Supporting Information

Au-Pd@ZnO Alloy Nanoparticles: Promising Heterogeneous Photocatalyst toward Decarboxylative Trifluoromethylation under Visible-Light Irradiation

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Table S1. Results of BET for Au-Pd@ZnO and ZnO

Sample	BET surface area ($m^2.g^{-1}$)	Mean pore diameter (nm)	Pore volume of pores ($cm^3.g^{-1}$)
Au-Pd@ZnO	40.3	35.0	0.43
ZnO	37.4	24.3	0.24

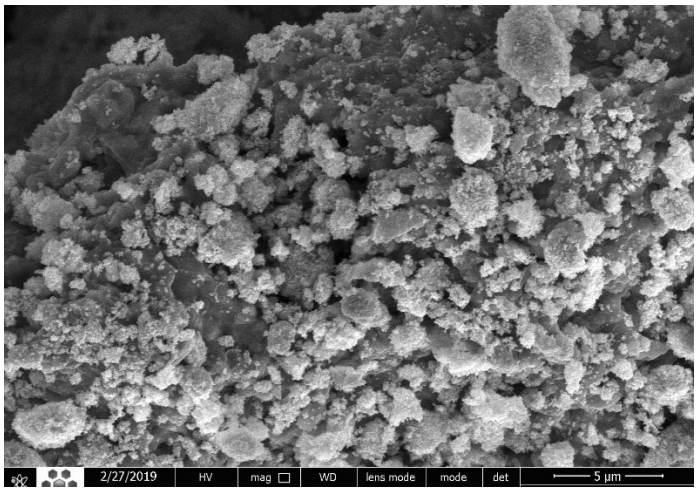
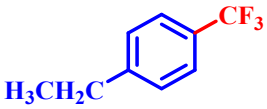


Figure S1. SEM image of the reused catalyst

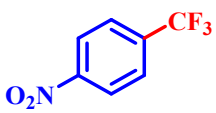
Experimental Data for Trifluoromethylation

1-Ethyl-4-(trifluoromethyl)benzene (2a) [3]



Colorless oil, TLC (Petroleumether: Ethyl acetate, 90:10 v/v): R_f = 0.72; IR (thin film) 3068, 2964, 2855,1593, 1515, 1476, 1370, 1248, 1168, 1076 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 7.75-7.73 (d, 2H, J = 4 Hz), 7.18–7.16 (d, 2H, J = 4 Hz), 2.60-2.58 (q, 2H, J = 8 Hz), 1.19-1.15 (t, 3H, J = 8 Hz), ^{13}C NMR (100 MHz, DMSO-d_6): δ 146.51, 145.67, 134.59 (q, $J_{C\text{-}F}$= 13 Hz), 134.24, 133.91, 133.56, 130.09 (q, $J_{C\text{-}F}$= 8 Hz), 126.8, 28.23, 15.47;^{19}F NMR (376 MHz, DMSO-d_6) δ -73.92 (s); UV/Vis (CH_3CN): λ_{max} 276 nm.

1-Nitro-4-(trifluoromethyl)benzene (2b) [3]

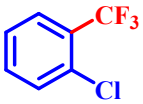


Colorless oil; TLC (Petroleumether: Ethyl acetate, 80:20 v/v): R_f = 0.65; IR (thin film) 3051, 1603, 1519, 1259, 1142, 1029 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.12-8.09 (d, 2H, *J* = 12 Hz), 6.87–6.83 (d, 2H, *J* = 12 Hz), ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.14, 129.26 (q, J^2_{C-F}= 84 Hz), 129.06 (q, J^3_{C-F}= 13 Hz), 126.74 (q, J^4_{C-F} = 3 Hz), 127.87 (q, J^1_{C-F}= 270 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.99 (s); UV/Vis (CH_3CN): λ_{max} 294 nm.

1-Nitro-2-(trifluoromethyl)benzene (2c) [3]

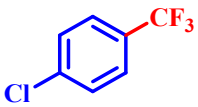
Colorless oil; TLC (Petroleumether: Ethyl acetate, 85:15 v/v): R_f= 0.67; IR (thin film) 3061, 1610, 1545, 1270, 1166 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.98-7.94 (d, 1H, *J* = 10 Hz), 7.79–7.75 (d, 1H, *J* = 10 Hz), 7.45-7.38 (t, 1H, *J* = 10 Hz), 7.23-7.16 (t, 1H, *J* = 10 Hz), ^{13}C NMR (100 MHz, $CDCl_3$): δ 132.88, 132.33, (d, J^4_{C-F}= 2 Hz), 131.42, 129.09 (q, J^2_{C-F}= 52 Hz), 127.59 (q, J^3_{C-F}= 5 Hz), 126.98 (q, J^1_{C-F}= 271 Hz), 126.69; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.26 (s); UV/Vis (CH_3CN): λ_{max} 276 nm.

1-Chloro-2-(trifluoromethyl)benzene (2d) [3]



Colorless oil; TLC (Petroleumether: Ethyl acetate, 90:10 v/v): R_f = 0.91; IR (thin film) 3024, 1595, 1488, 1193, 1133, 1089 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7. 73-7.71 (d, 1H, *J* = 8 Hz), 7.54–7.47 (m, 2H), 7.40-7.38 (d, 1H, *J* = 8 Hz), ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.59, 132.86, 129.18(q, J^2_{C-F}= 35 Hz), 126.53(q, J^4_{C-F}= 6 Hz), 123.73 (q, J^1_{C-F}= 277 Hz), 117.48, 117.12, 113.83 (q, J^3_{C-F} = 29 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.73 (s); UV/Vis (CH_3CN): λ_{max} 261 nm.

1-Chloro-4-(trifluoromethyl)benzene (2e) [3]

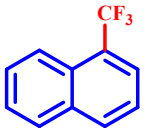


Colorless oil; TLC (Petroleumether: Ethyl acetate, 90:10 v/v): R_f = 0.90; IR (thin film) 3050, 1564, 1495, 1213, 1119, 1087 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.47-7.45 (d, 2H, *J* = 8 Hz), 7.36–7.34 (d, 2H, *J* = 8 Hz), ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.13(q, J^4_{C-F}= 1 Hz),129.57, (q, J^2_{C-F}= 33 Hz), 129.08, 127.83 (q, J^1_{C-F}= 269 Hz), 126.76 (q, J^3_{C-F}= 4 Hz), ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.26 (s); UV/Vis (CH_3CN): λ_{max} 267 nm.

(Trifluoromethyl)benzene (2f) [3]

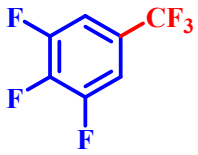
Clear colorless liquid; TLC (Petroleumether: Ethyl acetate, 90:10 v/v): R_f = 0.25; IR (thin film) 3039, 1550, 1229, 1138, cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.21-7.18 (t, 1H), 7.10-7.05 (t, 2H), 6.76-6.73 (d, 2H), ^{13}C NMR (100 MHz, DMSO-d_6): δ 138.35 (q, $J^2_{C\text{-}F}$= 11 Hz),134.42 (q, $J^1_{C\text{-}F}$= 203 Hz), 133.40, 129.97, 127.38 (q, $J^3_{C\text{-}F}$= 7 Hz), ^{19}F NMR (376 MHz, DMSO-d_6) δ -74.09 (s); UV/Vis (CH_3CN): λ_{max} 273nm.

1-(Trifluoromethyl)naphthalene (2g) [3]



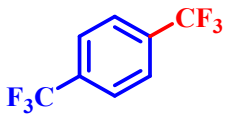
Colorless oil, TLC (Petroleumether: Ethyl acetate, 90:10 v/v): R_f = 0.51; IR (thin film) 3072, 1603, 1588, 1489, 1275, 1190, 1029 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.9 (d, 2H), 7.53 (d, 1H), 7.44 (t, 2H), 7.25 (t, 2H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 136.12, 133.75, 133.02, 132.83, 131.73, 129.61, 128.78, 128.07, 125.58, 125.15, 124.92, 124.38; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.72 (s); UV/Vis (CH_3CN): λ_{max} 270 nm.

1,2,3-Trifluoro-5-(trifluoromethyl)benzene (2h) [3]



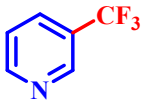
Clorless oil, TLC (Petroleumether: Ethyl acetate, 80:20 v/v): R_f = 0.24; IR (thin film) 3054, 1610, 1547, 1498, 1269, 1137, 1047, cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 7.75-7.45 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 151.20 (q, J = 9 Hz), 148.89 (q, J = 9 Hz), 141.21 (q, J = 15 Hz), 138.71 (q, J = 15 Hz), 135.38, 131.42, 128.98(q, J = 31 Hz), 125.95(q, J = 11 Hz), 117.81 (d, J= 17 Hz), 116.95(d, J = 17 Hz); ^{19}F NMR (376MHz, DMSO-d_6) δ -164.96 (s), -141.23 (s), -67.42 (s); UV/Vis (CH_3CN): λ_{max} 277 nm.

1,4-Bis(trifluoromethyl)benzene (2i) [3]



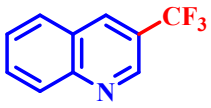
Clorless oil, TLC (Petroleumether: Ethyl acetate, 80:20 v/v): R_f = 0.26; IR (thin film) 3065, 1549, 1517, 1472, 1338, 1129, 1058, cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.02-7.89 (d, 4H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 134.59 (q, J = 180 Hz), 130.34 (q, J = 32 Hz), 123.76 (q, J = 81 Hz); ^{19}F NMR (376MHz, DMSO-d_6) δ -62.74 (d).

3-(Trifluoromethyl)pyridine (2j) [3]



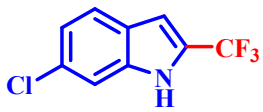
Colorless liquid, TLC (Petroleumether: Ethyl acetate, 80:20 v/v): R_f = 0.29; IR (thin film) 3079, 1585, 1496, 1445, 1215, 1165 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 9.01-8.99 (s, 1H), 8.53-8.50 (m, 2H), 7.80-7.72 (t, 1H), ^{19}F NMR (376 MHz, $CDCl_3$) δ -75.02 (s); UV/Vis (CH_3CN): λ_{max} 268 nm.

3-(Trifluoromethyl)quinolone (2k) [3]



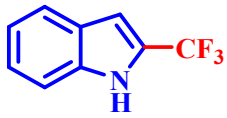
Clear oil, TLC (Petroleumether: Ethyl acetate, 70:30 v/v): R_f = 0.34; IR (thin film) 3043, 1607, 1562, 1523, 1458, 1343, 1249, 1194, 1104 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 9.10-9.08 (m, 1H), 8.25-8.21 (d, 1H), 8.08-8.07 (d, 1H), 8.04-8.01 (d, 1H), 7.63-7.55 (t, 1H), 7.53-7.50 (t, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.28, 136.28, 132.43, 128.72, 130.26 (q, J_{C-F}= 162 Hz), 128.10(q, J_{C-F}= 6 Hz), 125.21, 121.95; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.71 (s); UV/Vis (CH_3CN): λ_{max} 306 nm.

6-Chloro-2-(trifluoromethyl)-1H-indole (2l) [3]



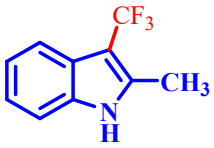
White powder; m.p: 145 ˚C (lit. **[**4]145 ˚C); TLC (Petroleumether: Ethyl acetate, 85:15 v/v): R_f = 0.13; IR (thin film) 3411, 3063, 1676, 1542, 1465, 1344, 1289, 1236, 1126 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 9.58 (s, 1H), 7.58-7.56 (d, J = 8 Hz, 1H), 7.50-7.48 (d, J = 8 Hz, 1H), 7.42-7.38 (t, 1H), 6.88-6.86 (d, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 154.69, 150.59, 145.80,137.67 (q, J_{C-F}= 39 Hz), 122.11 (q, J^1_{C-F}= 264 Hz), 119.47, 116.77, 114.08, 109.19; ^{19}F NMR (376 MHz, DMSO-d_6) δ -61.39 (s); UV/Vis (CH_3CN): λ_{max} 281 nm; analysis $C_9H_5ClF_3N$ (262.96): Calcd. C, 40.94; H, 1.91; N, 5.30; Found C, 40.95; H, 1.93; N, 5.28.

