Supporting Information

Site-specific hydroxyalkylation of chromones *via* alcohol mediated Minisci-type radical conjugate addition

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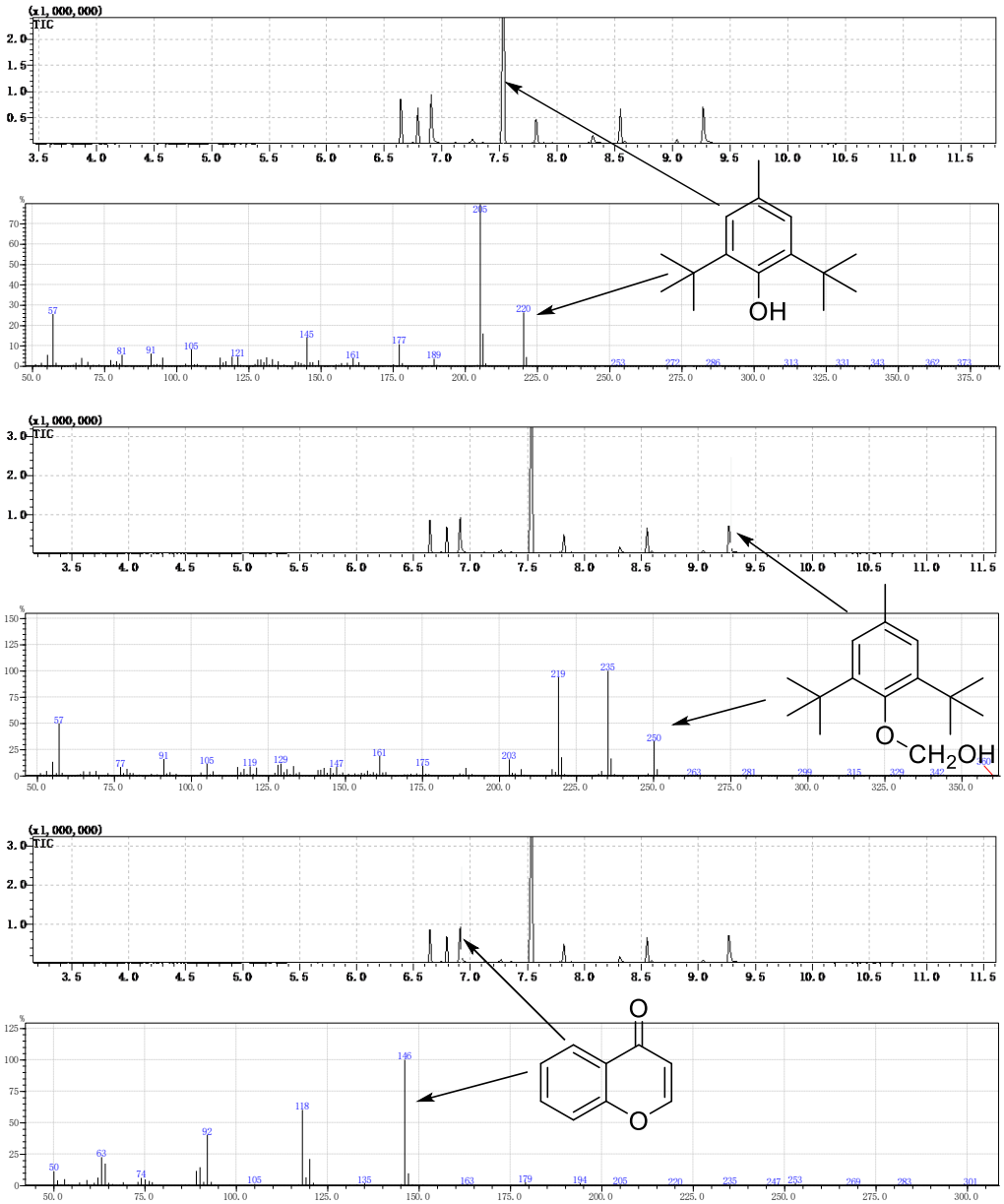
1. General experimental details

General Information: All chemicals were used as received without further purification unless stated otherwise. NMR spectra were recorded at ambient temperature on a 300 or 400 MHz NMR spectrometer. Chemical shifts (δ) are given in ppm relative to TMS, the coupling constants *J* are given in Hz. HRMS were recorded on a TOF LC/MS equipped with electrospray ionization (ESI) probe operating in positive or negative ion mode.

Experimental procedure: Under N_2, the mixture of **1** (0.2 mmol), **2** or **4** (1 mL) and DTBP (0.6 mmol) were added into the sealed tubed. The reaction mixture was vigorously stirred at 140 ^oC for 15h. Then, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography on silica gel to give the products.

2. Mechanism Studies

Standard Procedure + BHT (3.0 equiv)



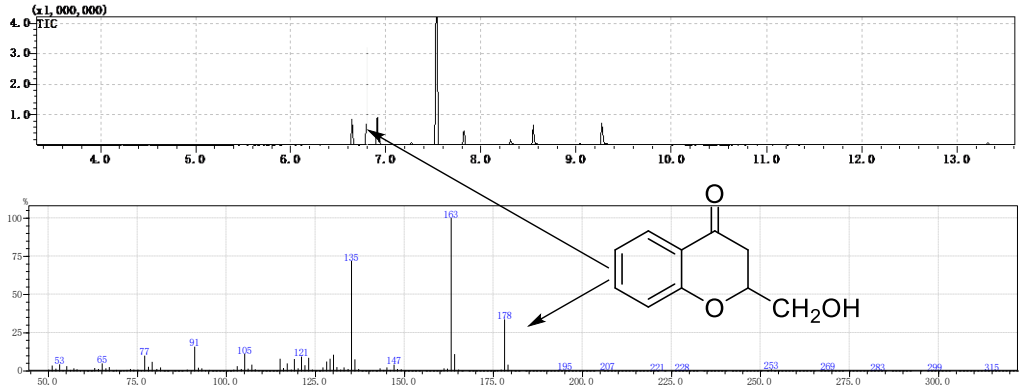
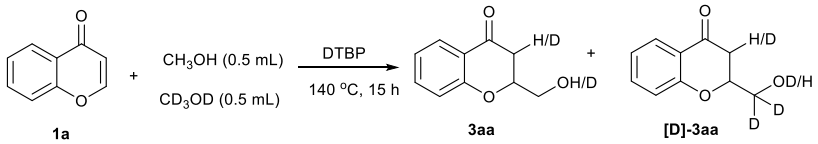
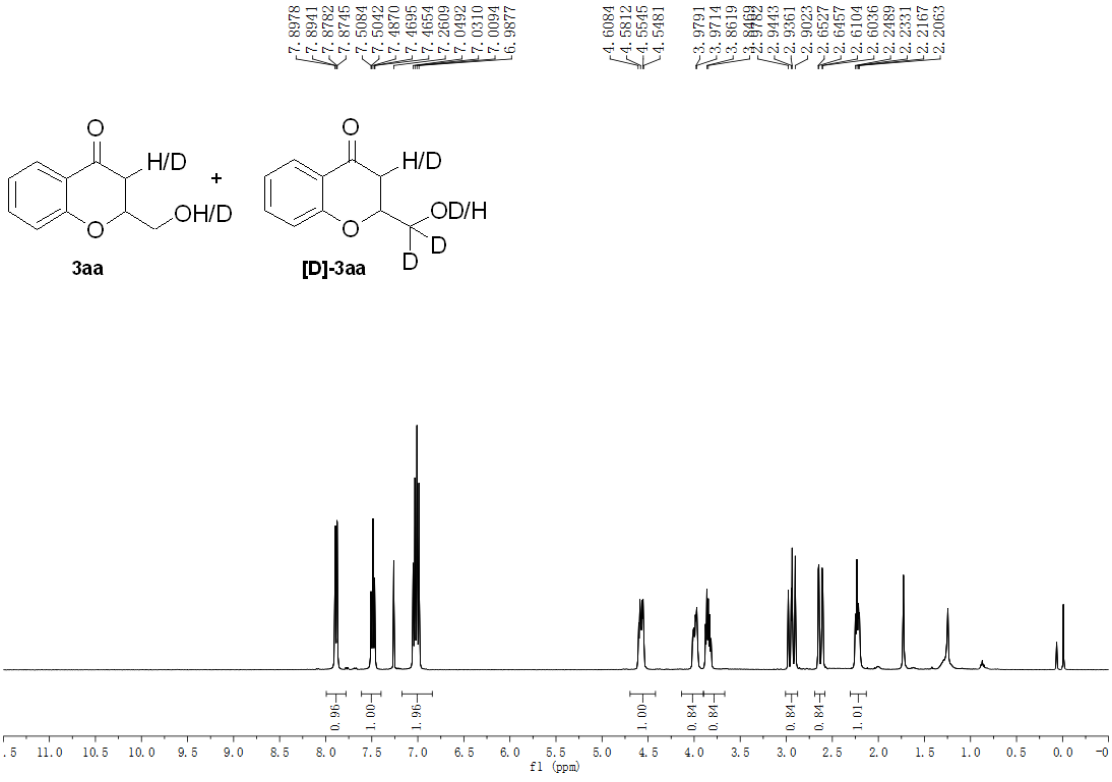


