Electronic Supplementary Material (ESI) for ChemComm.

Synthesis of polyfluoroarene substituted benzofuran derivatives via cooperative Pd/Cu Catalysis

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Supporting Information

Content:

1. General Remarks

Unless stated otherwise, all reactions were carried out in flame-dried glassware under a dry argon atmosphere. All solvents were purified and dried according to standard methods prior to use. For product purification by flash column chromatography, silica gel (200~300 mesh) and light petroleum ether (bp. 60~90 ^{o}C) are used. ^{1}H NMR spectra were recorded on a Bruker advance III 400 MHz in $CDCl_3$ and ^{13}C NMR spectra were recorded on 100 MHz in $CDCl_3$ using TMS as internal standard, ^{19}F NMR spectra were recorded on 376 MHz. Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s= singlet, d = doublet, t = triplet, m = multiplet or unresolved, br = broad singlet, coupling constant (s) in Hz, integration). Data for ^{13}C NMR is reported in terms of chemical shift (δ, ppm). High-resolution mass spectral analysis (HRMS) data were measured on a Bruker Apex II.

2. Preparation of Starting Materials 1[1]

General procedure for precursors 1 : To the corresponding phenol or tosylated aniline was added 5 equivalents K_2CO_3 and 10 equivalents of 1-bromo-2-chloroethane or 1-bromo-3-chloropropane (1M in acetone). The resulting solution was refluxed under argon for 12-24 hours. The mixture was the diluted with water and extracted with dichloromethane. The organic phase was dried over magnesium sulfate and evaporated under reduced pressure.

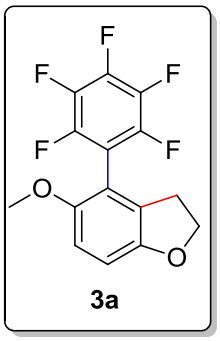
3. Preparation of Starting Materials polyfluoroarenes 2i-2l

Compound **2i-2l** were prepared according to literature procedure.[2]

4. General procedure for the preparation of the product 3

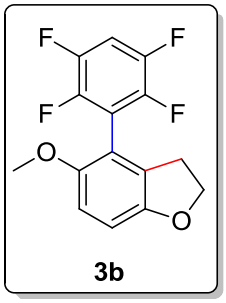
1 (0.3 mmol), **2** (0.6 mmol), $Pd(OAc)_2$ (10 mol %), 2-$PyPPh_2$ (30 mol %), CuI (5 mol %), Cs_2CO_3 (2.5 equiv), norbornene (2 equiv), were added to a sealed tube, MeCN (3.0 mL) was added. The mixture was flushed with Ar and stirred at 120 ℃ until completion (monitored by TLC). After cooling at room temperature, the mixture was diluted with diethyl ether, washed with water, dried over magnesium sulfate and purified by flash chromatography on silica gel (Hex/EA: 200/1-50/1).

5. Spectra Data.



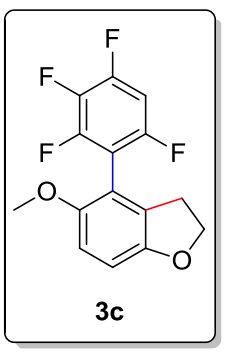
3a

5-methoxy-4-(perfluorophenyl)-2,3-dihydrobenzofuran (3a): 63.5 mg; 67% yield; white solid; **^{1}H NMR (400MHz, $CDCl_3$)** δ 6.82 (d, *J* = 8.8 Hz, 1H), 6.75 (d, *J* = 8.8 Hz, 1H), 4.55 (t, *J* = 8.4 Hz, 2H), 3.72 (s, 3H), 2.99 (t, *J* = 8.4 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 154.1, 151.5, 145.5-145.3 (m), 143.1-142.9 (m), 142.1-141.8 (m), 139.6-139.3 (m), 139.0-138.7 (m) 136.5-136.2 (m), 129.1, 112.4, 111.0-110.7(m), 110.5, 110.2, 71.2, 56.4, 29.6; **^{19}F NMR (376MHz, $CDCl_3$)** δ -139.3 (m, 2F), -155.4 (m, 1F), -162.7 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{15}H_9O_2F_5$: $[M]^+$ 316.0523; found: $[M]^+$ 316.0529.



3b

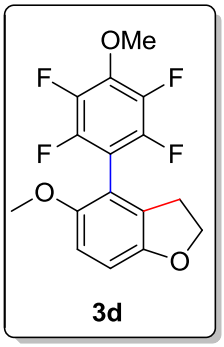
5-methoxy-4-(2,3,5,6-tetrafluorophenyl)-2,3-dihydrobenzofuran (3b): 38 mg; 42% yield; white solid; **^{1}H NMR (400MHz, $CDCl_3$)** δ 7.11-7.03 (m, 1H), 6.83 (d, *J* = 8.4 Hz, 1H), 6.76 (d, *J* = 8.4 Hz, 1H), 4.56 (t, *J* = 8.4 Hz, 2H), 3.73 (s, 3H), 3.01 (t, J = 8.4 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 154.0, 151.5, 147.1 (t, J_F = 20 Hz), 145.1-144.4 (m), 142.5 (t, J_F = 9 Hz), 129.0, 116.5 (t, J_F = 19 Hz), 113.6, 110.6, 110.0, 105.1 (t, J_F = 23 Hz), 71.2, 56.5, 29.6; **^{19}F NMR (376MHz, $CDCl_3$)** δ -139.6 (m, 2F), -140.0 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{15}H_{10}O_2F_4$: $[M]^+$ 298.0617; found: $[M]^+$ 298.0615.



3c

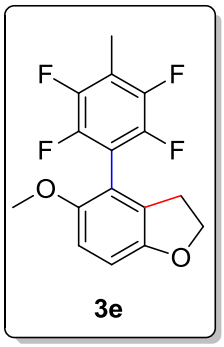
5-methoxy-4-(2,3,4,6-tetrafluorophenyl)-2,3-dihydrobenzofuran (3c): 31 mg; 34% yield; white

solid; **^{1}H NMR (400MHz, $CDCl_3$)** δ 6.77-6.71 (m, 2H), 6.65 (d, *J* = 8.8 Hz, 1H), 4.45 (t, *J* = 8.4 Hz, 2H), 3.62 (s, 3H), 2.90 (t, *J* = 8.4 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 155.6-155.155.5 (m), 153.9, 153.3-153.1 (m), 151.5, 150.4-150.2 (m), 149.0-148.8 (m), 147.9-147.8 (m), 138.7-138.3 (m), 136.2-135.8 (m), 129.2, 113.7, 110.4, 109.8, 100.9-100.3 (m), 71.2, 56.4, 29.6; **^{19}F NMR (376MHz, $CDCl_3$)** δ -114.8 (m, 1F), -131.7 (m, 1F), -133.3 (m, 1F), -165.3 (m, 1F); **HRMS (EI)** *m/z* calcd. $C_{15}H_{10}O_2F_4$: $[M]^+$ 298.0617; found: $[M]^+$ 298.0626.



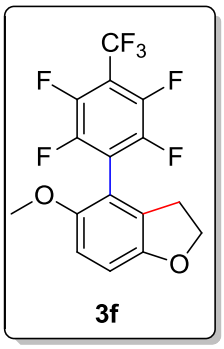
3d

5-methoxy-4-(2,3,5,6-tetrafluoro-4-methoxyphenyl)-2,3-dihydrobenzofuran (3d): 48 mg; 48% yield; yellow solid; **^{1}H NMR (400MHz, $CDCl_3$)** δ 6.81 (d, *J* = 8.4 Hz, 1H), 6.74 (d, *J* = 8.4 Hz, 1H), 4.55 (t, *J* = 8.4 Hz, 2H), 4.12 (t, J_F = 1.2 Hz, 3H), 3.73 (s, 3H), 3.01 (t, *J* = 8.4 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 154.0, 151.6, 145.6-145.4 (m), 143.2-143.0 (m), 142.3-142.0 (m), 139.8-139.6 (m), 137.9-137.6 (m), 129.3, 113.4, 110.5, 109.8, 109.0 (t, J_F = 20 Hz), 71.2, 62.0 (t, J_F = 4 Hz), 56.5, 29.7; **^{19}F NMR (376MHz, $CDCl_3$)** δ -141.1 (m, 2F), -158.6 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{16}H_{12}O_3F_4$: $[M]^+$ 328.0723; found: $[M]^+$ 328.0720.



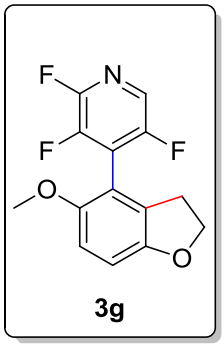
3e

5-methoxy-4-(2,3,5,6-tetrafluoro-4-methylphenyl)-2,3-dihydrobenzofuran (3e): 36 mg; 38% yield; white solid; **^{1}H NMR (400MHz, $CDCl_3$)** δ 6.72 (d, *J* = 8.4 Hz, 1H), 6.65 (d, *J* = 8.4 Hz, 1H), 4.45 (t, *J* = 8.4 Hz, 2H), 3.63 (s, 3H), 2.91 (t, *J* = 8.4 Hz, 2H), 2.19 (t, J_F = 2 Hz, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 153.9, 151.5, 146.4-146.1 (m), 144.9-144.7 (m), 143.9-143.6 (m), 142.5-142.2, 129.1, 115.4 (t, J_F = 19 Hz), 113.8, 112.8 (t, J_F = 20 Hz), 110.5, 109.7, 71.2, 56.5, 29.6, 7.5; **^{19}F NMR (376MHz, $CDCl_3$)** δ -141.6 (m, 2F), -144.4 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{16}H_{12}O_2F_4$: $[M]^+$ 312.0773; found: $[M]^+$ 312.0781.



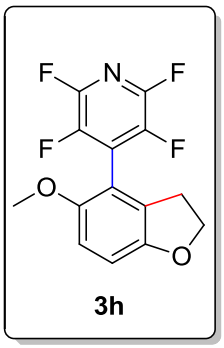
3f

5-methoxy-4-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)-2,3-dihydrobenzofuran (3f): 85 mg; 77% yield; colorless oil; **^{1}H NMR (400MHz, $CDCl_3$)** δ 6.86 (d, *J* = 8.8 Hz, 1H), 6.77 (d, *J* = 8.8 Hz, 1H), 4.57 (t, *J* = 8.8 Hz, 2H), 3.74 (s, 3H), 3.01 (t, *J* = 8.8 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 154.1, 151.2, 145.6-145.2 (m), 143.2-142.6 (m), 128.8, 122.3, 120.3 (t, J_F = 20 Hz), 119.5, 112.1, 110.7, 110.5, 71.2, 56.4, 29.6; **^{19}F NMR (376MHz, $CDCl_3$)** δ -56.2 (m, 3F), -137.4 (m, 2F), -141.3 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{16}H_9O_2F_7$: $[M]^+$ 366.0491; found: $[M]^+$ 366.0493.



3g

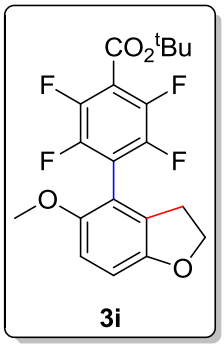
2,3,5-trifluoro-4-(5-methoxy-2,3-dihydrobenzofuran-4-yl)pyridine (3g): 40 mg; 47% yield; yellow oil; **^{1}H NMR (400MHz, $CDCl_3$)** δ 7.92 (s, 1H), 6.86 (d, *J* = 8.8 Hz, 1H), 6.77 (d, *J* = 8.8 Hz, 1H), 4.57 (t, *J* = 8.4 Hz, 2H), 3.74 (s, 3H), 3.02 (t, *J* = 8.4 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 155.6, 154.1, 153.1, 151.1, 149.6, 147.2 (d, J_F = 13 Hz), 143.9-143.6 (m), 141.3-141.0 (m), 128.6, 128.2-127.7 (m), 125.5 (t, J_F = 5 Hz), 122.3, 110.5, 71.2, 56.4, 29.5; **^{19}F NMR (376MHz, $CDCl_3$)** δ -89.7 (m, 1F), -128.7 (m, 1F), -135.9 (m, 1F); **HRMS (EI)** *m/z* calcd. $C_{14}H_{10}NO_2F_3$: $[M]^+$ 281.0664; found: $[M]^+$ 281.0668.



3h

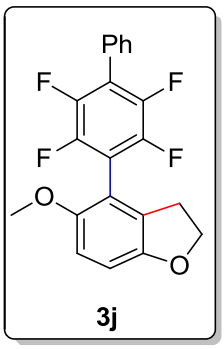
2,3,5,6-tetrafluoro-4-(5-methoxy-2,3-dihydrobenzofuran-4-yl)pyridine (3h): 47 mg; 52% yield; white solid; **^{1}H NMR (400MHz, $CDCl_3$)** δ 6.88 (d, *J* = 8.8 Hz, 1H), 6.78 (d, *J* = 8.8 Hz, 1H), 4.58 (t, *J* = 8.4 Hz, 2H), 3.75 (s, 3H), 3.03 (t, *J* = 8.4 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 154.1,

150.9, 144.8-144.5 (m), 142.4-142.0 (m), 141.0-140.6 (m), 138.4-138.1 (m), 129.4 (t, J_F = 17 Hz), 128.5, 111.1, 110.6, 71.2, 56.4, 29.5; **^{19}F NMR (376MHz, CDCl$_3$)** δ -91.4(m, 2F), -140.5 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{14}H_9NO_2F_4$: $[M]^+$ 299.0569; found: $[M]^+$ 299.0572.



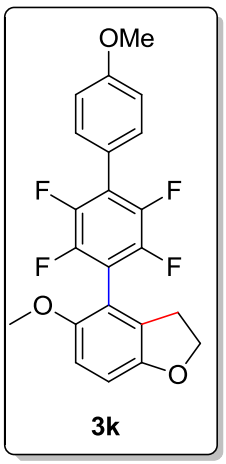
3i

tert-butyl 2,3,5,6-tetrafluoro-4-(5-methoxy-2,3-dihydrobenzofuran-4-yl)benzoate (3i): 55 mg; 46% yield; white solid; **^{1}H NMR (400MHz, CDCl$_3$)** δ 6.83 (d, *J* = 8.8 Hz, 1H), 6.75 (d, *J* = 8.8 Hz, 1H), 4.56 (t, *J* = 8.4 Hz, 2H), 3.72 (s, 3H), 3.00 (t, *J* = 8.4 Hz, 2H), 1.62 (s, 9H); **^{13}C NMR (100 MHz, CDCl$_3$)** δ 158.8, 154.0, 151.3, 145.5-145.0 (m), 143.0-142.5 (m), 128.9, 118.0 (t, J_F = 20 Hz), 113.7 (t, J_F = 17 Hz), 112.8, 110.4, 110.3, 84.6, 71.2, 56.4, 29.6, 28.0; **^{19}F NMR (376MHz, CDCl$_3$)** δ -138.9 (m, 2F), -141.8 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{20}H_{18}O_4F_4$: $[M]^+$ 398.1141; found: $[M]^+$ 398.1150.



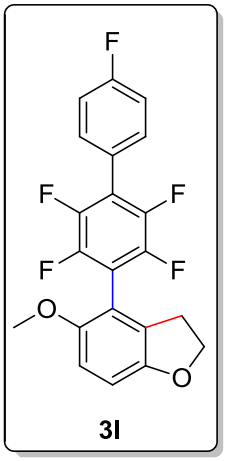
3j

5-methoxy-4-(2,3,5,6-tetrafluoro-[1,1'-biphenyl]-4-yl)-2,3-dihydrobenzofuran (3j): 68 mg; 60% yield; white solid **^{1}H NMR (400MHz, CDCl$_3$)** δ 7.51-7.45 (m, 5H), 6.84 (d, *J* = 8.8 Hz, 1H), 6.78 (d, *J* = 8.8 Hz, 1H), 4.58 (t, *J* = 8.4 Hz, 2H), 3.76 (s, 3H), 3.08 (t, *J* = 8.4 Hz, 2H); **^{13}C NMR (100 MHz, CDCl$_3$)** δ 154.0, 151.6, 145.5-144.9 (m), 143.0-142.4 (m), 130.2, 129.1, 128.6, 127.6, 119.9 (t, J_F = 16 Hz), 114.6 (t, J_F = 19 Hz), 113.6, 110.6, 110.0, 71.3, 56.6, 29.8; **^{19}F NMR (376MHz, CDCl$_3$)** δ -140.2 (m, 2F), -144.6 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{21}H_{14}O_2F_4$: $[M]^+$ 374.0930; found: $[M]^+$ 374.0931.



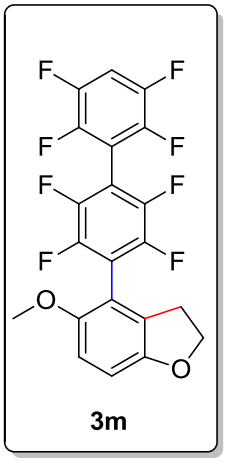
3k

5-methoxy-4-(2,3,5,6-tetrafluoro-4'-methoxy-[1,1'-biphenyl]-4-yl)-2,3-dihydrobenzofuran (3k): 66 mg; 54% yield; white solid; **^{1}H NMR (400MHz, $CDCl_3$)** δ 7.37 (d, *J* = 8.4 Hz, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 6.74 (d, *J* = 8.8 Hz, 1H), 6.67 (d, *J* = 8.8 Hz, 1H), 4.47 (t, *J* = 8.4 Hz, 2H), 3.76 (s, 3H), 3.66 (s, 3H), 2.97 (t, *J* = 8.4 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.0, 154.0, 151.6, 145.4-144.9 (m), 143.0-142.5 (m), 131.4, 129.2, 119.6 (t, J_F = 19 Hz), 114.0, 113.6, 110.5, 109.9, 71.2, 56.5, 55.2, 29.7; **^{19}F NMR (376MHz, $CDCl_3$)** δ -140.4 (m, 2F), -145.0 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{22}H_{16}O_3F_4$: $[M]^+$ 404.1036; found: $[M]^+$ 404.1043.

