Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Halogenation of aromatic compounds with *N*-halosuccinimides (NXS) catalysed by D-camphorsulfonic acid–$BiCl_3$

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Supplementary Information

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1. General information

Melting points were determined on a Yamato melting point apparatus MP-21 and are uncorrected. IR spectra were recorded using a JEOL FT/IR-4600ST spectrophotometer. NMR spectra were measured on a Varian NMR system 700 spectrometer (700 MHz) using tetramethylsilane as an internal standard. Column chromatography was performed on Merck Silica gel 60. Unless otherwise stated, anhydrous sodium sulfate was employed as the drying agent. Aromatic compounds and $PdCl_2(PPh_3)_2$ were purchased from TCI. $PdCl_2$(dppf) was purchased from Merck. Potassium carbonate (Fine powder for organic synthesis) and dry solvents (Super dehydrated for organic synthesis) were purchased from Fujifilm Wako Chemicals. IR and ^{1}H-NMR spectra of compounds **2a-i**, **2k-n**, **2v**, **2h'**, **2h''**, **2a'**, **2a''**, **3a**, **3d-g**, **3i**, **3k-m**, **3p**, **3a'**, **3e'**, **3m'**, **4d**, **4e**, **4v**, **5g**, **5l**, **5q**, **6l** and **7g** were completely in accordance with those of the commercially available samples purchased from TCI. IR and ^{1}H-NMR spectra of compounds **2u**, **3n** and **3u** were completely in accordance with those of the commercially available sample purchased from Aldrich. IR and ^{1}H-NMR spectra of compound **3v** were completely in accordance with those of the commercially available sample purchased from Fujifilm Wako Chemicals. IR and ^{1}H-NMR spectra of compounds **6g** and **6n** were completely in accordance with those of the commercially available sample purchased from Nacalai tesque. CH_2BrCN was identified by the comparison of ^{1}H-NMR spectra with that of the commercially available sample purchased from TCI. Compounds **2j, 2s, 2t, 3b, 3c, 3j, 3s, 3t, 4b, 4c**, **5e** and **5r** were identified by the comparison of spectroscopic characteristics with the authentic samples reported in the literature.[1-9]

2. Experimental procedures

General procedure for the bromination of aromatic compounds in MeCN

CSA (23 mg, 1 mol%) and $BiCl_3$ (32 mg, 1 mol%) were added to the solution of **1d** (1.20 g, 10 mmol) in dry MeCN (10 mL) at room temperature under an atmosphere of air. NBS (1.87 g, 10.5 mmol) was added to the solution. After stirring the mixture at room temperature for 1 h, saturated $NaHCO_3$ (15 mL) was added and the mixture was extracted with Et_2O (50 mL) twice. The combined extracts were washed with water (25 mL × 2), dried and evaporated. The residue was purified by column chromatography on silica gel using heptane as eluent to give **2d** (1.93 g, 97%).

General procedure for the chlorination of aromatic compounds in MeCN

CSA (46 mg, 2 mol%) and $BiCl_3$ (64 mg, 2 mol%) were added to the solution of **1d** (1.20 g, 10 mmol) in dry MeCN (10 mL) at room temperature under an atmosphere of air. NCS (1.40 g, 10.5 mmol) was added to the solution. After stirring the mixture at 80 °C for 3 h, saturated $NaHCO_3$ (15 mL) was added and the mixture was extracted with Et_2O (50 mL) twice. The combined extracts were washed with water (25 mL × 2), dried and evaporated. The residue was purified by column chromatography on silica gel using heptane as eluent to give **3d** (1.48 g, 96%).

General procedure for the iodination of aromatic compounds in MeCN

CSA (116 mg, 5 mol%) and $BiCl_3$ (158 mg, 5 mol%) were added to the solution of **1d** (1.20 g, 10 mmol) in dry MeCN (10 mL) at room temperature under an atmosphere of air. NIS (2.36 g, 10.5 mmol) was added to the solution. After stirring the mixture at 80 °C for 4 h, saturated $NaHCO_3$ (15

mL) was added and the mixture was extracted with Et_2O (50 mL) twice. The combined extracts were washed with water (25 mL × 2), dried and evaporated. The residue was purified by column chromatography on silica gel using heptane as eluent to give **4d** (2.36 g, 96%).

One-pot bromination followed by Suzuki-Miyaura cross-coupling

After the completion of the bromination of **1g**, $PhB(OH)_2$ (1.464 g, 12 mmol), K_2CO_3 (2.76 g, 20 mmol), H_2O (10 mL) and $PdCl_2(PPh_3)_2$ (210 mg, 3 mol%) were added in succession at room temperature. The mixture was degassed with nitrogen 4 times. After stirring the mixture at 80 °C for 4 h, water (30 mL) was added and the mixture was extracted with toluene (80 mL) twice. The combined extracts were washed with water (50 mL × 2), dried and evaporated. The residue was purified by column chromatography on silica gel using heptane as eluent to give **5g** (1.98 g, 97%).

One-pot bromination followed by Sonogashira coupling

After the completion of the bromination of **1g**, phenylacetylene (1.12 g, 11 mmol), dry MeCN (40 mL), Et_3N (2.02 g, 20 mmol), CuI (96 mg, 0.5 mmol, 5 mol%) and $PdCl_2(PPh_3)_2$ (210 mg, 0.3 mmol, 3 mol%) were added in succession at room temperature. The mixture was degassed with nitrogen 4 times. After stirring the mixture at 90 °C for 12 h, the reaction mixture was evaporated under reduced pressure. Water (50 mL) was added and the mixture was extracted with toluene (80 mL) twice. The combined extracts were washed with water (50 mL × 3), dried and evaporated. The residue was purified by column chromatography on silica gel using heptane as eluent to give **6g** (1.64 g, 72%).

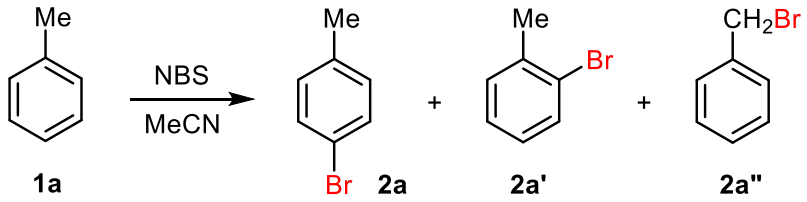
One-pot bromination followed by Miyaura borylation

After the completion of the bromination of **1g**, dry DMSO (60 mL), $(Bpin)_2$ (2.80 g, 11 mmol), KOAc (2.94 g, 30 mmol) and $PdCl_2(dppf)$ [dppf = 1,1'-bis(diphenylphosphino)ferrocece] (220 mg,

0.3 mmol, 3 mol%) were added in succession at room temperature. The mixture was degassed with nitrogen 4 times. After stirring the mixture at 80 °C for 24 h, the reaction mixture was extracted with toluene (80 mL) twice. The combined extracts were washed with water (50 mL × 3), dried and evaporated. The residue was purified by column chromatography on silica gel using heptane as eluent. Bromide **2g** was obtained in 82% (1.70 g).

3. Tables

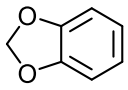
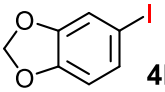
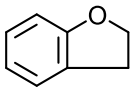
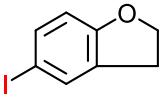
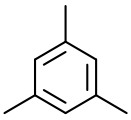
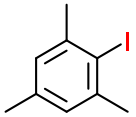
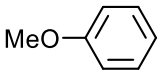
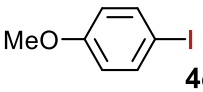
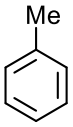
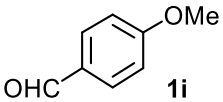
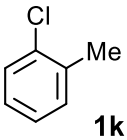
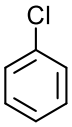
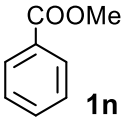
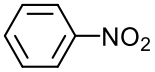
Table S1 Bromination of toluene (**1a**) using catalytic amounts of Lewis acids and additives[a]



Entry	Lewis acid	Additive	Time	**2a** (%)[b]	**2a'** (%)[b]	**2a"** (%)[b]
1	$NbCl_5$	1,2,2,6,6-penta-methylpiperidine	6 h	6	4	17
2	$NbCl_5$	Ph_3P	6 h	17	9	53
3	$B(C_6F_5)_3$	Ph_3P	6 h	17	10	30
4	$NbCl_5$	Bu_4PBPh_4	6 h	5	5	trace

[a] Conditions: toluene **1a** (10 mmol), Lewis acid (10 mol%), additive (10 mol%), NBS (10.5 mmol), dry MeCN (10 mL), room temp. [b] Determined by ^{1}H-NMR spectroscopy using TCE.

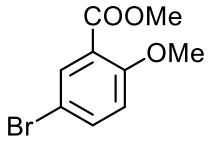
Table S2 Iodination of aromatic rings with NIS in MeCN[a]

Entry	ArH	$CSA–BiCl_3$ (mol%)	Temp (°C)	Time (h)	ArI / Yield (%)[b]
1	 **1b**	5	80	24	 **4b** 95
2	 **1c**	5	80	12	 **4c** 94
3	 **1d**	5	80	4	 **4d** 96
4	 **1e**	2	80	7	 **4e** 97
5	 **1a**	10	80	26	NR
6[c]		10	80	16	NR
7	 **1i**	10	80	16	NR
8[c]		10	80	16	NR
9[c]	 **1k**	10	80	16	NR
10[c]	 **1l**	10	80	16	NR
11[c]	 **1m**	10	80	16	NR
12[c]	 **1n**	10	100	16	NR
13[c]	 **1o**	10	120	24	NR

[a] Conditions: ArH **1** (10 mmol), NIS (10.5 mmol), dry MeCN (10 mL), [b] Isolated yield. [c] Without MeCN .

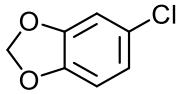
5. Analytical data of compounds 2j, 2s, 2t, 3b, 3c, 3j, 3s, 3t, 4b, **4c**, **5e** and **5r**

Methyl 5-bromo-2-methoxybenzoate (**2j**)[1]



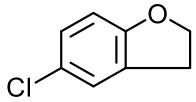
Colourless oil; IR (neat) 3106, 3078, 3005, 2950, 2905, 2842, 1732, 1717, 1594, 1572, 1488, 1463, 1435, 1395, 1300, 1275, 1251, 1182, 1151, 1099, 1083, 1023, 968, 899, 850, 813, 783, 707, 677, 625, 582 and 529 cm^{-1}; ^{1}H-NMR ($CDCl_3$) δ = 3.89 (6H, s), 6.87 (1H, d, *J* = 8.9 Hz), 7.55 (1H, dd, *J* = 8.9 and 2.6 Hz) and 7.91 (1H, d, *J* = 2.6 Hz); ^{13}C-NMR ($CDCl_3$) δ = 52.3, 56.3, 112.2, 113.9, 134.2, 136.1, 158.3 and 165.3.

5-Chlorobenzo[d][1,3]dioxole (**3b**)[2]



Colourless oil; IR (neat) 3110, 3080, 3011, 2979, 2898, 2779, 1625, 1606, 1504, 1476, 1425, 1341, 1236, 1156, 1124, 1105, 1039, 936, 889, 849, 801, 741, 724, 690, 662, 582, 443 and 419 cm^{-1}; ^{1}H-NMR ($CDCl_3$) δ = 5.97 (2H, s), 6.72 (1H, d, *J* = 8.3 Hz), 6.79 (1H, dd, *J* = 8.3 and 2.0 Hz) and 6.82 (1H, d, *J* = 2.0 Hz); ^{13}C-NMR ($CDCl_3$) δ = 101.7, 108.9, 109.6, 121.3, 126.3, 146.5 and 148.3.

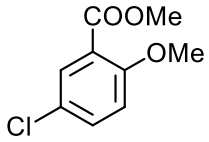
5-Chloro-2,3-dihydrobenzofuran (**3c**)[3]



Colourless plates, mp 36-37 °C; IR (KBr) 3098, 3062, 3038, 2979, 2948, 2904, 2861, 1634, 1605, 1591, 1482, 1469, 1441, 1424, 1362, 1302, 1279, 1233, 1161, 1108, 1066, 983, 943, 882, 809, 752, 709, 679, 581, 545 and 420 cm^{-1}; ^{1}H-NMR ($CDCl_3$) δ = 3.19 (2H, t, *J* = 8.7 Hz), 4.58 (2H, t, *J* = 8.7

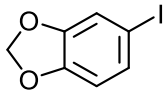
Hz), 6.69 (1H, d, *J* = 8.4 Hz), 7.05 (1H, dd, *J* = 8.4 and 2.2 Hz) and 7.14 (1H, d, *J* = 2.2 Hz) ; ^{13}C-NMR ($CDCl_3$) δ = 29.5, 71.4, 81.6, 111.7, 130.1, 133.7, 136.7 and 160.0.

Methyl 5-chloro-2-methoxybenzoate (**3j**)[4]



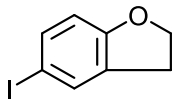
Colourless oil; IR (neat) 3078, 3004, 2950, 2904, 2841, 1733, 1595, 1578, 1489, 1463, 1436, 1396, 1301, 1275, 1250, 1182, 1151, 1131, 1098, 1084, 1050, 1023, 967, 899, 850, 813, 783, 758, 706, 676, 625 and 529 cm^{-1}; ^{1}H-NMR ($CDCl_3$) δ = 3.89 (6H, s), 6.92 (1H, d, *J* = 8.9 Hz), 7.42 (1H, dd, *J* = 8.9 and 2.7 Hz) and 7.77 (1H, d, *J* = 2.7 Hz); ^{13}C-NMR ($CDCl_3$) δ = 52.3, 56.3, 113.4, 121.2, 125.2, 131.4, 133.1, 157.8 and 165.4.

5-Iodobenzo[d][1,3]dioxole (**4b**)[5]



Colourless oil; IR (neat) 3090, 3071, 3006, 2971, 2982, 2776, 1617, 1596, 1498, 1472, 1413, 1398, 1334, 1230, 1155, 1105, 1040, 935, 864, 799, 740, 718, 662, 568, 429 and 412 cm^{-1}; ^{1}H-NMR ($CDCl_3$) δ = 5.95 (2H, s), 6.59 (1H, d, *J* = 8.1 Hz), 7.12 (1H, d, *J* = 1.6 Hz) and 7.14 (1H, dd, J = 8.1 and 1.6 Hz); ^{13}C-NMR ($CDCl_3$) δ = 82.2, 101.4, 110.5, 117.7, 130.6, 147.8 and 148.7.

