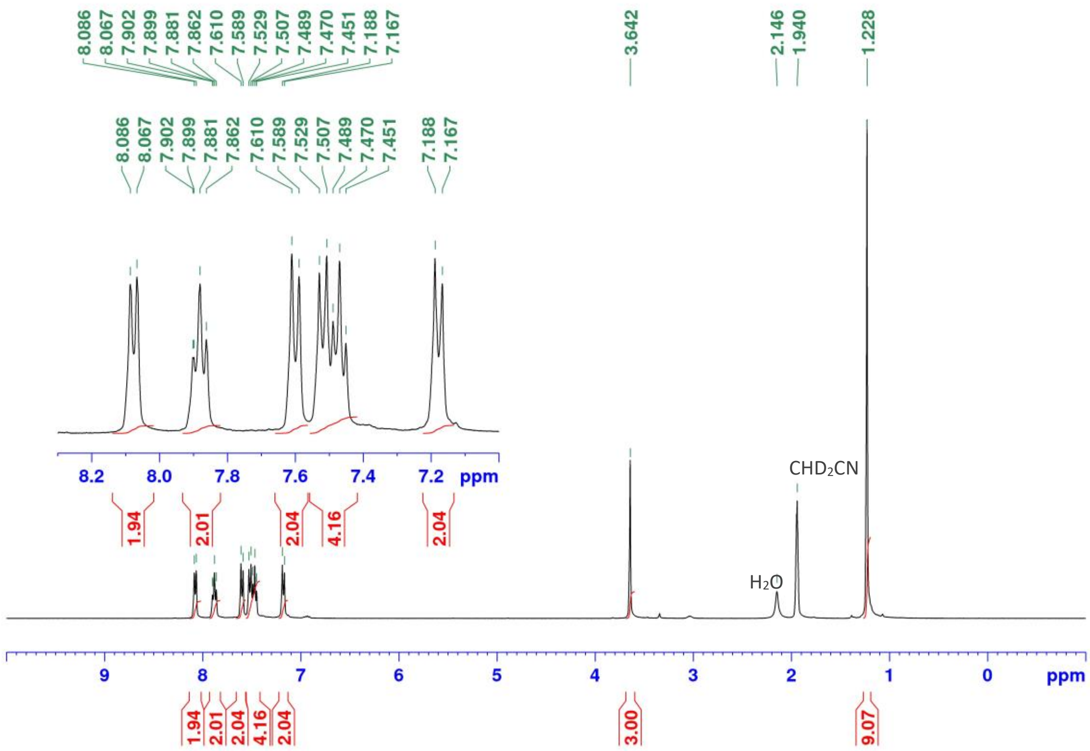
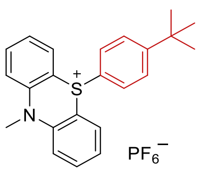


Figure S13. ^{1}H NMR (400 MHz) spectrum of **2c** in CD_3CN



2c

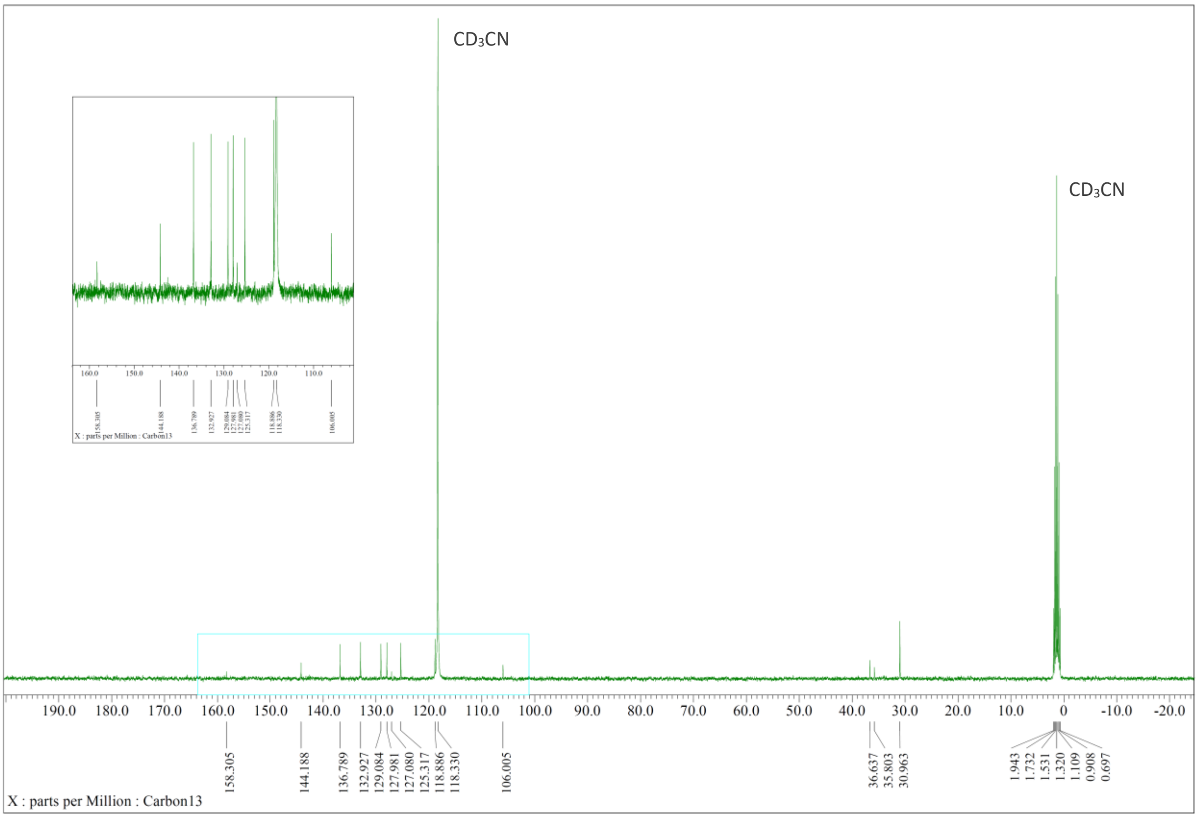
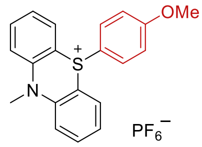


Figure S14. ^{13}C NMR (100 MHz) spectrum of **2c** in CD_3CN



2d

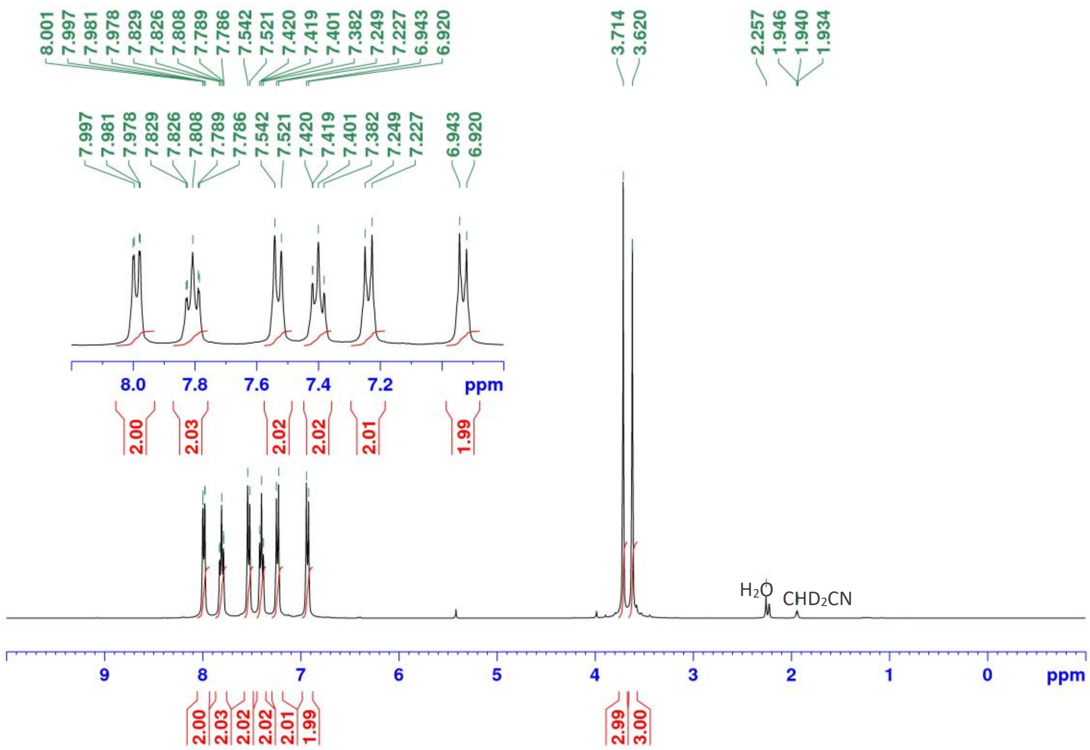
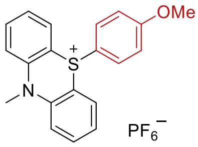


Figure S15. ^{1}H NMR (400 MHz) spectrum of **2d** in CD_3CN



2d

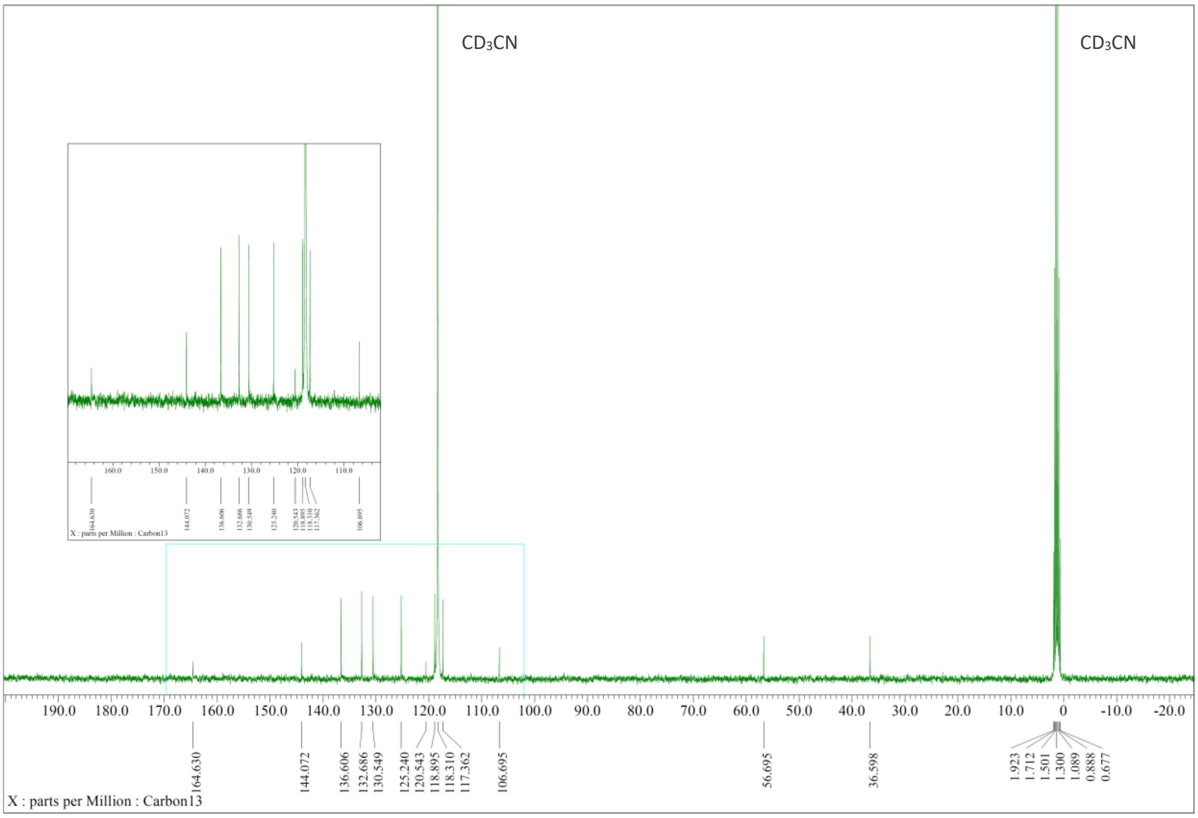
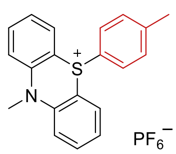


Figure S16. ^{13}C NMR (100 MHz) spectrum of **2d** in CD_3CN.



2e

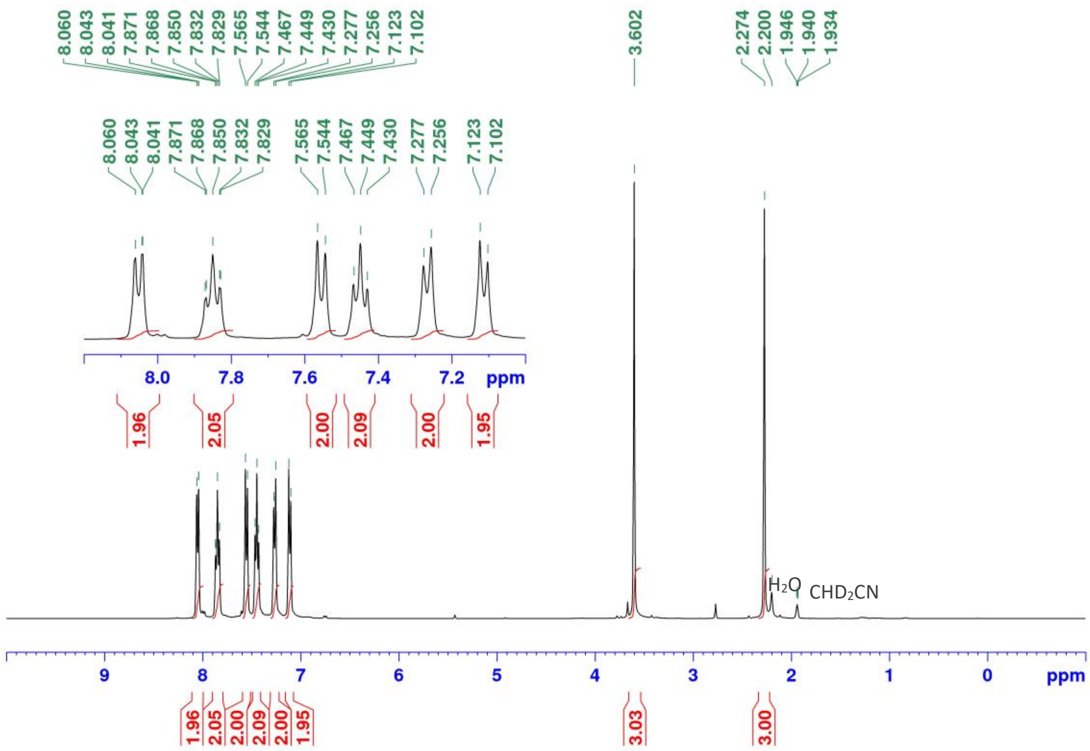
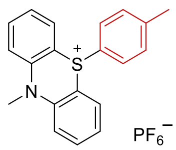


Figure S17. [1]H NMR (400 MHz) spectrum of **2e** in CD_3CN



2e

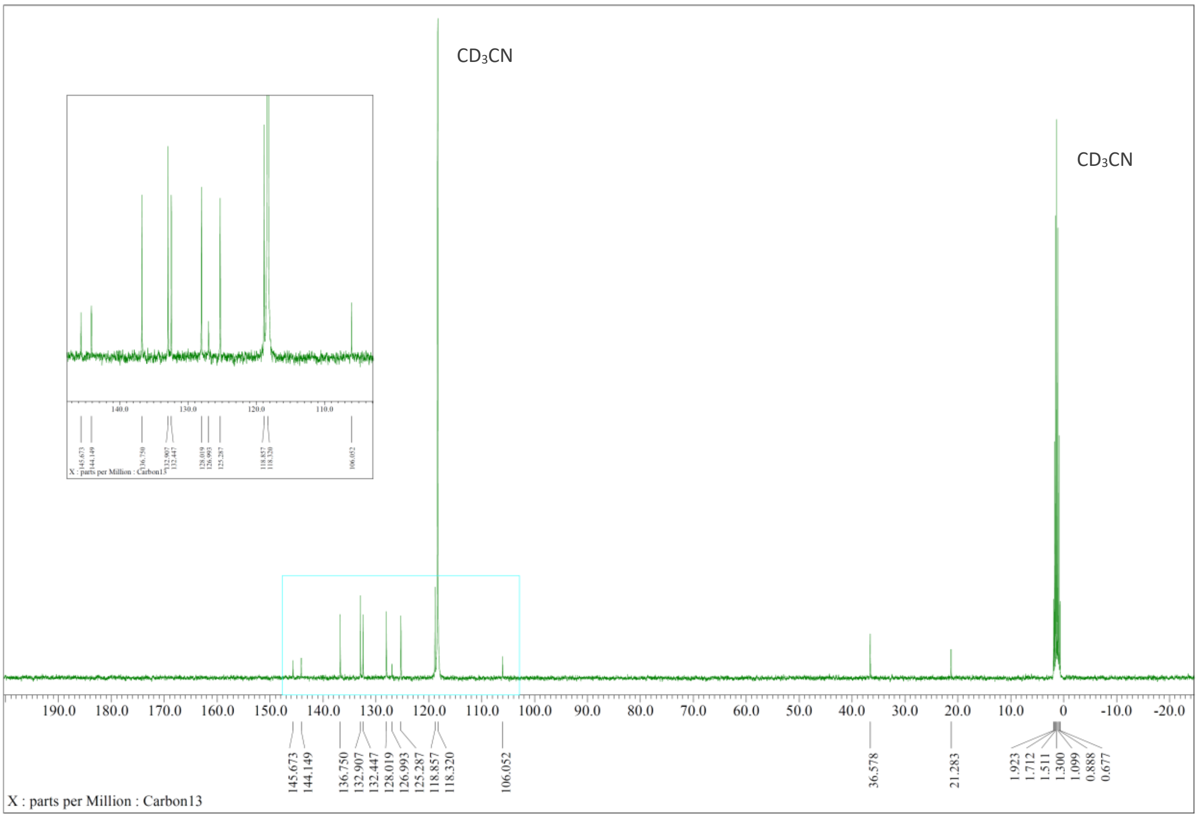
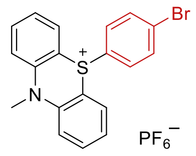


Figure S18. ^{13}C NMR (100 MHz) spectrum of **2e** in CD_3CN



2f

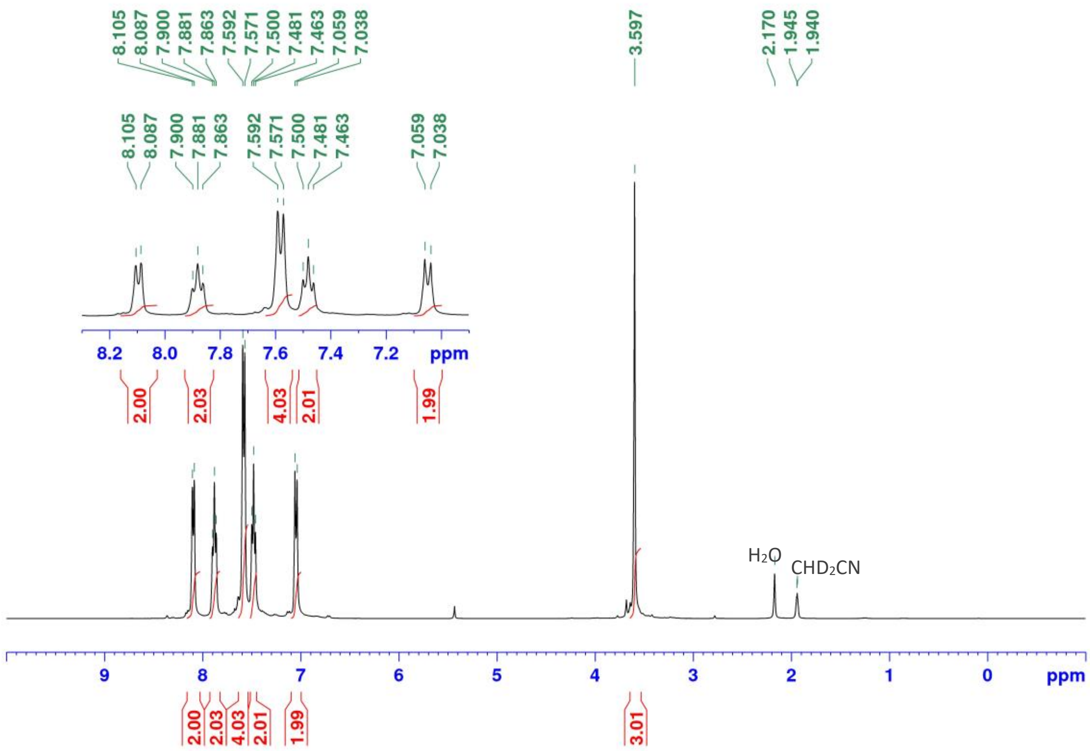
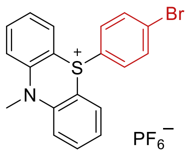


Figure S19. ^{1}H NMR (400 MHz) spectrum of **2f** in CD_3CN



2f

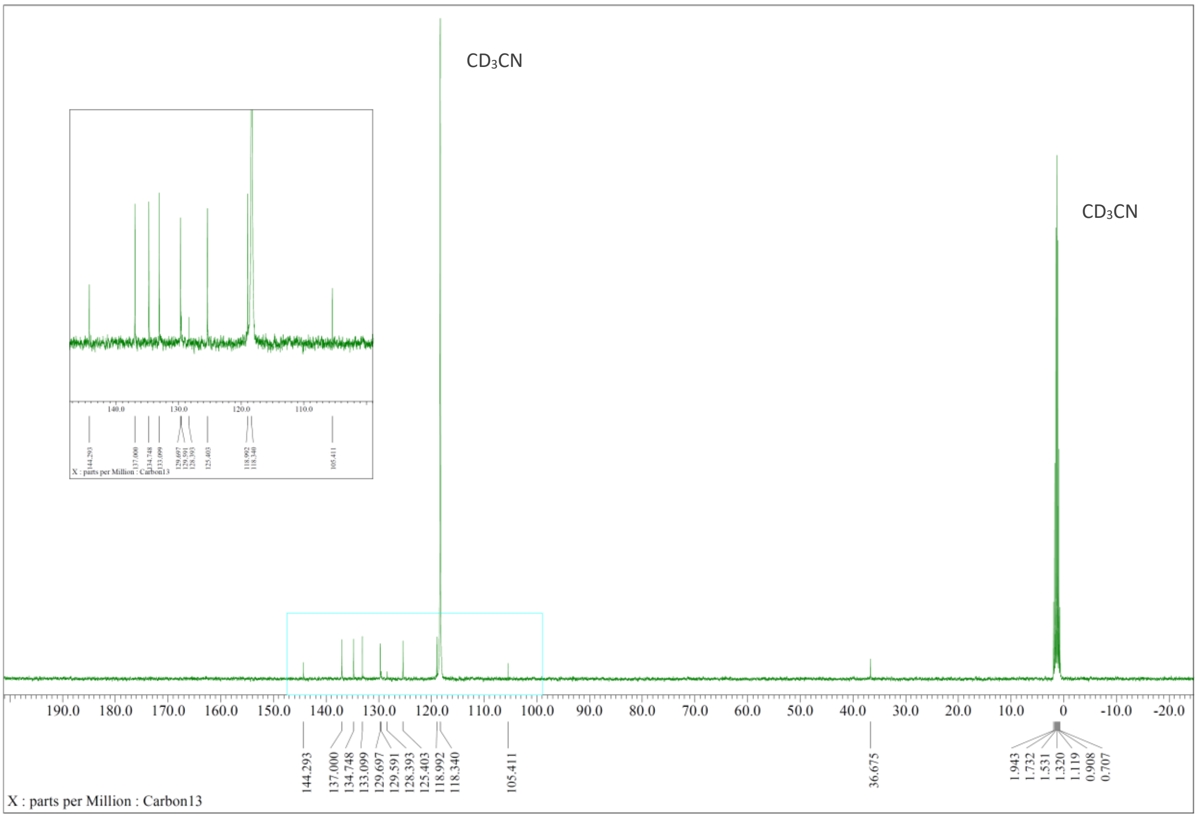
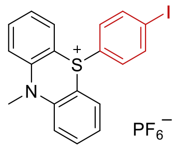


