Electronic Supporting Information (ESI)

Synthesis of 2-phenylnaphthalenes from styryl-2-methoxybenzenes

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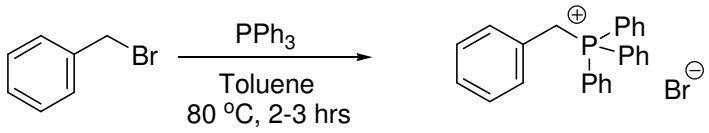
CONTENTS

S1. EXPERIMENTAL PROCEDURES AND SPECTRAL DATA

S1.a. General Information

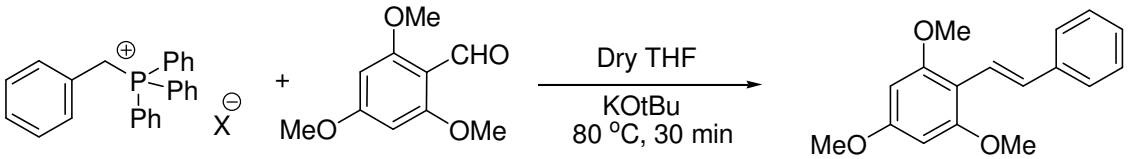
All chemicals were obtained from Sigma-Aldrich Company and used as received. ^{1}H, ^{13}C and DEPT NMR spectra were recorded on Brucker-Avance DPX FT-NMR 500 and 400 MHz instruments. Chemical data for protons are reported in parts per million (ppm) downfield from tetramethylsilane and are referenced to the residual proton in the NMR solvent ($CDCl_3$, 7.26 ppm). Carbon nuclear magnetic resonance spectra (^{13}C NMR) were recorded at 125 MHz or 100 MHz: chemical data for carbons are reported in parts per million (ppm, δ scale) downfield from tetramethylsilane and are referenced to the carbon resonance of the solvent ($CDCl_3$, 77 ppm). ESI-MS and HRMS spectra were recorded on Agilent 1100 LC-Q-TOF and HRMS-6540-UHD machines. IR spectra were recorded on Perkin-Elmer IR spectrophotometer. Melting points were recorded on digital melting point apparatus.

S1.b. General procedure for preparation of benzyl triphenylphosphinebromide salts (Wittig salts).



To the solution of benzyl bromide (1 g, 5.88 mmol) in toluene (15 ml) was added triphenylphosphine (1.69 g, 6.46 mmol) and the resulting reaction mixture was refluxed at 80 °C for 2-3 hrs. The formation of white solid was observed in the reaction mixture. The reaction mixture was allowed to cool to room temperature and then was filtered. The solid residue was washed with toluene (15 ml x 3). The obtained solid residue was dried under vacuum to get benzyltriphenylphosphine bromide salts (> 95% yield).

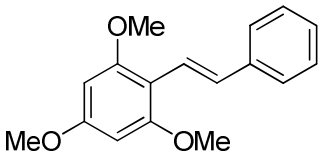
S1.c. General procedure for preparation of (E/Z)-1-styryl methoxybenzenes 1a-1z



1a

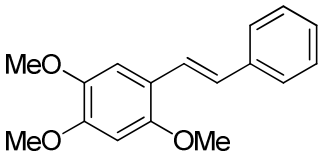
To the stirred solution of benzyl triphenylphosphine halide salts (2.8 mmol) in anhydrous THF (10 ml) under N_2 atmosphere, was added potassium tert-butoxide (3.0 mmol) in small portions at 0-5 °C and the

resulting mixture stirred at 80 °C for 30 min. Formation of orange color was observed in the reaction. Reaction was cooled to the room temperature and respective 2-methoxy benzaldehyde (0.5 g, 2.5 mmol) was added. The resulting reaction mixture was again refluxed at 80 °C for 30 min. Reaction mixture was quenched with ethyl acetate (10 ml), and solvent was evaporated under vaccum, followed by partitioning between water and ethyl acetate (50 ml x 2). The organic layer was collected, dried on anhydrous sodium sulphate and evaporated on rotary evaporator to get the crude product. The crude product was purified by silica gel (#100-200) column chromatography using 20% EtOAc: hexane to get (E/Z)-1-styryl methoxybenzenes **1a-1z** in 78-95% of yield. The ratio of cis/trans isomer in isolated products was determined by HPLC (ratios are mentioned below; and HPLC chromatograms are provided in section S9).



1a

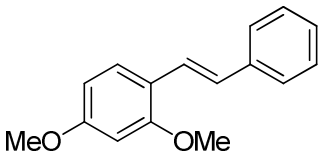
(E/Z)-1-Styryl-2,4,6-trimethoxybenzene (**1a).** mixture of cis/trans isomers (43: 56 ratio, determined based on HPLC); Light yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz) of trans-isomer: δ 7.51 (d, J = 7.6 Hz, 2H), 7.43 (d, J = 12.4 Hz, 1H), 7.33 (t, J = 7.6 Hz, 2H), 7.19 (m, 2H), 6.16 (s, 2H), 3.87 (s, 6H), 3.83 (s, 3H); ^{1}H NMR ($CDCl_3$, 400 MHz) of cis-isomer: δ 7.48 (m, 1H), 7.43 (m, 1H), 7.36 (m, 1H), 7.19 (d, J = 7.6 Hz, 1H), 7.12 (m, 1H), 6.67 (d, J = 12 Hz, 1H), 6.42 (d, J = 12.4 Hz, 1H), 6.10 (s, 2H), 3.82 (s, 3H), 3.57 (s, 6H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.8, 160.2, 159.5, 158.3, 139.6, 139.0, 131.1, 129.9, 128.4, 127.8, 127.6, 126.5, 126.1, 120.9, 119.8, 108.1, 90.7, 90.6, 55.8, 55.4, 55.3; IR ($CHCl_3$): ν_{max} 3436, 3079, 3056, 3000, 2959, 2936, 2533, 2155, 2109, 1955, 1726, 1605, 1594, 1584, 1514, 1497, 1466, 1455, 1436, 1377, 1331, 1271, 1214, 1205, 1190, 1155, 1140, 1122, 1072, 1060, 1038 cm^{-1}; ESI-MS: *m/z* 271.1 $[M+H]^+$.



1b

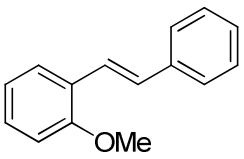
(E,Z)-1-Styryl-2,4,5-trimethoxybenzene (1b). mixture of cis/trans isomers (20: 80 ratio, determined by ^{1}H NMR); Light yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz) of mixture of cis/trans-isomer: δ 7.52 (d, J = 7.6 Hz, 1H), 7.46 (d, J = 16.4 Hz, 1H), 7.35 (m, 2H), 7.28 (m, 2H), 7.21 (m, 3H), 7.16 (m, 3H), 6.99 (d, J = 16.4 Hz, 1H), 6.70 (m, 2H), 6.55 (m, 3H), 3.91 (s, 12H), 3.81 (s, 3H), 3.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100

MHz): δ 151.8, 149.6, 149.1, 143.5, 142.4, 138.1, 137.7, 128.8, 128.6, 128.1, 127.0, 126.8, 126.3, 125.0, 123.0, 118.3, 117.4, 113.3, 109.5, 97.8, 97.3, 56.7, 56.6, 56.1, 56.0, 55.9; IR ($CHCl_3$): ν_{max} 3436, 3077, 3053, 2999, 2935, 2832, 1734, 1608, 1583, 1512, 1491, 1465, 1410, 1328, 1163, 1110 cm^{-1}; ESI-MS: *m/z* 271.1 $[M+H]^+$.



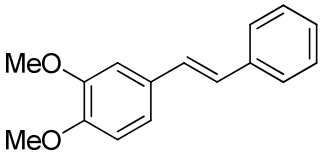
1c

(E,Z)-1-Styryl-2,4-dimethoxybenzene (1c). Mixture of cis/trans isomers (73: 25 ratio, determined based on HPLC), Light yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.50 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 16.4 Hz, 1H), 7.32-7.03 (m, 10H), 7.01 (d, *J* = 16.4 Hz, 1H), 6.63 (d, *J* = 12.4 Hz, 1H), 6.54-6.43 (m, 4H), 6.28 (d, 8.4 Hz, 1H), 3.82 (s, 3H), 3.79 (s, 3H), 3.76 (s, 3H), 3.74 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.6, 160.4, 158.3, 158.1, 138.3, 137.7, 130.6, 129.0, 128.8, 128.6, 128.1, 127.2, 127.0, 126.7, 126.3, 125.4, 123.3, 119.5, 118.8, 105.0, 104.2, 98.5, 98.3, 55.55, 55.50, 55.44, 55.34; IR ($CHCl_3$): ν_{max} 3053, 3003, 2957, 2936, 2835, 2592, 1950, 1882, 1608, 1576, 1503, 1490, 1463, 1438, 1417, 1288, 1208, 1183, 1159, 1118, 1107, 1072 cm^{-1} ; ESI-MS: *m/z* 241.1 $[M+H]^+$.



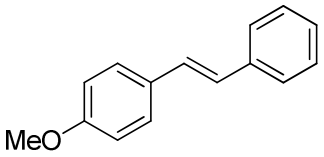
1d

(E,Z)-1-Styryl-2-methoxybenzene (1d). Mixture of cis/trans isomers (92.2: 7.8 ratio, determined based on HPLC), colourless oil; ^{1}H NMR ($CDCl_3$, 400 MHz) of cis-isomer (92%): δ 7.23-7.12 (m, 7H), 6.89 (d, *J* = 8.0 Hz, 1H), 6.76-6.60 (m, 3H), 3.81 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.2, 137.3, 130.2, 130.1, 128.8, 128.6, 128.0, 126.9, 126.2, 125.8, 120.2, 110.7, 55.4 ; IR ($CHCl_3$): ν_{max} 3436, 2938, 2850, 1590, 1513, 1462, 1446, 1418, 1311, 1259, 1224, 1153, 1138, 1025 cm^{-1} ; ESI-MS: *m/z* 211.1 $[M+H]^+$



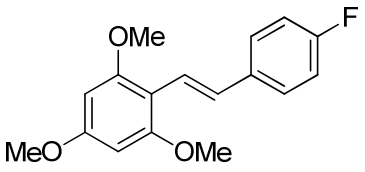
1e

(E)-1-Styryl-3,4-dimethoxybenzene (1e). Trans-isomer (100% determined based on HPLC); White amorphous solid; m.p. 121-122 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ 7.44 (d, J = 7.2 Hz, 2H), 7.30 (t, J = 7.2 Hz, 2H), 7.20 (d, J = 7.2 Hz, 1H), 7.01-6.89 (m, 4H), 6.74 (d, J = 8.4 Hz, 1H), 3.84 (s, 3H), 3.77 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 149.2, 149.0, 137.6, 130.5, 128.7, 128.5, 127.3, 126.8, 126.4, 120.0, 111.3, 109.0, 55.9, 55.8; IR ($CHCl_3$): ν_{max} 3436, 2938, 2839, 1590, 1513, 1462, 1446, 1418, 1311, 1259, 1224, 1154, 1138, 1025 cm^{-1}; ESI-MS: *m/z* 241.1 $[M+H]^+$.



1f

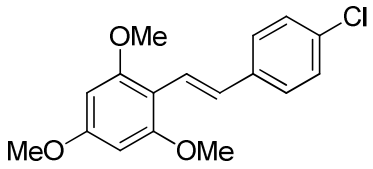
(E,Z)-1-Styryl-4-methoxybenzene (1f). Mixture of cis/trans isomers (1.3: 98.6 ratio determined based on HPLC); white amorphous solid; m.p. 106-108 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) of cis/trans isomers: δ 7.49 (dd, J = 7.2, 8.8 Hz, 3H), 7.34 (t, J = 7.6 Hz, 2H), 7.28-7.16 (m, 9H), 7.08-6.95 (m, 2H), 6.90 (d, J = 8.8 Hz, 2H), 6.76 (d, J = 8.8 Hz, 2H), 6.51 (d, J = 1.6 Hz, 2H), 3.82 (s, 3H), 3.77 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.3, 158.6, 137.6, 130.1, 129.7, 129.6, 128.8, 128.7, 128.69, 128.67, 128.25, 128.22, 127.7, 127.2, 126.9, 126.6, 126.5, 126.2, 114.1, 113.5, 55.3, 55.2; IR ($CHCl_3$): ν_{max} 3745, 3436, 3078, 3053, 3021, 2961, 2934, 2836, 1605, 1510, 1463, 1446, 1421, 1297, 1252, 1179, 1150, 1112, 1072 cm^{-1}; ESI-MS: *m/z* 211.1 $[M+H]^+$.



1g

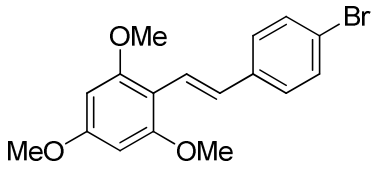
(E,Z)-1-(4′-Fluorostyryl)-2,4,6-trimethoxybenzene (1g). Mixture of cis/trans isomers (17.1: 82.8 ratio determined based on HPLC); brown crystalline solid; m.p. 70-72 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) of trans-isomer: δ 7.47 (m, 2H), 7.43-7.39 (d, J = 16.4 Hz, 1H), 7.31-7.27 (d, J = 16.4 Hz, 1H), 7.0 (t, J = 8.8 Hz, 2H), 6.16 (s, 2H), 3.86 (s, 6H), 3.82 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) of mixture of cis/trans isomers: δ 163.0 ($^1J_{CF}$ = 243.8 Hz), 160.3, 159.4, 158.4, 135.9, 135.8, 129.8, 129.46, 129.38, 128.7, 127.54, 127.46, 120.7, 119.64, 115.3 ($^2J_{CF}$ = 21.3 Hz), 114.5 ($^2J_{CF}$ = 21.3 Hz), 108.0, 90.8, 55.8, 55.4, 55.3; ^{19}F NMR ($CDCl_3$, 376.5 MHz): δ -115.63 (m, 1F), -116.29 (m, 1F); IR ($CHCl_3$): ν_{max} 3400, 2919,

2850, 1904, 1733, 1605, 1579, 1508, 1455, 1417, 1331, 1223, 1205, 1155, 1118, 1094, 1038, 1019 cm^{-1}; ESI-MS: *m/z* 289.1 $[M+H]^+$.



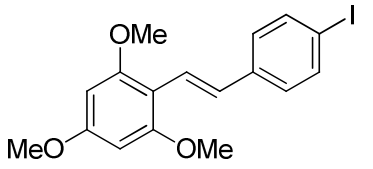
1h

(E)-1-(4′-Chlorostyryl)-2,4,6-trimethoxybenzene (1h). Trans-isomer (96.4% determined based on HPLC); white crystalline solid; m.p. 98-100 °C; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.43 (d, J = 8.8 Hz, 2H), 7.38 (d, J = 4.4 Hz, 2H), 7.27 (d, J = 8.8 Hz, 2H), 6.16 (s, 2H), 3.87 (s, 6H), 3.83 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.4, 159.6, 138.2, 131.9, 128.5, 128.4, 127.3, 120.5, 107.8, 90.8, 55.7, 55.3; IR ($CHCl_3$): ν_{max} 3400, 2922, 2851, 1741, 1603, 1581, 1494, 1385, 1331, 1205, 1118, 1156, 1020 cm^{-1} ; ESI-MS: *m/z* 305.0 $[M+H]^+$.



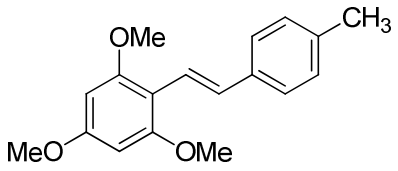
1i

(E)-1-(4′-Bromostyryl)-2,4,6-trimethoxybenzene (1i). Trans-isomer (96.9% determined based on HPLC); brown crystalline solid; m.p. 95-96 °C; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.41-7.33 (m, 6H), 6.13 (s, 2H), 3.84 (s, 6H), 3.80 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.7, 159.6, 138.7, 131.4, 128.4, 127.6, 120.6, 120.0, 107.8, 90.8, 55.7, 55.3; IR ($CHCl_3$) : ν_{max} 3368, 3000, 2924, 2850, 1740, 1602, 1580, 1492, 1466, 1455, 1435, 1330, 1214, 1205, 1189, 1175, 1156, 1120, 1062, 1038, 1006 cm^{-1}; ESI-MS: *m/z* 350.8 $[M+H]^+$.



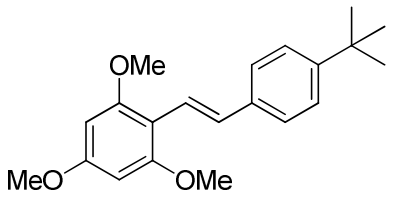
1j

(E)-1-(4′-Iodostyryl)-2,4,6-trimethoxybenzene (1j). Trans-isomer (95.1% determined based on HPLC); brown crystalline solid; m.p. 91-92 °C; ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 7.63 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 3.2 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 6.16 (s, 2H), 3.88 (s, 6H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.4, 159.6, 139.2, 137.4, 128.5, 127.9, 120.6, 107.6, 91.3, 90.7, 55.7, 55.3; IR ($CHCl_3$): ν_{max} 3435, 2924, 2851, 1744, 1603, 1578, 1455, 1416, 1204, 1155, 1121, 1059, 1017, 1002 cm^{-1}; ESI-MS: *m/z* 396.9 $[M+H]^+$.



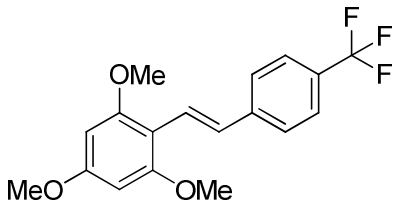
1k

(E/Z)-1-(4′-Methylstyryl)-2,4,6-trimethoxy-benzene (1k). mixture of cis/trans isomers (6.4: 88.8 ratio determined based on HPLC); brown crystalline solid; m.p. 90-92 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) of trans-isomer: δ 7.45-7.31 (m, 4H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.16 (s, 2H), 3.87 (s, 6H), 3.83 (s, 3H), 2.33 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.3, 158.7, 136.2, 135.6, 129.2, 128.5, 125.4, 118.1, 107.6, 90.1, 55.1, 54.7, 20.6; IR ($CHCl_3$) : ν_{max} 3785, 3436, 2923, 2850, 1604, 1585, 1491, 1437, 1416, 1384, 1330, 1214, 1205, 1191, 1155, 1119, 1060, 1033 cm^{-1} ; ESI-MS: *m/z* 285.1 $[M+H]^+$.



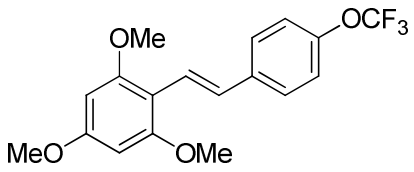
1l

(E)-1-(4′-(Tert-butyl)styryl)-2,4,6-trimethoxybenzene (1l). Trans-isomer (99.7% determined based on HPLC); white crystalline solid; m.p. 83-84 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.45 (t, *J* = 8.4 Hz, 3H), 7.35 (m, 3H), 6.16 (s, 2H), 3.86 (s, 6H), 3.83 (s, 3H), 1.32 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.0, 159.4, 149.5, 136.9, 129.8, 125.8, 125.3, 119.2, 108.3, 90.8, 55.8, 55.3, 34.5, 31.3; IR ($CHCl_3$): ν_{max} 2960, 1837, 1729, 1601, 1581, 1514, 1465, 1416, 1363, 1330, 1270, 1217, 1204, 1155, 1116, 1061, 1039 cm^{-1}; ESI-MS: *m/z* 327.1 $[M+H]^+$.



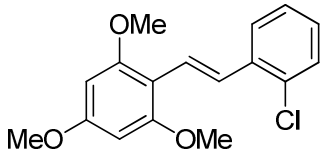
1m

(E/Z)-1-(4′-(Trifluoromethyl) styryl)-2,4,6-trimethoxybenzene (1m). Mixture of cis/trans isomers (5.5: 94.4 ratio based on HPLC); brown crystalline solid; m.p. 84-86 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) of trans-isomer: δ7.58-7.53 (m, 4H), 7.48 (s, 2H), 6.17 (s, 2H), 3.89 (s, 6H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.8, 159.7, 143.3, 128.0, 127.8, 126.1, 125.6, 125.35 (q, $^{1}J_{CF}$ = 3.7 Hz), 123.4, 122.4, 107.5, 90.7, 55.8, 55.3; ^{19}F NMR ($CDCl_3$, 376.5 Hz): δ-62.22 (s, 3F); IR ($CHCl_3$): ν_{max} 3435, 3002, 2938, 2638, 1919, 1725, 1601, 1516, 1490, 1468, 1457, 1437, 1419, 1270, 1217, 1206, 1193, 1184, 1156, 1119, 1108, 1065, 1038, 1014; ESI-MS: *m/z* 339.1 $[M+H]^+$.



1n

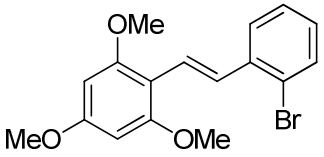
(E)-1-(4′-(Trifluoromethoxy)styryl)-2,4,6-trimethoxybenzene (1n). Trans-isomer (99.1% based on HPLC); white crystalline solid; m.p. 65-67 °C ; ^{1}H NMR ($CDCl_3$, 400 MHz): δ7.50 (m, 4H), 7.16 (d, *J* = 7.2 Hz, 2H), 6.17 (s, 2H), 3.88 (s, 6H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ160.4, 159.5, 147.7, 138.5, 128.2, 127.2, 121.0, 120.8, 107.7, 90.8, 55.8, 55.3; ^{19}F-NMR ($CDCl_3$, 376.5 Hz): δ-57.84 (s, 3F); IR ($CHCl_3$): ν_{max} 3401, 2938, 2840, 1605, 1507, 1456, 1419, 1331, 1257, 1218, 1203, 1156, 1121, 1062, 1039, 1016 cm^{-1}; ESI-MS: *m/z* 355.0 $[M+H]^+$.



1o

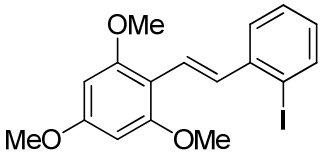
(E,Z)-1-(2′-Chlorostyryl)-2,4,6-trimethoxybenzene (1o). Mixture of cis/trans isomers (5.8: 94.1 ratio based on HPLC); White amorphous solid; m.p. 94-95 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) of trans-isomer: δ

7.87 (d, *J* = 16.4 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.38 (m, 2H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 1H), 6.16 (s, 2H), 3.88 (s, 6H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.6, 159.7, 137.8, 133.0, 129.5, 127.4, 126.7, 126.1, 125.8, 122.2, 108.1, 90.8, 55.8, 55.3; IR ($CHCl_3$): ν_{max} 3785, 2923, 2850, 1737, 1604, 1585, 1491, 1468, 1437, 1416, 1384, 1330, 1214, 1205, 1191, 1155, 1119, 1060, 1033 cm^{-1}; ESI-MS: 305.0 $[M+H]^+$.



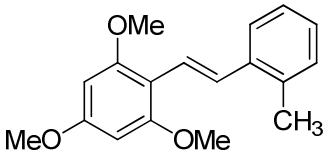
1p

(E)-1-(2′-Bromostyryl)-2,4,6-trimethoxybenzene (1p). Trans-isomer (98.2% determined based on HPLC); white crystalline solid; m.p. 109-111 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.84 (d, *J* = 16.8 Hz, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.35-7.26 (m, 2H), 7.06 (m, 1H), 6.18 (s, 2H), 3.90 (s, 6H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.6, 159.7, 139.4, 132.8, 128.5, 127.7, 127.4, 126.3, 123.9, 122.3, 107.9, 90.7, 55.8, 55.3; IR ($CHCl_3$): ν_{max} 3400, 3058, 3000, 2959, 2935, 2837, 2532, 1956, 1822, 1742, 1604, 1582, 1491, 1467, 1435, 1416, 1346, 1330, 1277, 1258, 1191, 1177, 1156, 1120, 1061, 1038, 1021 cm^{-1}; ESI-MS: *m/z* 350.8 $[M+H]^+$



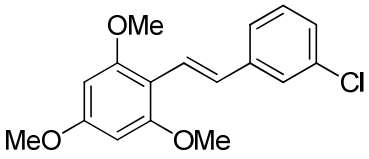
1q

(E)-1-(2′-Iodostyryl)-2,4,6-trimethoxybenzene (1q). Trans-isomer (99.2% determined based on HPLC); white crystalline solid; m.p. 121-122 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 16.5 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.32 (m, 2H), 6.88 (t, *J* = 7.5 Hz, 1H), 6.16 (s, 2H), 3.89 (s, 6H), 3.83 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.6, 159.7, 142.5, 139.4, 133.5, 128.8, 128.0, 125.7, 122.4, 107.8, 100.7, 90.7, 55.9, 55.4; IR ($CHCl_3$): ν_{max} 3436, 2921, 2850, 1603, 1578, 1457, 1432, 1416, 1384, 1330, 1216, 1155, 1119, 1020 cm^{-1}; ESI-MS: *m/z* 396.9 $[M+H]^+$.



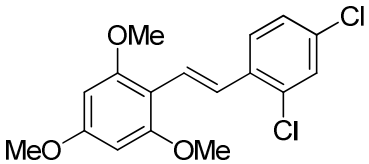
1r

(E)-1-(2′-Methylstyryl)-2,4,6-trimethoxy-benzene (1r). Trans-isomer (95.4% determined based on HPLC); white crystalline solid; m.p. 96-98 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.68 (m, 2H), 7.26-7.09 (m, 4H), 6.17 (s, 2H), 3.87 (s, 6H), 3.83 (s, 3H), 2.38 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.1, 159.4, 138.7, 135.3, 130.1, 128.1, 126.5, 126.0, 124.9, 120.7, 108.5, 90.8, 55.8, 55.3, 20.0; IR ($CHCl_3$): ν_{max} 3000, 2937, 2837, 1605, 1587, 1491, 168, 1455, 1418, 1330, 1212, 1191, 1156, 1120, 1061, 1038 cm^{-1}; ESI-MS: *m/z* 285.1 $[M+H]^+$.



1s

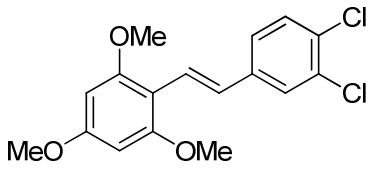
(E)-1-(3′-Chlorostyryl)-2,4,6-trimethoxybenzene (1s). Trans-isomer (98.6% determined based on HPLC); white crystalline solid; m.p. 81-83 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.49 (s, 1H), 7.39 (s, 2H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.15 (d, *J* = 8.0 Hz, 1H), 6.16 (s, 2H), 3.88 (s, 6H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.6, 159.7, 141.7, 134.4, 129.6, 128.3, 126.3, 125.9, 124.4, 121.3, 107.7, 90.8, 55.8, 55.3; IR ($CHCl_3$): ν_{max} 3000, 2937, 2837, 1605, 1587, 1491, 1468, 1455, 1410, 1330, 1212, 1156, 1120, 1061, 1038 cm^{-1}; ESI-MS: *m/z* 305.0 $[M+H]^+$.



1t

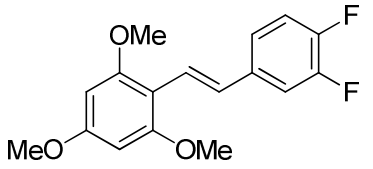
(E)-1-(2′,4′-Dichlorostyryl)-2,4,6-trimethoxybenzene (1t). Trans-isomer (99.2% determined based on HPLC); white crystalline solid; m.p. 129-131 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.79 (d, *J* = 16.4 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.36 (m, 2H), 7.20 (d, *J* = 8.4 Hz, 1H), 6.15 (s, 2H), 3.88 (s, 6H), 3.83 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.8, 159.7, 136.4, 133.3, 132.0, 129.2, 127.0, 126.8, 124.6, 122.7,

107.7, 90.7, 55.8, 55.3 ; IR ($CHCl_3$): ν_{max} 3435, 2922, 2851, 1743, 1603, 1579, 1513, 1466, 1414, 1384, 1327, 1249, 1215, 1204, 1156, 1118, 1099, 1019 cm^{-1}; ESI-MS: *m/z* 339.0 $[M+H]^+$.



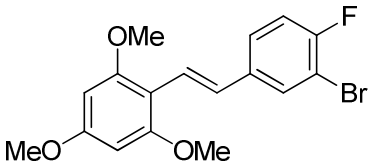
1u

(E,Z)-1-(3′,4′-Dichlorostyryl)-2,4,6-trimethoxybenzene(1u). Mixture of cis/trans isomers (10.6: 89.3 ratio determined based on HPLC); white amorphous solid; m.p. 104-105 °C; ^1H NMR ($CDCl_3$, 400 MHz) of trans-isomer: δ 7.56 (d, J = 2.0 Hz, 1H), 7.37-7.29 (m, 4H), 6.16 (s, 2H), 3.88 (s, 6H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.7, 159.7, 140.0, 132.3, 130.2, 129.6, 127.6, 127.0, 125.3, 121.7, 107.3, 90.6, 55.7, 55.3; IR ($CHCl_3$): ν_{max} 3436, 3003, 2936, 2839, 2483, 1898, 1605, 1587, 1577, 1507, 1469, 1457, 1437, 1420, 1384, 1331, 1258, 1219, 1204, 1188, 1156, 1121, 1062, 1039, 1016 cm^{-1}; ESI-MS: *m/z* 339.0 $[M+H]^+$.



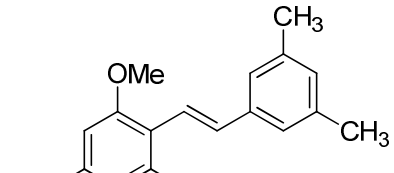
1v

(E,Z)-1-(3′,4′-Difluorostyryl)-2,4,6-trimethoxybenzene (1v). Mixture of cis/trans isomers (6.8: 93.1 ratio determined based on HPLC); white crystalline solid; m.p. 79-80 °C; ^1H NMR ($CDCl_3$, 400 MHz) of trans-isomer: δ 7.34-7.25 (m, 3H), 7.15 (m, 1H), 7.10- 7.04 (m, 1H), 6.16 (s, 2H), 3.88 (s, 6H), 3.83 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.5, 159.5, 151.5 ($^1J_{CF}$ = 176 Hz), 150.1 ($^1J_{CF}$ = 176 Hz), 137.1, 127.5, 122.2, 120.9, 117.0 (d, $^2J_{CF}$ = 17.1 Hz), 114.1 (d, $^2J_{CF}$ = 17.2 Hz), 107.4, 90.7, 55.7, 55.3; ^{19}F NMR ($CDCl_3$, 376.5 Hz): δ -138.73 (m, 1F), -141.08 (m, 1F); IR ($CHCl_3$): ν_{max} 3008, 2939, 2840, 2153, 1581, 1514, 1463, 1432, 1414, 1349, 1323, 1293,1201, 1271, 1223, 1150, 1120,1061, 1037 cm^{-1}; ESI-MS: *m/z* 307.1 $[M+H]^+$.



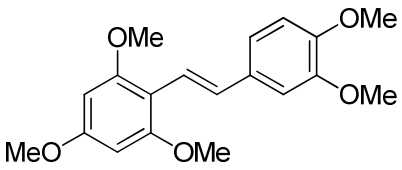
1w

(E)-1-(3′-Bromo-4′-fluorostyryl)-2,4,6-trimethoxybenzene (1w). Trans-isomer (90% determined based on HPLC); white amorphous solid; m.p. 110-112 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.67 (d, J = 7.0 Hz, 1H), 7.39-7.25 (m, 3H), 7.07 (t, J = 8.5 Hz, 1H), 6.16 (s, 2H), 3.88 (s, 6H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.7, 158.7, 157.8 (d, $^{1}J_{CF}$ = 244 Hz), 136.7, 129.7, 126.3, 125.6, 120.0, 115.5 (d, $^{2}J_{CF}$ = 22.2 Hz), 108.2 (d, $^{2}J_{CF}$ = 21 Hz), 106.6, 89.8, 54.9, 54.5; ^{19}F NMR ($CDCl_3$, 376.5 Hz): δ -111.06 (m, 1F); IR ($CHCl_3$): ν_{max} 3436, 3003, 2923, 2838, 1726, 1608, 1581, 1496, 1469, 1455, 1436, 1420, 1344, 1260, 1247, 1216, 1202, 1192, 1158, 1118, 1061, 1039 cm^{-1}; ESI-MS: *m/z* 366.9 $[M+H]^+$.



1x

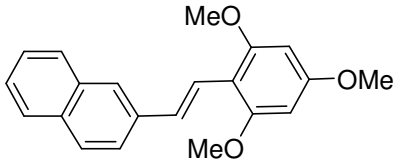
(E)-1-(3′,5′-Dimethylstyryl)-2,4,6-trimethoxybenzene (1x). Trans-isomer (98.3% determined based on HPLC); white crystalline solid; m.p. 145-147 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.42-7.31 (dd, J = 12.4, 16.8 Hz, 2H), 7.13 (s, 2H), 6.83 (s, 1H), 6.16 (s, 2H), 3.87 (s, 6H), 3.83 (s, 3H), 2.32 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.1, 159.5, 139.5, 137.7, 130.3, 128.3, 124.1, 119.4, 108.4, 90.9, 55.8, 55.3, 21.3; IR ($CHCl_3$): ν_{max} 3001, 2920, 2850, 1737, 1603, 1580, 1490, 1457, 1411, 1329, 1222, 1200, 1156, 1113, 1063, 1031 cm^{-1}; ESI-MS: *m/z* 299.1 $[M+H]^+$.



1y

(E)-1-(3′,4′-Dimethoxystyryl)-2,4,6-trimethoxybenzene (1y). Trans-isomer (93.7% determined based on HPLC); white amorphous solid; m.p. 124-126 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.41 (d, J = 16.4 Hz, 1H), 7.25 (d, J = 16.4 Hz, 1H), 7.06 (d, J = 13.6 Hz, 2H), 6.84 (d, J = 8.0 Hz, 1H), 6.17 (s, 2H), 3.94 (s,

3H), 3.88 (s, 9H), 3.83 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ159.9, 159.3, 148.9, 148.1, 132.8, 129.8, 119.1, 118.1, 111.1, 108.8, 108.2, 90.8, 55.9, 55.88, 55.81, 55.3; IR ($CHCl_3$): ν_{max} 3435, 2998, 2932, 2835, 1604, 1577, 1513, 1464, 1418, 1330, 1263, 1231, 1203, 1155, 1117, 1060, 1025 cm^{-1}; ESI-MS: *m/z* 331.1 $[M+H]^+$.

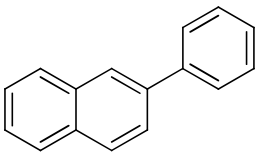


1z

(E,Z)-2-(2′,4′,6′-Trimethoxystyryl)naphthalene (1z). Mixture of cis/trans isomers (33: 67 ratio determined based on HPLC); white amorphous solid; m.p. 93-94 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ7.81 (m, 6H), 7.72 (m, 2H), 7.61 (s, 1H), 7.55 (m, 2H), 7.44-7.36 (m, 4H), 7.31 (d, *J* = 8.8 Hz, 1H), 6.82 (d, *J* = 12.0 Hz, 1H), 6.51 (d, *J* = 12.4 Hz, 1H), 6.19 (s, 2H), 6.12 (s, 2H), 3.91 (s, 6H), 3.84 (s, 6H), 3.53 (s, 6H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ160.9, 160.2, 159.5, 158.4, 137.2, 136.8, 133.8, 133.2, 132.6, 132.4, 130.9, 129.8, 128.0, 127.9, 127.8, 127.6, 127.4, 127.0, 126.7, 126.0, 125.9, 125.7, 125.6, 125.4, 125.2, 123.7, 121.3, 120.2, 108.0, 90.7, 90.5, 55.8, 55.4, 55.3, 53.4; IR ($CHCl_3$): ν_{max} 3436, 2923, 2849, 1737, 1603, 1455, 1415, 1330, 1224, 1204, 1156, 1060, 1038 cm^{-1}; ESI-MS: *m/z* 321.1 $[M+H]^+$.

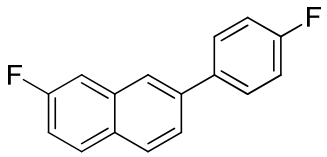
S1.(d). General procedure for synthesis of 2-phenylnaphthalenes 2a-2u

The solution of 2-methoxy-1-styrylbenzenes **1a**-**1z** (100 mg, 0.49 mmol) in 50% trifluoroacetic acid in water (1 ml) or 100% TFA (0.5 ml) was stirred at 80 °C for 30 min. Reaction was monitored with TLC using 100% n-hexane as an eluent. Reaction mixture was then cooled to room temperature and neutralized slowly with saturated $NaHCO_3$ solution; and extracted with ethyl acetate (25 ml x 2). The combined organic layer was dried over anhydrous sodium sulphate and evaporated on vacuo rotavapor to get crude product. The crude product was purified by silica gel (#60-120) column chromatography using 100% n-hexane as an eluent to get pure product **2a-2u** in 80-99% yield.



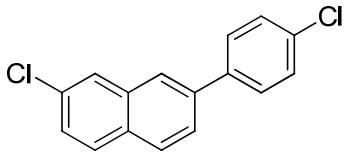
2a 1

2-Phenylnaphthalene (2a). Yield: 94%; white crystalline solid; m.p. 102-103 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.08 (s, 1H), 7.95 (m, 3H), 7.79 (t, J = 8.4 Hz, 3H), 7.55-7.49 (m, 4H), 7.42 (t, J = 6.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.2, 138.7, 133.8, 132.7, 128.9, 128.5, 128.3, 127.7, 127.5, 127.4, 126.4, 126.0, 125.9, 125.7; IR ($CHCl_3$): ν_{max} 3436, 3054, 2922, 2850, 1916, 1598, 1500, 1451, 1402, 1383, 1260, 1239,1192, 1129, 1090, 1019 cm^{-1}; GC-MS: *m/z* (EI) 204 (M^+, 100), 205 (M+1, 13), 203 (M-1, 23), 101.6 (5).



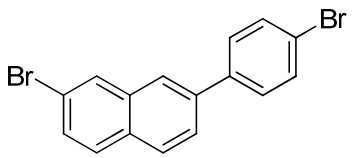
2b

2-(4′-Fluorophenyl)-7-fluoronaphthalene (2b). Yield: 98%; white crystalline solid; m.p. 91-92 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91-7.89 (m, 2H), 7.85 (dd, J = 5.6, 8.8 Hz, 1H), 7.68-7.64 (m, 3H), 7.50 (d, J = 10 Hz, 1H), 7.28-7.24 (m, 1H), 7.18 (t, J = 8.8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.7 (d, $^1J_{CF}$ = 207 Hz), 161.7 (d, $^1J_{CF}$ = 207 Hz), 138.6, 136.8, 134.5, 130.2, 129.5, 129.0, 128.6, 125.0, 124.8, 116.5 (d, $^2J_{CF}$ = 25 Hz), 115.9 (d, $^2J_{CF}$ = 21 Hz), 111.2 (d, $^2J_{CF}$ = 20 Hz); ^{19}F NMR ($CDCl_3$, 376.5 Hz): δ -114.16 (m, 1F), -115.17 (m, 1F); IR ($CHCl_3$): ν_{max} 3435, 3065, 2922, 2858, 1893, 1630, 1590, 1523, 1506, 1461, 1402, 1369, 1224, 1208, 1157, 1144, 1102, 1019 cm^{-1}; GC-MS: *m/z* (EI) 240 (M^+, 100), 241 (M+1, 16), 220 (8), 181 (1), 144 (1), 110 (5), 107 (2), 74 (2), 50 (1).



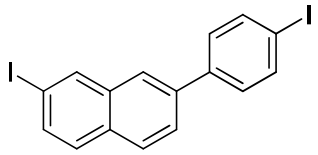
2c

2-(4′-Chlorophenyl)-7-chloronaphthalene (2c). Yield: 90%; white crystalline solid; m.p. 123-125 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.89 (m, 3H), 7.79 (d, J = 8.0 Hz, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.62 (d, J = 8.0 Hz, 2H), 7.46 (m , 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) : δ 139.1, 138.4, 134.2, 133.8, 132.2, 130.9, 129.2, 129.1, 128.6, 128.5, 127.1, 126.8, 125.5, 124.8; IR ($CHCl_3$): ν_{max} 3435, 2921, 2851, 1906, 1623, 1592, 1512, 1490, 1451, 1419, 1400, 1322, 1160, 1136, 1107, 1078, 1019 cm^{-1}; GC-MS: *m/z* (EI) 272 (M^+, 100), 273 (M+1, 15), 274 (M+2, 63), 236 (11), 202 (67), 136 (4), 118 (7), 100 (14), 87 (7).



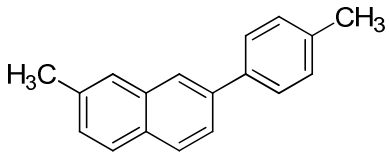
2d

2-(4′-Bromophenyl)-7-bromonaphthalene (2d). Yield: 92%; brown crystalline solid; m.p. 132-133 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.02 (s, 1H), 7.86 (d, *J* = 9.2 Hz, 2H), 7.71-7.65 (m, 2H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.55 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.5, 138.4, 134.7, 132.0, 131.1, 130.1, 129.5, 129.3, 128.9, 128.6, 127.8, 125.6, 124.7, 122.0, 120.5; IR ($CHCl_3$): ν_{max} 3436, 3057, 2852, 2924, 1908, 1754, 1590, 1457, 1395, 1323, 1205, 1152, 1066, 1019 cm^{-1}; GC-MS: *m/z* (EI) 360 (M^+, 48), 362 (M+2, 100), 202 (96), 150 (6), 101 (33), 88 (15), 75 (7), 50 (5).



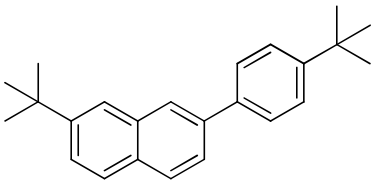
2e

2-(4′-Iodophenyl)-7-iodonaphthalene (2e). Yield: 97%; white amorphous solid; m.p. 191-192 °C; ^{1}H NMR ($CDCl_3$: DMSO-d_6 - 1: 1, 400 MHz): δ 8.38 (s, 1H), 8.10 (d, *J* = 8.4 Hz, 2H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.84-7.78 (m, 2H), 7.73 (m, 2H), 7.56 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR ($CDCl_3$: DMSO-d_6 - 1: 1, 100 MHz): δ 139.2, 137.6, 137.3, 136.3, 134.8, 134.2, 130.9, 129.1, 128.9, 128.4, 125.2, 124.0, 93.5, 92.1; IR ($CHCl_3$): ν_{max} 3435, 2955, 2852, 2347, 1743, 1620, 1582, 1541, 1444, 1410, 1384, 1323, 1219, 1140, 1095, 1019 cm^{-1}.



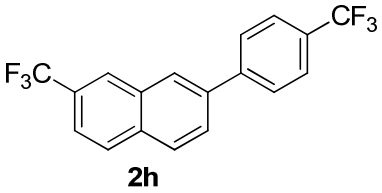
2f

2-(p-Tolyl)-7-methylnaphthalene (2f). Yield: 92%; white crystalline solid; m.p. 136-137 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (s, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.67 (m, 2H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.31 (m, 3H), 2.52 (s, 3H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 138.5, 138.4, 137.0, 135.9, 130.7, 129.6, 128.1, 128.0, 127.4, 127.2, 127.1, 124.8, 124.7, 21.8, 21.1; IR ($CHCl_3$): ν_{max} 3785, 3435, 3055, 3031, 2920, 2852, 1896, 1812, 1738, 1605, 1450, 1385, 1334, 1313, 1273, 1194, 1136, 1110, 1038, 1020 cm^{-1}; GC-MS: *m/z* (EI) 232 (M^+, 100), 233 (M+1, 18), 217 (25), 189 (5), 115 (8).



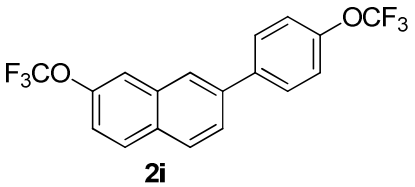
2g

2-(4′-(Tert-butyl) phenyl)-7-(tert-butyl) naphthalene (2g). Yield: 90%; white crystalline solid; m.p. 166-167 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.01 (s, 1H), 7.85 (m, 3H), 7.7 (m, 3H), 7.75 (d, J = 8.8 Hz, 1H), 7.51 (d, J = 8.4 Hz, 2H), 1.43 (s, 9H), 1.38 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 150.2, 148.9, 138.3, 138.2, 133.6, 130.7, 127.7, 127.2, 126.9, 125.7, 125.5, 124.9, 124.7, 123.1, 34.8, 34.5, 31.4, 31.2; IR ($CHCl_3$): ν_{max} 3436, 3065, 2952, 2862, 1737, 1628, 1500, 1461, 1362, 1019 cm^{-1}; GC-MS: *m/z* (EI) 316 (M^+, 90), 317 (M+1, 15), 301 (100), 273 (4), 245 (5), 215 (8), 202 (4), 165 (2), 129 (3), 115 (9).



2h

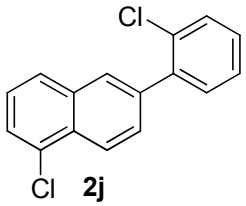
2-(4′-(Trifluoromethyl) phenyl)-7-(trifluoromethyl) naphthalene (2h). Yield: 90%; white crystalline solid; m.p. 85-87 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.23 (s, 1H), 8.14 (s, 1H), 8.02 (t, J = 8.4 Hz, 2H), 7.86 (m, 3H), 7.77 (d, J = 8.4 Hz, 2H), 7.69 (d, J = 8.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 143.8, 138.4, 134.0, 132.3, 129.9 (d, $^{2}J_{CF}$ = 32.3 Hz), 128.8, 128.6 (d, $^{2}J_{CF}$ = 32 Hz), 127.7, 127.4, 127.1, 126.0 (m), 125.3, 123.1, 122.0 (m); ^{19}F NMR ($CDCl_3$, 376.5 Hz): δ -62.39 (s, 3F), -62.47 (s, 3F); IR ($CHCl_3$): ν_{max} 3436, 2924, 2852, 1923, 1613, 1463, 1434, 1405, 1376, 1343, 1326, 1303, 1263, 1234, 1124, 1070, 1017 cm^{-1}; GC-MS: *m/z* (EI) 340 (M^+, 100), 341 (M+1, 18), 321 (10), 290 (3), 270 (7), 251 (11), 220 (5), 202 (19).



2i

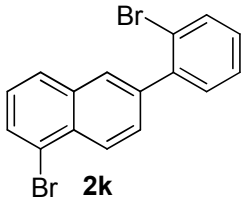
2-(4′-(Trifluoromethoxy)phenyl)-7-(trifluoromethoxy)naphthalene (2i). Yield: 99%; white amorphous solid; m.p. 58 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (s, 1H), 7.89 (dd, J = 8.8, 14 Hz, 2H), 7.68 (m, 4H), 7.34 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 148.9, 147.3, 139.3, 138.4, 133.8, 130.9, 129.8, 128.8, 128.5, 125.86, 125.75, 121.68 (d, $^{1}J_{CF}$ = 15.2 Hz), 121.4, 120.4, 119.5 (d, $^{1}J_{CF}$ = 13.7 Hz), 118.3; ^{19}F-

NMR ($CDCl_3$, 376.5 Hz): δ -57.65 (s, 3F), -57.78 (s, 3F) ; IR ($CHCl_3$): ν_{max} 3436, 2921, 2851, 1744, 1635, 1505, 1459, 1384, 1256, 1215, 1161, 1017 cm^{-1}; GC-MS: *m/z* (EI) 372 (M^+, 100), 373 (M+1, 20), 303 (21), 275 (36), 189 (15), 152 (7), 69 (20).



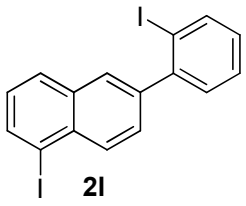
2j

2-(2′-Chlorophenyl)- 5-chloronaphthalene (2j). Yield: 90%; white amorphous solid; m.p. 77-78 °C; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.28 (d, *J* = 8.8 Hz, 1H), 7.83 (s, 1H), 7.70-7.64 (m, 2H), 7.50 (d, *J* = 6.8 Hz, 1H), 7.45 (d, *J* = 7.2 Hz, 1H), 7.35-7.21 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.9, 137.9, 134.3, 132.7, 131.9, 131.5, 130.0, 128.9, 128.8, 128.6, 127.4, 127.0, 126.5, 126.1, 124.1; IR ($CHCl_3$): ν_{max} 3435, 2922, 2851, 1919, 1741, 1627, 1405, 1021 cm^{-1}; GC-MS: *m/z* (EI) 272 (M^+, 100), 273 (M+1, 16), 274 (M+2, 66), 202 (72).



2k

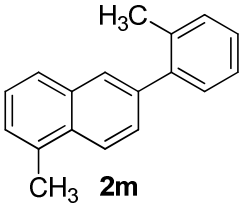
2-(2′-Bromophenyl)-5-bromonaphthalene (2k). Yield: 87%; white crystalline solid; m.p. 91-92 °C; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.30 (d, *J* = 8 Hz, 1H), 7.85 (m, 3H), 7.22 (d, *J* = 8 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.41-7.33 (m, 3H), 7.28 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.8, 139.5, 134.3, 133.2, 131.4, 131.2, 130.1, 129.1, 129.0, 128.6, 128.1, 127.5, 126.7, 126.6, 122.7, 122.6 ; IR ($CHCl_3$): ν_{max} 3436, 3053, 2920, 2850, 1927, 1595, 1555, 1494, 1474, 1452, 1428, 1343, 1254, 1198, 1137, 1019 cm^{-1}; GC-MS: *m/z* (EI) 362 (M^+, 80), 363 (M+1, 11), 360 (39), 202 (100), 174 (6), 101 (13), 74 (7).



2l

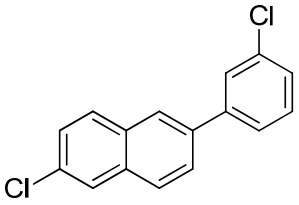
2-(2′-Iodophenyl)-5-iodonaphthalene (2l). Yield: 89%; white crystalline solid; m.p. 110-113 °C; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.14 (t, *J* = 9.6 Hz, 2H), 8.0 (d, *J* = 7.6 Hz, 1H), 7.87 (d, *J* = 8 Hz, 1H), 7.72

(s, 1H), 7.59 (d, *J* = 8.8 Hz, 1H), 7.45 (m, 2H), 7.24 (dd, *J* = 7.2, 14.8 Hz, 1H), 7.10 (t, *J* = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 145.7, 142.5, 139.6, 137.7, 133.7, 133.6, 131.7, 130.4, 129.3, 129.2, 129.1, 128.6, 128.2, 127.2, 99.3, 98.4; IR ($CHCl_3$): ν_{max} 3436, 3049, 2919, 2850, 2324, 1923, 1582, 1550, 1494, 1470, 1427, 1410, 1347, 1200, 1185, 1159, 1133, 1010 cm^{-1}.



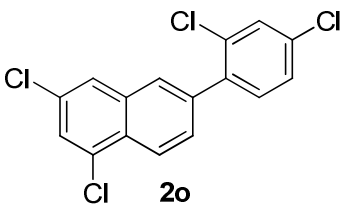
2m

2-(*O*-Tolyl)-5-methylnaphthalene (2m). Yield: 93%; white amorphous solid; m.p. 73-74 °C; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.00 (d, *J* = 8.0 Hz, 1H), 7.75 (s, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.37-7.26 (m, 6H), 2.68 (s, 3H), 2.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 141.9, 139.3, 135.7, 134.3, 133.6, 131.6, 130.5, 130.2, 128.6, 127.7, 127.5, 126.7, 126.6, 126.1, 126.0, 124.0, 20.7, 19.5; IR ($CHCl_3$): ν_{max} 3435, 3055, 3017, 2922, 1919, 1741, 1598, 1487, 1454, 1422, 1380, 1265, 1185, 1164, 1118, 1019 cm^{-1}; GC-MS: *m/z* (EI) 232 (M^+, 100), 233 (M+1, 18), 215 (35), 203 (8), 115 (8).



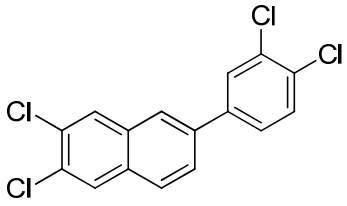
2n

6-Chloro-2-(3′-chlorophenyl)naphthalene (2n). Yield: 87%; white amorphous solid; m.p. 65-66 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) : δ 7.93 (s, 1H), 7.81-7.77 (m, 3H), 7.66 (m, 2H), 7.53 (d, *J* = 7.2 Hz, 1H), 7.43 (d, *J* = 8.8 Hz, 1H), 7.40-7.32 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 142.5, 137.4, 134.8, 133.3, 132.0, 131.8, 130.1, 129.8, 127.8, 127.5, 127.48, 127.45, 126.4, 126.3, 125.8, 125.4; IR ($CHCl_3$): ν_{max} 3435, 3057, 2954, 2924, 2852, 1725, 1640, 1566, 1481, 1423, 1329, 1269, 1224, 1175, 1098, 1076 cm^{-1}; GC-MS: *m/z* (EI) 270 (M^+, 100), 273 (M+1, 18), 275 (10), 236 (10), 202 (73), 175 (3), 136 (5), 118 (7), 100 (16), 87 (6).



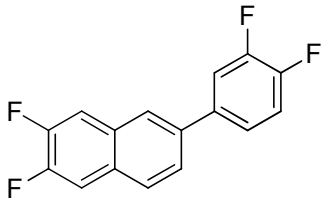
2o

2-(2′, 4′-Dichlorophenyl)-5,7-dichloronaphthalene (2o). Yield: 89%; white amorphous solid; m.p. 162-163 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.28 (d, J = 8.8 Hz, 1H), 7.79 (s, 2H), 7.66 (d, J = 8.4 Hz, 1H), 7.60 (s, 1H), 7.54 (s, 1H), 7.35 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 138.0, 137.9, 134.4, 134.3, 133.4, 132.9, 132.1, 131.4, 129.9, 128.7, 128.6, 127.8, 127.4, 127.2, 126.1, 124.4; IR ($CHCl_3$): ν_{max} 3436, 2920, 2851, 1737, 1625, 1587, 1470, 1020; GC-MS: *m/z* (EI) 340 (M^+, 73), 342 (M+2, 100), 343 (16), 344 (44), 346 (8), 270 (47), 234 (11), 200 (26), 171 (6), 135 (17), 99 (11), 74 (5).



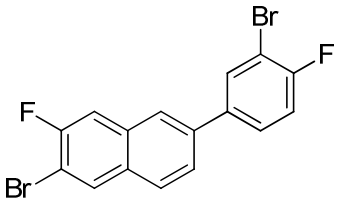
2p

2-(3′, 4′-Dichlorophenyl)-6,7-dichloronaphthalene (2p). Yield: 89%; white amorphous solid; m.p. 175-178 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.00 (d, J = 10 Hz, 2H), 7.83-7.82 (m, 2H), 7.77 (d, J = 2 Hz, 1H), 7.69 (d, J = 8.8 Hz, 1H), 7.57 (d, J = 8.4 Hz, 1H), 7.49 (d, J = 8.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100MHz): δ 140.3, 137.4, 133.2, 132.5, 132.1, 131.7, 131.1, 130.9, 130.8, 129.7, 129.1, 128.6, 127.8, 126.5, 126.2, 124.8; IR ($CHCl_3$): ν_{max} 3435, 2921, 2850, 1743, 1621, 1592, 1548, 1467, 1406, 1385, 1361, 1305, 1244, 1182, 1151, 1134, 1120, 1041, 1024 cm^{-1}.



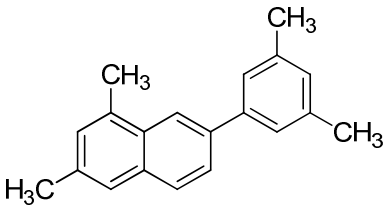
2q

2-(3′, 4′-Difluorophenyl)-6,7-difluoronaphthalene (2q). Yield: 90%; white amorphous solid; m.p. 87-88 °C ; ^{1}H NMR ($CDCl_3$, 500 MHz) : δ 7.87 (s, 1H), 7.84 (d, J = 8.5 Hz, 1H), 7.65-7.56 (m, 3H), 7.48 (m, 1H), 7.39 (m, 1H), 7.29-7.24 (dd, J = 8.5, 18.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 151.9 (m), 149.4 (m), 137.6, 136.9, 130.4, 129.5, 128.0, 125.4, 124.9, 123.2, 117.8 (d, $^{2}J_{CF}$ = 17.2 Hz), 116.2 (d, $^{2}J_{CF}$ = 17.7 Hz), 113.9 (d, $^{2}J_{CF}$ = 15.8 Hz), 113.5 (d, $^{2}J_{CF}$ = 16.2 Hz); ^{19}F NMR ($CDCl_3$, 376.5 Hz): δ -136.08 (m, 1F), -136.20 (m, 1F), -137.13 (m, 1F), -139.52 (m, 1F); IR ($CHCl_3$): ν_{max} 3850, 3745, 3671, 3647, 3435, 3003, 2964, 2931, 2441, 1948, 1602, 1579, 1490, 1466, 1455, 1414, 1386, 1350, 1326, 1270, 1238, 1215, 1203, 1191, 1176, 1155, 1118, 1099, 1059, 1047, 1034 cm^{-1}; GC-MS: *m/z* (EI) 276 (M^+ , 100), 277 (M+1, 16), 256.8 (18), 225 (4), 138 (4).



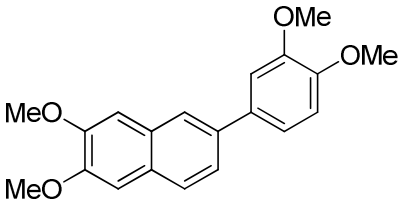
2r

2-(3′-Bromo-4′-fluorophenyl)-6-bromo-7-fluoronaphthalene (2r). Yield: 89%; white amorphous solid; m.p. 141-142 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.10 (d, J = 6.8 Hz, 1H), 7.85 (s, 2H), 7.82 (d, J = 8.4 Hz, 1H), 7.63-7.53 (m, 3H), 7.25 (m 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.5 (d, $^{1}J_{CF}$ = 247 Hz), 157.48 (d, $^{1}J_{CF}$ = 246 Hz), 137.6, 137.1, 132.8, 132.1, 131.9, 129.9, 127.4, 127.3, 125.0, 124.6, 116.1 (d, $^{2}J_{CF}$ = 22 Hz), 112.0 (d, $^{2}J_{CF}$ = 22 Hz), 109.5 (d, $^{2}J_{CF}$ = 24 Hz), 109.2 (d, $^{2}J_{CF}$ = 21 Hz); ^{19}F NMR ($CDCl_3$, 376.5 Hz): δ -109.03 (m, 1F), -109.15 (m, 1F); IR ($CHCl_3$): ν_{max} 3436, 2919, 2850, 1629, 1492, 1425, 1258, 1228, 1209, 1020 cm^{-1}; GC-MS: *m/z* (EI) 398 (M^+, 100), 399 (M+1, 15) 400 (M+2, 45), 238 (90), 199 (7), 119 (37).



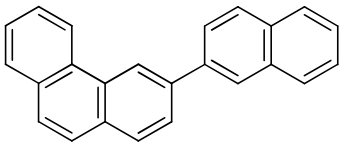
2s

2-(3′, 5′-Dimethylphenyl)-6, 8-dimethylnaphthalene (2s). Yield: 88%; white amorphous solid; m.p. 66-68 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.34 (s, 1H), 8.00 (d, J = 8.8 Hz, 1H), 7.92 (d, J = 8.4 Hz, 1H), 7.68 (s, 1H), 7.57 (s, 2H), 7.38 (s, 1H), 7.23 (s, 1H), 2.92 (s, 3H), 2.68 (s, 3H), 2.64 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 142.0, 138.5, 138.0, 135.2, 134.4, 133.3, 131.3, 129.5, 129.0, 128.5, 125.7, 125.6, 125.3, 122.2, 21.8, 21.7, 19.6; IR ($CHCl_3$): ν_{max} 3435, 2918, 2852, 1737, 1598, 1441, 1384, 1019 cm^{-1}; GC-MS: *m/z* (EI) 260 (M^+, 100), 245 (27), 229 (13), 115 (7).



2ta

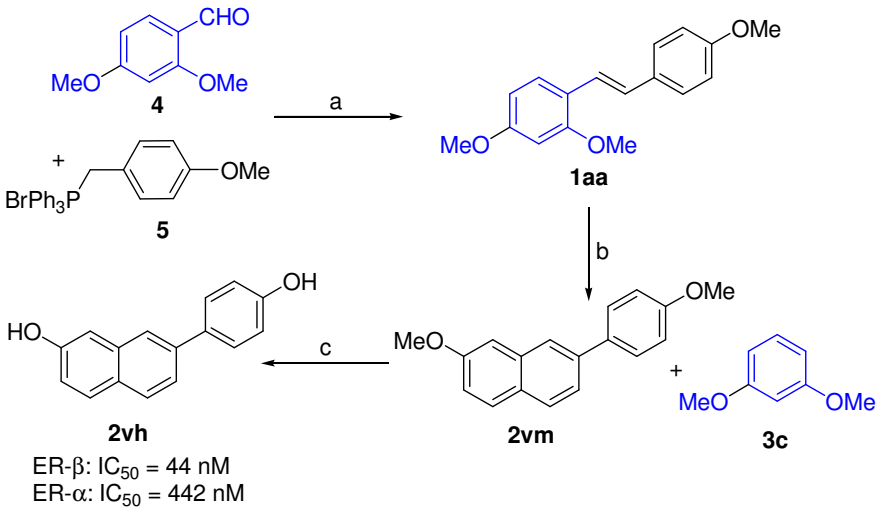
2-(3′, 4′-Dimethoxyphenyl)-6,7-dimethoxynaphthalene (2ta). Yield: 90%; white amorphous solid; m.p. 175-177 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.85 (s, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 8.0 Hz, 1H), 7.23 (m, 2H), 7.18 (s, 1H), 7.14 (s, 1H), 6.99 (d, J = 8.0 Hz, 1H), 4.02 (s, 6H), 3.99 (s, 3H), 3.94 (s, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 149.8, 149.4, 149.1, 148.4, 136.8, 134.4, 129.4, 128.1, 126.7, 123.8, 123.7, 119.4, 111.4, 110.4, 106.4, 106.0, 55.98, 55.94, 55.8; IR ($CHCl_3$): ν_{max} 3436, 2920, 2850, 1607, 1527, 1508, 1463, 1408, 1305, 1258, 1214, 1165, 1138, 1023 cm^{-1}; ESI-MS: *m/z* 325.0 $[M+H]^+$, 347 $[M+Na]^+$.



2u

2-(Naphthalen-2′-yl) phenanthrene (2u). Yield: 92%; brown amorphous solid; m.p. 109-111 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.01 (s, 1H), 8.84 (d, J = 8.4 Hz, 1H), 8.24 (s, 1H), 8.02-7.91 (m, 7H), 7.79 (dd, J = 8.8, 12.4 Hz, 2H), 7.72 (t, J = 8.0 Hz, 1H), 7.65 (t, J = 8.0 Hz, 1H), 7.57-7.49 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.3, 138.8, 133.8, 132.7, 132.3, 131.3, 130.6, 130.4, 129.2, 128.7, 128.6, 128.3, 127.7, 127.1, 126.8, 126.7, 126.6, 126.4, 126.3, 126.2, 126.1, 125.9, 122.7, 121.4; IR ($CHCl_3$): ν_{max} 3436, 3054, 2922, 2850, 1916, 1598, 1500, 1451, 1402, 1383, 1260, 1239, 1192, 1146, 1129, 1098, 1019 cm^{-1}.

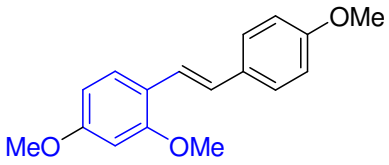
S1.d. Synthesis of ER-β agonist **2vh**



Synthesis of ER-β agonist 2vh. Reagents and conditions: (a) n-BuLi, THF, 30 min, 0 °C, 92%; (b) 50% TFA in water, 80 °C, 0.5 h, 92%; (c) BBr_3, anhydrous DCM, rt, 3 h, 84%.

S1.d.(a) Preparation of (E,Z)-2,4-dimethoxy-1-(4′-methoxystyryl)benzene (1aa).

To the stirred solution of (4-methoxybenzyl)-triphenylphosphine bromide salt **5** (1.1 equiv.) in anhydrous THF (10-15 ml) was added n-BuLi (2.5 M solution in hexane, 3 equiv.) at 0 °C for 2-3 minutes. After stirring for 30 min at 0 °C, 2,4-dimethoxy benzaldehyde (**4**, 1.0 equiv.) was added and the resulting reaction mixture was stirred at room temperature for 1 h. The reaction mixture was quenched with ethyl acetate (10 ml) and the solvent was evaporated under vaccum. The crude product was partitioned between water and ethyl acetate. The organic layer was colletced and was dried over anhydrous sodium sulphate and evaporated on rotary evaporator to get crude product. The crude product was purified by silica gel (#100-200) column chromatography (10% EtOAc: hexane) to get (E,Z)-2,4-dimethoxy-1-(4′-methoxystyryl)benzene (**1aa**) in 92% yield.



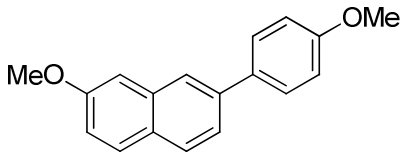
1aa

(E,Z)-2,4-Dimethoxy-1-(4′-methoxystyryl)benzene (1aa). mixture of cis/trans isomers (22.3: 77.6 ratio determined based on HPLC); light brown semisolid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.46 (m, 2H), 7.24 (d, J = 6.8 Hz, 1H), 7.19 (d, J = 8.8 Hz, 2H), 7.13 (d, J = 8.4 Hz, 1H), 6.97 (d, J = 8.4 Hz, 1H), 6.87 (d, J = 8.8 Hz, 1H), 6.73 (d, J = 8.8 Hz, 2H), 6.52 (m, 1H), 6.49 (d, J = 3.2 Hz, 2H), 6.46 (m, 3H), 6.32 (d, J = 2.4 Hz, 1H), 6.30 (d, J = 2.4 Hz, 1H), 3.85 (s, 3H), 3.82 (s, 3H), 3.81 (s, 3H), 3.78 (s, 3H), 3.79 (s, 3H), 3.76 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 160.2, 158.8, 158.4, 158.3, 157.8, 131.1, 130.5, 130.1, 130.0, 128.6, 127.5, 126.9, 126.6, 123.7, 121.2, 119.8, 119.1, 114.0, 113.4, 104.9, 104.2, 98.4, 98.3, 55.5, 55.4, 55.3, 55.18; IR ($CHCl_3$): ν_{max} 3787, 3436, 3034, 3000, 2956, 2936, 2835, 2058, 1879, 1608, 1577, 1499, 1464, 1455, 1438, 1418, 1332, 1320, 1288, 1276, 1249, 1207, 1158, 1118, 1032 cm^{-1}; ESI-MS: *m/z* 271.1 $[M+H]^+$.

S1.d.(b). Synthesis of 2-(4′-methoxyphenyl)-7-methoxynaphthalene (2vm)

The solution of (E,Z)-2,4-dimethoxy-1-(4-methoxystyryl)benzene (**1aa**, 100 mg, 0.49 mmol) in 50% trifluoroacetic acid in water (1 ml) was stirred at 80 °C for 30 min. Reaction was monitored with TLC using 10% EtOAc: n-Hexane as an eluent. Further the mixture was cooled to room temperature and neutralised slowly with saturated $NaHCO_3$ solution, and was extracted with EtOAc (50 ml x 2). The combined organic layer was dried over anhydrous sodium sulphate and evaporated on vacuo rotavapor to

get crude product. The crude product was purified by silica gel (#60-120) column chromatography using 10% EtOAc: n-Hexane as an eluent to get pure product **2vm** in 92% yield.

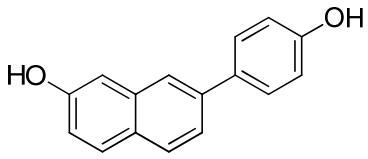


2vm

2-(4′-Methoxyphenyl)-7-methoxynaphthalene (2vm). Yield: 92%; white amorphous solid; m.p. 155-158 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.88 (s, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.66 (d, *J* = 9.2 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.17 (s, 1H), 7.13 (d, *J* = 8.8 Hz, 1H), 7.02 (d, *J* = 8.8 Hz, 2H), 3.93 (s, 3H), 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.2, 157.9, 138.6, 134.9, 133.8, 129.1, 128.4, 128.1, 127.8, 124.0, 123.2, 118.4, 114.3, 106.0, 55.39, 55.32; IR ($CHCl_3$): ν_{max} 3787, 3436, 2999, 2925, 2834, 1628, 1609, 1506, 1464, 1439, 1392, 1369, 1288, 1213, 1179, 1153, 1035 cm^{-1}; GC-MS: *m/z* (EI) 264 (M^+, 100), 265 (M+H, 18), 249 (33), 221 (31), 206 (8), 189 (8), 178 (20), 152 (8), 132 (6).

S1.d.(c) Procedure for synthesis of 2-(4′-hydroxyphenyl)-7-hydroxynaphthalene (2vh).

To the stirred solution of 2-(4′-methoxyphenyl)-7-methoxynaphthalene (**2vm**, 1 equiv.) in anhydrous DCM was slowly added BBr_3 (4 equiv.) at room temperature and the resulting mixture was stirred for 4-6 hrs. The reaction was monitored with TLC using 20% EtOAc: n-Hexane as an eluent. After completion of the reaction, it was neutralized with ice-cold water (slowly with caution). The product was extracted with EtOAc (50 ml x 2) and combined organic layer was dried over anhydrous sodium sulphate and evaporated on vacuo rotavapor. The crude product was purified by silica gel (#60-120) column chromatography using 20% EtOAc: n-Hexane as an eluent to get pure product **2vh** in 84% yield.



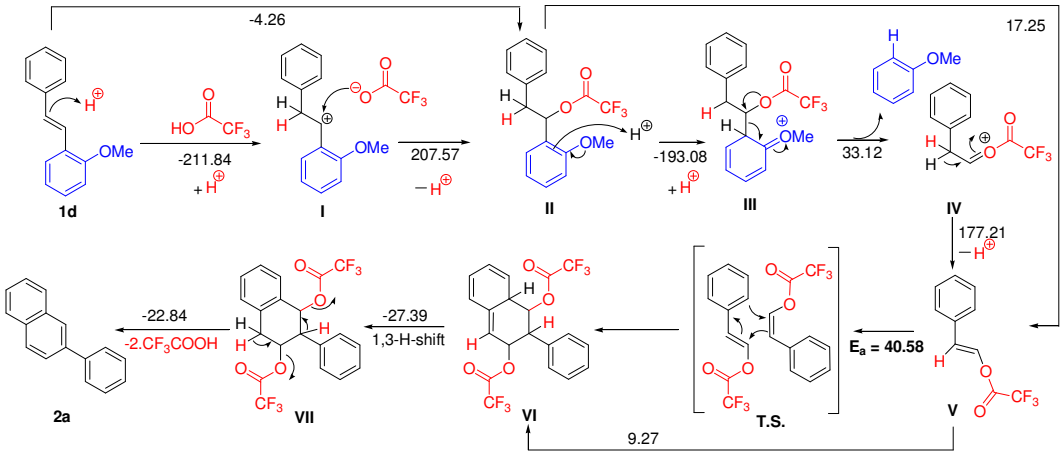
2vh

2-(4'-Hydroxyphenyl)naphthalen-7-ol (2vh): Yield: 84%; gray solid; m.p. 202-204 °C; ^{1}H NMR (CD_3OD, 400 MHz): δ 7.67 (s, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.59 (d, *J* = 8.8 Hz, 1H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.8 Hz, 1H), 7.04 (s, 1H), 6.93 (d, *J* = 8.8 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (CD_3OD, 125 MHz): δ 160.7, 159.2, 142.5, 139.3, 136.4, 132.6, 131.8, 131.6, 131.2, 126.5, 125.9,

121.4, 119.2, 112.6; IR ($CHCl_3$): ν_{max} 3776, 3431, 3354, 2923,2852, 2346, 1595, 1505, 1456, 1259, 1019. ESI-MS: *m/z* 237.0 $[M+H]^+$.

S2. Experimental protocol for density functional theory (DFT) studies to trace the reaction mechanism

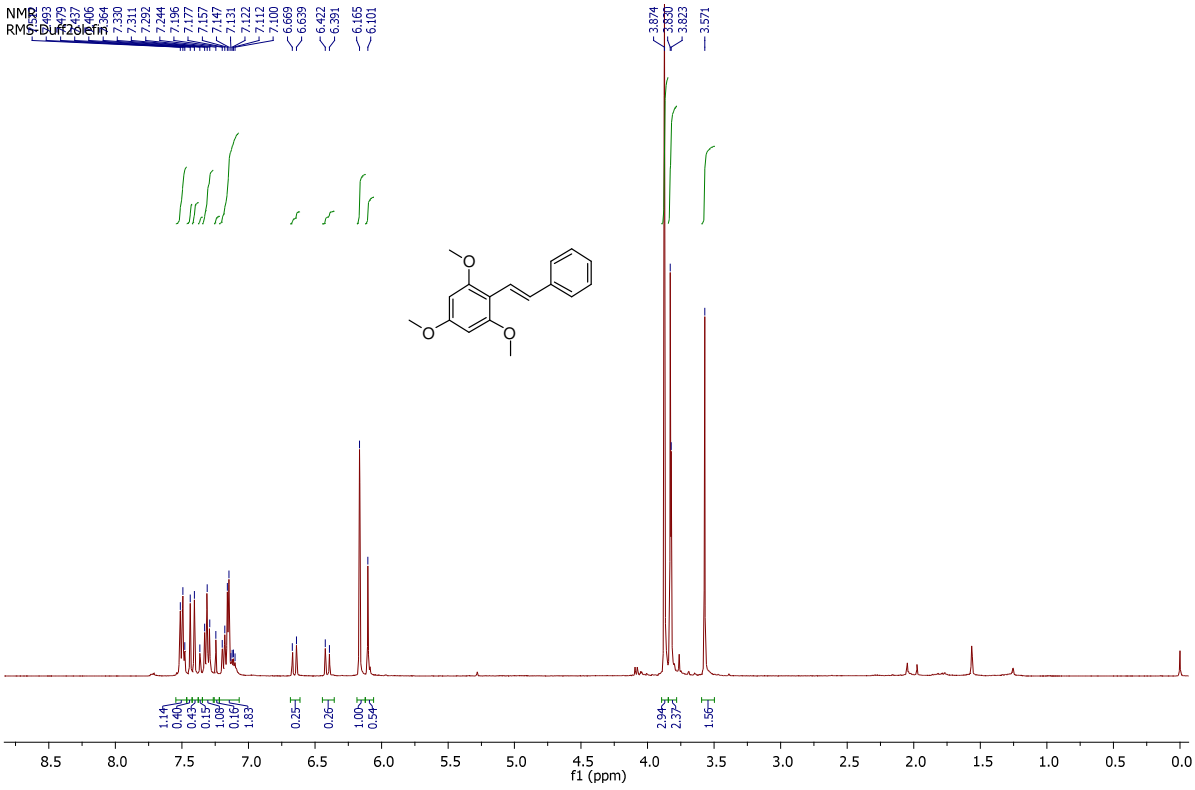
Density functional theory (DFT)[1] analysis was carried out to explore the mechanism of 2-phenylnaphthalene synthesis. The GAUSSIAN09 suite of programs[2] was used to carry out the geometry optimization of all the structures on the possible mechanistic path of the reaction and to estimate the absolute energies. Complete optimizations without any symmetry constraints were performed using Becke–Lee–Yang–Parr (B3LYP),[3-5] with the 6-311+G(d,p) basis set. Frequencies were computed analytically with the same basis set for all optimized species to characterize stationary points to minima and transition states to first-order saddle points with one imaginary frequency vibrational mode and also to estimate the zero point vibrational energies. Calculated ZPE values (at 298.15 K) were scaled by a factor of 0.9806.[6] Each transition state is a first-order saddle point with only one imaginary vibrational mode on the potential energy surface. The NBO analysis[7,8] using the B3LYP/6-311+G(d,p) level of theory was performed to estimate partial atomic charges.

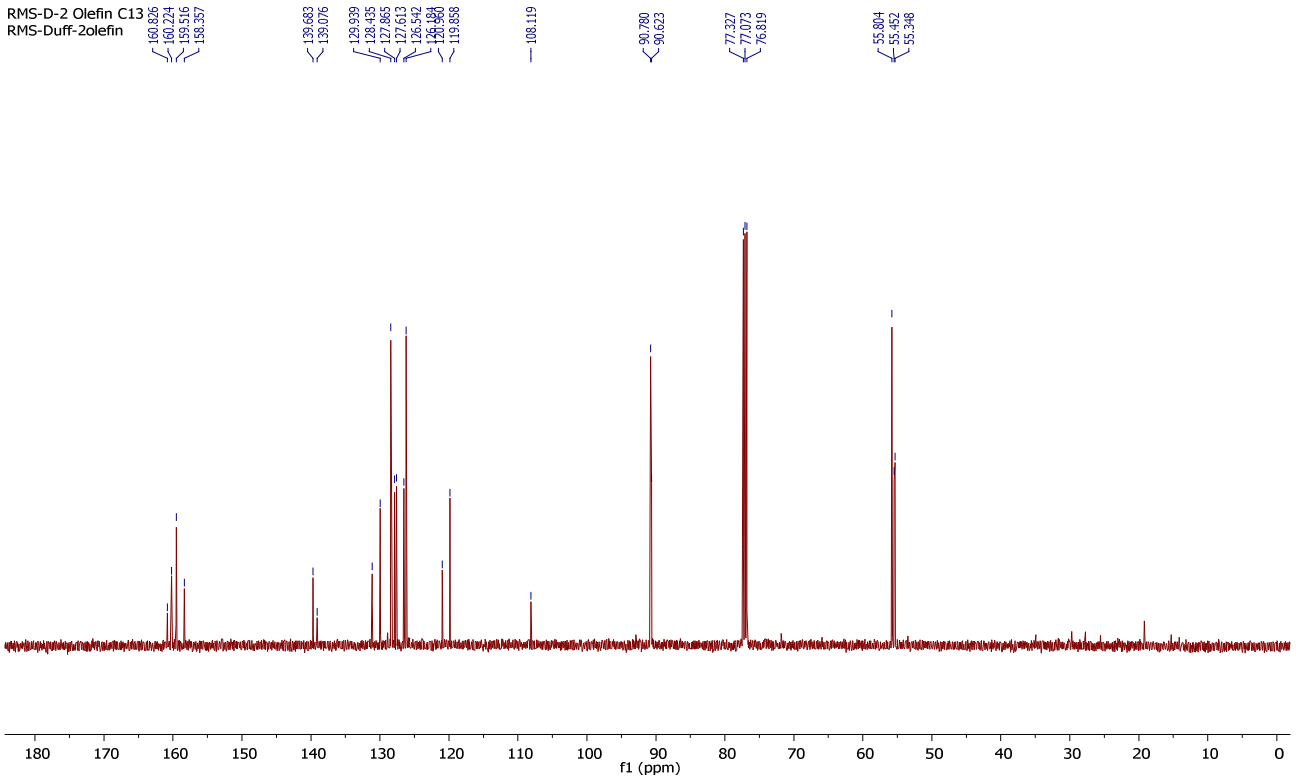


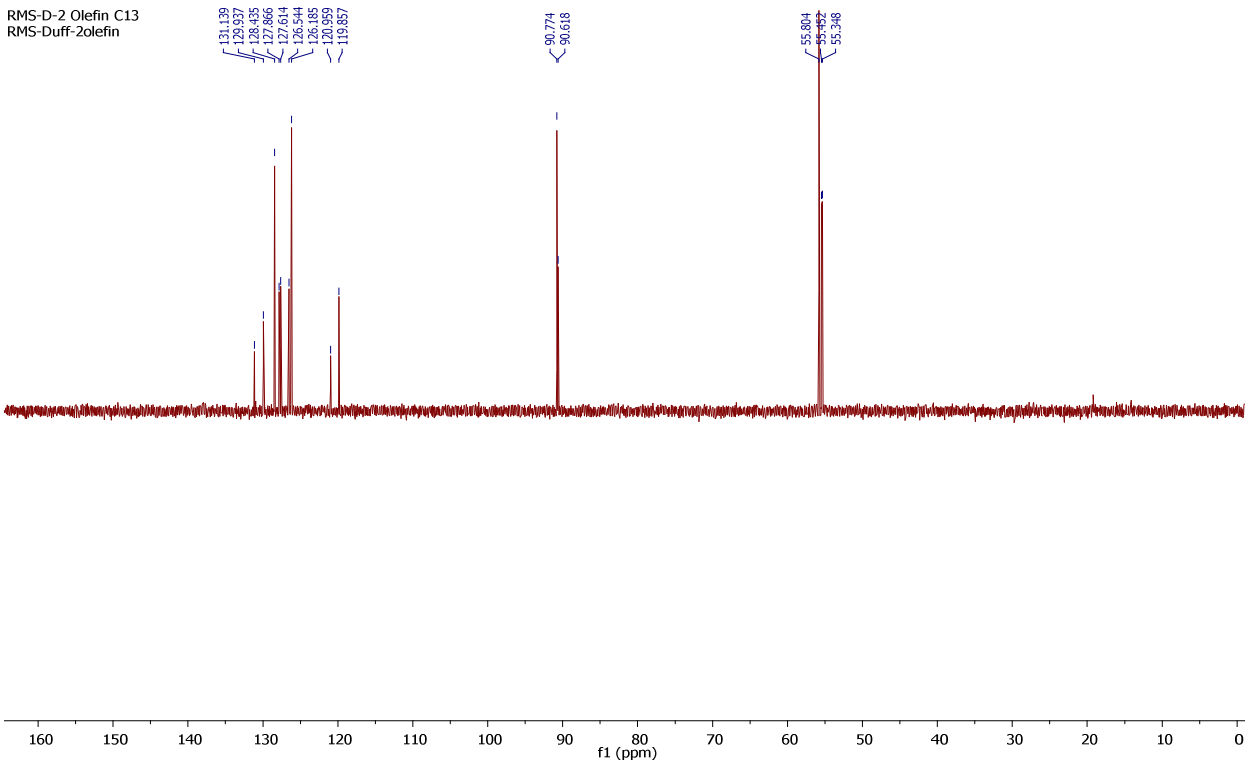
The stability of S-isomer over R-isomer in structure **I** is due to conformational change and is not due to configurational change. The optimized structure of the S-isomer is characterized by two C-H...O hydrogen bond interactions (~2.4 Å) and no oxygen-oxygen repulsions whereas the R-isomer is characterized by only one C-H...O hydrogen bond interaction (~2.4 Å) and one oxygen-oxygen repulsive interaction (~2.93 Å) which leads to the difference in the observed energies of R- and S- isomers.