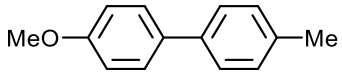
5-Iodo-2,3-dihydrobenzofuran (**4c**)[6]



Colourless needles, mp 64-65 °C; IR (KBr) 3088, 2989, 2960, 2898, 2846, 1597, 1574, 1473, 1433, 1407, 1363, 1297, 1284, 1231, 1187, 1158, 1132, 1107, 1084, 1047, 978, 942, 891, 816, 673, 632 and

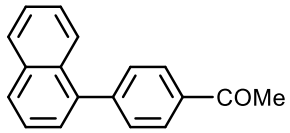
541 cm^{-1}; ^{1}H-NMR ($CDCl_3$) δ = 3.20 (2H, t, J = 8.8 Hz), 4.56 (2H, t, *J* = 8.8 Hz), 6.57 (1H, d, *J* = 8.4 Hz), 7.38 (1H, d, *J* = 8.4 and 1.0 Hz) and 7.47 (1H, s); ^{13}C-NMR ($CDCl_3$) δ = 29.5, 71.4, 81.6, 111.7, 130.1, 133.7, 136.7 and 160.0.

4-Methoxy-4'-methyl-1,1'-biphenyl (**5e**)[7]



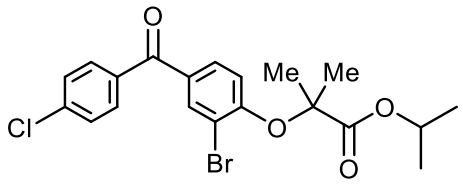
Colourless plates, mp 106-107 °C; IR (KBr) 3070, 3022, 2957, 2940, 2920, 2840, 1654, 1607, 1583, 1531, 1501, 1455, 1400, 1317, 1289, 1270, 1253, 1220, 1183, 1138, 1116, 1038, 1013, 842, 808, 784, 723 and 499 cm^{-1}; ^{1}H-NMR ($CDCl_3$) δ = 2.38 (3H, s), 3.84 (3H, s), 6.97 (2H, d, *J* = 7.8 Hz), 7.22 (2H, d, *J* = 8.8 Hz), 7.44 (2H, d, *J* = 7.8 Hz) and 7.51 (2H, d, *J* = 8.8 Hz); ^{13}C-NMR ($CDCl_3$) δ = 21.0, 55.3, 114.1, 126.6, 127.9, 129.4, 133.7, 136.3, 138.0 and 158.9.

1-(4-(Naphthalen-1-yl)phenyl)ethan-1-one (**5r**)[8]



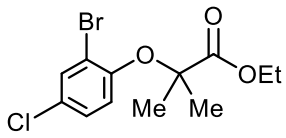
Colourless needles, mp 97-98 °C; IR (KBr) 3348, 3082, 3055, 3034, 3005, 1682, 1605, 1589, 1561, 1418, 1402, 1356, 1309, 1285, 1268, 1256, 1186, 1111, 1016, 959, 849, 806, 791, 780, 662, 605, 569 and 436 cm^{-1}; ^{1}H-NMR ($CDCl_3$) δ = 2.69 (3H, s), 7.42-7.46 (2H, m), 7.50-7.55 (2H, m), 7.61 (2H, d, *J* = 8.3 Hz), 7.84 (1H, d, *J* = 8.5 Hz), 7.90 (1H, d, *J* = 8.3 Hz), 7.92 (1H, d, *J* = 8.1 Hz) and 8.09 (2H, d, *J* = 8.3 Hz); ^{13}C-NMR ($CDCl_3$) δ = 26.7, 125.3, 125.6, 126.0, 126.4, 126.9, 128.4, 128.4, 128.4, 130.3, 131.2, 133.8, 136.0, 139.0 and 197.9.

Fenofibrate-Br (**2s**)[9]



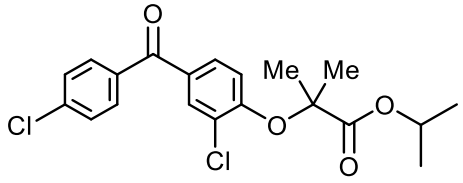
Colourless needles, mp 62-63 °C; IR (KBr) 3094, 3069, 3054, 2985, 2936, 1719, 1658, 1587, 1557, 1481, 1462, 1398, 1382, 1375, 1297, 1267, 1246, 1178, 1149, 1108, 1090, 1041, 1016, 970, 947, 934, 912, 847, 794, 761, 745, 700, 673, 659, 581, 485 and 423 cm^{-1}; ^{1}H-NMR ($CDCl_3$) δ = 1.22 (6H, d, *J* = 6.3 Hz), 1.70 (6H, s), 5.09 (1H, qq, *J* = 6.3 and 6.3 Hz), 6.82 (1H, d, *J* = 8.6 Hz), 7.47 (2H, d, *J* = 8.5 Hz), 7.63 (1H, dd, *J* = 8.6 and 2.2 Hz), 7.70 (2H, d, *J* = 8.5 Hz) and 8.03 (1H, d, *J* = 2.2 Hz); ^{13}C-NMR ($CDCl_3$) δ = 21.5, 25.3, 69.5, 81.1, 114.9, 116.5, 128.7, 130.2, 131.2, 131.5, 135.6, 135.8, 138.8, 156.4, 172.7 and 193.1.

Clofibrate-Br (**2t**)[9]



Colourless oil; IR (Neat) 3094, 3073, 2987, 2938, 2904, 2872, 1736, 1581, 1563, 1473, 1383, 1365, 1286, 1242, 1178, 1139, 1097, 1045, 1023, 968, 911, 867, 808, 767, 733, 720, 688, 653, 554 and 439 cm^{-1}; ^{1}H-NMR ($CDCl_3$) δ = 1.27 (3H, t, *J* = 7.1 Hz), 1.61 (6H, s), 4.25 (2H, q, *J* = 7.1 Hz), 6.82 (1H, d, *J* = 8.8 Hz), 7.14 (1H, dd, *J* = 8.8 and 2.5 Hz) and 7.54 (1H, d, *J* = 2.5 Hz); ^{13}C-NMR ($CDCl_3$) δ = 14.1, 25.1, 61.7, 81.2, 116.8, 120.1, 127.9, 133.0, 151.5 and 173.7.

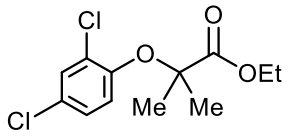
Fenofibrate-Cl (**3s**)[9]



Colourless prisms, mp 85-86 °C; IR (KBr) 3100, 3074, 3058, 2985, 2936, 2876, 1717, 1653, 1588,

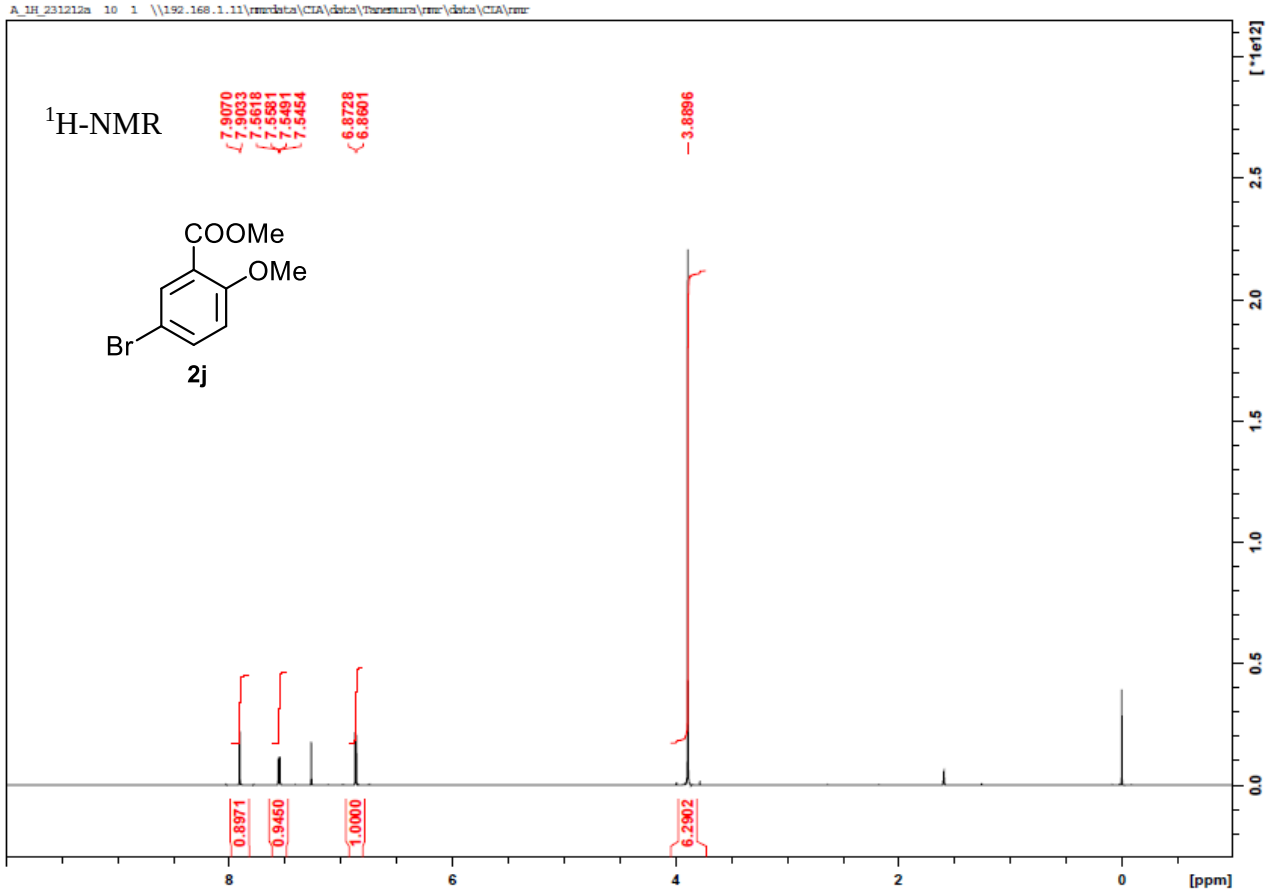
1562, 1485, 1461, 1399, 1382, 1297, 1268, 1241, 1199, 1179, 1156, 1107, 1089, 1053, 1014, 969, 935, 914, 850, 836, 821, 797, 764, 748, 704, 687, 656, 581, 545, 490, 480 and 427 cm^{-1}; ^{1}H-NMR ($CDCl_3$) δ = 1.22 (6H, d, *J* = 6.3 Hz), 1.69 (6H, s), 5.10 (1H, qq, *J* = 6.3 and 6.3Hz), 6.85 (1H, d, *J* = 8.6 Hz), 7.47 (2H, d, *J* = 8.5 Hz), 7.59 (1H, dd, *J* = 8.6 and 2.2 Hz), 7.70 (2H, d, *J* = 8.5 Hz) and 7.86 (1H, d, *J* = 2.2 Hz); ^{13}C-NMR ($CDCl_3$) δ = 21.5, 25.2, 69.5, 81.0, 116.9, 125.6, 128.7, 129.4, 131.2, 132.5, 135.8, 138.8, 155.5, 172.7 and 193.2.

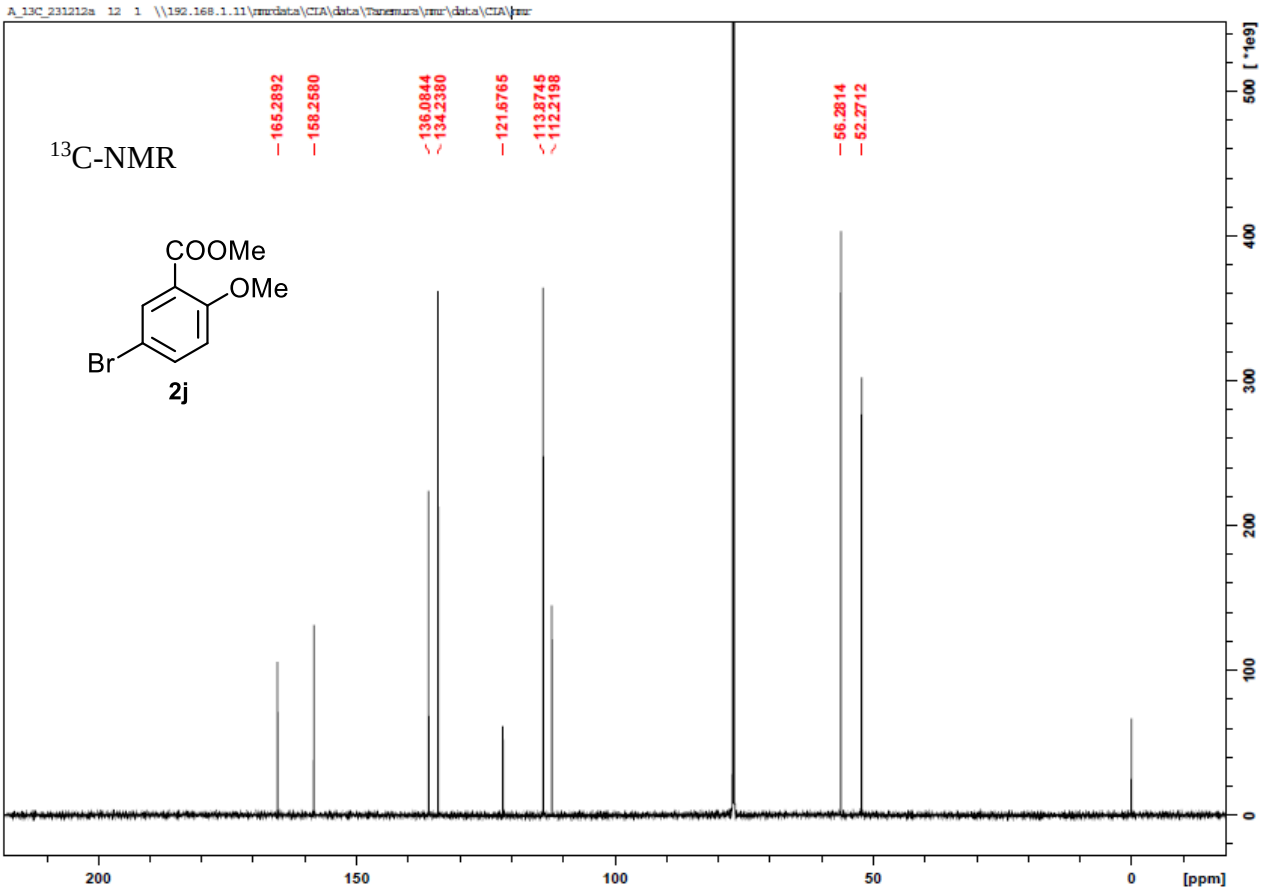
Clofibrate-Cl (**3t**)[9]