Figure S1 GC-MS spectra of the free radical capture results

Kinetic isotope effect experiments

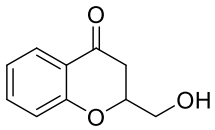


To a sealed tube, the mixture of **1a** (0.2 mmol), DTBP (0.6 mmol), CH_3OH (0.5 mL) and CD_3OD (0.5 mL) were added into the flask. The reaction mixture was vigorously stirred at 140 ^oC for 15 h. After the completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography on silica gel to afford the products **3aa** and **[D]-3aa**. ^1H NMR ($CDCl_3$, 400 MHz): δ 7.88 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.51-7.46 (m, 1H), 7.05-6.98 (m, 2H), 4.61-4.55 (m, 1H), 4.01-3.96 (m, 0.84H), 3.87-3.82 (m, 0.84H), 2.98-2.90 (m, 0.84H), 2.65-2.60 (m, 0.84H), 2.25-2.21 (m, 1H).



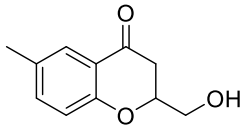
3. Characterization data of the products

2-(hydroxymethyl)chroman-4-one (3aa)



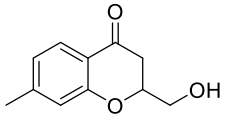
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (32.1 mg, 90%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.87 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.49-7.45 (m, 1H), 7.02-6.96 (m, 2H), 4.58-4.52 (m, 1H), 3.98-3.94 (m, 1H), 3.85-3.81 (m, 1H), 2.95-2.88 (m, 1H), 2.74 (s, 1H), 2.64-2.59 (m, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 192.3, 161.2, 136.2, 127.0, 121.7, 120.8, 117.8, 78.2, 64.4, 39.0. HRMS (ESI) *m/z* calcd for $C_{10}H_{11}O_3$ $(M+H)^+$ 179.0703, found 179.0704.

2-(hydroxymethyl)-6-methylchroman-4-one (3ba)



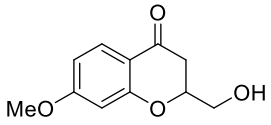
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (31.5 mg, 82%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.66 (s, 1H), 7.30-7.27 (m, 1H), 6.89 (d, *J* = 8.4 Hz, 1H), 4.57-4.51 (m, 1H), 3.99-3.95 (m, 1H), 3.86-3.82 (m, 1H), 2.95-2.87 (m, 1H), 2.63-2.58 (m, 2H), 2.30 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 192.4, 159.2, 137.3, 131.1 126.6, 120.4, 117.6, 78.2, 64.5, 39.1, 20.4. HRMS (ESI) *m/z* calcd for $C_{11}H_{13}O_3$ $(M+H)^+$ 193.0859, found 193.0861.

2-(hydroxymethyl)-7-methylchroman-4-one (3ca)



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (29.2 mg, 76%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.74 (d, *J* = 8.0 Hz, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 6.77 (s, 1H), 4.56-4.49 (m, 1H), 3.96-3.92 (m, 1H), 3.84-3.79 (m, 1H), 2.91-2.83 (m, 1H), 2.68 (s, 1H), 2.60-2.55 (m, 1H), 2.32 (s, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 191.9, 161.2, 147.8, 126.9, 123.0, 118.6, 117.9, 78.2, 64.4, 38.9, 21.9. HRMS (ESI) *m/z* calcd for $C_{11}H_{13}O_3$ $(M+H)^+$ 193.0859, found 193.0860.

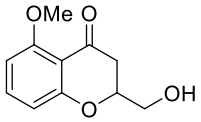
2-(hydroxymethyl)-7-methoxychroman-4-one (3da)



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave a yellow solid (32.0 mg, 77%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.78 (d, *J* = 8.8 Hz, 1H), 6.55 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.41 (d, *J* = 2.3 Hz, 1H), 4.57-4.50 (m, 1H), 3.95-3.92 (m, 1H), 3.84-3.80 (m, 1H), 3.79 (s, 3H), 2.88-2.81 (m, 1H), 2.72 (s, 1H), 2.57-2.52 (m, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 190.9,

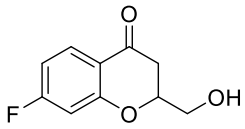
166.2, 163.2, 128.7, 114.7, 110.1, 100.8, 78.6, 64.4, 55.7, 38.6. HRMS (ESI) *m/z* calcd for $C_{11}H_{13}O_4$ $(M+H)^+$ 209.0808, found 209.0809.

2-(hydroxymethyl)-5-methoxychroman-4-one (3ea)



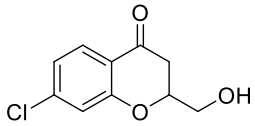
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave a yellow solid (28.3 mg, 68%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.35 (d, *J* = 8.4 Hz, 1H), 6.57 (d, *J* = 8.3 Hz, 1H), 6.49 (d, *J* = 8.3 Hz, 1H), 4.53-4.47 (m, 1H), 3.94-3.90 (m, 1H), 3.88 (s, 3H), 3.82-3.78 (m, 1H), 2.91-2.83 (m, 1H), 2.60 (s, 1H), 2.58-2.53 (m, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 191.0, 162.8, 160.7, 136.1, 111.2, 109.9, 104.0, 77.7, 64.3, 56.2, 40.4. HRMS (ESI) *m/z* calcd for $C_{11}H_{13}O_4$ $(M+H)^+$ 209.0808, found 209.0809.

7-fluoro-2-(hydroxymethyl)chroman-4-one (3fa)



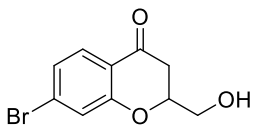
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow solid (27.4 mg, 70%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91-7.86 (m, 1H), 6.77-6.65 (m, 2H), 4.62-4.54 (m, 1H), 4.01-3.96 (m, 1H), 3.86-3.81 (m, 1H), 2.97-2.87 (m, 1H), 2.65-2.47 (m, 1H), 2.60 (s, 1H). ^{13}C NMR (DMSO-d_6, 75 MHz): δ 191.1, 167.1 (d, J_{C-F} = 251.2 Hz), 163.3 (d, J_{C-F} = 13.8 Hz), 129.5 (d, J_{C-F} = 11.6 Hz), 118.3, 109.6 (d, J_{C-F} = 22.7 Hz), 104.9 (d, J_{C-F} = 24.3 Hz), 79.6, 63.0, 38.9. HRMS (ESI) *m/z* calcd for $C_{10}H_{10}FO_3$ $(M+H)^+$ 197.0608, found 197.0609.

7-chloro-2-(hydroxymethyl)chroman-4-one (3ga)



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow solid (33.9 mg, 80%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.79 (d, *J* = 8.2 Hz, 1H), 7.00-6.97 (m, 2H), 4.60-4.54 (m, 1H), 3.99-3.96 (m, 1H), 3.85-3.81 (m, 1H), 2.96-2.88 (m, 1H), 2.65-2.60 (m, 1H), 2.49 (s, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 191.1, 161.5, 142.0, 128.3, 122.5, 119.4, 118.0, 78.7, 64.3, 38.8. HRMS (ESI) *m/z* calcd for $C_{10}H_{10}ClO_3$ $(M+H)^+$ 213.0313, found 213.0315.