Figure S20. ^{13}C NMR (100 MHz) spectrum of **2f** in CD_3CN



2g

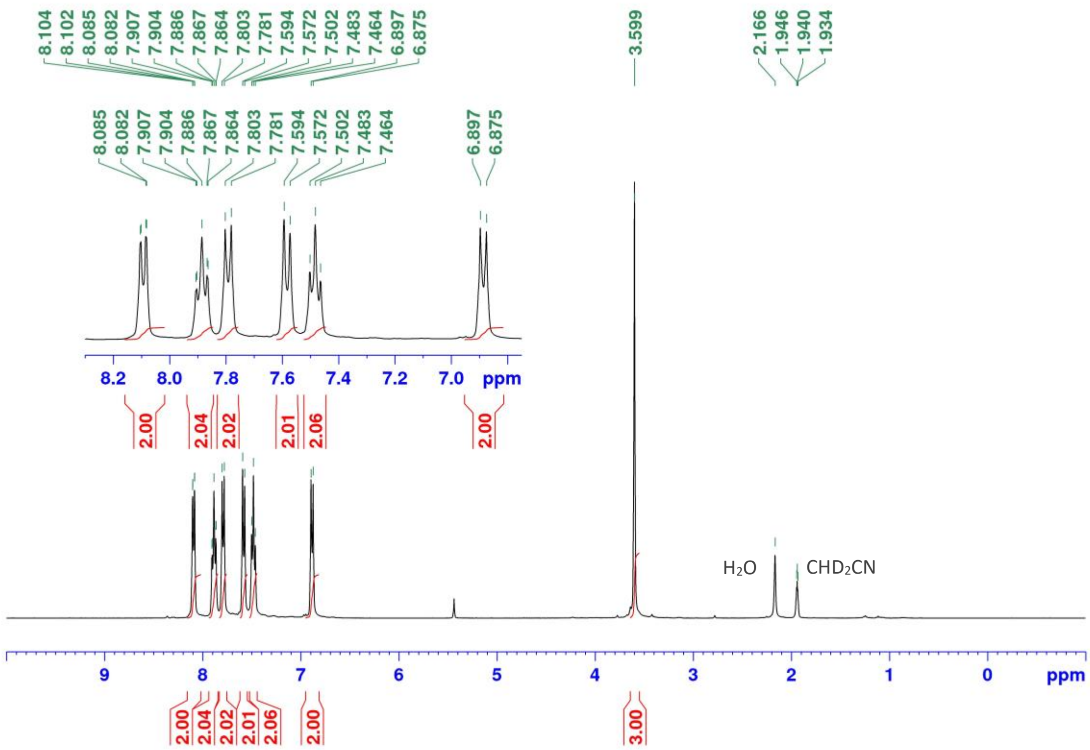
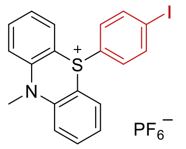


Figure S21. ^{1}H NMR (400 MHz) spectrum of **2g** in CD_3CN



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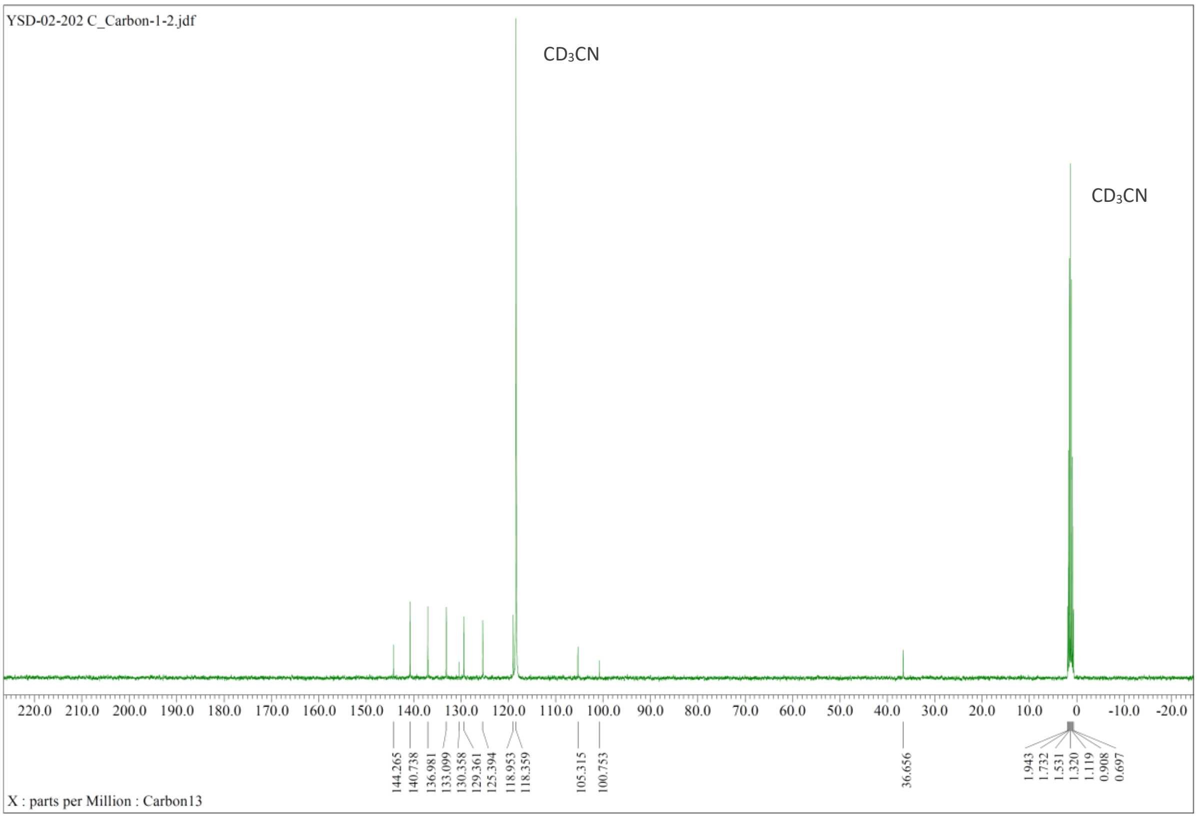
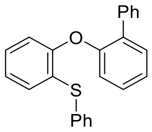


Figure S22. ^{13}C NMR (100 MHz) spectrum of **2g** in CD_3CN



7a

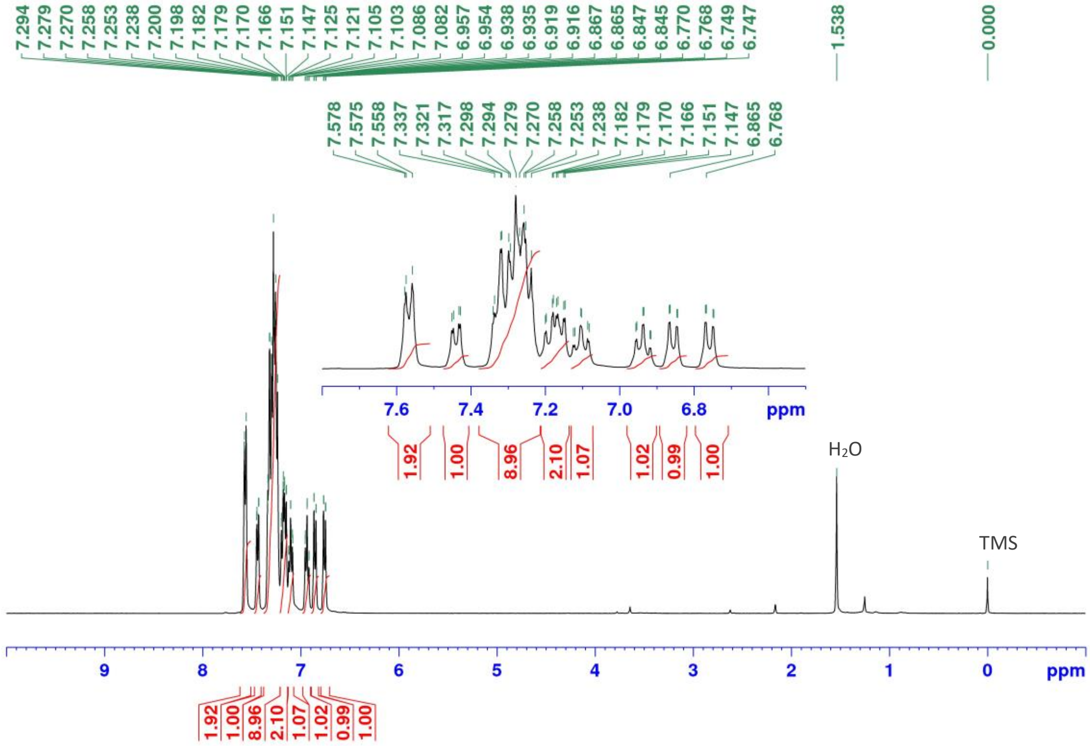
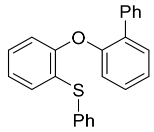


Figure S23. ^{1}H NMR (400 MHz) spectrum of **7a** in $CDCl_3$.



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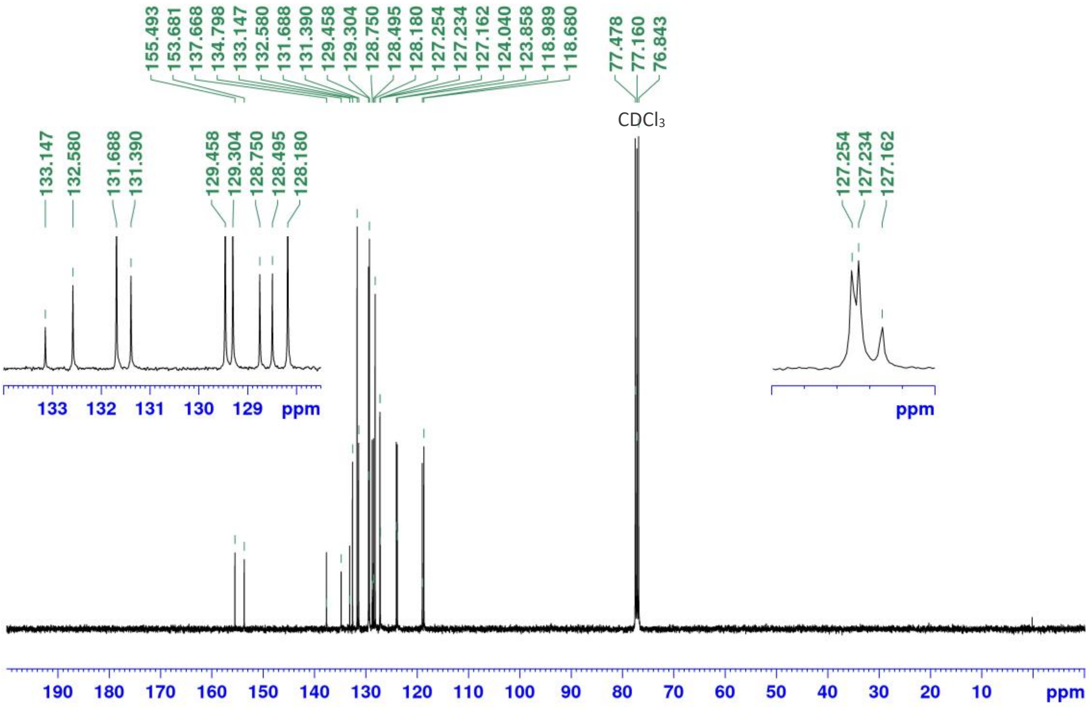
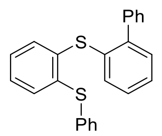


Figure S24. ^{13}C NMR (100 MHz) spectrum of **7a** in $CDCl_3$.



7b

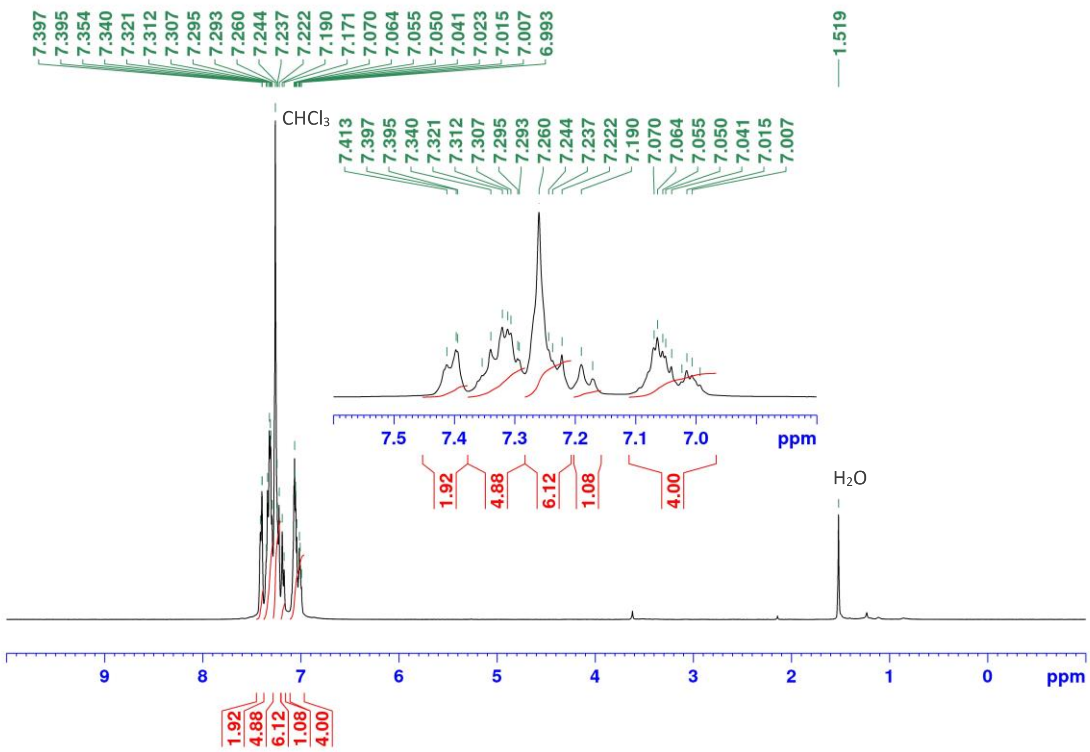
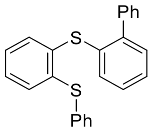


Figure S25. ^{1}H NMR (400 MHz) spectrum of **7b** in $CDCl_3$.



7b

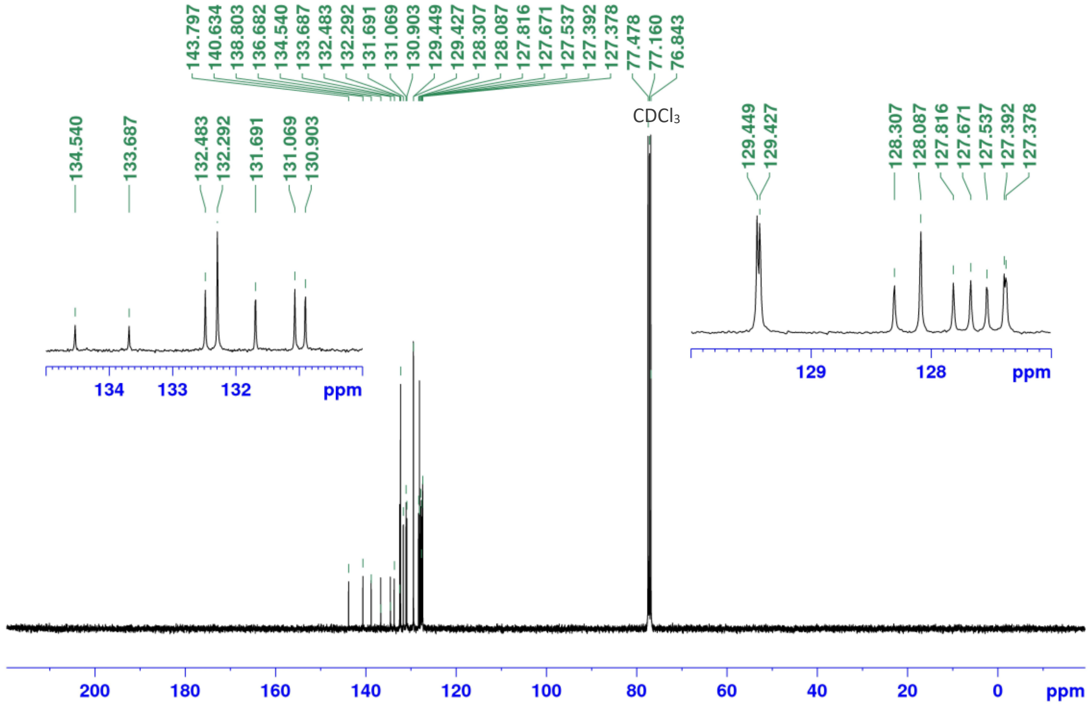
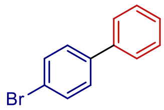


Figure S26. ^{13}C NMR (100 MHz) spectrum of **7b** in $CDCl_3$.



3b

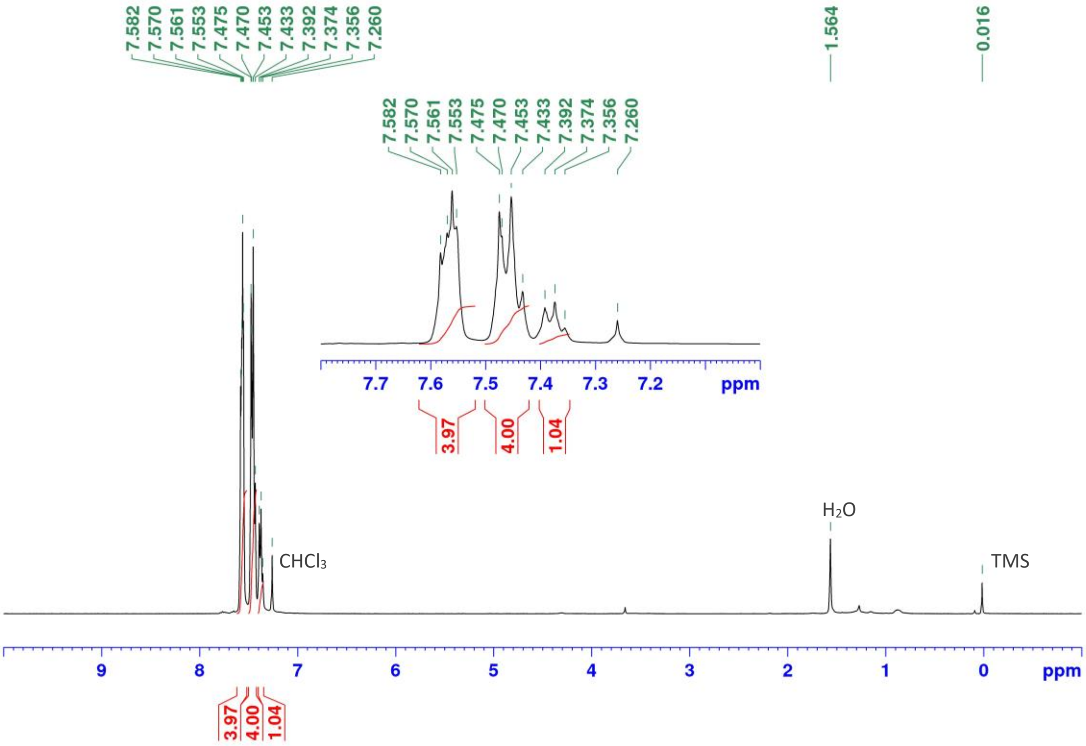
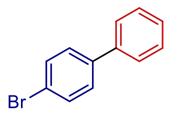


Figure S27. ^{1}H NMR (400 MHz) spectrum of **3b** in $CDCl_3$.



3b

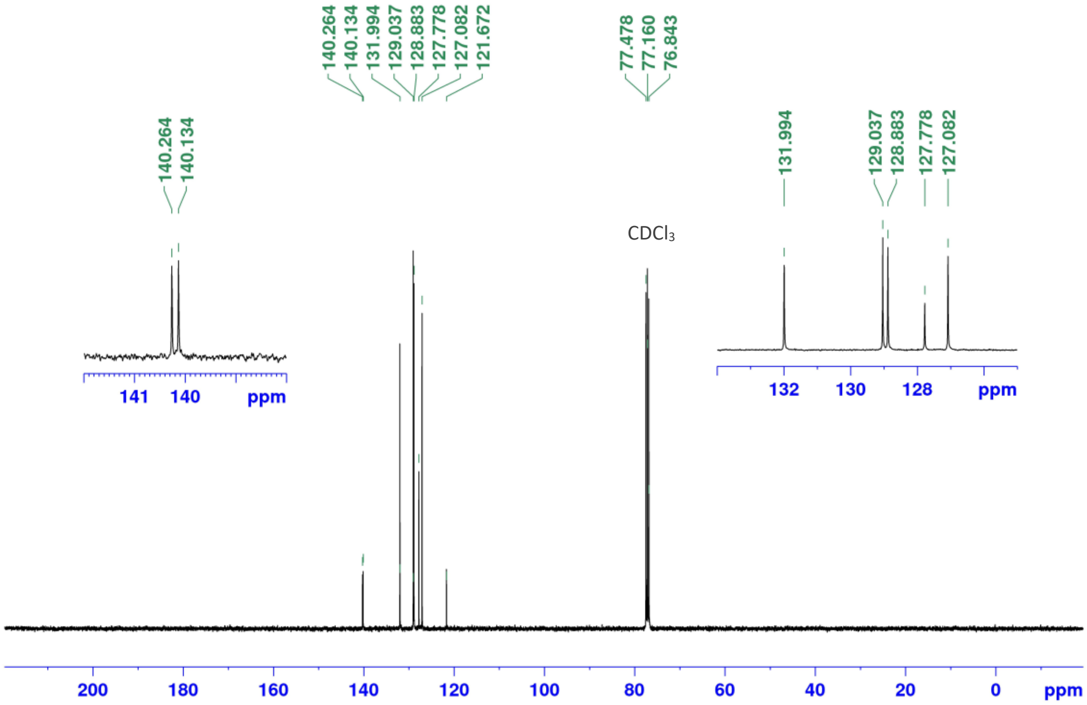
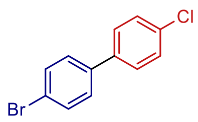


Figure S28. ^{13}C NMR (100 MHz) spectrum of **3b** in $CDCl_3$.



3c

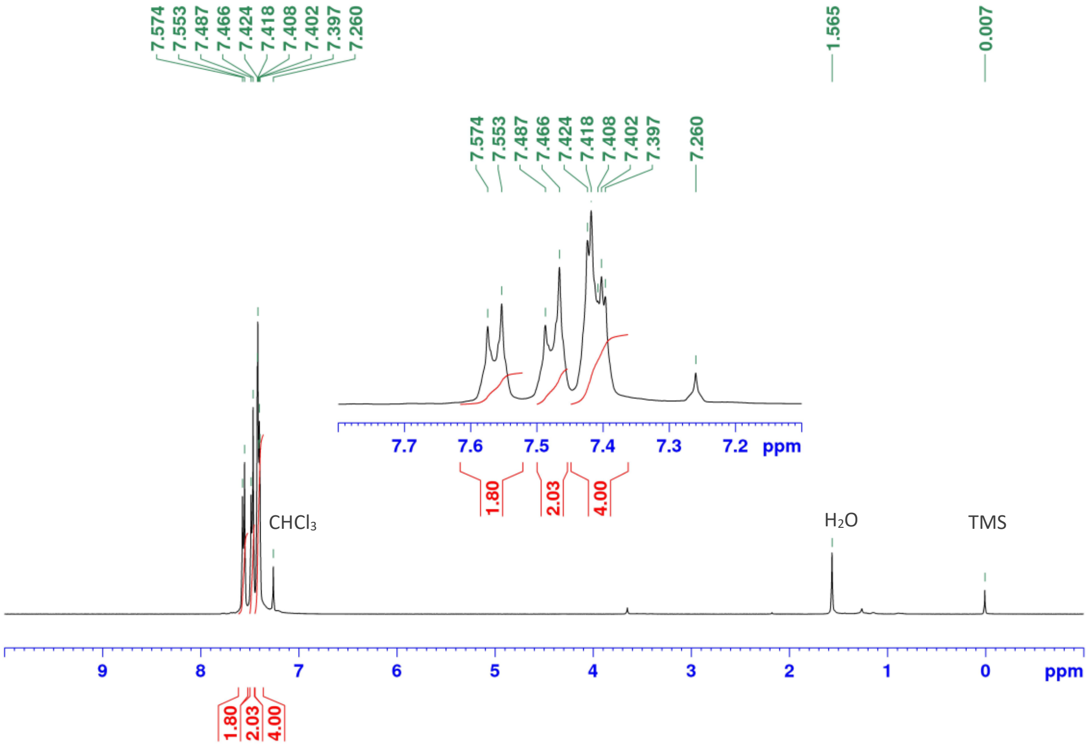
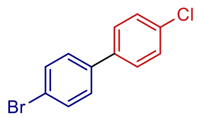


Figure S29. ^{1}H NMR (400 MHz) spectrum of **3c** in $CDCl_3$.



