Visible Light Mediated Synthesis of 6*H*-Benzo[*c*]chromenes: Transition-Metal-Free Intramolecular Direct C-H Arylation

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Supporting Information

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1. General Procedures and Equipment

1.1. General Methods. Purification of desired compounds was made by column chromatography on silica gel or by High Performance Liquid Chromatograpy (HPLC) preparative. Gas chromatographic (GC) analysis were performed with a flame-ionization detector, on 30 m capillary column of a 0.32 mm x 0.25 μm film thickness, with a 5% phenylpolysiloxane phase. Gas chromatography-mass spectroscopy (GC-MS) analysis were performed employing an electronic impact (EI) ionization method and a 25 m x 0.2 mm x 0.33 μm column with a 5% phenylpolysiloxane phase. ^{1}H NMR and ^{13}C NMR{1H} spectra were recorded on 400 and 500 MHz in spectrometer with $CDCl_3$ or DMSO-d_6 as solvents with TMS as internal standard. Coupling constants are given in Hz and chemical shifts are reported in δ values in ppm. Data are reported as followed: chemical shift, multiplicity (s = singlet, s br = broad singlet, d = doublet, t = triplet, dd = double doublet, dt = double triplet, ddd = double double doublet, m = multiplet), coupling constants (Hz), and integration. All new products were further characterized by high resolution mass spectrometry (HRMS). HRMS analyses were carried out using a time-of-flight mass spectrometry (TOF-MS) instrument with an electrospray ionization (ESI) source. Photoinduced reactions were conducted with blue LED (λ = (467 ± 20) nm), green LED (λ = (522 ± 20) nm) and violet LED (λ = (390 ± 20) nm) lights performing at 3W of potency and 700 mV of current emission spectra (Figure S1) and HPIT 400W lamps (λ≥ 350 nm) (Figure S2). Apparatus and irradiation setup is shown in Figure S3.

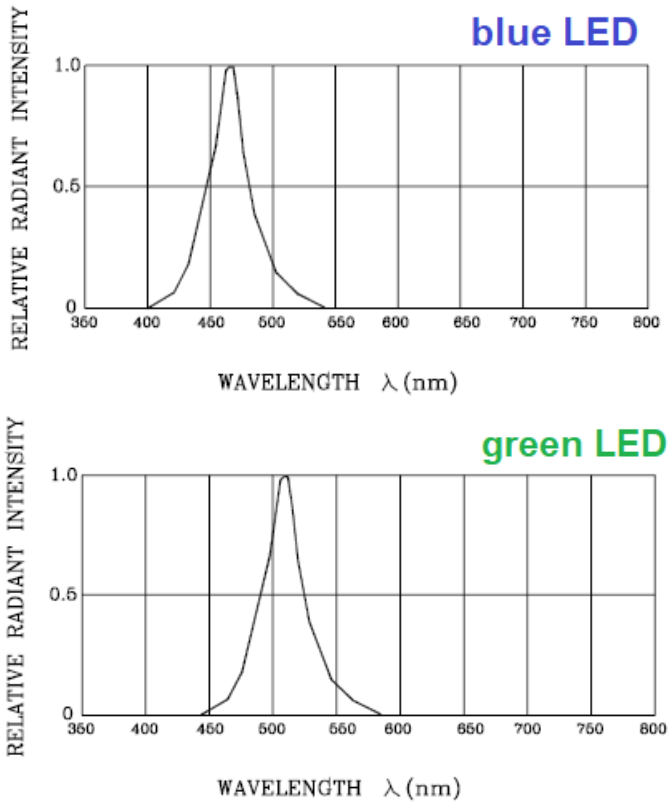


Figure S1. Emission spectra for blue and green LEDs as provided by the supplier.

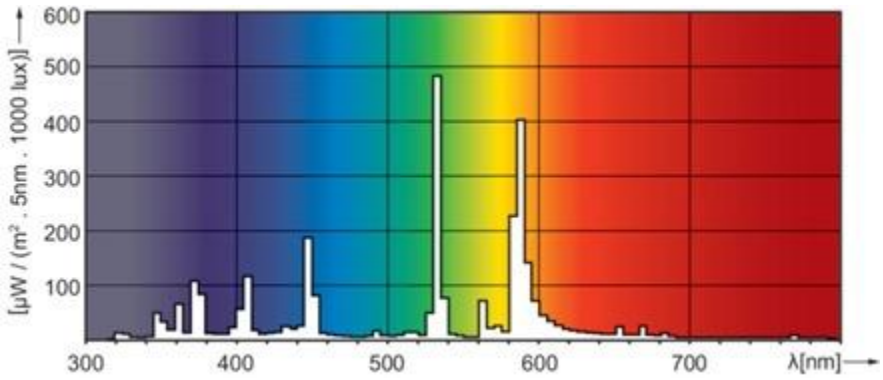


Figure S2. Emission spectrum for HPIT 400 W lamps ($\lambda \geq 350$ nm).

Table S1. Details of light sources employed

Light sources	blue LED	green LED	violet LED	HPIT
Manufacter and model	OSRAM Oslon	OSRAM Oslon	OSRAM Oslon	Philips HPIT
Potency	3 W	3 W	3 W	400 W
Wavelength of peak intensity	467 ± 20 nm	522 ± 20 nm	395 ± 20 nm	λ≥ 350 nm
Spectral distribution and intensity	See Figure S1	See Figure S1	--	See Figure S2
Distance from the light source	1 cm	1 cm	1 cm	15 cm
Material of the irradiation vessel	borosilicate glass	borosilicate glass	borosilicate glass	borosilicate glass

Figure S3. Apparatus and irradiation setup used.

1.2. Materials. Phenol, 2-Iodophenol, 2-Chlorophenol, 2-Methylphenol, 4-Methylphenol, 4-Methoxyphenol, 4-*tert*-Butylphenol, 4-Fluorophenol, 4-Cyanophenol, 4-Chlorophenol, 4-(Trifluoromethyl)phenol, 2,4-Di-*tert*-butylphenol, 2-Isopropyl-5-methylphenol, 1-Bromonaphtol, 1-Naphtol, 2-Naphtol, Benzyl chloride, Benzyl bromide, 2-Bromobenzyl bromide, 2-Iodobenzyl chloride, 2-Iodobenzyl bromide, 4-Methylbenzyl chloride, 4-Fluorobenzyl chloride, 5-Bromo-6-(bromomethyl)benzo[*d*][1,3]dioxole, KO^tBu, NaO^tBu, K_2CO_3, Cs_2CO_3 KOH, NaH, NH_4NO_3, NH_4Cl,

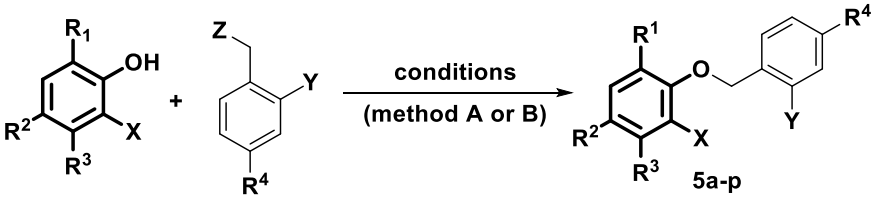
Na_2SO_4, 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO), 18-crown-6, 4-Nitroacetophenone and 2,4,6-trinitroanisole were purchased from commercial suppliers and used without further purification.
Acetone was previously distilled and DMSO, DMF, DMA, THF and MeCN were distilled and dried under molecular sieves (3 Å). MeOH HPLC was previously filtered. All solvents were analytical grade. The silica used in column chromatography corresponds to silica gel 60 (0.063−0.200 mm).

1.3. Typical Procedures for the Synthesis of Compounds 5a-u.

Method A: Employing previously described conditions,[1,2] to a solution of the corresponding phenol (1 equiv, 2 mmol) with K_2CO_3 (1 equiv, 2 mmol, 276 mg) in acetone (7.2 mL), the required benzyl bromide (1 equiv, 2 mmol) was added. The mixture was stirred followed by heating to 50 °C for 24 h. The reaction mixture was then cooled to room temperature and water was added and the layers separated. The organic layer was washed with water (3 x 20 mL), dried over Na_2SO_4 and concentrated under reduced pressure to afford the reaction crude which was analyzed by TLC, GC and isolated with column chromatography over silica gel.

Method B: To a solution of the corresponding phenol (1 equiv, 2 mmol) with K_2CO_3 (1 equiv, 2 mmol, 276 mg) in DMF (7.2 mL), 18-crown-6 (1 equiv, 2 mmol, 426 µL) and the required benzyl chloride (1 equiv, 2 mmol) were added. The mixture was stirred followed by heating to 120 °C for 24 h. The reaction mixture was then cooled to room temperature and water was added and the layers separated. The organic layer was washed with water (3 x 20 mL), dried over Na_2SO_4 and concentrated under reduced pressure to afford the reaction crude which was analyzed by TLC, GC and isolated with column chromatography over silica gel.

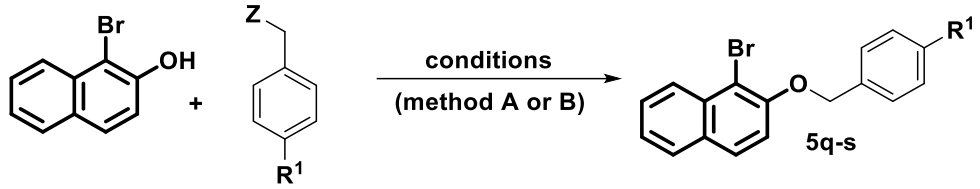
*Table S2. Preparation of Compounds **5a-p** from the corresponding phenols and benzyl halides*



Entry	R^1	R^2	R^3	X	Z	Y	R^4	**5**, yield (%)[a]
1	H	H	H	H	Br	Br	H	**5a**, 53[b]
2	H	H	H	H	Br	I	H	**5b**, 37[c]
3	H	CH_3	H	H	Br	I	H	**5c**, 56[c]
4	H	^{t}Bu	H	H	Cl	I	H	**5d**, 66[c]
5	H	OCH_3	H	H	Cl	I	H	**5e**, 53[c]
6	Me	H	H	H	Br	I	H	**5f,** 64[b]
7	H	CN	H	H	Br	I	H	**5g**, *79*[b]
8	H	CF_3	H	H	Br	I	H	**5h**, 75[b]
9	H	Cl	H	H	Br	I	H	**5i**, *36*[b]
10	Cl	H	H	H	Br	I	H	**5j**, *46*[b]
11	H	F	H	H	Cl	I	H	**5k**, *72*[c]
12	^{t}Bu	^{t}Bu	H	H	Br	I	H	**5l,** 17[b]
13	C_3H_7	H	CH_3	H	Br	I	H	**5m**, *46*[b]
14	H	H	H	I	Br	H	H	**5n**, 60[b]
15	H	H	H	I	Cl	H	F	**5o**, *37*[c]
16	H	H	H	I	Cl	H	CH_3	**5p**, 42[c]

Conditions: [a] Isolated yields. [b]**Method A:** Phenol (1 equiv) in acetone with K_2CO_3 (1 equiv) is treated with benzyl halide (1 equiv) at 50 °C for 24 h. [c]**Method B:** Phenol (1 equiv) in DMF with K_2CO_3 (1 equiv) and 18-crown-6 (1 equiv) is treated with benzyl halide (1 equiv) at 120 °C for 24 h.

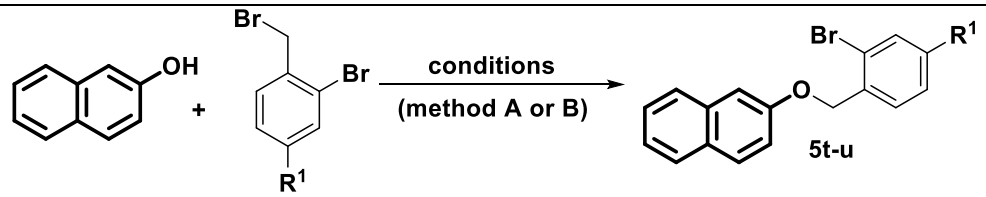
*Table S3: Preparation of Compounds **5q-s** from 1-Bromo-2-naphtol and the corresponding benzyl halides*



Entry	Z	R^1	**5**, yield (%)[a]
1	Br	H	**5q**, 85[b]
2	Cl	Me	**5r**, 34[b]
3	Cl	F	**5s**, *51*[b]

Conditions: [a] Isolated yields. **Method A:** Naphtol (1 eq.) in acetone with K_2CO_3 (1 eq.) is treated with benzyl halide (1 eq) at 50 °C for 24 h. [b]**Method B:** Naphtol (1 eq.) in DMF with K_2CO_3 (1 eq.) and 18-crown-6 (1 eq.) is treated with benzyl halide (1 eq.) at 120 °C for 24 h.

*Table S4: Preparation of Compounds **5t-u** from 2-naphtol and the corresponding benzyl halides*



Entry	R^1	**5**, yield (%)
1	H	**5t**, 53[a]
2	-OCH_2O-	**5u**, 43[b]

Conditions: [a]**Method A:** Naphtol (1 equiv) in acetone with K_2CO_3 (1 equiv) is treated with benzyl halide (1 equiv) at 50 °C for 24 h. [b]**Method B:** Naphtol (1 equiv) in DMF with K_2CO_3 (1 equiv) and 18-crown-6 (1 equiv) is treated with benzyl halide (1 equiv) at 120 °C for 24 h.

2. Characterization Data of compounds 5a-u

1-Bromo-2-(phenoxymethyl)benzene (**5a**).[1] Titled compound was obtained according to Method A and purified by column chromatography on silica gel eluting with hexane/EtOAc (90:10). White solid was isolated in 53% yield (1.07 mmol, 282 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.57 (ddd, *J* = 10.3, 7.9, 1.4 Hz, 2H), 7.35 – 7.27 (m, 3H), 7.18 (td, *J* = 7.7, 1.7 Hz, 1H), 7.03 – 6.92 (m, 3H), 5.14 (s, 2H). **GC/MS EI** *m*/*z* 264 (M^+ +2, 12), 262 (11), 183 (19), 171 (75), 169 (82), 92 (11), 91 (13), 90 (100), 89 (80), 77 (15), 65 (20), 64 (14), 63 (35), 51 (24).

1-Iodo-2-(phenoxymethyl)benzene (**5b**).[1] Titled compound was obtained according to Method A and purified by column chromatography on silica gel eluting with pentane. White solid was isolated in 37% yield (0.74 mmol, 226.8 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.52 (ddd, *J* = 6.4, 0.8 Hz, 1H), 7.36 (td, *J* = 7.5, 1.2 Hz, 1H), 7.33 – 7.29 (m, 2H), 7.02 (td, *J* = 7.7, 1.7 Hz, 1H), 7.00 – 6.97 (m, 3H), 5.05 (s, 2H).**^{13}C NMR{1H}** (126 MHz, $CDCl_3$) δ 158.6, 139.4, 139.3, 129.7, 129.6, 128.8, 128.5, 121.4, 115.1, 97.3, 74.0. **GC/MS EI** *m*/*z* 310 (M^+, 15), 217 (96), 207 (12), 183 (22), 91 (14), 90 (100), 89 (50), 65 (12), 63 (21), 51 (13).

1-Iodo-2-((*p*-tolyloxy)methyl)benzene (**5c**).[1] Titled compound was obtained according to Method A and purified by column chromatography on silica gel eluting with hexane/EtOAc (100:0→ 90:10). Yellow oil was isolated in 56% yield (1.12 mmol, 363 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 7.9, 1.2 Hz,

1H), 7.51 (ddd, *J* = 7.6, 1.6, 0.8 Hz, 1H), 7.35 (td, *J* = 7.5, 1.2 Hz, 1H), 7.10 (dd, *J* = 1.8, 0.8 Hz, 2H), 7.01 (td, *J* = 7.6, 1.8 Hz, 1H), 6.90 – 6.85 (m, 2H), 5.01 (s, 2H), 2.29 (s, 3H). **^{13}C NMR {1H}** (101 MHz, $CDCl_3$) δ 156.5, 139.5, 139.4, 130.6, 130.1, 129.5, 128.8, 128.5, 114.9, 97.3, 74.2, 20.7. **GC/MS EI** *m*/*z* 325 (M^+ +1, 3), 324 (M^+, 20), 217 (100), 197 (16), 91 (13), 90 (98), 89 (56), 77 (24), 64 (12), 63 (27), 51 (20).

1-((4-(*tert*-Butyl)phenoxy)methyl)-2-iodobenzene (**5d**).[1] Titled compound was obtained according to Method B and purified by column chromatography on silica gel eluting with hexane/EtOAc (100:0 → 80:20). Yellow oil was isolated in 66% yield (1.3 mmol, 473 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.56 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.42 – 7.35 (m, 3H), 7.05 (td, *J* = 7.6, 1.7 Hz, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 5.06 (s, 2H), 1.35 (s, 9H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 156.3, 144.0, 139.5, 139.3, 129.5, 128.8, 128.8, 128.5, 126.4, 114.4, 97.3, 74.1, 31.7. **GC/MS EI** *m*/*z* 367 (M^+ +1, 5), 366 (M^+, 23), 351 (17), 217 (100), 91 (27), 90 (78), 89 (37), 77 (12), 63 (14), 57 (55).

1-Iodo-2-((4-methoxyphenoxy)methyl)benzene (**5e**).[3] Titled compound was obtained according to Method B and purified by vacuum distillation using Kügelrohr apparatus. Brown oil was isolated in 53% yield (1.13 mmol, 386 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.49 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.33 (td, *J* = 7.5, 1.2 Hz, 1H), 6.98 (td, *J* = 7.7, 1.7 Hz, 1H), 6.93 – 6.87 (m, 2H), 6.87 – 6.79 (m, 2H), 4.96 (s, 2H), 3.74 (s, 3H).**^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 154.2, 152.6, 139.4, 139.3, 129.5, 128.7, 128.4, 115.95, 114.7, 97.3, 74.6, 55.8. **GC/MS EI** *m*/*z* 340 (M^+, 32), 217 (100), 123 (65), 95 (17), 90 (70), 89 (35), 77 (12), 63 (14).

1-Iodo-2-((*o*-tolyloxy)methyl)benzene (5f).[1] Titled compound was obtained according to Method A and purified by column chromatography on silica gel eluting with pentane/EtOAc (100:0 → 95:5). White solid was isolated in 64% yield (1.26 mmol, 409.4 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.8 Hz, 1H), 7.54 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.37 (td, *J* = 7.5, 1.2 Hz, 1H), 7.19 – 7.14 (m, 2H), 7.02 (td, *J* = 7.7, 1.7 Hz, 1H), 6.92 – 6.84 (m, 2H), 5.03 (s, 2H), 2.33 (s, 3H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 156.6, 139.7, 139.3, 130.9, 129.4, 128.5, 128.5, 127.2, 127.0, 121.0, 111.6, 97.0, 73.9, 16.6. **GC/MS EI** *m*/*z* 324 (M^+, 12), 217 (100), 197 (27), 91 (18), 90 (80), 89 (43), 77 (13), 63 (13).

4-((2-Iodobenzyl)oxy)benzonitrile (5g). Titled compound was obtained according to Method A and purified by column chromatography on silica gel eluting with pentane/EtOAc (100:0 → 80:20). White solid was isolated in 79% yield (1.57 mmol, 528 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.64 – 7.59 (m, 2H), 7.45 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.38 (td, *J* = 7.5, 1.3 Hz, 1H), 7.09 – 7.01 (m, 3H), 5.10 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 161.7, 139.6, 138.0, 134.2, 130.1, 128.8, 128.7, 119.2, 115.8, 104.7, 97.4, 74.3. **GC/MS EI** *m/z* 335 (M^+, 9), 217 (100), 90 (86), 89 (41), 63 (17), 50 (4). **FTIR** (cm^{-1}): 3064, 2912, 2222, 1307, 1261, 1168, 1038,1012, 837, 826, 751, 545.**HRMS (ESI-TOF$^+$)** *m/z*: $[M + Na]^+$ calcd for $C_{14}H_{10}INNaO$ 357.9699; found 357.9696.

1-Iodo-2-((4-trifluoromethyl)phenoxy)methyl)benzene (5h).[3] Titled compound was obtained according to Method A and purified by vacuum distillation using Kügelrohr apparatus. Light brown solid was isolated in 75% yield (1.43 mmol, 540 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.56 (d, *J* = 8.6 Hz, 2H), 7.47 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.37 (td, *J* = 7.5, 1.2 Hz, 1H), 7.06 – 7.01 (m, 3H), 5.08 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 160.9, 139.6, 138.5, 129.9, 128.8, 128.6, 127.1 (q, *J* = 3.7 Hz), 123.4 (q, *J* = 32 Hz), 123,1 (q, *J* = 272 Hz), 115.1, 97.4, 74.2. **GC/MS EI** *m*/*z* 378 (M^+, 8), 217 (100), 90 (78), 89 (39), 63 (15), 50 (3).

1-((4-Chlorophenoxy)methyl)-2-iodobenzene (5i).[1] Titled compound was obtained according to Method B and purified by column chromatography on silica gel eluting with pentane/EtOAc (100:0 → 90:10). White solid was isolated in 36% yield (0.70 mmol, 243 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 7.9, 1.2, 0.8 Hz, 1H), 7.47 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.37 (td, *J* = 7.5, 1.2 Hz, 1H), 7.27 – 7.23 (m, 2H), 7.03 (td, *J* = 7.7, 1.7 Hz, 1H), 6.93 – 6.88 (m, 2H), 5.01 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 157.2, 139.5, 138.9, 129.8, 129.6, 128.8, 128.6, 126.3, 116.4, 97.3, 74.4. **GC/MS EI** *m*/*z* 344 (M^+, 12), 217 (100), 91 (11), 90 (75), 89 (39), 63 (17), 50 (3).

1-Chloro-2-((2-iodobenzyl)oxy)benzene (5j). Titled compound was obtained according to Method A and purified by column chromatography on silica gel eluting with pentane/EtOAc (100:0 → 90:10). White solid was isolated in 46% yield (0.95 mmol, 233 mg). **^{1}H NMR (400 MHz $CDCl_3$)** δ 7.85 (d, *J* = 8 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.39 (td, *J* = 8.1, 1.4 Hz, 2H), 7.21 (td, *J* = 7.9, 1.7 Hz, 1H), 7.03 (td, *J* = 7.7, 1.7 Hz, 1H), 6.98 – 6.90 (m, 2H), 5.10 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 154.0, 139.2, 138.8, 130.6, 129.6, 128.6, 128.5, 127.9, 123.4, 122.1, 114.2, 96.6, 74.8. **GC/MS EI** *m/z* 344 (M+, 9), 217 (100), 90 (60), 89 (31), 63 (13). **FTIR** (cm^{-1}): 3064, 2912, 1253, 1064, 1041, 1010, 847, 746, 423.**HRMS** (ESI-TOF+) *m/z*: $[M + Na]^+$ calcd for $C_{13}H_{10}ClINaO$ 366.9357; found 366.9337.

1-((4-Fluorophenoxy)methyl)-2-iodobenzene (**5k**).[1] Titled compound was obtained according to Method B and purified by vacuum distillation using Kügelrohr apparatus. Brown oil was isolated in 72% yield (1.41 mmol, 463 mg). **^{1}H NMR** (400 MHz $CDCl_3$) δ 7.86 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.49 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.36 (td, *J* = 7.6, 1.2 Hz, 1H), 7.05 – 6.89 (m, 5H), 5.00 (s, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 158.7 (*J* = 240 Hz), 154.5 (*J* = 1 Hz), 139.3, 139.0, 129.6, 128.7, 128.5, 116.1 (x2, *J* = 3 Hz), 115.9 (x2, *J* = 12 Hz), 97.3, 74.5. **GC/MS EI** *m*/*z* 329 (M^+ +1, 2), 328 (M^+, 16), 217 (96), 90 (100), 89 (60), 83 (14), 64 (13), 63 (32), 57 (16) 51 (13).

2,4-Di-*tert*-butyl-1-((2-iodobenzyl)oxy)benzene (5l). Titled compound was obtained according to Method A and purified by column chromatography on silica gel eluting with pentane. White solid was isolated in 17% yield (0.33 mmol, 142 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8, 1H), 7.56 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.38 – 7.33 (m, 2H), 7.17 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.99 (td, *J* = 7.7, 1.7 Hz, 1H), 6.81 (d, *J* = 8.5 Hz, 1H), 5.07 (s, 2H), 1.44 (s, 9H), 1.31 (s, 9H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 155.1, 143.3, 139.9, 139.3, 137.7, 129.3, 128.6, 128.5, 124.2, 123.6, 112.4, 96.9, 74.8, 35.2, 34.5, 31.8, 30.2. **GC/MS** EI *m/z* 422 (M^+, 19), 217 (94), 207 (10), 91 (35), 90 (45), 89 (18), 57 (100). **FTIR** (cm^{-1}): 3059, 2956, 1358, 1230, 1012, 806, 744, 643, 496. **HRMS** (ESI-TOF$^+$) *m/z*: $[M + Na]^+$ calcd for $C_{21}H_{21}INaO$ 445.0975; found 445.0955.

2-((2-Iodobenzyl)oxy)1-isopropyl-4-methylbenzene (5m). Titled compound was obtained according to Method A and purified by column chromatography on silica gel eluting with pentane/EtOAc (80:20). White solid was isolated in 46% yield (0.91 mmol, 333.7 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.56 (ddd, *J* = 7.7, 1.8, 0.8 Hz, 1H), 7.39 (td, *J* = 7.5, 1.2 Hz, 1H), 7.14 (d, *J* = 7.7 Hz, 1H), 7.03 (td, *J* = 7.7, 1.7 Hz, 1H), 6.79 (dd, *J* = 7.7, 1.6 Hz, 1H), 6.72 (dd, *J* = 1.6, 1H), 5.01 (s, 2H), 3.40 (m,1H), 2.33 (s, 3H), 1.24 (d, *J* = 6.8, 6H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 155.5, 139.9, 139.3, 136.6, 134.5, 129.4, 128.5, 128.5, 126.2, 121.9, 112.9, 97.1, 74.2, 26.8, 23.0, 21.5. **GC/MS** EI *m/z* 366 (M^+, 73), 217 (100), 197 (20), 148 (12), 91 (17), 90 (46), 89 (20). **FTIR** (cm^{-1}): 3052, 2959, 1255, 1162, 1010, 746, 808, 594.**HRMS** (ESI-TOF$^+$) m/z: $[M + Na]^+$ calcd for $C_{17}H_{19}INaO$ 389.0373; found 389.0389.

1-(Benzyloxy)-2-iodobenzene (**5n**).[1] Titled compound was obtained according to Method B and purified by column chromatography on silica gel eluting with hexane/EtOAc (100:0 → 90:10). Yellow oil was isolated in 60% yield (1.2 mmol, 380 mg). **^{1}H NMR** (400 MHz $CDCl_3$) δ 7.80 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.51 – 7.49 (m, 2H), 7.41 – 7.37 (m, 2H), 7.34 – 7.30 (m, 1H), 7.29 – 7.25 (m, 1H), 6.86 (dd, *J* = 8.2, 1.3 Hz, 1H), 6.72 (td, *J* = 7.6, 1.4 Hz, 1H), 5.15 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.3, 139.7, 136.7, 129.6, 128.7, 128.0, 127.1, 123.0, 112.9, 87.0, 71.0. **GC/MS EI** *m/z* 310 (M^+, 1), 92 (14), 91 (100), 65 (26), 64 (12), 63 (15).

1-((4-Fluorobenzyl)oxy)-2-iodobenzene (5o). Titled compound was obtained according to Method B and purified by column chromatography on silica gel eluting with hexane/EtOAc (100:0 → 97:3). Yellow oil was isolated in 37% yield (0.71 mmol, 233 mg). **^{1}H NMR** (500 MHz $CDCl_3$) δ 7.81 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.48 (dd, *J* = 8.7, 5.4 Hz, 2H), 7.29 (ddd, *J* = 8.2, 7.5, 1.6 Hz, 1H), 7.09 (ddd, *J* = 9.6, 5.8, 2.5 Hz, 2H), 6.86 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.74 (td, *J* = 7.6, 1.3 Hz, 1H), 5.11 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 162.6 (*J* = 246 Hz), 157.2, 139.8, 132.4 (*J* = 3 Hz), 129.6, 129.0 (*J* = 8 Hz), 123.1, 115.4 (*J* = 8 Hz), 113.0, 87.0, 70.4. **GC/MS** EI *m/z* 328 (M+, 4), 109 (100), 50 (1). **FTIR** (cm^{-1}): 3062, 2925, 1274, 1224, 1051, 1018, 821, 749, 648, 599, 493.**HRMS** (ESI-TOF$^+$) *m/z*: $[M + Na]^+$ calcd for $C_{13}H_{10}FINaO$ 350.09653; found 350.9659.

1-Iodo-2-((4-methylbenzyl)oxy)benzene (5p).[3] Titled compound was obtained according to Method B and purified by vacuum distillation using Kügelrohr apparatus. Brown oil was isolated in 42% yield (0.47 mmol, 152.2 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.28 – 7.23 (m, 1H), 7.19 (d, *J* = 7.9 Hz, 2H), 6.85 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.70 (td, *J* = 7.6, 1.3 Hz, 1H), 5.10 (s, 2H), 2.35 (s, 3H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 157.4, 139.7, 137.7, 133.6, 129.5, 129.4, 127.3, 122.9, 113.0, 87.0, 71.0, 21.3 **GC/MS EI** *m/z* 324 (M^+, 3), 105 (100).

(2-Benzyloxy)-1-bromonaphthalene (5q)[4]: Titled compound was obtained according to Method A and purified by column chromatography on silica gel eluting with hexane/EtOAc (100:0 → 80:20). Brown solid was isolated in 85% yield (1.79 mmol, 537 mg). **^{1}H NMR** (400 MHz $CDCl_3$) δ 8.24 (dd, *J* = 8.6, 1.0 Hz, 1H), 7.77 – 7.73 (m, 2H), 7.58 – 7.50 (m, 3H), 7.39 (ddd, *J* = 7.8, 6.4, 1.3 Hz, 3H), 7.34 – 7.29 (m, 1H), 7.28 – 7.23 (m, 1H), 5.29 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 153.1, 136.9, 133.4, 130.2, 129.0, 128.7, 128.2, 128.1, 127.8, 127.3, 126.4, 124.7, 115.8, 110.2, 72.0 **GC/MS EI** *m/z* 314 (M^+ +2, 2), 312 (M^+, 2), 91 (100), 65 (13).

1-Bromo-2-((4-methylbenzyl)oxy)naphtalene (5r). Titled compound was obtained according to Method B and purified by column chromatography on silica gel eluting with hexane/EtOAc (100:0 → 90:10). Light brown solid was isolated in 34% yield (0.65 mmol, 212 mg. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.6 Hz, 1H), 7.73 (t, *J* = 6.8 Hz, 2H), 7.54 (t, *J* = 7.7 Hz, 1H), 7.38 (t, *J* = 5.5 Hz, 3H), 7.24 (d, *J* = 9.0 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 2H), 5.24 (s, 2H), 2.34 (s, 3H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 153.1, 137.9, 133.8, 133.3, 130.1, 129.4, 128.9, 128.1, 127.8, 127.4, 126.6, 124.6, 115.8, 110.1, 71.9, 21.4. **GC/MS EI** *m/z* 328 (M^+ +2, 1), 326 (M^+, 2), 105 (100), 79 (10), 77 (10). **FTIR** (cm^{-1}): 3049, 2915, 1266, 1067, 1018, 806, 764, 744, 483. **HRMS** (ESI-TOF$^+$) m/z: $[M + Na]^+$ calcd for $C_{18}H_{15}BrNaO$ 349.0174; found 349.0163.

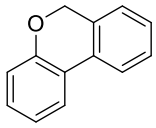
1-Bromo-2-((4-fluorobenzyl)oxy)naphtalene (5s). Titled compound was obtained according to Method B and purified by column chromatography on silica gel eluting with hexane/EtOAc (100:0

→ 80:20). White solid was isolated in 51% yield (1.27 mmol, 420.5 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.5 Hz, 1H), 7.76 (d, *J* = 8.8 Hz, 2H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.51 – 7.46 (m, 2H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.07 (t, *J* = 8.4 Hz, 2H), 5.23 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 162.7 (J = 247 Hz), 152.9, 133.3, 132.6 (*J* = 3 Hz), 130.3, 129.3 (*J* = 8 Hz), 129.0, 128.2, 127.9, 126.5, 124.8, 115.8 (*J* = 4 Hz), 115.6, 110.3, 71.4. **GC/MS** EI *m/z* 332 (M^+ +2, 4), 330 (M^+, 3), 114 (11), 109 (100), 83 (16). **FTIR** (cm^{-1}): 3065, 2933, 1261, 1053, 826, 795, 745, 410.**HRMS** (ESI-TOF$^+$) m/z: $[M + Na]^+$ calcd for $C_{17}H_{12}BrFNaO$ 352.9948; found 352.9926.

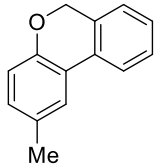
2-((2-Bromobenzyl)oxy)naphtalene (5t). Titled compound was obtained according to Method A and purified by column chromatography on silica gel eluting with pentane/EtOAc (100:0 → 90:10). White solid was isolated in 53% yield (1.05 mmol, 338 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.7 Hz, 2H), 7.73 (d, *J* = 8.3 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 2H), 7.45 – 7.42 (t, *J* = 6.8 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.28 – 7.17 (m, 3H), 5.25 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 156.6, 136.4, 134.7, 132.8, 129.7, 129.4, 129.4, 129.1, 127.8, 127.7, 127.0, 126.6, 124.0, 122.6, 119.0, 107.6, 69.6. **GC/MS** EI *m/z* 314 (M^+ +2, 1), 312 (M^+, 1), 233 (51), 171 (95), 169 (100), 115 (35), 90 (67), 89 (51), 63 (18). **FTIR** (cm^{-1}): 3052, 2930, 1268, 1240, 1095, 1064, 788, 770, 682. **HRMS** (ESI-TOF$^+$) *m/z*: $[M + Na]^+$ calcd for $C_{17}H_{13}BrNaO$ 335.0042; found 335.0034.

5-Bromo-6-((naphtalen-2-yloxy)methyl)benzo[*d*][1,3]dioxole (5u). Titled compound was obtained according to Method B and purified by column chromatography on silica gel eluting with pentane/EtOAc (100:0 → 90:10). Brown solid was isolated in 43% yield (0.83 mmol, 295 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 – 7.72 (m, 3H), 7.43 (ddd, *J* = 8.2, 6.8, 1.4 Hz, 1H), 7.34 (ddd, *J* = 8.1, 6.8, 1.3 Hz, 1H), 7.25 – 7.18 (m, 2H), 7.07 (s, 1H), 7.05 (s, 1H), 5.97 (s, 2H), 5.15 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 156.4, 148.2, 147.8, 134.6, 129.7, 129.6, 129.3, 127.8, 127.0, 126.6, 124.0, 119.0, 113.2, 112.9, 109.2, 107.5, 102.0, 69.5. **GC/MS** EI *m/z* 356 (M^+, 5), 277 (22), 215 (97), 213 (100), 207 (24), 157 (11), 115 (20), 78 (43), 77 (16), 76 (33), 75 (34), 50 (11). **FTIR** (cm^{-1}): 3059, 2902, 1475, 1498, 1237, 1036, 930, 811, 744. **HRMS** (ESI-TOF$^+$) *m/z*: $[M + Na]^+$ calcd for $C_{18}H_{13}BrNaO_3$ 378.9940; found 378.9933.

3. Characterization Data of 6*H*-Benzo[*c*]chromenes (1a-p)

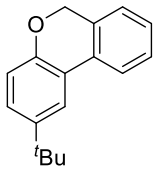


6*H*-Benzo[*c*]chromene (1a).[1] Titled compound was purified by HPLC preparative eluting with MeOH. Light yellow oil was isolated in 70% yield (0.05 mmol, 8.3 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.30 – 7.21 (m, 2H), 7.14 (d, *J* = 7.5 Hz, 1H), 7.05 (td, *J* = 7.5, 1.3 Hz, 1H), 6.99 (dd, *J* = 8.1, 1.3 Hz, 1H), 5.12 (s, 2H).**^{13}C NMR{1H}** 131.6, 130.3, 129.6, 128.6, 128.1, 127.8, 124.8, 123.4, 123.1, 122.3, 122.2, 117.5, 68.6. **GC/MS EI** *m*/*z* 183 (M^+ +1, 7), 182 (M^+ 61), 181 (100), 152 (36), 151 (13), 91 (27), 77 (15), 76 (50), 75 (13), 64 (10), 63 (24), 51 (13).

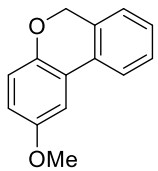


2-Methyl-6*H*-benzo[*c*]chromene (1c).[1] Titled compound was purified by HPLC preparative eluting with MeOH. Light yellow oil was isolated in 33% yield (0.03 mmol, 6.2 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.7 Hz, 1H), 7.53 (s, 1H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.28 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.14 (d, *J* = 7.5 Hz, 1H), 7.06 – 7.02 (m, 1H), 6.89 (d, *J* = 8.2 Hz, 1H), 5.08 (s, 2H), 2.36 (s, 3H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 152.8, 131.8, 131.5, 130.4, 130.2, 128.5, 127.7, 124.8, 123.8, 122.8, 122.1, 117.2, 68.7, 21.1.

GC/MS EI *m*/*z* 197 (M^+ +1, 11), 196 (M^+ 74), 195 (100), 165 (19), 153 (12), 152 (23), 97 (25), 82 (11), 63 (12).

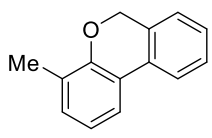


2-(*tert*-Butyl)-6*H*-benzo[*c*]chromene (1d).[1] Titled compound was purified by HPLC preparative eluting with MeOH. Light yellow oil was isolated in 21% yield (0.04 mmol, 10.2 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.77 – 7.71 (m, 2H), 7.37 (td, *J* = 7.6, 1.4 Hz, 1H), 7.30 – 7.24 (m, 2H), 7.14 (d, *J* = 7.6 Hz, 1H), 6.93 (d, *J* = 8.5 Hz, 1H), 5.09 (s, 2H), 1.36 (s, 9H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 152.7, 145.0, 131.8, 130.7, 128.5, 127.6, 126.7, 124.8, 122.3, 122.0, 120.0, 116.9, 68.7, 41.2, 31.7. **GC/MS EI** *m*/*z* 239 (M^+ +1, 8), 238 (M^+ 42), 224 (20), 223 (100), 195 (26), 180 (15), 165 (24), 153 (12), 152 (14), 115 (10), 97 (37).

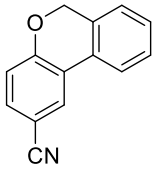


2-Methoxy-6*H*-benzo[*c*]chromene (1e).[5] Titled compound was purified by HPLC preparative eluting with MeOH. Light yellow oil was isolated in 37% yield (0.07 mmol, 15.0 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.37 (td, *J* = 7.6, 1.3 Hz, 1H), 7.30 – 7.24 (m, 2H), 7.15 (dd, *J* = 7.4, 0.7 Hz, 1H), 6.93 (d, *J* = 8.8 Hz, 1H), 6.80 (dd, *J* = 8.8, 3.0 Hz, 1H), 5.06 (s, 2H), 3.84 (s, 3H).**^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 155.0, 149.0, 132.0, 130.4, 128.5, 128.0, 124.8, 123.7, 122.2, 118.1, 115.2, 108.5, 68.7, 56.0.

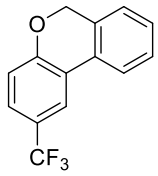
GC/MS EI *m*/*z* 213 (M^+ +1, 17), 212 (M^+ 100), 211 (67), 197 (31), 169 (30), 168 (23), 152(11), 141 (33), 139 (22), 115 (72), 89 (15), 76 (14), 63 (24, 51 (11).



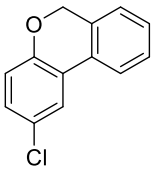
4-Methyl-6*H*-benzo[*c*]chromene (1f).[5] Titled compound was obtained and purified by HPLC preparative eluting with MeOH. Colorless oil was isolated in 24% yield (0.05 mmol, 9.1 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.8 Hz, 1H), 7.58 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.36 (td, *J* = 7.7, 1.1 Hz, 1H), 7.27 (dd, *J* = 7.4, 1.1 Hz, 1H), 7.15 (d, *J* = 7.4 Hz, 1H), 7.10 (dd, *J* = 7.4, 0.7 Hz, 1H), 6.95 (t, *J* = 7.6 Hz, 1H), 5.12 (s, 3H), 2.27 (s, 4H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 153.1, 131.6, 131.0, 130.7, 128.5, 127.6, 126.9, 124.7, 122.7, 122.4, 121.6, 121.1, 68.7, 16.1. **GC/MS EI** *m*/*z* 197 (M^+ +1, 10), 196 (M^+, 76), 195 (100), 165 (23), 153 (18), 152 (26), 97 (26), 82 (13).



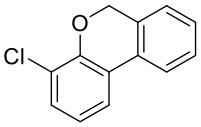
6*H*-Benzo[*c*]chromene-2-carbonitrile (1g).[5] Titled compound was purified by HPLC preparative eluting with MeOH. White solid was isolated in 12% yield (0.012 mmol, 2.5 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 2.0 Hz, 1H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.50 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.46 – 7.34 (m, 2H), 7.18 (d, *J* = 6.8 Hz, 1H), 7.03 (d, *J* = 4.8 Hz, 1H), 5.21 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 158.3, 133.2, 130.8, 129.1 (x2), 128.0, 127.7, 125.0, 123.8, 122.3, 119.2, 118.7, 105.7, 68.7. **GC/MS EI** *m*/*z* 208 (M^+ +1, 8), 207 (M^+, 60), 206 (100), 177 (13), 151 (21), 103 (10), 76 (17), 75 (11).



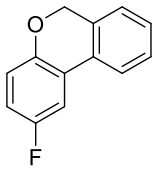
2-(Trifluoromethyl)-6*H*-benzo[*c*]chromene (1h).[6] Titled compound was purified by HPLC preparative eluting with MeOH. Brown oil was isolated in 33% yield (0.07 mmol, 16.3 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 2.1 Hz, 1H), 7.72 (d, *J* = 7.8, 1H), 7.47 (dd, *J* = 8.5, 2.2 Hz, 1H), 7.41 (t, *J* = 7.6, 1H), 7.33 (td, *J* = 7.5, 1.3 Hz, 1H), 7.16 (d, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 8.5 Hz, 1H), 5.17 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 157.4, 131.2, 128.9, 128.7, 126.5 (q, *J* = 3.7 Hz), 126.2 (q, *J* = 272.7 Hz), 124.9, 124.4 (q, *J* = 32.0 Hz), 123.2, 122.4, 120.8 (q, *J* = 3.7 Hz), 118.0, 68.7. **GC/MS EI** *m*/*z* 250 (M^+, 58), 249 (100), 207 (12), 201 (14), 152 (23), 115 (12), 76 (11).



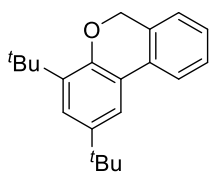
2-Chloro-6*H*-benzo[*c*]chromene (1i).[5] Titled compound was purified by HPLC preparative eluting with MeOH. Yellow oil was isolated in 39% yield (0.08 mmol, 16.9 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 2.5 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.38 (td, *J* = 7.6, 1.3 Hz, 1H), 7.31 (td, *J* = 7.5, 1.2 Hz, 1H), 7.20 – 7.13 (m, 2H), 6.92 (d, *J* = 8.6 Hz, 1H), 5.11 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 153.4, 131.4, 129.2 (x2), 128.8, 128.5, 127.3, 124.9, 124.5, 123.3, 122.3, 118.9, 68.7. **GC/MS EI** *m*/*z* 218 (M^+ +2, 22), 217 (M^+ +1, 38), 216 (M^+, 66), 215 (100), 181 (12), 153 (22), 152 (51), 151 (18), 90 (17), 76 (48), 75 (14), 63 (17).



4-Chloro-6*H*-benzo[*c*]chromene (1j).[7] The compound was obtained as a yellow oil (7 mg, 0.03 mmol, 30% isolated yield) in an unseparable mixture (9:1) with the reductive product 1-(benzyloxy)-2-chlorobenzene. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.5 Hz, 1H), 7.63 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.39 (ddd, *J* = 7.7, 1.4, 0.7 Hz, 1H), 7.34 – 7.28 (m, 2H), 7.17 (dd, *J* = 7.4, 0.7 Hz, 1H), 6.98 (t, *J* = 8 Hz, 1H), 5.22 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.67, 131.19, 130.00, 129.58, 128.79, 128.58, 128.43, 124.89, 122.52, 122.36, 121.85, 117.52, 69.05. **GC/MS EI** *m*/*z* 218 (M^+ +2, 24), 217 (M^+ +1, 40), 216 (M^+, 64), 215 (100), 207 (25), 181 (17), 153 (38), 152 (67), 151 29), 150 (14), 126 (10), 90 (17), 77 (13), 76 (57), 75 (22), 74 (11), 73 (17), 63 (26), 51 (16), 50 (10).

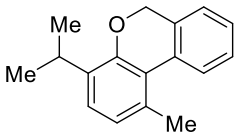


2-Fluoro-6*H*-benzo[*c*]chromene (1k).[1] Titled compound was purified by HPLC preparative eluting with MeOH. Brown oil was isolated in 23% yield (0.05 mmol, 9.1 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.6 Hz, 1H), 7.41– 7.37 (m, 2H), 7.31 (td, *J* = 7.5, 1.2 Hz, 1H), 7.16 (d, *J* = 7.4 Hz, 1H), 6.94 – 6.91 (m, 2H), 5.09 (s, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 159.6 (*J* = 240 Hz), 150.9, 131.7, 129.6 (*J* = 3 Hz), 128.7, 128.5, 124.9, 124.8 (*J* = 2 Hz), 122.4, 118.6 (*J* = 8 Hz), 115.9 (*J* = 23 Hz), 109.8 (*J* = 24 Hz), 68.7. **GC/MS EI** *m*/*z* 201 (M^+ +1, 8), 200 (M^+ 63), 211 (67), 199 (100), 171 (12), 170 (32), 85 (13), 76 (14).

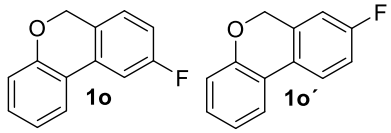


2,4-Di-*tert*-butyl-6*H*-benzo[*c*]chromene (1l).[5] Titled compound was obtained and purified by HPLC preparative eluting with MeOH. White solid was isolated in 71% yield (0.14 mmol, 41.3 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.7 Hz, 1H), 7.62 (d, *J* = 2.4 Hz, 1H), 7.37 (td, *J* = 7.6, 1.4 Hz, 1H), 7.30 (d, *J* = 2.2 Hz, 1H), 7.26

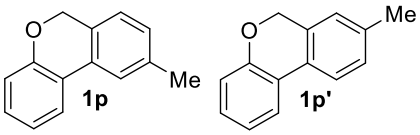
(td, *J* = 7.4, 1.2 Hz, 1H), 7.17 (d, *J* = 7.5 Hz, 1H), 5.03 (s, 2H), 1.42 (s, 9H), 1.37 (s, 9H).**^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 151.3, 143.8, 138.1, 132.0, 131.3, 128.2, 127.1, 124.4, 124.0, 123.1, 122.4, 118.1, 67.6, 34.8, 34.6, 31.6, 29.9. **GC/MS EI** *m*/*z* 295 (M^+ +1, 11), 294 (M^+, 49), 280 (22), 279 (100), 223 (23), 195 (15), 165 (11), 132 (12), 118 (16), 104 (14), 89 (11), 57 (84).



4-Isopropyl-1-methyl-6*H*-benzo[*c*]chromene (1m).[5] Titled compound was purified by HPLC preparative eluting with MeOH. White solid was isolated in 17% yield (0.03 mmol, 7.2 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.6 Hz, 1H), 7.37 (td, *J* = 7.5, 1.8 Hz, 1H), 7.30 – 7.23 (m, 2H), 7.09 (d, *J* = 7.8 Hz, 1H), 6.91 (d, *J* = 7.8 Hz, 1H), 4.93 (s, 2H), 3.32 (hept, *J* = 6.9 Hz, 1H), 2.65 (s, 3H), 1.24 (d, *J* = 6.9 Hz, 7H).**^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 153.8, 134.9, 134.2, 132.7, 131.4, 127.8, 126.8, 126.7, 125.5, 125.2, 124.8, 123.3, 69.1, 27.2, 22.9, 22.6. **GC/MS EI** *m*/*z* 239 (M^+ +1, 13), 238 (M^+, 62), 224 (17), 223 (100), 208 (20), 207 (10), 205 (12), 195 (32), 180 (11), 179 (14), 178 (19), 165 (35), 152 (13), 115 (12), 89 (17).

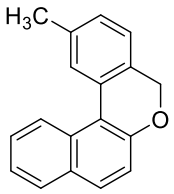


Compounds **1o** and **1o'**[9] were obtained as a yellow oil by HPLC preparative eluting with MeOH in 28% isolated yield (7 mg, 0.028 mmol), a mixture of unseparable isomers (**1o:1o'**=10:1). **9-Fluoro-6*H*-benzo[*c*]chromene (1o).** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.38 (dd, *J* = 9.9, 2.4 Hz, 1H), 7.30 – 7.20 (m, 1H), 7.10 (m, 2H), 7.02 – 6.96 (m, 2H), 5.09 (s, 2H). ^{13}C NMR{1H} (101 MHz, $CDCl_3$) δ 163.2 (*J* = 246 Hz), 155.0, 132.5, 132.4, 130.3, 127.2 (*J* = 3 Hz), 126.4 (*J* = 8 Hz), 123.6, 122.4, 117.6, 114.5 (*J* = 22 Hz), 109.2 (*J* = 23 Hz), 68.1. GC/MS EI m/z 201 (M^+ +1, 7), 200 (M^+, 56), 199 (100), 171 (12), 170 (30), 100 (11), 85 (17). **FTIR** (cm^{-1}): 3041, 2922, 1274, 1243, 1044, 1038, 806, 754, 534. HRMS (ESI-TOF$^+$) m/z: $[M - H]^+$ calcd for $C_{13}H_8FO$ 199.0565; found 199.0551.

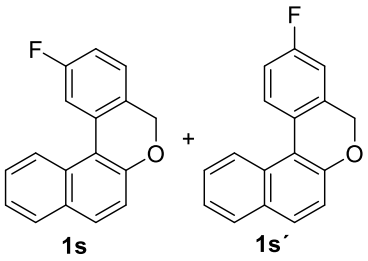


Compounds **1p**[8] and **1p'**[8] were obtained as a yellow oil by HPLC preparative in 9% isolated yield (17 mg, 0.08 mmol), a mixture of unseparable isomers (**1p:1p´**=1:3.5). **8-Methyl-6*H*-benzo[*c*]chromene (1p').**[8] **^{1}H NMR** (400 MHz, $CDCl_3$) δ ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.26 (m, 1H), 7.23 – 7.16 (m, 1H), 6.86 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.71 (td, *J* = 7.6, 1.3 Hz, 1H), 5.11 (s, 2H), 2.36 (s, 3H). **GC/MS EI** *m*/*z* 197 (M^+ +1, 10), 196 (M^+, 73), 195 (100), 181 (19), 165 (21), 153 (12), 152 (29), 97 (20), 82 (12). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.4, 139.7, 137.8, 133.6, 129.5, 129.4 (x2), 127.3, 125.4, 124.7, 122.9, 113.0, 71.0, 29.8. **9-Methyl-6*H*-benzo[*c*]chromene (1p)**.[8] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 – 7.68 (m, 1H), 7.51 (s, 1H), 7.23 – 7.15 (m, 1H), 7.11 – 6.94 (m, 4H), 5.09 (s, 2H), 2.37 (s, 3H). **GC/MS EI** *m*/*z* 196 (M^+, 61), 195 (100), 181 (21), 165 (22), 152 (25), 97 (16), 82 (11).

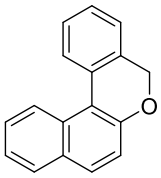
4. Characterization Data of 5*H*-Dibenzo[*c,f*]chromenes (1q-u)



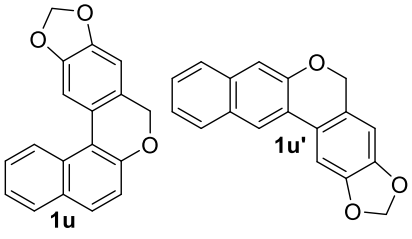
2-Methyl-5*H*-dibenzo[*c,f*]chromene (1r). Titled compound was purified by HPLC preparative eluting with MeOH. Yellow oil was isolated in 24% yield (0.024 mmol, 6 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 8.5 Hz, 1H), 7.86 (d, *J* = 6.6 Hz, 2H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.56 (ddd, *J* = 11.6, 6.5, 3.0 Hz, 1H), 7.43 (ddd, *J* = 8.0, 6.8, 1.1 Hz, 1H), 7.24 (dd, *J* = 8.2, 3.1 Hz, 2H), 7.17 (d, *J* = 7.6 Hz, 1H), 5.03 (s, 2H), 2.46 (s, 3H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 154.34, 137.93, 130.74, 130.43, 130.24, 130.07, 128.98, 127.86, 127.04, 126.93, 125.27, 124.96, 123.98, 118.42, 69.30, 21.87. **GC/MS** EI *m/z* 247 (M^+ +1, 20), 246 (M^+, 100), 245 (69), 231 (19), 229 (13), 215 (15), 203 (26), 202 (48), 123 (10), 101 (22), 95 (17). **FTIR** (cm^{-1}): 3054, 2925, 1240, 1204, 814, 742, 496.**HRMS** (ESI-TOF$^+$) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{15}O$ 247.1117; found 247.1111.



Compounds **1s** and **1s'** were obtained as a yellow oil by HPLC preparative eluting with MeOH in 60% isolated yield (0.12 mmol, 30 mg), a mixture of unseparable isomers (**1s:1s'**=10:1). **2-Fluoro-5*H*-dibenzo[*c,f*]chromene (1s). ^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 8.6 Hz, 1H), 7.86 (d, *J* = 2 Hz, 1H), 7.79 – 7.71 (m, 2H), 7.57 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.43 (ddd, *J* = 8.0, 6.9, 1.1 Hz, 1H), 7.28 (dd, *J* = 8.3, 5.8 Hz, 1H), 7.23 (d, *J* = 8.8 Hz, 1H), 7.04 (td, *J* = 8.4, 2.5 Hz, 1H), 5.02 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 162.8 (*J* = 245 Hz), 154.5, 133.8 (*J* = 4 Hz) 131.0, 130.7, 130.1, 129.1, 128.4 (*J* = 3 Hz), 127.5, 127.02, 126.7 (*J* = 4 Hz), 124.3 (x2), 122.6, 118.3, 113.7 (*J* = 23 Hz), 113.2 (*J* = 22 Hz), 68.9. **GC/MS** EI *m/z* 251 (M^+ +1, 22), 250 (M^+, 100), 249 (77), 233 (14), 222 (17), 221 (49), 220 (61), 218 (25), 207 (22), 201 (10), 125 (11), 110(31), 109 (12), 101 (13), 100 (10), 97 (20), 85 (10), 81 (11), 73 (19), 71 (11), 69 (13), 57 (22), 55 (18). **FTIR** (cm^{-1}): 3057, 2922, 1240, 1222, 1022, 824, 803, 589. **HRMS** (ESI-TOF$^+$) *m/z*: $[M - H]^+$ calcd for $C_{17}H_{10}FO$ 249.0721; found 249.0730.



5*H*-Dibenzo[*c,f*]chromene (1q).[10] Titled compound was purified by column chromatography on silica gel eluting with hexane/EtOAc (100:0 → 90:10). Yellow oil was isolated in 17% yield (0.02mmol, 4 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 8.5 Hz, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.76 (d, *J* = 8.8 Hz, 1H), 7.56 (m, 1H), 7.50 – 7.40 (m, 2H), 7.39 – 7.34 (m, 2H), 7.25 (d, *J* = 8.8 Hz, 1H), 5.07 (s, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.6, 132.1, 130.7, 130.3, 130.2, 129.3, 129.0, 128.3, 127.2, 127.00, 126.4, 125.4, 124.9, 124.1, 118.4, 112.5, 69.5. **GC/MS EI** *m/z* 233 (M^+ +1, 18), 232 (M^+ 100), 231 (76), 215 (13), 204 (12), 203 (35), 202 (53), 201 (14) 200 (12), 116 (20), 115 (10), 101 (62), 100 (22), 89 (16), 88 (33), 87 (10), 76 (15), 75 (14), 63 (12).



Compounds **1u** and **1u'** were obtained as a yellow oil by HPLC preparative in 85% isolated yield (46 mg, 0.17 mmol), a mixture of unseparable isomers (**1u:1u´**=15:1). **8*H*-[1,3]dioxolo [4',5':4,5]benzo[1,2-*c*]benzo [*f*] chromene (1u).** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.5 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.59 – 7.48 (m, 2H), 7.40 (m, 1H), 7.22 (d, *J* = 8.8 Hz, 1H), 6.81 (s, 1H), 6.03 (s, 2H), 4.94 (s, 2H). **^{13}C NMR{1H}** (101 MHz, $CDCl_3$) δ 153.5, 147.7, 146.7, 130.8, 130.1, 129.6, 129.0, 128.0, 126.9, 126.4, 124.7,

124.0, 121.8, 118.2, 107.3, 106.3, 101.4, 69.4. **GC/MS EI** *m/z* 276 (M+, 33), 275 (100), 209 (12), 208 (16), 207 (86), 191 (19), 180 (20), 177 (11), 163 (10), 137 (13), 133 (12), 101 (13), 96 (24), 94 (11), 88 (11), 87 (12), 75 (16), 73 (76), 61 (10). **FTIR** (cm^{-1}): 3057, 2922, 1240, 1222, 1012, 816, 751, 589. HRMS (ESI-TOF$^+$) m/z: $[M + Na]^+$ calcd for $C_{18}H_{12}NaO_3$ 299.0671; found 299.0671.

5. Spectroscopic Studies

5.1. Spectroscopic measurements. The UV-vis measurements were carried out in a Shimadzu UV-2101 PC. All measurements were carried out under an inert atmosphere of nitrogen, in quartz cuvettes, at room temperature. Solutions of KO^{t}Bu, NaO^{t}Bu and NaH in DMSO were prepared at time of use. UV-vis spectra were recorded on UV-vis spectrophotometer.

5.2. UV-Vis spectra in DMSO

UV-vis spectra of compound **5b** in DMSO and a solution of KO^{t}Bu in DMSO (3 equiv) are presented in Figure S4.

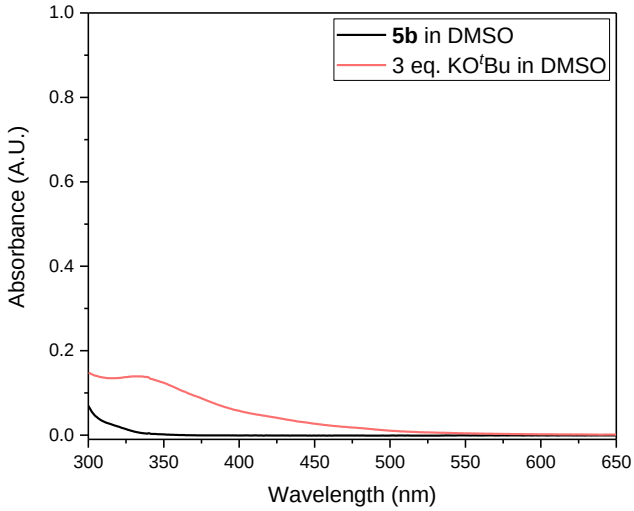


*Figure S4. UV-vis spectrum for compound **5b** (8.3 mM) in DMSO (in black) and dimsyl anion (in red) under N_2 atmosphere.*

UV-vis spectra of compound **5b** with increasing concentrations of KO^{t}Bu in DMSO are presented in Figure S5.

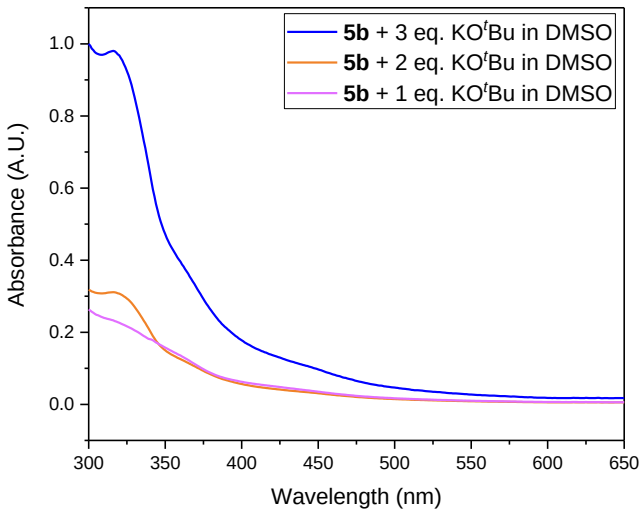


*Figure S5. UV-vis spectrum for compound **5b** in DMSO with KO^{t}Bu (8.3 mM) under N_2 atmosphere.*

A yellow coloration is observed when there is an increase in the concentration of the base in the mixture of the compound **5b** and KO^{t}Bu in DMSO. The same coloration was observed when NaO^{t}Bu or NaH were used (Figure S6).

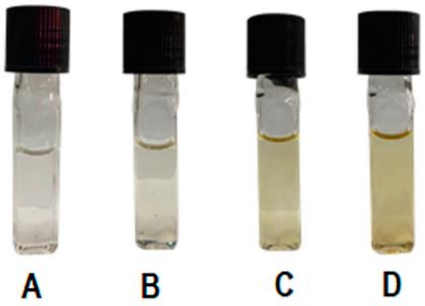


*Figure S6. Solution of compound **5b** in DMSO (**A**). Mixtures of: **1b** with 1 eq. of KO^{t}Bu in DMSO (**B**), **1b** with 2 eq. of KO^{t}Bu in DMSO (**C**) and **1b** with 3 eq. of KO^{t}Bu in DMSO (**D**).*

Next, Figure 7 shows the UV-vis spectra of compound **5b** with KO^{t}Bu or NaO^{t}Bu in DMSO.

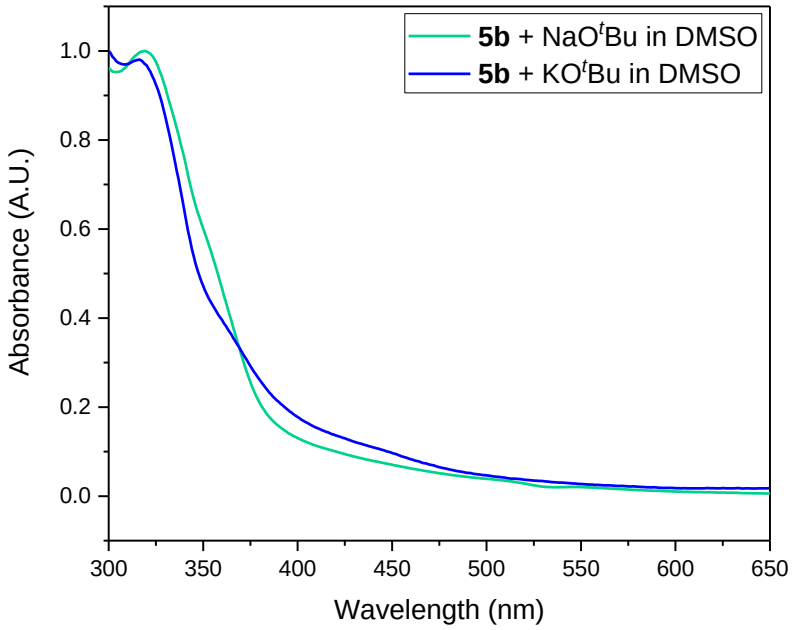


*Figure S7. UV-vis spectrum for compound **5b** (8.3 mM) in DMSO with bases as KO^{t}Bu or NaO^{t}Bu under N_2 atmosphere.*

The dimsyl anion was also formed using NaH (Figure S8). The same UV-vis spectrum was observed when a solution of compound **5b** in DMSO was treated with NaH. However, NaH was previously washed twice with hexane to eliminate the mineral oil presented in the dispersion; otherwise the λ_{max} changes because of the presence of the oil.

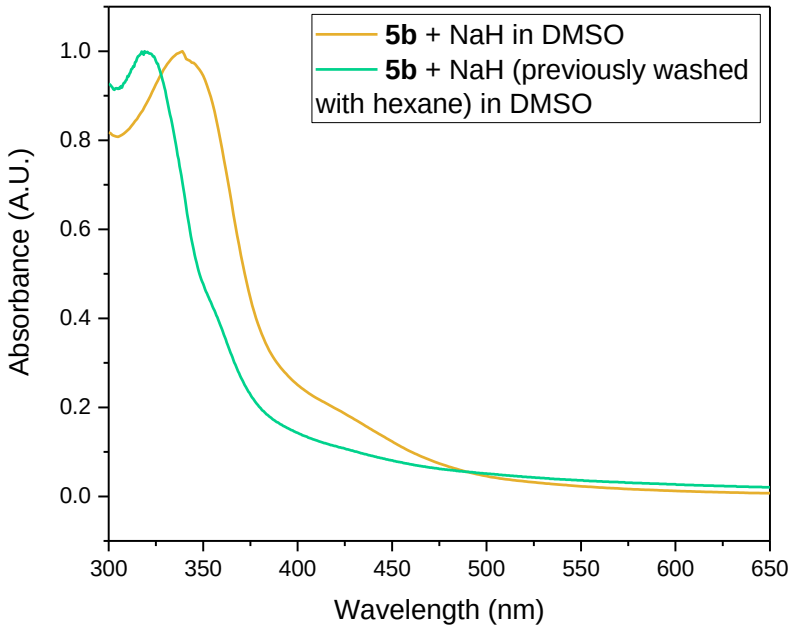


*Figure S8. UV-vis spectrum for compound **5b** in DMSO with NaH as base under N_2 atmosphere.*

6. Computational Procedure

6.1. General considerations. The experimental behavior of the system was investigated by molecular modeling calculations with the DFT methodology, the B3LYP,[11] M062X[12] and ωB97XD[13] functionals, the def2-tzvp basis set[14] with ECP for iodine,[15] downloaded from the BSE website,[16] and the PCM continuum solvent model (DMSO)[17] as implemented in Gaussian16 (Rev. C.01). Models of the reaction profiles were explored by using the distinguished reaction coordinate scan. The characterization of stationary points was done by Hessian matrix calculations. The energy informed for TSs, anions and radical anions includes zero-point and thermochemical corrections and corresponds to free energy differences at 298 K.

6.2 LUMO Orbital descriptions

Figures S9, S10 and S11 include a representation of the LUMO orbital for the molecules **5b**-**5p** with B3LYP and ωB97XD functionals. An isovalue of ± 0.03 was employed for all the representations.

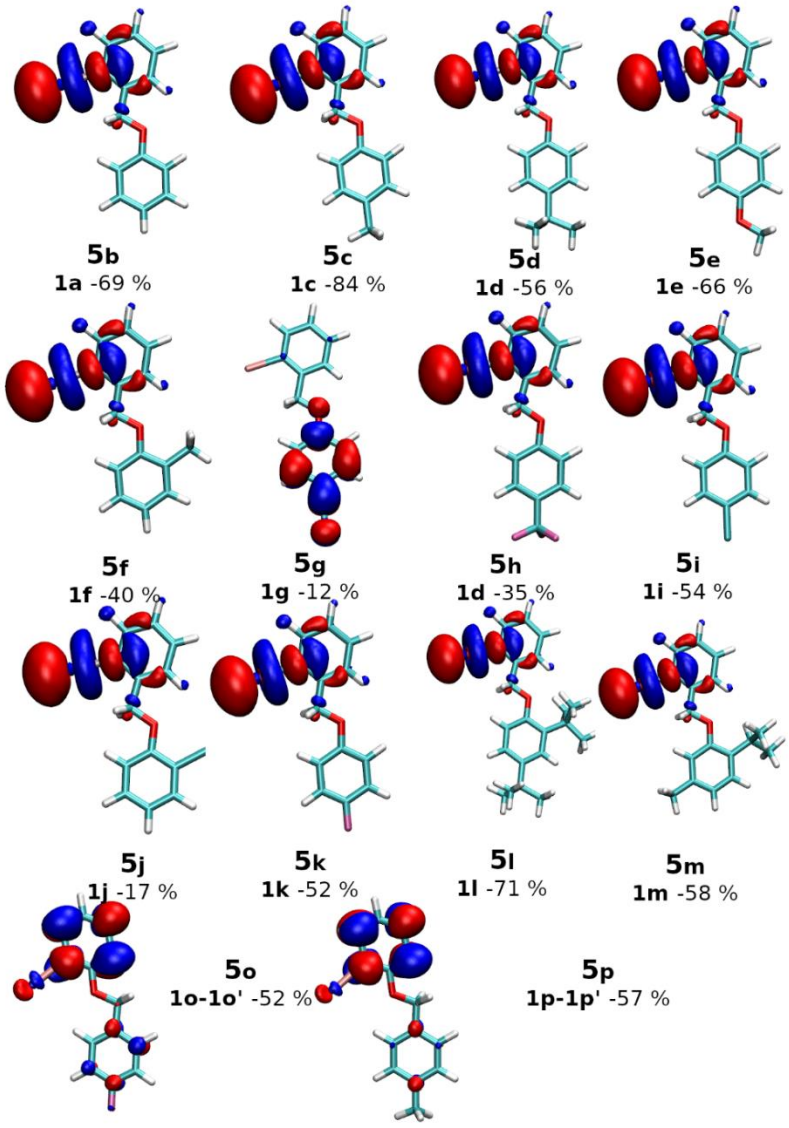


*Figure S9. LUMO representations of molecules **5b-5p** at B3LYP/def2-TZVP basis set and ECP for iodine. An isovalue of ± 0.03 was employed.*

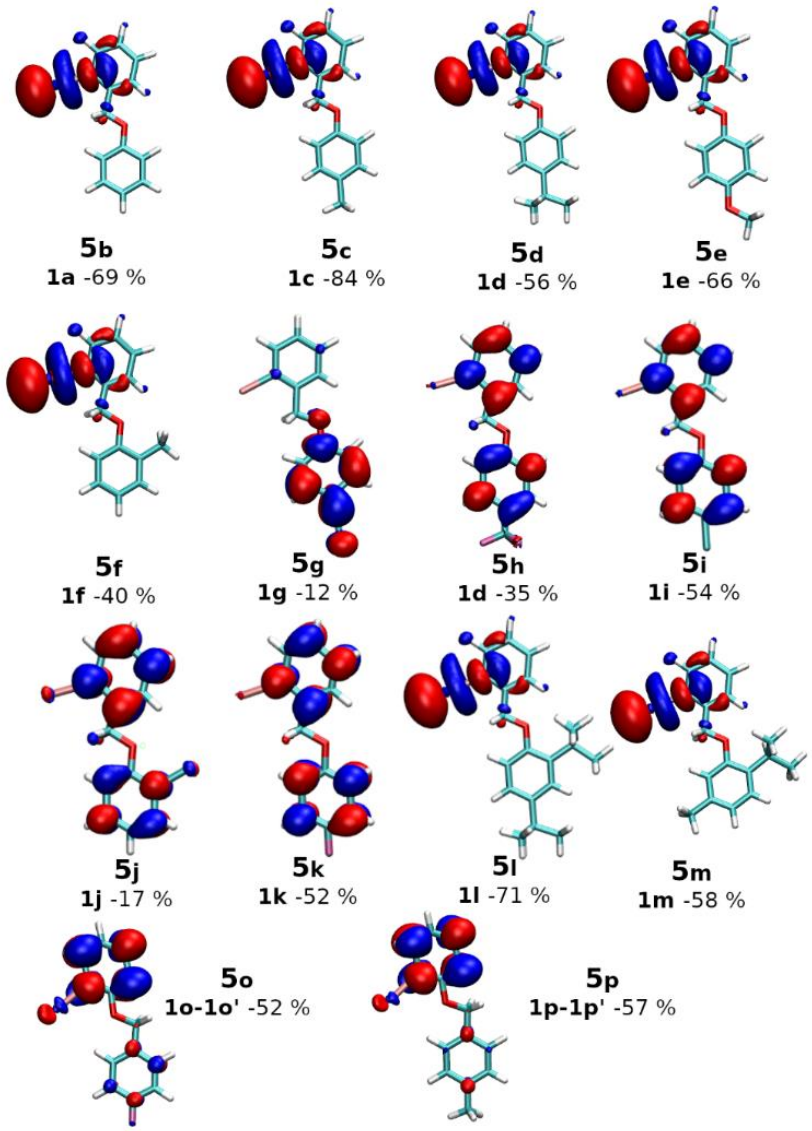


*Figure S10. LUMO representations of molecules **5b-5p** at M062X/def2-TZVP basis set and ECP for iodine. An isovalue of ± 0.03 was employed.*

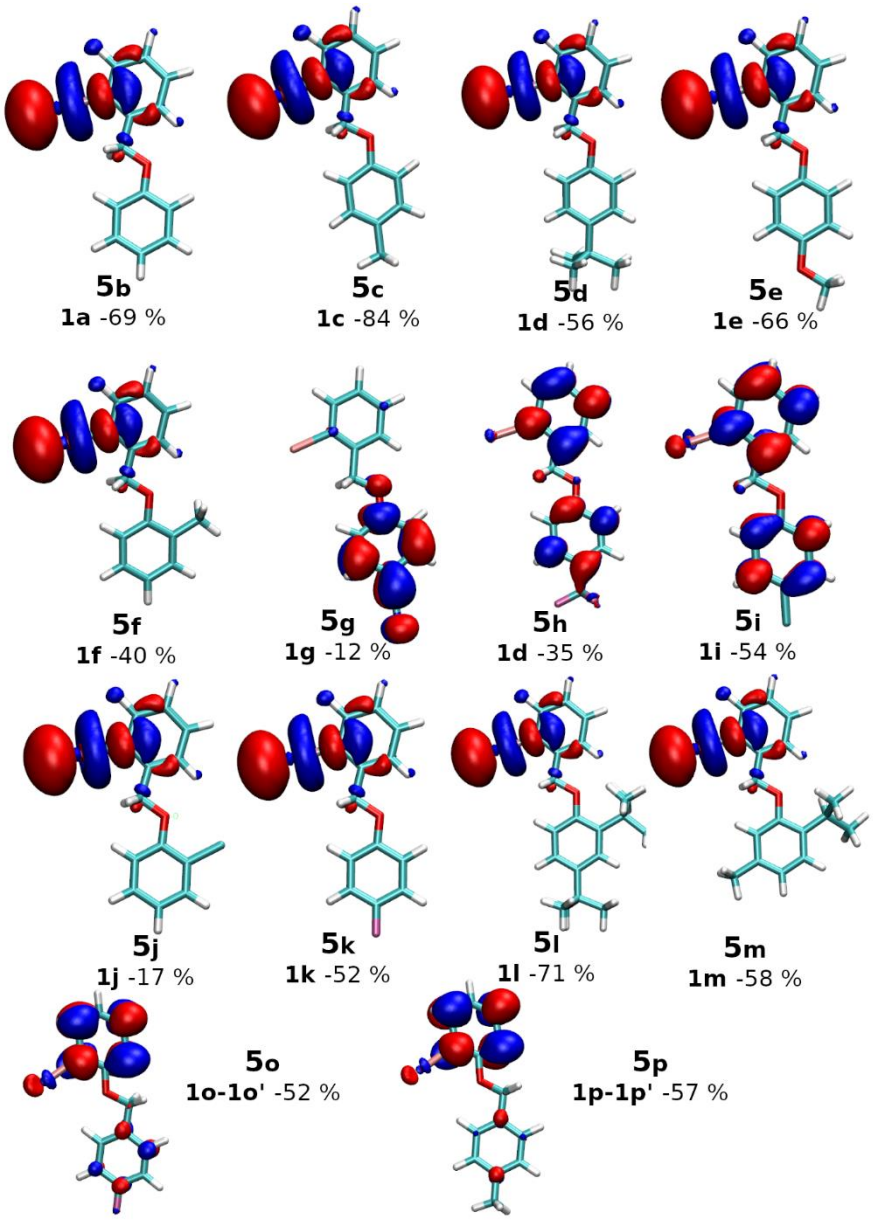


*Figure S11. LUMO representations of molecules **5b-5p** at ωB97XD/def2-TZVP basis set and ECP for iodine. An isovalue of ± 0.03 was employed.*

6.3 Analysis of the EDA complex formation.

In order to study the possible formation of an EDA complex, the CREST software was employed.[18]

Starting from an aleatory geometry of DMSO and substrate **5b**, 250 geometries of different complexes were obtained evaluated at TB-DFT level with the XTB+ approximation. The first 10 geometries were extracted, a H^+ from DSMO was removed, to form dimsyl anion, and this 10 tentative EDA complexes were evaluated with M062X/def2svp SCRF(IEFPCM, DMSO), Table S5.

*Table S5. Computed energies, in a.u. for the different evaluated geometries of **5b**-dimsyl anion complexes.*

COMPLEX	SCF ENERGY	Free ENERGY	Comp. rate
A	-1426.505166	-1426.284866	0.007
B	-1426.504966	-1426.284244	0.004
C	-1426.501516	-1426.281716	0.000
D	-1426.498813	-1426.279479	0.000
E	-1426.494878	-1426.274868	0.000
F	-1426.508752	-1426.286698	0.050
G	-1426.509567	-1426.28941	0.891
H	-1426.509677	-1426.286646	0.048

After carrying out a population analysis at 298 K, complex **G** was selected. The next step was the optimization at a higher level with B3LYP/def2tzvp SCRF(IEFPCM, DMSO) and M062X/deftzvp SCRF(IEFPCM, DMSO). These results are given in Table *S6* and in Figure *S12*.

Complexes obtained with:

B3LYP/ def2tzvp SCRF(IEFPCM, DMSO) **M062X/ def2tzvp SCRF(IEFPCM, DMSO)**

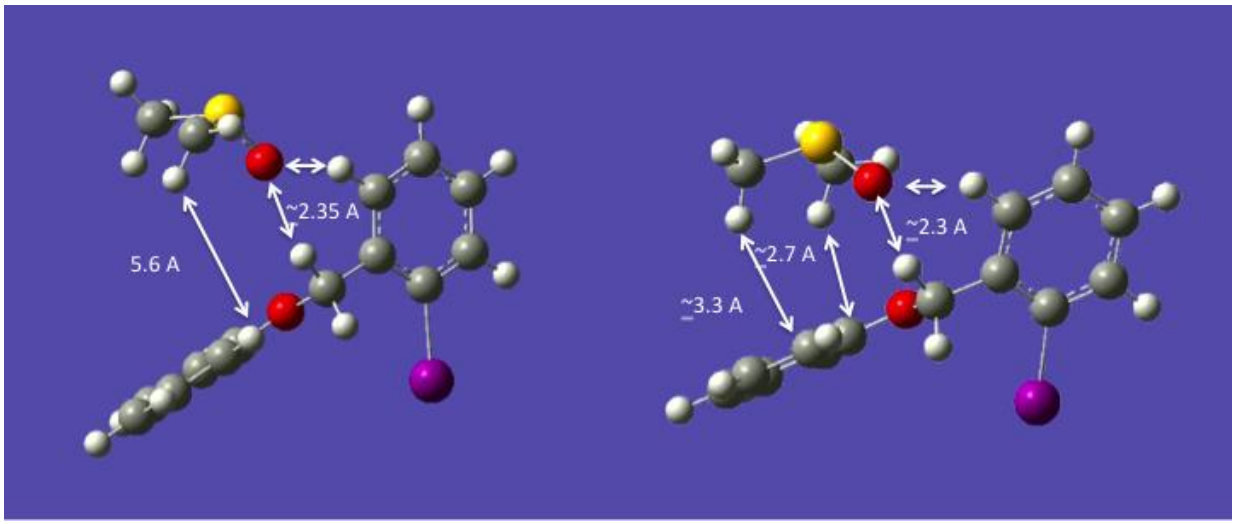


Figure S12. Most stable structure for EDA complex with B3LYP/ def2tzvp (left) and M062X/def2tzvp (right).