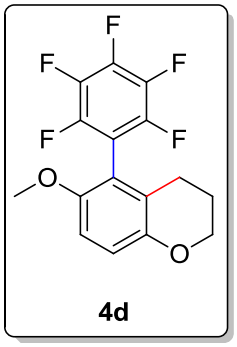


3l

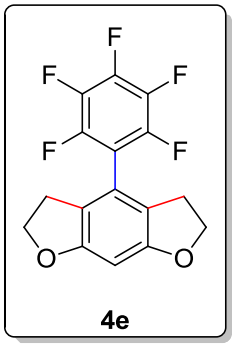
5-methoxy-4-(2,3,4',5,6-pentafluoro-[1,1'-biphenyl]-4-yl)-2,3-dihydrobenzofuran (3l): 60 mg; 51% yield; white solid; **^{1}H NMR (400MHz, $CDCl_3$)** δ 7.51 (t, *J* = 7.2 Hz, 2H), 7.20 (t, *J* = 8.8 Hz, 2H), 6.84 (d, *J* = 8.8 Hz, 1H), 6.78 (d, *J* = 8.8 Hz, 1H), 4.58 (t, *J* = 8.8 Hz, 2H), 3.77 (s, 3H), 3.07 (t, *J* = 8.8 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 164.2, 161.8, 154.0, 151.6, 145.5-144.8 (m), 143.1-142.4 (m), 132.0, 129.2, 123.4, 118.8 (t, J_F = 16 Hz), 115.8, 115.6, 114.8 (t, J_F = 19 Hz), 113.4, 110.6, 110.1, 71.3, 56.6, 29.8; **^{19}F NMR (376MHz, $CDCl_3$)** δ -111.6 (s, 1F), -140.0 (m, 2F), -144.8 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{21}H_{13}O_2F_5$: $[M]^+$ 392.0836; found: $[M]^+$ 392.0841.



5-methoxy-4-(2,2',3,3',5,5',6,6'-octafluoro-[1,1'-biphenyl]-4-yl)-2,3-dihydrobenzofuran (3m): 78 mg; 58% yield; white soild; **^{1}H NMR (400MHz, $CDCl_3$)** δ 7.30-7.24 (m, 1H), 6.86 (d, *J* = 8.8 Hz, 1H), 6.79 (d, *J* = 8.8 Hz, 1H), 4.59 (t, *J* = 8.8 Hz, 2H), 3.78 (s, 3H), 3.09 (t, *J* = 8.8 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 154.1, 151.4, 147.4-147.2 (m), 145.4-144.7 (m), 142.9-142.7 (m), 129.1, 118.0 (t, J_F = 19 Hz), 112.9, 110.4, 108.1-107.5 (m), 106.2 (t, J_F = 17 Hz), 71.3, 56.5, 29.8; **^{19}F NMR (376MHz, $CDCl_3$)** δ -137.7- -139.2 (m, 8F); **HRMS (EI)** *m/z* calcd. $C_{21}H_{10}O_2F_8$: $[M]^+$ 446.0553; found: $[M]^+$ 446.0555.

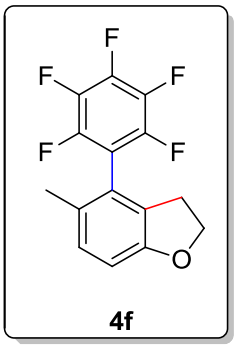


6-methoxy-5-(perfluorophenyl)chroman (4d): 28 mg; 28% yield; yellow oil; **^{1}H NMR (400MHz, $CDCl_3$)** δ 6.91 (d, *J* = 9.2 Hz, 1H), 6.79 (d, *J* = 9.2 Hz, 1H), 4.14 (t, *J* = 4.8 Hz, 2H), 3.70 (s, 3H), 2.42 (t, *J* = 6.4 Hz, 2H), 1.97-1.91 (m, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 150.9, 149.2, 145.4, 142.9, 141.8, 139.4, 138.8, 136.4, 122.8, 118.6, 114.7, 110.9-110.6 (m), 110.4, 65.8, 56.2, 23.2, 21.9; **^{19}F NMR (376MHz, $CDCl_3$)** δ -139.3 (m, 2F), -155.5 (m, 1F), -162.7 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{16}H_{11}O_2F_5$: $[M]^+$ 330.0679; found: $[M]^+$ 330.0685.



4-(perfluorophenyl)-2,3,5,6-tetrahydrobenzo[1,2-b:5,4-b']difuran (4e): 30 mg; 30% yield;

yellow solid; **^{1}H NMR (400MHz, $CDCl_3$)** δ 6.38 (s, 1H), 4.59 (t, *J* = 8.8 Hz, 4H), 2.93 (t, *J* = 8.8 Hz, 4H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.6, 145.0-144.9 (m), 142.6-142.4 (m), 142.2-141.9 (m), 139.6-138.8 (m), 136.6-136.3 (m), 119.0, 118.8, 112.6 (t, J_F = 16 Hz), 93.8, 72.0, 28.6; **^{19}F NMR (376MHz, $CDCl_3$)** δ -140.0 (m, 2F), -154.4 (m, 1F), -161.5 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{16}H_9O_2F_5$: $[M]^+$ 328.0523; found: $[M]^+$ 328.0524.

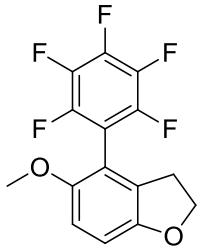


5-methyl-4-(perfluorophenyl)-2,3-dihydrobenzofuran (4f): 49 mg; 54% yield; white solid; **^{1}H NMR (400MHz, $CDCl_3$)** δ 7.07 (d, *J* = 8 Hz, 1H), 6.80 (d, *J* = 8 Hz, 1H), 4.57 (t, *J* = 8.8 Hz, 2H), 2.94 (t, *J* = 8.8 Hz, 2H), 2.07 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 158.2, 145.0-144.9 (m), 142.5-142.0 (m), 139.4-139.0 (m), 136.4, 129.8, 128.8, 127.6, 122.6, 113.4, 110.3, 71.2, 29.4, 18.8; **^{19}F NMR (376MHz, $CDCl_3$)** δ -140.0 (m, 2F), -154.7 (m, 1F), -161.6 (m, 2F); **HRMS (EI)** *m/z* calcd. $C_{15}H_9OF_5$: $[M]^+$ 300.0574; found: $[M]^+$ 300.0578.

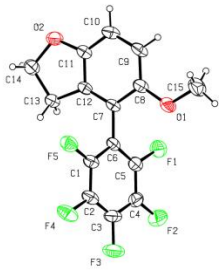
6. References

1. (a) B. Mariampillai, D. Alberico, V. Bidau, M. Lautens. *J. Am. Chem. Soc.*, **2006**, *128*, 14436. (b) S. Pache, M. Lautens. *Org. Lett.*, **2003**, *5*, 4827.
2. (a) M. Simonetti, G. J. Perry, X. C. Cambeiro, F. Julia´-Herna´ndez, J. N. Arokianathar, I. Larrosa. *J. Am. Chem. Soc.*, **2016**, *138*, 3596. (b) F. Chen, Q. Q. Min, X. Zhang, *J. Org. Chem.*, **2012**, *77*, 2992.

7. Crystallographic data of 3a and 3n



3a



Structure of 3a

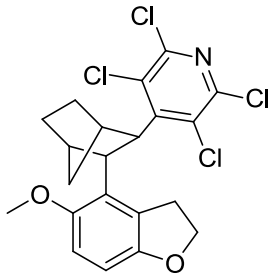
Datablock:

Bondprecision:	C-C = 0.0077 A	Wavelength=0.71073	
Cell:	a=10.7847(11)	b=8.7041(9)	c=28.524(4)
	alpha=90	beta=99.114(10)	gamma=90
Temperature:	297 K		

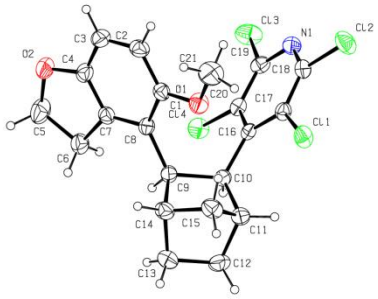
	Calculated	Reported
Volume	2643.8(5)	2643.8(5)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C15 H9 F5 O2	C15 H9 F5 O2
Sum formula	C15 H9 F5 O2	C15 H9 F5 O2
Mr	316.22	316.22
Dx,g cm-3	1.589	1.589
Z	8	8
Mu (mm-1)	0.151	0.151
F000	1280.0	1280.0
F000’	1281.11	
h,k,lmax	13,10,35	13,10,35
Nref	5210	5195
Tmin,Tmax	0.973,0.979	0.889,1.000
Tmin’	0.969	

Correction method = # Reported T Limits: Tmin = 0.889 Tmax = 1.000
AbsCorr = MULTI-SCAN

Datac ompleteness= 0.997	Theta(max)= 26.022
R(reflections)= 0.0790(2172)	wR2(reflections)= 0.2310(5195)
S = 1.036	Npar= 399



3n



Structure of 3n

Datablock:

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	alpha=90	beta=90	gamma=90
Temperature:	293 K		

	Calculated	Reported
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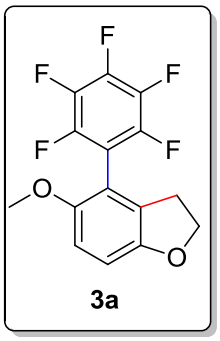
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C21 H19 Cl4 N O2	C21 H19 Cl4 N O2
Sum formula	C21 H19 Cl4 N O2	C21 H19 Cl4 N O2
Mr	459.17	459.17
Dx,g cm-3	1.499	1.499
Z	4	4
Mu (mm-1)	0.600	0.600
F000	944.0	944.0
F000’	946.68	
h,k,lmax	15,16,14	15,16,14
Nref	3992[2098]	2818
Tmin,Tmax	0.871,0.914	0.891,1.000
Tmin’	0.871	

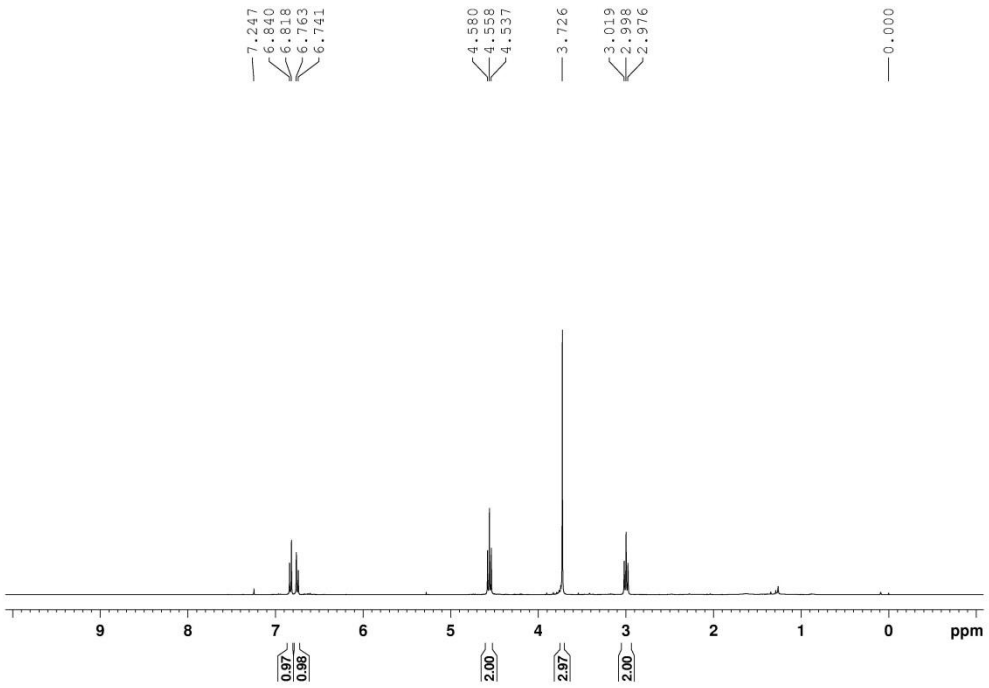
Correction method= # Reported T Limits: Tmin=0.891 Tmax=1.000
AbsCorr = MULTI-SCAN

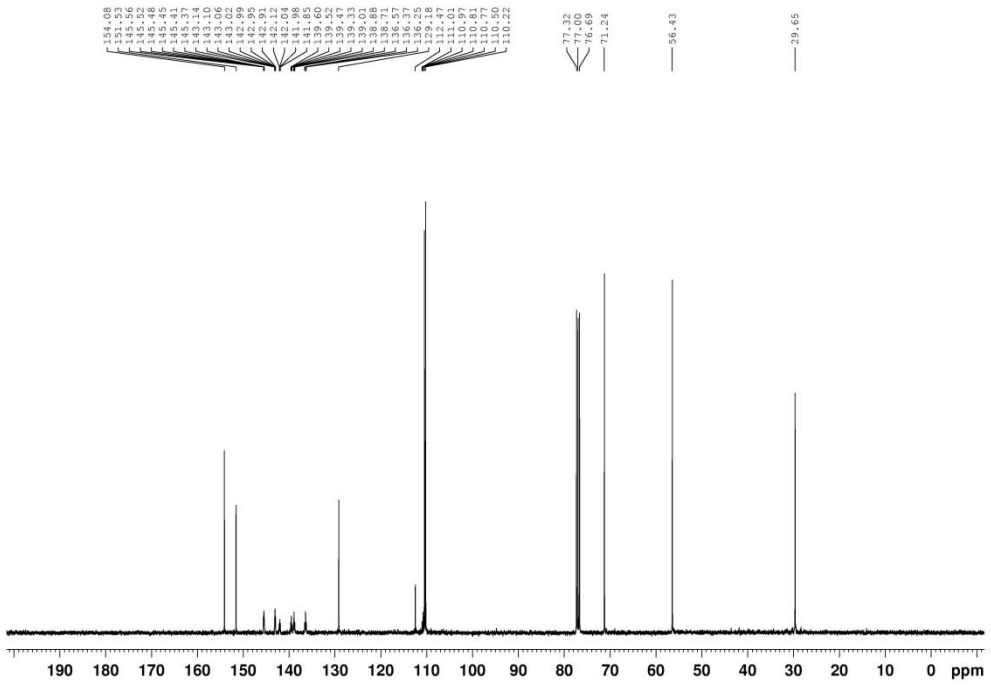
Data completeness= 1.34/0.71	Theta(max)= 26.010
R(reflections)= 0.0343(2416)	wR2(reflections)= 0.0782(2818)
S = 1.025	Npar= 254

8. Copies of ^{1}H, ^{19}F and ^{13}C spectra.



3a

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145.37
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143.10
143.06
143.02
142.99
142.95
142.91
142.12
142.04
141.98
141.85
141.60
139.52
139.47
139.33
139.01
138.88
138.71
136.57
136.37
136.25
136.18
112.47
111.01
110.97
110.61
110.17
110.50
110.22
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77.00
76.69
71.24
56.43
29.65
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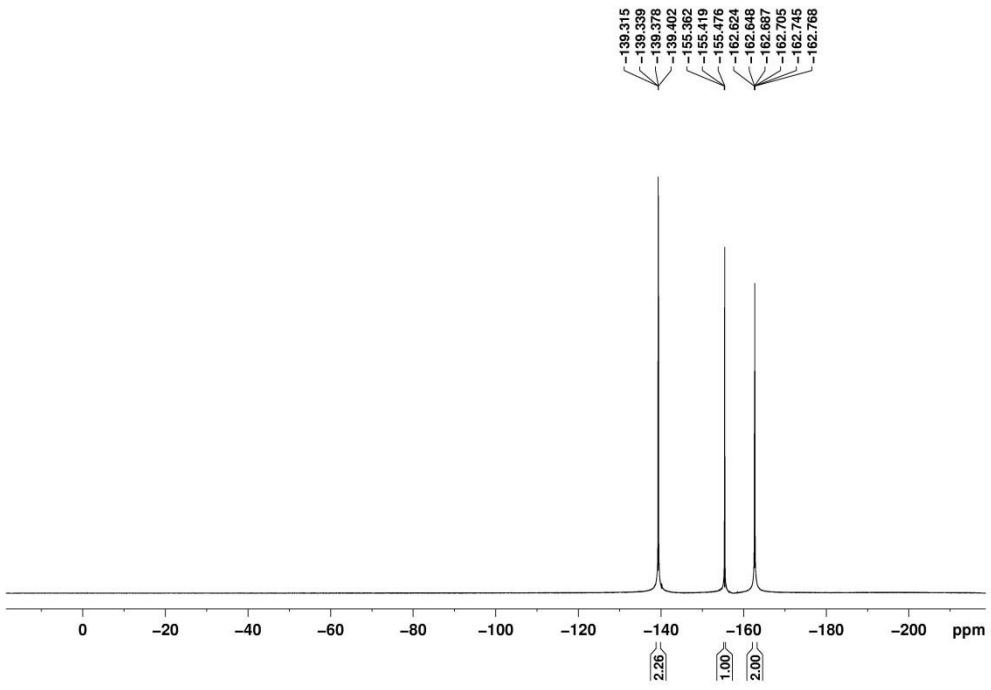
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-139.402
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-155.419
-155.476
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-162.648
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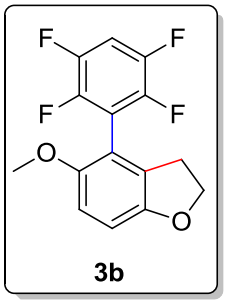
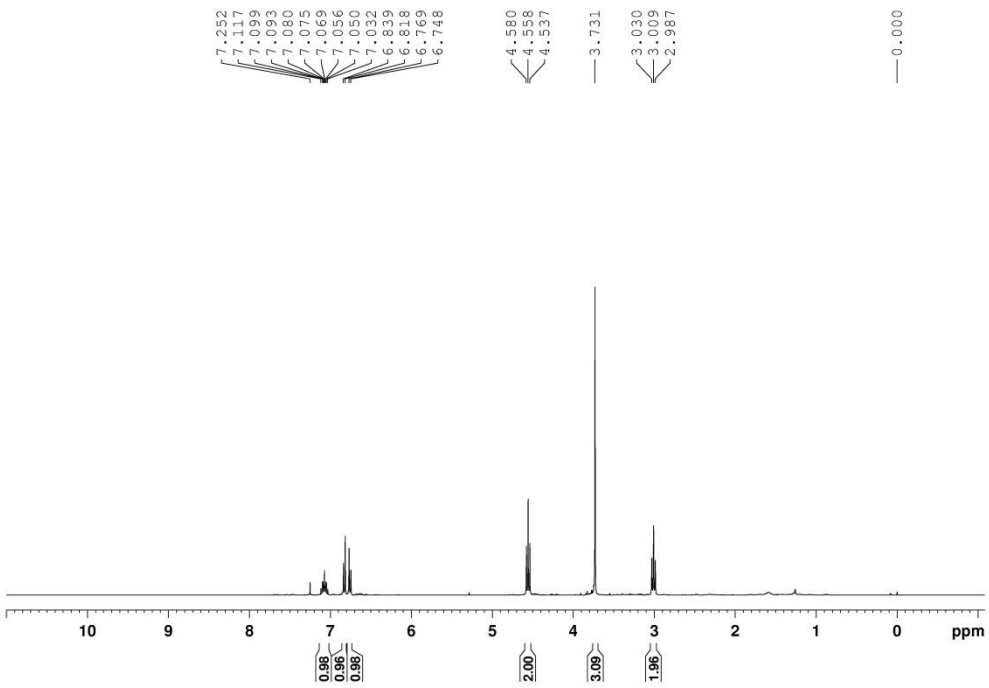
-162.745
-162.768
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm
2.26
1.00
2.00


