Supporting Information

One-Pot Synthesis of 3-Fluoroflavones *via* 1-(2- Hydroxyphenyl)-3-phenylpropane-1,3-diones and Selectfluor at Room Temperature

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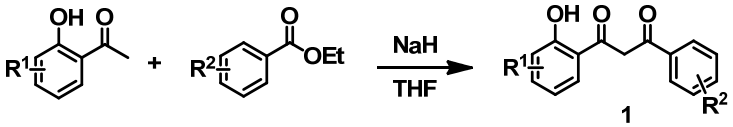
1. Synthetic Schemes.

Synthesis of 1-(2-Hydroxyphenyl)-3-phenylpropane-1,3-diones (1a-1s, 1u-1x)[1, 2]

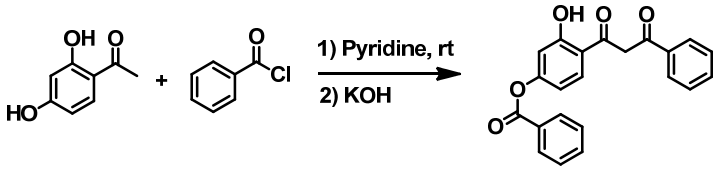
Sodium hydride (60 % in mineral oil; 1.76 g, 44.1 mmol) was suspended in THF (10 mL) at room temperature. A mixture of 1-(2-hydroxyphenyl)ethanone (1.50 g, 11mmol) and ethyl benzoate (4.13 g, 27.5mmol) in THF (2.5 mL) was added dropwise to the stirred suspension of sodium hydride. After completing the addition, the solution was heated at 65 °C stirring for 2 h. Then poured into crushed ice and acidified to pH = 6 with HCl and extracted with ethyl acetate (20 mL, ×3). Finally, the organic layer was combined, dried over Na_2SO_4, evaporated and purified by column chromatography (petroleum ether / ethyl acetate 15 : 1 as eluent) to gave 1-(2-Hydroxyphenyl)-3-phenylpropane-1,3-dione **1a** (1.9 g, 72%) as a yellow solid. Similarly, compounds **1a-1s** and **1u-1x** were prepared with the same method.



R^1 = H, Me, OMe, F, Br; R^2 = H, Me, OMe, F, COOEt, CF_3

Synthesis of 3-hydroxy-4-(3-oxo-3-phenylpropanoyl)phenyl benzoate (1t)[3]

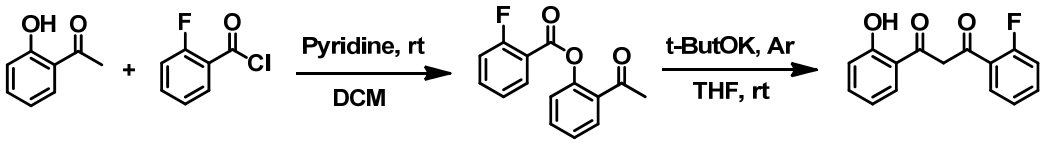
To a solution of benzoyl chloride (0.035 mol) and dry distilled pyridine (5 mL) was added 1-(2,4-dihydroxyphenyl)ethanone (0.025 mol) at room temperature. After 0.5 h, the mixture was poured into 120ml of 1M hydrochloric acid containing 50g of crushed ice. Then filtered and washed with ice-cold methanol and water, after recrystallized with ethanol, filtered and dried, 4-acetyl-1,3-phenylene dibenzoate was obtained. The 4-acetyl-1,3-phenylene dibenzoate (0.02 mol) was dissolved in 18ml of dry pyridine stirring at 50 °C, then potassium hydroxide (0.03 mol) was added which was preheated in an oven at 100 °C and was stirred for 2 h. The mixture was acidified with 10% aqueous acetic acid. The pale yellow precipitate was filtered and recrystallized with ethanol to give the product **1t**.



Synthesis of 1-(2-fluorophenyl)-3-(2-hydroxyphenyl)propane-1,3-dione (1y)[4]

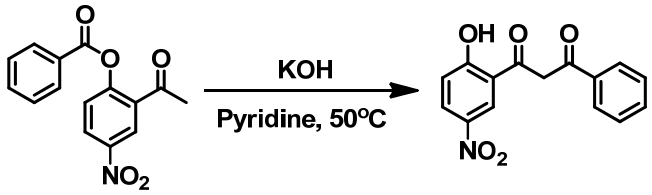
2-fluorobenzoyl chloride (1.9 g, 12.0mmol) in dichloromethane (10 mL) was added dropwise to the mixture of 2′-hydroxyacetophenone (1.8 g, 12.0mmol) and pyridine (2.88 mL, 36 mmol) in dichloromethane (30 mL) at 0 °C. After 1 h, the mixture was stirred at room temperature for 2 h. Then the mixture was washed with 3 M aqueous HCl and water,

the organic layer was dried over Na_2SO_4 and concentrated to get 2-acetylphenyl 2-fluorobenzoate. To a solution of 2-acetylphenyl 2-fluorobenzoate (3.0 mmol) in THF (25 mL) was added potassium tert-butoxide (438 mg, 3.9 mmol). The reaction mixture was stirred at room temperature for 12 h under argon and then was acidified to pH = 6 with 2 N aqueous HCl. The mixture was evaporated under vacuum to remove the THF. Then filtered and washed with hexane to get the product 1-(2-fluorophenyl)-3-(2-hydroxyphenyl)propane-1,3-dione.



Synthesis of 1-(2-hydroxy-5-nitrophenyl)-3-phenylpropane-1,3-dione (1z)[5]

The 2-acetyl-4-nitrophenyl benzoate (0.855 g, 3.0 mmol) was dissolved in pyridine (20 mL). The solution was heated to 50 °C and the pulverized potassium hydroxide (1.34 g, 24 mmol) was added. The reaction mixture was stirred for 12 h, after the staring material was consumed completely, The mixture was acidified with 20 mL of 10% aqueous acetic acid solution. The yellow precipitate was filtered and recrystallized with ethanol to give the product **1z.**



2. X-ray Parameters and Structures of 2v'

Table 1. Crystal data and structure refinement for 2v'

Empirical formula	$C_{16}H_{10}F_2O_3$
CCDC	1583436
Formula weight	288.24
Temperature/K	152.99
Crystal system	triclinic
Space group	P-1
a/Å	7.0746(17)
b/Å	8.499(2)
c/Å	10.459(2)
α/°	92.779(6)
β/°	104.832(6)
γ/°	93.958(6)

Volume/Å^3	605.0(2)
Z	2
ρ_{calc}g/cm^3	1.582
μ/mm^{-1}	1.108
F(000)	296.0
Crystal size/mm^3	0.5 × 0.4 × 0.3
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	10.458 to 136.618
Index ranges	-8 ≤ h ≤ 7, -10 ≤ k ≤ 10, -12 ≤ l ≤ 12
Reflections collected	14458
Independent reflections	2204 [R_{int} = 0.0533, R_{sigma} = 0.0386]
Data/restraints/parameters	2204/0/192
Goodness-of-fit on F^2	1.096
Final R indexes [I>=2σ (I)]	R_1 = 0.0430, wR_2 = 0.1112
Final R indexes [all data]	R_1 = 0.0431, wR_2 = 0.1113
Largest diff. peak/hole / e Å^{-3}	0.35/-0.30

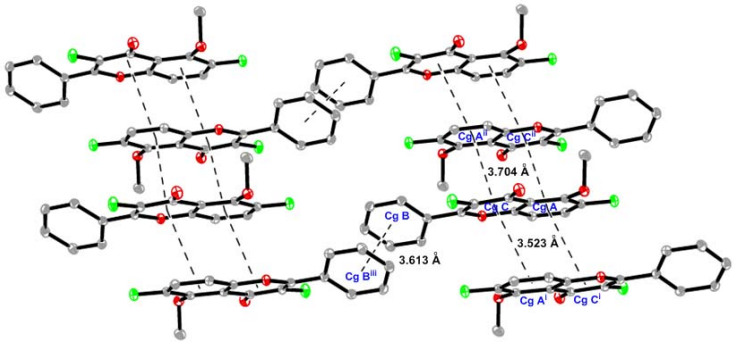


Figure 1. π···π stacking interactions of **2v'**

Symmetry codes: (i): 2−x, 1−y, 1−z; (ii): 1−x, 1−y, 1−z; (iii): 1−x, −y, −z

CgC-CgA^{i} = 3.523 Å, CgC-CgA^{ii} = 3.704 Å, CgB-CgB^{iii} = 3.613 Å, where Cg is the centroid of rings A, B, and C of the skeleton at (x, y, z), respectively, and Cg^{i} , Cg^{ii} and Cg^{iii} are the centroeds of rings A, B, and C of the neighbouring skeletons.

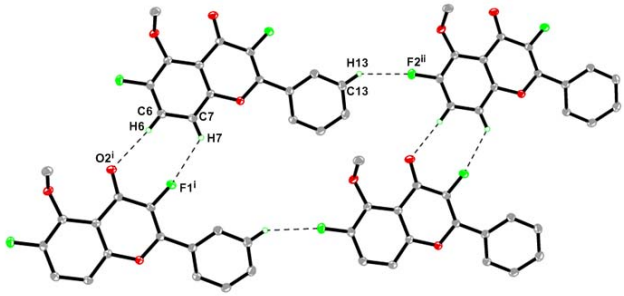


Figure 2. The hydrogen bonds in **2v'**

Symmetry codes: (i): x, y−1, z; (ii): x+1, y+1, z+1

Table 2 Hydrogen Bond Lengths (Å) and Bond Angles (°)

C—H···D	C—H	H···D	C—D	∠C—H···D
C6—H6···O2^{i}	0.950	2.495	3.434	169.7
C7—H7···F1^{i}	0.950	2.584	3.211	123.8
C13—H13···F2^{ii}	0.950	2.580	3.331	136.1

3. Spectroscopic data of 1

1-(2-hydroxyphenyl)-3-phenylpropane-1,3-dione (1a).

Yield: 72%, 1.9 g. Characteristic: a yellow solid as a 1:10 mixture of keto/enol tautomers. m.p. 87.5-88.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.55 (s, 1H), 12.11 (s, 1H), 11.96 (s, 0.1H*), 8.03-8.00 (m, 0.2H*), 7.98-7.91 (m, 2H), 7.79-7.45 (m, 1H and 0.1H*), 7.63-7.60 (m, 0.1H*), 7.57-7.54 (m, 1H), 7.52-7.46 (m, 3H), 7.45-7.44 (m, 0.3H*), 7.02-7.00 (m, 1H and 0.1H*), 6.95-6.90 (m, 1H and 0.1H*), 6.84 (s, 1H), 4.63 (s, 0.2H*); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) 200.3*, 195.8, 193.6*, 177.6, 162.9*, 162.6, 137.2*, 136.2*, 135.9, 134.0*, 133.7, 132.5, 131.0*, 129.0*, 128.9, 128.6, 126.9, 119.5*, 119.4*, 119.2, 119.1, 118.9, 118.8*, 92.4, 50.0*; * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 3058, 1903, 1797, 1610, 1298, 1188, 1039, 898, 729, 617, 449; HRMS (ESI): calc. for $C_{15}H_{12}O_3$ $[M+Na]^+$ 263.0684, found 263.0684.

1-(2-hydroxyphenyl)-3-(p-tolyl)propane-1,3-dione (1b).

Yield: 57%, 1.6 g. Characteristic: a yellow solid as a 1:6.7 mixture of keto/enol tautomers. m.p. 108.1-109.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.59 (s, 1H), 12.12 (s, 1H), 11.96 (s, 0.15H*), 7.88 (d, J = 8.1 Hz, 0.3H*), 7.81 (d, J = 8.12 Hz, 2H), 7.74 (d, J = 8.0 Hz, 0.15H* and 1H), 7.48-7.46 (m, 0.15H*), 7.42 (m, 1H), 7.25 (d, J = 8.0 Hz, 0.3H* and 2H), 6.98 (d, J = 8.3 Hz, 0.15H* and 1H), 6.92 (m, 0.15H* and 1H), 6.77 (s, 1H), 4.56 (s, 0.3H*), 2.40 (s, 0.45H* and 3H); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) 200.5*, 195.4, 193.1*, 177.9, 162.9*, 162.5, 145.1*, 143.4, 137.1*, 135.7, 133.8*, 131.0, 130.8, 130.2*, 129.7*, 129.6, 129.0*, 128.6, 126.9, 119.6*, 119.4*, 119.1, 118.8, 118.7*, 91.8, 50.0*, 21.8*, 21.7; * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 3448, 1909, 1785, 1618, 1487, 1396, 1292, 1188, 1029, 904, 746, 570, 464; HRMS (ESI): calc. for $C_{16}H_{14}O_3$ $[M+Na]^+$ 277.0841, found 277.0843.

1-(2-hydroxyphenyl)-3-(4-methoxyphenyl)propane-1,3-dione (1c).

Yield: 61%, 1.8 g. Characteristic: a yellow solid as a 1:5 mixture of keto/enol

tautomers. m.p. 107.3-108.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.76 (s, 1H), 12.14 (s, 1H), 11.99 (s, 0.2H*), 7.98 (d, *J* = 8.6 Hz, 0.4H*), 7.90 (d, *J* = 8.6 Hz, 2H), 7.79-7.73 (m, ,0.2H* and 1H), 7.48-7.42 (m, 0.2H* and 1H), 6.99-6.88 (m, 0.8H* and 4H), 6.74 (s, 1H), 6.74 (s, 0.40H*), 3.87 (s, 0.6* and 3H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) 200.6*, 194.9, 191.9*, 177.8, 164.3*, 163.3, 162.9*, 162.4, 137.1*, 135.6, 131.3, 131.1*, 129.3*, 128.9, 128.5, 125.9*, 119.6*, 119.4*, 119.2, 119.1, 118.8, 118.7*, 114.2, 114.1*, 91.1, 55.6*, 55.5, 50.0*; * = keto (minor) tautomer; IR (KBr), *v* (cm^{-1}) 3454, 3006, 2954, 2833, 1610, 1433, 1296, 1172, 1029, 840, 738, 576, 478; HRMS (ESI): calc. for $C_{16}H_{14}O_4$ $[M+Na]^+$ 293.0790, found 293.0789.

1-(2-hydroxyphenyl)-3-(4-fluorophenyl)propane-1,3-dione (1d).

Yield: 80%, 2.3 g. Characteristic: a yellow solid as a enol tautomer. m.p. 125.3-126.5 °C. ^{1}H NMR (400 MHz, DMSO-d_6), δ (ppm) 16.25 (s, 1H), 8.67-8.63 (m, 2H), 8.51 (d, *J* = 7.5 Hz, 1H), 7.91-7.86 (m, 3H), 7.41-7.38 (m, 2H), 7.14 (s, 1H), 4.48 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6), δ (ppm) 183.9, 182.3, 162.7, 163.0 (d, ^{1}J = 244.5 Hz), 139.6 (d, ^{4}J = 2.6 Hz), 131.6, 129.1 (d, ^{3}J = 8.5 Hz), 127.1, 122.0, 117.4, 117.1, 114.5 (d, ^{2}J = 21 Hz), 89.0; IR (KBr), *v* (cm^{-1}) 3444, 1915, 1622, 1494, 1301, 1207, 1161, 1037, 844, 744, 578, 482; HRMS (ESI): calc. for $C_{15}H_{11}FO_3$ $[M+Na]^+$ 281.0590, found 281.0597.

ethyl 4-(3-(2-hydroxyphenyl)-3-oxopropanoyl)benzoate (1e).

Yield: 50%,1.7 g. Characteristic: a yellow solid as a 1:20 mixture of keto/enol tautomers. m.p. 125.8-126.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.39 (s, 1H), 12.01 (s, 1H), 11.85 (s, 0.05H*), 8.15 (d, *J* = 8.3 Hz, 2H and 0.10H*), 7.99 (d, *J* = 8.2 Hz, 2H and 0.10H*), 7.80 (d, *J* = 8.0 Hz, 1H and 0.05H*), 7.49 (m, 1H and 0.05H*), 7.02 (d, *J* = 8.4 Hz, 1H and 0.05H*), 6.94 (m, 1H and 0.05H*), 6.88 (s, 1H), 4.67 (s, 0.10H*), 4.42 (q, *J* = 7.2 Hz, 2H and 0.10H*), 1.43 (t, *J* = 6.9 Hz, 3H and 0.15H*); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) 196.3, 175.8, 165.9, 137.7, 136.3, 133.8, 130.0, 128.8, 126.8, 119.3, 119.1, 119.0, 93.5, 61.6, 14.5; * = keto (minor) tautomer; IR (KBr), *v* (cm^{-1}) 2987, 1953, 1714, 1618, 1434, 1282, 1118, 1031, 864, 730, 511; HRMS (ESI): calc. for $C_{18}H_{16}O_5$ $[M+Na]^+$ 355.0895, found 355.0896.

1-(2-hydroxy-5-methylphenyl)-3-phenylpropane-1,3-dione (1f)[1].

Yield: 66%, 1.8 g. Characteristic: a yellow solid as a 1:10 mixture of keto/enol tautomers. m.p. 82.4-83.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.61 (s, 1H), 11.90 (s, 1H), 11.78 (s, 0.10H*), 8.02-8.00 (m, 0.20H*), 7.97-7.94 (m, 2H), 7.64-7.56

(m, 0.40H*), 7.55-7.48 (m, 4H), 7.33-7.30 (m, 0.10H*), 7.28 (dd, J = 8.6, 2.3 Hz, 1H), 6.91 (dd, J = 8.6 Hz, 1H), 6.90 (dd, J = 8.7 Hz, 0.10H*), 6.83 (s, 1H), 4.63 (s, 0.20H*), 2.34 (s, 3H), 2.31 (s, 0.30H*); * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 3448, 3028, 2921, 1897, 1618, 1454, 1290, 1193, 1039, 813, 773, 676, 503; HRMS (ESI): calc. for $C_{16}H_{14}O_3$ $[M+Na]^+$ 277.0841, found 277.0842.

1-(2-hydroxy-5-methylphenyl)-3-(p-tolyl)propane-1,3-dione (1g)[1].

Yield: 55%, 1.6 g. Characteristic: a yellow solid as a 1:6.7 mixture of keto/enol tautomers. m.p. 112.1-113.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.69 (s, 1H), 11.93 (s, 1H), 11.80 (s, 0.15H*), 7.91 (d, J = 8.1 Hz, 0.30H*), 7.85 (d, J = 8.0 Hz, 2H), 7.54-7.53 (m, 1H and 0.15H*), 7.30-7.26 (m, 3H and 0.45H*), 6.92-6.89 (m, 1H and 0.15H*), 6.80 (s, 1H), 4.60 (s, 0.3H*), 2.44 (s, 3H), 2.43 (s, 0.45H*), 2.34 (s, 3H), 2.30 (s, 0.45H*); * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 3452, 3062, 2918, 1917, 1787, 1560, 1444, 1288, 1191, 1041, 931, 813, 468; HRMS (ESI): calc. for $C_{17}H_{16}O_3$ $[M+Na]^+$ 291.0997, found 291.0995.

1-(2-hydroxy-5-methylphenyl)-3-(4-methoxyphenyl)propane-1,3-dione (1h)[1].

Yield: 57%, 1.8 g. Characteristic: a yellow solid as a 1:4.8 mixture of keto/enol tautomers. m.p. 136.4-137.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.84 (s, 1H), 11.93 (s, 1H), 11.81 (s, 0.21H*), 8.01-7.98 (m, 0.42H*), 7.95-7.91 (m, 2H), 7.57 (s, 0.21H*), 7.52 (s, 1H), 7.30 (dd, J = 8.5, 1.9 Hz, 0.21H*), 7.26 (dd, J = 8.4, 1.9 Hz, 1H), 7.00-6.95 (m, 2H and 0.42H*), 6.91-6.88 (m, 1H and 0.21H*), 6.75 (s, 1H), 4.57 (s, 0.42H*), 3.89 (s, 3H), 3.88 (s, 0.63H*), 2.34 (s, 3H), 2.30 (s, 0.63H*); * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 3452, 2937, 2842, 2569, 2036, 1920, 1610, 1487, 1257, 1182, 1020, 935, 796, 744, 588, 499; HRMS (ESI): calc. for $C_{17}H_{16}O_4$ $[M+Na]^+$ 307.0946, found 307.0942.

1-(2-hydroxy-5-methylphenyl)-3-(4-fluorophenyl)propane-1,3-dione (1i).

Yield: 55%, 1.5 g. Characteristic: a yellow solid as a 1:6.7 mixture of keto/enol tautomers. m.p. 122.9-123.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.66 (s, 1H), 11.84 (s, 1H), 11.73 (s, 0.15H*), 8.04 (dd, J = 8.7, 5.4 Hz, 0.3H*), 7.95 (dd, J = 8.7, 5.4 Hz, 2H), 7.54 (s, 0.15H*), 7.51 (s, 1H), 7.31 (m, 0.14H*), 7.27 (m, 1H), 7.16 (m, 2H and 0.3H*), 6.90 (d, J = 8.5 Hz, 1H and 0.15H*), 6.75 (s, 1H), 4.59 (s, 0.3H*), 2.33 (s, 3H), 2.31 (s, 0.45H*); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) 199.9*, 195.6, 192.1*, 176.4, 165.4* (d, ^1J = 252.4 Hz), 165.0*, 161.0*, 160.5, 138.5*, 137.1, 132.8* (d, ^4J = 2.9 Hz), 131.7* (d, ^3J = 9.5 Hz), 130.5*, 130.0 (d, ^4J = 3.0 Hz), 129.3

(d, ^{3}J = 8.9 Hz), 128.6*, 128.3, 128.2, 119.1*, 118.7, 118.6, 118.5, 116.2* (d, ^{2}J = 21.9 Hz), 116.1 (d, ^{2}J = 21.8 Hz), 92.1, 50.0*, 20.7, 20.6*; * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 2923, 1909, 1770, 1583, 1496, 1296, 1199, 1159, 1043, 910, 806, 723, 578, 499; HRMS (ESI): calc. for $C_{16}H_{13}FO_3$ $[M+Na]^+$ 295.0746, found 295.0755.

1-(5-bromo-2-hydroxyphenyl)-3-phenylpropane-1,3-dione (1j)[1].

Yield: 50%, 1.7 g. Characteristic: a yellow solid as a 1:16.7 mixture of keto/enol tautomers. m.p. 109.3-110.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.46 (s, 1H), 12.04 (s, 1H), 11.87 (s, 0.06H*), 7.99 (d, J = 7.7 Hz, 0.12H*), 7.94 (d, J = 7.9 Hz, 2H), 7.83-7.82 (m, 1H and 0.06H*), 7.65-7.61 (m, 0.06H*), 7.59-7.55 (m, 1H), 7.51-7.47 (m, 3H and 0.18H*), 6.90-6.89 (m, 1H and 0.06H*), 6.73-6.72 (m, 1H), 4.60 (s, 0.12H*); * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 3043, 1911, 1573, 1436, 1284, 1197, 1097, 1043, 829, 730, 676, 526; HRMS (ESI): calc. for $C_{15}H_{11}BrO_3$ $[M+Na]^+$ 340.9789, found 340.9786.

1-(5-bromo-2-hydroxyphenyl)-3-(p-tolyl)propane-1,3-dione (1k).

Yield: 66%, 2.4 g. Characteristic: a yellow solid as a keto tautomer. m.p. ＞ 300 °C. ^{1}H NMR (400 MHz, DMSO-d_6), δ (ppm) 16.06 (s, 1H), 7.89 (d, J = 2.5 Hz, 1H), 7.83 (d, J = 8.0 Hz, 2H), 7.32 (dd, J = 8.3, 2.6 Hz, 2H), 7.20 (d, J = 7.7 Hz, 2H), 6.67 (d, J = 8.8 Hz, 1H), 6.41 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6), δ (ppm) 184.5, 181.1, 162.3, 140.0, 139.4, 133.9, 128.9, 128.5, 127.0, 123.9, 119.9, 108.0, 89.3, 21.0; IR (KBr), ν (cm^{-1}) 3444, 3026, 2916, 1872, 1604, 1488, 1276, 1139, 1012, 935, 784, 746, 624, 491; HRMS (ESI): calc. for $C_{16}H_{13}BrO_3$ $[M+Na]^+$ 354.9946, found 354.9959.

1-(5-bromo-2-hydroxyphenyl)-3-(4-methoxyphenyl)propane-1,3-dione (1l).

Yield: 58%, 2.2 g. Characteristic: a yellow solid as a 1:10 mixture of keto/enol tautomers. m.p. 133.5-134.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.68 (s, 1H), 12.09 (s, 1H), 11.90 (s, 0.1H*), 7.98-7.88 (m, 2H and 0.2H*), 7.81 (s, 1H and 0.1H*), 7.56-7.48 (m, 1H and 0.1H*), 6.98 (d, J = 8.3 Hz, 2H and 0.2H*), 6.88 (d, J = 8.8 Hz, 1H and 0.1H*), 6.65 (s, 1H), 4.55 (s, 0.2H*), 3.88 (s, 3H and 0.3H*); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) 199.9*, 193.4, 191.4*, 178.8, 164.4*, 163.7, 161.9*, 161.3, 139.7*, 138.0, 133.3*, 131.3*, 130.6, 129.2, 125.6, 120.9*, 120.8, 120.7*, 120.6, 114.4, 114.2*, 110.9*, 110.8, 100.1*, 91.0, 55.7*, 55.6, 49.8*; * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 2947, 2840, 1897, 1774, 1604, 1473, 1259, 1174, 1020,

929, 804, 740, 590, 503; HRMS (ESI): calc. for $C_{16}H_{13}BrO_4$ $[M+Na]^+$ 370.9895, found 370.9905.

1-(5-fluoro-2-hydroxyphenyl)-3-phenylpropane-1,3-dione (1m).

Yield: 83%, 2.4 g. Characteristic: a yellow solid as a 1:14.3 mixture of keto/enol tautomers. m.p. 214.2-215.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.51 (s, 1H), 11.84 (s, 1H), 11.70 (s, 0.07H)*, 8.01 (d, J = 7.7 Hz, 0.14H*), 7.94 (d, J = 7.6 Hz, 2H), 7.65-7.62 (m, 0.07H*), 7.59-7.55 (m, 1H), 7.53-7.48 (m, 2H and 0.14H*), 7.45-7.42 (m, 1H and 0.07H*), 7.24-7.17 (m, 1H and 0.07H*), 6.97 (m, 1H and 0.07H*), 6.72 (s, 1H), 4.60 (s, 0.14H*); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) 199.6* (d, ^4J = 2.7 Hz), 194.6 (d, ^4J = 2.6 Hz), 193.2*， 178.5， 159.2* (d, ^4J = 1.3 Hz), 158.7 (d, ^4J = 1.3 Hz), 155.3 (d, ^1J = 236.7 Hz), 155.0* (d, ^1J = 237.8 Hz), 136.1*, 134.3, 133.5*,132.8, 129.3* (d, ^3J = 6.8 Hz), 129.1*, 129.0, 128.9*, 127.1, 124.9* (d, ^2J = 23.6 Hz), 123.3 (d, ^2J = 23.4 Hz), 120.2 (d, ^3J = 7.4 Hz), 119.0* (d, ^3J = 6.3 Hz), 118.3 (d, ^3J = 6.4 Hz), 115.8* (d, ^2J = 23.3 Hz), 113.6 (d, ^2J = 23.5 Hz), 92.3, 50.1*; * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 3058, 1901, 1600, 1488, 1274, 1188, 1041, 945, 817, 779, 678, 511; HRMS (ESI): calc. for $C_{15}H_{11}O_3$ $[M+Na]^+$ 281.0590, found 281.0597.

1-(5-fluoro-2-hydroxyphenyl)-3-(4-methoxyphenyl)propane-1,3-dione (1n)[6].

Yield: 69%, 2.2 g. Characteristic: a yellow solid as a 1:8.3 mixture of keto/enol tautomers. m.p. 141.2-141.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.74 (s, 1H), 11.87 (s, 1H), 11.73 (s, 0.12H*), 7.99 (d, J = 8.5 Hz, 0.24H*), 7.92 (d, J = 8.4 Hz, 2H), 7.48-7.45 (m, 0.12H*), 7.43-7.40 (m, 1H), 7.23-7.15 (m, 1H and 0.12H*), 7.00-7.94 (m, 3H and 0.36H*), 6.65 (s, 1H), 4.54 (s, 0.24H*), 3.89 (s, 3H and 0.36H*); * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 3448, 2960, 2837, 2032, 1905, 1608, 1502, 1247, 1178, 1029 ,790, 730, 582, 491; HRMS (ESI): calc. for $C_{16}H_{13}FO_4$ $[M+Na]^+$ 311.0696, found 311.0692.

1-(5-fluoro-2-hydroxyphenyl)-3-(4-fluorophenyl)propane-1,3-dione (1o)[6].

Yield: 67%, 2.0 g. Characteristic: a yellow solid as a 1:11.1 mixture of keto/enol tautomers. m.p. 165.0-165.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.57 (s, 1H), 11.77 (s, 1H), 11.65 (s, 0.09H*), 8.06-8.02 (m, 0.18H*), 7.98-7.93 (m, 2H), 7.46-7.43 (m, 0.09H*), 7.43-7.40 (m, 1H), 7.23-7.21 (m, 0.27H*), 7.20-7.15 (m, 3H), 6.99-6.95 (m, 1H and 0.09H*), 6.67 (s, 1H), 4.57 (s, 0.18H*); * = keto (minor) tautomer; IR

(KBr), ν (cm^{-1}) 3057, 2027, 1886, 1780, 1620, 1506, 1282, 1188, 1037, 946, 825, 736, 576, 499; HRMS (ESI): calc. for $C_{15}H_{10}F_2O_3$ $[M+Na]^+$ 299.0496, found 299.0505.

1-(2-hydroxy-4-methoxyphenyl)-3-phenylpropane-1,3-dione (1p)[1].

Yield: 32%, 1.0 g. Characteristic: a yellow solid as a 1:5.3 mixture of keto/enol tautomers. m.p. 99.8-100.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.36 (s, 1H), 12.58 (s, 1H), 12.41 (s, 0.19H*), 8.03-8.01 (m, 0.38H*), 7.92-7.91 (m, 2H), 7.70-7.69 (m, 1H and 0.19H*), 7.63-7.46 (m, 3H and 0.57H*), 6.72 (s, 1H), 6.51-6.42 (m, 2H and 0.38H*), 4.56 (s, 0.38H*), 3.85 (s, 3H), 3.84 (s, 0.57H*); * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 3448, 2960, 2923, 2835, 1780, 1602, 1448, 1332, 1230, 1018, 912, 777, 692, 580; HRMS (ESI): calc. for $C_{16}H_{14}O_4$ $[M+Na]^+$ 293.0790, found 293.0787.

1-(2-hydroxy-4-methoxyphenyl)-3-(p-tolyl)propane-1,3-dione (1q)[1].

Yield: 54%, 1.7 g. Characteristic: a yellow solid as a 1:4 mixture of keto/enol tautomers. m.p. 119.7-120.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.42 (s, 1H), 12.60 (s, 1H), 12.43 (s, 0.25H*), 7.92 (d, J = 8.1 Hz, 0.5H*), 7.81 (d, J = 8.2 Hz, 2H), 7.69 (d, J = 8.9 Hz, 0.25H*), 7.68 (d, J = 8.8 Hz, 1H), 7.28 (d, J = 8.2 Hz, 2H and 0.5H*), 6.68 (s, 1H), 6.49-6.41 (m, 2H and 0.5H*), 4.52 (s, 0.5H*), 3.85 (s, 3H), 3.83 (s, 0.75H*), 2.43 (s, 3H), 2.42 (s, 0.75H*); * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 3450, 2941, 1926, 1610, 1436, 1338, 1234, 1020, 900, 811, 561, 457; HRMS (ESI): calc. for $C_{17}H_{16}O_4$ $[M+Na]^+$ 307.0946, found 307.0943.

1-(2-hydroxy-4-methoxyphenyl)-3-(4-methoxyphenyl)propane-1,3-dione (1r)[1].

Yield: 42%, 1.4 g. Characteristic: a yellow solid as a 1:2.9 mixture of keto/enol tautomers. m.p. 108.7-109.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.55 (s, 1H), 12.61 (s, 1H), 12.45 (s, 0.35H*), 8.00-7.99 (m, 0.70H*), 7.90-7.87 (m, 2H), 7.71 (d, J = 9.0 Hz, 0.35H*), 7.66 (d, J = 8.7 Hz, 1H), 6.97-6.93 (m, 2H and 0.70H*), 6.63 (s, 1H), 6.48-6.41 (m, 2H and 0.70H*), 4.49 (s, 0.70H*), 3.87 (s, 3H), 3.86 (s, 1.05H*), 3.83 (s, 3H), 3.82 (s, 1.05H*); * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 3452, 2985, 2840, 2038, 1890, 1608, 1444, 1342, 1211, 1176, 1020, 825, 570, 453; HRMS (ESI): calc. for $C_{17}H_{16}O_5$ $[M+Na]^+$ 323.0895, found 323.0891.

1-(2-hydroxy-4-methoxyphenyl)-3-(4-fluorophenyl)propane-1,3-dione (1s).

Yield: 45%, 1.4 g. Characteristic: a yellow solid as a 1:4.5 mixture of keto/enol tautomers. m.p. 143.1-144.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.41 (s, 1H), 12.51 (s, 1H), 12.37 (s, 0.22H*), 8.05 (dd, J = 8.7, 5.4 Hz, 0.44H*), 7.91 (dd, J = 8.7,

5.4 Hz, 2H), 7.69 (d, *J* = 9 Hz, 0.22H*), 7.66 (d, *J* = 9 Hz, 1H), 7.17-7.13 (m, 2H and 0.44H*), 6.63 (s, 1H), 6.48-6.40 (m, 2H and 0.44H*), 4.51 (s, 0.44H*), 3.84 (s, 3H), 3.83 (s, 0.66H*); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) 197.6*, 194.5, 192.1*, 175.0, 167.6*, 166.9, 166.5 (d, ^{1}J = 251.9 Hz), 166.1, 166.0*, 165.5, 165.0*, 131.5* (d, ^{1}J = 225.4 Hz), 131.8* (d, ^{3}J = 9.5 Hz), 130.2, 130.1*, 129.1 (d, ^{3}J = 8.9 Hz), 116.2* (d, ^{2}J = 21.9 Hz), 116.0 (d, ^{2}J = 21.8 Hz), 113.8*, 112.6, 108.4*, 108.1, 101.5, 101.1*, 91.8, 55.8*, 55.7, 50.1*; * = keto (minor) tautomer; IR (KBr), *v* (cm^{-1}) 3072, 2950, 1905, 1728, 1614, 1450, 1334, 1218, 1107, 1016, 918, 794, 736, 561, 482; HRMS (ESI): calc. for $C_{16}H_{13}FO_4$ $[M+Na]^+$ 311.0696, found 311.0705.

3-hydroxy-4-(3-oxo-3-phenylpropanoyl)phenyl benzoate (1t)[3].

Yield: 35%, 2.5 g. Characteristic: a yellow solid as a 1:9.1 mixture of keto/enol tautomers. m.p. 168.1-168.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.46 (s, 1H), 12.34 (s, 1H), 12.16 (s, 0.11H*), 8.21-8.17 (m, 2H and 0.22H*), 8.03 (d, *J* = 7.8 Hz, 0.22H*), 7.95 (d, *J* = 7.6 Hz, 2H), 7.86-7.84 (m, 1H and 0.11H*), 7.68-7.63 (m, 1H and 0.11H*), 7.59-7.48 (m, 5H and 0.55H*), 6.91-6.90 (m, 1H and 0.11H*), 6.86-6.84 (m, 1H and 0.11H*), 6.81 (s, 1H), 4.64 (s, 0.22H*); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) 199.3*, 194.9, 193.4*, 177.7, 164.6*, 164.5, 164.3*, 164.2, 157.6*, 156.8, 136.2*, 134.2*, 134.1*, 134.0, 133.8*, 133.7, 132.6, 132.5*, 130.4, 129.9, 129.6*, 129.2, 129.1, 129.0*, 128.9*, 128.8, 128.7*, 127.0, 117.6*, 117.1, 113.6*, 113.3, 111.8, 111.6*, 92.4, 50.3*; * = keto (minor) tautomer; IR (KBr), *v* (cm^{-1}) 3730, 3519, 3033, 1745, 1537, 1290, 952, 528, 455, 422; HRMS (ESI): calc. for $C_{22}H_{16}O_5$ $[M+Na]^+$ 383.0895, found 383.0900.

1-(2-hydroxy-4,6-dimethoxyphenyl)-3-phenylpropane-1,3-dione (1u).

Yield: 50%, 1.7 g. Characteristic: a yellow solid as a 1:0.75 mixture of keto/enol tautomers. m.p. 121.1-122.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.51 (s, 0.75H), 13.72 (s, 1H*), 13.43 (s, 0.75H), 7.96 (d, *J* = 7.7 Hz, 2H*), 7.88 (d, *J* = 7.2 Hz, 1.5H), 7.61-7.43 (m, 3H* and 2.25H), 7.33 (s, 0.75H), 6.09 (d, *J* = 2.2 Hz, 0.75H), 6.07 (d, *J* = 2.2 Hz, 1H*), 5.98 (d, *J* = 2.3 Hz, 0.75H), 5.82 (d, *J* = 2.2 Hz, 1H*), 4.53 (s, 2H*), 3.91 (s, 2.25H), 3.81 (s, 2.25H), 3.79 (s, 3H*), 3.43 (s, 3H*); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) 198.7*, 194.7, 193.8*, 175.9, 168.0*, 167.1, 166.7*, 165.7, 162.1*, 162.0, 136.8*, 134.5, 133.4*, 131.8, 128.9*, 128.7, 128.2*, 126.7, 105.7*, 104.7, 98.2, 94.3, 94.0*, 91.5, 91.0*, 56.0*, 55.7*, 55.6, 55.5*, 54.7; * = keto tautomer; IR (KBr), *v* (cm^{-1}) 3344, 3062, 2949, 2709, 2607, 2050, 2003, 1593, 1417,

1290, 1217, 1110, 999, 825, 759, 680, 588, 457; HRMS (ESI): calc. for $C_{17}H_{16}O_5$ $[M+Na]^+$ 323.0895, found 323.0908.

1-(2-hydroxy-6-methoxyphenyl)-3-phenylpropane-1,3-dione (1v)[1].

Yield: 35%, 2.1 g. Characteristic: a yellow solid as a 1:1.1 mixture of keto/enol tautomers. m.p. 97.8-98.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.72 (s, 1H), 13.06 (s, 0.9H*), 12.53 (s, 1H), 7.98-7.96 (m, 1.8H*), 7.92-7.90 (m, 2H), 7.64-45 (m, 3H and 2.7H*), 7.37 (s, 1H), 7.35-7.31 (m, 1H and 0.9H*), 6.62-6.59 (m, 1H and 0.9H*), 6.44 (d, *J* = 8.1 Hz, 1H), 6.30 (d, *J* = 8.6 Hz, 0.9H*), 4.61 (s, 1.8H*), 3.96 (s, 3H), 3.48 (s, 2.7H*); * = keto (minor) tautomer; IR (KBr), *v* (cm^{-1}) 3452, 2933, 2671, 2501, 1957, 1602, 1458, 1321, 1242, 1087, 991, 788, 748, 634, 586, 472; HRMS (ESI): calc. for $C_{16}H_{14}O_4$ $[M+Na]^+$ 293.0790, found 293.0793.

1-(2-hydroxy-3-methylphenyl)-3-phenylpropane-1,3-dione (1w).

Yield: 37%, 1.0 g. Characteristic: a yellow solid as a 1:7.7 mixture of keto/enol tautomers. m.p. 96.7-97.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.51 (s, 1H), 12.40 (s, 1H), 12.25 (s, 0.13H), 8.01 (d, *J* = 7.9 Hz, 0.26H), 7.94 (d, *J* = 7.8 Hz, 2H), 7.65-7.63 (m, 1H and 0.13H*), 7.60-7.54 (M, 1H and 0.13H*), 7.51-7.47 (m, 2H and 0.26H*), 7.38-7.33 (m, 1H and 0.13H*), 6.85-6.81 (m, 2H and 0.26H*), 4.64 (s, 0.26H*), 2.29 (s, 3H), 2.26 (s, 0.39H*); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) 200.5*, 196.2, 193.7*, 177.2, 161.5*, 161.1, 137.9*, 136.7, 136.3*, 135.8*, 134.0*, 133.8, 132.4, 129.0*, 128.9, 128.5*, 127.9, 127.6*, 126.9, 126.3, 118.8*, 118.7, 118.5, 118.4*, 92.6, 50.1*, 15.8, 15.6*; * = keto (minor) tautomer; IR (KBr), *v* (cm^{-1}) 2877, 1508, 1367, 1259, 1112, 948, 842, 657; HRMS (ESI): calc. for $C_{16}H_{14}O_3$ $[M+Na]^+$ 277.0841, found 311.0705.

1-(2-hydroxyphenyl)-3-(4-(trifluoromethyl)phenyl)propane-1,3-dione (1x)[7, 8].

Yield: 34%, 1.2 g. Characteristic: a yellow solid as a 1:16.7mixture of keto/enol tautomers. m.p. 128.9-129.5°C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.38 (s, 1H), 11.97 (s, 1H), 11.82 (s, 0.06H), 8.12 (d, *J* = 8.1 Hz, 0.12H), 8.03 (d, *J* = 8.1 Hz, 2H), 7.79-7.73 (m, 3H and 0.18H*), 7.51-7.47 (m, 1H and 0.06H*), 7.02-7.00 (m, 1H and 0.06H*), 6.96-6.92 (m, 1H and 0.06H*), 6.86 (s, 1H), 4.67 (s, 0.12H); * = keto (minor) tautomer; IR (KBr), *v* (cm^{-1}) 2875, 2769, 1454, 1367, 1217, 1149, 1051, 655; HRMS (ESI): calc. for $C_{16}H_{11}F_3O_3$ $[M+Na]^+$ 331.0552, found 331.0549.

1-(2-fluorophenyl)-3-(2-hydroxyphenyl)propane-1,3-dione (1y)[4].

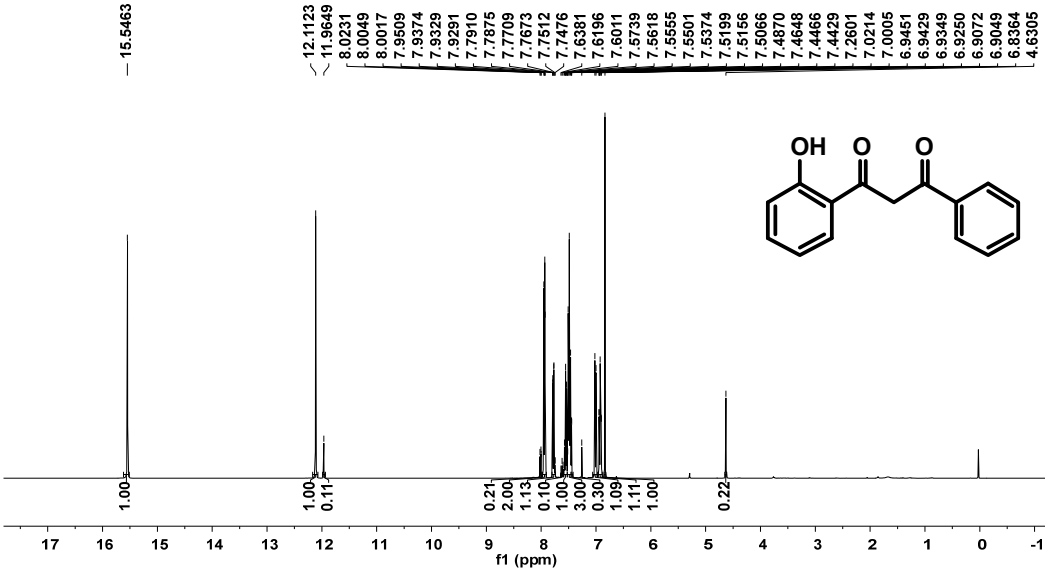
Yield: 21%, 0.16 g. Characteristic: a yellow solid as a 1:10 mixture of keto/enol tautomers. m.p. 91.0-91.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.50 (s, 1H), 12.03 (s, 1H), 11.85 (s, 0.1H*), 8.02-7.98 (m, 1H and 0.1H*), 7.76 (d, J = 8.1 Hz, 1H), 7.67 (d, J = 8.1 Hz, 0.1H*), 7.61-7.56 (m, 0.2H*), 7.53-7.45 (m, 2H), 7.31-7.26 (m, 1H and 0.1H*), 7.21-7.12 (m, 1H and 0.1H*), 7.04-6.99 (m, 2H and 0.2H*), 6.94-6.91 (m, 1H), 4.65 (d, J = 3.4 Hz, 0.2H); * = keto (minor) tautomer; IR (KBr), ν (cm^{-1}) 2873, 2767, 1448, 1369, 1255, 1220, 1172, 1095, 1058, 630; HRMS (ESI): calc. for $C_{15}H_{11}FO_3$ $[M+Na]^+$ 281.0590, found 281.0584.

1-(2-hydroxy-5-nitrophenyl)-3-phenylpropane-1,3-dione (1z).

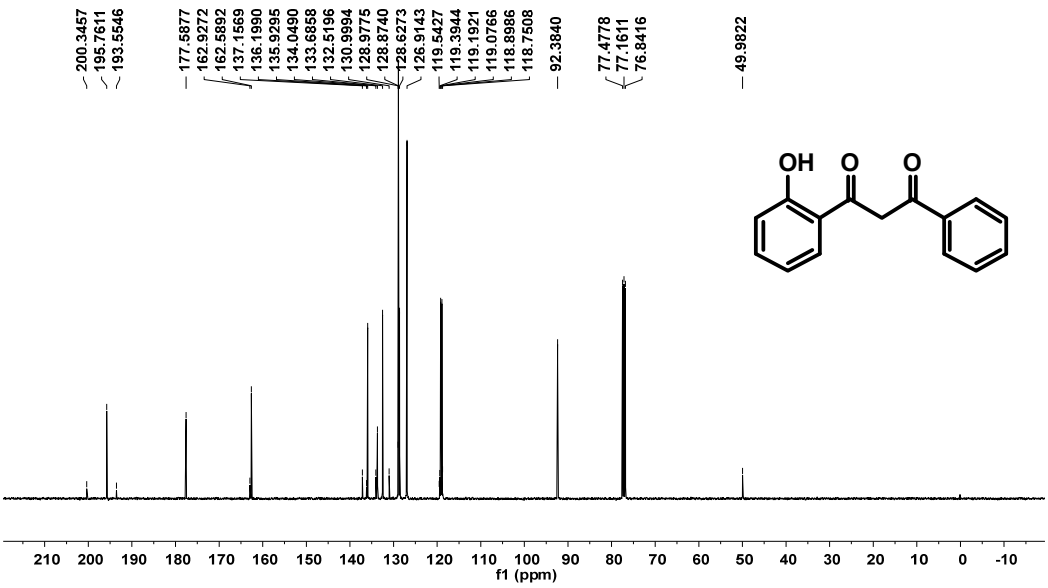
Yield: 20%, 0.17 g. Characteristic: a yellow solid as a enol tautomers. m.p. 182.7-183.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm) 15.34 (s, 1H), 12.89 (s, 1H), 8.74 (d, J = 1.0 Hz, 1H), 8.33 (d, J = 9.6 Hz, 1H), 8.00 (d, J = 7.6 Hz, 2H), 7.64-7.60 (m, 1H), 7.56-7.52 (m, 2H), 7.10 (d, J = 9.2 Hz, 1H), 6.90 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm) 193.9, 179.8, 167.5, 139.9, 133.4, 132.9, 130.4, 129.1, 127.4, 125.1, 119.9, 118.3, 92.1; IR (KBr), ν (cm^{-1}) 2871, 2769, 1436, 1367, 1309, 1226, 1149, 717, 653; HRMS (ESI): calc. for $C_{15}H_{11}NO_5$ $[M+Na]^+$ 308.0535, found 308.0526.