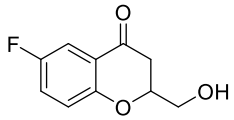
7-bromo-2-(hydroxymethyl)chroman-4-one (3ha)



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow solid (37.9 mg, 74%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.70 (d, *J* = 8.4 Hz, 1H), 7.18-7.13 (m, 2H),

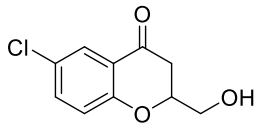
4.59-4.53 (m, 1H), 3.99-3.95 (m, 1H), 3.85-3.80 (m, 1H), 2.95-2.88 (m, 1H), 2.65-2.60 (m, 1H), 2.51 (s, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 191.3, 161.3, 130.6, 128.3, 125.3, 121.1, 119.7, 78.7, 64.3, 38.8. HRMS (ESI) *m/z* calcd for $C_{10}H_{10}BrO_3$ $(M+H)^+$ 256.9808, found 256.9813.

6-fluoro-2-(hydroxymethyl)chroman-4-one (3ia)



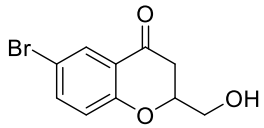
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (19.6 mg, 50%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.49 (dd, *J* = 8.2, 3.2Hz, 1H), 7.21-7.16 (m, 1H), 6.96 (d, *J* = 9.0 4.2 Hz, 1H), 4.57-4.50 (m, 1H), 3.99-3.80 (m, 1H), 2.95-2.87 (m, 1H), 2.64-2.59 (m, 1H), 2.54 (s, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 191.3 (d, J_{C-F} = 2.3 Hz), 157.4 (d, J_{C-F} = 2.3 Hz), 157.3 (d, J_{C-F} = 32.1 Hz), 123.7 (d, J_{C-F} = 32.5 Hz), 121.3 (d, J_{C-F} = 8.6 Hz), 119.5 (d, J_{C-F} = 9.8 Hz), 111.9 (d, J_{C-F} = 31.0 Hz), 78.4, 64.4, 38.8. HRMS (ESI) *m/z* calcd for $C_{10}H_{10}FO_3$ $(M+H)^+$ 197.0608, found 197.0609.

6-chloro-2-(hydroxymethyl)chroman-4-one (3ja)



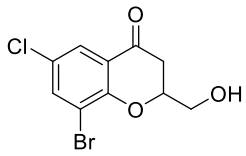
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow solid (17.8 mg, 42%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.77 (d, *J* = 2.5 Hz, 1H), 7.35 (dd, *J* = 8.8, 2.6 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 1H), 4.53-4.46 (m, 1H), 3.95-3.75 (m, 1H), 2.92-2.82 (m, 1H), 2.61-2.54 (m, 1H), 2.15 (s, 1H). ^{13}C NMR (DMSO-d_6, 75 MHz): δ 191.5, 160.3, 136.0, 125.6, 125.5, 122.0, 120.6, 79.2, 63.1, 38.9. HRMS (ESI) *m/z* calcd for $C_{10}H_{10}ClO_3$ $(M+H)^+$ 213.0313, found 213.0315.

6-bromo-2-(hydroxymethyl)chroman-4-one (3ka)



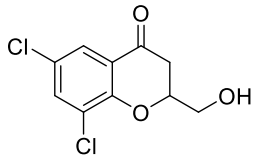
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow solid (21.0 mg, 41%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.97 (d, *J* = 2.5 Hz, 1H), 7.55 (d, *J* = 8.8, 2.5 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 1H), 4.58-4.53 (m, 1H), 4.00-3.98 (m, 1H), 3.85-3.82 (m, 1H), 2.97-2.89 (m, 1H), 2.66-2.61 (m, 1H), 2.77 (s, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 190.8, 160.0, 138.8, 129.5, 122.1, 119.9, 114.3, 78.4, 64.3, 38.7. HRMS (ESI) *m/z* calcd for $C_{10}H_{10}BrO_3$ $(M+H)^+$ 256.9808, found 256.9811.

8-bromo-6-chloro-2-(hydroxymethyl)chroman-4-one (3la)



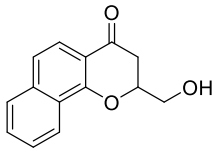
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow solid (20.3 mg, 35%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.81 (d, *J* = 2.5 Hz, 1H), 7.71 (d, *J* = 2.5 Hz, 1H), 4.67-4.59 (m, 1H), 4.08-4.03 (m, 1H), 3.90-3.86 (m, 1H), 3.02-2.92 (m, 1H), 2.72-2.65 (m, 1H), 2.32 (s, 1H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 190.8, 156.9, 138.1, 125.7, 125.3, 122.8, 112.8, 79.9, 63.1, 38.5. HRMS (ESI) *m/z* calcd for $C_{10}H_9BrClO_3$ $(M+H)^+$ 290.9418, found 290.9414.

6,8-dichloro-2-(hydroxymethyl)chroman-4-one (3ma)



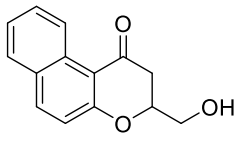
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow solid (20.2 mg, 41%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.76 (d, *J* = 2.4 Hz, 1H), 7.54 (d, *J* = 2.4 Hz, 1H), 4.66-4.59 (m, 1H), 4.08-4.04 (m, 1H), 3.89-3.86 (m, 1H), 3.03-2.92 (m, 1H), 2.72-2.65 (m, 1H), 2.34 (s, 1H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 190.8, 156.0, 135.3, 125.3, 124.6, 123.5, 123.0, 79.9, 63.0, 38.6. HRMS (ESI) *m/z* calcd for $C_{10}H_9Cl_2O_3$ $(M+H)^+$ 246.9923, found 246.9920.

2-(hydroxymethyl)-2,3-dihydro-4H-benzo[h]chromen-4-one (3na)



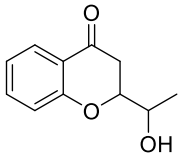
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow solid (25.1 mg, 55%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.30 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 8.7 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.63-7.58 (m, 1H), 7.53-7.49 (m, 1H), 7.39 (d, *J* = 8.7 Hz, 1H), 4.78-4.72 (m, 1H), 4.15-4.41 (m, 1H), 3.99-3.95 (m, 1H), 3.08-3.01 (m, 1H), 2.73-2.68 (m, 1H), 2.52 (s, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 191.9, 159.4, 137.5, 129.7, 127.9, 126.3, 124.6, 123.4, 121.6, 121.3, 115.4, 79.2, 64.5, 38.4. HRMS (ESI) *m/z* calcd for $C_{14}H_{13}O_3$ $(M+H)^+$ 229.0859, found 229.0860.

3-(hydroxymethyl)-2,3-dihydro-1H-benzo[f]chromen-1-one (3oa)



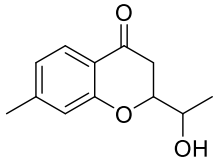
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow solid (18.2 mg, 40%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 9.44 (d, *J* = 8.6 Hz, 1H), 7.92 (d, *J* = 9.0 Hz, 1H), 7.74 (d, *J* = 7.9 Hz, 1H), 7.66-7.60 (m, 1H), 7.45-7.40 (m, 1H), 7.12 (d, *J* = 9.0 Hz, 1H), 4.73-4.64 (m, 1H), 4.05-3.88 (m, 2H), 3.11-3.01 (m, 1H), 2.73-2.66 (m, 1H), 2.29 (s, 1H). ^{13}C NMR (DMSO-d_6, 100 MHz): δ 193.9, 163.7, 137.9, 131.4, 129.8, 129.2, 129.1, 125.4, 125.0, 119.5, 112.1, 78.9, 62.9, 39.3. HRMS (ESI) *m/z* calcd for $C_{14}H_{13}O_3$ $(M+H)^+$ 229.0859, found 229.0862.