F
F
F
F
O
O

3b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7.075
7.069
7.056
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7.032
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6.818
6.769
6.748
4.580
4.558
4.537
3.731
3.030
3.009
2.987
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
0.96
0.98
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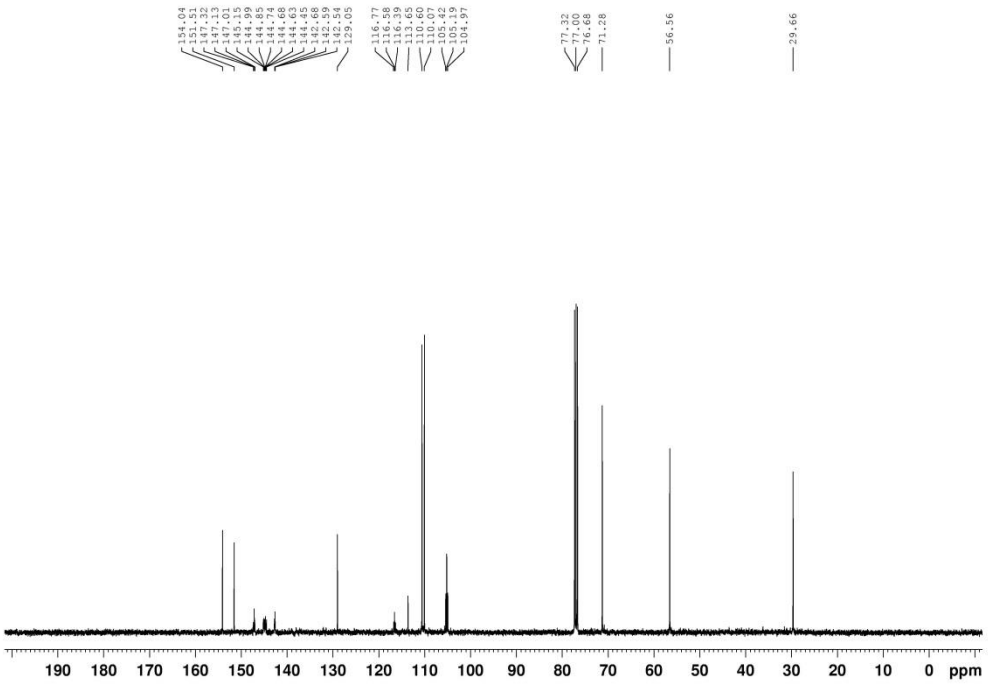
3.09
1.96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144.68
144.63
144.45
142.68
142.59
142.54
129.05
116.77
116.58
116.39
113.65
110.60
110.07
105.42
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104.97
77.32
77.00
76.68
71.28
56.56
29.66
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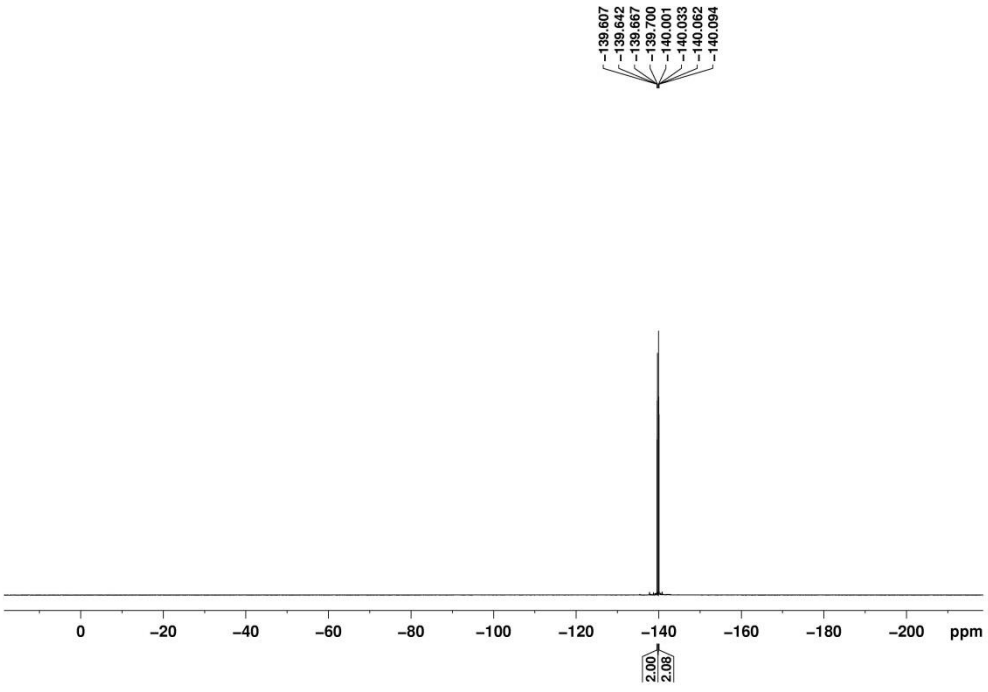
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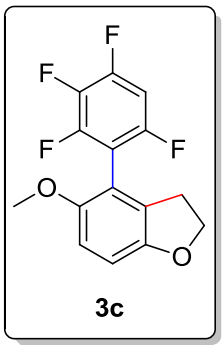
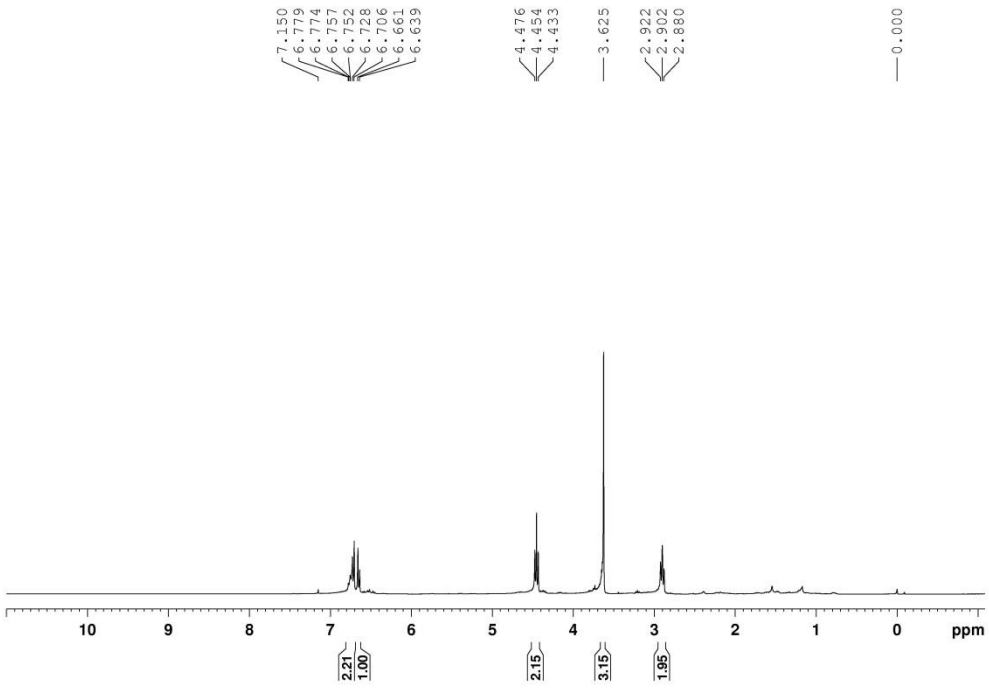
2.00
2.08


F
F
F
F
O
O

3c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6.661
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4.454
4.433
3.625
2.922
2.902
2.880
0.000
10
9
8
7
6
5
4
3
2
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ppm
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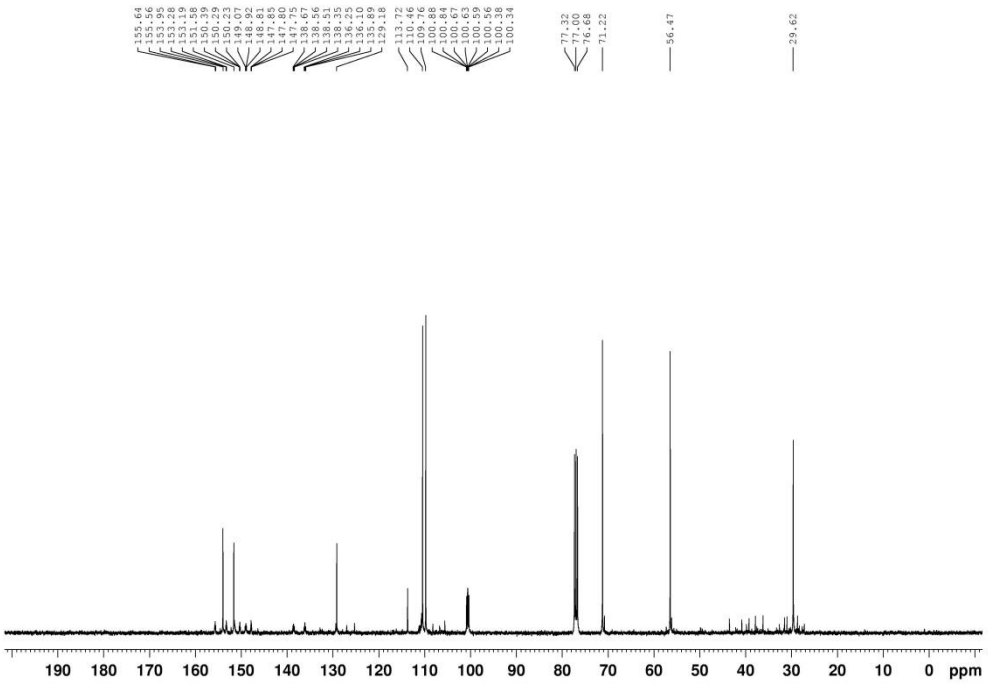
3.15
1.95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147.80
147.75
138.67
138.56
138.51
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136.25
136.10
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129.18
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110.46
109.76
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100.67
100.63
100.59
100.56
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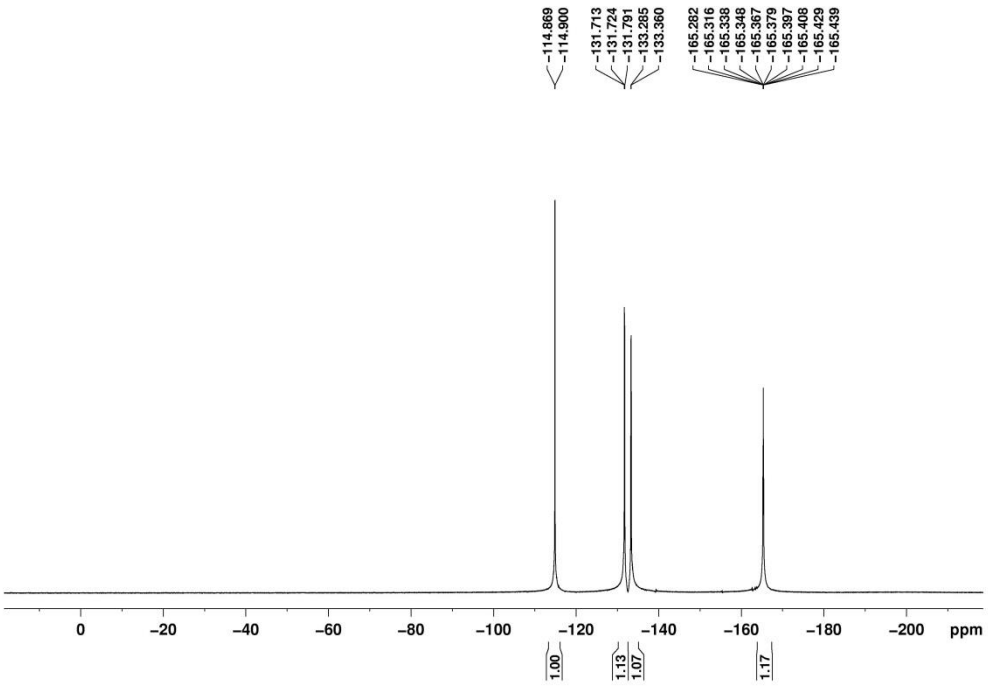
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-165.367
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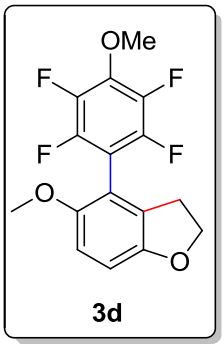
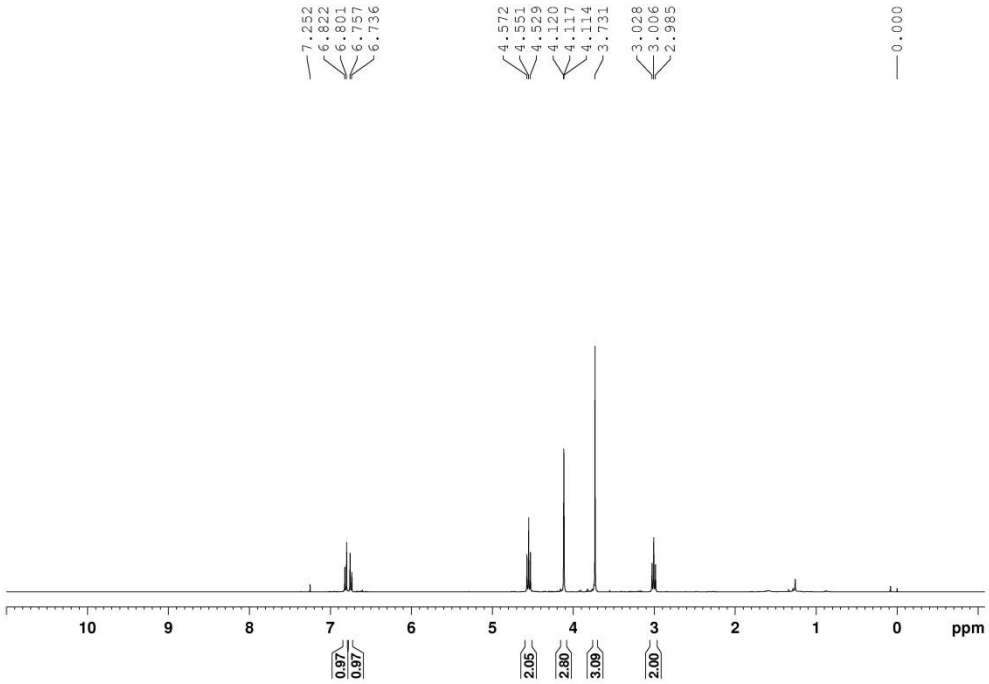
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm
1.00
1.13
1.07
1.17


