Supporting Information

Water-promoted catalytic hydrodecarboxylation of conjugated carboxylic acids under open air conditions at room temperature

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1. General Information

Unless otherwise stated, all reactions were carried out in anhydrous solvent and commercially available reagents were used as received. 1,8 Diazabicyclo[5.4.0]-7-Undecene (DBU, 98%) and *N,N'*-Carbonyldiimidazole (CDI, 98%) were purchased from Adamas and used as received. Anhydrous THF and MTBE were distilled from sodium and benzophenone, CH_3CN, CCl_4, EA and acetone were distilled from CaH_2. Dichloromethane (DCM) (Water≤50 ppm(by K.F.)，99.9%，SafeDry，with molecular sieves，Safeseal), *N,N*-dimethylformamide (DMF) (Water≤50 ppm(by K.F.)，99.8%，SafeDry，with molecular sieves，Safeseal), dimethyl sulfoxide (DMSO) (Water≤50 ppm(by K.F.)，99.7%，SafeDry，with molecular sieves，Safeseal), 1,4-dioxane (Water≤50 ppm(by K.F.)，99.8%，SafeDry，with molecular sieves，Safeseal), were all purchased from Adamas. NMR spectra were obtained in $CDCl_3$ or DMSO-d_6 using TMS as the internal standard at 400 (for ^{1}H NMR) or 100 MHz (for ^{13}C NMR), respectively. ^{1}H NMR spectra: J-values are reported in Hz. HRMS (m/z) were recorded on Thermo Scientific™ Q Exactive. Flash column chromatography was performed using Huanghai silica gel (300-400). The 2-Hydroxy-benzaldehydes were synthesized from the corresponding Phenols and Paraformaldehyde according to the literatures.[1] Coumarin-3-carboxylic acids **1** were synthesized according to the literatures.[2] The α,β-unsaturated carboxylic acids (**3a**-**3c**) were synthesized according to the literatures.[3] 4-Methyl-2-oxo-2H-chromene-3-carboxylic acid **5a** was synthesized according to the literatures.[4]

2. Experimental Section

General procedure for the hydrodecarboxylation of conjugated carboxylic acids (1, 3)

Conjugated carboxylic acids (**1, 3**) (0.3 mmol), CDI (0.36 mmol) were successively added into a 10 ml reaction tube, then dry anisole (2 ml) and water (16 μl) were added with stirring. The mixture was stirred in open air for 5 min and then DABCO (0.06 mmol) was added. The resulting mixture was continuously stirred at rt. After completion, the products (**2, 4**) were obtained by flash column chromatography on a short packed silica gel column eluting with petroleum ether/EtOAc (3:1).

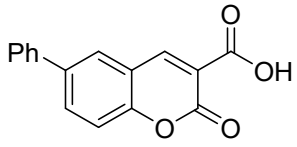
A typical procedure for the preparation of coumarin-3-carboxylic anhydride 6a.

Under standard conditions, coumarin-3-carboxylic acids **1a** (0.3 mmol), CDI (0.36 mmol) were successively added into a 10 ml reaction tube, then dry anisole (2 ml) and water (16 μl) were added with stirring, the mixture was stirred in open air for 5 min. The precipitates were formed and collected by filtration and wash with anisole to give the product **6a** (88.5mg, 98% yield).

Deuterization experiment of the hydrodecarboxylation of coumarin-3-carboxylic acid

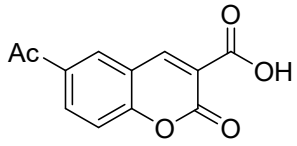
Under N_2 atmosphere, coumarin-3-carboxylic acids **1a** (0.3 mmol), CDI (0.36 mmol) were successively added into a 10 ml reaction tube, then dry anisole (2 ml) and D_2O (16 μl) were added with stirring. The mixture was stirred in open air for 5 min and then DABCO (0.06 mmol) was added. The resulting mixture was continuously stirred at rt. After completion, the products **2a'** was obtained by flash column chromatography on a short packed silica gel column eluting with petroleum ether/EtOAc (3:1).

3. The data of the products 1d, 1i, 1o, 2, 4, 6a, 2a'



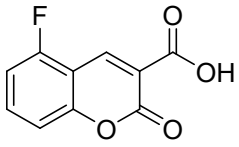
1d

2-oxo-6-phenyl-2*H*-chromene-3-carboxylic acid 1d: yellow solid, mp 208-209 °C, ^{1}H NMR (400 MHz, DMSO) δ 8.77 (s, 1H), 8.21 (s, 1H), 8.01 (d, *J* = 8.1 Hz, 1H), 7.71 (d, *J* = 7.5 Hz, 2H), 7.55 – 7.45 (m, 3H), 7.41 (t, *J* = 7.3 Hz, 1H); ^{13}C NMR (100 MHz, DMSO) δ 164.5, 157.1, 154.3, 148.7, 138.8, 137.1, 132.9, 129.6, 128.3, 127.2, 119.3, 118.8, 117.1. HRMS (FTMS-ESI): $[M + H]^+$ calcd for $C_{16}H_{11}O_4$+: 267.0657; found: 267.0648.



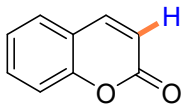
1i

6-acetyl-2-oxo-2*H*-chromene-3-carboxylic acid 1i: white solid, mp 253-254 °C, 1H NMR (400 MHz, DMSO) δ 13.37 (s, 1H), 8.82 (s, 1H), 8.57 (s, 1H), 8.24 (d, *J* = 8.7 Hz, 1H), 7.53 (d, *J* = 8.7 Hz, 1H), 2.63 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 196.7, 164.2, 157.7, 156.5, 148.6, 133.8, 133.7, 131.6, 119.7, 118.3, 117.1, 27.2. HRMS (FTMS-ESI): [M + H]+ calcd for $C_{12}H_9O_5$+: 233.0450; found: 233.0443.



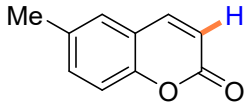
1o

5-fluoro-2-oxo-2*H*-chromene-3-carboxylic acid 1o: white solid, mp 177-178 °C, ^{1}H NMR (400 MHz, DMSO) δ 13.44 (s, 1H), 8.56 (s, 1H), 7.75 (dd, *J* = 15.2, 7.9 Hz, 1H), 7.32 – 7.23 (m, 2H); ^{13}C NMR (100 MHz, DMSO) δ 164.0, 159.0 (d, *J* = 254 Hz), 156.2, 155.3 (d, *J* = 4.6 Hz), 140.6 (d, *J* = 3.8 Hz), 135.6 (d, *J* = 10.1 Hz), 119.3, 113.0 (d, *J* = 3.7 Hz), 111.1 (d, *J* = 19.4 Hz), 108.4 (d, *J* = 19.0 Hz). HRMS (FTMS-ESI): [M + H]+ calcd for $C_{10}H_6FO_4$+: 209.0250; found: 209.0242.



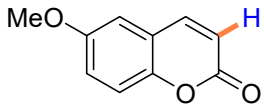
2a

2*H*-chromen-2-one 2a [5]: white solid, 99%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 9.5 Hz, 1H), 7.60 – 7.45 (m, 2H), 7.34 (d, *J* = 8.3 Hz, 1H), 7.31 – 7.27 (m, 1H), 6.43 (d, *J* = 9.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 154.1, 143.4, 131.9, 127.9, 124.4, 118.9, 116.9, 116.7.



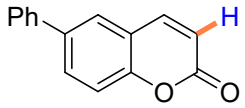
2b

6-methyl-2*H*-chromen-2-one 2b [5]: white solid, 96%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 9.5 Hz, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 7.27 (s, 1H), 7.21 (d, *J* = 8.4 Hz, 1H), 6.39 (d, *J* = 9.5 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.0, 152.2, 143.4, 134.1, 132.8, 127.7, 118.6, 116.5, 20.7.



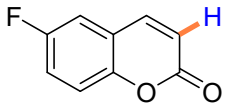
2c

6-methoxy-2*H*-chromen-2-one 2c [5]: white solid, 99%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 9.5 Hz, 1H), 7.26 (d, *J* = 9.1 Hz, 1H), 7.11 (d, *J* = 9.0 Hz, 1H), 6.92 (s, 1H), 6.42 (d, *J* = 9.5 Hz, 1H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 156.1, 148.5, 143.2, 119.5, 119.2, 117.9, 117.1, 110.0, 55.9.



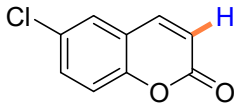
2d

6-phenyl-2*H*-chromen-2-one 2d [7]: white solid, 90%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (t, *J* = 8.0 Hz, 2H), 7.65 (s, 1H), 7.56 (d, *J* = 7.7 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 2H), 7.37 (t, *J* = 8.7 Hz, 2H), 6.44 (d, *J* = 9.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 153.4, 143.5, 139.4, 137.8, 130.7, 129.1, 127.8, 127.1, 126.1, 119.1, 117.3, 117.0.



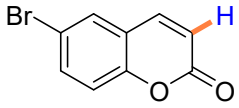
2e

6-fluoro-2*H*-chromen-2-one 2e [8]: white solid, 86%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 9.5 Hz, 1H), 7.48 (s, 2H), 7.28 (d, *J* = 9.0 Hz, 1H), 6.47 (d, *J* = 9.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 152.4, 142.2, 131.8, 129.7, 127.2, 119.8, 118.3, 117.8.



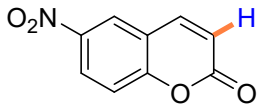
2f

6-chloro-2*H*-chromen-2-one 2f [6]: white solid, 98%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 9.6 Hz, 1H), 7.47 (d, *J* = 6.9 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 6.47 (d, *J* = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 152.4, 142.3, 131.7, 129.7, 127.2, 119.8, 118.3, 117.8.



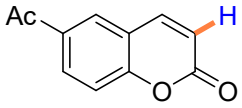
2g

6-bromo-2*H*-chromen-2-one 2g [5]: white solid, 89%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 – 8.35 (m, 2H), 7.82 (d, *J* = 9.6 Hz, 1H), 7.48 (d, *J* = 9.0 Hz, 1H), 6.60 (d, *J* = 9.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 157.6, 144.1, 142.2, 126.6, 123.8, 118.9, 118.8, 118.1.



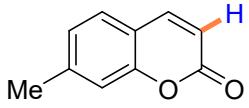
2h

6-nitro-2*H*-chromen-2-one 2h [5]: pale yellow solid, 63%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.57 (m, 3H), 7.22 (d, *J* = 8.5 Hz, 1H), 6.47 (d, *J* = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 152.9, 142.1, 134.6, 130.2, 120.3, 118.7, 117.9, 117.0.



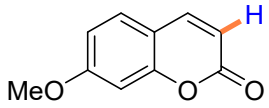
2i

6-acetyl-2*H*-chromen-2-one 2i [5]: white solid, 99%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 2H), 7.80 (d, *J* = 9.6 Hz, 1H), 7.40 (d, *J* = 9.0 Hz, 1H), 6.50 (d, *J* = 9.6 Hz, 1H), 2.66 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.0, 159.8, 156.9, 143.2, 133.5, 131.7, 128.6, 118.6, 117.6, 117.3, 26.6.



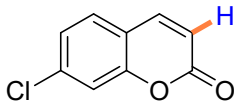
2j

7-methyl-2*H*-chromen-2-one 2j [7]: white solid, 96%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 9.5 Hz, 1H), 7.36 (d, *J* = 7.8 Hz, 1H), 7.23 – 7.04 (m, 2H), 6.35 (d, *J* = 9.5 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.1, 154.2, 143.4, 143.1, 127.5, 125.6, 117.1, 116.5, 115.4, 21.8.



2k

7-methoxy-2*H*-chromen-2-one 2k [6]: white solid, 89%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 9.5 Hz, 1H), 7.38 (d, *J* = 8.5 Hz, 1H), 6.89 – 6.77 (m, 2H), 6.25 (d, *J* = 9.5 Hz, 1H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9, 161.2, 155.9, 143.5, 128.8, 113.1, 112.6, 112.5, 100.9, 55.8.



2l

7-chloro-2*H*-chromen-2-one 2l [6]: white solid, 78%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 9.6 Hz, 1H), 7.48 (d, *J* = 6.6 Hz, 2H), 7.28 (d, *J* = 10.1 Hz, 1H), 6.47 (d, *J* = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 152.5, 142.2, 131.8, 129.7, 127.1, 119.8, 118.4, 117.9.

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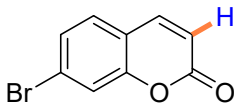
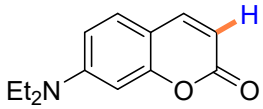


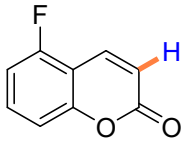
2m

7-bromo-2*H*-chromen-2-one 2m [6]: white solid, 74%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (t, *J* = 7.5 Hz, 3H), 7.25 (d, *J* = 11.0 Hz, 1H), 6.47 (d, *J* = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 153.0, 142.1, 134.6, 130.2, 120.3, 118.7, 117.9, 117.0.



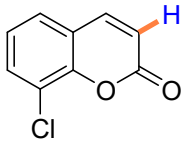
2n

7-(diethylamino)-2*H*-chromen-2-one 2n [9]: red solid, 83%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 9.3 Hz, 1H), 7.26 (d, *J* = 8.7 Hz, 1H), 6.58 (d, *J* = 8.8 Hz, 1H), 6.51 (s, 1H), 6.05 (d, *J* = 9.3 Hz, 1H), 3.43 (q, *J* = 7.0 Hz, 4H), 1.23 (t, *J* = 7.1 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 156.8, 150.7, 143.7, 128.8, 109.2, 108.7, 108.3, 97.5, 44.8, 12.4.



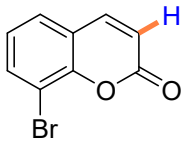
2o

5-fluoro-2*H*-chromen-2-one 2o [6]: white solid, 99%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 9.7 Hz, 1H), 7.49 (dd, *J* = 15.0, 7.9 Hz, 1H), 7.14 (d, *J* = 8.5 Hz, 1H), 7.00 (t, *J* = 8.7 Hz, 1H), 6.46 (d, *J* = 9.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8 (d, *J* = 7.3 Hz), 157.3, 154.7 (d, *J* = 5.1 Hz), 136.3 (d, *J* = 4.1 Hz), 132.2 (d, *J* = 9.6 Hz), 116.8 (d, *J* = 1.6 Hz), 112.7 (d, *J* = 4.0 Hz), 110.3 (d, *J* = 20.0 Hz), 109.0 (d, *J* = 19.2 Hz).



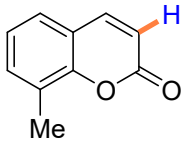
2p

8-chloro-2*H*-chromen-2-one 2p [6]: white solid, 90%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 9.6 Hz, 1H), 7.59 (d, *J* = 7.9 Hz, 1H), 7.41 (d, *J* = 7.7 Hz, 1H), 7.23 (t, *J* = 7.8 Hz, 1H), 6.47 (d, *J* = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 149.8, 143.1, 132.3, 126.4, 124.7, 121.8, 120.1, 117.4.



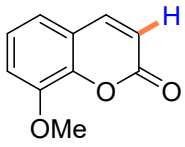
2q

8-bromo-2*H*-chromen-2-one 2q [6]: white solid, 98%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.9 Hz, 1H), 7.70 (d, *J* = 9.5 Hz, 1H), 7.46 (d, *J* = 7.7 Hz, 1H), 7.17 (t, *J* = 7.8 Hz, 1H), 6.45 (d, *J* = 9.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 150.8, 143.2, 135.4, 127.2, 125.2, 120.1, 117.3, 110.4.



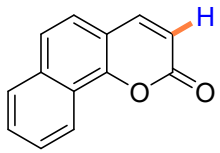
2r

8-methyl-2*H*-chromen-2-one 2r [7]: white solid, 75%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 9.5 Hz, 1H), 7.38 (d, *J* = 7.3 Hz, 1H), 7.32 (d, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 6.41 (d, *J* = 9.5 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.1, 152.4, 143.9, 133.2, 126.3, 125.6, 124.0, 118.6, 116.3, 15.4.



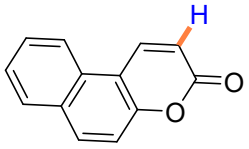
2s

8-methoxy-2*H*-chromen-2-one 2s [6]: white solid, 93%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 9.6 Hz, 1H), 7.21 (t, *J* = 7.9 Hz, 1H), 7.07 (t, *J* = 8.9 Hz, 2H), 6.43 (d, *J* = 9.5 Hz, 1H), 3.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 147.2, 143.71, 143.67, 124.3, 119.5, 119.3, 116.8, 113.8, 56.2.



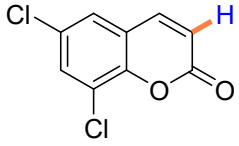
2t

2*H*-benzo[*h*]chromen-2-one 2t [5]: white solid, 97%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 – 8.43 (m, 1H), 7.89 – 7.80 (m, 1H), 7.76 (d, *J* = 9.4 Hz, 1H), 7.61 (dd, *J* = 11.0, 6.5 Hz, 3H), 7.39 (d, *J* = 8.5 Hz, 1H), 6.47 (d, *J* = 9.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 151.3, 144.2, 134.8, 128.7, 127.8, 127.2, 124.4, 123.6, 123.0, 122.2, 115.9, 114.2.



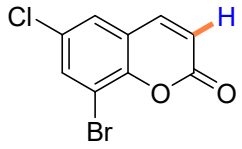
2u

2*H*-benzo[*g*]chromen-2-one 2u [6]: white solid, 98%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 9.8 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.93 (d, *J* = 9.0 Hz, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.66 (t, *J* = 7.7 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.39 (d, *J* = 9.0 Hz, 1H), 6.53 (d, *J* = 9.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 153.8, 139.1, 133.1, 130.2, 128.99, 128.96, 128.3, 126.1, 121.3, 117.0, 115.6, 112.9.



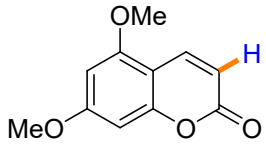
2v

6,8-dichloro-2*H*-chromen-2-one 2v [7]: white solid, 88%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 9.6 Hz, 1H), 7.59 (s, 1H), 7.40 (s, 1H), 6.52 (d, *J* = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 148.5, 142.0, 131.9, 129.6, 125.8, 122.8, 120.6, 118.6.



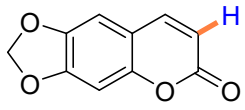
2w

6-bromo-8-chloro-2*H*-chromen-2-one 2w: white solid, 99%, mp 169-170 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.64 (d, *J* = 9.6 Hz, 1H), 7.45 (s, 1H), 6.50 (d, *J* = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 149.5, 142.1, 134.7, 129.9, 126.5, 120.6, 118.5, 111.2. HRMS (FTMS-ESI): [M + H]+ calcd for $C_9H_5BrClO_2$+: 258.9156; found: 258.9153.



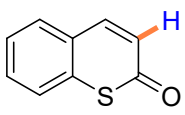
2x

5,7-dimethoxy-2*H*-chromen-2-one 2x [10]: white solid, 80%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 9.6 Hz, 1H), 6.38 (s, 1H), 6.27 (s, 1H), 6.13 (d, *J* = 9.6 Hz, 1H), 3.88 (s, 3H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 161.5, 157.0. 156.8, 138.7, 110.9, 104.0, 94.8, 92.8, 55.9, 55.8.



2y

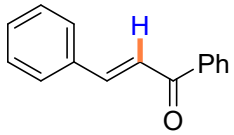
6*H*-[1,3]dioxolo[4,5-*g*]chromen-6-one 2y [10]: white solid, 99%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 9.5 Hz, 1H), 6.84 (d, *J* = 4.3 Hz, 2H), 6.29 (d, *J* = 9.5 Hz, 1H), 6.09 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.2, 151.29, 151.26, 144.9, 143.5, 113.4, 112.7, 105.0, 102.4, 98.4.



2z

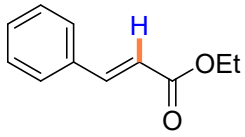
2*H*-thiochromen-2-one 2z [11]: brown solid, 80%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 10.6 Hz, 1H), 7.54 (d, *J* = 7.7 Hz, 1H), 7.47 – 7.35 (m, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 6.47 (d, *J* = 10.6 Hz, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 185.4, 143.8, 137.6, 131.6, 129.9, 126.5, 126.1, 125.9, 124.2.



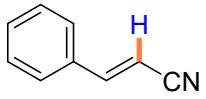
4a

(*E*)-chalcone 4a [12]: pale yellow, 63%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.7 Hz, 2H), 7.85 (d, *J* = 15.7 Hz, 1H), 7.67 (d, *J* = 4.6 Hz, 2H), 7.65 – 7.60 (m, 1H), 7.55 (dd, *J* = 16.5, 10.9 Hz, 3H), 7.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.6, 144.9, 138.3, 134.9, 132.8, 130.6, 129.0, 128.7, 128.53, 128.48, 122.1



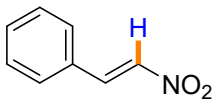
4b

ethyl cinnamate 4b [12]: colorless liquid, 70%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 16.0 Hz, 1H), 7.54 (d, *J* = 4.7 Hz, 2H), 7.48 – 7.35 (m, 3H), 6.47 (d, *J* = 16.0 Hz, 1H), 4.29 (q, *J* = 7.1 Hz, 2H), 1.36 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 144.6, 134.5, 130.2, 128.9, 128.1, 118.3, 60.5, 14.3.



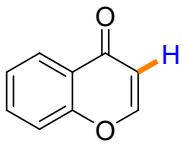
4c

cinnamonitrile 4c [13]: colorless liquid, 76%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.38 (m, 6H), 5.90 (d, *J* = 16.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.6, 133.6, 131.3, 129.2, 127.4, 118.2, 96.4.



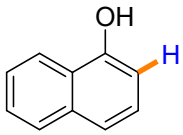
4d

(2-nitrovinyl)benzene 4d[15] yellow solid, 83%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 13.7 Hz, 1H), 7.59 (d, *J* = 13.8 Hz, 1H), 7.55 (d, *J* = 7.5 Hz, 2H), 7.52 – 7.41 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 137.1, 132.2, 130.1, 129.4, 129.2.



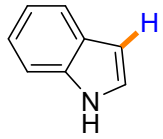
4e

4*H*-chromen-4-one 4e [14]: yellow solid, 90%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 6.0 Hz, 1H), 7.69 (t, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 8.5 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 1H), 6.36 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.6, 156.6, 155.3, 133.8, 125.8, 125.3, 124.9, 118.2, 113.0.



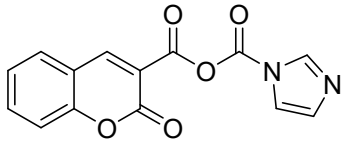
4f

naphthalen-1-ol 4f [16]: off-white solid, 80%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 – 8.21 (m, 1H), 7.99 – 7.87 (m, 1H), 7.59 (dt, *J* = 13.1, 7.0 Hz, 3H), 7.39 (t, *J* = 7.9 Hz, 1H), 6.85 (d, *J* = 7.5 Hz, 1H), 5.67 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.3, 134.9, 127.8, 126.6, 126.0, 125.5, 124.5, 121.6, 121.0, 109.0.



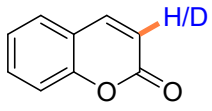
4g

1*H*-indole 4g [17]: pink solid, 30%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 8.1 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.23 (dd, *J* = 8.2, 5.4 Hz, 2H), 6.65 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.8, 127.9, 124.2, 122.1, 120.8, 119.9, 111.1, 102.6.



6a

1*H*-imidazole-1-carboxylic 2-oxo-2*H*-chromene-3-carboxylic 6a, mp 89-90 °C (decomposed), ^{1}H NMR (400 MHz, DMSO) δ 8.53 (s, 1H), 8.02 (s, 1H), 7.83 (d, *J* = 7.6 Hz, 1H), 7.68 (t, *J* = 7.8 Hz, 1H), 7.37 (dd, *J* = 11.9, 8.0 Hz, 2H), 7.19 (s, 2H); ^{13}C NMR (100 MHz, DMSO) δ 165.2, 157.8, 154.6, 146.6, 135.2, 134.1, 130.2, 125.2, 121.5, 121.4, 118.7, 116.5. MS (ITMS-ESI): $[M + Na]^+$ calcd for $C_{14}H_8N_2NaO_5^+$: 307.0; found: 307.0.



2a'

2a', ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 4.9 Hz, 2H), 7.51 – 7.38 (m, 4H), 7.27 (d, *J* = 8.3 Hz, 2H), 7.22 (d, *J* = 7.5 Hz, 2H), 6.36 (d, *J* = 9.5 Hz, 0.47H).

4. Reference

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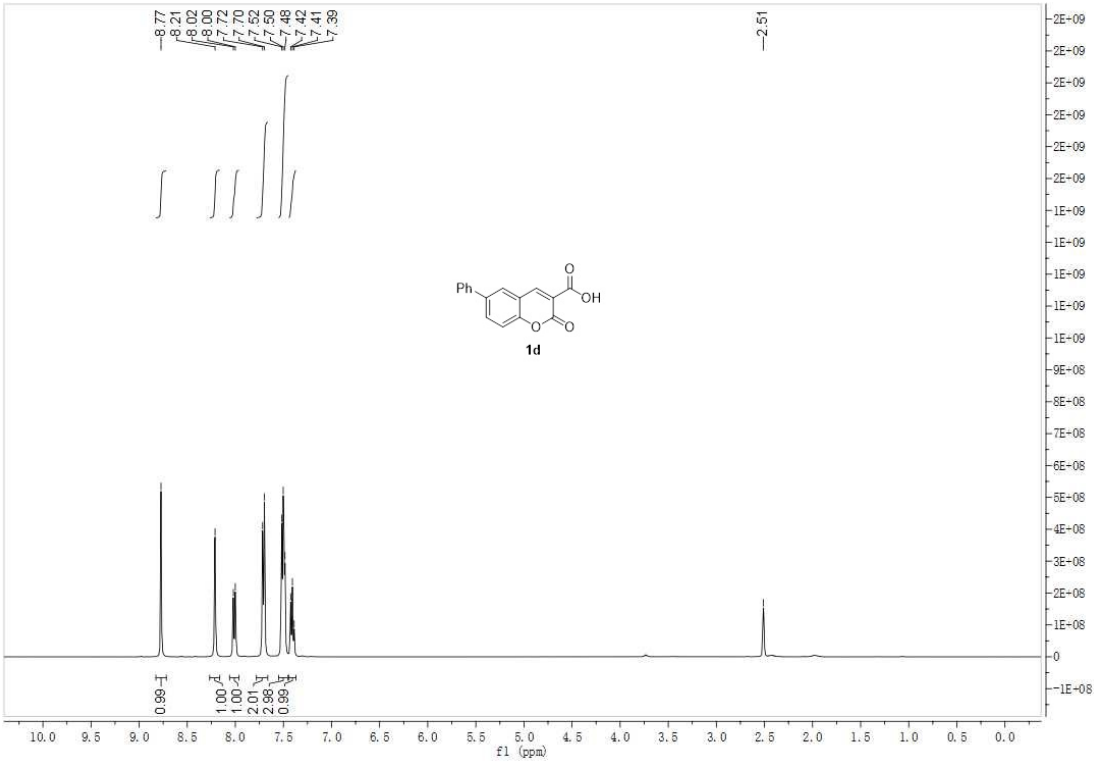
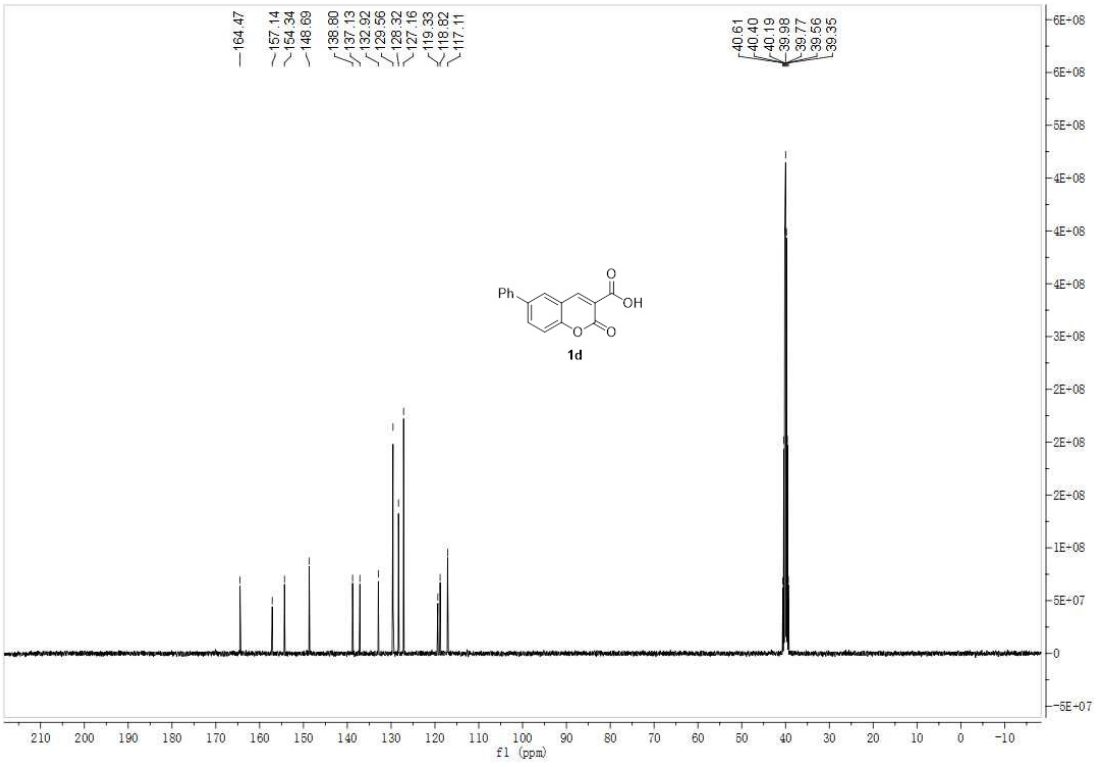
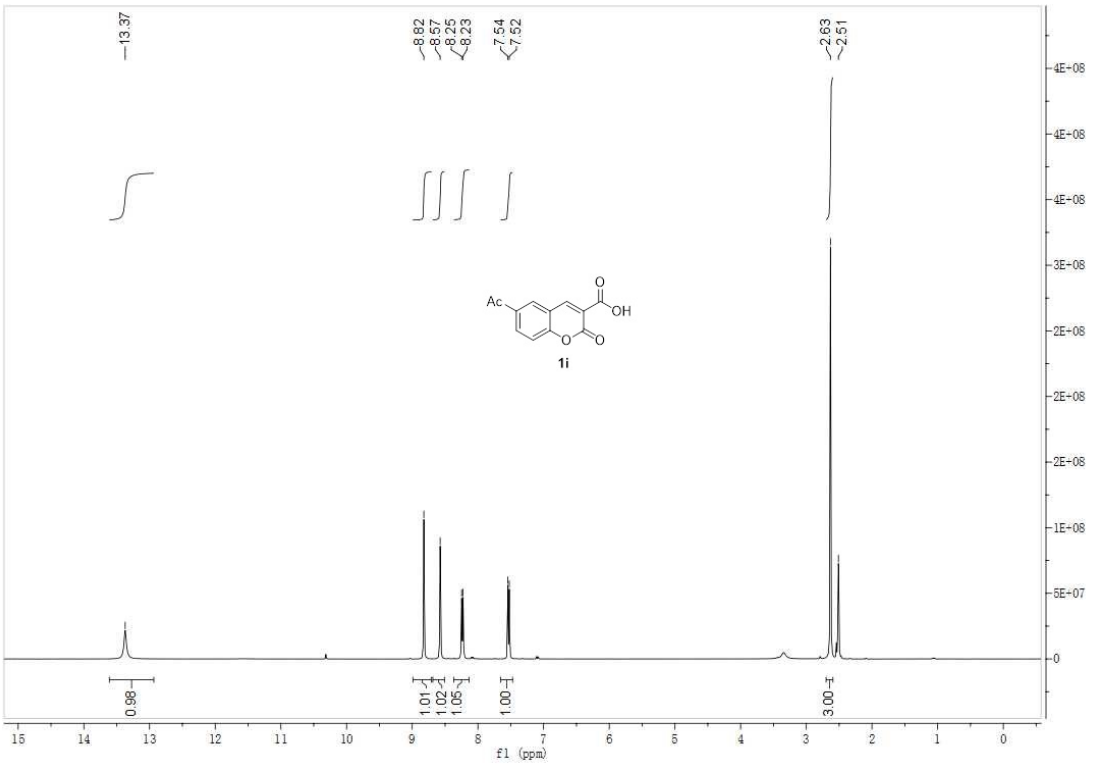
5 The NMR of 1d, 1i, 1o, 2, 4, 6a, 2a'



