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Supporting information

Copper-Catalyzed Stereoselective Oxytrifluoromethylation of Propargyl Amides for the Construction of Oxazolines

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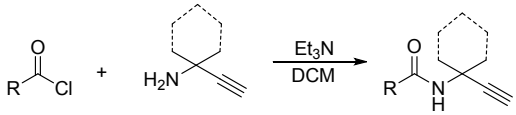
General information

All reagents were purchased from commercial sources and used as received. All solvents were purified by standard procedure prior to use. Unless otherwise mentioned, all reactions were performed under N_2. ^1H NMR spectra were recorded in $CDCl_3$ on a Bruker AM-300 spectrometer (300 MHz), Agilent AM-400 spectrometer (400 MHz), Bruker AM-400 spectrometer (400 MHz) or Varian AM-400 spectrometer (400 MHz) with TMS as internal standard. ^{19}F NMR spectra were taken on a Agilent AM-400 (376 MHz) spectrometer, Bruker AM-400 spectrometer (400 MHz) or Varian AM-400 spectrometer (376 MHz) using $CFCl_3$ as external standard. ^{13}C NMR spectra were recorded in $CDCl_3$ on a Varian AM-400 spectrometer (100 MHz) or Agilent AM-400 (100 MHz) spectrometer with TMS as internal standard. NMR data are reported as follows: chemical shift, multiplicity (s = singlet, bs = broad singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz). IR spectra were obtained with a Nicolet AV-360 spectrophotometer. Melting points were measured on a melt-Temp apparatus and uncorrected. Mass spectrum was obtained on a Finnigan GC-MS 4021. HRMS data were obtained on a high-resolution mass spectrometer. All reactions were monitored by TLC with Huanghai GF_{254} silica gel coated plates. Flash column chromatography was carried out using 300-400 mesh silica gels.

Typical procedure for the synthesis of propargyl amide.



To a solution of propargyl amine (3.0 mmol) in dry DCM (30 mL) was successively added acid chloride (5.4 mmol) and Et_3N (0.8 mL) at 0°C under N_2 atmosphere. The resulting solution was allowed to warm to room temperature, and stirred at the same temperature overnight. The reaction mixture was diluted with water. The aqueous layer was extracted with DCM (5 mL×3), and the combined organic solution was dried over anhydrous $MgSO_4$. After concentration, the residue was purified by flash column chromatography on silica gel to give the corresponding propargyl amide.

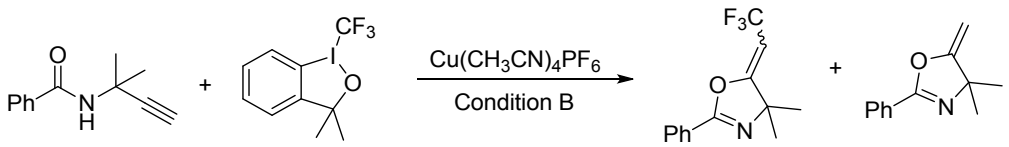
General procedure for the CuBr-catalyzed reaction

To a reactor charged with Togni I (0.12 mmol), CuBr (0.024 mmol) and propargyl amide (0.18 mmol) was added DMA (1.2 mL) under N_2 atmosphere. The mixture was stirred at room temperature for 3 h. After the completion of the reaction, the resulting mixture was diluted with EtOAc and washed with water (5 mL×2). The organic layer was dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The residue was purified by column chromatography to give the product.

General procedure for the $Cu(CH_3CN)_4PF_6$-catalyzed reaction

To a sealed tube charged with Togni I (0.12 mmol), $Cu(CH_3CN)_4PF_6$ (0.006 mmol) and propargyl amide (0.18 mmol) was added DCM (1.2 mL) under N_2 atmosphere. Unless otherwise mentioned, the mixture was stirred at 60 ^oC for 9 h. After the completion of the reaction, the solvent was removed under reduced pressure and the residue was purified by column chromatography to give the product.

Table S-1. Monitoring experiments for the $Cu(CH_3CN)_4PF_6$-catalyzed reaction



1a, 0.15 mmol **2**, 0.10 mmol **3a** **4**

Entry[a]	Time (h)	Z-**3a**[b]	**4**[c]
1	2	0.018 mmol	0.108 mmol
2	4	0.031 mmol	0.102 mmol
3	6	0.045 mmol	0.089 mmol
4	9	0.071 mmol	0.062 mmol

[a] Reaction condition B: **1** (0.15 mmol), **2** (0.10 mmol), $Cu(CN_3CN)_4PF_6$ (0.005 mmol), DCM (1.0 mL), 60 °C, time, under N_2. [b] Determined by ^1H NMR spectroscopy using anisole as internal standard. [c] Determined by ^{19}F NMR spectroscopy using hexafluorobenzene as internal standard.

Compound characterization

***N*-(1,1-dimethyl-2-propyn-1-yl)benzenecarboxamide (1a)**[a]. A white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.77 – 7.75 (m, 2H), 7.53 – 7.47 (m, 1H), 7.45 – 7.40 (m, 2H), 6.20 (bs, 1H), 2.40 (s, 1H), 1.78 (s, 6H).

***N*-(1,1-dimethyl-2-propyn-1-yl)-4-methylbenzamide (1b)**[b]. A white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 8.1Hz, 2H), 7.21 (d, J = 8.1Hz, 2H), 6.19 (bs, 1H), 2.38 (s, 4H), 1.76 (s, 6H).

***N*-(1,1-dimethyl-2-propyn-1-yl)-4-methoxylbenzamide (1c)**[b]. A white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.7Hz, 2H), 6.90 (d, J = 8.7Hz, 2H), 6.13 (bs, 1H), 3.84 (s, 3H), 2.38 (s, 1H), 1.76 (s, 6H).

***N*-(1,1-dimethyl-2-propyn-1-yl)-2-methylbenzamide (1d)**. A white solid. M.p. 97-99 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.27 (m, 2H), 7.25 – 7.05 (m, 2H), 5.89 (bs, 1H), 2.44 (s, 3H), 2.38 (s, 1H), 1.75 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.3, 136.8, 136.1, 131.0, 129.9, 126.6, 125.8, 87.2, 69.5, 48.1, 29.1, 19.7. HRMS (EI): *m/z* calcd. for $C_{13}H_{15}NO$ $[M]^+$ 201.1154, found: 201.1156. IR (KBr): 3281, 3047, 3021, 2985, 2931, 2842, 1644, 1535, 1315, 1223, 749, 669, 641 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)-3-methylbenzamide (1e)**. A white solid. M.p. 92-94 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (s, 1H), 7.52 – 7.51 (m, 1H), 7.29 – 7.26 (m, 2H), 6.24 (bs, 1H), 2.37 (s, 4H), 1.75 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8, 136.5, 134.9, 132.3, 128.5, 127.8, 123.9, 87.3, 69.4, 48.1, 29.1, 21.4. HRMS (EI): *m/z* calcd. for $C_{13}H_{15}NO$ $[M]^+$ 201.1154, found: 201.1157. IR (KBr): 3298, 3050, 2983, 2920, 2863, 1647, 1532, 1306, 1227, 747, 649 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)-2,4,6-trimethylbenzamide (1f)**. A white solid. M.p. 112-114 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.82 (s, 2H), 5.78 (bs, 1H), 2.38 (s, 1H), 2.30 (s, 6H), 2.26 (s, 3H), 1.74 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ ^{13}C NMR (101

MHz, $CDCl_3$) δ 169.7, 138.5, 135.1, 134.3, 128.2, 87.1, 69.6, 48.1, 29.0, 21.2, 19.0. HRMS (EI): *m/z* calcd. for $C_{15}H_{19}NO$ $[M]^+$ 229.1467, found: 229.1474. IR (KBr): 3284, 3263, 3054, 2984, 2919, 2857, 1639, 1538, 1222, 847 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)-3,4,5-trimethoxylbenzamide (1g)**. A white solid. M.p. 151-153 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 6.96 (s, 2H), 6.21 (bs, 1H), 3.87 (s, 6H), 3.84 (s, 3H), 2.38 (s, 1H), 1.74 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 153.2, 141.0, 130.4, 104.5, 87.2, 69.5, 61.0, 56.4, 48.1, 29.1. HRMS (EI): *m/z* calcd. for $C_{15}H_{19}NO_4$ $[M]^+$ 277.1314, found: 277.1309. IR (KBr): 3345, 3264, 3065, 3008, 2973, 2947, 2833, 1637, 1539, 1499, 1334, 1243, 1121, 996, 759 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)-4-fluorobenzamide (1h)**. A white solid. M.p. 114-116 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.76 (dd, J = 8.6, 5.3 Hz, 2H), 7.07 (t, J = 8.6 Hz, 2H), 6.22 (bs, 1H), 2.38 (s, 3H), 1.75 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.6, 164.8 (d, J = 251.8 Hz), 131.1, 129.4 (d, J = 8.9 Hz), 115.7 (d, J = 21.9 Hz), 87.1, 69.6, 48.2, 29.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -108.119 (tt, J = 8.6, 5.3 Hz, 1F). HRMS (EI): *m/z* calcd. for $C_{12}H_{12}FNO$ $[M]^+$ 205.0903, found: 205.0907. IR (KBr): 3344, 3305, 3293, 2985, 1645, 1530, 1503, 1221, 852, 768 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)-4-chlorobenzamide (1i)**[c]. A white solid. ^1H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 8.0 Hz, 2H), 7.39 (d, J = 8.0 Hz, 2H), 6.18 (bs, 1H), 2.39 (s, 1H), 1.76 (s, 6H).

***N*-(1,1-dimethyl-2-propyn-1-yl)-4-bromobenzamide (1j)**[b]. A white solid. ^1H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 8.5 Hz, 2H), 7.56 (d, J = 8.5 Hz, 2H), 6.15 (bs, 1H), 2.40 (s, 1H), 1.76 (s, 6H).

***N*-(1,1-dimethyl-2-propyn-1-yl)-4-iodobenzamide (1k)**. A white solid. M.p. 154-156 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.5 Hz, 2H), 7.45 (d, J = 8.5 Hz,

2H), 6.31 (bs, 1H), 2.37 (s, 1H), 1.73 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9, 137.8, 134.3, 129.0, 98.6, 87.0, 69.6, 48.2, 29.1. HRMS (EI): *m/z* calcd. for $C_{12}H_{12}INO$ $[M]^+$ 312.9964, found: 312.9967. IR (KBr): 3306, 3053, 2997, 2979, 2931, 1644, 1536, 1188, 845, 757, 612 cm^{-1}.

4-(methoxyacetyl)-*N*-(1,1-dimethyl-2-propyn-1-yl)benzenecarboxamide (1l). A white solid. M.p. 116-118 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.2 Hz, 2H), 7.78 (d, *J* = 8.2 Hz, 2H), 6.42 (bs, 1H), 3.90 (s, 3H), 2.39 (s, 1H), 1.75 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 165.8, 138.8, 132.7, 129.8, 127.1, 87.0, 69.7, 52.5, 48.3, 29.1. HRMS (EI): *m/z* calcd. for $C_{14}H_{15}NO_3$ $[M]^+$ 245.1052, found: 245.1051. IR (KBr): 3318, 3271, 3059, 3027, 2982, 2949, 1719, 1648, 1537, 1281, 1110, 871, 733 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)-4-nitrobenzamide (1m)**[c]. A white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.2 Hz, 2H), 7.90 (d, *J* = 8.2 Hz, 2H), 6.48 (bs, 1H), 2.40 (s, 1H), 1.75 (s, 6H).

4-(dimethylamino)-*N*-(1,1-dimethyl-2-propyn-1-yl)benzenecarboxamide (1n). A white solid. M.p. 126-128 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.7 Hz, 2H), 6.63 (d, *J* = 7.7 Hz, 2H), 6.09 (bs, 1H), 2.99 (s, 6H), 2.38 (s, 1H), 1.74 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 152.5, 128.5, 121.6, 111.1, 87.8, 69.1, 47.7, 40.2, 29.3. HRMS (EI): *m/z* calcd. for $C_{14}H_{18}N_2O$ $[M]^+$ 230.1419, found: 230.1415. IR (KBr): 3288, 3252, 3039, 2982, 1637, 1609, 1533, 1509, 1297, 1203, 827, 769 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)naphthalene-1-carboxamide (1o)**. A white solid. M.p. 162-164 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.2 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.72 – 7.49 (m, 3H), 7.45 – 7.41 (m, 1H), 6.12 (bs, 1H), 2.44 (s, 1H), 1.62 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.9, 134.8, 133.8, 130.6, 130.2, 128.4, 127.2, 126.5, 125.4, 124.9, 124.8, 87.1, 69.7, 48.4, 29.2. HRMS (EI): *m/z* calcd. for $C_{16}H_{15}NO$ $[M]^+$ 237.1154, found: 237.1150. IR (KBr):

3287, 3041, 3024, 2990, 1648, 1523, 1303, 780, 642 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)cinnamamide (1p)**[b]. A white solid. ^1H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 15.5 Hz, 1H), 7.50 – 7.48 (m, 2H), 7.36 – 7.34 (m, 3H), 6.36 (d, *J* = 15.5 Hz, 1H), 5.81 (bs, 1H), 2.38 (s, 1H), 1.73 (s, 6H).

***N*-(1,1-dimethyl-2-propyn-1-yl)-2-thiophencarboxamide (1q)**. A white solid. M.p. 107-109 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 4.1 Hz, 1H), 7.44 (d, *J* = 4.1 Hz, 1H), 7.03 (t, *J* = 4.1 Hz, 1H), 6.15 (bs, 1H), 2.38 (s, 1H), 1.74 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.1, 139.5, 130.1, 128.3, 127.7, 87.1, 69.7, 48.3, 29.2. HRMS (EI): *m/z* calcd. for $C_{10}H_{11}NOS$ $[M]^+$ 193.0561, found: 193.0555. IR (KBr): 3312, 3300, 3091, 2976, 1623, 1534, 1509, 1307, 734 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)-6-chloronicotinamide (1r)**. A white solid. M.p. 125-127 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.68 (s, 1H), 8.03 (d, *J* = 8.2 Hz, 1H), 7.35 (d, *J* = 8.2 Hz, 1H), 6.52 (bs, 1H), 2.39 (s, 1H), 1.73 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.8, 154.2, 148.1, 138.0, 129.5, 124.4, 86.6, 70.0, 48.5, 29.1. HRMS (EI): *m/z* calcd. for $C_{11}H_{11}ClN_2O$ $[M]^+$ 222.0560, found: 222.0565. IR (KBr): 3297, 3050, 2985, 2934, 2860, 1650, 1587, 1536, 1454, 1362, 1317, 1104, 766 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)cyclohexanecarboxamide (1s)**. A white solid. M.p. 95-97 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 5.64 (bs, 1H), 2.28 (s, 1H), 2.01 – 1.94 (m, 1H), 1.82 – 1.72 (m, 4H), 1.62 – 1.59 (m, 1H), 1.59 (s, 6H), 1.43 – 1.33 (m, 2H), 1.26 – 1.17 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.4, 87.6, 69.0, 47.5, 45.9, 29.6, 29.0, 25.8, 25.7. HRMS (EI): *m/z* calcd. for $C_{12}H_{19}NO$ $[M]^+$ 193.1467, found: 193.1460. IR (KBr): 3315, 3287, 3041, 2928, 2852, 1650, 1536, 1451, 1213, 630 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)adamantanecarbonycarboxamide (1t)**. A white solid. M.p. 110-112 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 5.63 (bs, 1H), 2.30 (s, 1H),

2.03 – 2.01 (m, 3H), 1.92 – 1.90 (m, 2H), 1.82 – 1.81 (m, 5H), 1.70 – 1.68 (m, 5H), 1.61 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.1, 87.7, 69.0, 47.5, 41.0, 39.3, 38.4, 36.6, 36.4, 29.0, 28.2, 27.8. HRMS (EI): *m/z* calcd. for $C_{16}H_{23}NO$ $[M]^+$ 245.1780, found: 245.1779. IR (KBr): 3330, 2982, 2904, 2849, 1646, 1523, 1451, 1282, 615 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)octanoylcarbonycarboxamide (1u)**. A white solid. M.p. 66-68 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.74 (bs, 1H), 2.29 (s, 1H), 2.10 (t, *J* = 7.5 Hz, 2H), 1.60 (s, 6H), 1.60 – 1.56 (m, 1H), 1.26 – 1.25 (m, 8H), 0.84 (t, *J* = 6.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.5, 87.4, 69.1, 47.5, 37.3, 31.8, 29.2, 29.1, 29.0, 25.7, 22.7, 14.1. HRMS (EI): *m/z* calcd. for $C_{13}H_{22}NO$ $[M-H]^+$ 208.1701, found: 208.1697. IR (KBr): 3318, 3221, 2957, 2927, 2856, 2104, 1643, 1544, 1468, 1434, 1361, 1225, 710, 604 cm^{-1}.

***N*-(cyclohexyl-2-propyn-1-yl)-4-methylbenzamide (1v)**. A white solid. M.p. 133-135 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.1 Hz, 2H), 7.21 (d, *J* = 8.1 Hz, 2H), 6.09 (bs, 1H), 2.44 (s, 1H), 2.38 (s, 3H), 2.24 – 2.21 (m, 2H), 1.96 – 1.91 (m, 2H), 1.77 – 1.59 (m, 5H), 1.34 – 1.31 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 141.9, 132.3, 129.3, 127.0, 85.7, 71.5, 52.1, 37.0, 25.4, 22.6, 21.5. HRMS (EI): *m/z* calcd. for $C_{16}H_{19}NO$ $[M]^+$ 241.1467, found: 241.1459. IR (KBr): 3304, 3066, 3036, 2858, 1644, 1533, 1502, 1449, 1307, 837, 754 cm^{-1}.

***N*-(1,1-dimethyl-2-propyn-1-yl)estra-1,3,5(10)-trien-17-one-3-methylcarboxamide (1w)**. Pale yellow solid. M.p. 158-160 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (s, 1H), 7.49 (d, *J* = 7.9 Hz, 1H), 7.33 (d, *J* = 7.9 Hz, 1H), 6.17 (bs, 1H), 2.96 – 2.94 (m, 2H), 2.55 – 2.42 (m, 2H), 2.38 (s, 1H), 2.34 – 2.30 (m, 1H), 2.17 – 2.06 (m, 4H), 1.76 (s, 6H), 1.64 – 1.44 (m, 6H), 0.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 220.7, 166.5, 143.6, 136.9, 132.3, 127.8, 125.5, 124.1, 87.4, 69.4, 50.5, 48.0, 44.5, 37.9, 35.9, 31.6, 29.3, 29.1, 26.4, 25.7, 21.6, 13.9. HRMS (EI): *m/z* calcd. for $C_{24}H_{29}NO_2$ $[M]^+$ 363.2198, found: 363.2190. IR (KBr): 3300, 3053, 2976, 2932, 2866, 1737, 1654,

1528, 1491, 1222, 669 cm^{-1}.

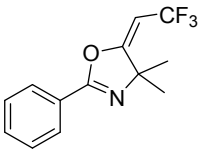
***N*-(prop-2-yn-1-yl)benzamide (1x)**. A white solid. ^1H NMR (300 MHz, $CDCl_3$) δ 7.81 – 7.77 (m, 2H), 7.55 – 7.50 (m, 1H), 7.47 – 7.42 (m, 2H), 6.32 (bs, 1H), 4.27 (dd, *J* = 5.2, 2.6 Hz, 2H), 2.29 (t, *J* = 2.6 Hz, 1H).

***N*-(3-phenylprop-2-yn-1-yl)benzamide (1y)**. A yellow solid. ^1H NMR (300 MHz, $CDCl_3$) δ 7.83 – 7.81 (m, 2H), 7.52 – 7.44 (m, 5H), 7.32 – 7.27 (m, 3H), 6.46 (bs, 1H), 4.50 (d, *J* = 5.0, 2H).

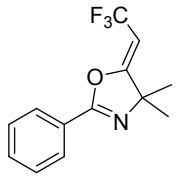
***N*-(1,1-dimethyl-4-phenyl-2-propyn-1-yl)benzamide (1z)**. A white solid. ^1H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.77 (m, 2H), 7.51 – 7.41 (m, 5H), 7.30 – 7.29 (m, 3H), 6.34 (bs, 1H), 1.87 (s, 6H).

A solution of **1a** (118 mg, 0.63 mmol) in dry THF (3.0 mL) was treated with 2.0 equiv. of n-BuLi (2.5 M solution in hexane, 0.5 mL, 1.25 mmol) at -78 °C. After 2 h, the reaction mixture was quenched with 0.5 mL D_2O (excess) and warmed to room temperature. The aqueous layer was extracted with DCM and the organic layer was dried over $MgSO_4$. The product was isolated as white solid.

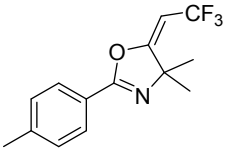
(1a-*d*)[c]. (93% D) ^1H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.74 (m, 2H), 7.50 – 7.46 (m, 1H), 7.42 – 7.39 (m, 2H), 6.25 (bs, 1H), 2.38 (s, 0.07 H), 1.76 (s, 6H).



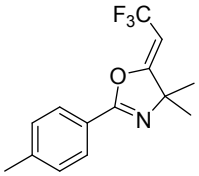
E-**3a**. Colorless oil. 76% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.94 (m, 2H), 7.56 – 7.52 (m, 1H), 7.48 – 7.43 (m, 2H), 5.60 (q, *J* = 9.2 Hz, 1H), 1.60 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.46 (d, *J* = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5 (q, *J* = 6.2 Hz), 158.2, 132.2, 128.6, 128.2, 125.8, 124.2 (q, *J* = 266.4 Hz), 92.8 (q, *J* = 37.6 Hz), 71.4, 26.9 (q, *J* = 3.5 Hz). HRMS (EI): *m/z* calcd. for $C_{13}H_{12}F_3NO$ $[M]^+$ 255.0871, found: 255.0876. IR (KBr): 3072, 3009, 2982, 2935, 2875, 1698, 1672, 1451, 1350, 1276, 1158, 1113, 1050, 1024, 965, 870, 693 cm^{-1}.



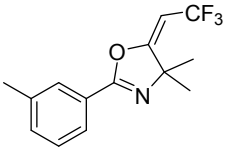
Z-**3a**. Colorless oil. 60% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 8.00 (m, 2H), 7.57 – 7.53 (m, 1H), 7.48 – 7.45 (m, 2H), 4.92 (q, *J* = 7.6 Hz, 1H), 1.49 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.51 (d, *J* = 7.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.8 (q, *J* = 5.0 Hz), 159.2, 132.3, 128.6, 128.4, 125.7, 123.2 (q, *J* = 268.8 Hz), 88.6 (q, *J* = 37.0 Hz), 71.6, 28.9 (q, *J* = 1.2 Hz). HRMS (EI): *m/z* calcd. for $C_{13}H_{12}F_3NO$ $[M]^+$ 255.0871, found: 255.0874. IR (KBr): 3092, 3065, 2980, 2931, 2866, 1710, 1663, 1452, 1358, 1257, 1156, 1115,1044, 1022, 968, 861, 696 cm^{-1}.



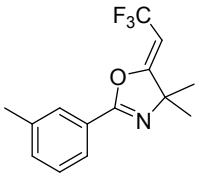
E-**3b**. Colorless oil. 76% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.2 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 5.58 (q, *J* = 9.2 Hz, 1H), 2.41 (s, 3H), 1.59 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.43 (d, *J* = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.6 (q, *J* = 5.9 Hz), 158.3, 142.7, 129.4, 128.1, 124.3 (q, *J* = 266.3 Hz), 123.0, 92.6 (q, *J* = 37.9 Hz), 71.4, 26.9, 21.6. HRMS (EI): *m/z* calcd. for $C_{14}H_{14}F_3NO$ $[M]^+$ 269.1027, found: 269.1022. IR (KBr): 3080, 3036, 2977, 2939, 2875, 1697, 1670, 1350, 1278, 1159, 1112, 1050, 1019, 966, 827, 725, 708 cm^{-1}.



Z-**3b**. Colorless oil. 69% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.2 Hz, 2H), 7.26 (d, *J* = 8.2 Hz, 2H), 4.90 (q, *J* = 7.6 Hz, 1H), 2.41 (s, 3H), 1.48 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.46 (d, *J* = 7.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.1 (q, *J* = 5.0 Hz), 159.4, 143.1, 129.5, 128.5, 123.4 (q, *J* = 268.8 Hz), 123.1, 88.5 (q, *J* = 37.0 Hz), 71.7, 29.1 (q, *J* = 0.9 Hz), 21.8. HRMS (EI): *m/z* calcd. for $C_{14}H_{14}F_3NO$ $[M]^+$ 269.1027, found: 269.1018. IR (KBr): 3069, 3036, 2979, 2932, 2864, 1709, 1663, 1357, 1257, 1156, 1114, 1043, 1017, 969, 828, 725, 676 cm^{-1}.

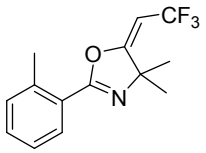


E-**3c**. Colorless oil. 73% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.75 – 7.72 (m, 1H), 7.35 – 7.26 (m, 2H), 5.59 (q, *J* = 9.2 Hz, 1H), 2.40 (s, 3H), 1.60 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.44 (d, *J* = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.6 (q, *J* = 6.3 Hz), 158.5, 138.7, 133.1, 128.8, 128.7, 125.8, 125.4, 124.4 (q, *J* = 266.5 Hz), 92.9 (q, *J* = 37.9 Hz), 71.5, 27.0 (q, *J* = 3.5 Hz), 21.4. HRMS (EI): *m/z* calcd. for $C_{14}H_{14}F_3NO$ $[M]^+$ 269.1027, found: 269.1030. IR (KBr): 3065, 3009, 2982, 2941, 2878, 1697, 1665, 1350, 1278, 1155, 1113,1066, 968, 870, 796, 711 cm^{-1}.

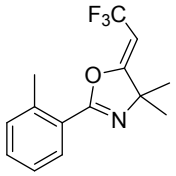


Z-**3c**. Colorless oil. 50% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.84 – 7.79 (m, 1H), 7.36 – 7.34 (m, 2H), 4.91 (q, *J* = 7.6 Hz, 1H), 2.41 (s, 3H), 1.48 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.47 (d, *J* = 7.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0 (q, *J* = 4.9 Hz), 159.5, 138.7, 133.3, 128.9, 128.7, 125.7, 124.9, 123.4 (q, *J* = 268.7 Hz), 88.7 (q, *J* = 37.0 Hz), 71.7, 29.0 (q, *J* = 0.9 Hz), 21.4. HRMS

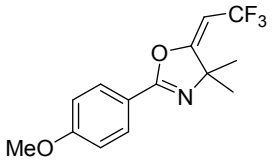
(EI): *m/z* calcd. for $C_{14}H_{14}F_3NO$ $[M]^+$ 269.1027, found: 269.1031. IR (KBr): 3066, 3039, 2979, 2932, 2866, 1709, 1662, 1357, 1258, 1152, 1116, 1058, 971, 861, 797, 714 cm^{-1}.



E-**3d**. Colorless oil. 70% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.79 (m, 1H), 7.41 – 7.37 (m, 1H), 7.29 – 7.25 (m, 2H), 5.56 (q, *J* = 9.2 Hz, 1H), 2.61 (s, 3H), 1.61 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.39 (d, *J* = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2 (q, *J* = 6.2 Hz), 158.2, 139.4, 131.5, 131.3, 129.7, 125.8, 125.0, 124.3 (q, *J* = 266.2 Hz), 92.2 (q, *J* = 37.9 Hz), 71.8, 27.0, 21.6. HRMS (EI): *m/z* calcd. for $C_{14}H_{14}F_3NO$ $[M]^+$ 269.1027, found: 269.1021. IR (KBr): 3071, 3027, 2979, 2937, 2875, 1695, 1659, 1350, 1264, 1162, 1112,1078, 1025, 966, 866, 726, 708 cm^{-1}.

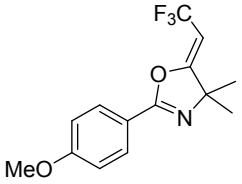


Z-**3d**. Colorless oil. 70% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.88 (m, 1H), 7.40 – 7.37 (m, 1H), 7.28 – 7.24 (m, 2H), 4.89 (q, *J* = 7.5 Hz, 1H), 2.61 (s, 3H), 1.48 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.51 (d, *J* = 7.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.6 (q, *J* = 4.1 Hz), 159.3, 139.6, 131.6, 130.2, 125.9, 124.9, 123.3 (q, *J* = 268.8 Hz), 88.2 (q, *J* = 37.0 Hz), 71.9, 29.0, 21.9. HRMS (EI): *m/z* calcd. for $C_{14}H_{14}F_3NO$ $[M]^+$ 269.1027, found: 269.1028. IR (KBr): 3069, 3027, 2977, 2926, 2869, 1708, 1655, 1357, 1260, 1159, 1116, 1018, 969, 860, 726, 677 cm^{-1}.

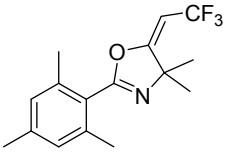


E-**3e**. Colorless oil. 77% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.87(m, 2H), 6.96 – 6.92 (m, 2H), 5.56 (q, *J* = 9.3 Hz, 1H), 3.85 (s, 3H), 1.58 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.38 (d, *J* = 9.3 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.6 (q, *J* = 6.3 Hz), 162.7, 157.9, 129.9, 124.3 (q, *J* = 266.4 Hz), 118.1, 114.0, 92.4

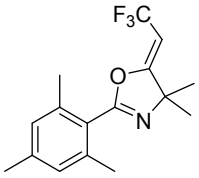
(q, J = 37.9 Hz), 71.2, 55.4, 26.9 (q, J = 3.5 Hz). HRMS (EI): *m/z* calcd. for $C_{14}H_{14}F_3NO_2$ $[M]^+$ 285.0977, found: 285.0980. IR (KBr): 2987, 2966, 2936, 2908, 2839, 1698, 1669, 1513, 1368, 1259, 1157, 1115, 1050, 837, 681 cm^{-1}.



Z-**3e**. Colorless oil. 60% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, J = 8.6 Hz, 2H), 6.96 (d, J = 8.6 Hz, 2H), 4.89 (q, J = 7.6 Hz, 1H), 3.86 (s, 3H), 1.47 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.43 (d, J = 7.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0 (q, J = 5.0 Hz), 162.8, 158.9, 130.2, 123.3 (q, J = 268.6 Hz), 118.0, 114.0, 88.2 (q, J = 37.0 Hz), 71.5, 55.4, 28.9 (q, J = 1.1 Hz). HRMS (EI): *m/z* calcd. for $C_{14}H_{14}F_3NO_2$ $[M]^+$ 285.0977, found: 285.0973. IR (KBr): 3077, 3044, 2976, 2931, 2839, 1662, 1611, 1513, 1359, 1259, 1155, 1113,1028, 840, 676 cm^{-1}.

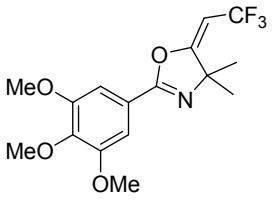


E-**3f**. A white solid. M.p. 54-56 °C. 25% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.24 (s, 2H), 5.48 (q, J = 9.2 Hz, 1H), 2.28 (s, 9H), 1.61 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.48 (d, J = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.6 (q, J = 6.3 Hz), 158.6, 140.4, 137.4, 128.6, 124.4 (q, J = 266.8 Hz), 123.7, 92.6 (q, J = 37.8 Hz), 71.6, 26.9 (q, J = 3.5 Hz), 21.4, 19.7. HRMS (EI): *m/z* calcd. for $C_{16}H_{18}F_3NO$ $[M]^+$ 297.1340, found: 297.1345. IR (KBr): 3009, 2979, 2937, 2875, 1700, 1678, 1351, 1265, 1173, 1111, 1076, 1014, 965, 850, 701 cm^{-1}.

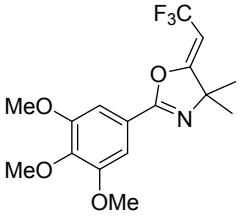


Z-**3f**. A white solid. M.p. 103-105 °C. 60% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 6.91 (s, 1H), 4.92 (q, J = 7.5 Hz, 1H), 2.32 (s, 6H), 2.30 (s, 3H), 1.48 (s, 6H). ^{19}F

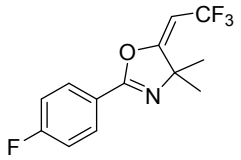
NMR (376 MHz, $CDCl_3$) δ -57.50 (d, *J* = 7.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0, 159.5, 140.6, 137.8, 128.7, 123.6, 123.3 (q, *J* = 268.8 Hz), 88.5 (q, *J* = 37.1 Hz), 71.9, 29.0, 21.4, 20.0. HRMS (EI): *m/z* calcd. for $C_{16}H_{18}F_3NO$ $[M]^+$ 297.1340, found: 297.1337. IR (KBr): 3086, 3039, 2980, 2929, 2866, 1709, 1670, 1612, 1360, 1263, 1147, 1112, 1010, 967, 853, 674 cm^{-1}.



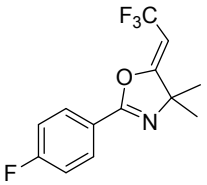
E-**3g**. A white solid. M.p. 69-71 °C. 83% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.17 (s, 2H), 5.60 (q, *J* = 9.2 Hz, 1H), 3.91 (s, 6H), 3.89 (s, 3H), 1.59 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.46 (d, *J* = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.6 (q, *J* = 6.4 Hz), 158.0, 153.4, 141.6, 124.3 (q, *J* = 266.5 Hz), 121.0, 105.5, 92.9 (q, *J* = 37.9 Hz), 71.6, 61.1, 56.4, 27.0 (q, *J* = 3.3 Hz). HRMS (EI): *m/z* calcd. for $C_{16}H_{18}F_3NO_4$ $[M]^+$ 345.1188, found: 345.1190. IR (KBr): 3077, 3006, 2976, 2942, 2839, 1697, 1665, 1589, 1505, 1461, 1417, 1350, 1227, 1183, 1130, 1073, 978, 849, 718 cm^{-1}.



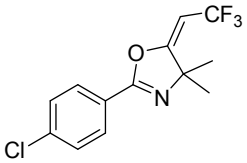
Z-**3g**. A white solid. M.p. 71-73 °C. 60% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.23 (s, 2H), 4.90 (q, *J* = 7.6 Hz, 1H), 3.91 (s, 6H), 3.90 (s, 3H), 1.48 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.55 (d, *J* = 7.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.9 (q, *J* = 5.0 Hz), 159.1, 153.4, 141.8, 123.4 (q, *J* = 268.7 Hz), 120.9, 105.7, 88.6 (q, *J* = 36.8 Hz), 71.9, 61.1, 56.4, 29.1. HRMS (EI): *m/z* calcd. for $C_{16}H_{18}F_3NO_4$ $[M]^+$ 345.1188, found: 345.1194. IR (KBr): 3101, 3000, 2977, 2942, 2837, 1708, 1661, 1588, 1504, 1463, 1418, 1341, 1257, 1192, 1130, 1084, 977, 860, 719 cm^{-1}.



E-**3h**. Colorless oil. 67% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.14 (t, *J* = 8.6 Hz, 2H), 5.59 (q, *J* = 9.2 Hz, 1H), 1.59 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.55 (d, *J* = 9.2 Hz, 3F), -106.48 (tt, *J* = 8.6, 5.4 Hz, 1F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5 (q, *J* = 6.4 Hz), 165.3 (d, *J* = 253.5 Hz), 157.4, 130.6 (d, *J* = 9.0 Hz), 124.3 (q, *J* = 266.6 Hz), 122.2 (d, *J* = 3.2 Hz), 116.0 (d, *J* = 22.1 Hz), 93.1 (q, *J* = 38.0 Hz), 71.6, 27.0 (q, *J* = 3.5 Hz). HRMS (EI): *m/z* calcd. for $C_{13}H_{11}F_4NO$ $[M]^+$ 273.0777, found: 273.0772. IR (KBr): 3077, 3006, 2979, 2940, 2875, 1699, 1673, 1607, 1510, 1351, 1280, 1158, 1115, 1051, 965, 846, 709 cm^{-1}.

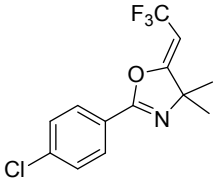


Z-**3h**. Colorless oil. 43% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (dd, *J* = 8.7, 5.4 Hz, 2H), 7.15 (t, *J* = 8.7 Hz, 2H), 4.92 (q, *J* = 7.6 Hz, 1H), 1.48 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.54 (d, *J* = 7.6 Hz, 3F), -106.17 (tt, *J* = 8.7, 5.4 Hz, 1F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.9 (q, *J* = 4.9 Hz), 165.4 (d, *J* = 253.5 Hz), 158.4, 130.9 (d, *J* = 9.1 Hz), 123.3 (q, *J* = 268.7 Hz), 122.1 (d, *J* = 3.2 Hz), 116.1 (d, *J* = 22.2 Hz), 89.0 (q, *J* = 37.1 Hz), 71.9, 29.0 (q, *J* = 1.4 Hz). HRMS (EI): *m/z* calcd. for $C_{13}H_{11}F_4NO$ $[M]^+$ 273.0777, found: 273.0779. IR (KBr): 3077, 3050, 2976, 2928, 2863, 1711, 1666, 1607, 1356, 1258, 1154, 1117, 1040, 968, 846, 675 cm^{-1}.

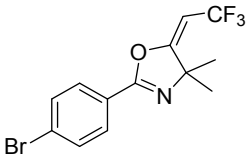


E-**3i**. Colorless oil. 68% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 5.59 (q, *J* = 9.2 Hz, 1H), 1.59 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.57 (d, *J* = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4 (q, *J* = 6.3 Hz), 157.5, 138.6, 129.6, 129.1, 124.4, 124.2 (q, *J* = 266.7 Hz), 93.3 (q, *J* = 38.0 Hz), 71.7, 26.9 (q, *J* = 3.5 Hz). HRMS (EI): *m/z* calcd. for $C_{13}H_{11}ClF_3NO$ $[M]^+$

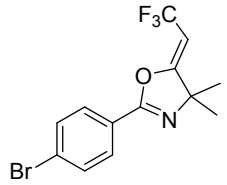
289.0481, found: 289.0479. IR (KBr): 3095, 3071, 2983, 2940, 2872, 1698, 1671, 1599, 1492, 1276, 1159, 1115, 1050, 966, 839, 679 cm^{-1}.



Z-**3i**. A white solid. M.p. 56-58 °C. 58% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.6 Hz, 2H), 7.44 (d, *J* = 8.6 Hz, 2H), 4.92 (q, *J* = 7.5 Hz, 1H), 1.48 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.57 (d, *J* = 7.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.6 (q, *J* = 5.0 Hz), 158.3, 138.6, 129.7, 129.0, 124.2, 123.1 (q, *J* = 268.9 Hz), 88.9 (q, *J* = 37.1 Hz), 71.8, 28.9 (q, *J* = 1.2 Hz). HRMS (EI): *m/z* calcd. for $C_{13}H_{11}ClF_3NO$ $[M]^+$ 289.0481, found: 289.0482. IR (KBr): 3104, 3089, 2979, 2931, 2866, 1711, 1664, 1599, 1491, 1256, 1155, 1114, 1043, 968, 839, 673 cm^{-1}.

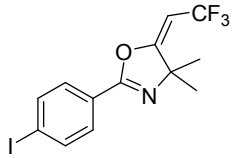


E-**3j**. Colorless oil. 72% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.5 Hz, 2H), 7.59 (d, *J* = 8.5 Hz, 2H), 5.59 (q, *J* = 9.2 Hz, 1H), 1.59 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.57 (d, *J* = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4 (q, *J* = 6.4 Hz), 157.6, 132.1, 129.7, 127.1, 124.9, 124.2 (q, *J* = 266.6 Hz), 93.3 (q, *J* = 37.9 Hz), 71.7, 26.9 (q, *J* = 3.5 Hz). HRMS (EI): *m/z* calcd. for $C_{13}H_{11}BrF_3NO$ $[M]^+$ 332.9976, found: 332.9982. IR (KBr): 3092, 3071, 2982, 2937, 2875, 1697, 1671, 1593, 1400, 1275, 1158, 1113,1050, 1011, 965, 836, 698 cm^{-1}.

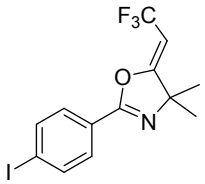


Z-**3j**. A white solid. M.p. 64-66 °C. 60% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 2H), 4.93 (q, *J* = 7.5 Hz, 1H), 1.48 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.54 (d, *J* = 7.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.8 (q, *J* = 4.9 Hz), 158.6, 132.2, 130.0, 127.3, 124.8, 123.3 (q, *J* = 268.8

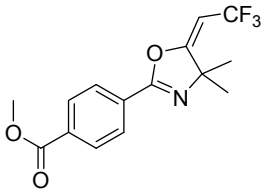
Hz), 89.1 (q, J = 37.2 Hz), 71.9, 29.0. HRMS (EI): *m/z* calcd. for $C_{13}H_{11}BrF_3NO$ $[M]^+$ 332.9976, found: 332.9973. IR (KBr): 3098, 3068, 2979, 2928, 2866, 1711, 1664, 1593, 1401, 1255, 1155, 1115,1042, 1010, 968, 836, 673 cm^{-1}.



E-**3k**. Colorless oil. 71% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 7.9 Hz, 2H), 7.66 (d, J = 7.9 Hz, 2H), 5.59 (q, J = 9.2 Hz, 1H), 1.58 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.55 (d, J = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4 (q, J = 6.2 Hz), 157.7, 138.1, 129.7, 125.4, 124.2 (q, J = 266.5 Hz), 99.5, 93.3 (t, J = 38.0 Hz), 71.7, 26.9 (q, J = 3.4 Hz). HRMS (EI): *m/z* calcd. for $C_{13}H_{11}F_3INO$ $[M]^+$ 380.9838, found: 380.9837. IR (KBr): 3071, 3009, 2979, 2937, 2875, 1697, 1670, 1589, 1483, 1396, 1274, 1158, 1113, 1060, 1007, 966, 832, 722, 693 cm^{-1}.

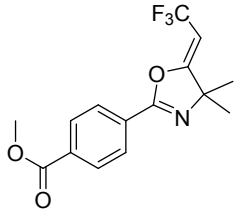


Z-**3j**. A white solid. M.p. 53-55 °C. 57% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 8.3 Hz, 2H), 7.71 (d, J = 8.3 Hz, 2H), 4.92 (q, J = 7.5 Hz, 1H), 1.48 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.54 (d, J = 7.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7 (q, J = 4.9 Hz), 158.8, 138.1, 129.9, 125.4, 123.3 (q, J = 268.9 Hz), 99.7, 89.1 (q, J = 37.2 Hz), 71.9, 29.0 (q, J = 1.0 Hz). HRMS (EI): *m/z* calcd. for $C_{13}H_{11}F_3INO$ $[M]^+$ 380.9838, found: 380.9834. IR (KBr): 3098, 3036, 2979, 2928, 2863, 1710, 1662, 1589, 1486, 1396, 1256, 1155, 1114, 1040, 1006, 968, 829, 723, 673 cm^{-1}.

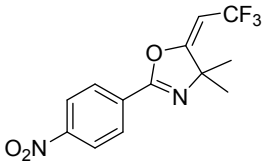


E-**3k**. A white solid. M.p. 97-99 °C. 73% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 8.5 Hz, 2H), 8.02 (d, J = 8.5 Hz, 2H), 5.62 (q, J = 9.2 Hz, 1H), 3.95 (s,

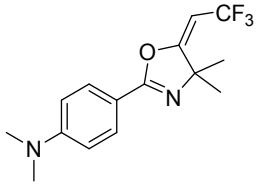
3H), 1.60 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.61 (d, J = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4 (q, J = 5.8 Hz), 166.3, 157.6, 133.4, 129.9, 128.3, 124.2 (q, J = 266.7 Hz), 93.5 (q, J = 37.9 Hz), 71.8, 52.6, 26.9. HRMS (EI): *m/z* calcd. for $C_{15}H_{14}F_3NO_3$ $[M]^+$ 313.0926, found: 313.0924. IR (KBr): 3009, 2985, 2940, 2875, 1718, 1694, 1671, 1408, 1284, 1156, 1097, 1043, 967, 861, 700 cm^{-1}.



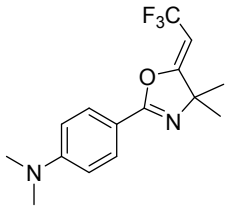
Z-**3k**. A white solid. M.p. 82-84 °C. 45% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 8.4 Hz, 2H), 8.07 (d, J = 8.4 Hz, 2H), 4.94 (q, J = 7.5 Hz, 1H), 3.95 (s, 3H), 1.49 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.59 (d, J = 7.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7 (q, J = 5.2 Hz), 166.3, 158.6, 133.5, 129.9, 129.8, 128.5, 123.2 (q, J = 268.9 Hz), 89.3 (q, J = 37.2 Hz), 72.0, 52.6, 29.0. HRMS (EI): *m/z* calcd. for $C_{15}H_{14}F_3NO_3$ $[M]^+$ 313.0926, found: 313.0930. IR (KBr): 3101, 3050, 2976, 2931, 2875, 1727, 1662, 1411, 1280, 1156, 1108, 1045, 968, 857, 710 cm^{-1}.



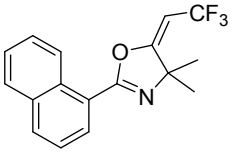
E-**3m**. Colorless oil. 60% isolated yield.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, J = 9.0 Hz, 2H), 8.14 (d, J = 9.0 Hz, 2H), 5.65 (q, J = 9.1 Hz, 1H), 1.62 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.73 (d, J = 9.1 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1 (q, J = 6.2 Hz), 156.6, 150.1, 131.7, 129.4, 124.1 (q, J = 266.8 Hz), 123.9, 94.0 (q, J = 38.1 Hz), 72.1, 26.9 (q, J = 3.5 Hz). HRMS (EI): *m/z* calcd. for $C_{13}H_{11}F_3N_2O_3$ $[M]^+$ 300.0722, found: 300.0719. IR (KBr): 3110, 3080, 2982, 2940, 2875, 1699, 1671, 1601, 1528, 1352, 1277, 1158, 1114,1053, 1014, 965, 866, 700 cm^{-1}.



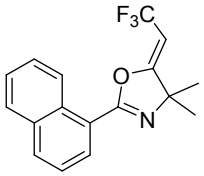
E-**3n**. A white solid. M.p. 82-84 °C. 70% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 9.1 Hz, 2H), 6.67 (d, *J* = 9.1 Hz, 2H), 5.54 (q, *J* = 9.3 Hz, 1H), 3.03 (s, 6H), 1.58 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.21 (d, *J* = 9.3 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.0 (q, *J* = 6.5 Hz), 158.7, 152.8, 129.7, 124.6 (q, *J* = 266.3 Hz), 112.5, 111.3, 92.0 (q, *J* = 37.7 Hz), 71.1, 40.2, 27.2 (q, *J* = 3.4 Hz). HRMS (EI): *m/z* calcd. for $C_{15}H_{17}F_3N_2O$ $[M]^+$ 298.1293, found: 298.1289. IR (KBr): 3000, 2978, 2938, 2812, 1696, 1659, 1529, 1365, 1230, 1158, 1111, 1078, 966, 821, 680 cm^{-1}.



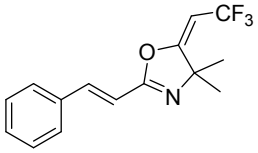
Z-**3n**. A white solid. M.p. 113-115 °C. 52% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 9.0 Hz, 2H), 6.68 (d, *J* = 9.0 Hz, 2H), 4.85 (q, *J* = 7.6 Hz, 1H), 3.04 (s, 6H), 1.46 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.31 (d, *J* = 7.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.4 (q, *J* = 4.8 Hz), 159.8, 152.9, 130.0, 123.6 (q, *J* = 268.8 Hz), 112.4, 111.3, 87.7 (q, *J* = 36.9 Hz), 71.4, 40.2, 29.2. HRMS (EI): *m/z* calcd. for $C_{15}H_{17}F_3N_2O$ $[M]^+$ 298.1293, found: 298.1288. IR (KBr): 2980, 2932, 2813, 1708, 1660, 1528, 1360, 1255, 1154, 1102,1035, 997, 823, 676 cm^{-1}.



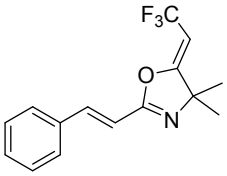
E-**3o**. A white solid. M.p. 62-64 °C. 60% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (d, *J* = 8.2 Hz, 1H), 8.12 (d, *J* = 8.2 Hz, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.66 (t, *J* = 8.2 Hz, 1H), 7.57 (t, *J* = 8.2 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 5.65 (q, *J* = 9.2 Hz, 1H), 1.72 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.32 (d, *J* = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.9 (q, *J* = 6.9 Hz), 157.7, 133.9, 133.0, 131.1, 129.5, 128.8, 128.0, 126.6, 126.2, 124.7, 124.5 (d, *J* = 266.5 Hz), 122.2, 92.5 (q, *J* = 37.8 Hz), 72.4, 27.2 (q, *J* = 3.5 Hz). HRMS (EI): *m/z* calcd. for $C_{17}H_{14}F_3NO$ $[M]^+$ 305.1027, found: 305.1029. IR (KBr): 3092, 3050, 3006, 2979, 2937, 2875, 1697, 1656, 1589, 1350, 1252, 1159, 1111, 1072, 982, 866, 774, 705 cm^{-1}.



Z-**3o**. A white solid. M.p. 97-99 °C. 33% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.24 (d, *J* = 8.5 Hz, 1H), 8.23 (dd, *J* = 7.3, 1.1 Hz, 1H), 8.03 (d, *J* = 8.2 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.70 – 7.62 (m, 1H), 7.59 – 7.52 (m, 2H). 4.97 (q, *J* = 7.6 Hz, 1H), 1.59 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.37 (d, *J* = 7.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.2 (q, *J* = 5.3 Hz), 158.6, 133.9, 133.2, 131.1, 130.1, 128.8, 128.1, 126.6, 126.2, 124.8, 123.5 (q, *J* = 267.4 Hz), 122.0, 88.3 (q, *J* = 37.0 Hz), 72.8, 29.2 (q, *J* = 1.4 Hz). HRMS (EI): *m/z* calcd. for $C_{17}H_{14}F_3NO$ $[M]^+$ 305.1027, found: 305.1031. IR (KBr): 3092, 3056, 2979, 2925, 2863, 1706, 1652, 1589, 1360, 1260, 1157, 1107, 1076, 923, 861, 677 cm^{-1}.

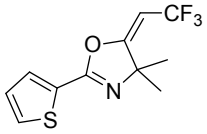


E-**3p**. Colorless oil. 61% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.49 (m, 2H), 7.43 (d, *J* = 16.3 Hz, 1H), 7.41 – 7.37 (m, 3H), 6.60 (d, *J* = 16.3 Hz, 1H), 5.55 (q, *J* = 9.2 Hz, 1H), 1.56 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.46 (d, *J* = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2 (q, *J* = 6.4 Hz), 158.1, 141.7, 134.7, 130.2, 129.1, 127.8, 124.3 (d, *J* = 266.5 Hz), 113.2, 92.7 (q, *J* = 37.9 Hz), 71.2, 26.9 (q, *J* = 3.5 Hz). HRMS (EI): *m/z* calcd. for $C_{15}H_{14}F_3NO$ $[M]^+$ 281.1027, found: 281.1028. IR (KBr): 3080, 3062, 3003, 2976, 2940, 2875, 1697, 1665, 1613, 1350, 1276, 1181, 1111,1074, 974, 869, 756, 695 cm^{-1}.

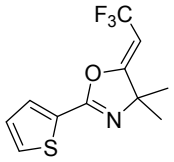


Z-**3p**. A white solid. M.p. 60-62 °C. 32% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.50 (m, 3H), 7.42 – 7.36 (m, 3H), 6.63 (d, *J* = 16.3 Hz, 1H), 4.87 (q, *J* = 7.6 Hz, 1H), 1.45 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.43 (d, *J* = 7.6 Hz, 3F). ^{13}C

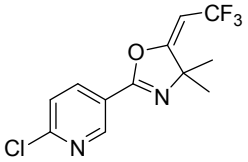
NMR (101 MHz, $CDCl_3$) δ 168.5 (q, *J* = 4.7 Hz), 158.9, 142.3, 134.6, 130.2, 129.0, 127.7, 123.2 (q, *J* = 268.6 Hz), 112.9, 88.3 (q, *J* = 36.9 Hz), 71.3, 28.9. HRMS (EI): *m/z* calcd. for $C_{15}H_{14}F_3NO$ $[M]^+$ 281.1027, found: 281.1031. IR (KBr): 3083, 3062, 3027, 2979, 2931, 2866, 1709, 1661, 1613, 1360, 1257, 1192, 1144,1113, 974, 854, 758, 697 cm^{-1}.



E-**3q**. Colorless oil. 61% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 3.6, 0.9 Hz, 1H), 7.53 (dd, *J* = 4.8, 0.9 Hz, 1H), 7.12 (dd, *J* = 4.8, 3.6 Hz, 1H), 5.58 (q, *J* = 9.2 Hz, 1H), 1.59 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.54 (d, *J* = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3 (q, *J* = 6.3 Hz), 154.2, 131.4, 131.1, 128.2, 128.0, 124.2 (q, *J* = 266.6 Hz), 93.1 (q, *J* = 38.0 Hz), 71.7, 27.0 (q, *J* = 3.5 Hz). HRMS (EI): *m/z* calcd. for $C_{11}H_{10}F_3NOS$ $[M]^+$ 261.0435, found: 261.0430. IR (KBr): 3087, 3006, 2980, 2941, 2872, 1699, 1669, 1429, 1276, 1155, 1113, 1072, 1008, 870, 714, 703 cm^{-1}.

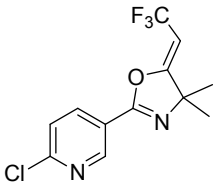


Z-**3q**. Colorless oil. 39% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 3.7, 1.1 Hz, 1H), 7.55 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.13 (dd, *J* = 5.0, 3.7 Hz, 1H), 4.90 (q, *J* = 7.5 Hz, 1H), 1.48 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.55 (d, *J* = 7.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7 (q, *J* = 3.5 Hz), 155.1, 132.0, 131.4, 128.2, 128.0, 123.2 (q, *J* = 268.7 Hz), 88.9 (q, *J* = 37.2 Hz), 71.9, 29.0. HRMS (EI): *m/z* calcd. for $C_{11}H_{10}F_3NSO$ $[M]^+$ 261.0435, found: 261.0441. IR (KBr): 3089, 2976, 2928, 2866, 1710, 1662, 1430, 1260, 1154, 1114, 1052, 1002, 853, 716, 677 cm^{-1}.

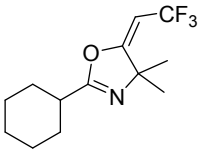


E-**3r**. A white solid. M.p. 152-154 °C. 53% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 8.91 (s, 1H), 8.18 (d, *J* = 8.3 Hz, 1H), 7.43 (d, *J* = 8.3 Hz, 1H), 5.62 (q, *J* = 9.1 Hz,

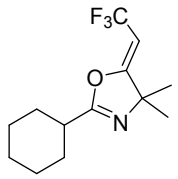
1H), 1.59 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.77 (d, *J* = 9.1 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.9 (q, *J* = 6.5 Hz), 155.7, 155.0, 149.5, 138.1, 124.5, 124.0 (q, *J* = 266.6 Hz), 121.2, 94.0 (q, *J* = 38.0 Hz), 71.8, 26.9 (q, *J* = 3.3 Hz). HRMS (EI): *m/z* calcd. for $C_{12}H_{10}ClF_3N_2O$ $[M]^+$ 290.0434, found: 290.0430. IR (KBr): 3104, 3044, 2984, 2941, 2881, 1713, 1673, 1554, 1459, 1364, 1286, 1162, 1085,1014, 837, 742, 693 cm^{-1}.



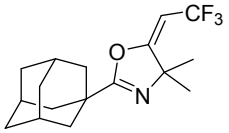
Z-**3r**. A white solid. M.p. 81-83 °C. 49% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (s, 1H), 8.20 (d, *J* = 8.4 Hz, 1H), 7.44 (d, *J* = 8.4 Hz, 1H), 4.96 (q, *J* = 7.5 Hz, 1H), 1.49 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.71 (d, *J* = 7.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1 (q, *J* = 5.0 Hz), 156.6, 155.2, 149.8, 138.2, 124.5, 123.1 (q, *J* = 269.0 Hz), 121.2, 89.8 (q, *J* = 37.1 Hz), 72.1, 28.9. HRMS (EI): *m/z* calcd. for $C_{12}H_{10}ClF_3N_2O$ $[M]^+$ 290.0434, found: 290.0428. IR (KBr): 3092, 3059, 2981, 2931, 2863, 1712, 1669, 1560, 1455, 1367, 1257, 1159,1109, 1012, 860, 744, 675 cm^{-1}.



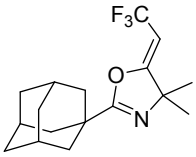
E-**3s**. A white solid. M.p. 114-116 °C. 55% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.40 (q, *J* = 9.3 Hz, 1H), 2.36 (tt, *J* = 11.4, 3.5 Hz, 1H), 1.96 – 1.93 (m, 2H), 1.80 – 1.77 (m, 2H), 1.69 – 1.65 (m, 1H), 1.47 (s, 6H), 1.43 – 1.40 (m, 1H), 1.35 – 1.20 (m, 4H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.44 (d, *J* = 9.3 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9 (q, *J* = 6.2 Hz), 165.1, 124.4 (q, *J* = 266.5 Hz), 92.0 (q, *J* = 37.8 Hz), 70.7, 36.9, 29.4, 26.8 (q, *J* = 3.3 Hz), 25.8, 25.5. HRMS (EI): *m/z* calcd. for $C_{13}H_{18}F_3NO$ $[M]^+$ 261.1340, found: 261.1342. IR (KBr): 3301, 3044, 3000, 2932, 2856, 1730, 1634, 1535, 1451, 1371, 1254, 1146, 1102, 668 cm^{-1}.



Z-**3s**. A white solid. M.p. 137-139 °C. 49% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.77 (q, *J* = 7.6 Hz, 1H), 2.47 (tt, *J* = 11.3, 3.6 Hz, 1H), 2.01 – 1.97 (m, 2H), 1.81 – 1.77 (m, 2H), 1.69 – 1.67 (m, 1H), 1.53 – 1.42 (m, 2H), 1.37 – 1.33 (m, 1H), 1.35 (s, 6H), 1.30 – 1.24 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.50 (d, *J* = 7.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.3 (q, *J* = 5.1 Hz), 166.3, 123.4 (q, *J* = 268.8 Hz), 87.8 (q, *J* = 36.9 Hz), 70.9, 37.0, 29.4, 28.9 (q, *J* = 1.5 Hz), 25.8, 25.5. HRMS (EI): *m/z* calcd. for $C_{13}H_{18}F_3NO$ $[M]^+$ 261.1340, found: 261.1345. IR (KBr): 3302, 3048, 3003, 2932, 2857, 1731, 1634, 1535, 1451, 1372, 1254, 1146,1102, 660 cm^{-1}.

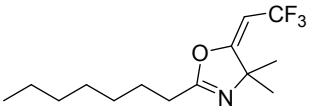


E-**3t**. A white solid. M.p. 72-74 °C. 77% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.39 (q, *J* = 9.3 Hz, 1H), 2.06 – 2.01 (m, 3H), 1.90 – 1.88 (m, 6H), 1.77 – 1.69 (m, 6H), 1.45 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.35 (d, *J* = 9.3 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9 (q, *J* = 6.4 Hz), 167.4, 124.3 (q, *J* = 266.3 Hz), 91.7 (q, *J* = 37.8 Hz), 70.3, 39.0, 36.4, 34.8, 27.6, 26.7 (q, *J* = 3.6 Hz). HRMS (EI): *m/z* calcd. for $C_{17}H_{22}F_3NO$ $[M]^+$ 313.1653, found: 313.1650. IR (KBr): 2982, 2913, 2854, 1691, 1676, 1452, 1241, 1176, 1078,1030, 983, 860, 653 cm^{-1}.

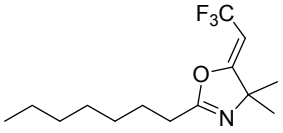


Z-**3t**. A white solid. M.p. 71-73 °C. 61% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.75 (q, *J* = 7.6 Hz, 1H), 2.06 – 2.01 (m, 3H), 1.94 – 1.91 (m, 6H), 1.77 – 1.70 (m, 6H), 1.33 (s, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.49 (d, *J* = 7.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.4 (q, *J* = 5.0 Hz), 168.8, 123.4 (q, *J* = 268.6 Hz), 87.7 (q, *J* = 36.9 Hz), 70.7, 39.1, 36.5, 35.2, 28.9 (q, *J* = 1.2 Hz), 27.8. HRMS (EI): *m/z* calcd. for $C_{17}H_{22}F_3NO$ $[M]^+$ 313.1653, found: 313.1647. IR (KBr): 2979, 2930, 2855, 1707,

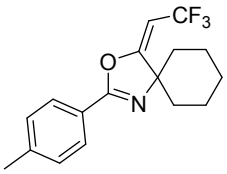
1673, 1453, 1256, 1153, 1102, 1030, 981, 861, 671 cm^{-1}.



E-**3u**. Colorless oil. 50% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.39 (q, *J* = 9.2 Hz, 1H), 2.34 (t, *J* = 7.6 Hz, 2H), 1.64 (dt, *J* = 14.8, 7.6 Hz, 2H), 1.46 (s, 6H), 1.39 – 1.21 (m, 8H), 0.86 (t, *J* = 6.7 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.55 (d, *J* = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8 (q, *J* = 6.2 Hz), 162.2, 124.4 (q, *J* = 266.4 Hz), 92.2 (q, *J* = 37.9 Hz), 70.8, 31.8, 29.1, 28.9, 27.7, 26.8 (q, *J* = 3.5 Hz), 25.6, 22.7, 14.2. HRMS (EI): *m/z* calcd. for $C_{14}H_{22}F_3NO$ $[M]^+$ 277.1653, found: 277.1646. IR (KBr): 2958, 2933, 2859, 1703, 1685, 1352, 1284, 1182, 1113, 1074, 971, 869 cm^{-1}.

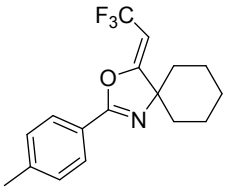


Z-**3u**. Colorless oil. 33% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.78 (q, *J* = 7.6 Hz, 1H), 2.42 (t, *J* = 7.6 Hz, 2H), 1.68 (dt, *J* = 15.0, 7.6 Hz, 2H), 1.42 – 1.24 (m, 8H), 1.35 (s, 6H), 0.87 (t, *J* = 6.8 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.56 (d, *J* = 7.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.3 (q, *J* = 5.1 Hz), 163.4, 123.3 (q, *J* = 268.8 Hz), 88.0 (q, *J* = 37.0 Hz), 71.1, 31.7, 29.1, 28.9, 28.9, 27.9, 25.5, 22.7, 14.2. HRMS (EI): *m/z* calcd. for $C_{14}H_{22}F_3NO$ $[M]^+$ 277.1653, found: 277.1644. IR (KBr): 2958, 2931, 2859, 1710, 1684, 1364, 1261, 1194, 1137, 1115, 972, 860 cm^{-1}.

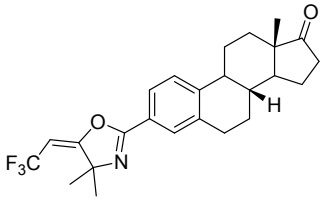


E-**3v**. Colorless oil. 33% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.2 Hz, 2H), 5.54 (q, *J* = 9.5 Hz, 1H), 2.40 (s, 3H), 2.13 – 2.00 (m, 2H), 1.99 – 1.89 (m, 2H), 1.84 – 1.81 (m, 1H), 1.68 – 1.63 (m, 4H), 1.41 – 1.34 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -51.86 (d, *J* = 9.5 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.3 (q, *J* = 6.3 Hz), 157.4, 142.5, 129.5, 128.3, 124.6 (q, *J* = 266.4 Hz), 123.7, 92.5 (q, *J* = 37.9 Hz), 75.1, 35.62 (q, *J* = 3.3 Hz), 25.5, 22.3, 21.8. HRMS

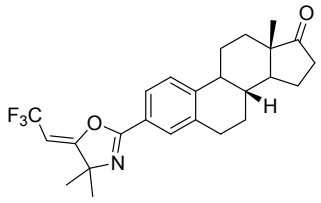
(EI): *m/z* calcd. for $C_{17}H_{18}F_3NO$ $[M]^+$ 309.1340, found: 309.1336. IR (KBr): 3039, 3009, 2931, 2860, 1694, 1668, 1449, 1359, 1285, 1156, 1097, 1043, 1018, 951, 827, 706 cm^{-1}.



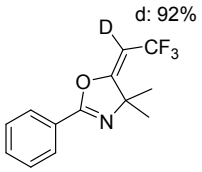
Z-**3v**. Colorless oil. 62% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.2 Hz, 2H), 7.26 (d, *J* = 8.2 Hz, 2H), 4.87 (q, *J* = 7.7 Hz, 1H), 2.42 (s, 3H), 1.92 – 1.88 (m, 1H), 1.86– 1.75 (m, 4H), 1.71 – 1.66 (m, 2H), 1.55 – 1.48 (m, 2H), 1.44 – 1.36 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.13 (d, *J* = 7.7 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.6 (q, *J* = 4.9 Hz), 158.6, 142.7, 129.4, 128.5, 123.7 (q, *J* = 268.7 Hz), 123.5, 88.7 (q, *J* = 36.8 Hz), 74.8, 38.7, 25.6, 22.2, 21.8. HRMS (EI): *m/z* calcd. for $C_{17}H_{18}F_3NO$ $[M]^+$ 309.1340, found: 309.1342. IR (KBr): 3042, 3006, 2936, 2859, 1707, 1663, 1448, 1356, 1280, 1212, 1115, 1049, 1017, 949, 828, 726 cm^{-1}.



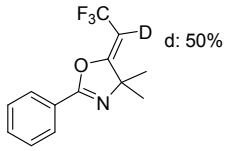
E-**3w**. A white solid. M.p. 193-195 °C. 75% isolated yield. ^1H NMR (400 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.69 (d, *J* = 8.1 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 1H), 5.57 (q, *J* = 9.2 Hz, 1H), 2.96 – 2.92 (m, 2H), 2.54 – 2.41 (m, 2H), 2.37 – 2.26 (m, 1H), 2.20 – 1.94 (m, 4H), 1.57 (s, 6H), 1.66 – 1.44 (m, 6H), 0.91 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -53.40 (d, *J* = 9.2 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.6 (q, *J* = 6.5 Hz), 158.4, 144.5, 137.2, 128.7, 125.8, 125.5, 124.3 (q, *J* = 266.5 Hz), 123.3, 92.7 (q, *J* = 37.8 Hz), 71.4, 50.6, 48.0, 44.7, 37.9, 35.9, 31.6, 29.3, 27.0 (q, *J* = 3.4 Hz), 26.3, 25.7, 21.7, 13.9. HRMS (EI): *m/z* calcd. for $C_{25}H_{28}F_3NO_2$ $[M]^+$ 431.2072, found: 431.2067. IR (KBr): 3000, 2968, 2920, 2875, 2855, 1739, 1664, 1271, 1178, 1114, 1076, 972, 709 cm^{-1}.



Z-**3w**. A white solid. M.p. 113-115 °C. 66% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.1 Hz, 1H), 7.73 (s, 1H), 7.37 (d, *J* = 8.1 Hz, 1H), 4.89 (q, *J* = 7.6 Hz, 1H), 2.96 – 2.93 (m, 2H), 2.53 – 2.41 (m, 2H), 2.36 – 2.29 (m, 1H), 2.16 – 1.96 (m, 4H), 1.66 – 1.44 (m, 6H), 1.43 (s, 6H), 0.91 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.41 (d, *J* = 7.6 Hz, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0 (q, *J* = 5.0 Hz), 159.4, 144.7, 137.3, 128.7, 125.8, 123.4 (q, *J* = 268.7 Hz), 123.2, 88.5 (q, *J* = 37.1 Hz), 71.6, 50.6, 48.0, 44.7, 37.9, 35.9, 31.6, 29.3, 29.0, 26.3, 25.7, 21.7, 13.9. HRMS (EI): *m/z* calcd. for $C_{25}H_{28}F_3NO_2$ $[M]^+$ 431.2072, found: 431.2076. IR (KBr): 29791, 2933, 2866, 1741, 1661, 1259, 1191, 1113, 971, 673 cm^{-1}.



E-**3a-*d***. Colorless oil. 74% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.95 (m, 2H), 7.56 – 7.52 (m, 1H), 7.47 – 7.44 (m, 2H), 5.60 (q, *J* = 9.1 Hz, 0.08H), 1.60 (s, 6H). HRMS (EI): *m/z* calcd. for $C_{13}H_{11}DF_3NO$ $[M]^+$ 256.0934, found: 256.0930.



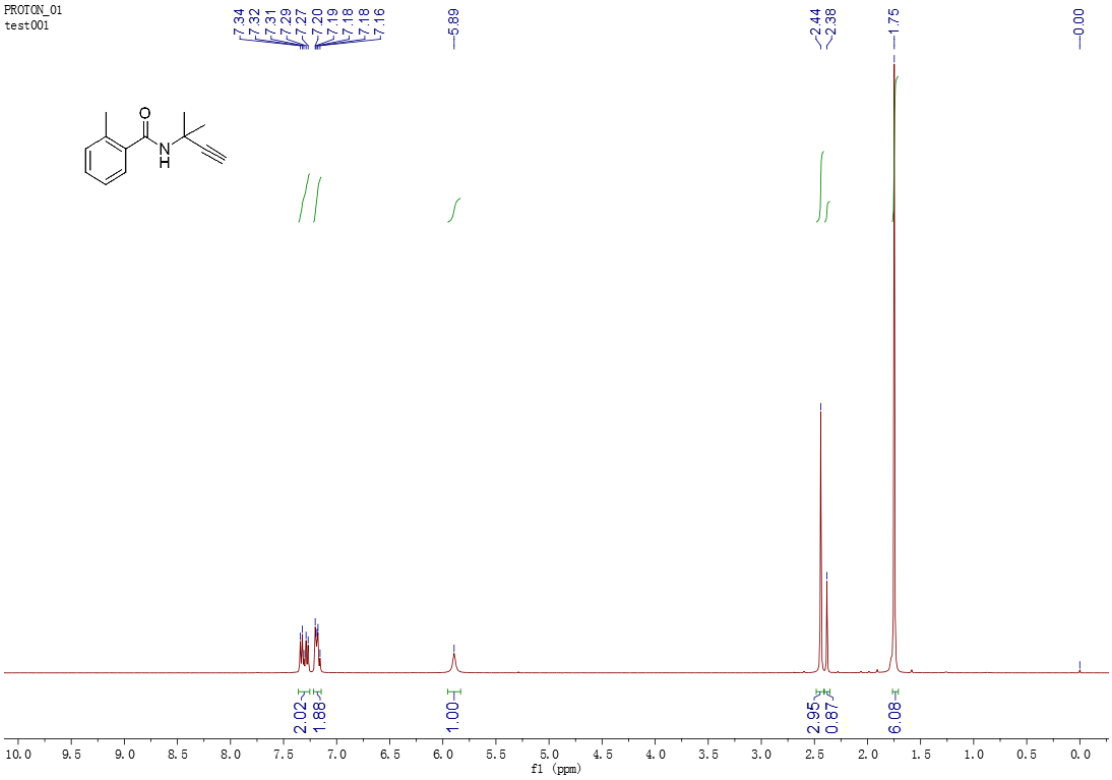
Z-**3a**:*Z*-**3a-*d*** = 1:1. *Z*-**3a-*d***. Colorless oil. 65% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 8.01 (m, 2H), 7.56 – 7.53 (m, 1H), 7.48 – 7.45 (m, 2H), 4.92 (q, *J* = 7.4 Hz, 0.5H), 1.49 (s, 6H). HRMS (EI): *m/z* calcd. for $C_{13}H_{11}DF_3NO$ $[M]^+$ 256.0934, found: 256.0936.

