

Supporting Information

Transition Metal Catalyst-Free, Base-Promoted 1,2-Additions of Polyfluorophenylboronates to Aldehydes and Ketones

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I. General Information

All NMR spectra were recorded on a Bruker AC-500 spectrometer (500 MHz for ^1H NMR, 125 MHz for $^{13}\text{C}\{^1\text{H}\}$ NMR, and 470 MHz for ^{19}F NMR) with CDCl_3 as the solvent. Chemical shifts (δ) are given in ppm and ^1H NMR spectra were referenced via residual proton resonances of CDCl_3 (7.26 ppm), $^{13}\text{C}\{^1\text{H}\}$ spectra were referenced to CDCl_3 (77.16 ppm) and ^{19}F spectra are referenced to external CFCl_3 . The following abbreviations were used to indicate multiplicities: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet. GCMS analyses were performed on an Agilent Technologies GCMS system (GC 7890A, EI-MS 5975C). HRMS were measured on a Thermo Scientific Exactive Plus equipped with an Orbitrap. ESI measurements were conducted using a HESI source with an aux-gas temperature of 50 °C. Measurements were conducted using an APCI source with a corona needle; aux-gas temperature was 400 °C. Chemical yields referred to pure isolated product. Automated flash chromatography was performed on silica gel (Biotage SNAP cartridge KP-Sil), obtained from Biotage, using a Biotage® Isolera Four Flash system. Unless otherwise stated, all reagents were commercially purchased and used without further purification. The degassed and dry solvents were used. B_2pin_2 was kindly provided by AllyChem Co. Ltd. (Dalian, China).

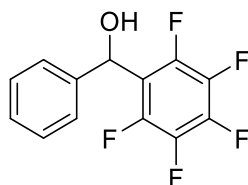
II. Borylation of Polyfluoroarenes

Pentafluorophenyl-Bpin, 2,3,5,6-tetrafluorophenyl-Bpin, 2,3,4,6-tetrafluorophenyl-Bpin and 2,4,6-trifluorophenyl-Bpin used were prepared according to the literature procedures.^[1] In an argon filled glovebox, a solution of $[(\text{COD})\text{Ir}(\text{OMe})]_2$ (0.5 mol%), 4,4'-di-tert-butyl-2,2'-bipyridine (2 mol%), bispinacolatodiboron (B_2pin_2) (0.5 equiv.) and pentafluoroarene (1 equiv.) in hexane (dry and degassed) was stirred at room temperature in a sealed reaction vessel for 48h. The volatile materials were removed *in vacuo* to give the crude product, together with unreacted starting arene. The residue was then purified by flash chromatography on silica gel to provide the corresponding product (~90 %).

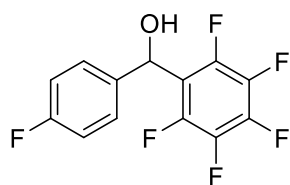
III. General Procedures

In an argon filled glovebox, a sealable reaction tube with a cap equipped with a magnetic stir bar was charged with polyfluorophenyl boronate esters **1** (0.45 mmol), aldehydes **2** (0.4 mmol) and K_2CO_3 (62.1 mg, 0.36 mmol) in toluene (3.0 mL, SPS and degassed) at room temperature. The sealed reaction vessel was placed in an oil bath at 60 °C for 36 h. After the reaction was completed, it was cooled to room temperature. The solvent was removed *in vacuo*. The residue was purified by flash chromatography on silica gel (eluant: *n*-pentane and EtOAc) to give the desired product.

IV. Characterization

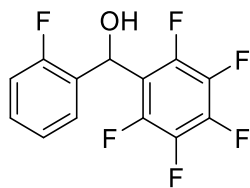


(3a):^[2] 101 mg, 92% yield, white solid. 1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.40-7.36 (m, 4H), 7.34-7.31 (m, 1H), 6.23 (s, 1H), 2.92 (s, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ (ppm) = 144.6 (dm, $^1J_{F-C} = 250$ Hz), 140.8 (dm, $^1J_{F-C} = 250$ Hz), 140.6, 137.6 (dm, $^1J_{F-C} = 250$ Hz), 128.7, 128.3, 125.4 (t, $J_{F-C} = 1$ Hz), 117.0 (tm, $J_{F-C} = 17$ Hz), 67.6. ^{19}F NMR (470 MHz, $CDCl_3$): δ (ppm) = -143 – -143.1 (m, 2F), -154.6 – -154.7 (m, 1F), -161.4 – -161.6 (m, 2F). HRMS (ASAP): Calcd. for $C_{13}H_7F_5O$ 274.0417, Found: 274.0403.

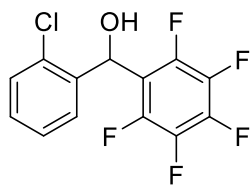


(3b):^[2] 109 mg, 93% yield, colorless oil. 1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.38-7.34 (m, 2H), 7.07-7.02 (m, 2H), 6.21 (s, 1H), 2.73 (s, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ (ppm) = 162.5 (d, $^1J_{F-C} = 250$ Hz), 144.6 (dm, $^1J_{F-C} = 250$ Hz), 140.9 (dm, $^1J_{F-C} = 250$ Hz), 137.7 (dm, $^1J_{F-C} = 250$ Hz), 136.3 (d, $J_{F-C} = 3$ Hz), 127.2 (m), 116.7 (tm, $J_{F-C} = 18$ Hz), 115.6 (d, $J_{F-C} = 22$ Hz), 66.7. ^{19}F NMR (470 MHz, $CDCl_3$): δ (ppm) = -113.7 – -113.8 (m, 1F),

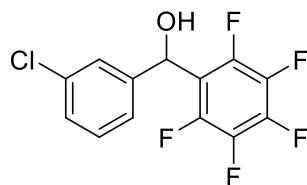
-143.1 – -143.2 (m, 2F), -154.2 – -154.3 (m, 1F), -161.2 – -161.3 (m, 2F). HRMS (ASAP):
Calcd. for C₁₃H₆F₆O 292.0323, Found: 292.0312.



(3c): 105 mg, 90% yield, colorless oil. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 7.69-7.65 (m, 1H), 7.33-7.29 (m, 1H), 7.22-7.19 (m, 1H), 7.02-6.98 (m, 1H), 6.42 (s, 1H), 3.04 (s, 1H). ¹³C{¹H} NMR (125 MHz, CDCl₃): δ (ppm) = 159.4 (d, ¹J_{F-C} = 250 Hz), 144.8 (dm, ¹J_{F-C} = 250 Hz), 141.0 (dm, ¹J_{F-C} = 250 Hz), 137.6 (dm, ¹J_{F-C} = 250 Hz), 129.9 (d, J_{F-C} = 8 Hz), 127.4 (d, J_{F-C} = 13 Hz), 126.9 (m), 124.2 (d, J_{F-C} = 4 Hz), 115.7 (tm, J_{F-C} = 15 Hz), 115.3 (d, J_{F-C} = 21 Hz), 62.0. ¹⁹F NMR (470 MHz, CDCl₃): δ (ppm) = -117.8 – -117.9 (m, 1F), -142.8 – -142.9 (m, 2F), -154.4 – -154.5 (m, 1F), -161.7 – -161.9 (m, 2F). HRMS (ASAP): Calcd. for C₁₃H₆F₆O 292.0323, Found: 292.0311.

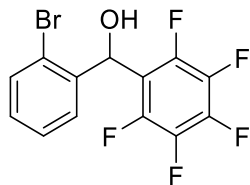


(3d):^[2] 108 mg, 88% yield, white solid. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 7.81-7.79 (m, 1H), 7.36-7.27 (m, 3H), 6.36 (s, 1H), 3.32 (s, 1H). ¹³C{¹H} NMR (125 MHz, CDCl₃): δ (ppm) = 145.1 (dm, ¹J_{F-C} = 250 Hz), 141.1 (dm, ¹J_{F-C} = 250 Hz), 137.6 (dm, ¹J_{F-C} = 250 Hz), 137.4, 131.7, 129.5, 129.4, 127.5 (t, J_{F-C} = 3 Hz), 126.8, 115.0 (tm, J_{F-C} = 17 Hz), 64.4. ¹⁹F NMR (470 MHz, CDCl₃): δ (ppm) = -141.6 – -141.7 (m, 2F), -153.9 (t, J_F = 21 Hz, 1F), -161.7 – -161.9 (m, 2F). HRMS (ASAP): Calcd. for C₁₃H₆F₅ClO 308.0027, Found: 308.0014.

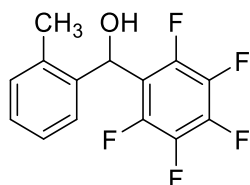


(3e): 108 mg, 87% yield, colorless oil. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 7.39 (s, 1H), 7.32-7.27 (m, 2H), 7.25-7.23 (m, 1H), 6.19 (s, 1H), 2.92 (s, 1H). ¹³C{¹H} NMR (125 MHz, CDCl₃): δ (ppm) = 144.7 (dm, ¹J_{F-C} = 250 Hz), 142.5, 141.1 (dm, ¹J_{F-C} = 250 Hz), 137.7 (dm,

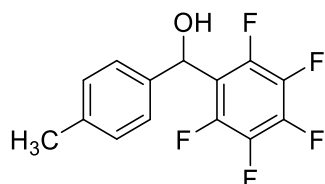
$^1J_{F-C} = 250$ Hz), 134.7, 130.0, 128.4, 125.6, 123.5, 116.3 (tm, $J_{F-C} = 15$ Hz), 66.7. ^{19}F NMR (470 MHz, $CDCl_3$): δ (ppm) = -142.8 – -142.9 (m, 2F), -153.7 – -153.8 (m, 1F), -160.9 – -161.1 (m, 2F). HRMS (ASAP): Calcd. for $C_{13}H_6F_5ClO$ 308.0027, Found: 308.0017.



(3f): 125 mg, 89% yield, white solid. 1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.80-7.78 (m, 1H), 7.51 (dd, $J = 8$ Hz, 1 Hz, 1H), 7.39 (tm, $J = 8$ Hz, 1H), 7.20 (tm, $J = 8$ Hz, 1H), 6.29 (s, 1H), 3.24 (s, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ (ppm) = 145.1 (dm, $^1J_{F-C} = 250$ Hz), 143.2 (dm, $^1J_{F-C} = 250$ Hz), 138.9, 137.6 (dm, $^1J_{F-C} = 250$ Hz), 132.8, 129.8, 128.1 (t, $J_{F-C} = 3$ Hz), 127.4, 121.5, 114.9 (tm, $J_{F-C} = 15$ Hz), 66.5. ^{19}F NMR (470 MHz, $CDCl_3$): δ (ppm) = -141.0 (m, 2F), -153.7 (t, $J_F = 20$ Hz, 1F), -161.6 – -161.8 (m, 2F). HRMS (ASAP): Calcd. for $C_{13}H_6F_5BrO$ 351.9522, Found: 351.9511.

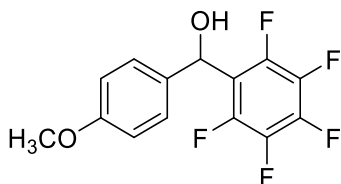


(3g):^[2] 91 mg, 79% yield, white solid. 1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.54-7.52 (m, 1H), 7.27-7.24 (m, 2H), 7.19-7.17 (m, 1H), 6.30 (s, 1H), 2.63 (s, 1H), 2.31 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ (ppm) = 144.8 (dm, $^1J_{F-C} = 250$ Hz), 140.8 (dm, $^1J_{F-C} = 250$ Hz), 137.9, 137.6 (dm, $^1J_{F-C} = 250$ Hz), 135.4, 130.8, 128.4, 126.2, 125.7 (t, $J_{F-C} = 3$ Hz), 115.8 (tm, $J_{F-C} = 15$ Hz), 65.3, 18.9. ^{19}F NMR (470 MHz, $CDCl_3$): δ (ppm) = -142.0 – -142.1 (m), -154.4 – -154.5 (m), -161.5 – -161.7 (m, 2F). HRMS (ASAP): Calcd. for $C_{14}H_9F_5O$ 288.0574, Found: 288.0563.

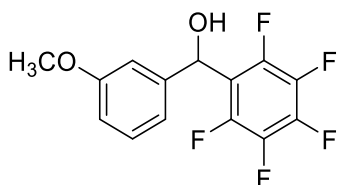


(3h):^[2] 93 mg, 81% yield, white solid. 1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.28-7.27 (m, 2H), 7.20-7.18 (m, 2H), 6.17 (s, 1H), 3.20 (s, 1H), 2.37 (s, 3H). $^{13}C\{^1H\}$ NMR (125 MHz,

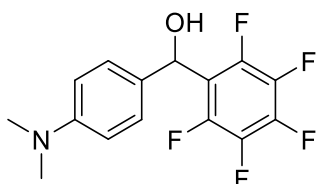
CDCl₃): δ (ppm) = 144.6 (dm, $^1J_{F-C}$ = 250 Hz), 140.7 (dm, $^1J_{F-C}$ = 250 Hz), 138.2, 137.7 (dm, $^1J_{F-C}$ = 251 Hz), 137.6, 129.4, 125.3, 117.1 (tm, J_{F-C} = 15 Hz), 67.5, 21.0. ^{19}F NMR (470 MHz, CDCl₃): δ (ppm) = -143.1 – -143.2 (m, 2F), -155.1 (t, J_F = 21 Hz, 1F), -161.7 – -161.8 (m, 2F). HRMS (ASAP): Calcd. for C₁₄H₉F₅O 288.0574, Found: 288.0563.



(3i):^[2] 86 mg, 71% yield, colorless oil. ^1H NMR (500 MHz, CDCl₃): δ (ppm) = 7.30-7.28 (m, 2H), 6.88-6.85 (m, 2H), 6.14 (s, 1H), 3.79 (s, 3H), 3.24 (s, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl₃): δ (ppm) = 159.5, 144.6 (dm, $^1J_{F-C}$ = 250 Hz), 140.7 (dm, $^1J_{F-C}$ = 250 Hz), 137.6 (dm, $^1J_{F-C}$ = 250 Hz), 132.7, 126.8, 117.2 (tm, J_{F-C} = 15 Hz), 114.0, 67.3, 55.2. ^{19}F NMR (470 MHz, CDCl₃): δ (ppm) = -143.2 – -143.3 (m, 2F), -155.2 (t, J_F = 21 Hz, 1F), -161.7 – -161.8 (m, 2F). HRMS (ASAP): Calcd. for C₁₄H₉F₅O₂ 304.0523, Found: 304.0512.

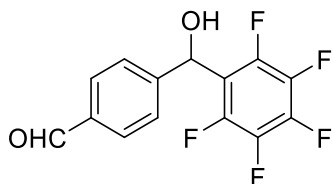


(3j):^[2] 86 mg, 71% yield, colorless oil. ^1H NMR (500 MHz, CDCl₃): δ (ppm) = 7.28-7.25 (m, 1H), 6.97 (s, 1H), 6.92-6.91 (m, 1H), 6.85-6.83 (m, 1H), 6.17 (s, 1H), 3.80 (s, 3H), 3.01 (s, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl₃): δ (ppm) = 159.9, 144.6 (dm, $^1J_{F-C}$ = 250 Hz), 142.3, 140.8 (dm, $^1J_{F-C}$ = 250 Hz), 137.6 (dm, $^1J_{F-C}$ = 250 Hz), 129.8, 117.6, 116.9 (tm, J_{F-C} = 15 Hz), 113.3, 111.3, 67.3, 55.3. ^{19}F NMR (470 MHz, CDCl₃): δ (ppm) = -143.0 – -143.1 (m, 2F), -154.7 (t, J_F = 21 Hz, 1F), -161.5 – -161.6 (m, 2F). HRMS (ASAP): Calcd. for C₁₄H₉F₅O₂ 304.0523, Found: 304.0509.

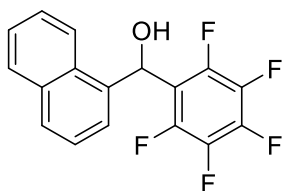


(3k): 108 mg, 85% yield, white solid. ^1H NMR (500 MHz, CDCl₃): δ (ppm) = 7.26-7.24 (m, 2H), 6.74-6.73 (m, 2H), 6.13 (s, 1H), 2.96 (s, 6H), 2.77 (s, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz,

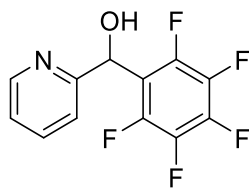
CDCl₃): δ (ppm) = 150.2, 144.5 (dm, $^1J_{F-C} = 250$ Hz), 140.5 (dm, $^1J_{F-C} = 250$ Hz), 137.6 (dm, $^1J_{F-C} = 250$ Hz), 128.7, 126.7, 117.4 (tm, $J_{F-C} = 15$ Hz), 112.7, 67.9, 40.7. ^{19}F NMR (470 MHz, CDCl₃): δ (ppm) = -142.9 – -143.0 (m, 2F), -155.6 (s, 1F), -161.5 – -161.6 (m, 2F). HRMS (ASAP): Calcd. for C₁₅H₁₂F₅NO [M+H]⁺ 318.0912, Found: 318.0903.



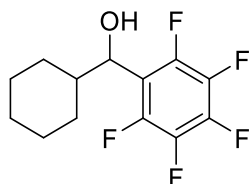
(3l): 97 mg, 80% yield, white solid. ^1H NMR (500 MHz, CDCl₃): δ (ppm) = 10.00 (s, 1H), 7.90-7.88 (m, 2H), 7.59-7.58 (m, 2H), 6.33 (s, 1H), 2.91 (s, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl₃): δ (ppm) = 191.9, 147.2, 144.7 (dm, $^1J_{F-C} = 250$ Hz), 141.2 (dm, $^1J_{F-C} = 250$ Hz), 137.7 (dm, $^1J_{F-C} = 250$ Hz), 136.0, 130.1, 126.0, 116.4 (tm, $J_{F-C} = 15$ Hz), 66.7. ^{19}F NMR (470 MHz, CDCl₃): δ (ppm) = -142.6 – -142.7 (m, 2F), -153.3 (m, 1F), -160.7 – -160.8 (m, 2F). HRMS (ASAP): Calcd. for C₁₄H₇F₅O₂ [M+H]⁺ 303.0439, Found: 303.0430.



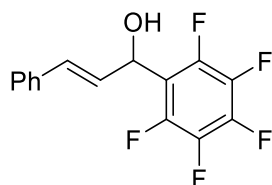
(3m):^[2] 91 mg, 70% yield, white solid. ^1H NMR (500 MHz, CDCl₃): δ (ppm) = 8.04 (d, $J = 9$ Hz, 1H), 7.91-7.85 (m, 1H), 7.85 (d, $J = 10$ Hz, 1H), 7.61 (d, $J = 8$ Hz, 1H), 7.58-7.51 (m, 2H), 7.49-7.46 (m, 1H), 6.85 (s, 1H), 2.94 (s, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl₃): δ (ppm) = 145.0 (dm, $^1J_{F-C} = 250$ Hz), 141.9 (dm, $^1J_{F-C} = 250$ Hz), 137.7 (dm, $^1J_{F-C} = 250$ Hz), 134.9, 133.9, 130.3, 129.4, 129.0, 126.8, 125.9, 125.1, 123.9 (t, $J_{F-C} = 2$ Hz), 122.7, 116.1 (tm, $J_{F-C} = 15$ Hz), 65.2. ^{19}F NMR (470 MHz, CDCl₃): δ (ppm) = -142.0 – -142.1 (m, 2F), -154.2 (t, $J_F = 21$ Hz, 1F), -161.3 – -161.4 (m, 2F). HRMS (ASAP): Calcd. for C₁₇H₉F₅O 324.0574, Found: 324.0561.



(3n): 90 mg, 82% yield, white solid. ^1H NMR (500 MHz, CDCl_3): δ (ppm) = 8.59 (d, J = 4 Hz, 1H), 7.72-7.69 (m, 1H), 7.30-7.28 (m, 1H), 7.16 (d, J = 8 Hz, 1H), 6.17 (s, 1H), 5.52 (s, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3): δ (ppm) = 157.3, 147.9, 145.3 (dm, $^1J_{\text{F-C}} = 250$ Hz), 141.1 (dm, $^1J_{\text{F-C}} = 250$ Hz), 137.6 (dm, $^1J_{\text{F-C}} = 250$ Hz), 137.3, 123.2, 120.4, 116.7 (tm, $J_{\text{F-C}} = 18$ Hz), 65.5. ^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -143.3 – -143.4 (m, 2F), -154.3 – -154.4 (m, 1F), -161.7 – -161.9 (m, 2F). HRMS (ASAP): Calcd. For $\text{C}_{12}\text{H}_6\text{F}_5\text{NO}$ $[\text{M}+\text{H}]^+$ 276.0442, Found: 276.0435.

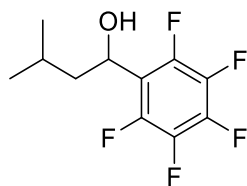


(3o): 90 mg, 80% yield, white solid. ^1H NMR (500 MHz, CDCl_3): δ (ppm) = 4.66 (d, J = 9 Hz, 1H), 2.45 (s, 1H), 2.16-2.13 (m, 1H), 1.83-1.78 (m, 2H), 1.68-1.66 (m, 2H), 1.29-1.13 (m, 4H), 1.05-1.03 (m, 1H), 0.96-0.88 (m, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3): δ (ppm) = 144.7 (dm, $^1J_{\text{F-C}} = 250$ Hz), 140.3 (dm, $^1J_{\text{F-C}} = 250$ Hz), 137.4 (dm, $^1J_{\text{F-C}} = 250$ Hz), 116.5 (tm, $J_{\text{F-C}} = 16$ Hz), 71.4, 43.3, 29.7, 28.9, 26.1, 25.6, 25.5. ^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -142.9 – -143.0 (m, 2F), -155.7 (t, $J_{\text{F}} = 19$ Hz, 1F), -162.2 – -162.3 (m, 2F). HRMS (ASAP): Calcd. for $\text{C}_{13}\text{H}_{13}\text{F}_5\text{O}$ $[\text{M}-\text{H}]^+$ 279.0803, Found: 279.0800.

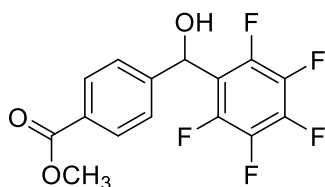


(3p):^[2] 101 mg, 84% yield, white solid. ^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.40-7.38 (m, 2H), 7.36-7.33 (m, 2H), 7.30-7.27 (m, 1H), 6.71-6.68 (m, 1H), 6.55-6.50 (m, 1H), 5.75 (d, J = 6 Hz, 1H), 2.57 (s, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3): δ (ppm) = 144.8 (dm, $^1J_{\text{F-C}} = 250$ Hz), 140.8 (dm, $^1J_{\text{F-C}} = 250$ Hz), 137.7 (dm, $^1J_{\text{F-C}} = 250$ Hz), 135.7, 132.8, 128.6, 128.4, 127.5, 126.7, 116.1 (tm, $J_{\text{F-C}} = 15$ Hz), 66.9. ^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -143.4

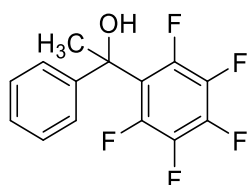
- -143.5 (m, 2F), -154.9 (t, $J_F = 20$ Hz, 1F), -161.7 – -161.8 (m, 2F). HRMS (ASAP): Calcd. for $C_{15}H_9F_5O$ 300.0574, Found: 300.0564.



(3q): 77 mg, 76% yield, white solid. 1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 5.13-5.10 (m, 1H), 2.34 (s, 1H), 1.94-1.88 (m, 1H), 1.68-1.59 (m, 2H), 0.96-0.93 (m, 6H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ (ppm) = 144.7 (dm, $^1J_{F-C} = 250$ Hz), 140.4 (dm, $^1J_{F-C} = 250$ Hz), 137.5 (dm, $^1J_{F-C} = 250$ Hz), 117.4 (tm, $J_{F-C} = 15$ Hz), 64.7 (m), 45.8, 25.1, 22.5, 22.1. ^{19}F NMR (470 MHz, $CDCl_3$): δ (ppm) = -144.2 – -144.3 (m, 2F), -155.6 – -155.7 (m, 1F), -161.9 – -162.1 (m, 2F). HRMS (ASAP): Calcd. for $C_{11}H_{11}F_5O$ $[M-H]^+$ 253.0646, Found: 253.0643.



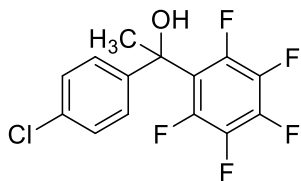
(3r): 114 mg, 86% yield, colorless oil. 1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.95-7.93 (m, 2H), 7.45-7.43 (m, 2H), 6.26 (s, 1H), 3.87 (s, 3H), 3.80 (s, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ (ppm) = 167.1, 145.9, 144.7 (dm, $^1J_{F-C} = 250$ Hz), 141.0 (dm, $^1J_{F-C} = 250$ Hz), 137.6 (dm, $^1J_{F-C} = 250$ Hz), 129.8, 129.4, 125.4, 116.7 (tm, $J_{F-C} = 17$ Hz), 66.5, 52.3. ^{19}F NMR (470 MHz, $CDCl_3$): δ (ppm) = -142.7 – -142.8 (m, 2F), -154.3 (t, $J_F = 21$ Hz, 1F), -161.4 – -161.5 (m, 2F). HRMS (ASAP): Calcd. for $C_{15}H_9F_5O_3$ $[M+H]^+$ 333.0545, Found: 333.0535.



(3s): 81 mg, 70% yield, colorless oil. 1H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.36-7.27 (m, 5H), 2.82 (s, 1H), 2.01 (t, $J = 4$ Hz, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ (ppm) = 146.8, 145.2 (dm, $^1J_{F-C} = 250$ Hz), 140.5 (dm, $^1J_{F-C} = 250$ Hz), 137.9 (dm, $^1J_{F-C} = 250$ Hz), 128.6, 127.7, 124.1, 120.7 (tm, $J_{F-C} = 14$ Hz), 76.9, 31.7 (t, $J_{F-C} = 6$ Hz). ^{19}F NMR (470 MHz,

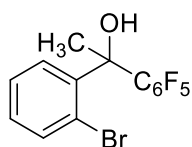
CDCl₃): δ (ppm) = -139.0 – -139.1 (m, 2F), -155.0 – -155.1 (m, 1F), -161.6 – -161.8 (m, 2F).

HRMS (ASAP): Calcd. for C₁₄H₉F₅O [M-OH]⁺ 271.0541, Found: 271.0534.

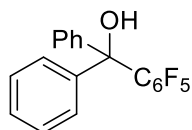


(**3t**): 92 mg, 71% yield, colorless oil. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 7.32-7.26 (m, 4H), 3.02 (s, 1H), 1.99 (t, *J* = 4 Hz, 3H). ¹³C{¹H} NMR (125 MHz, CDCl₃): δ (ppm) = 145.4, 145.2 (dm, ¹*J*_{F-C} = 250 Hz), 140.6 (dm, ¹*J*_{F-C} = 250 Hz), 138.9 (dm, ¹*J*_{F-C} = 250 Hz), 133.6, 128.7, 125.7, 120.1 (tm, *J*_{F-C} = 15 Hz), 76.5, 31.7 (t, *J*_{F-C} = 6 Hz). ¹⁹F NMR (470 MHz, CDCl₃): δ (ppm) = -138.9 – -139.1 (m, 2F), -154.4 – -154.5 (m, 1F), -161.2 – -161.4 (m, 2F).

HRMS (ASAP): Calcd. for C₁₄H₈F₅ClO 322.0184, Found: 322.0172.

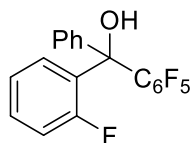


(**3u**): 89 mg, 61% yield, colorless oil. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 7.88-7.86 (m, 1H), 7.53-7.51 (m, 1H), 7.42-7.39 (m, 1H), 7.19-7.16 (m, 1H), 3.27 (s, 1H), 2.11 (t, *J* = 3 Hz, 3H). ¹³C{¹H} NMR (125 MHz, CDCl₃): δ (ppm) = 145.2 (dm, ¹*J*_{F-C} = 250 Hz), 144.4, 140.6 (dm, ¹*J*_{F-C} = 250 Hz), 137.7 (dm, ¹*J*_{F-C} = 250 Hz), 134.6, 129.5, 127.7, 126.7 (t, *J*_{F-C} = 2 Hz), 120.1, 119.7 (tm, *J*_{F-C} = 15 Hz), 76.2, 28.9 (t, *J*_{F-C} = 4 Hz). ¹⁹F NMR (470 MHz, CDCl₃): δ (ppm) = -139.1 – -139.2 (m, 2F), -155.4 – -155.5 (m, 1F), -162.3 – -162.5 (m, 2F). HRMS (ASAP): Calcd. for C₁₄H₈F₅BrO 365.9679, Found: 365.9668.

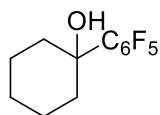


(**3v**): 84 mg, 60% yield, colorless oil. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 7.38-7.36 (m, 6H), 7.31-7.29 (m, 4H), 3.56 (s, 1H). ¹³C{¹H} NMR (125 MHz, CDCl₃): δ (ppm) = 145.1 (dm, ¹*J*_{F-C} = 250 Hz), 144.3, 140.7 (dm, ¹*J*_{F-C} = 250 Hz), 138.1 (dm, ¹*J*_{F-C} = 250 Hz), 128.4, 128.3, 126.9, 121.1 (tm, *J*_{F-C} = 12 Hz), 80.9. ¹⁹F NMR (470 MHz, CDCl₃): δ (ppm) = -136.4

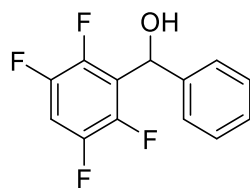
- -136.5 (m, 2F), -154.5 – -154.6 (m, 1F), -161.5 – -161.7 (m, 2F). HRMS (ASAP): Calcd. for C₁₉H₁₁F₅O 350.0730, Found: 350.0719.



(**3w**): 93 mg, 63% yield, colorless oil. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 7.41-7.33 (m, 6H), 7.11-7.05 (m, 2H), 6.94-6.90 (m, 1H), 3.69 (s, 1H). ¹³C{¹H} NMR (125 MHz, CDCl₃): δ (ppm) = 160.9 (d, ¹J_{F-C} = 250 Hz), 145.1 (dm, ¹J_{F-C} = 250 Hz), 142.5, 140.5 (dm, ¹J_{F-C} = 250 Hz), 137.7 (dm, ¹J_{F-C} = 250 Hz), 131.9 (d, J_{F-C} = 11 Hz), 130.4 (d, J_{F-C} = 9 Hz), 128.6, 128.5, 126.7, 124.0 (d, J_{F-C} = 3 Hz), 119.9 (tm, J_{F-C} = 15 Hz), 116.0 (d, J_{F-C} = 22 Hz), 78.5. ¹⁹F NMR (470 MHz, CDCl₃): δ (ppm) = -111.5 – -111.6 (m, 1F), -137.5 – -137.6 (m, 2F), -154.6 – -154.7 (m, 1F), -161.8 – -161.9 (m, 2F). HRMS (ASAP): Calcd. for C₁₉H₁₀F₆O 368.0636, Found: 368.0625.

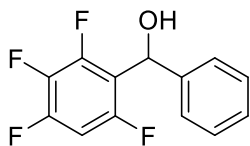


(**3x**): 76 mg, 71% yield, white solid. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 2.38 (s, 1H), 2.08-2.00 (m, 4H), 1.86-1.69 (m, 3H), 1.63-1.59 (m, 2H), 1.35-1.27 (m, 1H). ¹³C{¹H} NMR (125 MHz, CDCl₃): δ (ppm) = 145.2 (dm, ¹J_{F-C} = 250 Hz), 139.7 (dm, ¹J_{F-C} = 250 Hz), 137.8 (dm, ¹J_{F-C} = 250 Hz), 121.6 (tm, J_{F-C} = 12 Hz), 75.4, 37.3 (t, J_{F-C} = 4 Hz), 25.1, 21.4. ¹⁹F NMR (470 MHz, CDCl₃): δ (ppm) = -140.1 – -140.2 (m, 2F), -156.5 – -156.6 (m, 1F), -162.1 – -162.2 (m, 2F). HRMS (ASAP): Calcd. for C₁₂H₁₁F₅O 266.0730, Found: 266.0721.

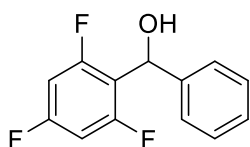


(**4a**): 84 mg, 82% yield, colorless oil. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 7.42-7.36 (m, 4H), 7.34-7.30 (m, 1H), 7.05-6.98 (m, 1H), 6.26 (s, 1H), 2.97 (s, 1H). ¹³C{¹H} NMR (125 MHz, CDCl₃): δ (ppm) = 146.1 (dm, ¹J_{F-C} = 250 Hz), 144.1 (dm, ¹J_{F-C} = 250 Hz), 140.7, 128.7, 128.2, 125.5, 122.7 (t, J_{F-C} = 15 Hz), 105.5 (t, J_{F-C} = 23 Hz), 67.9 (m). ¹⁹F NMR (470

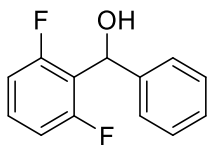
MHz, CDCl₃): δ (ppm) = -138.5 – -138.6 (m, 2F), -143.6 – -143.7 (m, 2F). HRMS (ASAP): calcd. for C₁₃H₈F₄O 256.0511, Found: 256.0500.



(4b): 86 mg, 84% yield, colorless oil. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 7.40-7.35 (m, 4H), 7.32-7.29 (m, 1H), 6.81-6.76 (m, 1H), 6.19 (s, 1H), 2.77 (s, 1H). ¹³C{¹H} NMR (125 MHz, CDCl₃): δ (ppm) = 154.8 (dm, ¹J_{F-C} = 250 Hz), 150.2 (dm, ¹J_{F-C} = 250 Hz), 149.6 (dm, ¹J_{F-C} = 250 Hz), 141.1 (m), 137.3 (dm, ¹J_{F-C} = 250 Hz), 128.6, 128.0, 125.4 (t, J_{F-C} = 1 Hz), 117.0 (tm, J_{F-C} = 19 Hz), 101.3 (m), 67.4 (m). ¹⁹F NMR (470 MHz, CDCl₃): δ (ppm) = -117.8 – -117.9 (m, 1F), -132.4 – -132.5 (m, 1F), -135.2 – -135.3 (m, 1F), -164.2 – -164.4 (m, 1F). HRMS (ASAP): calcd. for C₁₃H₈F₄O 256.0511, Found: 256.0499.

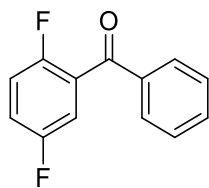


(4c): 76 mg, 80% yield, colorless oil. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 7.40-7.34 (m, 4H), 7.31-7.27 (m, 1H), 6.71-6.65 (m, 2H), 6.19 (s, 1H), 2.77 (s, 1H). ¹³C{¹H} NMR (125 MHz, CDCl₃): δ (ppm) = 162.2 (dt, ¹J_{F-C} = 250 Hz, J_{F-C} = 16 Hz), 161.1 (ddd, ¹J_{F-C} = 250 Hz, J_{F-C} = 15 Hz, 11 Hz), 141.8, 128.5, 127.7, 125.5 (t, J_{F-C} = 1 Hz), 115.9 (td, J_{F-C} = 17 Hz, 5 Hz), 100.8 (dd, J_{F-C} = 54 Hz, 2 Hz), 67.2 (t, J_{F-C} = 3 Hz). ¹⁹F NMR (470 MHz, CDCl₃): δ (ppm) = -108.1 – -108.2 (m, 1F), -111.1 – -111.2 (m, 2F). HRMS (ASAP): calcd. for C₁₃H₉F₃O 238.0600, Found: 238.0595.

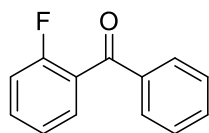


(4d): 70 mg, 80% yield, white solid. ¹H NMR (500 MHz, CDCl₃): δ (ppm) = 7.44-7.42 (m, 2H), 7.39-7.32 (m, 2H), 7.31-7.23 (m, 2H), 6.94-6.88 (m, 2H), 6.27 (s, 1H), 2.90 (s, 1H). ¹³C{¹H} NMR (125 MHz, CDCl₃): δ (ppm) = 160.8 (dd, ¹J_{F-C} = 250 Hz, J_{F-C} = 8 Hz), 142.1, 129.6 (t, J_{F-C} = 11 Hz), 128.4, 127.6, 125.6 (t, J_{F-C} = 1 Hz), 119.5 (t, J_{F-C} = 16 Hz), 112.0 (m),

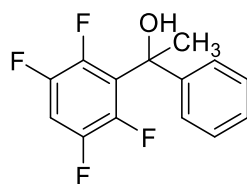
67.6 (t, $J_{F-C} = 3$ Hz). ^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -114.4 – -114.5 (m, 2F). HRMS (ASAP): calcd. for $\text{C}_{13}\text{H}_{10}\text{F}_2\text{O}$ 220.0694, Found: 220.0691.