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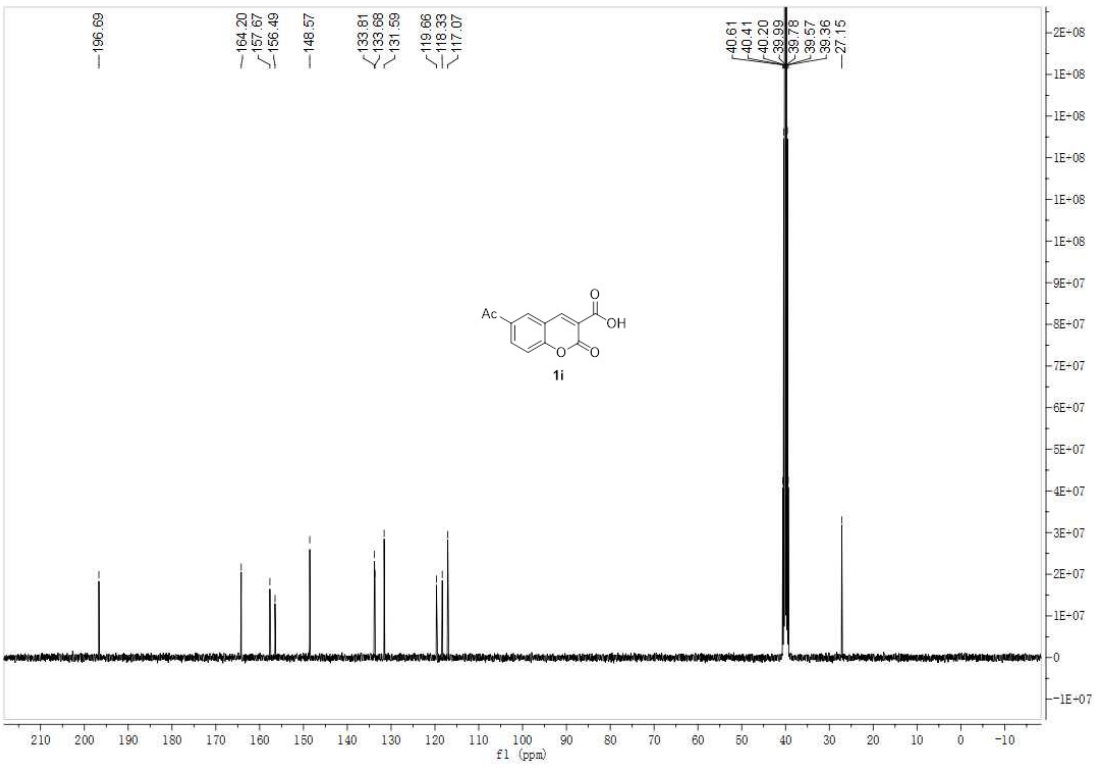
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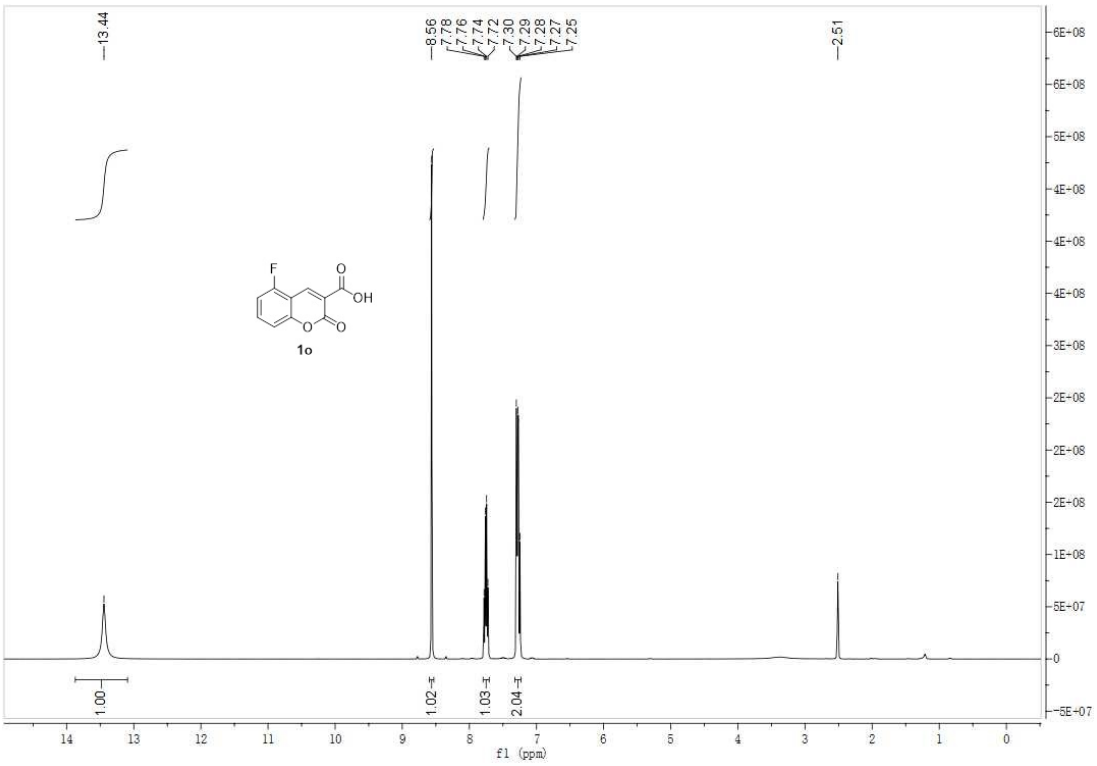
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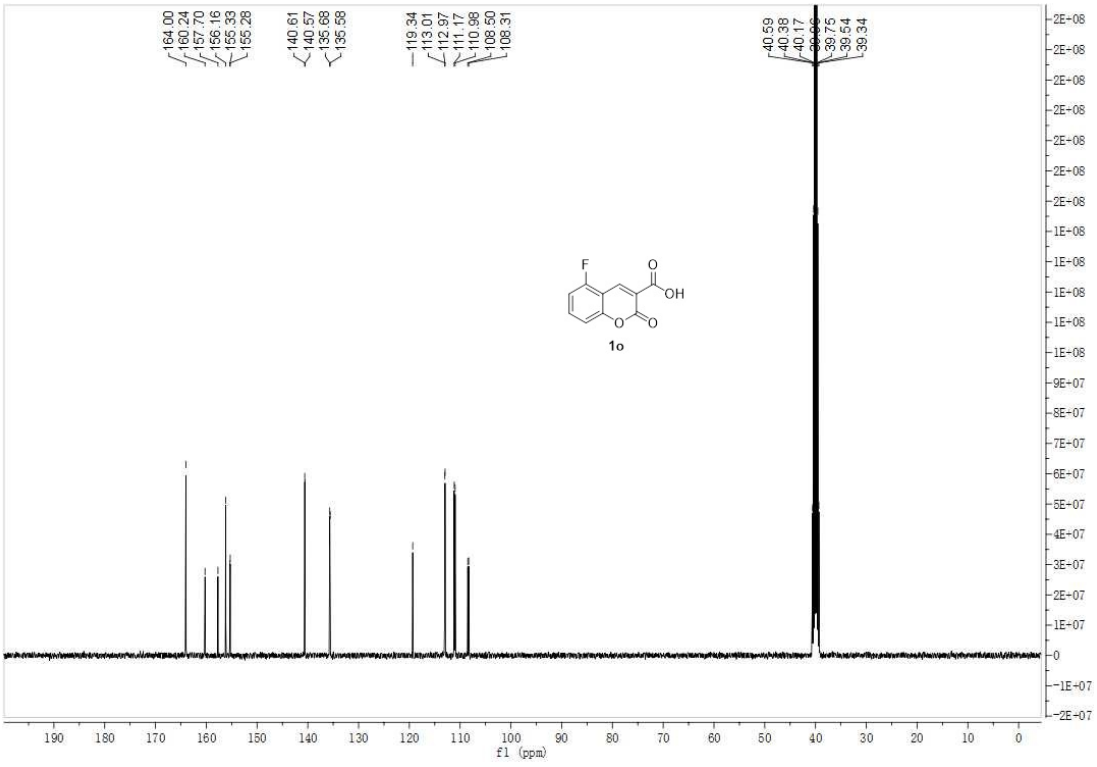
1.02
1.03
2.04
f1 (ppm)

1o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160.24
157.70
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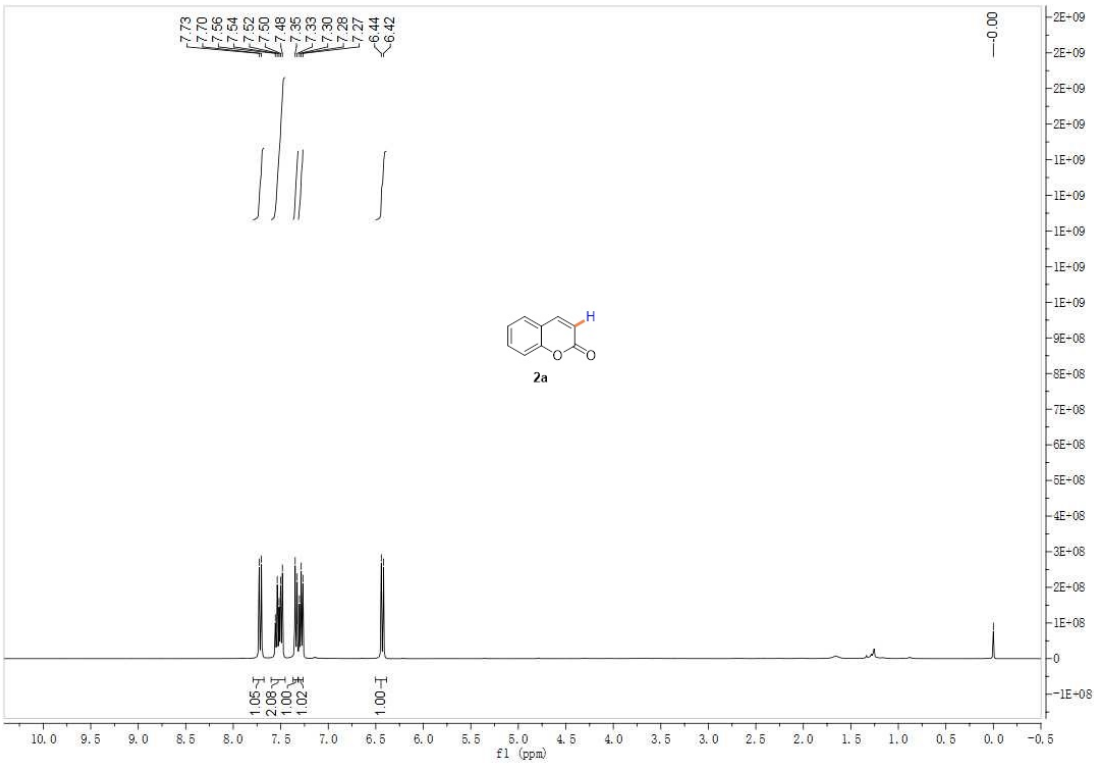
155.33
155.28
140.61
140.57
135.68
135.58
119.34
113.01
112.97
111.17
110.98
108.50
108.31
40.59
40.38
40.17
39.75
39.54
39.34
f1 (ppm)

1o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7.50
7.48
7.35
7.33
7.30
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7.27
6.44
6.42
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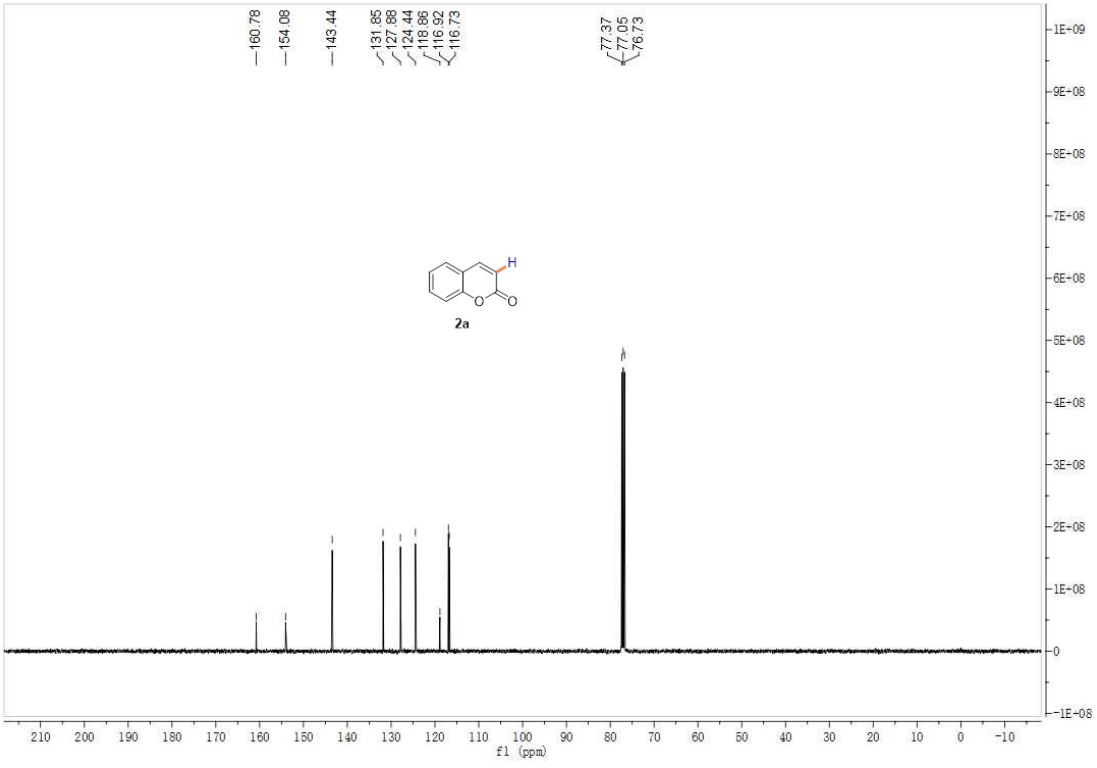
2.08
1.00
1.02
1.00
f1 (ppm)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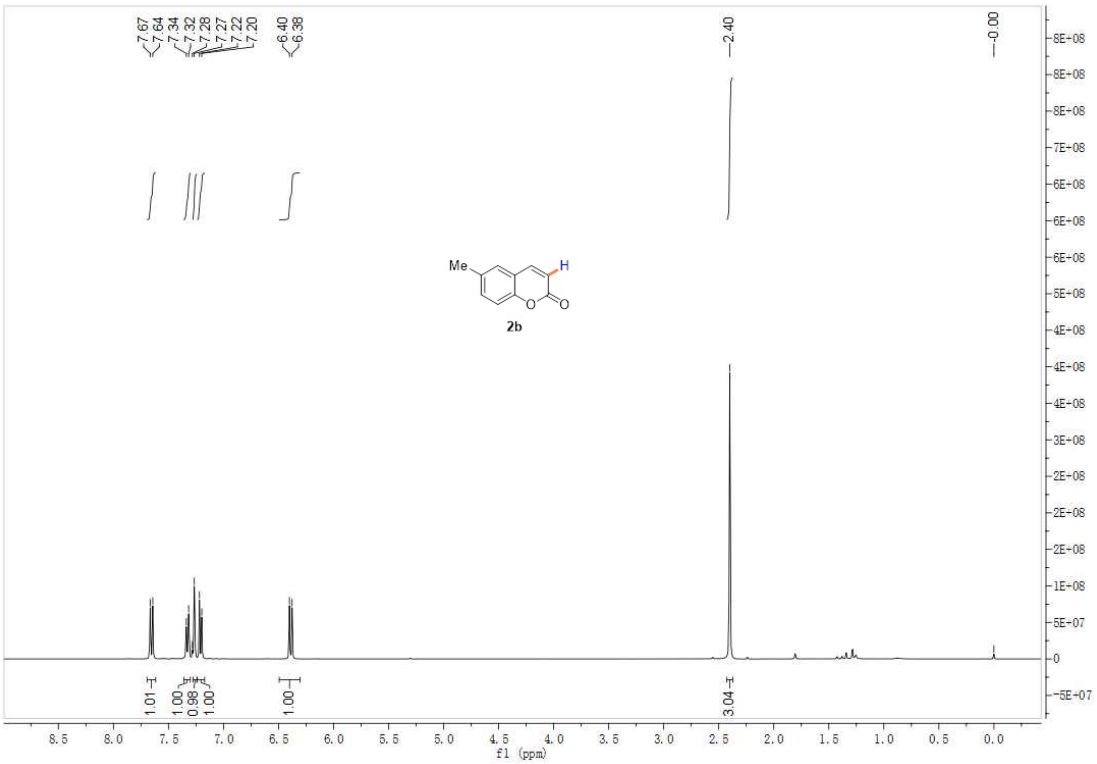
127.88
124.44
118.86
116.92
116.73
77.37
77.05
76.73
2a
f1 (ppm)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7.64
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7.32
7.28
7.27
7.22
7.20
6.40
6.38
2.40
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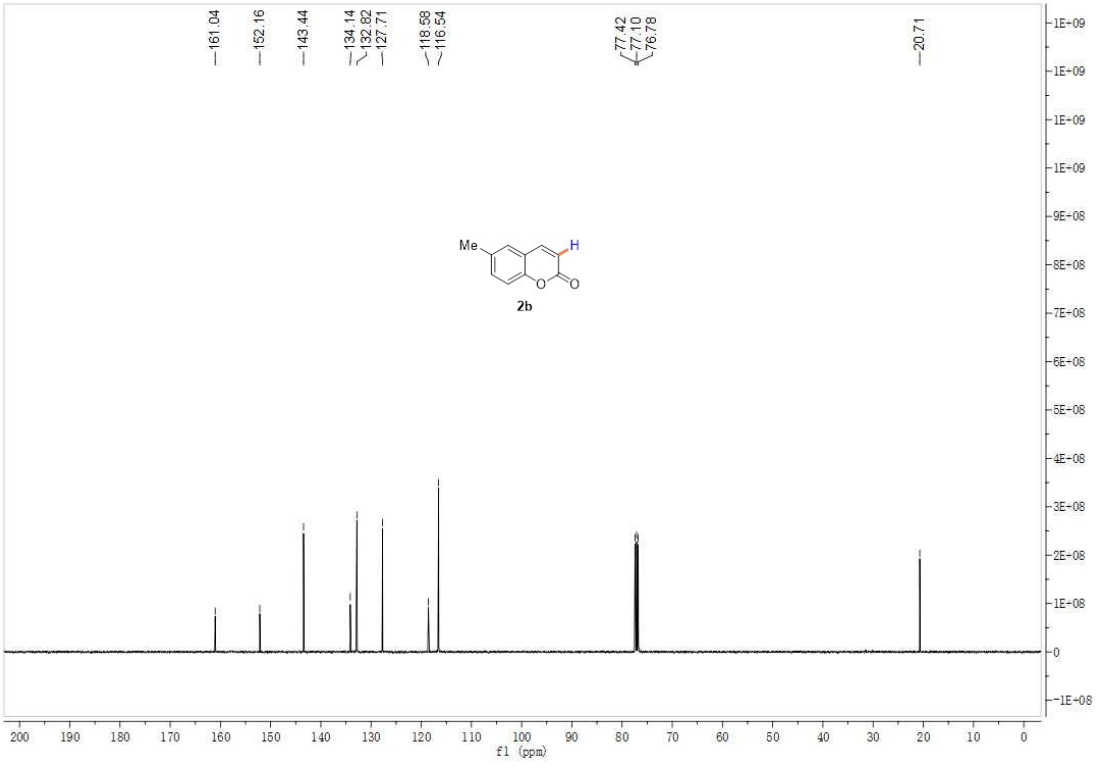
H
O
O
2b
1.01
1.00
0.98
1.00
1.00
3.04
f1 (ppm)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143.44
134.14
132.82
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77.10
76.78
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Me
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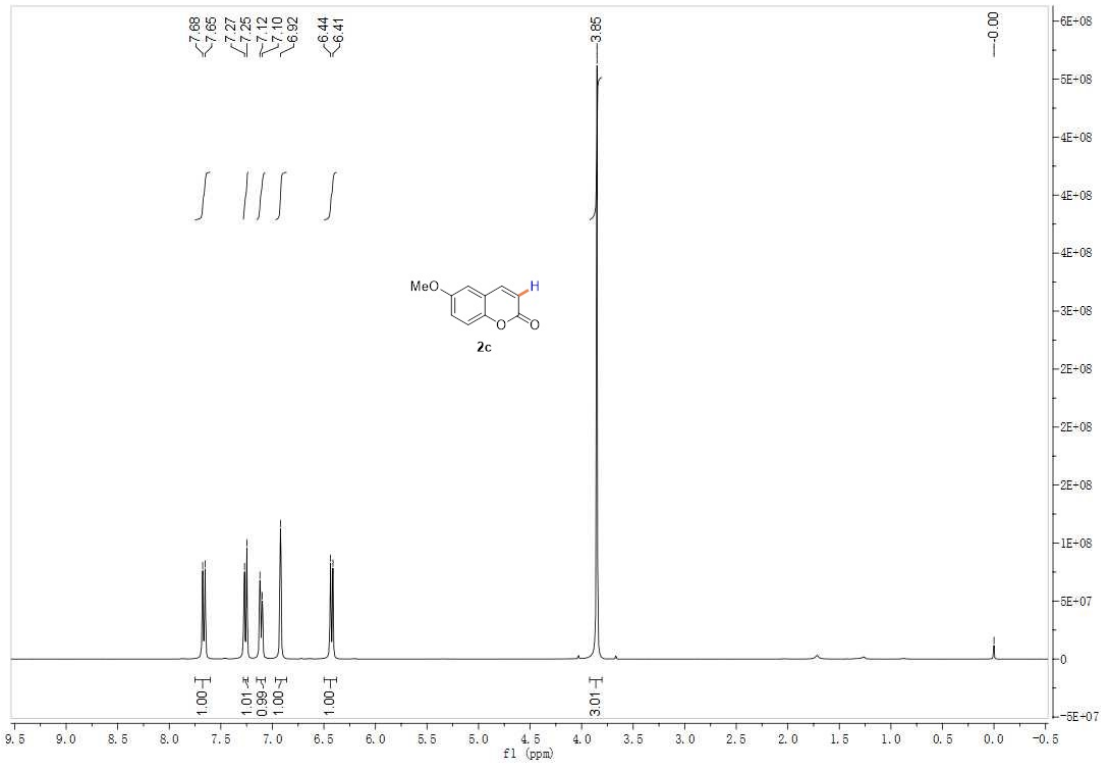
O
O
2b
f1 (ppm)