[a] X.-J. Meng, S. Kim, *Org. Biomol. Chem.* **2011**, *9*, 4429.

[b] S. Yasuhara, M. Sasa, T. Kusakabe, H. Takayama, M. Kimura, T. Mochida, K. Kato, *Angew.*

Chem. Int. Ed. **2011**, *50*, 3912; *Angew. Chem.* **2011**, *17*, 3998.

[c] A. Alhalib, W. J. Moran, *Org. Biomol. Chem.* **2014**, *12*, 795.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7.32
7.31
7.29
7.27
7.20
7.19
7.18
7.18
7.16
5.89
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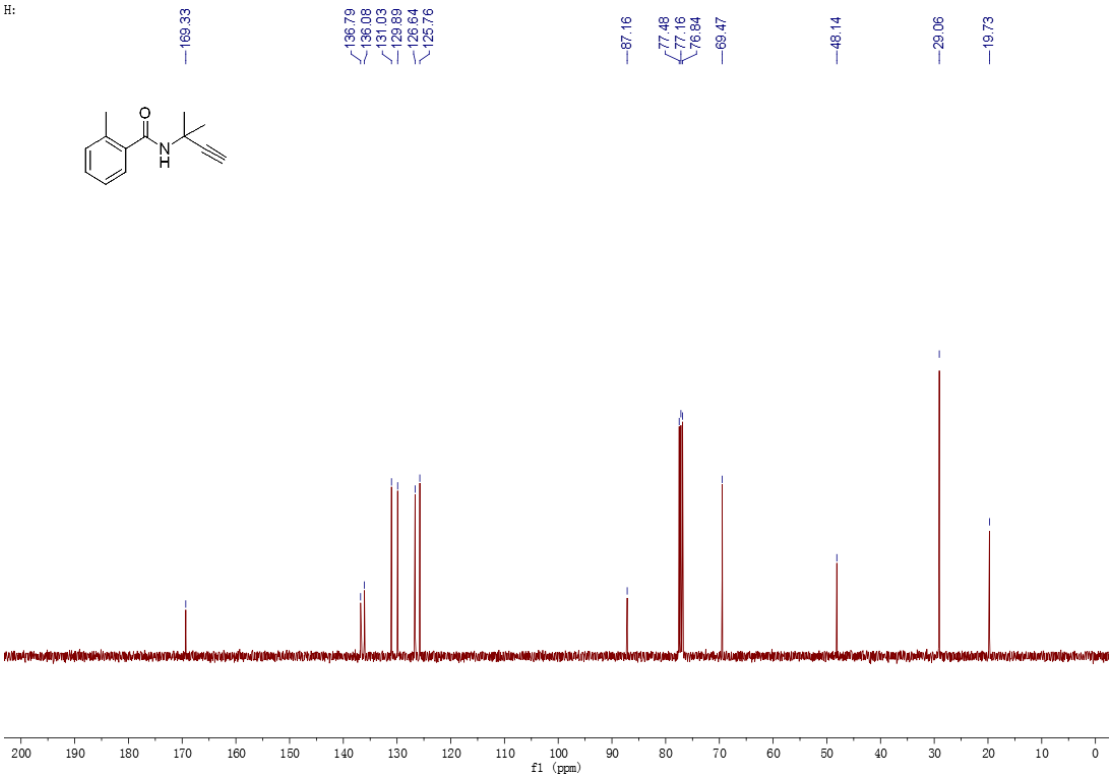
2.38
1.75
0.00
2.02
1.88
1.00
2.95
0.87
6.08
f1 (ppm)


H:
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136.79
136.08
131.03
129.89
126.64
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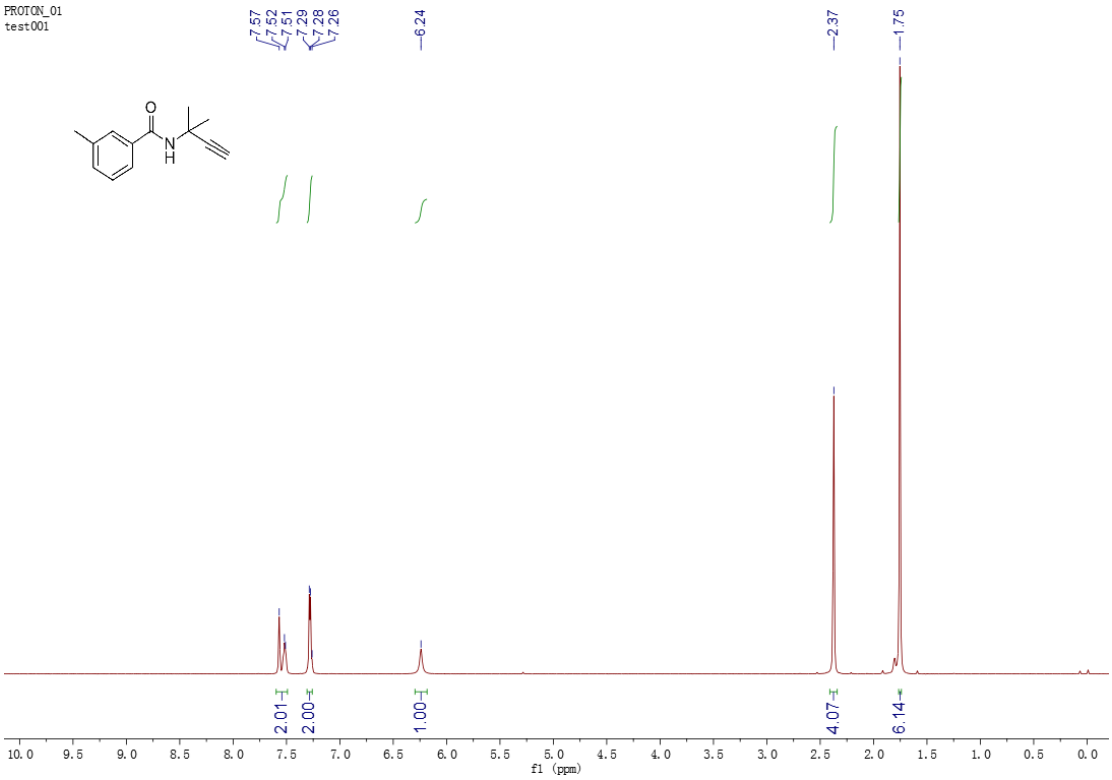
87.16
77.48
77.16
76.84
69.47
48.14
29.06
19.73
f1 (ppm)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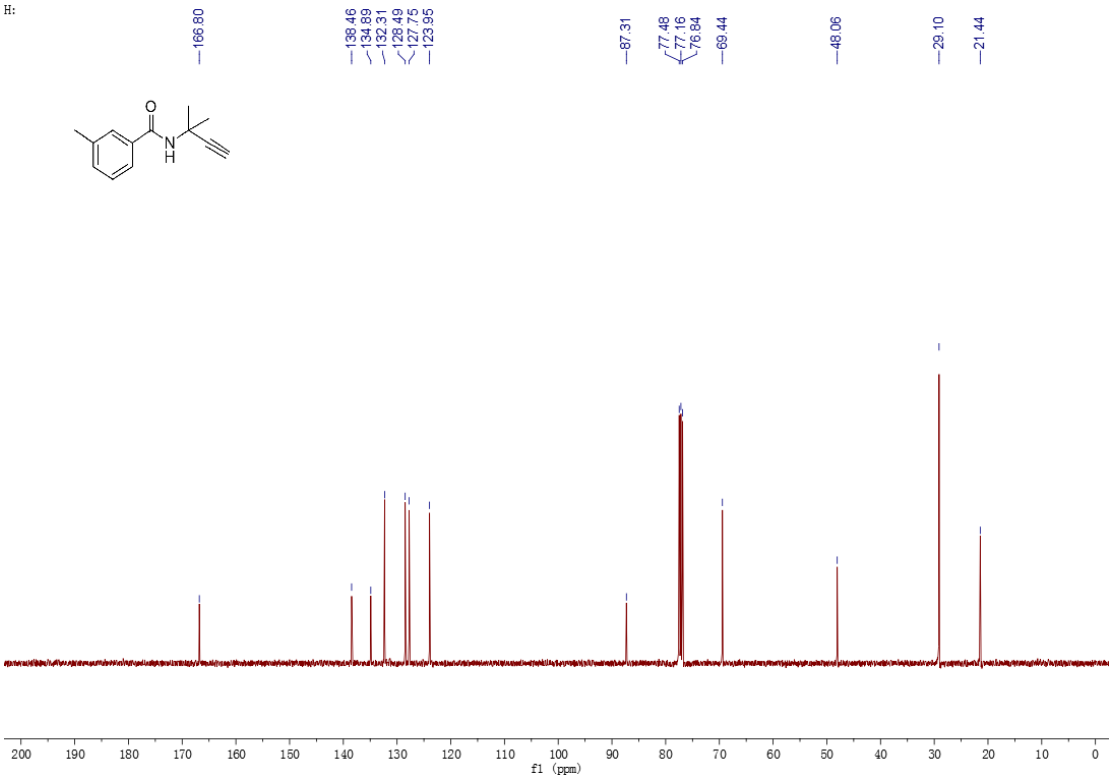
1.00
4.07
6.14
f1 (ppm)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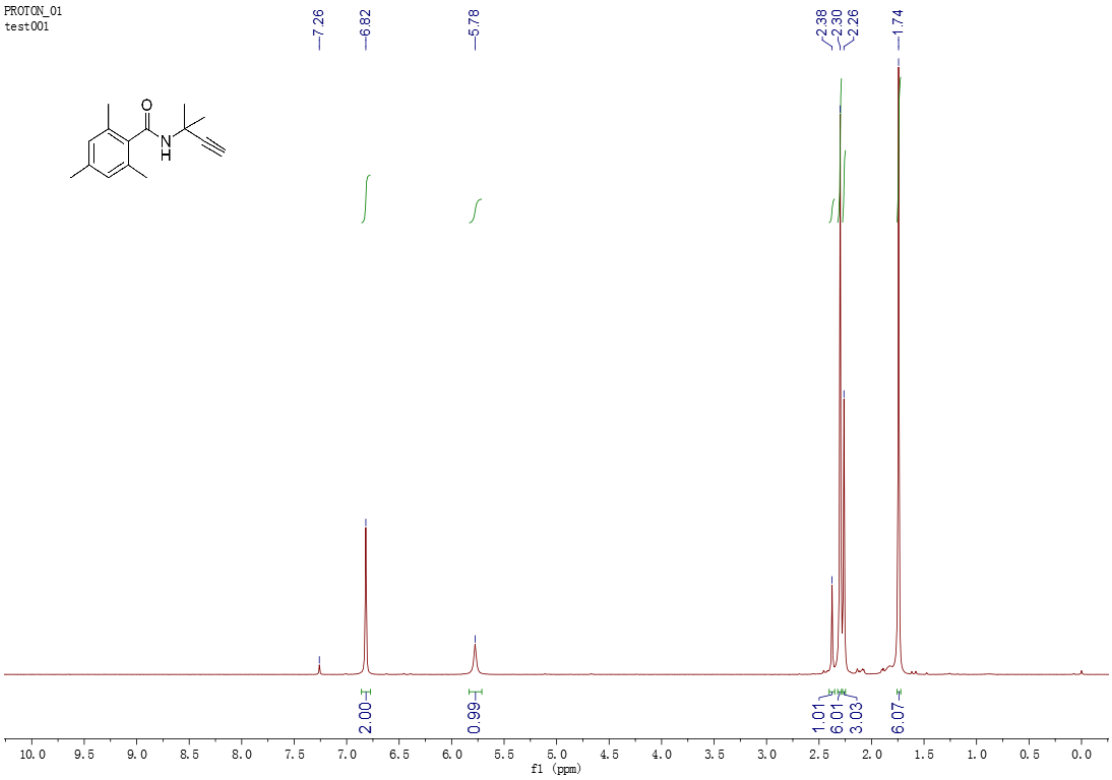
21.44
f1 (ppm)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2.00
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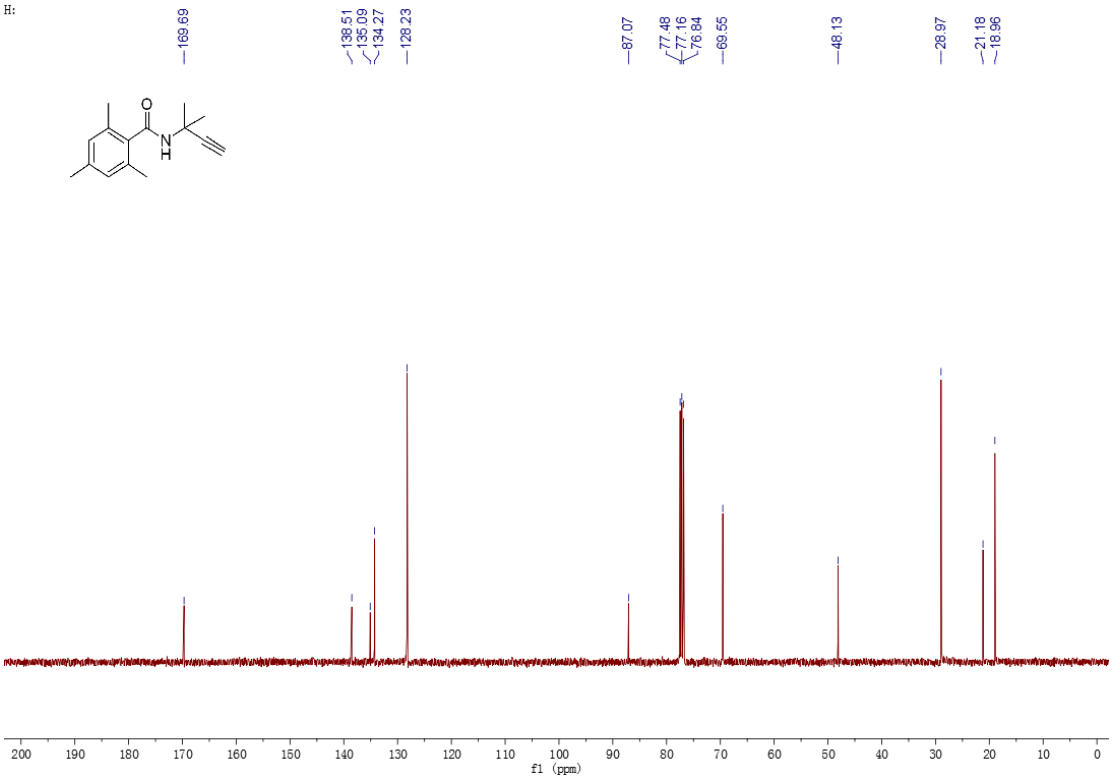
1.01
6.01
3.03
6.07
f1 (ppm)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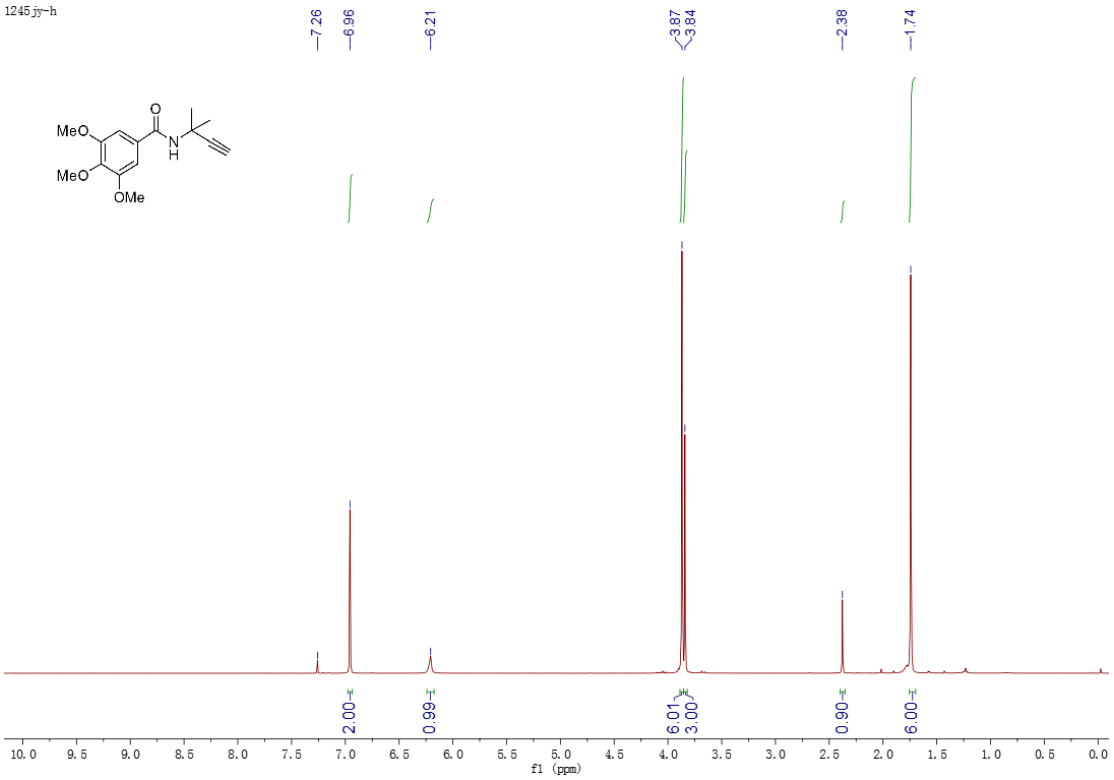
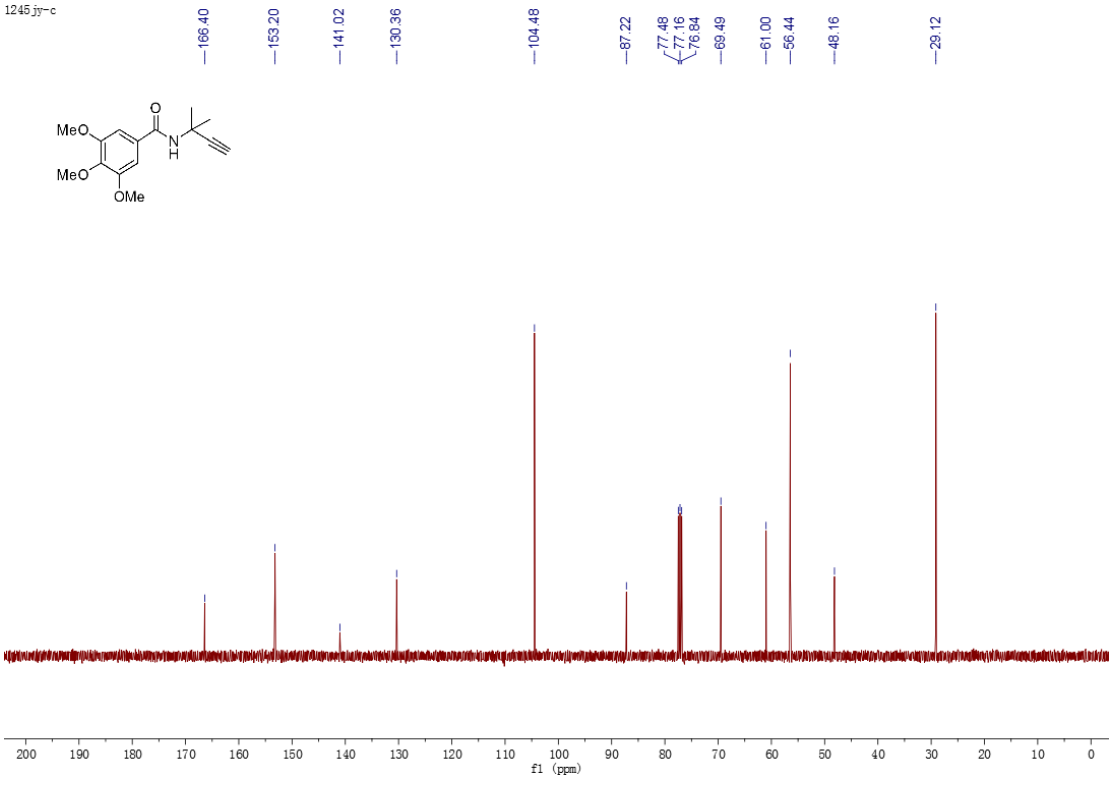
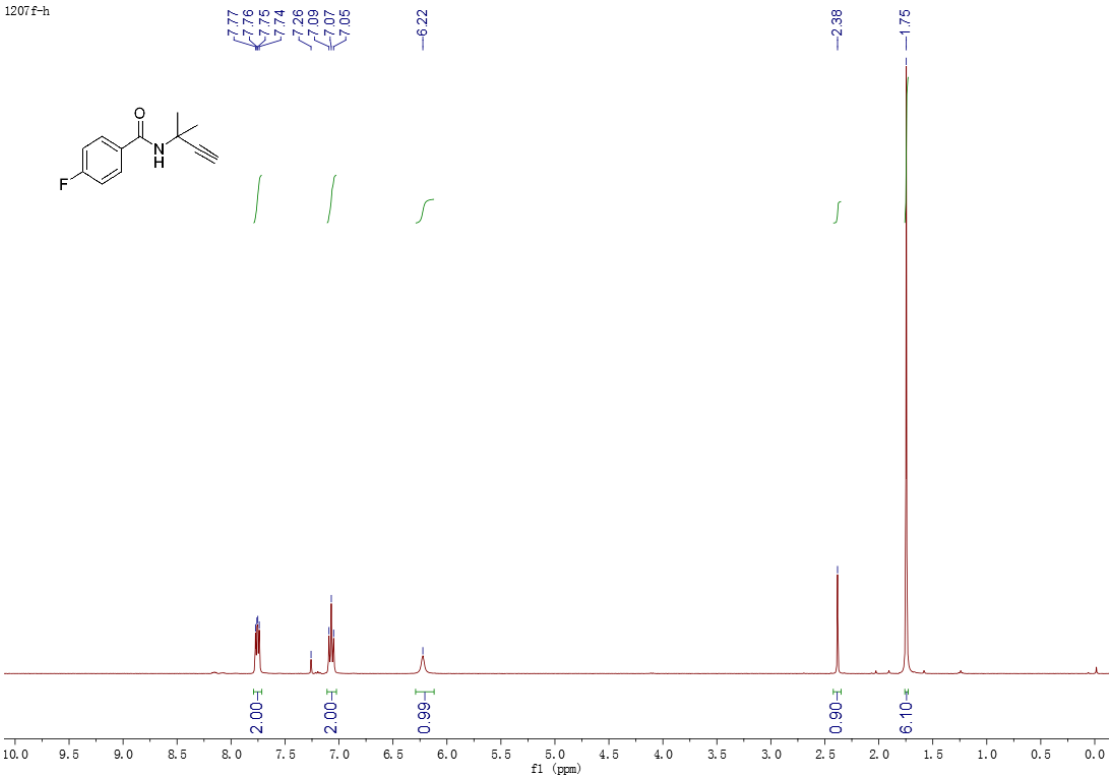
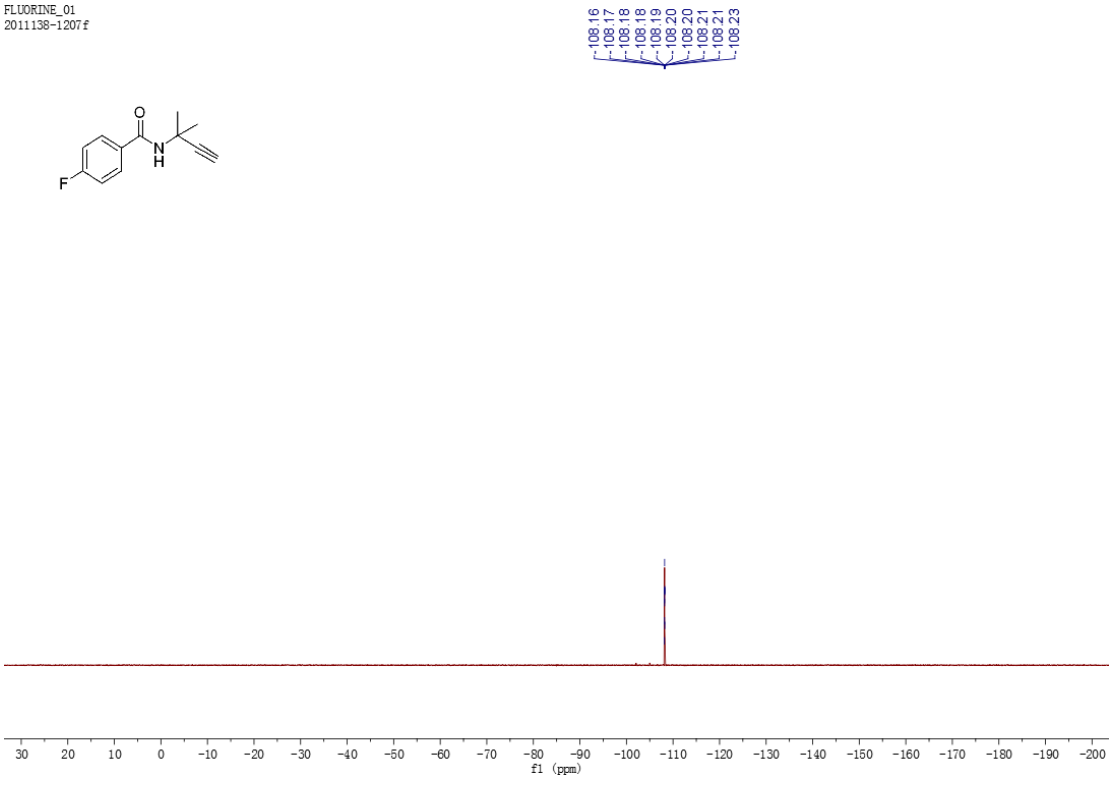
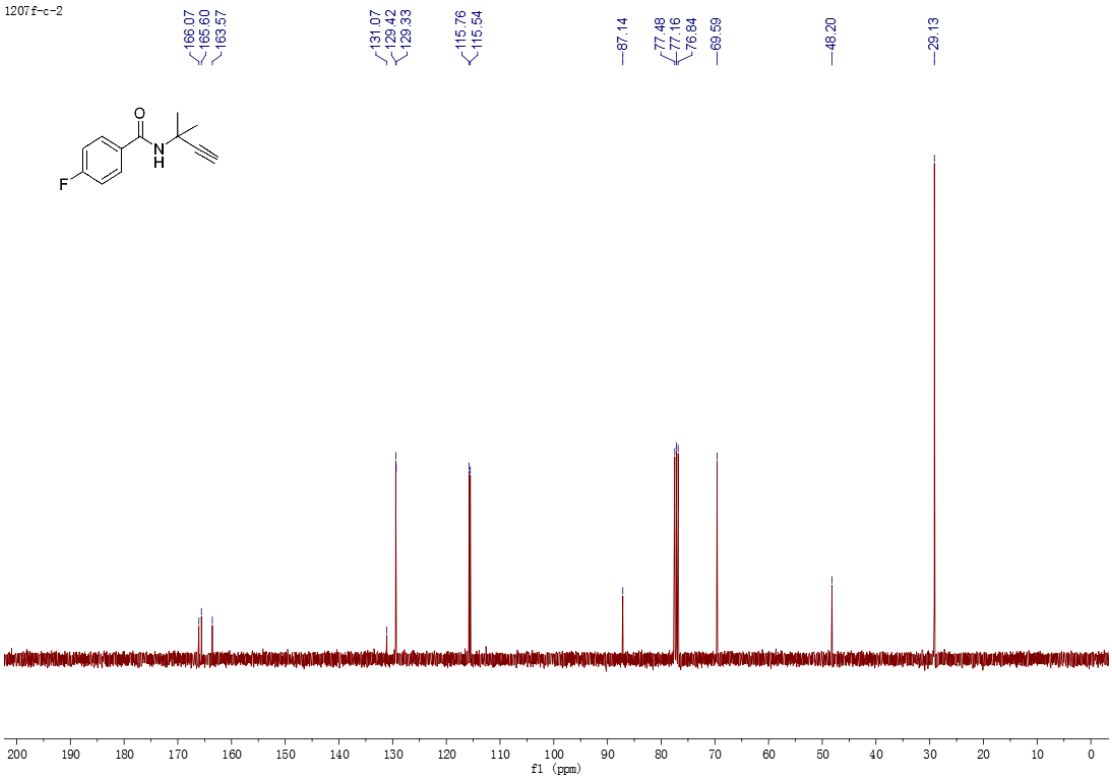
76.84
69.55
48.13
28.97
21.18
18.96
f1 (ppm)

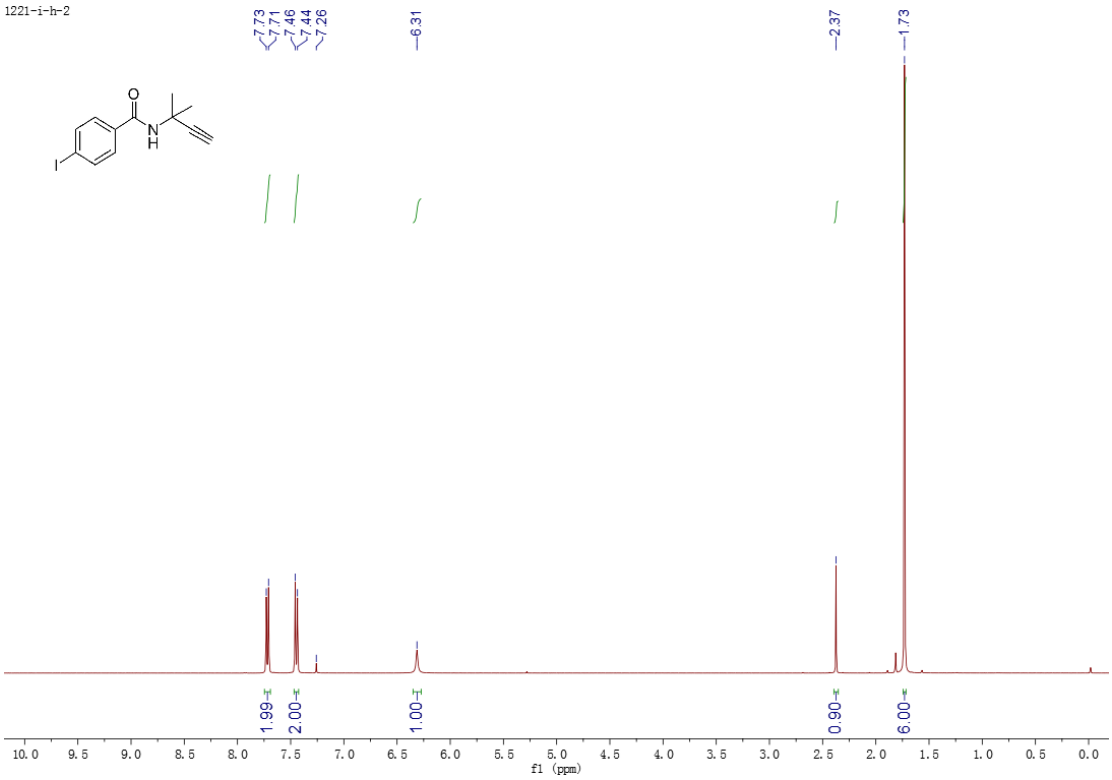

1245.jy-h
7.26
6.96
6.21
3.87
3.84
2.38
1.74
MeO
MeO
OMe
O
N
H
2.00
0.99
6.01
3.00
0.90
6.00
f1 (ppm)

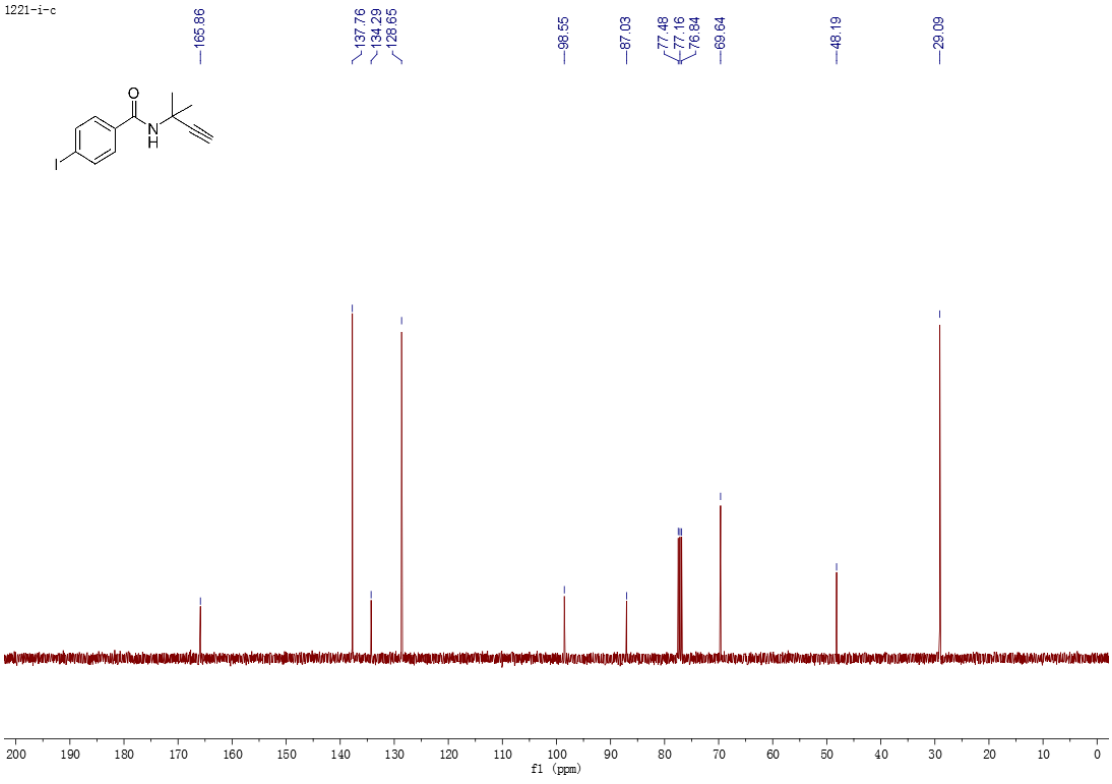

1245.jy-c
166.40
153.20
141.02
130.36
104.48
87.22
77.48
77.16
76.84
69.49
61.00
56.44
48.16
29.12
MeO
MeO
OMe
O
N
H
f1 (ppm)

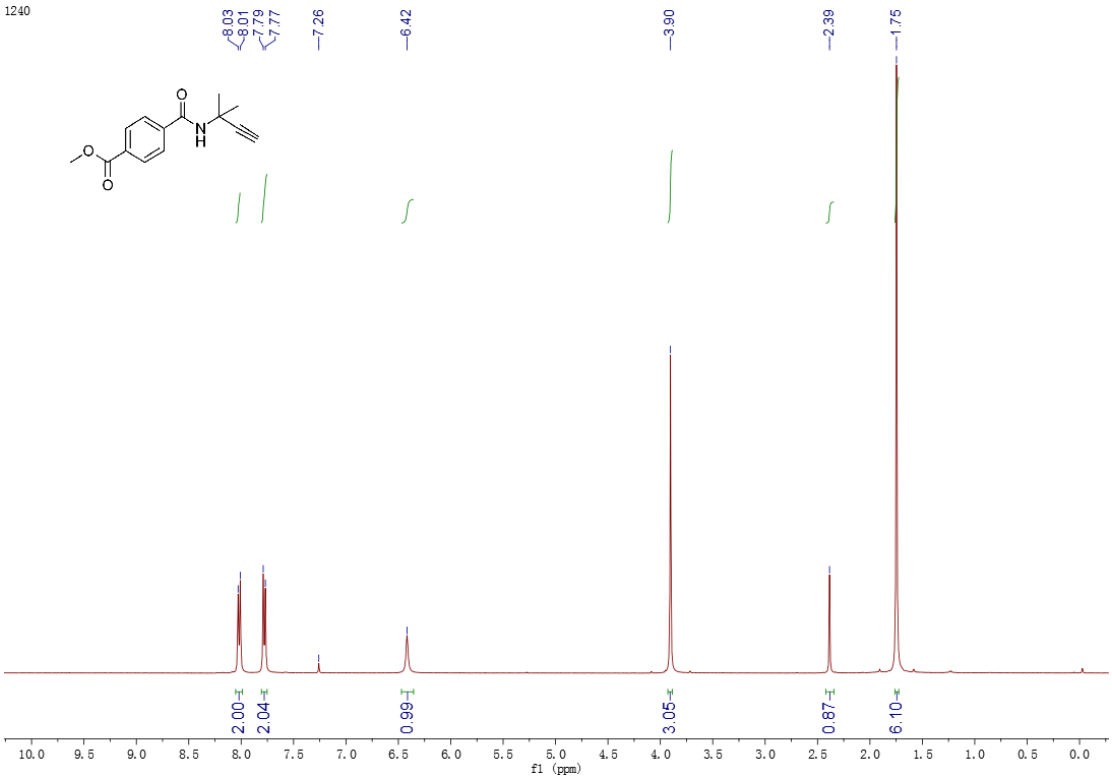

1207f-h
7.77
7.76
7.75
7.74
7.26
7.09
7.07
7.05
6.22
2.38
1.75
2.00
2.00
0.99
0.90
6.10
f1 (ppm)

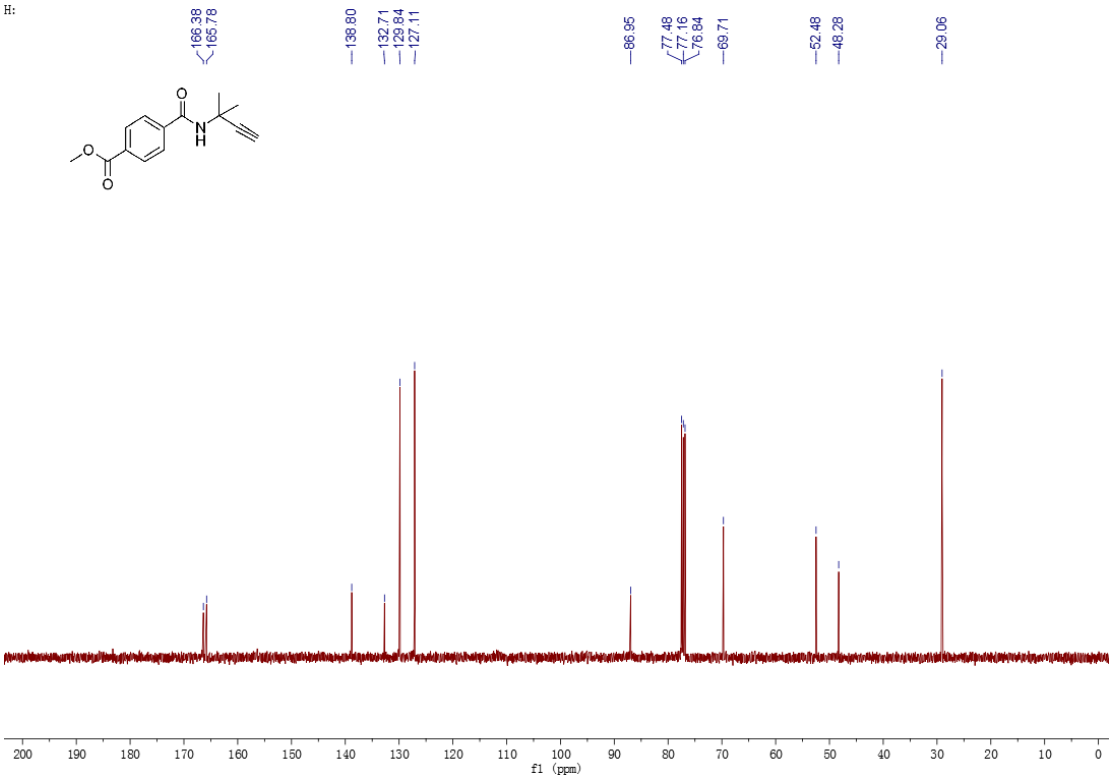

FLUORINE_01
2011138-1207f
-108.16
-108.17
-108.18
-108.18
-108.19
-108.20
-108.20
-108.21
-108.21
-108.23
f1 (ppm)

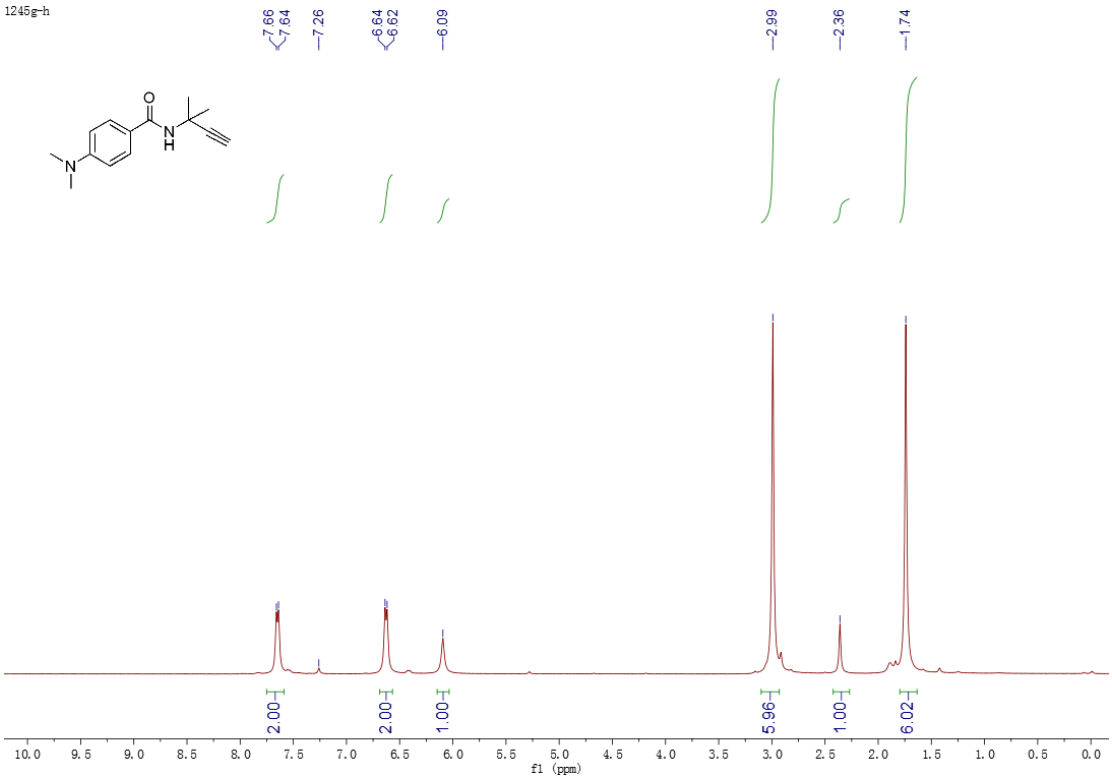

1207f-c-2
166.07
165.60
163.57
131.07
129.42
129.33
115.76
115.54
87.14
77.48
77.16
76.84
69.59
48.20
29.13
O
N
H
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

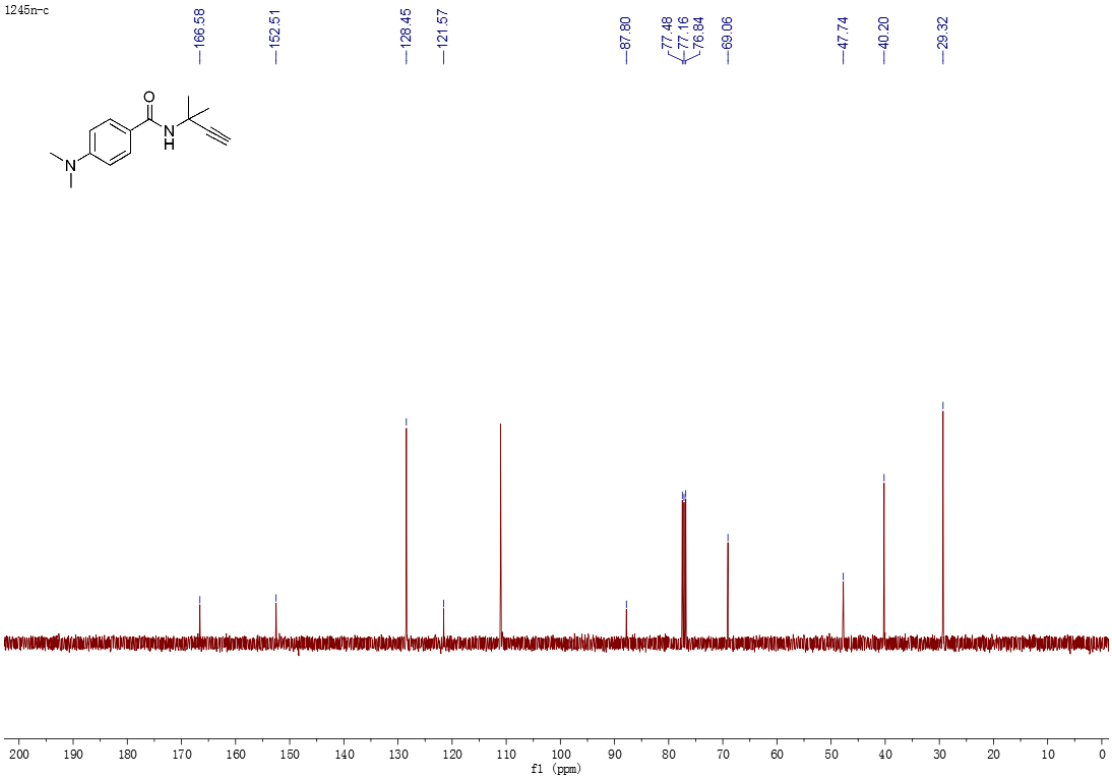

1221-i-h-2
7.73
7.71
7.46
7.44
7.26
6.31
2.37
1.73
1.99
2.00
1.00
0.90
6.00
f1 (ppm)

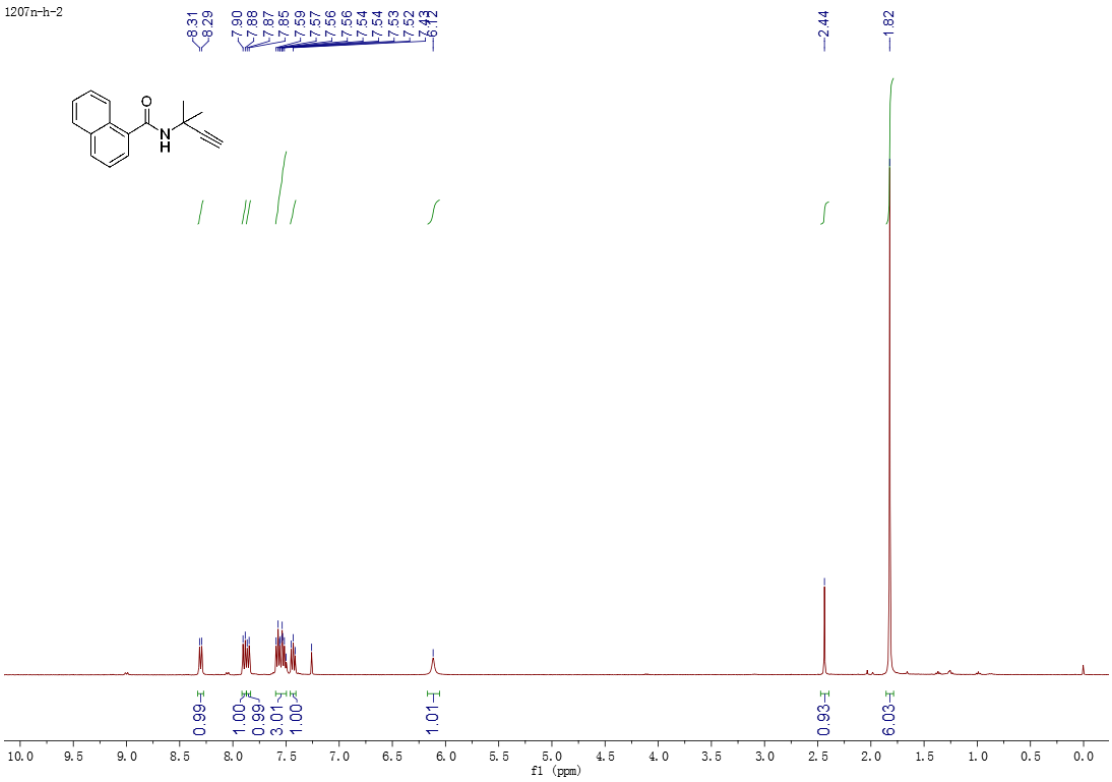

1221-i-c
165.86
137.76
134.29
128.65
98.55
87.03
77.48
77.16
76.84
69.64
48.19
29.09
f1 (ppm)

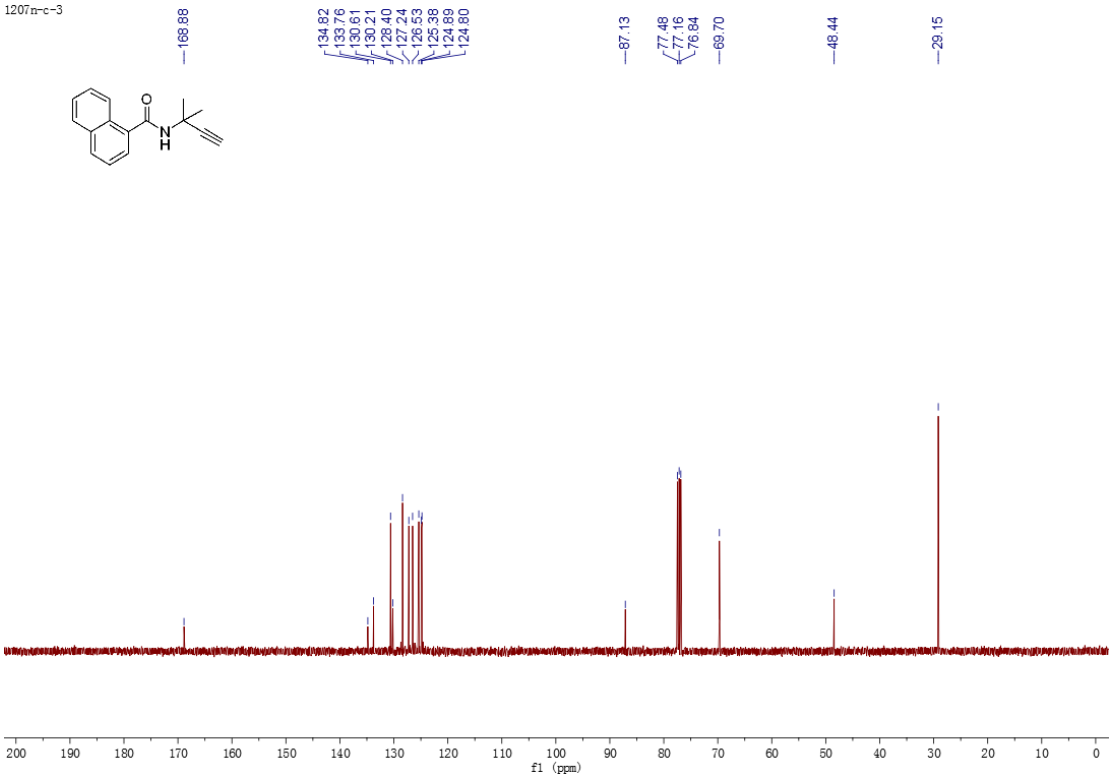

1240
8.03
8.01
7.79
7.77
7.26
6.42
3.90
2.39
1.75
2.00
2.04
0.99
3.05
0.87
6.10
f1 (ppm)

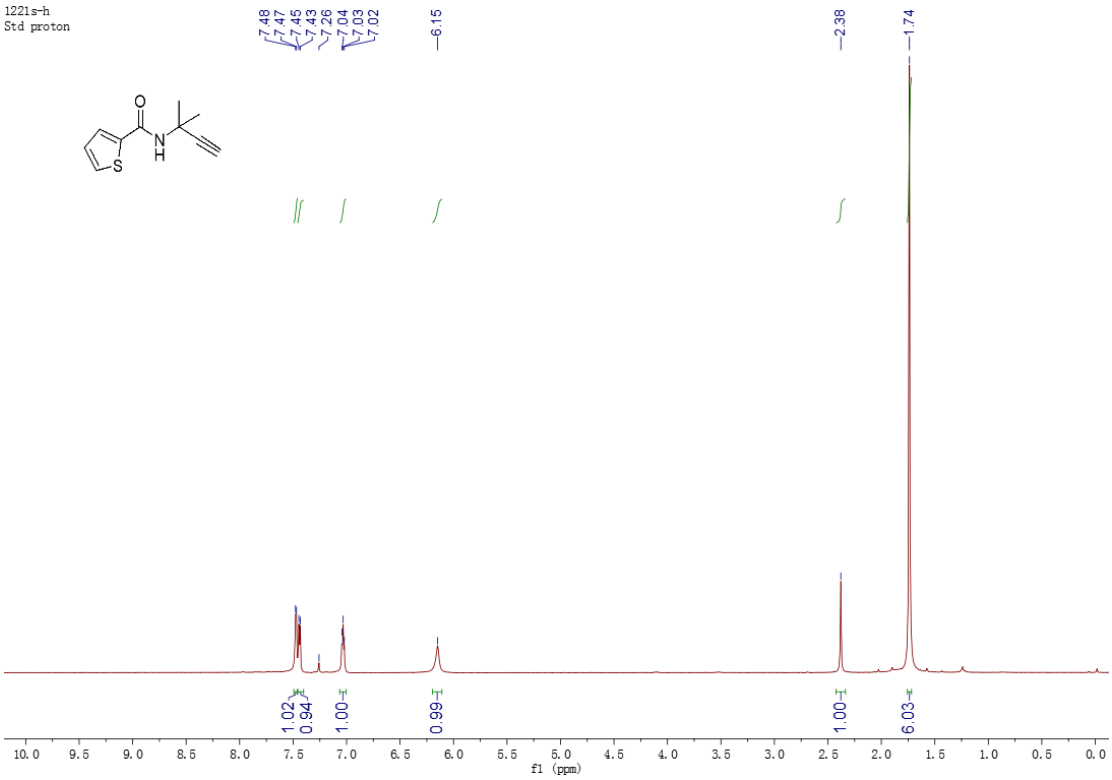

H:
166.38
165.78
138.80
132.71
129.84
127.11
86.95
77.48
77.16
76.84
69.71
52.48
48.28
29.06
f1 (ppm)

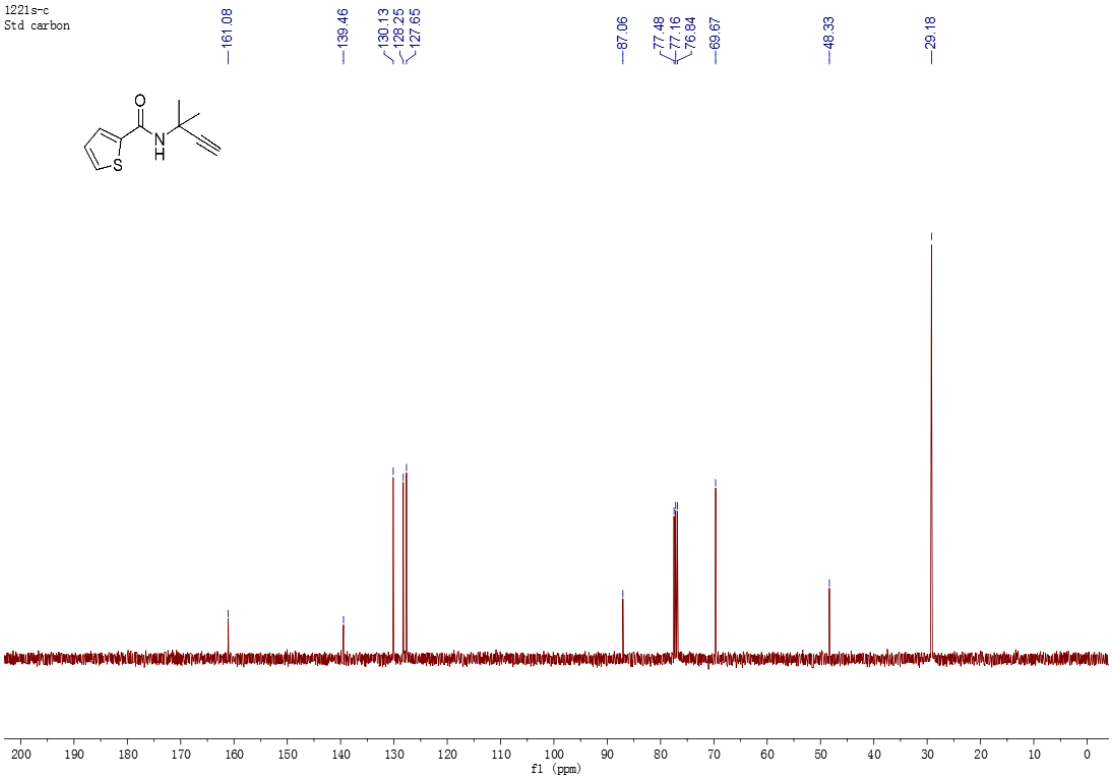

1245g-h
7.66
7.64
7.26
6.64
6.62
6.09
2.99
2.36
1.74
2.00
2.00
1.00
5.96
1.00
6.02
f1 (ppm)

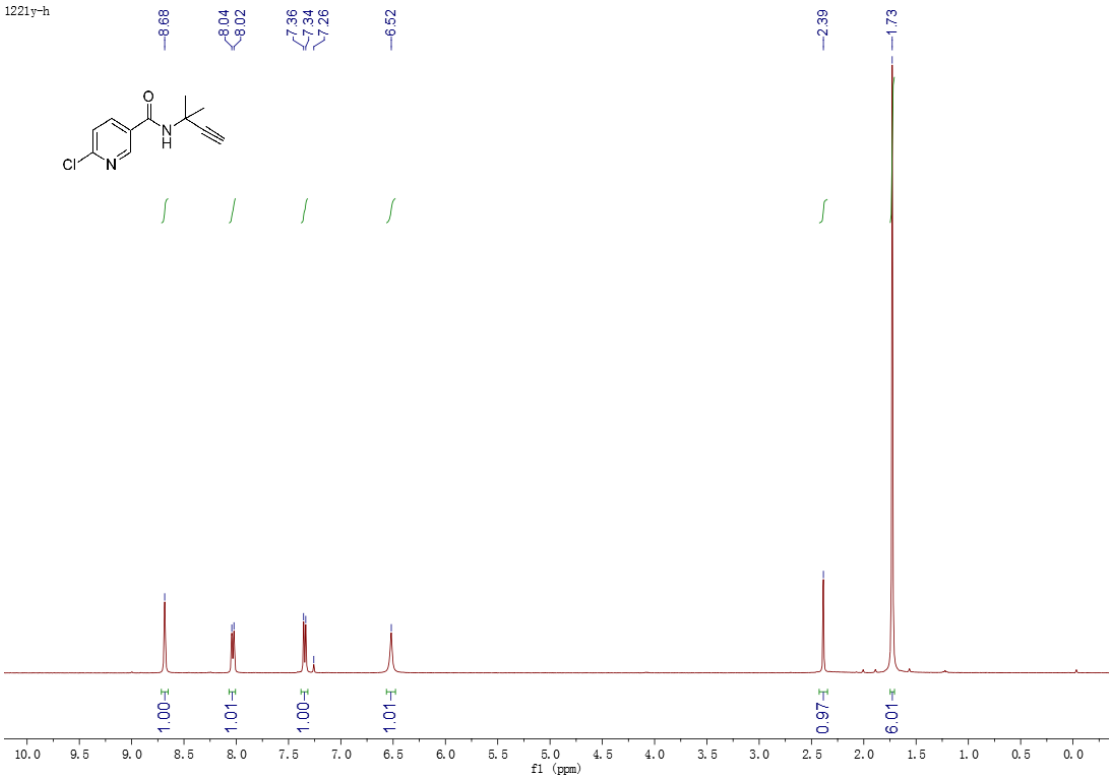

1245n-c
166.58
152.51
128.45
121.57
87.80
77.48
77.16
76.84
69.06
47.74
40.20
29.32
f1 (ppm)

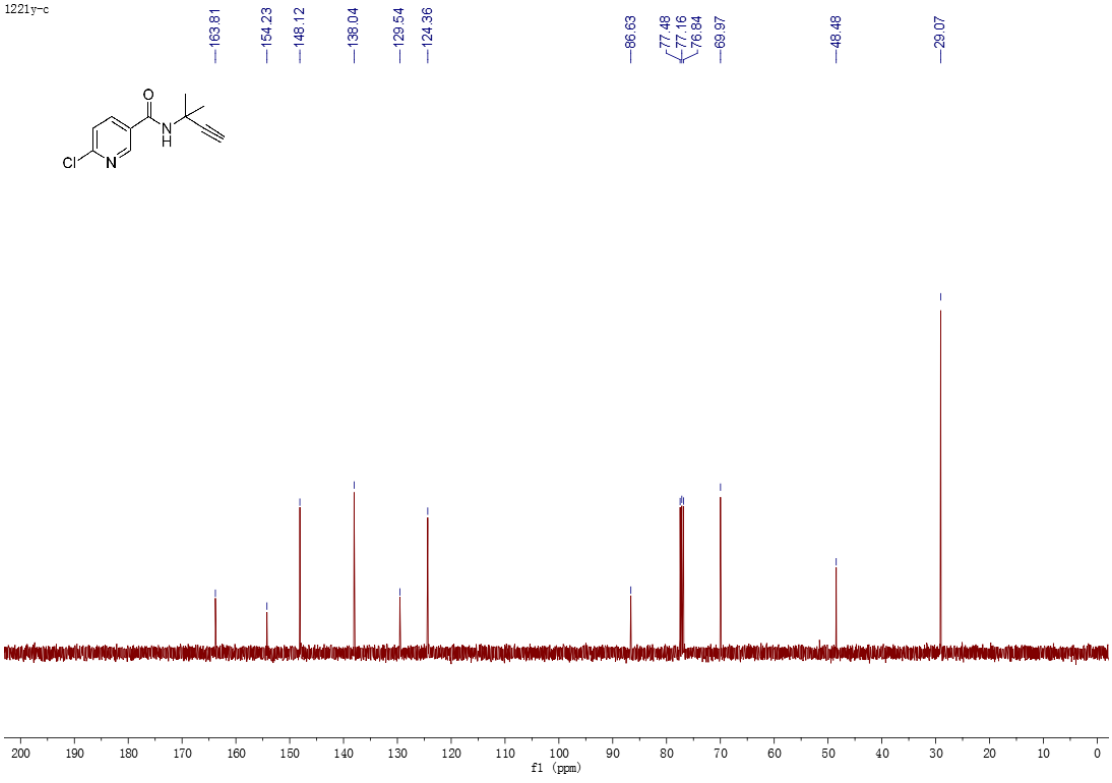

1207n-h-2
8.31
8.29
7.90
7.88
7.87
7.85
7.59
7.57
7.56
7.56
7.54
7.54
7.53
7.52
6.12
2.44
1.82
0.99
1.00
0.99
3.01
1.00
1.01
0.93
6.03
f1 (ppm)

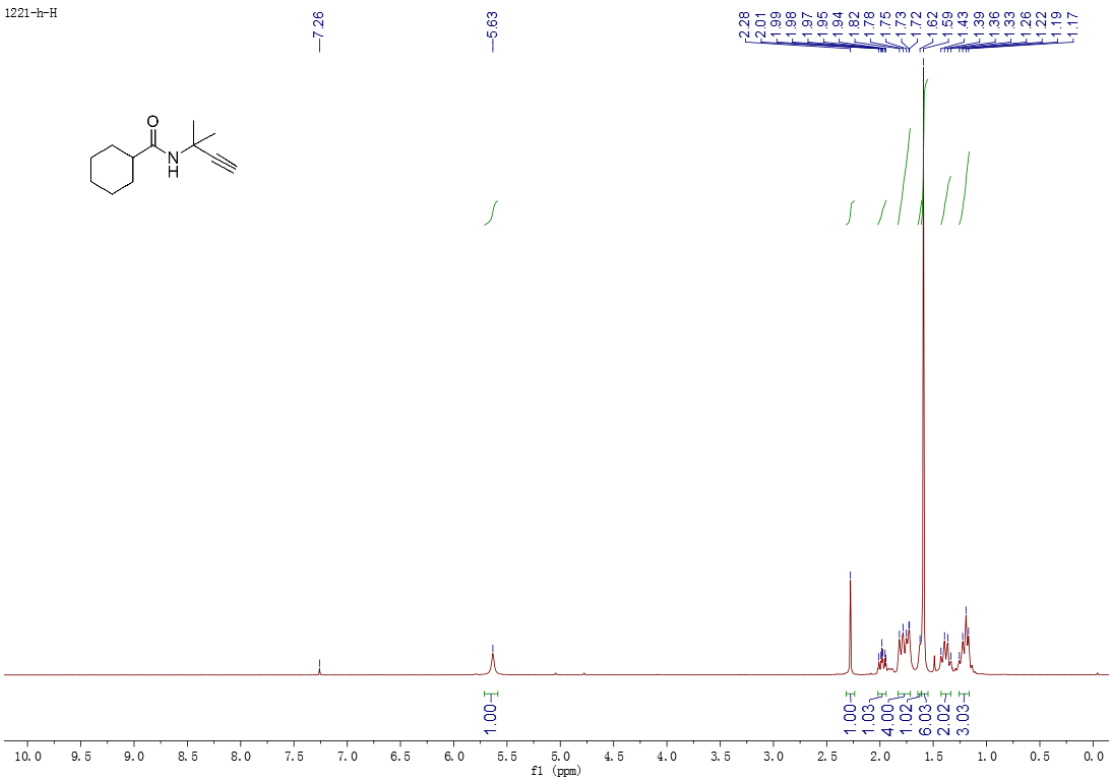

1207n-c-3
168.88
134.82
133.76
130.61
130.21
128.40
127.24
126.53
125.38
124.89
124.80
87.13
77.48
77.16
76.84
69.70
48.44
29.15
f1 (ppm)

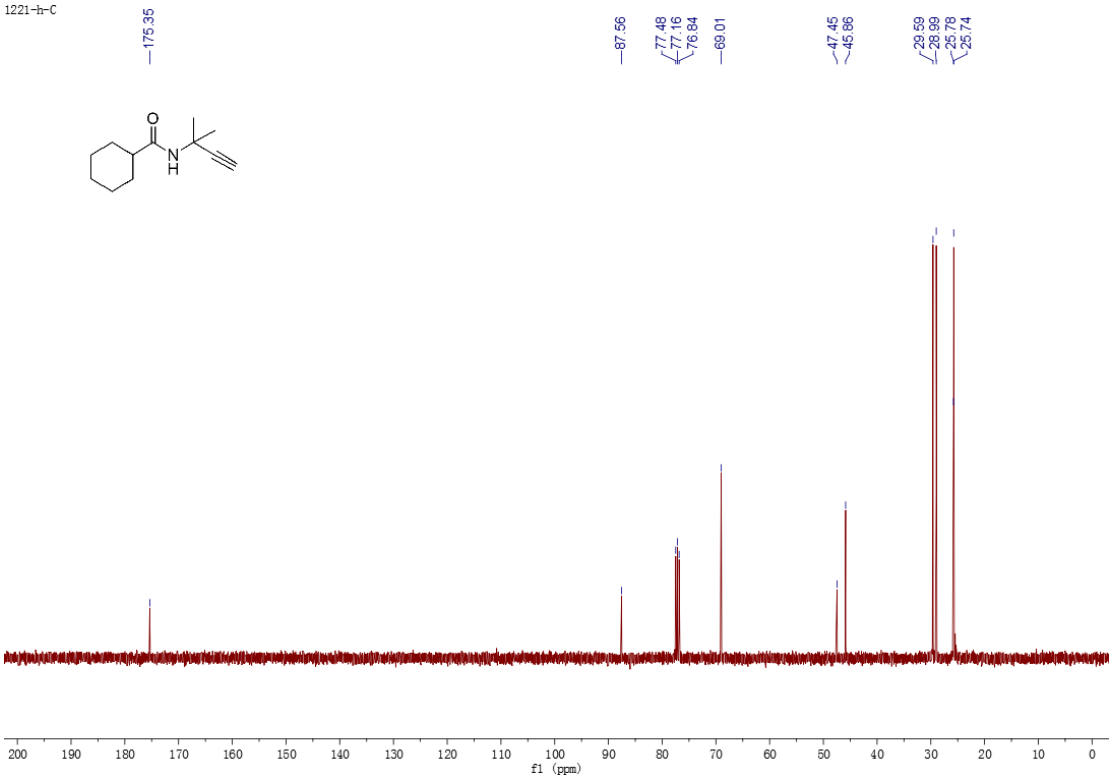

1221s-h
Std proton
7.48
7.47
7.45
7.43
7.26
7.04
7.03
7.02
6.15
2.38
1.74
1.02
0.94
1.00
0.99
1.00
6.03
f1 (ppm)


1221s-c
Std carbon
161.08
139.46
130.13
128.25
127.65
87.06
77.48
77.16
76.84
69.67
48.33
29.18
f1 (ppm)

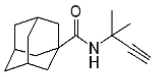

1221y-h
8.68
8.04
8.02
7.36
7.34
7.26
6.52
2.39
1.73
1.00
1.01
1.00
1.01
0.97
6.01
f1 (ppm)


1221y-c
163.81
154.23
148.12
138.04
129.54
124.36
86.63
77.48
77.16
76.84
69.97
48.48
29.07
f1 (ppm)

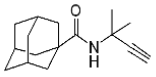

1221-h-H
7.26
5.63
2.28
2.01
1.99
1.98
1.97
1.95
1.94
1.82
1.78
1.75
1.73
1.72
1.62
1.59
1.43
1.39
1.36
1.33
1.26
1.22
1.19
1.17
1.00
1.00
1.03
4.00
1.02
6.03
2.02
3.03
f1 (ppm)

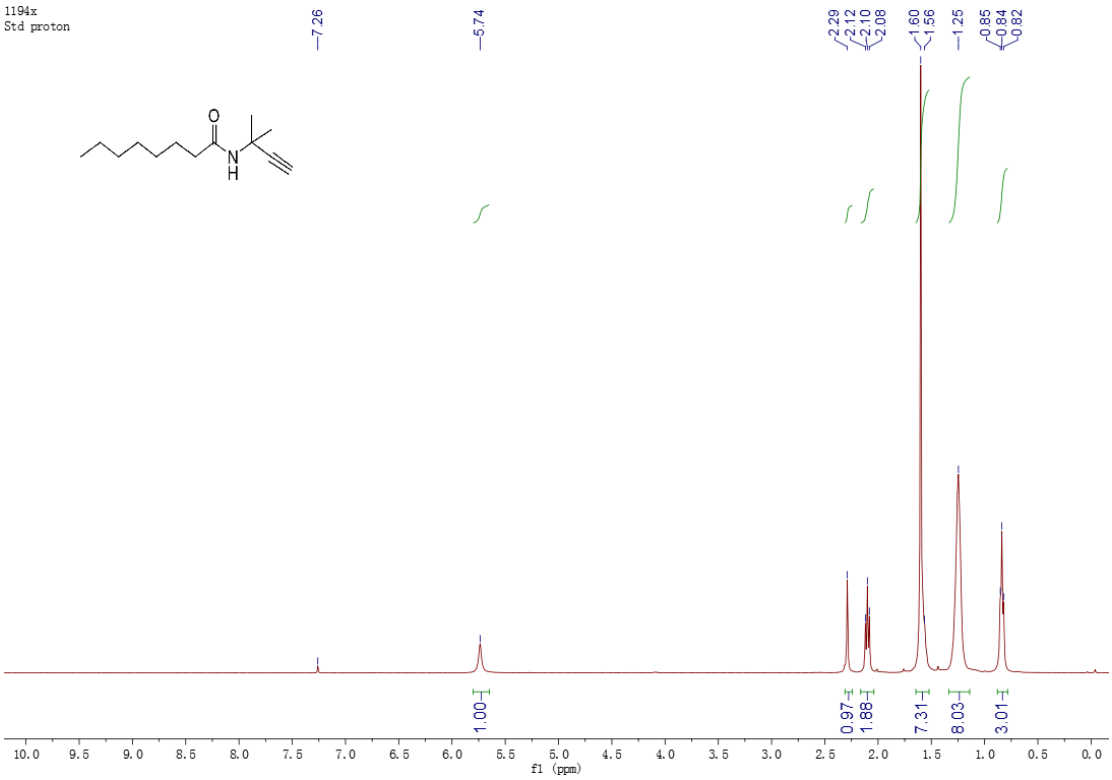

1221-h-C
175.35
87.56
77.48
77.16
76.84
69.01
47.45
45.86
29.59
28.99
25.78
25.74
f1 (ppm)