2-(1-hydroxyethyl)chroman-4-one (3ab)



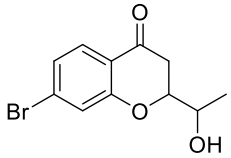
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (36.5 mg, 95%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.88-7.84 (m, 1H), 7.50-7.43 (m, 1H), 7.04-6.95 (m, 2H), 4.38-4.17 (m, 1.56H), 4.01-3.92 (m, 0.5H), 3.85-3.81 (m, 1H), 2.98-2.80 (m, 1H), 2.69-2.61 (m, 1.47H), 2.49 (s, 0.54H), 1.32 (d, *J* = 6.5 Hz, 1.46H), 1.27 (d, *J* = 6.5 Hz, 1.61H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 192.6, 192.1, 161.3, 160.9, 136.2, 136.1, 127.0, 126.9, 121.7, 121.5, 120.93, 120.91, 117.8, 81.5, 81.3, 69.2, 68.4, 39.6, 37.0, 18.5, 17.7. HRMS (ESI) *m/z* calcd for $C_{11}H_{13}O_3$ $(M+H)^+$ 193.0859, found 193.0860.

2-(1-hydroxyethyl)-7-methylchroman-4-one (3cb)



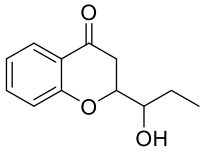
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (33.8 mg, 82%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.74-7.72 (m, 1H), 6.82-6.75 (m, 2H), 4.33-4.16 (m, 1H), 4.20-4.19 (m, 1H), 4.18-4.16 (m, 0.54H), 3.98-3.91 (m, 0.49H), 2.92-2.73 (m, 1.48H), 2.65-2.57 (m, 1.56H), 2.32 (d, 3H), 1.30 (d, *J* = 6.4 Hz, 1.48H), 1.25 (d, *J* = 6.4 Hz, 1.65H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 192.4, 191.8, 161.3, 161.0, 147.8, 147.7, 128.9, 126.8, 123.0, 122.9, 118.7, 118.6, 117.83, 117.82, 81.5, 81.3, 69.2, 68.4, 39.5, 36.9, 21.9, 18.5, 17.8. HRMS (ESI) *m/z* calcd for $C_{12}H_{15}O_3$ $(M+H)^+$ 207.1016, found 207.1018.

7-bromo-2-(1-hydroxyethyl)chroman-4-one (3gb)



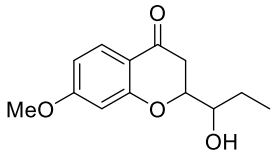
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (49.1 mg, 91%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.70-7.66 (m, 1H), 7.19-7.10 (m, 2H), 4.37-4.24 (m, 1H), 4.20-4.16 (m, 0.55H), 3.98-3.92 (m, 0.5H), 2.95-2.80 (m, 1H), 2.70-2.59 (m, 2H), 1.32 (d, *J* = 6.5 Hz, 1.47H), 1.25 (d, *J* = 6.5 Hz, 1.64H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 191.7, 191.3, 161.4, 161.2, 130.5, 130.4, 128.2, 128.1, 125.3, 125.2, 121.1, 121.0, 119.8, 119.7, 81.9, 81.8, 69.0, 68.3, 39.4, 36.8, 18.5, 17.8. HRMS (ESI) *m/z* calcd for $C_{11}H_{12}BrO_3$ $(M+H)^+$ 270.9964, found 270.9960.

2-(1-hydroxypropyl)chroman-4-one (3ac)



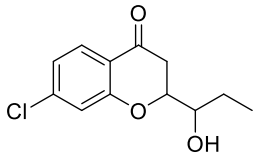
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (31.3 mg, 76%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.89-7.86 (m, 1H), 7.51-7.44 (m, 1H), 7.05-6.96 (m, 2H), 4.46-4.35 (m, 1H), 3.98-3.95 (m, 0.54H), 3.67-3.65 (m, 0.48H), 3.04-2.92 (m, 1H), 2.67-2.66 (m, 0.54H), 2.61-2.60 (m, 0.46H), 2.23 (s, 1H), 1.73-1.67 (m, 1H), 1.61-1.51 (m, 1H), 1.08-1.02 (m, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 192.7, 192.3, 161.3, 160.1, 136.12, 136.10, 127.0, 121.7, 121.6, 120.9, 117.9, 117.8, 80.4, 79.9, 74.3, 73.9, 39.8, 36.9, 25.8, 24.8, 10.3, 9.9. HRMS (ESI) *m/z* calcd for $C_{12}H_{15}O_3$ $(M+H)^+$ 207.1016, found 207.1018.

2-(1-hydroxypropyl)-7-methoxychroman-4-one (3dc)



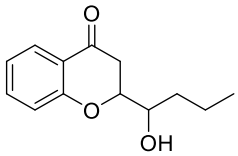
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave a yellow liquid (34.0 mg, 72%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.79-7.75 (m, 1H), 6.57-6.52 (m, 1H), 6.41-6.38 (m, 1H), 4.41-4.30 (m, 1H), 3.94-3.89 (m, 0.2H), 3.80 (d, 3H), 3.67-3.59 (m, 0.8H), 2.95-2.84 (m, 1H), 2.59-2.50 (m, 2H), 1.72-1.61 (m, 1.6H), 1.56-1.48 (m, 0.41H), 1.05-1.00 (m, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 191.4, 191.0, 166.1, 166.0, 163.3, 161.1, 128.7, 114.83, 114.80, 110.1, 109.9, 100.8, 80.8, 80.3, 74.2, 73.8, 55.7, 39.3, 36.6, 25.7, 24.9, 10.3, 9.9. HRMS (ESI) *m/z* calcd for $C_{13}H_{17}O_4$ $(M+H)^+$ 237.1121, found 237.1122.

7-chloro-2-(1-hydroxypropyl)chroman-4-one (3fc)



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (32.2 mg, 67%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.79-7.76 (m, 1H), 7.01-6.95 (m, 2H), 4.44-4.35 (m, 1H), 3.98-3.91 (m, 0.21H), 3.68-3.60 (m, 0.82H), 3.02-2.91 (m, 1H), 2.67-2.58 (m, 1H), 2.44-2.36 (m, 1H), 1.74-1.63 (m, 1.64H), 1.57-1.48 (m, 0.42H), 1.06-1.01 (m, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 191.6, 191.3, 161.6, 161.4, 141.9, 141.8, 128.2, 122.4, 122.3, 119.5, 118.0, 117.9, 80.9, 80.4, 74.2, 73.7, 39.5, 36.8, 25.8, 24.9, 10.2, 9.9. HRMS (ESI) *m/z* calcd for $C_{12}H_{14}ClO_3$ $(M+H)^+$ 241.0626, found 241.0624.

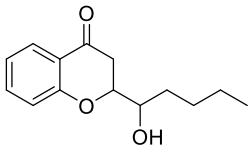
2-(1-hydroxybutyl)chroman-4-one (3ad)



Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (17.6 mg, 40%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.87-7.84 (m, 1H), 7.48-7.43 (m, 1H), 7.02-6.94 (m, 2H), 4.41-4.31 (m, 1H), 4.06-4.04 (m, 0.46H), 3.74-3.73 (m, 0.6H), 3.01-2.92 (m, 1H), 2.65-2.60 (m, 1H), 2.41 (s, 1H), 1.69-1.36 (m, 4H), 0.98-0.94 (m, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 192.8, 192.4, 161.3, 161.1, 136.1, 136.0, 126.9, 121.6, 121.5, 120.9, 117.9, 117.8, 80.7,

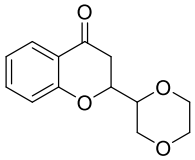
80.3, 72.7, 72.1, 39.8, 36.9, 34.8, 33.9, 19.0, 18.7, 14.0, 13.9. HRMS (ESI) *m/z* calcd for C13H17O3 $(M+H)^+$ 221.1172, found 221.1174.