7.68
7.65
7.27
7.25
7.12
7.10
6.92
6.44
6.41
3.85
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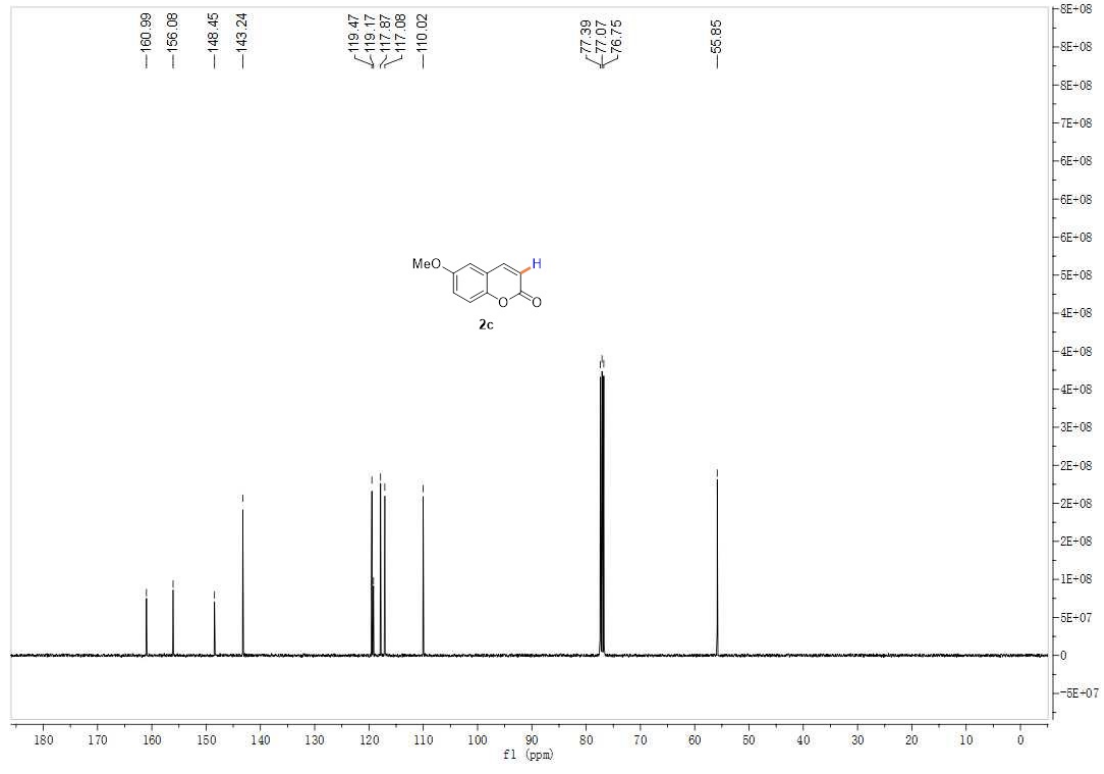
O
O
2c
1.00
1.01
0.99
1.00
1.00
3.01
f1 (ppm)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156.08
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119.17
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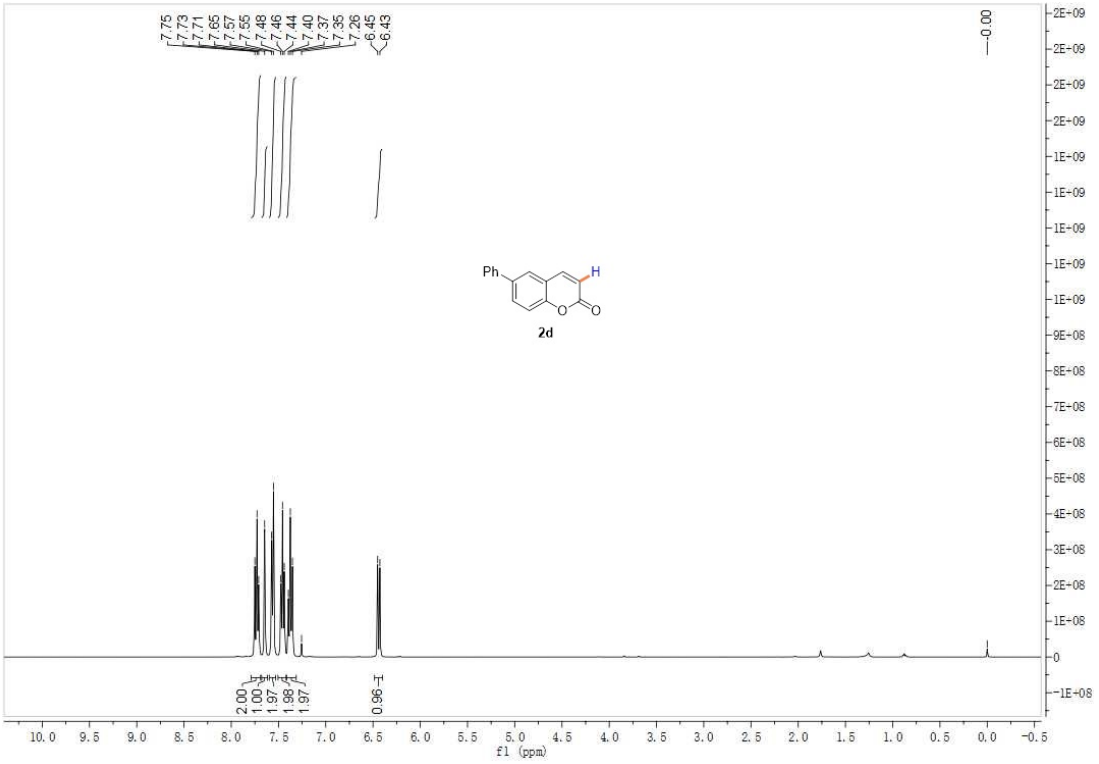
77.39
77.07
76.75
55.85
MeO
H
O
O
2c
f1 (ppm)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7.73
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7.55
7.48
7.46
7.44
7.40
7.37
7.35
7.26
6.45
6.43
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Ph
H
O
O
2d
2.00
1.00
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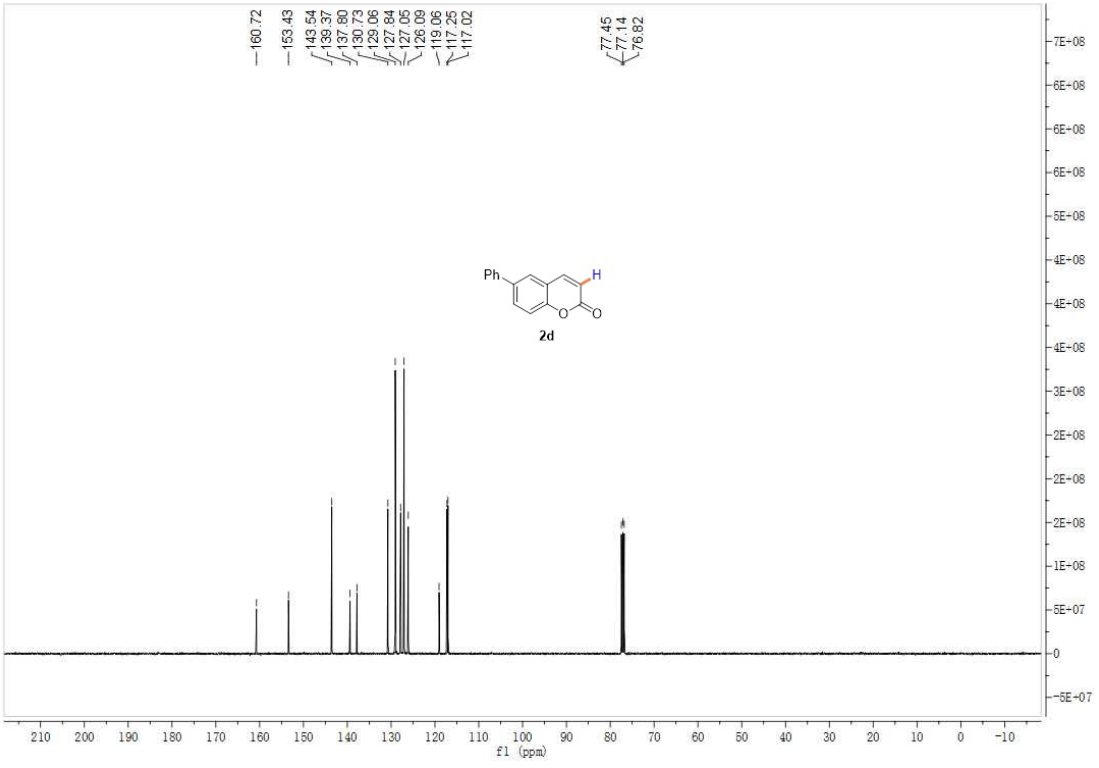
1.98
1.97
0.96
f1 (ppm)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130.73
129.06
127.84
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117.25
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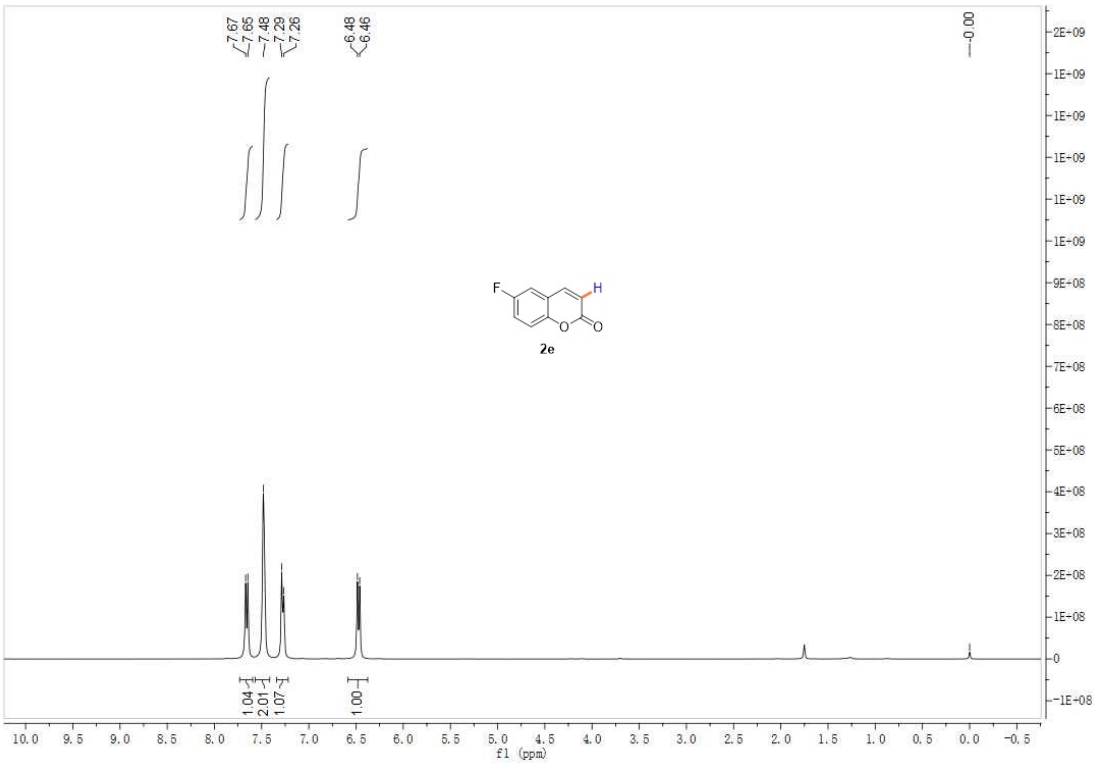
76.82
Ph
H
O
O
2d
f1 (ppm)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7.29
7.26
6.48
6.46
0.00
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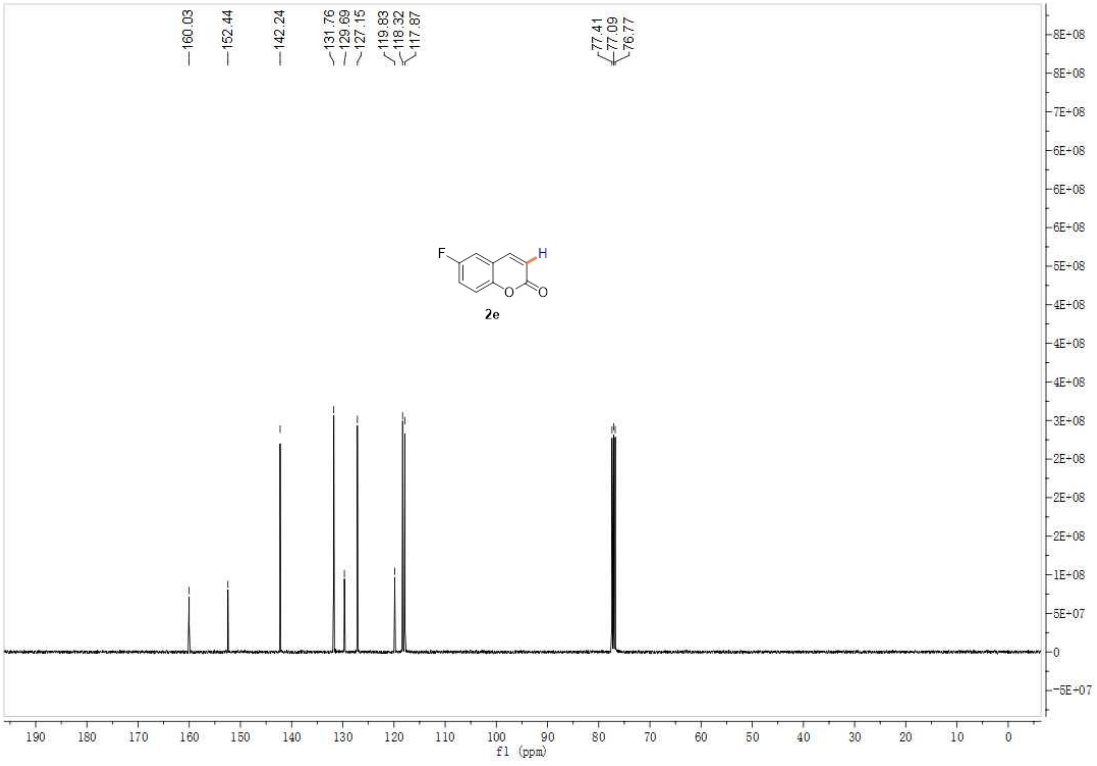
H
O
O
2e
1.04
2.01
1.07
1.00
f1 (ppm)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152.44
142.24
131.76
129.69
127.15
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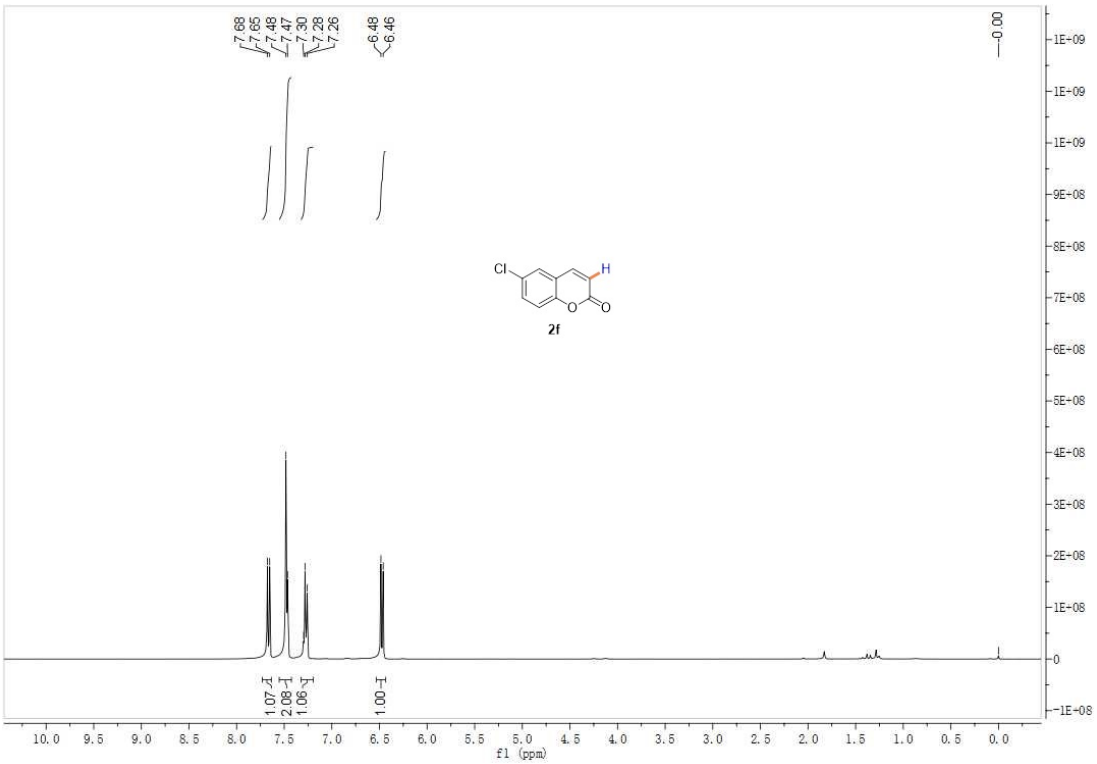
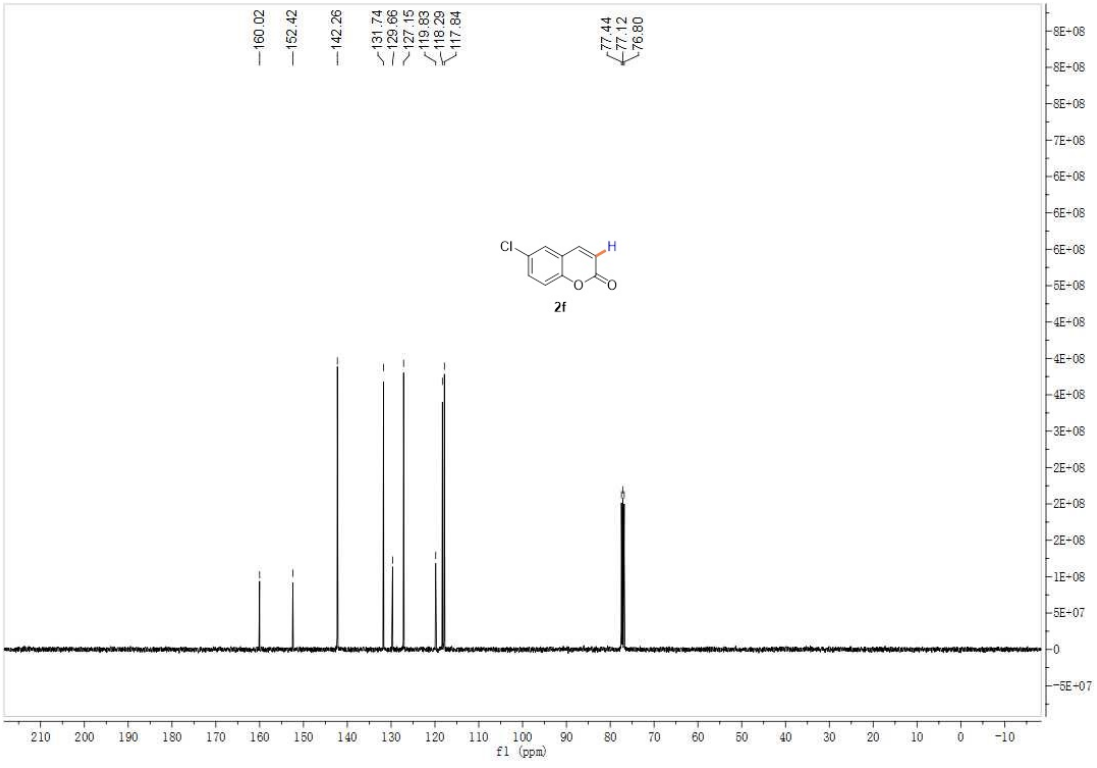
118.32
117.87
77.41
77.09
76.77
F
H
O
O
2e
f1 (ppm)


7.68
7.65
7.48
7.47
7.30
7.28
7.26
6.48
6.46
0.00
Cl
H
O
O
2f
1.07
2.08
1.06
1.00
f1 (ppm)


160.02
152.42
142.26
131.74
129.66
127.15
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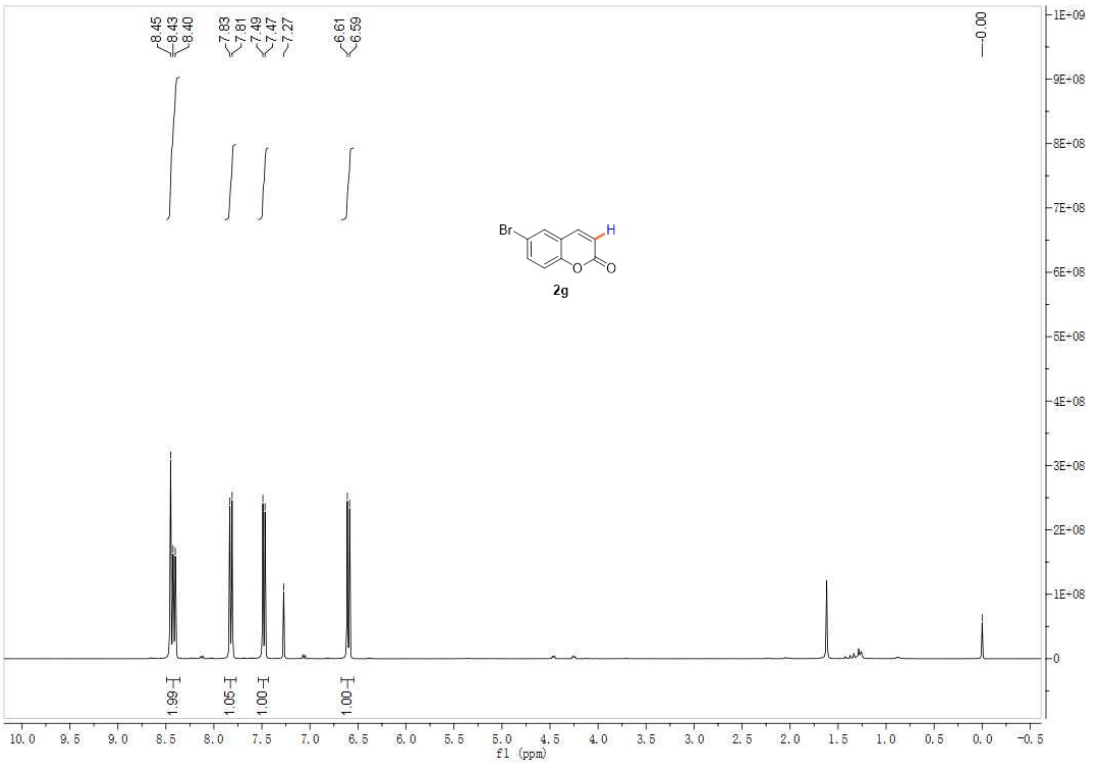
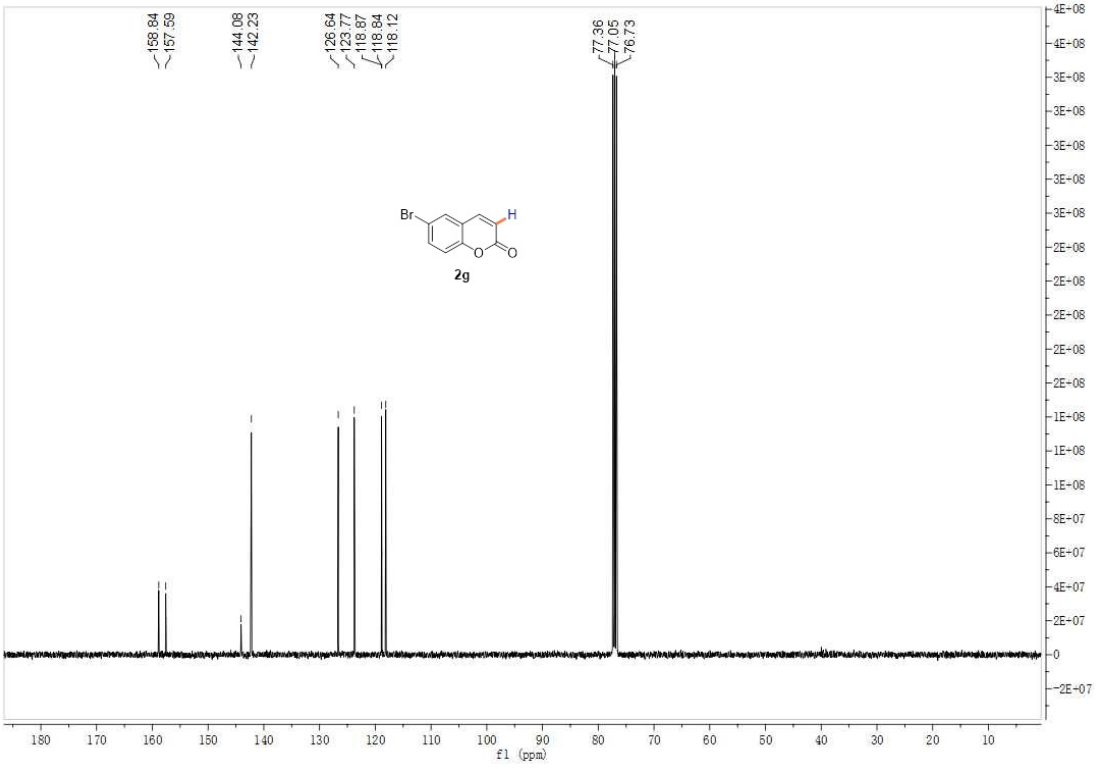
118.29
117.84
77.44
77.12
76.80
Cl
H
O
O
2f
f1 (ppm)


8.45
8.43
8.40
7.83
7.81
7.49
7.47
7.27
6.61
6.59
0.00
Br
H
O
O
2g
1.99
1.05
1.00
1.00
f1 (ppm)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157.59
144.06
142.23
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118.12
77.36
77.05
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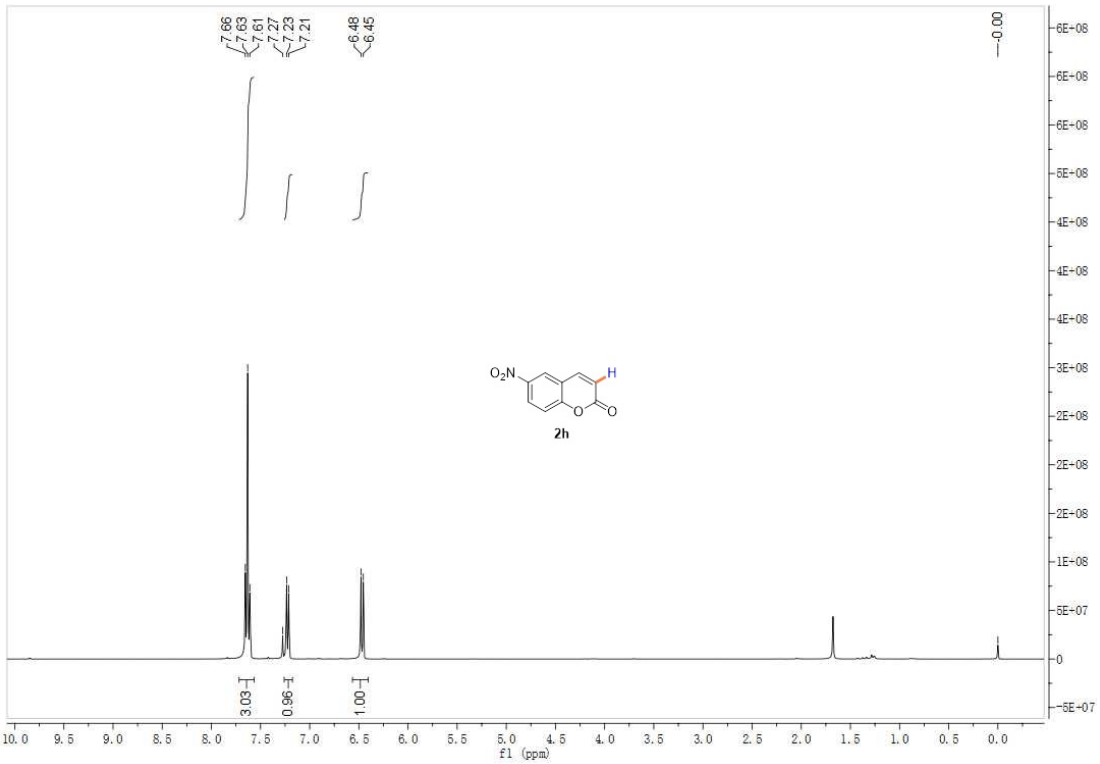
Br
H
O
O
2g
f1 (ppm)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7.63
7.61
7.27
7.23
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6.45
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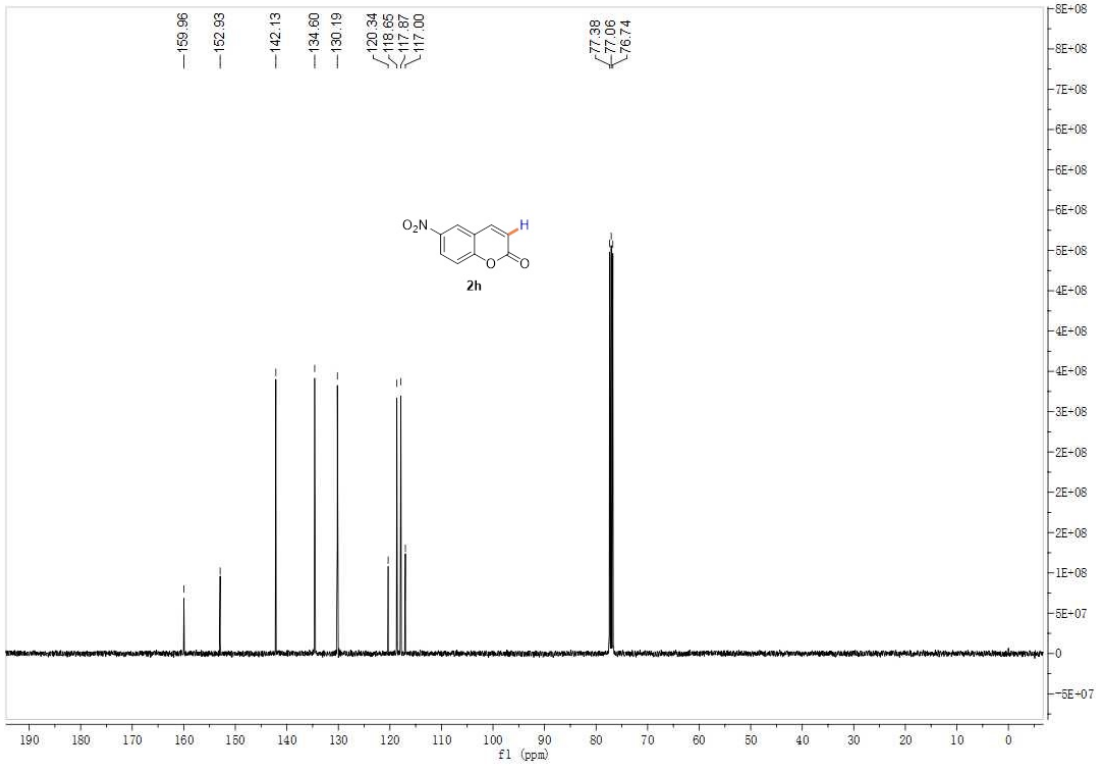
1.00
O2N
H
O
O
2h
f1 (ppm)


159.96
152.93
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134.60
130.19
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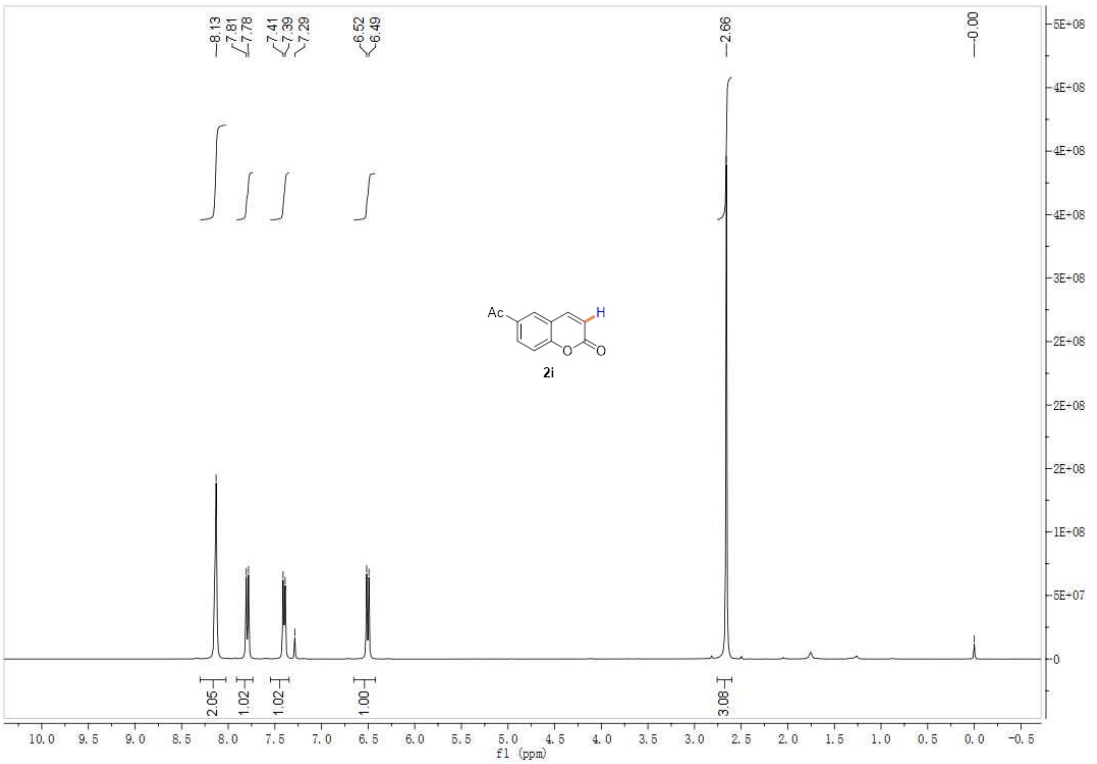
118.65
117.87
117.00
77.38
77.06
76.74
O2N
H
O
O
2h
f1 (ppm)