3c

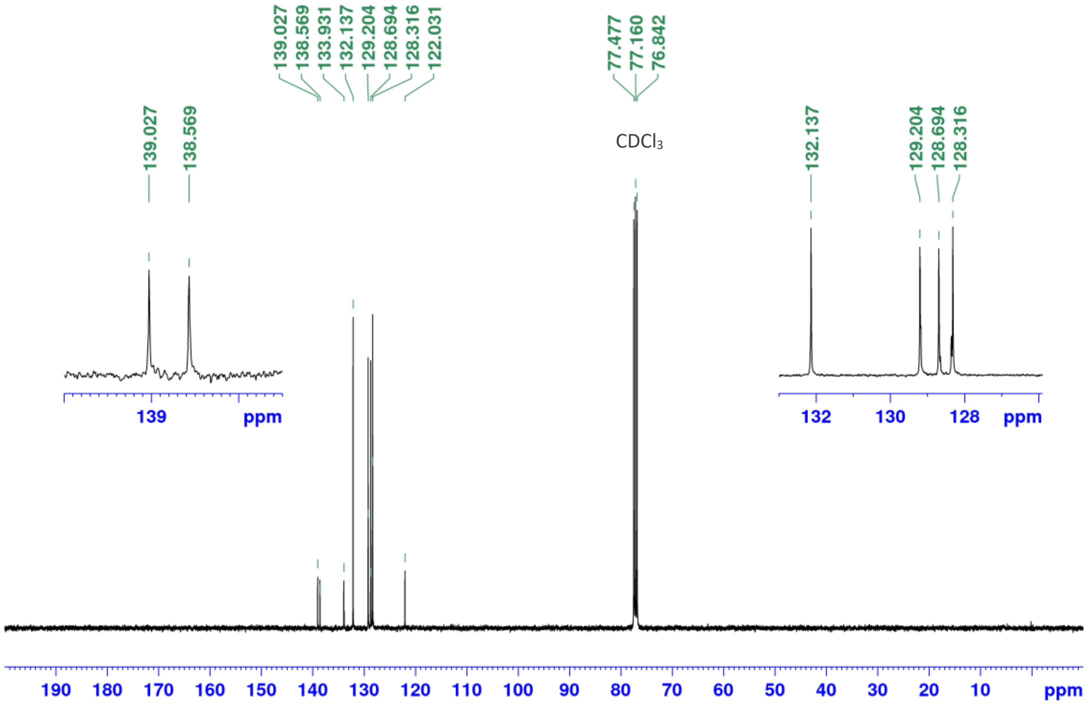
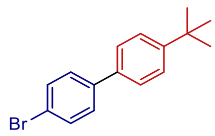


Figure S30. ^{13}C NMR (100 MHz) spectrum of **3c** in $CDCl_3$.



3d

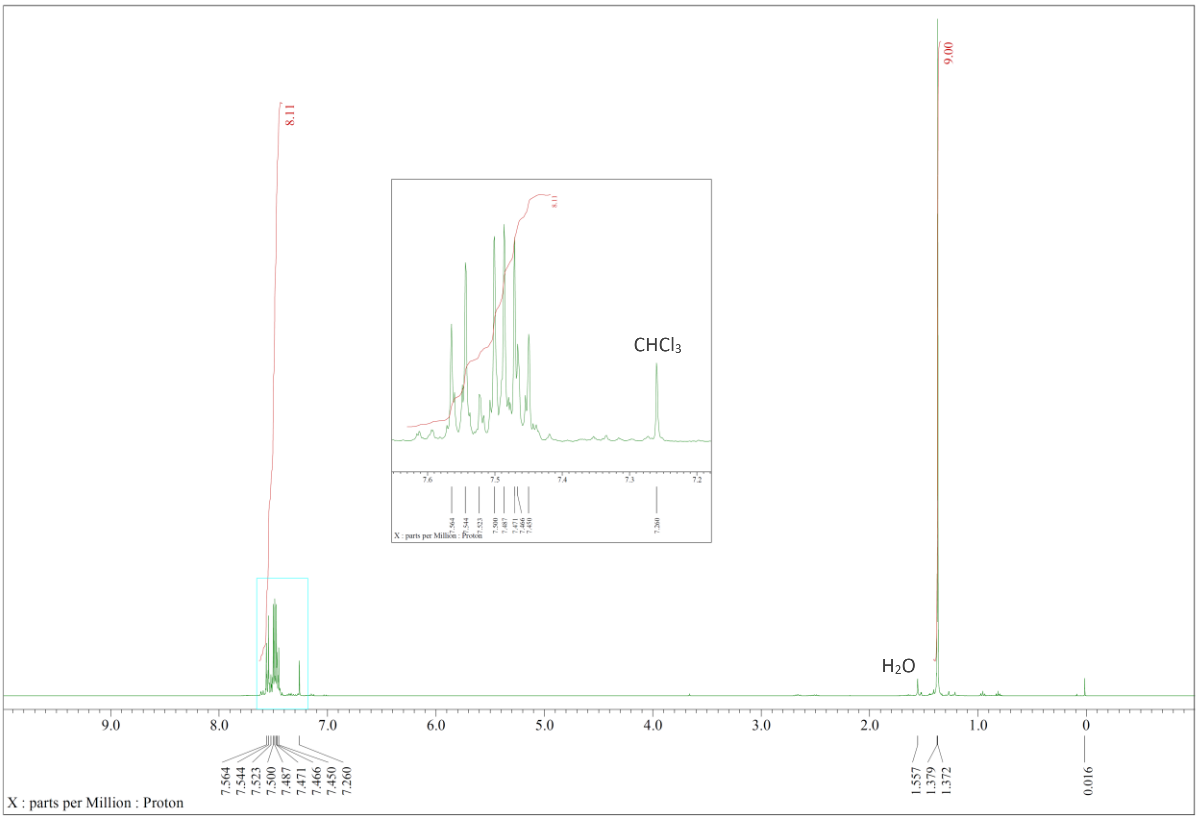
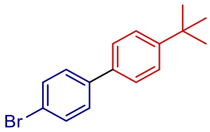


Figure S31. ^{1}H NMR (400 MHz) spectrum of **3d** in $CDCl_3$.



3d

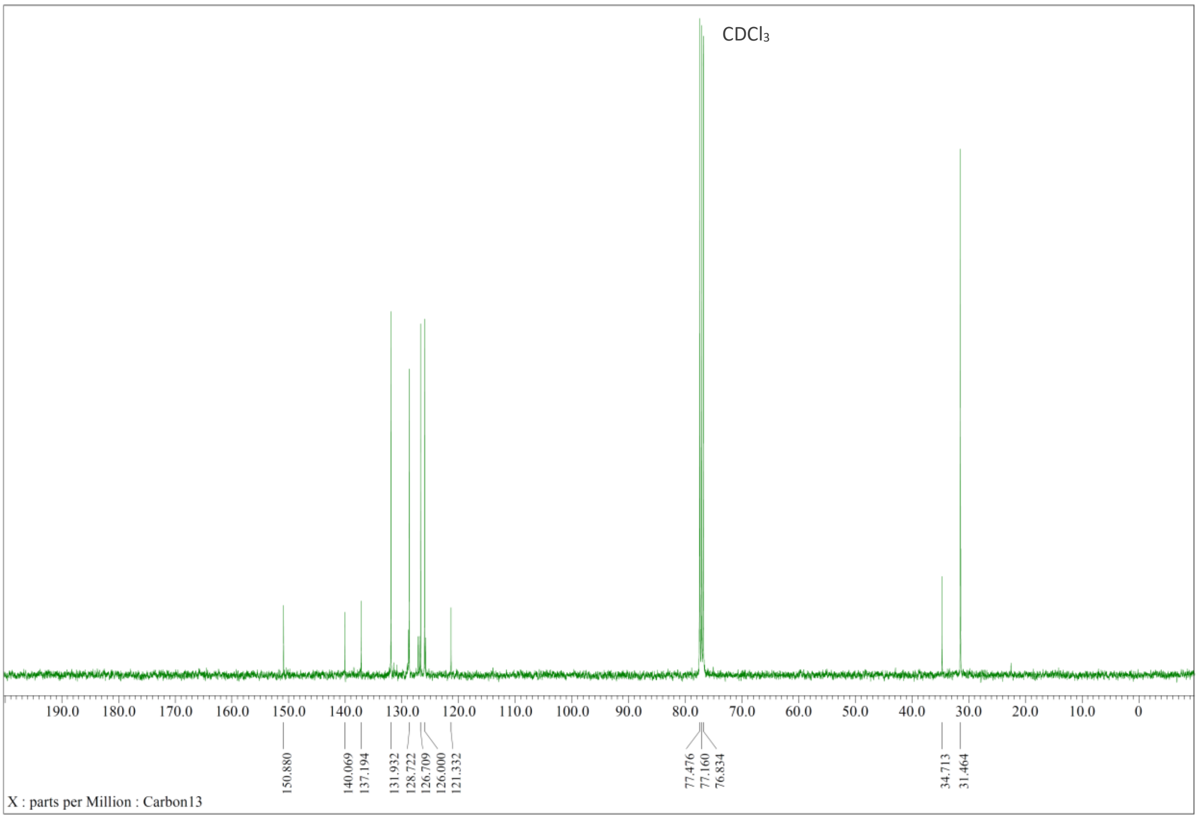
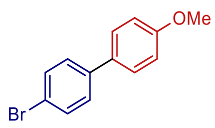


Figure S32. ^{13}C NMR (100 MHz) spectrum of **3d** in $CDCl_3$.



3e

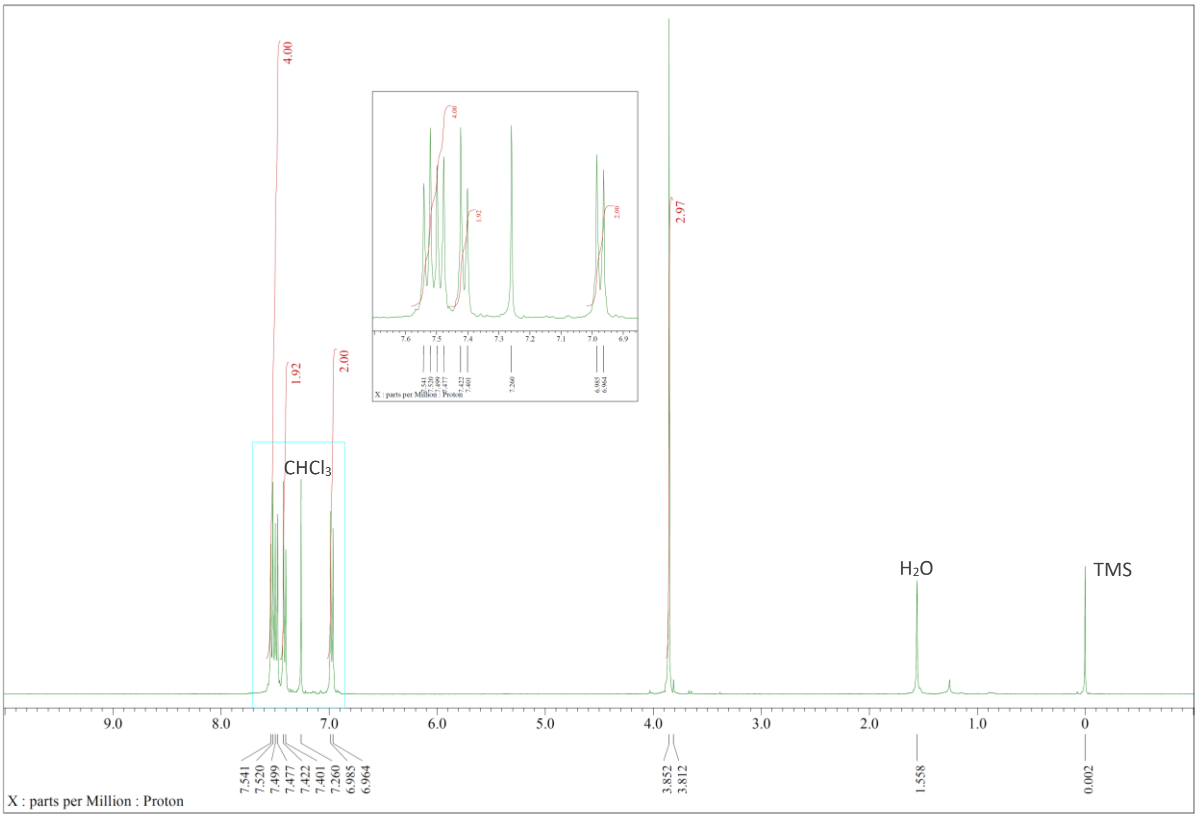
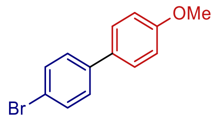


Figure S33. ^{1}H NMR (400 MHz) spectrum of **3e** in $CDCl_3$.



3e

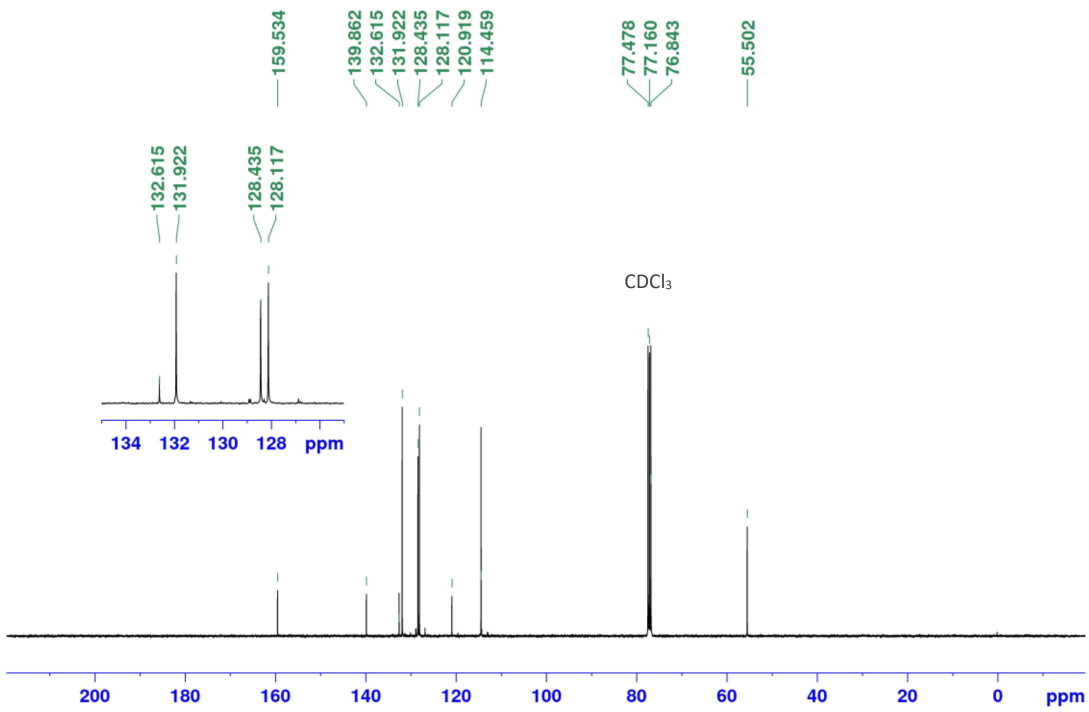
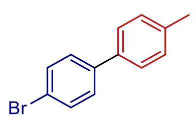


Figure S34. ^{13}C NMR (100 MHz) spectrum of **3e** in $CDCl_3$.



3f

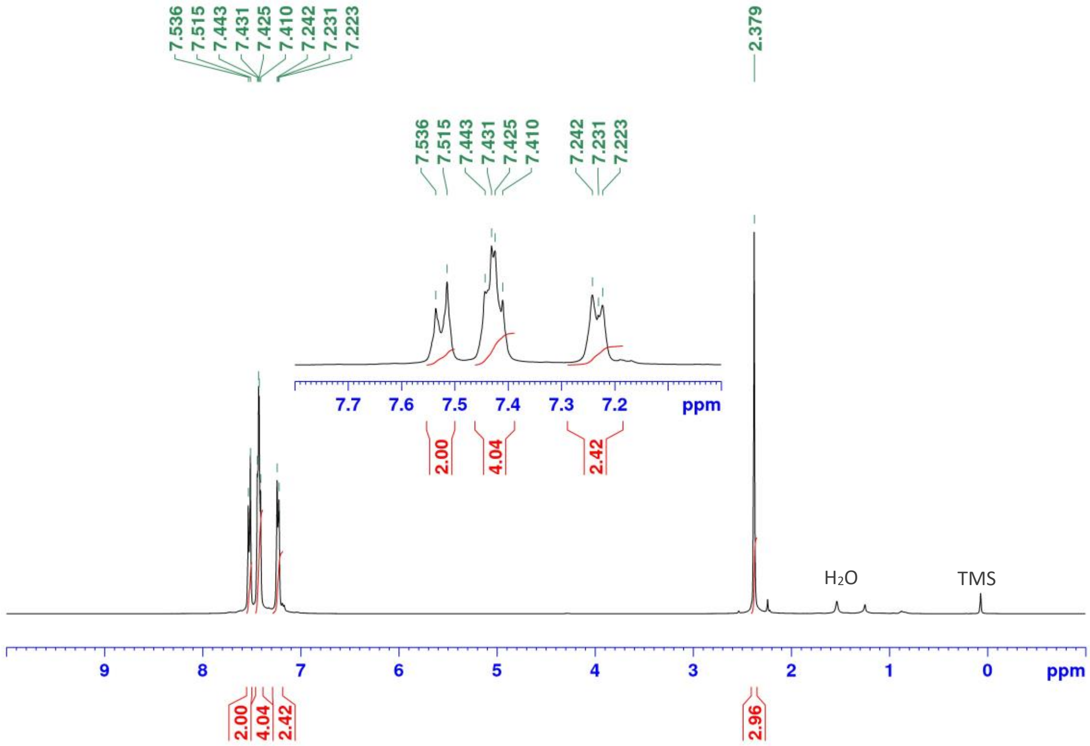
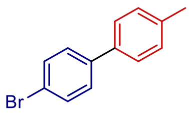


Figure S35. ^{1}H NMR (400 MHz) spectrum of **3f** in $CDCl_3$.



3f

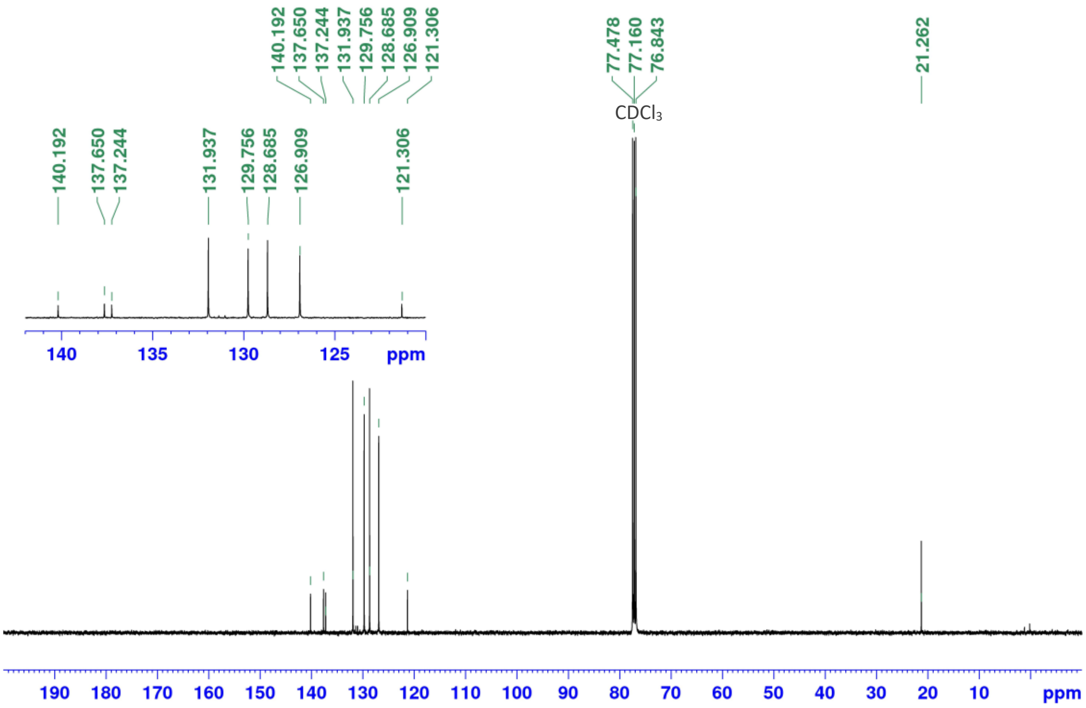
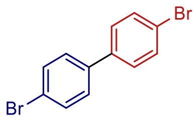


Figure S36. ^{13}C NMR (100 MHz) spectrum of **3f** in $CDCl_3$.



3g

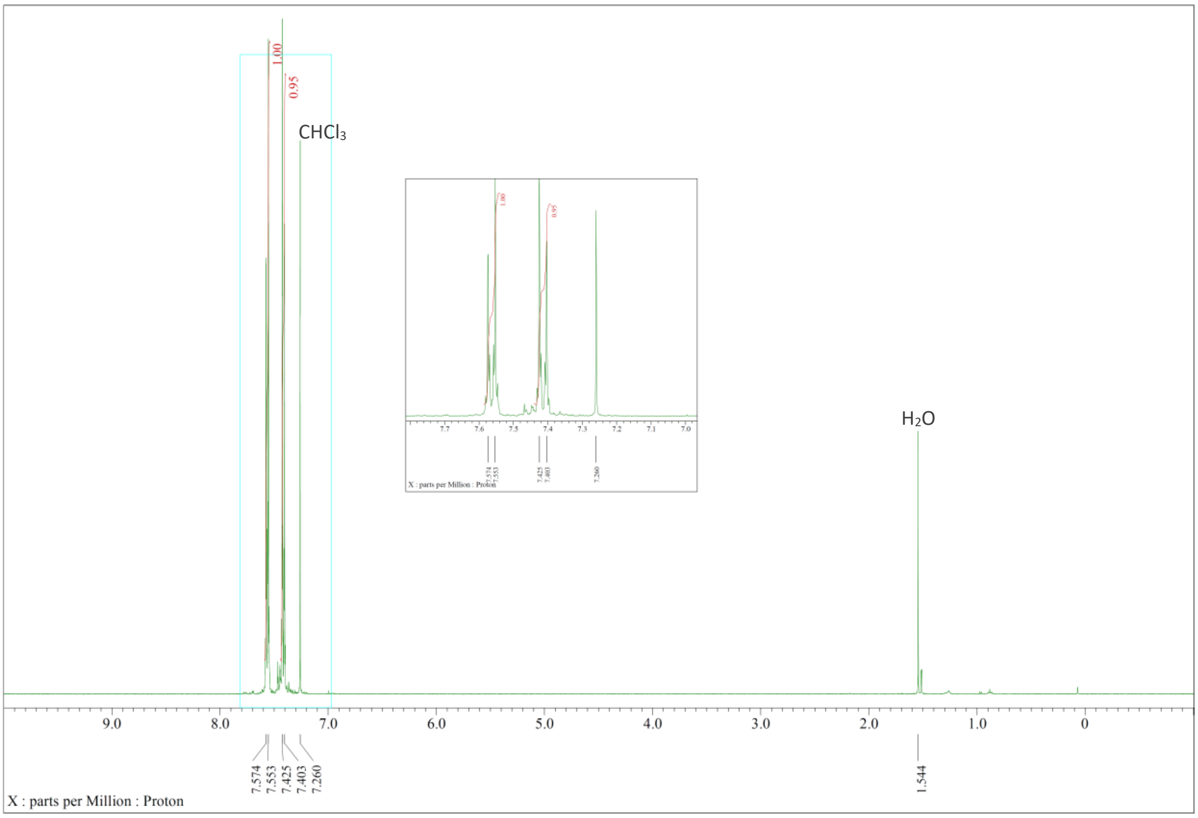
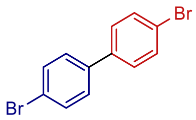


Figure S37. [1]H NMR (400 MHz) spectrum of **3g** in $CDCl_3$.