2-(Trifluoromethyl)-1H-indole (2m) [3]



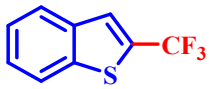
White solid, m.p: 107-108 ˚C (lit. **[**5] 107-109 ˚C); TLC (Petroleumether: Ethyl acetate, 70:30 v/v): R_f = 0.28; IR (thin film) 3409, 3053, 1618, 1509, 1428, 1383, 1337, 1265, 1141 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 12.69 (s, 1H), 8.48-8.46 (s, 2H), 8.19-8.16 (d, J = 8 Hz, 1H), 7.60-7.58 (d, J = 8 Hz, 1H), 7.57-7.28 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 138.11 (q, J_{C-F}= 5 Hz), 137.12, 126.11,124.78, 123.87, 121.66 (q, J^1_{C-F}= 298 Hz), 121.56, 113.46, 109.31; ^{19}F NMR (376 MHz, DMSO-d_6) δ -71.39 (s); UV/Vis (CH_3CN): λ_{max} 311 nm; analysis $C_9H_6F_3N$ (185.05): Calcd. C, 58.38; H, 3.27; N, 7.57; Found C, 58.37; H, 3.29; N, 7.55.

2-Methyl-3-(trifluoromethyl)-1H-indole (2n) [3]



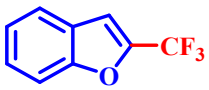
White solid, m.p: 146-147 °C (lit. [6] 147.5 °C); TLC (Petroleumether: Ethyl acetate, 85:15 v/v): R_f = 0.17; IR (thin film) 3405, 3058, 2934, 2867, 1644, 1599, 1532, 1458, 1357, 1278, 1158, 1035, cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.9 (s, 1H), 8.04-8.00 (d, 1H), 7.32-7.29 (d, 1H), 7.28 (t, *J* = 12 Hz, 1H), 7.26-7.18 (t, *J* = 12 Hz, 1H), 2.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.34, 132.60, 123.99,121.61, 121.27, 119.35 (q, J^1_{C-F}= 284 Hz), 119.03(q, J_{C-F}= 32 Hz), 116.51, 109.18, 106.16, 13.74; ^{19}F NMR (376 MHz, $CDCl_3$) δ -74.33 (s); UV/Vis (CH_3CN): λ_{max} 271 nm; analysis $C_{10}H_8F_3N$ (199.06) : Calcd. C, 60.30; H, 4.05; N, 7.03; Found C, 60.31; H, 4.03; N, 7.04.

2-(Trifluoromethyl)benzo[b]thiophene (2o) [3]



Colorless oil; TLC (Petroleumether: Ethyl acetate, 80:20 v/v): R_f = 0.39; IR (thin film) 3079, 1521, 1458, 1284, 1171 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.64 (s, 1H), 7.98-7.89 (m, 2H), 7.37-7.35 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 142.64, 140.48, 139.36 (q, J^2_{C-F}= 31 Hz), 137.37(q, J^4C-F = 5 Hz), 132.70, 127.23 (q, J^1_{C-F}= 304 Hz), 124.84,124.01(d, J^3C-F = 6 Hz), 122.39; ^{19}F NMR (376 MHz, DMSO-d_6) δ -73.78 (s); UV/Vis (CH_3CN): λ_{max} 330 nm.

2-(Trifluoromethyl)benzofuran (2p) [3]



Colorless oil; TLC (Petroleumether: Ethyl acetate, 80:20 v/v): R_f = 0.39; IR (thin film) 3058, 1575, 1449, 1308, 1280, 1127, 1126, 1071 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ 8.3-8.21(d, H), 7.67-7.65 (d, H), 7.57-7.54 (d, H), 7.45-7.37 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 156.42, 127.64, 125.25, 124.18 (q, J^2_{C-F}= 138 Hz), 122.48, 121.74, 117.41, 111.33, 111.13 (q, J^1_{C-F}= 270 Hz), ^{19}F NMR (376 MHz, DMSO-d_6) δ -73.74 (s).

NMR (^{1}HNMR, ^{13}CNMR, ^{19}FNMR purified products)

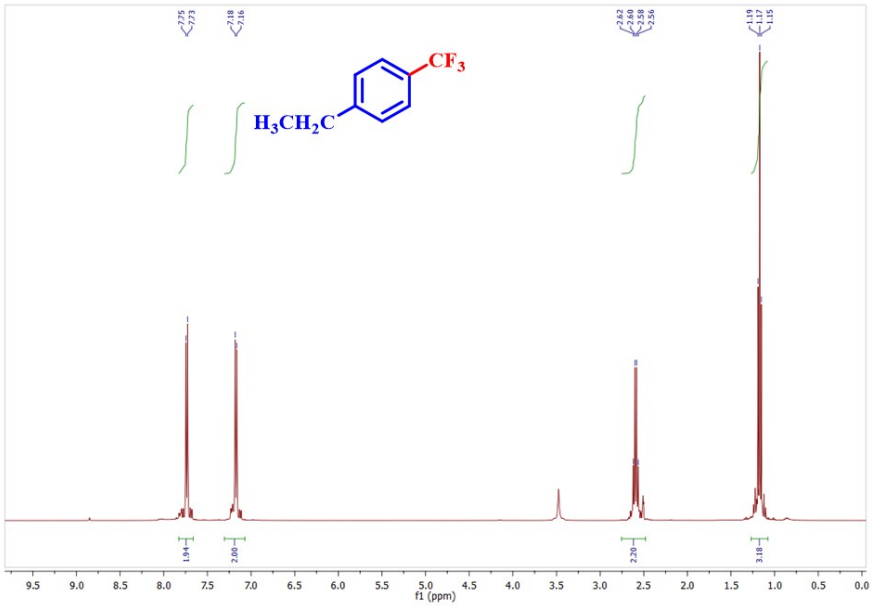


Figure S2. [1]H NMR spectram of **1-ethyl-4-(trifluoromethyl)benzene** [3].

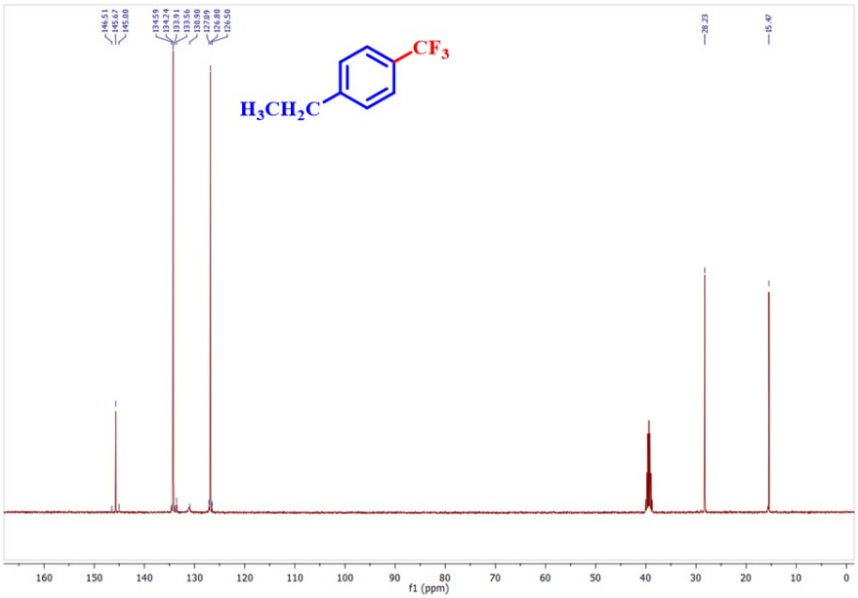


Figure S3.[13]C NMR spectram of **1-ethyl-4-(trifluoromethyl)benzene** [3].

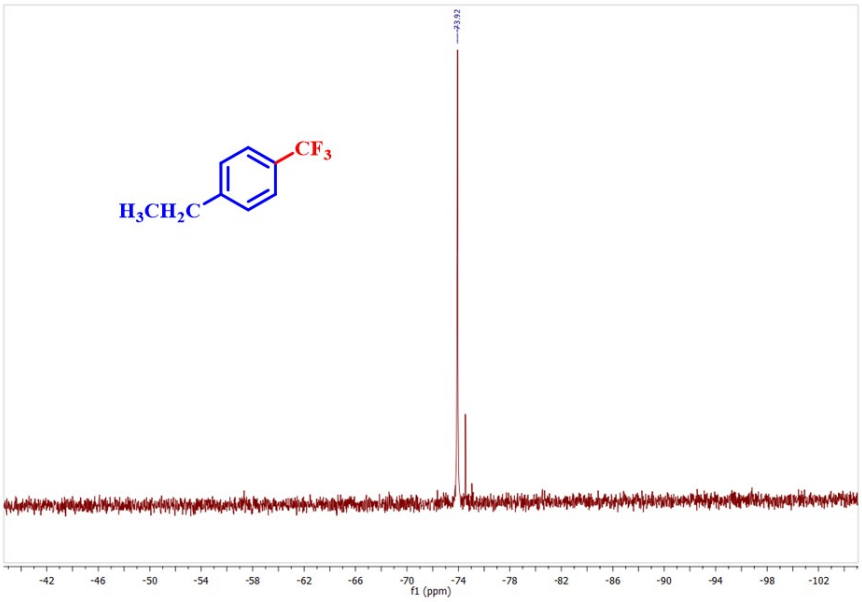


Figure S4.[19]F NMR spectram of **1-ethyl-4-(trifluoromethyl)benzene** [3].

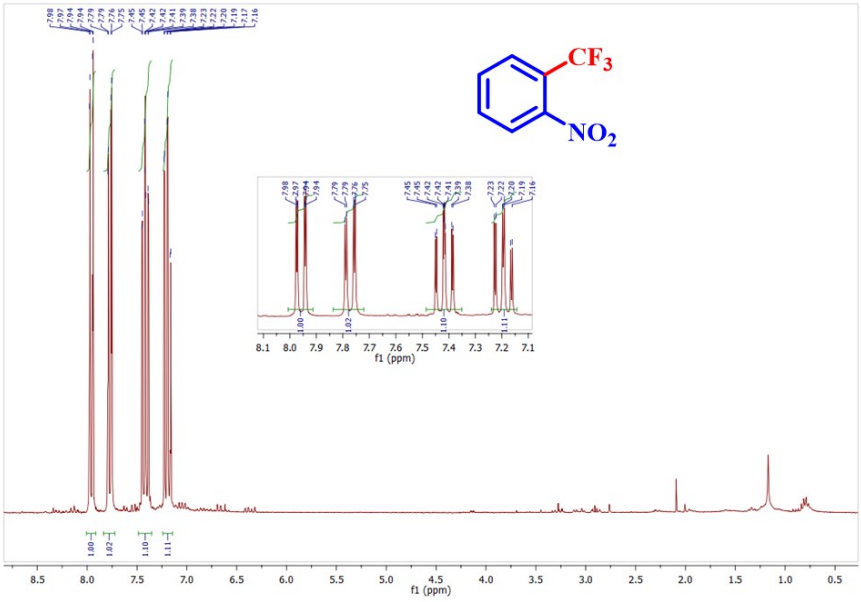


Figure S5.[1]H NMR spectram of **1-nitro-2-(trifluoromethyl)benzene** [3].