4. ^{1}H NMR ^{13}C NMR and HRMS Spectra of 1, 4 and 2

1a

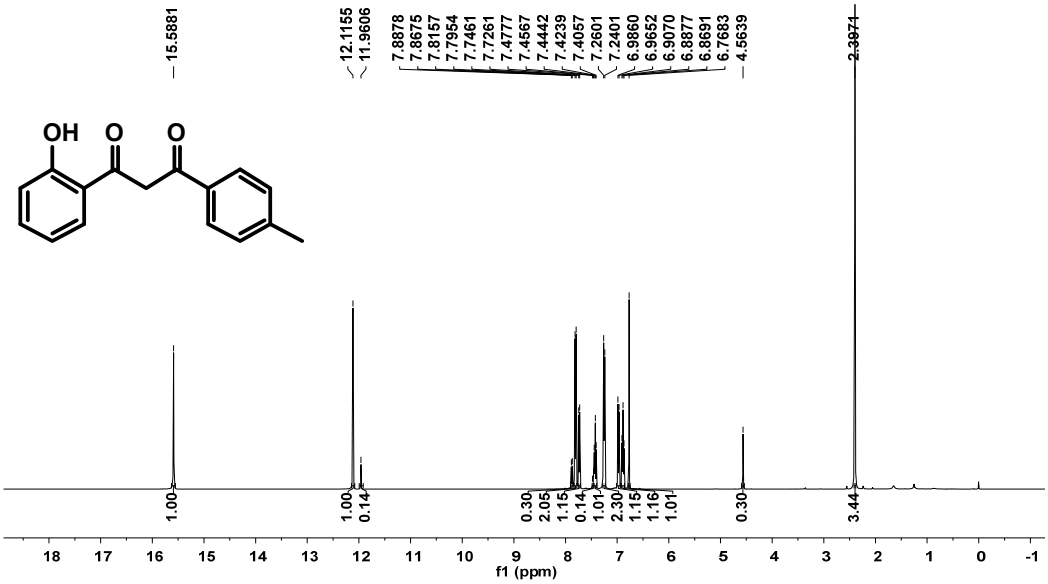


^{1}H NMR spectrum of **1a** ($CDCl_3$)



^{13}C NMR spectrum of **1a** ($CDCl_3$)

1b



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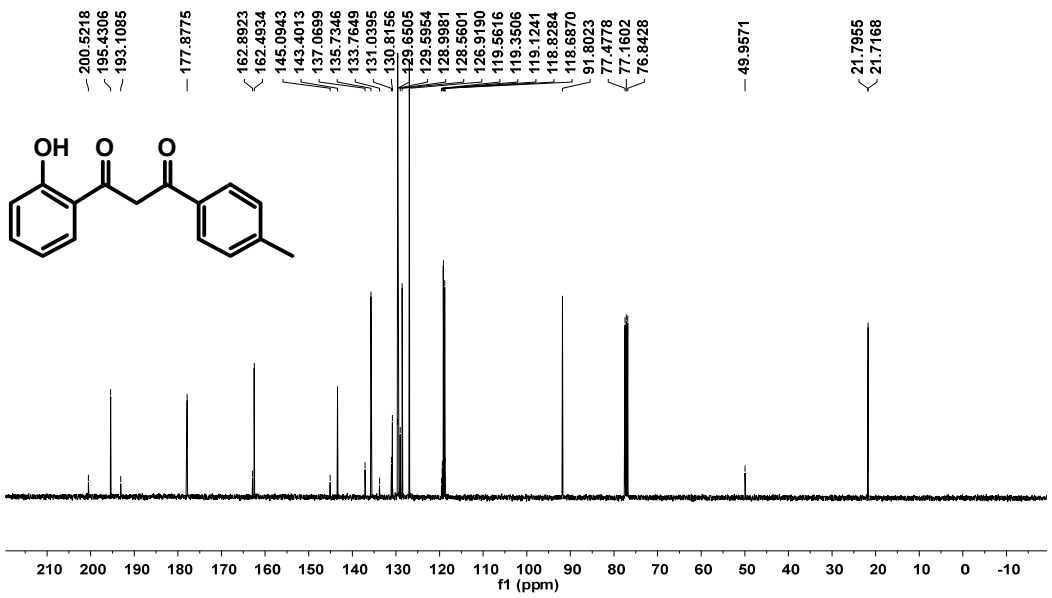
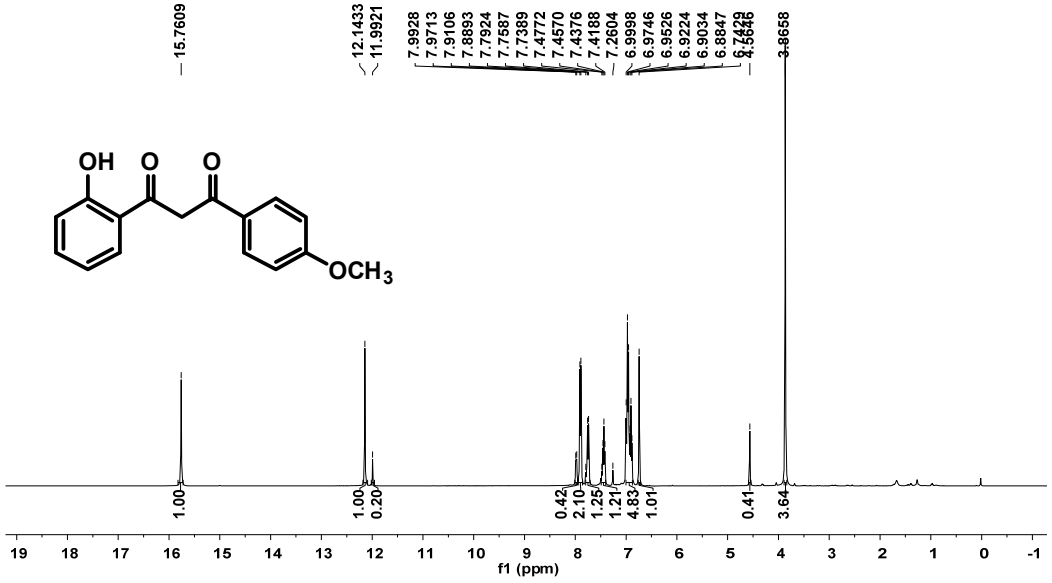
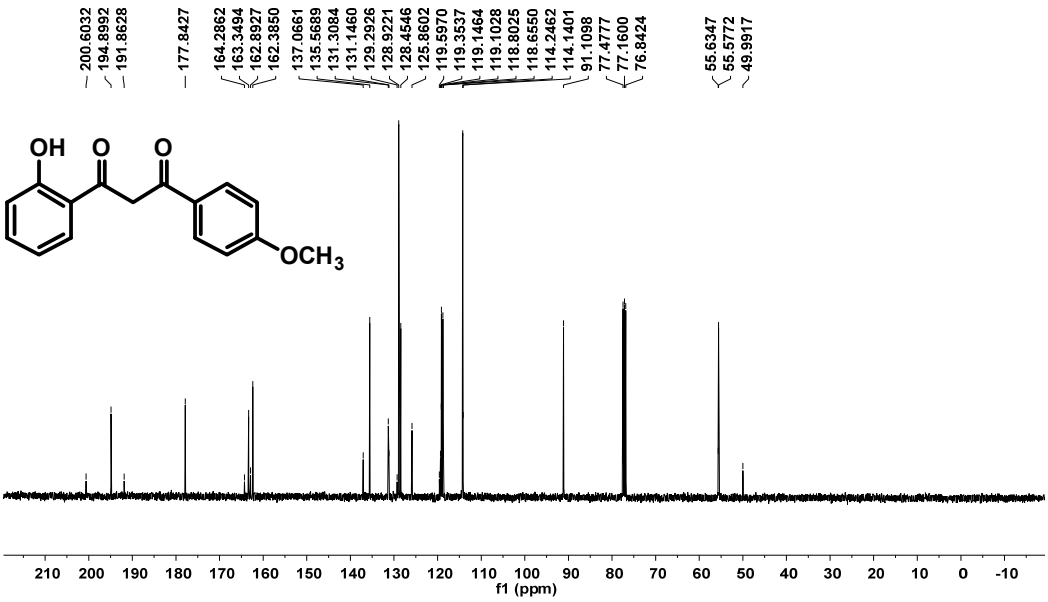


^{13}C NMR spectrum of **1b** ($CDCl_3$)

1c

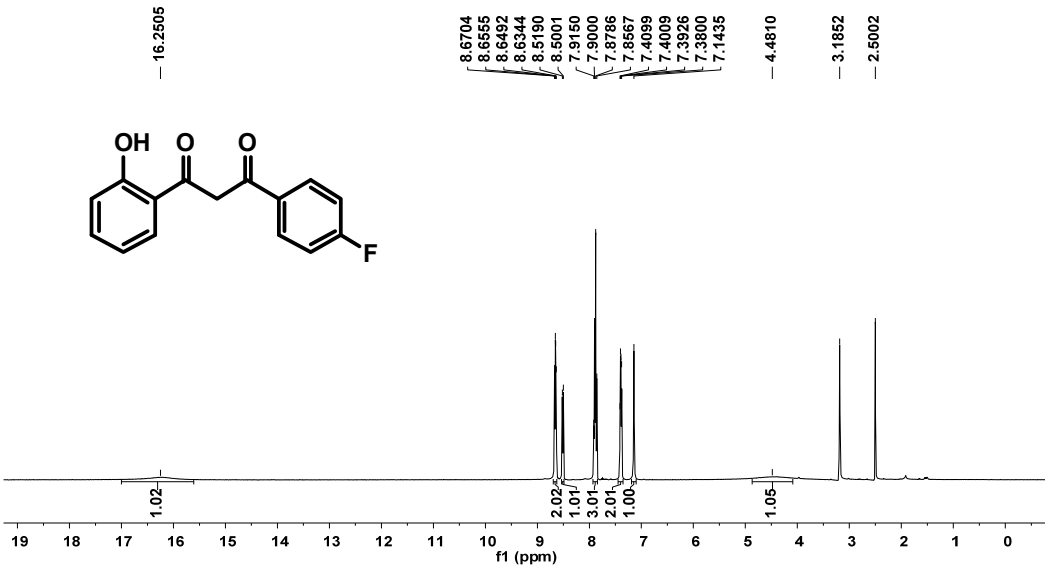


^{1}H NMR spectrum of **1c** ($CDCl_3$)

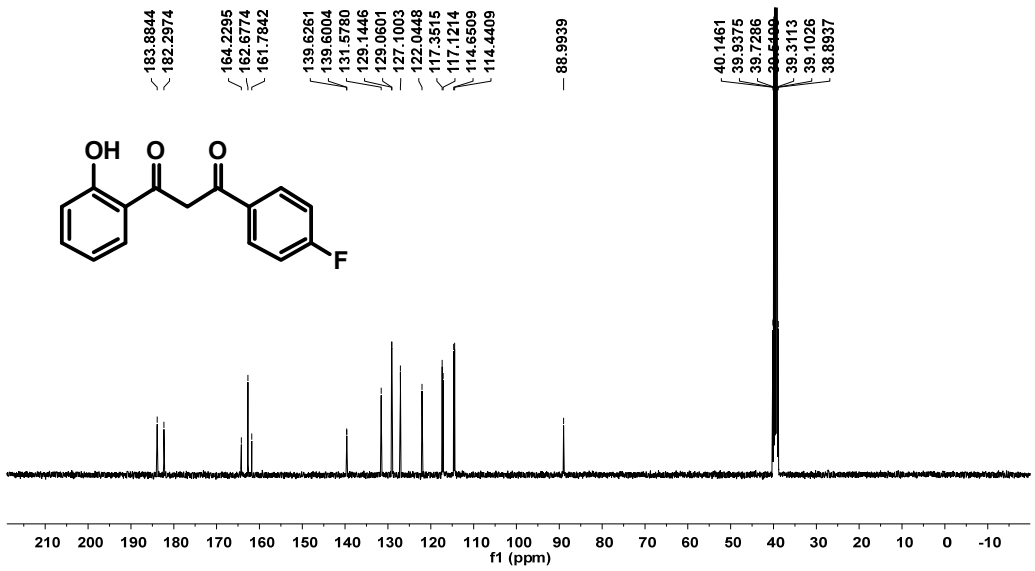


^{13}C NMR spectrum of **1c** ($CDCl_3$)

1d

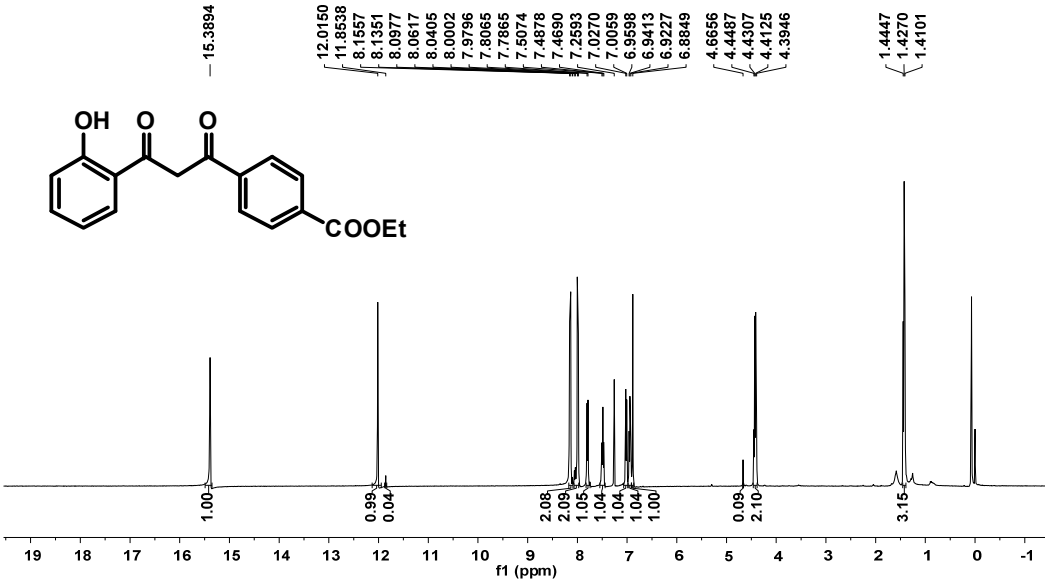


^{1}H NMR spectrum of **1d** (DMSO-d_6)

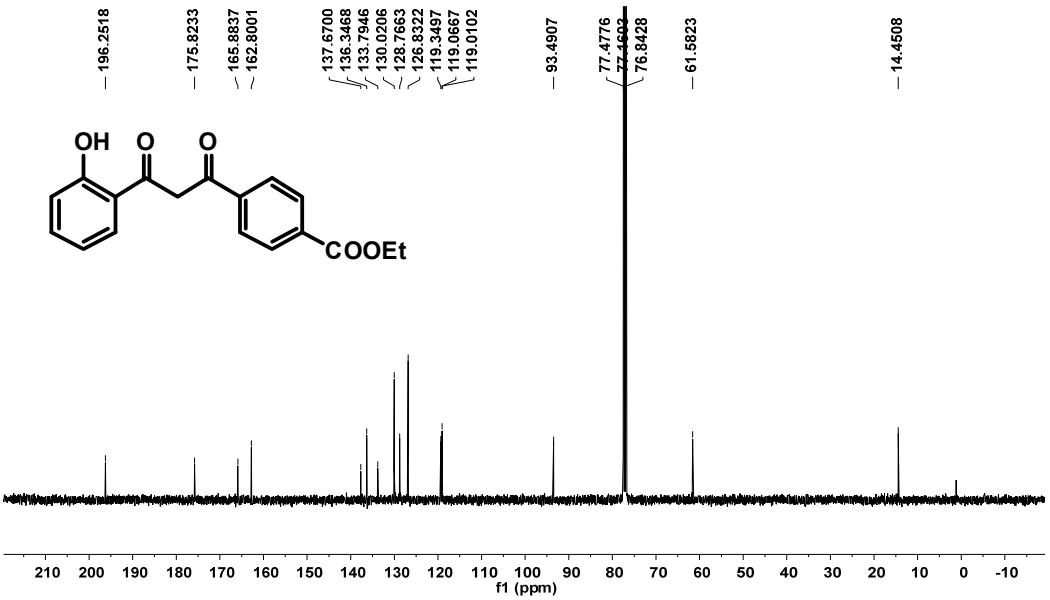


^{13}C NMR spectrum of **1d** (DMSO-d_6)

1e

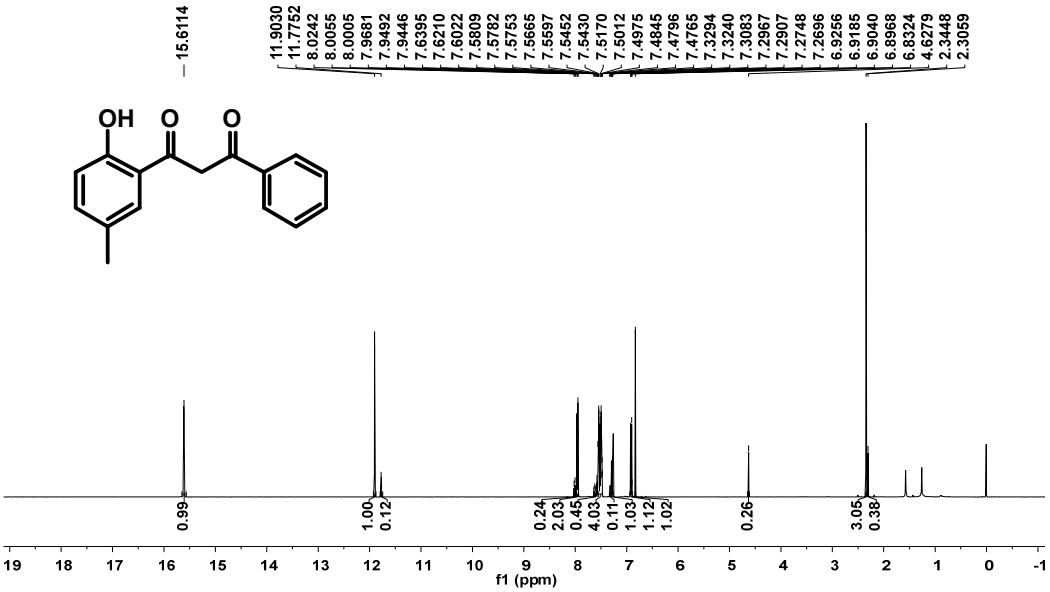


^{1}H NMR spectrum of **1e** ($CDCl_3$)



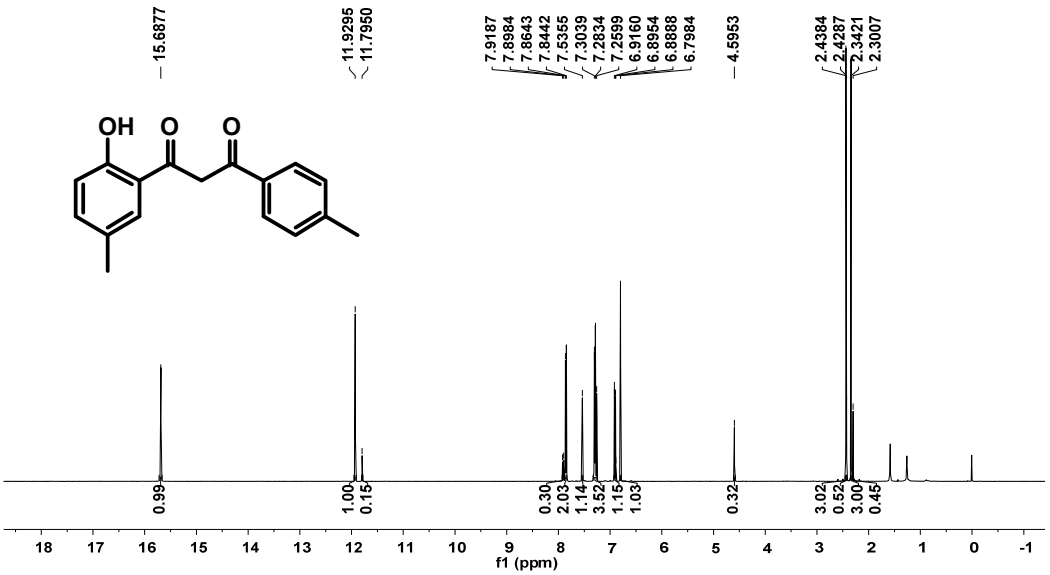
^{13}C NMR spectrum of **1e** ($CDCl_3$)

1f



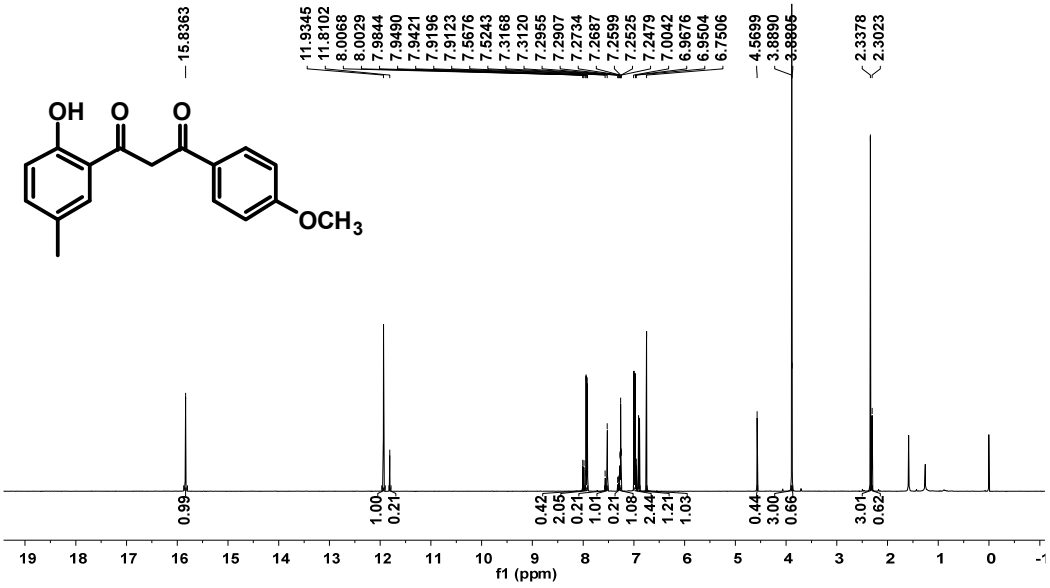
^{1}H NMR spectrum of **1f** ($CDCl_3$)

1g



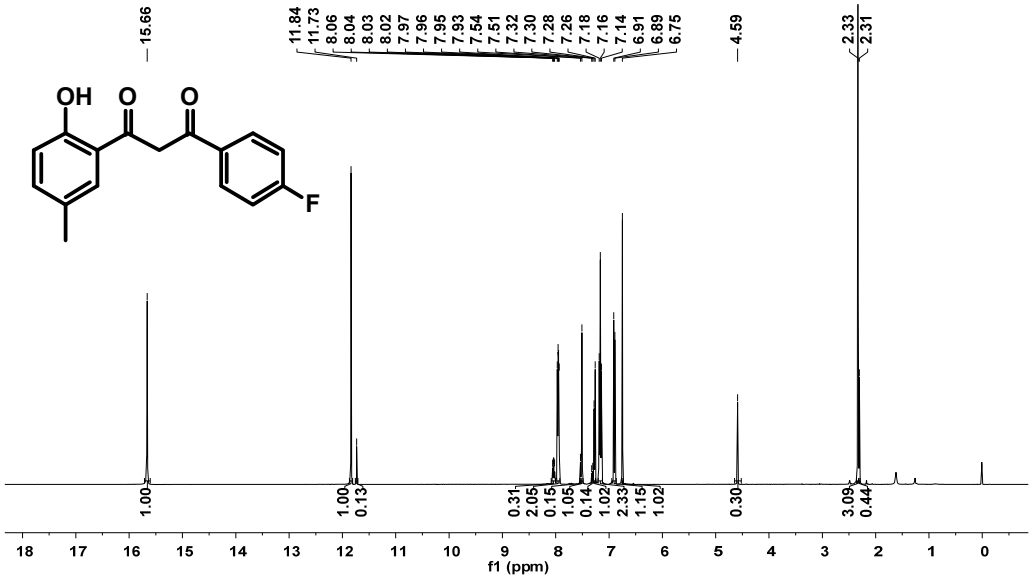
^{1}H NMR spectrum of **1g** ($CDCl_3$)

1h

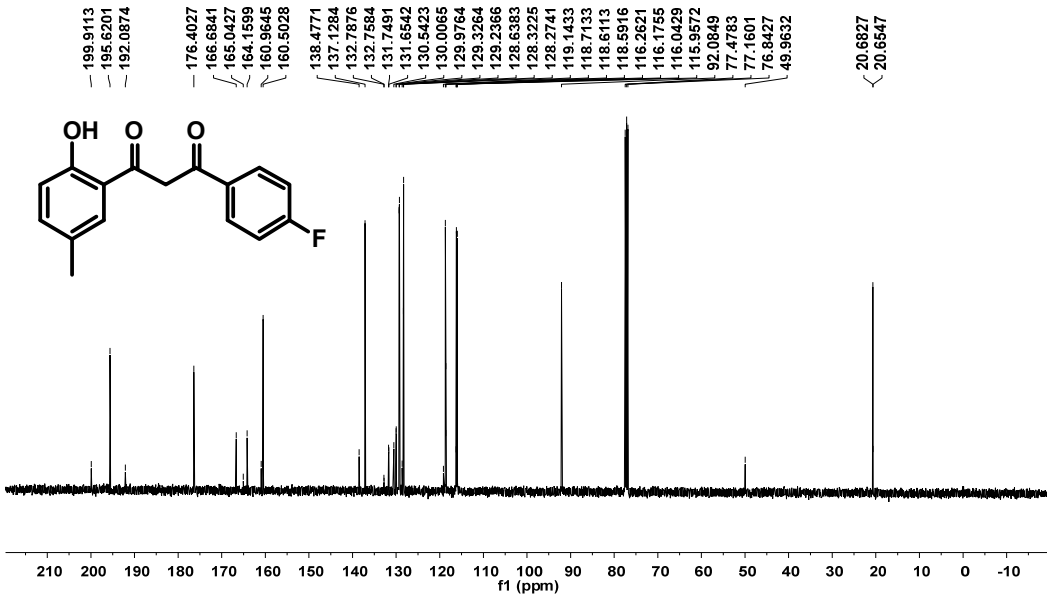


^{1}H NMR spectrum of **1h** ($CDCl_3$)

1i

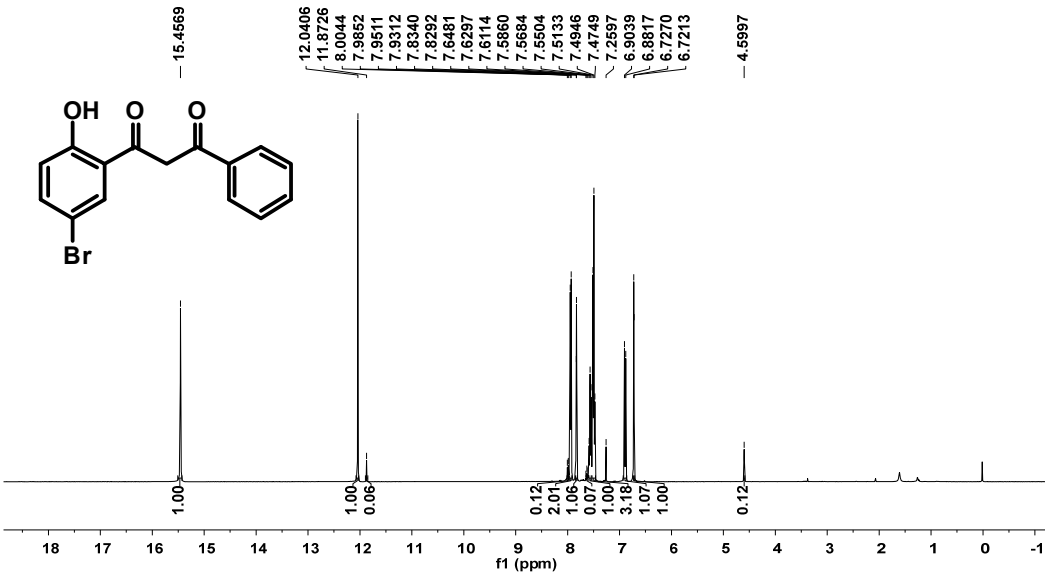


^{1}H NMR spectrum of **1i** ($CDCl_3$)



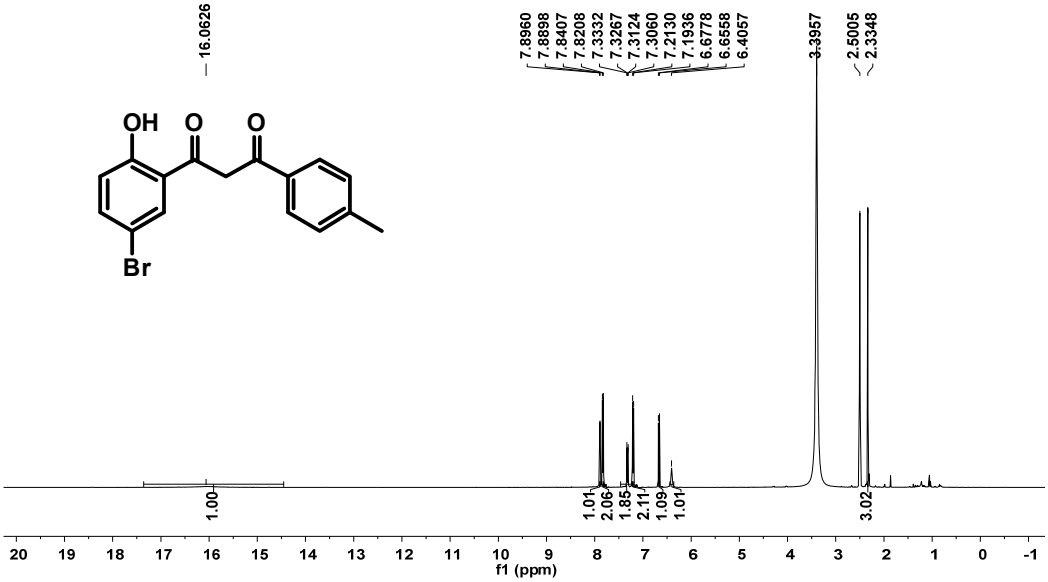
^{13}C NMR spectrum of **1i** ($CDCl_3$)

1j

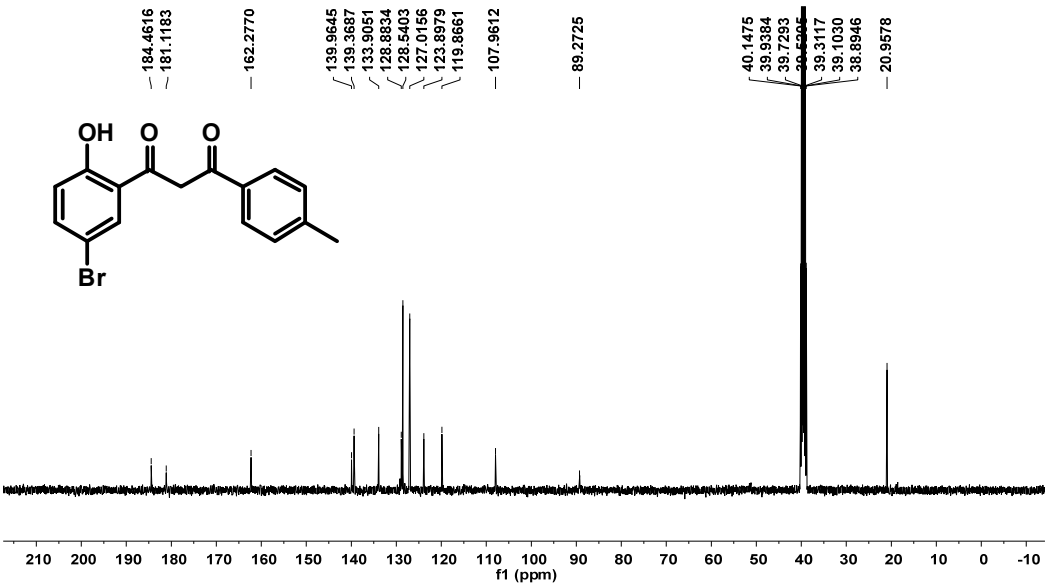


^{1}H NMR spectrum of **1j** ($CDCl_3$)

1k

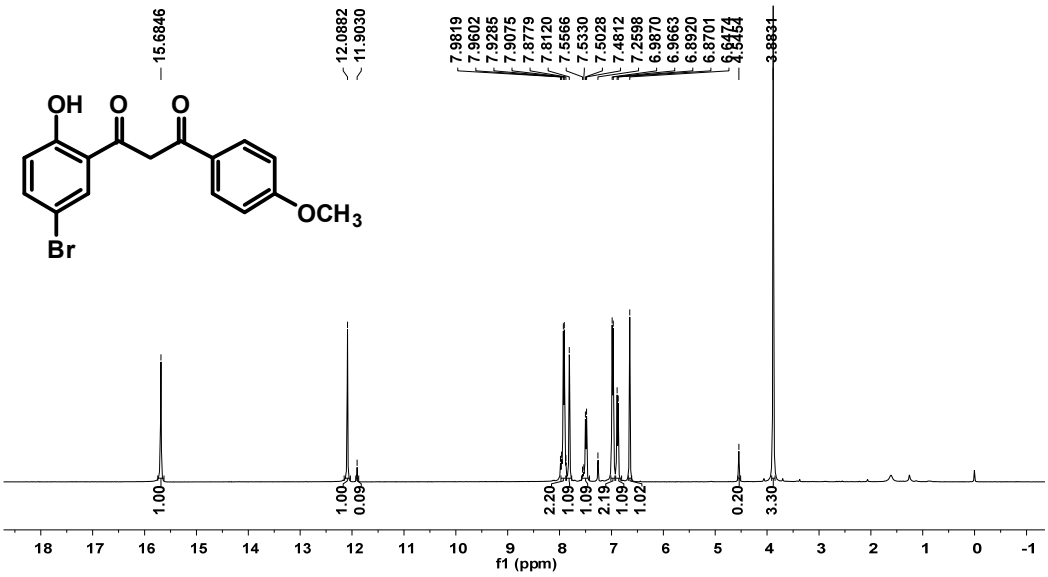


^{1}H NMR spectrum of **1k** (DMSO-d_6)

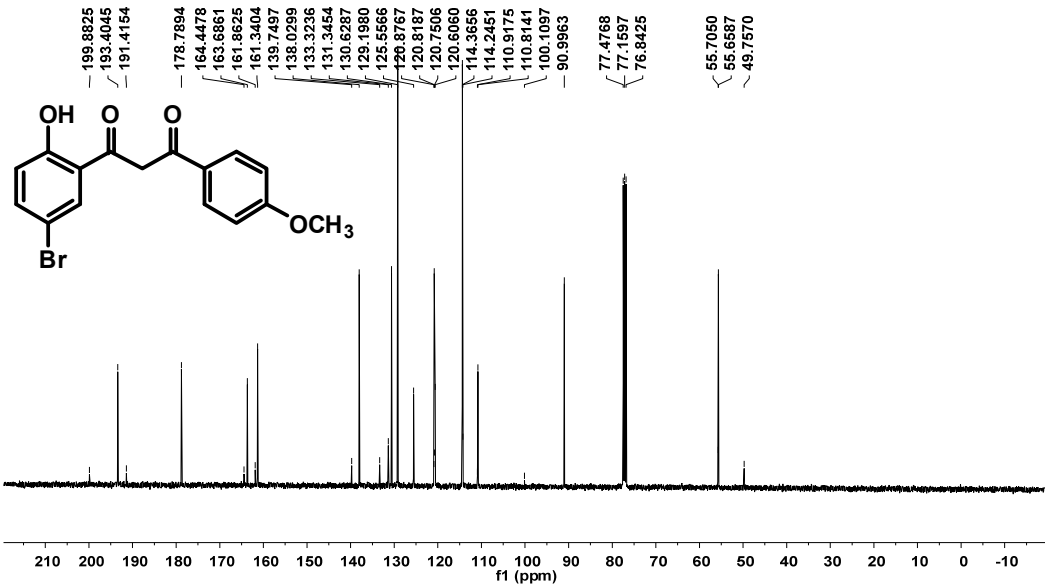


^{13}C NMR spectrum of **1k** (DMSO-d_6)

1l

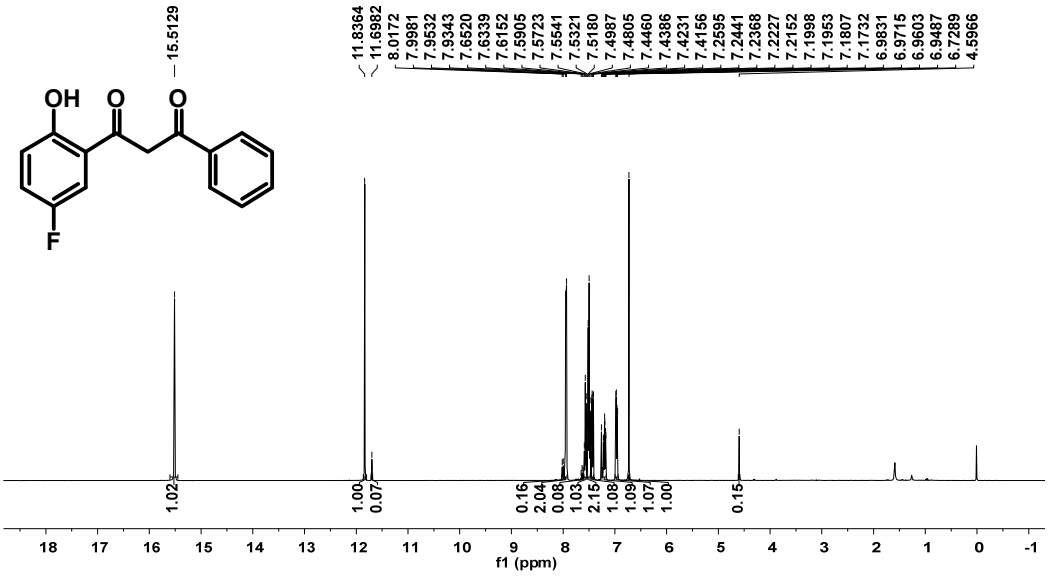


^{1}H NMR spectrum of **1l** ($CDCl_3$)



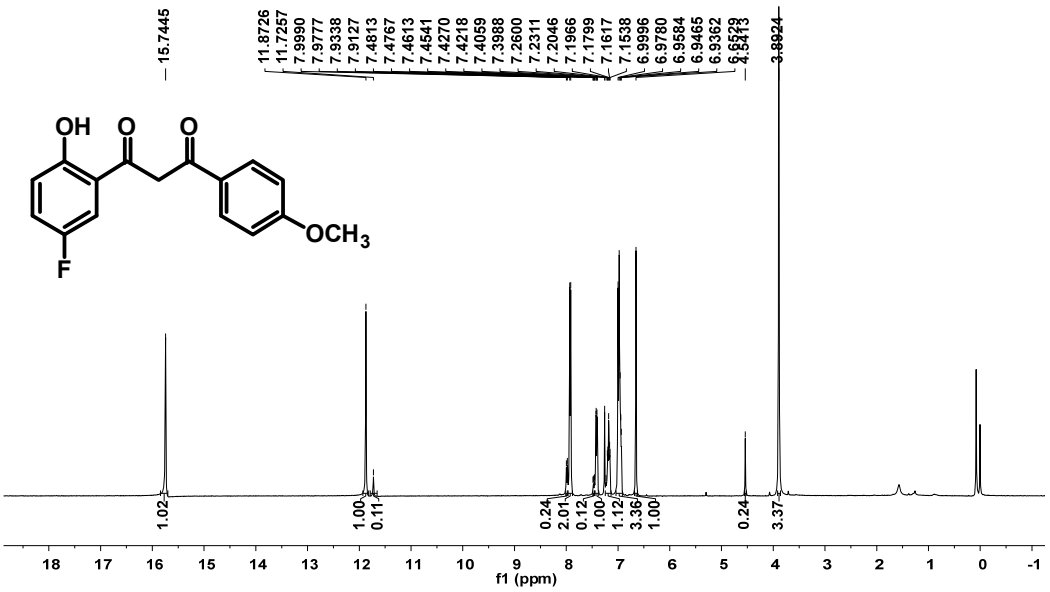
^{13}C NMR spectrum of **1l** ($CDCl_3$)

1m



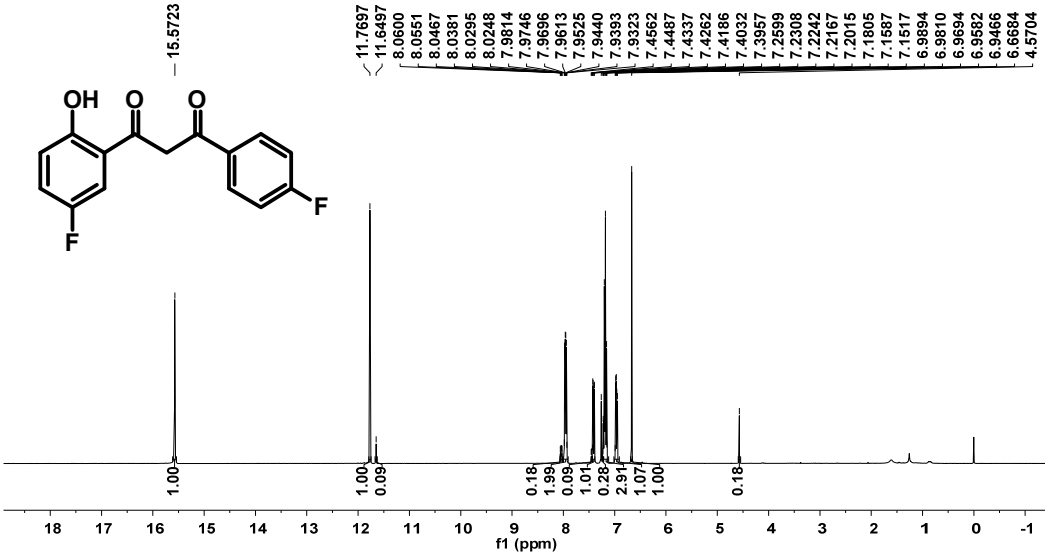
^{1}H NMR spectrum of **1m** ($CDCl_3$)

1n



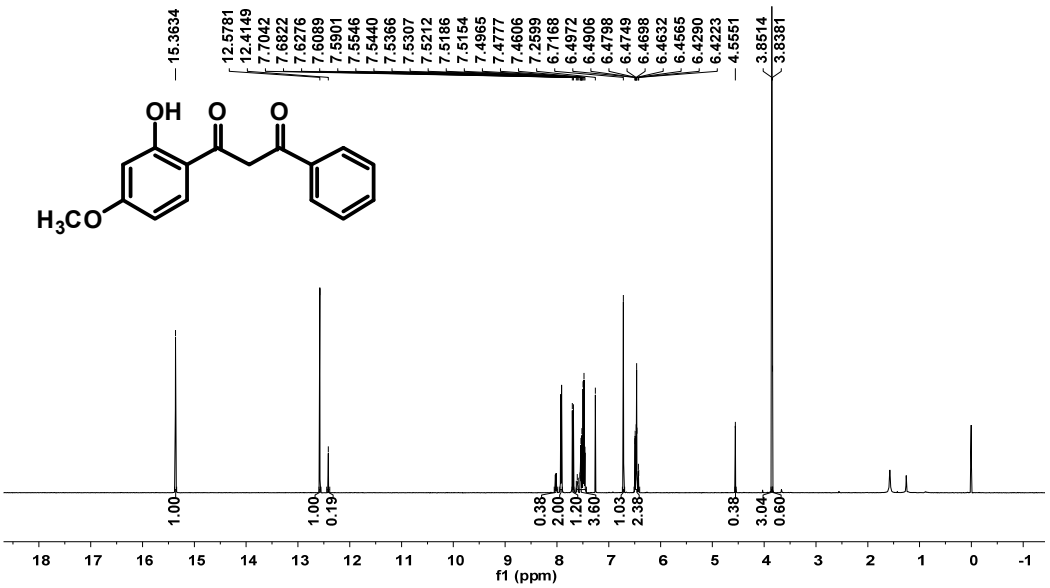
^{1}H NMR spectrum of **1n** ($CDCl_3$)

1o



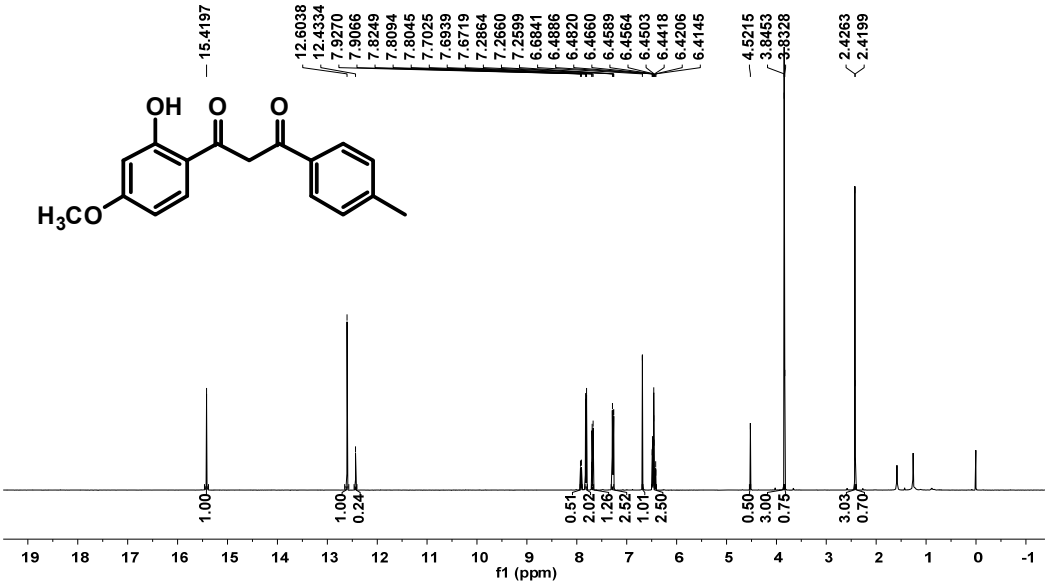
^{1}H NMR spectrum of **1o** ($CDCl_3$)