2-(1-hydroxypentyl)chroman-4-one (3ae)



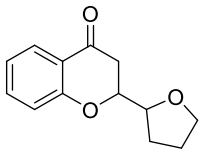
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (14.0 mg, 30%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.87-7.84 (m, 1H), 7.48-7.43 (m, 1H), 7.02-6.94 (m, 2H), 4.41-4.32 (m, 1H), 4.03 (s, 0.5H), 3.72 (s, 0.51H), 3.01-2.92 (m, 1H), 2.65-2.59 (m, 1H), 2.44 (s, 1H), 1.68-1.24 (m, 6H), 0.93-0.89 (m, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 192.8, 192.4, 161.3, 161.1, 136.1, 136.0, 126.9, 121.6, 121.5, 120.9, 117.9, 117.8, 80.7, 80.3, 72.9, 72.3, 39.8, 36.9, 32.4, 31.5, 27.9, 27.6, 22.7, 22.6, 14.03, 14.00. HRMS (ESI) *m/z* calcd for $C_{14}H_{19}O_3$ $(M+H)^+$ 235.1329, found 235.1330.

2-(1,4-dioxan-2-yl)chroman-4-one (5a)



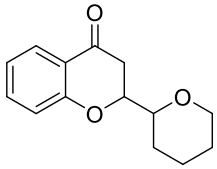
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (23.4 mg, 50%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.87-7.84 (m, 1H), 7.48-7.43 (m, 1H), 7.02-6.94 (m, 2H), 4.46-4.35 (m, 1H), 4.04-4.03 (m, 0.61H), 3.92-3.59 (m, 6H), 3.53-3.48 (m, 0.62H), 3.08-3.00 (m, 0.43H), 2.83-2.81 (m, 1H), 2.59-2.54 (m, 0.43H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 191.9, 191.5, 161.0, 160.7, 136.1, 136.0, 126.97, 126.91, 121.7, 121.1, 120.9, 118.1, 117.9, 76.9, 76.8, 75.7, 75.5, 68.2, 67.4, 67.3, 66.7, 66.5, 66.4, 39.1, 38.9. HRMS (ESI) *m/z* calcd for $C_{13}H_{15}O_4$ $(M+H)^+$ 235.0965, found 235.0966.

2-(tetrahydrofuran-2-yl)chroman-4-one (5b)



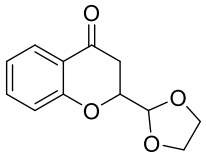
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (37.5 mg, 86%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.83 (d, *J* = 7.8 Hz, 1H), 7.45-7.40 (m, 1H), 7.02-6.94 (m, 2H), 4.39-4.32 (m, 1H), 4.15-4.10 (m, 0.53H), 4.09-4.04 (m, 0.48H), 3.92-3.77 (m, 2H), 2.90-2.59 (m, 2H), 2.10-1.81 (m, 4H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 192.1, 192.0, 161.4, 161.3, 136.0, 135.9, 126.9, 126.8, 121.3, 120.0, 120.9, 118.1, 117.9, 79.8, 79.6, 79.4, 68.9, 68.8, 39.8, 39.0, 27.6, 27.5, 25.9, 25.7. HRMS (ESI) *m/z* calcd for $C_{13}H_{15}O_3$ $(M+H)^+$ 219.1016, found 219.1018.

2-(tetrahydro-2*H*-pyran-2-yl)chroman-4-one (5c)



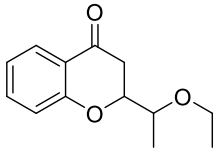
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (33.9 mg, 73%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.86-7.83 (m, 1H), 7.46-7.42 (m, 1H), 7.03-6.96 (m, 2H), 4.38-4.29 (m, 1H), 4.10-4.02 (m, 1H), 3.64-3.59 (m, 0.66H), 3.52-3.44 (m, 1.42H), 3.02-2.84 (m, 1H), 2.76-2.71 (m, 0.63H), 2.61-2.56 (m, 0.40H), 1.96-1.39 (m, 6H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 192.7, 192.6, 161.5, 161.4, 135.9, 126.9, 126.8, 121.3, 121.1, 120.9, 118.2, 118.0, 80.1, 79.6, 78.2, 78.1, 77.5, 77.1, 76.7, 69.1, 68.8, 39.3, 38.5, 27.3, 26.9, 25.9, 25.8, 23.2, 23.0. HRMS (ESI) *m/z* calcd for $C_{14}H_{17}O_3$ $(M+H)^+$ 233.1172, found 233.1175.

2-(1,3-dioxolan-2-yl)chroman-4-one (5d)



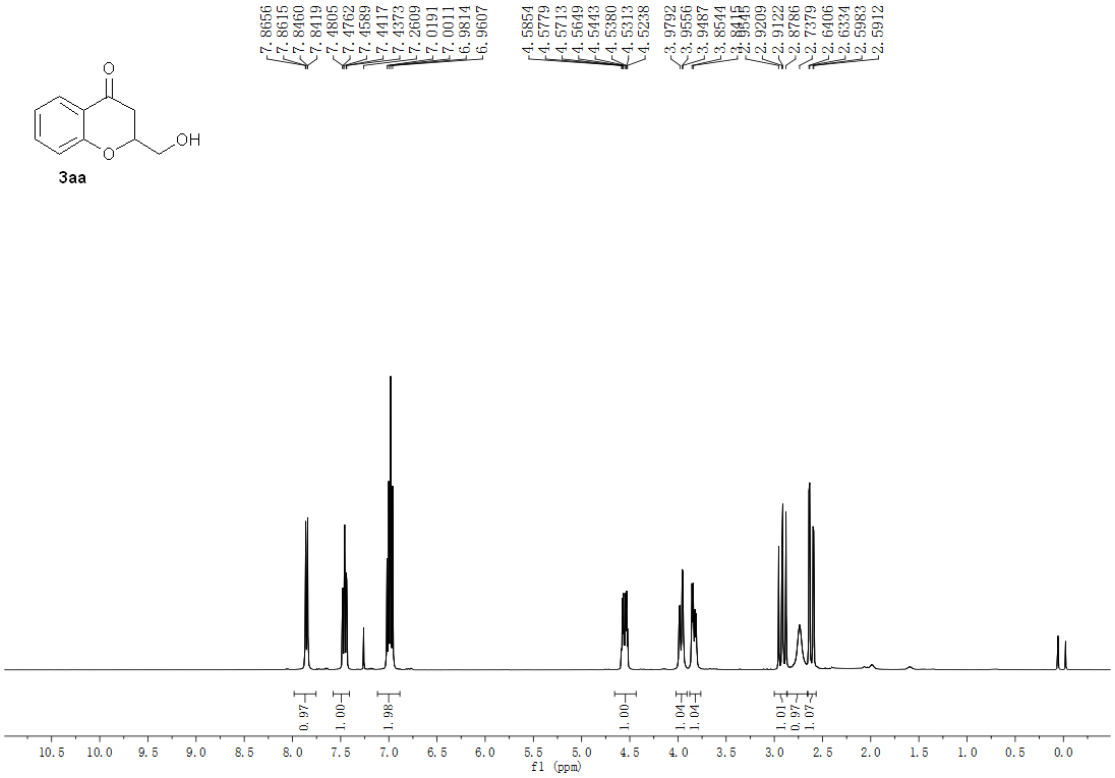
Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (17.6 mg, 40%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.88-7.85 (m, 1H), 7.49-7.45 (m, 1H), 7.04-6.97 (m, 2H), 5.20 (d, *J* = 3.5 Hz, 1H), 4.54-4.51 (m, 1H), 4.07-3.95 (m, 4H), 2.92-2.85 (m, 1H), 2.79-2.72 (m, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 192.4, 160.7, 136.1, 126.8, 121.6, 121.1, 117.9, 103.0, 77.6, 65.8, 65.5, 37.1. HRMS (ESI) *m/z* calcd for $C_{12}H_{13}O_4$ $(M+H)^+$ 221.0808, found 221.0806.