(**4e**):^[3,4] 69 mg, 79% yield, colorless oil. ^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.85-7.83 (m, 2H), 7.64-7.61 (m, 1H), 7.51-7.47 (m, 2H), 7.28-7.20 (m, 2H), 7.17-7.12 (m, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3): δ (ppm) = 191.9 (m), 158.4 (dd, $^1J_{F-C} = 250$ Hz, $J_{F-C} = 2$ Hz), 155.9 (dd, $^1J_{F-C} = 250$ Hz, $J_{F-C} = 2$ Hz), 136.7, 133.8, 129.8 (d, $J_{F-C} = 1$ Hz), 128.6, 128.1 (dd, $J_{F-C} = 18$ Hz, 7 Hz), 119.5 (dd, $J_{F-C} = 24$ Hz, 9 Hz), 117.6 (dd, $J_{F-C} = 25$ Hz, 8 Hz), 116.9 (dd, $J_{F-C} = 25$ Hz, 4 Hz). ^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -117.0 – -117.1 (m, 1F), -117.6 – -117.7 (m, 1F). HRMS (ASAP): calcd. for $\text{C}_{13}\text{H}_8\text{F}_2\text{O}$ $[\text{M}+\text{H}]^+$ 219.0618, Found: 219.0614.



(**4f**):^[5,6] 60 mg, 75% yield, colorless oil. ^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.85-7.83 (m, 2H), 7.60-7.44 (m, 5H), 7.22-7.24 (m, 1H), 7.17-7.12 (m, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3): δ (ppm) = 193.5, 160.1 (d, $^1J_{F-C} = 250$ Hz), 137.4 (d, $J_{F-C} = 1$ Hz), 133.5, 133.1 (d, $J_{F-C} = 8$ Hz), 130.7 (d, $J_{F-C} = 3$ Hz), 129.8 (d, $J_{F-C} = 1$ Hz), 128.5, 127.0 (d, $J_{F-C} = 15$ Hz), 124.3 (d, $J_{F-C} = 4$ Hz), 116.3 (d, $J_{F-C} = 21$ Hz). ^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -111.0 – -111.1 (m, 1F). HRMS (ASAP): calcd. for $\text{C}_{13}\text{H}_9\text{FO}$ $[\text{M}+\text{H}]^+$ 201.0710, Found: 201.0706.

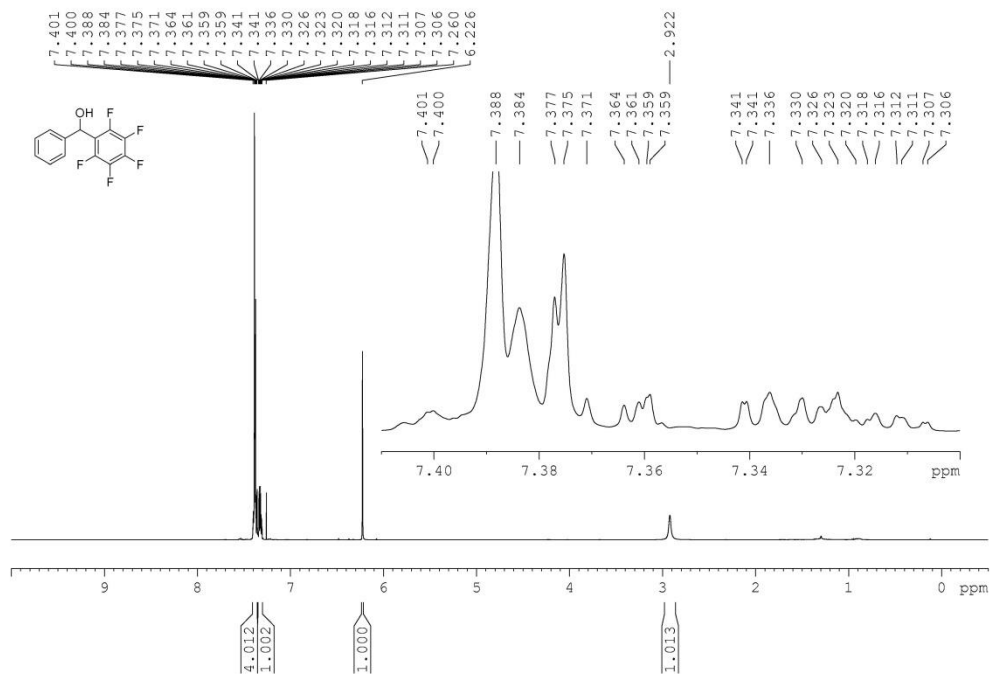


(**4g**): 73 mg, 68% yield, colorless oil. ^1H NMR (500 MHz, CDCl_3): δ (ppm) = 7.35-7.34 (m, 4H), 7.30-7.27 (m, 1H), 7.08-7.01 (m, 1H), 3.21 (s, 1H), 2.03 (t, $J = 4$ Hz, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3): δ (ppm) = 147.1, 146.4 (dm, $^1J_{F-C} = 250$ Hz), 144.8 (dm, $^1J_{F-C} = 250$ Hz), 128.5, 127.6, 126.1 (t, $J_{F-C} = 12$ Hz), 124.2, 105.2 (t, $J_{F-C} = 22$ Hz), 77.1, 31.5 (t,

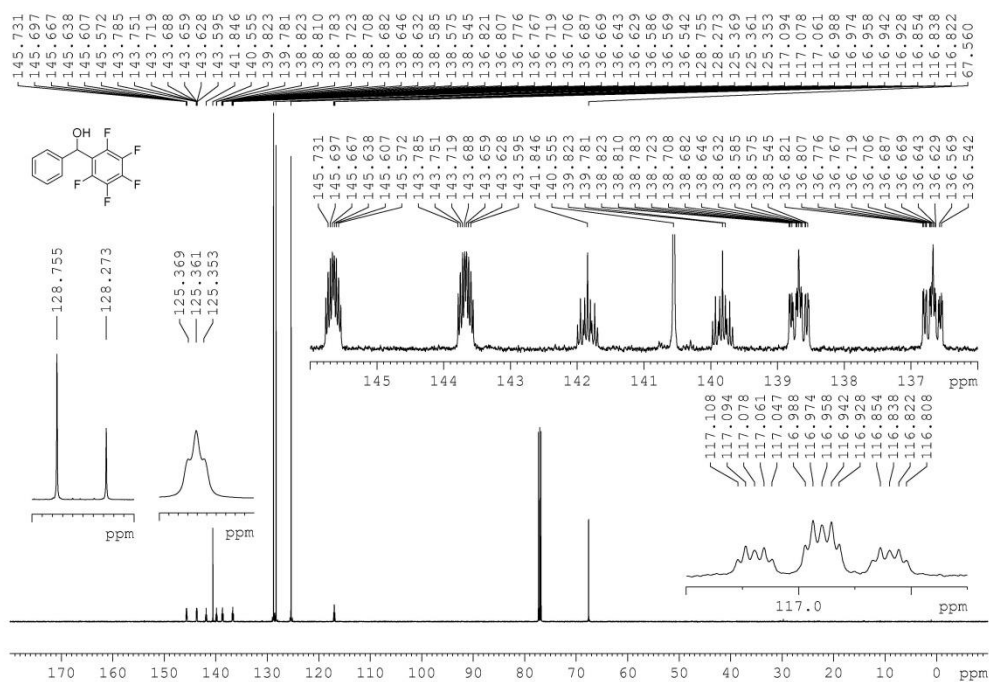
$J_{F-C} = 7$ Hz). ^{19}F NMR (470 MHz, CDCl_3): δ (ppm) = -138.5 – -138.6 (m, 2F), -139.6 – -139.7 (m, 2F). HRMS (ASAP): calcd. for $\text{C}_{14}\text{H}_{10}\text{F}_4\text{O}$ $[\text{M-OH}]^+$ 253.0635, Found: 253.0630.

V. ^1H NMR, ^{19}F NMR and ^{13}C NMR Spectra

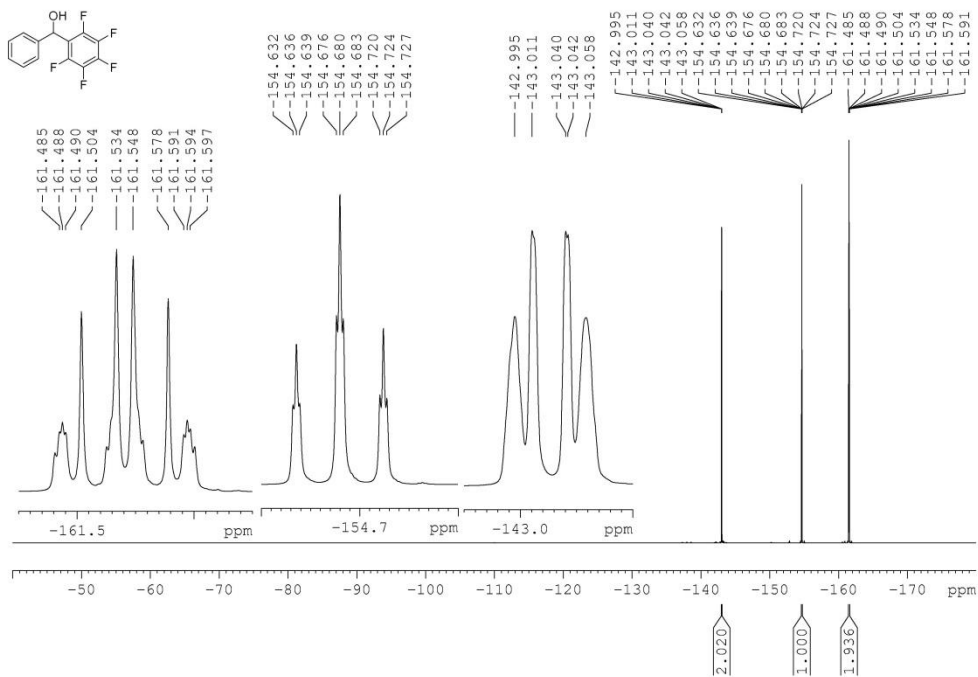
Compound 3a: ^1H NMR spectrum (500 MHz, CDCl_3).



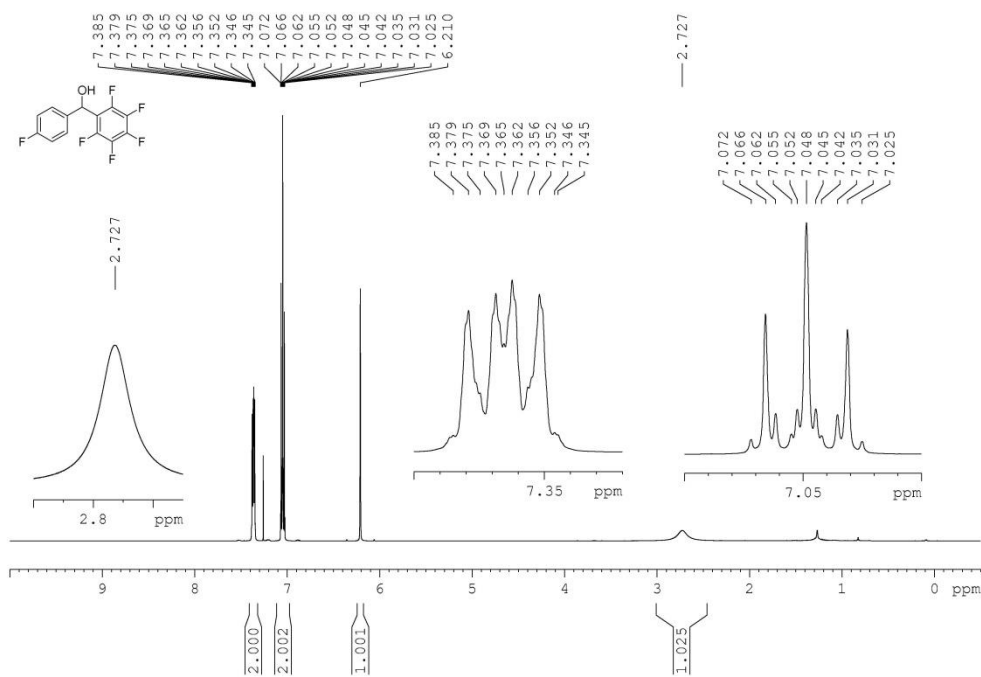
Compound 3a: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



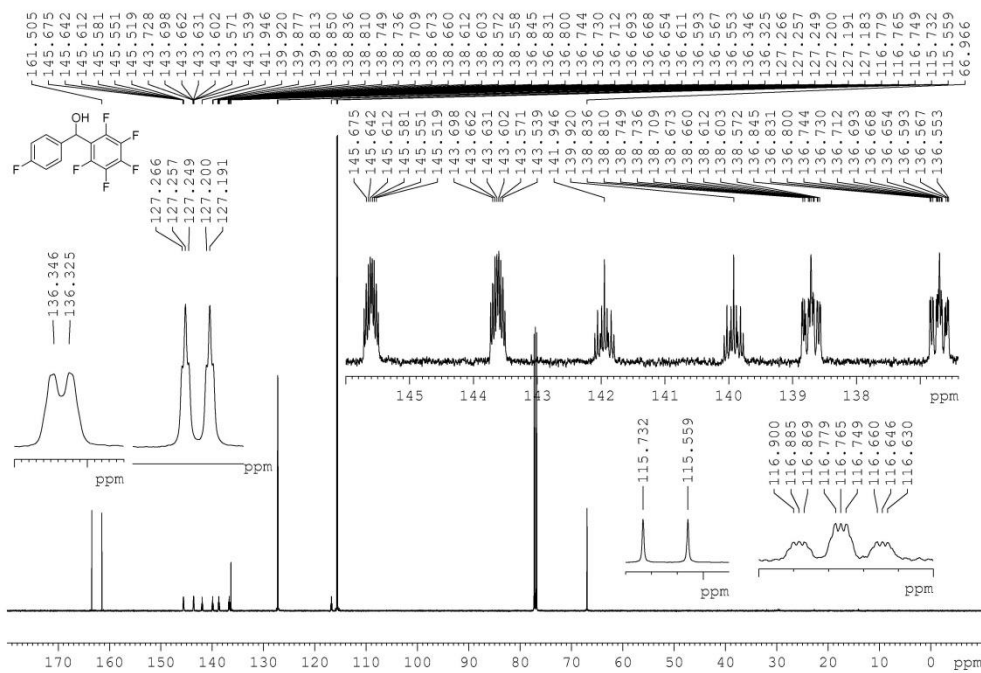
Compound 3a: ^{19}F NMR spectrum (470 MHz, CDCl_3).



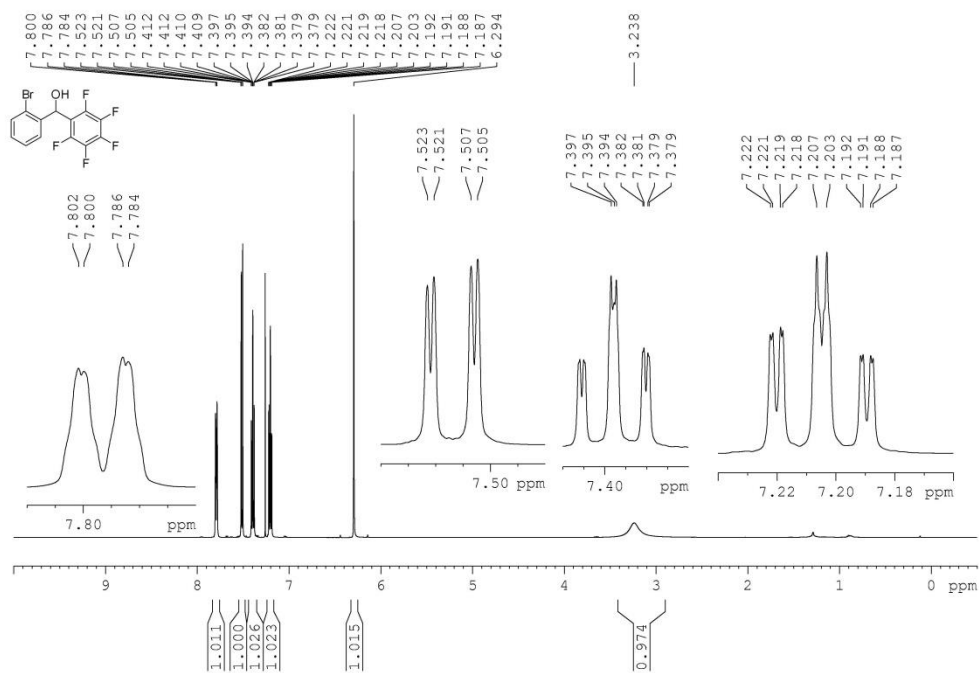
Compound 3b: ^1H NMR spectrum (500 MHz, CDCl_3).



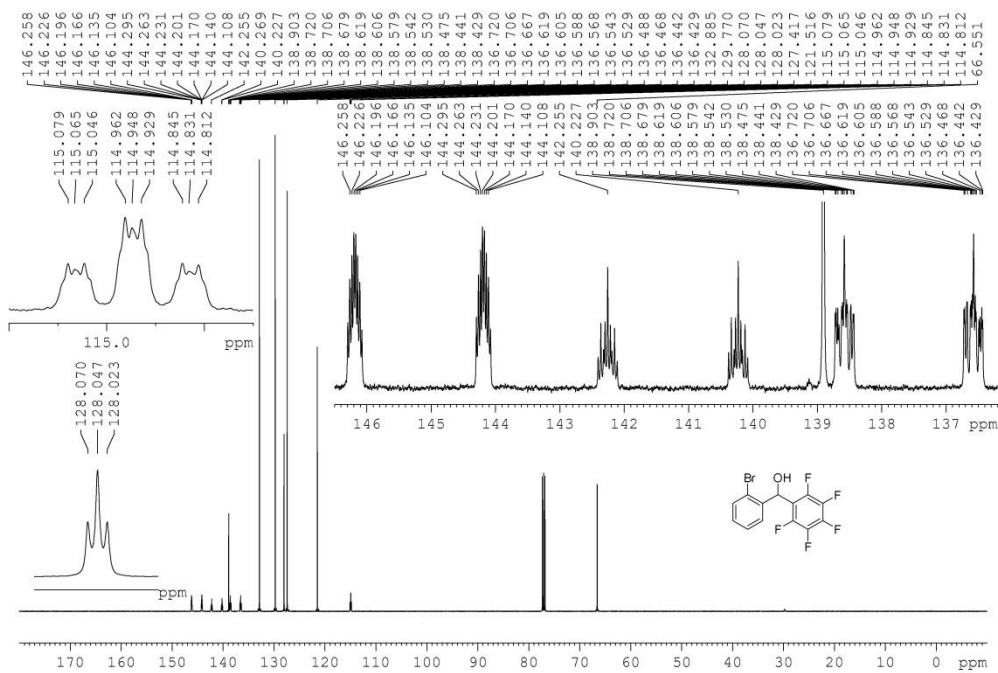
Compound 3b: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



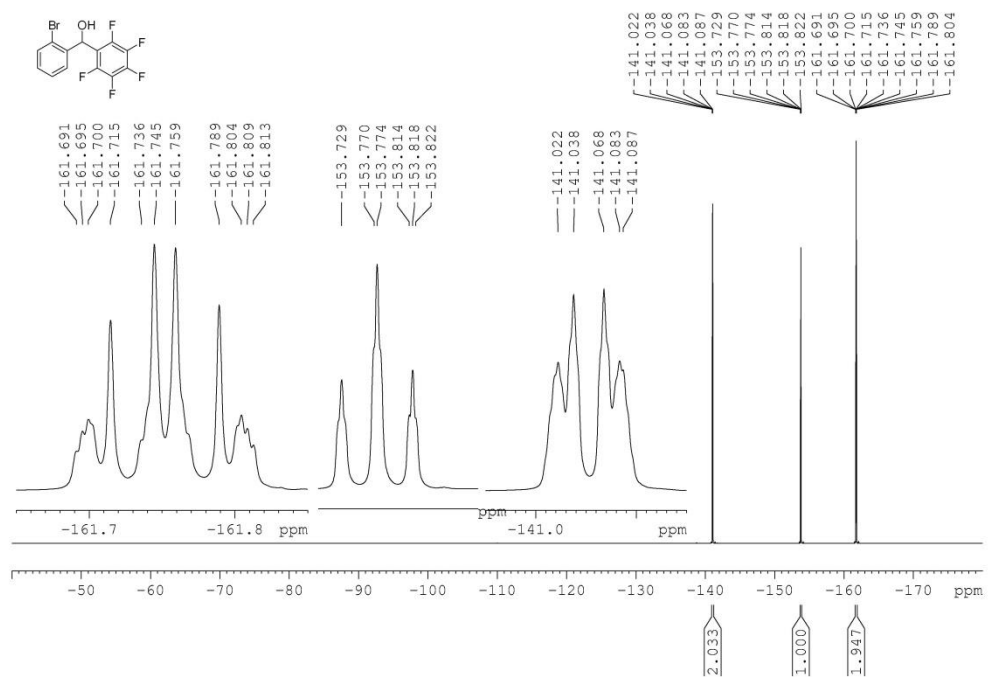
Compound 3f: ^1H NMR spectrum (500 MHz, CDCl_3).



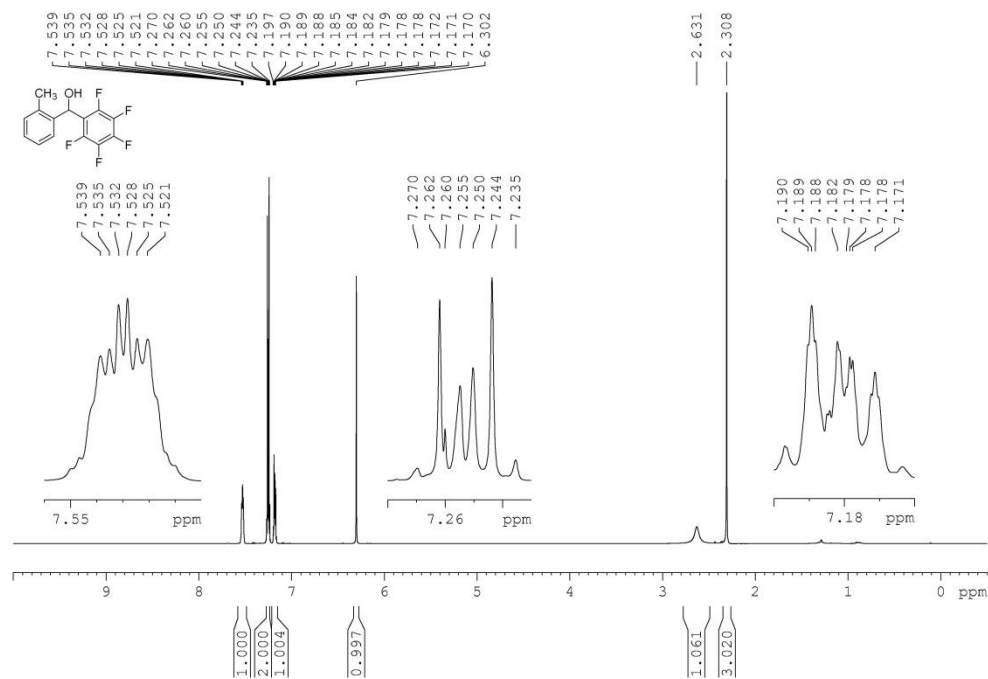
Compound 3f: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



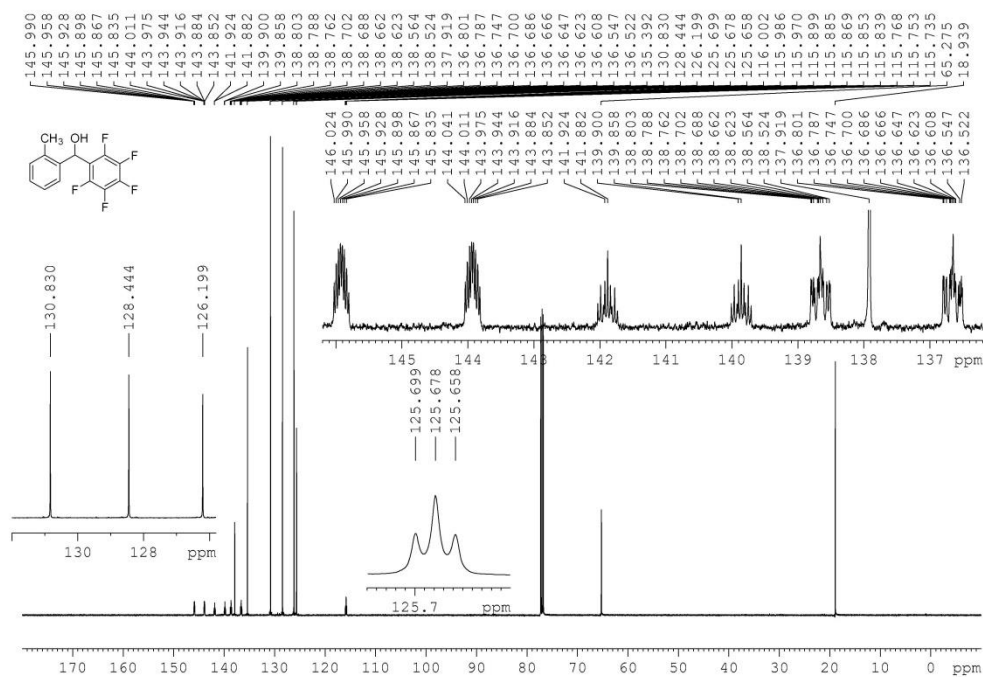
Compound 3f: ^{19}F NMR spectrum (470 MHz, CDCl_3).



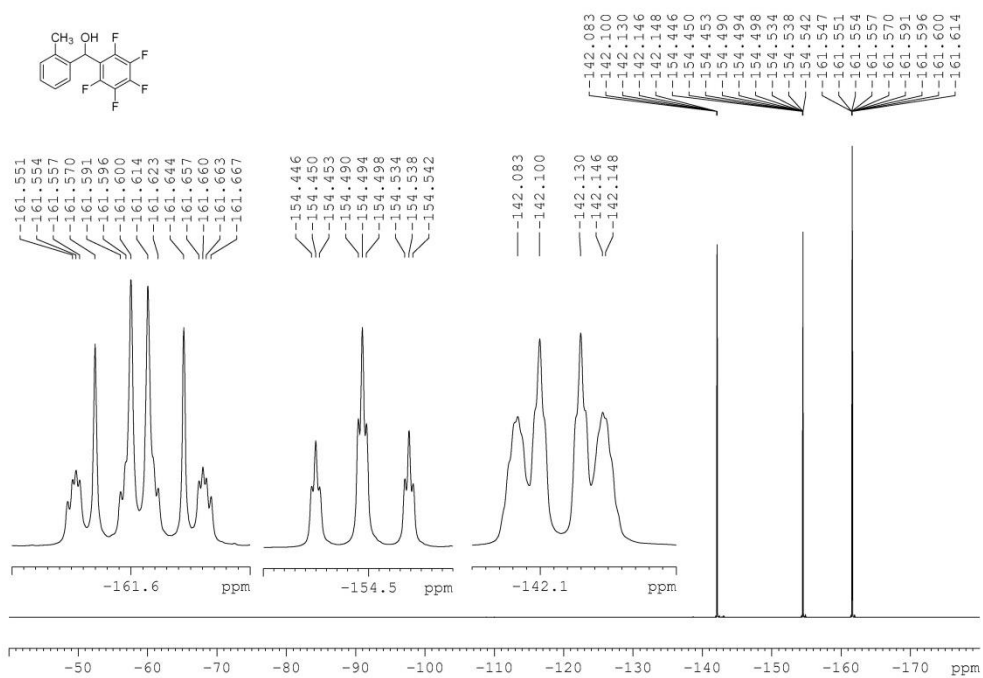
Compound 3g: ^1H NMR spectrum (500 MHz, CDCl_3).



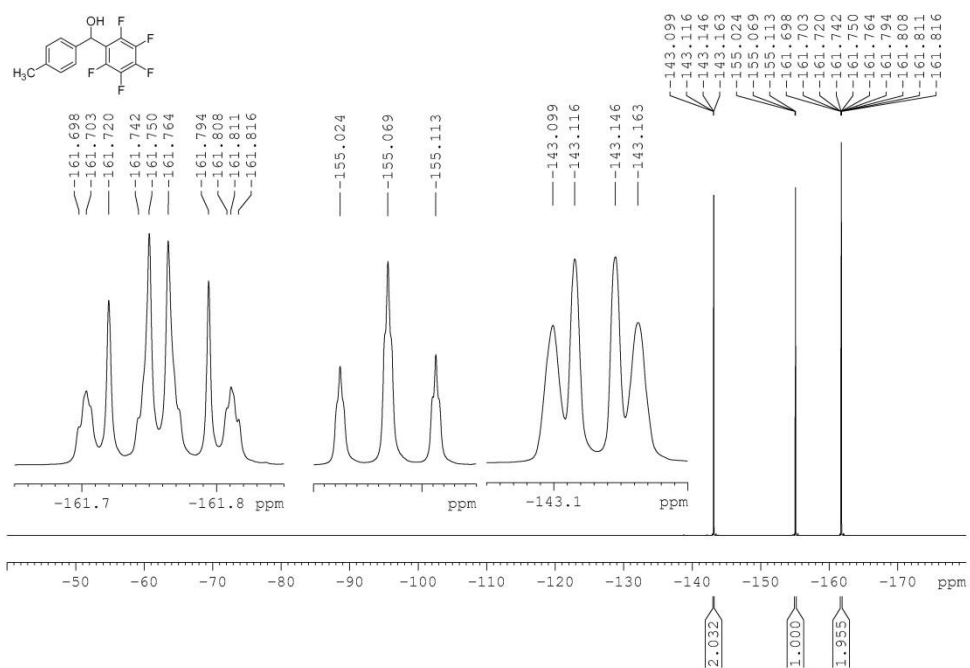
Compound 3g: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



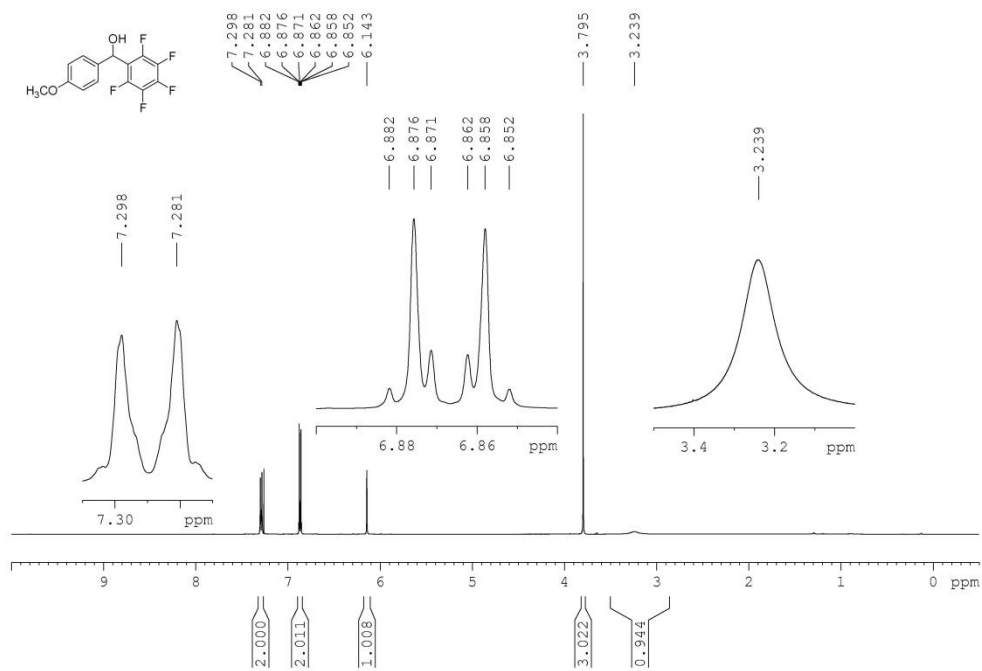
Compound 3g: ^{19}F NMR spectrum (470 MHz, CDCl_3).



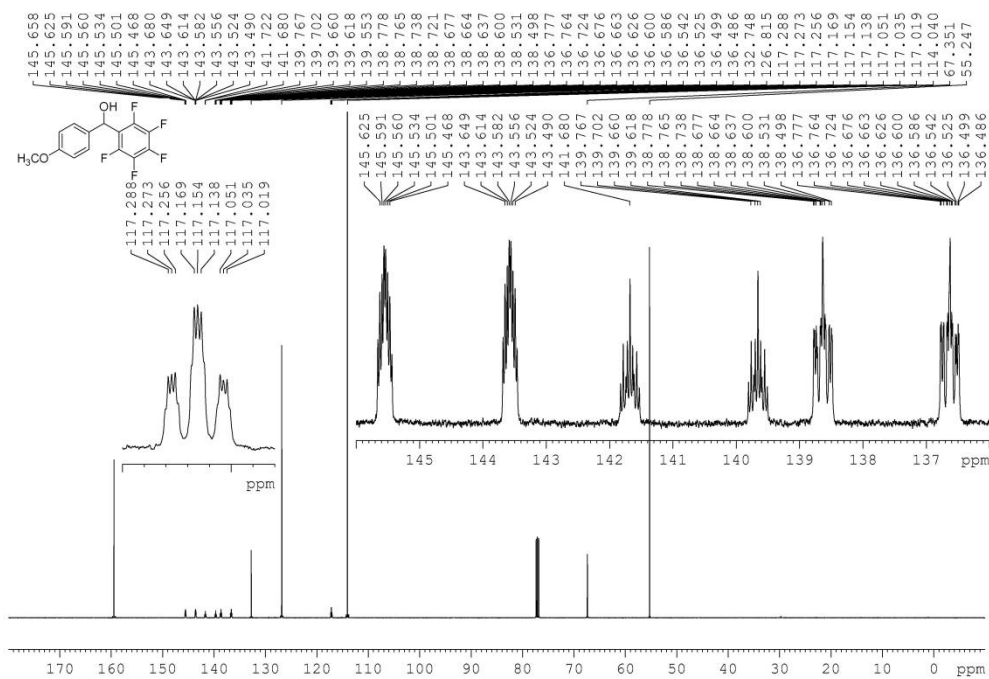
Compound 3h: ^{19}F NMR spectrum (470 MHz, CDCl_3).



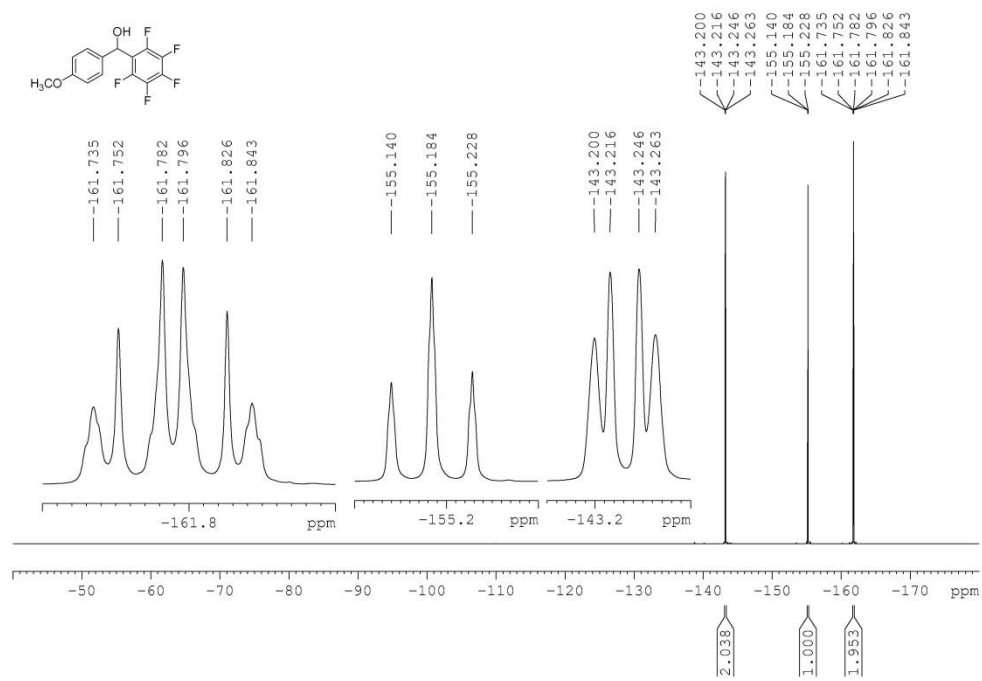
Compound 3i: ^1H NMR spectrum (500 MHz, CDCl_3).



