A CONVENIENT SYNTHESIS OF 5-TRIFLUOROMETHYL-5-CYCLOPROPYL-SUBSTITUTED PYRAZOLINES

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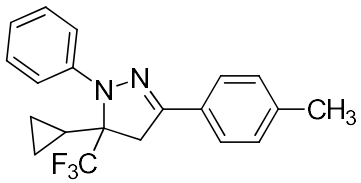
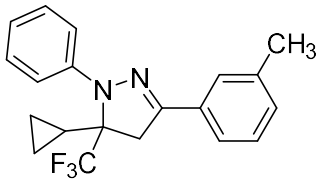
Supporting Information

Spectral data of Pyrazoles



5-cyclopropyl-1-phenyl-3-(*p*-tolyl)-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3aa)

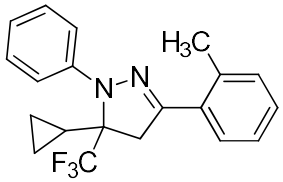
Yield: 83%. Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.2 Hz, 2H), 7.40 (d, *J* = 8.3 Hz, 2H), 7.37-7.32 (m, 2H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.17-7.13 (m, 1H), 3.23 (d, *J* = 17.7 Hz, 1H), 2.71 (d, *J* = 17.7 Hz, 1H), 2.40 (s, 3H), 1.26-1.19 (m, 1H), 0.72-0.63 (m, 1H), 0.52-0.45 (m, 1H), 0.38-0.25 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.43 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.45 (s), 144.60 (s), 139.37 (s), 129.40 (s), 129.02 (s), 128.52 (s), 126.43 (q, *J* = 284.4 Hz), 125.81 (s), 124.42 (s), 123.53 (s), 74.27 (q, *J* = 26.5 Hz), 36.01 (s), 21.44 (s), 9.91 (s), 2.62 (s), -0.18 (s) ppm. IR (KBr): 3032, 2923, 1685, 1597, 1516, 1494, 1452, 1431, 1413, 1372, 1308, 1231, 1167, 1085, 1064, 1043, 1020, 910, 880, 815, 764, 731, 713, 698, 634, 536, 480 cm^{-1}. MS (EI): *m/z* (%) 344 (M^+, 27.91), 275 (100), 276, 119, 91, 77, 65, 51. HRMS (EI): Mass calculated for $C_{20}H_{19}N_2F_3$: 344.1500; Found: 344.1498.



5-cyclopropyl-1-phenyl-3-(*m*-tolyl)-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ba)

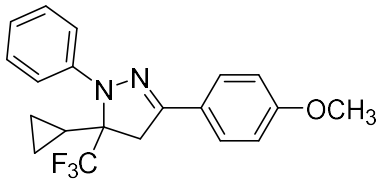
Yield: 81%. Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (s, 1H), 7.49 (d, *J* = 7.7 Hz, 1H), 7.41 (d, *J* = 8.1 Hz, 2H), 7.37-7.28 (m, 3H), 7.22-7.13 (m, 2H), 3.24 (d, *J* = 17.7 Hz, 1H), 2.72 (d, *J* = 17.7 Hz, 1H), 2.41 (s, 3H), 1.27-1.19 (m, 1H), 0.73-0.63 (m, 1H), 0.53-0.46 (m, 1H), 0.38-0.26 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.46 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.43 (s), 144.50 (s), 138.41 (s), 131.70 (s), 130.03 (s), 128.60 (s), 128.55 (s), 126.41 (q, *J* = 284.5 Hz), 126.41 (s), 124.52 (s),

123.59 (s), 123.03 (s), 74.33 (q, J = 26.6 Hz), 35.98 (s), 21.43 (s), 9.93 (s), 2.62 (s), -0.17 (s) ppm. IR (KBr): 3039, 2923, 1687, 1597, 1493, 1453, 1432, 1373, 1307, 1237, 1211, 1167, 1093, 1043, 1024, 908, 883, 851, 819, 784, 764, 729, 696, 638, 581, 564, 524, 481, 443 cm^{-1}. MS (EI): *m/z* (%) 344 (M^+, 23.03), 275 (100), 276, 187, 119, 91, 77, 65. HRMS (EI): Mass calculated for $C_{20}H_{19}N_2F_3$: 344.1500; Found: 344.1492.



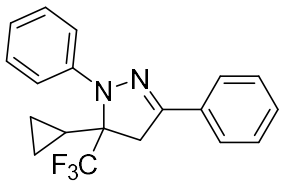
5-cyclopropyl-1-phenyl-3-(*o*-tolyl)-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ca)

Yield: 84%. Yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, J = 8.3 Hz, 2H), 7.38-7.22 (m, 6H), 7.16-7.11 (m, 1H), 3.33 (d, J = 17.6 Hz, 1H), 2.77 (d, J = 17.6 Hz, 1H), 2.68 (s, 3H), 1.35-1.25 (m, 1H), 0.74-0.64 (m, 1H), 0.54-0.46 (m, 1H), 0.42-0.29 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.01 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.05 (s), 144.54 (s), 137.74 (s), 131.85 (s), 130.60 (s), 128.59 (s), 128.52 (s), 127.96 (s), 126.51 (q, J = 285.1 Hz), 125.83 (s), 124.03 (s), 122.52 (d, J = 1.5 Hz), 73.49 (q, J = 26.6 Hz), 38.44 (s), 23.52 (s), 10.06 (s), 2.82 (s), -0.09 (s) ppm. IR (KBr): 3027, 2966, 2927, 1946, 1800, 1695, 1592, 1580, 1563, 1492, 1457, 1450, 1430, 1383, 1367, 1284, 1231, 1209, 1159, 1145, 1085, 1066, 1051, 1037, 1011, 943, 907, 874, 862, 853, 835, 809, 795, 760, 722, 699, 667, 628, 585, 549, 538, 508, 491, 457 cm^{-1}. MS (EI): *m/z* (%) 344 (M^+, 19.10), 275 (100), 276, 91, 77, 65, 64, 51. HRMS (EI): Mass calculated for $C_{20}H_{19}N_2F_3$: 344.1500; Found: 344.1502.



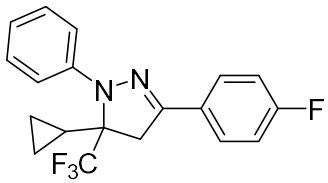
5-cyclopropyl-3-(4-methoxyphenyl)-1-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3da)

Yield: 78%. Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.62 (m, 2H), 7.39 (d, *J* = 8.1 Hz, 2H), 7.33 (dd, *J* = 10.5, 5.3 Hz, 2H), 7.14 (t, *J* = 7.2 Hz, 1H), 6.96-6.91 (m, 2H), 3.85 (s, 3H), 3.20 (d, *J* = 17.7 Hz, 1H), 2.68 (d, *J* = 17.7 Hz, 1H), 1.26-1.16 (m, 1H), 0.71-0.60 (m, 1H), 0.52-0.42 (m, 1H), 0.37-0.23 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.47 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.57 (s), 147.29 (s), 144.73 (s), 128.50 (s), 127.35 (s), 126.45 (q, *J* = 284.6 Hz), 124.54 (s), 124.33 (s), 123.48 (d, *J* = 1.0 Hz), 114.15 (s), 74.19 (dd, *J* = 53.1, 26.5 Hz), 55.44 (s), 36.11 (s), 9.90 (s), 2.63 (s), -0.17 (s) ppm. IR (KBr): 3011, 2961, 2963, 2839, 1679, 1609, 1518, 1493, 1465, 1423, 1374, 1308, 1253, 1233, 1211, 1170, 1112, 1085, 1062, 1016, 910, 880, 833, 794, 764, 731, 698, 541 cm^{-1}. MS (EI): *m/z* (%) 360 (M^+, 27.99), 291 (100), 292, 275, 135, 91, 77, 64. HRMS (EI): Mass calculated for $C_{20}H_{19}N_2OF_3$: 360.1449; Found: 360.1445.



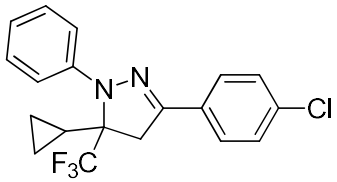
5-cyclopropyl-1,3-diphenyl-5-(trifluoromethyl)-4,5-dihydro-1H-pyrazole (3ea)

Yield: 84%. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.70 (m, 2H), 7.45-7.32 (m, 7H), 7.19-7.14 (m, 1H), 3.25 (d, *J* = 17.7 Hz, 1H), 2.73 (d, *J* = 17.8 Hz, 1H), 1.28-1.20 (m, 1H), 0.73-0.64 (m, 1H), 0.55-0.45 (m, 1H), 0.40-0.25 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.45 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.26 (s), 144.42 (s), 131.78 (s), 129.21 (q, *J* = 284.6 Hz), 129.19 (s), 128.70 (s), 128.56 (s), 125.82 (s), 124.53 (s), 123.54 (d, *J* = 1.2 Hz), 74.40 (q, *J* = 26.7 Hz), 35.90 (s), 9.92 (s), 2.65 (s), -0.17 (s) ppm. IR (KBr): 3061, 3029, 2922, 1690, 1596, 1493, 1448, 1431, 1374, 1308, 1231, 1211, 1167, 1088, 1062, 1043, 1016, 910, 880, 847, 759, 730, 693, 637, 578, 563, 536, 478 cm^{-1}. MS (EI): *m/z* (%) 330 (M^+, 18.77), 261 (100), 262, 104, 91, 77, 64, 51. HRMS (EI): Mass calculated for $C_{19}H_{17}N_2F_3$: 330.1344; Found: 330.1339.



5-cyclopropyl-3-(4-fluorophenyl)-1-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3fa)

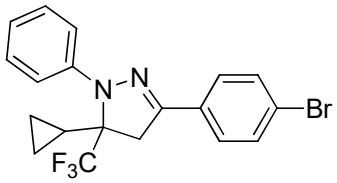
Yield: 85%. Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71-7.64 (m, 2H), 7.40-7.30 (m, 4H), 7.18-7.06 (m, 3H), 3.20 (d, *J* = 17.7 Hz, 1H), 2.68 (d, *J* = 17.7 Hz, 1H), 1.26-1.17 (m, 1H), 0.72-0.63 (m, 1H), 0.51-0.43 (m, 1H), 0.39-0.32 (m, 1H), 0.32-0.24 (m, 1H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.51 (s, 3F), -110.59– -113.17 (m, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.59 (s), 162.10 (s), 146.32 (s), 144.34 (s), 128.59 (s), 127.65 (d, *J* = 8.3 Hz), 126.35 (q, *J* = 284.6 Hz), 124.63 (s), 123.55 (d, *J* = 1.3 Hz), 115.80 (d, *J* = 21.9 Hz), 74.54 (q, *J* = 26.7 Hz), 35.99 (s), 9.93 (s), 2.68 (s), -0.13 (s) ppm. IR (KBr): 3061, 3019, 1690, 1604, 1578, 1494, 1453, 1431, 1415, 1371, 1307, 1232, 1157, 1086, 1065, 1043, 1018, 910, 880, 836, 810, 765, 728, 698, 631, 614, 574, 536, 483, 427 cm^{-1}. MS (EI): *m/z* (%) 348 (M^+, 22.80), 279 (100), 280, 93, 91, 77, 64, 51. HRMS (EI): Mass calculated for $C_{19}H_{16}N_2F_4$: 348.1250; Found: 348.1249.



3-(4-chlorophenyl)-5-cyclopropyl-1-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ga)

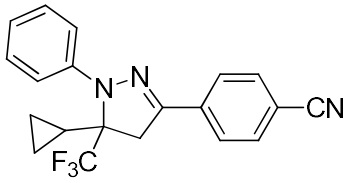
Yield: 90%. Yellow oil.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64-7.59 (m, 2H), 7.39-7.31 (m, 6H), 7.18-7.13 (m, 1H), 3.20 (d, *J* = 17.7 Hz, 1H), 2.67 (d, *J* = 17.7 Hz, 1H), 1.26-1.18 (m, 1H), 0.72-0.64 (m, 1H), 0.51-0.44 (m, 1H), 0.40-0.32 (m, 1H), 0.32-0.24 (m, 1H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.47 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.08 (s), 144.16 (s), 135.00 (s), 130.33 (s), 128.94 (s), 128.62 (s), 127.00 (s), 126.30 (q, *J* = 284.8 Hz), 124.74 (s), 123.56 (d, *J* = 1.3 Hz), 74.68 (q, *J* = 26.7 Hz), 35.81 (s), 9.99 (d, *J* = 1.1 Hz), 2.71 (s), -0.11 (s) ppm. IR (KBr): 3062, 2922, 1942, 1690, 1598,

1560, 1492, 1453, 1432, 1406, 1371, 1306, 1232, 1211, 1167, 1092, 1066, 1043, 1012, 909, 880, 830, 765, 738, 720, 697, 638, 533, 488, 408 cm^{-1}. MS (EI): *m/z* (%) 364 (M^+, 21.34), 295 (100), 297, 296, 105, 91, 77, 64. HRMS (EI): Mass calculated for $C_{19}H_{16}N_2F_3Cl$: 364.0954; Found: 364.0949.



3-(4-bromophenyl)-5-cyclopropyl-1-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ha)

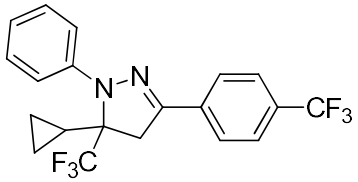
Yield: 60%. Yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.58-7.50 (m, 4H), 7.41-7.32 (m, 4H), 7.19-7.14 (m, 1H), 3.20 (d, *J* = 17.7 Hz, 1H), 2.68 (d, *J* = 17.7 Hz, 1H), 1.28-1.18 (m, 1H), 0.73-0.65 (m, 1H), 0.52-0.45 (m, 1H), 0.41-0.32 (m, 1H), 0.32-0.24 (m, 1H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.41 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.11 (s), 144.11 (s), 131.88 (s), 130.75 (s), 128.63 (s), 127.23 (s), 126.28 (q, *J* = 284.5 Hz), 124.77 (s), 123.58 (d, *J* = 1.3 Hz), 123.23 (s), 74.70 (q, *J* = 26.7 Hz), 35.73 (s), 9.97 (s), 2.70 (s), -0.11 (s) ppm. IR (KBr): 3062, 3039, 2928, 2855, 1690, 1596, 1557, 1491, 1453, 1431, 1402, 1370, 1305, 1232, 1211, 1166, 1070, 1008, 909, 880, 820, 764, 733, 697, 670, 637, 581 cm^{-1}. MS (EI): *m/z* (%) 408 (M^+, 18.71), 77 (100), 91, 339, 341, 64, 51, 261, 102. HRMS (EI): Mass calculated for $C_{19}H_{16}N_2F_3Br$: 408.0449; Found: 408.0450.