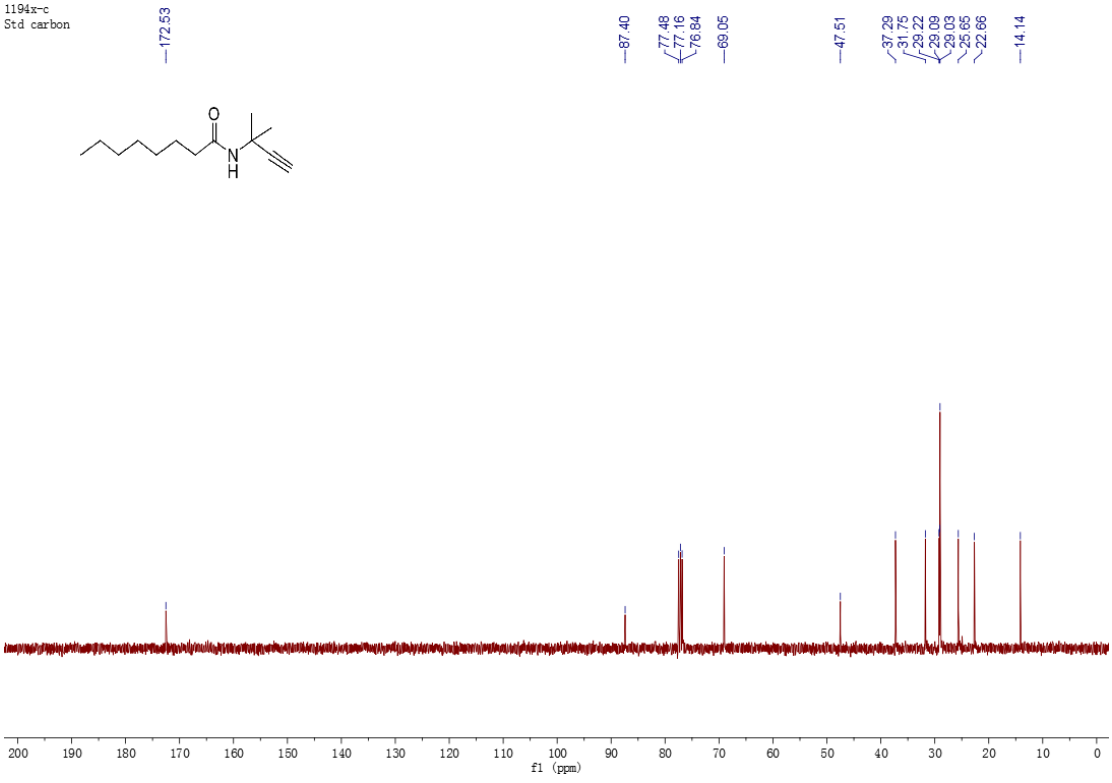
1195j-h

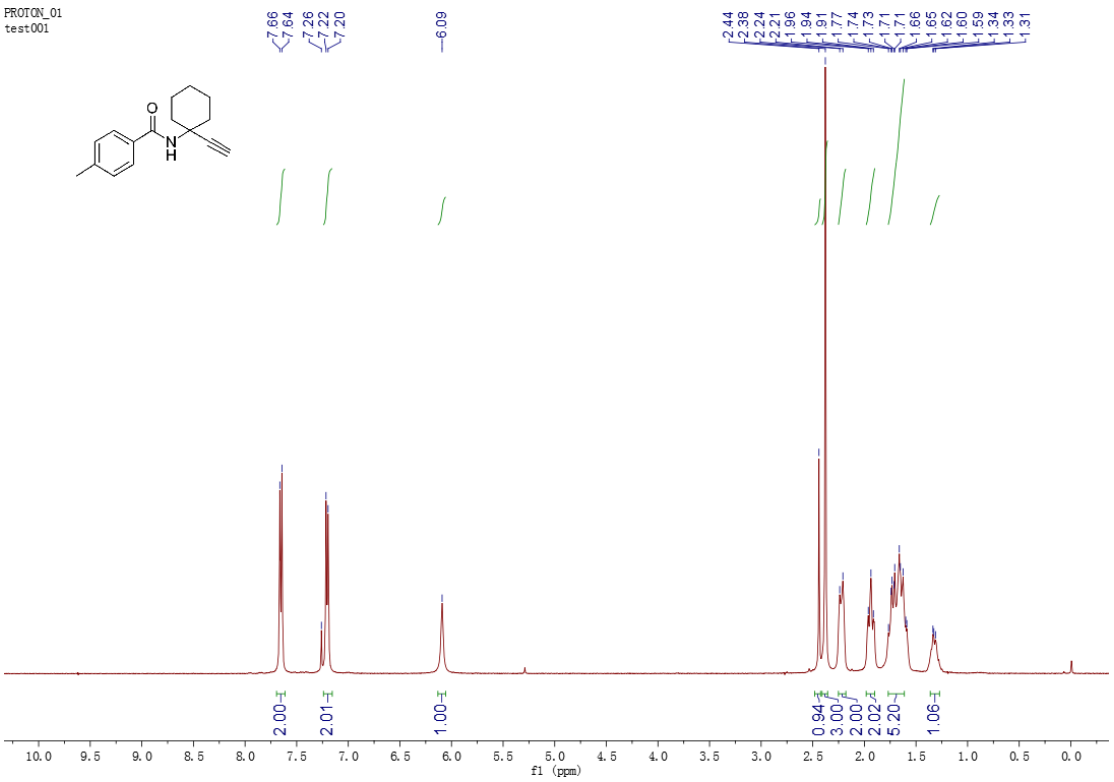


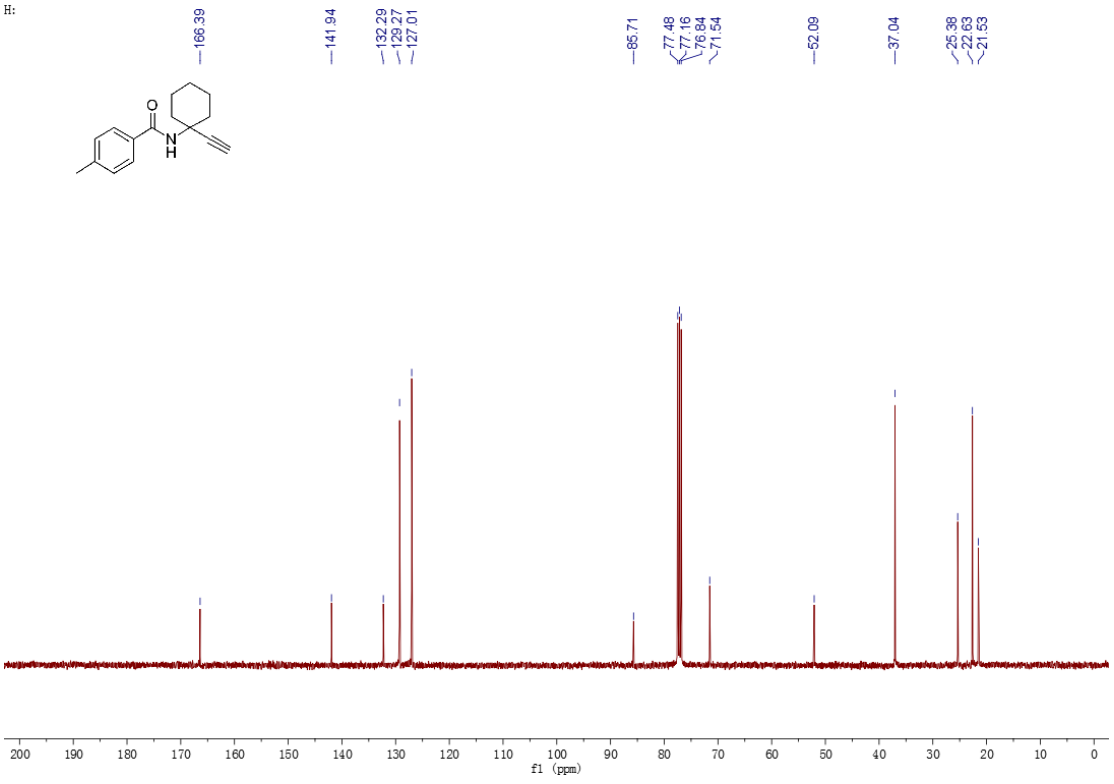
1195j-c-2

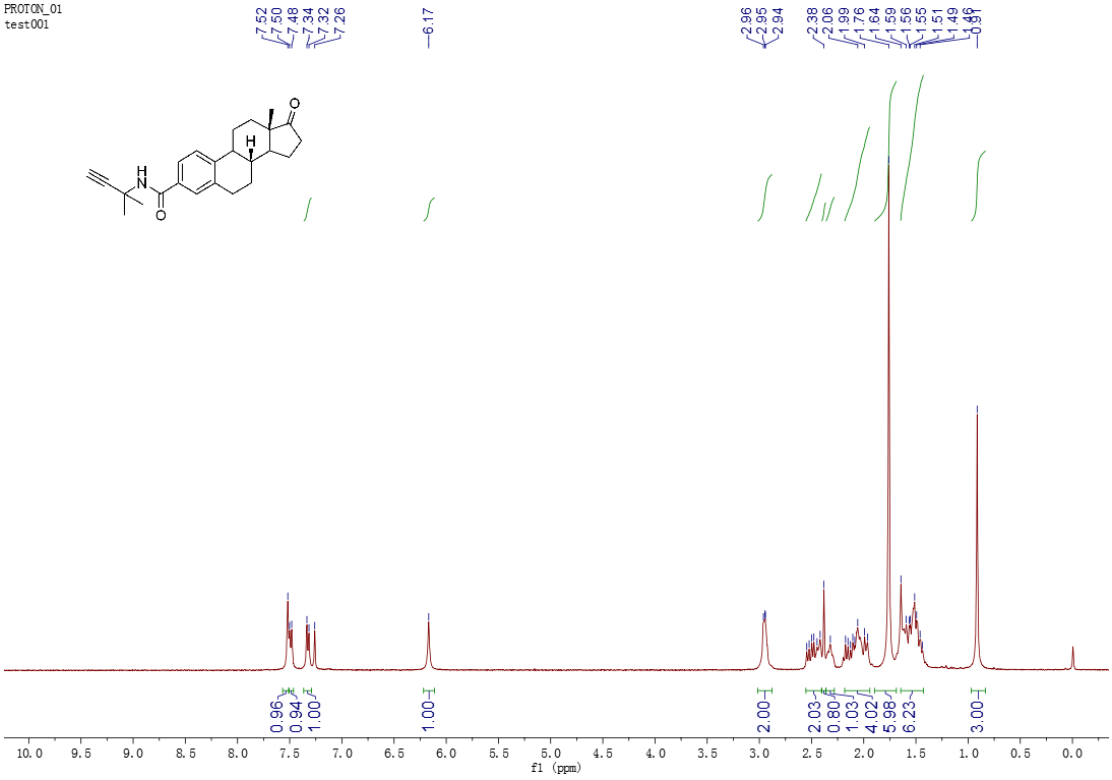


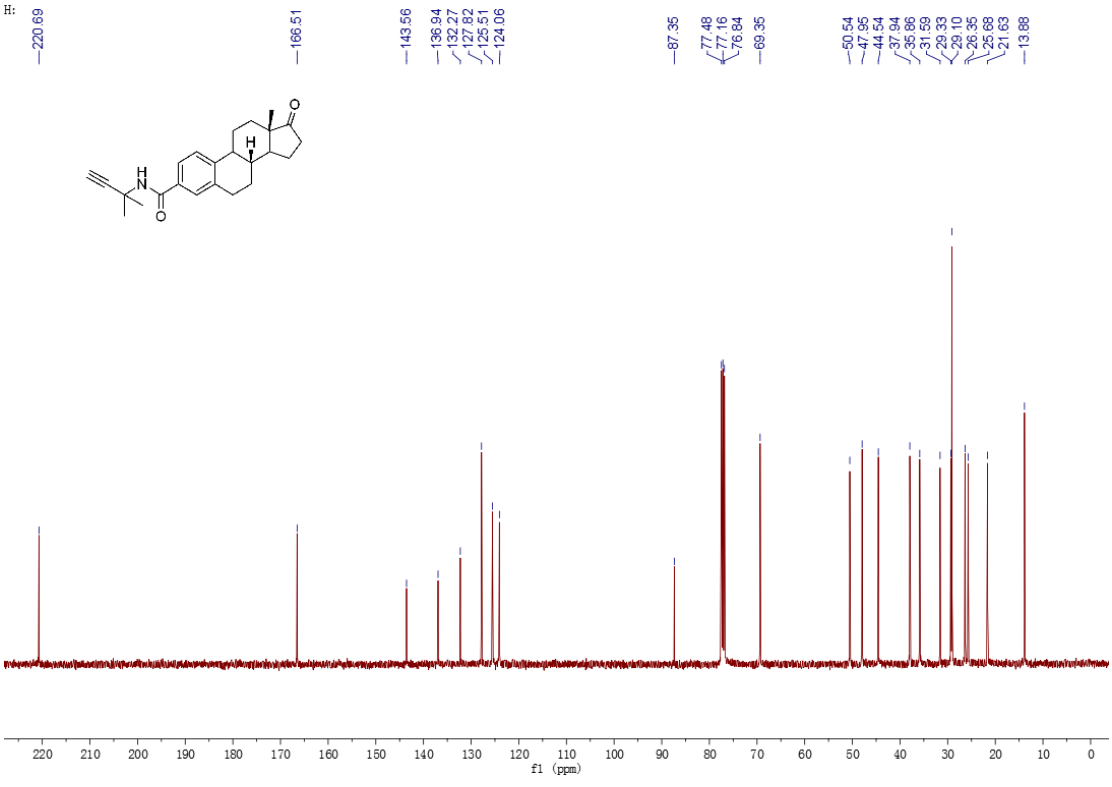

1194x
Std proton
7.26
5.74
2.29
2.12
2.10
2.08
1.60
1.56
1.25
0.85
0.84
0.82
1.00
0.97
1.88
7.31
8.03
3.01
f1 (ppm)

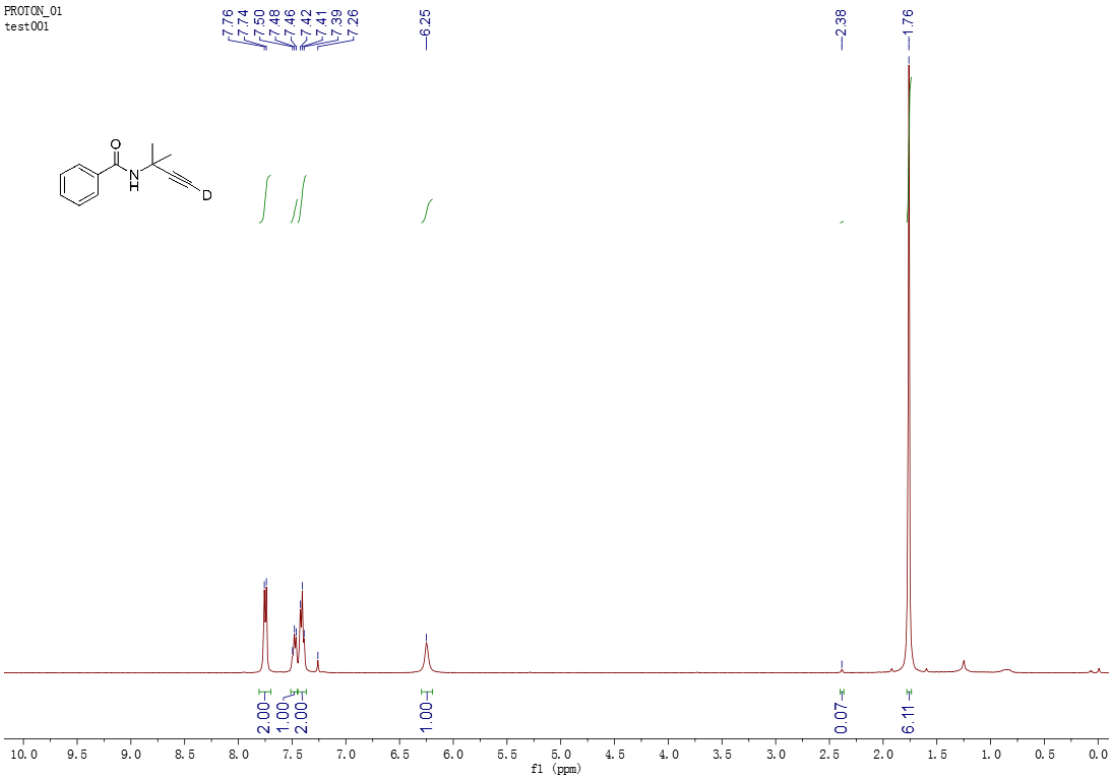

1194x-c
Std carbon
172.53
87.40
77.48
77.16
76.84
69.05
47.51
37.29
31.75
29.22
29.09
29.03
25.65
22.66
14.14
f1 (ppm)

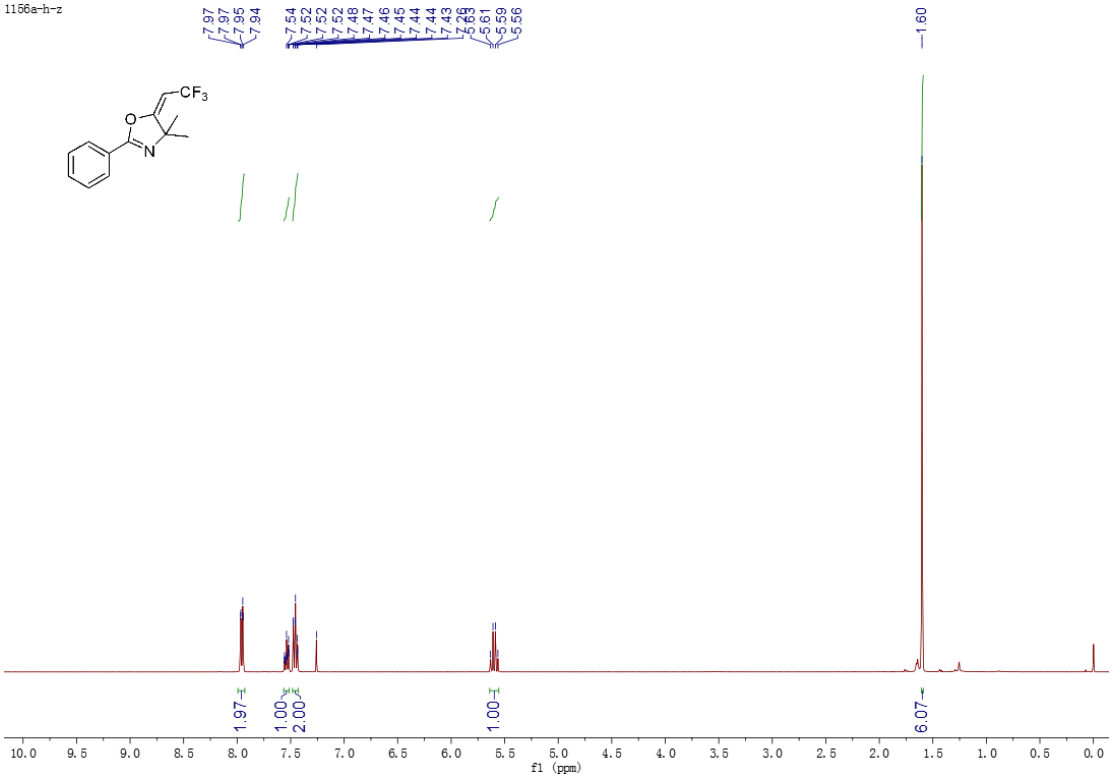

PROTON_01
test001
7.66
7.64
7.26
7.22
7.20
6.09
2.44
2.38
2.24
2.21
1.96
1.94
1.91
1.77
1.74
1.73
1.71
1.71
1.66
1.65
1.62
1.60
1.59
1.34
1.33
1.31
2.00
2.01
1.00
0.94
3.00
2.00
2.02
5.20
1.06
f1 (ppm)

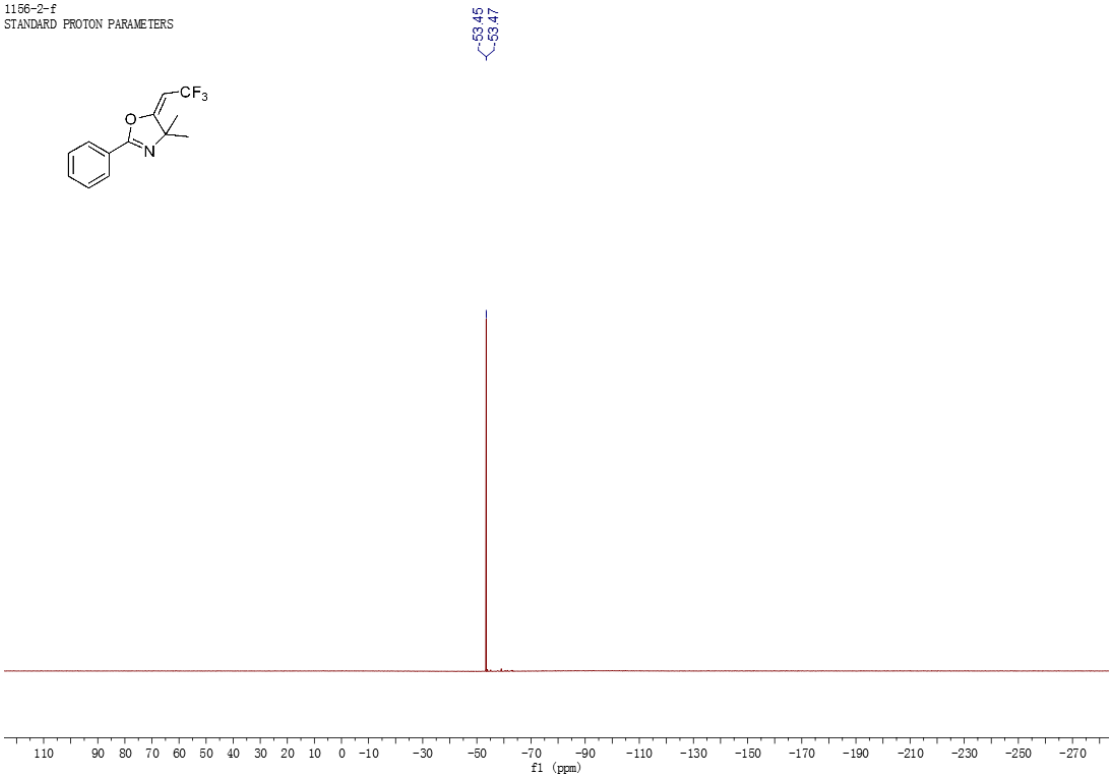

H:
166.39
141.94
132.29
129.27
127.01
85.71
77.48
77.16
76.84
71.54
52.09
37.04
25.38
22.63
21.53
f1 (ppm)

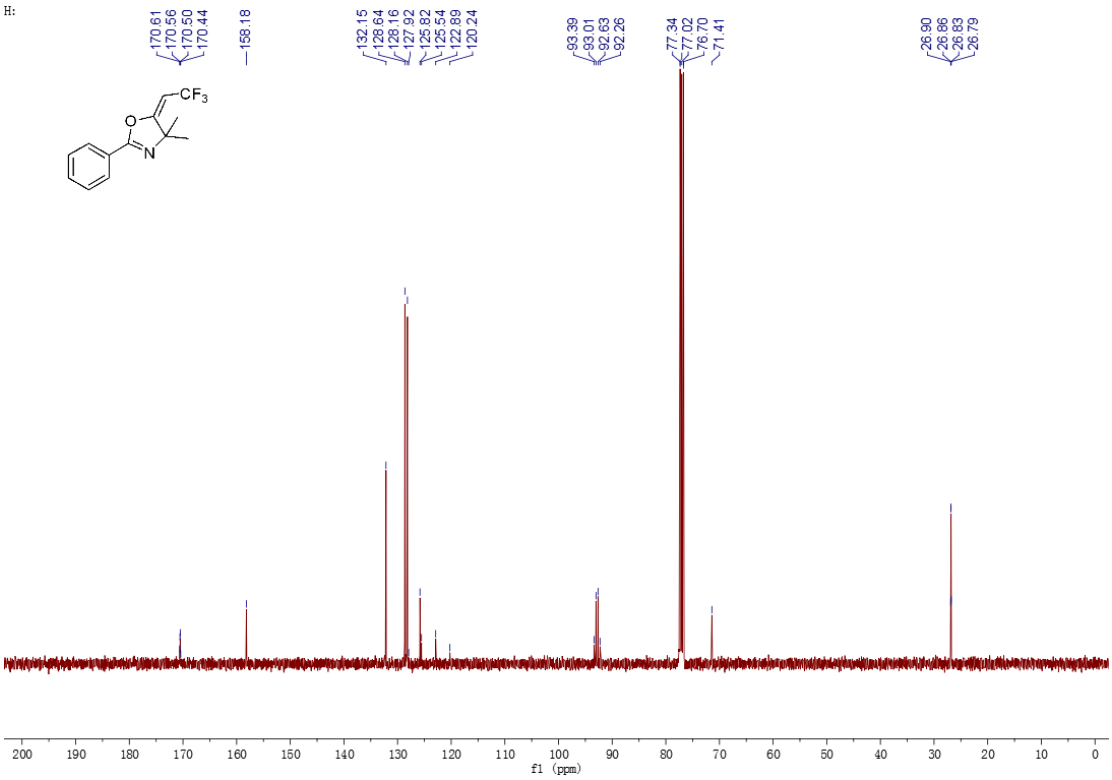

PROTON_01
test001
7.52
7.50
7.48
7.34
7.32
7.26
6.17
2.96
2.95
2.94
2.38
2.06
1.99
1.76
1.64
1.59
1.56
1.55
1.51
1.49
1.46
0.91
0.96
0.94
1.00
1.00
2.00
2.03
0.80
1.03
4.02
5.98
6.23
3.00
f1 (ppm)

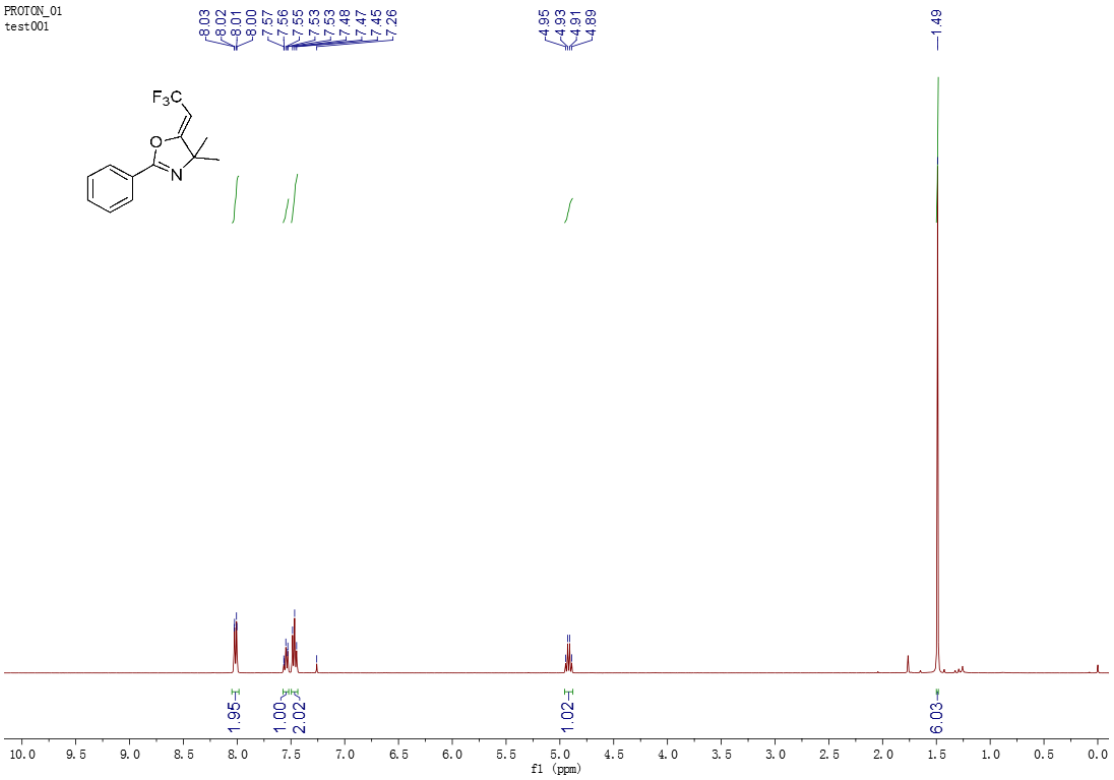

H:
220.69
166.51
143.56
136.94
132.27
127.82
125.51
124.06
87.35
77.48
77.16
76.84
69.35
50.54
47.95
44.54
37.94
35.86
31.59
29.33
29.10
26.35
25.68
21.63
13.88
f1 (ppm)

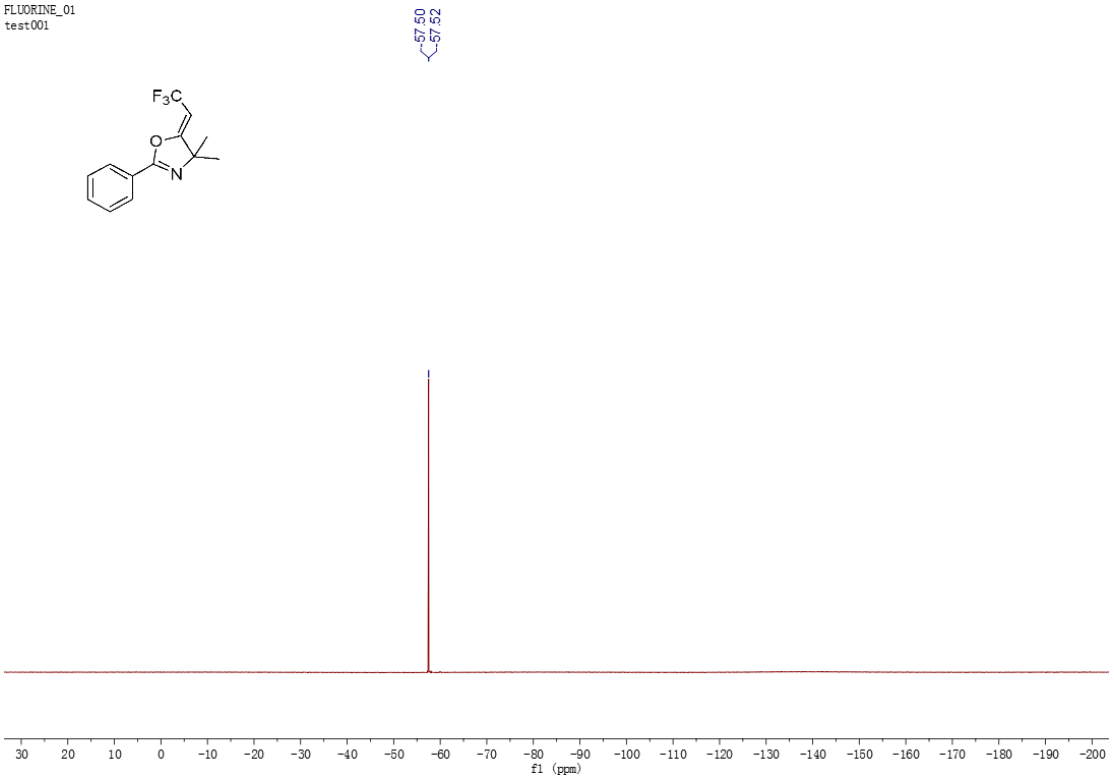

PROTON_01
test001
7.76
7.74
7.50
7.48
7.46
7.42
7.41
7.39
7.26
6.25
2.38
1.76
O
N
H
D
2.00
1.00
2.00
1.00
0.07
6.11
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

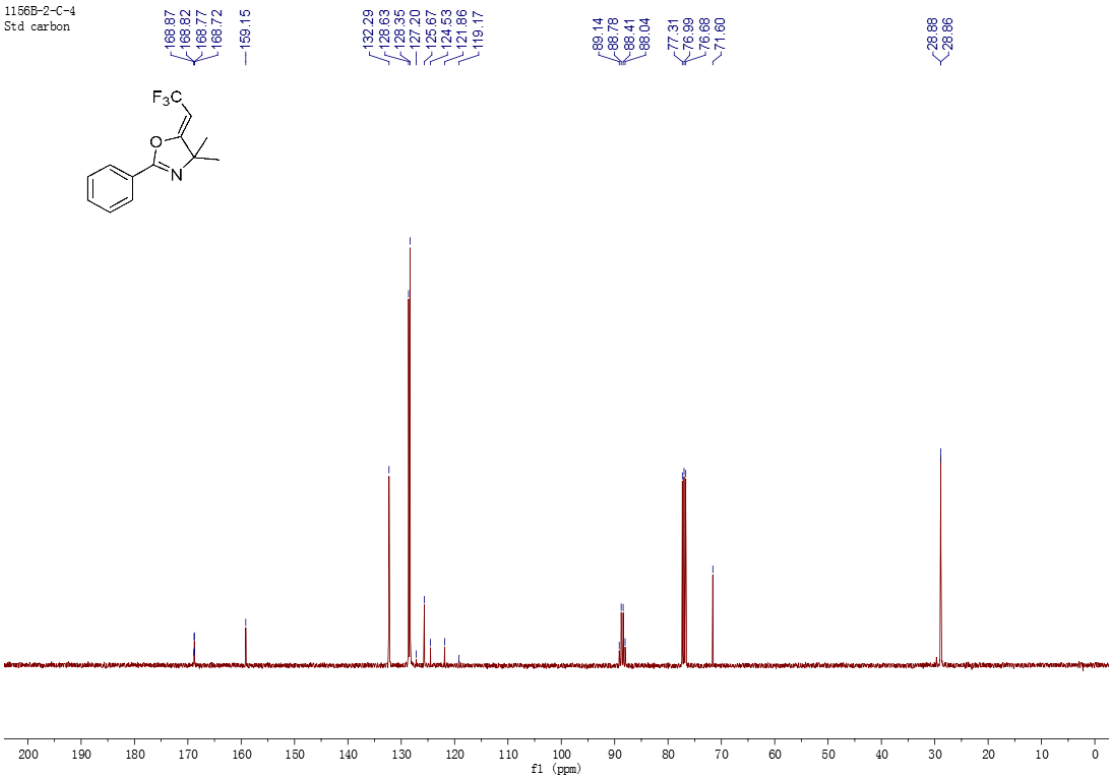

1156a-h-z
7.97
7.97
7.95
7.94
7.54
7.52
7.52
7.52
7.48
7.47
7.46
7.45
7.44
7.44
7.43
7.26
5.63
5.61
5.59
5.56
1.60
CF3
O
N
1.97
1.00
2.00
1.00
6.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

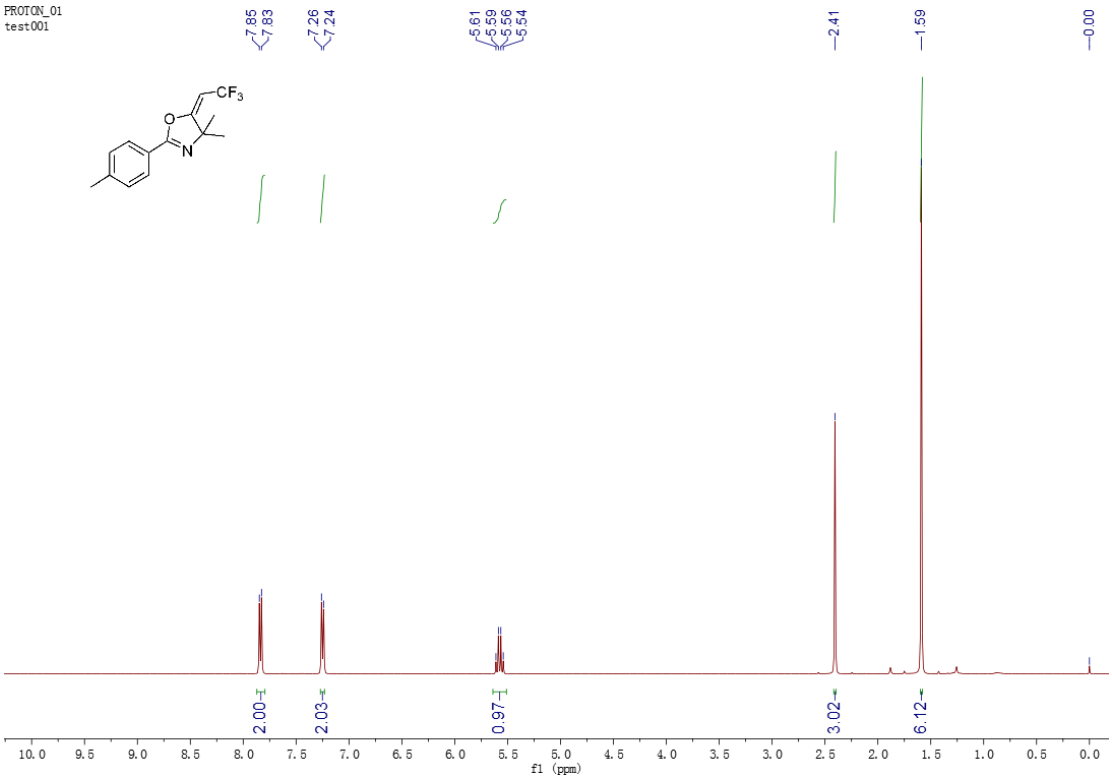

1156-2-f
STANDARD PROTON PARAMETERS
-53.45
-53.47
CF3
O
N
110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)

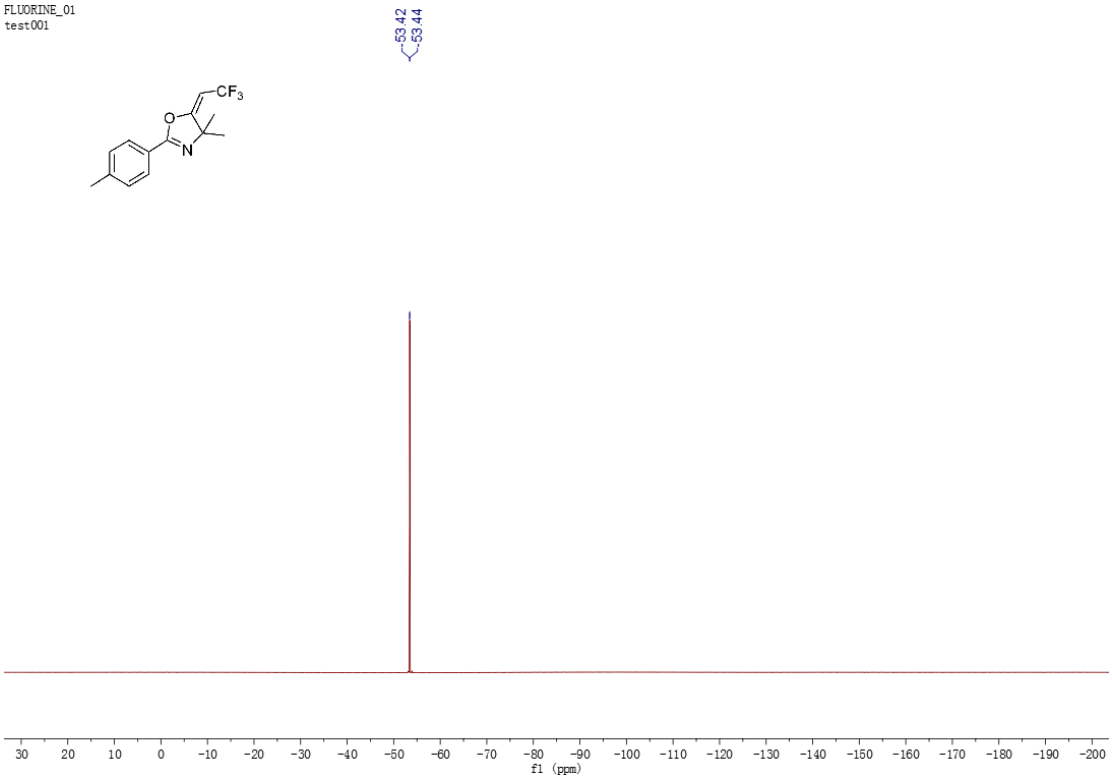

H:
170.61
170.56
170.50
170.44
158.18
132.15
128.64
128.16
127.92
125.82
125.54
122.89
120.24
93.39
93.01
92.63
92.26
77.34
77.02
76.70
71.41
26.90
26.86
26.83
26.79
CF3
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

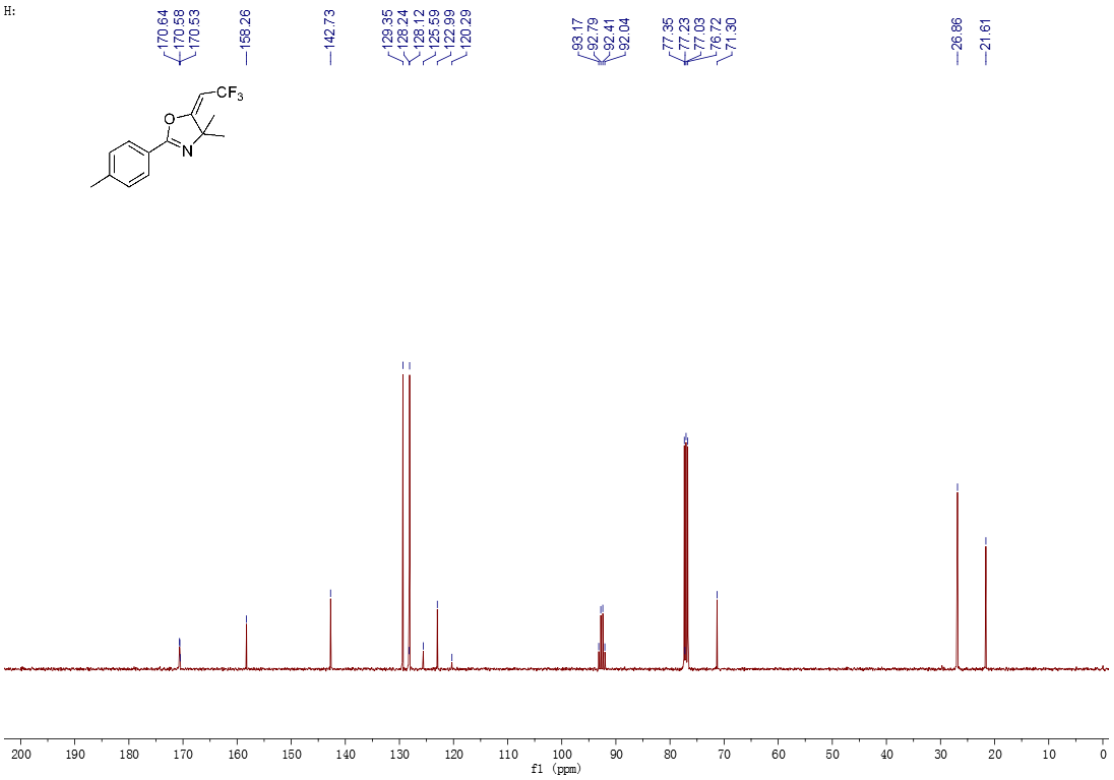

PROTON_01
test001
8.03
8.02
8.01
8.00
7.57
7.56
7.55
7.53
7.48
7.47
7.45
7.26
4.95
4.93
4.91
4.89
1.49
F3C
O
N
1.95
1.00
2.02
1.02
6.03
f1 (ppm)

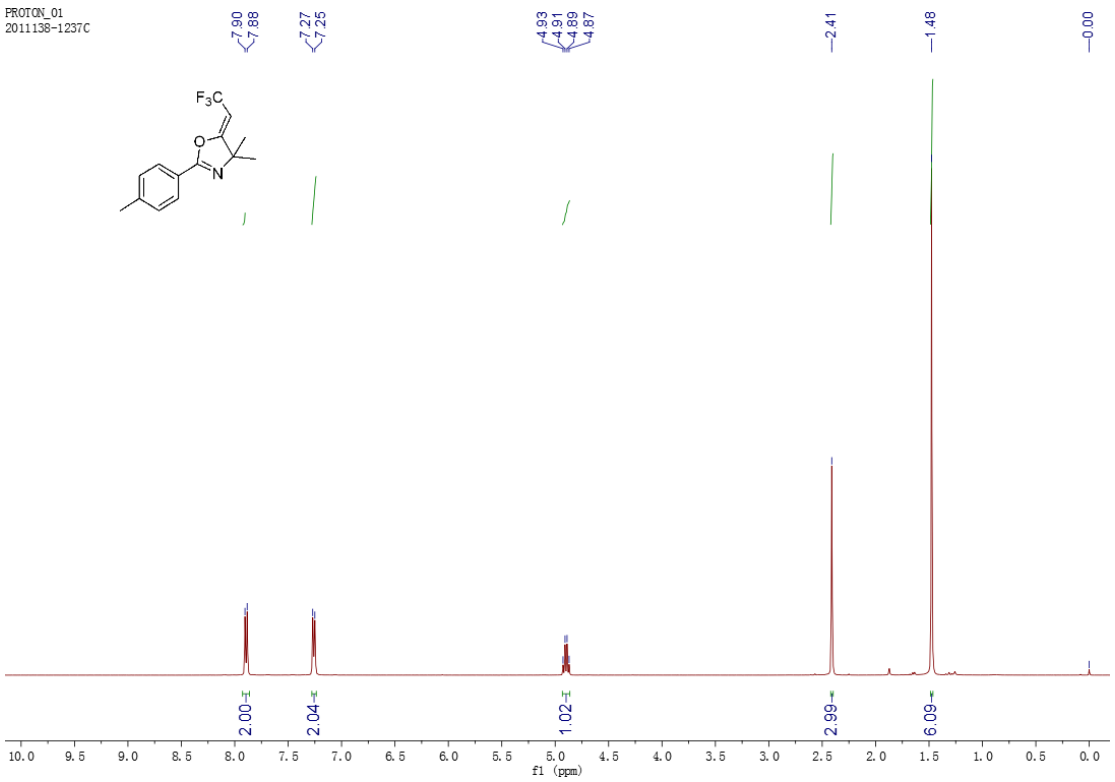

FLUORINE_01
test001
-57.50
-57.52
F3C
O
N
f1 (ppm)

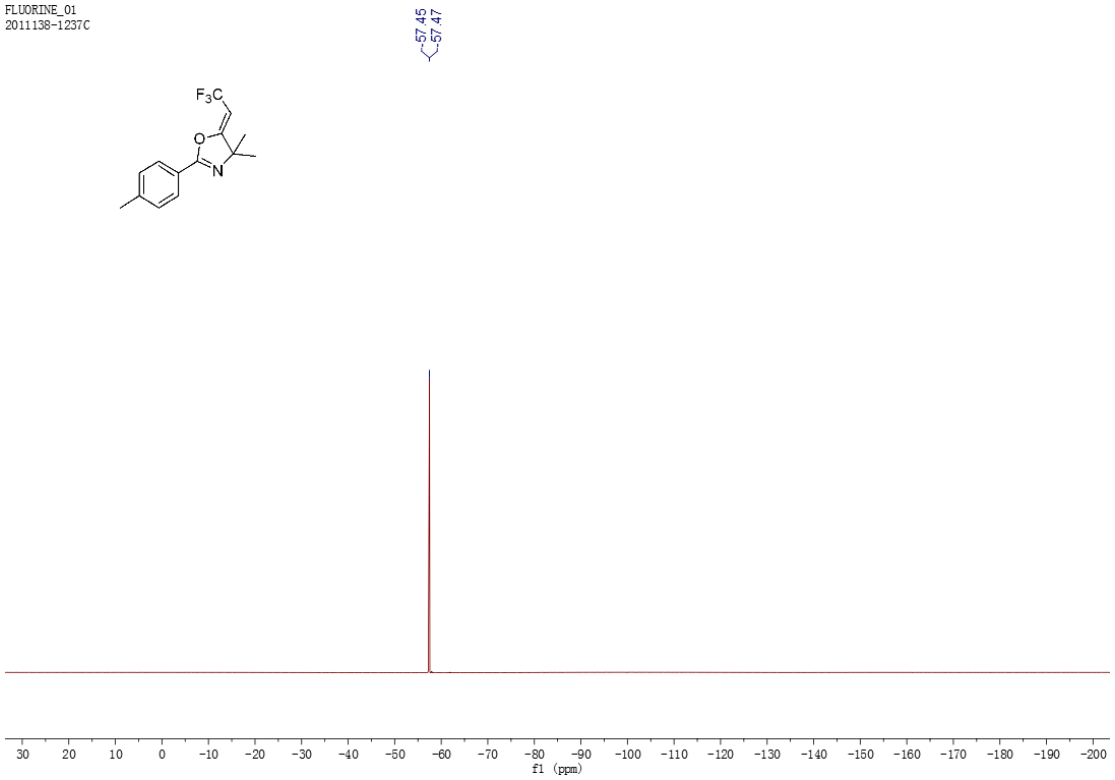

1156B-2-C-4
Std carbon
168.87
168.82
168.77
168.72
159.15
132.29
128.63
128.35
127.20
125.67
124.53
121.86
119.17
89.14
88.78
88.41
88.04
77.31
76.99
76.68
71.60
28.88
28.86
F3C
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

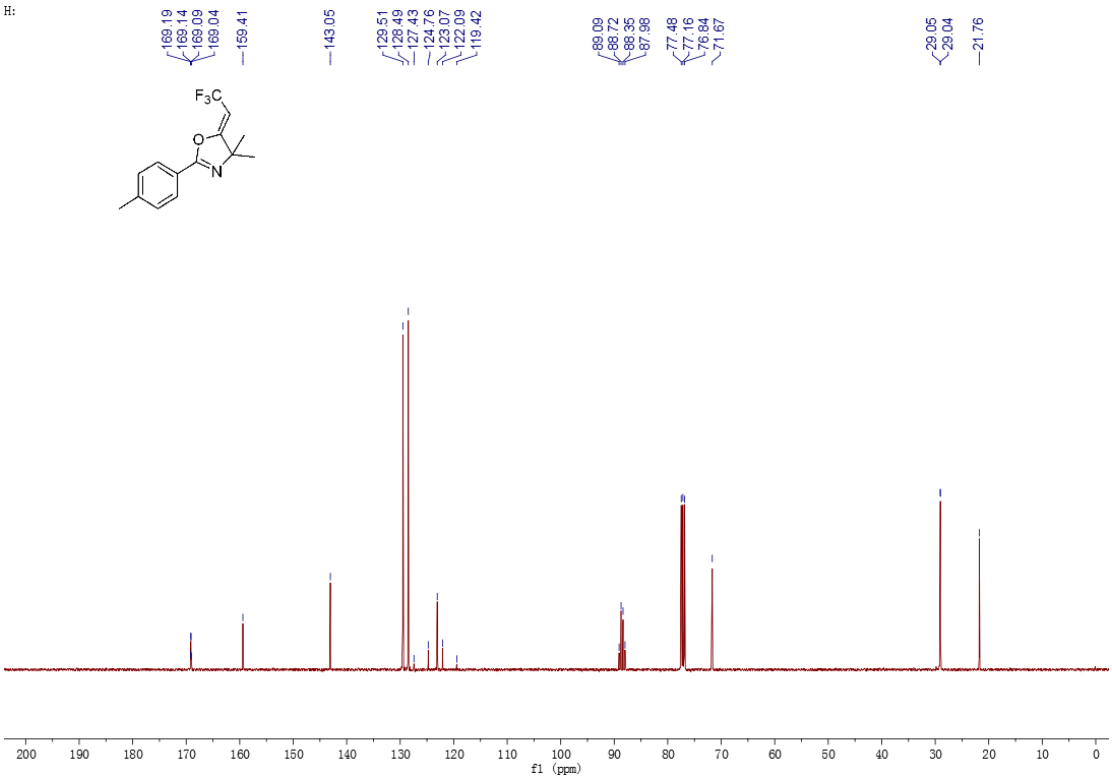

PROTON_01
test001
7.85
7.83
7.26
7.24
5.61
5.59
5.56
5.54
2.41
1.59
0.00
CF3
O
N
2.00
2.03
0.97
3.02
6.12
f1 (ppm)

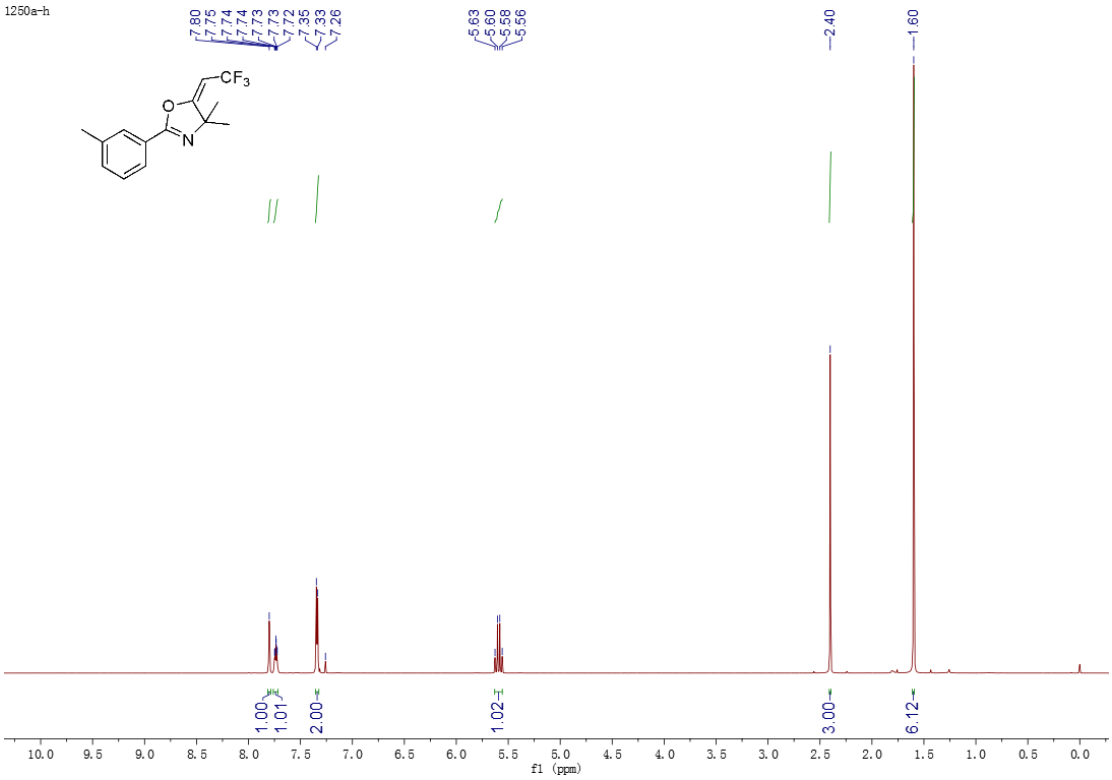

FLUORINE_01
test001
-53.42
-53.44
CF3
O
N
f1 (ppm)

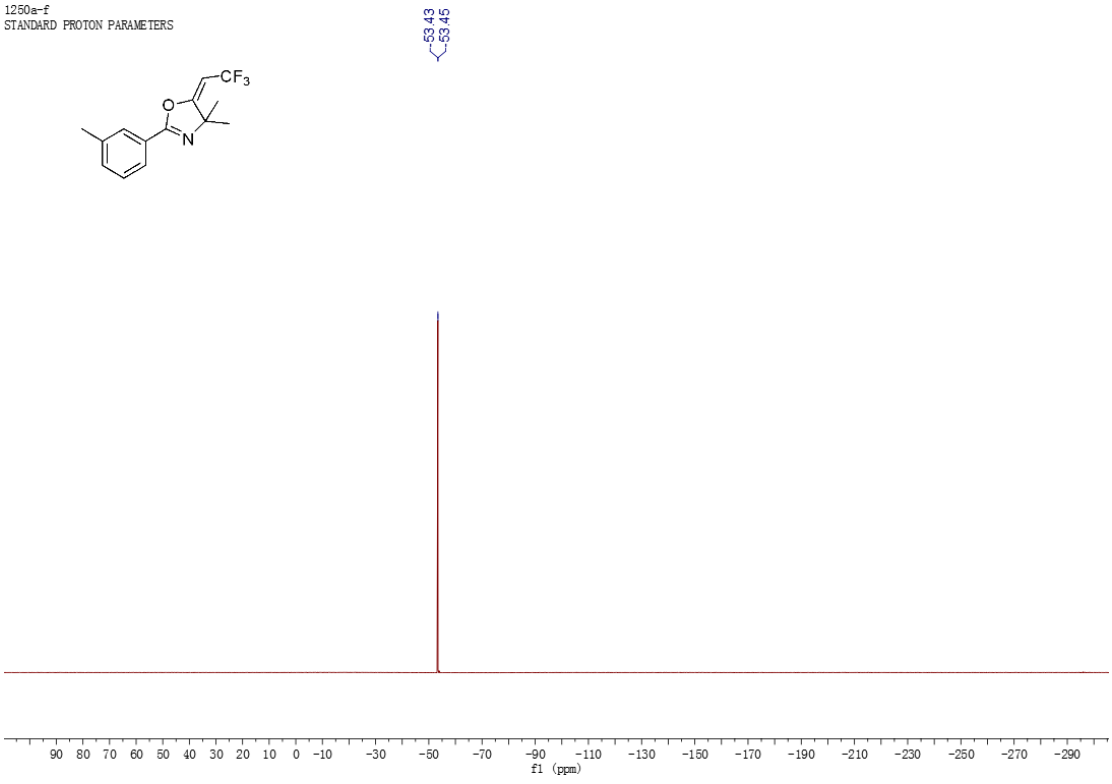

H:
170.64
170.58
170.53
158.26
142.73
129.35
128.24
128.12
125.59
122.99
120.29
93.17
92.79
92.41
92.04
77.35
77.23
77.03
76.72
71.30
26.86
21.61
CF3
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

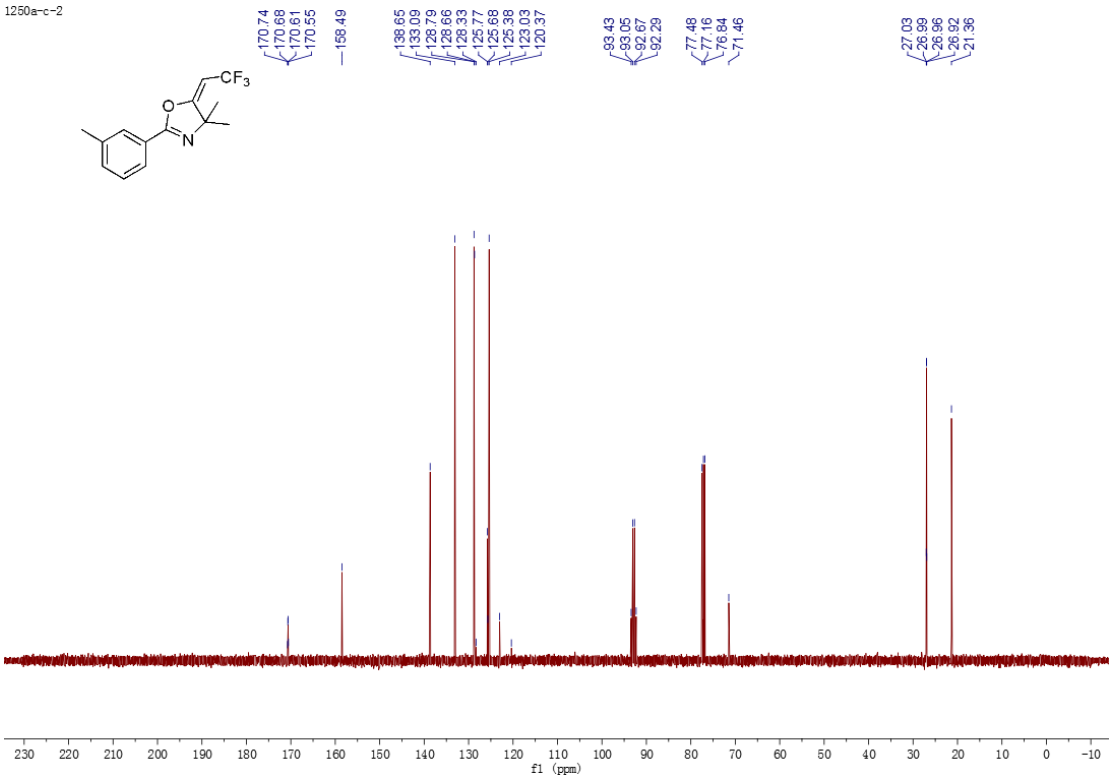

PROTON_01
2011138-1237C
7.90
7.88
7.27
7.25
4.93
4.91
4.89
4.87
2.41
1.48
0.00
F3C
O
N
2.00
2.04
1.02
2.99
6.09
f1 (ppm)

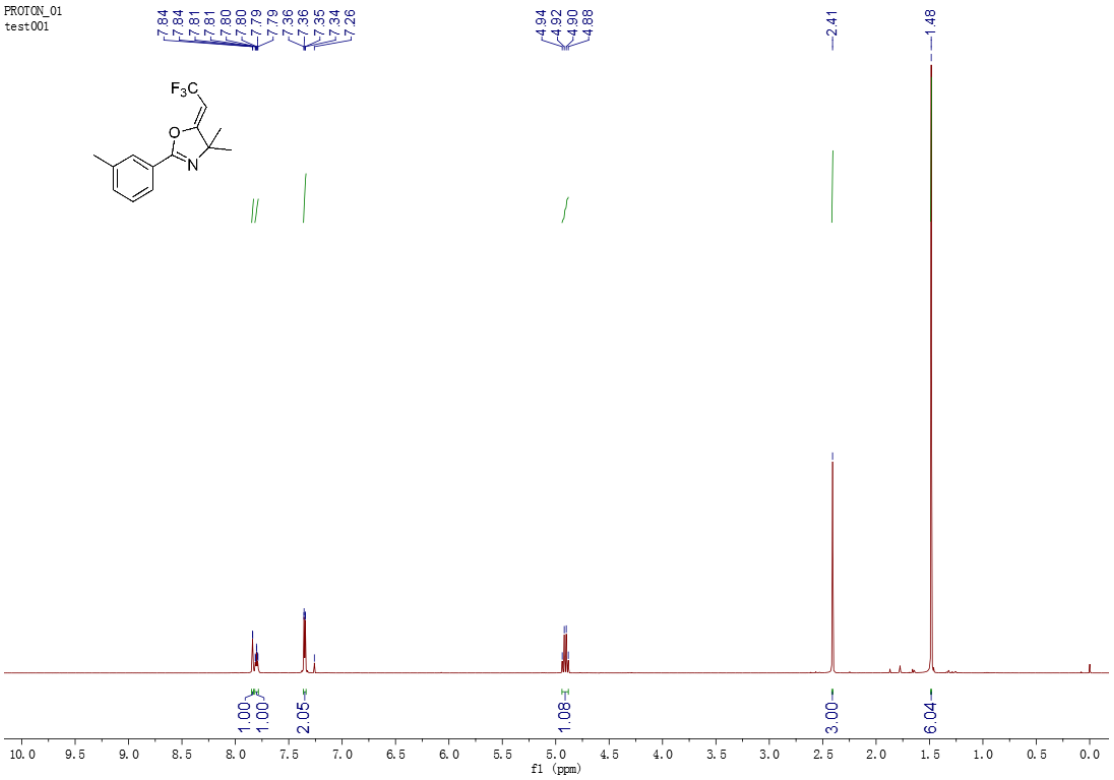

FLUORINE_01
2011138-1237C
-57.45
-57.47
F3C
O
N
f1 (ppm)

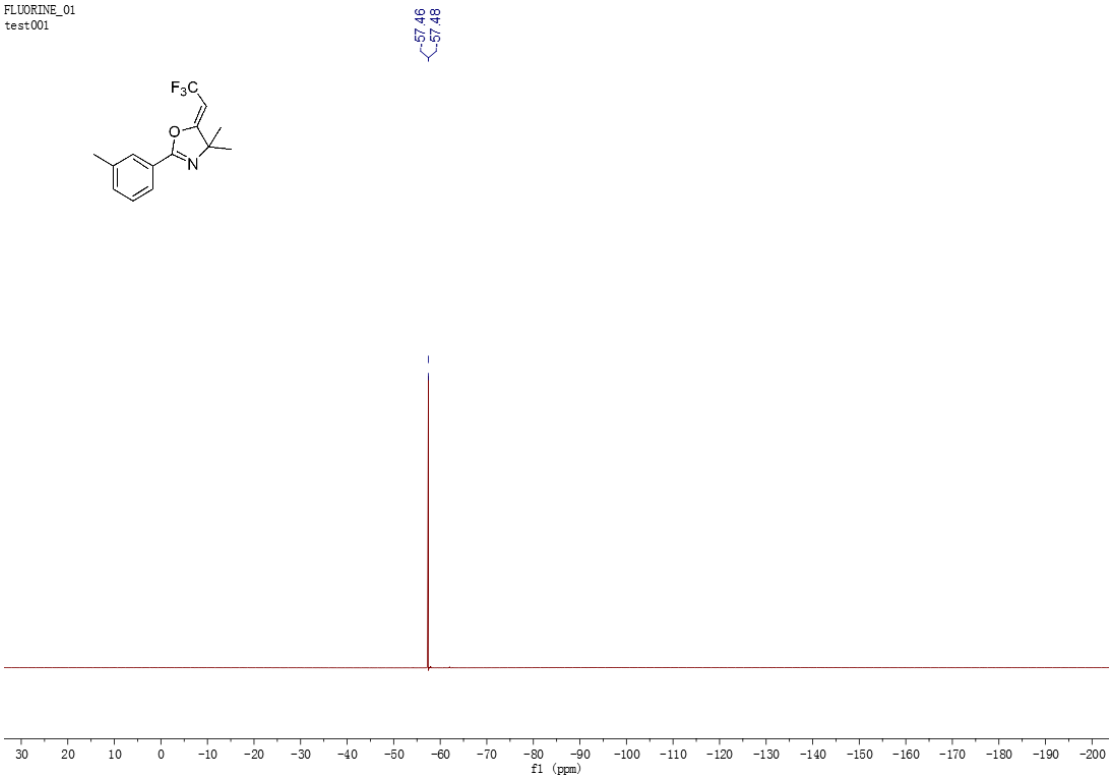

H:
169.19
169.14
169.09
169.04
159.41
143.05
129.51
128.49
127.43
124.76
123.07
122.09
119.42
89.09
88.72
88.35
87.98
77.48
77.16
76.84
71.67
29.05
29.04
21.76
F3C
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

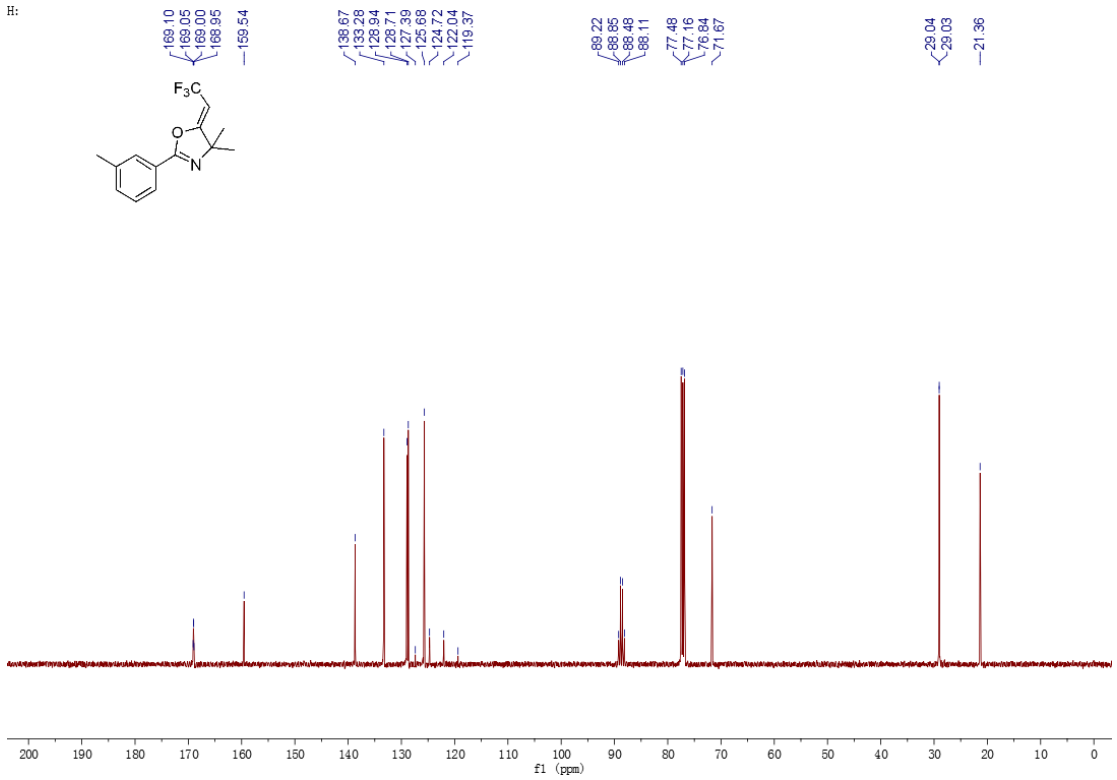

1250a-h
7.80
7.75
7.74
7.74
7.73
7.73
7.72
7.35
7.33
7.26
5.63
5.60
5.58
5.56
2.40
1.60
CF3
O
N
1.00
1.01
2.00
1.02
3.00
6.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

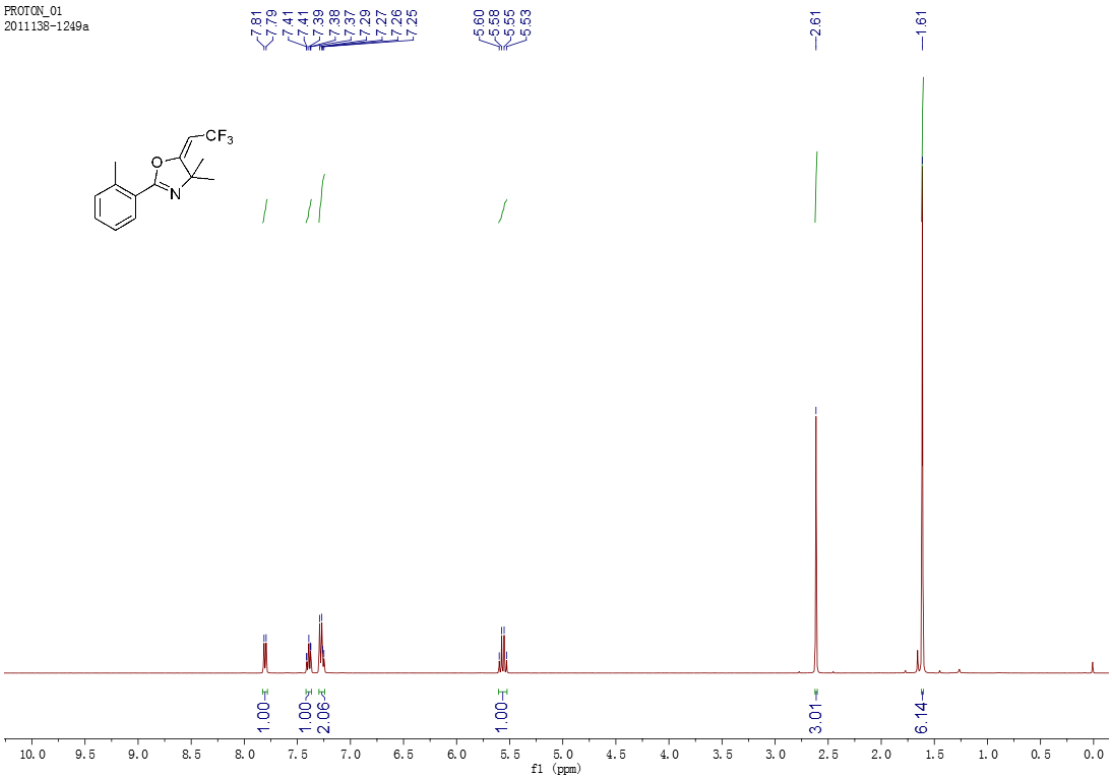

1250a-f
STANDARD PROTON PARAMETERS
-53.43
-53.45
CF3
O
N
90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