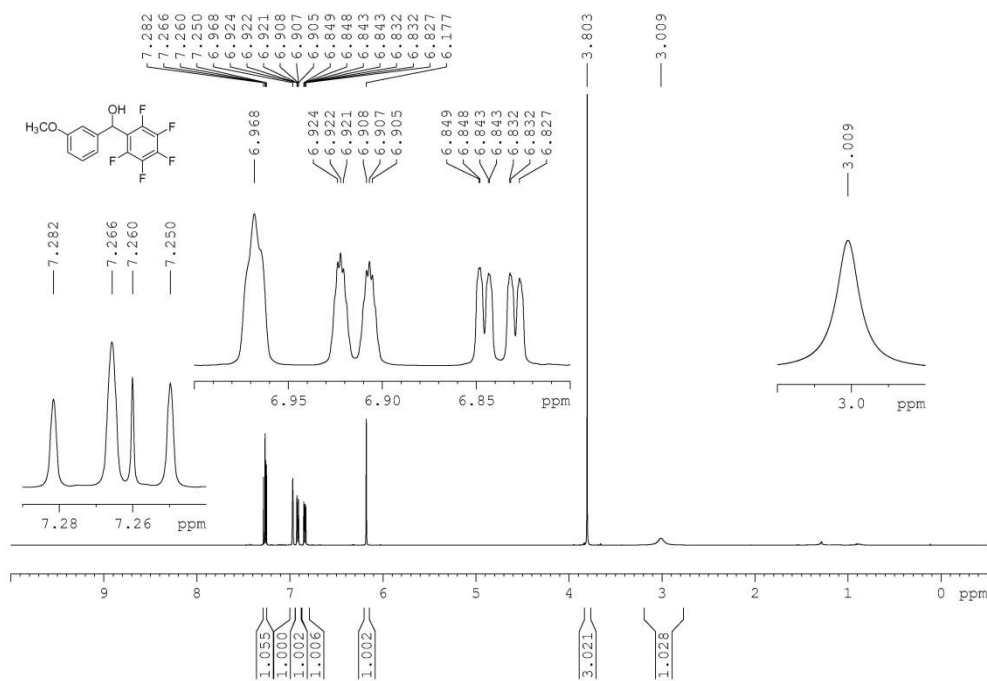
Compound 3i: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



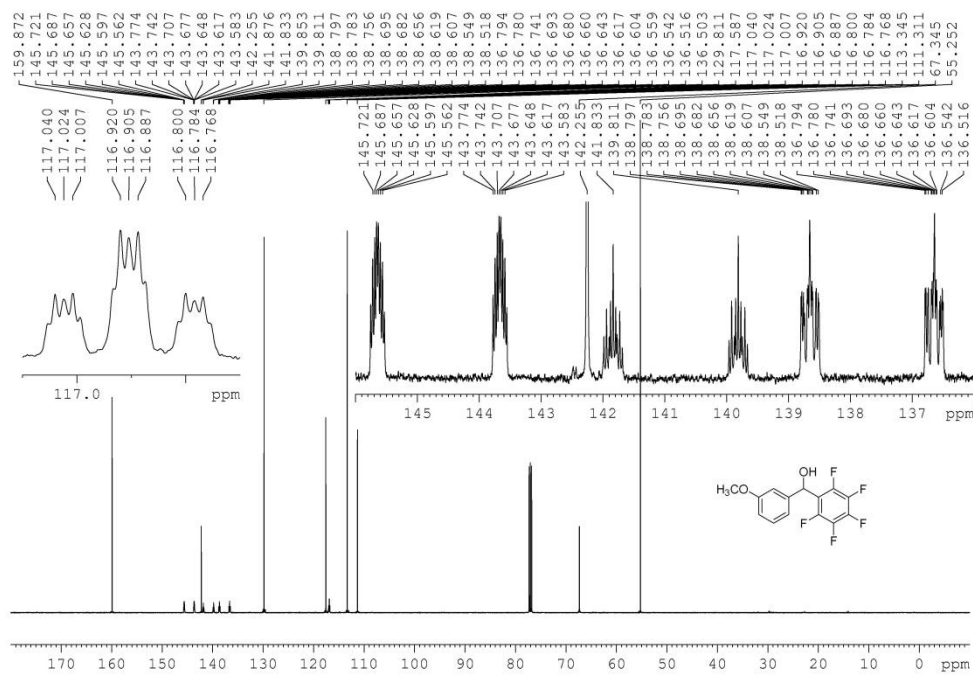
Compound 3i: ^{19}F NMR spectrum (470 MHz, CDCl_3).



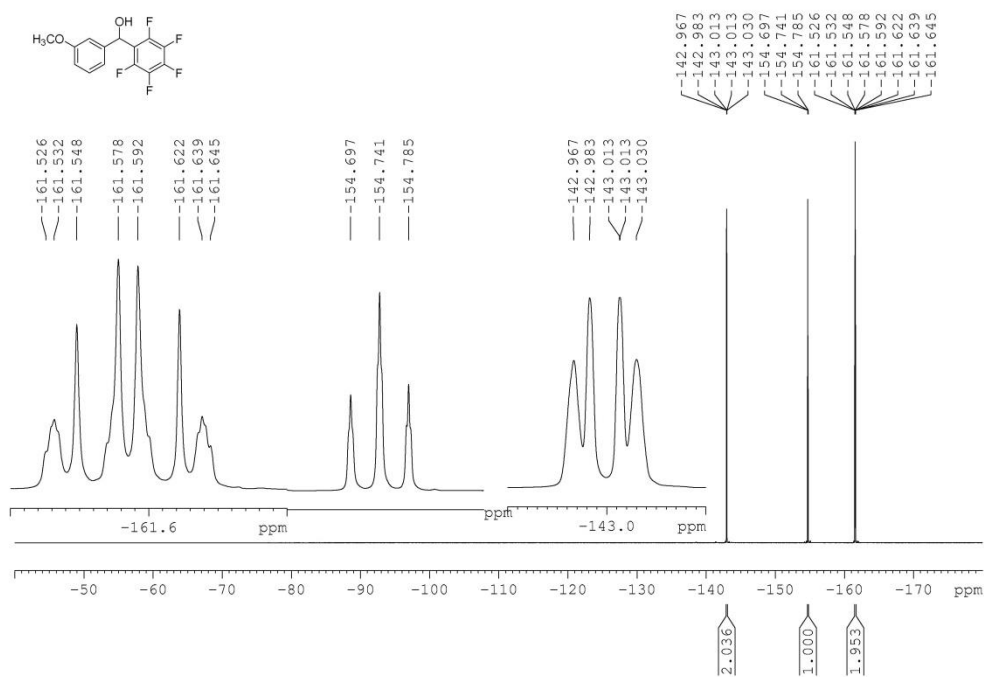
Compound 3j: ^1H NMR spectrum (500 MHz, CDCl_3).



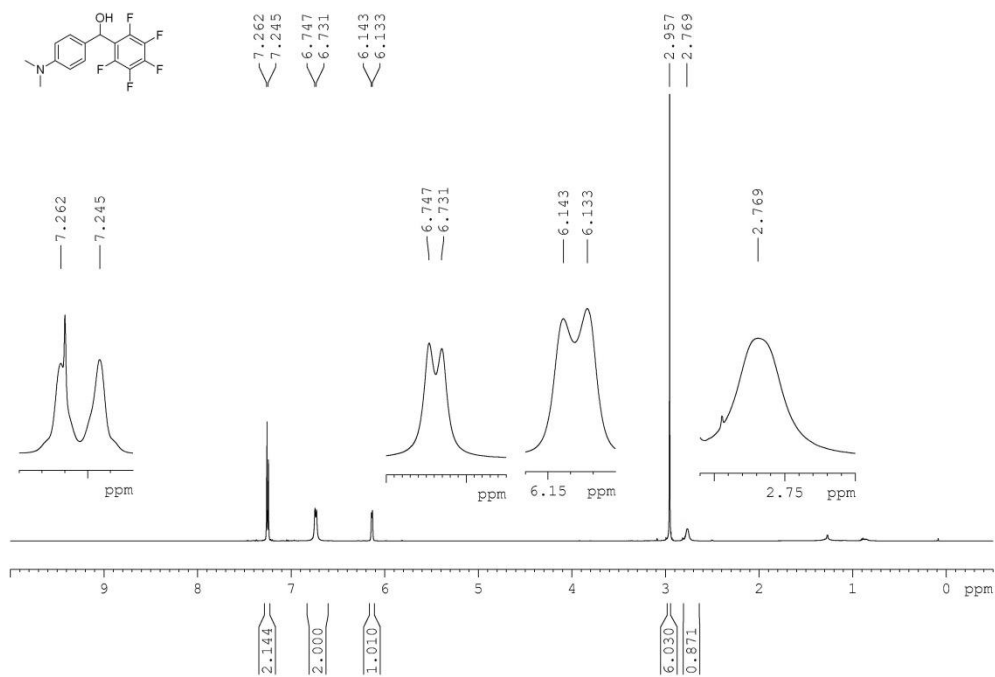
Compound 3j: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



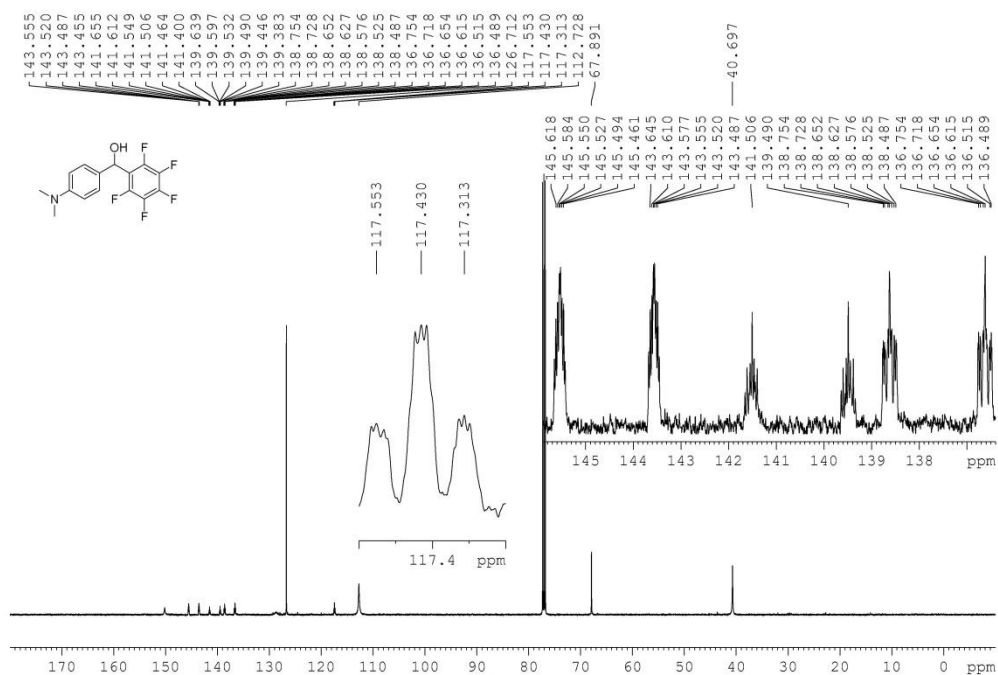
Compound 3j: ^{19}F NMR spectrum (470 MHz, CDCl_3).



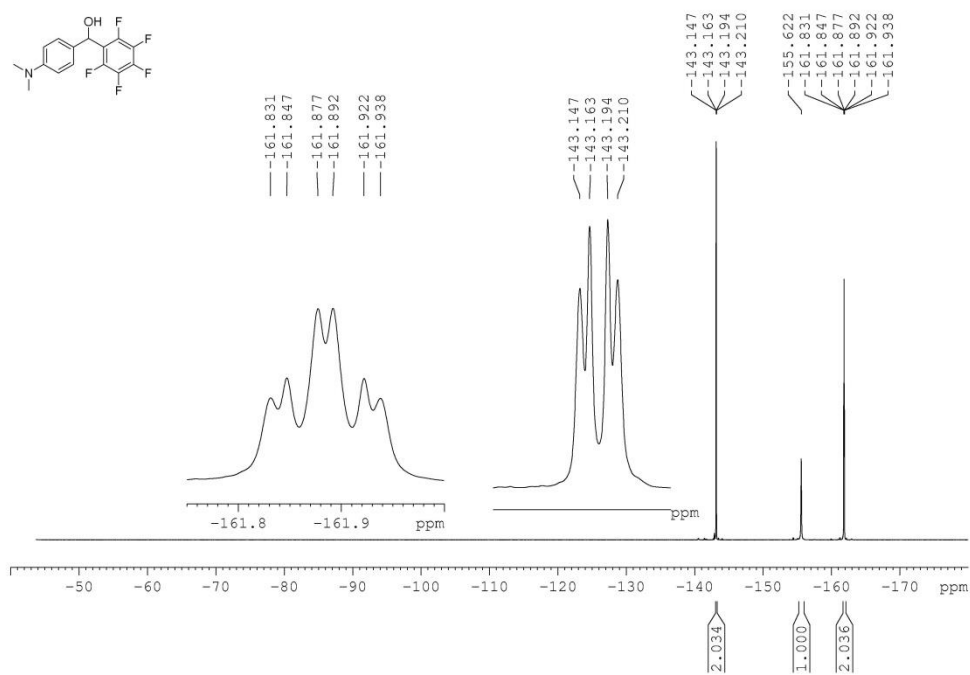
Compound 3k: ^1H NMR spectrum (500 MHz, CDCl_3).



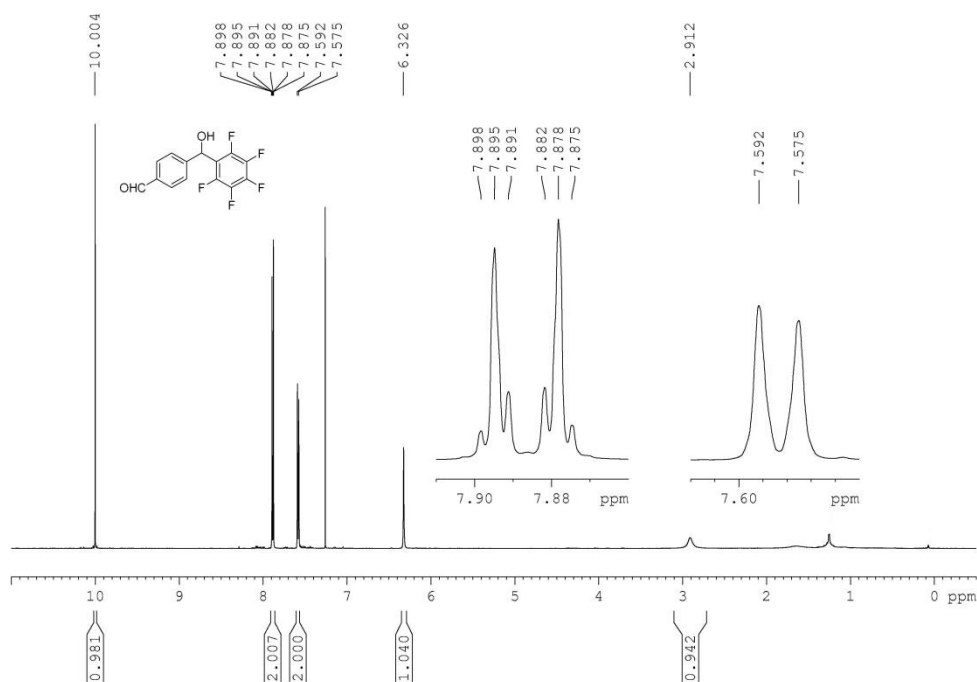
Compound 3k: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



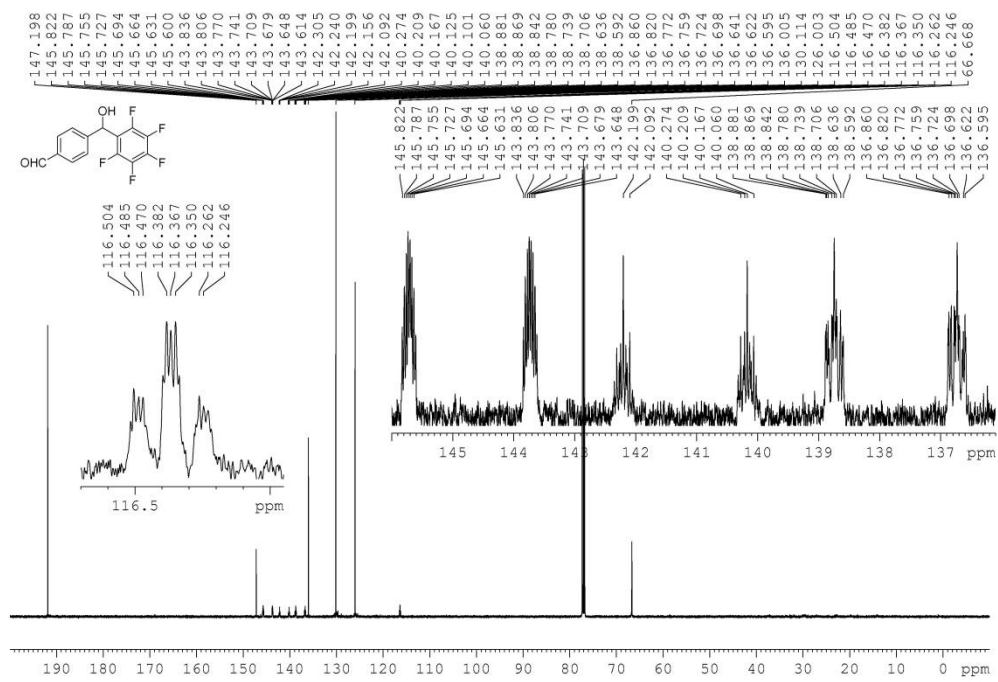
Compound 3k: ^{19}F NMR spectrum (470 MHz, CDCl_3).



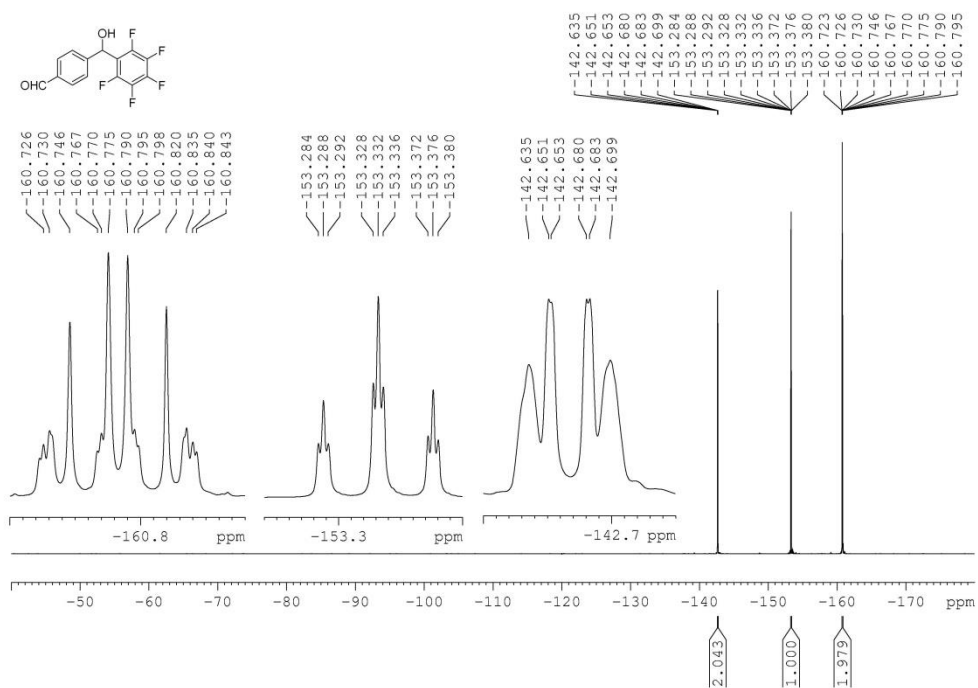
Compound 3l: ^1H NMR spectrum (500 MHz, CDCl_3).



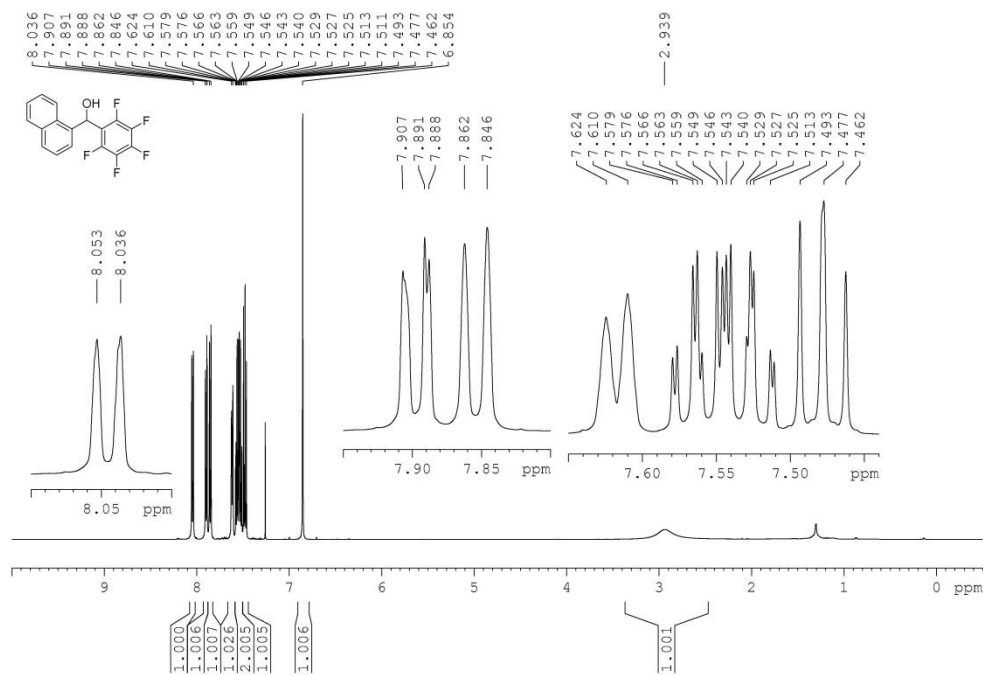
Compound 3l: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



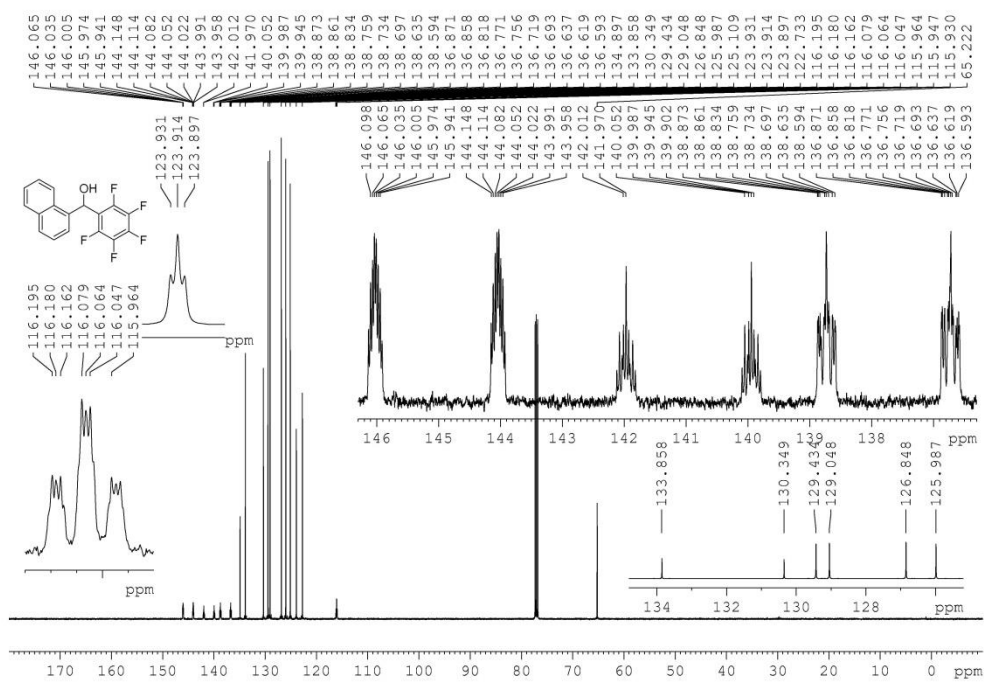
Compound 3l: ^{19}F NMR spectrum (470 MHz, CDCl_3).



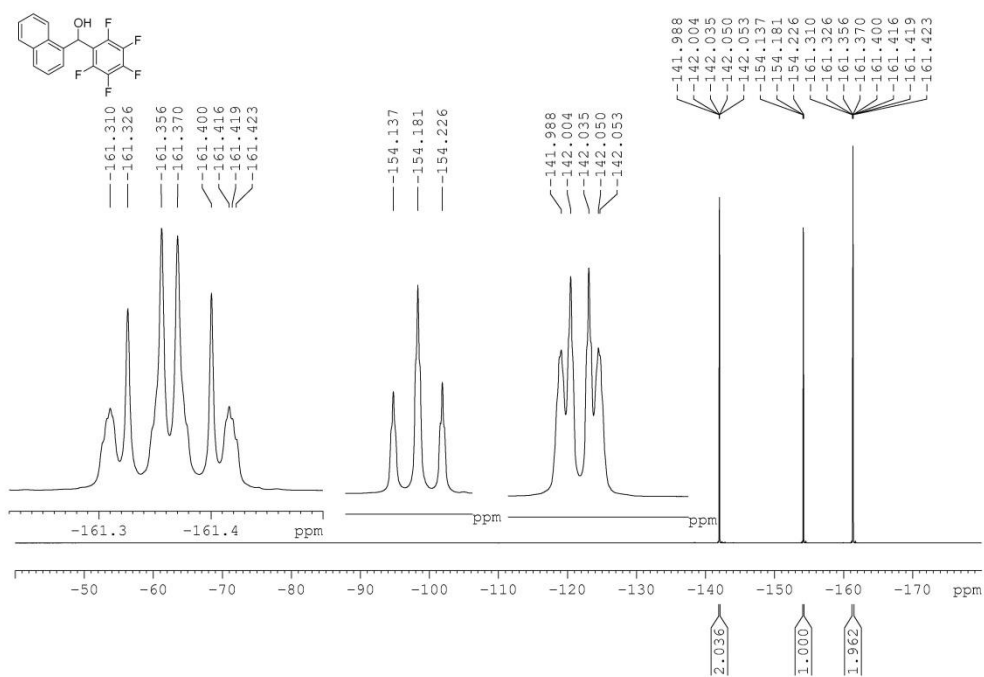
Compound 3m: ^1H NMR spectrum (500 MHz, CDCl_3).



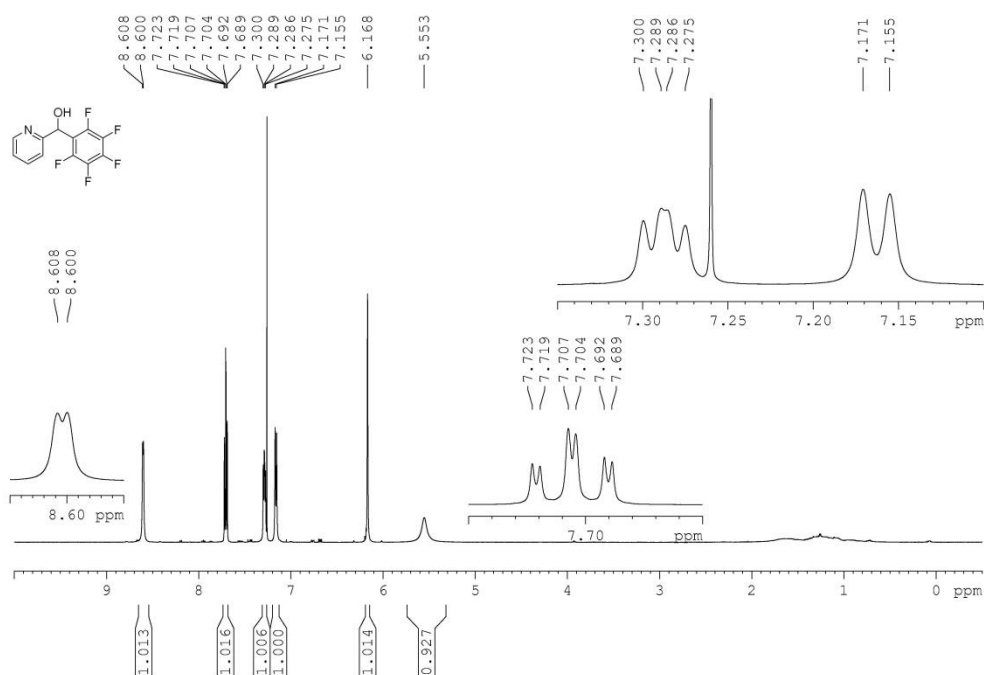
Compound 3m: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



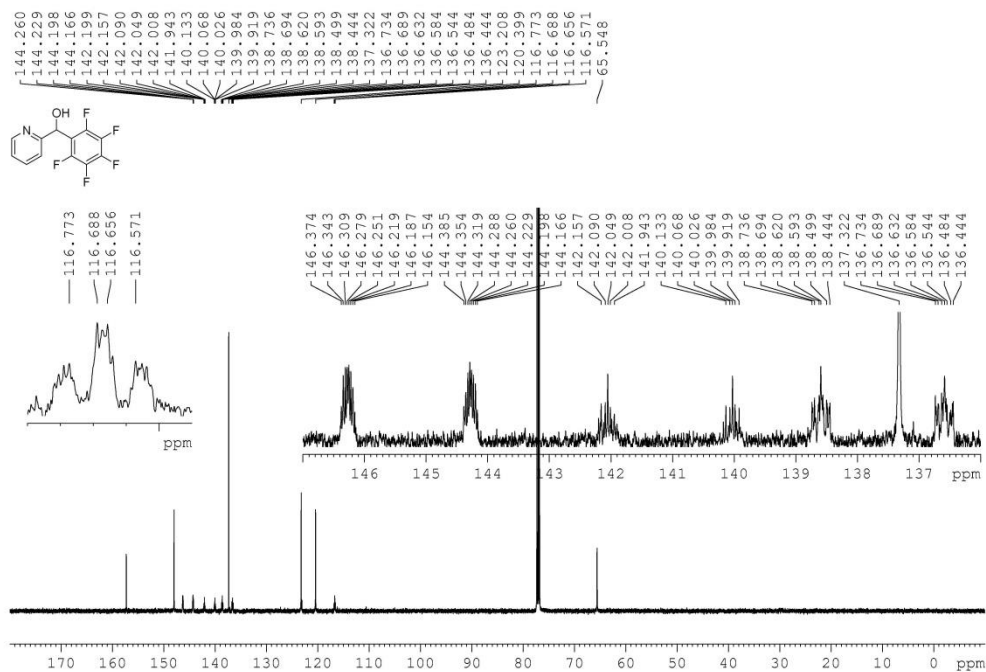
Compound 3m: ^{19}F NMR spectrum (470 MHz, CDCl_3).



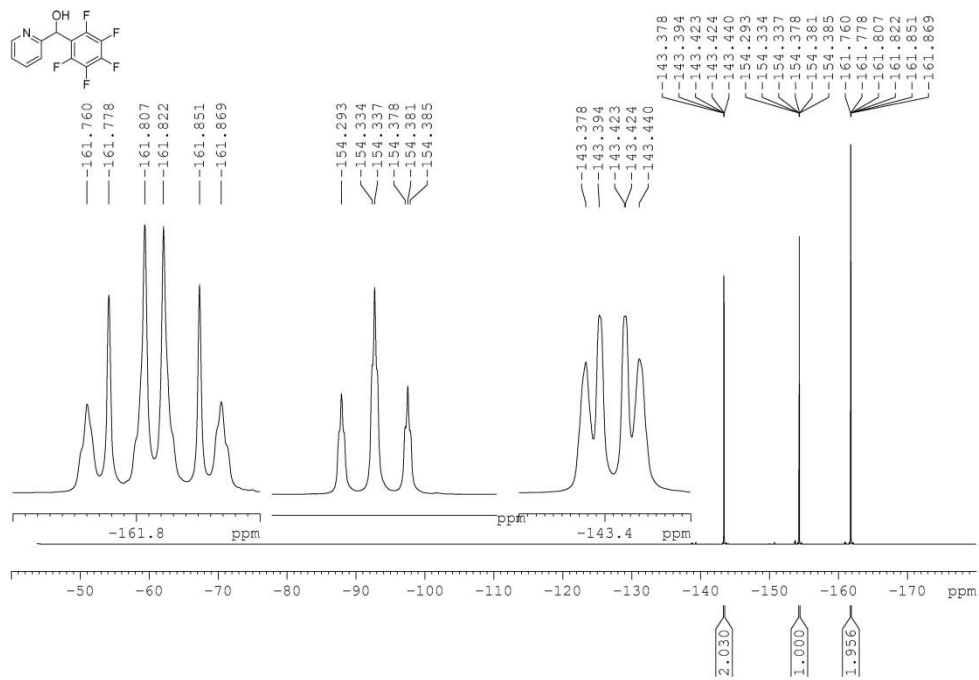
Compound 3n: ^1H NMR spectrum (500 MHz, CDCl_3).



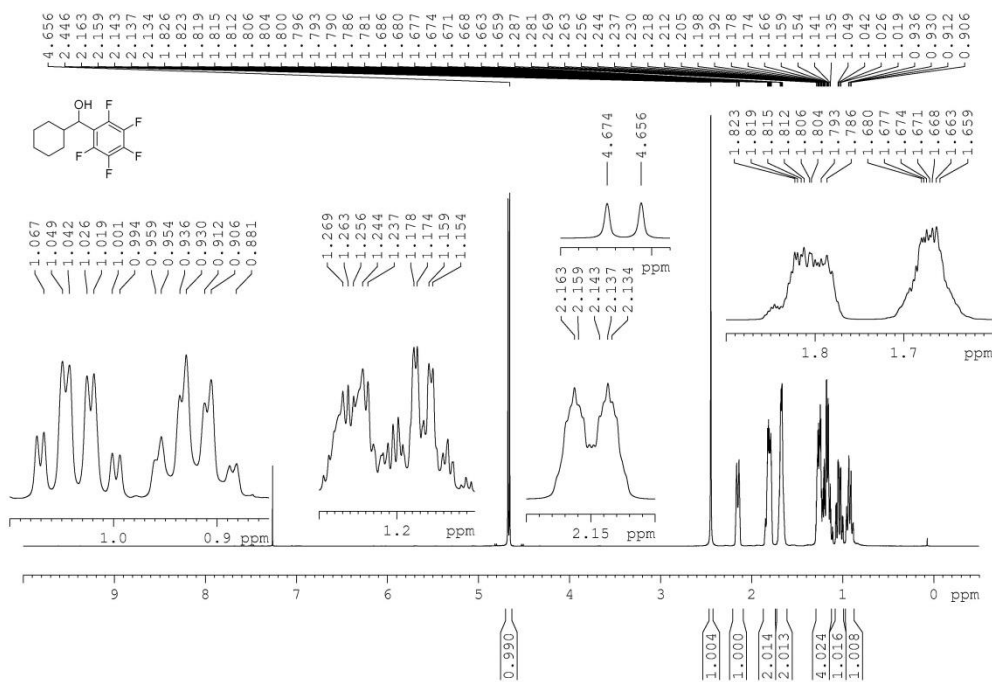
Compound 3n: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



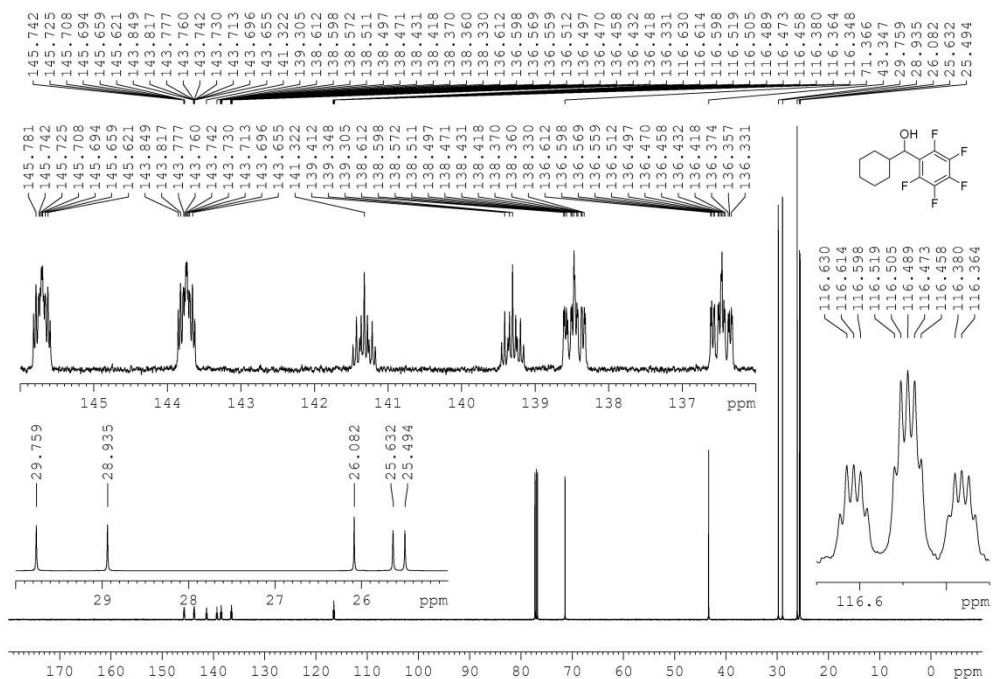
Compound 3n: ^{19}F NMR spectrum (470 MHz, CDCl_3).