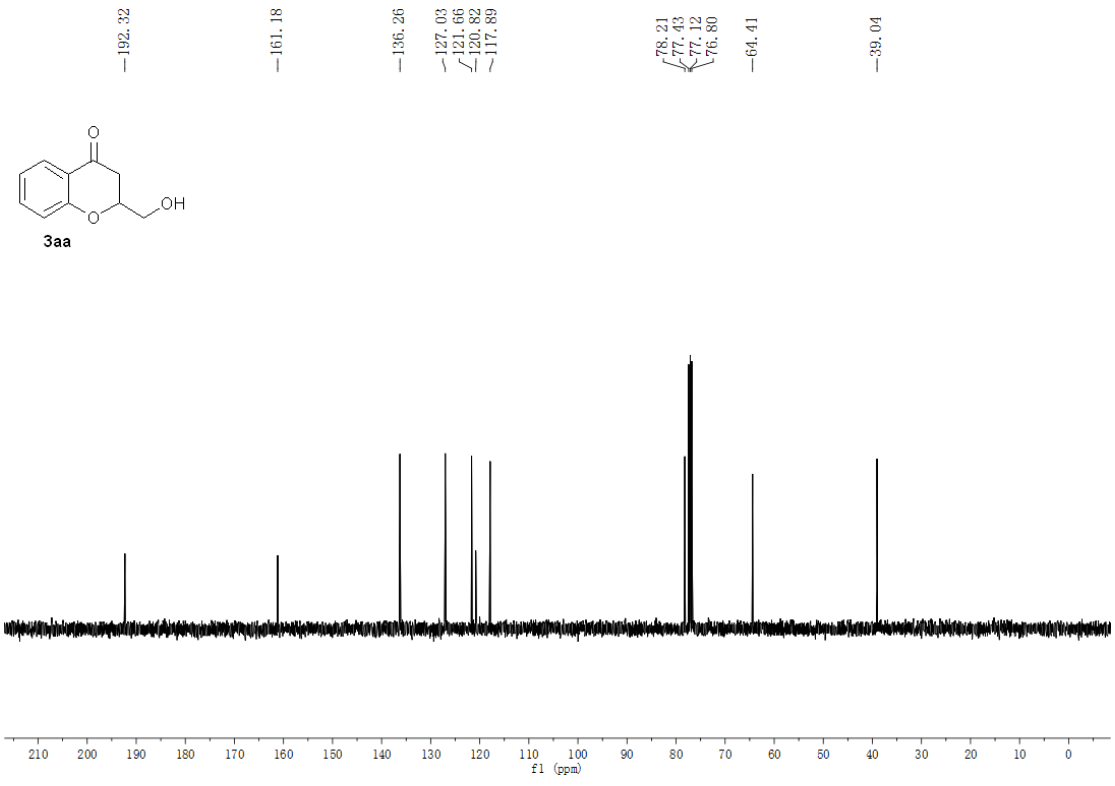
2-(1-ethoxyethyl)chroman-4-one (5e)

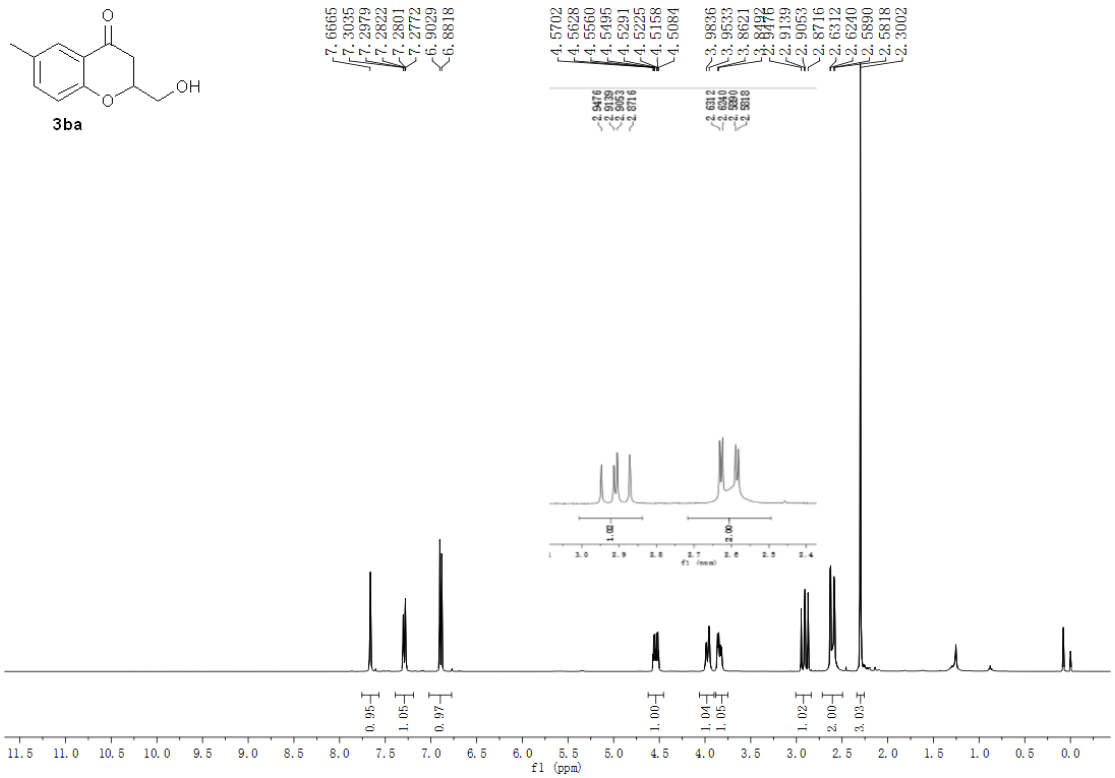


Flash column chromatography on silica gel (petroleum ether/ethyl acetate 3/1) gave a yellow liquid (22.0 mg, 50%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.86-7.83 (m, 1H), 7.47-7.42 (m, 1H), 6.99-6.96 (m, 2H), 4.44-4.38 (m, 0.38H), 4.34-4.29 (m, 0.61H), 3.75-3.61 (m, 2H), 3.58-3.46 (m, 1H), 2.96-2.74 (m, 1.66H), 2.64-2.59 (m, 0.41H), 1.32-1.25 (m, 3H), 1.21-1.16 (m, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 192.8, 192.6, 161.5, 161.3, 135.9, 135.8, 126.9, 126.8, 121.3, 121.1, 121.0, 118.1, 117.9, 80.6, 79.8, 75.9, 75.5, 65.4, 65.2, 38.9, 38.4, 16.2, 15.5, 15.48, 15.40. HRMS (ESI) *m/z* calcd for $C_{13}H_{17}O_3$ $(M+H)^+$ 221.1172, found 221.1171.