4-(5-cyclopropyl-1-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazol-3-yl)benzonitrile (3ia)

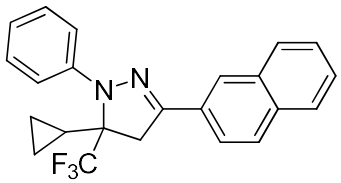
Yield: 85%. Yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.6 Hz, 2H), 7.66 (d, *J* = 8.6 Hz, 2H), 7.40-7.32 (m, 4H), 7.21-7.16 (m, 1H), 3.21 (d, *J* = 17.7 Hz, 1H), 2.69 (d, *J* = 17.8 Hz, 1H), 1.31-1.23 (m, 1H), 0.77-0.67 (m, 1H), 0.54-0.46 (m, 1H),

0.45-0.37 (m, 1H), 0.34-0.26 (m, 1H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.48 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.79 (s), 143.50 (s), 136.07 (s), 132.47 (s), 128.76 (s), 126.13 (q, *J* = 285.2 Hz), 125.99 (s), 125.21 (s), 123.61 (d, *J* = 1.4 Hz), 118.79 (s), 111.96 (s), 75.25 (q, *J* = 26.8 Hz), 35.42 (d, *J* = 0.8 Hz), 10.13 (d, *J* = 1.0 Hz), 2.87 (s), 0.07 (s) ppm. IR (KBr): 3063, 3016, 2924, 2852, 2227, 1691, 1592, 1579, 1550, 1493, 1454, 1430, 1414, 1376, 1309, 1232, 1211, 1170, 1096, 1044, 1072, 1019, 912, 881, 851, 764, 738, 698, 637, 559, 540, 511, 472 cm^{-1}. MS (EI): *m/z* (%) 355 (M^+, 19.39), 77 (100), 286, 130,105, 102, 91, 51. HRMS (EI): Mass calculated for $C_{20}H_{16}N_3F_3$: 355.1296; Found: 355.1302.



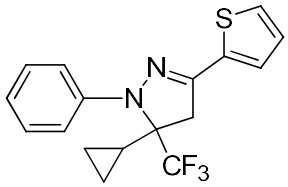
5-cyclopropyl-1-phenyl-5-(trifluoromethyl)-3-(4-(trifluoromethyl)phenyl)-4,5-dihydro-1*H*-pyrazole (3ja)

Yield: 85%. Yellow oil. ^{1}H NMR (400 MHz, CDCl3) δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.42-7.31 (m, 4H), 7.18 (t, *J* = 7.0 Hz, 1H), 3.23 (d, *J* = 17.7 Hz, 1H), 2.72 (d, *J* = 17.7 Hz, 1H), 1.29-1.21 (m, 1H), 0.75-0.67 (m, 1H), 0.54-0.46 (m, 1H), 0.43-0.35 (m, 1H), 0.33-0.26 (m, 1H) ppm. ^{19}F NMR (376 MHz, CDCl3) δ -62.72 (s, 3F), -76.47 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.52 (s), 143.83 (s), 135.17 (d, *J* = 1.3 Hz), 130.63 (q, *J* = 32.6 Hz), 128.71 (s), 126.80 (q, *J* = 272.0 Hz), 126.22 (q, *J* = 284.8 Hz), 125.86 (s), 125.68 (q, *J* = 3.8 Hz), 125.03 (s), 123.67 (d, *J* = 1.4 Hz), 74.95 (q, *J* = 26.8 Hz), 35.63 (d, *J* = 0.9 Hz), 10.02 (d, *J* = 1.2 Hz), 2.76 (s), -0.09 (s) ppm. IR (KBr): 3064, 2925, 1618, 1596, 1565, 1495, 1415, 1377, 1326, 1232, 1212, 1169, 1127, 1068, 1044, 1014, 880, 850, 764, 729, 699, 599, 529, 483 cm^{-1}. MS (EI): *m/z* (%) 398 (M^+, 35.33), 329 (100), 330, 173, 145, 91, 77, 64. HRMS (EI): Mass calculated for $C_{20}H_{16}N_2F_6$: 398.1218; Found: 398.1212.



5-cyclopropyl-3-(naphthalen-2-yl)-1-phenyl-5-(trifluoromethyl)-4,5-dihydro-1H-pyrazole (3ka)

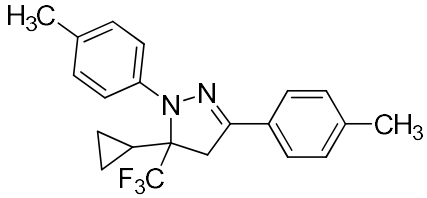
Yield: 93%. Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 8.8, 1.5 Hz, 1H), 7.87-7.82 (m, 4H), 7.54-7.48 (m, 2H), 7.44 (d, *J* = 8.3 Hz, 2H), 7.39-7.33 (m, 2H), 7.20-7.15 (m, 1H), 3.37 (d, *J* = 17.6 Hz, 1H), 2.84 (d, *J* = 17.6 Hz, 1H), 1.32-1.22 (m, 1H), 0.76-0.66 (m, 1H), 0.60-0.50 (m, 1H), 0.42-0.30 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.29 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.32 (s), 144.38 (s), 133.69 (s), 133.25 (s), 129.46 (s), 128.61 (s), 128.45 (s), 128.21 (s), 127.92 (s), 126.74 (s), 126.70 (s), 126.42 (q, *J* = 284.7 Hz), 125.30 (s), 124.63 (s), 123.61 (d, *J* = 1.3 Hz), 123.36 (s), 74.62 (q, *J* = 26.6 Hz), 35.90 (s), 10.03 (d, *J* = 0.9 Hz), 2.72 (s), -0.10 (s) ppm. IR (KBr): 3060, 2922, 2849, 2247, 1946, 1684, 1629, 1597, 1493, 1476, 1452, 1431, 1396, 1379, 1348, 1306, 1242, 1226, 1211, 1166, 1088, 1066, 1044, 1022, 948, 909, 886, 860, 821, 749, 733, 698, 672, 649, 638, 574, 545, 476 cm^{-1}. MS (EI): *m/z* (%) 380 (M^+, 27.05), 311 (100), 312, 155, 127, 126, 91, 77. HRMS (EI): Mass calculated for $C_{23}H_{19}N_2F_3$: 380.1500; Found: 380.1494.



5-cyclopropyl-1-phenyl-3-(thiophen-2-yl)-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3la)

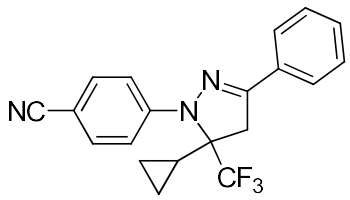
Yield: 75%. Yellow oil. 1H NMR (400 MHz, $CDCl_3$) δ 7.39-7.28 (m, 5H), 7.15 (d, *J* = 6.9 Hz, 1H), 7.11 (d, *J* = 3.6 Hz, 1H), 7.07-7.03 (m, 1H), 3.23 (d, *J* = 17.6 Hz, 1H), 2.70 (d, *J* = 17.6 Hz, 1H), 1.24-1.15 (m, 1H), 0.72-0.63 (m, 1H), 0.50-0.42 (m, 1H), 0.39-0.25 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.46 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.15 (s), 143.43 (s), 135.49 (s), 128.51 (s), 127.35 (s), 127.19

(s), 126.18 (q, J = 284.5 Hz), 124.65 (s), 123.72 (s), 123.71 (s), 74.50 (q, J = 26.8 Hz), 36.53 (d, J = 1.1 Hz), 9.80 (d, J = 1.2 Hz), 2.59 (s), -0.19 (s) ppm. IR (KBr): 3084, 3015, 2923, 2849, 1663, 1598, 1522, 1493, 1470, 1443, 1415, 1369, 1344, 1305, 1267, 1228, 1210, 1167, 1085, 1044, 1026, 908, 880, 865, 838, 764, 698, 625, 577, 564, 547, 523, 471, 419 cm^{-1}. MS (EI): *m/z* (%) 336 (M^+, 51.35), 267 (100), 269, 268, 111, 97, 91, 77. HRMS (EI): Mass calculated for $C_{17}H_{15}N_2F_3S$: 336.0909; Found: 336.0908.



5-cyclopropyl-1,3-di-*p*-tolyl-5-(trifluoromethyl)-4,5-dihydro-1H-pyrazole (3ab)

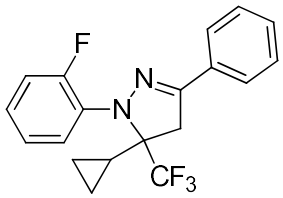
Yield: 60%. Yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.2 Hz, 2H), 7.26 (d, J = 8.3 Hz, 2H), 7.20 (d, J = 8.0 Hz, 2H), 7.12 (d, J = 8.3 Hz, 2H), 3.19 (d, J = 17.7 Hz, 1H), 2.66 (d, J = 17.6 Hz, 1H), 2.38 (s, 3H), 2.34 (s, 3H), 1.16-1.07 (m, 1H), 0.67-0.59 (m, 1H), 0.48-0.40 (m, 1H), 0.36-0.23 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.33 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.98 (s), 141.98 (s), 139.13 (s), 134.31 (s), 129.29 (s), 129.07 (s), 129.01 (s), 126.38 (q, J = 284.2 Hz), 125.67 (s), 124.11 (s), 74.27 (q, J = 26.4 Hz), 35.64 (s), 21.35 (s), 20.88 (s), 9.76 (s), 2.24 (s), -0.28 (s) ppm. IR (KBr): 3031, 2923, 2858, 1653, 1611, 1576, 1559, 1541, 1509, 1457, 1431, 1412, 1371, 1308, 1231, 1209, 1165, 1112, 1069, 1041, 1020, 933, 881, 816, 792, 719, 535, 484, 419 cm^{-1}. MS (EI): *m/z* (%) 358 (M^+, 42.38), 289 (100), 359, 290, 221, 143, 105, 91. HRMS (EI): Mass calculated for $C_{21}H_{21}N_2F_3$: 358.1645; Found: 358.1657.



4-(5-cyclopropyl-3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1H-pyrazol-1-yl)benzonitrile (3ec)

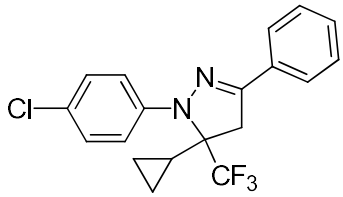
Yield: 40%. Yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.74-7.68 (m, 2H), 7.59-7.55 (m, 2H), 7.53-7.48 (m, 2H), 7.46-7.40 (m, 3H), 3.34 (d, J = 18.0 Hz, 1H), 2.86 (d, J =

18.0 Hz, 1H), 1.65-1.57 (m, 2H), 0.90-0.81 (m, 2H), 0.71-0.63 (m, 1H), 0.55-0.47 (m, 1H), 0.36-0.28 (m, 1H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.39 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.77 (s), 147.55 (s), 132.92 (s), 130.94 (s), 130.03 (s), 128.88 (s), 126.11 (q, *J* = 286.0 Hz), 126.10 (s), 119.66 (s), 118.85 (d, *J* = 2.0 Hz), 104.46 (s), 74.03 (q, *J* = 27.5 Hz), 37.86 (d, *J* = 1.0 Hz), 10.52 (s), 4.44 (s), 0.51 (s) ppm. IR (KBr): 3055, 2925, 2852, 2221, 1606, 1559, 1541, 1508, 1498, 1448, 1431, 1392, 1298, 1266, 1235, 1215, 1177, 1122, 1084, 1071, 1046, 1018, 1008, 940, 880, 835, 760, 739, 692, 546 cm^{-1}. MS (EI): *m/z* (%) 355 (M^+, 34.42), 286 (100), 287, 97, 83, 69, 57, 55. HRMS (EI): Mass calculated for $C_{20}H_{16}N_3F_3$: 355.1295; Found: 355.1296.



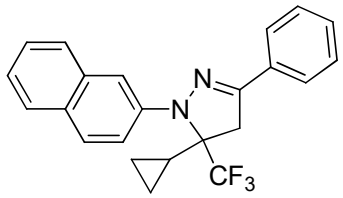
5-cyclopropyl-1-(2-fluorophenyl)-3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ed)

Yield: 68%. Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.63 (m, 2H), 7.48-7.42 (m, 1H), 7.41-7.33 (m, 3H), 7.29-7.22 (m, 1H), 7.16-7.08 (m, 2H), 3.21 (d, *J* = 17.6 Hz, 1H), 2.68 (d, *J* = 17.6 Hz, 1H), 1.03-0.94 (m, 1H), 0.70-0.61 (m, 1H), 0.52-0.38 (m, 3H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -77.16 (d, *J* = 7.6 Hz, 3F), -117.26– -117.40 (m, 1F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.65 (d, *J* = 252.5 Hz), 147.72 (s), 131.72 (s), 131.36 (d, *J* = 10.3 Hz), 130.75 (s), 129.25 (s), 128.69 (s), 128.59 (s), 126.31 (q, *J* = 284.3 Hz), 125.90 (s), 123.92 (d, *J* = 3.7 Hz), 116.58 (d, *J* = 20.8 Hz), 74.77 (q, *J* = 26.7 Hz), 34.98 (s), 9.40 (s), 2.03 (s), 0.10 (s) ppm. IR (KBr): 3066, 3029, 2927, 2853, 1953, 1805, 1724, 1690, 1599, 1570, 1497, 1448, 1432, 1370, 1308, 1264, 1241, 1210, 1166, 1111, 1065, 1042, 1017, 936, 888, 872, 812, 801, 758, 740, 725, 692, 667, 632, 582, 563, 549, 537, 458 cm^{-1}. MS (EI): *m/z* (%) 348 (M^+, 32.37), 279 (100), 349, 280, 109, 95, 77, 82. HRMS (EI): Mass calculated for $C_{19}H_{16}N_2F_4$: 348.1257; Found: 348.1250.



1-(4-chlorophenyl)-5-cyclopropyl-3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ee)

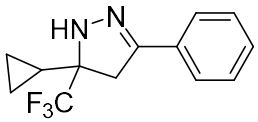
Yield: 75%. Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72-7.65 (m, 2H), 7.44-7.35 (m, 3H), 7.30 (q, *J* = 9.0 Hz, 4H), 3.23 (d, *J* = 17.8 Hz, 1H), 2.71 (d, *J* = 17.9 Hz, 1H), 1.26-1.17 (m, 1H), 0.70 (ddd, *J* = 14.8, 8.7, 6.1 Hz, 1H), 0.50 (td, *J* = 11.0, 5.7 Hz, 1H), 0.40-0.31 (m, 1H), 0.26 (td, *J* = 11.3, 5.6 Hz, 1H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.59 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.83 (s), 143.02 (s), 131.43 (s), 129.60 (s), 129.40 (s), 128.70 (s), 128.57 (s), 126.20 (q, *J* = 284.6 Hz), 125.83 (s), 124.31 (d, *J* = 1.6 Hz), 74.30 (q, *J* = 26.7 Hz), 36.00 (d, *J* = 0.9 Hz), 9.83 (d, *J* = 1.1 Hz), 2.79 (s), -0.22 (s) ppm. IR (KBr): 3030, 2927, 2853, 1675, 1593, 1568, 1489, 1448, 1374, 1307, 1232, 1211, 1169, 1109, 1092, 1063, 1040, 1013, 911, 880, 829, 759, 740, 717, 691, 649, 626, 583, 536, 508 cm^{-1}. MS (EI): *m/z* (%) 364 (M^+, 41.37), 295 (100), 297, 296, 212, 111, 105, 77. HRMS (EI): Mass calculated for $C_{19}H_{16}N_2F_3Cl$: 364.0958; Found: 364.0954.