OMe
F
F
F
F
O
O

3d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4.529
4.120
4.117
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3.028
3.006
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10
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4
3
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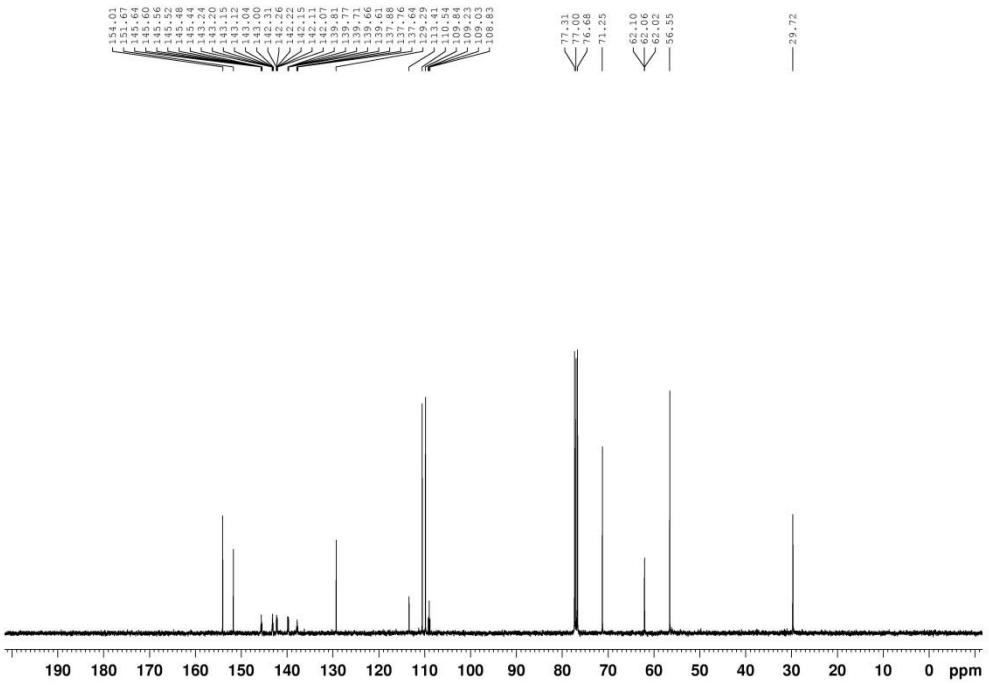
2.00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142.11
142.07
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139.66
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129.29
113.41
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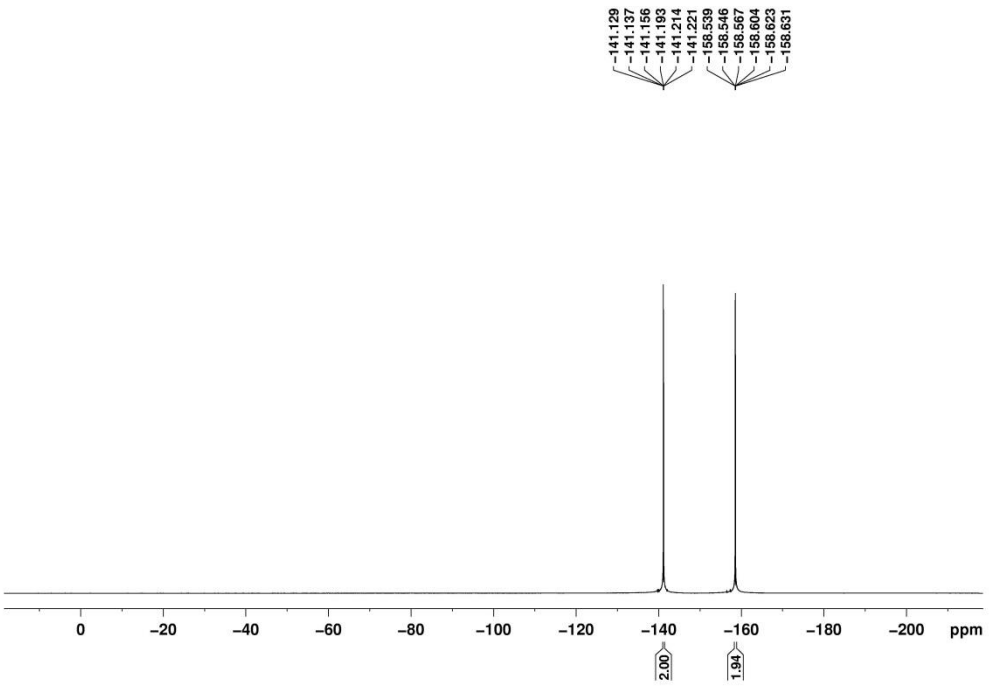
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-158.623
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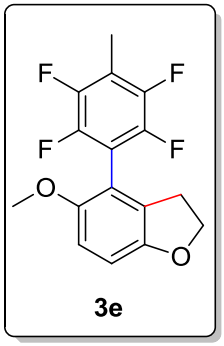
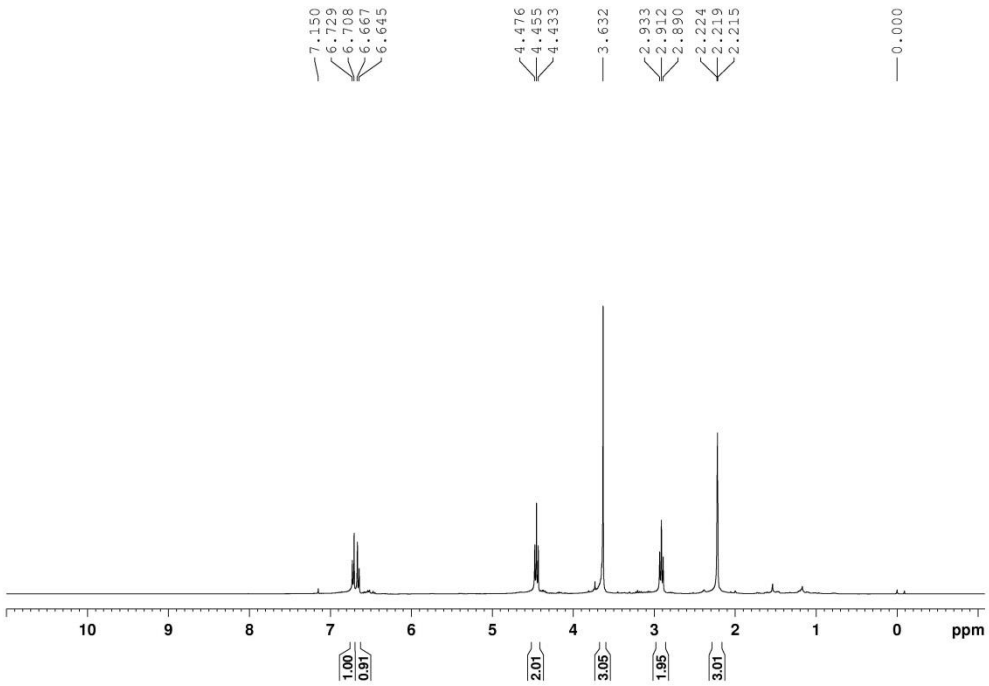
2.00
1.94


F
F
F
F
O
O

3e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2.890
2.224
2.219
2.215
0.000
10
9
8
7
6
5
4
3
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1
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ppm
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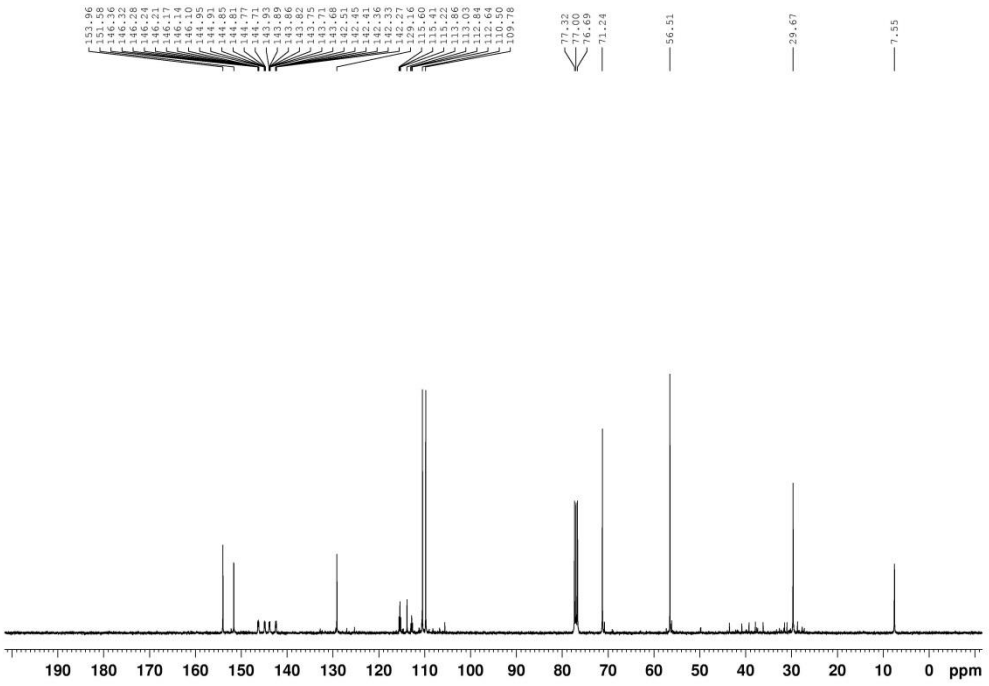
3.05
1.95
3.01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144.95
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144.71
143.93
143.89
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143.82
143.75
143.71
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143.51
142.45
142.41
142.36
142.33
142.27
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113.22
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113.03
112.84
112.64
110.50
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76.69
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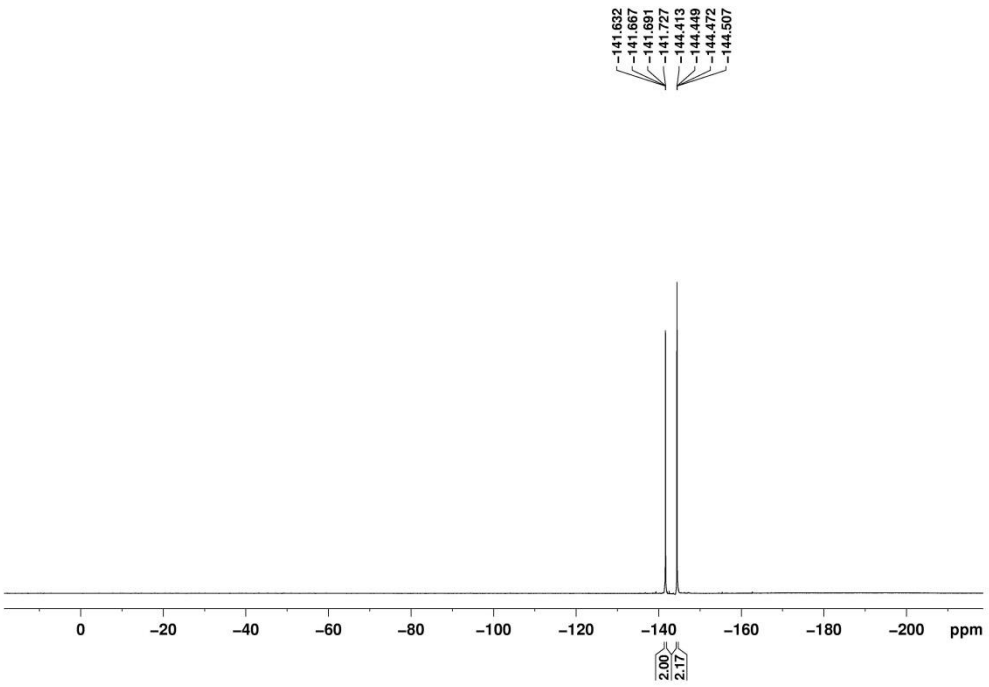
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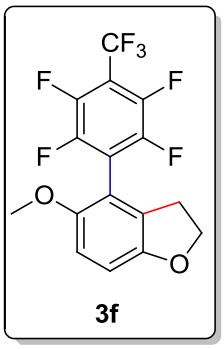
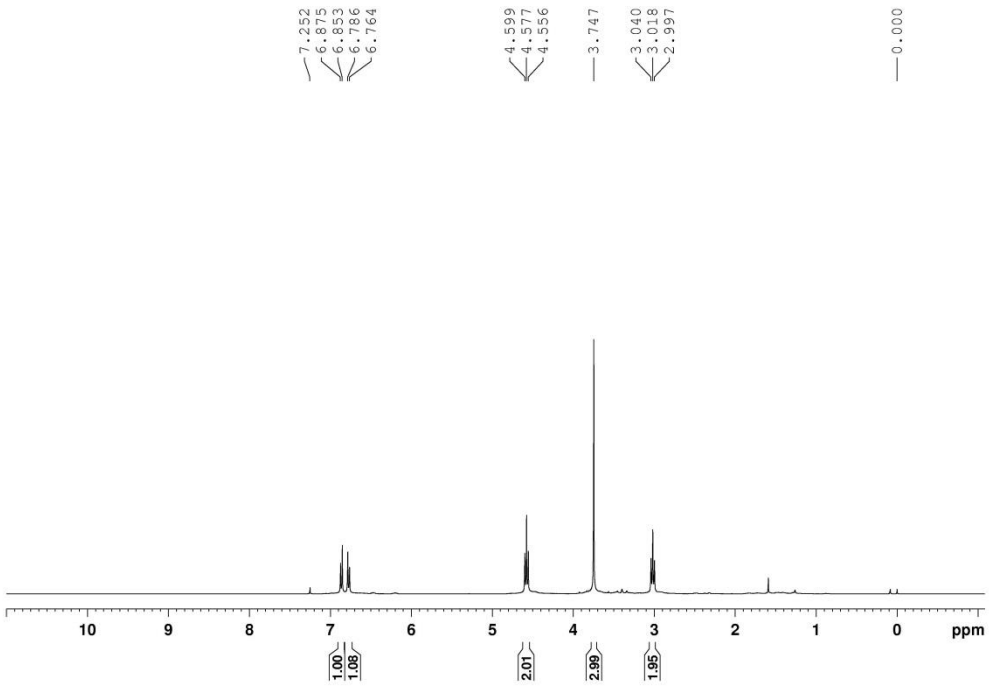
2.00
2.17


CF3
F
F
F
F
O
O

3f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3.747
3.040
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2.997
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
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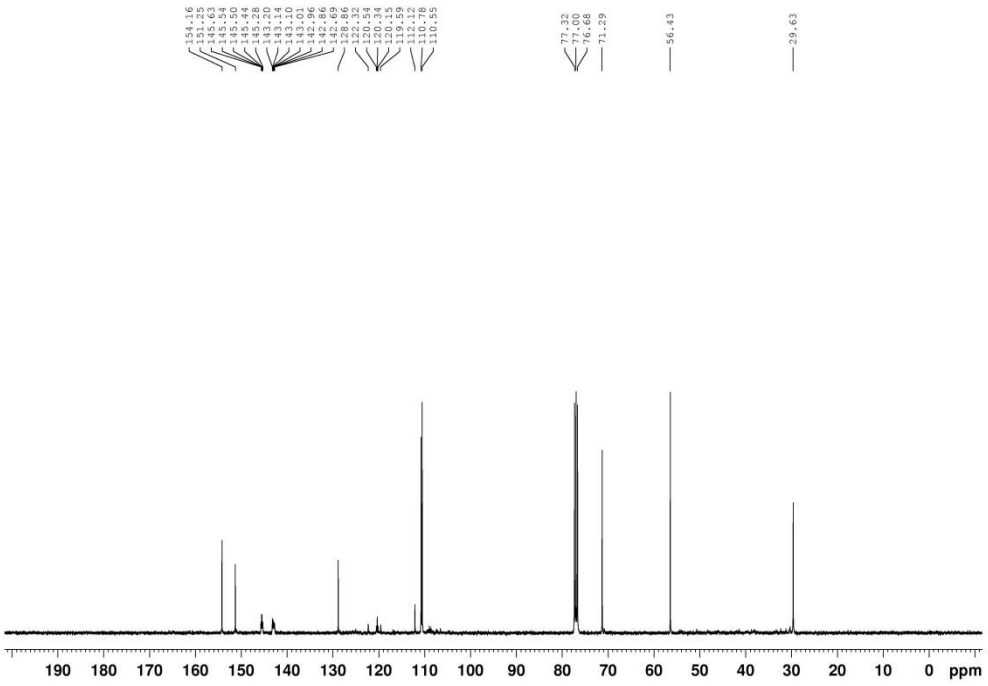
1.95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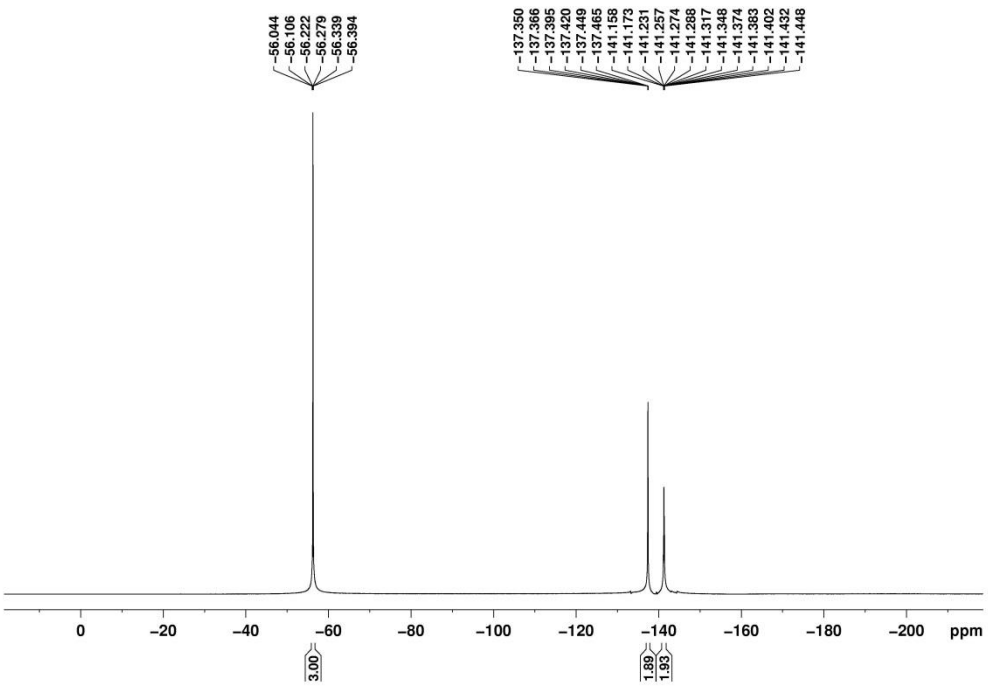
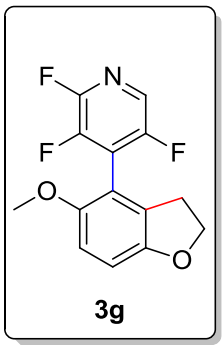
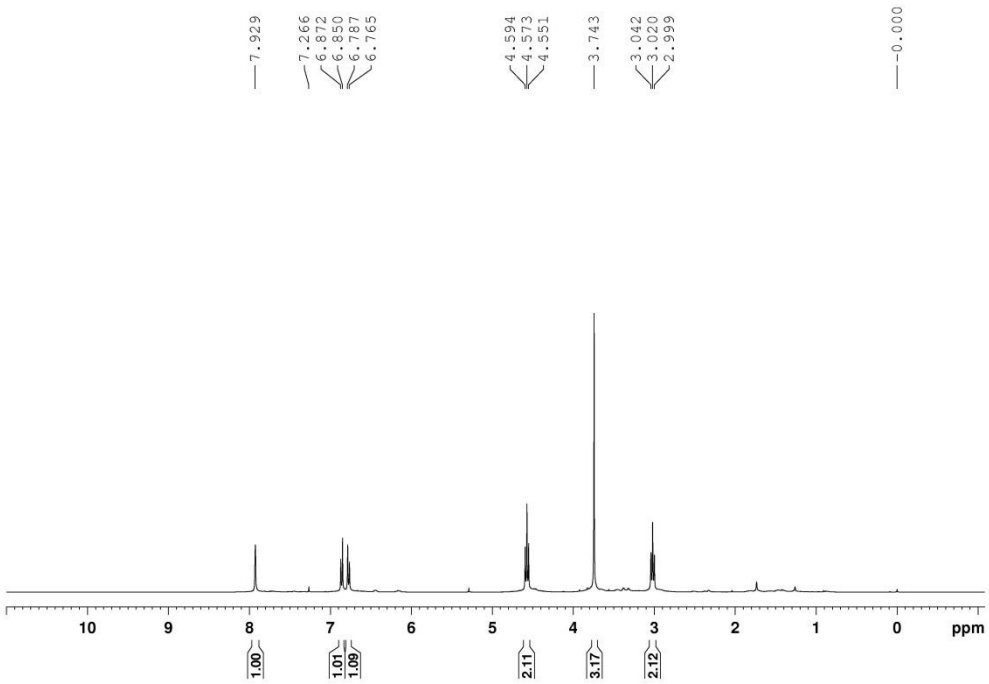
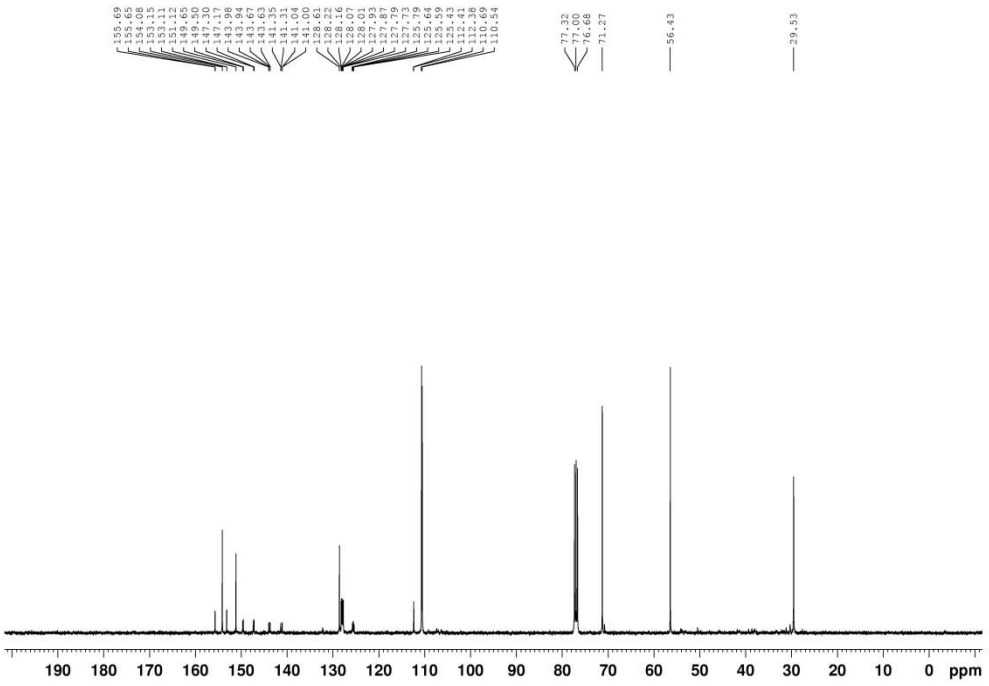
143.01
142.96
142.86
142.69
128.86
128.32
120.54
120.34
120.15
119.59
112.12
110.78
110.55
77.32
77.00
76.68
71.29
56.43
29.63
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