1p



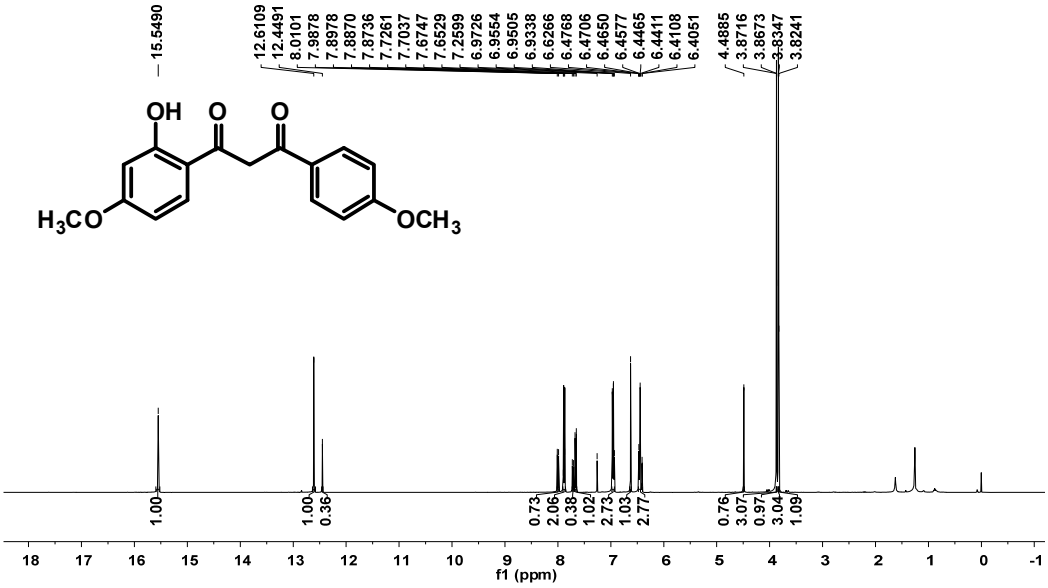
^{1}H NMR spectrum of **1p** ($CDCl_3$)

1q



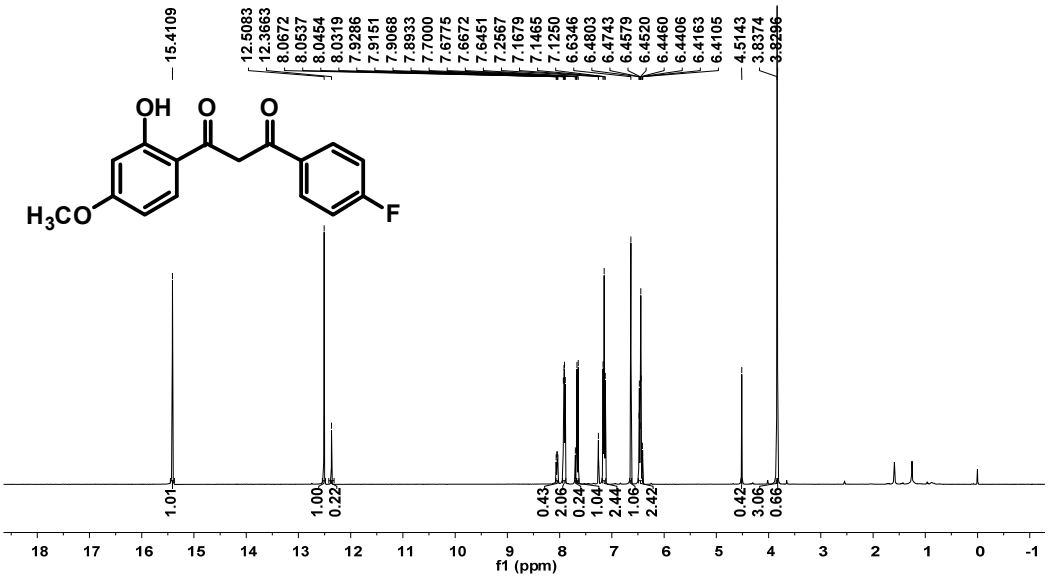
^{1}H NMR spectrum of **1q** ($CDCl_3$)

1r

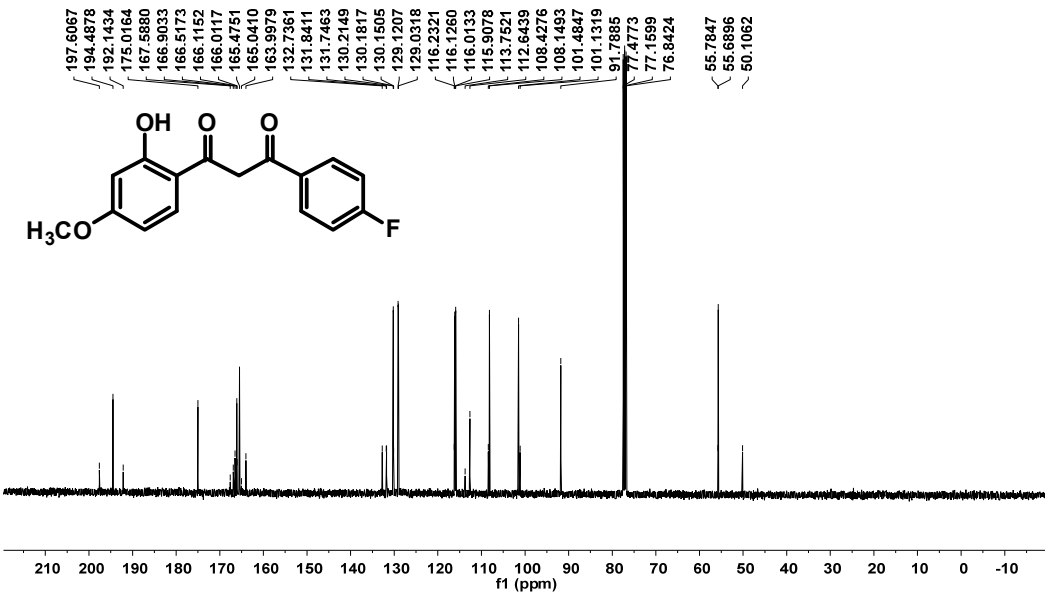


^{1}H NMR spectrum of **1r** ($CDCl_3$)

1s

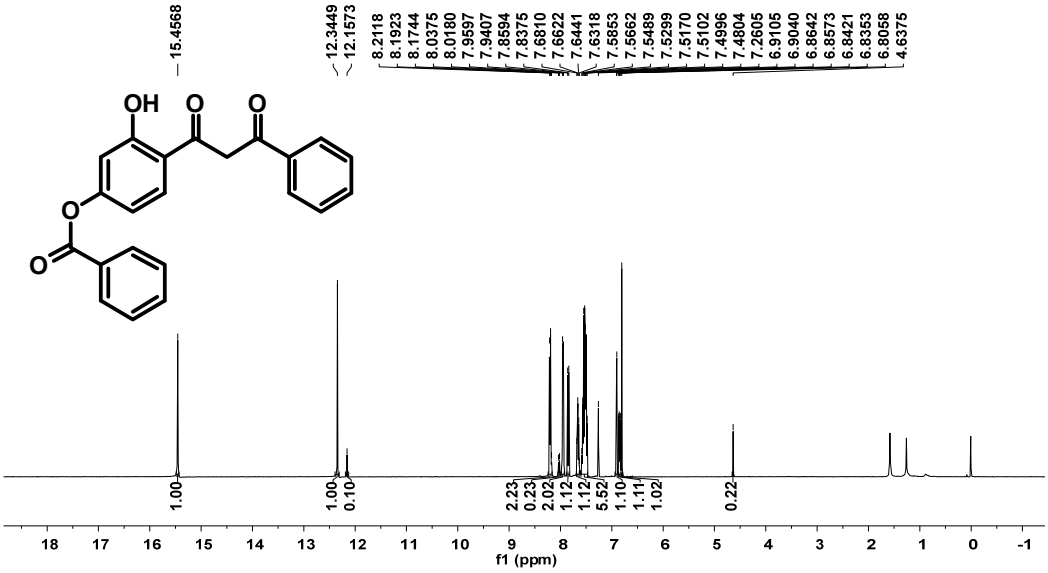


^{1}H NMR spectrum of **1s** ($CDCl_3$)

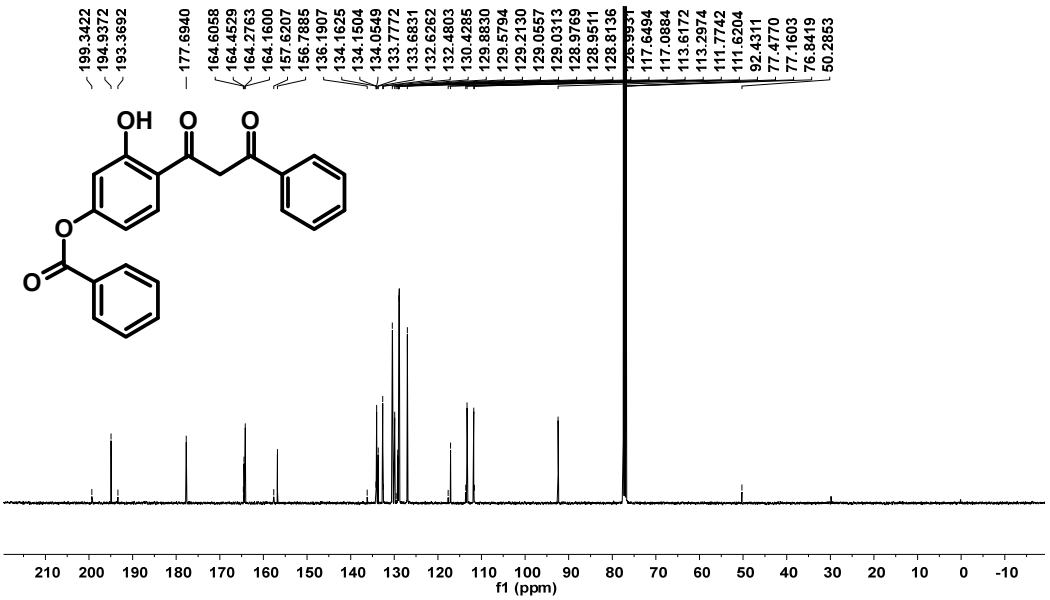


^{13}C NMR spectrum of **1s** ($CDCl_3$)

1t

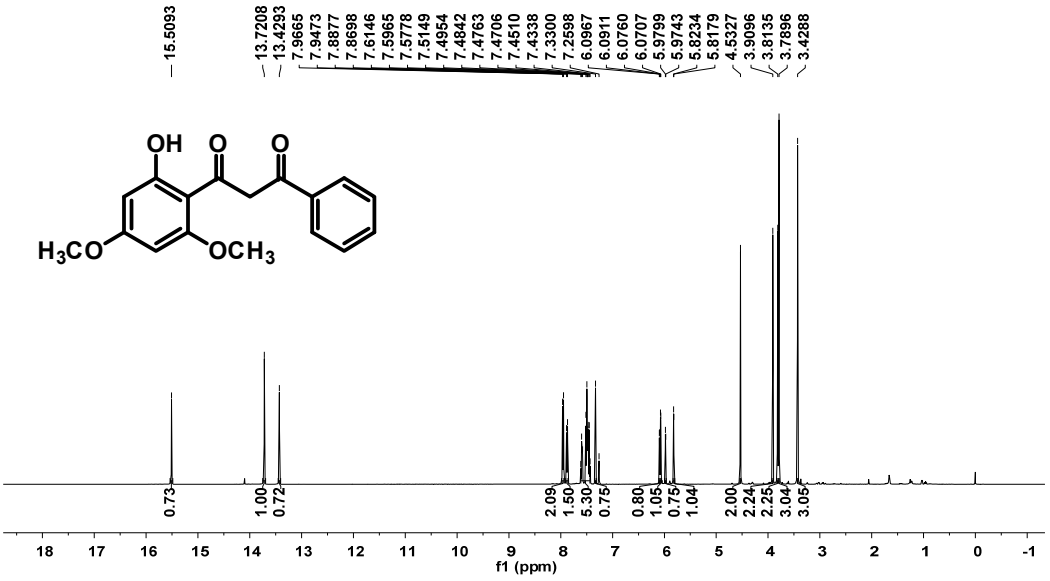


^{1}H NMR spectrum of **1t** ($CDCl_3$)

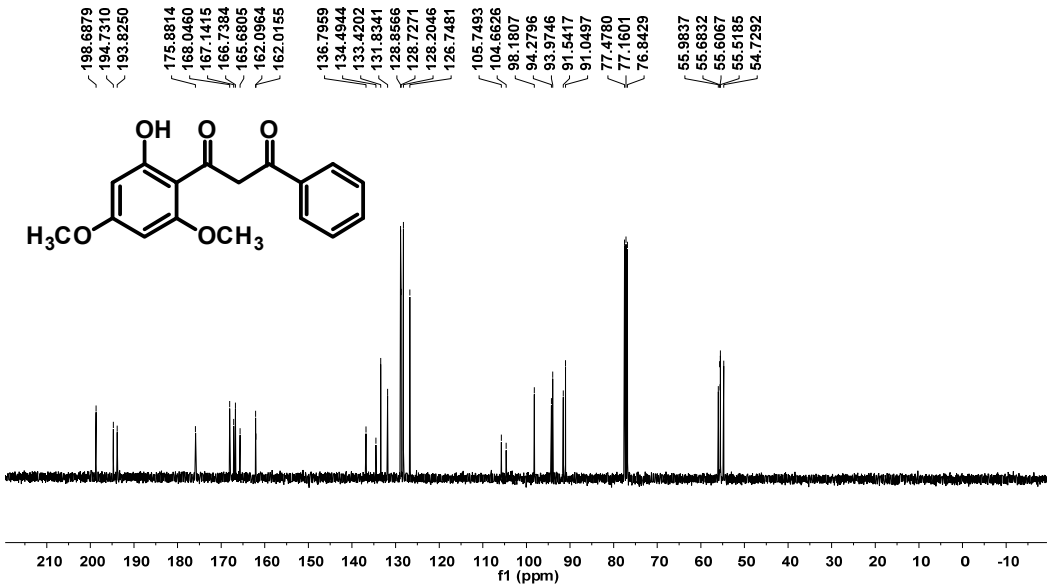


^{13}C NMR spectrum of **1t** ($CDCl_3$)

1u

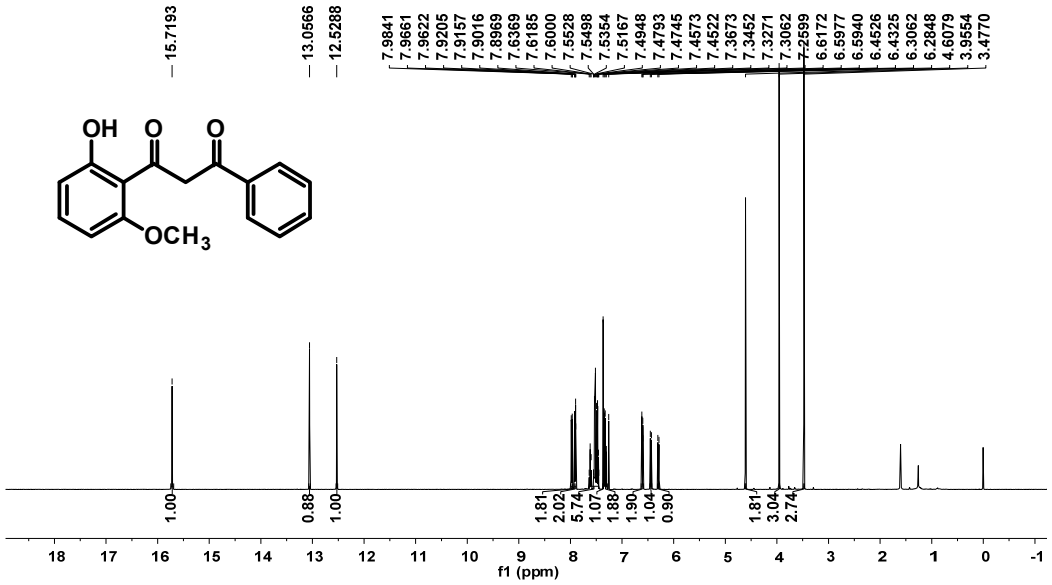


^{1}H NMR spectrum of **1u** ($CDCl_3$)



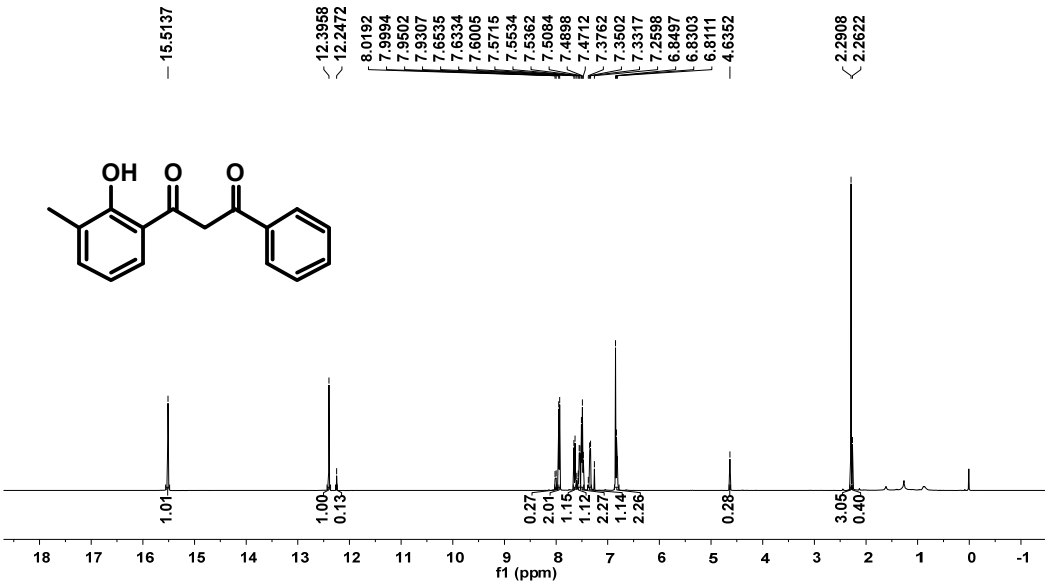
^{13}C NMR spectrum of **1u** ($CDCl_3$)

1v

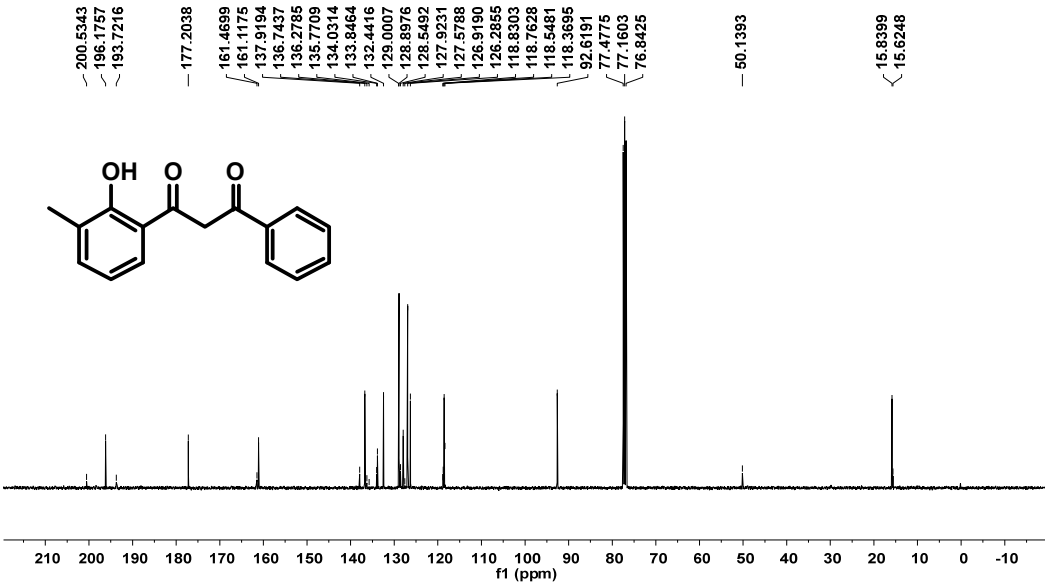


^{1}H NMR spectrum of **1v** ($CDCl_3$)

1w

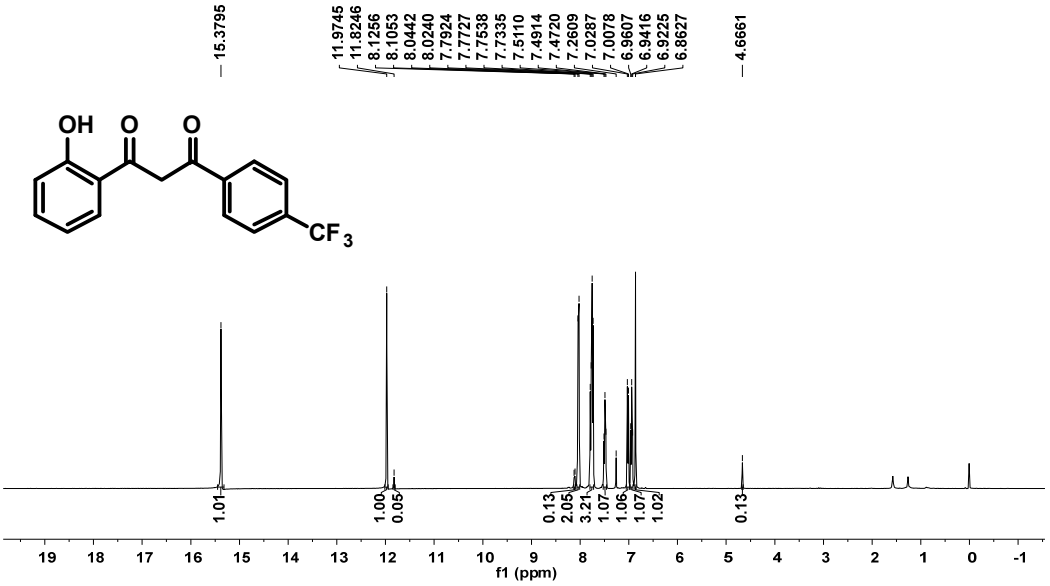


^{1}H NMR spectrum of **1w** ($CDCl_3$)



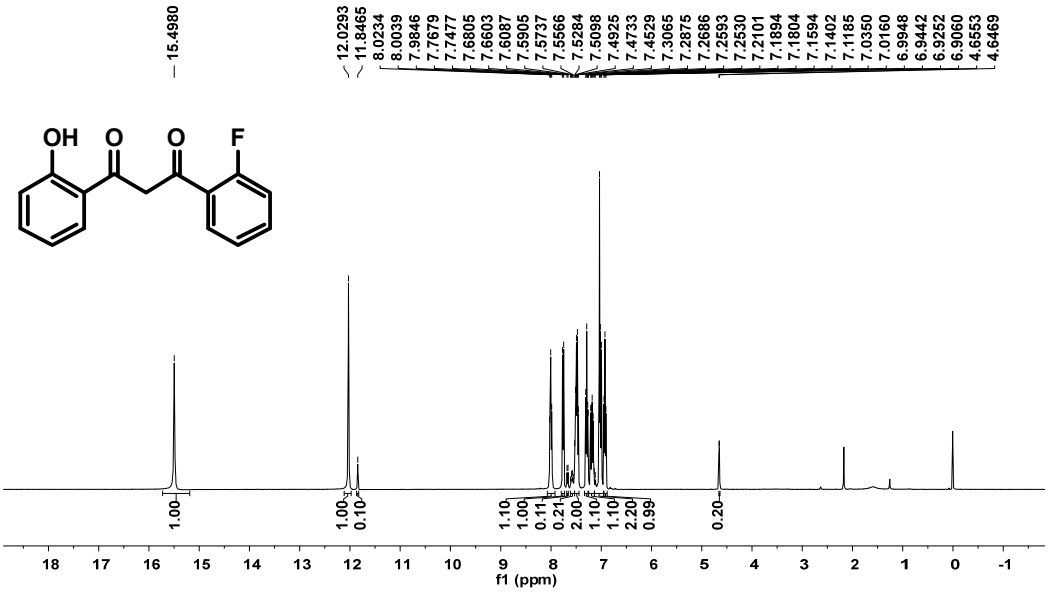
^{13}C NMR spectrum of **1w** ($CDCl_3$)

1x



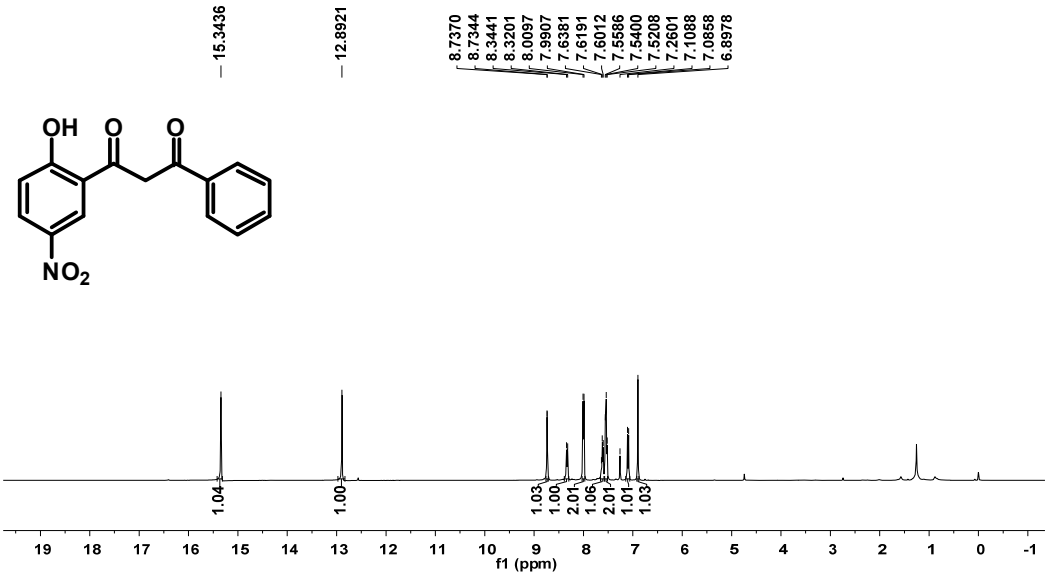
^{1}H NMR spectrum of **1x** ($CDCl_3$)

1y

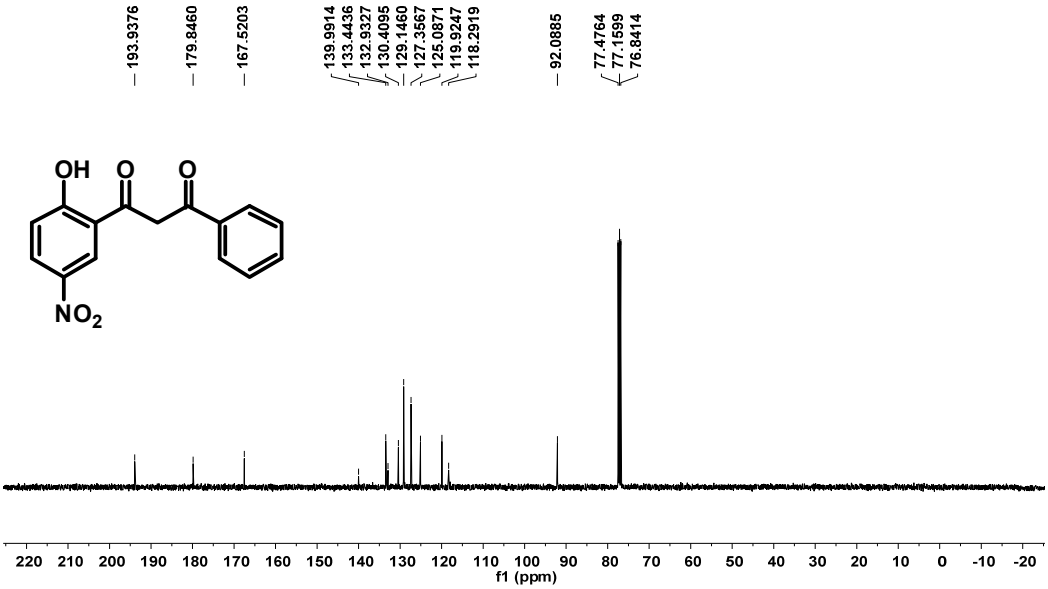


^{1}H NMR spectrum of **1y** ($CDCl_3$)

1z

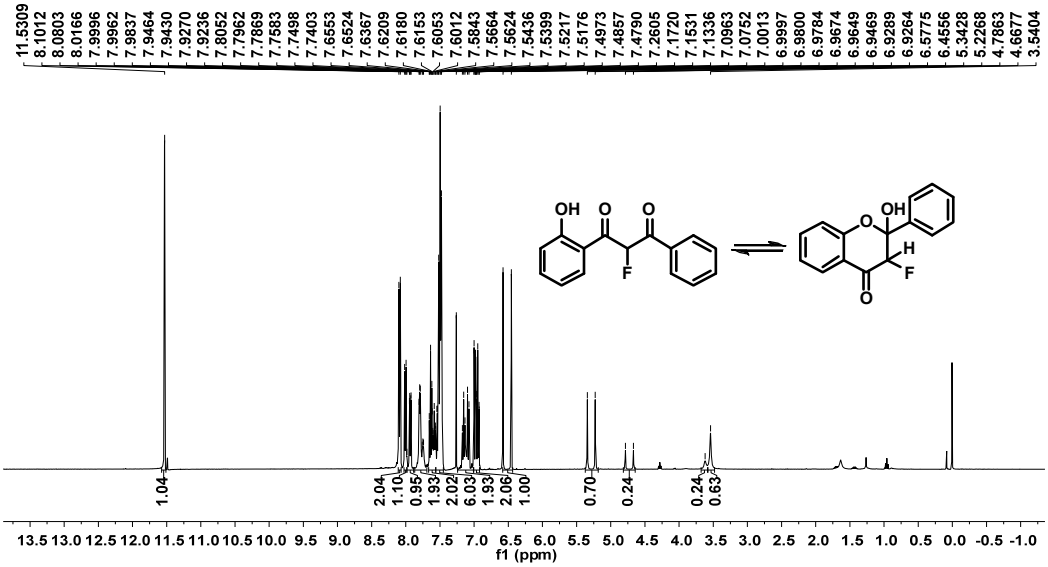


^{1}H NMR spectrum of **1z** ($CDCl_3$)

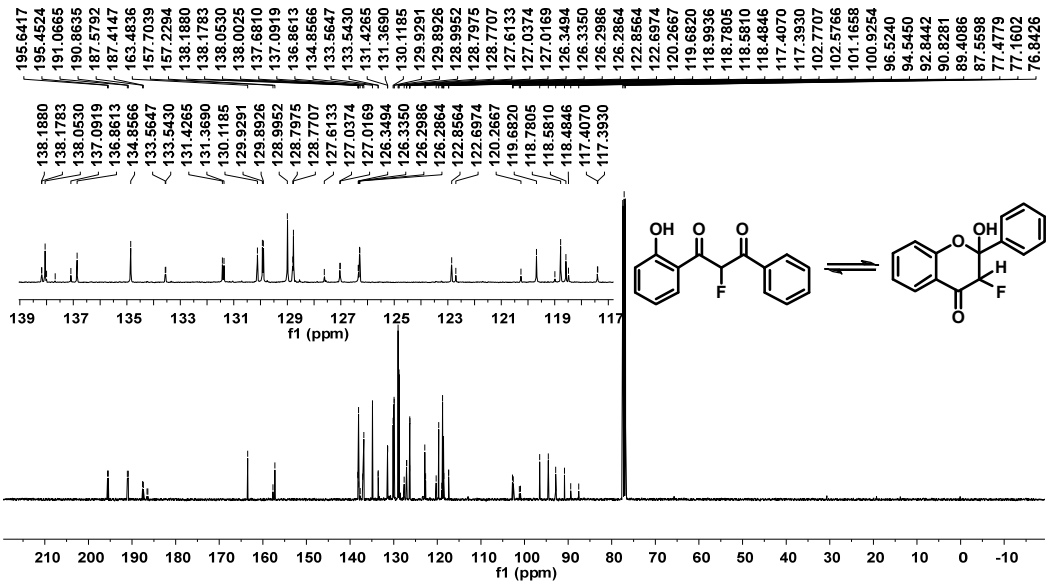


^{13}C NMR spectrum of **1z** ($CDCl_3$)

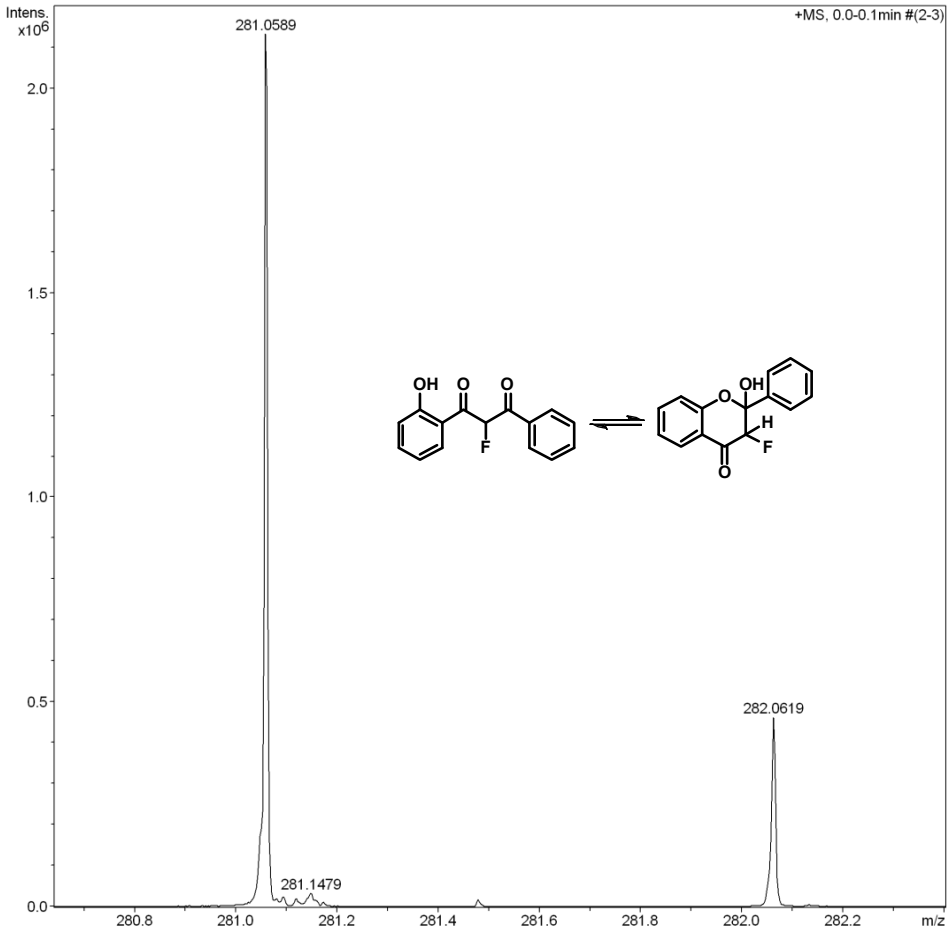
4



^{1}H NMR spectrum of **4** ($CDCl_3$)

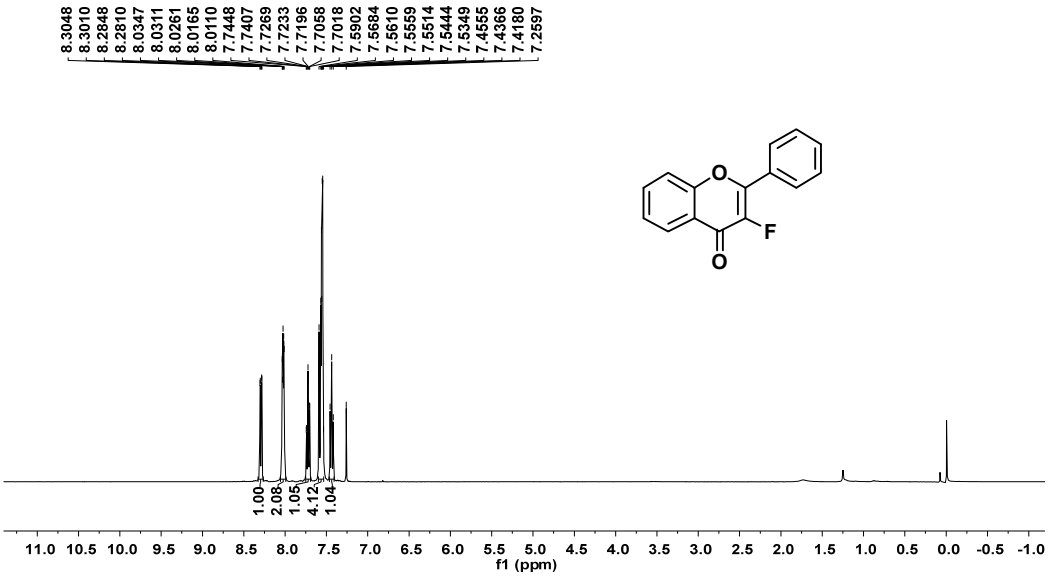


^{13}C NMR spectrum of **4** ($CDCl_3$)

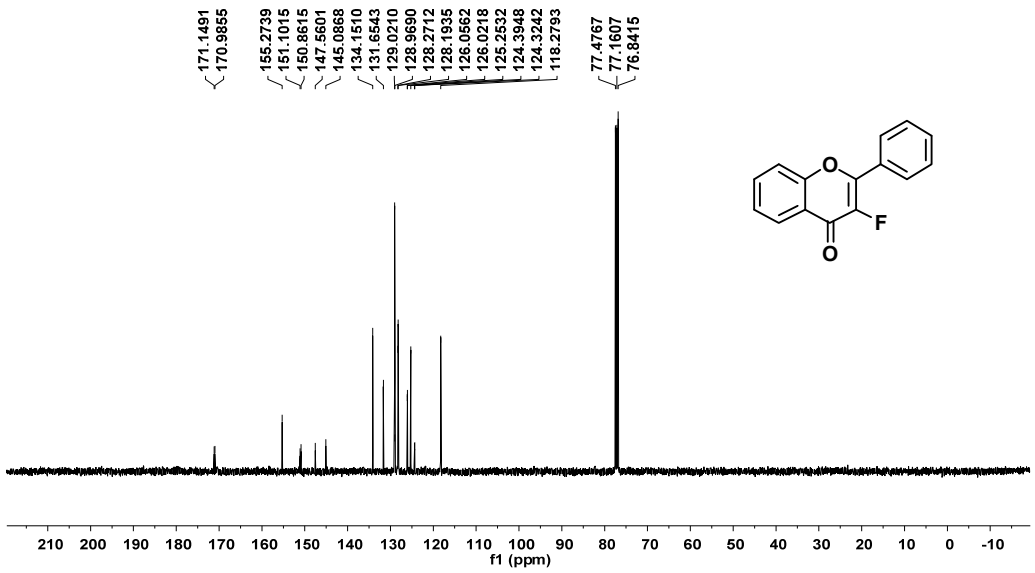


HRMS spectrum of **4** (MeOH)

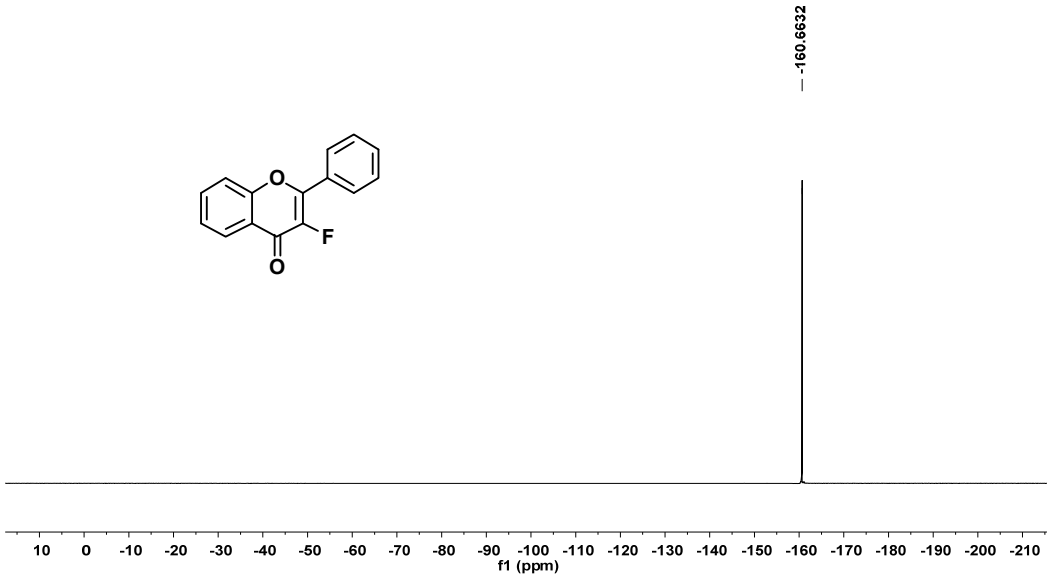
2a



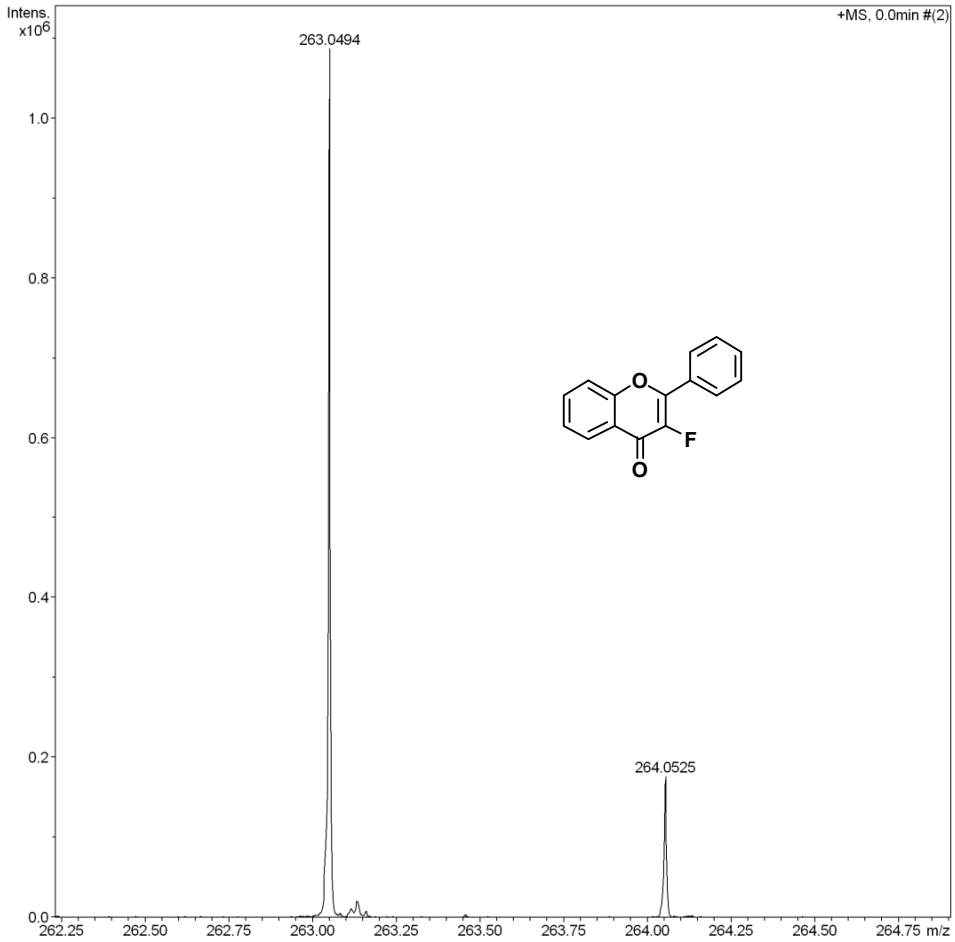
^{1}H NMR spectrum of **2a** ($CDCl_3$)



^{13}C NMR spectrum of **2a** ($CDCl_3$)

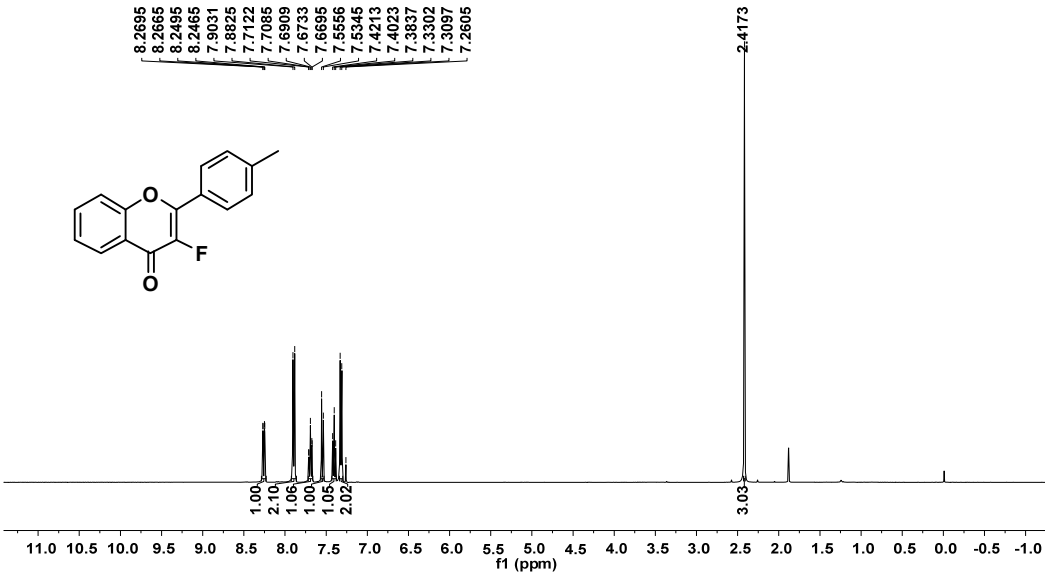


^{19}F NMR spectrum of **2a** ($CDCl_3$)