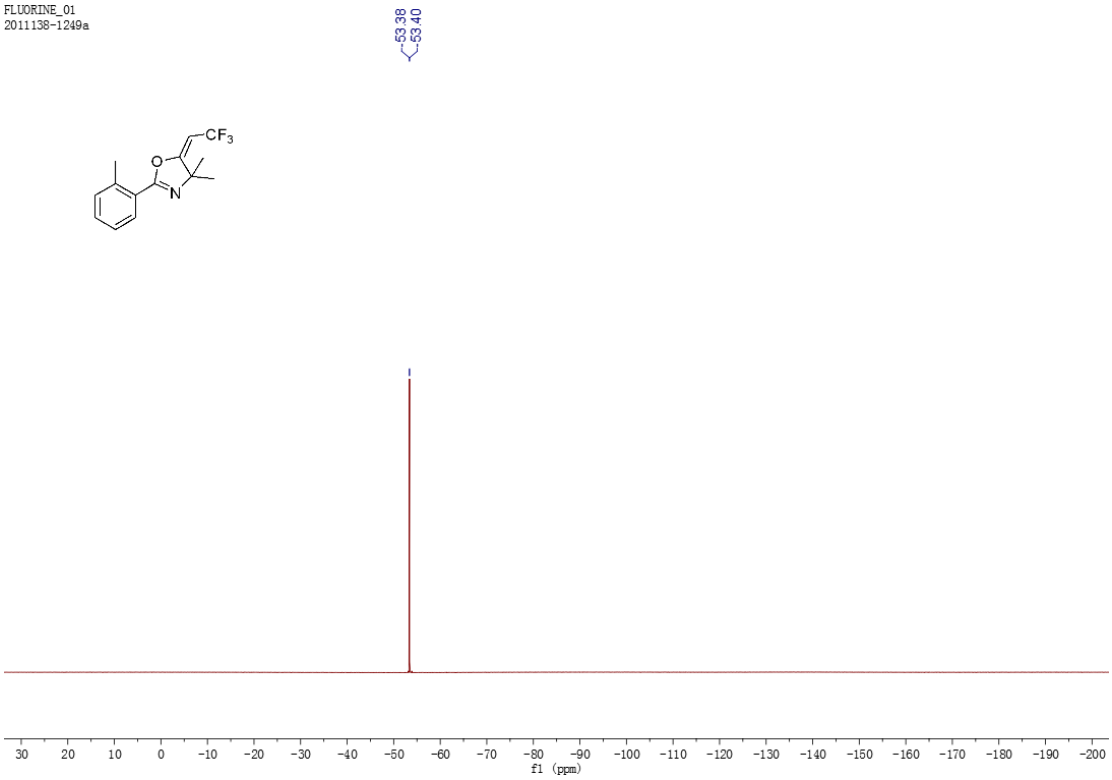

1250a-c-2
170.74
170.68
170.61
170.55
158.49
138.65
133.09
128.79
128.66
128.33
125.77
125.68
125.38
123.03
120.37
93.43
93.05
92.67
92.29
77.48
77.16
76.84
71.46
27.03
26.99
26.96
26.92
21.36
CF3
O
N
f1 (ppm)

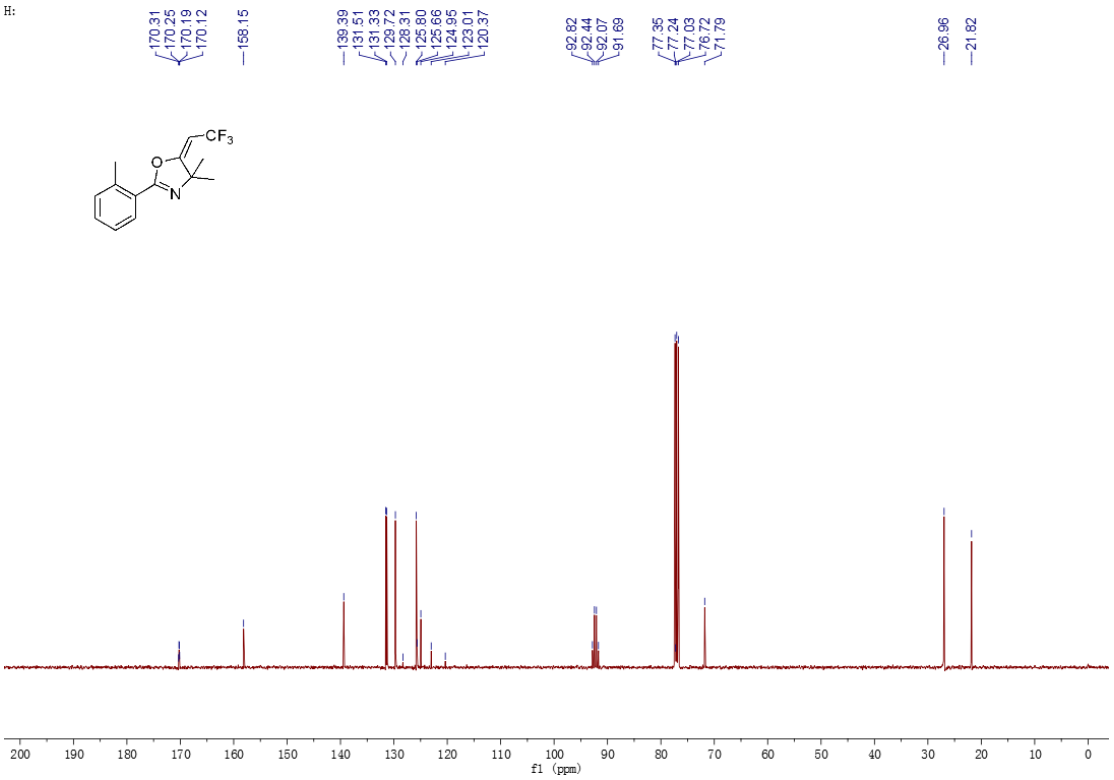

PROTON_01
test001
7.84
7.84
7.81
7.81
7.80
7.80
7.79
7.79
7.36
7.35
7.34
7.26
4.94
4.92
4.90
4.88
2.41
1.48
F3C
O
N
1.00
1.00
2.05
1.08
3.00
6.04
f1 (ppm)

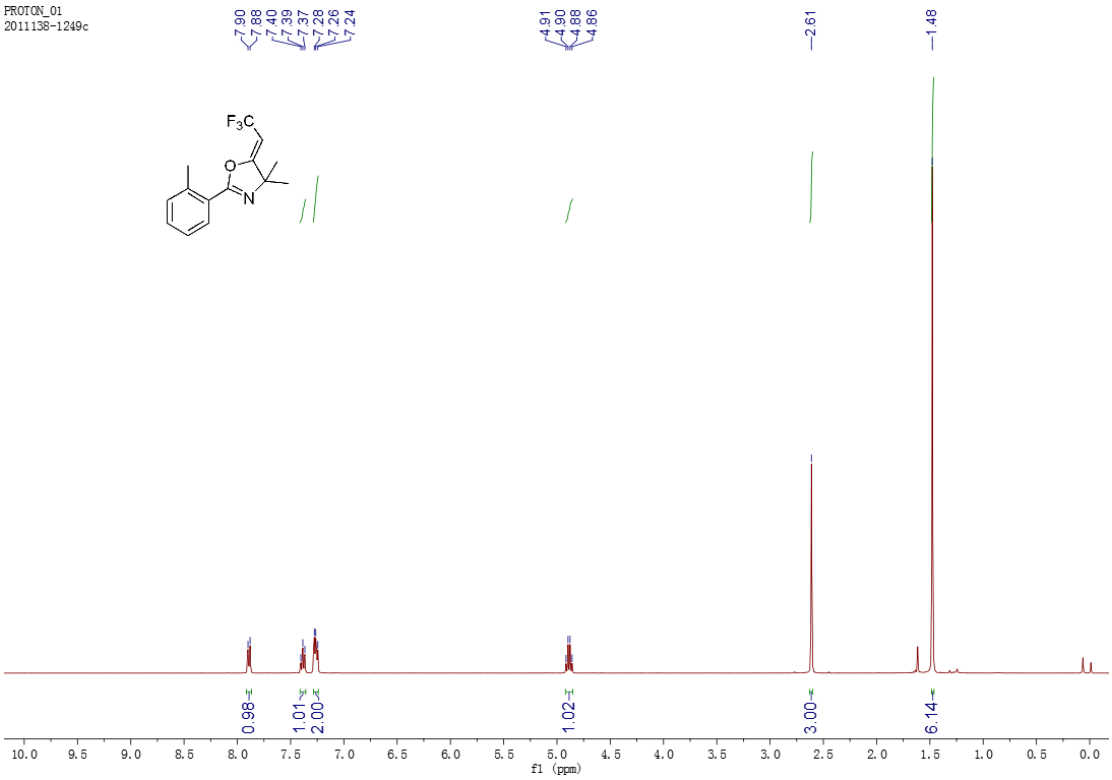

FLUORINE_01
test001
-57.46
-57.48
F3C
O
N
f1 (ppm)

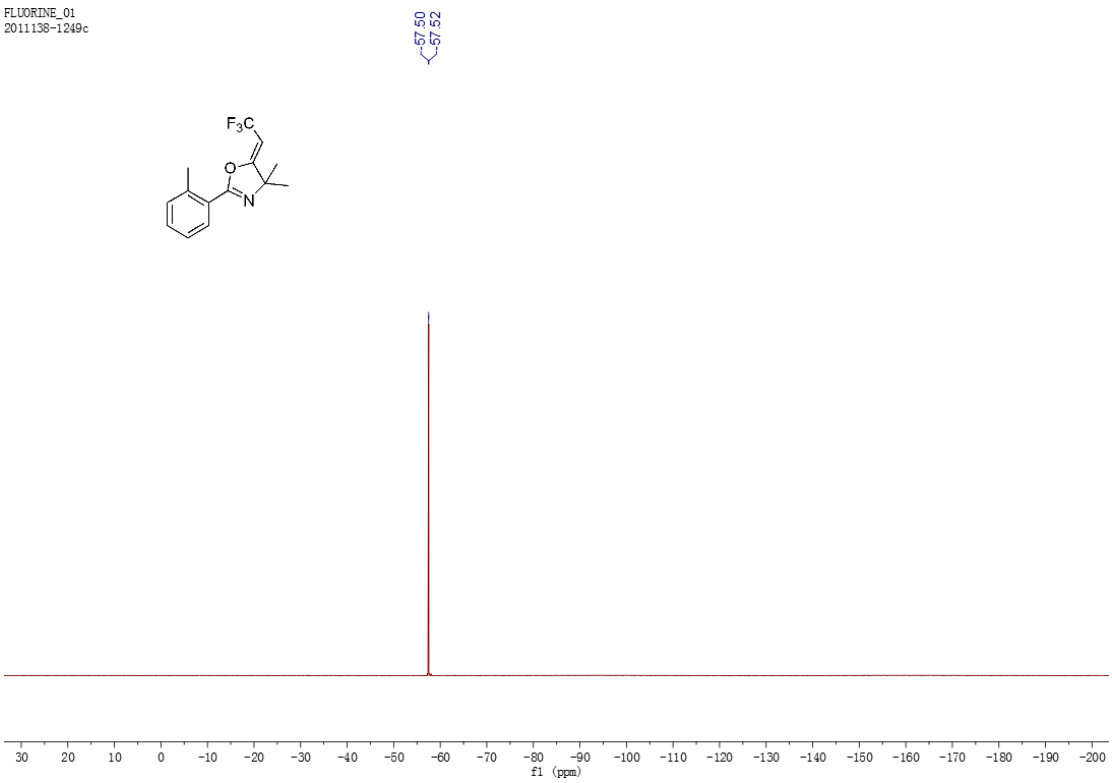

H:
169.10
169.05
169.00
168.95
159.54
138.67
133.28
128.94
128.71
127.39
125.68
124.72
122.04
119.37
89.22
88.85
88.48
88.11
77.48
77.16
76.84
71.67
29.04
29.03
21.36
F3C
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

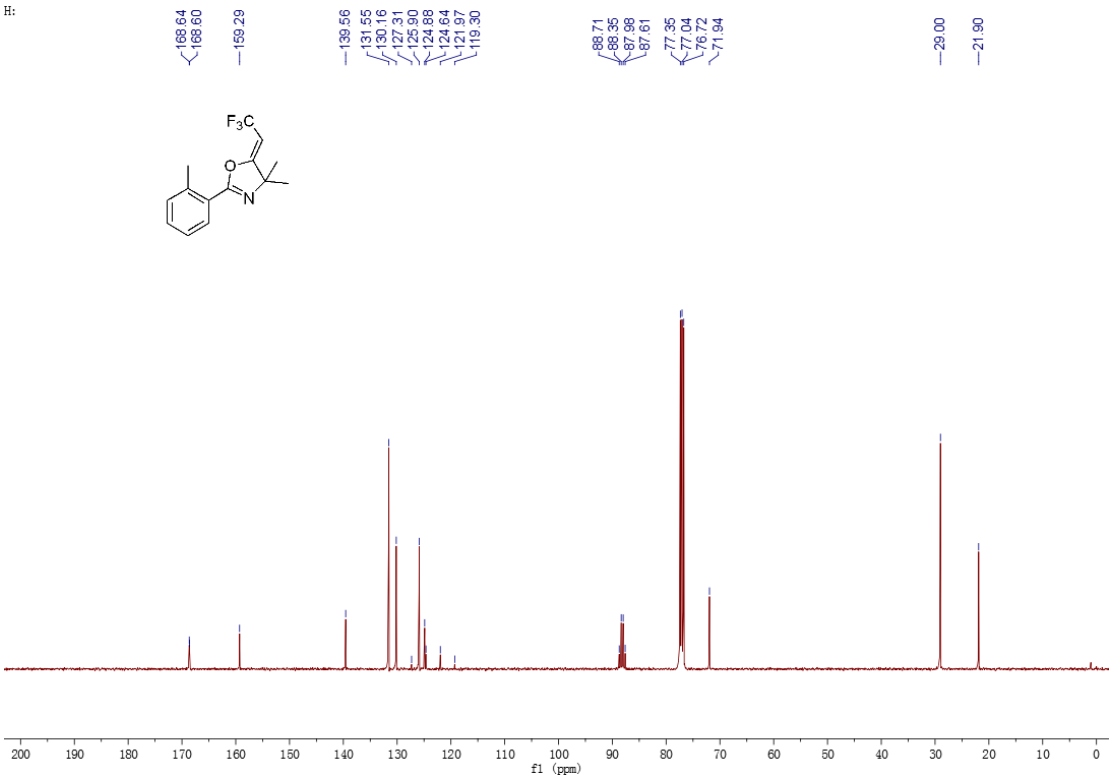

PROTON_01
2011138-1249a
7.81
7.79
7.41
7.41
7.39
7.38
7.37
7.29
7.27
7.26
7.25
5.60
5.58
5.55
5.53
2.61
1.61
CF3
O
N
1.00
1.00
2.06
1.00
3.01
6.14
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

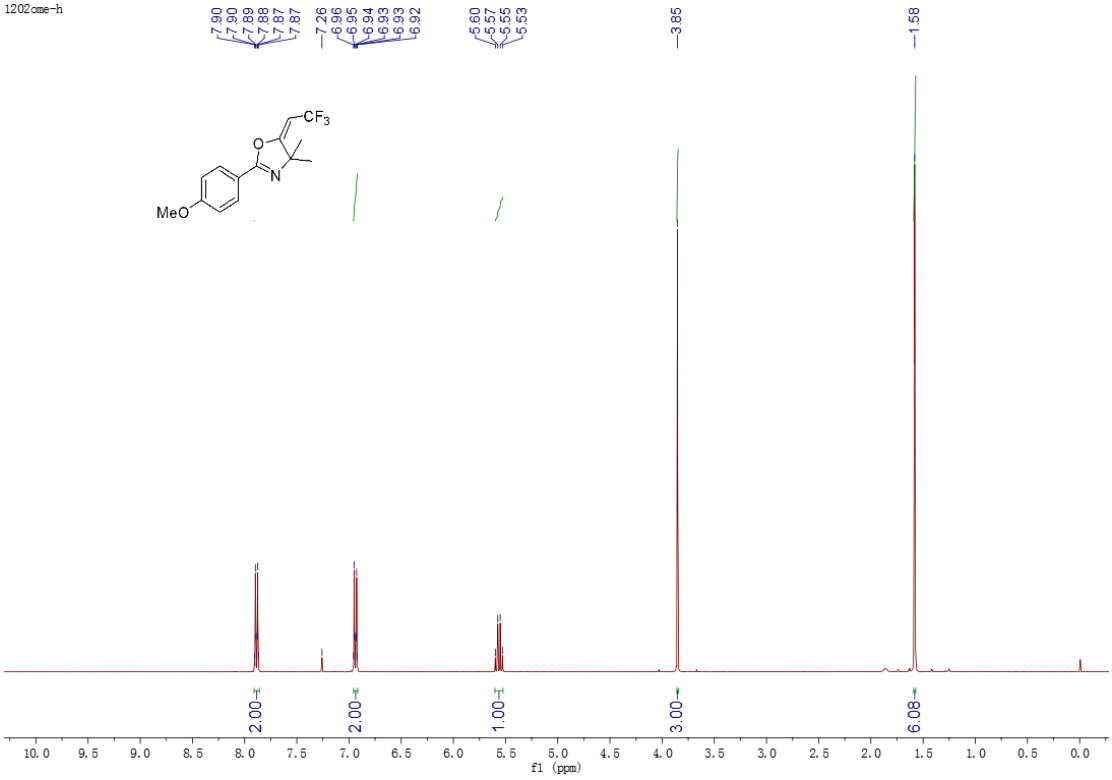

FLUORINE_01
2011138-1249a
-53.38
-53.40
CF3
O
N
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

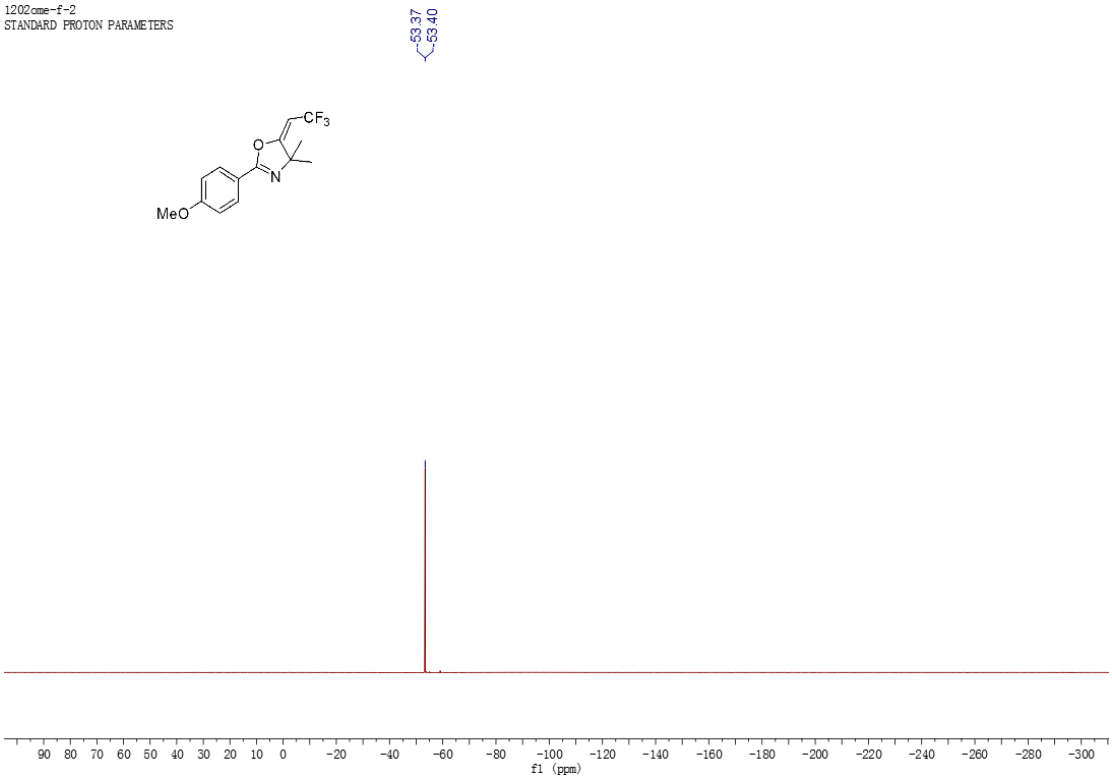

H:
170.31
170.25
170.19
170.12
158.15
139.39
131.51
131.33
129.72
128.31
125.80
125.66
124.95
123.01
120.37
92.82
92.44
92.07
91.69
77.35
77.24
77.03
76.72
71.79
26.96
21.82
CF3
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

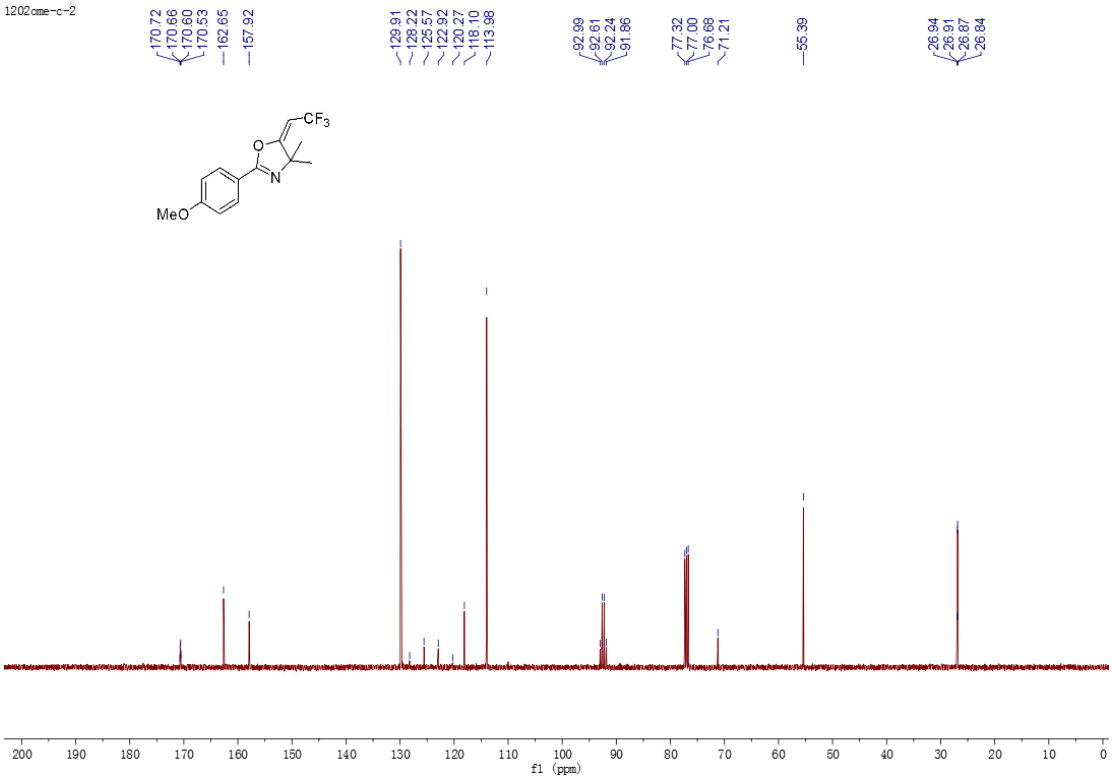

PROTON_01
2011138-1249c
7.90
7.88
7.40
7.39
7.37
7.28
7.26
7.24
4.91
4.90
4.88
4.86
2.61
1.48
F3C
O
N
0.98
1.01
2.00
1.02
3.00
6.14
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

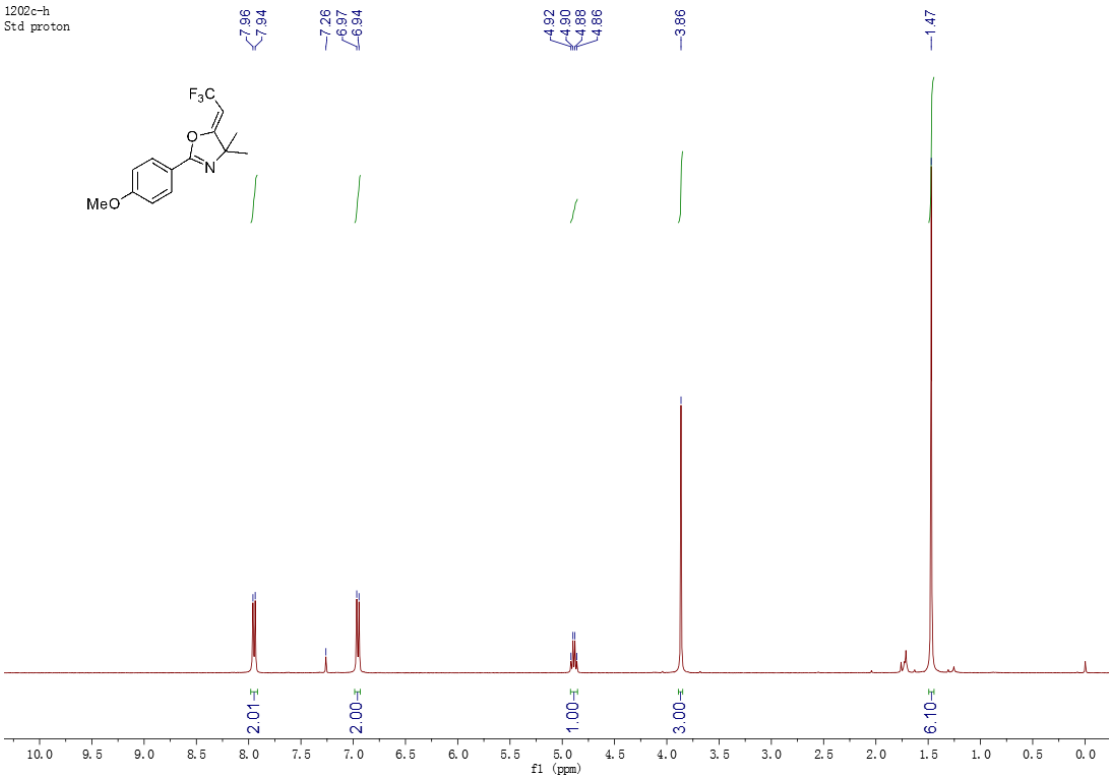

FLUORINE_01
2011138-1249c
-57.50
-57.52
F3C
O
N
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

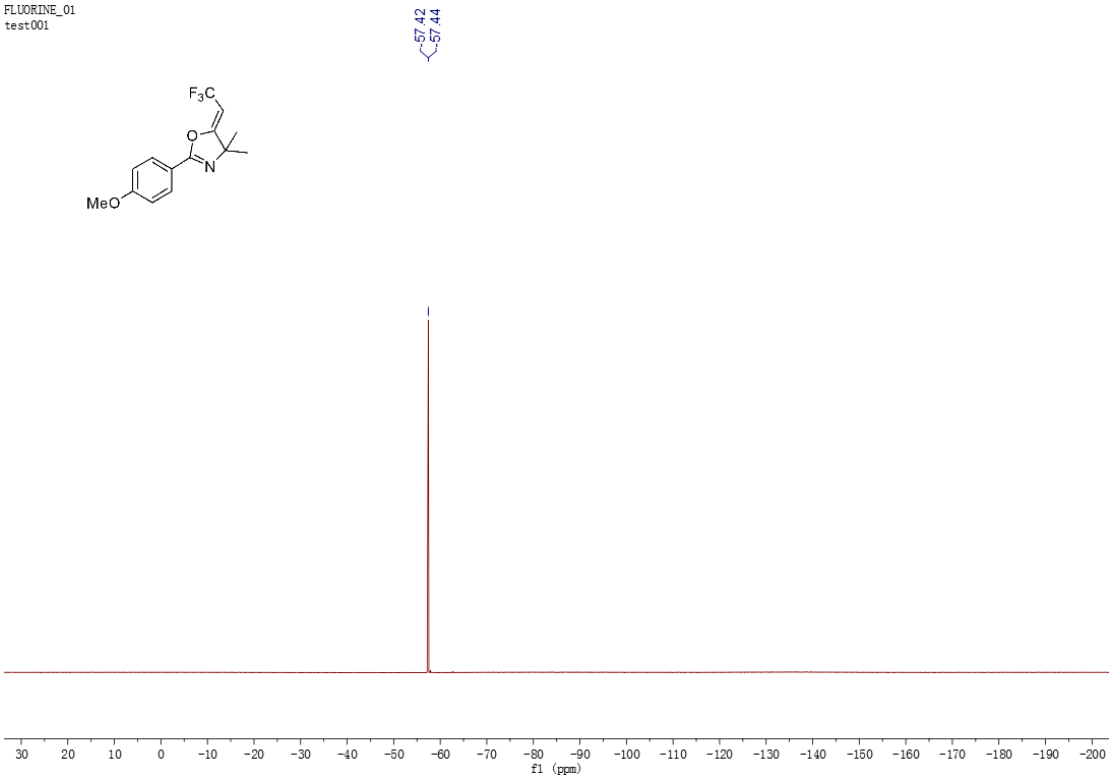

H:
168.64
168.60
159.29
139.56
131.55
130.16
127.31
125.90
124.88
124.64
121.97
119.30
88.71
88.35
87.98
87.61
77.35
77.04
76.72
71.94
29.00
21.90
F3C
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

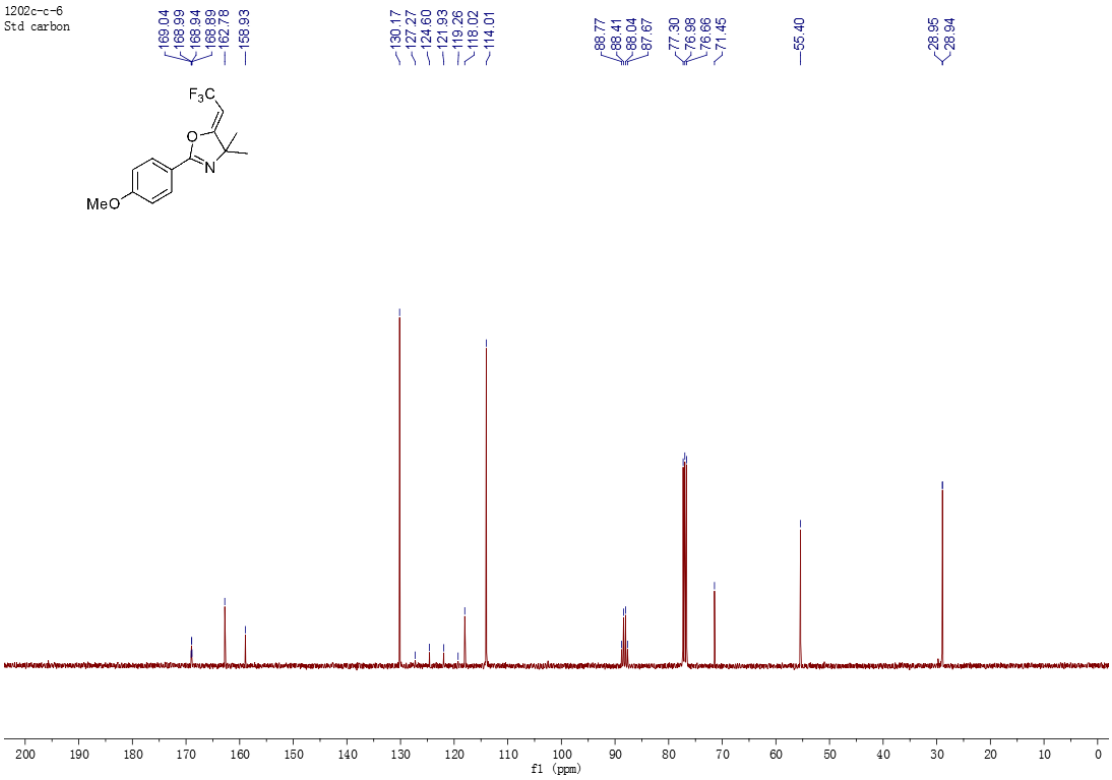

1202ome-h
7.90
7.90
7.89
7.88
7.87
7.87
7.26
6.96
6.95
6.94
6.93
6.93
6.92
5.60
5.57
5.55
5.53
3.85
1.58
CF3
O
N
MeO
2.00
2.00
1.00
3.00
6.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

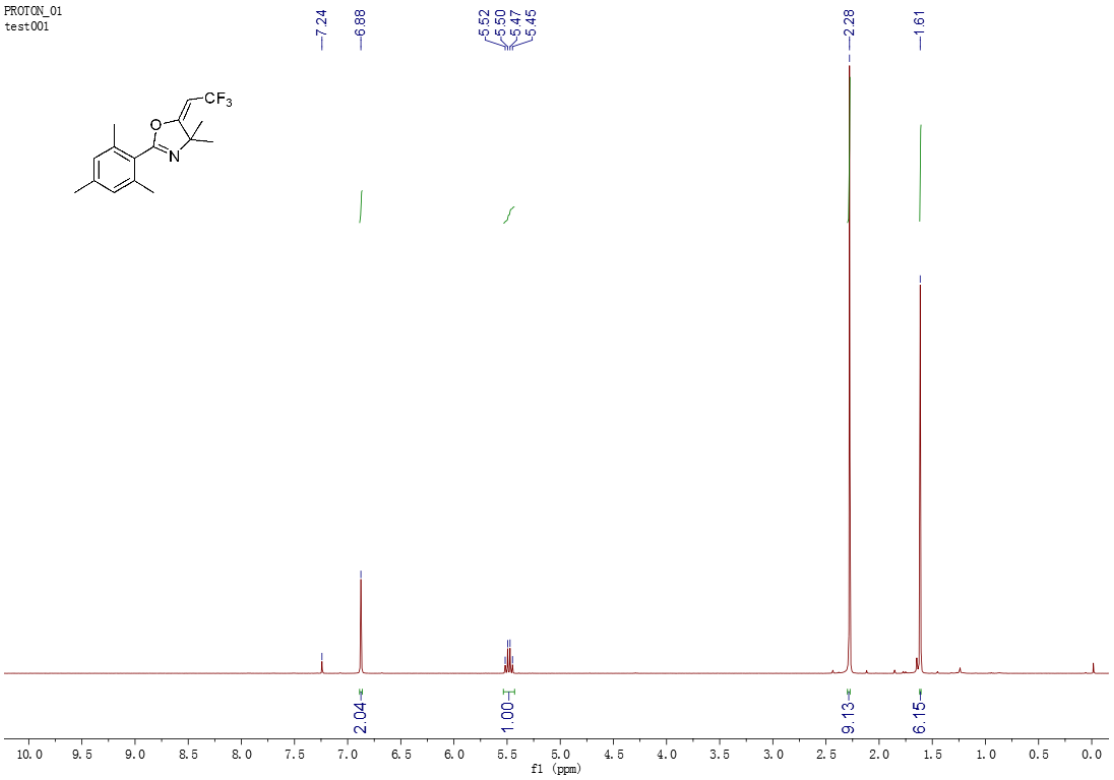

1202ome-f-2
STANDARD PROTON PARAMETERS
-53.37
-53.40
CF3
O
N
MeO
90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300
f1 (ppm)

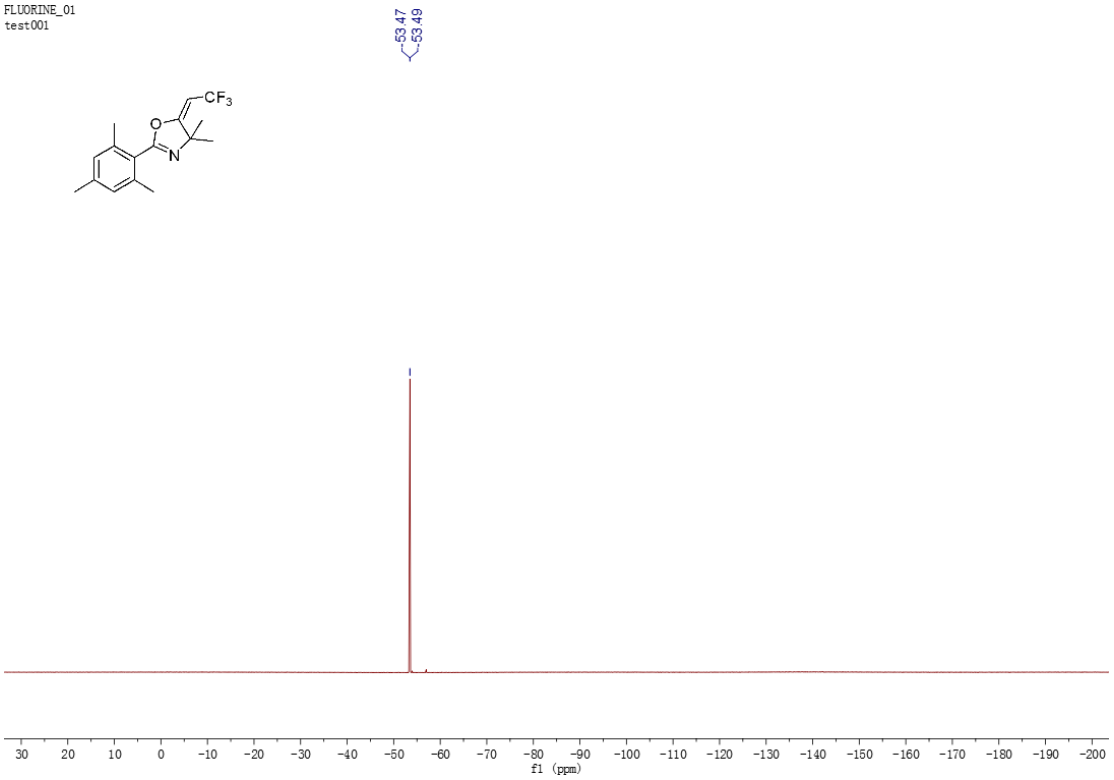

1202ome-c-2
170.72
170.66
170.60
170.53
162.65
157.92
129.91
128.22
125.57
122.92
120.27
118.10
113.98
92.99
92.61
92.24
91.86
77.32
77.00
76.68
71.21
55.39
26.94
26.91
26.87
26.84
CF3
O
N
MeO
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

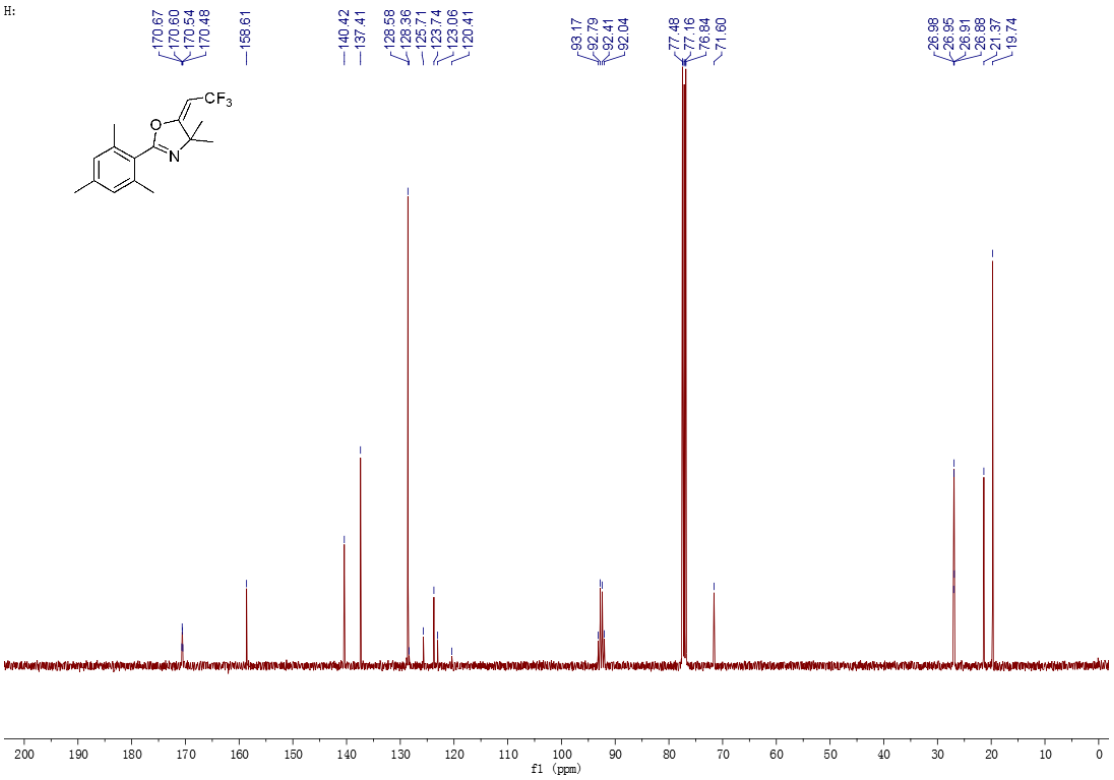

1202c-h
Std proton
7.96
7.94
7.26
6.97
6.94
4.92
4.90
4.88
4.86
3.86
1.47
F3C
O
N
MeO
2.01
2.00
1.00
3.00
6.10
f1 (ppm)

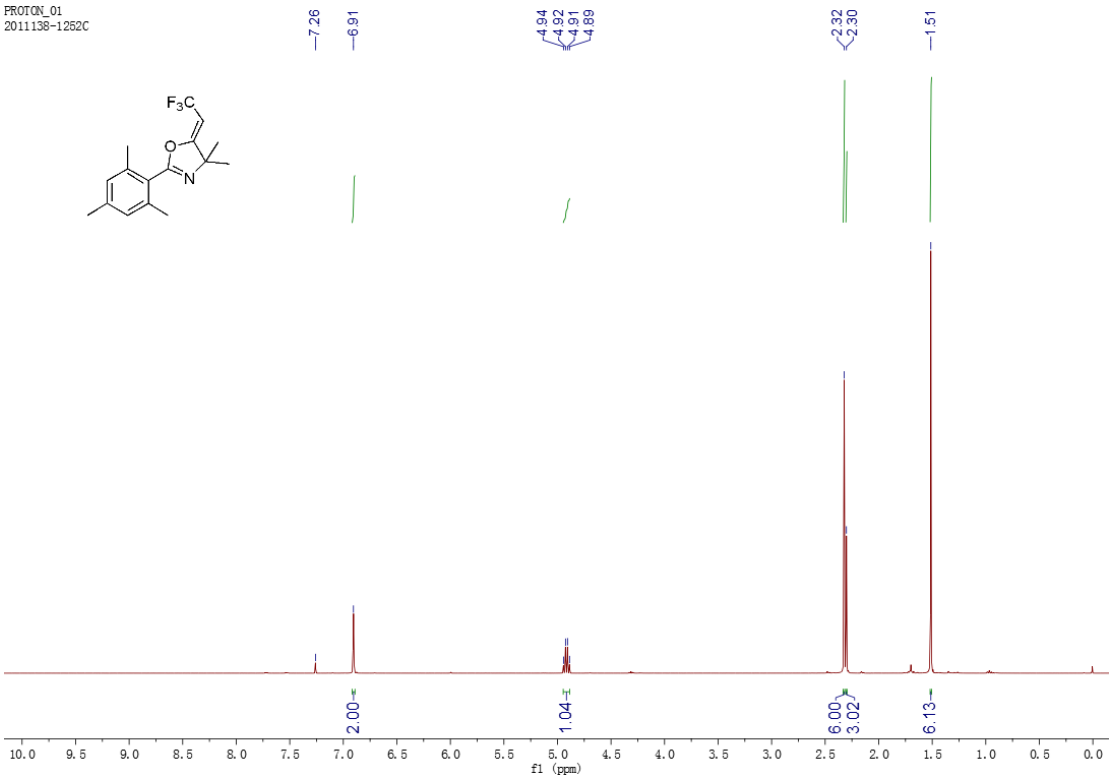

FLUORINE_01
test001
57.42
57.44
F3C
O
N
MeO
f1 (ppm)

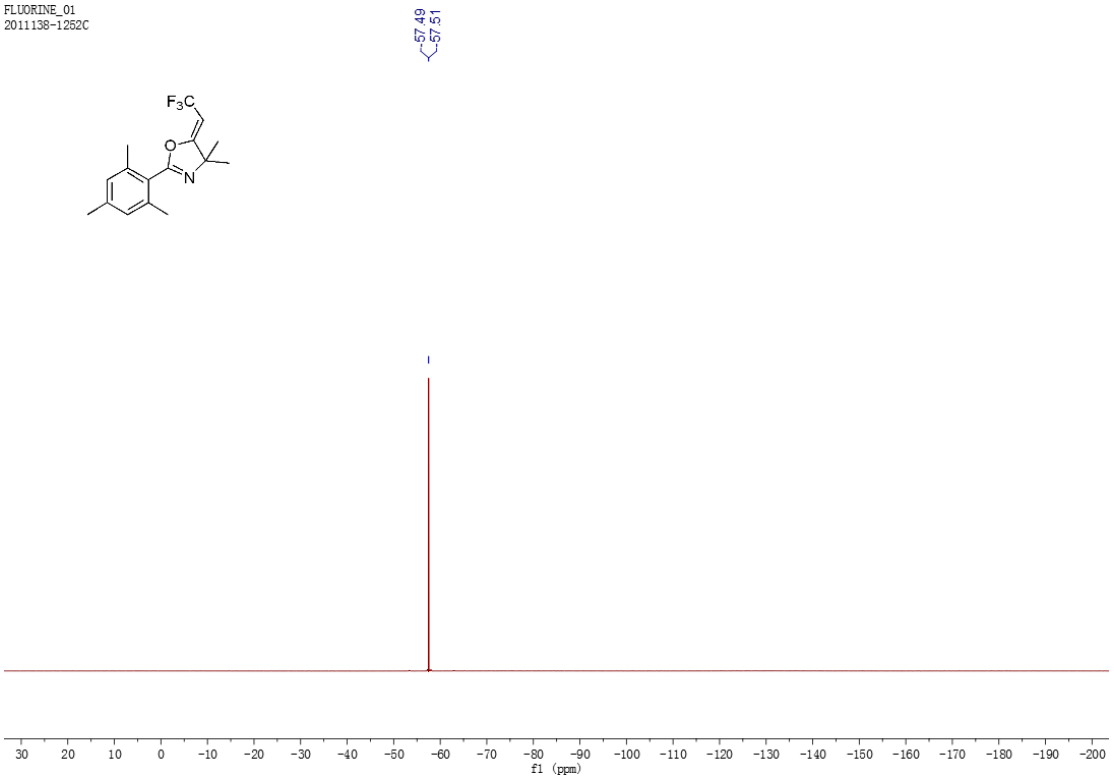

1202c-c-6
Std carbon
169.04
168.99
168.94
168.89
162.78
158.93
130.17
127.27
124.60
121.93
119.26
118.02
114.01
88.77
88.41
88.04
87.67
77.30
76.98
76.66
71.45
55.40
28.95
28.94
F3C
O
N
MeO
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

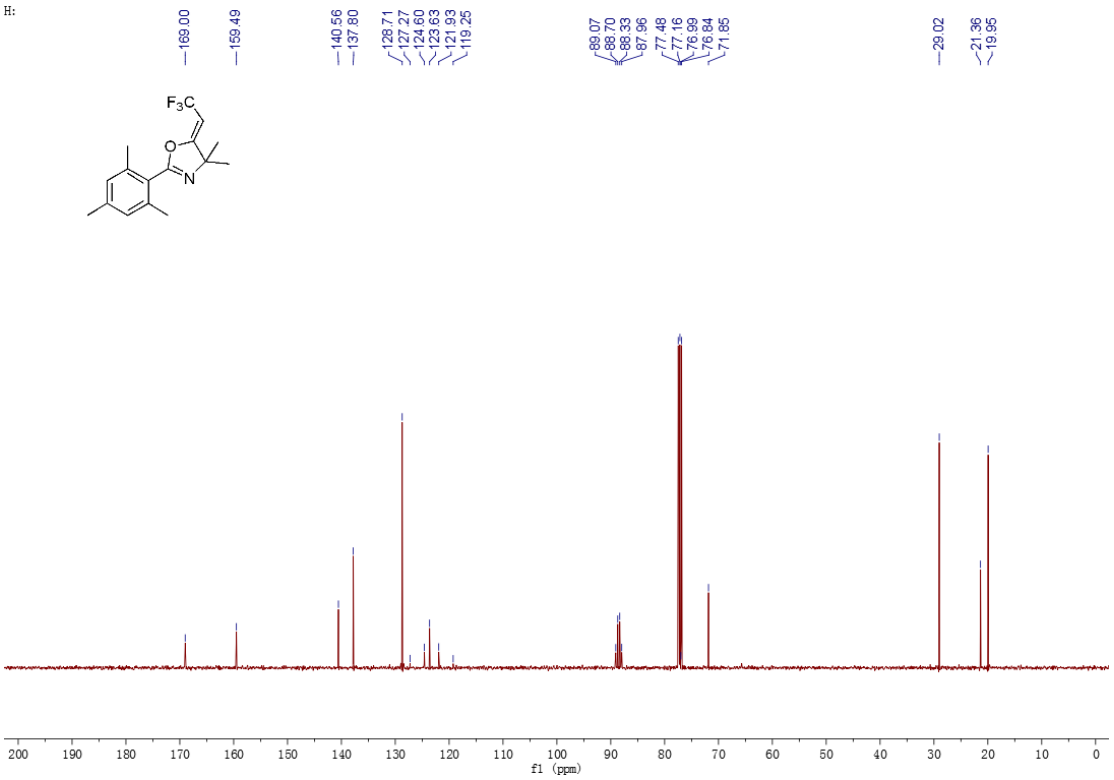

PROTON_01
test001
7.24
6.88
5.52
5.50
5.47
5.45
2.28
1.61
CF3
O
N
2.04
1.00
9.13
6.15
f1 (ppm)

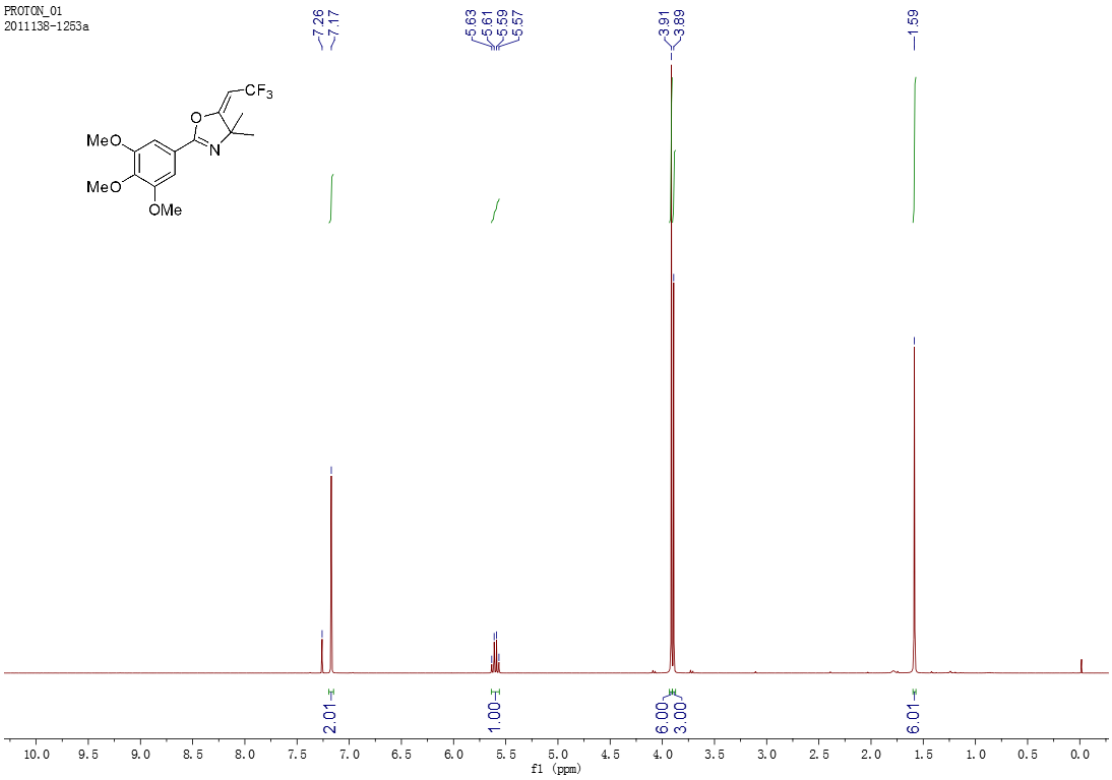

FLUORINE_01
test001
-53.47
-53.49
CF3
O
N
f1 (ppm)

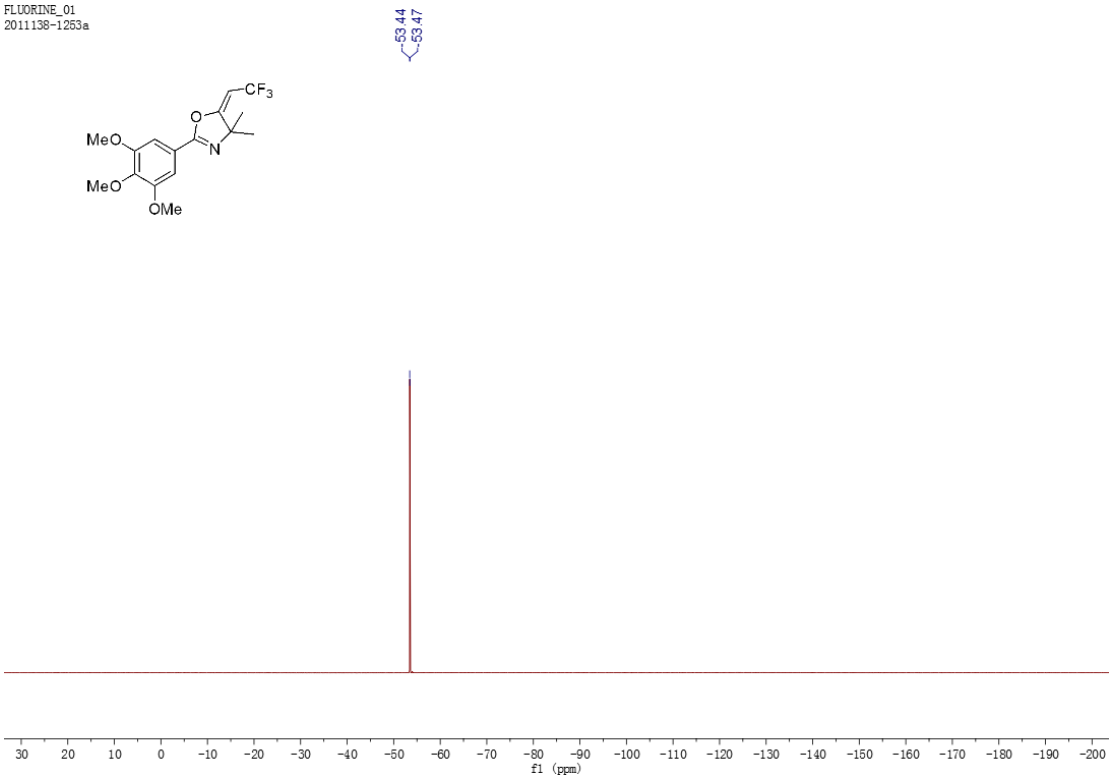

H:
170.67
170.60
170.54
170.48
158.61
140.42
137.41
128.58
128.36
125.71
123.74
123.06
120.41
93.17
92.79
92.41
92.04
77.48
77.16
76.84
71.60
26.98
26.95
26.91
26.88
21.37
19.74
CF3
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

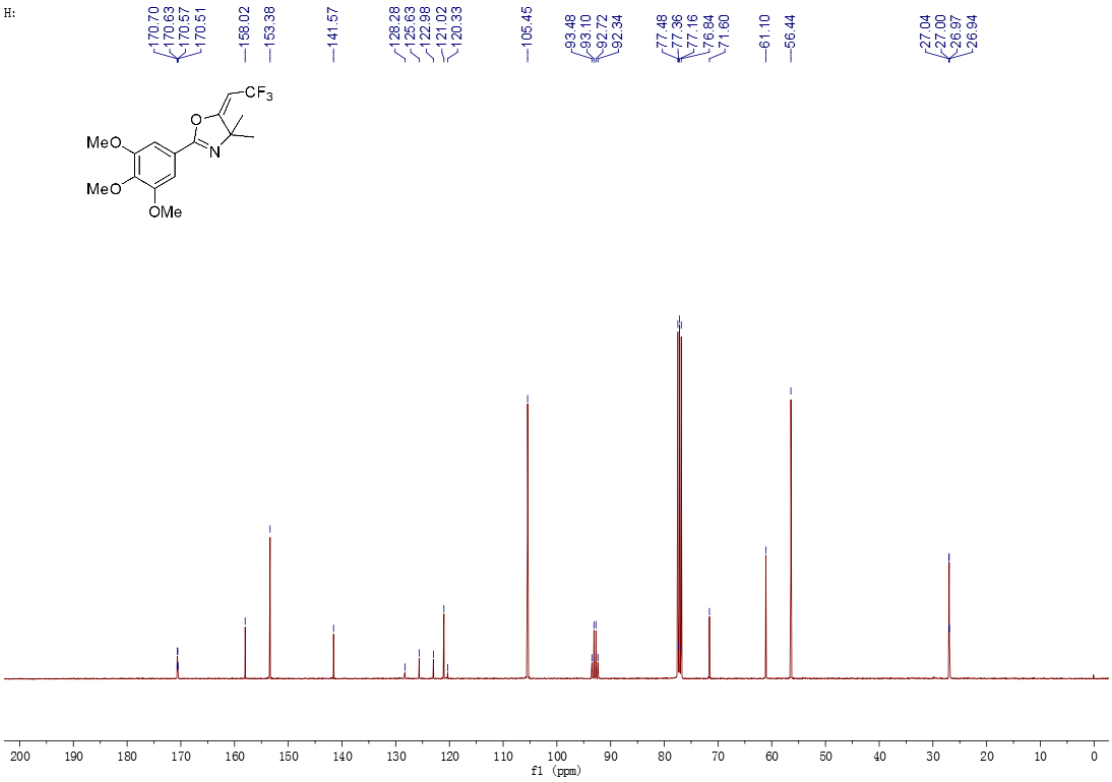

PROTON_01
2011138-1252C
7.26
6.91
4.94
4.92
4.91
4.89
2.32
2.30
1.51
F3C
O
N
2.00
1.04
6.00
3.02
6.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

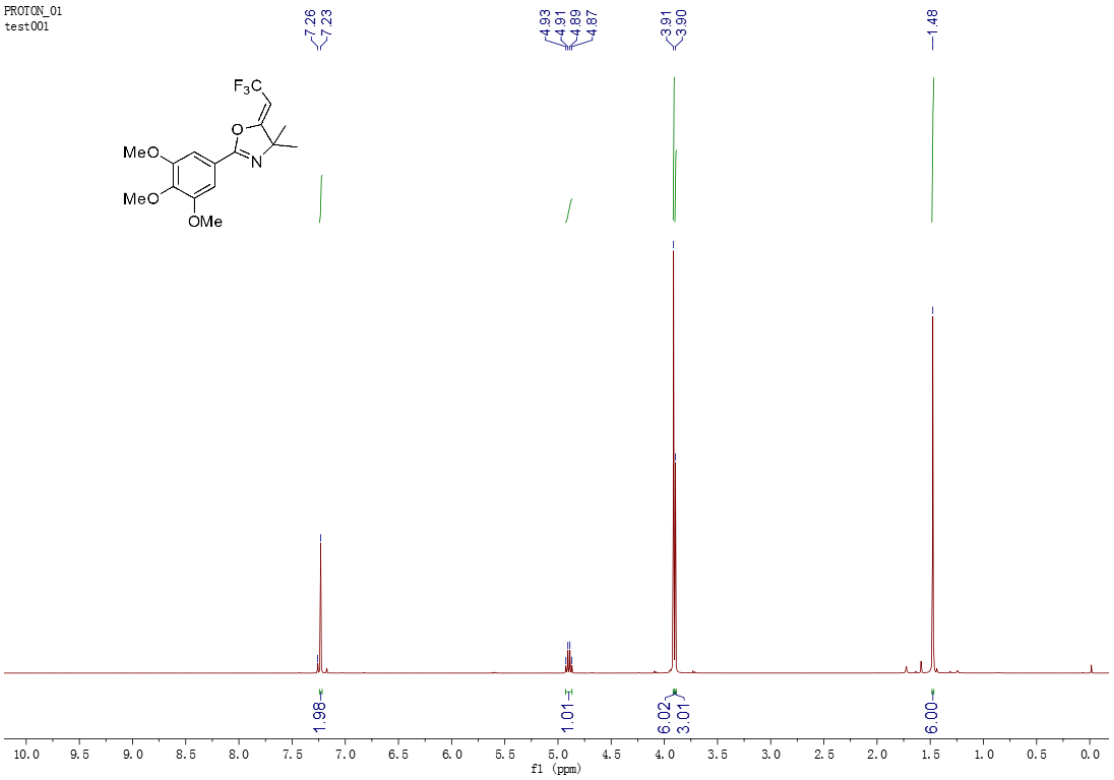

FLUORINE_01
2011138-1252C
-57.49
-57.51
F3C
O
N
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

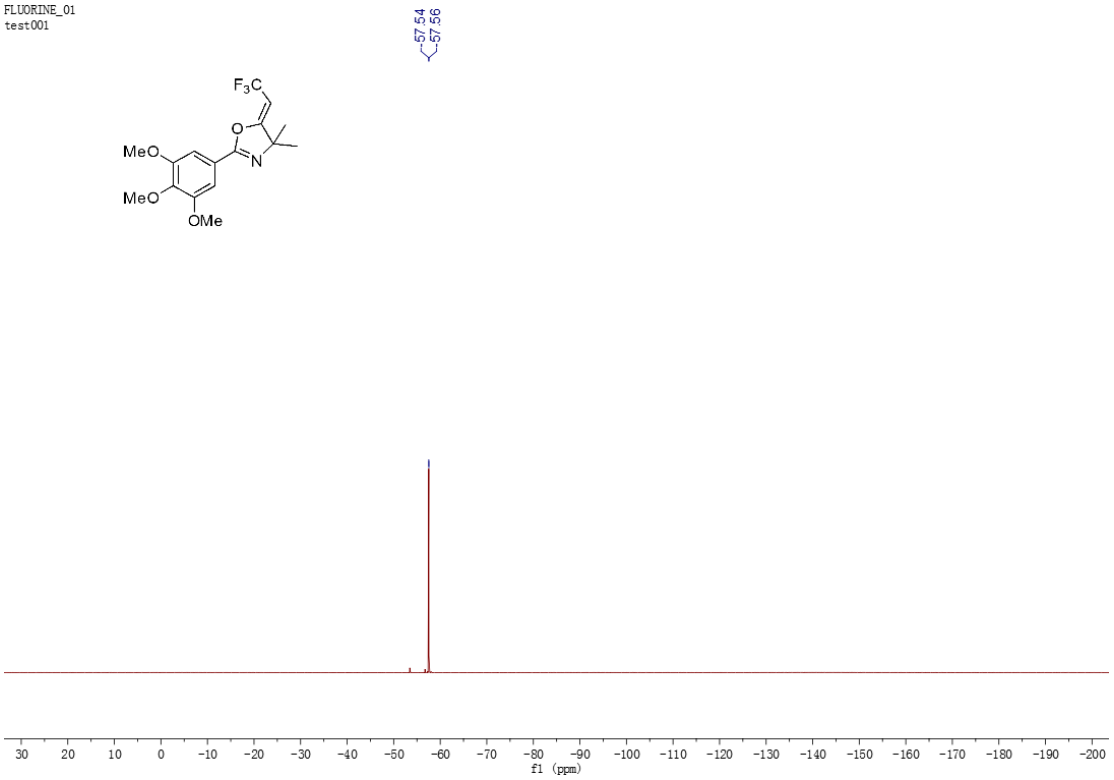

H:
169.00
159.49
140.56
137.80
128.71
127.27
124.60
123.63
121.93
119.25
89.07
88.70
88.33
87.96
77.48
77.16
76.99
76.84
71.85
29.02
21.36
19.95
F3C
O
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

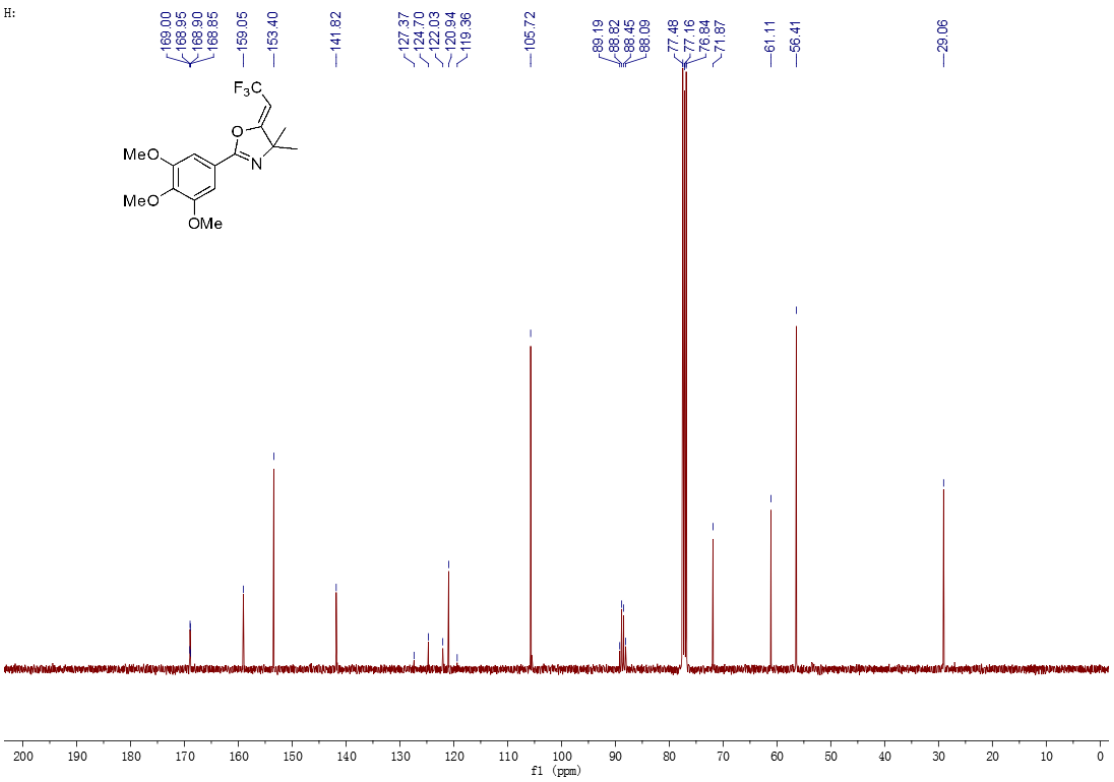

PROTON_01
2011138-1253a
7.26
7.17
5.63
5.61
5.59
5.57
3.91
3.89
1.59
CF3
O
N
MeO
MeO
OMe
2.01
1.00
6.00
3.00
6.01
f1 (ppm)

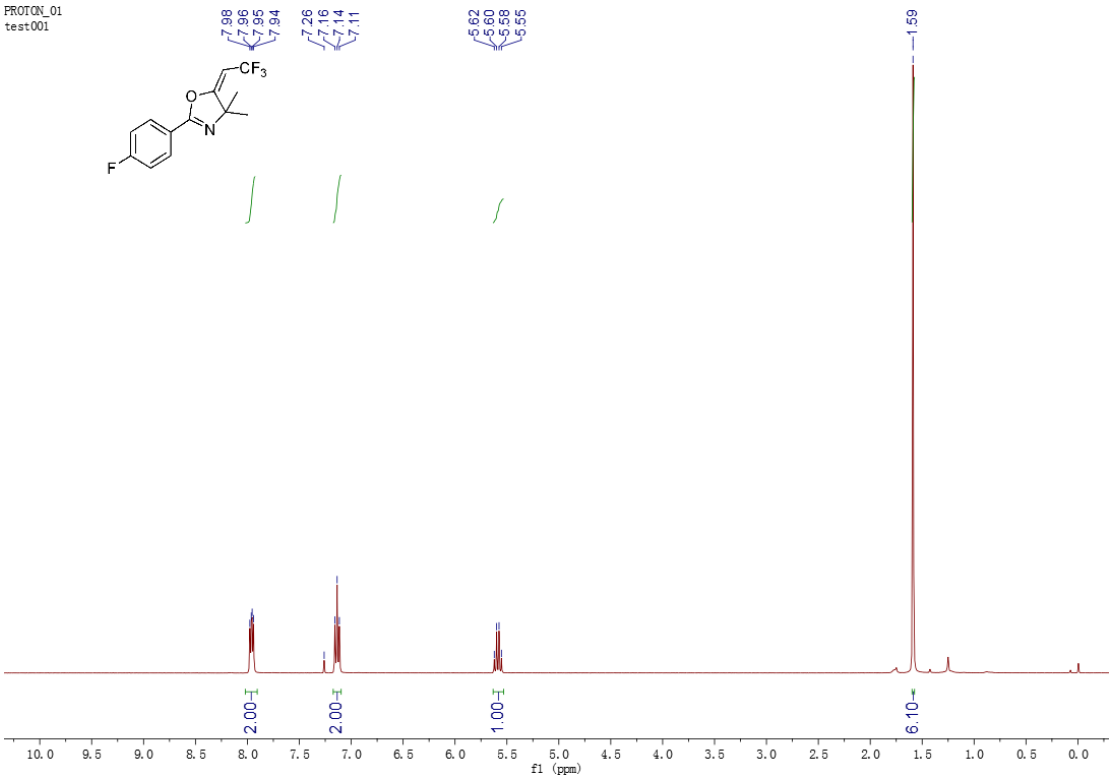

FLUORINE_01
2011138-1253a
-53.44
-53.47
CF3
O
N
MeO
MeO
OMe
f1 (ppm)

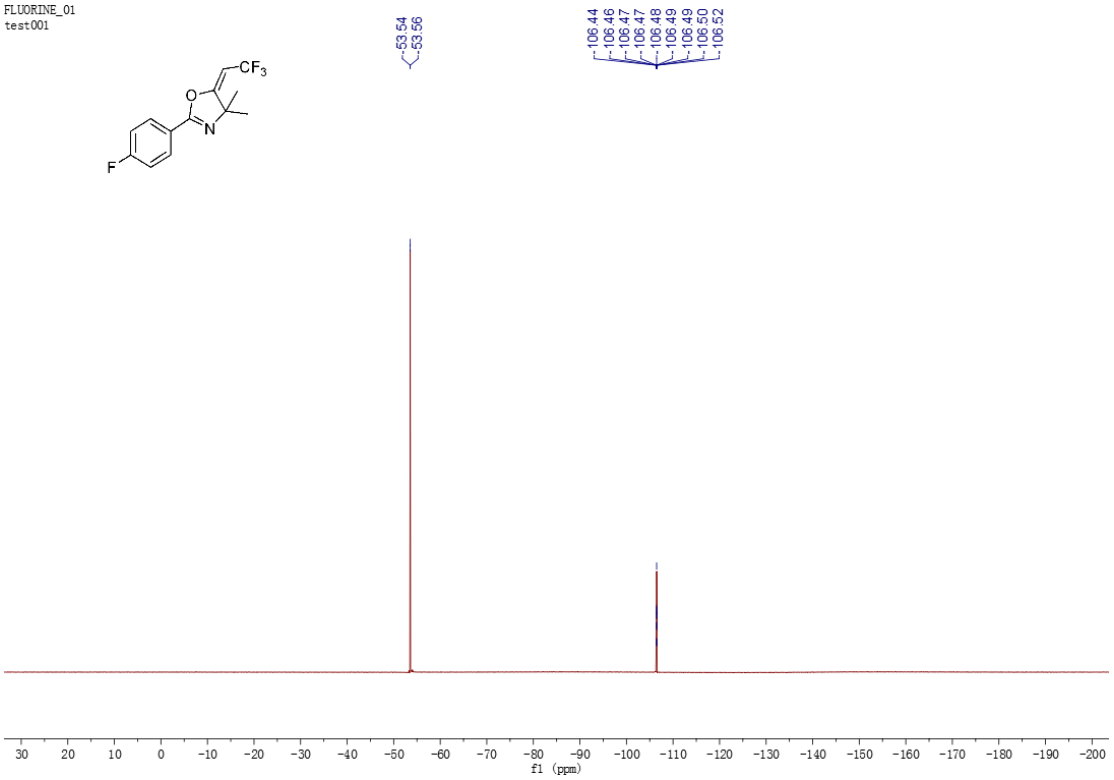

H:
170.70
170.63
170.57
170.51
158.02
153.38
141.57
128.28
125.63
122.98
121.02
120.33
105.45
93.48
93.10
92.72
92.34
77.48
77.36
77.16
76.84
71.60
61.10
56.44
27.04
27.00
26.97
26.94
CF3
O
N
MeO
MeO
OMe
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