3g

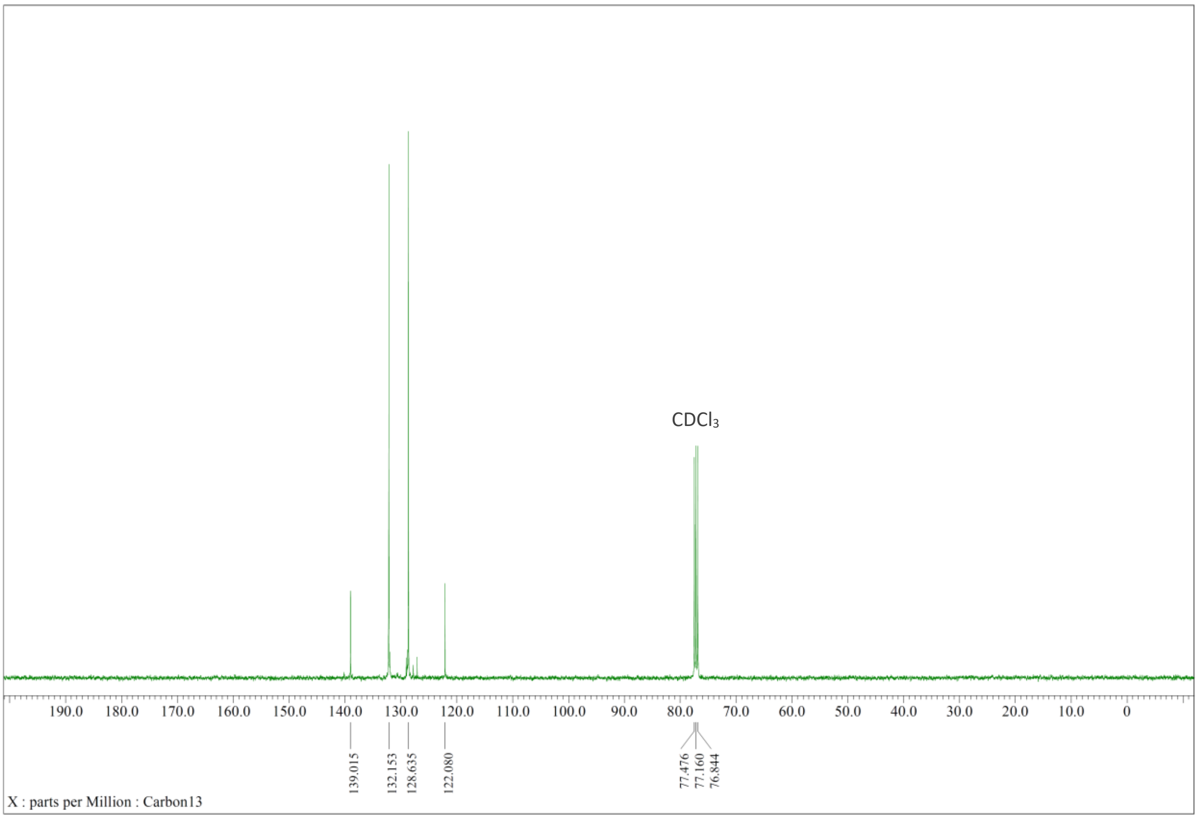
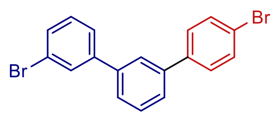


Figure S38. ^{13}C NMR (100 MHz) spectrum of **3g** in $CDCl_3$.



3h

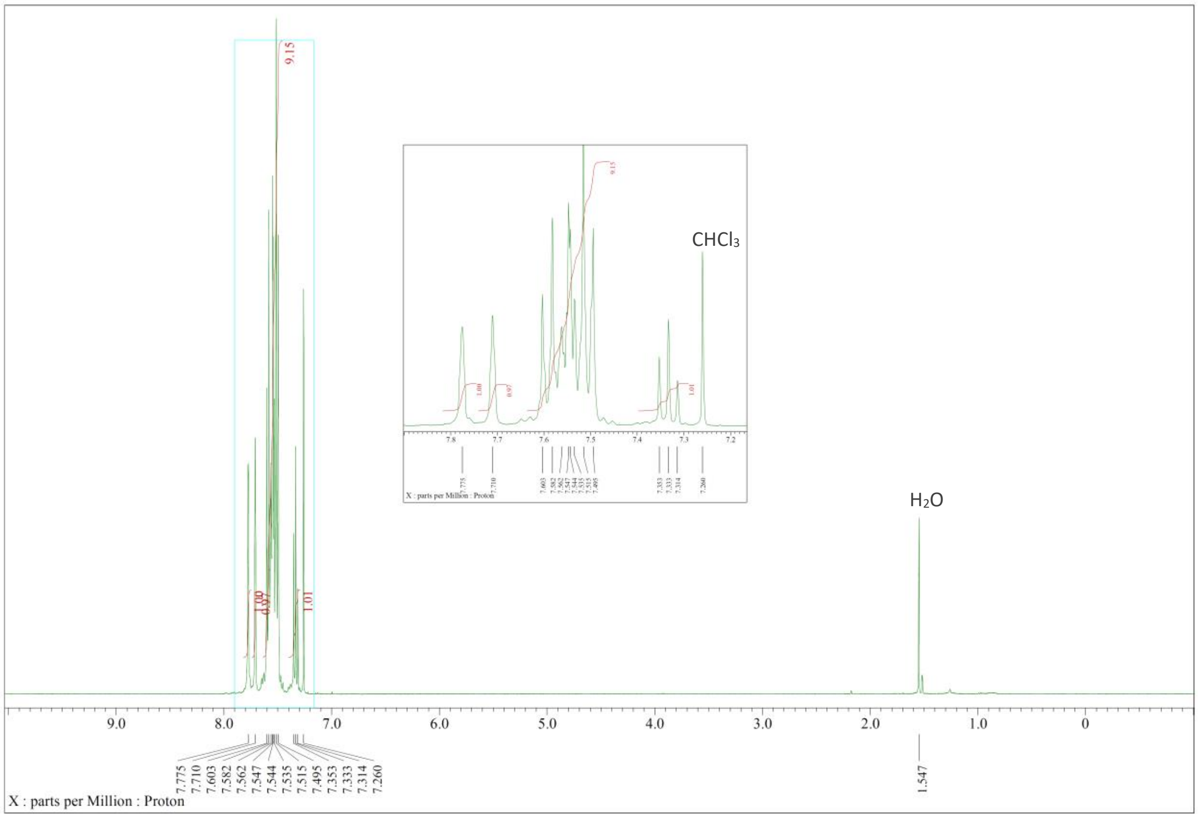
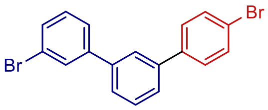


Figure S39. ^{1}H NMR (400 MHz) spectrum of **3h** in $CDCl_3$.



3h

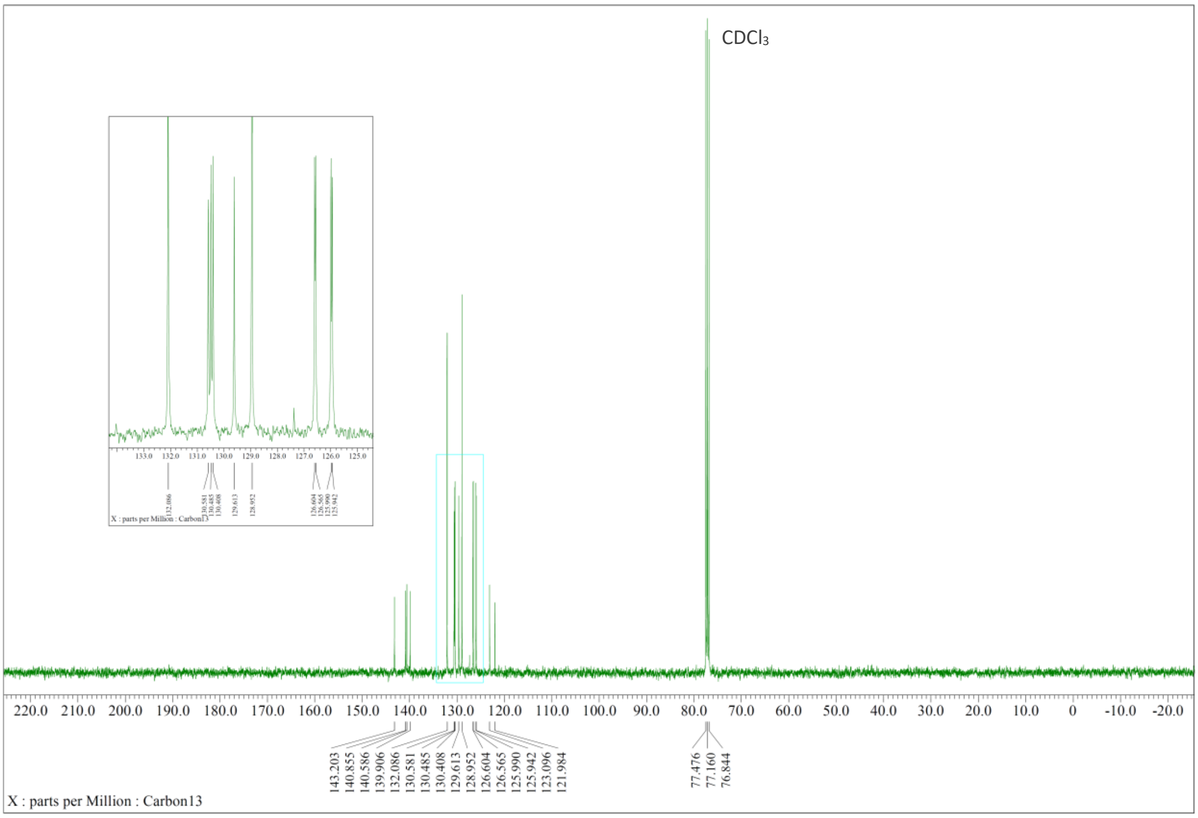
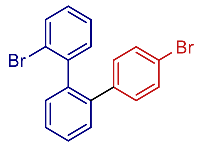


Figure S40. ^{13}C NMR (100 MHz) spectrum of **3h** in $CDCl_3$.



3i

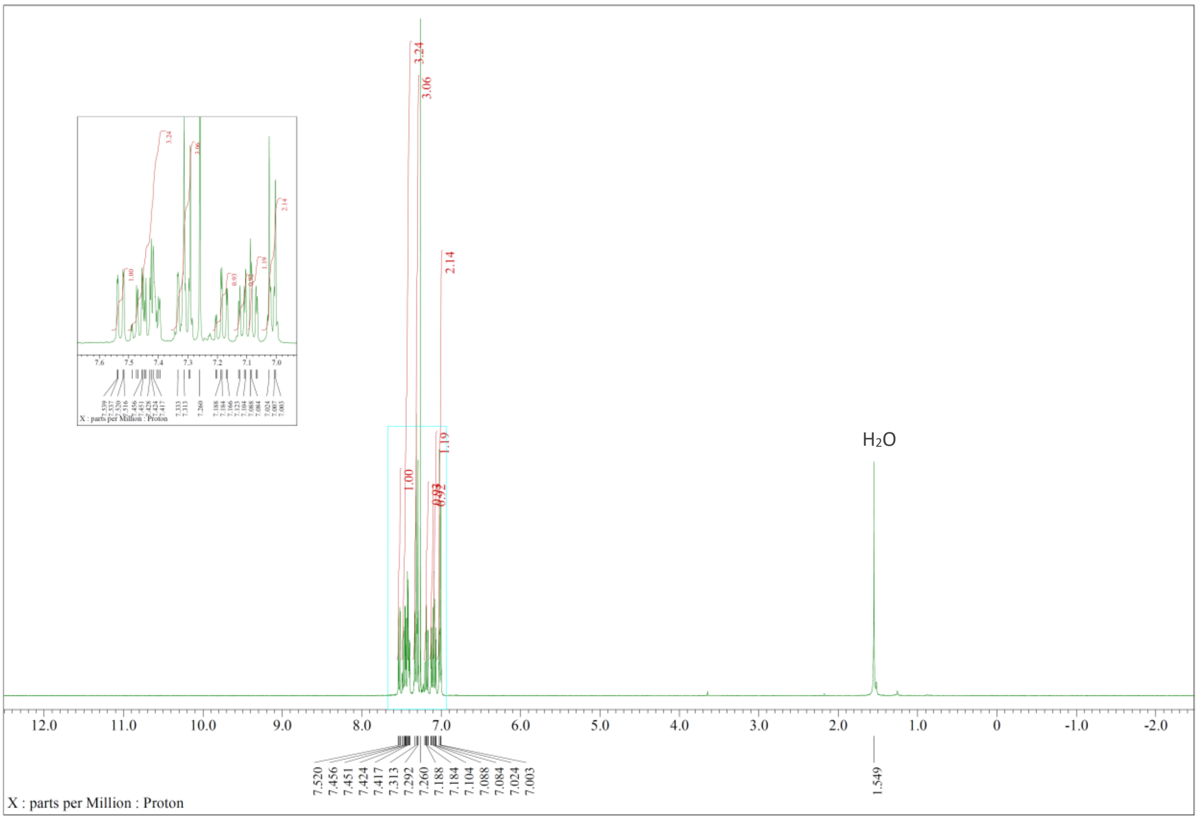
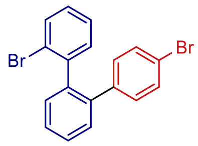


Figure S41. ^{1}H NMR (400 MHz) spectrum of **3i** in $CDCl_3$.



3i

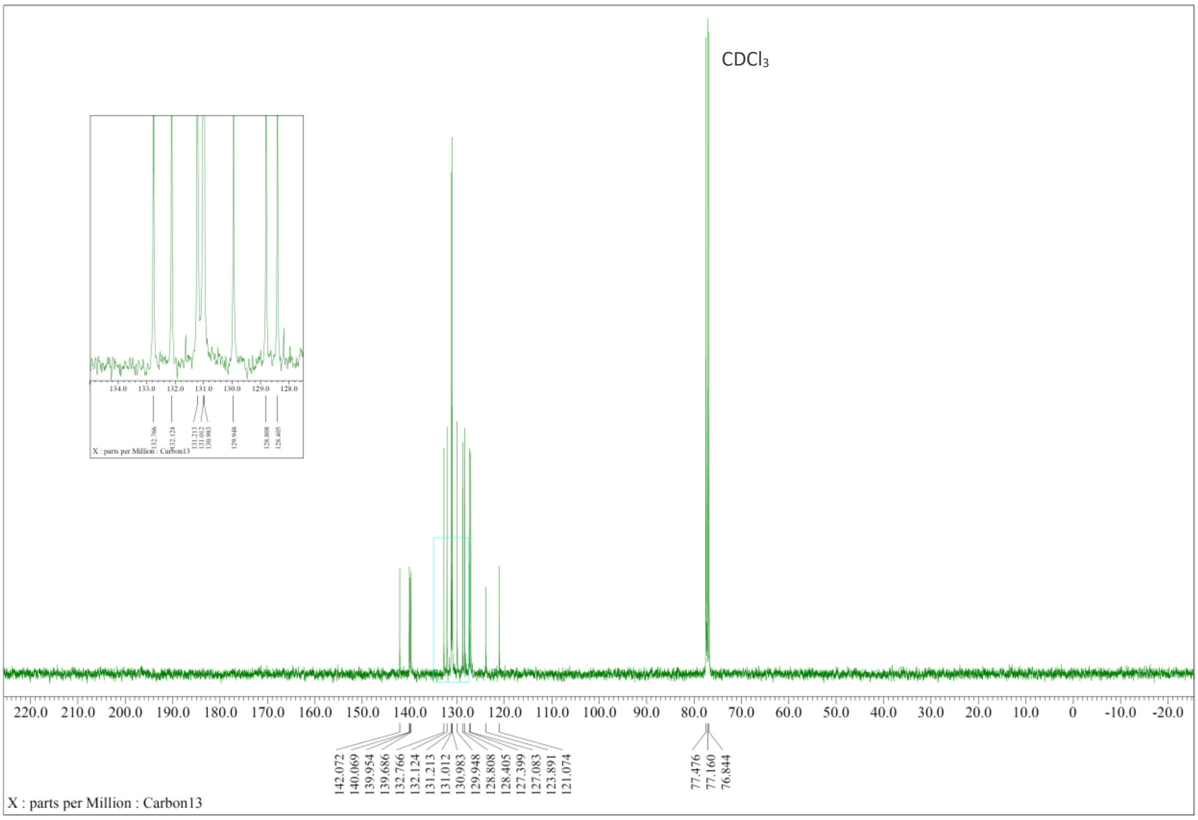
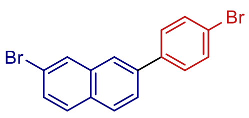


Figure S42. ^{13}C NMR (100 MHz) spectrum of **3i** in $CDCl_3$.



3j

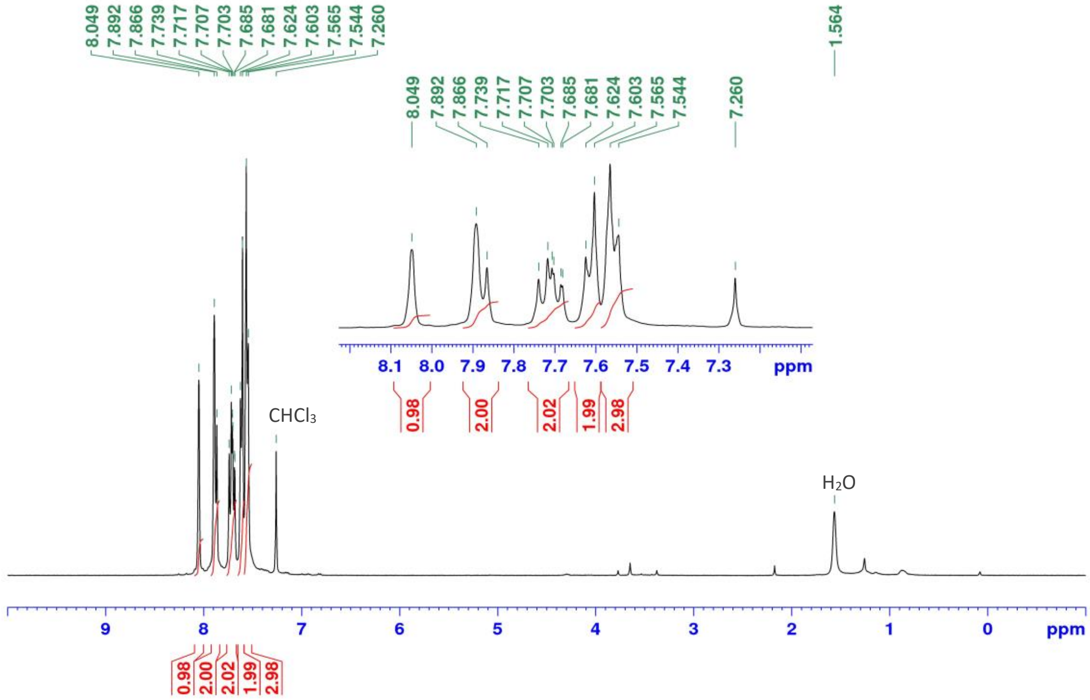
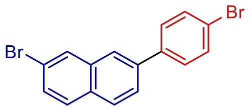


Figure S43. ^{1}H NMR (400 MHz) spectrum of **3j** in $CDCl_3$.



3j

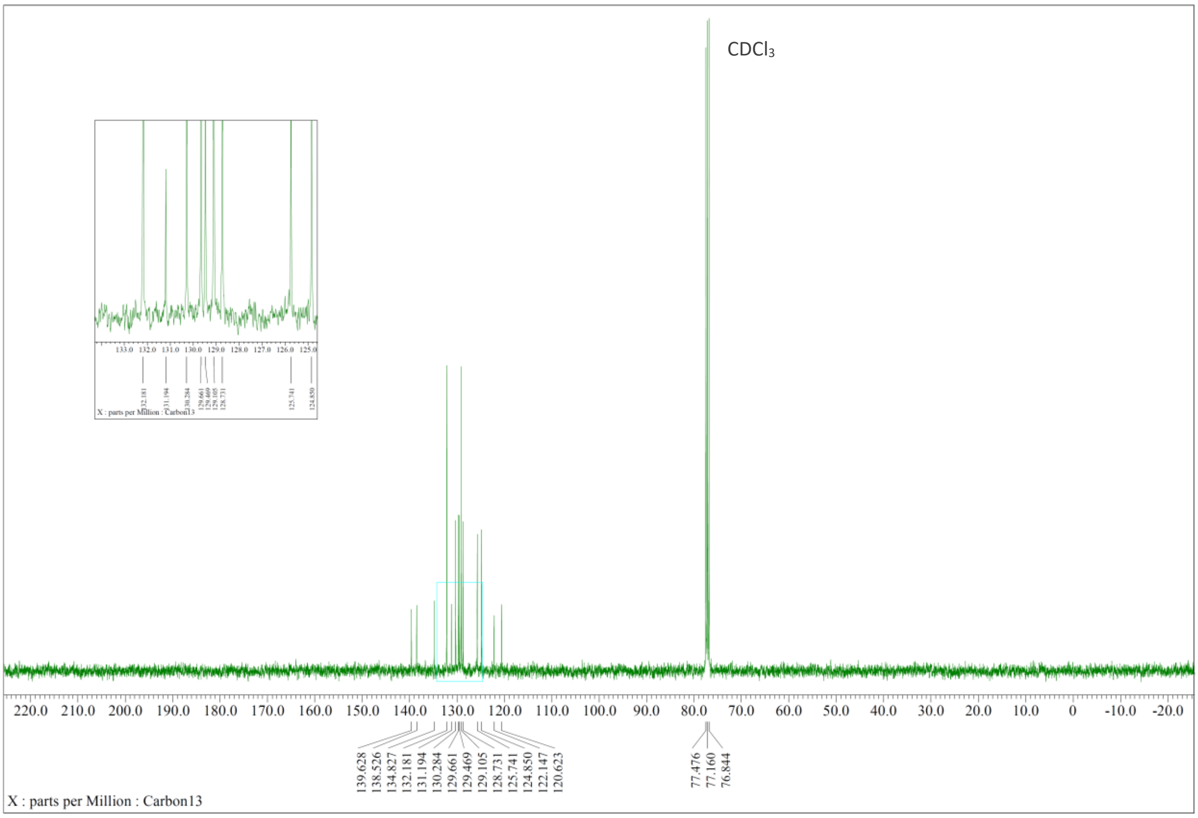
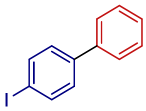


Figure S44. ^{13}C NMR (100 MHz) spectrum of **3j** in $CDCl_3$.



3k

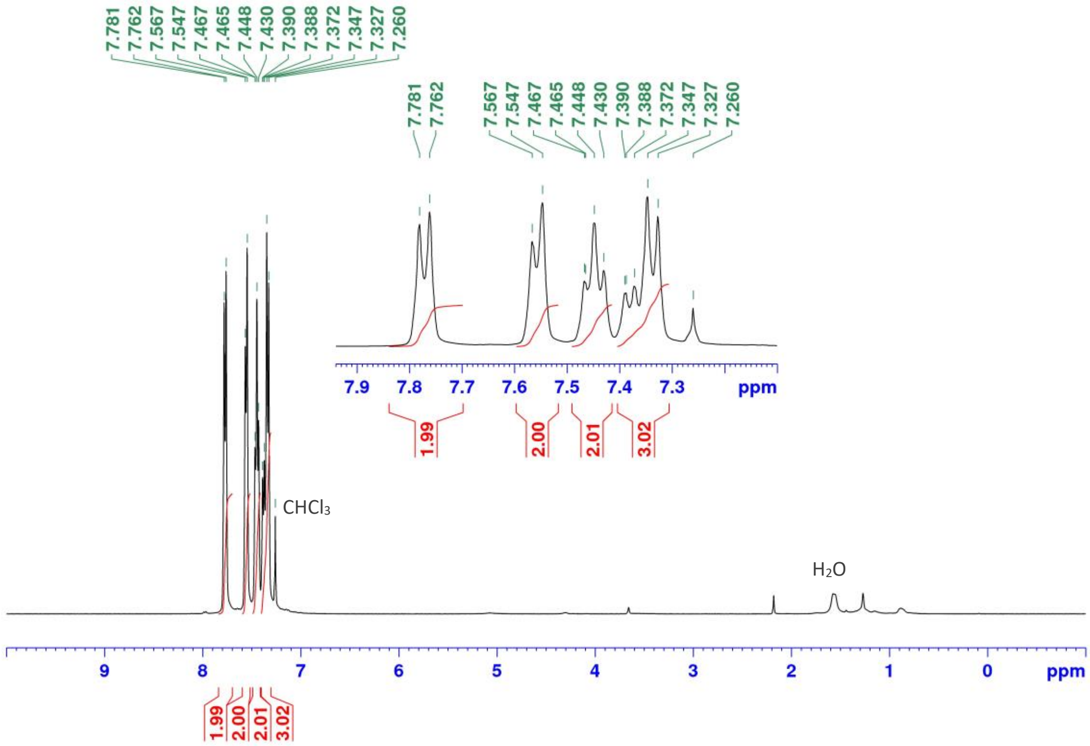
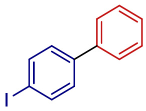


Figure S45. ^{1}H NMR (400 MHz) spectrum of **3k** in $CDCl_3$.