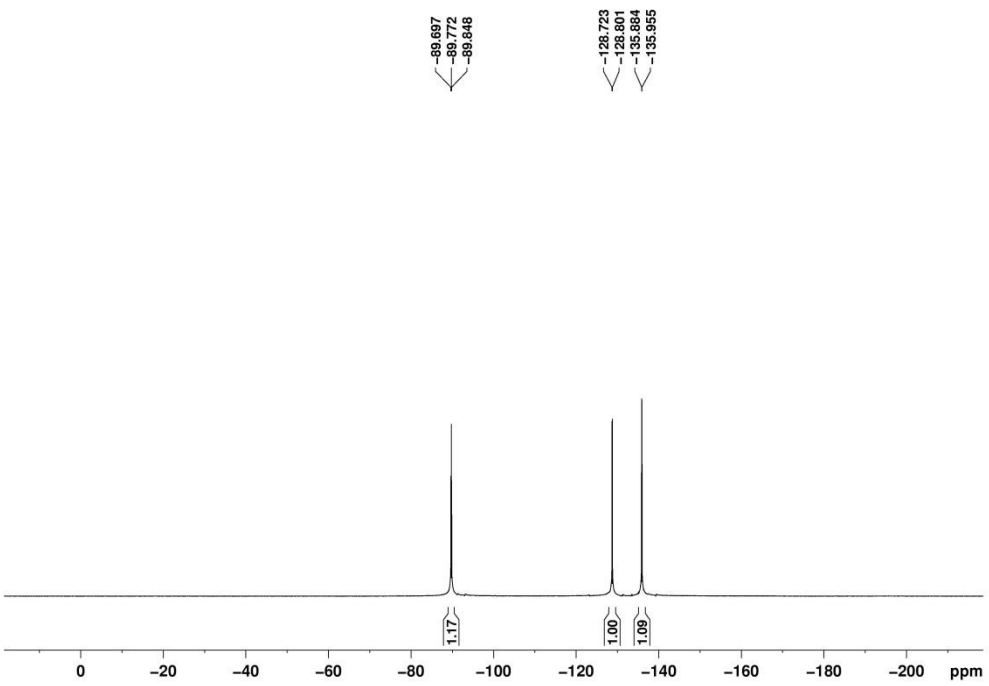

56.044
56.106
56.222
56.279
56.339
56.394
137.350
137.366
137.395
137.420
137.449
137.465
141.158
141.173
141.231
141.257
141.274
141.288
141.317
141.348
141.374
141.383
141.402
141.432
141.448
0 −20 −40 −60 −80 −100 −120 −140 −160 −180 −200 ppm
3.00
1.89
1.93

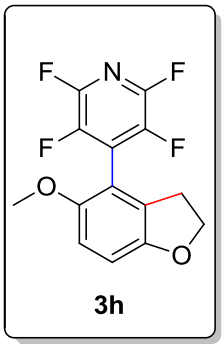

F
N
F
F
O
O

3g

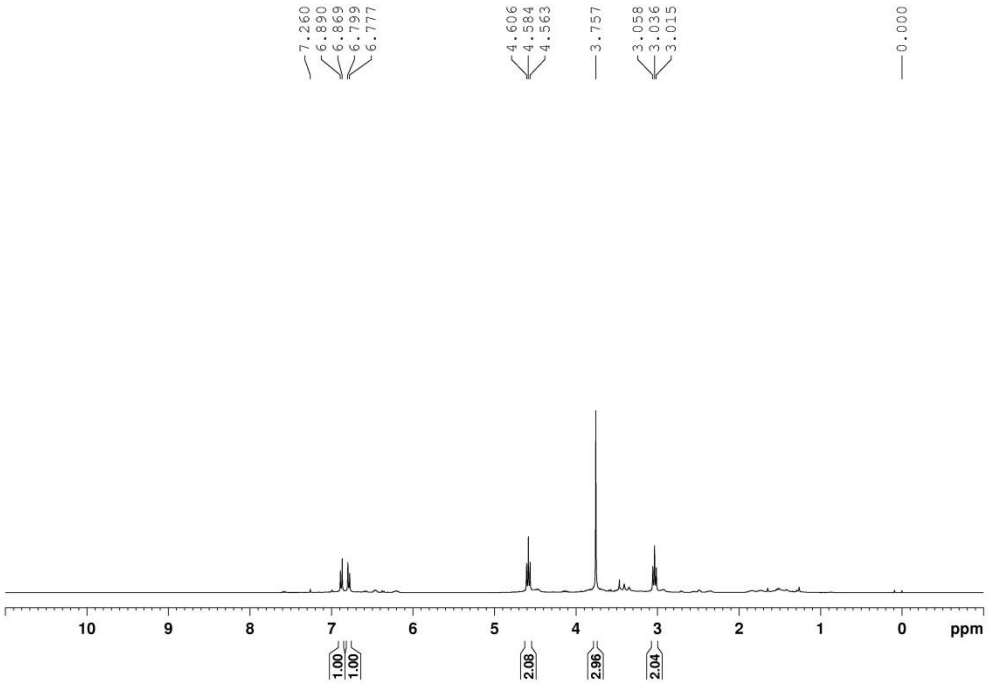

7.929
7.266
6.872
6.850
6.787
6.765
4.594
4.573
4.551
3.743
3.042
3.020
2.999
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.09
2.11
3.17
2.12

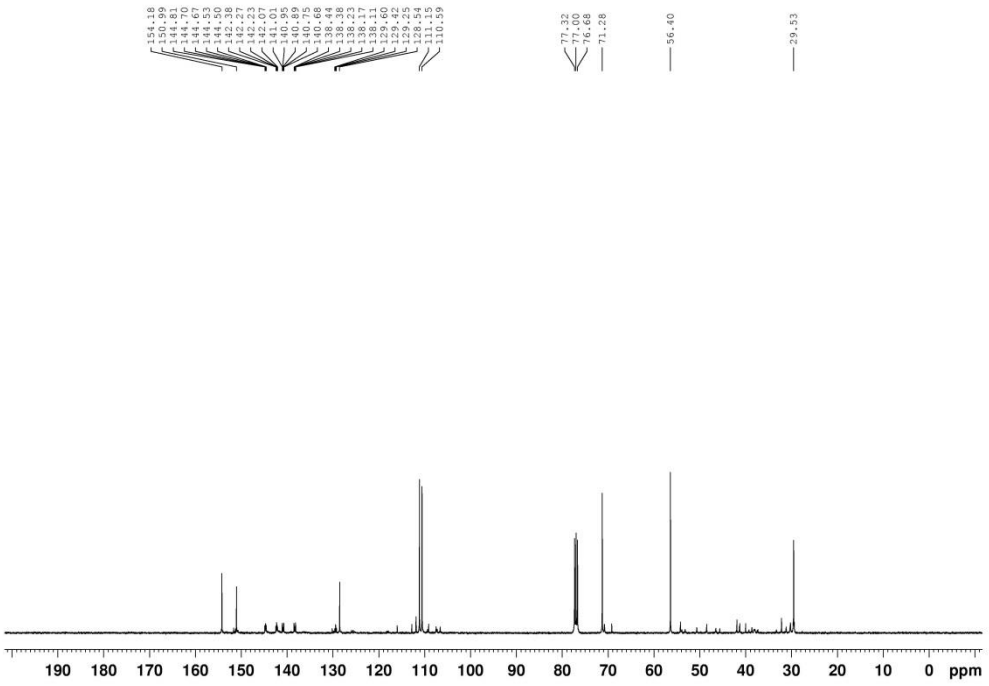

155.69
155.65
154.08
153.15
153.11
151.12
149.65
149.50
147.30
147.17
143.98
143.94
143.67
143.63
141.35
141.31
141.04
141.00
128.61
128.22
128.16
128.07
128.01
127.93
127.87
127.79
127.73
125.79
125.64
125.59
125.43
112.41
112.38
110.69
110.54
77.32
77.00
76.68
71.27
56.43
29.53
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

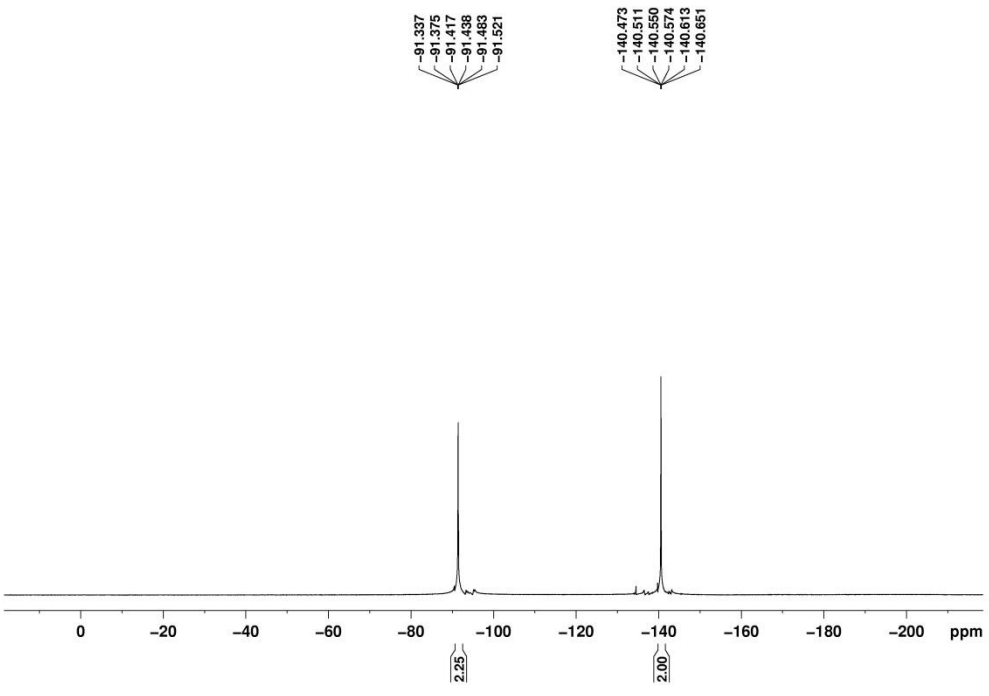

-89.697
-89.772
-89.848
-128.723
-128.801
-135.884
-135.955
1.17
1.00
1.09
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm

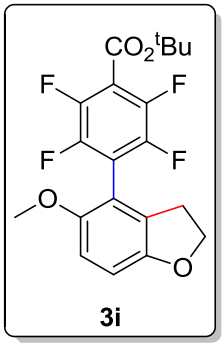

F
N
F
F
F
O
O

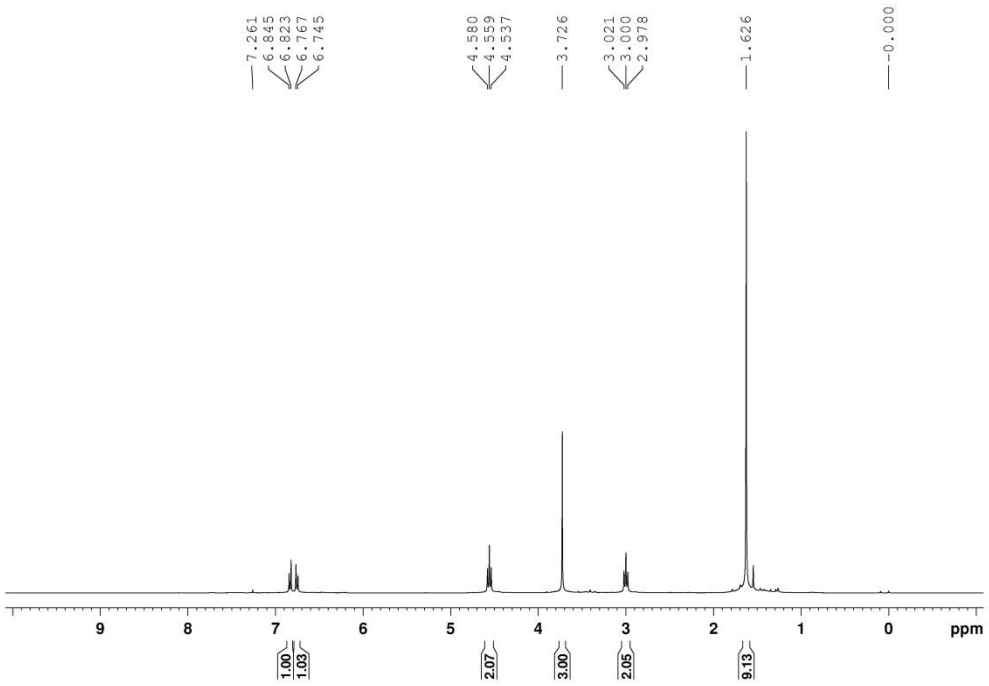
3h

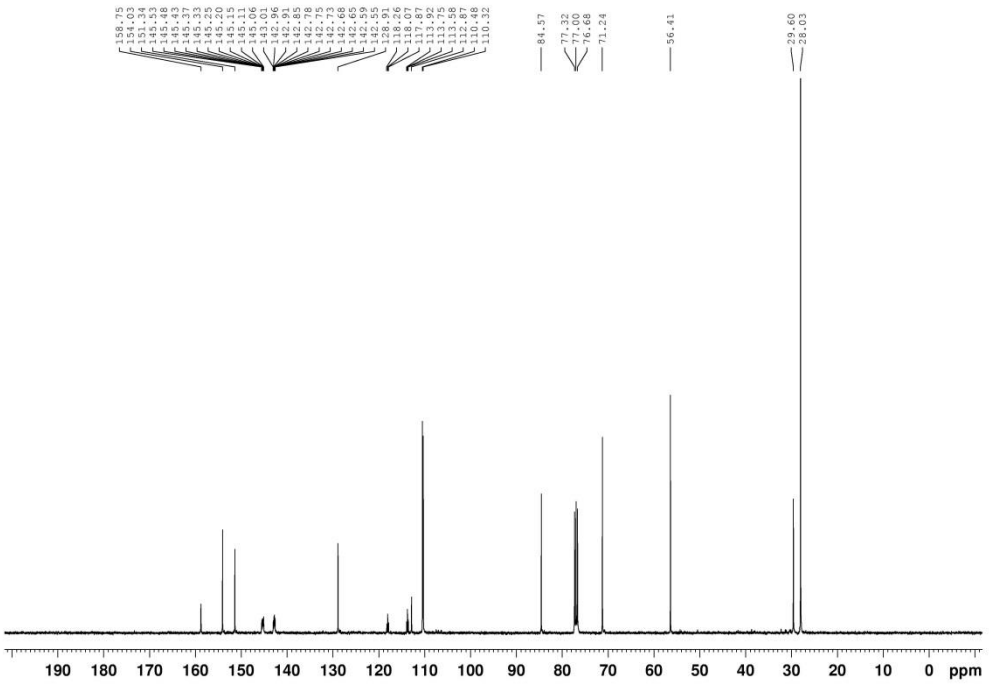

7.260
6.890
6.869
6.799
6.777
4.606
4.584
4.563
3.757
3.058
3.036
3.015
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
2.08
2.96
2.04

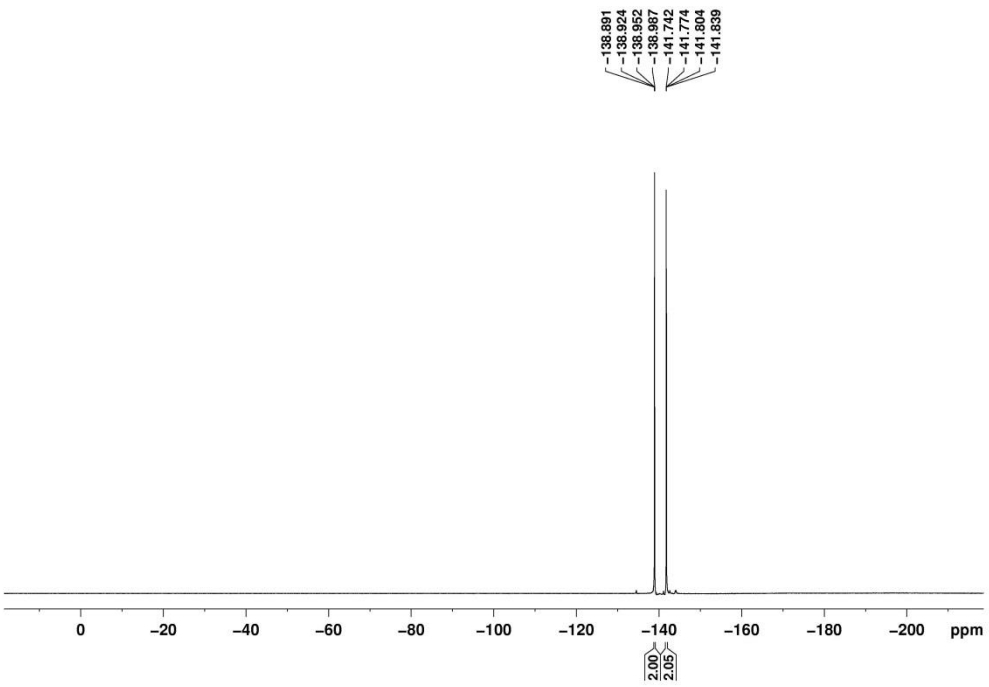

154.18
151.09
149.81
144.70
144.67
144.53
144.50
142.38
142.27
142.23
142.07
141.01
140.95
140.89
140.75
140.68
140.44
138.38
138.23
138.17
138.11
129.60
129.42
129.25
128.54
111.15
110.59
77.32
77.00
76.68
71.28
56.40
29.53
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