5-cyclopropyl-1-(naphthalen-2-yl)-3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1H-pyrazole (3ef)

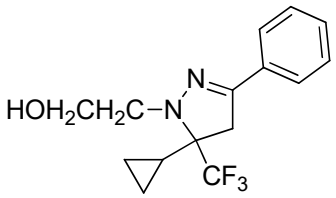
Yield: 32%. Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84-7.71 (m, 6H), 7.60 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.49-7.36 (m, 5H), 3.28 (d, *J* = 17.8 Hz, 1H), 2.77 (d, *J* = 17.7 Hz, 1H), 1.36-1.23 (m, 1H), 0.73-0.61 (m, 1H), 0.56-0.44 (m, 1H), 0.36-0.25 (m, 2H) ppm. ^{19}F NMR (376 MHz, cdcl3) δ -76.44 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.60 (s), 142.03 (s), 133.77 (s), 131.70 (s), 130.93 (s), 129.26 (s), 128.70 (s), 128.10 (s), 127.68 (s), 127.51 (s), 126.37 (q, *J* = 284.4 Hz), 126.17 (s), 125.86 (s), 124.92 (s),

123.13 (s), 120.06 (s), 74.50 (q, J = 26.7 Hz), 36.05 (s), 10.01 (s), 2.72 (s), -0.12 (s) ppm. IR (KBr): 3058, 2925, 2851, 1951, 1810, 1689, 1630, 1596, 1569, 1508, 1469, 1447, 1375, 1306, 1244, 1211, 1166, 1066, 1042, 1015, 964, 910, 876, 856, 815, 786, 758, 692, 651, 591, 549, 536, 475 cm^{-1}. MS (EI): *m/z* (%) 380 (M^+, 49.69), 311 (100), 312, 158, 128, 127, 105, 77. HRMS (EI): Mass calculated for $C_{23}H_{19}N_2F_3$: 380.1492; Found: 380.1500.



5-cyclopropyl-3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3eg)

Yield: 81%. Yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.65-7.59 (m, 2H), 7.45-7.32 (m, 3H), 5.53 (s, 1H), 3.41 (dd, J = 17.2, 1.3 Hz, 1H), 3.03 (d, J = 17.2 Hz, 1H), 1.31-1.22 (m, 1H), 0.64-0.39 (m, 4H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.21 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.73 (s), 131.75 (s), 129.25 (s), 128.57 (s), 126.73 (q, J = 283.5 Hz), 125.95 (s), 69.11 (q, J = 26.6 Hz), 39.34 (s), 13.18 (d, J = 1.8 Hz), 1.09 (s), -0.25 (s) ppm. IR (KBr): 3347, 3063, 3018, 2927, 2333, 1683, 1598, 1581, 1498, 1449, 1356, 1320, 1296, 1170, 1032, 914, 872, 830, 759, 692, 643, 550 cm^{-1}. MS (EI): *m/z* (%) 254 (M^+, 0.38), 105 (100), 213, 212, 189, 115, 106, 77, 51. HRMS (EI): Mass calculated for $C_{13}H_{13}N_2F_3$: 254.1031; Found: 254.1044.

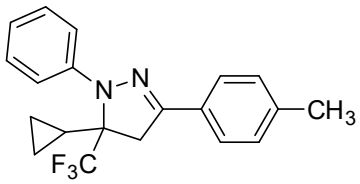


2-(5-cyclopropyl-3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1H-pyrazol-1-yl)ethane (3eh)

Yield: 67%. Yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.58-7.50 (m, 2H), 7.42-7.29 (m, 3H), 4.10-3.97 (m, 2H), 3.48 (ddd, J = 12.5, 6.7, 2.8 Hz, 1H), 3.36 (ddd, J = 12.4, 5.8, 2.8 Hz, 1H), 3.14 (d, J = 17.6 Hz, 1H), 2.58 (d, J = 17.7 Hz, 1H), 1.34-1.25 (m, 2H), 0.75-0.66 (m, 1H), 0.65-0.56 (m, 1H), 0.53-0.44 (m, 1H), 0.39-0.31 (m, 1H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -76.05 (s, 3F) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ

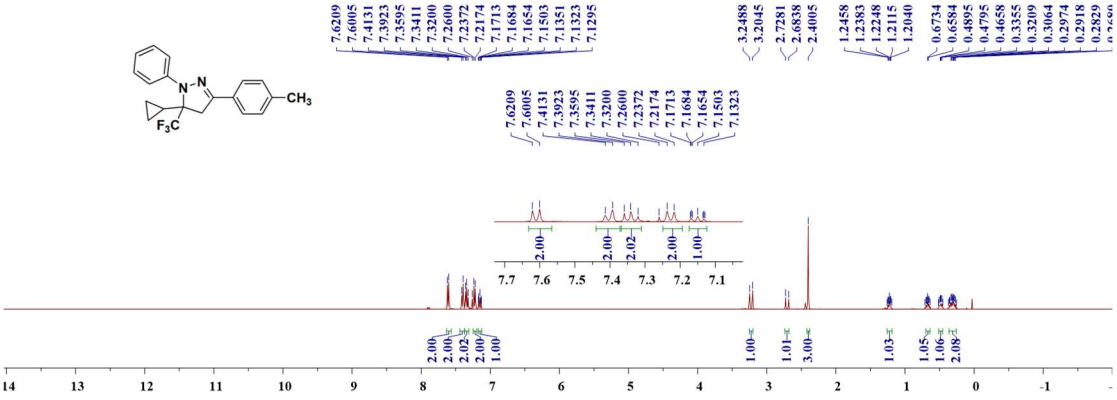
146.24 (s), 131.27 (s), 129.25 (s), 128.72 (s), 126.55 (q, J = 284.2 Hz), 125.66 (s), 73.47 (q, J = 26.2 Hz), 62.56 (s), 51.56 (s), 35.03 (s), 8.97 (s), 1.26 (s), -0.02 (s) ppm. IR (KBr): 3567, 3447, 3061, 3027, 2926, 2856, 1596, 1569, 1498, 1448, 1368, 1312, 1255, 1159, 1036, 972, 936, 921, 878, 845, 759, 730, 693, 660, 621, 549, 537, 506, 437, 417 cm^{-1}. MS (EI): *m/z* (%) 298 (M^+, 19.08), 267 (100), 268, 229, 131, 104, 77, 55. HRMS (EI): Mass calculated for $C_{15}H_{17}N_2OF_3$: 298.1292; Found: 298.1293.

^{1}H, ^{19}F and ^{13}C NMR Spectrum of Pyrazoles

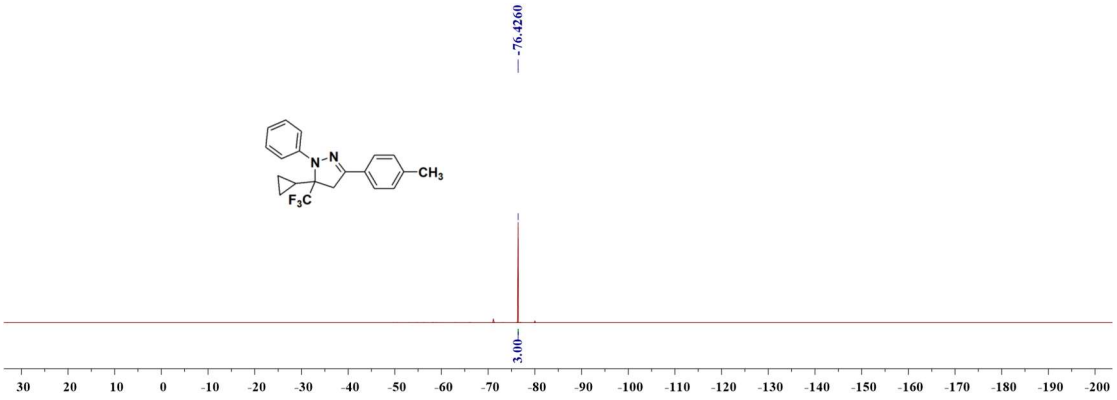


Spectrum of 5-cyclopropyl-1-phenyl-3-(*p*-tolyl)-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3aa)

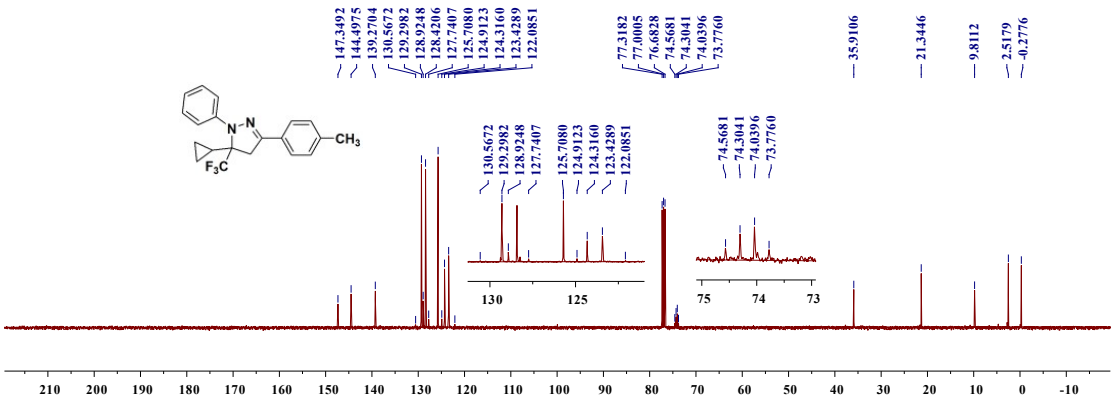
^{1}H NMR

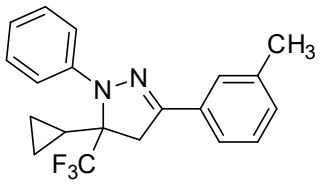


^{19}F NMR



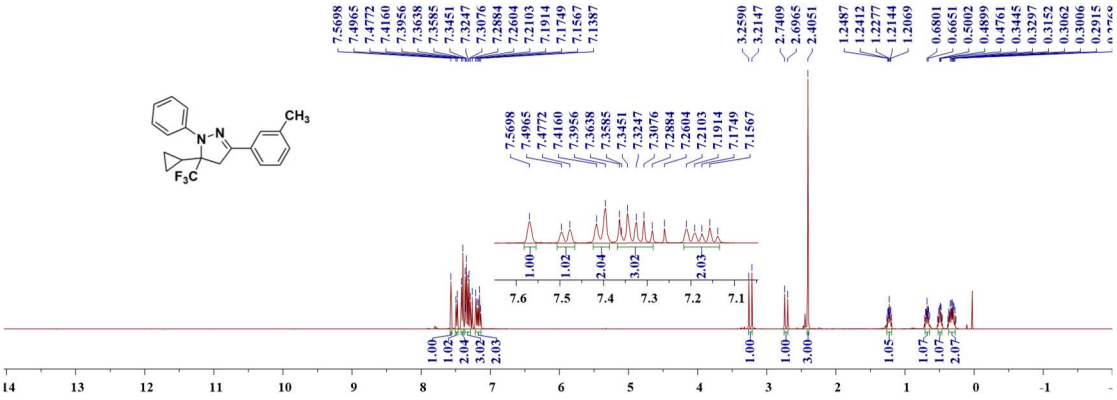
^{13}C NMR



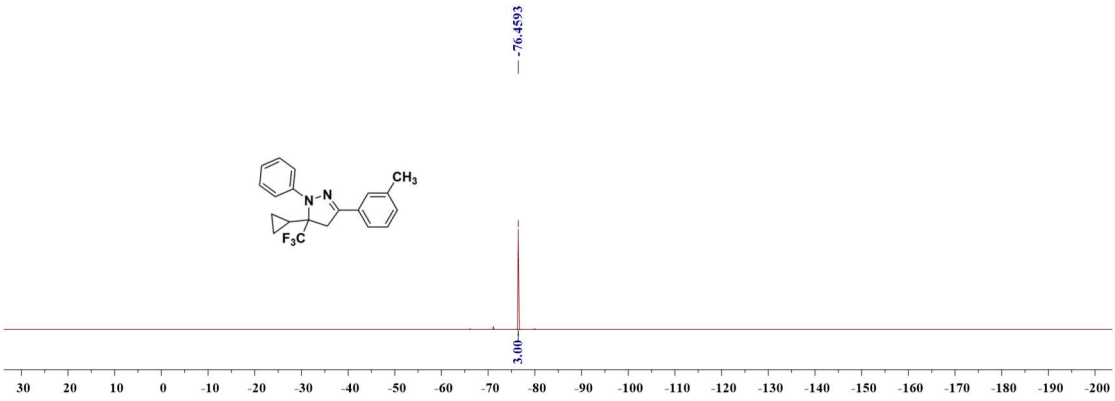


Spectrum of 5-cyclopropyl-1-phenyl-3-(*m*-tolyl)-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ba)

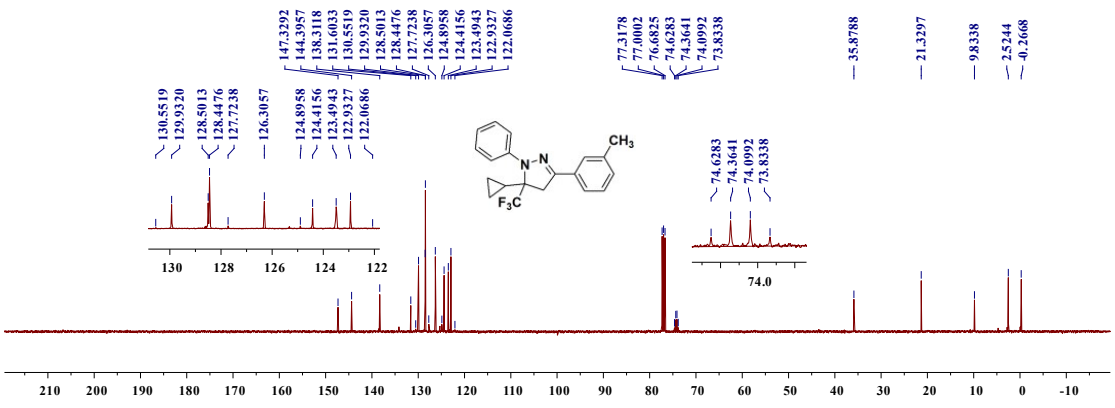
^{1}H NMR

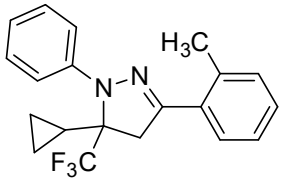


^{19}F NMR



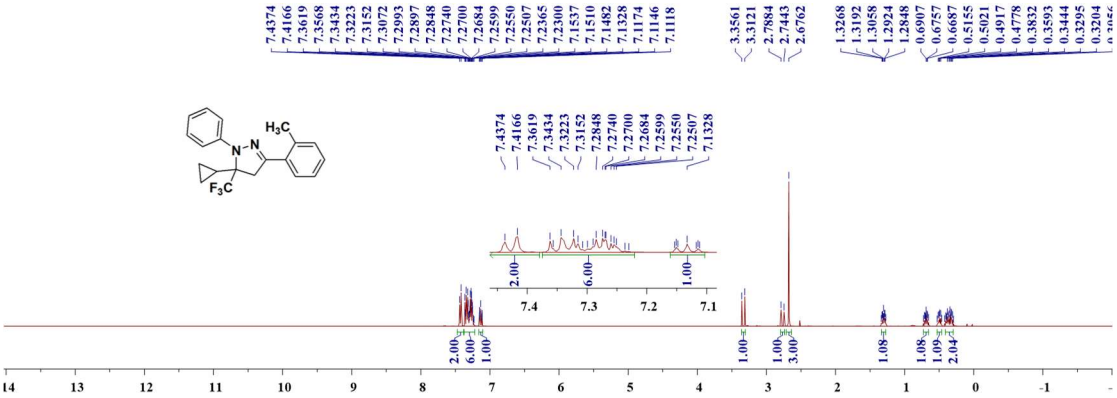
^{13}C NMR



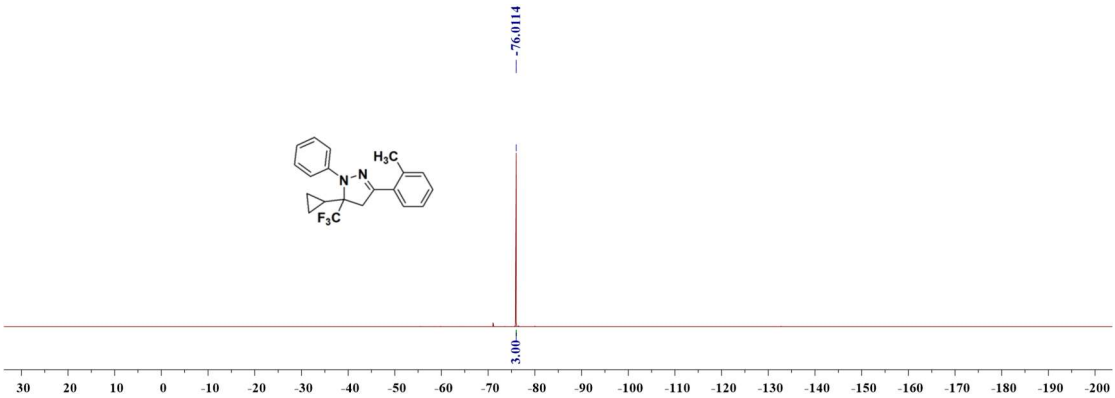


Spectrum of 5-cyclopropyl-1-phenyl-3-(*o*-tolyl)-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ca)