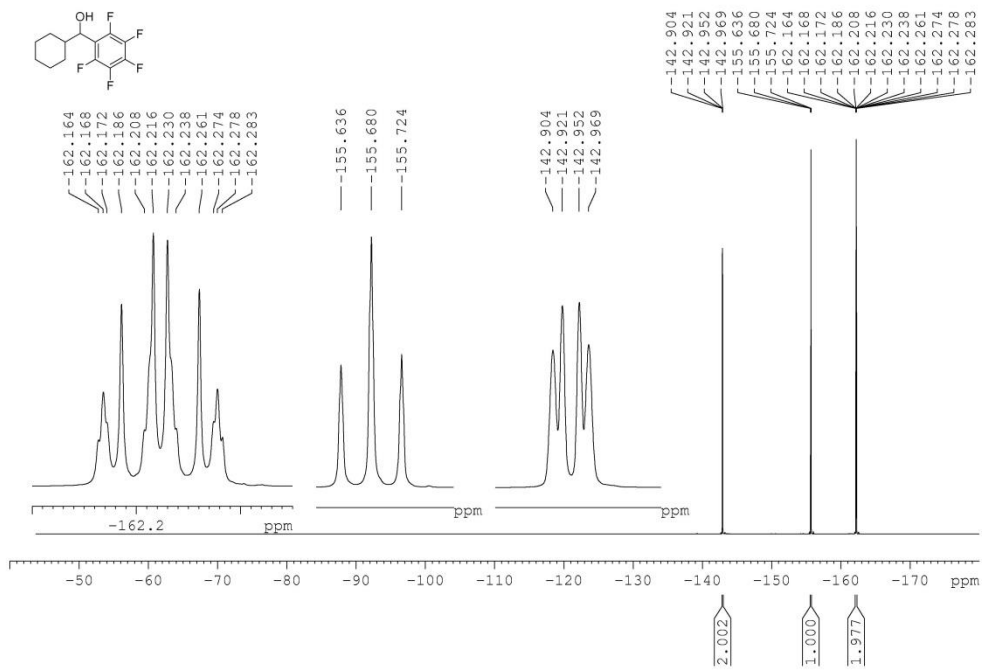
Compound 3o: ^1H NMR spectrum (500 MHz, CDCl_3).



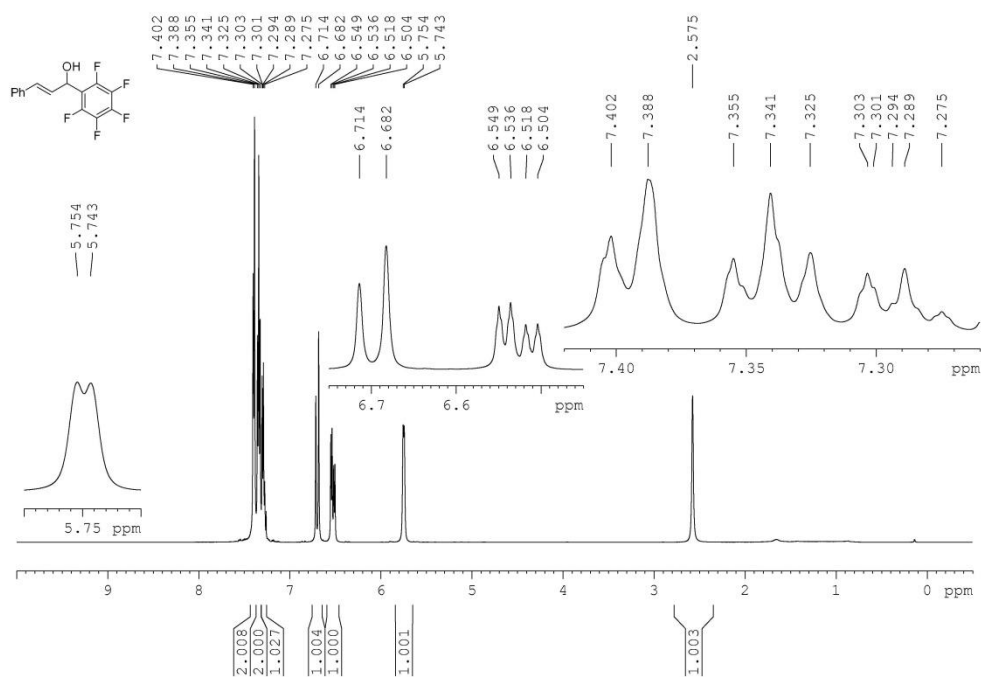
Compound 3o: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



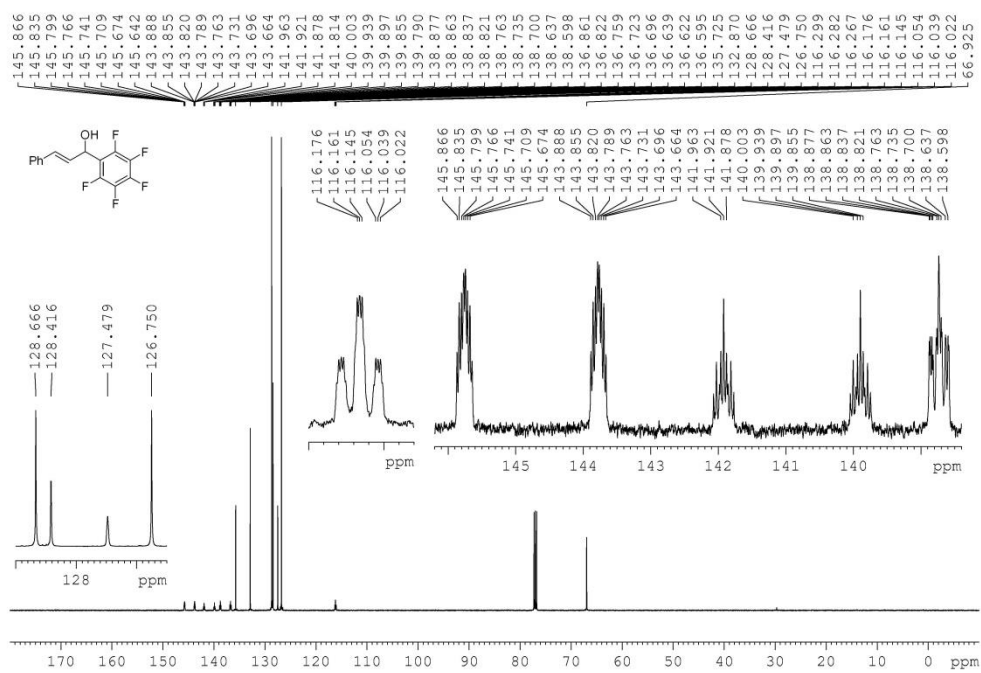
Compound 3o: ^{19}F NMR spectrum (470 MHz, CDCl_3).



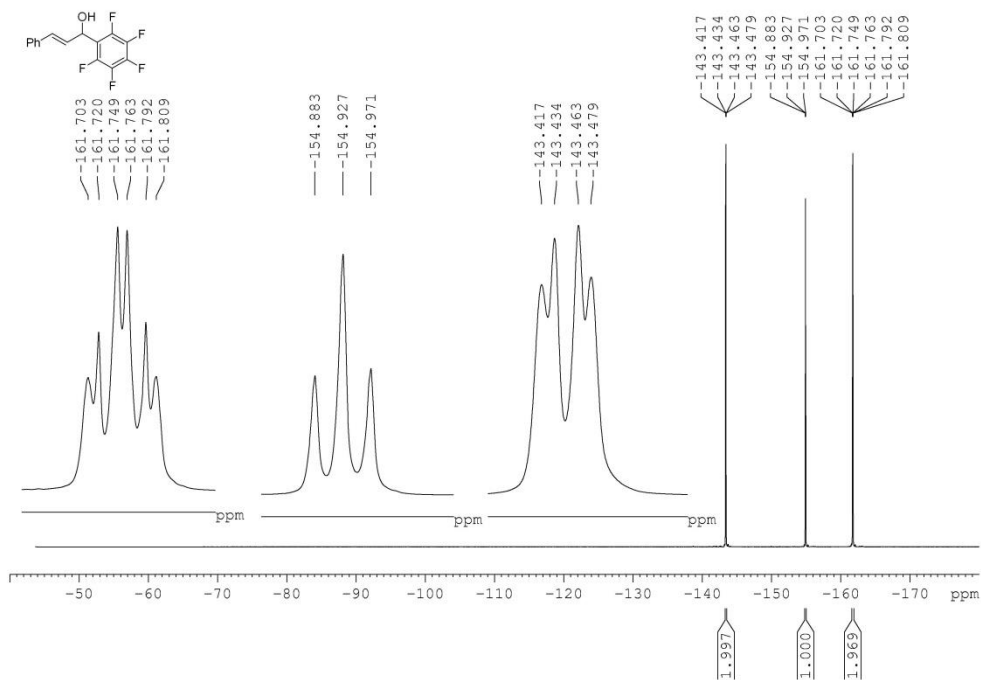
Compound 3p: ¹H NMR spectrum (500 MHz, CDCl₃).



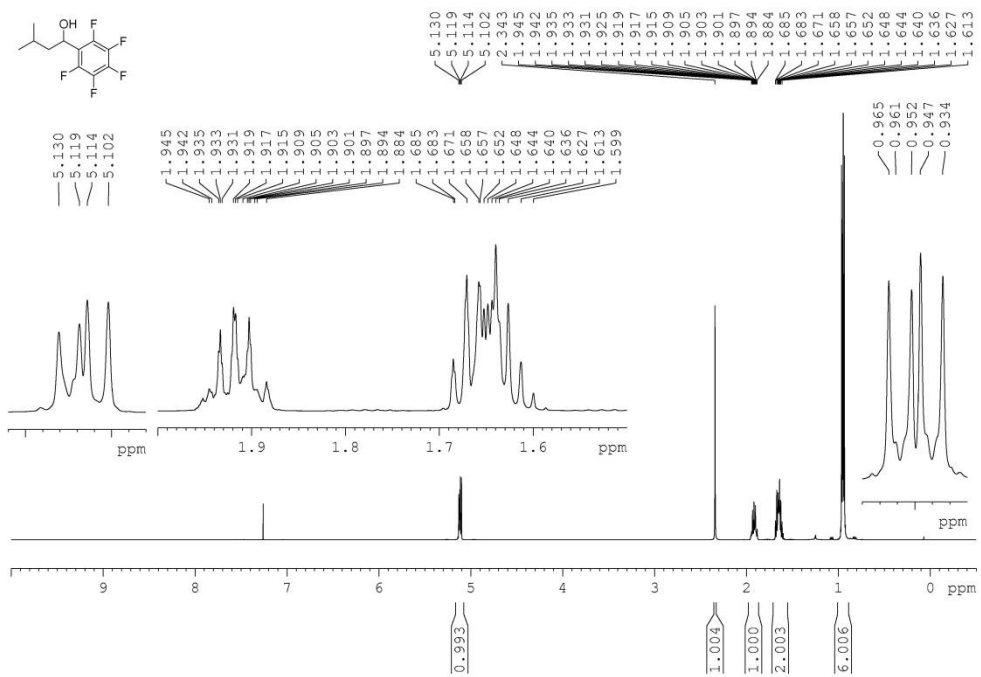
Compound 3p: ¹³C{¹H} NMR spectrum (125 MHz, CDCl₃).



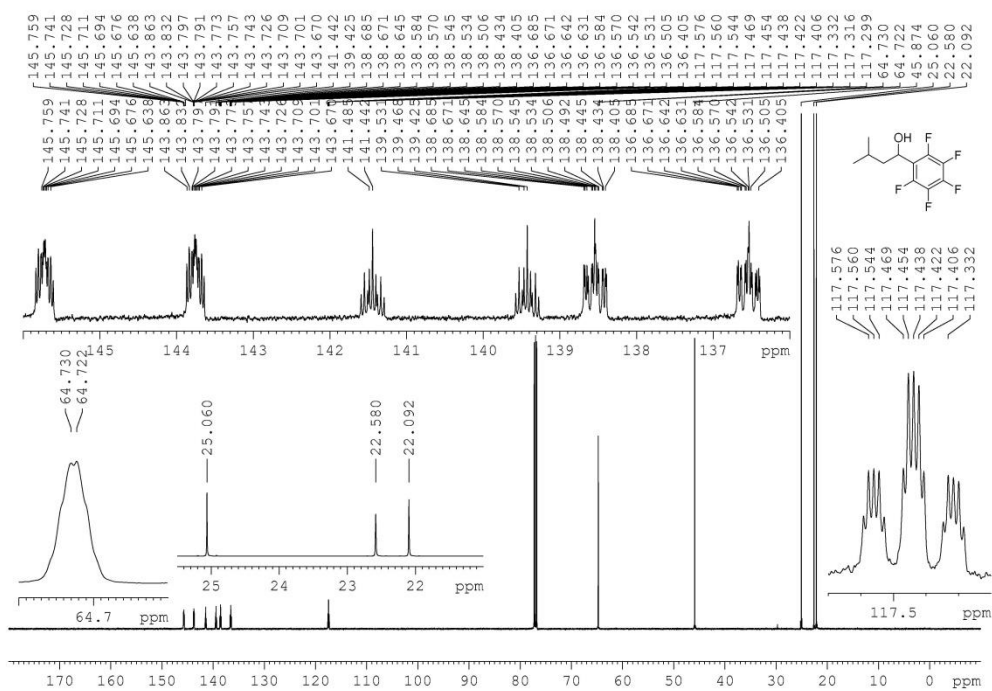
Compound 3p: ^{19}F NMR spectrum (470 MHz, CDCl_3).



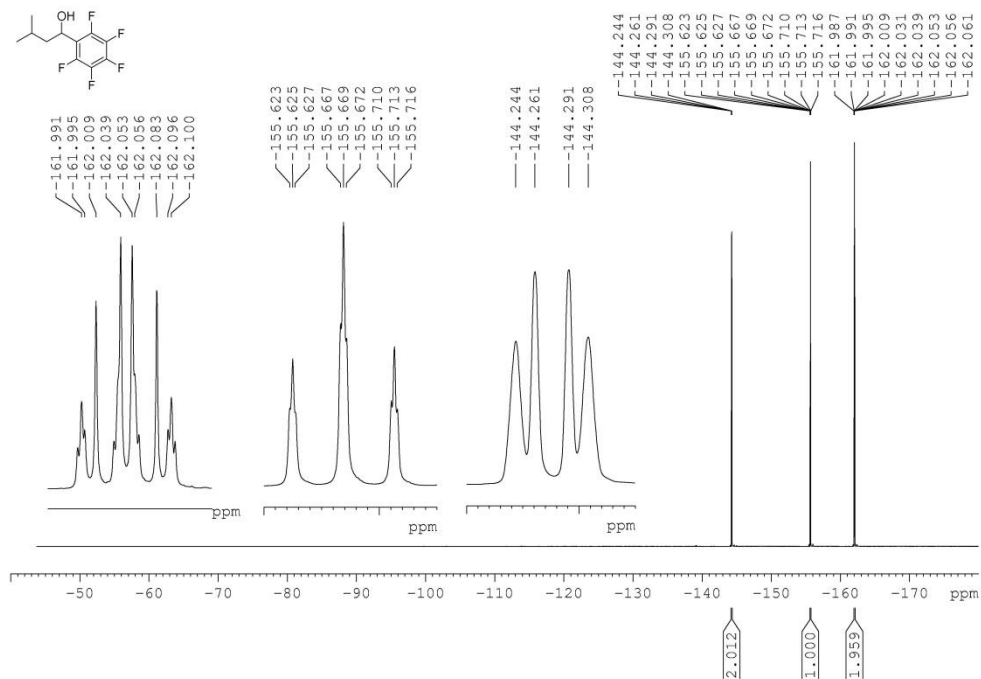
Compound 3q: ^1H NMR spectrum (500 MHz, CDCl_3).



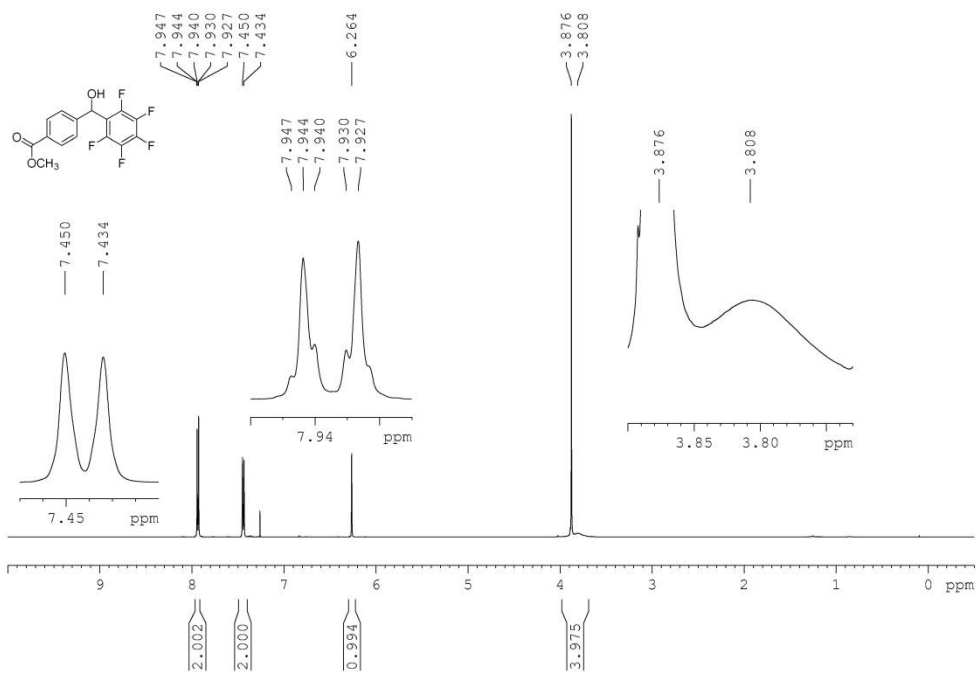
Compound 3q: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



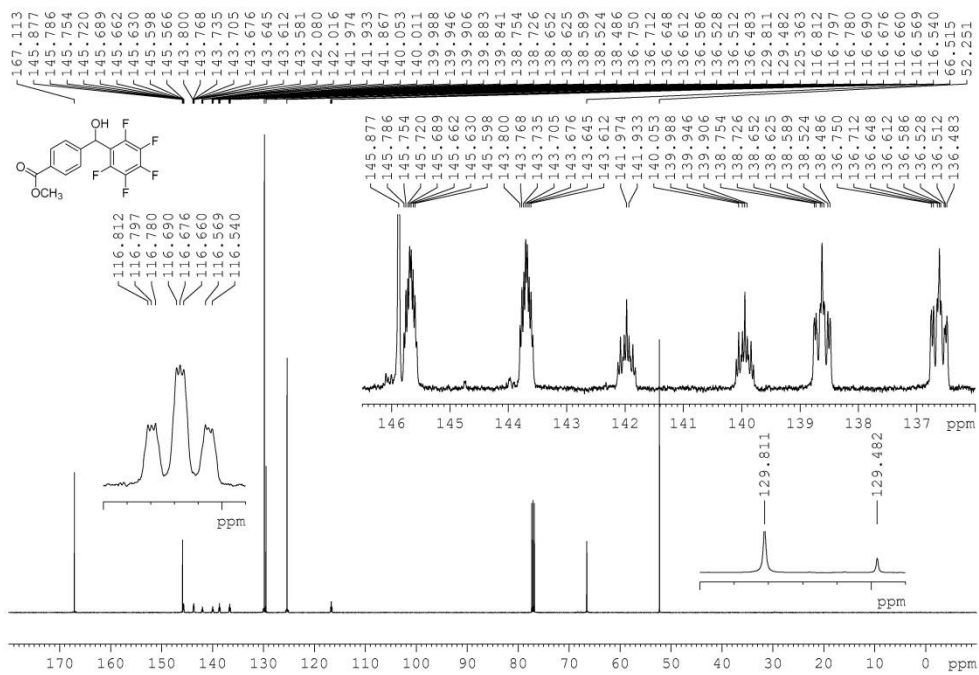
Compound 3q: ^{19}F NMR spectrum (470 MHz, CDCl_3).



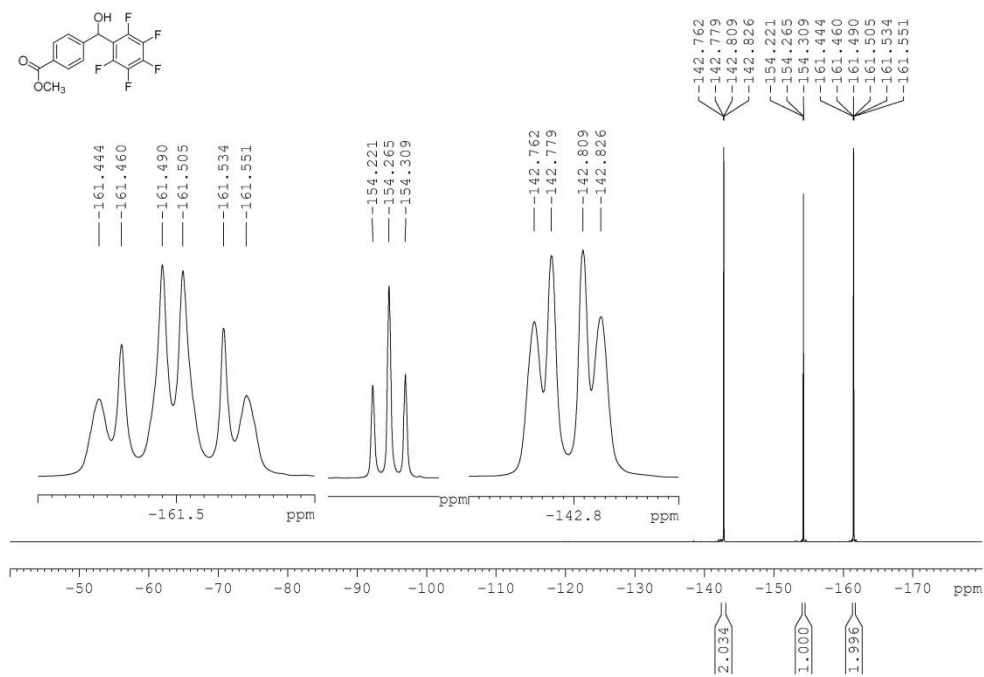
Compound 3r: ^1H NMR spectrum (500 MHz, CDCl_3).



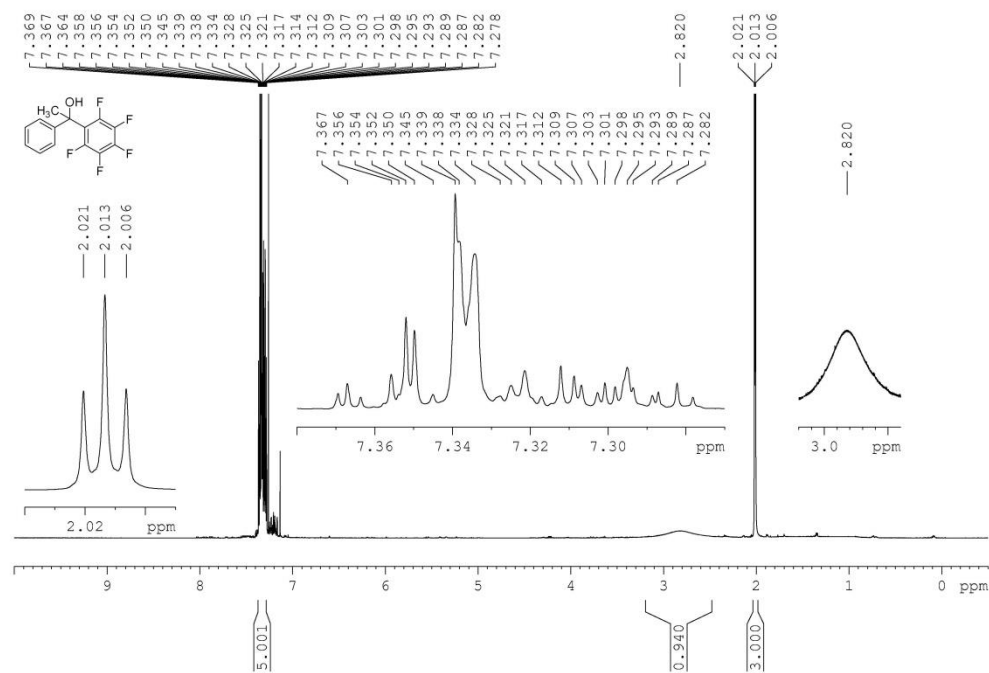
Compound 3r: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



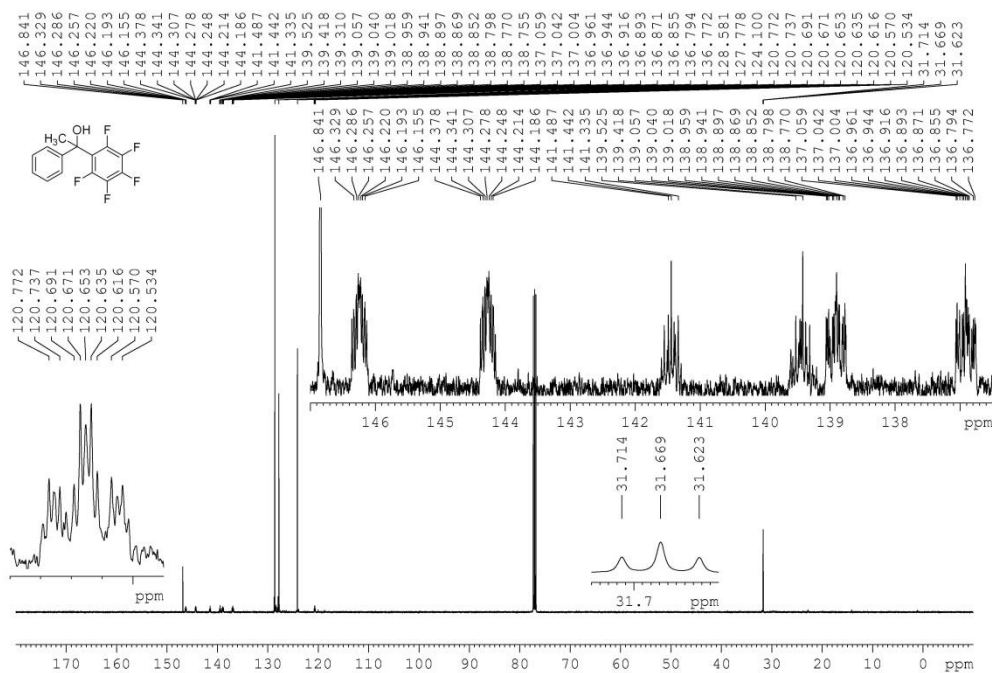
Compound 3r: ^{19}F NMR spectrum (470 MHz, CDCl_3).



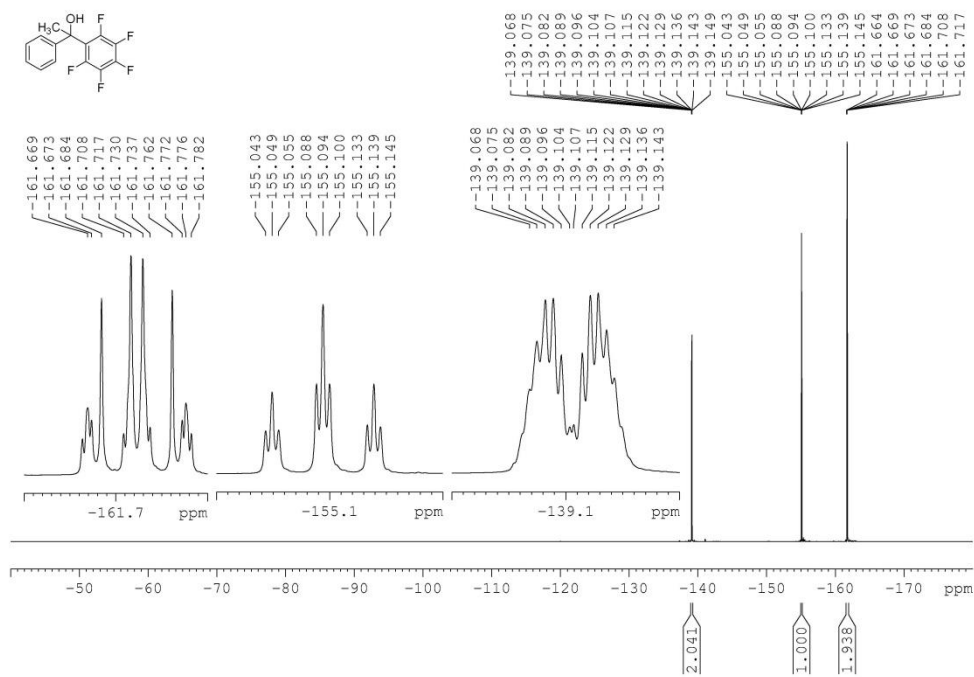
Compound 3s: ^1H NMR spectrum (500 MHz, CDCl_3).



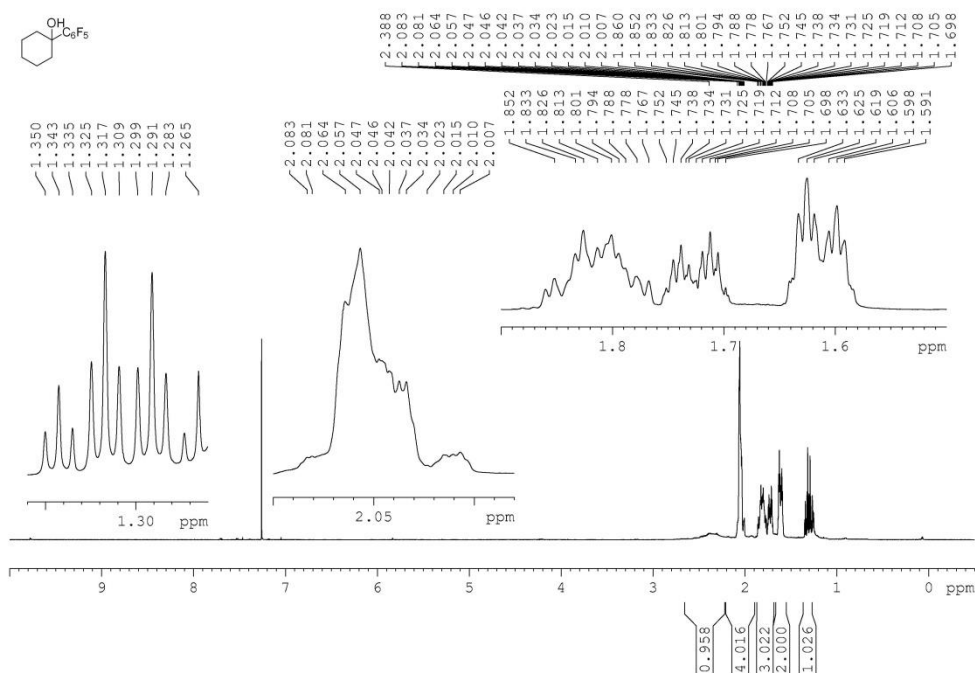
Compound 3s: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



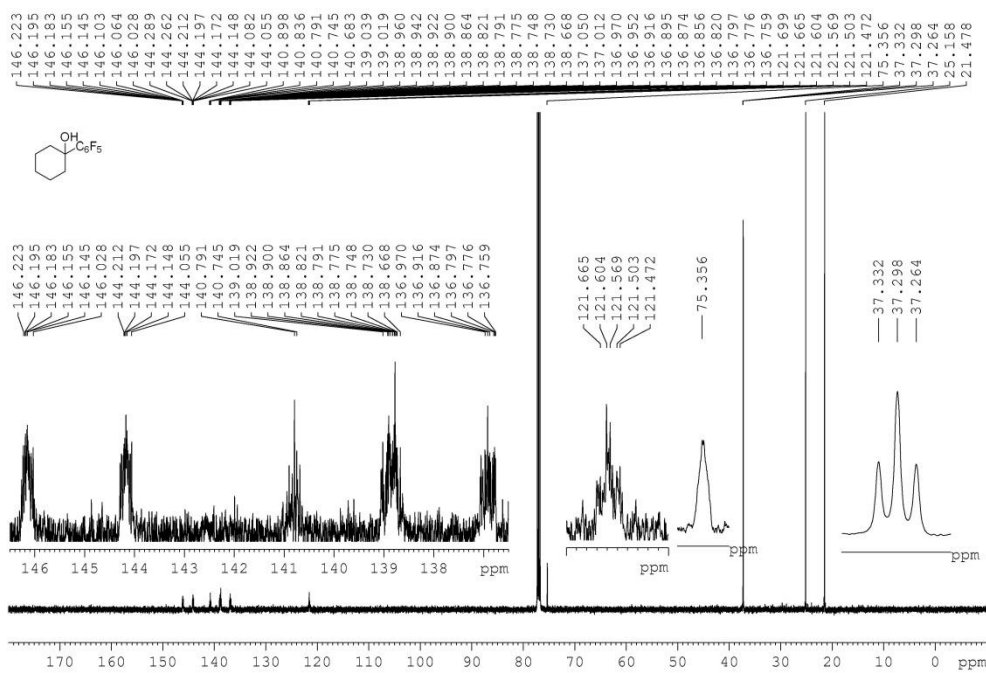
Compound 3s: ^{19}F NMR spectrum (470 MHz, CDCl_3).



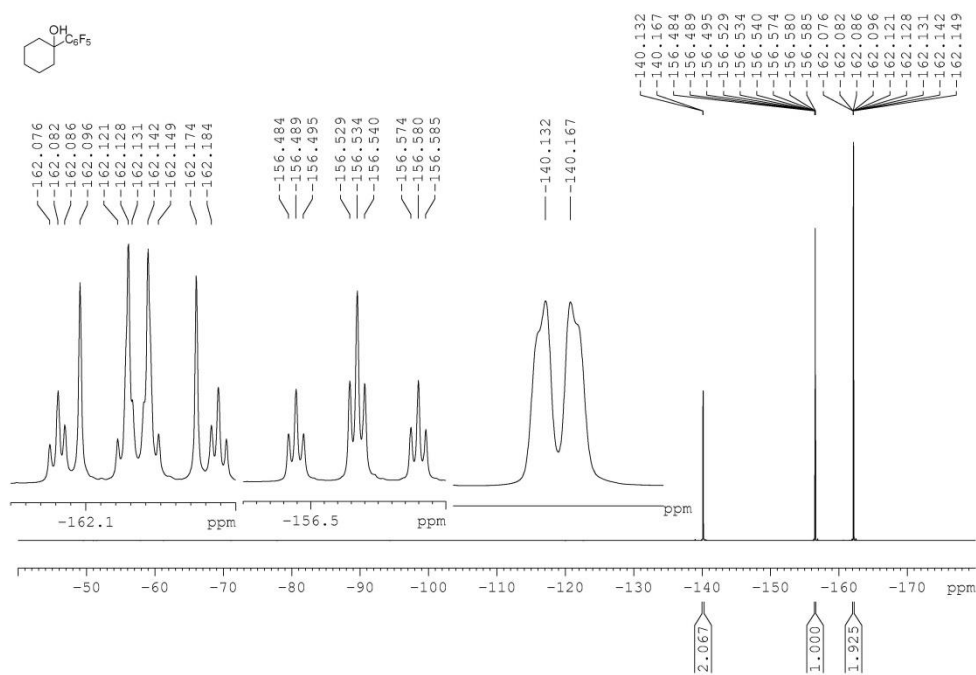
Compound 3x: ^1H NMR spectrum (500 MHz, CDCl_3).