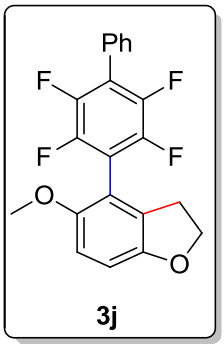

-91.337
-91.375
-91.417
-91.438
-91.483
-91.521
-140.473
-140.511
-140.550
-140.574
-140.613
-140.651
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm
2.25
2.00


CO2tBu
F
F
F
F
O
O
3i

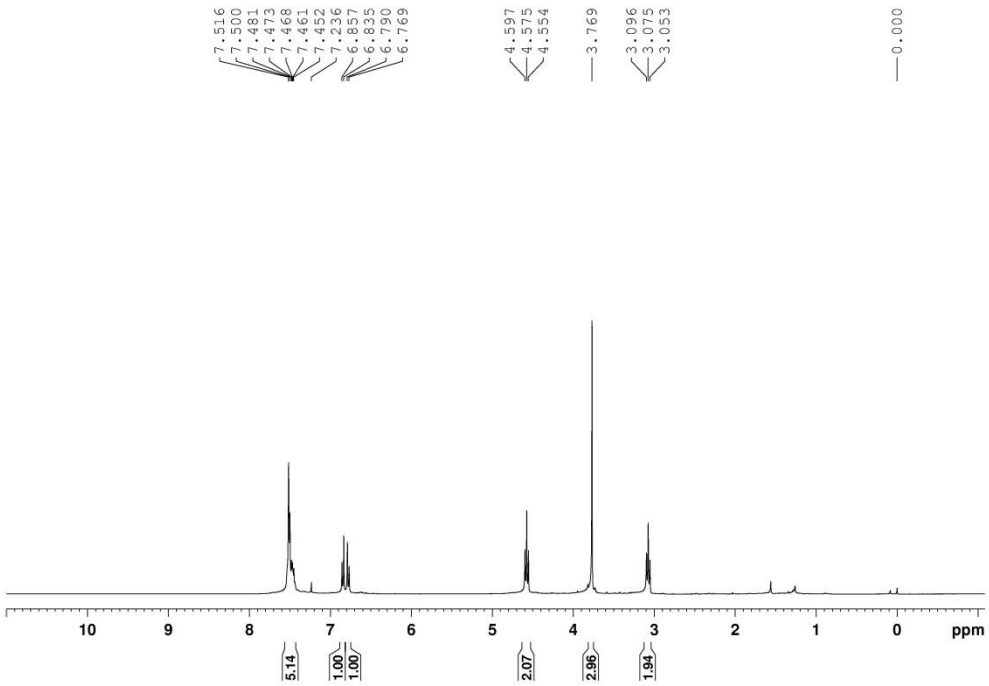

7.261
6.845
6.823
6.767
6.745
4.580
4.559
4.537
3.726
3.021
3.000
2.978
1.626
0.000
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
2.07
3.00
2.05
9.13

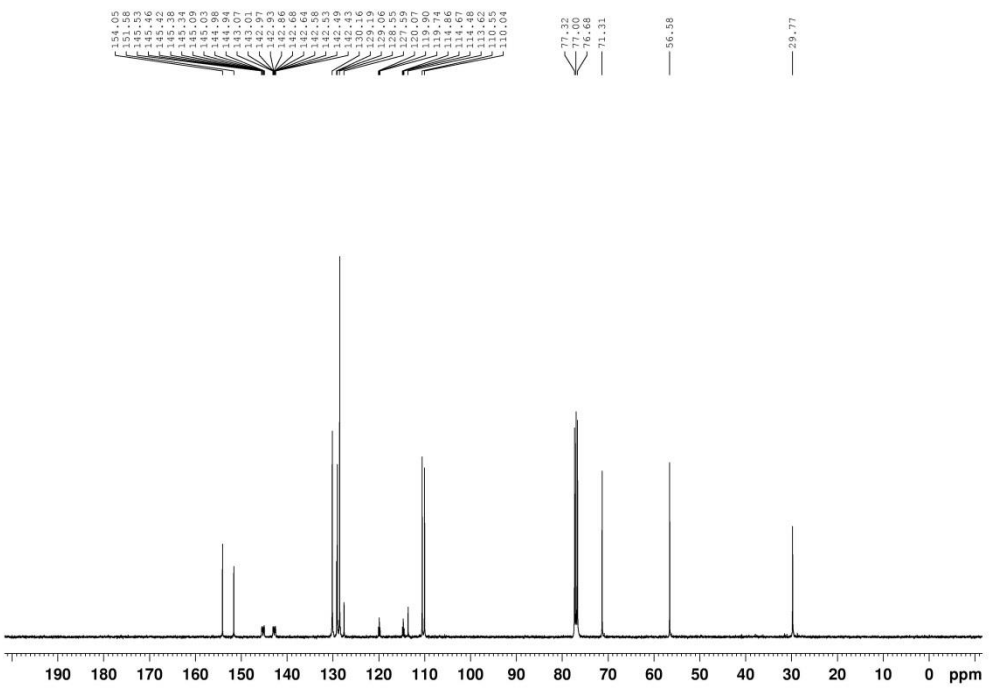

158.75
154.03
151.34
145.53
145.48
145.43
145.37
145.33
145.25
145.20
145.15
145.11
145.06
143.01
142.96
142.91
142.85
142.78
142.75
142.73
142.68
142.65
142.59
142.55
142.51
118.26
118.07
117.87
113.92
113.75
113.58
112.87
110.48
110.32
84.57
77.32
77.00
76.68
71.24
56.41
29.60
28.03
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

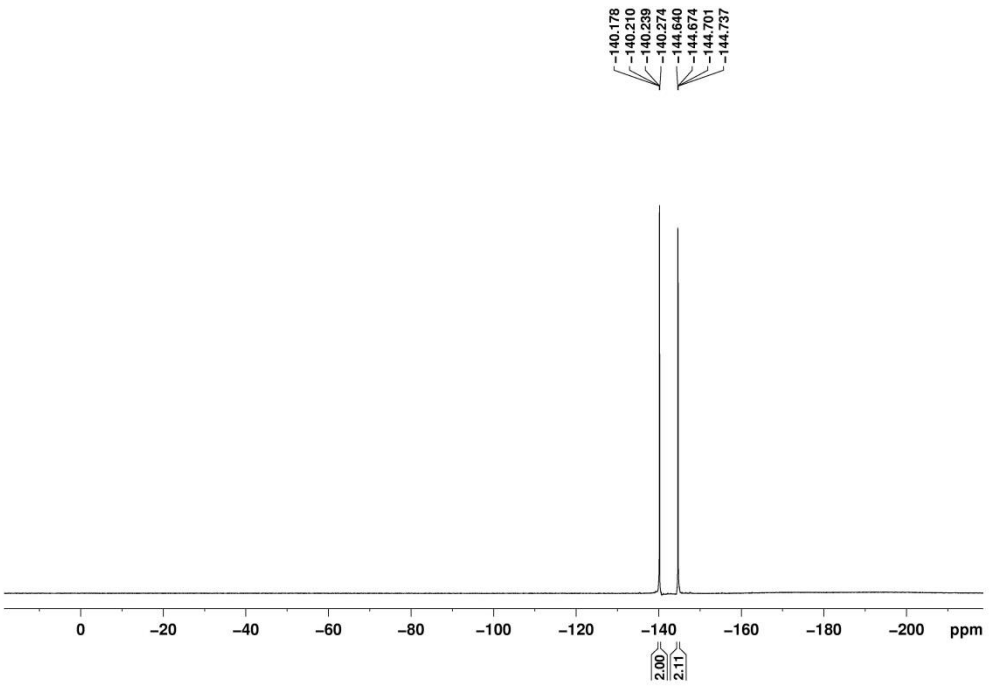

-138.891
-138.924
-138.952
-138.987
-141.742
-141.774
-141.804
-141.839
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm
2.00
2.05

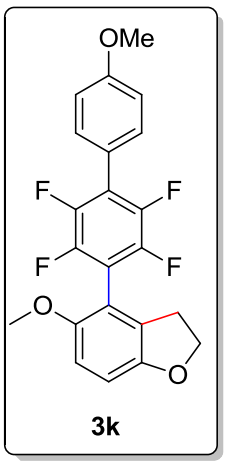

Ph
F
F
F
F
O
O

3j

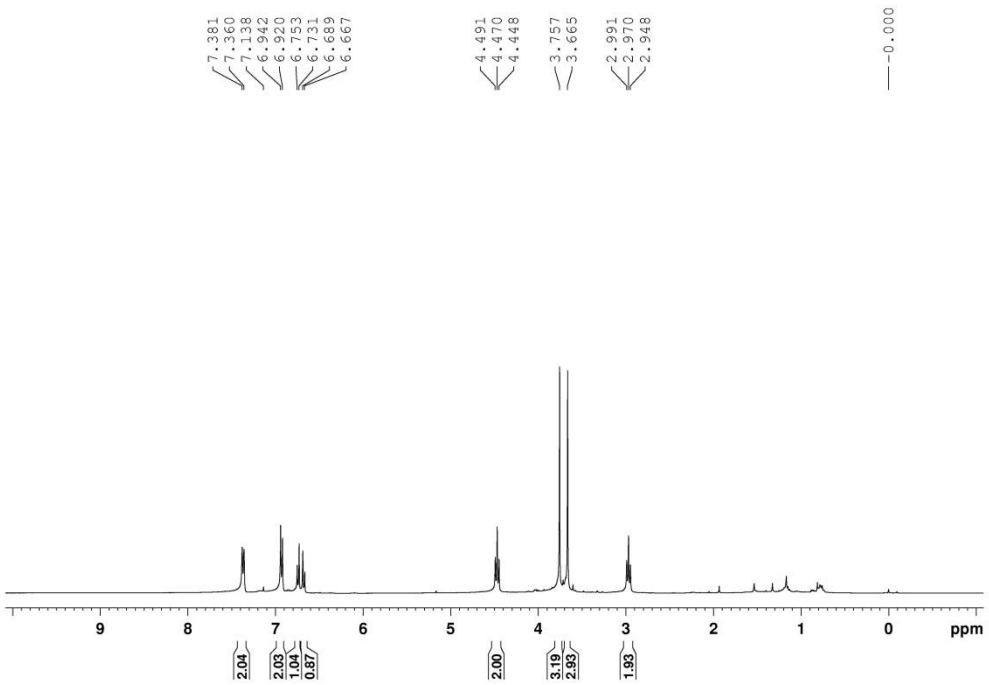

7.516
7.500
7.481
7.473
7.468
7.461
7.452
7.236
6.857
6.835
6.790
6.769
4.597
4.575
4.554
3.769
3.096
3.075
3.053
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
5.14
1.00
1.00
2.07
2.96
1.94

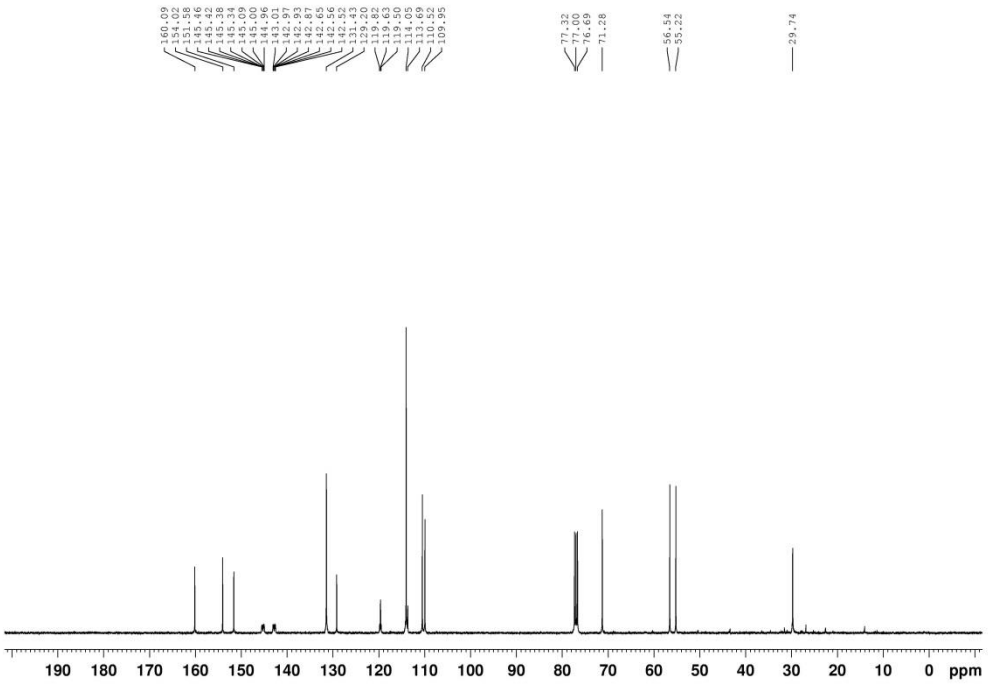

154.05
151.58
145.53
145.46
145.42
145.38
145.34
145.09
145.03
144.98
144.94
143.07
143.01
142.97
142.93
142.86
142.68
142.64
142.58
142.53
142.49
142.43
130.16
129.18
129.06
128.55
127.59
120.97
119.90
119.74
114.86
114.67
114.48
113.62
110.55
110.04
77.32
77.00
76.68
71.31
56.58
29.77
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

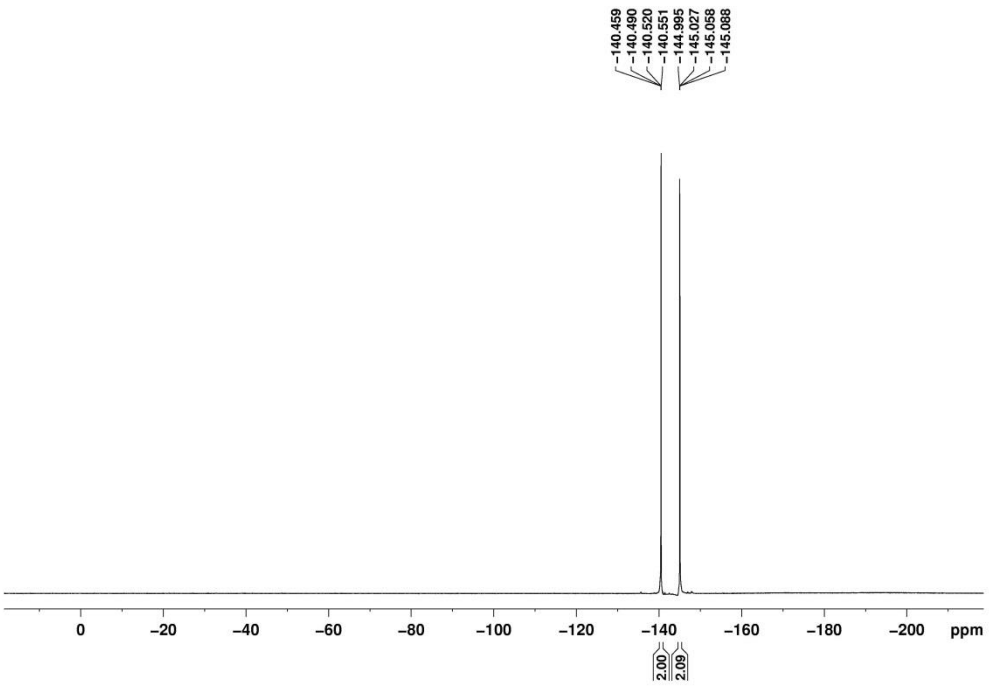

-140.178
-140.210
-140.239
-140.274
-144.640
-144.674
-144.701
-144.737
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm
2.00
2.11

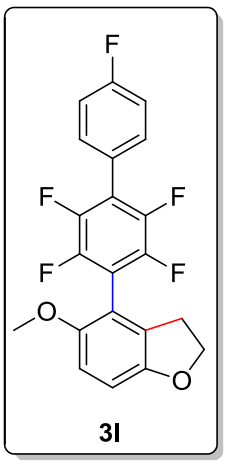

OMe
F
F
F
F
O
O

3k

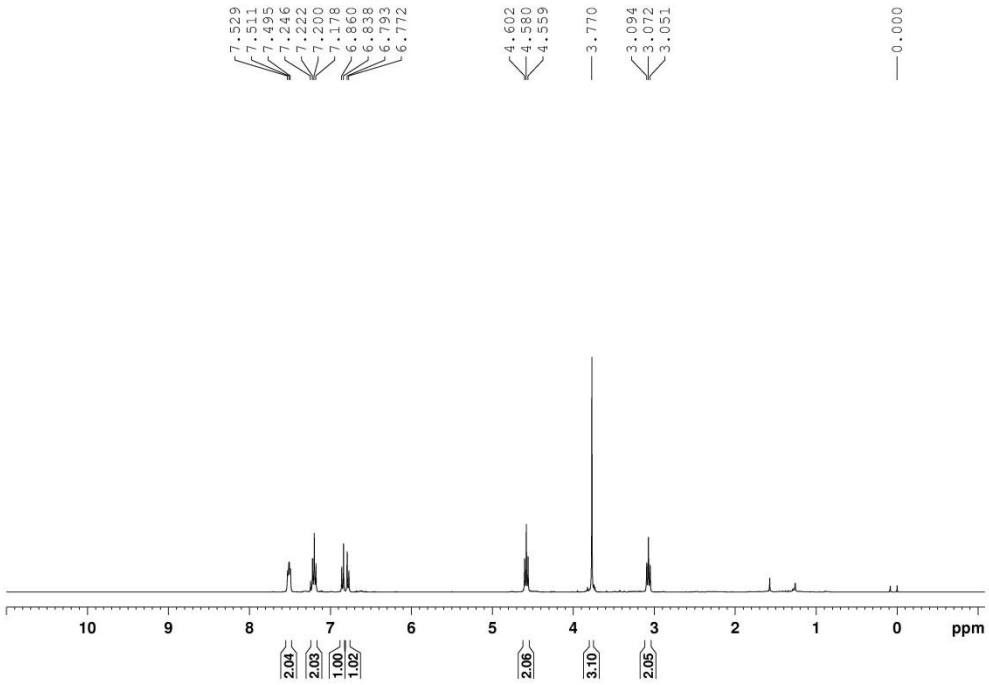

7.381
7.360
7.138
6.942
6.920
6.753
6.731
6.689
6.667
4.491
4.470
4.448
3.757
3.665
2.991
2.970
2.948
0.000
9
8
7
6
5
4
3
2
1
0
ppm
2.04
2.03
1.04
0.87
2.00
3.19
2.93
1.93