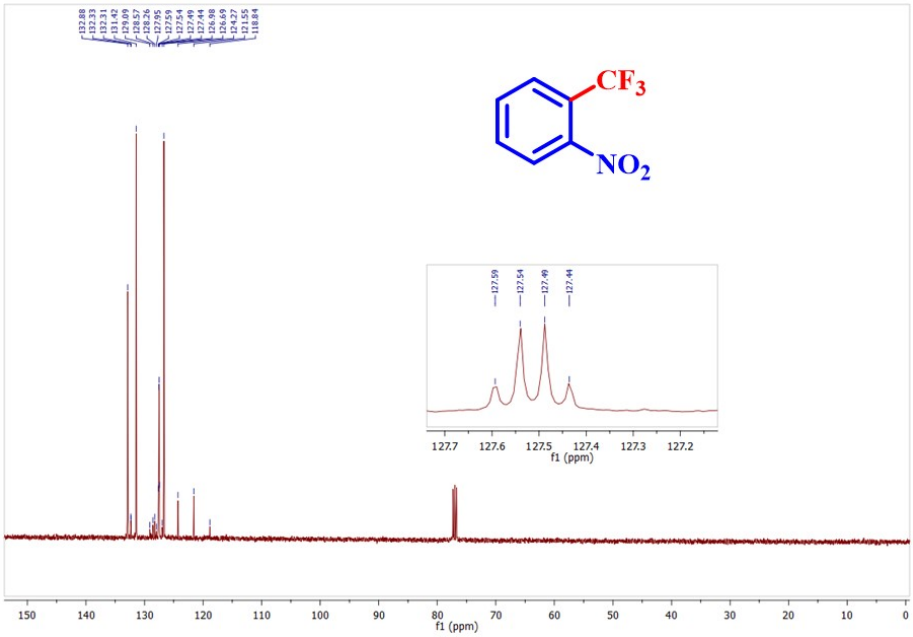


Figure S6.[13]C NMR spectram of **1-nitro-2-(trifluoromethyl)benzene** [3].

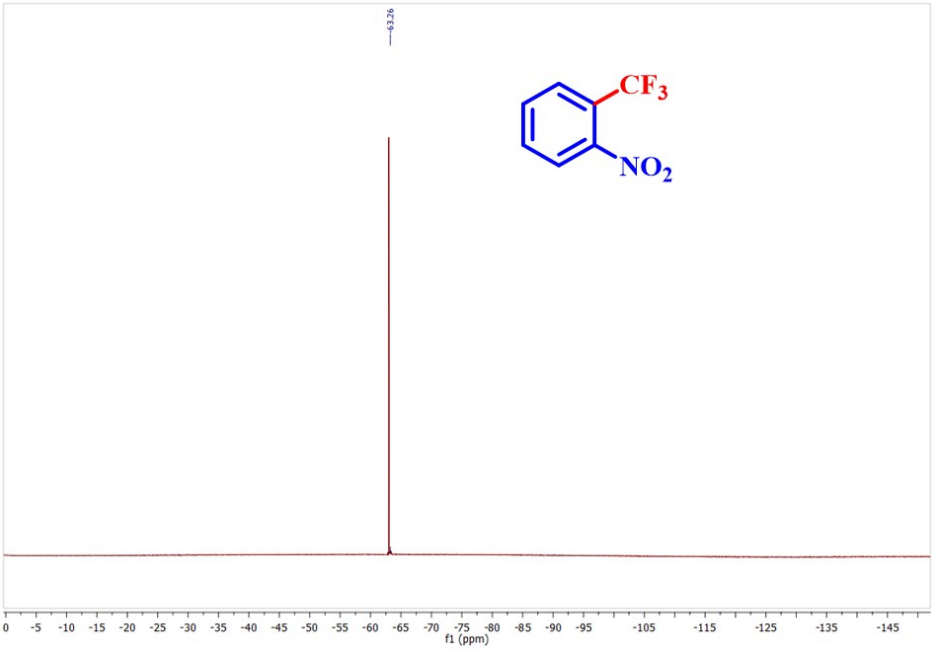


Figure S7.[19]F NMR spectram of **1-nitro-2-(trifluoromethyl)benzene** [3].

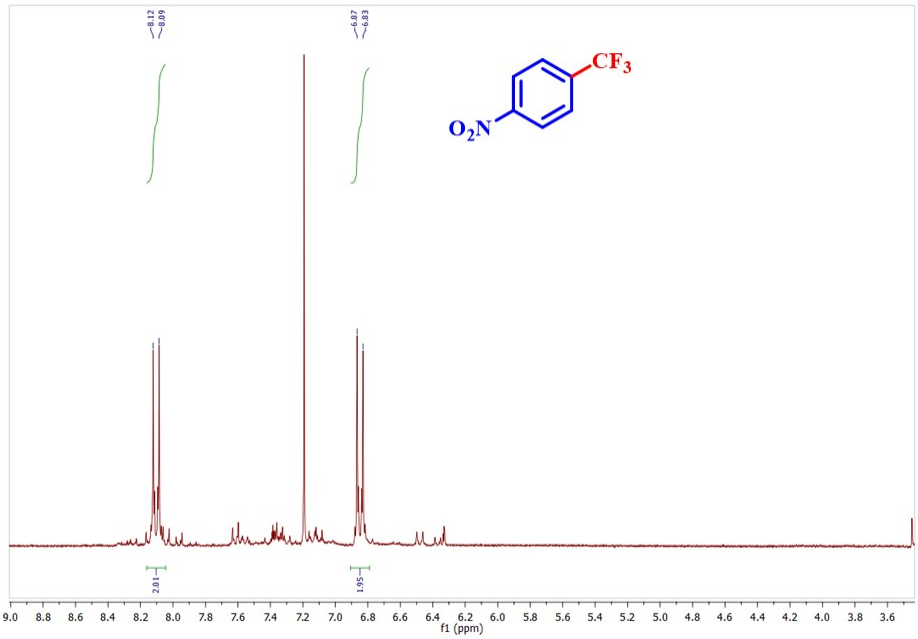


Figure S8.[1]H NMR spectram of **1-nitro-4-(trifluoromethyl)benzene [**3].

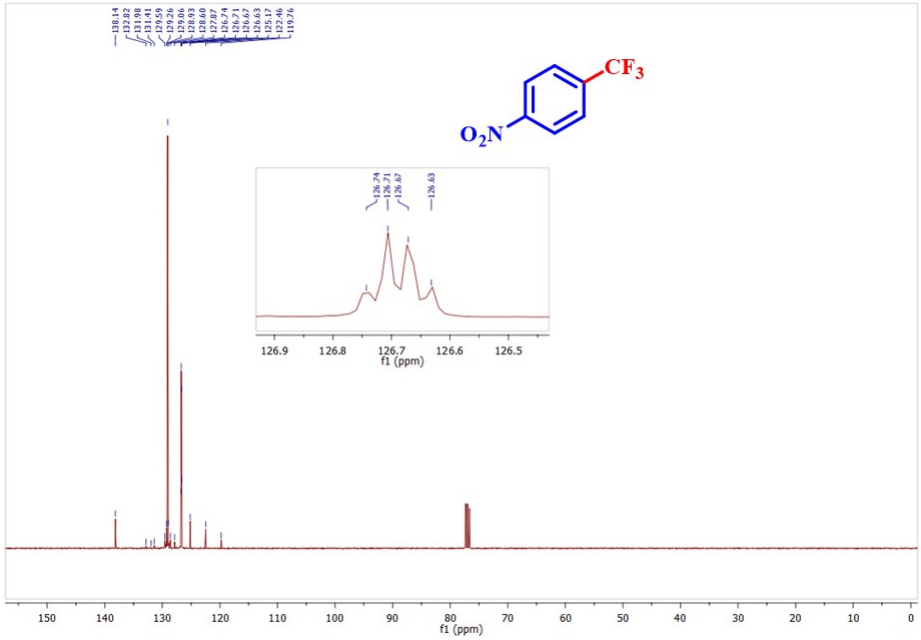


Figure S9.[13]C NMR spectram of **1-nitro-4-(trifluoromethyl)benzene [**3].

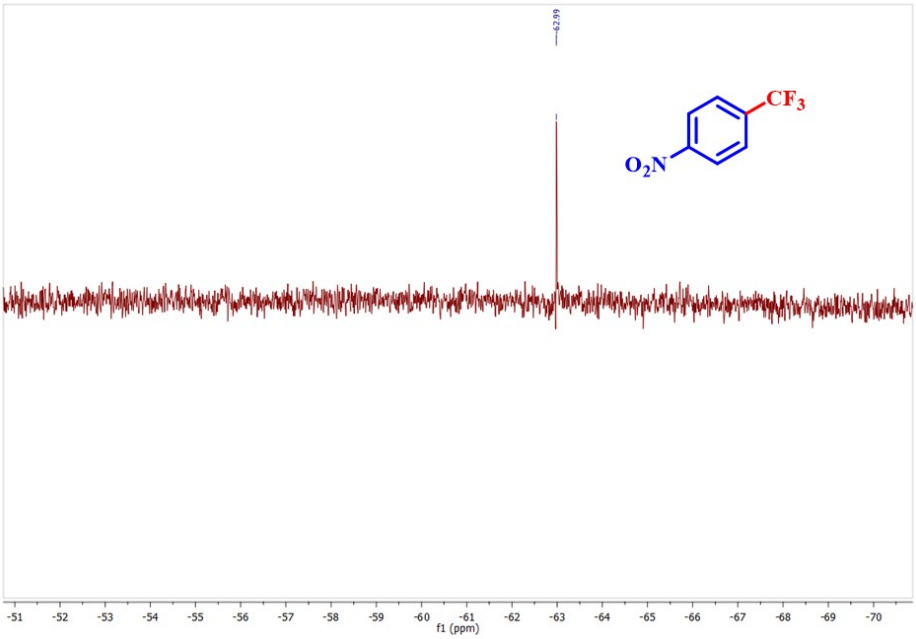


Figure S10.[19]F NMR spectram of **1-nitro-4-(trifluoromethyl)benzene [**3].

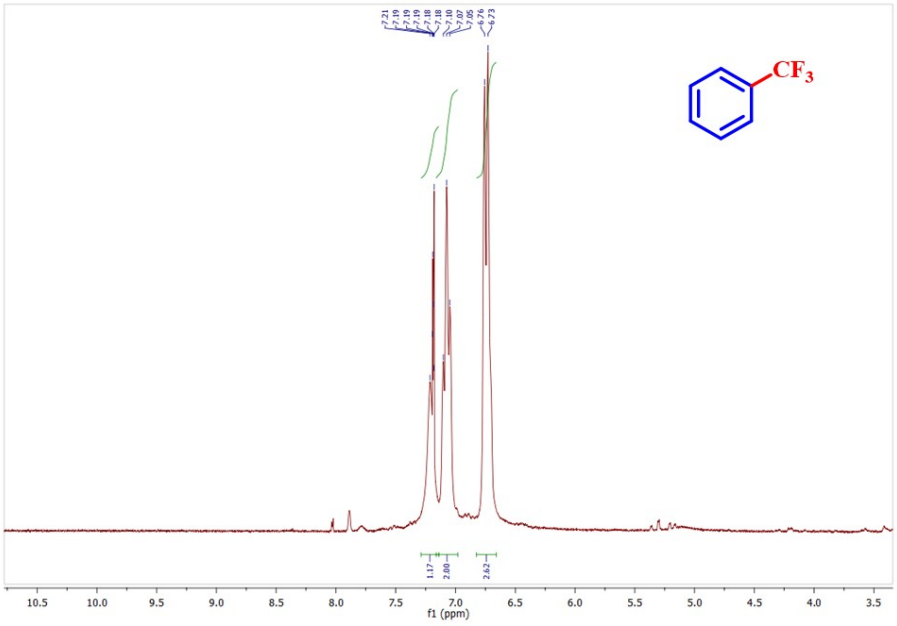


Figure S11.[1]H NMR spectram of **(trifluoromethyl)benzene [**3].