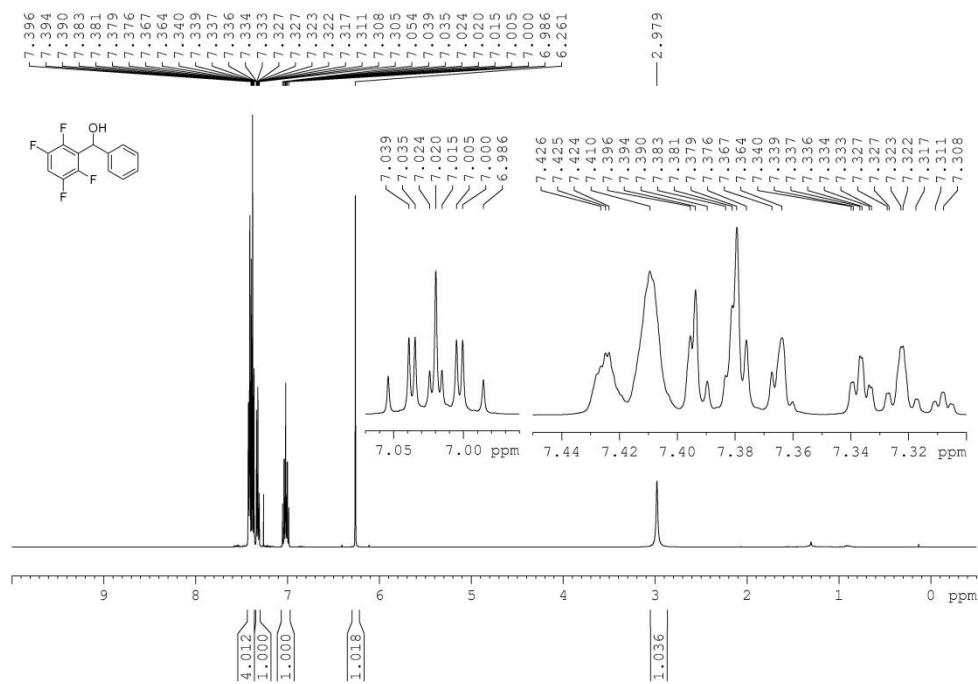
Compound 3x: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



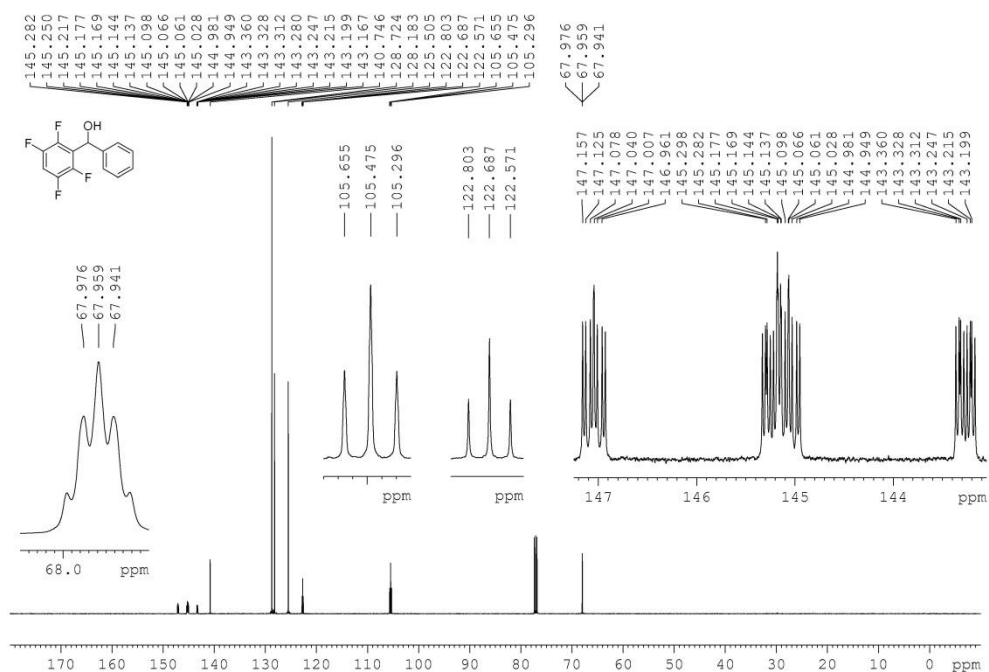
Compound 3x: ^{19}F NMR spectrum (470 MHz, CDCl_3).



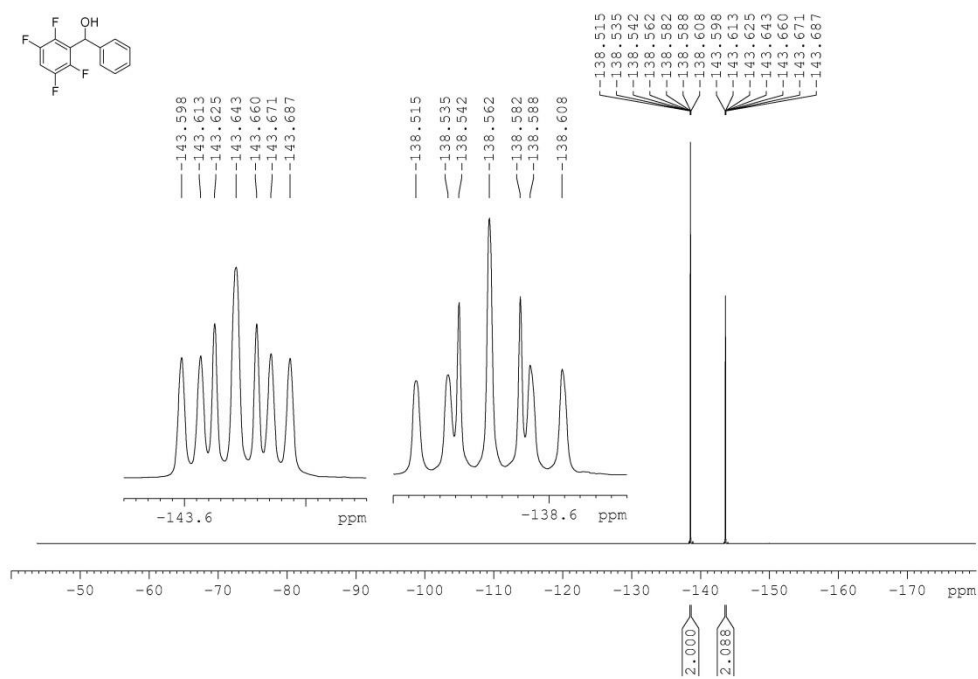
Compound 4a: ^1H NMR spectrum (500 MHz, CDCl_3).



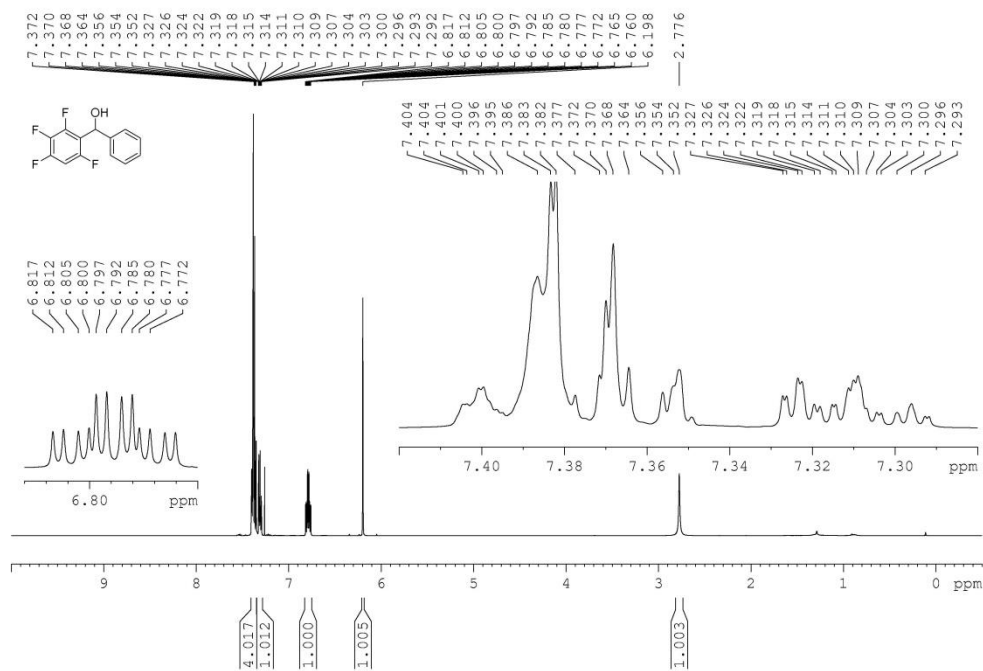
Compound 4a: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



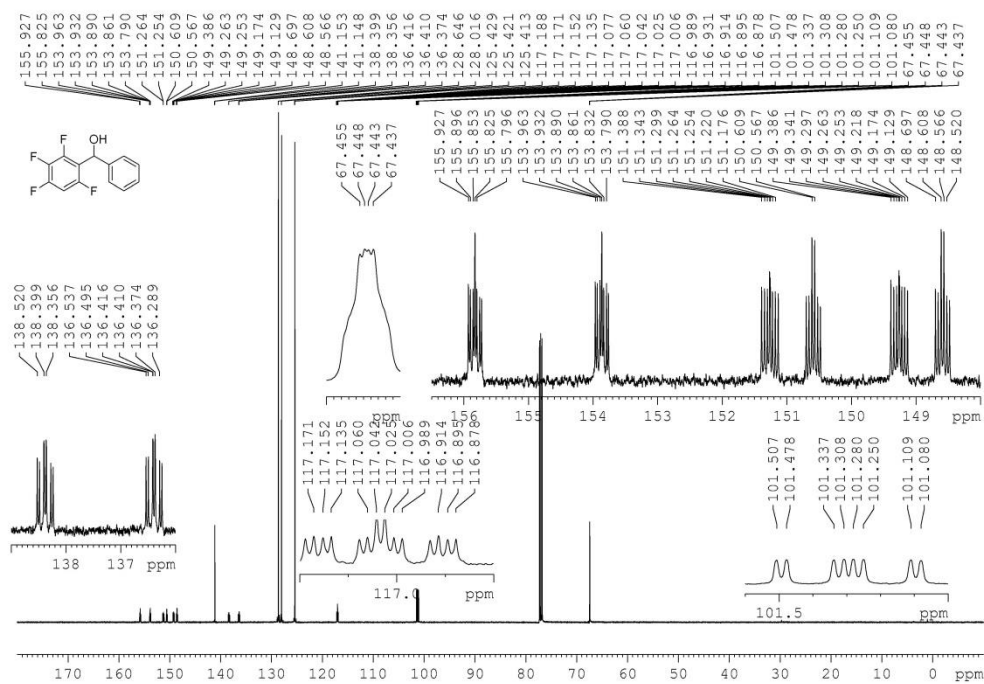
Compound 4a: ^{19}F NMR spectrum (470 MHz, CDCl_3).



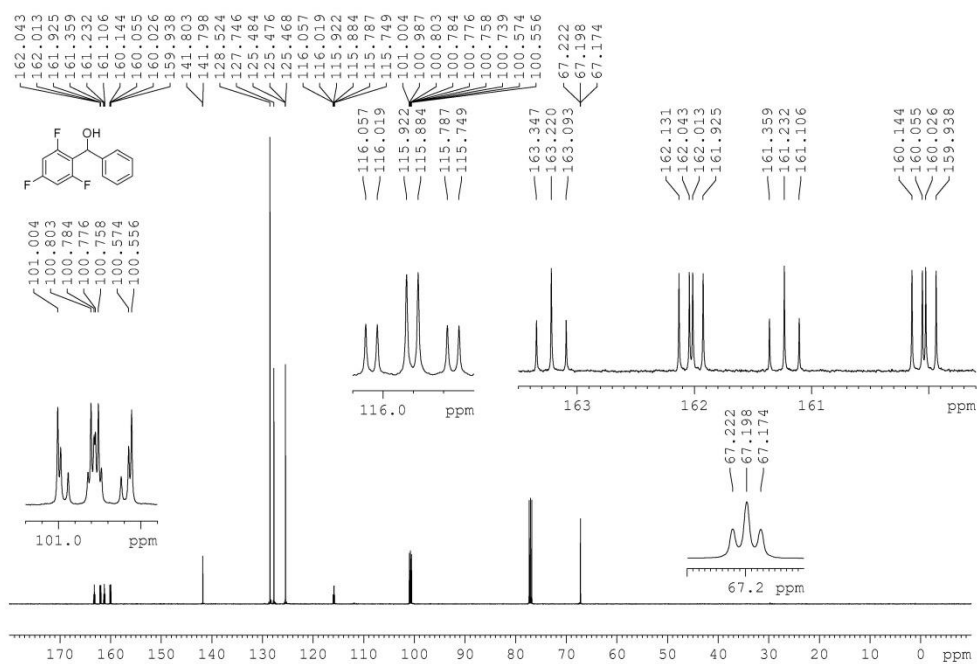
Compound 4b: ^1H NMR spectrum (500 MHz, CDCl_3).



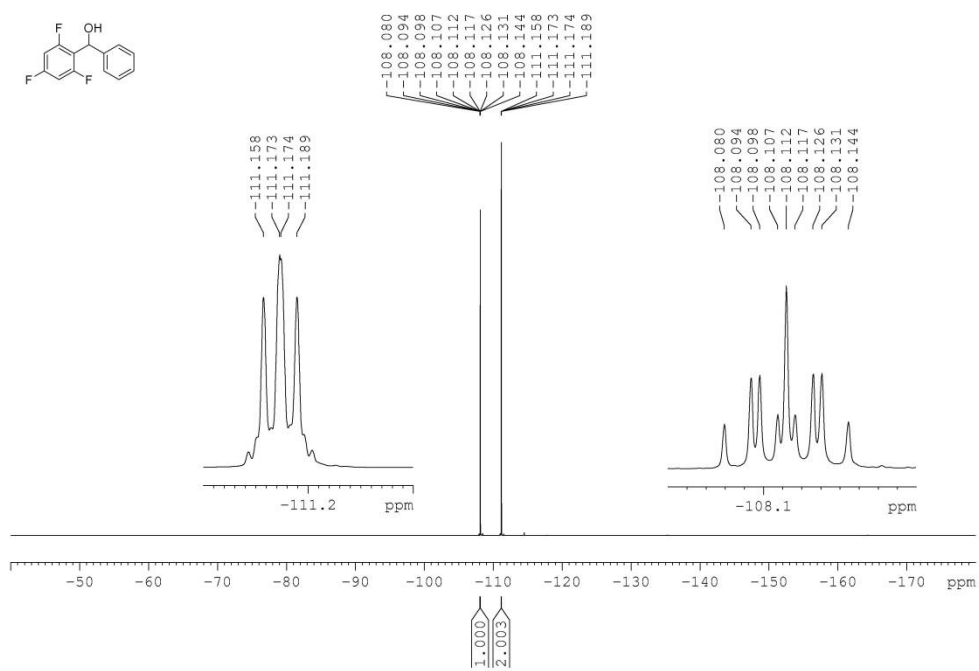
Compound 4b: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



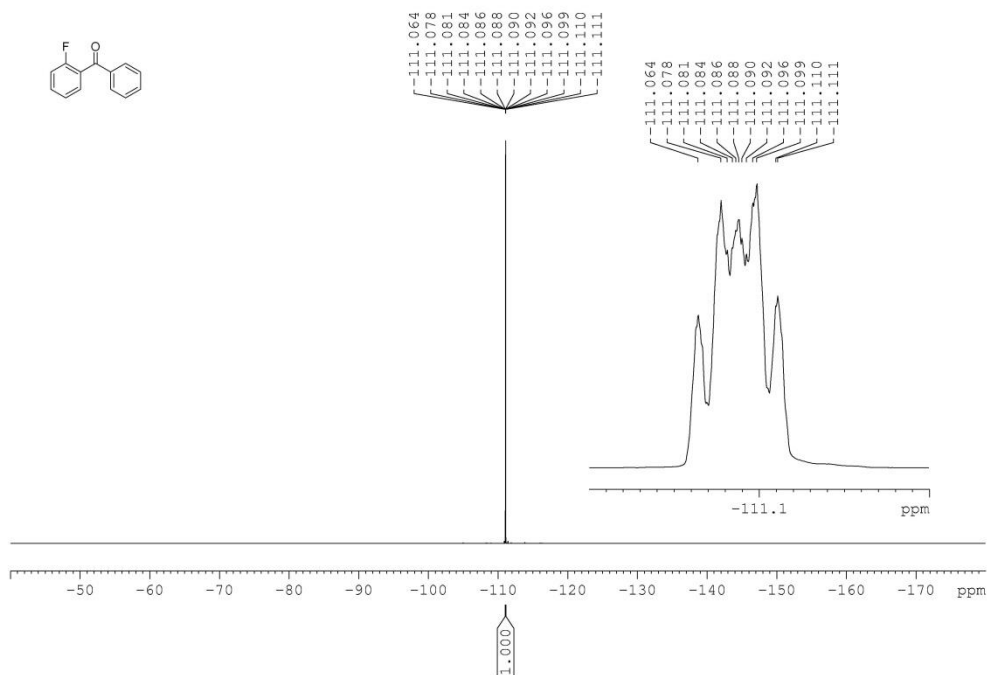
Compound 4c: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



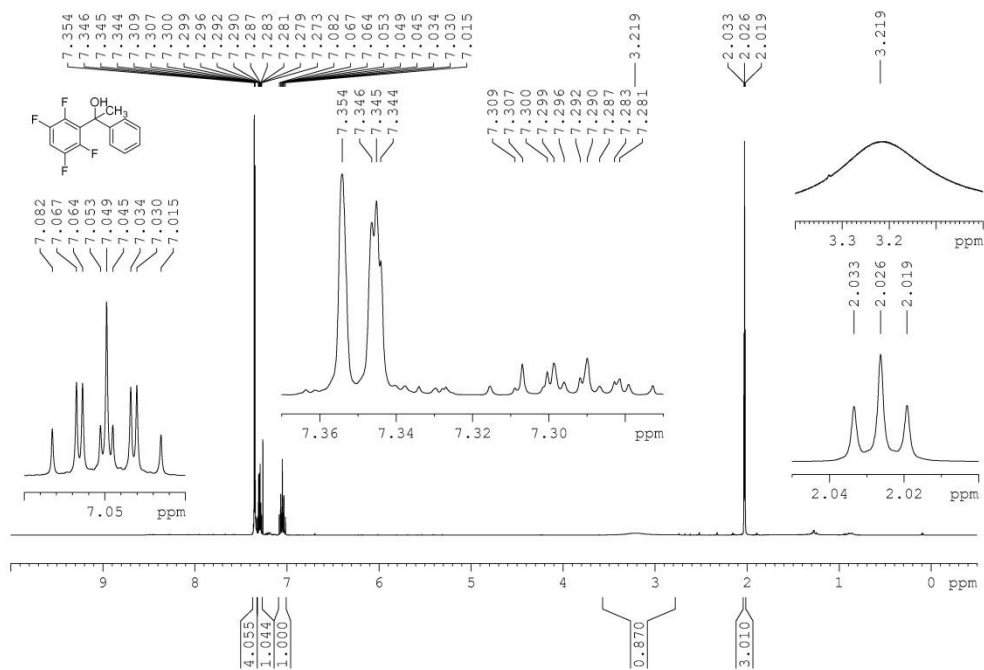
Compound 4c: ^{19}F NMR spectrum (470 MHz, CDCl_3).



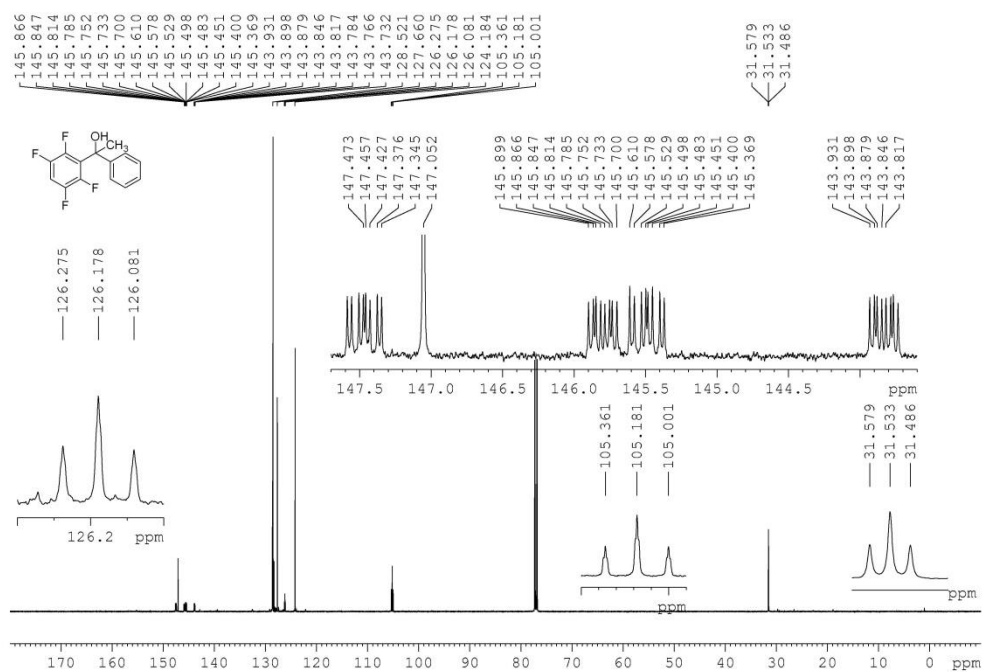
Compound 4f: ^{19}F NMR spectrum (470 MHz, CDCl_3).



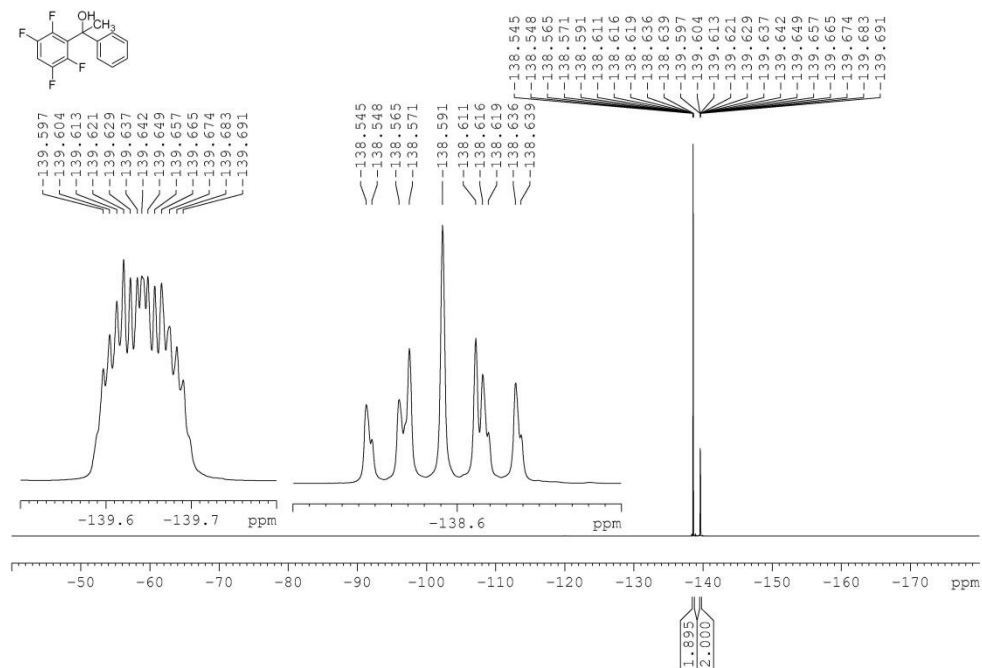
Compound 4g: ^1H NMR spectrum (500 MHz, CDCl_3).



Compound 4g: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3).



Compound 4g: ^{19}F NMR spectrum (470 MHz, CDCl_3).



VI. Single Crystal X-Ray Diffraction

Single crystals suitable for X-ray diffraction were selected, coated in perfluoropolyether oil, and mounted on MiTeGen sample holders. Diffraction data were collected on Bruker X8 Apex II 4-circle diffractometers with CCD area detectors using Mo-K α radiation monochromated by graphite or multi-layer focusing mirrors. The crystals were cooled using an Oxford Cryostream low-temperature device. Diffraction data were collected at 100 K. The images were processed and corrected for Lorentz-polarization effects and absorption effects by employing the Bruker software packages. The structure was solved using the intrinsic phasing method (SHELXT)^[7d] and expanded using Fourier techniques. All the non-hydrogen atoms were refined in anisotropic approximation, with hydrogen atoms ‘riding’ in idealized positions, by full-matrix least squares against F^2 on all data, using SHELXL^[7a,c] software and the SHELXLE^[7b] graphical user interface. Crystal data and experimental details are listed in Table S1; full structural information has been deposited with the Cambridge Crystallographic Data Centre. CCDC-2045652 (**3f**), 2045653 (**3l**), 2045654 (**3m**), 2045655 (**3n**), and 2045656 (**4d**).

Table S1. Single-crystal X-ray diffraction data and structure refinements of 3f, 3l, 3m, 3n, and 4d.

Compounds	3f	3l	3m	3n	4d
CCDC number	2045652	2045653	2045654	2045655	2045656
Empirical formula	C ₁₃ H ₆ BrF ₅ O	C ₁₄ H ₇ F ₅ O ₂	C ₁₇ H ₉ F ₅ O	C ₁₂ H ₆ F ₅ NO	C ₁₃ H ₁₀ F ₂ O
Formula weight (g mol ⁻¹)	353.09	302.20	324.24	275.18	220.21
Temperature (K)	100(2)	100(2)	100(2)	100(2)	100(2)
Radiation, λ (Å)	Mo-Kα 0.71073	Mo-Kα 0.71073	Mo-Kα 0.71073	Mo-Kα 0.71073	Mo-Kα 0.71073
Crystal color, habit	Colorless, block	Colorless, block	Colorless, block	Colorless, block	Colorless, block
Crystal size (mm ³)	0.17×0.26×0.34	0.57×0.55×0.28	0.30×0.33×0.41	0.54×0.39×0.23	0.44×0.35×0.22
Crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 1	<i>P</i> $\bar{1}$	<i>P</i> 2 ₁ / <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>C</i> 2/ <i>c</i>
<i>Unit cell dimensions</i>					
<i>a</i> (Å)	14.964(6)	6.9938(7)	8.422(5)	22.136(7)	20.058(3)
<i>b</i> (Å)	19.077(8)	7.7520(8)	23.486(13)	10.023(3)	10.796(3)
<i>c</i> (Å)	19.488(8)	11.9114(12)	14.108(9)	9.945(3)	9.2708(17)
α (°)	90.142(12)	71.116(2)	90	90	90
β (°)	109.530(7)	87.313(2)	99.583(17)	105.237(8)	98.046(8)
γ (°)	106.160(7)	82.190(2)	90	90	90
Volume (Å ³)	5008(4)	605.36(11)	2751(3)	2128.8(12)	1987.9(7)
<i>Z</i>	16	2	8	8	8
Calc. density (Mg·m ⁻³)	1.873	1.658	1.565	1.717	1.472
μ (mm ⁻¹)	3.337	0.161	0.143	0.170	0.117
<i>F</i> (000)	2752	304	1312	1104	912
θ range (°)	1.493 - 26.370	2.800 - 27.103	1.701 - 26.369	1.907 - 26.371	2.051 - 26.372
Reflections collected	165215	25240	62274	51503	15767
Independent reflections	40933	2658	5627	2178	2035
Minimum/maximum transmission	0.486 / 0.533	0.679 / 0.717	0.621 / 0.702	0.711 / 0.746	0.691 / 0.746
Parameters / restraints	2963 / 208	191 / 0	618 / 615	173 / 0	148 / 0
Goof on <i>F</i> ²	1.003	1.070	1.089	1.072	1.037
<i>R</i> ₁ [<i>I</i> >2σ(<i>I</i>)]	0.0351	0.0388	0.0945	0.0300	0.0397
<i>wR</i> ² (all data)	0.0755	0.1099	0.2297	0.0842	0.1057
Maximum/minimum residual electron density (e·Å ⁻³)	1.476 / -0.515	0.475 / -0.204	0.757 / -0.594	0.282 / -0.194	0.484 / -0.217

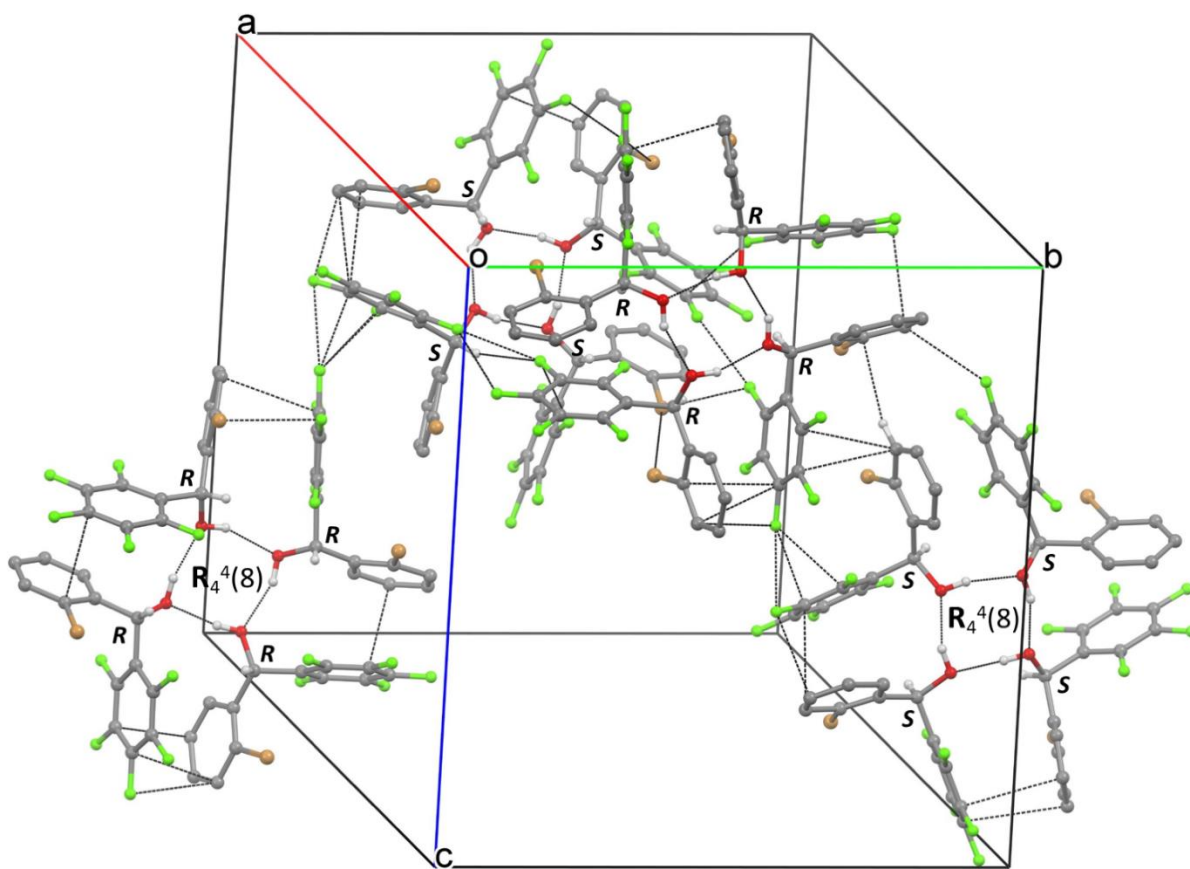


Figure S1. The asymmetric unit of **3f** and the unit cell metric are drawn. It consists of a racemic mixture of 16 symmetry-independent molecules which form four hydrogen-bonded tetramers of $R_4^4(8)$ graphset. The chirality of all 16 molecules are shown. Each tetramer contains only one type of chirality. In addition to hydrogen bonding interactions, other interactions, such as $\pi \cdots \pi$, $C-F \cdots \pi(C)$, $C-H \cdots \pi$, $F \cdots F$, $F \cdots Br$, etc. are also observed. The interplanar separations and angles between the phenyl and pentafluorophenyl rings lie in the range of 3.281(7) – 3.687(14) Å and 4.96(19) – 16.8(3)°, respectively.

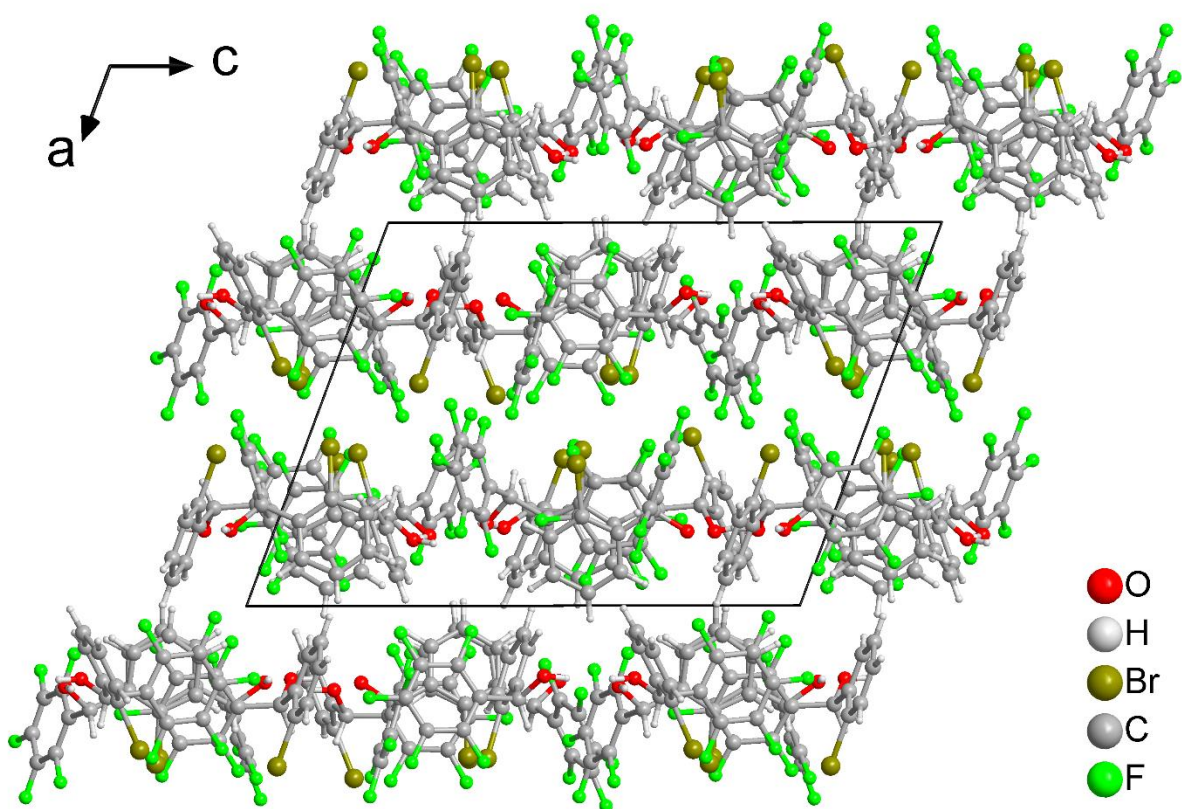


Figure S2. Tetramers of **3f** are arranged in sheets parallel to the \vec{b}, \vec{c} -plane with bromine atoms all pointing up or down within a sheet. Parallel sheets face each other either with the bromine atoms or without.