3k

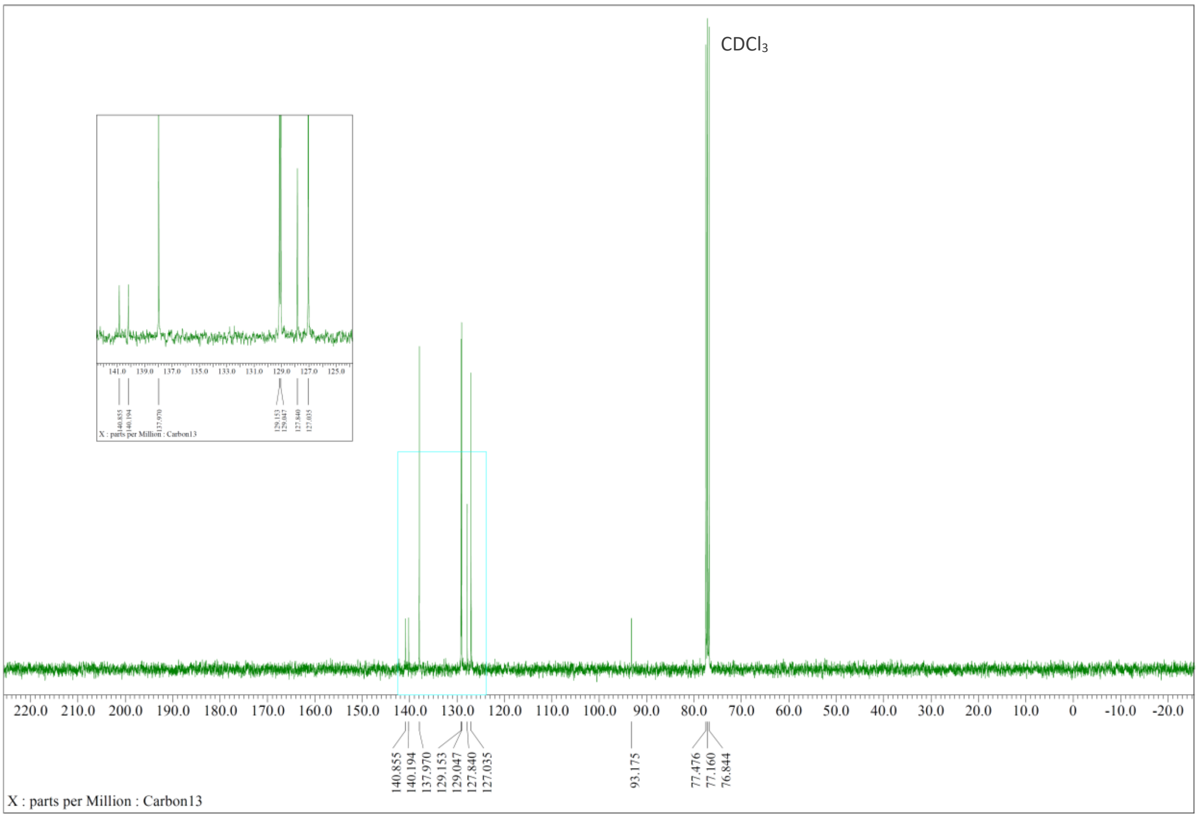
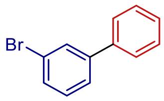


Figure S46. ^{13}C NMR (100 MHz) spectrum of **3k** in $CDCl_3$.



3l

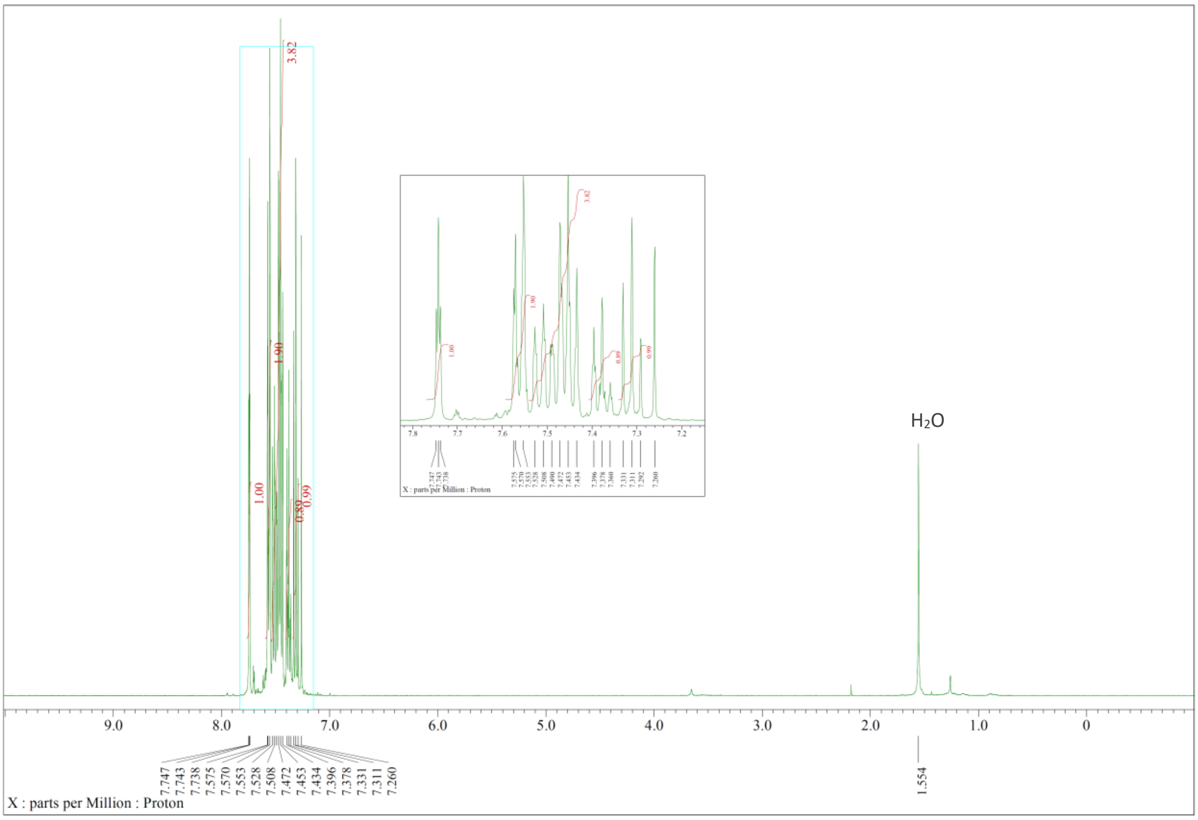
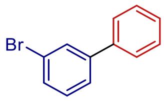


Figure S47. ^{1}H NMR (400 MHz) spectrum of **3l** in $CDCl_3$.



3l

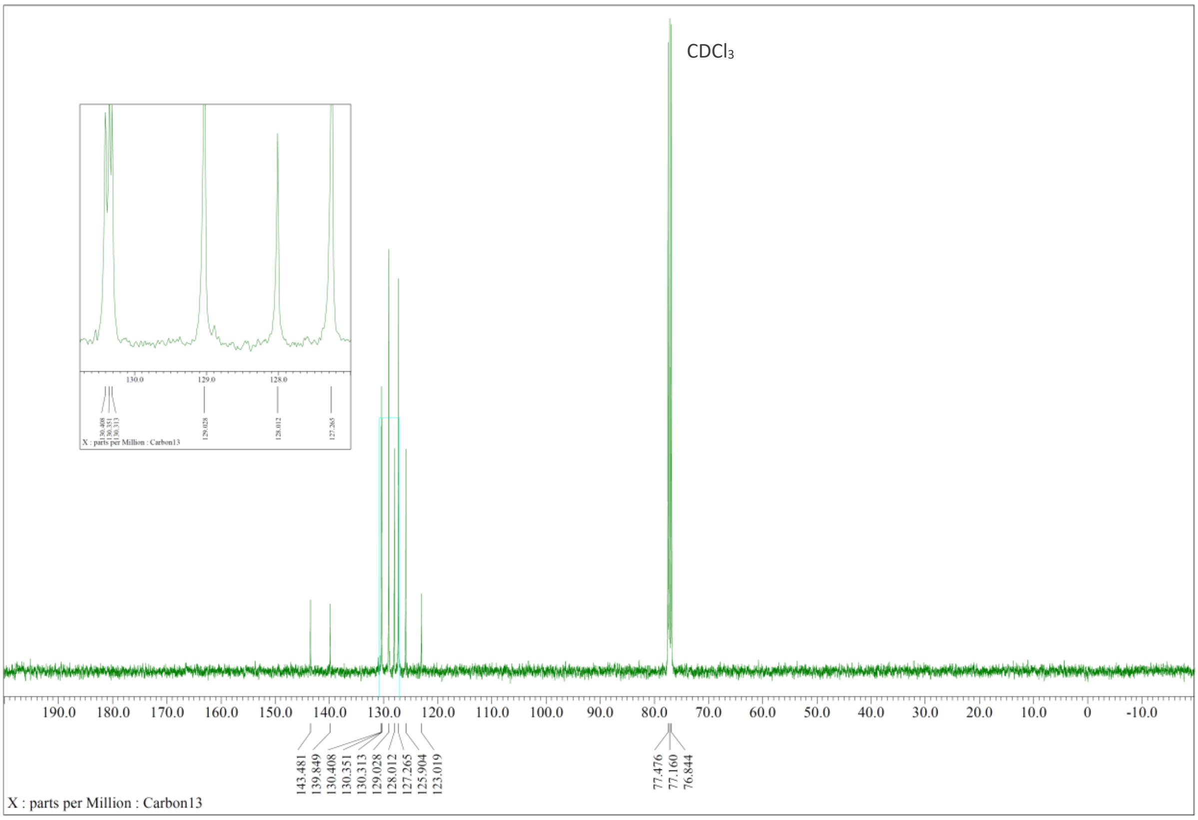
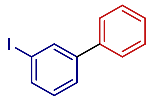


Figure S48. ^{13}C NMR (100 MHz) spectrum of **3l** in $CDCl_3$.



3m

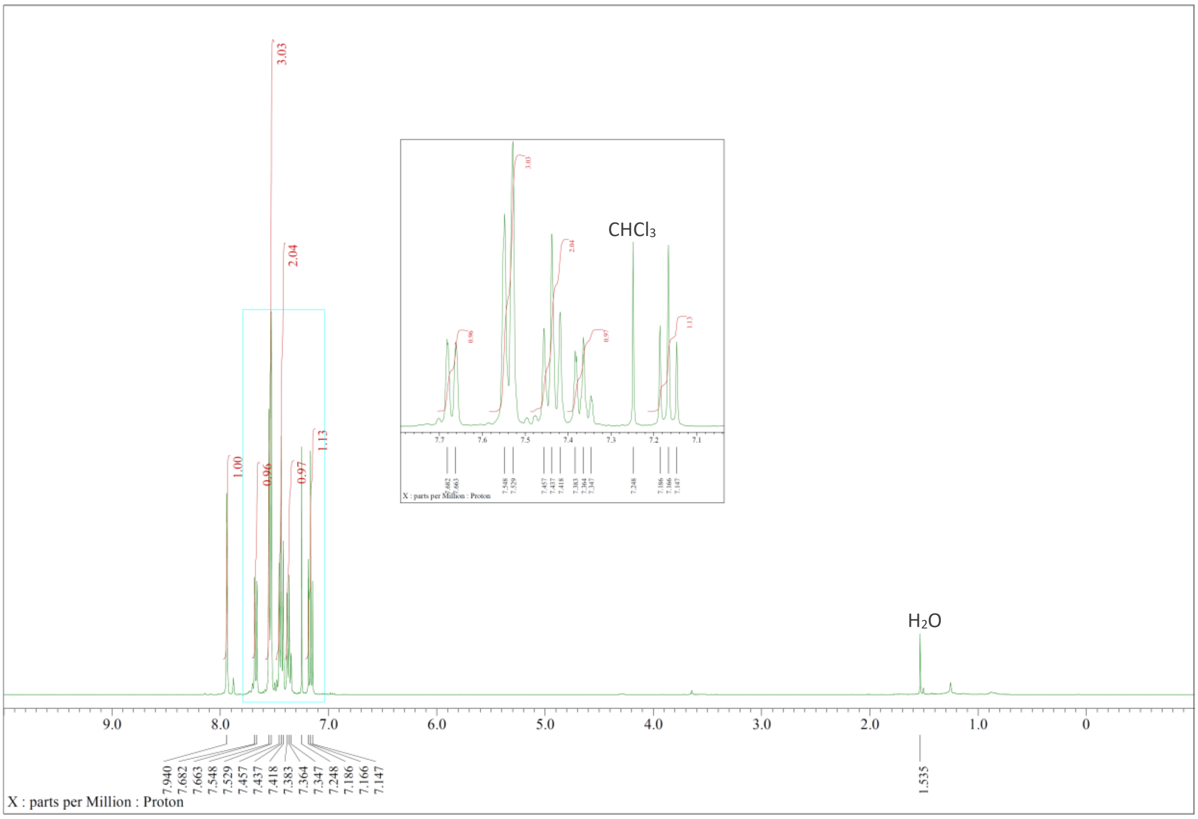
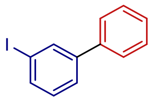


Figure S49. ^{1}H NMR (400 MHz) spectrum of **3m** in $CDCl_3$.



3m

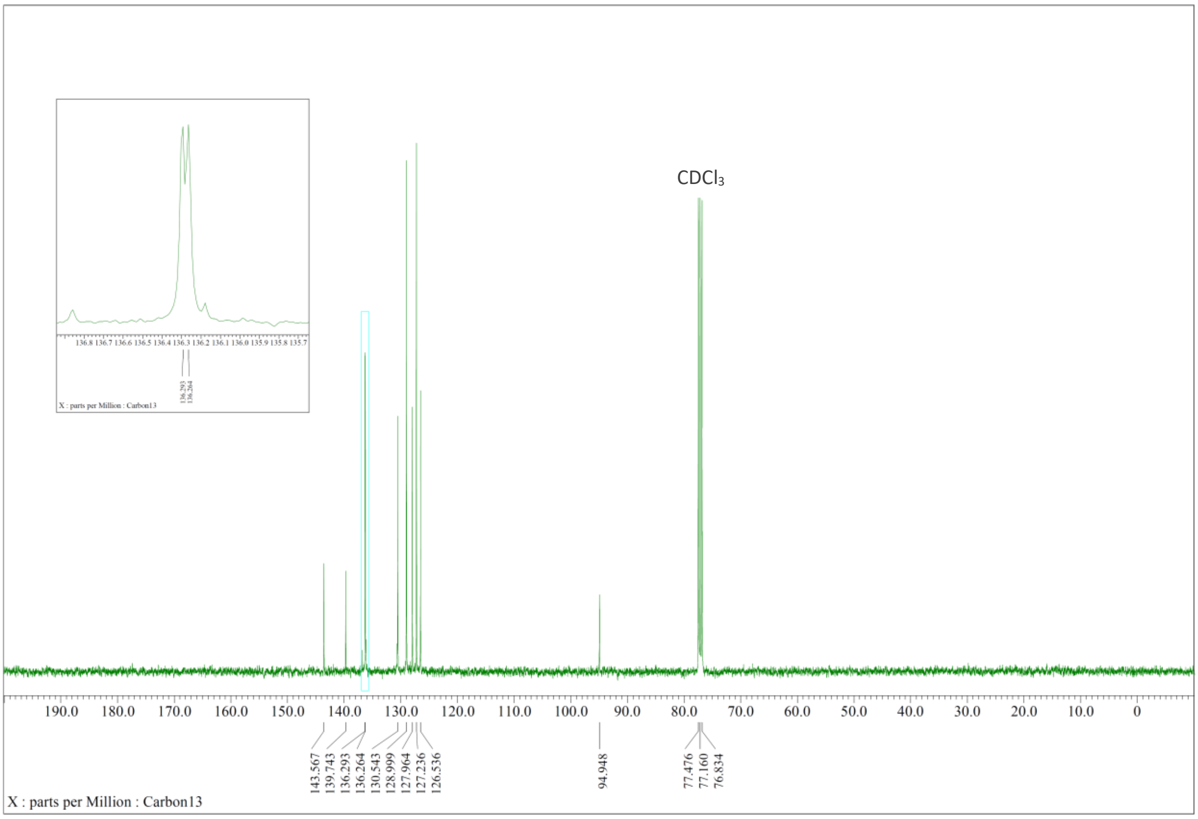
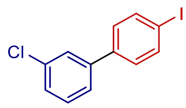


Figure S50. ^{13}C NMR (100 MHz) spectrum of **3m** in $CDCl_3$.



3n

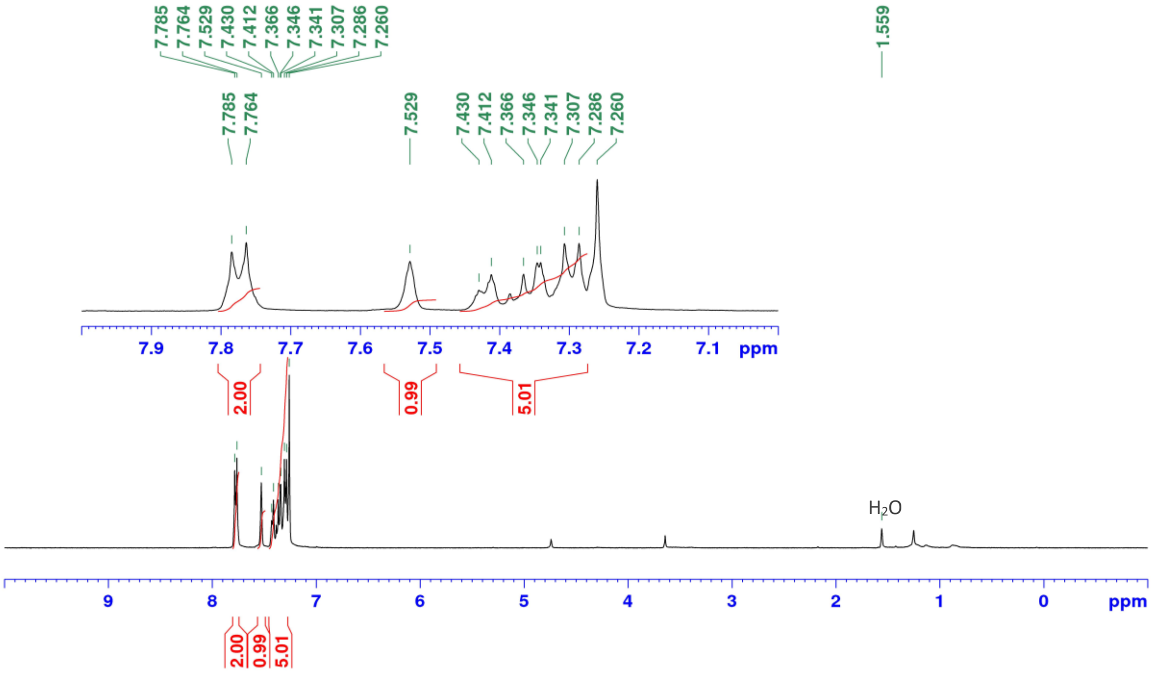
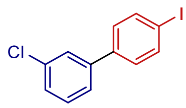


Figure S51. [1]H NMR (400 MHz) spectrum of **3n** in $CDCl_3$.



3n

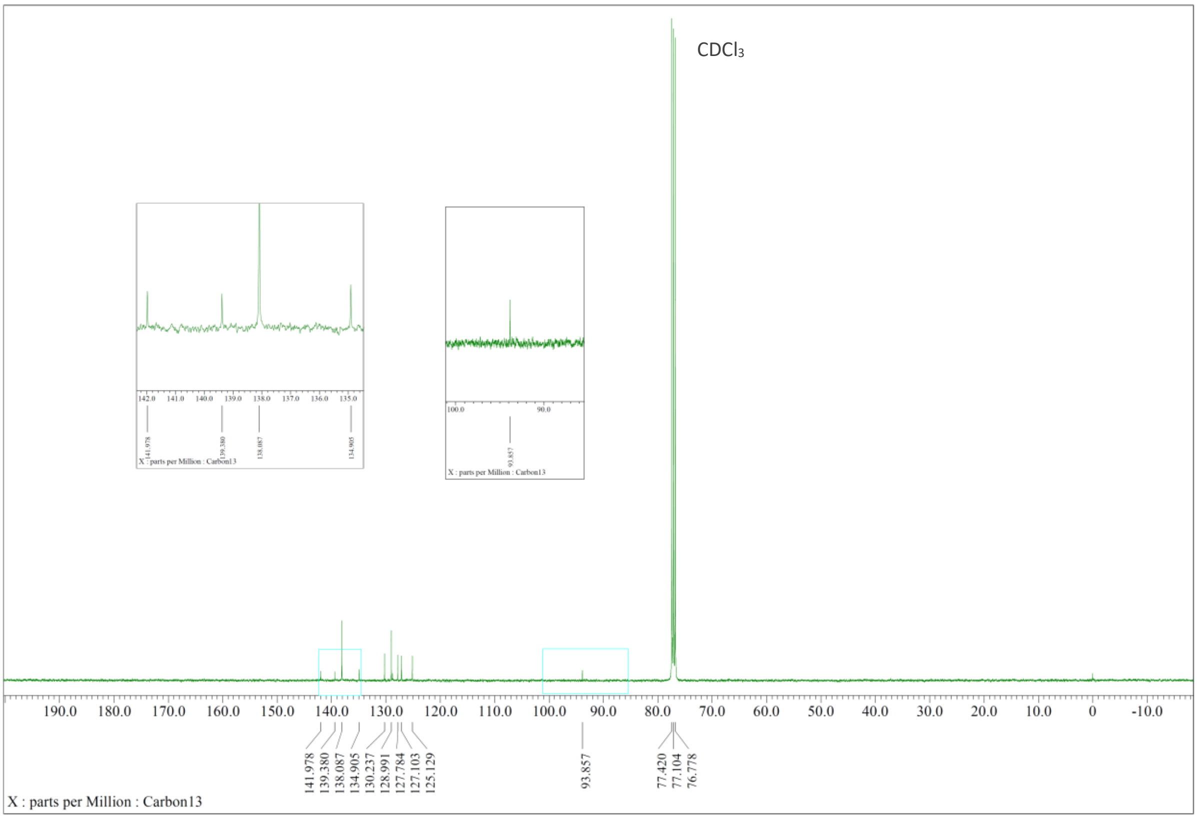
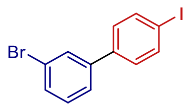


Figure S52. ^{13}C NMR (100 MHz) spectrum of **3n** in $CDCl_3$.