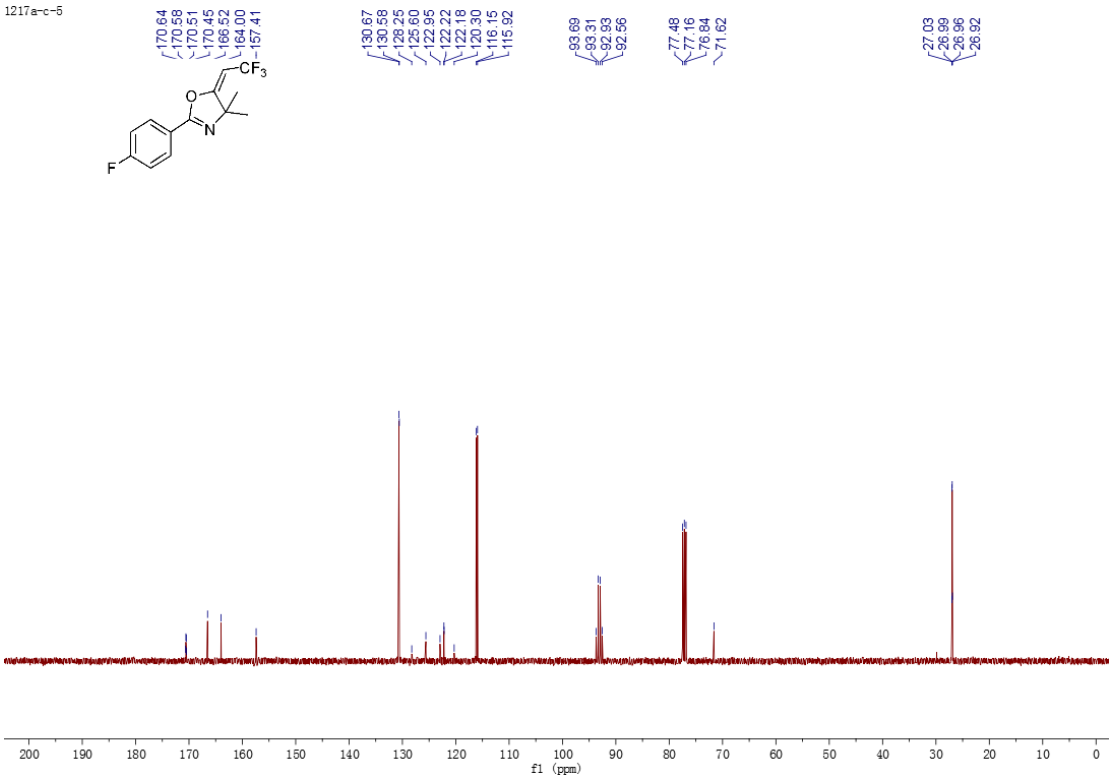

PROTON_01
test001
7.26
7.23
4.93
4.91
4.89
4.87
3.91
3.90
1.48
F3C
O
N
MeO
MeO
OMe
1.98
1.01
6.02
3.01
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

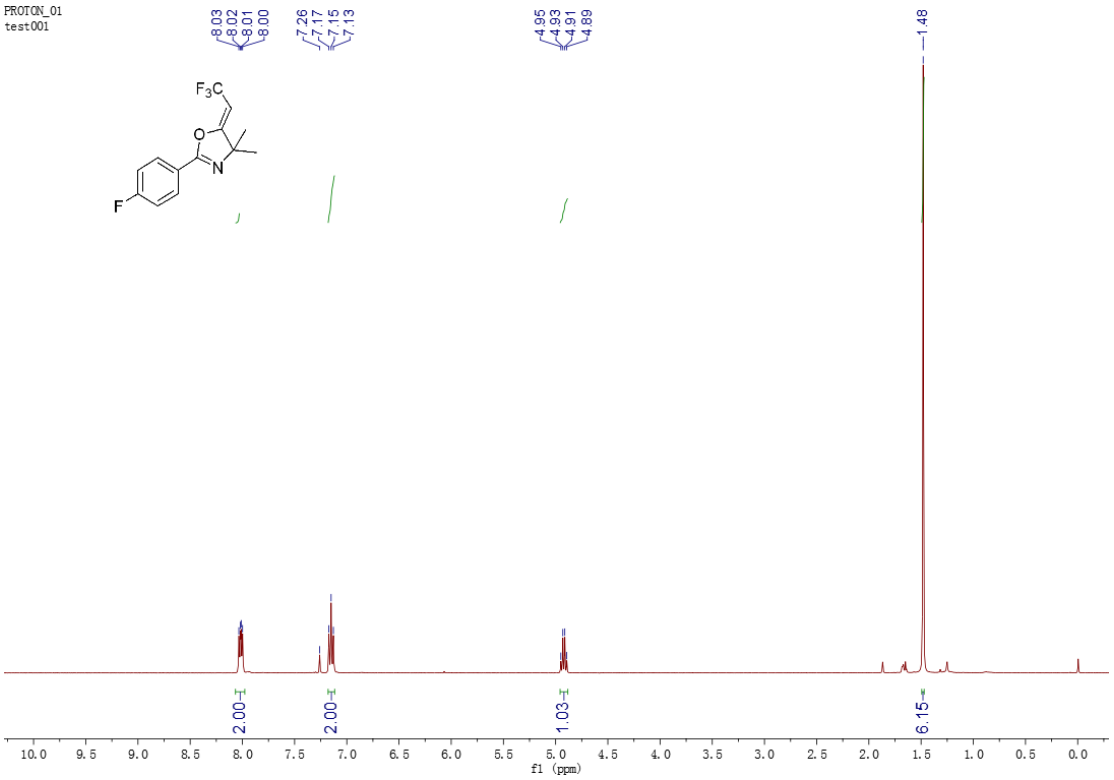

FLUORINE_01
test001
-57.54
-57.56
F3C
O
N
MeO
MeO
OMe
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

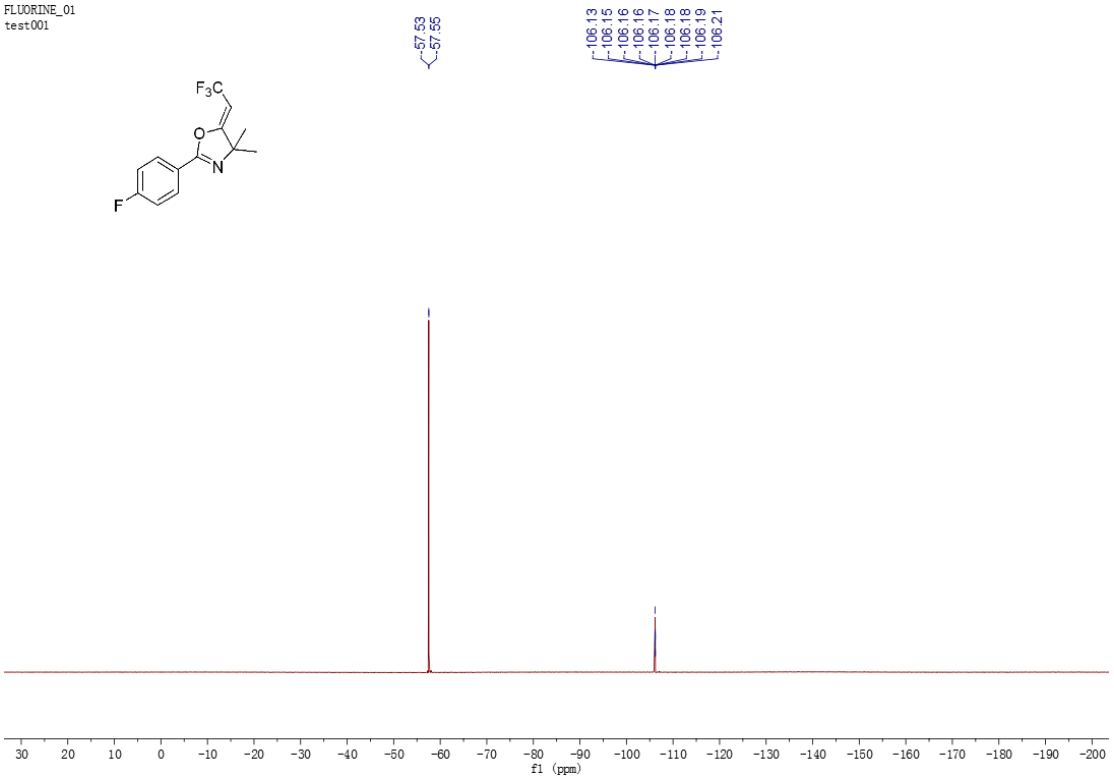

H:
169.00
168.95
168.90
168.85
159.05
153.40
141.82
127.37
124.70
122.03
120.94
119.36
105.72
89.19
88.82
88.45
88.09
77.48
77.16
76.84
71.87
61.11
56.41
29.06
F3C
O
N
MeO
MeO
OMe
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

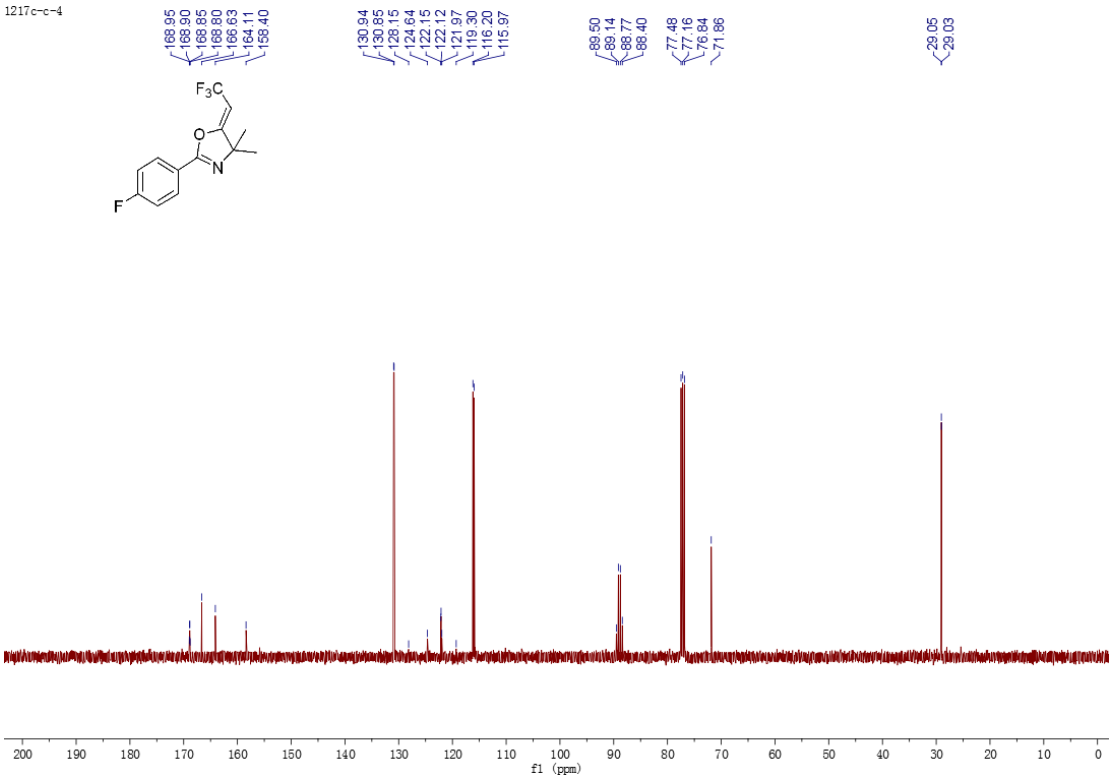

PROTON_01
test001
7.98
7.96
7.95
7.94
7.26
7.16
7.14
7.11
5.62
5.60
5.58
5.55
1.59
CF3
O
N
F
2.00
2.00
1.00
6.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

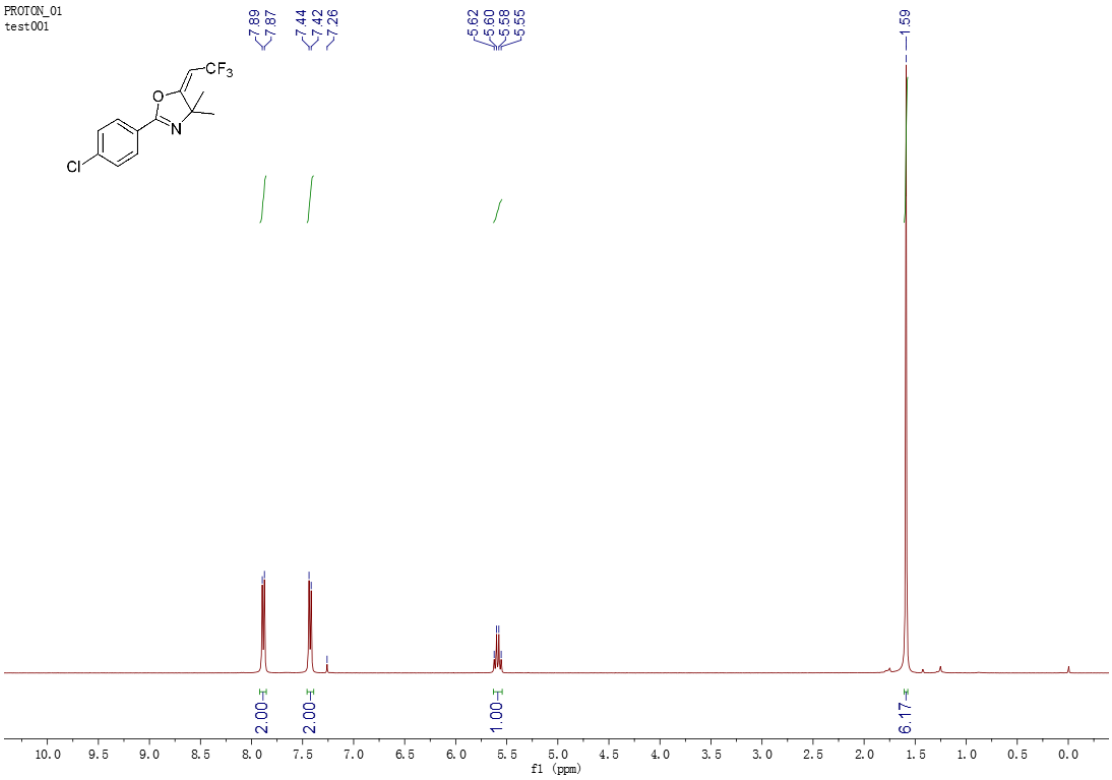

FLUORINE_01
test001
-53.54
-53.56
-106.44
-106.46
-106.47
-106.47
-106.48
-106.49
-106.49
-106.50
-106.52
CF3
O
N
F
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

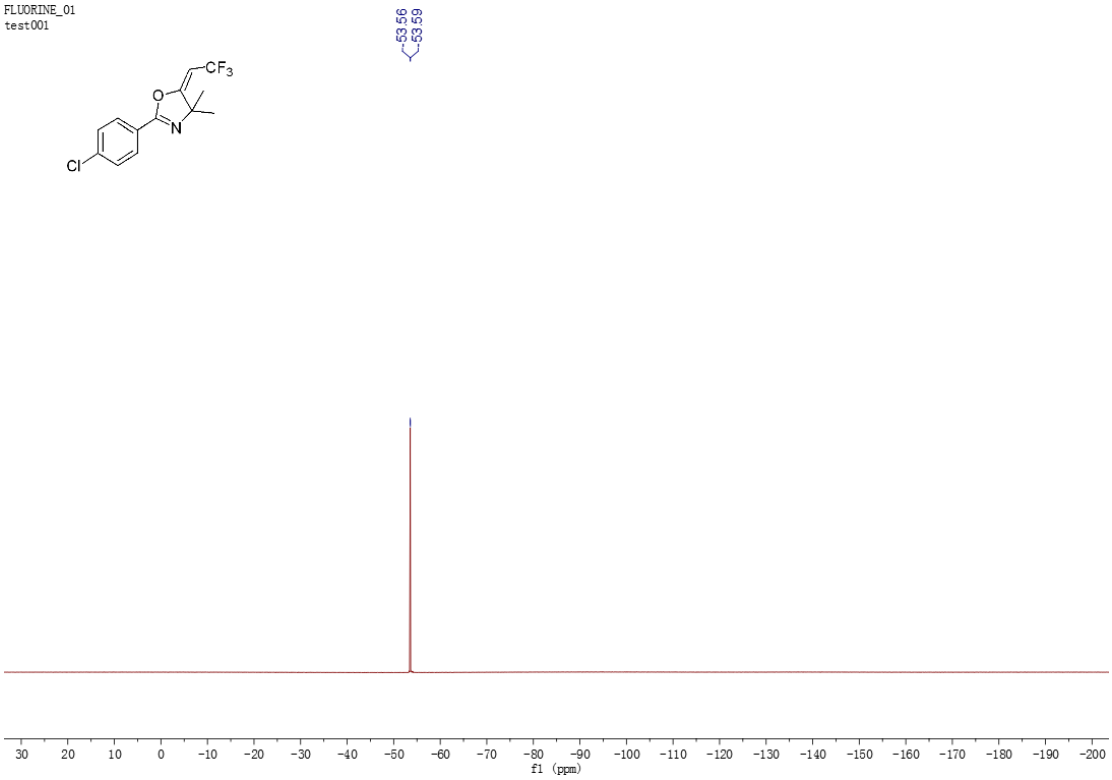

1217a-c-5
170.64
170.58
170.51
170.45
166.52
164.00
157.41
130.67
130.58
128.25
125.60
122.95
122.22
122.18
120.30
116.15
115.92
93.69
93.31
92.93
92.56
77.48
77.16
76.84
71.62
27.03
26.99
26.96
26.92
CF3
O
N
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

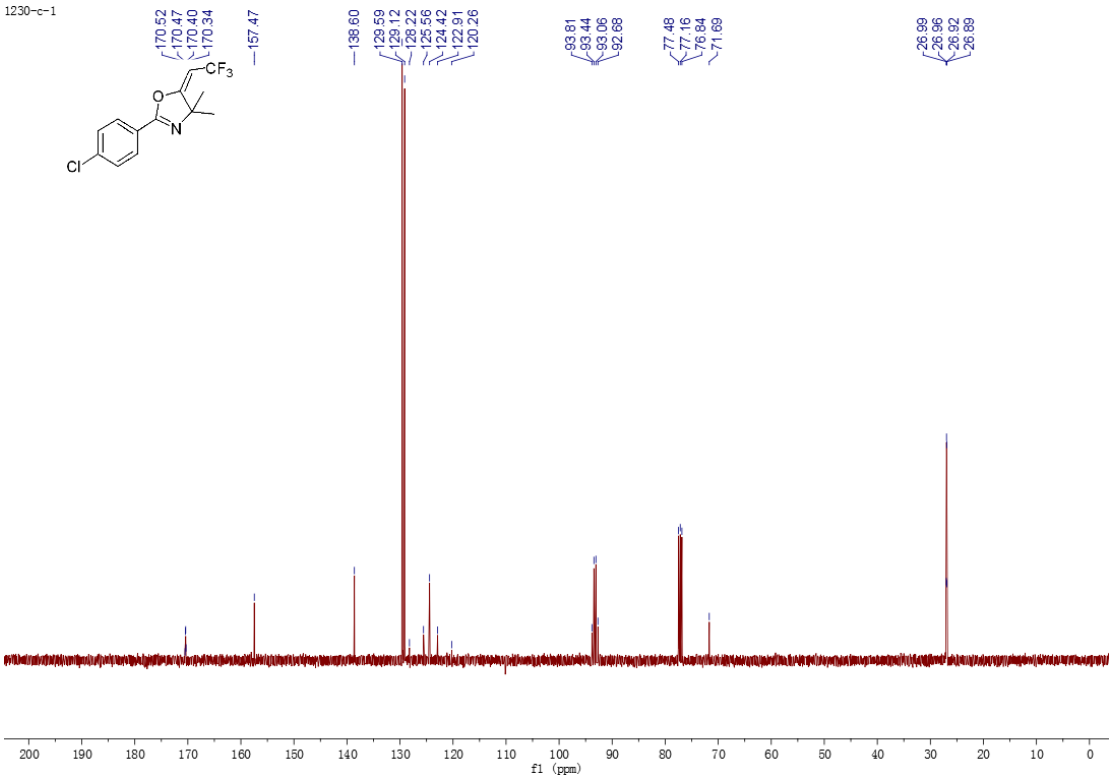

PROTON_01
test001
8.03
8.02
8.01
8.00
7.26
7.17
7.15
7.13
4.95
4.93
4.91
4.89
1.48
F3C
O
N
F
2.00
2.00
1.03
6.15
f1 (ppm)

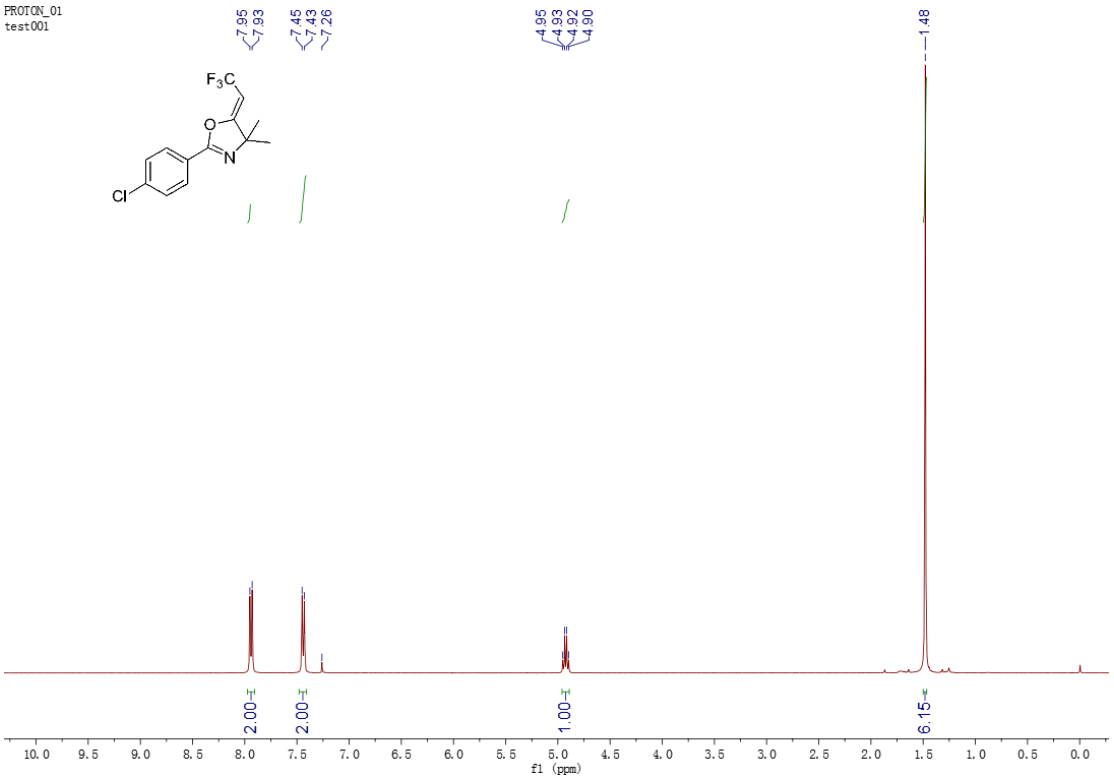

FLUORINE_01
test001
-57.53
-57.55
-106.13
-106.15
-106.16
-106.16
-106.17
-106.18
-106.18
-106.19
-106.21
F3C
O
N
F
f1 (ppm)

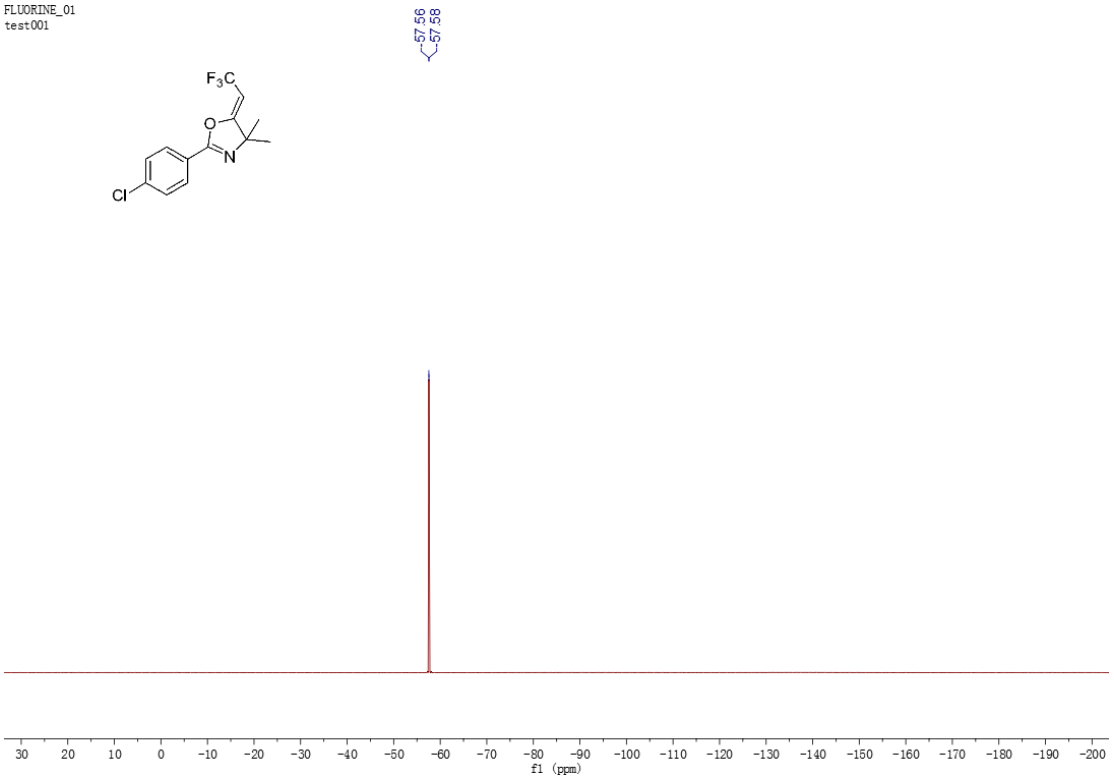

1217c-c-4
168.95
168.90
168.85
168.80
166.63
164.11
158.40
130.94
130.85
128.15
124.64
122.15
122.12
121.97
119.30
116.20
115.97
89.50
89.14
88.77
88.40
77.48
77.16
76.84
71.86
29.05
29.03
F3C
O
N
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

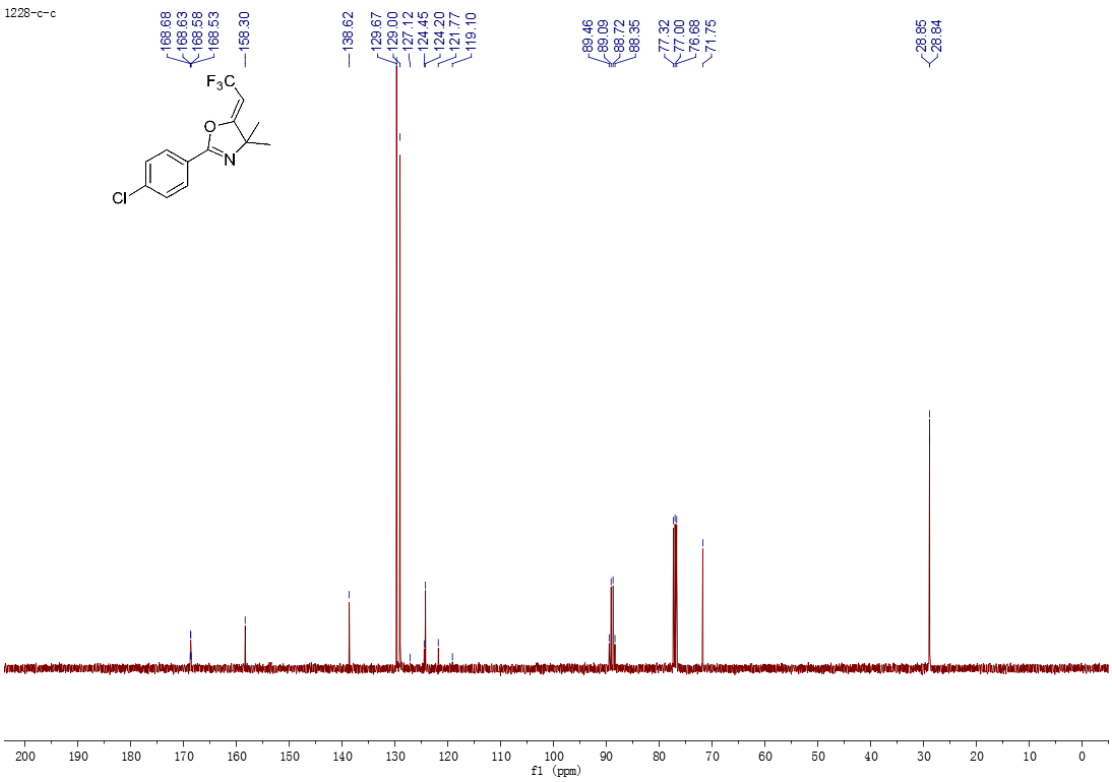

PROTON_01
test001
7.89
7.87
7.44
7.42
7.26
5.62
5.60
5.58
5.55
1.59
CF3
O
N
Cl
2.00
2.00
1.00
6.17
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

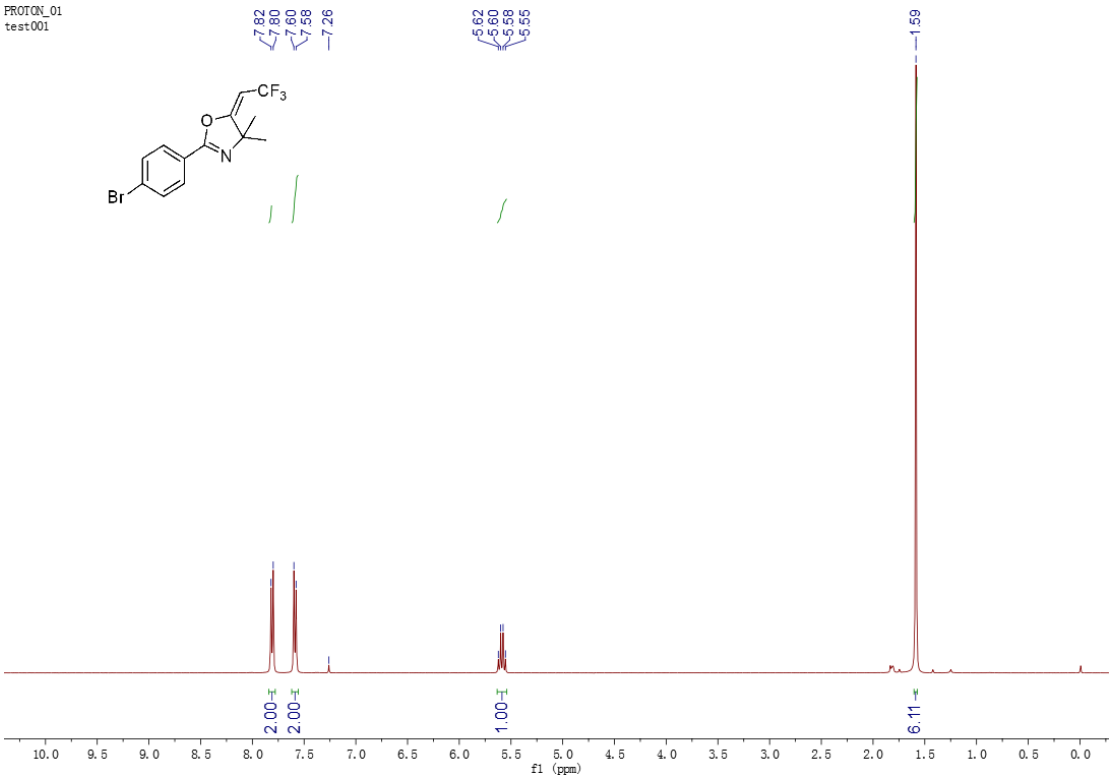

FLUORINE_01
test001
-53.56
-53.59
CF3
O
N
Cl
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

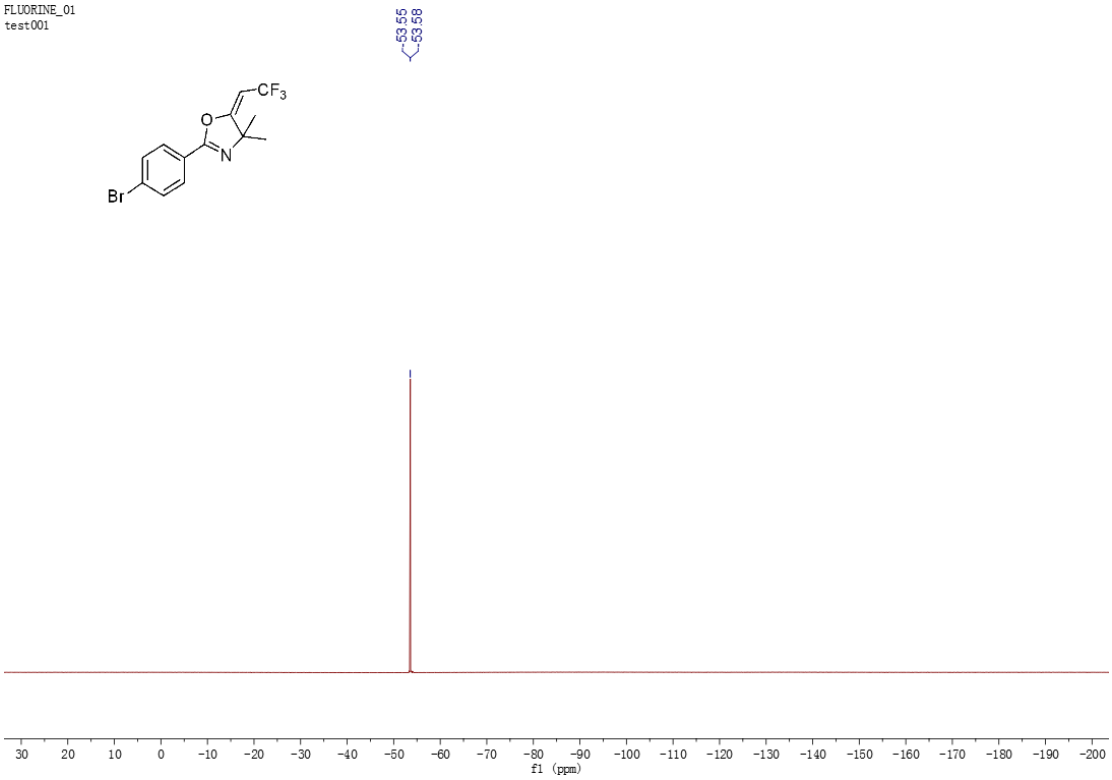

1230-c-1
170.52
170.47
170.40
170.34
157.47
138.60
129.59
129.12
128.22
125.56
124.42
122.91
120.26
93.81
93.44
93.06
92.68
77.48
77.16
76.84
71.69
26.99
26.96
26.92
26.89
CF3
O
N
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

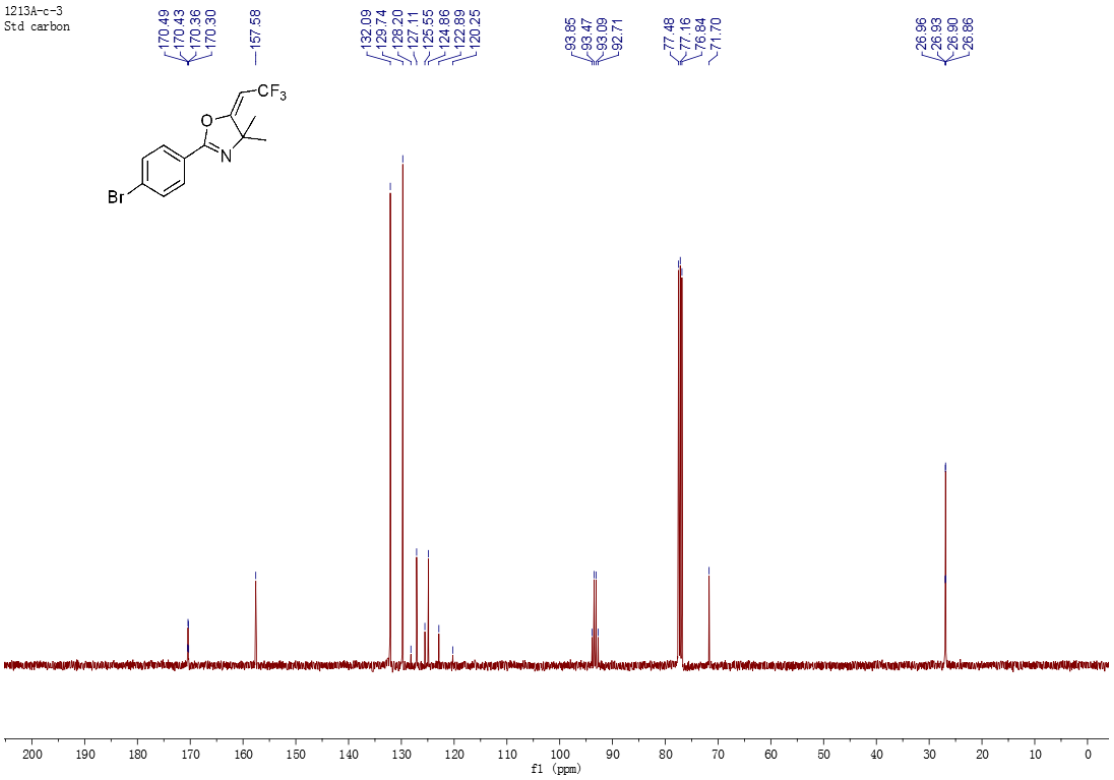

PROTON_01
test001
7.95
7.93
7.45
7.43
7.26
4.95
4.93
4.92
4.90
1.48
F3C
O
N
Cl
2.00
2.00
1.00
6.15
f1 (ppm)

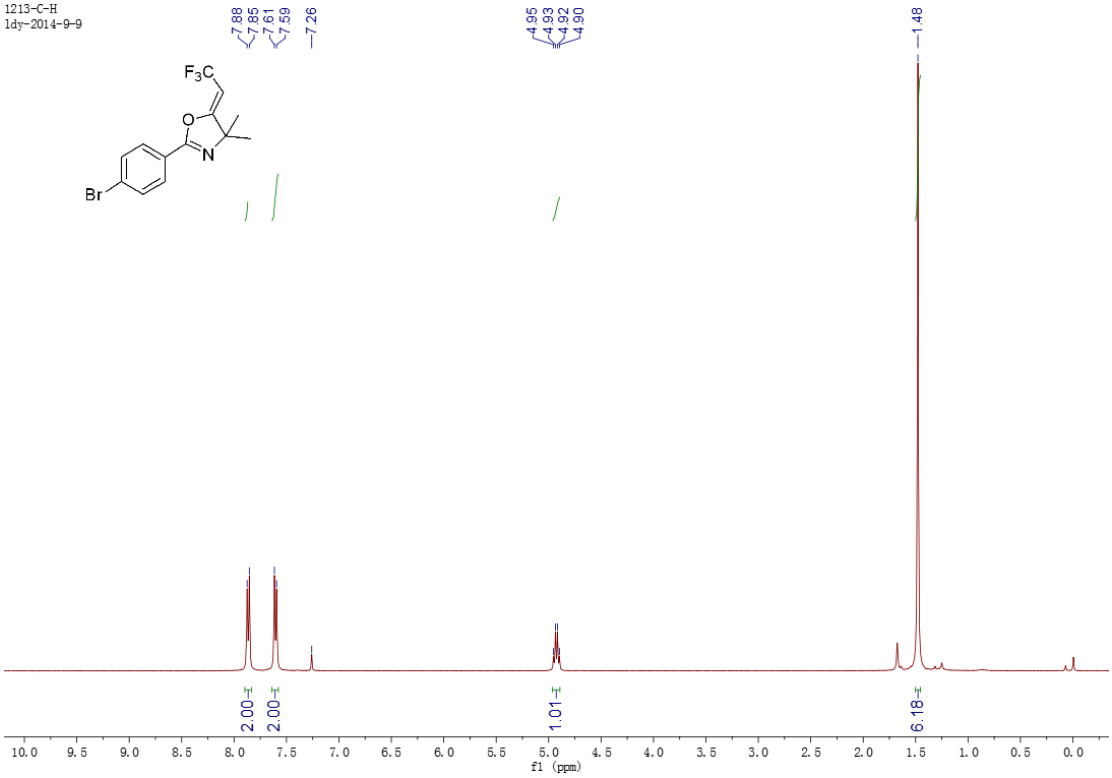

FLUORINE_01
test001
-57.56
-57.58
F3C
O
N
Cl
f1 (ppm)

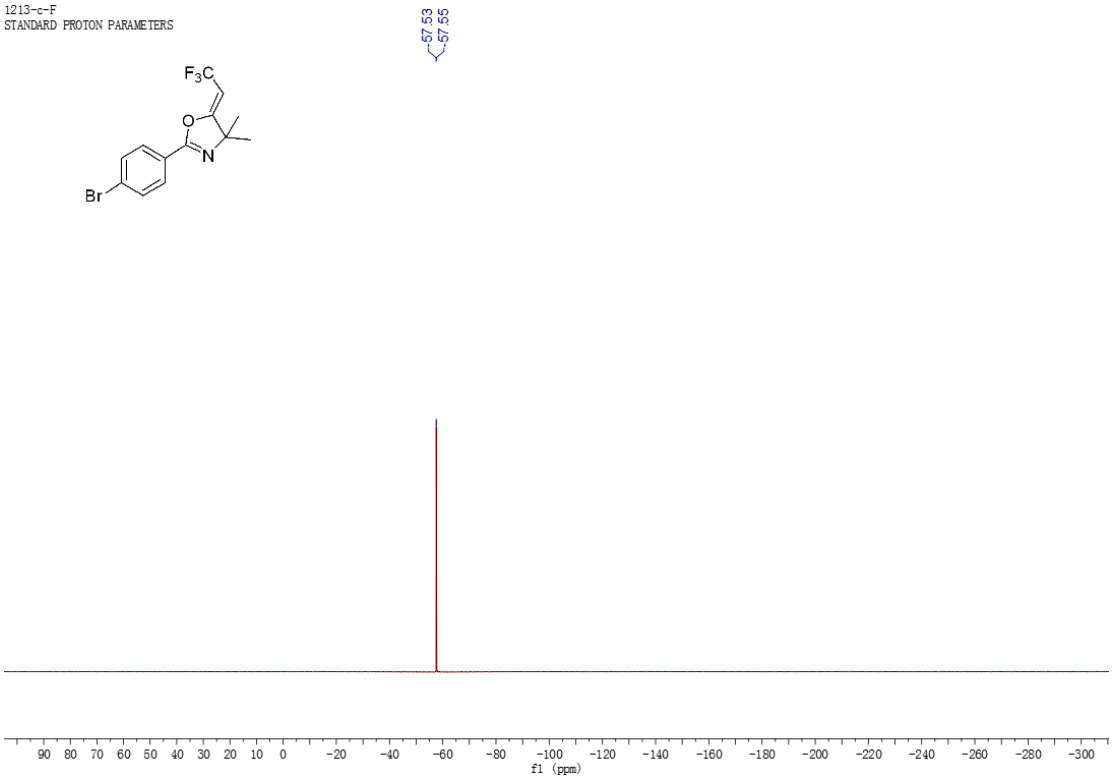

1228-c-c
168.68
168.63
168.58
168.53
158.30
138.62
129.67
129.00
127.12
124.45
124.20
121.77
119.10
89.46
88.09
87.72
86.35
77.32
77.00
76.68
71.75
28.85
28.84
F3C
O
N
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

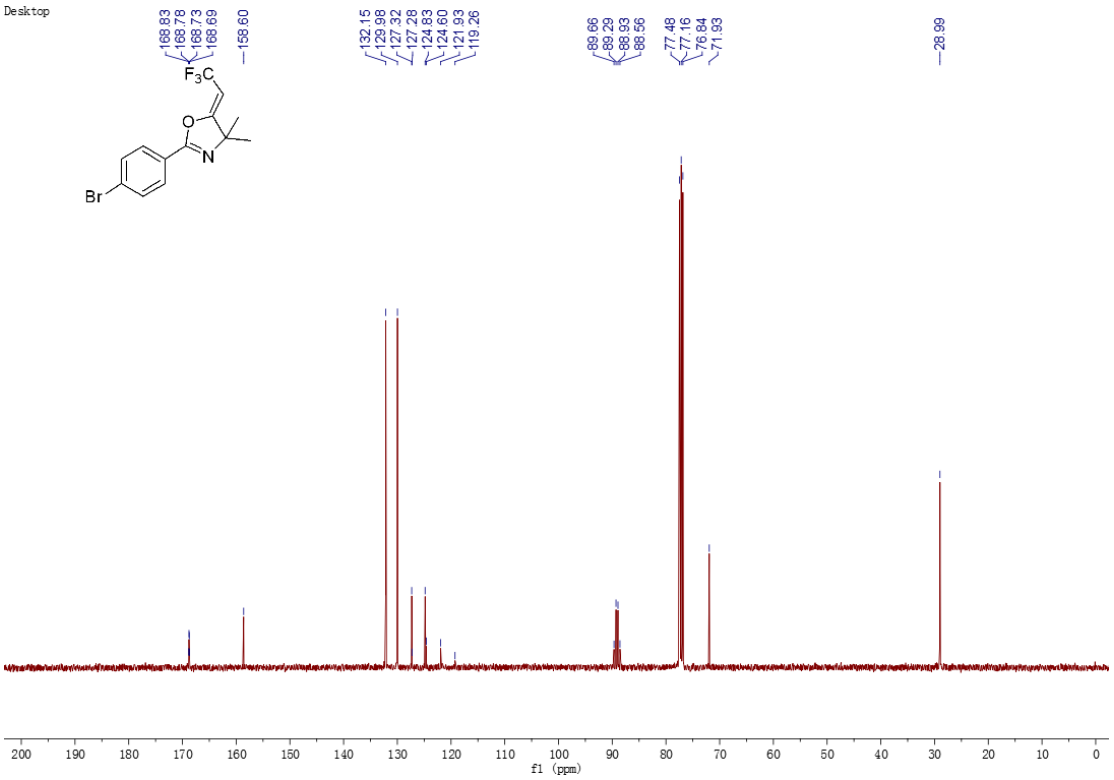

PROTON_01
test001
7.82
7.80
7.60
7.58
7.26
5.62
5.60
5.58
5.55
1.59
CF3
O
N
Br
2.00
2.00
1.00
6.11
f1 (ppm)

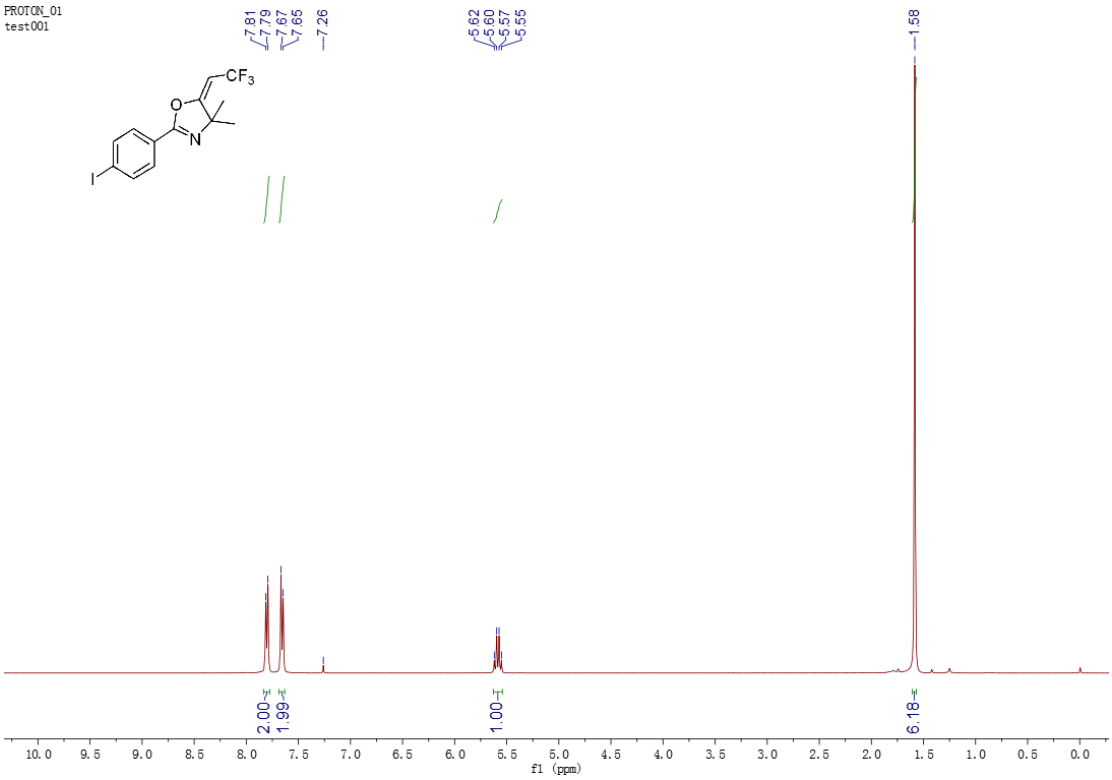

FLUORINE_01
test001
-53.55
-53.58
CF3
O
N
Br
f1 (ppm)

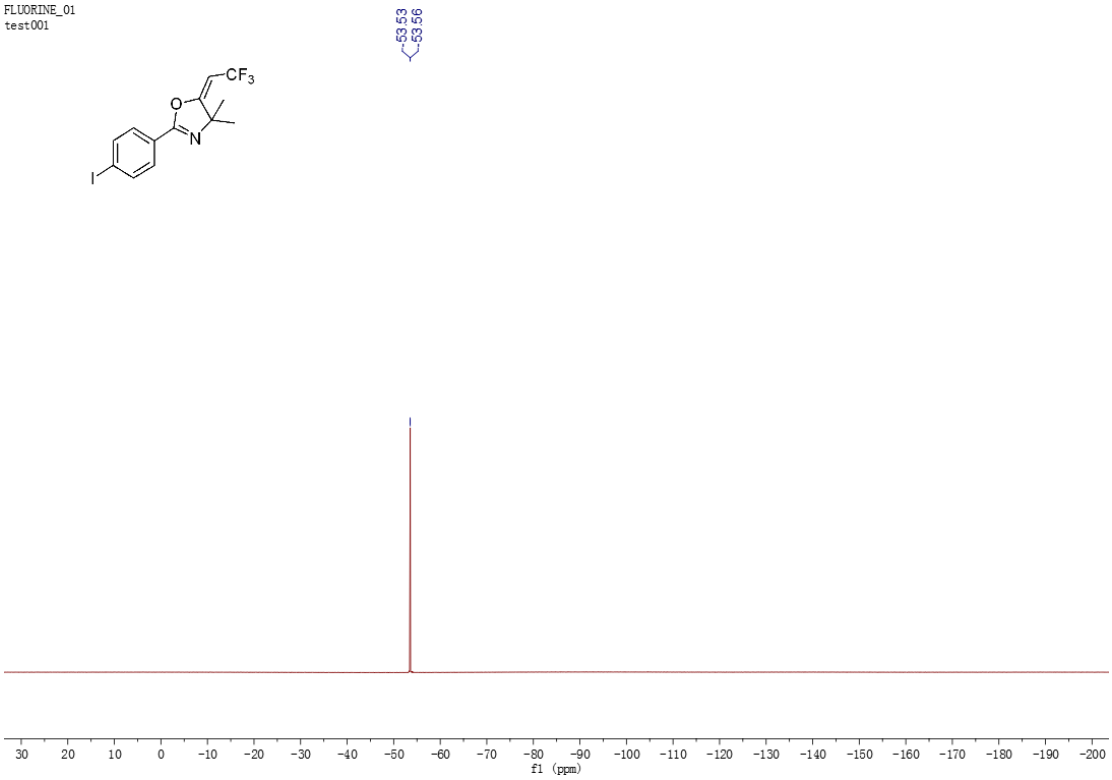

1213A-c-3
Std carbon
170.49
170.43
170.36
170.30
157.58
132.09
129.74
128.20
127.11
125.55
124.86
122.89
120.25
93.85
93.47
93.09
92.71
77.48
77.16
76.84
71.70
26.96
26.93
26.90
26.86
CF3
O
N
Br
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

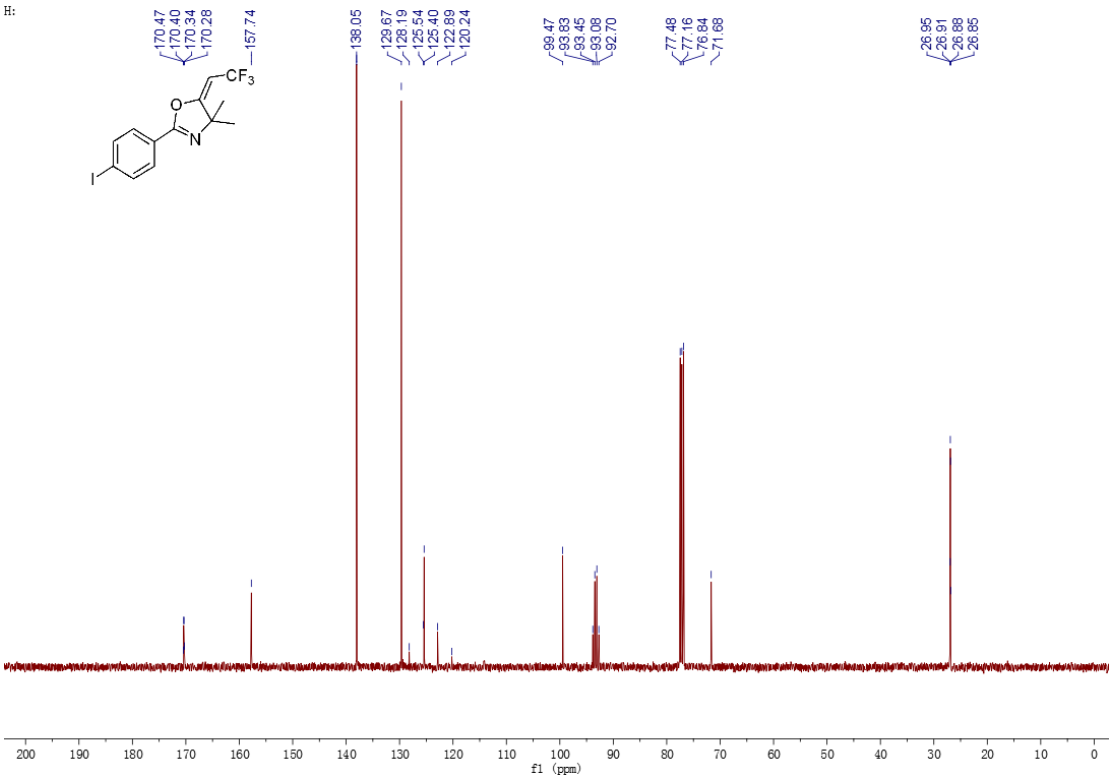

1213-C-H
1dy-2014-9-9
7.88
7.85
7.61
7.59
7.26
4.95
4.93
4.92
4.90
1.48
F3C
O
N
Br
2.00
2.00
1.01
6.18
f1 (ppm)

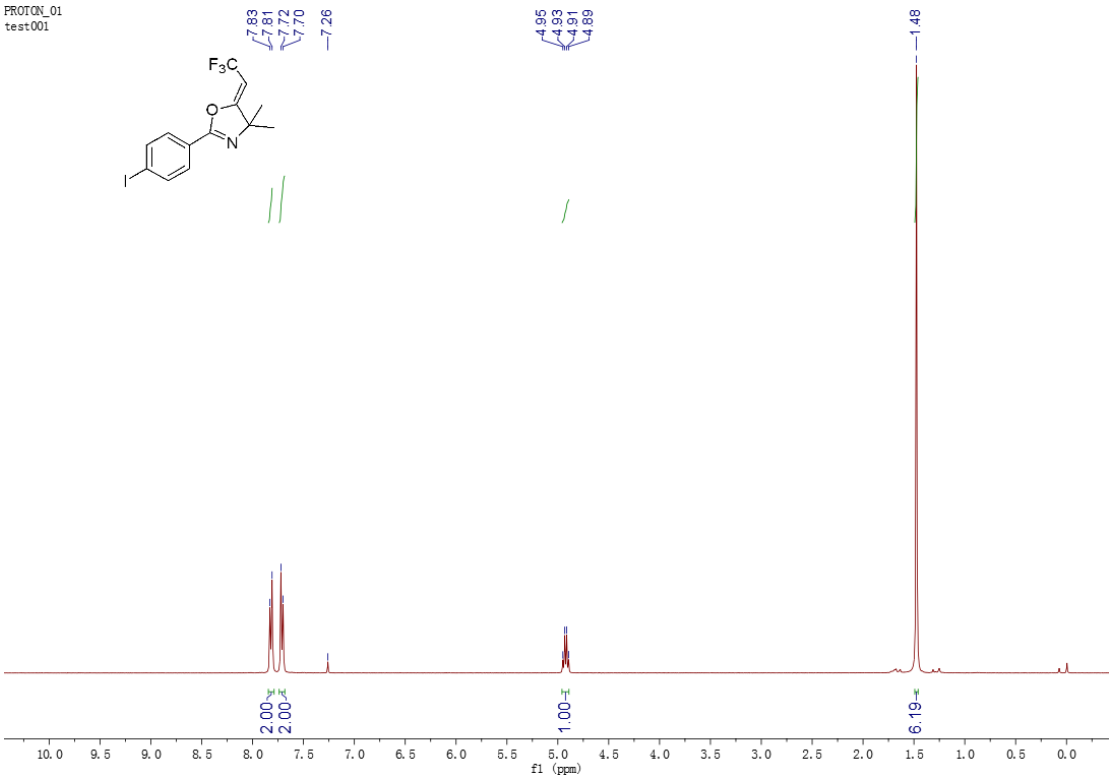

1213-c-F
STANDARD PROTON PARAMETERS
-57.53
-57.55
F3C
O
N
Br
f1 (ppm)

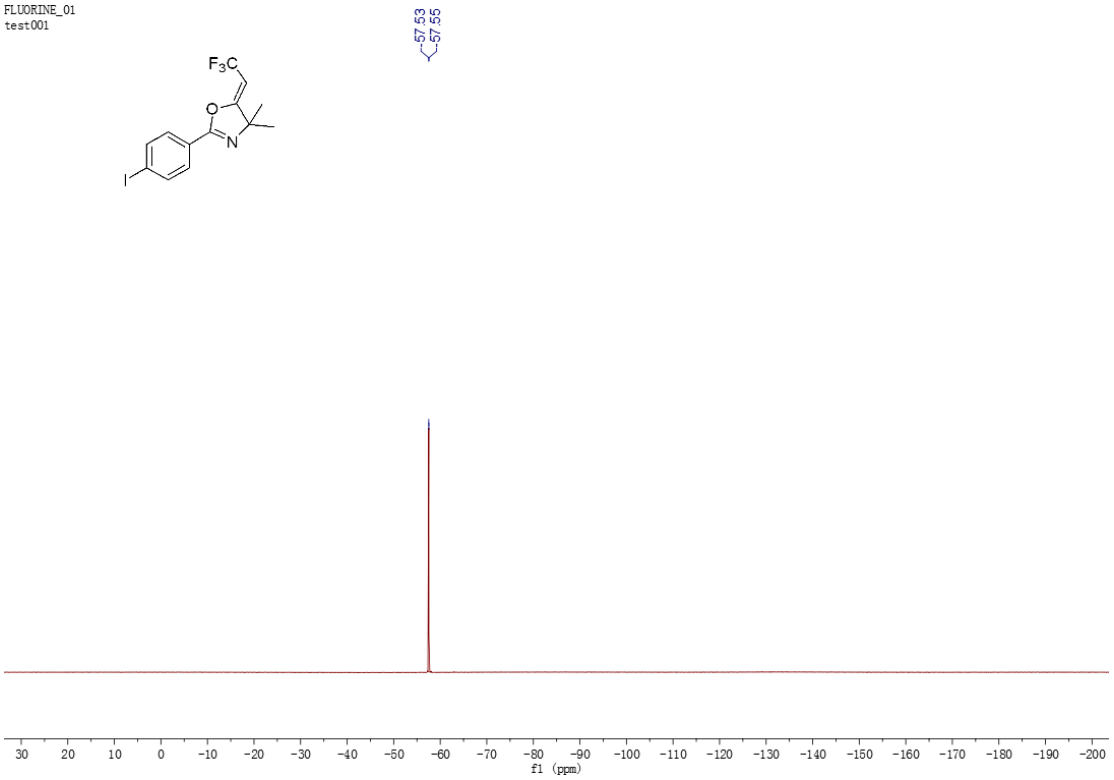

Desktop
168.83
168.78
168.73
168.69
158.60
132.15
129.98
127.32
127.28
124.83
124.60
121.93
119.26
89.66
89.29
88.93
88.56
77.48
77.16
76.84
71.93
28.99
F3C
O
N
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

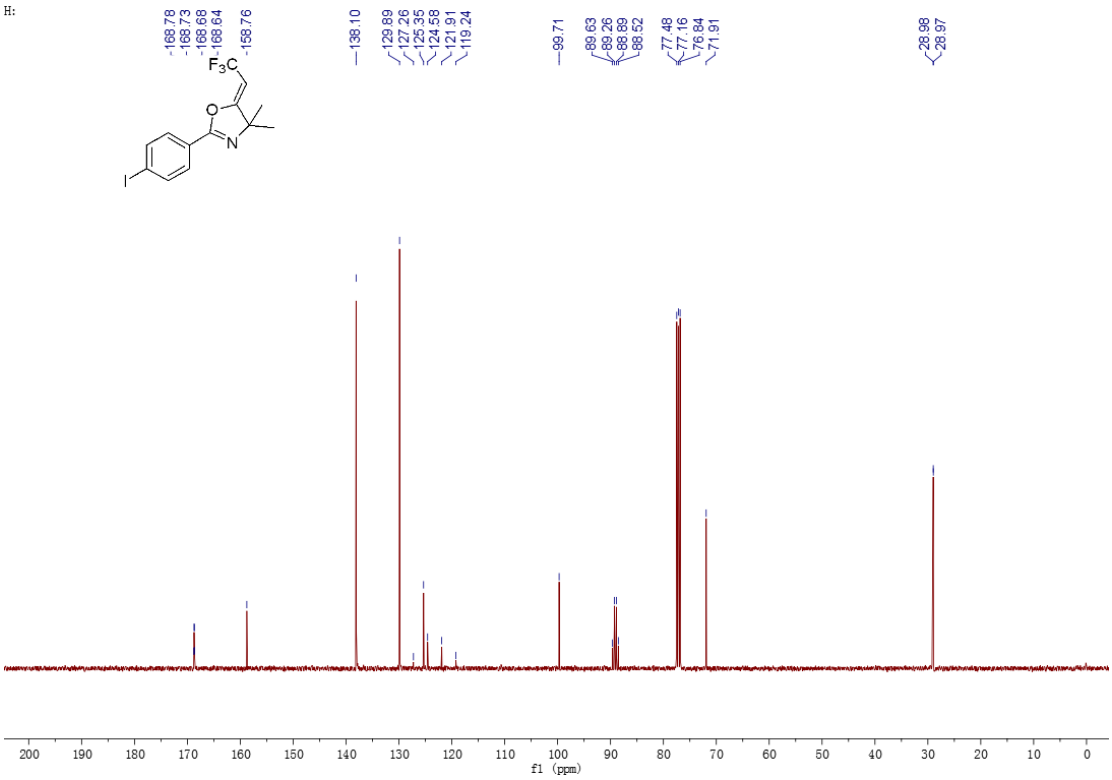

PROTON_01
test001
7.81
7.79
7.67
7.65
7.26
5.62
5.60
5.57
5.55
1.58
CF3
O
N
I
2.00
1.99
1.00
6.18
f1 (ppm)

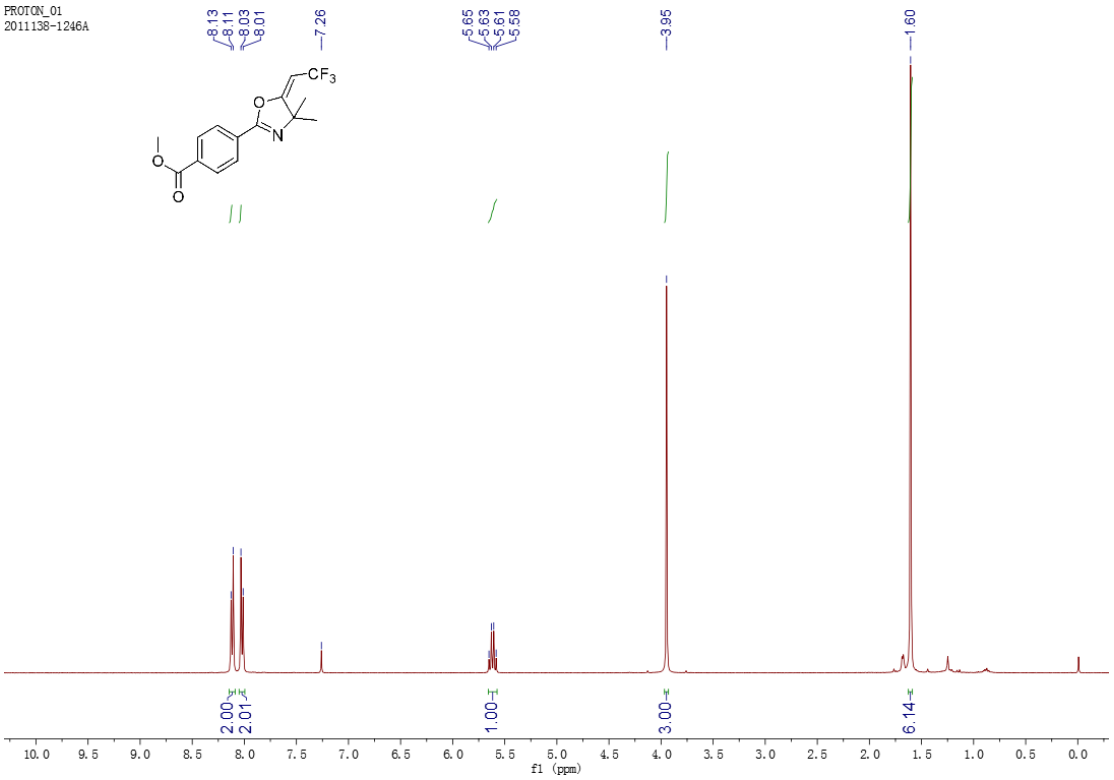

FLUORINE_01
test001
-53.53
-53.56
CF3
O
N
I
f1 (ppm)

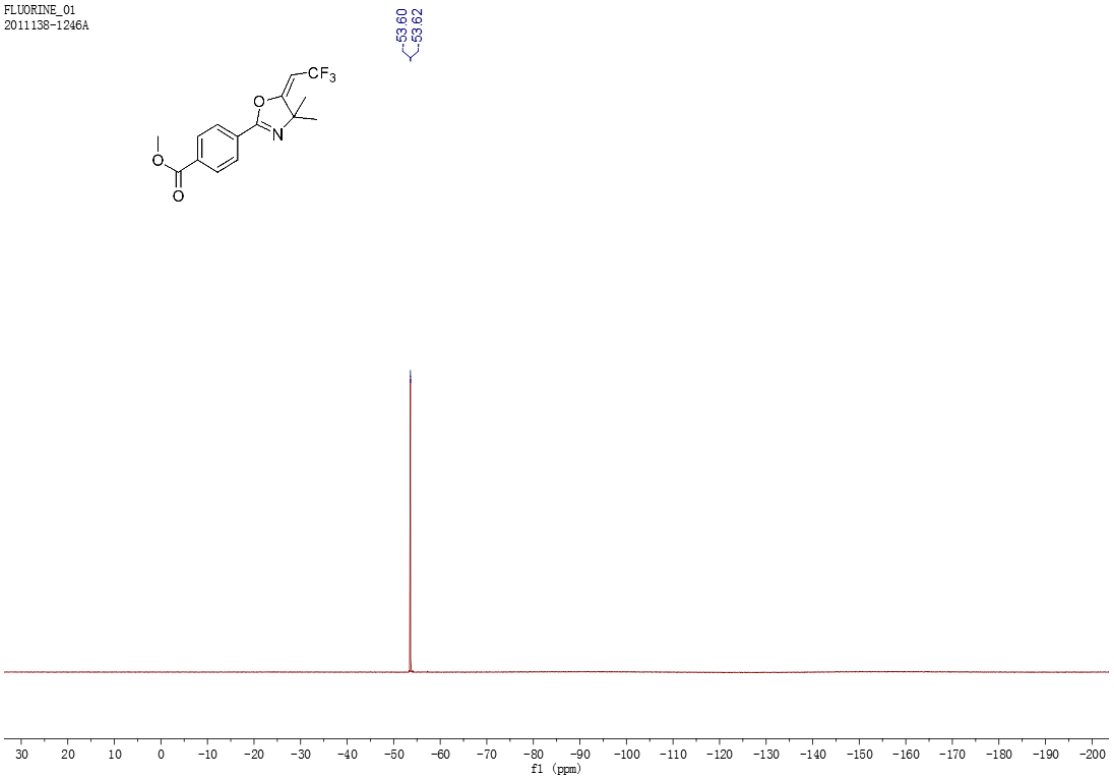

H:
170.47
170.40
170.34
170.28
157.74
138.05
129.67
128.19
125.54
125.40
122.89
120.24
99.47
93.83
93.45
93.08
92.70
77.48
77.16
76.84
71.68
26.95
26.91
26.88
26.85
CF3
O
N
I
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