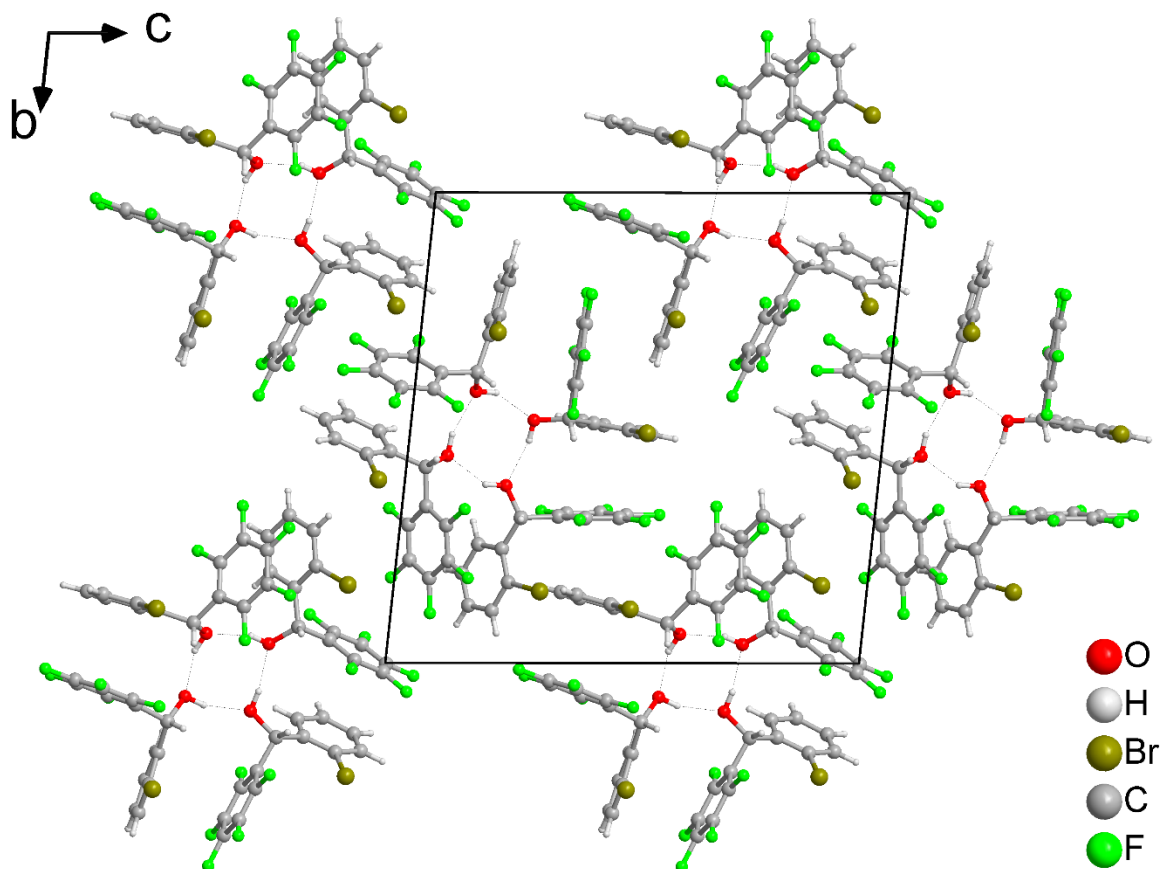


Figure S3. One of two symmetry-independent sheets of tetramers of **3f** containing two of four symmetry-independent tetramers. Tetramers within the sheet show alternating chirality.

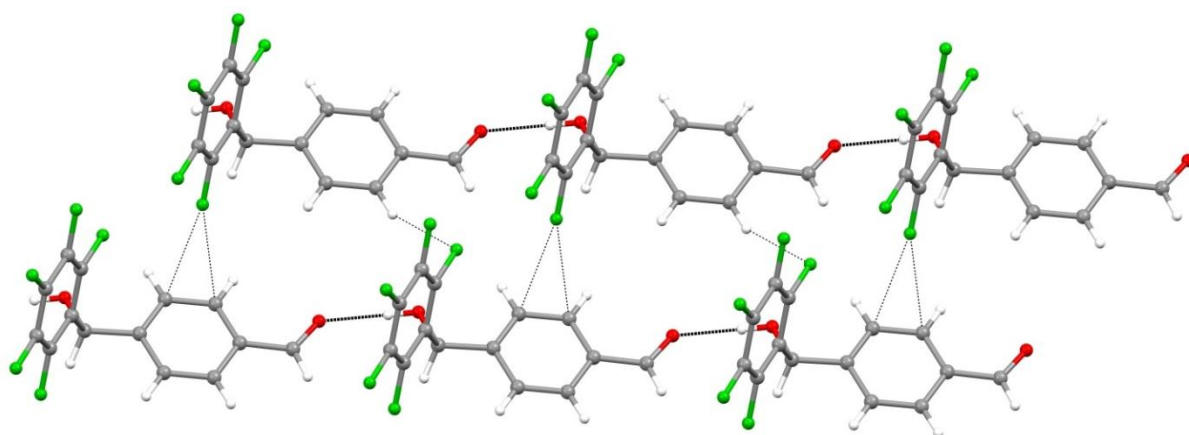


Figure S4. One-dimensional hydrogen bonded ($\text{O-H}\cdots\text{O}$) chains also exhibit $\text{C-F}\cdots\pi(\text{C})$ and $\text{C-H}\cdots\text{F}$ interactions between phenyl and pentafluorophenyl groups in **3l**.

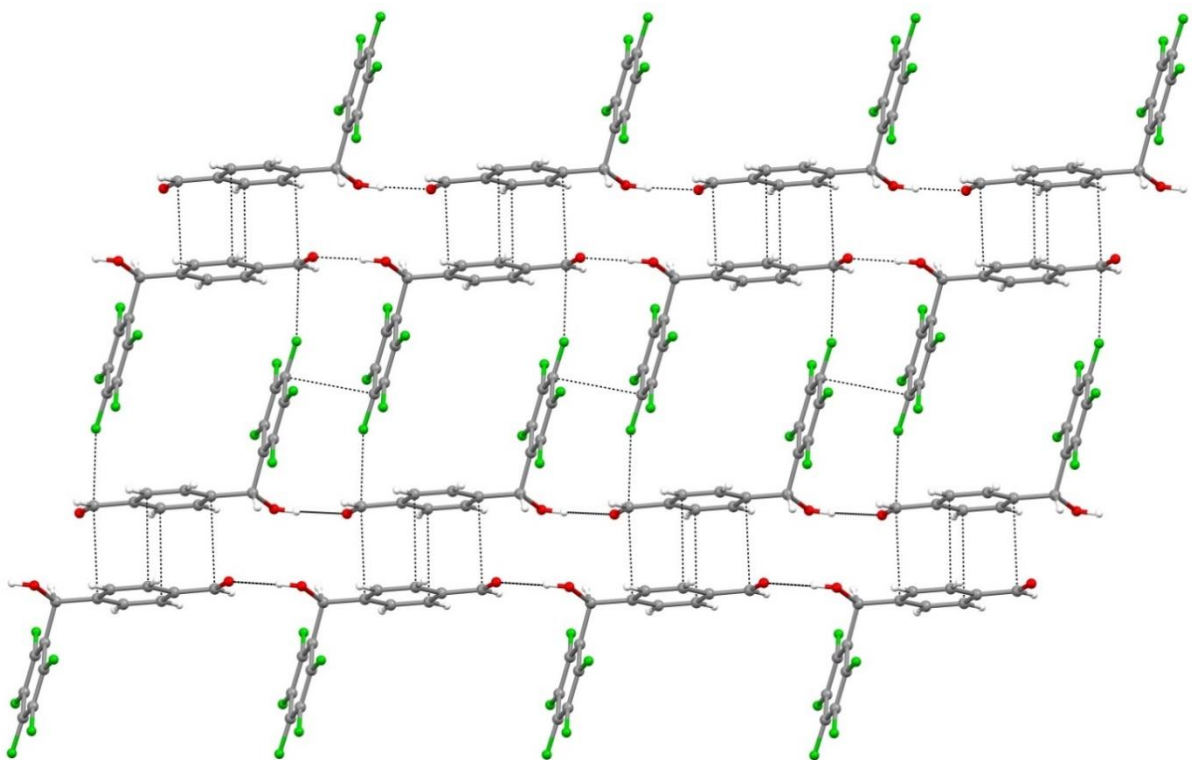


Figure S5. The π -stacked hydrogen-bonded chains further interdigitate⁸ (viewed approximately along a -axis) and there exist partial $\pi \cdots \pi$ interactions between fluorinated moieties and $C-F \cdots \pi$ interactions between pentafluorophenyl and carbonyl groups in **3I**.

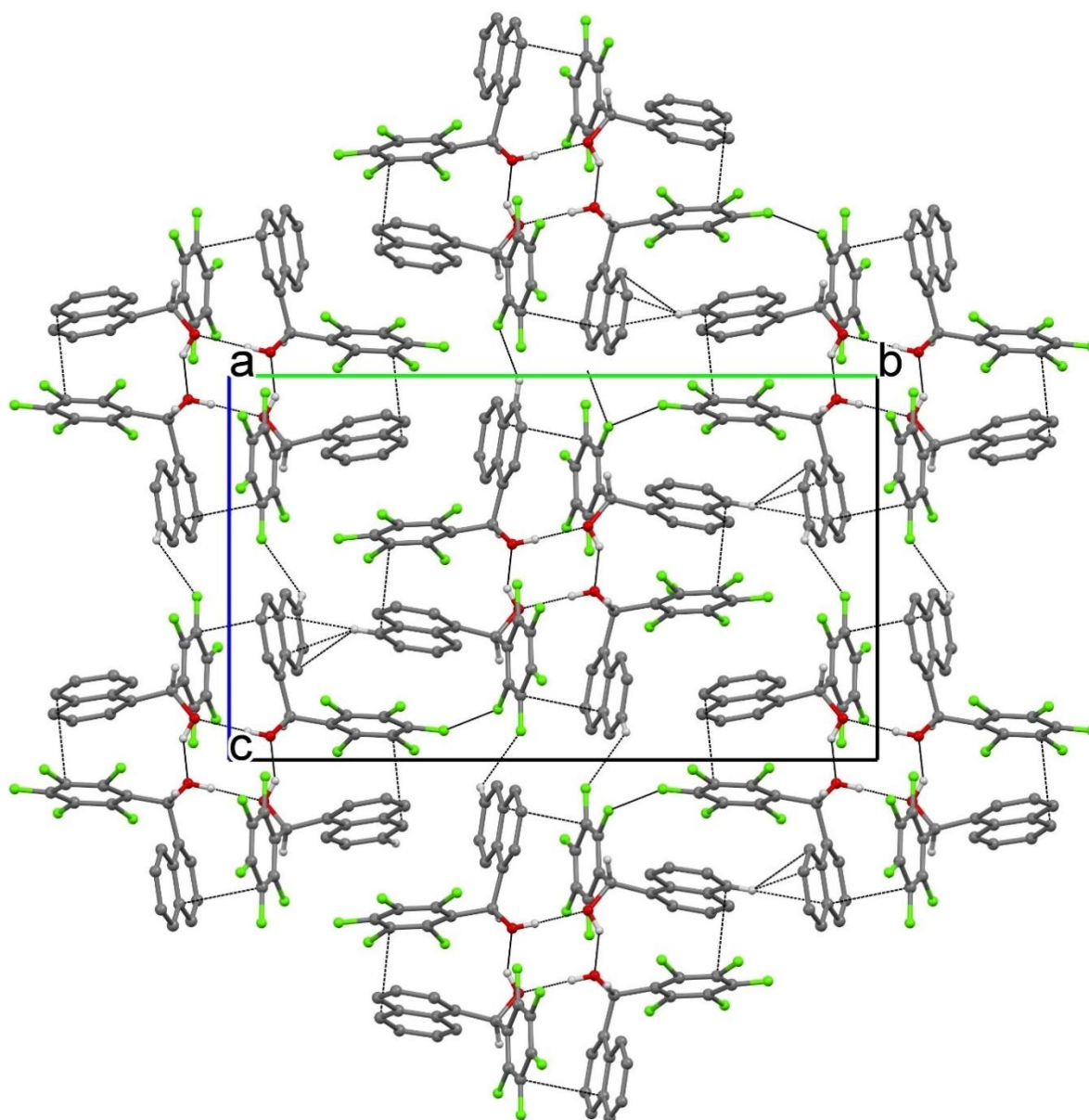


Figure S6. The crystal packing of compound **3m** is viewed along the *a*-axis. In addition to O–H···O hydrogen bonding, various intermolecular interactions, such as $\pi\cdots\pi$, C–H··· π , C–H···F, and F···F, are also observed. Interplanar separations and angles between the planes of naphthalene and pentafluorophenyl rings are 3.416(5) – 3.637(3) Å and 6.47(13) – 16.05(13)°.

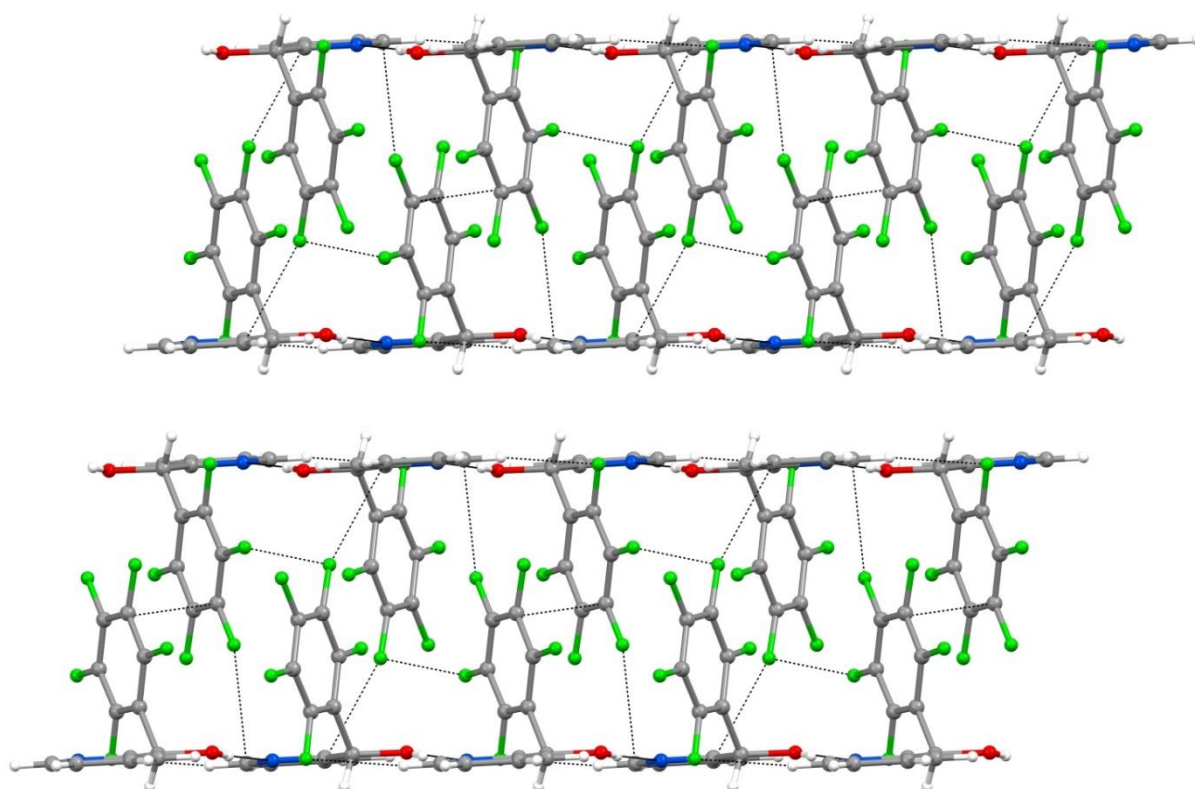


Figure S7. The crystal packing of **3n** is viewed along the *b*-axis. The pyridyl rings lie coplanar and the pentafluorophenyl groups interdigitate to form a parallel ribbon-like arrangement. Various types of weak interactions include, besides O–H···N hydrogen bonding, C–H··· π , C–F··· π , and F···F interactions ($d_{\text{F-F}} = 2.72 \text{ \AA}$, $F_{\text{vdW-radius}} = 1.47 \text{ \AA}$). Alternating hydrophobic and hydrophilic regions can be seen.

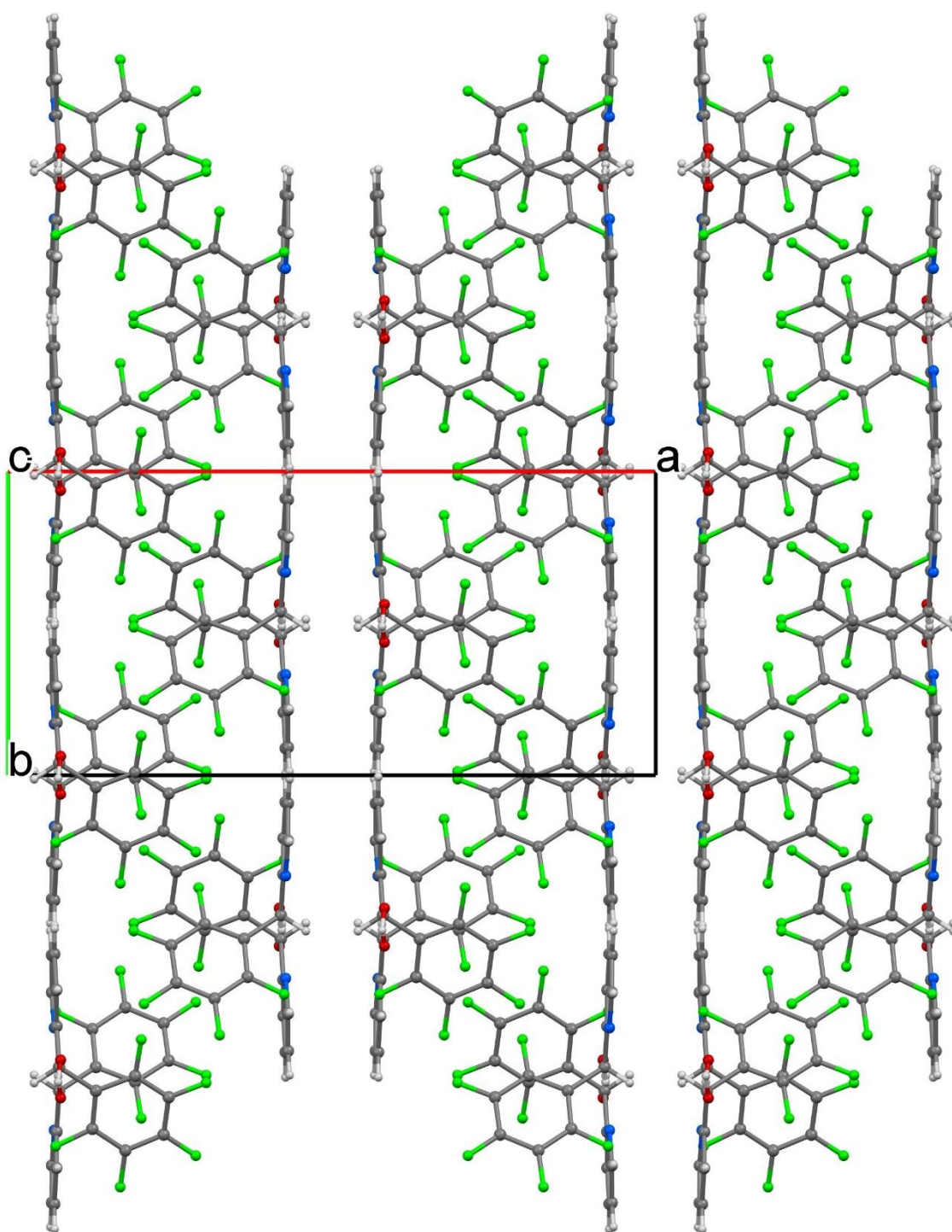


Figure S8. The crystal packing of **3n** is viewed along the *c*-axis. Alternating hydrophobic and hydrophilic regions can be seen.

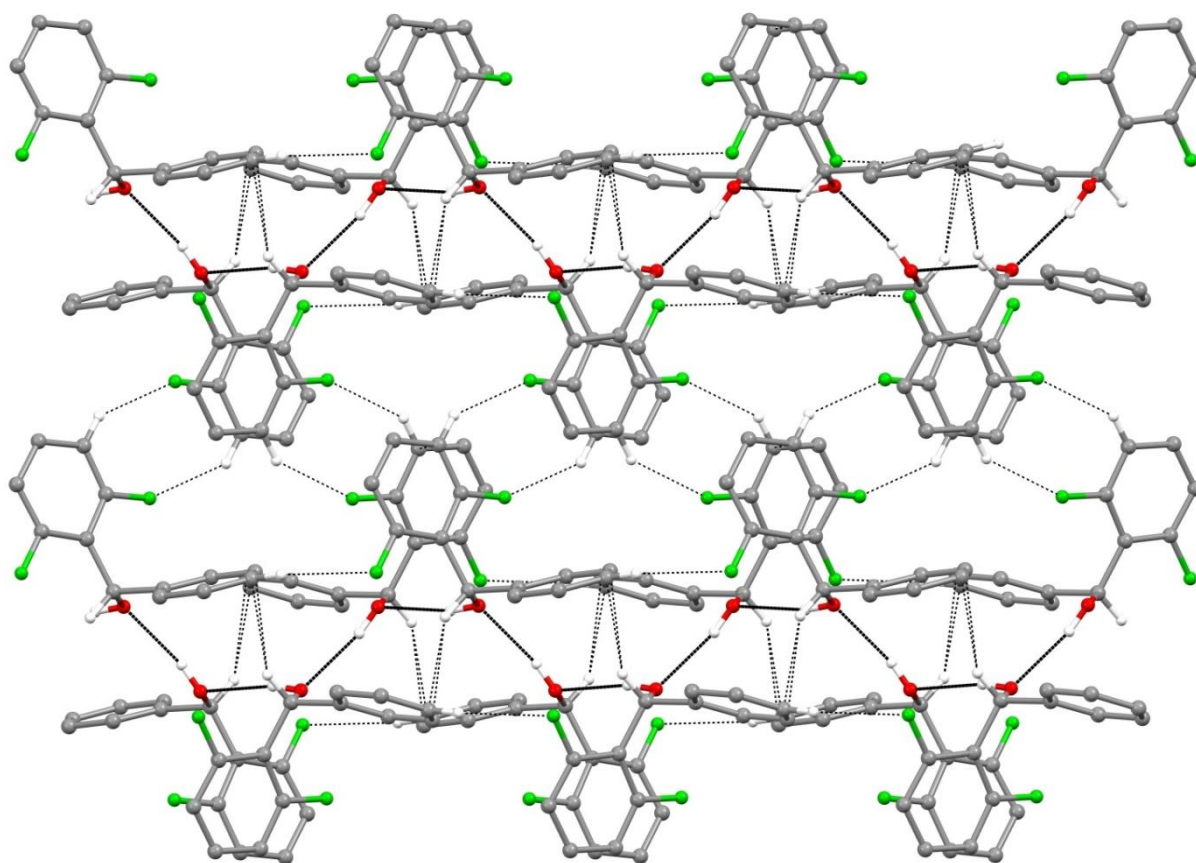


Figure S9. Crystal packing of **4d**, viewed along the *a*-axis, shows corrugated one-dimensional hydrogen bonded (O–H···O) chains propagating along the *c*-axis. In addition, several other intermolecular interactions, including C–H···F, C–H··· π , and π ··· π , can be observed.

Table S2. Parameters for hydrogen bonding in 3f, 3l, 3m 3n and 4d.

Donor(D)–H···Acceptor(A) ^a	H···A (Å) ^a	D···A (Å)	D–H···A (°)
Compound 3f			
O1–H1A···O2	1.90	2.693(5)	157.4
O2–H2A···O3	1.87	2.702(6)	171.0
O3–H3A···O4	1.90	2.704(5)	160.2
O4–H4A···O1	1.97	2.765(6)	156.5
O5–H5A···O8	1.91	2.697(6)	156.2
O8–H8A···O7	1.86	2.681(6)	166.6
O7–H7A···O6_1/11	2.02/2.07	2.703(14)/2.646(16)	138.4/125.4
O6_1/11–H6_1/11···O5	1.87/1.84	2.700(19)/2.666(11)	171.0/166.8
O9–H9A···O12	1.95	2.698(6)	148.1
O10–H10A···O9	1.97	2.756(5)	155.7
O11–H11A···O10	1.95	2.711(6)	150.3
O12–H12A···O11	1.92	2.740(5)	166.1
O13–H13A···O14	1.88	2.690(5)	162.0
O14–H14A···O15	1.90	2.716(5)	163.0
O15–H15A···O16	1.89	2.699(6)	161.0
O16–H16A···O13	1.88	2.677(6)	158.8
Compound 3l			
O1–H1···O2	1.90	2.7412(16)	176.4
Compound 3m			
O1_1–H1a_1···O1a_3	1.99	2.65(2)	135.3
O1_1–H1a_1···O1_3	2.11	2.72(2)	129.1
O1a_3–H1ab_3···O1_1	1.91	2.65(2)	145.6
O1a_3–H1ab_3···O1a_1	1.82	2.41(3)	125.4
Compound 3n			
O1–H1···N1	1.95	2.7880(17)	173.5
Compound 4d			
O1–H1A···O1	2.16	2.9815(17)	165.4
O1–H1B···O1	2.04	2.8661(16)	167.3

^a The donor–H distance was constrained to be 0.84 Å for all H atoms. H atoms were refined riding in idealized positions.

Table S3. Aryl...aryl ($\pi\cdots\pi$) distances (Å) and angles ($^\circ$) in **3f, **3l**, and **3m** at 100 K.**

Aryl...aryl	Centroid-centroid distance	Interplanar separation	Offset shift ^a	Plane normal angle
Compound 3f				
Ar _{Br1} ...Ar _F	3.648(4)	3.529(5)/3.330(7)	0.924(11)/1.490(12)	9.6(3)
Ar _{Br2} ...Ar _F	3.536(4)	3.470(4)/3.284(5)	0.682(9) / 1.311(8)	11.04(19)
Ar _{Br3} ...Ar _F	3.800(4)	3.570(5)/3.348(6)	1.301(11)/1.797(9)	9.9(2)
Ar _{Br4} ...Ar _F	3.648(4)	3.525(5)/3.386(6)	0.940(11)/1.357(10)	9.5(2)
Ar _{Br5} ...Ar _F	3.657(3)	3.538(4)/3.362(5)	0.927(9)/1.439(9)	8.75(19)
Ar _{Br6_1} ...Ar _F	3.694(14)	3.640(14)/3.687(14)	0.631(14)/0.23(5)	10.7(8)
Ar _{Br6_11} ...Ar _F	3.719(15)	3.717(14)/3.682(14)	0.12(5)/0.518(15)	9.9(8)
Ar _{Br7} ...Ar _F	3.783(5)	3.285(8)/3.659(6)	1.875(12)/0.959(13)	16.8(3)
Ar _{Br8} ...Ar _F	3.523(4)	3.416(4)/3.514(4)	0.729(10)/0.25(1)	8.0(2)
Ar _{Br9} ...Ar _F	3.674(5)	3.494(6)/3.276(8)	1.138(12)/1.663(12)	8.9(3)
Ar _{Br10} ...Ar _F	3.719(4)	3.528(5)/3.317(5)	1.179(10)/1.682(9)	11.43(19)
Ar _{Br11} ...Ar _F	3.728(4)	3.554(5)/3.362(5)	1.128(10)/1.611(9)	8.8(2)
Ar _{Br12} ...Ar _F	3.564(4)	3.484(4)/3.343(6)	0.754(11)/1.237(10)	9.7(2)
Ar _{Br13} ...Ar _F	3.739(4)	3.357(6)/3.635(4)	1.646(10)/0.877(10)	13.3(2)
Ar _{Br14} ...Ar _F	3.610(4)	3.593(4)/3.523(4)	0.35(1)/0.788(10)	12.5(2)
Ar _{Br15} ...Ar _F	3.706(5)	3.559(5)/3.281(7)	1.034(12)/1.723(11)	12.9(3)
Ar _{Br16} ...Ar _F	3.592(4)	3.577(4)/3.539(4)	0.330(9)/0.614(9)	4.96(19)
Compound 3l				
Ar...Ar	3.6667(10)	3.3379(13)	1.5176(19)	0.00(7)
Ar _F ...Ar _F	4.6778(14)	3.375(2)	3.238(3)	0.00(1)
Compound 3m ^b				
Ar _d ...Ar _F	3.650(3)	3.637(3)/3.564(3)	0.305(7)/0.787(6)	16.05(13)
Ar...Ar _{F_d}	3.538(3)	3.448(3)/3.357(4)	0.794(5)/1.119(7)	6.47(13)
Ar _d ...Ar _F (T...T)	3.886(3)	3.613(4)/3.416(5)	1.431(5)/1.854(7)	6.89(13)
Compound 3n				
Ar _F ...Ar _F	4.2972(15)	3.193(2)	2.876(2)	0.0(5)
Compound 4d				
Ar...Ar	4.8860(13)	3.177(3)	3.712(2)	0.00(1)
Ar _{HF} ...Ar _{HF}	4.5100(14)	3.358(2)	3.010(3)	17.65(7)

^a The offset shift, also called inter-centroid shift, is the distance within a plane of an aryl ring between the centroid of the respective aryl ring and the intersection point with the normal to the plane through the centroid of the other aryl ring.

^b Only interactions with the main parts (85%) of the disordered (d) pentafluorophenyl and naphthalene moieties are reported here.

VII. Computational Methods

All the calculations were performed with the Gaussian09 programs.^[9] The geometries of the different structures were optimized at the DFT level using the B3-LYP^[10-11] hybrid functional with 6-31+G(d) basis set. Frequency analysis was carried out at the same level to verify the stationary points as an intermediate or transition state and to obtain the thermodynamic energy corrections assuming a standard state of 1 atm and 298.15 K. Intrinsic reaction coordinates (IRC)^[12] were calculated to confirm the connection between the transition state and the correct reactant/product. The solvent effects were taken into consideration by single point calculations of the gas-phase stationary points with the SMD^[13-15] continuum solvation model. To obtain more accurate energy information, single-point calculations were carried out with the M06^[16] functional and 6-311++G(d,p) basis set in toluene solvent (using the SMD solvent model). All of the three-dimensional molecular diagrams of the molecules were generated with CYLView.^[17]

Table S4. Absolute calculated electronic energies, correction of enthalpies, and free energies.

Geometry	$E_{(\text{elec-B3LYP})}^1$	$G_{(\text{corr-B3LYP})}^2$	$H_{(\text{corr-B3LYP})}^3$	$E_{(\text{M06 toluene})}^4$	IF ⁵
6	-2602.91354	0.19189	0.276362	-2602.613003	
7-ts	-2602.862623	0.187452	0.27543	-2602.566437	-135.94
8	-2602.899113	0.183295	0.276536	-2602.586769	
9	-2948.493833	0.283666	0.395715	-2948.028436	
10-ts	-2948.48623	0.2872	0.395038	-2948.022579	-104.87
11	-2948.514631	0.289305	0.397303	-2948.048797	
12-ts	-2948.483194	0.291873	0.396411	-2948.029586	-71.99
13	-2948.526205	0.29542	0.397854	-2948.072049	
14-ts	-4087.664887	0.503267	0.650296	-4086.926819	-74.41
15	-4087.674391	0.503786	0.651069	-4086.934931	
16-ts	-4087.667933	0.502938	0.650055	-4086.930499	-106.81
17	-1484.742692	0.286987	0.373107	-1484.297391	
18	-2503.68739	0.201261	0.283462	-2503.387159	
19-ts	-2503.634465	0.196446	0.282443	-2503.338675	-135.57
20	-2404.458457	0.210645	0.290577	-2404.158042	
21-ts	-2404.40159	0.205886	0.289656	-2404.105012	-137.3
22	-2305.218418	0.220156	0.297974	-2304.918703	
23-ts	-2305.159478	0.215332	0.297033	-2304.863907	-141.31
24	-2205.970598	0.228529	0.305459	-2205.671805	
25-ts	-2205.908151	0.223326	0.304145	-2205.612351	-104.72
26	-2205.963365	0.228374	0.305711	-2205.664144	
27-ts	-2205.892339	0.222338	0.304343	-2205.595884	-114.48
28	-1402.96216	0.191335	0.268364	-1402.767999	
29-ts	-1402.951039	0.18894	0.266972	-1402.754229	-132.93
30	-675.200515	0.156661	0.211906	-675.04524	

31	-727.84762	0.011433	0.055189	-727.754167	
32-ts	-1073.433312	0.110004	0.173384	-1073.176777	-121.88
33	-1073.441942	0.113864	0.175008	-1073.188879	
34-ts	-1748.560884	0.292987	0.387263	-1748.200815	-108.2
35	-1748.578555	0.295372	0.389196	-1748.223167	

¹ The electronic energy calculated by B3-LYP/6-31+g(d) in gas phase. ² The thermal correction to Gibbs free energy calculated by B3-LYP/6-31+g(d) in gas phase. ³ The thermal correction to enthalpy calculated by B3-LYP/6-31+g(d) in gas phase. ⁴ The electronic energy calculated by M06/6-311++G(d,p) in toluene. ⁵ The B3-LYP calculated imaginary frequencies for the transition states.

B3LYP geometries for all the optimized compounds and transition state.