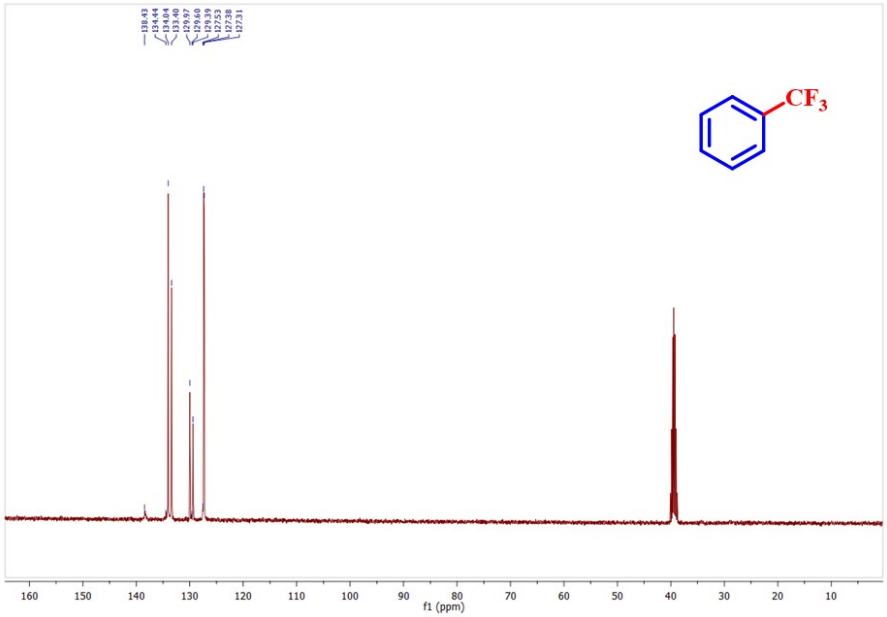


Figure S12.[13]C NMR spectram of **(trifluoromethyl)benzene [**3].

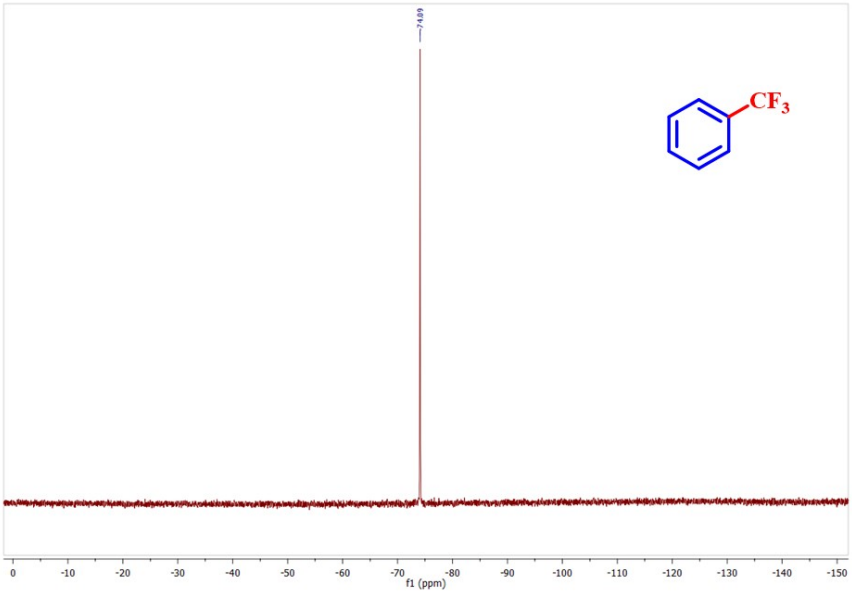


Figure S13. [1]F NMR spectram of **(trifluoromethyl)benzene [**3].

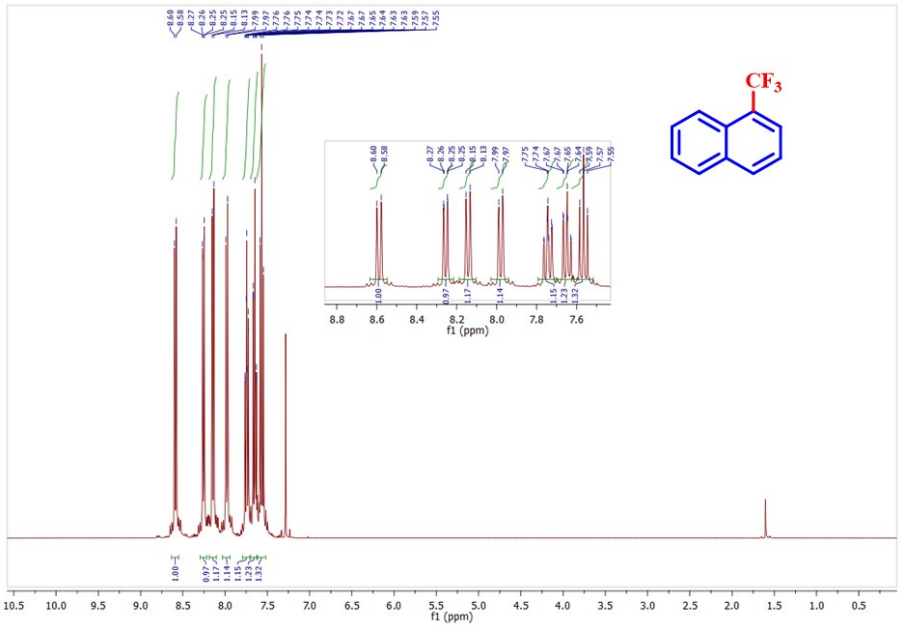


Figure S14. ^{1}H NMR spectram of **1-(trifluoromethyl)naphthalene** [3].

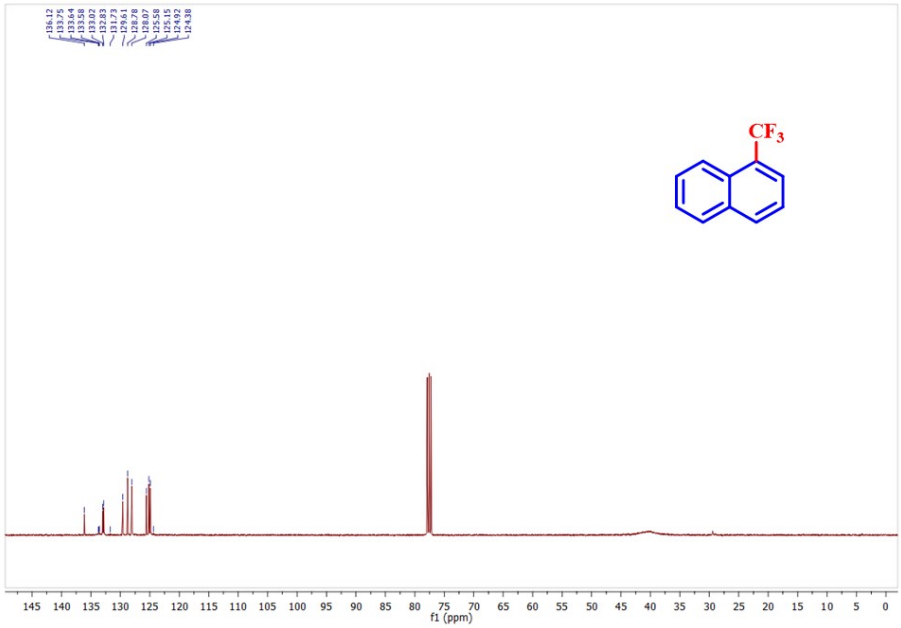


Figure S15. ^{13}C NMR spectram of **1-(trifluoromethyl)naphthalene** [3].

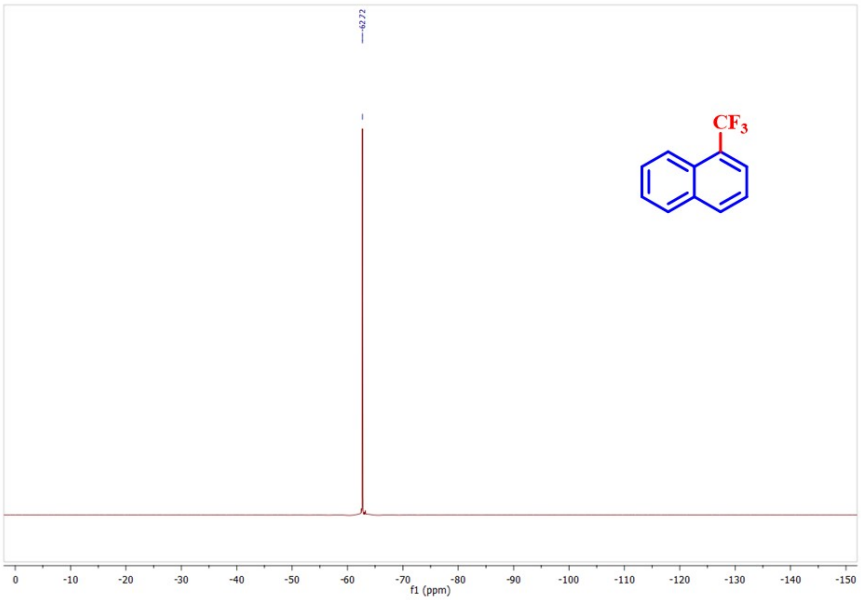


Figure S16. ^{19}F NMR spectram of **1-(trifluoromethyl)naphthalene [**3].

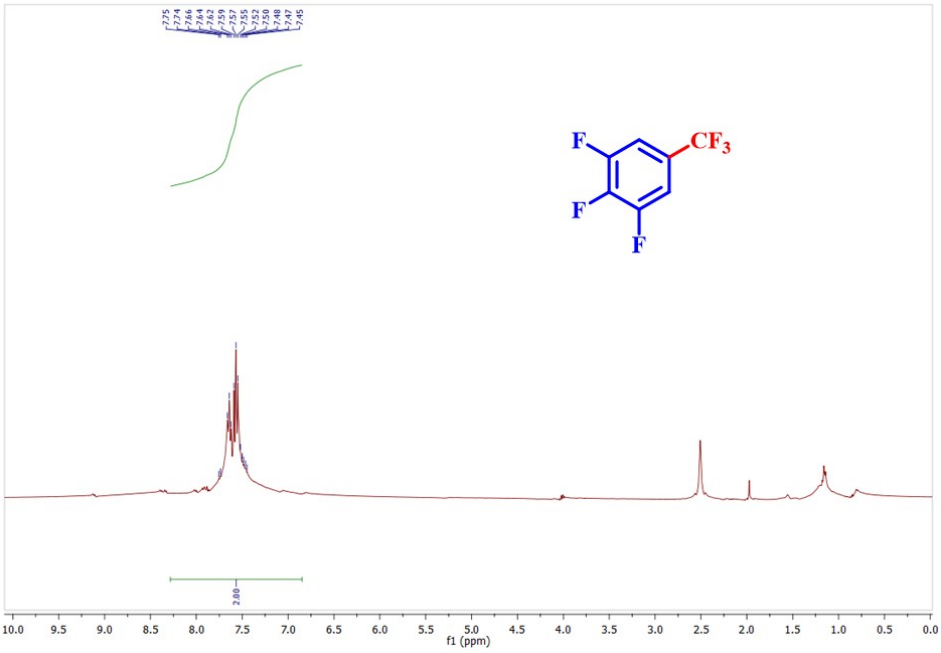


Figure S17. ^{1}H NMR spectram of **1,2,3-Trifluoro-5-(trifluoromethyl)benzene [**3].