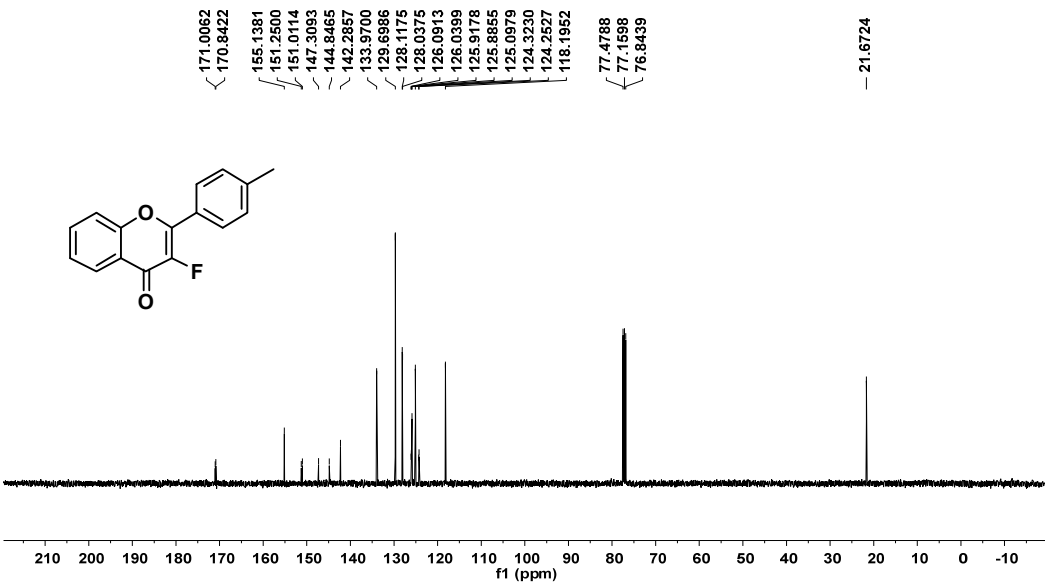


HRMS spectrum of **2a** (MeOH)

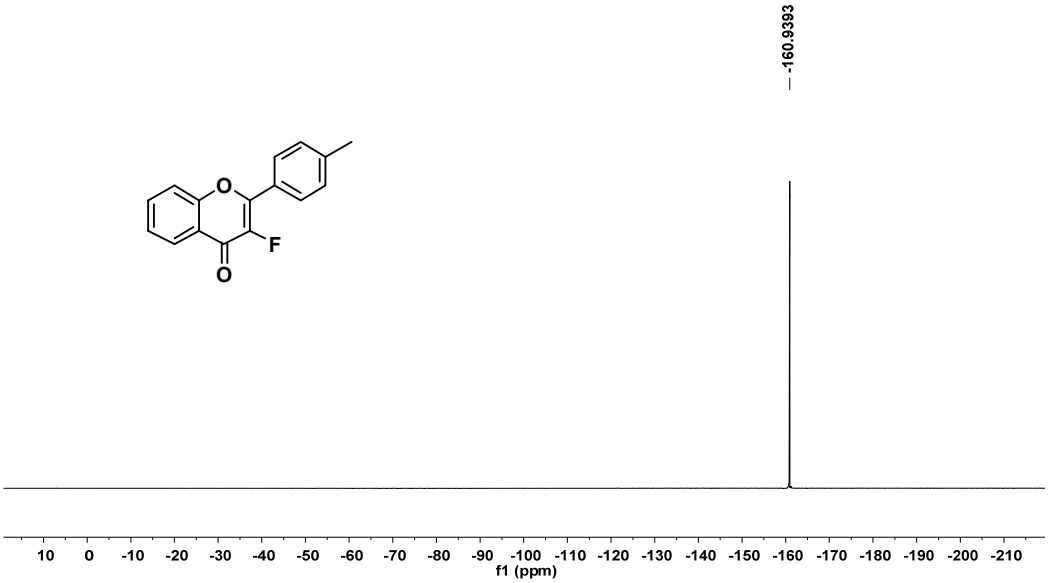
2b



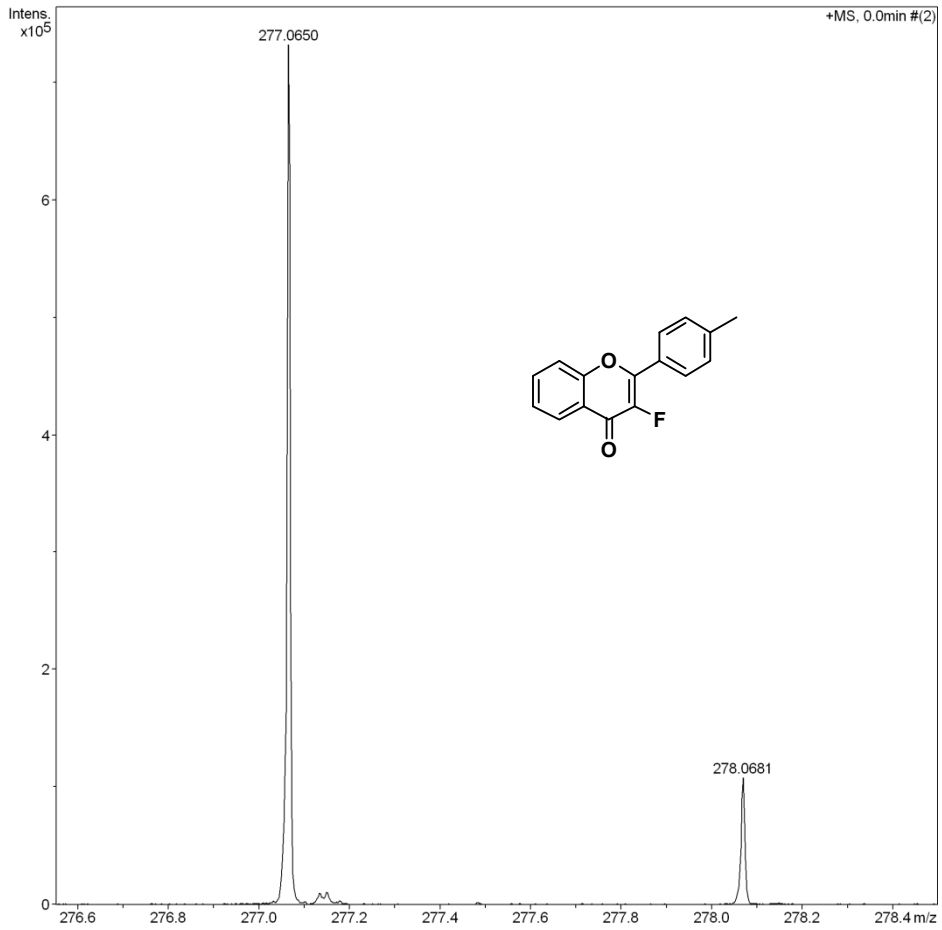
^{1}H NMR spectrum of **2b** ($CDCl_3$)



^{13}C NMR spectrum of **2b** ($CDCl_3$)

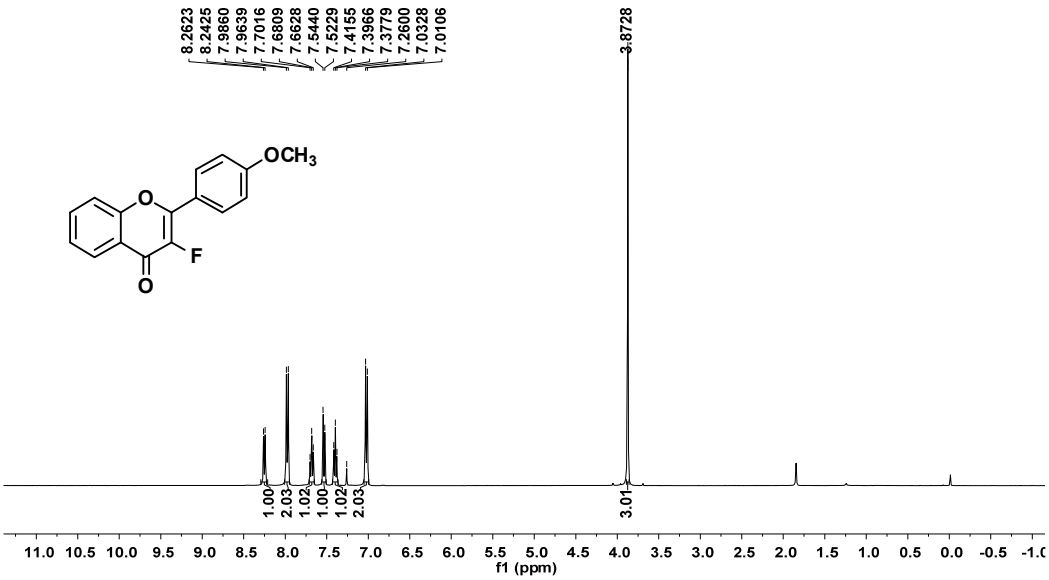


^{19}F NMR spectrum of **2b** ($CDCl_3$)

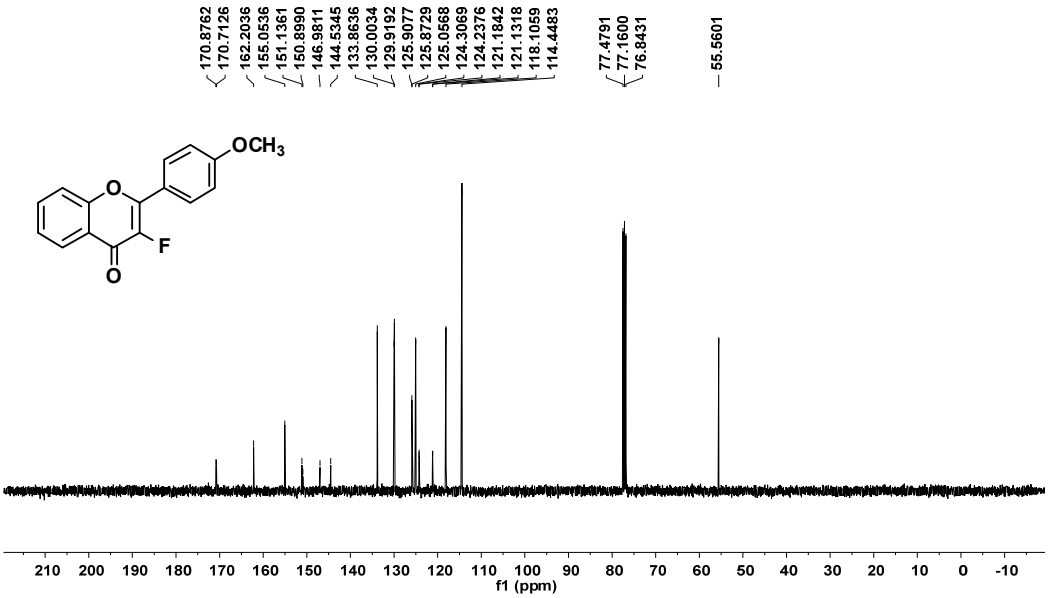


HRMS spectrum of **2b** (MeOH)

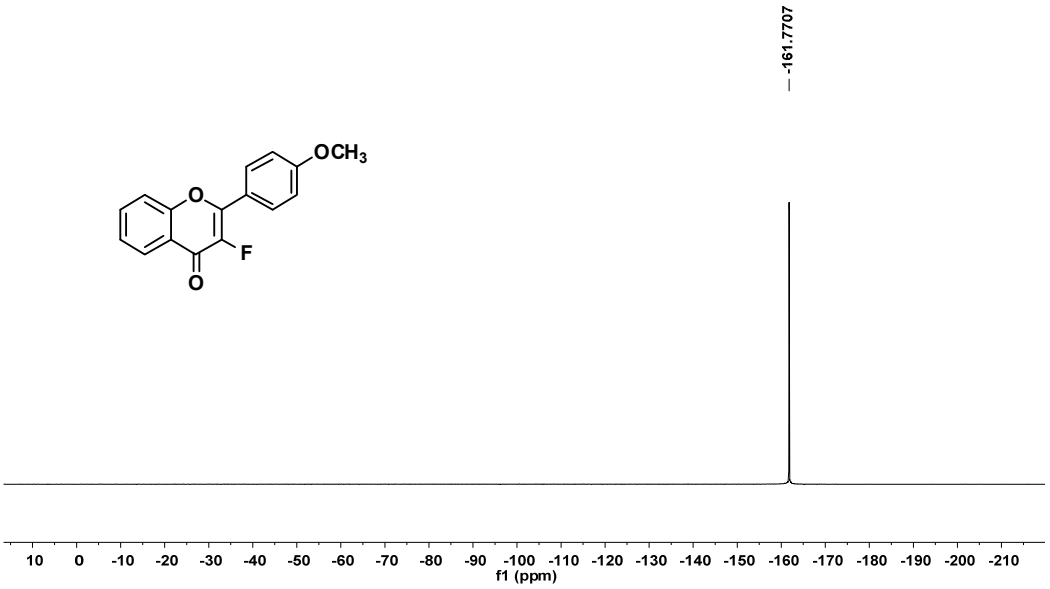
2c



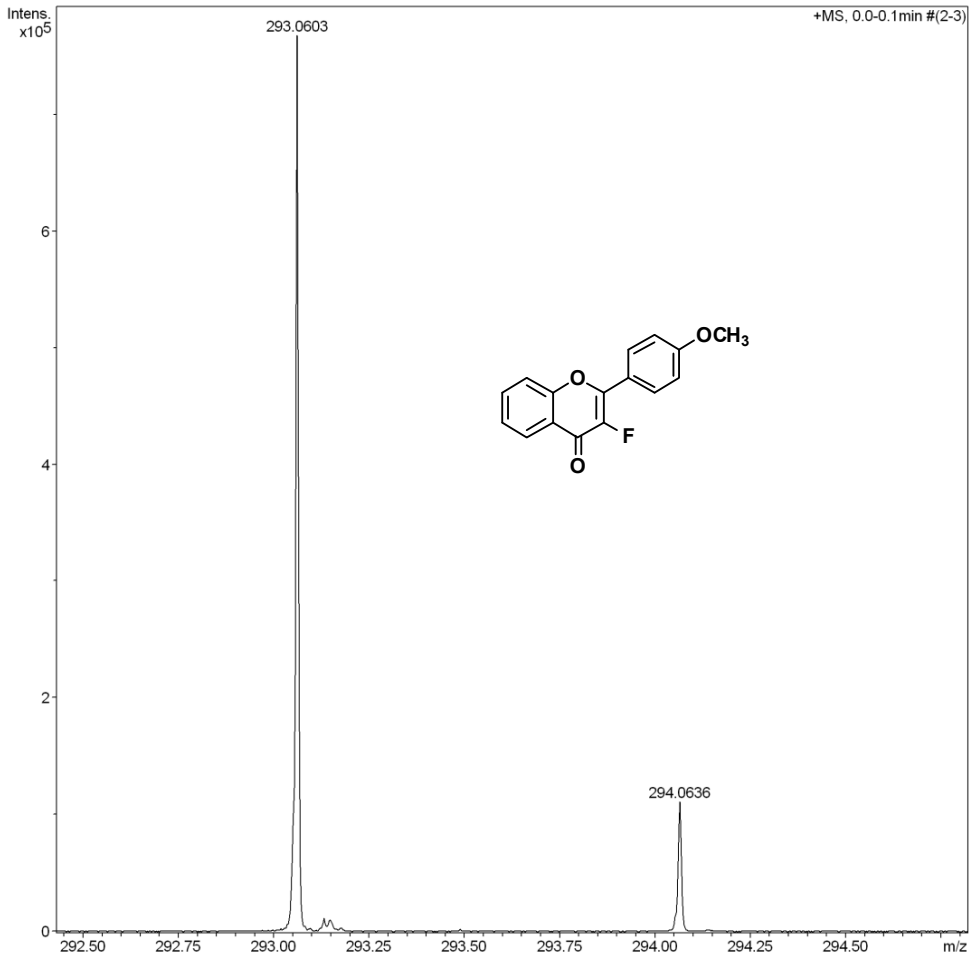
^{1}H NMR spectrum of **2c** ($CDCl_3$)



^{13}C NMR spectrum of **2c** ($CDCl_3$)

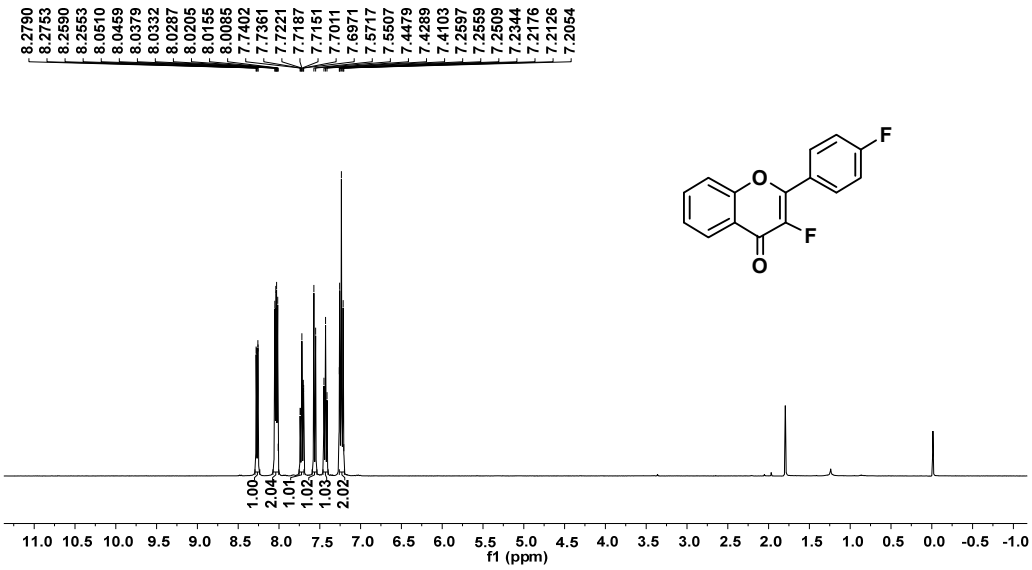


^{19}F NMR spectrum of **2c** ($CDCl_3$)

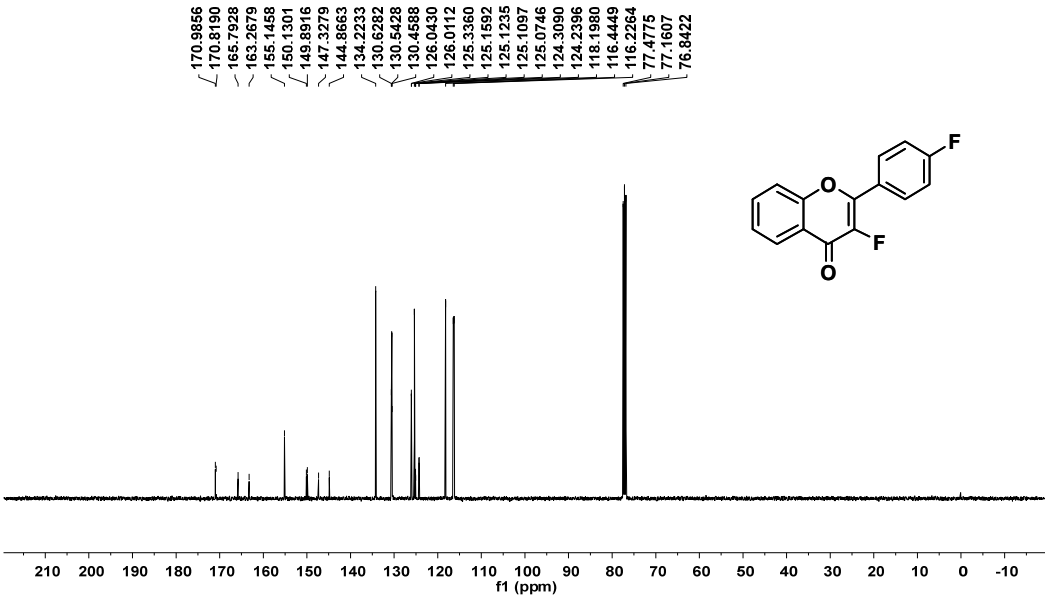


HRMS spectrum of **2c** (MeOH)

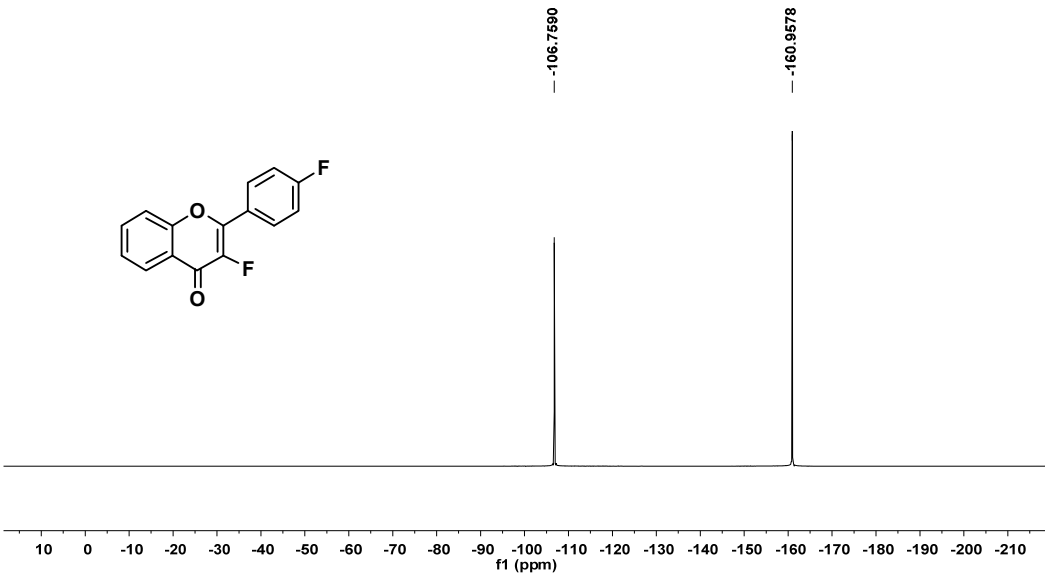
2d



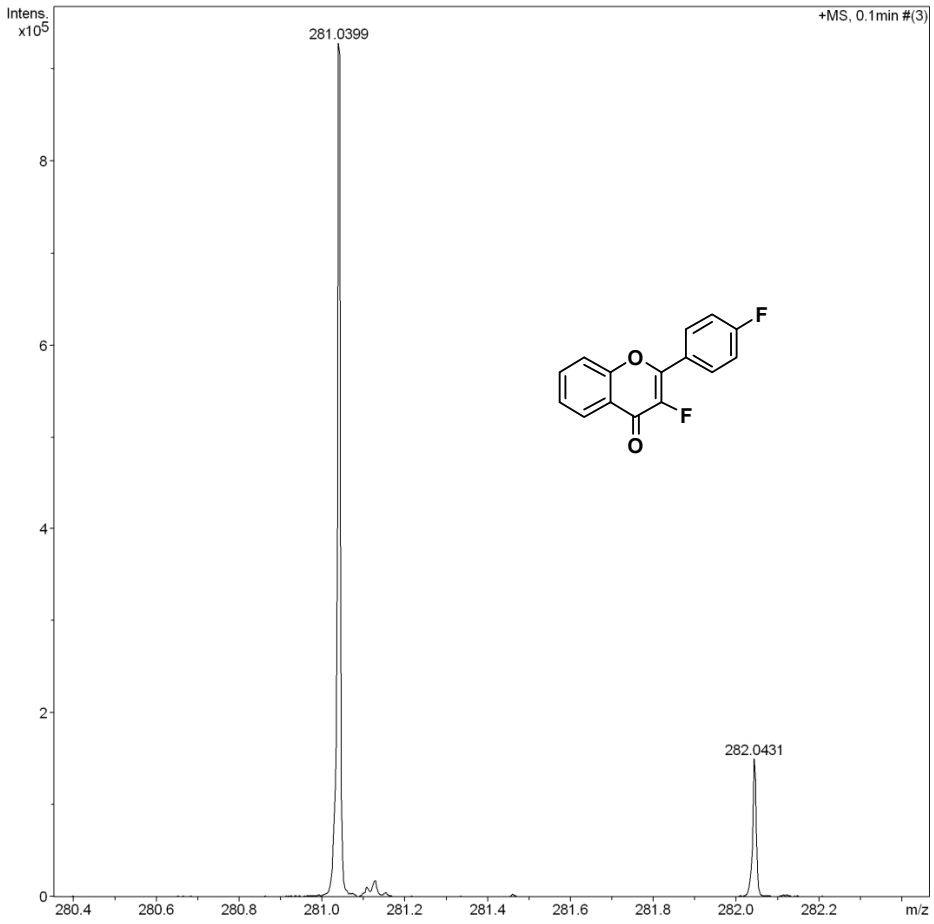
^{1}H NMR spectrum of **2d** ($CDCl_3$)



^{13}C NMR spectrum of **2d** ($CDCl_3$)

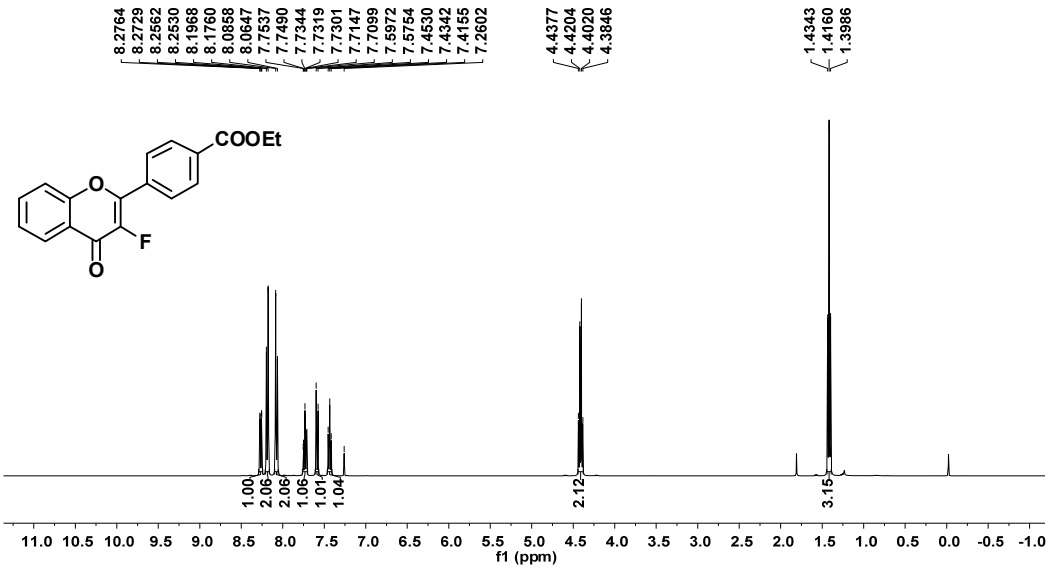


^{19}F NMR spectrum of **2d** ($CDCl_3$)

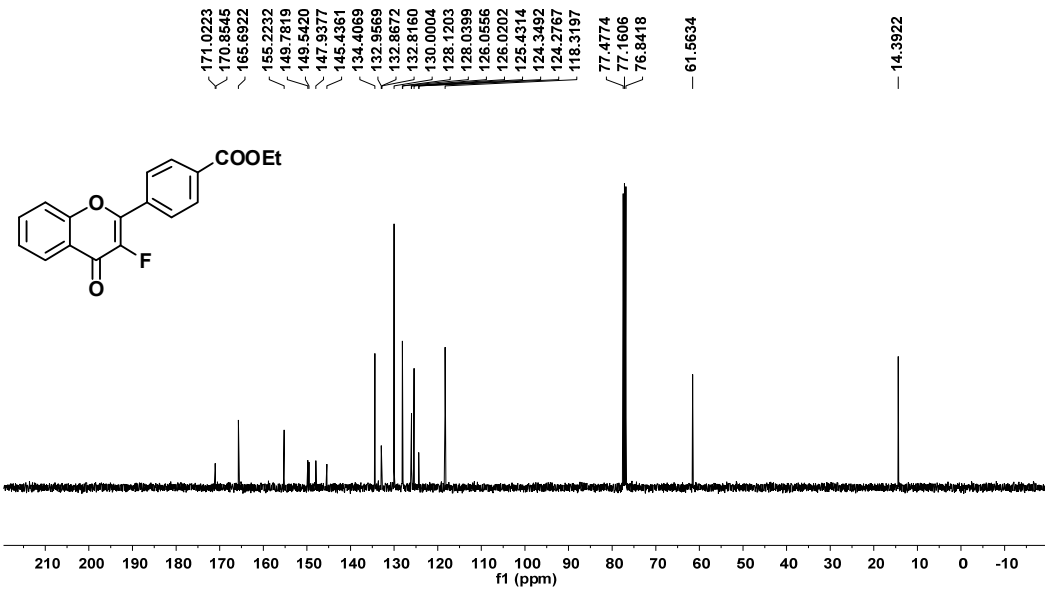


HRMS spectrum of **2d** (MeOH)

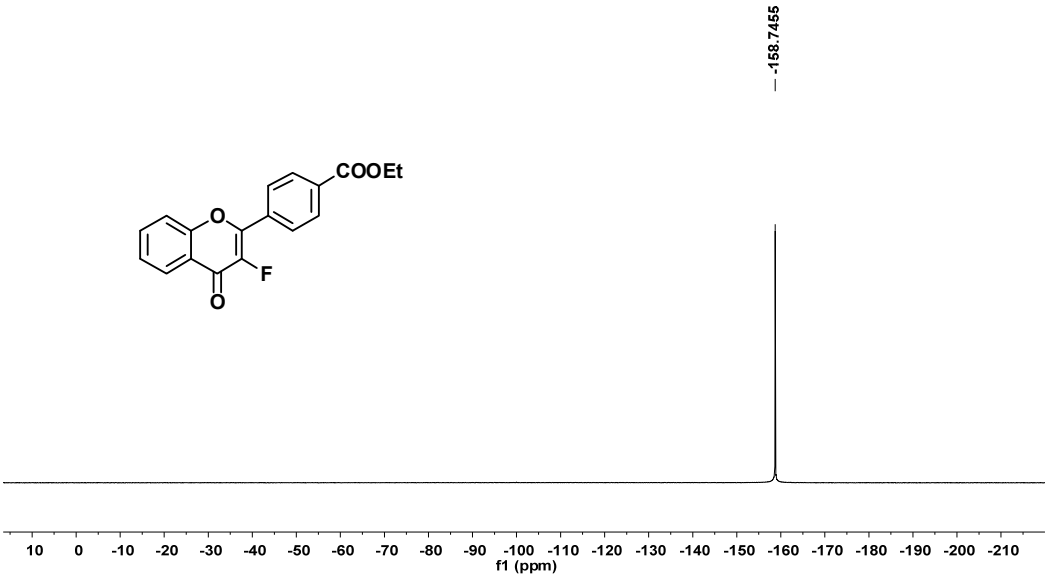
2e



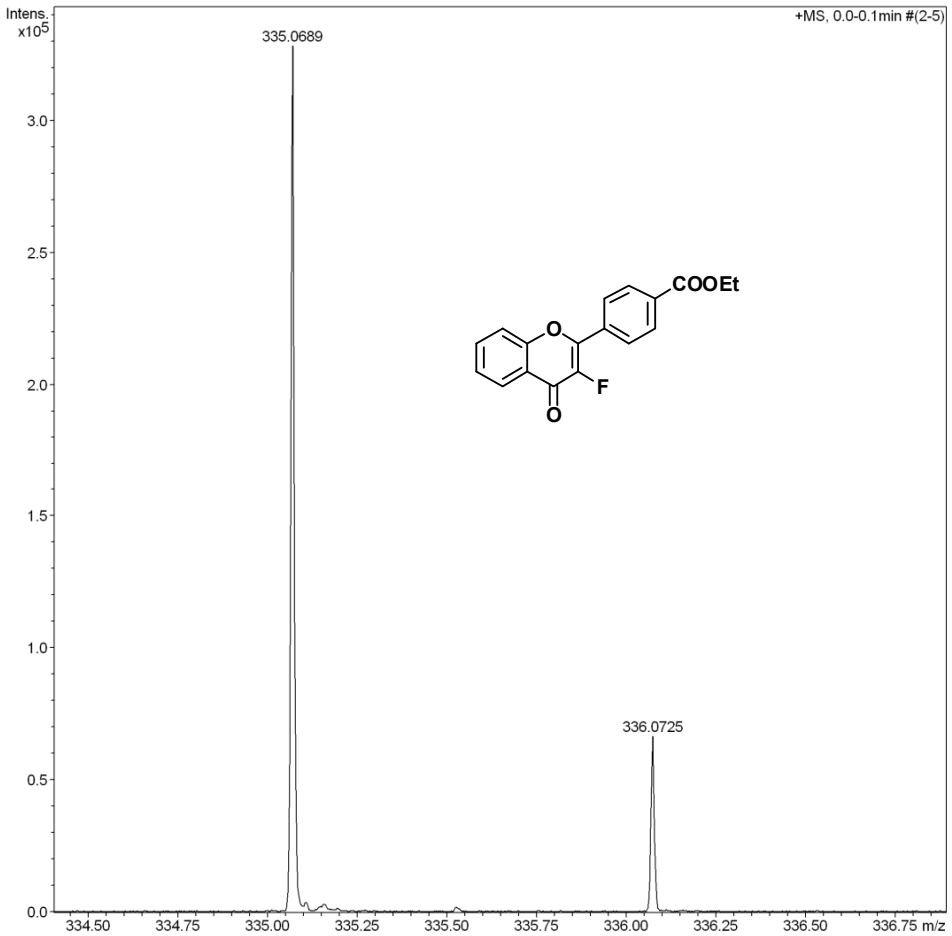
^{1}H NMR spectrum of **2e** ($CDCl_3$)



^{13}C NMR spectrum of **2e** ($CDCl_3$)

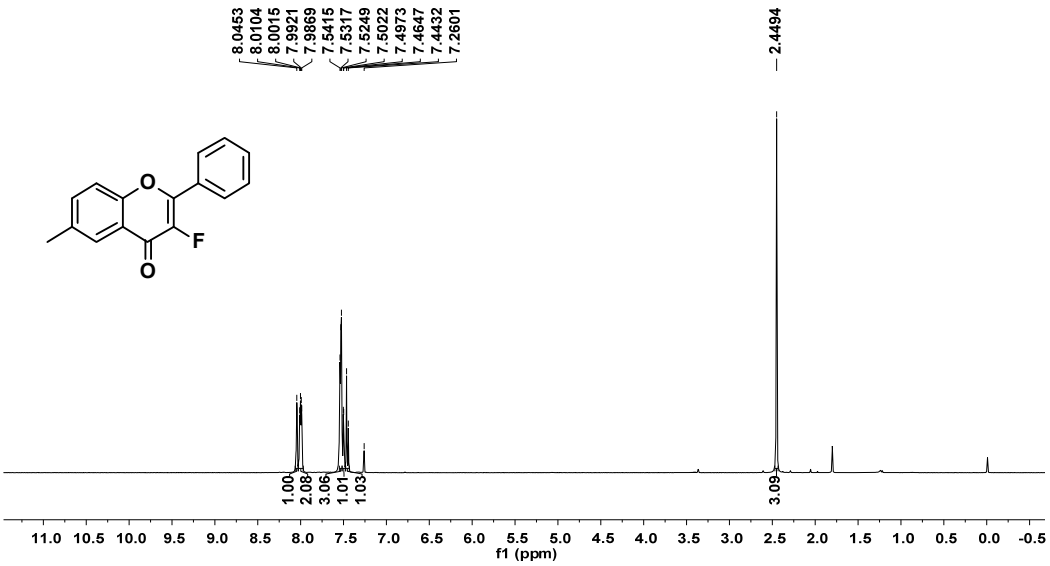


^{19}F NMR spectrum of **2e** ($CDCl_3$)

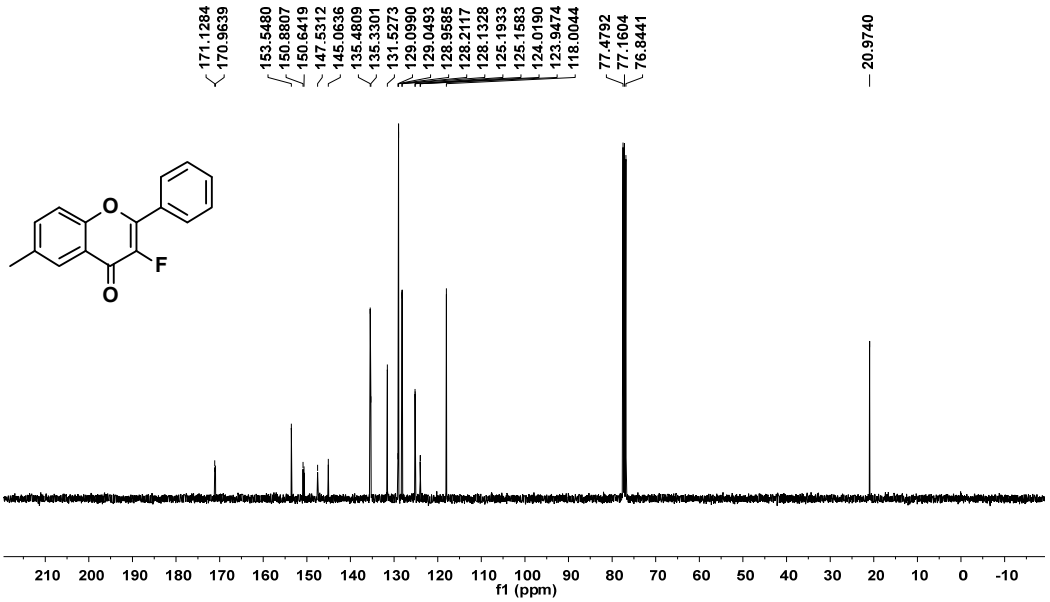


HRMS spectrum of **2e** (MeOH)

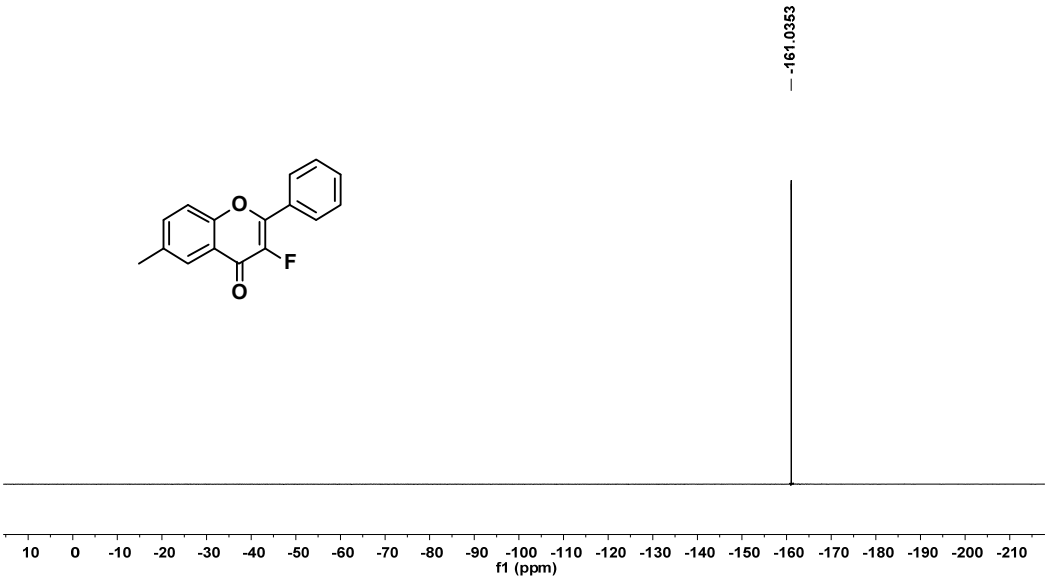
2f



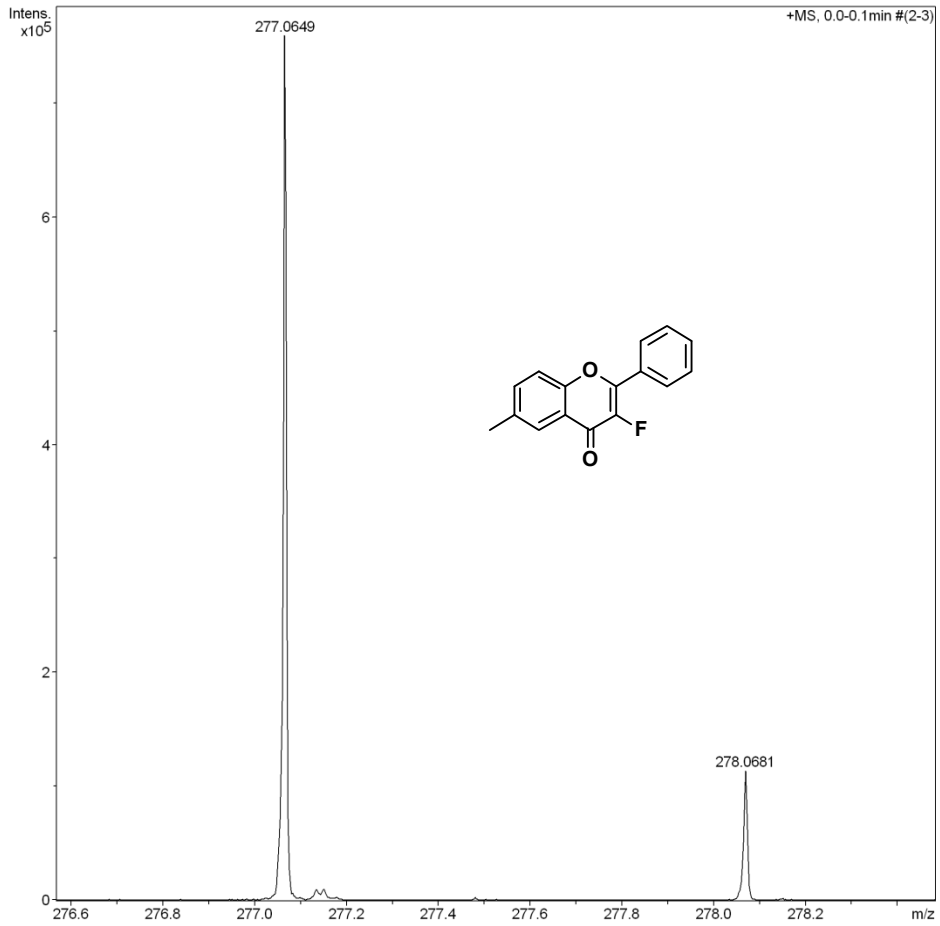
^{1}H NMR spectrum of **2f** ($CDCl_3$)



^{13}C NMR spectrum of **2f** ($CDCl_3$)

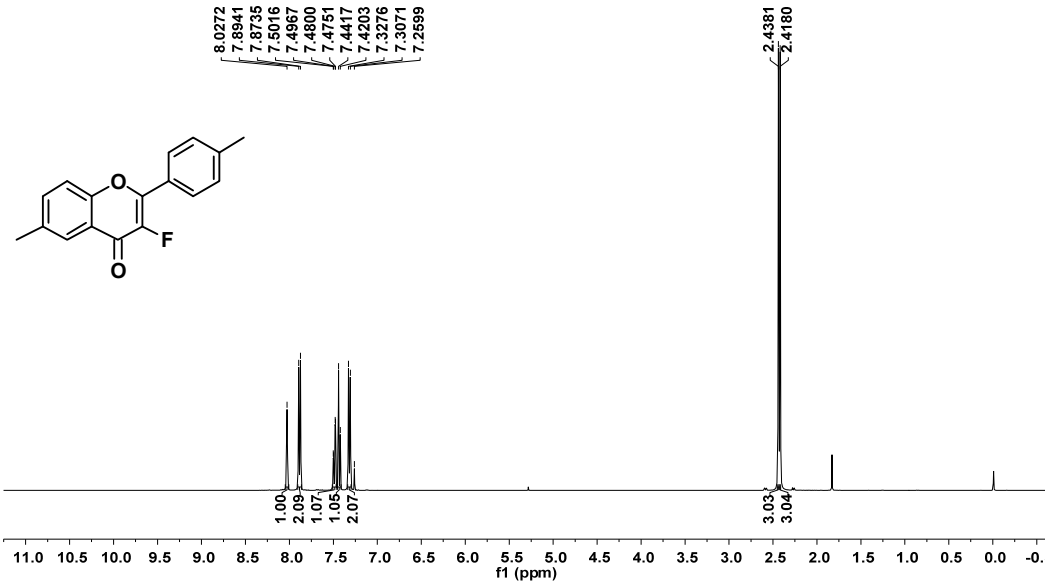


^{19}F NMR spectrum of **2f** ($CDCl_3$)

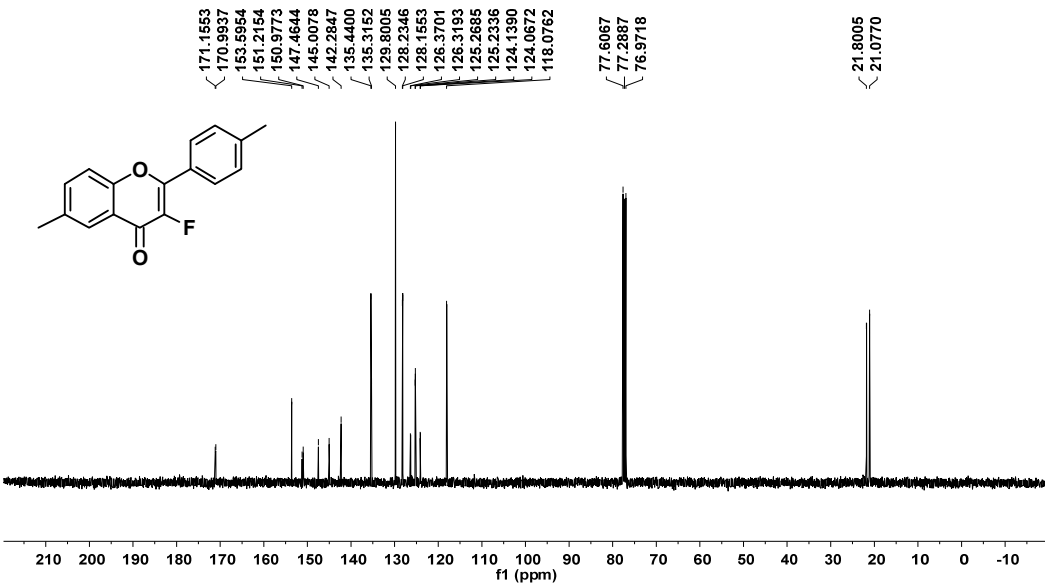


HRMS spectrum of **2f** (MeOH)