Table S6. Energies involved in the computation of EDA complexes.

Molecule	B3LYP		M062X	
	SCF energy (a.u)	Free Energy (a.u)	SCF energy (a.u)	Free Energy (a.u)
5b	-875.242601	-875.082772	-874.828819	-874.665770
Dimsyl anion	-552.783902	-552.748008	-552.674133	-552.635852
EDA Complex	-1428.033321	-1427.818981	-1427.511353	-1427.291785
ΔE (kcal/mol)	-4.3	7.4	-5.3	6.2

6.4 Extract of important information from TD-DFT calculation of the excited states of the EDA complex.

For the B3LYP complex:

Excited state symmetry could not be determined.
Excited State 1: Singlet-?Sym 3.1855 eV 389.21 nm f=0.0049 <S**2>=0.000
82 -> 83 0.70101
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1427.91617334

For the M062X complex (Figures S13 and S14):

Excited state symmetry could not be determined.
Excited State 2: Singlet-?Sym 4.9733 eV 249.30 nm f=0.0033 <S**2>=0.000
80 -> 86 -0.10931
82 -> 83 -0.25120
82 -> 84 0.28497
82 -> 85 -0.28768
82 -> 86 0.49774

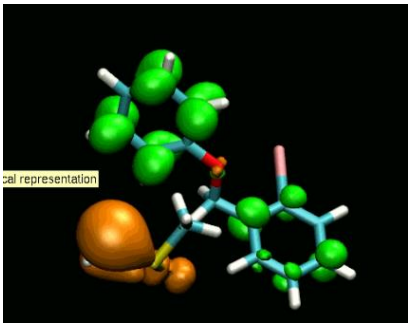


Figure S13. Isosurfaces of hole (orange) and electron (green) distributios, with an isovalue of 0.002. Second excited state.

Excited state symmetry could not be determined.
Excited State 3: Singlet-?Sym 5.0438 eV 245.82 nm f=0.0019 <S**2>=0.000
82 -> 83 0.48125
82 -> 84 -0.34253
82 -> 85 -0.13999
82 -> 86 0.32736

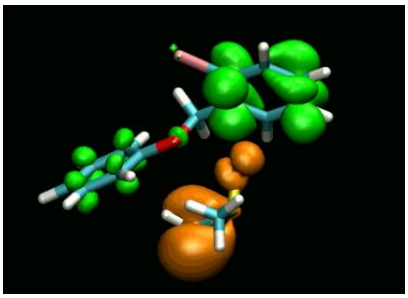


Figure S14. Isosurfaces of hole (orange) and electron (green) distributios, with an isovalue of 0.002. Third excited state.

6.5 Energy of the species involved in the initiation step.

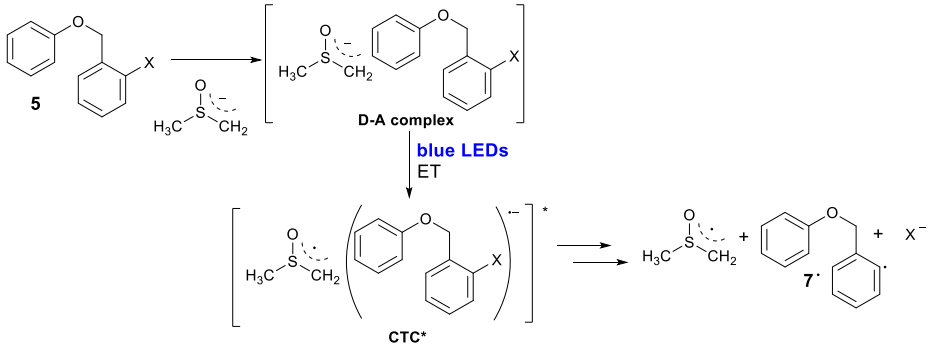


*Figure S15. Initiation step mechanism for substrate **5**.*

Table S7. Energies involved in the computation of ET in the initiation step.

	Molecule	B3LYP		M062X	
		SCF energy (a.u)	Free Energy (a.u)	SCF energy (a.u)	Free Energy (a.u)
Reactant 1 (R1)	**5b**	-875.242601	-875.082772	-874.828819	-874.665770
	Dimsyl anion	-552.783902	-552.748008	-552.674133	-552.635852
Reactant 2 (R2)	EDA Complex	-1428.033321	-1427.818981	-1427.511353	-1427.291785
Reactant 3 (R3)	(EDA Complex)*	-1427.916173	--	-1427.362512	--
Product	Dimsyl radical	-552.6481779	-552.612038	-552.529832	-552,493139
	7a•	-577.358607	-577.19824	-577,112113	-576,948676
	I^-	-297.992643	-298.009491	-297,819076768	-297,835925
ΔEnergy (kcal/mol)	**Prod – R1**	17.0	6.9	26.3	15.0
	Prod – R2	21.3	-0.49	31.6	8.8
	Prod – R3	-52.2	--	-61.8	--

The excited states could not be optimized since they dissociate in radical **7•** and I^-.

6.6 Energies of the species involved in the propagation cycle.

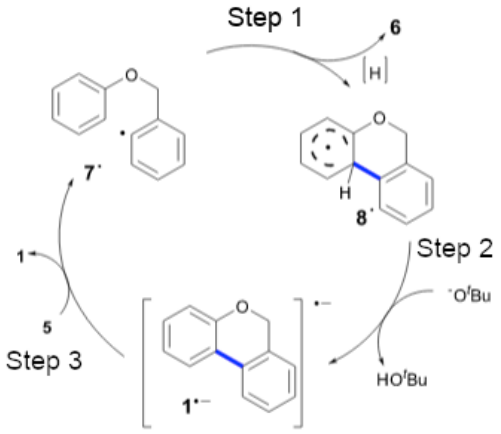


Figure S16. Propagation cycle for BHAS mechanism.

Table S8. Energies involved in the propagation cycle.

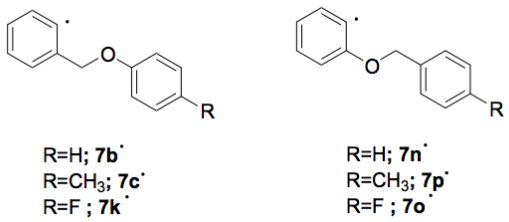
	Molecule	B3LYP		M062X	
		SCF energy (a.u)	Free Energy (a.u)	SCF energy (a.u)	Free Energy (a.u)
Step 1	**7a**$^{\bullet}$	-577.358607	-577.19824	-577.112113	-576.948676
	8a$^{\bullet}$	-577.386968	-577.222247	-577.1418527	-576.974649
ΔEnergy (kcal/mol)		-17.8	-15.1	-18.7	-16.3

	Molecule	B3LYP		M062X	
		SCF energy (a.u)	Free Energy (a.u)	SCF energy (a.u)	Free Energy (a.u)
Step 2	**8a**$^{\bullet}$	-577.386968	-577.222247	-577.1418527	-576.974649
	^{t}BuO^{-}	-233.258565	-233.166688	-233.138394	-233.044735
	1a$^{\bullet-}$	-576.91506498	-576.76349	-576.915065	-576.76349
	^{t}BuOH	-233.779098768	-233.673234	-233.657789	-233.5506358
ΔEnergy (kcal/mol)		-30.5	-30.0	-33.1	-32.6

	Molecule	B3LYP		M062X	
		SCF energy (a.u)	Free Energy (a.u)	SCF energy (a.u)	Free Energy (a.u)
Step 3	**1a**$^{\bullet-}$	-576.91506498	-576.76349	-576.915065	-576.76349
	5a	-875.242601	-875.082772	-874.828819	-874.665770
	7a$^{\bullet}$	-577.358607	-577.19824	-577.112113	-576.948676
	I^{-}	-297.992643	-298.009491	-297.819076	-297.835925
	1a	-576.851127	-576.693460	-576.612217182	-576.452307
ΔEnergy (kcal/mol)		-1.2	-1.5	5.5	5.2

6.7 Product regiochemistry Discussion

The studies of the regiochemistry of the coupling of the different substrates were divided in two sections, one for 2-halobenzylphenyl ethers **5a**-**m** and the other for 2-halophenylbenzyl ethers **5n**-**p**. The six model radicals shown in the Figure S17 were employed.



R=H; **7b**$^{\bullet}$
R=CH_3; **7c**$^{\bullet}$
R=F ; **7k**$^{\bullet}$

R=H; **7n**$^{\bullet}$
R=CH_3; **7p**$^{\bullet}$
R=F ; **7o**$^{\bullet}$

Figure S17: Starting radicals employed as reactant for the DFT studies

6.7.1 6-*endo vs* 5-*exo* coupling of radicals 7b,7c and 7k

In Figure S18 is represented the proposed mechanism for the reaction of radicals **7a**-**7m**, formed from the respective 2-halobenzyl-phenyl ethers, which will finally give compounds **1a**-**1m**. It should be mentioned that with these substrates only the product from 6-*endo* radical coupling was experimentally obtained. This regiochemsitry could be explained based on the differences in the activation energies of the 6-*endo* vs 5-*exo*, presented in Tables S9 and S10.

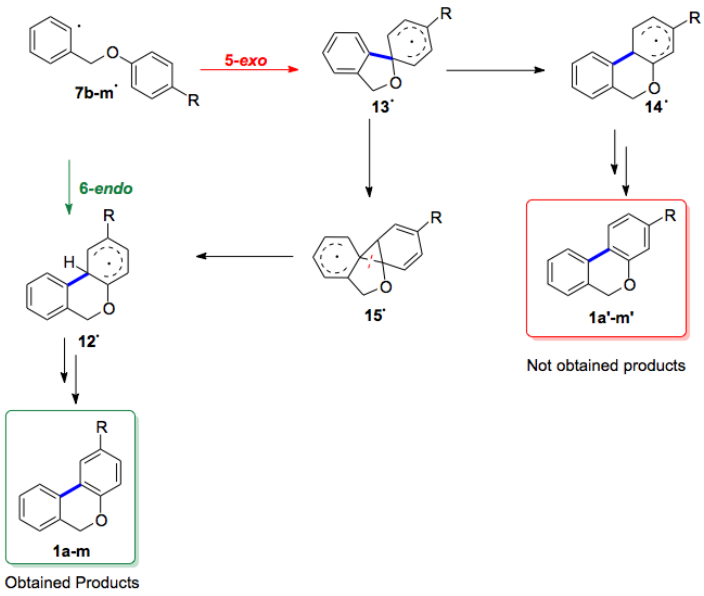


*Figure S18. Possible radical pathway for the intramolecular photocyclization reaction of **7b-m**.*

*Table S9. Free activation energy and ΔG (in kcal.mol^{-1}) for 6-endo cyclization for **7b**, **7c** and **7k***

7, R/Energies	**B3LYP**		**M062X**	
	ΔG_R	ΔG_{act} (E_{act})	ΔG_R	ΔG_{act} (E_{act})
7c, CH_3	-13.9	11.2	-17.1	10.1
7k, F	-18.2	8.6	-20.4	9.5
7b, H	-16.8	8.8	-19.0	9.9

*Table S10. Free activation energy and ΔG (in kcal.mol^{-1}) for 5-exo cyclization for **7b**, **7c** and **7k***

7, R/Energies	**B3LYP**		**M062X**	
	ΔG_R	ΔG_{act} (E_{act})	ΔG_R	ΔG_{act} (E_{act})
7c, CH_3	-15.5	15.1	-16.5	10.4
7k, F	-14.7	14.6	-14.3	11.0
7b, H	-13.7	14.0	-14.0	11.3

Table S11. Activation energies differences for 6-*endo* vs 5-*exo* (in kcal.mol^{-1})

7, R/Energies	**B3LYP**	**M062X**
	ΔG_{act} ($\Delta E_{act=}$ $E_{act\ 6\text{-}endo}$ - $E_{act\ 5\text{-}exo}$)	ΔG_{act} ($\Delta E_{act=}$ $E_{act\ 6\text{-}endo}$ - $E_{act\ 5\text{-}exo}$)
7c, CH_3	-3.9	-0.3
7k, F	-6.0	-1.5
7b, H	-5.2	-1.4

As it is shown in Tables *S9* and *S10* the 6-*endo* coupling is favored over 5-*exo* due to lower free activation energies barriers for this radical cyclization. A higher energy difference between both activation barrier (for example, for B3LYP: ΔEa = -3.9 kcal.mol^{-1} for CH_3, ΔEa = -6.0 kcal.mol^{-1} for F and ΔEa = -5.2 kcal.mol^{-1} for H) was found (Table *S11*).

6.7.2 6-*endo* vs 5-*exo* coupling of radicals 7n,7o and 7p

In Figure S19 is represented the proposed mechanism for the reaction of radicals **7n**-**7p**, formed from the respective 2-halophenylbenzyl ethers, which will finally give compounds **1a**, and **1o**-**1p**. It should be mentioned that with these substrates two regioisomers of the products formed from 6-*endo* and 5-*exo* radical coupling were experimentally obtained. This regiochemsitry could be explained based on the differences in the activation energies of the 6-*endo vs* 5-*exo*, presented in Tables S12 and S13.

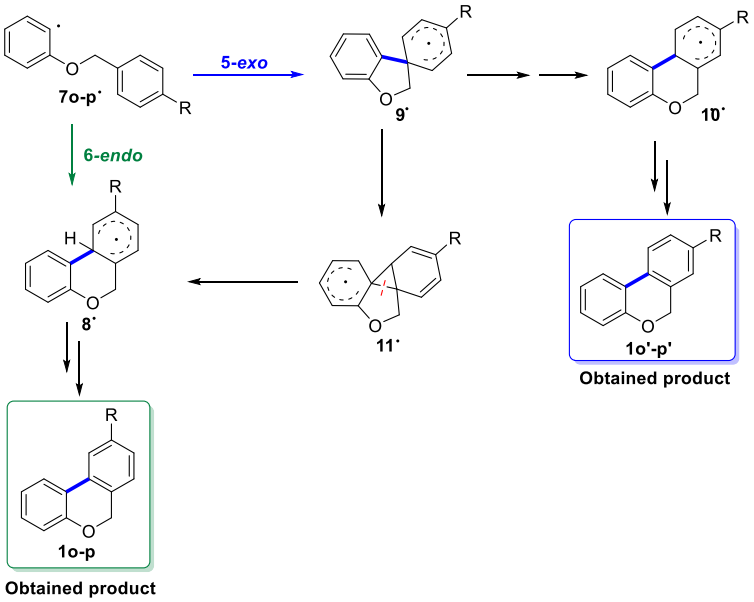


*Figure S19. Possible radical pathway for the intramolecular photocyclization reaction of **7n-o**.*

*Table S12. Free activation energy and ΔG (in kcal.mol^{-1}) for 6-endo cyclization for **7n**, **7o** and **7p***

7, R/Energies	**B3LYP**		**M062X**	
	ΔG_R	ΔG_{act} (E_{act})	ΔG_R	ΔG_{act} (E_{act})
7p, CH_3	-14.3	9.6	-16.0	10.8
7o, F	-15.3	9.2	-16.4	10.7
7n, H	-15.0	9.4	-16.0	10.8

*Table S13. Free activation energy and ΔG (in kcal.mol^{-1}) for 5-exo cyclization for **7n**, **7o** and **7p***

7, R/Energies	**B3LYP**		**M062X**	
	ΔG_R	ΔG_{act} (E_{act})	ΔG_R	ΔG_{act} (E_{act})
7p, CH_3	-13.7	8.1	-15.0	9.3
7o, F	-13.0	8.2	-14.3	9.8
7n, H	-13.2	8.1	-14.5	9.6

Table S14. Activation energies differences for 6-endo vs 5-exo (in kcal.mol^{-1})

7, R/Energies	**B3LYP**	**M062X**
	ΔG_{act} (ΔE_{act}= $E_{act\ 6\text{-}endo}$ - $E_{act\ 5\text{-}exo}$)	ΔG_{act} (ΔE_{act}= $E_{act\ 6\text{-}endo}$ - $E_{act\ 5\text{-}exo}$)
7p, CH_3	1.5	1.5
7o, F	1.0	0.9
7n, H	1.3	1.3

As it is shown in Tables *S12* and *S13* the free activation energies (Ea) of 5-*exo* are lower Ea 6-*endo.* However, a low energy difference between both activation barriers (for example, for B3LYP: ΔEa = 1.5 kcal.mol^{-1} for CH_3, ΔEa = 0.9 kcal.mol^{-1} for F, and ΔEa = 1.3 kcal.mol^{-1} for H) was found. According to this, a mixture products **1o-p**/**1o´-p´** were experimentally obtained.

6.8 Energies of the species involved in the comparation of EAs of 1a-m and 5b-m.

*Table S15 Energies of the species involved in the comparation of EAs of **5b-m** with B3LYP*

Substrate 5x	Neutral B3LYP		RA B3LYP	Eas
x	SCF Energy	Free Energy	SCF Energy	Vert EA
5b	−875,2426	−875,08277	−875,29525	−1,43
5c	−875,2426	−875,08277	−875,29525	−1,43
5d	−1032,55244	−1032,28794	−1032,60493	−1,43
5e	−989,81161	−989,62314	−989,86404	−1,43
5f	−914,57391	−914,38837	−914,62646	−1,43
5g	−967,52704	−967,37097	−967,58512	−1,58
5h	−1212,43889	−1212,28137	−1212,49211	−1,45
5i	−1334,8681	−1334,72	−1334,92105	−1,44
5j	−1334,86586	−1334,71754	−1334,91893	−1,44
5k	−974,52313	−974,37292	−974,57594	−1,44
5k5	−1189,85612		−1189,90863	−1,43
5l	−1067,23889	−1067,02084	−1067,28855	−1,35
5m	−1032,55773	−1032,29478	−1032,61019	−1,43
5p	−974,52604	−974,37626	−974,63157	
5q	−875,2426	−875,08277	−875,29525	−1,43

Note: Comma is employed as decimal separator

*Table S16 Energies of the species involved in the comparation of EAs of **5b-m** with M062X*

Substrate 5x	Neutral M062X		RA M062X	Eas
x	SCF Energy	Free Energy	SCF Energy	Vert EA
5b	−874,82882	−874,66577	−874,87554	−1,27
5c	−914,13863	−913,95068	−914,18516	−1,27
5d	−1032,0615	−1031,79229	−1032,10813	−1,27
5e	−989,35384	−989,16147	−989,40036	−1,27
5f	−914,14058	−913,9515	−914,18721	−1,27
5g	−967,08509	−966,92586	−967,14059	−1,51
5h	−1211,92404	−1211,76263	−1211,95580	−0,86
5i	−1334,43244	−1334,28111	−1334,46335	−0,84
5j	−1334,43133	−1334,27999	−1334,46934	−1,03
5k	−974,08125	−973,92777	−974,11114	−0,81
5k5	−1189,29155	−1188,91448	−1189,33828	−1,27
5l	−1066,74565	−1066,52352	−1066,79364	−1,31
5m	−1032,06516	−1031,79701	−1032,11173	−1,27
5p	−974,08232	−973,93023	−974,12033	−1,03
5q	−914,13875	−913,95263	−914,17638	−1,02

*Table S17 Energies of the species involved in the comparation of EAs of **1a-m** with B3LYP*

Product	Neutral B3LYP		RA B3LYP		Eas	
	SCF Energy	Free Energy	SCF Energy	Free Energy	Vert EA	Ad EA
1a	−576,851127	−576,693460	−576,91506	−576,76349	−1,74	−1,91
1c	−616,181804	−615,998443	−616,24512	−616,06955	−1,72	−1,93
1d	−734,160874	−733,898429	−734,22278	−733,96665	−1,68	−1,86
1e	−691,420398	−691,234156	−691,48520	−691,30508	−1,76	−1,93
1f	−616,182558	−615,999411	−616,24430	−616,06784	−1,68	−1,86
1g	−669,134891	−668,981152	−669,20894	−669,06155	−2,01	−2,19
1h	−914,046897	−913,891430	−914,11798	−913,96889	−1,93	−2,11
1i	−1036,476417	−1036,330498	−1036,54675	−1036,40673	−1,91	−2,07
1j	−1036,474262	−1036,328177	−1036,54347	−1036,40337	−1,88	−2,05
1k	−676,13177	−675,983695	−676,20138	−676,05918	−1,89	−2,05
1l	−891,466432	−891,098202	−891,52529	−891,16347	−1,60	−1,78
1m	−773,481633	−773,191845	−773,53979	−773,25609	−1,58	−1,75
1o	−676,132983	−675,984882	−676,20220	−676,06004	−1,88	−2,05
1p	−616,182571	−616,001436	−616,24579	−616,06935	−1,72	−1,85

*Table S18 Energies of the species involved in the comparation of EAs of **1a-m** with M062X*

Product	Neutral M062X		RA M062X		Eas	
	SCF Energy	Free Energy	SCF Energy	Free Energy	Vert EA	Ad EA
1a	−576,61222	−576,452310	−576,67526	−576,52076	−1,72	−1,86
1c	−615,92196	−615,736140	−615,98467	−615,80555	−1,71	−1,89
1d	−733,84498	−733,578860	−733,90677	−733,64622	−1,68	−1,83
1e	−691,13756	−690,948200	−691,20223	−691,01834	−1,76	−1,91
1f	−615,92353	−615,737810	−615,98456	−615,80491	−1,66	−1,83
1g	−668,86774	−668,711760	−668,94056	−668,79008	−1,98	−2,13
1h	−913,7068	−913,548820	−913,77739	−913,62427	−1,92	−2,05
1i	−1036,21559	−1036,067470	−1036,28532	−1036,14245	−1,90	−2,04
1j	−1036,2141	−1036,065740	−1036,28258	−1036,13954	−1,86	−2,01
1k	−675,86472	−675,714360	−675,93368	−675,78857	−1,88	−2,02
1l	−891,07545	−890,702250	−891,13473	−890,76711	−1,61	−1,76
1m	−773,14883	−772,854930	−773,20664	−772,91826	−1,57	−1,72
1o	−675,866	−675,715610	−675,93452	−675,78944	−1,86	−2,01
1p	−615,92269	−615,738540	−615,98532	−615,80577	−1,70	−1,83

6.9. xyz-stationary points of calculated structures

XYZ Coordinates of Substrate 5b-p

Substrate 5b
26

C	3.129541821168	1.389875790441	2.484560077193
C	4.110575516802	1.309575473178	3.455778183551
C	4.177779515506	0.206210244447	4.303066035794
C	3.249918178457	-0.812146184047	4.161755159269
C	2.255492762930	-0.747450906509	3.188966055687
C	2.198397515975	0.360066438935	2.348806627678
O	1.270856064174	0.527150156275	1.366513330196
C	0.317011815729	-0.494693677255	1.189747616414
C	-0.612344854027	-0.130972017036	0.064079174984
C	-0.476899388006	1.067646191116	-0.631167487276
C	-1.339781359731	1.396064478890	-1.667362841636
C	-2.357978294414	0.526702688449	-2.027717782532
C	-2.511936224924	-0.674298073965	-1.348592016241
C	-1.642522629295	-0.989737201013	-0.315091495062
I	-1.922067766497	-2.820553023401	0.676412338139
H	3.064752111923	2.240721426151	1.818847719160
H	4.828735923008	2.113634606124	3.553084433825
H	4.945902494943	0.145429192763	5.062078420292
H	3.289266621315	-1.676181550241	4.812674951826
H	1.544949294935	-1.556580042930	3.102040775599
H	-0.258875378291	-0.638364449715	2.111199030472
H	0.817252285200	-1.443235933043	0.963888055089
H	0.316826368308	1.744858812375	-0.349687401972
H	-1.213727697063	2.333779443554	-2.192249656201
H	-3.035006489776	0.774765138088	-2.834359174532
H	-3.302778208350	-1.358957021634	-1.622830129718

Substrate 5c
29

C	3.168204138178	1.360191705082	2.450520828882
C	4.141230159816	1.277556140757	3.426687093144
C	4.192981761291	0.199354643093	4.315464369168
C	3.229849799629	-0.789264467853	4.183230949972
C	2.237648022521	-0.726813337989	3.205505646534
C	2.208118304917	0.354210827813	2.334925069000
O	1.287681570016	0.519771841245	1.342792310911
C	0.301502421789	-0.475649715209	1.204077566579
C	-0.620523232165	-0.123442798296	0.068709582043
C	-0.436403673846	1.032965473872	-0.684349153236
C	-1.291212729925	1.350281635370	-1.730663800737
C	-2.349988692850	0.511620537561	-2.043744633144
C	-2.553024489017	-0.647051310686	-1.306607283960
C	-1.691453235945	-0.951506005868	-0.263320572765
I	-2.048599817322	-2.715999730620	0.818830116779
H	3.131904029074	2.196664237299	1.764456480027
H	4.880465338688	2.066767400128	3.504395599702
H	3.242496965719	-1.638509790646	4.856363188484
H	1.508773435958	-1.521967986548	3.142431783188
H	-0.274669587775	-0.568963356628	2.131871250246
H	0.769556423468	-1.447926058350	1.010718080193
H	0.389203894667	1.685955975056	-0.439808686429
H	-1.127003070734	2.255179314092	-2.300625566286
H	-3.020973962170	0.751247063643	-2.857937846278
H	-3.376027465687	-1.307391267824	-1.543235203649
C	5.260573012245	0.128115533161	5.372677485963
H	5.163493317475	-0.779265857662	5.967033344517
H	6.255903728121	0.136779614398	4.925173897191
H	5.201225083862	0.984031121609	6.047268443963

Substrate 5d
38

C	3.099952906826	1.404069932701	2.460300614790
C	4.090780168432	1.340982383562	3.430556504736
C	4.205746681373	0.251095543711	4.300117165284
C	3.270545736146	-0.774311433633	4.142481832389
C	2.268697826395	-0.732770772052	3.177068894431
C	2.179727277949	0.366880270271	2.324904799707
O	1.240899852254	0.517192968934	1.342098702905
C	0.281470489796	-0.511731181039	1.161710765419
C	-0.653660201677	-0.148390506334	0.035540619986
C	-0.507378011142	1.045966791429	-0.673033177710
C	-1.368025404800	1.381029768775	-1.711268087337
C	-2.400101876833	0.522245490116	-2.065010933781
C	-2.567726559385	-0.673438365796	-1.375442799115
C	-1.699945999386	-0.995990713137	-0.339175176247
I	-2.025323192978	-2.842406509303	0.663629773671
H	3.030881078059	2.258269713622	1.798639538959
H	4.782352185555	2.168598194756	3.498501915242
H	3.309093361591	-1.643901762073	4.786315336452
H	1.574370680833	-1.557156412493	3.104668829648
H	-0.289568518649	-0.658821303755	2.085131830250
H	0.784448137328	-1.458556846618	0.935232189358
H	0.295015510397	1.715168897751	-0.399150186676
H	-1.229033983461	2.314156076329	-2.241795703174
H	-3.076151179921	0.773236164668	-2.872105920243
H	-3.368999029275	-1.347018877943	-1.645240930364
C	5.291043890796	0.151449990756	5.382680320205
C	4.627662113564	0.035507023247	6.771056141078
C	6.158726241169	-1.099448362227	5.130477290072
C	6.214240118806	1.378885565748	5.395441171434
H	4.013936182927	0.913535714243	6.983685154033
H	3.989395718221	-0.846267436757	6.841814774568
H	5.390671076840	-0.041543746793	7.549382812567
H	6.651612841679	-1.041414188128	4.157602303574
H	6.931928912428	-1.184354396020	5.897874875016
H	5.565021817373	-2.014332007479	5.152806578132
H	6.964969983035	1.261527270457	6.179173879747
H	6.742527997954	1.500377500028	4.447719484865
H	5.663975359780	2.299401500478	5.600247976128

Substrate 5e
30

C	2.880923592790	1.495845938392	2.707936438777
C	3.819916540225	1.463057568070	3.731784060531
C	3.917473615632	0.338081768088	4.552954650143
C	3.063931184461	-0.740021555737	4.328568274382
C	2.124842971166	-0.707667982859	3.304708944785
C	2.028543034725	0.417755056929	2.485031028191
O	1.139970480653	0.554747851704	1.449984991316
C	0.253587359925	-0.516958883867	1.179311089072
C	-0.633462029298	-0.166064177478	0.010947633106
C	-0.526088598053	1.066016196662	-0.637366473339
C	-1.343198004769	1.390864818835	-1.713347900262
C	-2.291555573483	0.483579011874	-2.166495690369
C	-2.419067797050	-0.750364978725	-1.538454203040
C	-1.595437438163	-1.062080290752	-0.463603857568
I	-1.855379218860	-2.969112673598	0.440071501347
H	2.803921909886	2.367197207697	2.070403234811
H	4.465207608204	2.317014686912	3.876190273088
H	3.140963167122	-1.611549703050	4.965926409620
H	1.480769315389	-1.562784997237	3.161816281585
H	-0.362469861719	-0.728713898780	2.060846063028

H	0.820842861136	-1.427096810710	0.953171852630
H	0.211195243818	1.772860484339	-0.285922617127
H	-1.235996022116	2.354072774751	-2.195243963977
H	-2.933171632937	0.726096350429	-3.003719678322
H	-3.155122438854	-1.461816982781	-1.885717721415
O	4.804389913113	0.205677283299	5.584236436400
C	5.697742871789	1.281084446125	5.849963816740
H	6.303118067498	0.965703168171	6.696176609431
H	6.347976416317	1.479639268718	4.993891568036
H	5.155977951452	2.193528034579	6.112755238400

Substrate 5f

29

C	3.127468290393	1.413390269797	2.475759895941
C	4.105827562462	1.317373573526	3.459156799970
C	4.189686376160	0.215205011007	4.308738150878
C	3.274452384817	-0.817068505425	4.173345194263
C	2.280599783104	-0.752958967111	3.197893549878
C	2.208483221060	0.354677517041	2.355611571028
O	1.269897188685	0.504015716178	1.372574973766
C	0.307055444047	-0.520769541814	1.187198589660
C	-0.624528870445	-0.149872699991	0.060582827157
C	-0.472881526557	1.047108995656	-0.642439876560
C	-1.330319176946	1.389270466461	-1.681016725314
C	-2.364335259202	0.535229166761	-2.040586790962
C	-2.537235508692	-0.662852724143	-1.356511505829
C	-1.672653427763	-0.992584952794	-0.319811996443
I	-2.006138946631	-2.842050717114	0.674721106547
H	4.819075344163	2.127154626050	3.560910594560
H	4.962661570729	0.169302040348	5.064904608932
H	3.322476050290	-1.681833570335	4.823130886647
H	1.575862755498	-1.566261928745	3.106946481809
H	-0.265935449514	-0.668586645121	2.109118518858
H	0.807118760554	-1.468423038663	0.958557643502
H	0.331088458932	1.712350316412	-0.363704809581
H	-1.187344296351	2.324212107901	-2.207274537046
H	-3.037878044041	0.791800481159	-2.848021862983
H	-3.340087465898	-1.332696219901	-1.630866100415
C	3.041037487119	2.604284533692	1.562173497593
H	3.141688593755	2.311070174116	0.514465315474
H	2.076174342427	3.108574066857	1.654821756320
H	3.826605127844	3.322814758195	1.793714832352

Substrate 5g

27

C	3.119685060500	1.391059058427	2.497149560627
C	4.105962730434	1.337782019928	3.458296880190
C	4.197416919453	0.227303311495	4.312597185430
C	3.281384120847	-0.819604705741	4.178962438250
C	2.287897737005	-0.769462008986	3.213345759908
C	2.203189672171	0.339269032445	2.366170393922
O	1.276339111308	0.489473465892	1.393454848924
C	0.307454223988	-0.536523685548	1.195027852472
C	-0.616811495175	-0.150703573507	0.068107290324
C	-0.457065050046	1.049742469303	-0.626670744282
C	-1.310333219079	1.401526255329	-1.665421420486
C	-2.346953020858	0.554135097528	-2.032588026937
C	-2.527219563919	-0.647212052255	-1.356297697845
C	-1.667355254598	-0.987448188176	-0.319207440488
I	-2.010804536443	-2.840387851918	0.663802751061
H	3.039099136293	2.241103631764	1.833342188553
H	4.810858604092	2.152091473756	3.555062955328
H	3.345730385766	-1.678077255453	4.833492632335

H	1.593479838112	-1.591616110003	3.132238083119
H	-0.265405056738	-0.685518828951	2.115577378300
H	0.811854405200	-1.479236913285	0.960411538374
H	0.348380902704	1.711410647840	-0.343725528736
H	-1.161712741394	2.338866653392	-2.185625303762
H	-3.017091956119	0.818558258855	-2.840265193334
H	-3.332318068958	-1.311683595889	-1.636920552233
C	5.216281945304	0.168042804943	5.307355489421
N	6.042226320148	0.120518708816	6.112452451566

Substrate 5h

29

C	3.158330174905	1.347214861870	2.451793640300
C	4.137846966742	1.289190080869	3.422230726741
C	4.178840612656	0.216547711584	4.317871683014
C	3.229196801439	-0.791553993185	4.222736414520
C	2.237199338820	-0.742127181027	3.248845847954
C	2.199965121692	0.330452219669	2.357773347773
O	1.280144893927	0.480325806814	1.372324911995
C	0.273872331880	-0.513501642673	1.215183764065
C	-0.633942429410	-0.142498555640	0.069869266843
C	-0.431461971533	1.023215886059	-0.671444730059
C	-1.269430342518	1.362742667056	-1.726619763320
C	-2.333859224299	0.537659849741	-2.063985704735
C	-2.557001126379	-0.629040122665	-1.341377493495
C	-1.711785025193	-0.957106167653	-0.288442159366
I	-2.121508189455	-2.757260227651	0.765116349535
H	3.115557244663	2.173966508570	1.755629506837
H	4.871153141250	2.082200717084	3.487137920652
H	3.250257983418	-1.625747834876	4.909853847482
H	1.509638784935	-1.537912175265	3.200832957700
H	-0.306959983554	-0.601919117946	2.138991405348
H	0.739956452612	-1.485451435767	1.023097407743
H	0.395809772254	1.667115786415	-0.411357335844
H	-1.087231055723	2.273040942985	-2.282961629715
H	-2.992524305726	0.792697613245	-2.884036849181
H	-3.383833933303	-1.276107575566	-1.598519800534
C	5.268921137647	0.157582116874	5.341310553234
F	5.444075773719	1.342433295259	5.975780124931
F	6.476115747826	-0.147542147622	4.793829087775
F	5.042832106708	-0.766342016559	6.297555891809

Substrate 5i

26

C	3.120240936949	1.392523940984	2.495484234338
C	4.109413502839	1.335220135100	3.462363958325
C	4.183654960523	0.227163995420	4.300270498393
C	3.280567718482	-0.814741762998	4.176218176405
C	2.284427669737	-0.758680332117	3.203771822820
C	2.201697267345	0.347683712297	2.358976621347
O	1.269802667163	0.503231680248	1.377915988946
C	0.306185981347	-0.522933742419	1.186120428141
C	-0.623249334823	-0.146557446449	0.059868210474
C	-0.470331355061	1.052541056600	-0.638995605421
C	-1.326863640872	1.398082748979	-1.677181076922
C	-2.360742813928	0.545432111485	-2.040164580907
C	-2.534618531460	-0.654740550704	-1.360069066553
C	-1.671184930223	-0.988209413500	-0.323674459953
I	-2.005570249328	-2.840314231256	0.664848662857
H	3.047682619302	2.246694558769	1.835356486151
H	4.817720040619	2.145665893055	3.564318852724
H	3.343839522088	-1.673046137921	4.830656805982
H	1.589879484076	-1.581334381297	3.123587723158
H	-0.266783860267	-0.673213273599	2.107390112793

H	0.809228266085	-1.467921845858	0.953938137549
H	0.333258971645	1.717526747674	-0.358467779972
H	-1.183141660702	2.334598027360	-2.200343998870
H	-3.033521502416	0.804763629696	-2.847330423261
H	-3.337443660992	-1.323436820981	-1.637237501825
Cl	5.435725811872	0.152234431432	5.526016583281

Substrate 5j
26

C	3.126740072377	1.394566169502	2.502023919285
C	4.113587696730	1.331902602308	3.471694887291
C	4.194305747280	0.226008483303	4.312355348098
C	3.280076712527	-0.807882629853	4.169227048916
C	2.287123510824	-0.748199810467	3.195922201830
C	2.196033929535	0.355774038522	2.346693727944
O	1.265691282861	0.502835127689	1.371872016630
C	0.303282470033	-0.527610106798	1.184393185513
C	-0.626434804191	-0.150908726051	0.058733754579
C	-0.471072291100	1.047163431493	-0.641496510204
C	-1.328011770509	1.392548648612	-1.679378691627
C	-2.363887176995	0.541346776274	-2.040195623435
C	-2.539720544070	-0.657561304062	-1.358408231443
C	-1.676087858332	-0.991372499267	-0.322281326781
I	-2.012505899686	-2.841286511611	0.669428731860
H	4.814948599046	2.149780013180	3.564644405891
H	4.966302713236	0.180643688266	5.068535793267
H	3.330858860054	-1.674013970145	4.816092210667
H	1.586537248105	-1.564624442362	3.103403605071
H	-0.266911744454	-0.676084771957	2.107120631973
H	0.808938121146	-1.470760363098	0.952545427073
H	0.334316528824	1.710585154376	-0.362081156297
H	-1.183041740538	2.327988079596	-2.204110511396
H	-3.036843504615	0.800907683327	-2.847142376068
H	-3.344136122691	-1.324994276695	-1.633987011429
Cl	3.039369404605	2.790945845915	1.455224772790

Substrate 5k
26

C	3.120866477855	1.394275471579	2.495925379108
C	4.111471727578	1.337041271055	3.463240139814
C	4.172798600682	0.226777718490	4.289512658996
C	3.280007615039	-0.817782961736	4.176886855899
C	2.283490043066	-0.758846474678	3.203006974526
C	2.202758063305	0.348970207951	2.359974543588
O	1.268739837391	0.506356944285	1.376404461619
C	0.306812218684	-0.519625043035	1.185735033071
C	-0.623589391810	-0.145486569115	0.059395388342
C	-0.471774150268	1.053128115237	-0.640599613648
C	-1.328666683969	1.397265496924	-1.678957903328
C	-2.362025633724	0.543598451724	-2.041122994969
C	-2.534913132208	-0.656133335242	-1.359980558261
C	-1.671021212471	-0.988047260733	-0.323447821711
I	-2.004065119455	-2.839768483649	0.666503930709
H	3.046827163112	2.247970148119	1.835528225021
H	4.827234232751	2.139820879089	3.577727143296
H	3.355537410738	-1.670387626957	4.838139121380
H	1.587511267606	-1.579908929483	3.120333342610
H	-0.266697250520	-0.670676728805	2.106884814167
H	0.809441435245	-1.465272828287	0.954010598960
H	0.331505733120	1.718670932988	-0.360473256316
H	-1.185687866717	2.333453778818	-2.202937869260
H	-3.035114717095	0.801770716047	-2.848410303090
H	-3.337294151866	-1.325656077098	-1.636460298290
F	5.143969113932	0.168199426511	5.239558787768

Substrate 5l
50

C	3.121284748976	1.457463166170	2.430463650813
C	4.083472496704	1.309709804521	3.434128261229
C	4.171936270603	0.210243606109	4.292430596590
C	3.225998365472	-0.795239700057	4.117388236965
C	2.248676673728	-0.699791925334	3.136349055900
C	2.184512061065	0.409610245713	2.293569768364
O	1.224918089416	0.521980812580	1.317444093846
C	0.280110579423	-0.526260711402	1.174224111687
C	-0.684620829157	-0.218499649119	0.056241685405
C	-0.590805232652	0.955668545439	-0.692960152666
C	-1.482279444685	1.232521883677	-1.722425444393
C	-2.494991353480	0.333183380130	-2.027024195588
C	-2.611606459777	-0.844167505185	-1.296658990289
C	-1.713202073305	-1.107799195794	-0.269962204716
I	-1.965124581553	-2.931581195714	0.794498873587
H	4.804558007795	2.100505041272	3.550880841266
H	3.232595069172	-1.676846413019	4.745597866766
H	1.536645128740	-1.505141791760	3.039275061821
H	-0.274984162240	-0.662175977240	2.108852275483
H	0.795002641397	-1.469888070814	0.962715486924
H	0.194951505723	1.657846117925	-0.459934336112
H	-1.382005906473	2.152185920935	-2.284239137375
H	-3.194985463978	0.538122781291	-2.826656320793
H	-3.397456092165	-1.549591542217	-1.527569250741
C	5.246949897917	0.085347486942	5.383623316485
C	4.568414018457	-0.032243370136	6.764658932891
C	6.094781545726	-1.178679640745	5.128711555908
C	6.193281144178	1.294633756305	5.419355616955
H	3.968813658804	0.854822162898	6.980310975391
H	3.913198920451	-0.902618644812	6.819912141633
H	5.322004733207	-0.131226990504	7.549783964943
H	6.598690397610	-1.120532800582	4.161453041339
H	6.858468720516	-1.285133556929	5.903042615253
H	5.484201102754	-2.082610332422	5.135953290750
H	6.933077561689	1.153889628084	6.209730850196
H	6.734541454235	1.416325885265	4.478990330339
H	5.659294140937	2.223607193491	5.629011615149
C	3.104988775174	2.711048163783	1.532376519093
C	3.312917163274	2.310953261765	0.054830501231
C	1.771696663820	3.472195986640	1.703974341878
C	4.230078838927	3.698751608810	1.888411638003
H	4.287972302546	1.836118175060	-0.076709050134
H	2.550620993138	1.619879697045	-0.295409874949
H	3.286266150870	3.200997853086	-0.578612426698
H	1.659385977587	3.814121464359	2.735464177462
H	1.760386258740	4.352605649500	1.056754929101
H	0.911321960997	2.855802101261	1.456698287047
H	4.165742479703	4.560607520901	1.221636511677
H	4.145739926967	4.068545504587	2.911927322567
H	5.220812133031	3.258631768242	1.761297422519

Substrate 5m
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C	3.295819904670	1.301876484945	2.347929938076
C	4.290174107751	1.146314317437	3.305880822312
C	4.301675453580	0.077619492939	4.201931057087
C	3.302270269860	-0.885575499619	4.161591376236
C	2.291023355053	-0.750987964527	3.204026934589
C	2.282679157124	0.320967231150	2.316281865378

O	1.310796890639	0.496739764578	1.367347291623
C	0.282012304093	-0.471291466031	1.253558004137
C	-0.660654838203	-0.091636511124	0.138846638410
C	-0.474055639933	1.074659114380	-0.605932916085
C	-1.343007394608	1.424780611855	-1.632248627354
C	-2.424718086136	0.609508718309	-1.937324271359
C	-2.633763912102	-0.557299884380	-1.210621190680
C	-1.757086560405	-0.895123059789	-0.186768627535
I	-2.150223372155	-2.694408200678	0.875852855977
H	5.087707971146	1.875644672650	3.361401493034
H	5.098990746517	-0.001073369202	4.931179341255
H	1.510905610729	-1.498317538399	3.166428906288
H	-0.271876714098	-0.544975266336	2.196077021101
H	0.714617321583	-1.457614822259	1.052788914332
H	0.366354663684	1.710314629515	-0.369349506233
H	-1.171600989516	2.335446908607	-2.191540246813
H	-3.107621408385	0.872236121506	-2.734853453680
H	-3.473952916358	-1.196835271977	-1.442198044549
C	3.290806214819	-2.053100126768	5.113809138087
H	2.377674298421	-2.065767763364	5.714141384092
H	3.333201823992	-3.003608278871	4.576107530091
H	4.140768250370	-2.013624931065	5.794923531519
C	3.255280280351	2.479408792011	1.387408203328
C	4.634741093446	3.059407089792	1.060625144063
C	2.317231353033	3.581391051959	1.911694000488
H	2.829063732671	2.110669284147	0.451484923006
H	5.319616140011	2.289579540787	0.699935090541
H	4.540112534209	3.818560573608	0.281678782552
H	5.092704560681	3.540671235896	1.927449325154
H	1.316914333797	3.192493792426	2.105122088194
H	2.703942774150	4.003056733182	2.842960924785
H	2.231799415522	4.391927762710	1.183960168552

Substrate 5o
26

C	2.097306912945	-0.914458557265	-1.358565035425
C	3.070160379386	-0.017352404008	-1.762018714242
C	2.777610935200	1.339937944657	-1.834658418093
C	1.508271594531	1.782134246763	-1.501721985960
C	0.526901368328	0.885580574157	-1.097064443516
C	0.812822688121	-0.475498115817	-1.020939069691
O	-0.079791692265	-1.415663108263	-0.641465783918
C	-1.368323700785	-0.998581809008	-0.228426585739
C	-2.151312763423	-2.207272225054	0.206973143943
C	-1.522296923560	-3.394097484476	0.565633597608
C	-2.265402190822	-4.485371330466	0.997821233781
C	-3.637575954141	-4.362436126788	1.067503861414
C	-4.295412416186	-3.198755680552	0.718553240793
C	-3.538597958613	-2.121660207375	0.283473487099
I	2.542764682843	-2.952283848962	-1.243741932685
H	4.057650808393	-0.376639672129	-2.018156646626
H	3.540852117111	2.038135816296	-2.149574645767
H	1.267482034275	2.835671516637	-1.554737900315
H	-0.457566221535	1.251663310063	-0.844688571326
H	-1.882593747335	-0.492770806372	-1.050680050760
H	-1.274695629512	-0.288744918138	0.600470343906
H	-0.445203129119	-3.470696067085	0.500935007652
H	-1.793137389625	-5.417603665697	1.276548145696
H	-5.373781847209	-3.148160619912	0.781376309837
H	-4.038103703928	-1.203738649287	-0.002885733345
F	-4.364321893078	-5.416511741917	1.485675215678

Substrate 5p
29

C	2.112117883536	-0.905040469203	-1.338679802129
C	3.080034279268	-0.003789091787	-1.744622184027
C	2.776074210317	1.349983636967	-1.834542189246
C	1.500199779255	1.784091502487	-1.516244943575
C	0.523842371330	0.883264334350	-1.108938125517
C	0.820852466854	-0.474621141218	-1.015168208761
O	-0.065411056969	-1.418008331266	-0.631310491663
C	-1.363912513756	-1.008542894070	-0.240569321512
C	-2.145766225798	-2.215671486266	0.199744390850
C	-1.528703625907	-3.413048204023	0.534777565933
C	-2.287135751128	-4.494854406276	0.970132622785
C	-3.669943569067	-4.408486822740	1.084632356080
C	-4.280062388916	-3.199420109609	0.747378514714
C	-3.531493380336	-2.120438456487	0.308129389464
I	2.574789439715	-2.937708796998	-1.200319704978
C	-4.494460192678	-5.581837695010	1.537223961414
H	4.072542074119	-0.357086429003	-1.989485575806
H	3.535436879769	2.051529460781	-2.151394435344
H	1.250327881514	2.834765242644	-1.582795485594
H	-0.465648808725	1.243297086569	-0.867940610600
H	-1.869593994477	-0.516354379699	-1.076737935052
H	-1.287553852299	-0.286416355008	0.579620206596
H	-0.453432069719	-3.503251960797	0.451983391494
H	-1.789873808770	-5.423180806999	1.226463663226
H	-5.357216130617	-3.106673539638	0.826499173746
H	-4.027750923991	-1.192888744997	0.045051291822
H	-5.213968260149	-5.283327638219	2.300458830378
H	-5.060726206343	-6.001265257692	0.703174983344
H	-3.864784506035	-6.370658246791	1.946198671960

XYZ Coordinates of intermediates of proposed Mechanism in Figure S18

Radical 7c

C	0.002181496618	0.008770421972	0.001590747440
C	0.005128293407	0.008451329791	1.410016300191
C	1.166871486030	0.004005524242	2.121612499964
C	2.506724422372	0.043902060502	1.446279127585
C	2.408462143348	-0.096864463738	-0.047571006012
C	1.225497137387	-0.076243652266	-0.721736555132
C	1.233889139656	-0.099390082294	3.601415067933
O	1.940979152826	-1.299383354034	3.994770051817
C	3.114863501881	-1.550058390176	3.340872189691
C	3.465164530281	-0.945315972061	2.125051798653
C	4.706188422273	-1.265637027044	1.571550752145
C	5.564664634354	-2.175254040375	2.174754872178
C	5.184800081667	-2.790451653674	3.364881206413
C	3.967360425155	-2.475831788074	3.946927659307
C	1.179646805455	-0.156341497269	-2.225832528615
H	3.657610228459	-2.930317731664	4.879445549505
H	5.839694193512	-3.506585972434	3.845016945765
H	6.518932101197	-2.403843324965	1.718319813135
H	5.008323361677	-0.795803996077	0.644337628151
H	1.762495937094	0.755934486925	4.041014009958
H	0.248806483482	-0.176774575819	4.056252357692
H	-0.941254749552	-0.006608072541	1.940221183522
H	3.333889028026	-0.159398524698	-0.605751173470
H	-0.937656477918	0.025045813704	-0.535144070581
H	2.937860485580	1.046280375988	1.645132586773
H	0.599445929386	-1.022358216874	-2.554120441452
H	2.179800121983	-0.234496916780	-2.651538059853
H	0.697799224735	0.729315293444	-2.647950282399

Radical 7k

C	-0.002375424498	0.016505867562	0.002521771011
C	0.003178651448	0.015114869005	1.413346479454
C	1.165356513661	0.005629011432	2.122984200135

C	2.514784614451	0.032700386708	1.460586110164
C	2.435868104917	-0.090919633774	-0.034804991679
C	1.236810416484	-0.058855906459	-0.658143746398
C	1.225578003474	-0.093629103465	3.604744257954
O	1.913226775950	-1.301183089839	4.003158070946
C	3.084421055209	-1.574297629893	3.354141748355
C	3.449991541937	-0.979644055936	2.138536591806
C	4.683110278722	-1.326615771018	1.584467289563
C	5.521822332198	-2.252137416588	2.190600234027
C	5.128657125373	-2.855447818855	3.382531050982
C	3.917594858605	-2.515354261619	3.963124674714
F	1.202011383955	-0.116664796771	-2.017883641613
H	2.954700902635	1.026467224432	1.676552890837
H	3.597595113168	-2.961947763850	4.895858119018
H	5.768427677301	-3.583604061768	3.864777581803
H	6.470848665435	-2.502373045898	1.734930487706
H	4.994862191092	-0.866409775342	0.655667472592
H	1.762815481111	0.757352566185	4.041041067635
H	0.237548677271	-0.155448368570	4.054744412522
H	-0.943909024088	0.005696614208	1.940239996903
H	3.342123712861	-0.143815081450	-0.620654197431
H	-0.920683841244	0.032764035310	-0.565869807471

Radical 7b

C	-0.002501801911	0.043456958897	0.003905348800
C	0.000895200657	0.037131158257	1.415698134374
C	1.163243497683	0.004570689801	2.124571403693
C	2.510685061183	0.023090107312	1.457178761981
C	2.415448172873	-0.116630567169	-0.037412956658
C	1.224067964407	-0.065818574963	-0.692078030036
C	1.224628681018	-0.104676767532	3.605030629494
O	1.907935531070	-1.318154087726	3.996069771080
C	3.083415599255	-1.583395621689	3.350906016976
C	3.450857943391	-0.979659341413	2.140035456641
C	4.691465682785	-1.314057154405	1.594094347016
C	5.533083293842	-2.237087900417	2.200476630940
C	5.136090072953	-2.851263996825	3.385604271160
C	3.918802044073	-2.522497285488	3.960033500833
H	2.955296890007	1.019493922037	1.656224403281
H	3.596314171117	-2.975708912515	4.888813564357
H	5.777893670244	-3.577633942510	3.867967697965
H	6.487623635652	-2.476801884388	1.750471868897
H	5.006656046065	-0.844840478486	0.670873426916
H	1.767263580613	0.740317615240	4.047425850210
H	0.236968932585	-0.165008755332	4.056656775016
H	-0.944049473292	0.037534657290	1.948329638924
H	3.335298693325	-0.202923124810	-0.599825180410
H	-0.936915477576	0.081914064007	-0.538626052902
H	1.211348177980	-0.125093647175	-1.774174278546

TS-6-*endo* from radical 7c

NI=1 Freq=-324.4193

C	0.04579000	0.07747100	0.00876100
C	0.04287200	0.03151300	1.42518000
C	1.24925200	-0.06312800	2.09853300
C	2.45171200	-0.15181000	1.39826900
C	2.47310000	-0.14498100	-0.00534600
C	1.26680600	-0.05760100	-0.68642000
C	-1.24594500	0.32462600	2.12638300
O	-1.45189500	1.74892900	2.30181900
C	-1.26528200	2.55773000	1.21778600
C	-1.68167500	3.89024400	1.33691200
C	-1.49869500	4.77328800	0.27975800
C	-0.90307000	4.35454100	-0.90833400
C	-0.48281600	3.02780900	-1.03066600

C	-0.67619700	2.16814700	0.02667200
C	3.78030000	-0.25253700	-0.74472200
H	-2.14441800	4.21446300	2.26165700
H	-1.82673800	5.79969000	0.38670800
H	-0.76374100	5.04830300	-1.72811400
H	-0.00872000	2.68567100	-1.94433200
H	-2.09614700	-0.07750600	1.56845400
H	-1.26274400	-0.07549400	3.13796100
H	1.25902700	-0.05919700	3.18248700
H	1.25777000	-0.09121000	-1.76903800
H	3.38330100	-0.23704200	1.94489100
H	4.39281100	0.63818000	-0.58218400
H	3.62224600	-0.35954000	-1.81759100
H	4.36185400	-1.10885400	-0.39673900
H	-0.87625900	-0.11352700	-0.52538100

TS 6-*endo* from radical 7k

NI=1 ; Freq=-317.7000

C	0.03543300	0.02054300	1.43154800
C	1.23547100	-0.08008500	2.11455500
C	2.44694000	-0.18064600	1.42766900
C	2.41650500	-0.17400400	0.03970700
C	1.25094400	-0.08688900	-0.68811200
C	-1.25449600	0.32166000	2.12920800
O	-1.45042800	1.74636600	2.30479000
C	-1.26161400	2.55157600	1.21935700
C	-1.67294600	3.88622300	1.33167300
C	-1.48547900	4.76350100	0.27071000
C	-0.89034800	4.33818700	-0.91532400
C	-0.47444900	3.00972600	-1.03294400
C	-0.67341700	2.15896400	0.02954900
F	3.59058400	-0.29328100	-0.62685800
H	-2.13533000	4.21584500	2.25457100
H	-1.80967800	5.79152000	0.37297500
H	-0.74779000	5.02794800	-1.73775000
H	-0.00107600	2.66131900	-1.94432000
H	-2.10471000	-0.07528100	1.56819600
H	-1.27608500	-0.08014600	3.13971000
H	1.23966100	-0.07050100	3.19765800
H	1.27719600	-0.13145000	-1.76790700
H	3.39036300	-0.26819200	1.94819000
H	-0.88699500	-0.12260200	-0.52043600

TS 6-*endo* from radical 7b

NI=1 ; Freq=-330.6575

C	0.04609200	0.08243100	0.00605900
C	0.04954200	0.03276600	1.42434600
C	1.25090100	-0.06734500	2.10429300
C	2.45779500	-0.15774300	1.40590900
C	2.45735100	-0.14427900	0.00966600
C	1.26621300	-0.05283000	-0.69102900
C	-1.24103800	0.32537000	2.12544800
O	-1.44408700	1.74884000	2.30051100
C	-1.26190800	2.55811800	1.21571900
C	-1.68087900	3.88962300	1.33582000
C	-1.50188900	4.77308700	0.27841500
C	-0.90785200	4.35589200	-0.91103100
C	-0.48496600	3.03021800	-1.03483200
C	-0.67450100	2.17087000	0.02326100
H	-2.14254000	4.21249400	2.26154300
H	-1.83189700	5.79874100	0.38616900
H	-0.77171000	5.05007500	-1.73093800
H	-0.01226400	2.68909000	-1.94950200
H	-2.09048600	-0.07685800	1.56653600

H	-1.25788800	-0.07568300	3.13655100
H	1.25375500	-0.06548200	3.18809700
H	1.26467000	-0.08180700	-1.77287100
H	3.39065300	-0.24614700	1.94732900
H	-0.87883300	-0.10722100	-0.52336200
H	3.39311700	-0.23270800	-0.52829000

radical 12c

C	0.996341708676	-0.979777823339	3.314870749168
C	0.417673145605	0.089026926682	4.009600955825
C	0.324701132704	1.316253524987	3.356292003305
C	0.785409287679	1.472724732792	2.051297883882
C	1.361409136591	0.407159697735	1.365836806931
C	1.464759795879	-0.824008389142	2.019246996819
C	1.895139159657	0.581734402586	-0.032657059606
O	1.356724334469	-0.366775939033	-0.975307151725
C	0.084348110077	-0.166826126690	-1.403569778533
C	-0.465914553206	-1.092390321184	-2.302653413924
C	-0.728715569989	0.886634288594	-1.042832274906
C	-2.010201354930	1.093567017484	-1.480392363480
C	-2.540670846064	0.162063517011	-2.379773142822
C	-1.759665047002	-0.921035835790	-2.779153496243
C	-0.091154790650	-0.092793958035	5.415130086065
H	1.086359083816	-1.944477629047	3.801295462909
H	-0.118216222580	2.161970213655	3.869163218569
H	0.694680256428	2.436592954274	1.564327646963
H	1.913399876415	-1.666569297581	1.506435425294
H	1.709051856897	1.597000019458	-0.390674858246
H	2.968440030900	0.394652920920	-0.064012829267
H	0.137679764078	-1.937367085863	-2.612701865843
H	-2.596109778989	1.943020730231	-1.149741675680
H	-3.547762591387	0.286377937628	-2.756655554460
H	-2.164084634245	-1.646809200290	-3.473245543497
H	0.682937339268	-0.507003169886	6.065028537678
H	-0.935286415705	-0.786785311930	5.440610183826
H	-0.422452214391	0.853511203770	5.842405051000

Radical 12k

C	0.019403979826	-0.066577322623	-0.106433127944
C	0.009199574497	0.055399533606	1.277469844000
C	1.210296812317	0.001887771799	1.999639482414
C	2.358530071596	-0.173552900064	1.257342932494
C	2.419016472719	-0.292317970386	-0.105920330145
C	1.210416455098	-0.240619015267	-0.809098748873
O	1.151589342104	0.111038758243	3.352218987955
C	2.397852446632	0.082352870464	4.072639330657
C	3.173795001894	1.371775358307	3.975212376055
C	2.581668914787	2.581384356381	4.346465421007
C	3.290518474965	3.773373629767	4.282344369475
C	4.605856595553	3.734017881457	3.850952961364
C	5.230507137333	2.558614005723	3.481346264215
C	4.499007364326	1.376250574344	3.543545647609
F	5.305547891723	4.893809850960	3.789867990708
H	6.259189102590	2.571158248603	3.147708211803
H	2.841527200325	4.715678922391	4.565744482151
H	1.553613415228	2.594460624413	4.686168675642
H	4.971330526383	0.446991208246	3.250281007635
H	3.003514510758	-0.757194795854	3.724102257829
H	2.098531771757	-0.110883442763	5.102473114289
H	-0.918186028736	0.193704054181	1.820791485298
H	3.360254566828	-0.423052101670	-0.626549803840
H	1.207531785800	-0.334346347413	-1.887471453683
H	-0.919170967349	-0.023776691493	-0.644250637817

Radical 12b

C	0.944821338881	-0.994579836886	3.288888716571
C	0.428204158273	0.092524770958	3.990537913176
C	0.374414997083	1.341738257646	3.383213665950
C	0.830368550380	1.501661618828	2.077613575352
C	1.352384208899	0.420308845393	1.369622811821
C	1.408443430182	-0.829972094695	1.989825729385
C	1.885896568179	0.604945217843	-0.029665865496
O	1.364163939539	-0.348636698399	-0.972807899835
C	0.088823636948	-0.165436786135	-1.401912982640
C	-0.447110028116	-1.094983450007	-2.305127390804
C	-0.739326278927	0.874490278569	-1.036948473729
C	-2.023277250997	1.065378184258	-1.474317039314
C	-2.539624612483	0.129972578910	-2.377828779892
C	-1.743003247561	-0.940101275739	-2.781460939037
H	0.991244770868	-1.969513937325	3.757806356830
H	-0.028365478131	2.190903714701	3.920869235776
H	0.778279525233	2.475167680557	1.604685081443
H	1.813010884438	-1.677456182365	1.449890260121
H	1.686754895709	1.618578566086	-0.385193714654
H	2.962337304010	0.435119589655	-0.055802254549
H	0.168834885403	-1.929742878863	-2.618481530522
H	-2.621352134268	1.905037296575	-1.140568863688
H	-3.548192729277	0.241407830962	-2.754754719604
H	-2.136720160932	-1.668546591743	-3.478863579370
H	0.069873336667	-0.035692888784	5.004117086711

TS 5-*exo* from radical 7c

NI=1; Freq=-334.8375

C	0.528853453045	-0.933186795259	3.017007607443
C	0.195252918650	0.239264918922	3.714335542069
C	0.456739939257	1.466759711736	3.090552447662
C	0.985714272177	1.529482374095	1.816403688109
C	1.230671302289	0.350231079103	1.065760371070
C	1.062564100319	-0.888154823856	1.747100254517
C	2.140867390639	0.422519627911	-0.147014855200
O	1.682959409538	-0.381757917749	-1.249986498590
C	0.331203427650	-0.278913122813	-1.401448179613
C	-0.315339334058	-0.732914431404	-2.550061171480
C	-0.410014830254	0.263374815484	-0.376613554313
C	-1.778824561402	0.377265569412	-0.415680118225
C	-2.437540708112	-0.072757978866	-1.567483108325
C	-1.703252243558	-0.623172470639	-2.616729833068
C	-0.415638393053	0.176618306384	5.085868599855
H	0.383318773388	-1.893729787420	3.498034704216
H	0.251410278901	2.387011228054	3.625158323766
H	1.188949234381	2.491969393586	1.362593361084
H	1.334529666961	-1.806689057858	1.241309032609
H	2.222485360830	1.461036215063	-0.478851328820
H	3.135761820552	0.046687494923	0.088256624874
H	0.254936675605	-1.159116968403	-3.366597320607
H	-2.340934488838	0.798911649403	0.410261103374
H	-3.515323400603	0.005878931922	-1.639659852473
H	-2.216838376153	-0.971227352087	-3.504165478600
H	-0.218342635265	1.087838151741	5.651608118821
H	-0.033028949830	-0.673208796463	5.653493748668
H	-1.502317103056	0.059650035080	5.024715771178

TS 5-*exo* from radical 7k

NI=1; Freq=-348.1453

C	0.52224200	-0.94992600	3.01263200
C	0.20424400	0.24052300	3.65520400
C	0.44372600	1.48237100	3.08322900

C	0.98071100	1.53330600	1.81161900
C	1.22813500	0.34861400	1.06709000
C	1.06423800	-0.89349400	1.74546300
C	2.14334000	0.42006900	-0.14339600
O	1.68627500	-0.38485800	-1.24469500
C	0.33452700	-0.28080500	-1.39653100
C	-0.31397900	-0.73061600	-2.54542100
C	-0.40578800	0.25892600	-0.37002400
C	-1.77425900	0.37544000	-0.40501100
C	-2.43418500	-0.07040200	-1.55755800
C	-1.70174300	-0.61863800	-2.60931100
H	0.36271600	-1.89325000	3.51752500
H	0.22133600	2.38382400	3.63814600
H	1.18268200	2.49376000	1.35500600
H	1.34052700	-1.80984500	1.23977200
H	2.22553300	1.45834300	-0.47511100
H	3.13711300	0.04451900	0.09599400
H	0.25464300	-1.15489500	-3.36397900
H	-2.33419300	0.79544100	0.42299200
H	-3.51185900	0.00976500	-1.62823200
H	-2.21710700	-0.96328900	-3.49696600
F	-0.32427500	0.18687700	4.90051500

TS 5-*exo* from radical 7b

C	0.522890814167	-0.940375319920	3.012979413438
C	0.195240234803	0.239705706136	3.688049974368
C	0.444977652901	1.473360509942	3.082854368339
C	0.980717353131	1.533158358843	1.810310885760
C	1.232287122559	0.348417094596	1.068108870438
C	1.063504594618	-0.893527229573	1.744156777345
C	2.143652952371	0.420775162565	-0.145065054329
O	1.686889343595	-0.385768405436	-1.246147941908
C	0.335564943114	-0.282131939347	-1.397409618529
C	-0.313768220675	-0.730927973363	-2.546388236323
C	-0.405557358248	0.256995319371	-0.371164832885
C	-1.773550409123	0.374853621605	-0.405619325062
C	-2.433738464918	-0.070068854689	-1.558525339604
C	-1.701518530670	-0.618316331360	-2.610356442746
H	0.370354502812	-1.897319477216	3.496411160800
H	0.229082481738	2.390186694247	3.617025013008
H	1.181510740885	2.492507553652	1.349327338078
H	1.337144893620	-1.809134366616	1.234377400431
H	2.224074016743	1.458762615732	-0.478388382883
H	3.138349774498	0.046749607804	0.093393012839
H	0.254670123241	-1.154978085997	-3.365224468091
H	-2.332877878394	0.794532790541	0.422900433303
H	-3.511359897372	0.010853453240	-1.629155896057
H	-2.216943359495	-0.962319134361	-3.498235557134
H	-0.223172425900	0.197437629602	4.685184447404

Radical 13c

C	0.490084446174	-0.881724573468	3.116606332715
C	0.207662885410	0.379447070652	3.722962735506
C	0.128431147387	1.542367507309	2.902889956573
C	0.333909354617	1.479946511210	1.550451320678
C	0.671289112581	0.192645082287	0.848020310438
C	0.704200416614	-0.996300024908	1.770468453475
C	2.048786968101	0.333231790087	0.107467405946
O	1.807996681307	0.163064885389	-1.344344677323
C	0.456085220527	-0.057534124339	-1.525001581951
C	-0.128676549702	-0.261620538572	-2.767366831105
C	-0.277818305861	-0.054212808169	-0.312196330296
C	-1.644881591463	-0.261252617765	-0.345422760543

C	-2.262504920271	-0.470275399556	-1.594327341928
C	-1.518812006275	-0.470383424540	-2.775976845299
C	-0.012717676227	0.463348466360	5.188696926202
H	0.529377365373	-1.766341519685	3.755662646999
H	-0.105113747229	2.498529375384	3.375993877158
H	0.258966435404	2.362241647250	0.921382599840
H	0.903885168556	-1.956906446160	1.304081831570
H	2.503849247941	1.330157564625	0.200767473983
H	2.773841642472	-0.452534633457	0.364844828465
H	0.453245214773	-0.261162903903	-3.683428615030
H	-2.234880186095	-0.264032815825	0.570554003089
H	-3.338535800905	-0.634516699111	-1.633529899490
H	-2.021122045280	-0.635335479224	-3.731413180262
H	0.818453350513	0.011717444936	5.751825377300
H	-0.924809943064	-0.077618465721	5.487193515913
H	-0.121372885376	1.494723128915	5.551306467377

Radical 13k

C	0.505890154342	-0.907516050152	3.057100521516
C	0.205399744209	0.317388962733	3.672519126682
C	0.144717550213	1.523050210923	2.957907715133
C	0.378233815928	1.525008916048	1.617049751035
C	0.696791648571	0.279199472354	0.836467372769
C	0.744172061047	-0.946501110762	1.718331620708
C	2.030541922649	0.443428907767	0.018884475111
O	1.824146663645	-0.161391037804	-1.279371699933
C	0.476777312983	-0.225828056881	-1.483368462725
C	-0.122666013204	-0.541913791751	-2.692331568213
C	-0.264025415403	0.043345948973	-0.338750764206
C	-1.646789297605	0.006220870570	-0.382024974025
C	-2.275599380262	-0.301707589050	-1.590439200981
C	-1.517020246432	-0.575556617451	-2.726960324042
H	0.546158851397	-1.806367146402	3.659426988941
H	-0.087929098821	2.439327848801	3.485639732956
H	0.329118829269	2.452630590724	1.060775453301
H	0.978017427911	-1.887781311759	1.236715777813
H	2.254567295176	1.502521426524	-0.127939672978
H	2.877578271769	-0.048739310253	0.490605759215
H	0.471204547914	-0.747887305162	-3.572953468306
H	-2.232694695606	0.211160842466	0.505752879004
H	-3.356049117623	-0.328954569303	-1.644297306436
H	-2.015289276806	-0.814075443693	-3.658187089263
F	-0.030610885263	0.336957172542	5.006059476926

Radical 13b

C	0.505339480626	-0.898182990846	3.055223548206
C	0.200272468185	0.317218036897	3.710260946097
C	0.147351907296	1.513038026973	2.959721920150
C	0.378830045928	1.522347378014	1.618342842112
C	0.696462584725	0.280659109209	0.835287841978
C	0.743254299102	-0.942656878410	1.716742863566
C	2.029290827622	0.445585869884	0.016986003591
O	1.823943624756	-0.164125972006	-1.279849754806
C	0.476667554626	-0.227826905917	-1.484228422191
C	-0.122424340447	-0.545720375509	-2.693002000638
C	-0.264132507364	0.044651437433	-0.340175353962
C	-1.646899347518	0.009129173418	-0.385012002329
C	-2.275492397662	-0.300659447595	-1.593219209630
C	-1.516822753697	-0.577920804428	-2.728799795235
H	0.552371479743	-1.813235228037	3.634042810444
H	-0.082001518929	2.444679408205	3.463640656091
H	0.330933923856	2.450545693192	1.061173908988
H	0.976384613928	-1.883421317637	1.231755060693
H	2.250651568631	1.504570432946	-0.134454520617

H	2.877985116641	-0.043106535064	0.489272186134
H	0.471915804511	-0.754069721901	-3.572793773656
H	-2.233108621975	0.216689942753	0.501954543962
H	-3.355994829815	-0.326636458830	-1.647518789467
H	-2.014756135706	-0.817761944316	-3.659887235021
H	0.013040182934	0.331111941573	4.775368565539

XYZ Coordinates of intermediates of proposed Mechanism in Figure S19

Radical 7p

C	-0.006685451621	-0.038981120067	-0.007504684097
C	-0.008635206879	-0.019372980294	1.379216411079
C	1.189236368641	0.010399343078	2.095858578556
C	2.407653370256	0.030711503932	1.413494397414
C	2.399514442026	-0.001669151661	0.017287502905
C	1.205967799880	-0.033944600053	-0.691118011741
C	1.131688275820	0.039989270295	3.601661413139
O	2.391076136416	-0.208881822591	4.243997853334
C	3.469643280023	0.382162198820	3.649140641709
C	3.713836310475	0.029875672519	2.212173418507
C	4.840026288014	0.839536371399	1.625575117892
C	5.677875277176	1.606430034786	2.376460477868
C	5.453942391062	1.740079081319	3.776532921644
C	4.327560090702	1.147185713625	4.378895481497
C	6.839839826025	2.335975560702	1.751681977390
H	4.115944382150	1.310824984835	5.428872773972
H	6.122039105417	2.348626301899	4.371957167247
H	5.024625693825	0.739249325986	0.564024948679
H	0.757654969967	1.011837145896	3.945288875412
H	0.454698791291	-0.728235368755	3.974824110893
H	-0.950033902151	-0.032597263071	1.917171787804
H	3.333478074511	-0.005443454522	-0.528697063838
H	1.222489580248	-0.057719386082	-1.773409993385
H	-0.942203995221	-0.065625982142	-0.551536690559
H	4.041299360935	-1.030624760821	2.212085169729
H	7.785920579620	2.013520230720	2.194256403877
H	6.890684107469	2.159030604774	0.677483920106
H	6.761672051684	3.413603446306	1.916676100323

Radical 7o

C	-6.207717550639	-0.435326505388	2.717594798093
C	-7.338511240326	-0.672521102623	3.446980588386
C	-7.443805641948	-1.811491655234	4.267202992821
C	-6.342900068619	-2.686645147983	4.332548934176
C	-5.187405286198	-2.520354599017	3.653826381491
C	-5.013017590096	-1.360169778761	2.719354855471
C	-4.885636251885	0.931983930092	1.269258003902
O	-6.128709874303	0.689805497515	1.968936121047
C	-3.755595976621	-0.513395833266	2.913168967272
C	-3.705889945990	0.657907812107	2.152182323434
C	-2.611144873001	1.509462122439	2.246313465225
C	-2.707986323493	-0.821115476918	3.772588152747
C	-1.604047605773	0.024834994929	3.852587771950
C	-1.552369612122	1.186490669302	3.089961210209
F	-6.475746031227	-3.774201816820	5.145553233177
H	-8.153219937337	0.038481441540	3.395028051772
H	-8.331692175475	-2.011800673696	4.848258802625
H	-4.397457080514	-3.253650348787	3.734450336003
H	-4.929522996198	1.970865165127	0.951884289300
H	-4.868815182958	0.299591285122	0.374585006774
H	-2.585464348584	2.423136127251	1.664480561496
H	-2.745893498468	-1.713881723976	4.382495569076
H	-0.787172425394	-0.222315130604	4.518812234199

H	-0.696944480384	1.845982369651	3.160515780807
H	-4.926354002447	-1.765111622003	1.692041568547

Radical 7n

C	-6.209272625358	-0.432714465048	2.718170555460
C	-7.341008685611	-0.674172874021	3.441491450490
C	-7.443913652316	-1.818171301002	4.260133575371
C	-6.353091197191	-2.712793376180	4.355415402217
C	-5.198950704837	-2.513255022436	3.662204464332
C	-5.015577790775	-1.356522667469	2.722523113468
C	-4.885701088348	0.936616506751	1.271192627713
O	-6.128281504984	0.696381102418	1.969894165200
C	-3.755890052989	-0.512286336993	2.912483016784
C	-3.705034986513	0.660018056636	2.152613021830
C	-2.609042163935	1.510448184063	2.245350549865
C	-2.705850512109	-0.821011312489	3.769461111087
C	-1.600564710610	0.023340422470	3.847951602422
C	-1.548736258099	1.185810945123	3.086410479598
H	-8.155657056646	0.037748951693	3.385070893961
H	-8.348430416948	-1.996940407836	4.824564985851
H	-4.387249015621	-3.225431500835	3.734151350677
H	-4.926635467703	1.976165659141	0.954871926559
H	-4.868382237157	0.306065233516	0.375020616459
H	-2.583766123625	2.424688751520	1.664206555059
H	-2.743259097935	-1.714072593665	4.378958288964
H	-0.782514759364	-0.225450591294	4.512280632732
H	-0.692198685705	1.844075438322	3.155823137967
H	-4.925379895504	-1.766496473012	1.696354432024
H	-6.439970930117	-3.580860489374	4.998619573909

TS 6-*endo* from radical 7p

NI=1 ; Freq=-320.3094

C	0.064734960573	0.059023792857	0.014937457829
C	0.049075920361	0.009374703671	1.394233858154
C	1.289337465914	-0.088595584064	2.040160738527
C	2.469552079067	-0.123509435801	1.305145164621
C	2.438634177656	-0.065288212885	-0.086472444334
C	1.211426032513	0.023131195952	-0.747139513968
C	-1.224285884484	0.105439614582	2.207627696009
O	-2.412172212436	-0.201895572850	1.460667750933
C	-2.536612099391	0.530356081749	0.299312795969
C	-3.109282167016	1.786853892386	0.291417987228
C	-3.158095640262	2.517457016696	-0.897155695387
C	-2.636926955743	1.998542915377	-2.092001577341
C	-2.075959140315	0.728385904763	-2.074381033142
C	-1.965580755170	-0.008808343621	-0.874654292947
C	-2.708281333111	2.801787746381	-3.364814723174
H	-3.510285596336	2.197534980114	1.209731964641
H	-3.617301458490	3.498795671101	-0.897198359795
H	-1.708712478745	0.290686852442	-2.994678090652
H	-1.206206120352	-0.604979823155	3.033539382200
H	-1.318547492116	1.111895609554	2.632202234000
H	1.328059442527	-0.136958365075	3.123505332373
H	1.171105897780	0.059932959796	-1.830157397527
H	3.360656989449	-0.094532149222	-0.654898649202
H	3.418297245049	-0.200886891775	1.821053155287
H	-1.776019377394	-1.072582573535	-0.918771959136
H	-3.716817735226	3.182739935602	-3.538239787216
H	-2.417010409604	2.203245536649	-4.227844618322
H	-2.041741088768	3.667184974601	-3.318449145513

TS 6-*endo* from radical 7o

NI=1 ; Freq= -314.4023

C	0.02386800	-0.00088800	0.00476700
C	0.01981200	0.00036400	1.38509900
C	1.25848000	-0.01230900	2.03354900
C	2.43523800	-0.03664000	1.28794900
C	2.39311500	-0.03277200	-0.10371900
C	1.16116600	-0.00863200	-0.76731800
C	-1.28897300	0.02318800	2.13374500
O	-2.15594400	1.07772100	1.67037200
C	-2.38508400	1.16357300	0.33150900
C	-2.80881600	2.38690900	-0.16807700
C	-3.01857800	2.55657900	-1.53446000
C	-2.79630600	1.47767800	-2.38032900
C	-2.39675000	0.24510700	-1.92256800
C	-2.13349400	0.07669500	-0.54598800
F	-3.01560700	1.64471200	-3.71185800
H	-2.96054900	3.21002500	0.51741100
H	-3.34489400	3.50489400	-1.93829500
H	-2.28377300	-0.58238200	-2.60914300
H	-1.81009000	-0.93566700	2.04880300
H	-1.13614800	0.23013600	3.19017700
H	1.30203900	-0.00253400	3.11708100
H	1.11814300	-0.00040700	-1.85057500
H	3.31376900	-0.04470100	-0.67515200
H	3.39052100	-0.04898800	1.79714400
H	-2.09996300	-0.93061800	-0.15798200