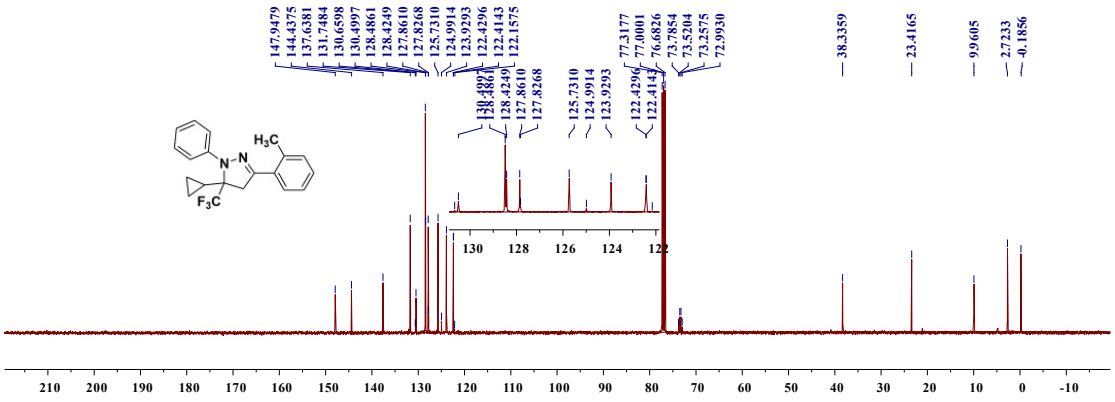
^{1}H NMR

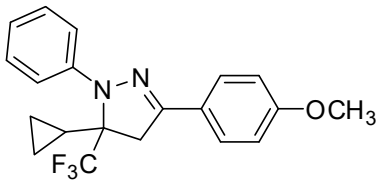


^{19}F NMR



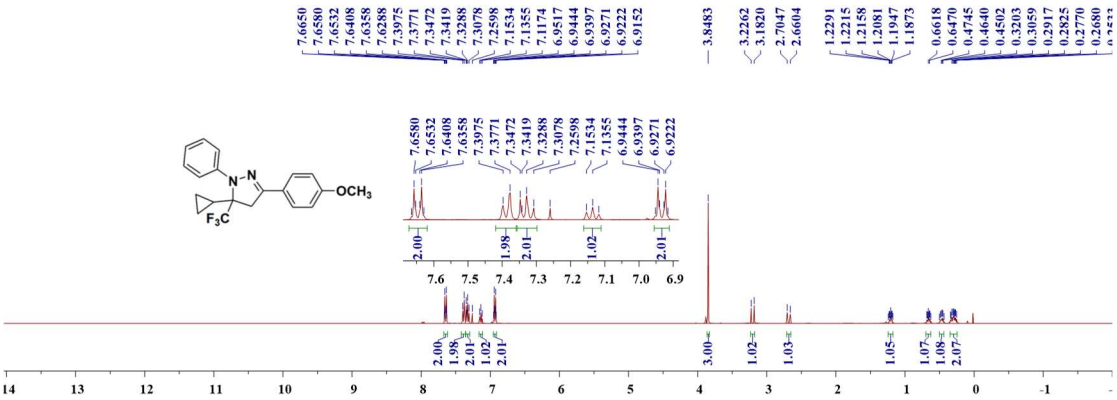
^{13}C NMR



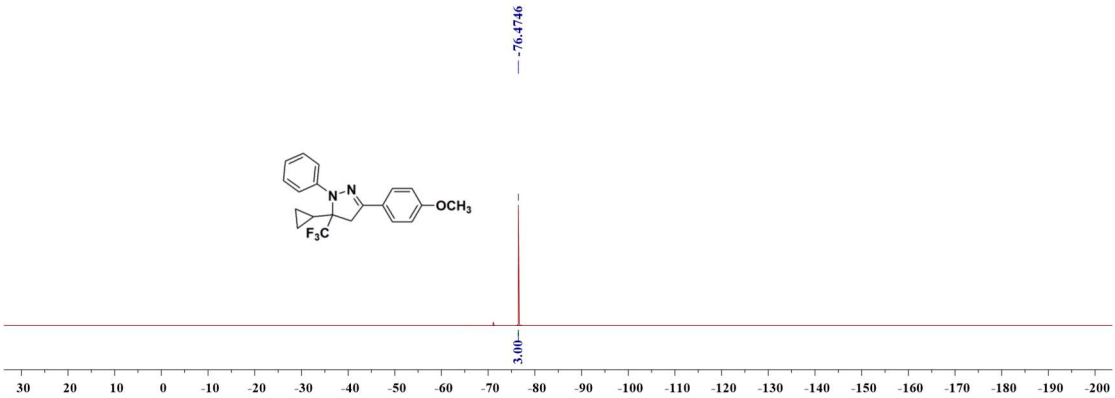


Spectrum of 5-cyclopropyl-3-(4-methoxyphenyl)-1-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3da)

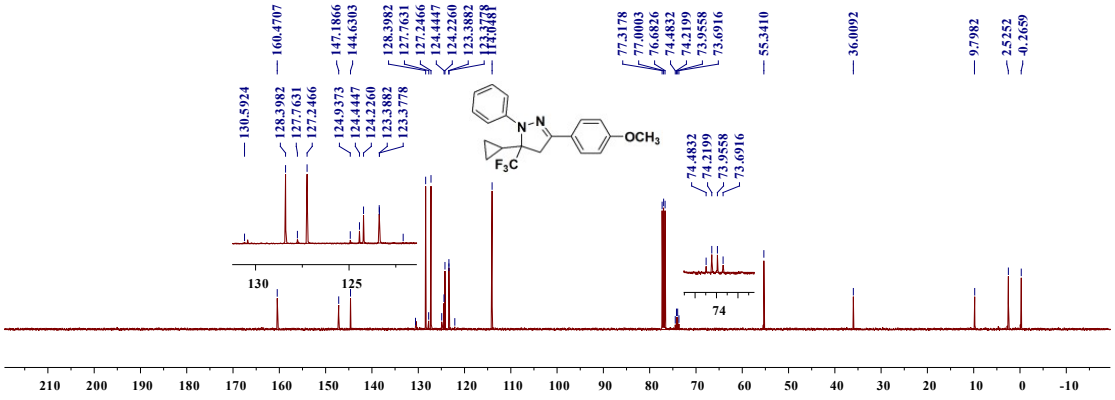
^{1}H NMR

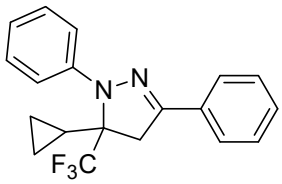


^{19}F NMR



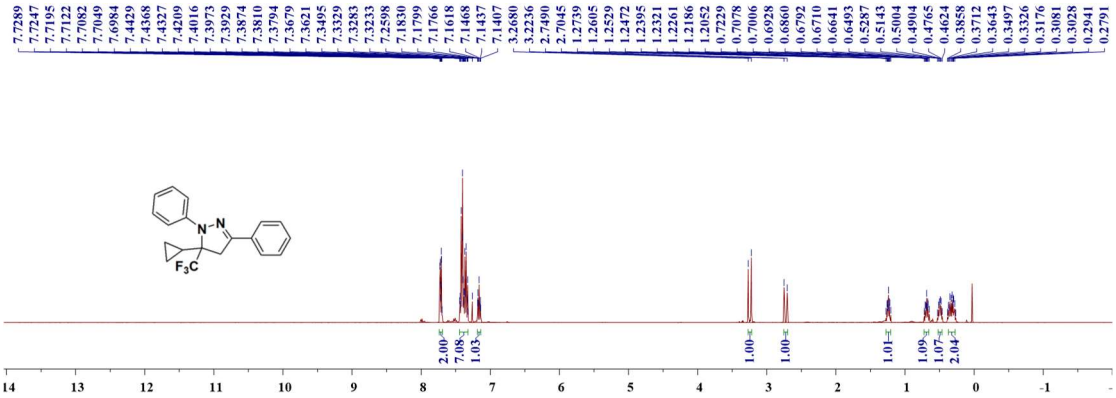
^{13}C NMR



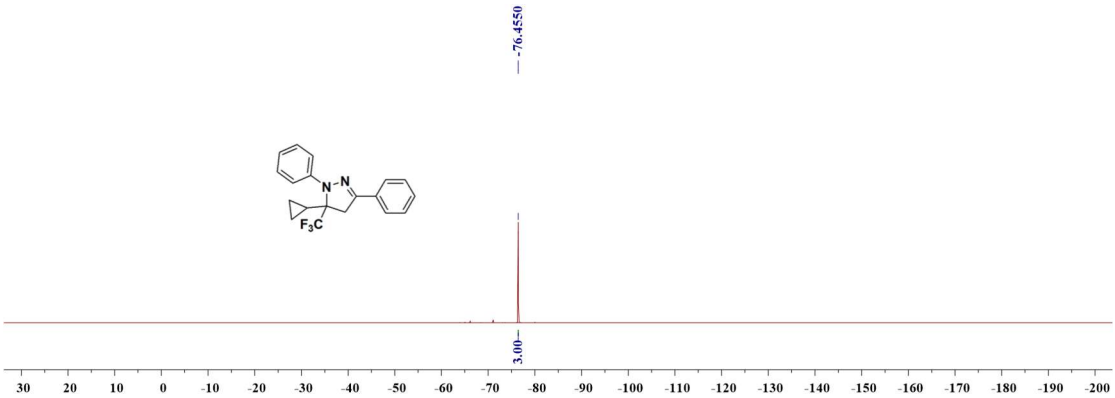


Spectrum of 5-cyclopropyl-1,3-diphenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ea)

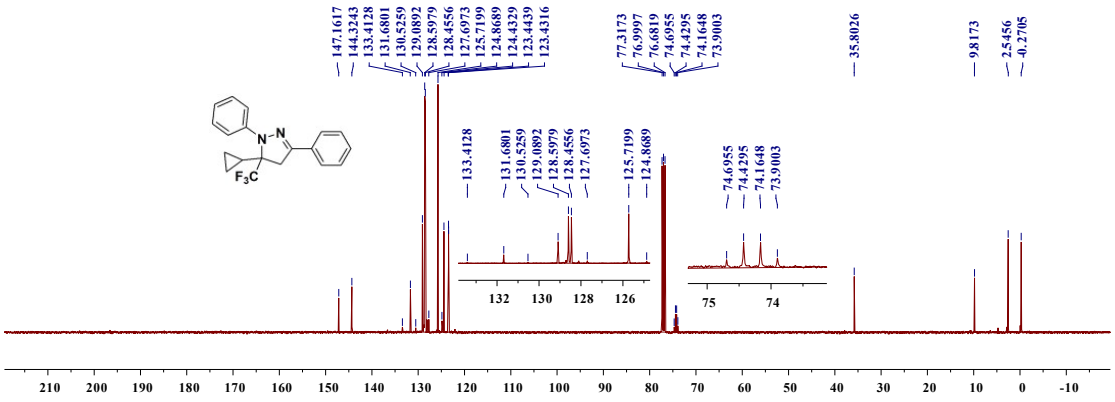
^{1}H NMR

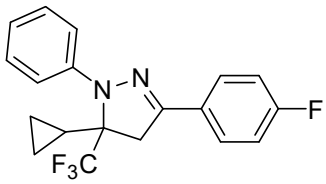


^{19}F NMR



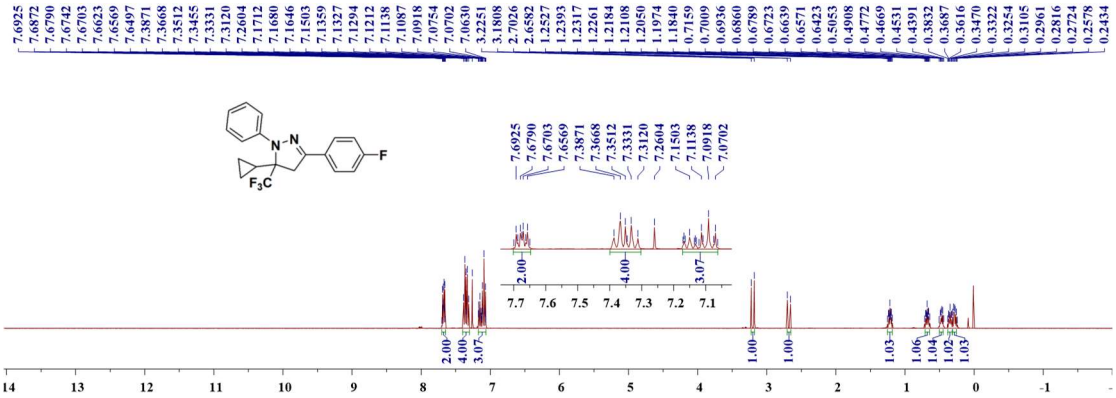
^{13}C NMR



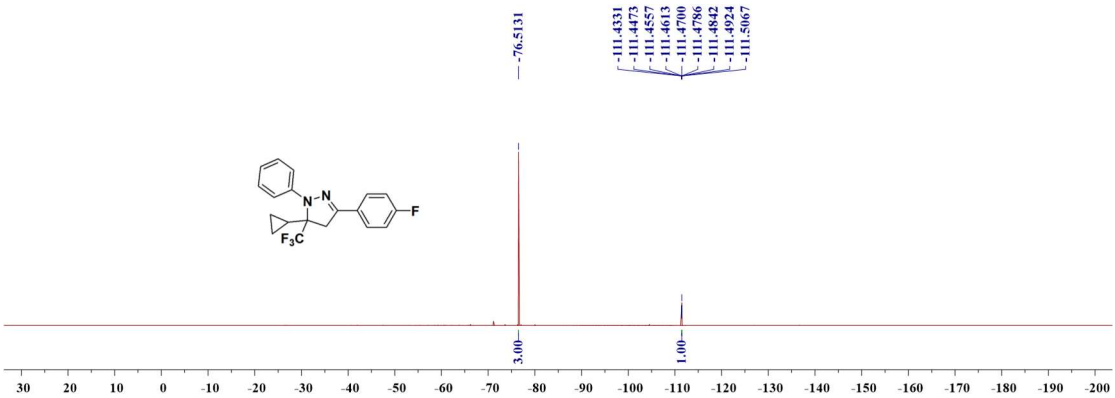


Spectrum of 5-cyclopropyl-3-(4-fluorophenyl)-1-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3fa)