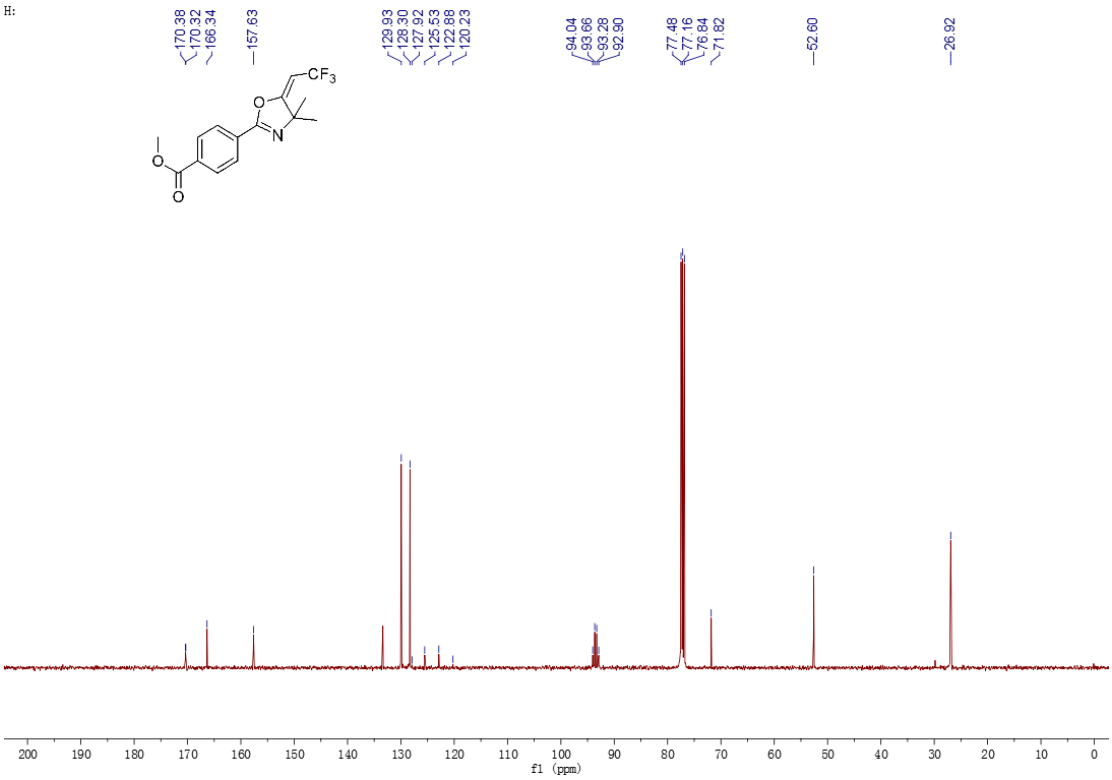

PROTON_01
test001
7.83
7.81
7.72
7.70
7.26
4.95
4.93
4.91
4.89
1.48
2.00
2.00
1.00
6.19
f1 (ppm)

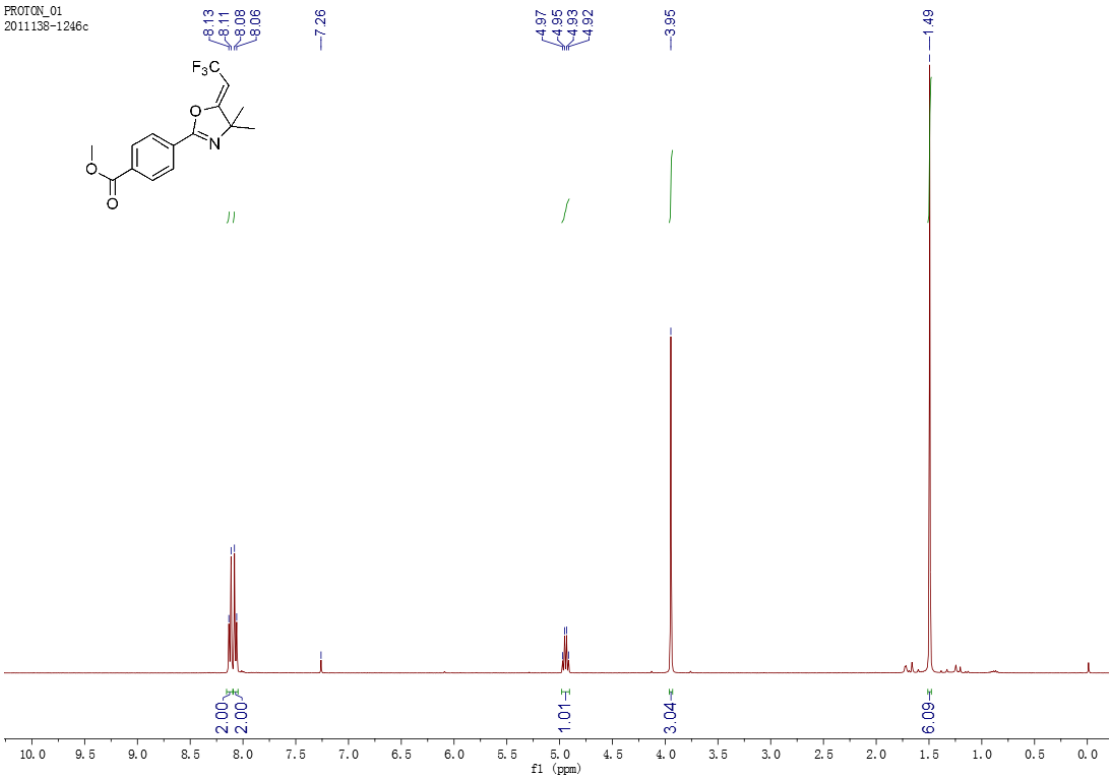

FLUORINE_01
test001
-57.53
-57.55
f1 (ppm)

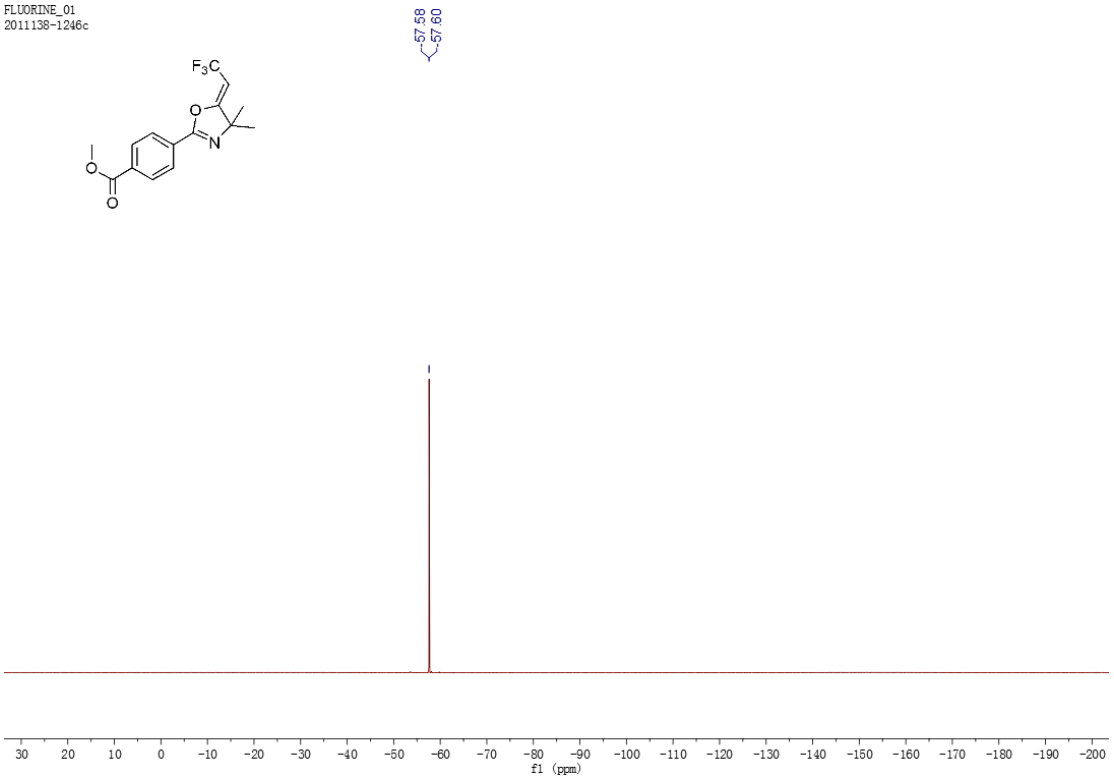

H:
168.78
168.73
168.68
168.64
158.76
138.10
129.89
127.26
125.35
124.58
121.91
119.24
99.71
89.63
89.26
88.89
88.52
77.48
77.16
76.84
71.91
28.98
28.97
F3C
O
N
I
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

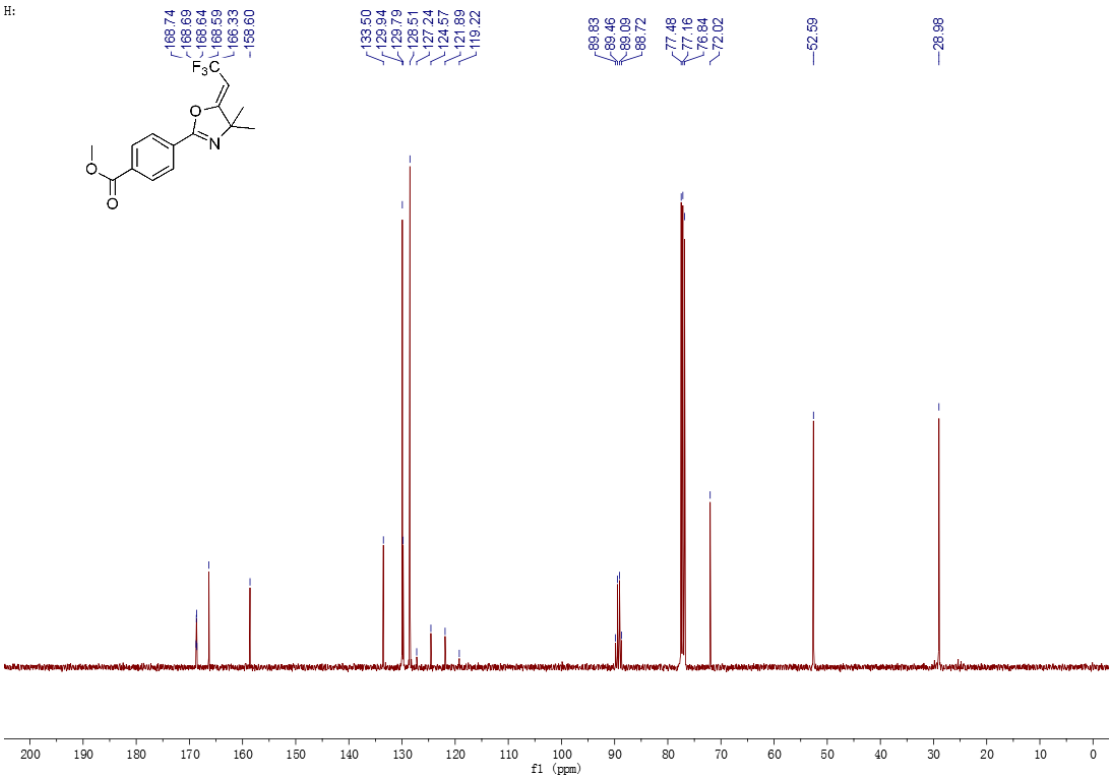

PROTON_01
2011138-1246A
8.13
8.11
8.03
8.01
7.26
5.65
5.63
5.61
5.58
3.95
1.60
CF3
O
N
O
O
2.00
2.01
1.00
3.00
6.14
f1 (ppm)

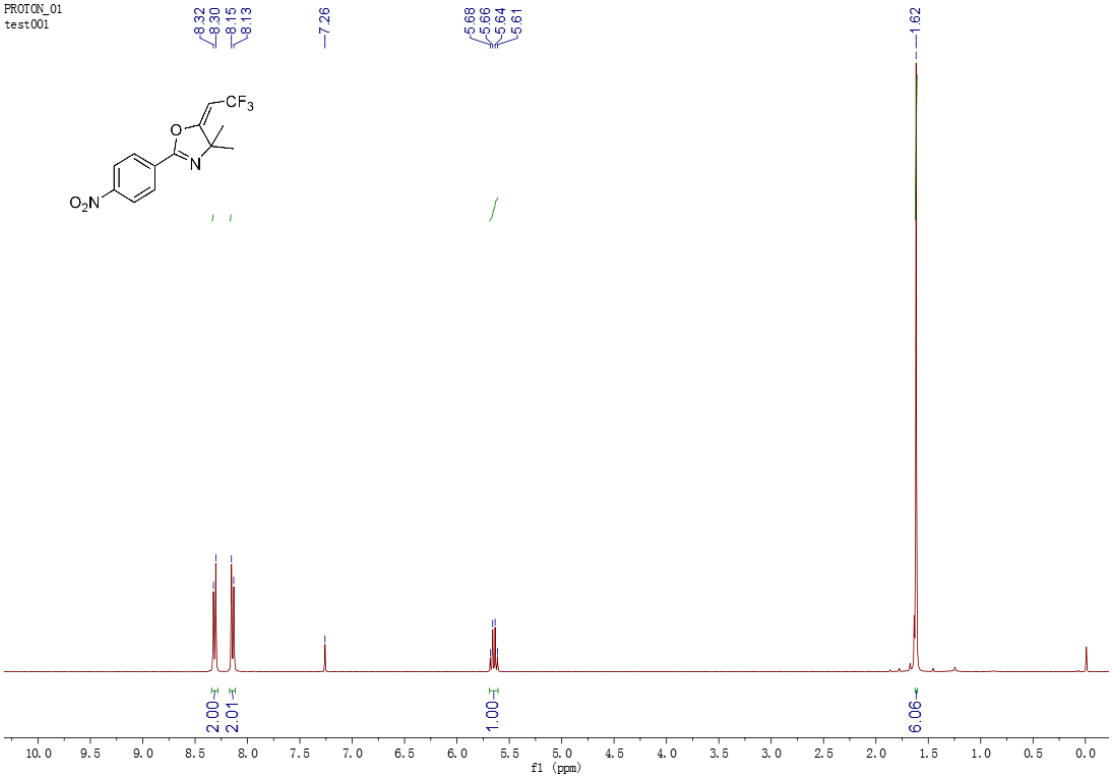

FLUORINE_01
2011138-1246A
-53.60
-53.62
CF3
O
N
O
O
f1 (ppm)

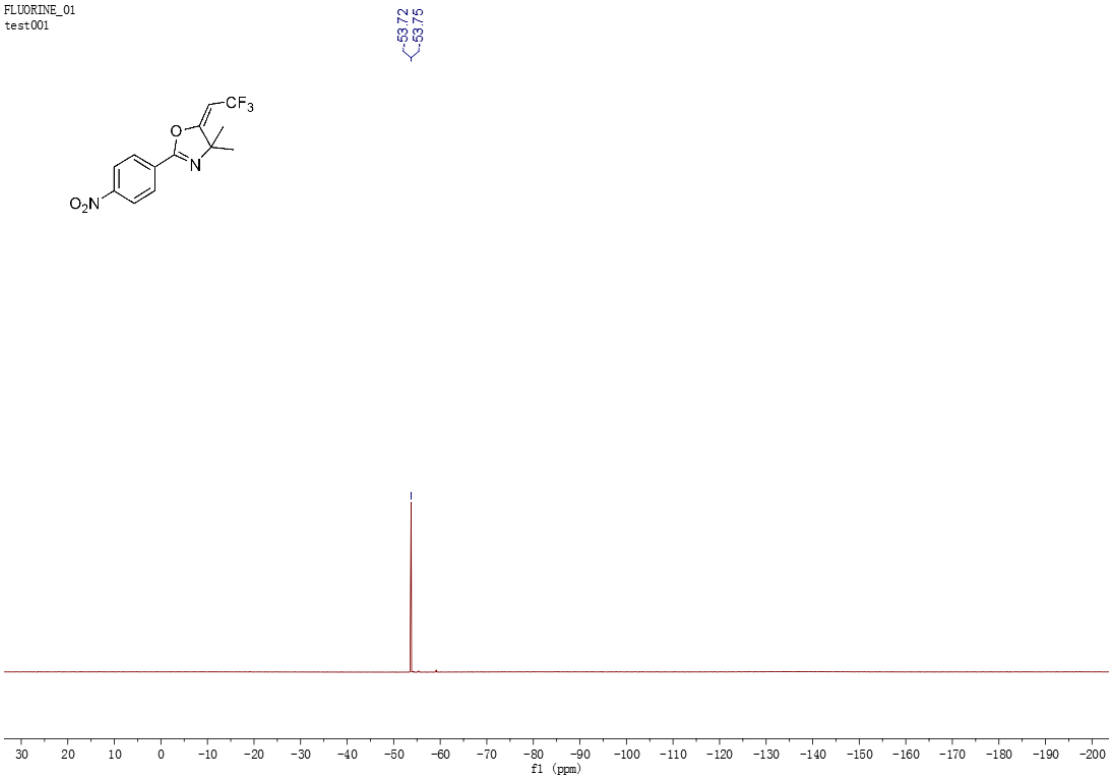

H:
170.38
170.32
166.34
157.63
129.93
128.30
127.92
125.53
122.88
120.23
94.04
93.66
93.28
92.90
77.48
77.16
76.84
71.82
52.60
26.92
CF3
O
N
O
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

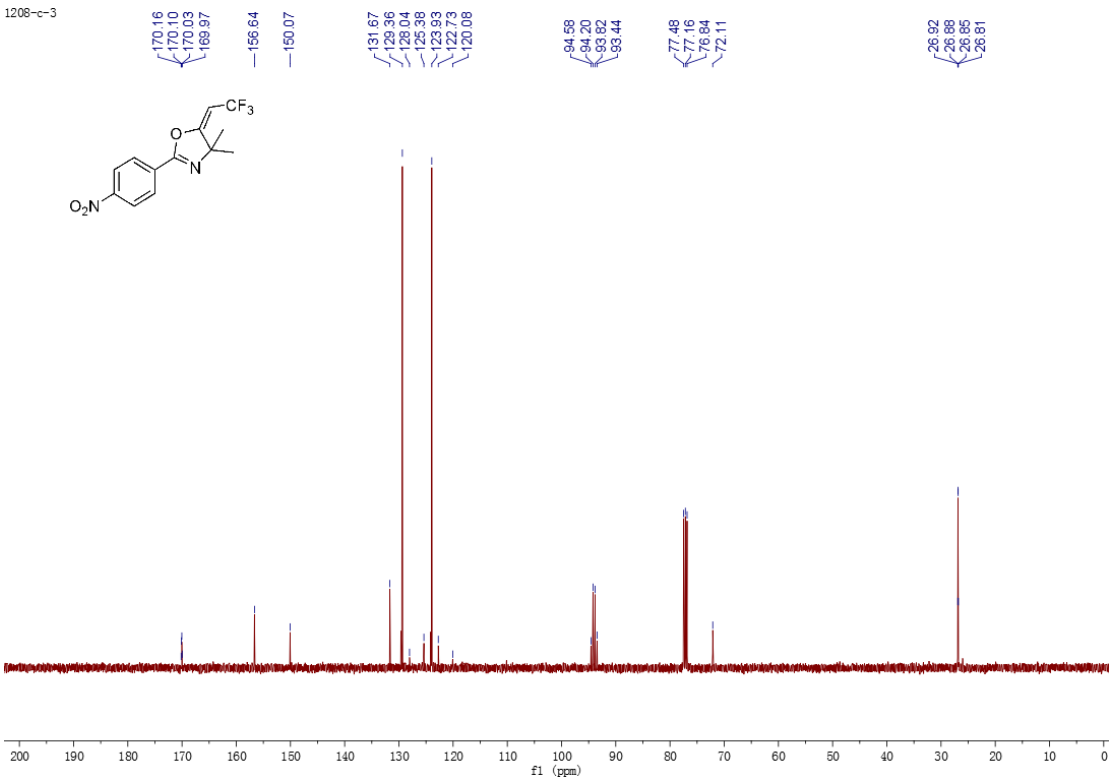

PROTON_01
2011138-1246c
8.13
8.11
8.08
8.06
7.26
4.97
4.95
4.93
4.92
3.95
1.49
F3C
O
N
O
O
2.00
2.00
1.01
3.04
6.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

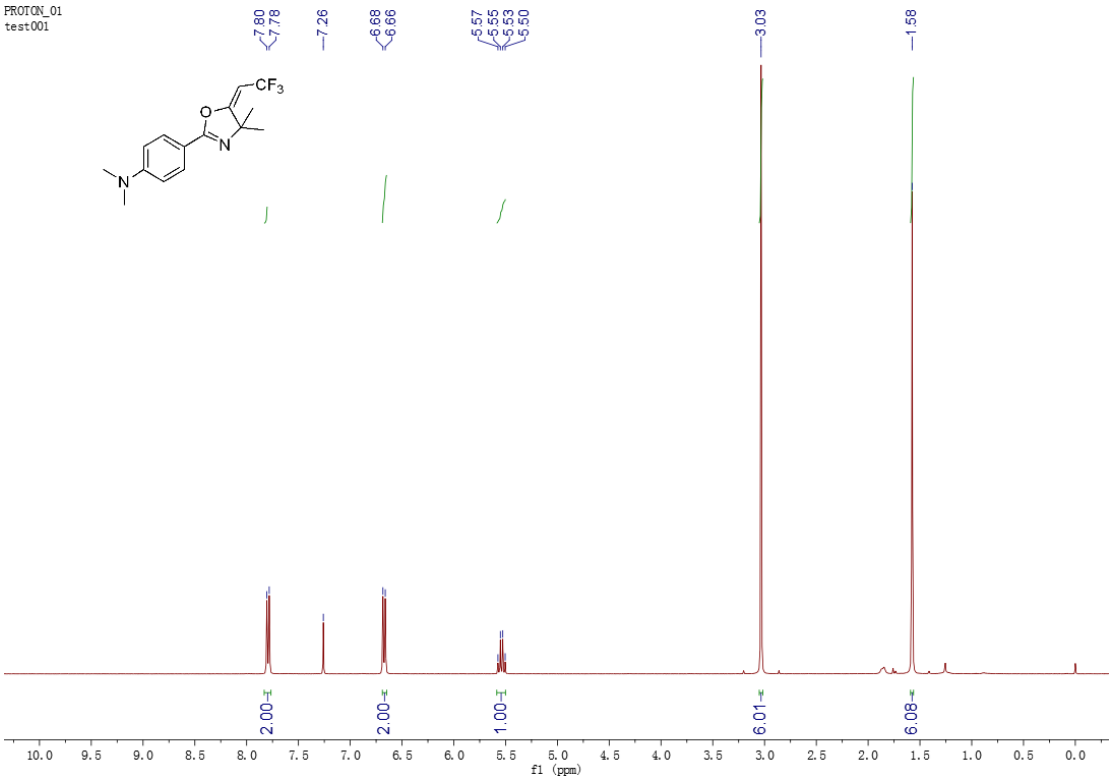

FLUORINE_01
2011138-1246c
-57.58
-57.60
F3C
O
N
O
O
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

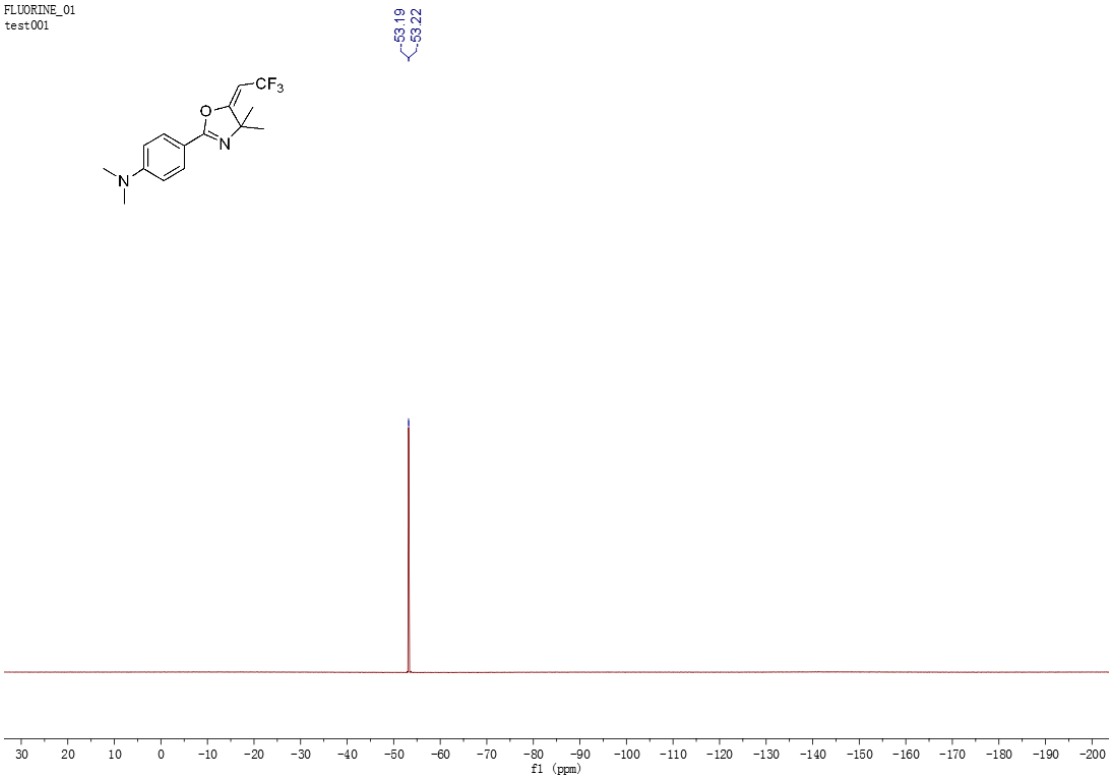

H:
168.74
168.69
168.64
168.59
166.33
158.60
133.50
129.94
129.79
128.51
127.24
124.57
121.89
119.22
89.83
89.46
89.09
88.72
77.48
77.16
76.84
72.02
52.59
28.98
F3C
O
N
O
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

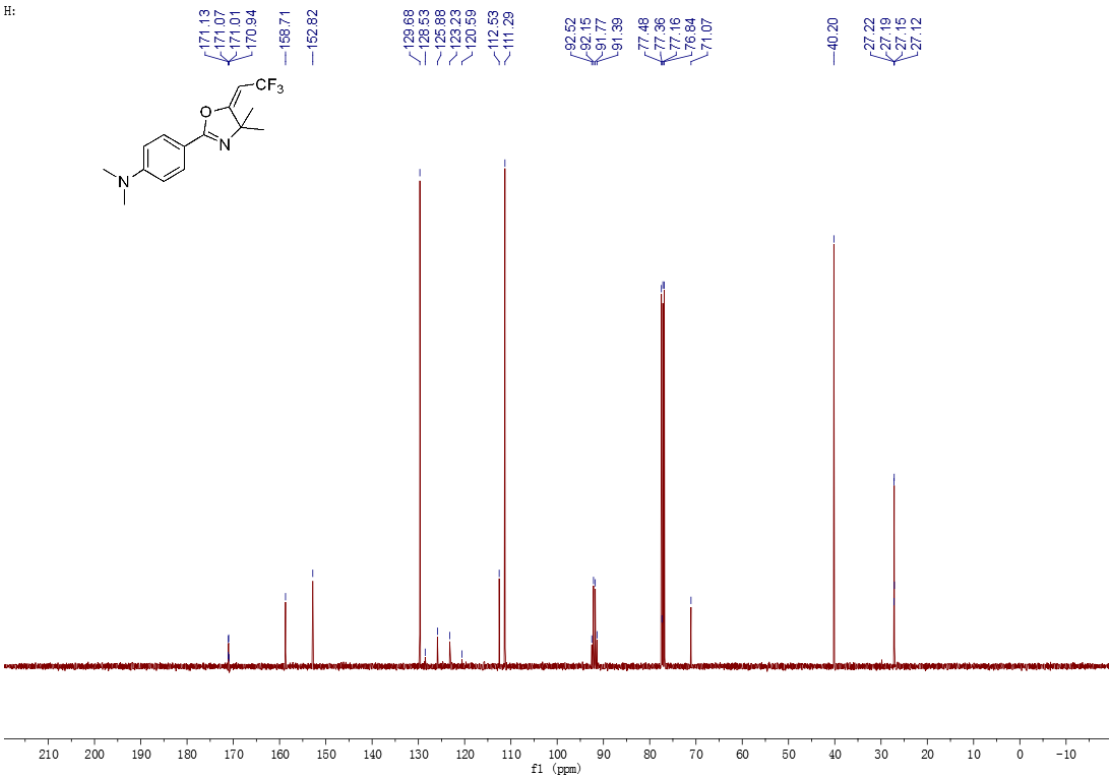

PROTON_01
test001
8.32
8.30
8.15
8.13
7.26
5.68
5.66
5.64
5.61
1.62
CF3
O
N
O2N
2.00
2.01
1.00
6.06
f1 (ppm)

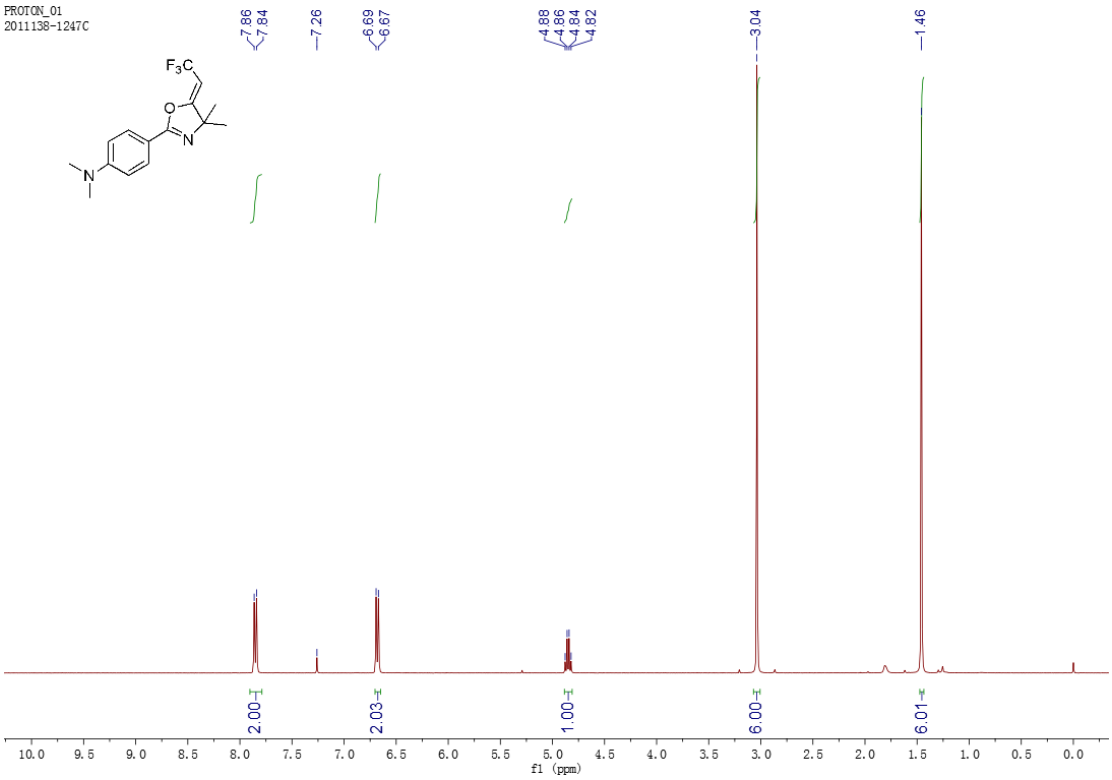

FLUORINE_01
test001
-53.72
-53.75
CF3
O
N
O2N
f1 (ppm)

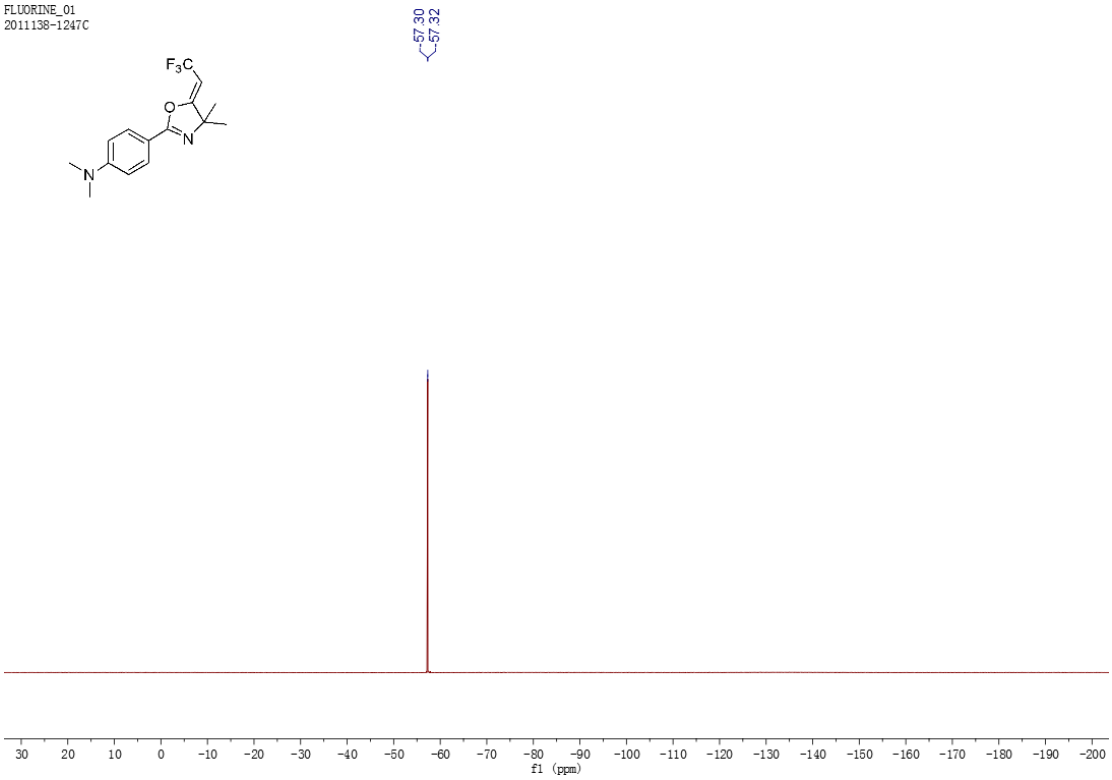

1208-c-3
170.16
170.10
170.03
169.97
156.64
150.07
131.67
129.36
128.04
125.38
123.93
122.73
120.08
94.58
94.20
93.82
93.44
77.48
77.16
76.84
72.11
26.92
26.88
26.85
26.81
CF3
O
N
O2N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

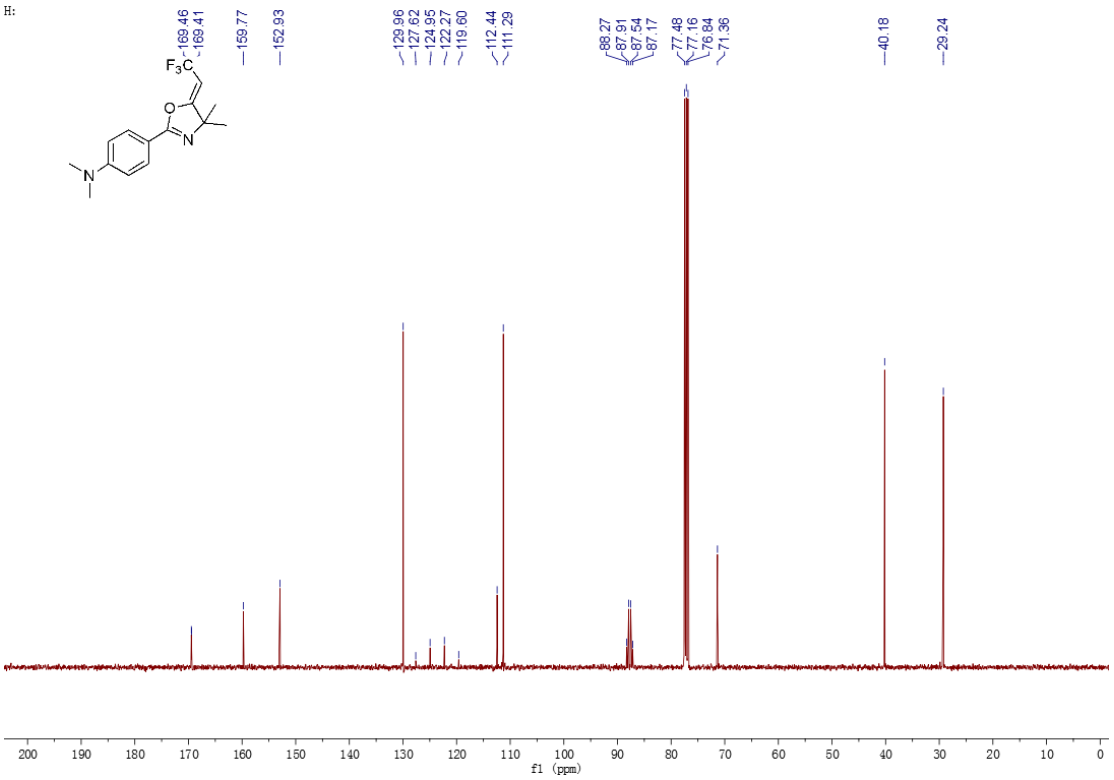

PROTON_01
test001
7.80
7.78
7.26
6.68
6.66
5.57
5.55
5.53
5.50
3.03
1.58
CF3
O
N
N
2.00
2.00
1.00
6.01
6.08
f1 (ppm)

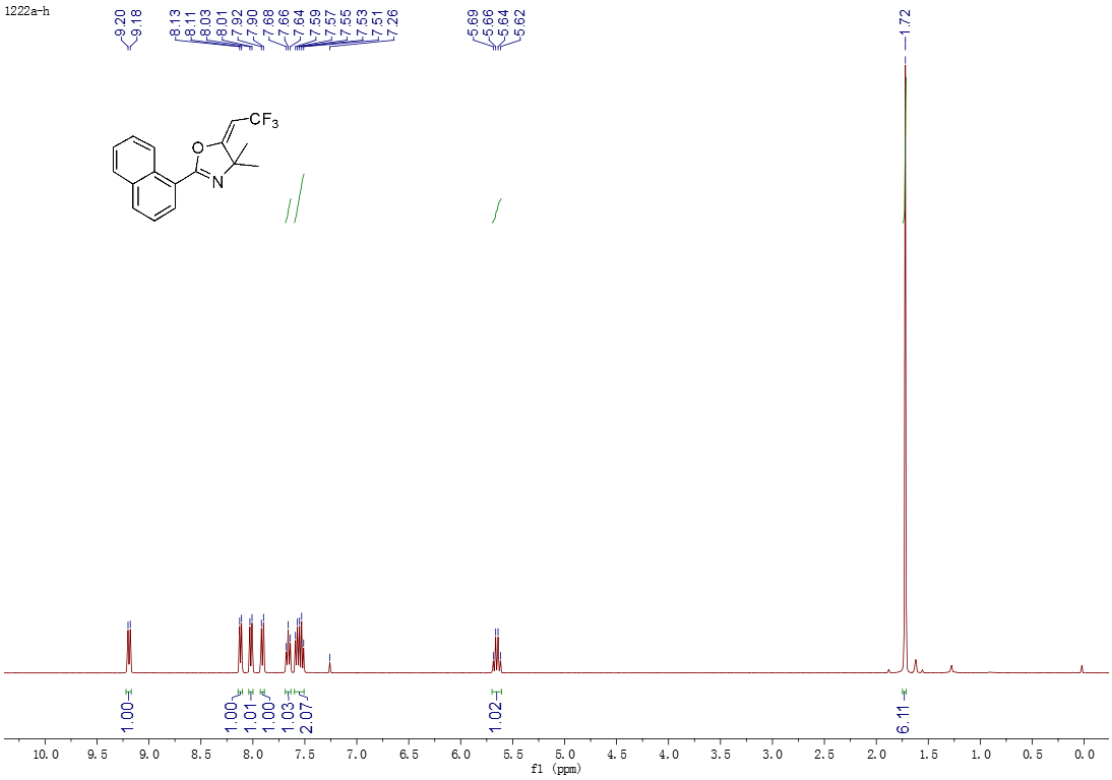

FLUORINE_01
test001
-53.19
-53.22
CF3
O
N
N
f1 (ppm)

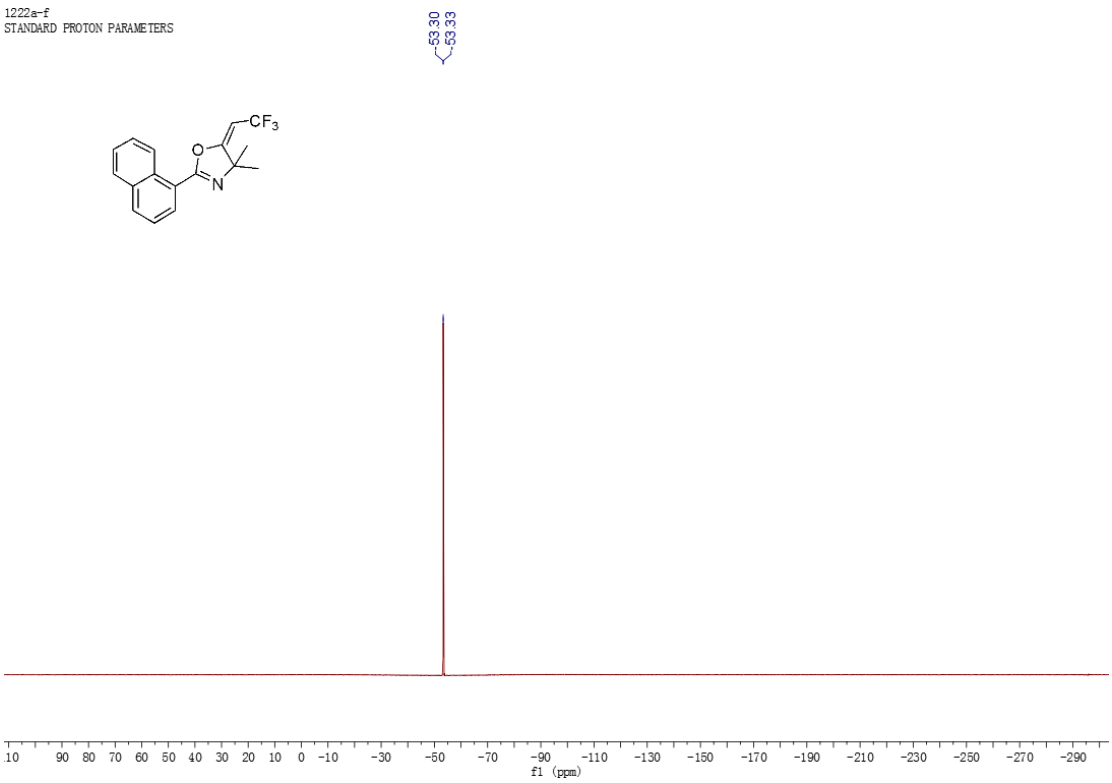

H:
171.13
171.07
171.01
170.94
158.71
152.82
129.68
128.53
125.88
123.23
120.59
112.53
111.29
92.52
92.15
91.77
91.39
77.48
77.36
77.16
76.84
71.07
40.20
27.22
27.19
27.15
27.12
CF3
O
N
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

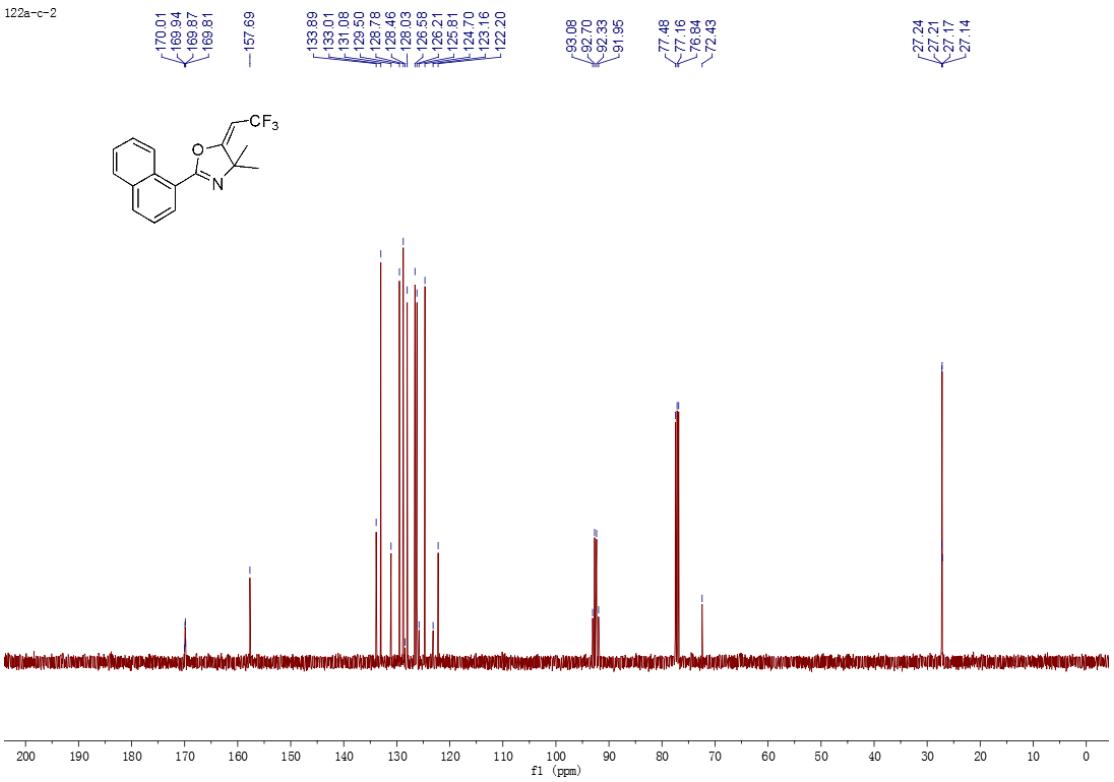

PROTON_01
2011138-1247C
7.86
7.84
7.26
6.69
6.67
4.88
4.86
4.84
4.82
3.04
1.46
2.00
2.03
1.00
6.00
6.01
f1 (ppm)

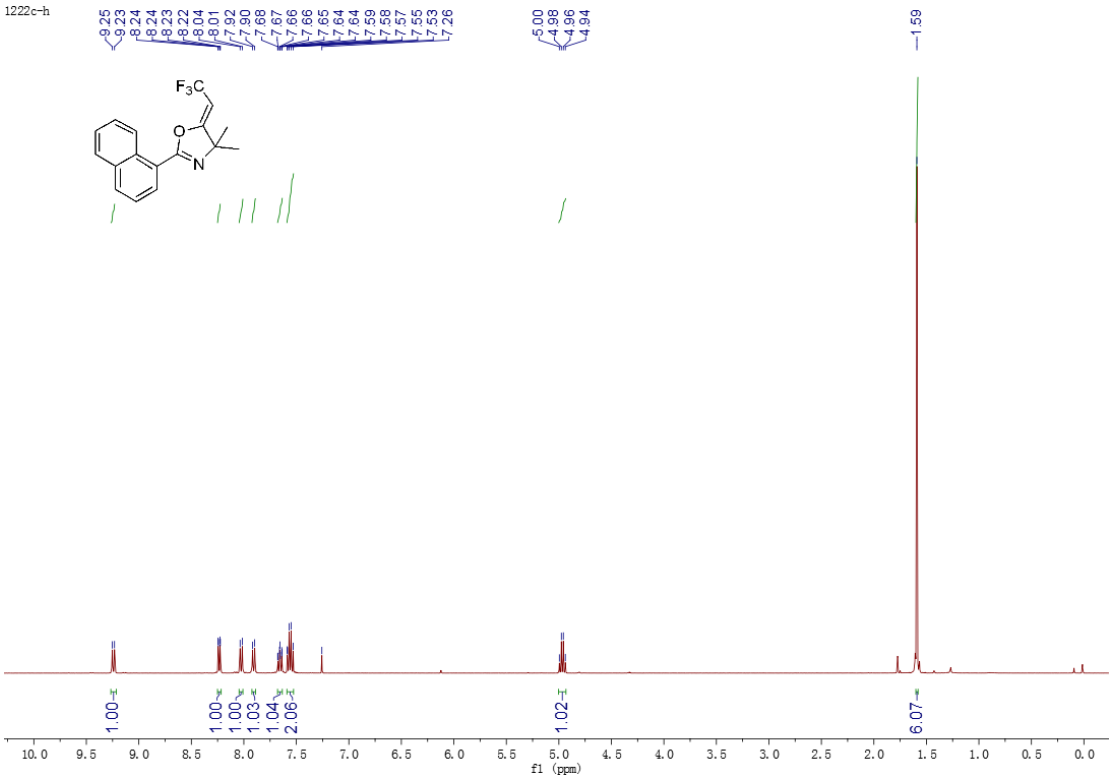

FLUORINE_01
2011138-1247C
-57.30
-57.32
f1 (ppm)

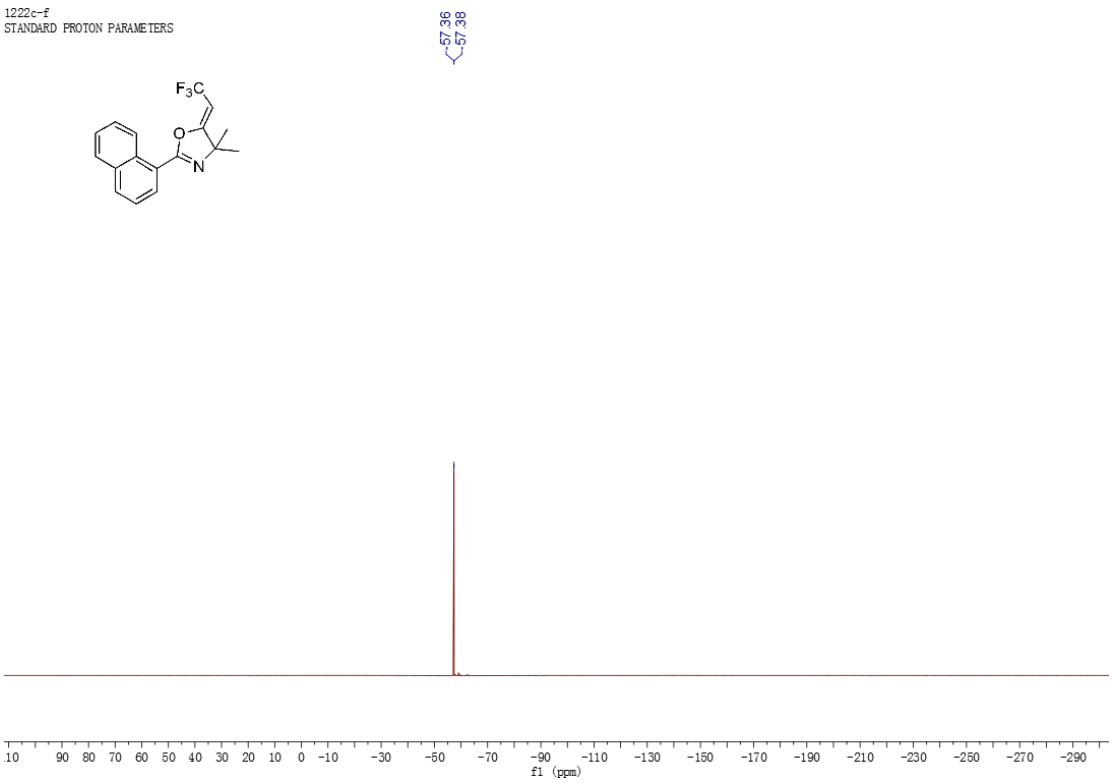

H:
169.46
169.41
159.77
152.93
129.96
127.62
124.95
122.27
119.60
112.44
111.29
88.27
87.91
87.54
87.17
77.48
77.16
76.84
71.36
40.18
29.24
F3C
O
N
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

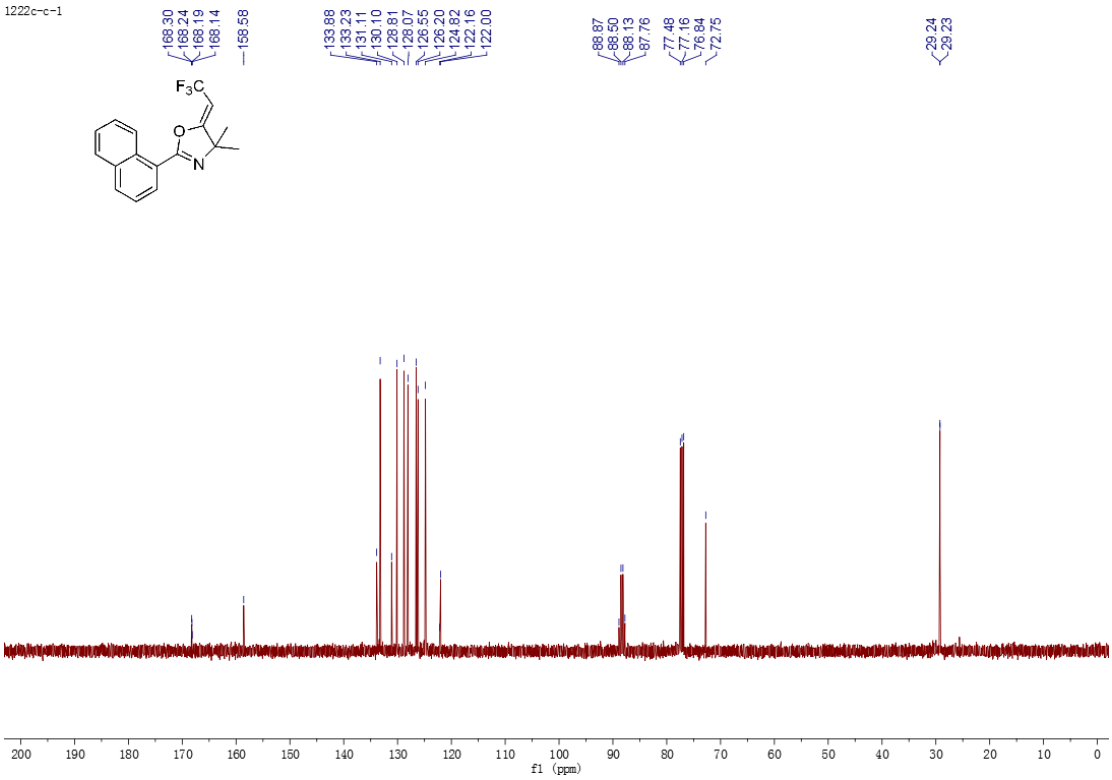

1222a-h
9.20
9.18
8.13
8.11
8.03
8.01
7.92
7.90
7.68
7.66
7.64
7.59
7.57
7.55
7.53
7.51
7.26
5.69
5.66
5.64
5.62
1.72
CF3
O
N
1.00
1.00
1.01
1.00
1.03
2.07
1.02
6.11
f1 (ppm)

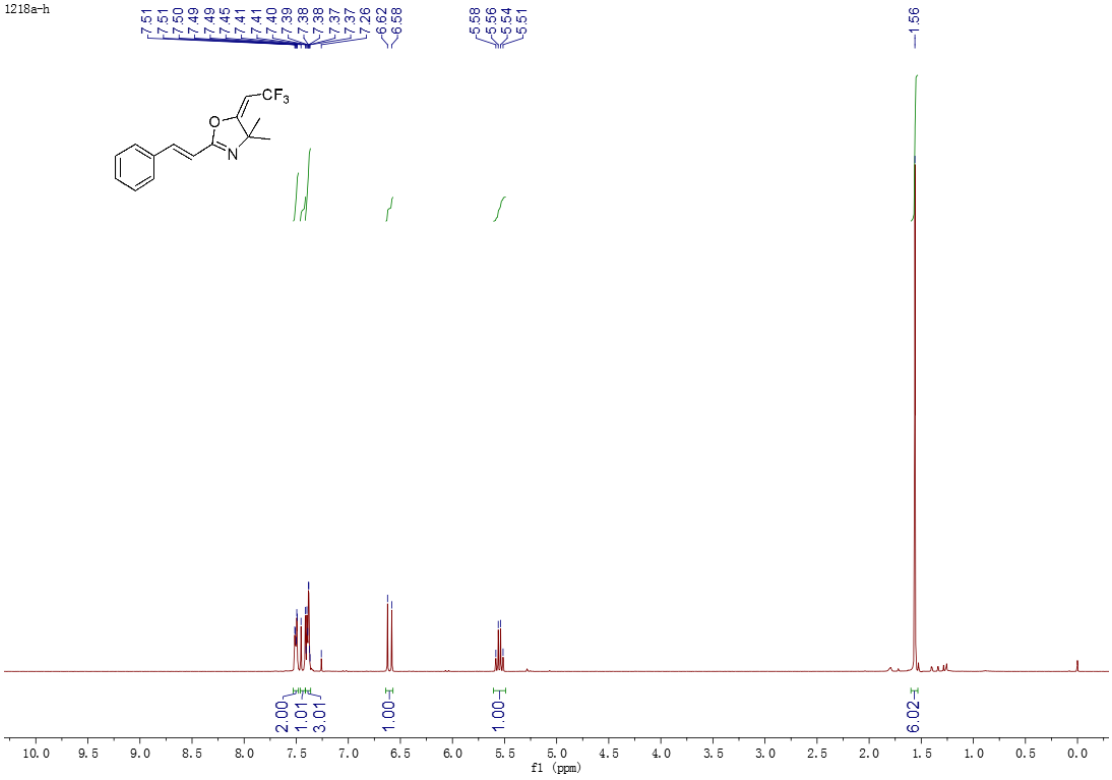

1222a-f
STANDARD PROTON PARAMETERS
53.30
53.33
CF3
O
N
f1 (ppm)

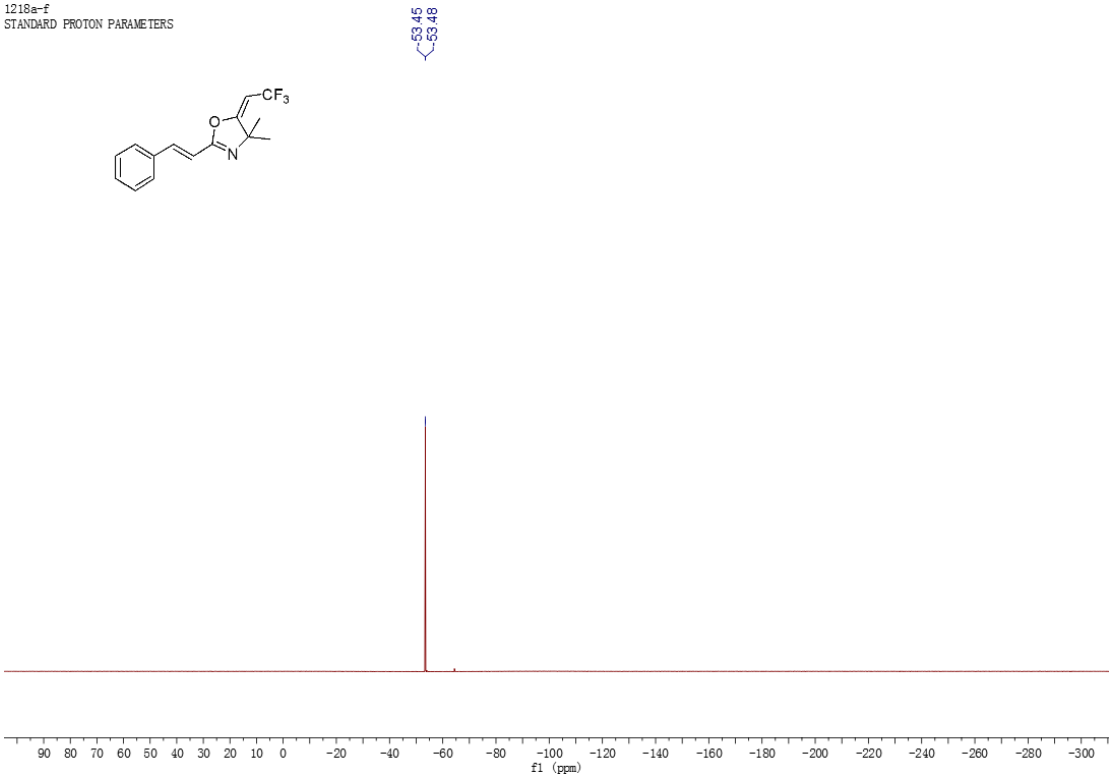

122a-c-2
170.01
169.94
169.87
169.81
157.69
133.89
133.01
131.08
129.50
128.78
128.46
128.03
126.58
126.21
125.81
124.70
123.16
122.20
93.08
92.70
92.33
91.95
77.48
77.16
76.84
72.43
27.24
27.21
27.17
27.14
CF3
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

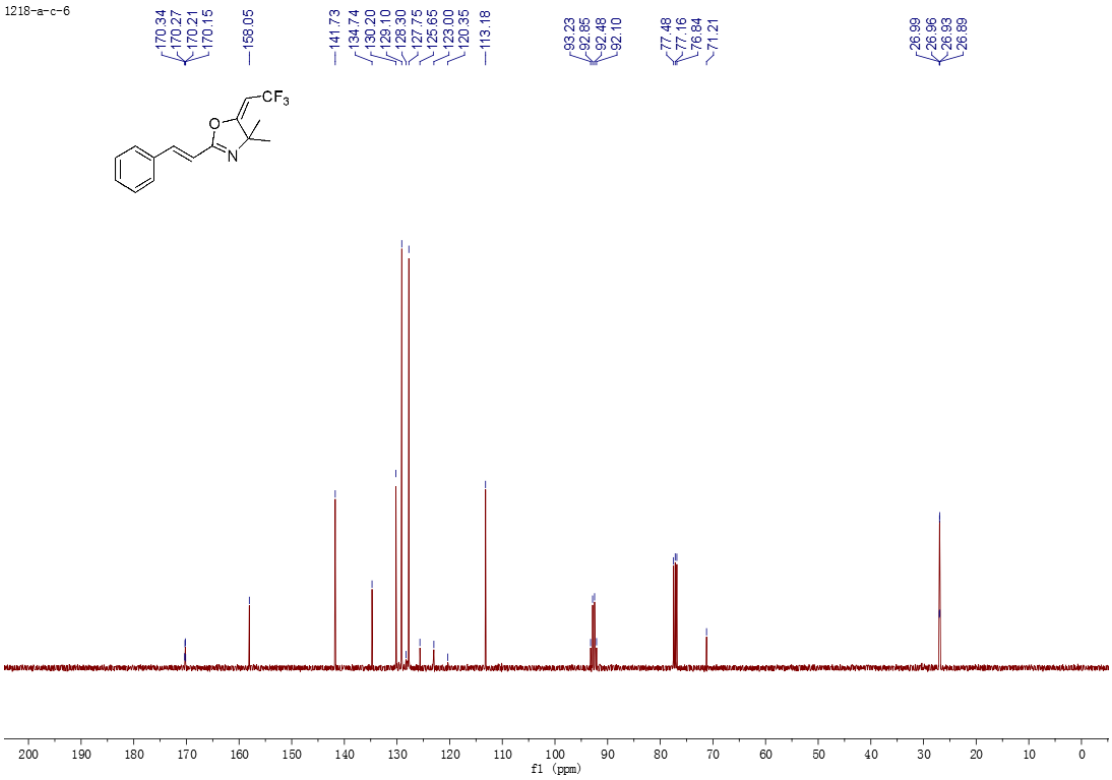

1222c-h
9.25
9.23
8.24
8.24
8.23
8.22
8.04
8.01
7.92
7.90
7.68
7.67
7.66
7.66
7.65
7.64
7.64
7.59
7.58
7.57
7.55
7.53
7.26
5.00
4.98
4.96
4.94
1.59
F3C
O
N
1.00
1.00
1.00
1.03
1.04
2.06
1.02
6.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

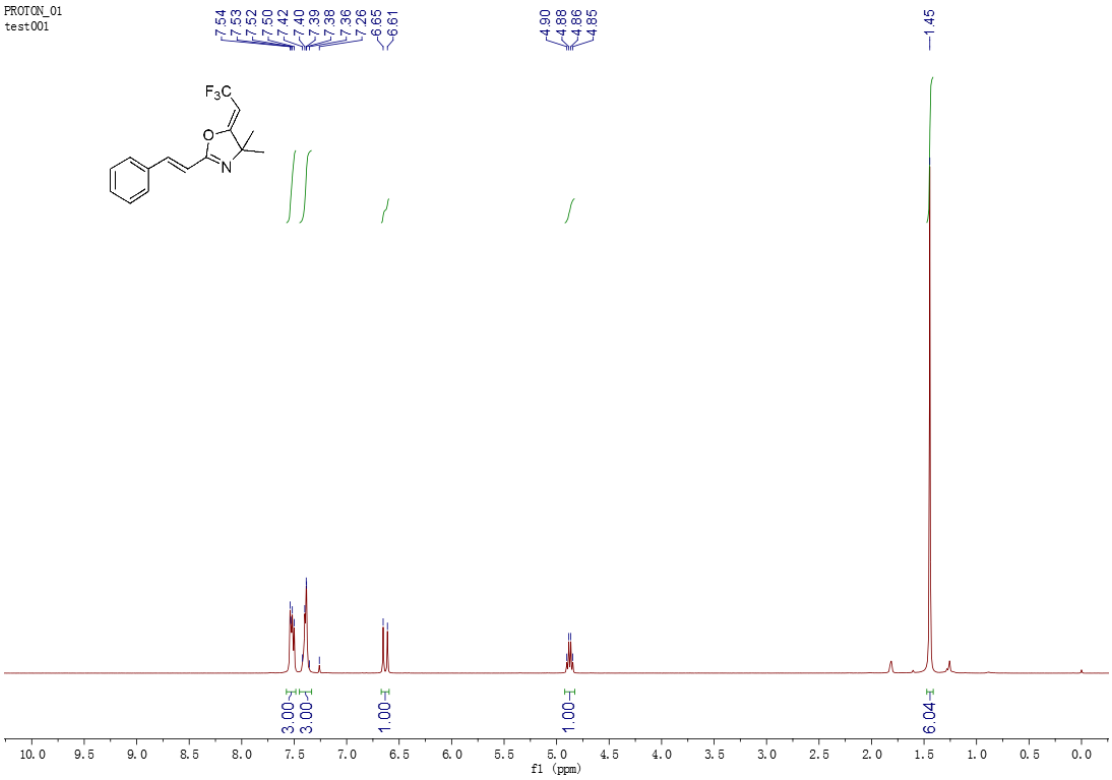

1222c-f
STANDARD PROTON PARAMETERS
57.36
57.38
F3C
O
N
10
90
80
70
60
50
40
30
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
-250
-270
-290
f1 (ppm)

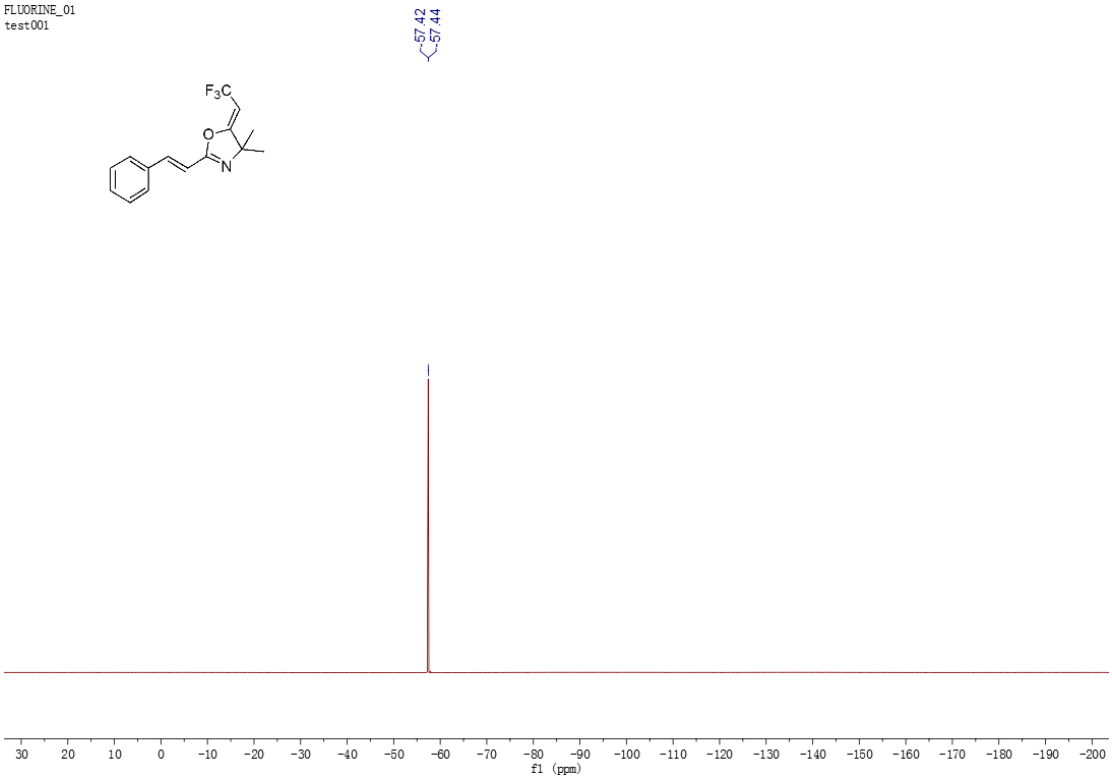

1222c-c-1
168.30
168.24
168.19
168.14
158.58
133.88
133.23
131.11
130.10
128.81
128.07
126.55
126.20
124.82
122.16
122.00
88.87
88.50
88.13
87.76
77.48
77.16
76.84
72.75
29.24
29.23
F3C
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

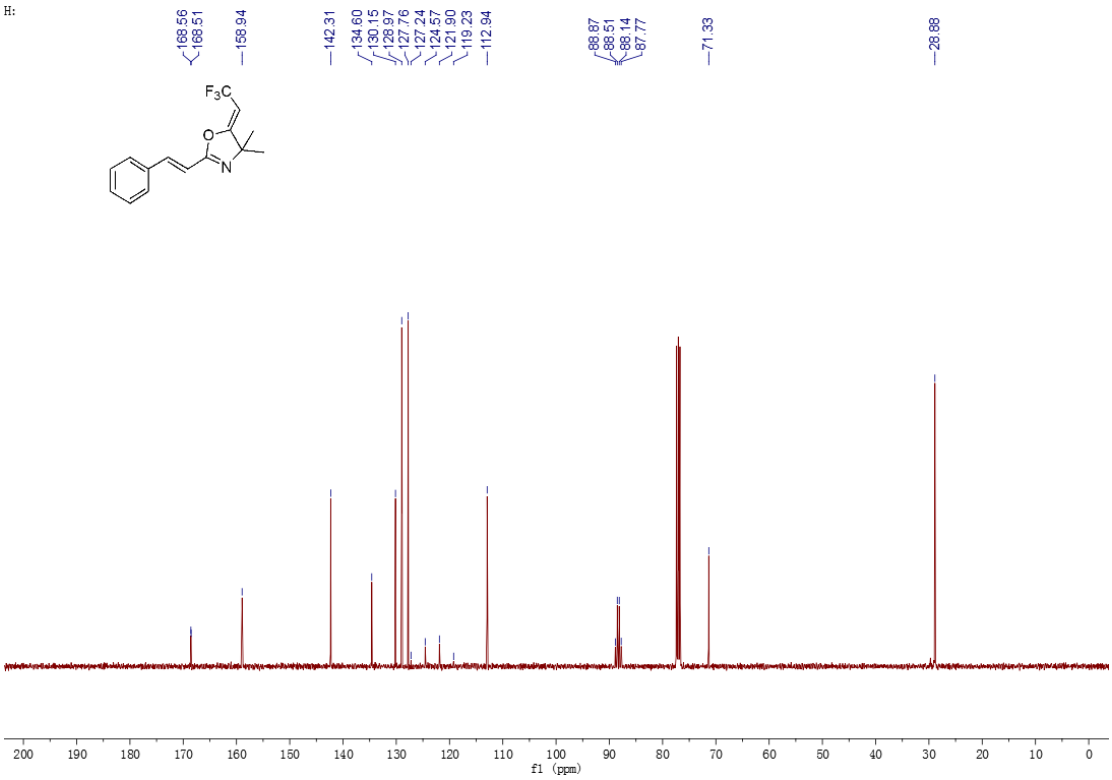

1218a-h
7.51
7.51
7.50
7.49
7.49
7.45
7.41
7.41
7.40
7.39
7.38
7.38
7.37
7.37
7.26
6.62
6.58
5.58
5.56
5.54
5.51
1.56
CF3
O
N
2.00
1.01
3.01
1.00
1.00
6.02
f1 (ppm)