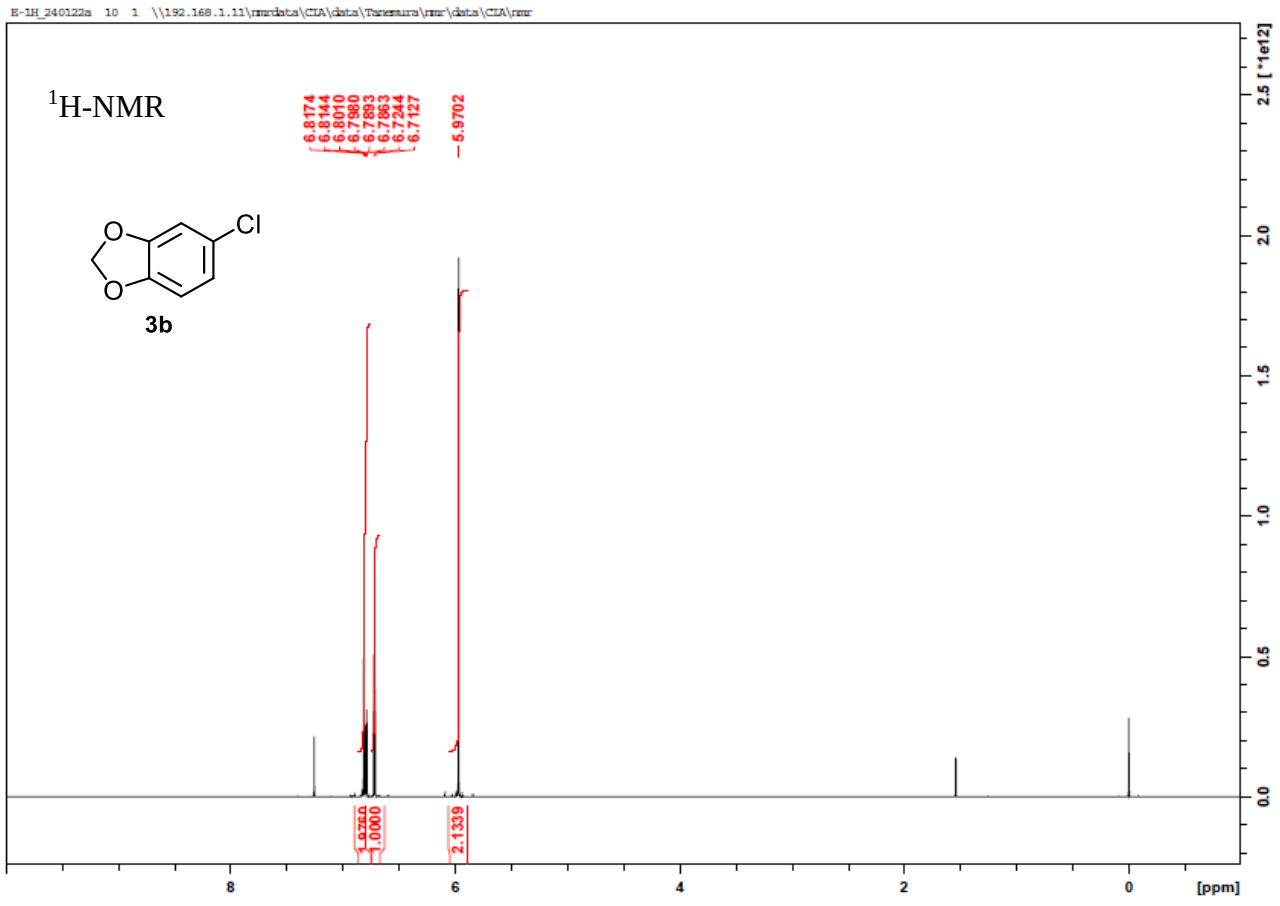


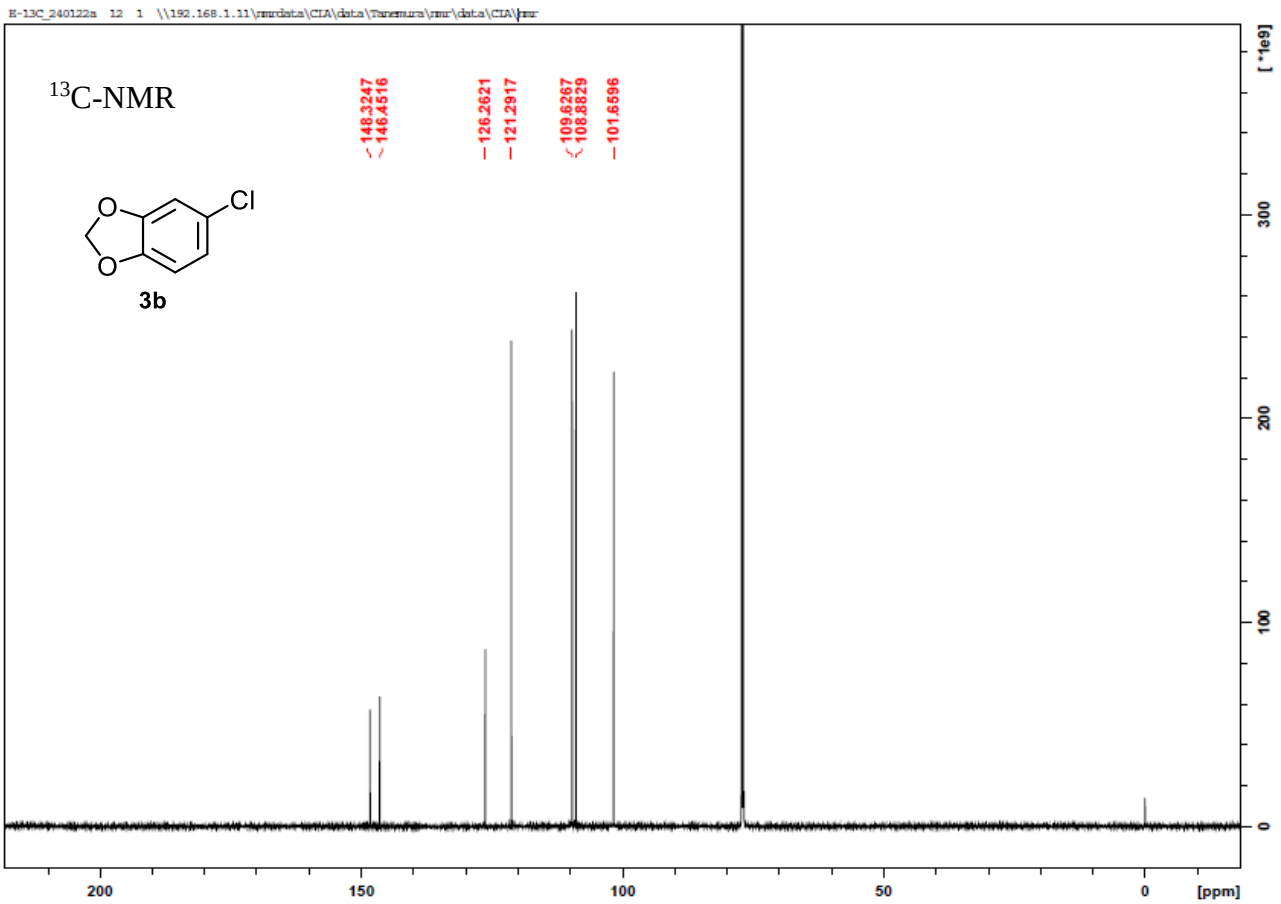
Colourless oil; IR (Neat) 3076, 2987, 2939, 2905, 2872, 1737, 1584, 1476, 1387, 1366, 1288, 1244, 1178, 1138, 1103, 1059, 1023, 968, 910, 866, 808, 768, 741, 698, 657, 559 and 442 cm^{-1}; ^{1}H-NMR ($CDCl_3$) δ = 1.27 (3H, t, *J* = 7.1 Hz), 1.60 (6H, s), 4.25 (2H, q, *J* = 7.1 Hz), 6.85 (1H, d, *J* = 8.8 Hz), 7.10 (1H, dd, *J* = 8.8 and 2.5 Hz) and 7.37 (1H, d, *J* = 2.5 Hz); ^{13}C-NMR ($CDCl_3$) δ = 14.1, 25.0, 61.6, 81.2, 120.7, 127.2, 127.6, 127.7, 130.1, 150.4 and 173.7.

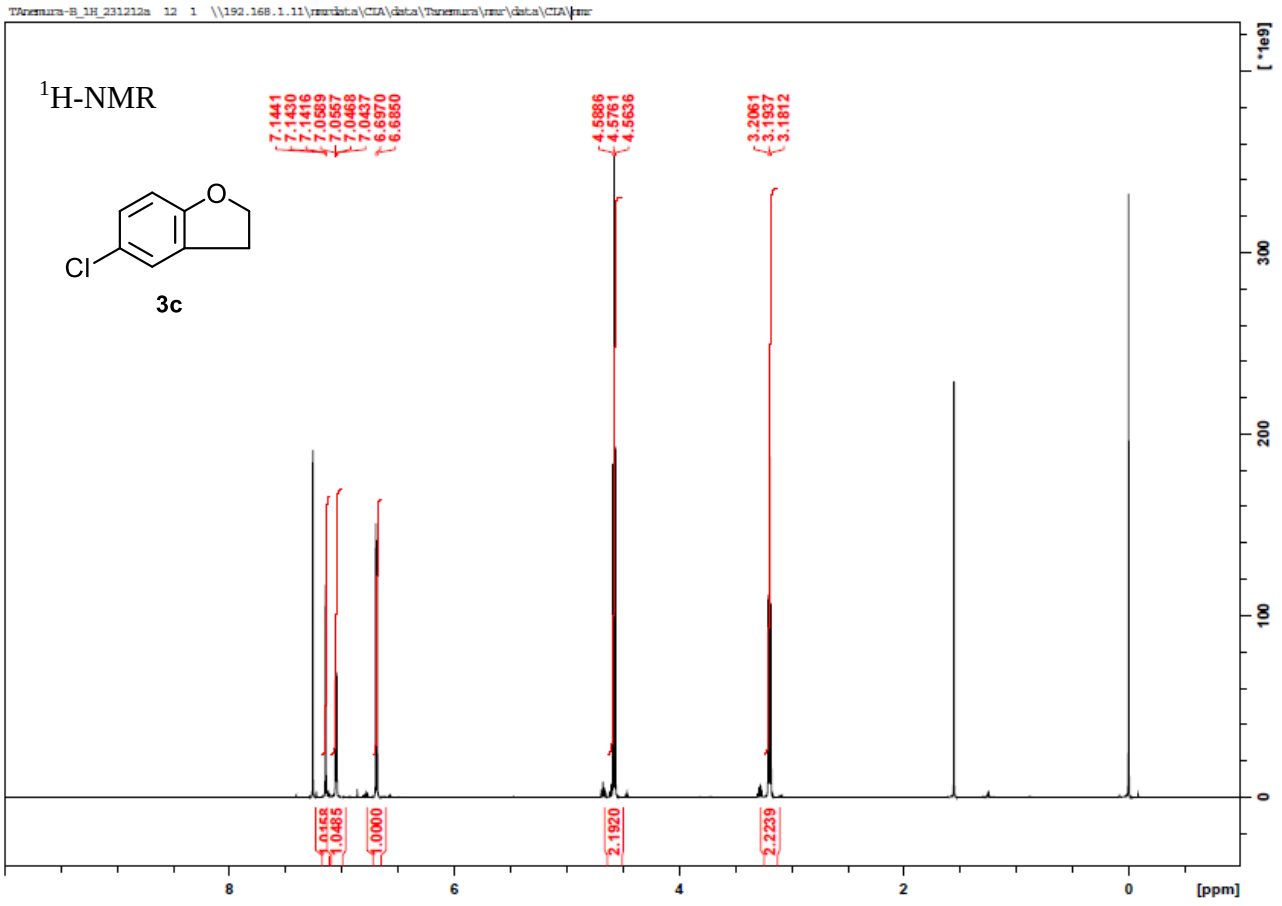
6. ^{1}H- and ^{13}C-NMR spectra of 2j, 2s, 2t, 3b, 3c, 3j, 3s, 3t, 4b, 4c, 5e and 5r