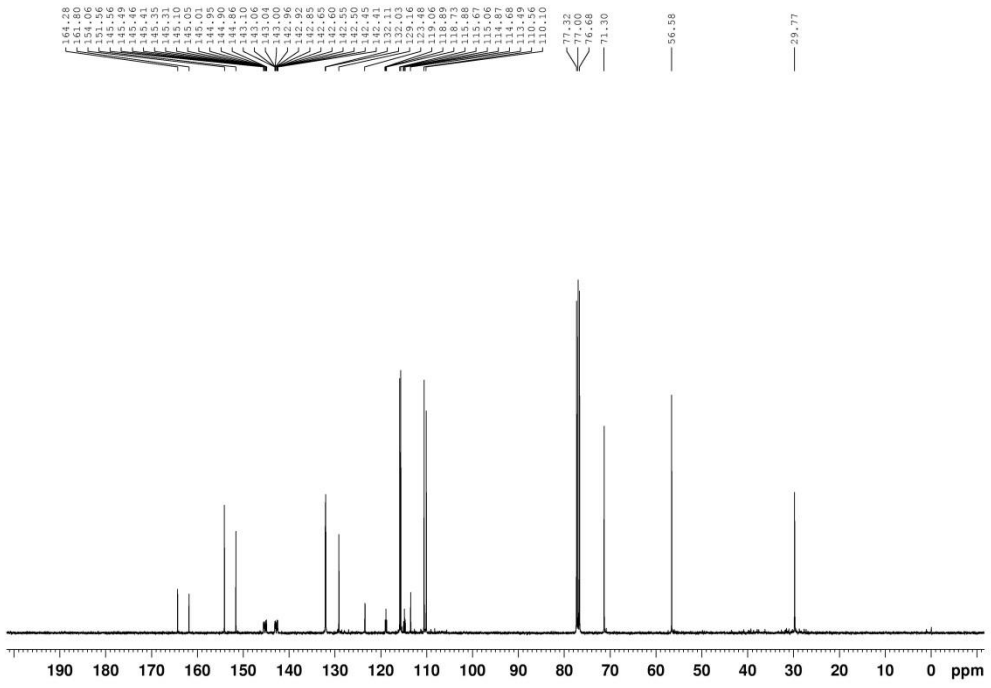

160.09
154.02
151.58
145.46
145.42
145.38
145.34
145.09
145.00
144.96
143.01
142.97
142.93
142.87
142.65
142.56
142.52
131.43
129.20
119.82
119.63
119.50
114.05
113.69
110.52
109.95
77.32
77.00
76.69
71.28
56.54
55.22
29.74
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

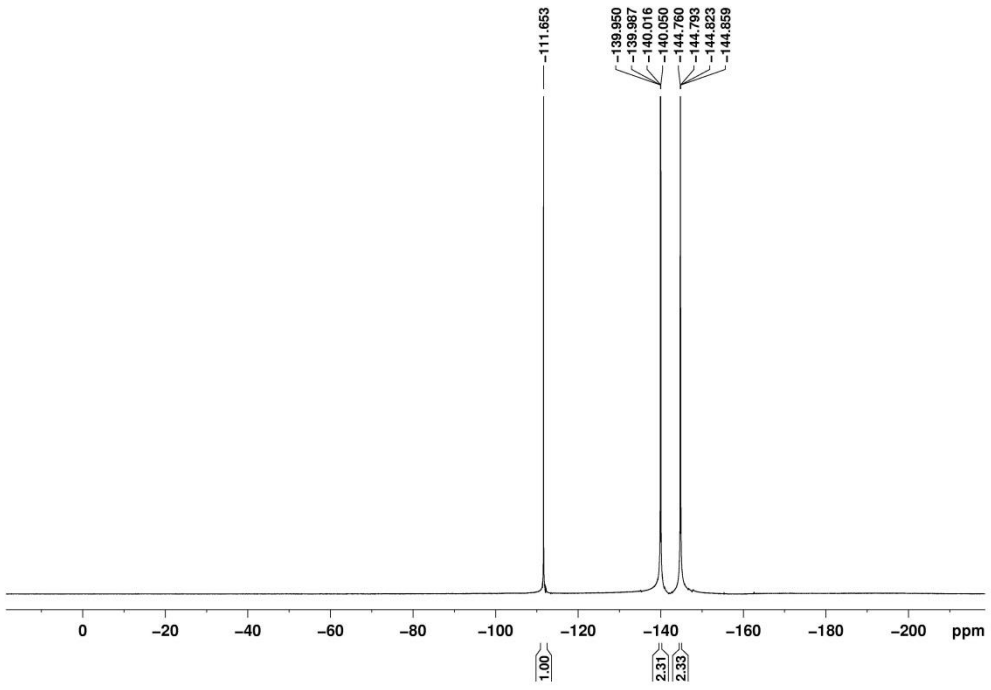

-140.459
-140.490
-140.520
-140.551
-144.995
-145.027
-145.058
-145.088
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm
2.00
2.09

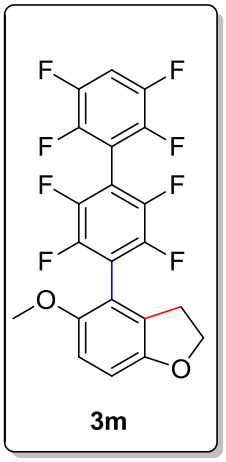

F
F
F
F
F
O
O

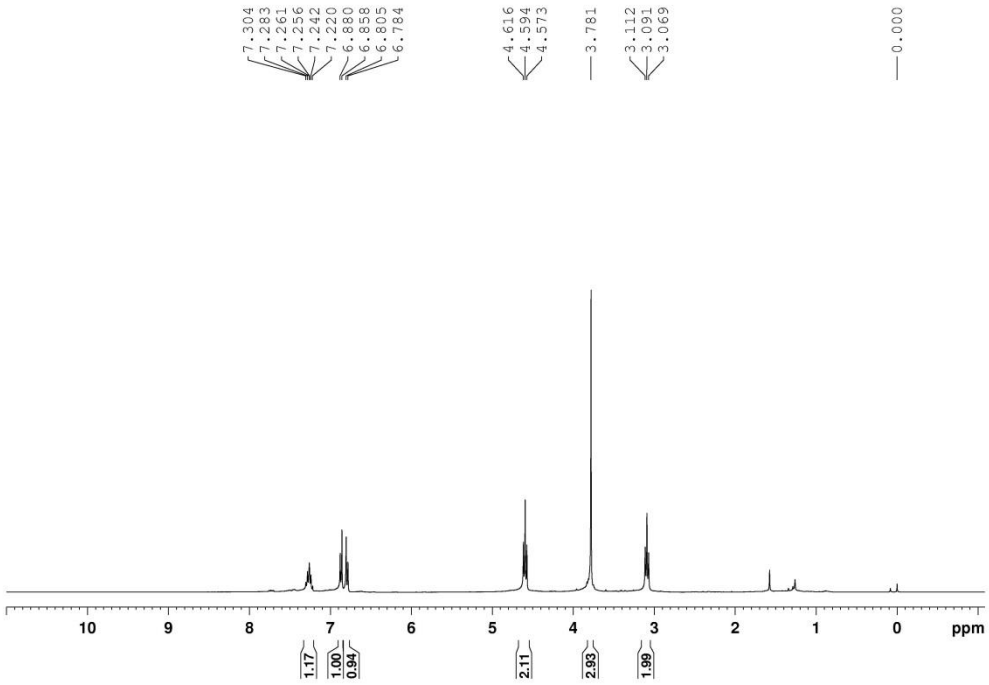
3l

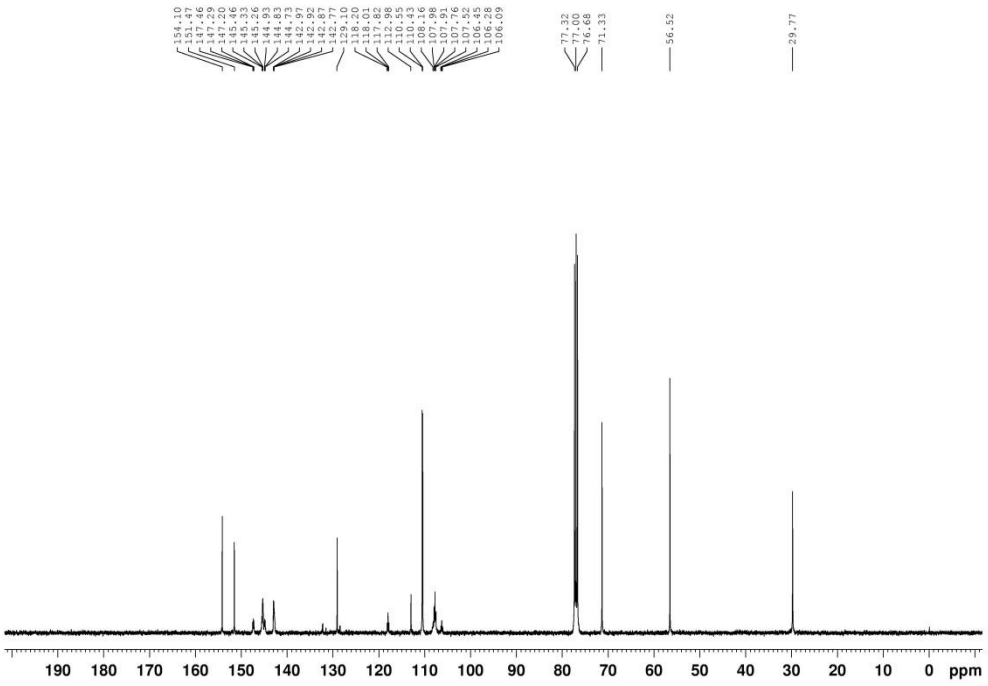

7.529
7.511
7.495
7.246
7.222
7.200
7.178
6.860
6.838
6.793
6.772
4.602
4.580
4.559
3.770
3.094
3.072
3.051
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
2.04
2.03
1.00
1.02
2.06
3.10
2.05

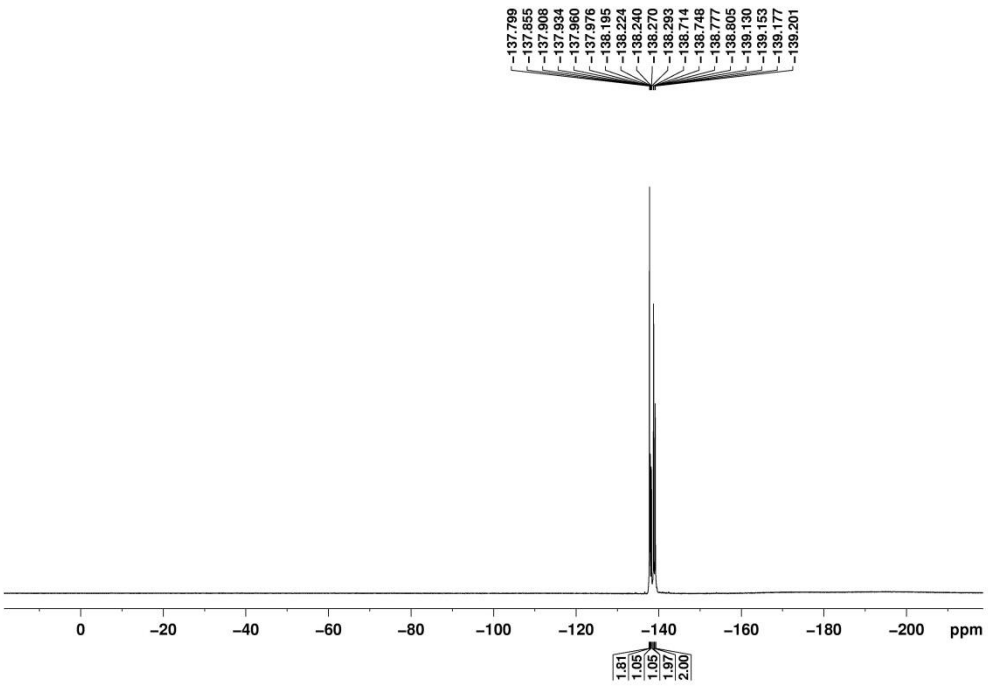

164.28
161.80
154.06
151.56
145.56
145.49
145.46
145.41
145.35
145.31
145.10
145.05
145.01
144.95
144.90
144.86
143.10
143.06
143.04
143.00
142.96
142.92
142.85
142.65
142.60
142.55
142.50
142.45
142.41
132.11
132.03
129.16
123.48
119.06
118.89
118.73
115.88
115.67
115.06
114.87
114.68
113.49
110.56
110.10
77.32
77.00
76.68
71.30
56.58
29.77
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

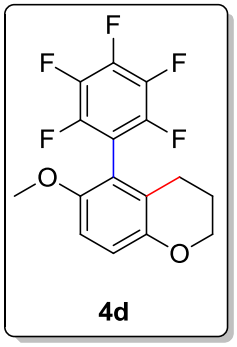

-111.653
-139.950
-139.987
-140.016
-140.050
-144.760
-144.793
-144.823
-144.859
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm
1.00
2.31
2.33


F
F
F
F
F
F
F
F
O
O
3m

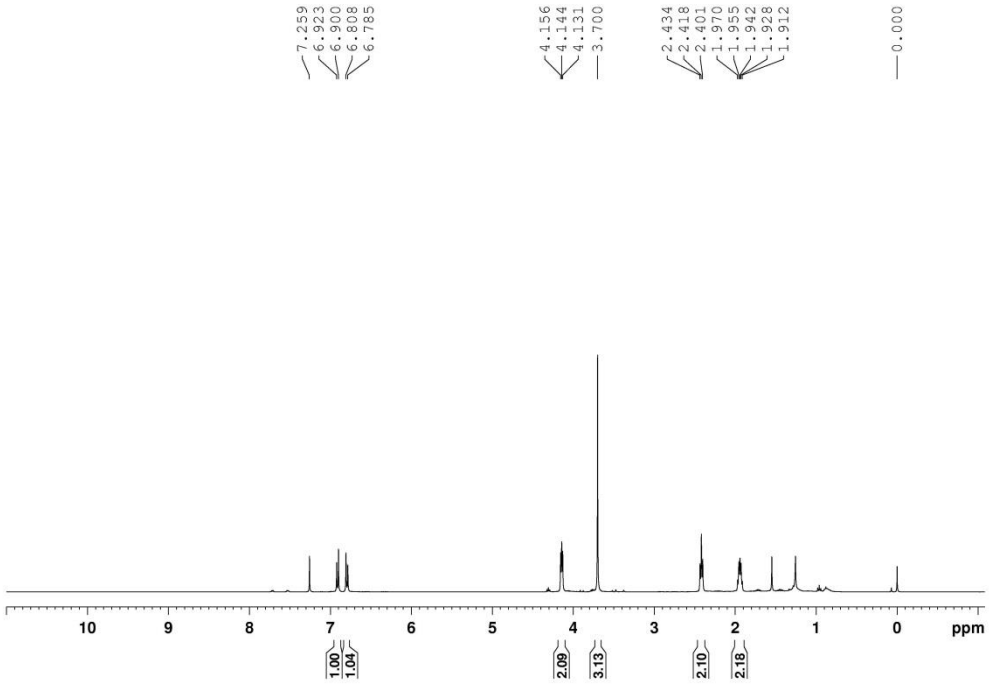

7.304
7.283
7.261
7.256
7.242
7.220
6.880
6.858
6.805
6.784
4.616
4.594
4.573
3.781
3.112
3.091
3.069
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
1.17
1.00
0.94
2.11
2.93
1.99

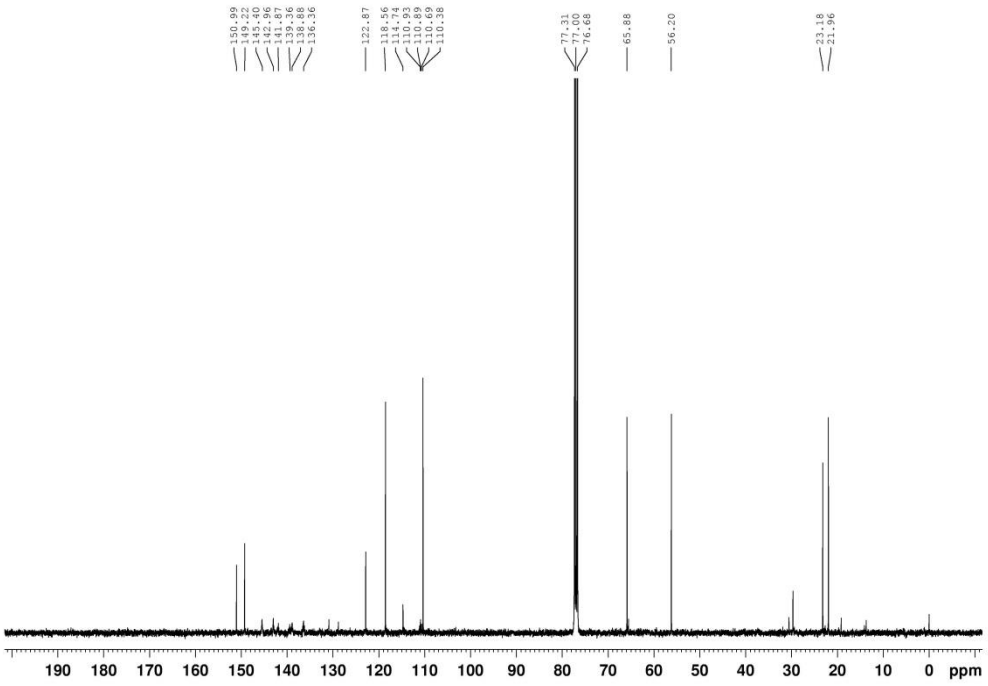

154.10
151.47
147.46
147.29
147.20
145.46
145.33
145.26
144.93
144.83
144.73
142.97
142.92
142.87
142.77
119.10
118.20
118.01
117.82
112.98
110.55
110.43
108.16
107.98
107.91
107.76
107.52
106.45
106.28
106.09
77.32
77.00
76.68
71.33
56.52
29.77
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