8.13
7.81
7.78
7.41
7.39
7.29
6.52
6.49
2.66
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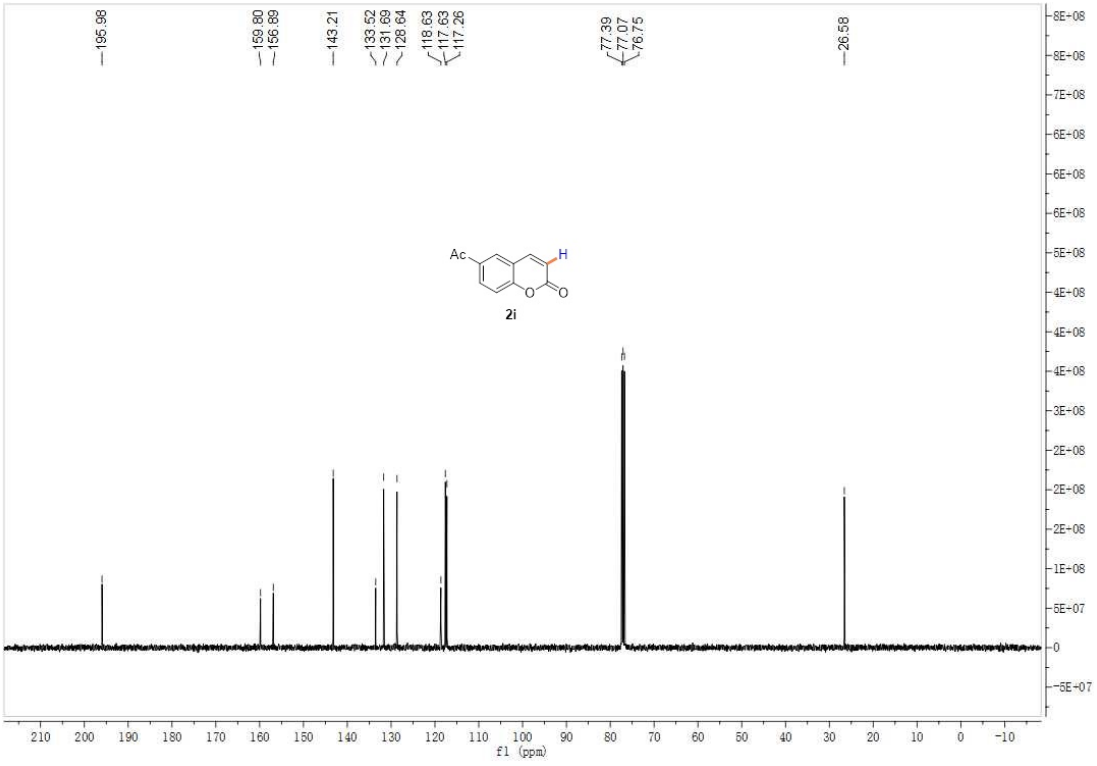
Ac
H
O
O
2i
2.05
1.02
1.02
1.00
3.08
f1 (ppm)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156.89
143.21
133.52
131.69
128.64
118.63
117.63
117.26
77.39
77.07
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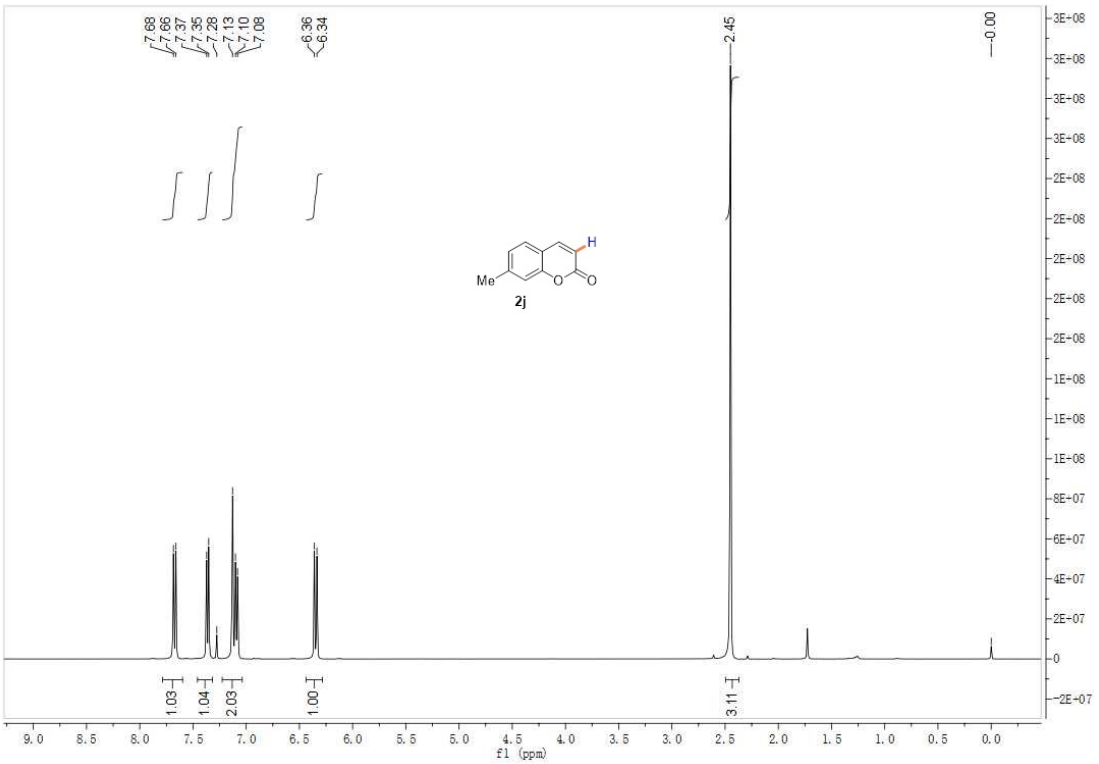
26.58
Ac
H
O
O
2i
f1 (ppm)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7.66
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7.35
7.28
7.13
7.10
7.08
6.36
6.34
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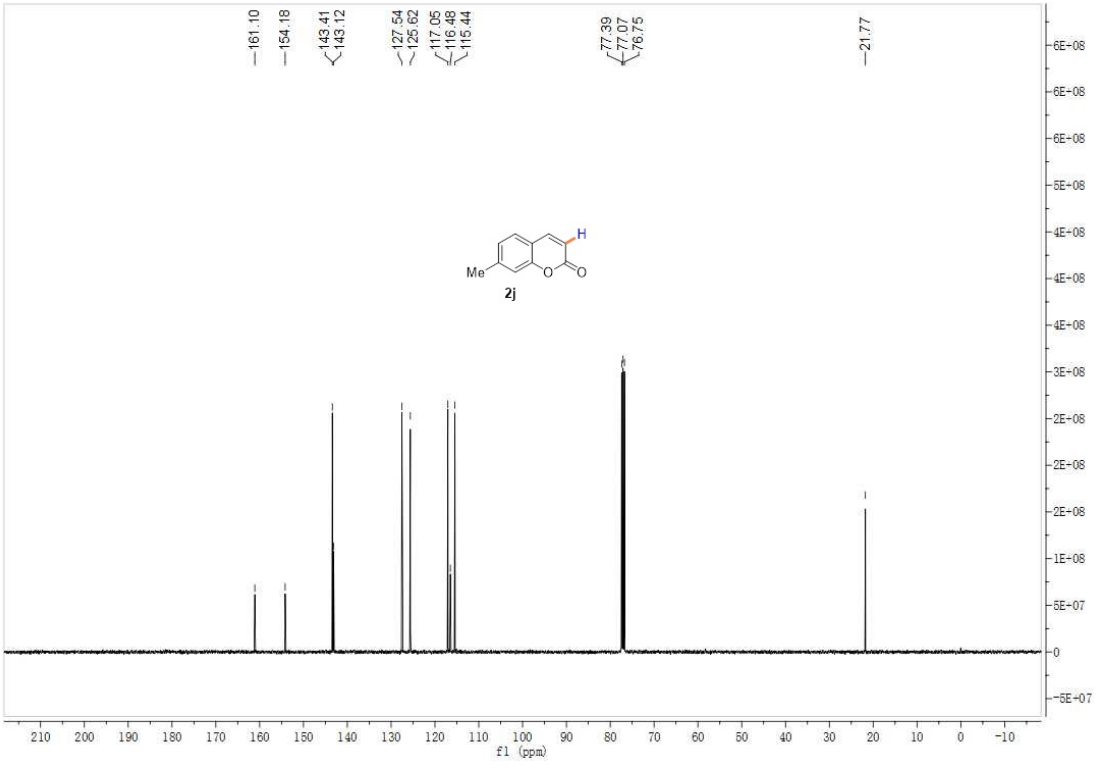
Me
O
O
H
2j
1.03
1.04
2.03
1.00
3.11
f1 (ppm)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143.12
127.54
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115.44
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77.07
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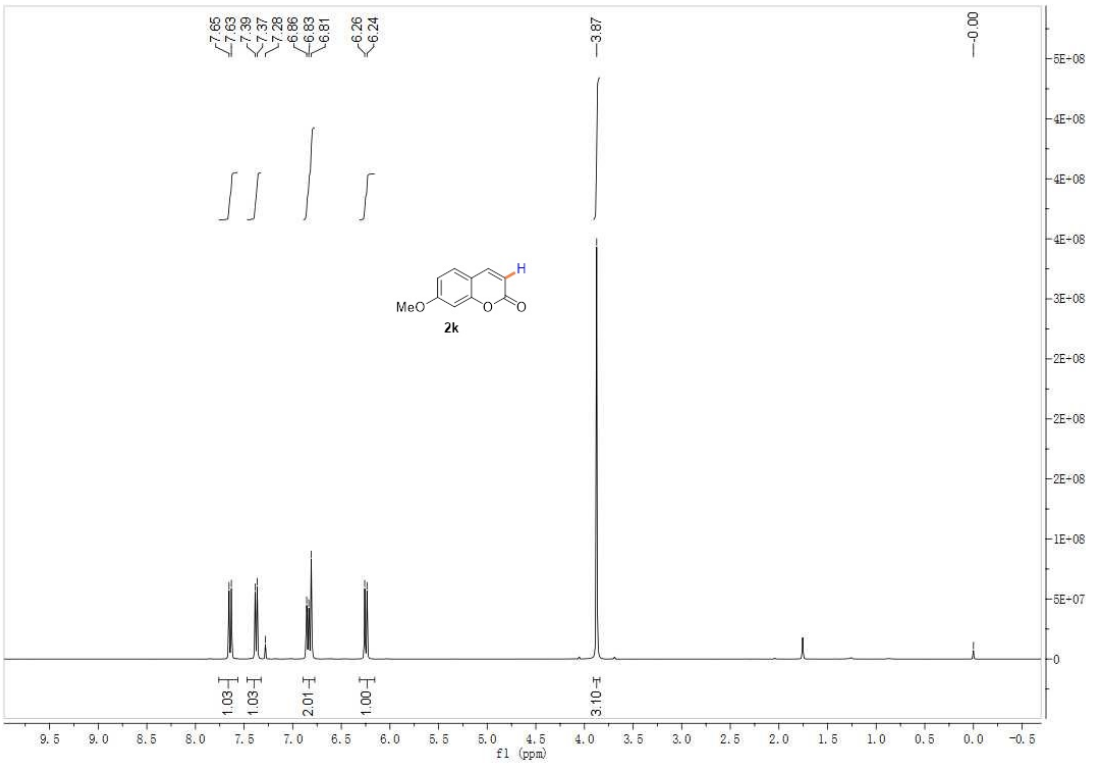
Me
O
O
H
2j
f1 (ppm)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7.37
7.28
6.86
6.83
6.81
6.26
6.24
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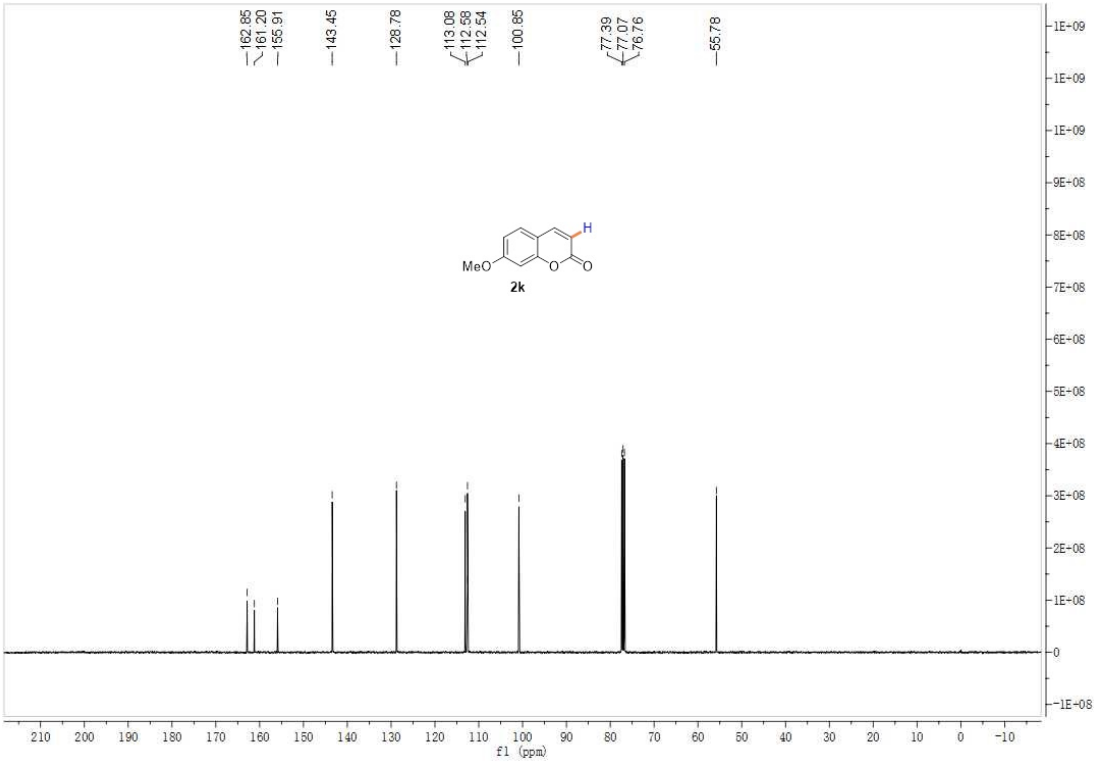
1.03
2.01
1.00
3.10
MeO
O
O
H
2k
f1 (ppm)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128.78
113.08
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77.07
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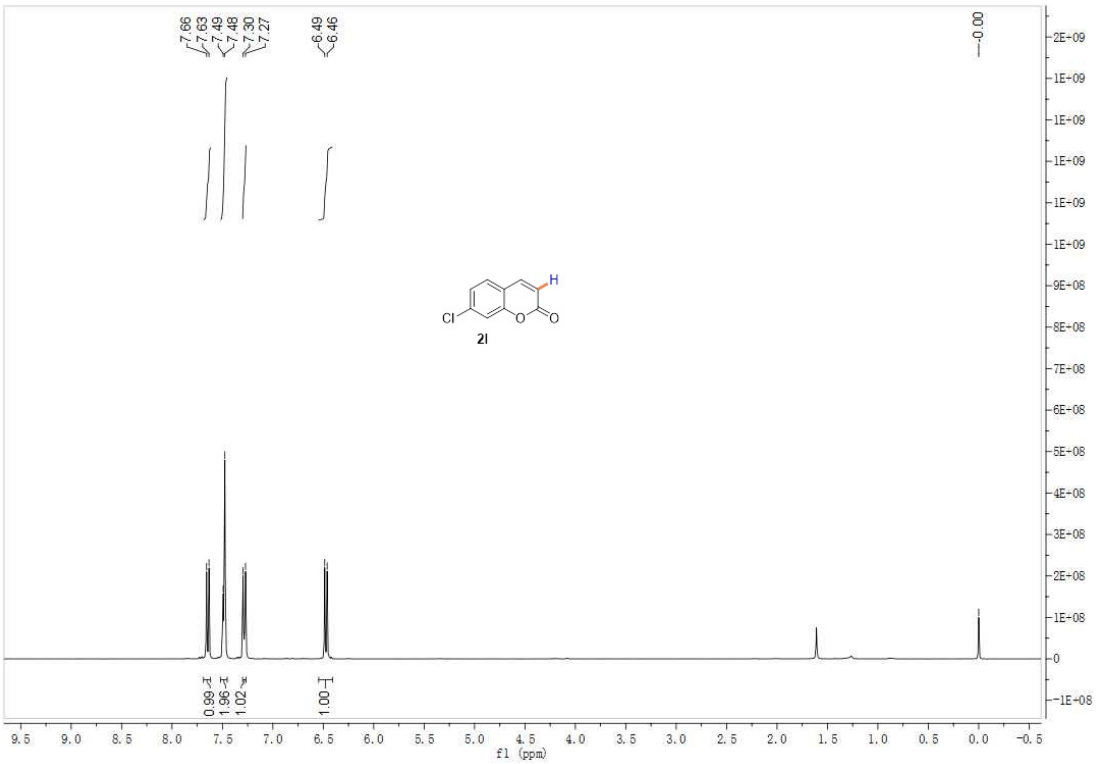
55.78
MeO
O
O
H
2k
f1 (ppm)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7.63
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7.48
7.30
7.27
6.49
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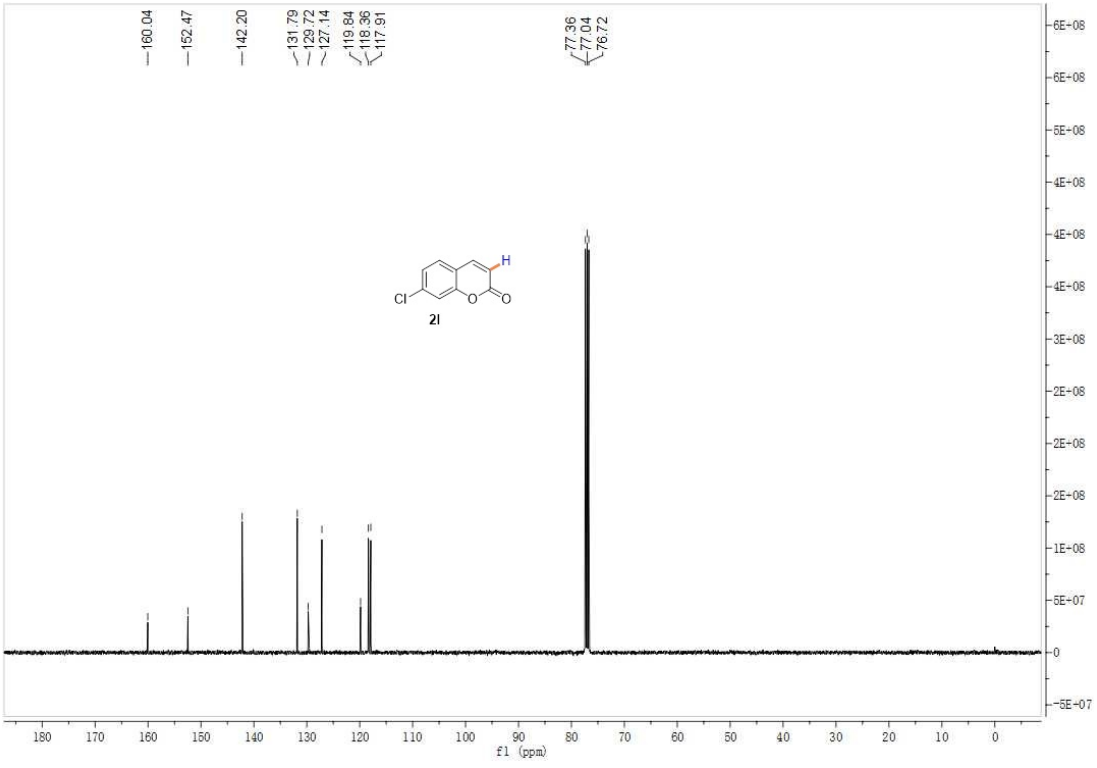
0.99
1.96
1.02
1.00
Cl
O
O
H
2l
f1 (ppm)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129.72
127.14
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118.36
117.91
77.36
77.04
76.72
Cl
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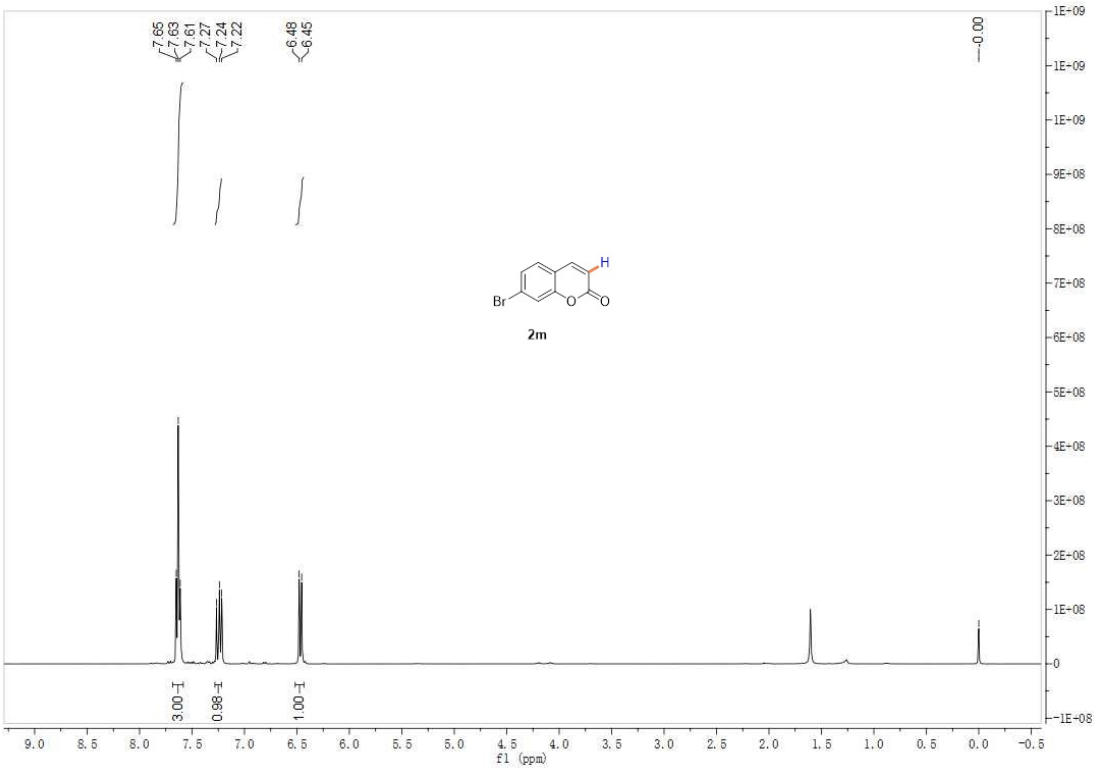
O
H
2l
f1 (ppm)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7.63
7.61
7.27
7.24
7.22
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6.45
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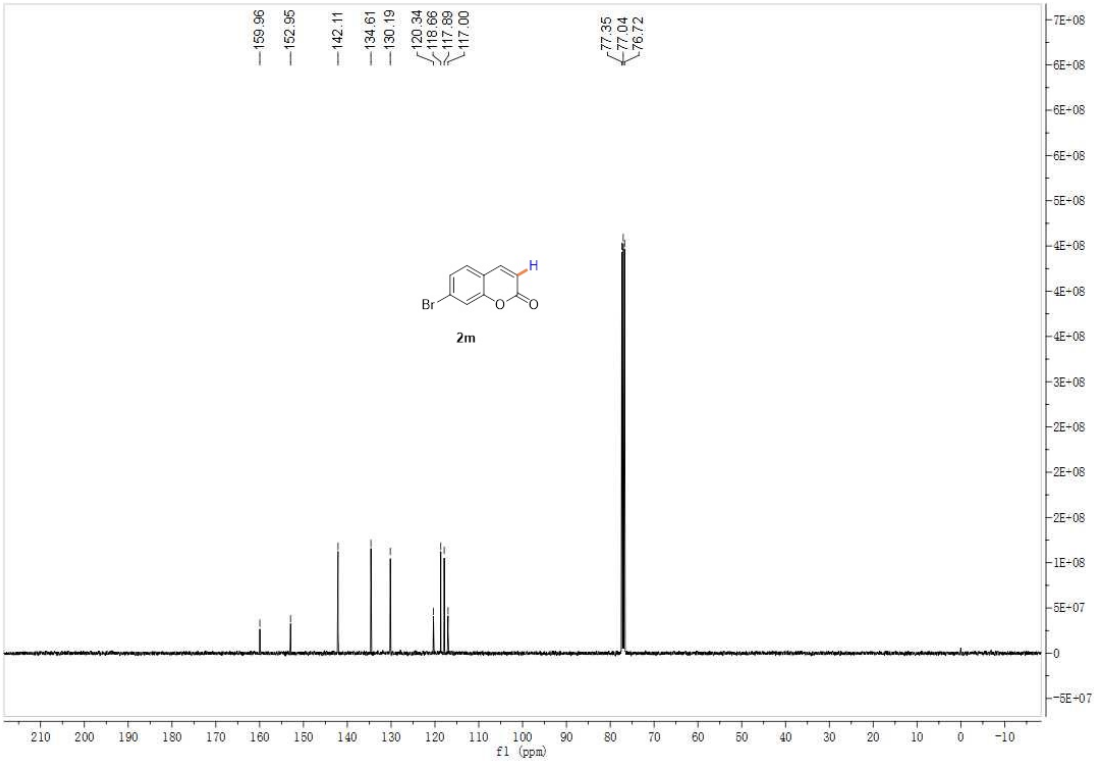
Br
O
O
H
2m
3.00
0.98
1.00
f1 (ppm)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142.11
134.61
130.19
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117.00
77.35
77.04
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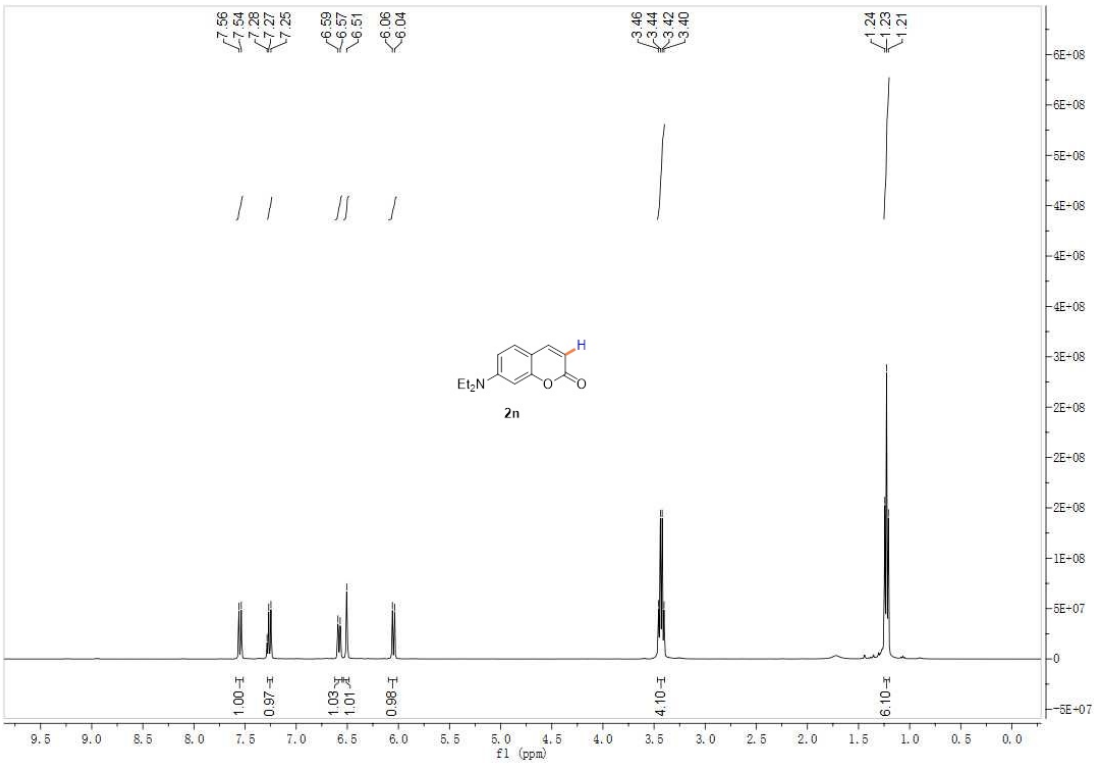
Br
O
O
H
2m