6

C	-2.27197500	0.88043600	-1.53236400
C	-2.65585600	-0.62458300	-1.26977200
O	-1.50658800	-1.11901800	-0.57012800
O	-1.52181800	1.20667900	-0.35807100
B	-0.82930300	-0.00536400	0.14312500
C	0.81156600	-0.00311700	-0.20654500
C	1.57578400	1.16182700	-0.26982500
C	1.54782400	-1.16102800	-0.45624800
C	2.93231300	1.20292500	-0.58179700
C	2.90348000	-1.18470400	-0.77289900
C	3.60583200	0.01408700	-0.84209000
O	-1.03623900	-0.09693500	1.60633000
C	-0.02050700	-0.16995300	2.61978200
O	0.33486200	-1.32923400	2.92791100
O	0.33160600	0.93346200	3.09209100
C	-3.88967900	-0.76451400	-0.35566100
H	-4.81443900	-0.45330500	-0.85606700
H	-4.00876800	-1.81920100	-0.07493400
H	-3.76934400	-0.18045300	0.56199600
C	-2.86422200	-1.46237000	-2.53519300
H	-3.13209500	-2.49061300	-2.26257100
H	-3.67923300	-1.05863100	-3.14923800
H	-1.95640700	-1.50483400	-3.14221000
C	-3.46281000	1.83876300	-1.63913700
H	-3.10237700	2.85735100	-1.82798000
H	-4.12221100	1.56149300	-2.47087500
H	-4.05557800	1.85240900	-0.71940700
C	-1.37274000	1.05628800	-2.77092000
H	-1.92916100	0.90706000	-3.70377100

H	-0.96944700	2.07510200	-2.77334300
H	-0.52928100	0.35996600	-2.75615700
F	1.00950400	2.37975900	-0.00637500
F	3.59563500	2.37278600	-0.63053400
F	4.91280700	0.02264500	-1.14748600
F	3.53950500	-2.34771000	-1.00564700
F	0.95227900	-2.39118300	-0.38382100
K	-1.04721800	-2.87445200	1.41987500
K	-1.04337900	2.67075900	1.79668500
7-ts			
C	0.46292300	2.80457500	-0.28914600
C	0.93411000	2.36303100	1.16428300
O	0.87683100	0.91600700	1.09949800
O	0.74813000	1.63109200	-1.08854900
B	0.85999100	0.54819300	-0.24076000
C	-1.31576800	-0.51892500	-0.33293200
C	-2.26133100	-0.08870200	-1.25197100
C	-1.86771100	-1.09607000	0.79104800
C	-3.64089400	-0.16870500	-1.05798600
C	-3.22770800	-1.21845600	1.06731000
C	-4.12723600	-0.73266400	0.12163900
O	1.51143300	-0.64889100	-0.66281000
C	2.83025300	-0.92611000	-0.45547200
O	3.66663800	-0.00183500	-0.32608100
O	3.09202800	-2.18298700	-0.43336200
C	2.39361100	2.73219200	1.47641400
H	2.52668100	3.81639300	1.57357700
H	2.67368000	2.26678300	2.42853100
H	3.07010100	2.35019600	0.70696100
C	0.03030000	2.83613500	2.30474800
H	0.41221200	2.44826600	3.25580400
H	0.01638800	3.93156600	2.36603700
H	-0.99545900	2.47979900	2.18548300
C	1.24801100	3.97521600	-0.88729600
H	0.87359700	4.18332900	-1.89564900
H	1.12174100	4.88282900	-0.28394900
H	2.31424600	3.74801700	-0.96396200
C	-1.04009200	3.10287600	-0.38850800
H	-1.29525600	4.03636500	0.12697000
H	-1.31041400	3.20420500	-1.44443900
H	-1.64393300	2.29651200	0.03300100
F	-1.86829200	0.45997600	-2.44177900
F	-4.52419900	0.27623100	-1.98186400
F	-5.45583100	-0.82835800	0.33350600
F	-3.69504800	-1.80380000	2.19687600

F	-1.01943300	-1.67657400	1.74561600
K	5.61649200	-1.62245000	-0.19876500
K	0.45353000	-2.92102000	-0.21376700
8			
C	5.27663600	1.00011600	-0.46195400
C	5.40606700	-0.48068100	0.08284100
O	4.12362500	-0.67871900	0.74640200
O	3.83438000	1.14029100	-0.63301200
B	3.24118600	0.20198900	0.18236900
C	-3.10863500	1.35634300	-0.42346400
C	-4.37302000	1.75597400	-0.03626100
C	-3.02269700	0.02479900	-0.71918100
C	-5.47480000	0.90413400	0.06419200
C	-4.04871500	-0.90520200	-0.61153400
C	-5.30537500	-0.45243300	-0.22182000
O	1.89177800	0.27594500	0.43221300
C	1.06562400	-0.83599600	0.76323300
O	1.37994000	-1.95077400	0.31481000
O	0.03991600	-0.49648300	1.40842900
C	5.49761700	-1.53551300	-1.02858300
H	6.46620600	-1.49763500	-1.53953600
H	5.37924300	-2.52811800	-0.58281300
H	4.70507100	-1.40857800	-1.77337500
C	6.51783300	-0.69971100	1.10688100
H	6.50898800	-1.74351300	1.43793600
H	7.50013300	-0.49181600	0.66590700
H	6.38874600	-0.06699400	1.98856800
C	5.95120700	1.25762500	-1.80756200
H	5.77862700	2.29543300	-2.11263500
H	7.03429900	1.10170600	-1.73613400
H	5.55559600	0.60653200	-2.59064200
C	5.70937700	2.06356700	0.55700400
H	6.79481400	2.06027400	0.70533400
H	5.41738500	3.05163200	0.18562200
H	5.22789800	1.91042000	1.52872800
F	-4.60299700	3.06369700	0.31317600
F	-6.69539600	1.34037300	0.44678400
F	-6.33777700	-1.31272000	-0.11097600
F	-3.84415100	-2.24808800	-0.83563000
F	-1.78009700	-0.51937500	-1.13495500
K	-1.19472100	-2.64939000	0.40126200
K	-0.40122600	1.89915500	0.28674400
9			
C	-4.83159700	0.03947600	0.36536300
C	-3.49213300	0.24315000	0.68414400

C	-2.43332400	-0.53403600	0.27153600
C	-2.82305300	-1.58400600	-0.52603000
C	-4.12916000	-1.88013400	-0.90604300
C	-5.15007300	-1.04698000	-0.44920900
C	-0.37872300	0.88334000	-1.84999700
H	-1.27348100	0.58003400	-2.42326600
C	-0.44116900	2.23293200	-1.25529700
C	0.62058800	2.74491200	-0.48514200
C	-1.59250300	3.00967300	-1.46242400
C	0.51966500	4.01975600	0.06988800
H	1.51168400	2.14438100	-0.32993100
C	-1.68897500	4.28654800	-0.90766900
H	-2.41496600	2.60399800	-2.04707200
C	-0.63356800	4.79065300	-0.14099000
H	1.34062500	4.41833400	0.66043400
H	-2.58369000	4.88211100	-1.06469900
H	-0.70650500	5.78474200	0.29266300
F	-1.85890200	-2.46842500	-1.03805700
F	-4.43643200	-2.93252400	-1.69759100
F	-6.43029900	-1.28964000	-0.79055800
F	-5.81969700	0.84875200	0.80924500
F	-3.24472100	1.35183000	1.51118600
O	0.57984300	0.12177200	-1.76178100
O	3.65752800	0.84274600	0.57060500
C	4.62415000	0.58634500	-0.48781100
C	4.65022600	-0.99420000	-0.54638300
O	3.32079500	-1.34269300	-0.05939500
B	2.87710000	-0.28772200	0.72954200
C	4.08528000	1.23626000	-1.76957700
H	3.94488600	2.30785800	-1.59133100
H	4.78897400	1.12321300	-2.60195000
H	3.12057900	0.81270200	-2.06457400
C	5.95184100	1.23396700	-0.09535100
H	5.83277500	2.32221900	-0.06045200
H	6.29170000	0.90220100	0.88859700
H	6.73099800	1.00304200	-0.83178500
C	5.65526100	-1.62696700	0.42654800
H	5.47767500	-2.70628700	0.46994000
H	6.68824300	-1.45871100	0.10277300
H	5.54061200	-1.22988100	1.44038800
C	4.83004000	-1.58777200	-1.94256100
H	5.79602600	-1.29241200	-2.36837800
H	4.81309300	-2.68189100	-1.88306500
H	4.04022100	-1.26755500	-2.62751400
C	1.30141900	-1.49565800	2.38753300

O	1.53720200	-2.59471600	1.88829000
O	0.70973000	-1.07937200	3.38076300
O	1.78250000	-0.29397100	1.53411200
K	0.76793500	-2.38861300	-0.62091400
K	-0.65111500	0.86371200	2.22826100
10-ts			
C	-4.54637200	-0.41225900	0.76349200
C	-3.33810500	0.25411600	0.57317800
C	-2.37179400	-0.11990500	-0.33549000
C	-2.67609700	-1.25320400	-1.05445500
C	-3.85607600	-1.98087500	-0.93371900
C	-4.80613100	-1.54372100	-0.01036800
C	-0.58362500	1.06853900	-1.27705500
H	-1.03388200	0.68935200	-2.20450900
C	-0.97613300	2.47374700	-0.94180800
C	-0.12585800	3.27618800	-0.16589300
C	-2.15157600	3.03132400	-1.46687100
C	-0.46165700	4.60508900	0.10757200
H	0.81990900	2.86415100	0.17869300
C	-2.48809300	4.35632200	-1.19500200
H	-2.81087600	2.41333700	-2.07218700
C	-1.64721400	5.14533100	-0.39992900
H	0.20746000	5.22231000	0.70212400
H	-3.40627000	4.77581800	-1.59775900
H	-1.91059400	6.17819900	-0.18761800
F	-1.75561900	-1.74898500	-1.98136500
F	-4.10047400	-3.08522100	-1.66895500
F	-5.95916200	-2.21708500	0.14230800
F	-5.45672000	-0.00721700	1.67205100
F	-3.10710800	1.34515100	1.40033900
O	0.47453200	0.55807700	-0.83552700
O	4.02001300	0.37935600	1.33521400
C	4.84093600	0.64420500	0.16679500
C	4.67583600	-0.68770000	-0.66440800
O	3.34898100	-1.13929700	-0.25567200
B	3.09113500	-0.58237300	0.99253600
C	4.24355600	1.87427700	-0.53299100
H	4.22527000	2.70725400	0.17799800
H	4.84292700	2.17960700	-1.39819300
H	3.21687900	1.68841700	-0.86576800
C	6.26656500	0.94184900	0.62838100
H	6.27687000	1.87010400	1.20943800
H	6.66248900	0.14491400	1.26248800
H	6.93545600	1.07288600	-0.23090000
C	5.66487900	-1.78797200	-0.25705100

H	5.36450100	-2.73152700	-0.72454600
H	6.68418900	-1.55188500	-0.58188700
H	5.67182100	-1.94027800	0.82686000
C	4.68288500	-0.50636700	-2.18128300
H	5.63773800	-0.08548700	-2.51738800
H	4.56110900	-1.47872500	-2.67344500
H	3.87881300	0.15521800	-2.51497800
C	1.15081400	-2.02615600	1.78849700
O	1.51918500	-2.95555800	1.05640000
O	0.15020500	-1.84525800	2.49447100
O	2.03232600	-0.83270200	1.80841200
K	0.95562400	-2.07751000	-1.33046900
K	-0.38773600	0.64195700	1.94486700
11			
C	-4.57005300	-0.52949400	0.97168100
C	-3.34564900	0.06554300	0.68935500
C	-2.79054200	0.11619700	-0.59074600
C	-3.55133400	-0.48849100	-1.59300200
C	-4.78212100	-1.10006400	-1.35250300
C	-5.29673900	-1.12143900	-0.06020900
C	-1.36341900	0.66500100	-0.86330400
H	-1.27959800	0.67893000	-1.96956100
C	-1.24796900	2.15370800	-0.45533700
C	-0.01404700	2.63591400	0.00206400
C	-2.30409900	3.06609200	-0.59744200
C	0.15914700	3.98645400	0.32670200
H	0.81757500	1.93902800	0.06898300
C	-2.13892400	4.41514400	-0.27074800
H	-3.26997500	2.72357800	-0.96319000
C	-0.90635900	4.88176200	0.19792500
H	1.12803600	4.33987400	0.67338000
H	-2.97477900	5.10218600	-0.38060700
H	-0.77771800	5.93057600	0.45311300
F	-3.10373500	-0.50559700	-2.87133500
F	-5.47150300	-1.66845300	-2.35561200
F	-6.47669500	-1.70542800	0.19250400
F	-5.05539500	-0.54118400	2.22434400
F	-2.68220500	0.61538900	1.74379100
O	-0.42919200	-0.15664300	-0.28967200
O	4.51886000	0.22993500	1.08804600
C	5.12505300	0.67400700	-0.15479700
C	4.69150900	-0.46229300	-1.16321400
O	3.43319400	-0.91895200	-0.57925000
B	3.47349000	-0.61306600	0.77892900
C	4.51917800	2.04516900	-0.48788100

H	4.69708500	2.72309500	0.35333700
H	4.97485900	2.48307400	-1.38293400
H	3.43759300	1.98093000	-0.64836300
C	6.63216400	0.80570000	0.05854100
H	6.83003200	1.59927800	0.78682400
H	7.06894500	-0.11885000	0.44345700
H	7.13784300	1.07128700	-0.87775000
C	5.64386300	-1.66566500	-1.17006300
H	5.18743100	-2.48338700	-1.73767200
H	6.60130500	-1.41513000	-1.63968800
H	5.83738900	-2.03203100	-0.15707100
C	4.42473400	0.00799000	-2.59197700
H	5.33166200	0.43590500	-3.03496200
H	4.12547000	-0.84331500	-3.21490000
H	3.63221200	0.75975800	-2.63348300
C	1.84176600	-2.28350400	1.77295800
O	2.19402500	-3.11587800	0.92493500
O	0.97067400	-2.27405100	2.65026200
O	2.56076600	-0.97988100	1.71918700
K	0.99258900	-2.07938200	-1.18248800
K	0.00159100	0.12966500	2.31128400
12-ts			
C	1.89045500	2.92142600	-0.25955200
C	2.13961800	2.72834400	1.29886300
O	2.23954700	1.61858200	-0.79508900
O	2.00559600	1.29308700	1.47715200
B	2.14545000	0.71290600	0.23655800
O	2.52961100	-0.62853100	0.06541200
C	3.63837400	-1.04055900	-0.62428700
O	4.68272500	-0.34817200	-0.59777600
O	3.49295300	-2.16249400	-1.22074000
C	3.56846900	3.08554500	1.73776300
H	3.75494900	4.16447600	1.68188900
H	3.70549900	2.76704900	2.77693800
H	4.31273800	2.56528100	1.12630100
C	1.12625000	3.43028200	2.20249300
H	1.35322500	3.20298200	3.25006100
H	1.17374400	4.51879400	2.07318000
H	0.10520500	3.09903500	1.99908700
C	2.78935300	3.96647100	-0.92377800
H	2.56979300	4.00469000	-1.99667800
H	2.60450300	4.96380200	-0.50576700
H	3.84893800	3.72641200	-0.80426400
C	0.42454900	3.18806200	-0.62443900
H	0.08546800	4.16240400	-0.25446700

H	0.32872600	3.18254800	-1.71613100
H	-0.22022400	2.39872600	-0.23396500
C	-3.89777800	-0.83607500	-1.79066000
C	-2.82175400	-0.93308100	-0.91654600
C	-2.47539500	0.06991900	-0.00799300
C	-3.30320200	1.19337000	-0.01905400
C	-4.39051400	1.33159000	-0.88340400
C	-4.69060000	0.31027100	-1.77783500
C	-1.17276300	-0.00880700	0.83901700
H	-1.15257800	0.93312300	1.42669800
C	-1.27863000	-1.13186400	1.90456200
C	-0.09042300	-1.70315000	2.38673100
C	-2.49301100	-1.56927700	2.45365200
C	-0.11709200	-2.69171100	3.37614200
H	0.85545600	-1.33823800	1.99749900
C	-2.52515200	-2.56273300	3.43844600
H	-3.43007100	-1.13537200	2.11119500
C	-1.33602200	-3.13279900	3.90204800
H	0.81773300	-3.10976400	3.74478500
H	-3.48067000	-2.89077400	3.84215700
H	-1.35862800	-3.90364800	4.66881200
F	-3.07300800	2.21828600	0.83327800
F	-5.15160000	2.44025900	-0.85716800
F	-5.73234900	0.42278200	-2.61893400
F	-4.18317800	-1.83734300	-2.64592600
F	-2.09523100	-2.08456200	-0.98485100
O	-0.10308700	-0.11906800	0.00354600
K	0.72419900	-2.32606400	-0.88250400
K	5.95106900	-2.00180100	-2.04595700
13			
C	-2.77645200	-1.03077300	-1.83590800
C	-2.02983700	-2.19903700	-1.08119300
O	-2.68870200	0.04941800	-0.89683100
O	-1.01744600	-1.50285700	-0.35248700
B	-1.49844500	-0.14750500	-0.04837100
O	-1.76316200	-0.10227800	1.40337600
C	-2.23819300	0.93610300	2.21767200
O	-2.21538600	0.63768700	3.44165100
O	-2.60966000	2.00371800	1.67569200
C	-2.95040000	-2.92977900	-0.08045500
H	-3.71029600	-3.54198100	-0.58090100
H	-2.33422300	-3.60262100	0.53090400
H	-3.45450000	-2.21857800	0.58143200
C	-1.36323300	-3.23042400	-1.99724400
H	-0.87672000	-4.00348100	-1.39032100

H	-2.09767100	-3.72590000	-2.64519800
H	-0.59764300	-2.76808700	-2.62553900
C	-4.25396400	-1.30244300	-2.13722800
H	-4.68806900	-0.44910400	-2.67307400
H	-4.37429700	-2.18898900	-2.77272800
H	-4.82945800	-1.44716700	-1.21913800
C	-2.05675700	-0.61884800	-3.13490100
H	-2.14281200	-1.38527600	-3.91441300
H	-2.51774300	0.29932500	-3.52199600
H	-0.99727700	-0.41752000	-2.95255100
C	3.08564400	-1.37432200	-1.37021600
C	2.21427100	-0.30935900	-1.15622300
C	1.66113500	-0.02602600	0.09672300
C	2.03336800	-0.89119800	1.12326600
C	2.89704700	-1.96778400	0.94724200
C	3.43191000	-2.21193300	-0.31234400
C	0.63845300	1.10578600	0.33083000
H	0.38521600	1.07042200	1.39600100
C	1.24214500	2.48616900	0.06825400
C	1.08385400	3.13974800	-1.16160200
C	1.95182200	3.13326200	1.08892100
C	1.62529100	4.41312800	-1.36442900
H	0.55136500	2.63679000	-1.96288200
C	2.49761600	4.40385000	0.88798200
H	2.06483100	2.64646100	2.05578200
C	2.33507400	5.04947200	-0.34126200
H	1.50174500	4.90433400	-2.32705900
H	3.03848600	4.89268400	1.69439600
H	2.75515400	6.03945900	-0.49971700
F	1.52251600	-0.73000200	2.38016300
F	3.20025100	-2.77628900	1.98073700
F	4.26691300	-3.24210400	-0.50670700
F	3.59176100	-1.60473100	-2.59186300
F	1.90565600	0.44573400	-2.22472900
O	-0.51162200	0.91133900	-0.44375500
K	-2.54950400	2.69329300	-0.72126700
K	-1.04484700	-1.65468800	3.26768700
14-ts			
C	1.48107000	3.56279300	-0.48309300
C	1.63257800	2.68805100	-1.78999800
O	0.82984900	2.65782700	0.42348300
O	1.80481600	1.36737600	-1.26742400
B	1.17347400	1.28001000	0.04602700
O	-0.00237100	0.37060400	-0.09034100
C	-0.88228100	-0.05335400	0.87674000

O	-1.57730800	-1.05392300	0.49078700
O	-0.94527300	0.52819200	1.97924000
C	0.36445900	2.71277500	-2.66496500
H	0.21412100	3.68229300	-3.15406000
H	0.46929500	1.95582900	-3.45270900
H	-0.52940900	2.48144200	-2.07838400
C	2.84659100	3.04130100	-2.65551900
H	2.87793700	2.38319100	-3.53200900
H	2.79259100	4.07665800	-3.01534700
H	3.78284400	2.91072900	-2.10659100
C	0.60715300	4.81049600	-0.64488000
H	0.55678500	5.35689800	0.30520700
H	1.02381300	5.49175500	-1.39744100
H	-0.41386900	4.55137500	-0.93600400
C	2.84210600	3.96487500	0.11702300
H	3.36585200	4.69961000	-0.50564200
H	2.67645800	4.42520100	1.10016500
H	3.48871200	3.09293000	0.25122800
C	5.42859900	-0.65892300	-1.35313400
C	4.62318100	-0.38620000	-0.25071100
C	3.36170500	-0.96329800	-0.07538300
C	2.95200400	-1.82868800	-1.08844200
C	3.72752200	-2.12098800	-2.20635200
C	4.97981800	-1.53264900	-2.34076200
C	2.43241400	-0.61448700	1.10444200
H	1.53372800	-1.22619300	0.96929800
C	3.03685600	-1.01416500	2.45104900
C	3.72332600	-0.09479000	3.25600500
C	2.88384000	-2.32936200	2.91078800
C	4.24596600	-0.48434500	4.49320000
H	3.86320600	0.92040800	2.89778300
C	3.40847000	-2.72281600	4.14470700
H	2.33696800	-3.04938300	2.30479200
C	4.09218700	-1.79989800	4.94167200
H	4.78464600	0.23813000	5.10223600
H	3.27398800	-3.74588000	4.48682200
H	4.49930400	-2.10212500	5.90314400
F	1.72348100	-2.41763300	-1.03833000
F	3.26473900	-2.95281300	-3.15895200
F	5.74444300	-1.80104300	-3.40801600
F	6.63357800	-0.08036700	-1.47546100
F	5.10451900	0.48633000	0.65218000
O	2.09280500	0.74762000	1.10217700
C	-4.06972800	-3.46346200	0.54778100
C	-3.91110800	-3.35999200	-1.02222800

O	-3.39140100	-2.01037400	-1.20493300
O	-4.24832000	-2.07626100	0.92716800
B	-3.67629300	-1.28333900	-0.03837900
C	-3.92206600	0.28673500	-0.05176700
C	-3.59245800	1.09632800	-1.14052600
C	-4.46497900	0.96592200	1.04674300
C	-3.78061100	2.47384800	-1.16985000
C	-4.66557100	2.34606400	1.05911000
C	-4.32333200	3.10548600	-0.05493600
C	-2.81675800	-3.98492800	1.26803200
H	-2.96465100	-3.87018600	2.34691100
H	-2.64545700	-5.04716700	1.05598000
H	-1.93100000	-3.40535300	0.99754600
C	-5.29813100	-4.24521100	1.01700100
H	-5.24159800	-5.29288300	0.69650100
H	-5.34110600	-4.22747800	2.11095600
H	-6.22723800	-3.81192500	0.63851200
C	-5.24448700	-3.42364900	-1.78164800
H	-5.07030400	-3.16866500	-2.83279500
H	-5.68759900	-4.42498400	-1.73985900
H	-5.96695300	-2.70747400	-1.37779000
C	-2.91987200	-4.35154600	-1.63324700
H	-3.25703900	-5.38384000	-1.48287300
H	-2.84467600	-4.18444400	-2.71495800
H	-1.92372400	-4.25556700	-1.19127300
F	-4.82153700	0.30379200	2.15750600
F	-5.18383600	2.95330300	2.14085100
F	-4.50948100	4.43408300	-0.05425500
F	-3.43650700	3.19639200	-2.25146000
F	-3.02811900	0.55116000	-2.25660200
K	0.72278300	2.10386900	3.01686000
K	-0.80574100	-1.17676900	-2.03249700
15			
C	1.47875000	3.70467900	-0.03358300
C	1.72915200	3.00949800	-1.42837700
O	0.86344200	2.64946500	0.73117400
O	1.98688700	1.64925600	-1.05477600
B	1.29023300	1.36352100	0.18177200
O	0.12384900	0.44884600	-0.17639500
C	-0.82342500	-0.01879400	0.64069200
O	-1.47788000	-0.99276800	0.04567300
O	-1.03420000	0.39207700	1.78408600
C	0.48697500	3.04791200	-2.33956900
H	0.28251600	4.05545700	-2.71961200
H	0.67104900	2.39779800	-3.20427500

H	-0.40534600	2.68829800	-1.81855400
C	2.93846200	3.54393100	-2.20150200
H	3.03739100	3.00333800	-3.14997500
H	2.82341200	4.61015000	-2.43376500
H	3.86612700	3.40598200	-1.63997000
C	0.52487000	4.90149800	-0.07403100
H	0.41069000	5.32276200	0.93237100
H	0.91423000	5.69546200	-0.72324900
H	-0.46712700	4.61330200	-0.43070100
C	2.78864600	4.10975200	0.66672800
H	3.28054800	4.95084500	0.16459700
H	2.56231900	4.42630300	1.69330000
H	3.48914400	3.27053400	0.71263200
C	5.57570200	-0.34516200	-1.27290300
C	4.72416900	-0.23745500	-0.17667200
C	3.46235600	-0.83826000	-0.14043900
C	3.09868300	-1.54772300	-1.28461600
C	3.92212100	-1.67224600	-2.39939600
C	5.17450700	-1.06819300	-2.39403600
C	2.48217500	-0.67226400	1.03428300
H	1.60261600	-1.27031000	0.77291300
C	3.02709000	-1.24425300	2.34258200
C	3.65575200	-0.43576400	3.29950000
C	2.87216100	-2.61133200	2.61028300
C	4.12015900	-0.98558000	4.49856600
H	3.79768100	0.61994800	3.09024300
C	3.33936400	-3.16403100	3.80559500
H	2.36997200	-3.24774500	1.88406700
C	3.96516000	-2.35136800	4.75541400
H	4.61480400	-0.34803200	5.22777700
H	3.20513200	-4.22538400	3.99792200
H	4.32708200	-2.77780000	5.68736700
F	1.87463900	-2.13835300	-1.36936500
F	3.50534600	-2.35670400	-3.48092500
F	5.98401000	-1.17745200	-3.45561700
F	6.77872600	0.24902600	-1.26078300
F	5.15873200	0.49713100	0.86229500
O	2.11174000	0.67537000	1.20952200
C	-3.54583200	-3.56089300	0.25083300
C	-3.82668500	-3.16267500	-1.24866500
O	-3.08700800	-1.93631600	-1.37840800
O	-3.46080800	-2.28477400	0.89323800
B	-2.99713900	-1.30800300	-0.04078100
C	-3.78440900	0.14374800	0.05598900
C	-3.69283900	1.08346800	-0.96940900

C	-4.58446100	0.54357300	1.13102300
C	-4.34192700	2.31404300	-0.97800200
C	-5.25593700	1.76753800	1.17100800
C	-5.13692400	2.65949600	0.11001100
C	-2.20634200	-4.30212300	0.43269200
H	-1.98315600	-4.35798900	1.50371700
H	-2.24459000	-5.32399500	0.03523100
H	-1.38320000	-3.76653700	-0.05069900
C	-4.66222900	-4.36864300	0.91967200
H	-4.82832800	-5.32252300	0.40221200
H	-4.38398300	-4.58903600	1.95637800
H	-5.60183200	-3.81083000	0.93981900
C	-5.31268900	-2.86481500	-1.51895300
H	-5.40850900	-2.40079300	-2.50736100
H	-5.92190500	-3.77627800	-1.50778700
H	-5.71725000	-2.16883900	-0.77784900
C	-3.31390100	-4.16184800	-2.29032400
H	-3.80755400	-5.13531600	-2.18085800
H	-3.53126200	-3.79170900	-3.30015600
H	-2.23369600	-4.31824800	-2.20592600
F	-4.74467300	-0.24473900	2.21043200
F	-6.01360900	2.10261100	2.23315200
F	-5.77651900	3.84150600	0.13650800
F	-4.20273600	3.16966200	-2.01065300
F	-2.90171900	0.83402900	-2.06398200
K	0.59412200	1.74635000	3.20938700
K	-0.76476900	-0.89373800	-2.44852300
16-ts			
C	1.74961600	-3.46780700	-1.39753700
C	2.01912300	-3.40549000	0.16252000
O	1.27412000	-2.12794100	-1.69321700
O	2.33988800	-2.01158200	0.36008300
B	1.76417300	-1.27282800	-0.67168700
O	-1.99581800	-0.07607300	0.93371500
C	-0.61411700	-0.01434200	0.87375800
O	-0.08957700	-0.76195200	-0.00844400
O	-0.03394200	0.70935700	1.71292900
C	0.78774700	-3.74545500	1.01768600
H	0.54018900	-4.81222400	0.96150400
H	1.01287100	-3.50212800	2.06158300
H	-0.08347700	-3.15515400	0.72332800
C	3.21080500	-4.24202300	0.63476100
H	3.33731000	-4.11704100	1.71561400
H	3.04738000	-5.30833500	0.43508800
H	4.14048500	-3.93390300	0.15018200

C	0.68021300	-4.47626100	-1.82222100
H	0.53136200	-4.42595300	-2.90810600
H	0.98755900	-5.50050600	-1.58025300
H	-0.27815100	-4.28981600	-1.32761000
C	3.02337300	-3.68740800	-2.22855200
H	3.42350500	-4.69995800	-2.10354200
H	2.78646500	-3.54054300	-3.28811000
H	3.80272200	-2.96819200	-1.95949500
C	6.42656500	-0.40381100	-0.00347200
C	5.18136000	0.02803700	-0.45435200
C	4.15316200	0.39351600	0.41952500
C	4.44907500	0.32003200	1.78206900
C	5.68604800	-0.10353700	2.26292700
C	6.68191700	-0.47098700	1.36375100
C	2.76983300	0.85703000	-0.05973000
H	2.10582300	0.87253200	0.81021700
C	2.85620900	2.27237000	-0.62499300
C	2.94461100	2.51352800	-2.00098500
C	2.87137600	3.35988000	0.25965400
C	3.05305800	3.82166200	-2.48264000
H	2.92483300	1.67354600	-2.68711300
C	2.98172800	4.66725300	-0.22057500
H	2.79123000	3.18102400	1.33007700
C	3.07427300	4.90260700	-1.59617300
H	3.12305400	3.99569800	-3.55396400
H	2.99186900	5.50059400	0.47810100
H	3.16042300	5.91880700	-1.97314700
F	3.52095500	0.66776800	2.69683800
F	5.92247800	-0.16172400	3.58484700
F	7.87949100	-0.88041500	1.80897200
F	7.38486000	-0.75281300	-0.87930100
F	4.99711800	0.07566600	-1.78703300
O	2.23723300	-0.02197000	-1.03905600
C	-2.40794700	2.27768200	-1.61406700
C	-3.25915800	2.97820900	-0.48841000
O	-3.10576400	2.07244900	0.61194200
O	-2.58362200	0.87747200	-1.31276000
B	-2.95711800	0.69310800	0.09424800
C	-4.35428200	-0.21054900	0.27337300
C	-5.13626000	-0.12803400	1.42419200
C	-4.80608100	-1.15436700	-0.64533500
C	-6.29596000	-0.86626500	1.64441400
C	-5.95827000	-1.92160600	-0.48285400
C	-6.71783500	-1.77065500	0.67330500
C	-0.91213400	2.61875600	-1.52756800

H	-0.34583300	1.96585300	-2.20086200
H	-0.71099900	3.65286000	-1.82961100
H	-0.51674300	2.46870600	-0.51973300
C	-2.90734500	2.53557700	-3.04012500
H	-2.88944500	3.60657400	-3.27683600
H	-2.25357400	2.03186500	-3.76339300
H	-3.92429100	2.16252800	-3.18752600
C	-4.75461200	3.08643300	-0.84298300
H	-5.30918900	3.39625700	0.04993200
H	-4.93338300	3.82881100	-1.62949100
H	-5.16256100	2.12760500	-1.17617800
C	-2.74555200	4.35822500	-0.06556500
H	-2.76760400	5.06458500	-0.90435700
H	-3.38839200	4.76406200	0.72532400
H	-1.72027900	4.31048600	0.31226500
F	-4.09312600	-1.41089300	-1.78686900
F	-6.33453800	-2.81322900	-1.41854000
F	-7.83189400	-2.49675000	0.85657300
F	-7.00332800	-0.72719000	2.78090400
F	-4.76604700	0.70132900	2.45009000
K	-2.10589500	1.67069500	3.00688600
K	-1.27650100	-1.24948800	-2.24053600
17			
C	-4.00064800	-0.33220600	-0.79214500
C	-3.71036500	-0.34294100	0.76461900
O	-2.92200500	0.50349600	-1.30547900
O	-2.26370400	-0.14139000	0.80776100
B	-1.90990000	0.46139700	-0.37944500
C	-4.34511300	0.83778900	1.51186900
H	-5.43429300	0.73613800	1.57105600
H	-3.94744300	0.86803800	2.53165300
H	-4.11330500	1.79328400	1.02944100
C	-4.03728400	-1.65344200	1.47647400
H	-3.77480400	-1.57174900	2.53663100
H	-5.10913400	-1.87440400	1.40871300
H	-3.48062000	-2.49418300	1.05564800
C	-5.33273600	0.29644100	-1.19573400
H	-5.43252700	0.27563500	-2.28612200
H	-6.17307300	-0.26274800	-0.76725200
H	-5.40350300	1.33755300	-0.87198300
C	-3.84743200	-1.71066900	-1.45008900
H	-4.66239100	-2.38583000	-1.16672400
H	-3.86548800	-1.58659900	-2.53765100
H	-2.89700400	-2.18345300	-1.18061600
C	2.60390000	-1.72384700	-1.28367300

C	1.81963700	-0.58738800	-1.10061400
C	1.23235400	-0.27803700	0.13173000
C	1.48173100	-1.16563600	1.18086100
C	2.26668900	-2.30710600	1.02775300
C	2.82783200	-2.58912600	-0.21415000
C	0.35641800	0.95886900	0.33848800
H	-0.08988000	0.87227000	1.33266000
C	1.16695500	2.25028300	0.28342600
C	1.12947700	3.09801200	-0.82874000
C	1.97120900	2.59033400	1.38061400
C	1.89372100	4.26909800	-0.84315700
H	0.50115500	2.84036200	-1.67427800
C	2.73623700	3.75831200	1.36375600
H	1.99648300	1.94333600	2.25573400
C	2.69989000	4.60182000	0.24864500
H	1.85702700	4.92183400	-1.71173400
H	3.35323000	4.01202600	2.22201600
H	3.29229800	5.51306500	0.23379300
F	0.96585600	-0.92921200	2.40495000
F	2.47980000	-3.13274800	2.06353200
F	3.58235200	-3.68252700	-0.38007600
F	3.14727000	-1.99046000	-2.48045900
F	1.64297400	0.22024100	-2.15786800
O	-0.67758300	0.98132300	-0.64404000
18			
C	2.23586900	-0.89264300	-1.34664000
C	2.58542700	0.61772200	-1.06332100
O	1.36882900	1.11524500	-0.49251100
O	1.36497800	-1.20841700	-0.25634100
B	0.62298700	0.00728200	0.15995600
C	-0.97174600	-0.00315100	-0.35230900
C	-1.72148100	-1.17293100	-0.48610700
C	-1.68210000	1.15210900	-0.68207100
C	-3.03954100	-1.20463100	-0.93223400
C	-2.99966000	1.15355800	-1.13031100
C	-3.70415400	-0.03400200	-1.26912600
O	0.68595400	0.11536700	1.63626400
C	-0.41534000	0.19683700	2.55383800
O	-0.78394900	1.35928100	2.83422300
O	-0.82029800	-0.90321300	2.99105200
C	3.71820500	0.77429900	-0.02898800
H	4.69137400	0.46584400	-0.42934200
H	3.80148900	1.83235400	0.25223300
H	3.50838500	0.19714500	0.87670200
C	2.92084000	1.44027000	-2.31152900

H	3.15483800	2.47352500	-2.02689800
H	3.79646900	1.03223000	-2.83222100
H	2.08001000	1.46849300	-3.00894400
C	3.43466300	-1.84664900	-1.31164300
H	3.09930800	-2.86954800	-1.52211100
H	4.17839500	-1.57893200	-2.07234000
H	3.92523800	-1.84261500	-0.33345600
C	1.47616800	-1.08756900	-2.67312000
H	2.12914300	-0.94518200	-3.54243900
H	1.08028000	-2.10875500	-2.70743600
H	0.63245200	-0.39656700	-2.75787000
F	-1.17662200	-2.38804500	-0.15993300
F	-3.68079300	-2.39191300	-1.03449200
F	-3.60164100	2.32821300	-1.42930800
F	-1.09622900	2.38538700	-0.55728100
K	0.70624300	2.89049100	1.41887200
K	0.66167000	-2.65403100	1.84669300
H	-4.73211600	-0.04533900	-1.61240900
19-ts			
C	0.12417100	2.78847800	-0.29409900
C	0.63787500	2.37005800	1.15225300
O	0.65748300	0.92253600	1.08506500
O	0.45936900	1.63218700	-1.09939700
B	0.63969800	0.55668700	-0.25483900
C	-1.50837300	-0.62278100	-0.30314000
C	-2.49882400	-0.23715600	-1.19568800
C	-2.00704700	-1.22972100	0.83238700
C	-3.86466700	-0.39289000	-0.95509300
C	-3.35565200	-1.41442600	1.12704600
C	-4.31844600	-0.98115100	0.22286300
O	1.33629500	-0.60868800	-0.68988300
C	2.66490300	-0.83501400	-0.48407400
O	3.46492900	0.12150600	-0.35622000
O	2.97599600	-2.08041400	-0.46218100
C	2.07973200	2.81656700	1.44525500
H	2.15567000	3.90623600	1.54276700
H	2.39807000	2.36544800	2.39222100
H	2.76508100	2.47270900	0.66563700
C	-0.27464400	2.79245600	2.30569300
H	0.14230000	2.42794100	3.25131200
H	-0.34983700	3.88544600	2.36660400
H	-1.27991300	2.37794400	2.20134500
C	0.83976800	3.99875000	-0.90046400
H	0.43938100	4.19026600	-1.90210100
H	0.67746300	4.89719200	-0.29195800

H	1.91477400	3.82593100	-0.99466000
C	-1.39325100	3.00928800	-0.37184800
H	-1.68724200	3.93014100	0.14592400
H	-1.68408600	3.09386400	-1.42373000
H	-1.94904400	2.17434400	0.05943100
F	-2.16286500	0.33525600	-2.39446600
F	-4.78063800	0.02186600	-1.87314300
F	-3.74712700	-2.02836900	2.27988300
F	-1.10621700	-1.77114500	1.76553200
K	5.47290900	-1.42247700	-0.21026600
K	0.36403200	-2.92031000	-0.23513700
H	-5.37723100	-1.10819700	0.41819300
20			
C	2.14090500	-1.11386400	-1.19806800
C	2.48651400	0.42358600	-1.18342000
O	1.27151300	1.00991900	-0.70443600
O	1.27462500	-1.23776900	-0.06802300
B	0.52248800	0.02920800	0.13097900
C	-1.06495900	-0.07197100	-0.36804500
C	-1.83110100	-1.23877000	-0.30657100
C	-1.79666700	0.99001900	-0.90559600
C	-3.14112200	-1.39791200	-0.74686200
C	-3.10509900	0.94525800	-1.37568400
C	-3.75457500	-0.27716300	-1.28658700
O	0.59876100	0.38748700	1.57079400
C	-0.49425900	0.63866900	2.46483400
O	-0.87738200	1.82950800	2.51508300
O	-0.88018800	-0.35628100	3.11886500
C	3.62364900	0.76214100	-0.19813900
H	4.59512300	0.38441100	-0.53886100
H	3.70958700	1.85361300	-0.11318100
H	3.41611500	0.35948200	0.79804100
C	2.81388600	1.01776400	-2.55760200
H	3.04006800	2.08662200	-2.45772500
H	3.69165400	0.53270800	-3.00361500
H	1.97123400	0.91833700	-3.24633900
C	3.34251900	-2.04487200	-1.00164900
H	3.00823300	-3.08938000	-1.02743100
H	4.08335800	-1.91486300	-1.80047500
H	3.83703800	-1.86928600	-0.04138800
C	1.37835100	-1.53789000	-2.46836400
H	2.02738200	-1.54520800	-3.35219100
H	0.98696500	-2.55111100	-2.32355200
H	0.53131500	-0.87450300	-2.66497400
F	-1.27284000	-2.37323100	0.24453300