S3. Scanned copies of ^{1}H, ^{13}C and DEPT135 NMR spectra's of 1-styryl methoxybenzenes 1a-1z

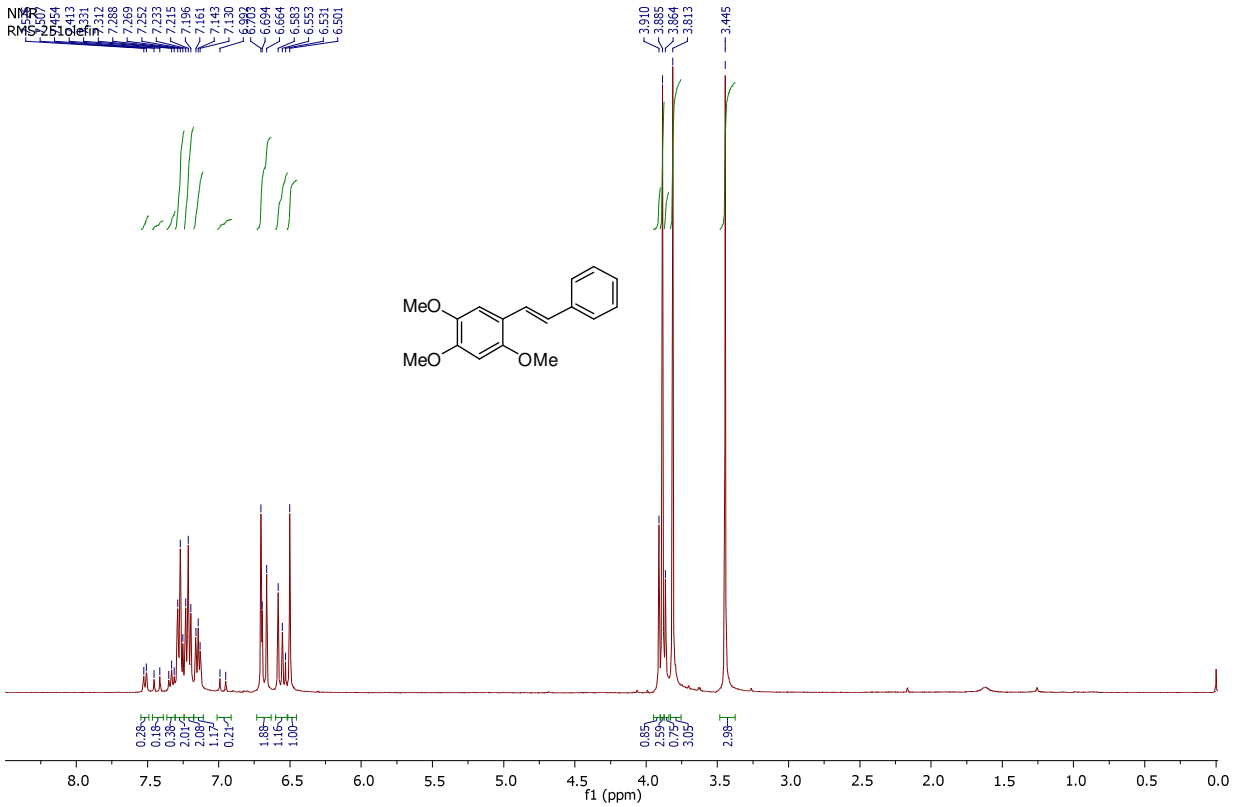
S3.1. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E,Z)-1-styryl-2,4,6-trimethoxy-benzene (**1a**):

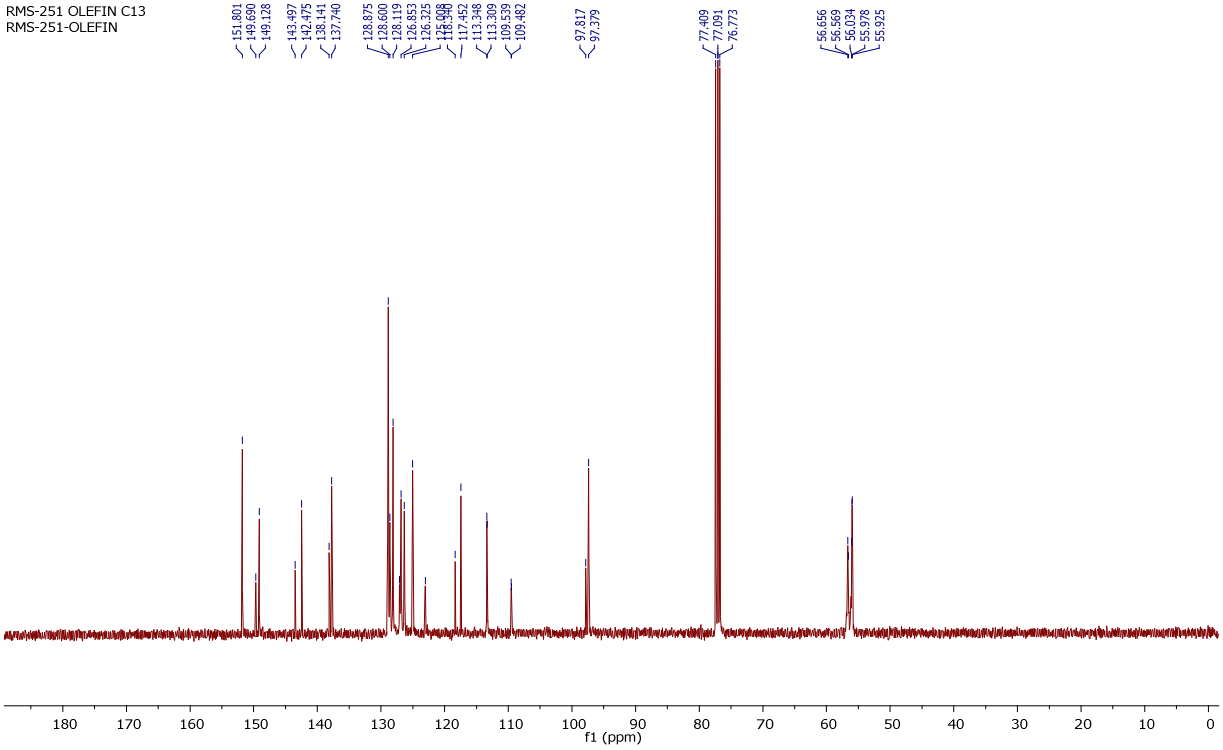


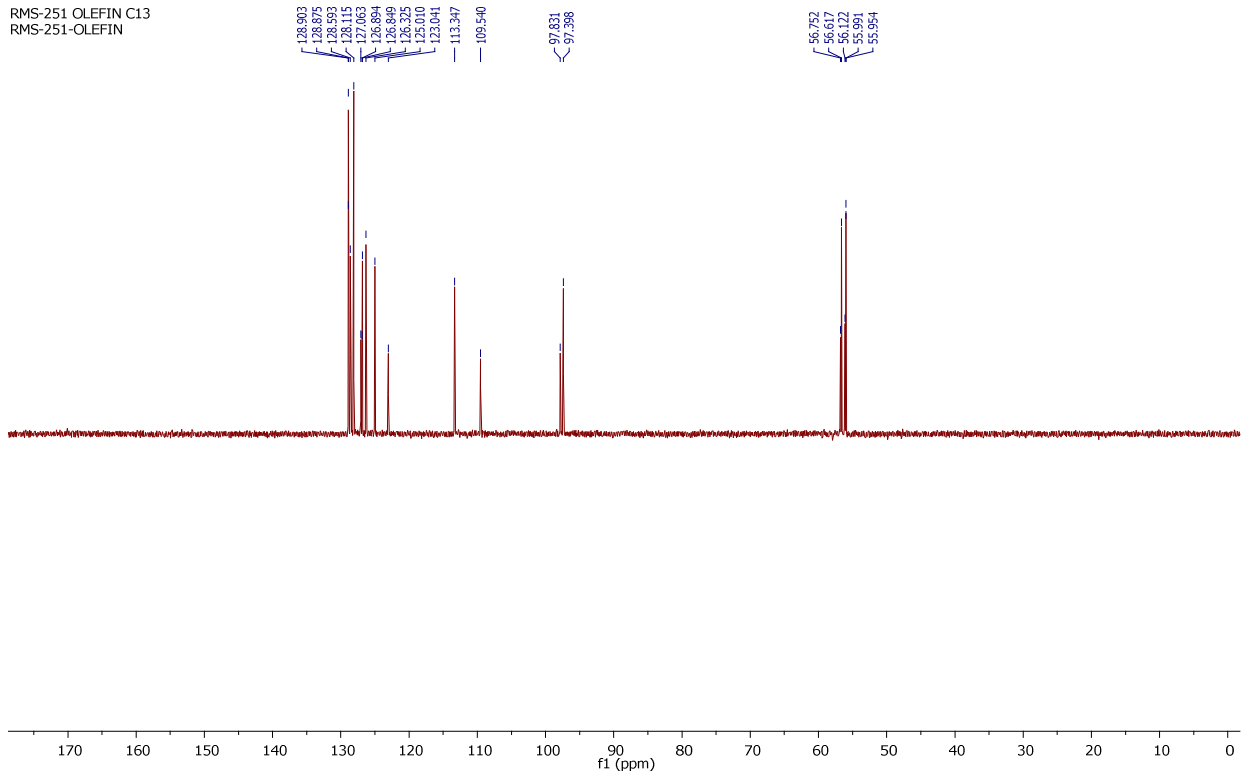

RMS-D-2 Olefin C13
RMS-Duff-2olefin
160.826
160.224
159.516
158.357
139.683
139.076
129.939
128.435
127.865
127.613
126.542
126.184
126.060
119.858
108.119
90.780
90.623
77.327
77.073
76.819
55.804
55.452
55.348
f1 (ppm)


RMS-D-2 Olefin C13
RMS-Duff-2olefin
131.139
129.937
128.435
127.866
127.614
126.544
126.185
120.959
119.857
90.774
90.618
55.804
55.452
55.348
f1 (ppm)

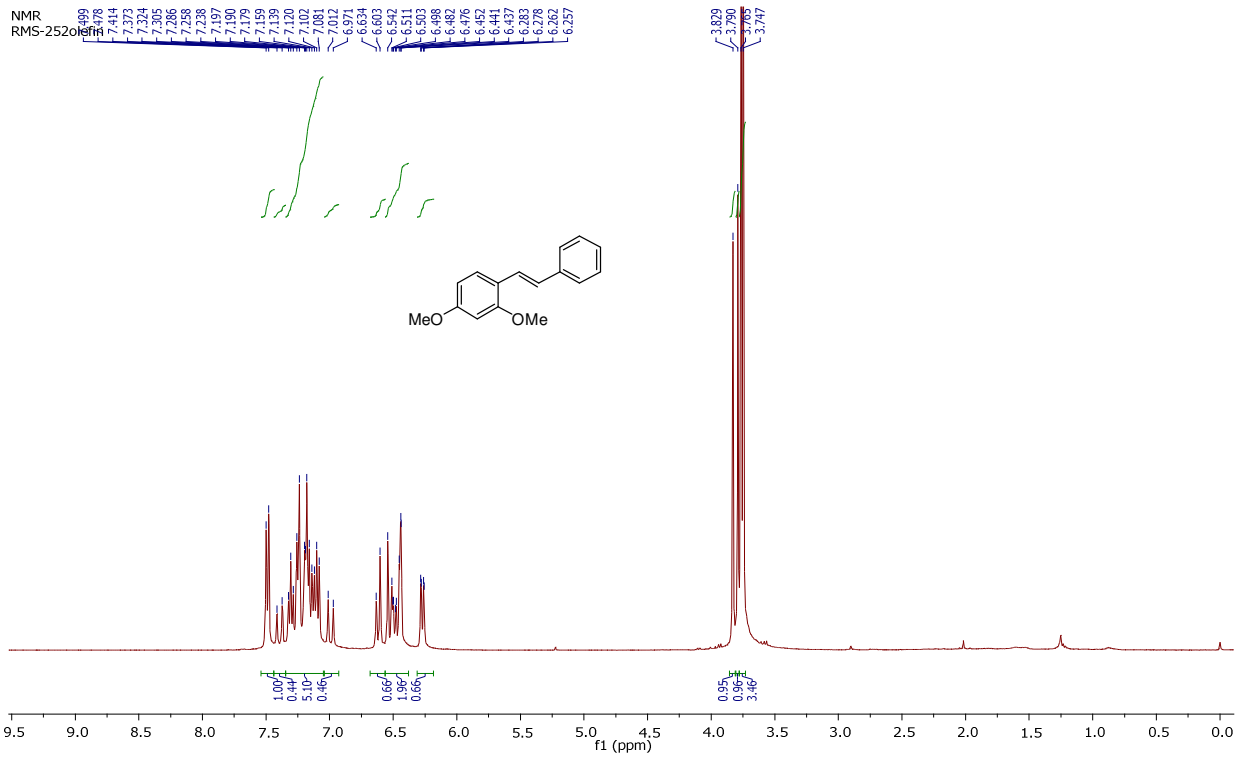
S3.2 ^{1}H, ^{13}C and DEPT135 NMR spectra of (E/Z)- 2,4,5-Trimethoxy-1-styrylbenzene (**1b**)

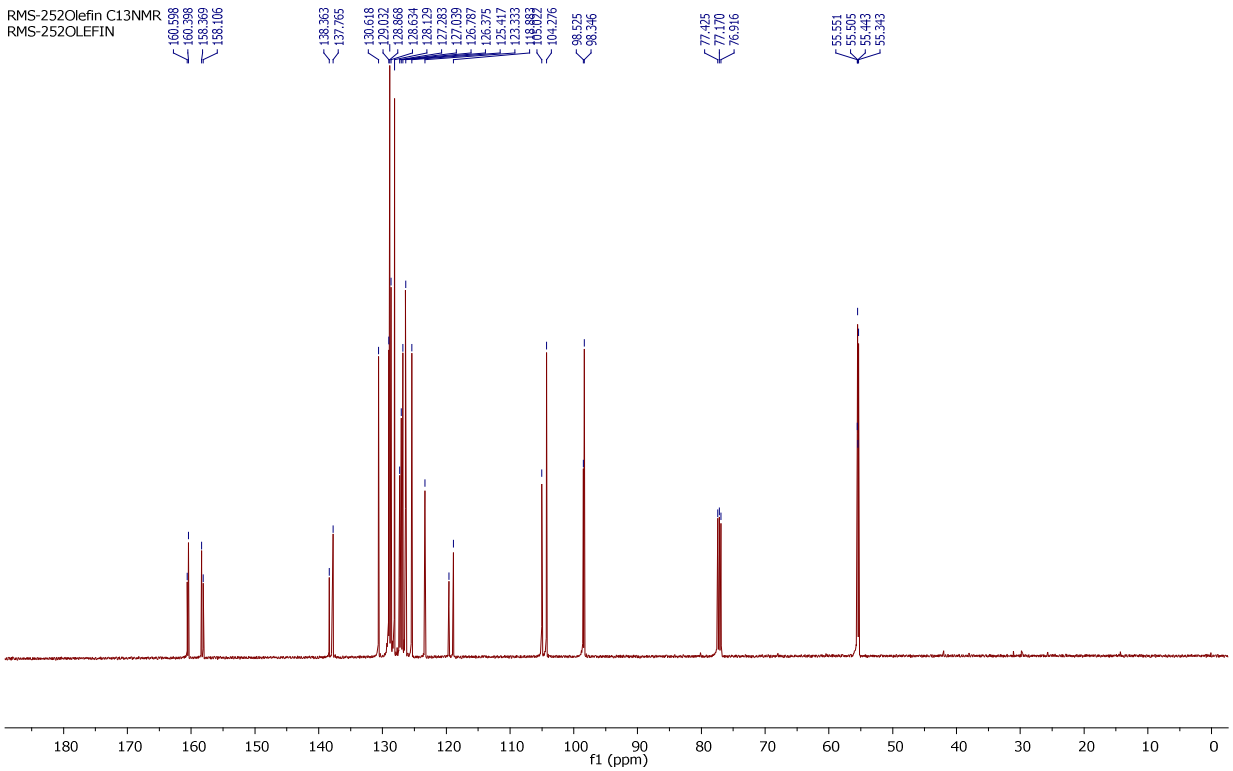


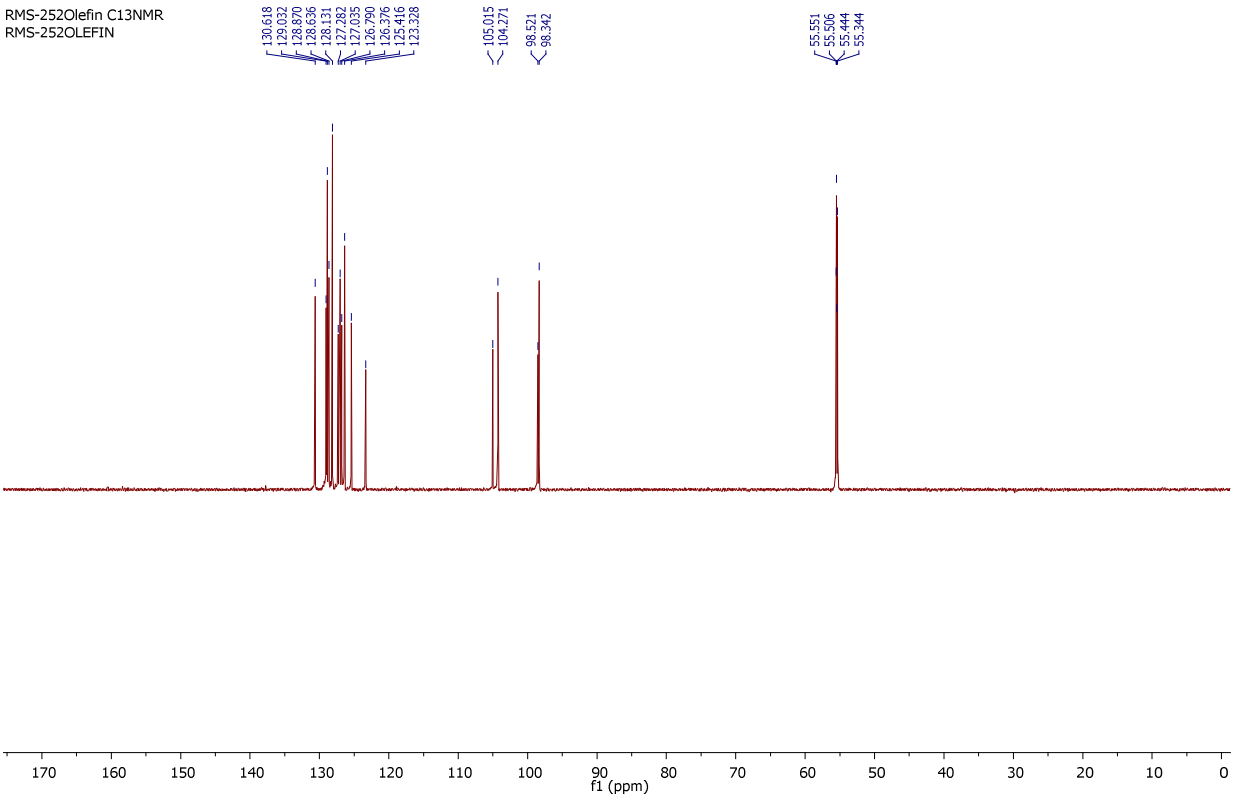




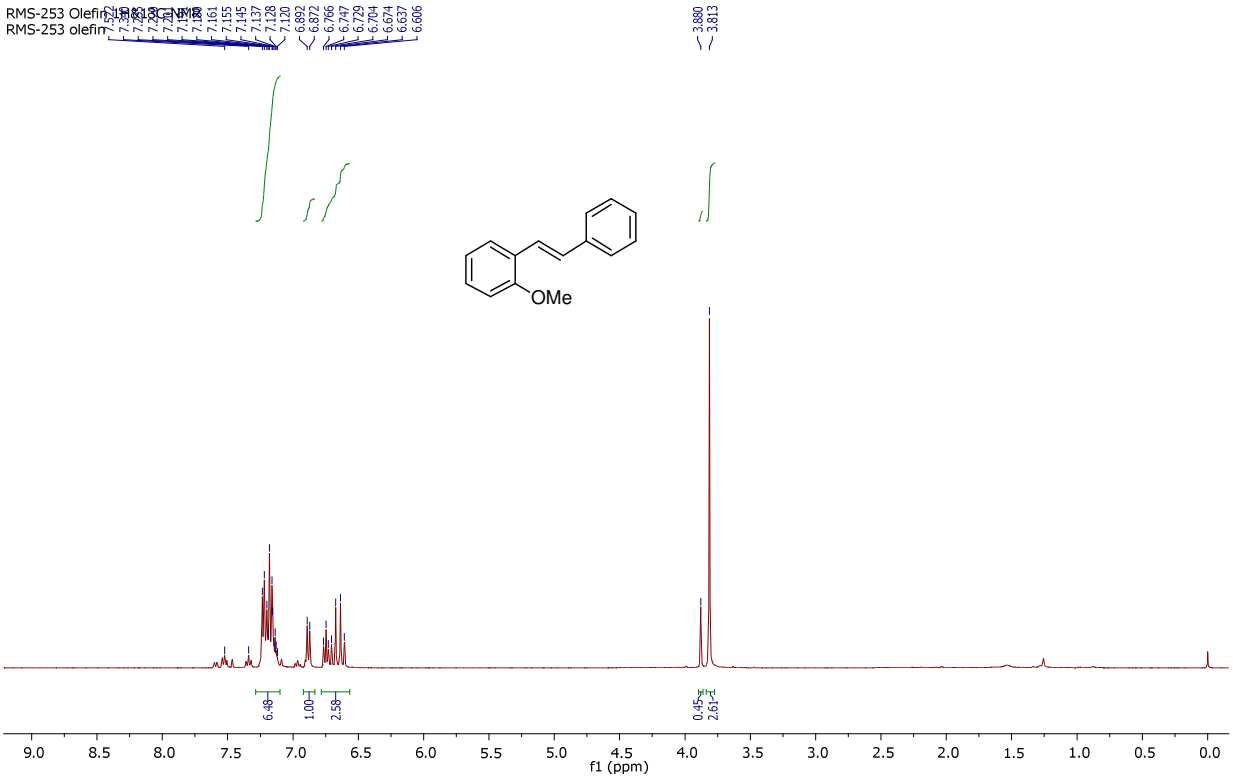
S3.3. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E/Z)-2,4-dimethoxy-1-styrylbenzene (**1c**)

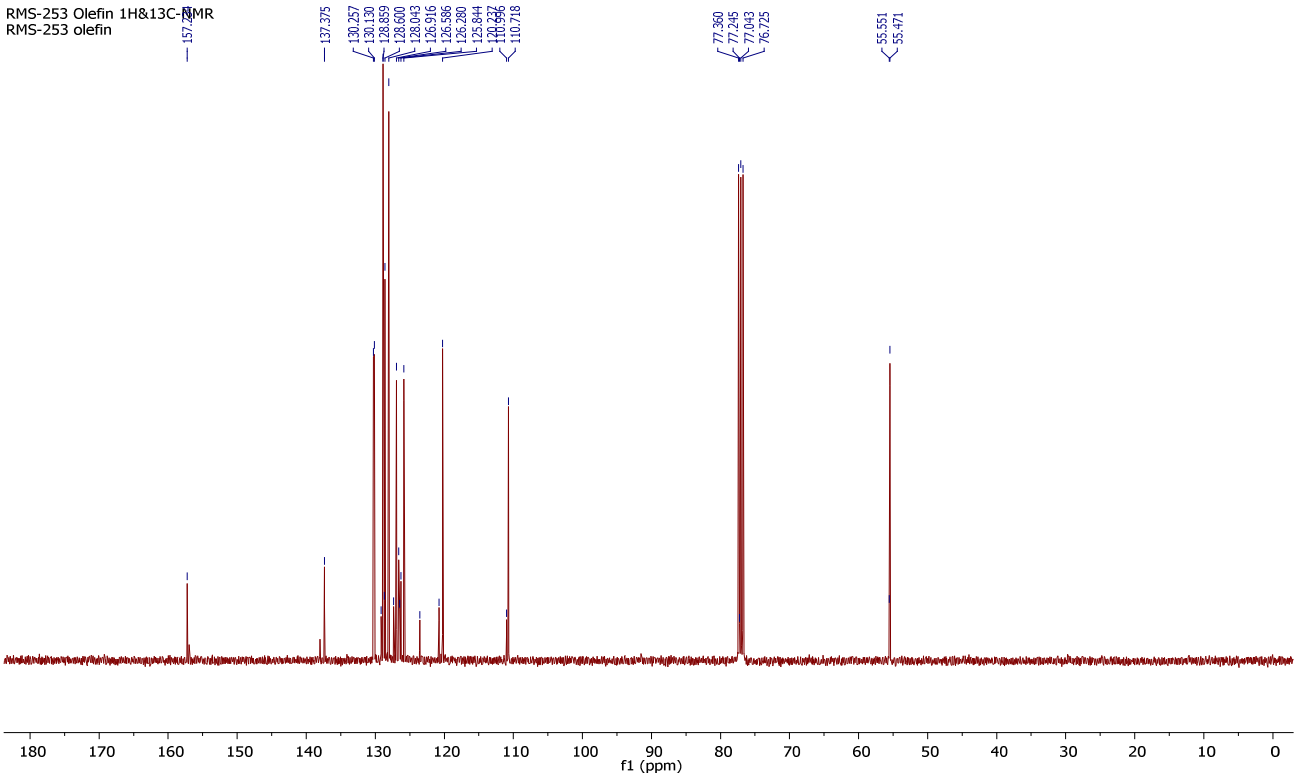


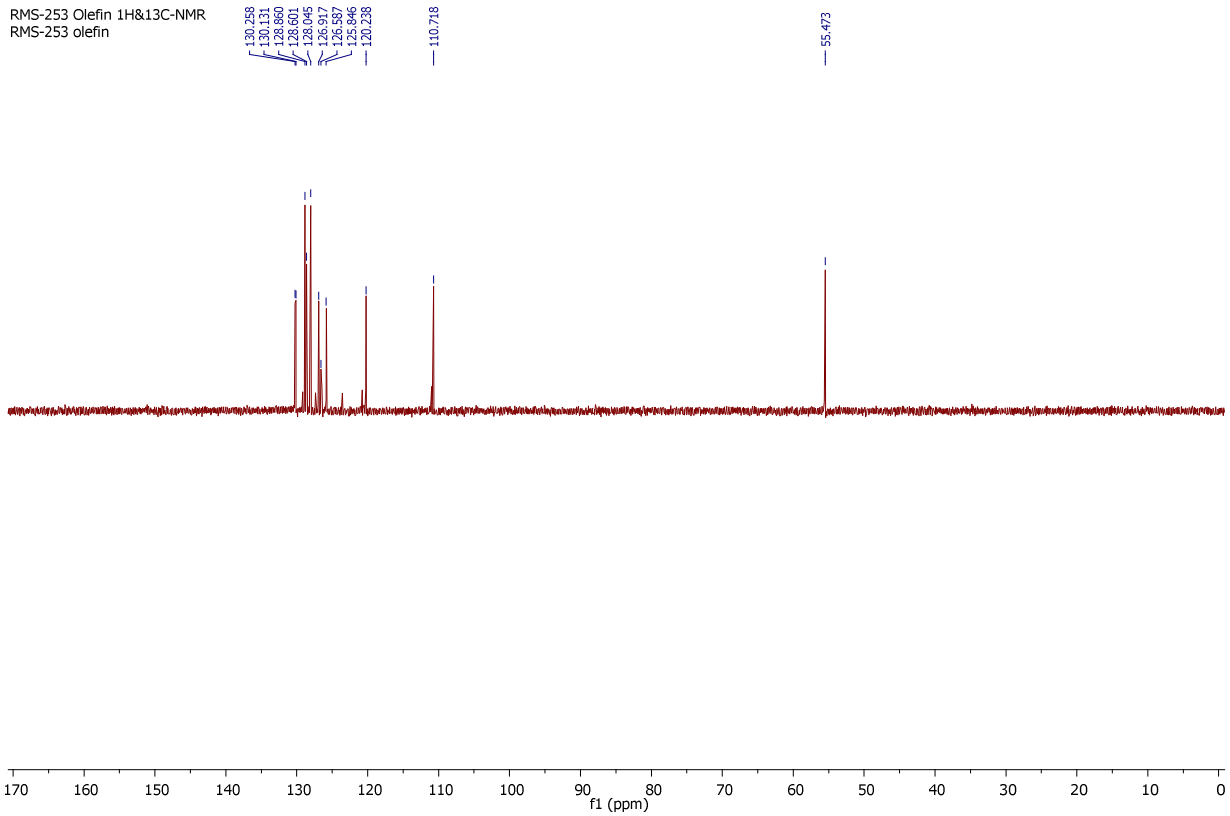

RMS-252Olefin C13NMR
RMS-252OLEFIN
160.598
160.398
158.369
158.106
138.363
137.765
130.618
129.032
128.868
128.634
128.129
127.283
127.039
126.787
126.375
125.417
123.333
105.015
104.276
98.525
98.346
77.425
77.170
76.916
55.551
55.505
55.443
55.343
f1 (ppm)


RMS-252Olefin C13NMR
RMS-252OLEFIN
130.618
129.032
128.870
128.636
128.131
127.282
127.035
126.790
126.376
125.416
123.328
105.015
104.271
98.521
98.342
55.551
55.506
55.444
55.344
f1 (ppm)

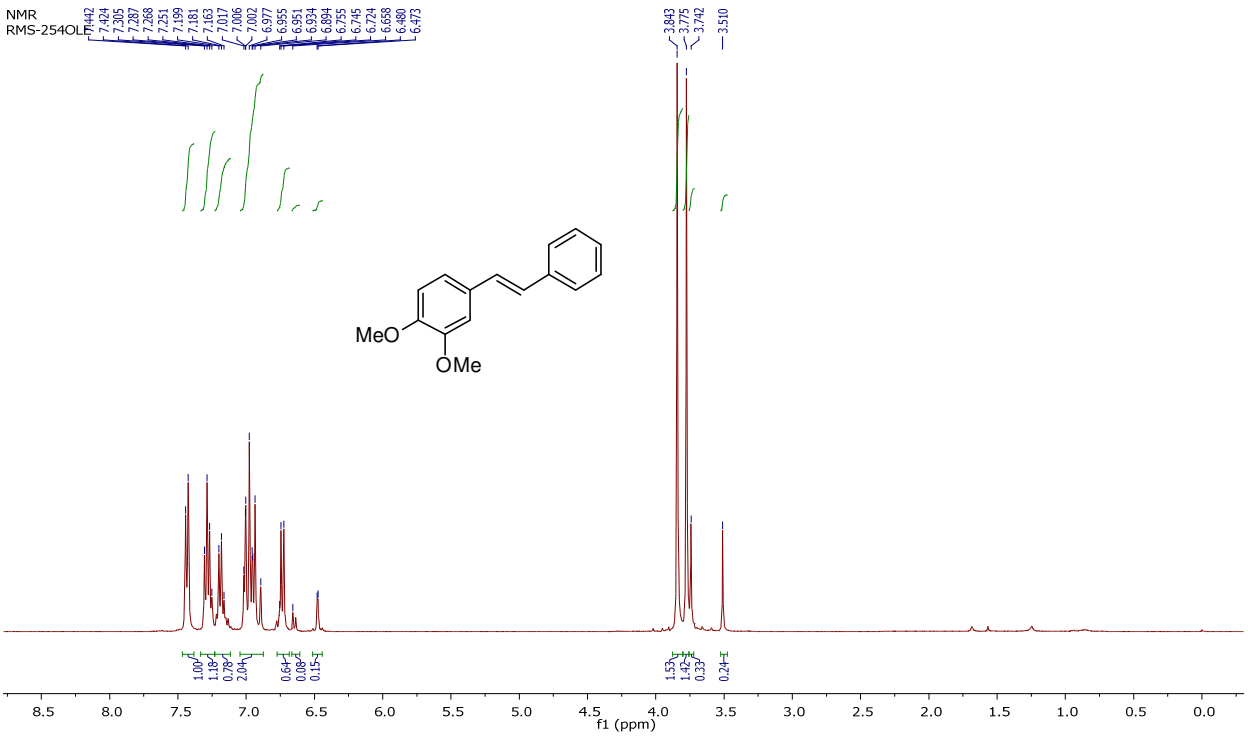
S3.4 ^{1}H, ^{13}C and DEPT135 NMR spectra of (E,Z)-2-methoxy-1-styrylbenzene (**1d**)

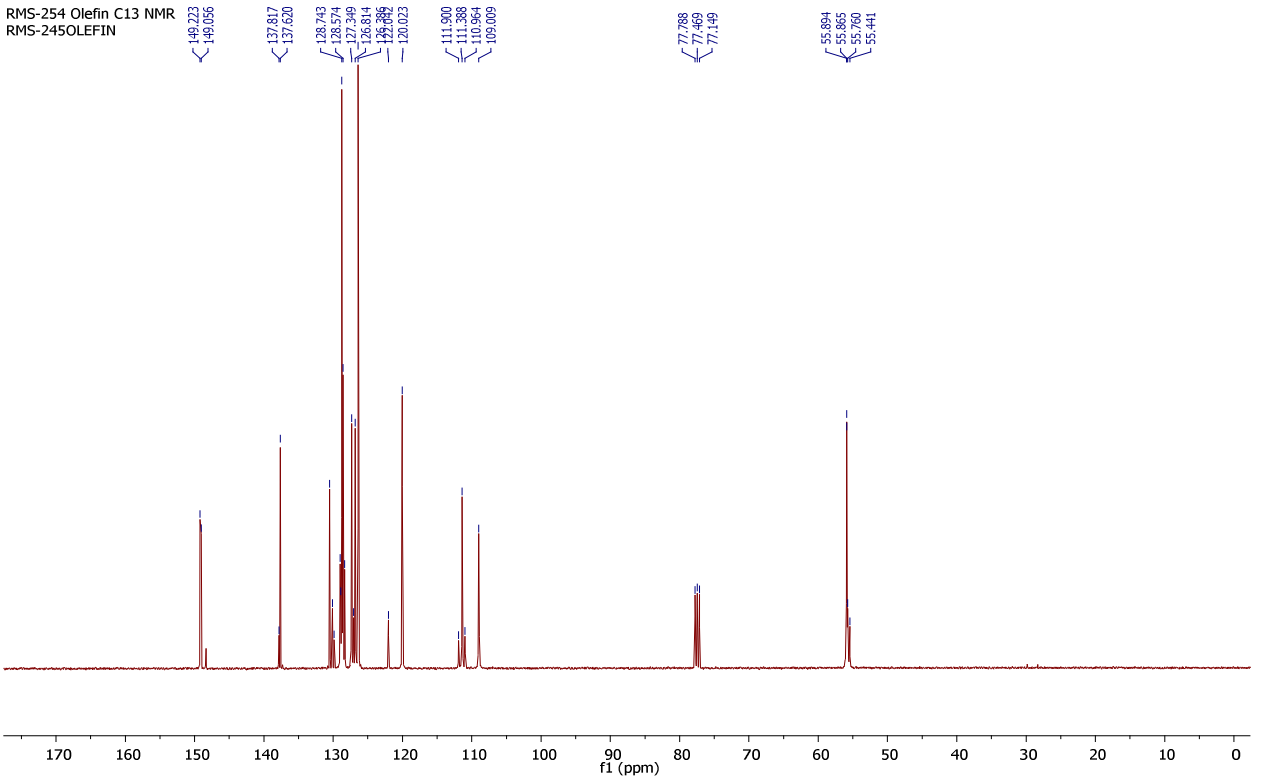


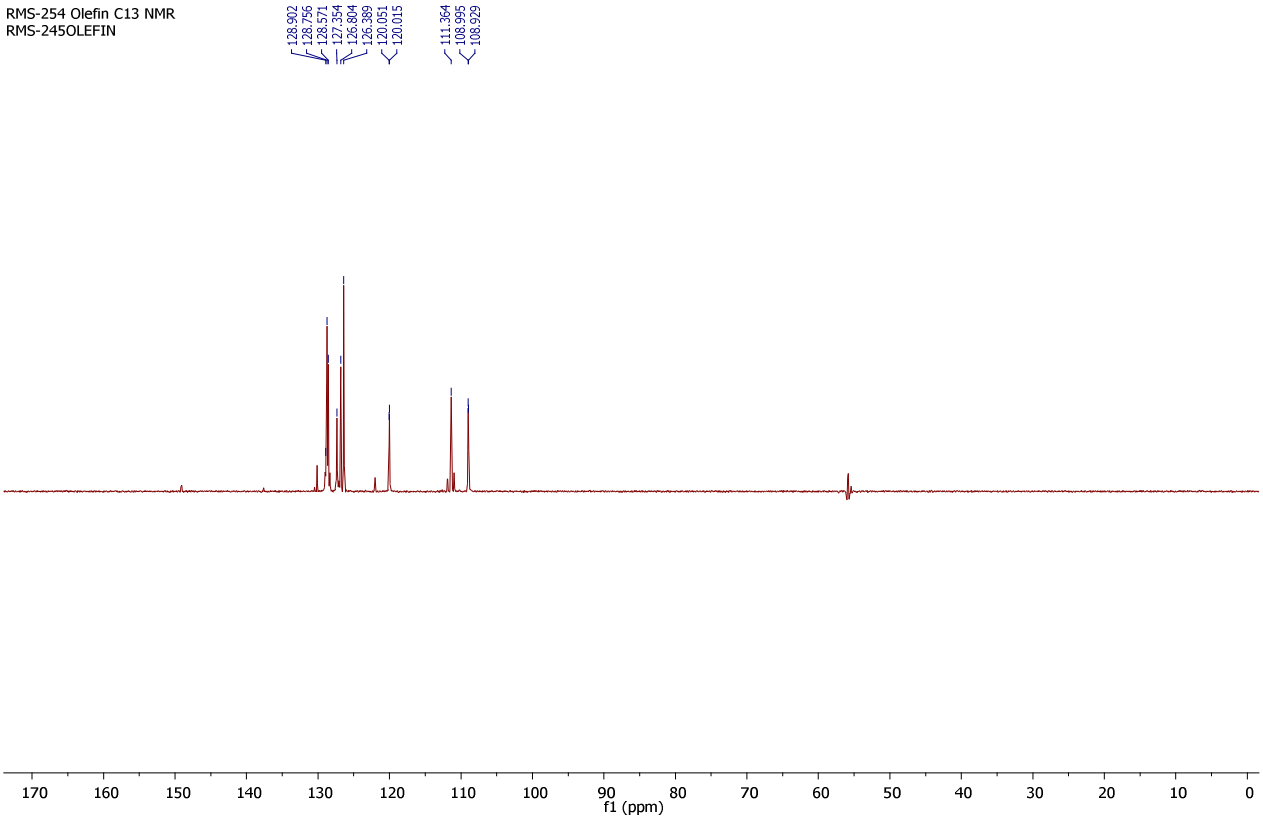




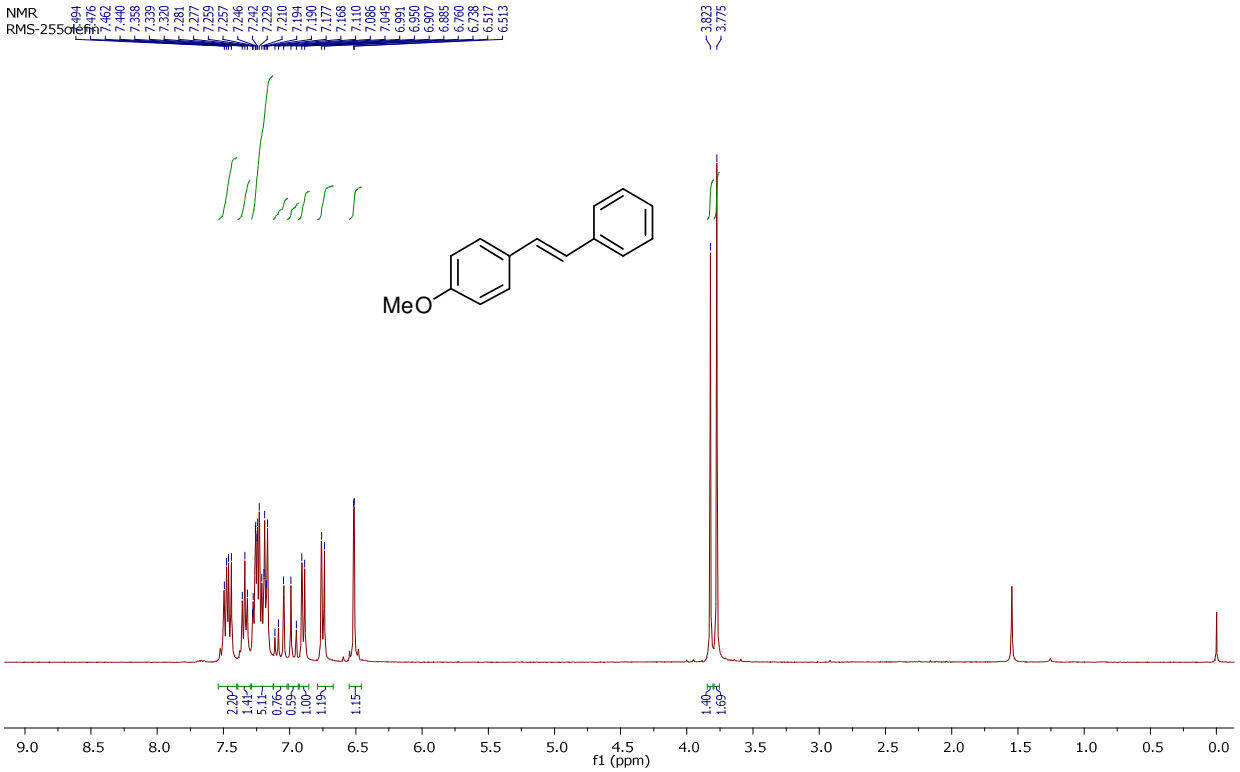
S3.5 ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-3,4-dimethoxy-1-styrylbenzene (**1e**)

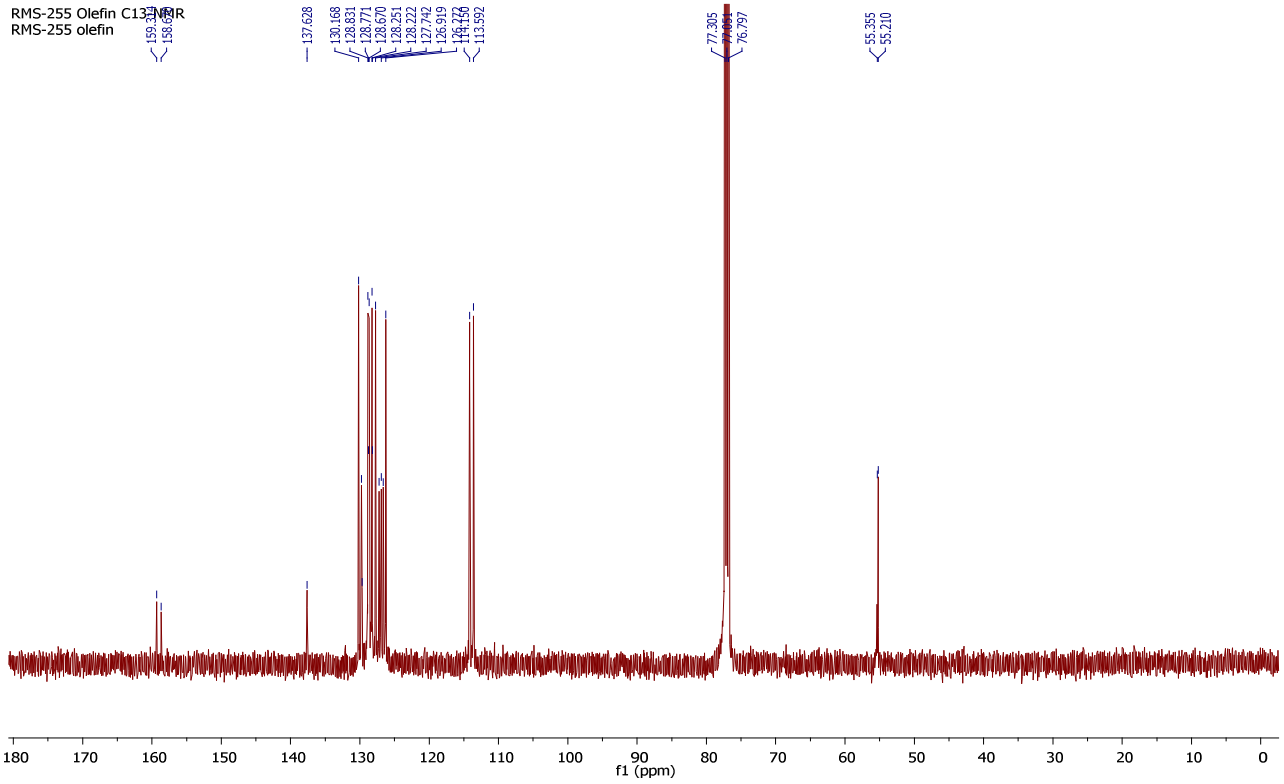


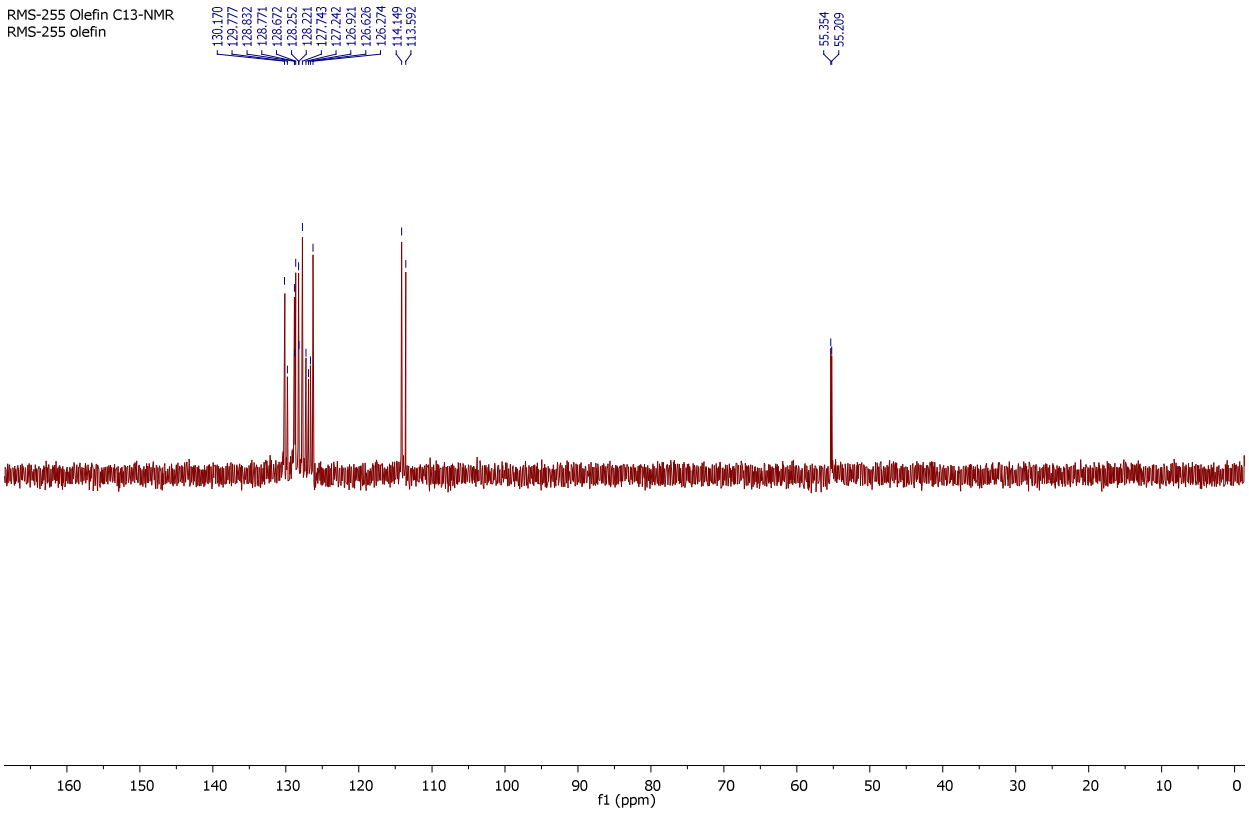

RMS-254 Olefin C13 NMR
RMS-245OLEFIN
149.223
149.056
137.817
137.620
128.743
128.574
127.349
126.814
122.042
120.023
111.900
111.388
110.964
109.009
77.788
77.469
77.149
55.894
55.865
55.760
55.441
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


RMS-254 Olefin C13 NMR
RMS-245OLEFIN
128.902
128.756
128.571
127.354
126.804
126.389
120.051
120.015
111.364
108.995
108.929
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

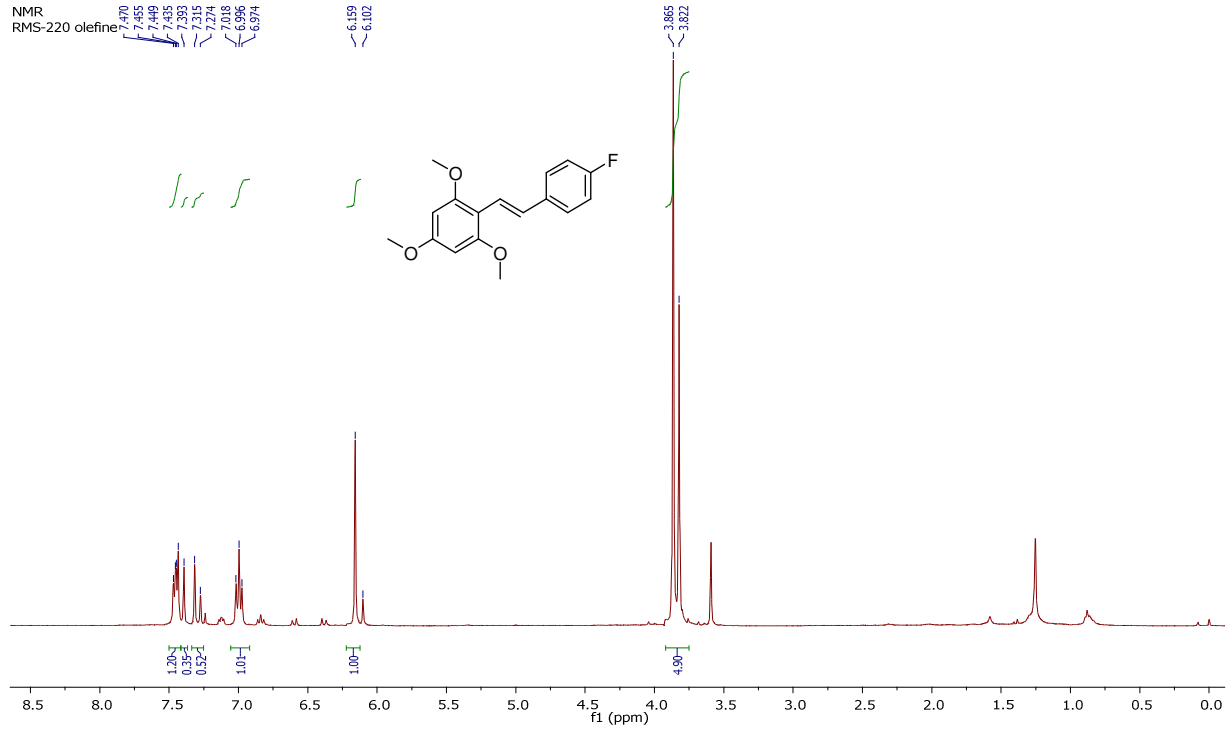
S3.6 ^{1}H, ^{13}C and DEPT135 NMR spectra of (E,Z)-4-methoxy-1-styrylbenzene (**1f**)

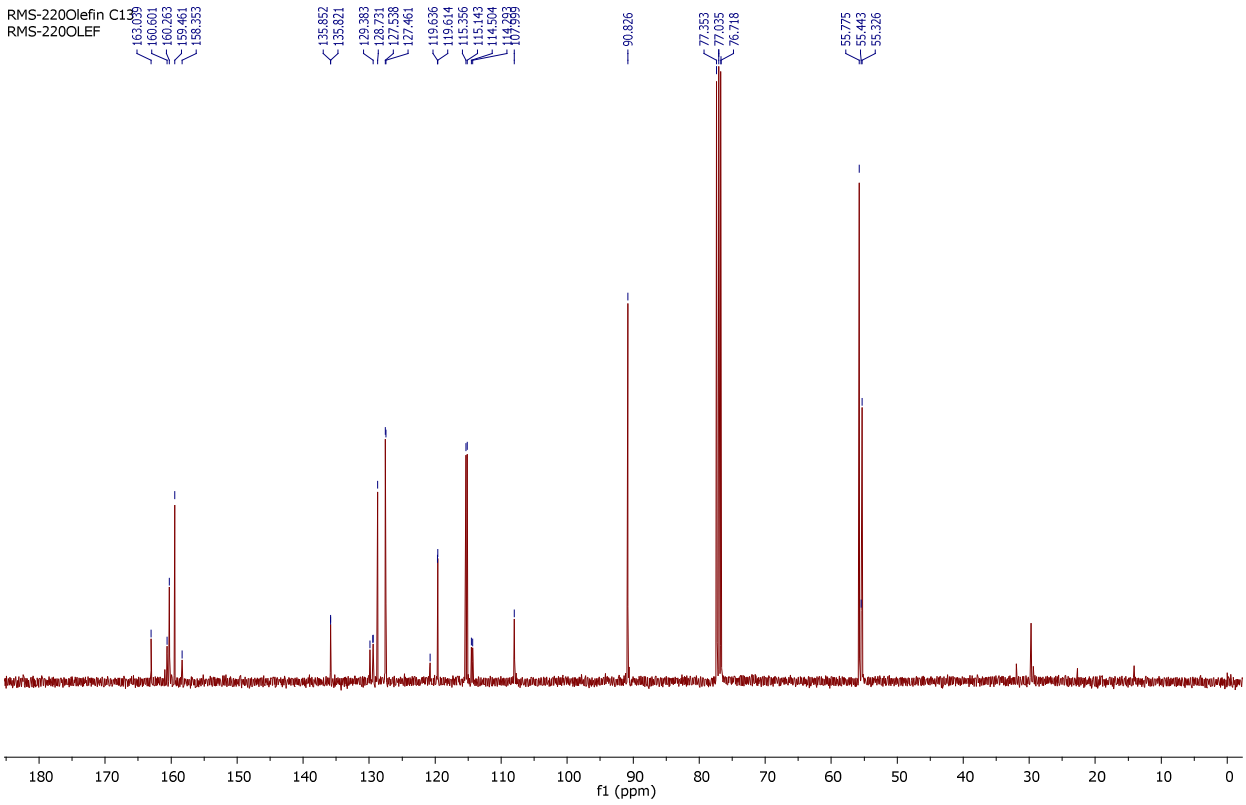


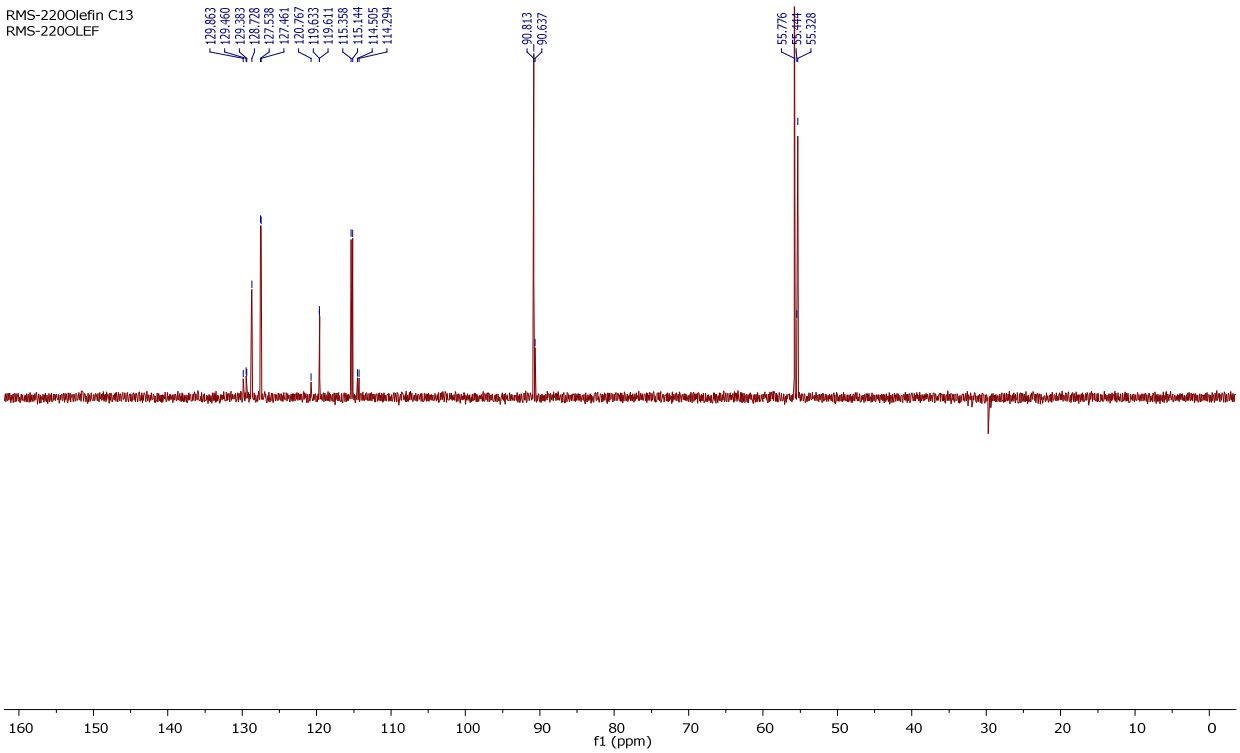


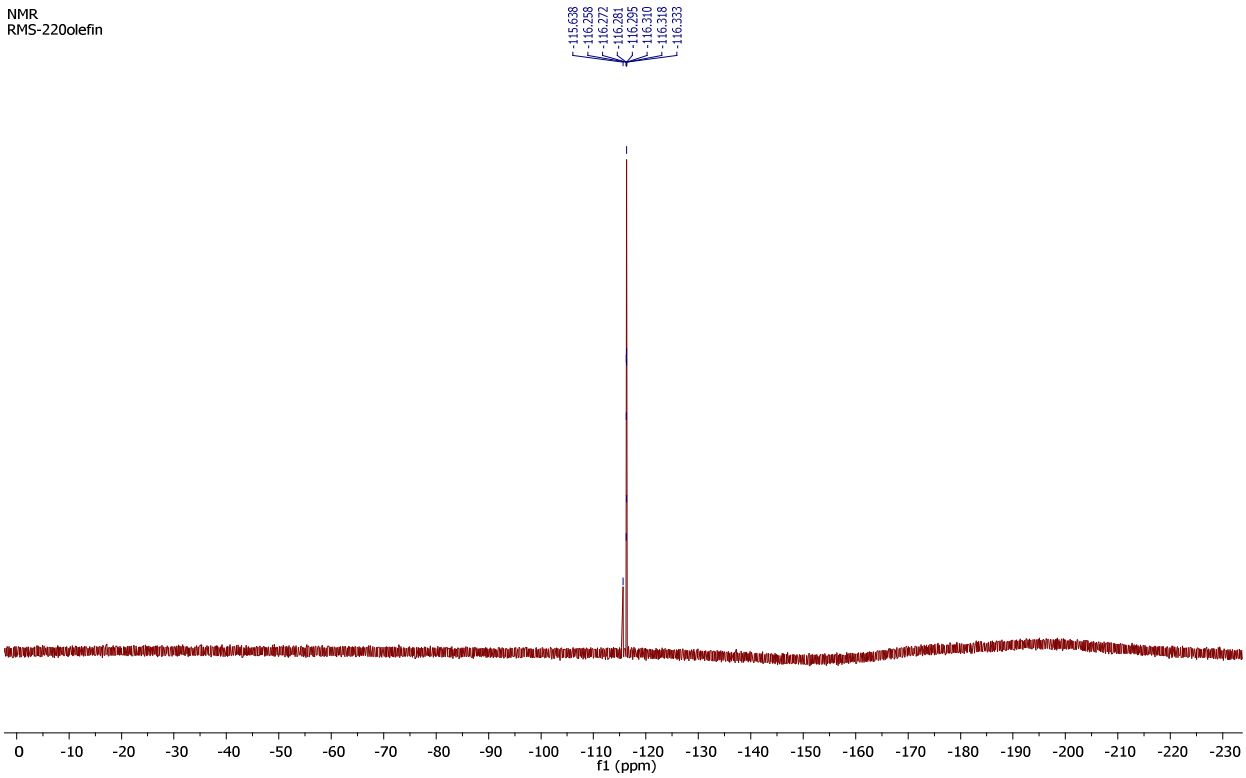


S3.7. ^{1}H, ^{13}C, DEPT135 and ^{19}F NMR spectra of (E,Z)-1-(4′-fluorostyryl)-2,4,6-trimethoxybenzene (**1g**)

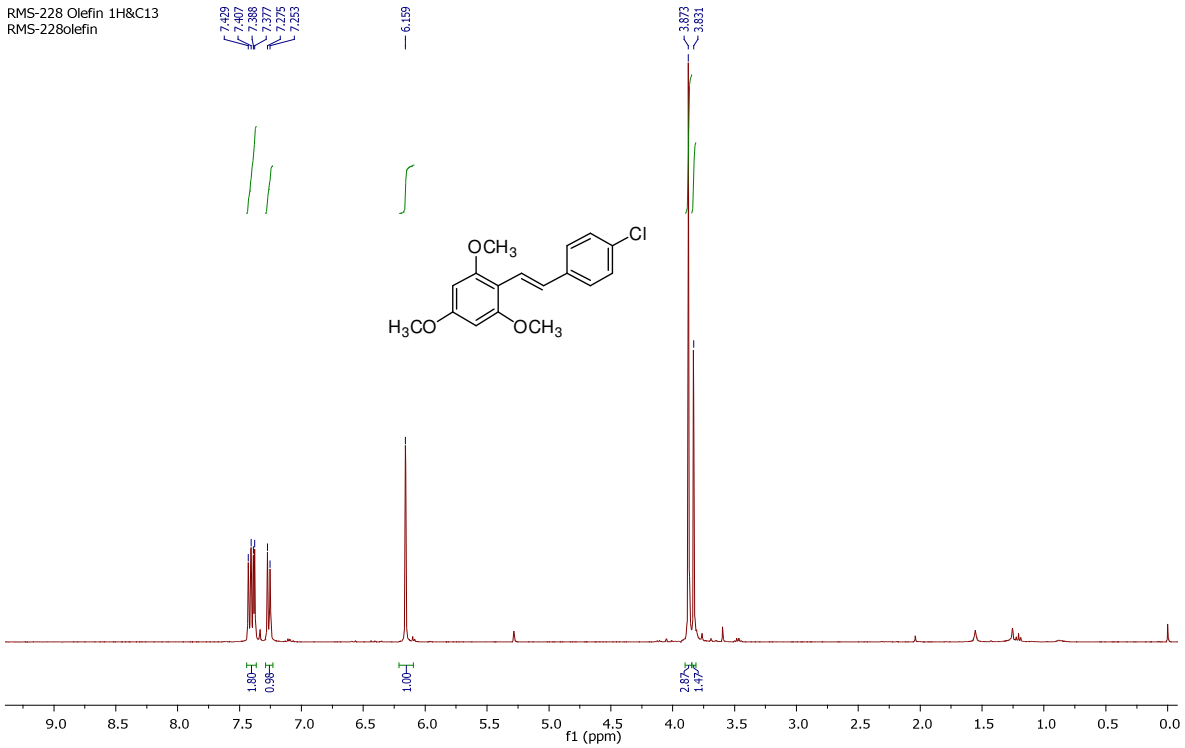


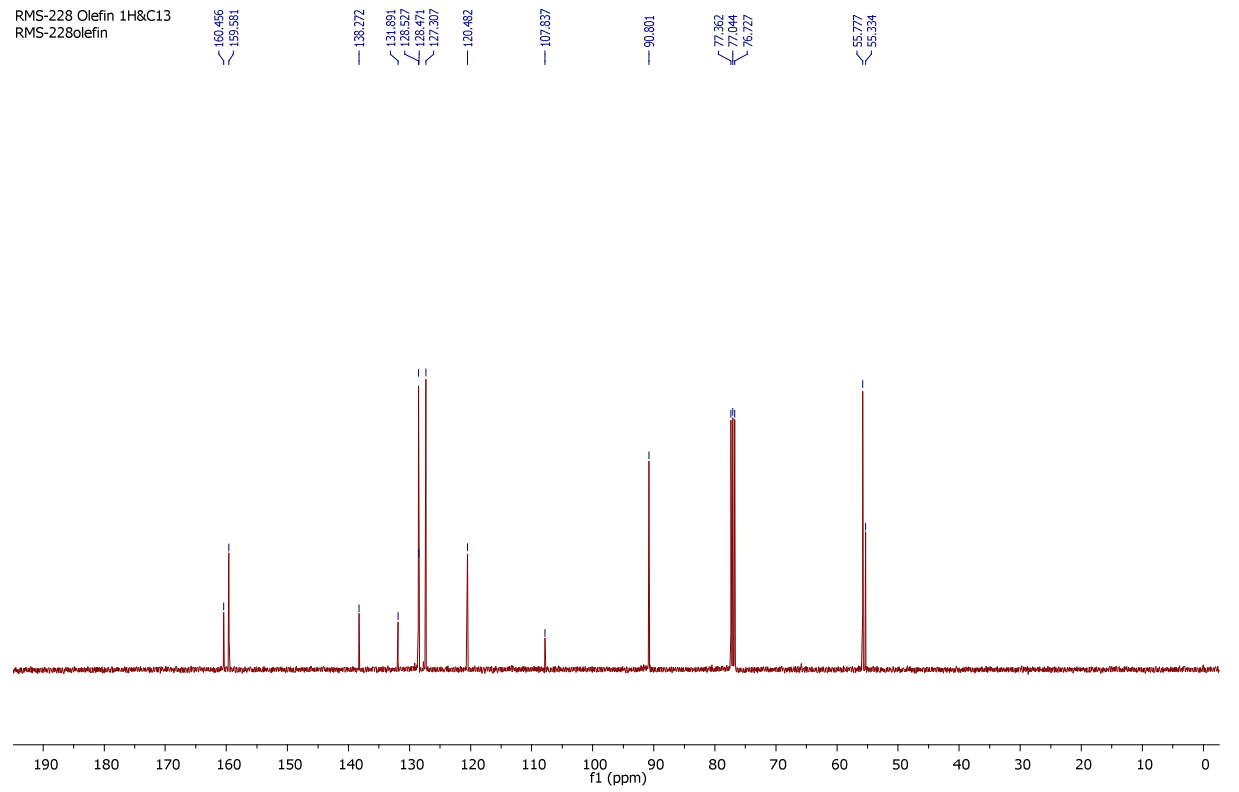

RMS-220Olefin C13
RMS-220OLEF
163.039
160.601
160.263
159.461
158.353
135.852
135.821
129.383
128.731
127.538
127.461
119.636
119.614
115.356
115.143
114.504
114.283
107.999
90.826
77.353
77.035
76.718
55.775
55.443
55.326
f1 (ppm)

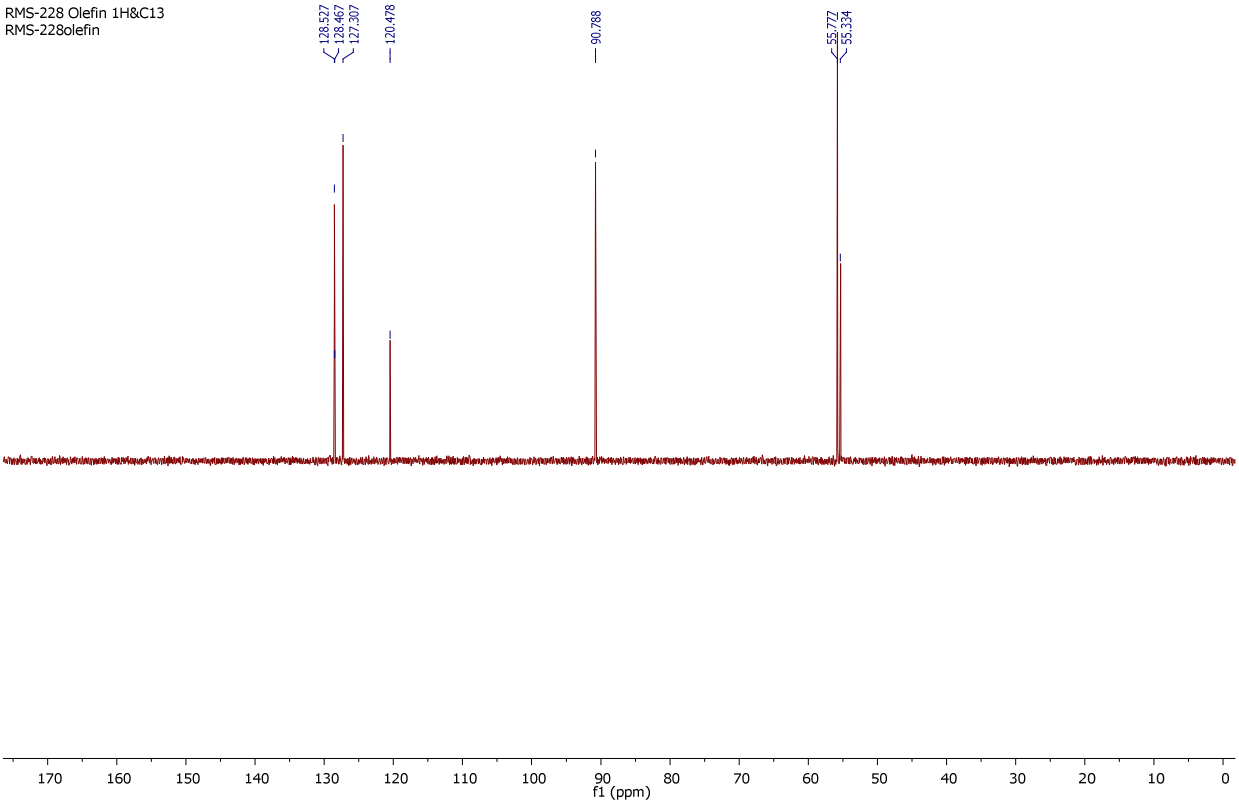

RMS-220Olefin C13
RMS-220OLEF
129.863
129.460
129.383
128.728
127.538
127.461
120.767
119.633
119.611
115.358
115.144
114.505
114.294
90.813
90.637
55.776
55.444
55.328
f1 (ppm)



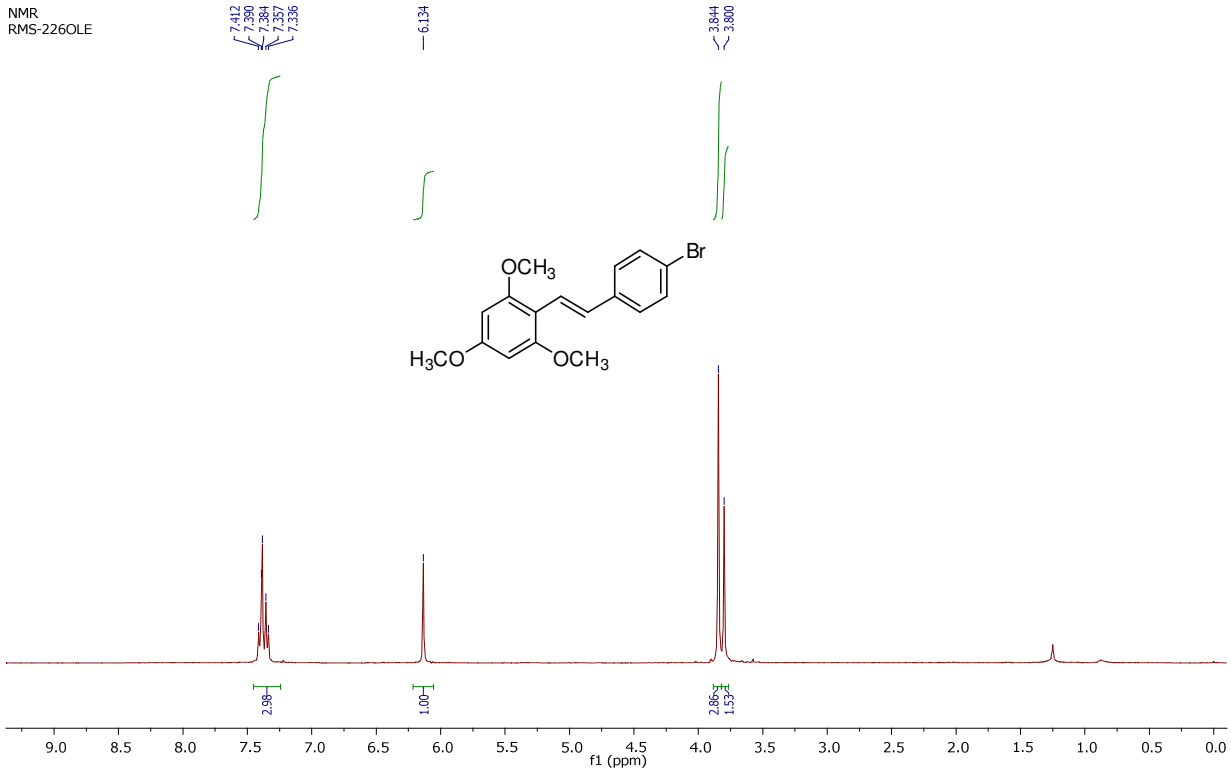
S3.8. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-1-(4′-Chlorostyryl)-2,4,6-trimethoxybenzene (**1h**)

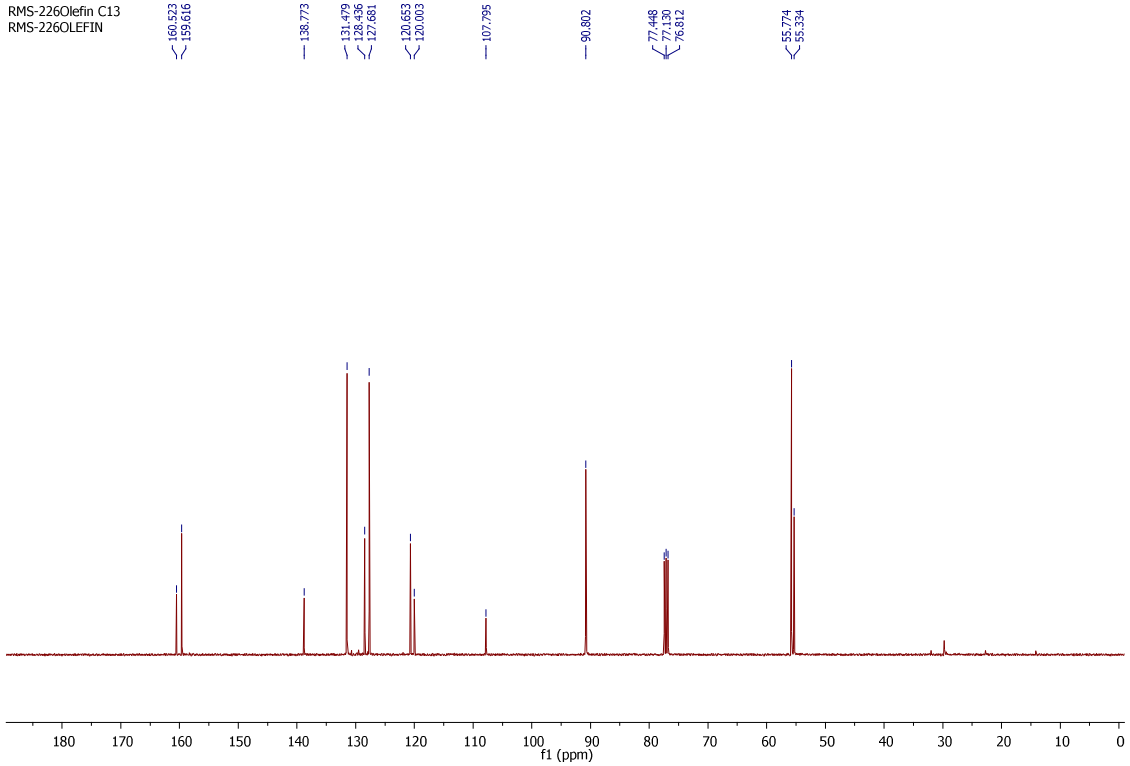


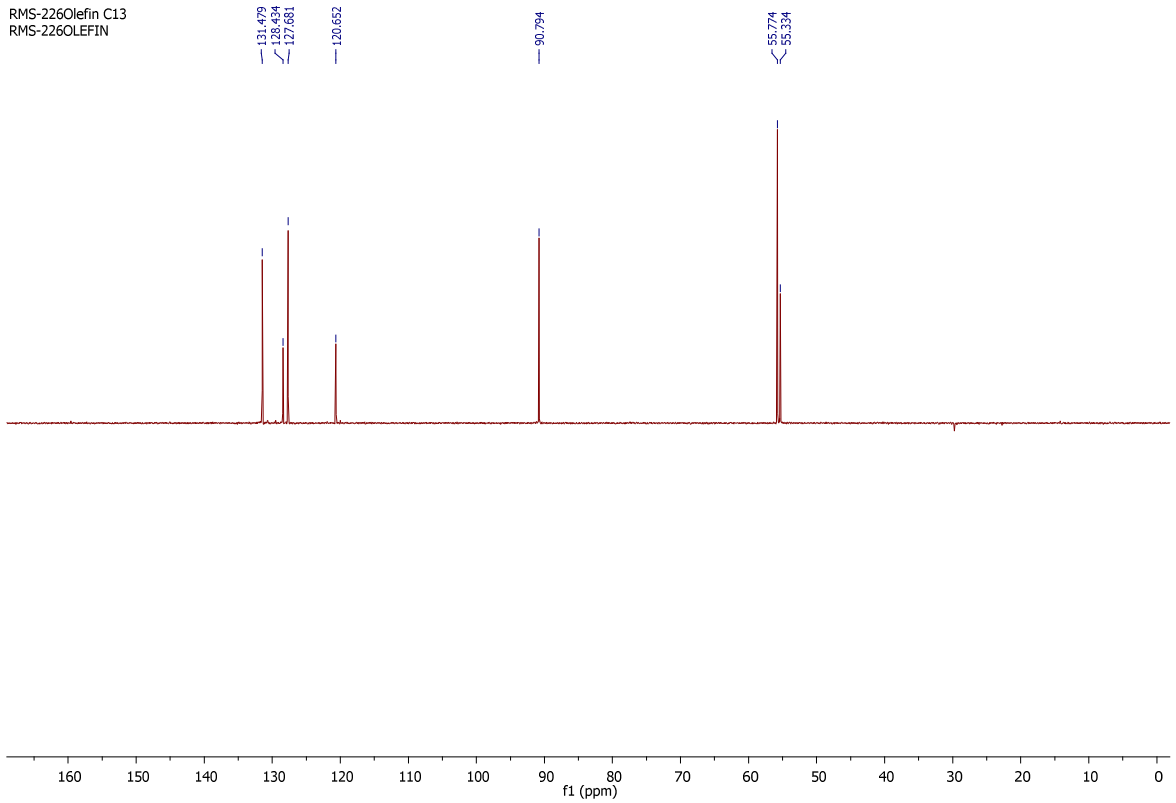

RMS-228 Olefin 1H&C13
RMS-228olefin
160.456
159.581
138.272
131.891
128.527
128.471
127.307
120.482
107.837
90.801
77.362
77.044
76.727
55.777
55.334
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