TS 6-*endo* from radical 7n

NI=1 ; Freq=-330.2804

C	0.034654750410	0.063556941437	0.016600400135
C	0.034860087763	0.019316600066	1.435066258924
C	1.234224711911	-0.084922372724	2.117926499330
C	2.442044051679	-0.184706967107	1.422443423807
C	2.444598835178	-0.176569531660	0.026154684490
C	1.255462909488	-0.081144885968	-0.677386374362
C	-1.255484214391	0.321791663847	2.132383022487
O	-1.450839108319	1.747044224345	2.301953450801
C	-1.261504501401	2.551413979268	1.214751732506
C	-1.672397243408	3.885914376966	1.329364429893
C	-1.486079946039	4.764447053144	0.269115454055
C	-0.892551084503	4.339318851460	-0.917772997098
C	-0.477580010541	3.010635073155	-1.036050832630
C	-0.674322834646	2.156293459682	0.024779992313
H	-2.133689739483	4.214959455814	2.253095322801
H	-1.809918896176	5.792503147230	0.372609311691
H	-0.750736535768	5.029697458961	-1.739928006135
H	-0.005329193873	2.663334843770	-1.948625614808
H	-2.106041110419	-0.077552918055	1.573105758203
H	-1.276737585722	-0.075550642078	3.144865260659
H	1.234804479050	-0.078941558431	3.201720973552
H	1.256024949886	-0.114139131965	-1.759114918359
H	3.373270481773	-0.276206475442	1.966147516711
H	-0.890193441373	-0.122855790946	-0.514096184192
H	3.380981268926	-0.272365144766	-0.509472214773

TS 5-*exo* from 7p

NI=1 ; Freq= -354.4482

C	1.556979000000	-1.819792000000	-1.144335000000
C	2.918106000000	-1.503008000000	-0.985490000000
C	3.333004000000	-0.443298000000	-0.166100000000
C	2.384345000000	0.338649000000	0.528492000000
C	1.086042000000	-0.031059000000	0.322405000000
C	0.598179000000	-1.055317000000	-0.464395000000
C	-0.882744000000	-1.246042000000	-0.502816000000

O	-1.533910000000	-0.026376000000	-0.025144000000
C	-0.872416000000	0.638357000000	1.014624000000
C	-0.333501000000	0.845779000000	3.362714000000
C	-0.736790000000	0.044431000000	2.296531000000
C	-0.710165000000	2.035616000000	0.827632000000
C	-0.311882000000	2.811542000000	1.913654000000
C	-0.112356000000	2.228649000000	3.184465000000
C	0.331774000000	3.073655000000	4.328724000000
H	1.254410000000	-2.646962000000	-1.784107000000
H	3.665515000000	-2.096470000000	-1.512715000000
H	4.393775000000	-0.218782000000	-0.061467000000
H	2.675213000000	1.163229000000	1.171109000000
H	-1.302701000000	-1.349417000000	-1.520922000000
H	-1.219806000000	-2.082654000000	0.136828000000
H	-0.197677000000	0.401173000000	4.348907000000
H	-0.928327000000	-1.017082000000	2.427889000000
H	-0.886420000000	2.472622000000	-0.151544000000
H	-0.157965000000	3.883072000000	1.782987000000
H	1.421408000000	3.232574000000	4.301369000000
H	-0.133192000000	4.070058000000	4.318224000000
H	0.101235000000	2.625579000000	5.305197000000

TS 5-*exo* from 7o

NI=1 ; Freq=-355.3481

C	1.556979000000	-1.819792000000	-1.144335000000
C	2.918106000000	-1.503008000000	-0.985490000000
C	3.333004000000	-0.443298000000	-0.166100000000
C	2.384345000000	0.338649000000	0.528492000000
C	1.086042000000	-0.031059000000	0.322405000000
C	0.598179000000	-1.055317000000	-0.464395000000
C	-0.882744000000	-1.246042000000	-0.502816000000
O	-1.533910000000	-0.026376000000	-0.025144000000
C	-0.872416000000	0.638357000000	1.014624000000
C	-0.333501000000	0.845779000000	3.362714000000
C	-0.736790000000	0.044431000000	2.296531000000
C	-0.710165000000	2.035616000000	0.827632000000
C	-0.311882000000	2.811542000000	1.913654000000
C	-0.112356000000	2.228649000000	3.184465000000
H	1.254410000000	-2.646962000000	-1.784107000000
H	3.665515000000	-2.096470000000	-1.512715000000
H	4.393775000000	-0.218782000000	-0.061467000000
H	2.675213000000	1.163229000000	1.171109000000
H	-1.302701000000	-1.349417000000	-1.520922000000
H	-1.219806000000	-2.082654000000	0.136828000000
H	-0.197677000000	0.401173000000	4.348907000000
H	-0.928327000000	-1.017082000000	2.427889000000
H	-0.886420000000	2.472622000000	-0.151544000000
H	-0.157965000000	3.883072000000	1.782987000000
F	0.289996980000	2.994169630000	4.221089450000

TS 5-*exo* from 7n

NI=1 ; Freq=-346.7244

C	1.556979000000	-1.819792000000	-1.144335000000
C	2.918106000000	-1.503008000000	-0.985490000000
C	3.333004000000	-0.443298000000	-0.166100000000
C	2.384345000000	0.338649000000	0.528492000000
C	1.086042000000	-0.031059000000	0.322405000000
C	0.598179000000	-1.055317000000	-0.464395000000
C	-0.882744000000	-1.246042000000	-0.502816000000
O	-1.533910000000	-0.026376000000	-0.025144000000
C	-0.872416000000	0.638357000000	1.014624000000
C	-0.333501000000	0.845779000000	3.362714000000
C	-0.736790000000	0.044431000000	2.296531000000
C	-0.710165000000	2.035616000000	0.827632000000

C	-0.311882000000	2.811542000000	1.913654000000
C	-0.112356000000	2.228649000000	3.184465000000
H	1.254410000000	-2.646962000000	-1.784107000000
H	3.665515000000	-2.096470000000	-1.512715000000
H	4.393775000000	-0.218782000000	-0.061467000000
H	2.675213000000	1.163229000000	1.171109000000
H	-1.302701000000	-1.349417000000	-1.520922000000
H	-1.219806000000	-2.082654000000	0.136828000000
H	-0.197677000000	0.401173000000	4.348907000000
H	-0.928327000000	-1.017082000000	2.427889000000
H	-0.886420000000	2.472622000000	-0.151544000000
H	-0.157965000000	3.883072000000	1.782987000000
H	0.206545990000	2.835394980000	4.006085860000

Radical 9p

C	1.392276645502	-1.801125527945	-1.445152271444
C	2.765915467197	-1.641071457897	-1.281799932921
C	3.268721518686	-0.783101698069	-0.303404457442
C	2.403357939617	-0.073293396699	0.524956176281
C	1.035060496925	-0.238250426904	0.356820975563
C	0.534272042915	-1.090757524438	-0.615042262712
C	-0.962908948274	-1.070891902163	-0.571567213356
O	-1.299740930126	-0.177291649811	0.499194675175
C	-0.100734460069	0.420702642471	1.126299940078
C	-0.144859499790	0.989288859635	3.574200126826
C	-0.098713228939	0.059060228696	2.581463281123
C	-0.146541417677	1.906232521830	0.918993111976
C	-0.191291833747	2.792597723782	1.945547909429
C	-0.187380463315	2.379481997380	3.306800198640
C	-0.248074288467	3.390438768279	4.409511078721
H	1.004995905507	-2.468196740698	-2.205815988827
H	3.449702619355	-2.187257253016	-1.919227116836
H	4.339028741557	-0.668743921034	-0.187555936993
H	2.793284371026	0.593162960967	1.284546545444
H	-1.400668673403	-0.703960272395	-1.506362311909
H	-1.388536703038	-2.058596902662	-0.365973485004
H	-0.152824634988	0.659300513927	4.607346828931
H	-0.072323291071	-0.998690100334	2.813443961094
H	-0.155845286951	2.247105149641	-0.109290510012
H	-0.235422144022	3.854230204135	1.726444674346
H	0.550670807106	4.131863203869	4.312581371113
H	-1.191766519837	3.945785553400	4.386860436250
H	-0.159520231680	2.920703446053	5.388895196468

Radical 9o

C	1.425170027653	-1.791212652294	-1.410338692154
C	2.792710786854	-1.603301137767	-1.227188514355
C	3.264477038689	-0.724614316831	-0.251853215401
C	2.373542697382	-0.021239664175	0.554485983470
C	1.011724727386	-0.213980281995	0.365680139750
C	0.541187623759	-1.086635972785	-0.603018785828
C	-0.956293665152	-1.095227676933	-0.582235099127
O	-1.325852691276	-0.171728932910	0.454028476484
C	-0.149361690204	0.429854769751	1.110289077723
C	-0.274287867393	0.964127646048	3.567051235640
C	-0.178425210790	0.049429014772	2.564303859353
C	-0.207883601398	1.917533591848	0.902959630113
C	-0.303313822357	2.804946482314	1.929972535340
C	-0.331707584630	2.330235862478	3.250426951284
H	1.062566583221	-2.474344618134	-2.168748504652
H	3.496351092703	-2.143911080854	-1.847428481988
H	4.330450071309	-0.588757633617	-0.121153988964
H	2.739423757785	0.661114827834	1.311807080203
H	-1.389637062782	-0.765540987832	-1.531984288946

H	-1.365001950258	-2.083891115695	-0.349500532616
H	-0.310362633093	0.660450782482	4.605473322329
H	-0.138539418565	-1.009072920177	2.786557989002
H	-0.189858300923	2.262363212017	-0.122776502402
H	-0.360824363800	3.870916681687	1.750356048784
F	-0.423620334118	3.225168040767	4.258474896957

Radical 9n

C	1.432228150865	-1.788023100469	-1.407242967581
C	2.797576236502	-1.593110162032	-1.215470875740
C	3.258062330795	-0.712613041716	-0.236255025339
C	2.358111230128	-0.014756309368	0.564832751964
C	0.998377157781	-0.214266928373	0.367655779955
C	0.539143748206	-1.088960881850	-0.604987285830
C	-0.958289585337	-1.105656744257	-0.594055949279
O	-1.340221948827	-0.187334283573	0.441322291754
C	-0.172515980095	0.422804455821	1.104747415917
C	-0.262107430952	0.969342690554	3.556583085984
C	-0.201442329892	0.046483025947	2.558455904609
C	-0.232191188116	1.909239023513	0.898233973874
C	-0.292165599083	2.793954834198	1.930330577668
C	-0.301250684246	2.353655614027	3.273454071812
H	1.078024879887	-2.472504855513	-2.168490510004
H	3.508083486065	-2.129413310050	-1.831654087599
H	4.322448960817	-0.571010125304	-0.098450330319
H	2.715395756163	0.668976448462	1.325027308226
H	-1.386659018740	-0.776847410781	-1.546640520952
H	-1.362985352766	-2.097522922450	-0.367082994750
H	-0.288253196116	0.639778588535	4.588458353636
H	-0.181187137232	-1.013846465544	2.778724696581
H	-0.234901112064	2.249699795131	-0.130001565583
H	-0.341186669926	3.856100716262	1.721798215017
H	-0.353315443817	3.071955508832	4.080314225978

Product-1a

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C	-6.207111662653	-0.321573169181	2.997455940375
C	-7.473053629196	-0.832354335472	3.250381934498
C	-7.601992214171	-2.059755738946	3.881012880430
C	-6.469773146394	-2.777511739560	4.253194705762
C	-5.210917821883	-2.250644041116	4.013933205180
C	-5.054044752364	-1.008540215327	3.398215086212
C	-4.971122435693	1.053505403802	1.560212285988
O	-6.117797134096	0.897764204801	2.392955863825
C	-3.753321755074	-0.346603043744	3.198131660358
C	-3.707190471181	0.723672150244	2.299764023038
C	-2.523060674450	1.413355834891	2.088020423652
C	-2.594258395660	-0.702828118169	3.886291026362
C	-1.407749538485	-0.020128527938	3.661781733149
C	-1.367969703398	1.038063970852	2.761825447303
H	-8.338481599885	-0.261379645084	2.940656796886
H	-8.588322479373	-2.462942039942	4.070066124896
H	-4.333670579845	-2.812372253141	4.308238366497
H	-4.977536225864	2.087263594931	1.222605985536
H	-5.083459402363	0.398631267840	0.687334999760
H	-2.503937250349	2.244728300397	1.393245214372
H	-2.617374295713	-1.506478154231	4.610717801401
H	-0.513766438704	-0.307492461539	4.199741697216
H	-0.443625322890	1.574835978131	2.593667638218
H	-6.569444070318	-3.743540222500	4.729413159085

Product-1c

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C	-6.216180913077	-0.321543284441	2.980500599207

C	-7.477839642995	-0.841326398397	3.235206856857
C	-7.603271532080	-2.068591988770	3.874615700296
C	-6.478415505159	-2.798770392471	4.263970455833
C	-5.222827551425	-2.248684175222	4.013385600767
C	-5.060194393842	-1.007545162756	3.391250708160
C	-4.964208316723	1.078968719022	1.554557482063
O	-6.131693970252	0.902096829960	2.370888382914
C	-3.758082140148	-0.348638484976	3.191858839189
C	-3.706816062665	0.733924058677	2.299880875972
C	-2.517317249133	1.422886976511	2.095846956805
C	-2.591730887852	-0.712337876340	3.873113359907
C	-1.401445730058	-0.030911293176	3.653722489493
C	-1.359402767367	1.038615181752	2.763998564569
H	-8.350672724650	-0.283207072424	2.921461158495
H	-8.592608504636	-2.470301264426	4.058449650546
H	-4.342685835813	-2.805239955578	4.312240884938
H	-4.973256498656	2.121258992248	1.242438473632
H	-5.068693650017	0.450090254437	0.660245027824
H	-2.494668845559	2.261391050902	1.409565441821
H	-2.612278663078	-1.522903549280	4.589424296784
H	-0.507652437129	-0.327902612350	4.187665027853
H	-0.434131077074	1.575642197835	2.599319232902
C	-6.610864484512	-4.137391159757	4.944771387167
H	-6.013911765406	-4.900970162116	4.441322360819
H	-6.266118386379	-4.091586522445	5.981190224077
H	-7.647893624316	-4.473116066421	4.954545251112

Product-1d.

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C	-6.210179483110	-0.308210864193	2.917104944935
C	-7.475242878930	-0.828449163086	3.142057829858
C	-7.620896038303	-2.049033647682	3.792211282607
C	-6.512728682627	-2.781855671057	4.226936836854
C	-5.252551780142	-2.222410888073	4.004018390921
C	-5.069449916952	-0.989847627798	3.373030270836
C	-4.913014996436	1.076320654942	1.517114252037
O	-6.107266168087	0.907500200284	2.295850928822
C	-3.760730597212	-0.333386759155	3.208724949125
C	-3.680711489367	0.739210355668	2.306754603133
C	-2.485260155255	1.426324290396	2.133121732469
C	-2.616667928680	-0.688274255021	3.931241100984
C	-1.419934717696	-0.008971523444	3.742321851608
C	-1.349248673083	1.050262836634	2.842228139569
H	-8.341038903043	-0.276834587040	2.798352387143
H	-8.621382139857	-2.428225348771	3.941542362725
H	-4.373094139239	-2.760371584070	4.331656955073
H	-4.911602746681	2.115393689339	1.194326244002
H	-4.988096823263	0.438485102014	0.626244733744
H	-2.440689351982	2.256957768218	1.438356622192
H	-2.659523464778	-1.490215239080	4.656179438153
H	-0.543849814352	-0.299374759941	4.308289500722
H	-0.419210710252	1.585774395216	2.701169996915
C	-6.634532370997	-4.146681338896	4.923189641700
C	-6.006859666647	-4.068416225058	6.330742914800
H	-6.085297087717	-5.035479662509	6.833118743468
H	-4.950455418939	-3.799753183201	6.289185743817
H	-6.519665001529	-3.324912262870	6.944702703735
C	-5.892006933866	-5.216884832536	4.095865434229
H	-5.970641826585	-6.191902187070	4.582611828727
H	-6.320802398089	-5.302025217725	3.095054979850
H	-4.831992346625	-4.982748615174	3.988975396404
C	-8.096387262422	-4.592321474569	5.077306388911
H	-8.674179303977	-3.890439266026	5.681848311448
H	-8.592805435281	-4.700530385170	4.110960851302
H	-8.129640598000	-5.562647273494	5.576141157183

Product-1e

28

C	-6.227604496381	-0.278210469802	2.918657762834
C	-7.496003233448	-0.795428962473	3.125080346926
C	-7.664136445434	-2.045904898274	3.713651460461
C	-6.542232737951	-2.784901960110	4.090038289367
C	-5.268573947453	-2.254087875076	3.894178939366
C	-5.086965539320	-0.994300018039	3.325258307889
C	-4.936788052364	1.157091943568	1.568835757578
O	-6.114303730878	0.973863258724	2.367032167677
C	-3.773300691018	-0.346320577781	3.170726216360
C	-3.694312102118	0.765083656908	2.317001838821
C	-2.491232717163	1.441014827745	2.152781829139
C	-2.623080159574	-0.751684397140	3.855273844742
C	-1.419809231284	-0.081516949223	3.676466723105
C	-1.349247794843	1.016300816976	2.823777252175
H	-8.357292094109	-0.216092878132	2.818508065978
H	-8.662747271946	-2.430785236521	3.856554207711
H	-4.417547733994	-2.848626602978	4.198520358301
H	-4.922952570621	2.209430720526	1.292359744093
H	-5.040186753364	0.560698220404	0.652164224411
H	-2.445594495842	2.301681942457	1.495730603235
H	-2.666441624452	-1.586458267059	4.542220626800
H	-0.538375436118	-0.409939385304	4.212441579737
H	-0.413737963523	1.544164747772	2.690232685193
O	-6.590170930917	-4.028402060031	4.653792635385
C	-7.864626947858	-4.623105806911	4.874189457117
H	-7.668202232469	-5.593802095780	5.322541576431
H	-8.470373964902	-4.023949866061	5.558967318202
H	-8.407192570657	-4.760862668385	3.935318480966

Product-1f

27

C	-6.212308754769	-0.330905502390	2.983260805719
C	-7.497146695260	-0.823851090454	3.241682202940
C	-7.600615743756	-2.052505035474	3.888449106390
C	-6.468340938730	-2.770625458648	4.266779505046
C	-5.207158404159	-2.251422173159	4.023424765713
C	-5.053508203075	-1.011729723807	3.392175671673
C	-4.955179353127	1.061084361075	1.544374415837
O	-6.122620151664	0.885477408509	2.360845497616
C	-3.752640197490	-0.350243342699	3.191298742341
C	-3.698867530043	0.727213550176	2.294331884579
C	-2.510472511007	1.418116111387	2.091067640127
C	-2.588114183835	-0.708279057597	3.878963182375
C	-1.398253636244	-0.025677493083	3.660584276252
C	-1.354466573627	1.039581155620	2.765787478532
H	-8.585802709882	-2.458449970166	4.085311360168
H	-4.331840035938	-2.811754706836	4.324103128382
H	-4.969561763538	2.100624998906	1.223352400589
H	-5.056598121232	0.423849764053	0.655867418746
H	-2.487118684340	2.252967260527	1.400364145469
H	-2.609781473392	-1.514955931120	4.599569875405
H	-0.506037903365	-0.318418263435	4.199514981437
H	-0.429477685976	1.577380414144	2.602056868106
H	-6.573978822072	-3.732411031620	4.751840992106
C	-8.712165643245	-0.043208454068	2.822909340317
H	-8.745720098773	0.934215742052	3.310059983784
H	-8.713828498687	0.142523334472	1.746588251327
H	-9.622437462773	-0.583576256368	3.080606959024

Product-1g.

25

C	-6.215526042635	-0.352663927757	2.975654144639
C	-7.484365866438	-0.861162637371	3.249668853629
C	-7.618227353639	-2.073930901770	3.896331949647

C	-6.472146486581	-2.788061593328	4.273850289069
C	-5.203327506169	-2.259569111735	4.022009384453
C	-5.050471322304	-1.029176408422	3.389398614133
C	-4.962008546718	1.063532721136	1.551156369227
O	-6.145757188927	0.842934392088	2.343445962137
C	-3.752228358204	-0.363864835284	3.188800090536
C	-3.709645337234	0.722447926841	2.303548904066
C	-2.524919691307	1.421096791239	2.104865791320
C	-2.586099838933	-0.725157427358	3.870631560246
C	-1.400905577627	-0.034616797873	3.656240458406
C	-1.366313030280	1.040123797705	2.772549988559
H	-8.600144352951	-2.479119355336	4.097431461607
H	-4.332295916911	-2.819906179426	4.330884100833
H	-4.991182891016	2.113318535912	1.269391507710
H	-5.048785432206	0.457978589793	0.640987098677
H	-2.506851294808	2.263329114698	1.423495637522
H	-2.601071779686	-1.538537837462	4.583704985450
H	-0.505877907277	-0.328178131796	4.189459907652
H	-0.444777331617	1.584536828921	2.612172666352
H	-8.353075140446	-0.298470906986	2.936022542177
C	-6.599146317659	-4.053883739096	4.918285272706
N	-6.703742428426	-5.078046247335	5.440188149248

Product-1h

27

C	-6.214048301458	-0.323880601306	3.000227793501
C	-7.480690584788	-0.830739712667	3.279298677661
C	-7.610733033122	-2.058422737041	3.904186464935
C	-6.469916035501	-2.784936242839	4.247329153390
C	-5.207754999220	-2.263915093424	3.992106114511
C	-5.051664875345	-1.019072338976	3.381005118740
C	-4.973543232836	1.101315583600	1.578343842639
O	-6.140641667735	0.889891616779	2.394023474846
C	-3.749817439893	-0.364345715761	3.170081486266
C	-3.710170465415	0.736292123850	2.301744033657
C	-2.521649955807	1.425747919558	2.094149644232
C	-2.575591275081	-0.748625157063	3.825228985733
C	-1.386769514792	-0.066802936954	3.601798975520
C	-1.355618092228	1.022036766755	2.735413466176
H	-8.595321589091	-2.457894758017	4.104768156838
H	-4.332985375942	-2.833995143726	4.270514130259
H	-4.992594113099	2.153900106991	1.305520145718
H	-5.085323369562	0.505035632094	0.664169717086
H	-2.506343331099	2.278875918010	1.426292367191
H	-2.586912288216	-1.573911202376	4.524612732169
H	-0.485824268404	-0.378494725757	4.114510041565
H	-0.431114817845	1.559342345477	2.568019083154
H	-8.351070606056	-0.258452134090	2.987996332187
C	-6.611731191116	-4.103996529323	4.943431999219
F	-7.697807479692	-4.793726264692	4.527138557134
F	-6.752515515929	-3.964927934397	6.289523995080
F	-5.542846590730	-4.908842094706	4.760737240593

Product-1i

24

C	-6.214115710433	-0.332822907543	2.982280365191
C	-7.478923995116	-0.848515085599	3.243410725200
C	-7.614880259059	-2.068537483510	3.889659225048
C	-6.471013864323	-2.763145000156	4.264328445328
C	-5.207079535307	-2.250301233037	4.027314135417
C	-5.054810780752	-1.012032993563	3.395720483808
C	-4.964233023645	1.068202542418	1.551852210862
O	-6.135486811679	0.880819802820	2.363869054457
C	-3.754285281553	-0.352001319085	3.194213056118
C	-3.707707479415	0.728277472928	2.300174303765
C	-2.519951365756	1.419635035007	2.095001045545

C	-2.588374233952	-0.713044262875	3.876734275456
C	-1.400226532366	-0.028890604329	3.656167749022
C	-1.361759202375	1.038959147588	2.764367239684
H	-8.595321272585	-2.479443925087	4.084886967328
H	-4.338630377677	-2.813936573415	4.336505379345
H	-4.980480543065	2.111668818964	1.245204752852
H	-5.063683579074	0.442593297247	0.655431870743
H	-2.498901720363	2.256626476374	1.407095763555
H	-2.606413148356	-1.521953092036	4.594949933506
H	-0.505716987434	-0.322380786926	4.190505419486
H	-0.437903009986	1.577969742204	2.598690209035
H	-8.350940434763	-0.290604715352	2.929011412310
Cl	-6.630986790966	-4.321706203036	5.053618816938

Product-1j

24

C	-6.213121799041	-0.317174373737	2.975986691061
C	-7.475314994490	-0.846592636418	3.251366526106
C	-7.610770999586	-2.068304685622	3.893749625428
C	-6.472588094300	-2.774579891603	4.266429532091
C	-5.213851708134	-2.247307707371	4.019296309141
C	-5.059418415164	-1.008459883491	3.391249974517
C	-4.957171647468	1.070591733052	1.543006233218
O	-6.128600428195	0.889953722533	2.359137069991
C	-3.758330930300	-0.346476958632	3.190047937468
C	-3.703427407788	0.730641963694	2.293553590656
C	-2.513561998384	1.418870341931	2.090535377338
C	-2.596075159585	-0.707649964613	3.879182938914
C	-1.405226345964	-0.027221472502	3.661448259847
C	-1.359377147744	1.037448794116	2.766166298659
H	-8.598591156579	-2.464121000297	4.084370554099
H	-4.337748866300	-2.805725627688	4.319370194806
H	-4.974067534869	2.112935367116	1.233231015574
H	-5.062001588393	0.441041493236	0.650601277215
H	-2.487960062465	2.253713129531	1.400200235887
H	-2.619763052160	-1.513624904907	4.600269748996
H	-0.514090001132	-0.321062387253	4.201254387121
H	-0.433359552684	1.573507803698	2.603076279064
H	-6.573867728101	-3.735961149899	4.751744162770
Cl	-8.901804011172	0.041333995126	2.774428630034

Product-1k

24

C	-6.213688808740	-0.331262823696	2.985959120154
C	-7.479492448697	-0.847939636522	3.239983038678
C	-7.617835890066	-2.069843961480	3.885201214916
C	-6.470282328214	-2.748437830853	4.257074785357
C	-5.205030043337	-2.249184184993	4.030990829684
C	-5.053694640262	-1.009482406601	3.399727206778
C	-4.966310125303	1.068555758274	1.554777061652
O	-6.132598429063	0.888996793322	2.373336821318
C	-3.754052118682	-0.349332180858	3.196800357071
C	-3.707735866975	0.729524626031	2.300688769237
C	-2.519435454219	1.419010273310	2.092857832586
C	-2.587528894750	-0.710948727277	3.877918932962
C	-1.398971432896	-0.028163593852	3.655067152416
C	-1.360736058919	1.038341712720	2.761619559196
H	-8.592062019561	-2.495238371702	4.082919509050
H	-4.346886917549	-2.825161684677	4.348084252532
H	-4.980210229921	2.110326234288	1.241878450934
H	-5.069466097740	0.437849223370	0.661966232375
H	-2.498185826708	2.254693125902	1.403335356868
H	-2.605815521859	-1.519671518939	4.596457496692
H	-0.503939635097	-0.321821134231	4.188467741009
H	-0.436523804410	1.576128582397	2.593841695845
H	-8.349633345051	-0.289026739492	2.922641396754

F	-6.593929031982	-3.956295904443	4.868884365936

Product-1l

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C	-6.197841759748	-0.284282196820	2.969503647749
C	-7.488849413581	-0.782988256126	3.205785549404
C	-7.572436833773	-2.022272958185	3.849651609469
C	-6.461329267737	-2.765869004748	4.254389292085
C	-5.205859880015	-2.214211947341	4.020593833302
C	-5.050570876131	-0.974481351771	3.401632041150
C	-4.884305940363	1.057186831001	1.531600334228
O	-6.050943487405	0.935405900080	2.355127348511
C	-3.736421223111	-0.328123834809	3.224772890611
C	-3.642354577723	0.723333911871	2.301797120175
C	-2.439383556114	1.390997203740	2.107250944133
C	-2.594944421737	-0.680829812966	3.953302421468
C	-1.389856757674	-0.021605714739	3.745992630101
C	-1.306277399835	1.015310841832	2.821127552799
H	-8.552342043685	-2.430484241681	4.028896531646
H	-4.318336268825	-2.754345767257	4.320743223496
H	-4.876113395350	2.085700906559	1.176023972386
H	-4.997143946235	0.392438491245	0.664420196447
H	-2.387336735065	2.205816555614	1.394466327172
H	-2.645784717279	-1.464456289548	4.697394567752
H	-0.516587483541	-0.310230007246	4.317311681386
H	-0.369138009387	1.534277781793	2.665717147706
C	-6.582789648855	-4.141268309626	4.931585169537
C	-8.043372065548	-4.582144330506	5.110055621512
H	-8.070366230519	-5.560003028321	5.594538233916
H	-8.604856114785	-3.887542772099	5.737961976380
H	-8.561352177127	-4.673699489024	4.153358655410
C	-5.925600706147	-4.090840133984	6.326968381500
H	-6.000517556125	-5.065408704772	6.815355417877
H	-4.868428798498	-3.828667090915	6.267765592255
H	-6.420176597285	-3.353905300182	6.963472619953
C	-5.864585556943	-5.203114732471	4.072423893853
H	-5.938973098978	-6.185476954614	4.545061591498
H	-6.314734738923	-5.269733763024	3.079562800421
H	-4.805712412793	-4.973137883655	3.946819114204
C	-8.756135783583	-0.017351442179	2.775820695979
C	-10.043065003909	-0.769885455374	3.155465557866
H	-10.110796444599	-1.743461142682	2.666361981853
H	-10.129218614177	-0.919697943837	4.233332590673
H	-10.904449278343	-0.180905326290	2.835409735106
C	-8.773022997771	0.169892079479	1.242668450419
H	-9.683168584964	0.696074594534	0.944300077034
H	-7.918288058172	0.745684700595	0.895556252628
H	-8.765434275871	-0.798456633885	0.737136518649
C	-8.809684727397	1.358513218795	3.475600076815
H	-7.952437354131	1.977197585727	3.220083602679
H	-9.716816942384	1.890283425350	3.177920588897
H	-8.834682547860	1.236338792463	4.560995879910

Product-1m

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C	-6.155476503408	-0.346718915733	2.976298179142
C	-7.458471969236	-0.802316145331	3.245047642313
C	-7.543018158763	-2.041819207561	3.877015215639
C	-6.416787169864	-2.788153847950	4.195592566096
C	-5.129930836870	-2.314512421727	3.966837597645
C	-4.989667064353	-1.033612663113	3.390491042098
C	-4.886378689493	0.892600142577	1.428109474688
O	-6.016770968855	0.844589087672	2.308468129710
C	-3.702682797138	-0.320843064042	3.211592988483
C	-3.633742493866	0.663700402432	2.211719788051
C	-2.474062438189	1.398574665031	2.003690987462

C	-2.578884174292	-0.496530956165	4.029461738462
C	-1.416034599240	0.234532601347	3.815499897970
C	-1.351321316142	1.174215031559	2.792824811483
H	-8.510840278759	-2.465414428145	4.099621536503
H	-4.905281564486	1.877531300842	0.966152931645
H	-5.018986895442	0.135029176517	0.644538313758
H	-2.452065849961	2.154437466742	1.227344366316
H	-2.608251481541	-1.188098719488	4.856236382754
H	-0.561348928095	0.074829063593	4.460822353081
H	-0.445310449771	1.742816326355	2.626849863186
H	-6.544496723613	-3.772289633934	4.630446248316
C	-8.717060648513	-0.005801186166	2.851190604852
C	-10.003492446425	-0.717602842664	3.304666756724
H	-10.864117263726	-0.108572622916	3.022493314716
H	-10.122612991338	-1.693985802605	2.831374068694
H	-10.036547768809	-0.854256543993	4.387289558629
C	-8.798226578405	0.151331894327	1.316868931178
H	-7.947361567112	0.700296185536	0.920445892610
H	-8.834631743708	-0.826674168836	0.831605482259
H	-9.709072115537	0.692253163973	1.048360092714
C	-8.704501627172	1.384098926997	3.524028730471
H	-8.686048657206	1.283971911163	4.611816880897
H	-7.843354048896	1.974532677403	3.219698018983
H	-9.609395730954	1.934131339780	3.254206758240
C	-3.973752319860	-3.221692735433	4.311865510402
H	-3.145318182921	-3.120616860826	3.611259694856
H	-3.580509305350	-3.029130894932	5.313352240903
H	-4.307938262691	-4.259336642285	4.296328568069

Product-1o

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C	-6.212939738165	-0.331740443019	2.981099295537
C	-7.479920983673	-0.842924253060	3.243906445618
C	-7.608791905223	-2.063444805118	3.892144723270
C	-6.473988666317	-2.776422880438	4.274420286866
C	-5.214333881776	-2.250677015783	4.027798305199
C	-5.054371170302	-1.013765213726	3.392986263935
C	-4.962580330546	1.065694754430	1.547487325594
O	-6.132539620078	0.883049152526	2.360888082564
C	-3.755870170670	-0.352280204390	3.190487659865
C	-3.706550940308	0.730276424291	2.298429898029
C	-2.519381695641	1.423274512559	2.098543198303
C	-2.594102596582	-0.719693036494	3.876506227673
C	-1.428558687455	-0.018795092200	3.639524579936
C	-1.356691388890	1.050137099381	2.764736298855
H	-8.595266343861	-2.464788467800	4.086083892656
H	-4.978102322881	2.107047309658	1.233466884127
H	-5.062684402157	0.433857351566	0.655367495617
H	-2.494161928600	2.261857590131	1.413494968260
H	-2.586461878327	-1.525672829289	4.596679466458
H	-0.423096806683	1.575853699713	2.620065386034
H	-6.572047608025	-3.736382521299	4.763896876729
H	-8.348013032158	-0.279415869604	2.927475400038
H	-4.339319466332	-2.809625807327	4.332833705292
F	-0.307353805351	-0.388371024710	4.308606303547

Product-1p

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C	-6.217311672798	-0.327100499088	2.974490841815
C	-7.486642374705	-0.828369508859	3.244626376348
C	-7.622090036483	-2.031782669127	3.923684216179
C	-6.490113711211	-2.736609357277	4.327537425433
C	-5.227748528284	-2.219989650568	4.071628887059
C	-5.060434371868	-0.999376739694	3.407611836045
C	-4.959184415941	1.031282596472	1.508420651255
O	-6.132580555127	0.872016513820	2.322991022381

C	-3.758158250549	-0.346839936645	3.190174622569
C	-3.706826949593	0.707664915387	2.269363819947
C	-2.512461859448	1.386563957615	2.059580805794
C	-2.595053989290	-0.691927120624	3.887266184946
C	-1.388723147777	-0.030704138002	3.670574207260
C	-1.362800436182	1.017631738613	2.745834076754
H	-8.610374346580	-2.425599212056	4.124024690753
H	-4.970255046504	2.065544743344	1.170717870003
H	-5.061322699905	0.380678697637	0.629690928355
H	-2.478894948815	2.208615367796	1.353877517689
H	-2.628289693600	-1.482241935137	4.626671219157
H	-0.438509751058	1.555697906494	2.571109005724
H	-6.591733427701	-3.683831083830	4.840869383578
H	-8.351982502408	-0.270856274267	2.910117542674
H	-4.355293280676	-2.773407718827	4.393480801141
C	-0.139790836228	-0.431933292785	4.411536145597
H	-0.365583173152	-1.115054800901	5.230273972597
H	0.566286922028	-0.933690659004	3.744313475352
H	0.372784823854	0.438947719512	4.824710193596

RA of Product-1a

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C	-6.228669014855	-0.347327048600	2.957879162481
C	-7.485000608907	-0.856366467757	3.194850744687
C	-7.646059015549	-2.075936439651	3.894936727668
C	-6.500394833104	-2.753900040914	4.321068898670
C	-5.232171302863	-2.247281808228	4.080376660216
C	-5.033111375379	-1.007802120002	3.388416779713
C	-4.951454596466	1.062539668161	1.547494322700
O	-6.137571947328	0.890603673612	2.350466843913
C	-3.772345609070	-0.367215458044	3.194781984424
C	-3.707109420672	0.768108082590	2.322957739821
C	-2.539412595071	1.478315145526	2.147366678100
C	-2.543984546659	-0.763681813641	3.815752709297
C	-1.377705276545	-0.049045350902	3.612185681071
C	-1.345505042124	1.089443149895	2.790461255776
H	-8.345401619369	-0.295959947529	2.846661437481
H	-8.634993890196	-2.471935880580	4.085492922107
H	-4.368788768893	-2.804464324577	4.422799485061
H	-4.979216693791	2.090361047399	1.186075820218
H	-5.037587475726	0.390561025351	0.680451940570
H	-2.538333380211	2.336681647003	1.481446965811
H	-2.526704409738	-1.623006778097	4.474992712966
H	-0.468391324041	-0.374873887999	4.107559473831
H	-0.428924842749	1.645742665289	2.643662650972
H	-6.600143410693	-3.695881738307	4.850724402448

RA of Product-1c

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C	-6.226848642548	-0.320093719541	2.990120314996
C	-7.478805920104	-0.828576283654	3.246564556910
C	-7.631009292696	-2.063768145450	3.917324019277
C	-6.489023559083	-2.781513181864	4.305881013155
C	-5.229886972513	-2.260829161267	4.039746721735
C	-5.033113123108	-1.005817029800	3.375454931289
C	-4.969082887185	1.112845648446	1.589288940618
O	-6.136654288422	0.936149183501	2.416442028667
C	-3.768193493883	-0.377223957034	3.167684501318
C	-3.709863984179	0.781128345429	2.325530393423
C	-2.537718033636	1.481758866122	2.140686172282
C	-2.529502994857	-0.806709628940	3.744305192764
C	-1.359262840104	-0.101406631380	3.530596905047
C	-1.332974755593	1.059988546152	2.741465637605
H	-8.345965687274	-0.254714258562	2.938752154185
H	-8.621525971785	-2.452122734872	4.121849412209

H	-4.360075858728	-2.830754606273	4.345714803522
H	-4.989988925017	2.150029752313	1.254769049568
H	-5.084977888263	0.464798915936	0.707291616987
H	-2.542184781596	2.358422010081	1.498980460053
H	-2.506544252696	-1.684514857456	4.378497564516
H	-0.441870824836	-0.453039937745	3.992349459940
H	-0.413200253428	1.608881949710	2.586848356591
C	-6.634224547932	-4.118916104661	4.992357439741
H	-5.672427448855	-4.488806823265	5.351096004366
H	-7.311408254788	-4.057189568087	5.848938201375
H	-7.048527676891	-4.874099747839	4.316899437859

RA of Product-1d

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C	-6.213928620806	-0.329012415121	2.877045481072
C	-7.466816069316	-0.853964001384	3.076184829673
C	-7.637970612710	-2.084508018442	3.755365678717
C	-6.518708437126	-2.788322643950	4.218741750130
C	-5.252663418921	-2.240740993173	4.006049314804
C	-5.036722205074	-0.993147646182	3.339232510423
C	-4.899221773655	1.098734139545	1.524573495780
O	-6.110548285587	0.916519063411	2.286206080773
C	-3.770639615259	-0.348148739042	3.193526007363
C	-3.680190870630	0.797791811432	2.337097616394
C	-2.510141038920	1.513199537543	2.207339466322
C	-2.560733774922	-0.748029895935	3.850089443237
C	-1.390946304291	-0.027573700388	3.692311824870
C	-1.335226987812	1.120644129123	2.885248223508
H	-8.327574036514	-0.302162559805	2.714791654585
H	-8.639273811437	-2.461971652336	3.898151379362
H	-4.382310323373	-2.779837514312	4.357312827539
H	-4.916551951875	2.130257222580	1.172973824720
H	-4.955719870310	0.435420953124	0.648206838025
H	-2.490267653536	2.378673044312	1.550879741877
H	-2.561097158380	-1.615192604922	4.499143114995
H	-0.496980683890	-0.356671536564	4.213081241446
H	-0.415850850620	1.680522863867	2.773605096061
C	-6.646277479599	-4.145124551243	4.939381691284
C	-6.014818966133	-4.059490095904	6.344514975242
H	-6.100523719519	-5.019342238878	6.861638406283
H	-4.957197289107	-3.798363034000	6.295610153897
H	-6.519223581588	-3.303207698795	6.950543465197
C	-5.917162764829	-5.237647735386	4.129080812278
H	-6.003910836967	-6.207240308066	4.627714075014
H	-6.348996464877	-5.331805075126	3.129898471867
H	-4.856304178333	-5.011836224563	4.015329144504
C	-8.108532742332	-4.586253054563	5.110123263227
H	-8.681088421018	-3.869572919096	5.702152801856
H	-8.610091817546	-4.708661097738	4.148250036260
H	-8.143424633189	-5.547909360024	5.627144711415

RA of Product-1e

28

C	-6.230720582246	-0.305480925677	2.885341593802
C	-7.482994461566	-0.821648439461	3.068649514472
C	-7.676032612938	-2.081282779597	3.692544470938
C	-6.544516038339	-2.782266018725	4.101792334071
C	-5.265838221385	-2.271408786952	3.916443719455
C	-5.053707722381	-1.002577926362	3.300267880219
C	-4.933095153116	1.148017650763	1.578509675974
O	-6.112922067835	0.966080711991	2.363655857362
C	-3.788930033868	-0.366253949969	3.163819448990
C	-3.699692150176	0.807021001688	2.352605443530
C	-2.525188812599	1.508845199598	2.227749350318
C	-2.580313645027	-0.810205545536	3.781438492096
C	-1.405484482933	-0.099353012149	3.629500449593

C	-1.348524522776	1.074665562830	2.868726264186
H	-8.336381725657	-0.238917739344	2.742784476460
H	-8.674452499729	-2.464270253557	3.833325203108
H	-4.427399639764	-2.869014502737	4.250220236849
H	-4.935656634459	2.187065134795	1.251167028679
H	-5.014092379908	0.501874755600	0.692575529938
H	-2.506396300567	2.397769692864	1.604050144496
H	-2.584437347478	-1.702741410773	4.395004033345
H	-0.507303267345	-0.459150683681	4.120308784104
H	-0.423574563963	1.624947743143	2.762809624899
O	-6.603345604887	-4.014408712957	4.708250847852
C	-7.878521754898	-4.581378264541	4.908045908456
H	-7.717061694844	-5.543394130912	5.388503813712
H	-8.496942597906	-3.953611180843	5.555144114266
H	-8.399506951410	-4.733974029500	3.959068058829

RA of Product-1f

27

C	-6.228717636622	-0.331995576603	2.980162716540
C	-7.498868562442	-0.824322417280	3.216781632546
C	-7.633658796682	-2.048830950867	3.917573208129
C	-6.491030407052	-2.733994425964	4.339887376018
C	-5.223026510152	-2.234183257378	4.096407322689
C	-5.031108557254	-0.997353675593	3.404143701469
C	-4.946994627911	1.067356283327	1.557509346763
O	-6.126286622517	0.906984477506	2.372077551144
C	-3.767438715664	-0.365100499632	3.199153463647
C	-3.699266687048	0.768713017645	2.324169837390
C	-2.528359739294	1.470688447139	2.138720529532
C	-2.535080306487	-0.769745116071	3.809990157110
C	-1.366187129822	-0.063389895257	3.597259012347
C	-1.331686744062	1.075716794358	2.774122823481
H	-8.622357928098	-2.447249165286	4.110409319391
H	-4.358881246225	-2.793822675721	4.432588363203
H	-4.971229716842	2.093451957258	1.190328229788
H	-5.045193910138	0.391289496896	0.694851453653
H	-2.526885390104	2.327426949684	1.470455746661
H	-2.517464396829	-1.628984494850	4.469423244454
H	-0.455333259908	-0.395587149313	4.085764818730
H	-0.412444681919	1.625679337737	2.620241550985
H	-6.597145863833	-3.676954747727	4.866703395219
C	-8.719269570175	-0.062093879259	2.766795136394
H	-8.886144594879	0.838895160629	3.365913156996
H	-8.632508803599	0.266486482532	1.728859087246
H	-9.611471374442	-0.684059867911	2.854878698478

RA of Product-1g

25

C	-6.239306657321	-0.356949625762	2.960175513158
C	-7.489722551914	-0.879315094656	3.182955549300
C	-7.657246416661	-2.104182503854	3.863805409590
C	-6.487717793373	-2.778890758248	4.294744218965
C	-5.219036804216	-2.252357330786	4.066150943311
C	-5.030811034232	-1.019529649522	3.392551780528
C	-4.958165273330	1.071250923022	1.568737668104
O	-6.147171154187	0.879264559250	2.367532204211
C	-3.767828037014	-0.376836736677	3.200017887530
C	-3.711584451479	0.758541560291	2.334491684775
C	-2.540335475213	1.467529341003	2.154576194644
C	-2.545005302625	-0.771335974263	3.817994122231
C	-1.376624422454	-0.061687122682	3.608839299514
C	-1.349745334891	1.074256071049	2.786495879715
H	-8.637837660729	-2.517132781081	4.047508114513
H	-4.359085885158	-2.807561728508	4.416541704117
H	-4.987058589226	2.108393902972	1.236959729850
H	-5.046491131227	0.425660754387	0.683998874324

H	-2.541176303763	2.330350254460	1.495241159043
H	-2.526570053471	-1.628293018468	4.480087083384
H	-0.466682365918	-0.387580674123	4.101405806960
H	-0.434005145370	1.631208219353	2.637658259719
H	-8.352412828213	-0.323122473768	2.835727771244
C	-6.600641920062	-4.022800707416	4.975925052752
N	-6.706630347955	-5.033926745973	5.530053778516

RA of Product-1h

27

C	-6.227805560803	-0.329699698674	2.990389745013
C	-7.479853919131	-0.839545597542	3.240024453557
C	-7.636869008293	-2.081872659688	3.894974849464
C	-6.476428272610	-2.780553732506	4.266520698851
C	-5.211818030820	-2.275129544293	4.015550897576
C	-5.024448998086	-1.017193553349	3.364178781131
C	-4.970518202884	1.123103471333	1.604522142183
O	-6.140956955931	0.922950890324	2.427189039097
C	-3.761082333201	-0.384569124011	3.160489306976
C	-3.710050337195	0.781888256855	2.333351464734
C	-2.538213373478	1.486708537613	2.153395300439
C	-2.524547608558	-0.816766665163	3.730781190280
C	-1.354998335206	-0.108845144542	3.520743599902
C	-1.334713617513	1.059291809132	2.744108428722
H	-8.621063290408	-2.481642399952	4.092683850409
H	-4.346400269677	-2.846112875760	4.319281562324
H	-4.998505685910	2.167230239426	1.294802930773
H	-5.085185686292	0.495799591713	0.708903194698
H	-2.545330861880	2.371769397578	1.523960680751
H	-2.498323766930	-1.700068715232	4.356996380011
H	-0.436346004289	-0.463104838257	3.976880225812
H	-0.416657276456	1.612029858045	2.593643236146
H	-8.345843575756	-0.264553545800	2.934679123999
C	-6.631278914920	-4.077818150638	4.987888965789
F	-7.523837662660	-4.913395686613	4.387836088594
F	-7.098522579526	-3.921112563658	6.262932839066
F	-5.481399881588	-4.781330866342	5.105462753704

RA of Product-1i

24

C	-6.228339246531	-0.349062967759	2.952722731475
C	-7.481736068175	-0.858464191537	3.193276315066
C	-7.648573729087	-2.080646114079	3.895098112018
C	-6.491646289435	-2.736633528561	4.301410800193
C	-5.219282885757	-2.254459810920	4.069605712701
C	-5.032097248553	-1.009043668582	3.380493991492
C	-4.951645044409	1.064588848341	1.547635897970
O	-6.138719562853	0.887561574196	2.348003284070
C	-3.771764873299	-0.366883368669	3.193382098657
C	-3.707982383048	0.767642421612	2.323568424524
C	-2.538915072623	1.477615634449	2.150663856819
C	-2.548960311080	-0.762676643668	3.818205685047
C	-1.381017021245	-0.048600423861	3.616683817419
C	-1.348941931140	1.087184980837	2.794802557973
H	-8.629318012407	-2.484065003188	4.097370665999
H	-4.364064450536	-2.821506723620	4.408007414960
H	-4.980358643629	2.094173432107	1.192166983470
H	-5.034883398197	0.397272764599	0.677144686194
H	-2.535489076015	2.337082474790	1.486702382705
H	-2.534085579707	-1.620616215446	4.479056505728
H	-0.473049652699	-0.373488500805	4.114334283021
H	-0.432170618670	1.643455169028	2.649339083174
H	-8.346990639681	-0.303902505998	2.850572396439
Cl	-6.661794201225	-4.281091483265	5.160745152888

RA of Product-1j

24

C	-6.227816742847	-0.328239890805	2.950471203859
C	-7.472680455257	-0.859979333376	3.205090614796
C	-7.646840713367	-2.076638432656	3.901461025852
C	-6.493888867150	-2.749899129357	4.317582057355
C	-5.230209810482	-2.243724370618	4.073092430351
C	-5.036641275949	-1.003172640266	3.383010297355
C	-4.944686564037	1.068859611705	1.542023203355
O	-6.132661548869	0.900131795575	2.347261626381
C	-3.775322416080	-0.362325843702	3.191179899682
C	-3.704004953060	0.770518519712	2.319122676633
C	-2.532538060790	1.476492518808	2.146005401413
C	-2.553029935531	-0.760886802829	3.817638852074
C	-1.382930645985	-0.051565822602	3.616372609377
C	-1.344809271927	1.083884768550	2.792403965661
H	-8.637784889261	-2.463360826996	4.087661393083
H	-4.365295195009	-2.800892066768	4.409151967023
H	-4.973293092390	2.097151077664	1.183458516775
H	-5.035780018260	0.397839955560	0.675905957764
H	-2.526002170260	2.334426177894	1.480003831663
H	-2.541443477785	-1.617552359674	4.479974935273
H	-0.476972931787	-0.379120872182	4.116059421131
H	-0.425964708656	1.636912781847	2.647908642326
H	-6.596571662300	-3.692839213974	4.843605887696
Cl	-8.912921222962	0.009756098489	2.673256433120

RA of Product-1k

24

C	-6.227606349553	-0.348185682102	2.954731438585
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C	-7.650285877546	-2.081081836987	3.892387846933
C	-6.492477193502	-2.723598182356	4.299844854380
C	-5.219503285512	-2.250154428353	4.078611275786
C	-5.031409530441	-1.006084407154	3.385549768284
C	-4.952807073413	1.064549628807	1.548410991829
O	-6.136657937977	0.892801864509	2.352340410718
C	-3.771924246676	-0.364448805404	3.195336978011
C	-3.707770769653	0.768674389289	2.323072858404
C	-2.538379207641	1.476993728907	2.147736148125
C	-2.548158804651	-0.761051879917	3.818909835549
C	-1.379863600134	-0.048095626496	3.615316064994
C	-1.347543715787	1.086704613588	2.791857458447
H	-8.625824525281	-2.497907659829	4.096318279616
H	-4.375042076042	-2.827328473691	4.429304059874
H	-4.979820277707	2.092755161856	1.188351237821
H	-5.037854680059	0.393443298803	0.680555799111
H	-2.534649067280	2.334989110287	1.481785882337
H	-2.533617080339	-1.619208399538	4.479618327488
H	-0.471420348386	-0.373420525276	4.111963474948
H	-0.430321534610	1.641716956427	2.644282859490
H	-8.345472681800	-0.302289716532	2.845061346236
F	-6.623460858808	-3.920420948313	4.968327745225

RA of Product-1l

48

C	-6.209921340832	-0.284514000915	2.977782742942
C	-7.485905545698	-0.788276625472	3.191927741956
C	-7.592456447957	-2.041887051954	3.855520817602
C	-6.467605215121	-2.763636191269	4.273693840389
C	-5.207653926044	-2.226801851689	4.037537625721
C	-5.020824484916	-0.971424744142	3.389573708739
C	-4.892420854782	1.126115602331	1.594892976736
O	-6.064224759156	0.974627214477	2.417352521541
C	-3.745862677114	-0.348440407596	3.209693105904
C	-3.649438082402	0.796218013748	2.353434166651
C	-2.467194235697	1.481430750181	2.183146396703

C	-2.522464889008	-0.783121087892	3.822956244757
C	-1.340490041799	-0.093266812055	3.626974602180
C	-1.279371598675	1.056418539015	2.820467557623
H	-8.572417984434	-2.447079460643	4.034053882261
H	-4.328104458233	-2.776126697380	4.346779782851
H	-4.902377889498	2.157889809275	1.242544090419
H	-5.006816481074	0.464045793269	0.722916428332
H	-2.448298937509	2.346957127679	1.526488123843
H	-2.521273373738	-1.651327948150	4.470453487352
H	-0.438802972103	-0.448317795896	4.116855484640
H	-0.349391337752	1.591677907109	2.679584654740
C	-6.590769093288	-4.133710068143	4.971374354089
C	-8.050492139928	-4.569842467419	5.174017784645
H	-8.076185232715	-5.540997873702	5.673665522240
H	-8.602665722399	-3.862158907423	5.795501773081
H	-8.579459837056	-4.672094058392	4.224528877186
C	-5.921255692823	-4.079429454387	6.360574072153
H	-5.999308053586	-5.048443160487	6.861727293457
H	-4.863639515909	-3.823803403669	6.287863251517
H	-6.404030214186	-3.331726177254	6.994296625973
C	-5.891621274142	-5.216348969436	4.122137987806
H	-5.971316350124	-6.194389373232	4.605337819767
H	-6.351169870342	-5.289595599205	3.133588273515
H	-4.832721142098	-4.995386249521	3.983301411133
C	-8.753891870467	-0.026341809801	2.745076844983
C	-10.045458745286	-0.801331390833	3.063345627231
H	-10.076784908126	-1.770133290000	2.561293802925
H	-10.171129468625	-0.968417299461	4.134664880822
H	-10.903987060020	-0.221279774721	2.717272993709
C	-8.735113255136	0.201871154787	1.217612735887
H	-9.637329317088	0.735149988234	0.903877889504
H	-7.869327905600	0.784537947781	0.911331241876
H	-8.711863391683	-0.754118391636	0.688564873663
C	-8.856429325041	1.332282239125	3.472594518853
H	-8.000345083005	1.967433953134	3.256554676674
H	-9.764424415836	1.859208561147	3.164171189943
H	-8.908787891949	1.183474792485	4.554175633483

RA of Product-1m

39

C	-6.170590366346	-0.342348510250	3.005564742655
C	-7.460458168497	-0.795448995391	3.267273669848
C	-7.574514177762	-2.023939668642	3.959447254142
C	-6.432160348240	-2.753165202382	4.293127685910
C	-5.145346714643	-2.312195579831	4.031383302760
C	-4.960879881573	-1.021446501203	3.412331791785
C	-4.896237585532	0.948891032586	1.488545519041
O	-6.035075337099	0.879297298293	2.366301839967
C	-3.704489565881	-0.345481483088	3.216724891502
C	-3.646588747710	0.733071821594	2.265201378086
C	-2.511171848427	1.489150048336	2.070001038602
C	-2.481363273997	-0.585145531895	3.931024064540
C	-1.345685092050	0.168553351746	3.708589774660
C	-1.323360622281	1.224496736460	2.777790691675
H	-8.543069651185	-2.433713403662	4.199689847546
H	-4.931144186493	1.931046566457	1.016609196759
H	-5.026253331593	0.183279302828	0.708647427325
H	-2.538696139588	2.294937255695	1.341297971370
H	-2.437025664838	-1.352090694974	4.688301739712
H	-0.453184706626	-0.054055786744	4.285398978916
H	-0.431662508143	1.816714836474	2.619228863428
H	-6.557189708941	-3.726735065625	4.758608846879
C	-8.718368630819	-0.012536292098	2.830491505774
C	-10.015698684959	-0.734443848828	3.238697619337
H	-10.872987967964	-0.143134231446	2.909138355341
H	-10.097942929615	-1.721070142104	2.779070282929

H	-10.094089115442	-0.855330224209	4.320749460778
C	-8.755851063222	0.139448155887	1.294031858937
H	-7.889284363986	0.683038553944	0.924911759725
H	-8.777638150289	-0.841870417846	0.813475180929
H	-9.656971316163	0.680024660814	0.989736295088
C	-8.756455030368	1.381501773424	3.493983304684
H	-8.773396702468	1.286001915552	4.582723963996
H	-7.892388860200	1.981032329621	3.217436572393
H	-9.660819898164	1.918572438334	3.192628326745
C	-4.004071374755	-3.249962633529	4.344450080058
H	-3.261211976209	-3.269055261955	3.543000311947
H	-3.465106292568	-2.995568454913	5.262939020716
H	-4.385322625363	-4.264829087430	4.472958743517

RA of Product-1o

24

C	-6.229562735389	-0.348176004167	2.954008146046
C	-7.484985659220	-0.862340648505	3.186688584553
C	-7.642810967626	-2.080308893363	3.886062266926
C	-6.498642775234	-2.752849446769	4.321261291177
C	-5.231221687452	-2.240278731303	4.086368024273
C	-5.035758735647	-1.004845547364	3.391695497442
C	-4.952861947251	1.067933310768	1.549734394701
O	-6.140133826455	0.888938968390	2.346976077650
C	-3.776769912591	-0.363784731942	3.197954354063
C	-3.709048996031	0.770115865430	2.327033925917
C	-2.541773172364	1.475649654411	2.146763384695
C	-2.550638201901	-0.769015963790	3.826589419429
C	-1.410695117425	-0.038483932411	3.598055652295
C	-1.339441104372	1.089411910475	2.787413043857
H	-8.631151272795	-2.480402641894	4.071044527173
H	-4.980591827759	2.098496626595	1.196846675876
H	-5.033799307952	0.403577463460	0.676711779508
H	-2.534452474534	2.331999366800	1.480178015869
H	-2.507186582153	-1.616604955481	4.496667700049
H	-0.409283888443	1.621200507165	2.649567821299
H	-6.597737386419	-3.693340423758	4.853065974523
H	-8.346595206204	-0.306217316623	2.835223441177
H	-4.366879789810	-2.790911813351	4.436668524276
F	-0.255106794971	-0.442714192772	4.224350447224

RA of Product-1p

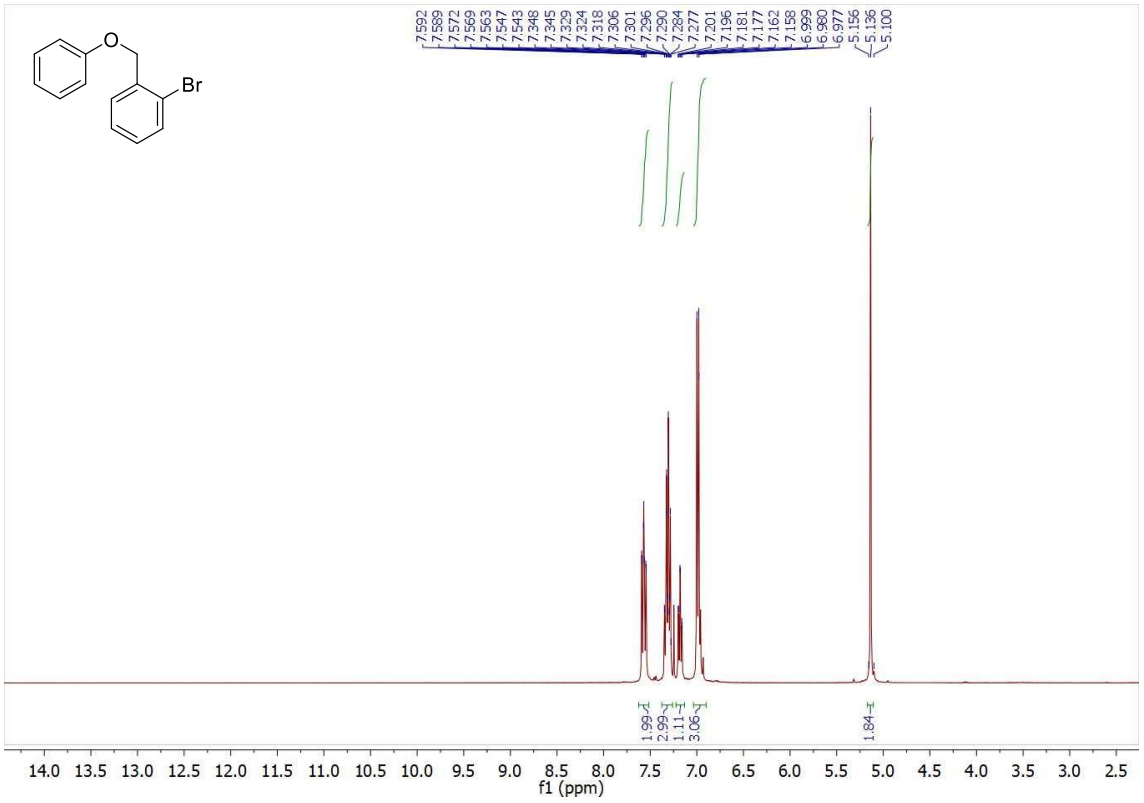
27

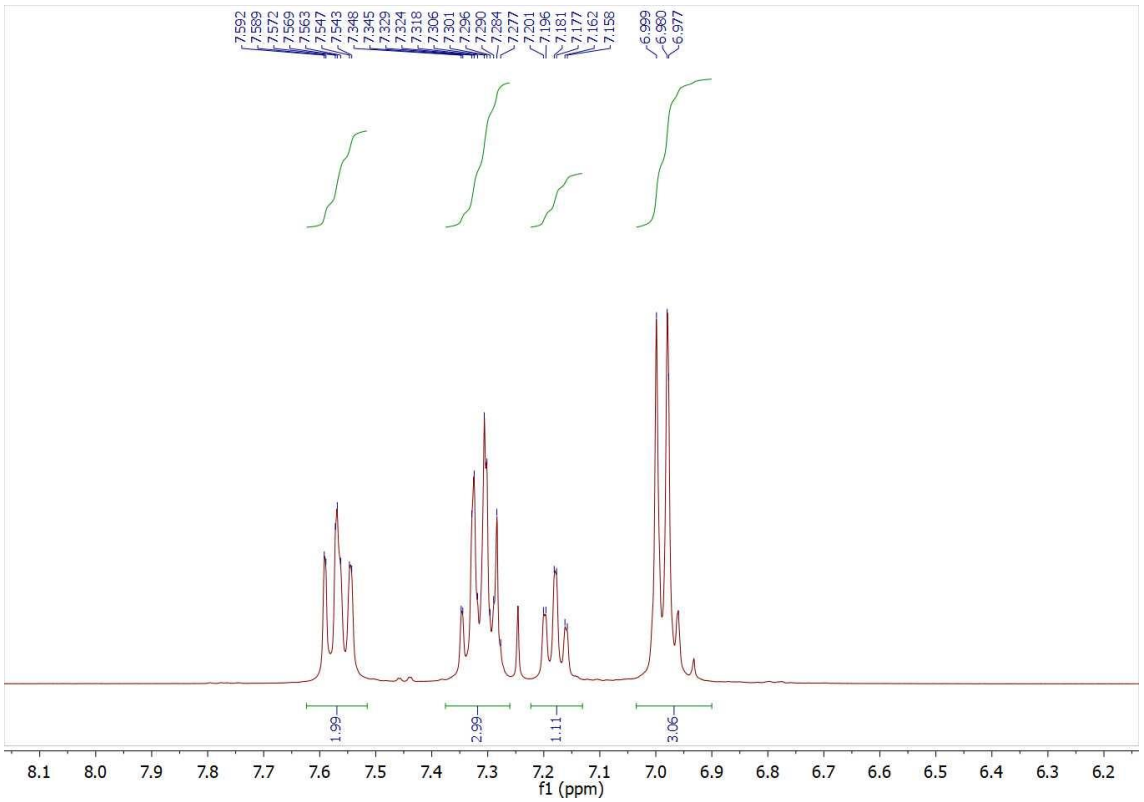
C	-6.234873107432	-0.344666188027	2.942170334843
C	-7.493956866436	-0.844940070590	3.183755927198
C	-7.663670500627	-2.036776064140	3.928015675086
C	-6.523323003235	-2.696024098377	4.395401077192
C	-5.252282868365	-2.198435157789	4.150111733583
C	-5.044279333399	-0.987525693759	3.412036820487
C	-4.942290284266	1.010653987416	1.491859154786
O	-6.138024319025	0.868844090877	2.287736013665
C	-3.780903150832	-0.355109237386	3.204781590119
C	-3.708382348652	0.743814319433	2.292115067690
C	-2.532519364379	1.438102410923	2.106828263070
C	-2.560808345887	-0.728306370278	3.855906188653
C	-1.377028299227	-0.039023440101	3.652449538115
C	-1.351577901270	1.068778037274	2.779835466846
H	-8.654938236252	-2.425353090179	4.121841927221
H	-4.965201662058	2.024681132501	1.092655358016
H	-5.022146347974	0.308066976292	0.648503695289
H	-2.514132147228	2.271394129412	1.409740105903
H	-2.560504577563	-1.561873080903	4.548965872501
H	-0.431689674528	1.617962491828	2.618357987626
H	-6.629325032852	-3.616153990128	4.961048483452
H	-8.350230970952	-0.299133283211	2.803667873203
H	-4.393366596056	-2.740968811678	4.525524296457

C	-0.114773905509	-0.456619269245	4.366362072578
H	-0.289049737136	-1.315084057874	5.016648534333
H	0.673394954080	-0.727087215659	3.656978979349
H	0.282795367060	0.356111103371	4.981879682740

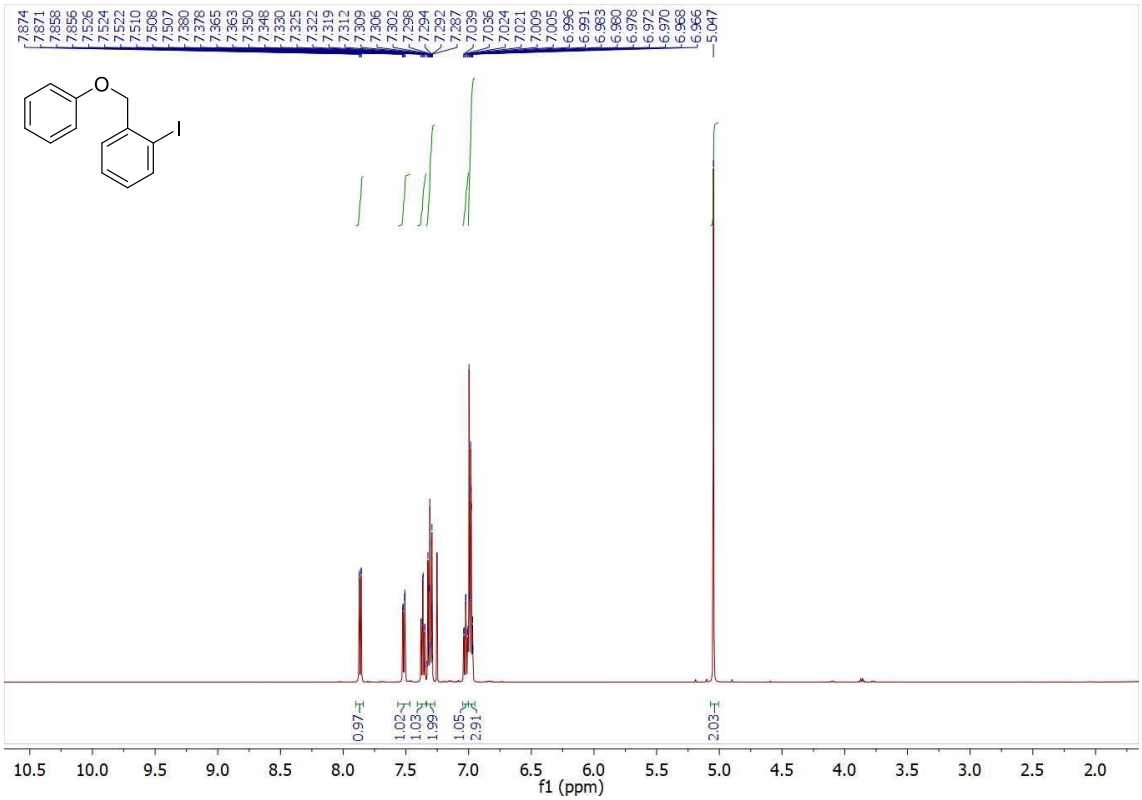
7. NMR spectra of compounds 5a-u

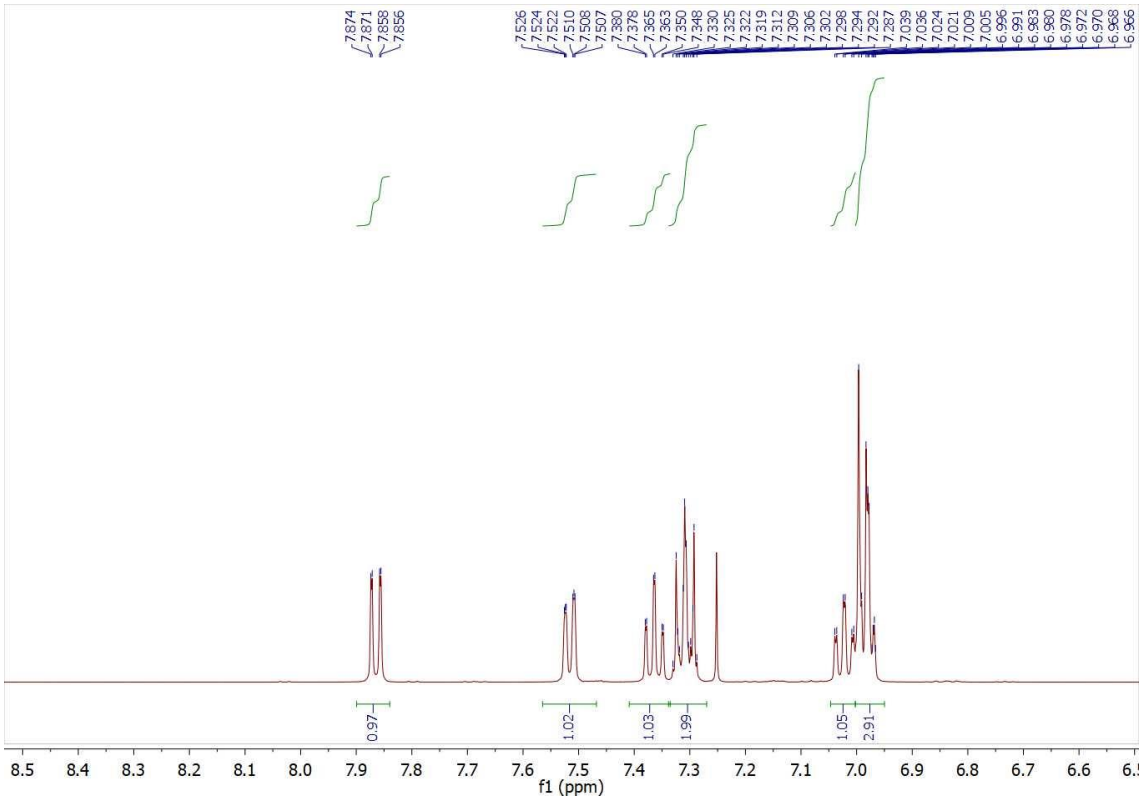
^{1}H-NMR (400 MHz, $CDCl_3$). 1-Bromo-2-(phenoxymethyl)benzene (**5a**)



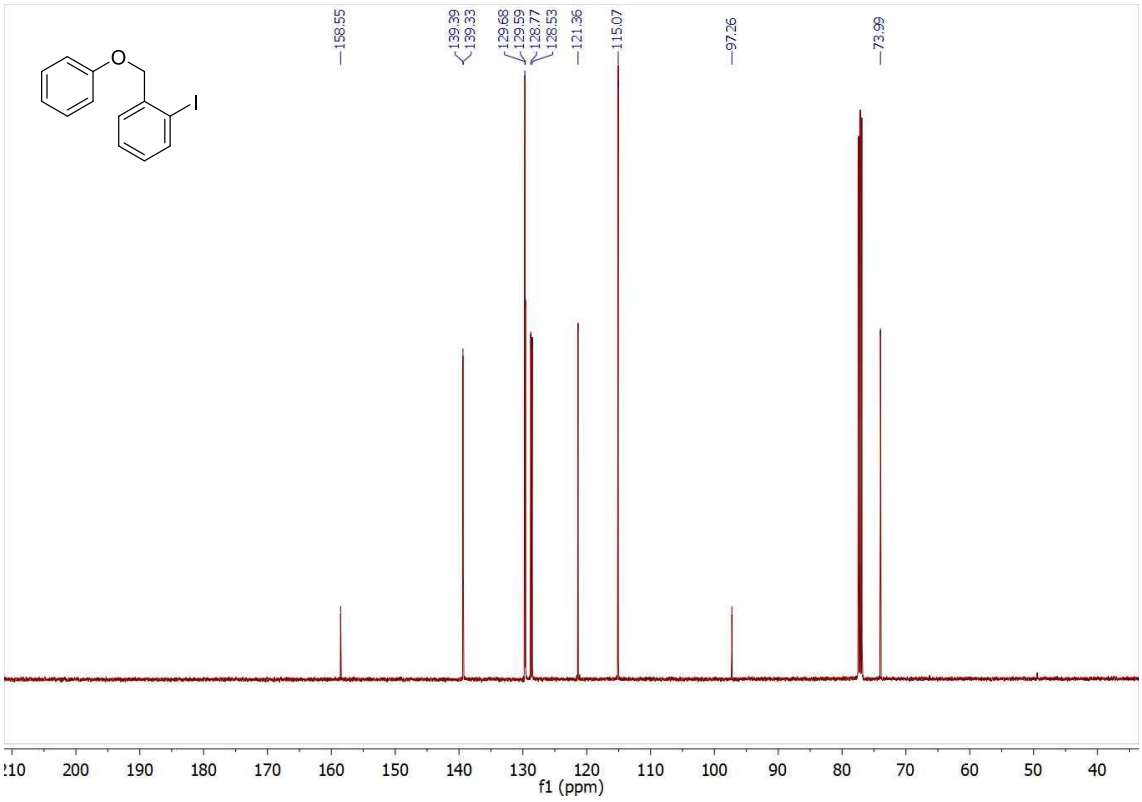


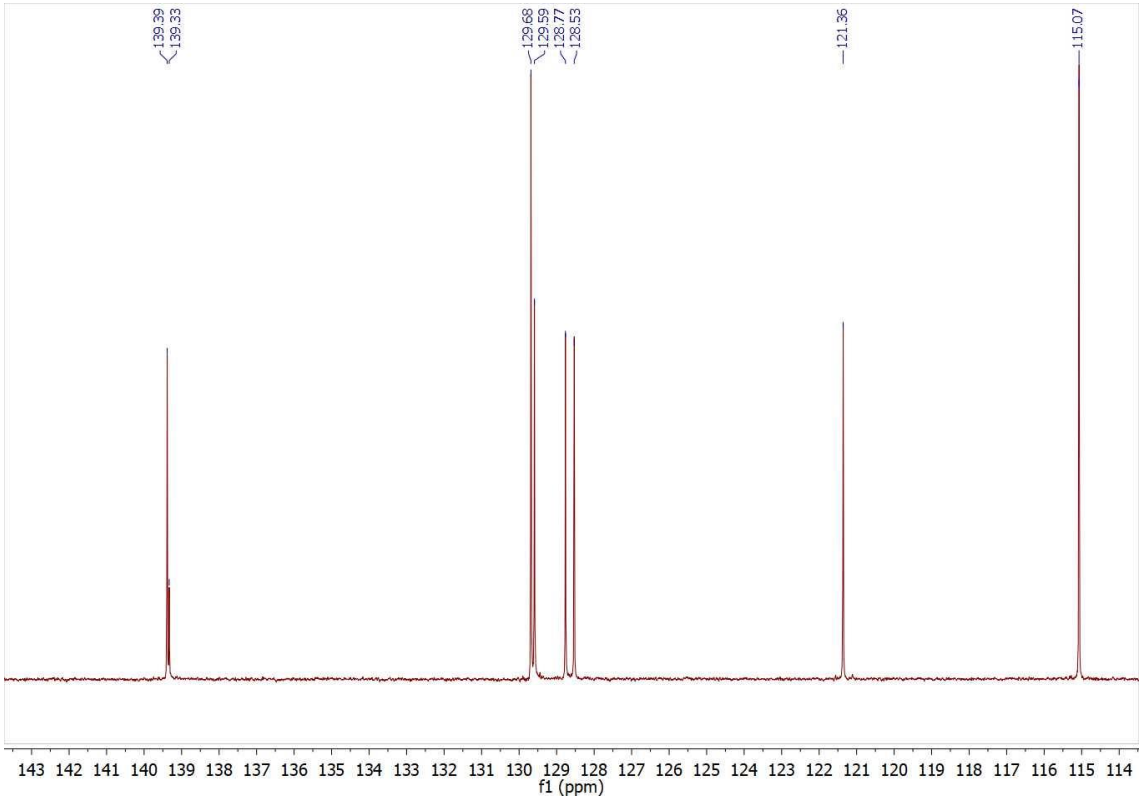
^{1}H-NMR (500 MHz, $CDCl_3$). 1-Iodo-2-(phenoxymethyl)benzene (**5b**)