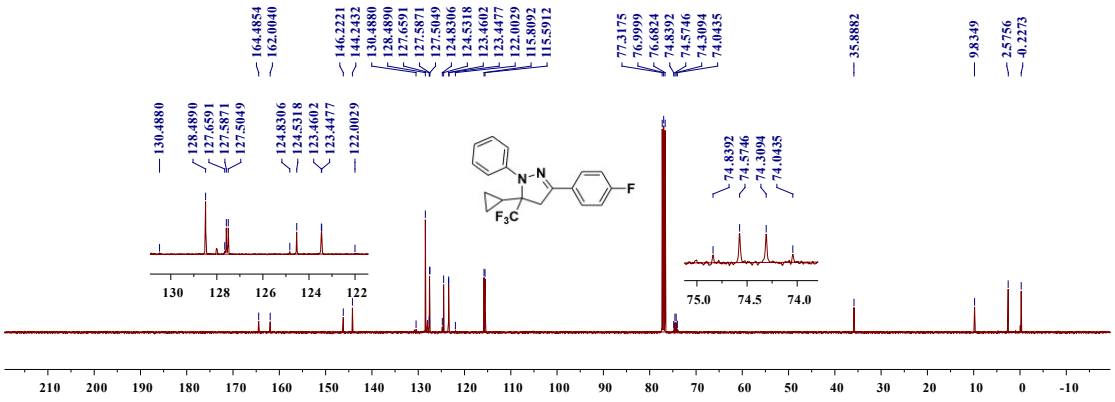
^{1}H NMR

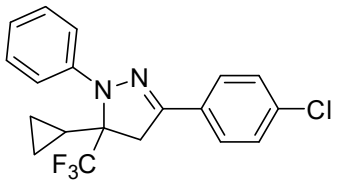


^{19}F NMR



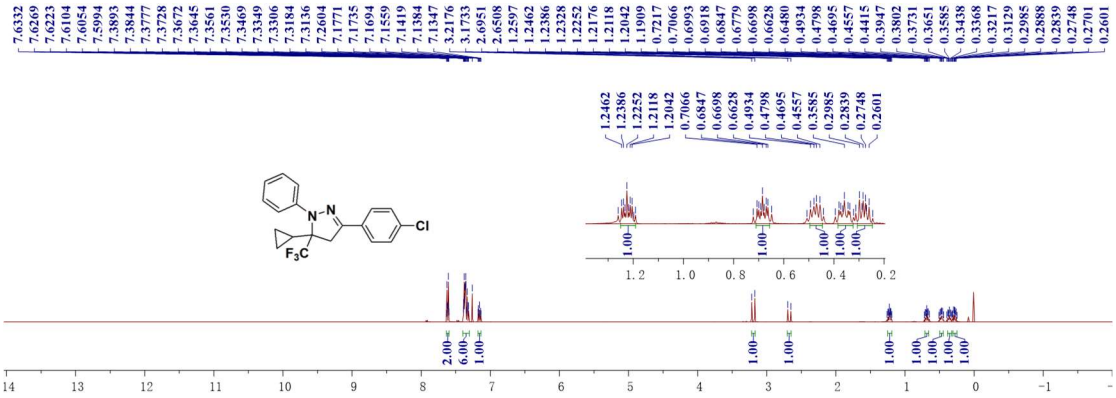
^{13}C NMR



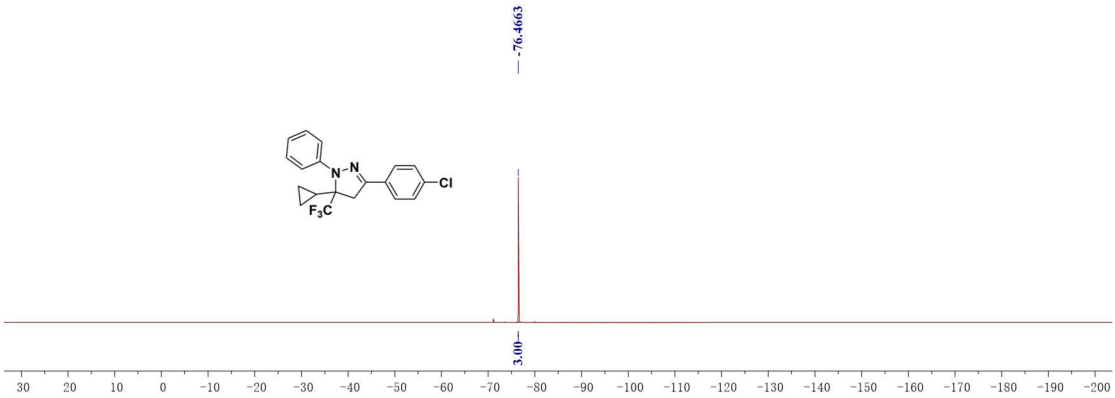


Spectrum of 3-(4-chlorophenyl)-5-cyclopropyl-1-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ga)

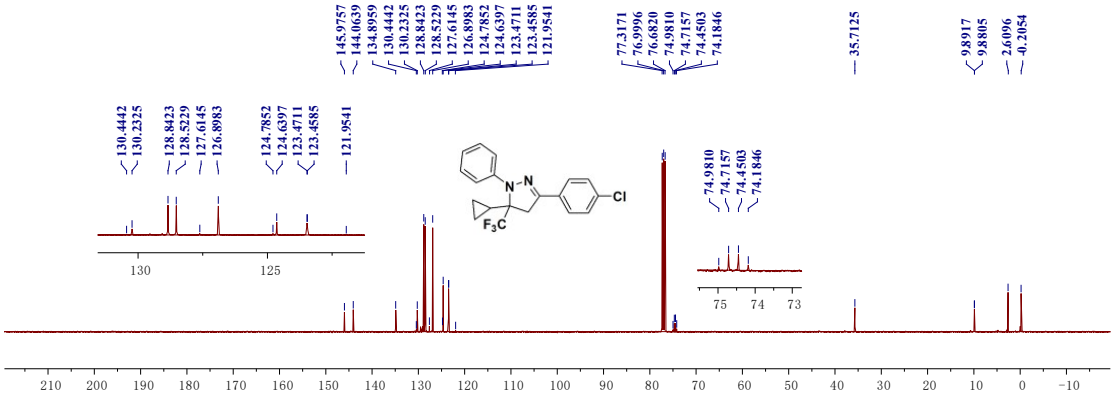
^{1}H NMR

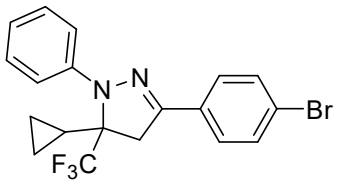


^{19}F NMR



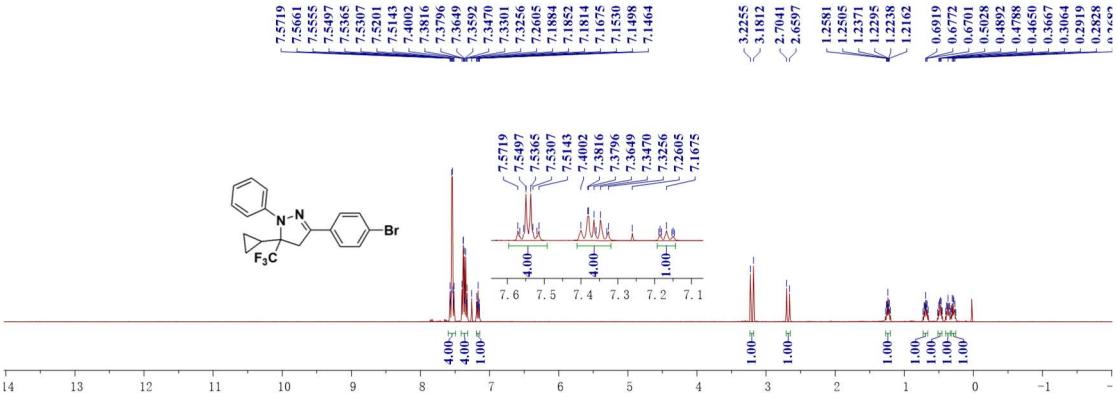
^{13}C NMR



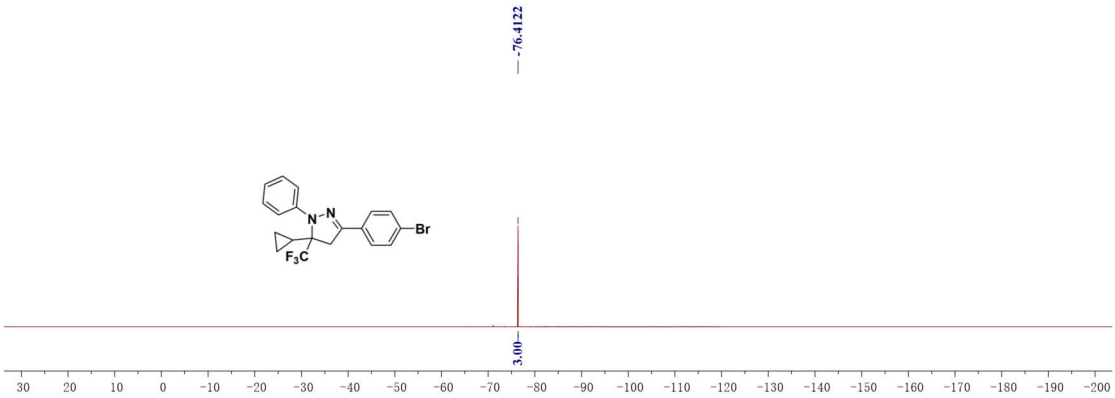


Spectrum of 3-(4-bromophenyl)-5-cyclopropyl-1-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ha)

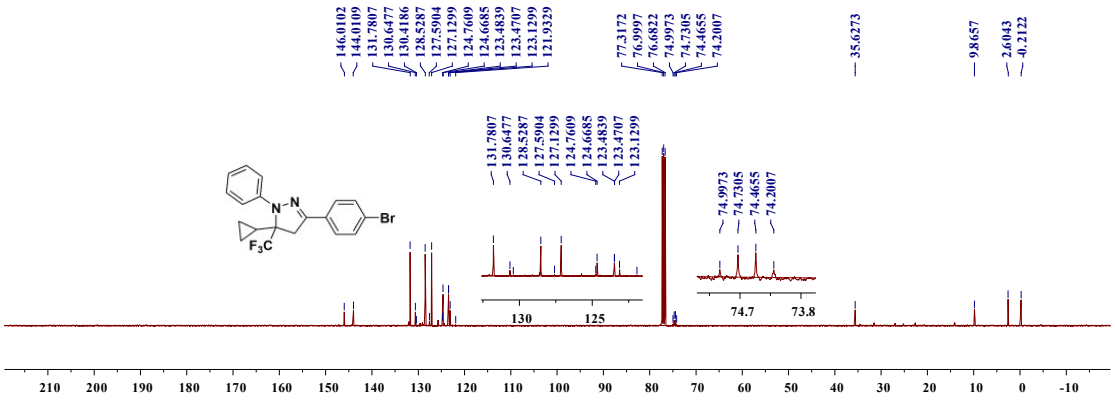
^{1}H NMR

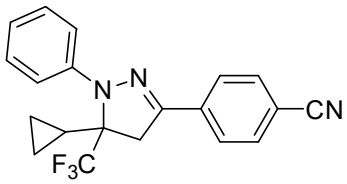


^{19}F NMR



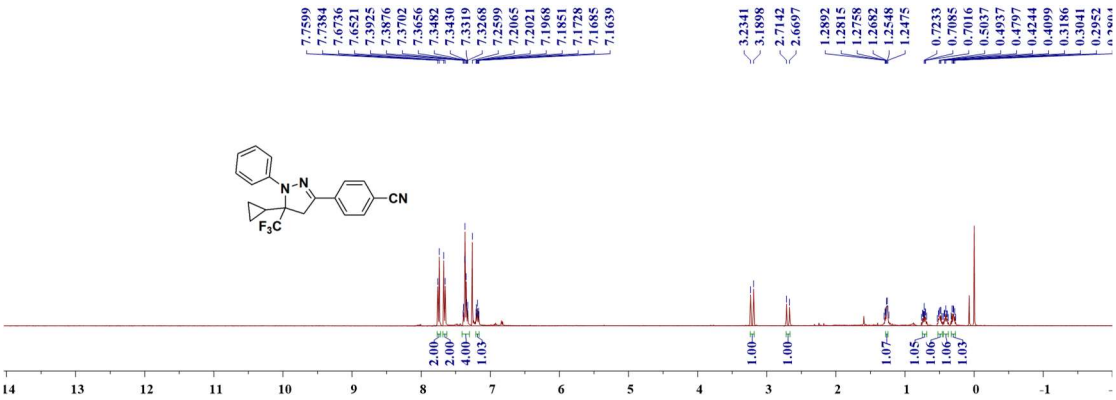
^{13}C NMR



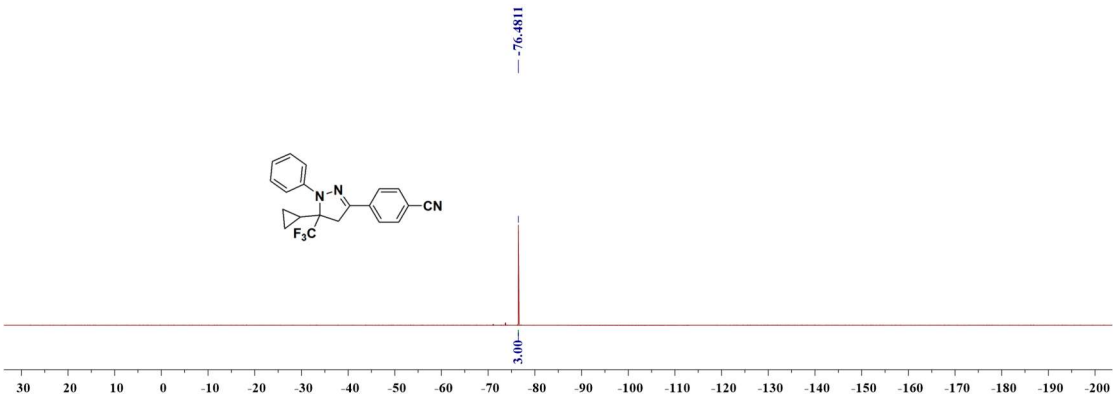


Spectrum of 4-(5-cyclopropyl-1-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazol-3-yl)benzonitrile (3ia)