f1 (ppm)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7.25
6.59
6.57
6.51
6.06
6.04
3.46
3.44
3.42
3.40
1.24
1.23
1.21
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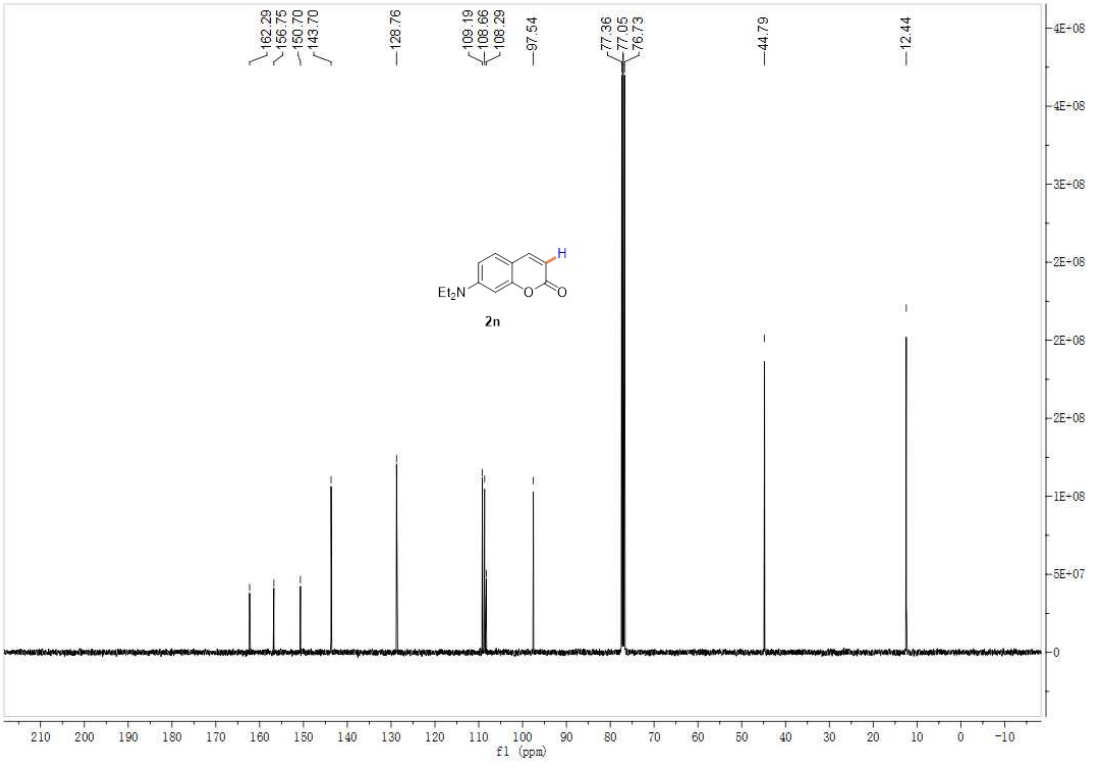
1.01
0.98
4.10
6.10
Et2N
O
O
H
2n
f1 (ppm)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128.76
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77.36
77.05
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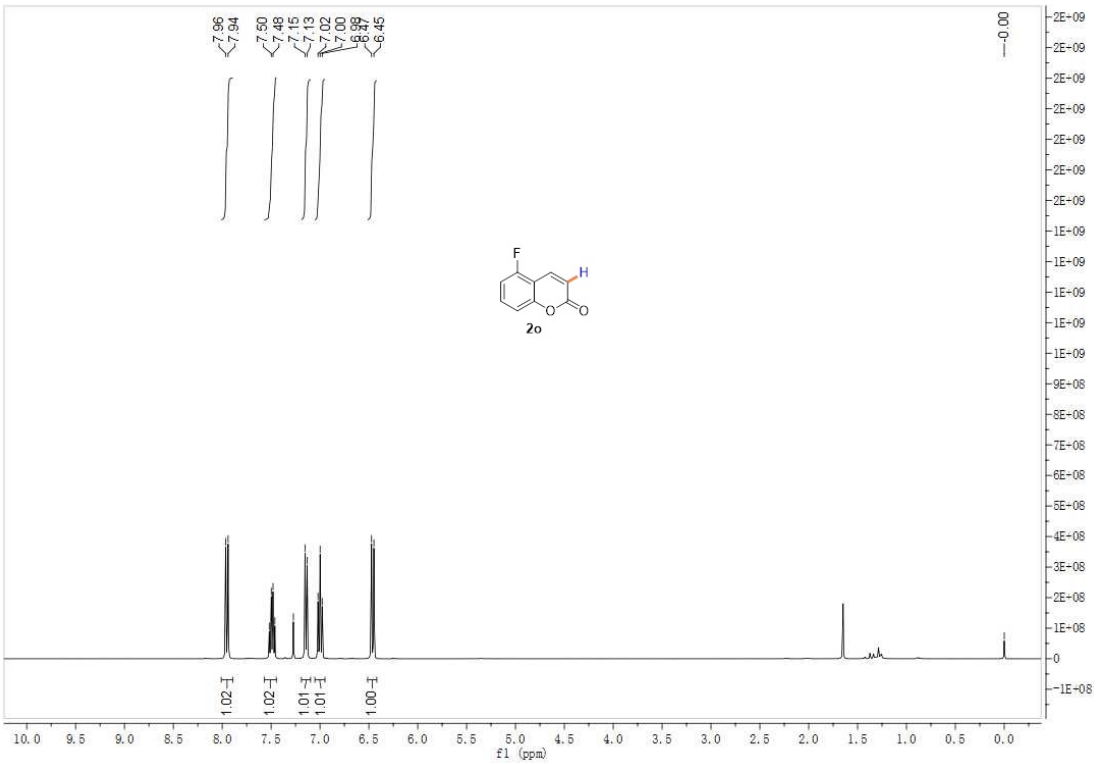
12.44
Et2N
O
O
H
2n
f1 (ppm)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7.48
7.15
7.13
7.02
7.00
6.45
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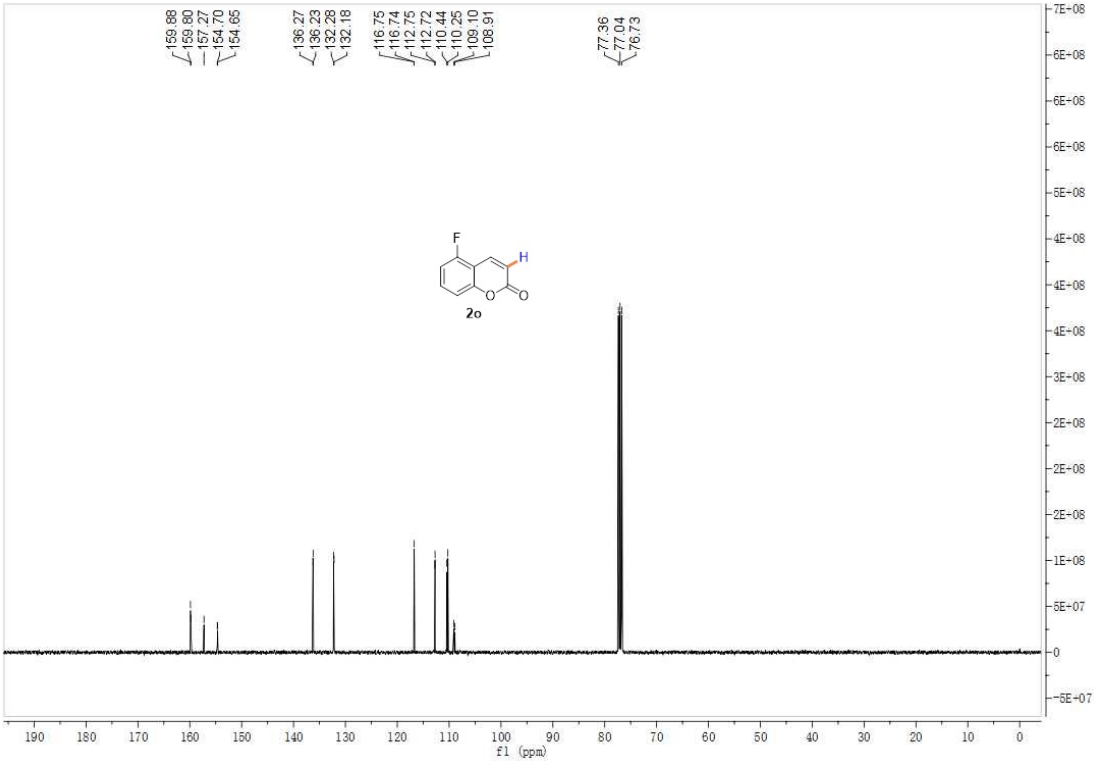
F
H
O
O
2o
1.02
1.02
1.01
1.01
1.00
fl (ppm)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132.28
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116.74
112.75
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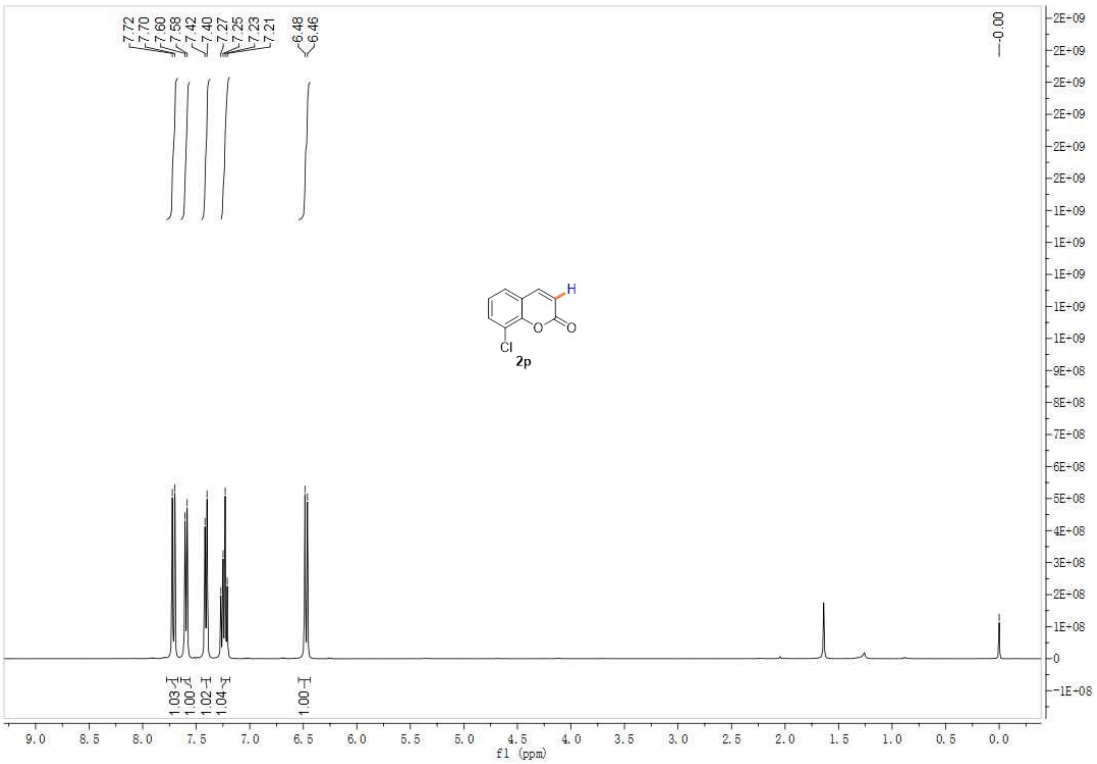
110.25
109.10
108.91
77.36
77.04
76.73
F
H
O
O
2o
fl (ppm)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7.40
7.27
7.25
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6.46
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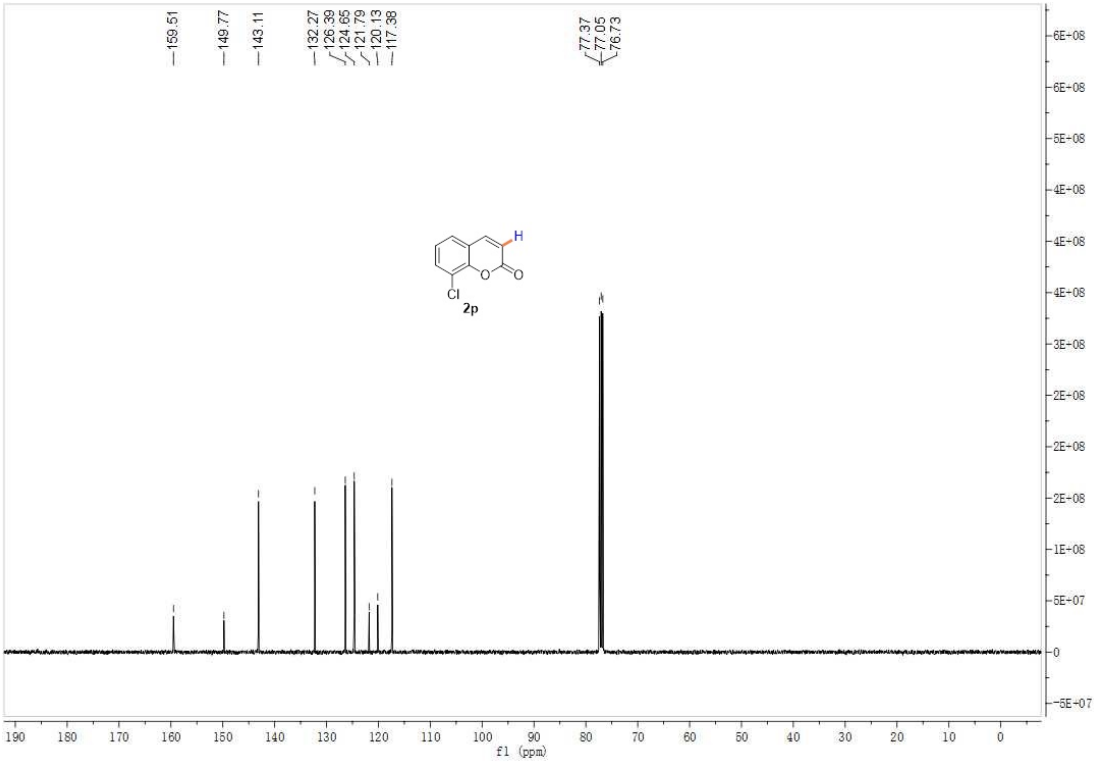
1.00
1.02
1.04
1.00
2p
f1 (ppm)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124.65
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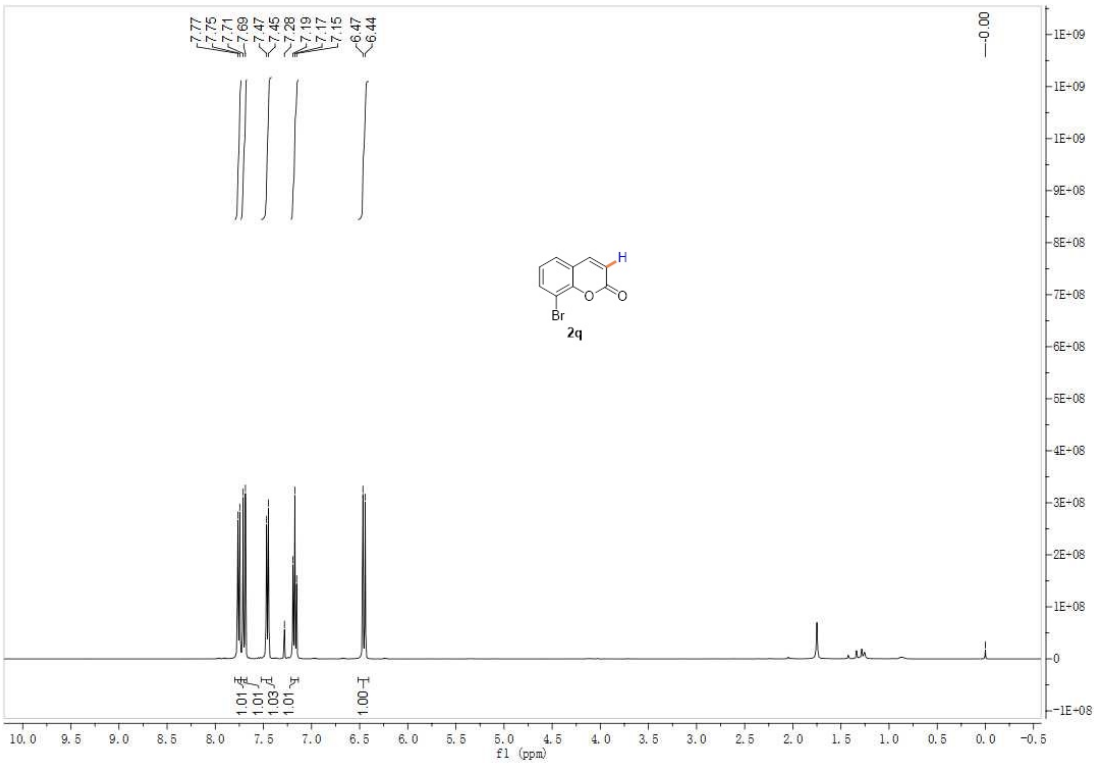
120.13
117.38
77.37
77.05
76.73
2p
f1 (ppm)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7.69
7.47
7.45
7.28
7.19
7.17
7.15
6.47
6.44
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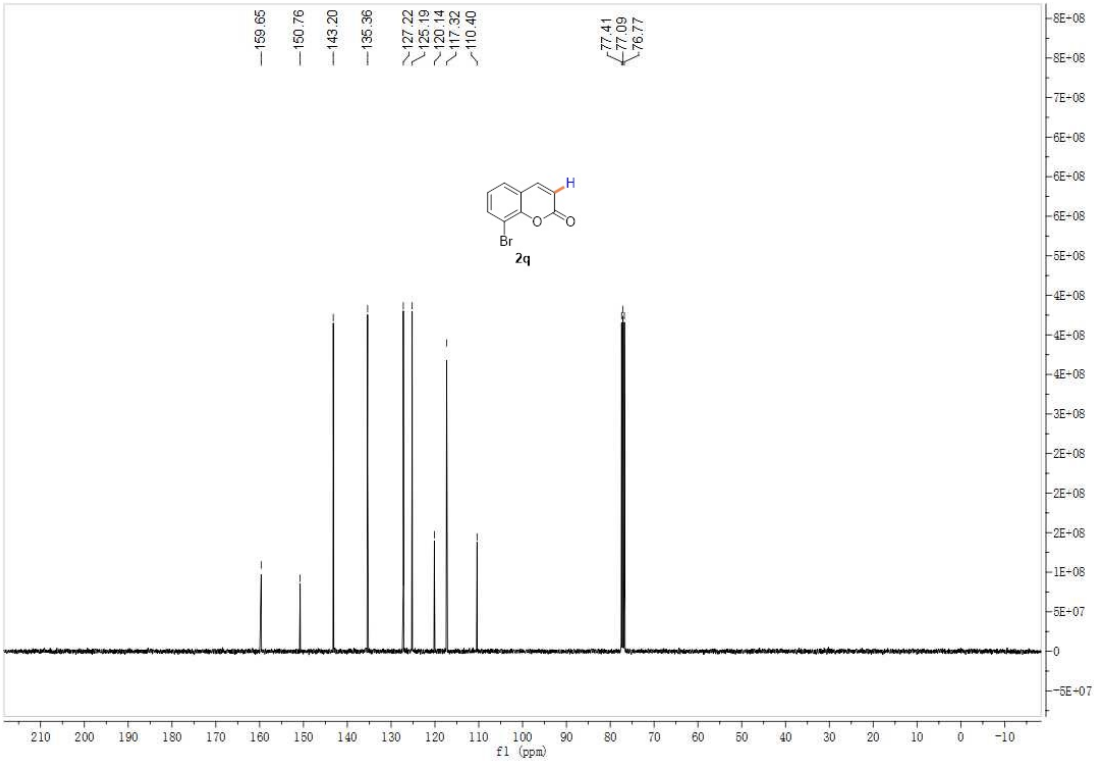
H
O
O
Br
2q
1.01
1.01
1.03
1.01
1.00
f1 (ppm)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135.36
127.22
125.19
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117.32
110.40
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77.09
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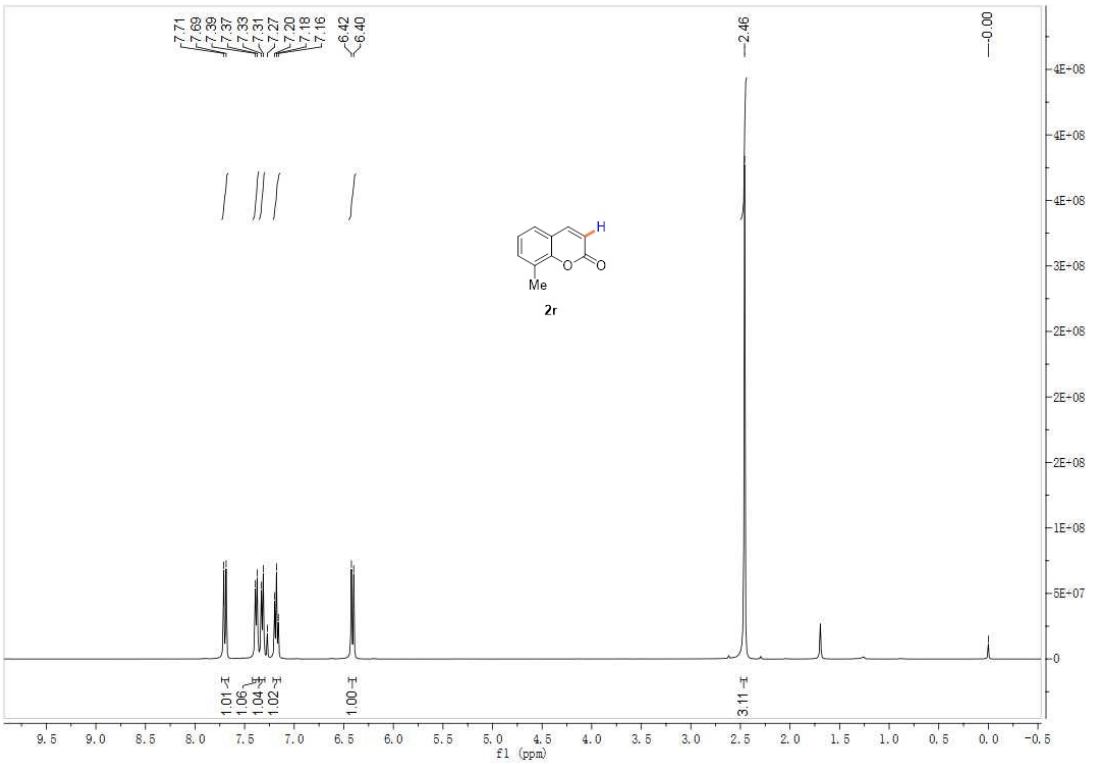
O
O
Br
2q
f1 (ppm)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7.33
7.31
7.27
7.20
7.18
7.16
6.42
6.40
2.46
0.00
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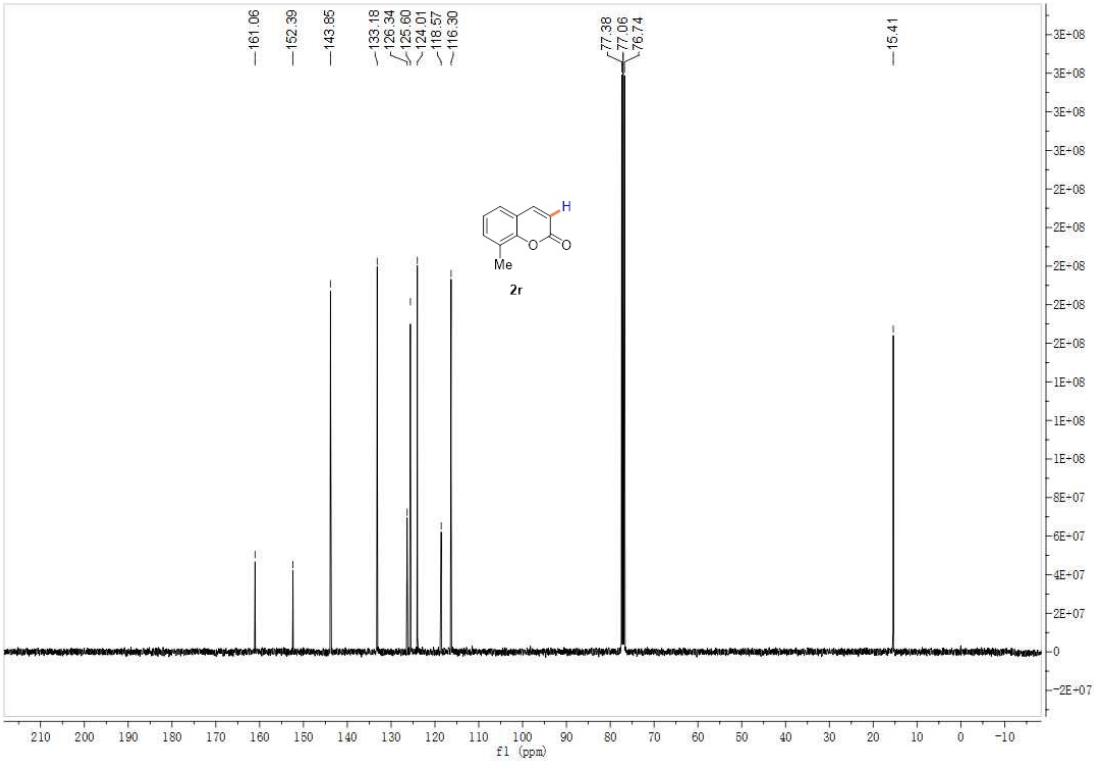
O
O
Me
2r
1.01
1.06
1.04
1.02
1.00
3.11
f1 (ppm)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125.60
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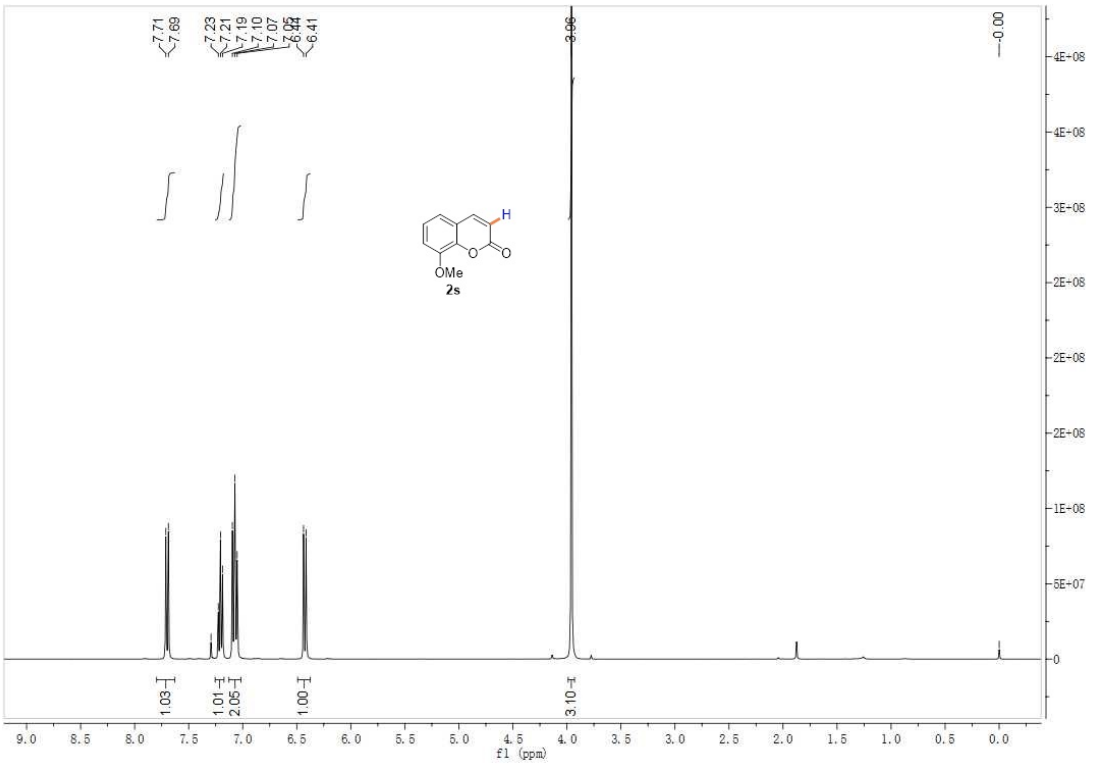
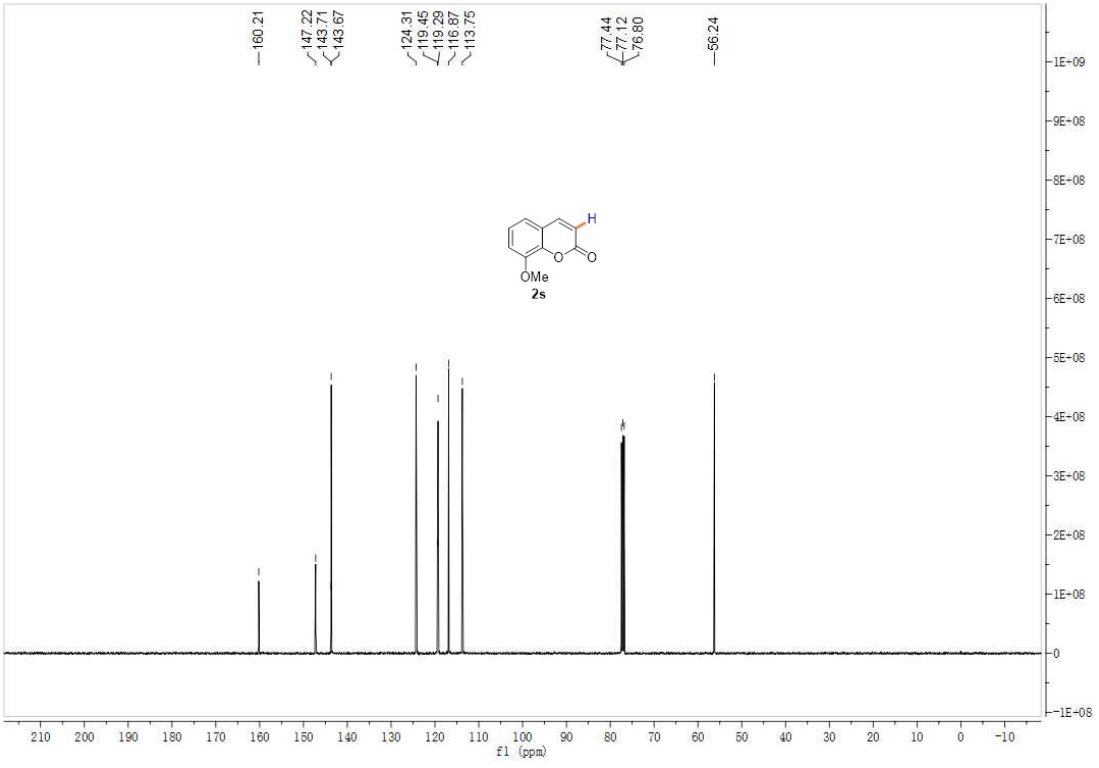
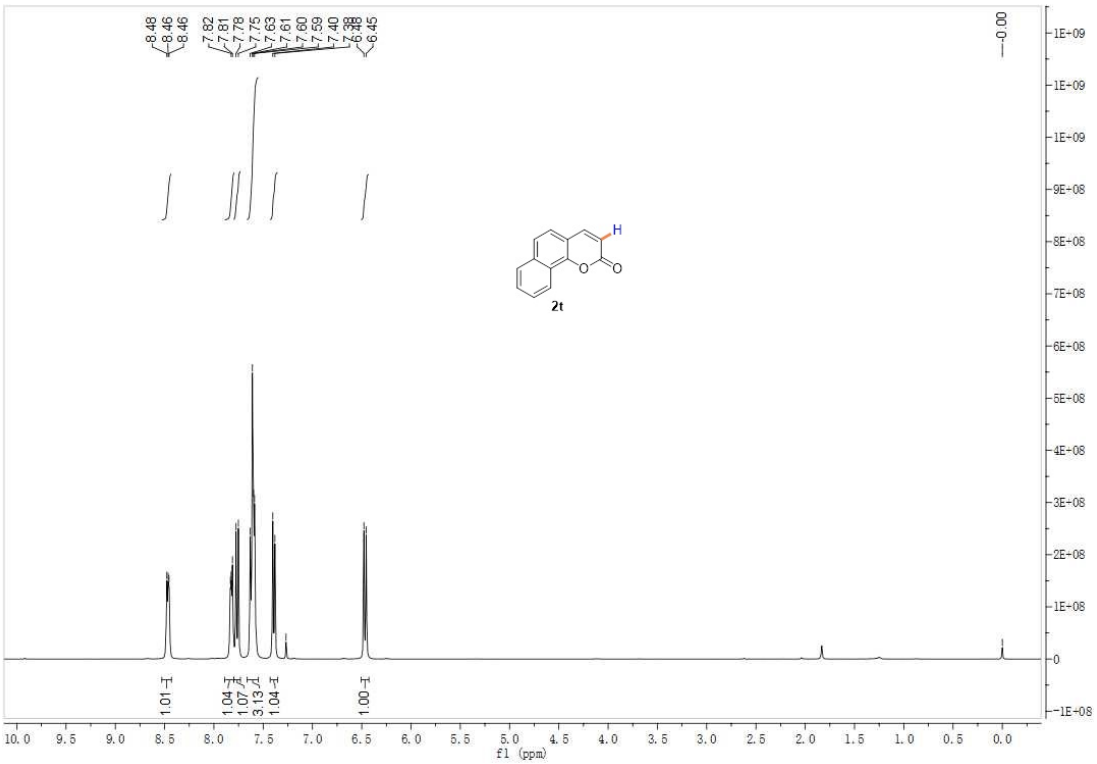
116.30
77.38
77.06
76.74
15.41
H
O
O
Me
2r
f1 (ppm)