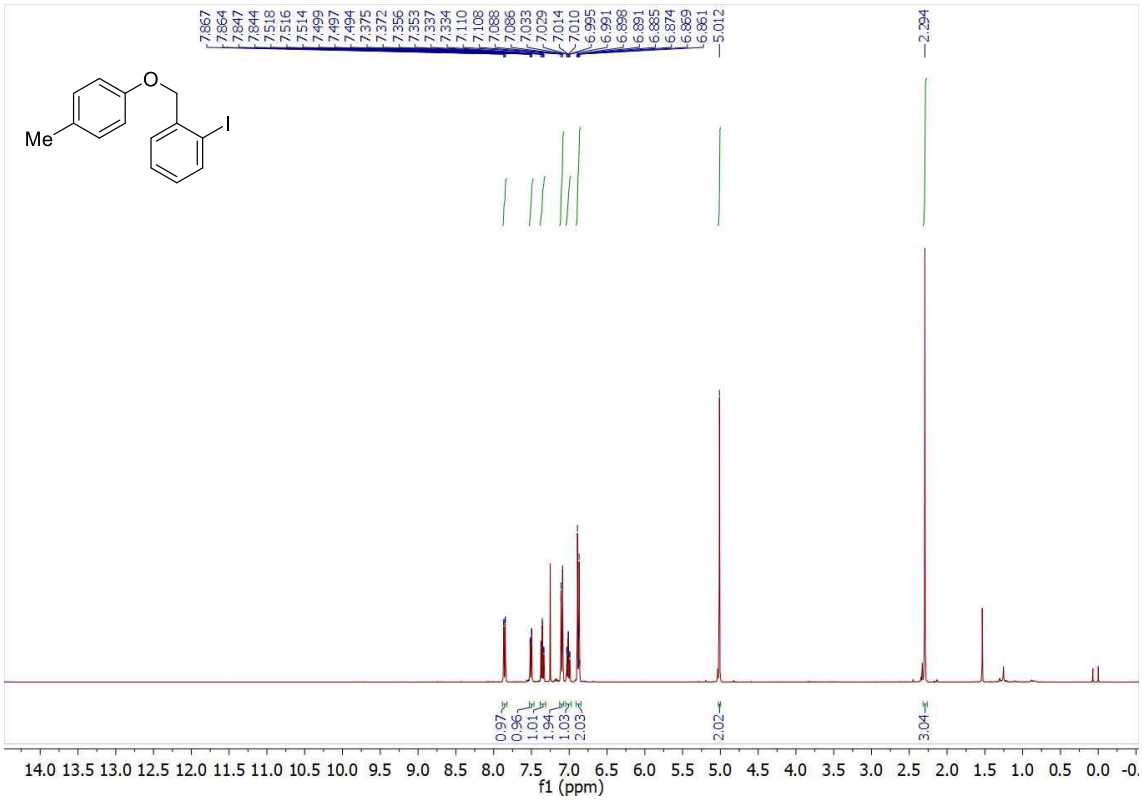


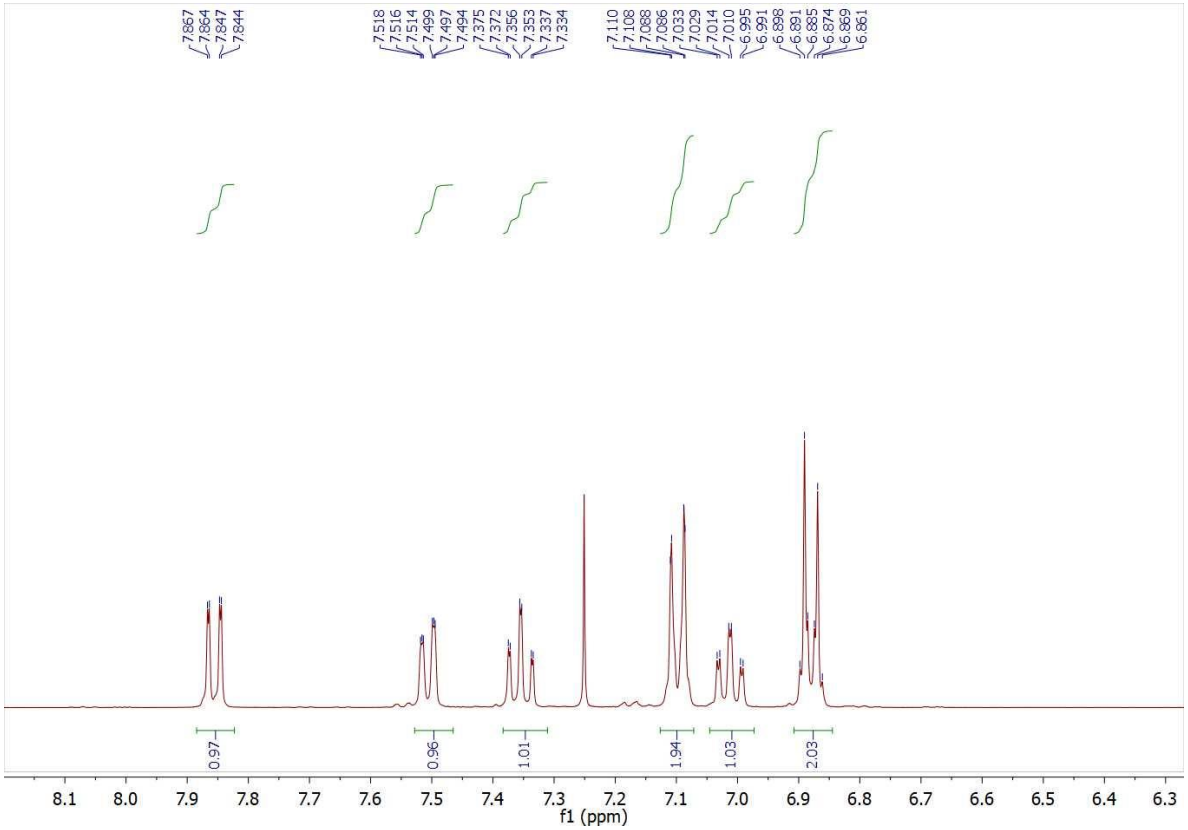
^{13}C NMR{1H} (126 MHz, $CDCl_3$). 1-Iodo-2-(phenoxymethyl)benzene (**5b**)



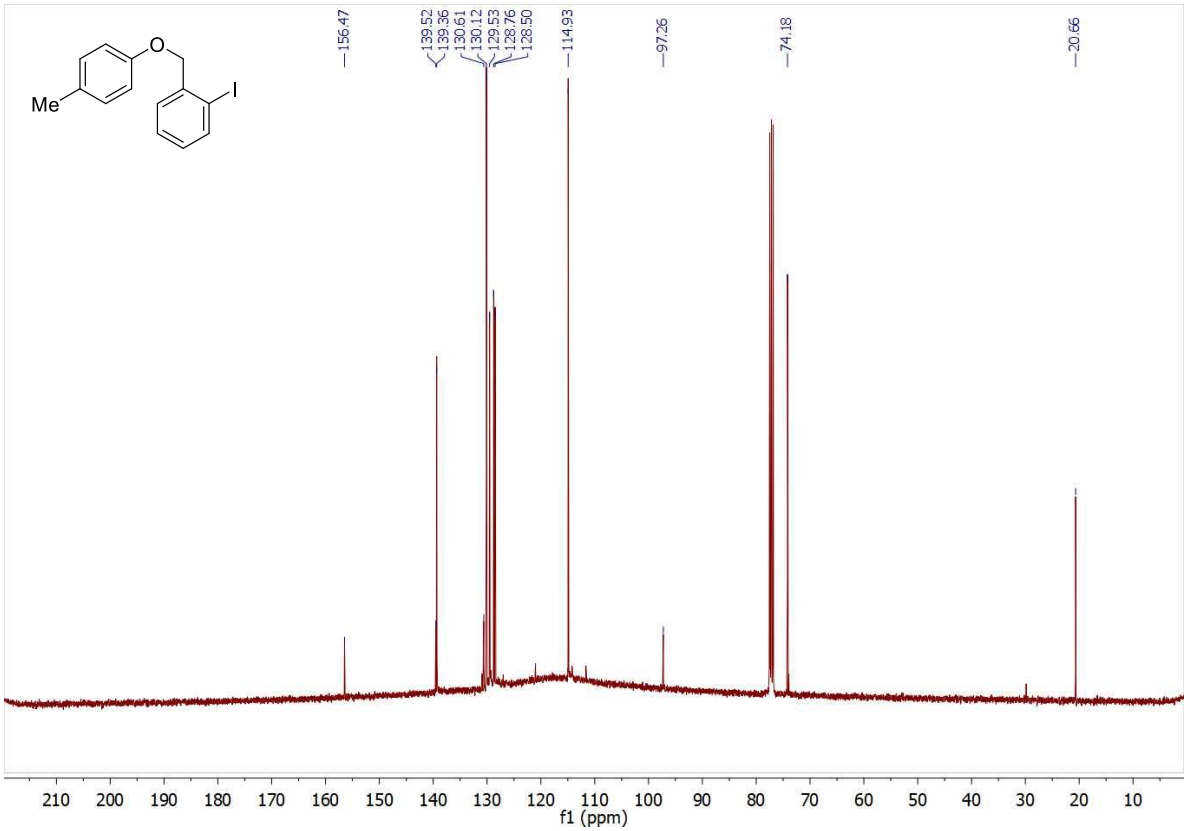


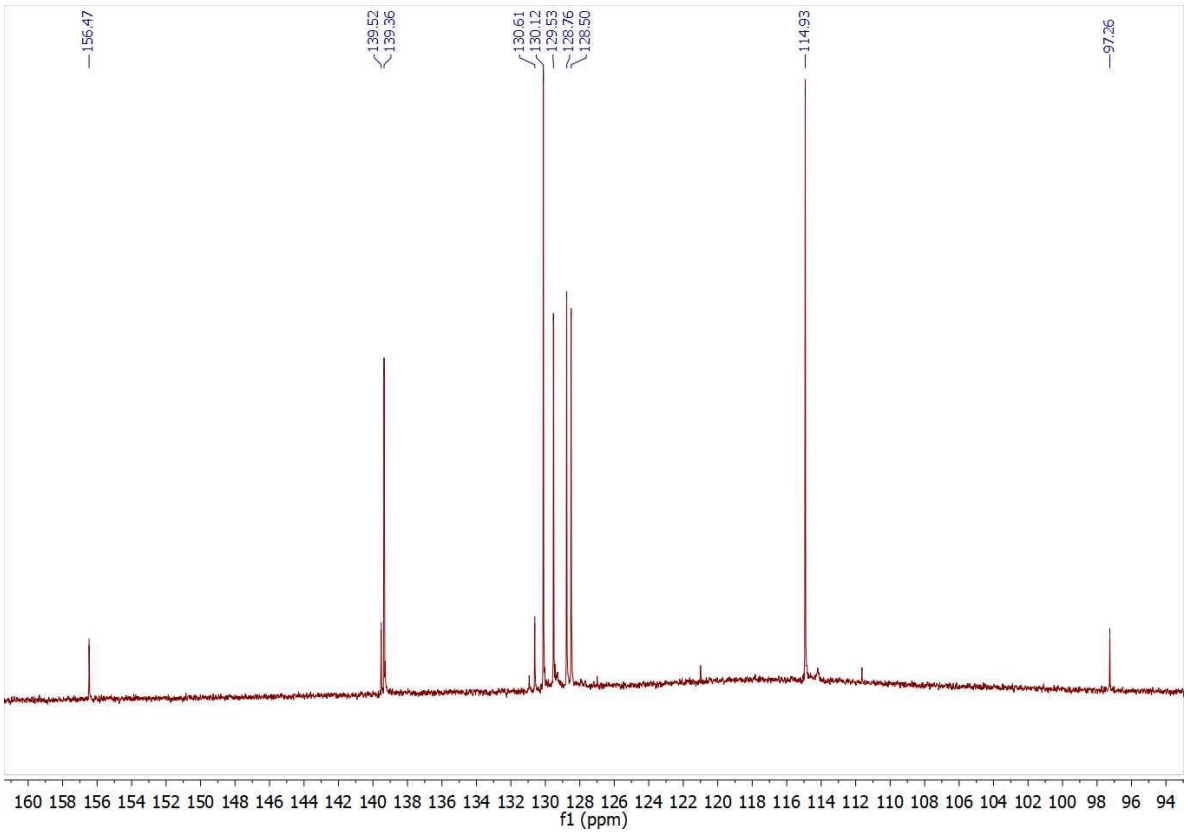
^{1}H-NMR (400 MHz, $CDCl_3$). 1-Iodo-2-((*p*-tolyloxy)methyl)benzene (**5c**)



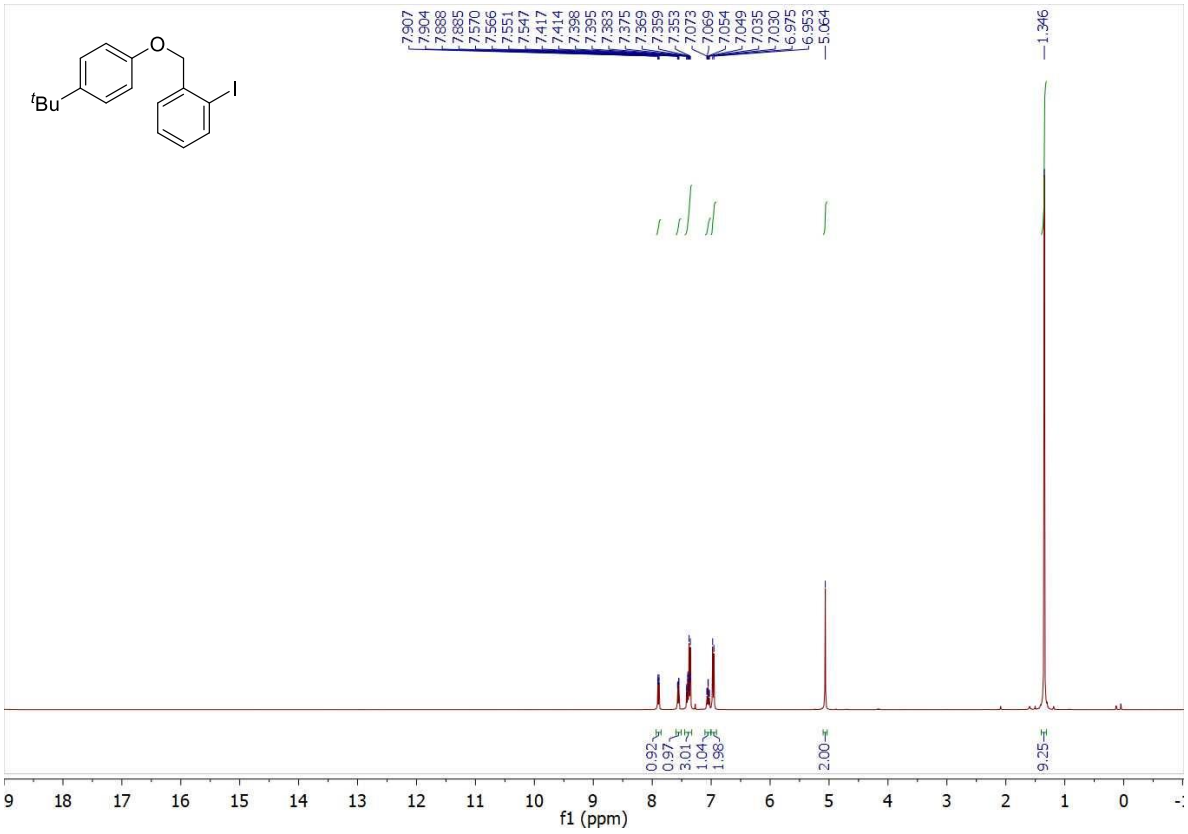


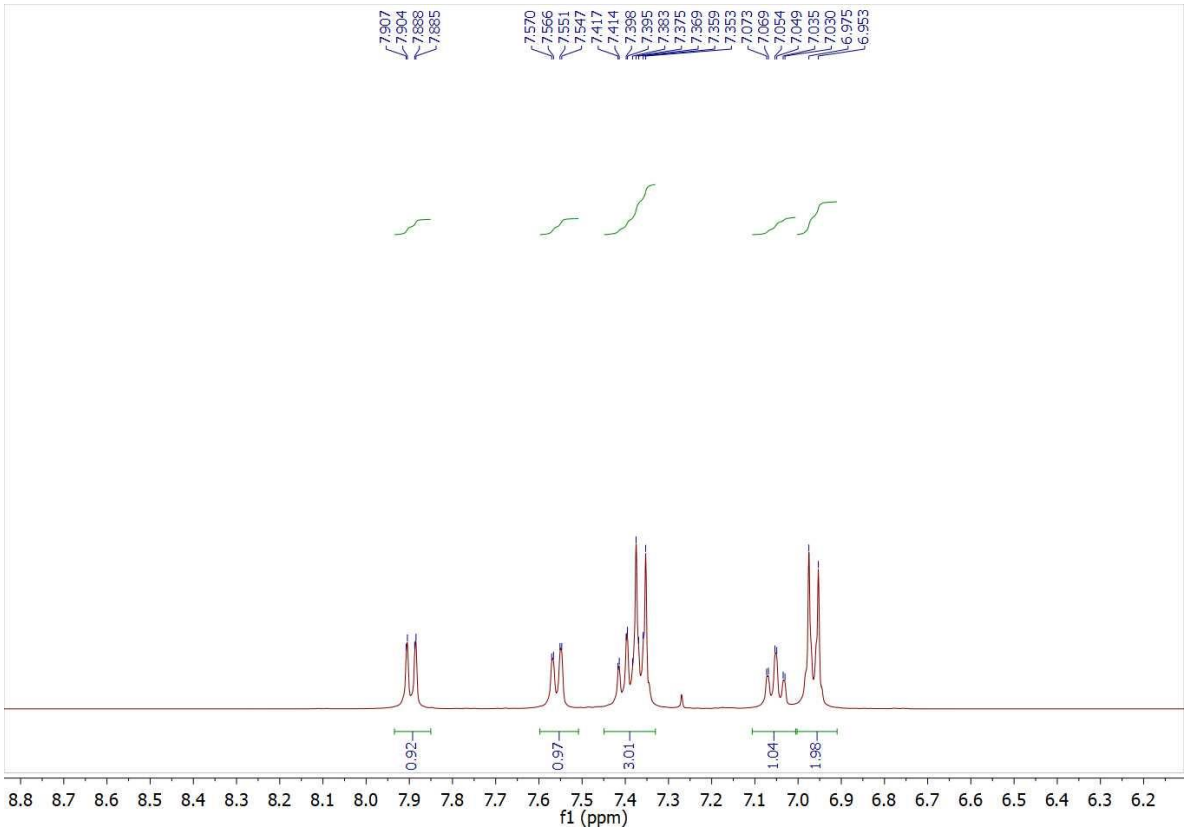
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-Iodo-2-((*p*-tolyloxy)methyl)benzene (**5c**)



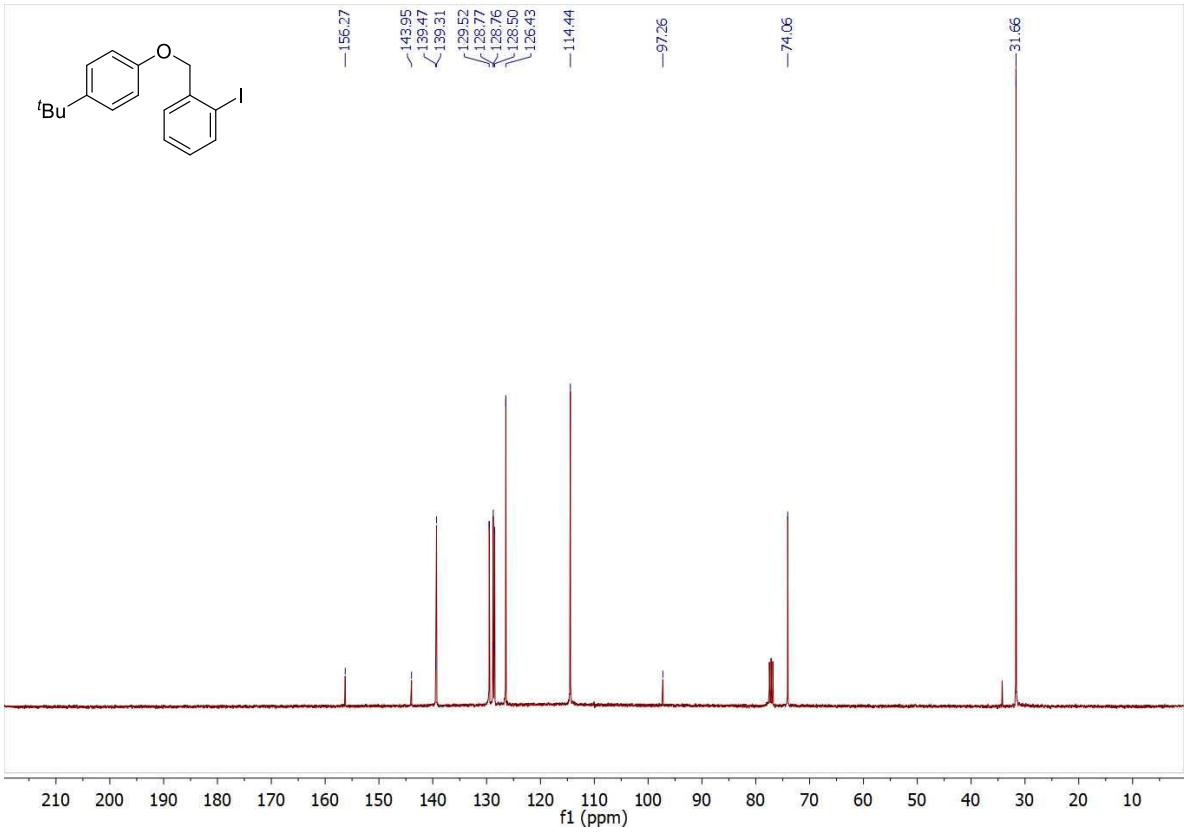


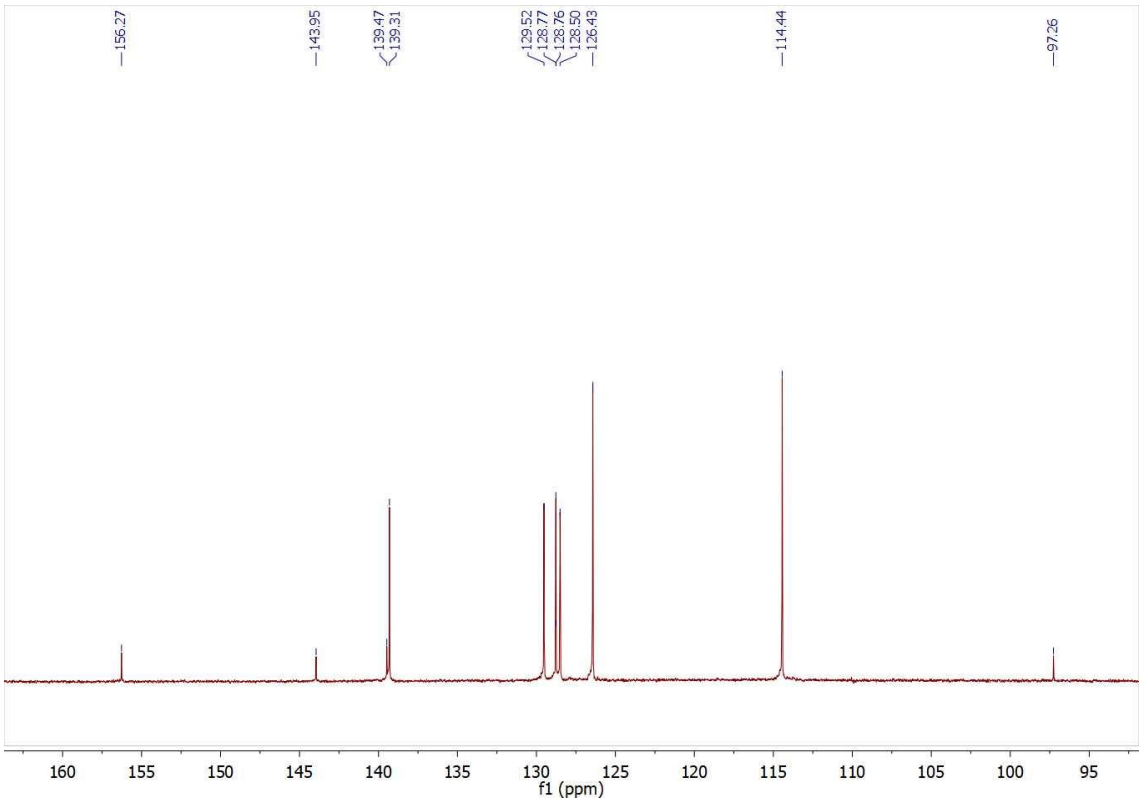
^{1}H-NMR (400 MHz, $CDCl_3$). 1-((4-(*tert*-Butyl)phenoxy)methyl)-2-iodobenzene (**5d**)



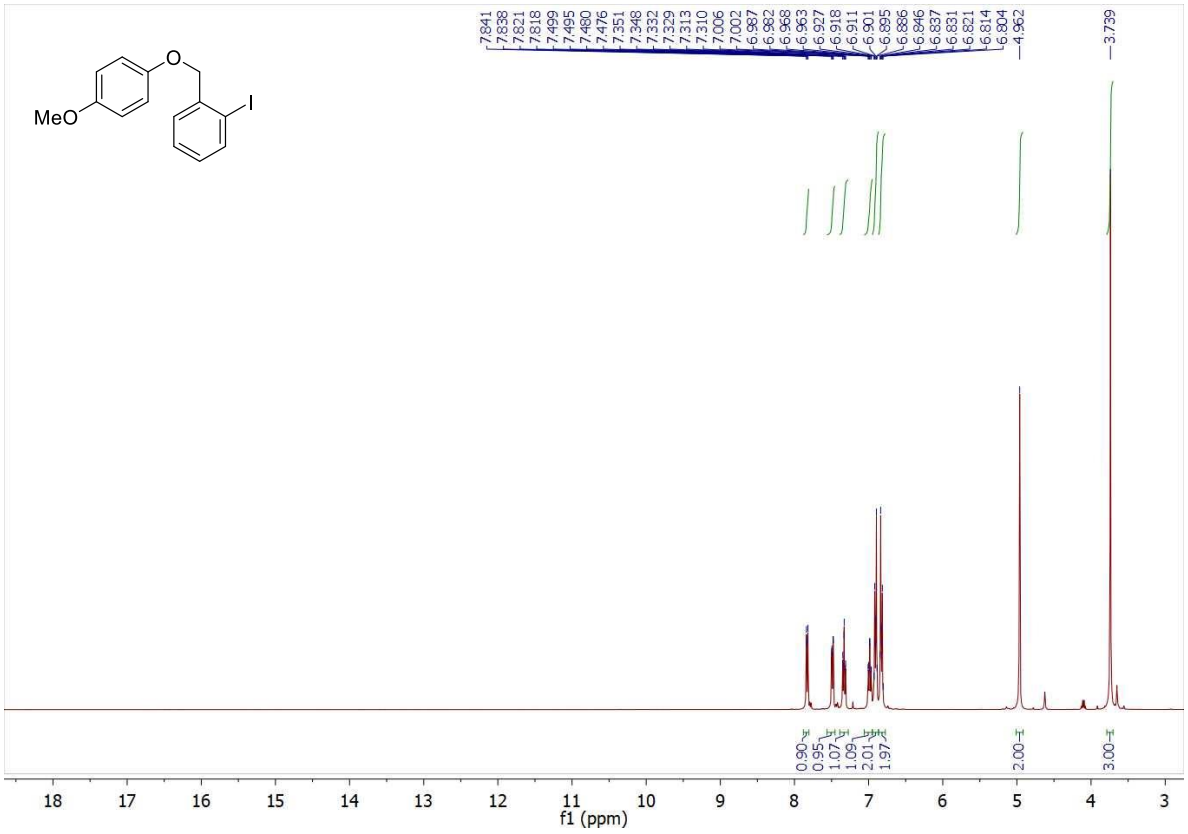


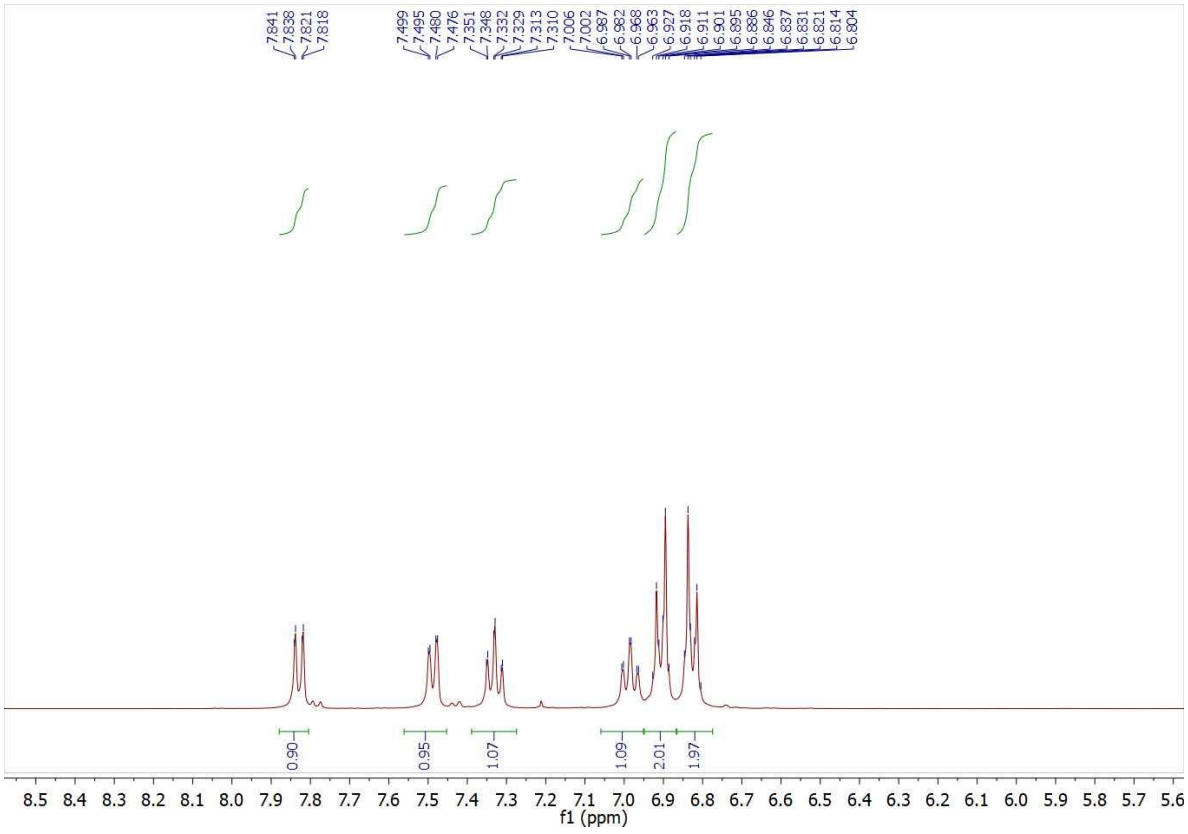
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-((4-(*tert*-Butyl)phenoxy)methyl)-2-iodobenzene (**5d**)



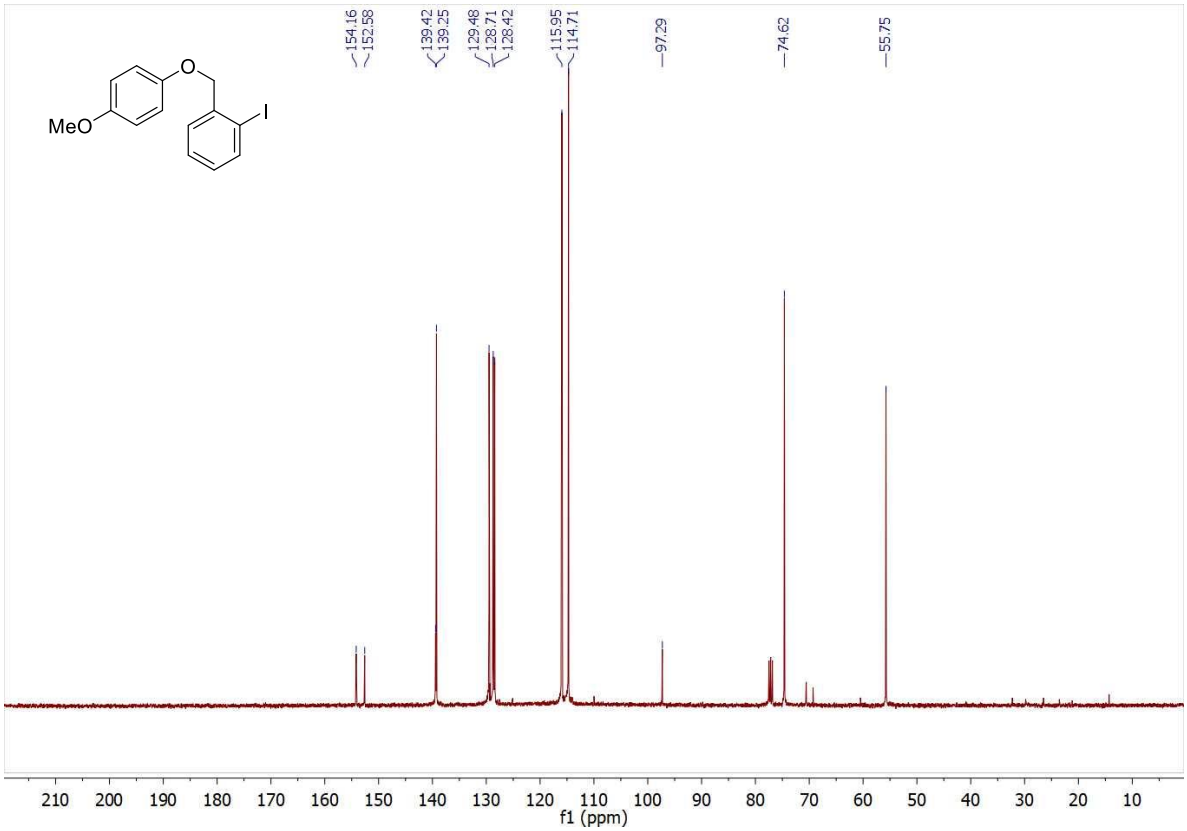


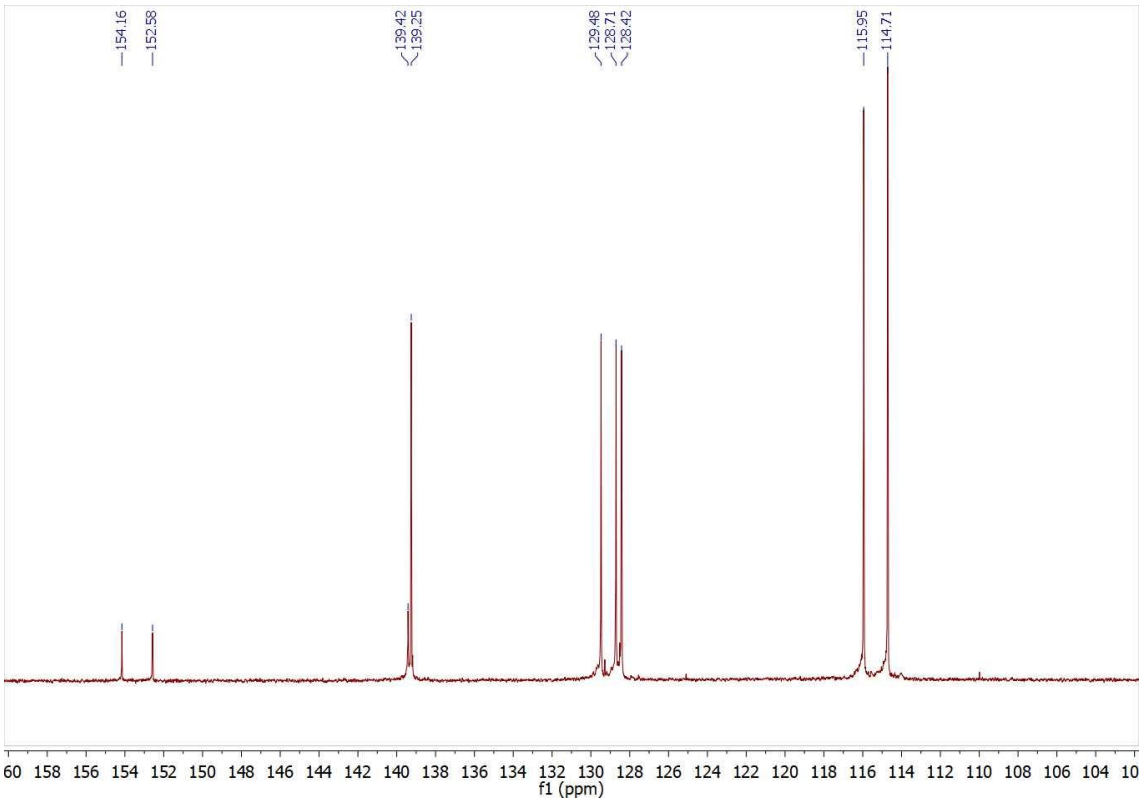
^{1}H-NMR (400 MHz, $CDCl_3$). 1-Iodo-2-((4-methoxyphenoxy)methyl)benzene (**5e**)



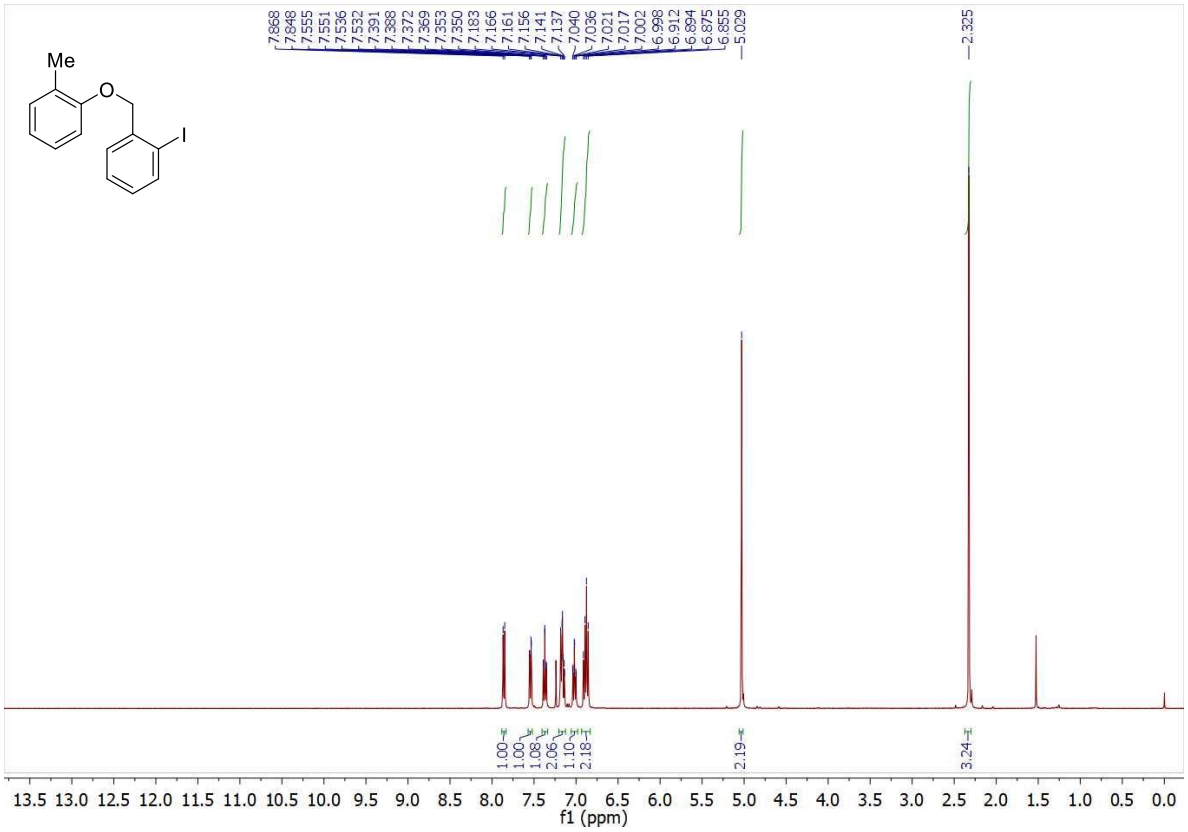


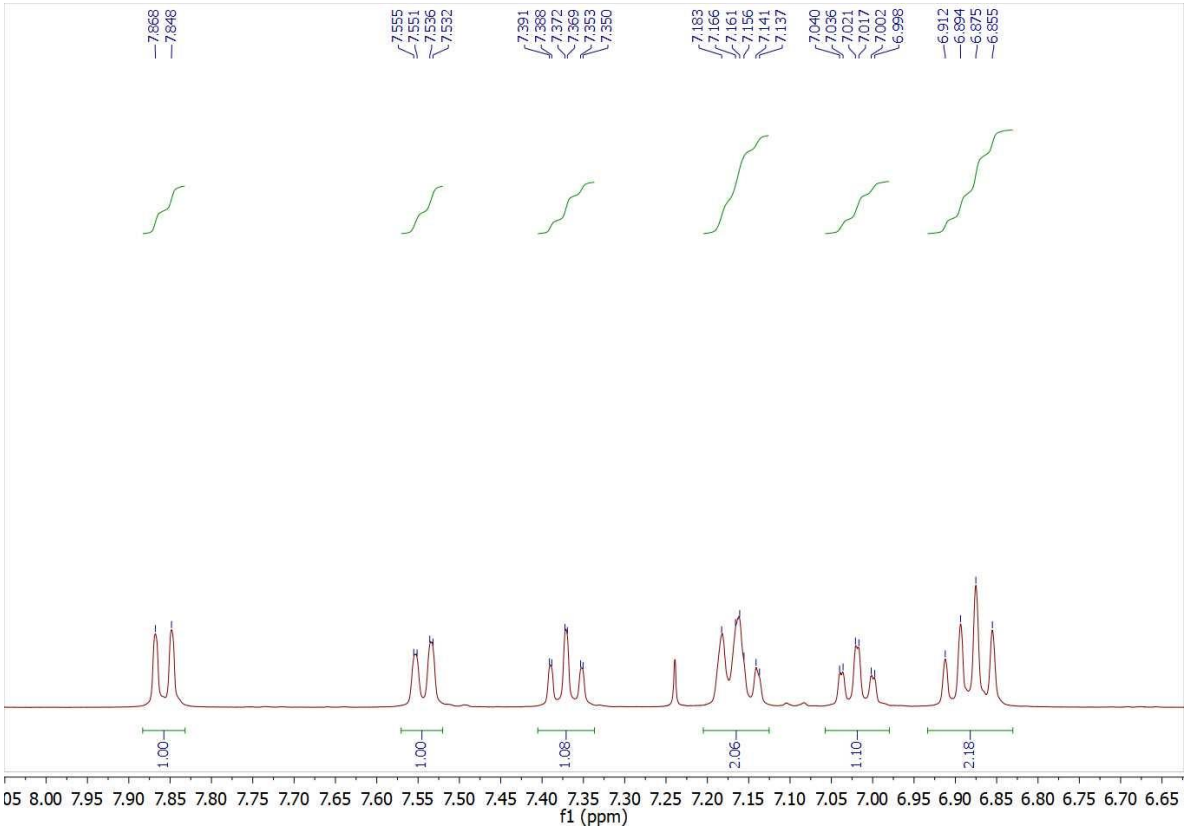
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-Iodo-2-((4-methoxyphenoxy)methyl)benzene (**5e**)



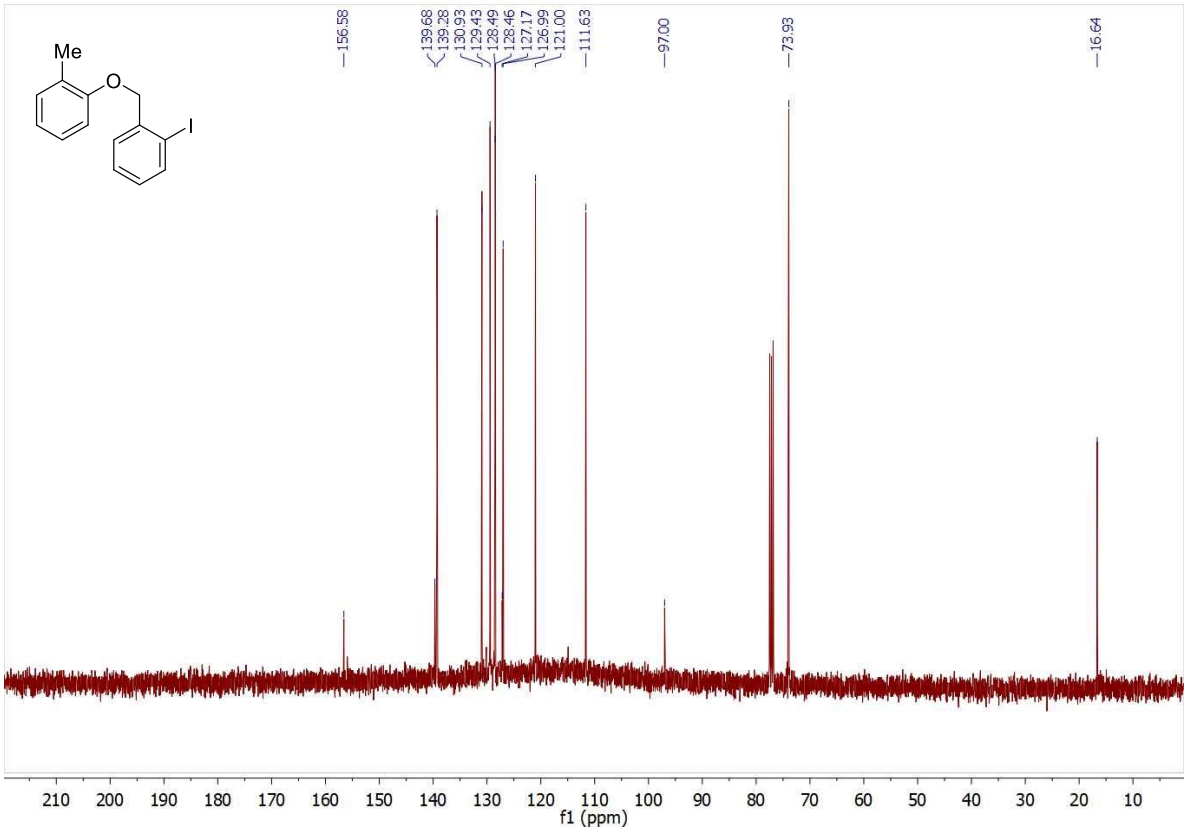


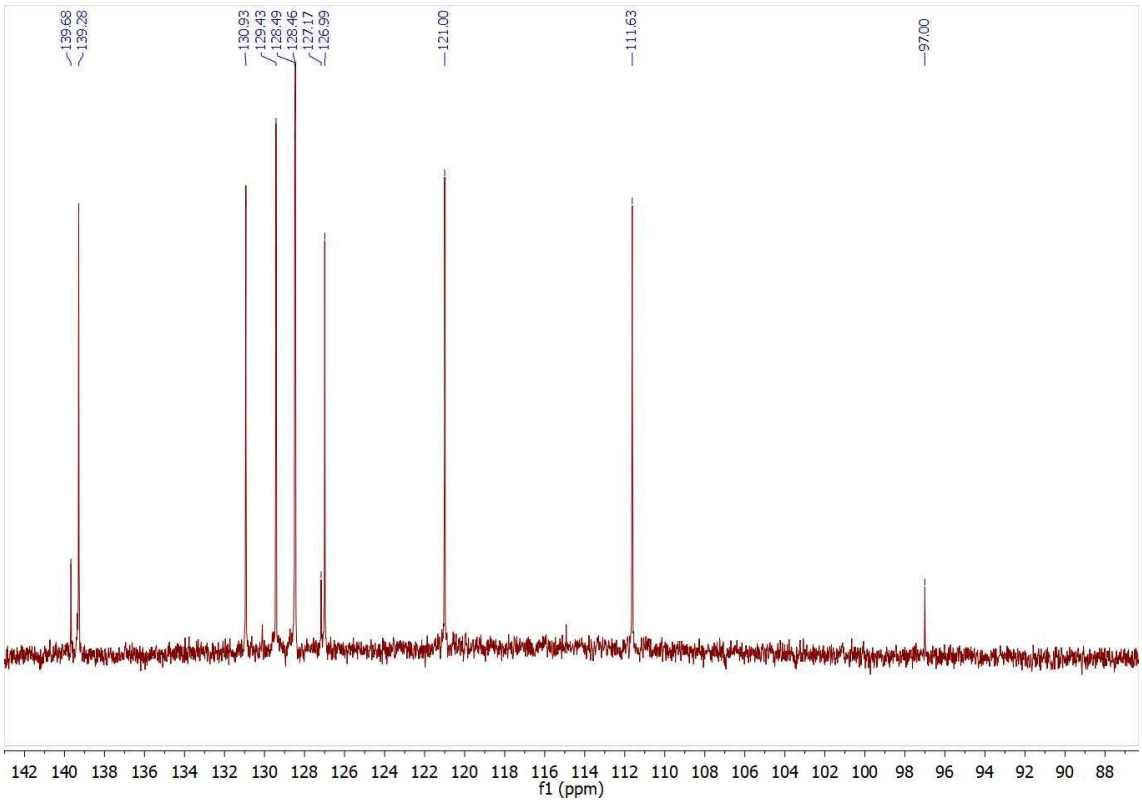
^{1}H-NMR (400 MHz, $CDCl_3$). 1-Iodo-2-((*o*-tolyloxy)methyl)benzene (**5f**)



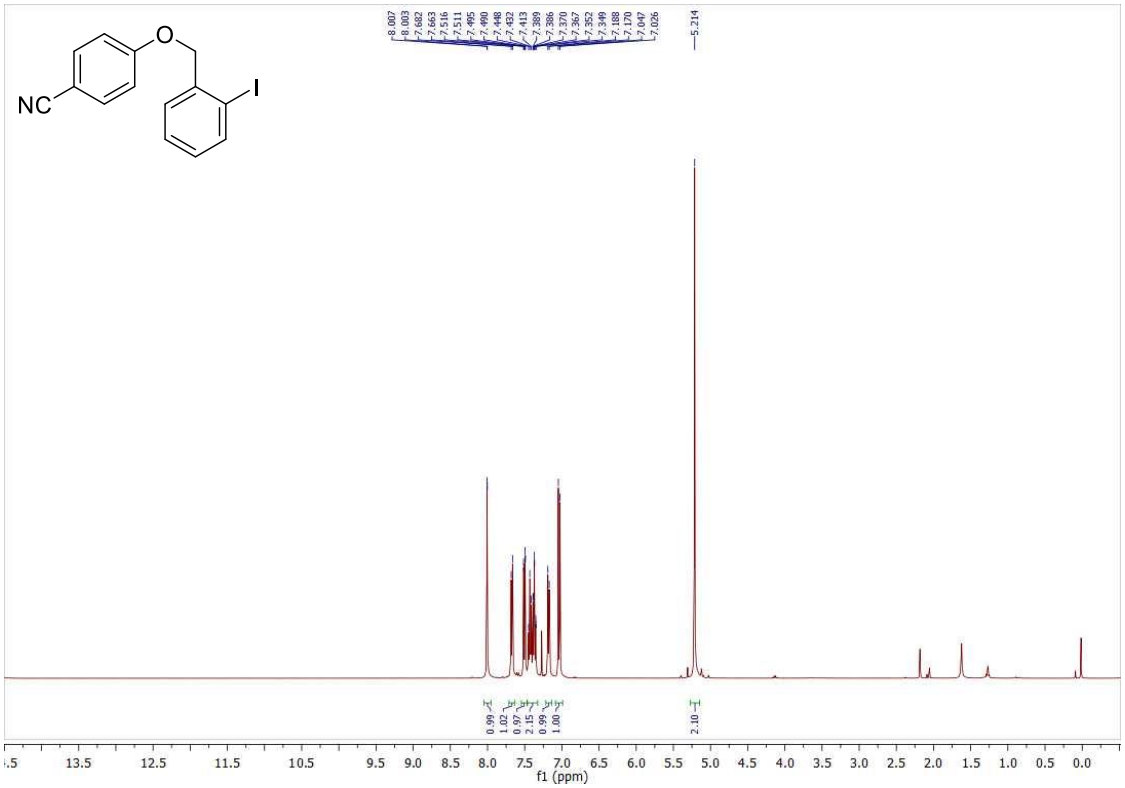


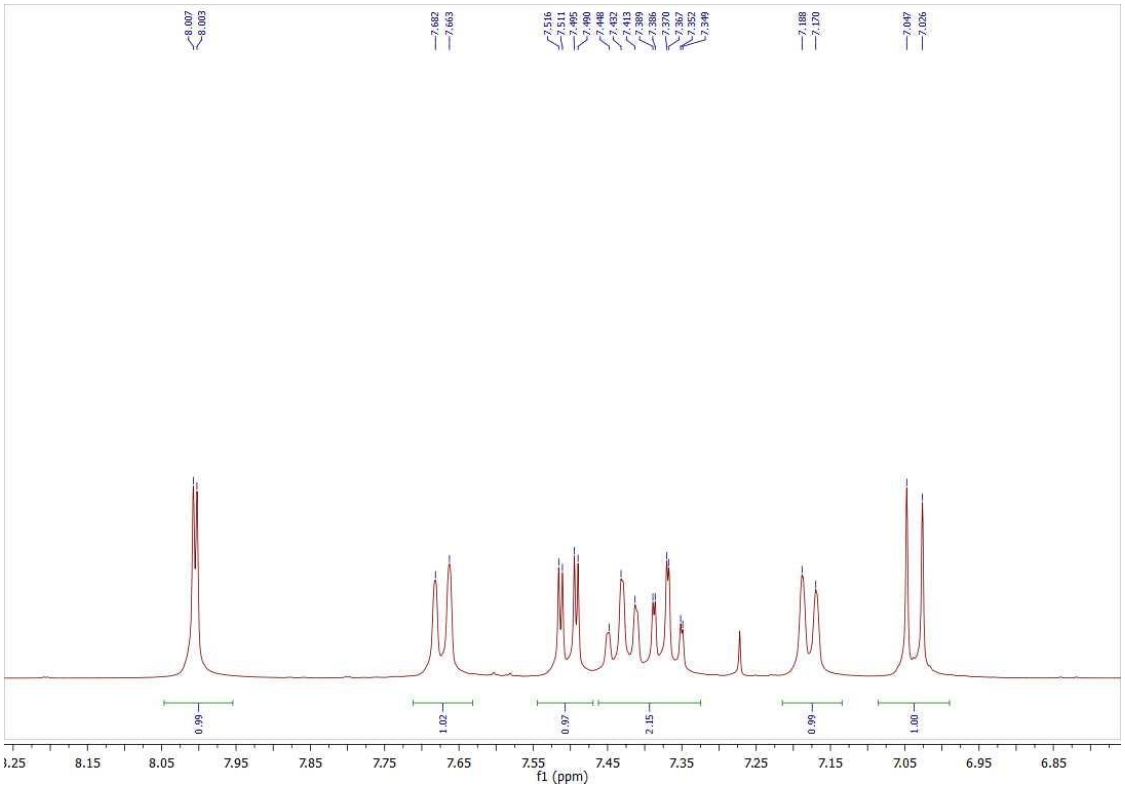
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-Iodo-2-((*o*-tolyloxy)methyl)benzene (**5f**)



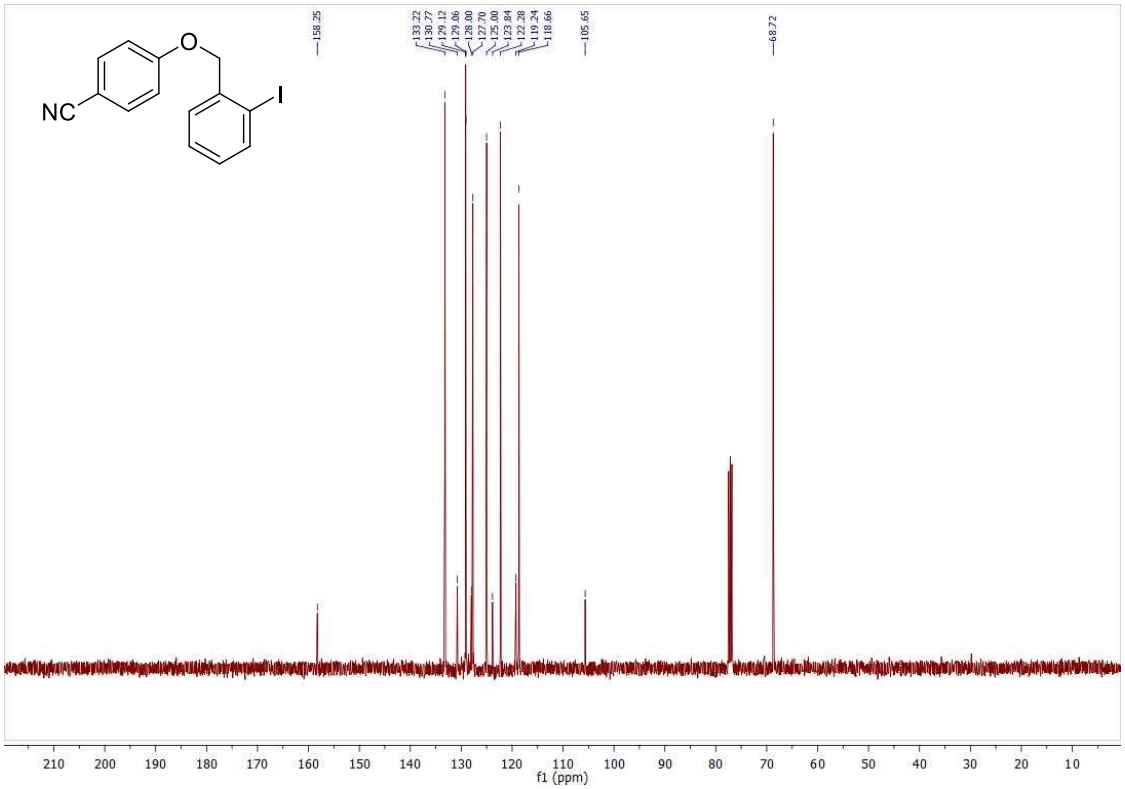


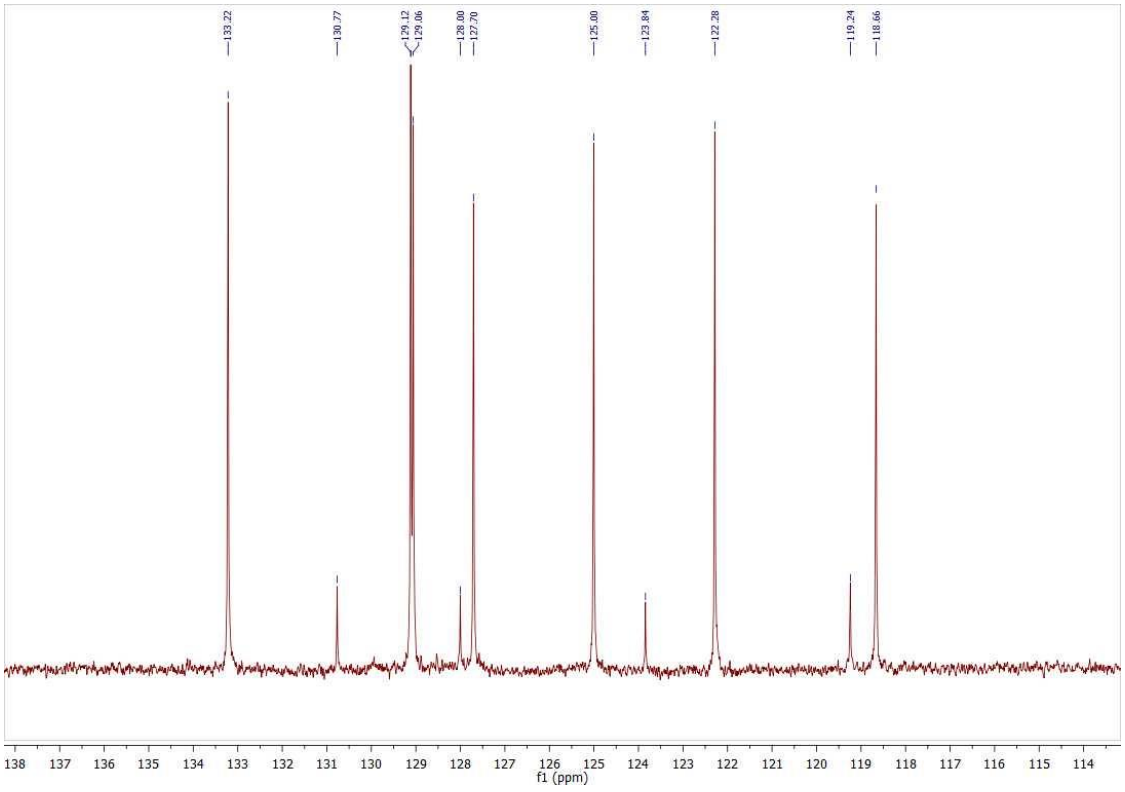
1H-NMR (400 MHz, $CDCl_3$). 4-((2-Iodobenzyl)oxy)benzonitrile **(5g).**



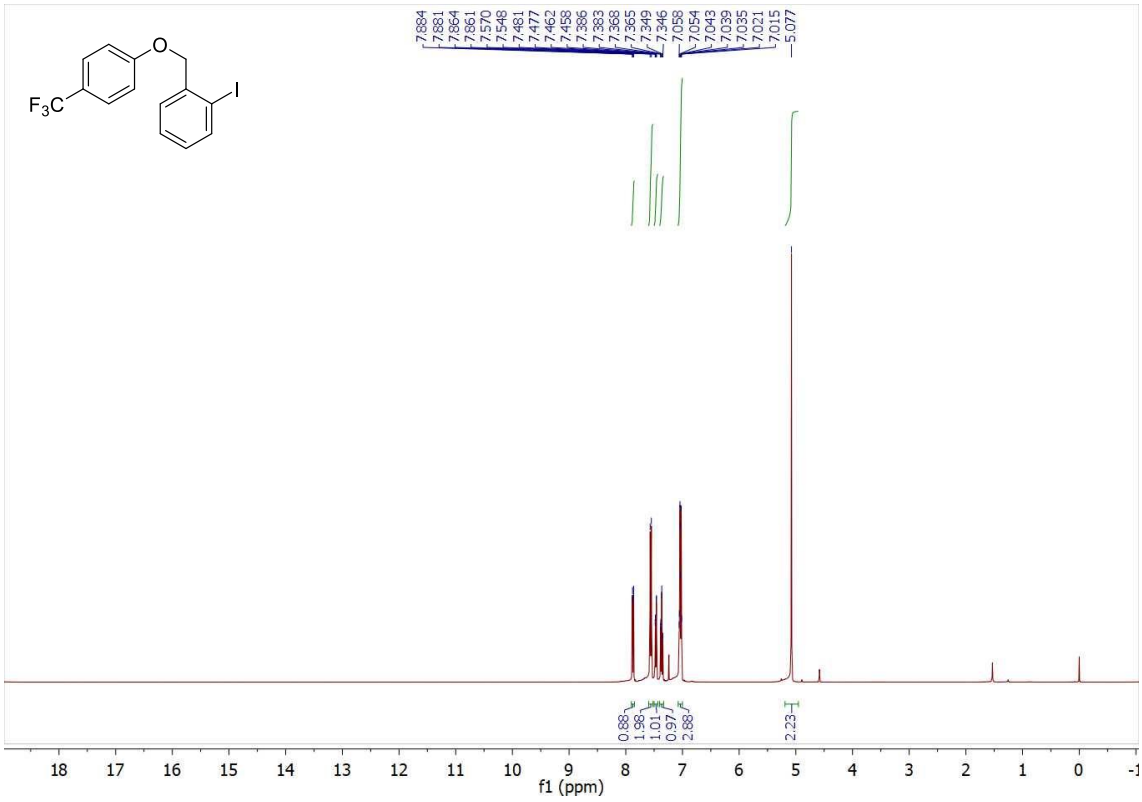


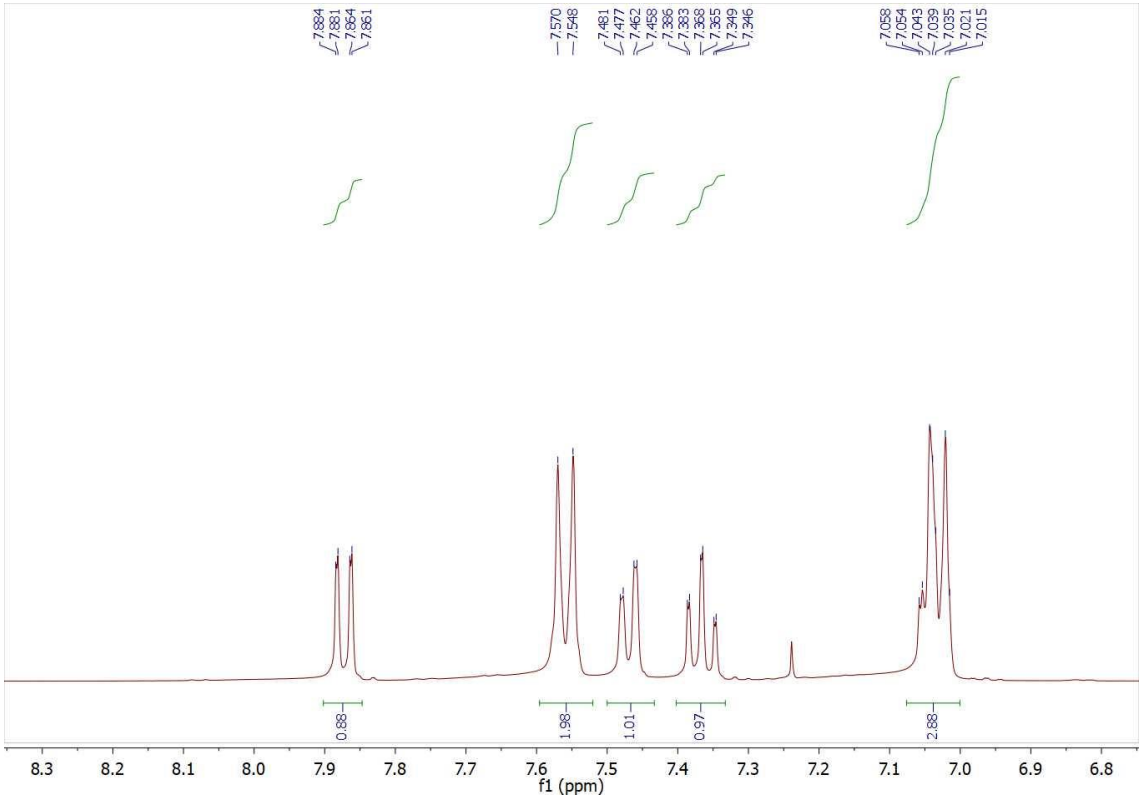
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 4-((2-Iodobenzyl)oxy)benzonitrile **(5g).**



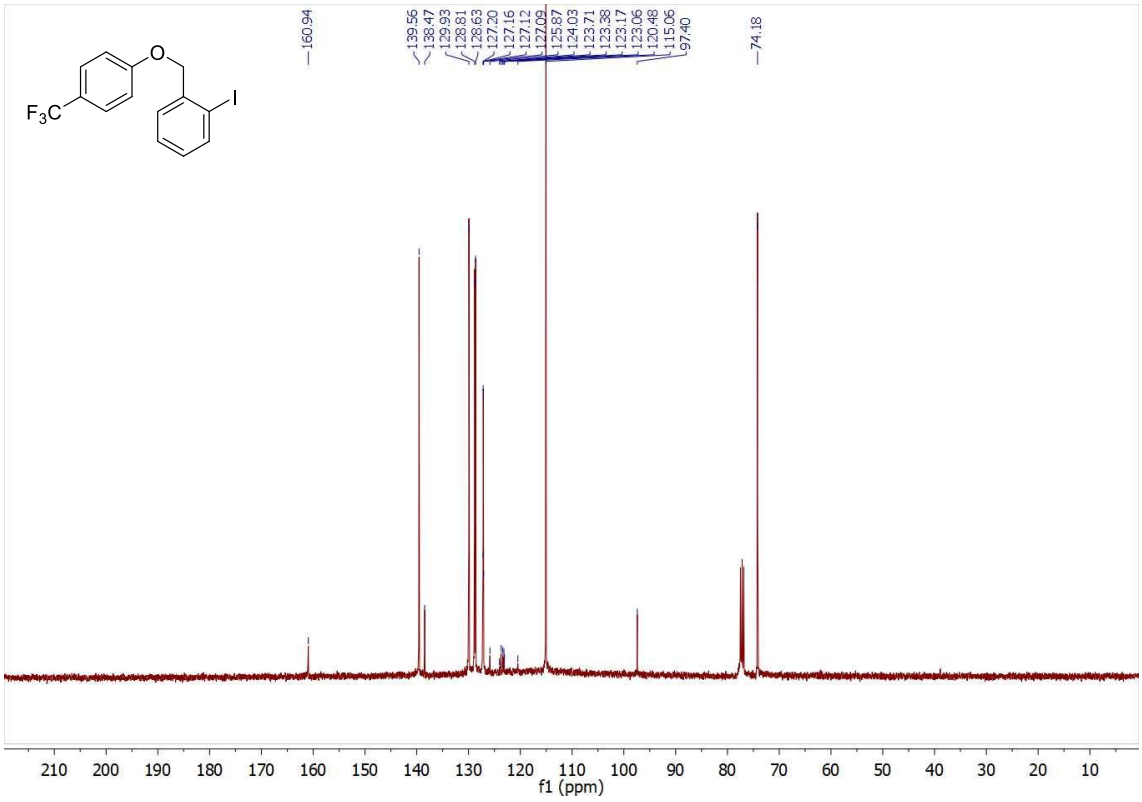


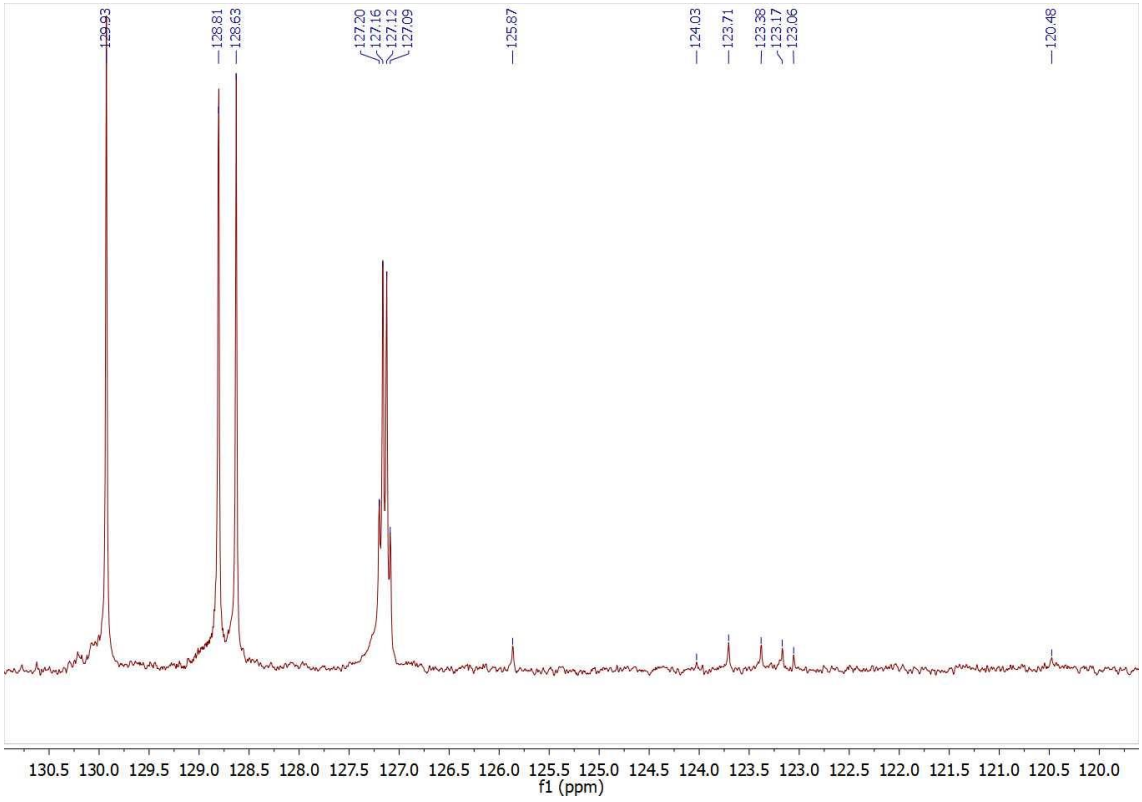
^{1}H-NMR (400 MHz, $CDCl_3$). 1-Iodo-2-((4-trifluoromethyl)phenoxy)methyl)benzene (**5h**)



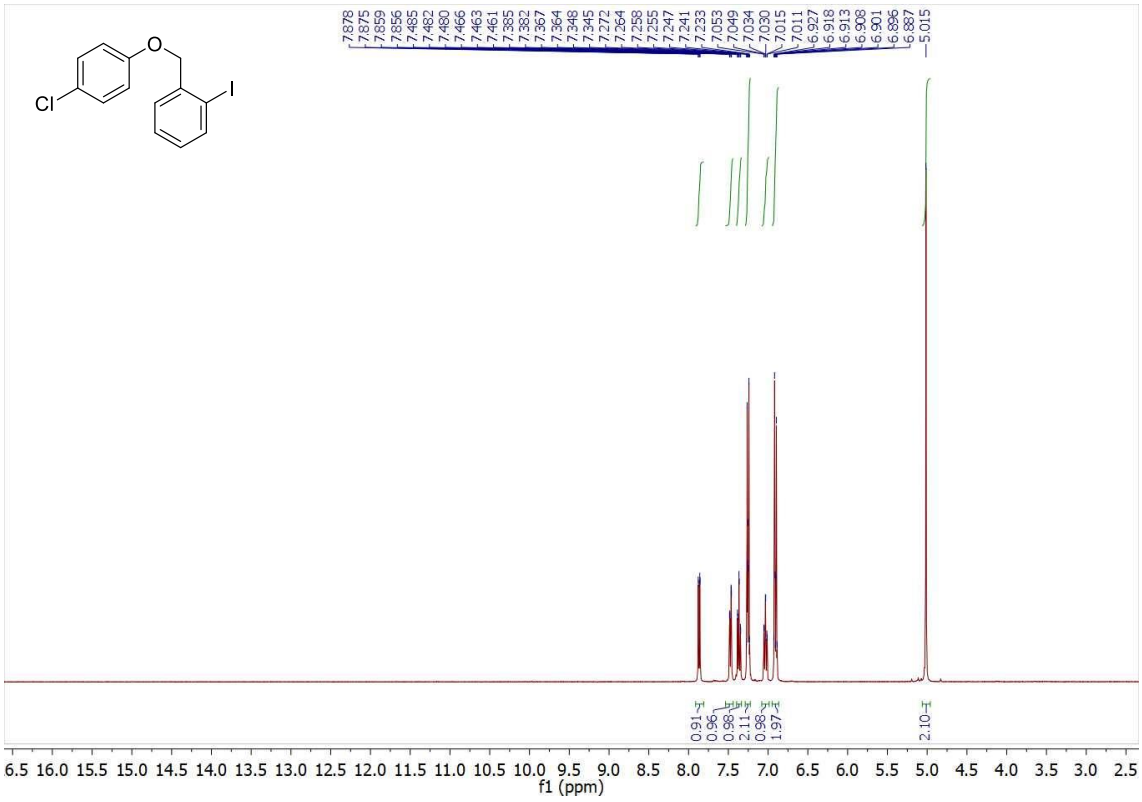


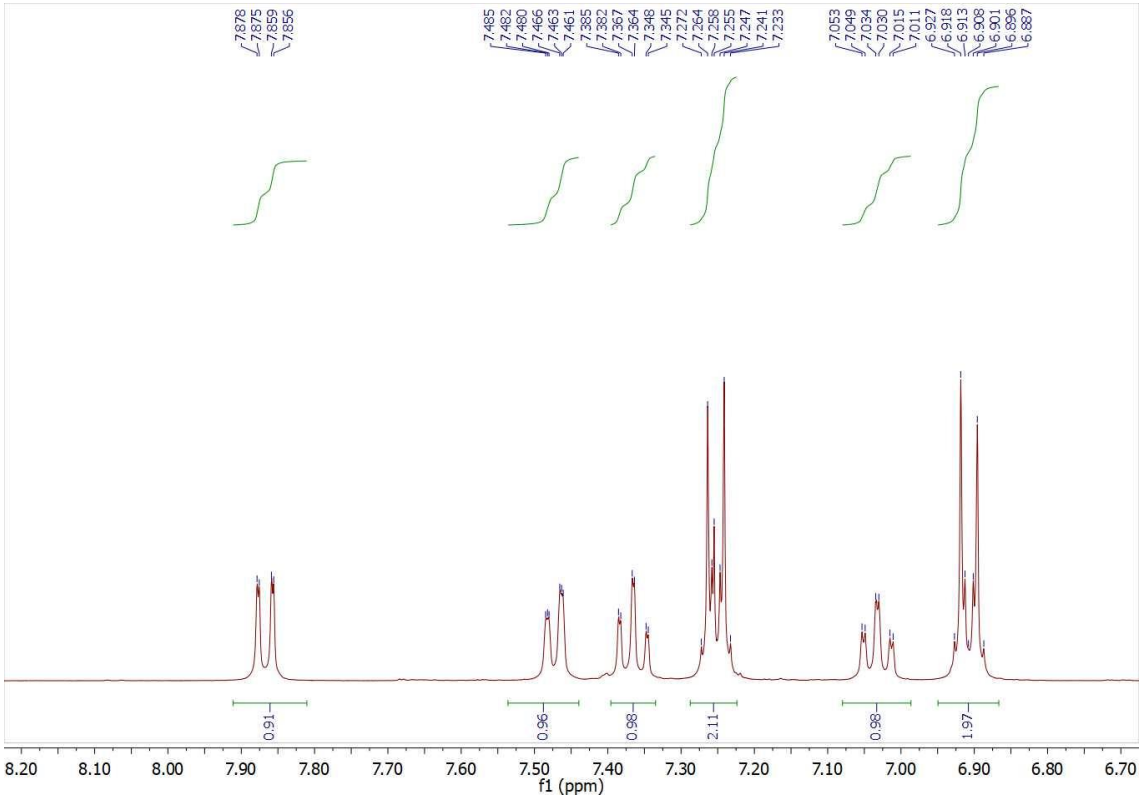
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-Iodo-2-((4-trifluoromethyl)phenoxy)methyl)benzene (**5h**)



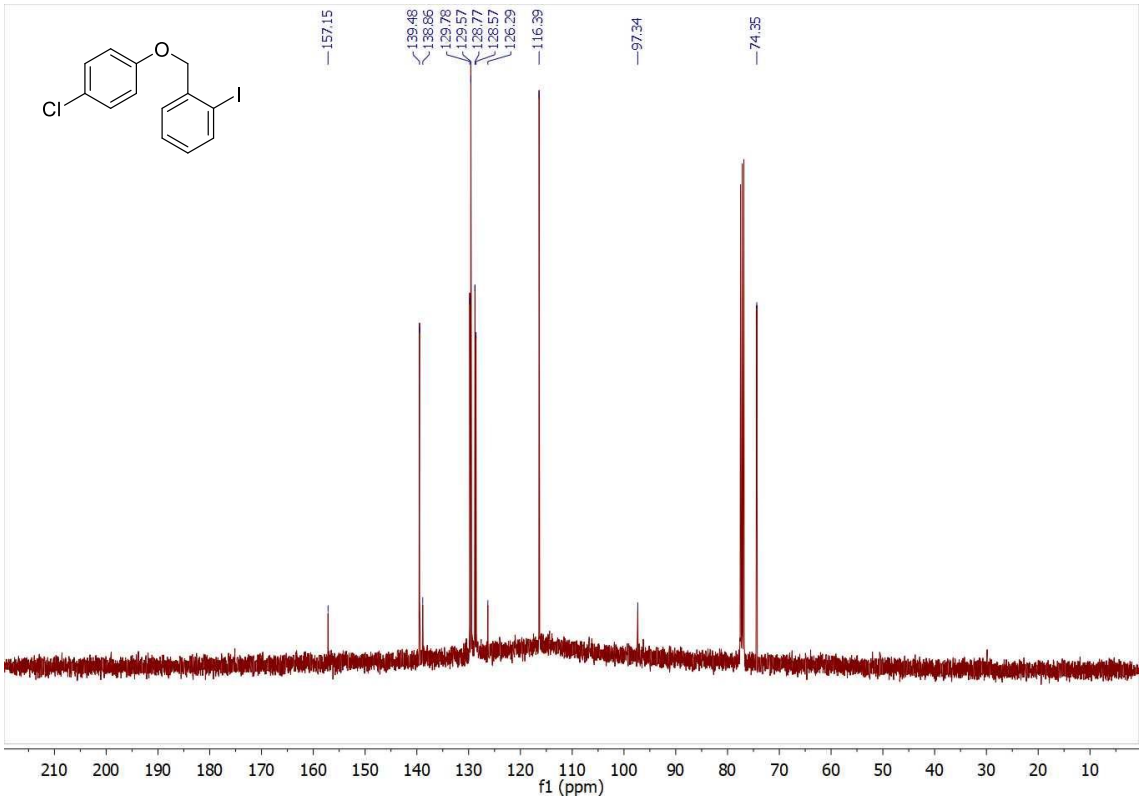


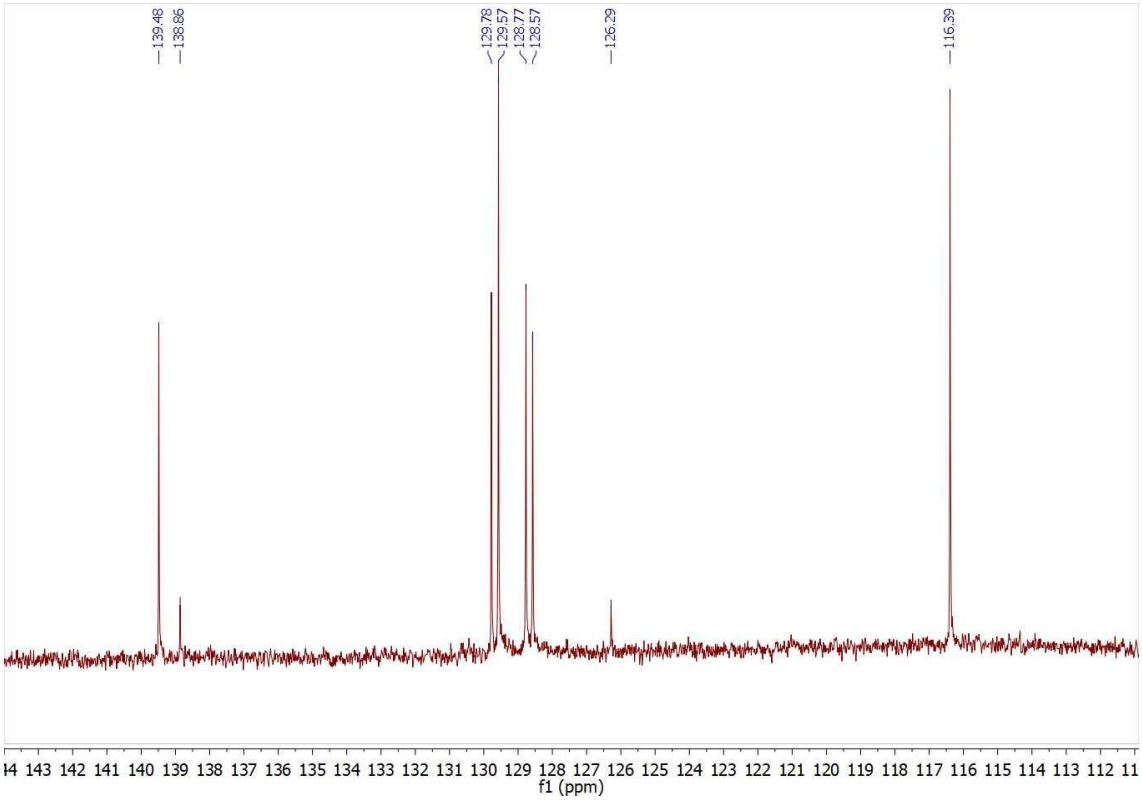
^{1}H-NMR (400 MHz, $CDCl_3$). 1-((4-Chlorophenoxy)methyl)-2-iodobenzene (**5i**)