3o

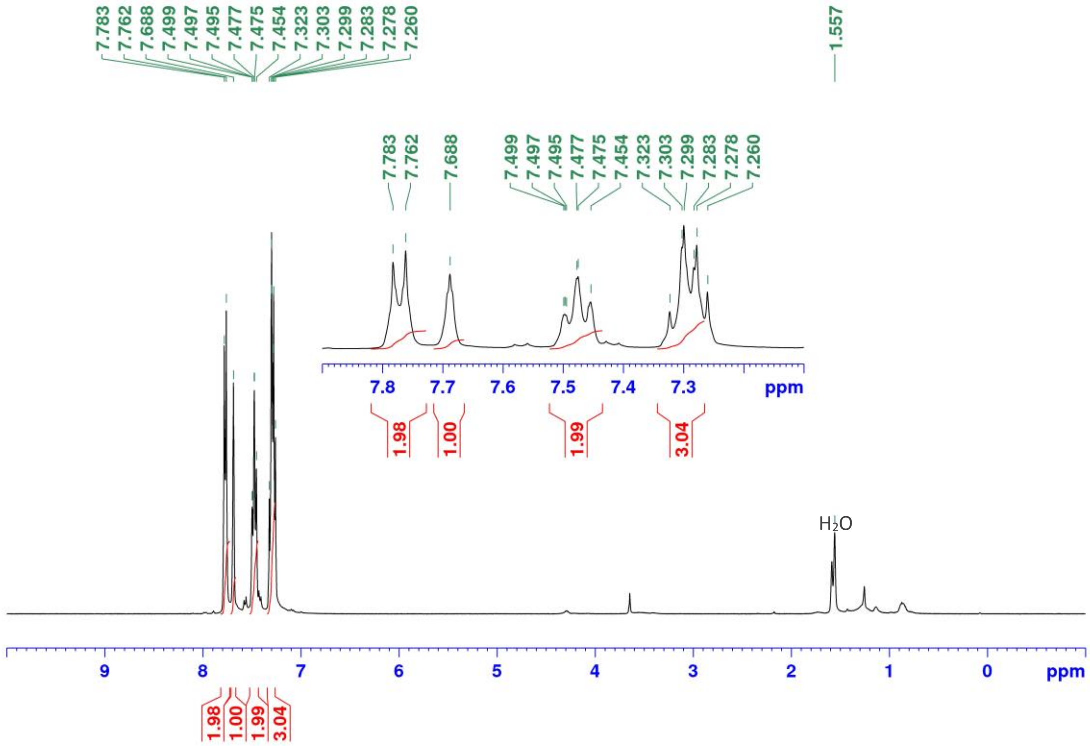
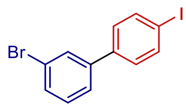


Figure S53. ^{1}H NMR (400 MHz) spectrum of **3o** in $CDCl_3$.



3o

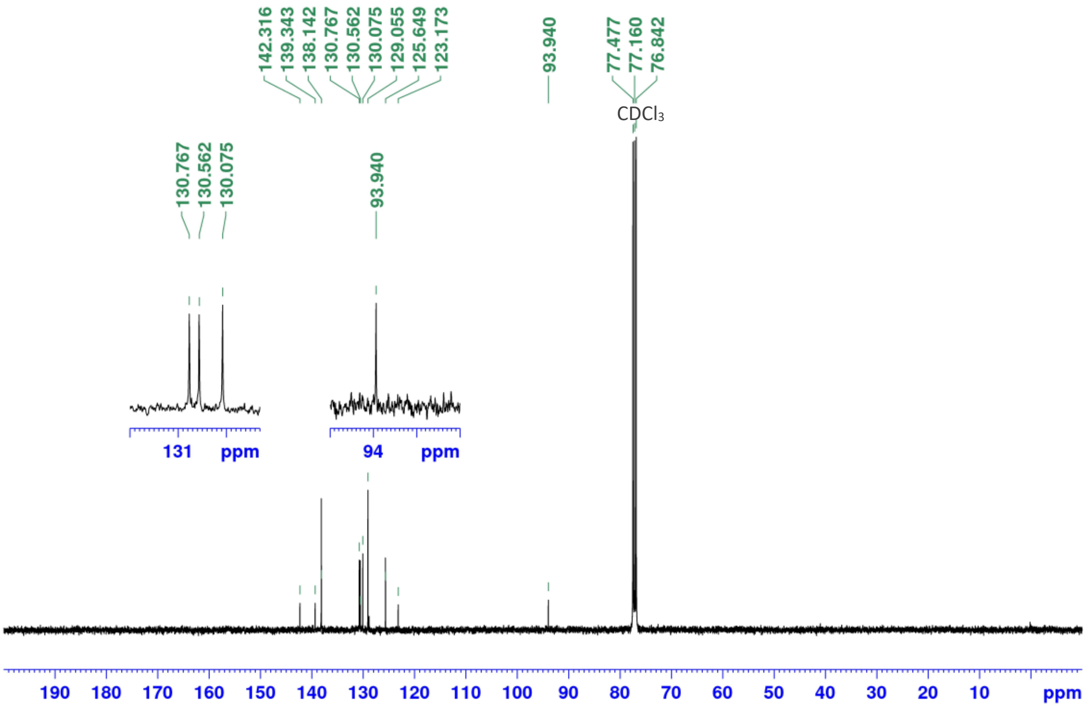
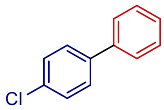


Figure S54. ^{13}C NMR (100 MHz) spectrum of **3o** in $CDCl_3$.



3p

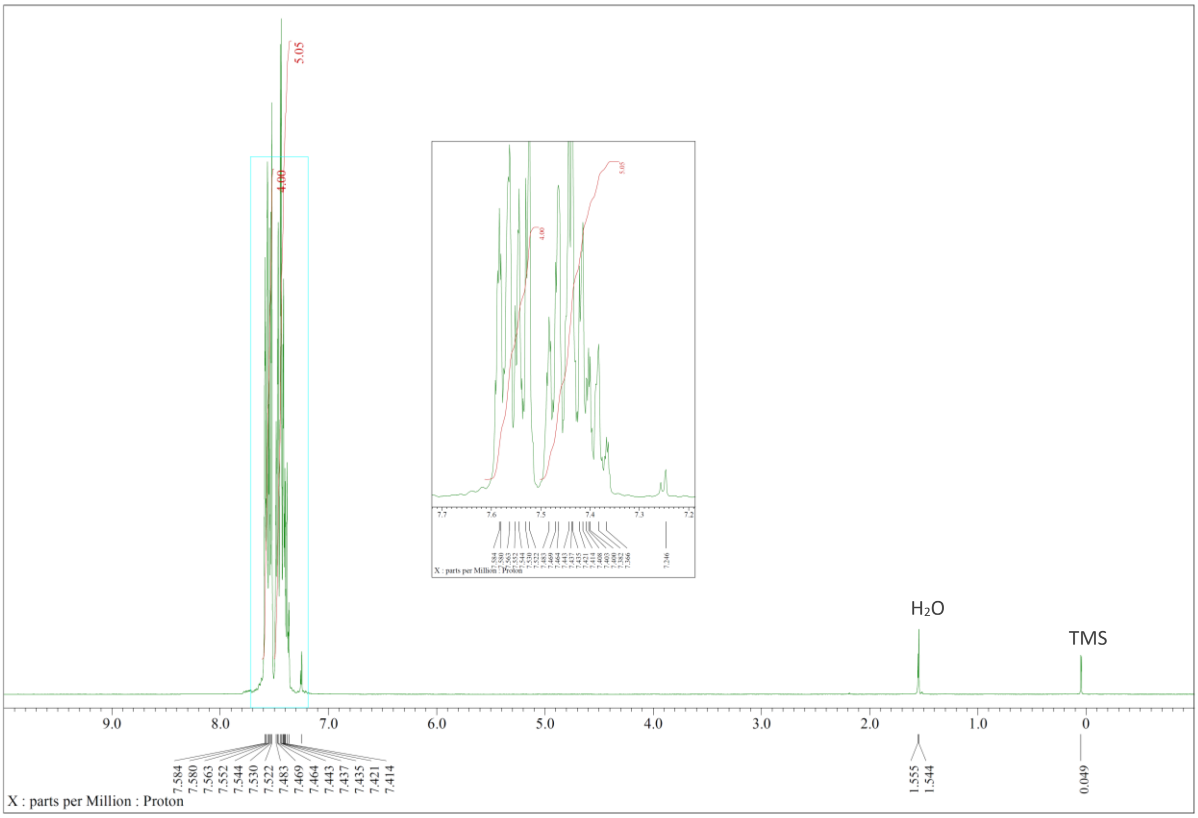
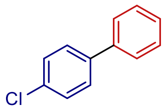


Figure S55. ^{1}H NMR (400 MHz) spectrum of **3p** in $CDCl_3$.



3p

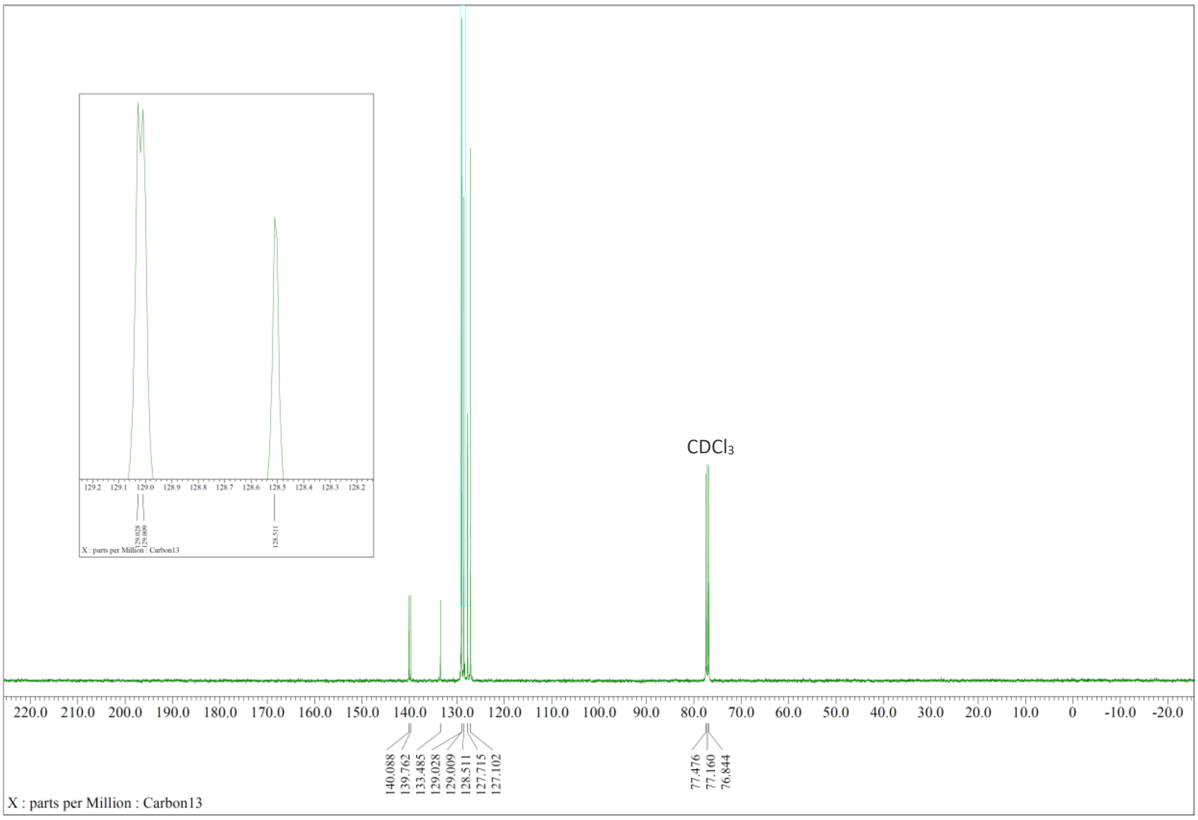
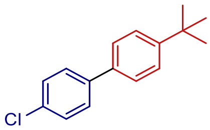


Figure S56. ^{13}C NMR (100 MHz) spectrum of **3p** in $CDCl_3$.



3q

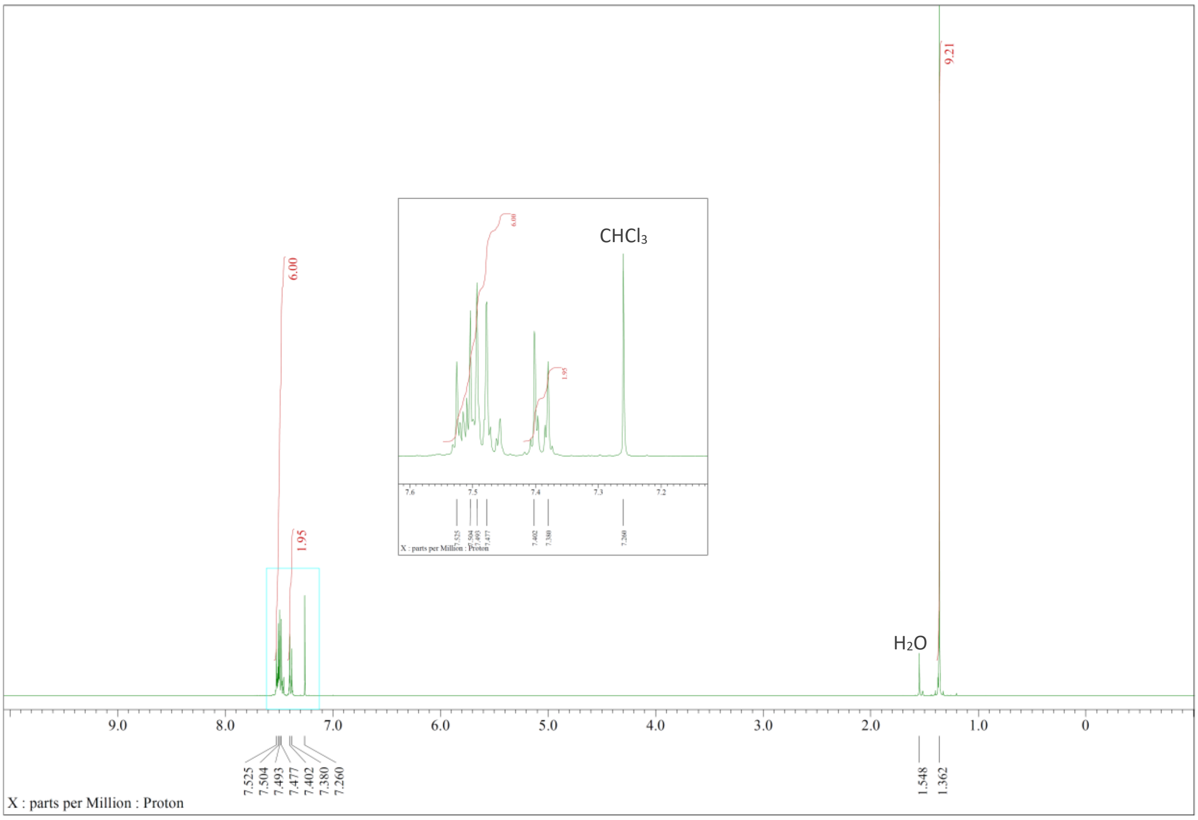
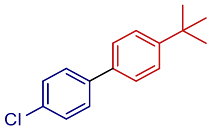


Figure S57. ^{1}H NMR (400 MHz) spectrum of **3q** in $CDCl_3$.



3q

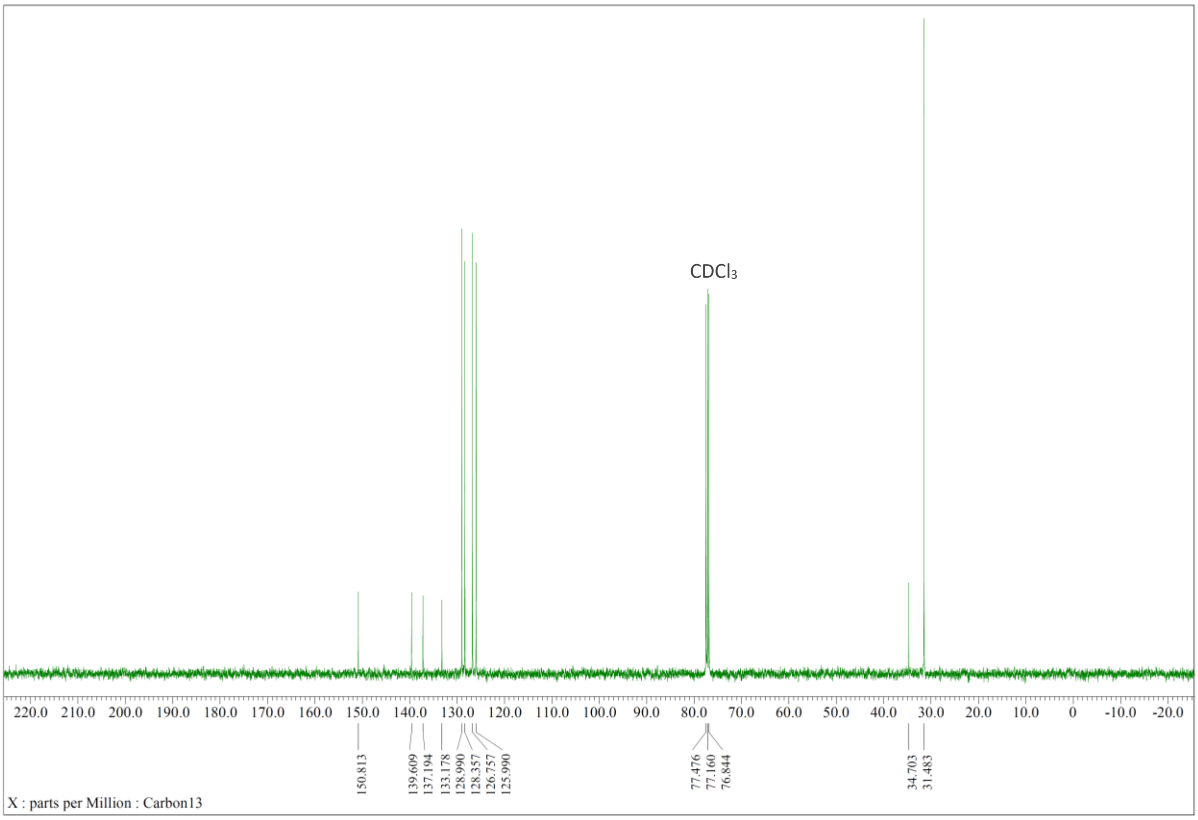
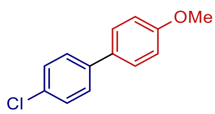


Figure S58. ^{13}C NMR (100 MHz) spectrum of **3q** in $CDCl_3$.



3r

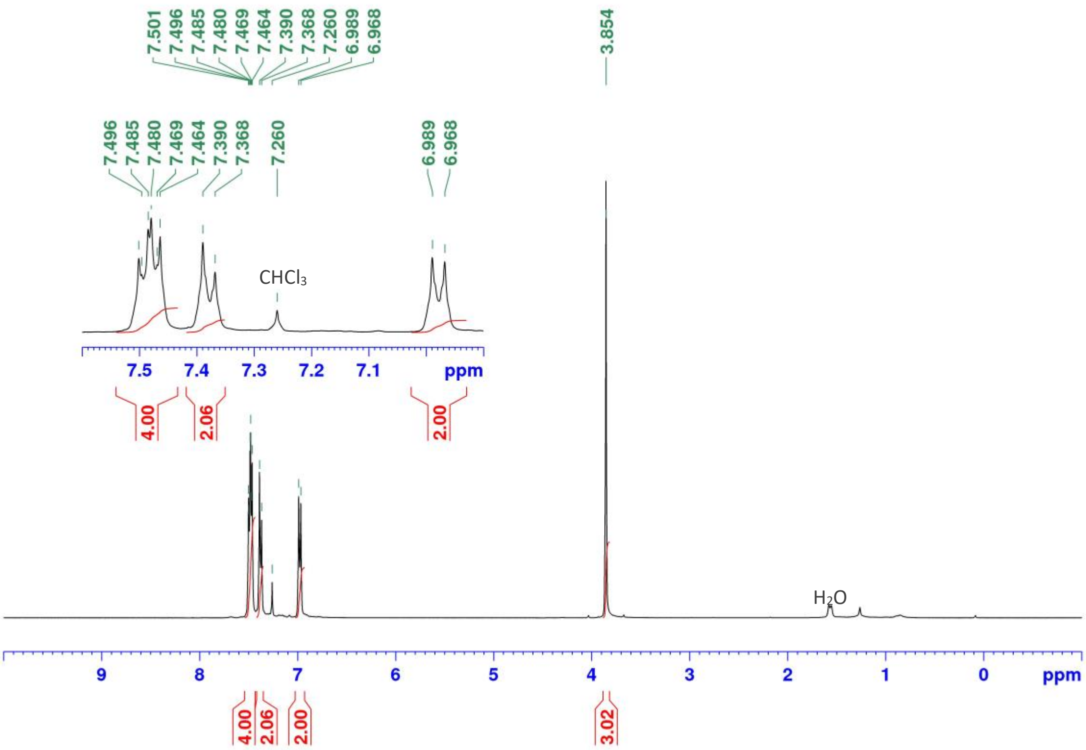
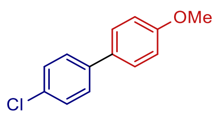


Figure S59. ^{1}H NMR (400 MHz) spectrum of **3r** in $CDCl_3$.



3r

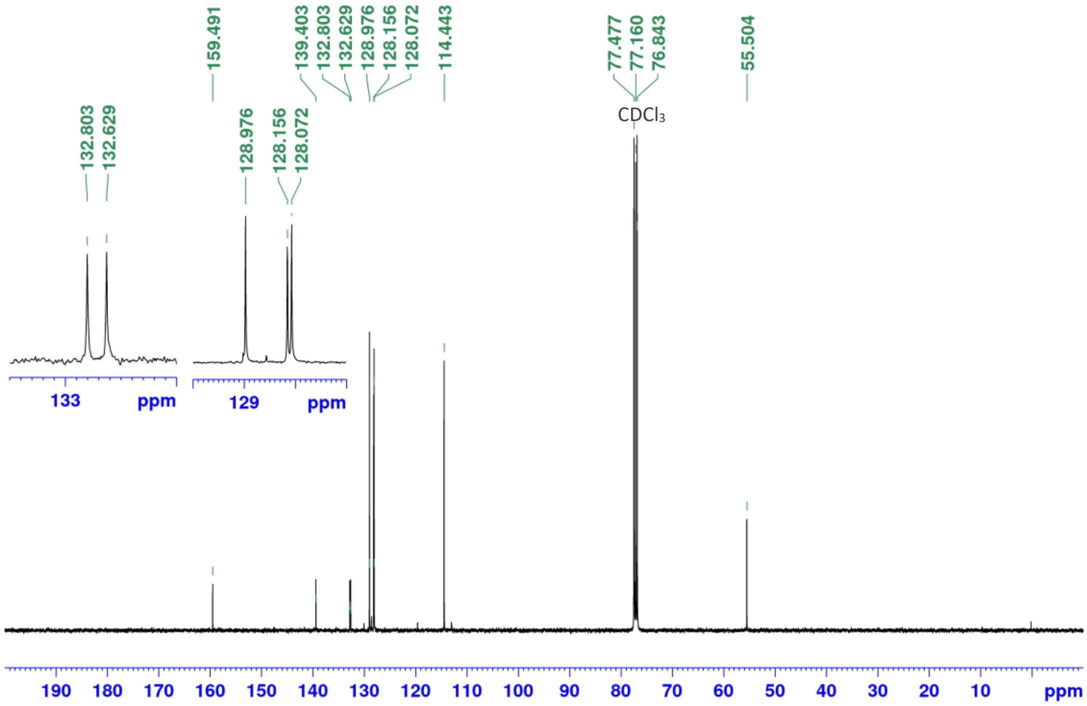
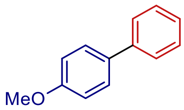


Figure S60. ^{13}C NMR (100 MHz) spectrum of **3r** in $CDCl_3$.