RMS-228 Olefin 1H&C13
RMS-228olefin
128.527
128.467
127.307
120.478
90.788
55.777
55.334
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

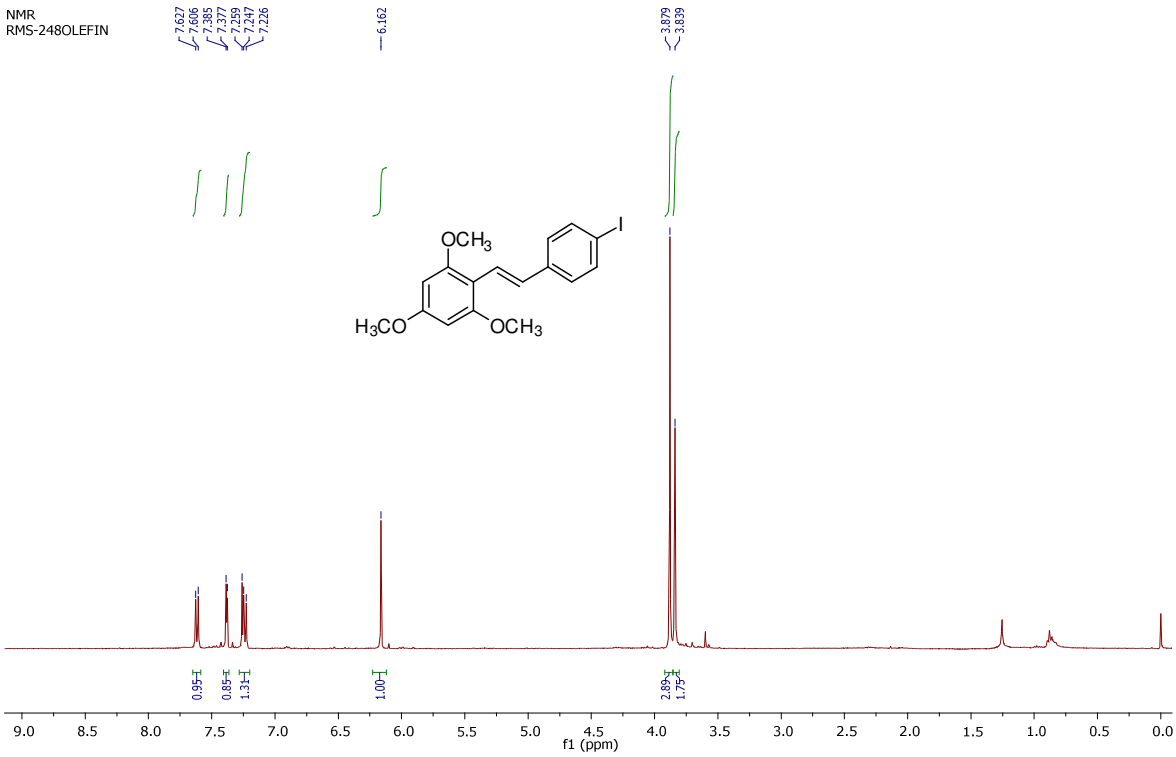
S3.9. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-1-(4′-bromostyryl)-2,4,6-trimethoxybenzene (**1i**)

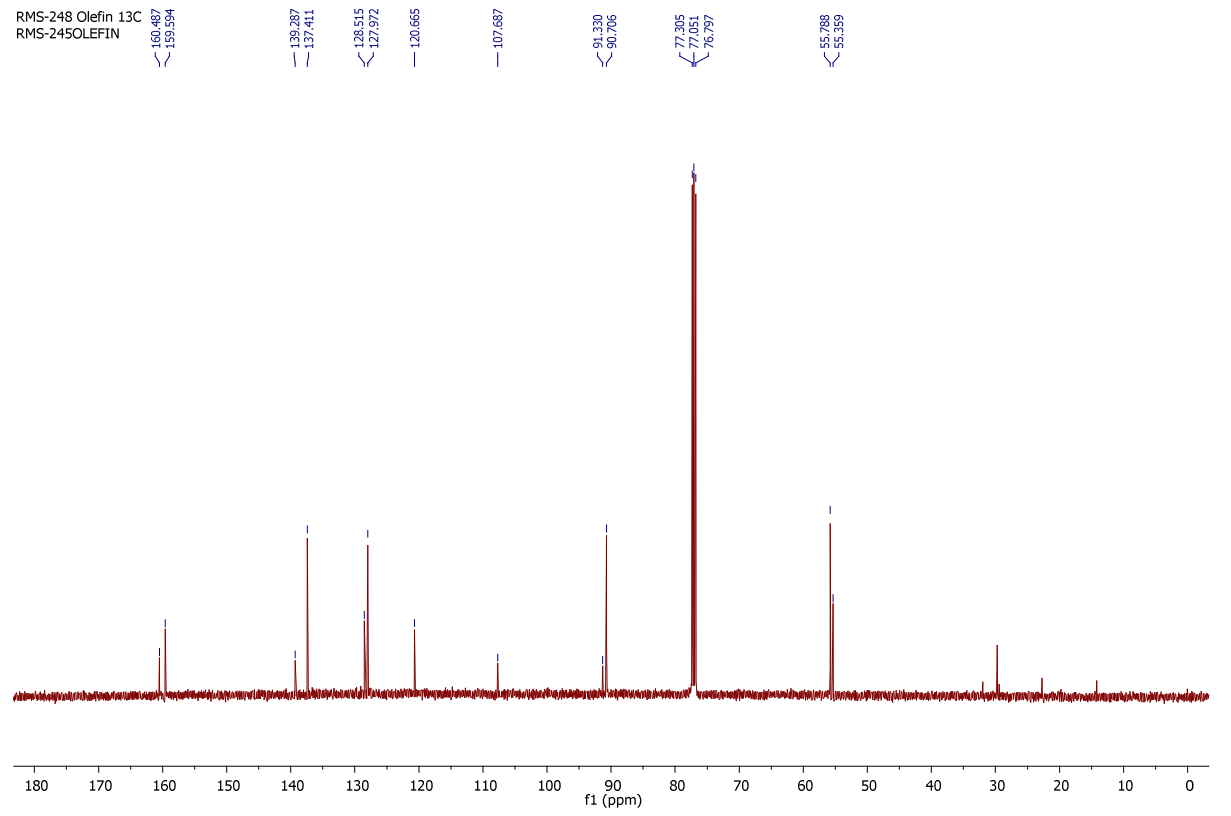


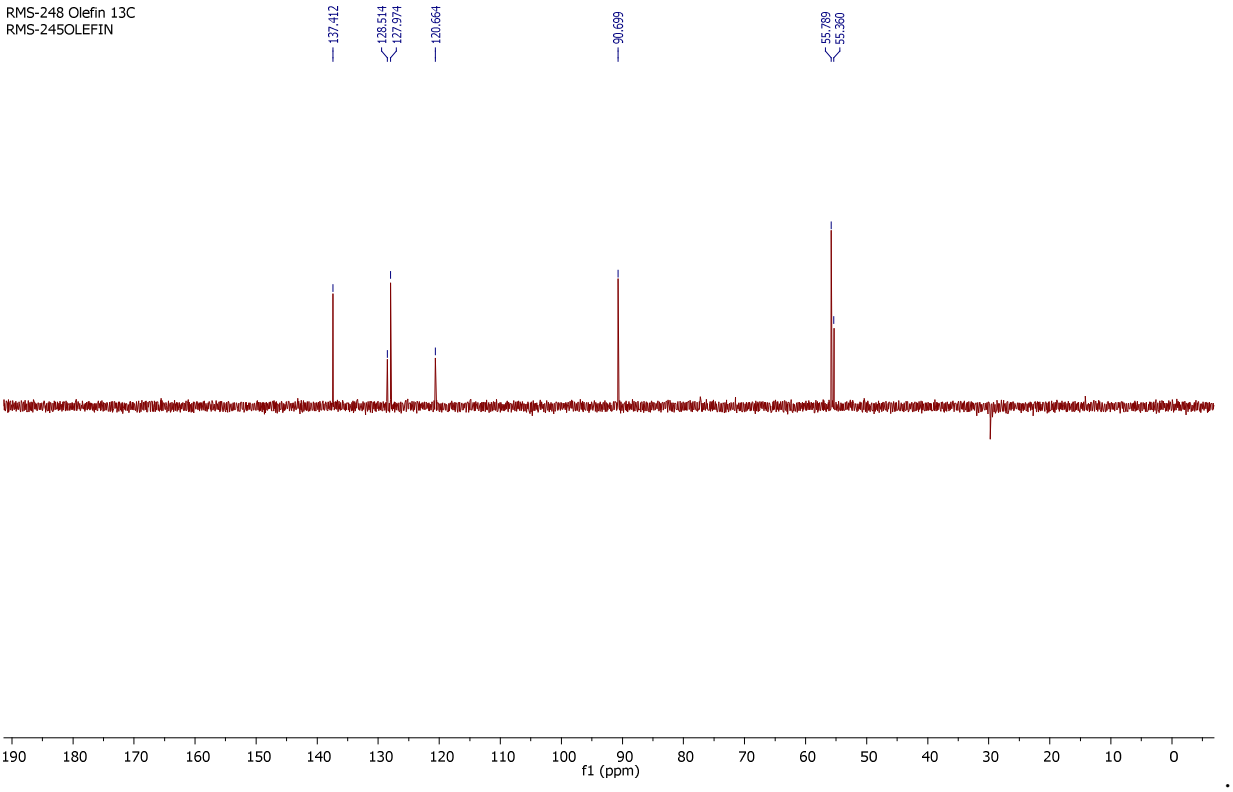




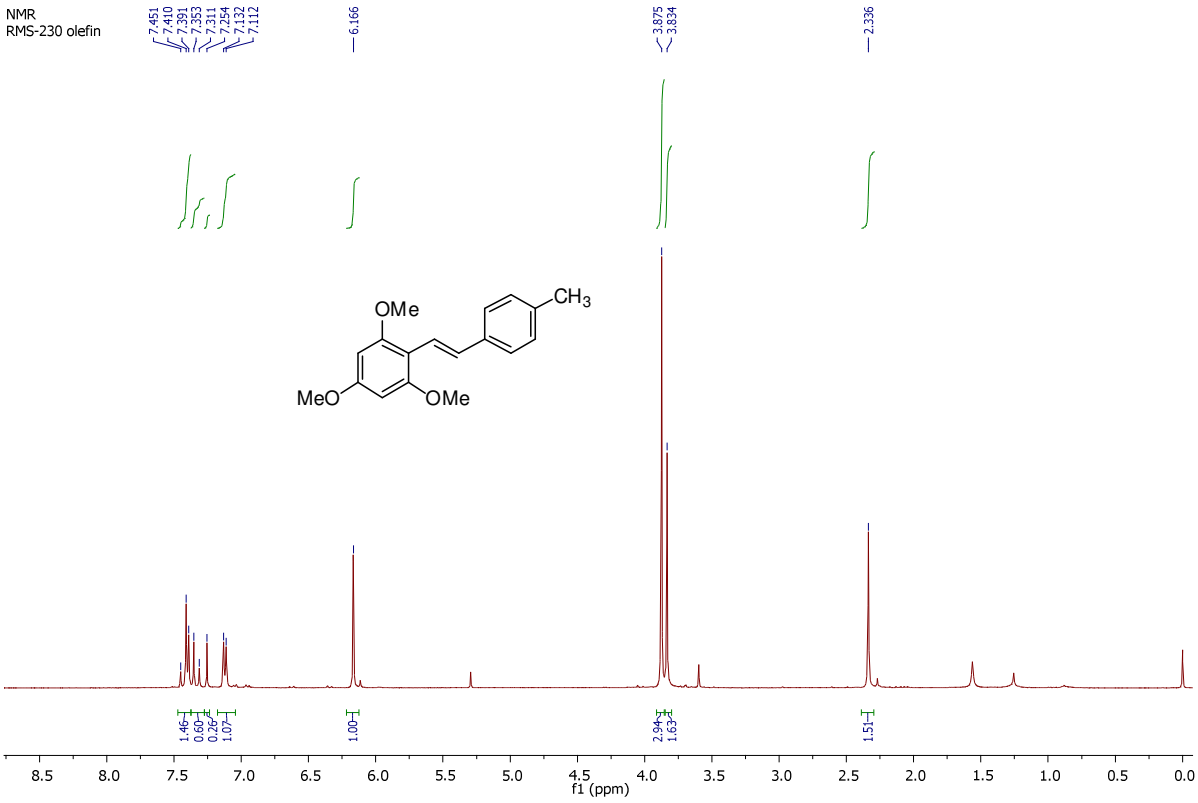
S3.10. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-1-(4′-iodostyryl)-2,4,6-trimethoxybenzene (**1j**)

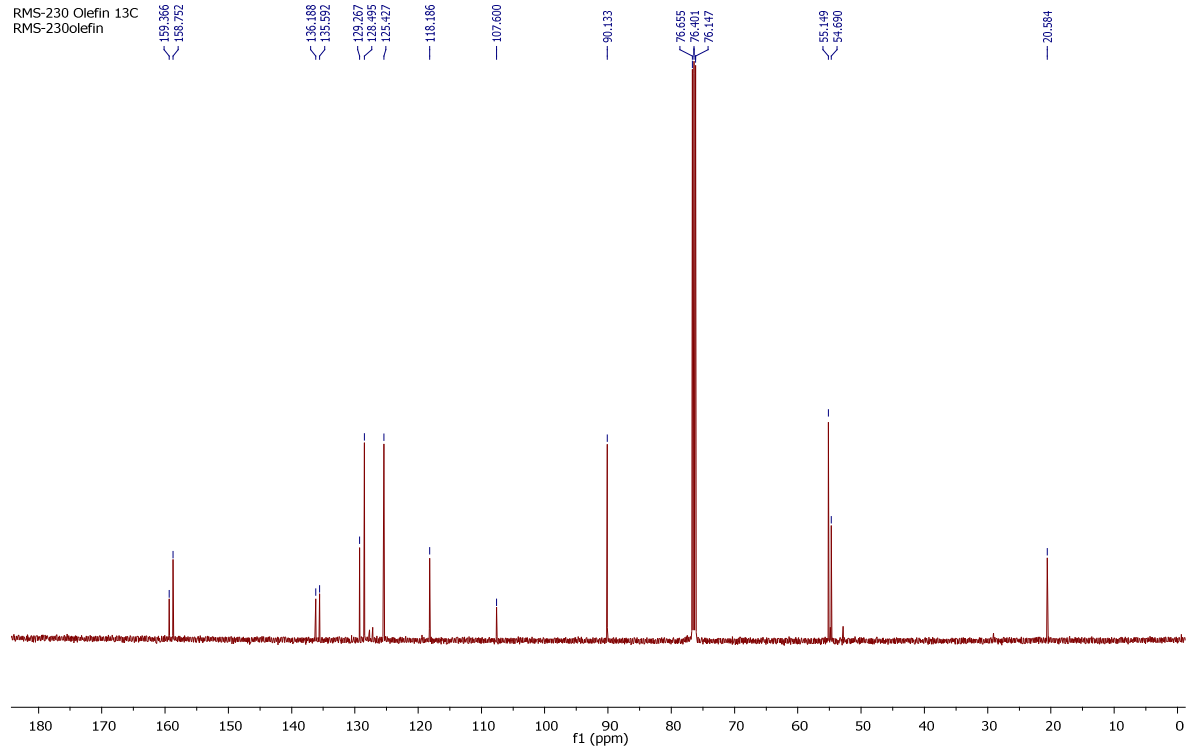


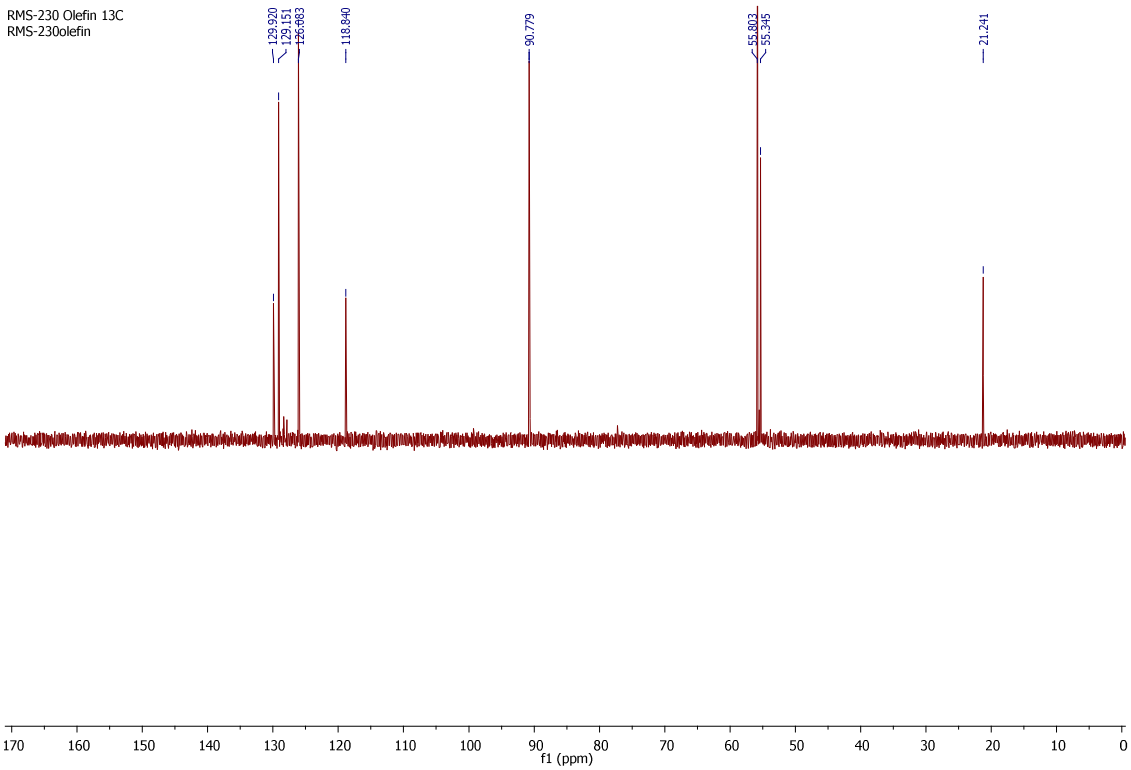

RMS-248 Olefin 13C
RMS-245OLEFIN
160.487
159.594
139.287
137.411
128.515
127.972
120.665
107.687
91.330
90.706
77.305
77.051
76.797
55.788
55.359
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


RMS-248 Olefin 13C
RMS-245OLEFIN
137.412
128.514
127.974
120.664
90.699
55.789
55.360
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

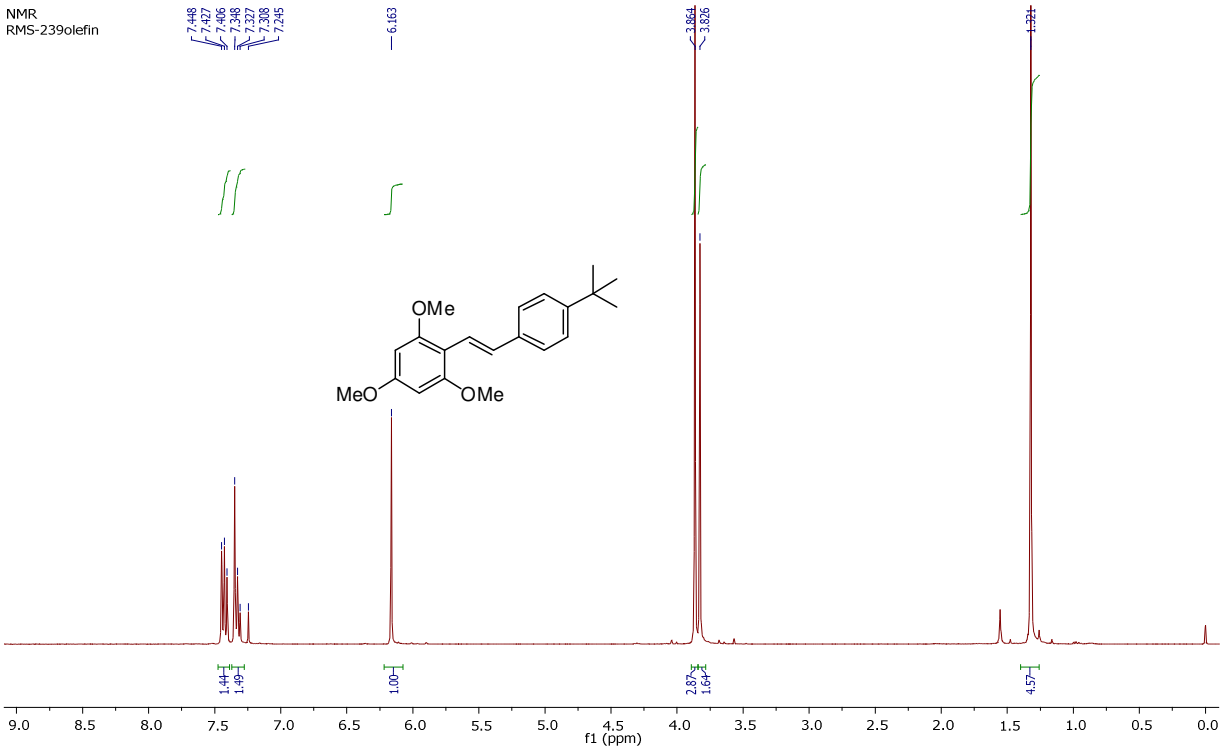
S3.11 ^{1}H, ^{13}C and DEPT135 NMR spectra of (E/Z)-1-(4′-methylstyryl)-2,4,6-trimethoxy-benzene (**1k**)

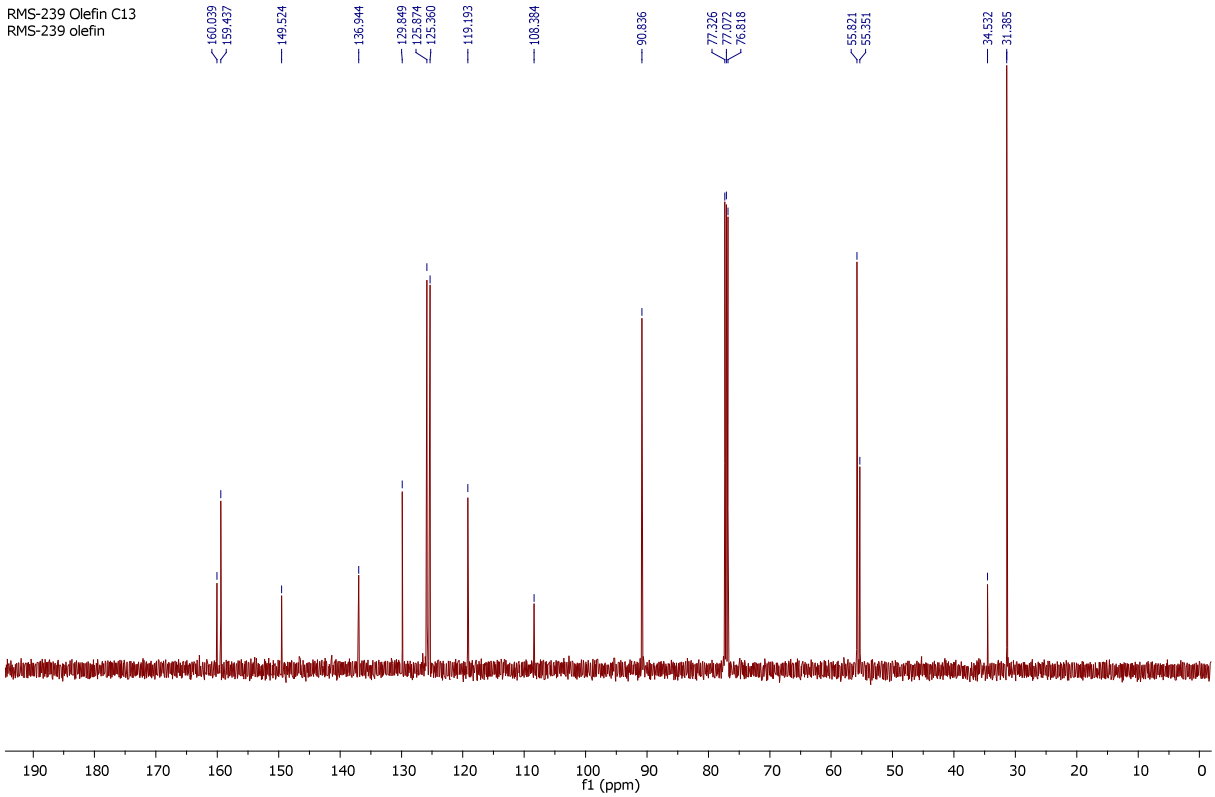


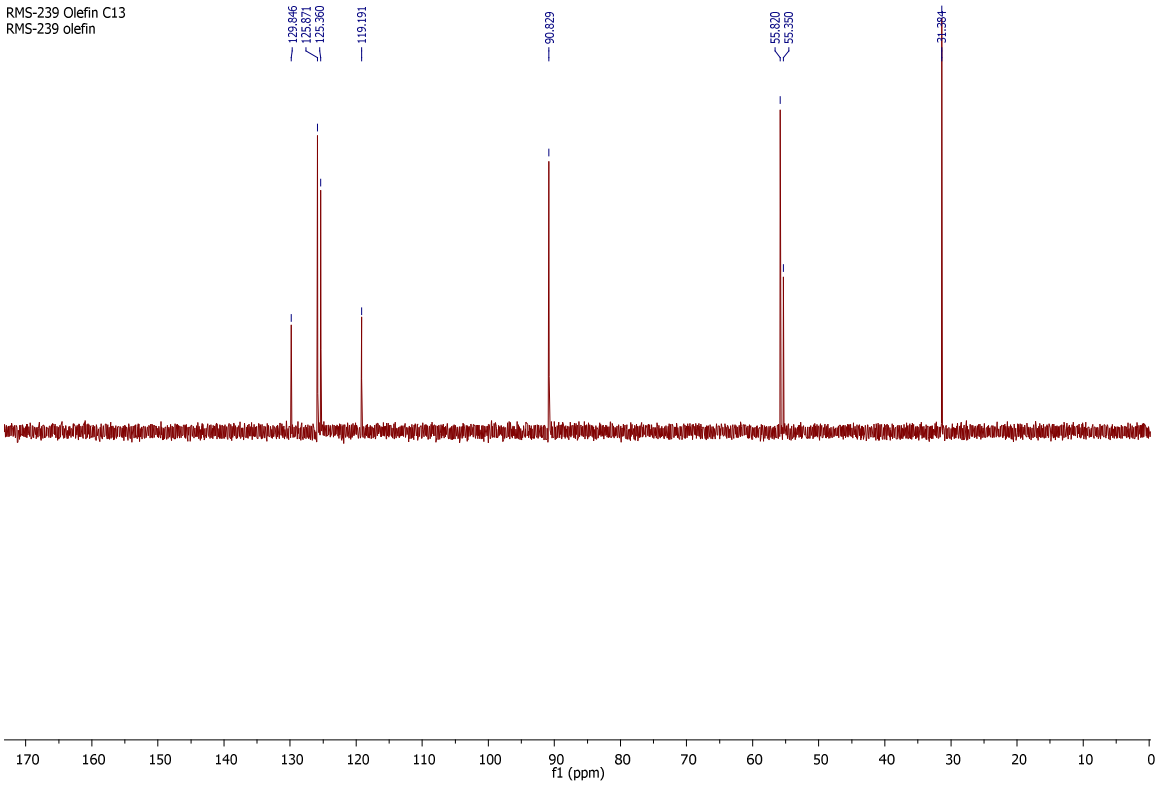




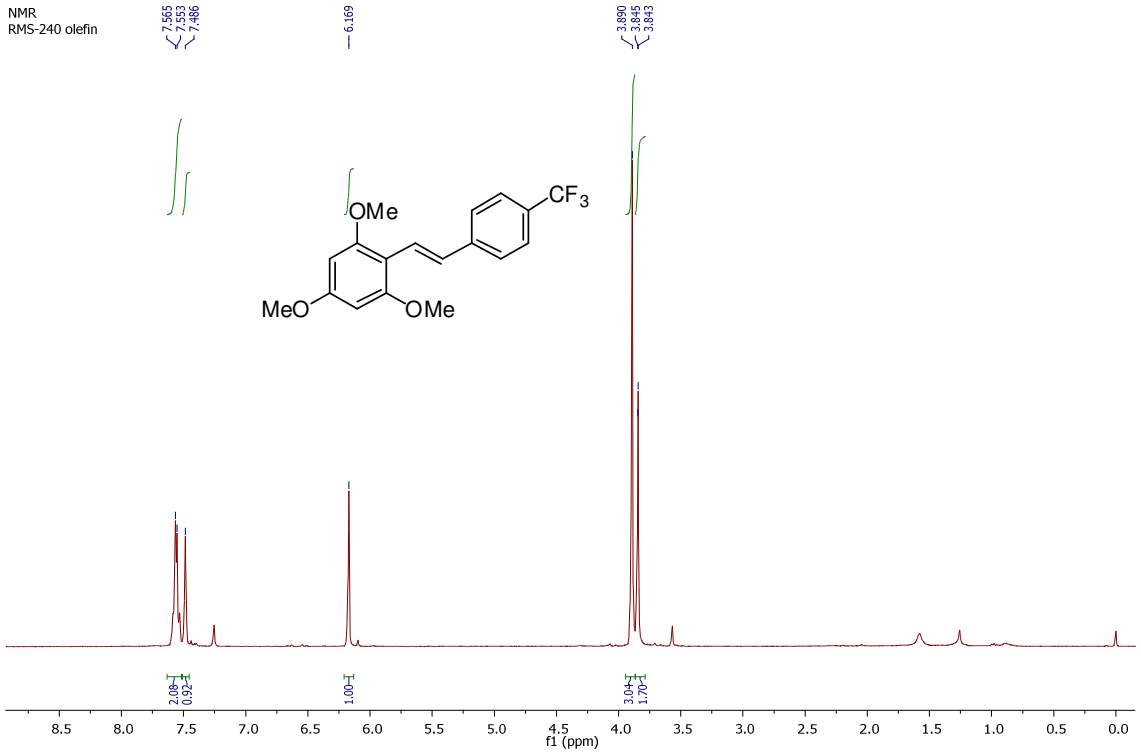
S3.12. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-1-(4′-(tert-butyl)styryl)-2,4,6-trimethoxybenzene (**1l**)

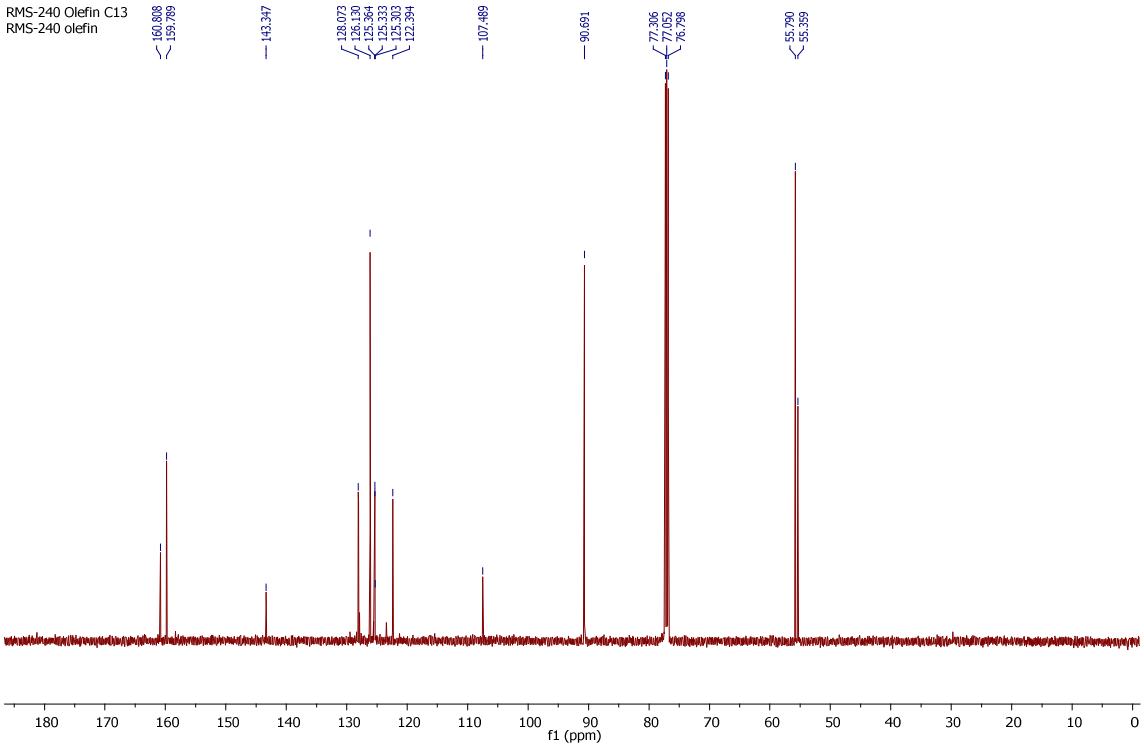


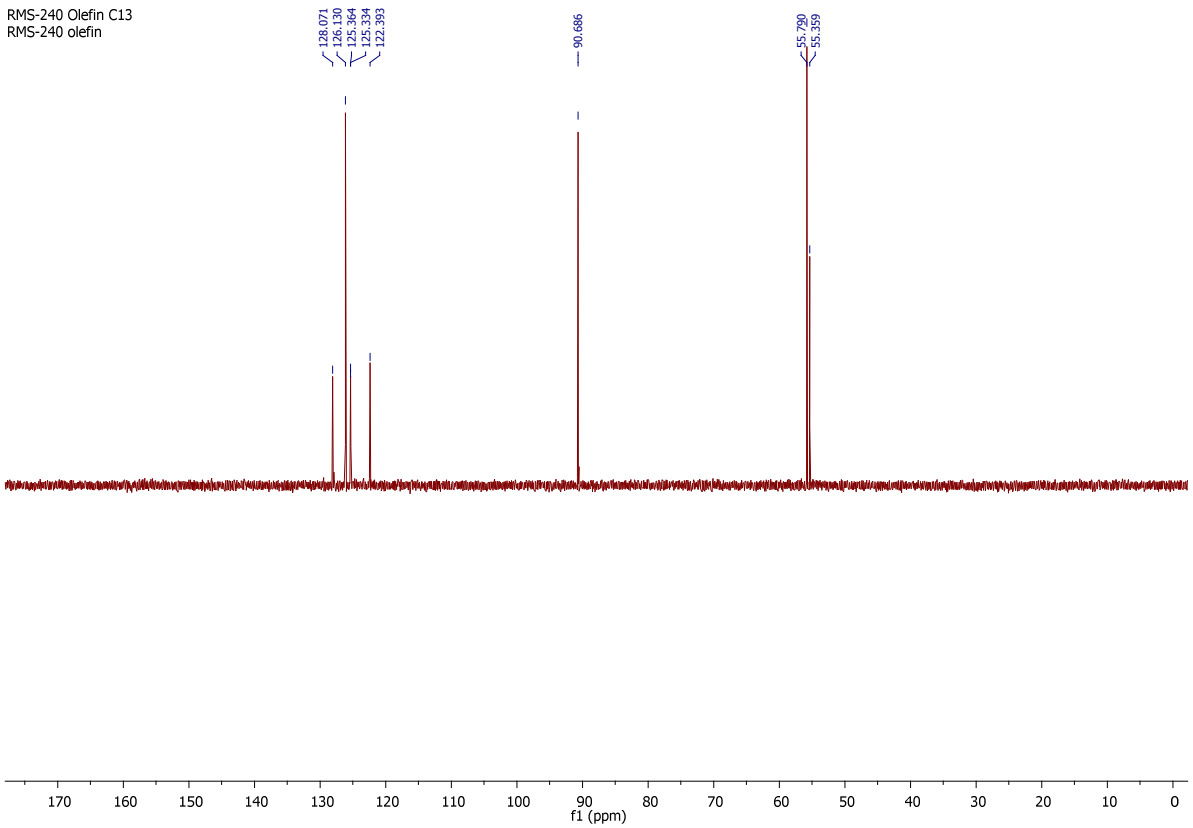

RMS-239 Olefin C13
RMS-239 olefin
160.039
159.437
149.524
136.944
129.849
125.874
125.360
119.193
108.384
90.836
77.326
77.072
76.818
55.821
55.351
34.532
31.385
f1 (ppm)

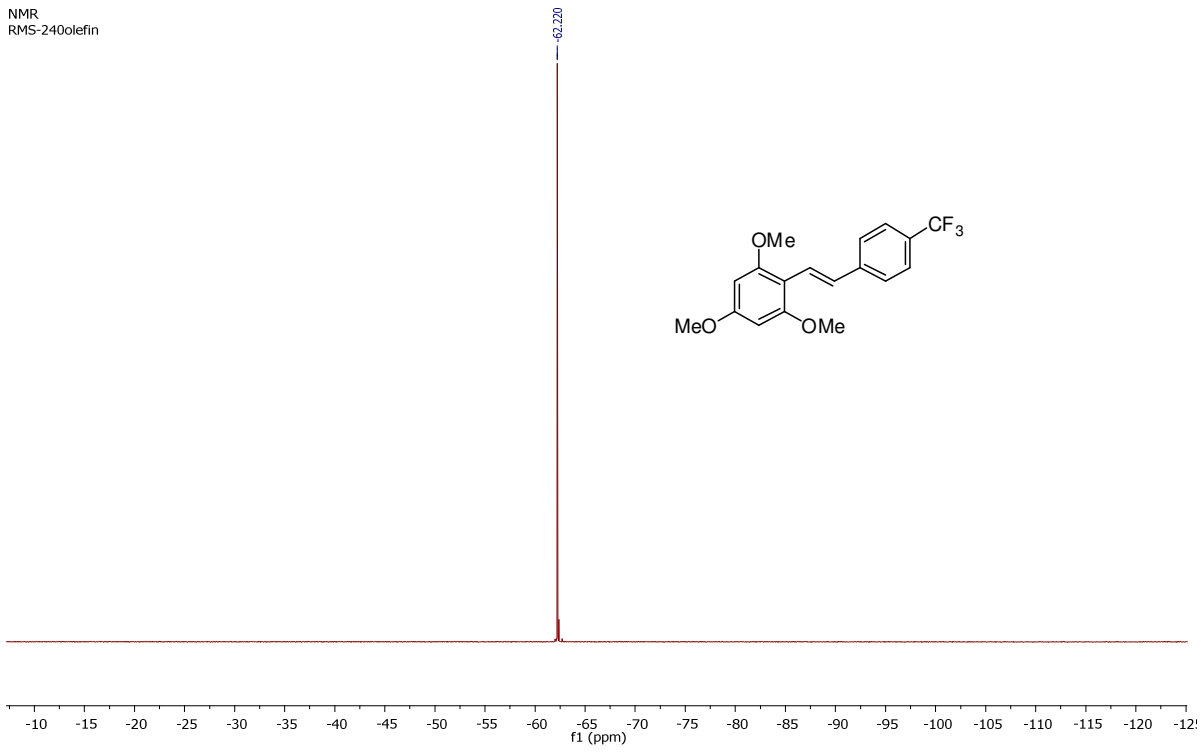

RMS-239 Olefin C13
RMS-239 olefin
129.846
125.871
125.360
119.191
90.829
55.820
55.350
31.384
f1 (ppm)

S3.13 ^{1}H, ^{13}C, DEPT135 and ^{19}F NMR spectra of (E/Z)-1-(4′-(trifluoromethyl) styryl)-2,4,6-trimethoxybenzene (**1m**)

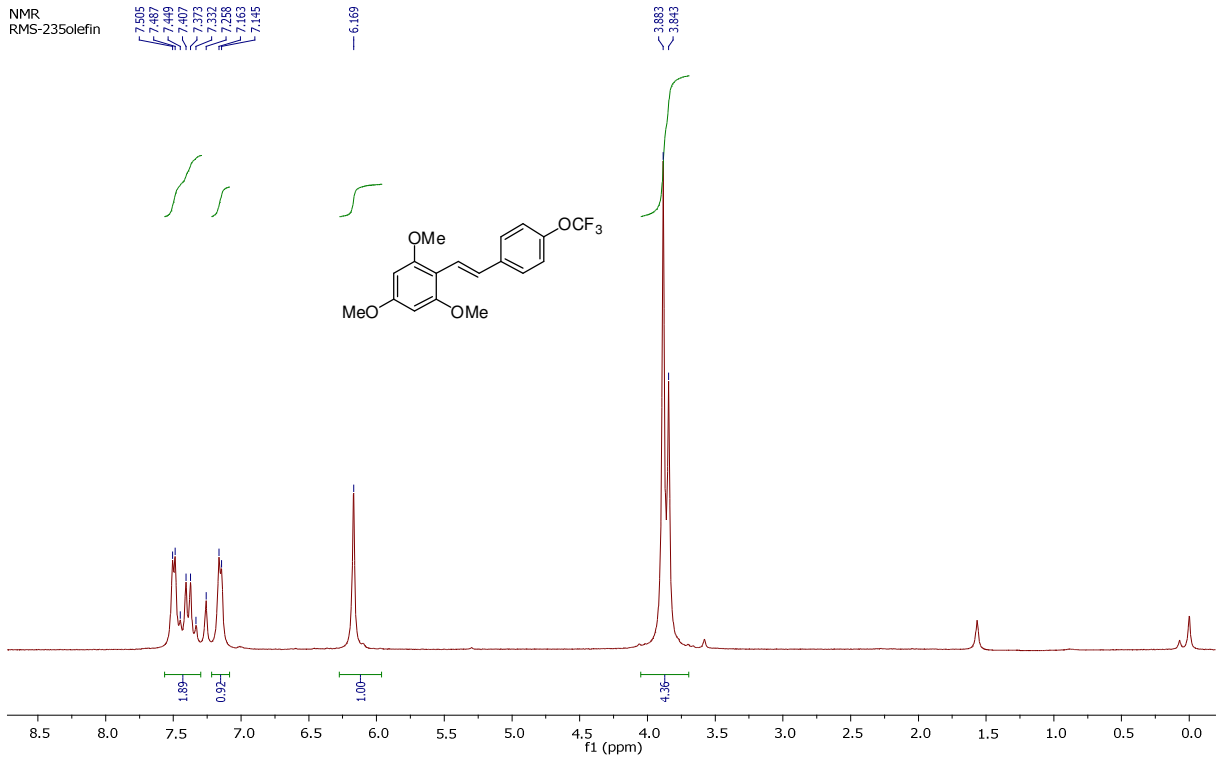


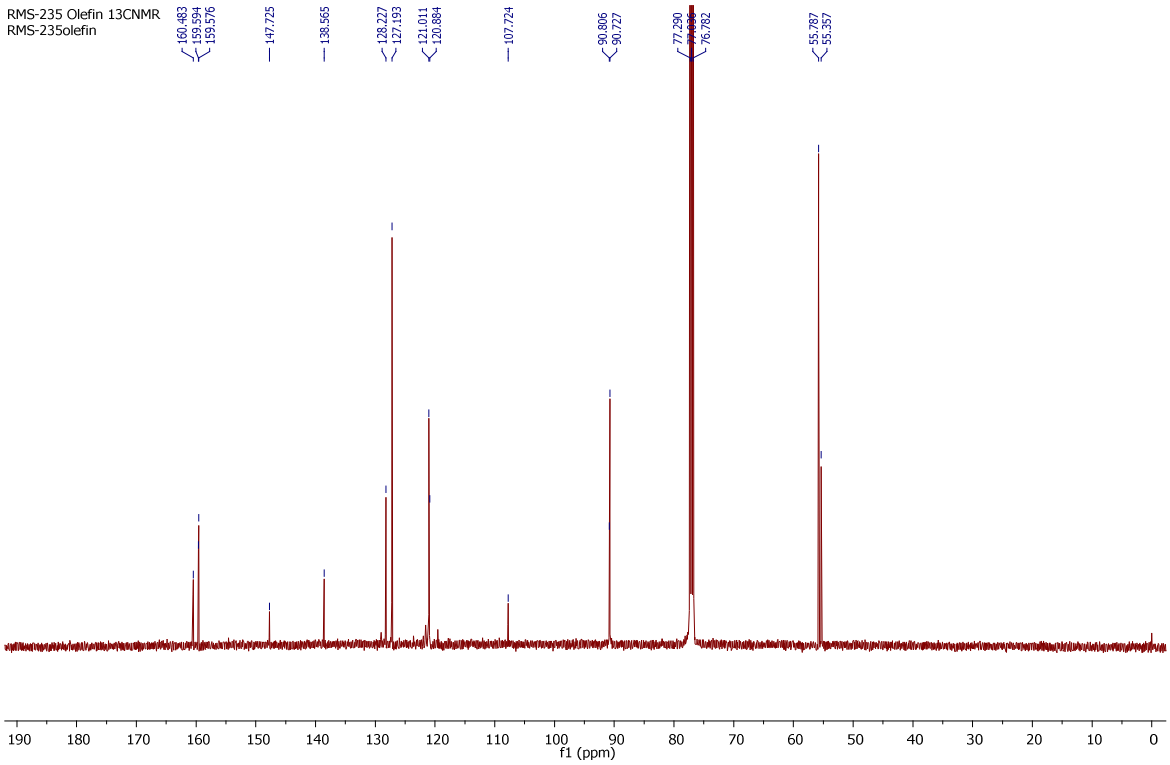


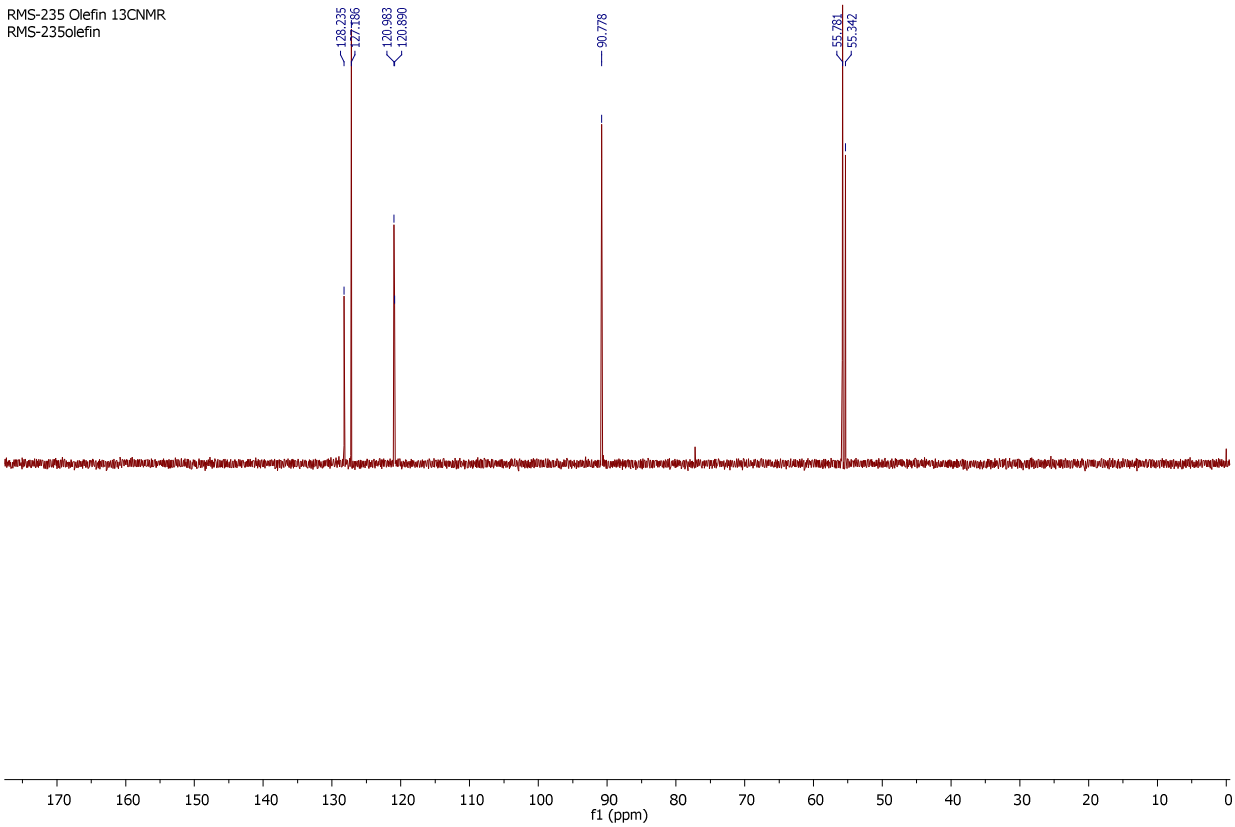

RMS-240 Olefin C13
RMS-240 olefin
128.071
126.130
125.364
125.334
122.393
90.686
55.790
55.599
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

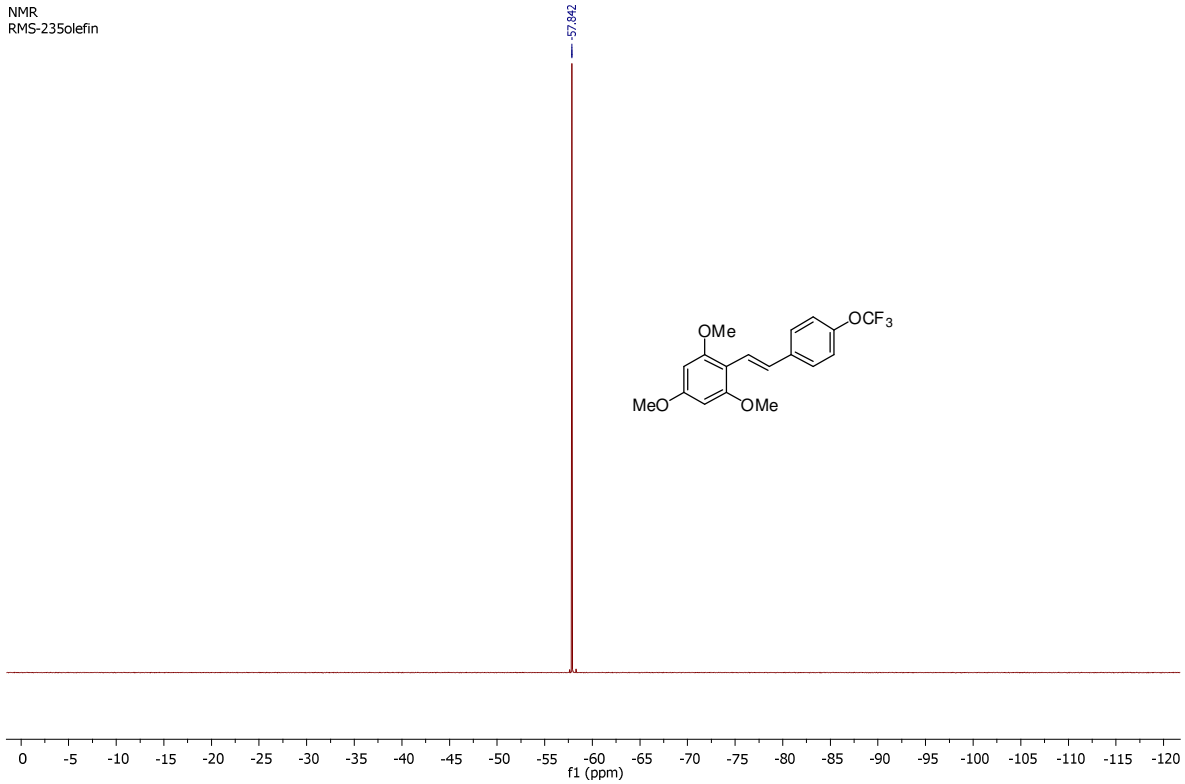

NMR
RMS-240olefin
-62.220
OMe
CF3
MeO
OMe
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
f1 (ppm)

S3.14. ^{1}H, ^{13}C, DEPT135 and ^{19}F NMR spectra of (E)-1-(4′-(trifluoromethoxy)styryl)-2,4,6-trimethoxybenzene (**1n**)

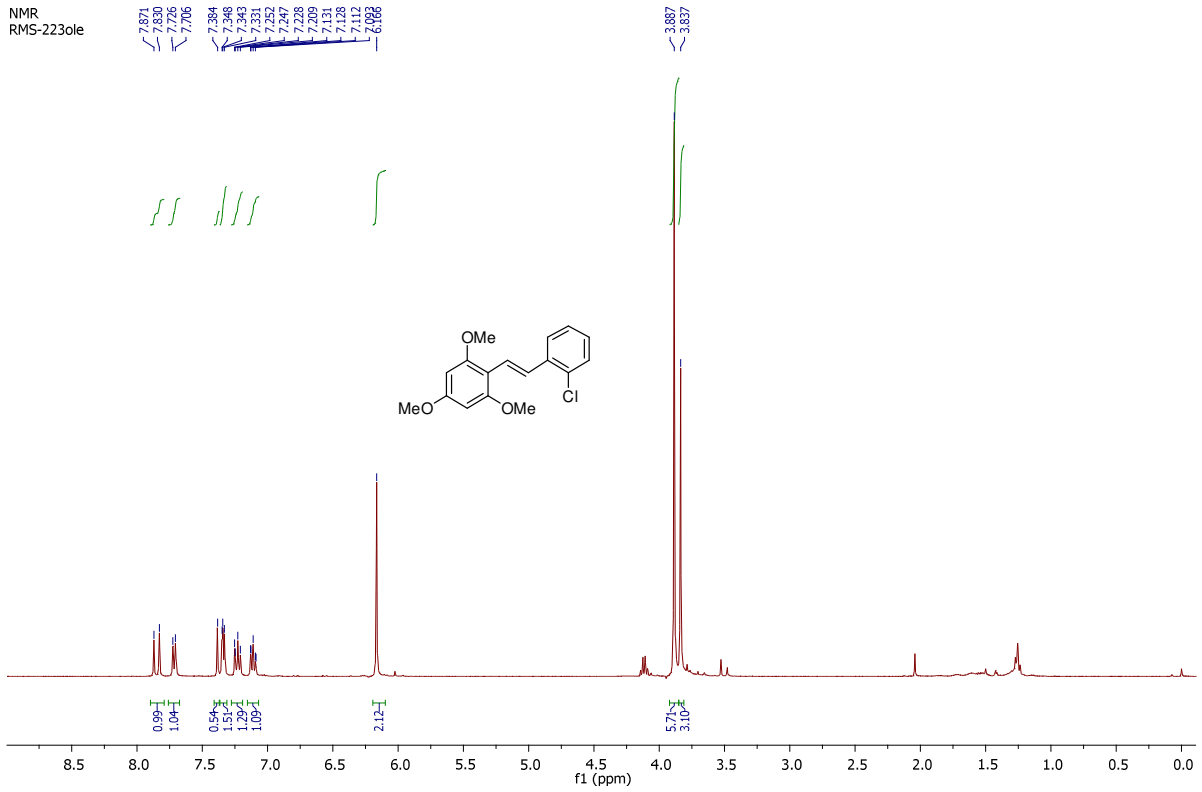


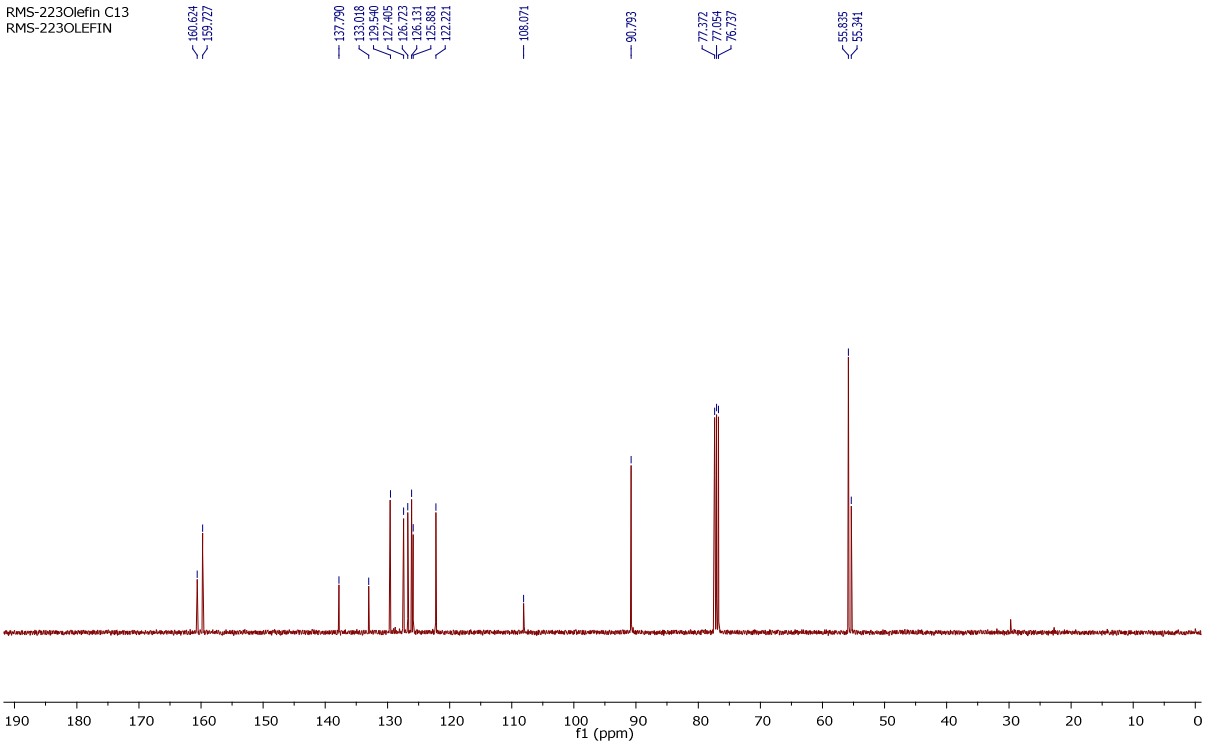


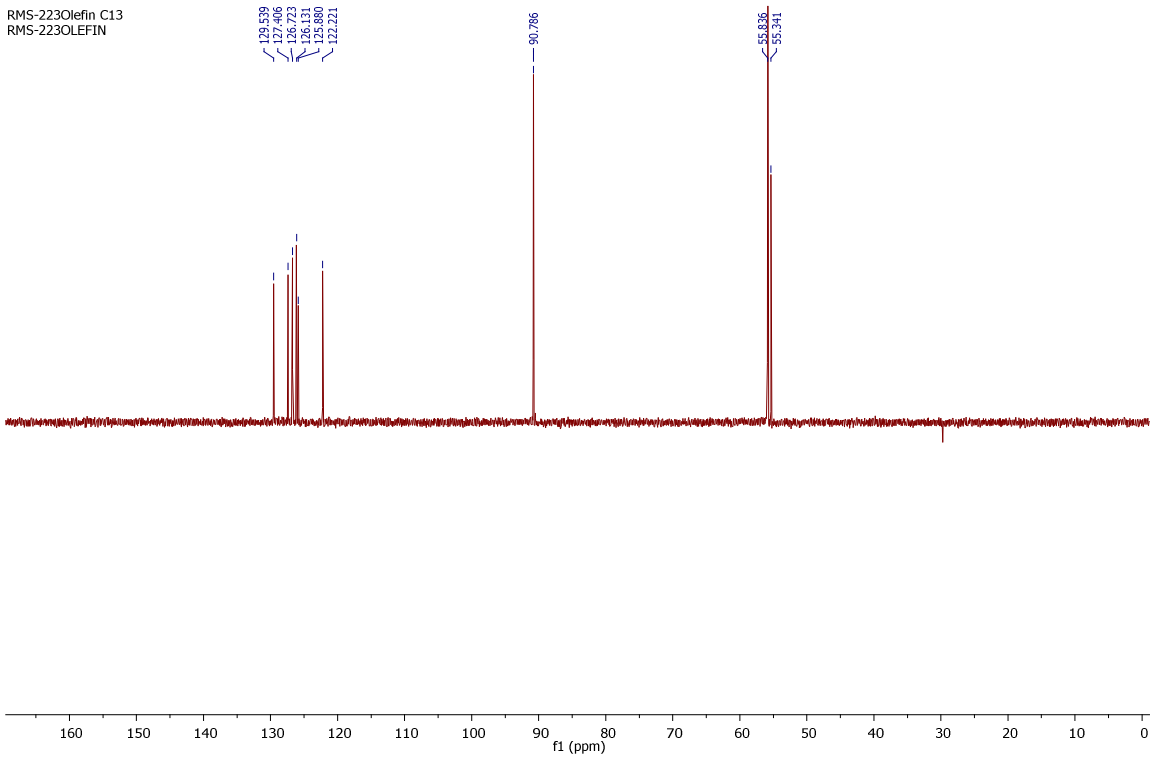

RMS-235 Olefin 13CNMR
RMS-235olefin
128.235
127.186
120.983
120.890
90.778
55.781
55.342
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


NMR
RMS-235olefin
-57.842
OMe
OCF3
MeO
OMe
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120
f1 (ppm)

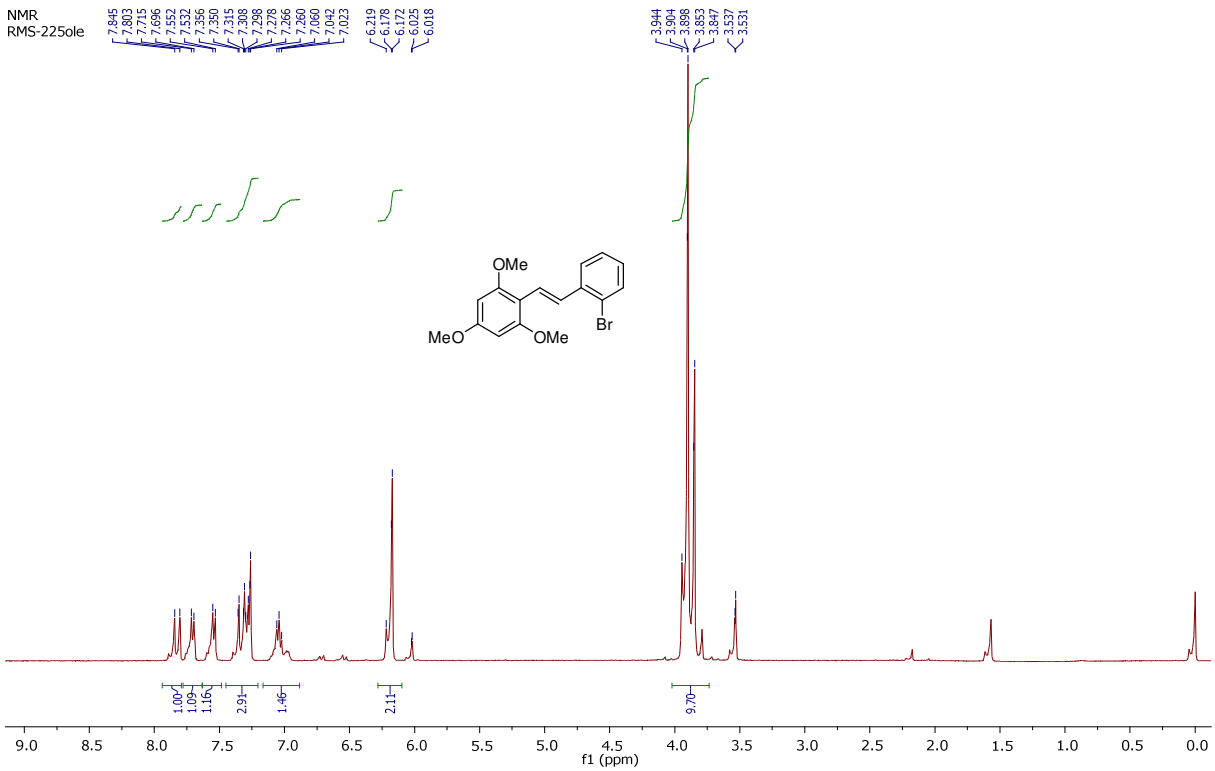
S3.15. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E,Z)-1-(2′-chlorostyryl)-2,4,6-trimethoxybenzene (**1o**)

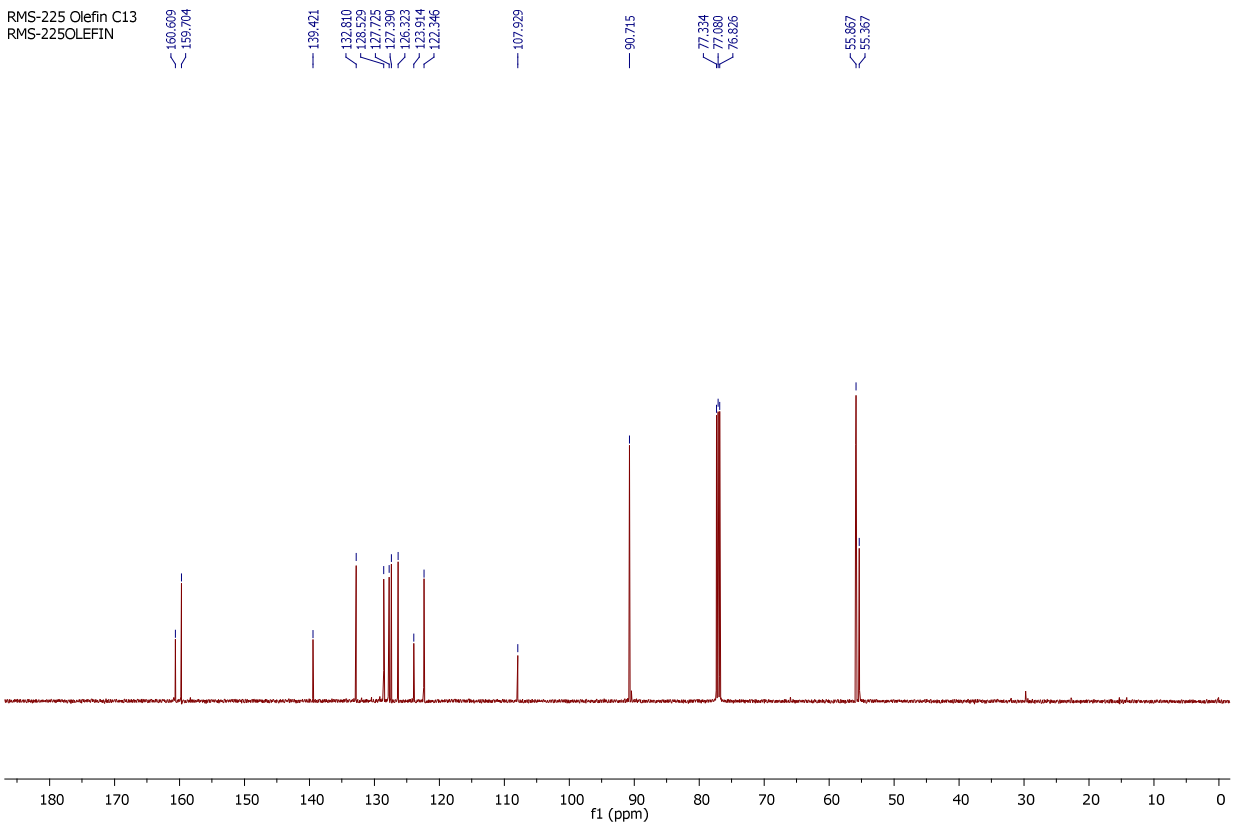


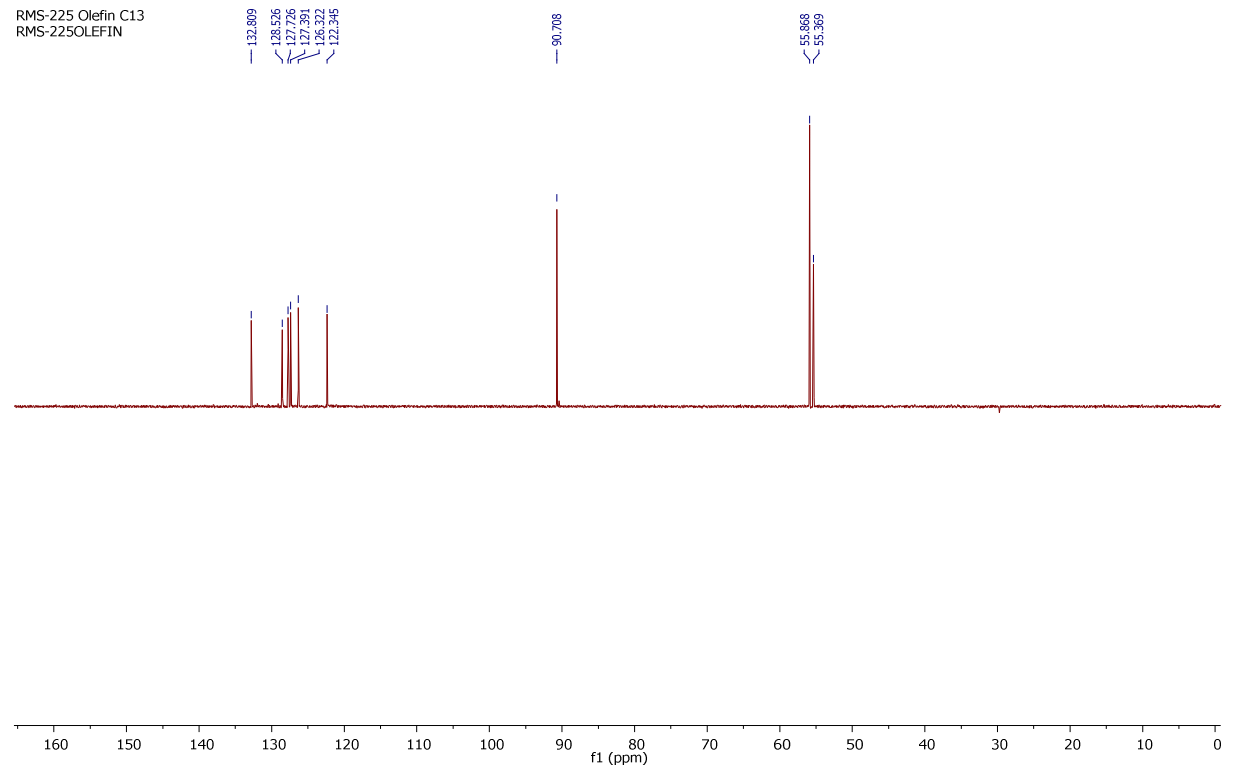




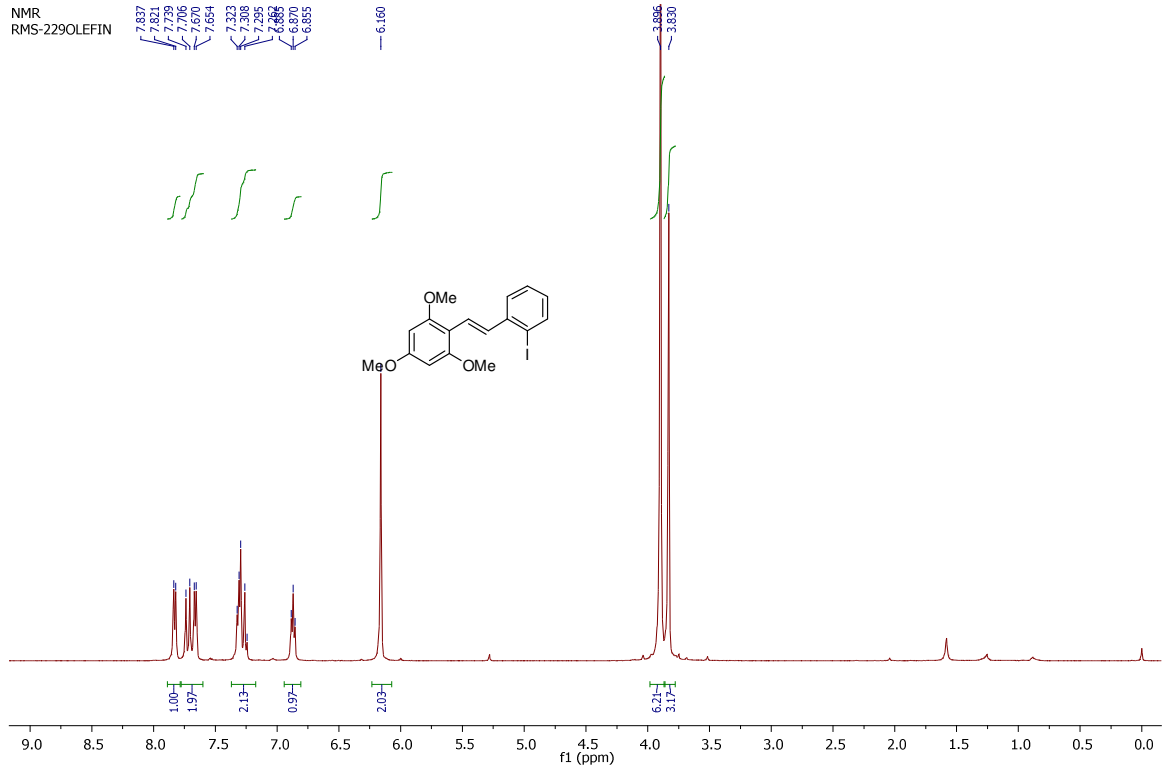
S3.16. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-1-(2′-bromostyryl)-2,4,6-trimethoxybenzene (**1p**)

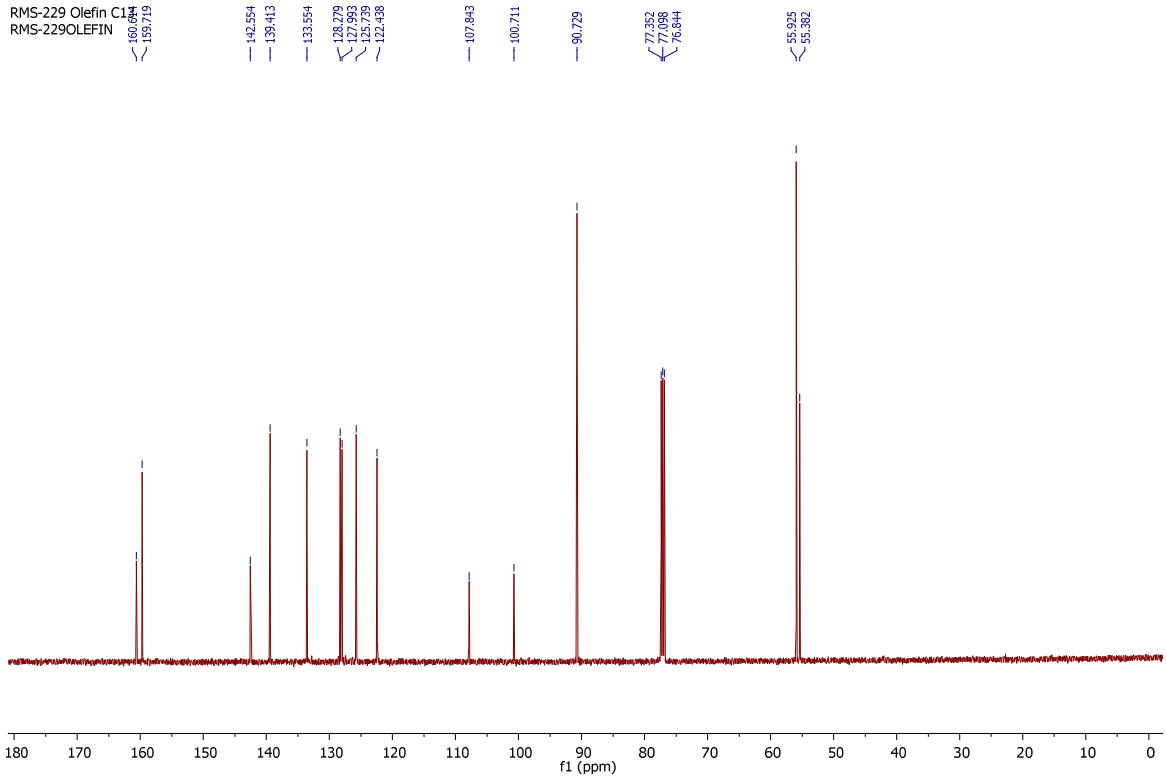


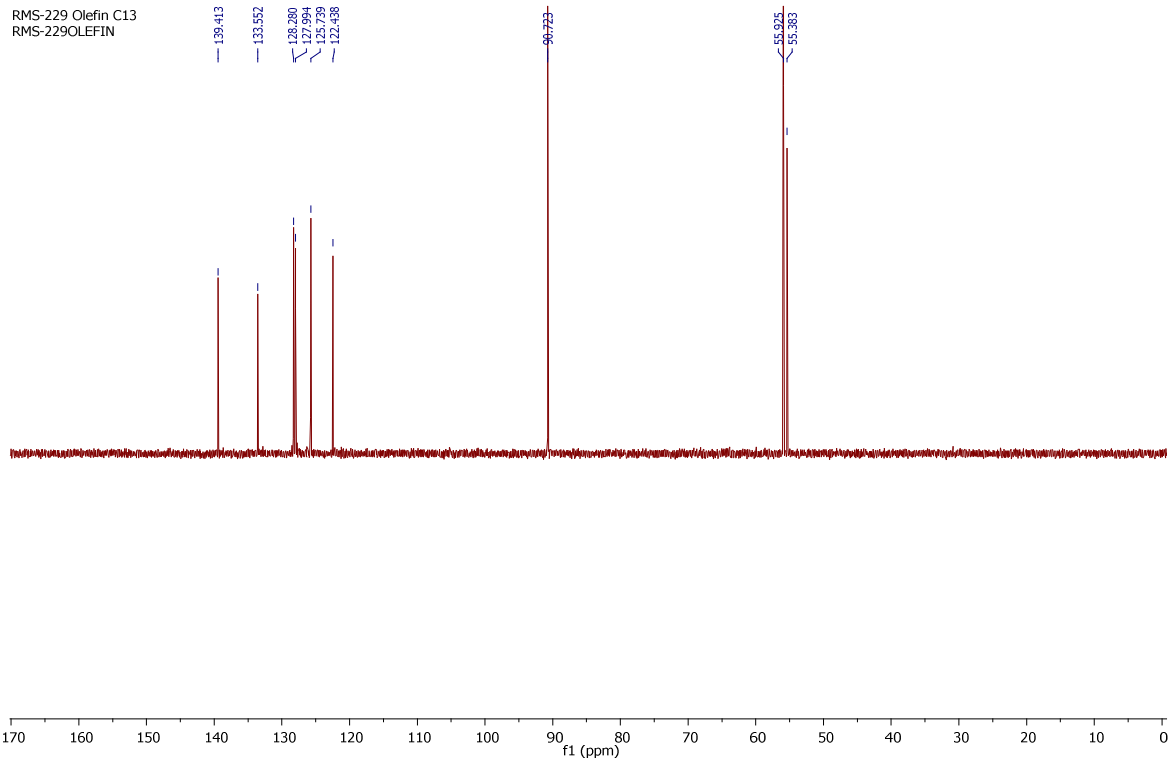

RMS-225 Olefin C13
RMS-225OLEFIN
160.609
159.704
139.421
132.810
128.529
127.725
127.390
126.323
123.914
122.346
107.929
90.715
77.334
77.080
76.826
55.867
55.367
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


RMS-225 Olefin C13
RMS-225OLEFIN
132.809
128.526
127.726
127.391
126.322
122.345
90.708
55.868
55.369
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

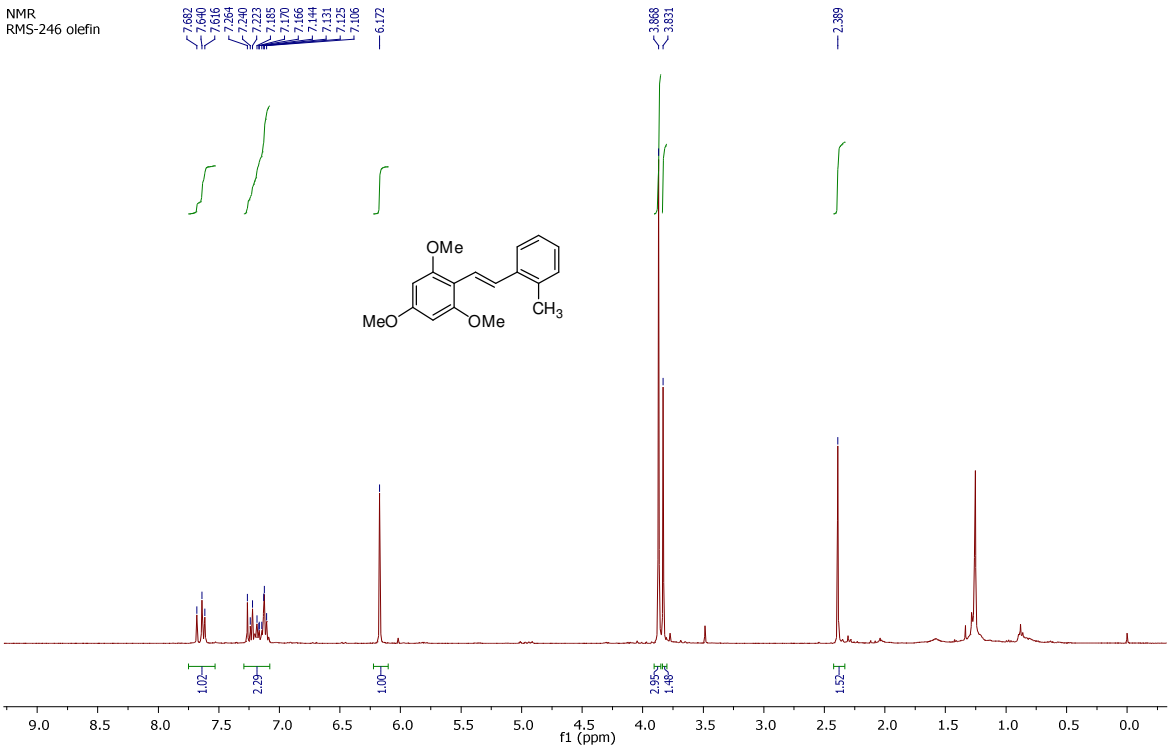
S3.17. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-1-(2′-iodostyryl)-2,4,6-trimethoxybenzene (**1q**)