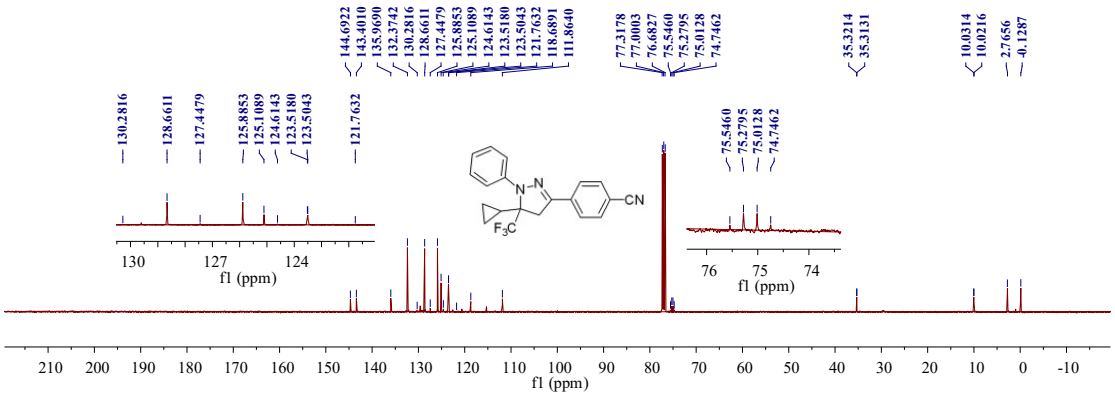
^{1}H NMR

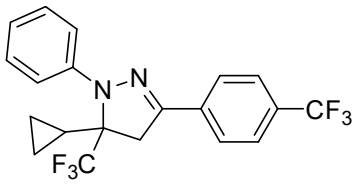


^{19}F NMR



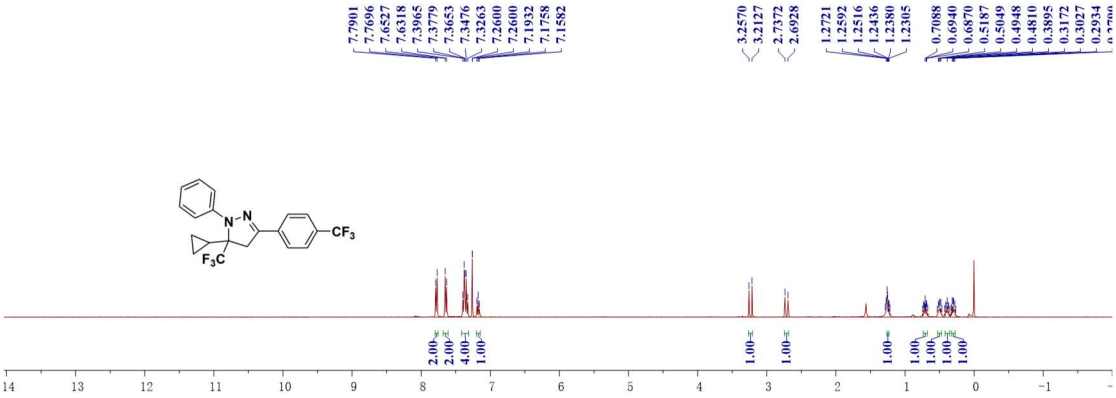
^{13}C NMR



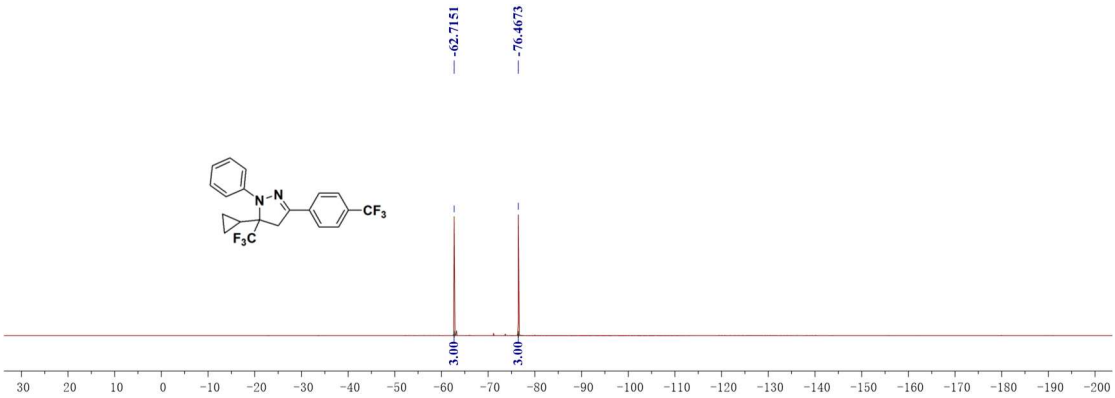


Spectrum of 5-cyclopropyl-1-phenyl-5-(trifluoromethyl)-3-(4-(trifluoromethyl)phenyl)-4,5-dihydro-1*H*-pyrazole (3ja)

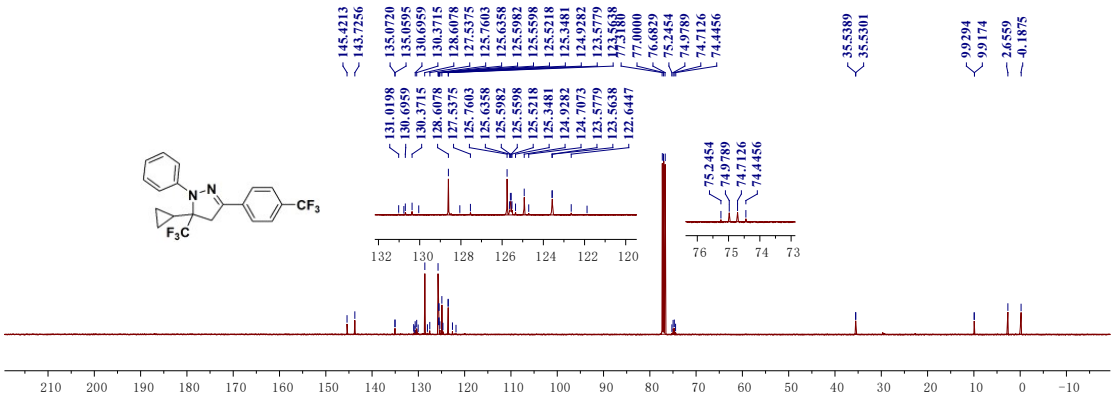
^{1}H NMR

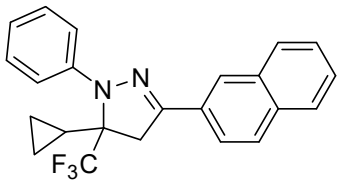


^{19}F NMR



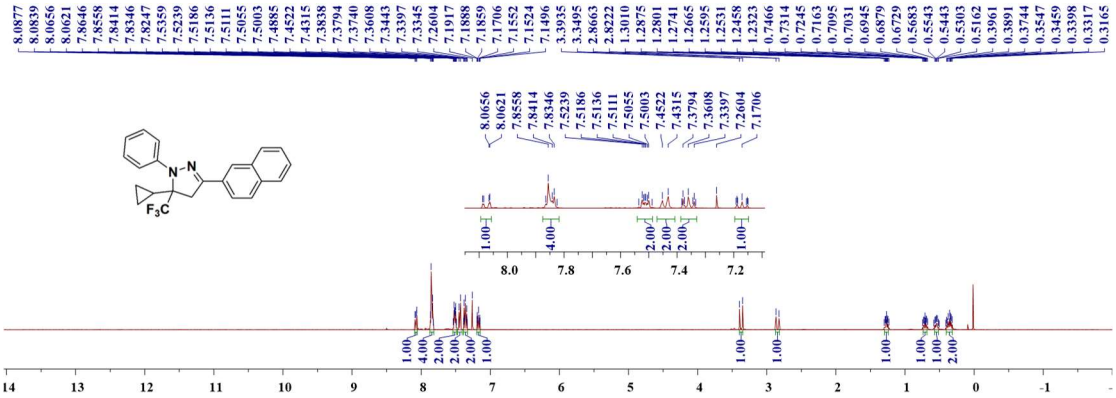
^{13}C NMR



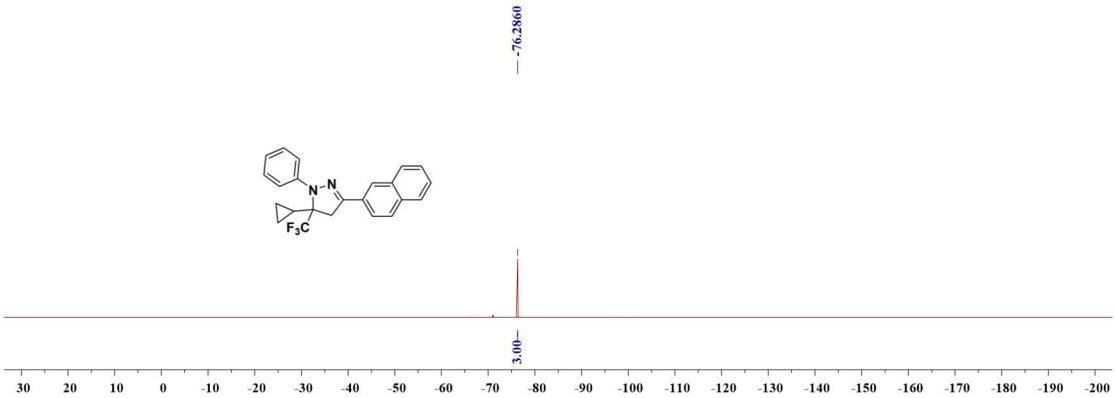


Spectrum of 5-cyclopropyl-3-(naphthalen-2-yl)-1-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ka)

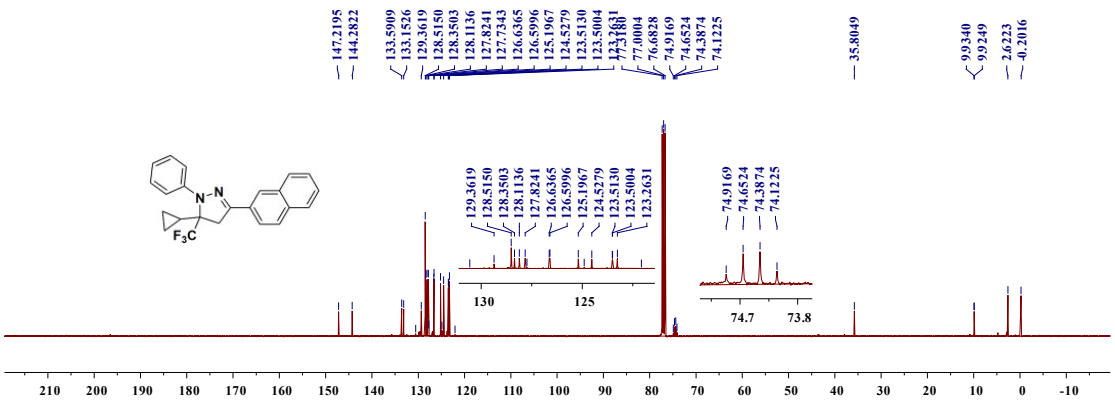
^{1}H NMR

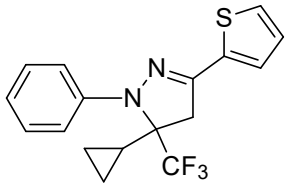


^{19}F NMR



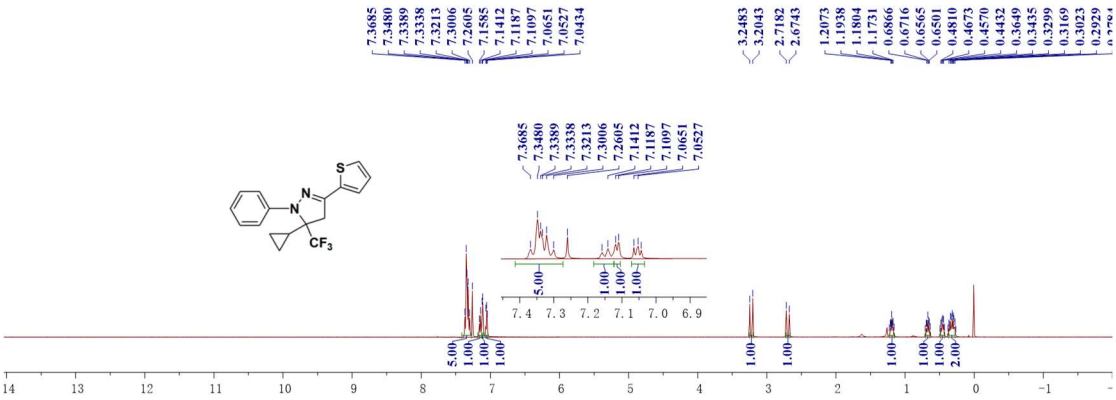
^{13}C NMR



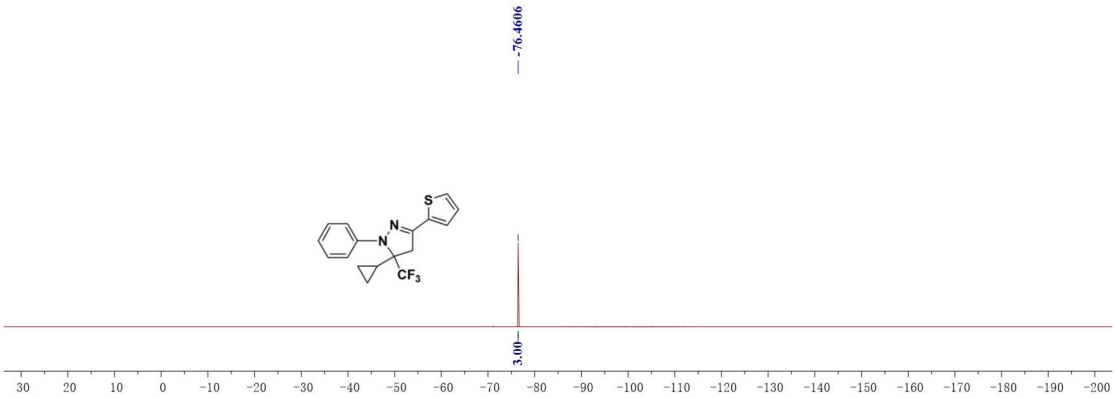


Spectrum of 5-cyclopropyl-1-phenyl-3-(thiophen-2-yl)-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3la)

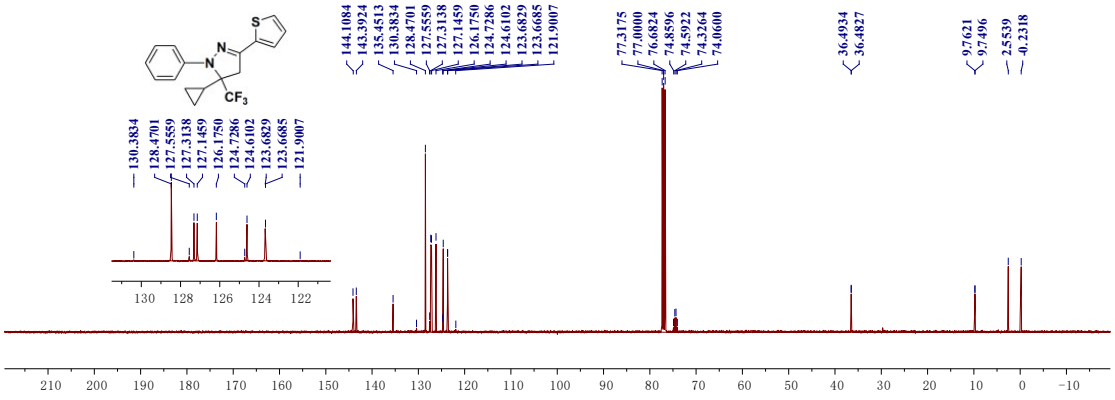
^{1}H NMR

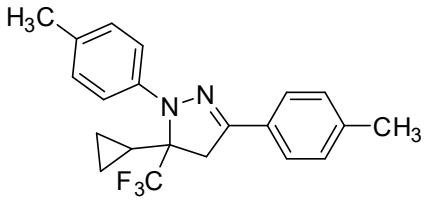


^{19}F NMR



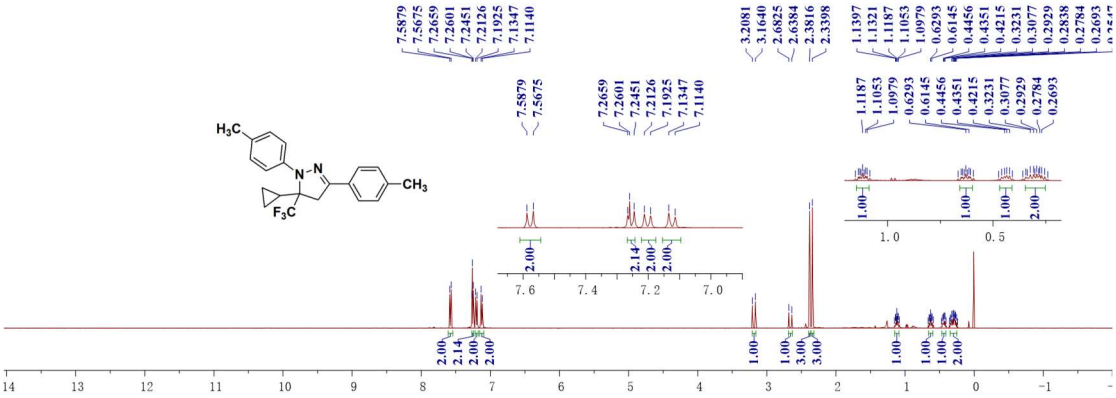
^{13}C NMR



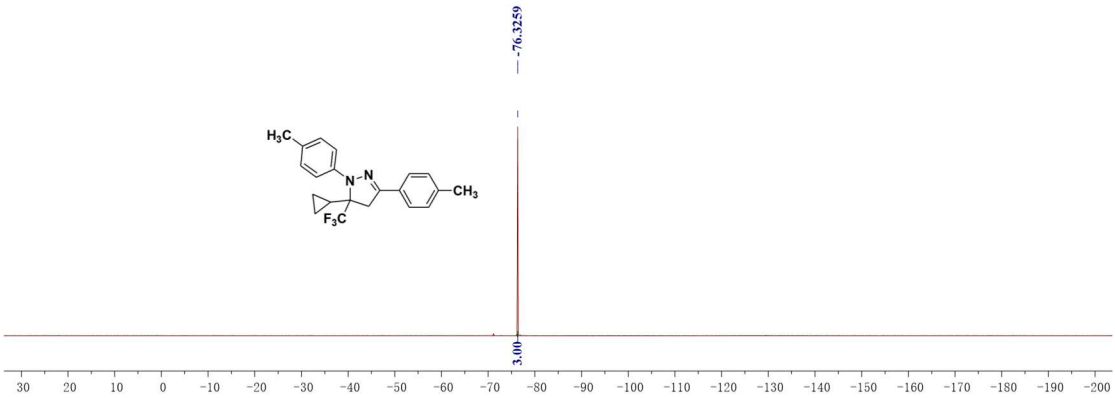


Spectrum of 5-cyclopropyl-1,3-di-*p*-tolyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ab)