7.71
7.69
7.23
7.21
7.19
7.10
7.07
6.42
6.41
3.96
0.00
OMe
2s
1.03
1.01
2.05
1.00
3.10
f1 (ppm)


160.21
147.22
143.71
143.67
124.31
119.45
119.29
116.87
113.75
77.44
77.12
76.80
56.24
OMe
2s
f1 (ppm)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7.81
7.78
7.75
7.63
7.61
7.60
7.59
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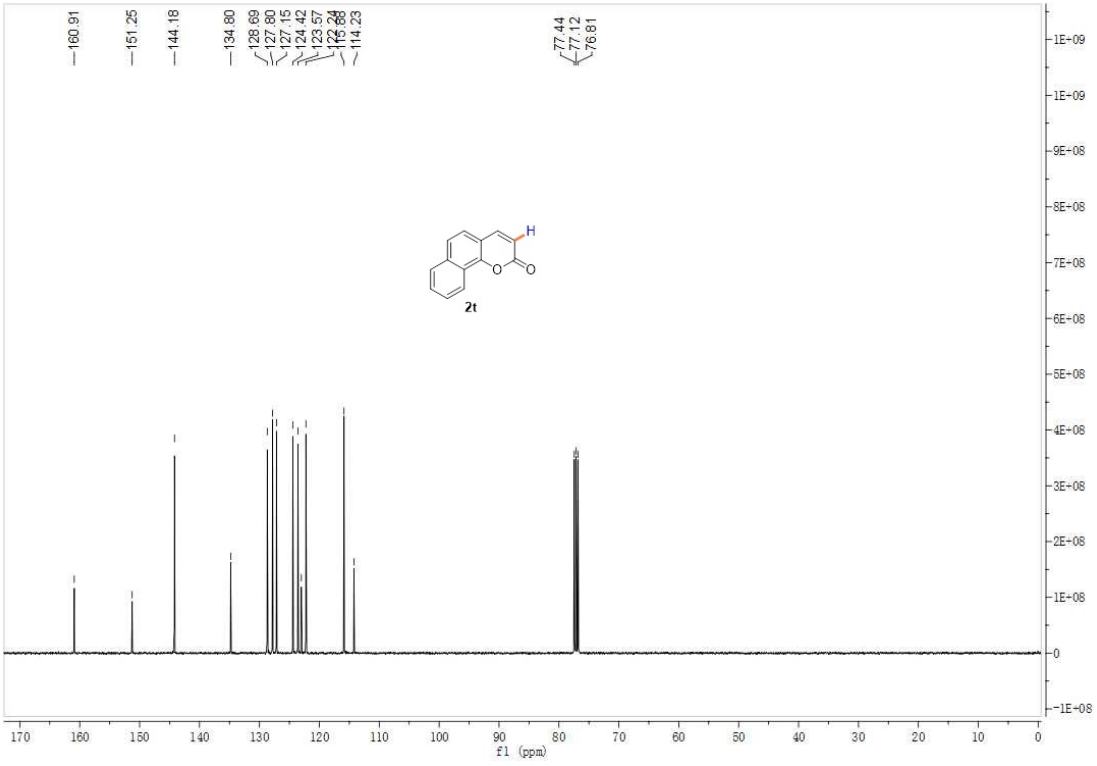
6.45
0.00
2t
1.01
1.04
1.07
3.13
1.04
1.00
f1 (ppm)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127.80
127.15
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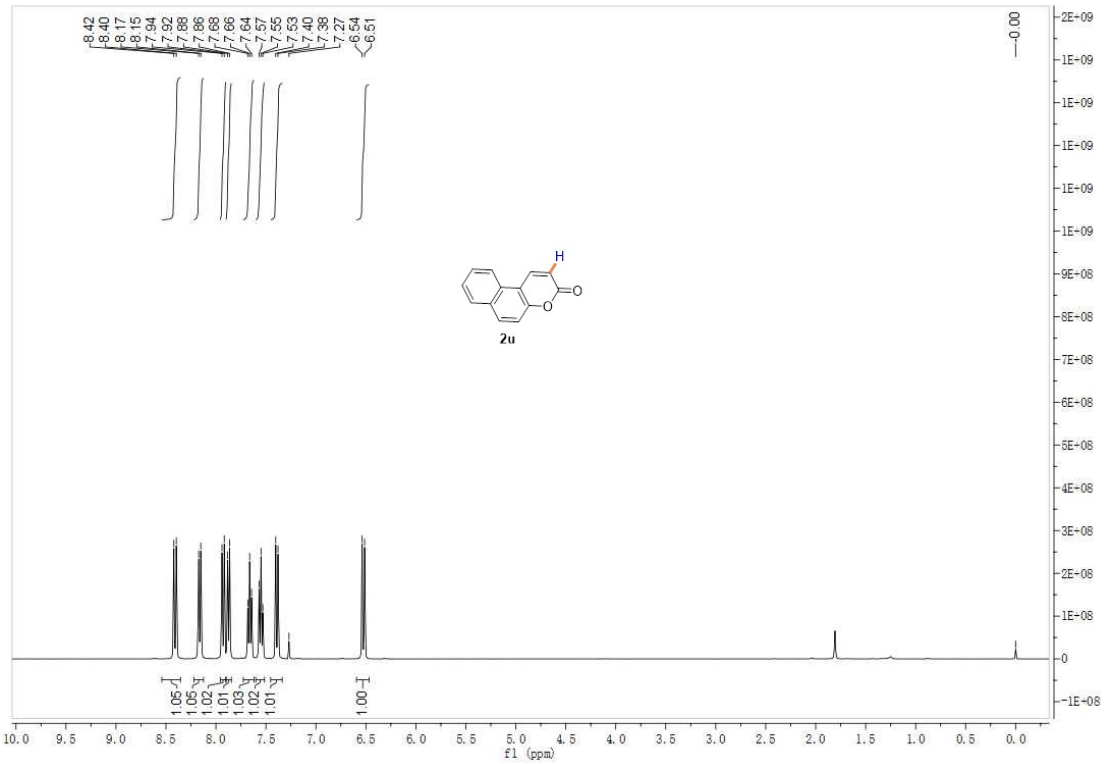
123.57
114.23
77.44
77.12
76.81
2t
f1 (ppm)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8.15
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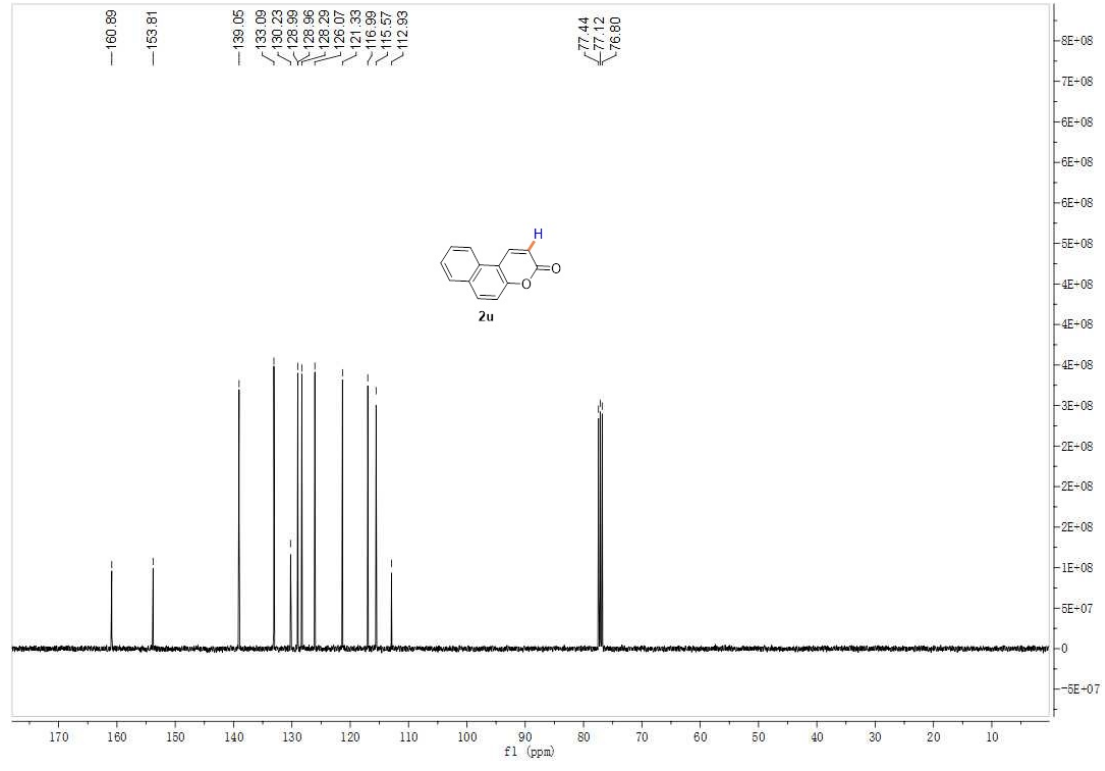
7.92
7.88
7.86
7.68
7.66
7.64
7.57
7.55
7.53
7.40
7.38
7.27
6.54
6.51
0.00
H
O
O
2u
1.05
1.05
1.02
1.01
1.03
1.02
1.01
1.00
f1 (ppm)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153.81
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133.09
130.23
128.99
128.96
128.29
126.07
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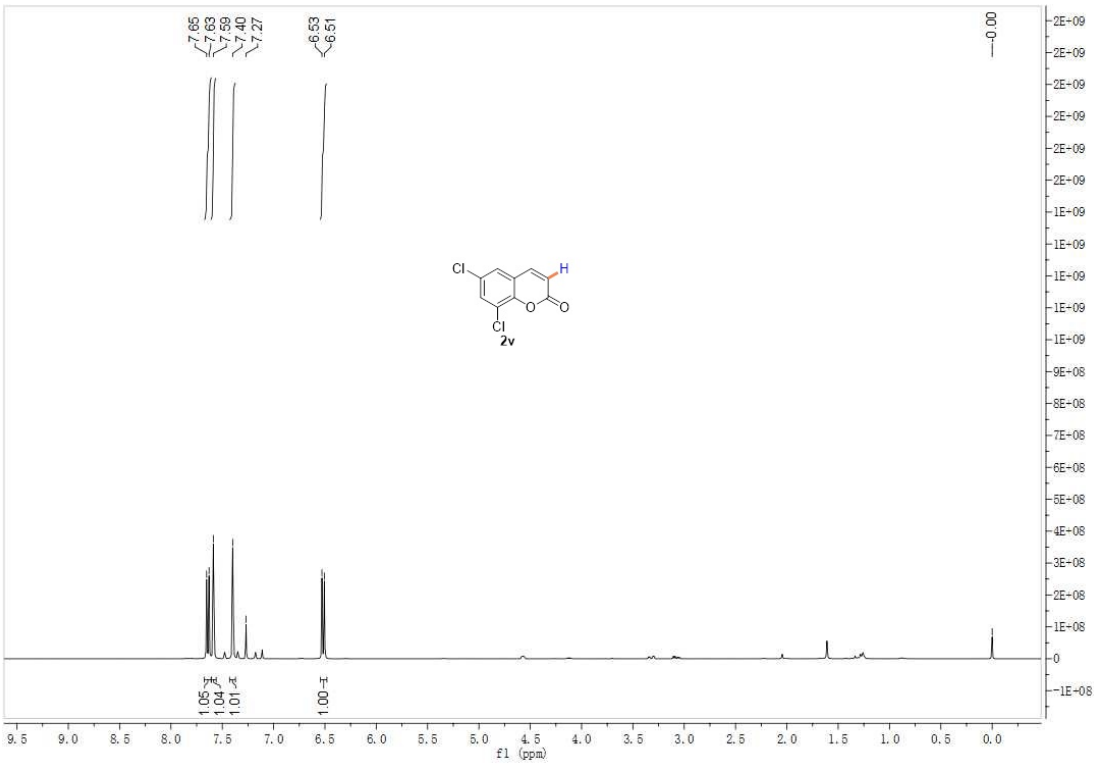
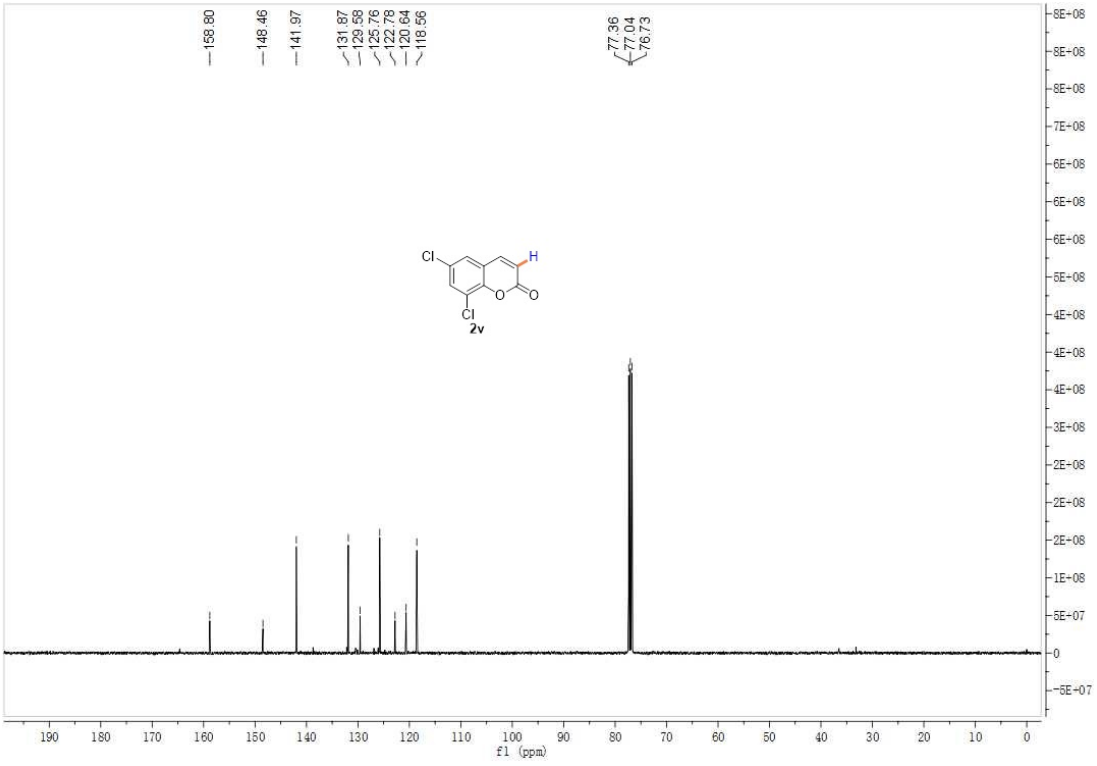
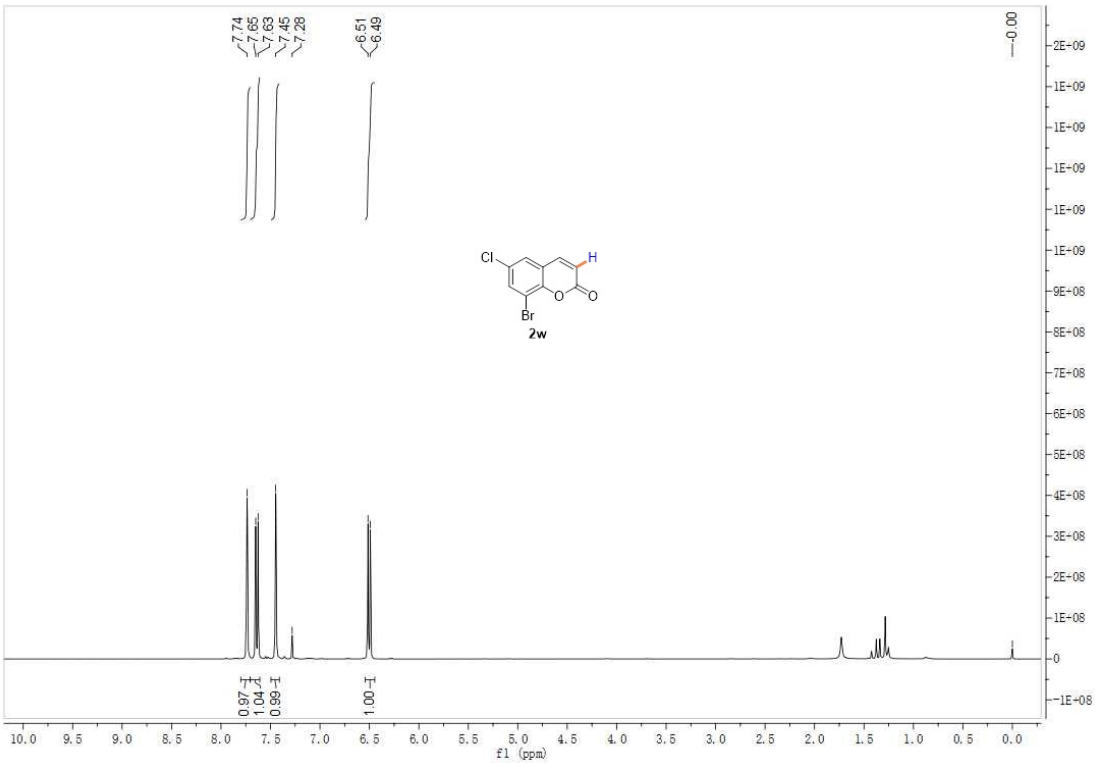
116.99
115.57
112.93
77.44
77.12
76.80
H
O
O
2u
f1 (ppm)


7.65
7.63
7.59
7.40
7.27
6.53
6.51
0.00
Cl
H
O
O
Cl
2v
1.05
1.04
1.01
1.00
f1 (ppm)


158.80
148.46
141.97
131.87
129.58
125.76
122.78
120.64
118.56
77.36
77.04
76.73
Cl
H
O
O
Cl
2v
f1 (ppm)


7.74
7.65
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7.45
7.28
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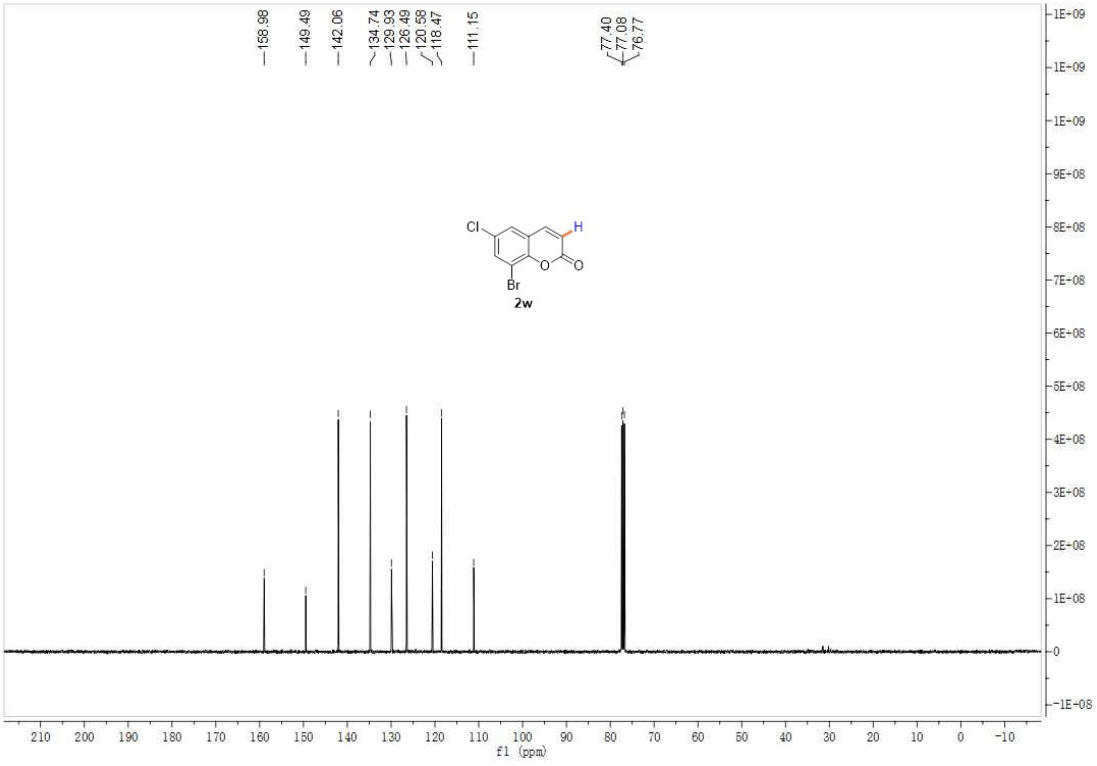
6.49
0.00
Cl
H
O
O
Br
2w
0.97
1.04
0.99
1.00
f1 (ppm)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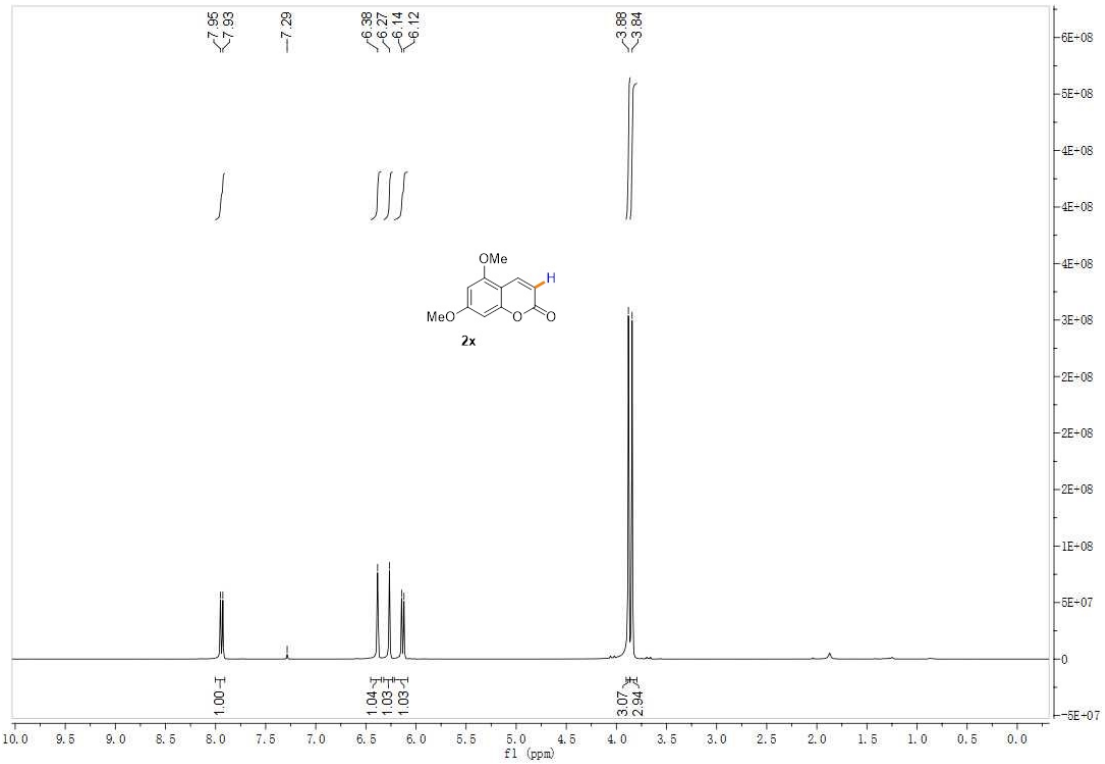
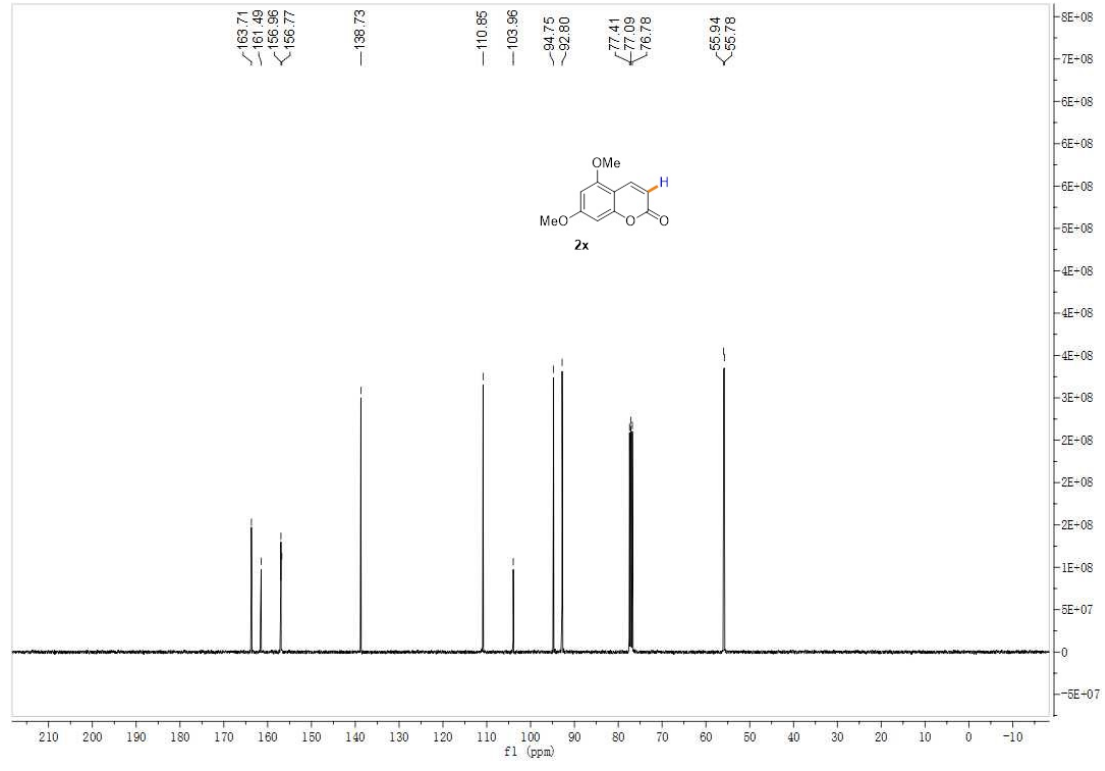
149.49
142.06
134.74
129.93
126.49
120.58
118.47
111.15
77.40
77.08
76.77
Cl
H
O
O
Br
2w
f1 (ppm)


7.95
7.93
7.29
6.38
6.27
6.14
6.12
3.88
3.84
OMe
MeO
H
O
O
2x
1.00
1.04
1.03
1.03
3.07
2.94
f1 (ppm)