3s

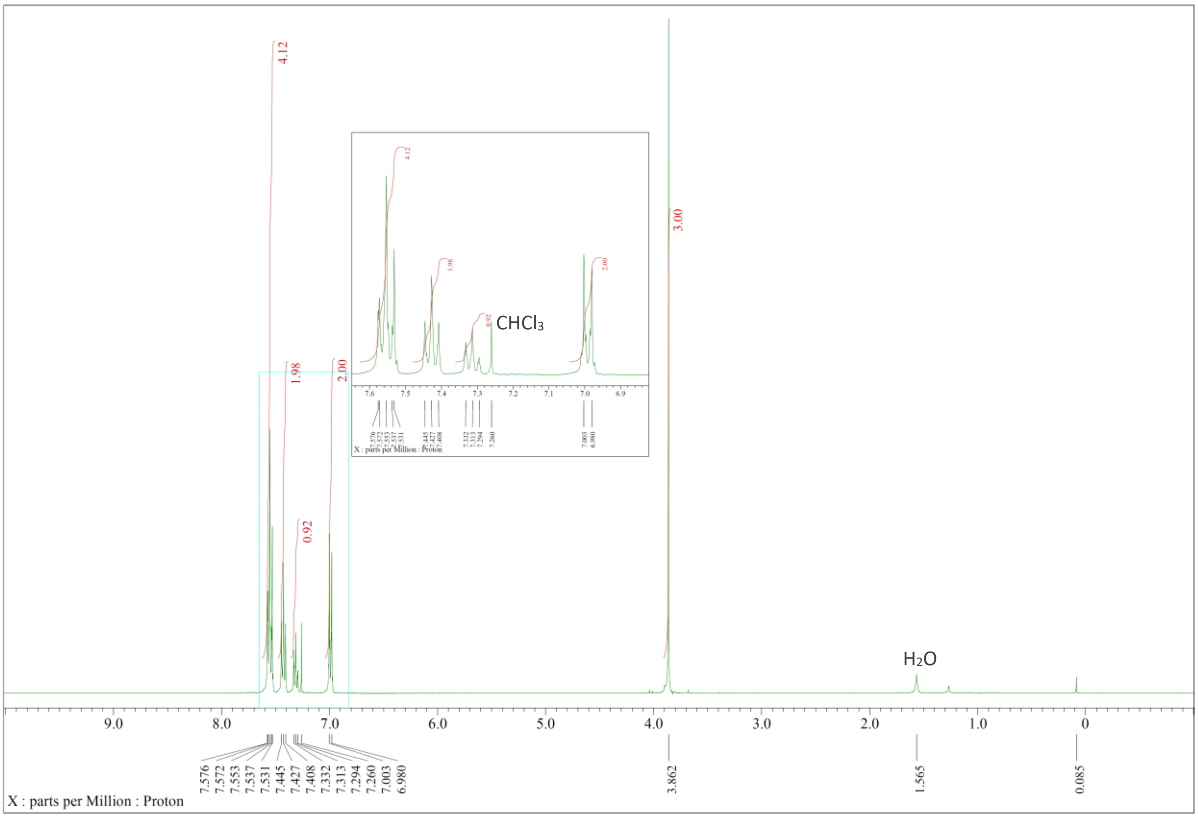
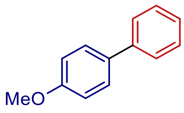


Figure S61. ^{1}H NMR (400 MHz) spectrum of **3s** in $CDCl_3$.



3s

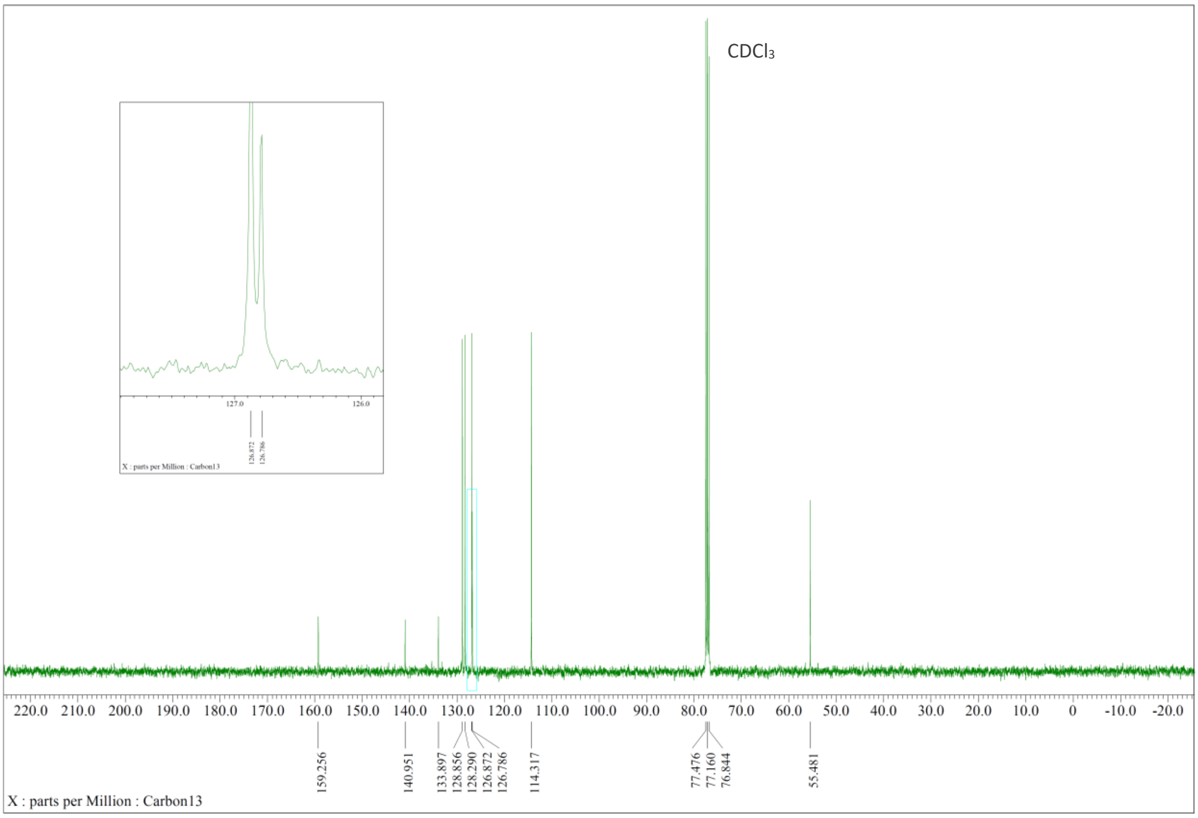
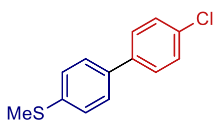


Figure S62. ^{13}C NMR (100 MHz) spectrum of **3s** in in $CDCl_3$.



3t

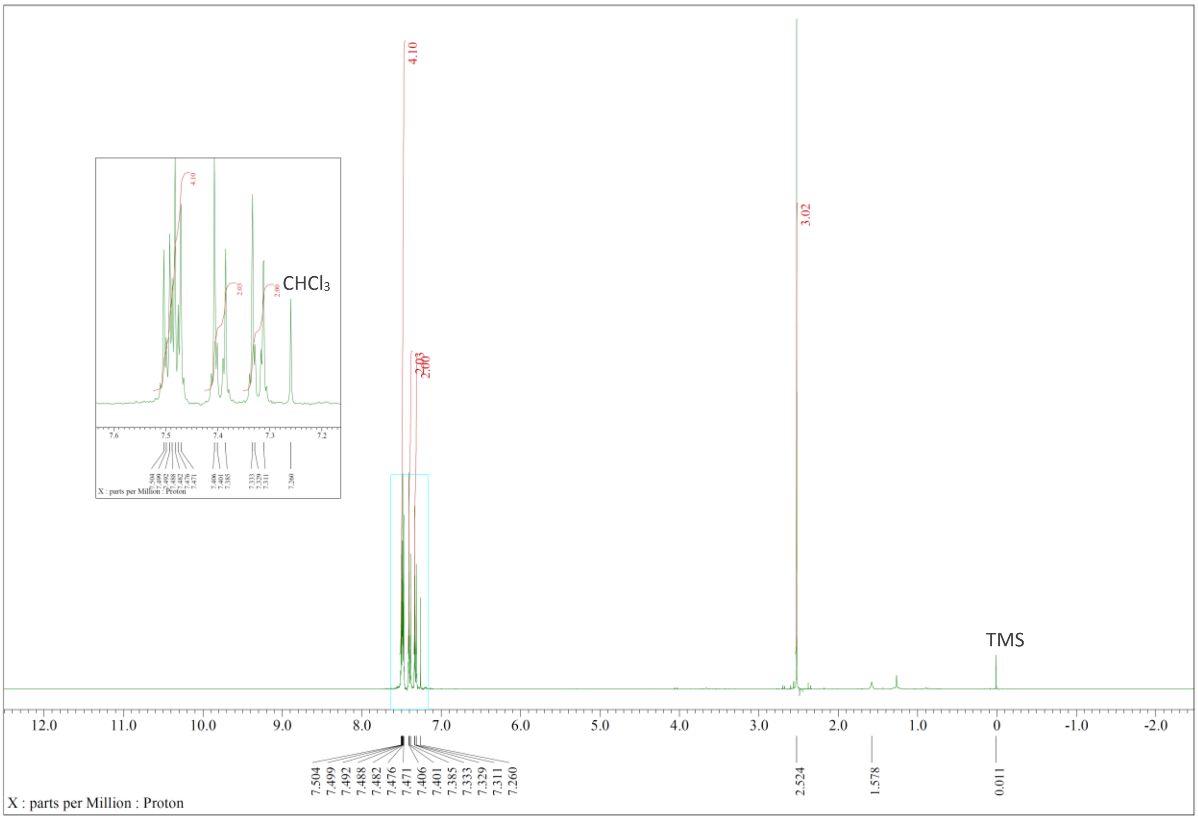
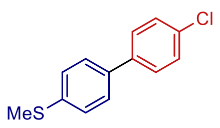


Figure S63. ^{1}H NMR (400 MHz) spectrum of **3t** in $CDCl_3$.



3t

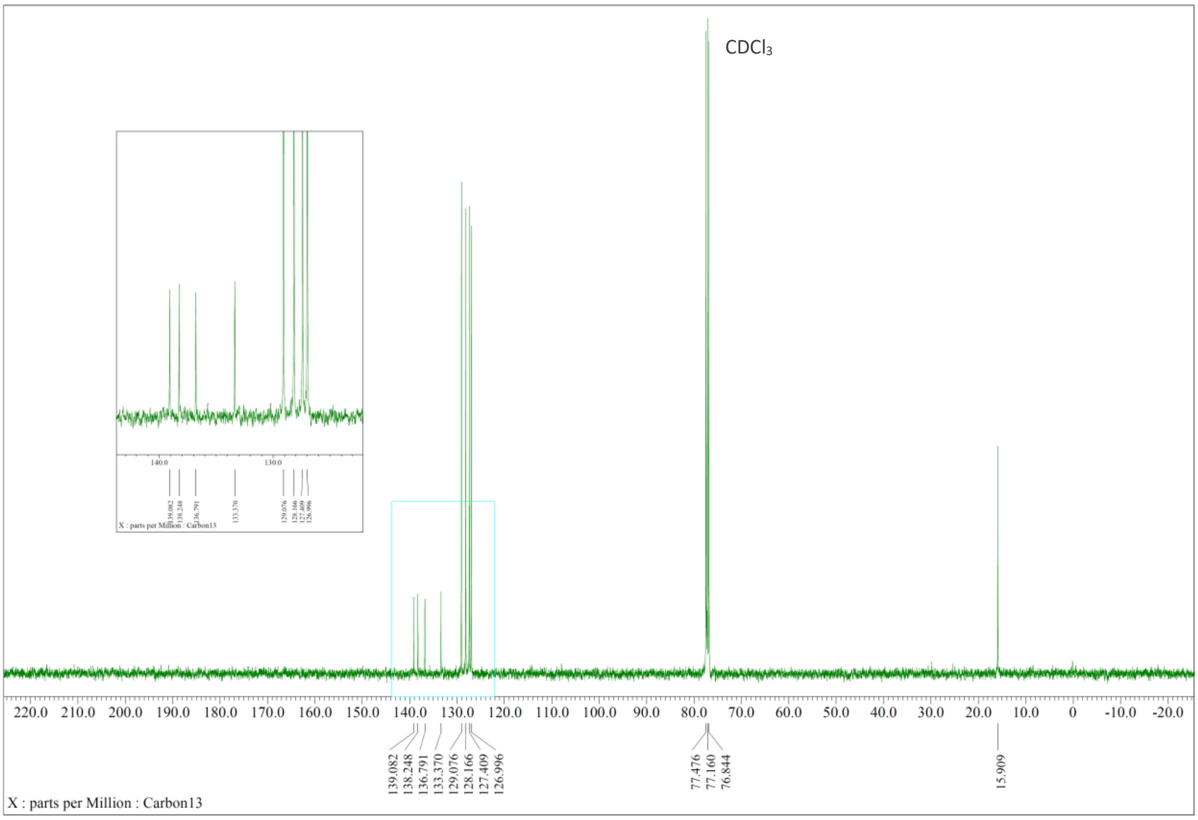
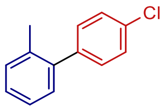


Figure S64. ^{13}C NMR (100 MHz) spectrum of **3t** in $CDCl_3$.



3u

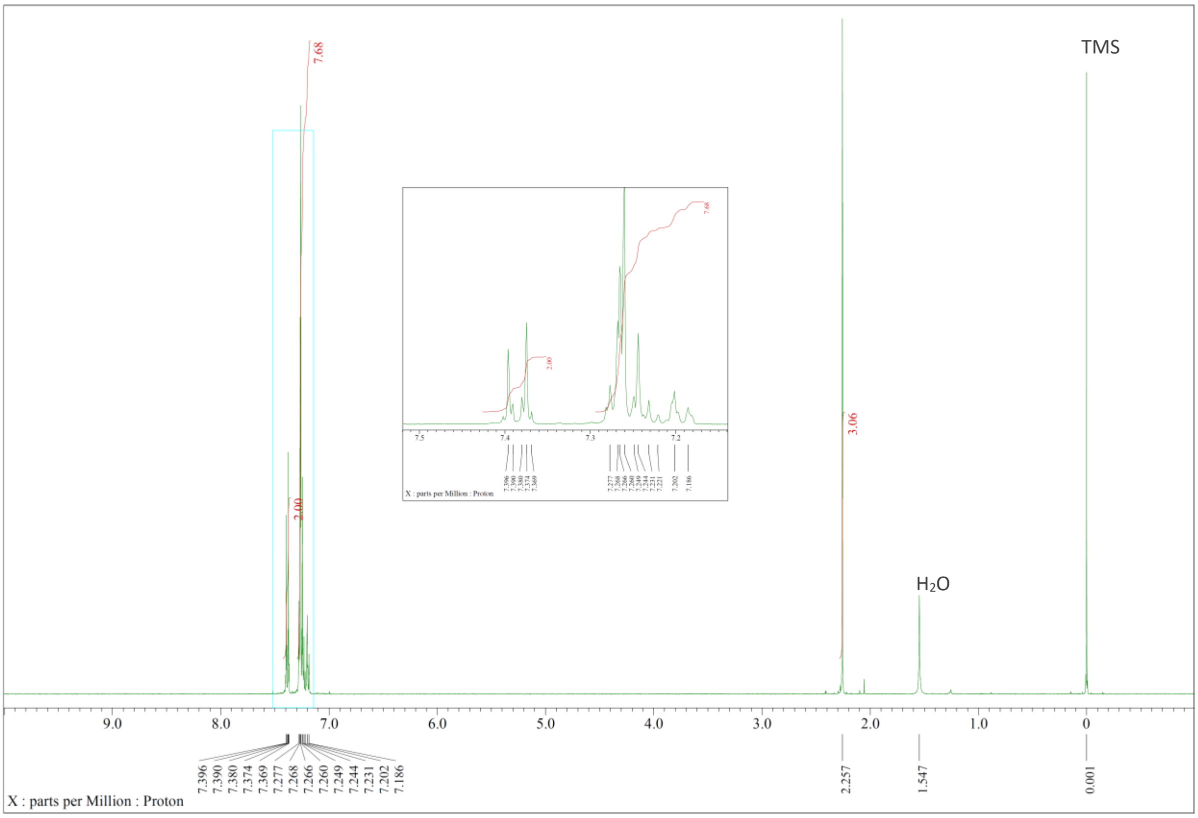
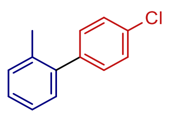


Figure S65. ^{1}H NMR (400 MHz) spectrum of **3u** in $CDCl_3$.



3u

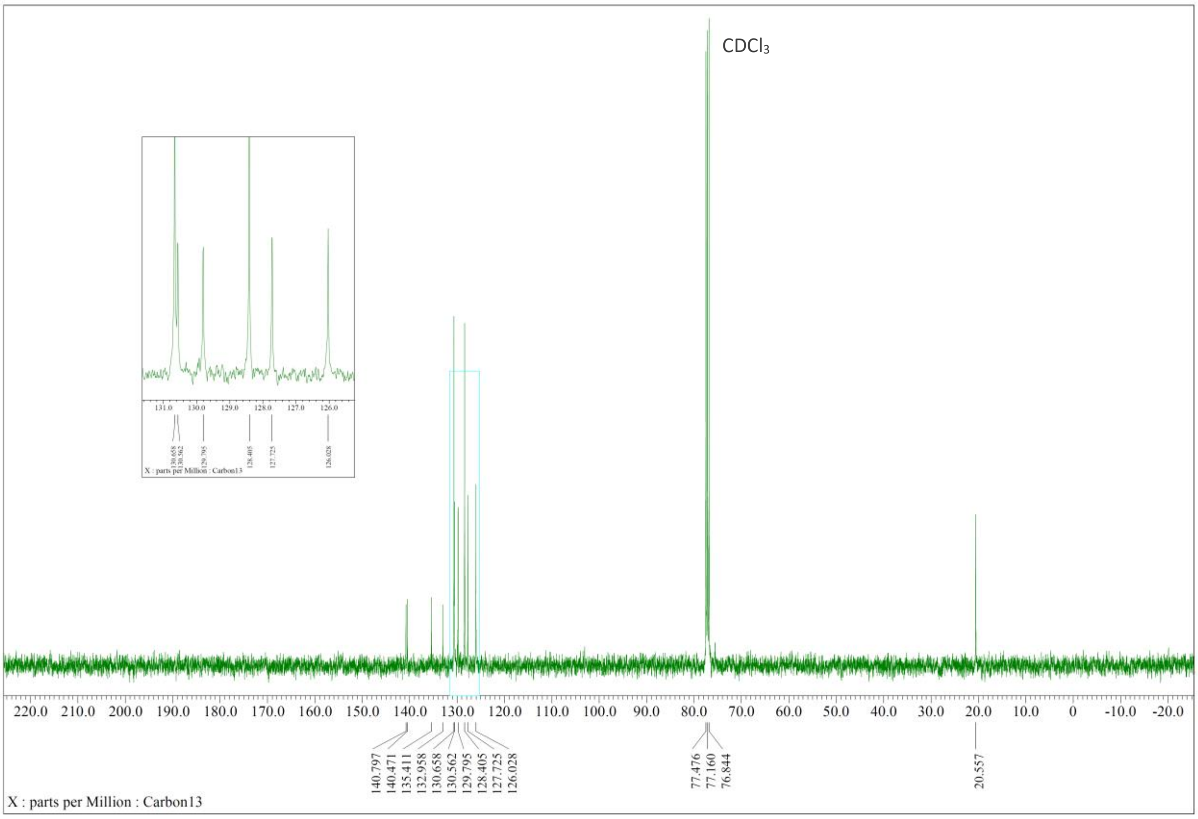
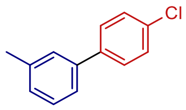


Figure S66. ^{13}C NMR (100 MHz) spectrum of **3u** in $CDCl_3$.



3v

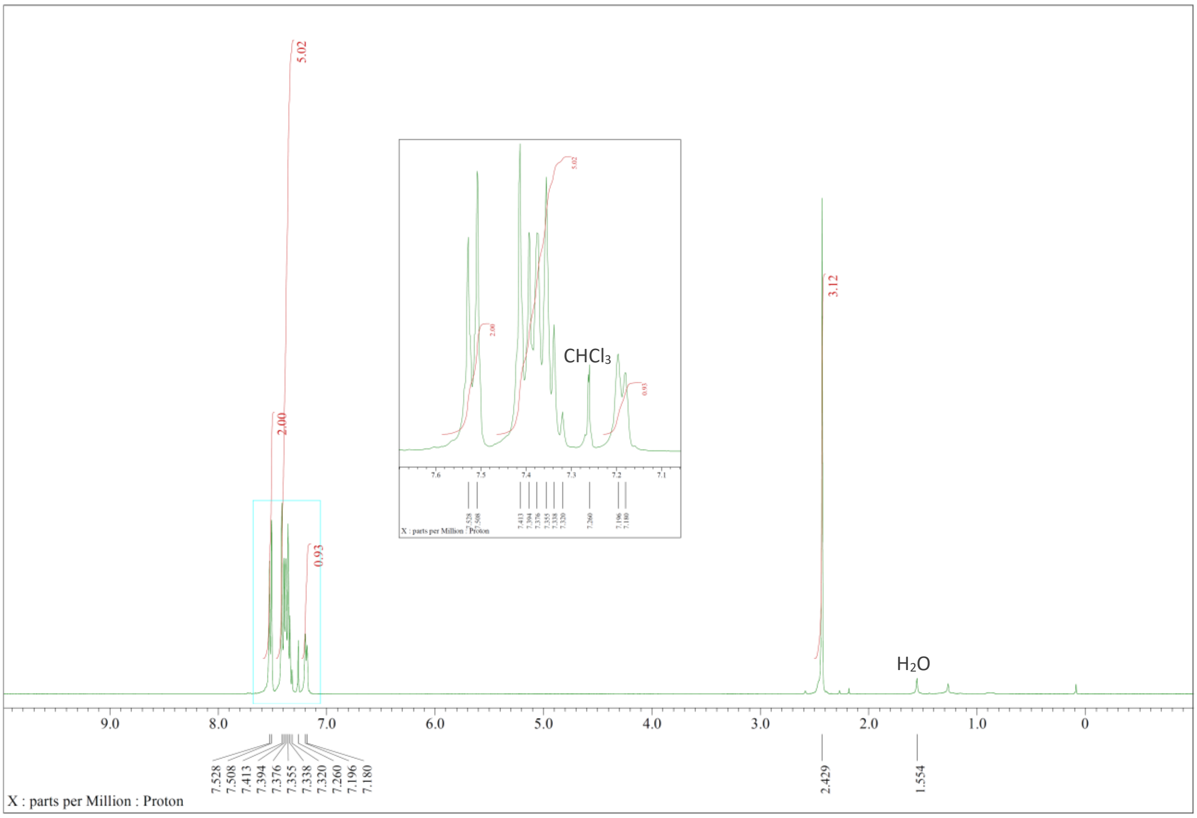
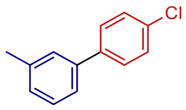


Figure S67. ^{1}H NMR (400 MHz) spectrum of **3v** in $CDCl_3$.



3v

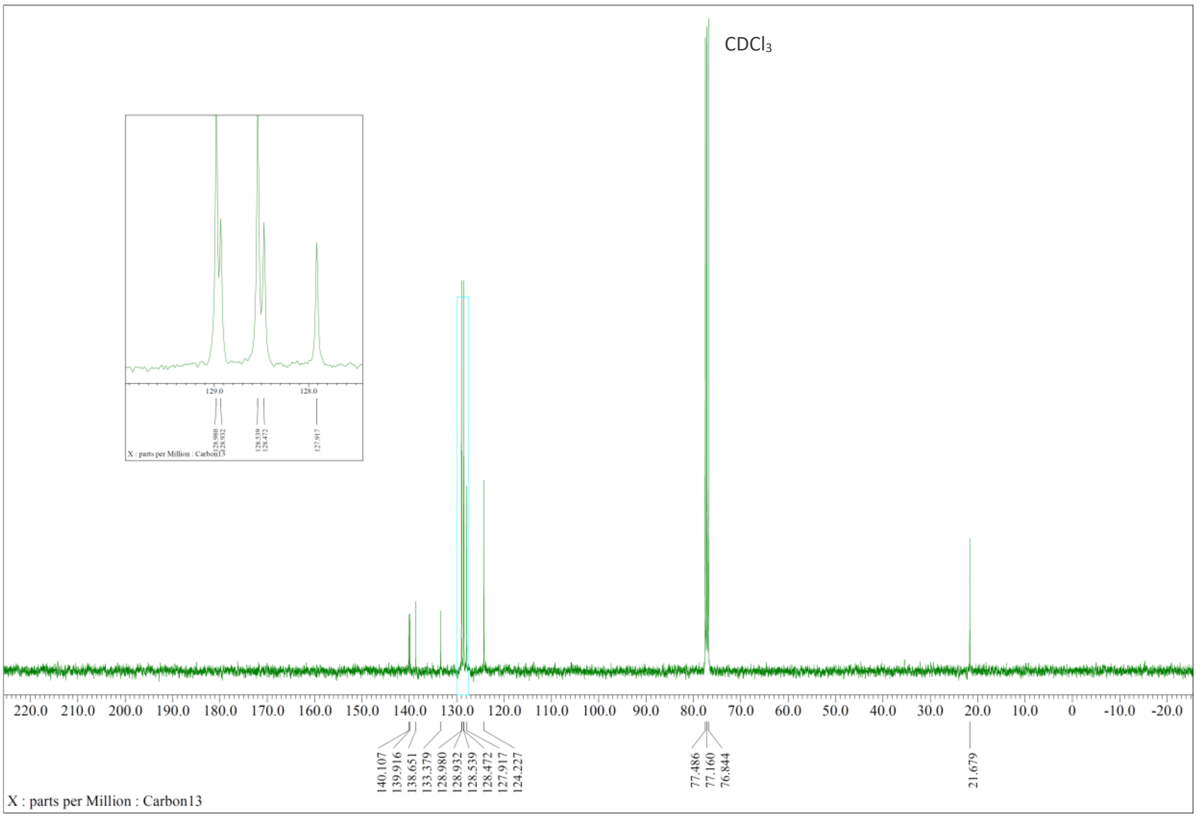
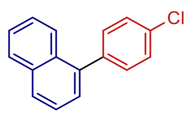


Figure S68. ^{13}C NMR (100 MHz) spectrum of **3v** in $CDCl_3$.