2g

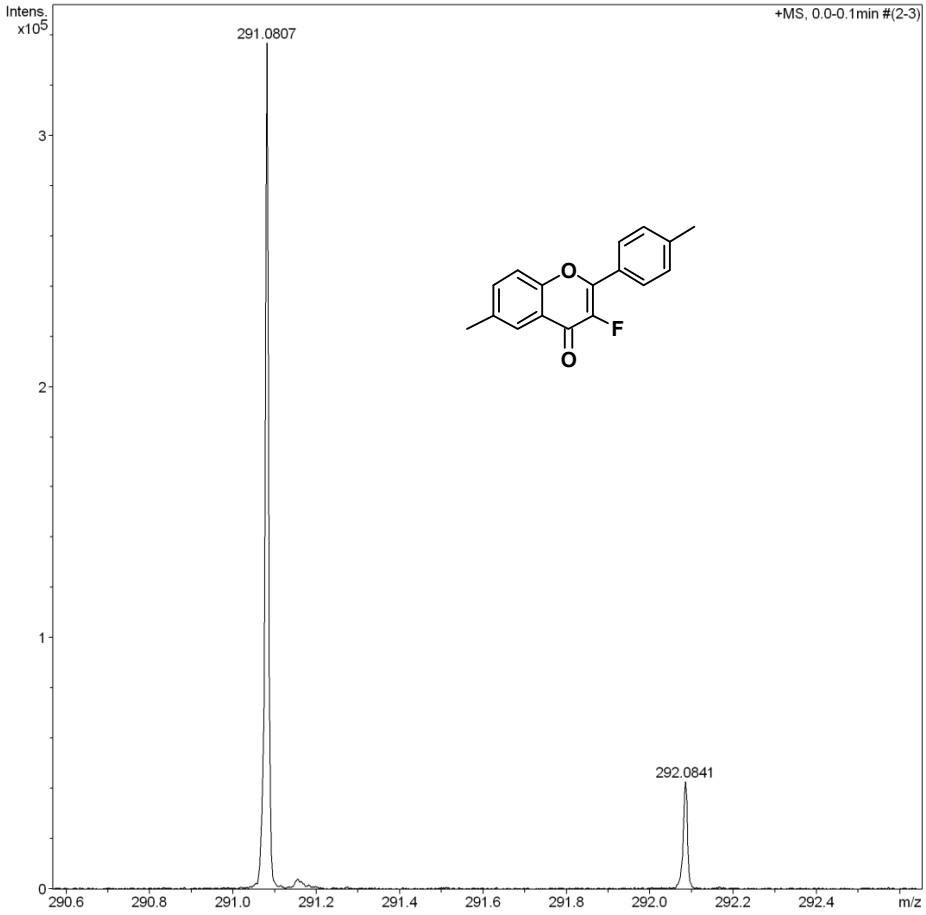


^{1}H NMR spectrum of **2g** ($CDCl_3$)



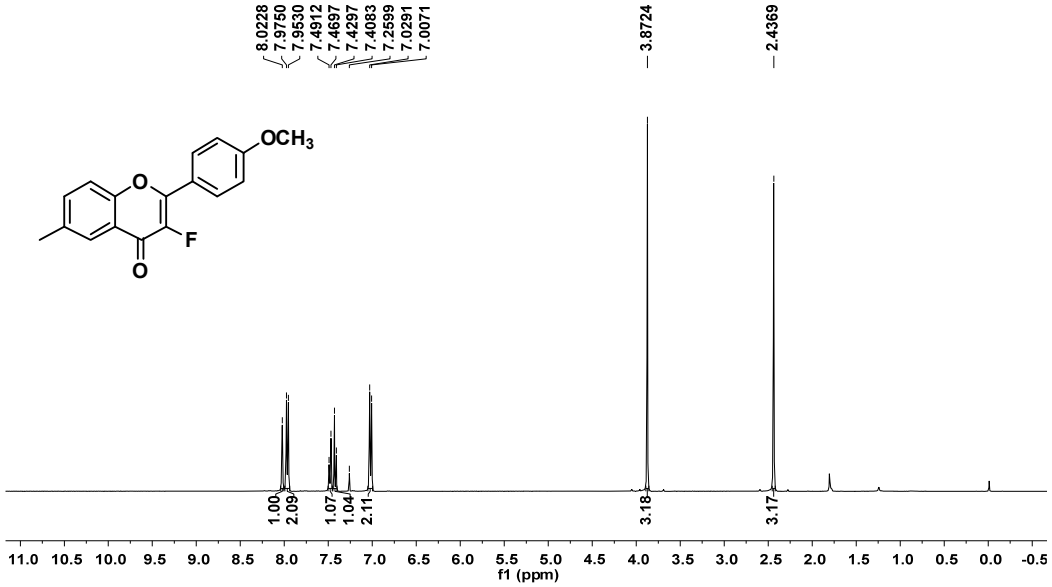
^{13}C NMR spectrum of **2g** ($CDCl_3$)

^{19}F NMR spectrum of **2g** ($CDCl_3$)

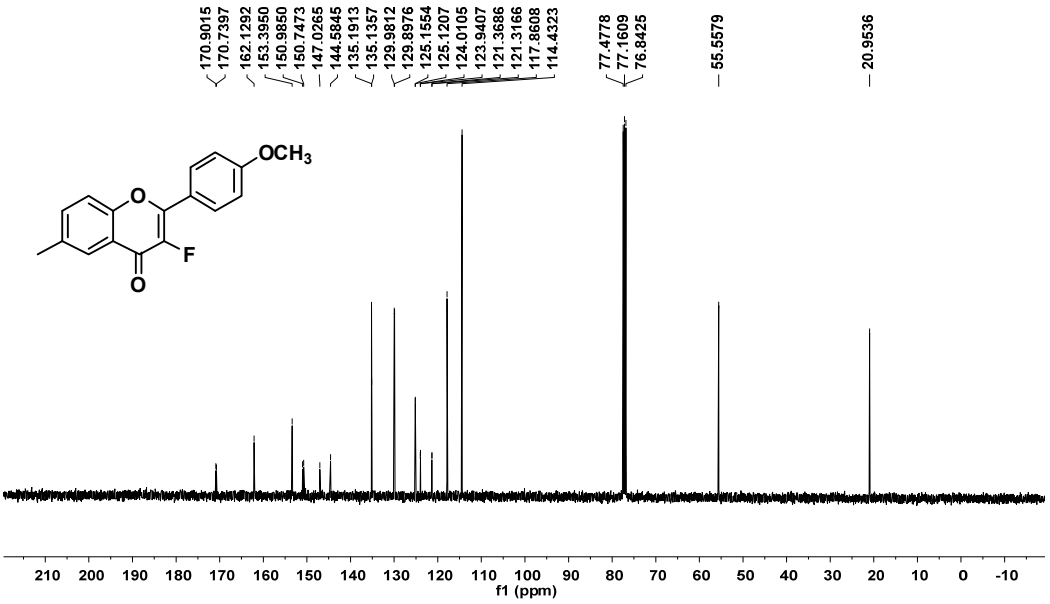


HRMS spectrum of **2g** (MeOH)

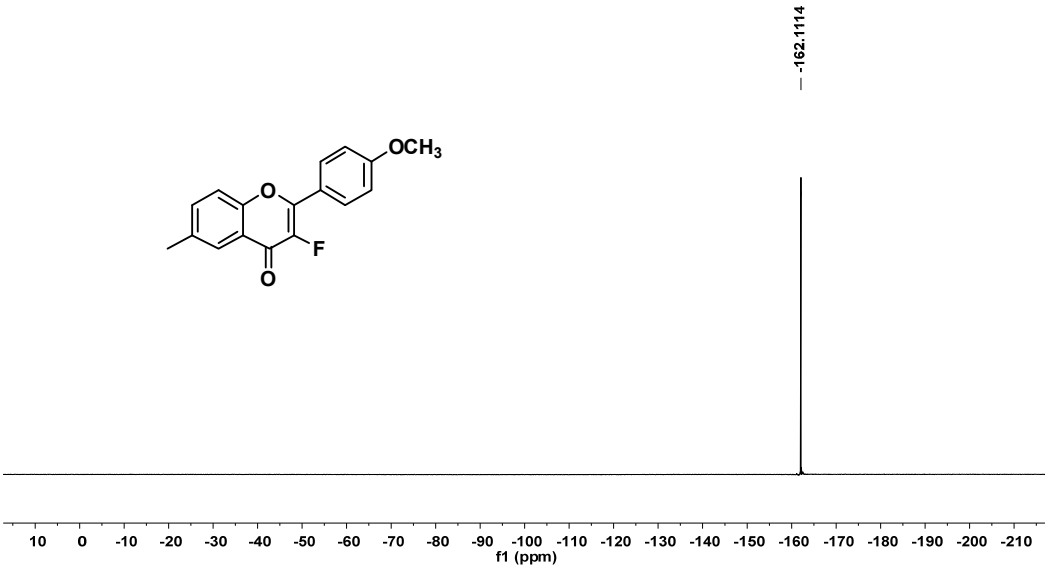
2h



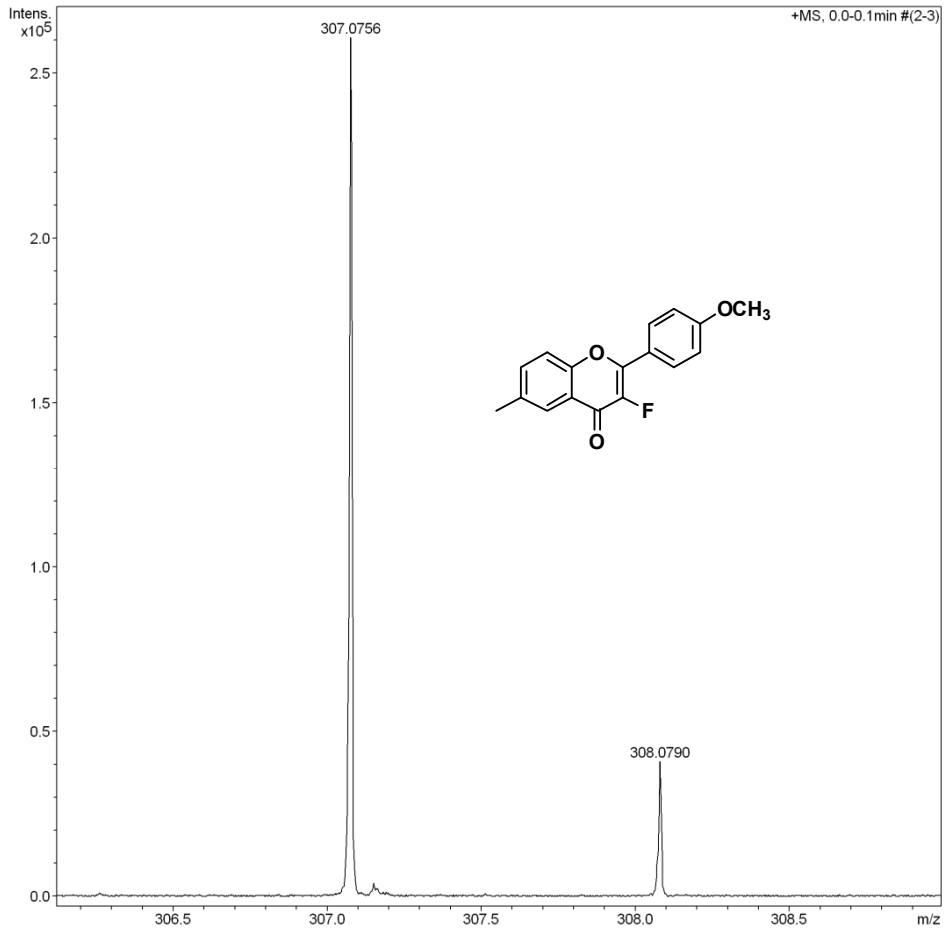
^{1}H NMR spectrum of **2h** ($CDCl_3$)



^{13}C NMR spectrum of **2h** ($CDCl_3$)

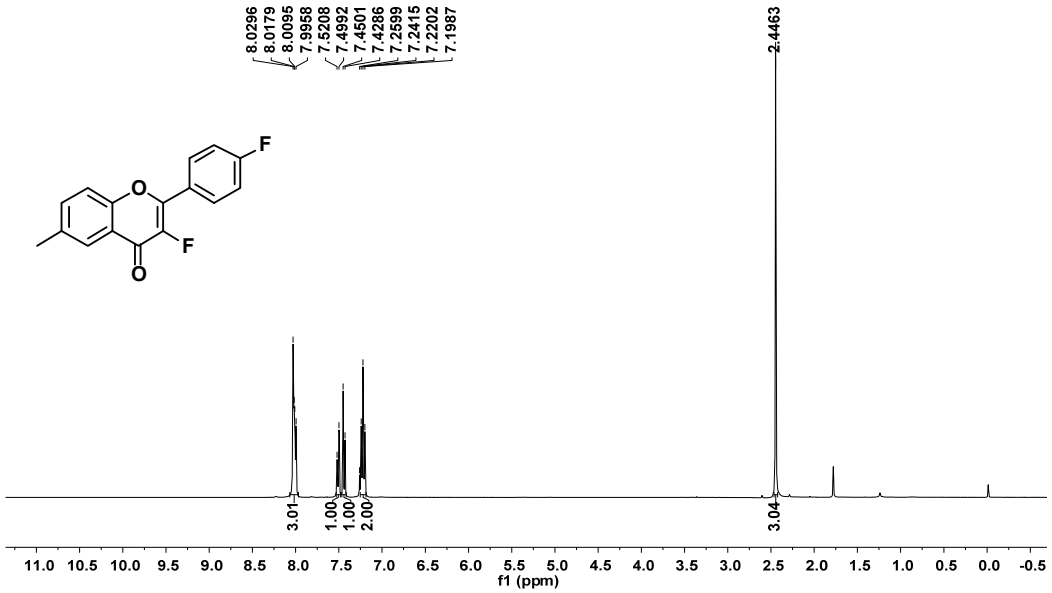


^{19}F NMR spectrum of **2h** ($CDCl_3$)

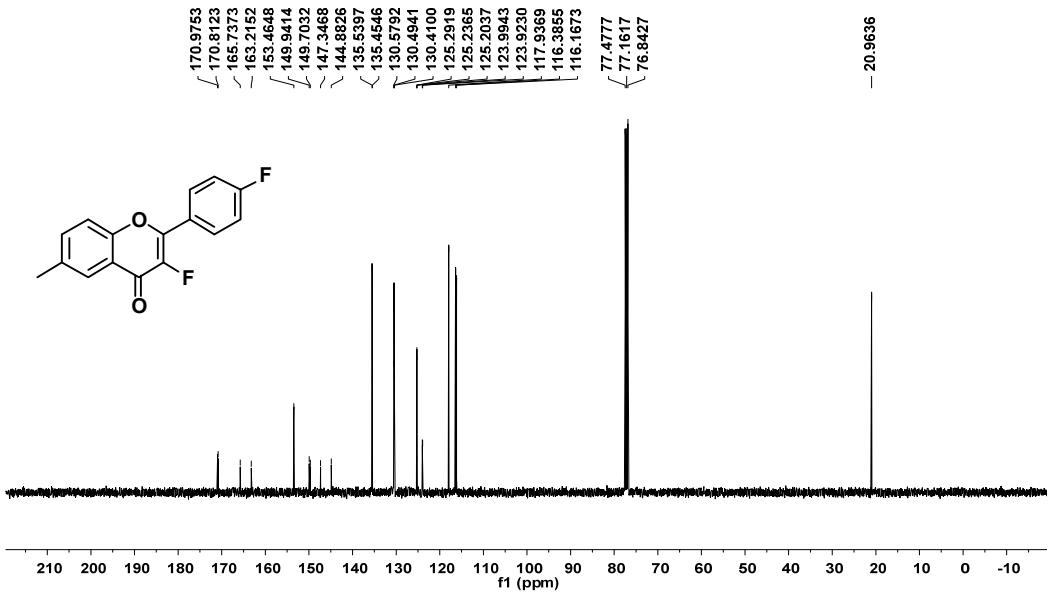


HRMS spectrum of **2h** (MeOH)

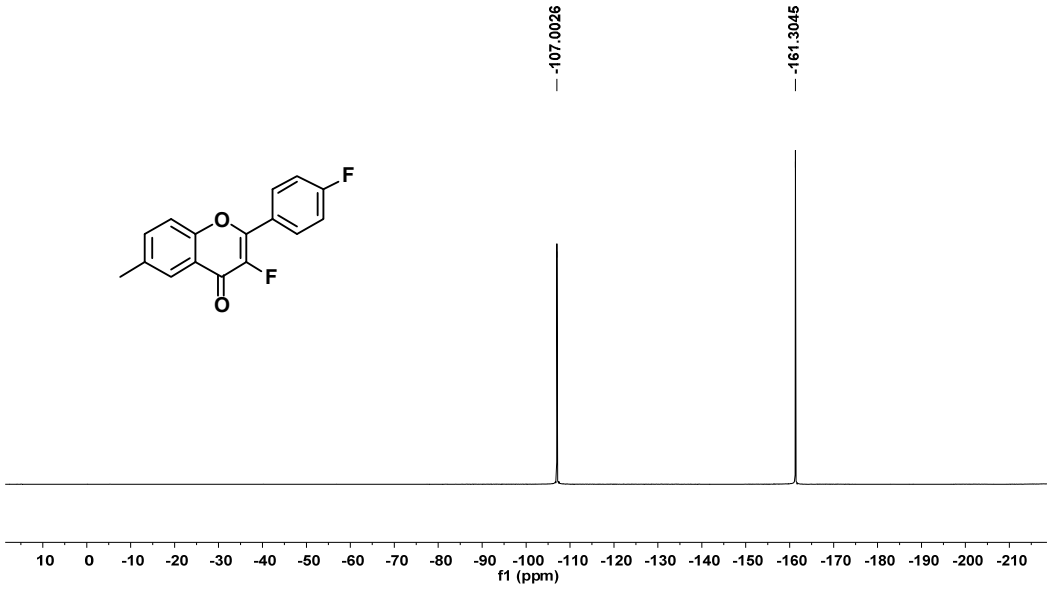
2i



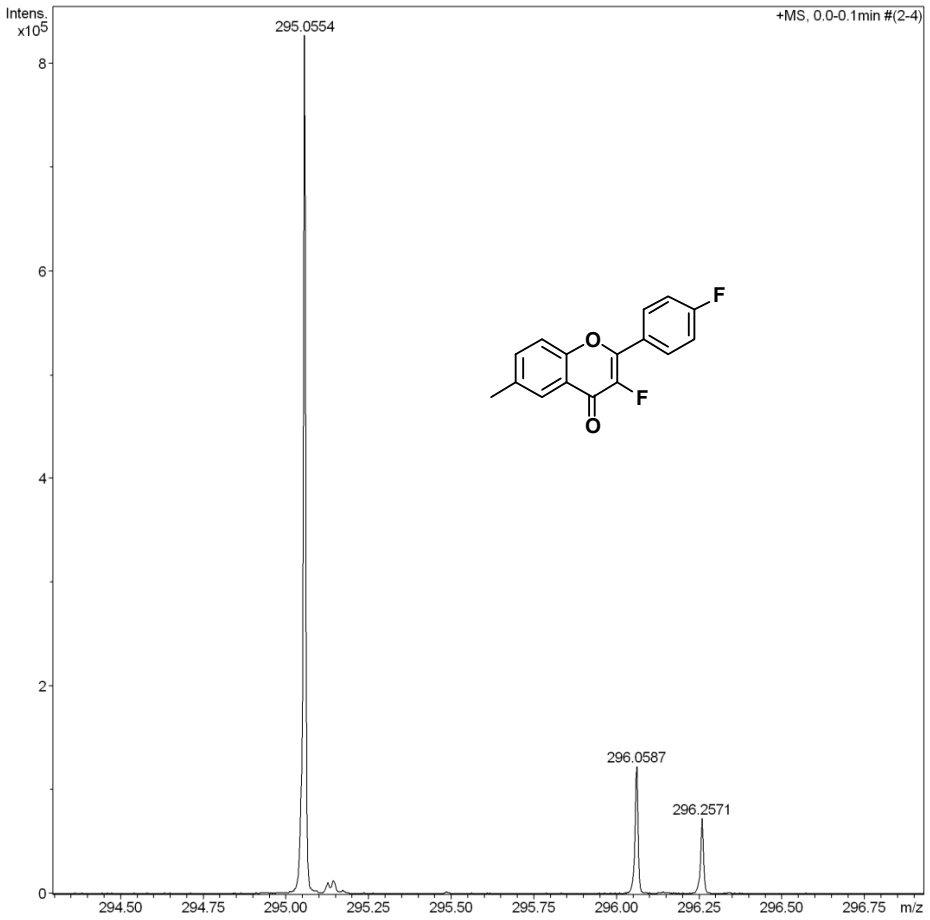
^{1}H NMR spectrum of **2i** ($CDCl_3$)



^{13}C NMR spectrum of **2i** ($CDCl_3$)

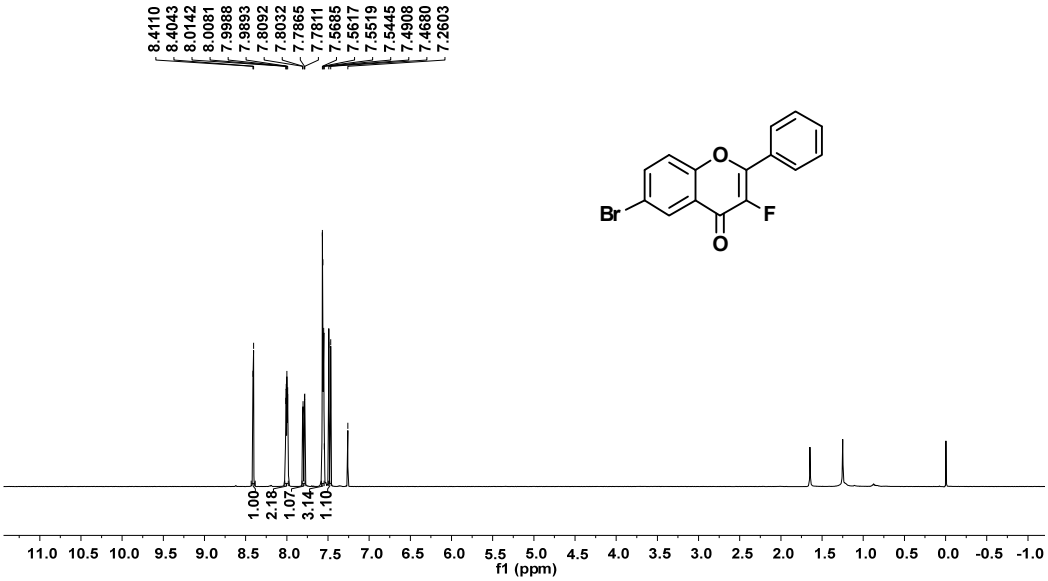


^{19}F NMR spectrum of **2i** ($CDCl_3$)

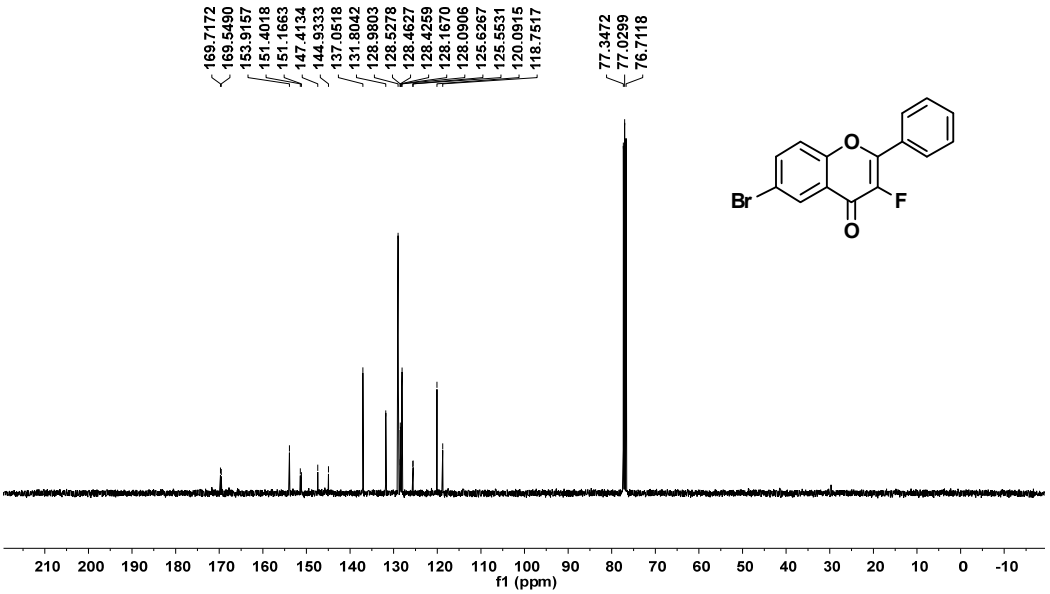


HRMS spectrum of **2i** (MeOH)

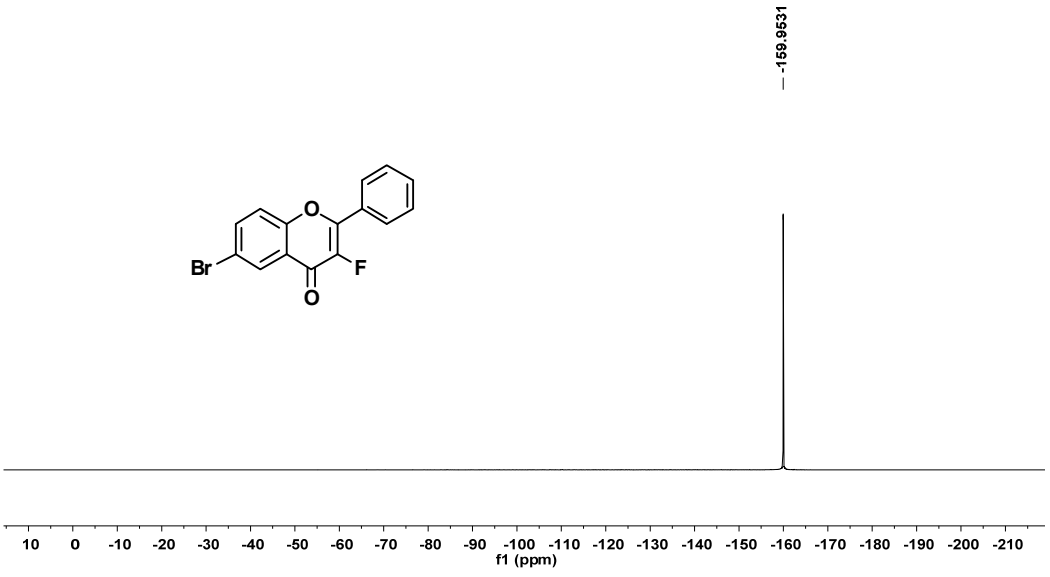
2j



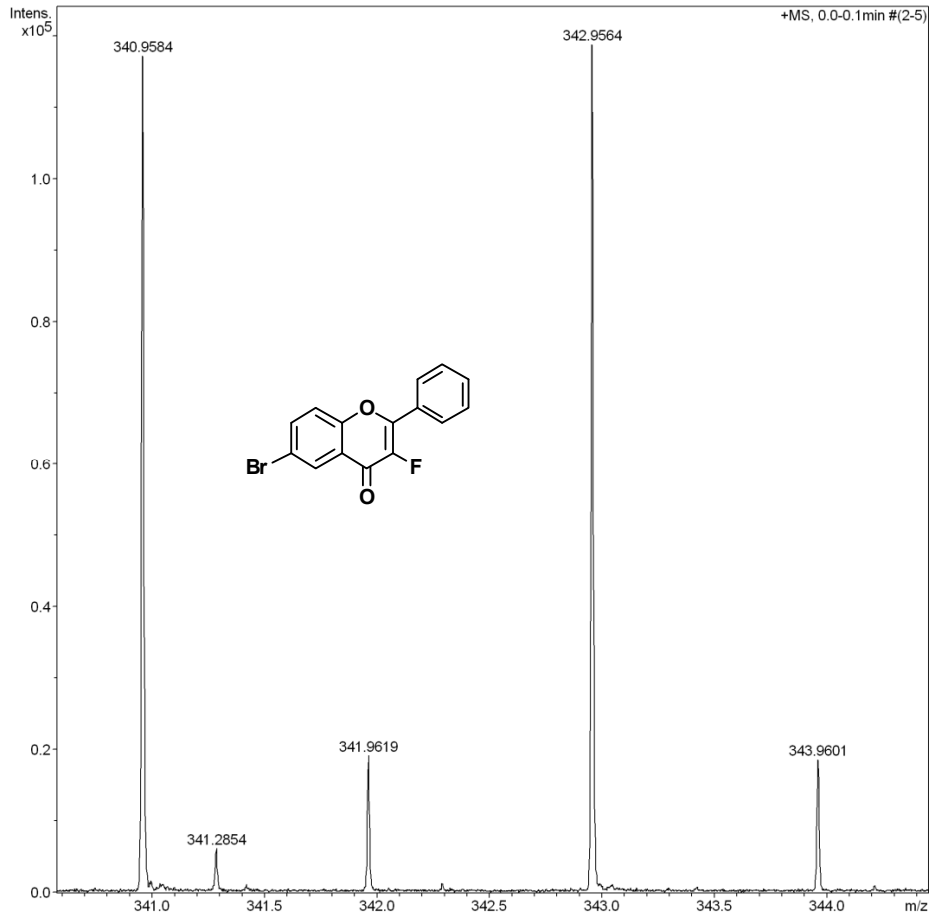
^{1}H NMR spectrum of **2j** ($CDCl_3$)



^{13}C NMR spectrum of **2j** ($CDCl_3$)

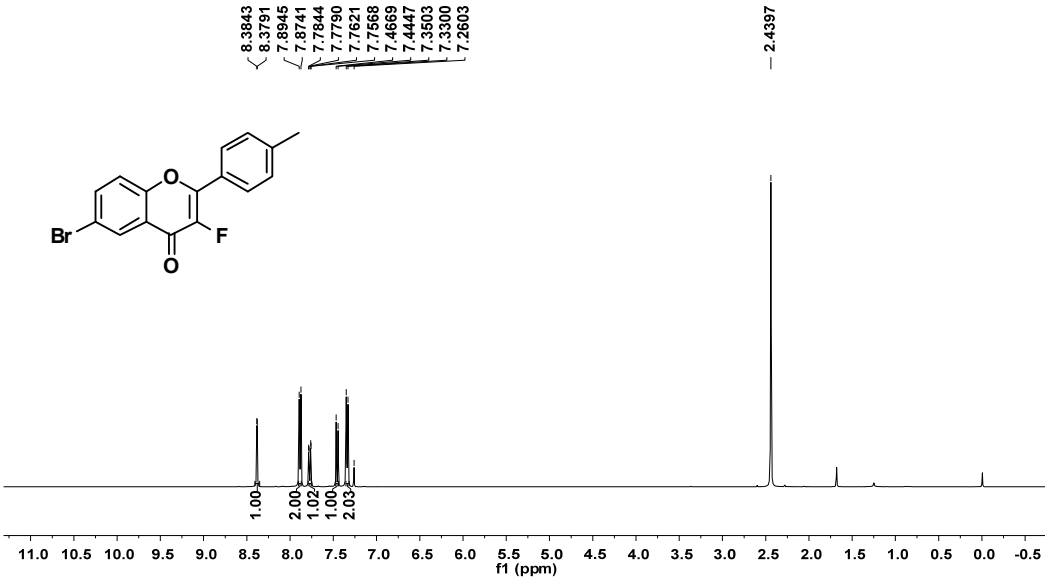


^{19}F NMR spectrum of **2j** ($CDCl_3$)

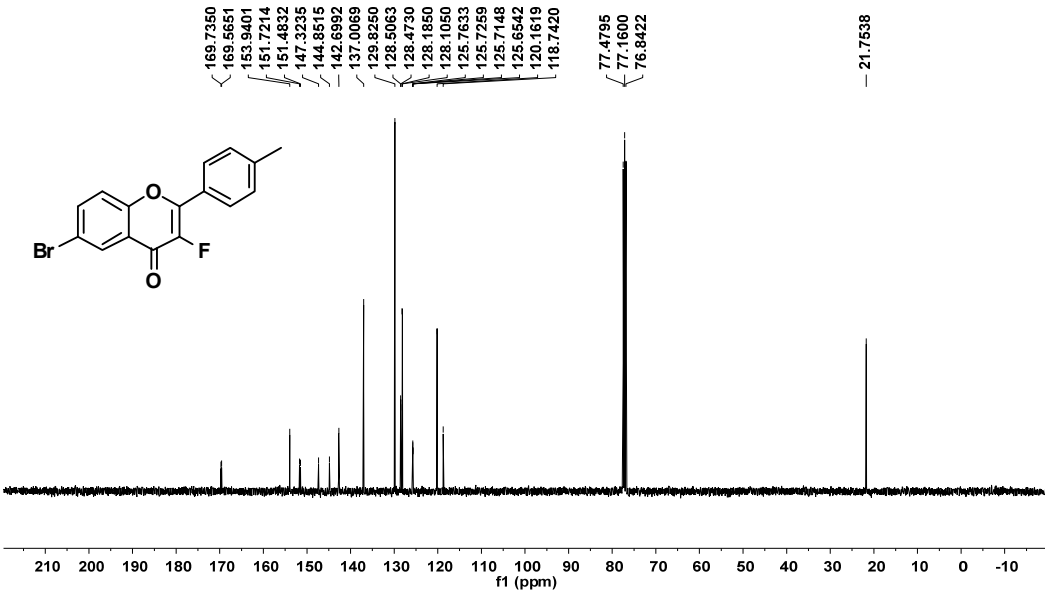


HRMS spectrum of **2j** (MeOH)

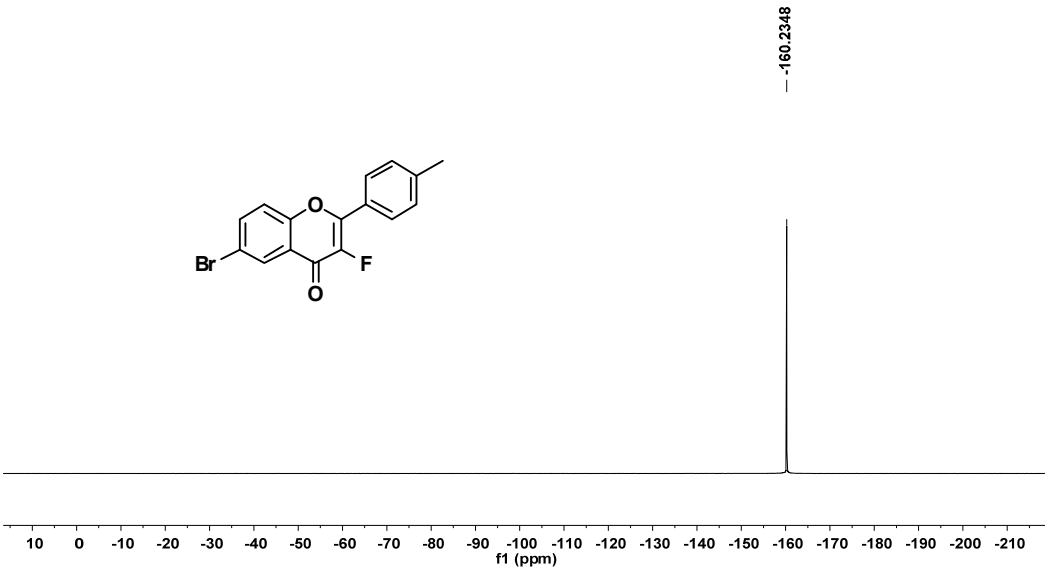
2k



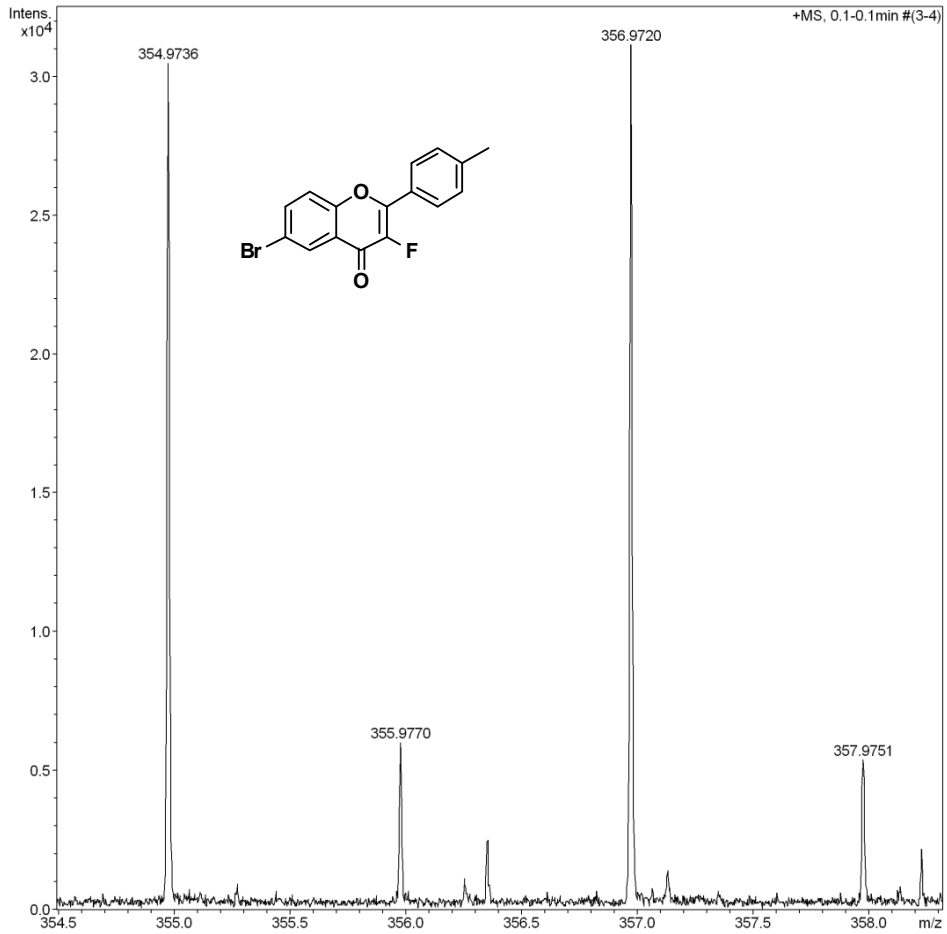
^{1}H NMR spectrum of **2k** ($CDCl_3$)



^{13}C NMR spectrum of **2k** ($CDCl_3$)

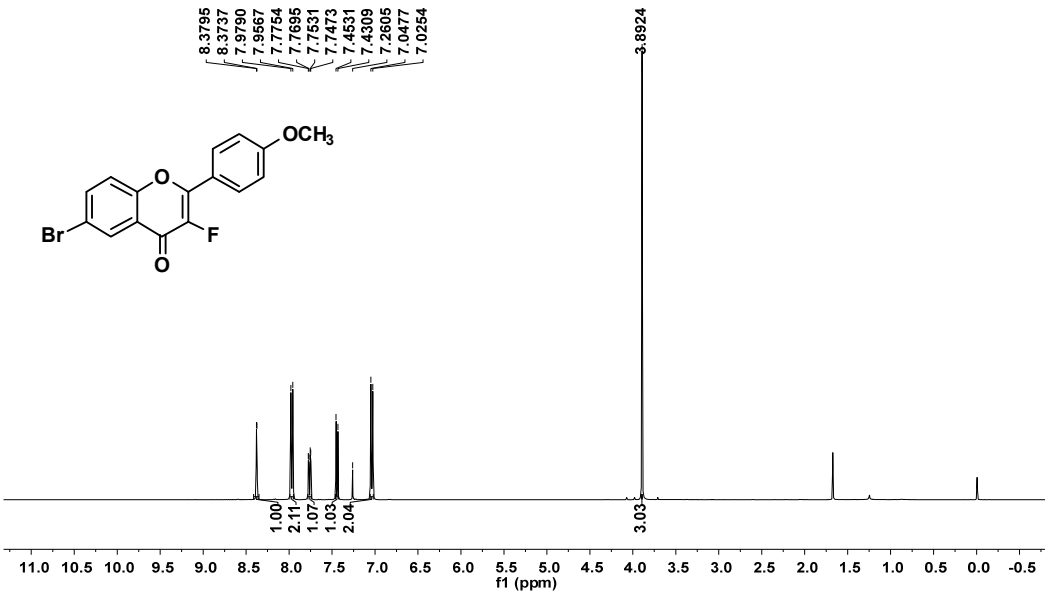


^{19}F NMR spectrum of **2k** ($CDCl_3$)

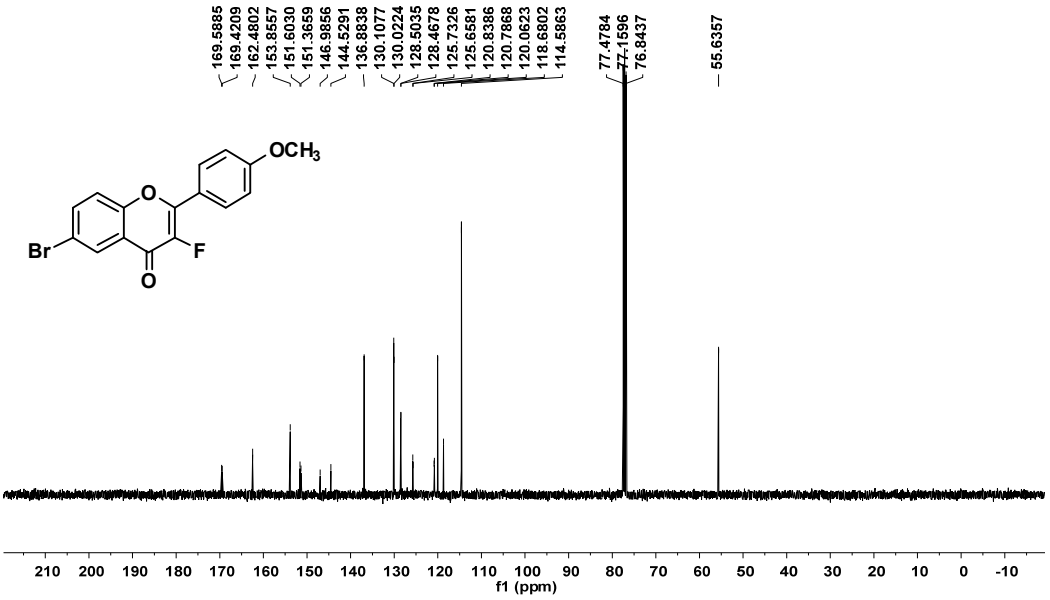


HRMS spectrum of **2k** (MeOH)

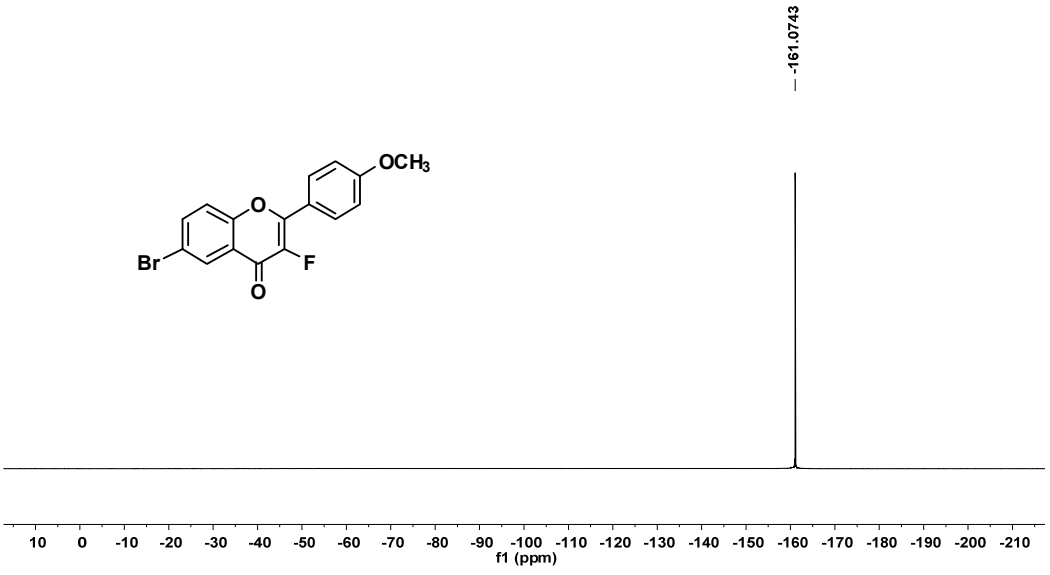
2l



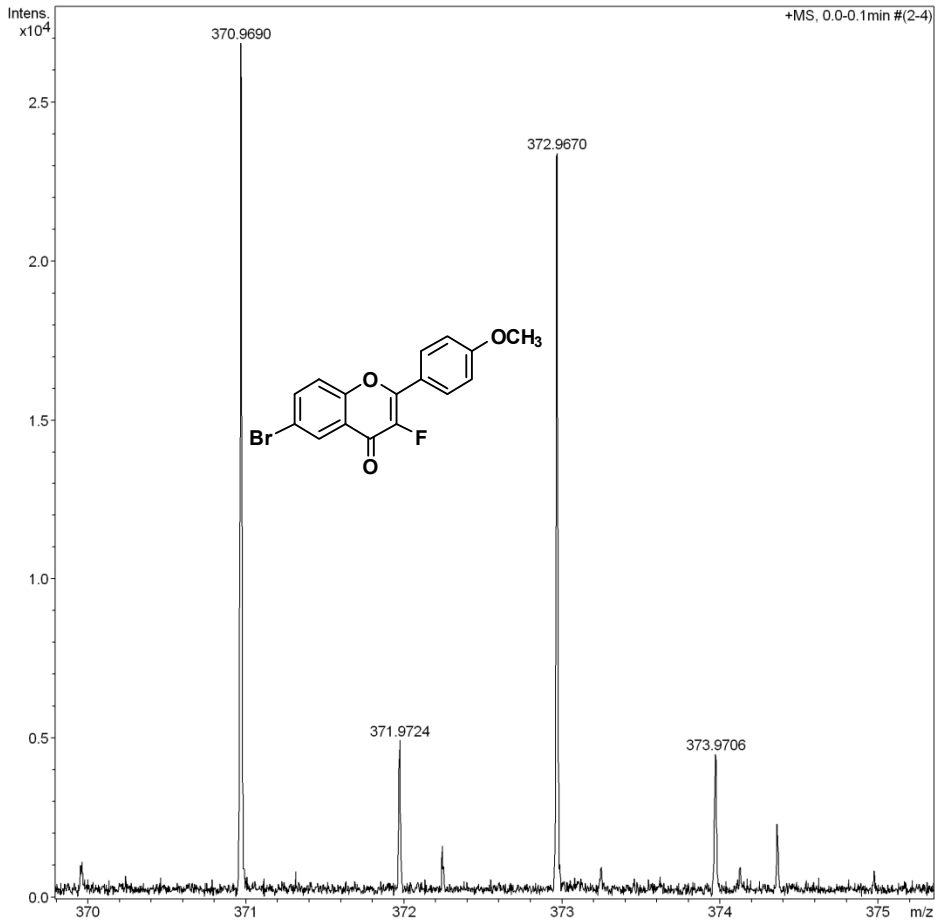
^{1}H NMR spectrum of **2l** ($CDCl_3$)