4. Copies of ^{1}H NMR and ^{13}C NMR spectra of the products



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7.2801
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4.5560
4.5495
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4.5225
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4.5084
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3.9533
3.8621
2.9139
2.9053
2.8716
2.6312
2.6240
2.5890
2.5818
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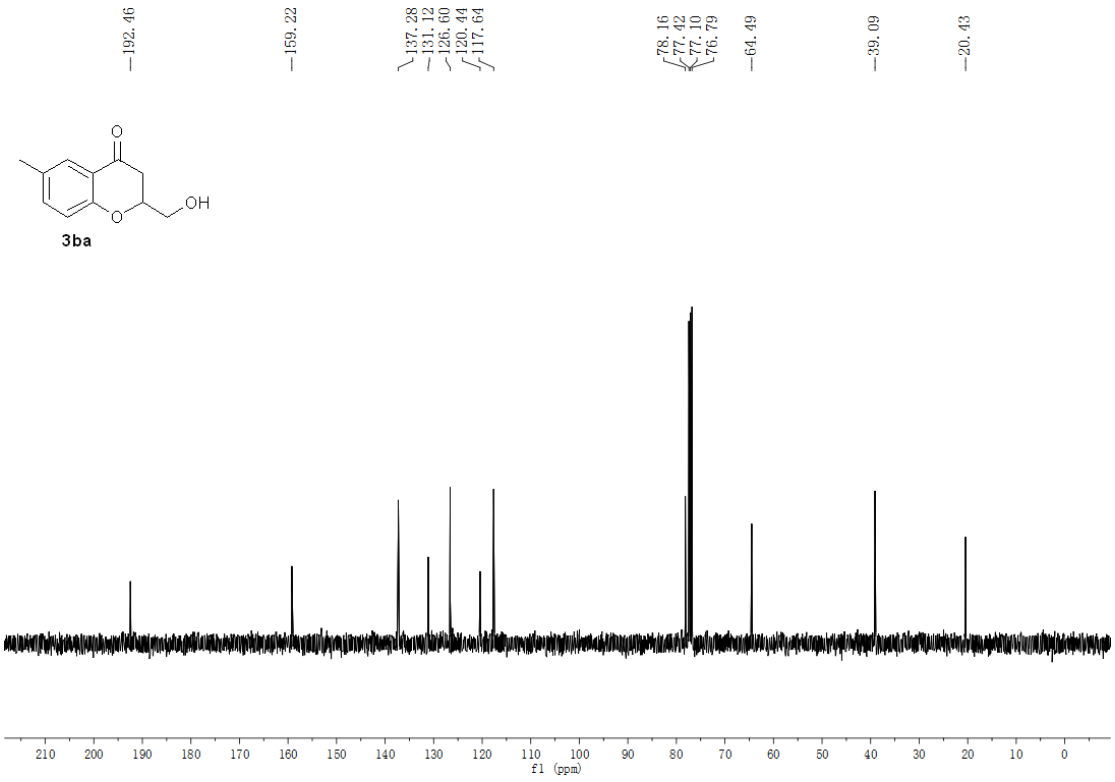
0.95
1.05
0.97
1.00
1.04
1.05
1.02
2.00
3.03
f1 (ppm)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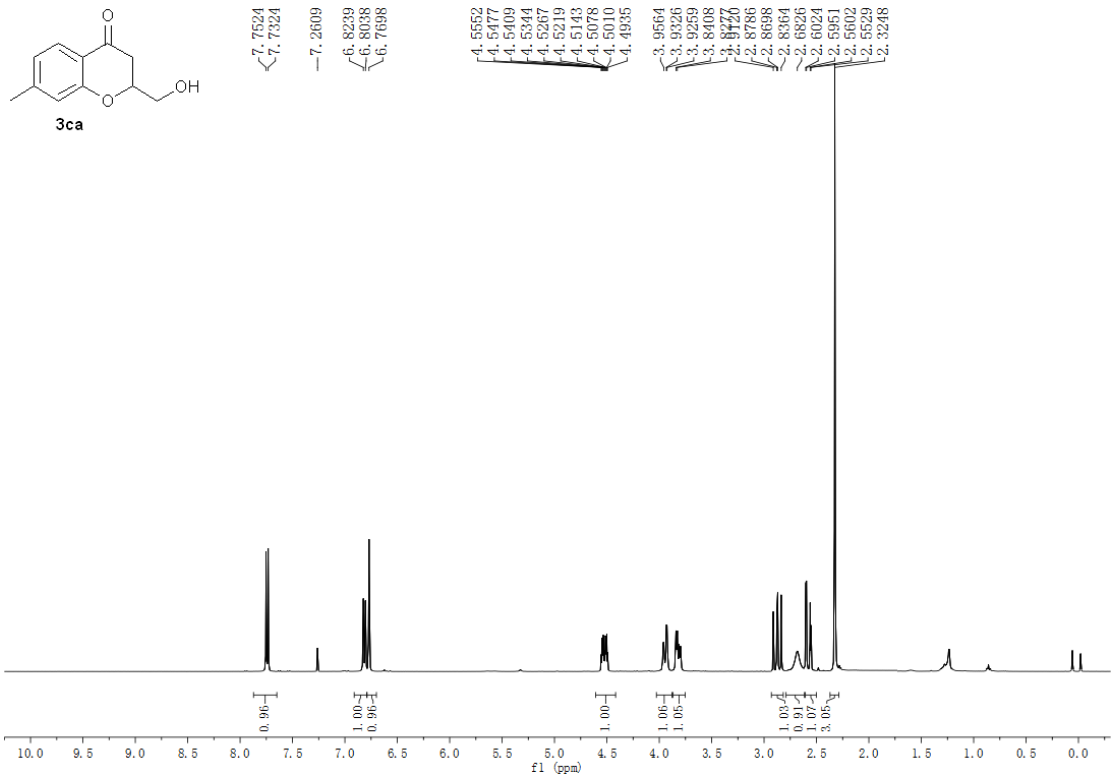
117.64
78.16
77.42
77.10
76.79
64.49
39.09
20.43
3ba
f1 (ppm)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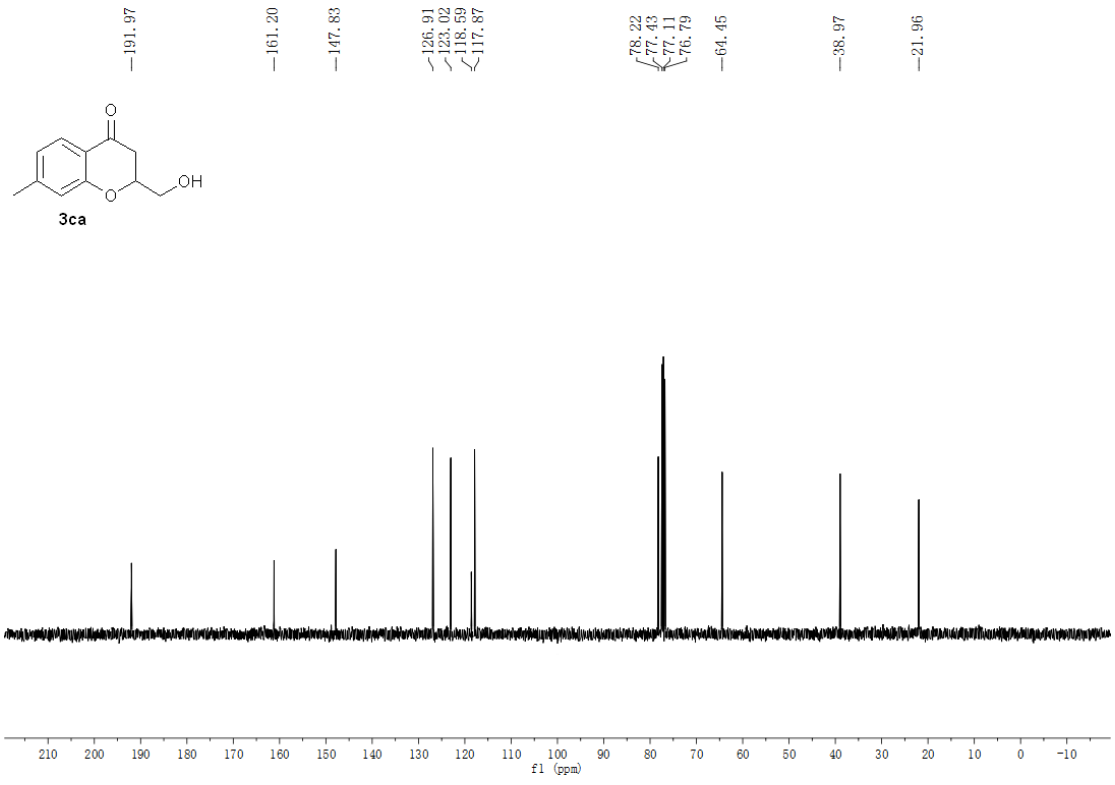