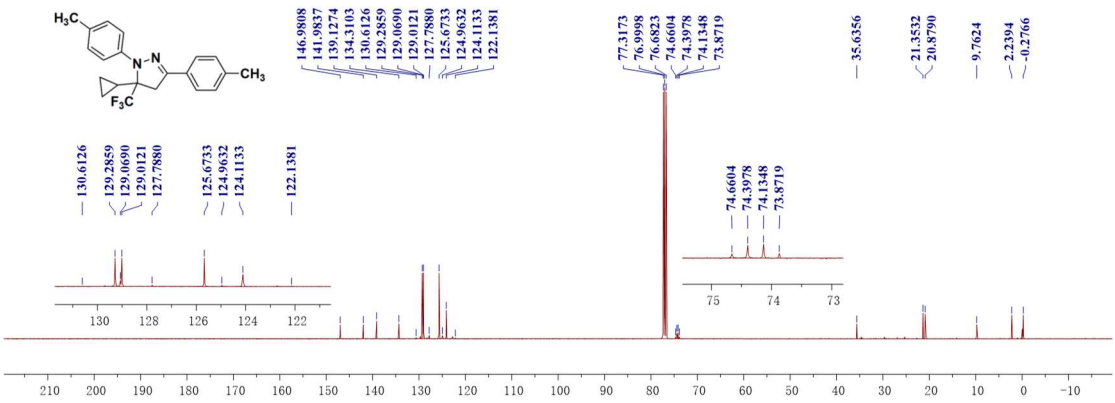
^{1}H NMR

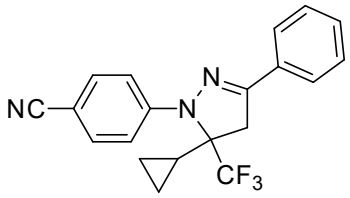


^{19}F NMR



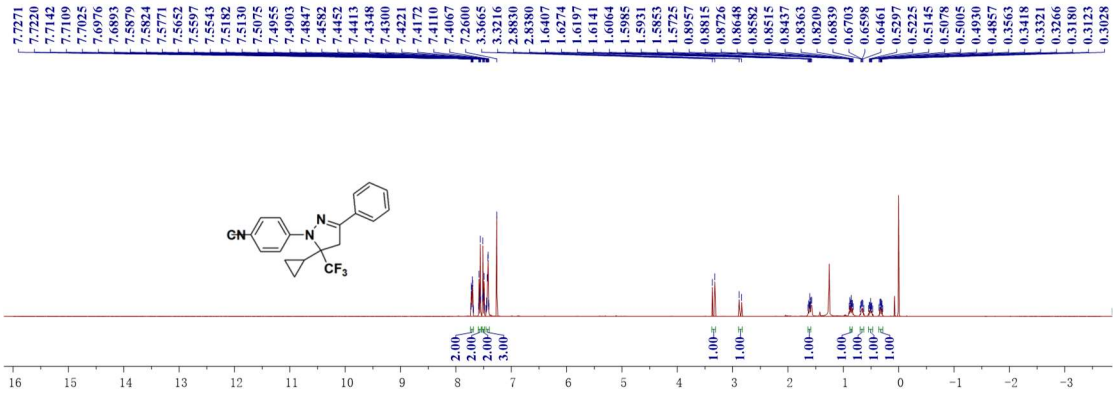
^{13}C NMR



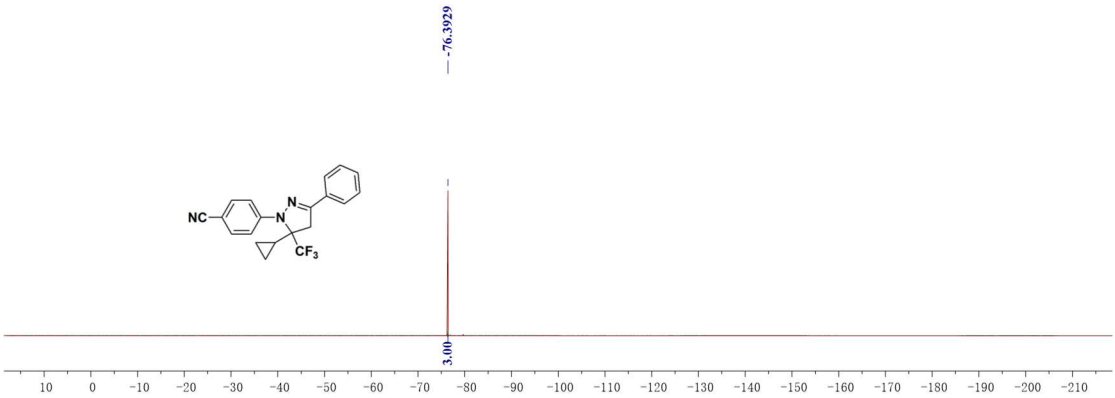


Spectrum of 4-(5-cyclopropyl-3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazol-1-yl)benzonitrile (3ec)

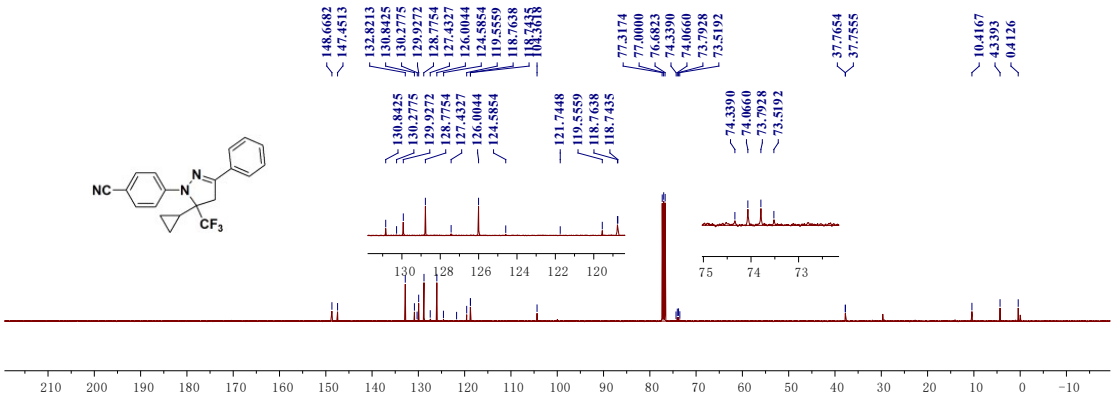
^{1}H NMR

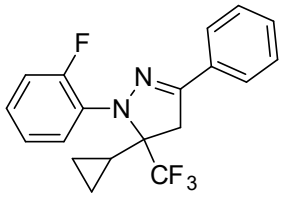


^{19}F NMR



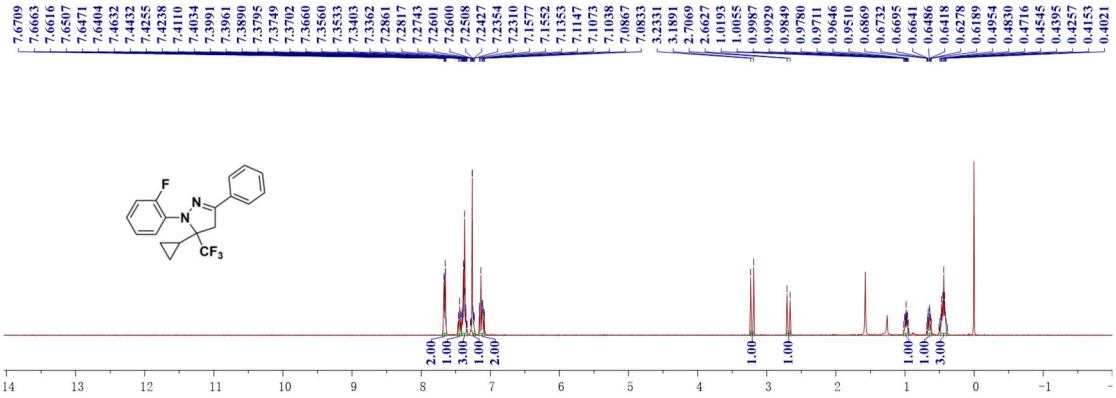
^{13}C NMR



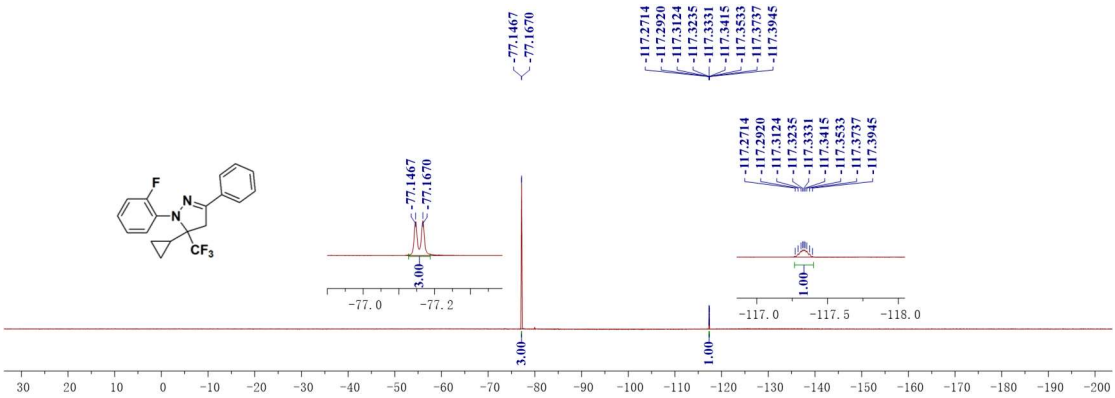


Spectrum of 5-cyclopropyl-1-(2-fluorophenyl)-3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ed)

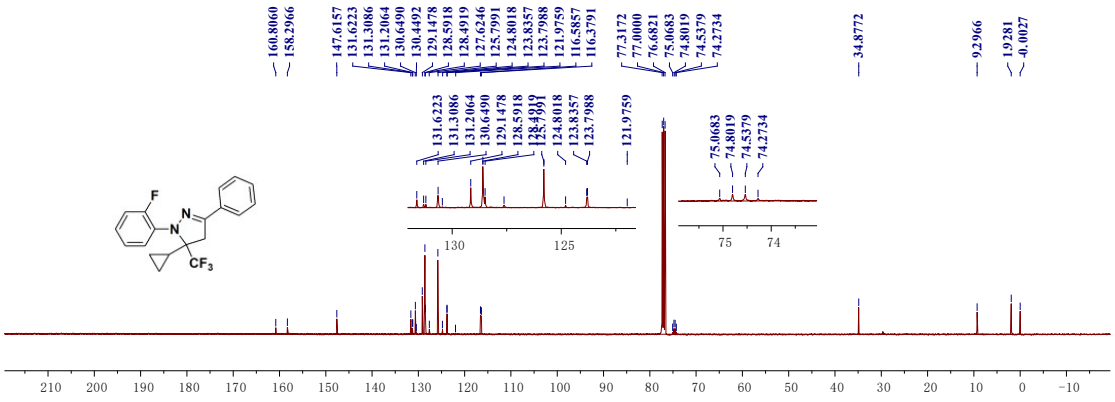
^{1}H NMR

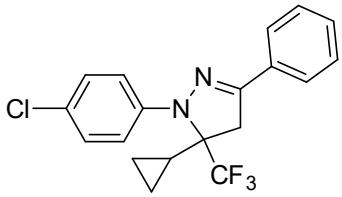


^{19}F NMR



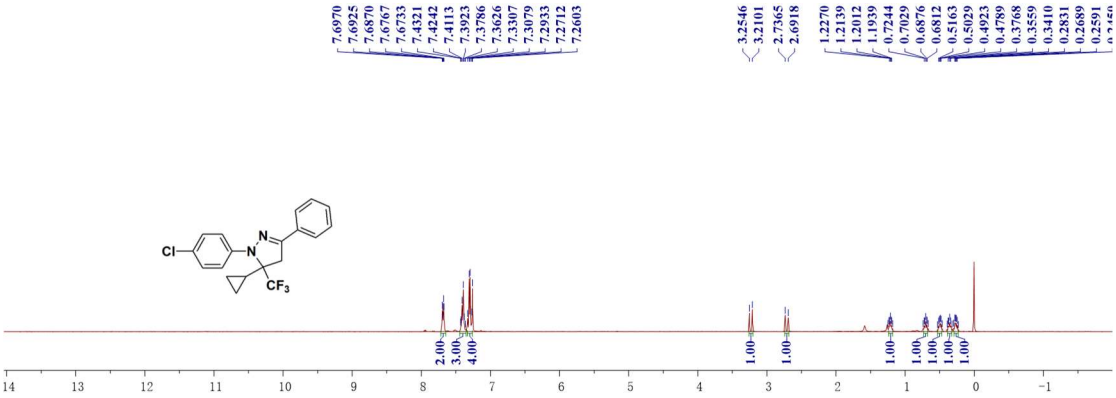
^{13}C NMR



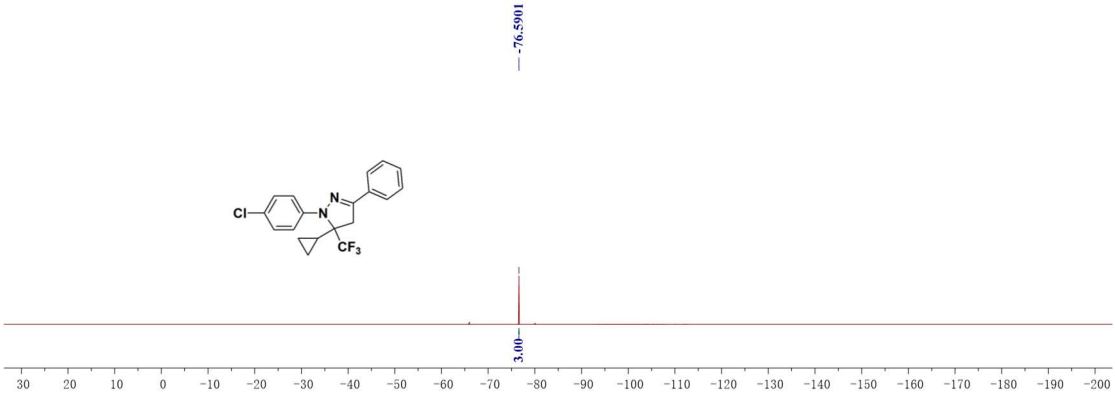


Spectrum of 1-(4-chlorophenyl)-5-cyclopropyl-3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ee)