163.71
161.49
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156.77
138.73
110.85
103.96
94.75
92.80
77.41
77.09
76.78
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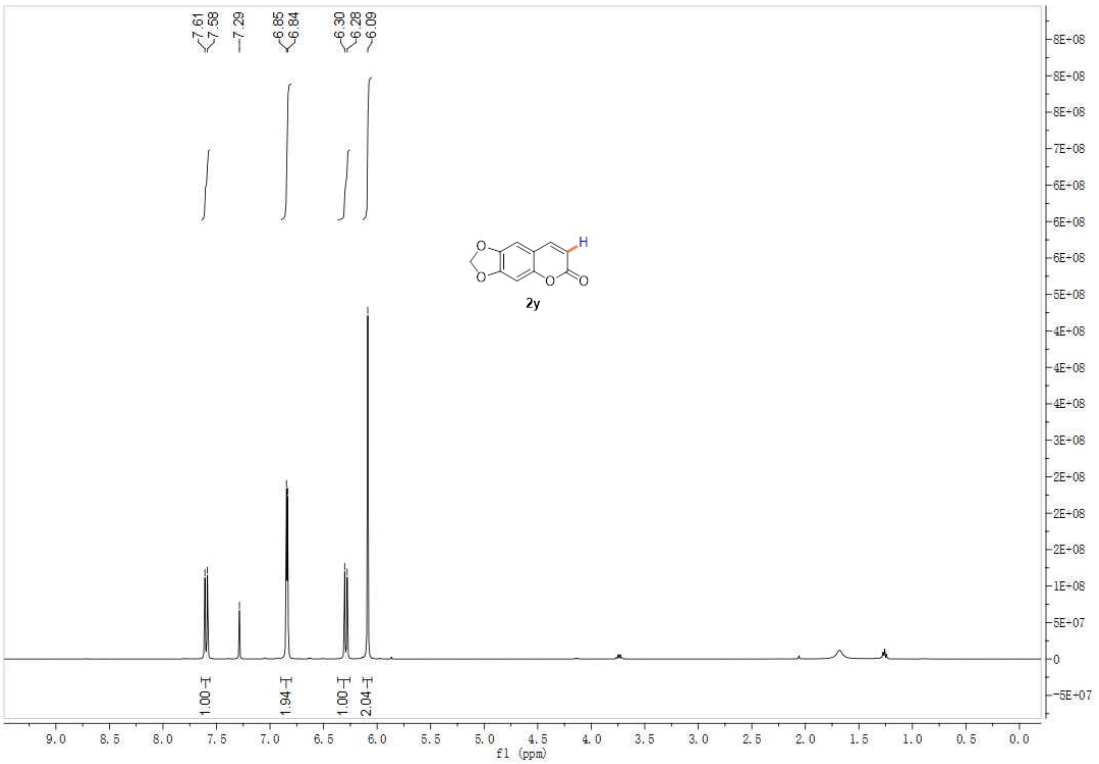
55.78
OMe
MeO
H
O
O
2x
f1 (ppm)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7.58
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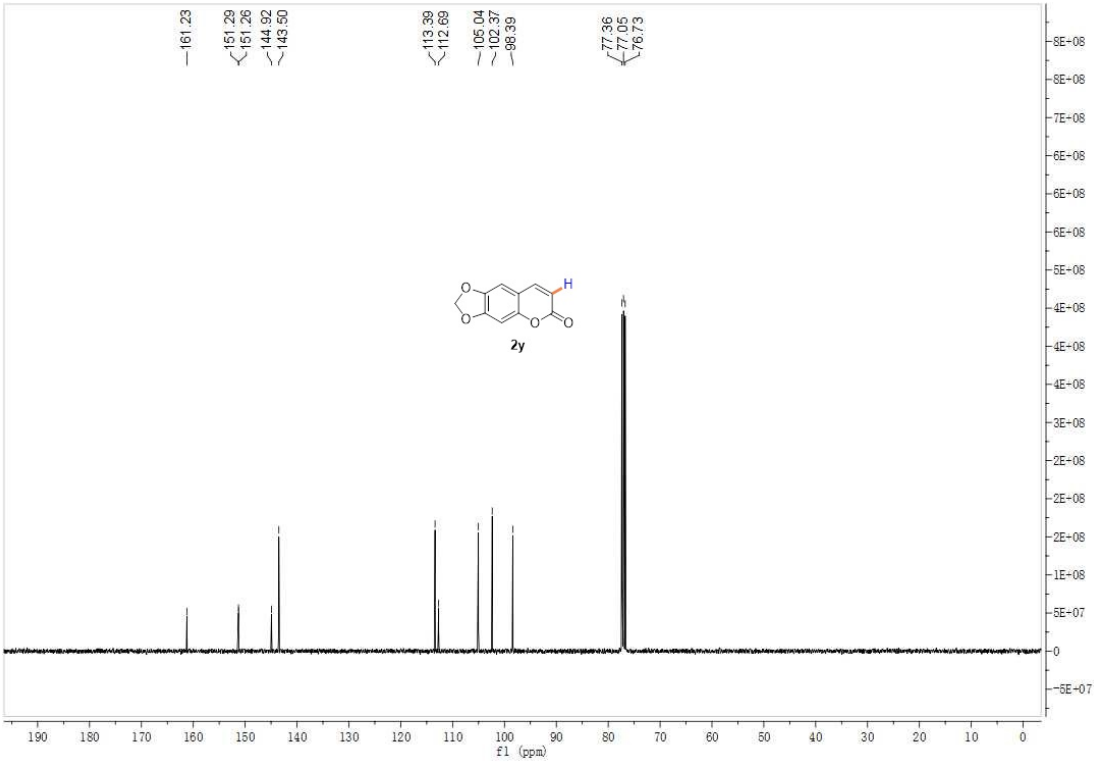
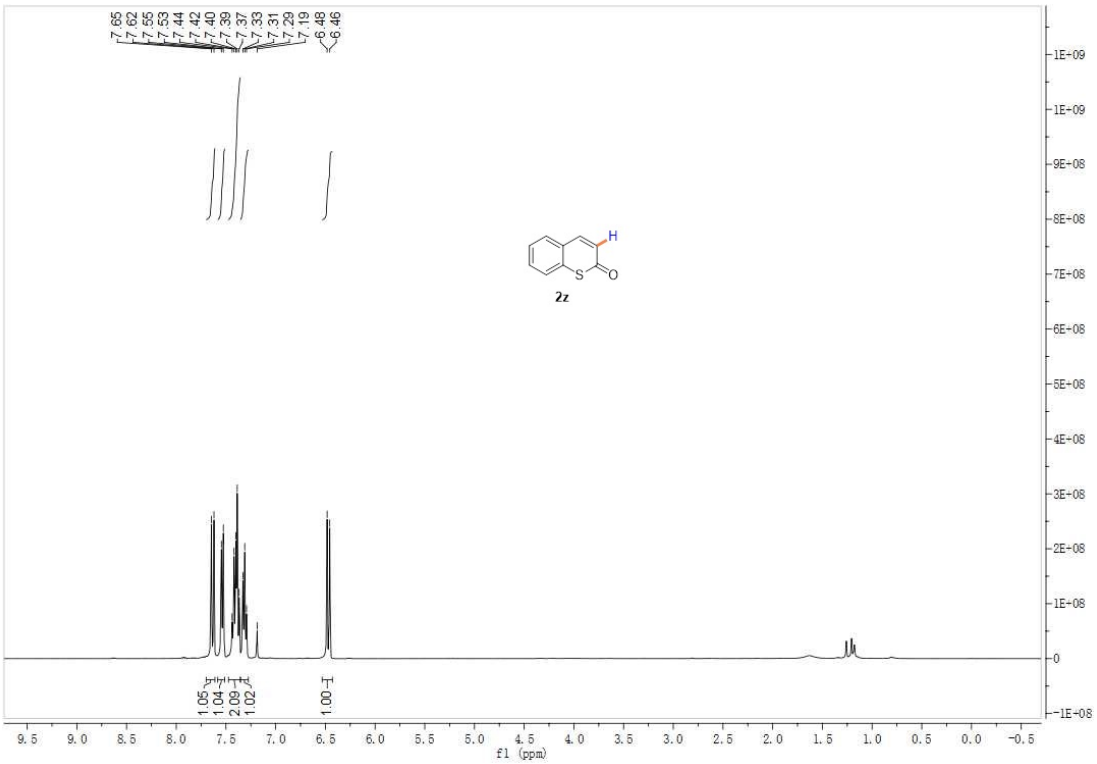
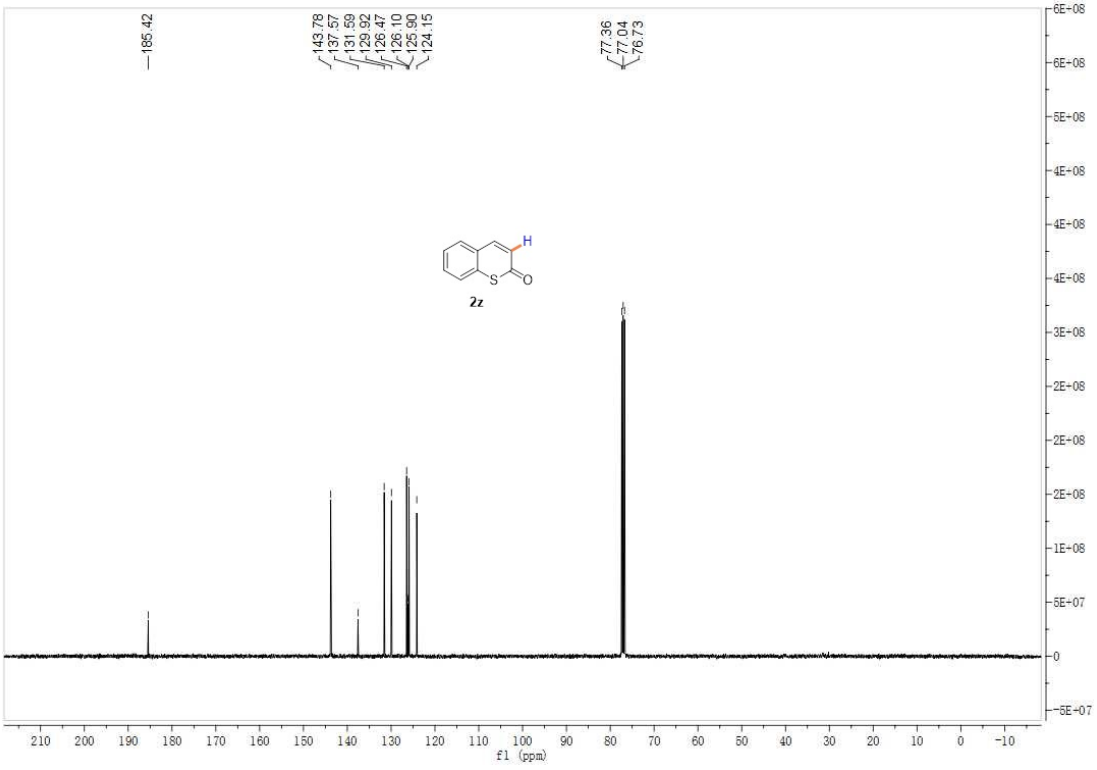
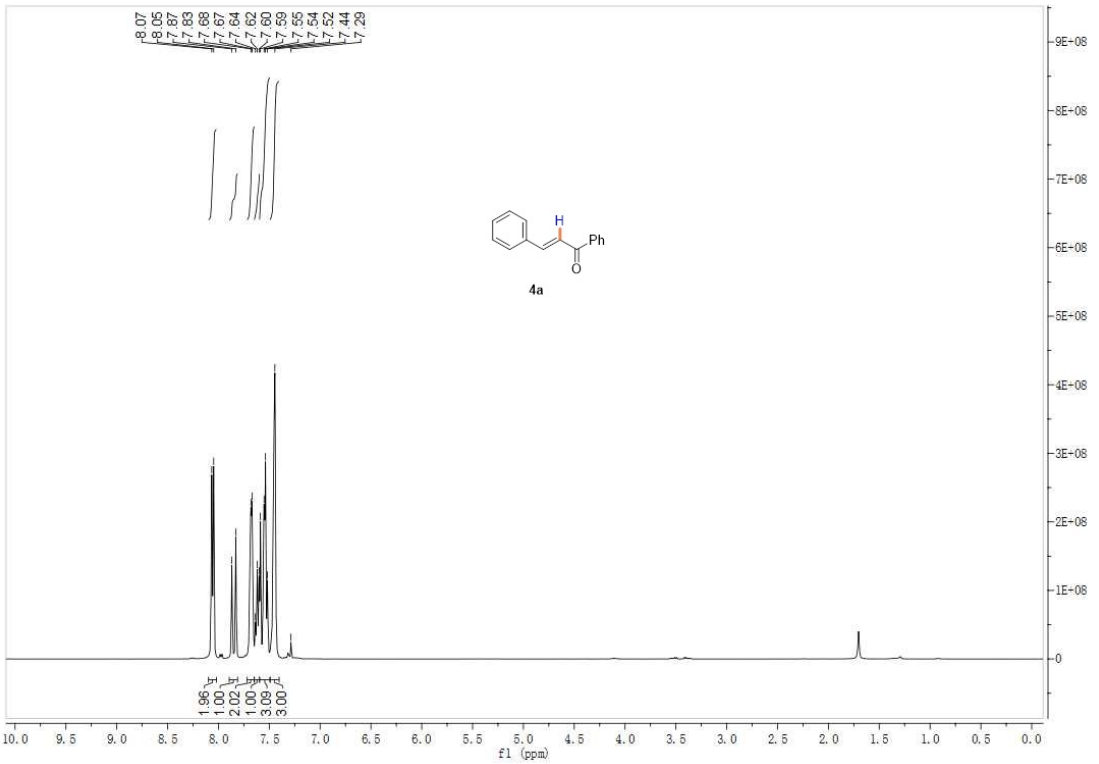
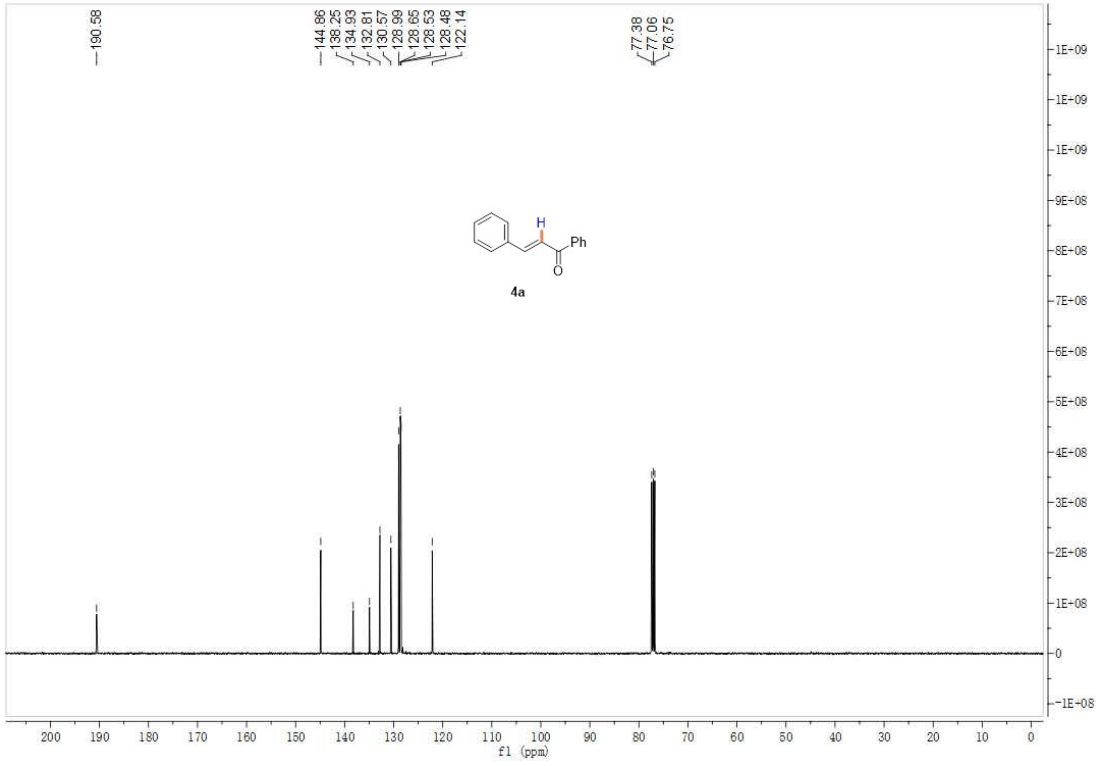
6.85
6.84
6.30
6.28
6.09
2y
1.00
1.94
1.00
2.04
f1 (ppm)

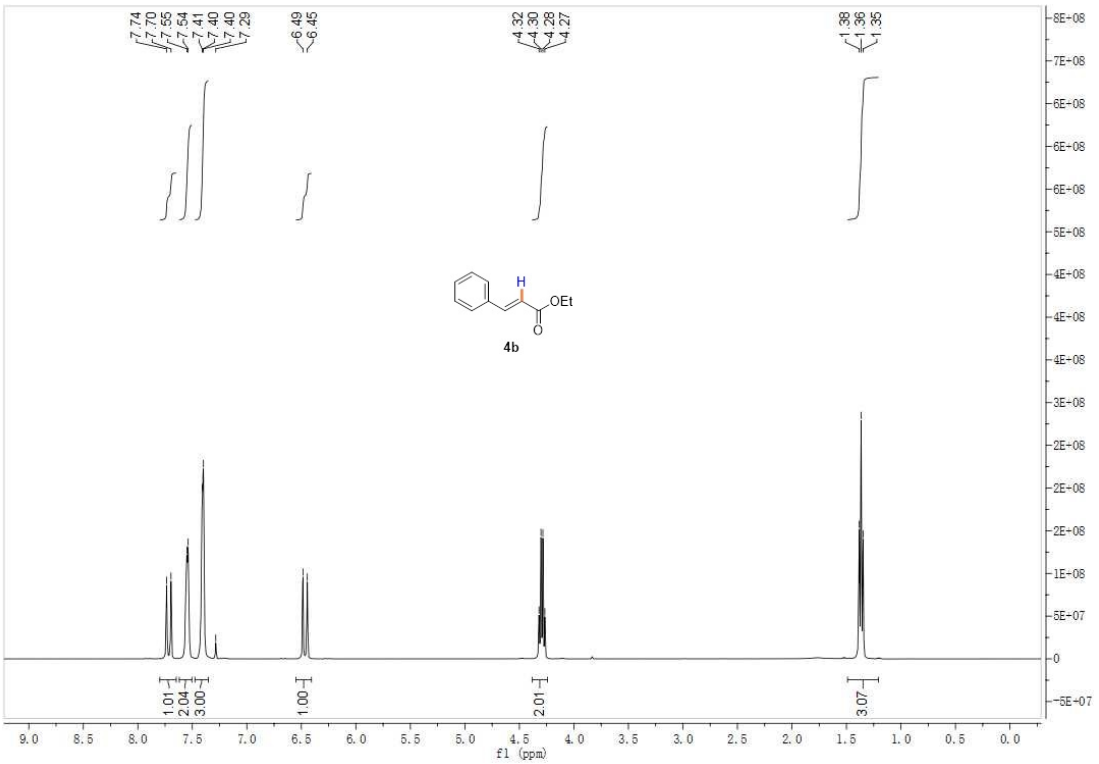

161.23
151.29
151.26
144.92
143.50
113.39
112.69
105.04
102.37
98.39
77.36
77.05
76.73
2y
f1 (ppm)

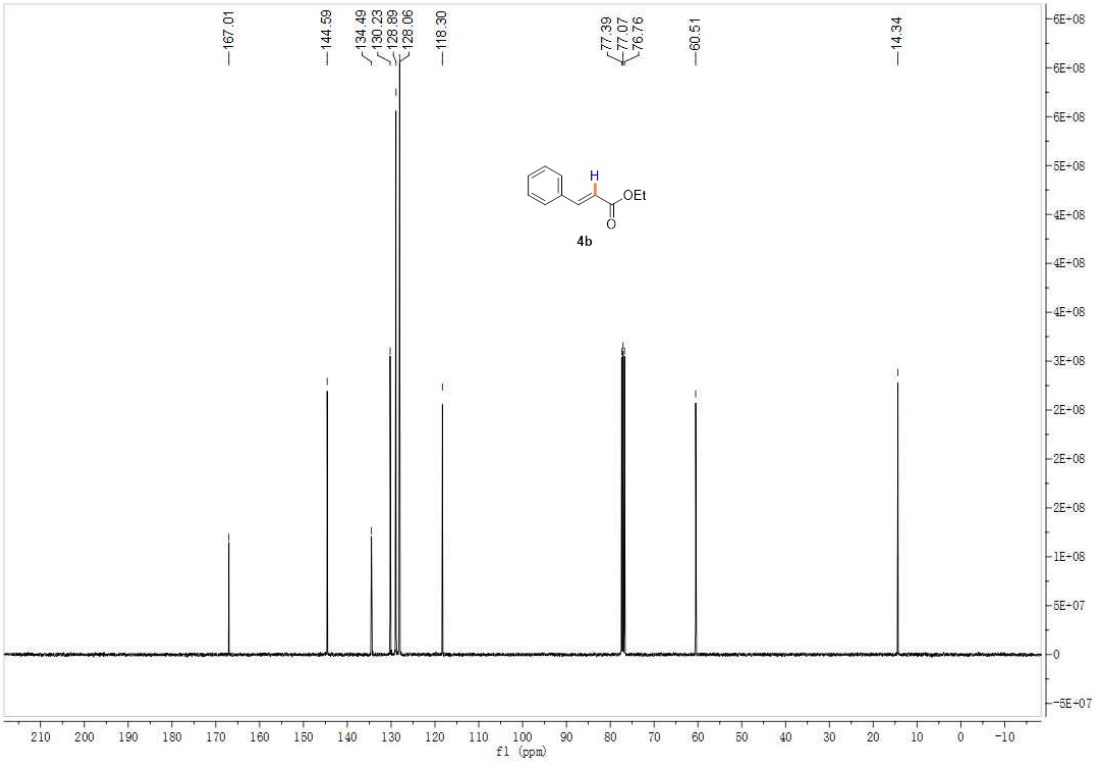

7.65
7.62
7.55
7.53
7.44
7.42
7.40
7.39
7.37
7.33
7.31
7.29
7.19
6.48
6.46
1.05
1.04
2.09
1.02
1.00
2z
f1 (ppm)

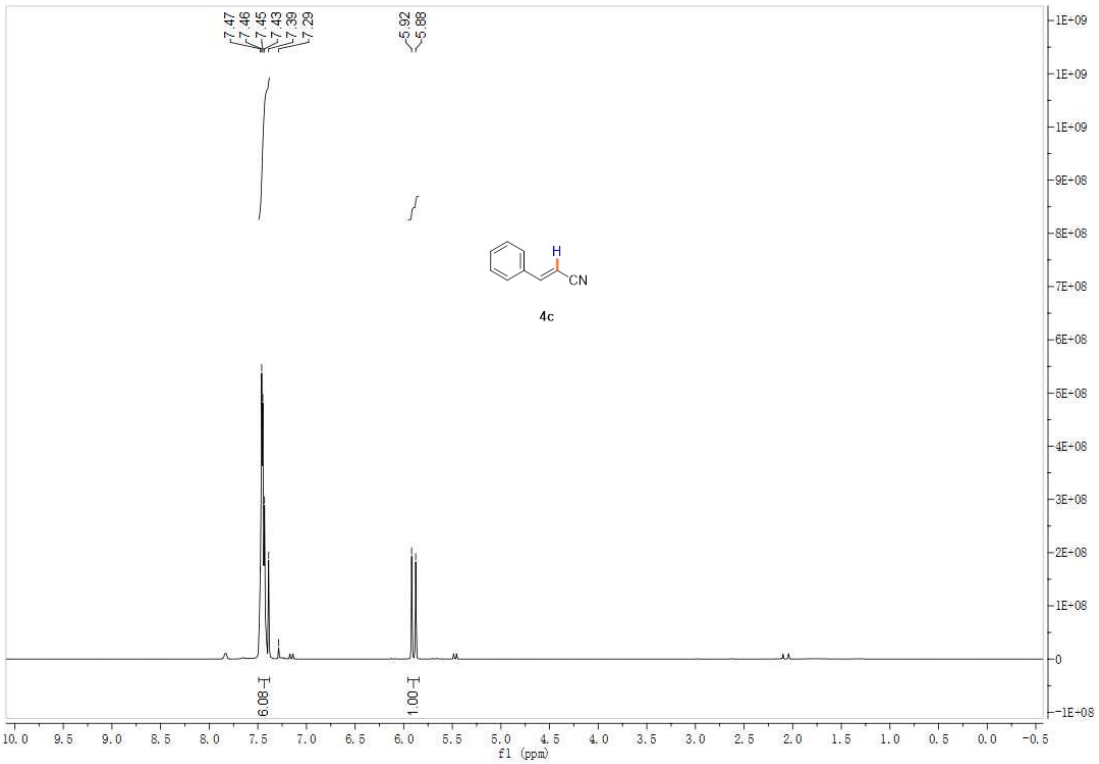

185.42
143.78
137.57
131.59
129.92
126.47
126.10
125.90
124.15
77.36
77.04
76.73
2z
f1 (ppm)

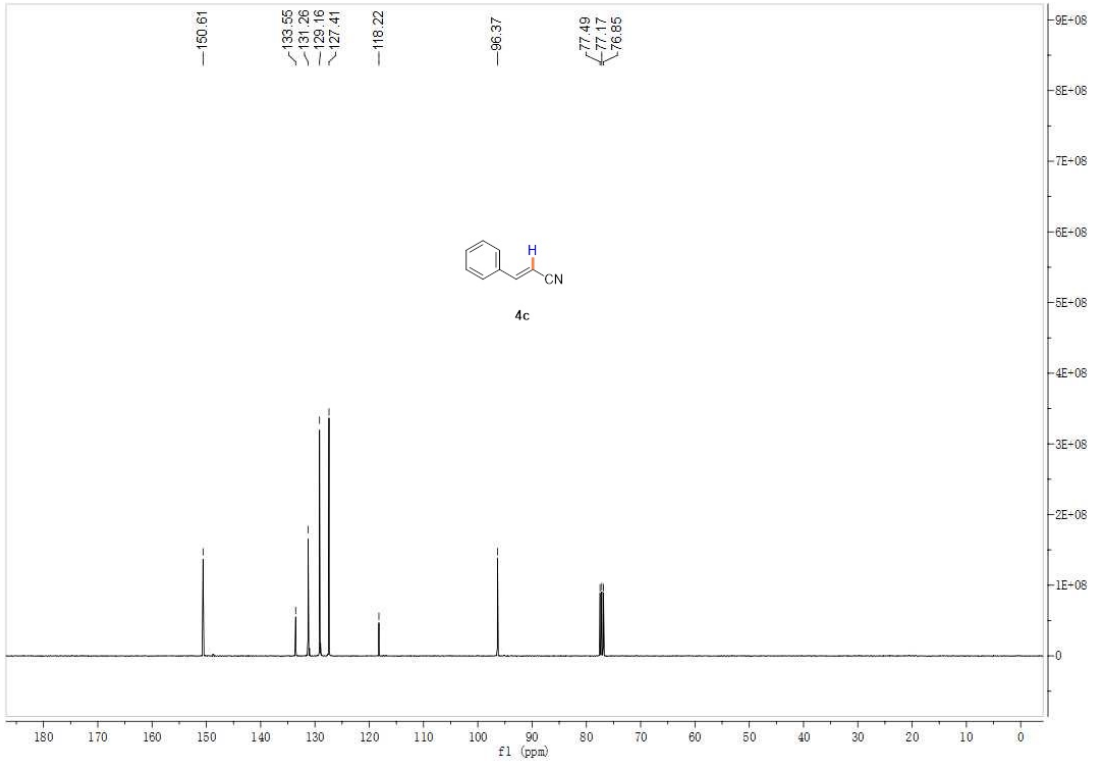

8.07
8.05
7.87
7.83
7.68
7.67
7.64
7.62
7.60
7.59
7.55
7.54
7.52
7.44
7.29
H
Ph
O
4a
1.96
1.00
2.02
1.00
3.09
3.00
f1 (ppm)

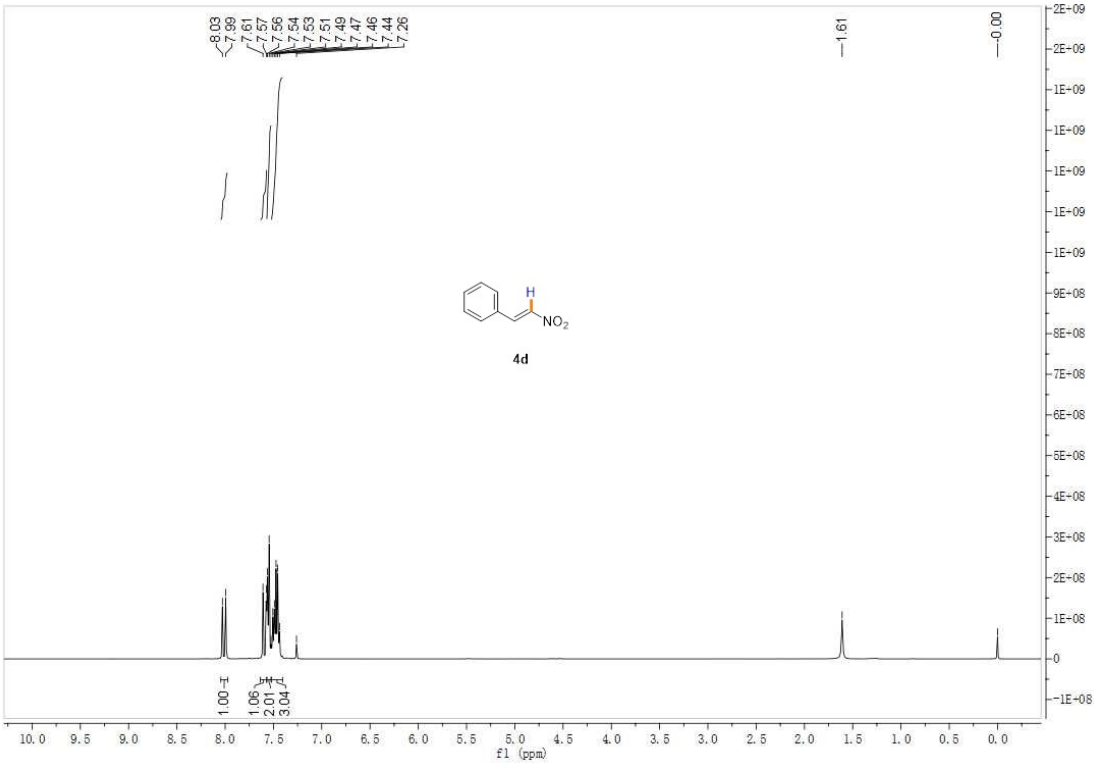

190.58
144.86
138.25
134.93
132.81
130.57
128.99
128.65
128.53
128.48
122.14
77.38
77.06
76.75
H
Ph
O
4a
f1 (ppm)


7.74
7.70
7.55
7.54
7.41
7.40
7.40
7.29
6.49
6.45
4.32
4.30
4.28
4.27
1.38
1.36
1.35
H
OEt
O
4b
1.01
2.04
3.00
1.00
2.01
3.07
f1 (ppm)


167.01
144.59
134.49
130.23
128.89
128.06
118.30
77.39
77.07
76.76
60.51
14.34
H
OEt
O
4b
f1 (ppm)


7.47
7.46
7.45
7.43
7.39
7.29
5.92
5.88
H
CN
4c
6.08
1.00
f1 (ppm)


150.61
133.55
131.26
129.16
127.41
118.22
96.37
77.49
77.17
76.85
H
CN
4c
f1 (ppm)


8.03
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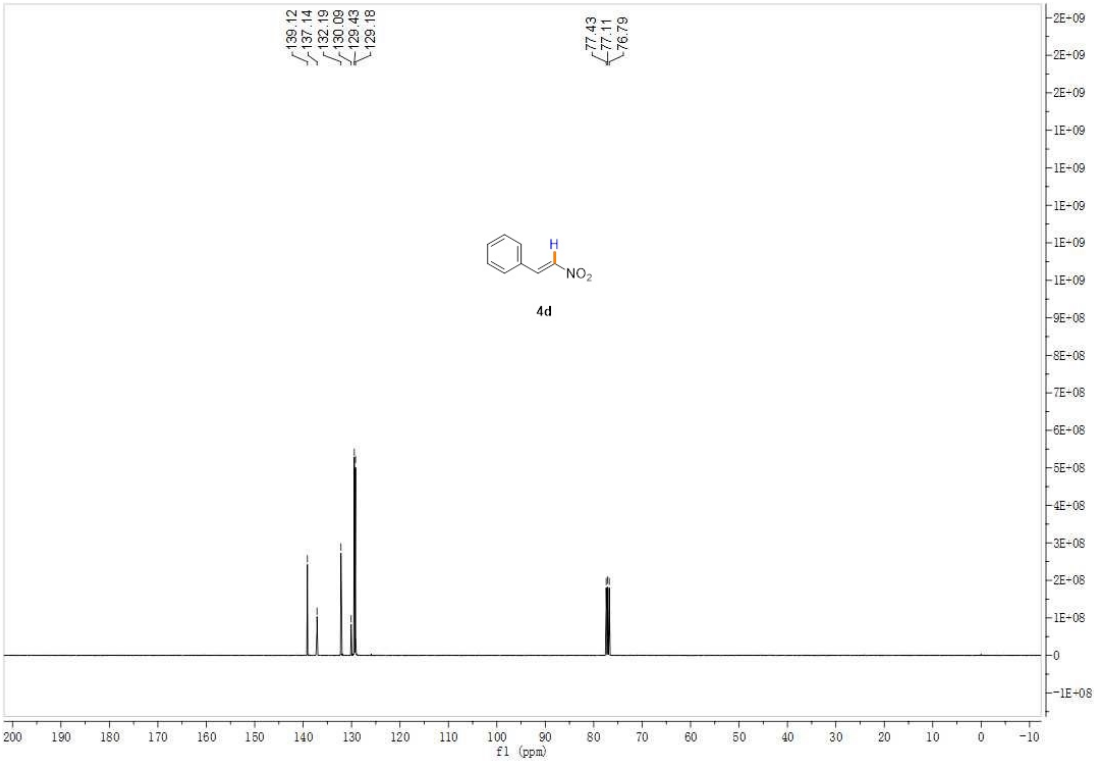
7.57
7.56
7.54
7.53
7.51
7.49
7.47
7.46
7.44
7.26
1.61
0.00
4d
1.00
1.06
2.01
3.04
f1 (ppm)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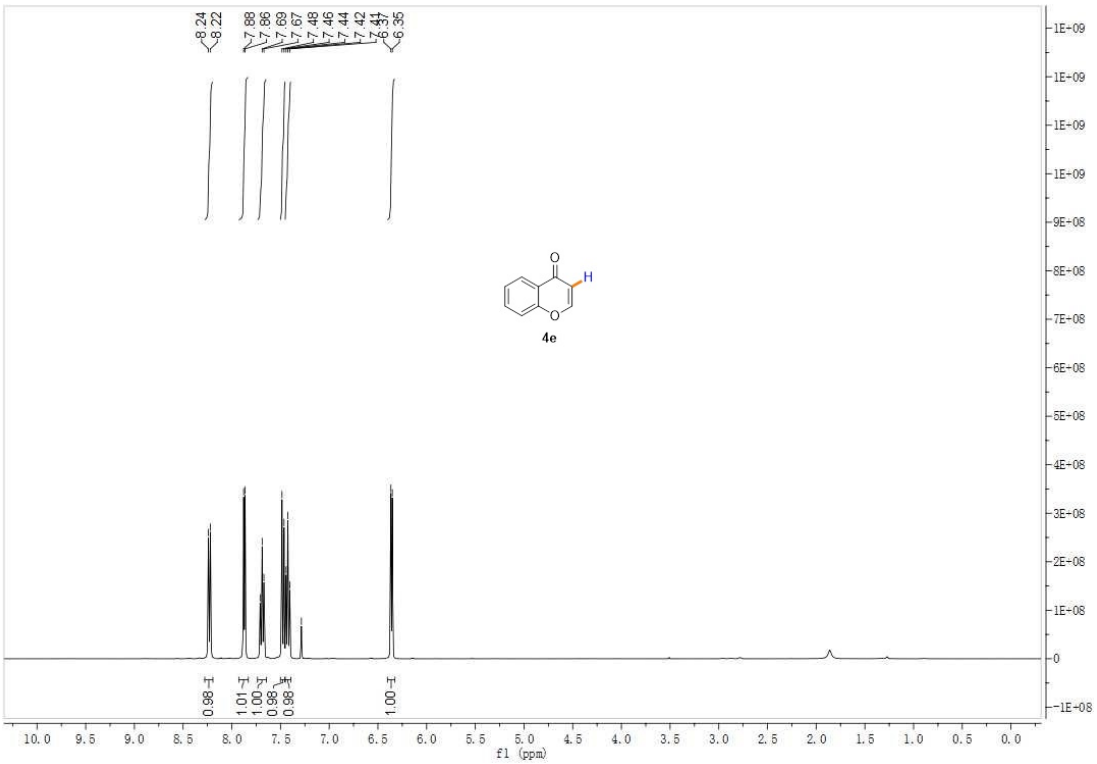
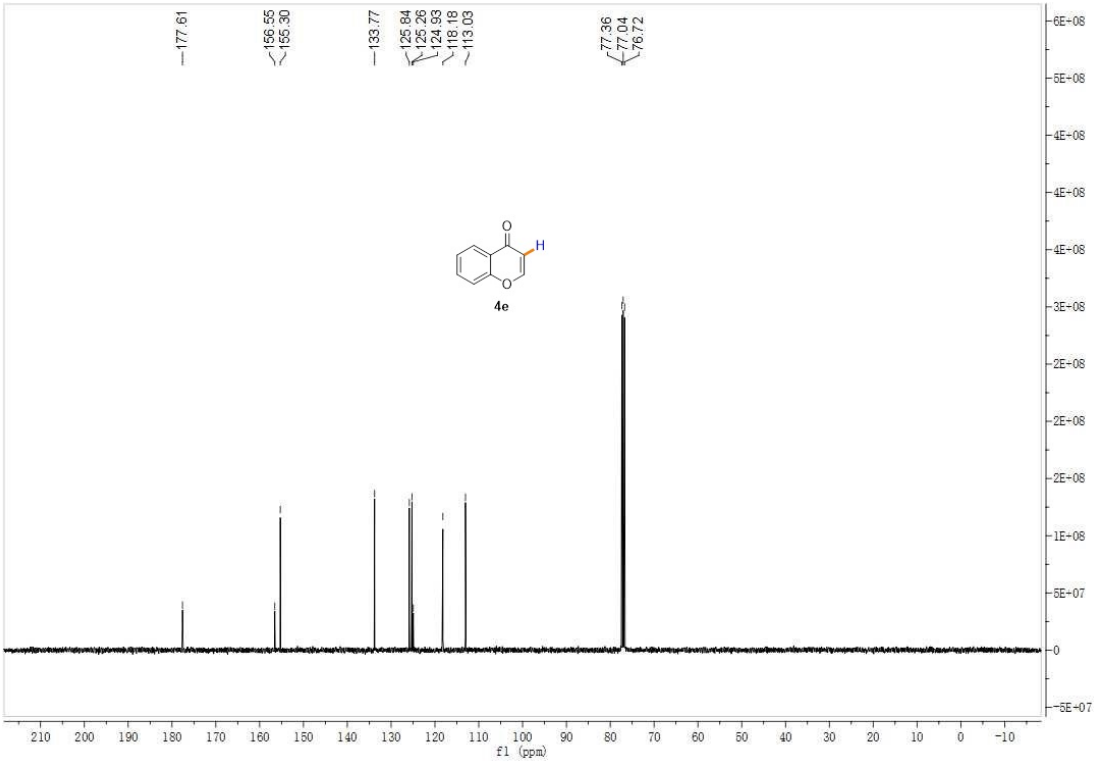
137.14
132.19
130.09
129.43
129.18
77.43
77.11
76.79
4d
f1 (ppm)