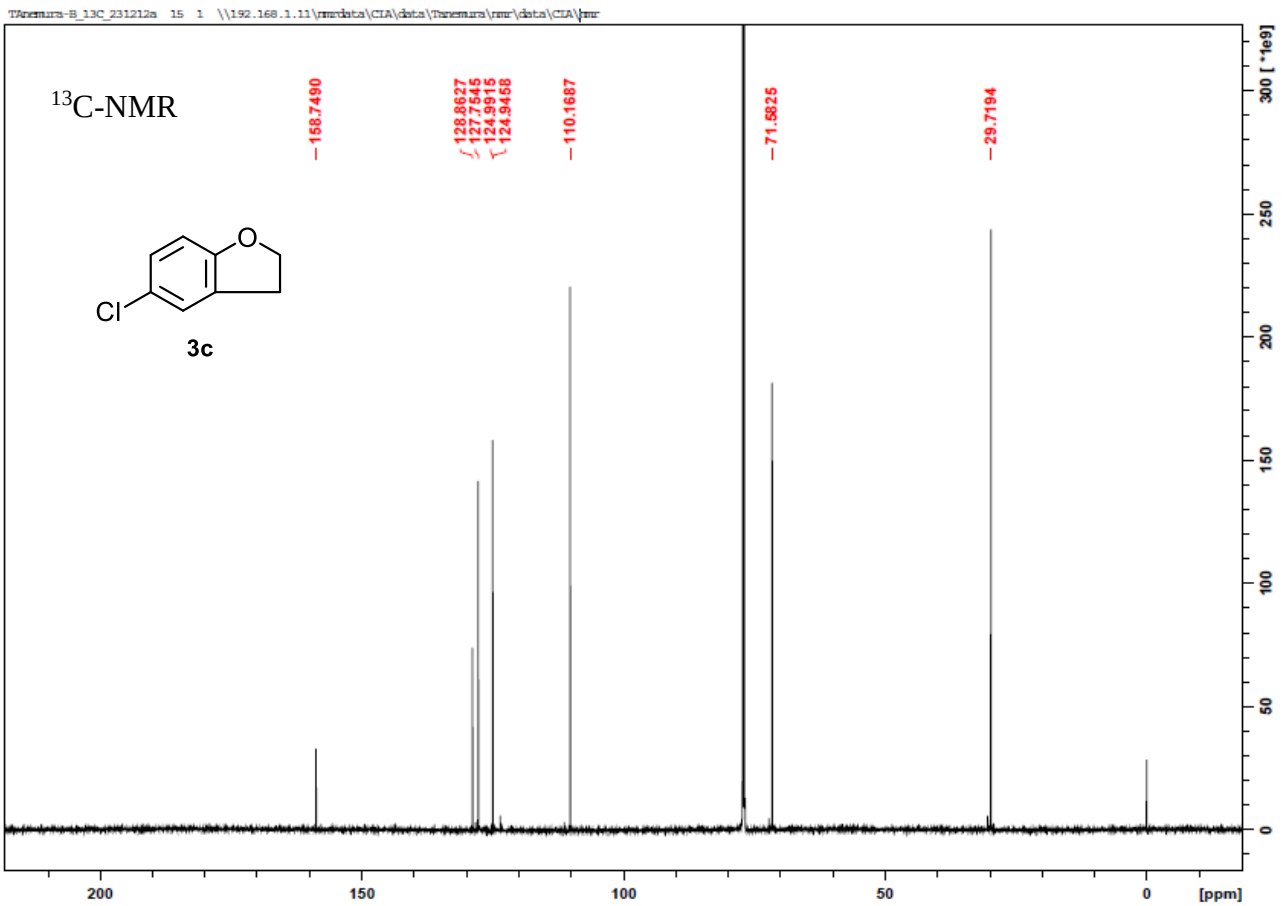


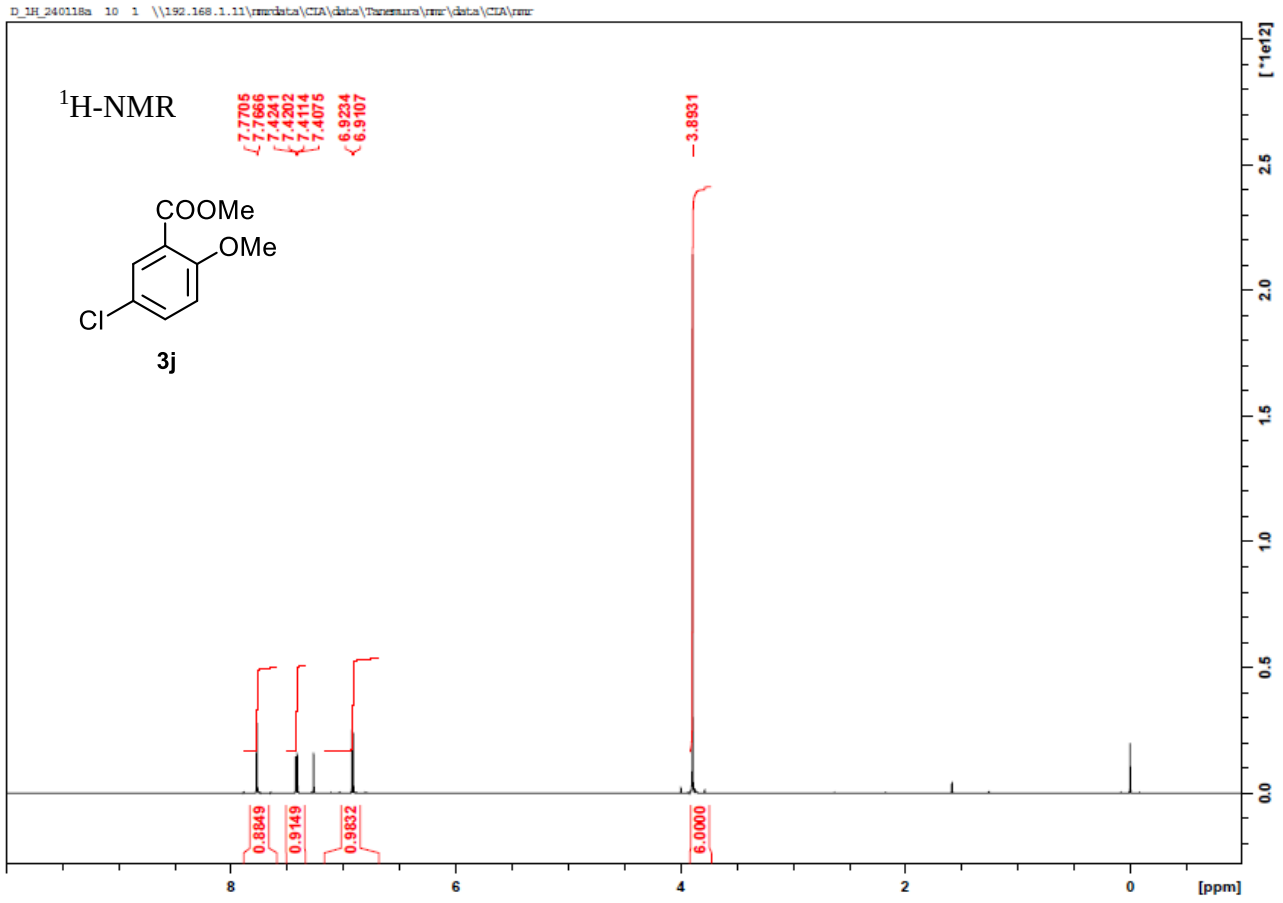


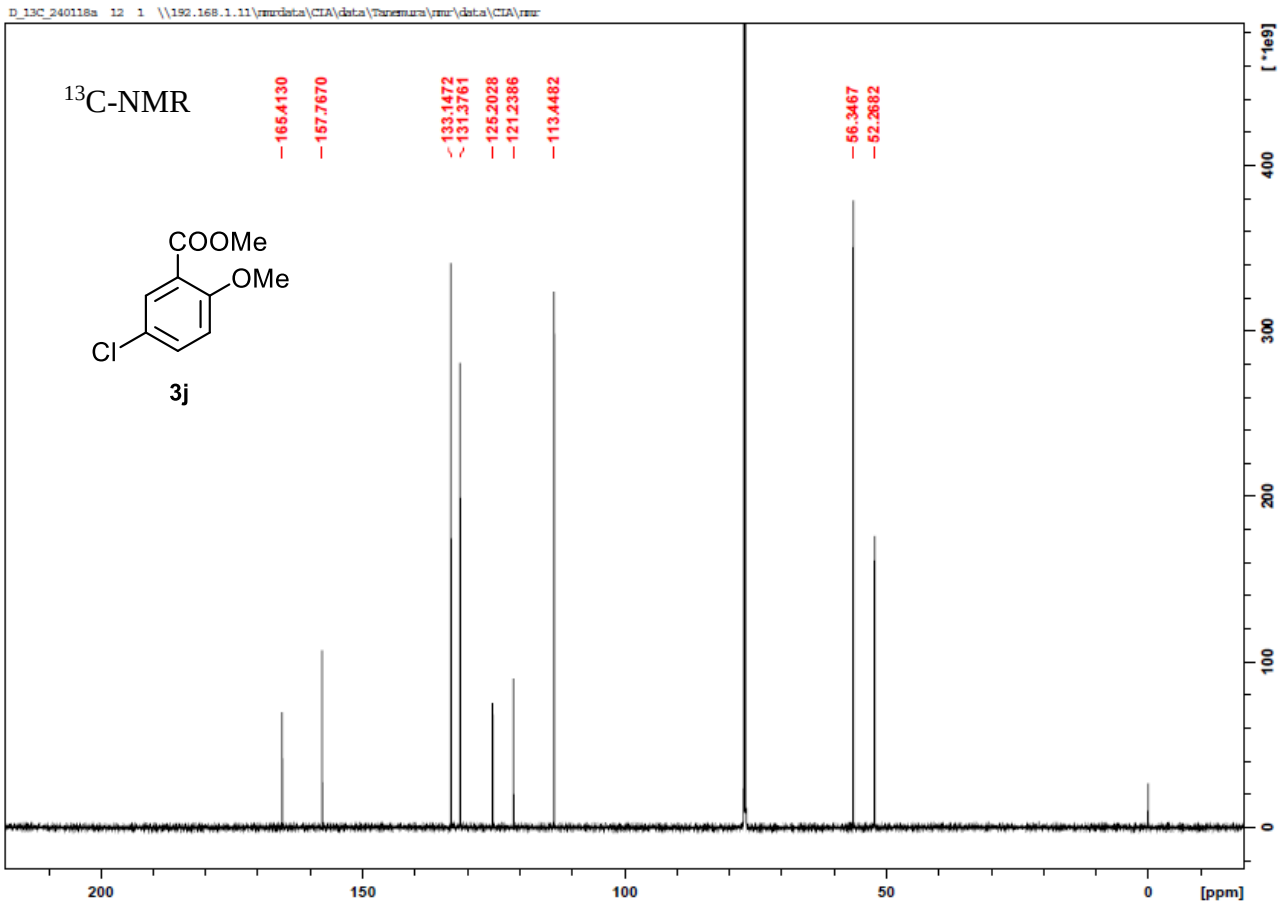

^{1}H-NMR
6.8174
6.8144
6.8010
6.7980
6.7893
6.7863
6.7244
6.7127
5.9702
Cl
O
O
3b
1.0000
2.1339
8
6
4
2
0
[ppm]
2.5 [*1e12]
2.0
1.5
1.0
0.5
0.0

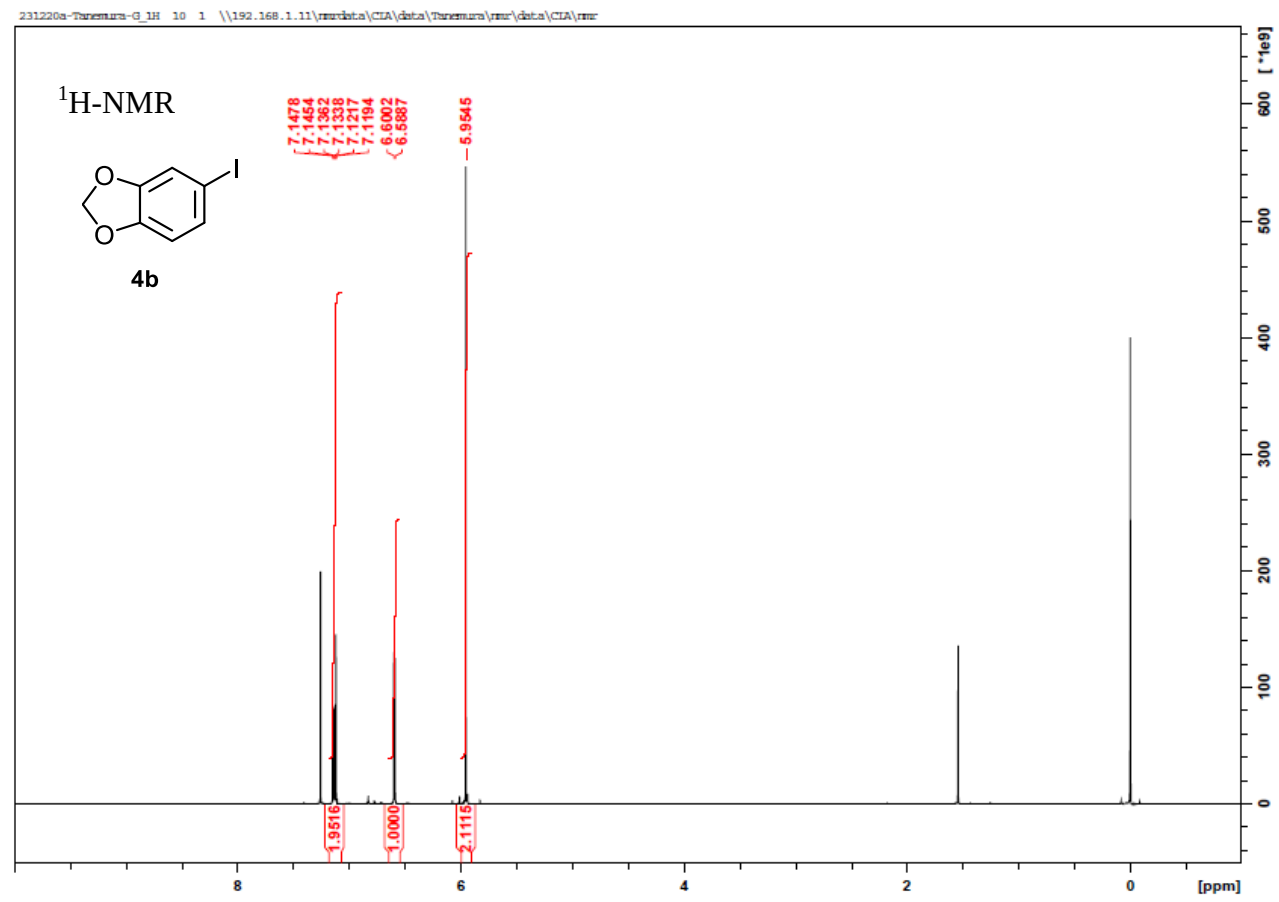

^{13}C-NMR
148.3247
146.4516
126.2621
121.2917
109.6267
108.8829
101.6596
Cl
O
O
3b
200
150
100
50
0
[ppm]
[*1e9]
300
200
100
0