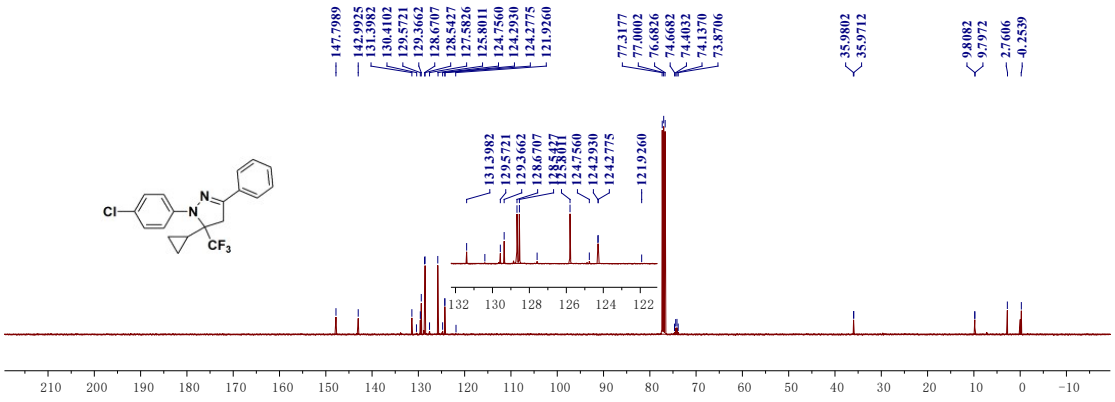
^{1}H NMR

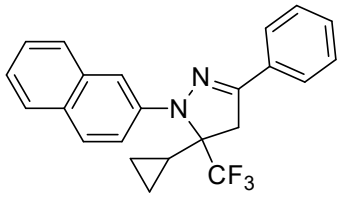


^{19}F NMR



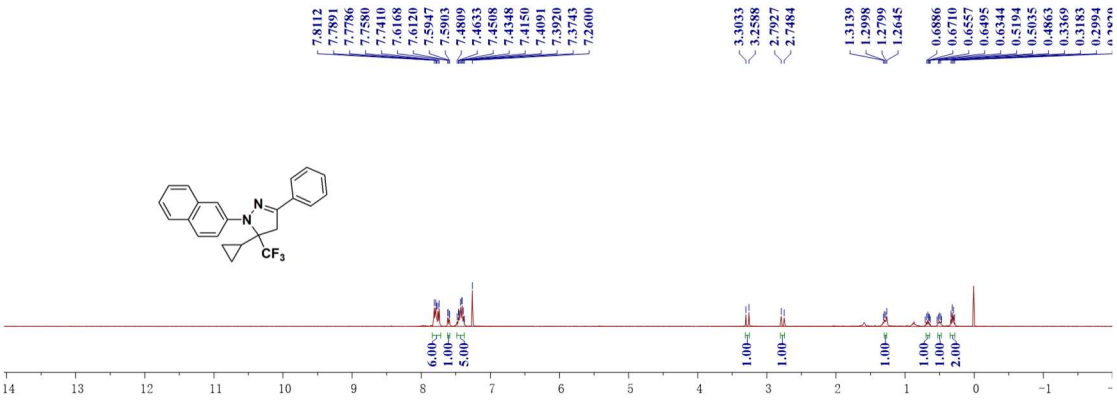
^{13}C NMR



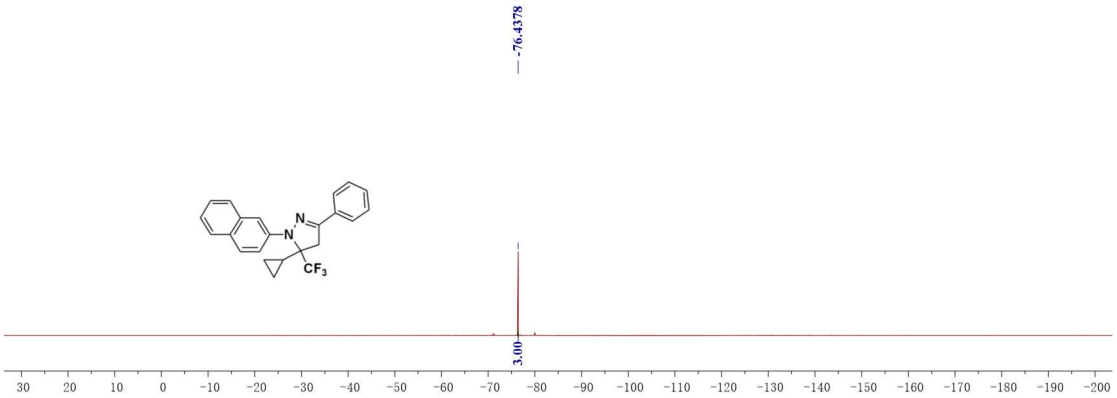


Spectrum of 5-cyclopropyl-1-(naphthalen-2-yl)-3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3ef)

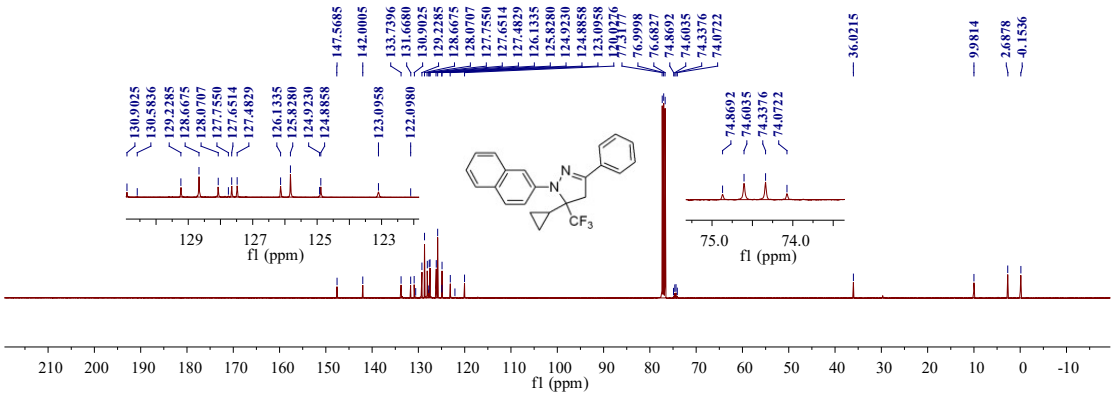
^{1}H NMR

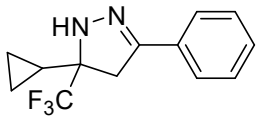


^{19}F NMR



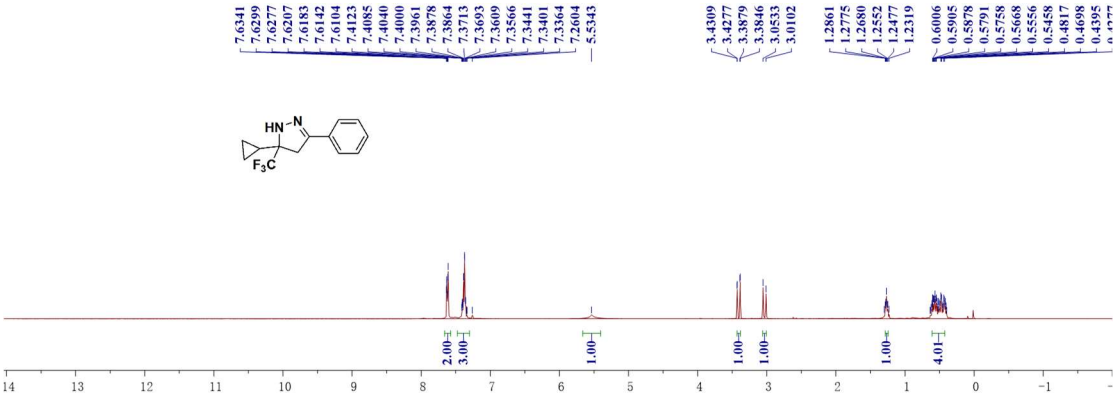
^{13}C NMR



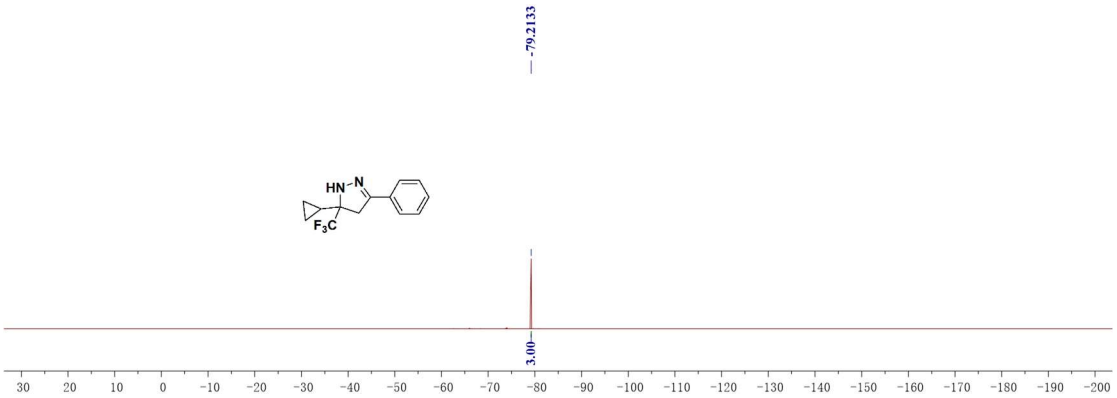


Spectrum of 5-cyclopropyl-3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazole (3eg)

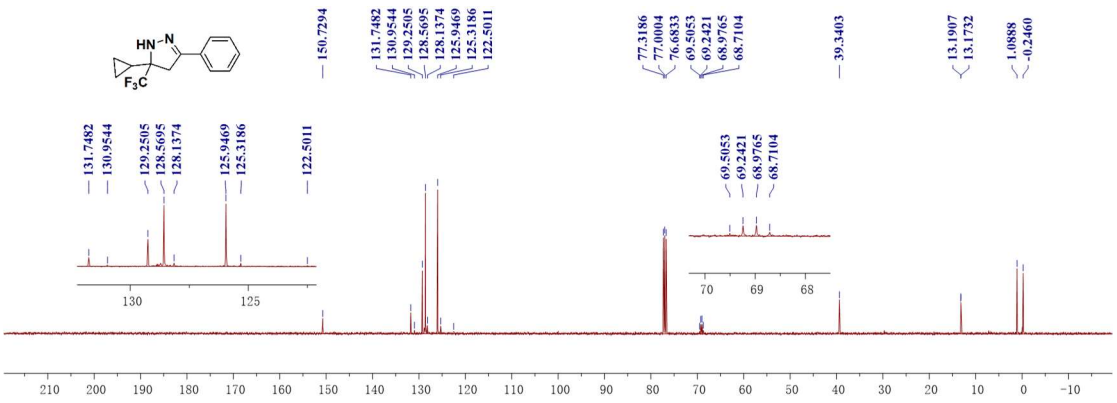
^{1}H NMR

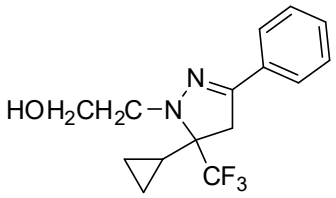


^{19}F NMR



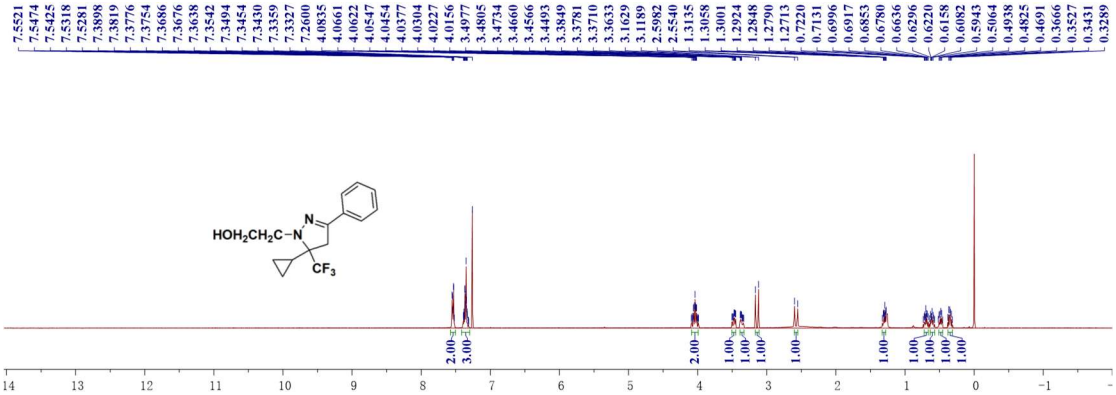
^{13}C NMR



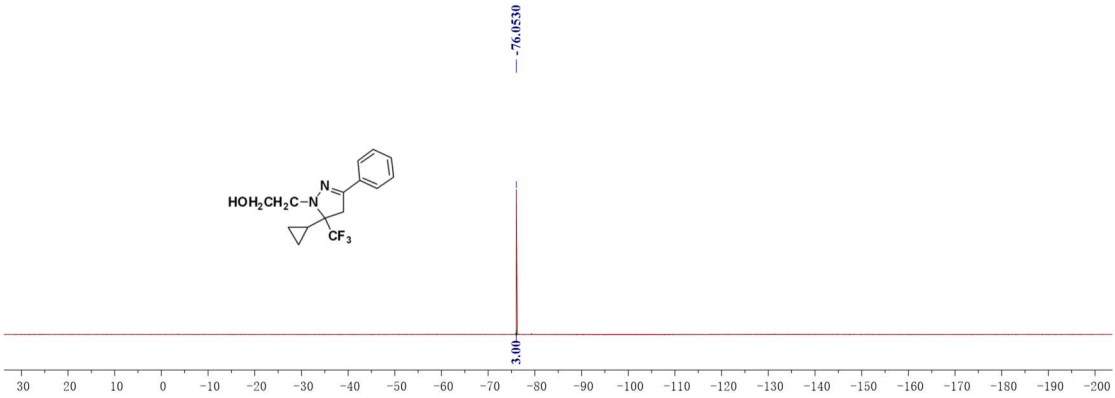


Spectrum of 2-(5-cyclopropyl-3-phenyl-5-(trifluoromethyl)-4,5-dihydro-1*H*-pyrazol-1-yl)ethane (3eh)

^{1}H NMR



^{19}F NMR



^{13}C NMR