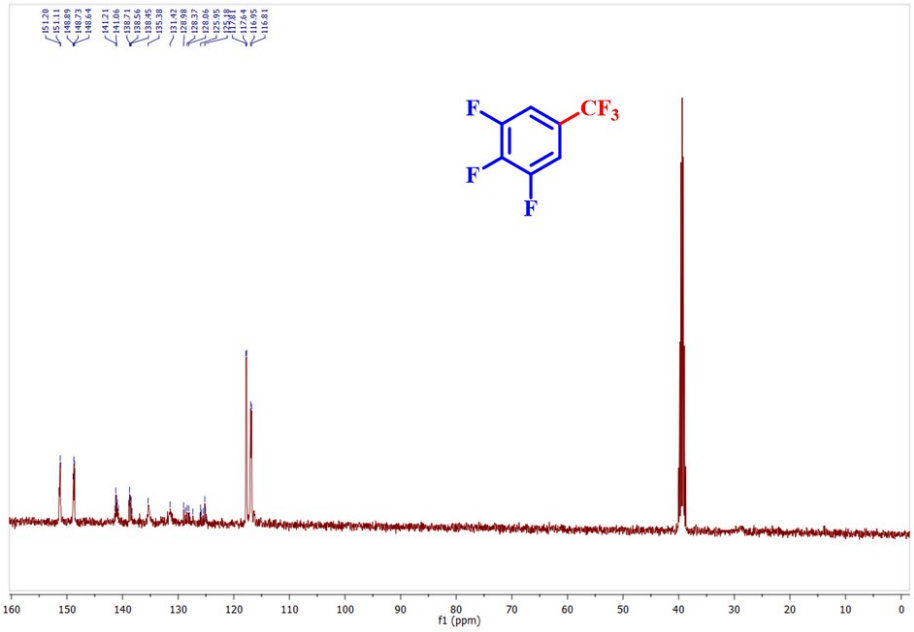


Figure S18. ^{13}C NMR spectram of **1,2,3-Trifluoro-5-(trifluoromethyl)benzene [**3].

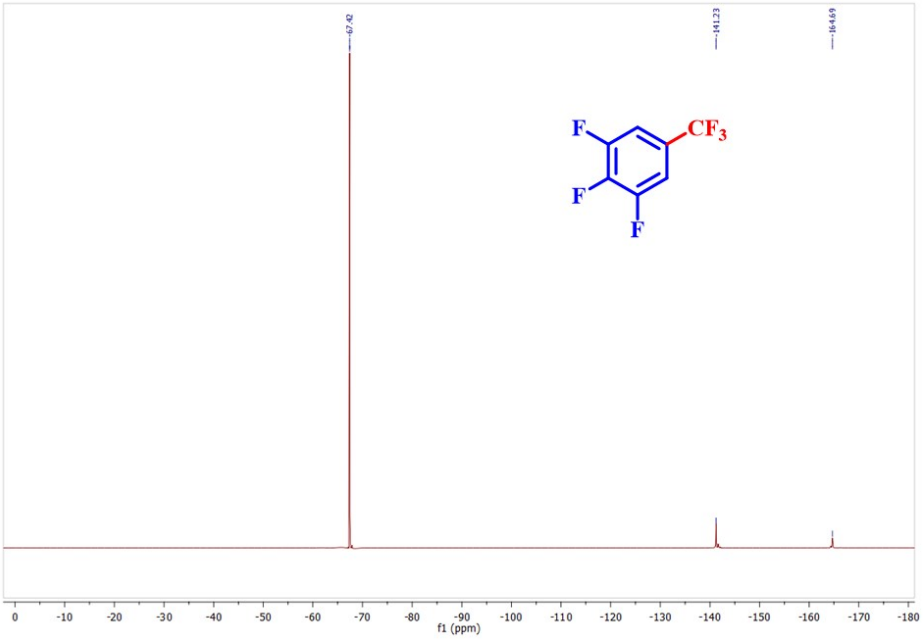


Figure S19. ^{19}F NMR spectram of **1,2,3-Trifluoro-5-(trifluoromethyl)benzene [**3].

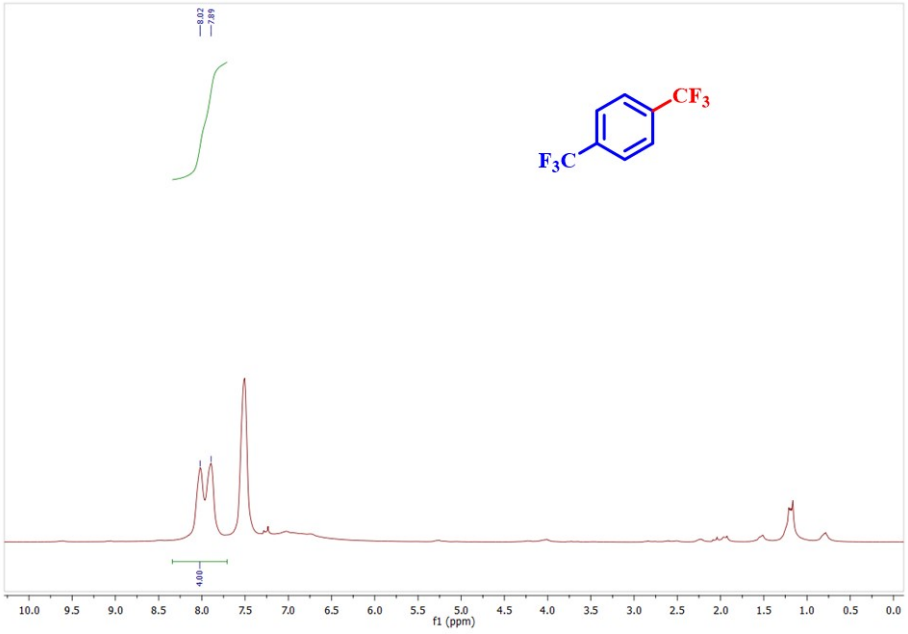


Figure S20.[1]H NMR spectram of **1,4-bis(trifluoromethyl)benzene [**3**].**

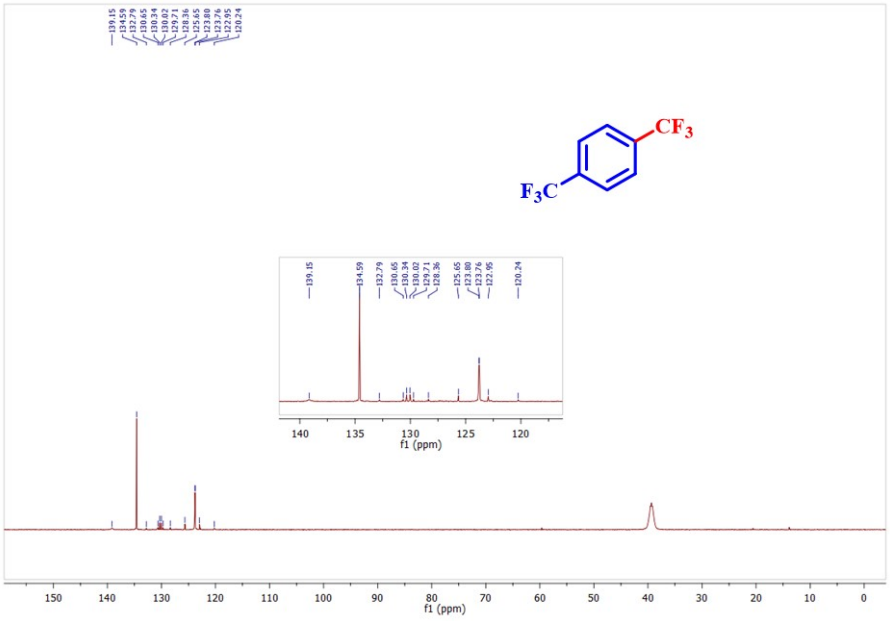


Figure S21.[13]C NMR spectram of **1,4-bis(trifluoromethyl)benzene [**3**].**

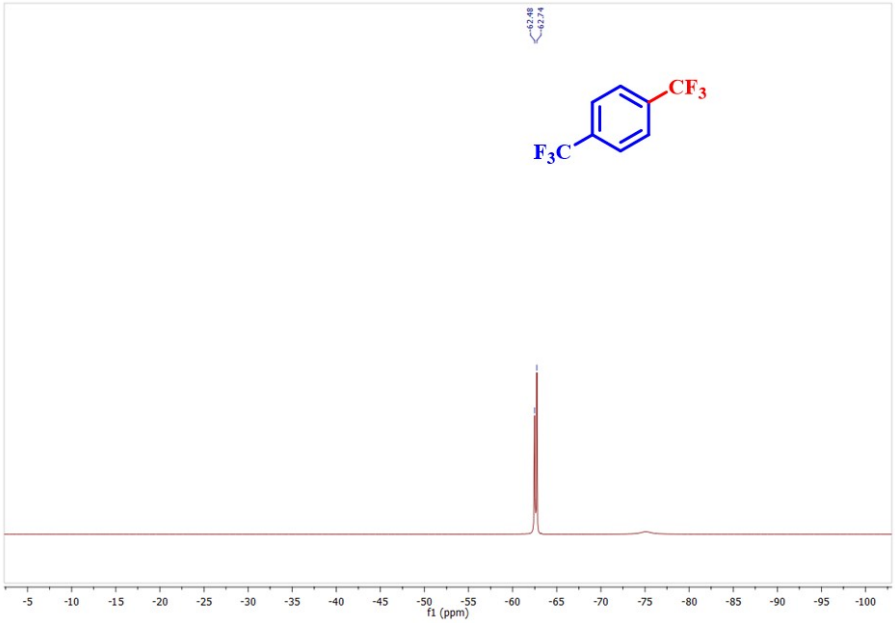


Figure S22.[19]F NMR spectram of **1,4-bis(trifluoromethyl)benzene [**3**].**

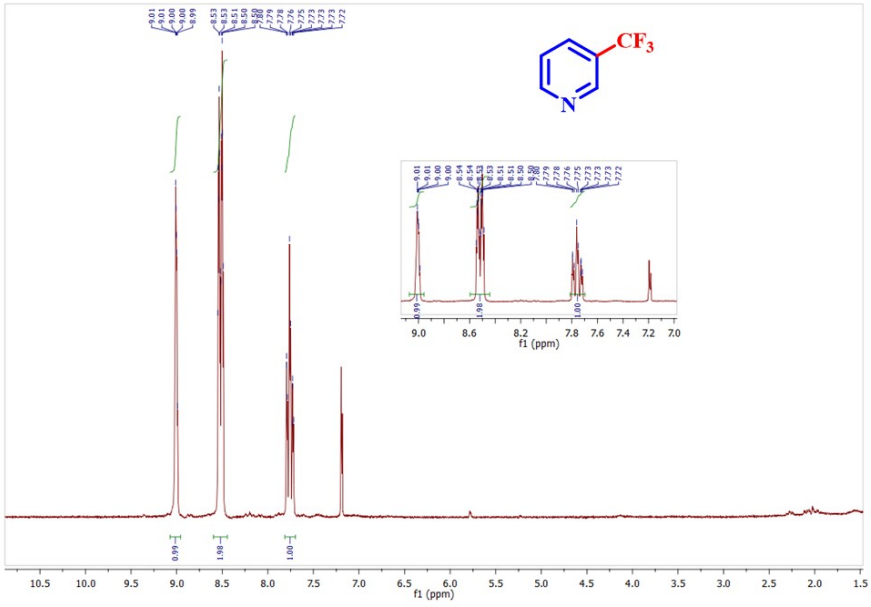


Figure S23.[1]H NMR spectram of **3-(trifluoromethyl)pyridine [**3].