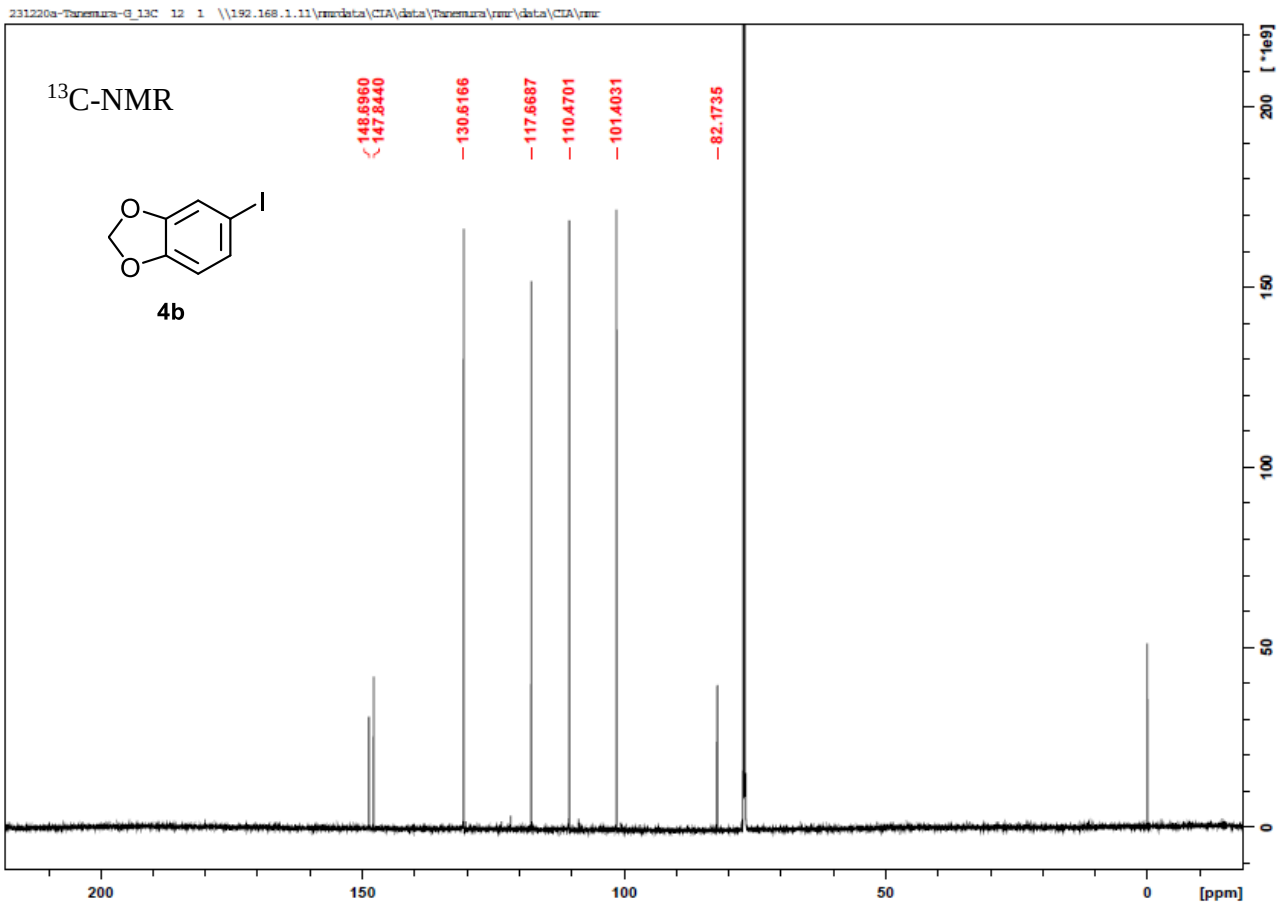

^{1}H-NMR
7.1441
7.1430
7.1416
7.0589
7.0557
7.0468
7.0437
6.6970
6.6850
4.5886
4.5761
4.5636
3.2061
3.1937
3.1812
1.0158
1.0485
1.0000
2.1920
2.2239
[*1e9]
[ppm]
Cl
O
3c

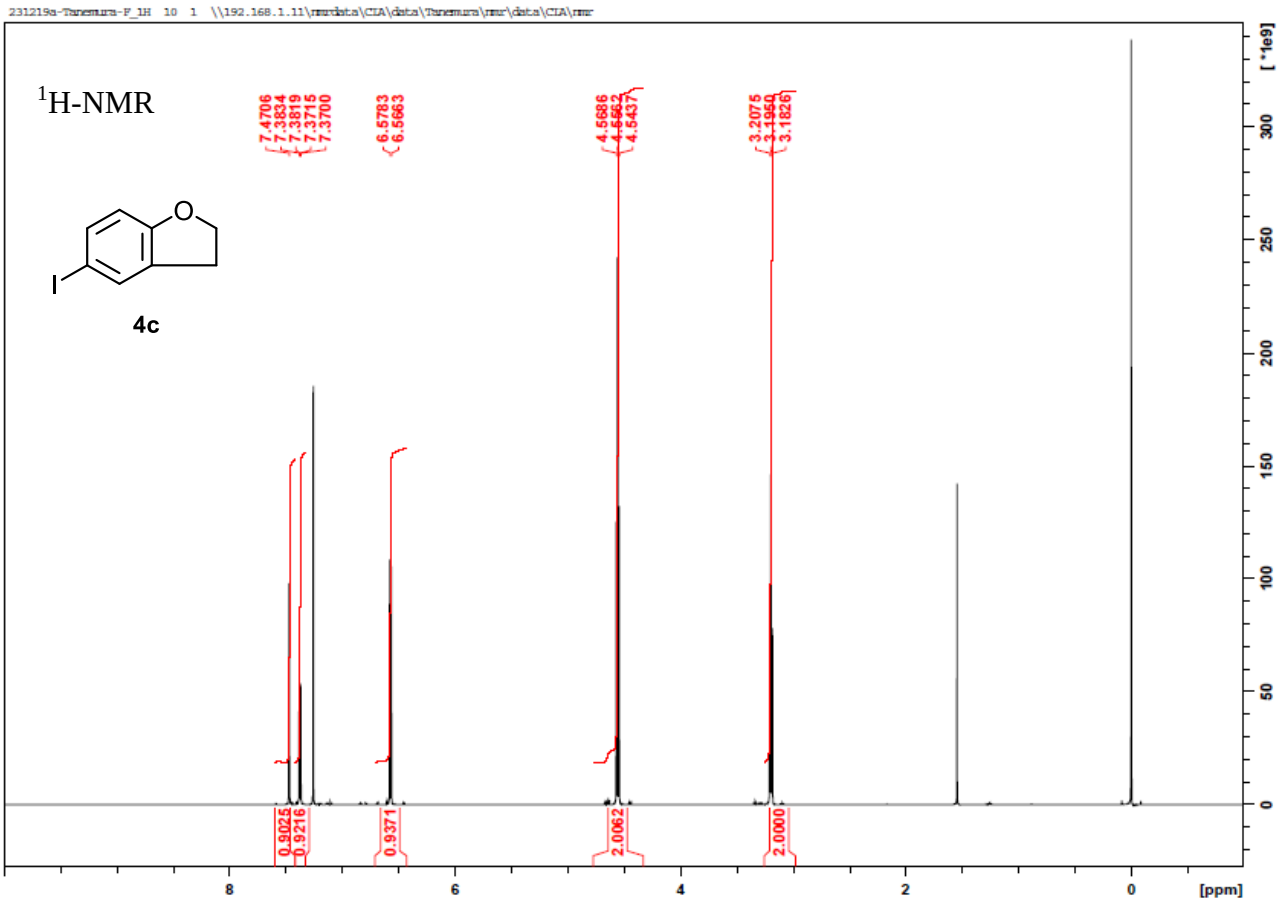

^{13}C-NMR
158.7490
128.8627
127.7545
124.9915
124.9458
110.1687
71.5825
29.7194
300 [*1e9]
[ppm]
Cl
O
3c

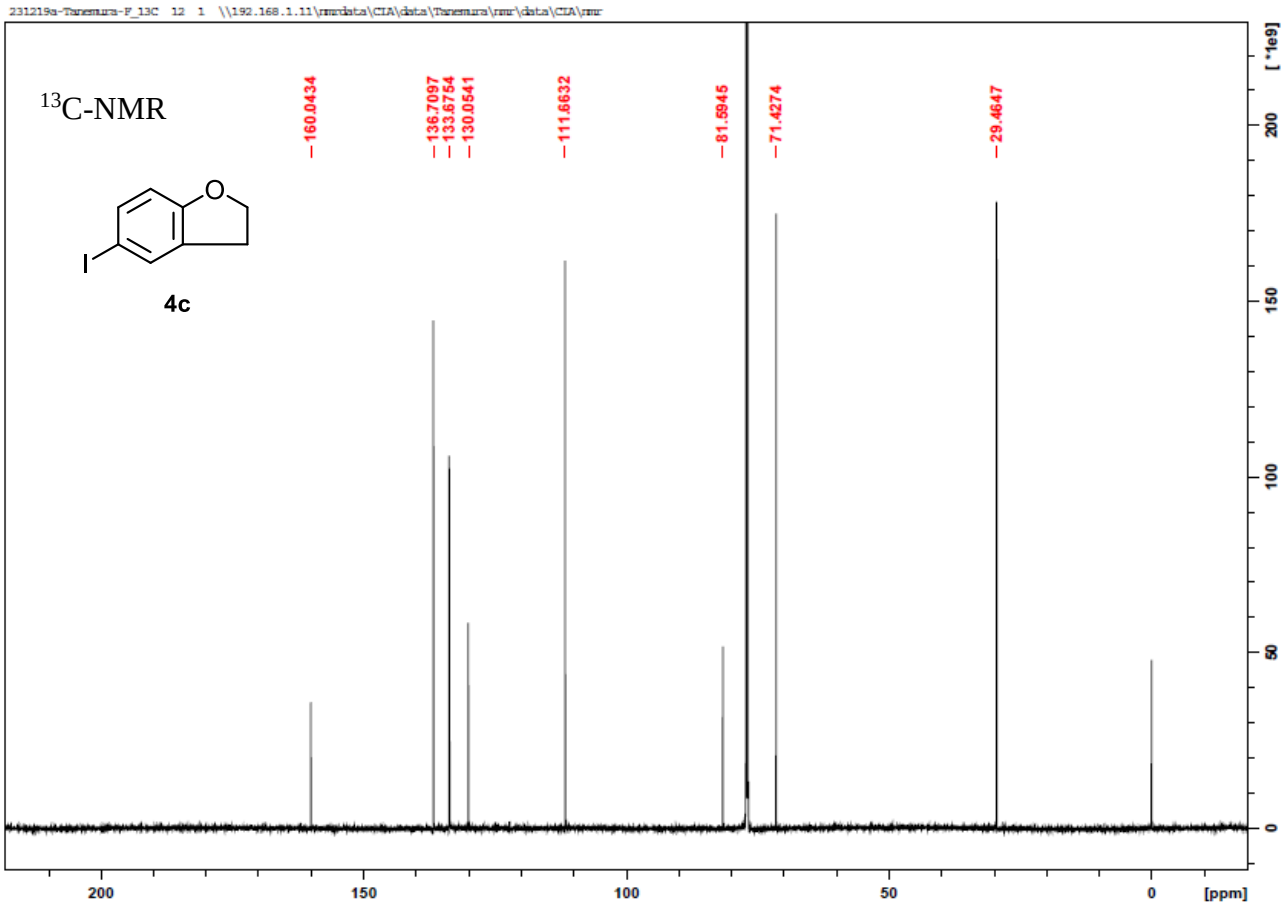

^{1}H-NMR
7.7705
7.7666
7.4261
7.4202
7.4114
7.4075
6.9234
6.9107
3.8931
COOMe
OMe
Cl
3j
0.8849
0.9149
0.9832
6.0000
[*1e12]
[ppm]

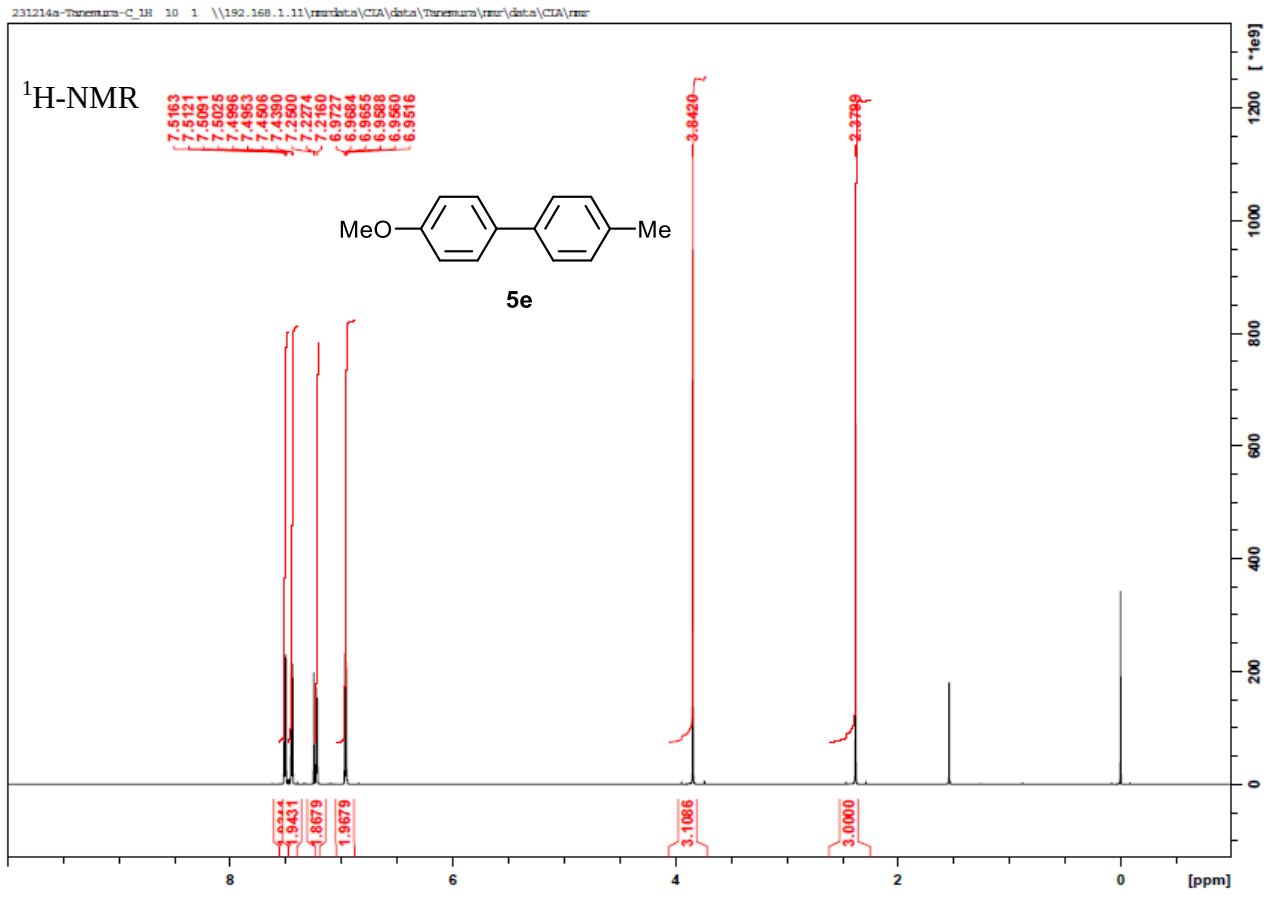

^{13}C-NMR
165.4130
157.7670
133.1472
131.3761
125.2028
121.2386
113.4482
56.3467
52.2682
COOMe
OMe
Cl
3j
[*1e9]
[ppm]