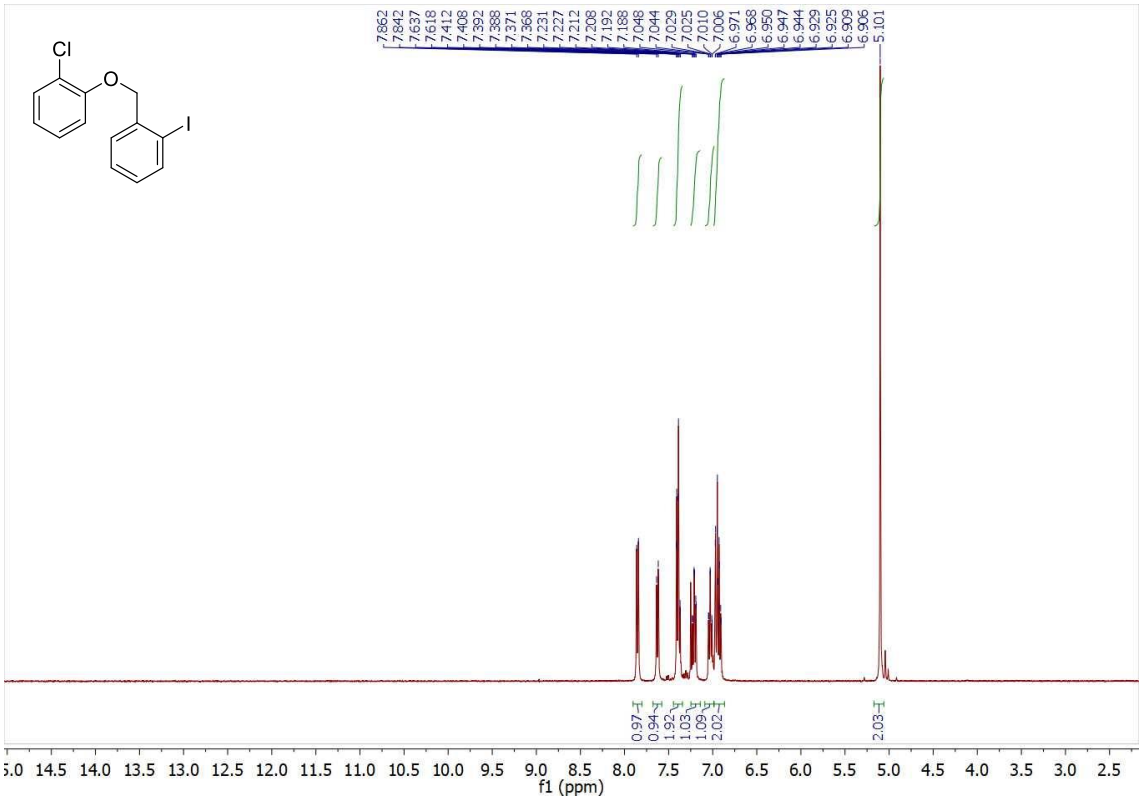


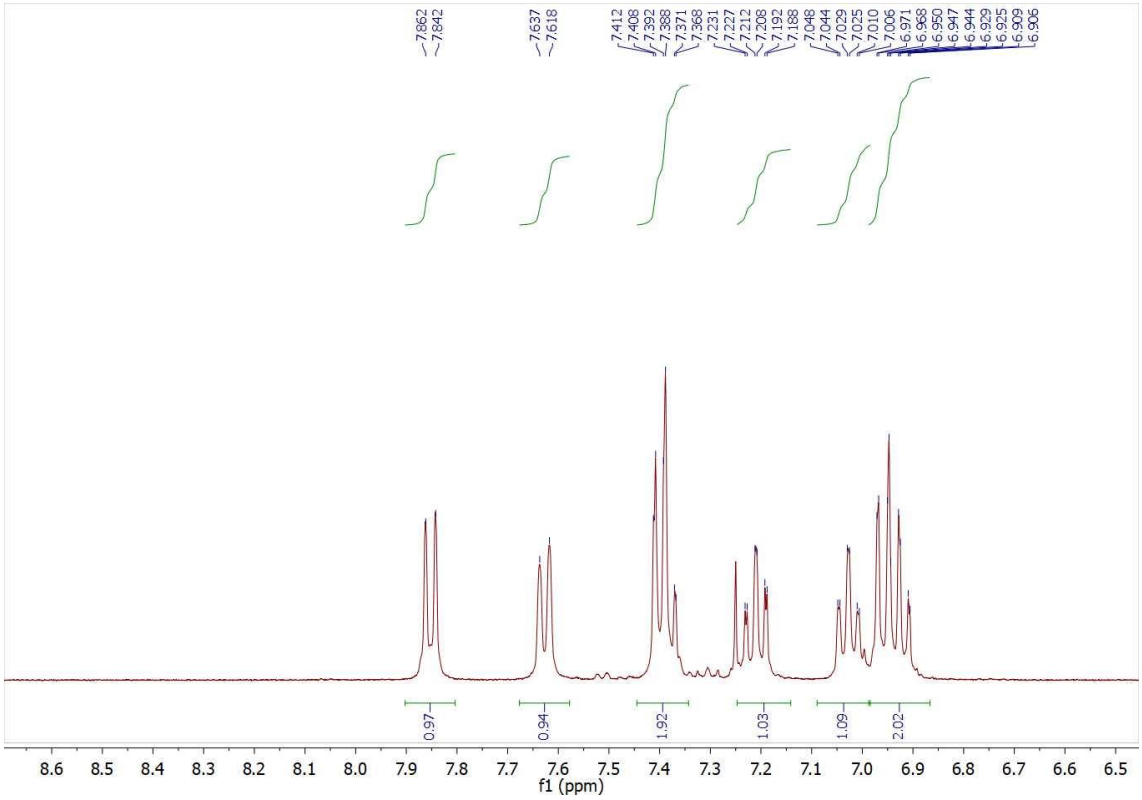
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-((4-Chlorophenoxy)methyl)-2-iodobenzene (**5i**)



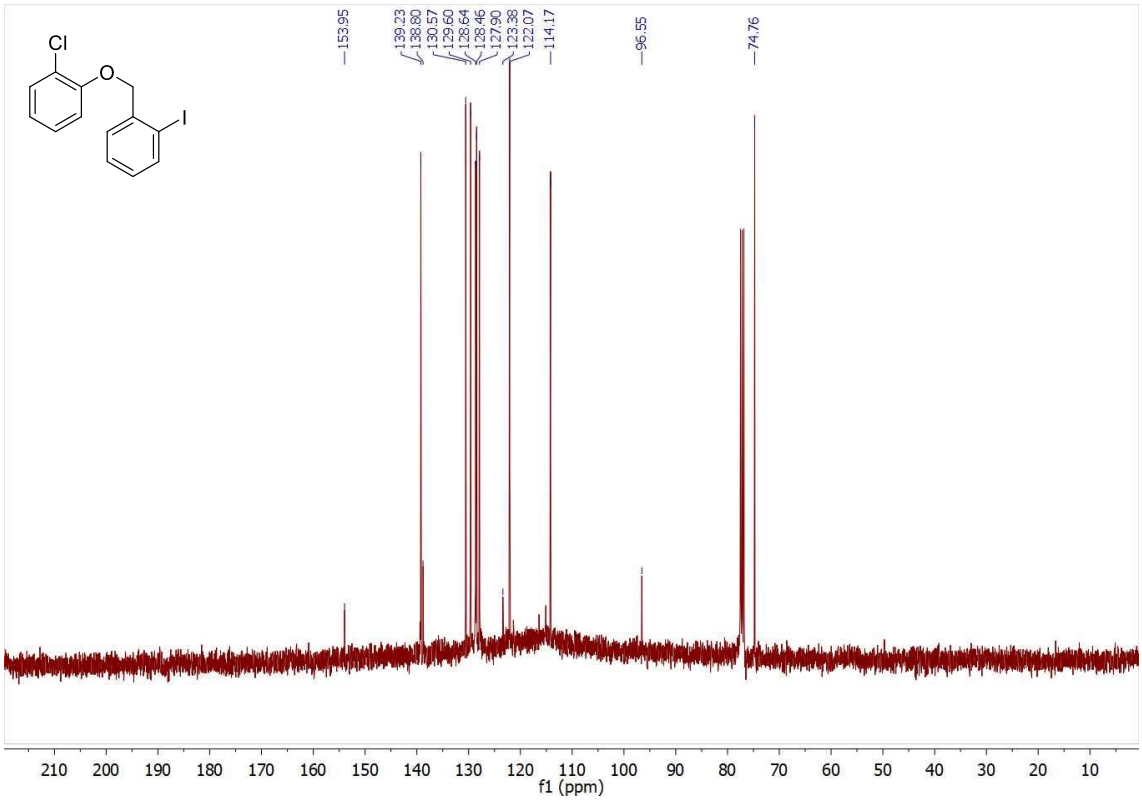


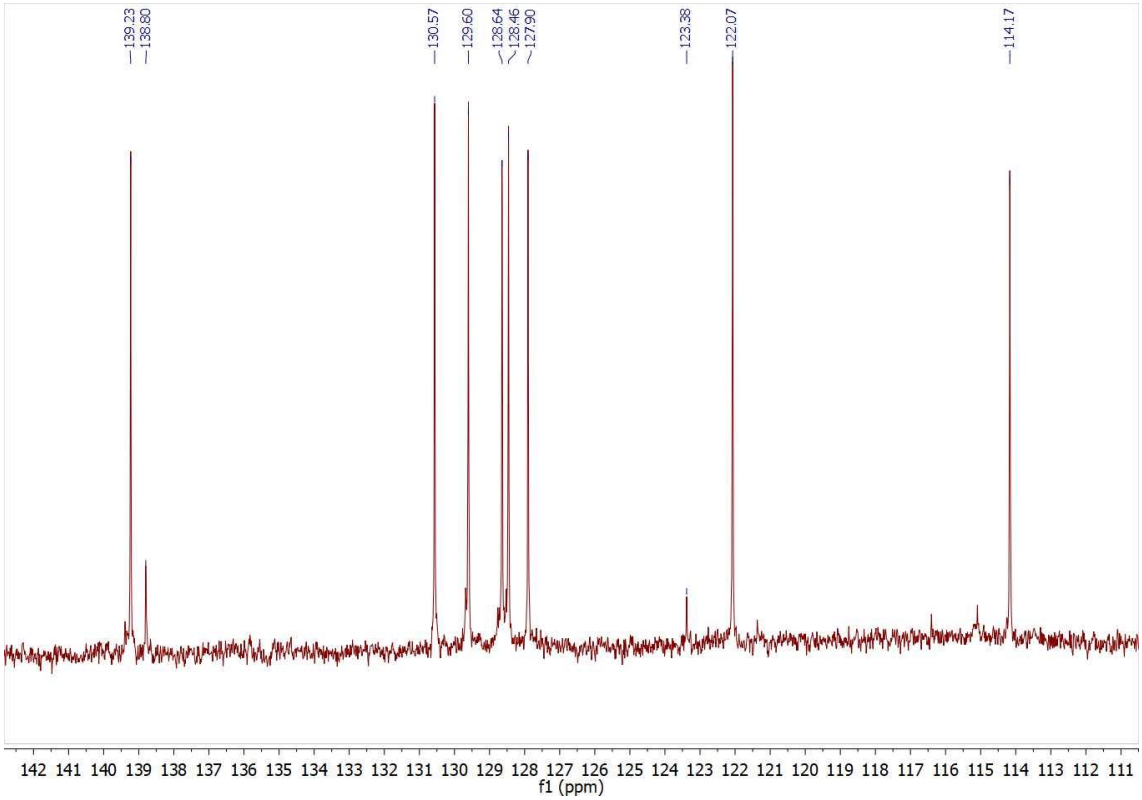
^{1}H-NMR (400 MHz, $CDCl_3$). 1-Chloro-2-((2-iodobenzyl)oxy)benzene (**5j**)



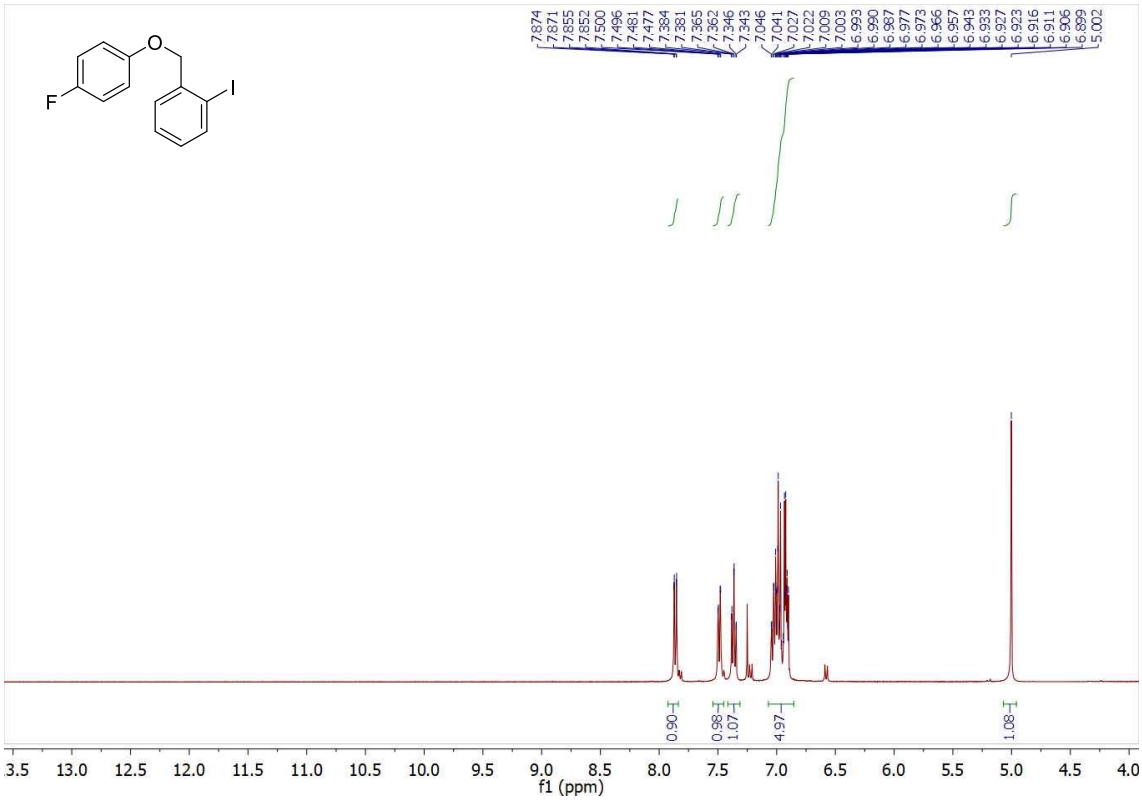


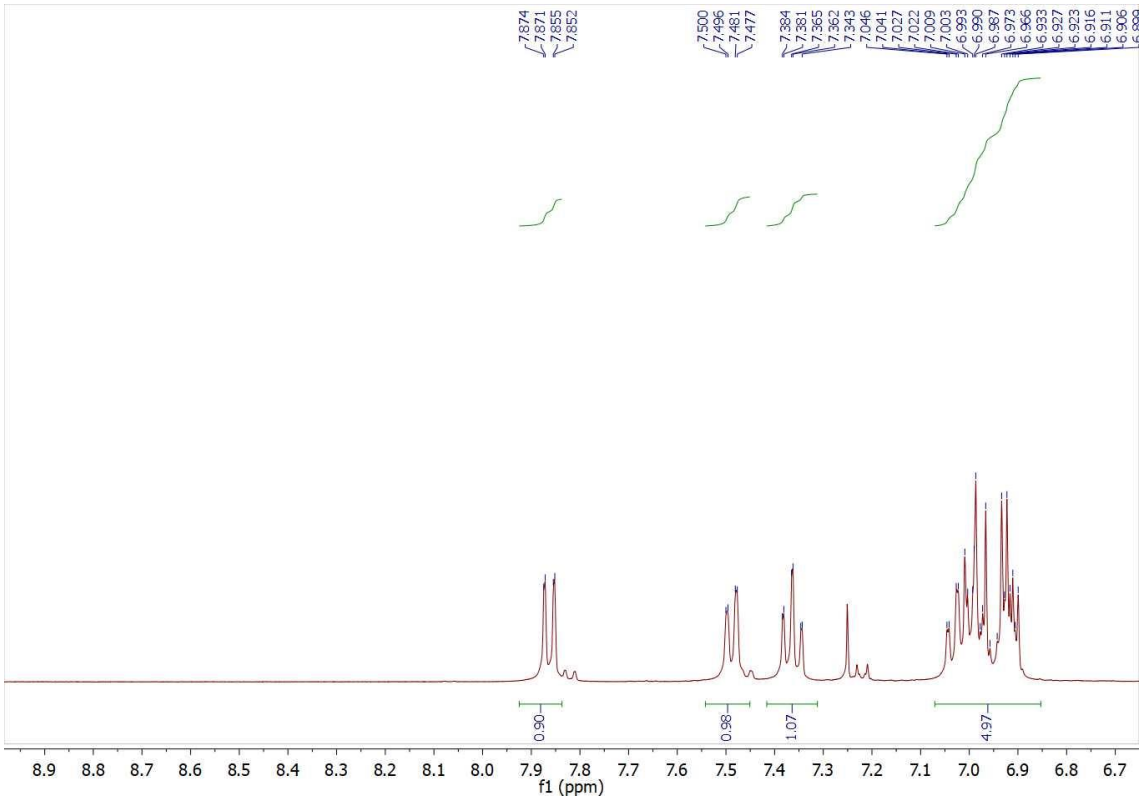
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-Chloro-2-((2-iodobenzyl)oxy)benzene (**5j**)



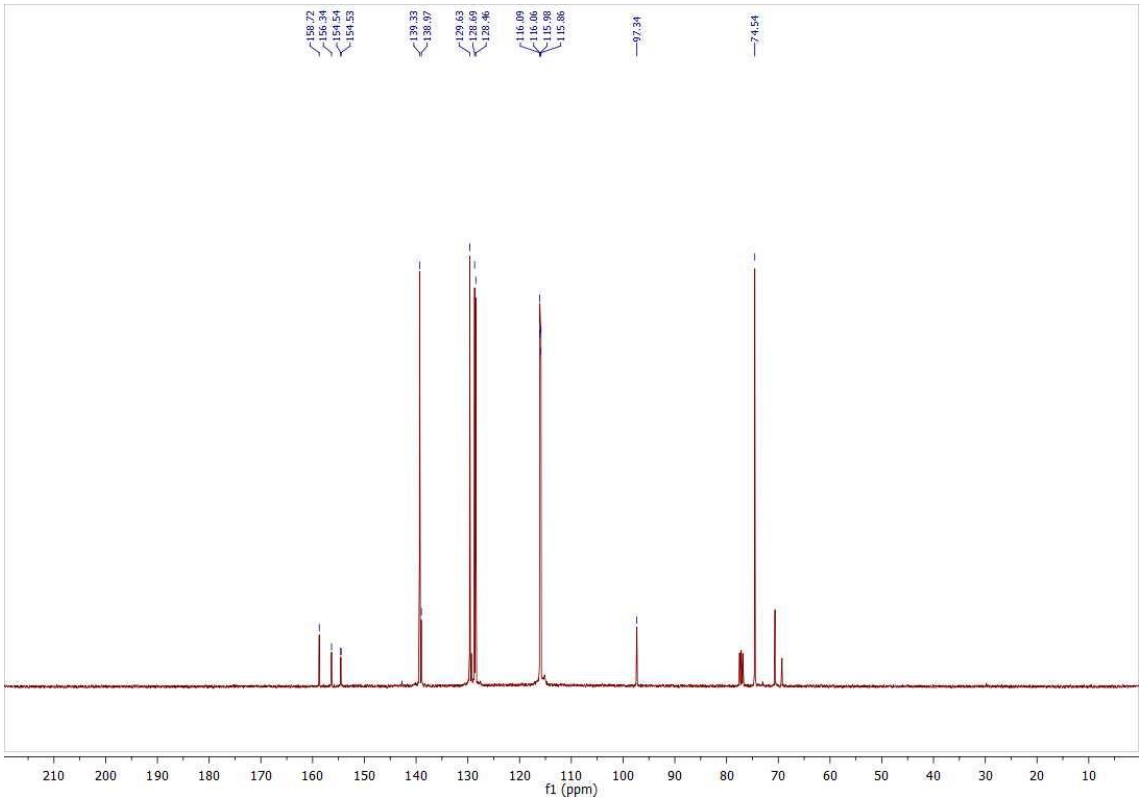


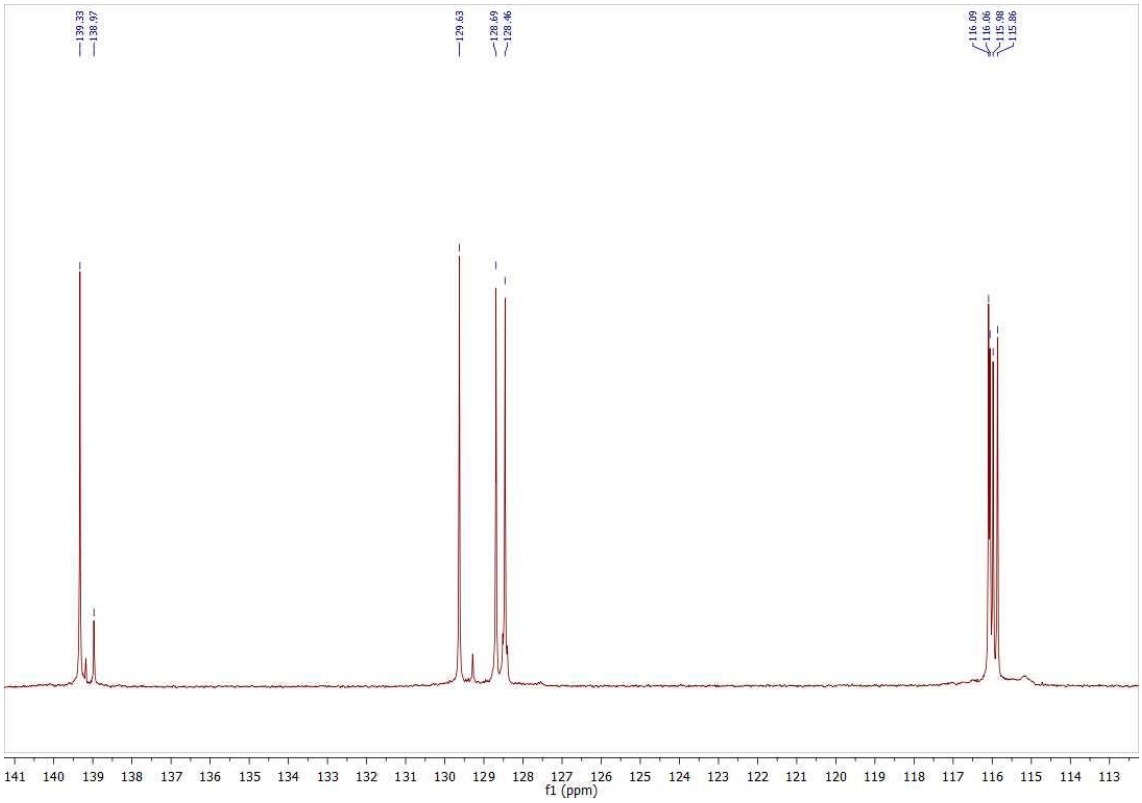
^{1}H-NMR (400 MHz, $CDCl_3$). 1-((4-Fluorophenoxy)methyl)-2-iodobenzene (**5k**)



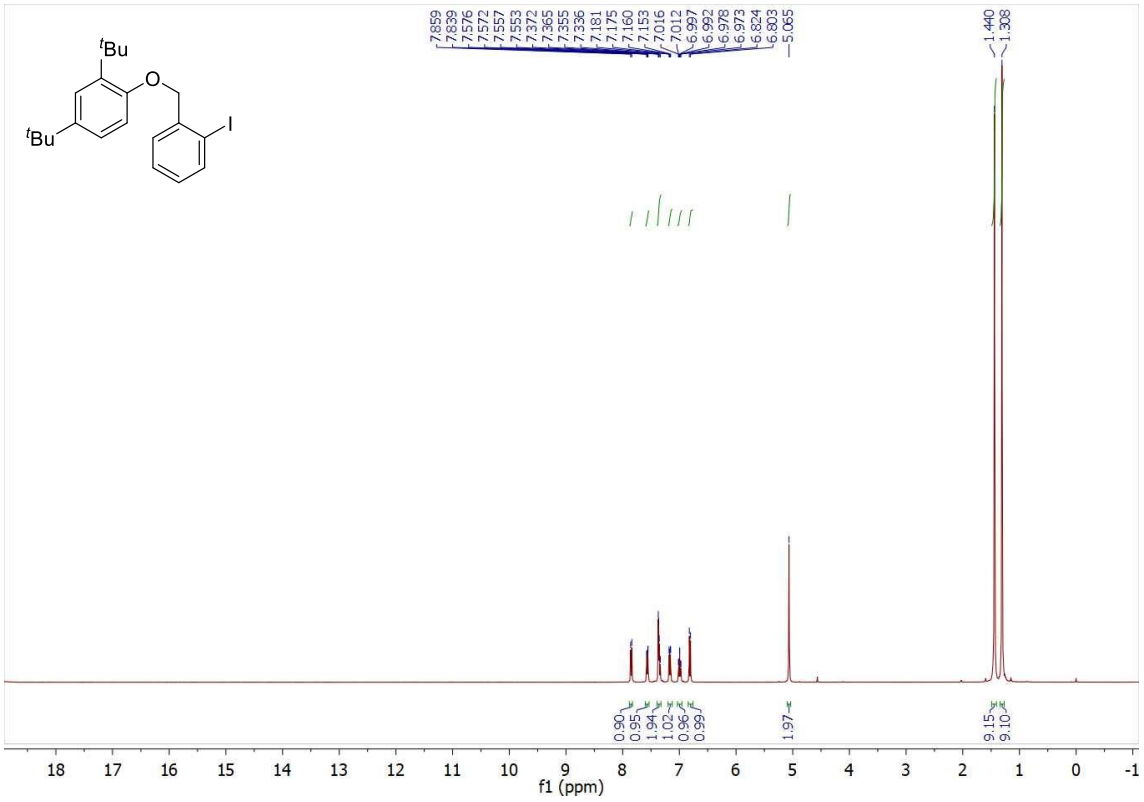


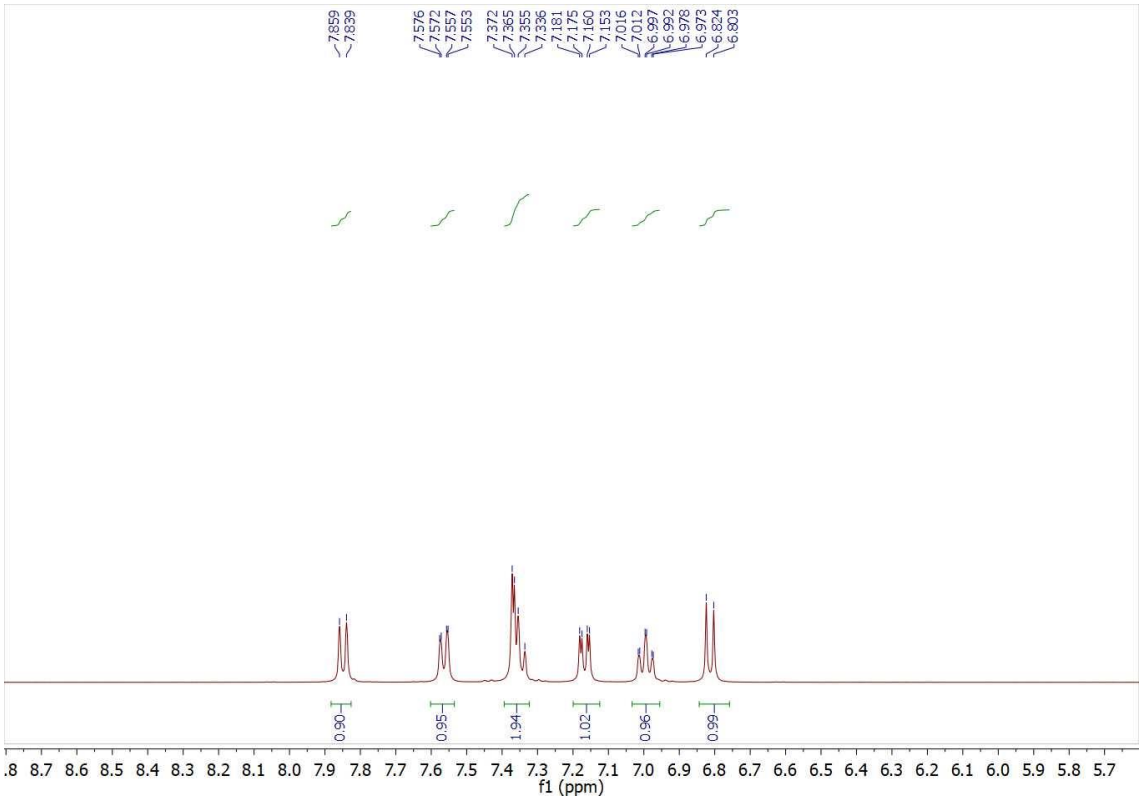
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-((4-Fluorophenoxy)methyl)-2-iodobenzene (**5k**)



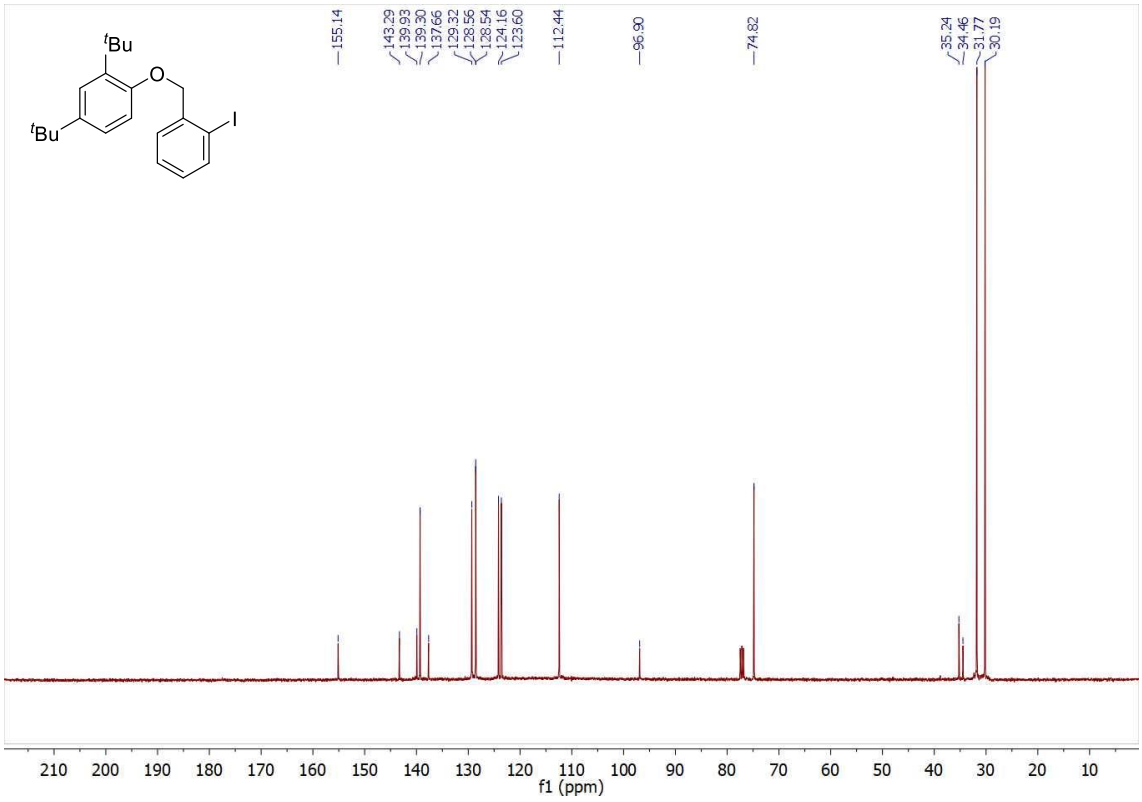


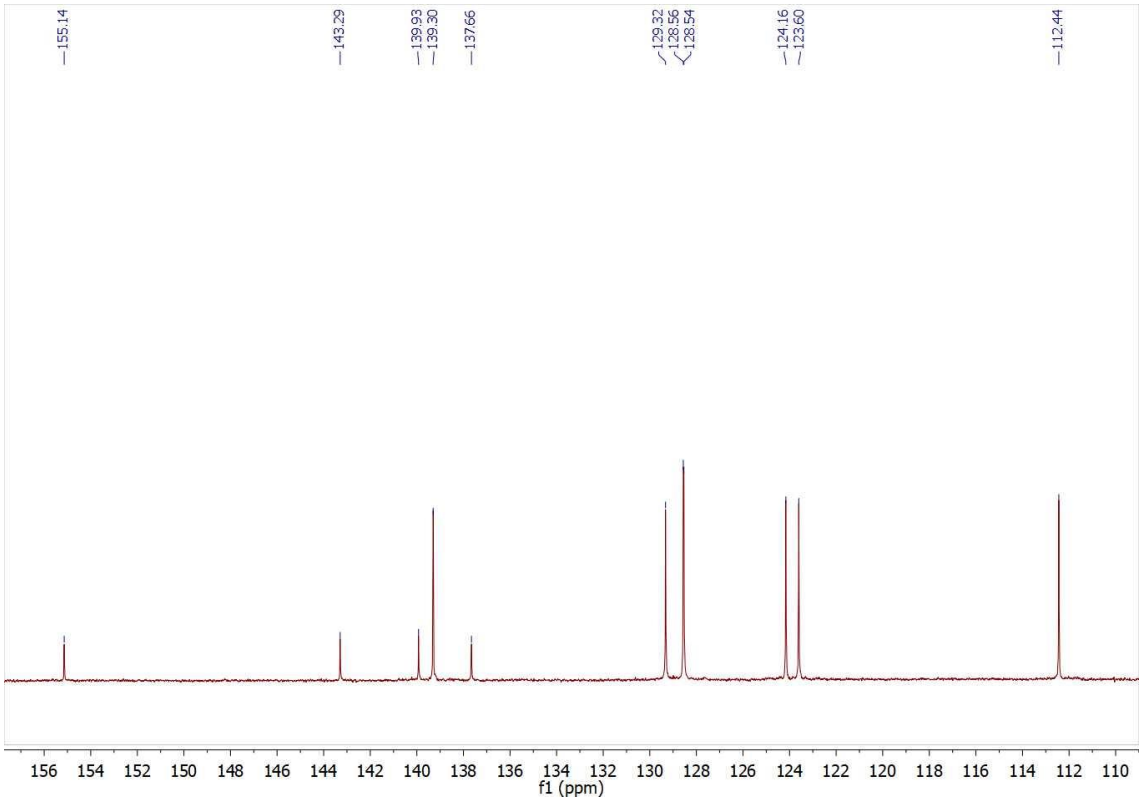
^{1}H-NMR (400 MHz, $CDCl_3$). 2,4-Di-*tert*-butyl-1-((2-iodobenzyl)oxy)benzene (**5l**).



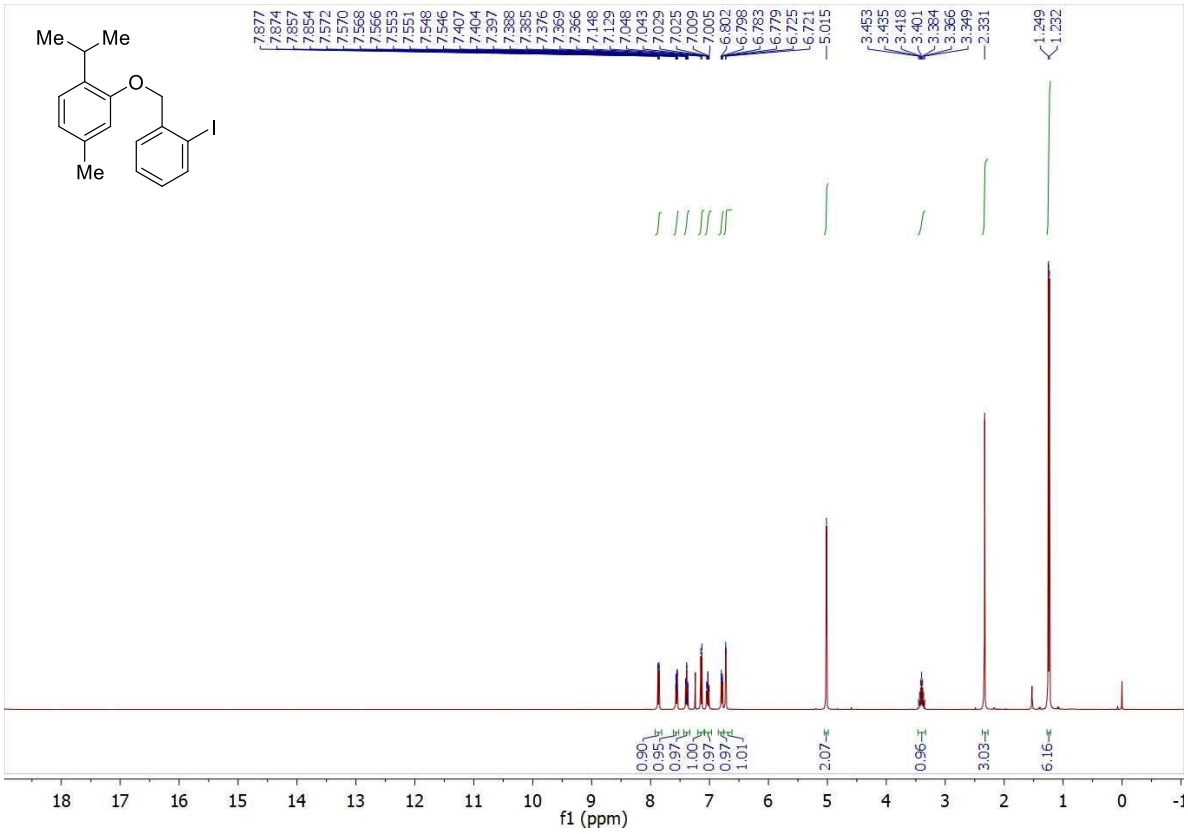


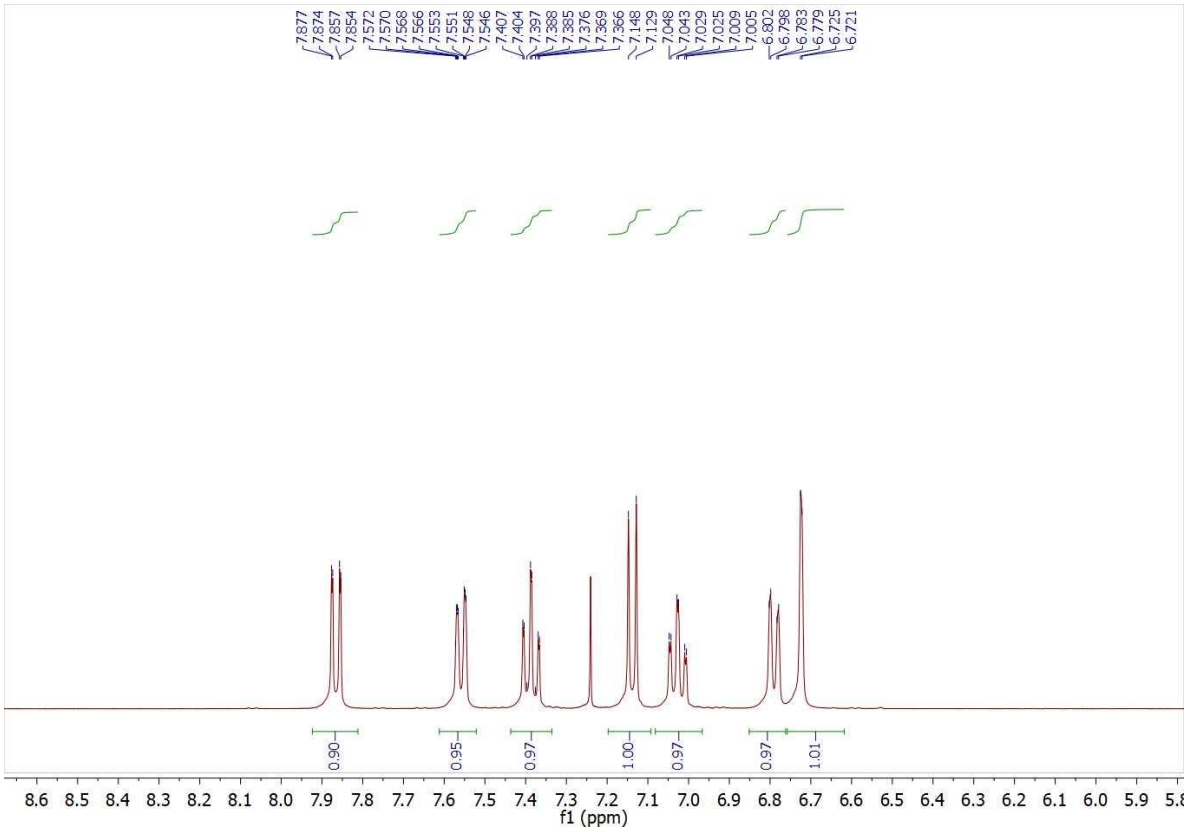
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 2,4-Di-*tert*-butyl-1-((2-iodobenzyl)oxy)benzene (**5l**).



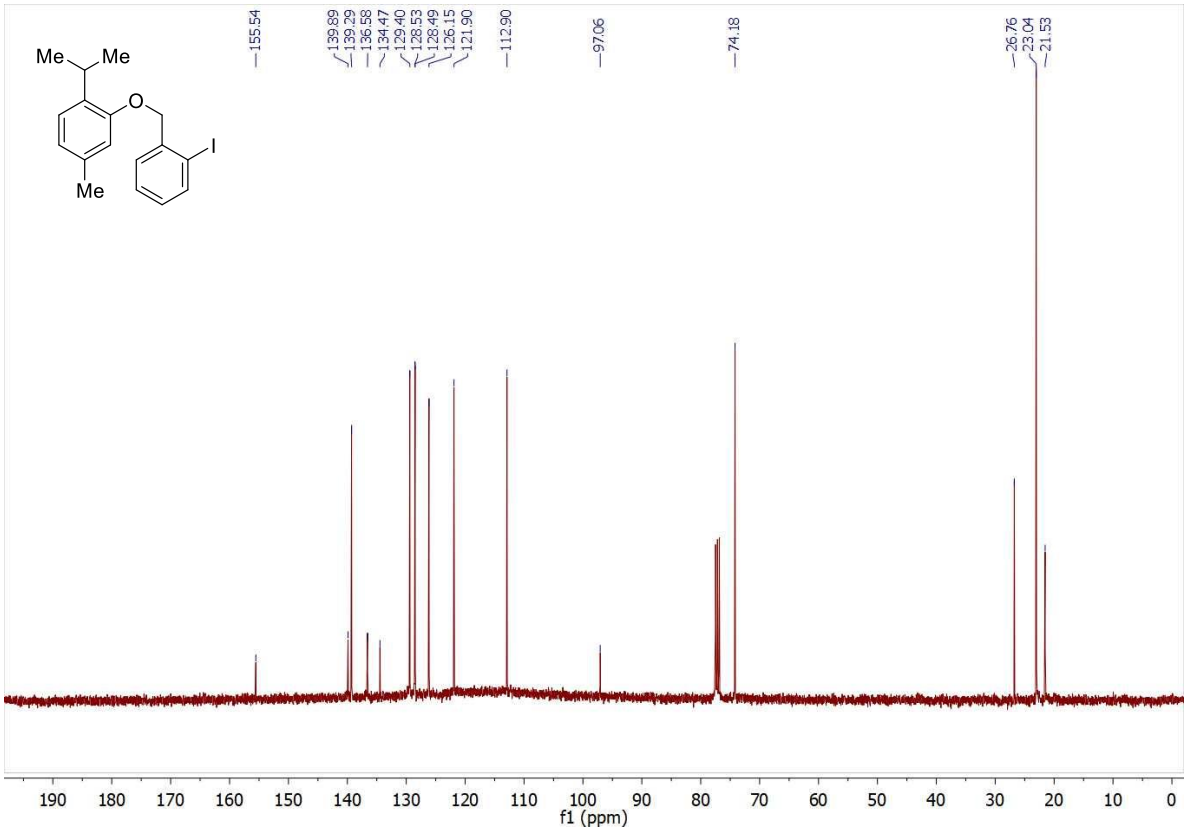


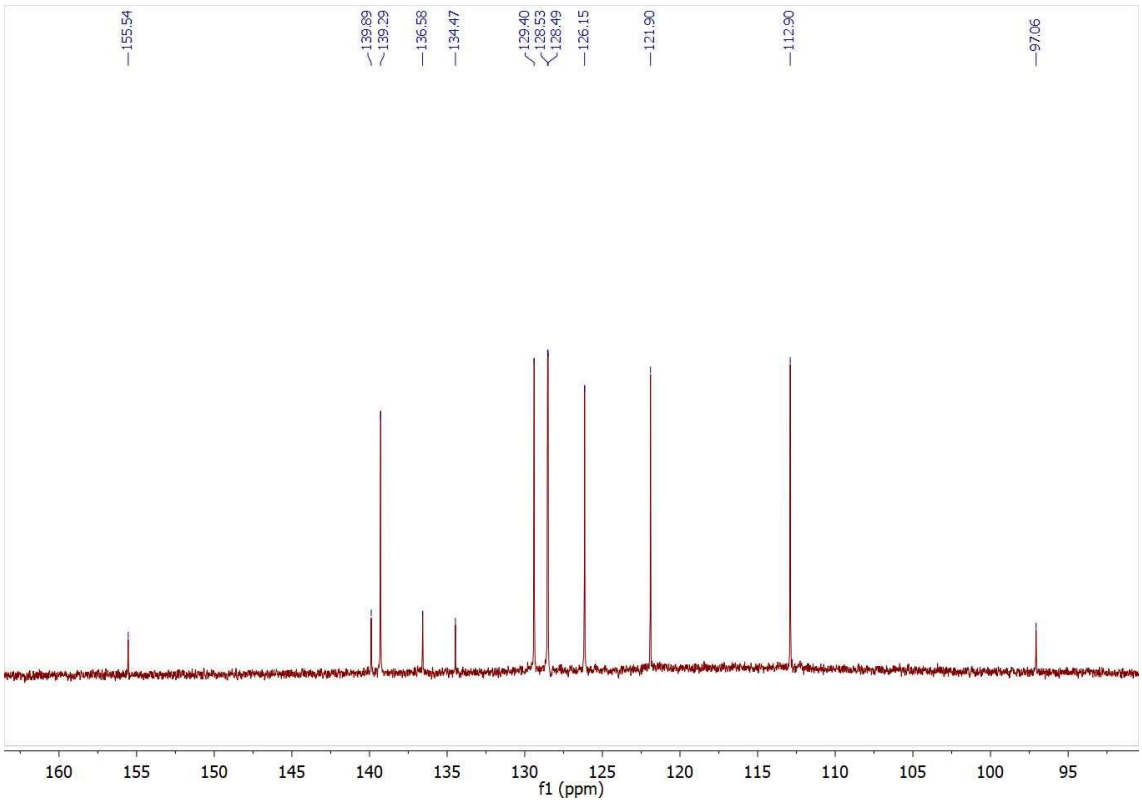
^{1}H-NMR (400 MHz, $CDCl_3$). 2-((2-Iodobenzyl)oxy)1-isopropyl-4-methylbenzene (**5m**).



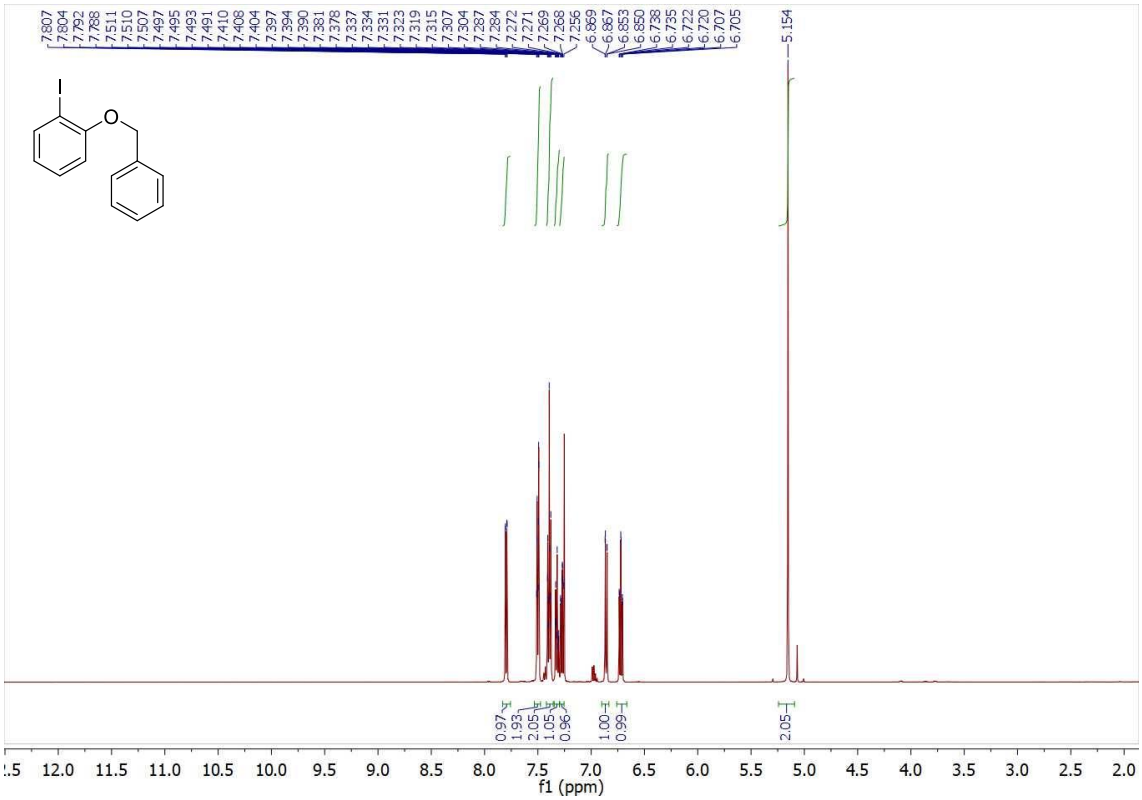


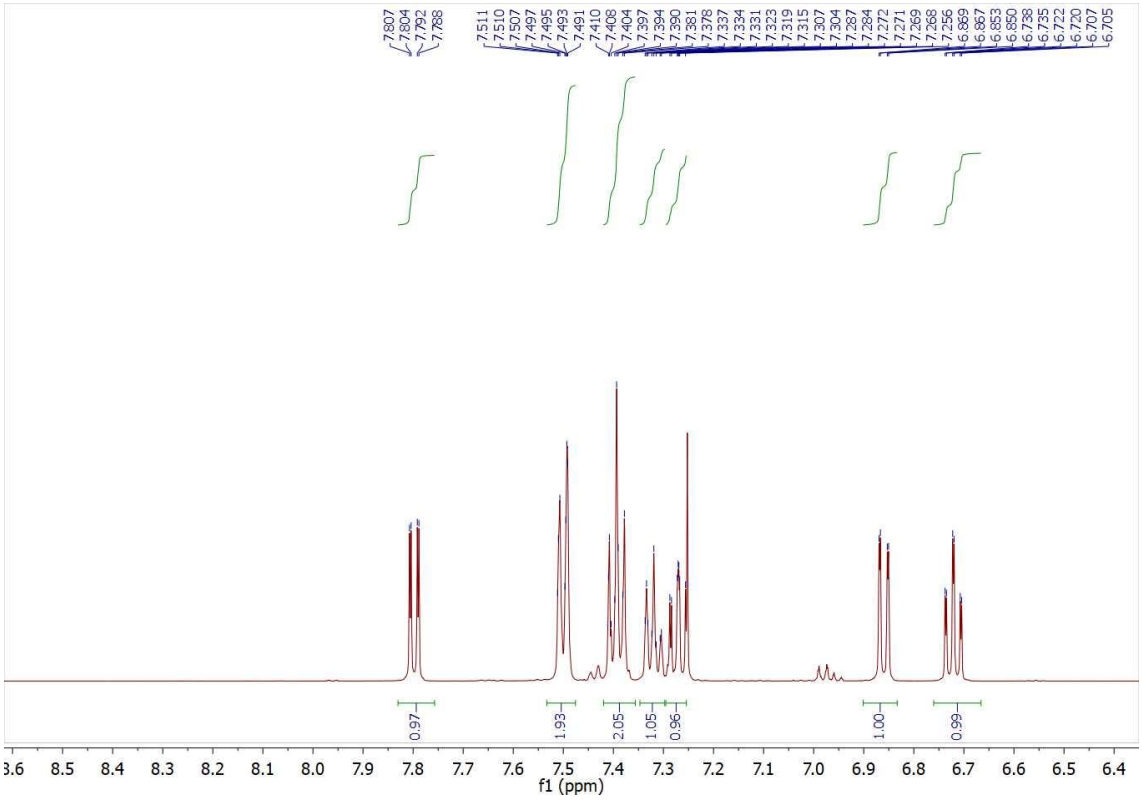
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 2-((2-Iodobenzyl)oxy)1-isopropyl-4-methylbenzene (**5m**).



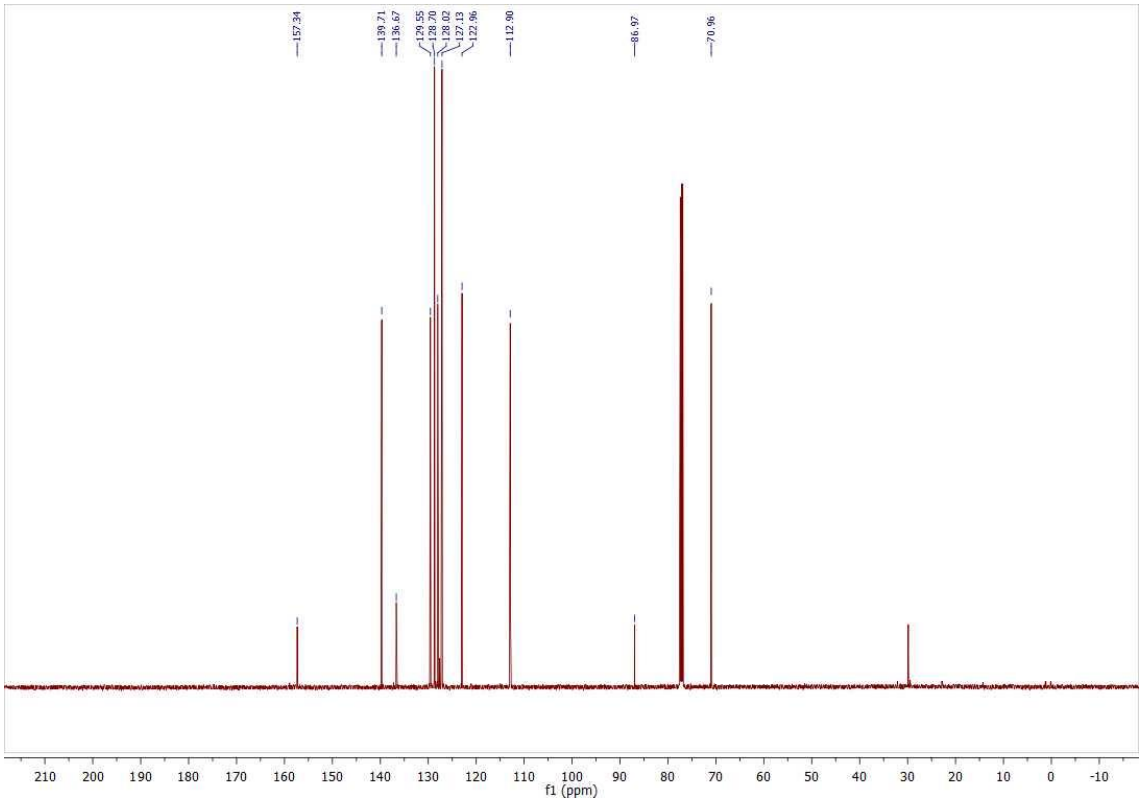


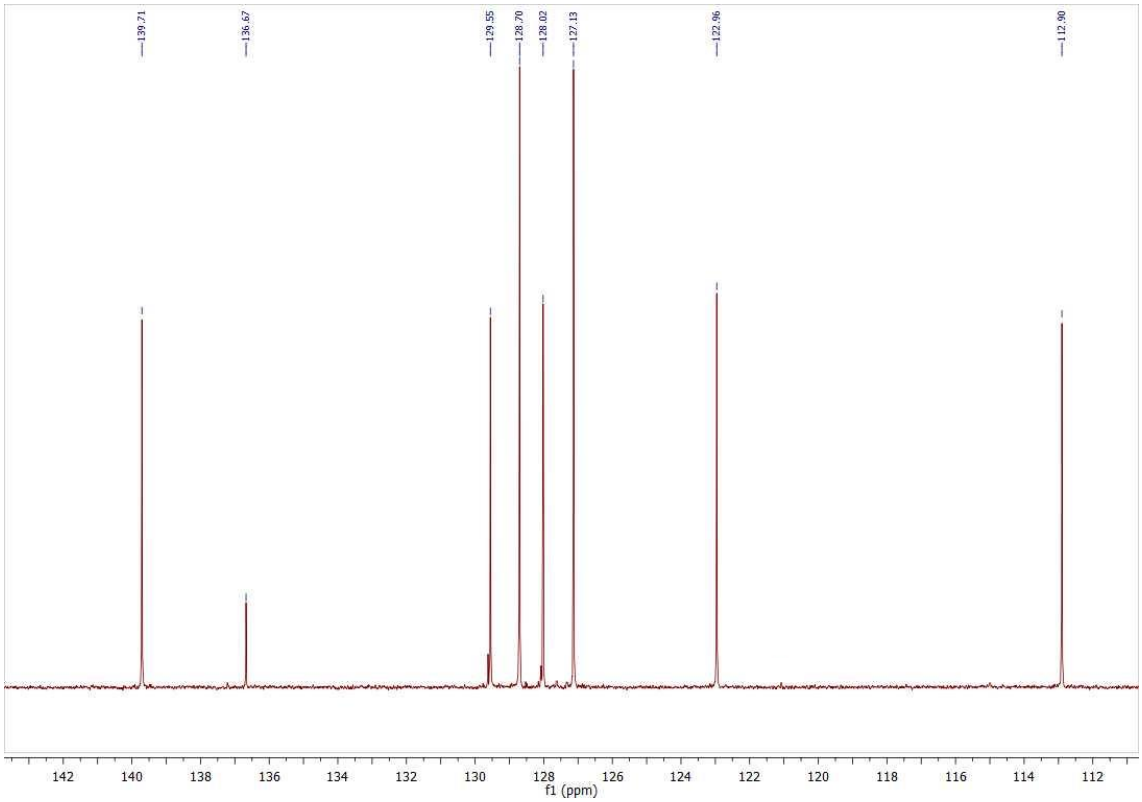
^{1}H-NMR (400 MHz, $CDCl_3$). 1-(Benzyloxy)-2-iodobenzene (**5n**).



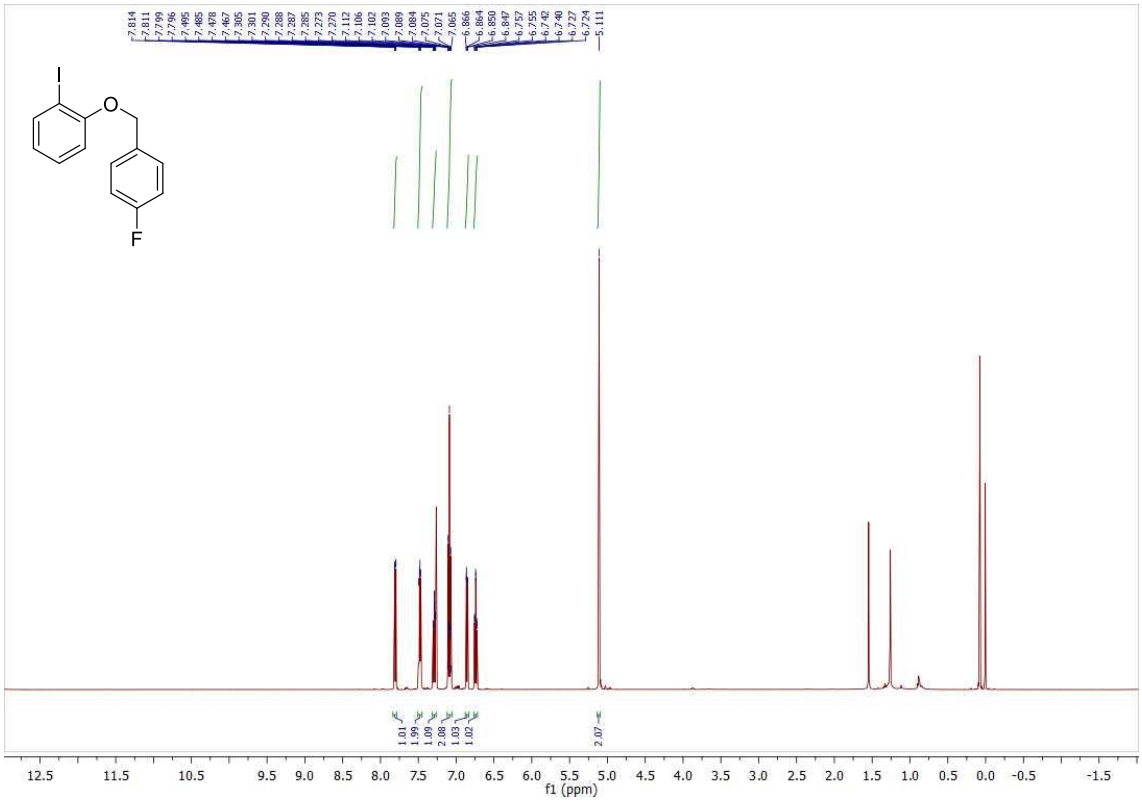


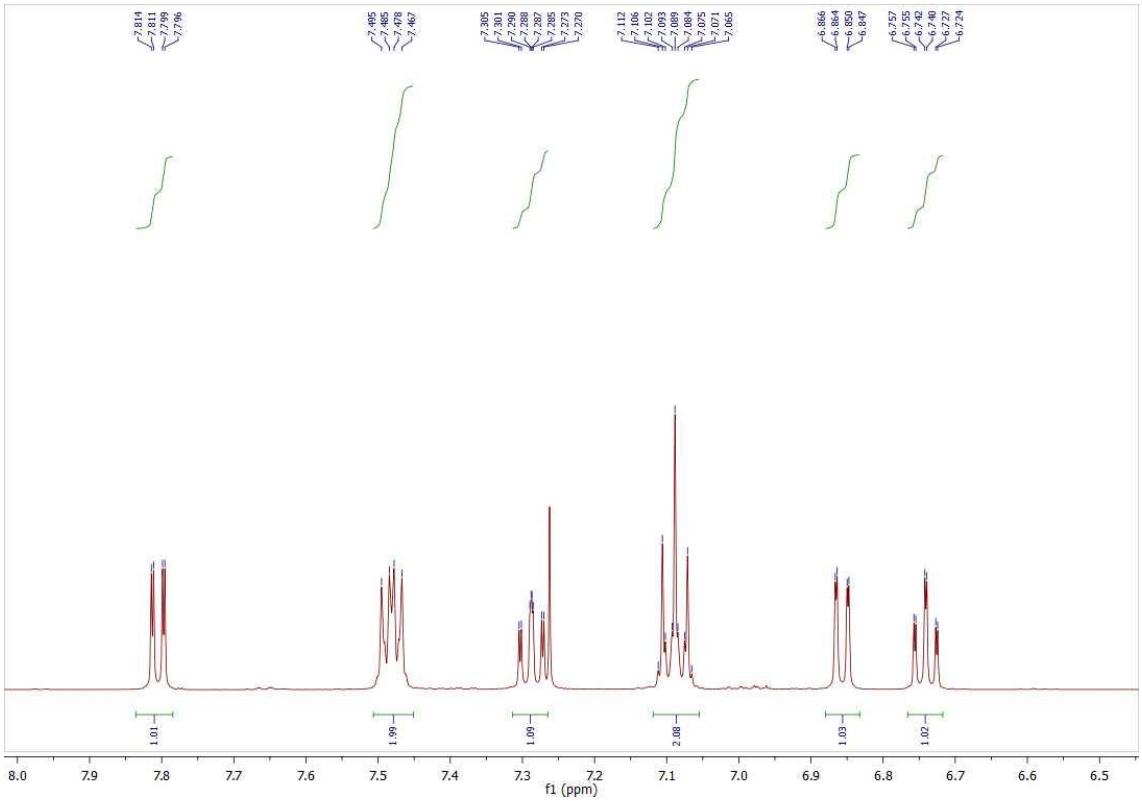
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-(Benzyloxy)-2-iodobenzene (**5n**).



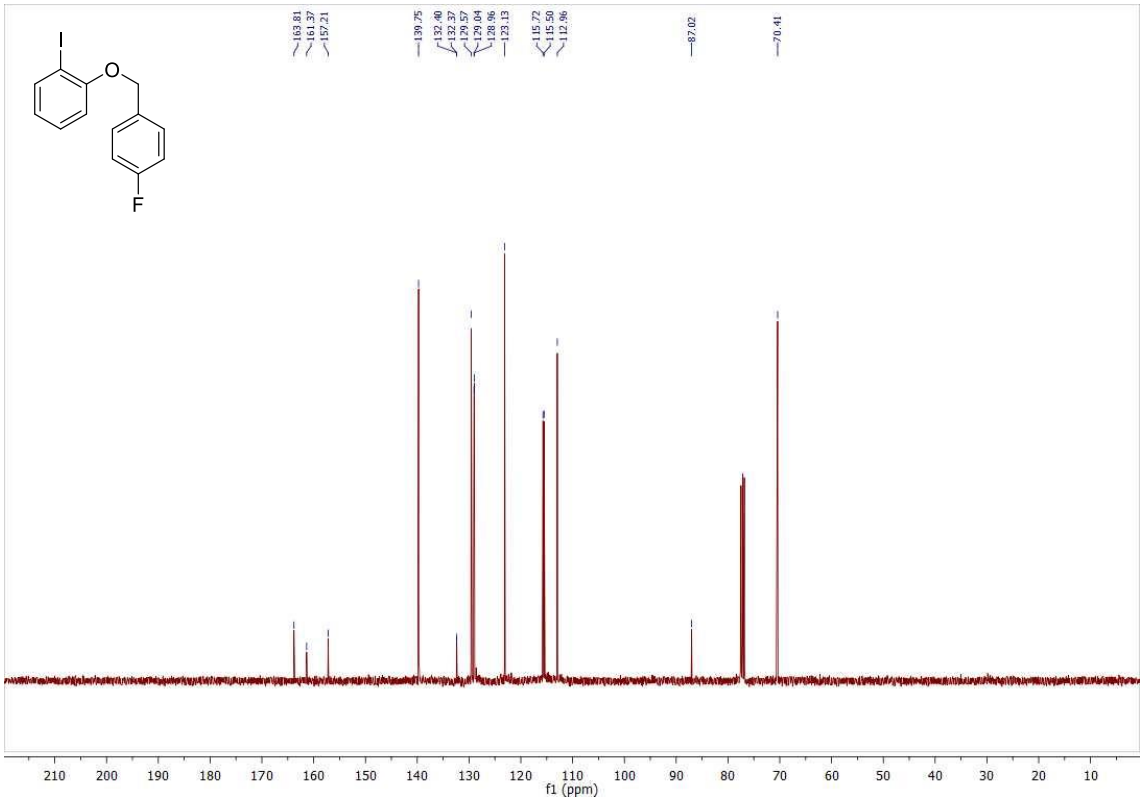


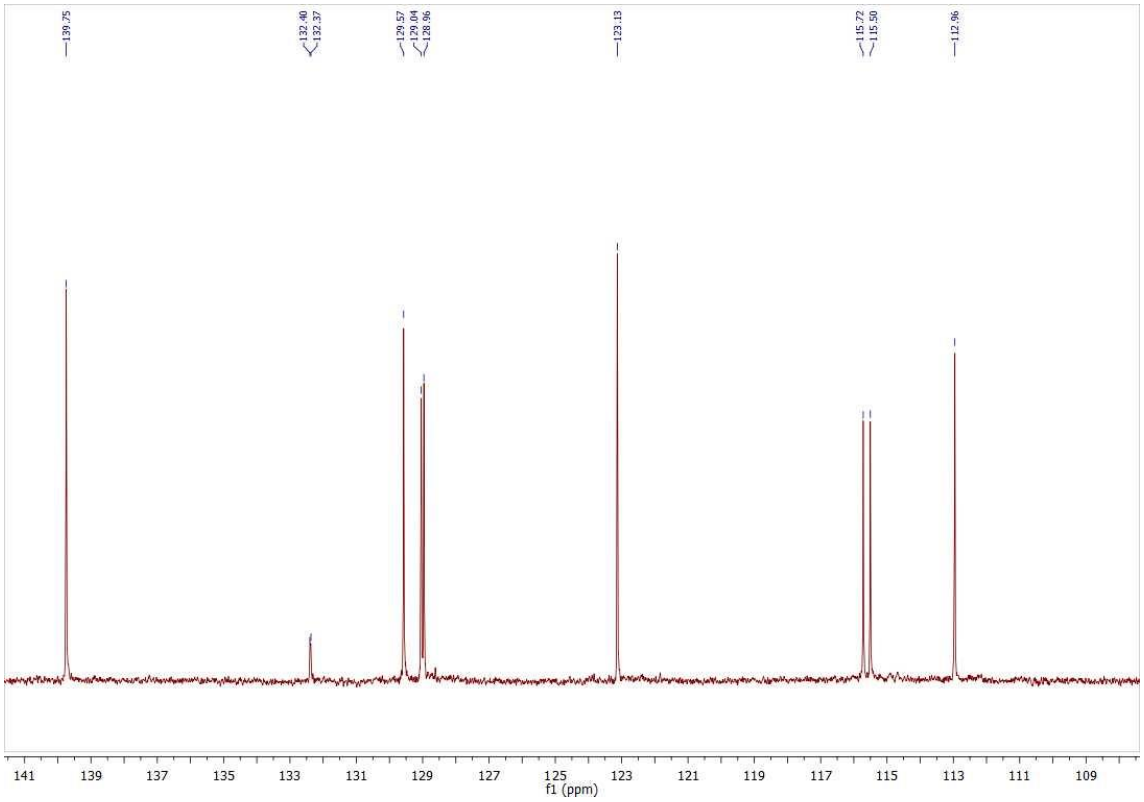
^{1}H-NMR (500 MHz, $CDCl_3$). 1-((4-Fluorobenzyl)oxy)-2-iodobenzene (**5o**).



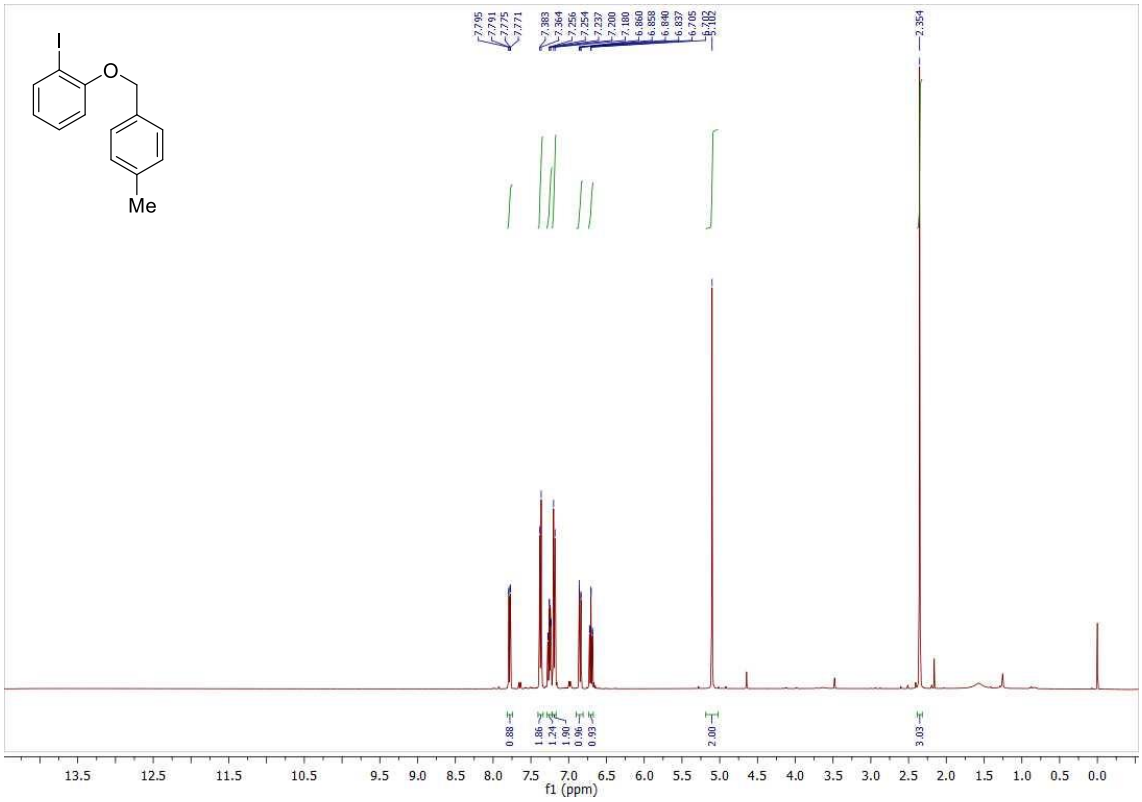


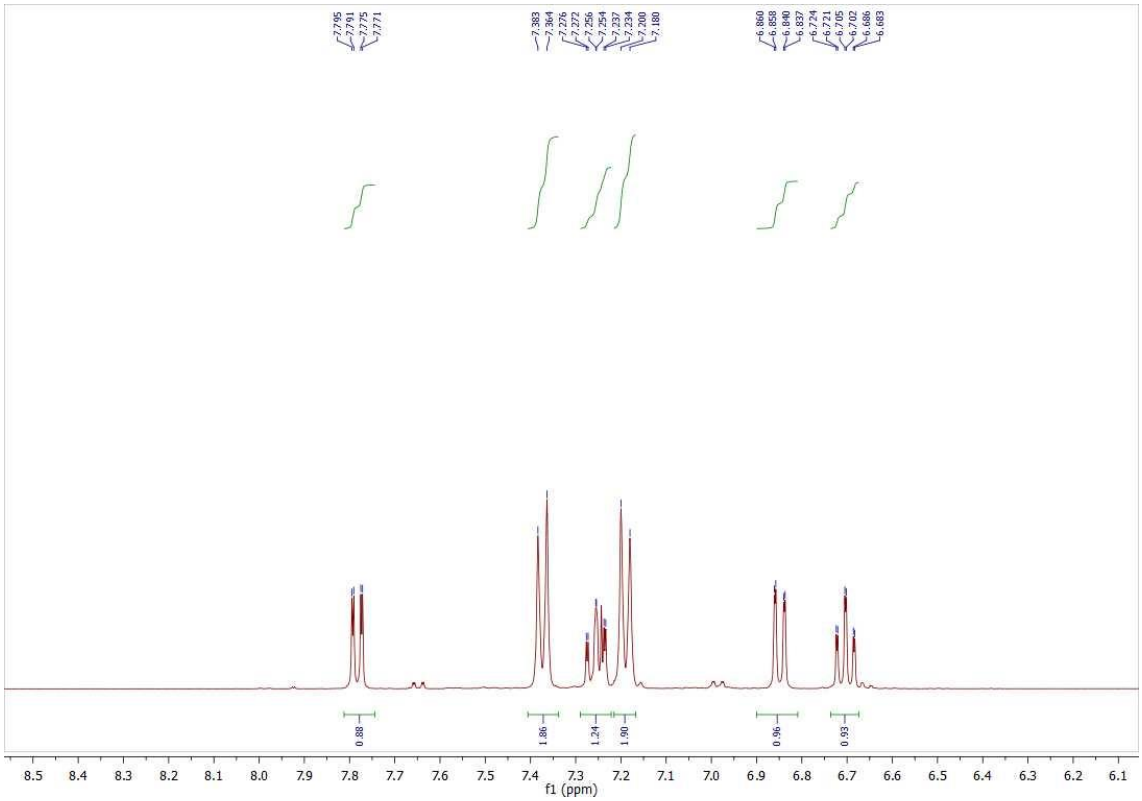
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-((4-Fluorobenzyl)oxy)-2-iodobenzene (**5o**).