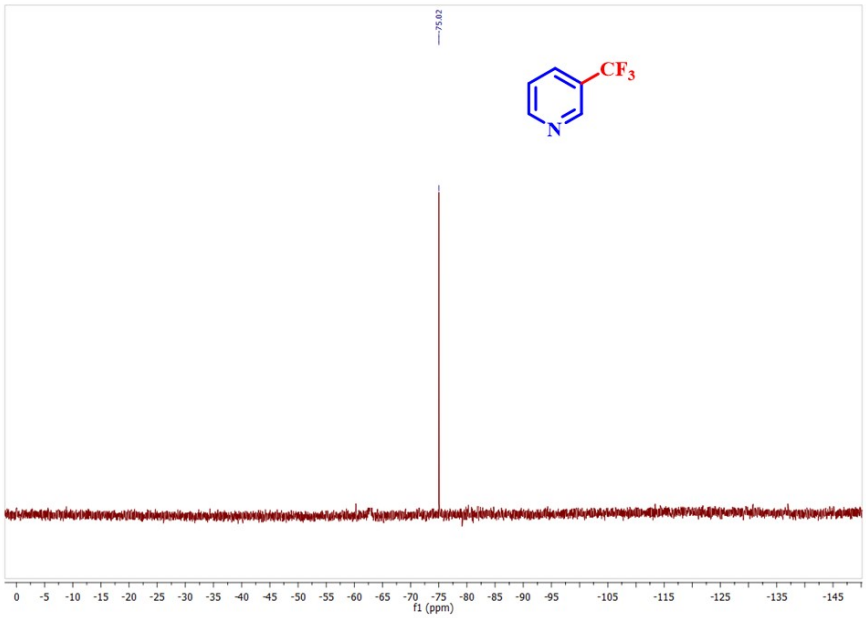


Figure S24.[19]F NMR spectram of **3-(trifluoromethyl)pyridine** [3].

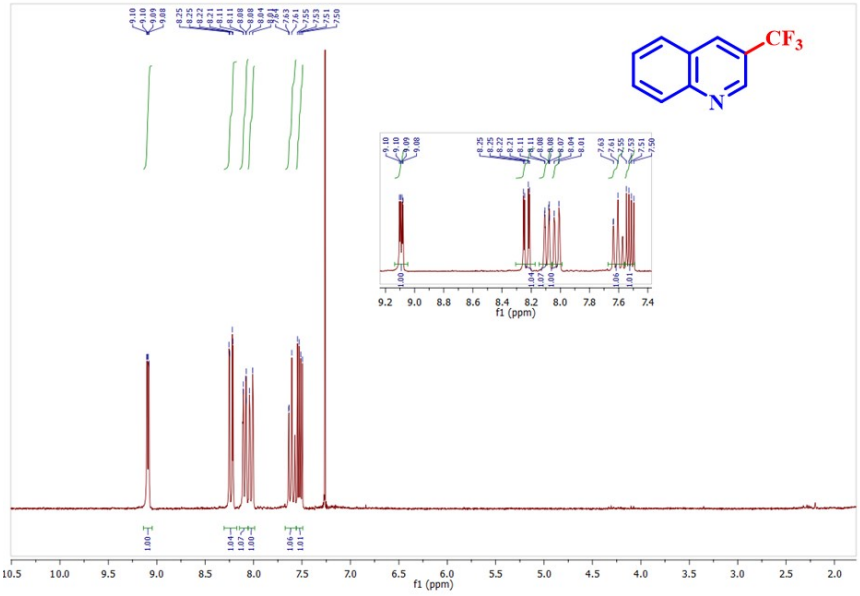


Figure S25.[1]H NMR spectram of **3-(trifluoromethyl)quinolone** [3].

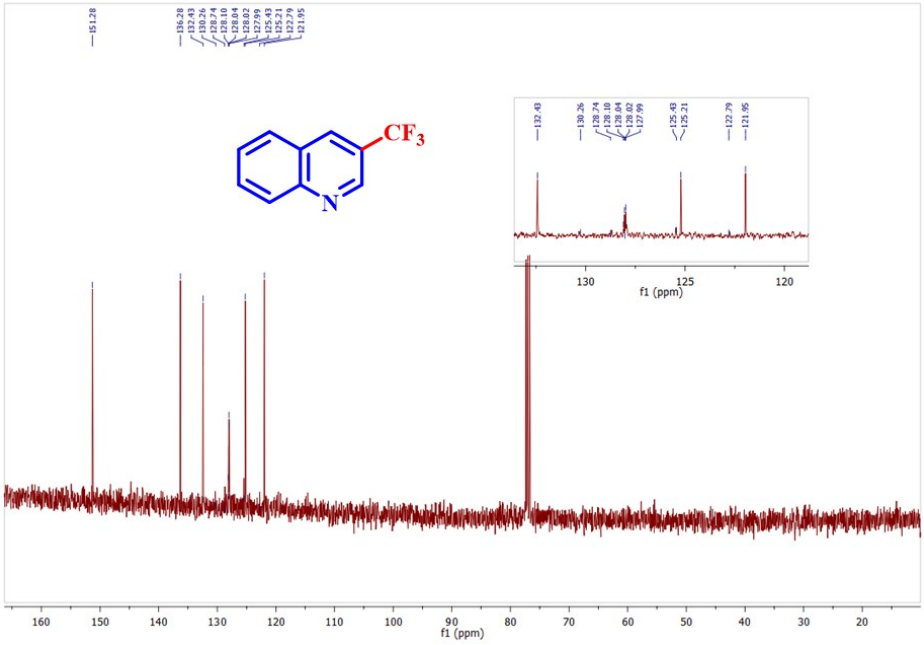


Figure S26.[13]C NMR spectram of **3-(trifluoromethyl)quinolone [**3].

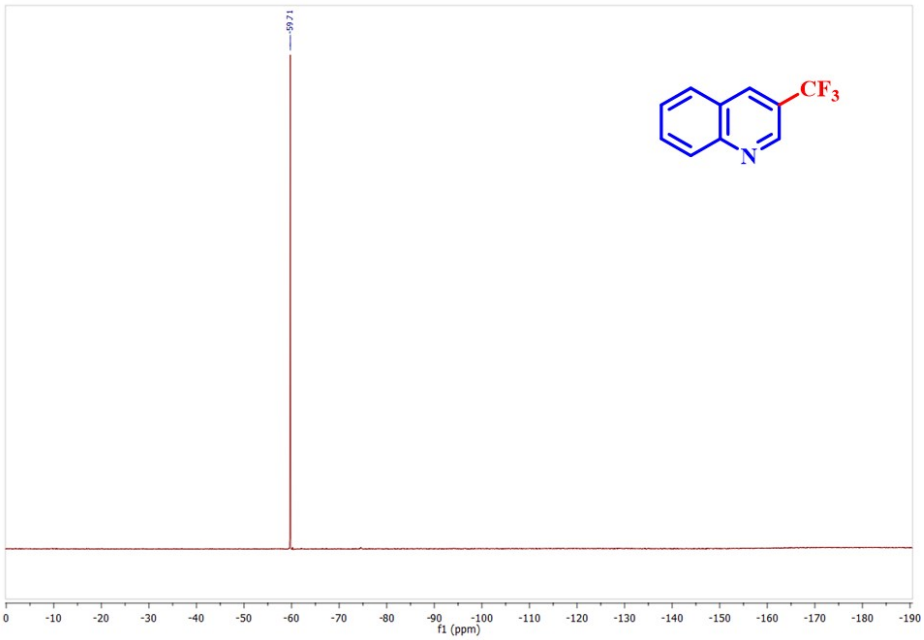


Figure S27.[19]F NMR spectram of **3-(trifluoromethyl)quinolone [**3].

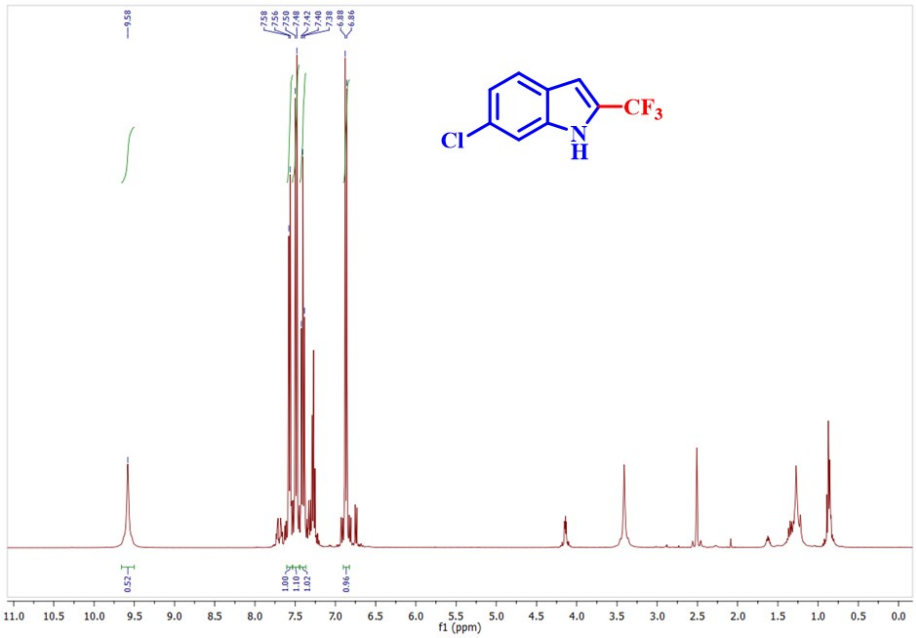


Figure S28. ^{1}H NMR spectram of **6-Chloro-2-(trifluoromethyl)-1H-indole [**3**].**

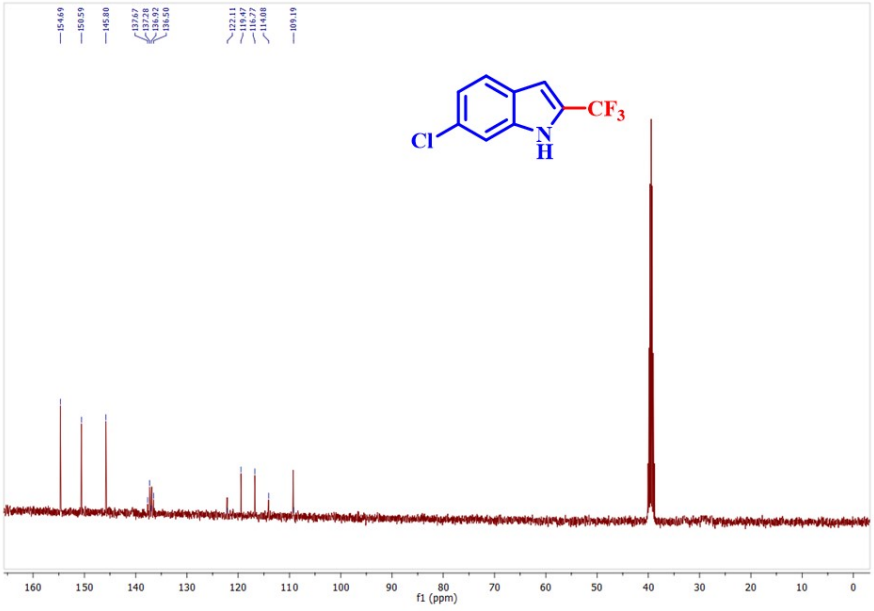


Figure S29. ^{13}C NMR spectram of **6-Chloro-2-(trifluoromethyl)-1H-indole [**3**].**

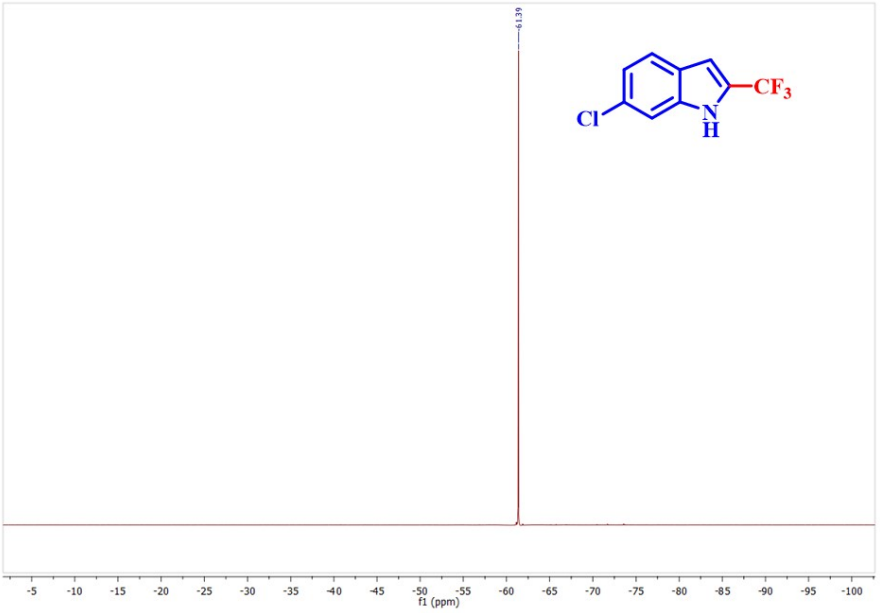


Figure S30. ^{19}F NMR spectram of **6-Chloro-2-(trifluoromethyl)-1H-indole [**3**].**