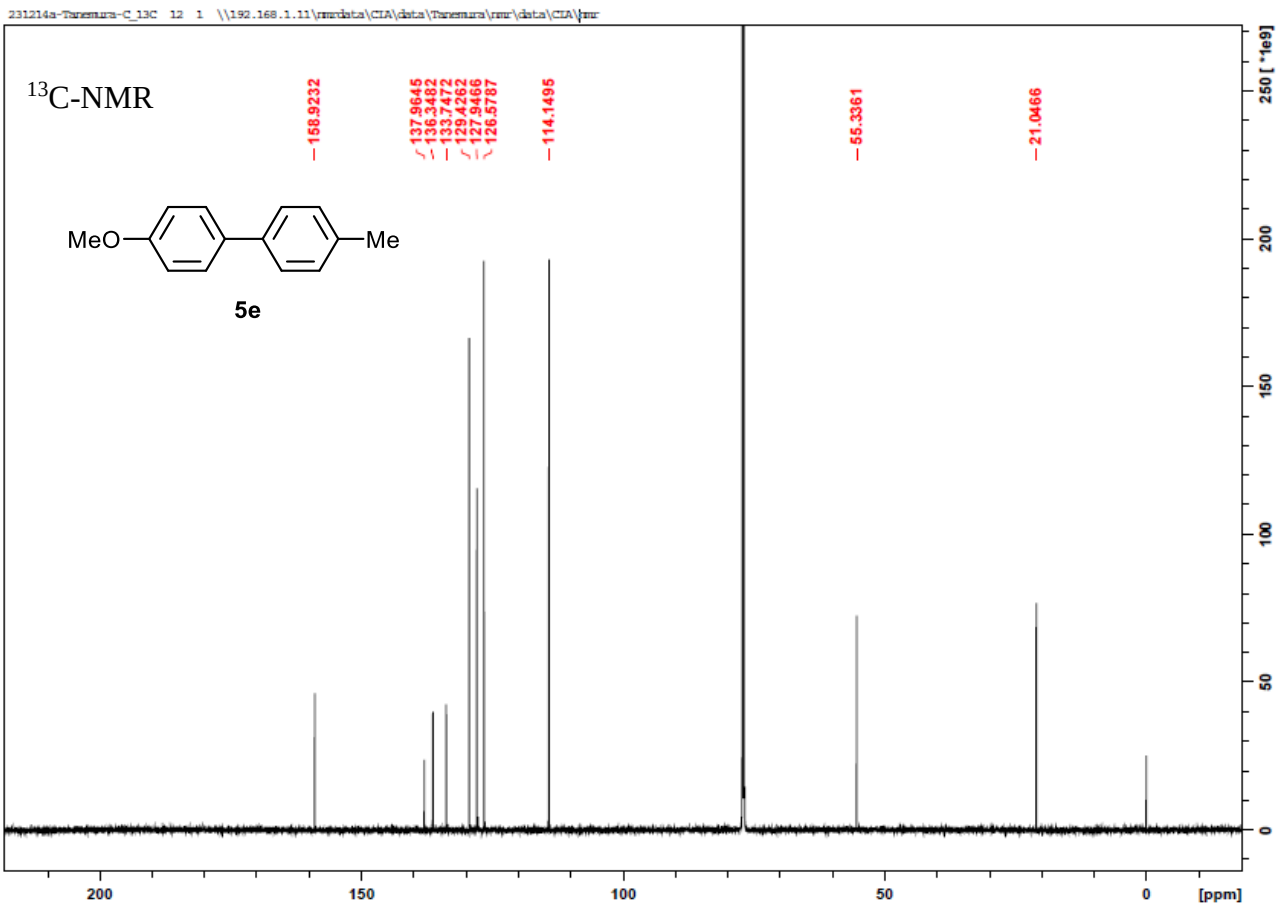

231220a-Tanemura-G_1H 10 1 \\192.168.1.11\nmrdata\CIA\data\Tanemura\nmr\data\CIA\nmr
1H-NMR
4b
7.1478
7.1454
7.1362
7.1338
7.1217
7.1194
6.6002
6.5887
5.9545
1.9516
1.0000
2.1115
8
6
4
2
0
[ppm]
[*1e9]

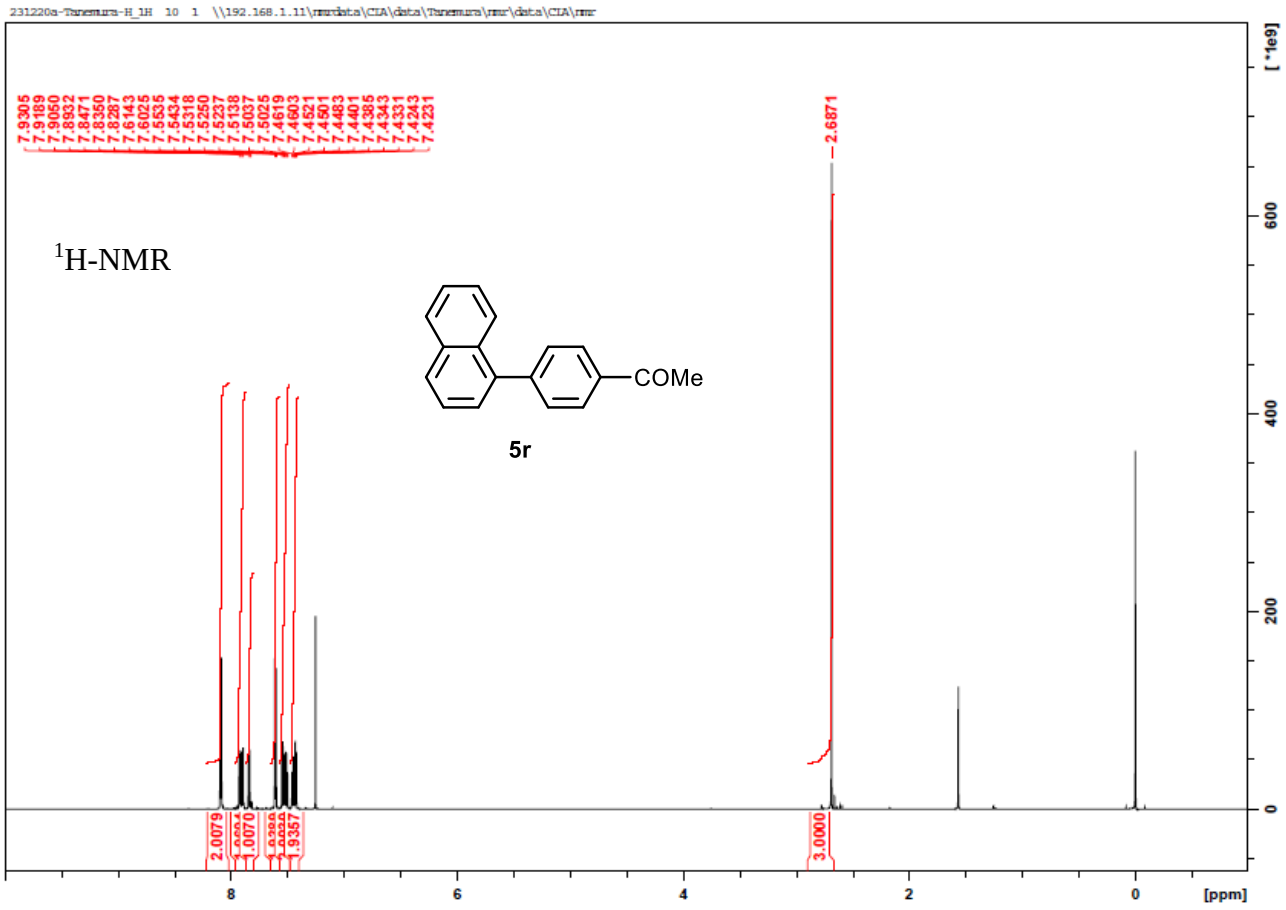

231220a-Tanemura-G_13C 12 1 \\192.168.1.11\nmrdata\CIA\data\Tanemura\nmr\data\CIA\nmr
13C-NMR
4b
148.6960
147.8440
130.6166
117.6687
110.4701
101.4031
82.1735
200
150
100
50
0
[ppm]
[*1e9]

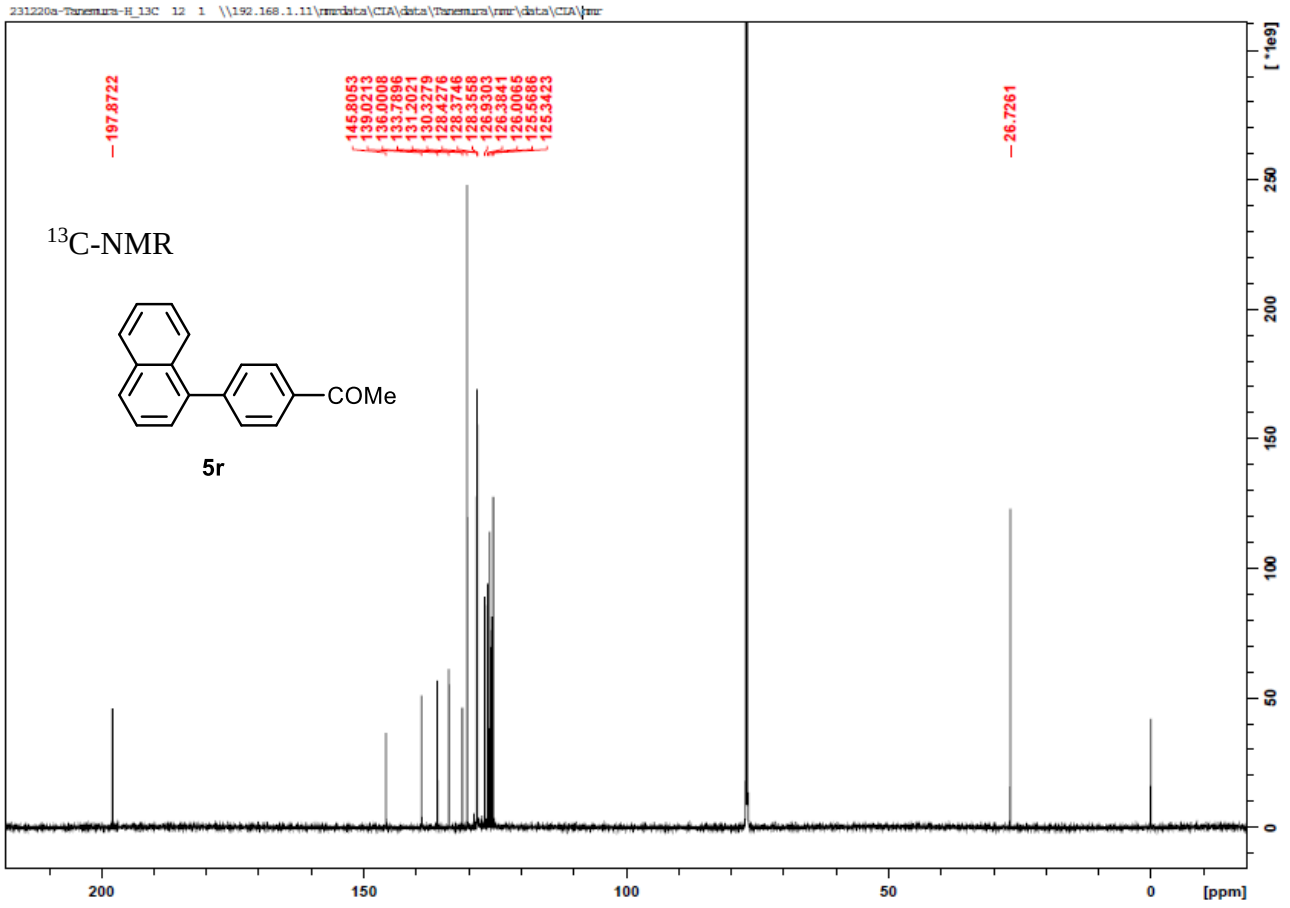

231219a-Tanemura-F_1H 10 1 \\192.168.1.11\nmrdata\CIA\data\Tanemura\nmr\data\CIA\nmr
^{1}H-NMR
7.4706
7.3834
7.3819
7.3715
7.3700
6.5783
6.5663
4.5686
4.5662
4.5437
3.2075
3.1950
3.1826
0.9025
0.9216
0.9371
2.0062
2.0000
4c
[*1e9]
[ppm]

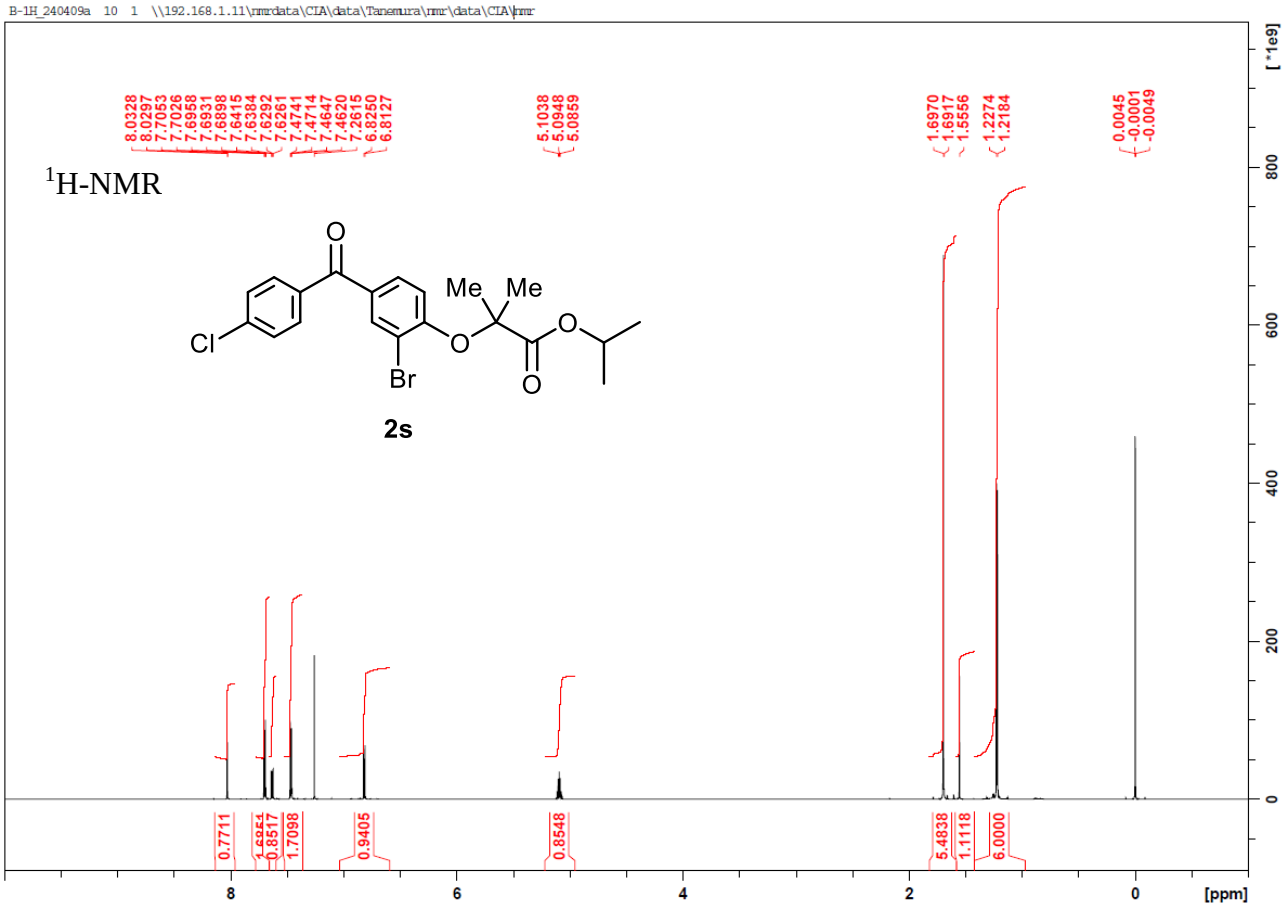

231219a-Tanemura-F_13C 12 1 \\192.168.1.11\nmrdata\CIA\data\Tanemura\nmr\data\CIA\nmr
^{13}C-NMR
160.0434
136.7097
133.6754
130.0541
111.6632
81.5945
71.4274
29.4647
4c
[*1e9]
[ppm]