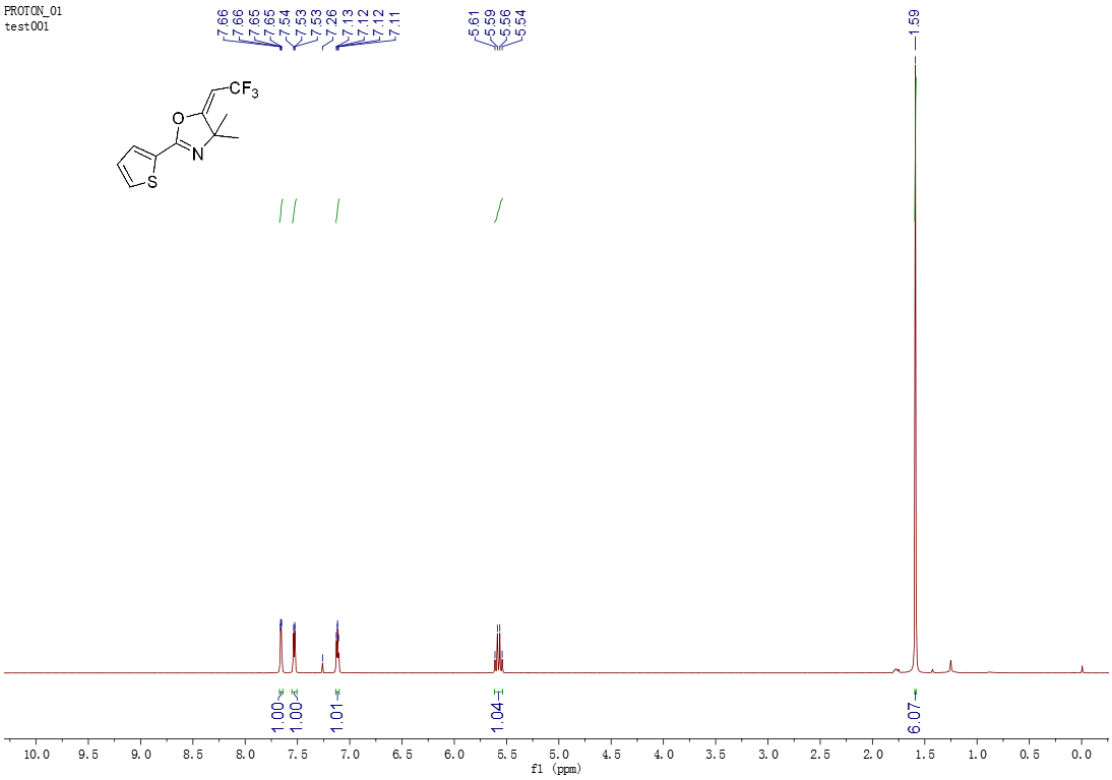

1218a-f
STANDARD PROTON PARAMETERS
-53.45
-53.48
CF3
O
N
f1 (ppm)

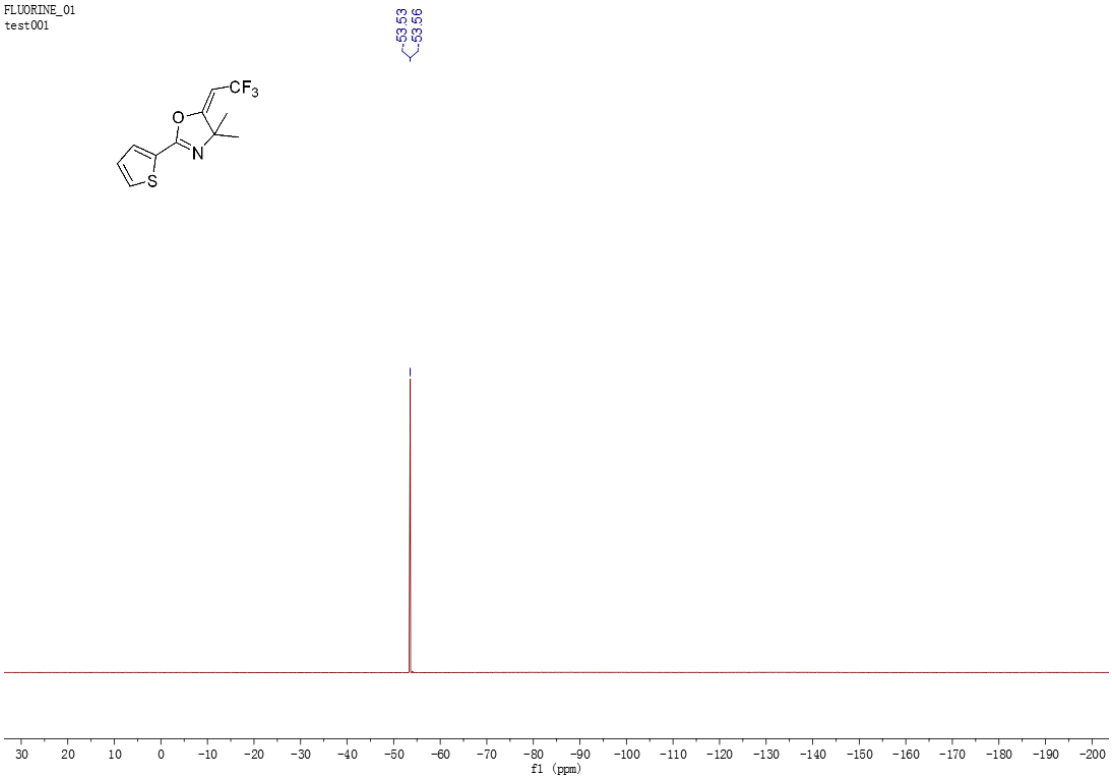

1218-a-c-6
170.34
170.27
170.21
170.15
158.05
141.73
134.74
130.20
129.10
128.30
127.75
125.65
123.00
120.35
113.18
93.23
92.85
92.48
92.10
77.48
77.16
76.84
71.21
26.99
26.96
26.93
26.89
CF3
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

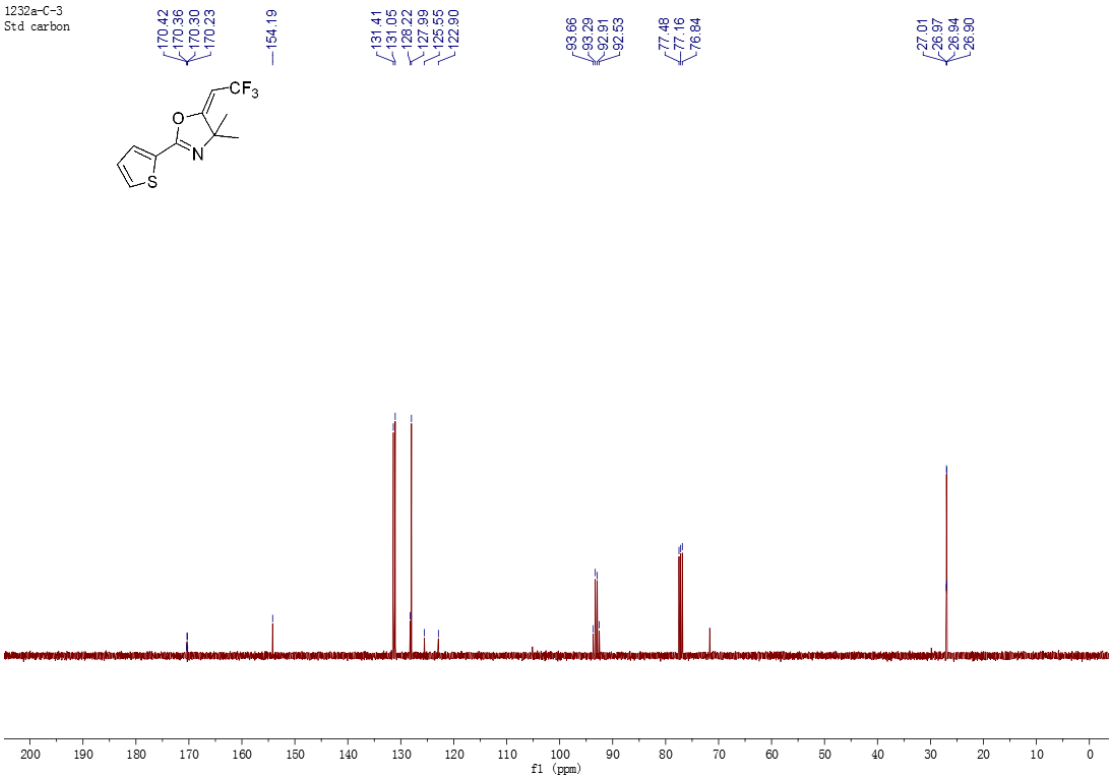

PROTON_01
test001
7.54
7.53
7.52
7.50
7.42
7.40
7.39
7.38
7.36
7.26
6.65
6.61
4.90
4.88
4.86
4.85
1.45
F3C
O
N
3.00
3.00
1.00
1.00
6.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

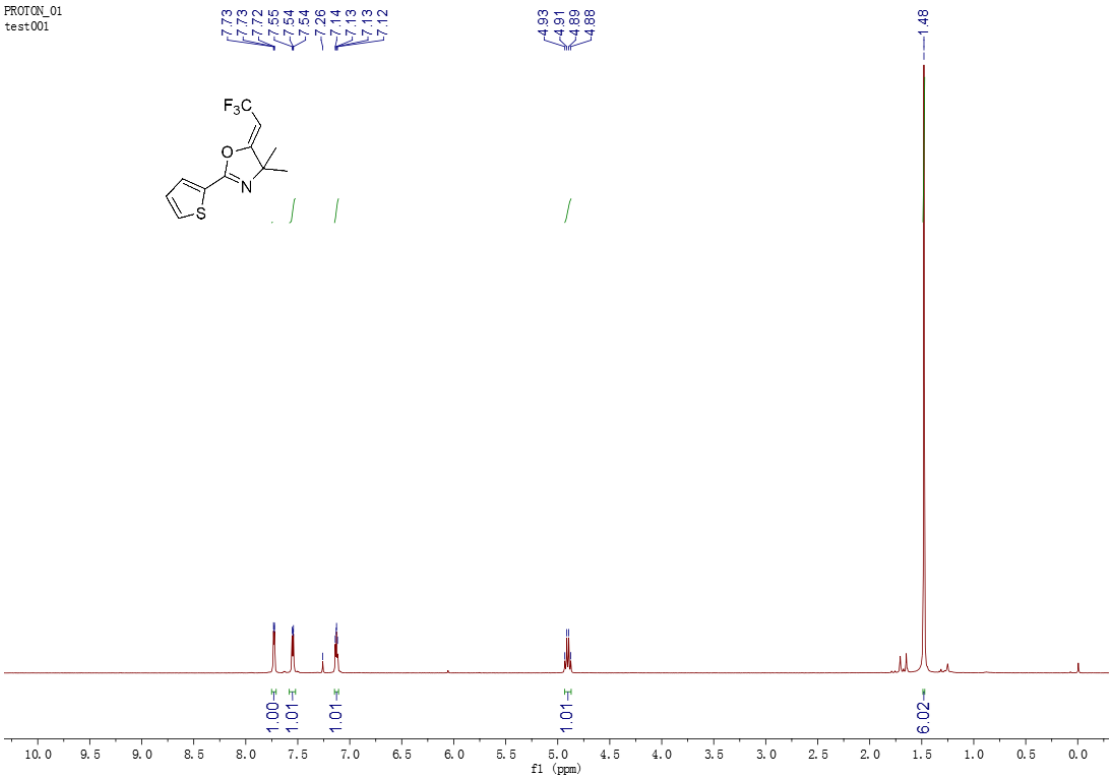

FLUORINE_01
test001
-57.42
-57.44
F3C
O
N
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

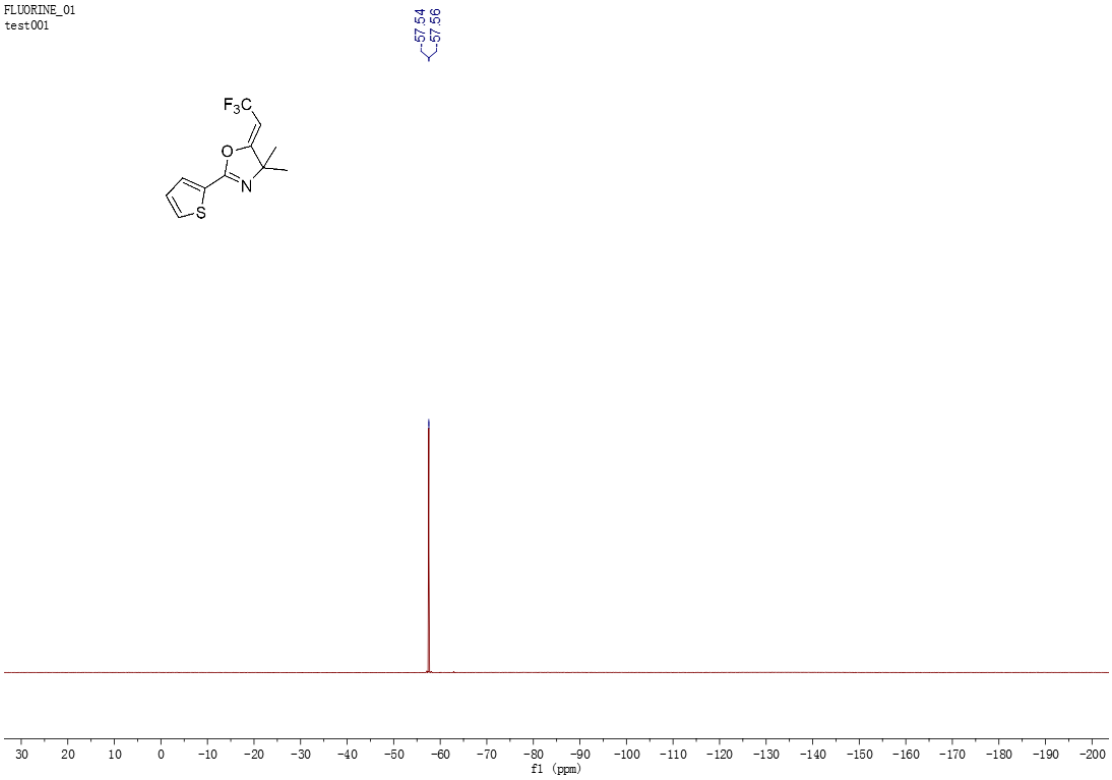

H:
168.56
168.51
158.94
142.31
134.60
130.15
128.97
127.76
127.24
124.57
121.90
119.23
112.94
88.87
88.51
88.14
87.77
71.33
28.88
F3C
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

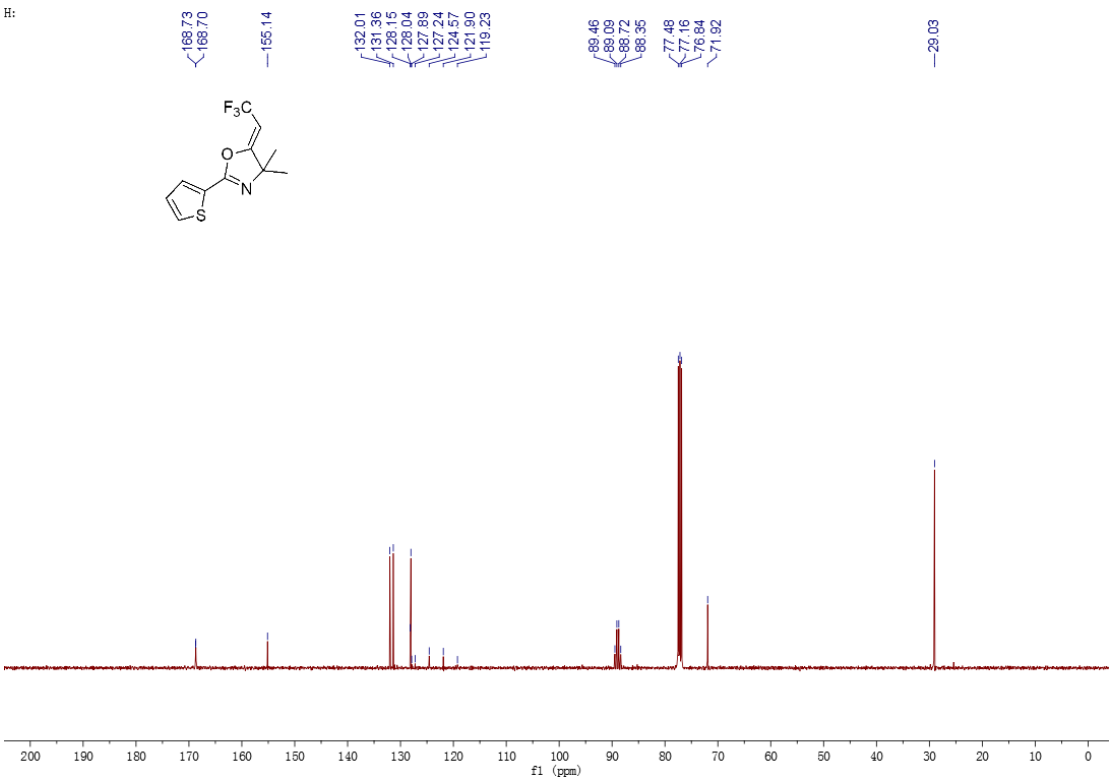

PROTON_01
test001
7.66
7.66
7.65
7.65
7.54
7.53
7.53
7.26
7.13
7.12
7.12
7.11
5.61
5.59
5.56
5.54
1.59
CF3
O
N
S
1.00
1.00
1.01
1.04
6.07
f1 (ppm)

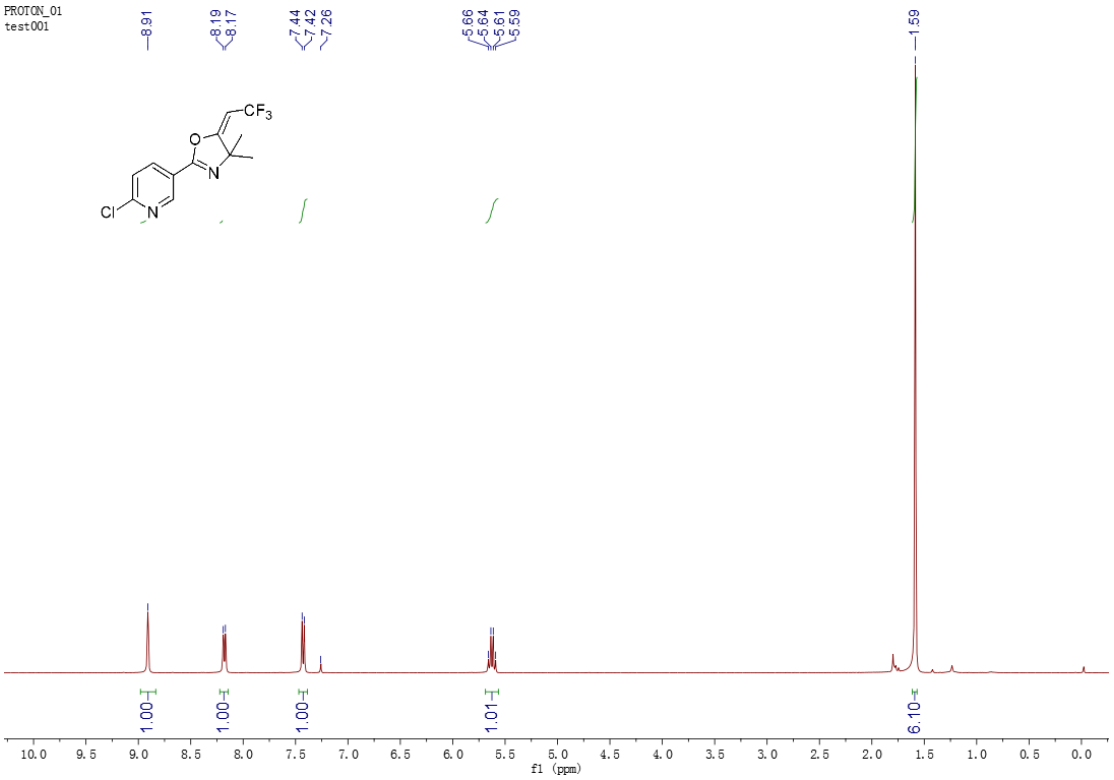

FLUORINE_01
test001
-53.53
-53.56
CF3
O
N
S
f1 (ppm)

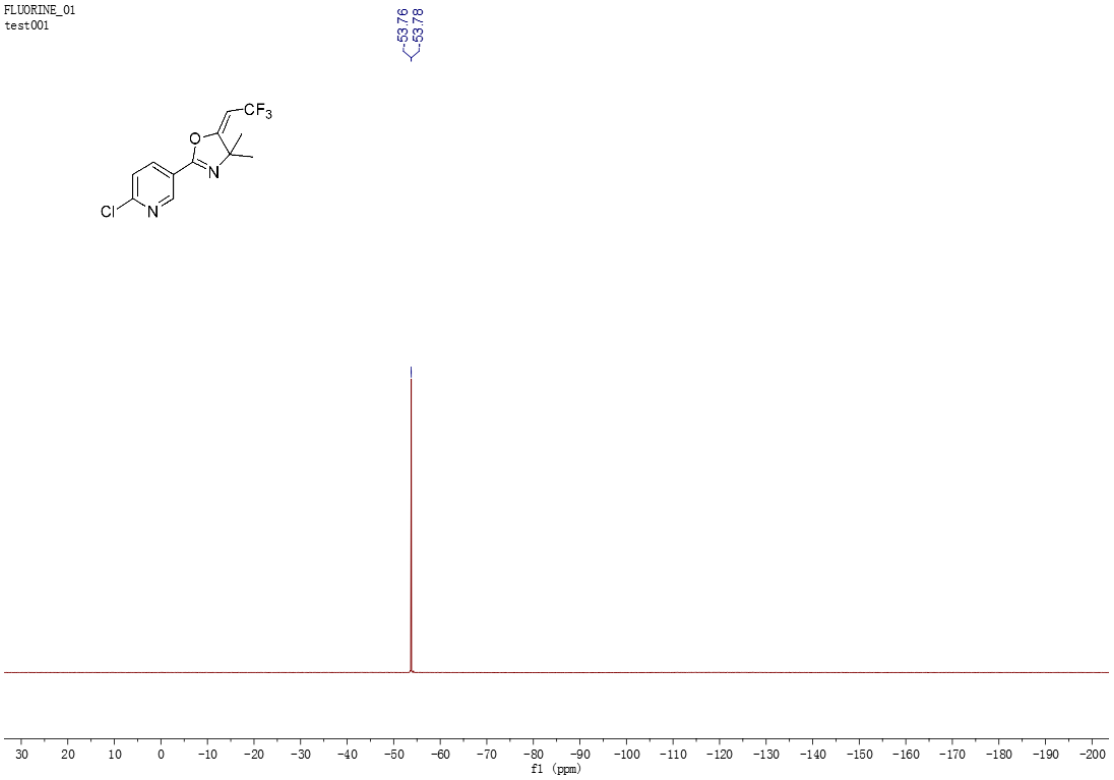

1232a-C-3
Std carbon
170.42
170.36
170.30
170.23
154.19
131.41
131.05
128.22
127.99
125.55
122.90
93.66
93.29
92.91
92.53
77.48
77.16
76.84
27.01
26.97
26.94
26.90
CF3
O
N
S
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

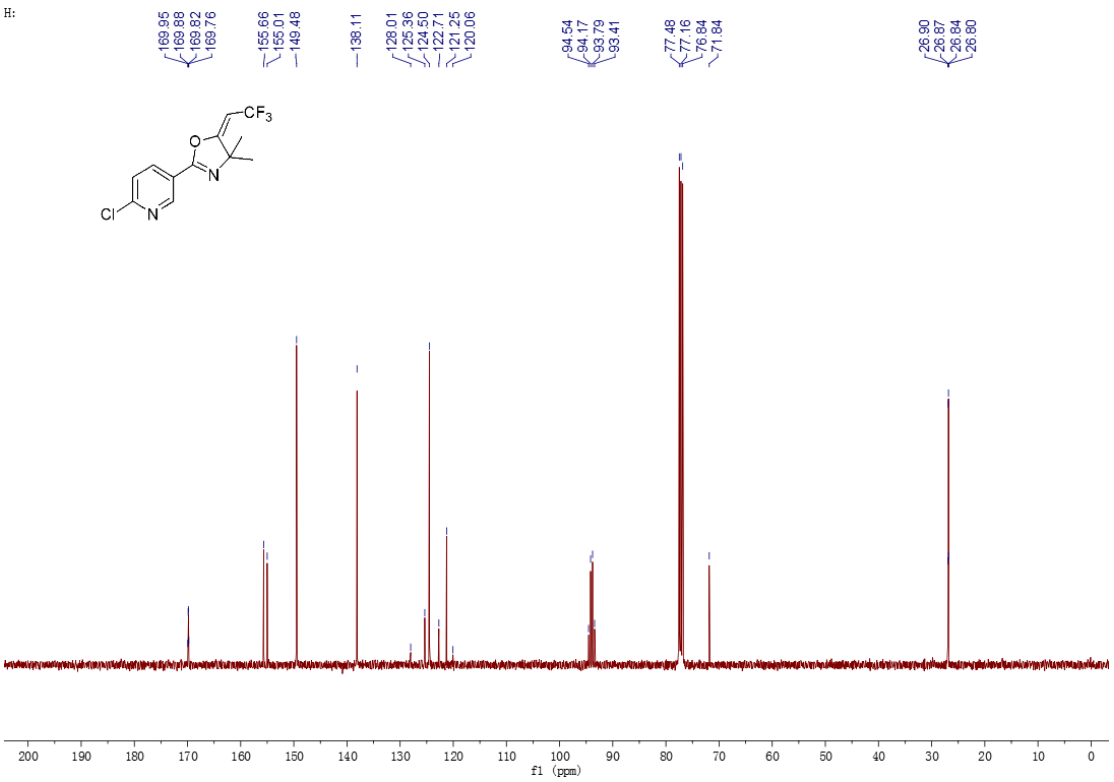

PROTON_01
test001
7.73
7.73
7.72
7.55
7.54
7.54
7.26
7.14
7.13
7.13
7.12
4.93
4.91
4.89
4.88
1.48
F3C
O
N
S
1.00
1.01
1.01
1.01
6.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

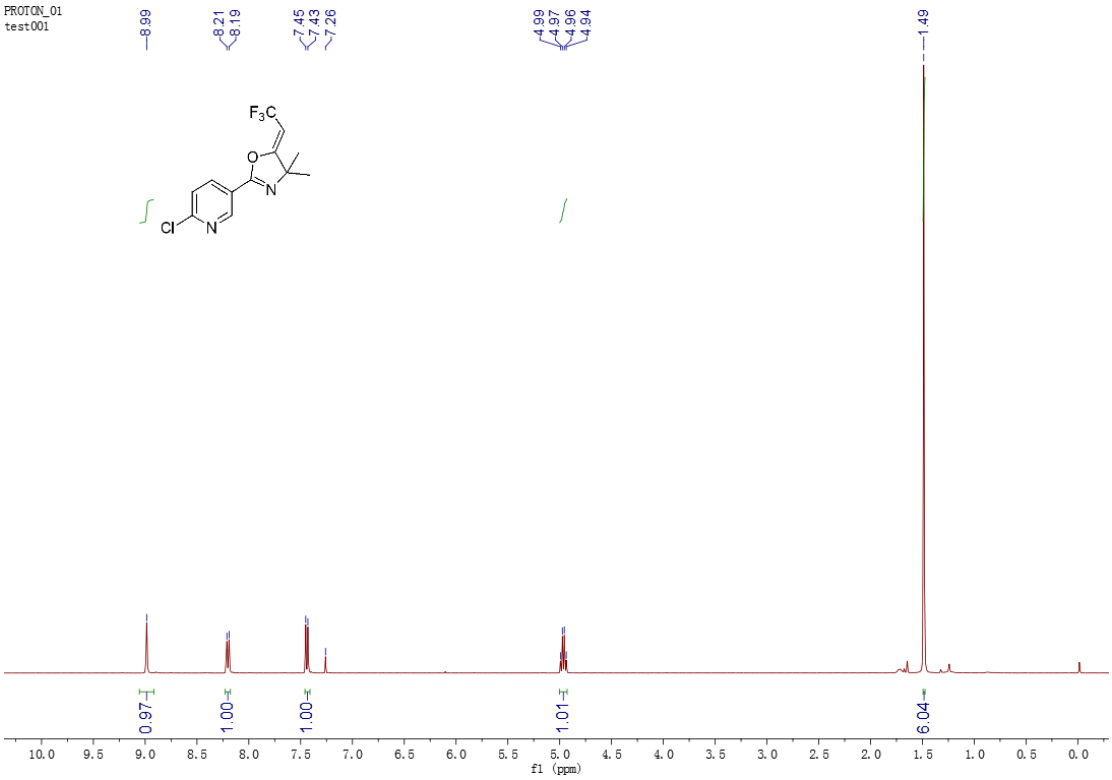

FLUORINE_01
test001
-57.54
-57.56
F3C
O
N
S
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

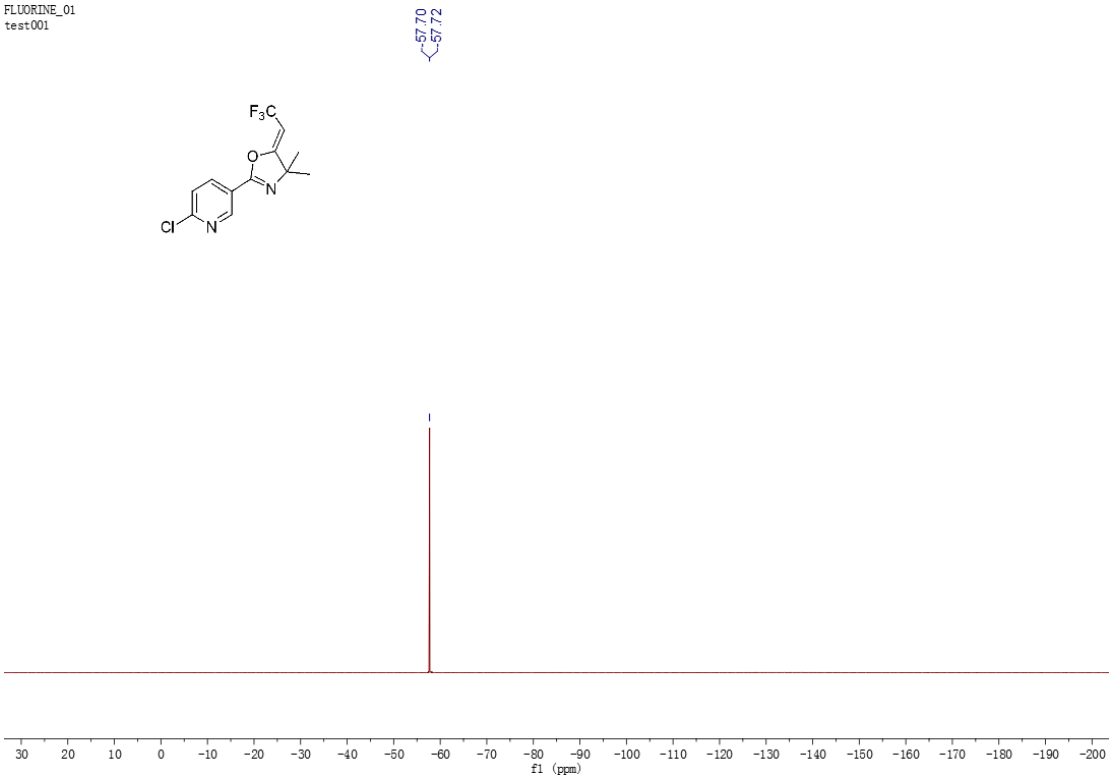

H:
168.73
168.70
155.14
132.01
131.36
128.15
128.04
127.89
127.24
124.57
121.90
119.23
89.46
89.09
88.72
88.35
77.48
77.16
76.84
71.92
29.03
F3C
O
N
S
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

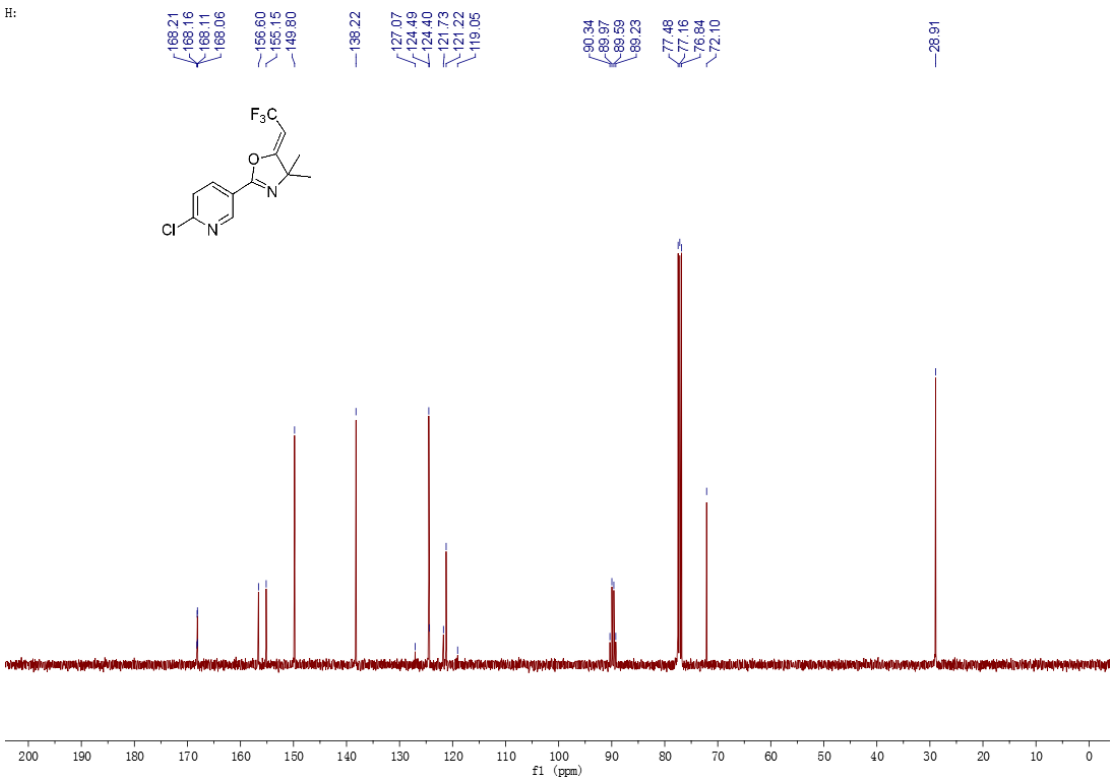

PROTON_01
test001
8.91
8.19
8.17
7.44
7.42
7.26
5.66
5.64
5.61
5.59
1.59
CF3
O
N
Cl
N
1.00
1.00
1.00
1.01
6.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

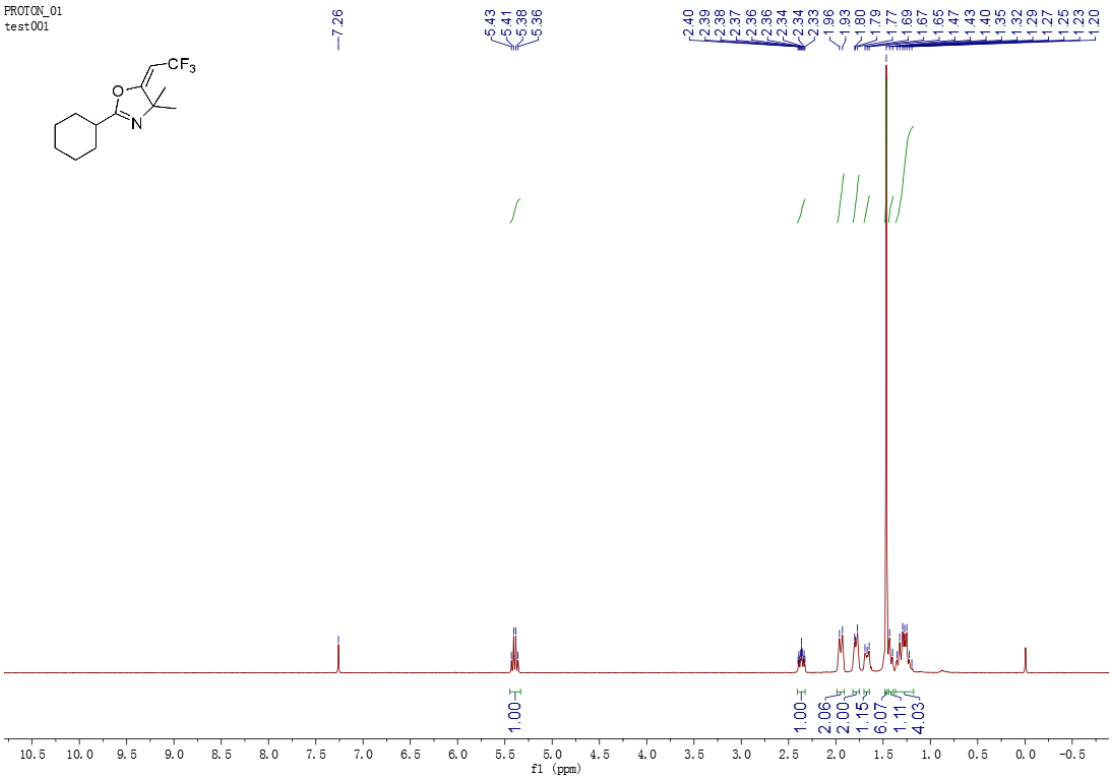

FLUORINE_01
test001
-53.76
-53.78
CF3
O
N
Cl
N
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

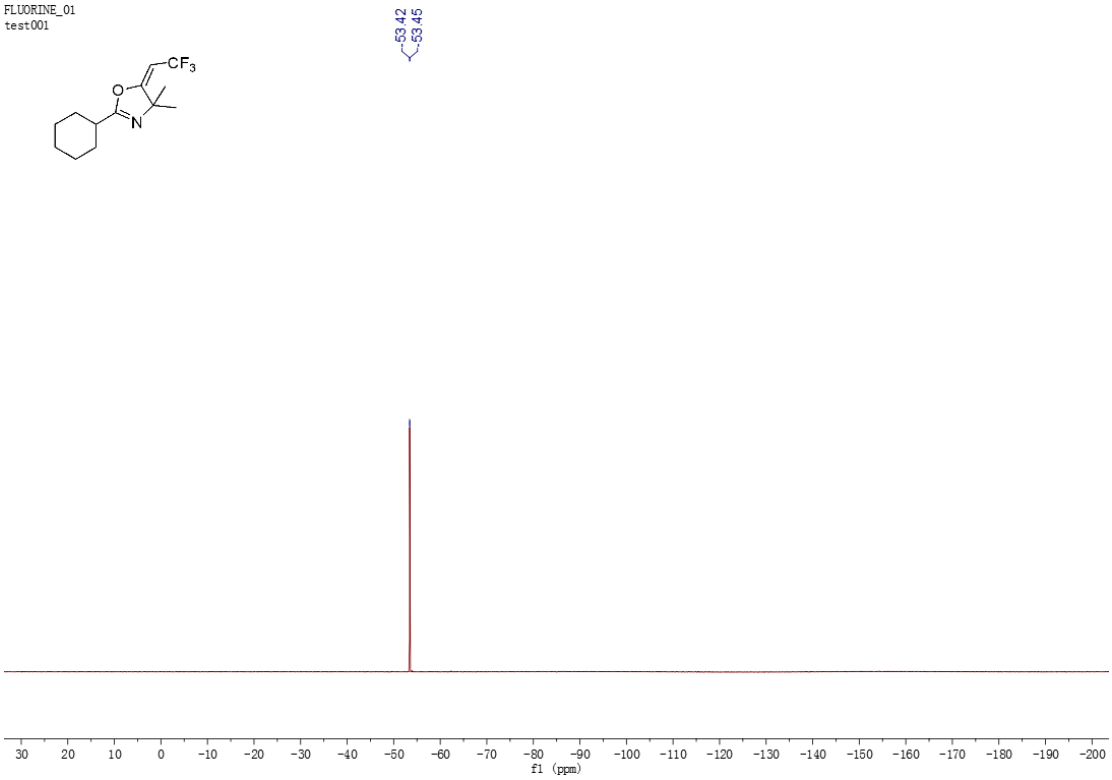

H:
169.95
169.88
169.82
169.76
155.66
155.01
149.48
138.11
128.01
125.36
124.50
122.71
121.25
120.06
94.54
94.17
93.79
93.41
77.48
77.16
76.84
71.84
26.90
26.87
26.84
26.80
CF3
O
N
Cl
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

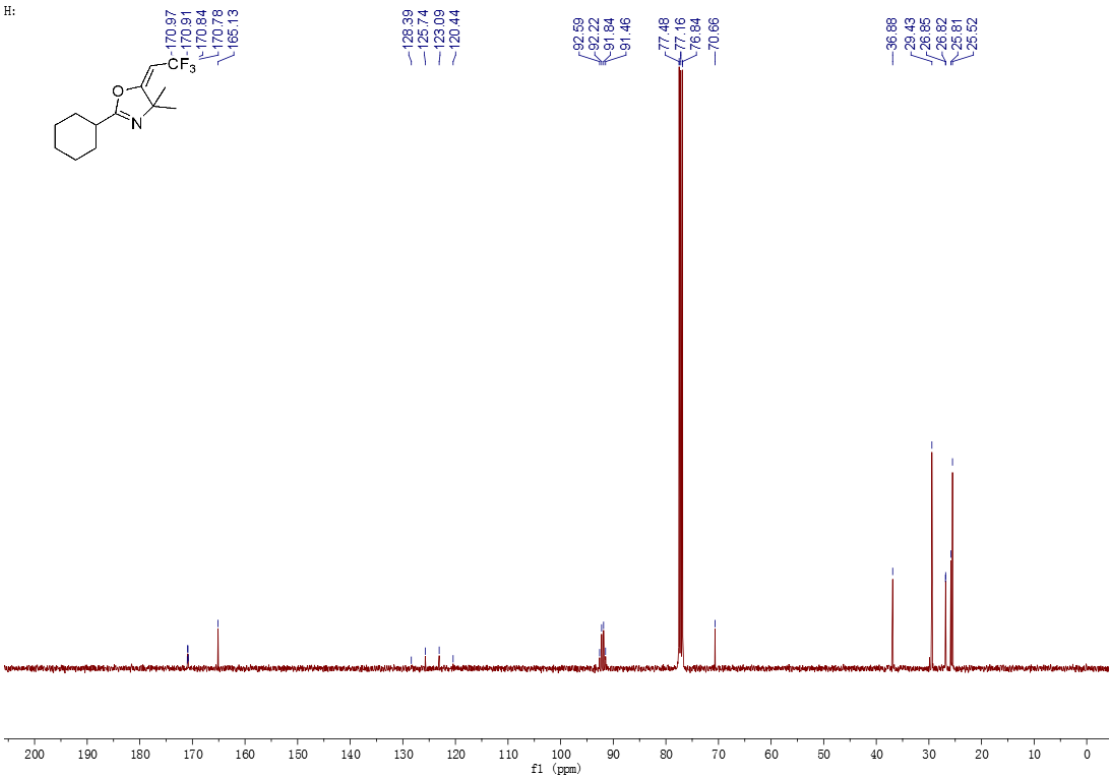

PROTON_01
test001
8.99
8.21
8.19
7.45
7.43
7.26
4.99
4.97
4.96
4.94
1.49
F3C
O
N
Cl
N
0.97
1.00
1.00
1.01
6.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

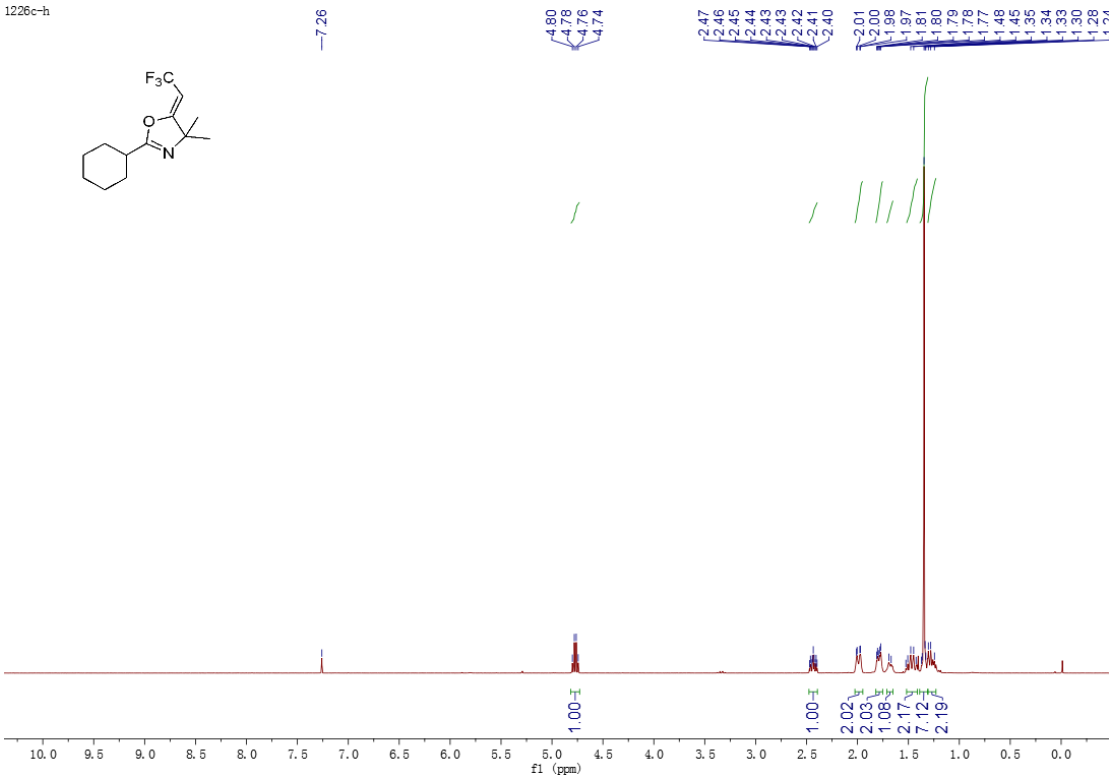

FLUORINE_01
test001
-57.70
-57.72
F3C
O
N
Cl
N
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

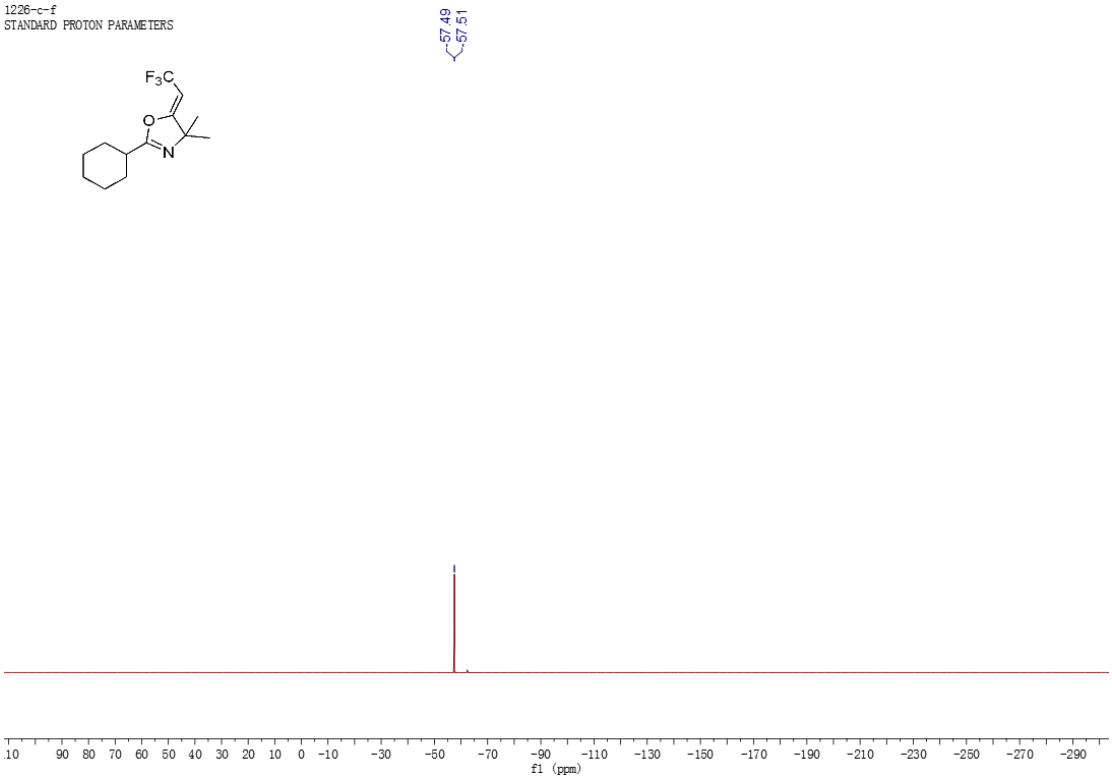

H:
168.21
168.16
168.11
168.06
156.60
155.15
149.80
138.22
127.07
124.49
124.40
121.73
121.22
119.05
90.34
89.97
89.59
89.23
77.48
77.16
76.84
72.10
28.91
F3C
O
N
Cl
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

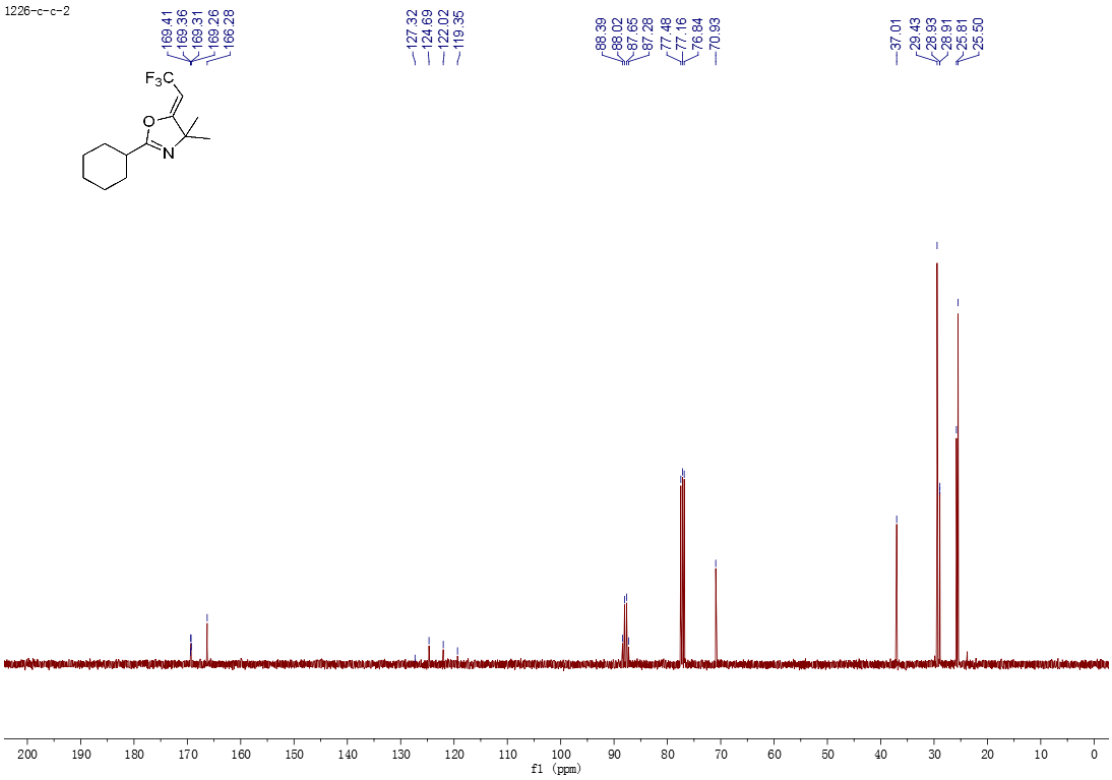

PROTON_01
test001
7.26
5.43
5.41
5.38
5.36
2.40
2.39
2.38
2.37
2.36
2.36
2.34
2.34
2.33
1.96
1.93
1.80
1.79
1.77
1.69
1.67
1.65
1.47
1.43
1.40
1.35
1.32
1.29
1.27
1.25
1.23
1.20
CF3
O
N
1.00
1.00
2.06
2.00
1.15
6.07
1.11
4.03
f1 (ppm)

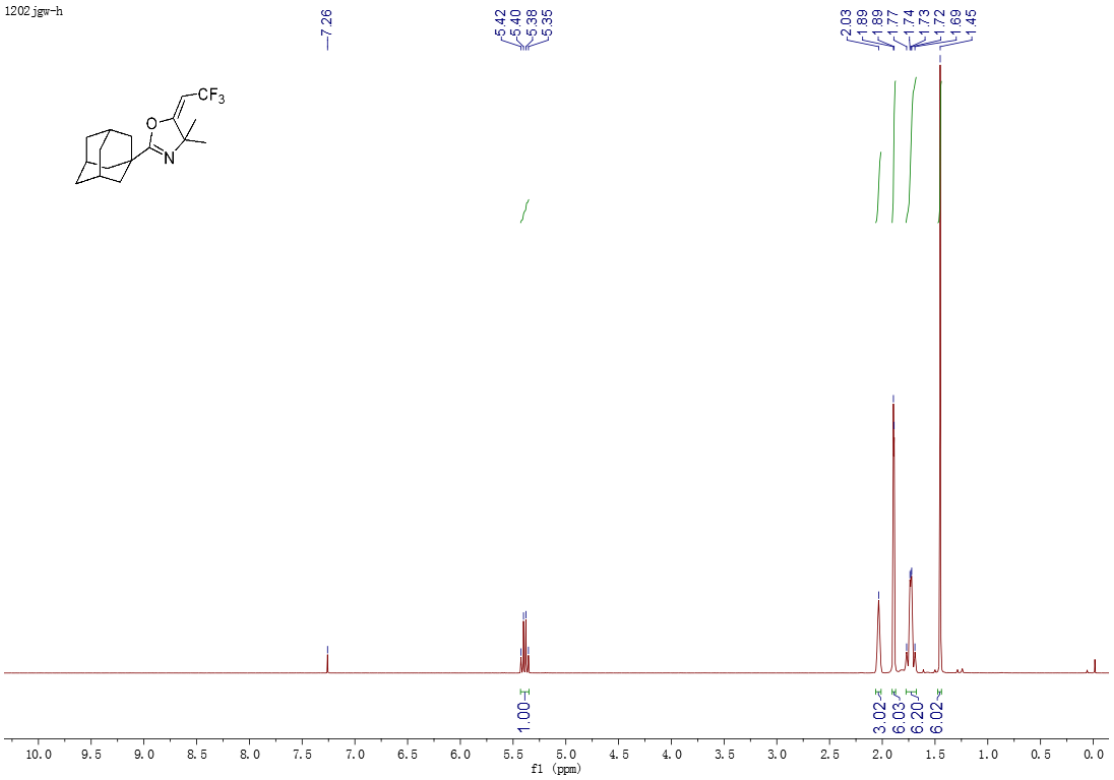

FLUORINE_01
test001
-53.42
-53.45
CF3
O
N
f1 (ppm)

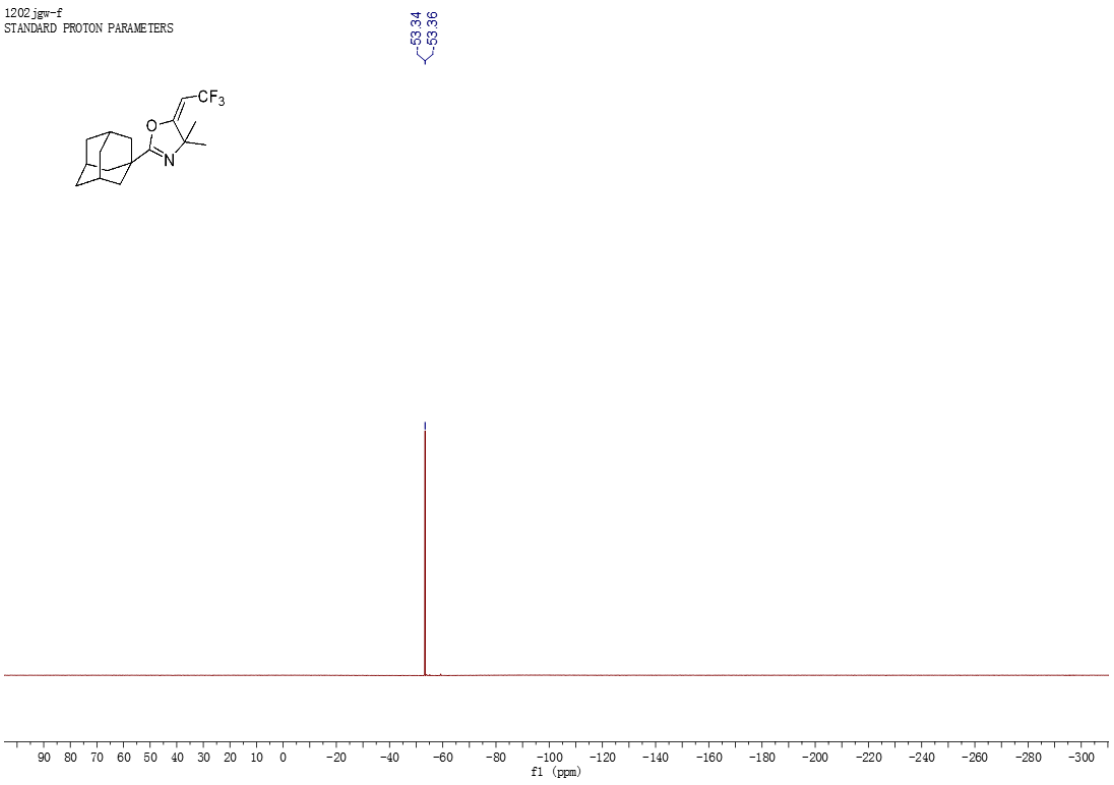

H:
170.97
170.91
170.84
170.78
165.13
128.39
125.74
123.09
120.44
92.59
92.22
91.84
91.46
77.48
77.16
76.84
70.66
36.88
29.43
26.85
26.82
25.81
25.52
CF3
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

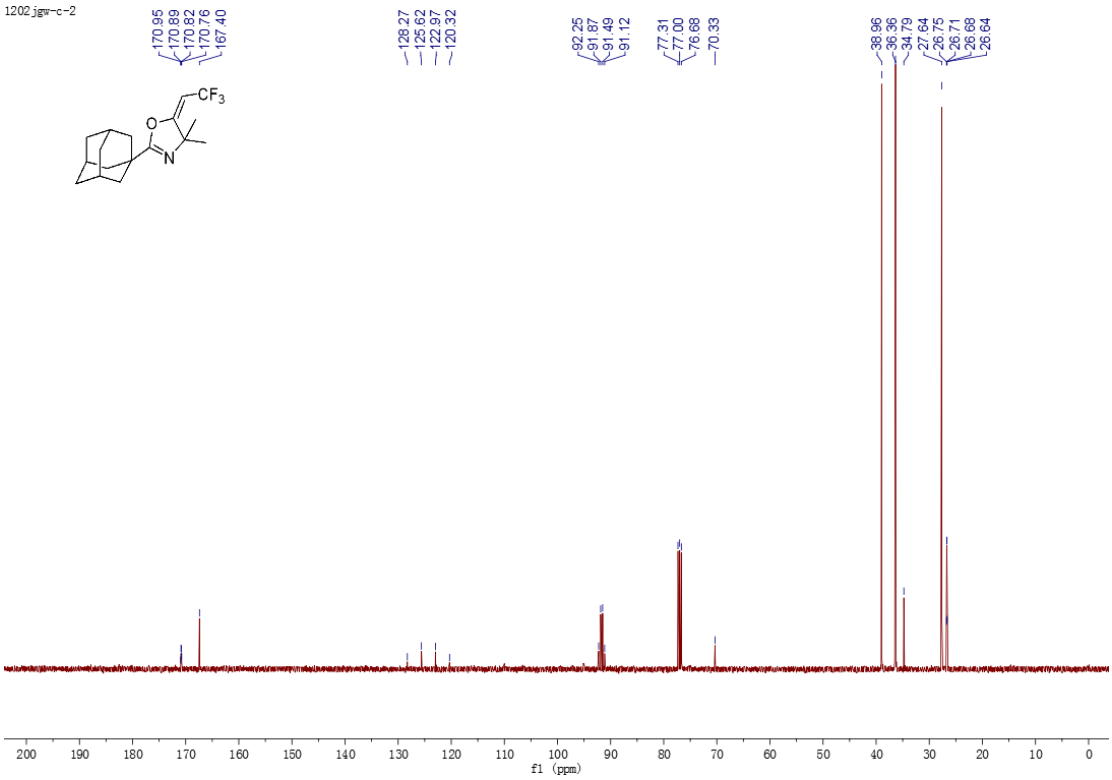

1226c-h
7.26
4.80
4.78
4.76
4.74
2.47
2.46
2.45
2.44
2.43
2.43
2.42
2.41
2.40
2.01
2.00
1.98
1.97
1.81
1.80
1.79
1.78
1.77
1.48
1.45
1.35
1.34
1.33
1.30
1.28
F3C
O
N
1.00
1.00
2.02
2.03
1.08
2.17
7.12
2.19
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

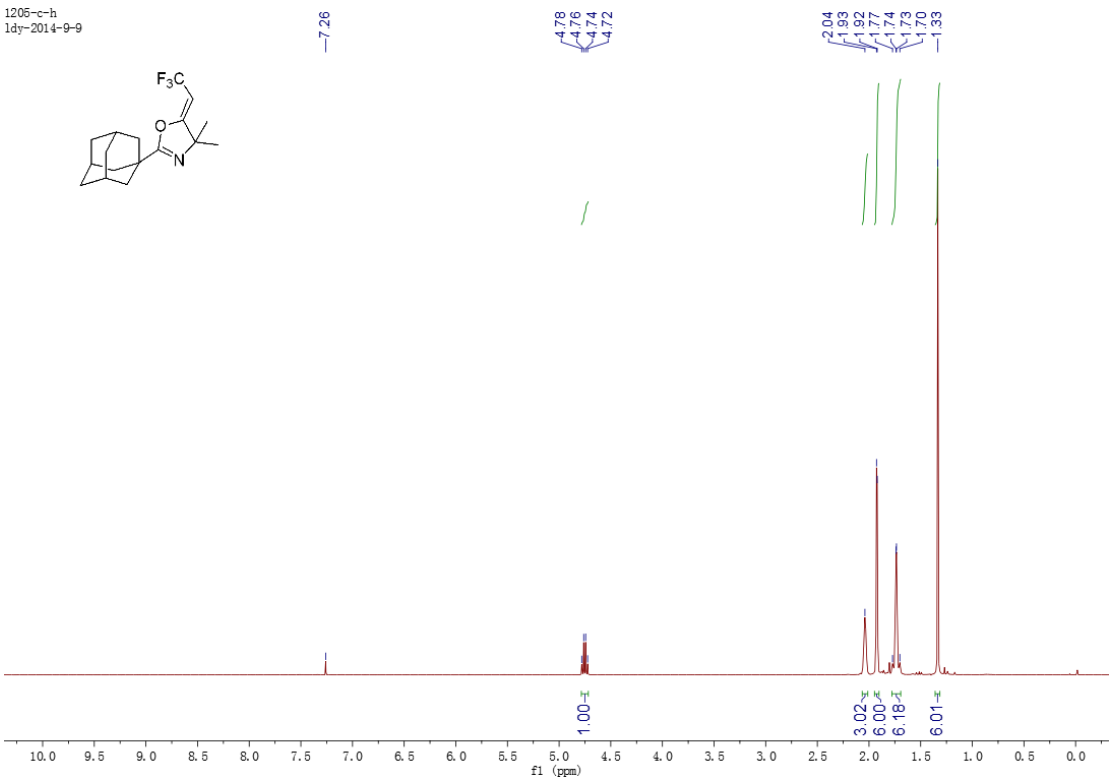

1226-c-f
STANDARD PROTON PARAMETERS
57.49
57.51
F3C
O
N
10
90
80
70
60
50
40
30
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
-250
-270
-290
f1 (ppm)

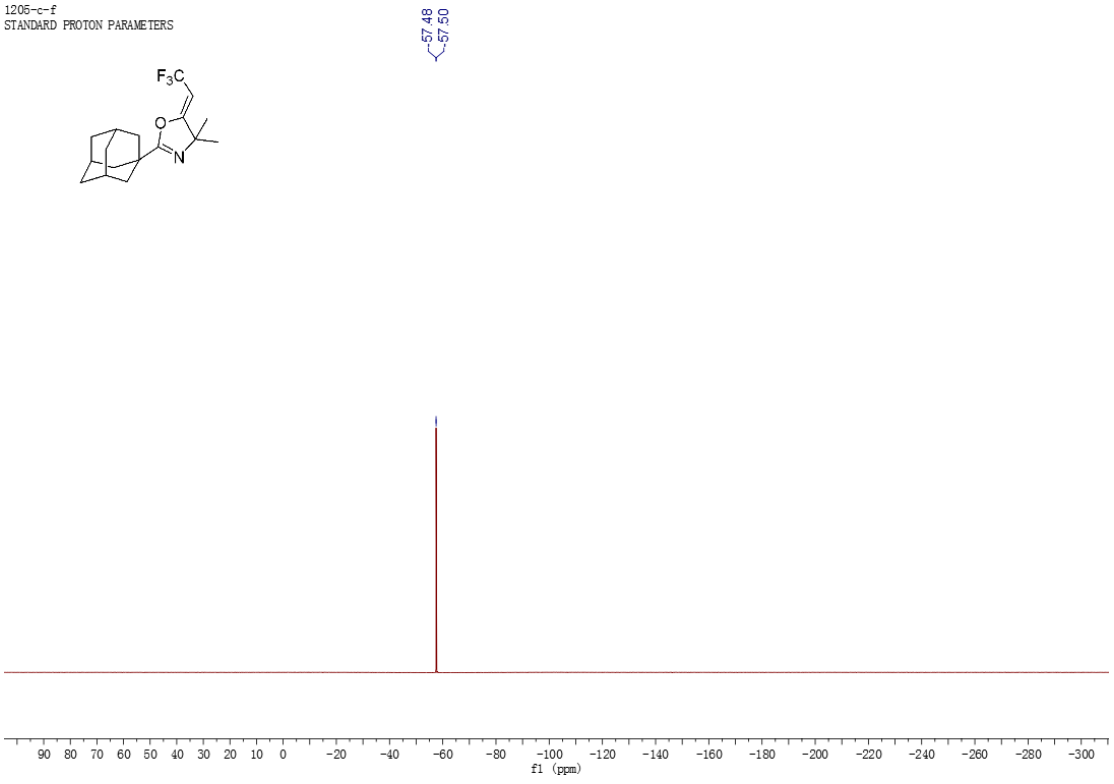

1226-c-c-2
169.41
169.36
169.31
169.26
166.28
127.32
124.69
122.02
119.35
88.39
88.02
87.65
87.28
77.48
77.16
76.84
70.93
37.01
29.43
28.93
28.91
25.81
25.50
F3C
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

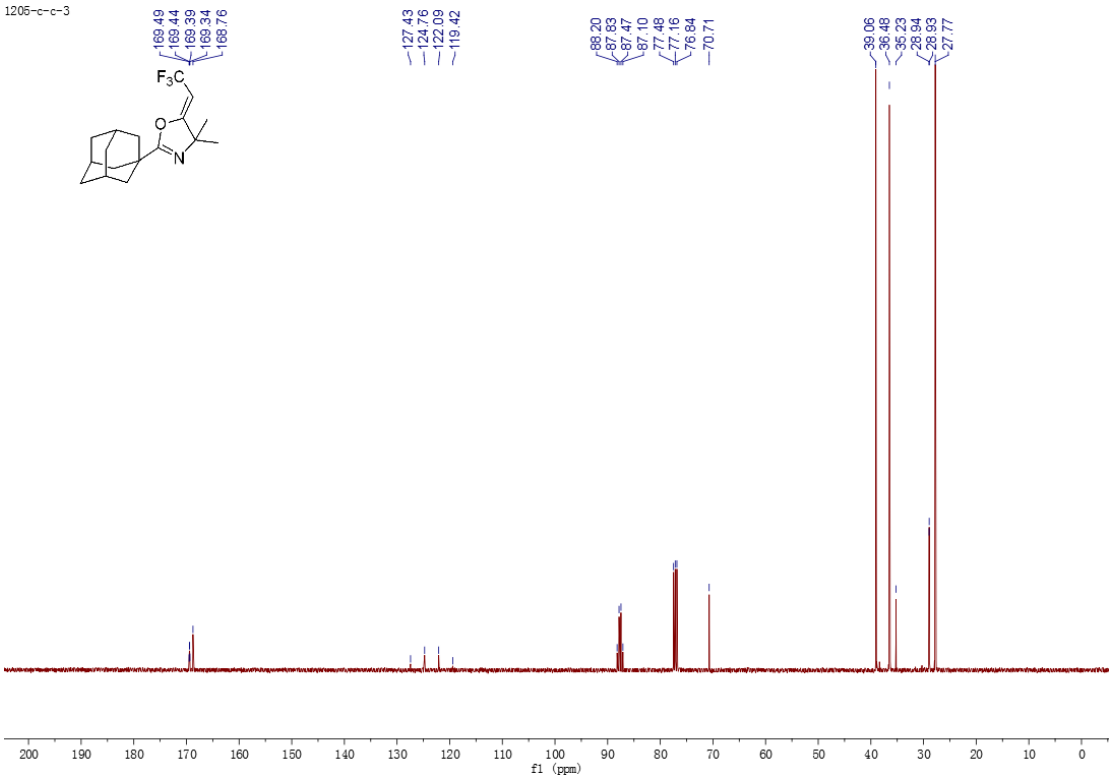

1202.jgw-h
7.26
5.42
5.40
5.38
5.35
2.03
1.89
1.89
1.77
1.74
1.73
1.72
1.69
1.45
CF3
O
N
1.00
3.02
6.03
6.20
6.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

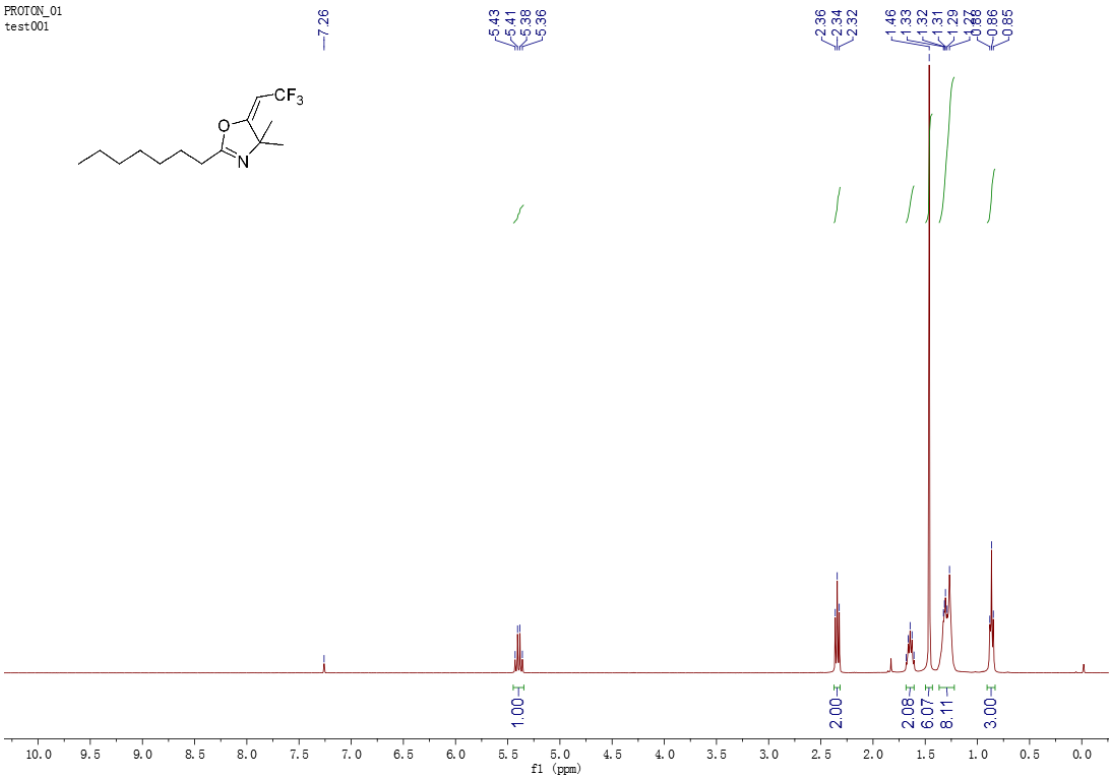

1202.jgw-f
STANDARD PROTON PARAMETERS
53.34
53.36
CF3
O
N
90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300
f1 (ppm)