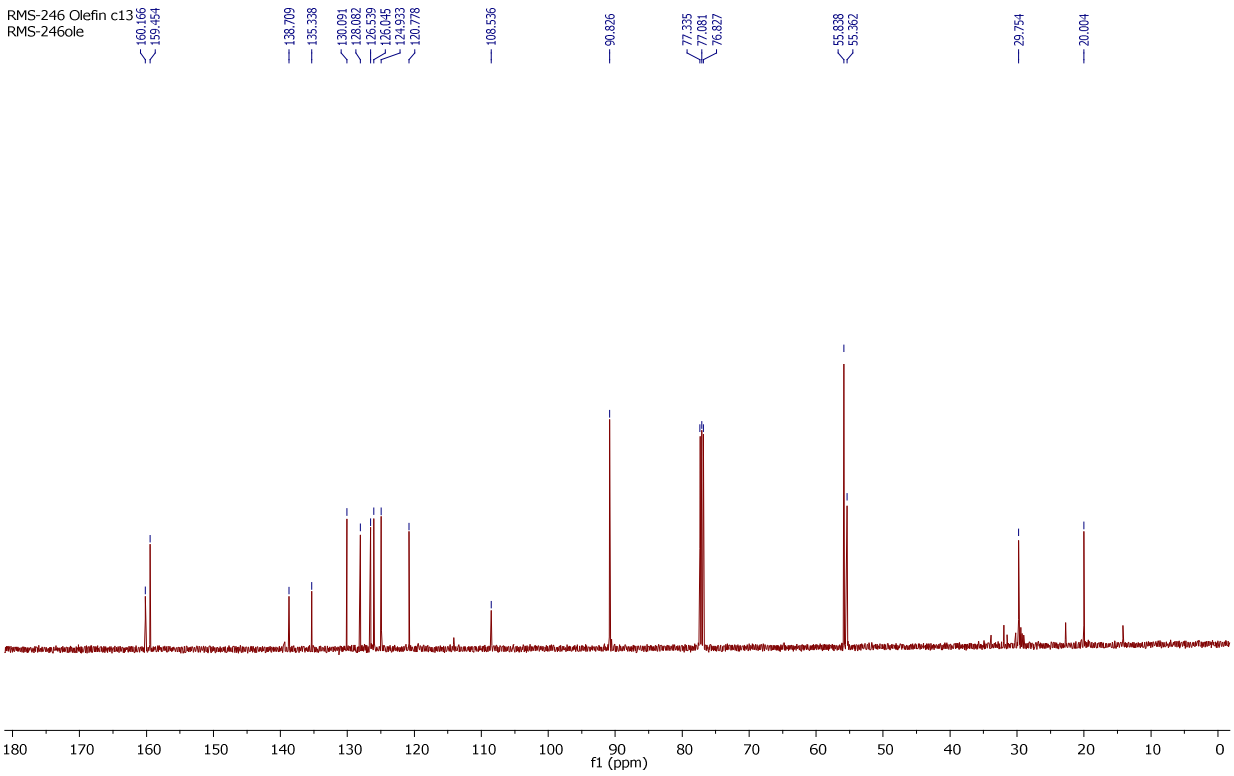


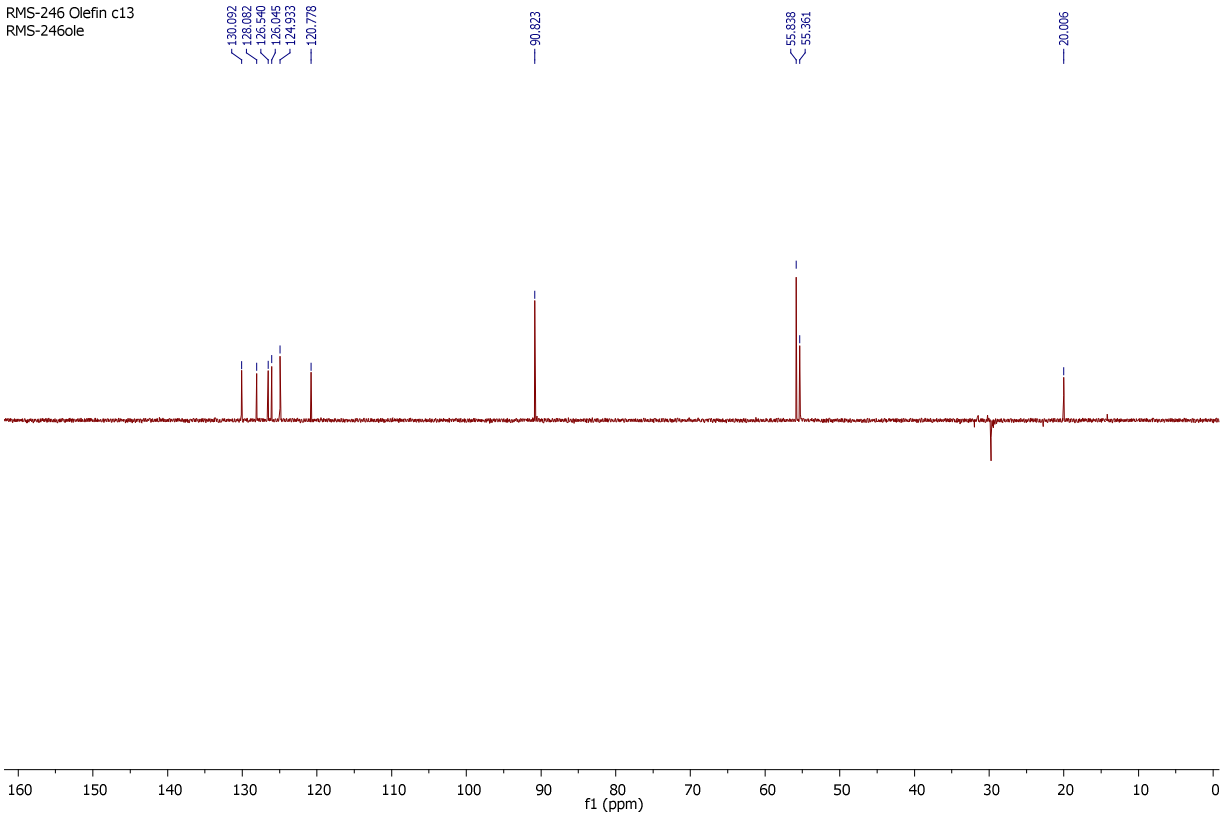




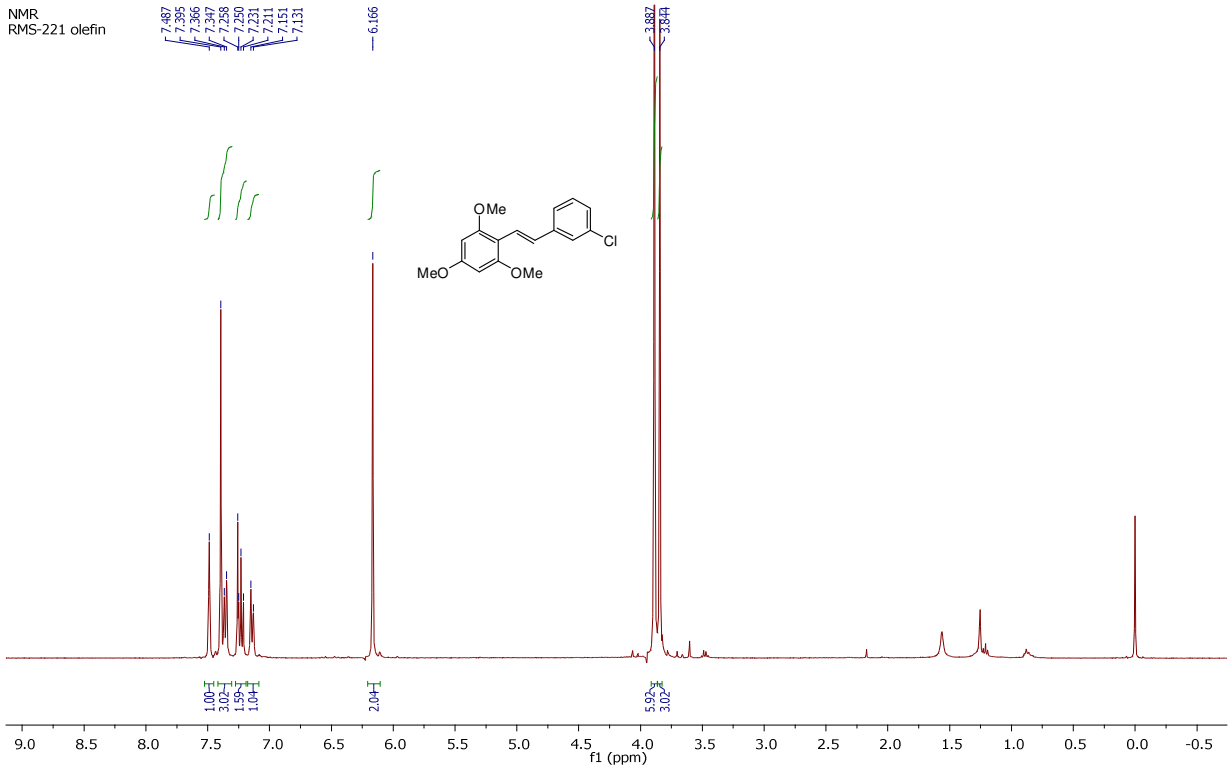
S3.18. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-1-(2′-methylstyryl)-2,4,6-trimethoxy-benzene (**1r**)

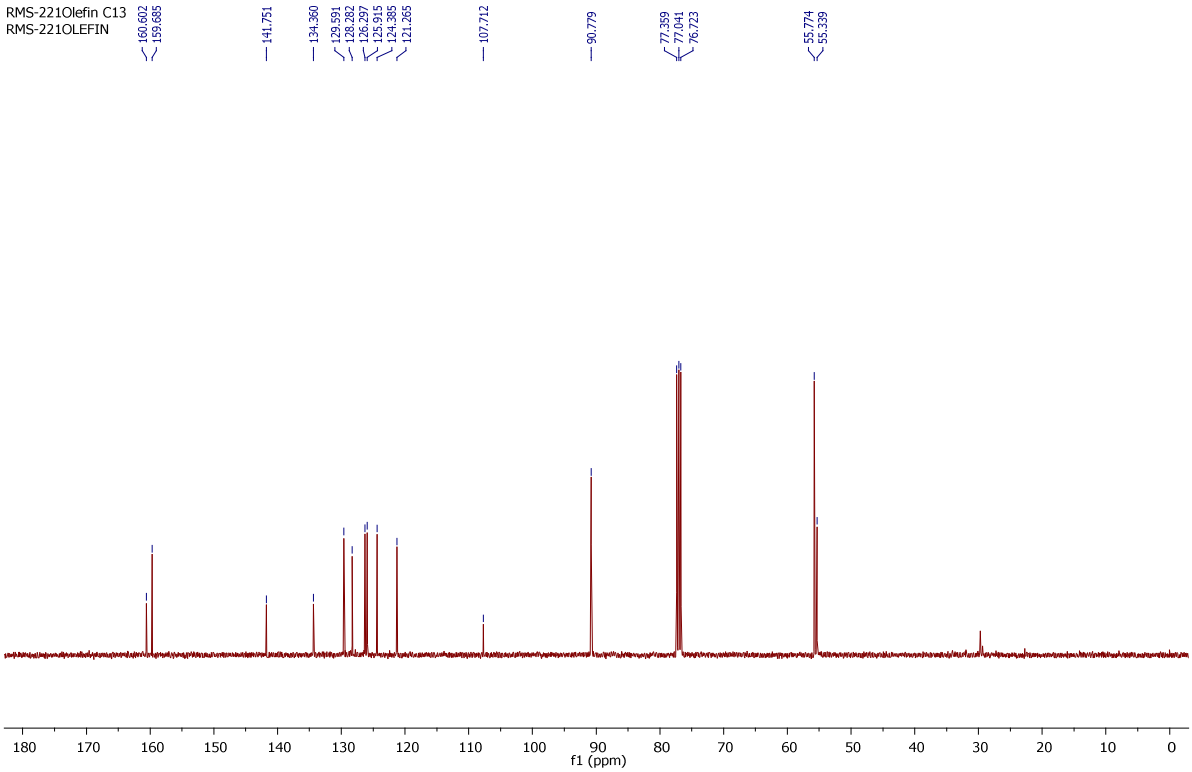


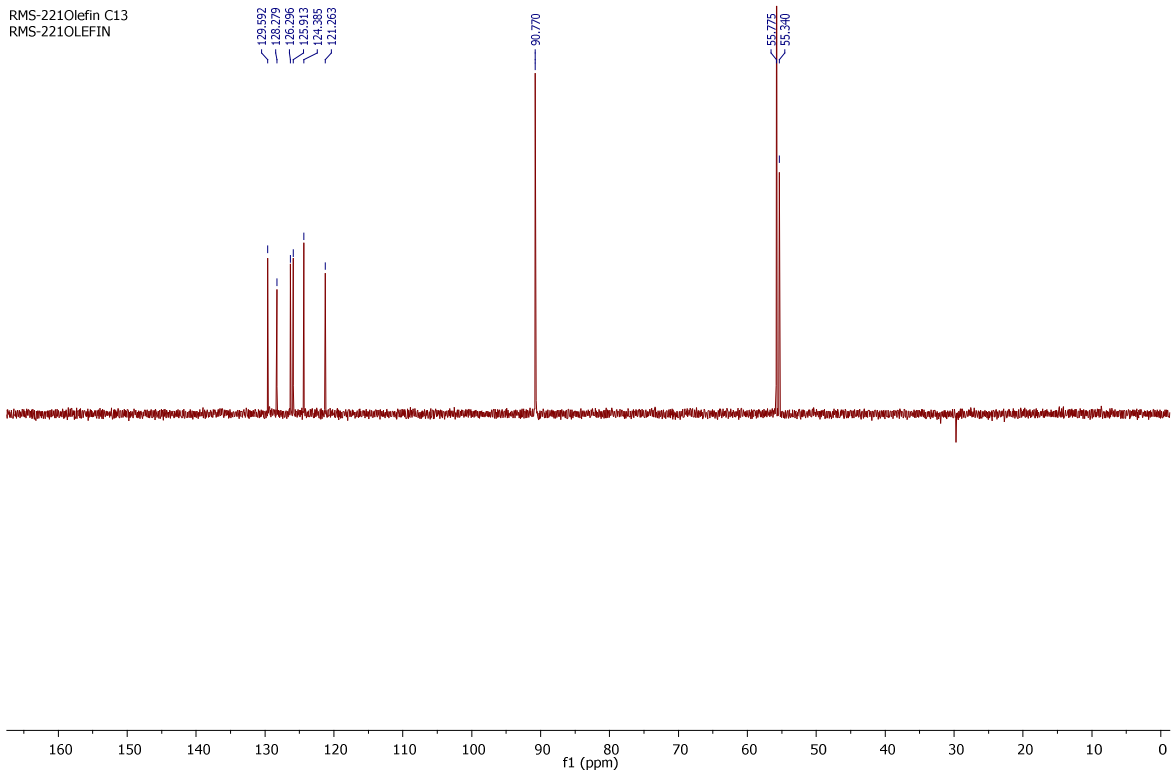

RMS-246 Olefin c13
RMS-246ole
160.166
159.454
138.709
135.338
130.091
128.082
126.539
126.045
124.933
120.778
108.536
90.826
77.335
77.081
76.827
55.838
55.362
29.754
20.004
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


RMS-246 Olefin c13
RMS-246ole
130.092
128.082
126.540
126.045
124.933
120.778
90.823
55.838
55.361
20.006
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

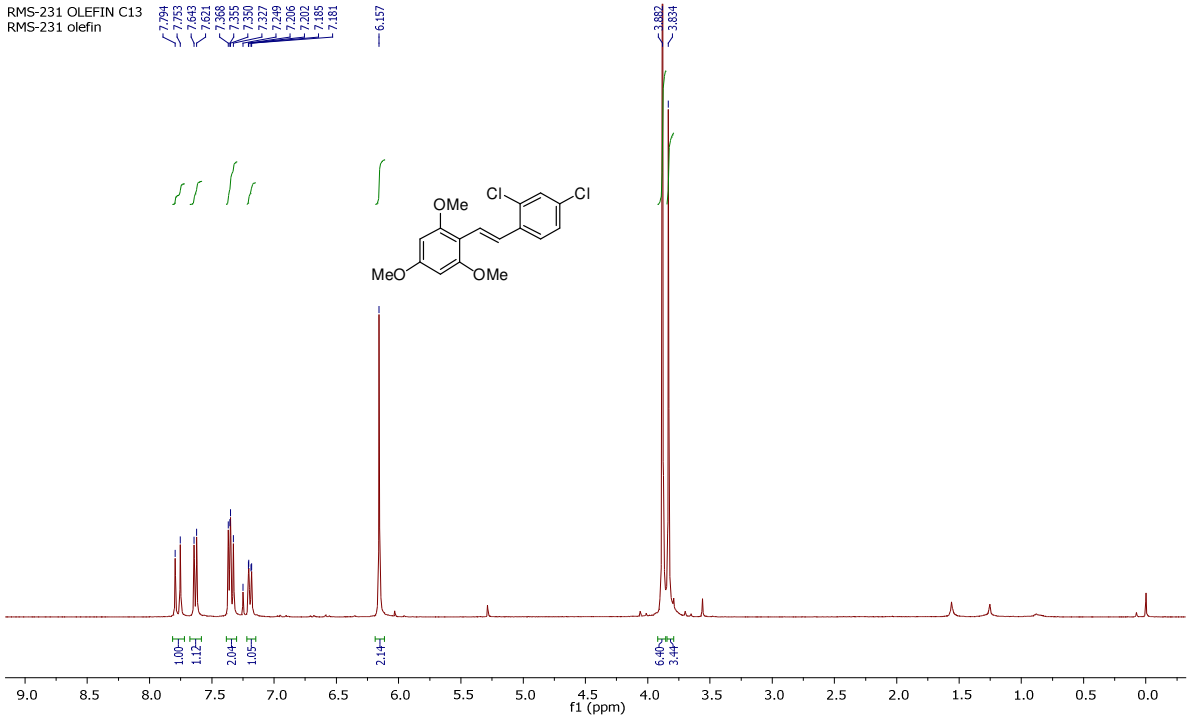
S3.19. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-1-(3′-chlorostyryl)-2,4,6-trimethoxybenzene (**1s**)

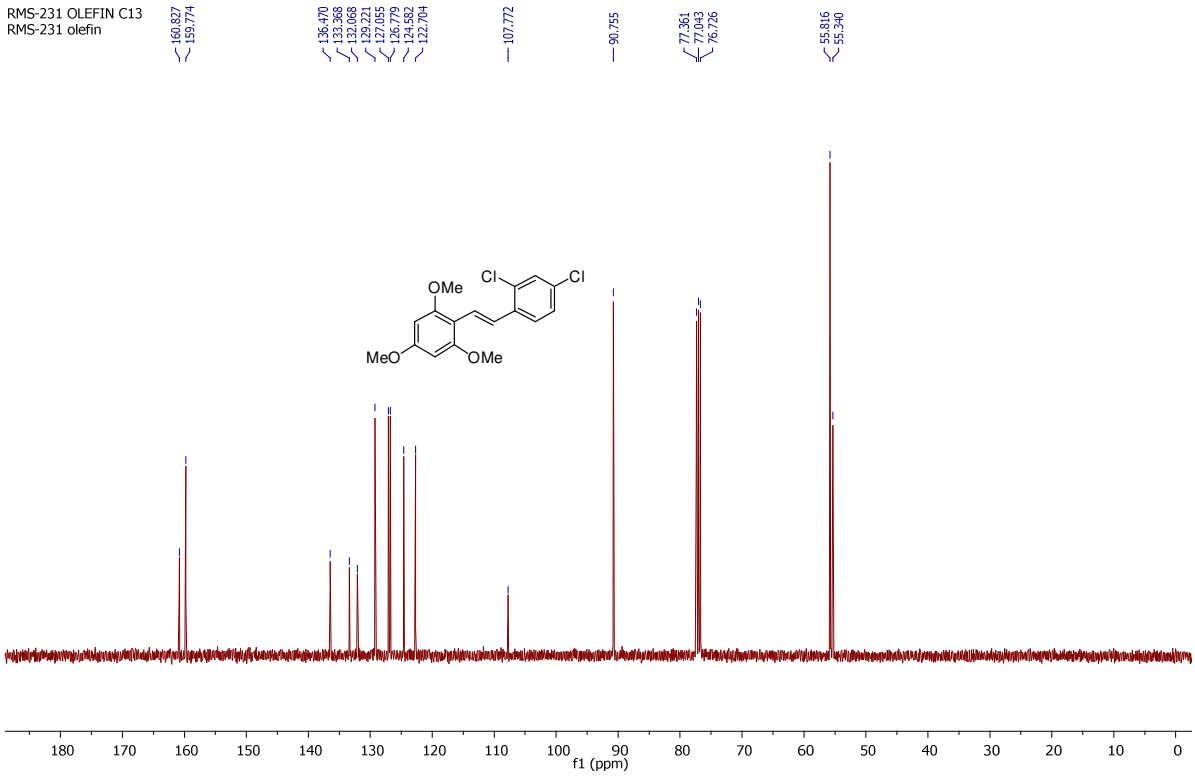


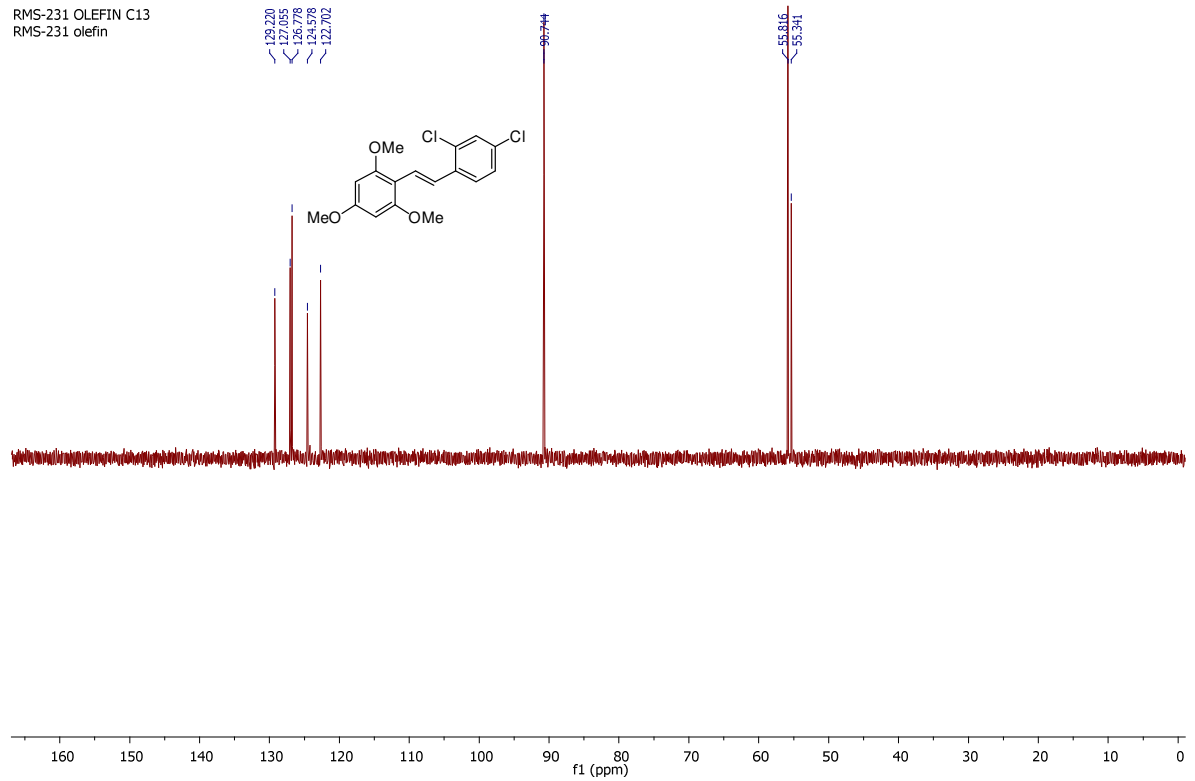




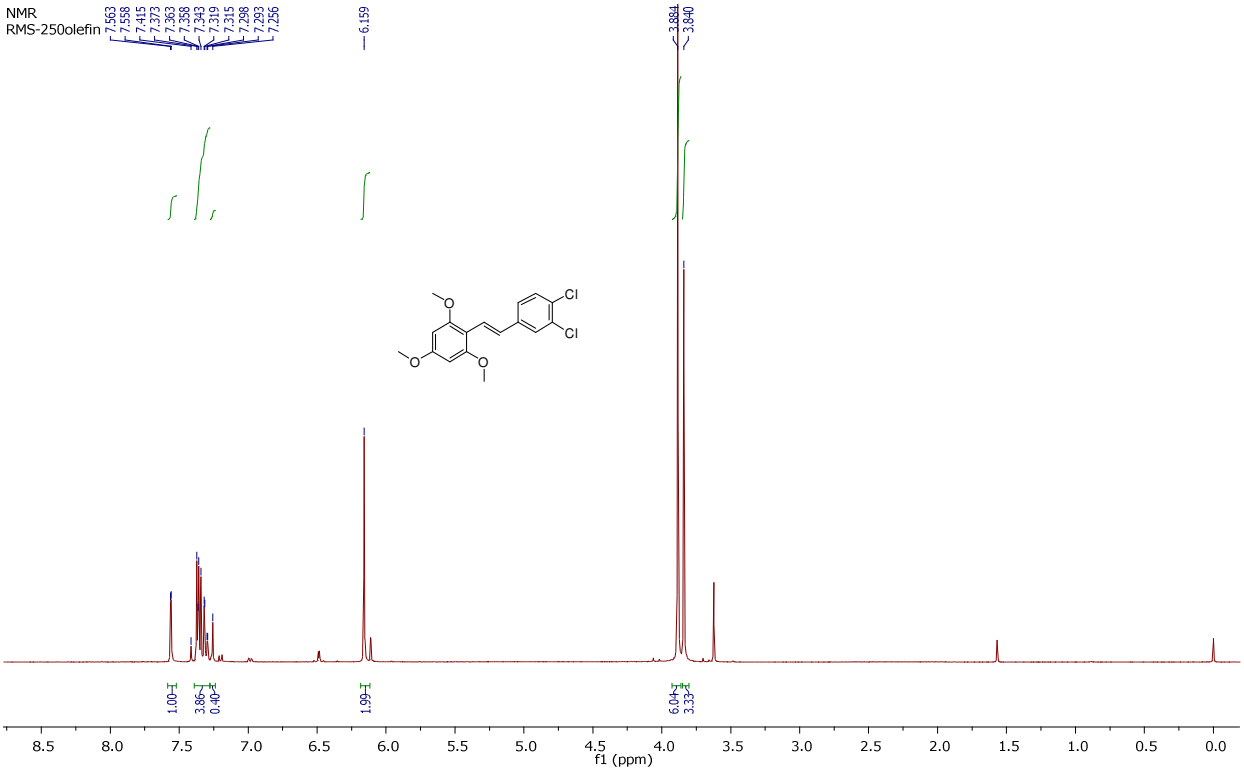
S3.20. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-1-(2′,4′-dichlorostyryl)-2,4,6-trimethoxybenzene (**1t**)

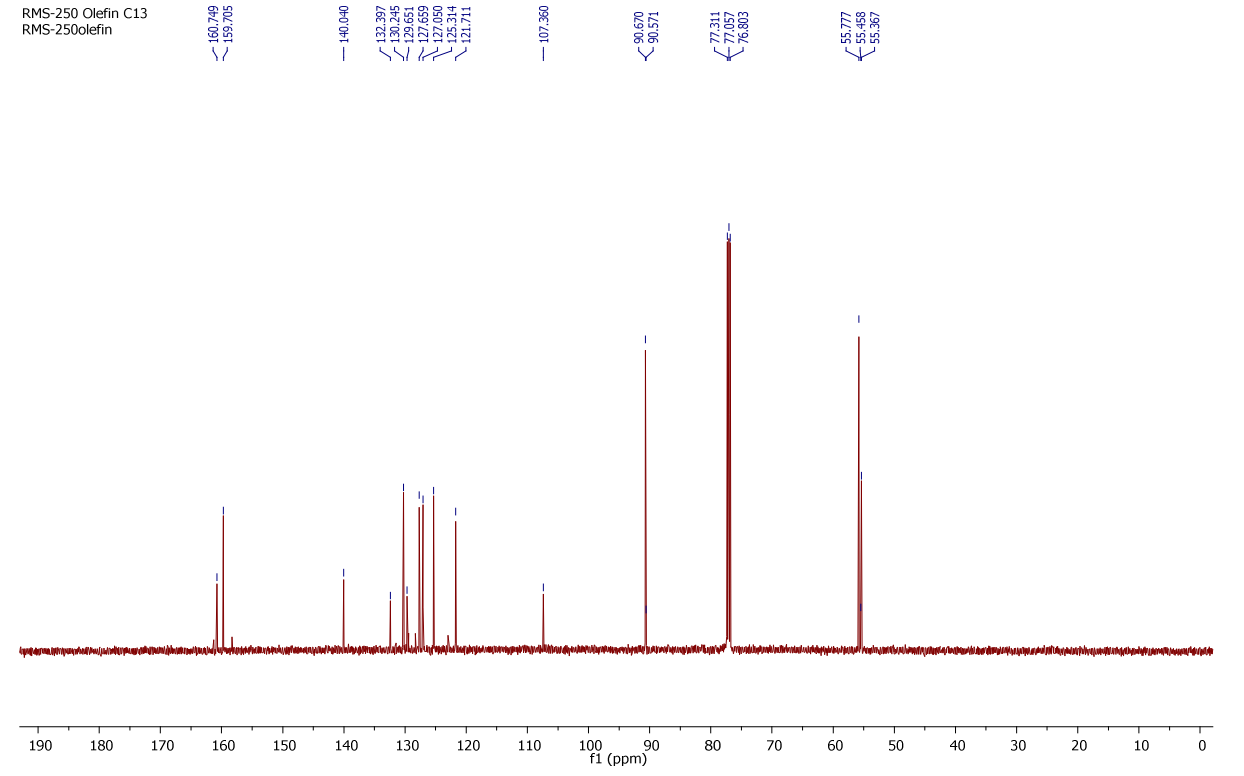


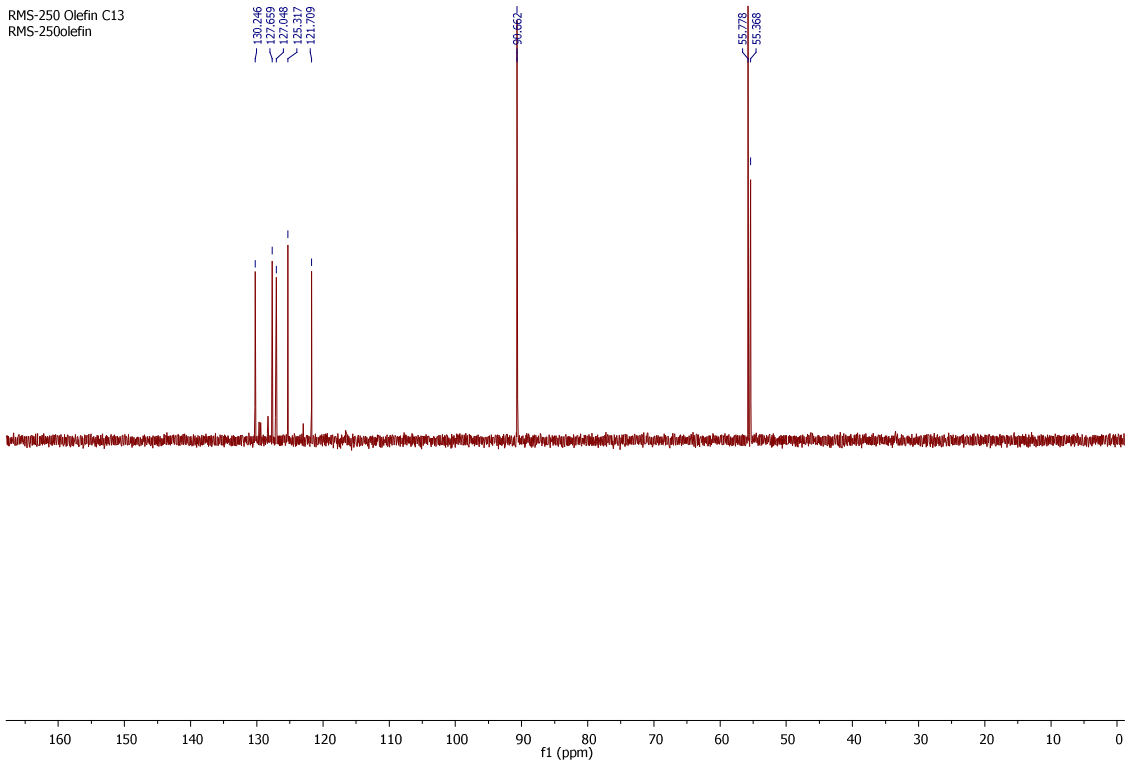

RMS-231 OLEFIN C13
RMS-231 olefin
160.827
159.774
136.470
133.368
132.068
129.221
127.055
126.779
124.582
122.704
107.772
90.755
77.361
77.043
76.726
55.816
55.340
OMe
Cl
Cl
MeO
OMe
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


RMS-231 OLEFIN C13
RMS-231 olefin
129.220
127.055
126.778
124.578
122.702
90.744
55.816
55.341
OMe
Cl
Cl
MeO
OMe
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

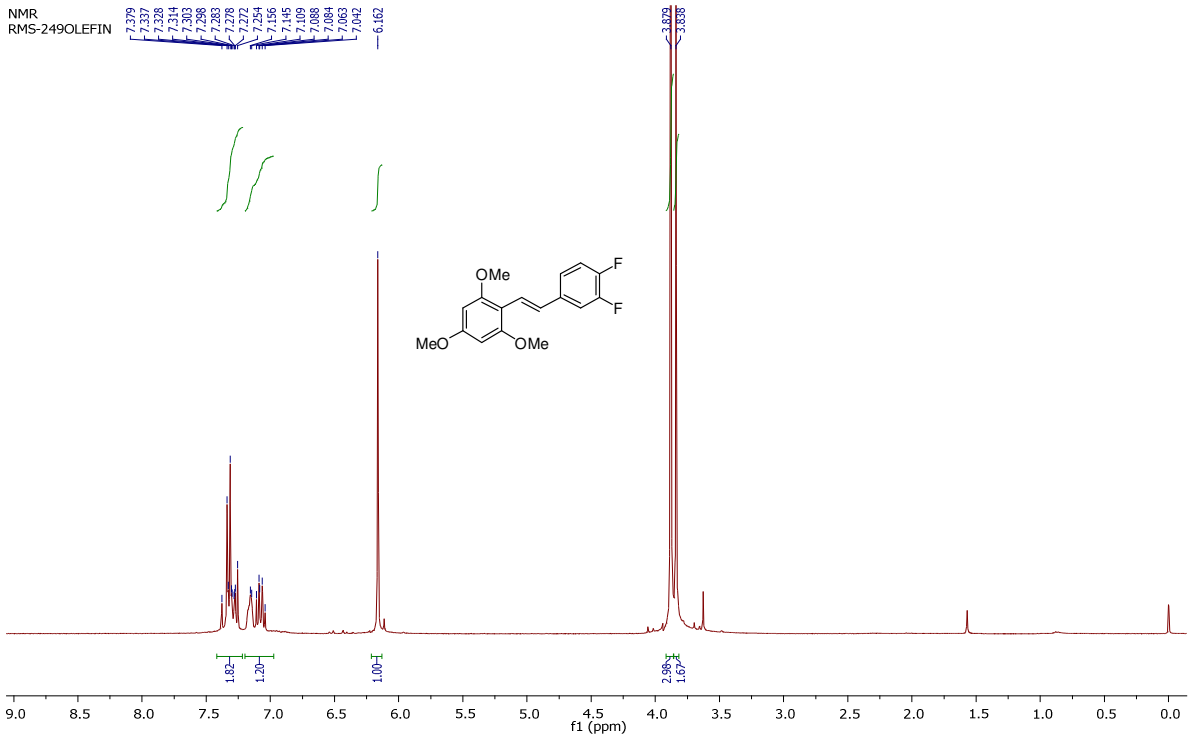
S3.21. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E/Z)-1-(3′,4′-dichlorostyryl)-2,4,6-trimethoxybenzene (**1u**)

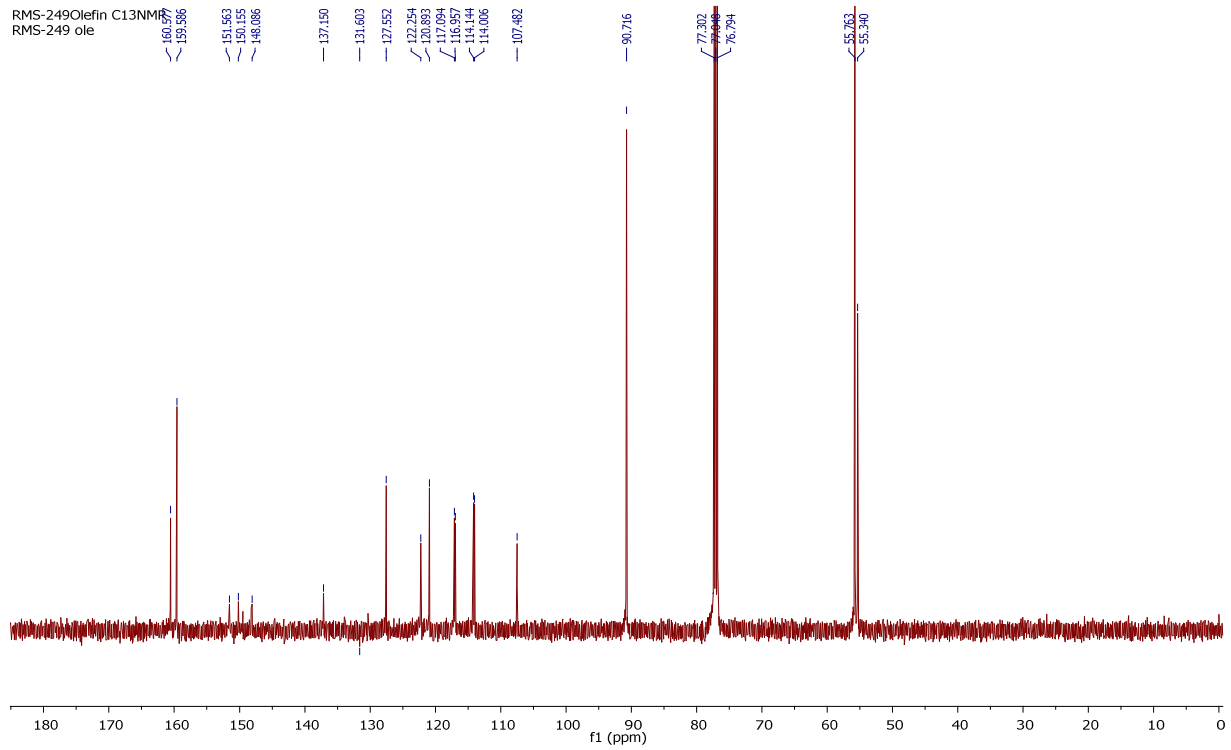


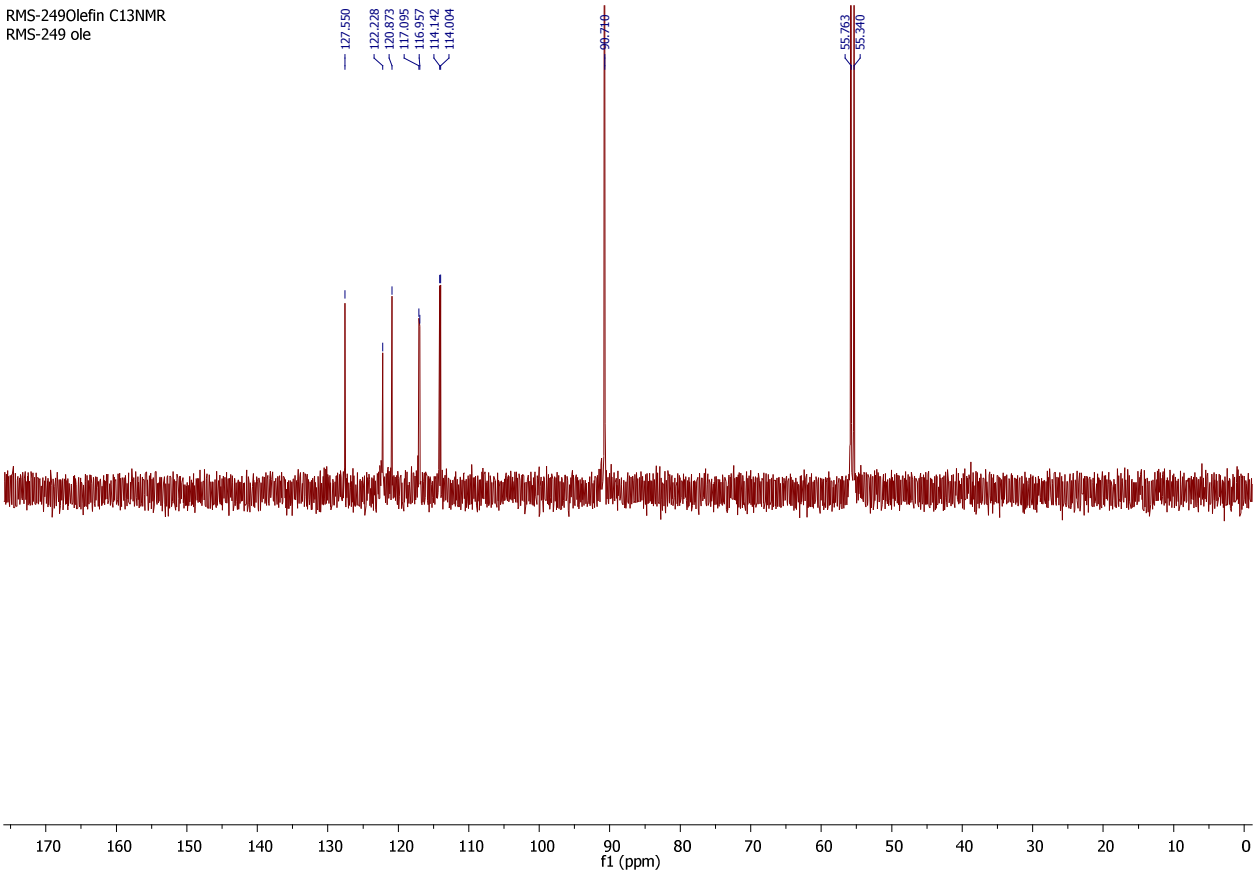


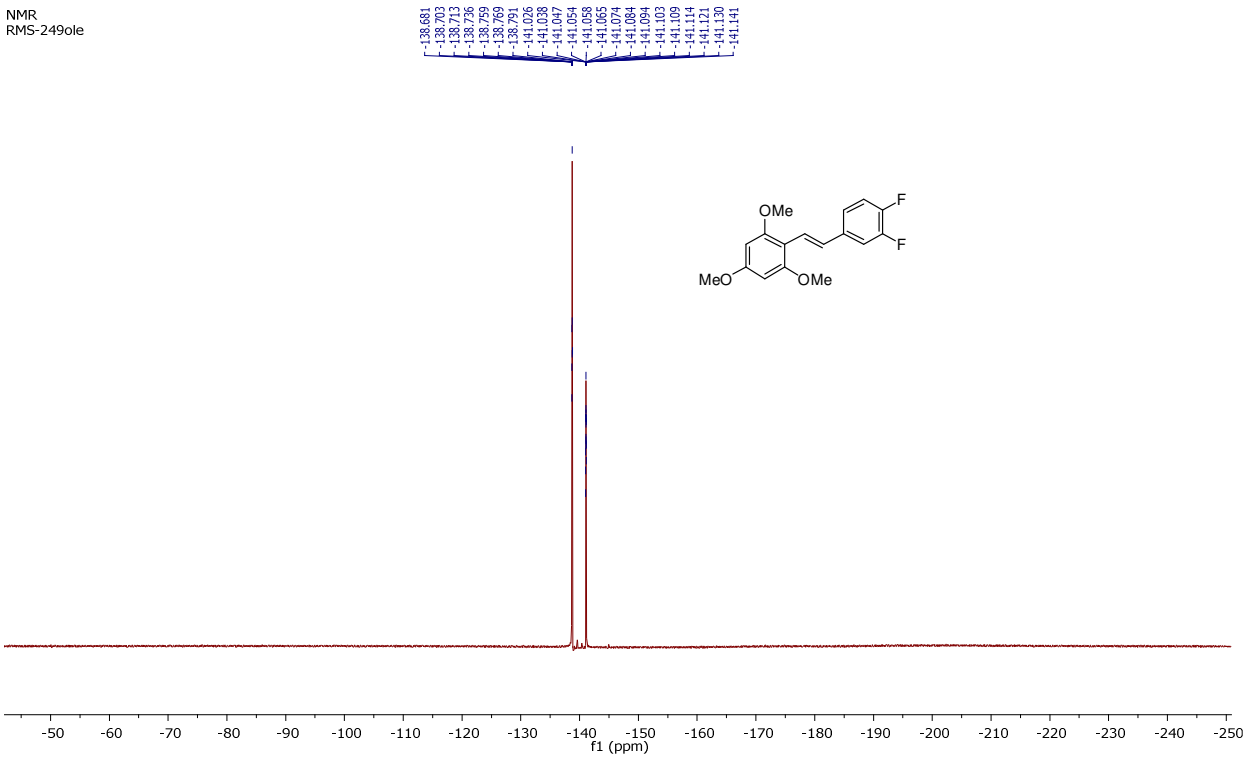


S3.22. ^{1}H, ^{13}C, DEPT135 and ^{19}F NMR spectra of (E/Z)-1-(3′,4′-difluorostyryl)-2,4,6-trimethoxybenzene (**1v**)

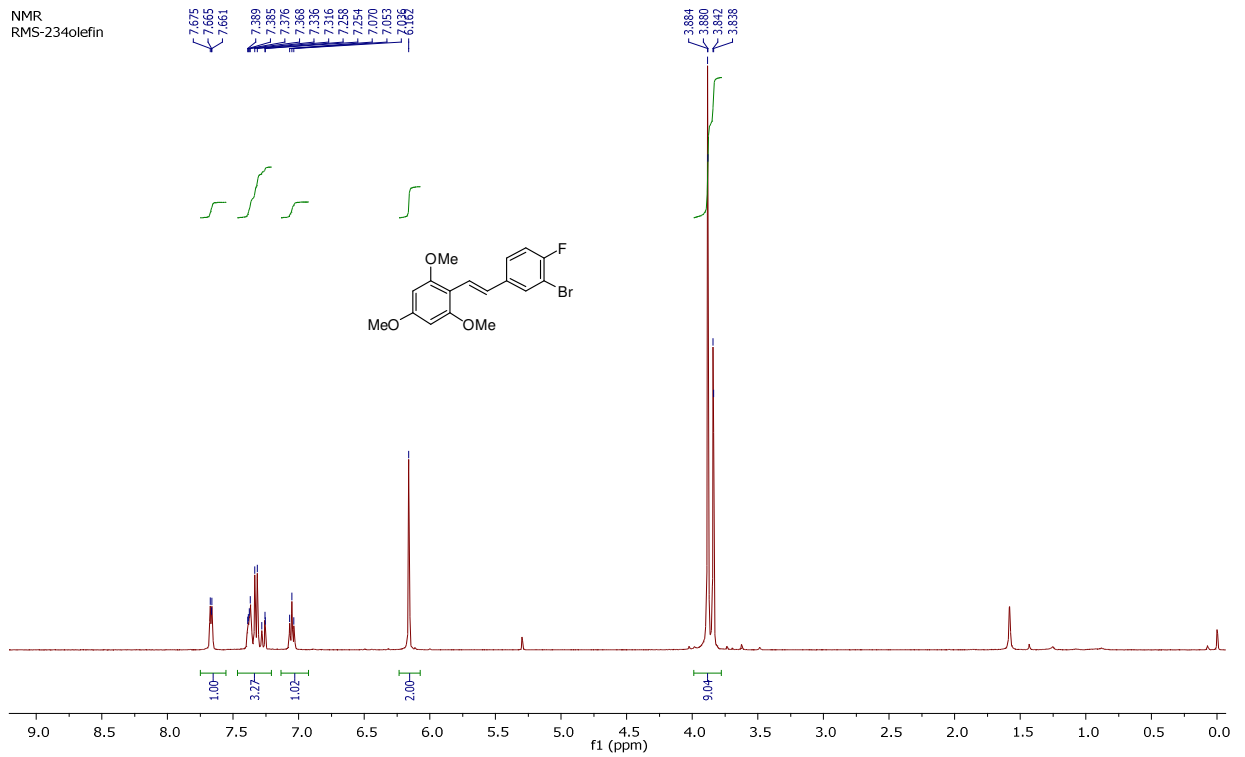


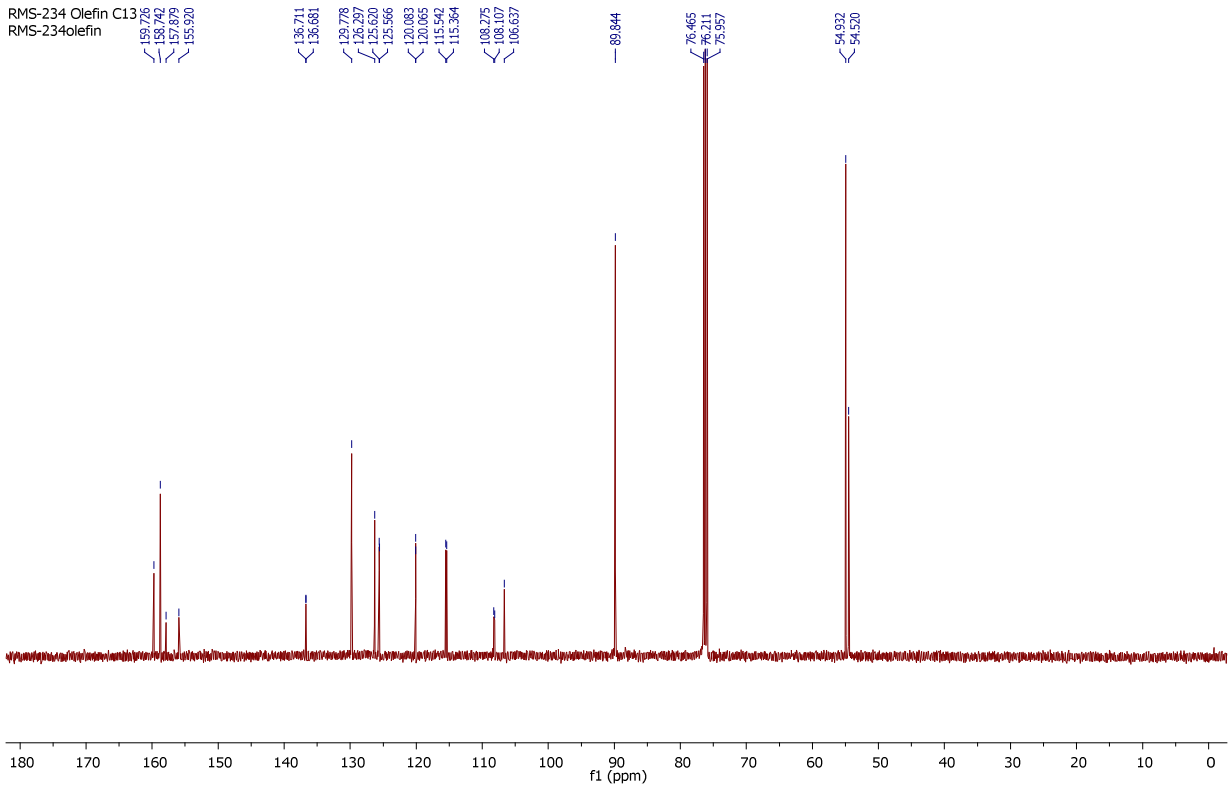

RMS-249Olefin C13NMR
RMS-249 ole
160.377
159.586
151.563
150.155
148.086
137.150
131.603
127.552
122.254
120.893
117.094
116.957
114.144
114.006
107.482
90.716
77.302
77.048
76.794
55.763
55.340
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

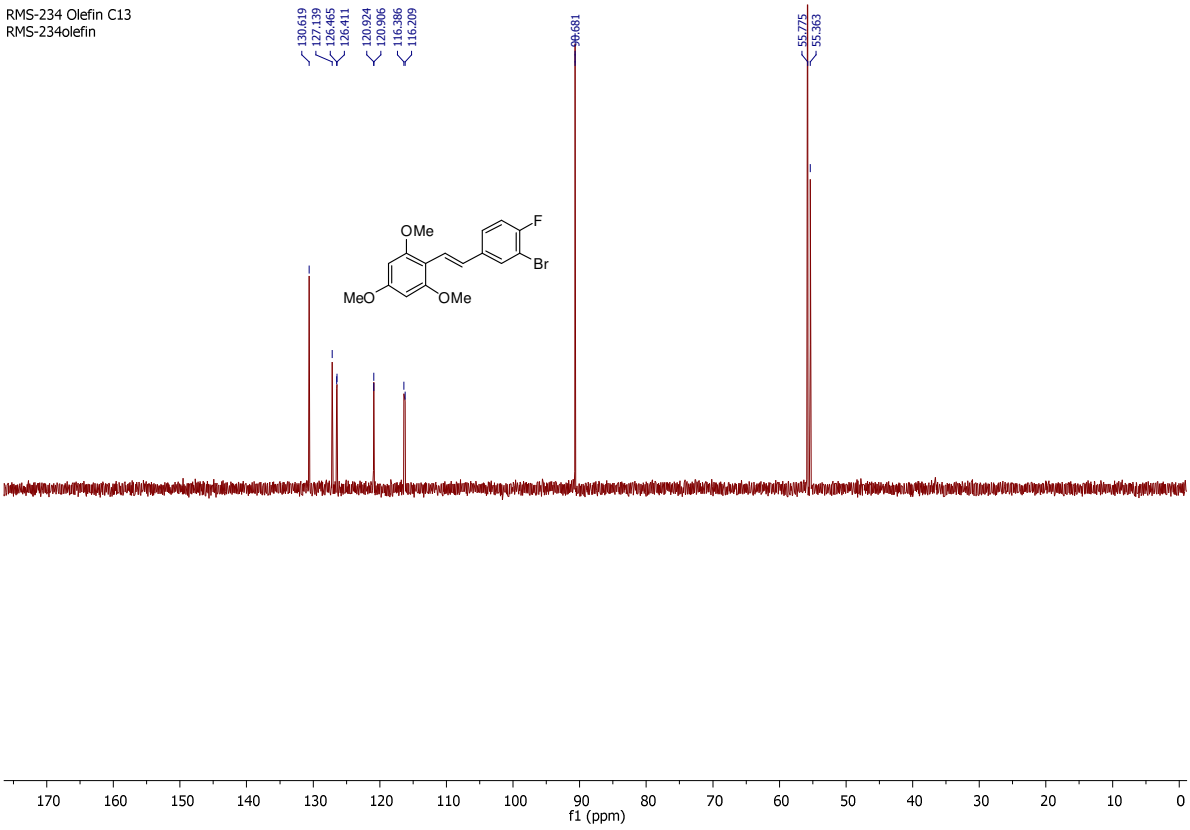

RMS-249Olefin C13NMR
RMS-249 ole
127.550
122.228
120.873
117.095
116.957
114.142
114.004
90.710
55.763
55.340
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



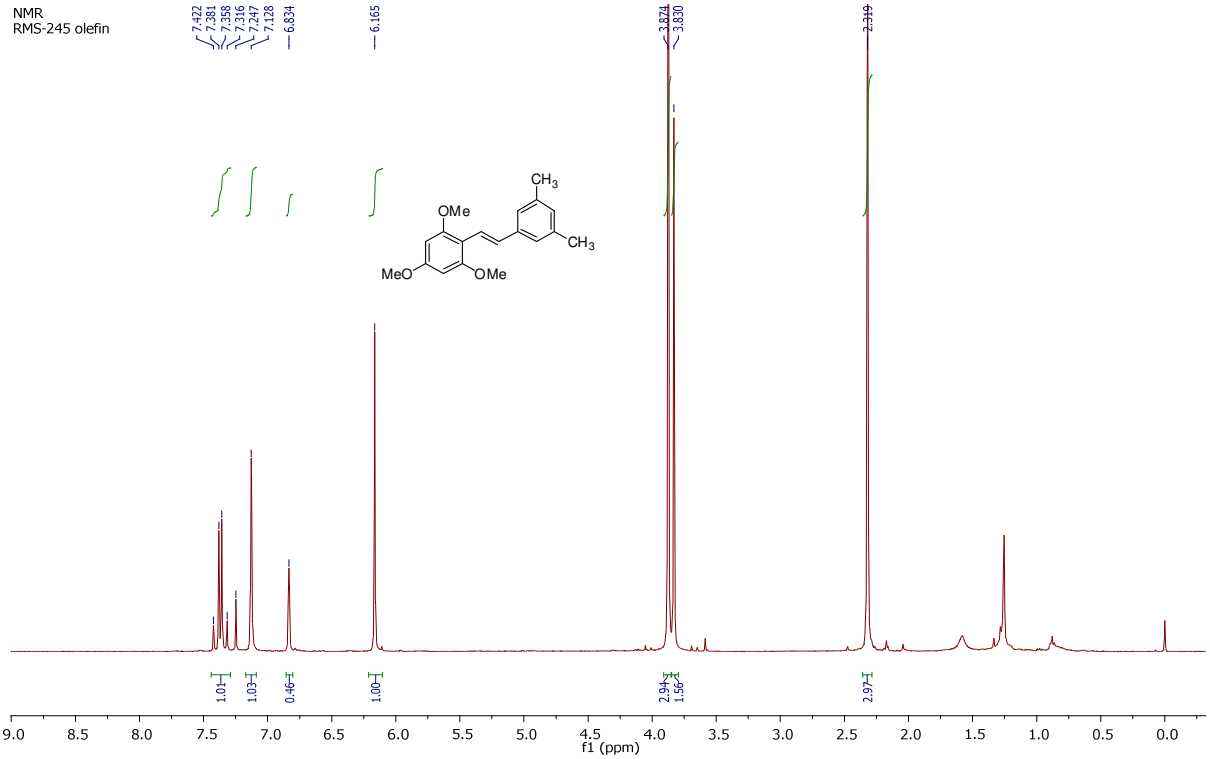
S3.23. ^{1}H, ^{13}C, DEPT135 and ^{19}F NMR spectra of (E)-1-(3′-bromo-4′-fluorostyryl)-2,4,6-trimethoxybenzene (**1w**)

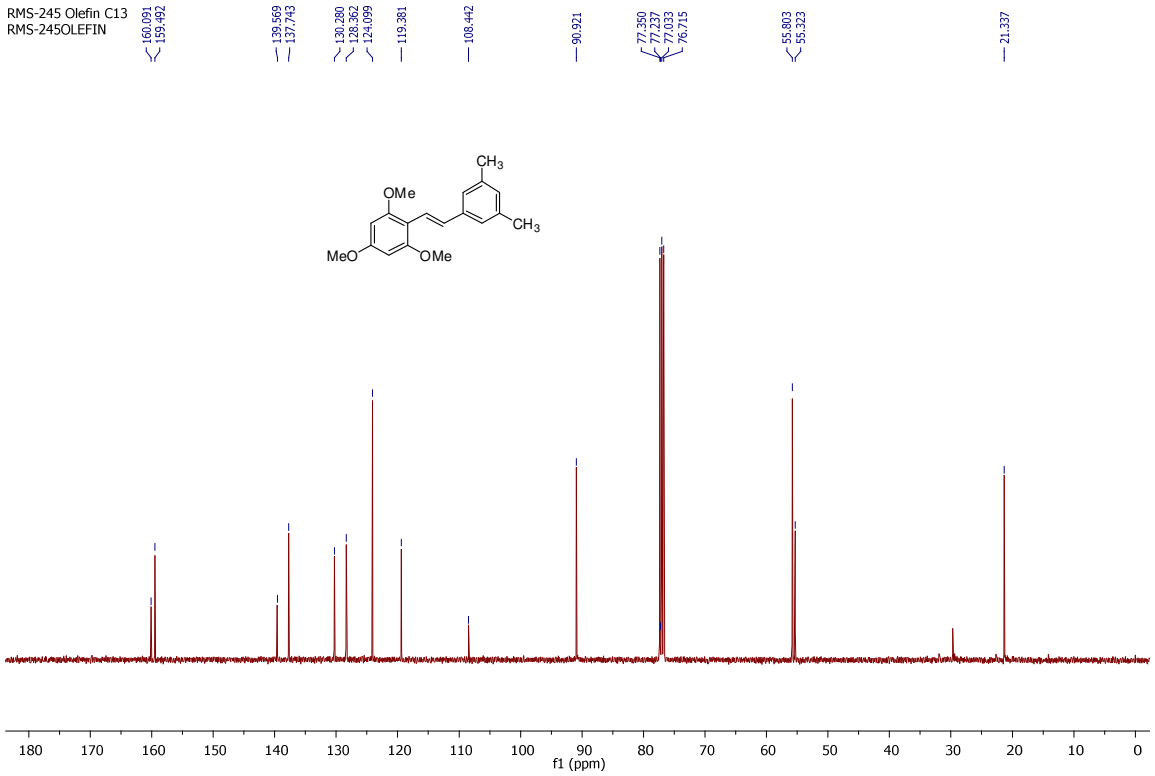


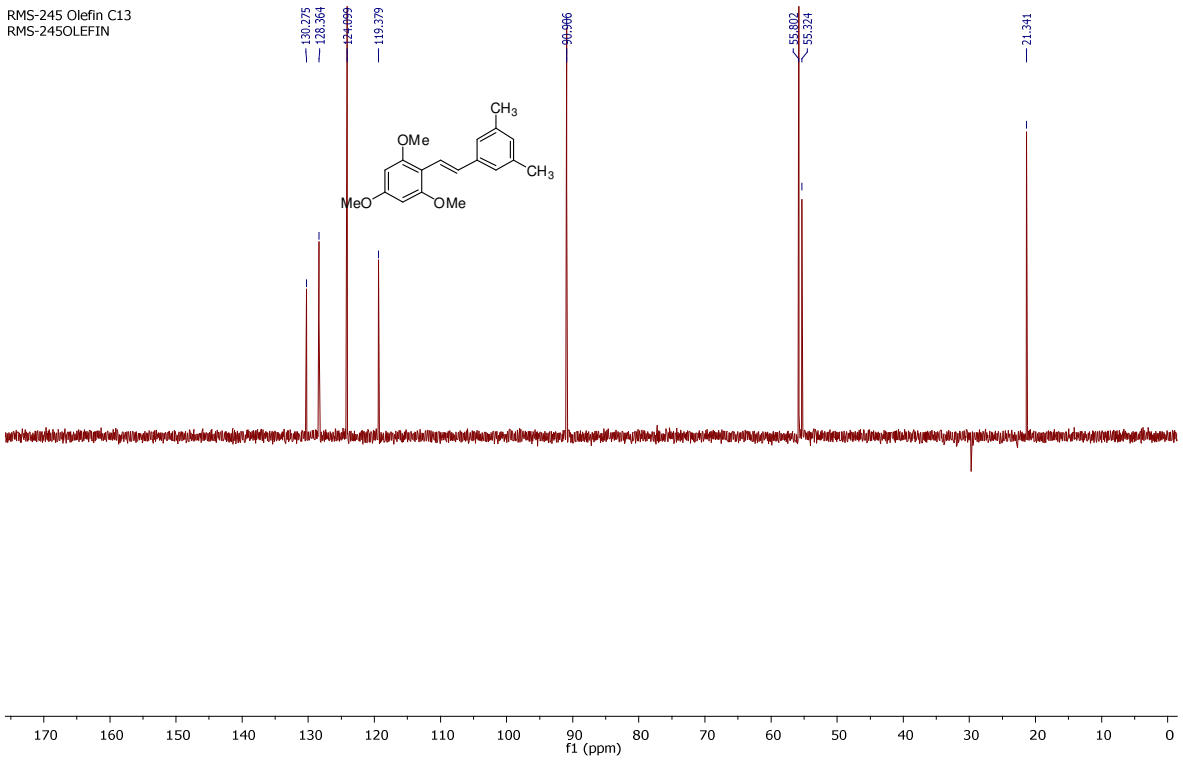

RMS-234 Olefin C13
RMS-234olefin
159.726
158.742
157.879
155.920
136.711
136.681
129.778
126.297
125.620
125.566
120.083
120.065
115.542
115.364
108.275
108.107
106.637
89.844
76.465
76.211
75.957
54.932
54.520
f1 (ppm)


RMS-234 Olefin C13
RMS-234olefin
130.619
127.139
126.465
126.411
120.924
120.906
116.386
116.209
90.681
55.775
55.363
OMe
F
Br
MeO
OMe
f1 (ppm)

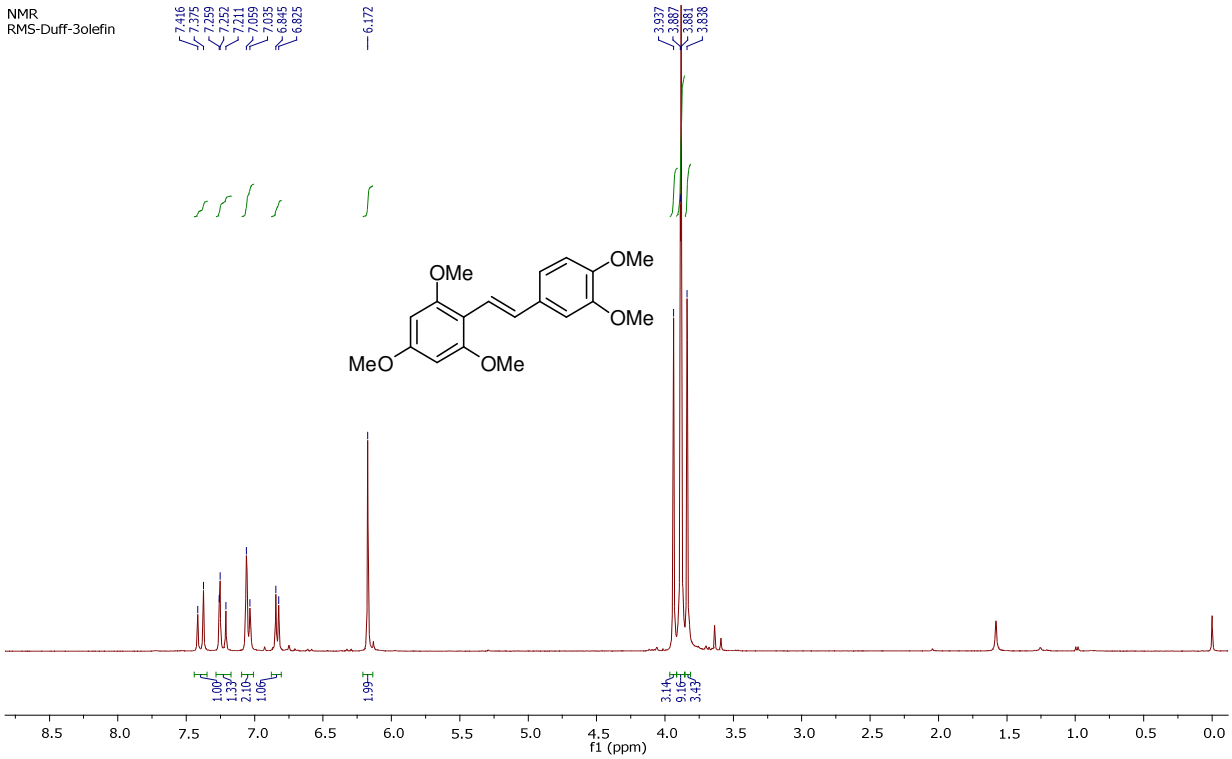
S3.24. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-1-(3′,5′-dimethylstyryl)-2,4,6-trimethoxybenzene (**1x**)

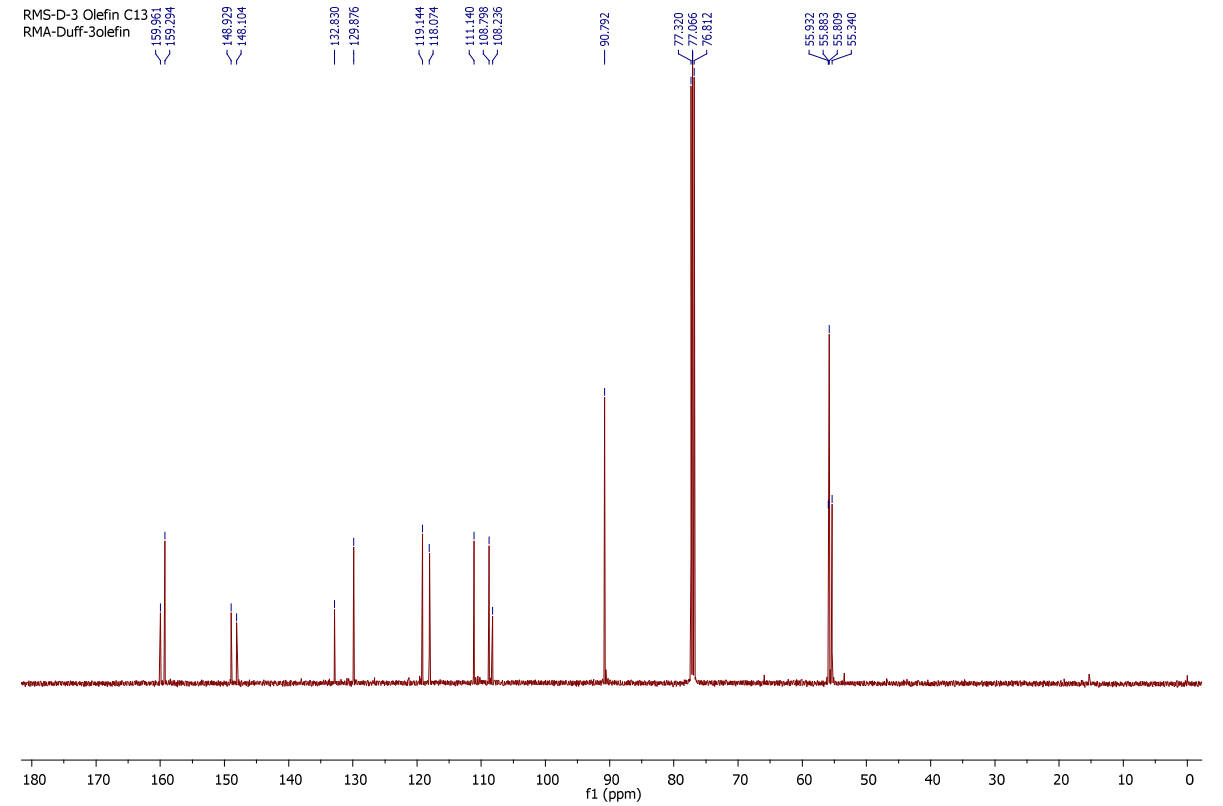


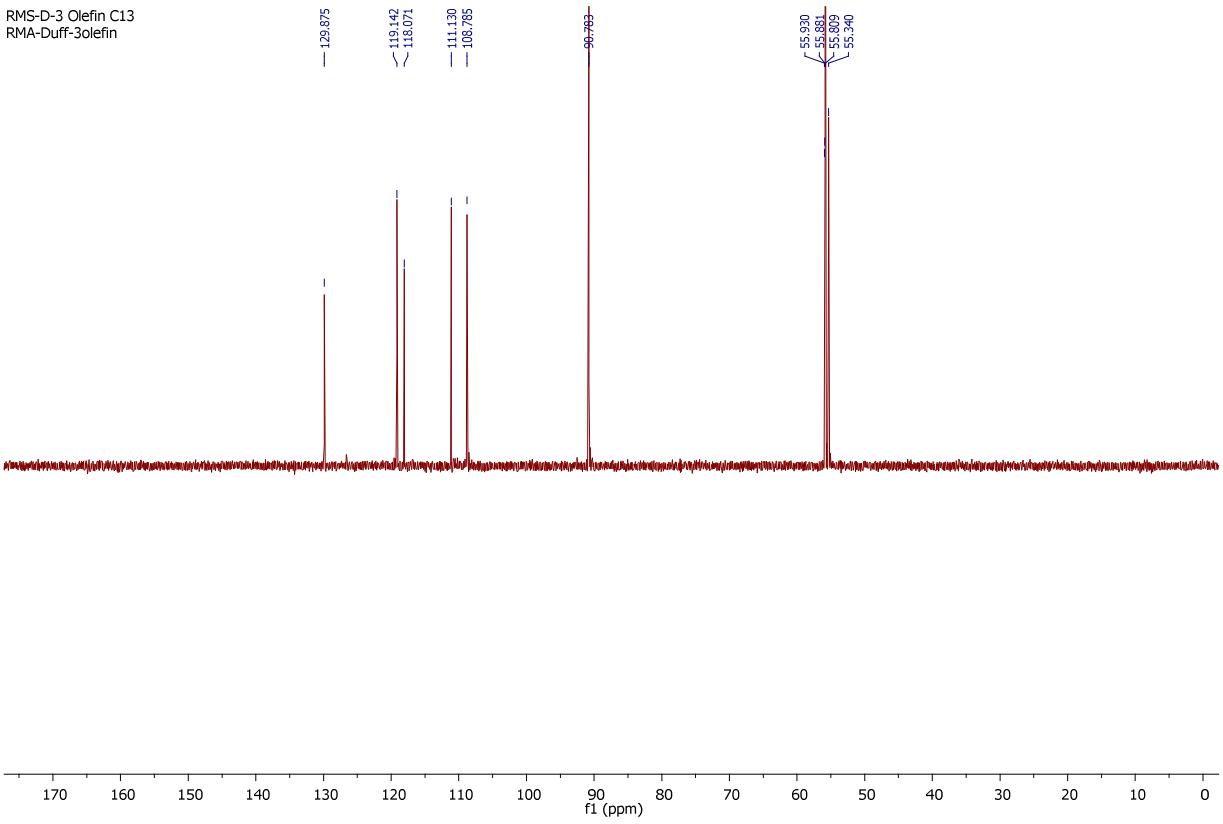




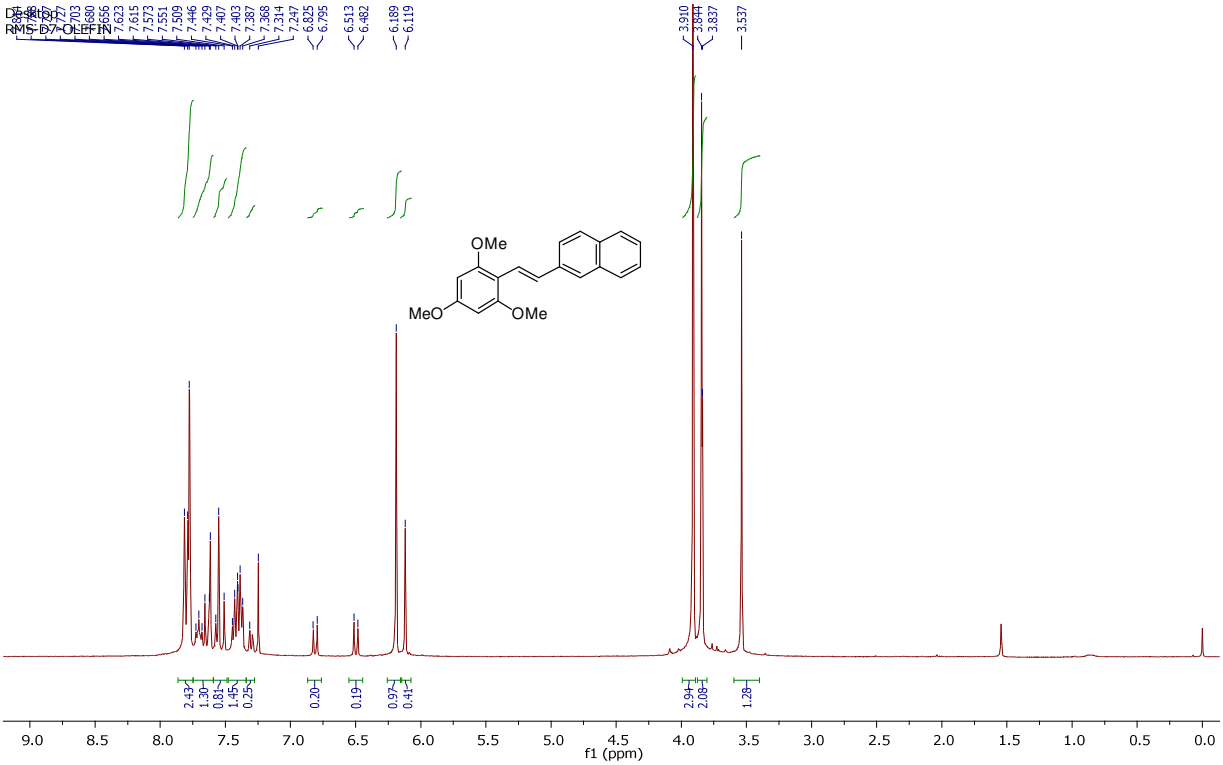
S3.25. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-1-(3′,4′-dimethoxystyryl)-2,4,6-trimethoxybenzene (**1y**)

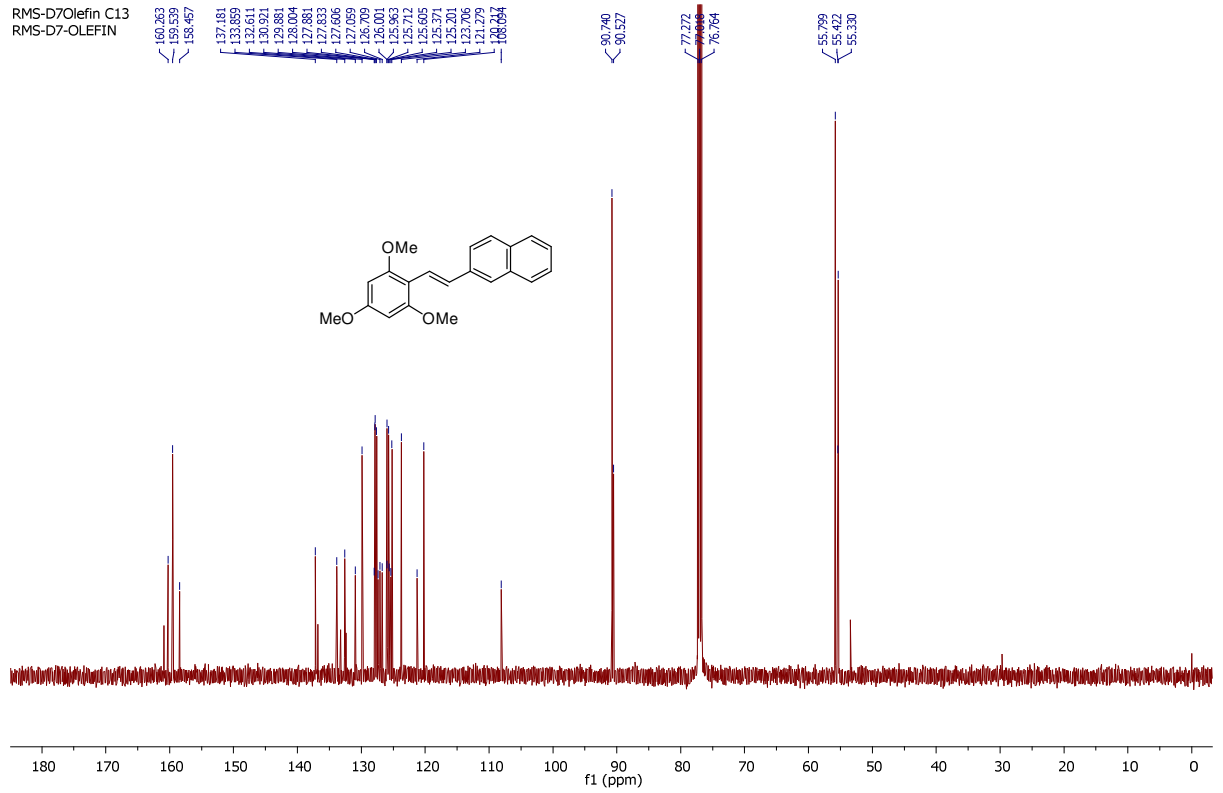


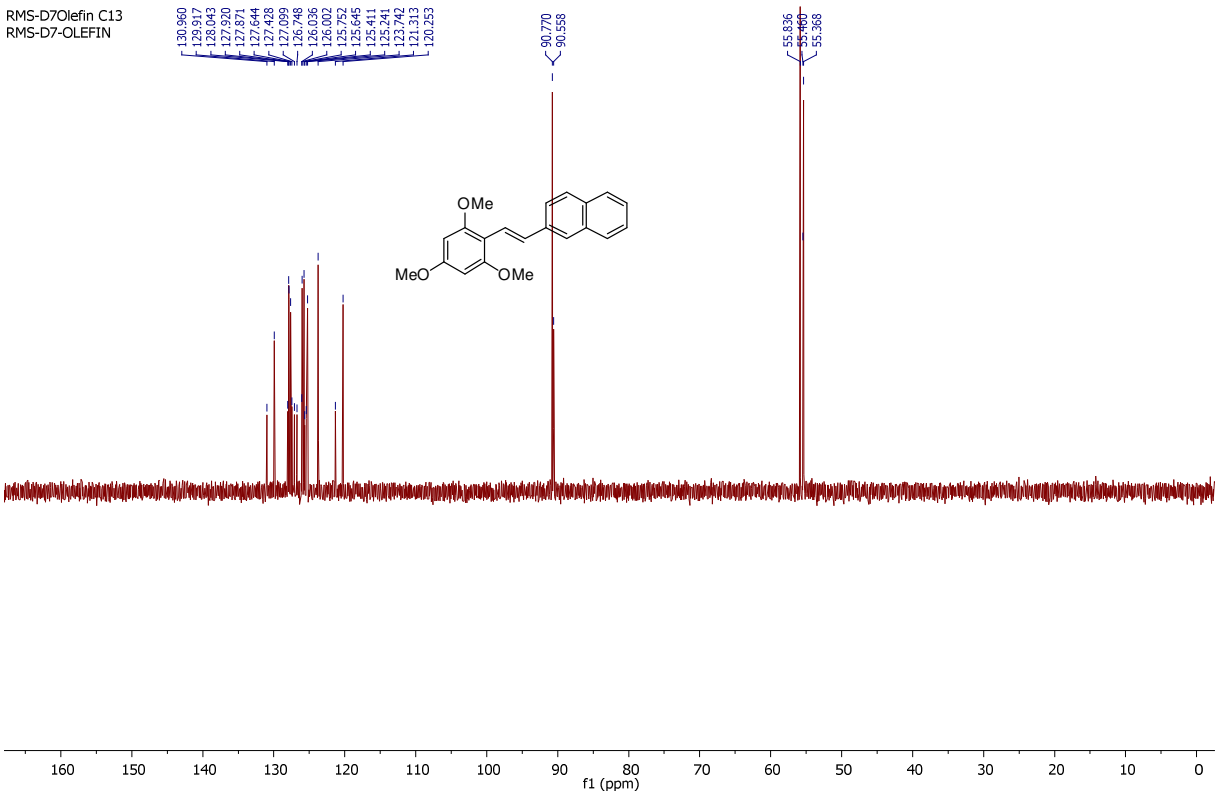

RMS-D-3 Olefin C13
RMA-Duff-3olefin
159.961
159.294
148.929
148.104
132.830
129.876
119.144
118.074
111.140
108.798
108.236
90.792
77.320
77.066
76.812
55.932
55.883
55.809
55.340
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