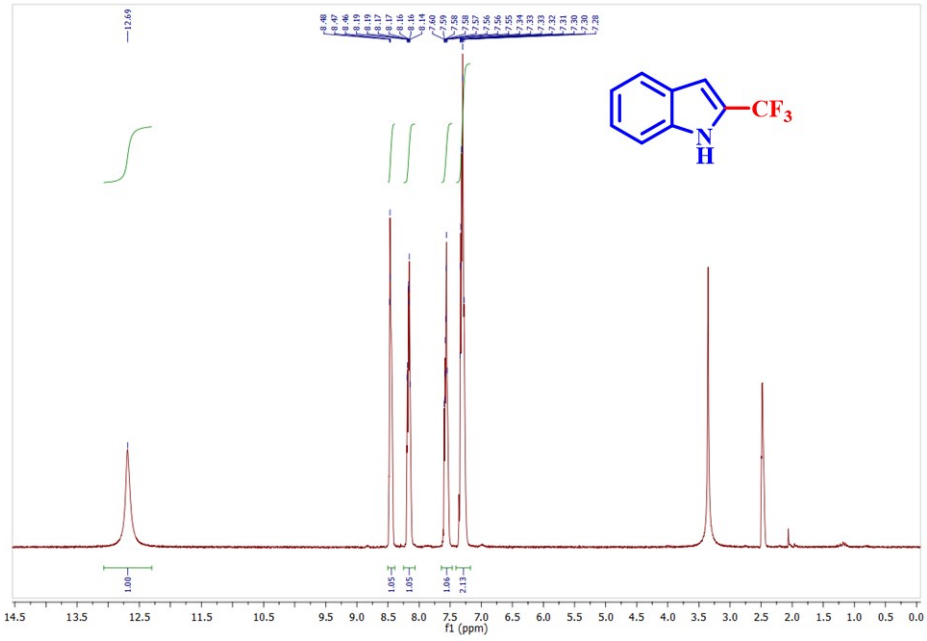


Figure S31. ^{1}H NMR spectram of **2-(trifluoromethyl)-1H-indole [**3**].**

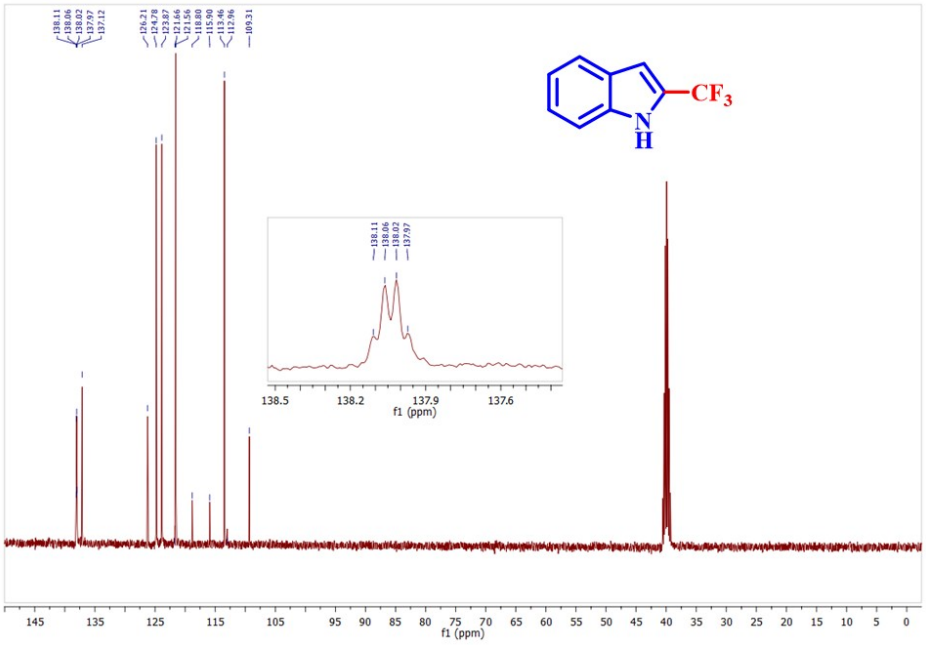


Figure S32. ^{13}C NMR spectram of **2-(trifluoromethyl)-1H-indole [**3].

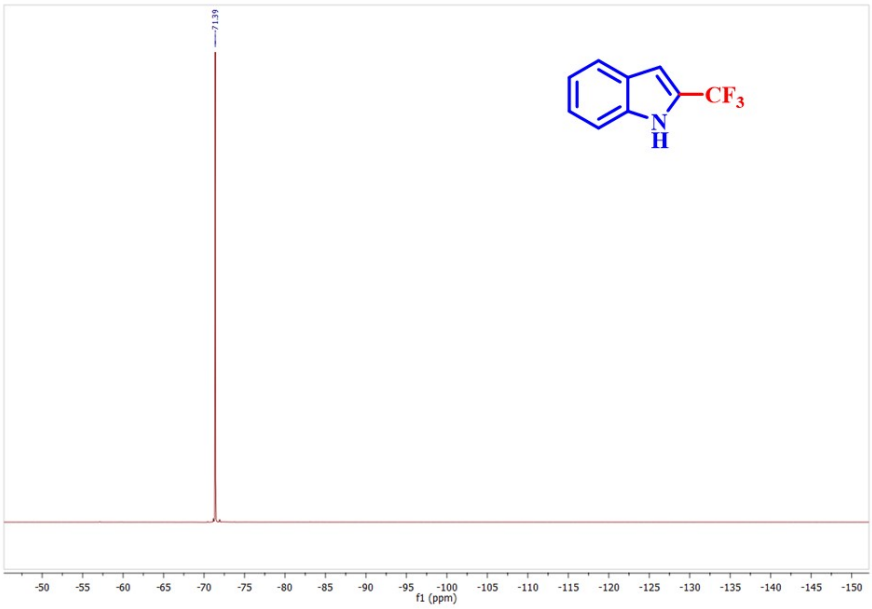


Figure S33. ^{19}F NMR spectram of **2-(trifluoromethyl)-1H-indole [**3].

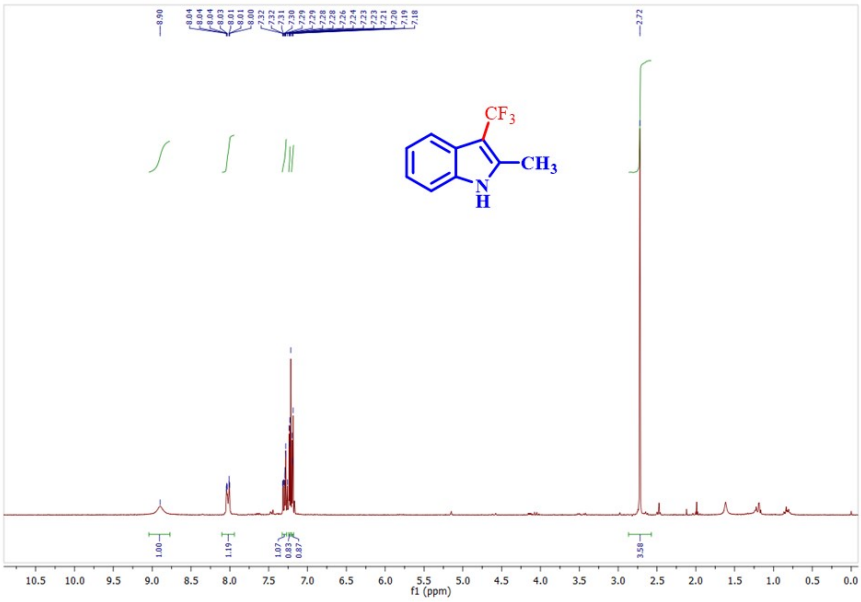


Figure S34.[1]H NMR spectram of **2-Methyl-3-(trifluoromethyl)-1H-indole [**3**].**

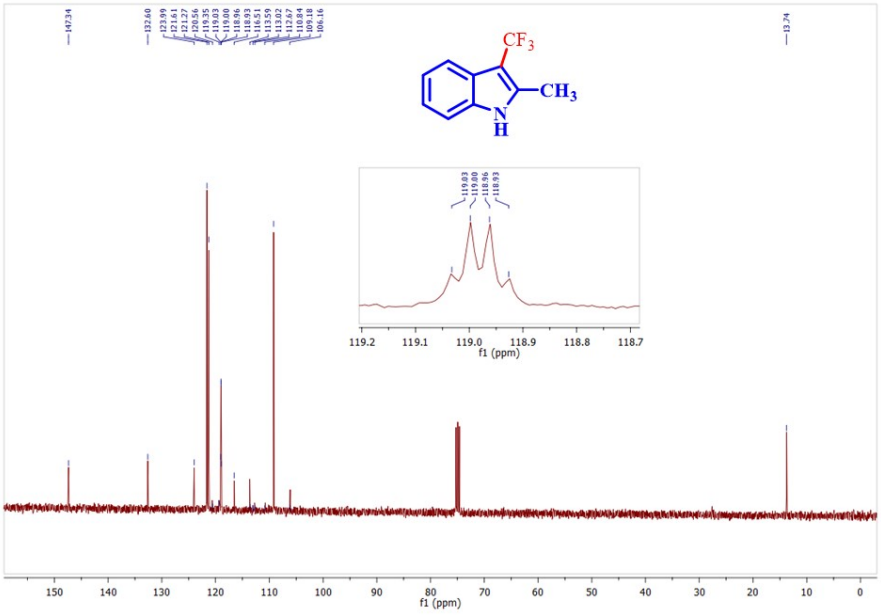


Figure S35.[13]C NMR spectram of **2-Methyl-3-(trifluoromethyl)-1H-indole [**3**].**

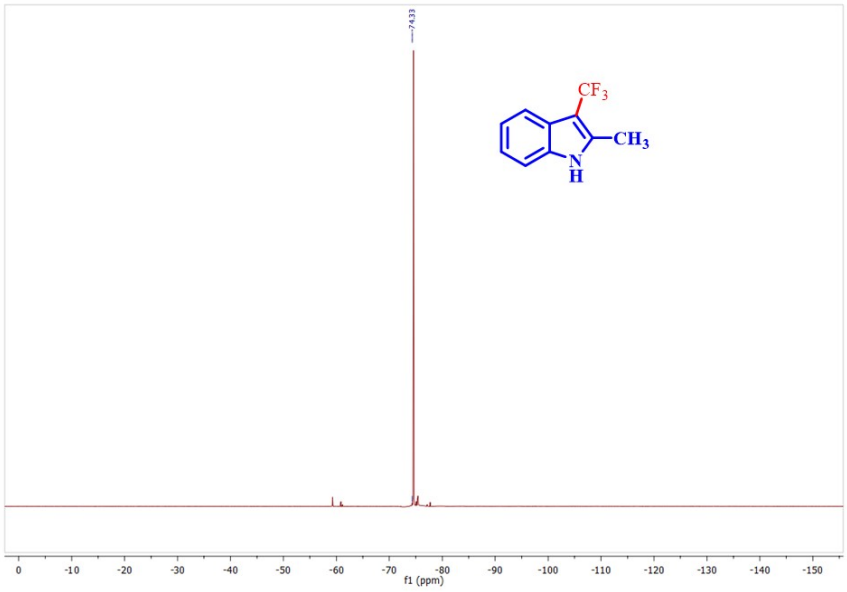


Figure S36.[19]F NMR spectram of **2-Methyl-3-(trifluoromethyl)-1H-indole [**3**].**