^{1}H-NMR
7.5163
7.5121
7.5091
7.5025
7.4996
7.4953
7.4506
7.4390
7.2500
7.2274
7.2160
6.9727
6.9684
6.9655
6.9588
6.9560
6.9516
3.8420
2.3799
MeO
Me
5e
1.9431
1.8679
1.9679
3.1086
3.0000
[*1e9]
[ppm]


^{13}C-NMR
158.9232
137.9645
136.3482
133.7472
129.4262
127.9466
126.5787
114.1495
55.3361
21.0466
MeO
Me
5e
250 [*1e9]
[ppm]

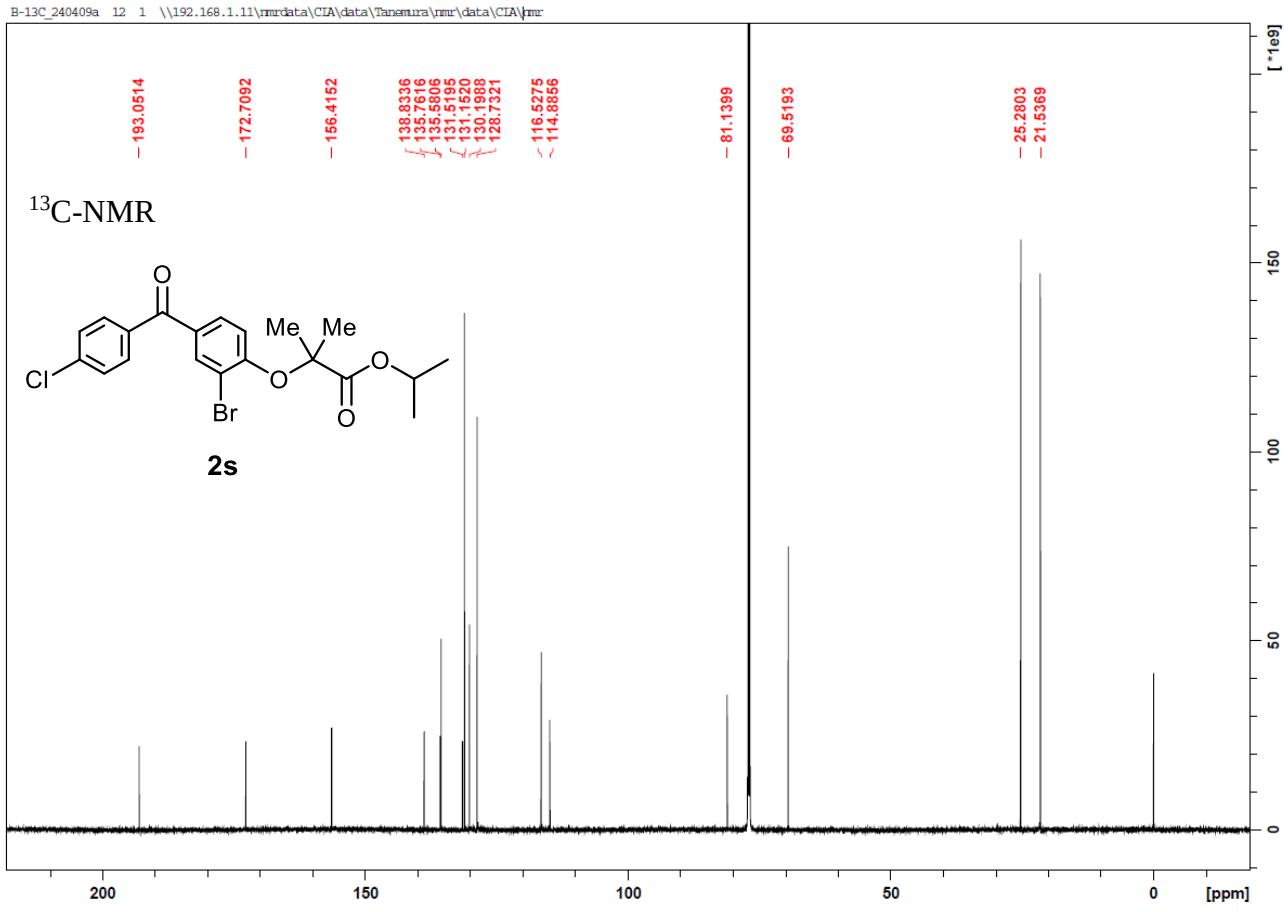

^{1}H-NMR
COMe
5r
[*1e9]
[ppm]


^{13}C-NMR
COMe
5r
[*1e9]
[ppm]