RMS-D-3 Olefin C13
RMA-Duff-3olefin
129.875
119.142
118.071
111.130
108.785
90.783
55.930
55.881
55.809
55.340
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

S3.26. ^{1}H, ^{13}C and DEPT135 NMR spectra of (E)-2-(2′,4′,6′-trimethoxystyryl)naphthalene (**1z**)

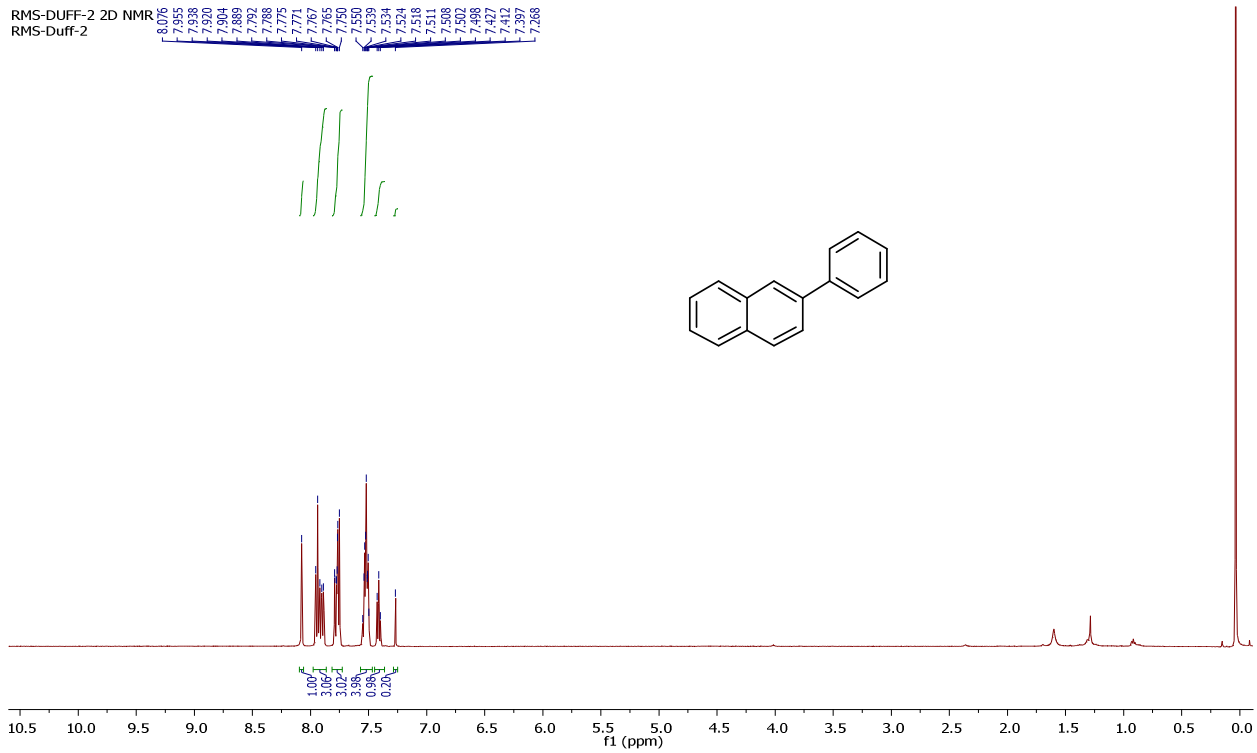


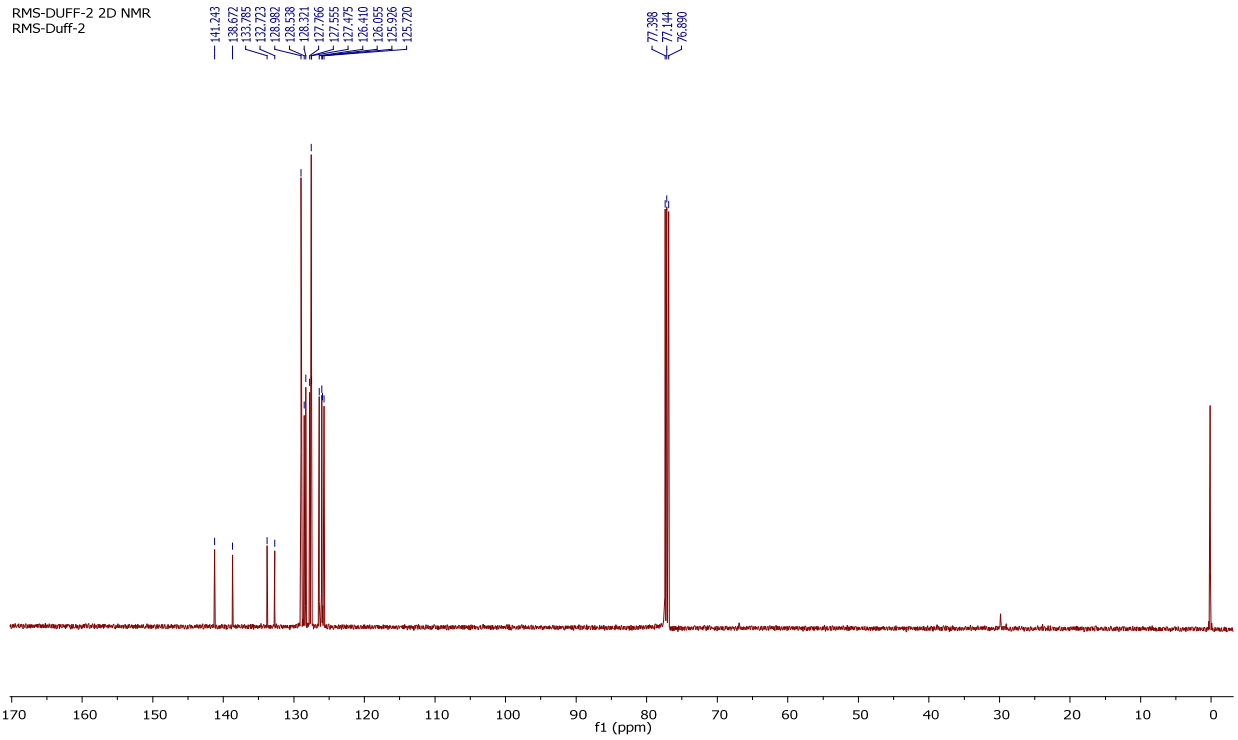


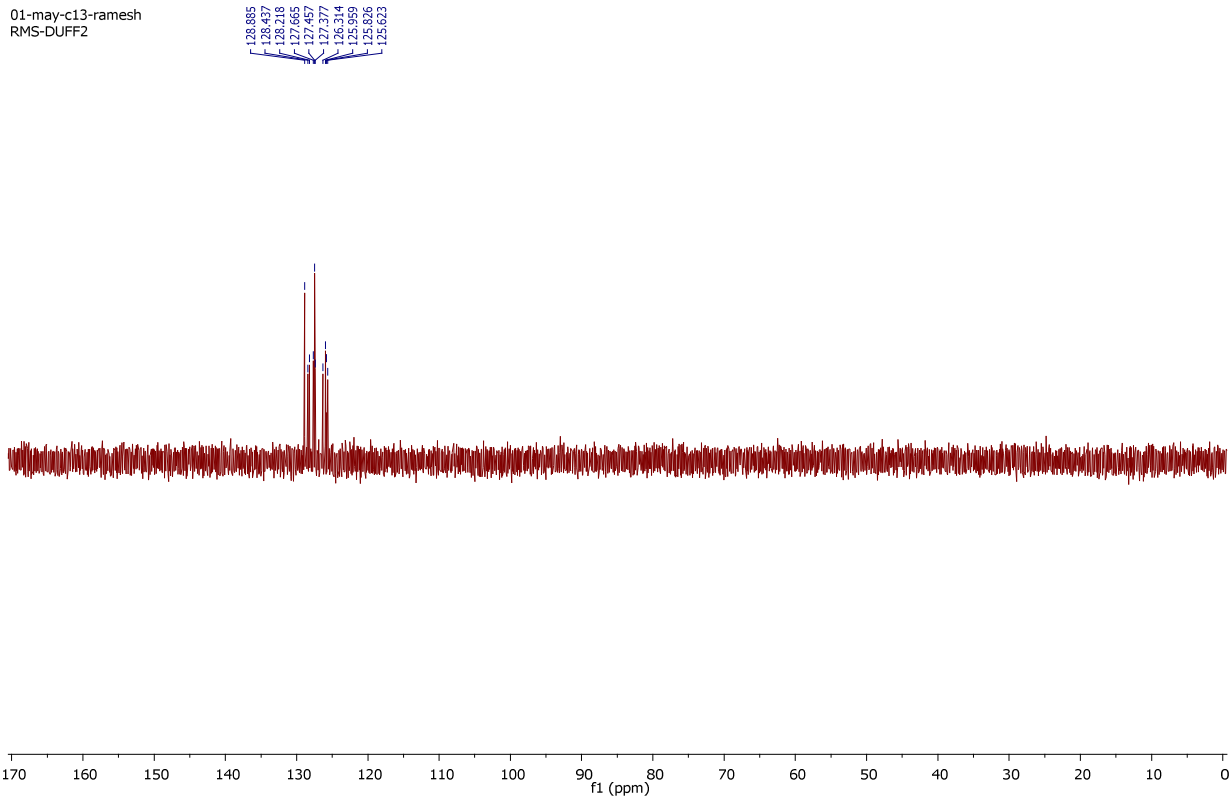

RMS-D7Olefin C13
RMS-D7-OLEFIN
130.960
129.917
128.043
127.920
127.871
127.644
127.428
127.099
126.748
126.036
126.002
125.752
125.645
125.411
125.241
123.742
121.313
120.253
90.770
90.558
55.836
55.460
55.368
OMe
MeO
OMe
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

S4. SCANNED COPIES OF ^{1}H, ^{13}C AND DEPT135 NMR SPECTRAS OF ALL COMPOUNDS

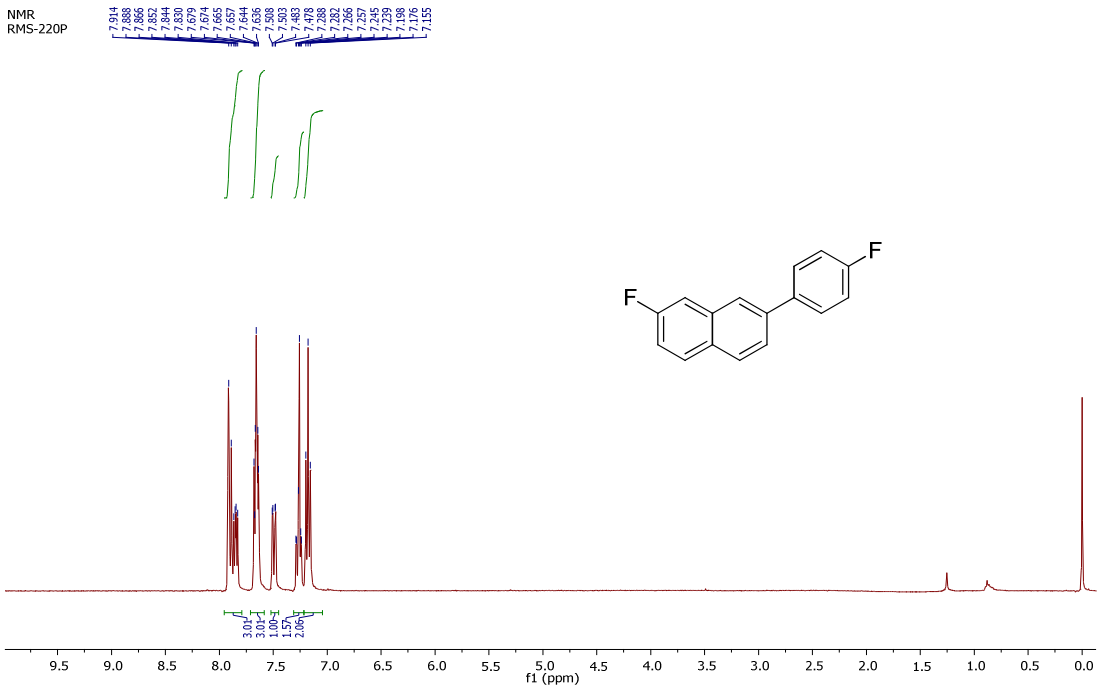
S4.1. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-phenylnaphthalene (**2a**)

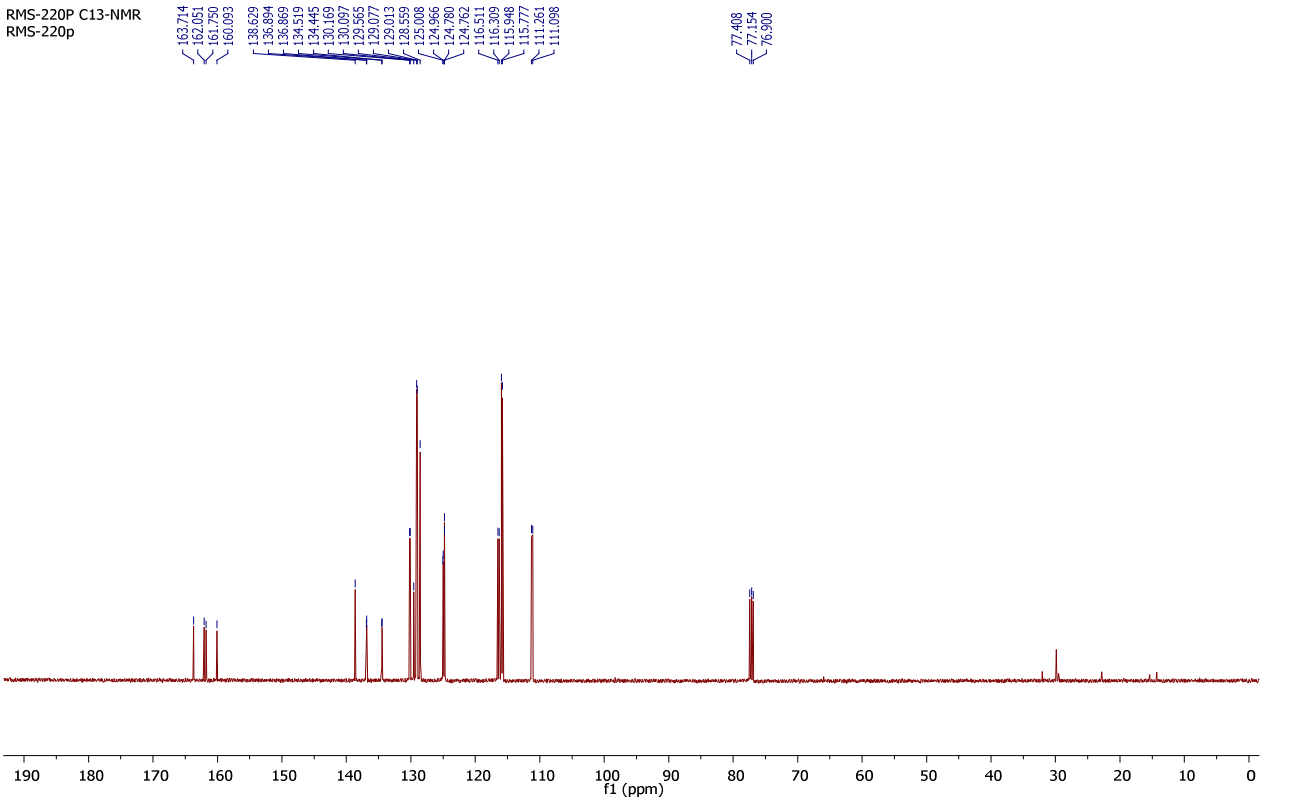


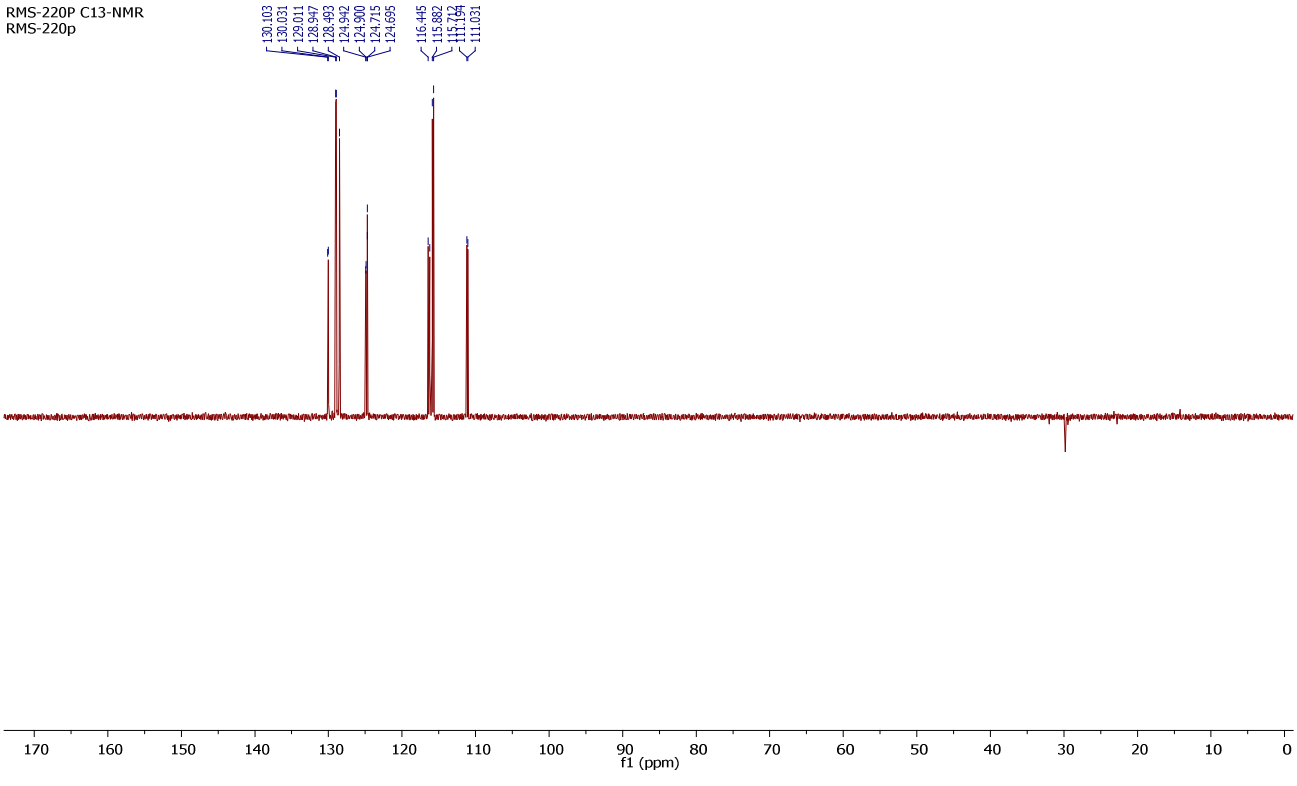


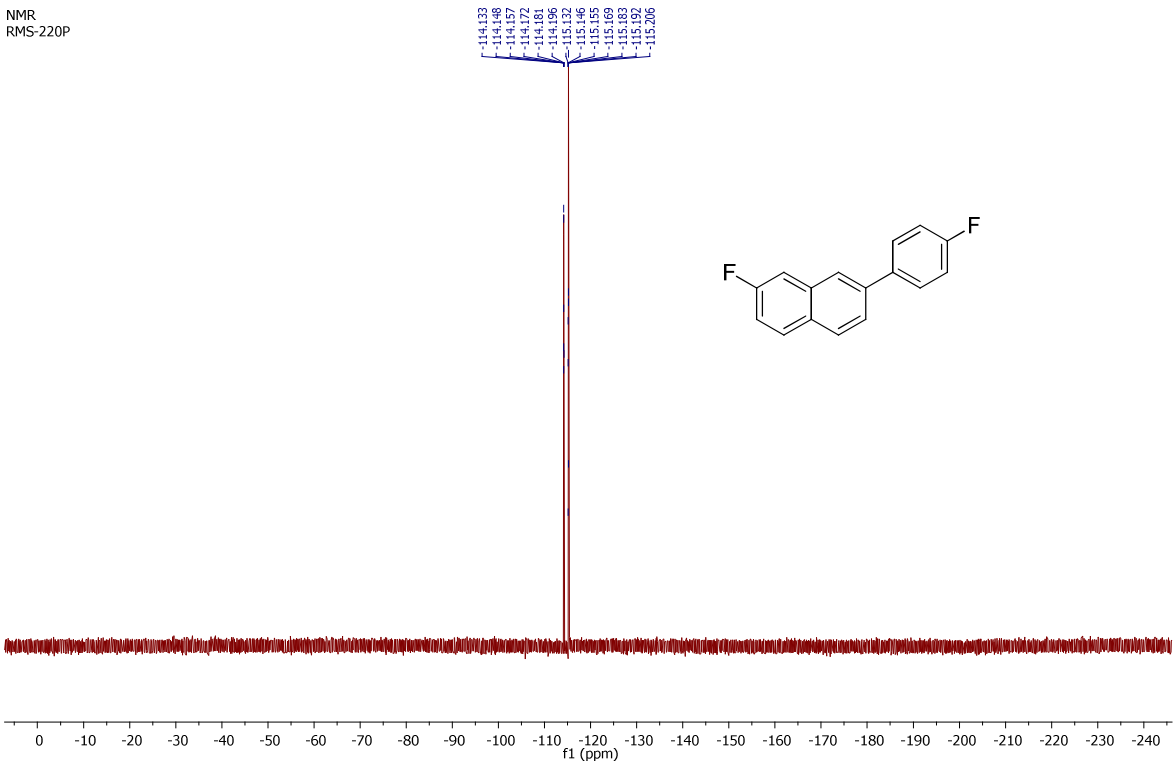


S4.2. ^{1}H, ^{13}C, DEPT135 and ^{19}F NMR spectra of 2-(4′-fluorophenyl)-7-fluoronaphthalene (**2b**)

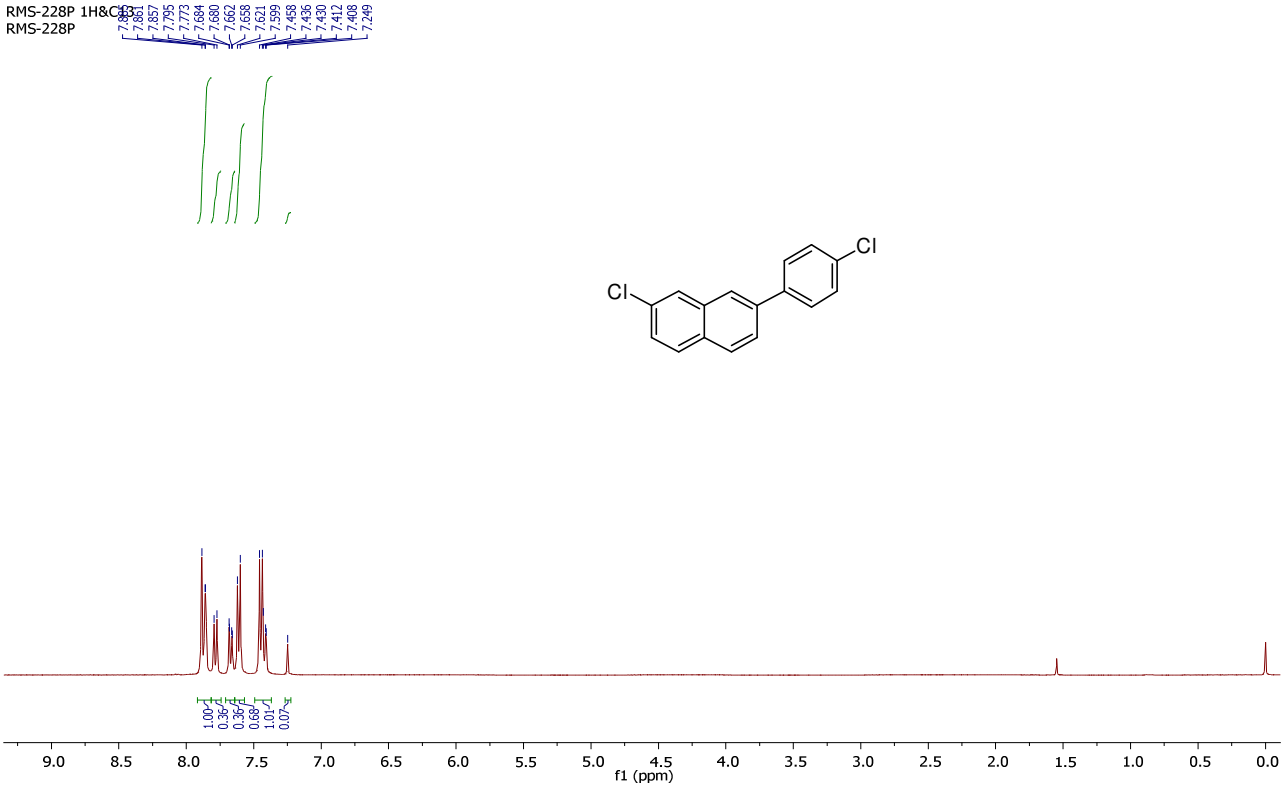


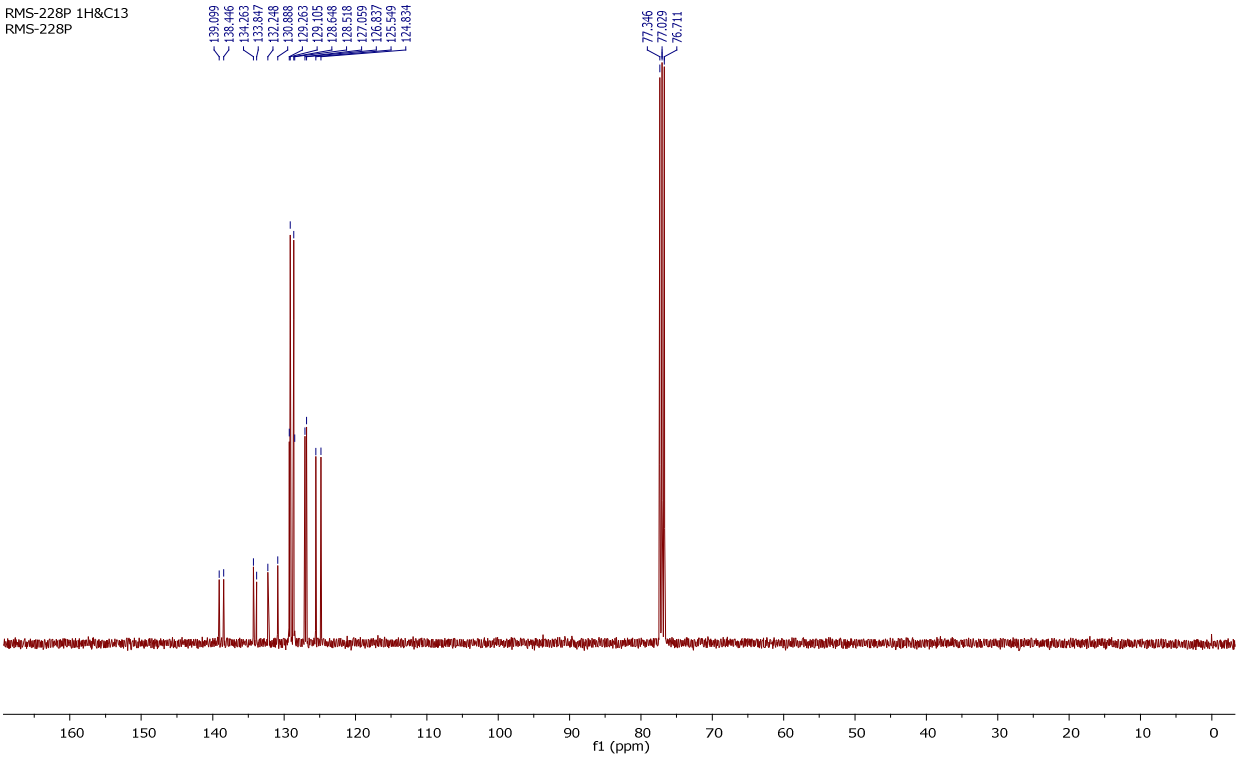

RMS-220P C13-NMR
RMS-220p
163.714
162.051
161.750
160.093
138.629
136.894
136.869
134.519
134.445
130.169
130.097
129.565
129.077
129.013
128.559
125.008
124.966
124.780
124.762
116.511
116.309
115.948
115.777
111.261
111.098
77.408
77.154
76.900
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

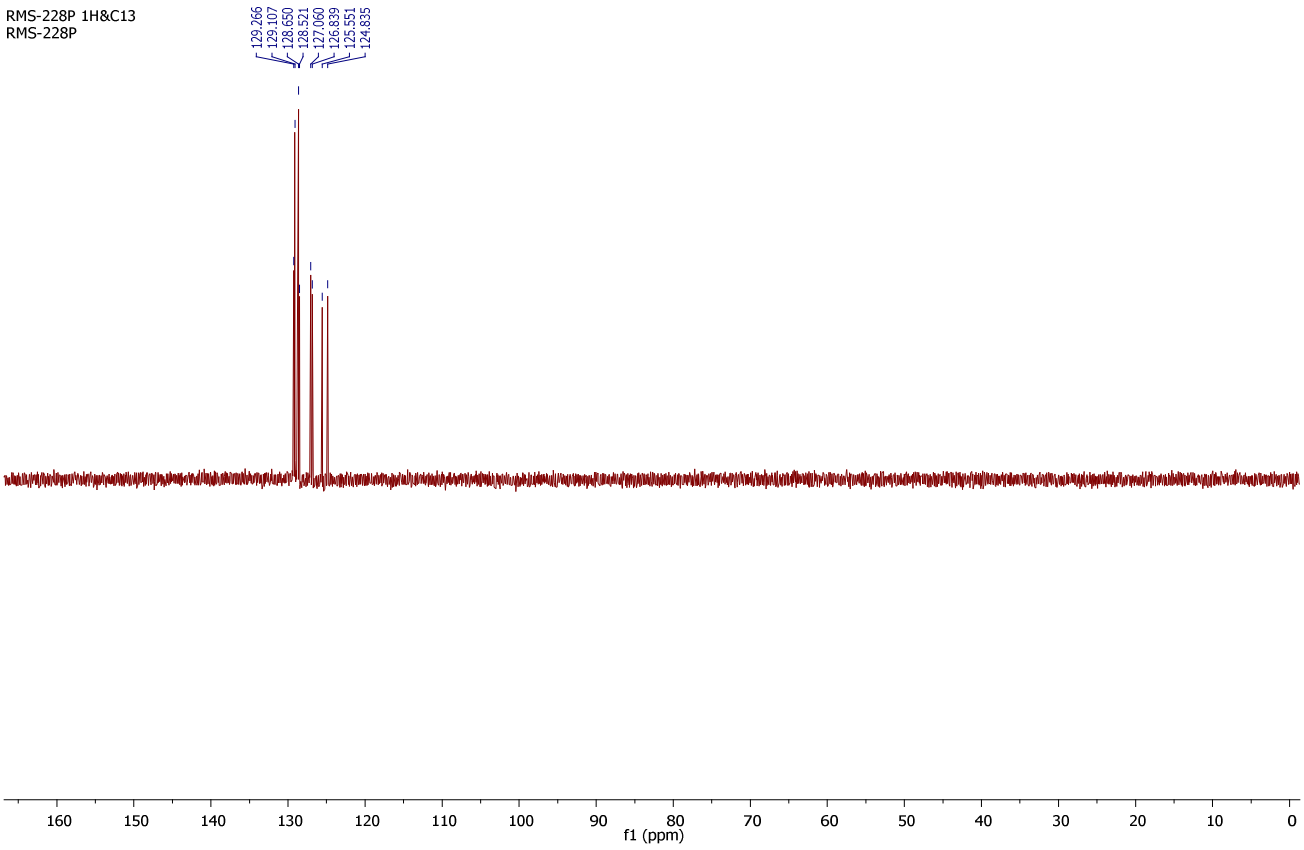

RMS-220P C13-NMR
RMS-220p
130.103
130.031
129.011
128.947
128.493
124.942
124.900
124.715
124.695
116.445
115.882
115.712
111.194
111.031
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



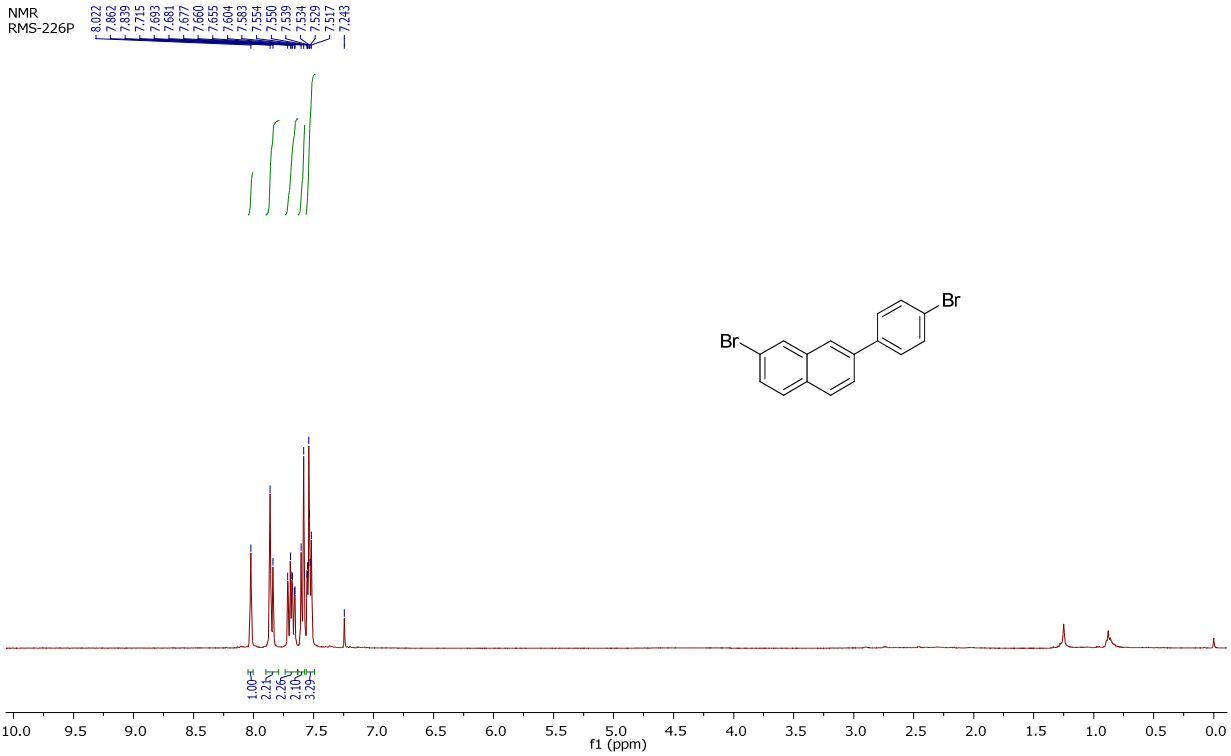
S3.3. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(4′-chlorophenyl)-7-chloronaphthalene (**2c**)

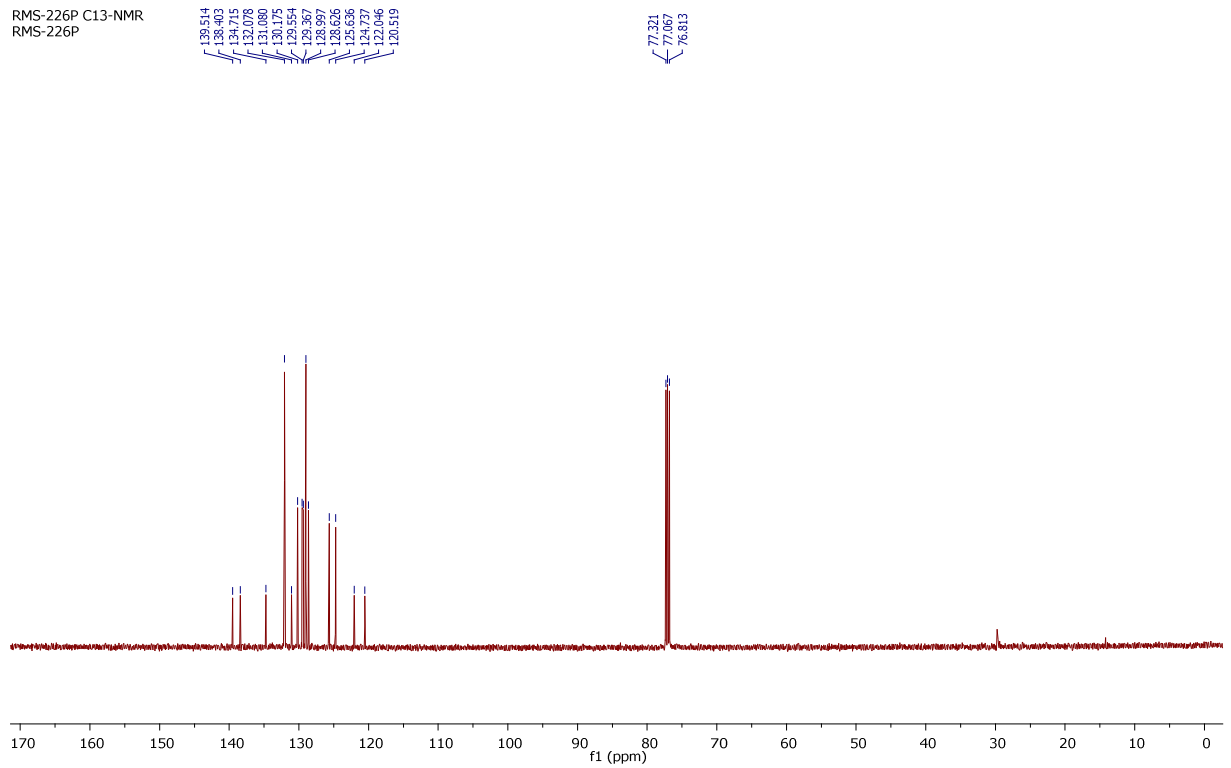


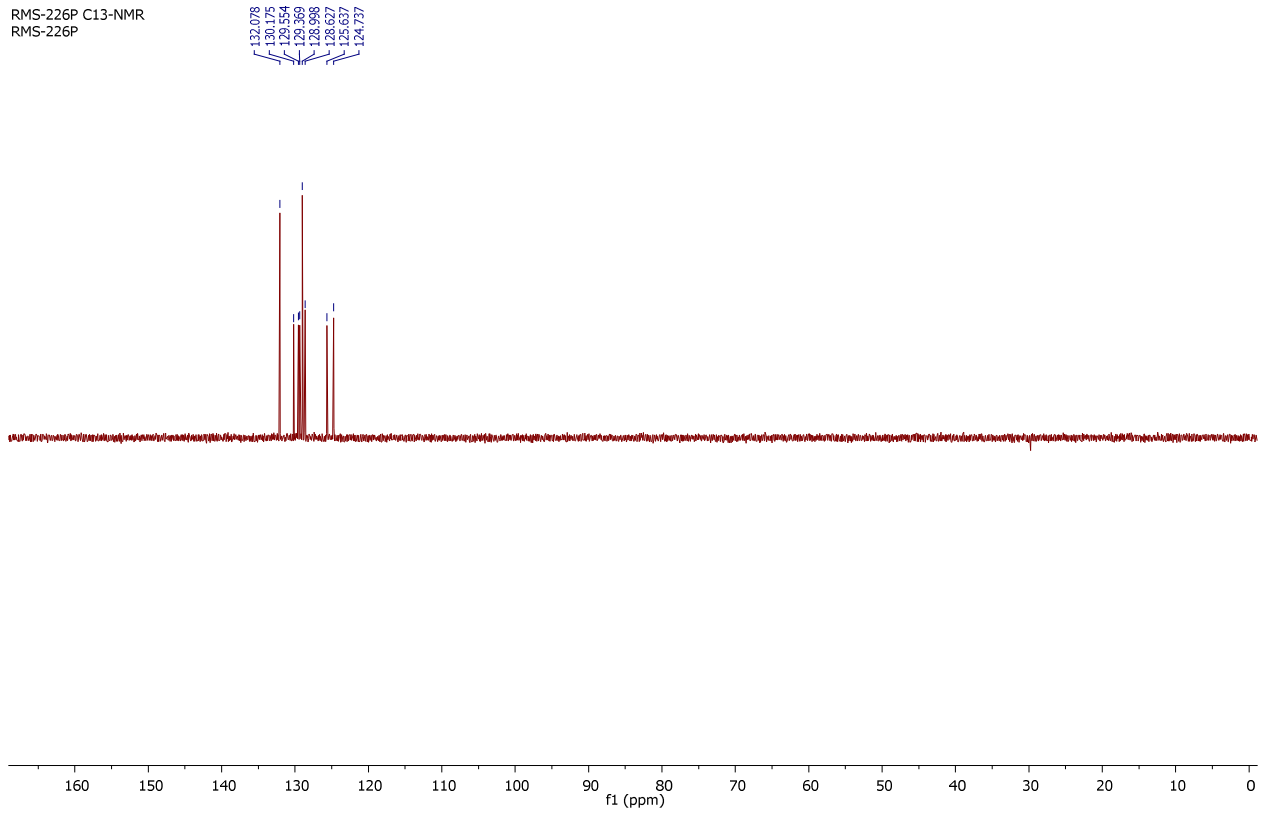

RMS-228P 1H&C13
RMS-228P
139.099
138.446
134.263
133.847
132.248
130.888
129.263
129.105
128.648
128.518
127.059
126.837
125.549
124.834
77.346
77.029
76.711
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


RMS-228P 1H&C13
RMS-228P
129.266
129.107
128.650
128.521
127.060
126.839
125.551
124.835
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

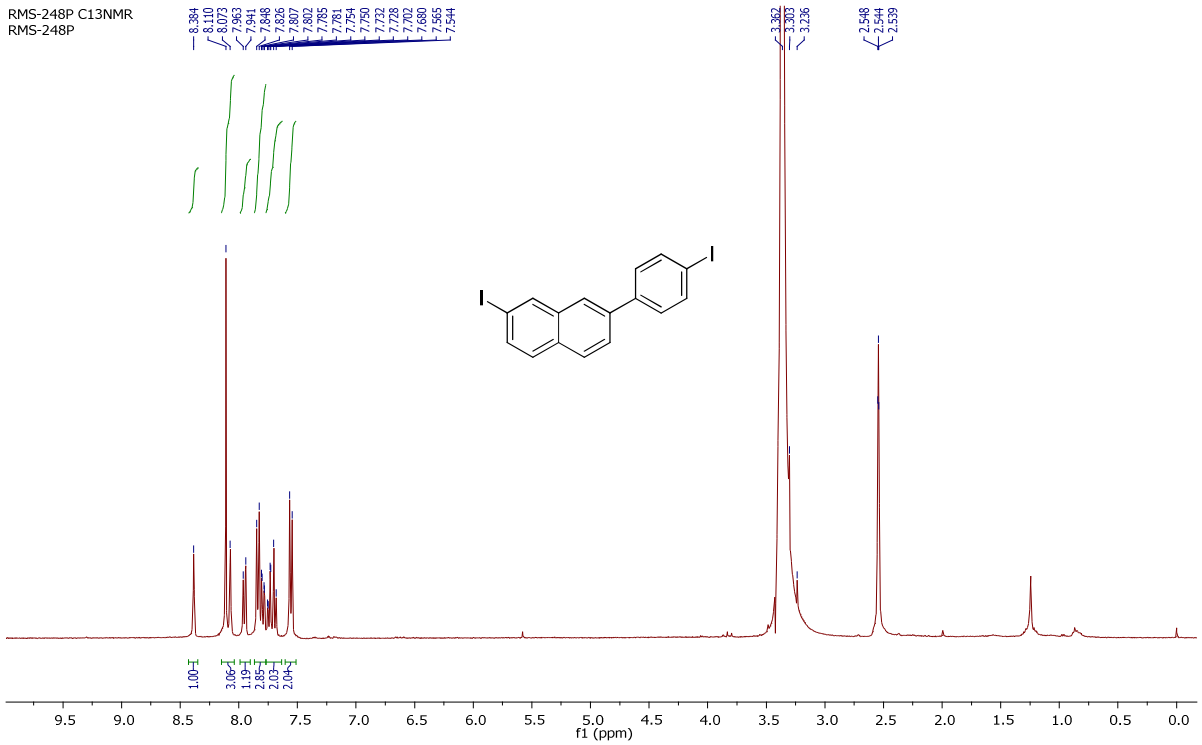
S4.4. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(4′-bromophenyl)-7-bromonaphthalene (**2d**)

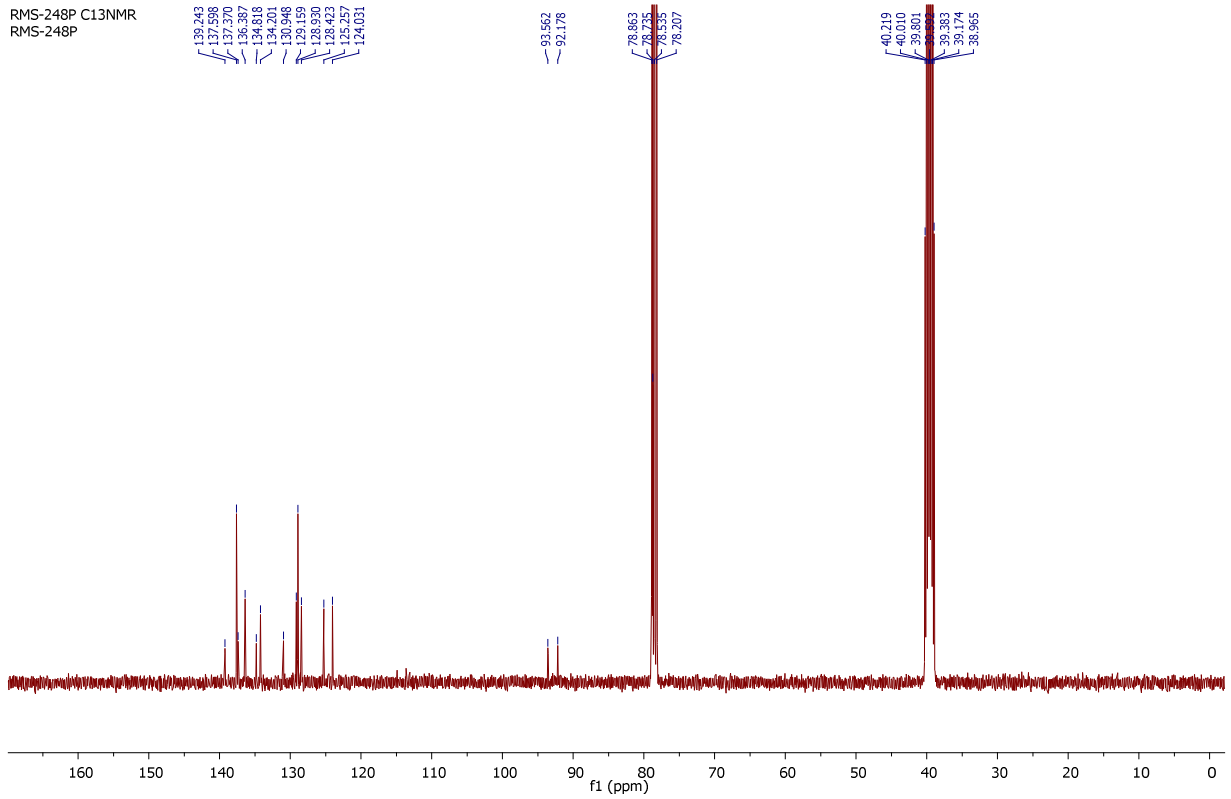


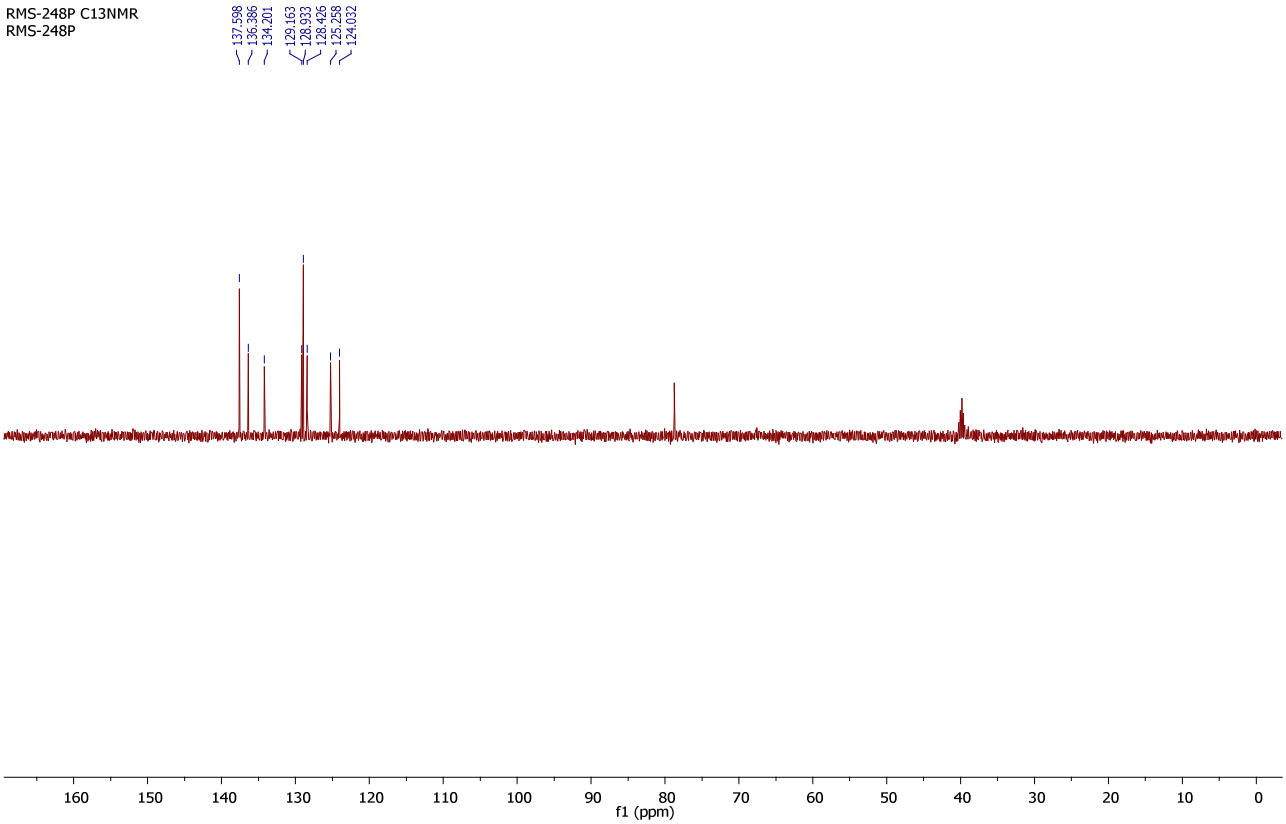




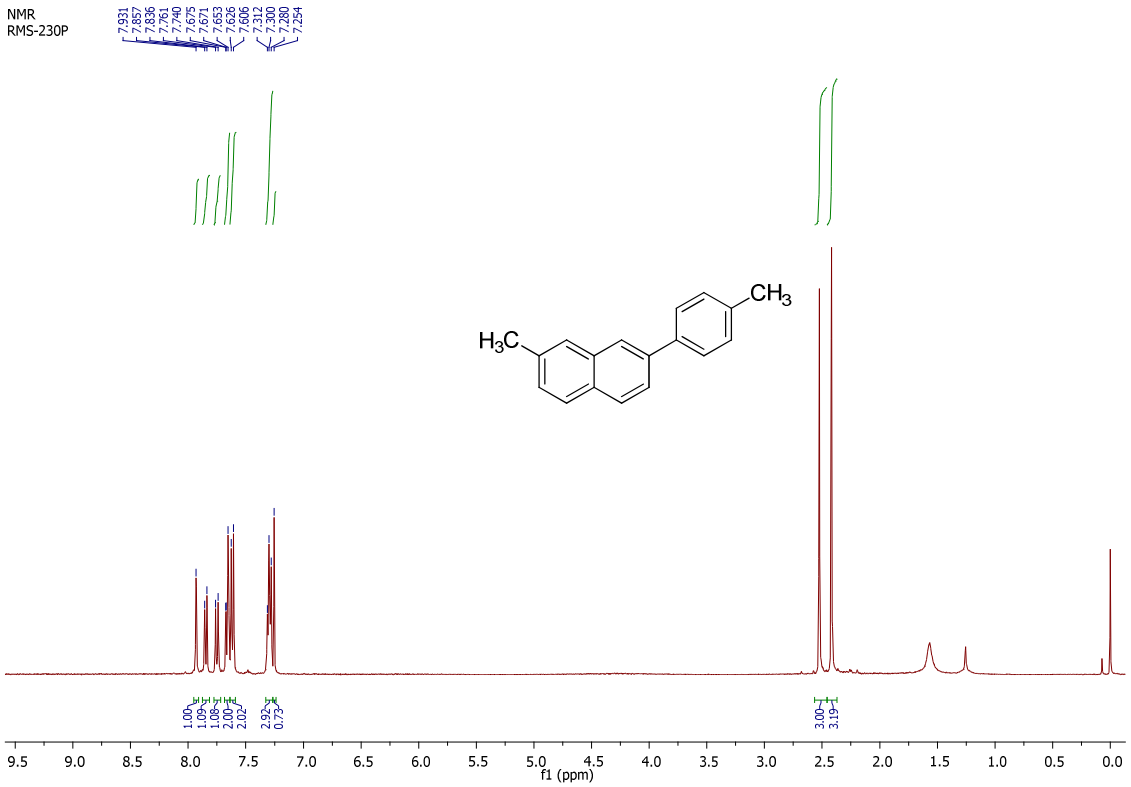
S4.5. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(4′-iodophenyl)- 7-iodonaphthalene (**2e**)

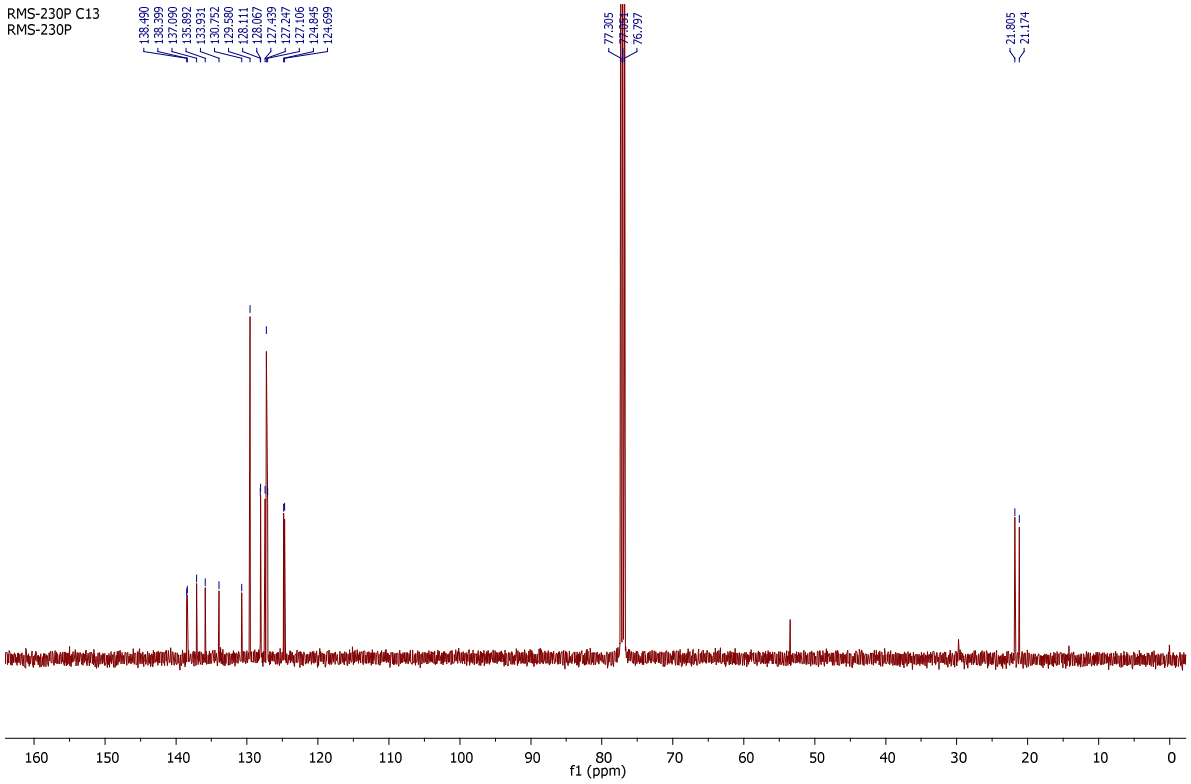


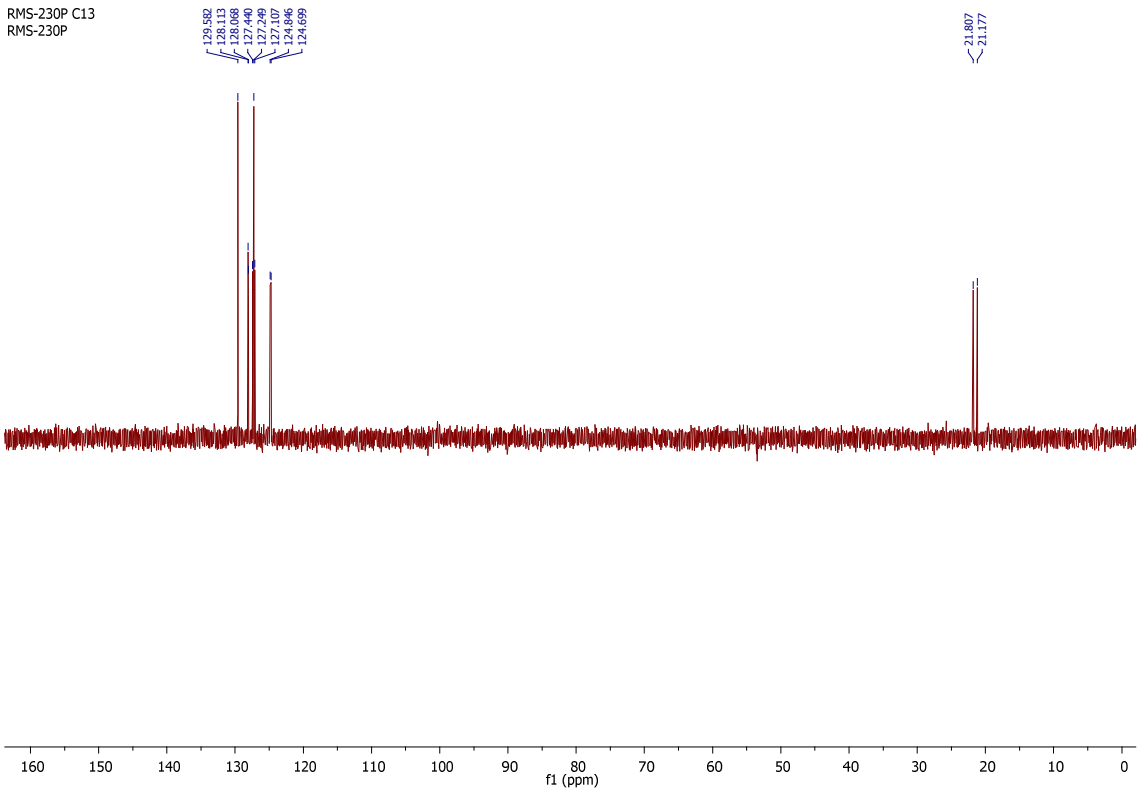

RMS-248P C13NMR
RMS-248P
139.243
137.598
137.370
136.387
134.818
134.201
130.948
129.159
128.930
128.423
125.257
124.031
93.562
92.178
78.863
78.735
78.535
78.207
40.219
40.010
39.801
39.592
39.383
39.174
38.965
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


RMS-248P C13NMR
RMS-248P
137.598
136.386
134.201
129.163
128.933
128.426
125.258
124.032
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

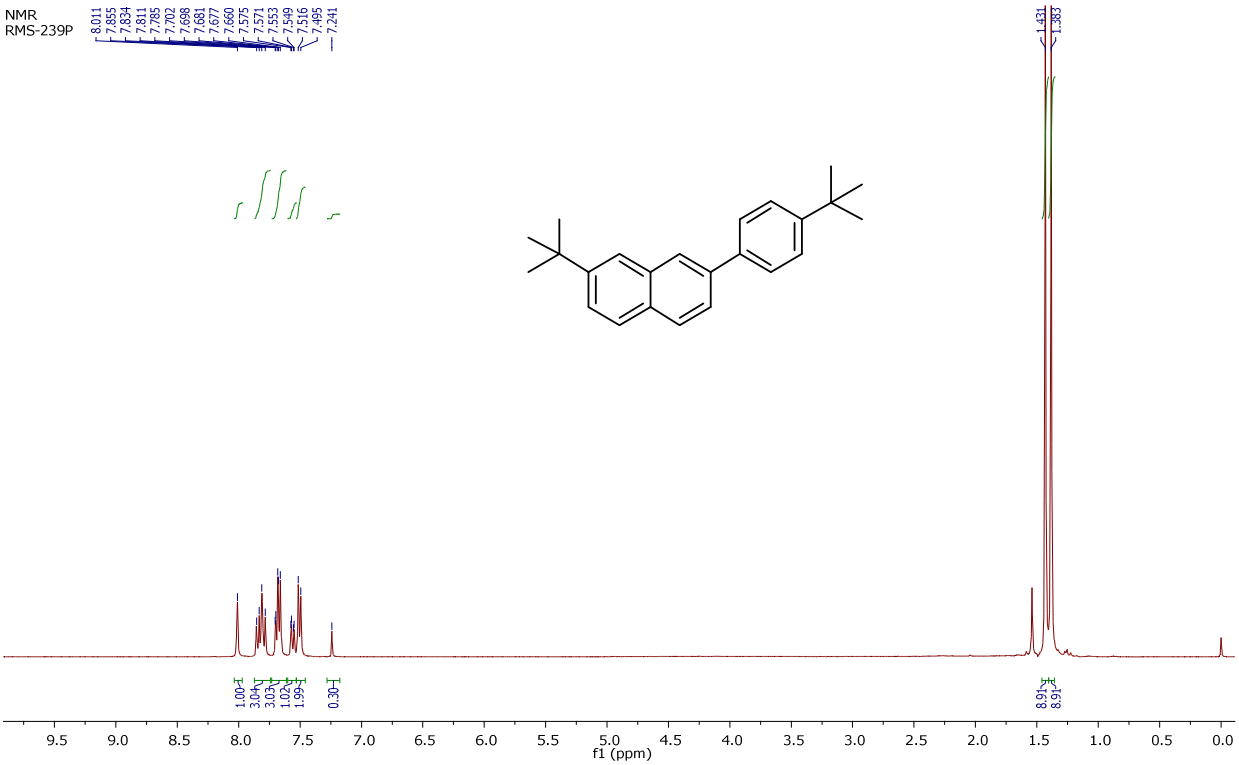
S4.6. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(p-tolyl)-7-methylnaphthalene (**2f**).

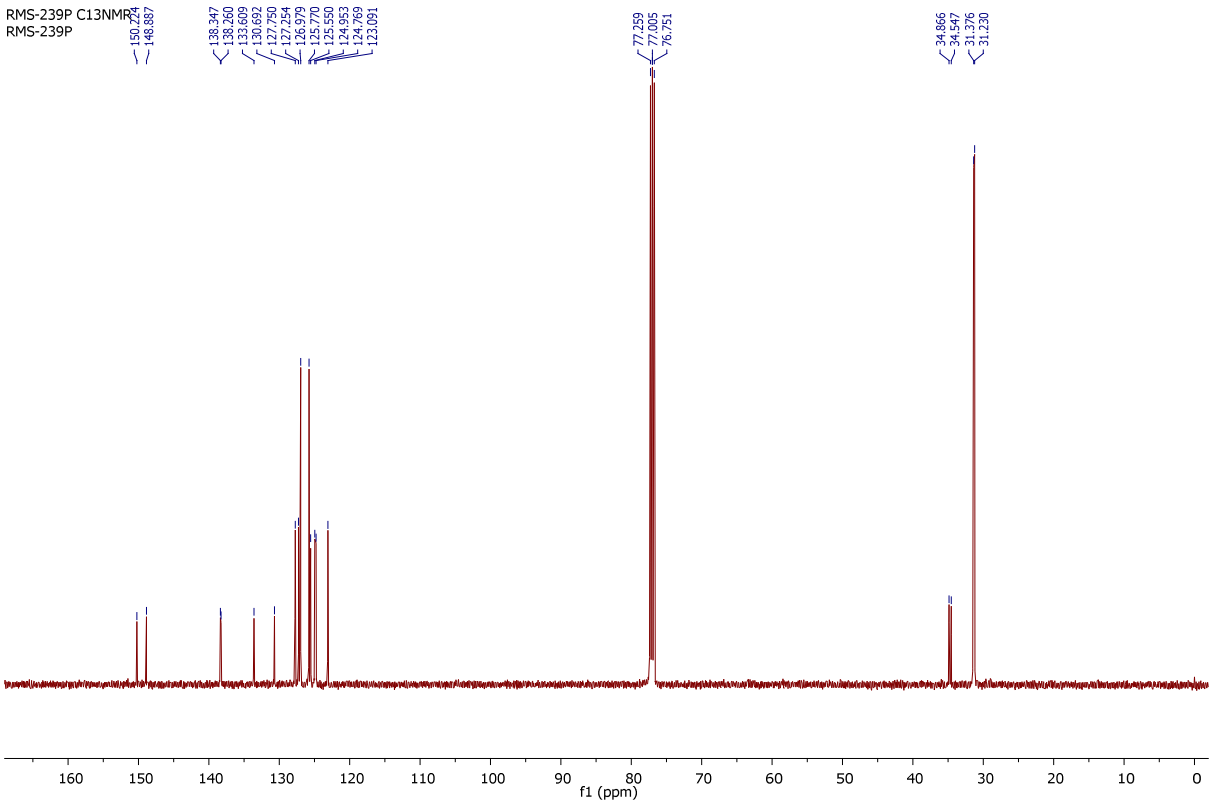


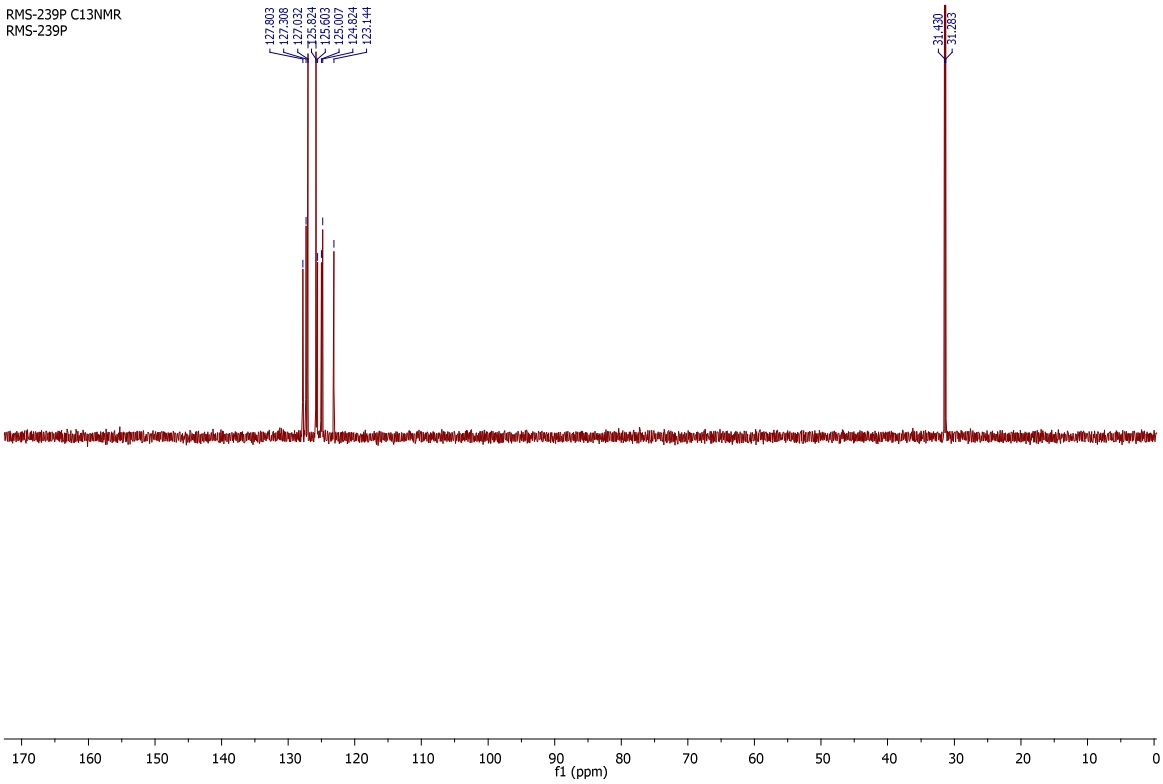




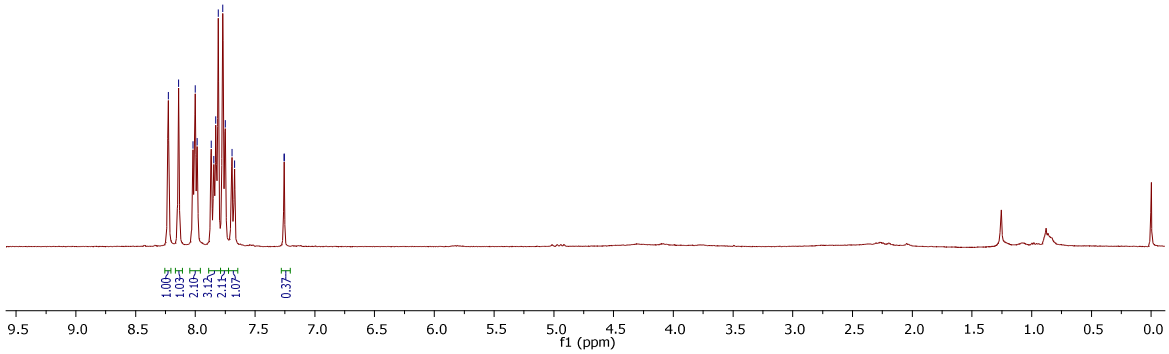
S3.7. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(4′-(tert-butyl)phenyl)-7-(tert-butyl)naphthalene (**2g**)

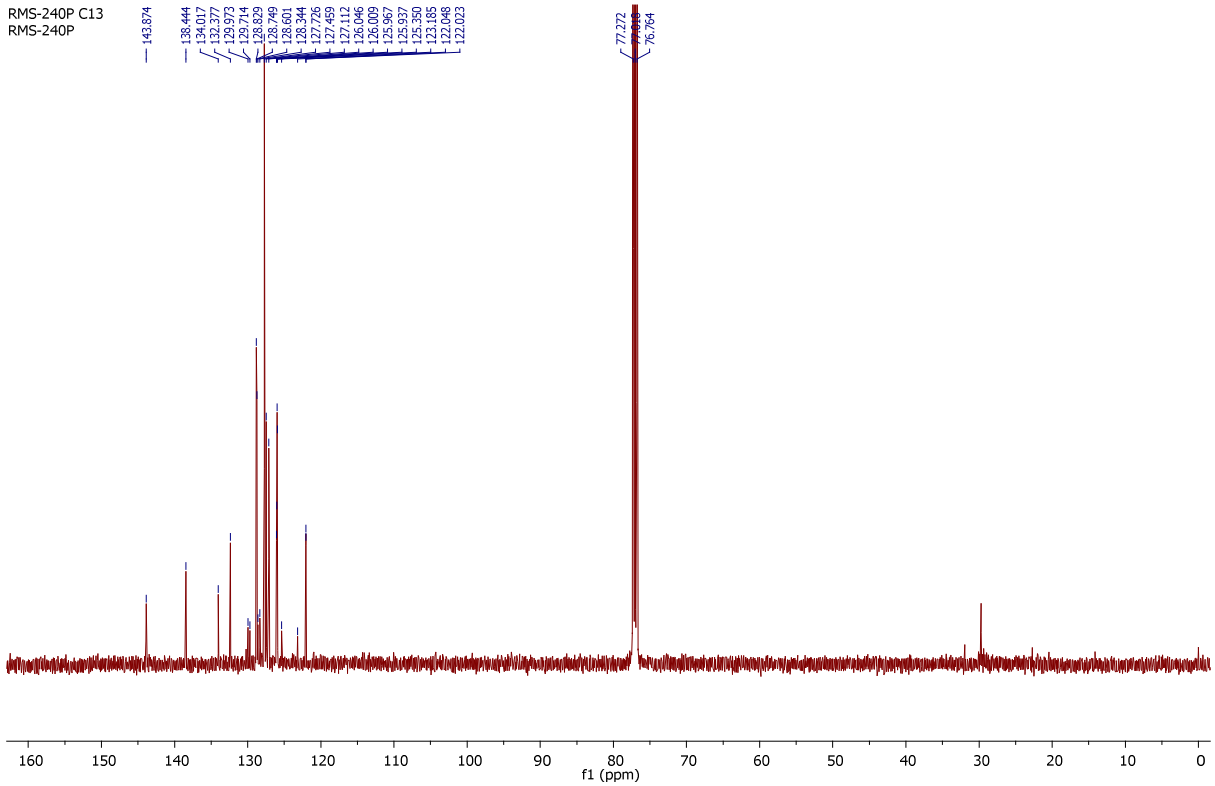


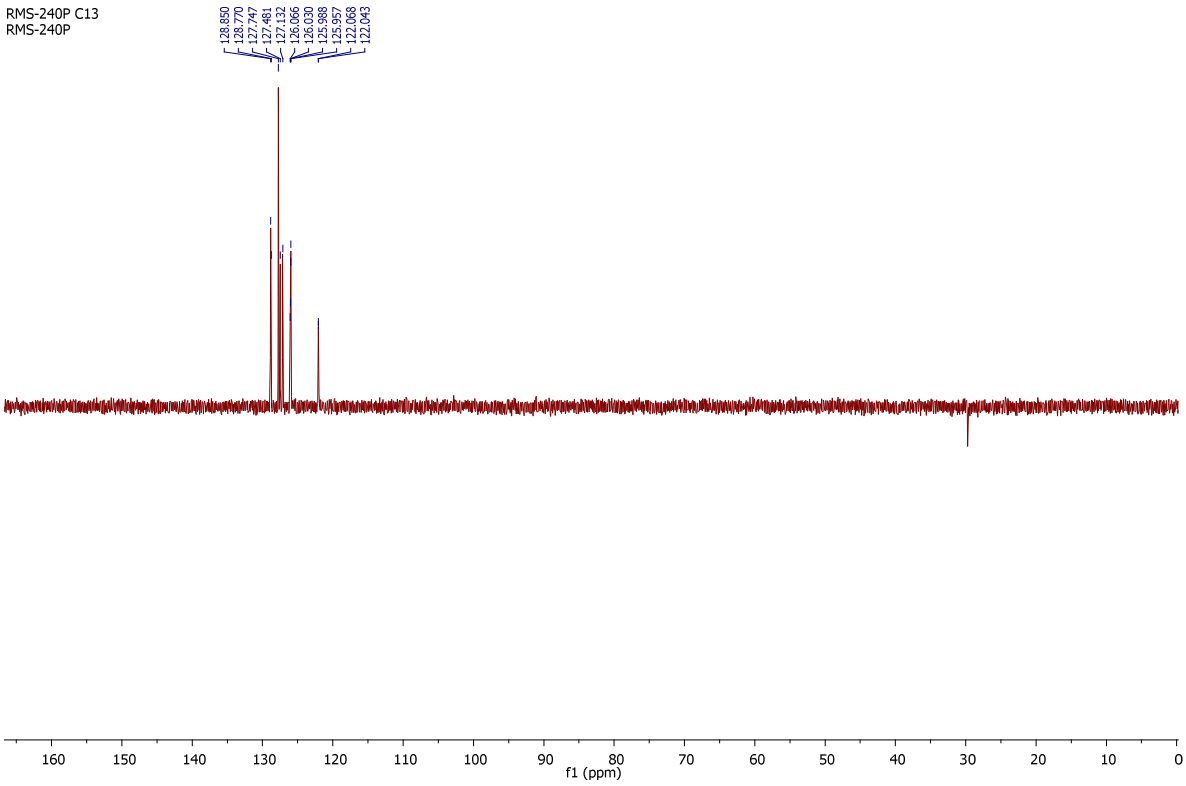

RMS-239P C13NMR
RMS-239P
150.224
148.887
138.347
138.260
133.609
130.692
127.750
127.254
126.979
125.770
125.550
124.953
124.769
123.091
77.259
77.005
76.751
34.866
34.547
31.376
31.230
f1 (ppm)

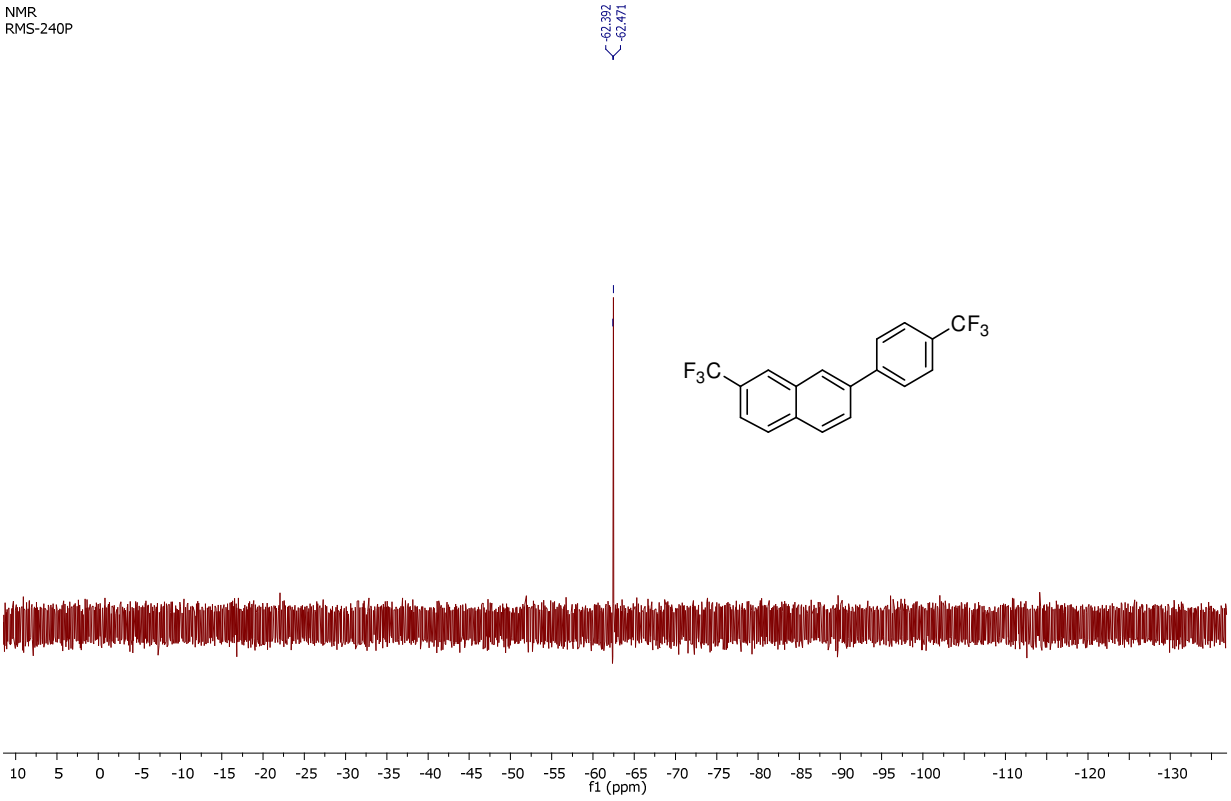

RMS-239P C13NMR
RMS-239P
127.803
127.308
127.032
125.824
125.603
125.007
124.824
123.144
31.430
31.283
f1 (ppm)