^{13}C NMR spectrum of **2l** ($CDCl_3$)

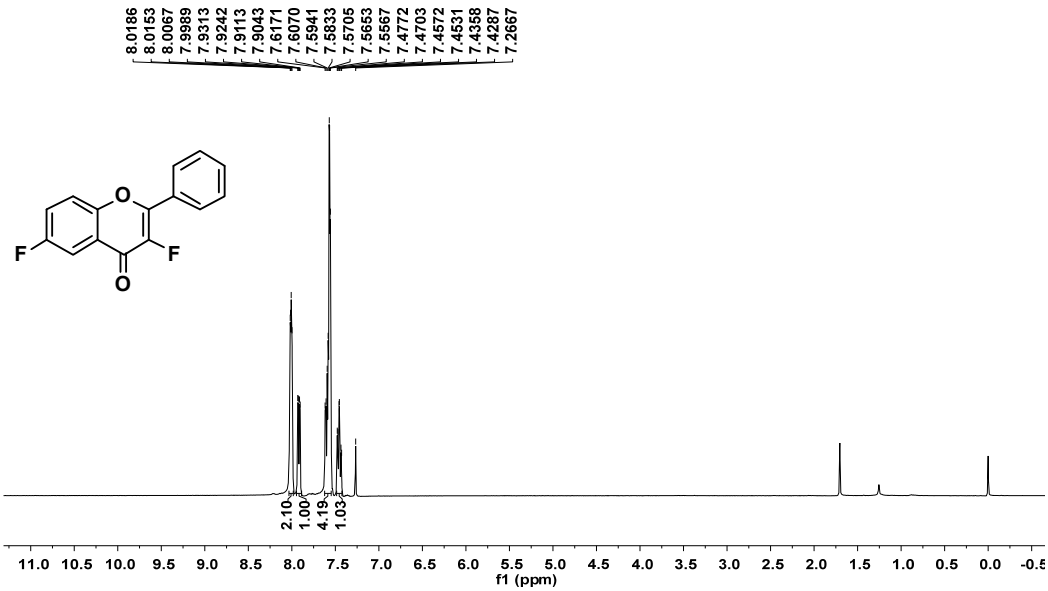


^{19}F NMR spectrum of **2l** ($CDCl_3$)

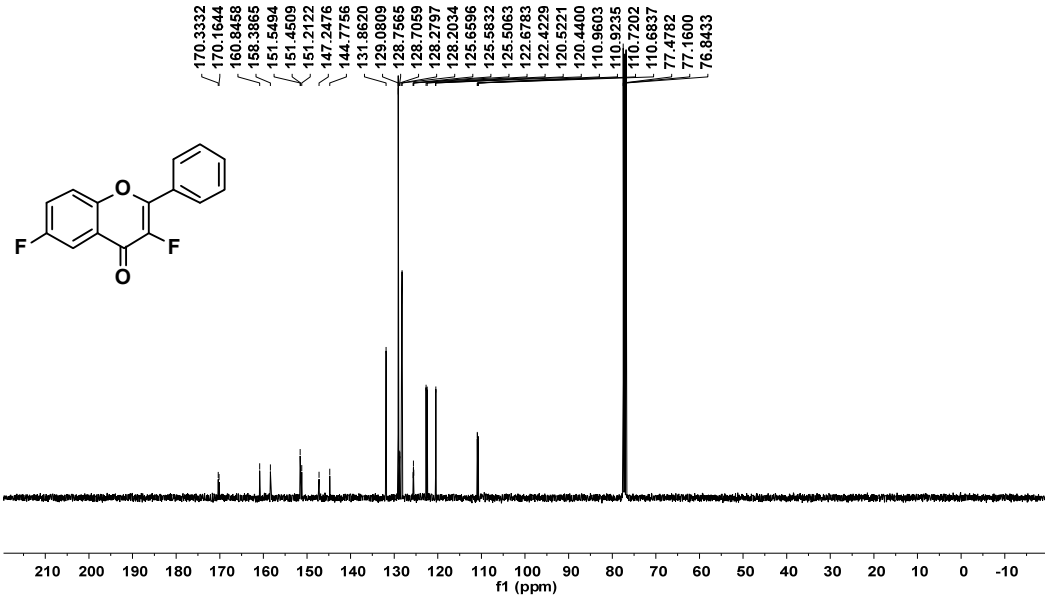


HRMS spectrum of **2l** (MeOH)

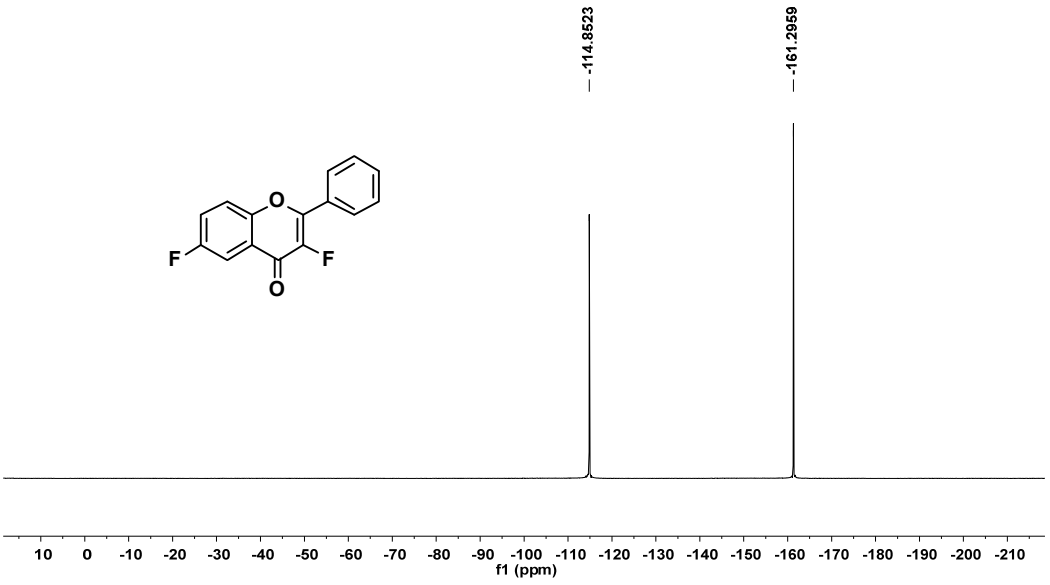
2m



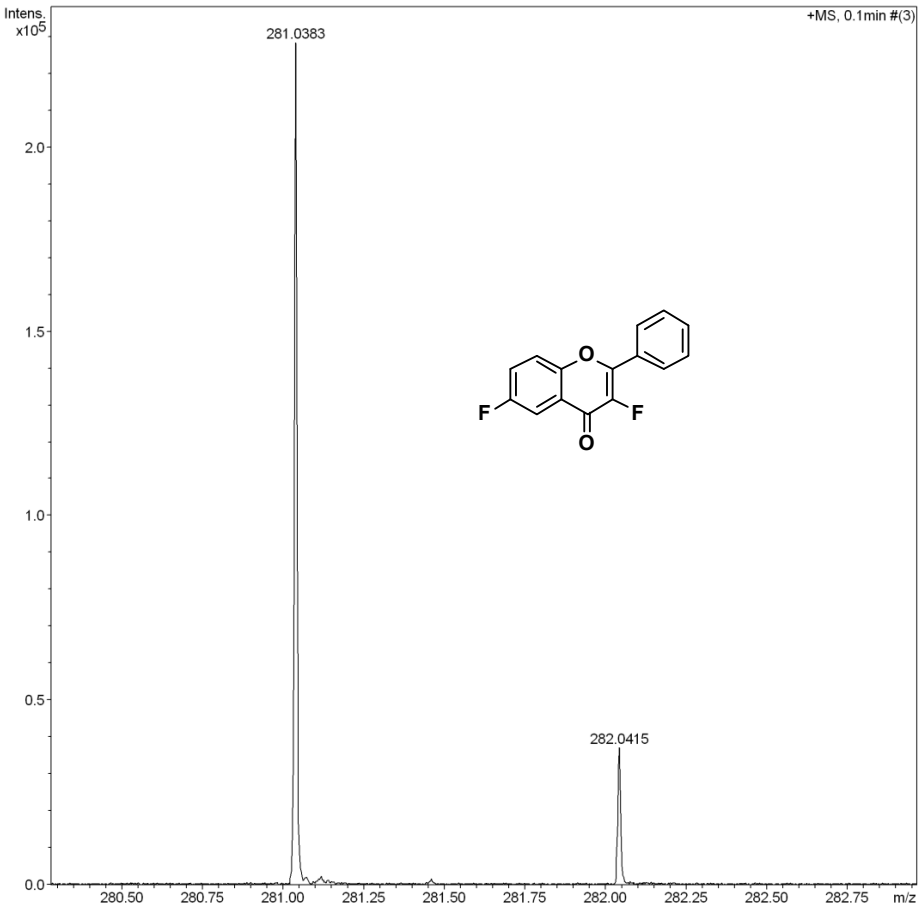
^{1}H NMR spectrum of **2m** ($CDCl_3$)



^{13}C NMR spectrum of **2m** ($CDCl_3$)

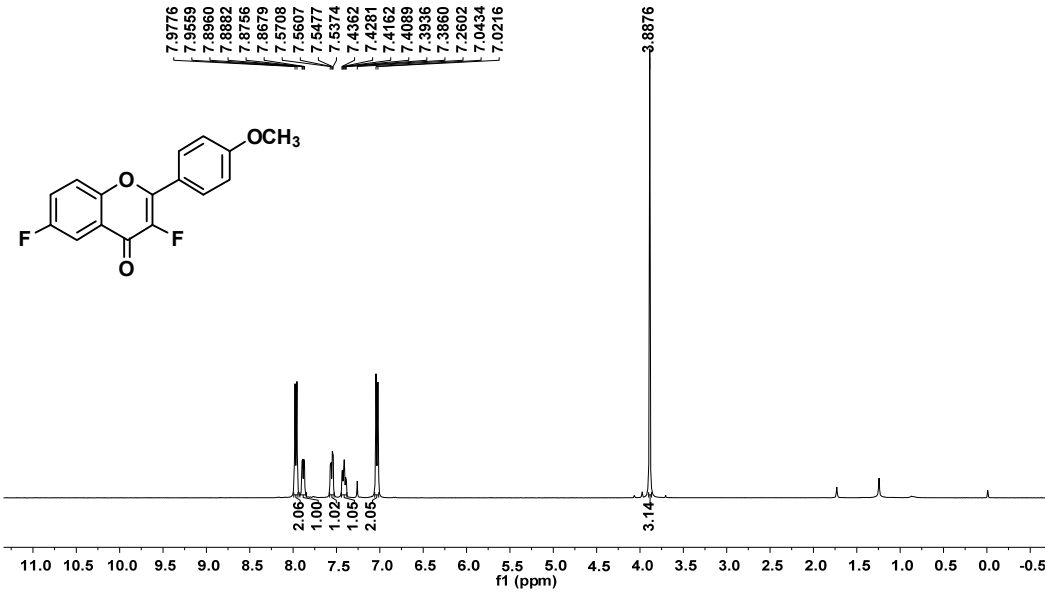


^{19}F NMR spectrum of **2m** ($CDCl_3$)

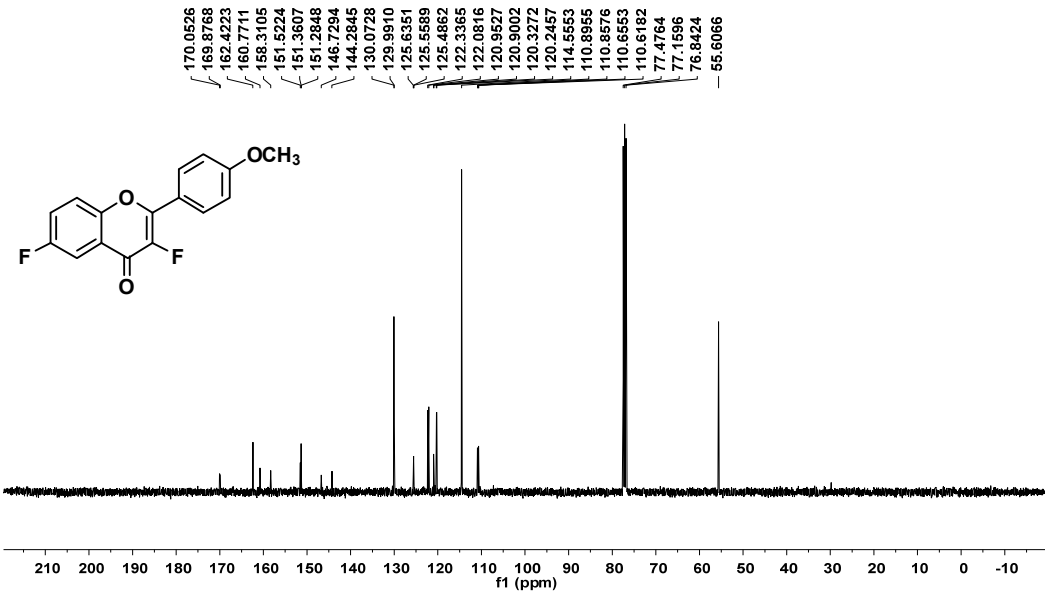


HRMS spectrum of **2m** (MeOH)

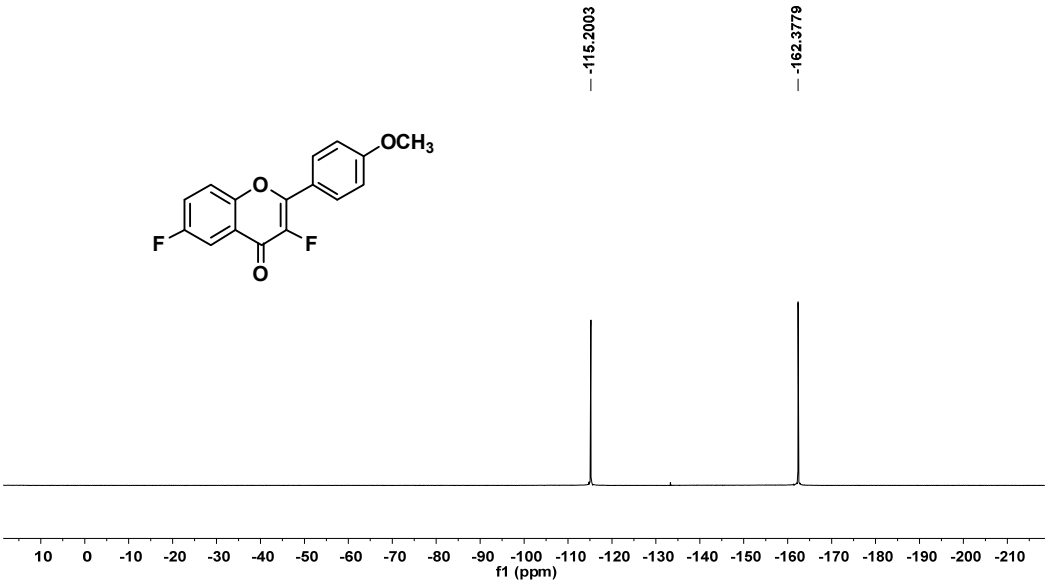
2n



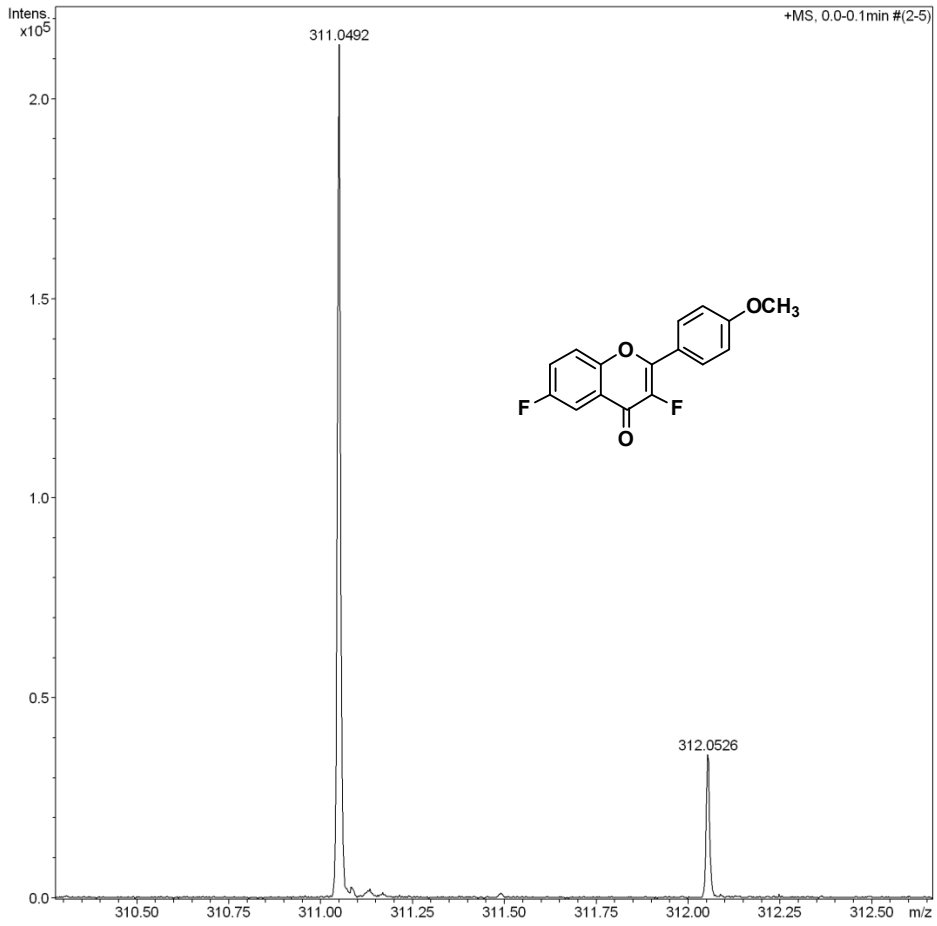
^{1}H NMR spectrum of **2n** ($CDCl_3$)



^{13}C NMR spectrum of **2n** ($CDCl_3$)

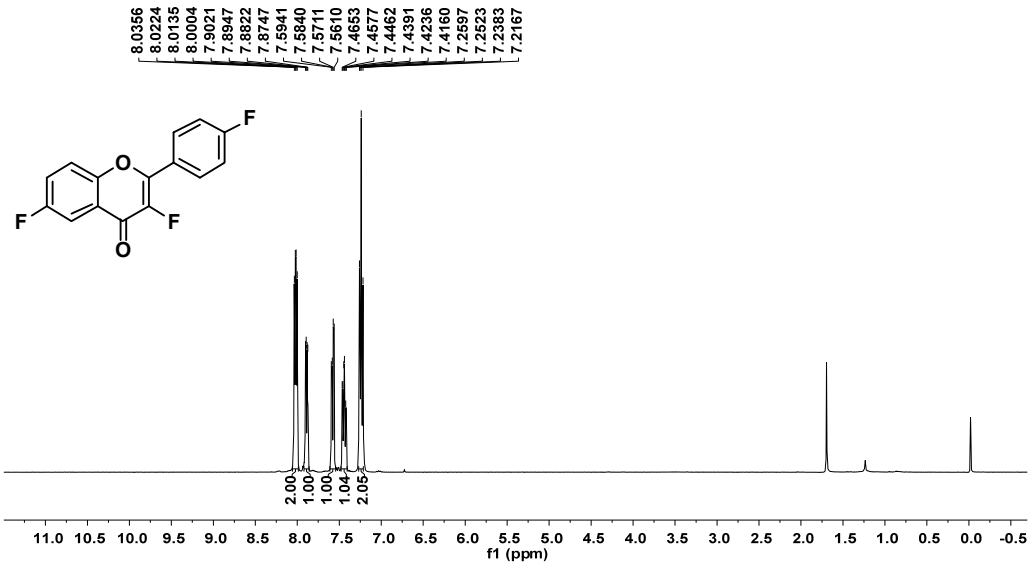


^{19}F NMR spectrum of **2n** ($CDCl_3$)

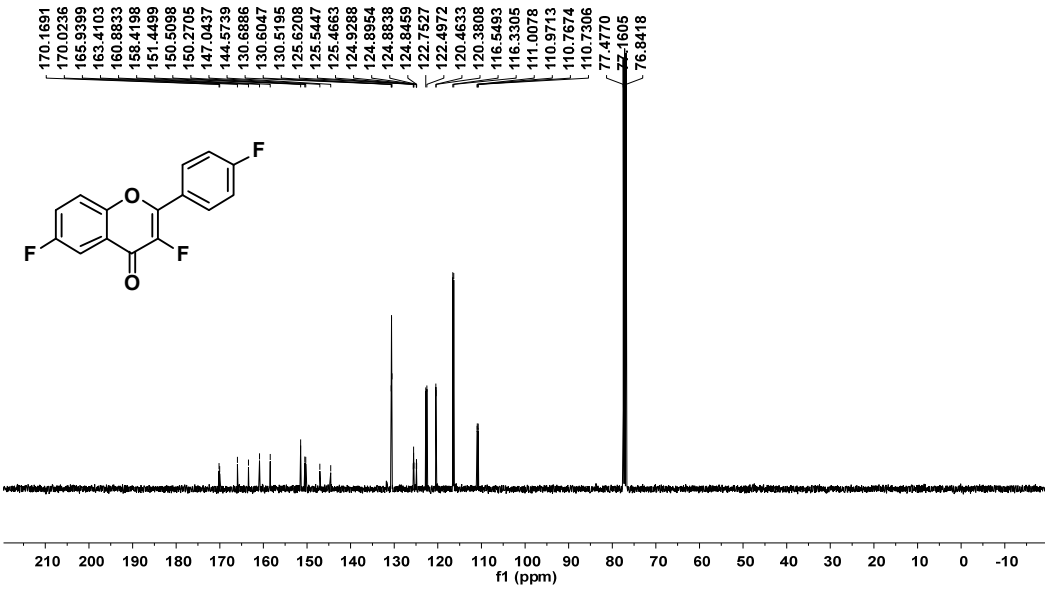


HRMS spectrum of **2n** (MeOH)

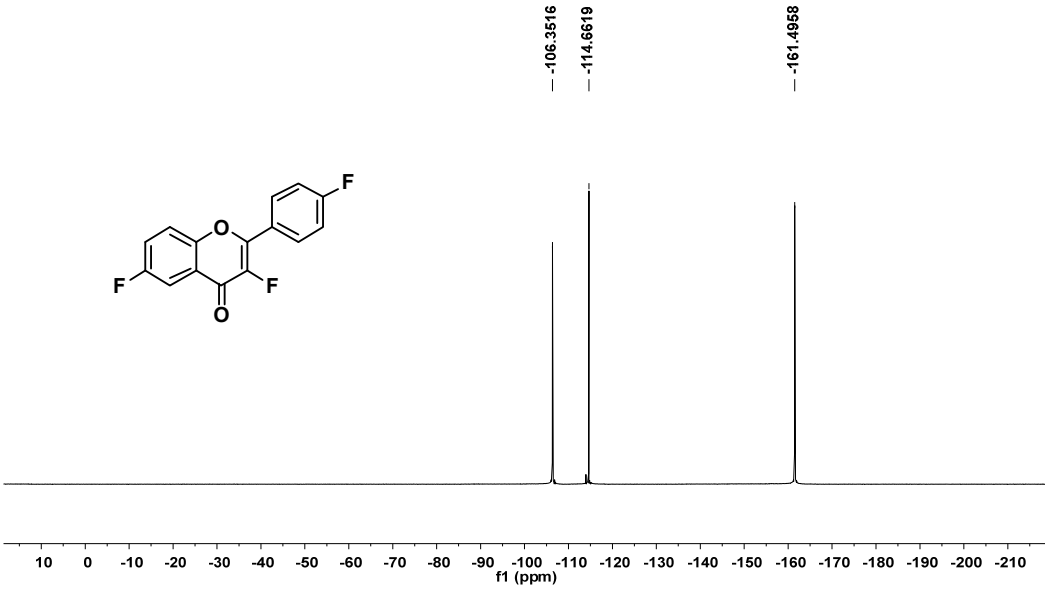
2o



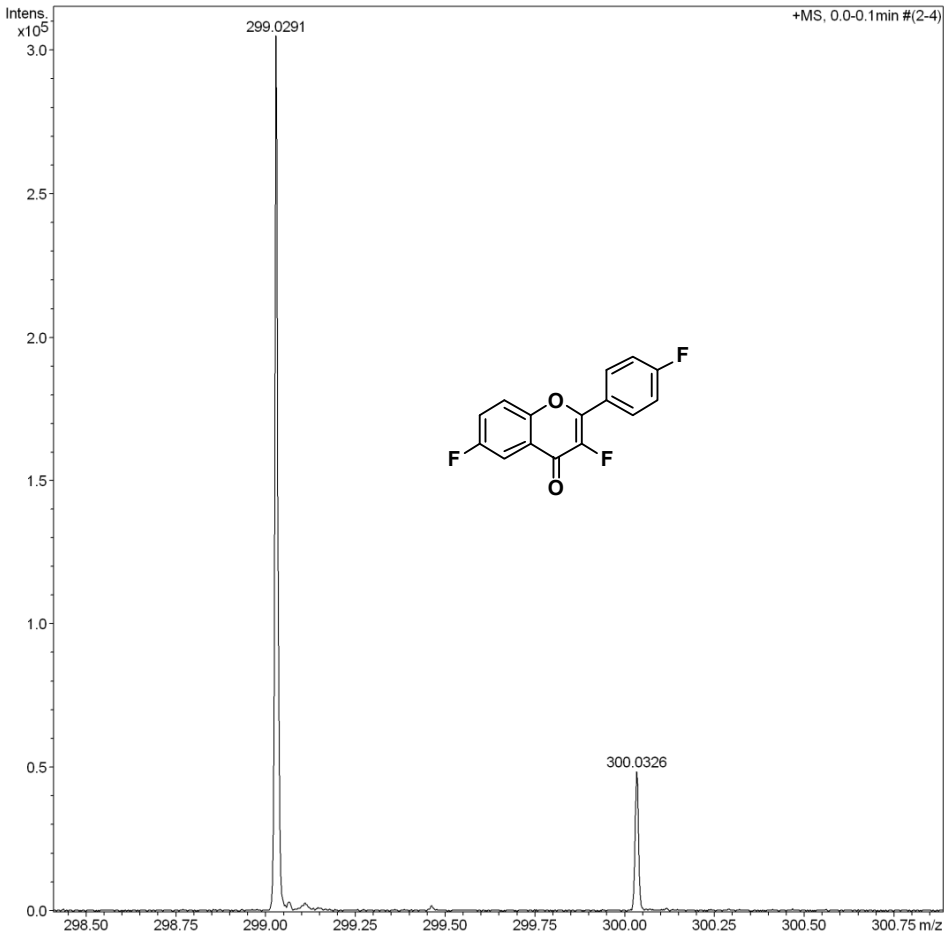
^{1}H NMR spectrum of **2o** ($CDCl_3$)



^{13}C NMR spectrum of **2o** ($CDCl_3$)

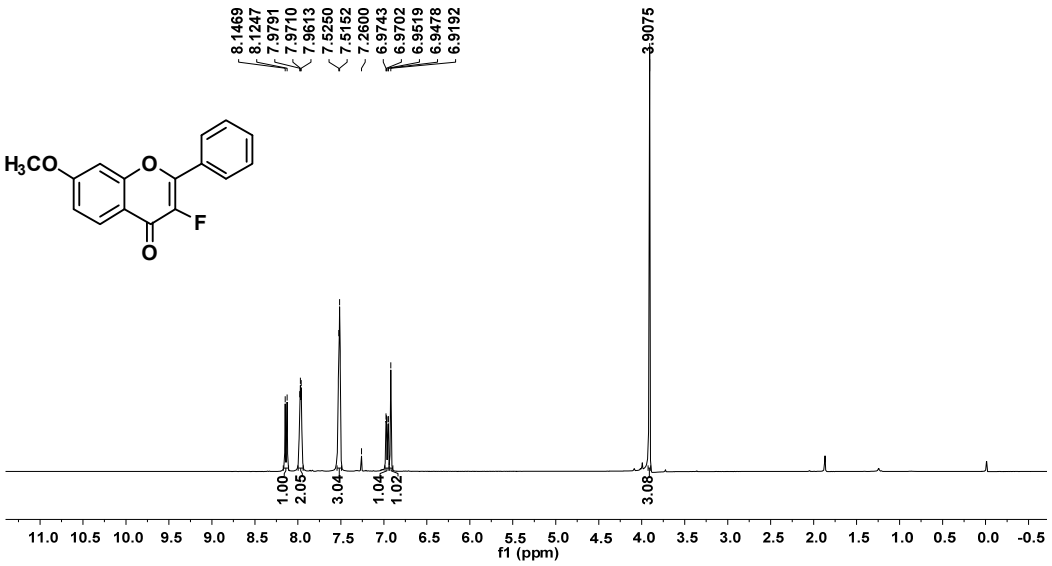


^{19}F NMR spectrum of **2o** ($CDCl_3$)

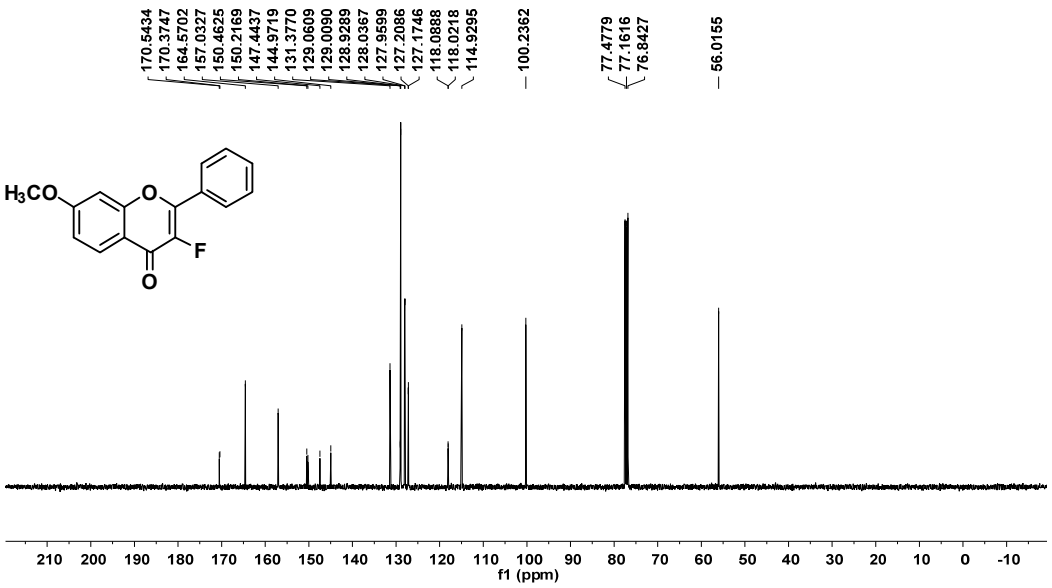


HRMS spectrum of **2o** (MeOH)

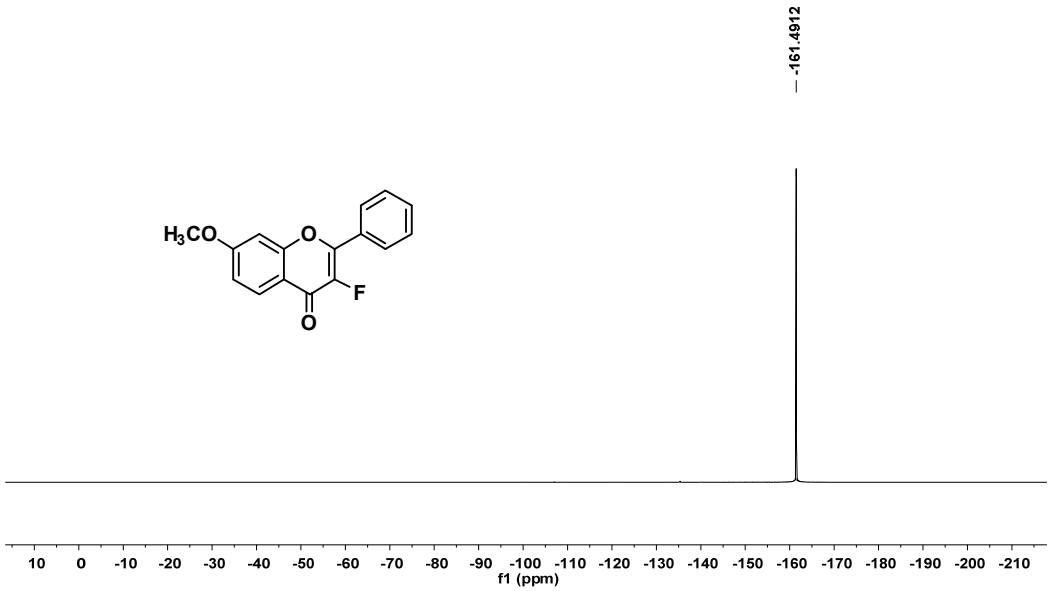
2p



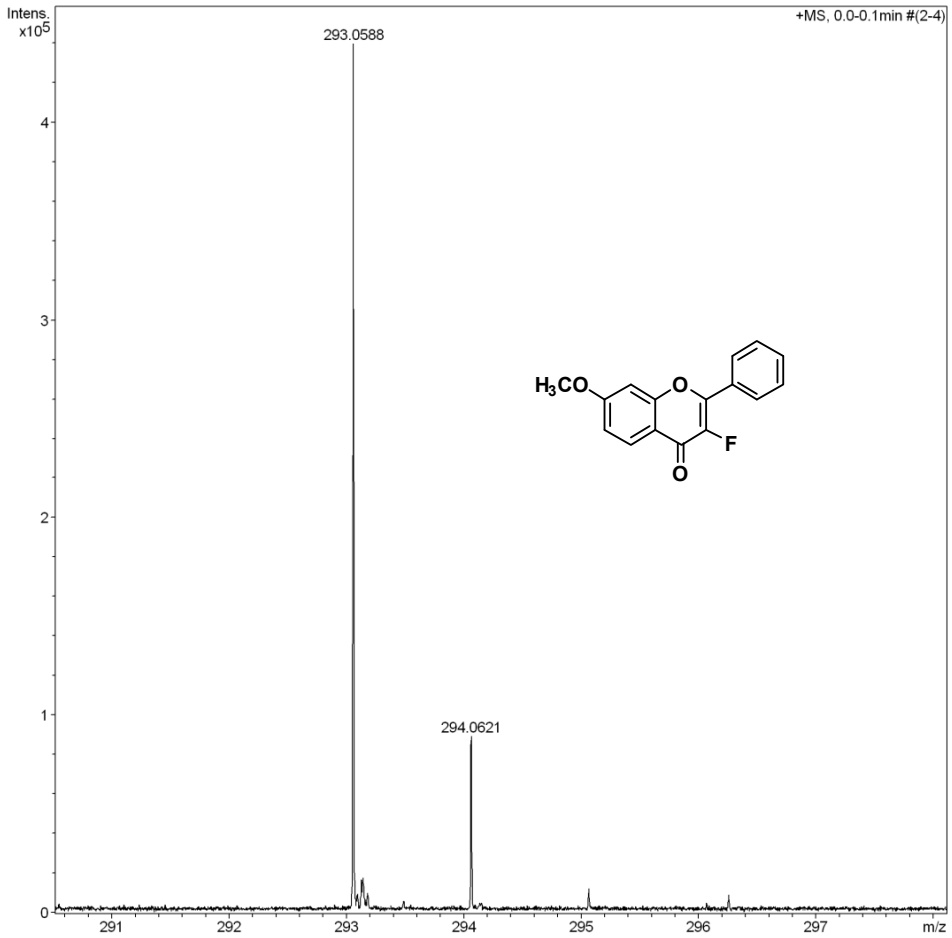
^{1}H NMR spectrum of **2p** ($CDCl_3$)



^{13}C NMR spectrum of **2p** ($CDCl_3$)

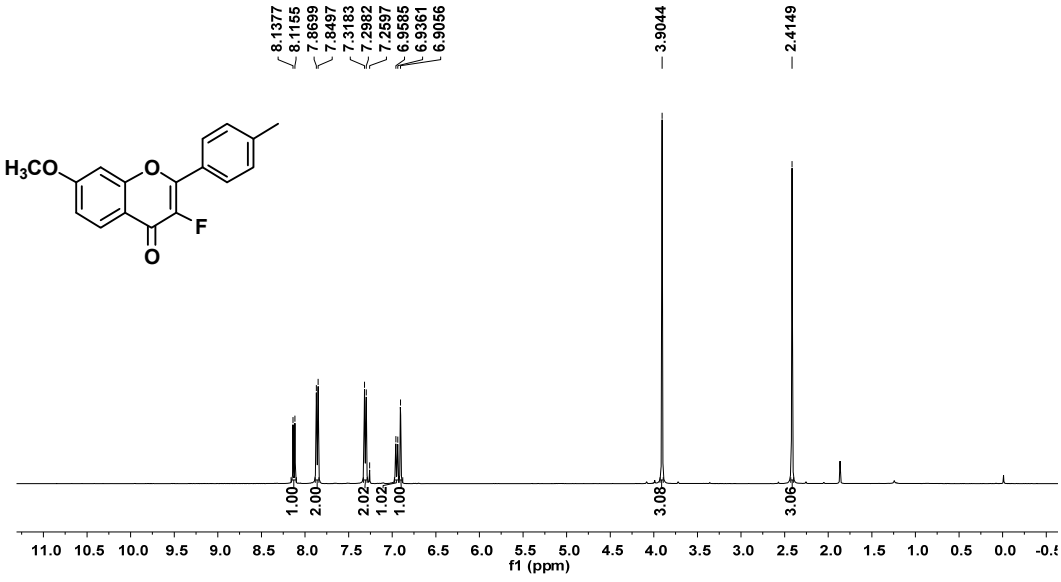


^{19}F NMR spectrum of **2p** ($CDCl_3$)

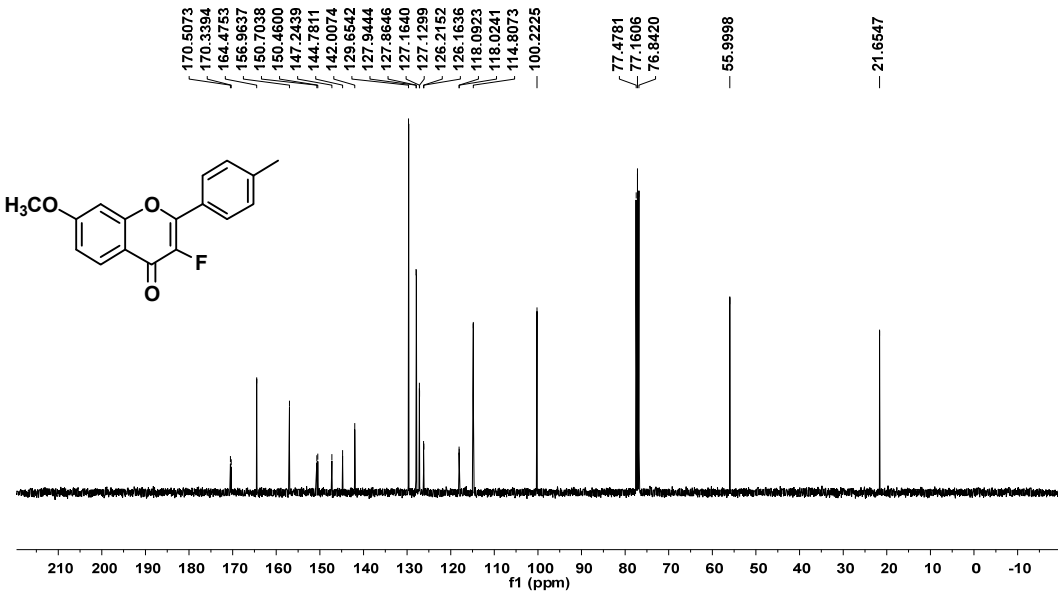


HRMS spectrum of **2p** (MeOH)

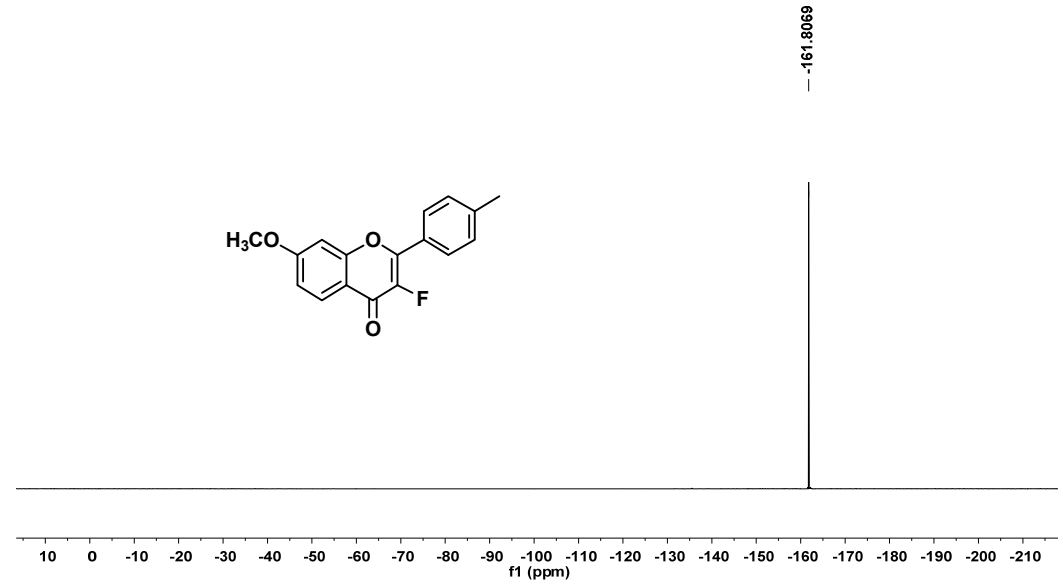
2q



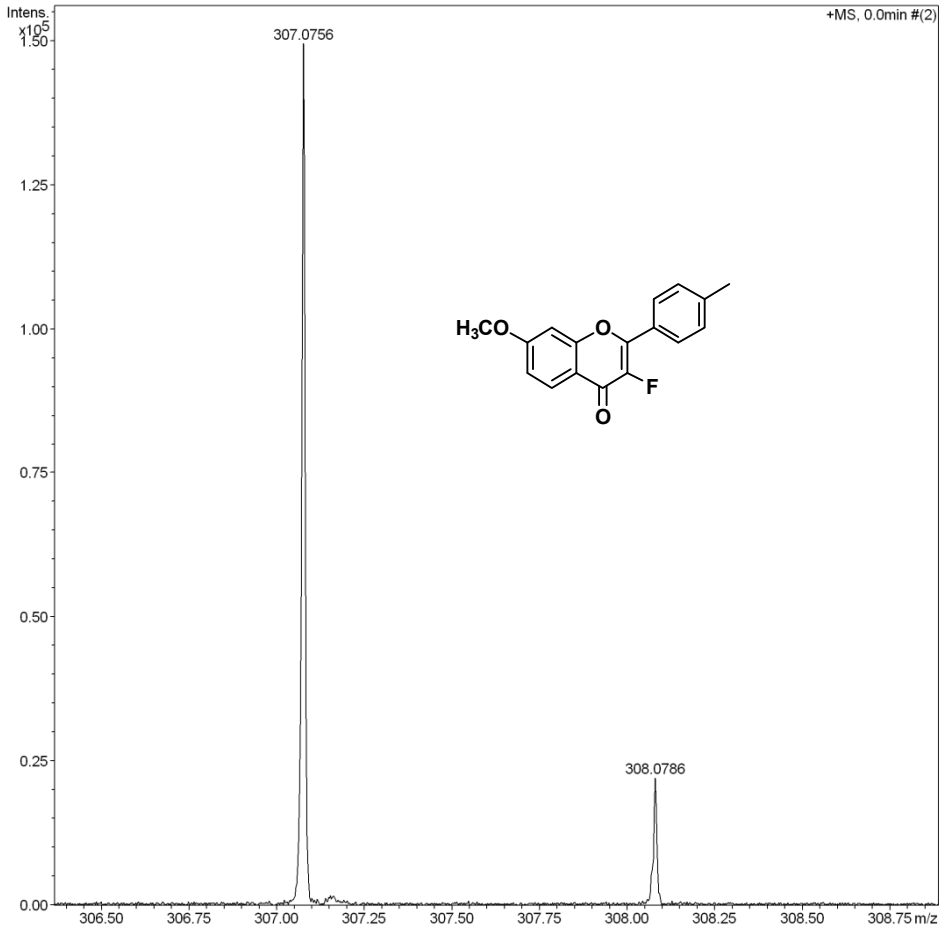
^{1}H NMR spectrum of **2q** ($CDCl_3$)



^{13}C NMR spectrum of **2q** ($CDCl_3$)

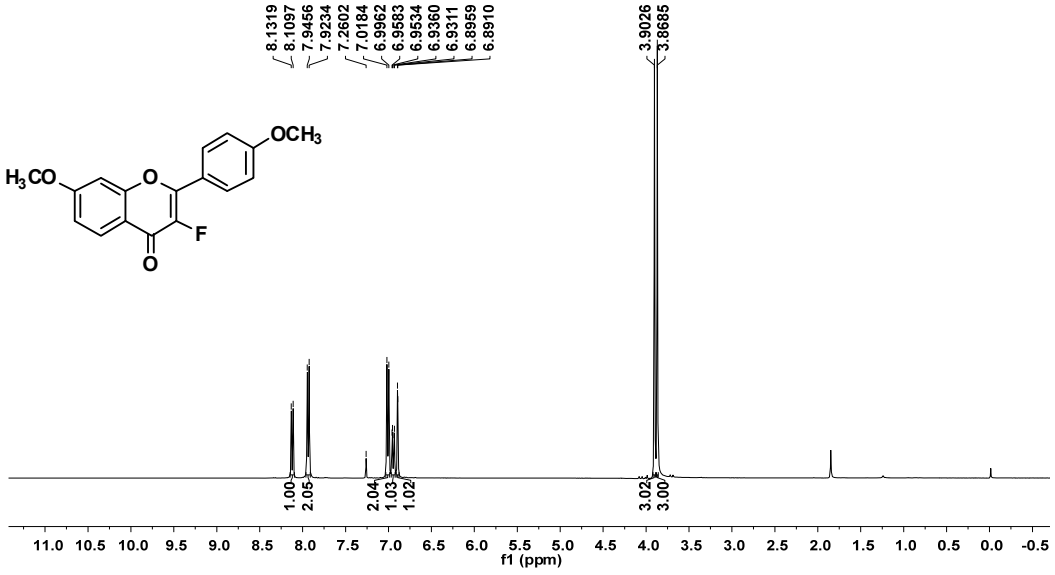


^{19}F NMR spectrum of **2q** ($CDCl_3$)