F	-1.20373200	2.23242300	-0.98584700
K	0.61074500	3.07726400	0.85519700
K	0.58093500	-2.28174200	2.25813500
F	-5.03304700	-0.37722900	-1.73247100
H	-3.59463700	1.82406100	-1.77846400
H	-3.65811800	-2.34640100	-0.66173700
21-ts			
C	-0.08195000	2.71444500	-0.46642300
C	0.43722900	2.39517200	1.00472600
O	0.53324100	0.94986600	1.01157600
O	0.31133500	1.53454400	-1.20787800
B	0.54114700	0.51559000	-0.30726400
C	-1.58923500	-0.77025800	-0.30856700
C	-2.60253800	-0.44491800	-1.20462400
C	-2.12431800	-1.28718800	0.85599300
C	-3.98125200	-0.55007500	-0.99317600
C	-3.46570400	-1.44767500	1.21043900
C	-4.37890800	-1.04903000	0.24175500
O	1.29012200	-0.63620200	-0.68013100
C	2.61152100	-0.82072700	-0.39982700
O	3.38419700	0.16065100	-0.28885200
O	2.94861100	-2.05481900	-0.29626700
C	1.84970100	2.93346500	1.28473000
H	1.86634900	4.02953300	1.31526600
H	2.18040300	2.55795900	2.26008800
H	2.56158600	2.58034600	0.53357100
C	-0.50921100	2.82614200	2.12742400
H	-0.08485900	2.53056100	3.09365400
H	-0.64112700	3.91546800	2.13339400
H	-1.49058700	2.35542200	2.03418000
C	0.58589000	3.92166000	-1.13131200
H	0.18990900	4.03873600	-2.14614800
H	0.37524700	4.84424400	-0.57596400
H	1.66880000	3.79415400	-1.20512900
C	-1.60649100	2.86570400	-0.56539900
H	-1.94325600	3.79645200	-0.09331900
H	-1.89033100	2.88963100	-1.62243800
H	-2.13024400	2.02842300	-0.10051000
F	-2.25232500	0.03868700	-2.44603000
F	-1.21594400	-1.78386100	1.82199800
K	5.41185200	-1.32333500	0.04637900
K	0.33280300	-2.93652900	-0.13529200
F	-5.71320100	-1.17021600	0.50612600
H	-4.70703700	-0.26036800	-1.74575100
H	-3.78424600	-1.85520000	2.16388800

22

C	2.25218800	-0.89522500	-0.86253000
C	2.48956800	0.63543900	-0.57535400
O	1.16020000	1.11848100	-0.35874100
O	1.14472400	-1.19122600	-0.00995600
B	0.28684700	0.01648800	0.13792600
C	-1.11692400	-0.06926400	-0.75556900
C	-1.80386300	-1.25647900	-1.02440400
C	-1.75363700	1.02907900	-1.34029500
C	-2.94838200	-1.39023300	-1.80138300
C	-2.89573000	0.99668600	-2.13134800
C	-3.49737300	-0.23980400	-2.36867100
O	-0.01611700	0.19127700	1.58189900
C	-1.30266200	0.28871100	2.20720700
O	-1.75758900	1.45071400	2.30981700
O	-1.77188700	-0.79499500	2.62235800
C	3.32066900	0.87009200	0.70271000
H	4.36856100	0.57150500	0.57714700
H	3.31203800	1.94146900	0.94330800
H	2.89704200	0.32764000	1.55343900
C	3.11570200	1.41535500	-1.73646800
H	3.24422400	2.46735400	-1.45278300
H	4.10518300	1.01781000	-1.99616100
H	2.48101800	1.38491100	-2.62562100
C	3.42303600	-1.80949400	-0.48475300
H	3.16877400	-2.85069700	-0.71849900
H	4.32748400	-1.55440100	-1.05108100
H	3.65577600	-1.74708200	0.58275100
C	1.85159200	-1.16823700	-2.32543700
H	2.69677200	-1.03894000	-3.01217100
H	1.49906600	-2.20252500	-2.40768400
H	1.03909600	-0.50985000	-2.64584700
F	-1.33257300	-2.43567500	-0.47407400
F	-1.23165200	2.29164500	-1.12067800
K	-0.00630100	2.94623200	1.20178400
K	-0.04347300	-2.55004200	1.91336700
H	-3.29907100	1.91973300	-2.53486600
H	-3.39296100	-2.36995500	-1.94271700
H	-4.39327600	-0.30451300	-2.97918700

23-ts

C	-0.59147600	2.61627100	-0.46004900
C	0.00057900	2.36578000	0.99684600
O	0.25220100	0.93934100	1.00736800
O	-0.09819700	1.47827000	-1.20697700
B	0.26379200	0.49739200	-0.30836600

C	-1.74745200	-1.00132000	-0.23540400
C	-2.80497500	-0.78552200	-1.11370300
C	-2.20863300	-1.55742900	0.94379500
C	-4.15897000	-1.02440700	-0.86650600
C	-3.52106700	-1.84069300	1.31949000
C	-4.51672400	-1.55039500	0.38014900
O	1.10946600	-0.57930400	-0.69576300
C	2.44701300	-0.63432800	-0.43715400
O	3.12550400	0.41767400	-0.35800100
O	2.90136200	-1.82854000	-0.31893200
C	1.35426500	3.05398100	1.23548400
H	1.25461500	4.14568900	1.26699000
H	1.75127700	2.71807700	2.20047500
H	2.07856000	2.77789800	0.46420500
C	-0.95521000	2.69894100	2.14466900
H	-0.47672000	2.45045400	3.09882200
H	-1.19899000	3.76876500	2.15519500
H	-1.88440100	2.12857300	2.07692800
C	-0.07429400	3.88143700	-1.15170300
H	-0.50630200	3.94387600	-2.15667400
H	-0.36957600	4.78204500	-0.59876600
H	1.01389300	3.87103300	-1.25328300
C	-2.12573700	2.60479900	-0.51458400
H	-2.54519400	3.49523000	-0.03094200
H	-2.44061700	2.59727400	-1.56303000
H	-2.54333000	1.71629300	-0.03753500
F	-2.52126100	-0.28090000	-2.36845300
F	-1.22902800	-1.95230500	1.89674800
K	5.28756600	-0.86133200	-0.02872800
K	0.37623900	-2.94657200	-0.07568600
H	-4.90485900	-0.80447800	-1.62562500
H	-3.75278800	-2.26662400	2.29185100
H	-5.56085200	-1.74425300	0.61288100
24			
C	2.18119800	-0.24902100	-1.26275800
C	2.51853400	0.69289500	-0.04181300
O	1.22026900	1.06100500	0.43738300
O	0.99098700	-0.90424000	-0.82391200
B	0.22114700	0.00113200	0.07864200
C	-1.08655300	0.69968500	-0.63069400
C	-2.06563000	0.00913600	-1.34170900
C	-1.30101600	2.09219000	-0.57973400
C	-3.18122700	0.57430300	-1.94566500
C	-2.40720500	2.71892200	-1.16278700
C	-3.35811500	1.95630600	-1.84612500

O	-0.14081500	-0.79753800	1.28714600
C	-1.41267700	-1.00632100	1.91013000
O	-1.81757800	-0.07250500	2.64390400
O	-1.91982600	-2.12931800	1.69742800
C	3.26781800	-0.05061800	1.08245400
H	4.29149700	-0.31767700	0.79383200
H	3.33676900	0.60400600	1.96181600
H	2.73269100	-0.95872100	1.37591600
C	3.29051100	1.96460000	-0.41056600
H	3.47716800	2.56199000	0.49090800
H	4.26442700	1.72571100	-0.85653400
H	2.72769600	2.58420300	-1.11345200
C	3.24701100	-1.30946800	-1.56346400
H	2.93337800	-1.91319600	-2.42393700
H	4.20996900	-0.84813600	-1.81602500
H	3.39895300	-1.98184900	-0.71355700
C	1.87991000	0.53848700	-2.55295700
H	2.78526700	0.98677700	-2.97996600
H	1.45758600	-0.14961000	-3.29393300
H	1.14673100	1.33046300	-2.37711800
F	-1.93712100	-1.36487700	-1.49995700
K	0.11457500	1.53679600	2.78957400
K	-0.39628400	-3.07701600	-0.14963800
H	-0.54652100	2.70590900	-0.09102000
H	-2.52233400	3.79812700	-1.09185100
H	-4.22426900	2.42671800	-2.30419100
H	-3.88783800	-0.05809600	-2.47473700
25-ts			
C	-0.62447200	2.55692500	-0.46082000
C	0.10154600	2.27489700	0.93015400
O	0.44578400	0.86481400	0.84070600
O	-0.13537100	1.48258300	-1.30755400
B	0.34387000	0.48770000	-0.49773100
C	-1.91798300	-1.03698700	-0.38376900
C	-2.49417700	-1.02403500	-1.67864900
C	-2.83241500	-1.43107500	0.57082300
C	-3.83231800	-1.35450000	-1.93950900
C	-4.17391000	-1.77120200	0.41441900
C	-4.68237600	-1.72465400	-0.88805300
O	1.07728200	-0.62041400	-0.93820800
C	2.40433000	-0.76867300	-0.59486400
O	3.22641900	0.10767400	-0.95236300
O	2.68041500	-1.84030300	0.04147000
C	1.42810900	3.03180700	1.09780000
H	1.26903500	4.11176700	1.19707800

H	1.92465900	2.67525000	2.00762400
H	2.10081000	2.84818800	0.25440900
C	-0.77712300	2.48280300	2.16413800
H	-0.20312300	2.24268800	3.06691600
H	-1.10309600	3.52723000	2.24146600
H	-1.66036700	1.84056000	2.14262900
C	-0.23161400	3.88048900	-1.12308900
H	-0.75069000	3.96857300	-2.08344600
H	-0.52646100	4.73345200	-0.49928600
H	0.84260900	3.93850000	-1.31605000
C	-2.15381300	2.45479300	-0.39431800
H	-2.57985800	3.28023500	0.18841500
H	-2.55418000	2.50996300	-1.41193800
H	-2.47645700	1.50369200	0.03263800
F	-2.36203000	-1.53926300	1.93042900
K	5.20223600	-1.37534500	-0.34319200
K	0.17786600	-2.04870600	1.22920100
H	-1.87302700	-0.72840100	-2.52680400
H	-4.21736000	-1.32165100	-2.95836500
H	-5.72364900	-1.97795600	-1.07553200
H	-4.79078300	-2.05861000	1.26288500
26			
C	-2.10667900	-1.24804700	-0.95217600
C	-2.22453600	-1.33643100	0.62094100
O	-0.93698200	-0.88960200	1.05381100
O	-1.26170300	-0.10886200	-1.13652100
B	-0.35211100	0.04960000	0.04651600
C	1.21077400	-0.35049600	-0.23406000
C	2.07417700	0.44090900	-1.02053700
C	1.75792200	-1.54481700	0.27559400
C	3.39408300	0.07063500	-1.29416100
C	3.07890700	-1.94281000	0.02601300
C	3.87100700	-1.12093700	-0.76215700
O	-0.51954300	1.46349200	0.52555000
C	0.42506500	2.52042800	0.64193200
O	1.11007600	2.53173200	1.68977700
O	0.40650600	3.34808300	-0.30426100
C	-3.29864100	-0.38796000	1.19093700
H	-4.31574400	-0.71554200	0.94375400
H	-3.21153200	-0.36971000	2.28422200
H	-3.15429600	0.63495200	0.83108200
C	-2.46661700	-2.75043700	1.16122400
H	-2.53455700	-2.72327000	2.25583600
H	-3.40725700	-3.16898100	0.78094600
H	-1.65170500	-3.42750300	0.89143600

C	-3.43663700	-0.99916400	-1.67502200
H	-3.26422600	-0.94042600	-2.75691400
H	-4.14700900	-1.81596300	-1.49735300
H	-3.90692500	-0.06529600	-1.34951200
C	-1.42704300	-2.48323000	-1.57287200
H	-2.07034700	-3.37057300	-1.53224700
H	-1.20383300	-2.27020600	-2.62441100
H	-0.48200800	-2.71165100	-1.07398800
K	0.53050600	0.37485100	2.90416900
K	-1.43635500	2.42257800	-1.81179000
H	3.48418800	-2.87063400	0.42045900
H	4.04885700	0.69473300	-1.89540200
H	1.72690800	1.39270000	-1.41491200
H	1.12348700	-2.19930600	0.87048700
F	5.16001700	-1.49300800	-1.02022500
27-ts			
C	-0.45211200	2.61635100	-0.76955600
C	0.17186100	2.50828700	0.69199400
O	0.54912300	1.11016900	0.78927700
O	0.13014300	1.47413200	-1.45086400
B	0.57829100	0.59693200	-0.48869700
C	-1.66393800	-1.02537100	-0.13635900
C	-2.67254500	-1.26542800	-1.10426100
C	-2.15766200	-0.99726200	1.19204500
C	-4.03722900	-1.44876200	-0.80865900
C	-3.50866200	-1.17343700	1.54368200
C	-4.42354400	-1.39755300	0.52319800
O	1.37806800	-0.50392800	-0.85788200
C	2.61560600	-0.77923000	-0.33904000
O	3.38959600	0.15571700	-0.03187800
O	2.87449100	-2.03087100	-0.25088300
C	1.46446300	3.32017600	0.87248500
H	1.27256800	4.39934000	0.84605600
H	1.90039400	3.07172000	1.84642000
H	2.20395600	3.06948600	0.10618600
C	-0.80266000	2.82700900	1.82673400
H	-0.29603000	2.69313900	2.78948700
H	-1.14687300	3.86705100	1.76776300
H	-1.67208900	2.16644700	1.80733900
C	-0.04577500	3.87432400	-1.54236800
H	-0.48843400	3.84068800	-2.54390900
H	-0.41255900	4.77843800	-1.04072100
H	1.03860600	3.95140200	-1.65651000
C	-1.97841700	2.46521700	-0.80806400
H	-2.47508700	3.32805200	-0.34856900

H	-2.29808400	2.40358300	-1.85415800
H	-2.30498300	1.55134100	-0.30891500
K	5.19068900	-1.44307800	0.76705700
K	0.30508400	-2.86782000	-0.75739100
H	-4.78404700	-1.61584600	-1.58272100
H	-3.85118500	-1.13486900	2.57627100
H	-1.46299700	-0.79878700	2.01325800
H	-2.40712700	-1.28090500	-2.16741600
F	-5.75053800	-1.57283900	0.84186900
28			
C	-2.59640000	-1.20318400	-0.35307100
C	-2.79583400	-0.48706500	1.04172800
O	-1.52667900	0.07929200	1.27191000
O	-1.71079200	-0.34550600	-1.02649500
B	-0.94434400	0.49788200	-0.05378700
C	0.69080200	0.08292100	0.00501800
C	1.36716800	-0.72112500	-0.91550400
C	1.48846900	0.53253200	1.06024600
C	2.71985600	-1.04701500	-0.81232100
C	2.84315800	0.23361000	1.20071500
C	3.46921000	-0.56569500	0.25343200
O	-1.13974900	1.90929100	-0.26682700
C	-0.50416600	2.70172500	-1.24093100
O	-1.01218500	3.84392500	-1.38602600
O	0.49065400	2.20154300	-1.83548900
C	-3.85752900	0.63740800	0.97698200
H	-4.87823500	0.24481500	0.84550300
H	-3.82002600	1.20059300	1.91830700
H	-3.61901700	1.33524300	0.16967300
C	-3.14214500	-1.42864800	2.20799100
H	-3.25052900	-0.84125800	3.12987800
H	-4.08830300	-1.96286800	2.03030500
H	-2.34851400	-2.16433800	2.37395800
C	-3.87947800	-1.35459300	-1.18924900
H	-3.64078900	-1.85983400	-2.13502900
H	-4.64151300	-1.95135500	-0.66375400
H	-4.30039200	-0.37501900	-1.43311400
C	-1.94105000	-2.59970100	-0.20371500
H	-2.62491400	-3.34645300	0.22954500
H	-1.63191400	-2.94341200	-1.19822700
H	-1.04507200	-2.53732000	0.42246000
F	0.74291700	-1.24545800	-1.99780900
F	3.33030000	-1.83816600	-1.74267900
F	4.78971800	-0.88516000	0.37577000
F	3.56950700	0.70175500	2.25734200

F	0.97073400	1.32440800	2.03347800
29-ts			
C	-2.27974700	-1.44925100	-0.64061000
C	-2.62142500	-1.08127600	0.86676200
O	-1.71118400	-0.02536800	1.15269300
O	-1.73768700	-0.23876500	-1.14817400
B	-1.28353300	0.56673800	-0.07050900
C	1.01945200	0.05342700	0.00505600
C	1.78095400	-0.12407800	-1.13435700
C	1.76034600	0.14496700	1.16826600
C	3.17376900	-0.20188000	-1.15482700
C	3.15281700	0.07625500	1.22821600
C	3.86715500	-0.09736700	0.04692100
O	-1.04793100	1.92028400	-0.21960500
C	-2.13246400	2.86548000	-0.32801800
O	-3.29300200	2.38397500	-0.28667000
O	-1.75275500	4.04719200	-0.44968200
C	-4.04774900	-0.52136200	1.04301900
H	-4.82118500	-1.27701600	0.83750400
H	-4.15944900	-0.18755600	2.08286000
H	-4.18315000	0.35781800	0.40405700
C	-2.39032700	-2.22097600	1.87102400
H	-2.61004900	-1.85638700	2.88253600
H	-3.05034700	-3.07710500	1.66506600
H	-1.35159400	-2.56331700	1.85913600
C	-3.49951700	-1.82370100	-1.49604100
H	-3.16935300	-2.03790000	-2.52095200
H	-4.00660500	-2.71805600	-1.10433400
H	-4.21302400	-0.99652800	-1.53730000
C	-1.21512100	-2.55828200	-0.77314900
H	-1.60046700	-3.53956600	-0.45937200
H	-0.90943800	-2.62164900	-1.82444200
H	-0.32536000	-2.31441600	-0.18708400
F	1.18458100	-0.25682600	-2.37187400
F	3.89216600	-0.38472500	-2.31071200
F	5.23204200	-0.17074100	0.06770100
F	3.85165600	0.16588400	2.40680200
F	1.14503200	0.30504400	2.39172600
30			
C	-1.65964000	-0.64237800	-0.15132900
C	-1.19571600	0.81906300	0.23147700
O	-0.45551700	-1.21579200	-0.68159800
O	0.18906400	0.62403300	0.54803400
B	0.64278300	-0.51073900	-0.14208700
O	1.89331500	-0.93621500	-0.26181800

C	3.11636100	-0.01039400	-0.03371000
O	3.86114000	-0.45826300	0.83581300
O	3.11509400	0.95579000	-0.79936800
C	-1.26608000	1.80260700	-0.95038500
H	-2.30105700	2.05759200	-1.21276000
H	-0.73872700	2.72083600	-0.67068100
H	-0.76666300	1.39365300	-1.83460400
C	-1.89938100	1.42654300	1.44791700
H	-1.48845600	2.42338800	1.64504700
H	-2.97857100	1.52973300	1.27190500
H	-1.74542000	0.81938300	2.34403200
C	-2.75503700	-0.71627900	-1.21871700
H	-2.99040900	-1.76625100	-1.43021800
H	-3.67491800	-0.22207500	-0.87838400
H	-2.43233400	-0.25103000	-2.15395800
C	-2.07437400	-1.47941700	1.07260900
H	-3.02741500	-1.14146300	1.49926100
H	-2.18439600	-2.52471400	0.76212900
H	-1.30712500	-1.44024600	1.85298400
31			
C	-1.20366400	0.37401300	0.00006500
C	-1.15470000	-1.01887200	0.00022700
C	0.00000000	-1.76188400	0.00001000
C	1.15470100	-1.01887300	-0.00019300
C	1.20366400	0.37401300	-0.00003600
C	0.00000000	1.07647500	0.00001200
F	2.37562900	1.08460400	0.00006600
F	0.00000000	2.43947900	-0.00000600
F	-2.37562900	1.08460400	-0.00006600
F	-2.40160600	-1.64596700	-0.00013800
F	2.40160500	-1.64596700	0.00008800
32-ts			
C	2.15407200	-1.31467300	-0.23889700
C	0.85791200	-1.08848800	0.22299700
C	0.35956300	0.16798600	0.50722400
C	1.23236200	1.21344000	0.29821400
C	2.54056200	1.05949100	-0.15818000
C	3.00307500	-0.22577800	-0.42648600
C	-1.45152300	0.43034700	1.60914200
H	-1.17504000	1.49028400	1.76167300
C	-2.41693600	0.26099600	0.44882400
C	-3.15807800	-0.91997800	0.31828400
C	-2.64315700	1.30625900	-0.45743600
C	-4.09085200	-1.06243600	-0.71243200
H	-2.98075900	-1.71309800	1.03933800

C	-3.57940500	1.17155200	-1.48560400
H	-2.06506700	2.22420600	-0.35920000
C	-4.30710000	-0.01778300	-1.61965200
H	-4.65423700	-1.98940300	-0.80895800
H	-3.74145500	1.99110800	-2.18404900
H	-5.03515600	-0.12769200	-2.42145400
F	0.83007000	2.51485800	0.53023500
F	3.37716100	2.11717000	-0.35042600
F	4.27046100	-0.41695900	-0.87193700
F	2.61772800	-2.56342500	-0.51954700
F	0.07524900	-2.20178500	0.37371500
O	-1.48590900	-0.35122000	2.58478800
33			
C	-1.84919400	1.43657800	0.03808500
C	-0.59573400	0.90880200	0.33214900
C	-0.33167200	-0.46615300	0.34194700
C	-1.41702000	-1.28084500	0.01492600
C	-2.68849900	-0.78784100	-0.27526000
C	-2.90985400	0.58353600	-0.25965700
C	1.00728900	-1.06771000	0.94136100
H	0.98035600	-2.13985700	0.61835500
C	2.22795600	-0.48587200	0.17343000
C	3.24404100	0.13810400	0.90332300
C	2.38652000	-0.63012400	-1.21190300
C	4.39141700	0.61938000	0.26325900
H	3.08985600	0.22604500	1.97615000
C	3.52900400	-0.14965400	-1.86015600
H	1.60624500	-1.12568900	-1.79081600
C	4.53976200	0.47987500	-1.12187400
H	5.17414100	1.10587300	0.84469800
H	3.63324700	-0.26556900	-2.93849500
H	5.43183200	0.85428900	-1.62174600
F	-1.27284100	-2.63213400	-0.04697000
F	-3.70870900	-1.62575000	-0.58356700
F	-4.13713500	1.08587900	-0.53171300
F	-2.05588000	2.77557000	0.02574400
F	0.38163200	1.80028300	0.60083800
O	1.00208000	-0.88477000	2.25688600
34-ts			
C	-2.43523700	-2.35826100	-0.70621800
C	-2.70331900	-2.04640400	0.83127500
O	-2.64685300	-1.09213300	-1.32598500
O	-2.43337500	-0.64792800	0.93246900
B	-2.52030600	-0.07952200	-0.35814800
O	-2.89482800	1.22202000	-0.60021000

C	-4.29070300	1.60469500	-0.56335800
O	-4.47713700	2.81156300	-0.81115400
O	-5.10008700	0.68492200	-0.29272500
C	-4.17685500	-2.24566600	1.24003700
H	-4.48513800	-3.30018100	1.18750700
H	-4.29614700	-1.90223100	2.27560000
H	-4.82780200	-1.62494300	0.61568000
C	-1.78964200	-2.80318000	1.80321600
H	-2.02607600	-2.50030800	2.83126800
H	-1.93850500	-3.89021400	1.72504800
H	-0.73597300	-2.57688700	1.62226600
C	-3.41563000	-3.36483200	-1.32662000
H	-3.17937800	-3.48578200	-2.39164800
H	-3.33520600	-4.35038000	-0.84487200
H	-4.44783700	-3.01263900	-1.24869200
C	-0.99075400	-2.80225300	-1.00422600
H	-0.74907500	-3.76994900	-0.54176600
H	-0.87641600	-2.90057300	-2.09168400
H	-0.29354700	-2.02755600	-0.67256500
C	3.86698700	-0.32370100	-1.21896900
C	2.70959100	0.38579900	-0.91382900
C	1.91518000	0.09655300	0.20551600
C	2.38236200	-0.94149400	1.01339200
C	3.53182800	-1.67936200	0.72954900
C	4.27960300	-1.37223700	-0.39884800
C	0.49185000	0.74570400	0.39579100
H	0.15322400	0.40522300	1.40223400
C	0.62465500	2.28484500	0.52883200
C	-0.35396400	3.09308300	-0.06484100
C	1.63700000	2.89349400	1.28600400
C	-0.30942100	4.48296700	0.09271400
H	-1.16082700	2.61058200	-0.61152800
C	1.69114100	4.28419000	1.43492300
H	2.39756400	2.27583700	1.76537800
C	0.71390500	5.08721900	0.83374100
H	-1.09209800	5.09045000	-0.35803300
H	2.49266100	4.73854300	2.01850600
H	0.74582900	6.17048200	0.95057600
F	1.72614600	-1.27848800	2.15539200
F	3.93986100	-2.68398900	1.54758900
F	5.39826600	-2.07967800	-0.69947600
F	4.61702400	-0.00355300	-2.30395700
F	2.38968500	1.39438000	-1.74544200
O	-0.27947300	0.29444700	-0.60464200

C	3.17789600	0.05272200	-1.53301500
C	2.83728200	1.27642100	-0.57184700
O	2.74973800	-1.07358400	-0.80513600
O	1.74129200	0.79911600	0.18003800
B	1.70472300	-0.69858700	0.15506000
O	1.70023300	-1.36718100	1.42563100
C	2.69738400	-1.47131500	2.41721300
O	2.31754000	-2.09144200	3.44404800
O	3.82471800	-0.96157900	2.18115200
C	3.99231500	1.62117000	0.39199900
H	4.87645400	2.01254800	-0.13661900
H	3.63878300	2.39671600	1.08608700
H	4.25050100	0.73834000	0.98892600
C	2.41261600	2.55883700	-1.31425100
H	2.16712000	3.33423900	-0.57610900
H	3.22199900	2.94437900	-1.95341900
H	1.52545100	2.39354200	-1.93436400
C	4.67610100	-0.11024500	-1.84256200
H	4.81770100	-0.98075000	-2.49853000
H	5.08698500	0.77414500	-2.35377500
H	5.23746500	-0.28742900	-0.92133000
C	2.39743900	0.10596100	-2.86998800
H	2.72241600	0.93324400	-3.51959400
H	2.56610400	-0.83917300	-3.40339900
H	1.32303200	0.19302100	-2.68385200
C	-2.34071200	2.18533100	-0.97670400
C	-1.83368600	0.89091700	-0.91661700
C	-1.44417600	0.28834300	0.28400700
C	-1.61443700	1.05756700	1.43595700
C	-2.11914100	2.35828900	1.40621000
C	-2.47923000	2.92756900	0.19211700
C	-0.76484100	-1.10603600	0.31167900
H	-0.47889100	-1.30652200	1.35629400
C	-1.75524500	-2.19836200	-0.11164300
C	-1.34095800	-3.18899300	-1.01122700
C	-3.05028500	-2.27727300	0.42235500
C	-2.20402200	-4.22751100	-1.37427100
H	-0.33151500	-3.11425300	-1.40376600
C	-3.91628700	-3.31438400	0.06209500
H	-3.38479500	-1.52303800	1.13290900
C	-3.49700600	-4.29667900	-0.84269000
H	-1.86335400	-4.98976500	-2.07389300
H	-4.91697600	-3.35707600	0.49072900
H	-4.16814900	-5.10680800	-1.12501300
F	-1.31612900	0.55325900	2.64806000

F	-2.27607200	3.06988700	2.54694000
F	-2.97822200	4.18587400	0.14523000
F	-2.71629800	2.73175200	-2.15876700
F	-1.74802300	0.22031600	-2.08151600
O	0.35556800	-1.10110500	-0.48811000

VIII. Investigation of the Reaction Mechanism

(a) Reactivity test of acetophenone with pentafluorophenyl-Bpin and K_2CO_3

A mixture of acetophenone (0.04 mmol, 4.8 mg), pentafluorophenyl-Bpin (0.04 mmol, 6.7 mg) and K_2CO_3 (0.04 mmol, 5.5 mg, 1 equiv.) was dissolved in 0.7 mL C_6D_6 in a Young's tap NMR tube. The 1H and ^{11}B NMR spectra of the mixture were recorded immediately. Then, the mixture was heated at 120 °C for 4 h. They subsequently were studied by 1H and ^{11}B NMR spectra, which revealed that the formation of product **3s-2** was observed.

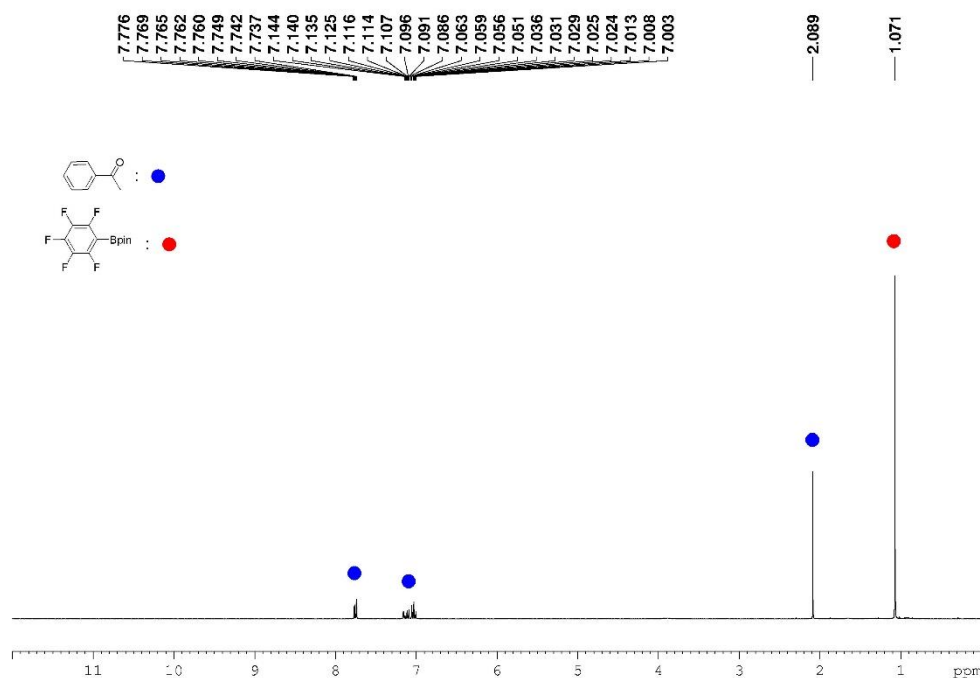
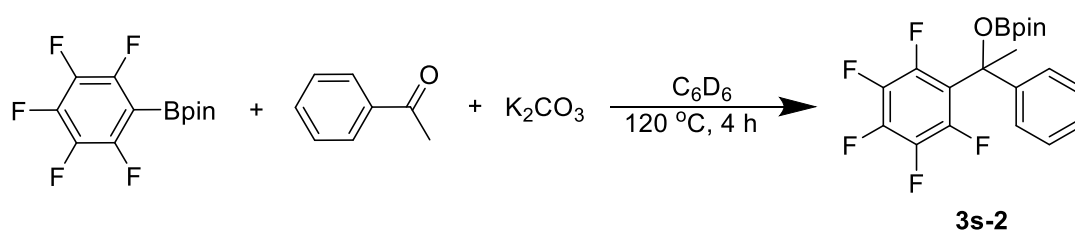


Figure S10. 1H NMR spectrum at 0 min (300 MHz, C_6D_6).

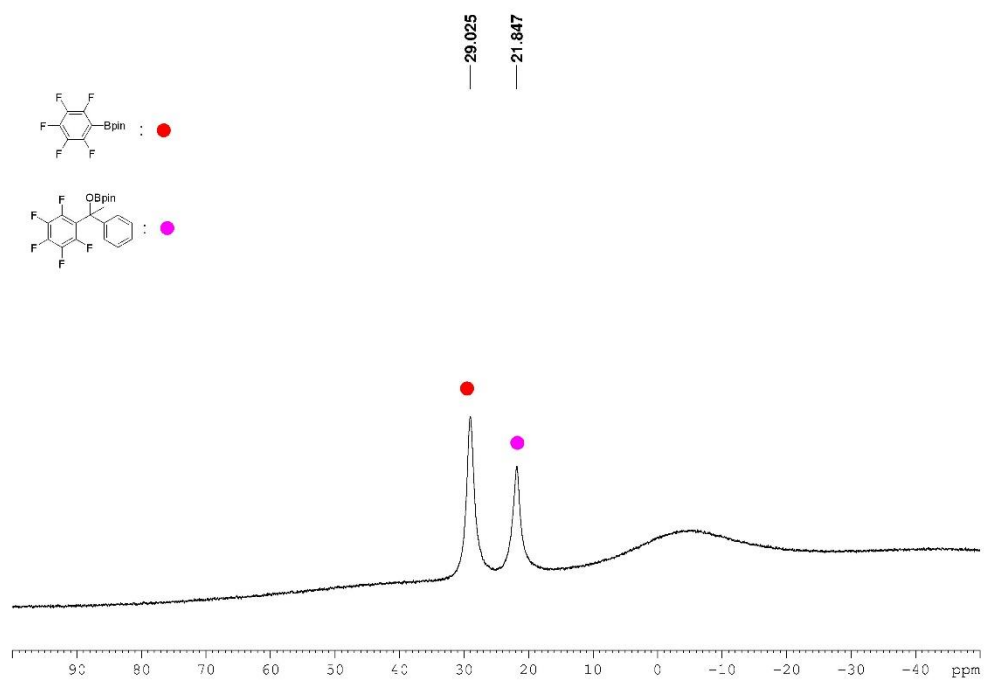
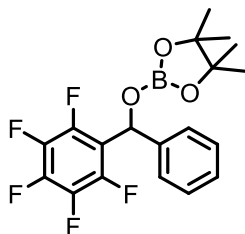
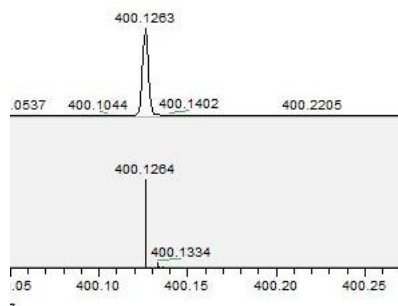


Figure S13. ^{11}B NMR spectrum after 4 h heating (96 MHz, C_6D_6).

HRMS data of intermediate D



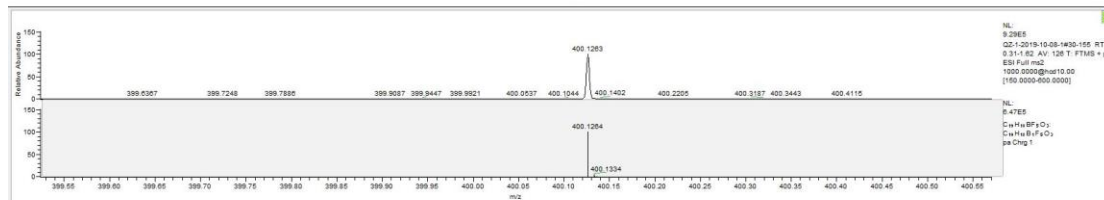
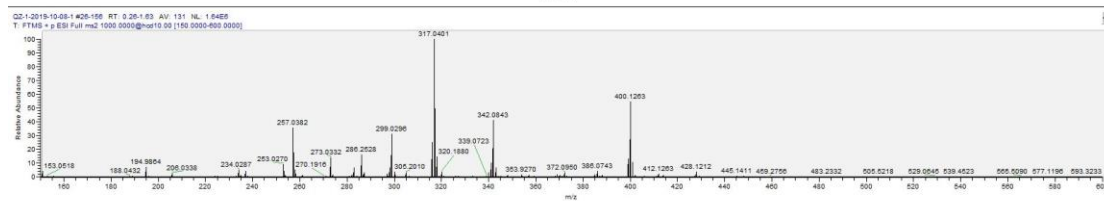
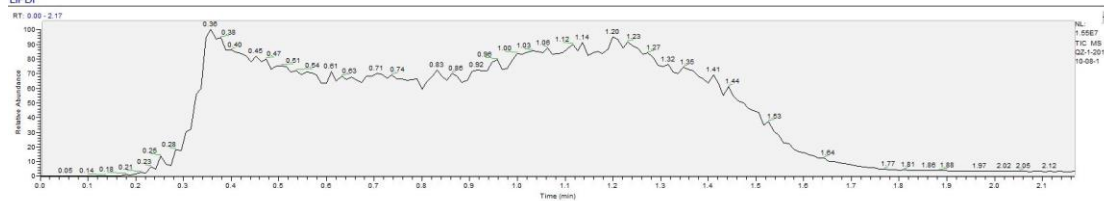
Formula: C₁₉H₁₈BF₅O₃
 Exact Mass: 400.1269
 Found: 400.1263



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