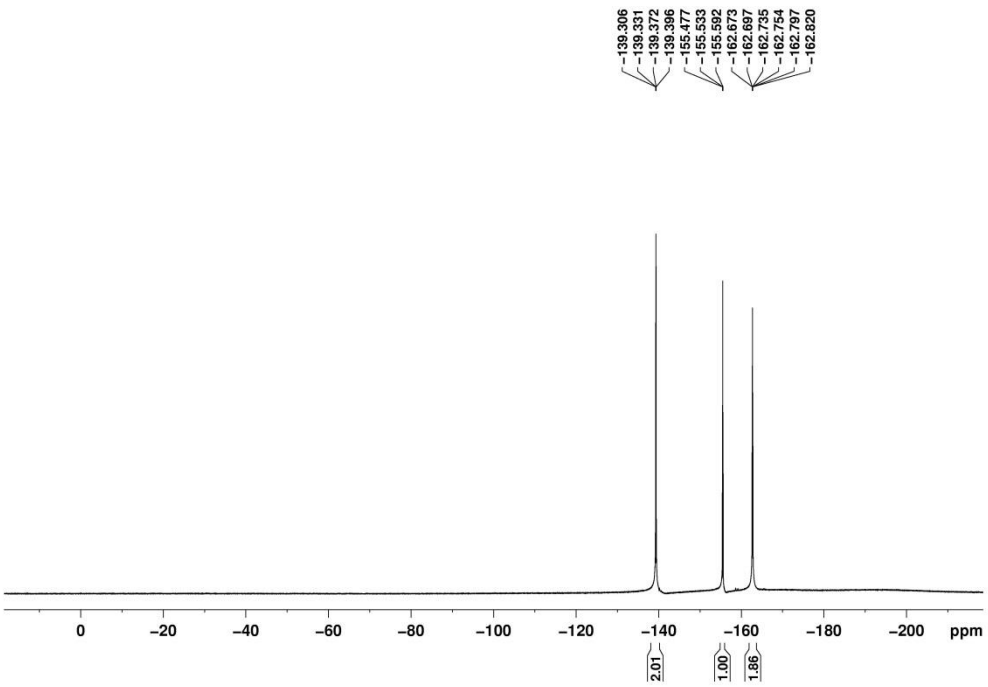

-137.799
-137.855
-137.908
-137.934
-137.960
-137.976
-138.195
-138.224
-138.240
-138.270
-138.293
-138.714
-138.748
-138.777
-138.805
-139.130
-139.153
-139.177
-139.201
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm
1.81
1.05
1.05
1.97
2.00


F
F
F
F
F
O
O

4d


7.259
6.923
6.900
6.808
6.785
4.156
4.144
4.131
3.700
2.434
2.418
2.401
1.970
1.955
1.942
1.928
1.912
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.04
2.09
3.13
2.10
2.18


150.99
149.22
145.40
142.96
141.87
139.36
138.88
136.36
122.87
118.56
114.74
110.93
110.89
110.69
110.58
77.31
77.00
76.68
65.88
56.20
23.18
21.96
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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-139.331
-139.372
-139.396
-155.477
-155.533
-155.592
-162.673
-162.697
-162.735
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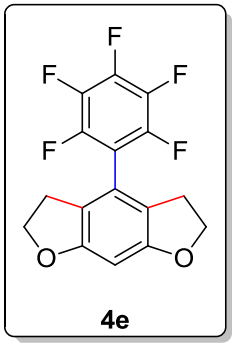
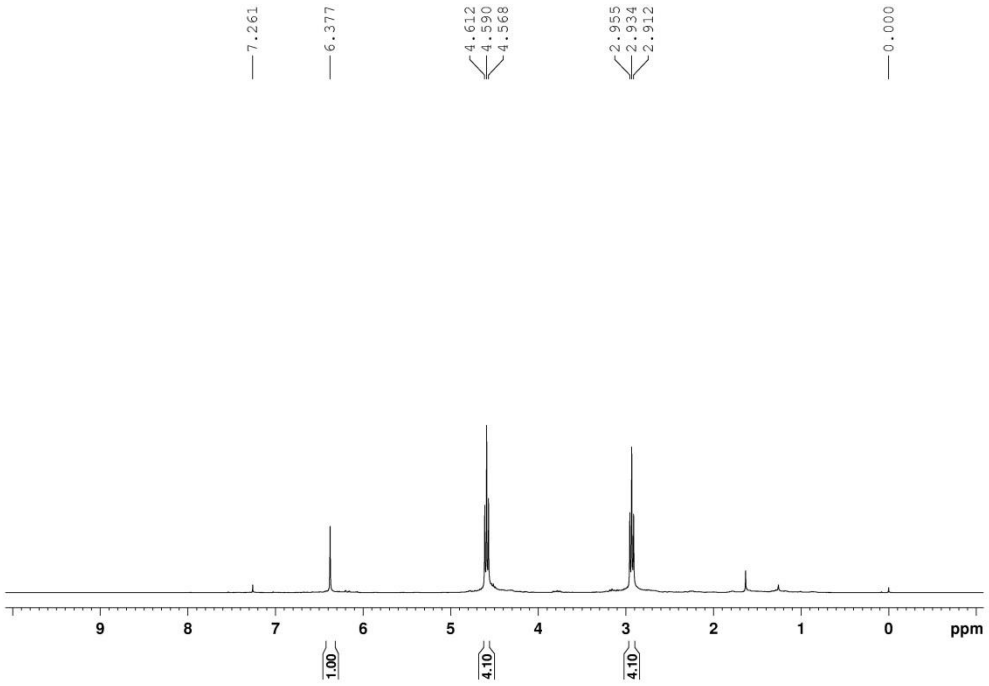
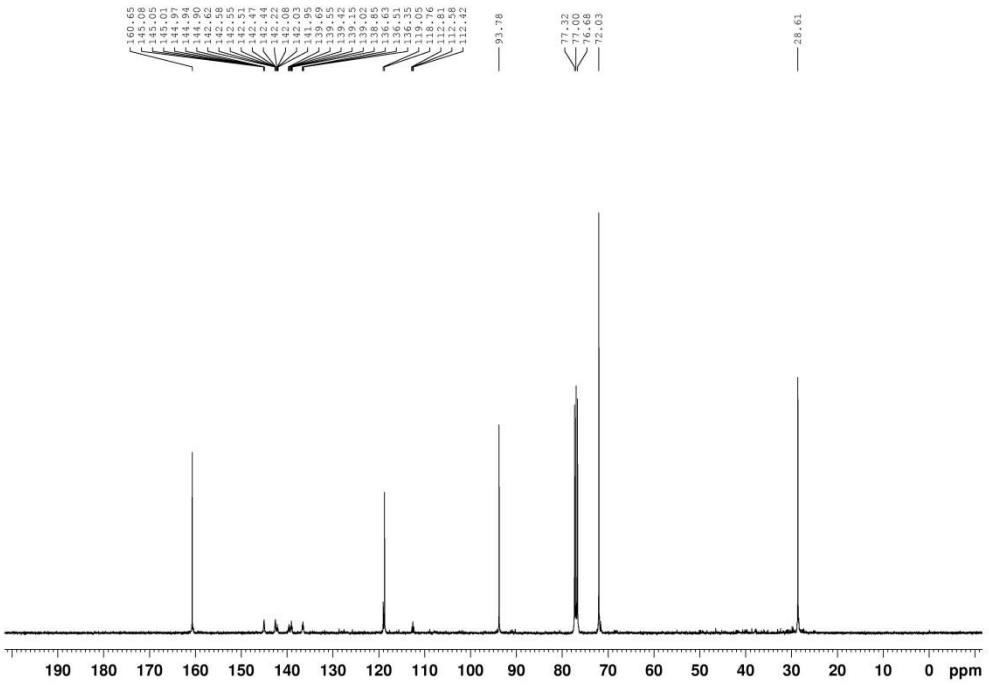
-162.797
-162.820
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm
2.01
1.00
1.86


F
F
F
F
F
O
O
4e


7.261
6.377
4.612
4.590
4.568
2.955
2.934
2.912
0.000
9
8
7
6
5
4
3
2
1
0
ppm
1.00
4.10
4.10


160.65
145.08
145.05
145.01
144.97
144.94
144.90
142.62
142.58
142.55
142.51
142.47
142.44
142.22
142.08
142.03
141.95
139.69
139.55
139.42
139.15
139.02
138.85
136.63
136.51
136.35
119.05
118.76
112.81
112.58
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28.61
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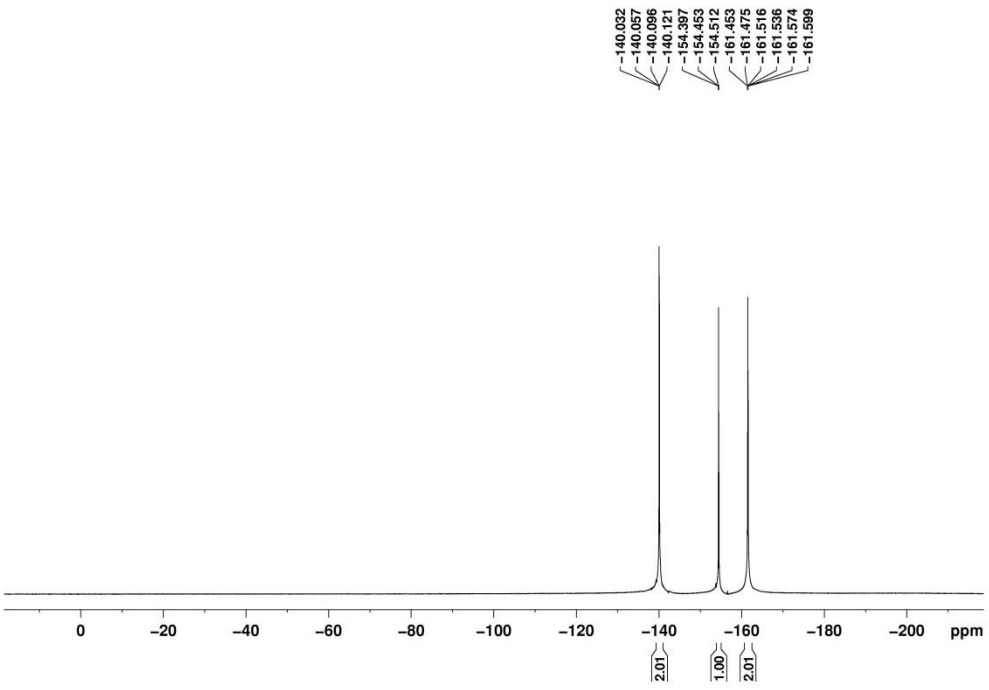
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-140.057
-140.096
-140.121
-154.397
-154.453
-154.512
-161.453
-161.475
-161.516
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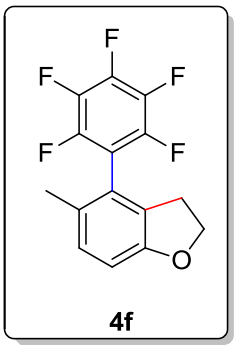
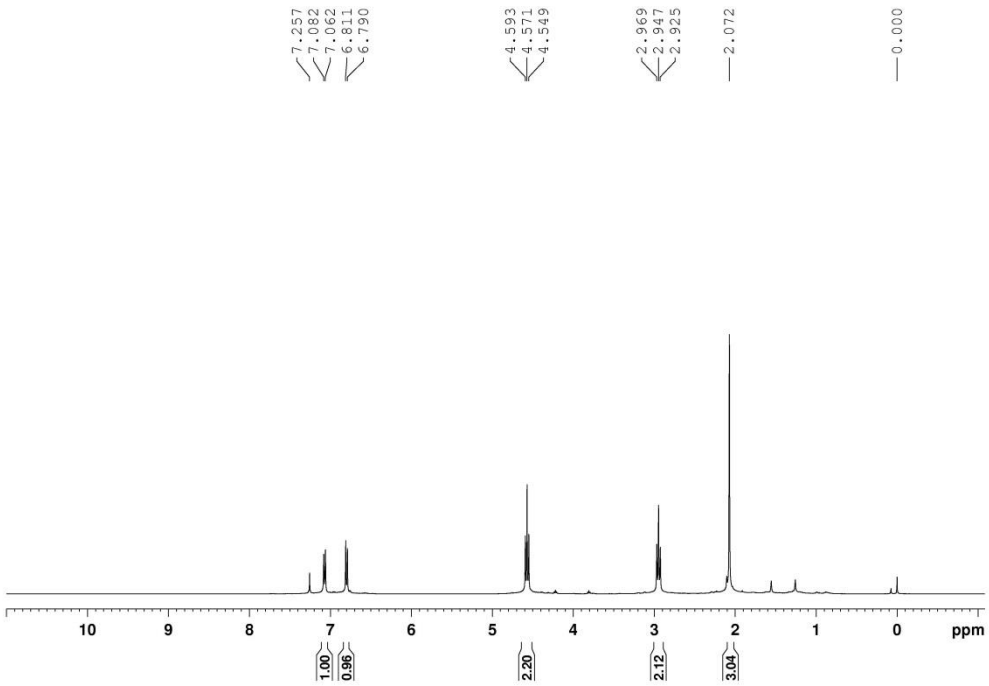
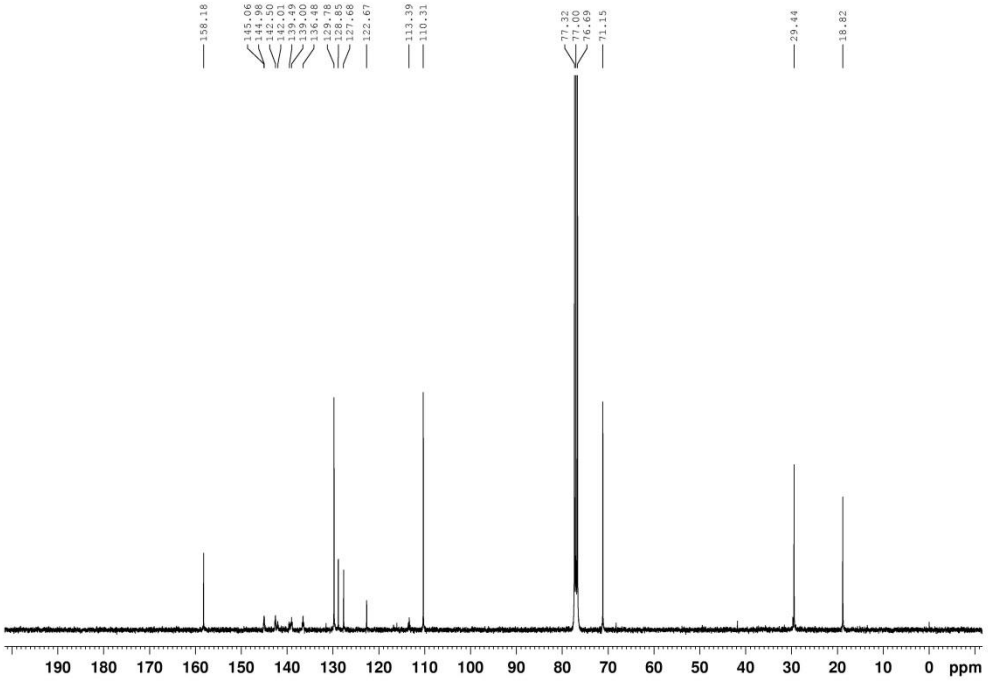
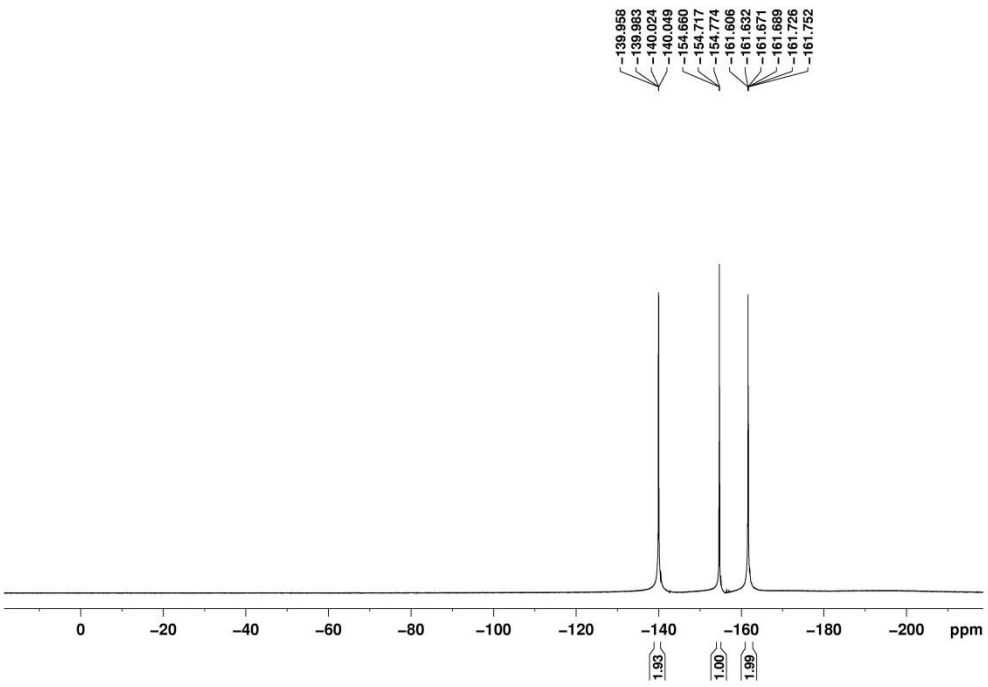
-161.599
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm
2.01
1.00
2.01


F
F
F
F
F
O

4f


7.257
7.082
7.062
6.811
6.790
4.593
4.571
4.549
2.969
2.947
2.925
2.072
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.96
2.20
2.12
3.04


158.18
145.06
144.98
142.50
142.01
139.49
139.00
136.48
129.78
128.85
127.68
122.67
113.39
110.31
77.32
77.00
76.69
71.15
29.44
18.82
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


-139.958
-139.983
-140.024
-140.049
-154.660
-154.717
-154.774
-161.606
-161.632
-161.671
-161.689
-161.726
-161.752
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm
1.93
1.00
1.99