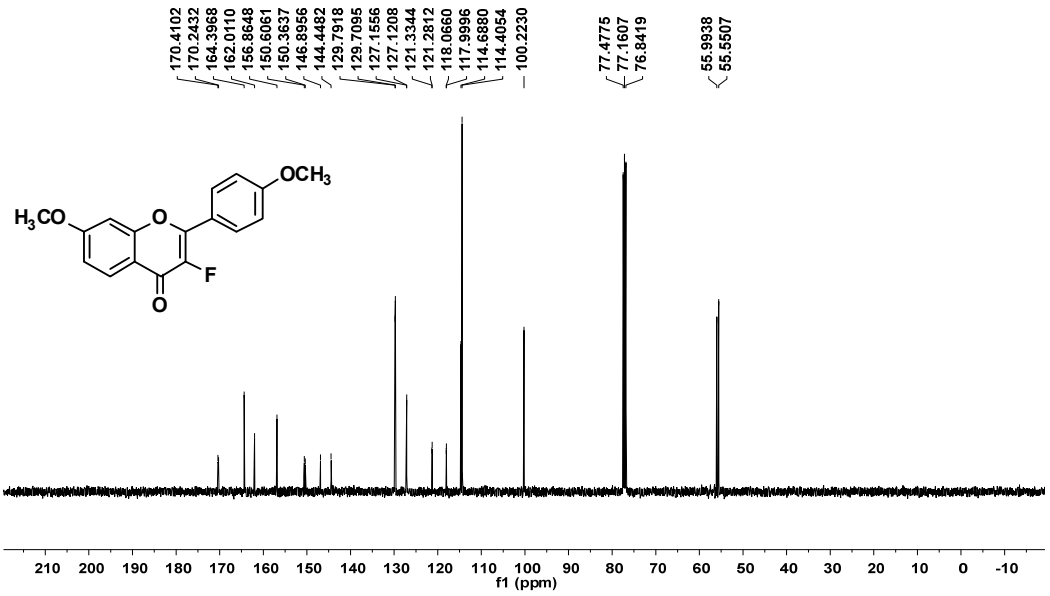


HRMS spectrum of **2q** (MeOH)

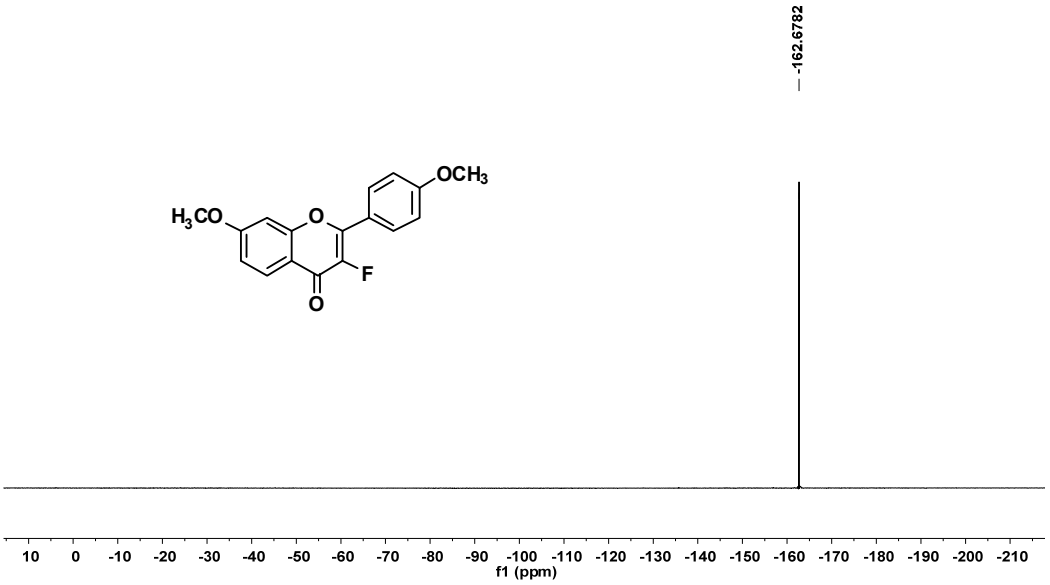
2r



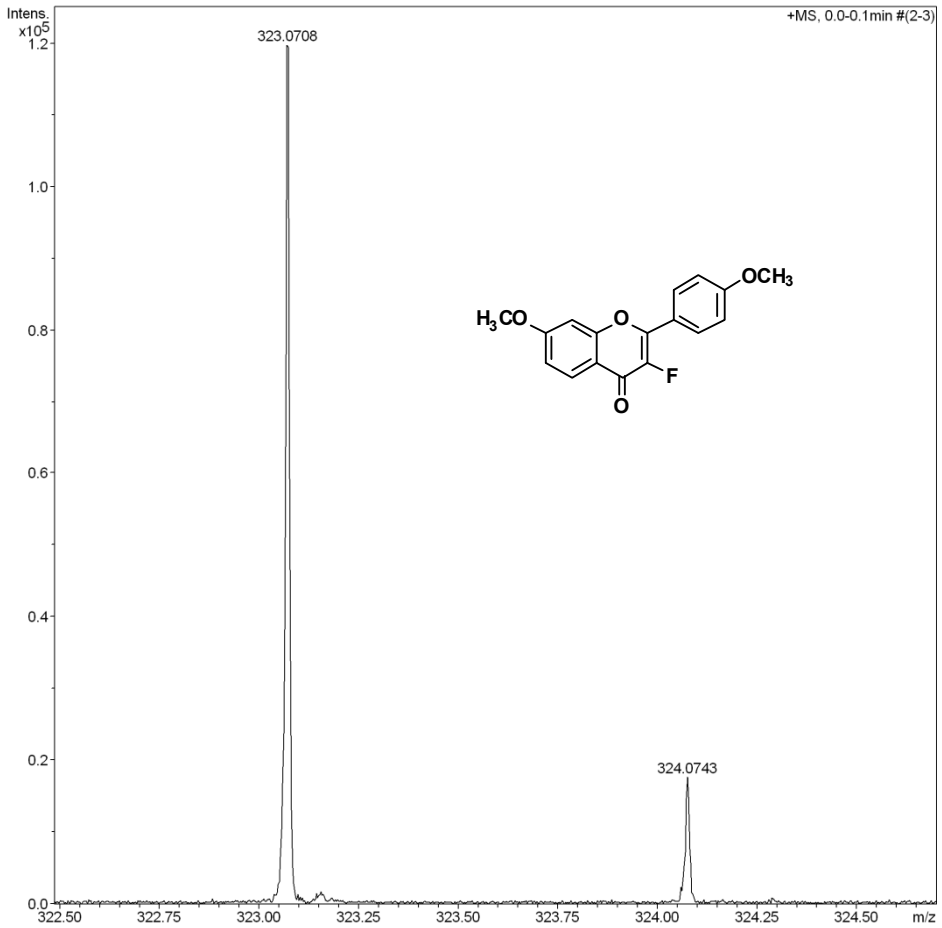
^{1}H NMR spectrum of **2r** ($CDCl_3$)



^{13}C NMR spectrum of **2r** ($CDCl_3$)

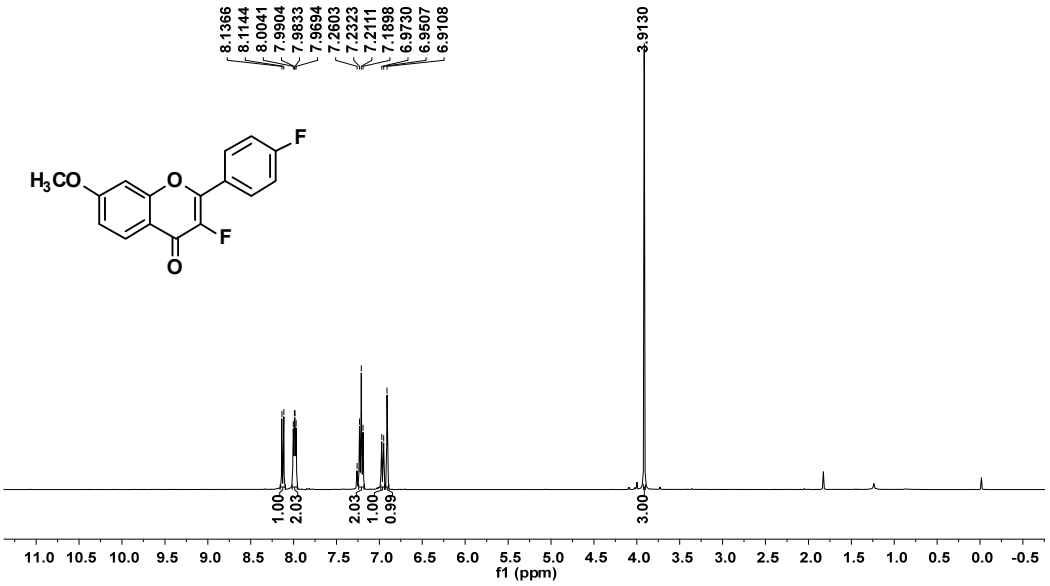


^{19}F NMR spectrum of **2r** ($CDCl_3$)

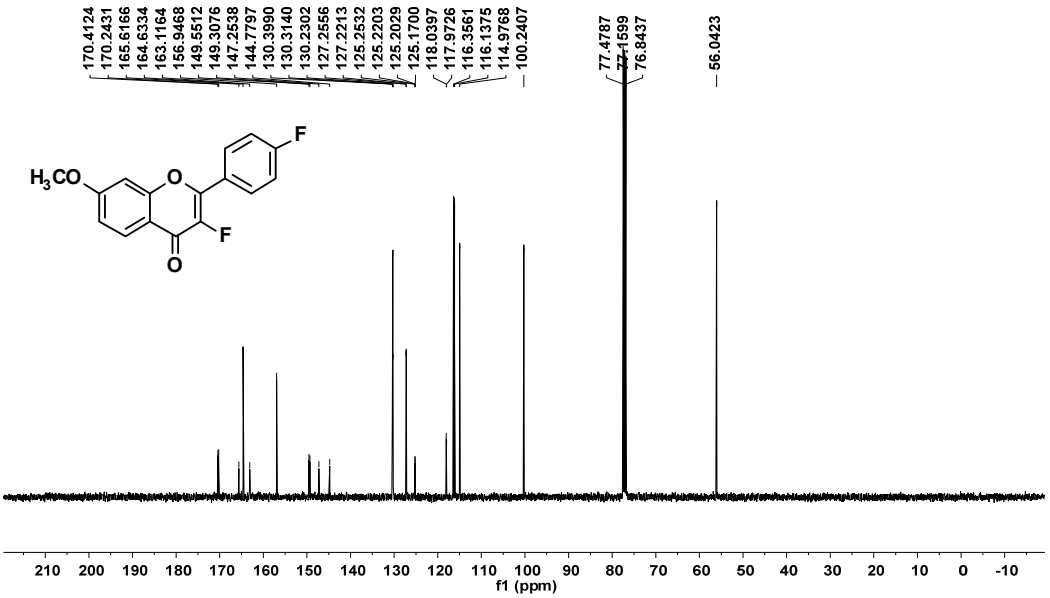


HRMS spectrum of **2r** (MeOH)

2s

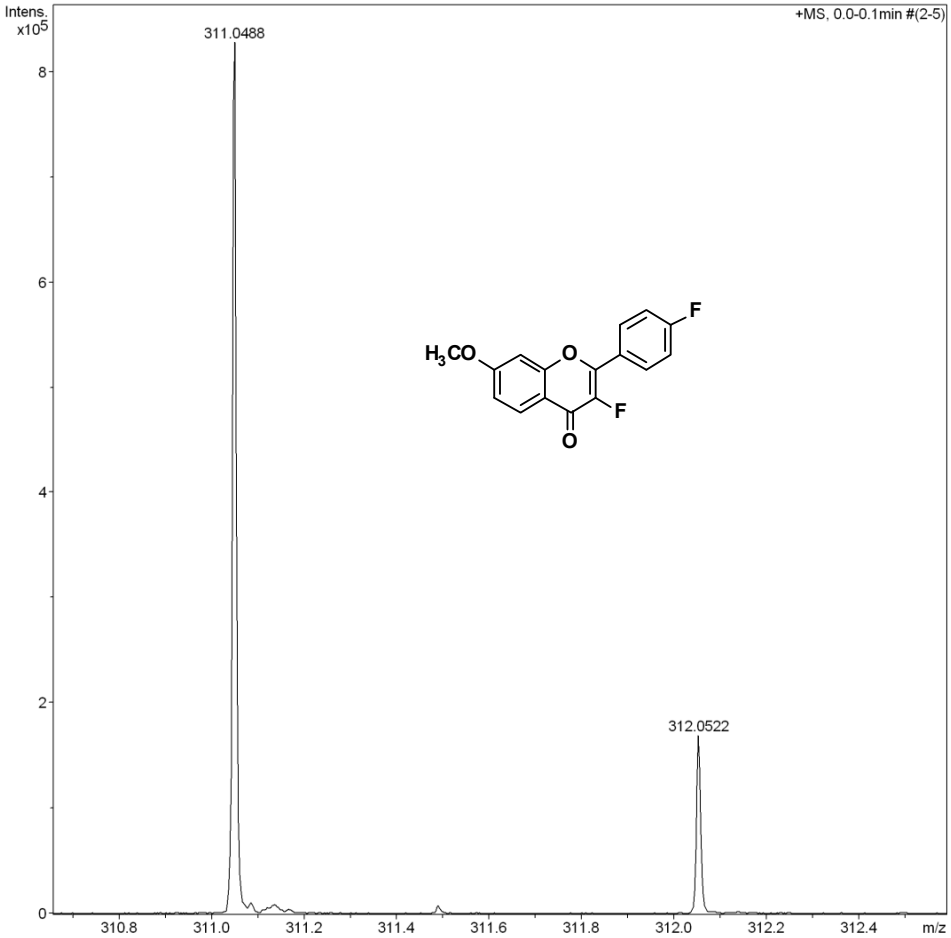


^{1}H NMR spectrum of **2s** ($CDCl_3$)



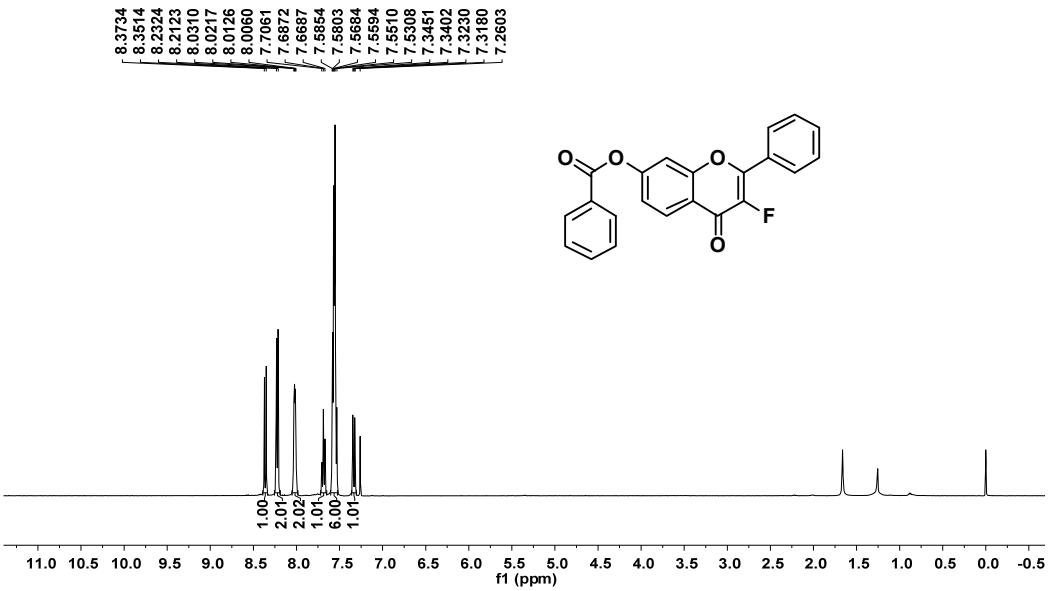
^{13}C NMR spectrum of **2s** ($CDCl_3$)

^{19}F NMR spectrum of **2s** ($CDCl_3$)

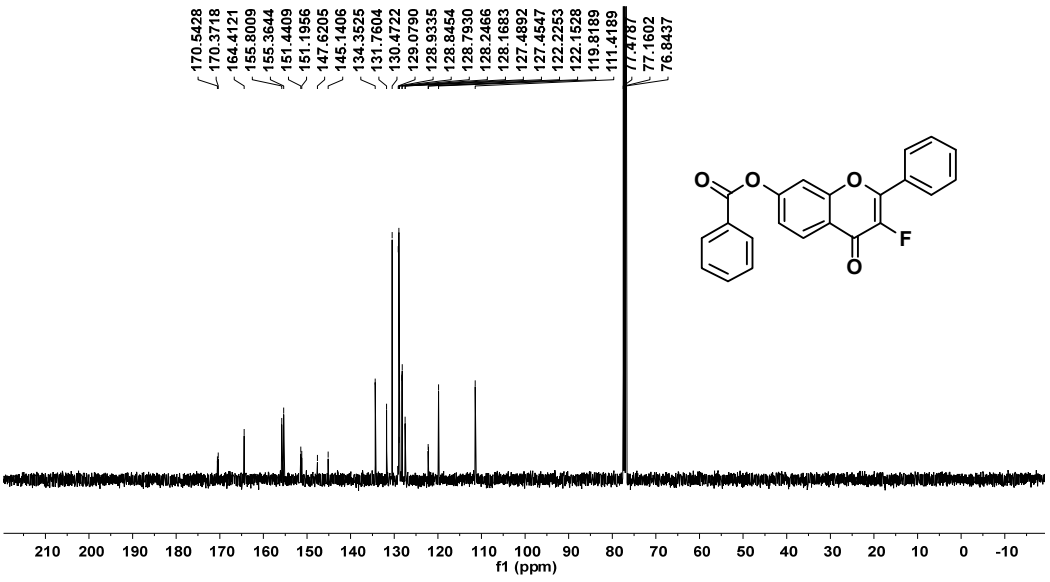


HRMS spectrum of **2s** (MeOH)

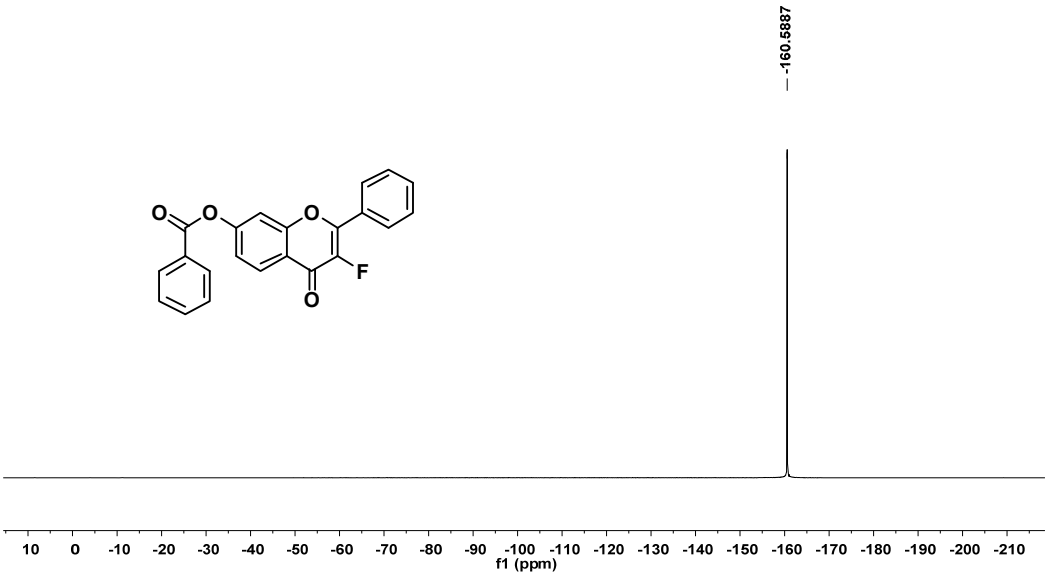
2t



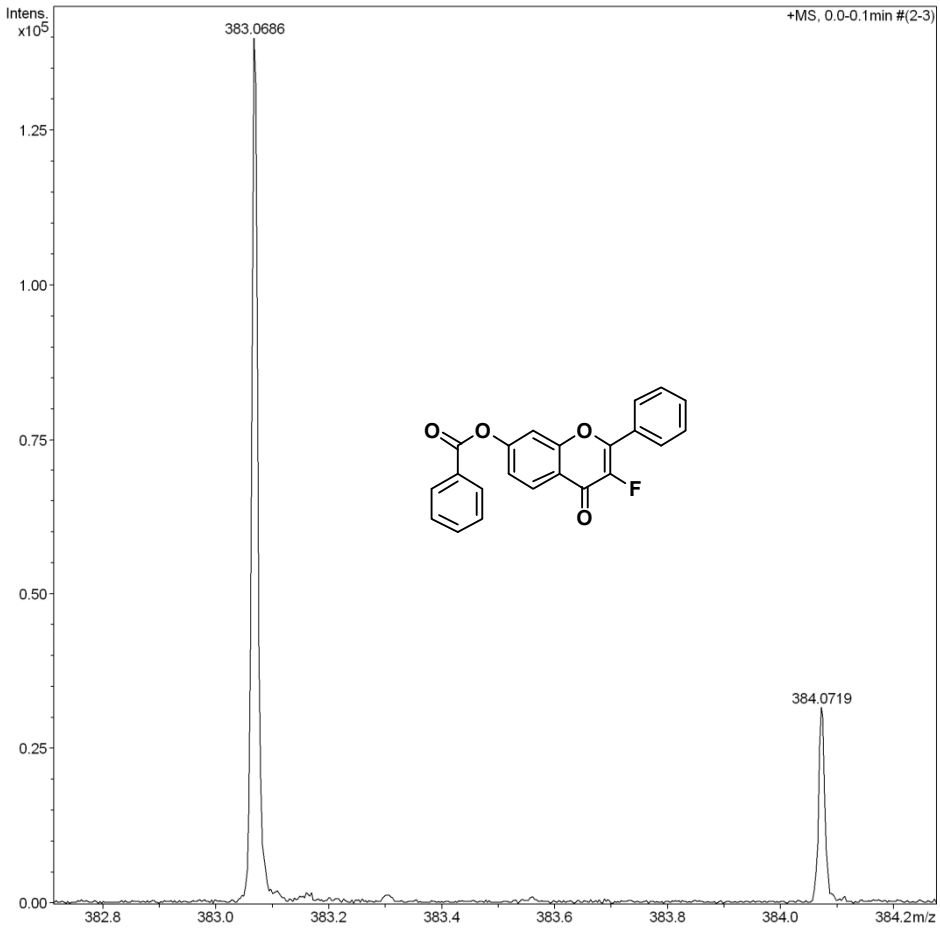
^{1}H NMR spectrum of **2t** ($CDCl_3$)



^{13}C NMR spectrum of **2t** ($CDCl_3$)

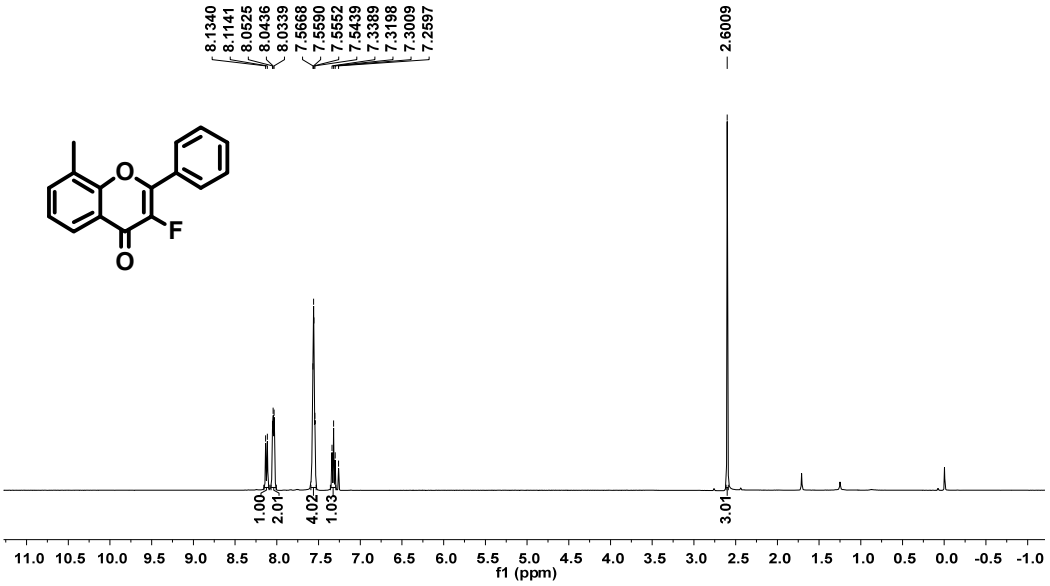


^{19}F NMR spectrum of **2t** ($CDCl_3$)

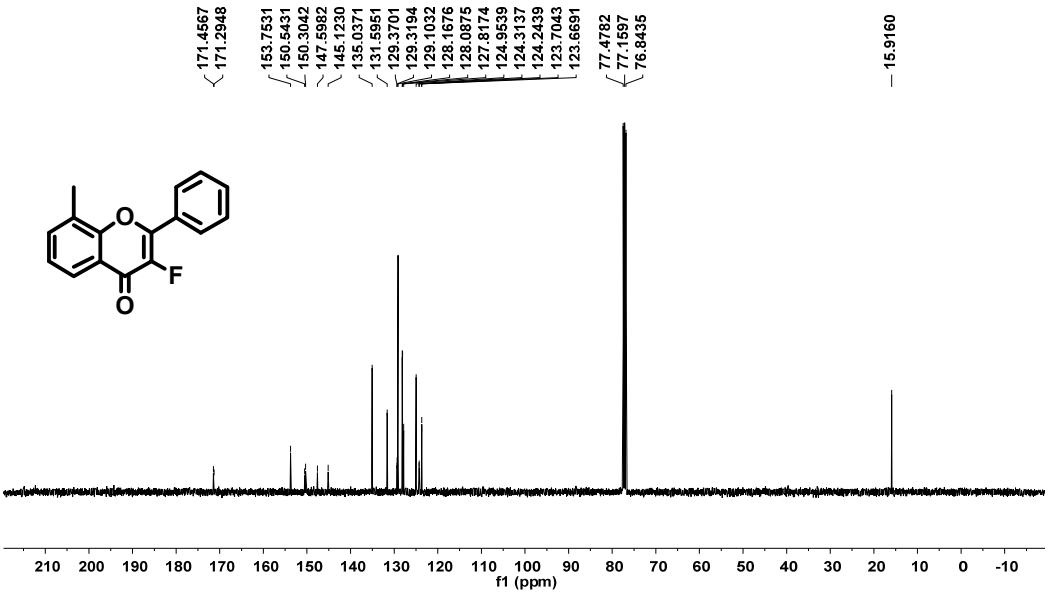


HRMS spectrum of **2t** (MeOH)

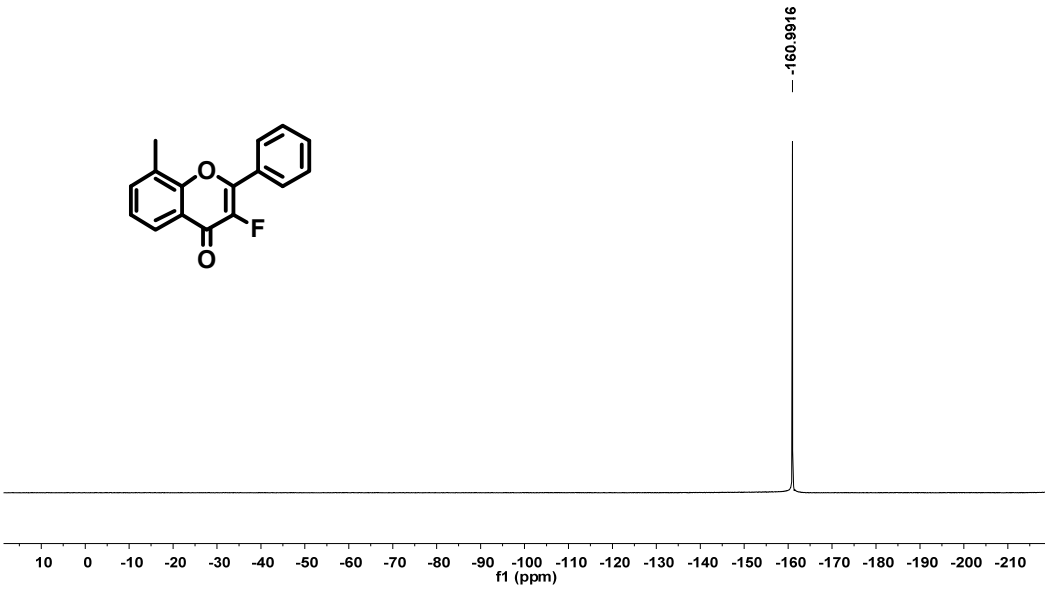
2w



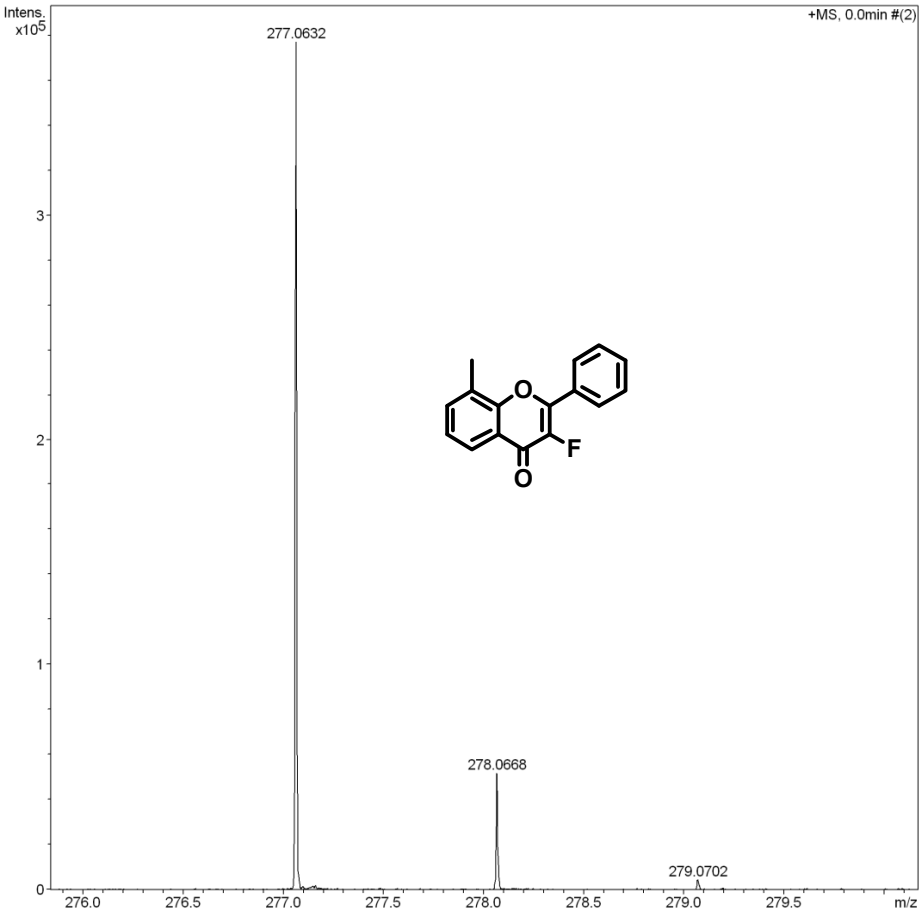
^{1}H NMR spectrum of **2w** ($CDCl_3$)



^{13}C NMR spectrum of **2w** ($CDCl_3$)

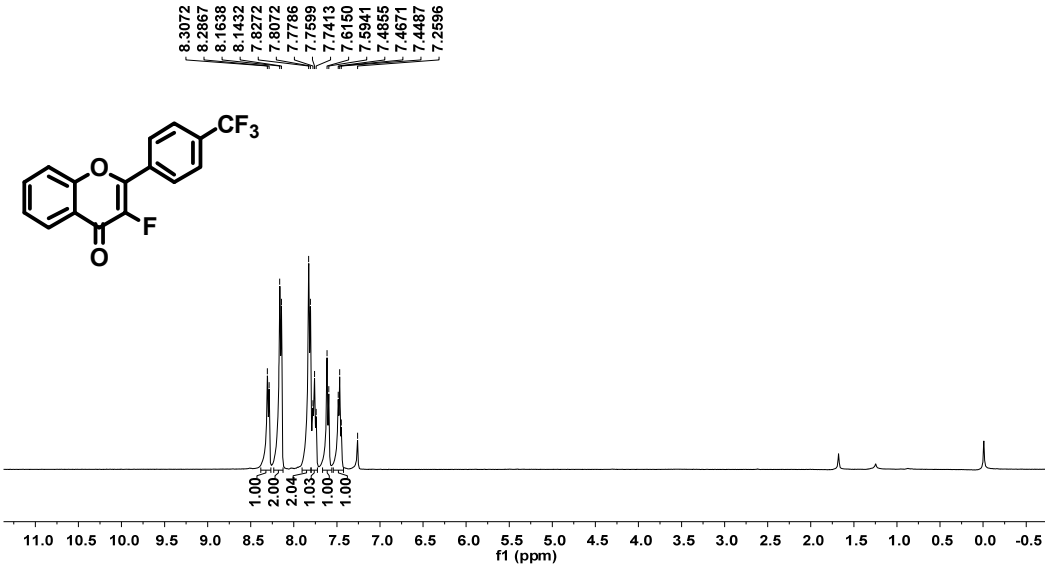


^{19}F NMR spectrum of **2w** ($CDCl_3$)

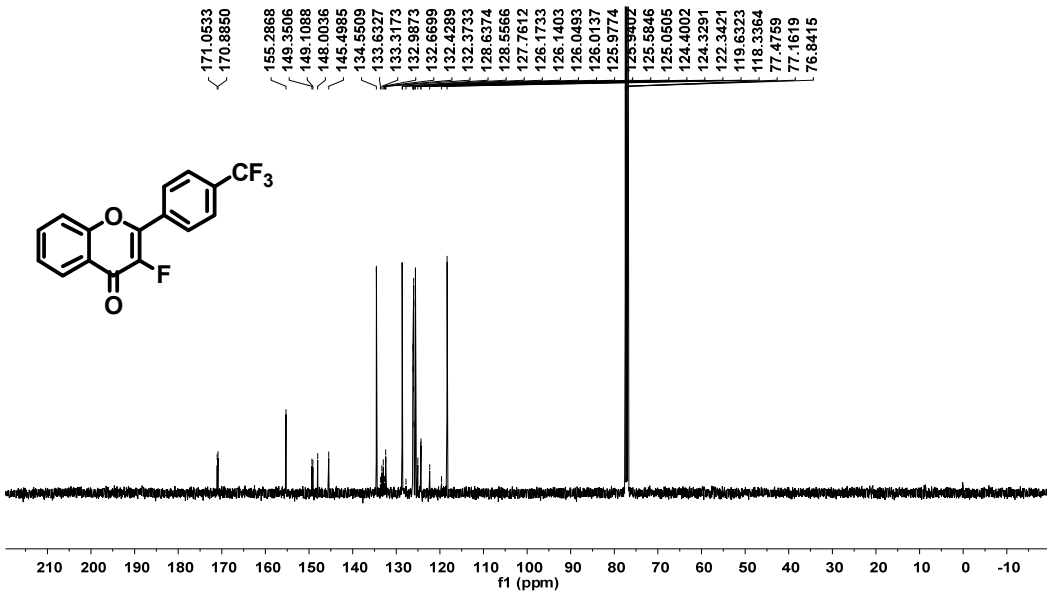


HRMS spectrum of **2w** (MeOH)

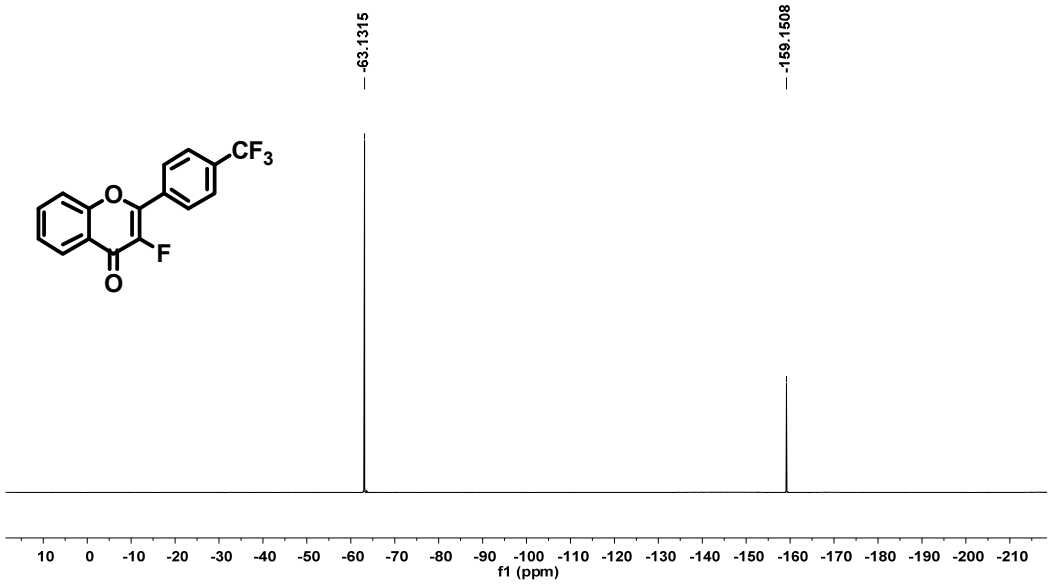
2x



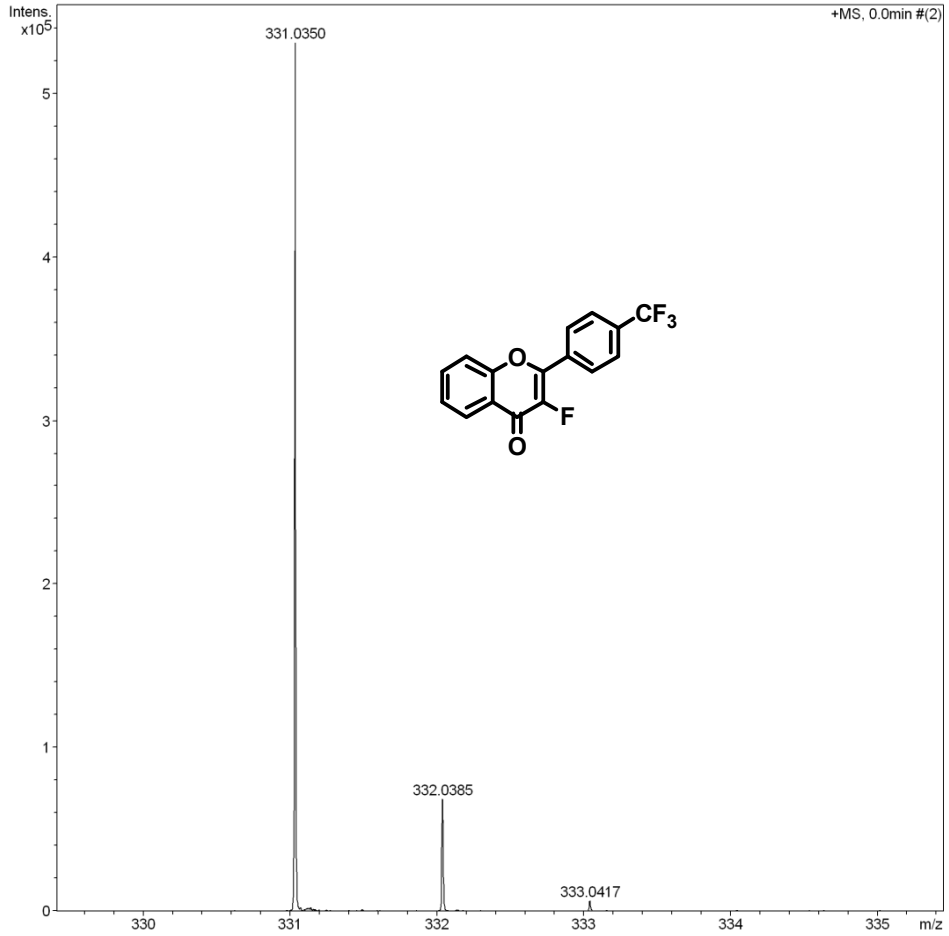
^{1}H NMR spectrum of **2x** ($CDCl_3$)



^{13}C NMR spectrum of **2x** ($CDCl_3$)

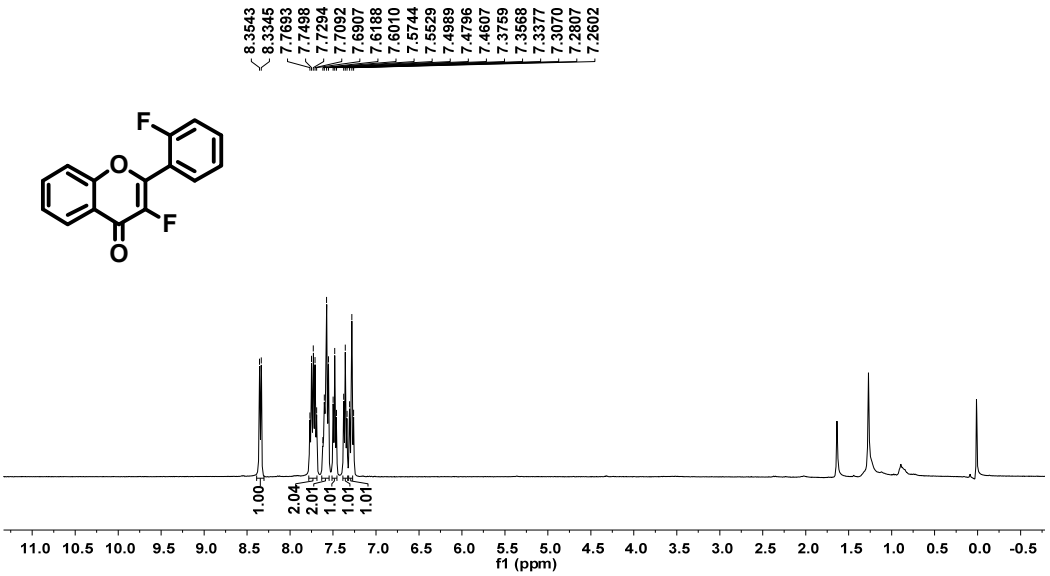


^{19}F NMR spectrum of **2x** ($CDCl_3$)

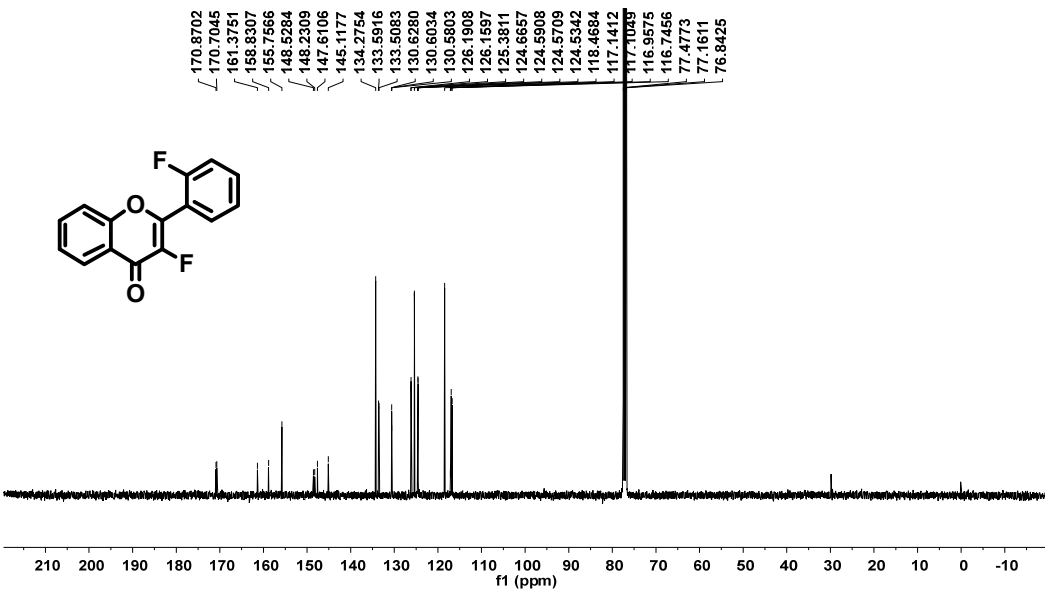


HRMS spectrum of **2x** (MeOH)