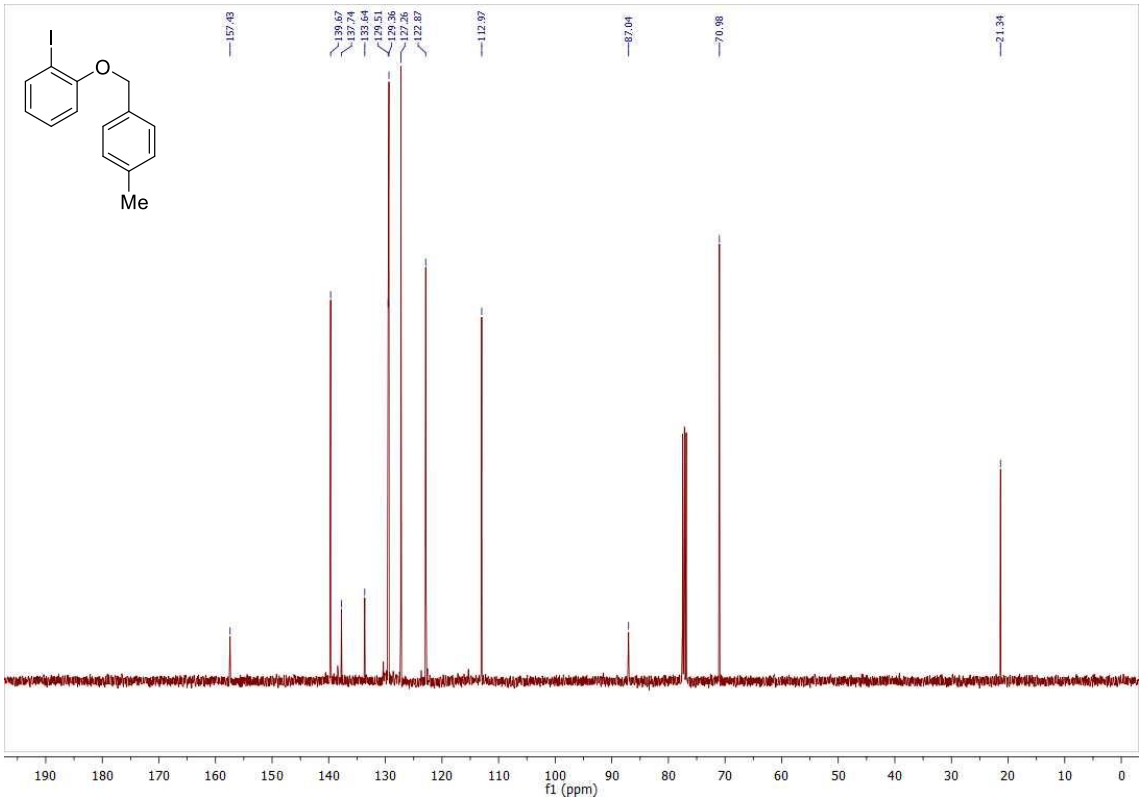


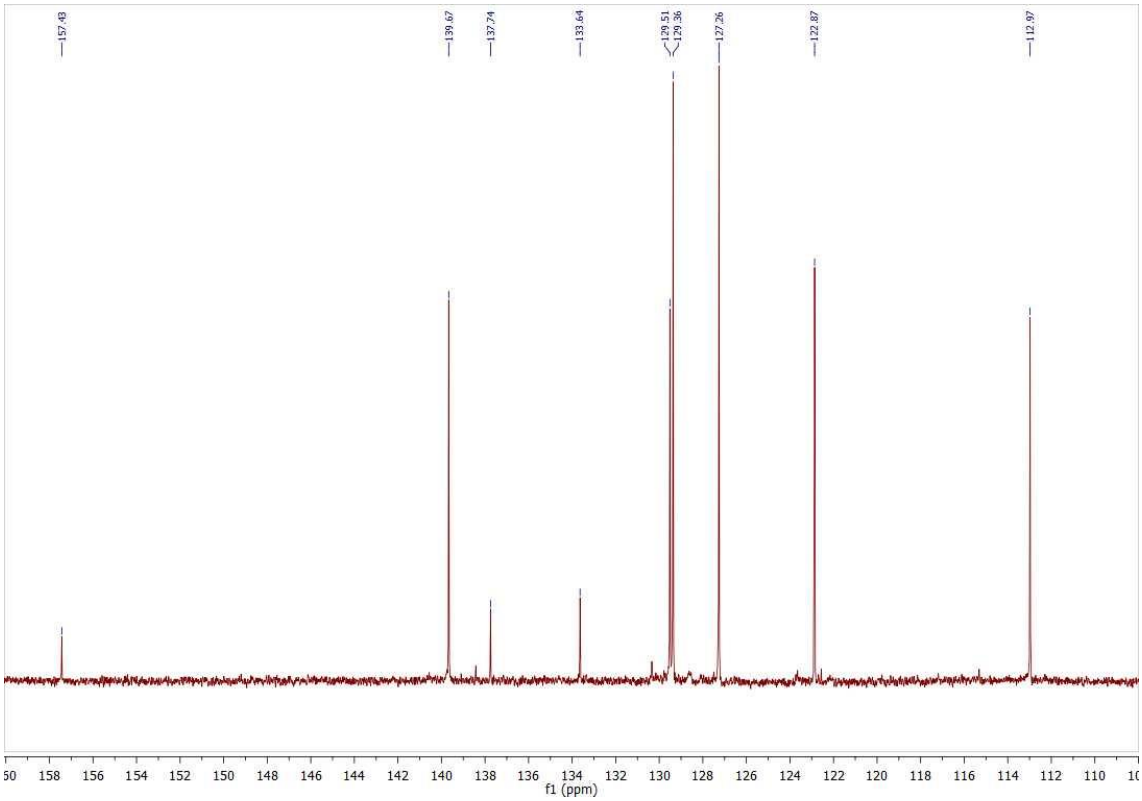
^{1}H-NMR (400 MHz, $CDCl_3$). 1-Iodo-2-((4-methylbenzyl)oxy)benzene (**5p**).



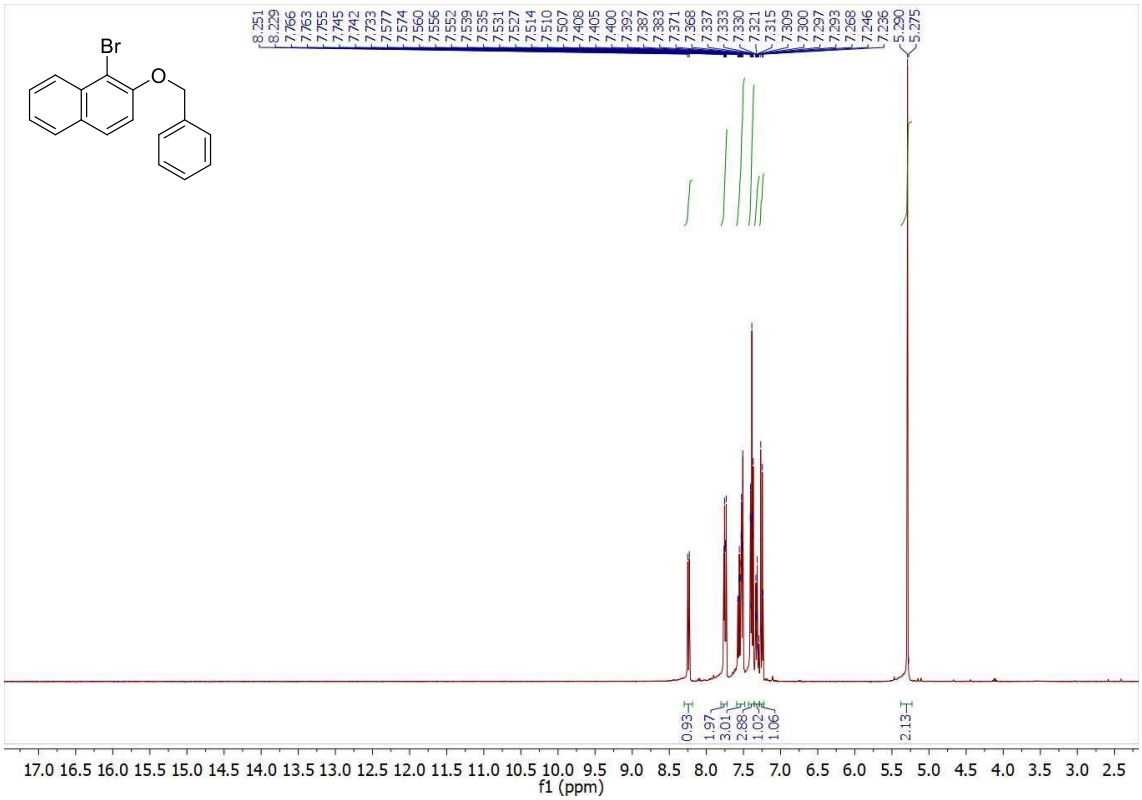


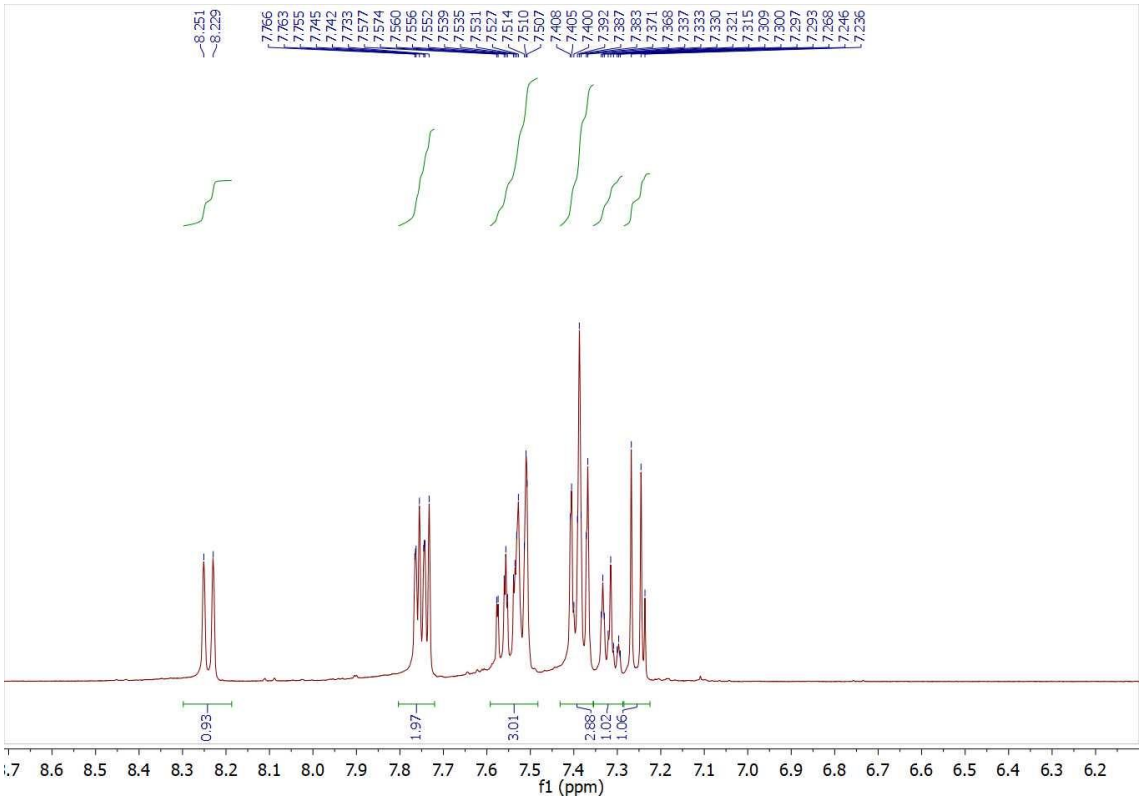
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-Iodo-2-((4-methylbenzyl)oxy)benzene (**5p**).



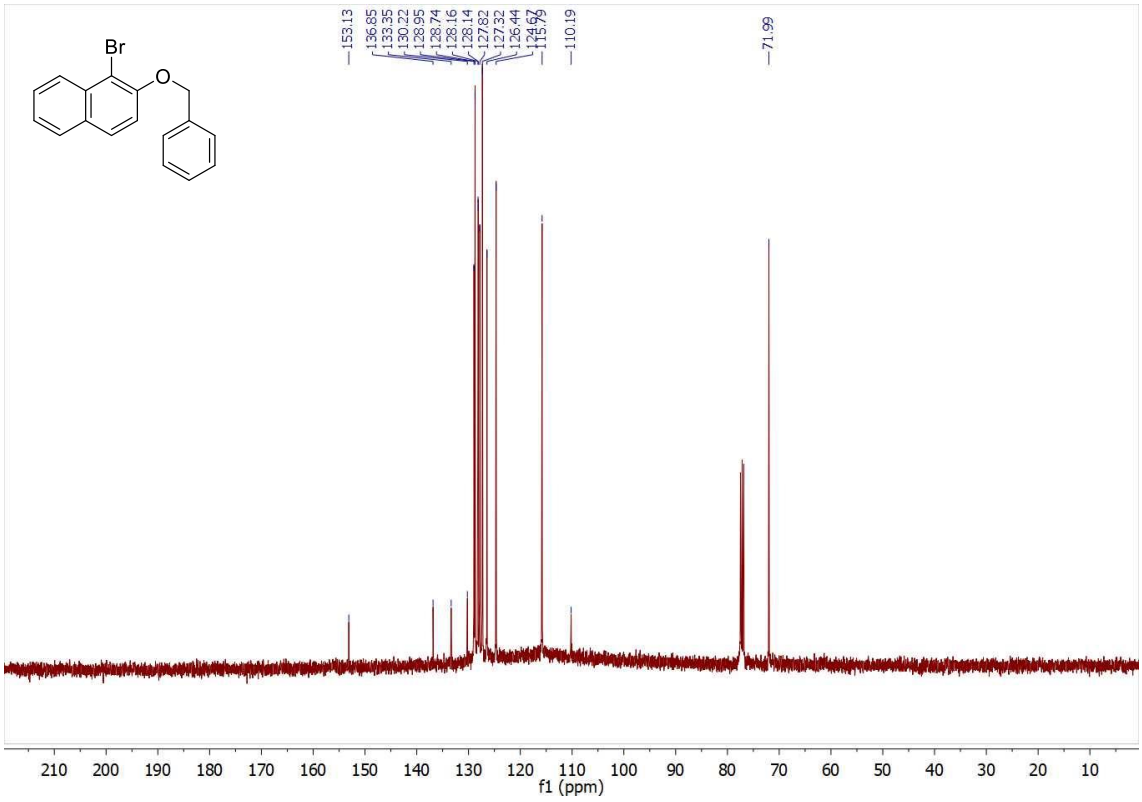


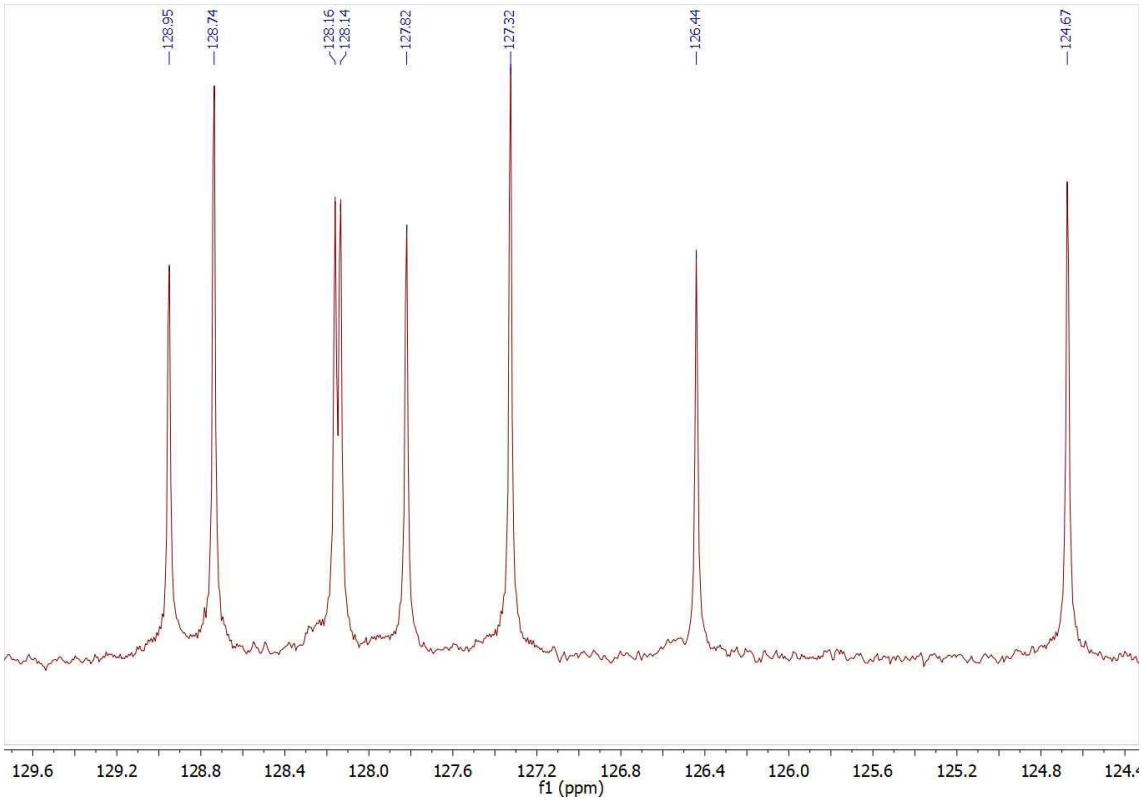
^{1}H-NMR (400 MHz, $CDCl_3$). (2-Benzyloxy)-1-bromonaphthalene (**5q**)



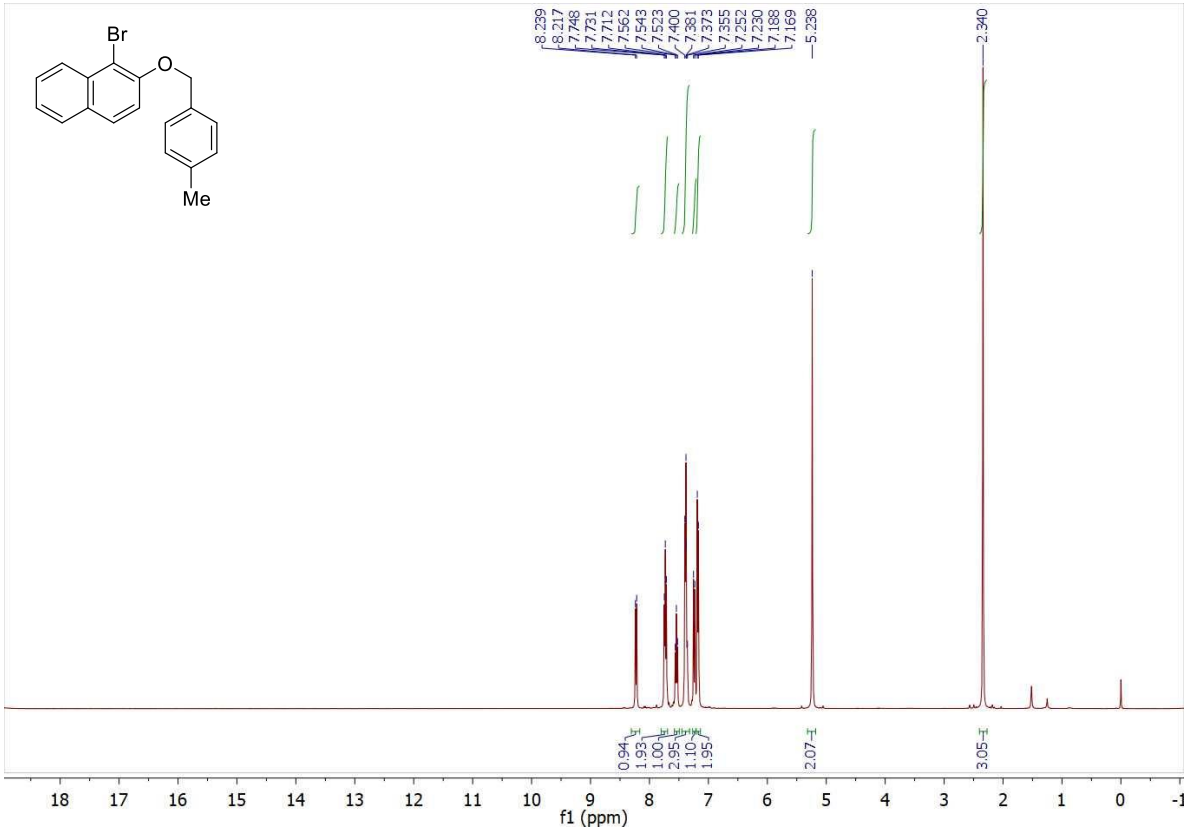


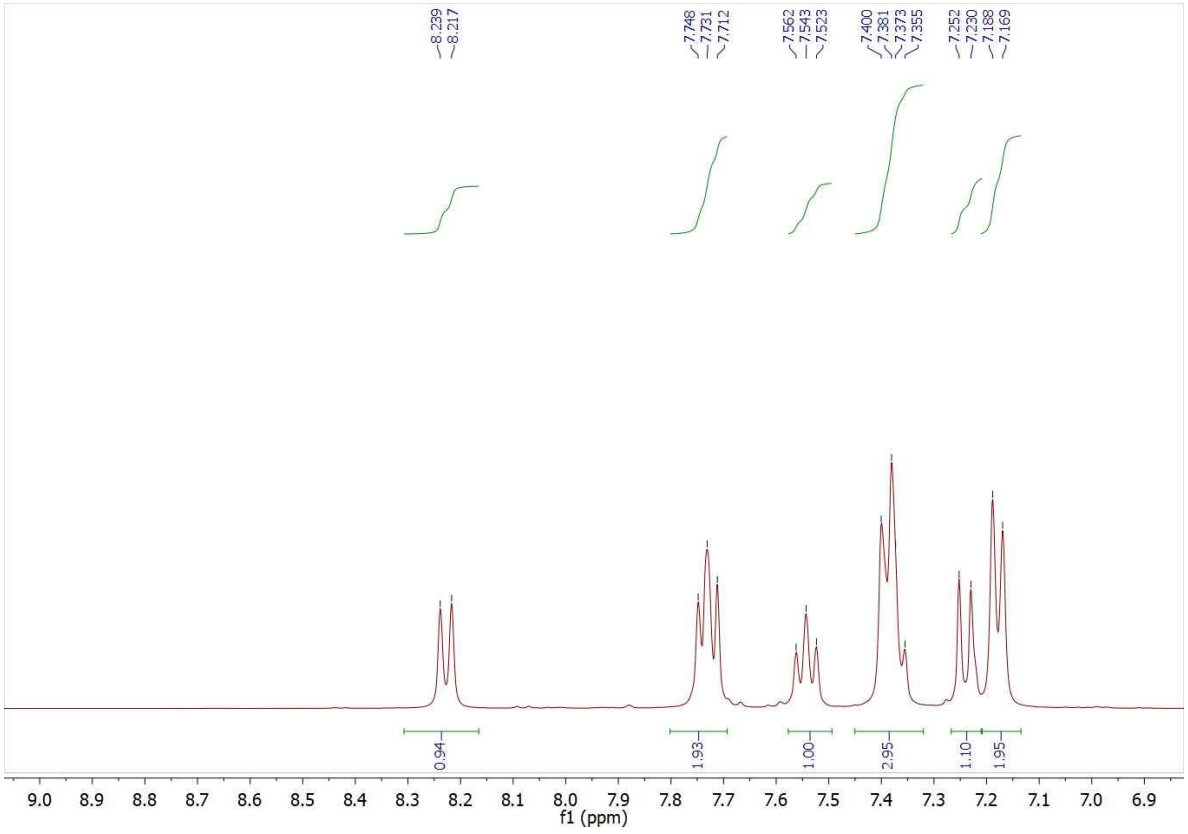
^{13}C NMR{1H} (101 MHz, $CDCl_3$). (2-Benzyloxy)-1-bromonaphthalene (**5q**)



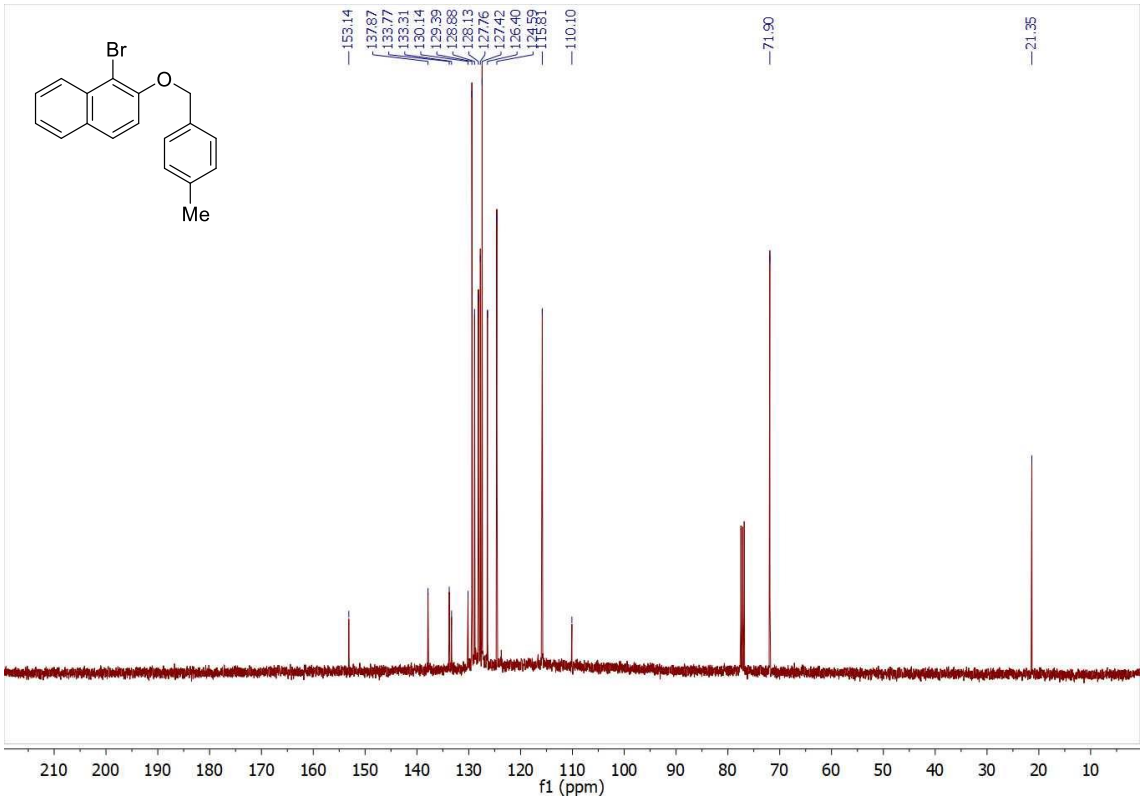


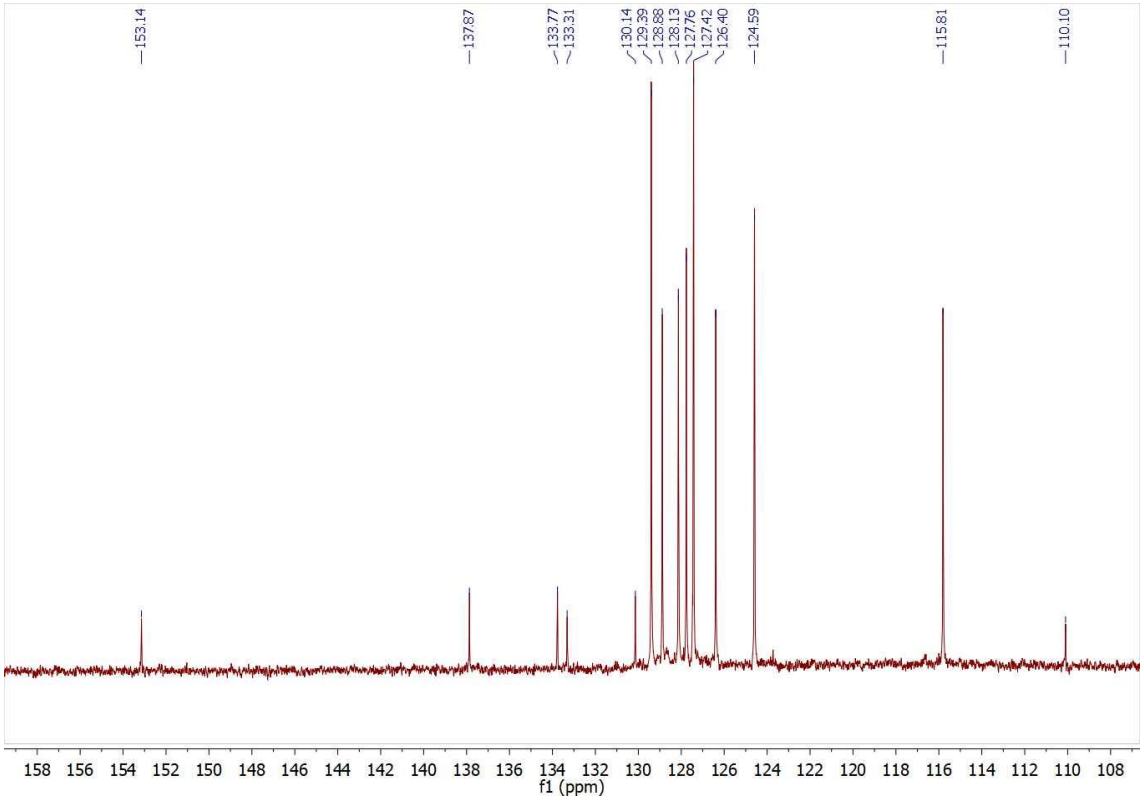
^{1}H-NMR (400 MHz, $CDCl_3$). 1-Bromo-2-((4-methylbenzyl)oxy)naphtalene (**5r**)



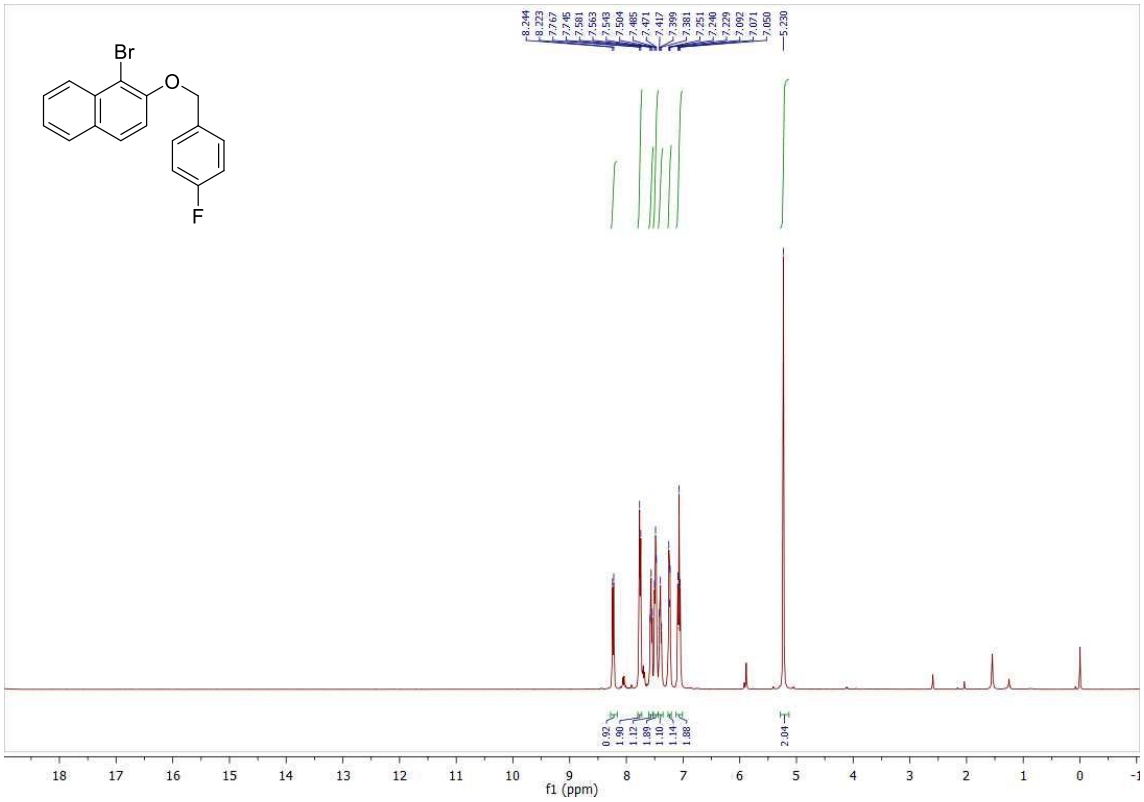


^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-Bromo-2-((4-methylbenzyl)oxy)naphtalene (**5r**)

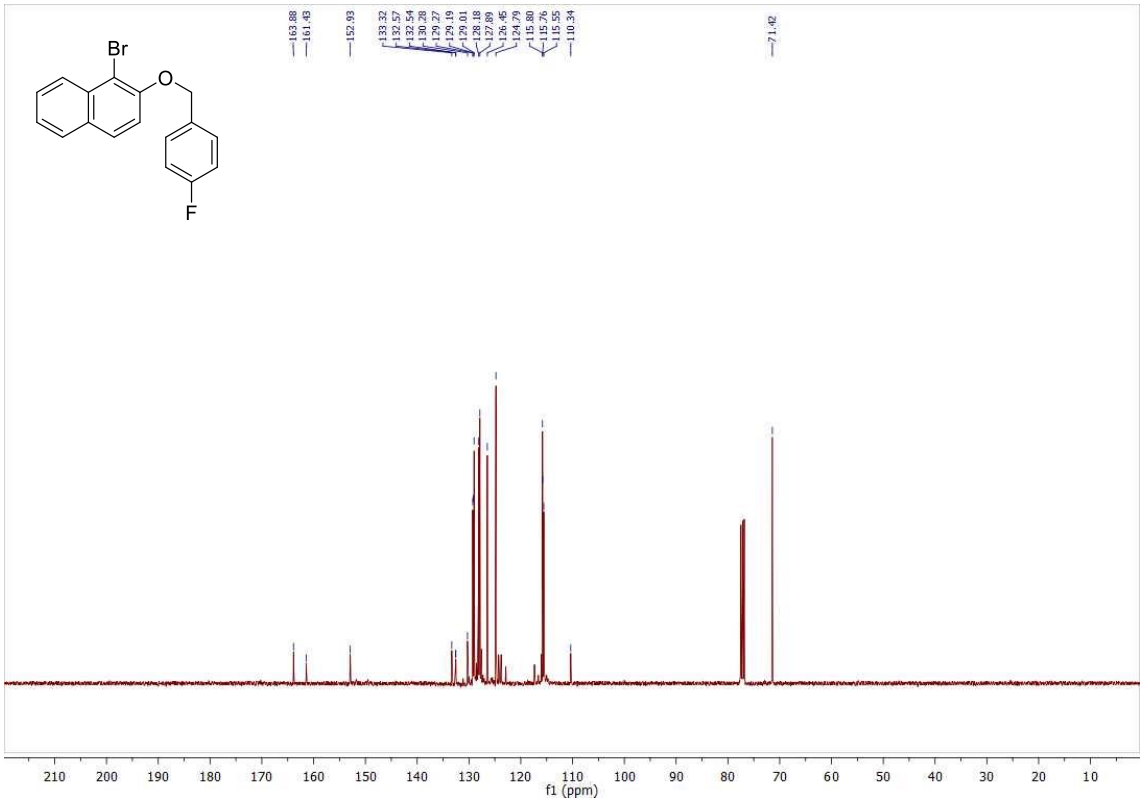




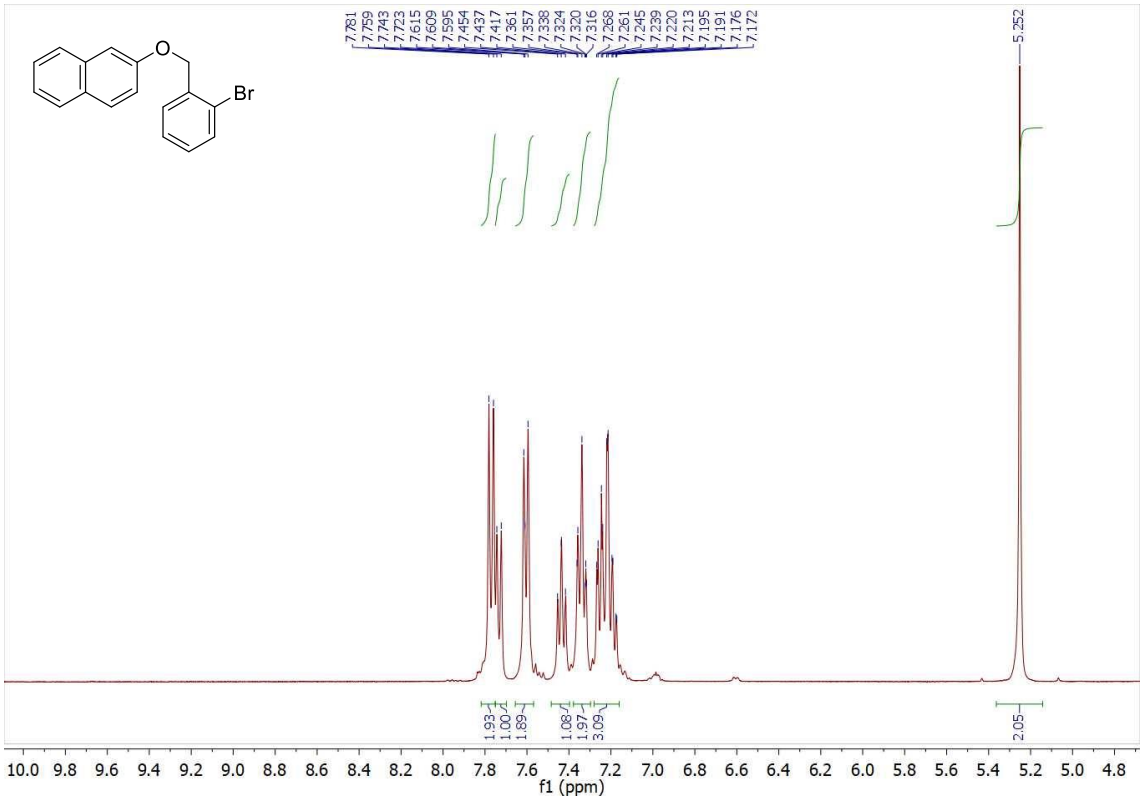
^{1}H-NMR (400 MHz, $CDCl_3$). 1-Bromo-2-((4-fluorobenzyl)oxy)naphtalene (**5s**).

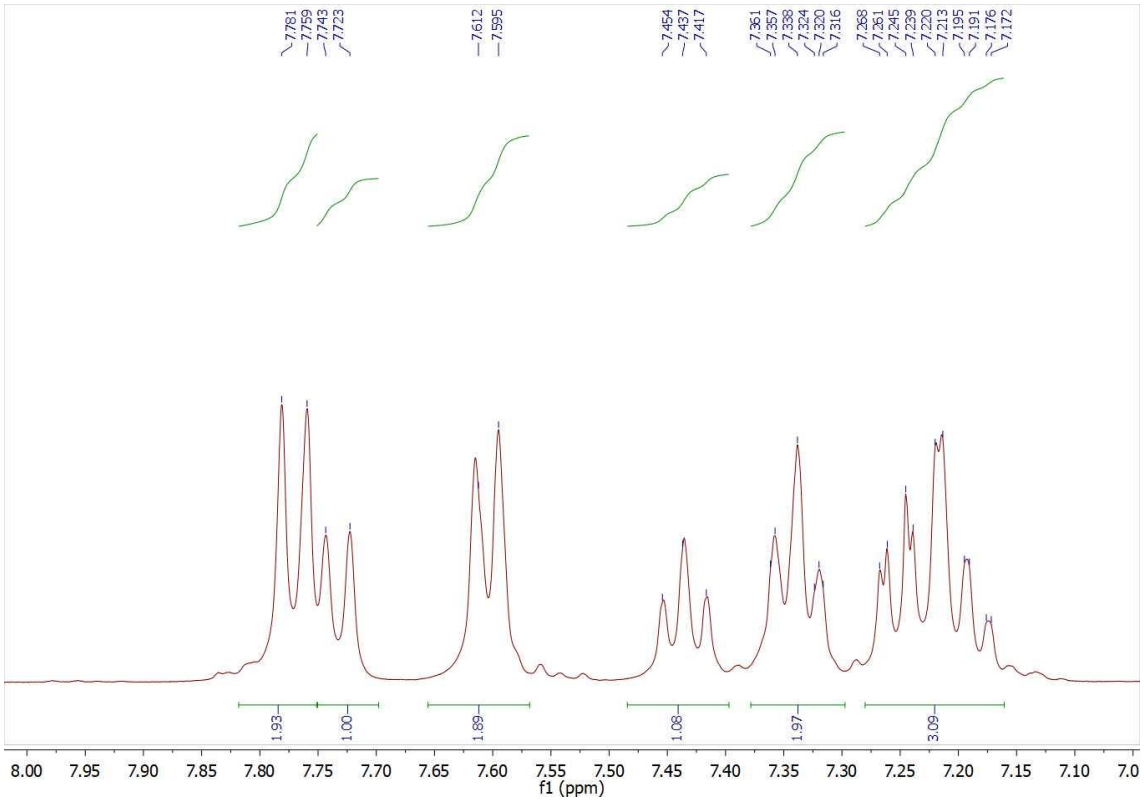


^{13}C NMR{1H} (101 MHz, $CDCl_3$). 1-Bromo-2-((4-fluorobenzyl)oxy)naphtalene (**5s**).

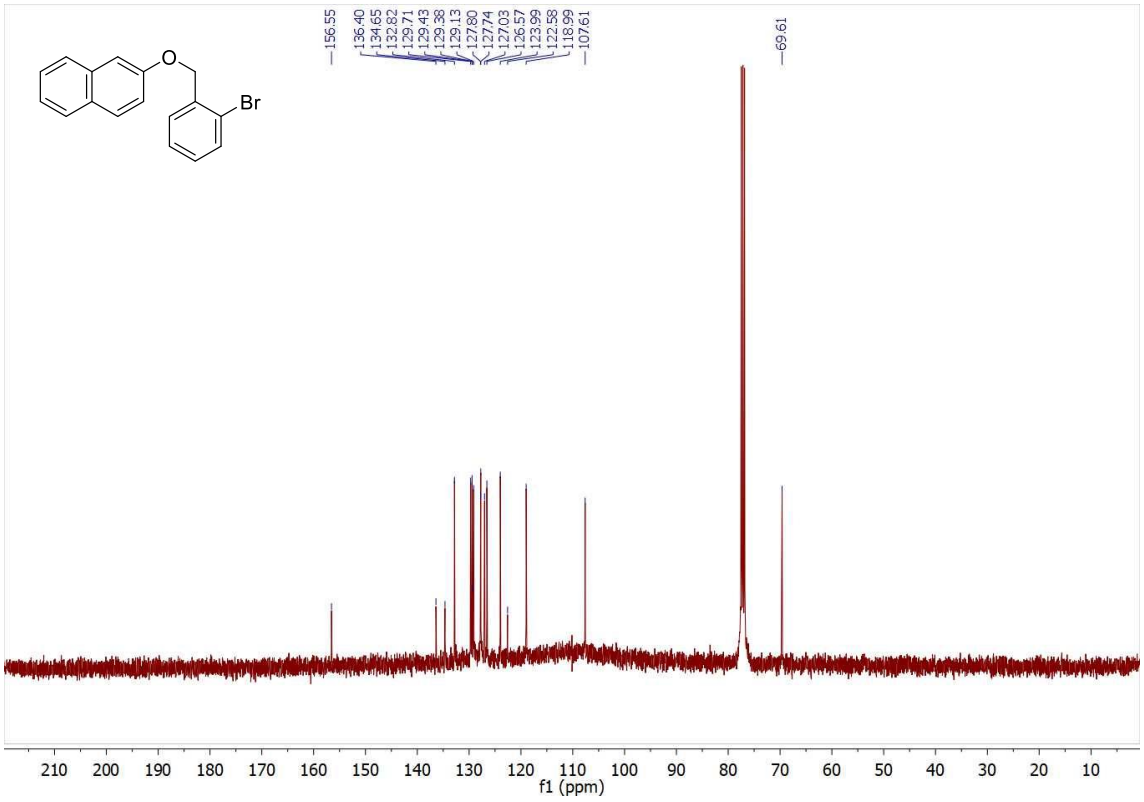


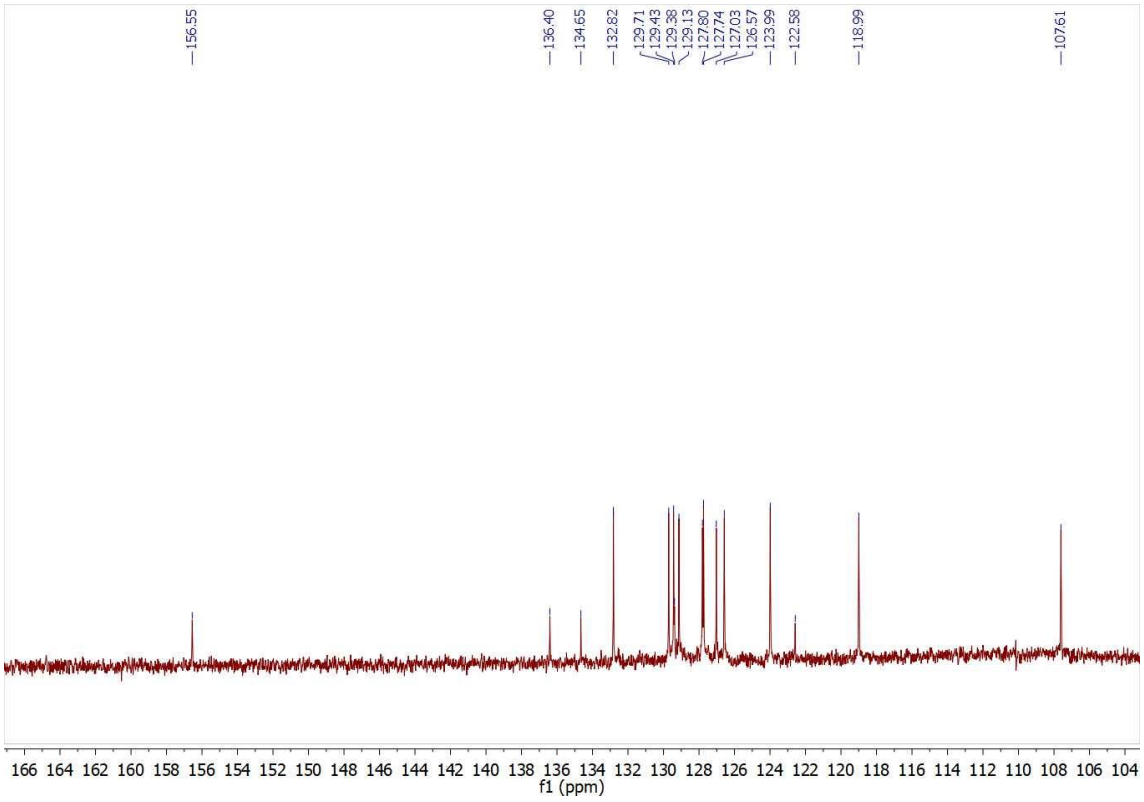
^{1}H-NMR (400 MHz, $CDCl_3$). 2-((2-Bromobenzyl)oxy)naphtalene (**5t**)



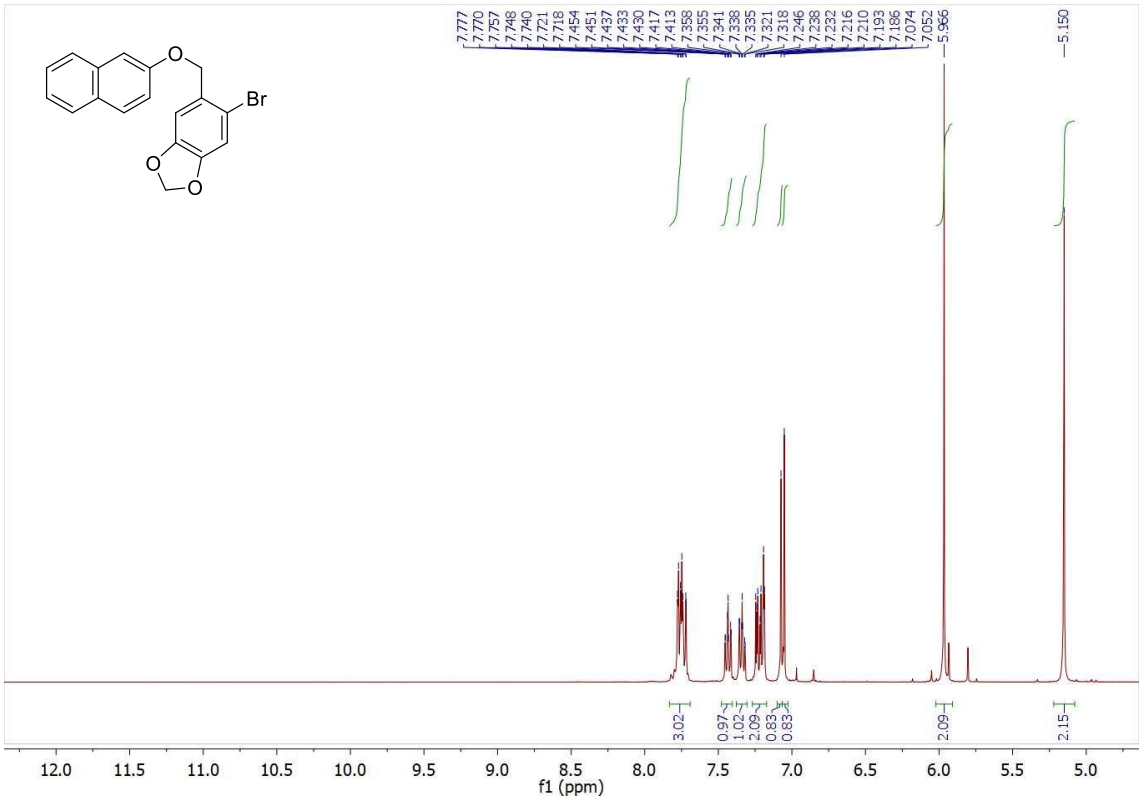


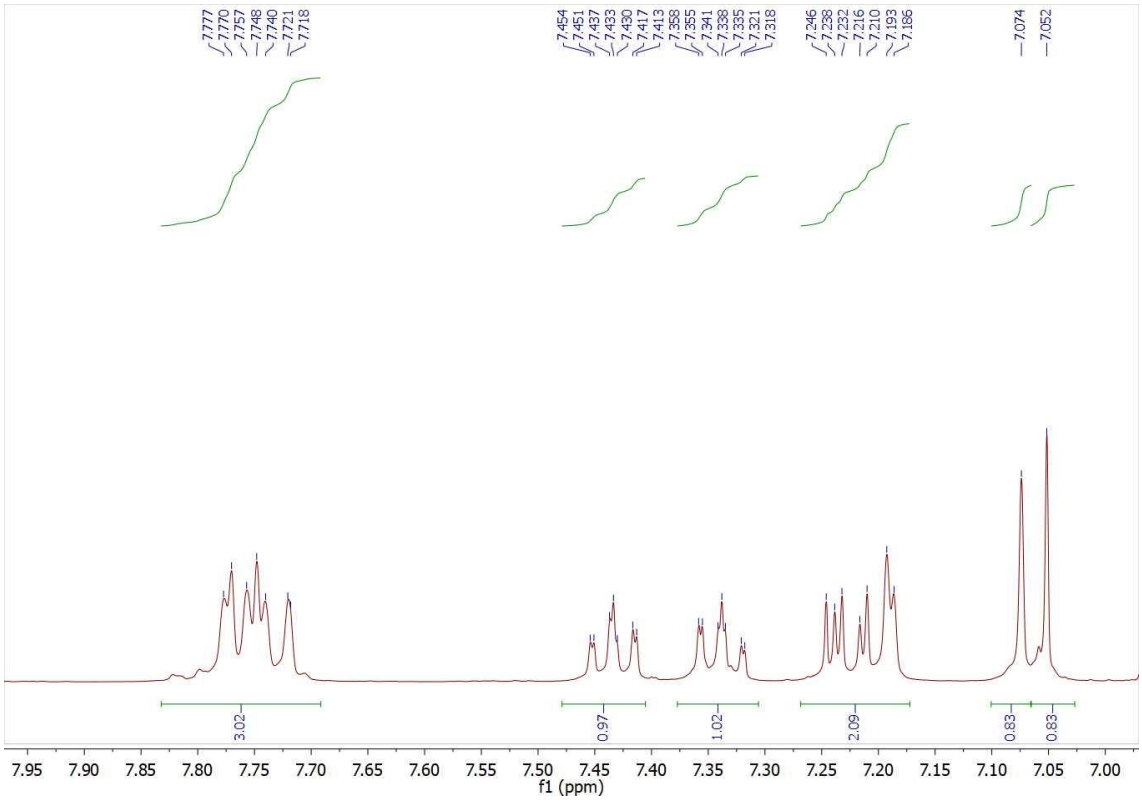
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 2-((2-Bromobenzyl)oxy)naphtalene (**5t**)



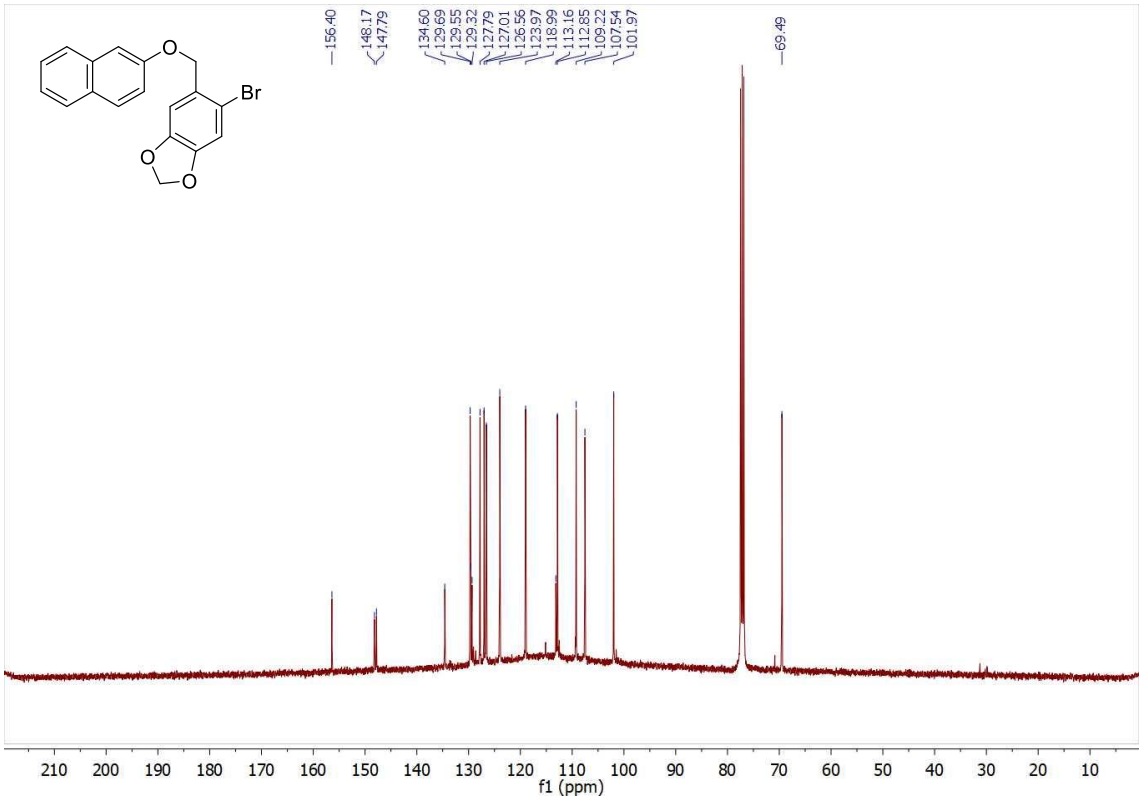


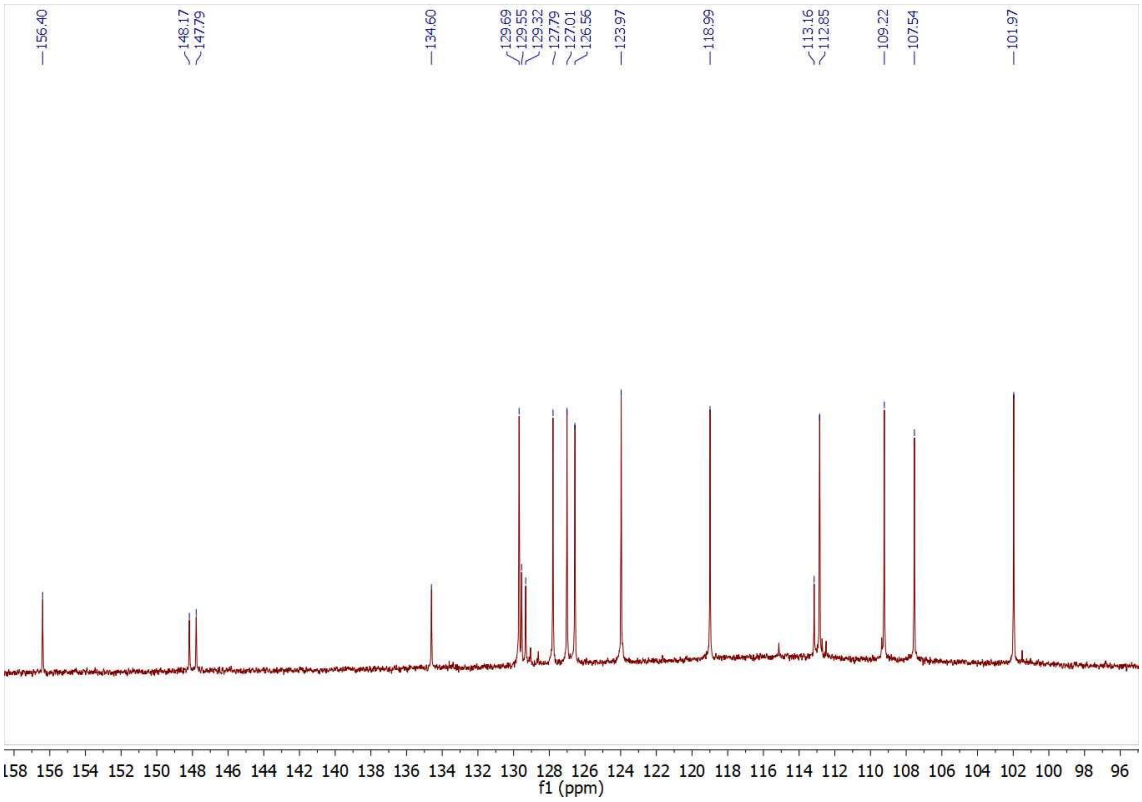
^{1}H-NMR (400 MHz, $CDCl_3$). 5-Bromo-6-((naphtalen-2-yloxy)methyl)benzo[d][1,3]dioxole (**5u**)





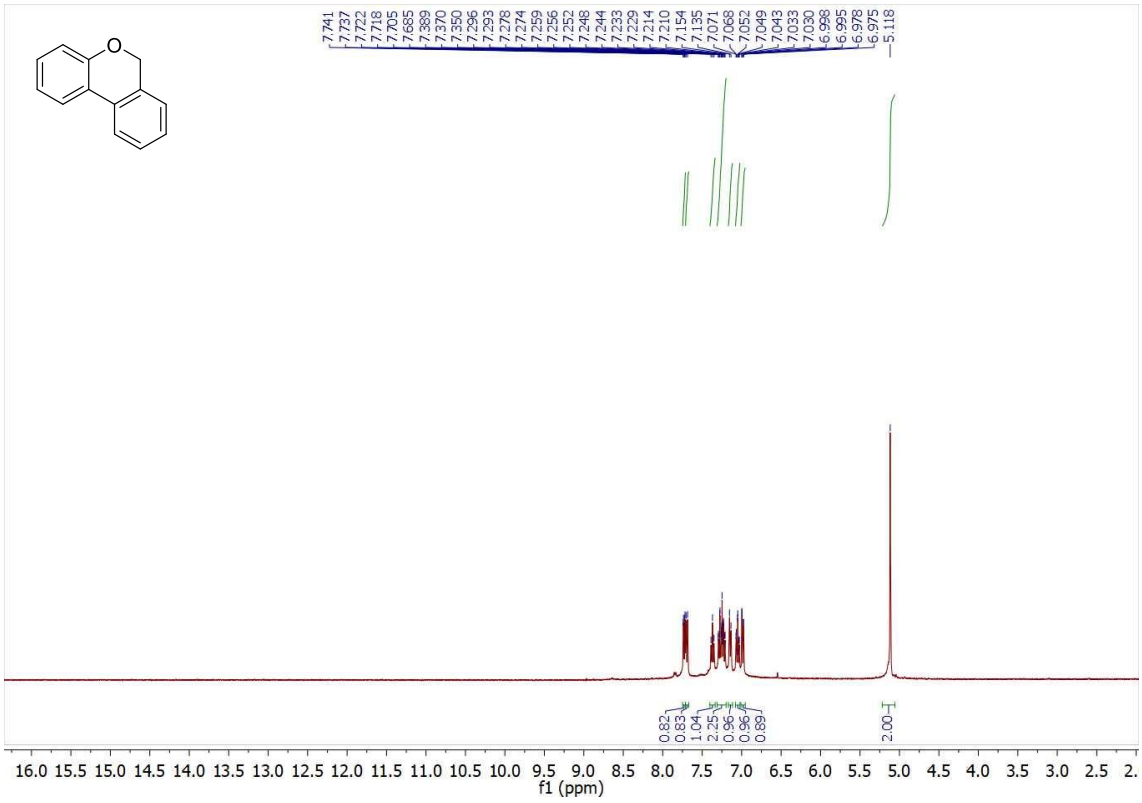
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 5-Bromo-6-((naphtalen-2-yloxy)methyl)benzo[d][1,3]dioxole (**5u**)

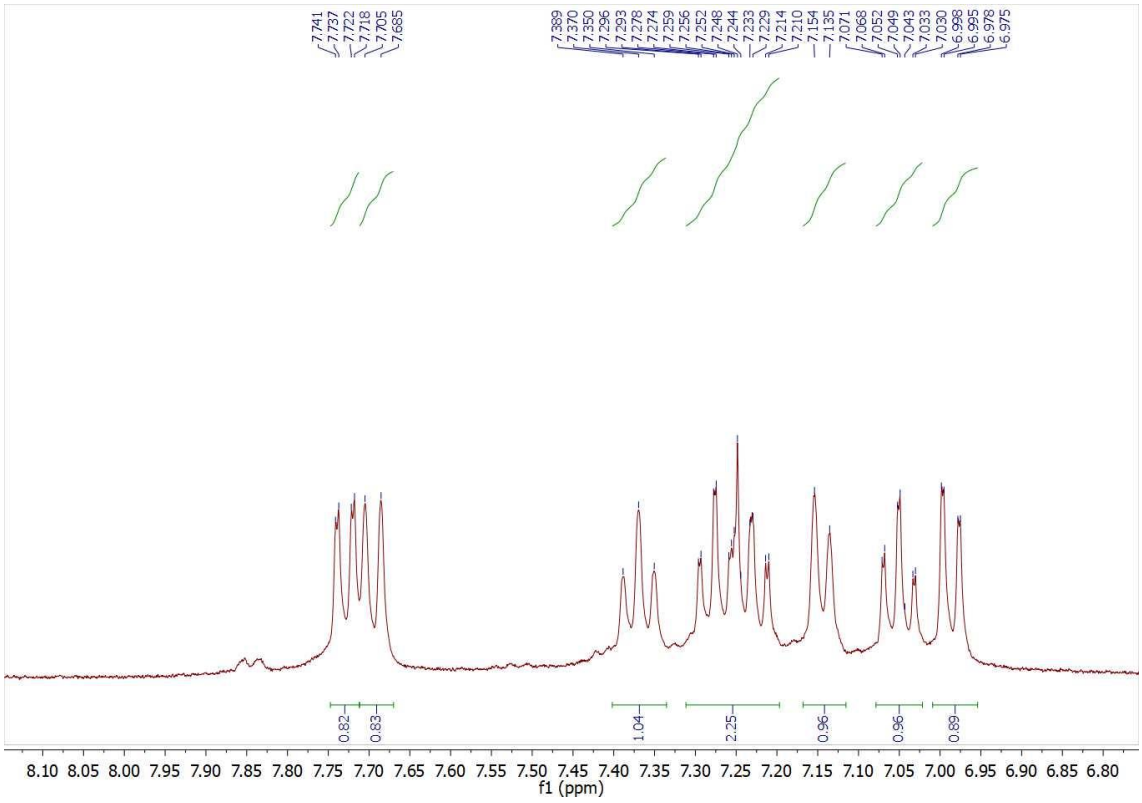




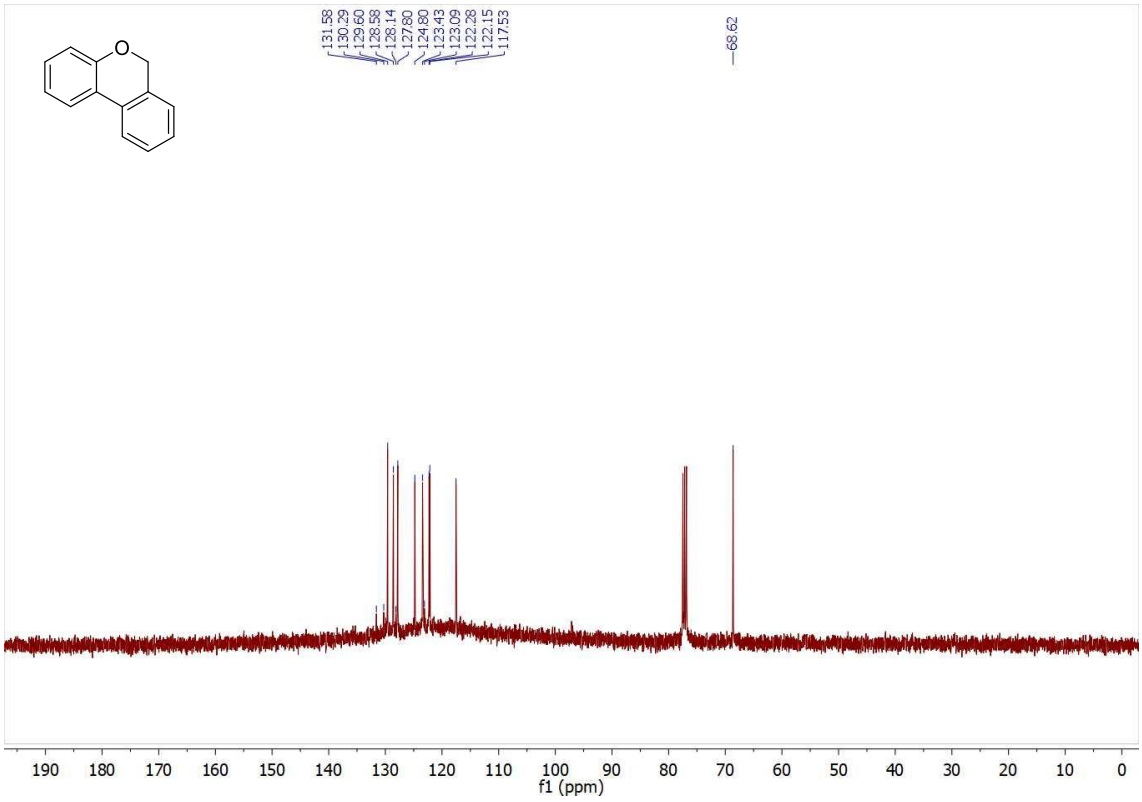
8. NMR spectra of compounds 1a-u

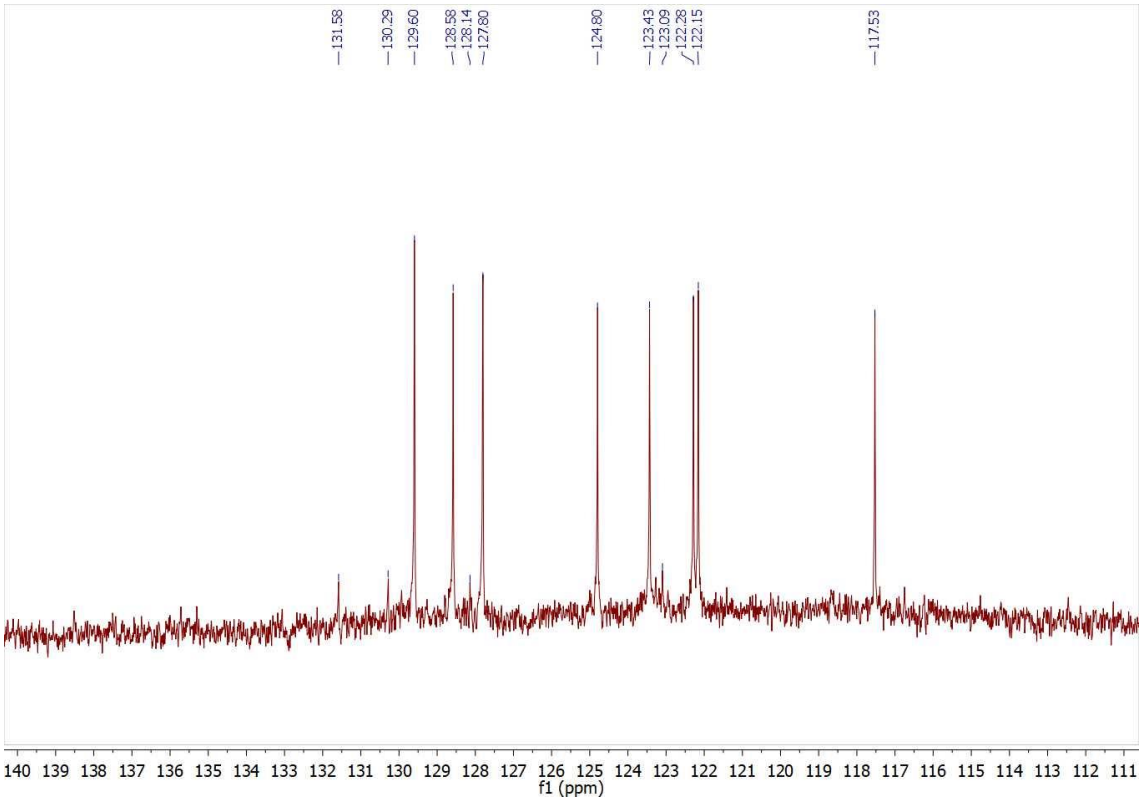
^{1}H-NMR (400 MHz, $CDCl_3$). 6*H*-Benzo[*c*]chromene (**1a**)



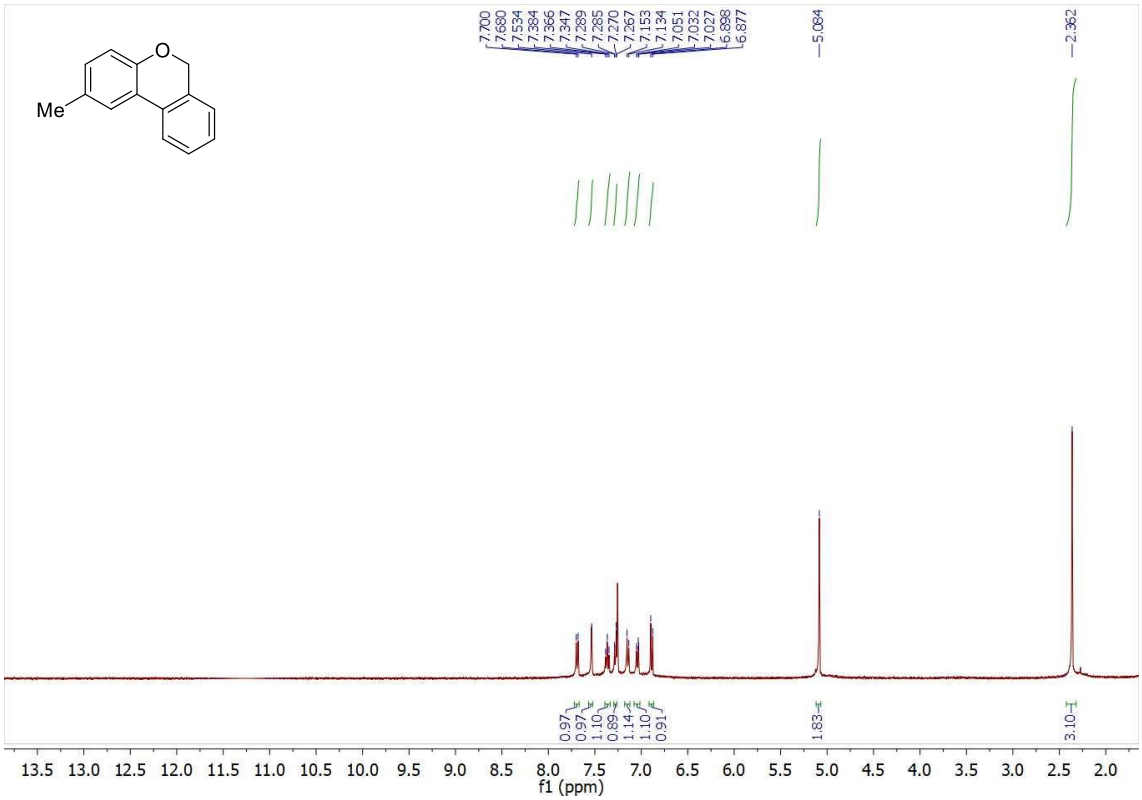


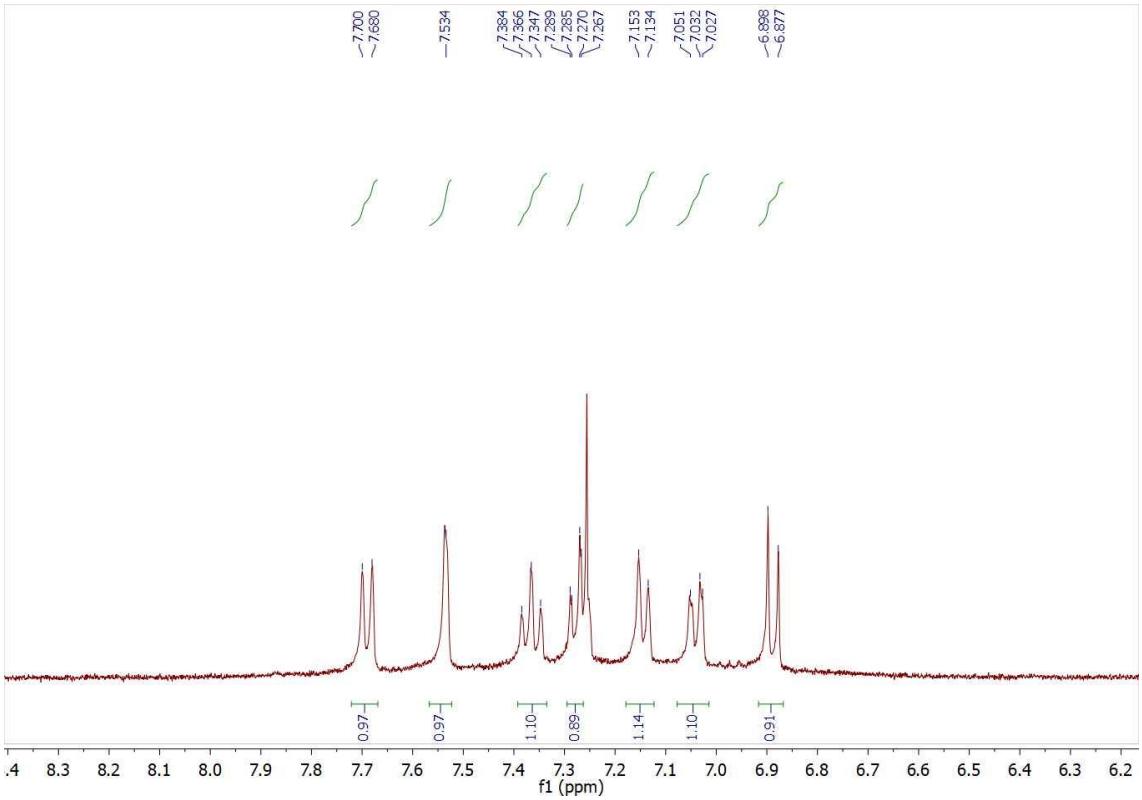
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 6*H*-Benzo[*c*]chromene (**1a**)