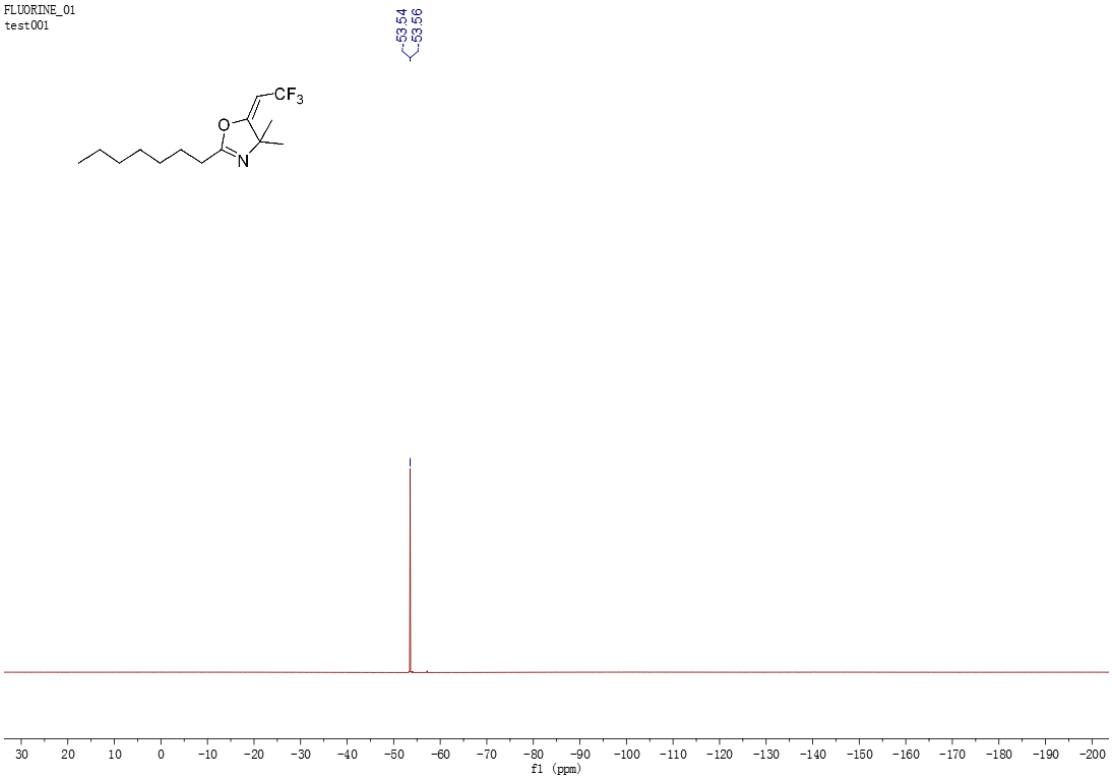

1202.jgw-c-2
170.95
170.89
170.82
170.76
167.40
128.27
125.62
122.97
120.32
92.25
91.87
91.49
91.12
77.31
77.00
76.68
70.33
38.96
36.36
34.79
27.64
26.75
26.71
26.68
26.64
CF3
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

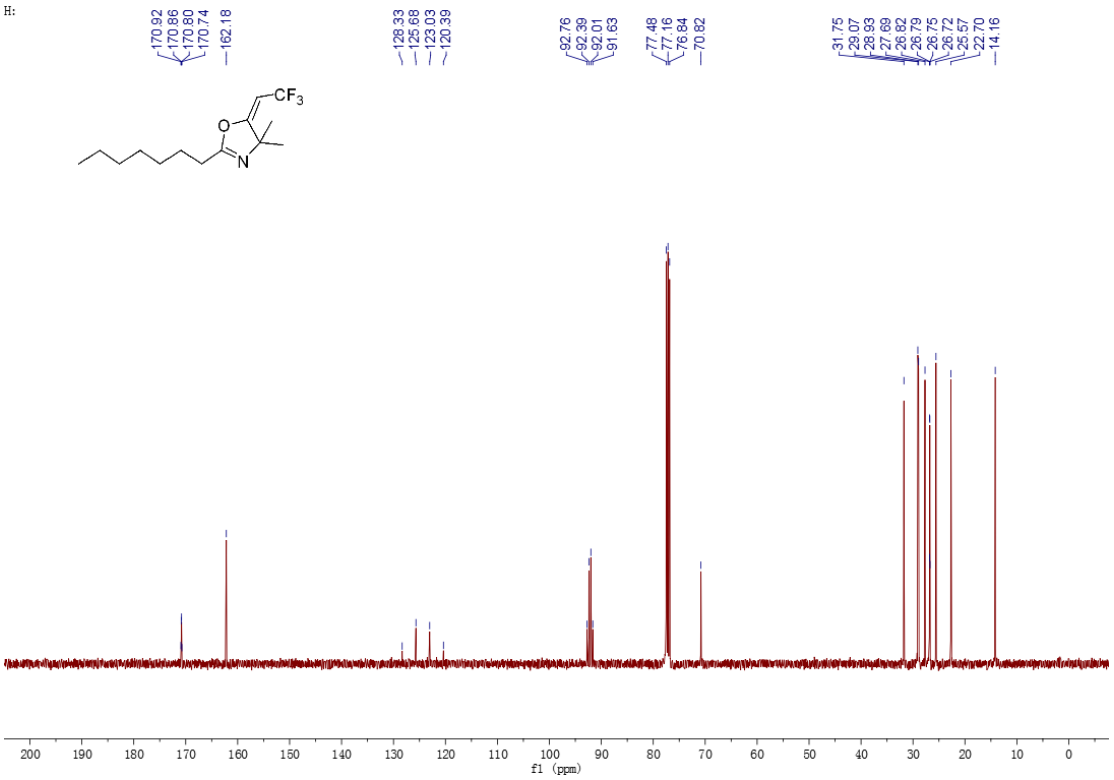

1205-c-h
1dy-2014-9-9
7.26
4.78
4.76
4.74
4.72
2.04
1.93
1.92
1.77
1.74
1.73
1.70
1.33
F3C
O
N
1.00
3.02
6.00
6.18
6.01
f1 (ppm)

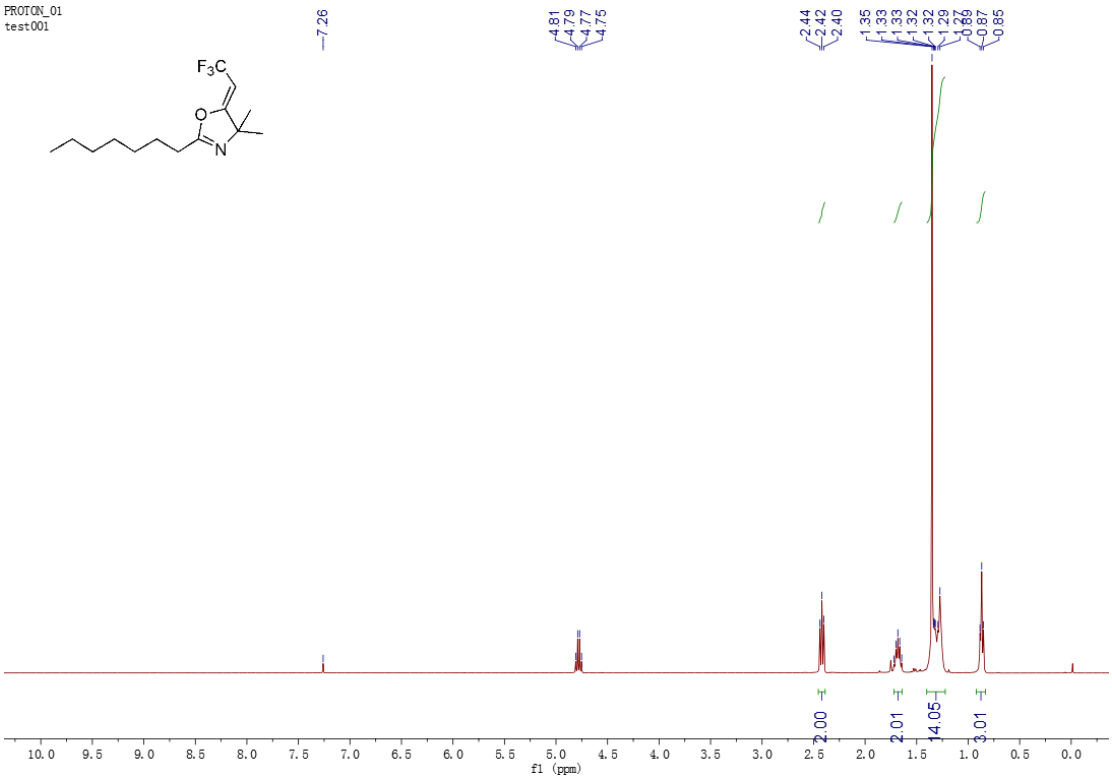

1205-c-f
STANDARD PROTON PARAMETERS
-57.48
-57.50
F3C
O
N
f1 (ppm)

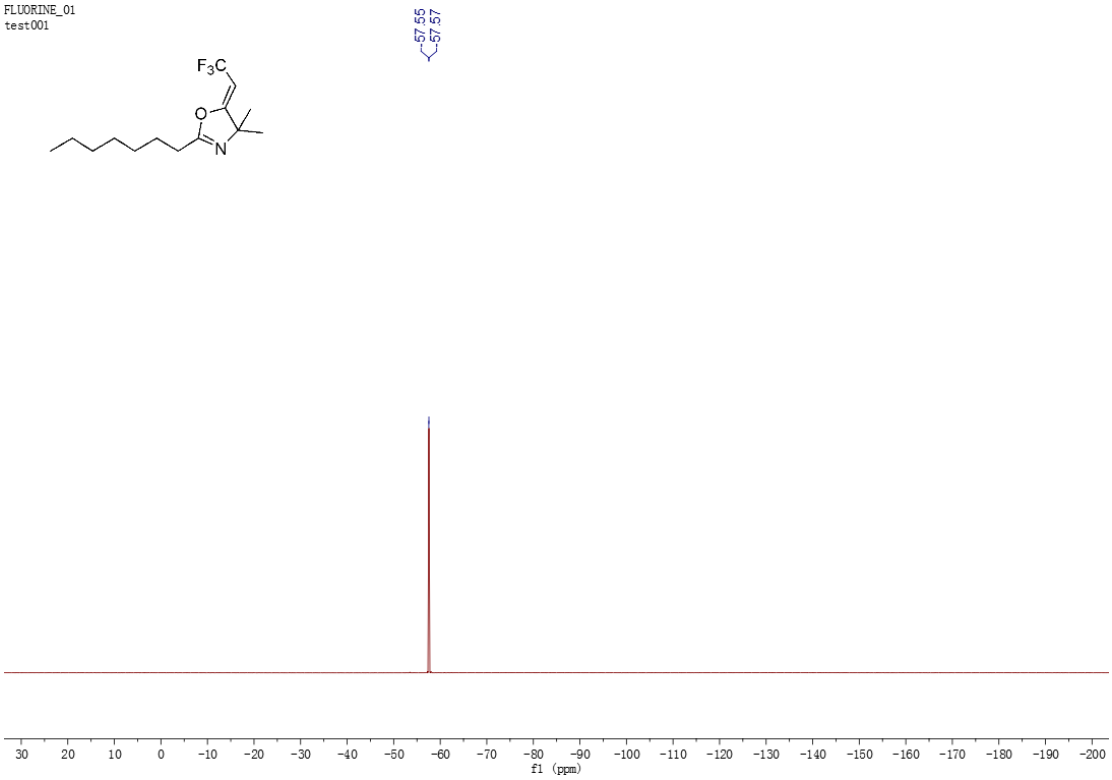

1205-c-c-3
169.49
169.44
169.39
169.34
168.76
127.43
124.76
122.09
119.42
88.20
87.83
87.47
87.10
77.48
77.16
76.84
70.71
39.06
36.48
35.23
28.94
28.93
27.77
F3C
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

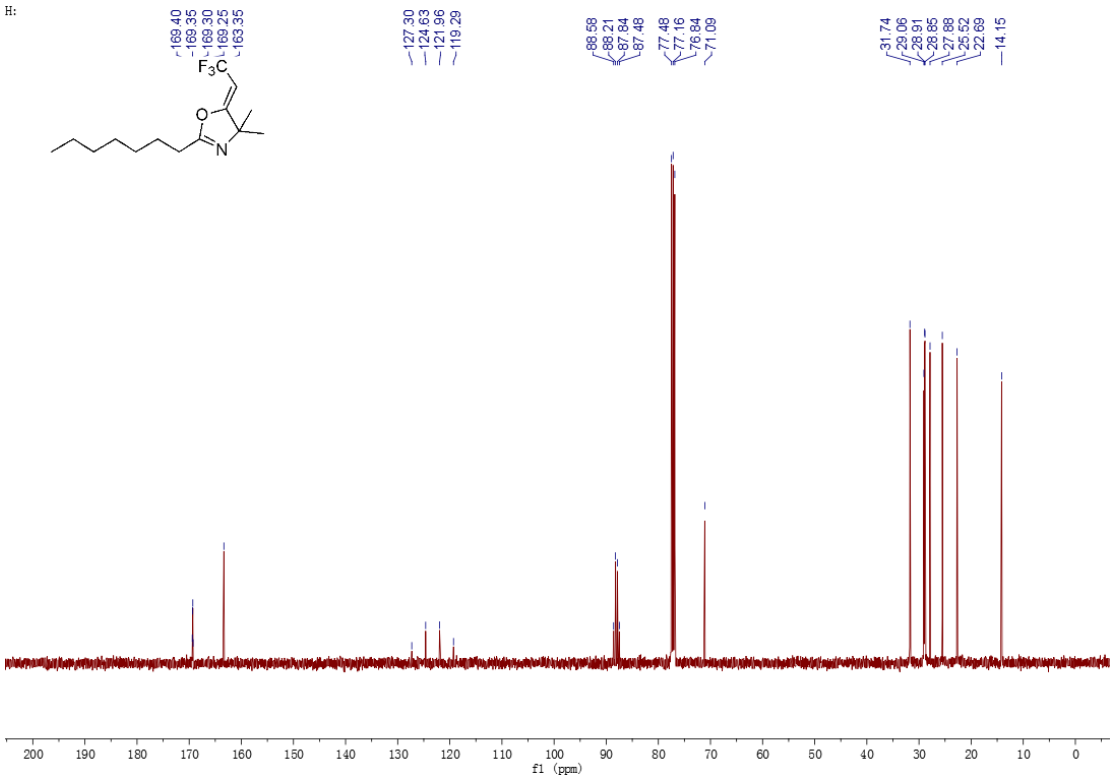

PROTON_01
test001
7.26
5.43
5.41
5.38
5.36
2.36
2.34
2.32
1.46
1.33
1.32
1.31
1.29
0.88
0.86
0.85
CF3
O
N
1.00
2.00
2.08
6.07
8.11
3.00
f1 (ppm)

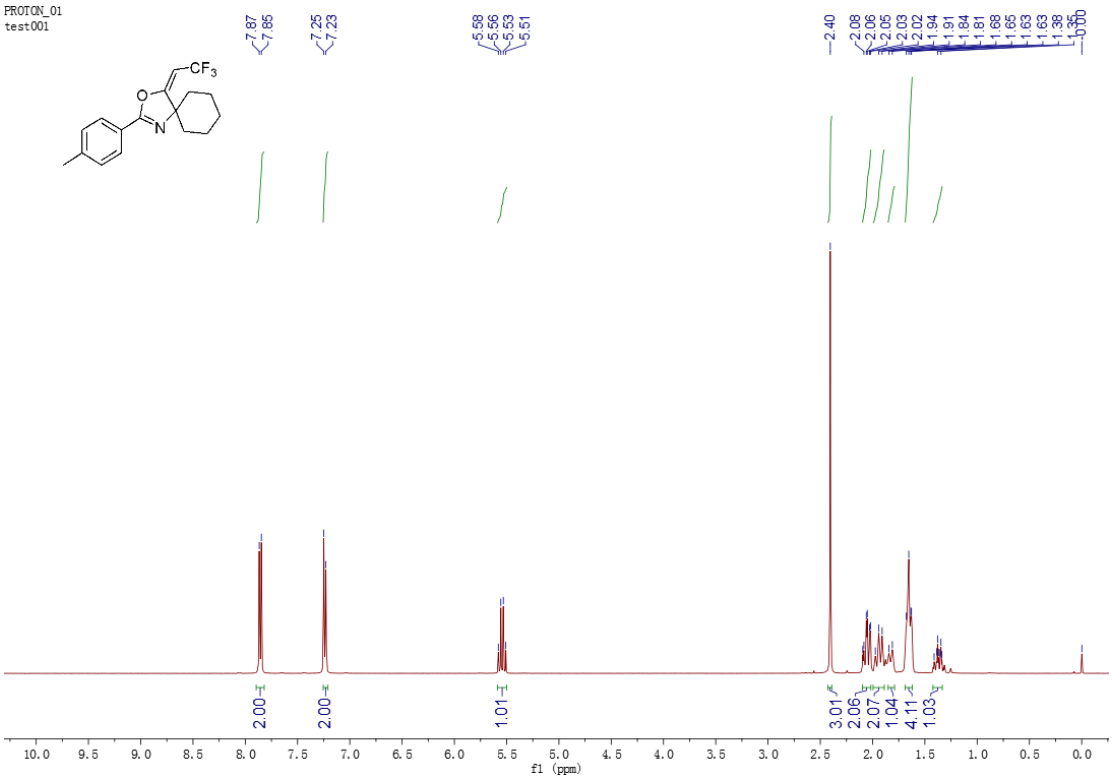

FLUORINE_01
test001
-53.54
-53.56
CF3
O
N
f1 (ppm)

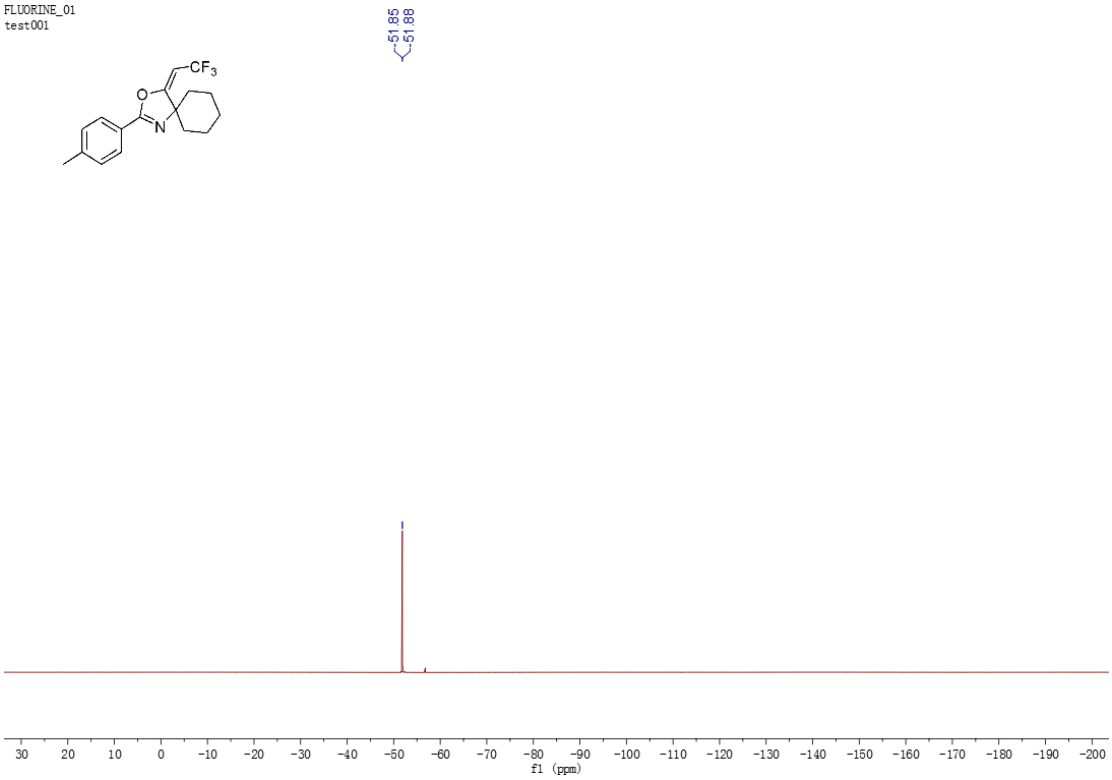

H:
170.92
170.86
170.80
170.74
162.18
128.33
125.68
123.03
120.39
92.76
92.39
92.01
91.63
77.48
77.16
76.84
70.82
31.75
29.07
28.93
27.69
26.82
26.79
26.75
26.72
25.57
22.70
14.16
CF3
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

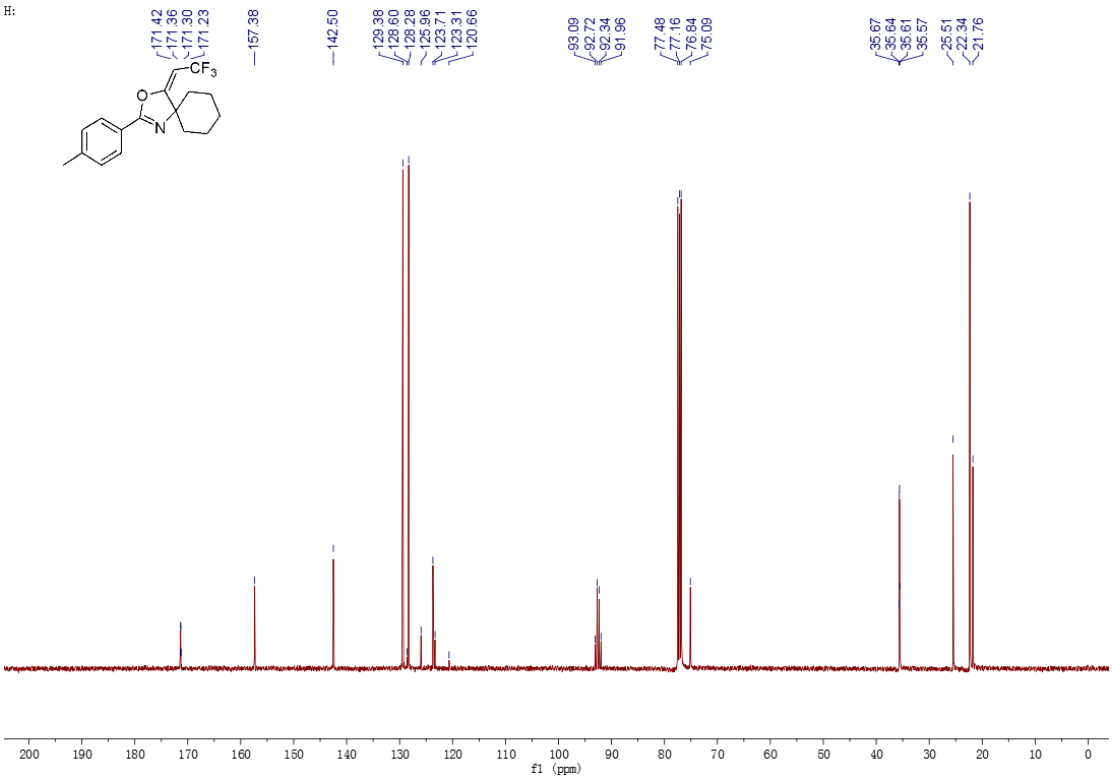

PROTON_01
test001
7.26
4.81
4.79
4.77
4.75
2.44
2.42
2.40
1.35
1.33
1.33
1.32
1.32
1.29
0.89
0.87
0.85
F3C
O
N
2.00
2.01
14.05
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

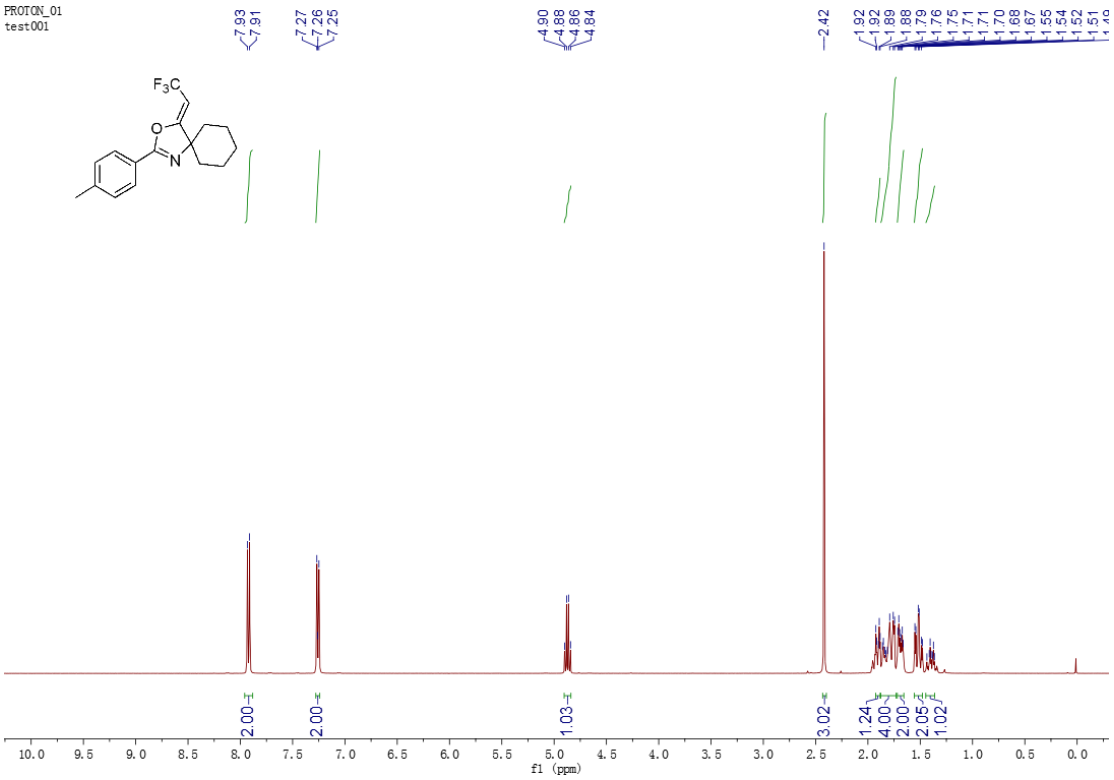

FLUORINE_01
test001
-57.55
-57.57
F3C
O
N
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

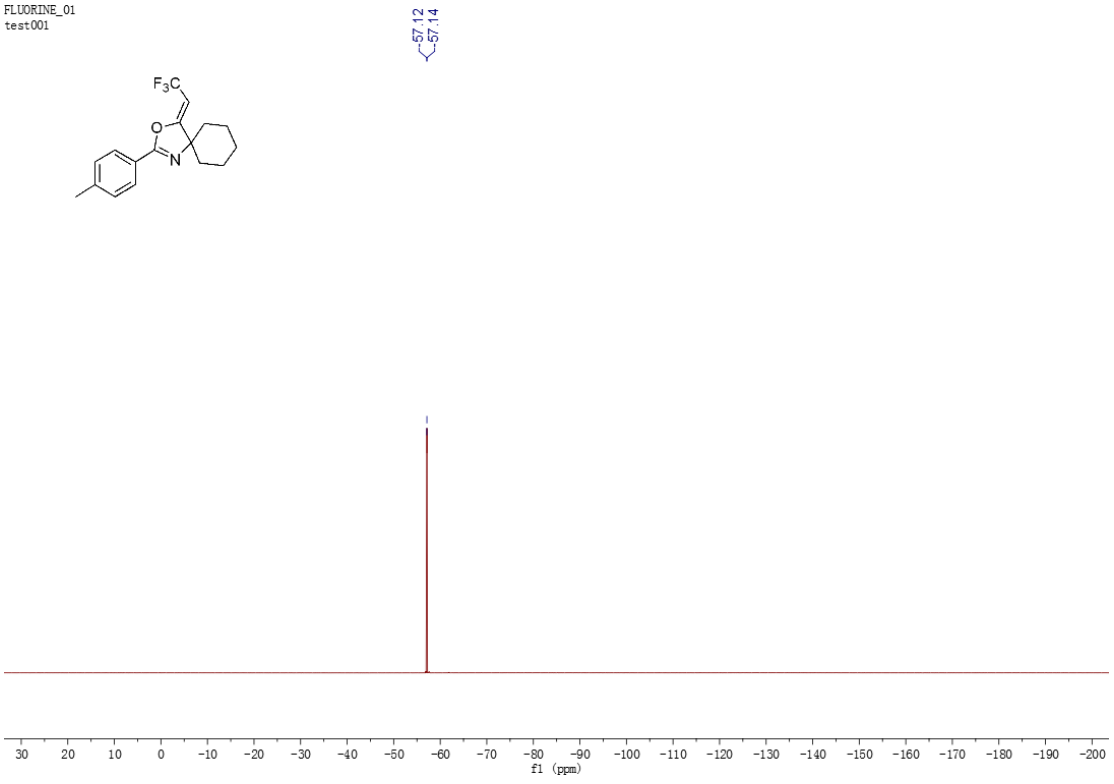

H:
169.40
169.35
169.30
169.25
163.35
127.30
124.63
121.96
119.29
88.58
88.21
87.84
87.48
77.48
77.16
76.84
71.09
31.74
29.06
28.91
28.85
27.88
25.52
22.69
14.15
F3C
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

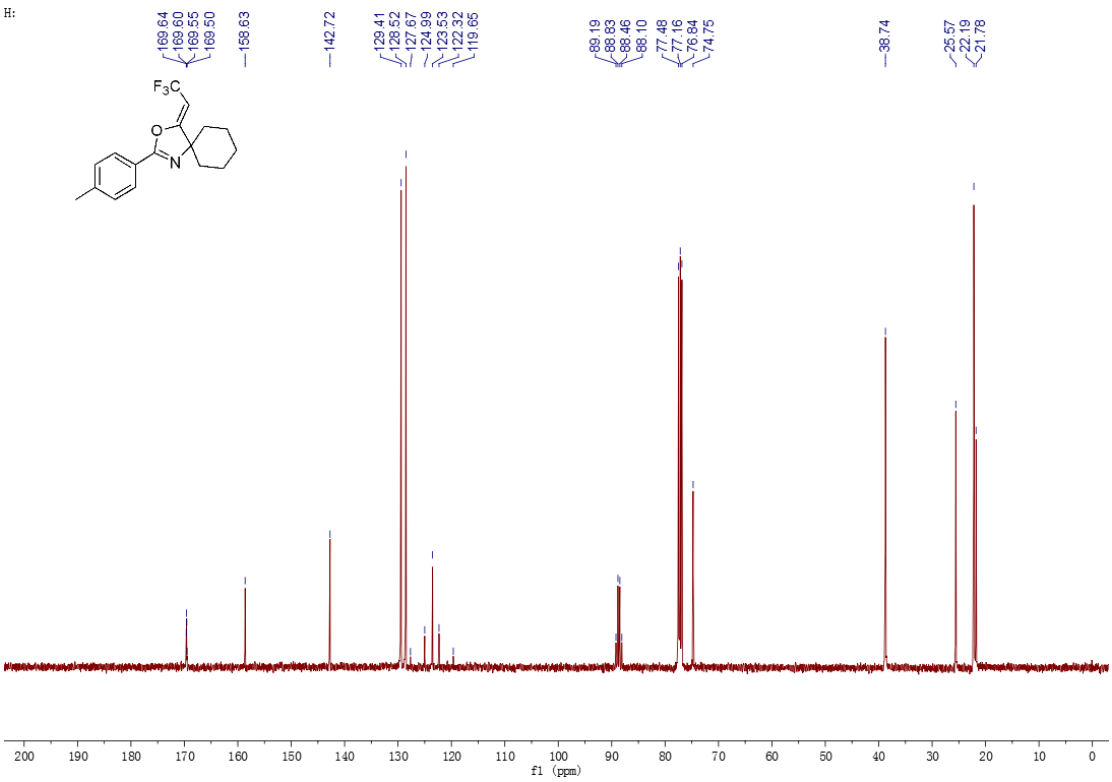

PROTON_01
test001
7.87
7.85
7.25
7.23
5.58
5.56
5.53
5.51
2.40
2.08
2.06
2.05
2.03
2.02
1.94
1.91
1.84
1.81
1.68
1.65
1.63
1.38
1.35
0.00
CF3
O
N
2.00
2.00
1.01
3.01
2.06
2.07
1.04
4.11
1.03
f1 (ppm)

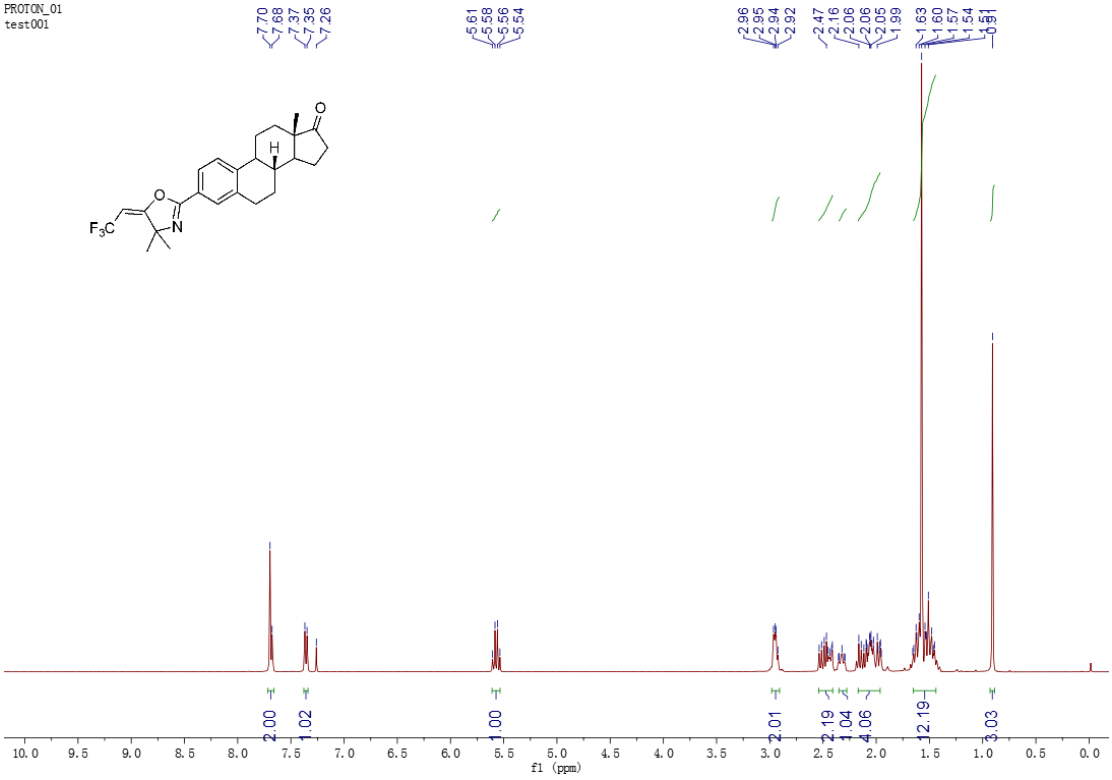

FLUORINE_01
test001
-51.85
-51.88
CF3
O
N
f1 (ppm)

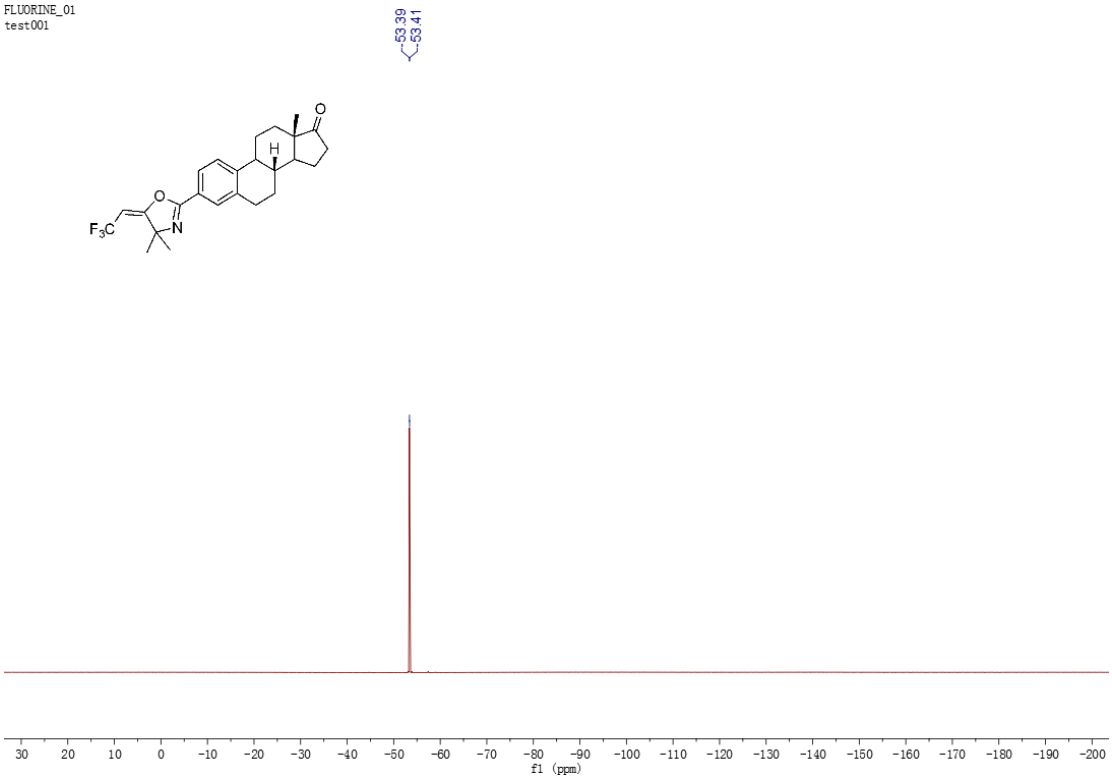

H:
171.42
171.36
171.30
171.23
157.38
142.50
129.38
128.60
128.28
125.96
123.71
123.31
120.66
93.09
92.72
92.34
91.96
77.48
77.16
76.84
75.09
35.67
35.64
35.61
35.57
25.51
22.34
21.76
CF3
O
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

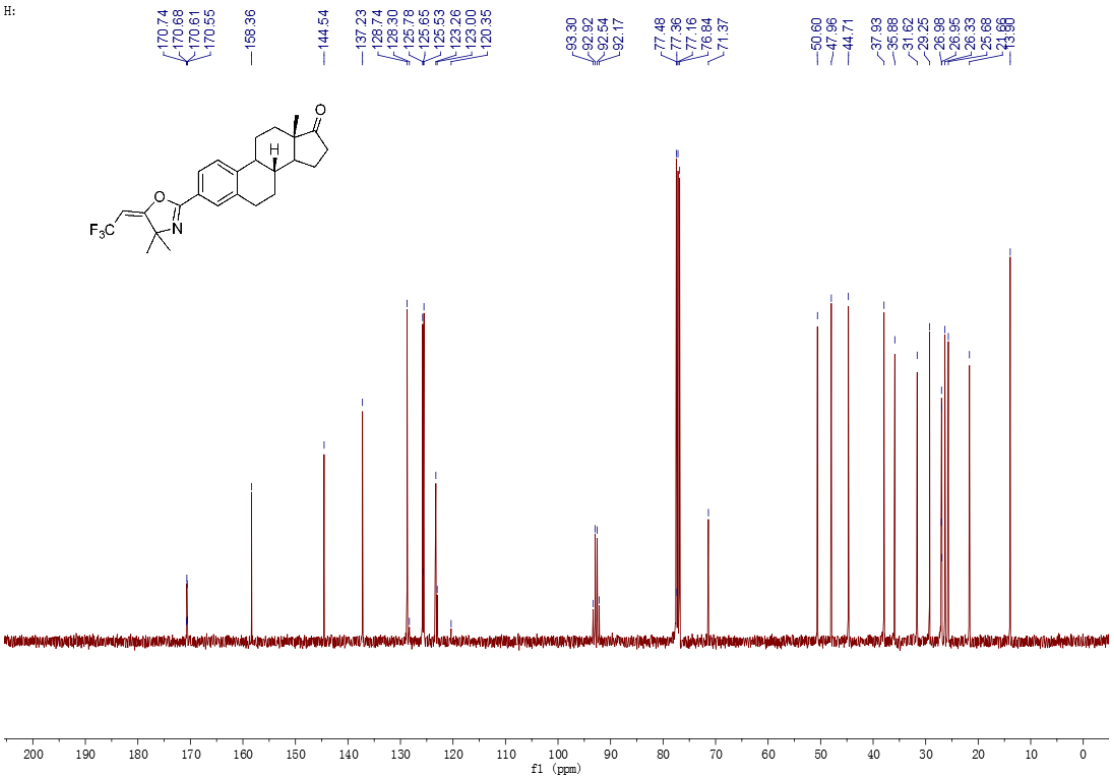

PROTON_01
test001
7.93
7.91
7.27
7.26
7.25
4.90
4.88
4.86
4.84
2.42
1.92
1.92
1.89
1.88
1.79
1.76
1.75
1.71
1.71
1.70
1.68
1.67
1.55
1.54
1.52
1.51
F3C
O
N
2.00
2.00
1.03
3.02
1.24
4.00
2.00
2.05
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

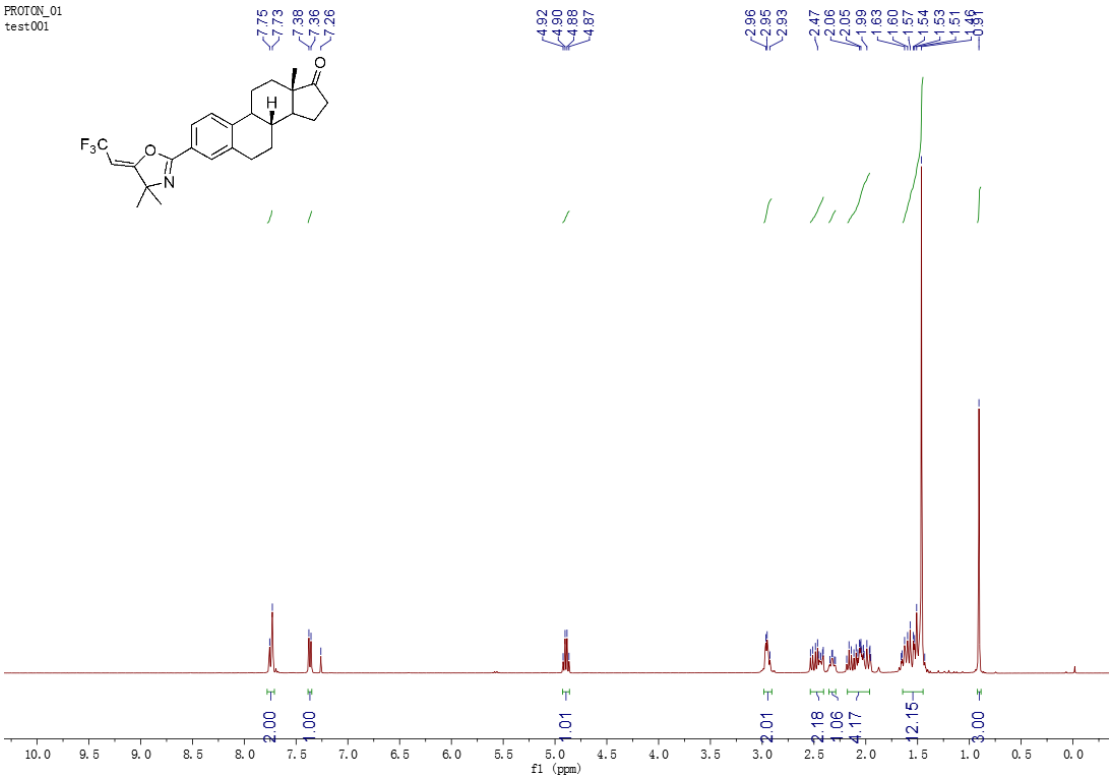

FLUORINE_01
test001
-57.12
-57.14
F3C
O
N
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

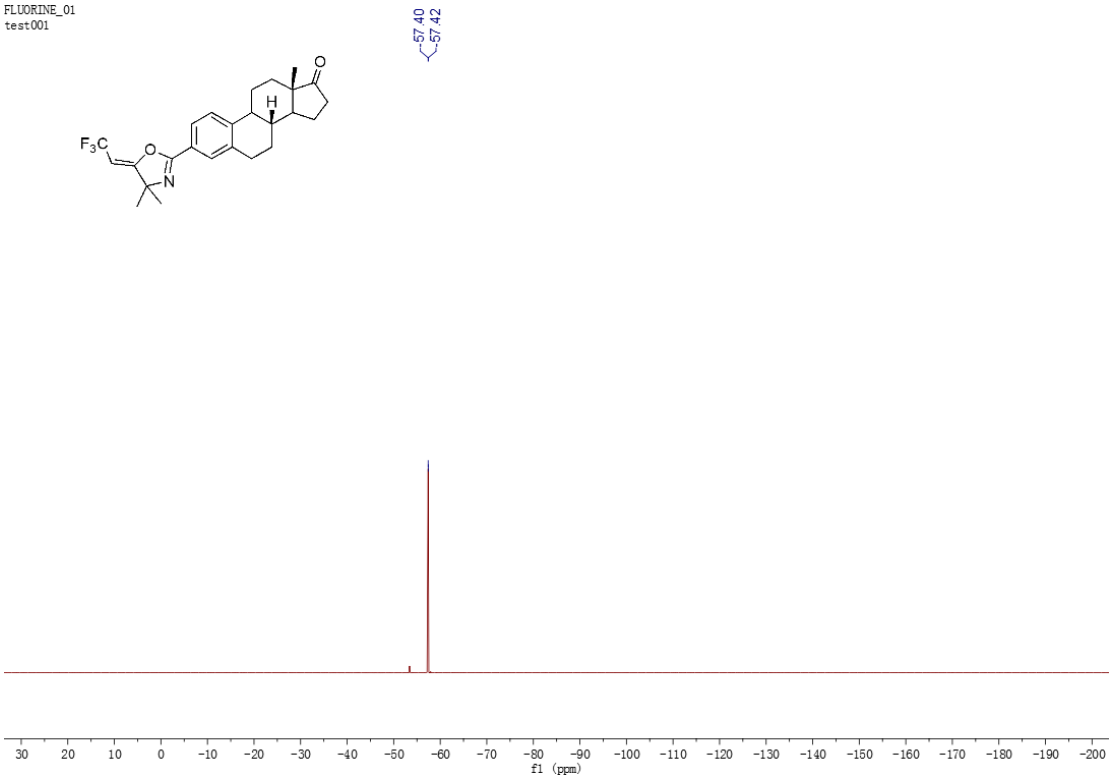

H:
169.64
169.60
169.55
169.50
158.63
142.72
129.41
128.52
127.67
124.99
123.53
122.32
119.65
89.19
88.83
88.46
88.10
77.48
77.16
76.84
74.75
38.74
25.57
22.19
21.78
F3C
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

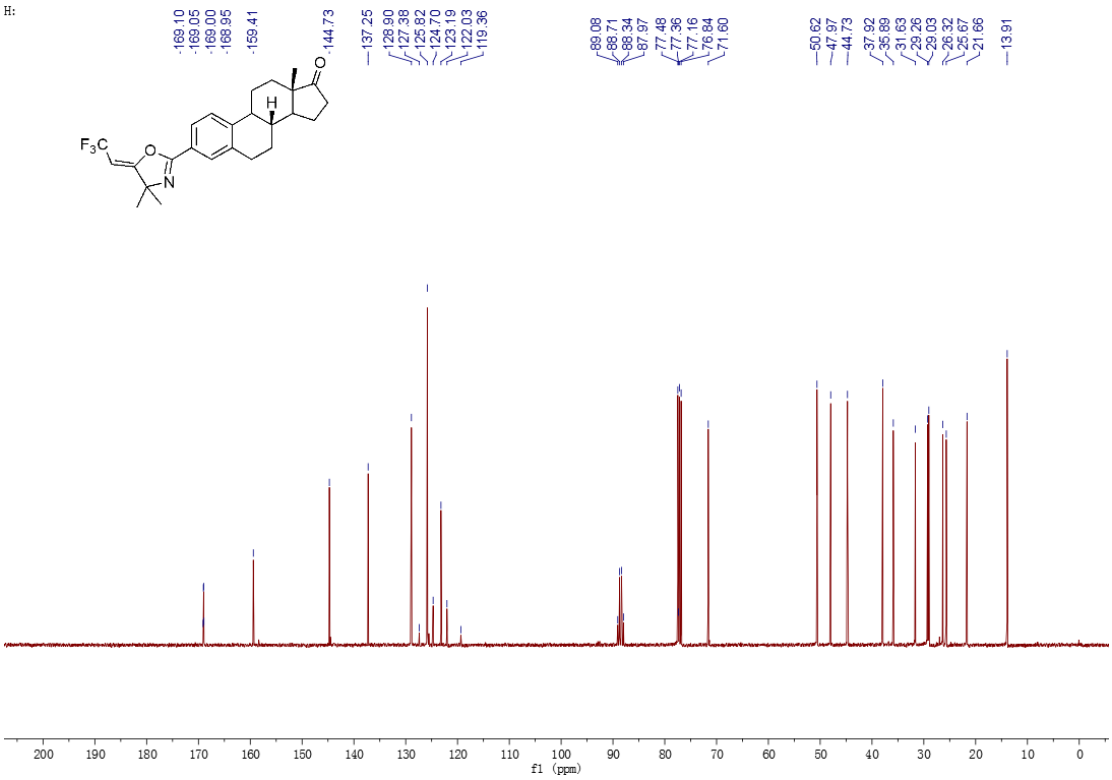

PROTON_01
test001
7.70
7.68
7.37
7.35
7.26
5.61
5.58
5.56
5.54
2.96
2.95
2.94
2.92
2.47
2.16
2.06
2.06
2.05
1.99
1.63
1.60
1.57
1.54
0.91
2.00
1.02
1.00
2.01
2.19
1.04
4.06
12.19
3.03
f1 (ppm)

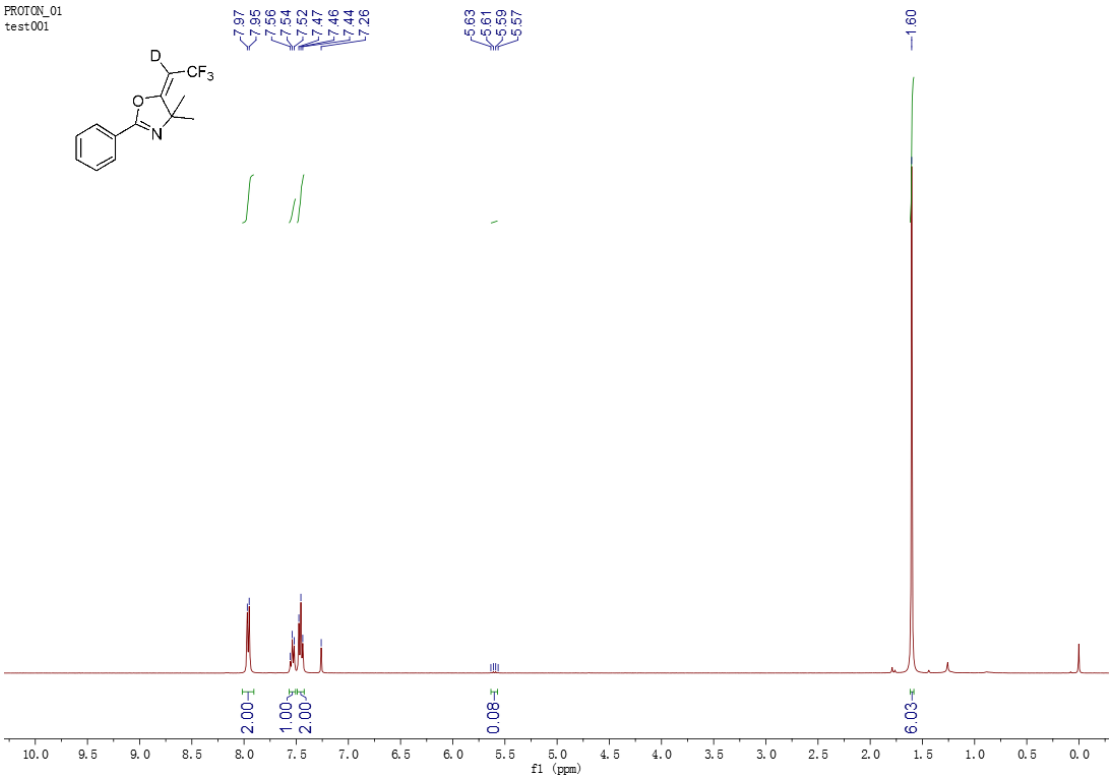

FLUORINE_01
test001
-53.39
-53.41
f1 (ppm)

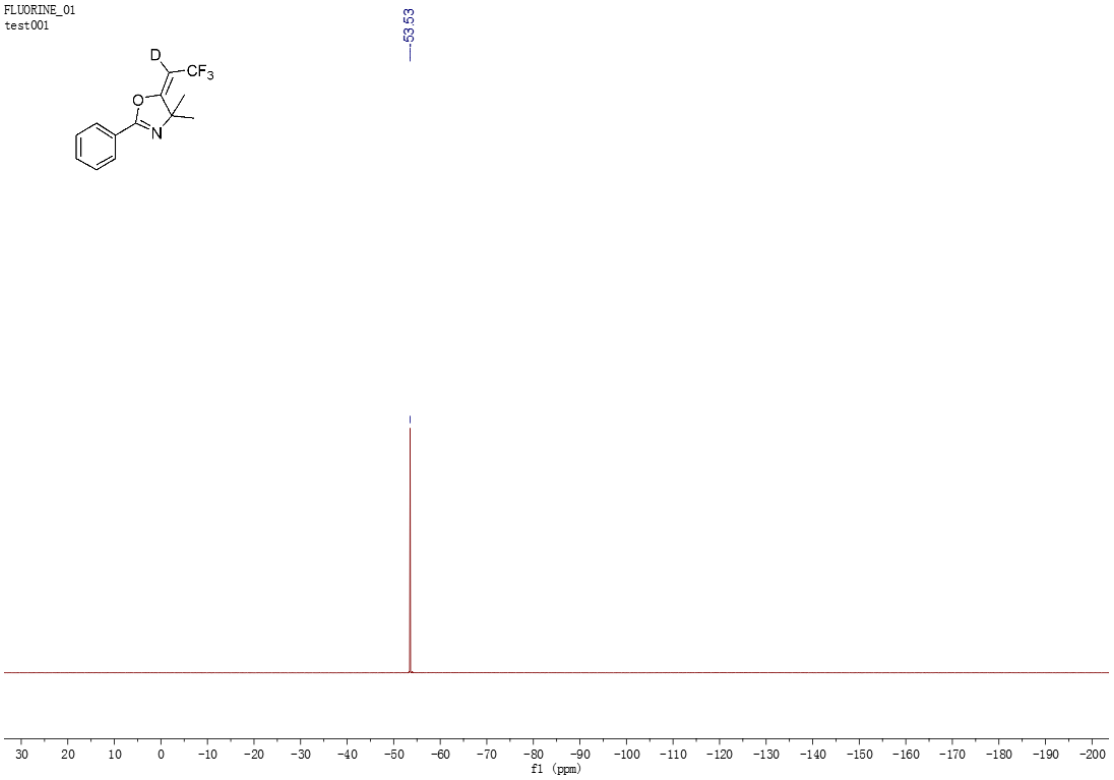

H:
170.74
170.68
170.61
170.55
158.36
144.54
137.23
128.74
128.30
125.78
125.65
125.53
123.26
123.00
120.35
93.30
92.92
92.54
92.17
77.48
77.36
77.16
76.84
71.37
50.60
47.96
44.71
37.93
35.88
31.62
29.25
26.98
26.95
26.33
25.68
21.86
13.90
O
H
O
N
F3C
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

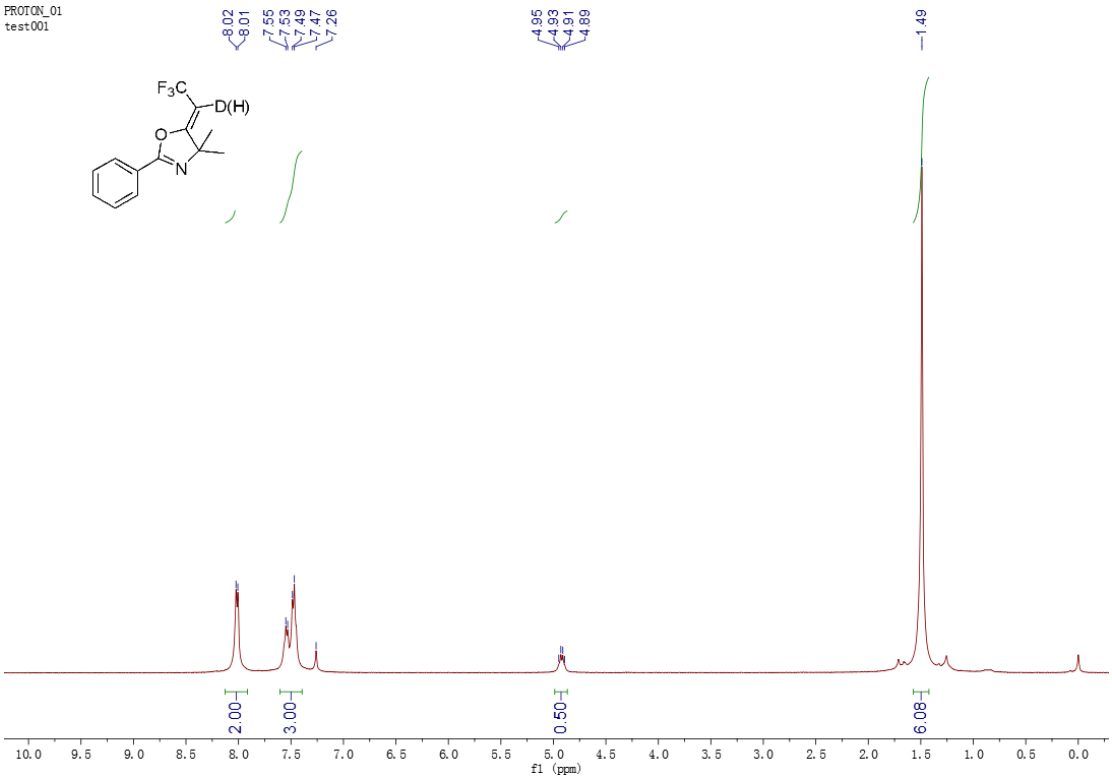

PROTON_01
test001
7.75
7.73
7.38
7.36
7.26
4.92
4.90
4.88
4.87
2.96
2.95
2.93
2.47
2.06
2.05
1.99
1.63
1.60
1.57
1.54
1.53
1.51
1.46
0.91
F3C
O
N
H
2.00
1.00
1.01
2.01
2.18
1.06
4.17
12.15
3.00
f1 (ppm)

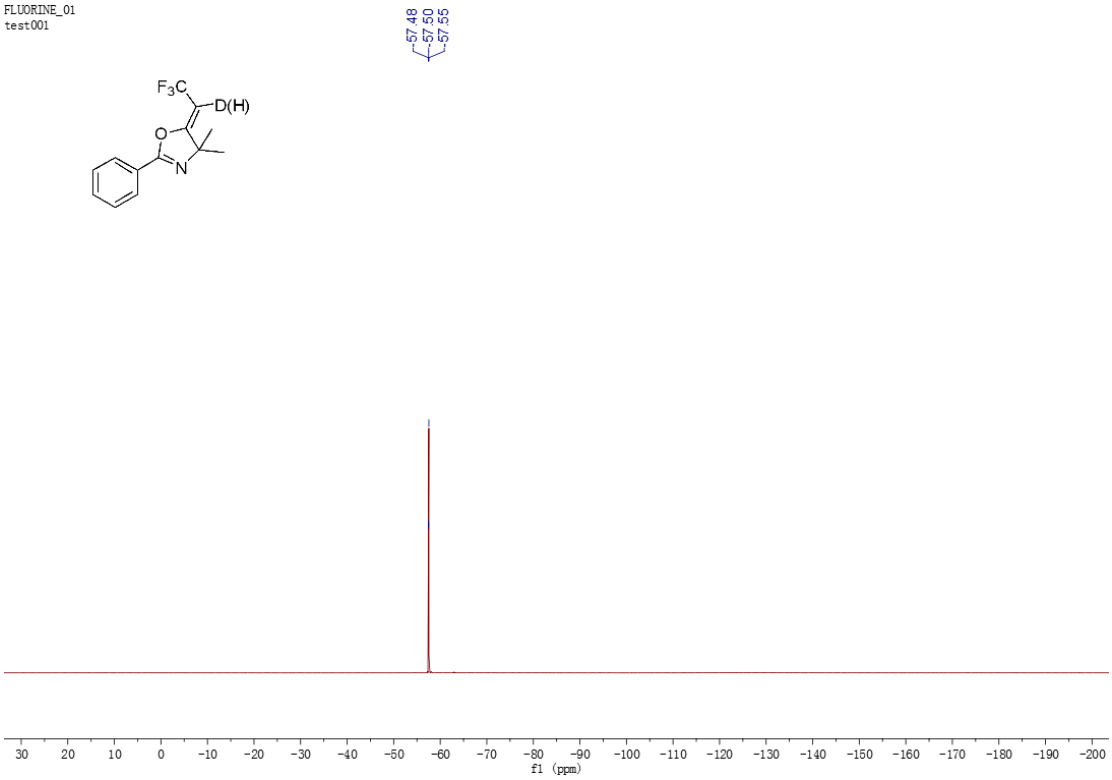

FLUORINE_01
test001
-57.40
-57.42
F3C
O
N
H
f1 (ppm)

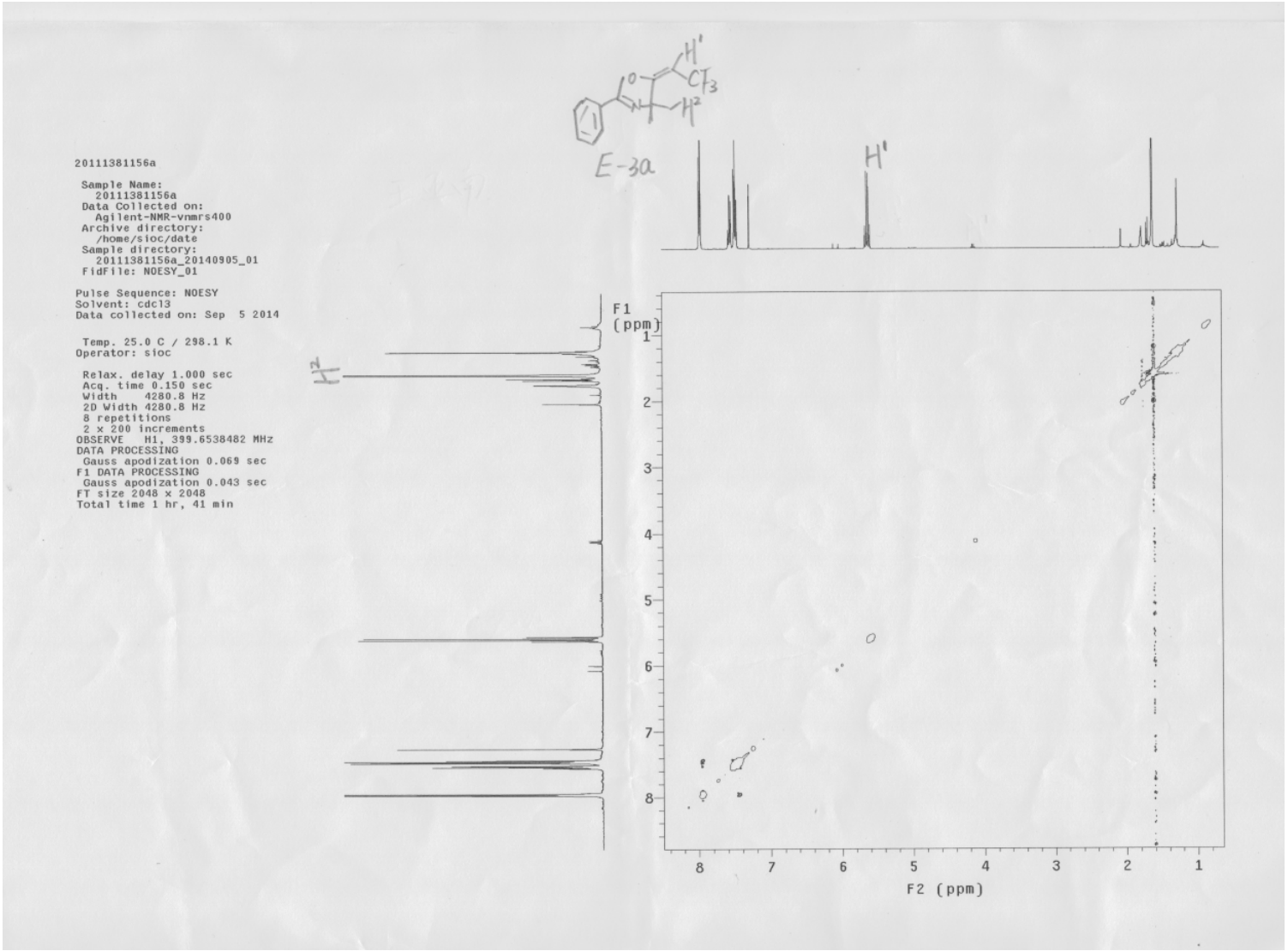

H:
169.10
169.05
169.00
168.95
159.41
144.73
137.25
128.90
127.38
125.82
124.70
123.19
122.03
119.36
89.08
88.71
88.34
87.97
77.48
77.36
77.16
76.84
71.60
50.62
47.97
44.73
37.92
35.89
31.63
29.26
29.03
26.32
25.67
21.66
13.91
F3C
O
N
H
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

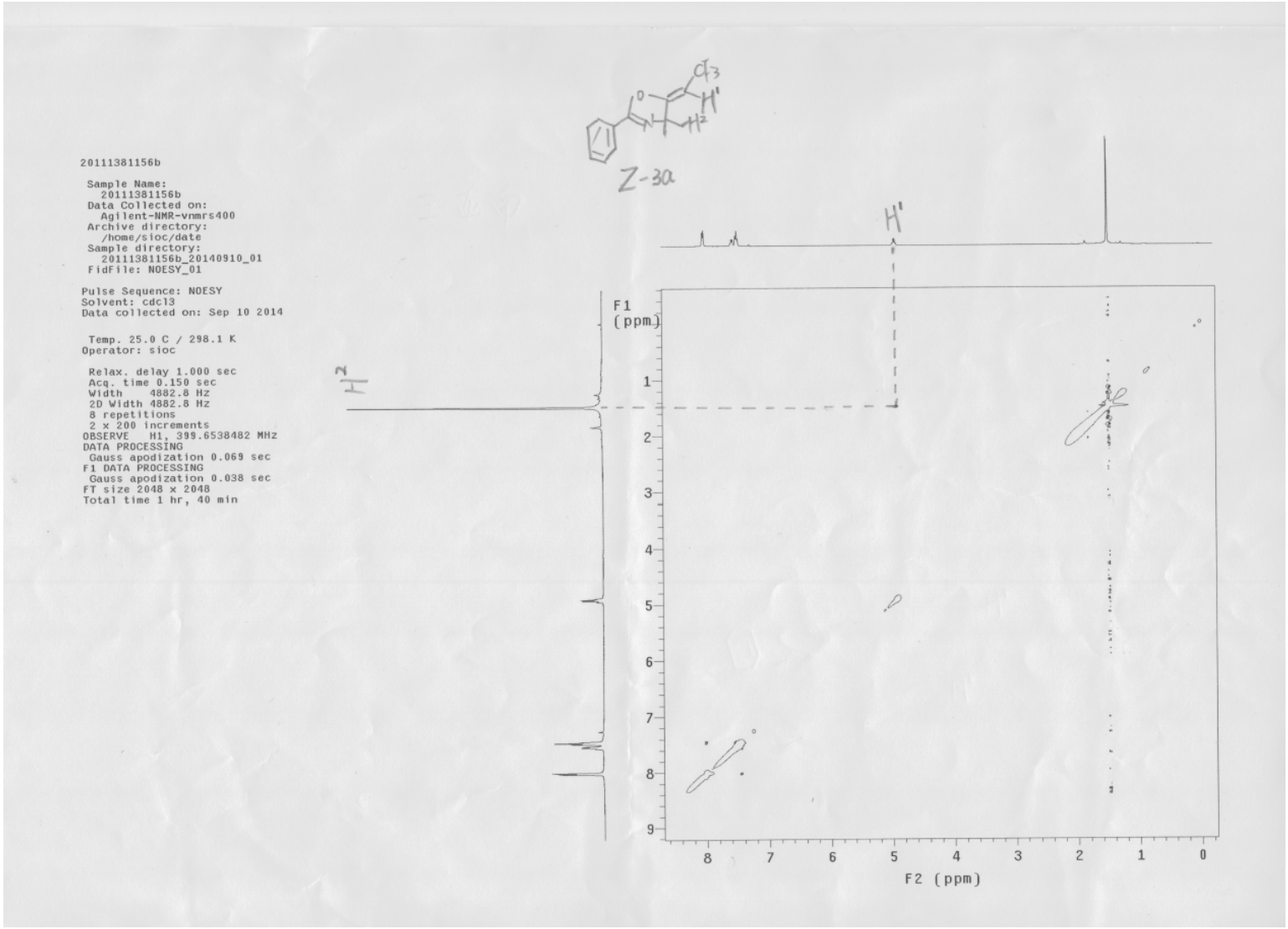

PROTON_01
test001
7.97
7.95
7.56
7.54
7.52
7.47
7.46
7.44
7.26
5.63
5.61
5.59
5.57
1.60
D
CF3
O
N
2.00
1.00
2.00
0.08
6.03
f1 (ppm)


FLUORINE_01
test001
-53.53
D
CF3
O
N
f1 (ppm)


PROTON_01
test001
8.02
8.01
7.55
7.53
7.49
7.47
7.26
4.95
4.93
4.91
4.89
1.49
F3C
D(H)
O
N
2.00
3.00
0.50
6.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


FLUORINE_01
test001
-57.48
-57.50
-57.55
F3C
D(H)
O
N
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


20111381156a
Sample Name:
20111381156a
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/sioc/date
Sample directory:
20111381156a_20140905_01
FidFile: NOESY_01
Pulse Sequence: NOESY
Solvent: cdcl3
Data collected on: Sep 5 2014
Temp. 25.0 C / 298.1 K
Operator: sioc
Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 4280.8 Hz
2D Width 4280.8 Hz
8 repetitions
2 x 200 increments
OBSERVE H1, 399.6538482 MHz
DATA PROCESSING
Gauss apodization 0.069 sec
F1 DATA PROCESSING
Gauss apodization 0.043 sec
FT size 2048 x 2048
Total time 1 hr, 41 min
E-3a
H'
H²
F1 (ppm)
F2 (ppm)


20111381156b
Sample Name:
20111381156b
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
/home/sioc/date
Sample directory:
20111381156b_20140910_01
FidFile: NOESY_01
Pulse Sequence: NOESY
Solvent: cdcl3
Data collected on: Sep 10 2014
Temp. 25.0 C / 298.1 K
Operator: sioc
Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 4882.8 Hz
2D Width 4882.8 Hz
8 repetitions
2 x 200 increments
OBSERVE H1, 399.6538482 MHz
DATA PROCESSING
Gauss apodization 0.069 sec
F1 DATA PROCESSING
Gauss apodization 0.038 sec
FT size 2048 x 2048
Total time 1 hr, 40 min
Z-3a
H'
H2
F1 (ppm)
F2 (ppm)