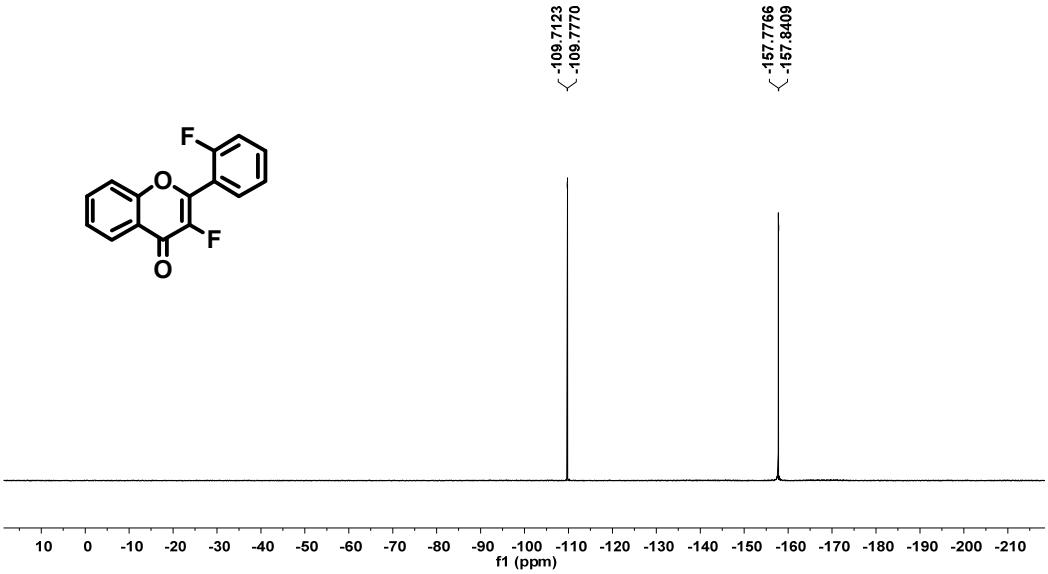
2y



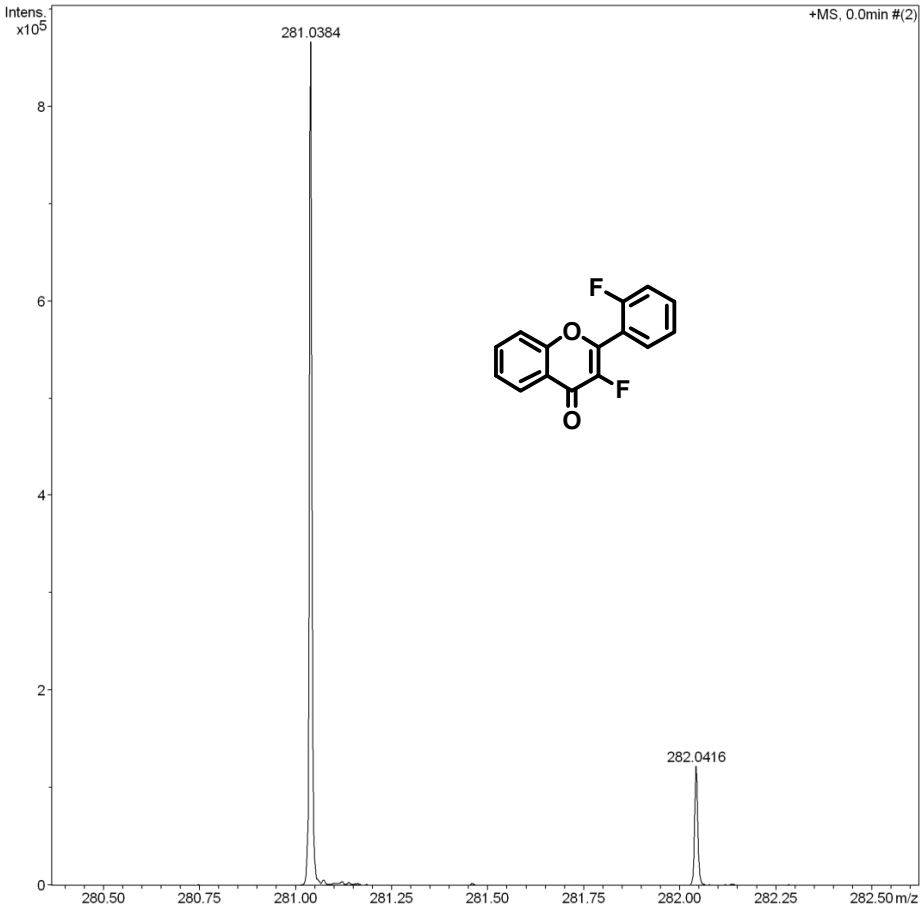
^{1}H NMR spectrum of **2y** ($CDCl_3$)



^{13}C NMR spectrum of **2y** ($CDCl_3$)

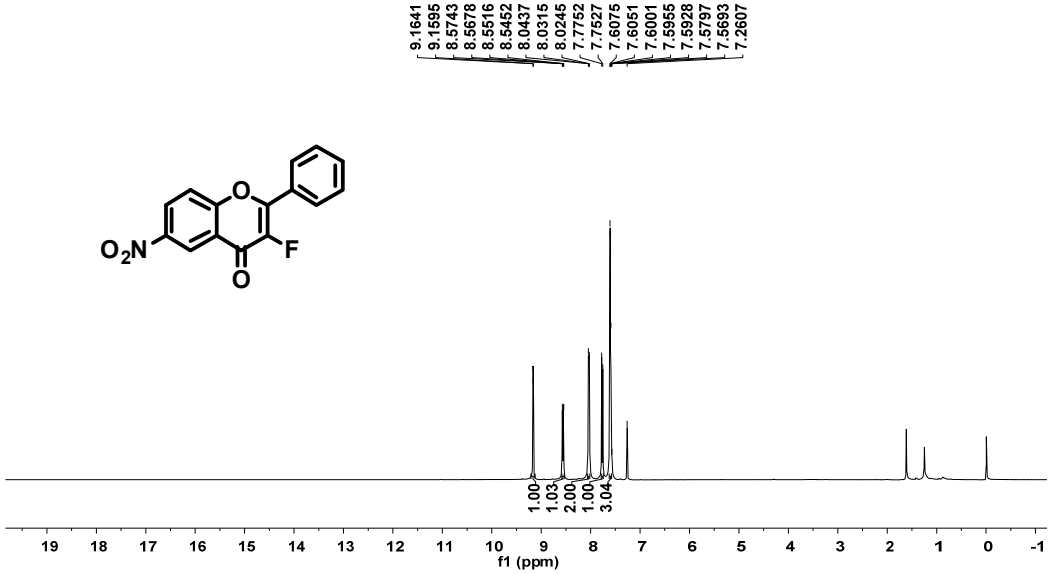


^{19}F NMR spectrum of **2y** ($CDCl_3$)

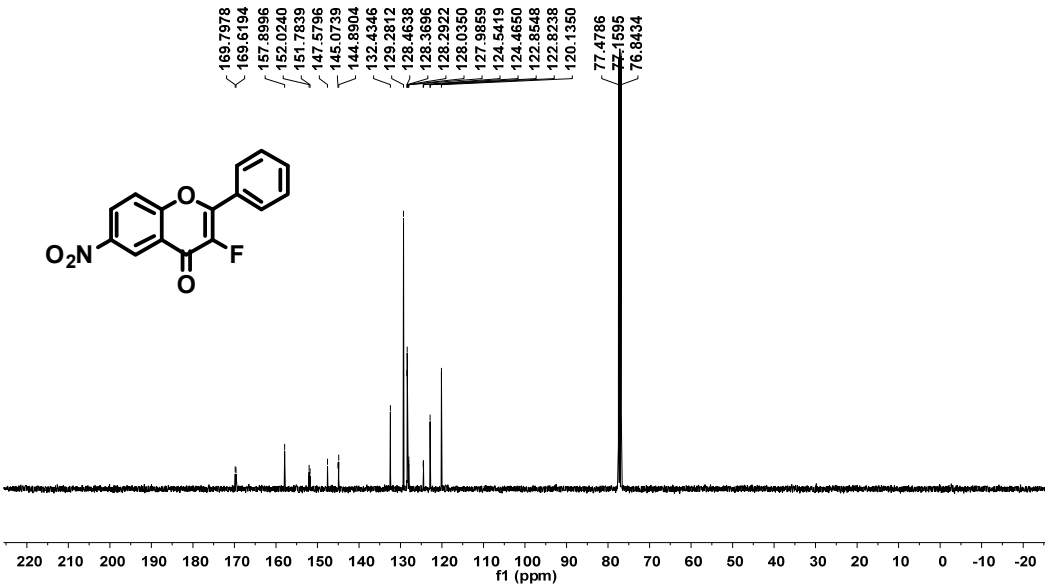


HRMS spectrum of **2y** (MeOH)

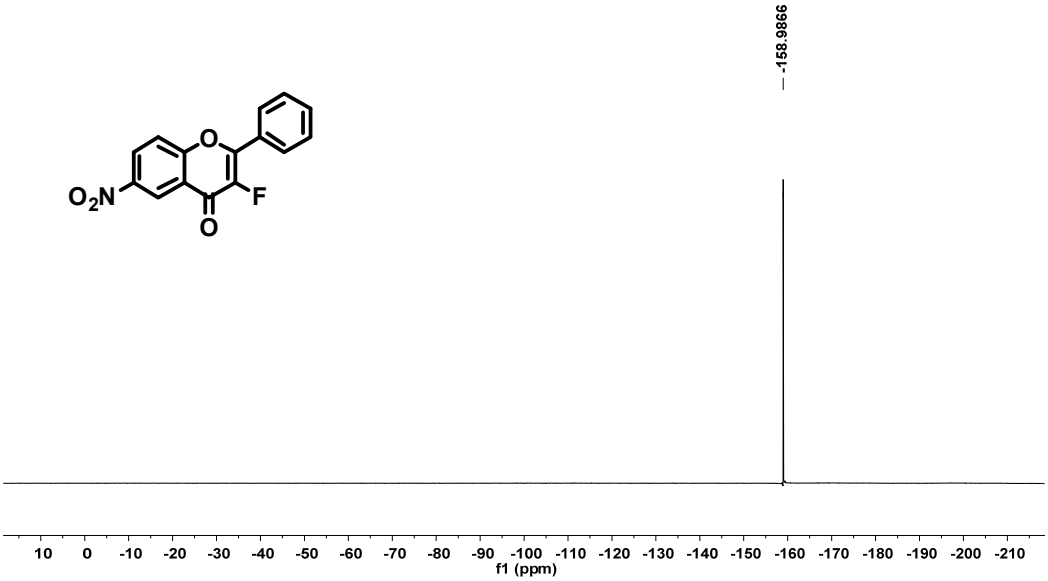
2z



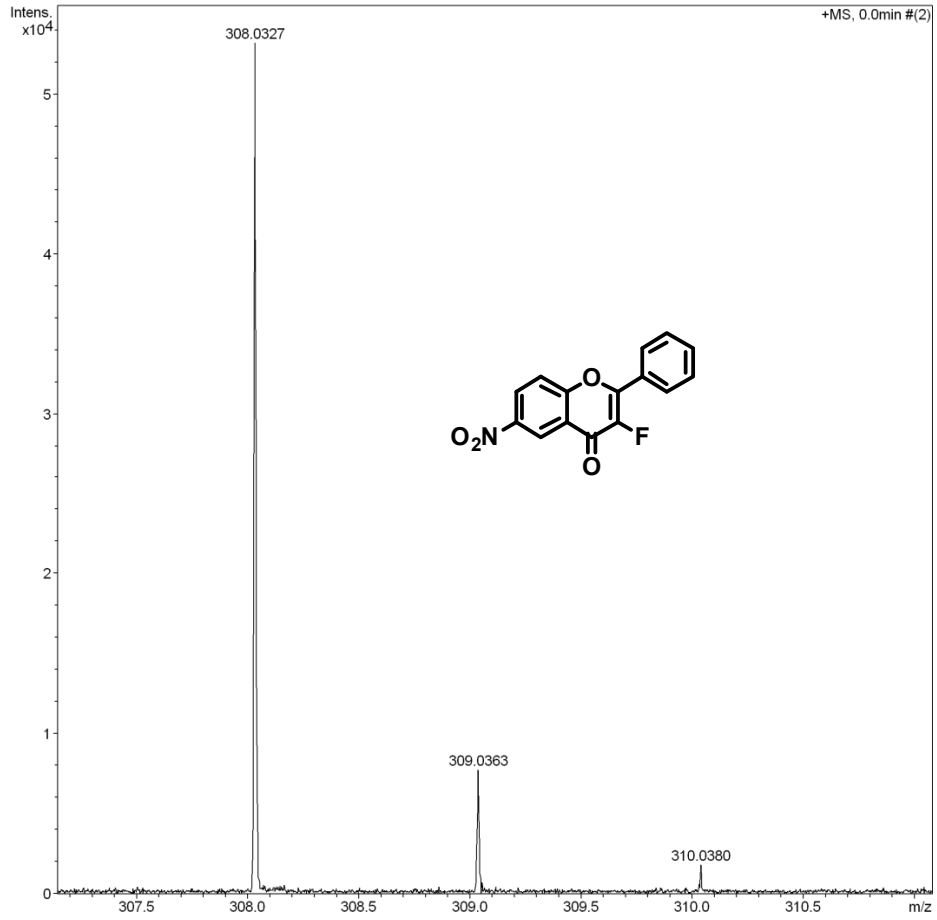
^{1}H NMR spectrum of **2z** ($CDCl_3$)



^{13}C NMR spectrum of **2z** ($CDCl_3$)

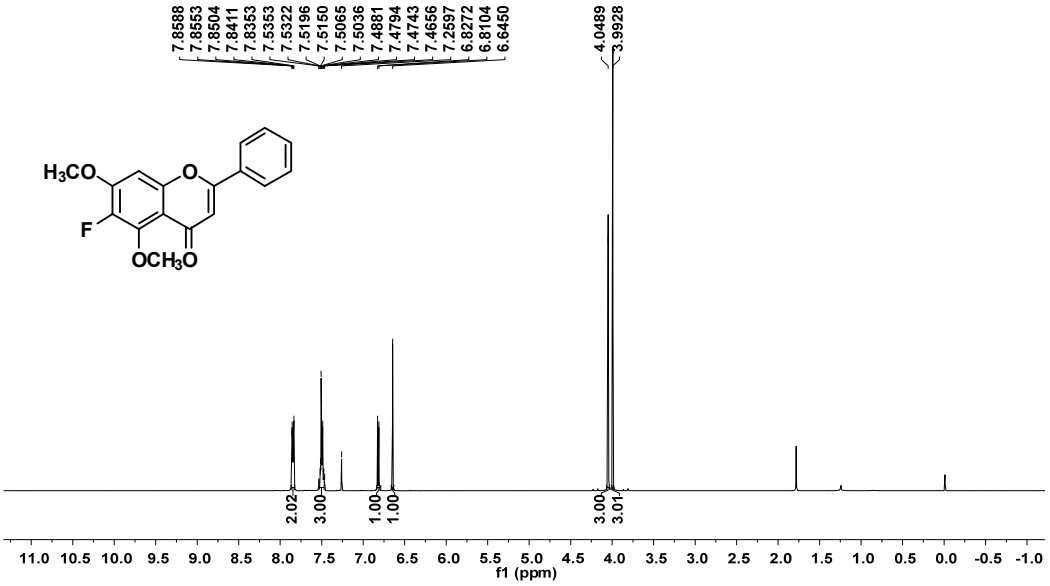


^{19}F NMR spectrum of **2z** ($CDCl_3$)

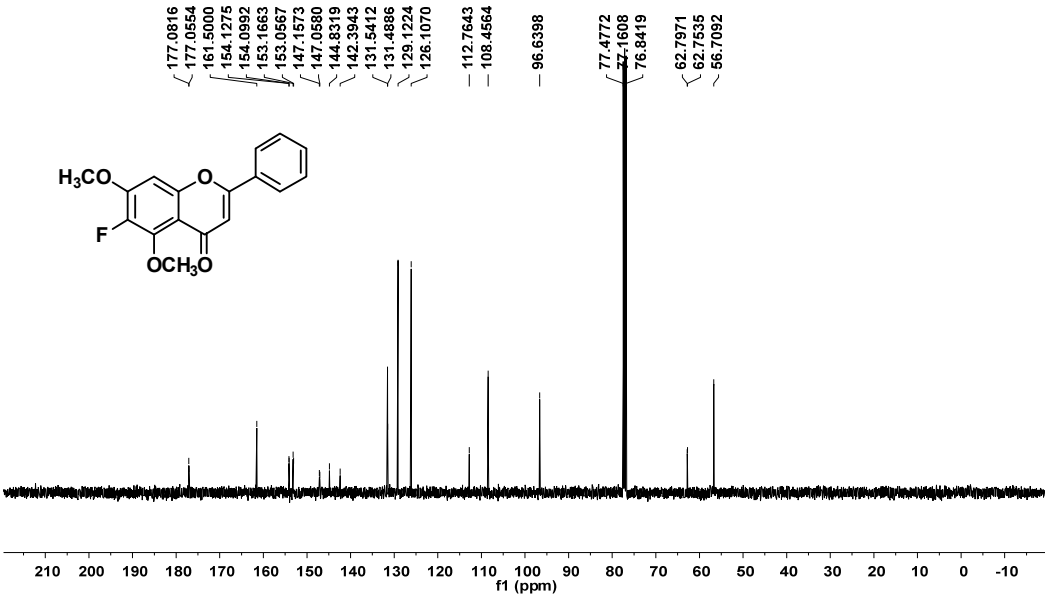


HRMS spectrum of **2z** (MeOH)

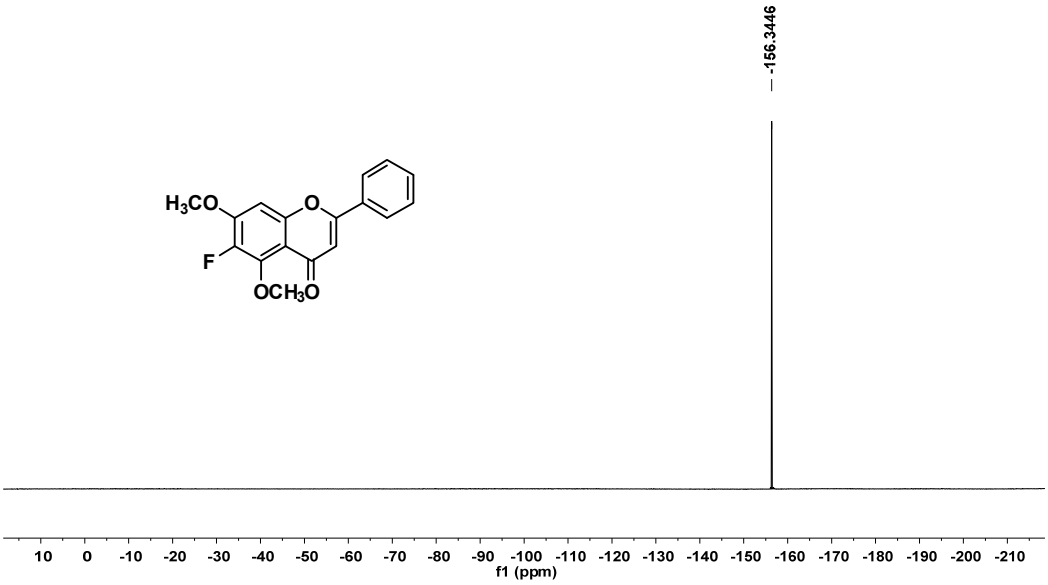
2u



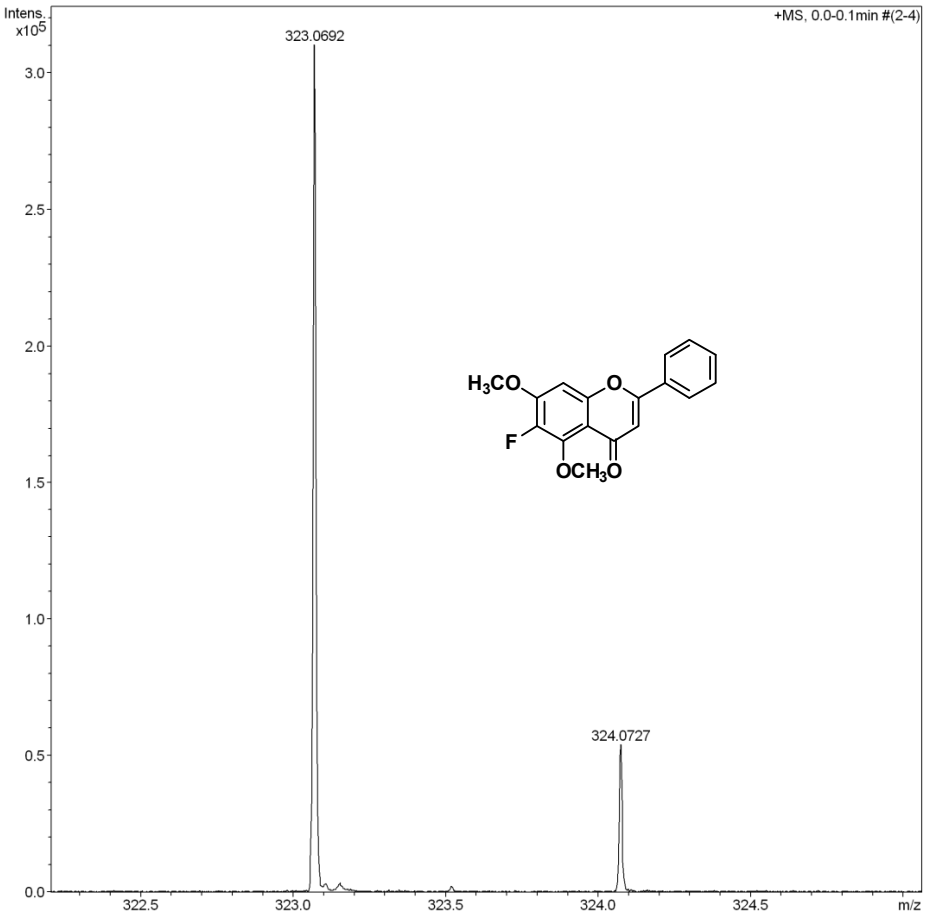
^{1}H NMR spectrum of **2u** ($CDCl_3$)



^{13}C NMR spectrum of **2u** ($CDCl_3$)

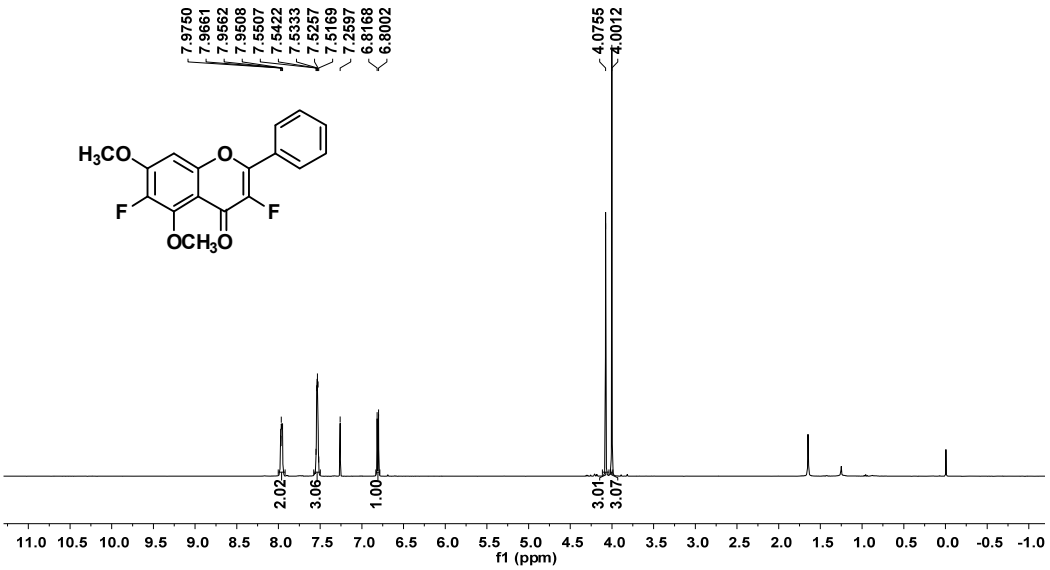


^{19}F NMR spectrum of **2u** ($CDCl_3$)

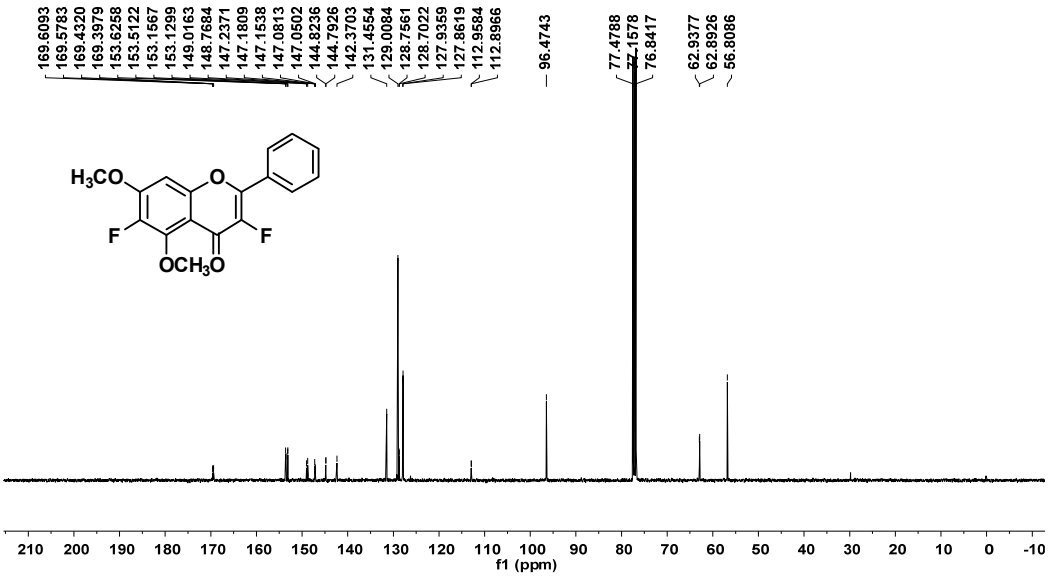


HRMS spectrum of **2u** (MeOH)

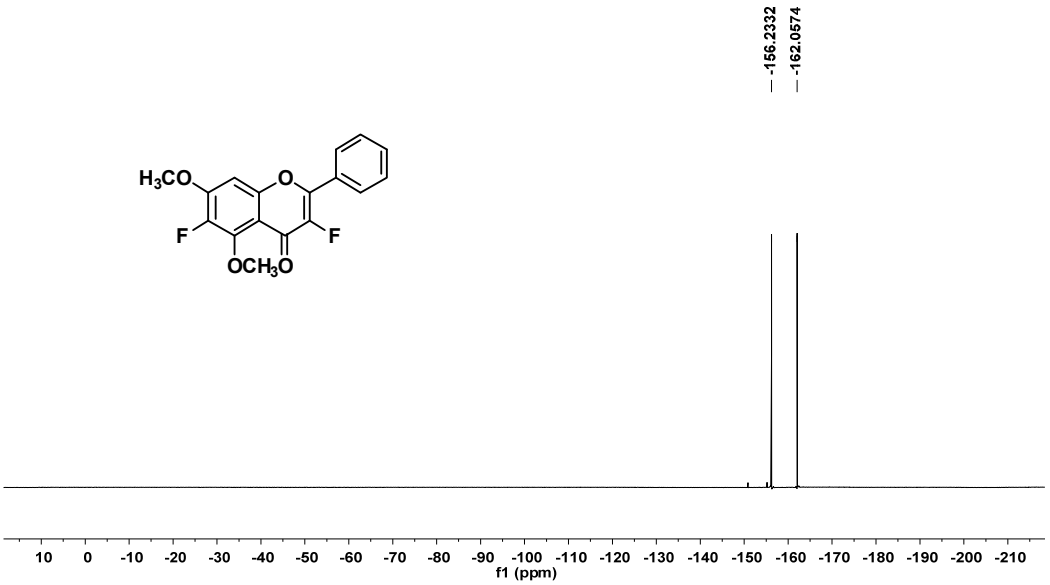
2u'



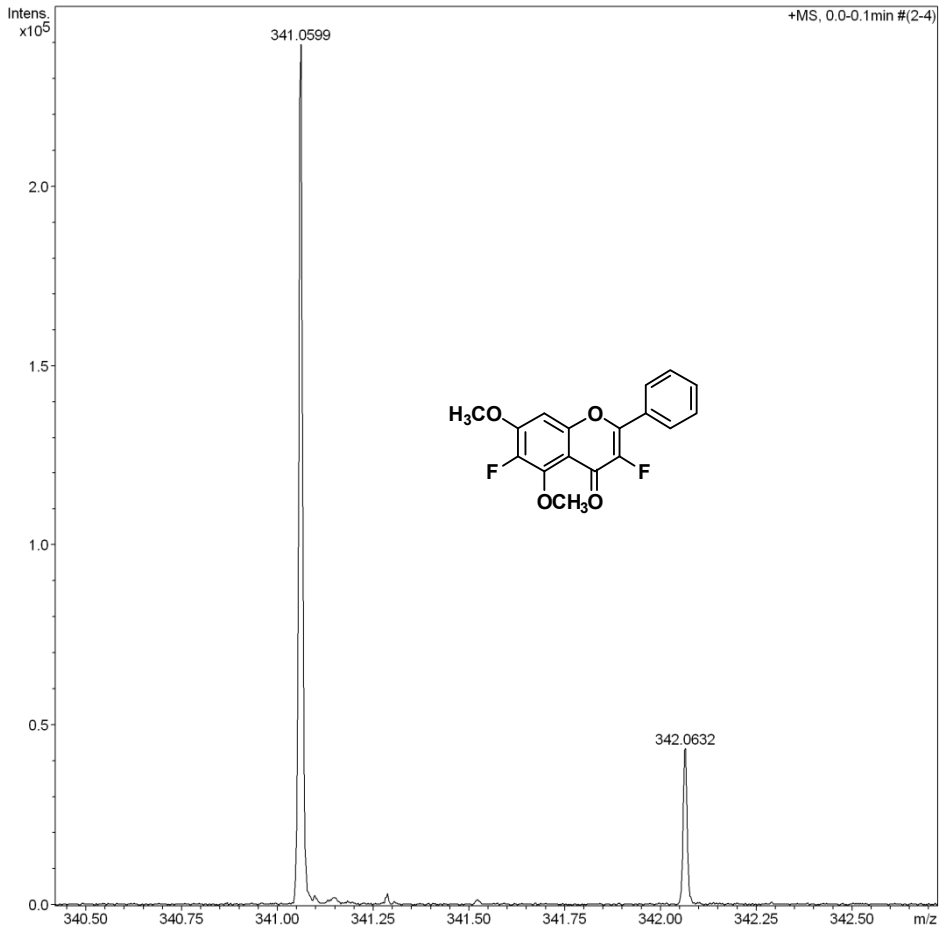
^{1}H NMR spectrum of **2u'** ($CDCl_3$)



^{13}C NMR spectrum of **2u'** ($CDCl_3$)

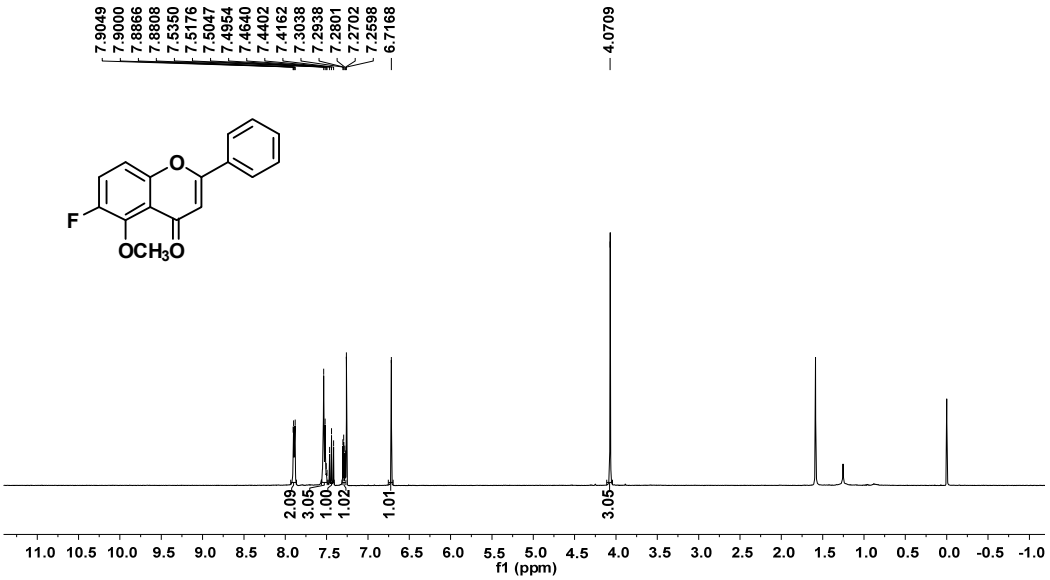


^{19}F NMR spectrum of **2u'** ($CDCl_3$)

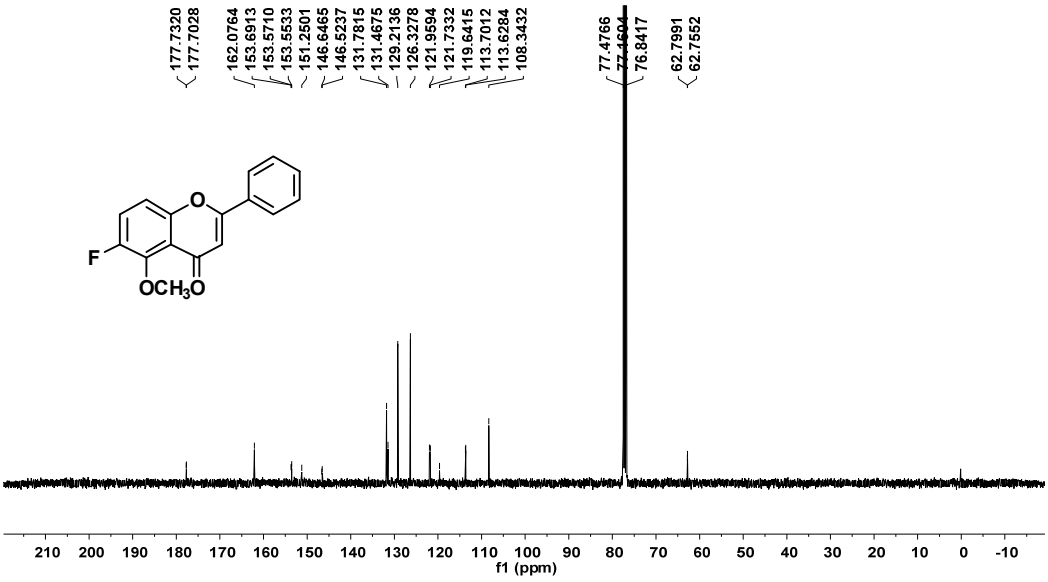


HRMS spectrum of **2u'** (MeOH)

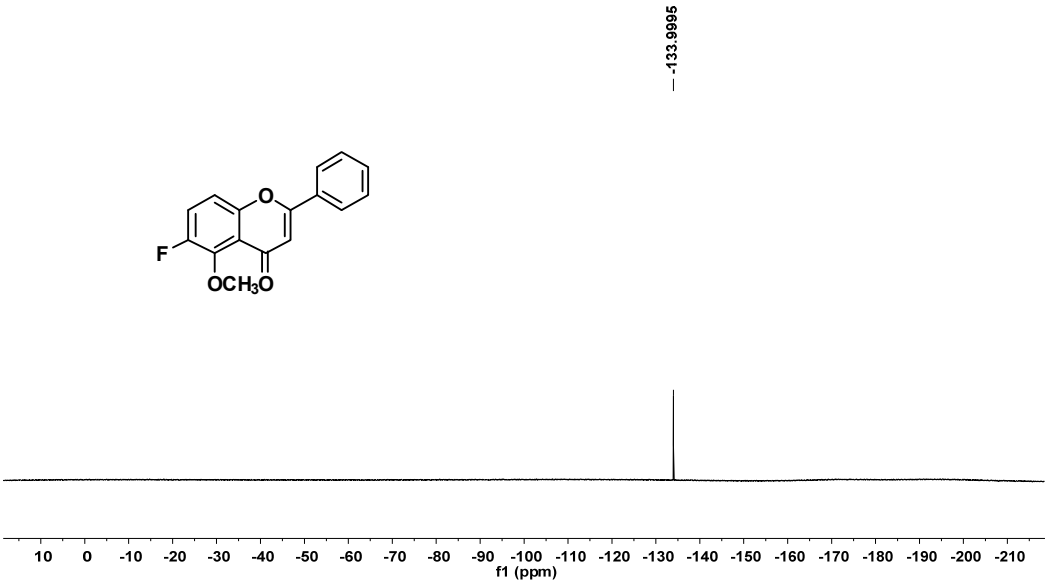
2v



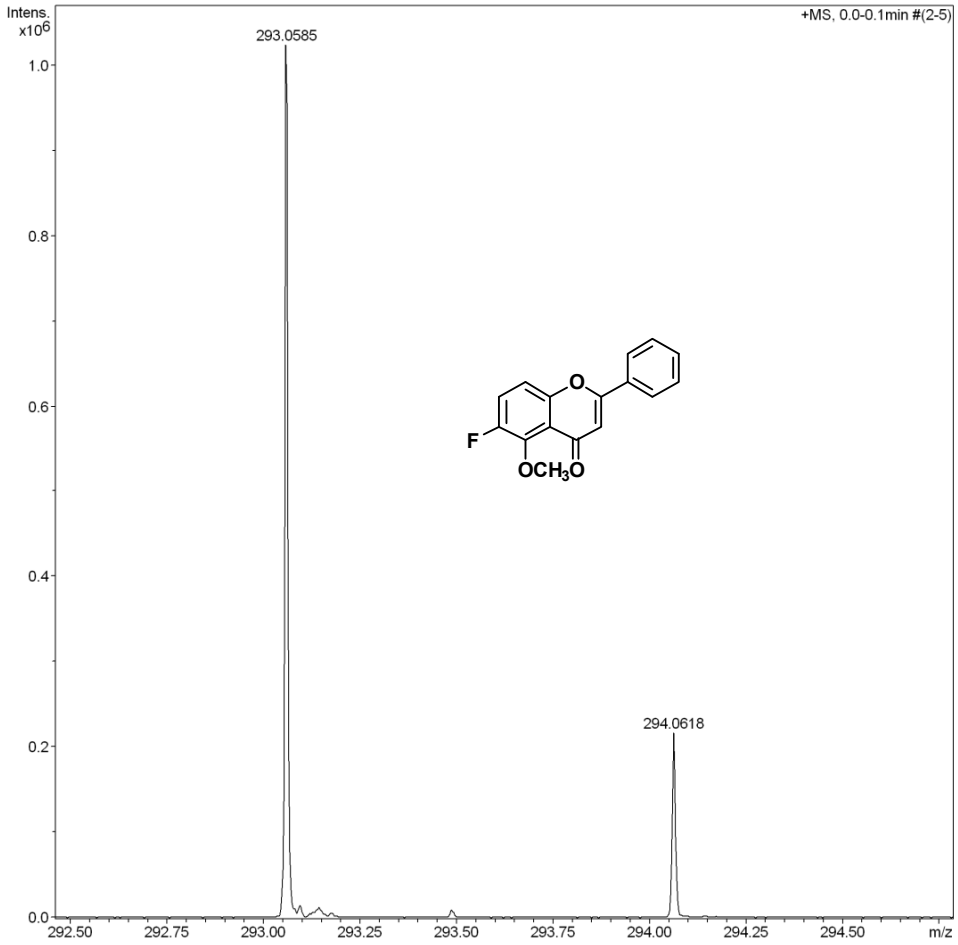
^{1}H NMR spectrum of **2v** ($CDCl_3$)



^{13}C NMR spectrum of **2v** ($CDCl_3$)

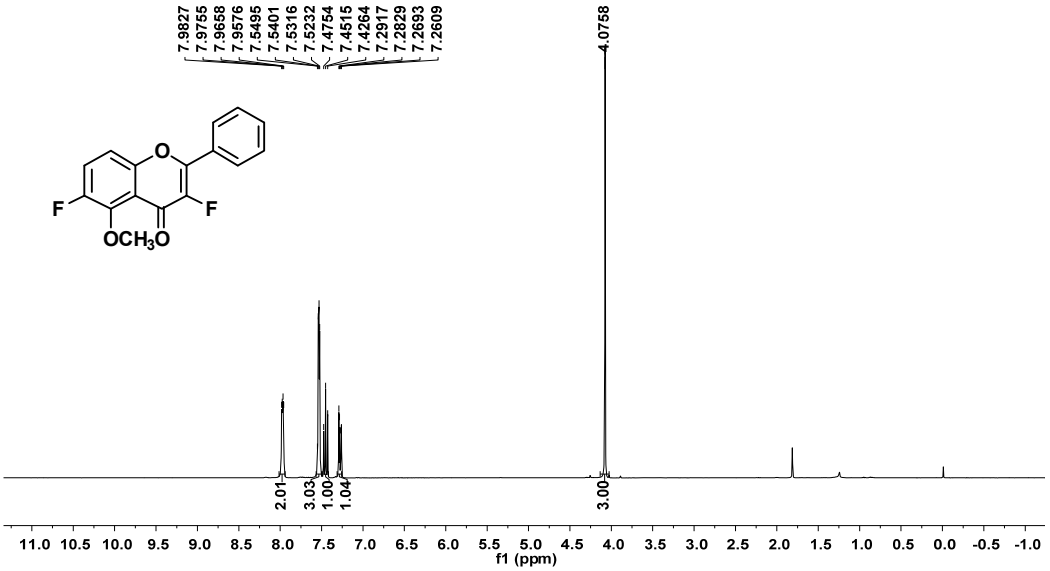


^{19}F NMR spectrum of **2v** ($CDCl_3$)

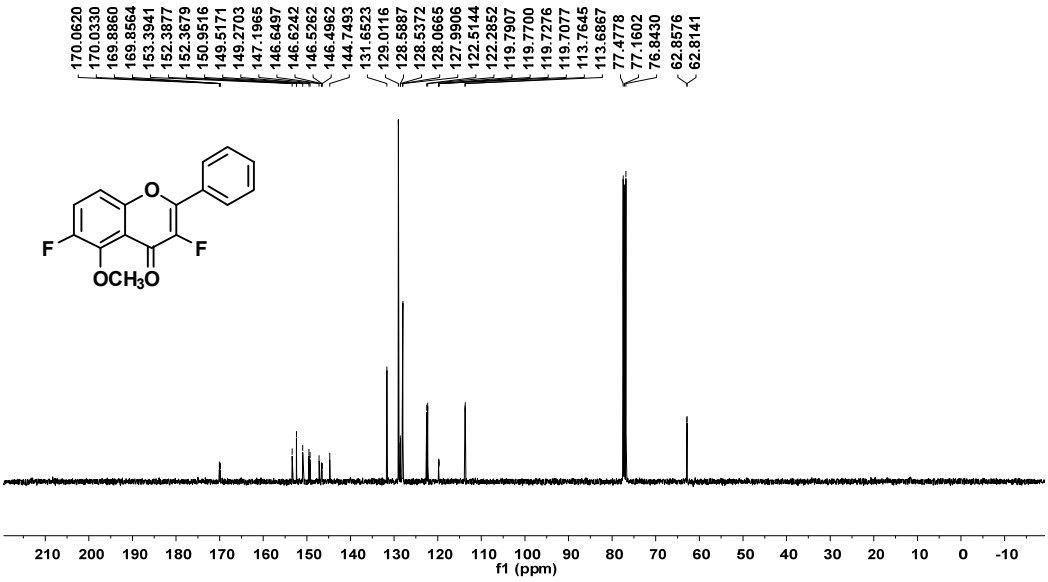


HRMS spectrum of **2v** (MeOH)

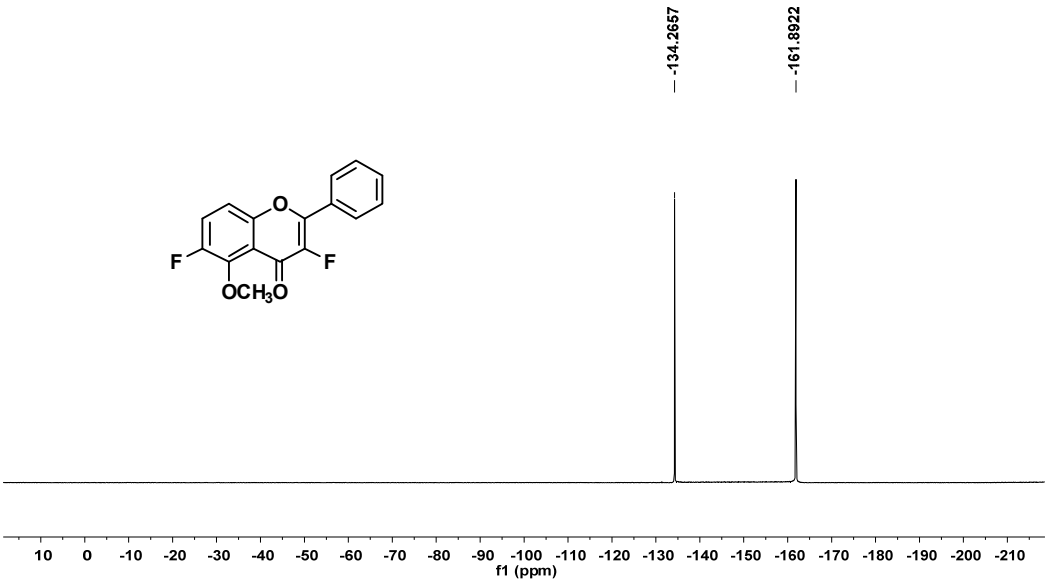
2v'



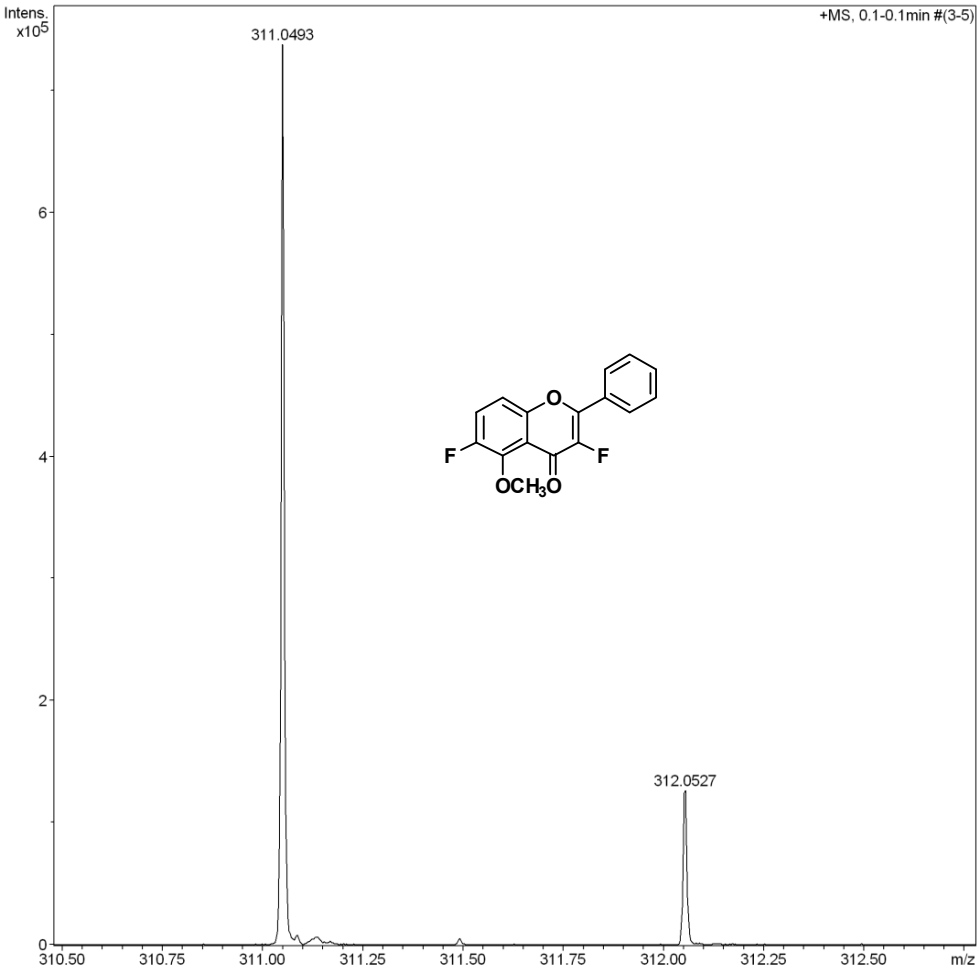
^{1}H NMR spectrum of **2v'** ($CDCl_3$)



^{13}C NMR spectrum of **2v'** ($CDCl_3$)



^{19}F NMR spectrum of **2v'** ($CDCl_3$)



HRMS spectrum of **2v'** (MeOH)

5. References

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