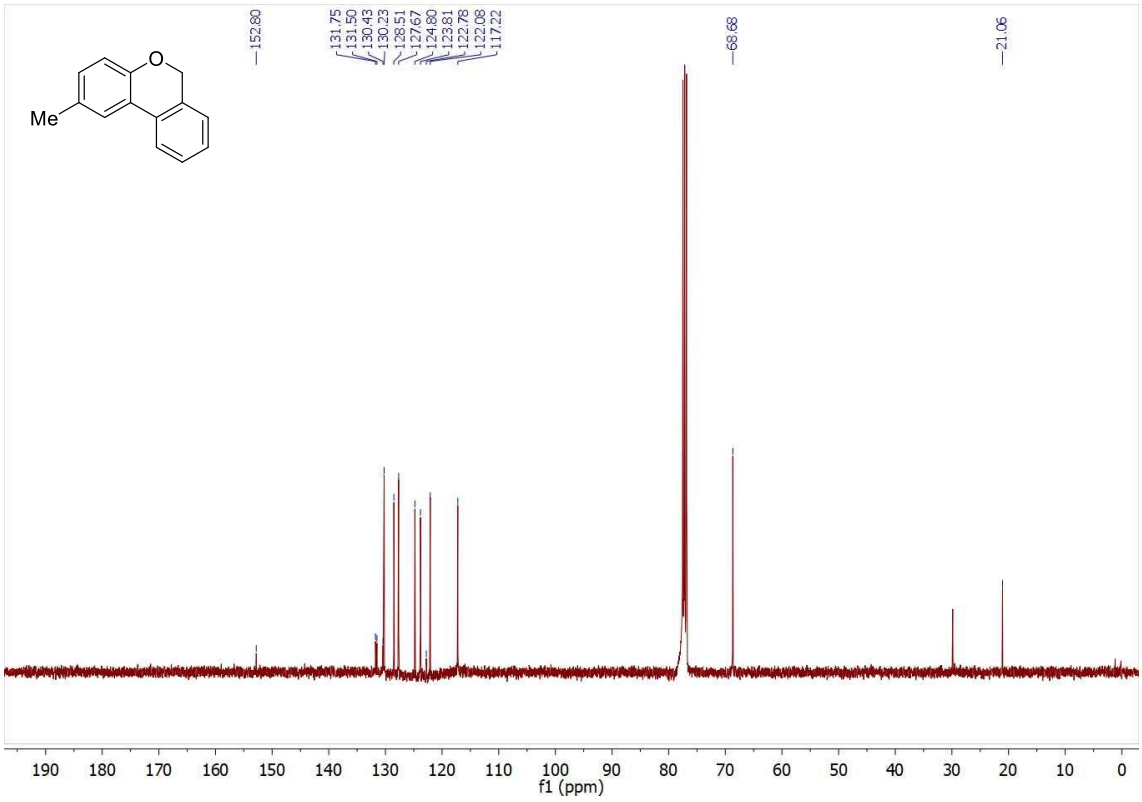


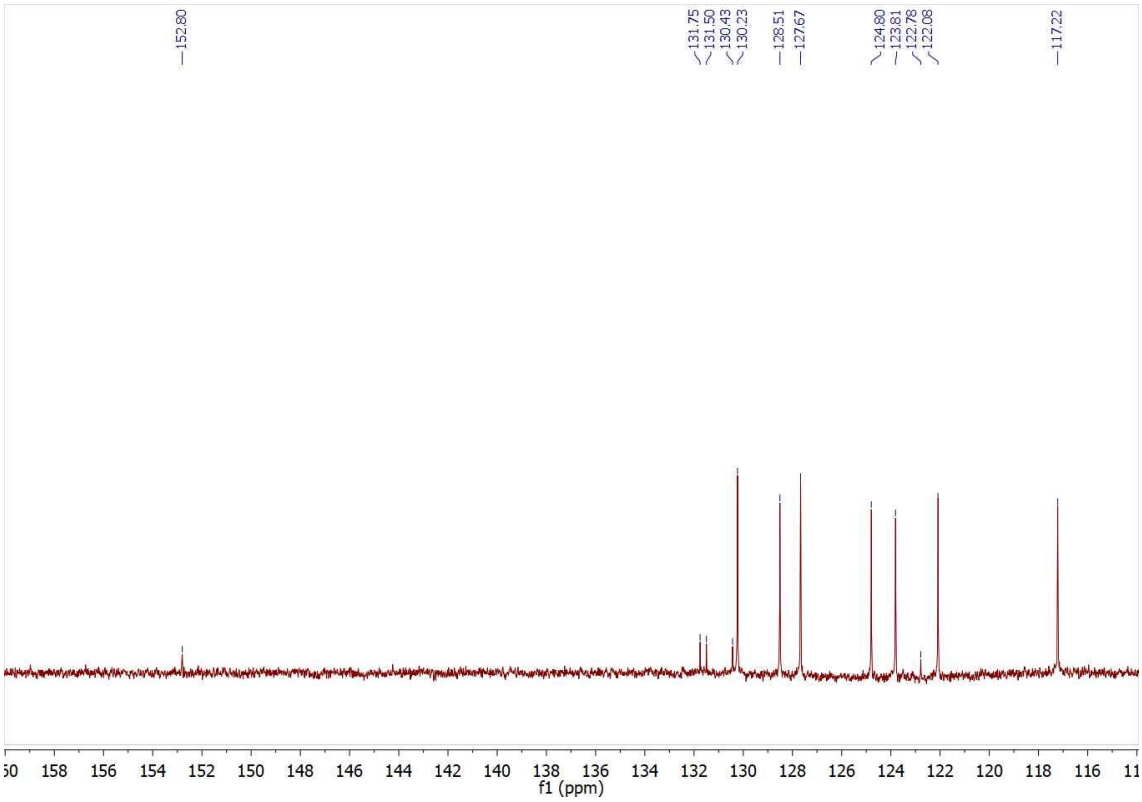
^{1}H-NMR (400 MHz, $CDCl_3$). 2-Methyl-6*H*-benzo[*c*]chromene (**1c**)



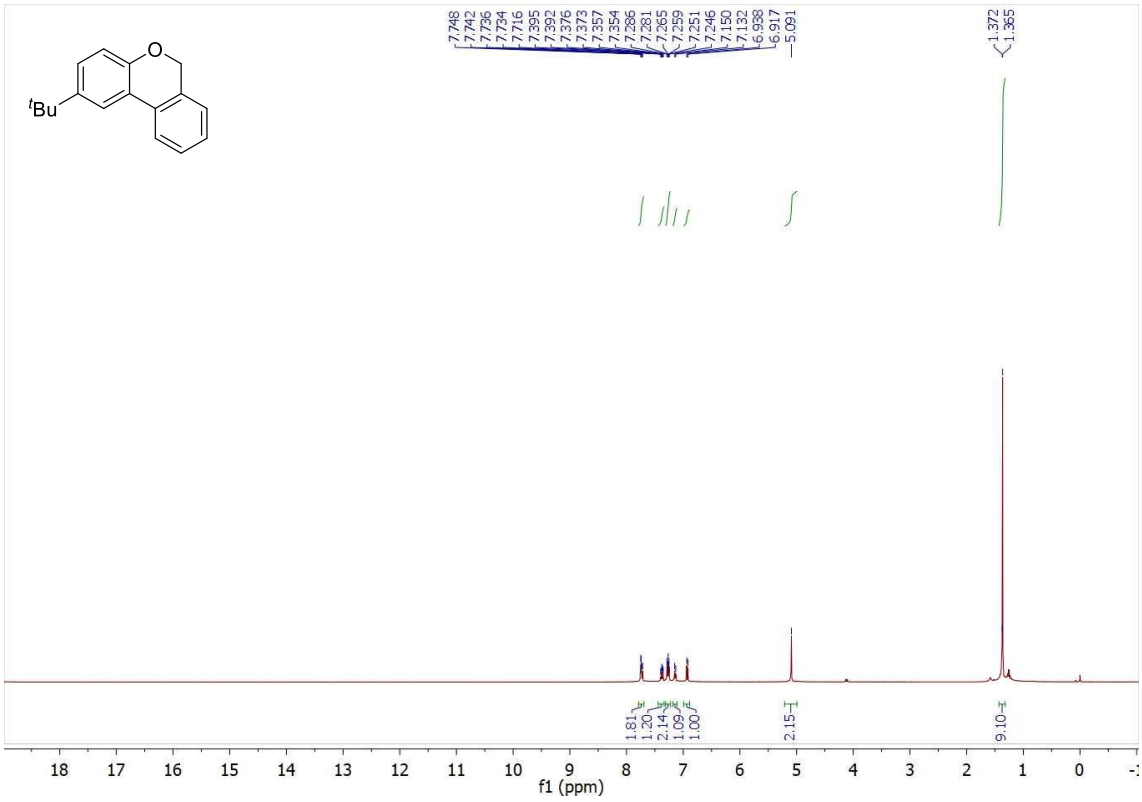


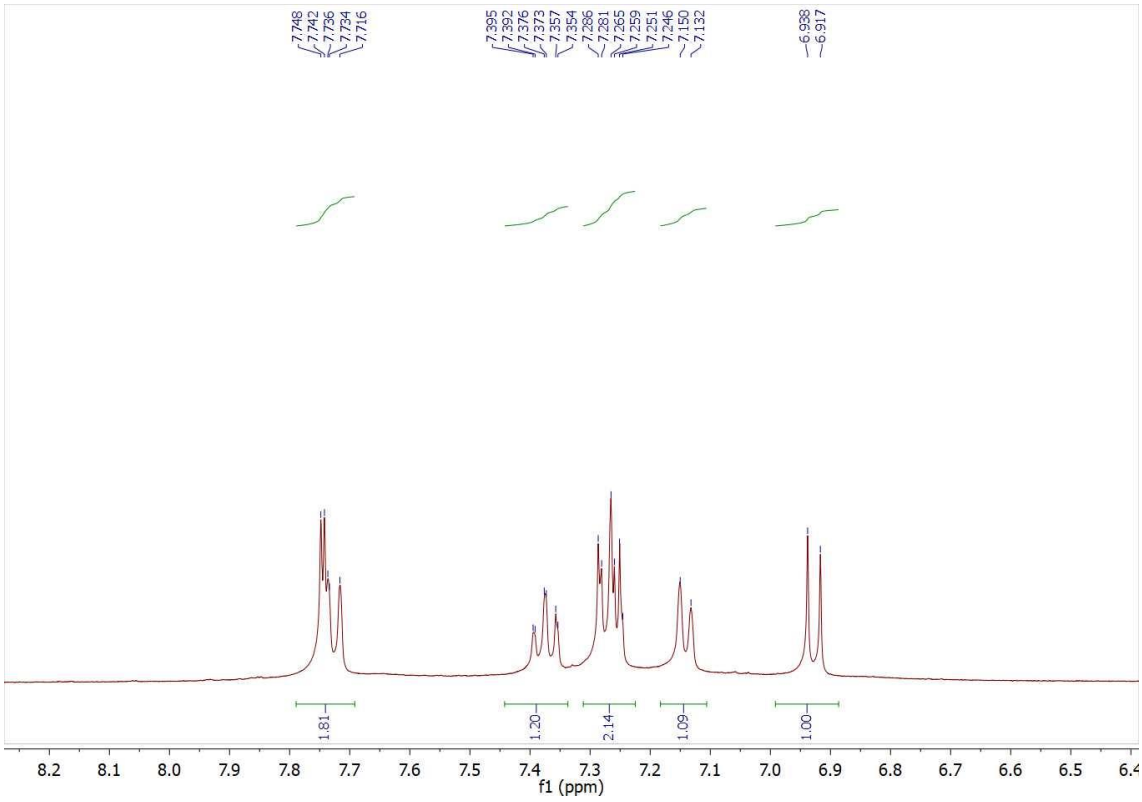
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 2-Methyl-6*H*-benzo[*c*]chromene (**1c**)



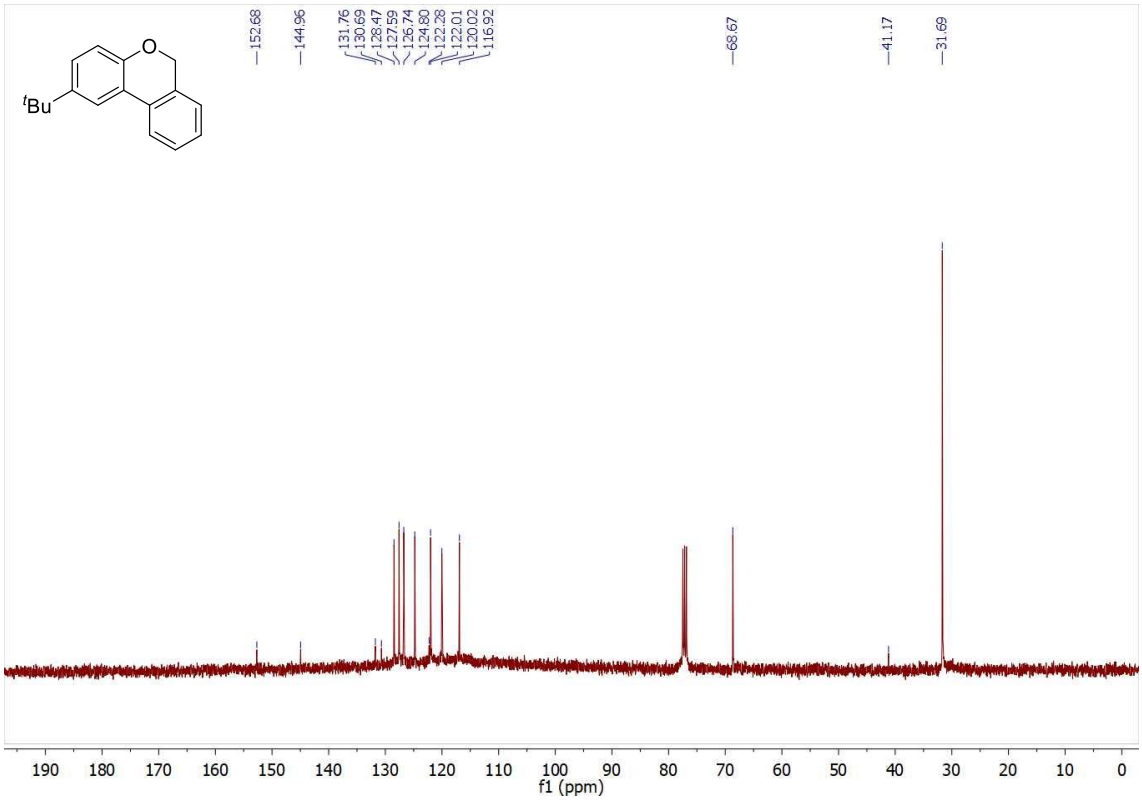


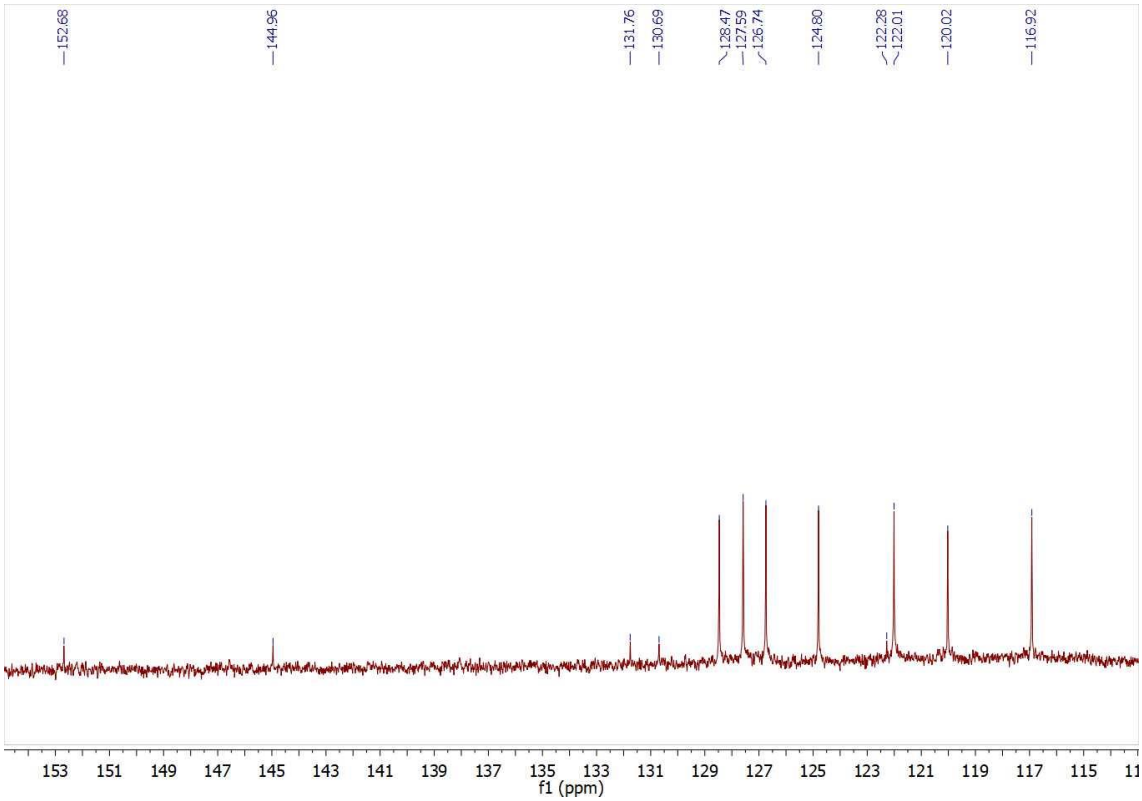
^{1}H-NMR (400 MHz, $CDCl_3$). 2-(*tert*-Butyl)-6*H*-benzo[*c*]chromene (**1d**)



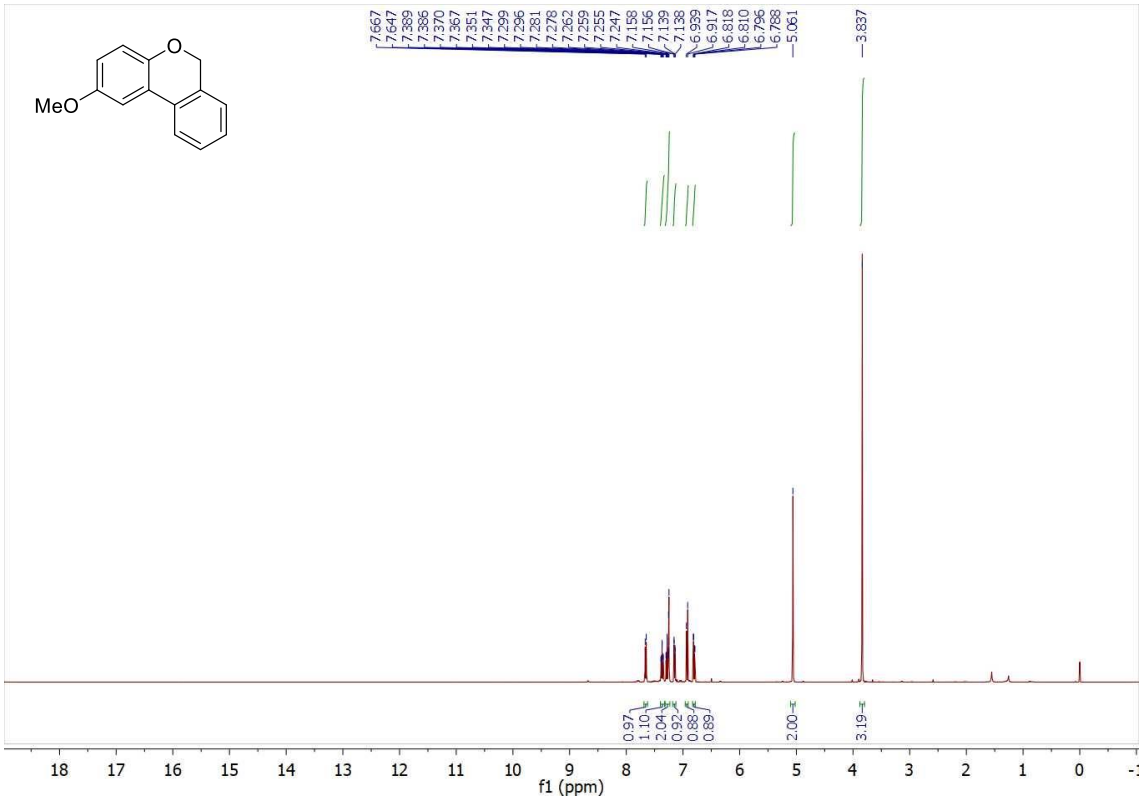


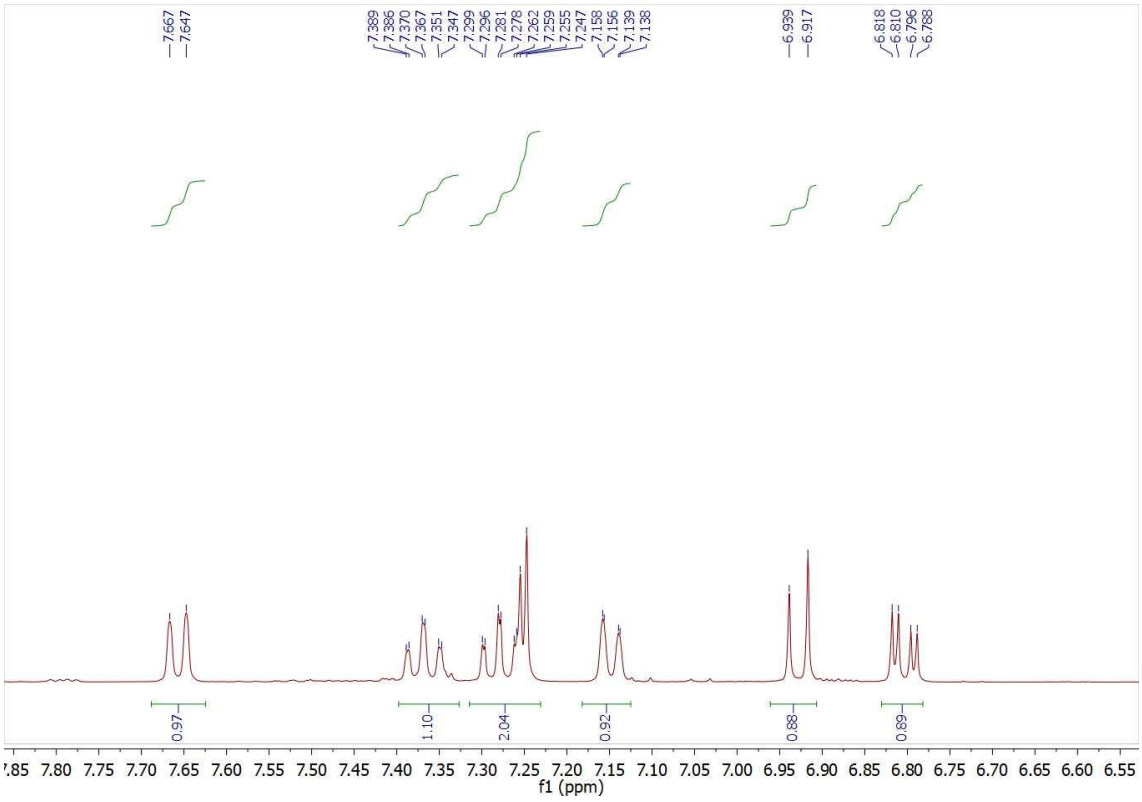
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 2-(*tert*-Butyl)-6*H*-benzo[*c*]chromene (**1d**)



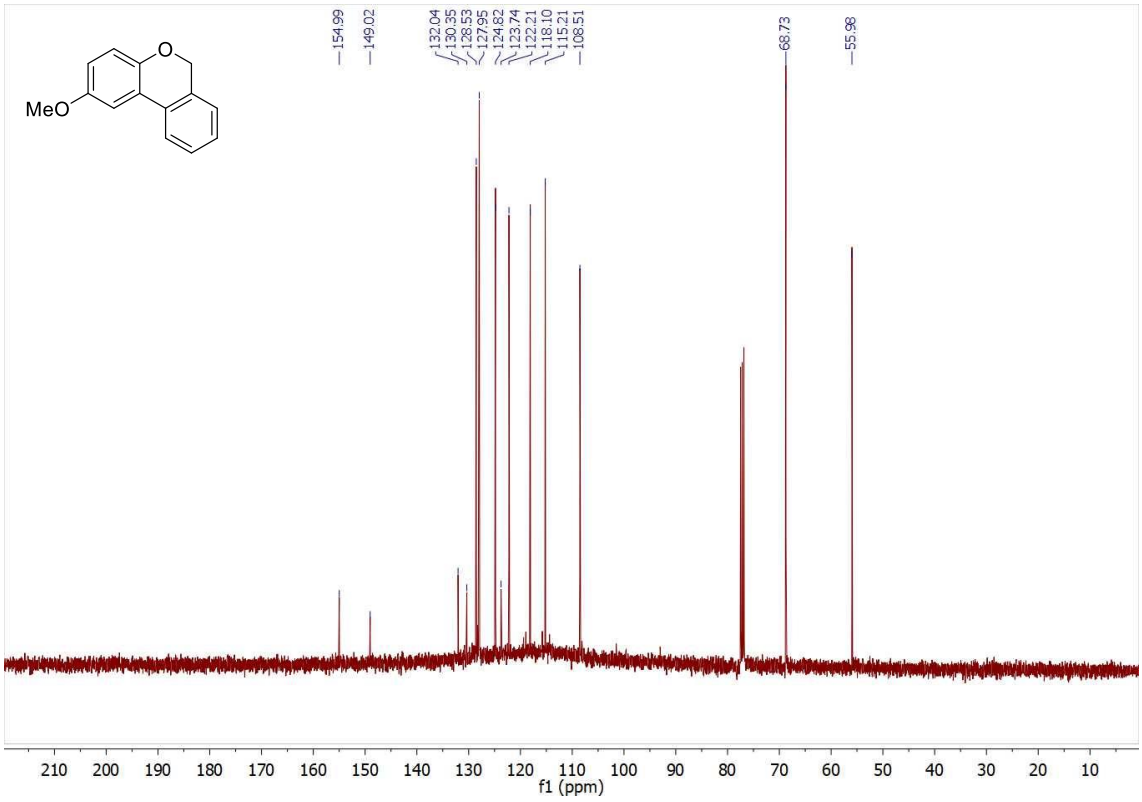


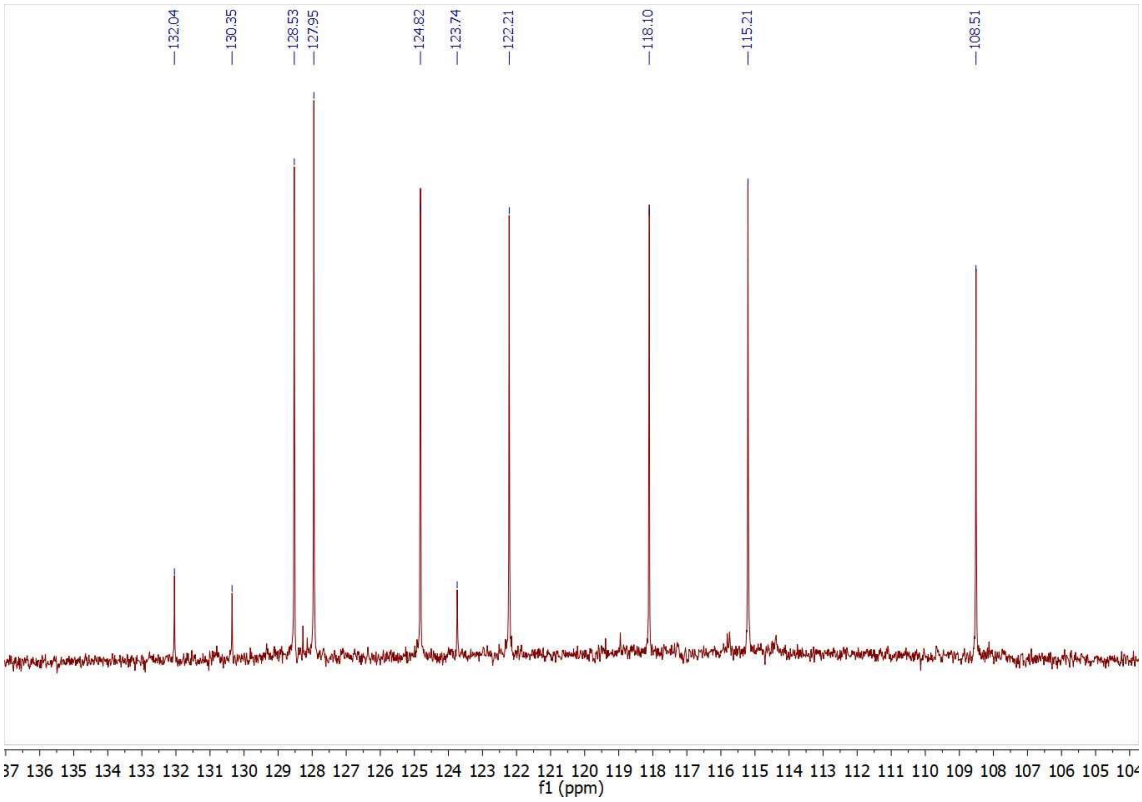
^{1}H-NMR (400 MHz, $CDCl_3$). 2-Methoxy-6*H*-benzo[*c*]chromene (**1e**)



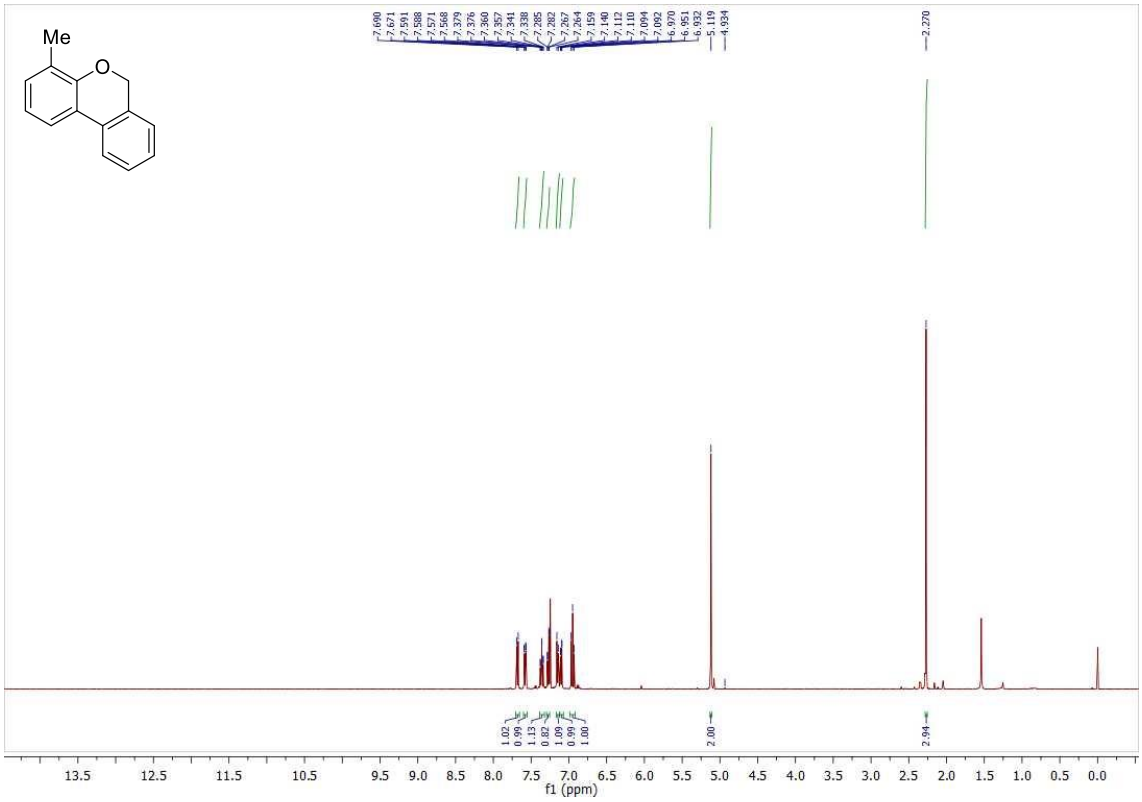


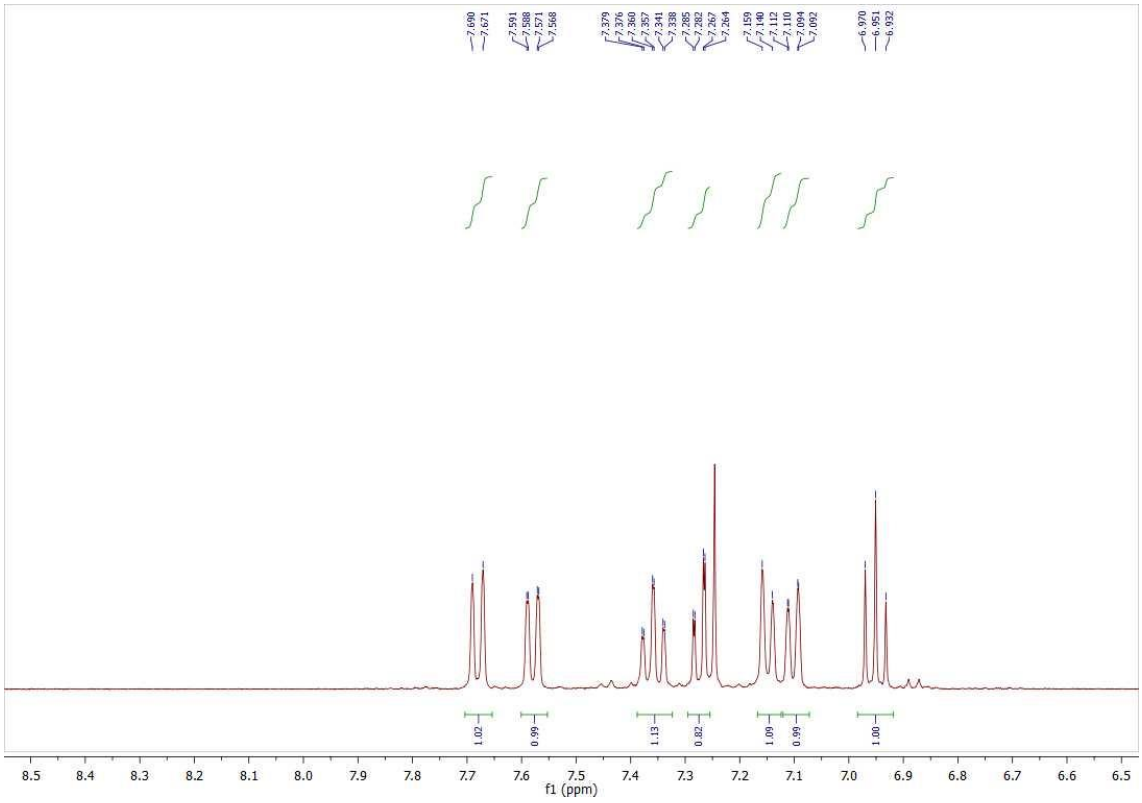
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 2-Methoxy-6*H*-benzo[*c*]chromene (**1e**)



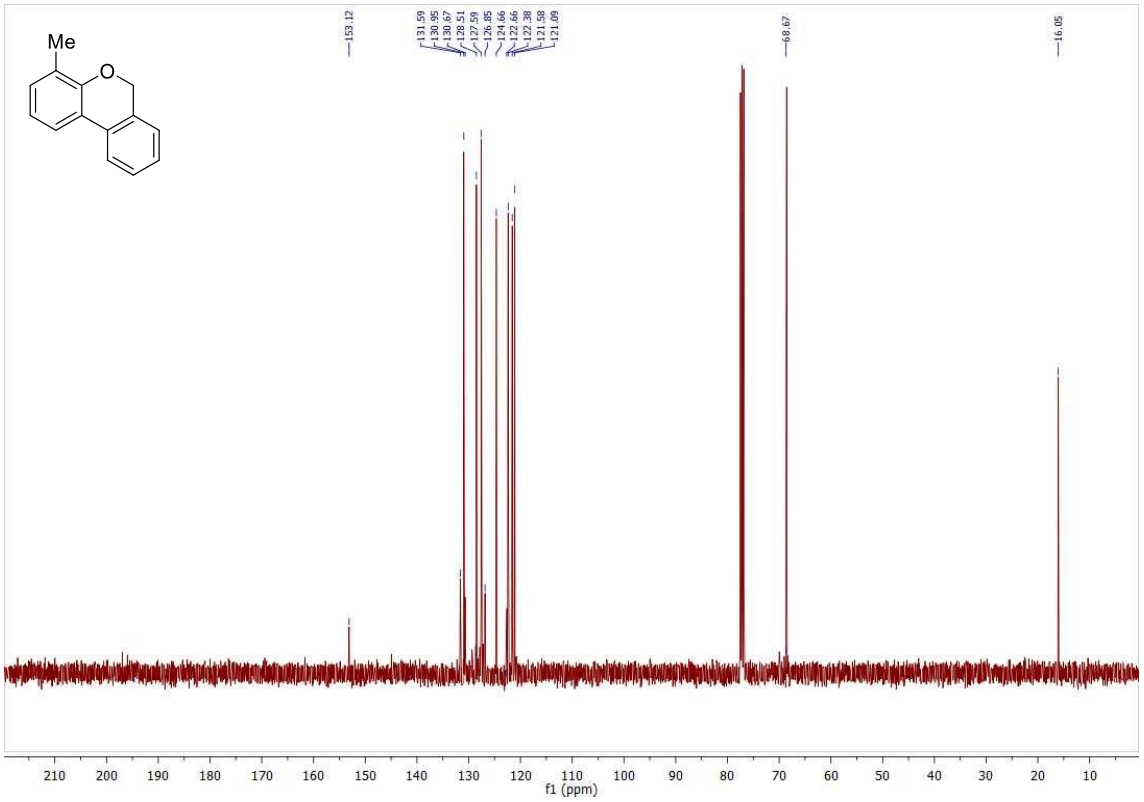


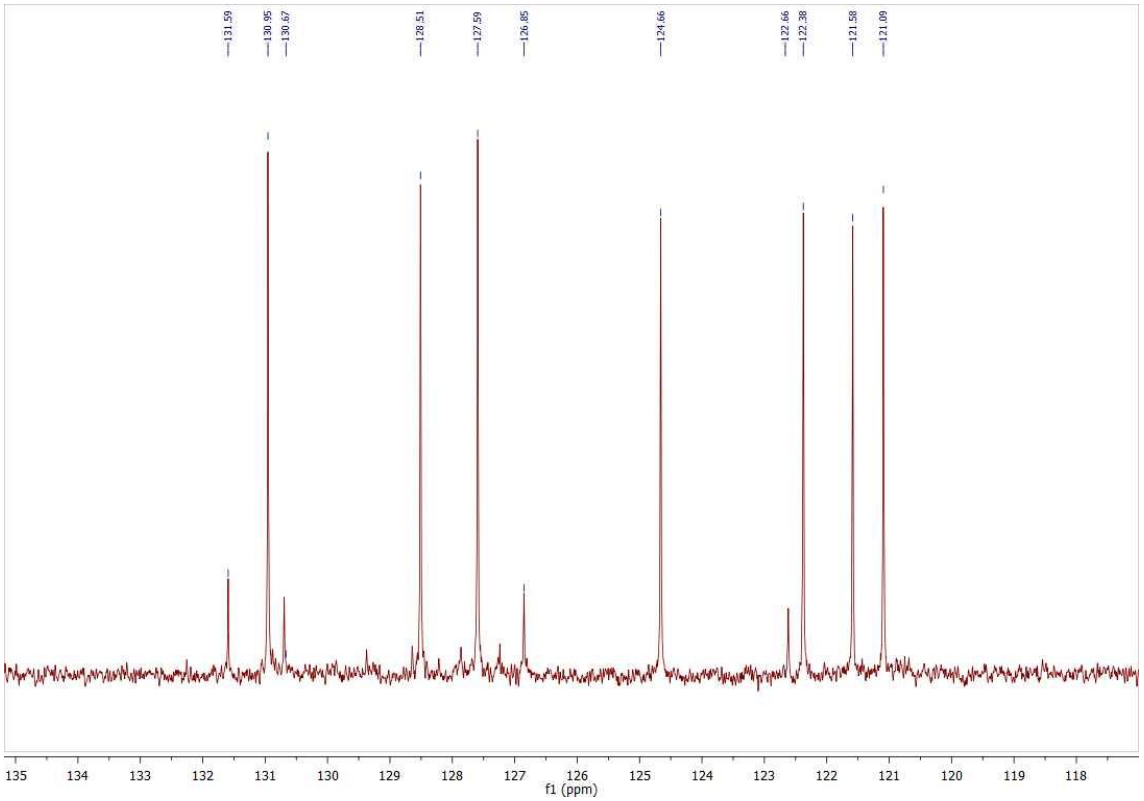
^{1}H-NMR (400 MHz, $CDCl_3$). 4-Methyl-6*H*-benzo[*c*]chromene (**1f**).



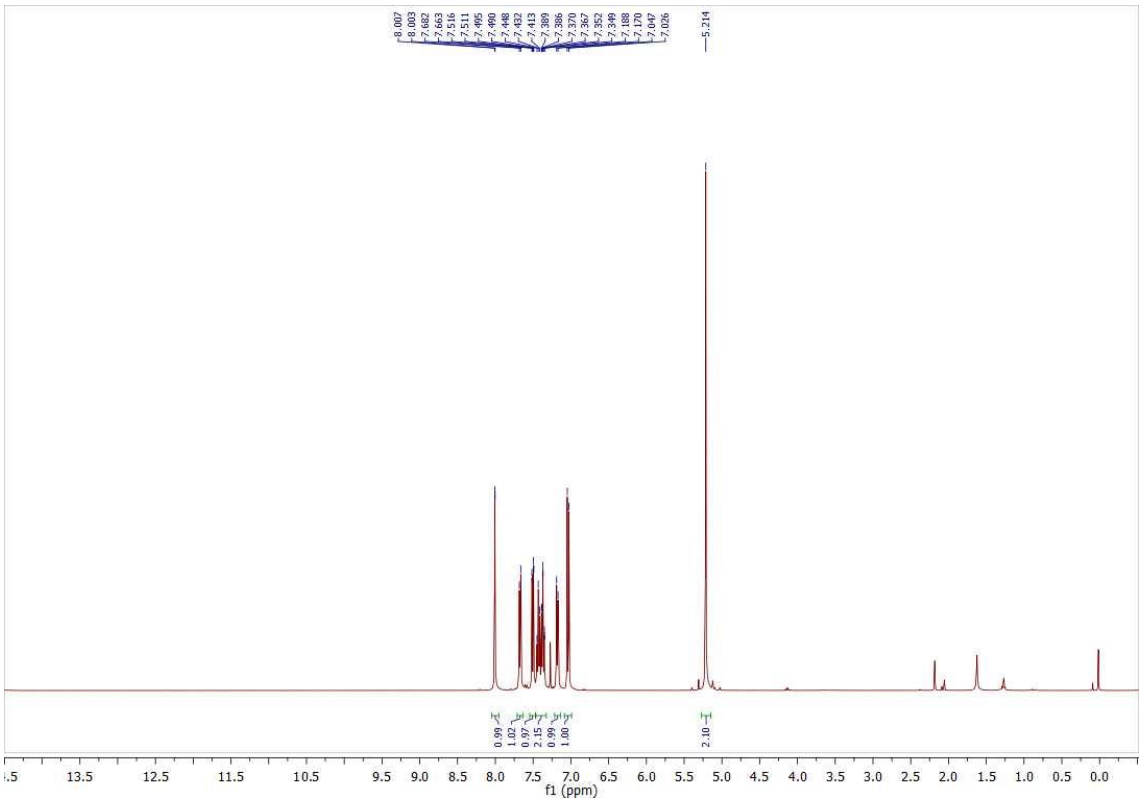


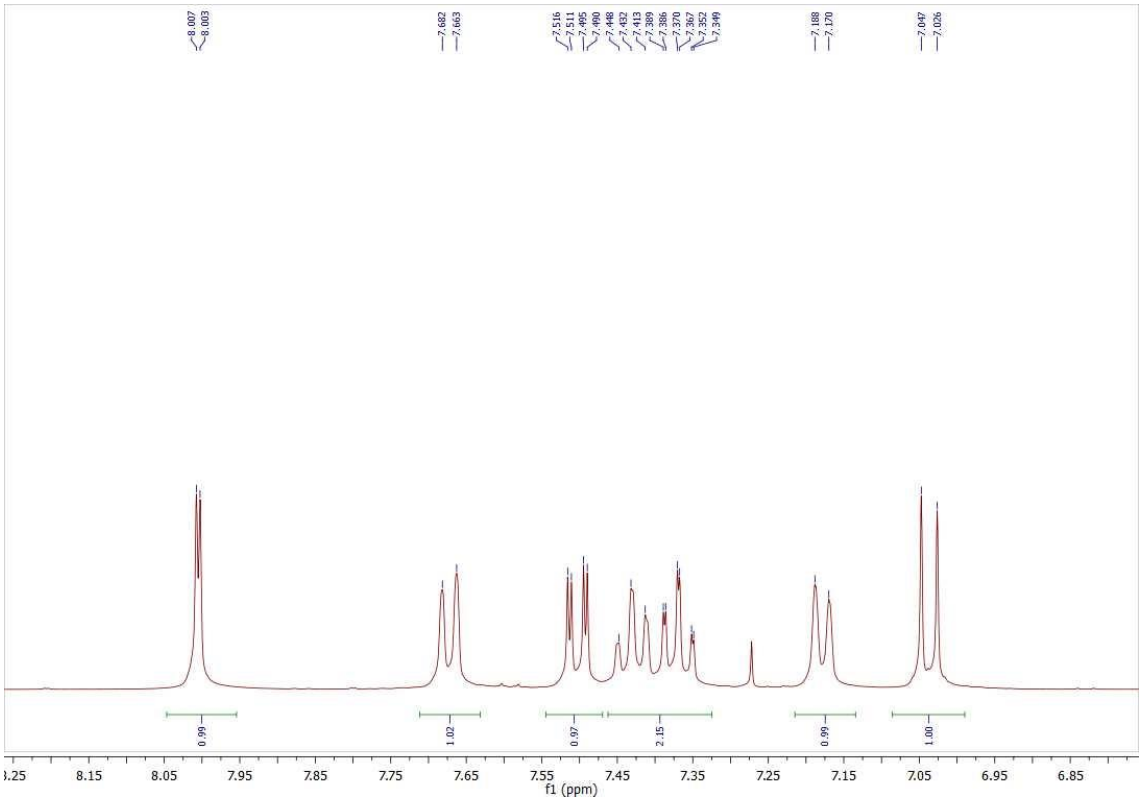
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 4-Methyl-6*H*-benzo[*c*]chromene (**1f**).



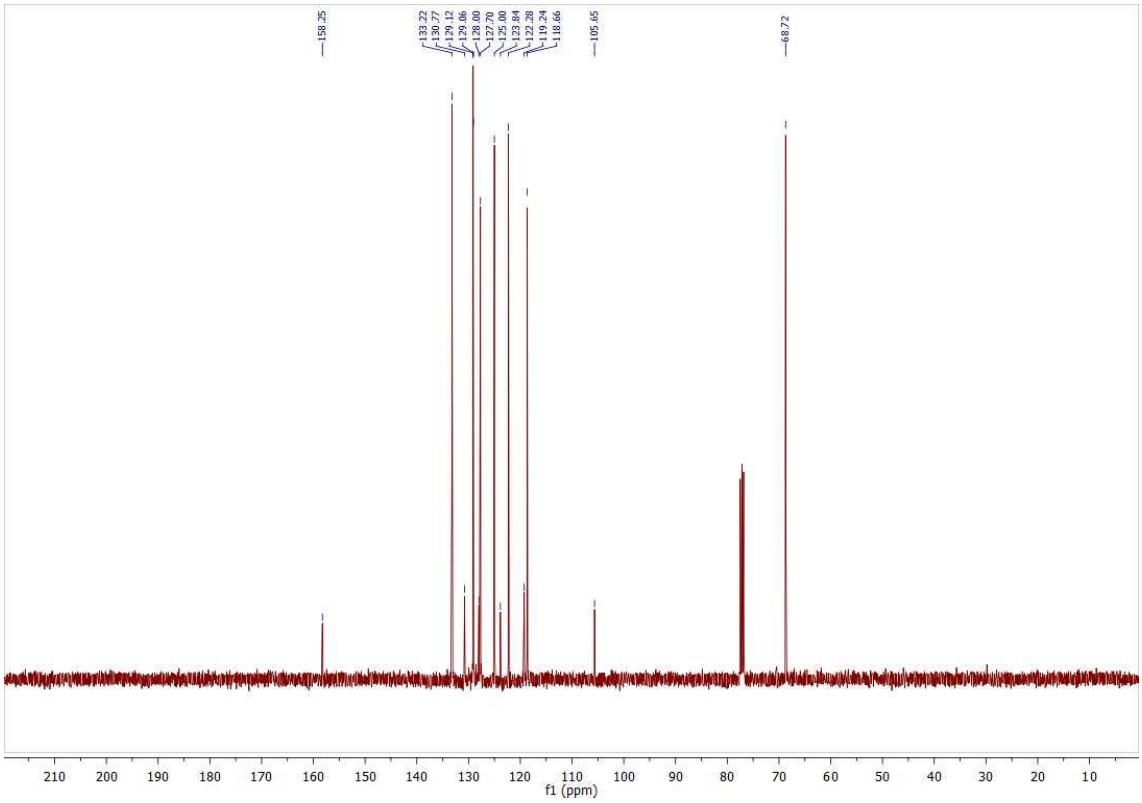


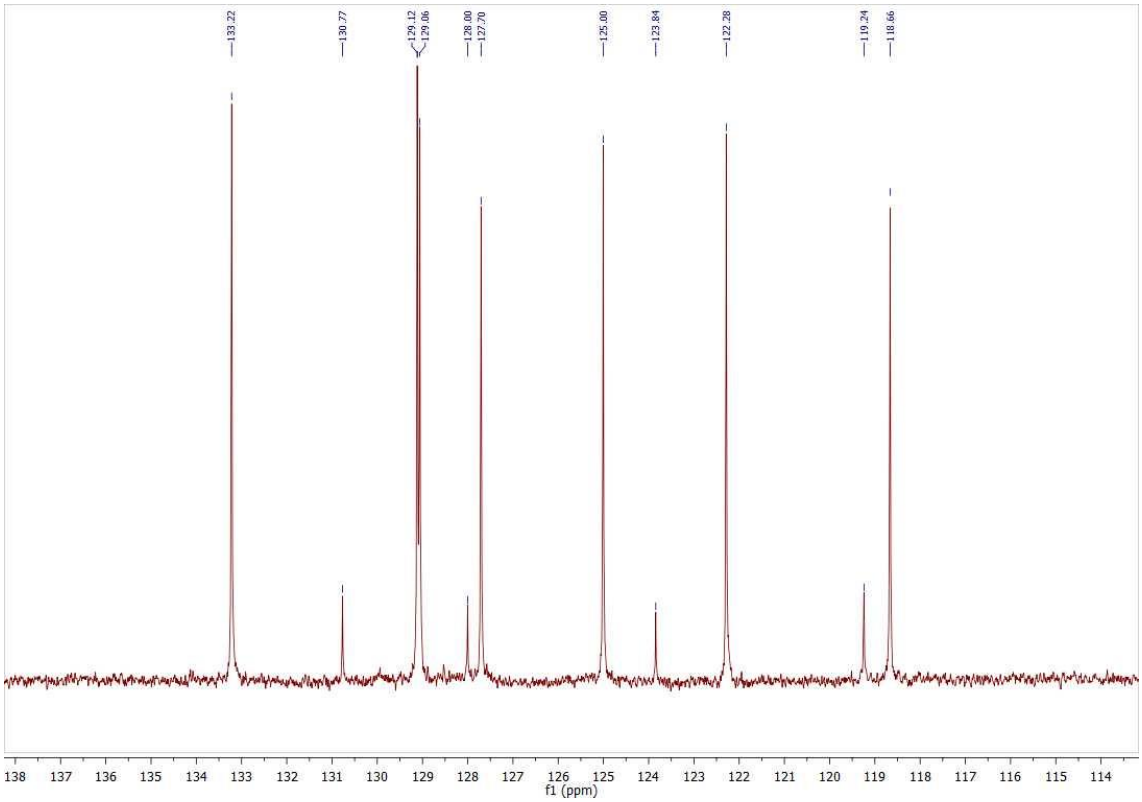
^{1}H-NMR (400 MHz, $CDCl_3$). 6*H*-Benzo[*c*]chromene-2-carbonitrile **(1g)**



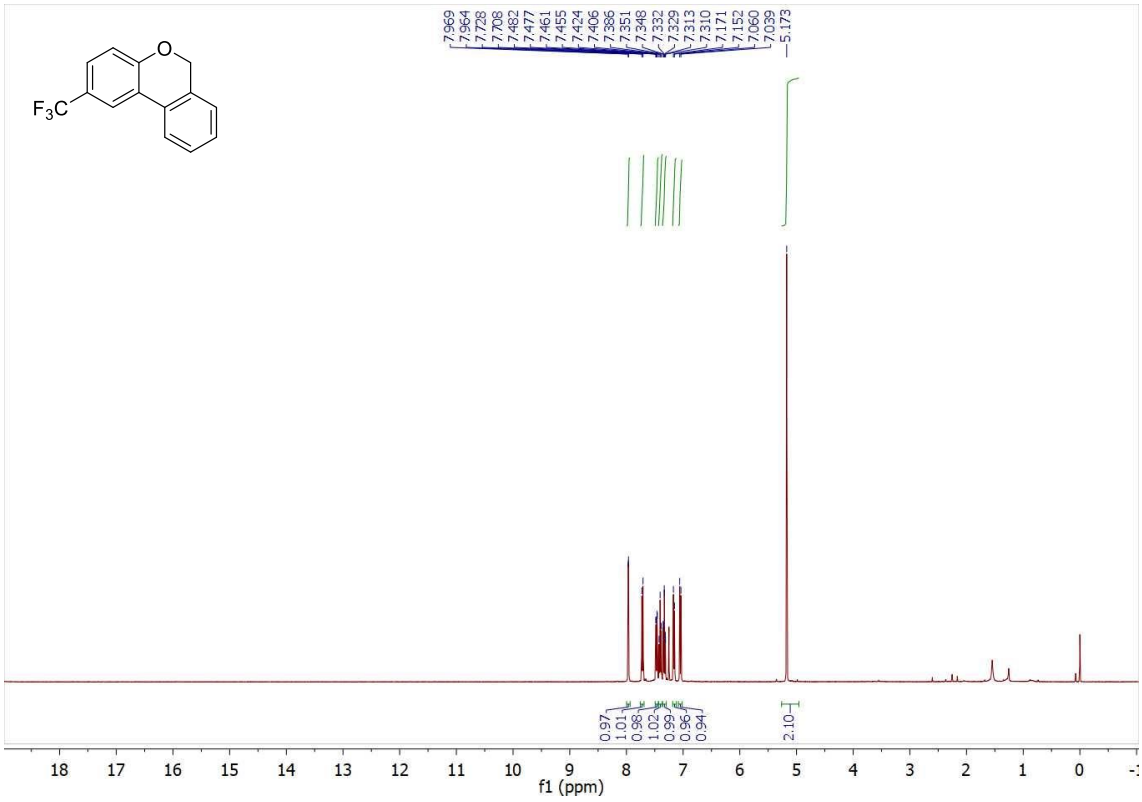


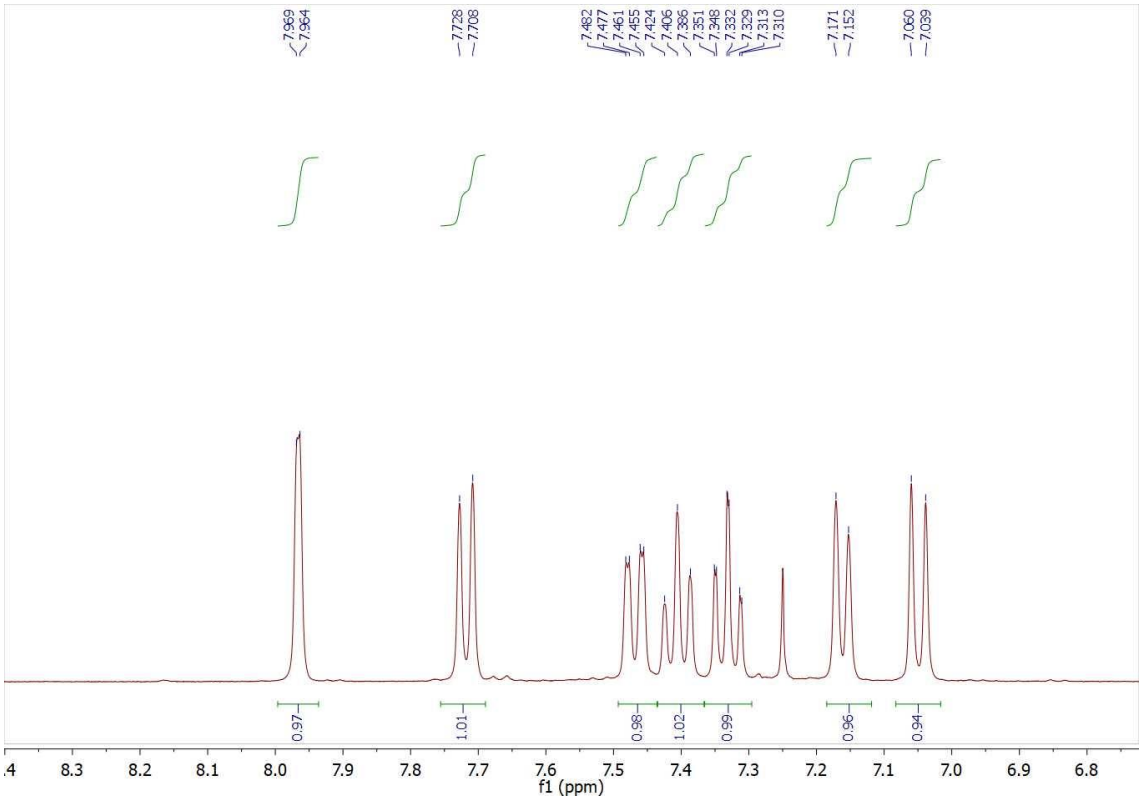
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 6*H*-Benzo[*c*]chromene-2-carbonitrile **(1g)**



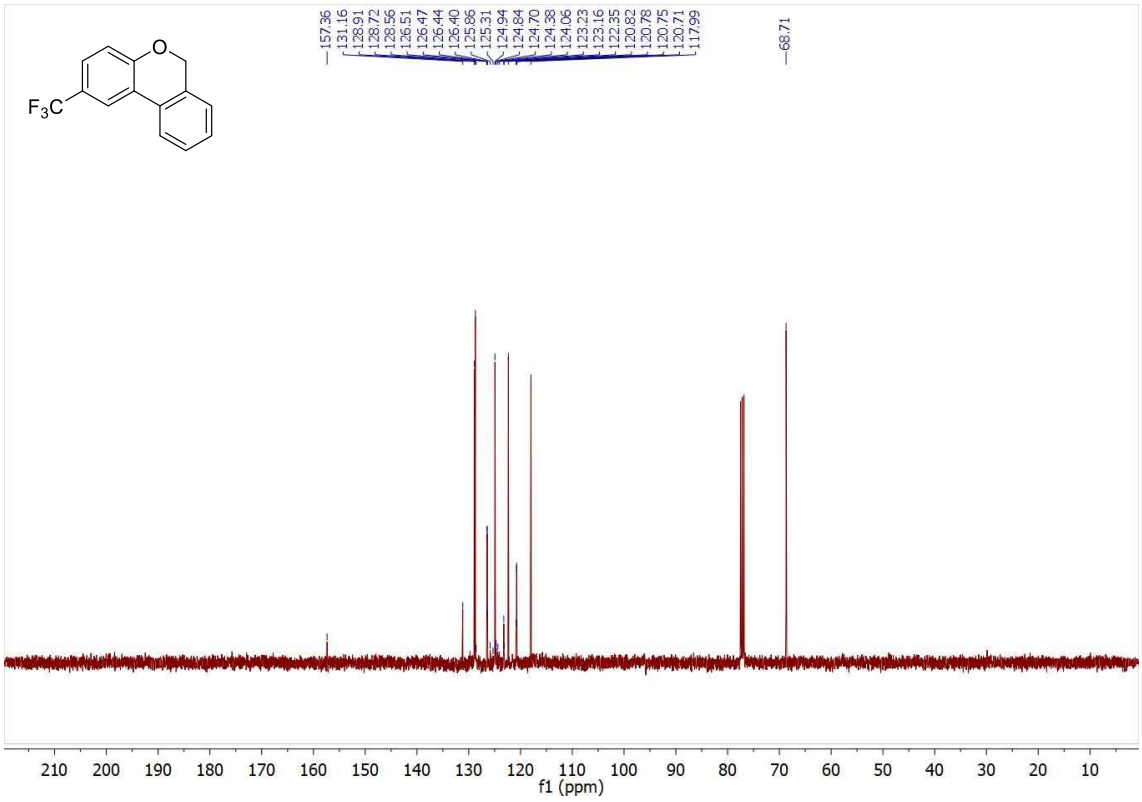


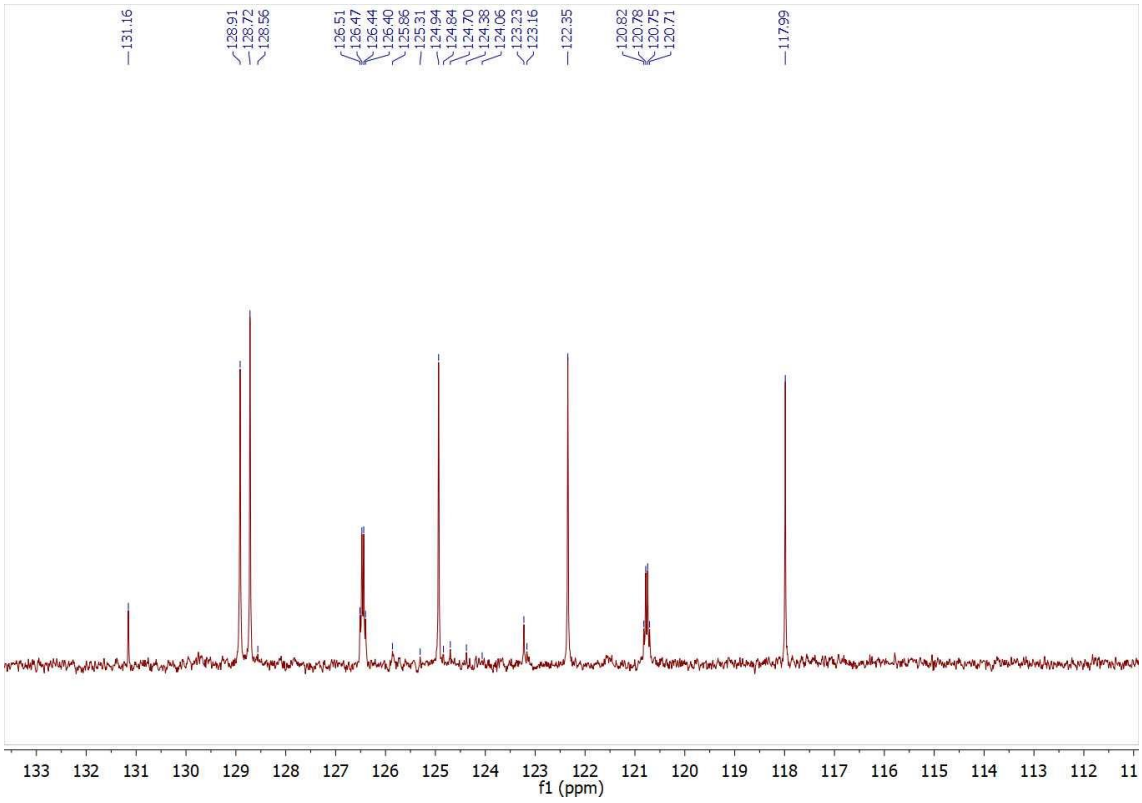
^{1}H-NMR (400 MHz, $CDCl_3$). 2-(Trifluoromethyl)-6*H*-benzo[*c*]chromene (**1h**).



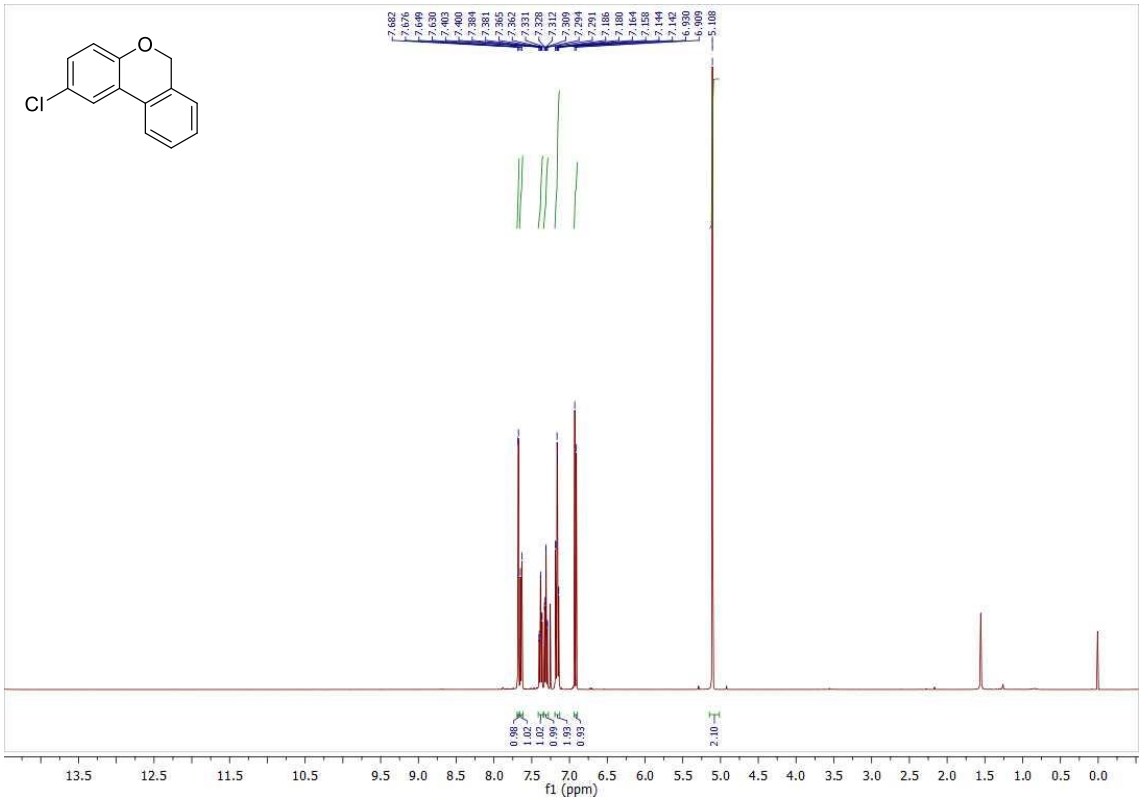


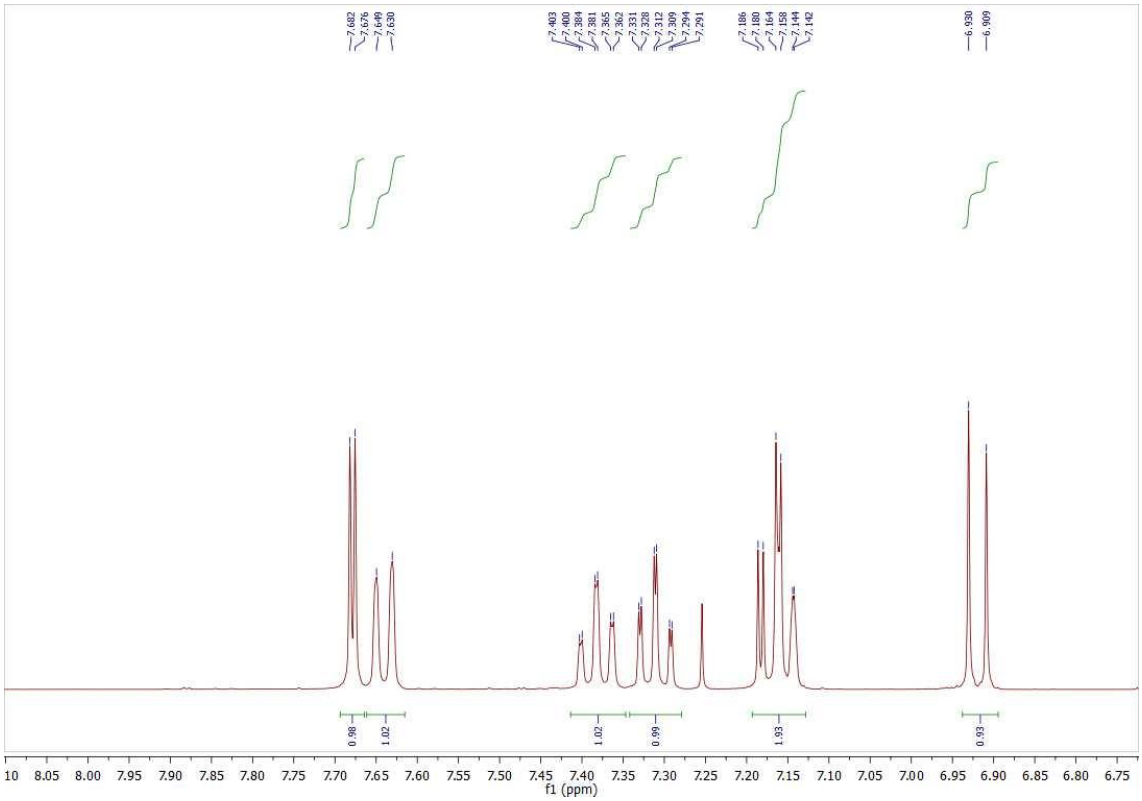
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 2-(Trifluoromethyl)-6*H*-benzo[*c*]chromene (**1h**).



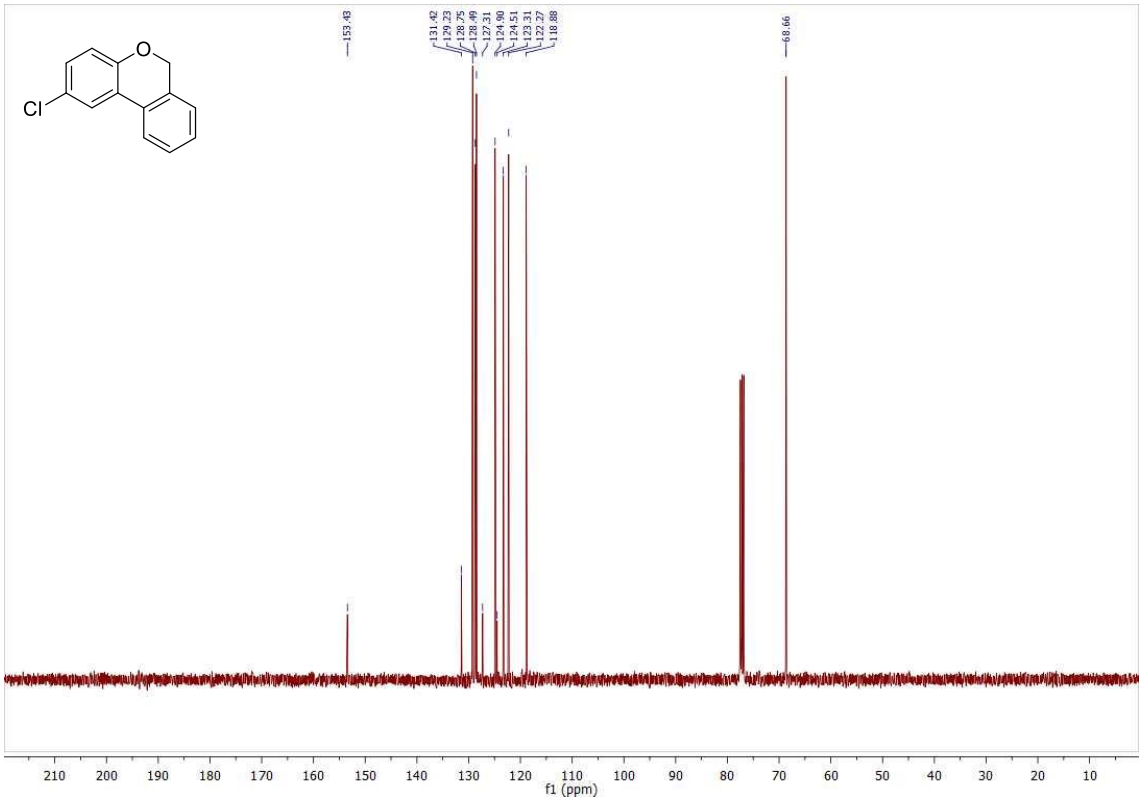


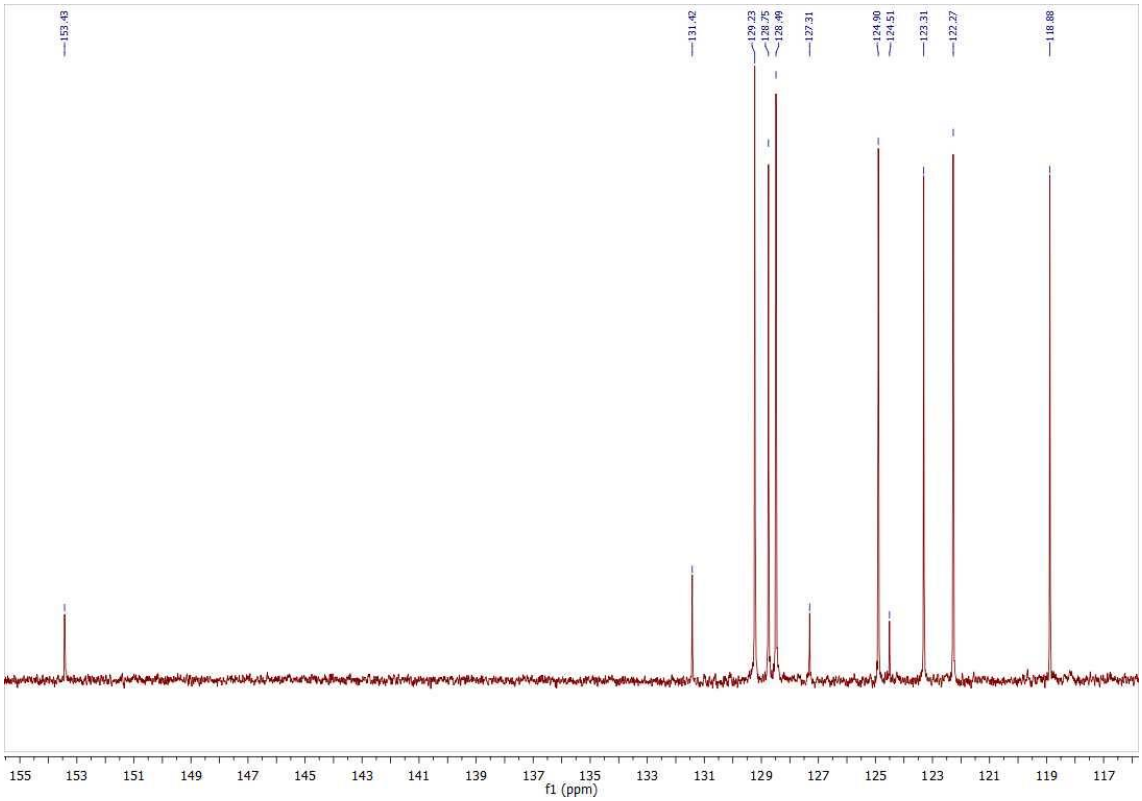
^{1}H-NMR (400 MHz, $CDCl_3$). 2-Chloro-6*H*-benzo[*c*]chromene (**1i**).



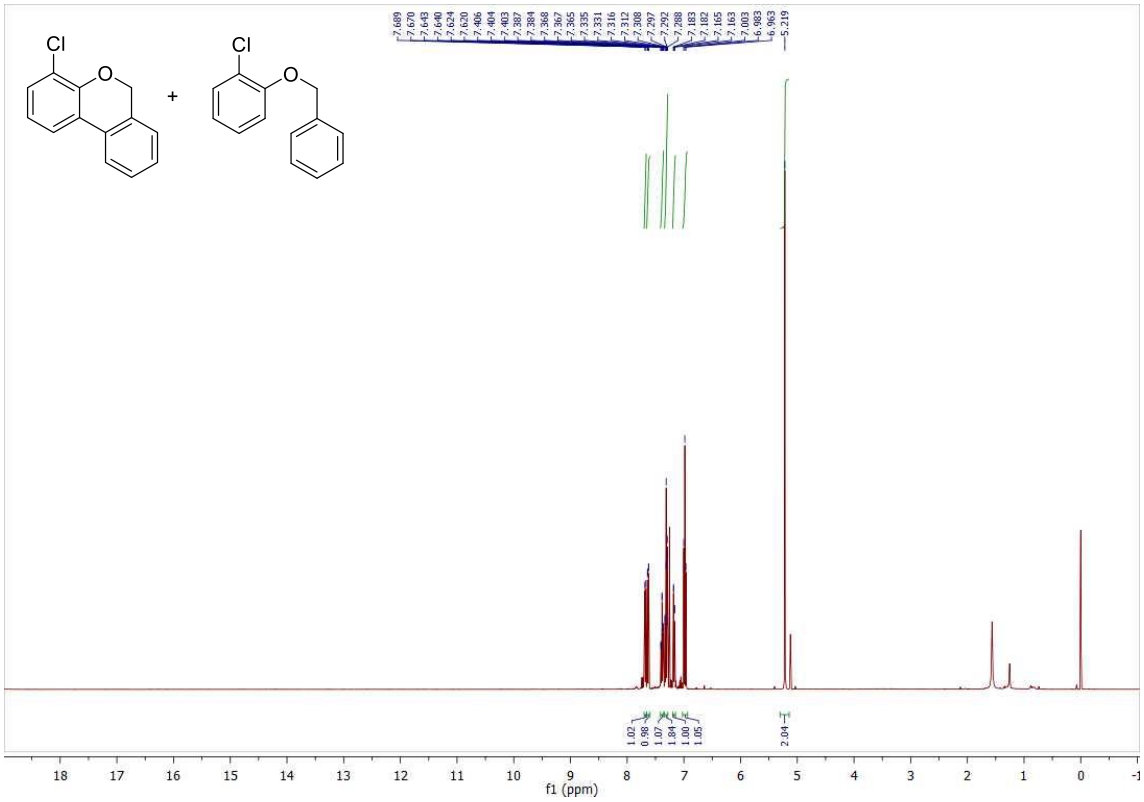


^{13}C NMR{1H} (101 MHz, $CDCl_3$). 2-Chloro-6*H*-benzo[*c*]chromene (**1i**).