8.24
8.22
7.88
7.86
7.69
7.67
7.48
7.46
7.44
7.42
7.41
7.37
6.35
4e
0.98
1.01
1.00
0.98
0.98
1.00
f1 (ppm)


177.61
156.55
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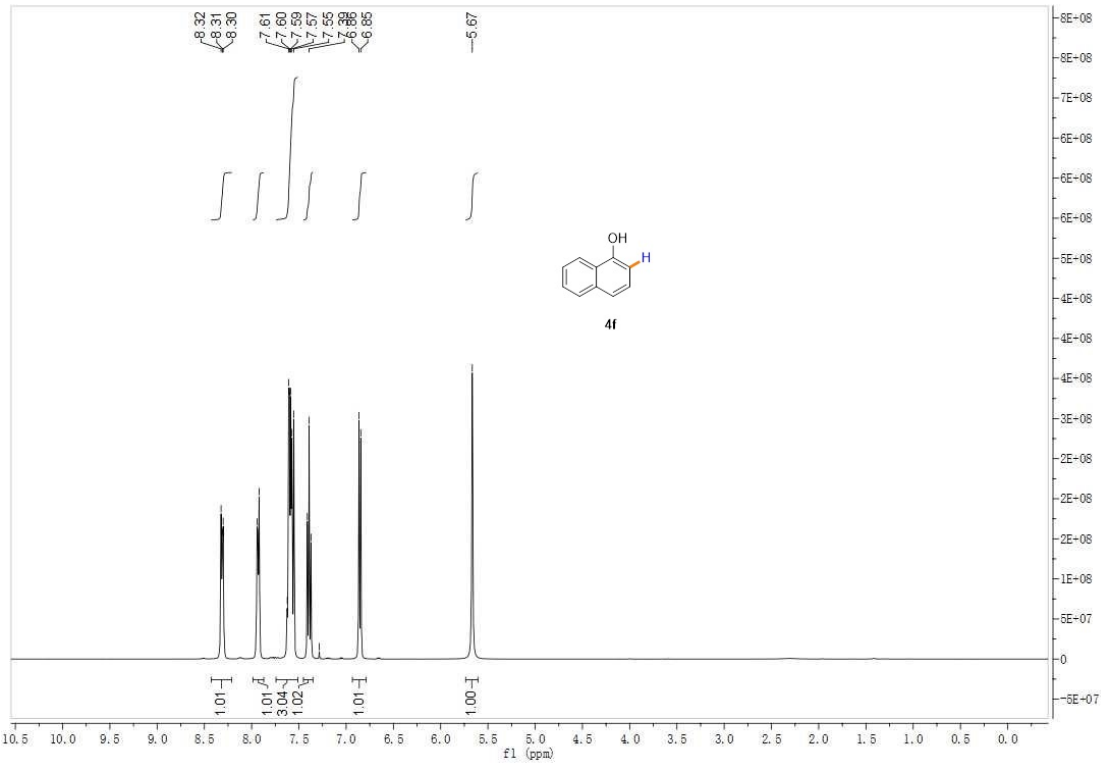
125.84
125.26
124.93
118.18
113.03
77.36
77.04
76.72
4e
f1 (ppm)


8.32
8.31
8.30
7.61
7.60
7.59
7.57
7.55
7.39
6.86
6.85
5.67
OH
H
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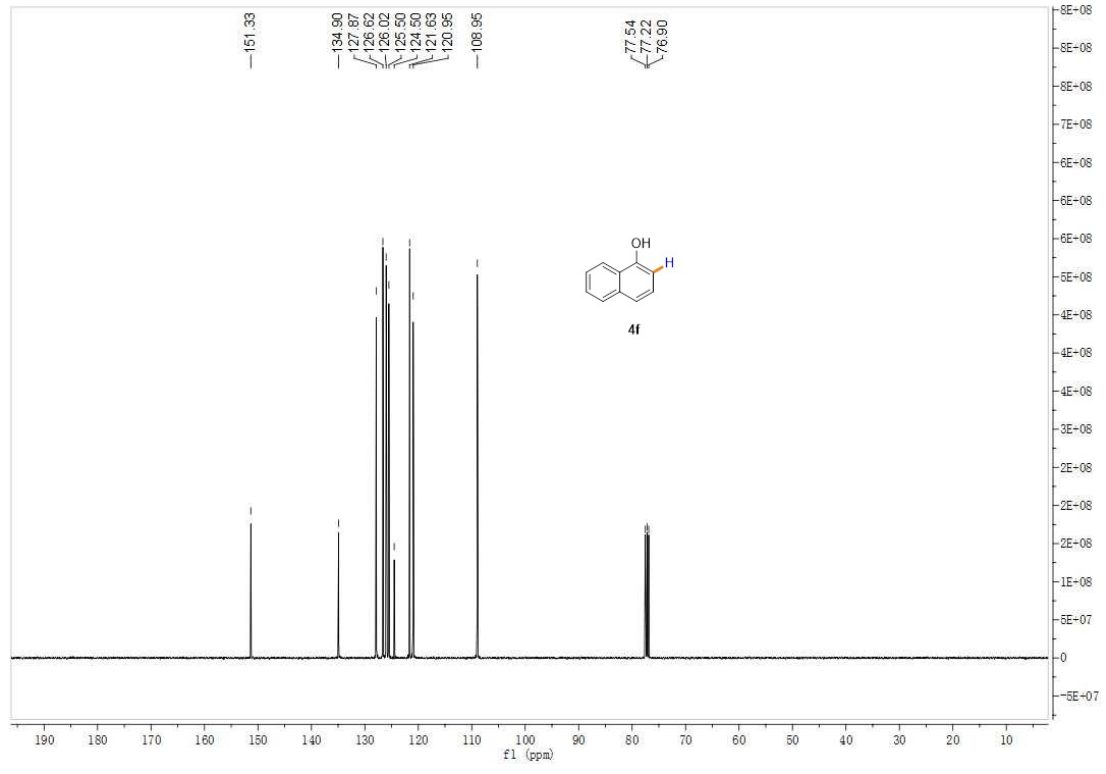
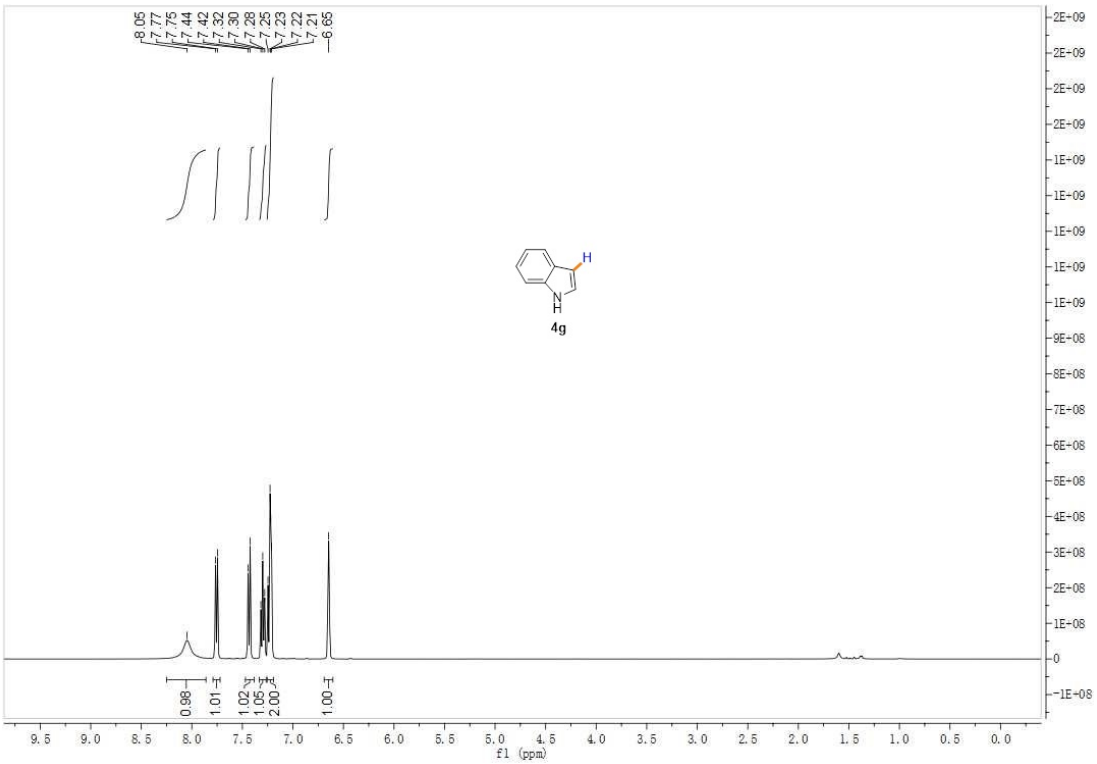
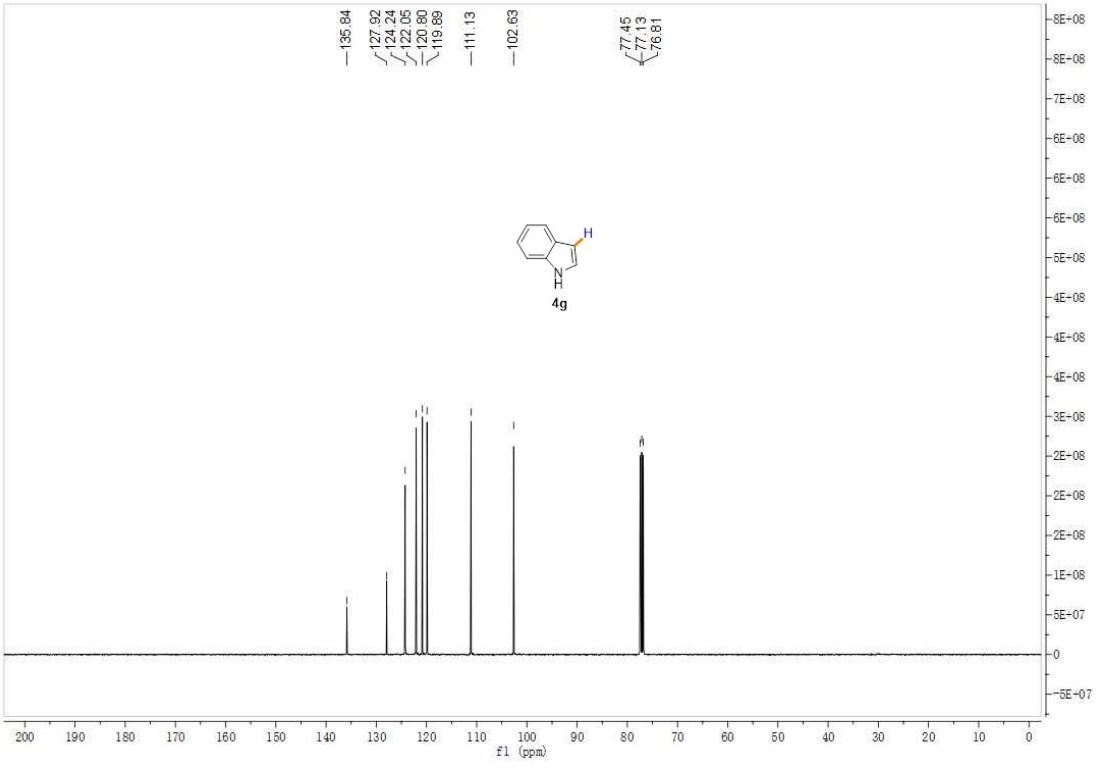
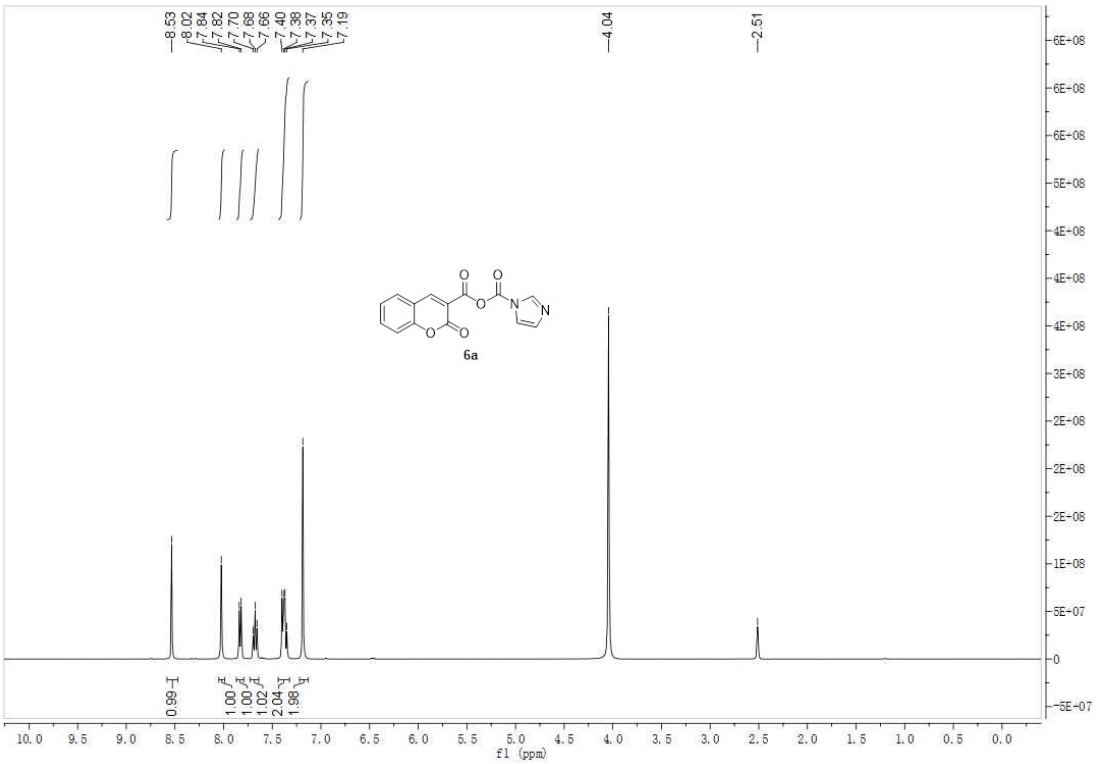
3.04
1.02
1.01
1.00
f1 (ppm)


151.33
134.90
127.87
126.62
126.02
125.50
124.50
121.63
120.95
108.96
77.54
77.22
76.90
OH
H
4f
f1 (ppm)


8.05
7.77
7.75
7.44
7.42
7.32
7.30
7.28
7.25
7.23
7.22
7.21
6.65
4g
0.98
1.01
1.02
1.05
2.00
1.00
f1 (ppm)


135.84
127.92
124.24
122.05
120.80
119.89
111.13
102.63
77.45
77.13
76.81
4g
f1 (ppm)


8.53
8.02
7.84
7.82
7.70
7.68
7.66
7.40
7.38
7.37
7.35
7.19
4.04
2.51
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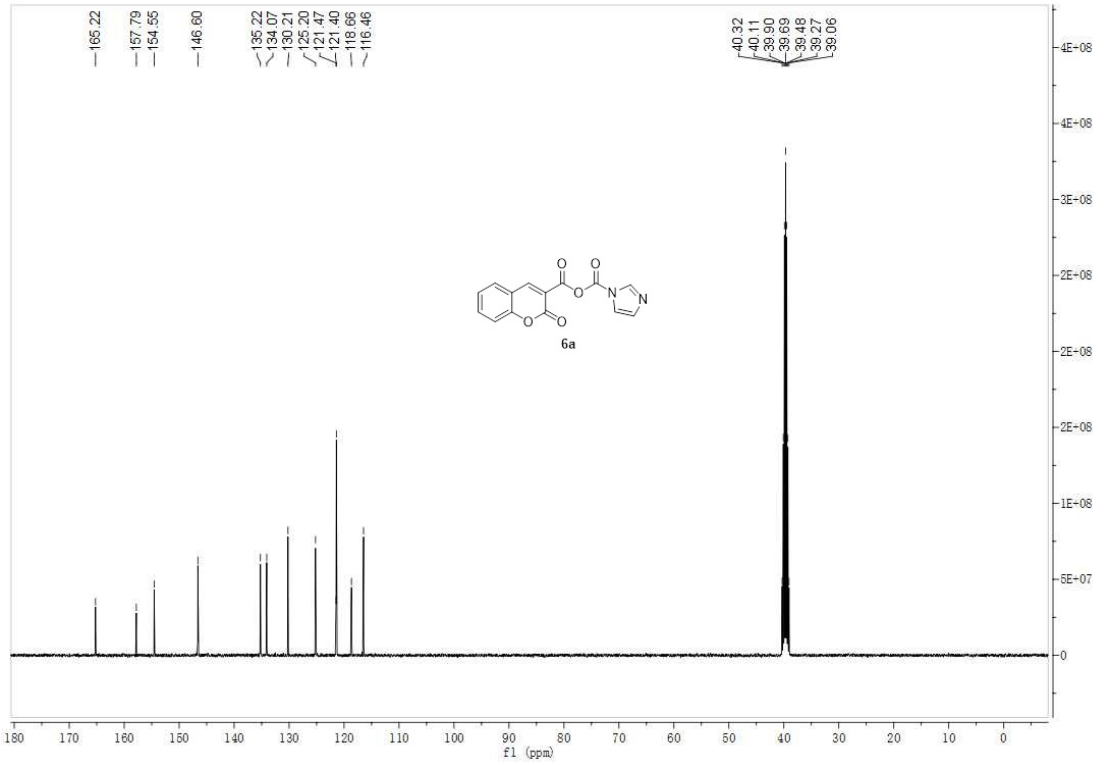
1.00
1.00
1.02
2.04
1.98
6a
f1 (ppm)


165.22
157.79
154.55
146.60
135.22
134.07
130.21
125.20
121.47
121.40
118.66
116.46
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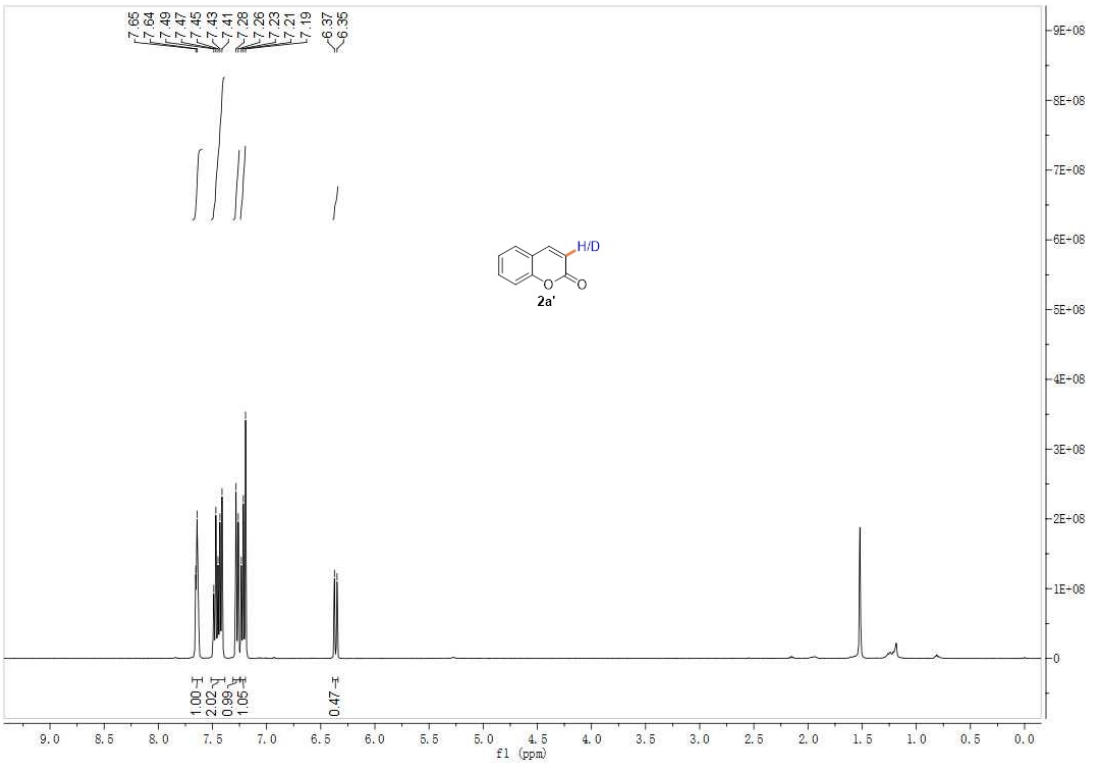
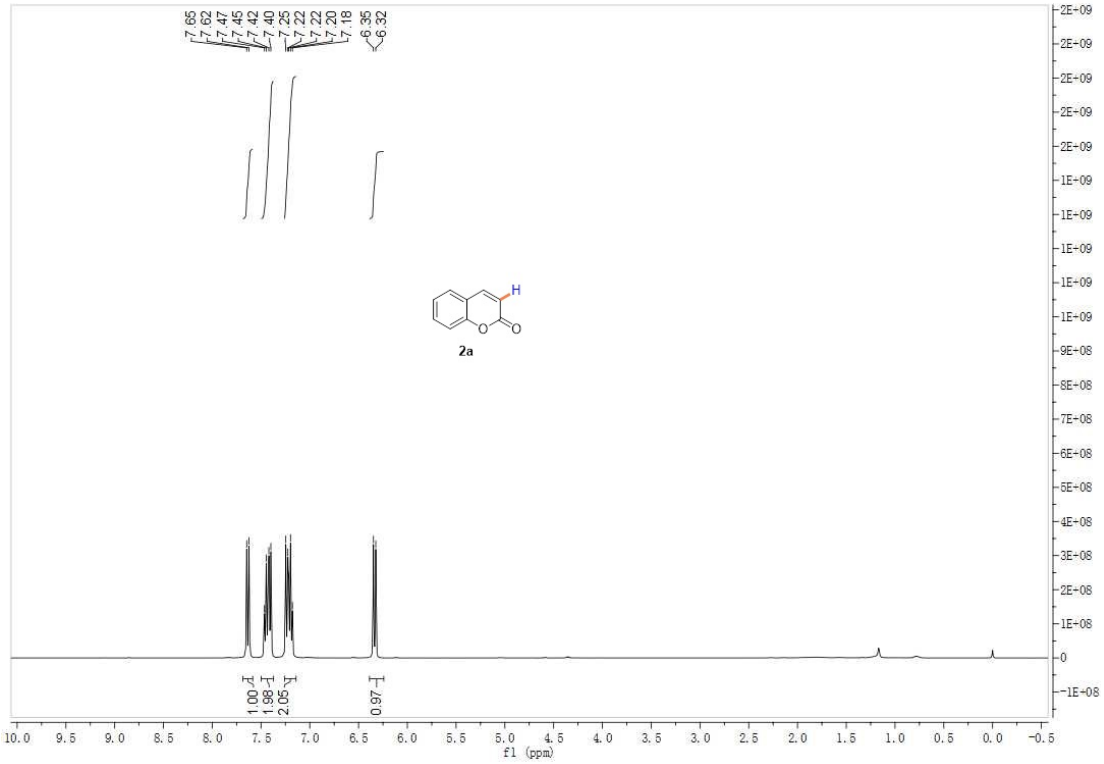
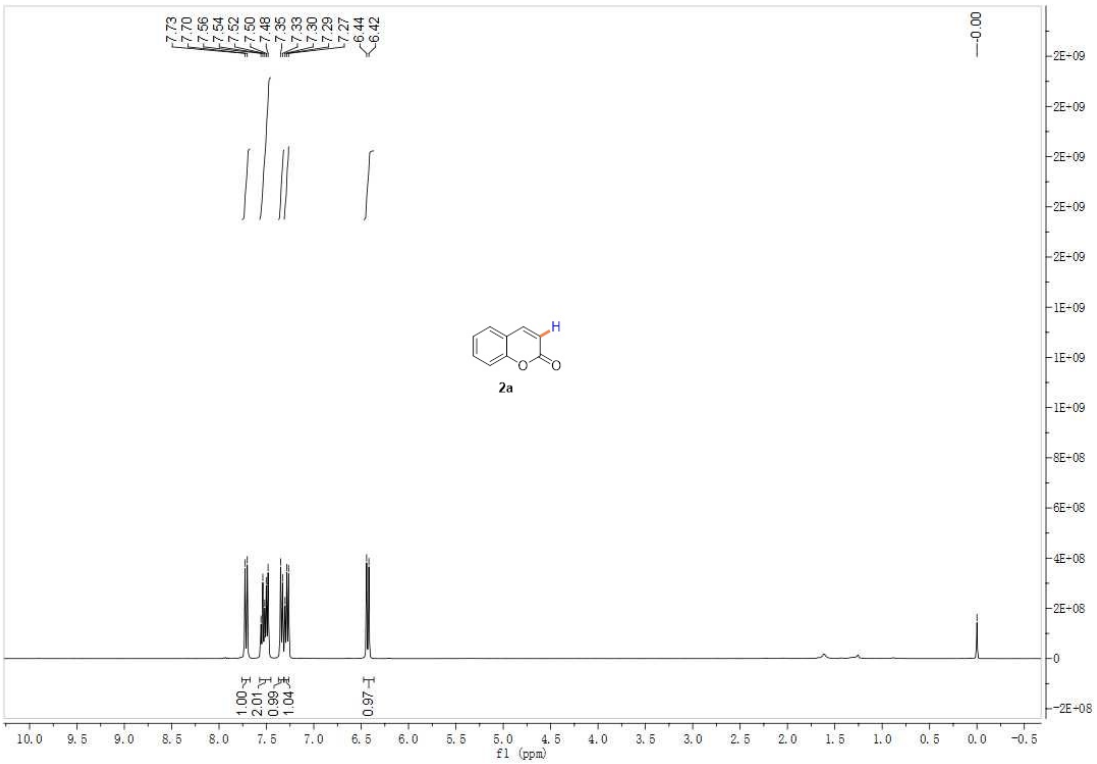
39.48
39.27
39.06
6a
f1 (ppm)



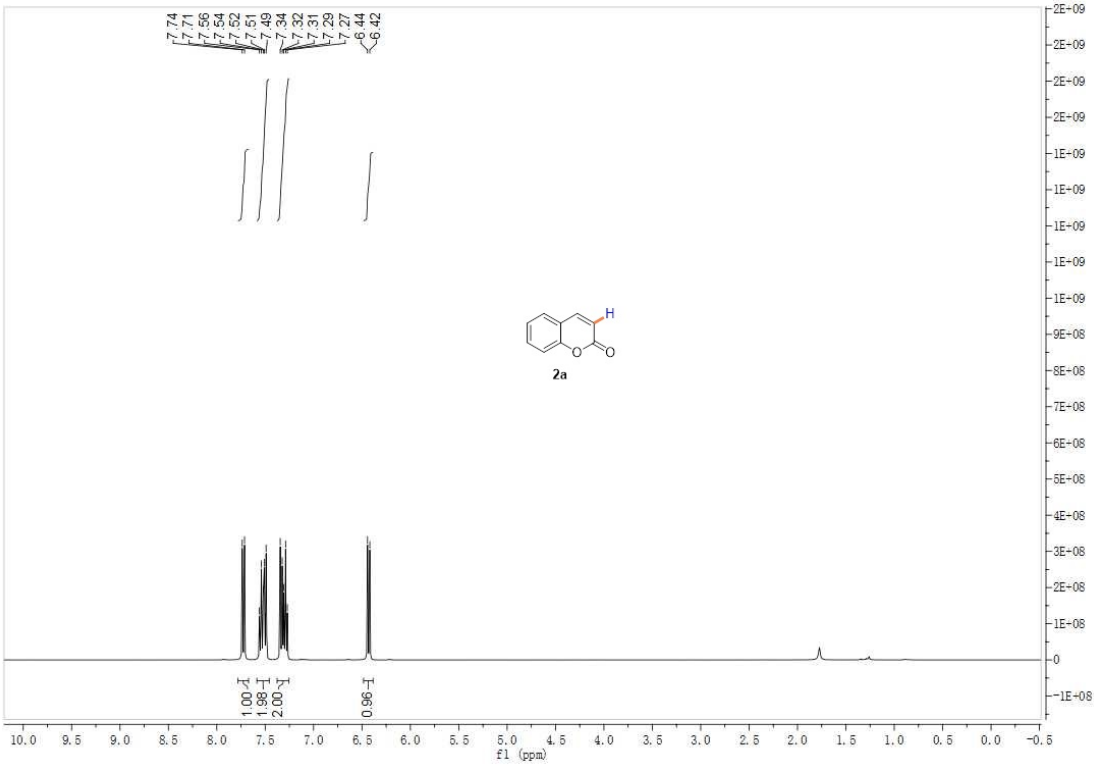
6 Scanned copies of ^{1}H-NMR, for 2*H*-chromen-2-one (2a) (isolated from the experiment carried out in the presence of TEMPO, BHT, p-benzoquinone as a radical scavenger)



(Isolated from the experiment carried out in the presence of TEMPO as a radical scavenger)



(Isolated from the experiment carried out in the presence of BHT as a radical scavenger)



(Isolated from the experiment carried out in the presence of p-benzoquinone as a radical scavenger)