S4.8. ^{1}H, ^{13}C, DEPT135 and ^{19}F NMR spectra of 2-(4′-(trifluoromethyl)phenyl)-7-(trifluoromethyl) naphthalene (**2h**)

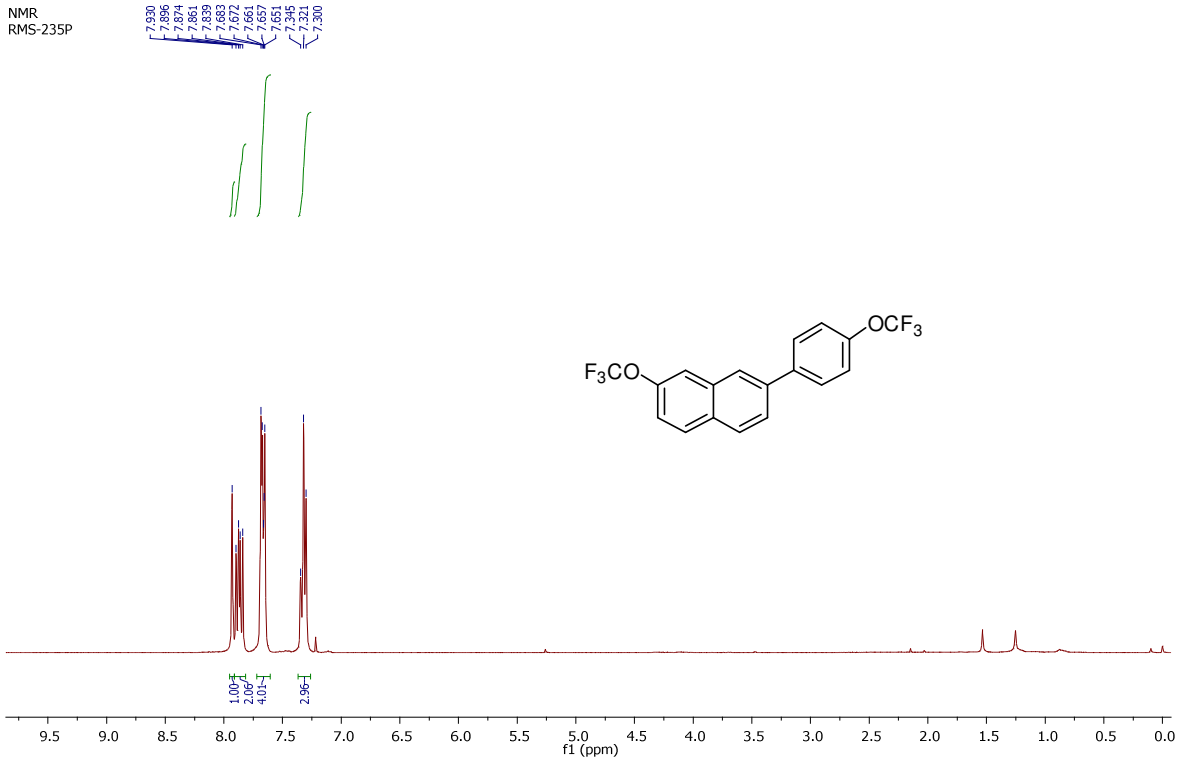


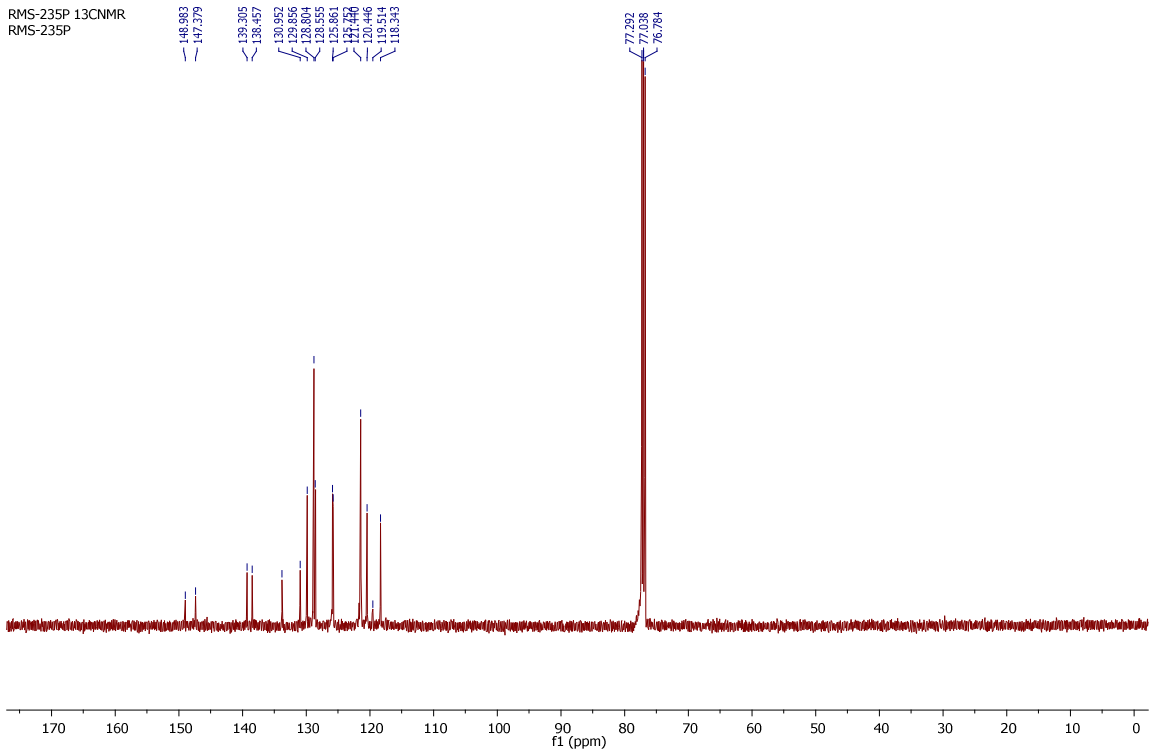


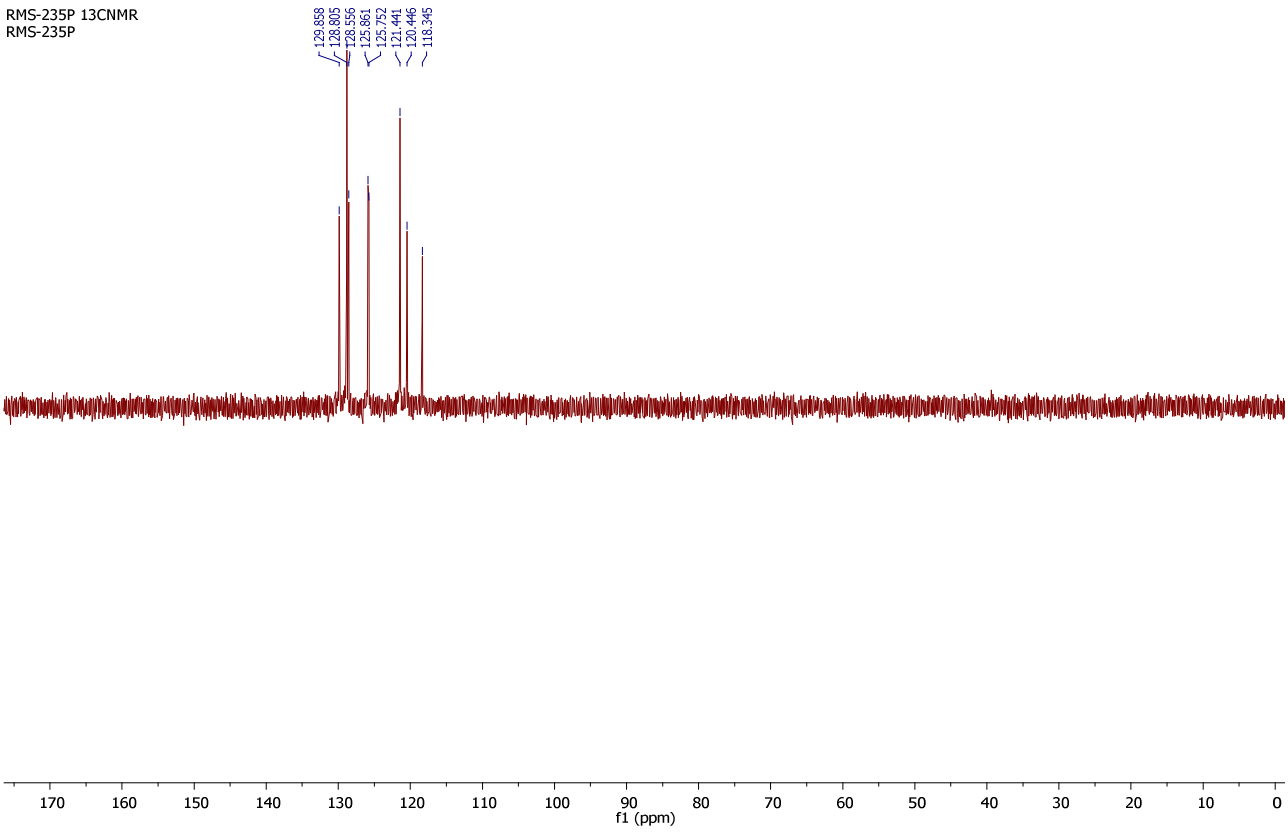

RMS-240P C13
RMS-240P
128.850
128.770
127.747
127.481
127.132
126.066
126.030
125.988
125.957
122.068
122.043
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

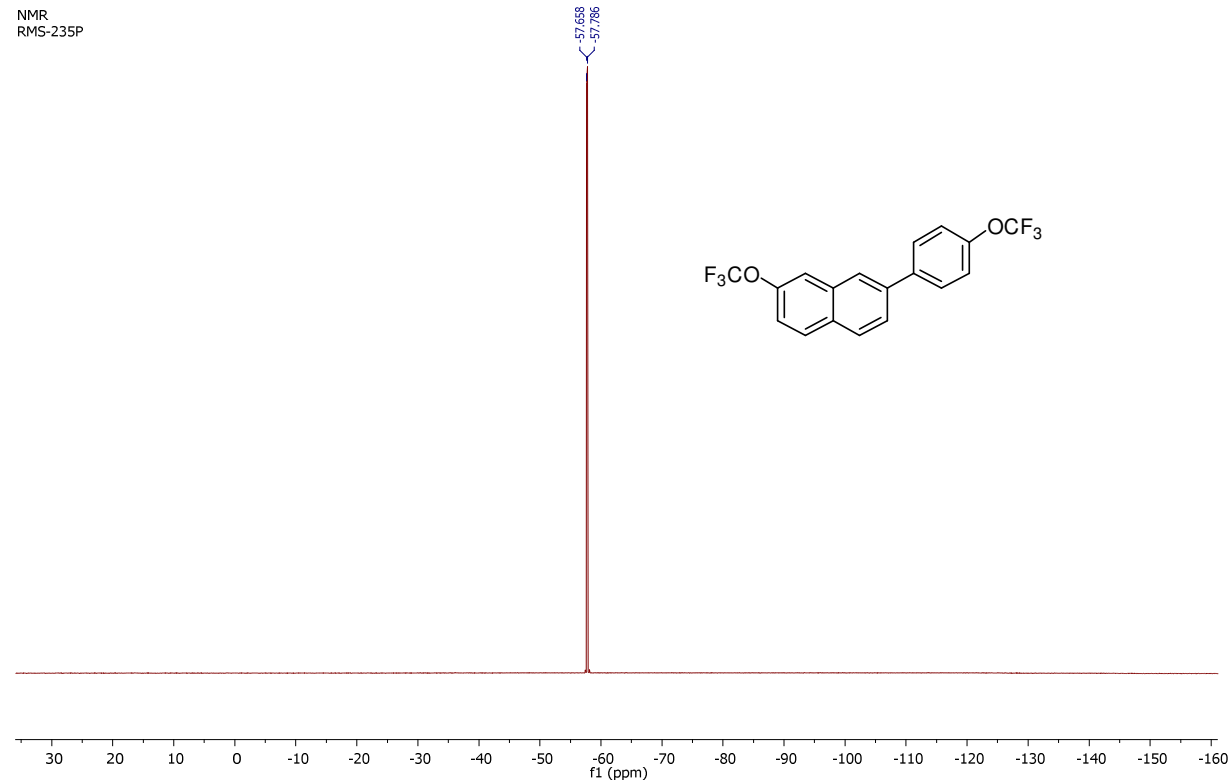

NMR
RMS-240P
-62.392
-62.471
CF3
F3C
10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -110 -120 -130
f1 (ppm)

S4.9. ^{1}H, ^{13}C, DEPT135 and ^{19}F NMR spectra of 7-(trifluoromethoxy)-2-(4'-(trifluoromethoxy)phenyl) naphthalene (**2i**)

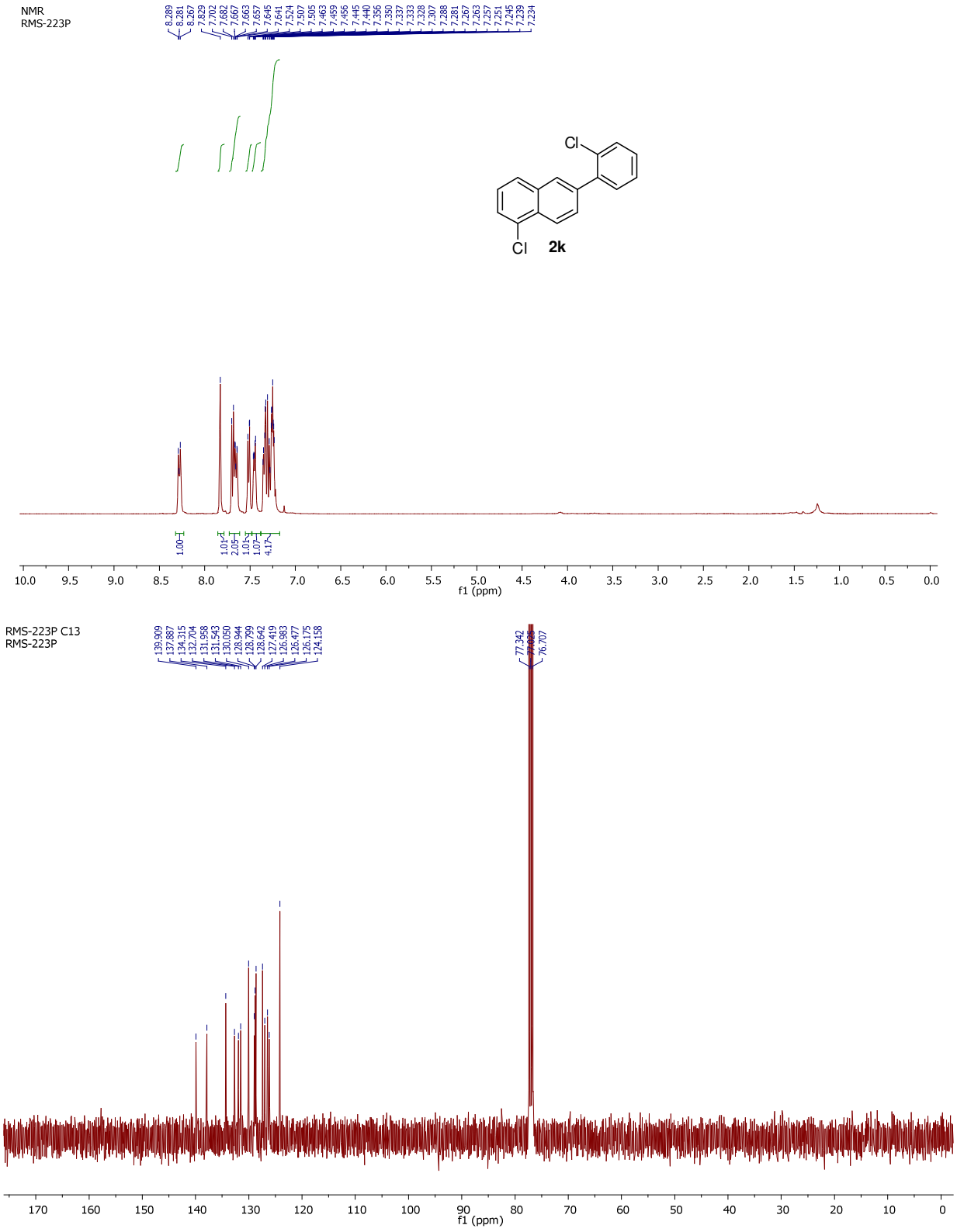


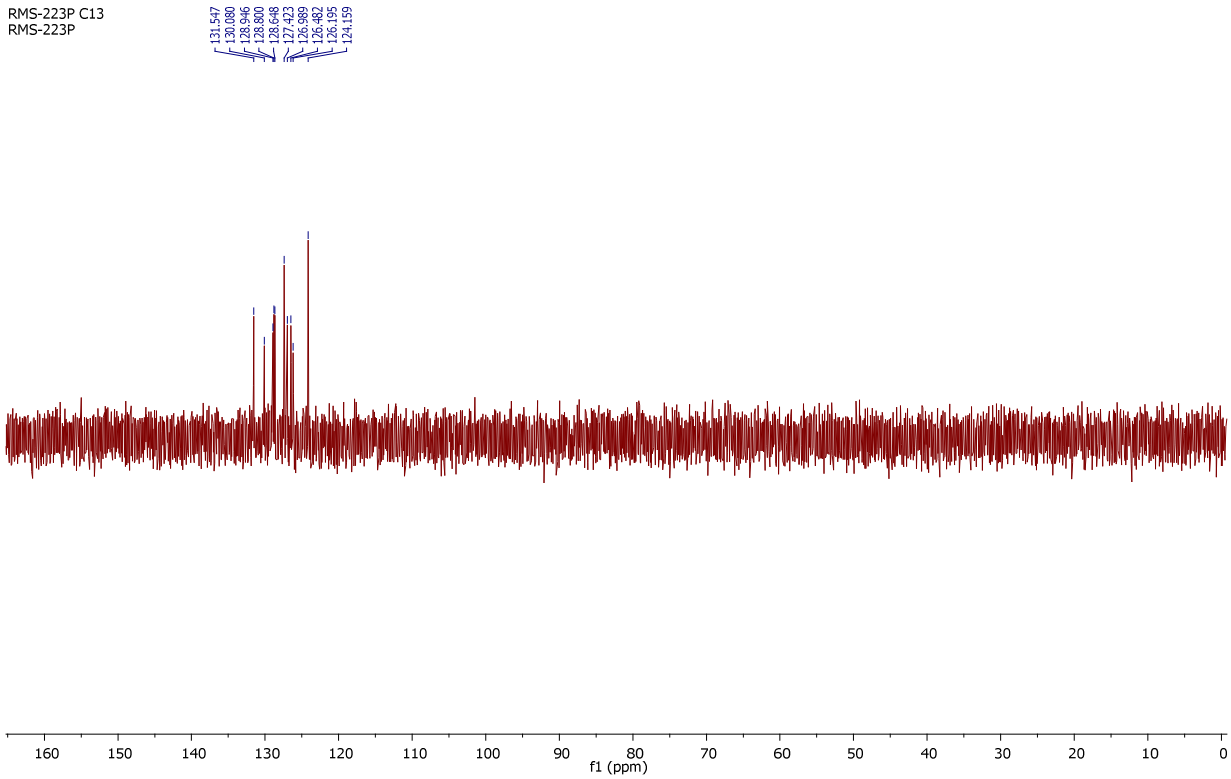



RMS-235P 13CNMR
RMS-235P
129.858
128.805
128.556
125.861
125.752
121.441
120.446
118.345
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

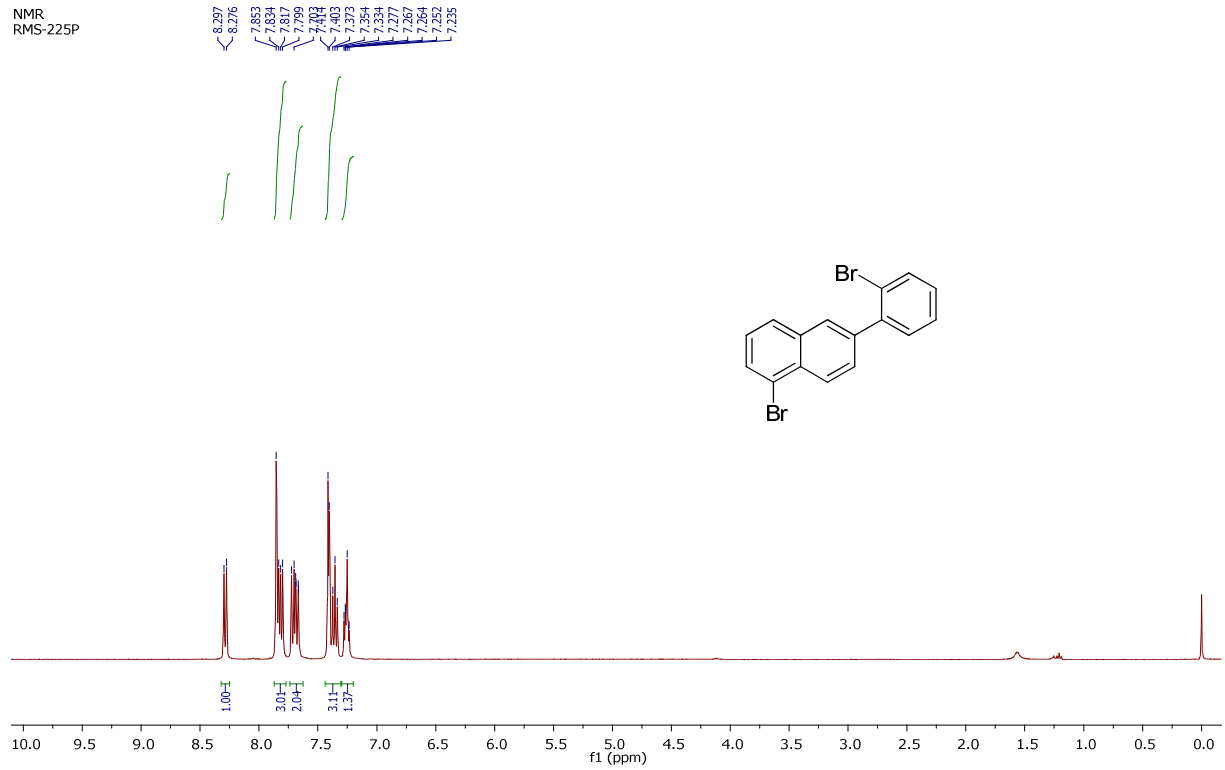

NMR
RMS-235P
-57.658
-57.786
OCF3
F3CO
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
f1 (ppm)

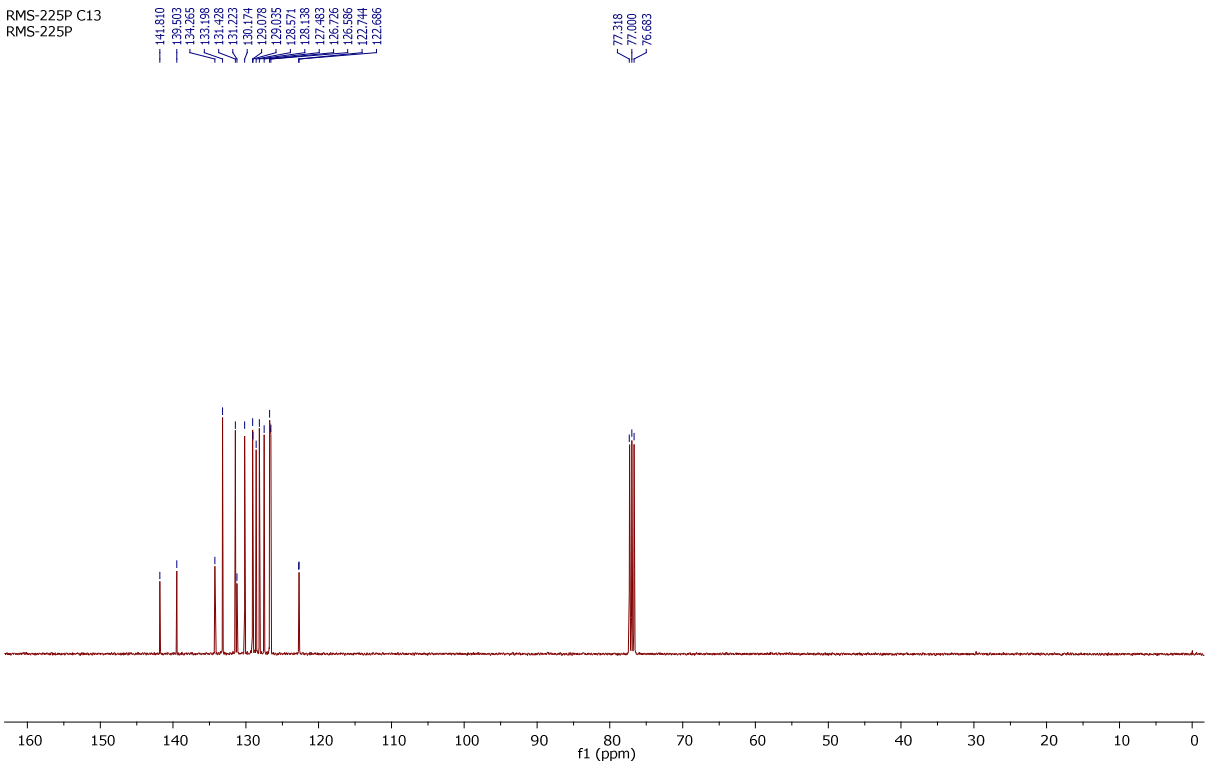
S4.10. ^{1}H,^{13}C and DEPT135 NMR spectra of 2-(2′-chlorophenyl)-5-chloronaphthalene (**2j**)

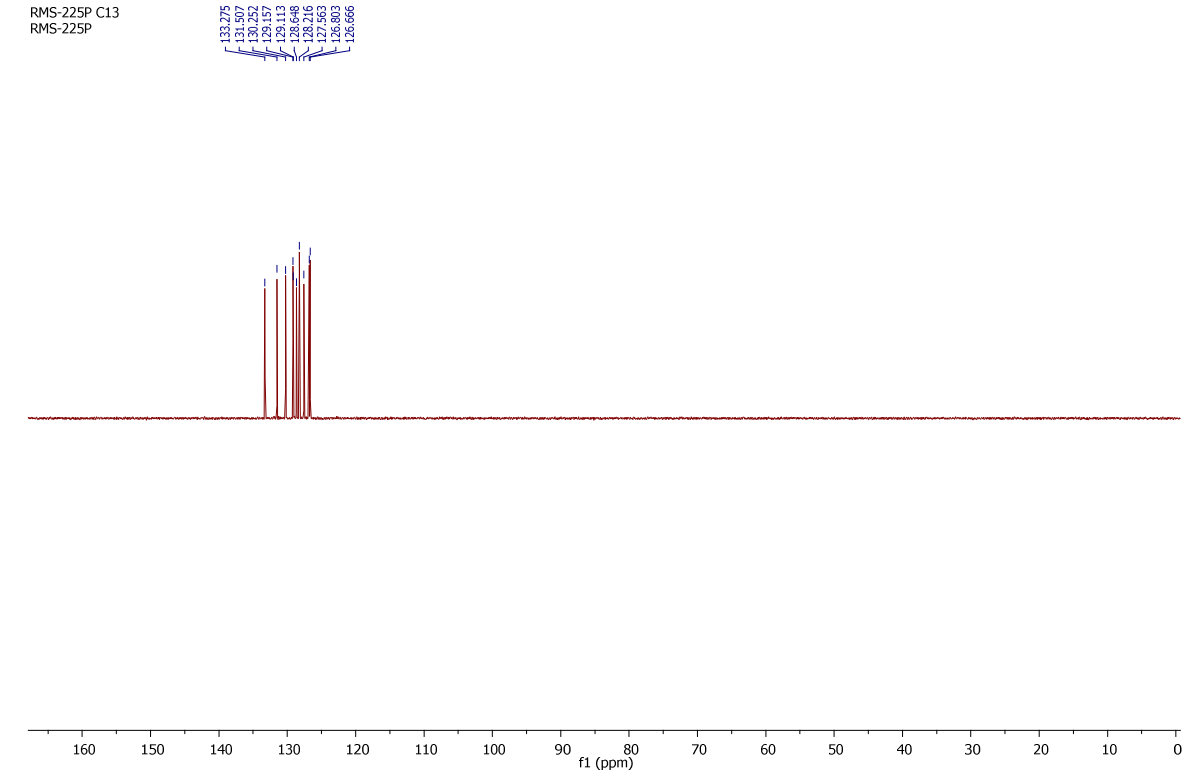




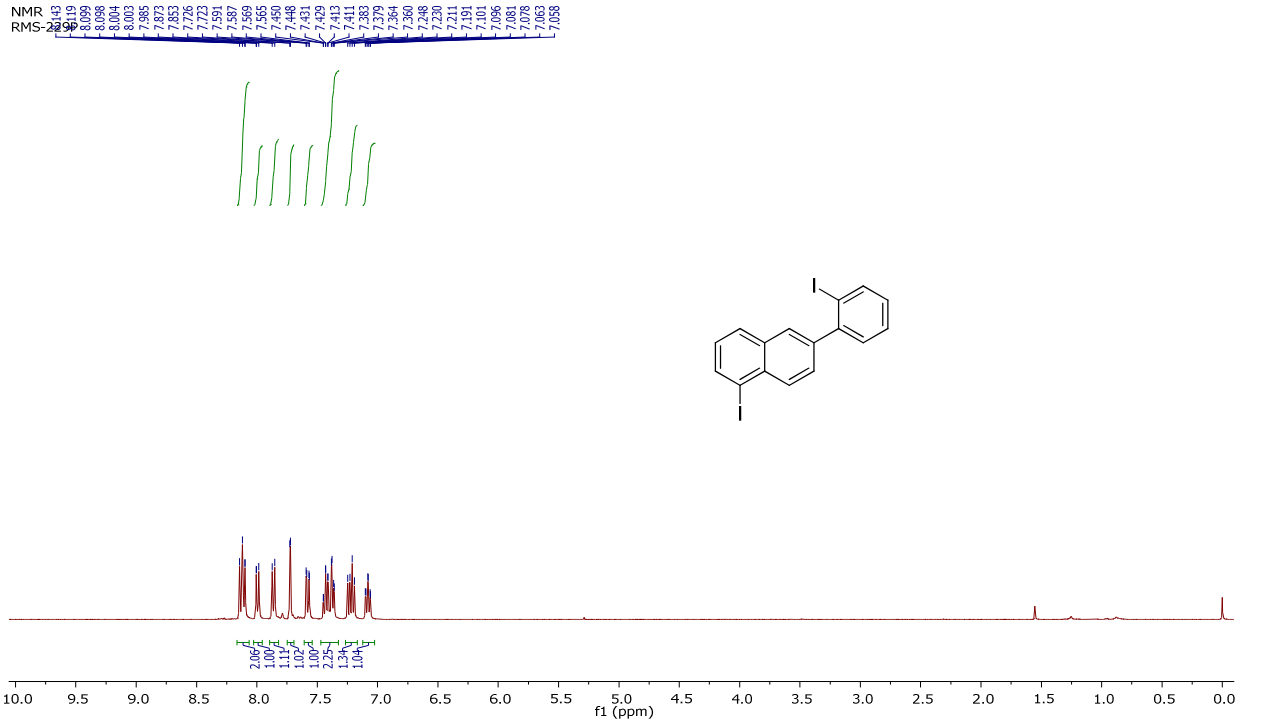
S4.11. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(2′-bromophenyl)-5-bromonaphthalene (**2k**)

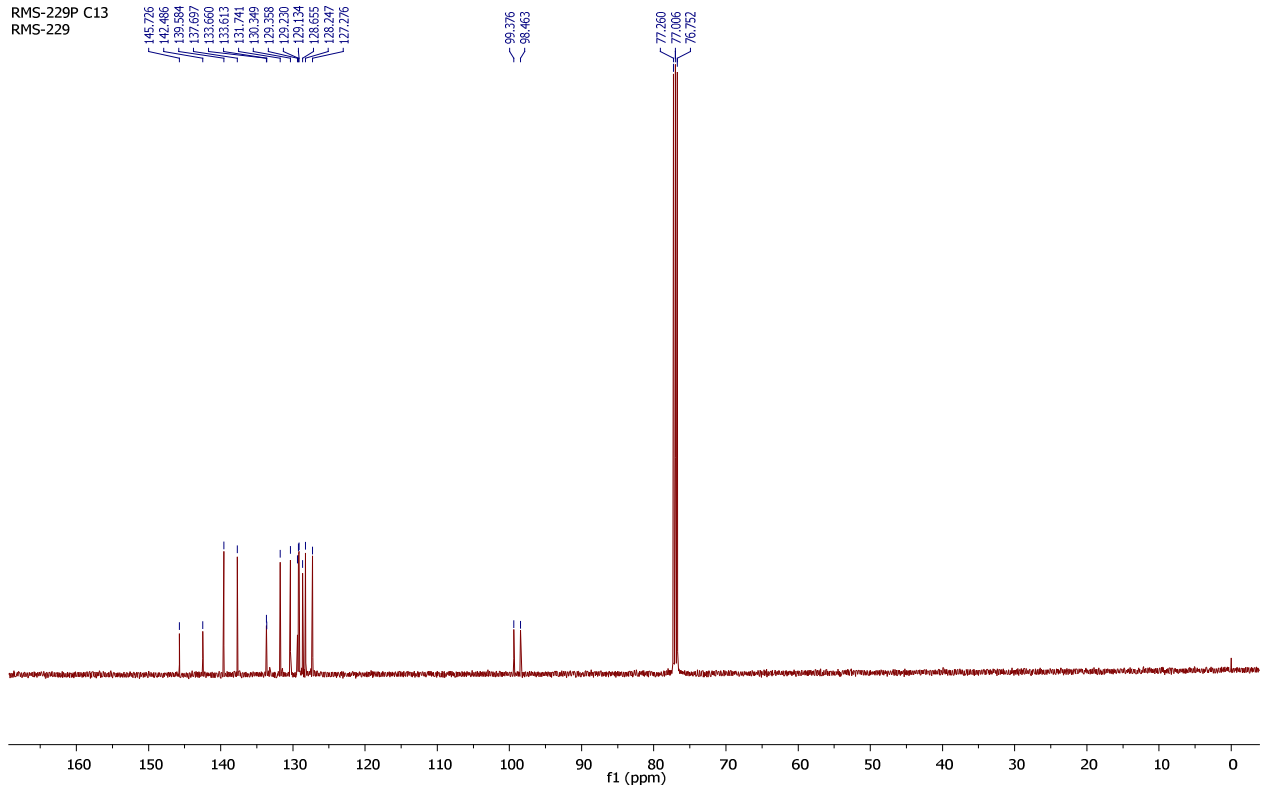


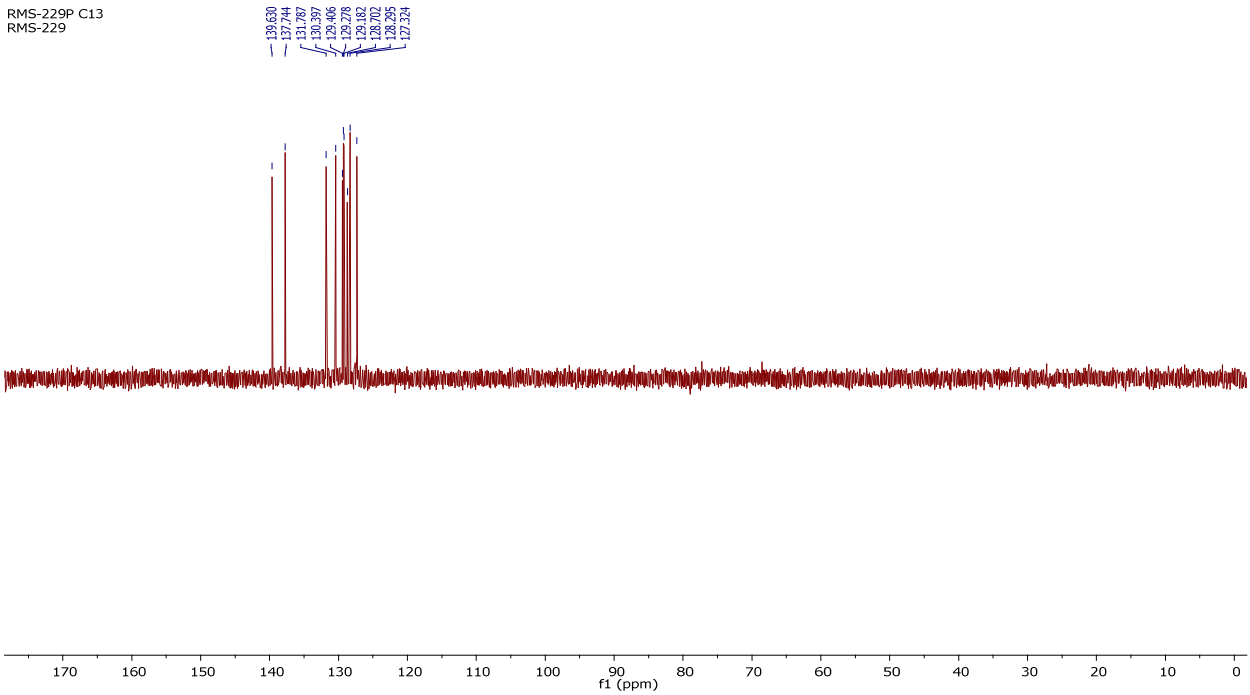

RMS-225P C13
RMS-225P
141.810
139.503
134.265
133.198
131.428
131.223
130.174
129.078
129.035
128.571
128.138
127.483
126.726
126.586
122.744
122.686
77.318
77.000
76.683
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


RMS-225P C13
RMS-225P
133.275
131.507
130.252
129.157
129.113
128.648
128.216
127.563
126.803
126.666
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

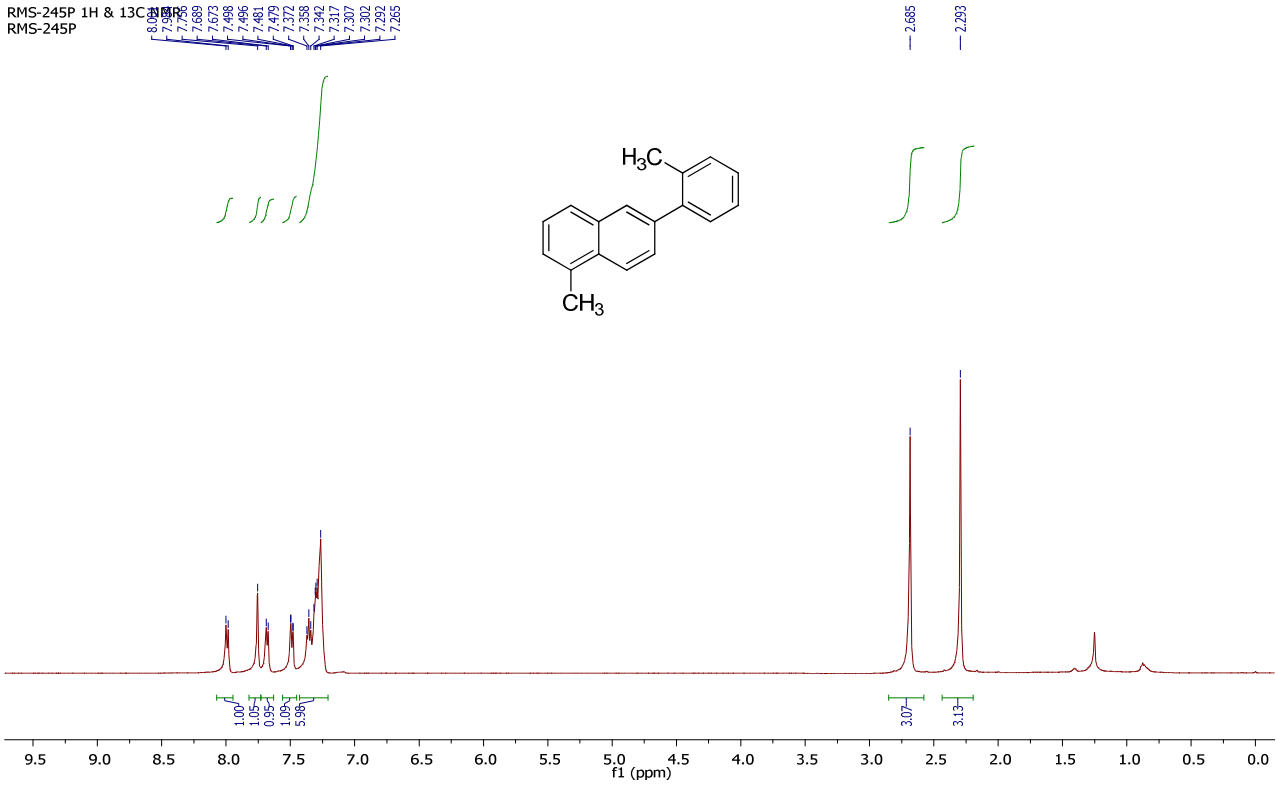
S4.12 ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(2′-iodophenyl)-5-iodonaphthalene (**2l**)

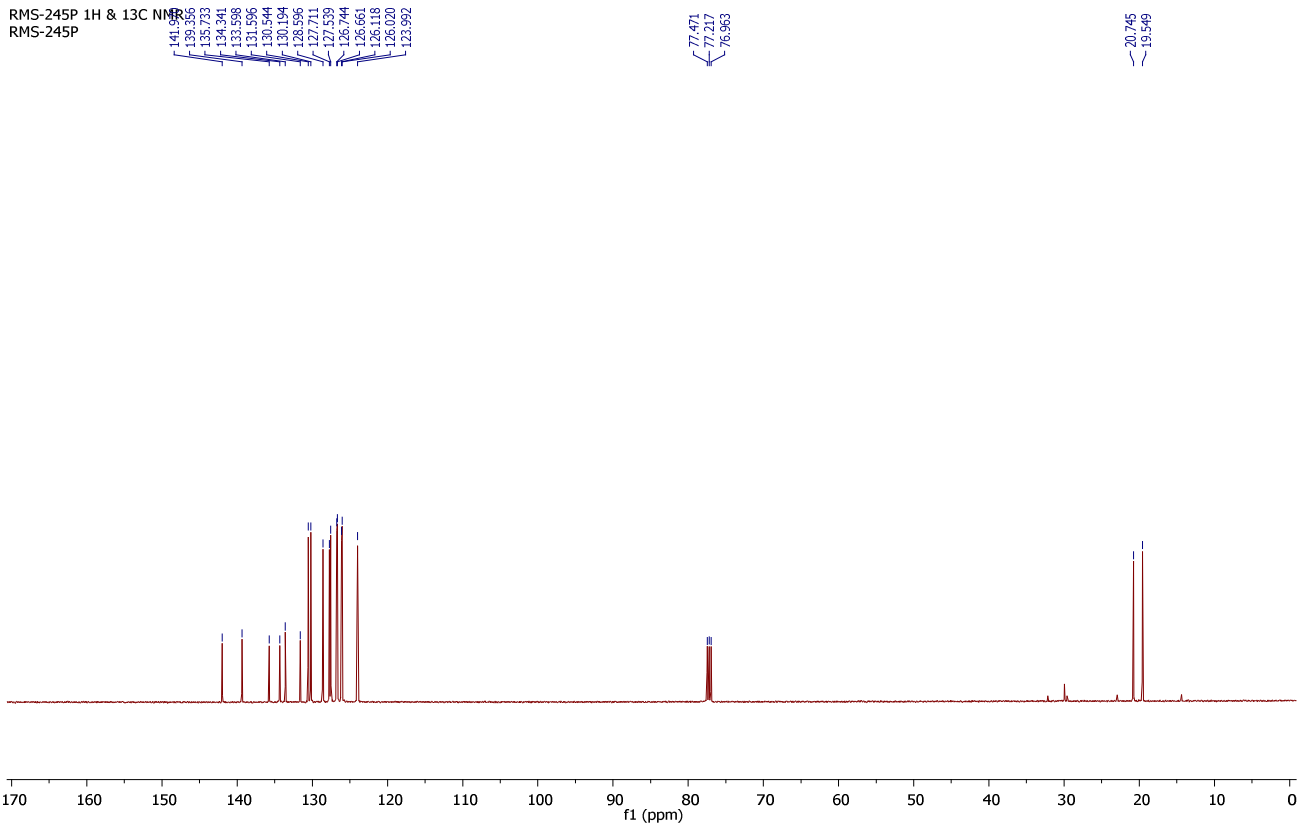


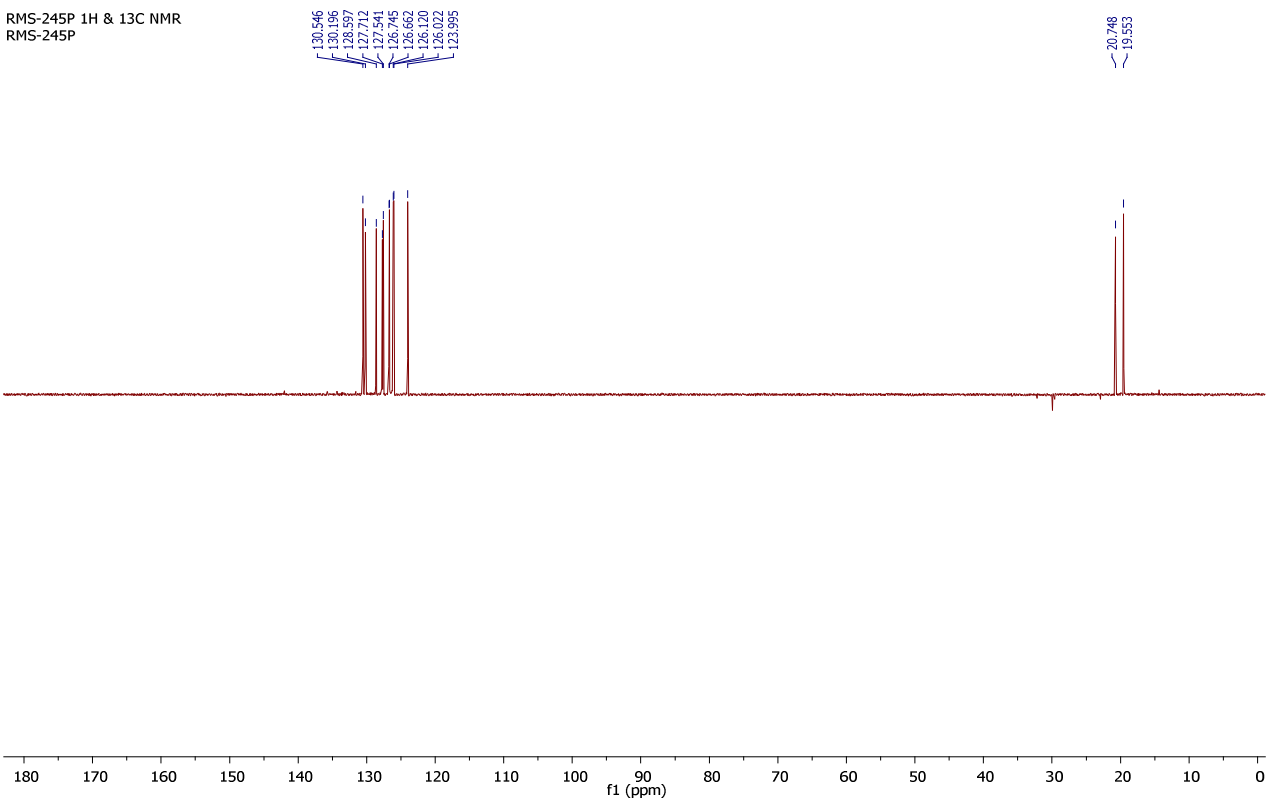




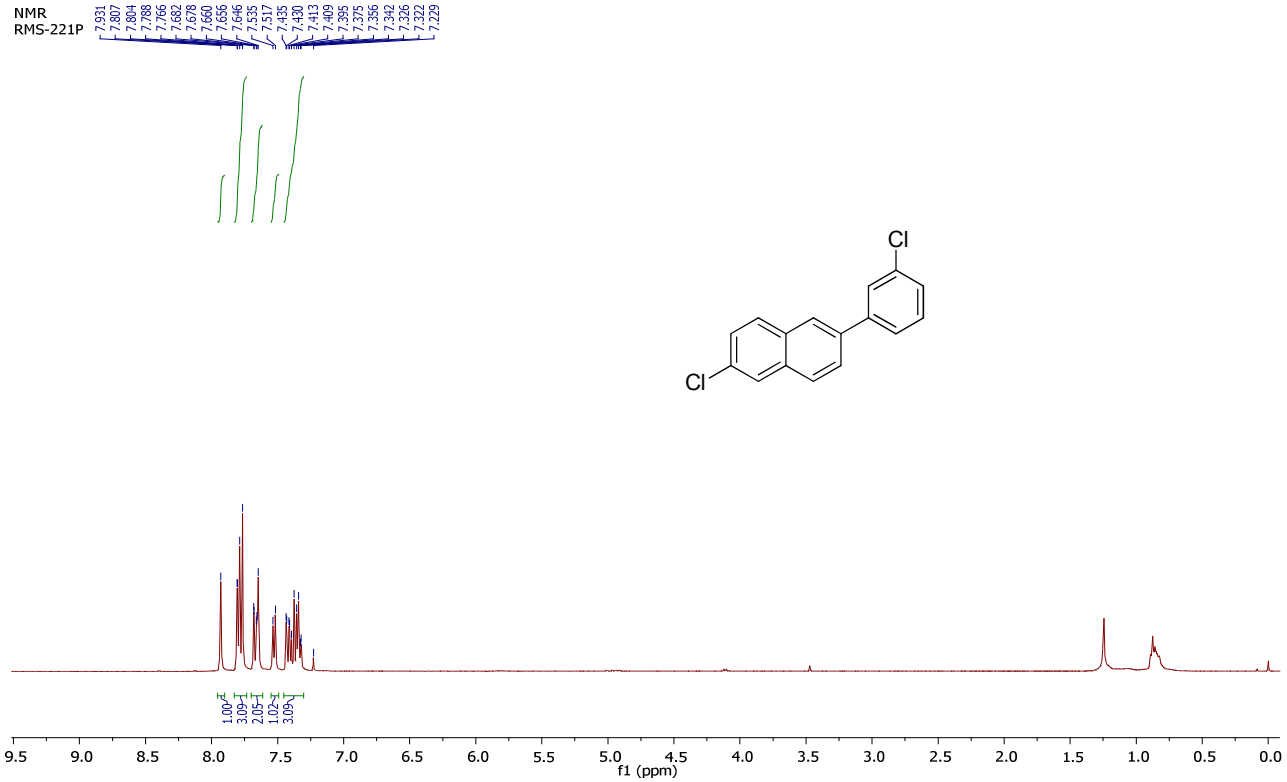
S4.13. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(o-tolyl)-5-methylnaphthalene (**2m**)

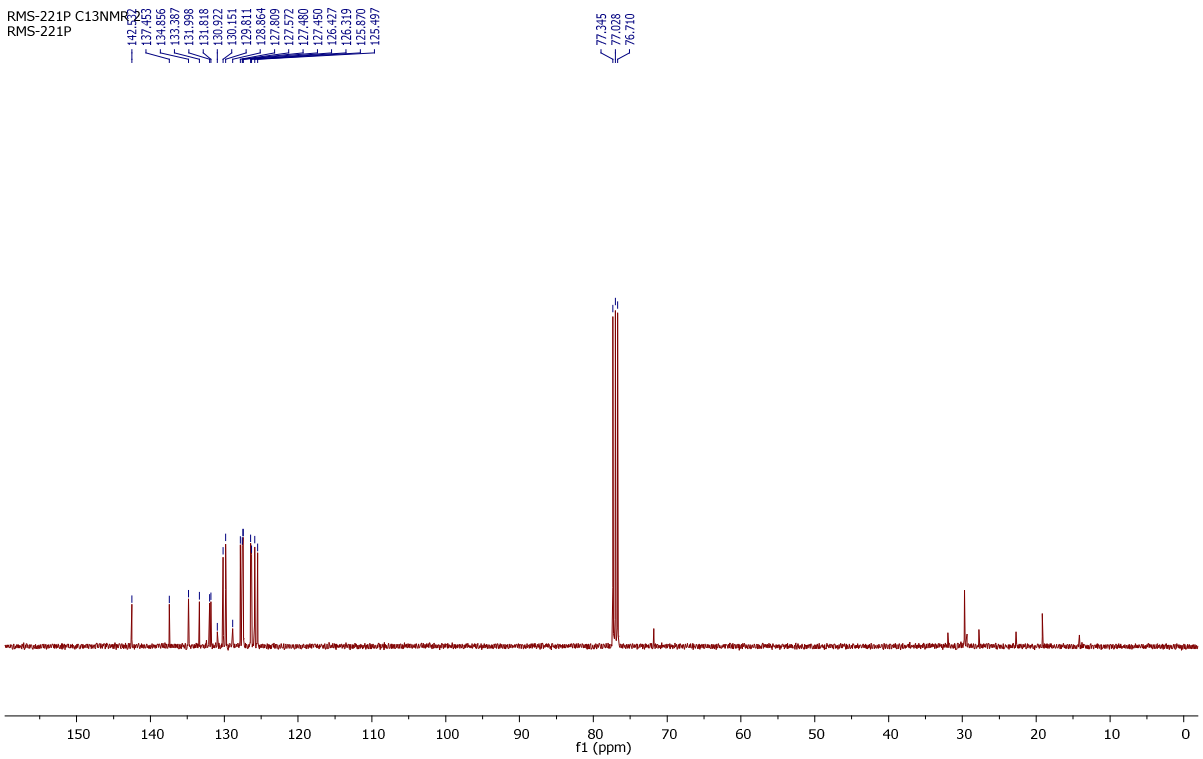


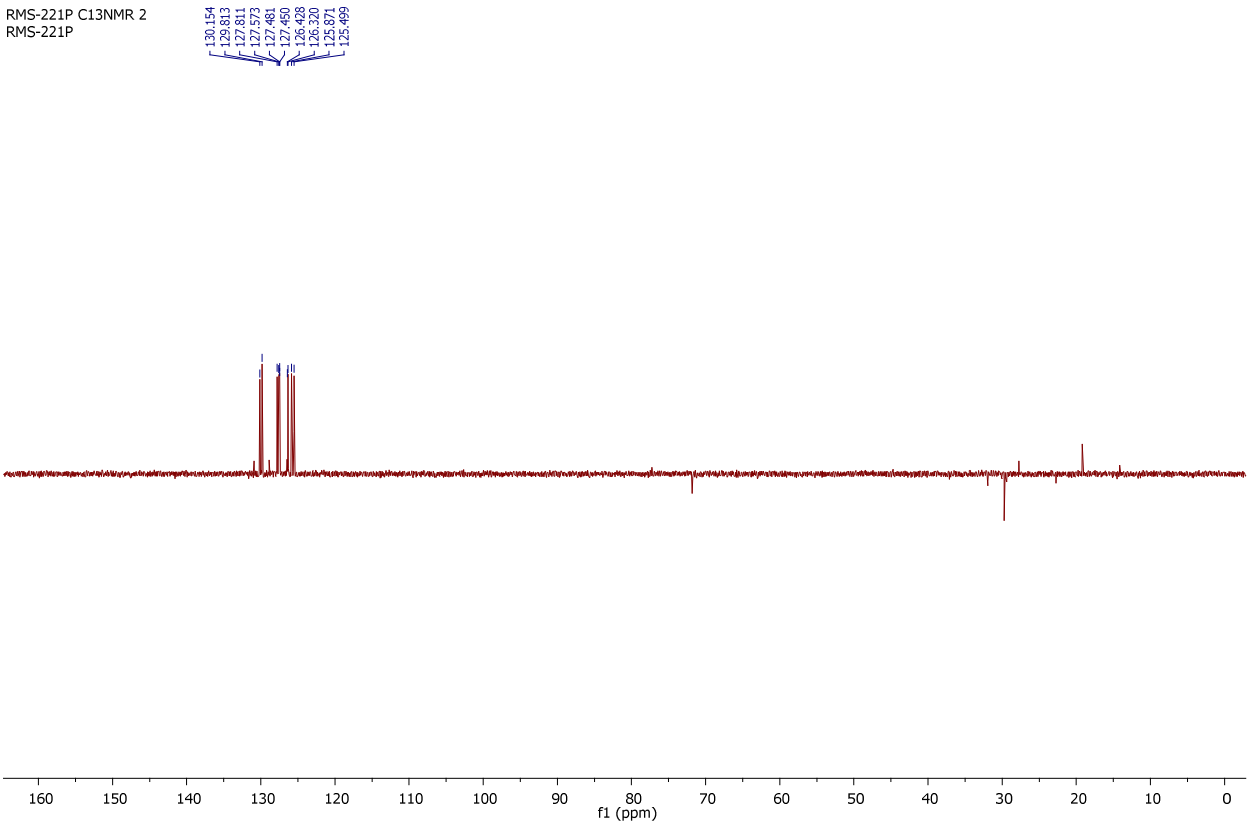

RMS-245P 1H & 13C NMR
RMS-245P
141.598
139.356
135.733
134.341
133.598
131.596
130.544
130.194
128.596
127.711
127.539
126.744
126.661
126.118
126.020
123.992
77.471
77.217
76.963
20.745
19.549
f1 (ppm)


RMS-245P 1H & 13C NMR
RMS-245P
130.546
130.196
128.597
127.712
127.541
126.745
126.662
126.120
126.022
123.995
20.748
19.553
f1 (ppm)

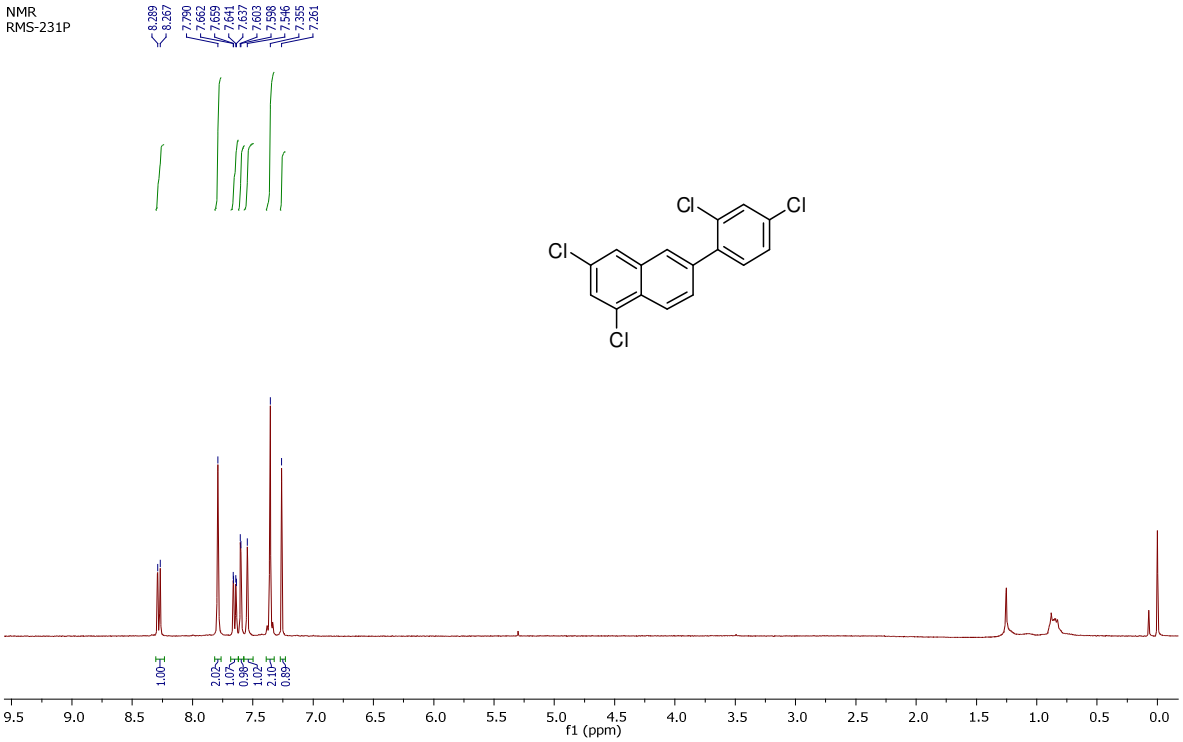
S4.14. ^{1}H, ^{13}C and DEPT135 NMR spectra of 6-chloro-2-(3′-chlorophenyl) naphthalene (**2n**)

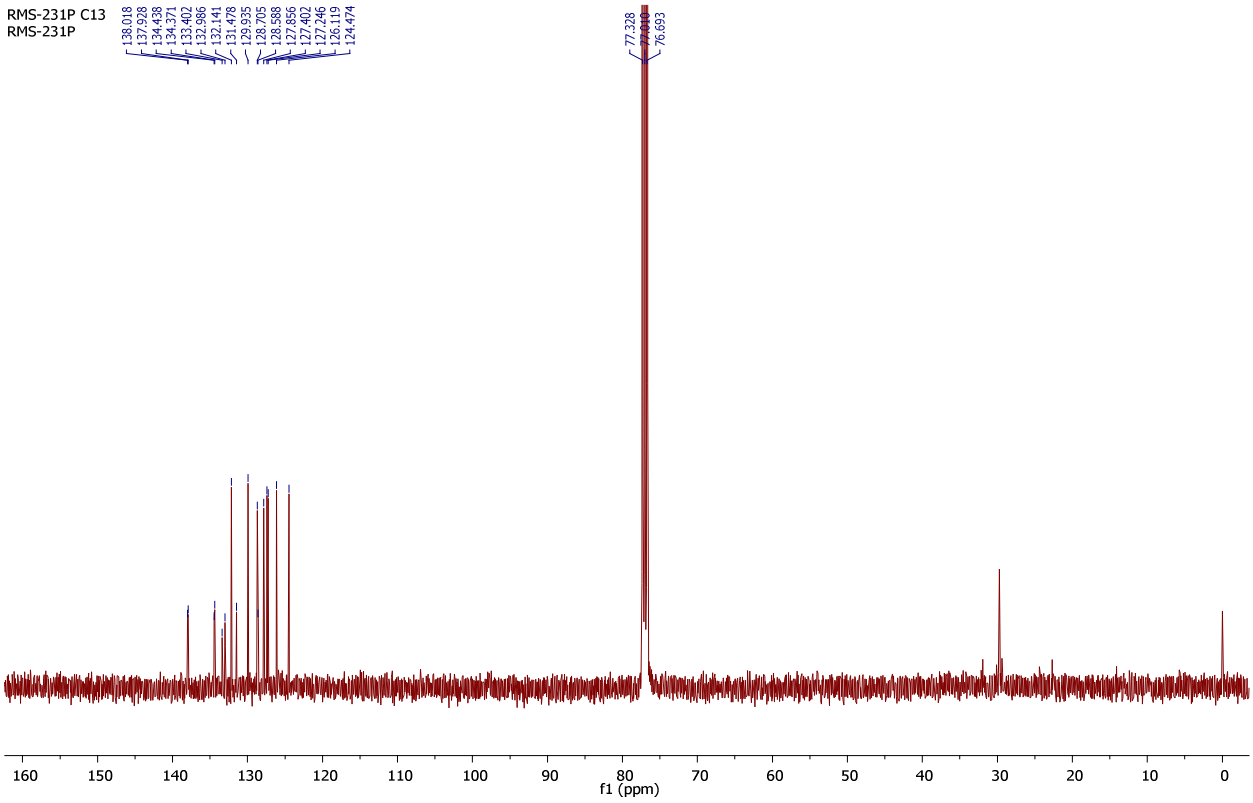


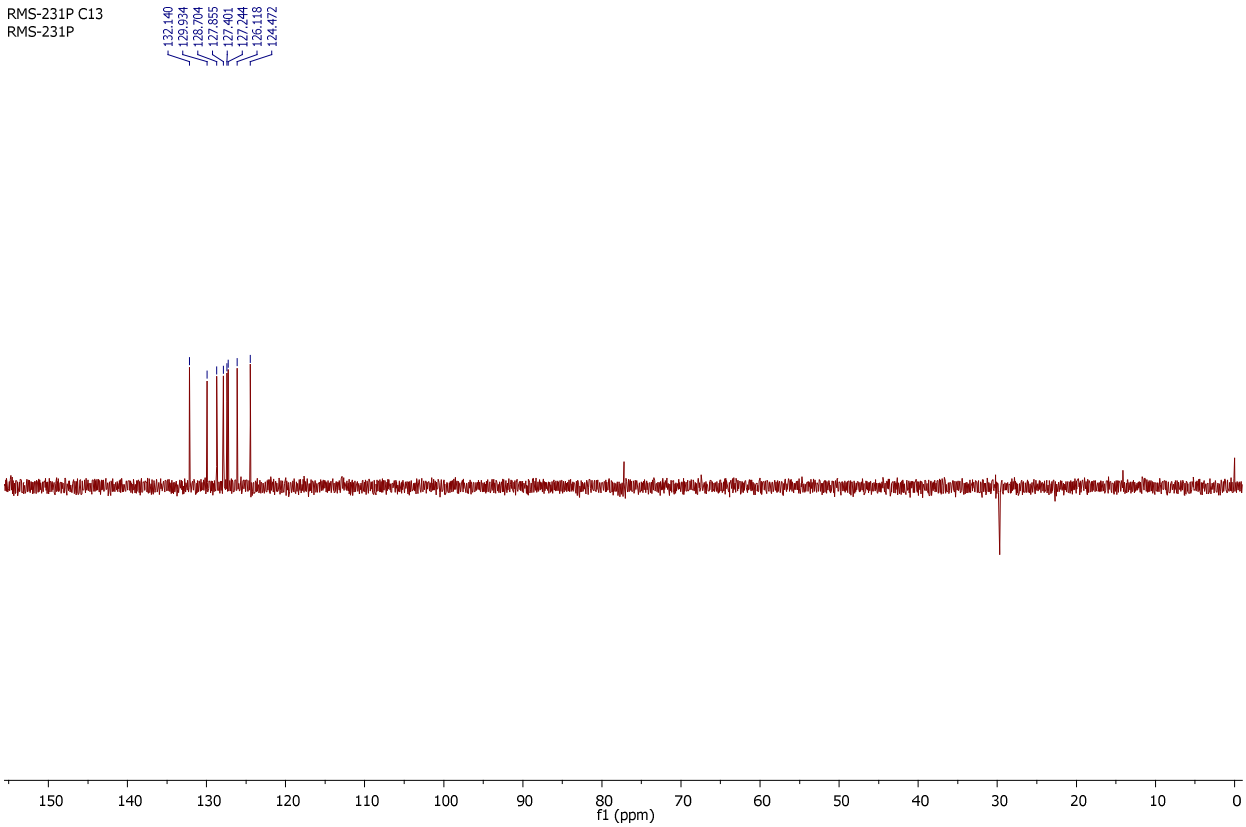




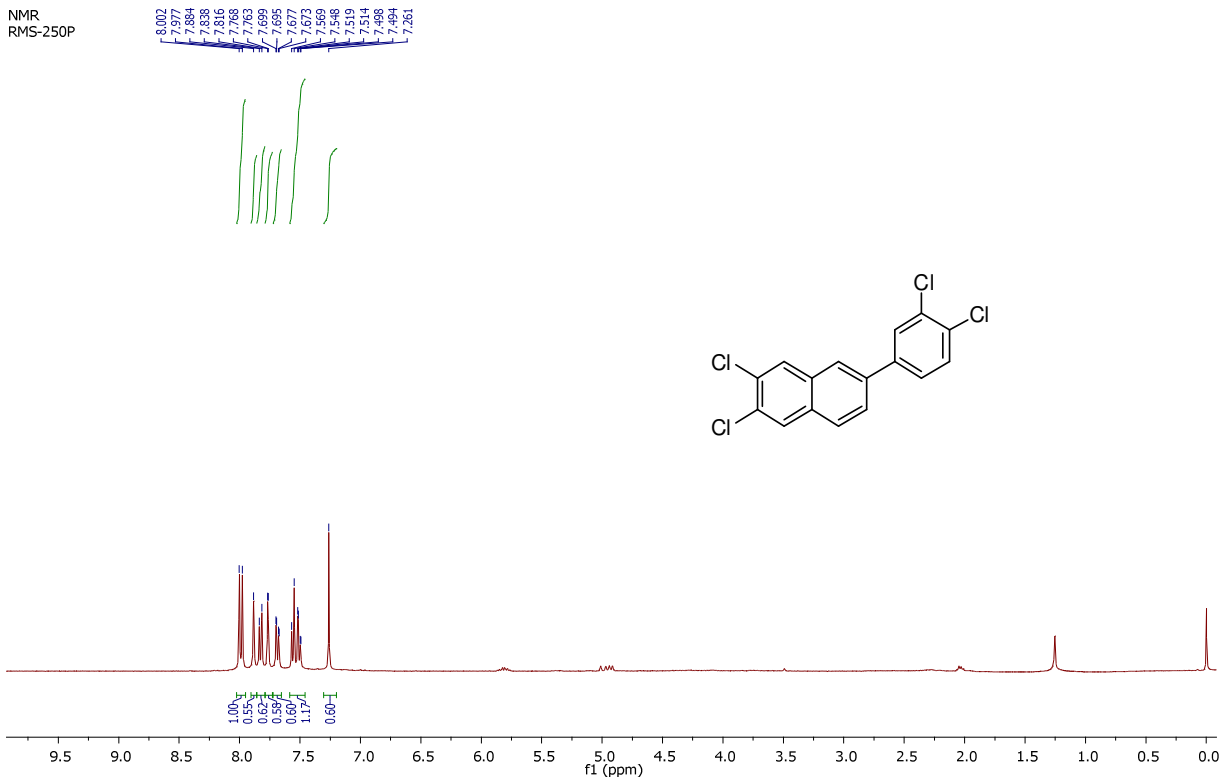
S4.15. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(2′, 4′-dichlorophenyl)-5,7-dichloronaphthalene (**2o**)

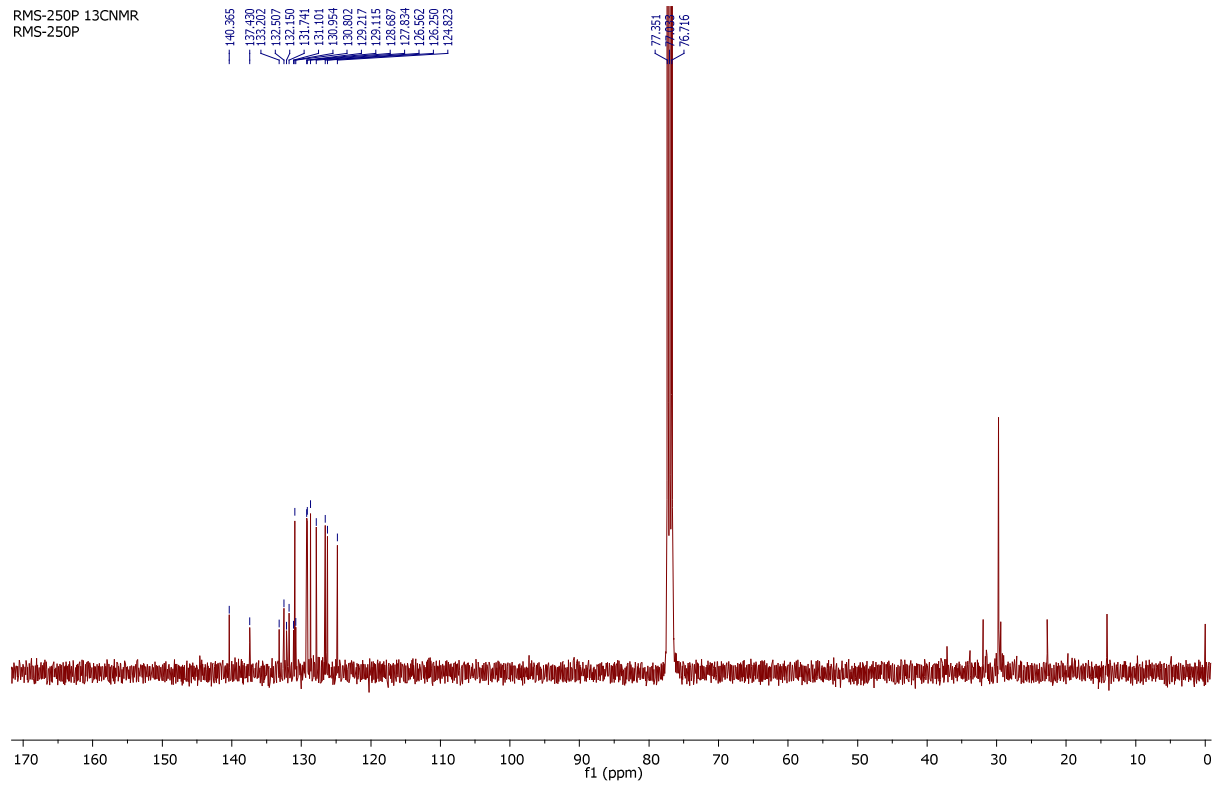


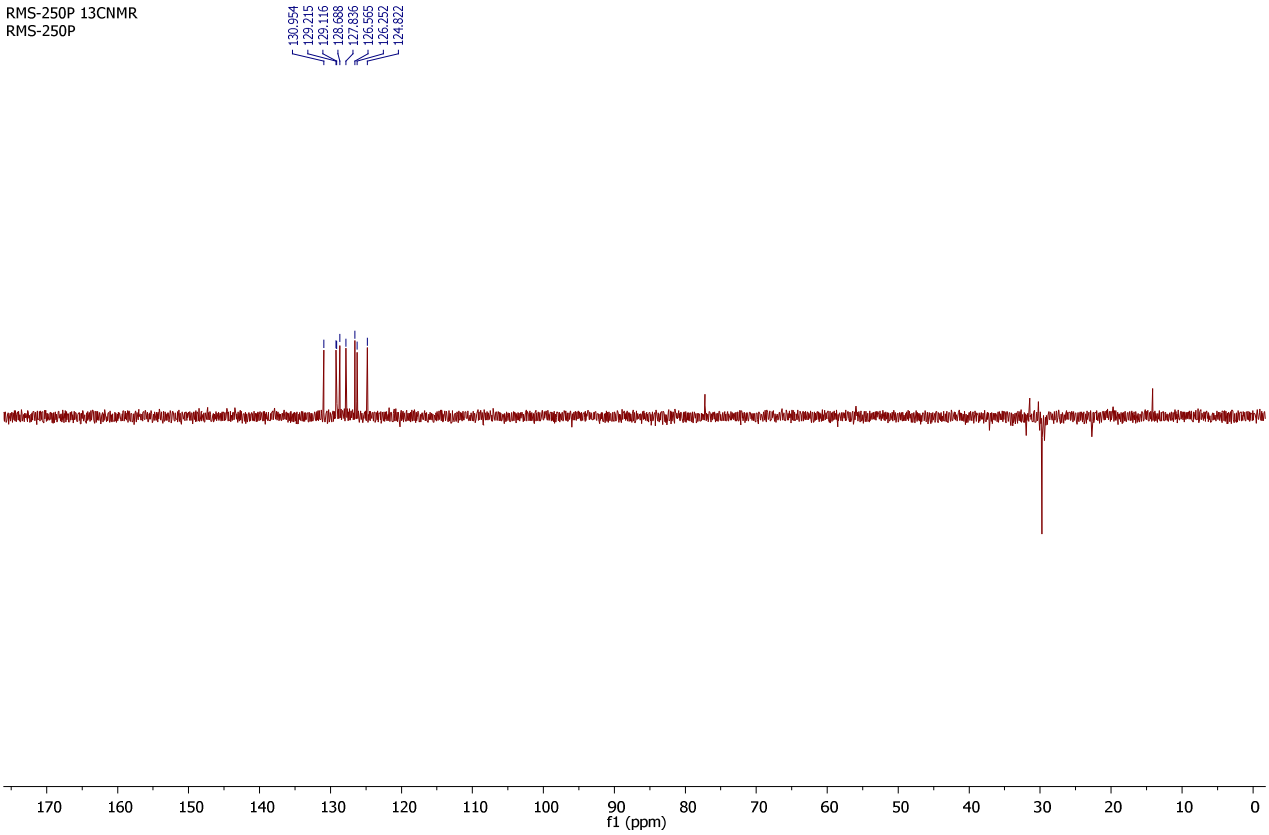

RMS-231P C13
RMS-231P
138.018
137.928
134.438
134.371
133.402
132.986
132.141
131.478
129.935
128.705
128.588
127.855
127.402
127.246
126.119
124.474
77.328
77.010
76.693
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


RMS-231P C13
RMS-231P
132.140
129.934
128.704
127.855
127.401
127.244
126.118
124.472
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

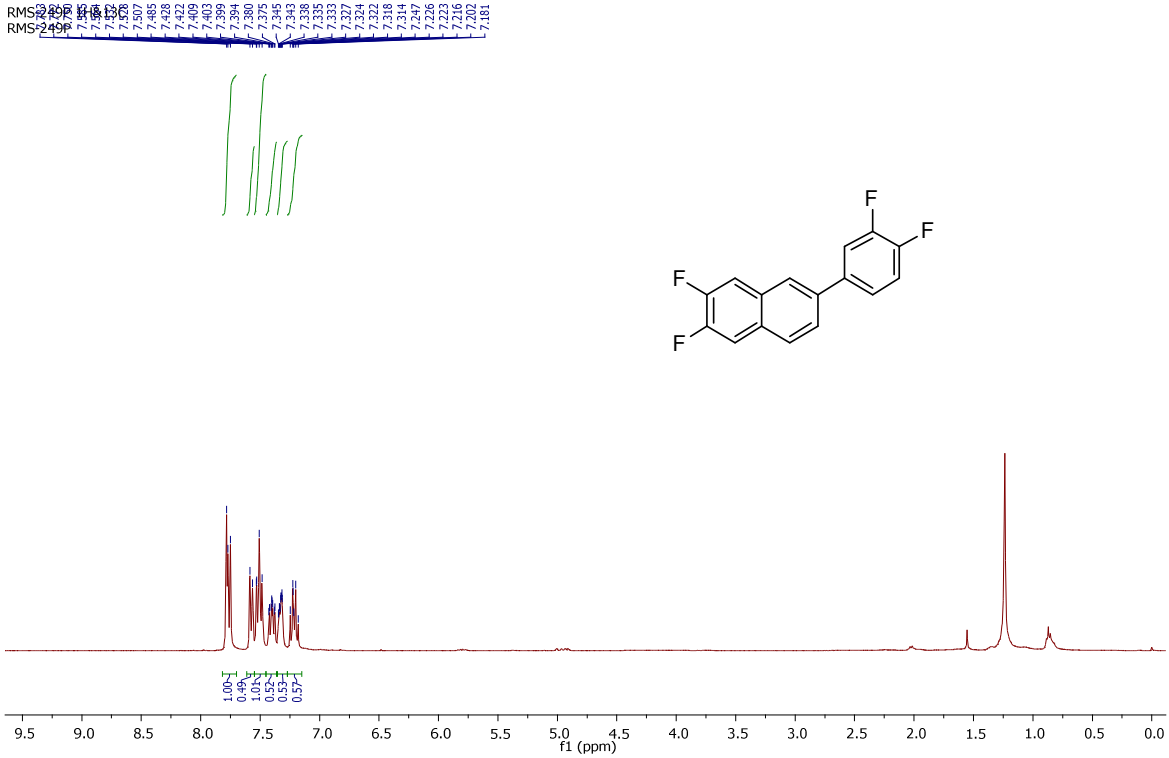
S4.16. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(3′,4′-dichlorophenyl)- 6,7-dichloronaphthalene (**2p**)