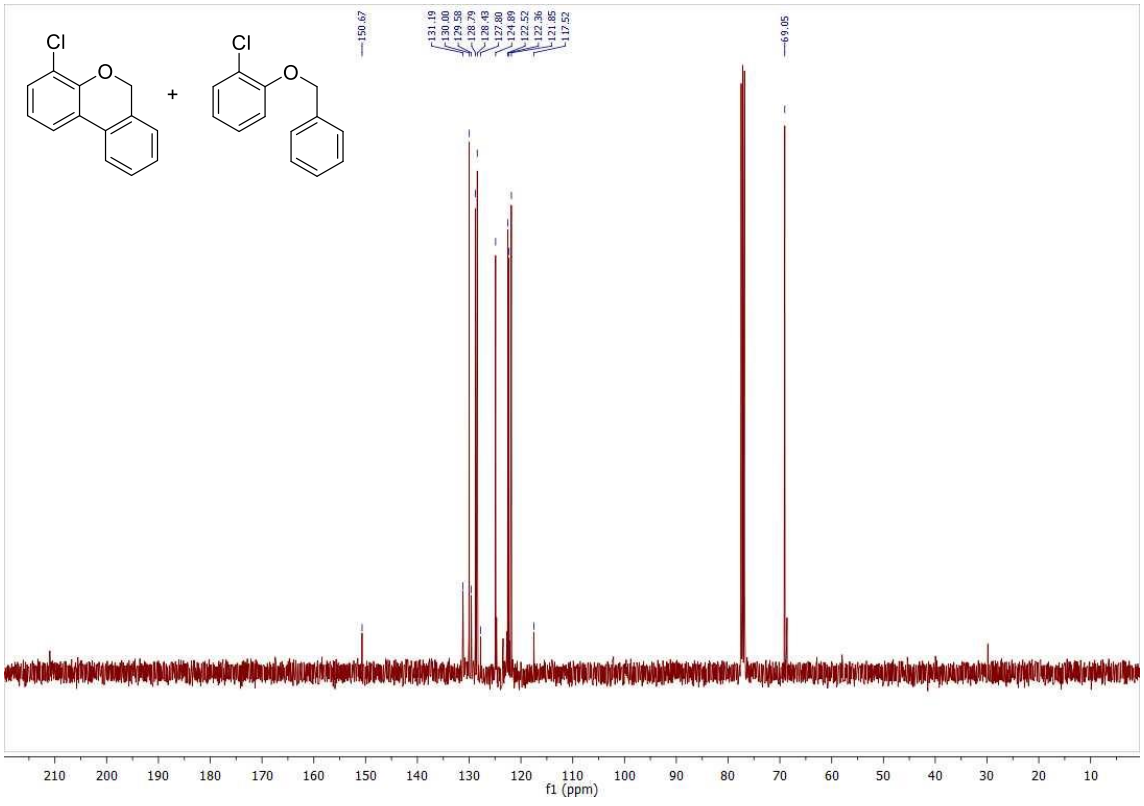




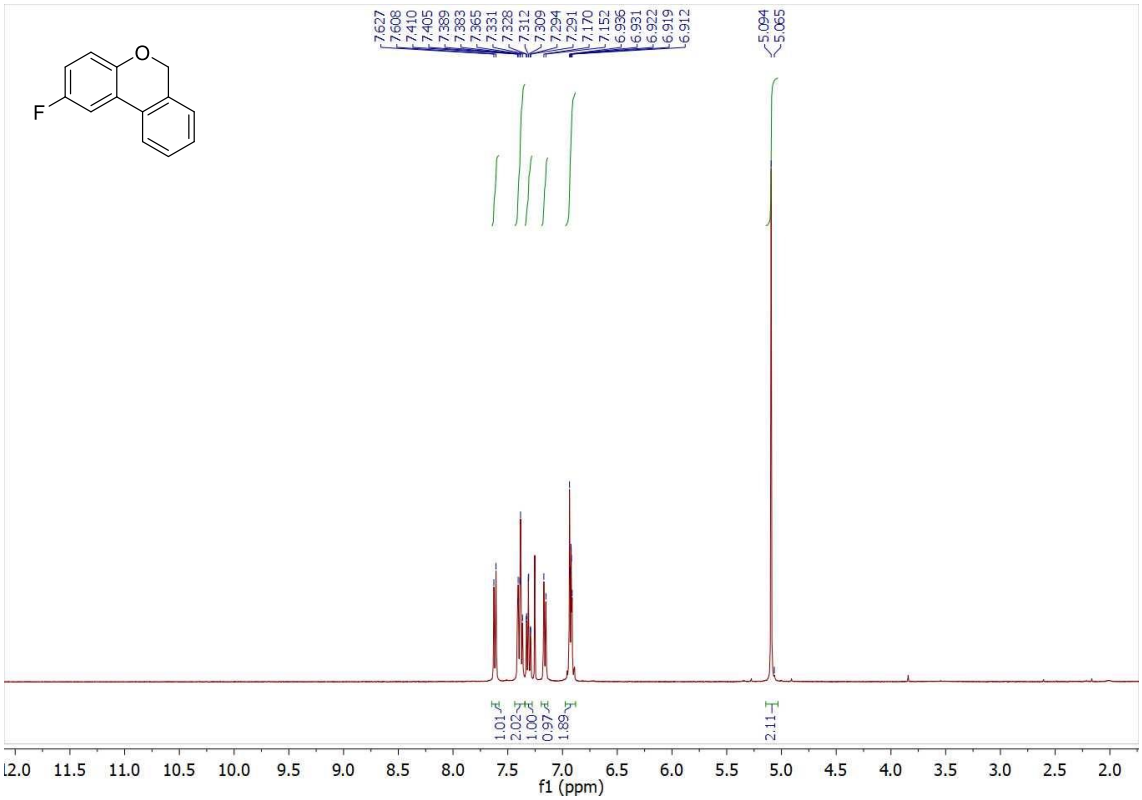
^{1}H-NMR (400 MHz, $CDCl_3$). 4-Chloro-6*H*-benzo[*c*]chromene (**1j**).

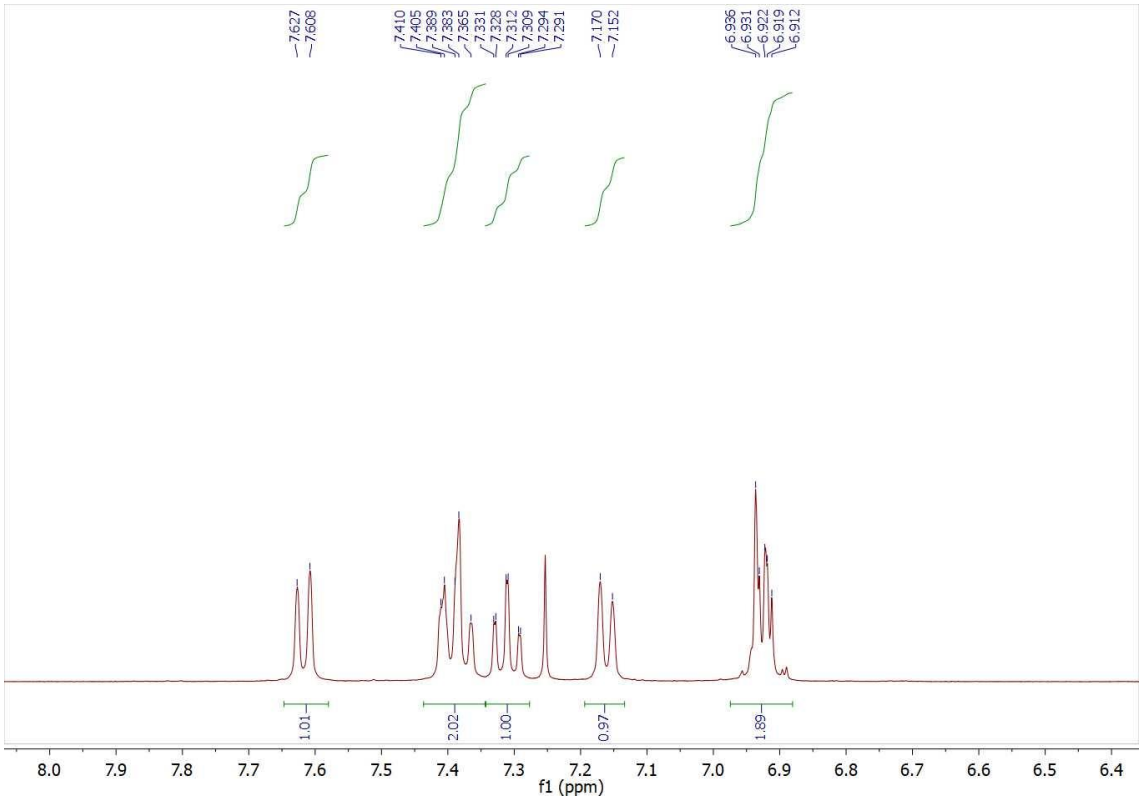


^{13}C NMR{1H} (101 MHz, $CDCl_3$). 4-Chloro-6*H*-benzo[*c*]chromene (**1j**).

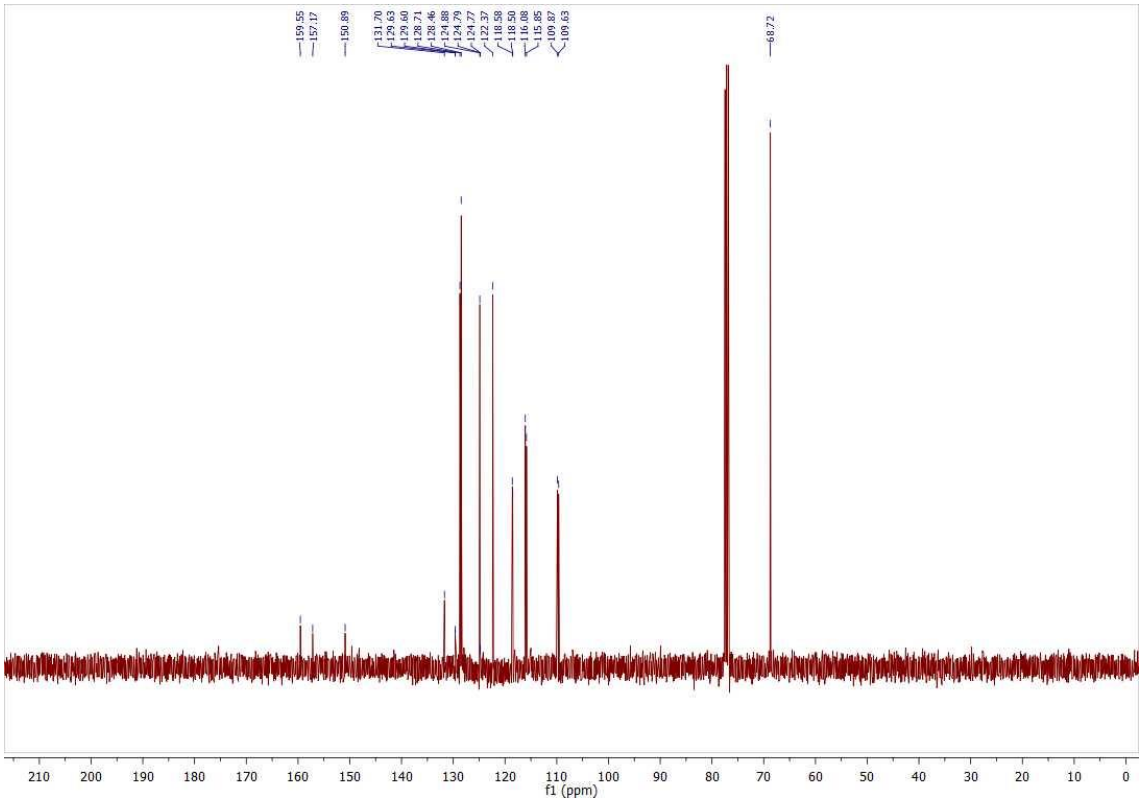


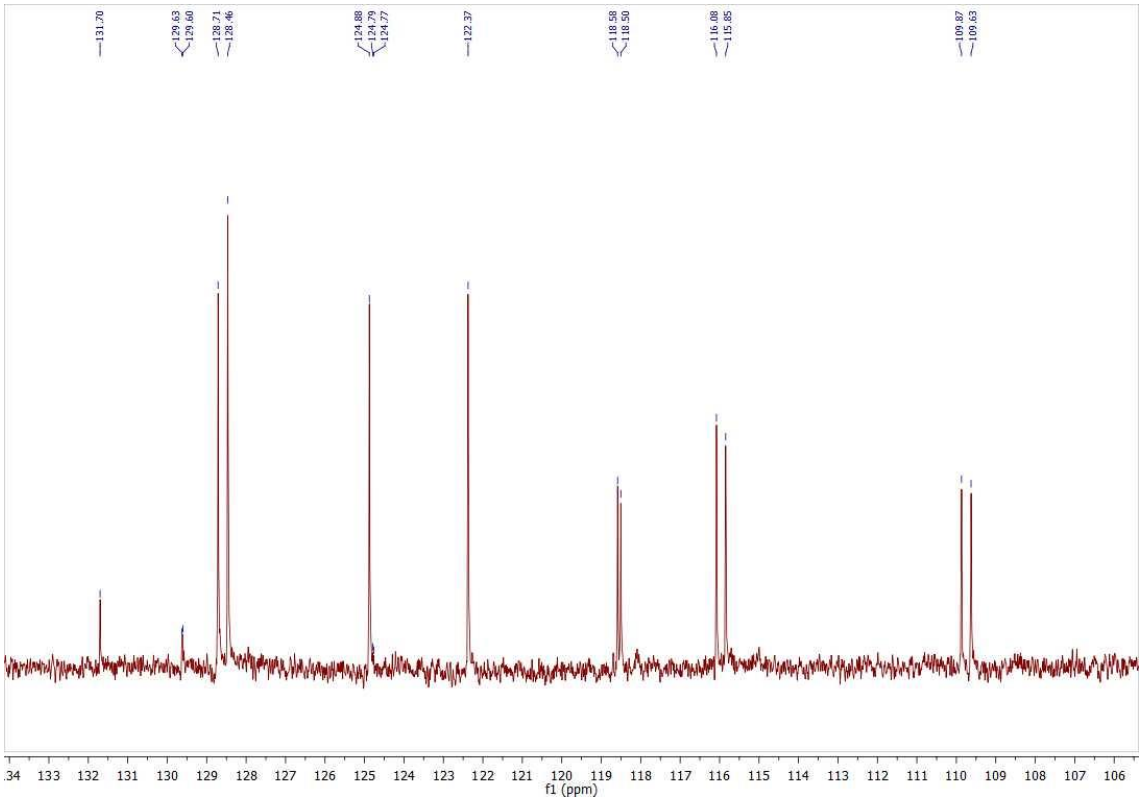
^{1}H-NMR (400 MHz, $CDCl_3$). 2-Fluoro-6*H*-benzo[*c*]chromene (**1k**).



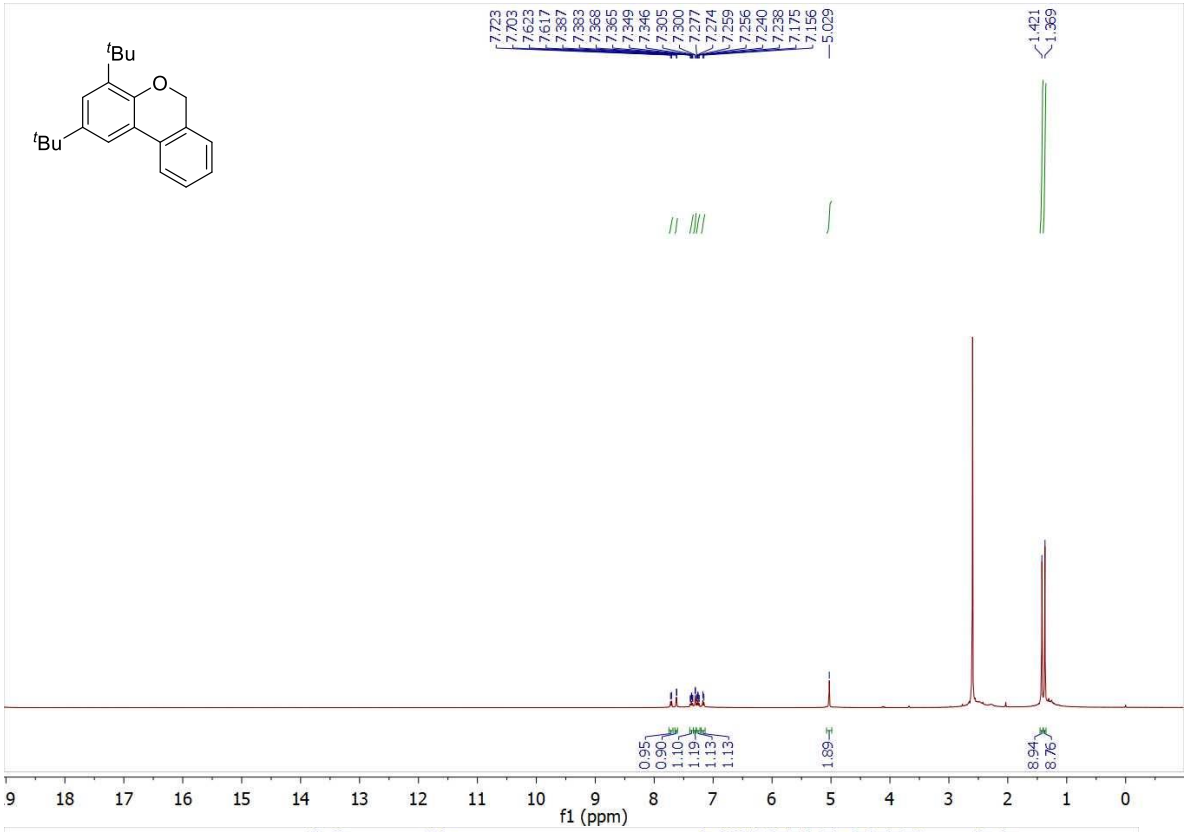


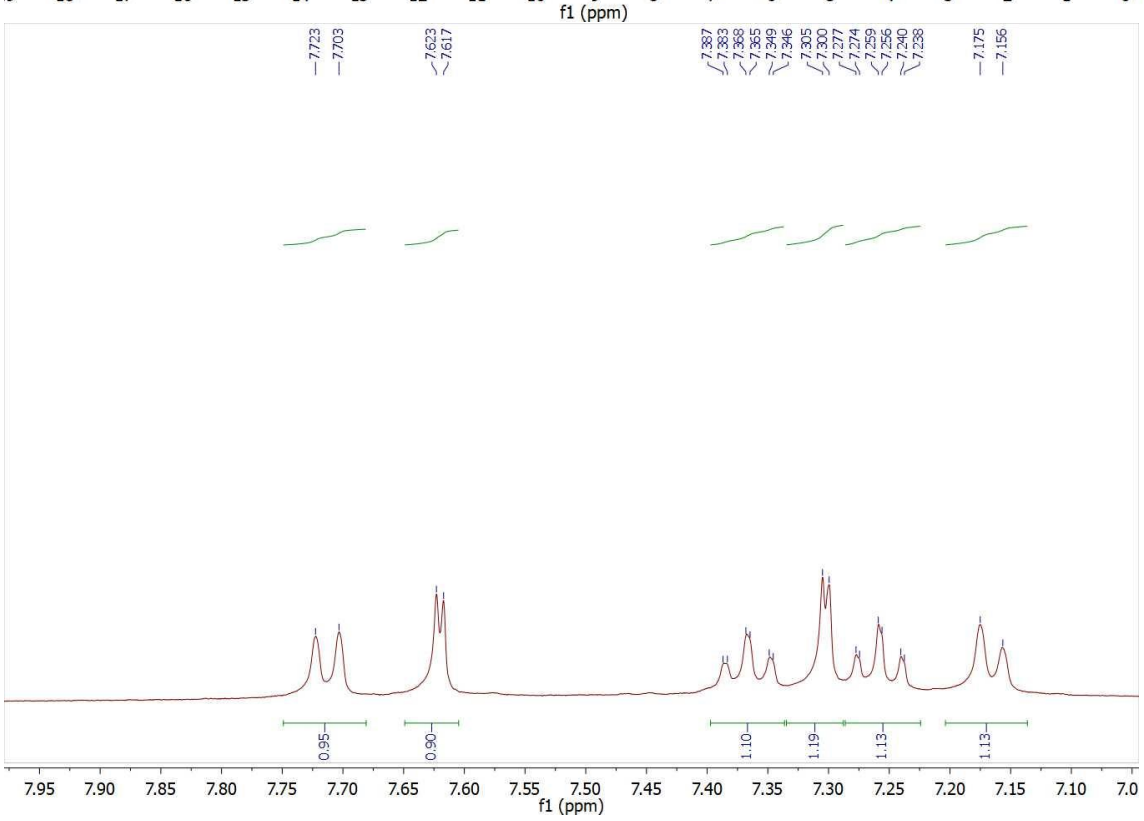
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 2-Fluoro-6*H*-benzo[*c*]chromene (**1k**).



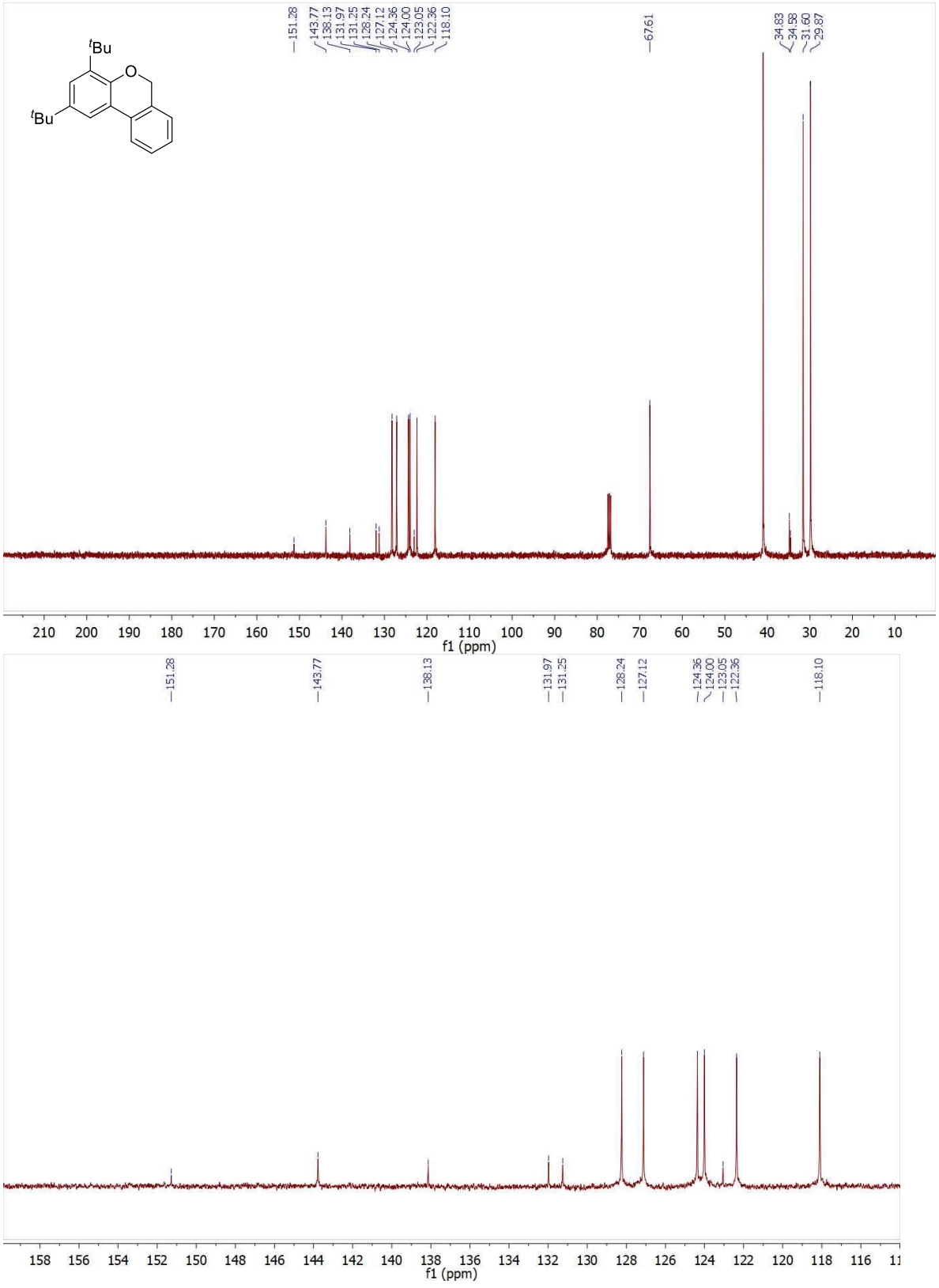


^{1}H-NMR (400 MHz, $CDCl_3$). 2,4-Di-*tert*-butyl-6*H*-benzo[*c*]chromene (**1l**)

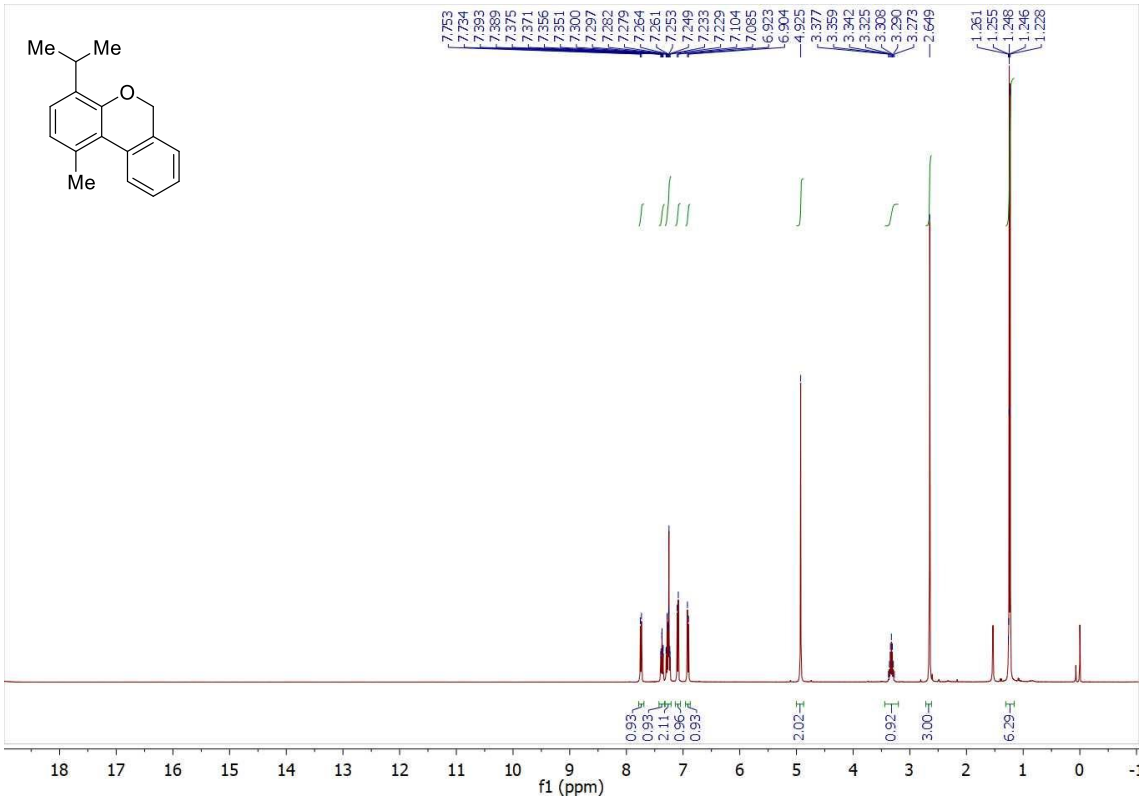


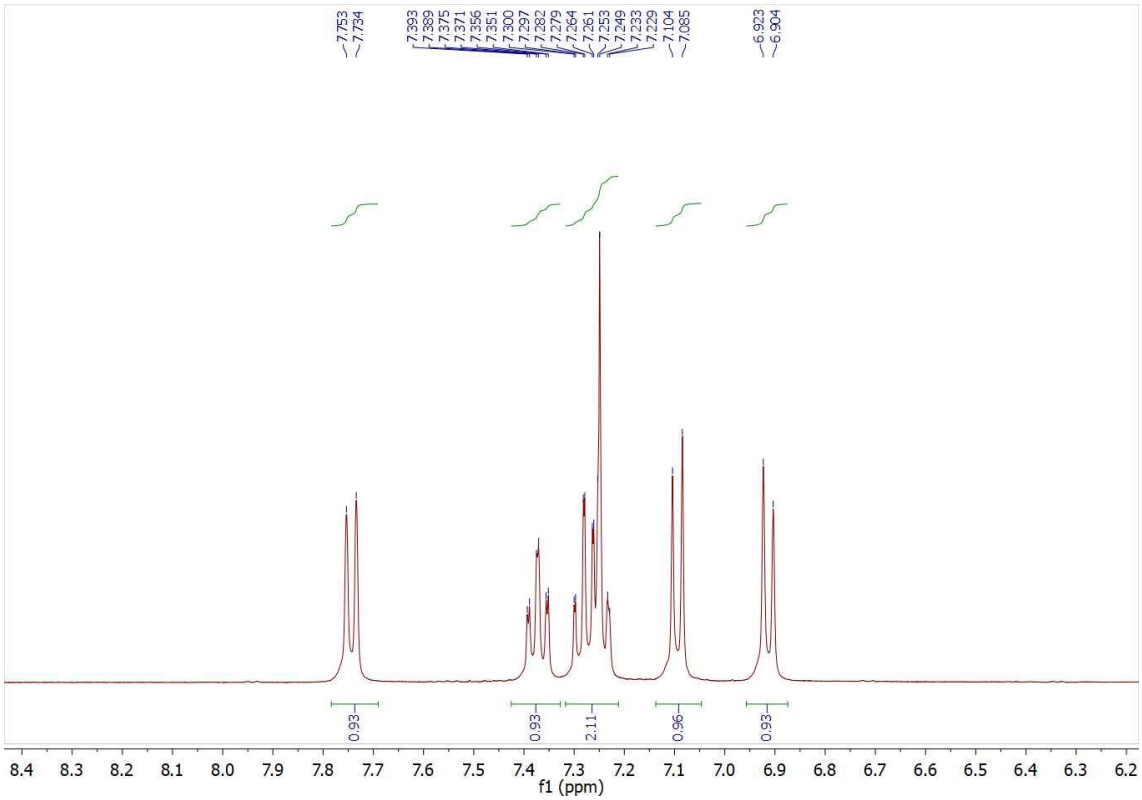


^{13}C NMR{1H} (101 MHz, $CDCl_3$). 2,4-Di-*tert*-butyl-6*H*-benzo[*c*]chromene (**1l**).

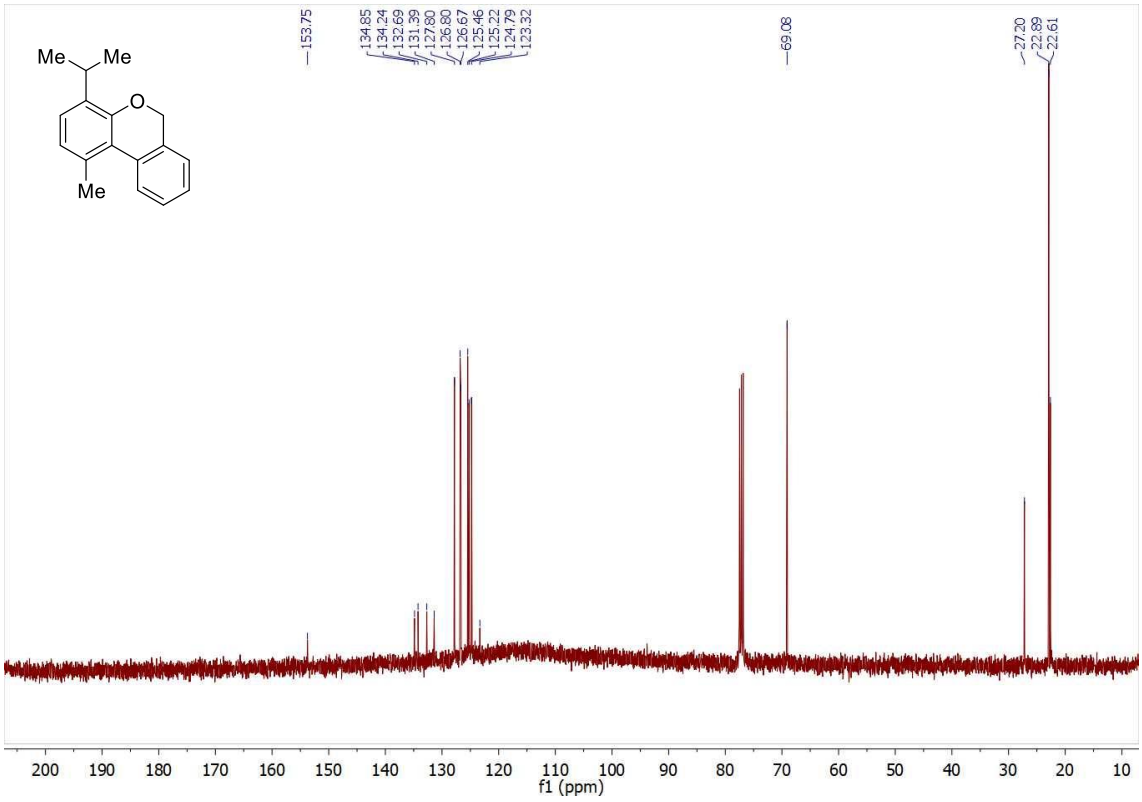


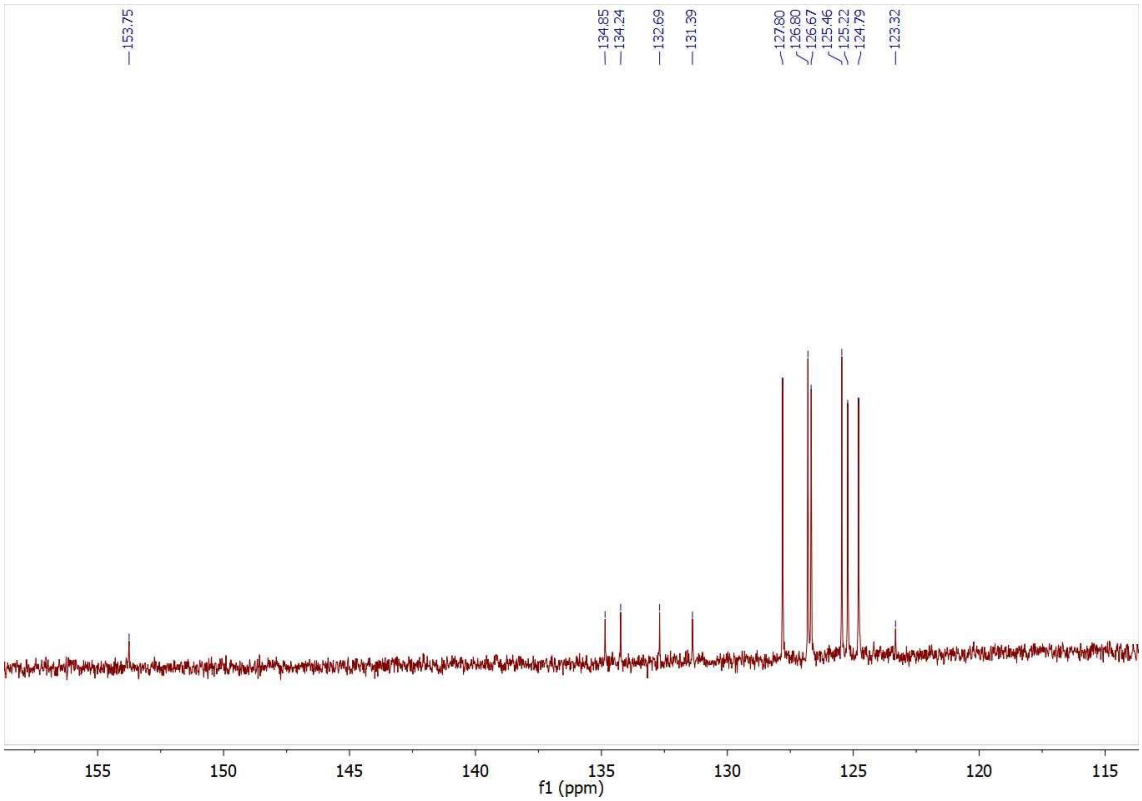
^{1}H-NMR (400 MHz, $CDCl_3$). 4-Isopropyl-1-methyl-6*H*-benzo[*c*]chromene (**1m**)



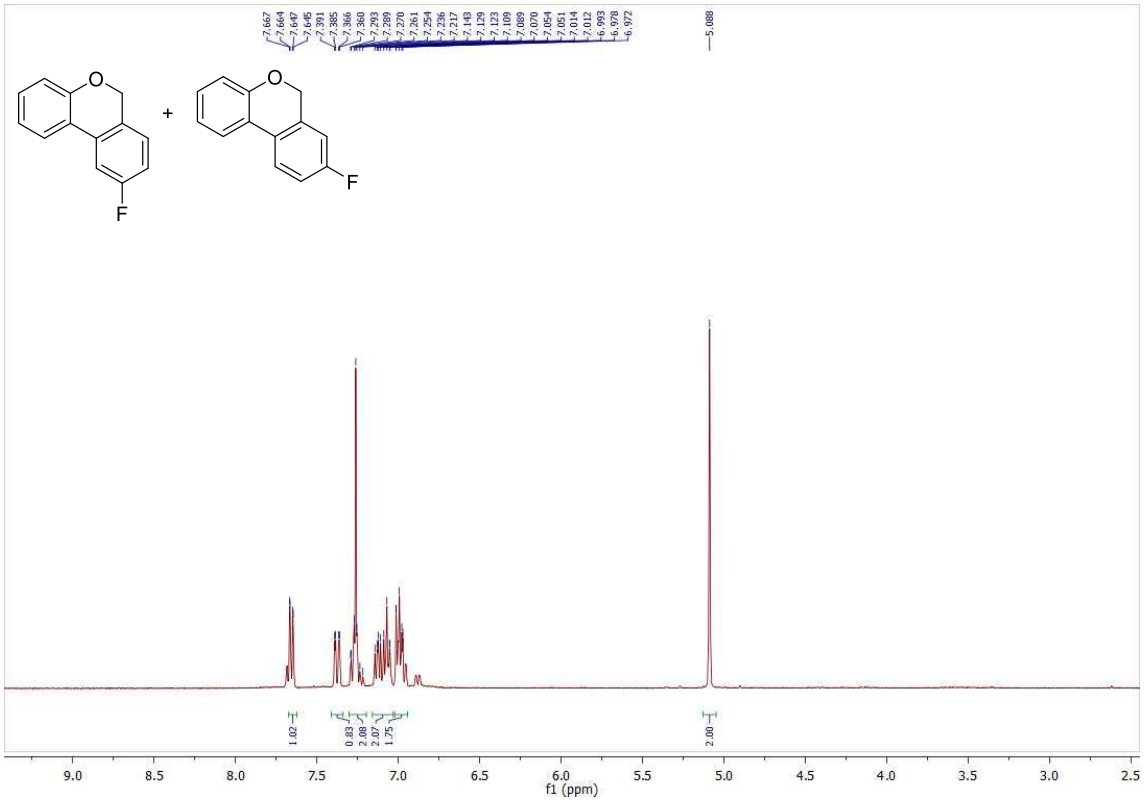


^{13}C NMR{1H} (101 MHz, $CDCl_3$). 4-Isopropyl-1-methyl-6*H*-benzo[*c*]chromene (**1m**)

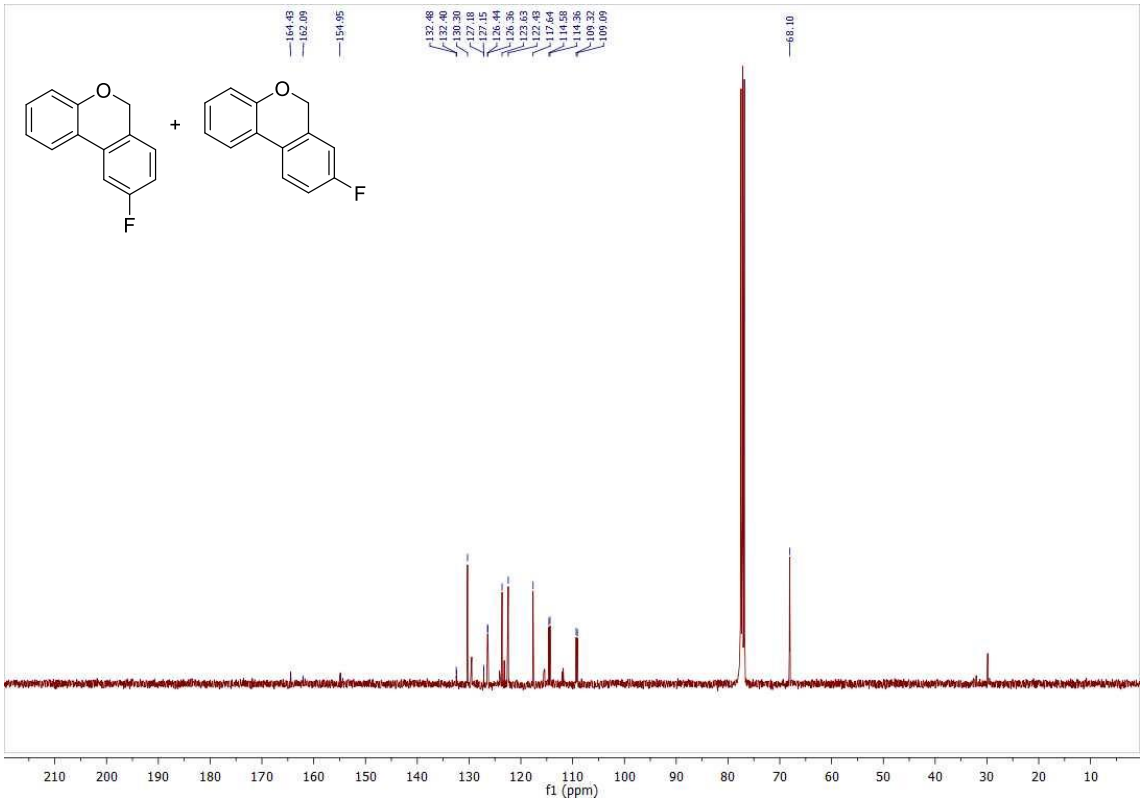


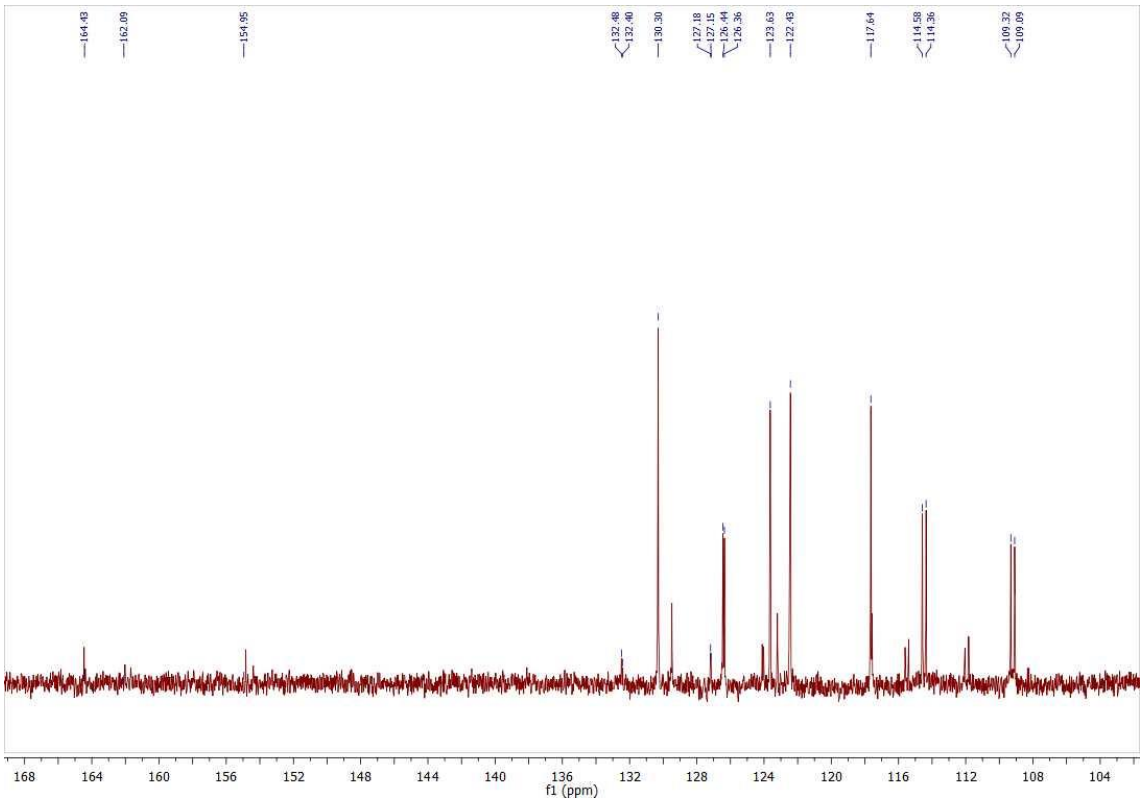


^{1}H-NMR (400 MHz, $CDCl_3$). 9-Fluoro-6*H*-benzo[*c*]chromene (**1o**).

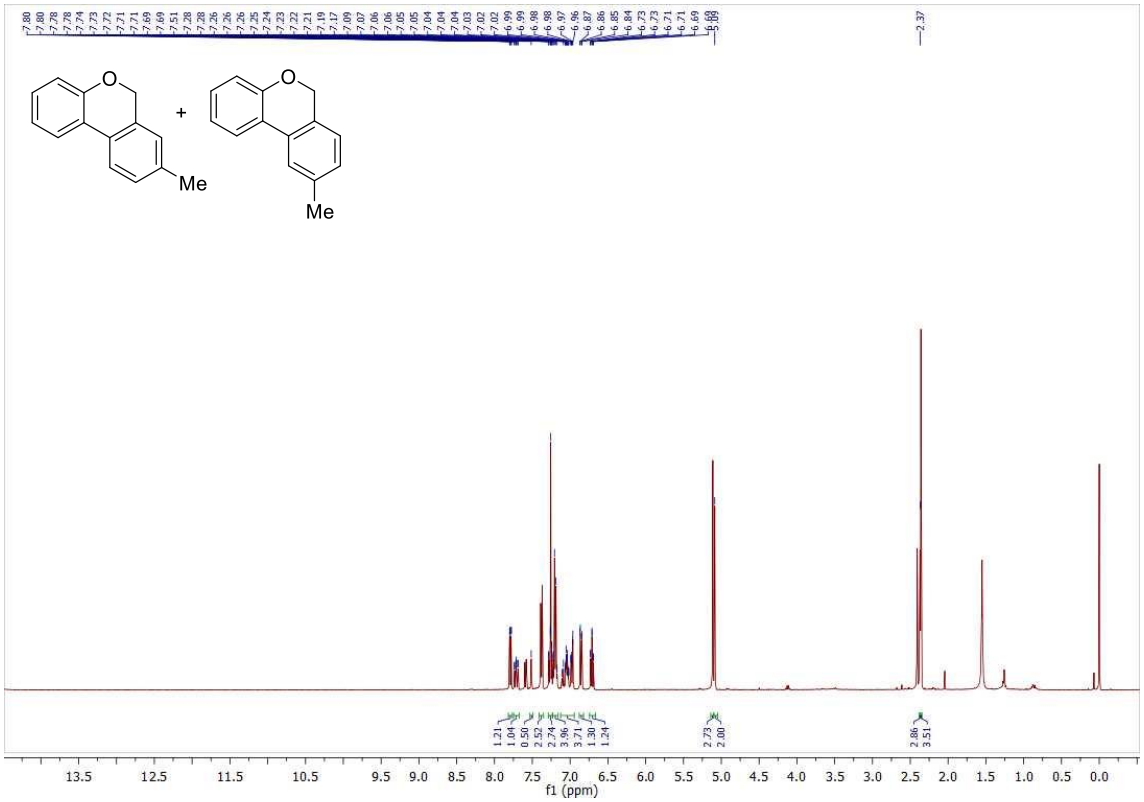


^{13}C NMR{1H} (101 MHz, $CDCl_3$).). 9-Fluoro-6*H*-benzo[*c*]chromene (**1o**).

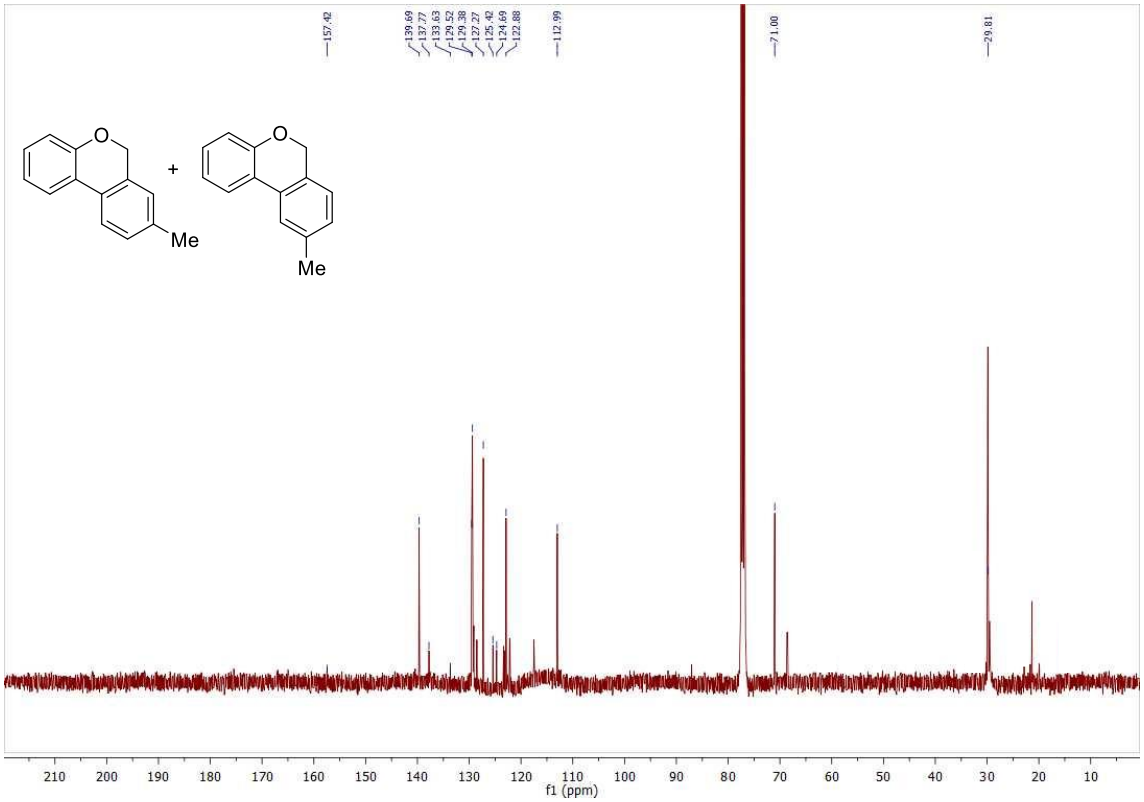




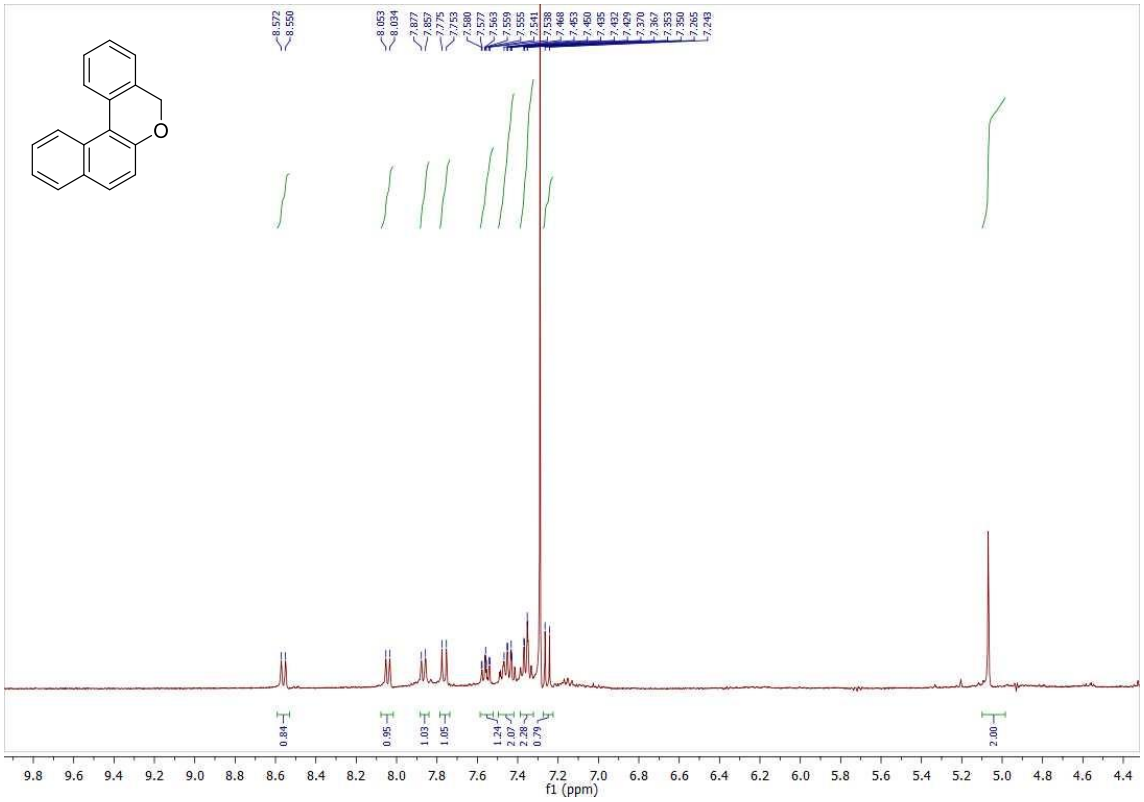
^{1}H-NMR (400 MHz, $CDCl_3$). 8-Methyl-6*H*-benzo[*c*]chromene (**1p**). 9-Methyl-6*H*-benzo[*c*]chromene (**1p´**).



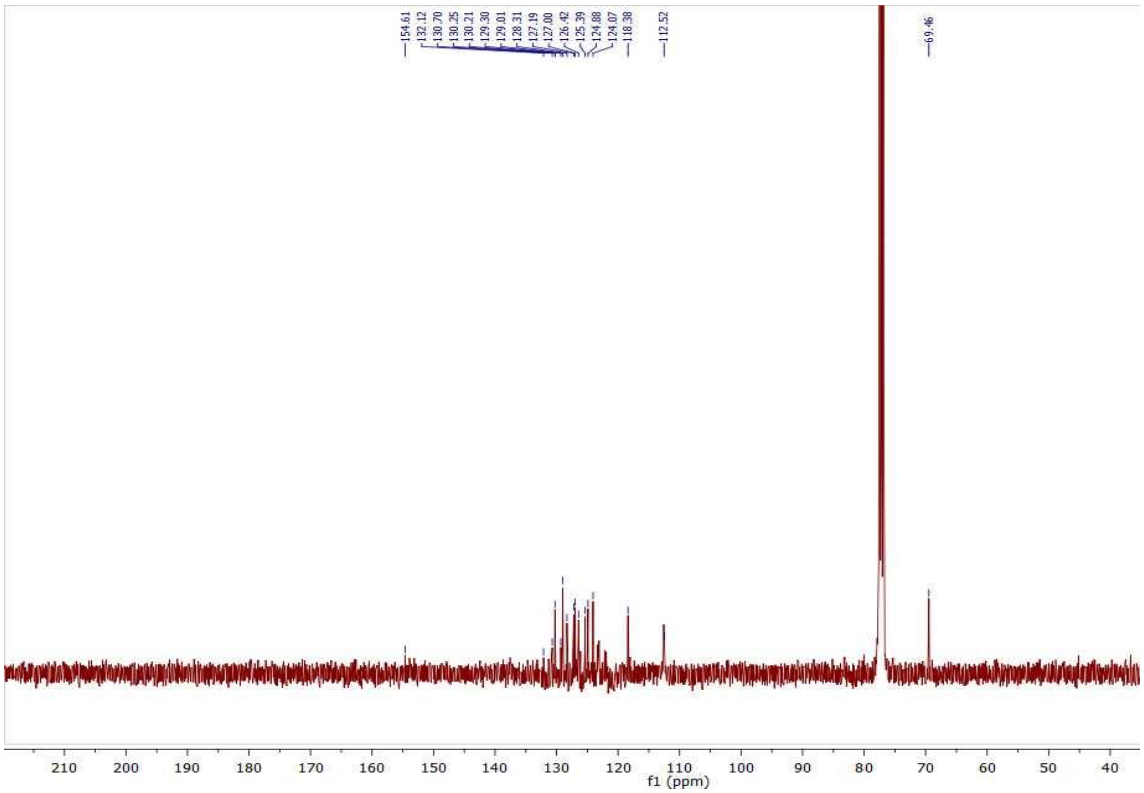
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 8-Methyl-6*H*-benzo[*c*]chromene (**1p**). 9-Methyl-6*H*-benzo[*c*]chromene (**1p´**).



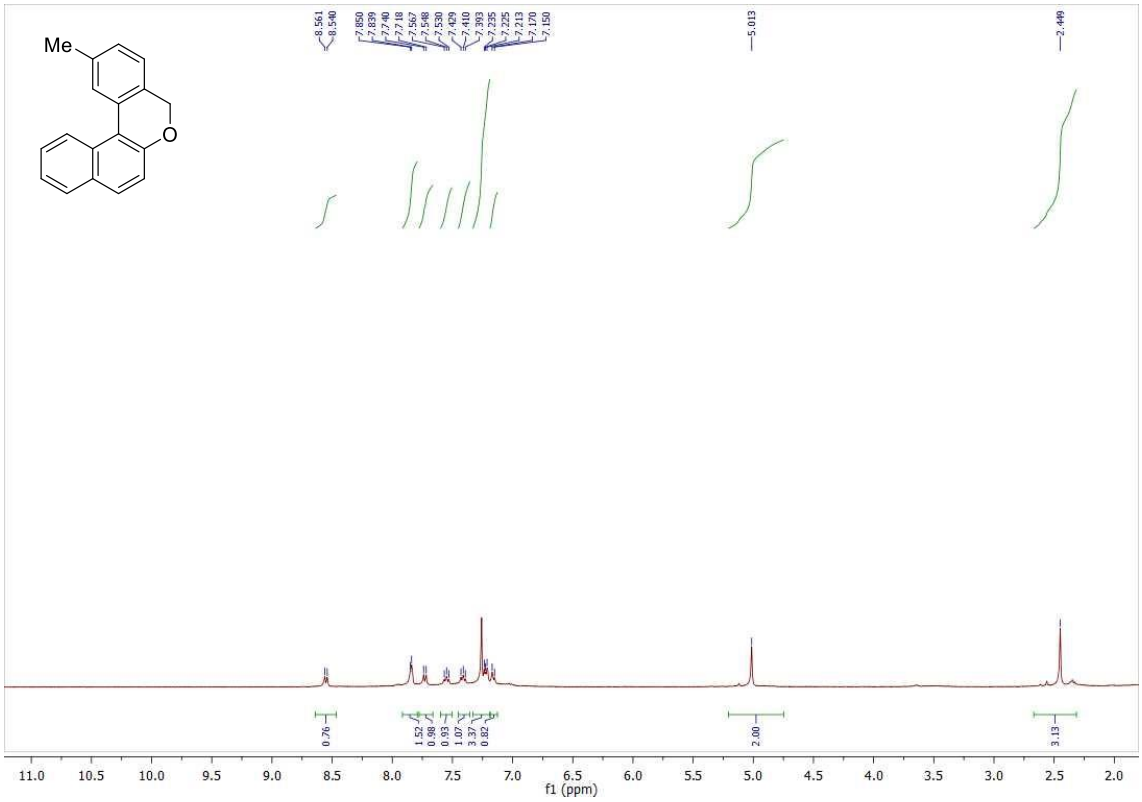
^{1}H-NMR (400 MHz, $CDCl_3$). 5*H*-Dibenzo[*c,f*]chromene (**1q**).



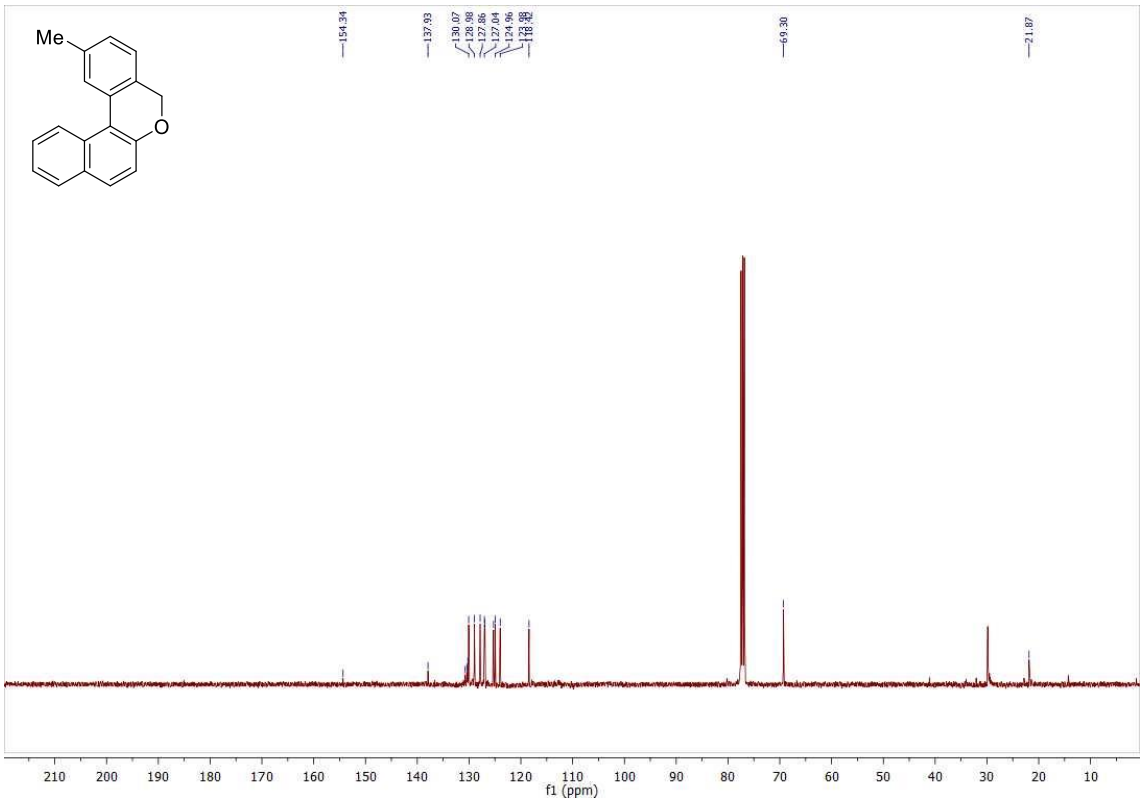
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 5*H*-Dibenzo[*c,f*]chromene (**1q**).



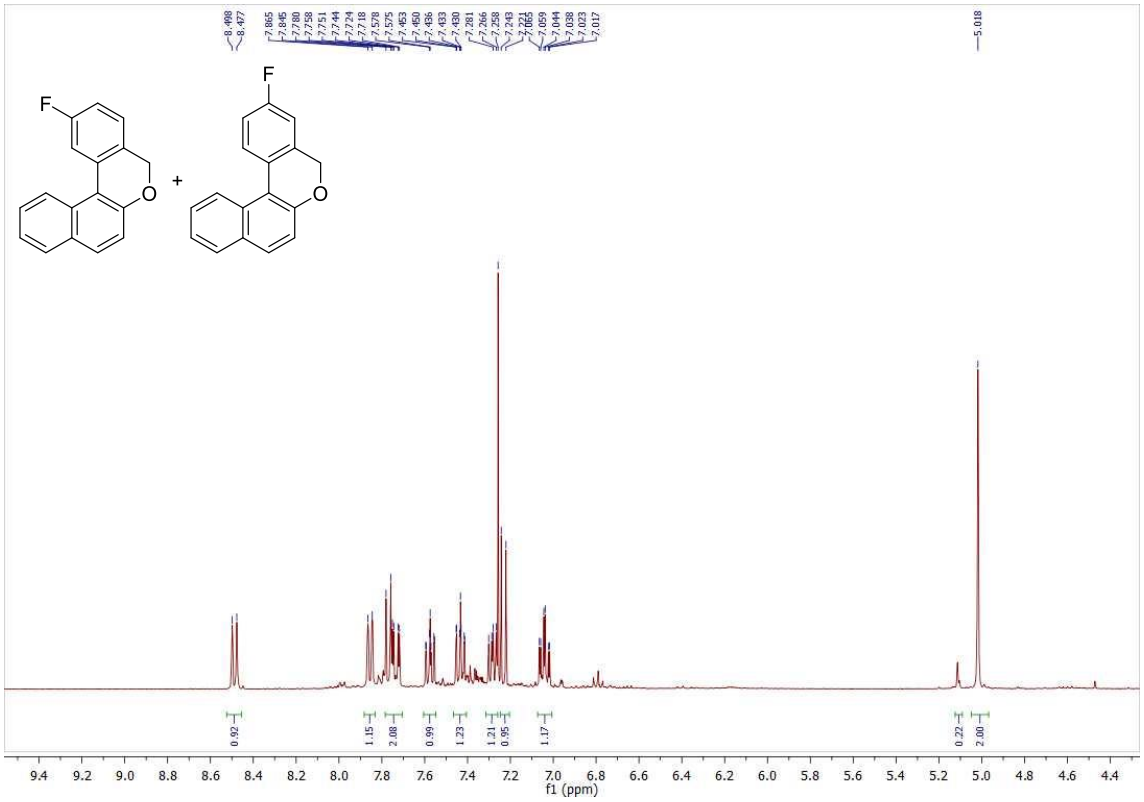
^{1}H-NMR (400 MHz, $CDCl_3$). 2-Methyl-5*H*-dibenzo[*c,f*]chromene (**1r**).



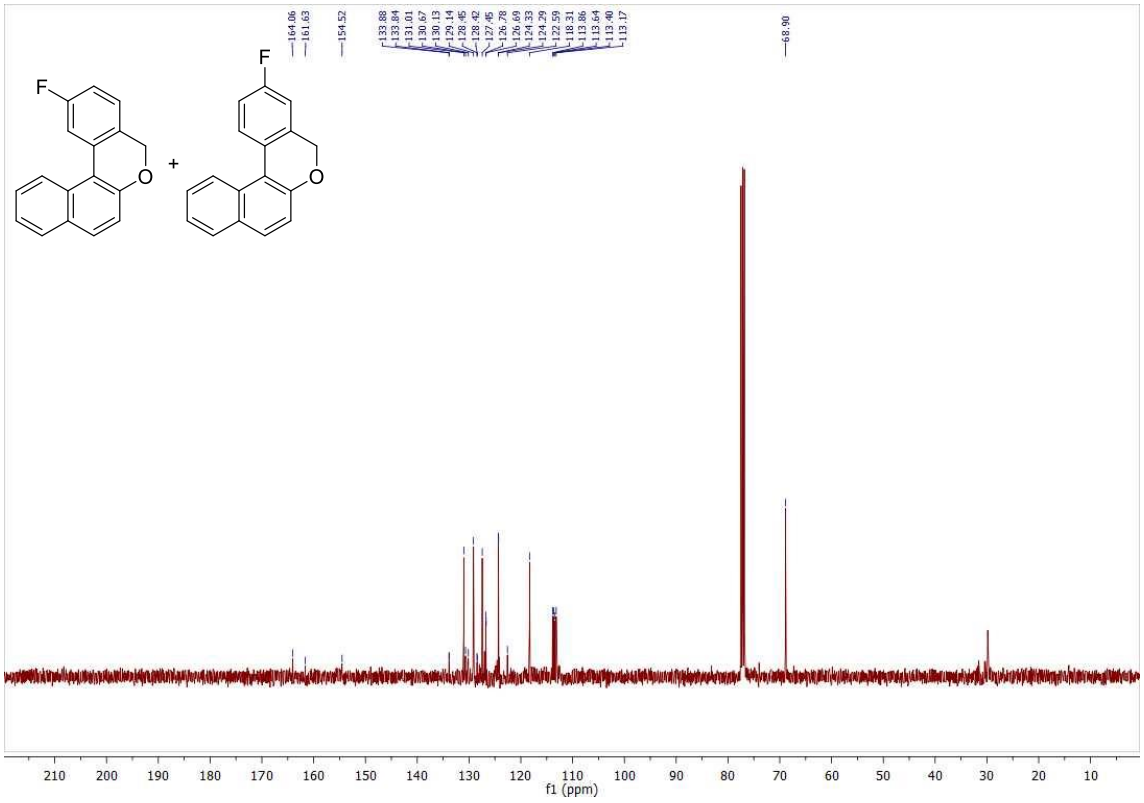
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 2-Methyl-5*H*-dibenzo[*c,f*]chromene (**1r**).

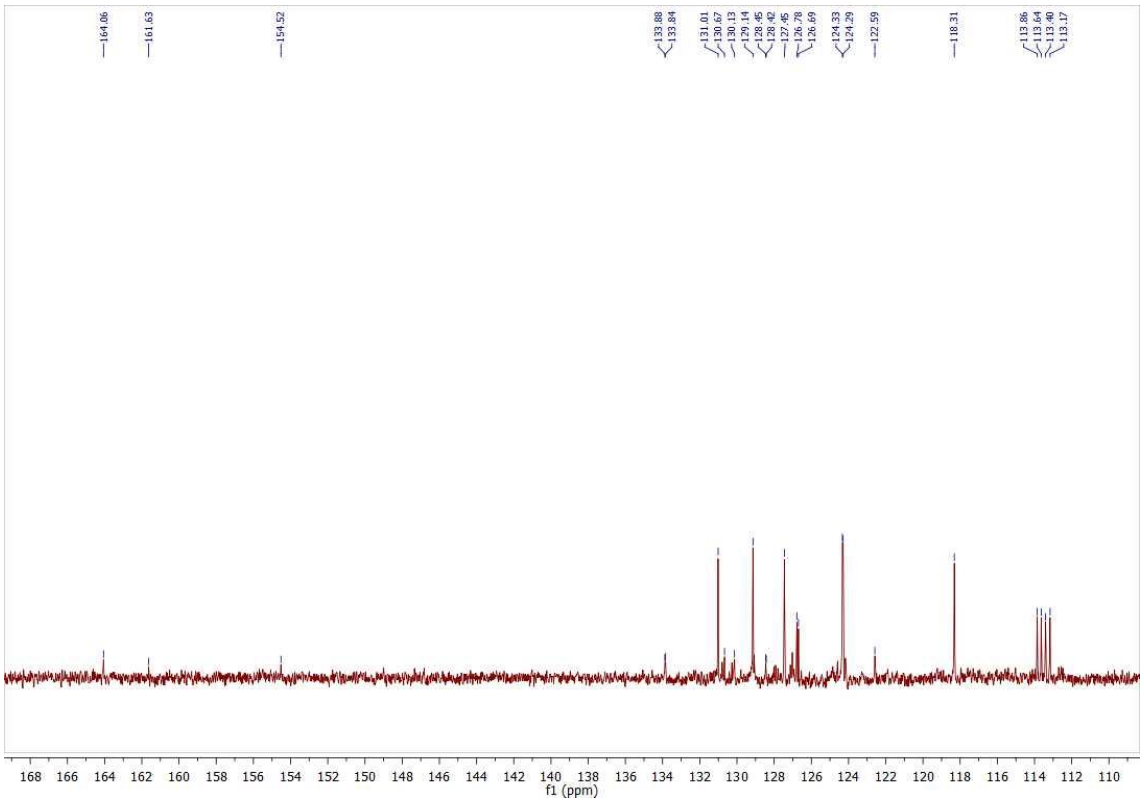


^{1}H-NMR (400 MHz, $CDCl_3$). 2-Fluoro-5*H*-dibenzo[*c,f*]chromene (**1s**).

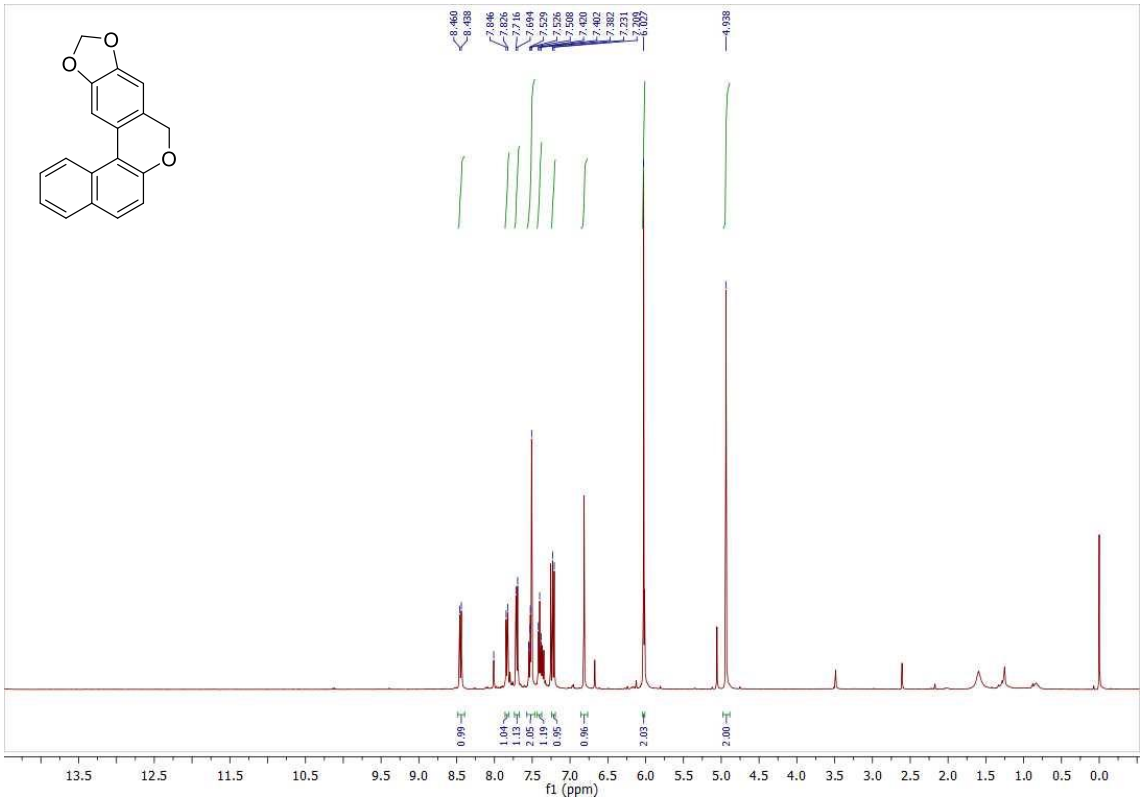


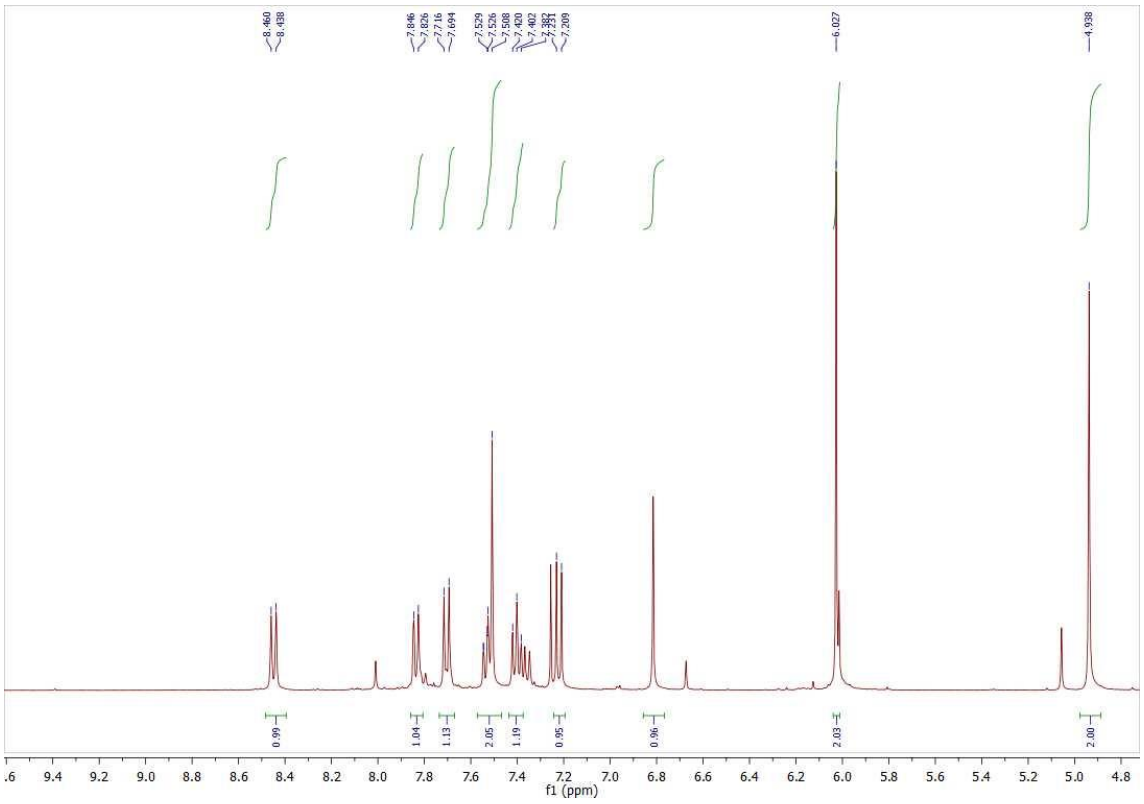
^{13}C NMR{1H} (101 MHz, $CDCl_3$). 2-Fluoro-5*H*-dibenzo[*c,f*]chromene (**1s**).



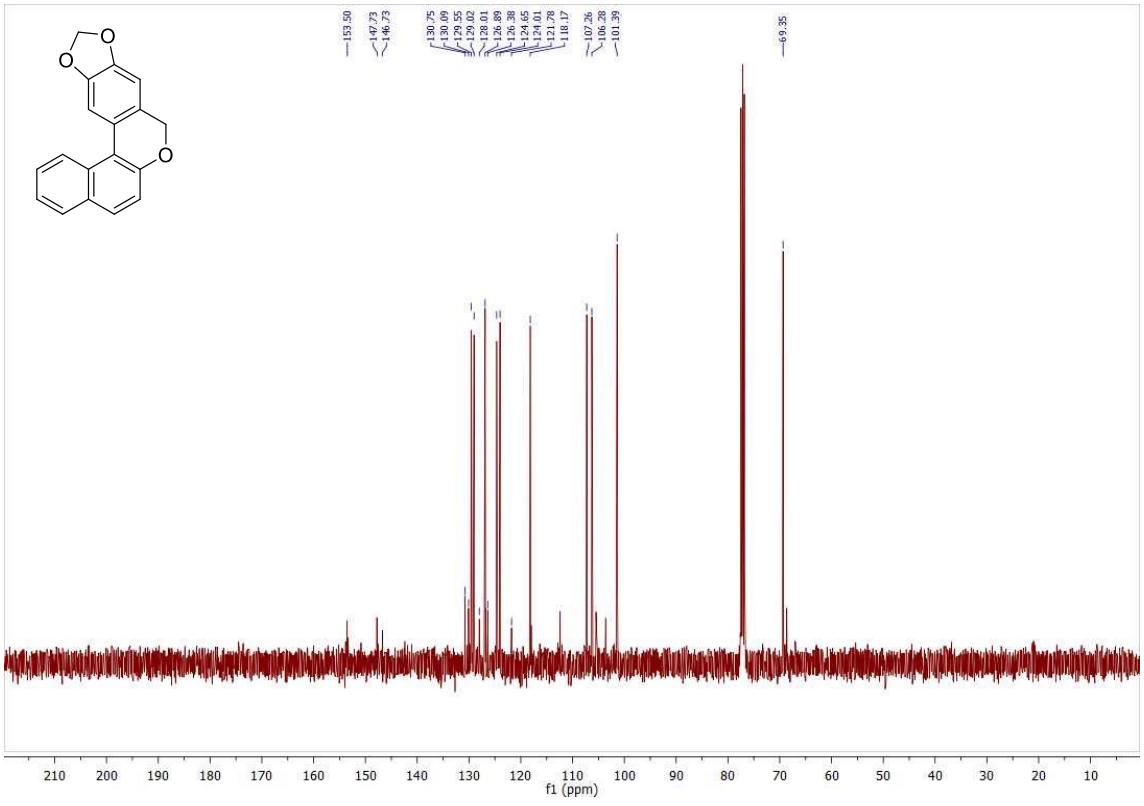


^{1}H-NMR (400 MHz, $CDCl_3$). 8H-[1,3]dioxolo[4',5':4,5]benzo[1,2-c]benzo[f]chromene (**1u**).





^{13}C NMR{1H} (101 MHz, $CDCl_3$). 8H-[1,3]dioxolo[4',5':4,5]benzo[1,2-c]benzo[f]chromene (**1u**).



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