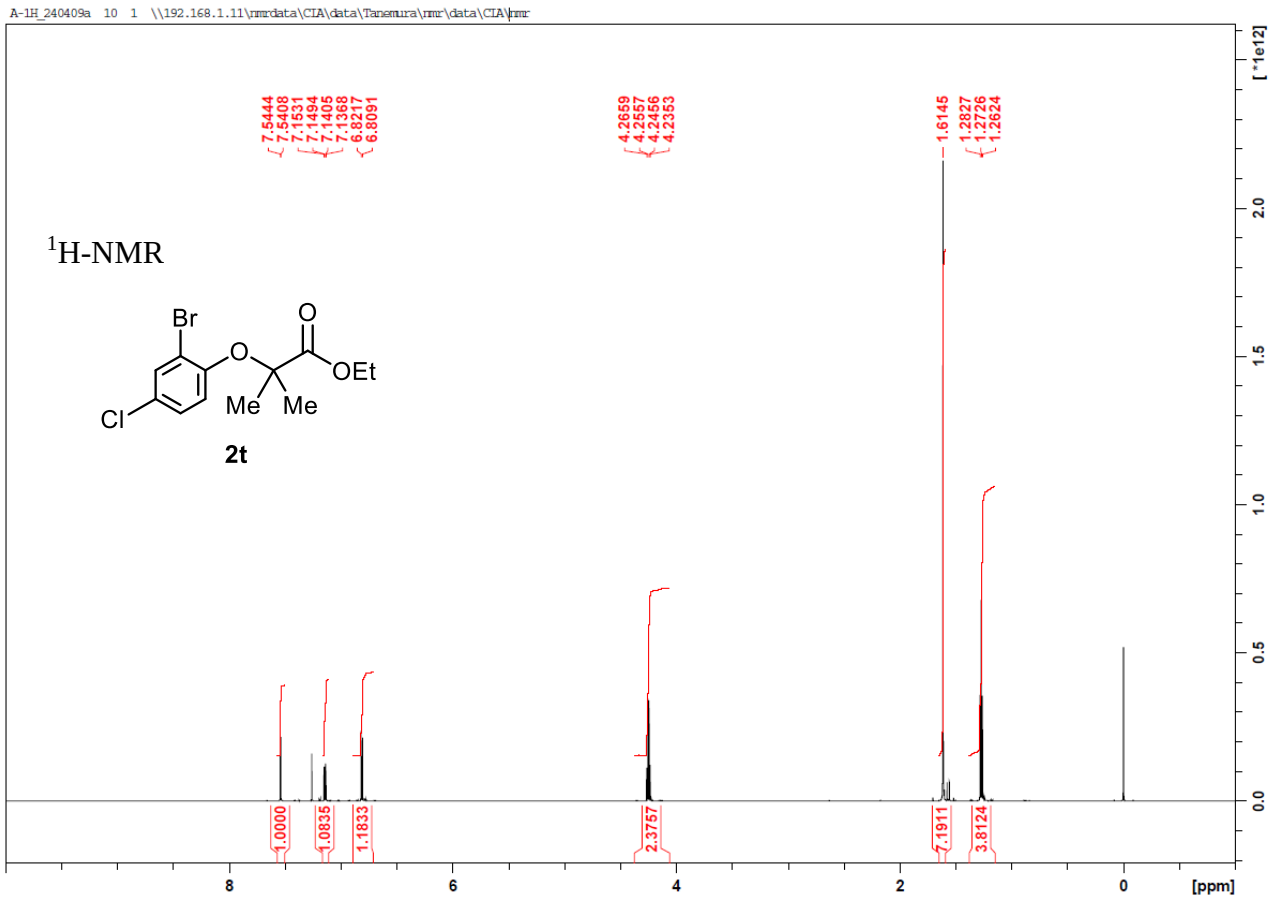
^{1}H-NMR

2s



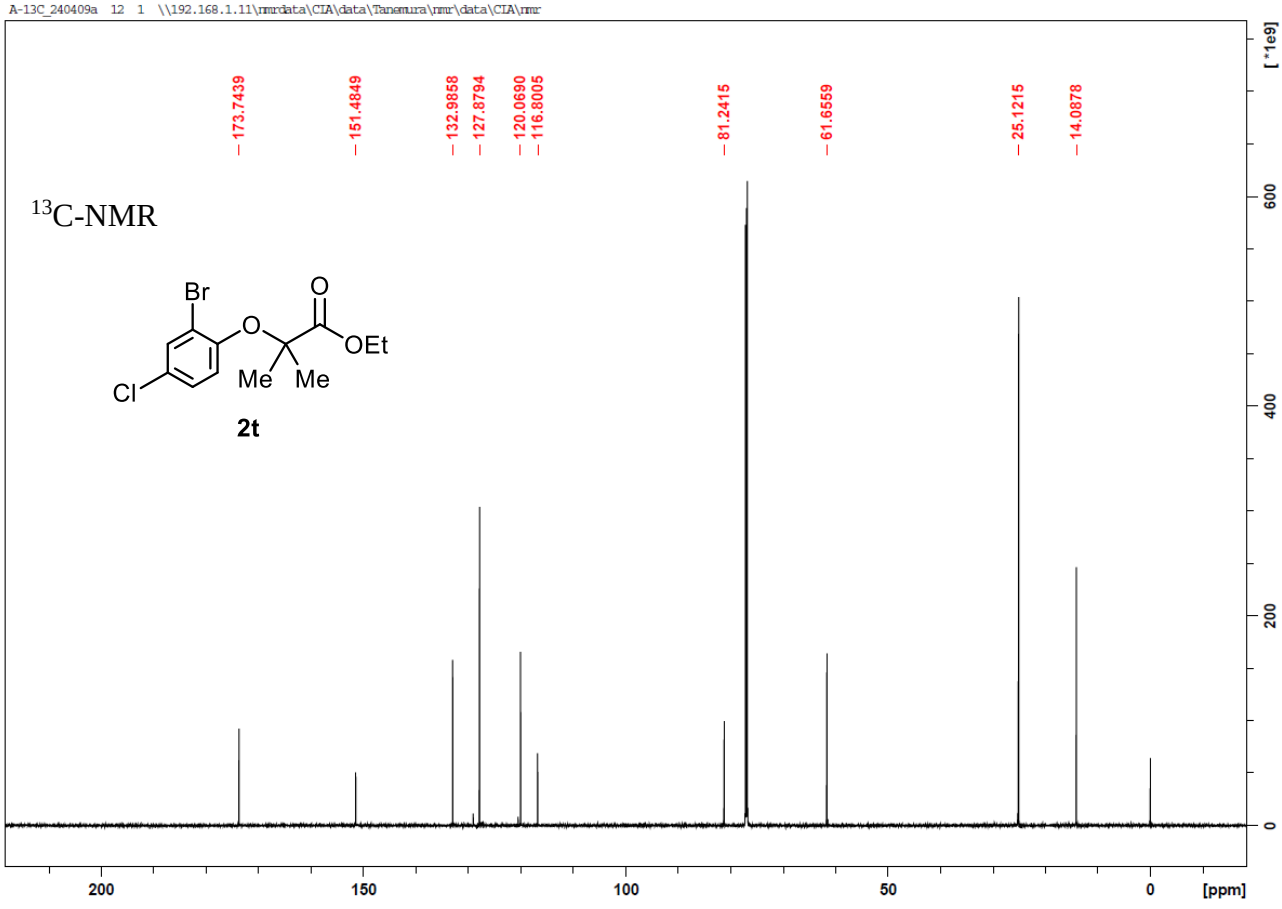
^{13}C-NMR

2s



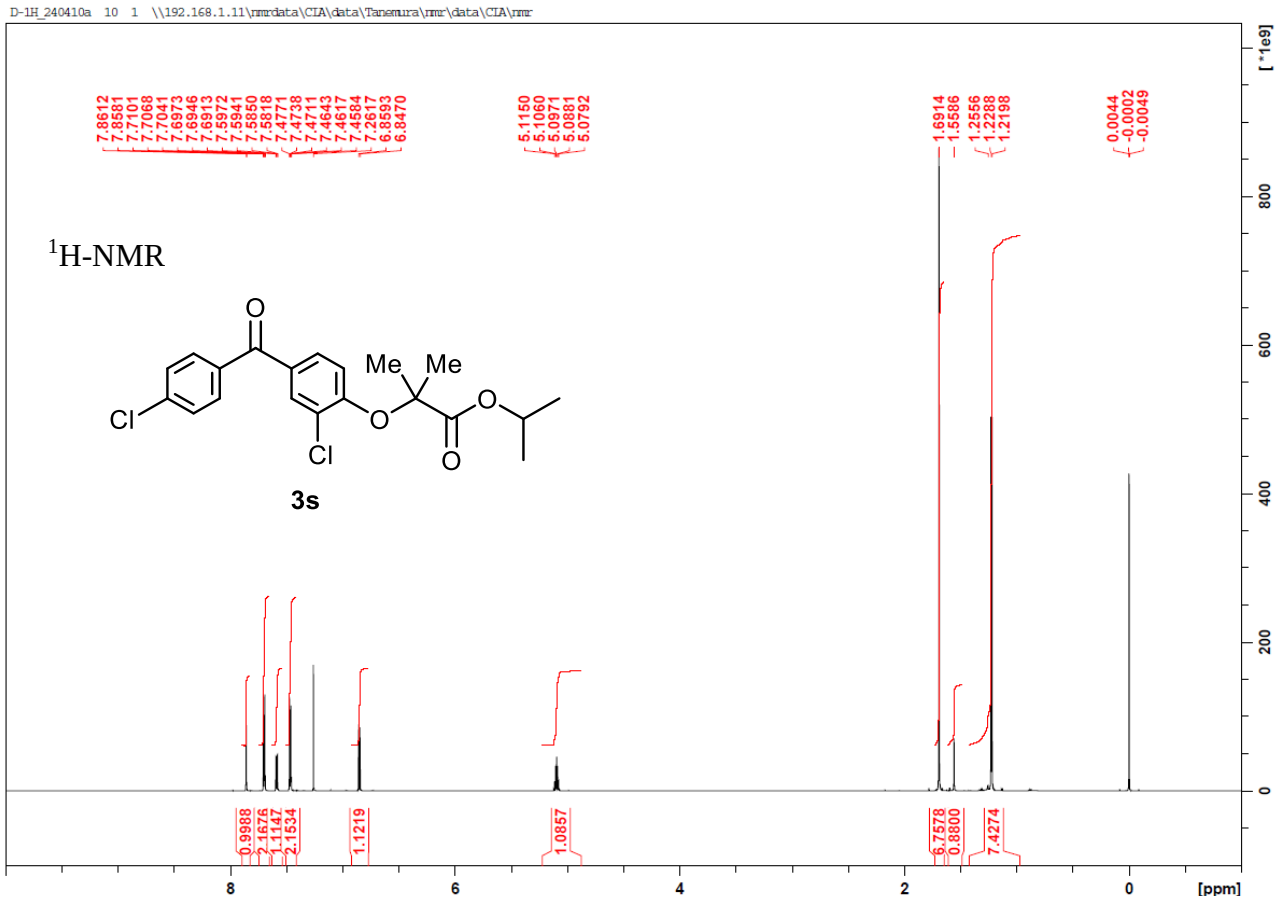
^{1}H-NMR

2t



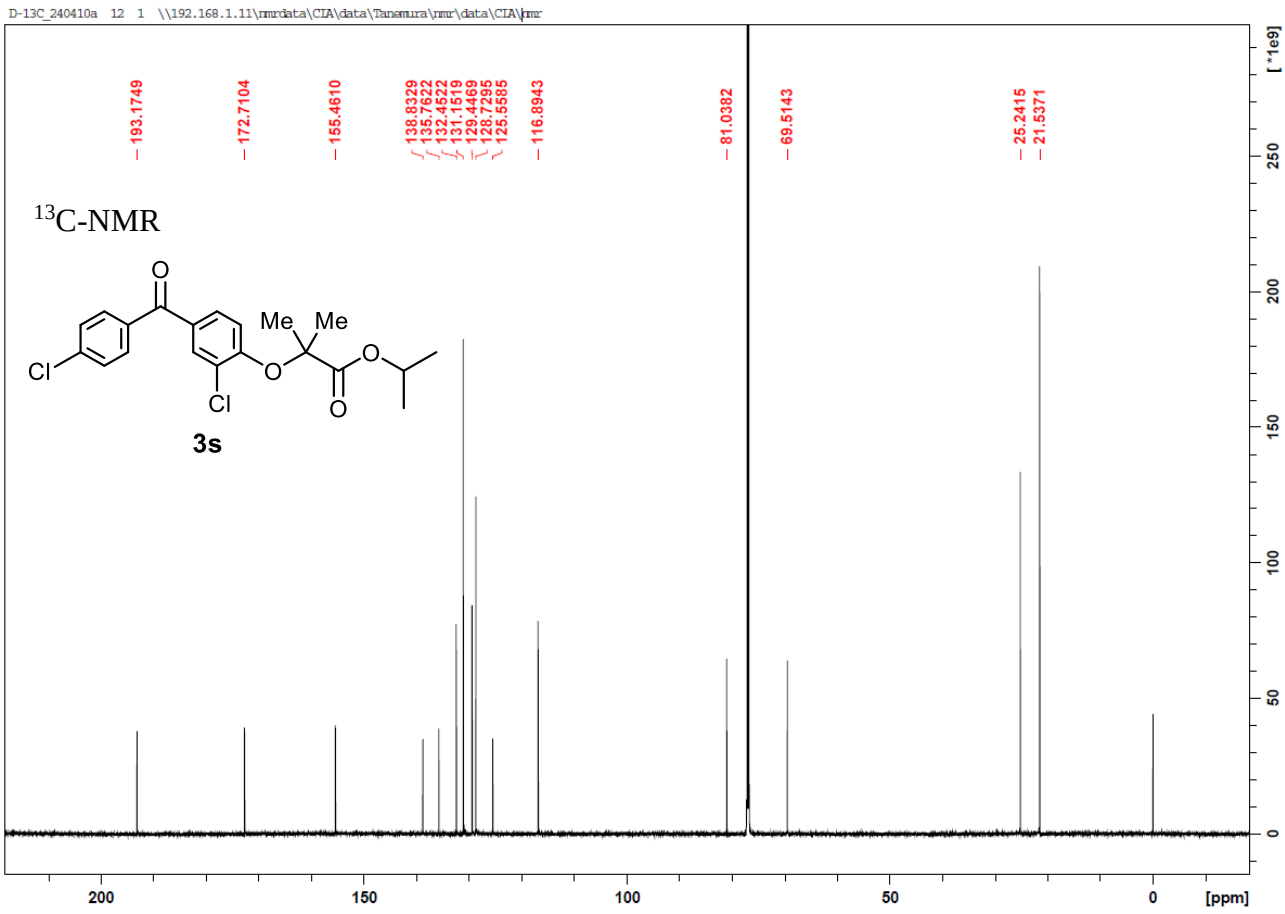
^{13}C-NMR

2t



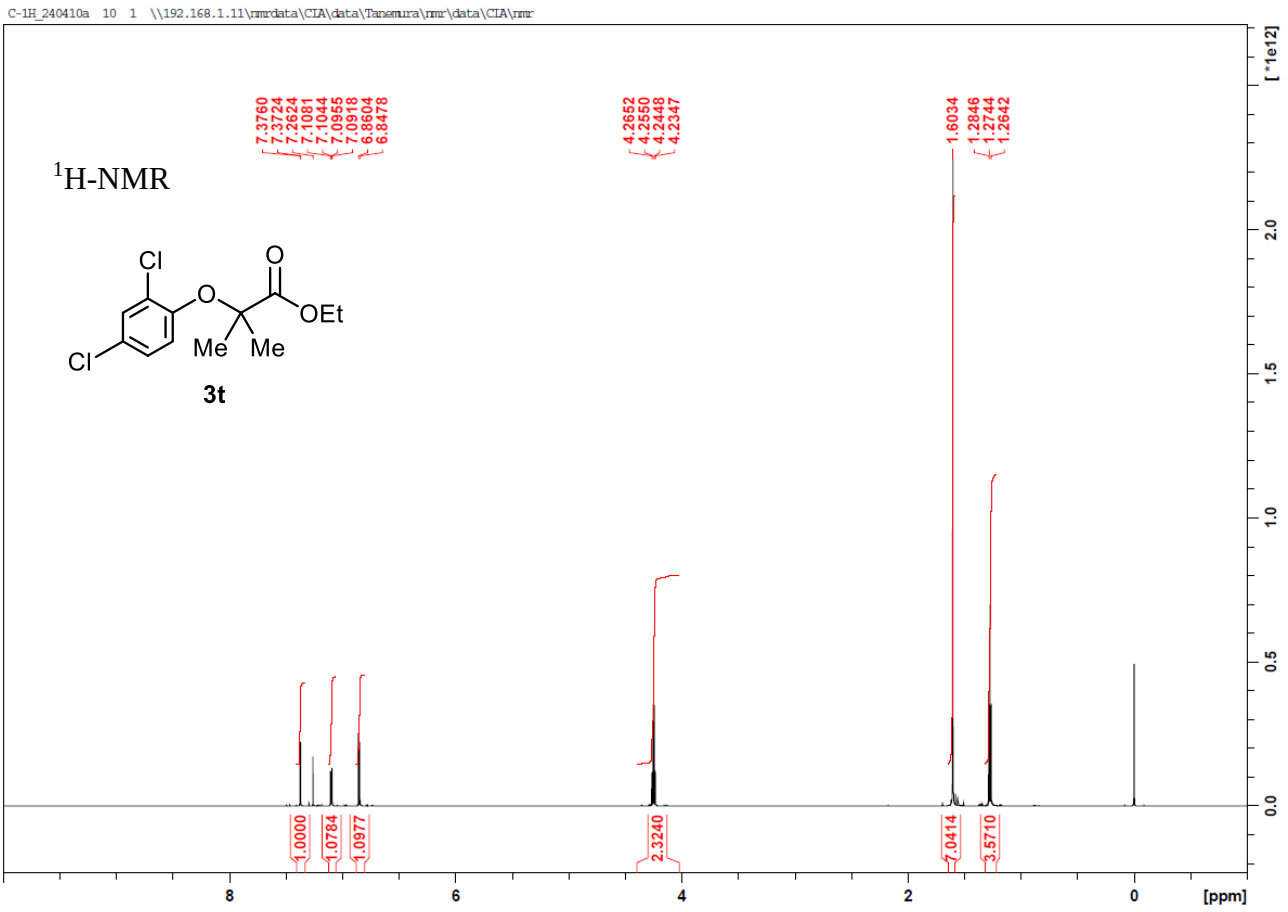
^{1}H-NMR

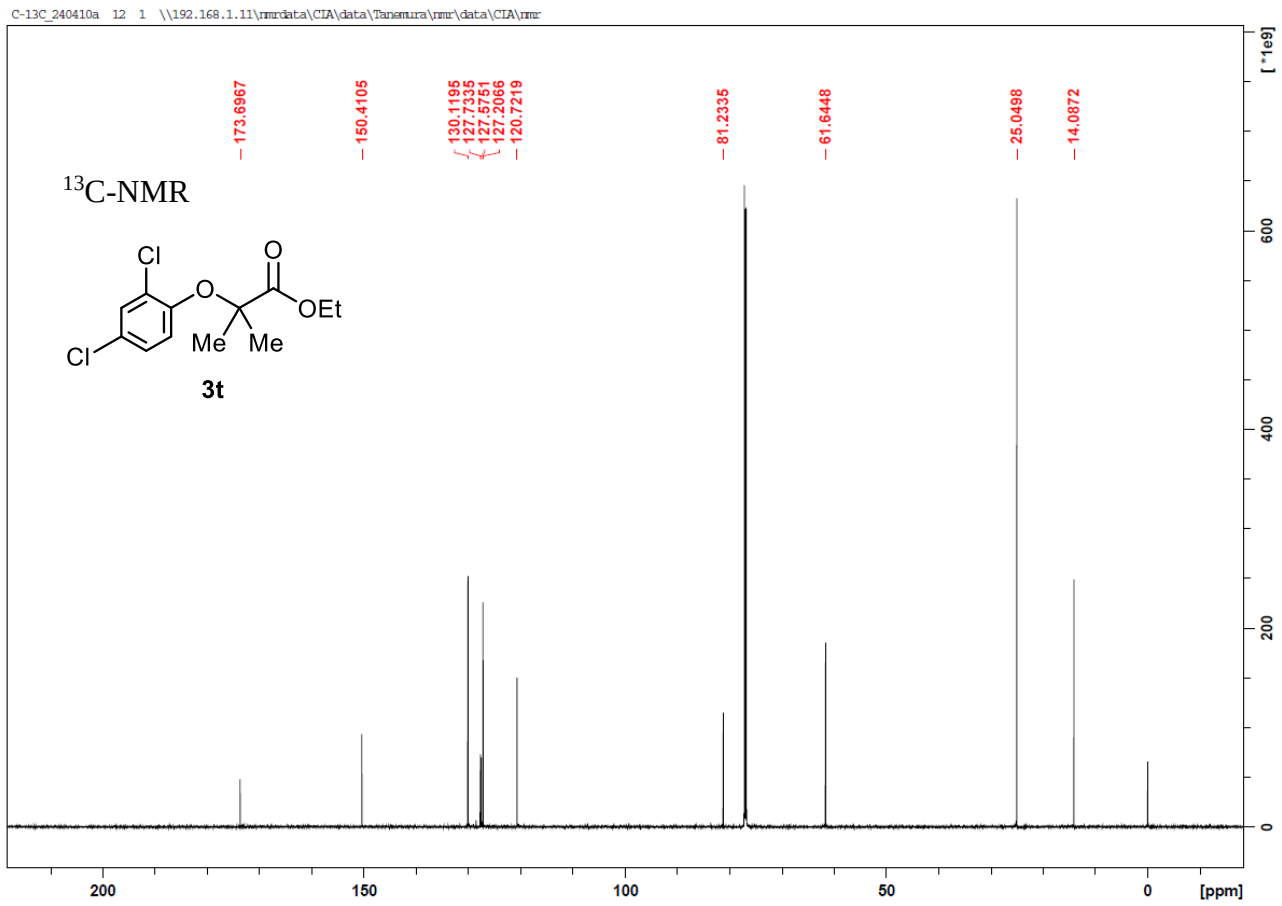
3s



^{13}C-NMR

3s


C-1H_240410a 10 1 \\192.168.1.11\nmrdata\CIA\data\Tanemura\nmr\data\CIA\nmr
1H-NMR
Cl
O
O
OEt
Me Me
Cl
3t
7.3760
7.3724
7.2624
7.1081
7.1044
7.0955
7.0918
6.8604
6.8478
4.2652
4.2550
4.2448
4.2347
1.6034
1.2846
1.2744
1.2642
1.0000
1.0784
1.0977
2.3240
7.0414
3.5710
[*1e12]
2.0
1.5
1.0
0.5
0.0
8
6
4
2
0
[ppm]


C-13C_240410a 12 1 \\192.168.1.11\nmrdata\CIA\data\Tanemura\nmr\data\CIA\nmr
13C-NMR
Cl
O
O
OEt
Me Me
Cl
3t
173.6967
150.4105
130.1195
127.7335
127.5751
127.2066
120.7219
81.2335
61.6448
25.0498
14.0872
[*1e9]
600
400
200
0
200
150
100
50
0
[ppm]

7. References

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