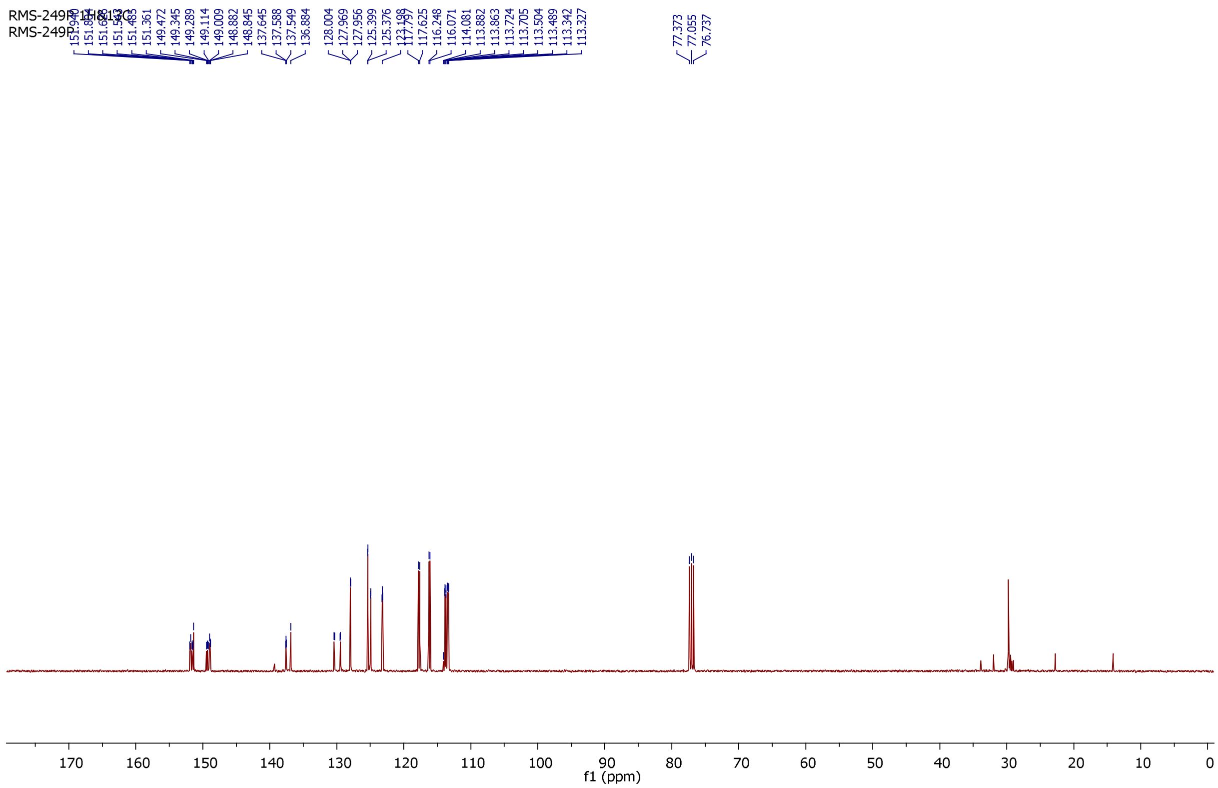


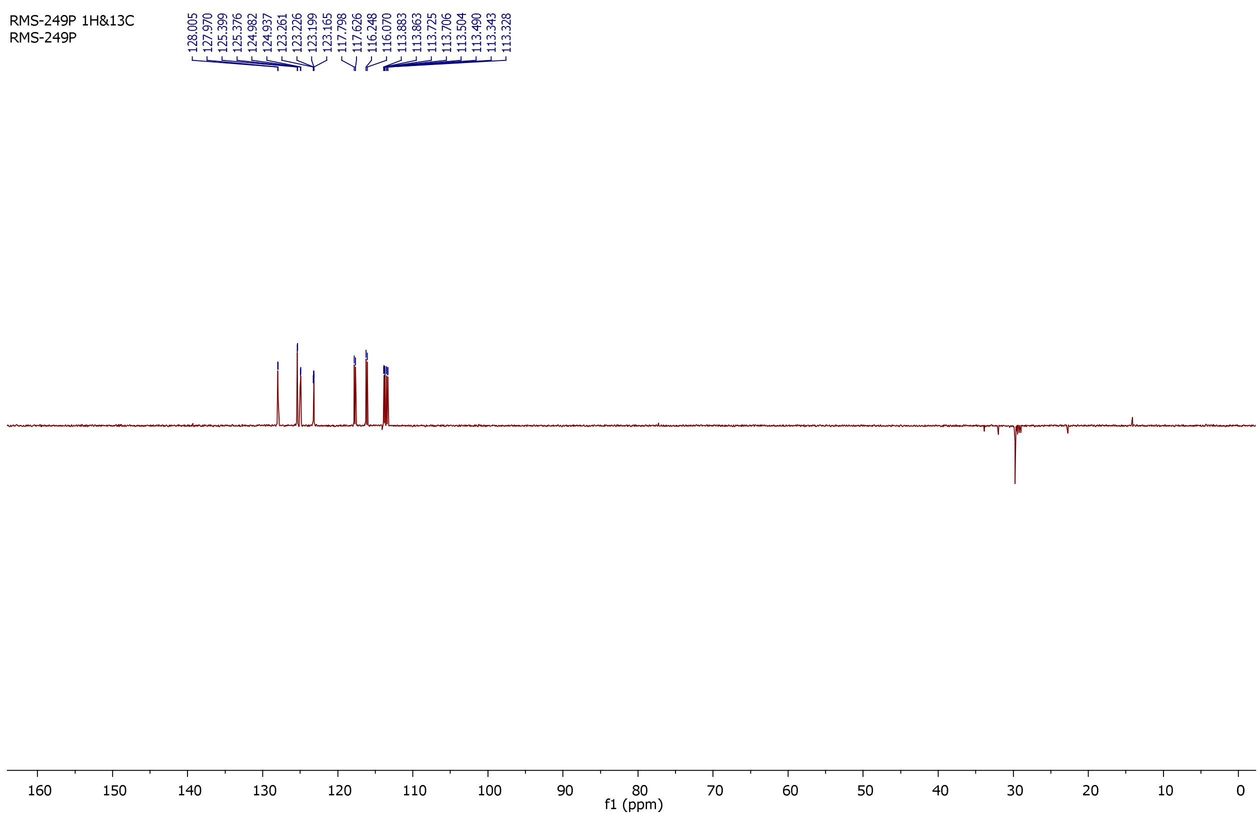


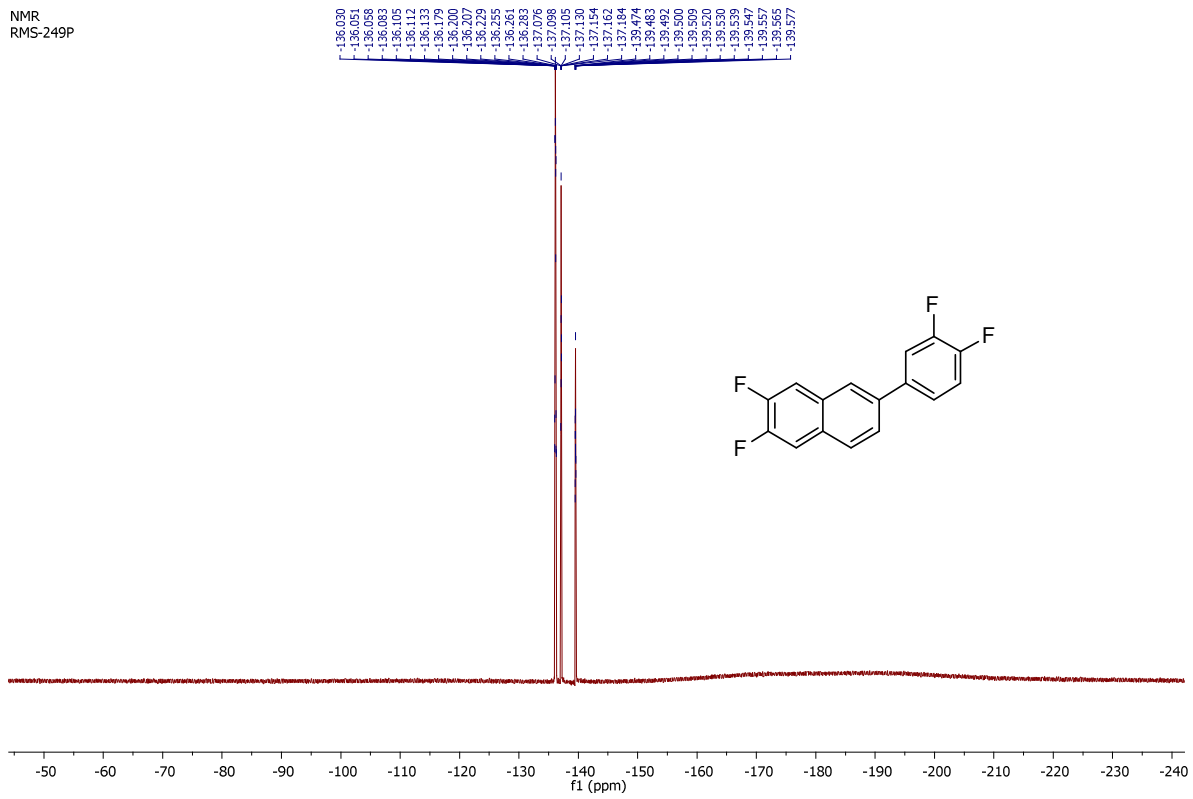


S4.17. ^{1}H, ^{13}C, DEPT135 and ^{19}F NMR spectra of 2-(3′,4′-difluorophenyl)-6,7-difluoronaphthalene (**2q**)

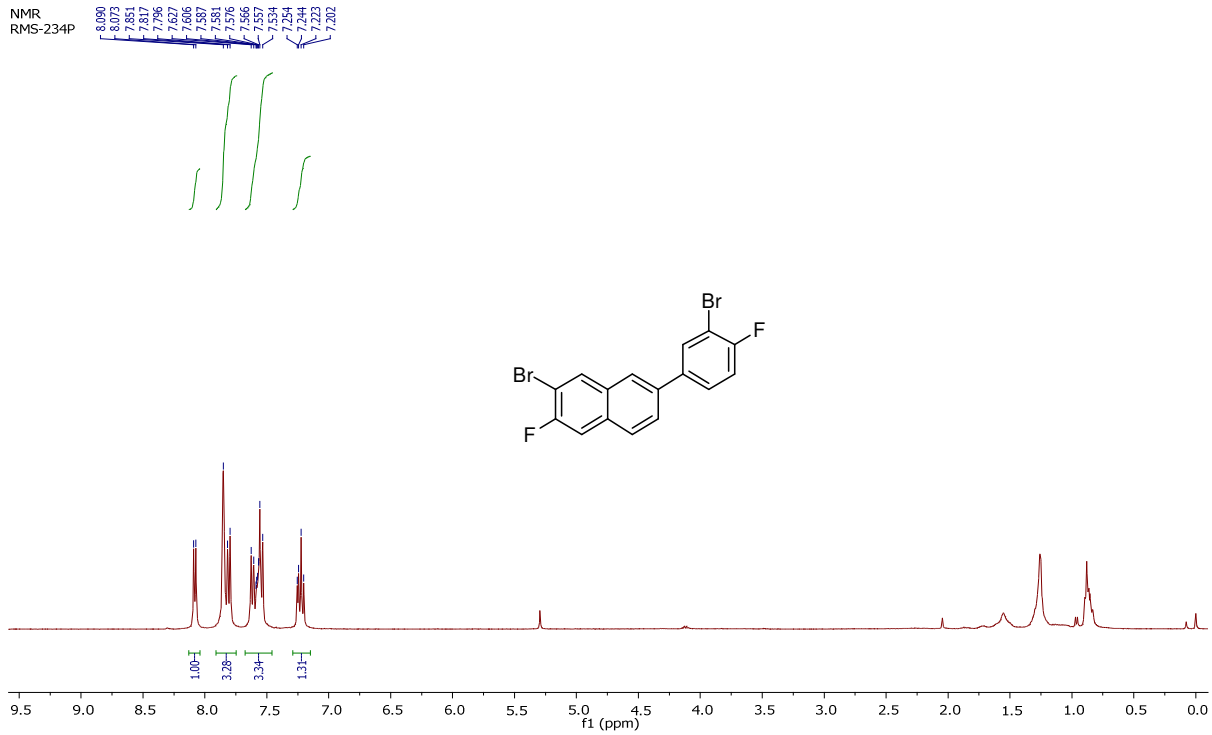


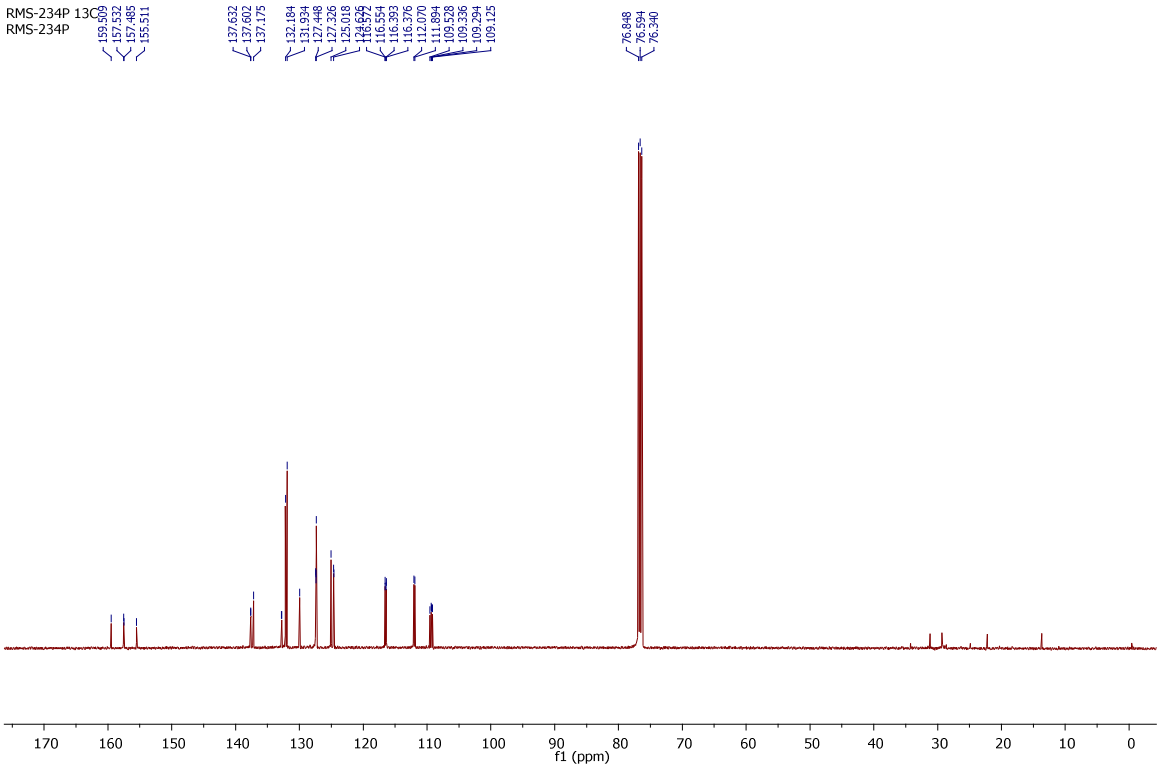

RMS-249P 1H&13C
RMS-249P
151.361
149.472
149.345
149.289
149.114
149.009
148.882
148.845
137.645
137.588
137.549
136.884
128.004
127.969
127.956
125.399
125.376
117.625
116.248
116.071
114.081
113.882
113.863
113.724
113.705
113.504
113.489
113.342
113.327
77.373
77.055
76.737
f1 (ppm)

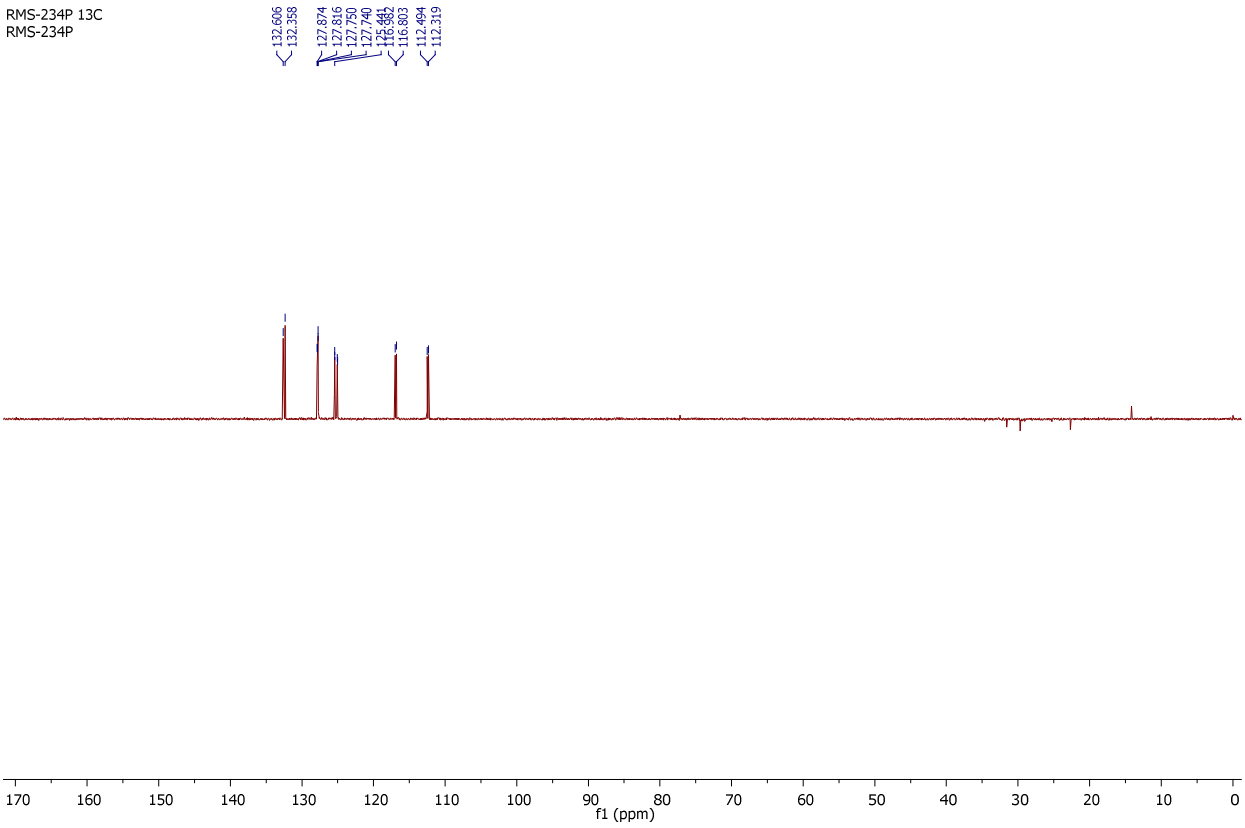

RMS-249P 1H&13C
RMS-249P
128.005
127.970
125.399
125.376
124.982
124.937
123.261
123.226
123.199
123.165
117.798
117.626
116.248
116.070
113.883
113.863
113.725
113.706
113.504
113.490
113.343
113.328
f1 (ppm)

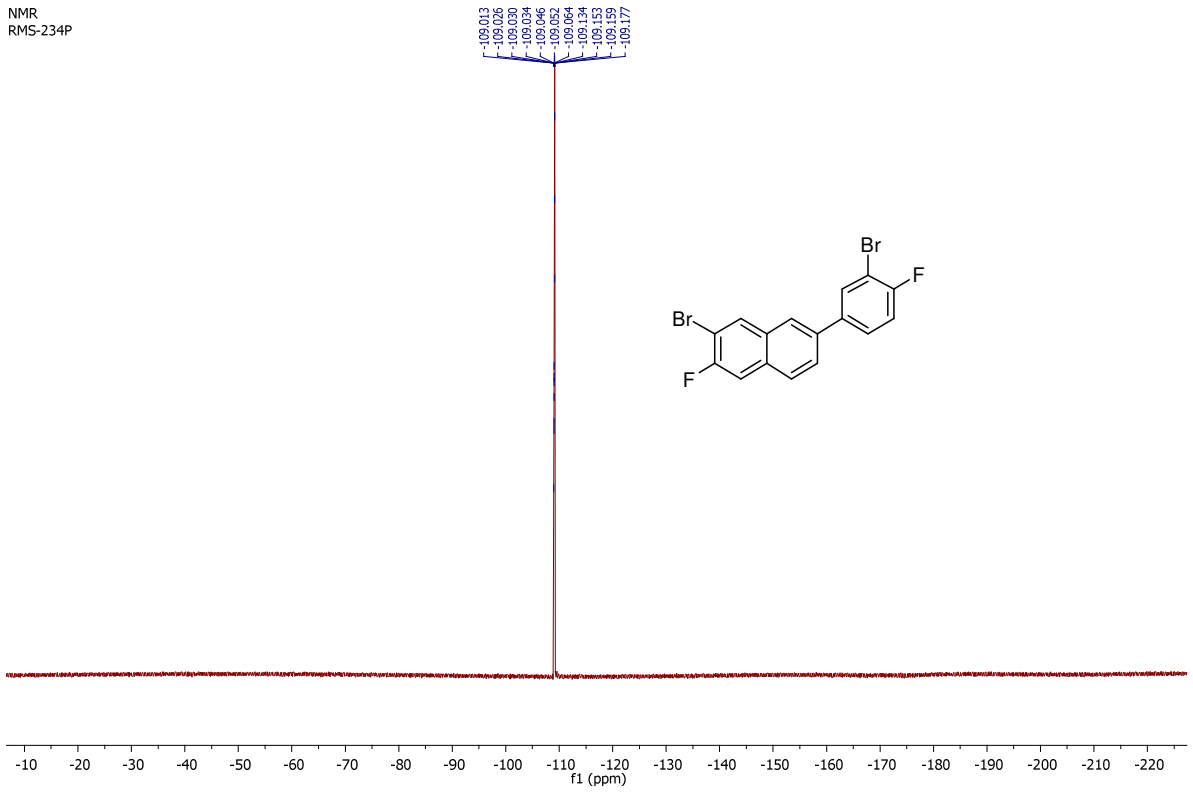


S4.18. ^{1}H, ^{13}C, DEPT135 and ^{19}F NMR spectra of 2-(3′-bromo-4′-fluorophenyl)-6-bromo-7-fluoronaphthalene (**2r**)

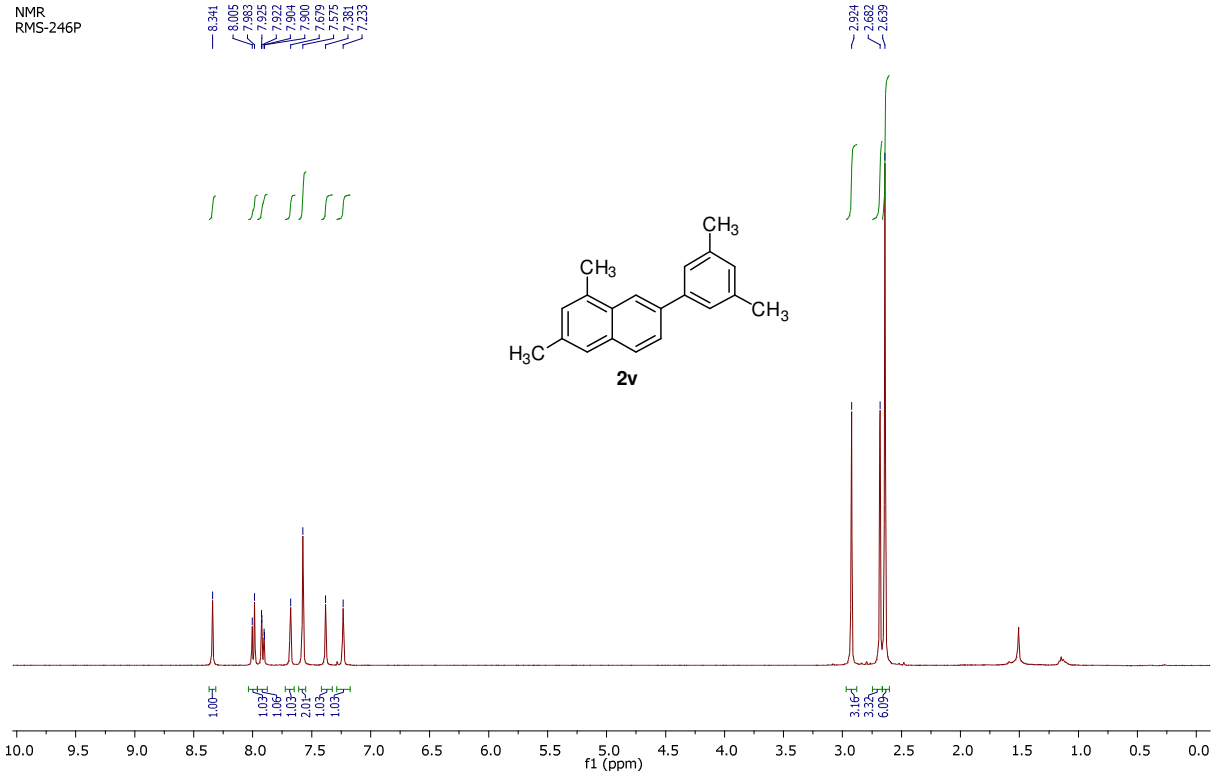



RMS-234P 13C
RMS-234P
159.509
157.532
157.485
155.511
137.632
137.602
137.175
132.184
131.934
127.448
127.326
125.018
116.554
116.393
116.376
112.070
111.894
109.528
109.336
109.294
109.125
76.848
76.594
76.340
f1 (ppm)


RMS-234P 13C
RMS-234P
132.606
132.358
127.874
127.816
127.750
127.740
116.982
116.803
112.494
112.319
f1 (ppm)



S4.19. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(3′,5′dimethylphenyl)-6,8-dimethylnaphthalene (**2s**)

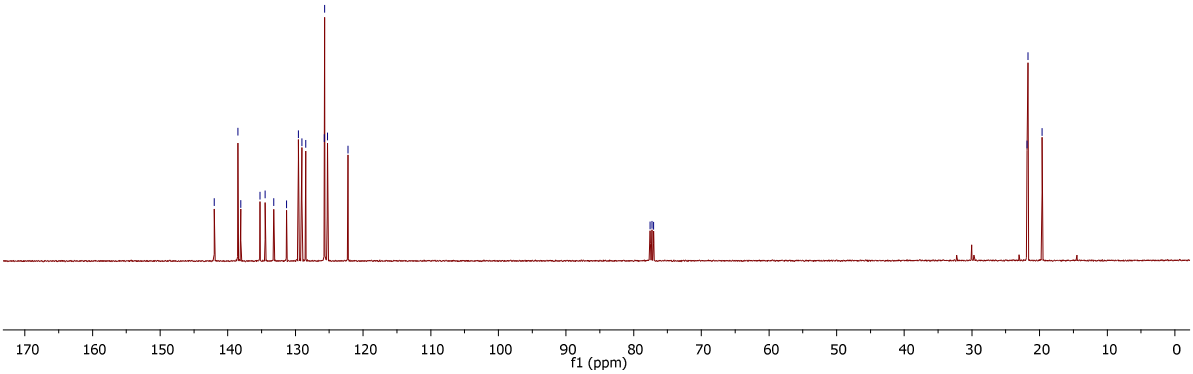


RMS-246P C13NMR
RMS-246P

141.999
138.522
138.086
135.250
134.463
133.223
131.319
129.550
129.065
128.490
125.715
125.667
125.278
122.224

77.557
77.303
77.049

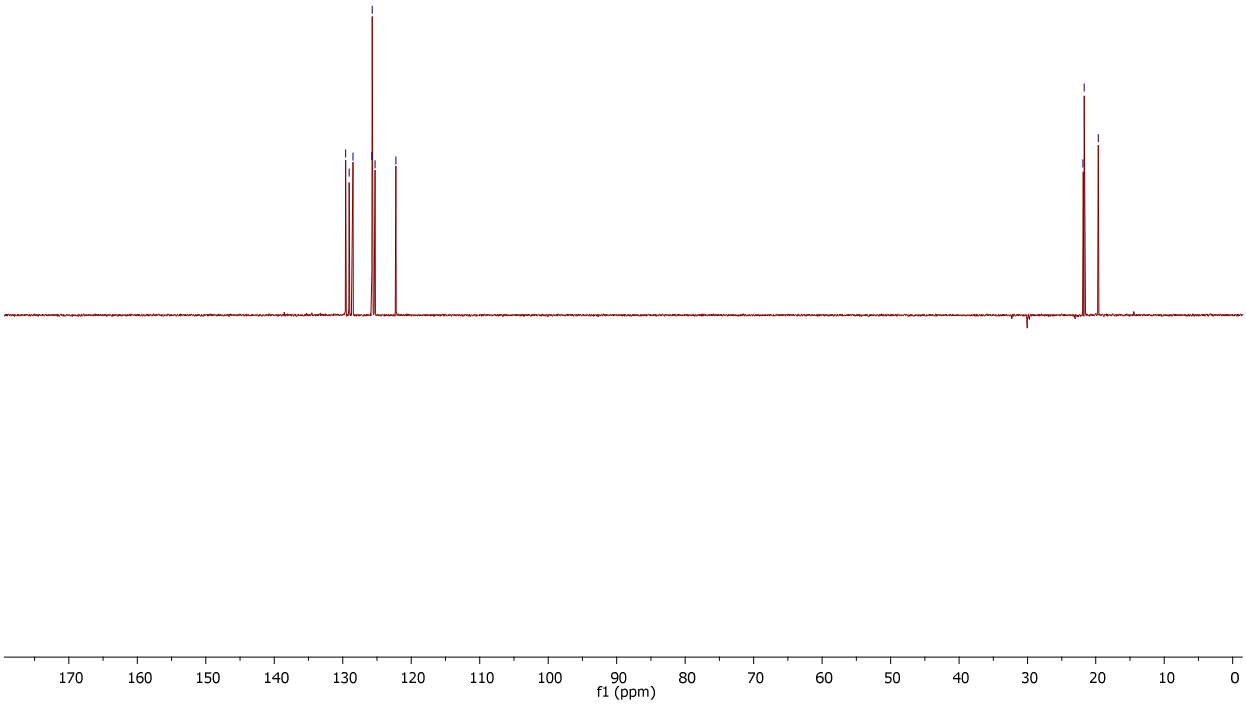
21.869
21.712
19.633



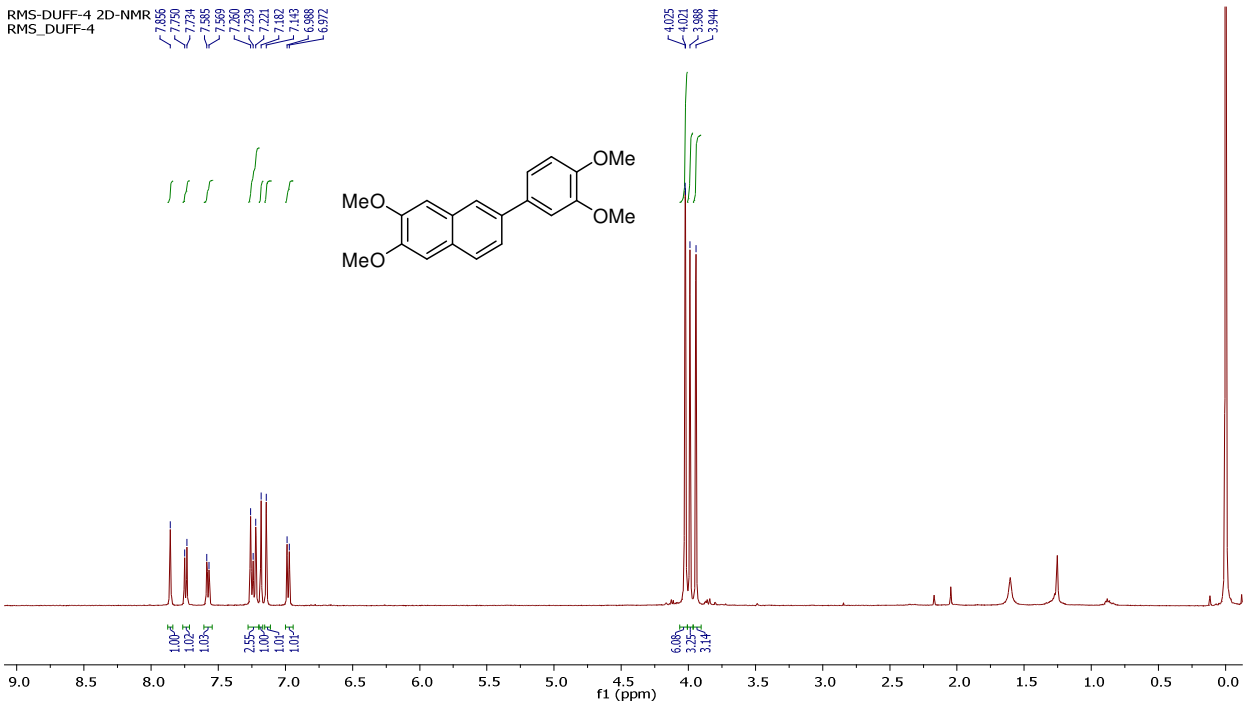
RMS-246P C13NMR
RMS-246P

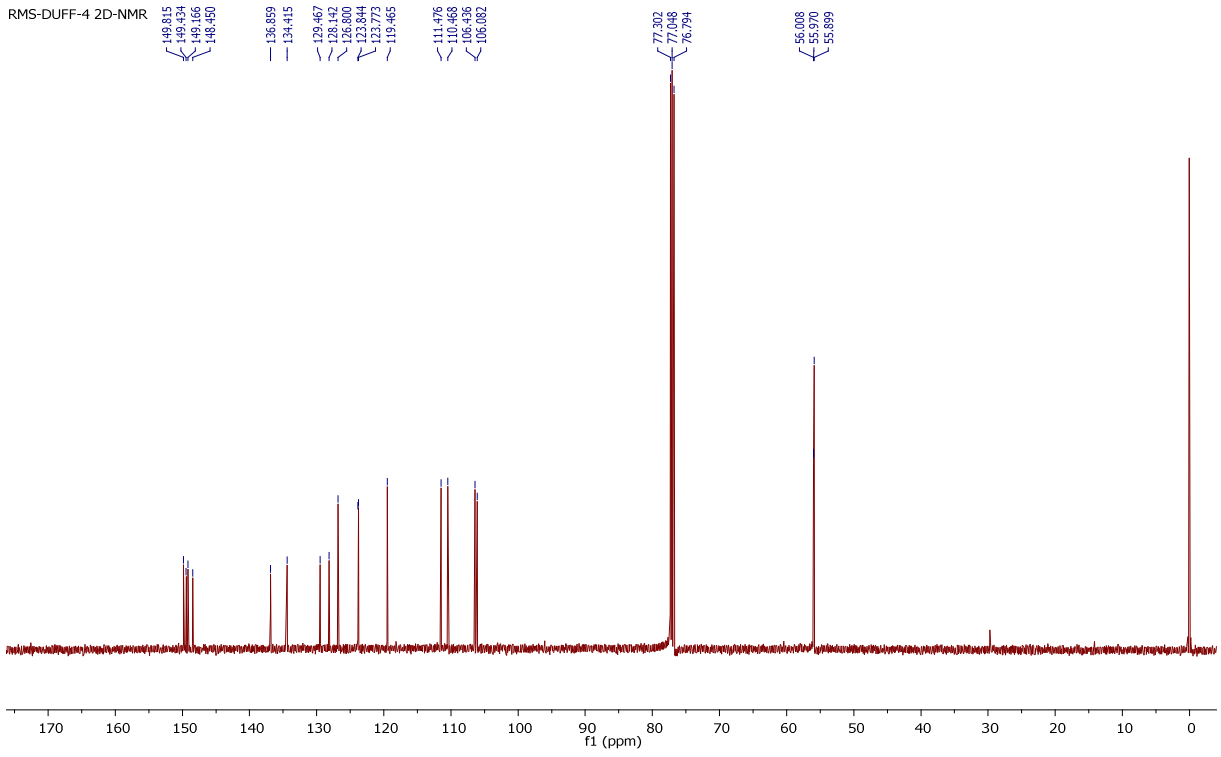
129.552
129.066
128.492
125.715
125.668
125.279
122.225

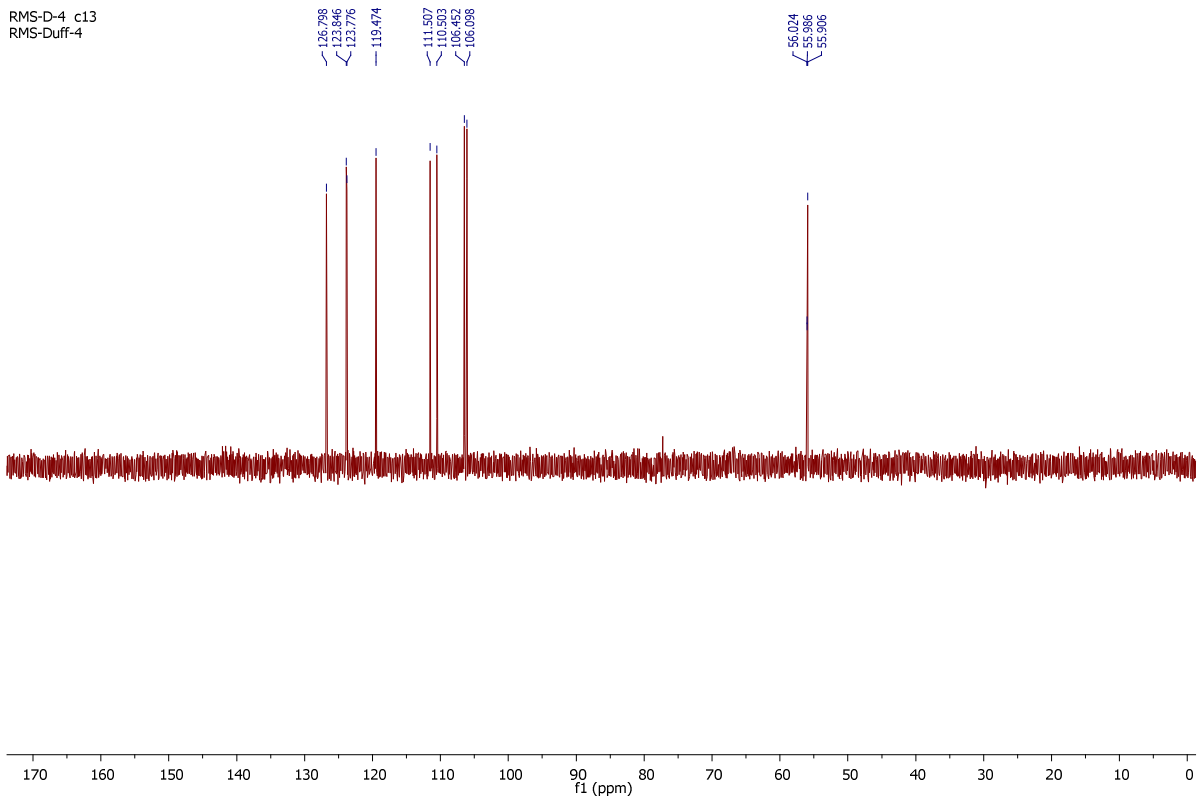
21.870
21.713
19.636



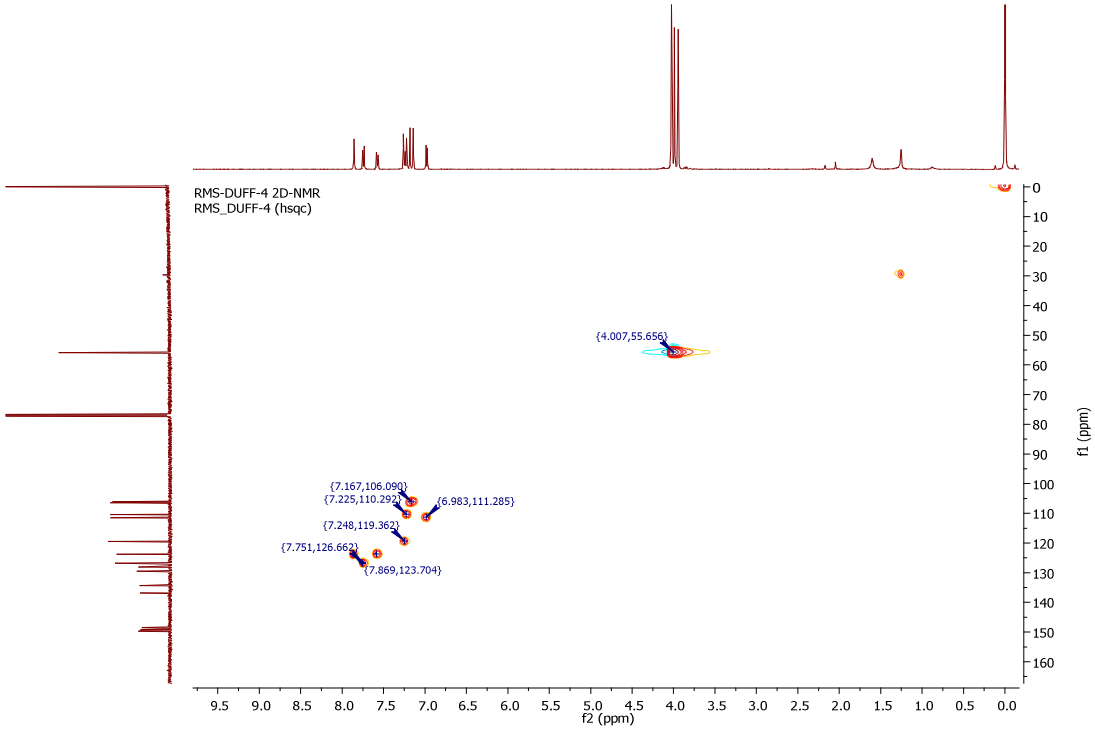
S4.20. ^{1}H, ^{13}C, DEPT135, HSQC and HMBC NMR spectra of 6-(3',4'-dimethoxyphenyl)-6,7-dimethoxynaphthalene (**2ta**).

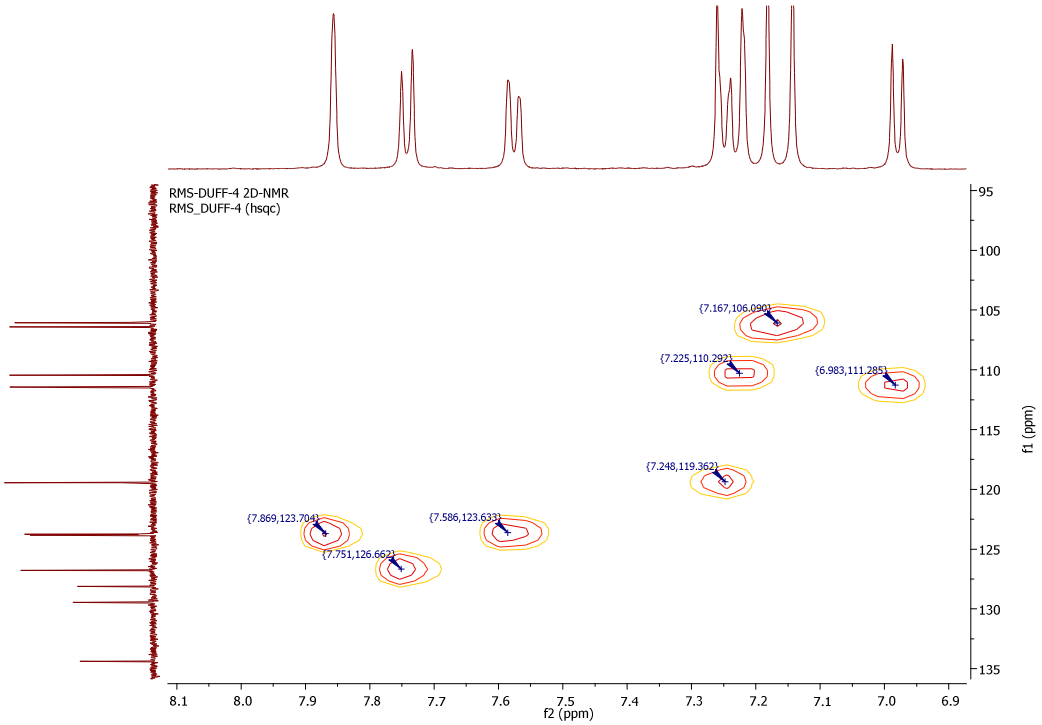




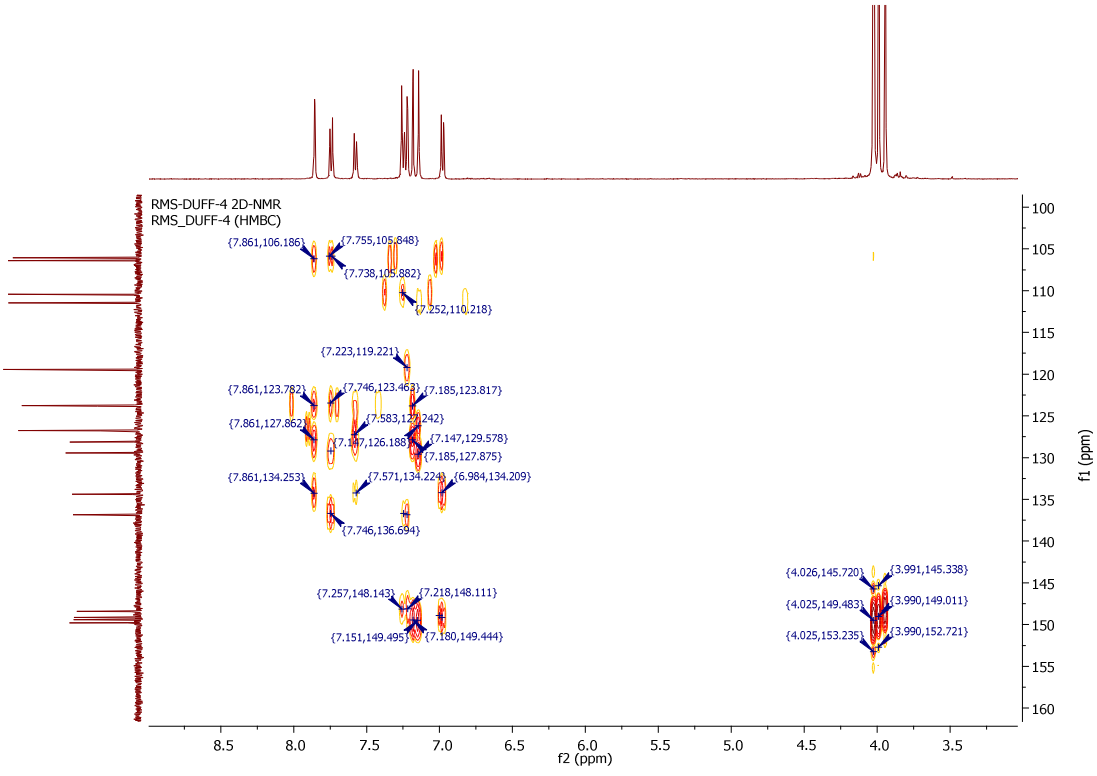


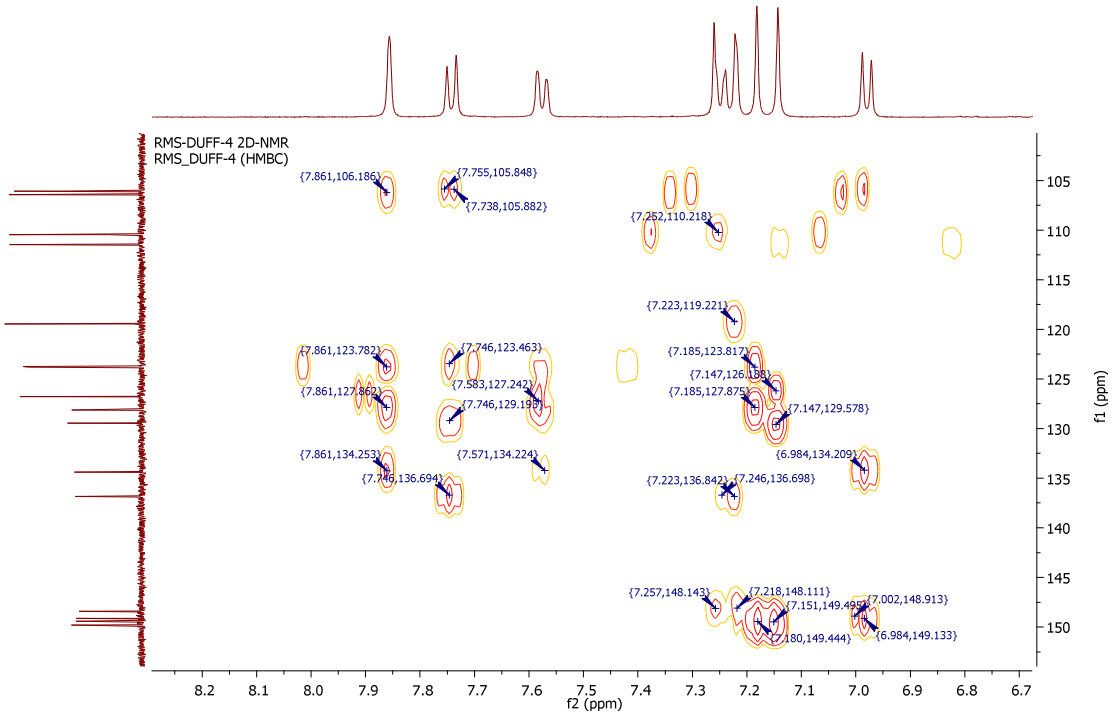
HSQC Correlations of 6-(3', 4'-dimethoxyphenyl)-2,3-dimethoxynaphthalene (**2ta**).



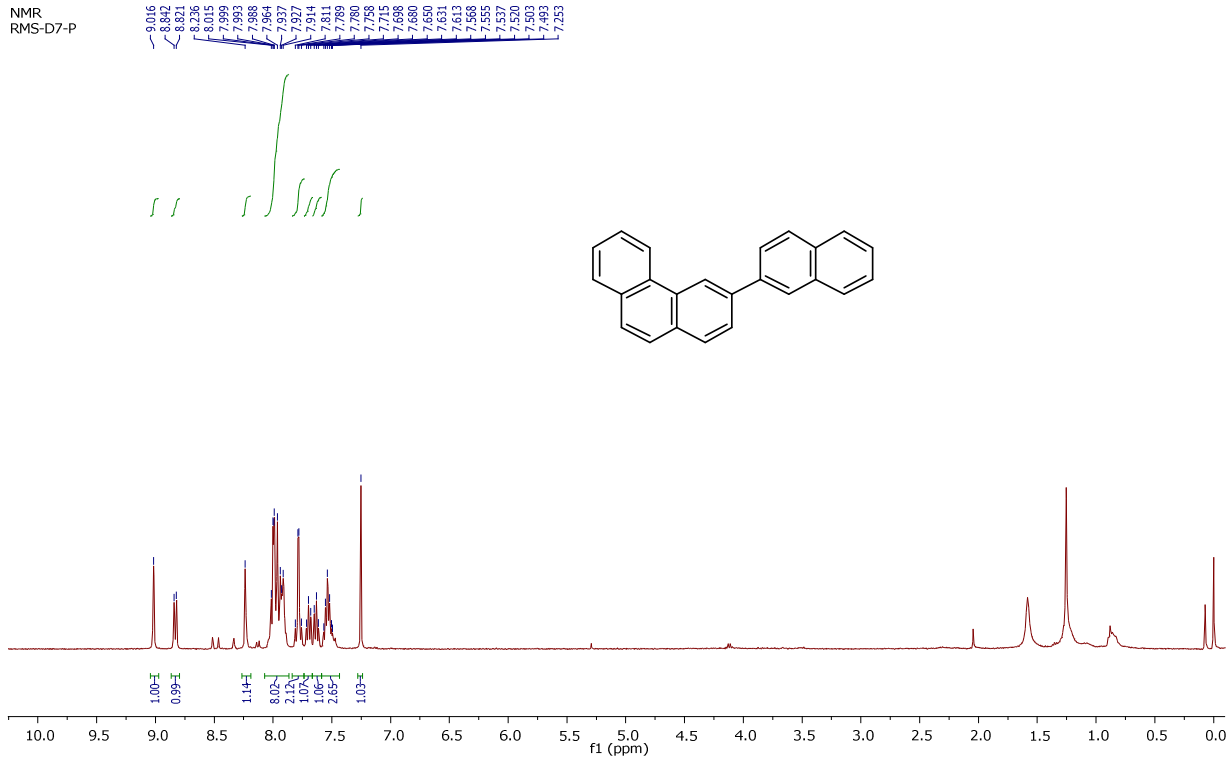


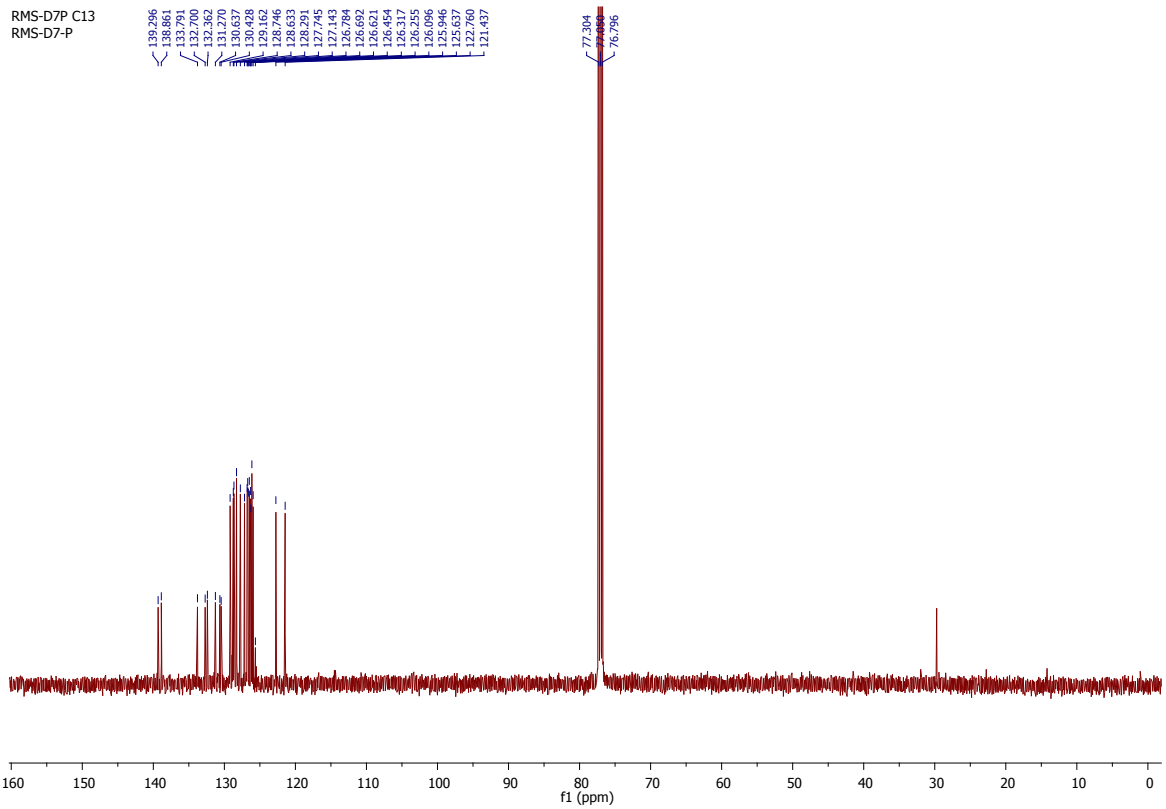
HMBC Correlations of 6-(3', 4'-dimethoxyphenyl)-2,3-dimethoxynaphthalene (**2ta**).



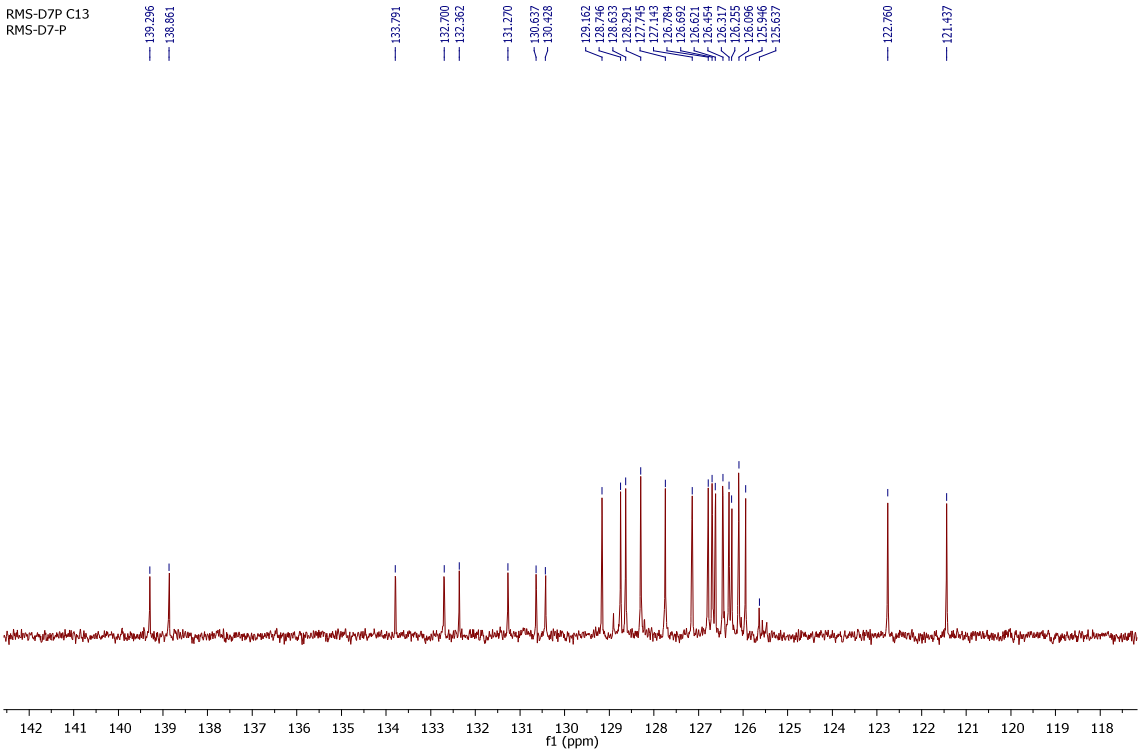


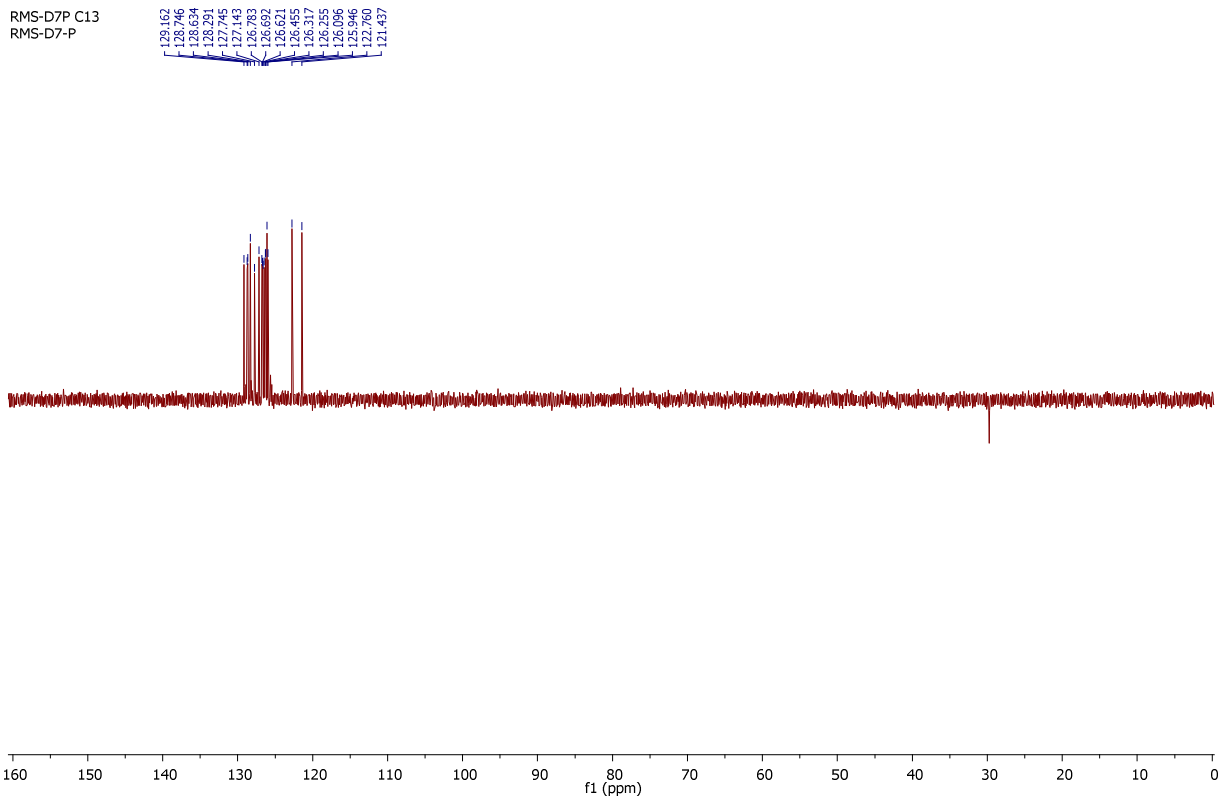
S4.21. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(naphthalen-2′-yl) phenanthrene (**2u**)





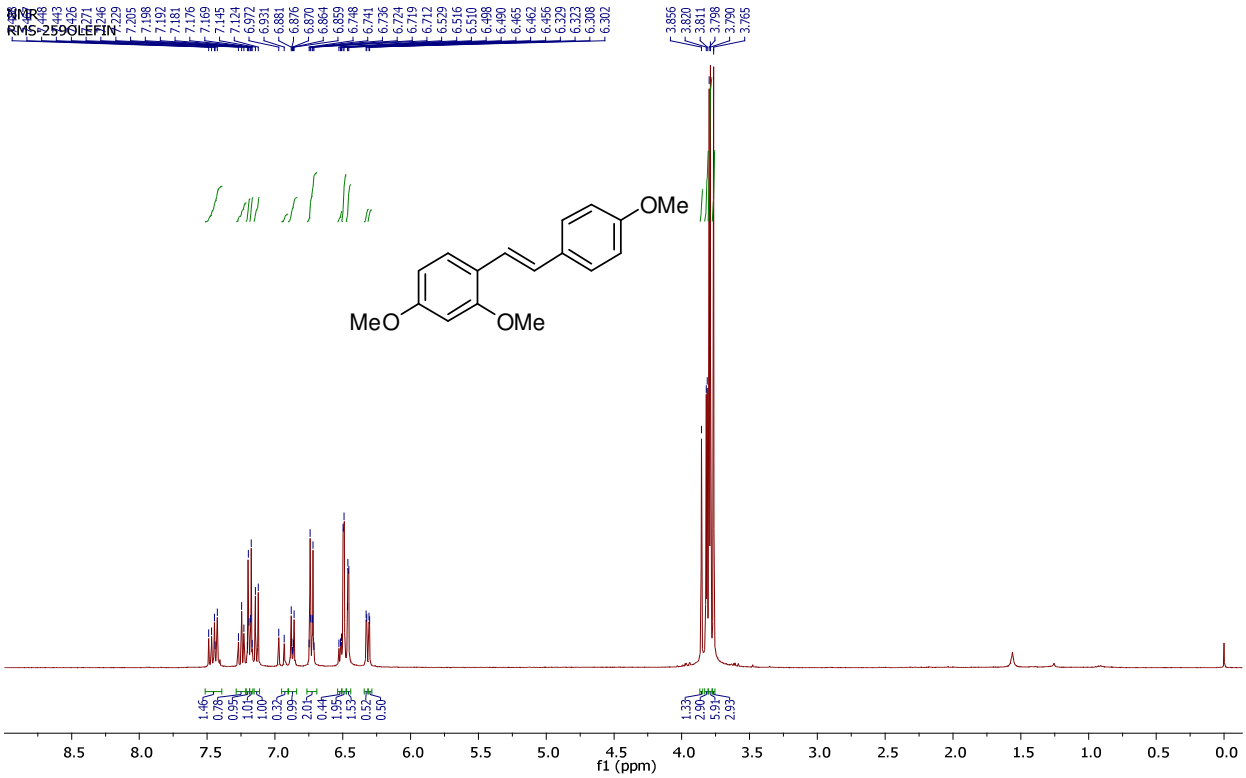
^{13}C-NMR Expantion of **2u**

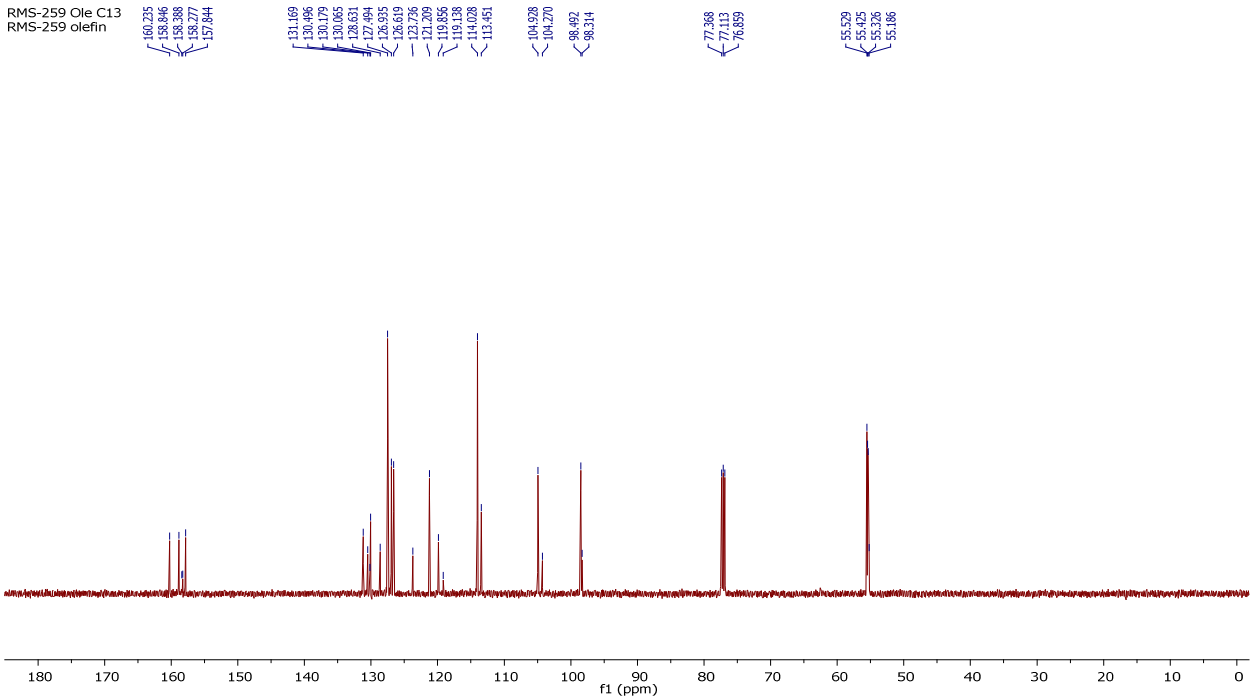


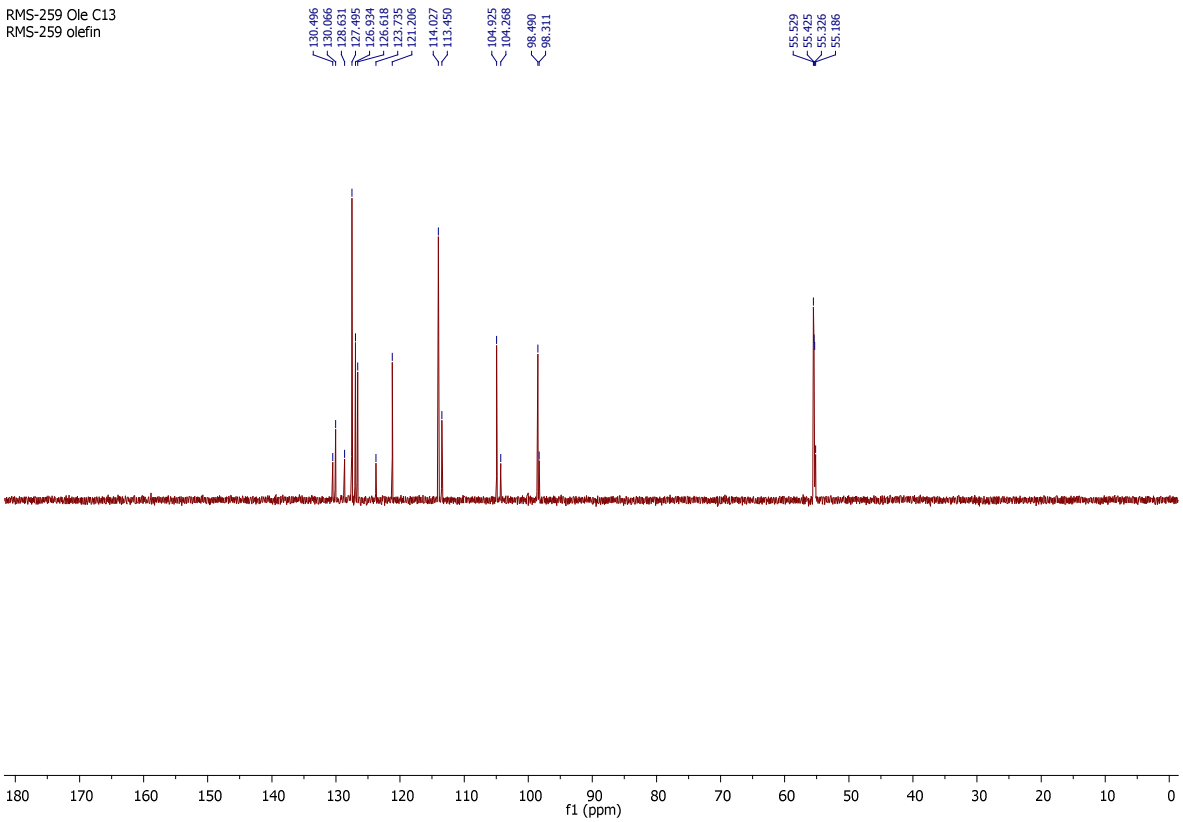

RMS-D7P C13
RMS-D7-P
129.162
128.746
128.634
128.291
127.745
127.143
126.783
126.692
126.621
126.455
126.317
126.255
126.096
125.946
122.760
121.437
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

S5. NMR spectra scans of ER-β agonist 2vh and its intermediates 1aa, 2vm

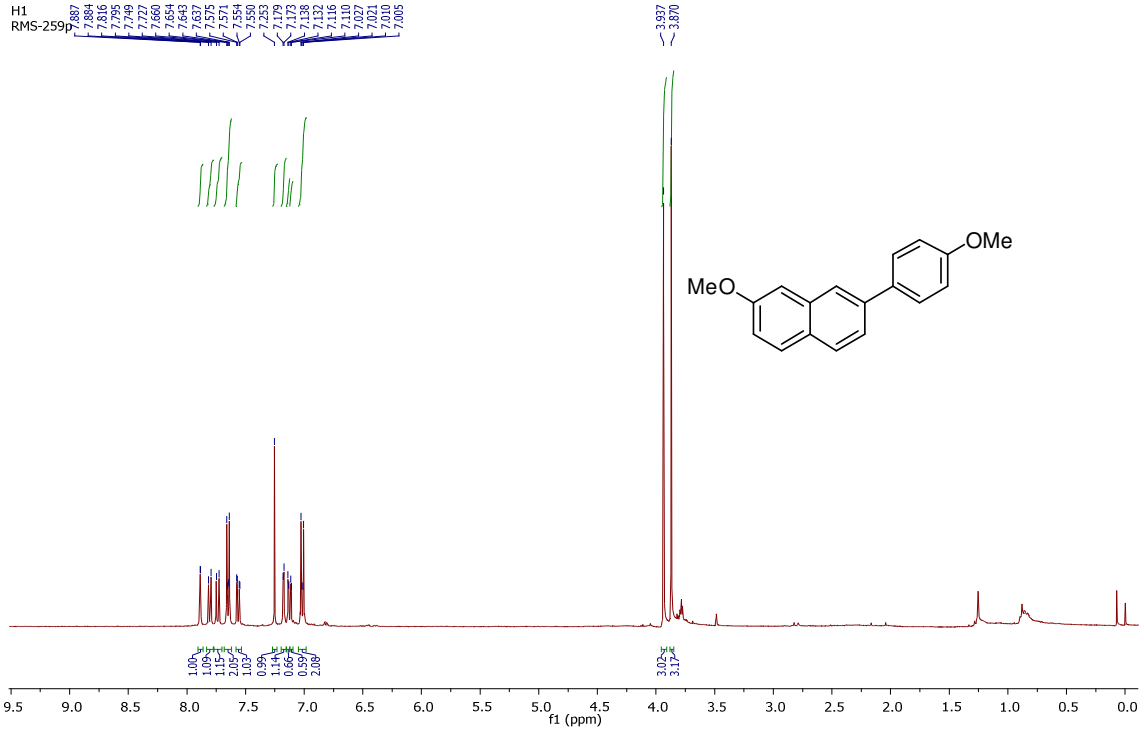
S5.1.^{1}H, ^{13}C and DEPT135 NMR spectra of (E,Z)-1-(4′-methoxystyryl)-2,4-dimethoxybenzene (**1aa**)

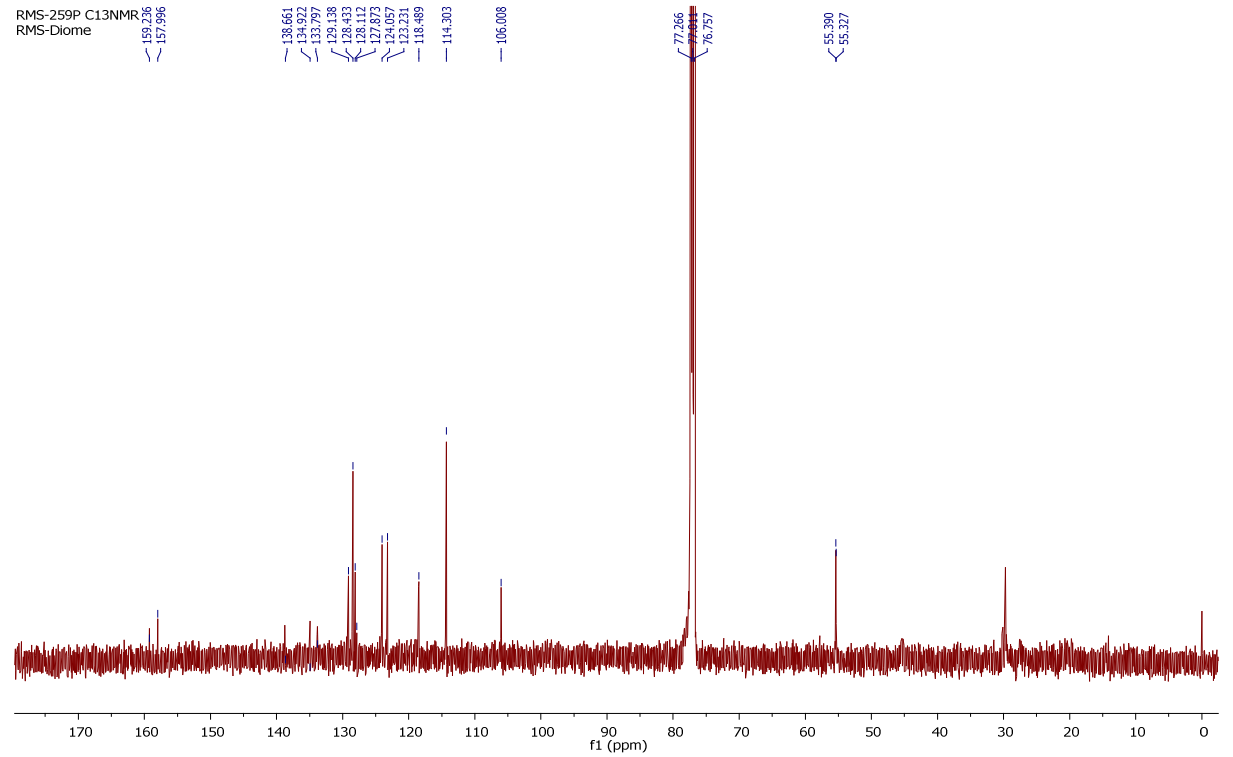


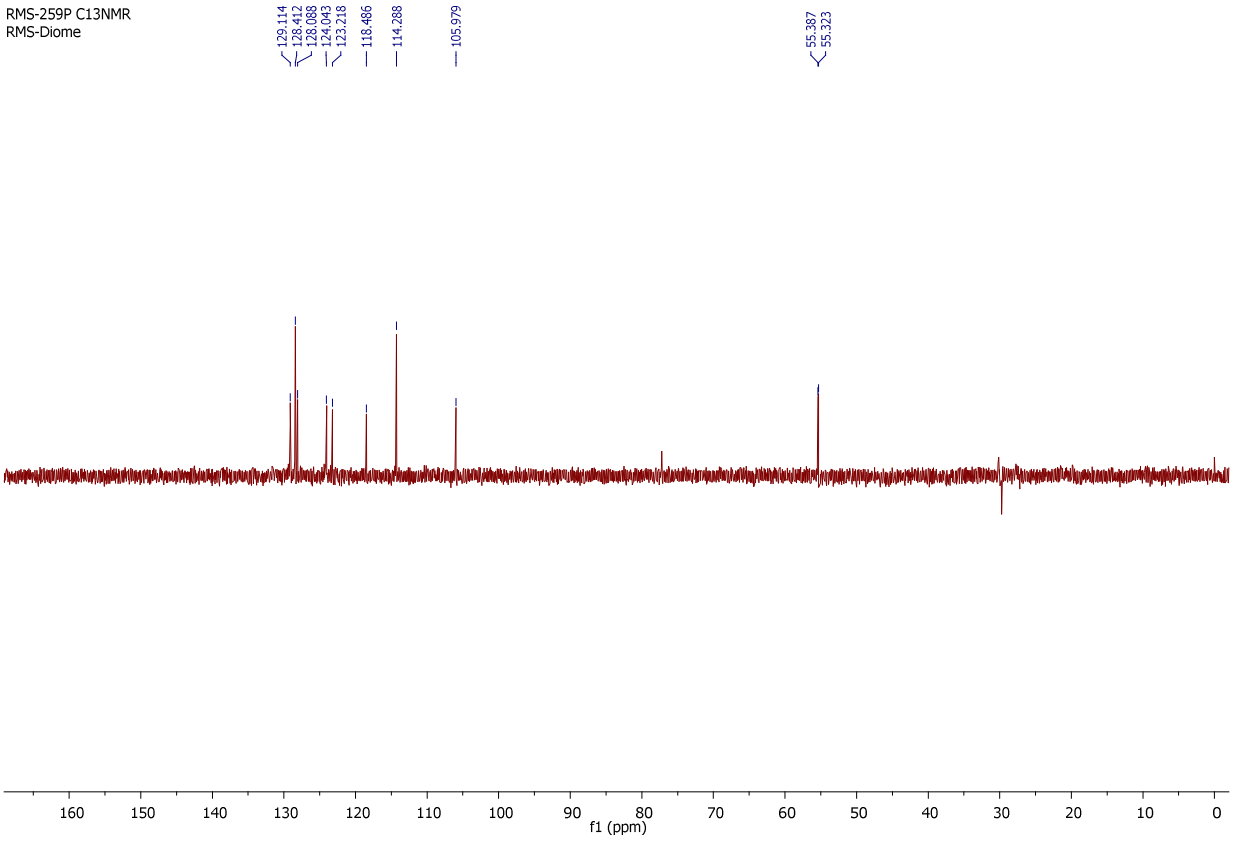




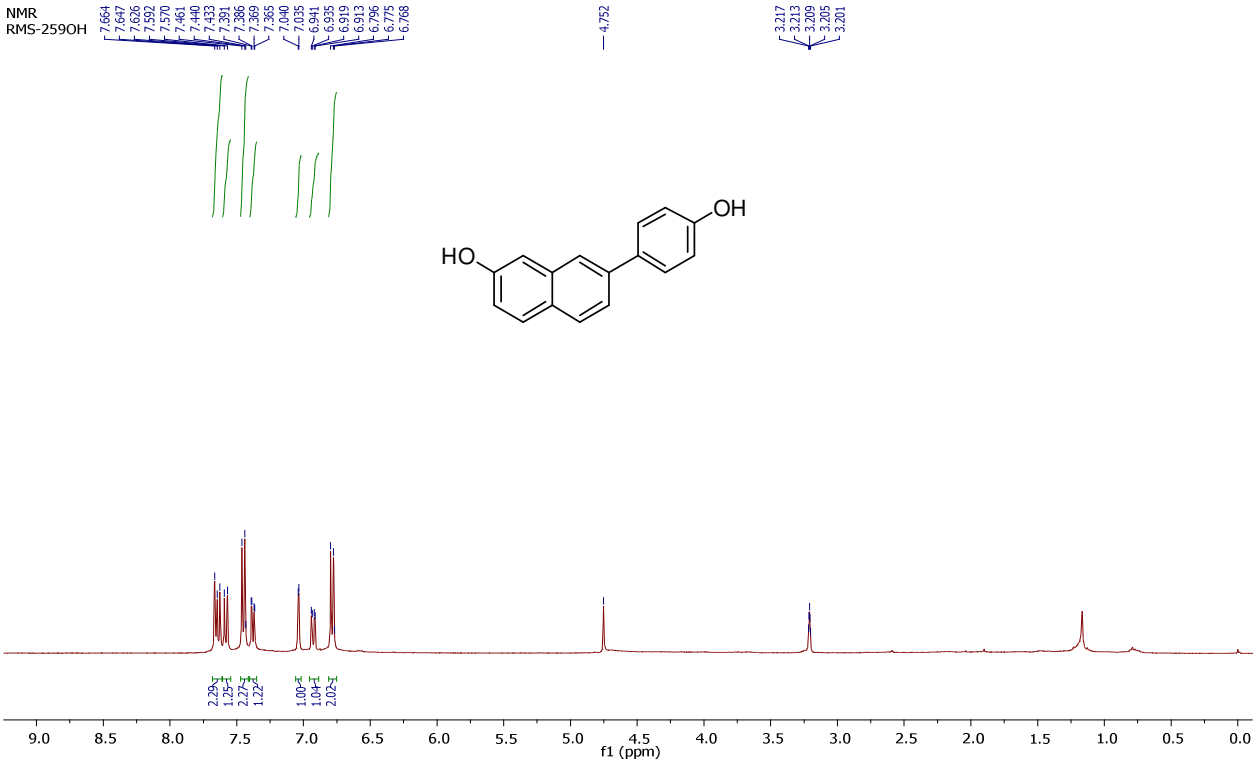
S5.2. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(4′-methoxyphenyl)-7-methoxynaphthalene (**2vm**)

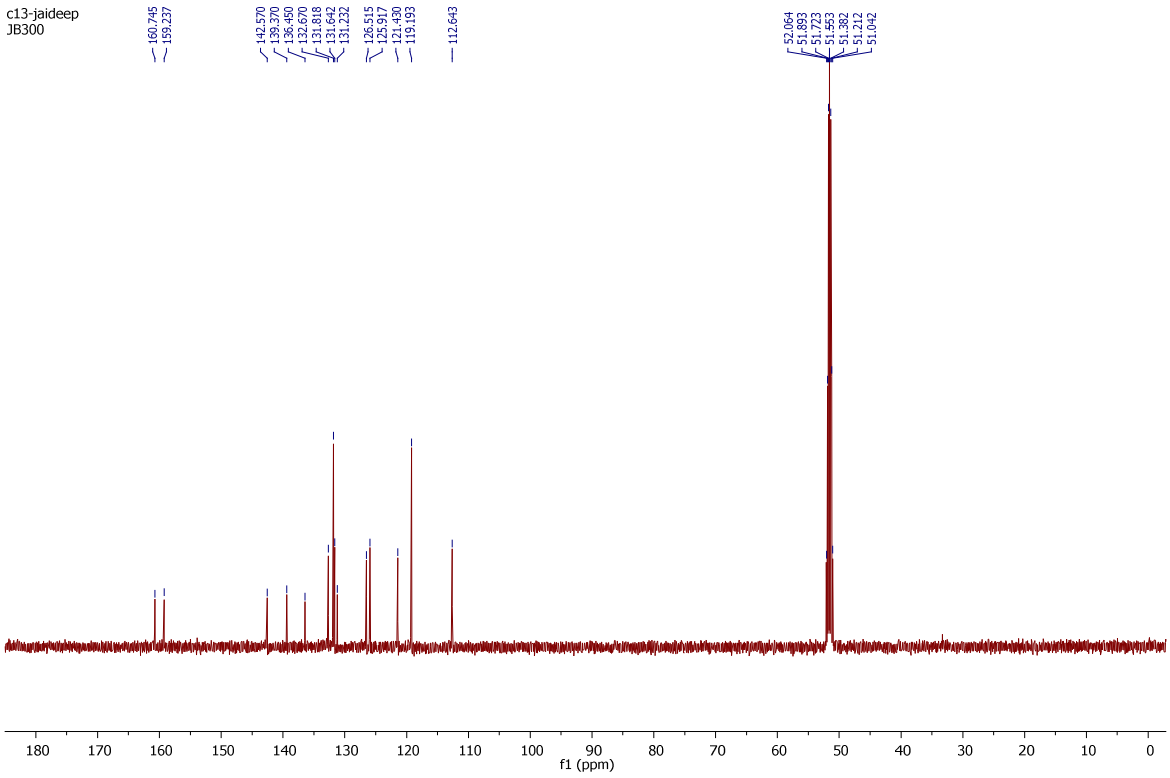


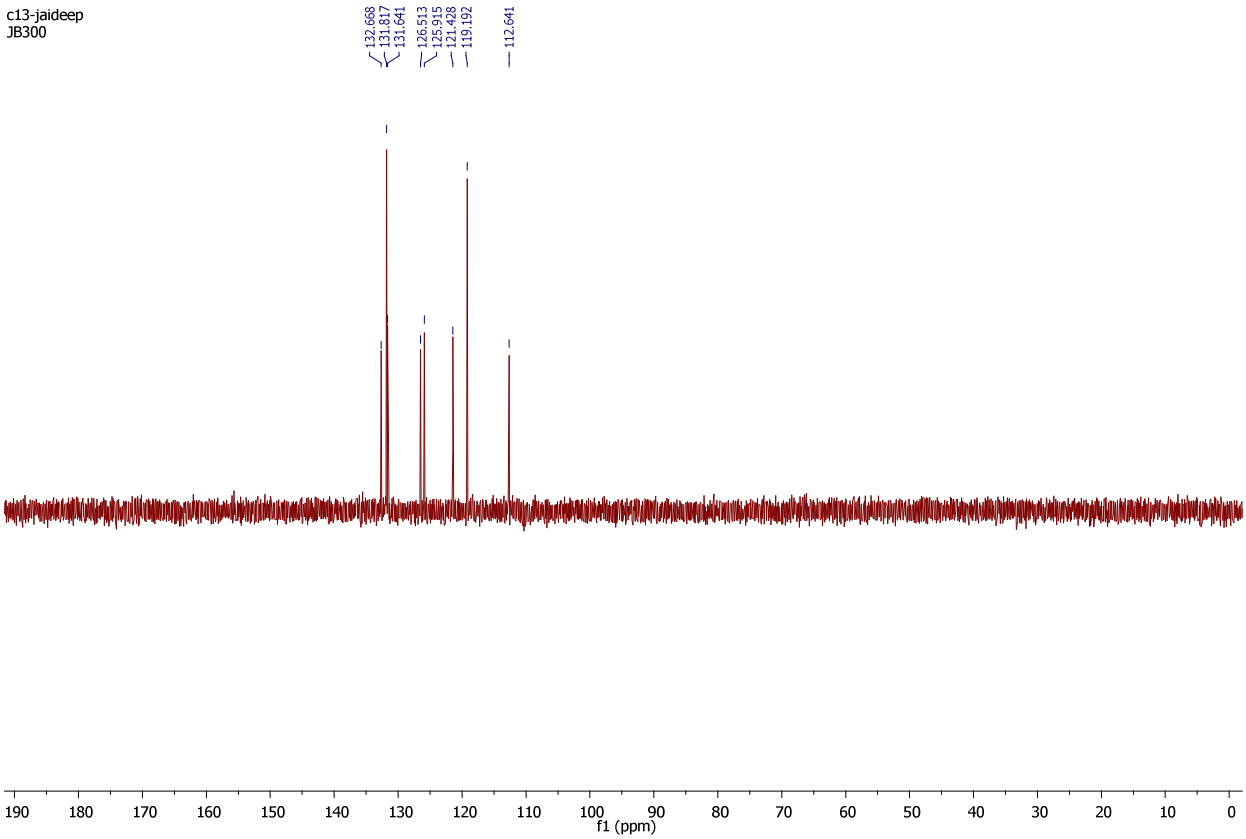

RMS-259P C13NMR
RMS-Diome
159.236
157.996
138.661
134.922
133.797
129.138
128.433
128.112
127.873
124.057
123.231
118.489
114.303
106.008
77.266
77.011
76.757
55.390
55.327
f1 (ppm)


RMS-259P C13NMR
RMS-Diome
129.114
128.412
128.088
124.043
123.218
118.486
114.288
105.979
55.387
55.323
f1 (ppm)

S5.3. ^{1}H, ^{13}C and DEPT135 NMR spectra of 2-(4′-hydroxyphenyl)naphthalen-7-ol (**2vh**)






c13-jaideep
JB300
132.668
131.817
131.641
126.513
125.915
121.428
119.192
112.641
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

S6. Confirmation of the formation of product **2ta** *versus* **2tb** (using HMBC correlations)

The HMBC spectra scans are shown in section of S4.20 of ESI.