3w

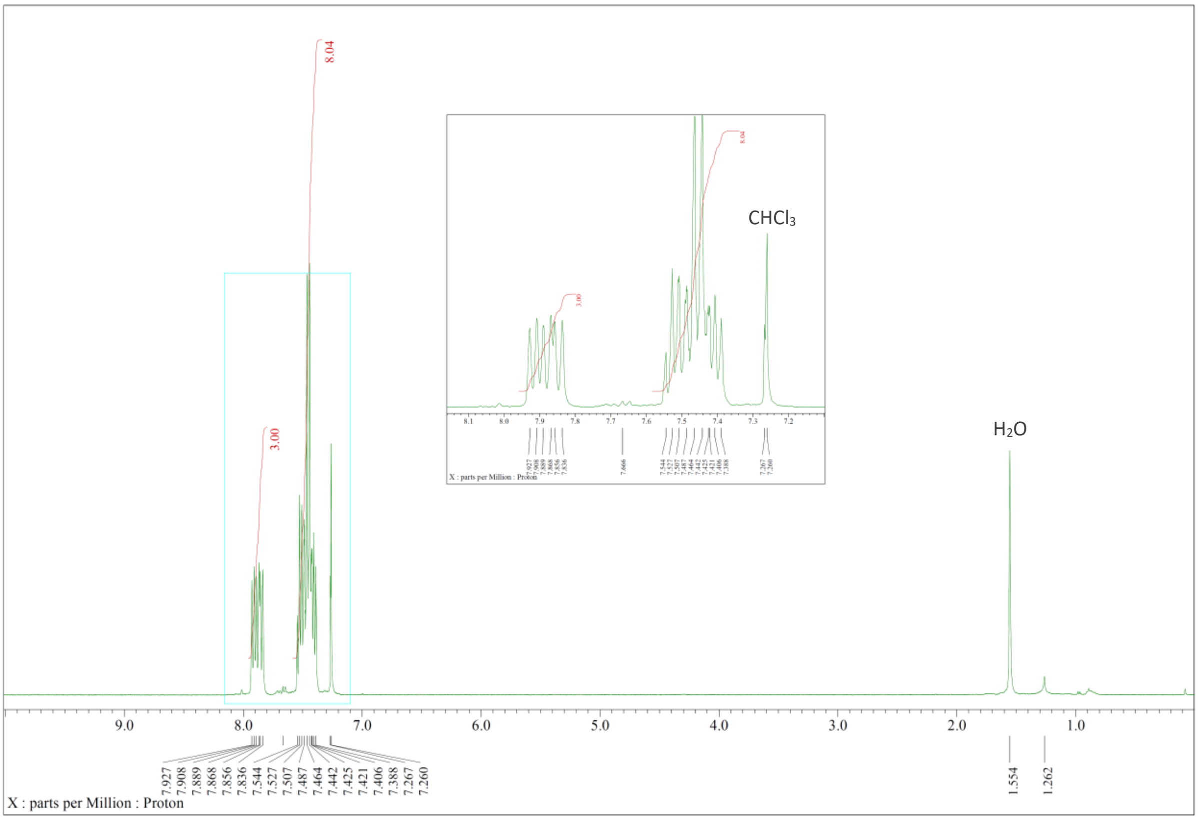
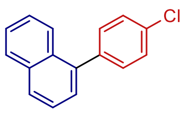


Figure S69. ^{1}H NMR (400 MHz) spectrum of **3w** in $CDCl_3$.



3w

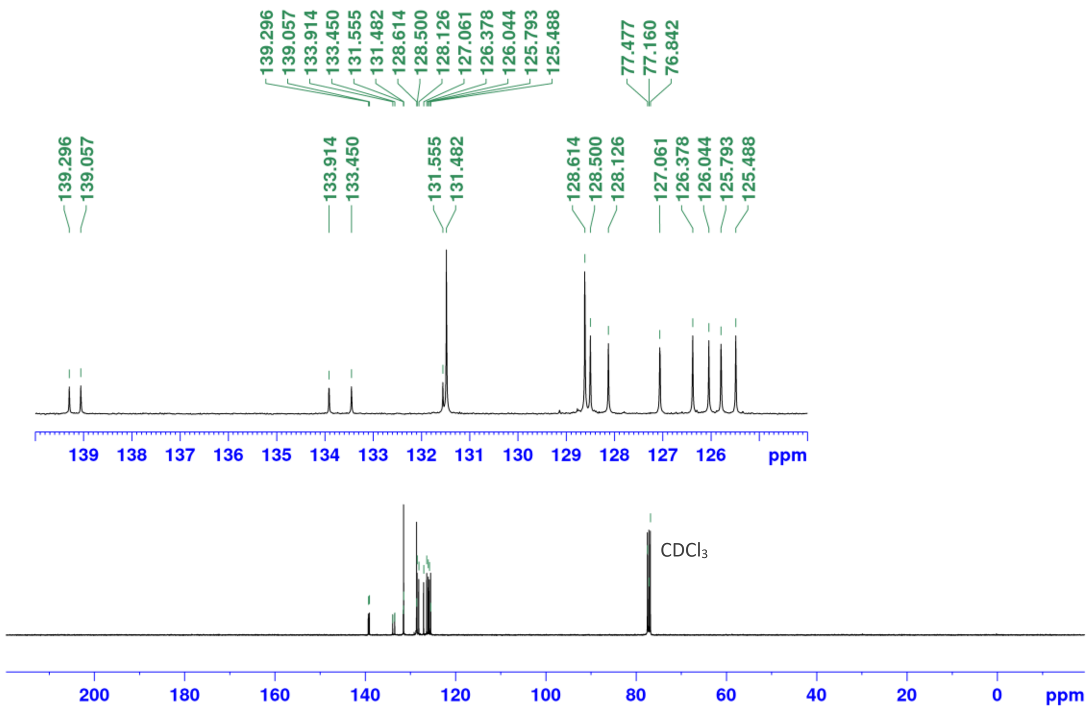
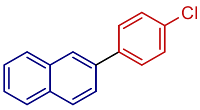


Figure S70. ^{13}C NMR (100 MHz) spectrum of **3w** in $CDCl_3$.



3x

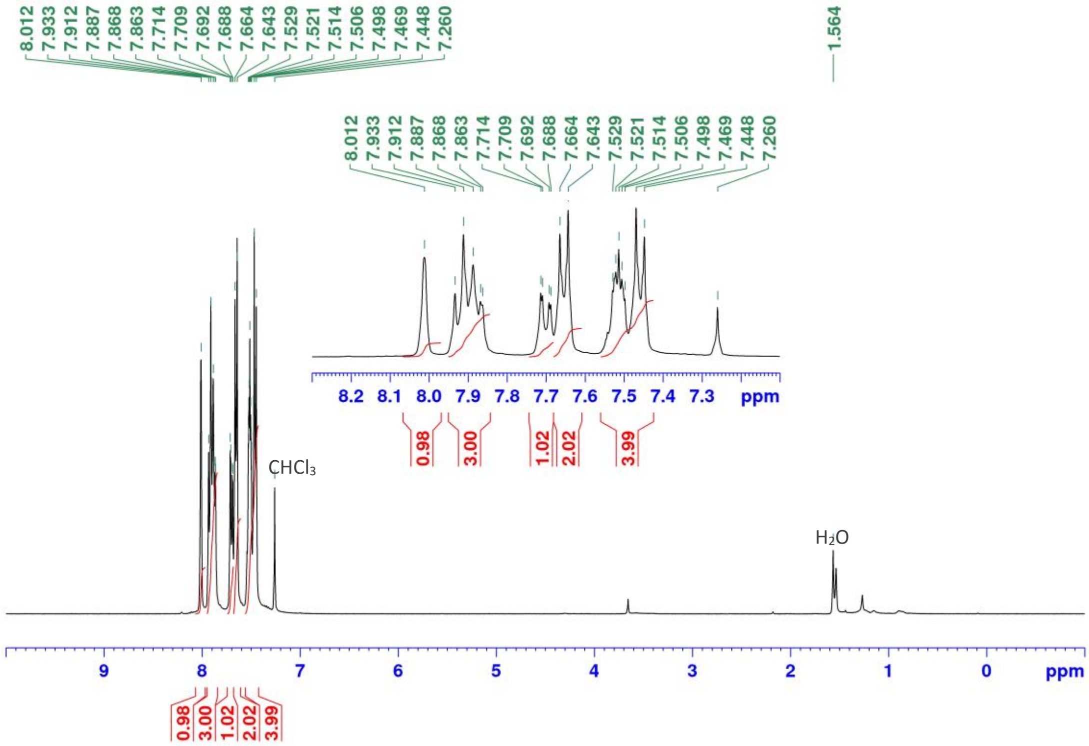
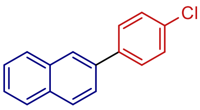


Figure S71. ^{1}H NMR (400 MHz) spectrum of **3x** in $CDCl_3$.



3x

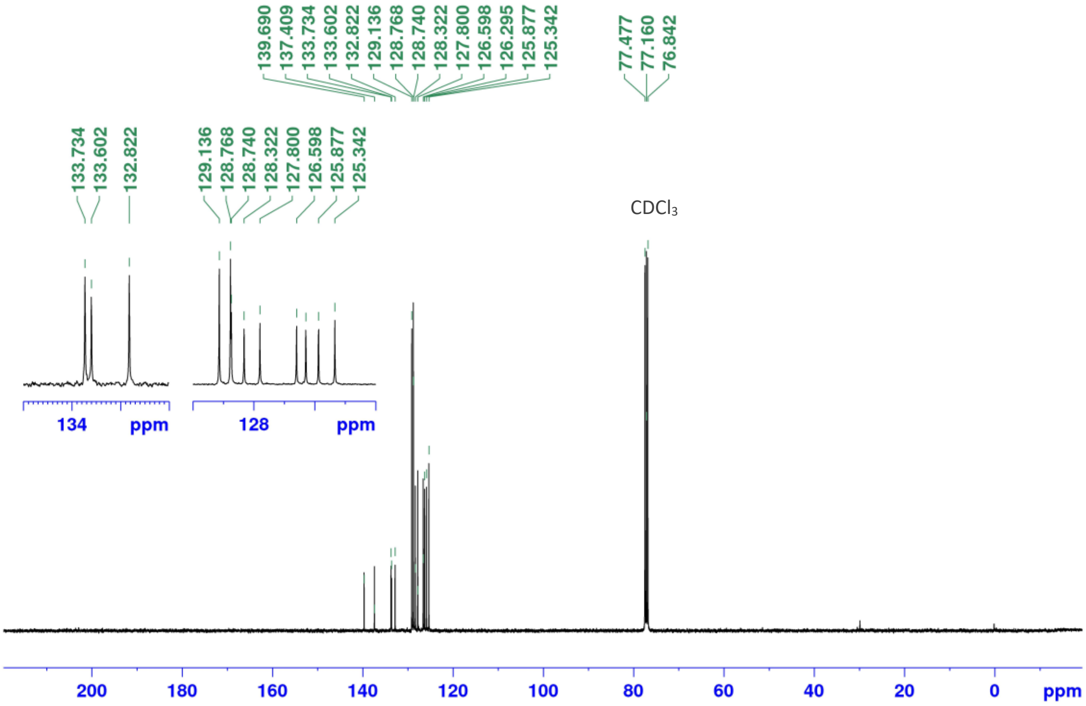
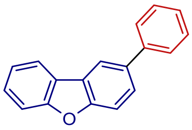


Figure S72. ^{13}C NMR (100 MHz) spectrum of **3x** in $CDCl_3$.



3y

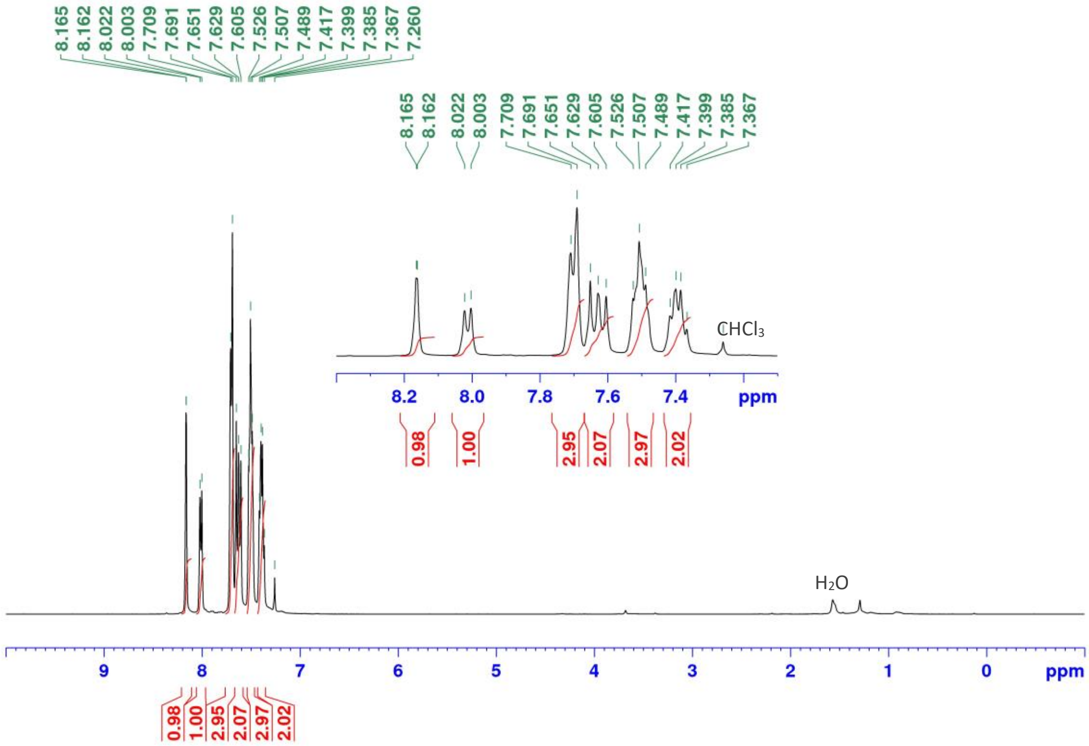
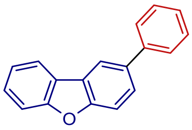


Figure S73. ^{1}H NMR (400 MHz) spectrum of **3y** in $CDCl_3$.



3y

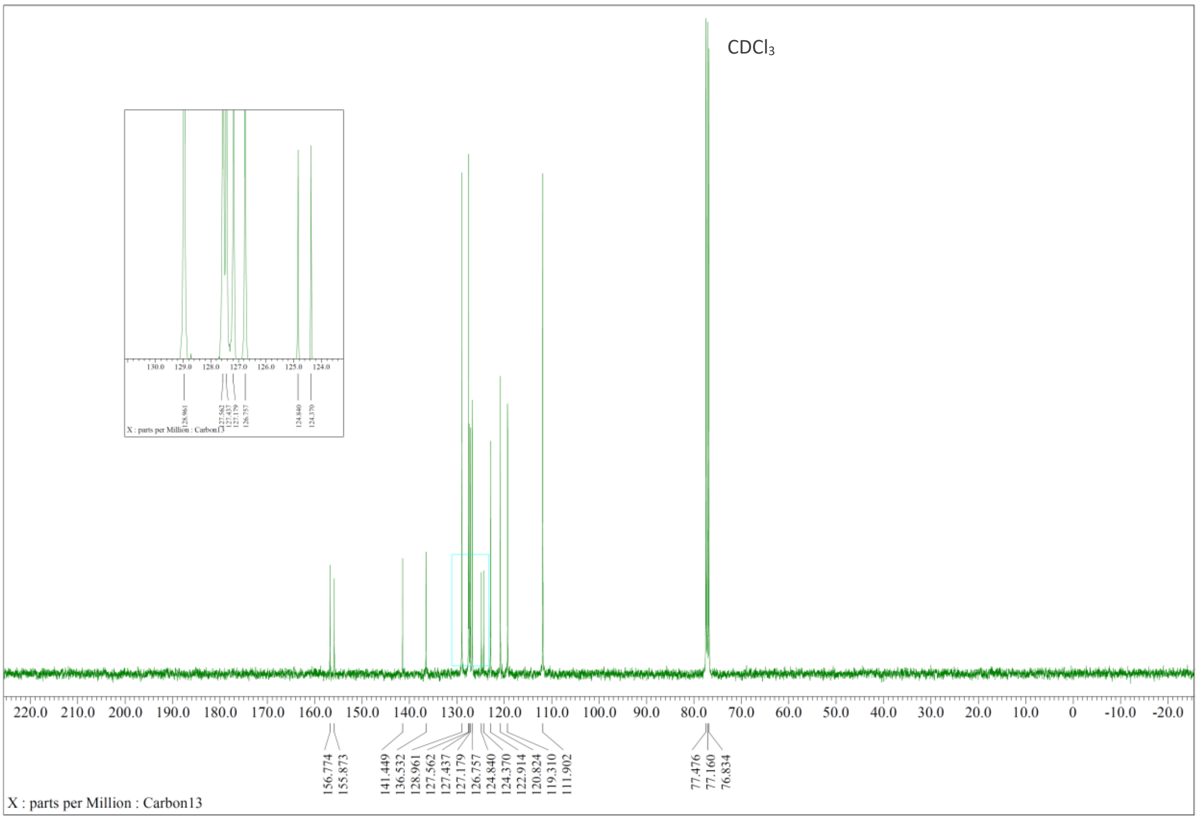
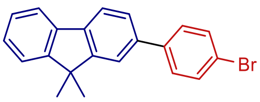


Figure S74. ^{13}C NMR (100 MHz) spectrum of **3y** in $CDCl_3$.



3z

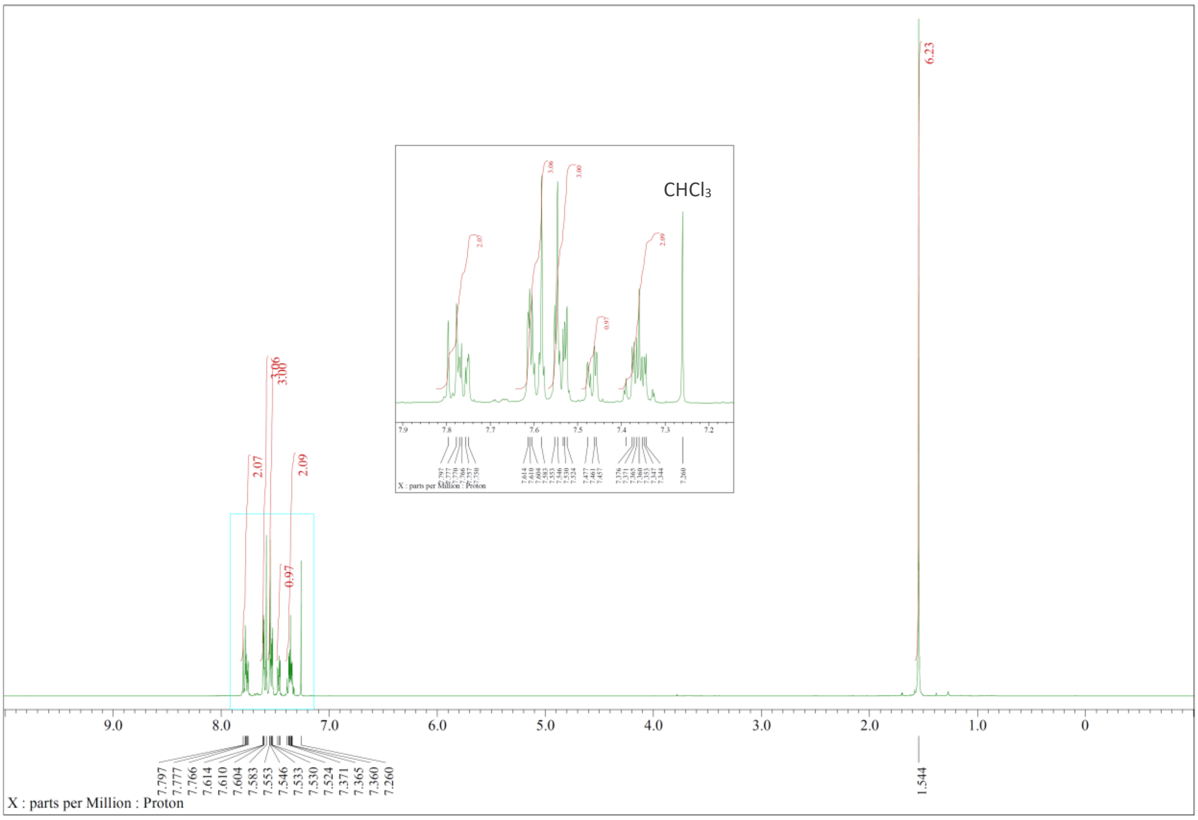
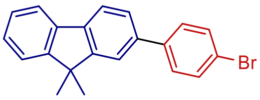


Figure S75. ^{1}H NMR (400 MHz) spectrum of **3z** in $CDCl_3$.



3z

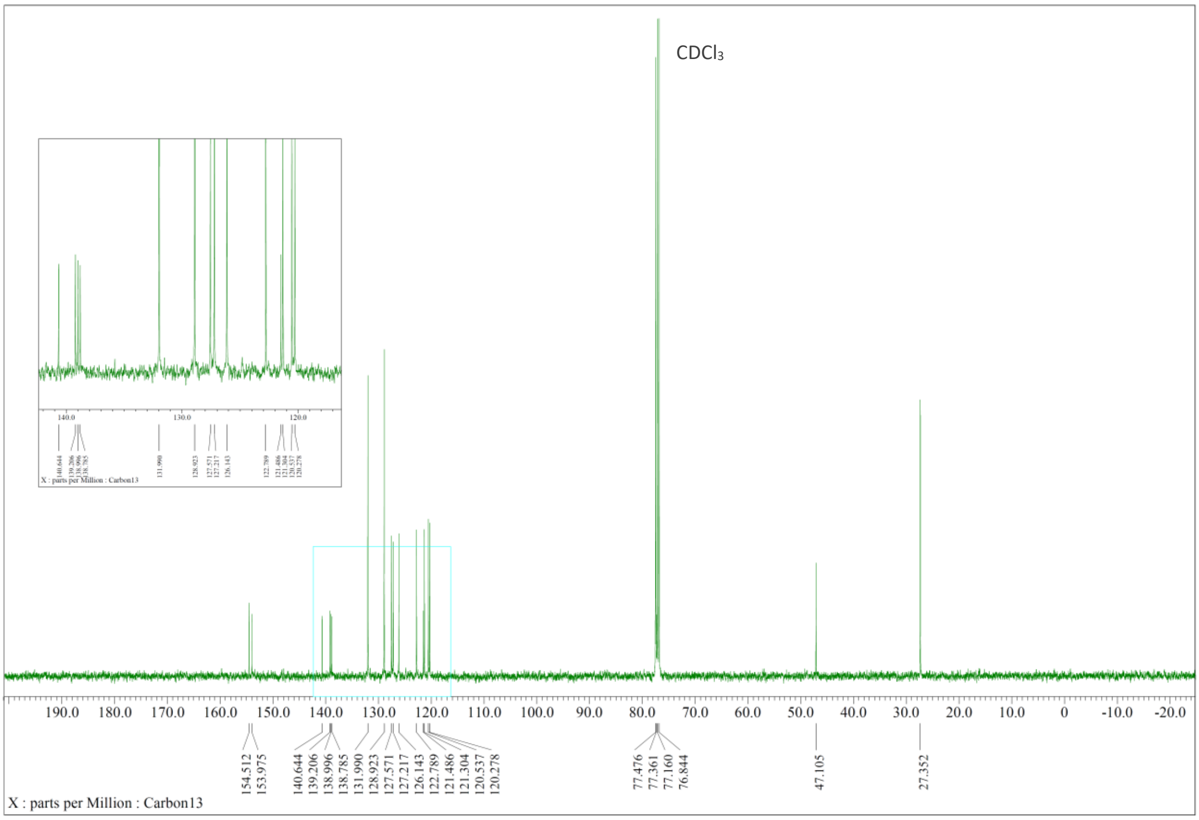


Figure S76. ^{13}C NMR (100 MHz) spectrum of **3z** in $CDCl_3$.