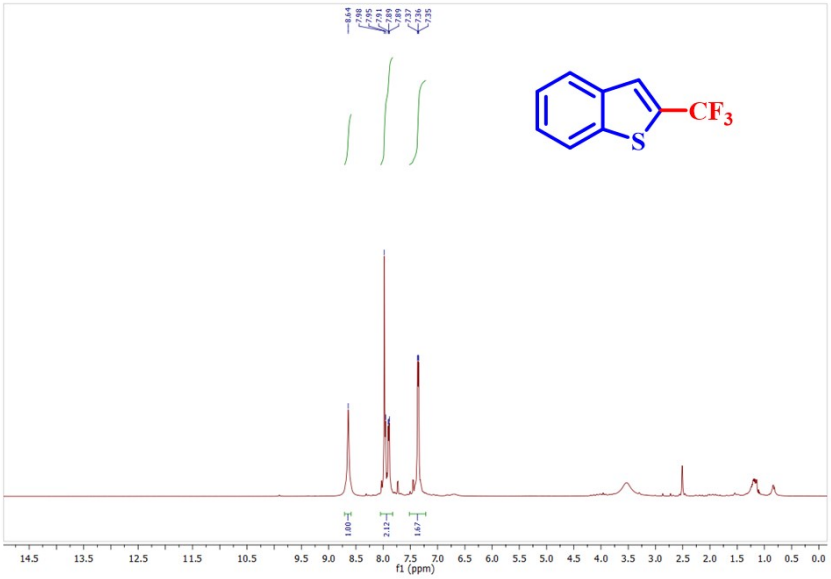


Figure S37.[1]H NMR spectram of **2-(Trifluoromethyl)benzo[b]thiophene [**3**].**

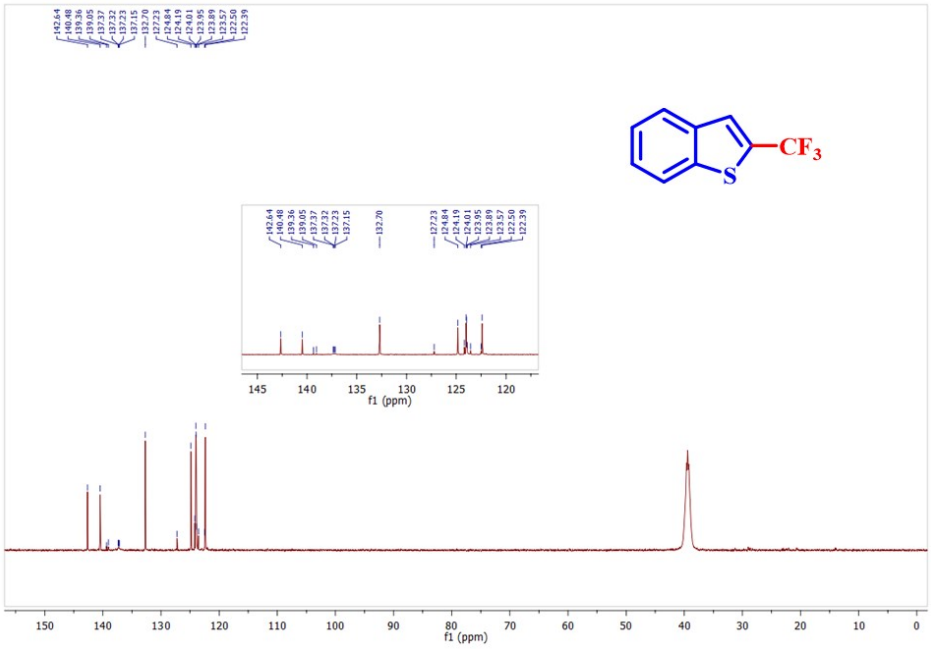


Figure S38.[13]C NMR spectram of **2-(Trifluoromethyl)benzo[b]thiophene [**3**].**

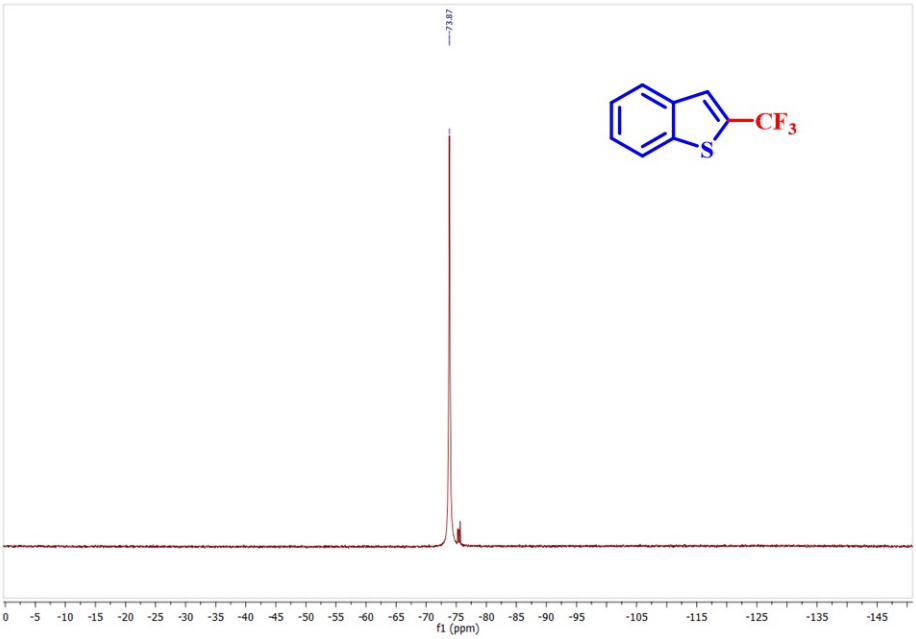


Figure S39.[19]F NMR spectram of **2-(Trifluoromethyl)benzo[b]thiophene [**3**].**

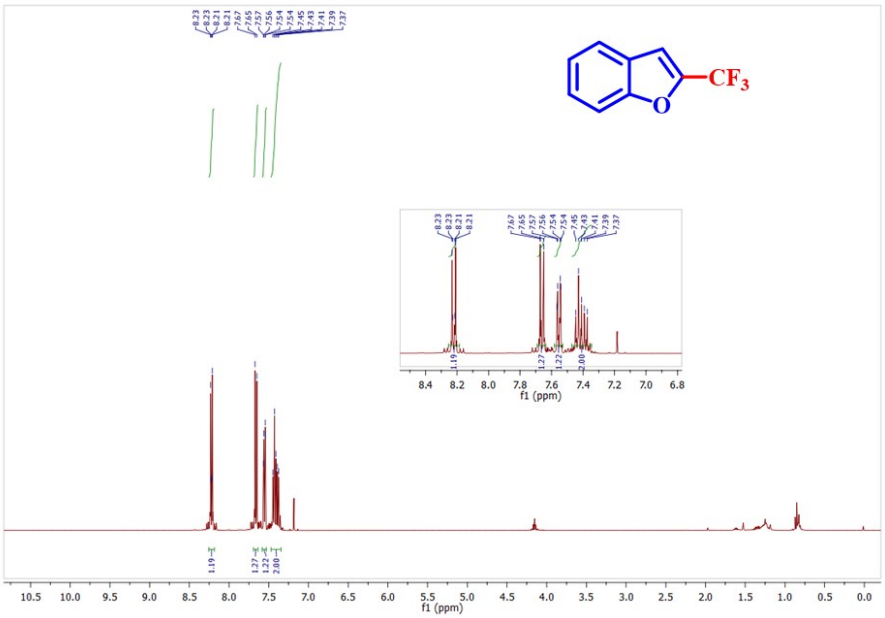


Figure S40.[1]H NMR spectram of **2-(Trifluoromethyl)benzofuran [**3**].**

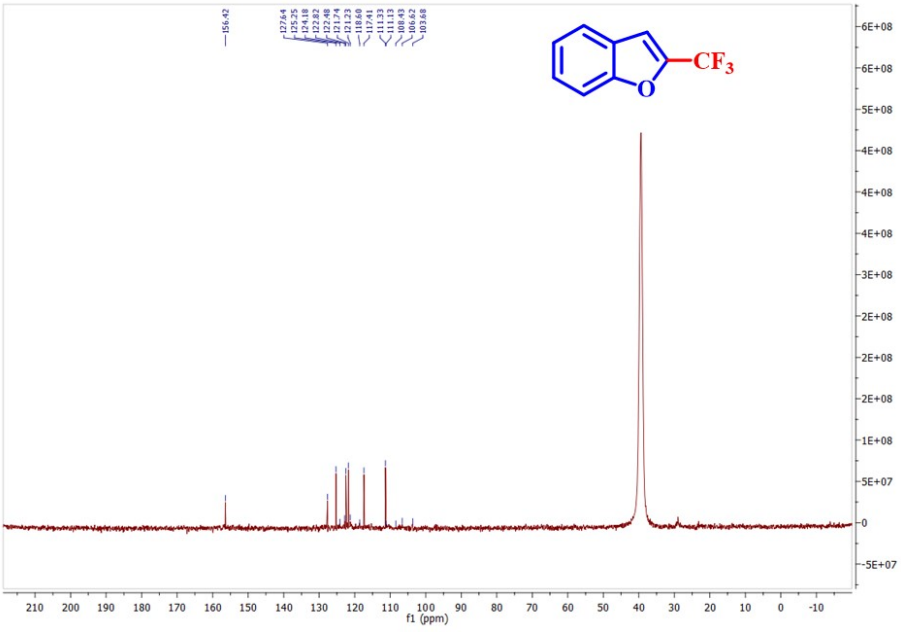


Figure S41.[13]C NMR spectram of **2-(Trifluoromethyl)benzofuran [**3**].**

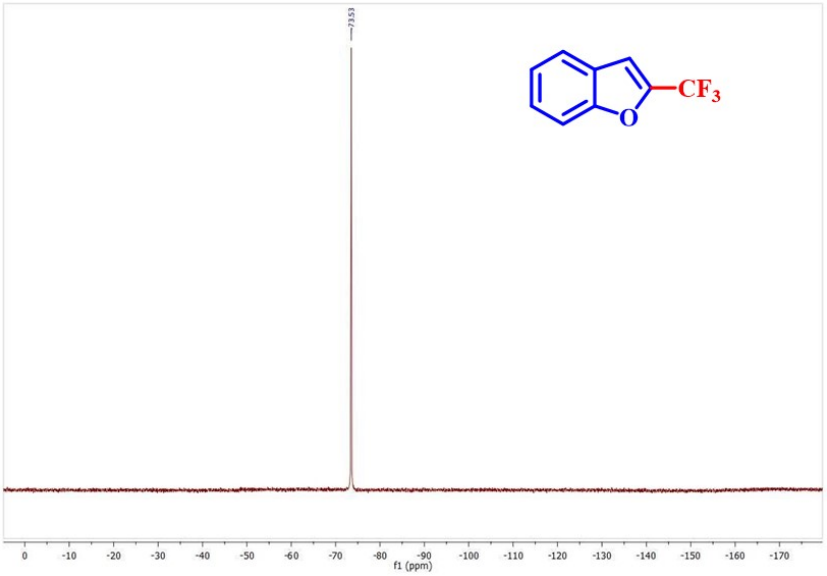


Figure S42.[19]F NMR spectram of **2-(Trifluoromethyl)benzofuran [**3**].**

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