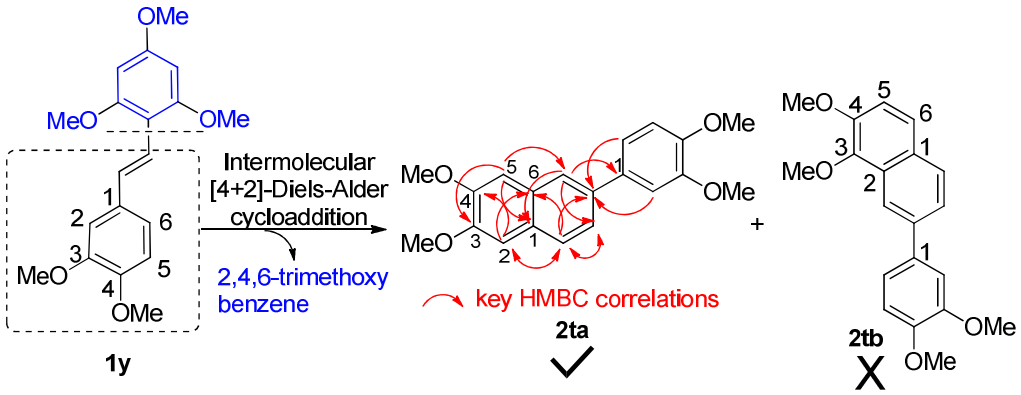
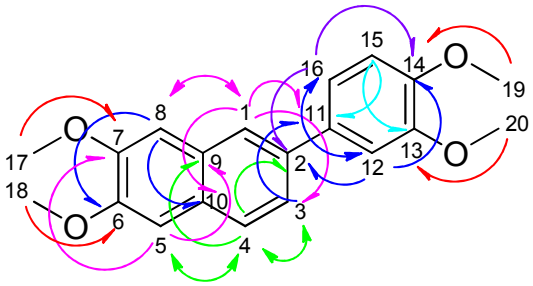


Figure S1. The possible products from the reaction of disubstituted styryl methoxybenzene with TFA. The HMBC correlations are shown.

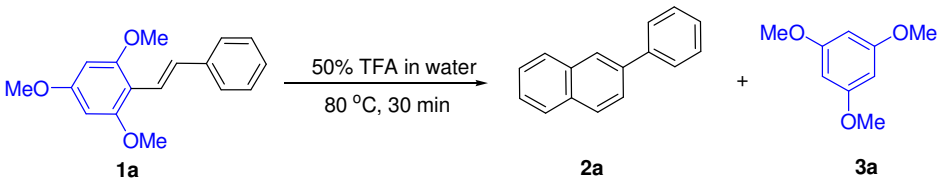
HMBC Correlations of 2-(3', 4'-dimethoxyphenyl)-6,7-dimethoxynaphthalene (**2ta**).



Carbon Number	^{1}H-value	^{13}C-NMR	HSQc	HMBC Correlations
C_1	7.85 (s)	123.8	123.8	C_3 (123.8), C_8 (106.4), C_{10} (128.1), C_{11}(134.4)
C_2	-	136.8	-	
C_3	7.57 (d)	123.7	123.7	C_4 (126.7), C_{11} (134.4)
C_4	7.74 (d)	126.7	126.7	C_2 (136.8), C_3 (123.7), C_5 (106.0), C_9 (129.4)

C_5	7.14 (s)	106.0	106.0	C_4 (126.7), C_7 (149.8), C_9 (129.4)
C_6	-	149.4	-	-
C_7	-	149.8	-	-
C_8	7.18 (s)	106.4	106.4	C_1 (123.8), C_6 (149.4)C_{10} (128.1)
C_9	-	129.4	-	-
C_{10}	-	128.1	-	-
C_{11}	-	134.4	-	-
C_{12}	7.22	110.4	110.4	C_2 (136.8), C_{14} (148.4), C_{16} (119.4)
C_{13}	-	149.1	-	-
C_{14}	-	148.4	-	-
C_{15}	6.98 (d)	111.4	111.4	C_{11} (134.4), C_{13} (149.1)
C_{16}	7.25 (d)	119.4	119.4	C_{12} (110.4), C_{14} (148.4)
C_{17}	4.02 (s)	55.9	55.89	C_7 (149.8)
C_{18}	4.02 (s)	55.9	55.89	C_6 (149.4)
C_{19}	3.94 (s)	55.87	55.89	C_{14} (148.4)
C_{20}	3.98 (s)	55.87	55.89	C_{13} (149.1)

S7. HPLC analysis of 2-phenylnaphthalene synthesis



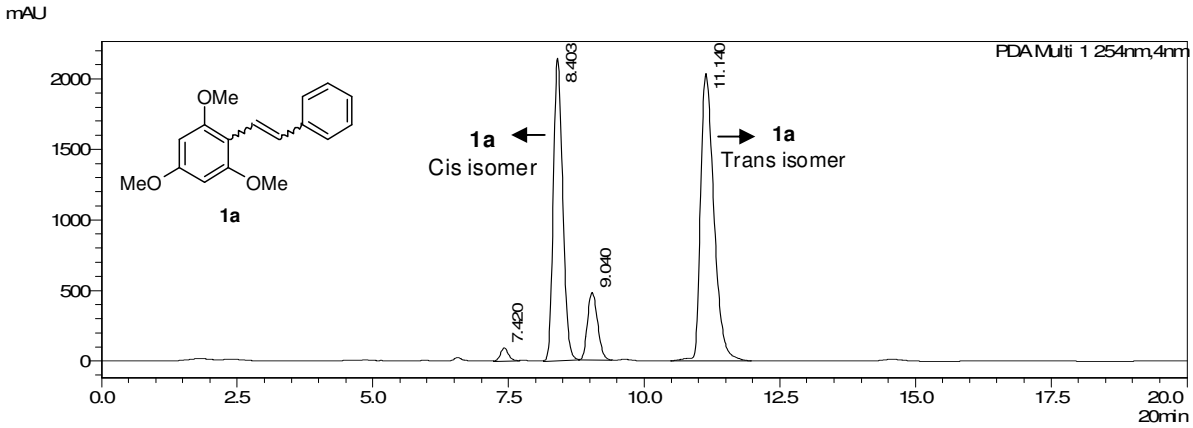
1a **2a** **3a**

HPLC conditions: HPLC analysis was done on Shimadzu HPLC system (model: LC-6AD) equipped with a PDA detector (model: SPD-M20A). Analysis was done on Inertsil C_8 (3.5 µ, 4.6 × 250 mm) column.

Mobile phase: Methanol: water (70:30) isocratic elution at flow rate of 1 ml/min.

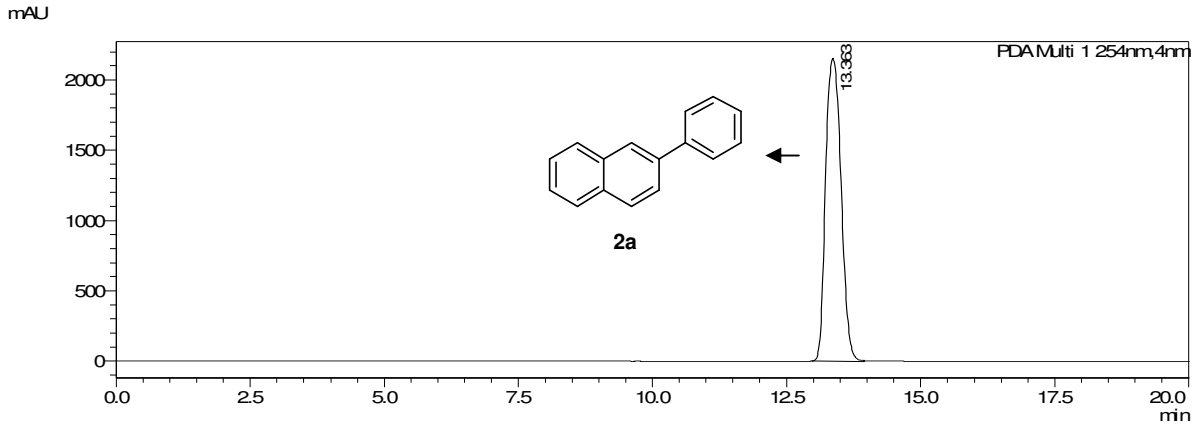
Samples: The HPLC analysis of starting material **1a**, pure products **2a** and **3a** and crude reaction mixture was done in order to undertand % conversion of the reaction and number of products formed.

S7.a. HPLC chromatogram of 1-styryl 2,4,6-trimethoxybenzene (1a):



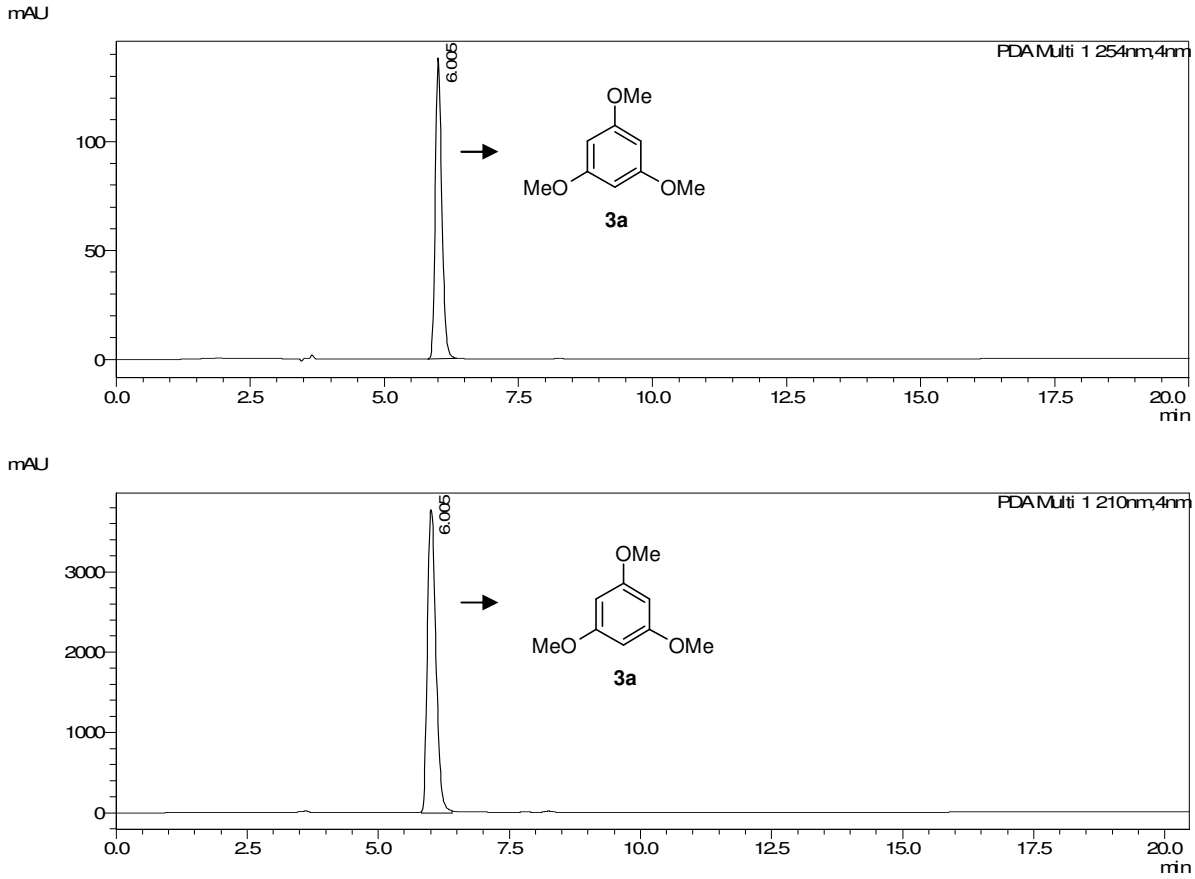
Sr.No	Compound	Retention time	Area (%) of peaks
1	*Cis*-isomer of **1a**	8.4 min	38.0
2	Unknown impurity	9.04 min	9.2
3	*Trans*-isomer of **1a**	11.14 min	51.2

S7.b. HPLC chromatogram of pure 2-phenynaphthalene (2a)



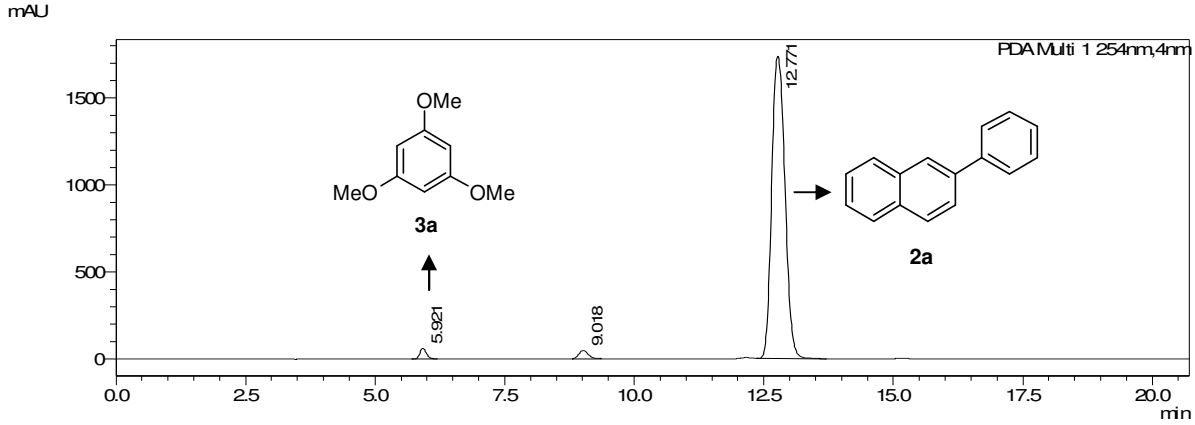
Sr.No	Compound	Retention time	Area (%) of peaks
1	2-phenylnaphthalene (**2a**)	13.36 min	100

S7.c. HPLC chromatogram of pure 1,3,5-trimethoxy benzene (3a)

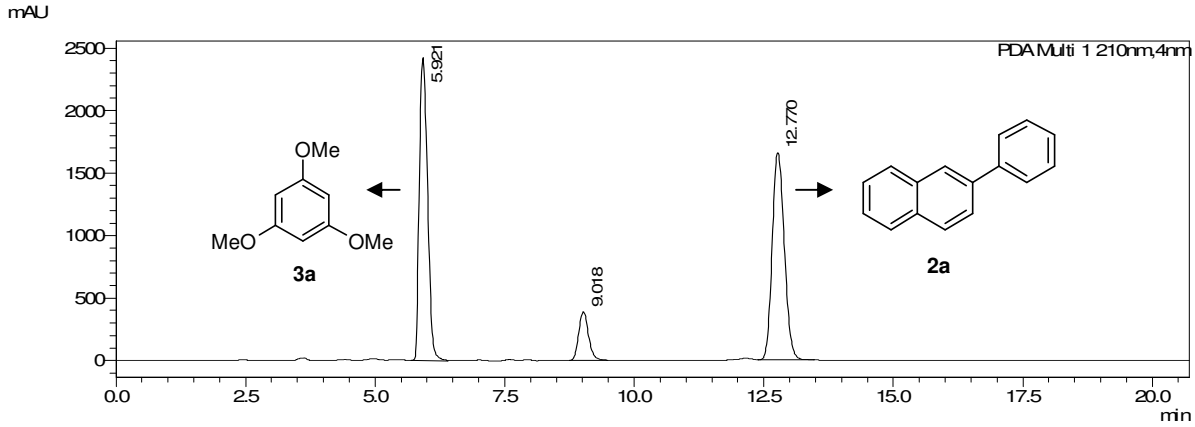


Sr.No	Compound	Retention time	Area (%) of peaks
1	1,3,5-Trimethoxybenzene (**3a**)	6.00 min	100

S7.d. HPLC chromatogram of crude reaction mixture after 30 min reaction time (at 254 and 210 nm)

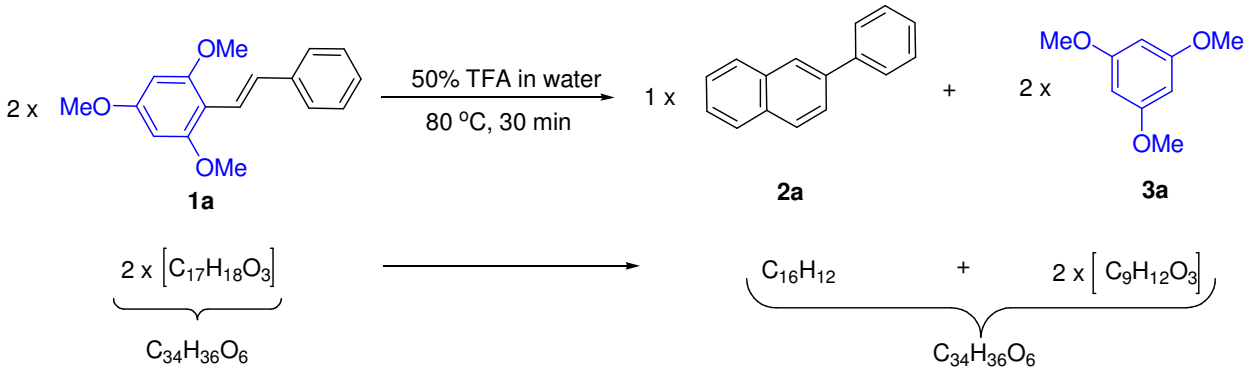


Sr.No	Compound	Retention time	Area (%) of peaks
1	1,3,5-Trimethoxy benzene (**3a**)	5.92 min	1.19
2	Impurity from starting material **1a**	9.01 min	2.38
3	2-phenylnaphthalene (**2a**)	12.77 min	96.41



Sr.No	Compound	Retention time	Area (%) of peaks
1	1,3,5-Trimethoxy benzene (**3a**)	5.92 min	45.13
2	Impurity from starting material **1a**	9.01 min	8.89
3	2-phenylnaphthalene (**2a**)	12.77 min	45.97

S8. Yield calculation of the 2-phenylnaphthalene product



2 moles of starting material **1a** gives 1 mole of product **2a**. Therefore, this fact was taken into consideration while calculating % yield of the product **2a**.

	1a	**2a**
Mol. wt.	**270**	**204**
Amount	**0.1 g**	**0.035 g (isolated amount)**
Theoretical yield	**-**	$= \frac{\text{mol.wt of 2a x amount of 2a x moles of 2a}}{\text{mol. wt. of 1a x moles of 1a}}$ $= \frac{204 \times 0.1 \times 1}{270 \times 2} = 0.037$ g
Practical yield (%)	**-**	$\text{Practical yield (\%)} = \frac{\text{Isolated amount}}{\text{Theoretical yield}} \times 100$ $= \frac{0.035}{0.037} \times 100 = 94\%$

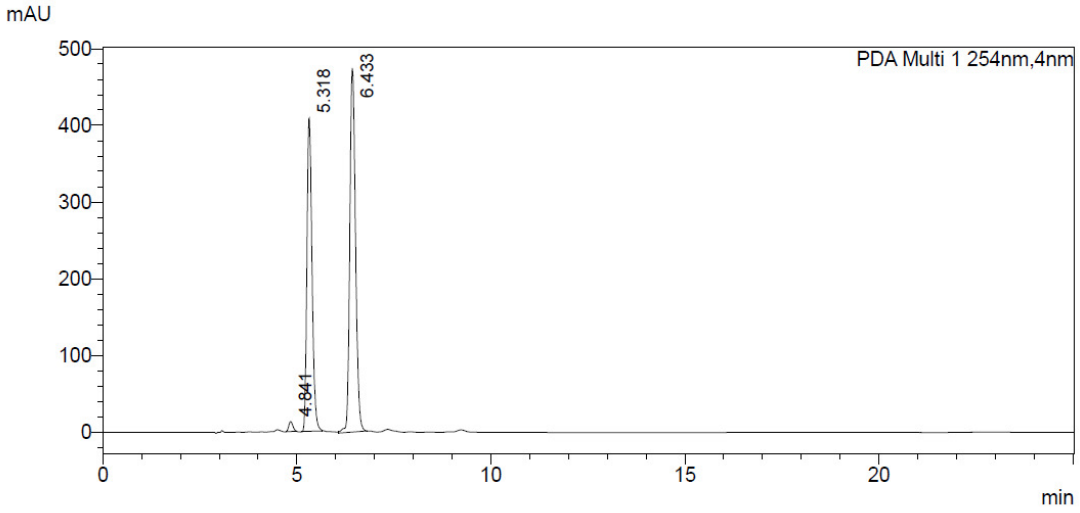
S9. HPLC chromatograms of intermediates 1a-1aa

HPLC conditions: HPLC analysis was done on Shimadzu HPLC system (model: LC-6AD) equipped with a PDA detector (model: SPD-M20A). Analysis was done on Inertsil C_8 (3.5 µ, 4.6 × 250 mm) column.

Mobile phase: Methanol: water (90:10) isocratic elution at flow rate of 1 ml/min.

HPLC chromatogram of 1a:

<Chromatogram>



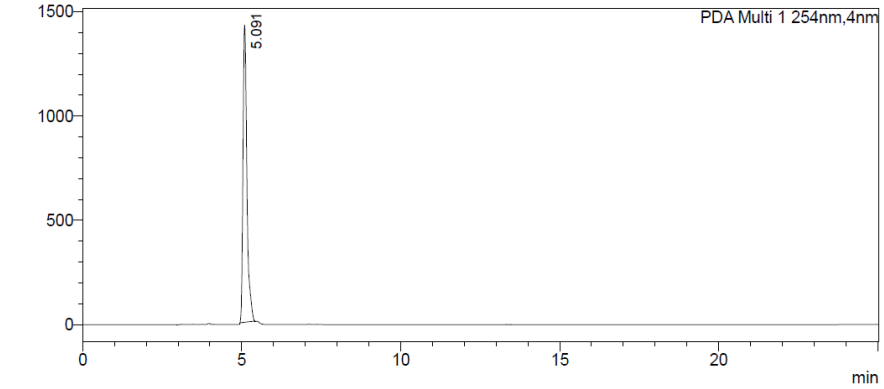
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.841	94176	12897	4.725	4.992	1.083
2	5.318	3734992	408261	5.120	5.653	42.952
3	6.433	4866596	474489	6.080	6.805	55.965
Total		8695764	895647			100.000

HPLC Chromatogram of 1b:

<Chromatogram>



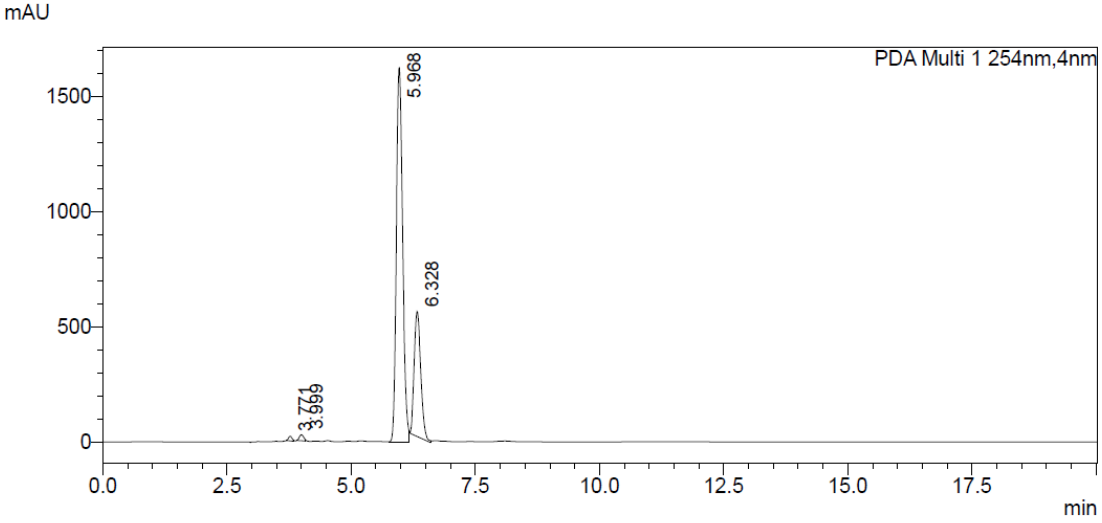
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	5.091	12228277	1425418	4.928	5.419	100.000
Total		12228277	1425418			100.000

HPLC Chromatogram of 1c:

<Chromatogram>



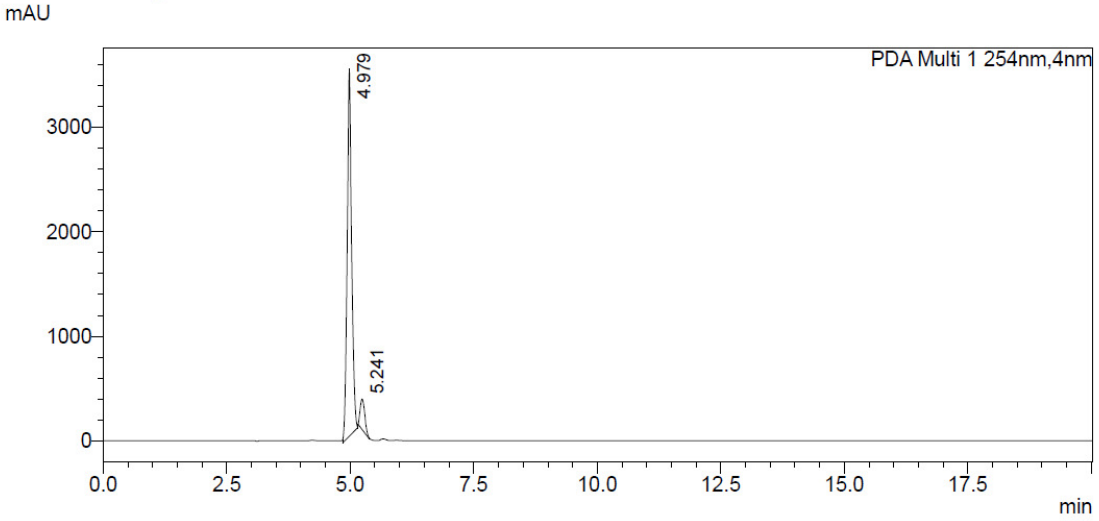
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	3.771	104474	20456	3.701	3.840	0.531
2	3.999	154973	26529	3.915	4.075	0.788
3	5.968	14396096	1625483	5.771	6.165	73.213
4	6.328	5007701	543153	6.187	6.603	25.467
Total		19663244	2215620			100.000

HPLC Chromatogram of 1d:

<Chromatogram>



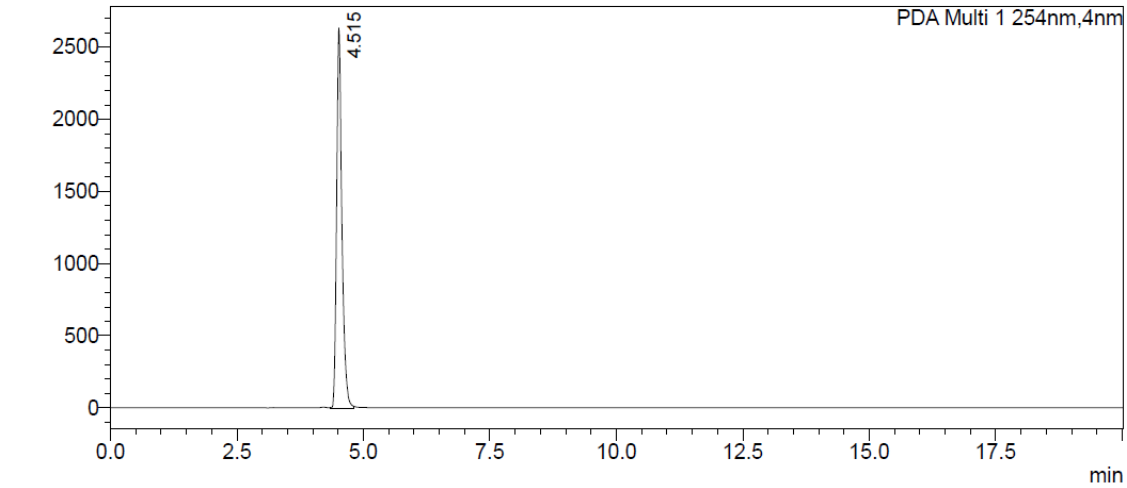
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.979	21932847	3514002	4.843	5.141	92.200
2	5.241	1855391	291160	5.152	5.387	7.800
Total		23788239	3805162			100.000

HPLC Chromatogram of 1e:

<Chromatogram>



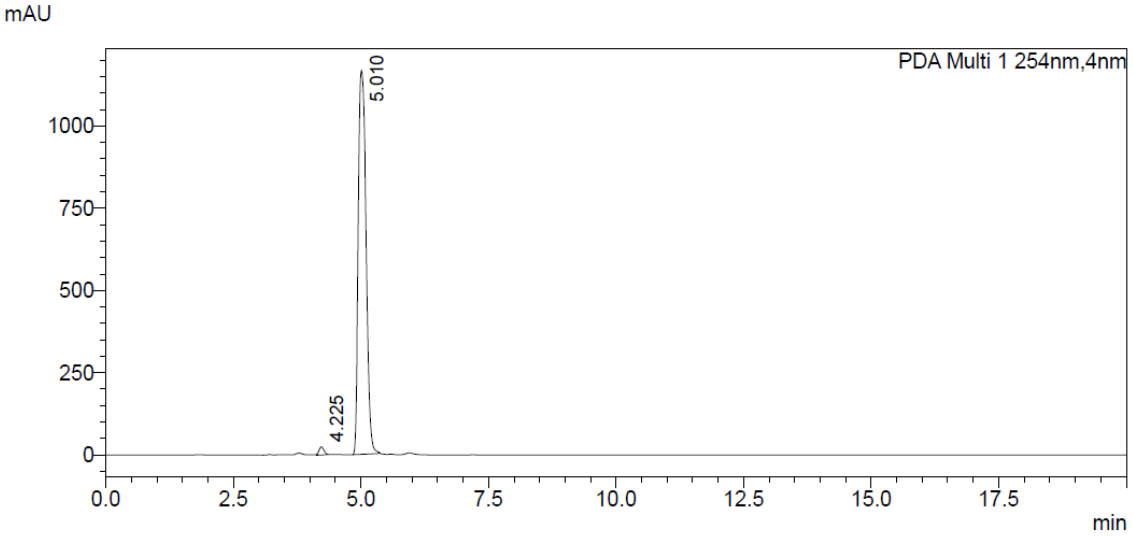
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.515	19250736	2637425	4.352	4.800	100.000
Total		19250736	2637425			100.000

HPLC Chromatogram of 1f:

<Chromatogram>



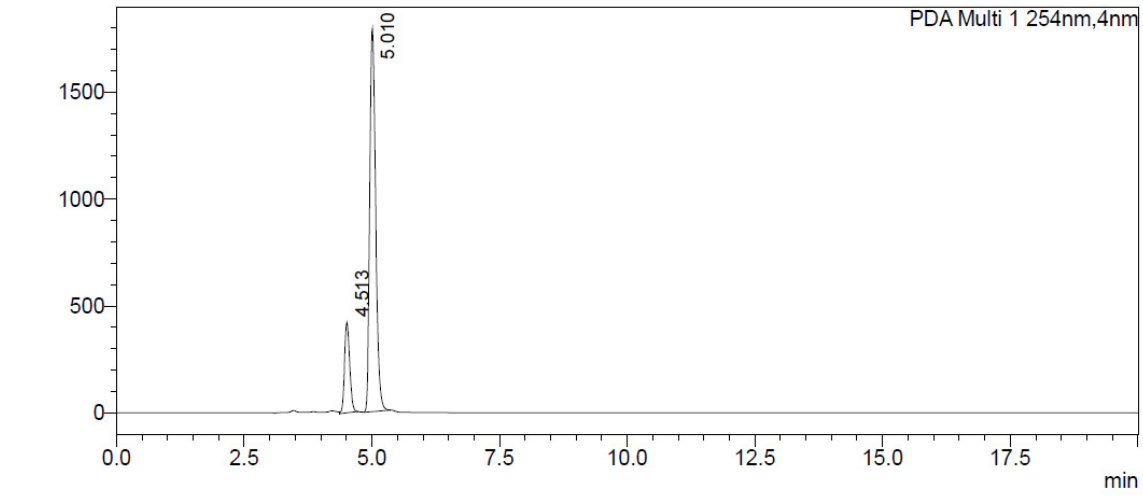
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.225	164543	25057	4.128	4.341	1.314
2	5.010	12362359	1166530	4.843	5.344	98.686
Total		12526903	1191587			100.000

HPLC Chromatogram of 1g:

<Chromatogram>



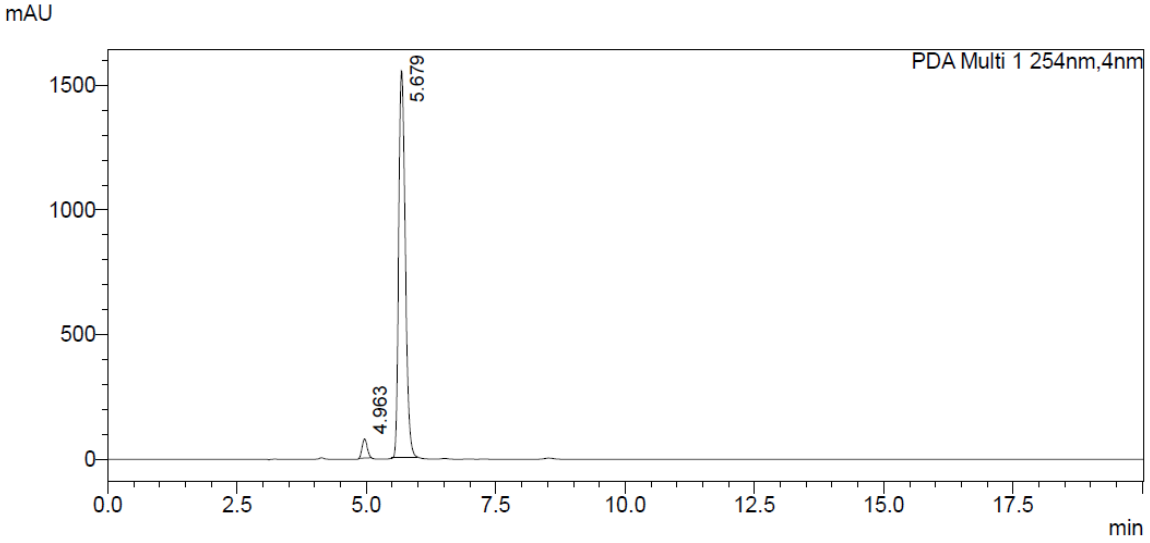
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.513	2970405	423936	4.363	4.725	17.138
2	5.010	14361981	1791654	4.843	5.365	82.862
Total		17332386	2215590			100.000

HPLC Chromatogram of 1h:

<Chromatogram>



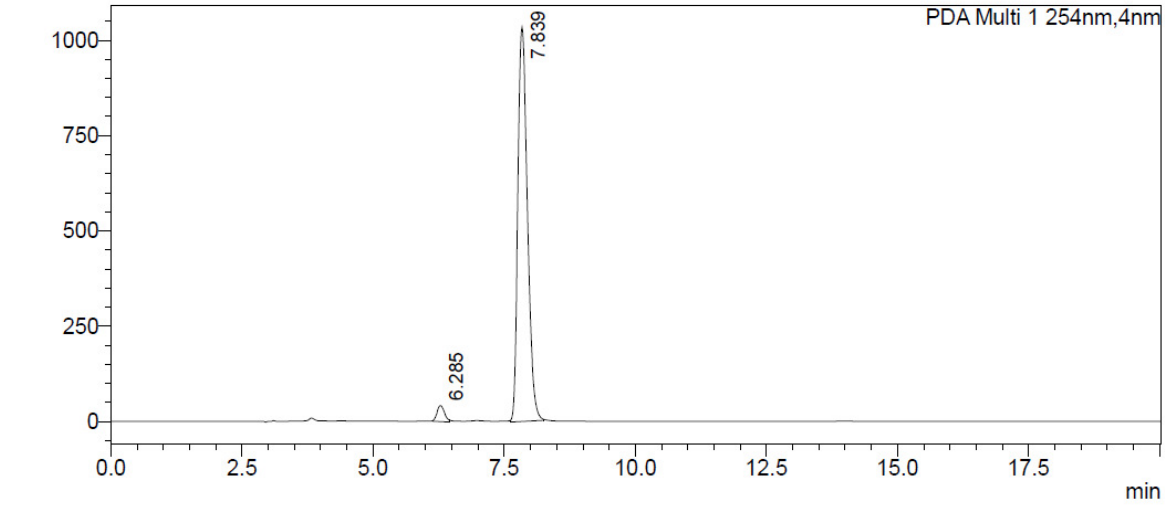
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.963	512999	75796	4.843	5.088	3.596
2	5.679	13753802	1550220	5.493	5.984	96.404
Total		14266801	1626016			100.000

HPLC Chromatogram of 1i:

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	6.285	417600	42138	6.133	6.453	3.084
2	7.839	13124564	1034246	7.616	8.245	96.916
Total		13542164	1076385			100.000

HPLC Chromatogram of 1j:

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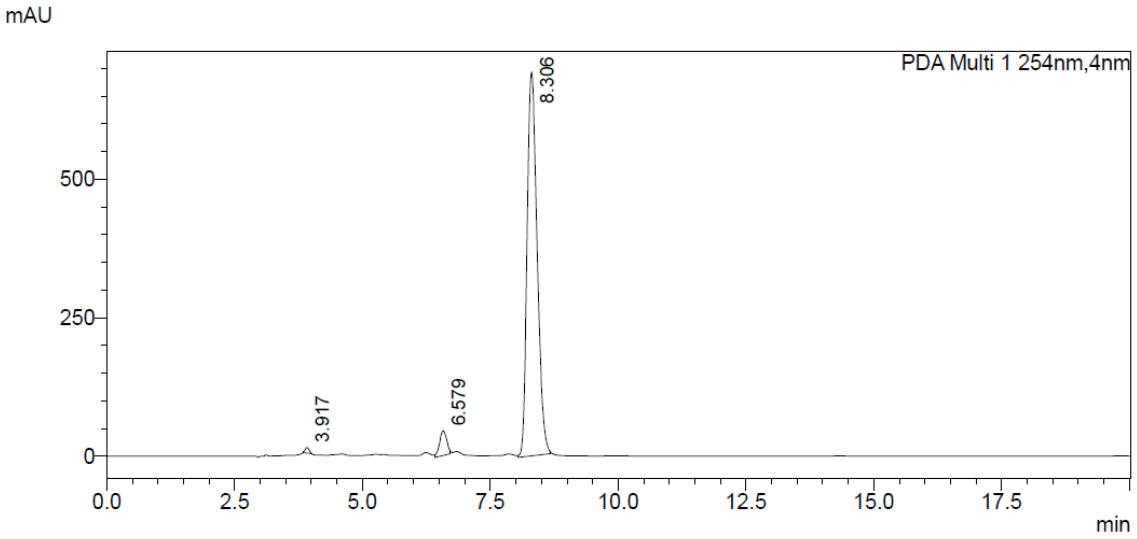


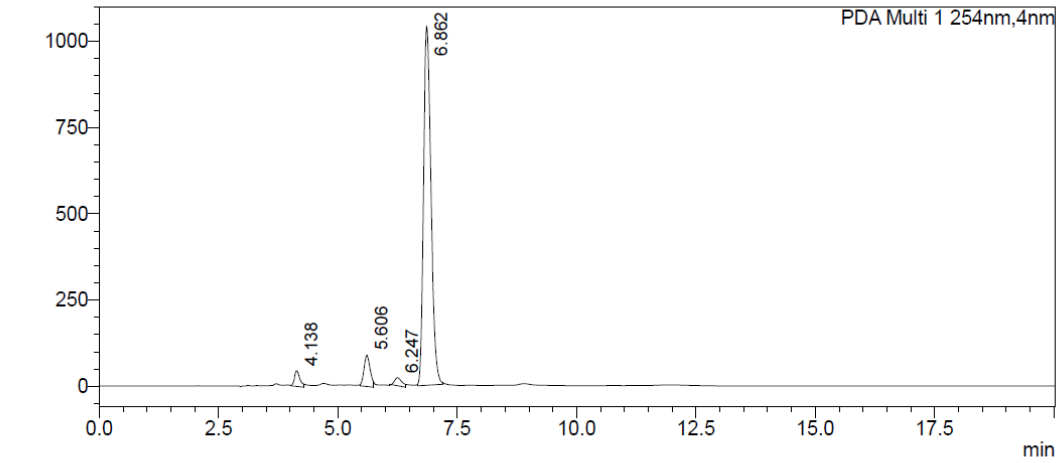
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	3.917	52832	9768	3.851	4.000	0.532
2	6.579	436295	44433	6.421	6.720	4.396
3	8.306	9436598	692199	8.053	8.672	95.072
Total		9925724	746400			100.000

HPLC Chromatogram of 1k:

<Chromatogram>



<Peak Table>

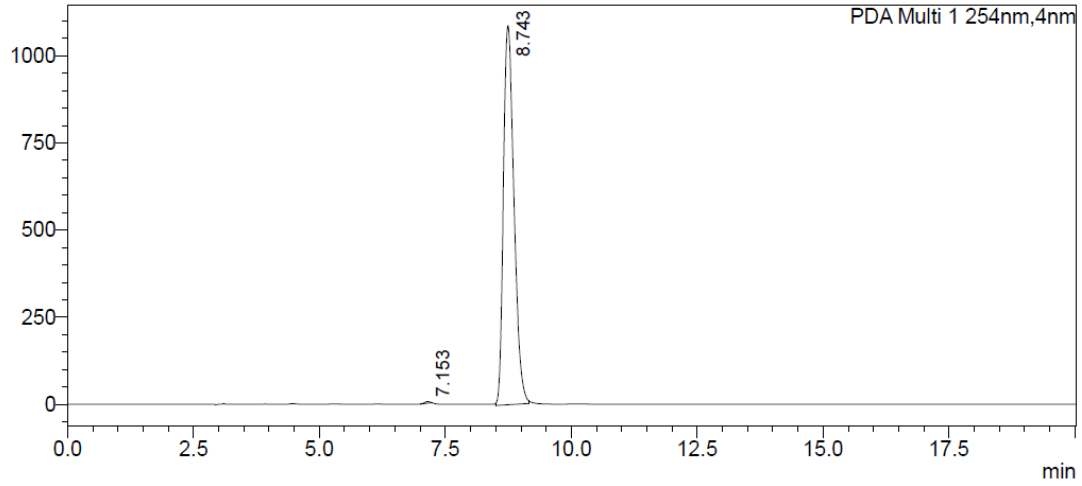
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.138	354803	45344	4.021	4.288	2.794
2	5.606	813565	90282	5.461	5.749	6.407
3	6.247	245400	23186	6.080	6.411	1.933
4	6.862	11284272	1039359	6.667	7.200	88.866
Total		12698040	1198171			100.000

HPLC Chromatogram of 1l:

<Chromatogram>

mAU



<Peak Table>

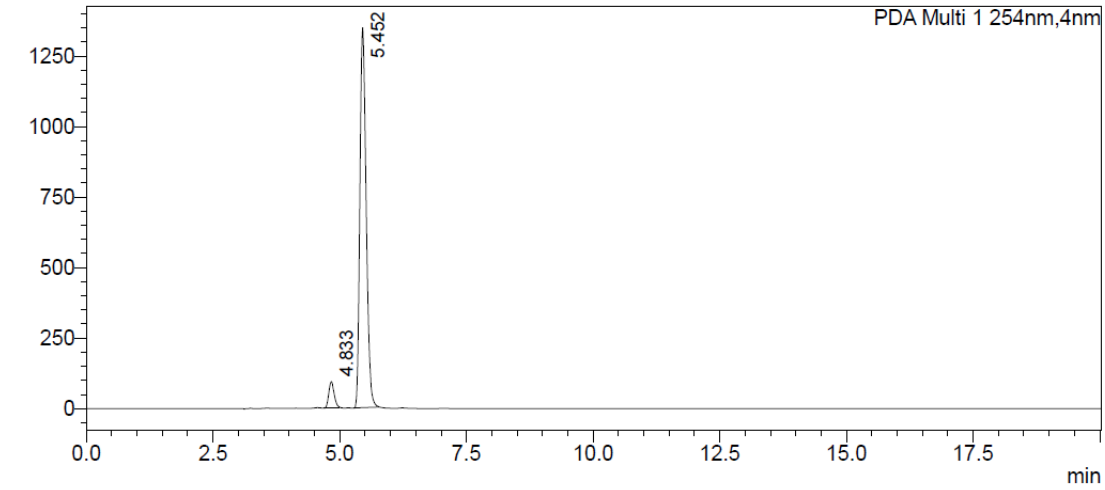
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	7.153	35708	4545	7.008	7.232	0.225
2	8.743	15863346	1086278	8.501	9.152	99.775
Total		15899054	1090823			100.000

HPLC Chromatogram of 1m:

<Chromatogram>

mAU



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.833	690517	93311	4.693	4.981	5.593
2	5.452	11655777	1348181	5.280	5.760	94.407
Total		12346294	1441492			100.000

HPLC Chromatogram of 1n:

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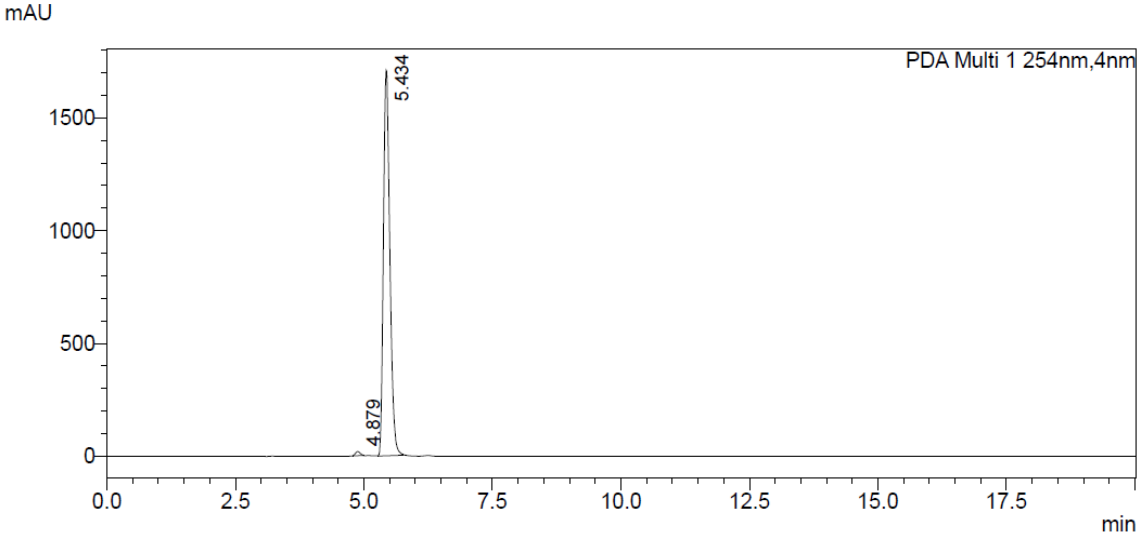


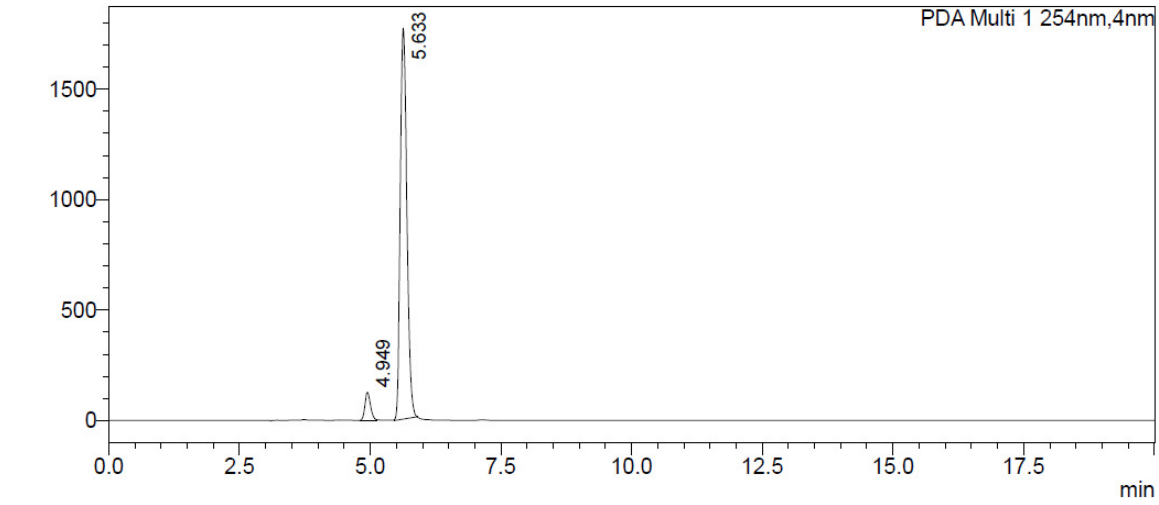
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.879	120351	17906	4.779	4.992	0.803
2	5.434	14870068	1707856	5.269	5.749	99.197
Total		14990418	1725761			100.000

HPLC Chromatogram of 1o:

<Chromatogram>



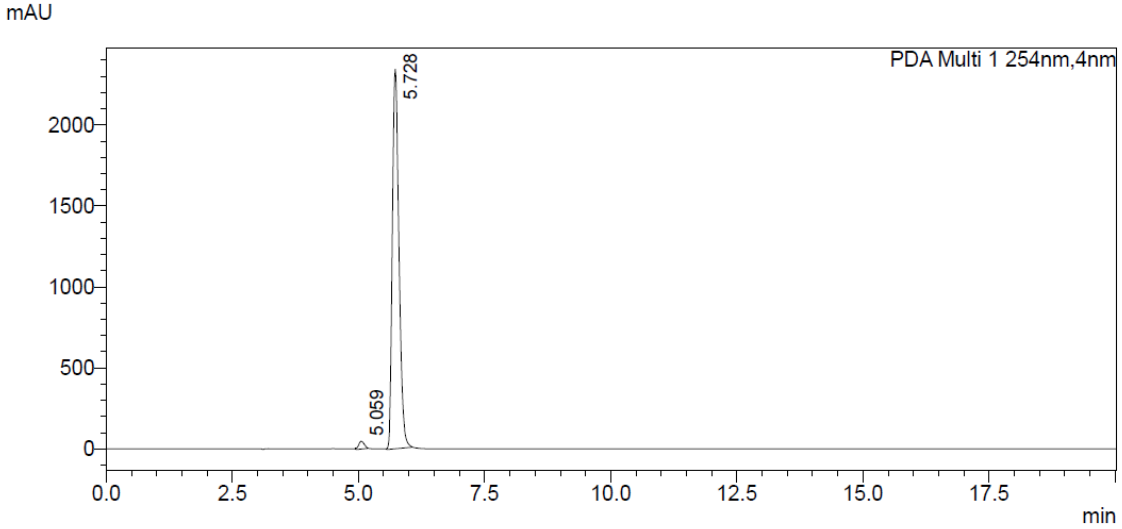
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.949	962992	128430	4.821	5.120	5.819
2	5.633	15586309	1770284	5.461	5.899	94.181
Total		16549301	1898714			100.000

HPLC Chromatogram of 1p:

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	5.059	376229	48213	4.949	5.184	1.731
2	5.728	21364758	2344784	5.557	6.048	98.269
Total		21740987	2392998			100.000

HPLC Chromatogram of 1q:

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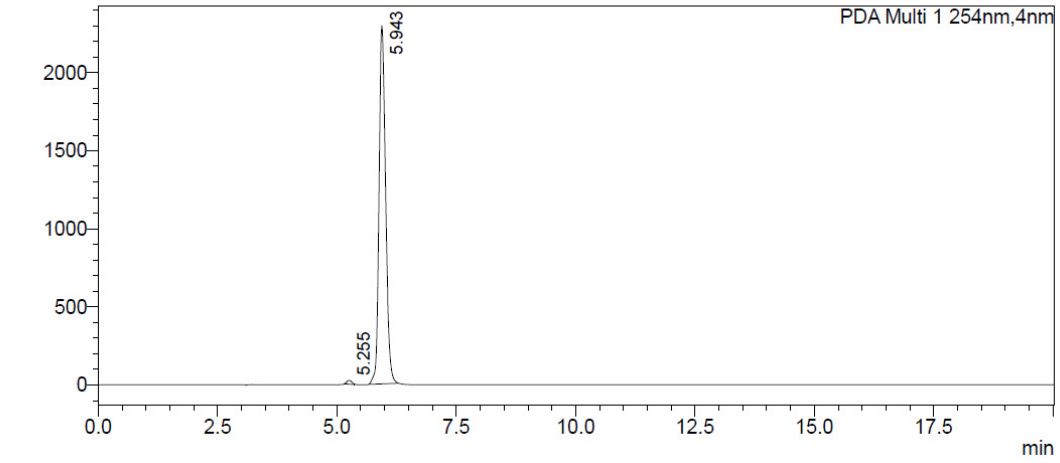

<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	5.255	175101	24859	5.152	5.365	0.788
2	5.943	22035952	2293759	5.685	6.261	99.212
Total		22211053	2318618			100.000

HPLC Chromatogram of 1r:

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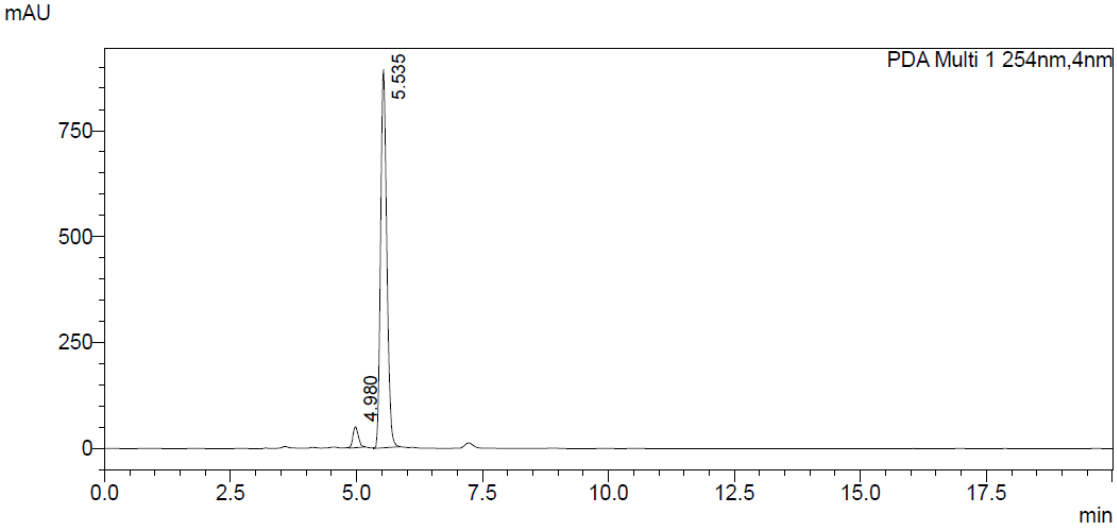


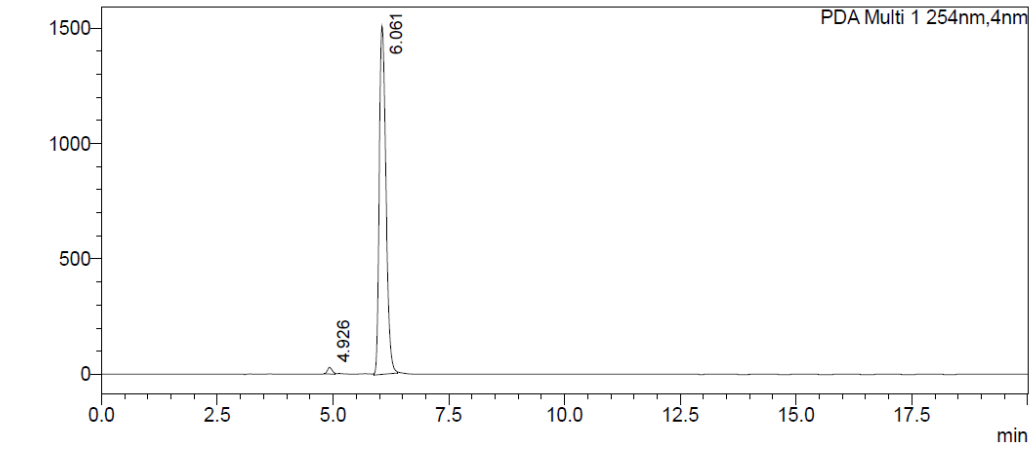
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.980	366754	49010	4.843	5.163	4.563
2	5.535	7671063	892805	5.344	5.845	95.437
Total		8037817	941815			100.000

HPLC Chromatogram of 1s:

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.926	205463	29091	4.821	5.045	1.342
2	6.061	15102997	1509556	5.888	6.400	98.658
Total		15308460	1538647			100.000

HPLC Chromatogram of 1t:

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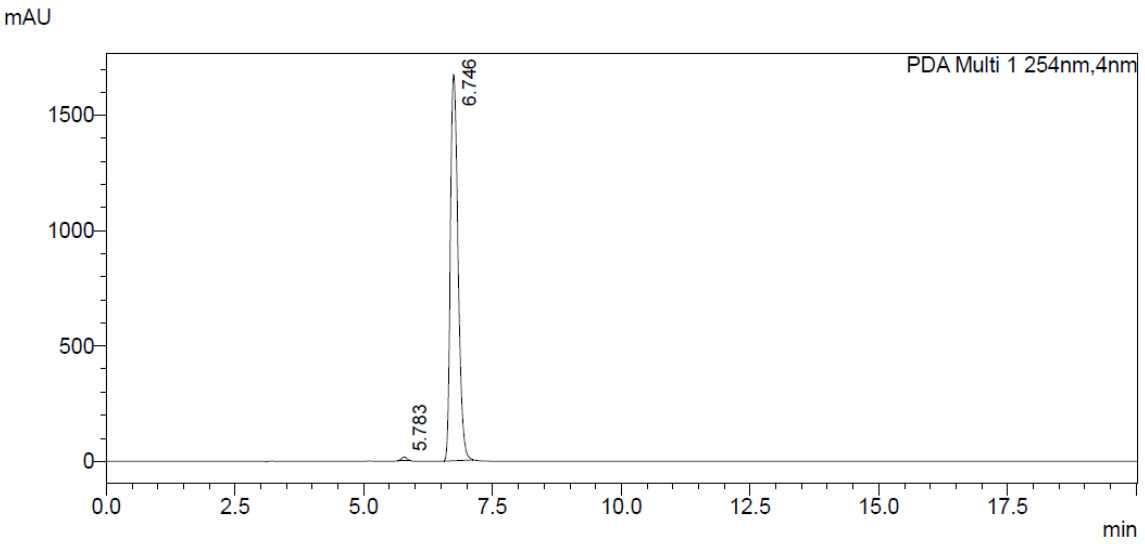


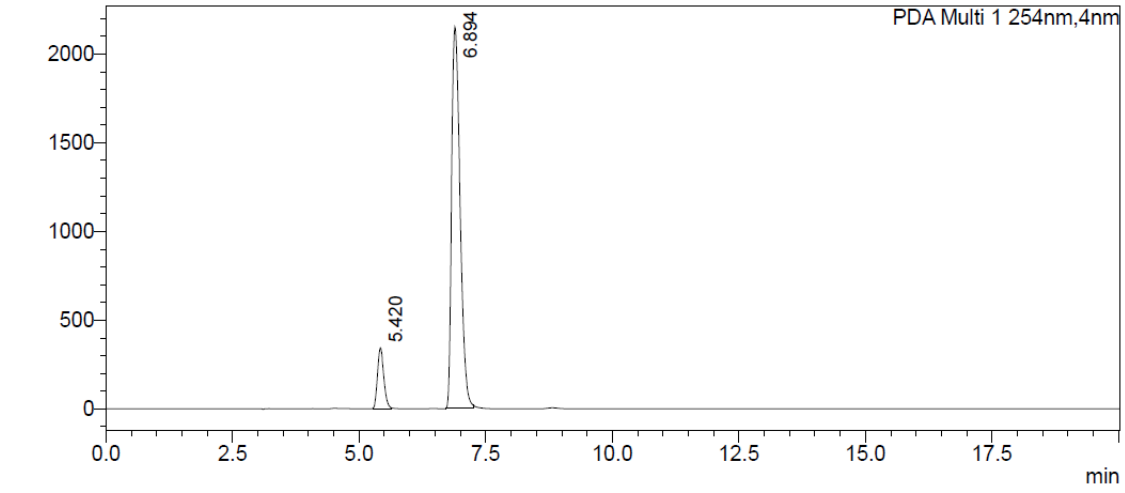
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	5.783	123269	16625	5.664	5.899	0.706
2	6.746	17330241	1672963	6.560	7.104	99.294
Total		17453510	1689588			100.000

HPLC Chromatogram of 1u:

<Chromatogram>



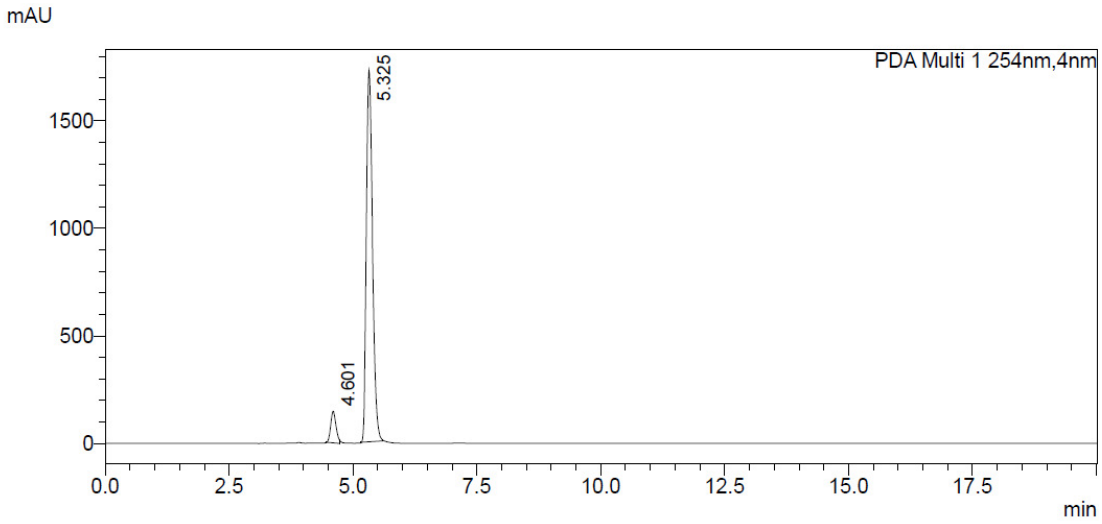
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	5.420	2958200	343483	5.269	5.632	10.651
2	6.894	24814520	2146056	6.709	7.253	89.349
Total		27772720	2489539			100.000

HPLC Chromatogram of 1v:

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.601	1090101	146747	4.469	4.725	6.832
2	5.325	14864624	1725869	5.163	5.600	93.168
Total		15954725	1872616			100.000

HPLC Chromatogram of 1w:

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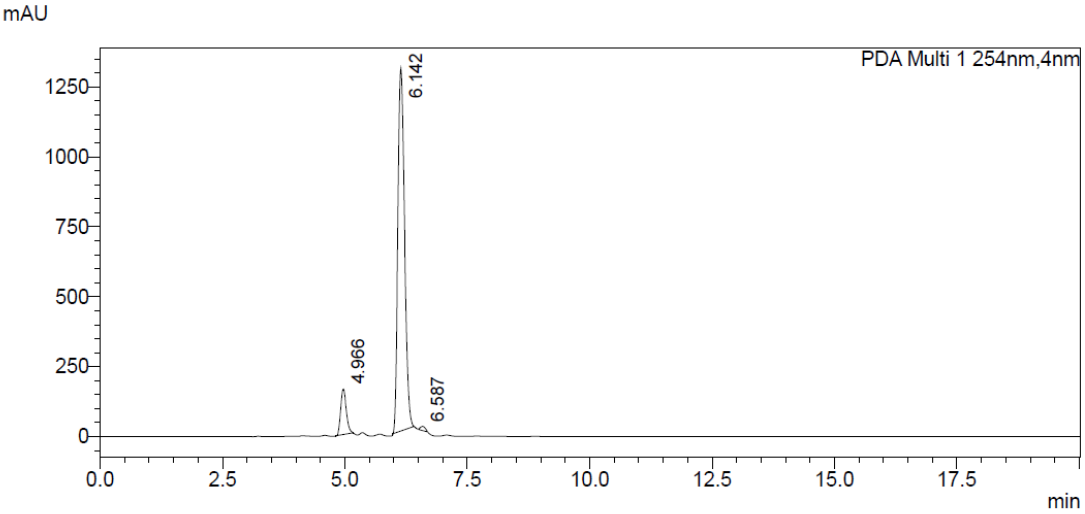


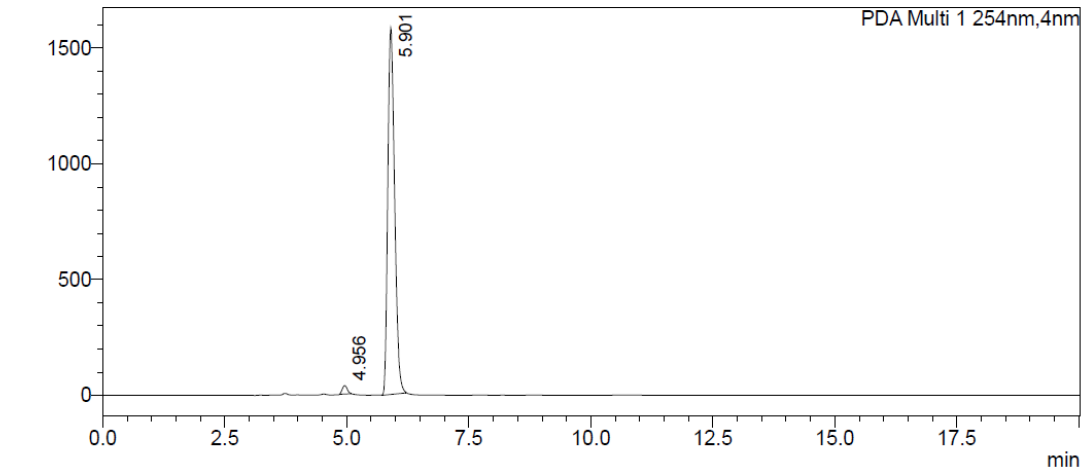
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.966	1277011	162198	4.811	5.173	9.342
2	6.142	12291953	1297194	5.973	6.400	89.924
3	6.587	100338	15080	6.507	6.677	0.734
Total		13669301	1474472			100.000

HPLC Chromatogram of 1x:

<Chromatogram>



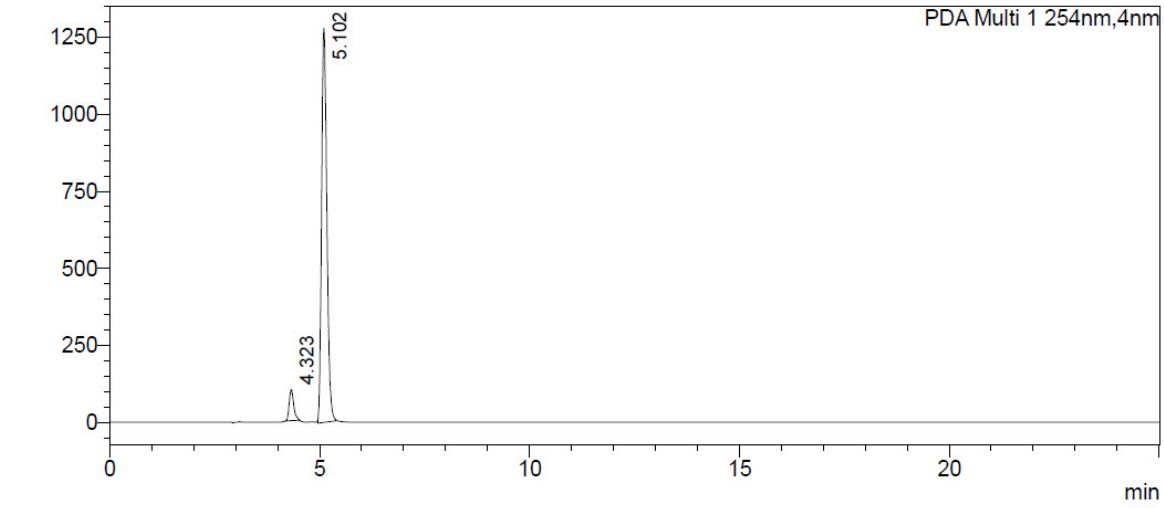
<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.956	261202	36754	4.853	5.088	1.663
2	5.901	15449015	1582986	5.717	6.208	98.337
Total		15710217	1619741			100.000

HPLC Chromatogram of 1y:

<Chromatogram>



<Peak Table>

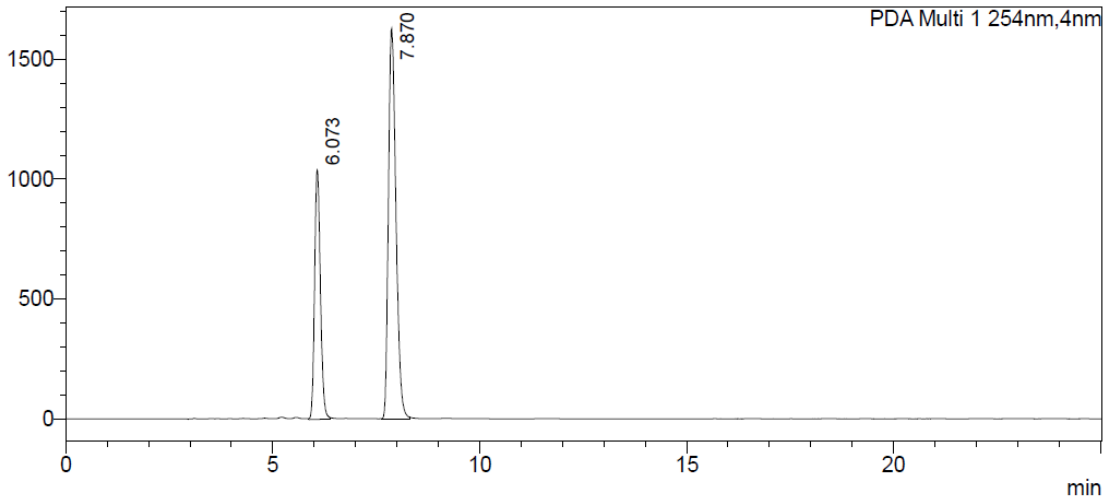
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.323	748419	100651	4.203	4.501	6.288
2	5.102	11153256	1279689	4.949	5.387	93.712
Total		11901675	1380340			100.000

HPLC Chromatogram of 1z:

<Chromatogram>

mAU



<Peak Table>

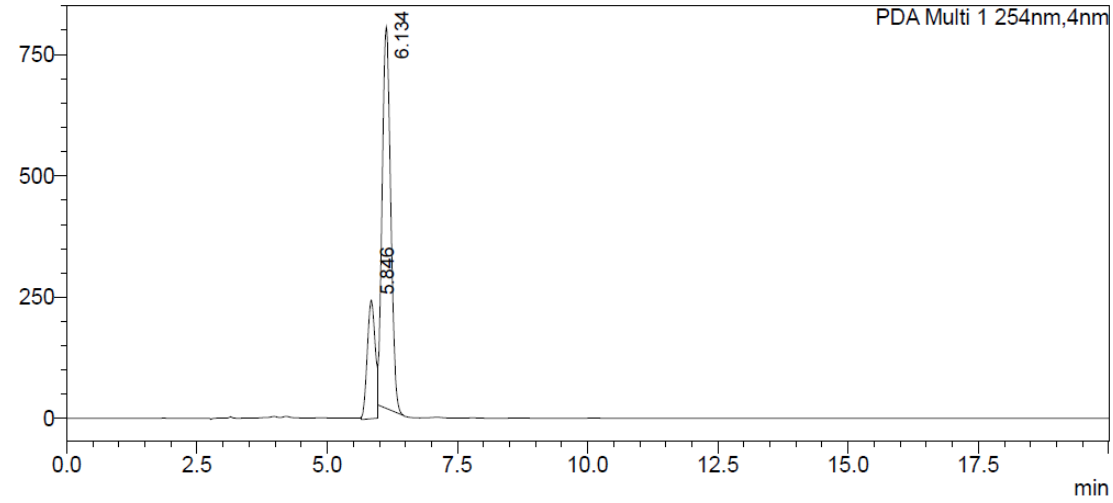
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	6.073	10172896	1039626	5.867	6.389	33.019
2	7.870	20636009	1628585	7.637	8.309	66.981
Total		30808905	2668211			100.000

HPLC Chromatogram of 1aa:

<Chromatogram>

mAU



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	5.846	2559187	244068	5.653	5.963	22.331
2	6.134	8901249	785605	5.973	6.453	77.669
Total		11460436	1029673			100.000

S10. References associated with ESI.

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