3.05
f1 (ppm)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77.43
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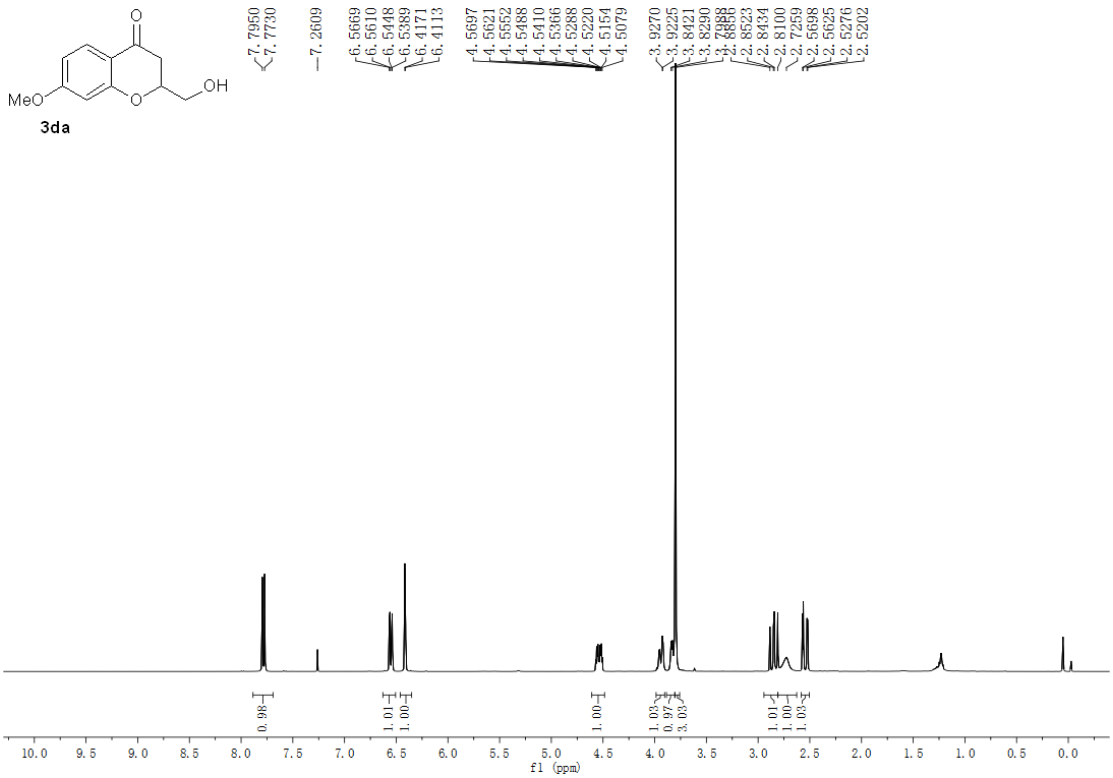
38.97
21.96
f1 (ppm)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4.5220
4.5154
4.5079
3.9270
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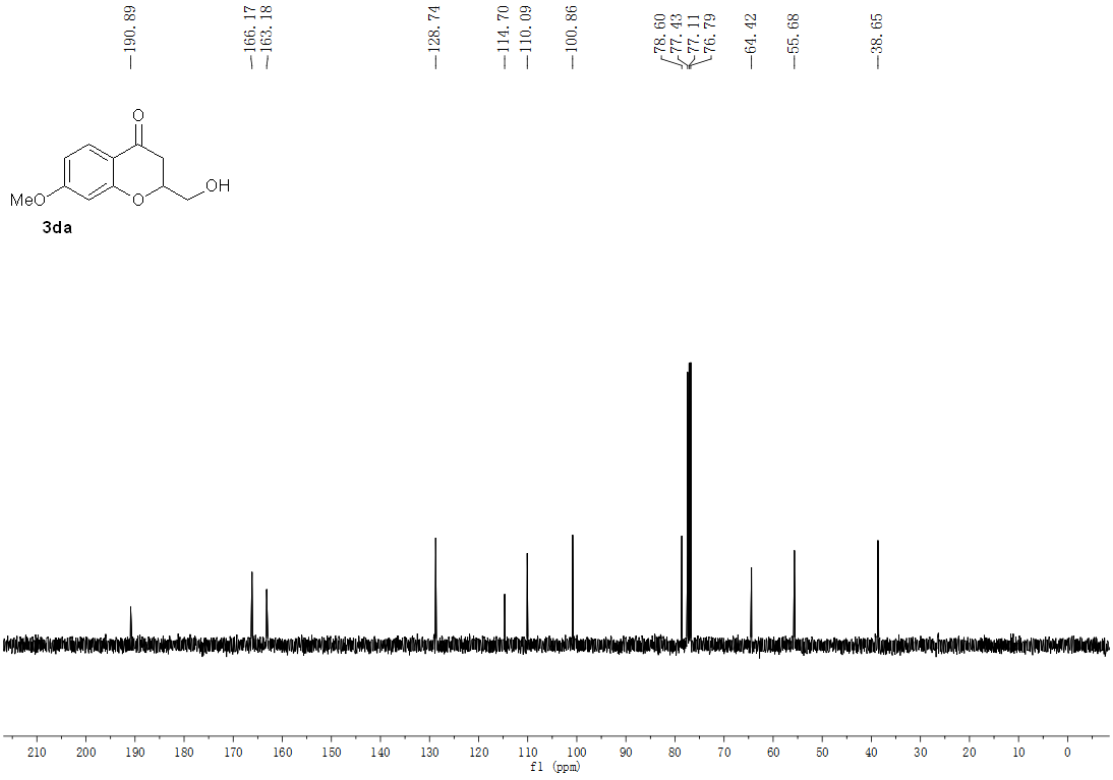
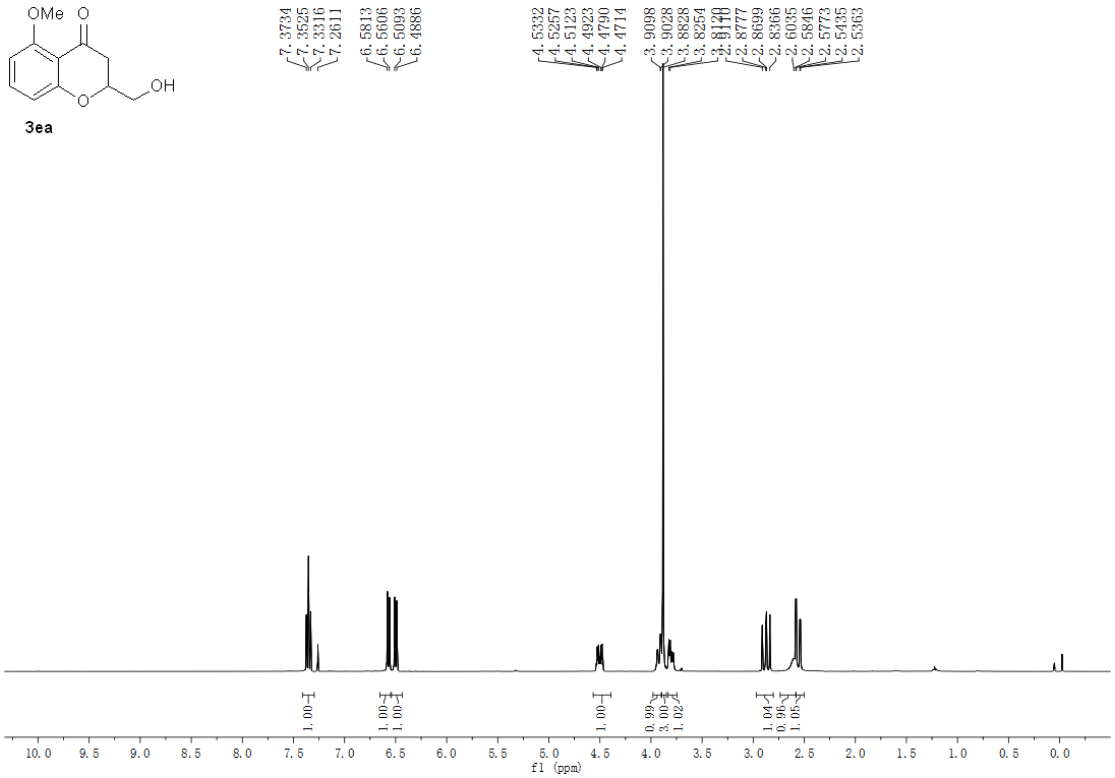
3.8421
3.8290
2.8523
2.8434
2.8100
2.7959
2.5698
2.5625
2.5276
2.5202
0.98
1.01
1.00
1.00
1.03
0.97
3.03
1.01
1.00
1.03
f1 (ppm)


3da
190.89
166.17
163.18
128.74
114.70
110.09
100.86
78.60
77.43
77.11
76.79
64.42
55.68
38.65
f1 (ppm)


OMe
O
OH
3ea
7.3734
7.3525
7.3316
7.2611
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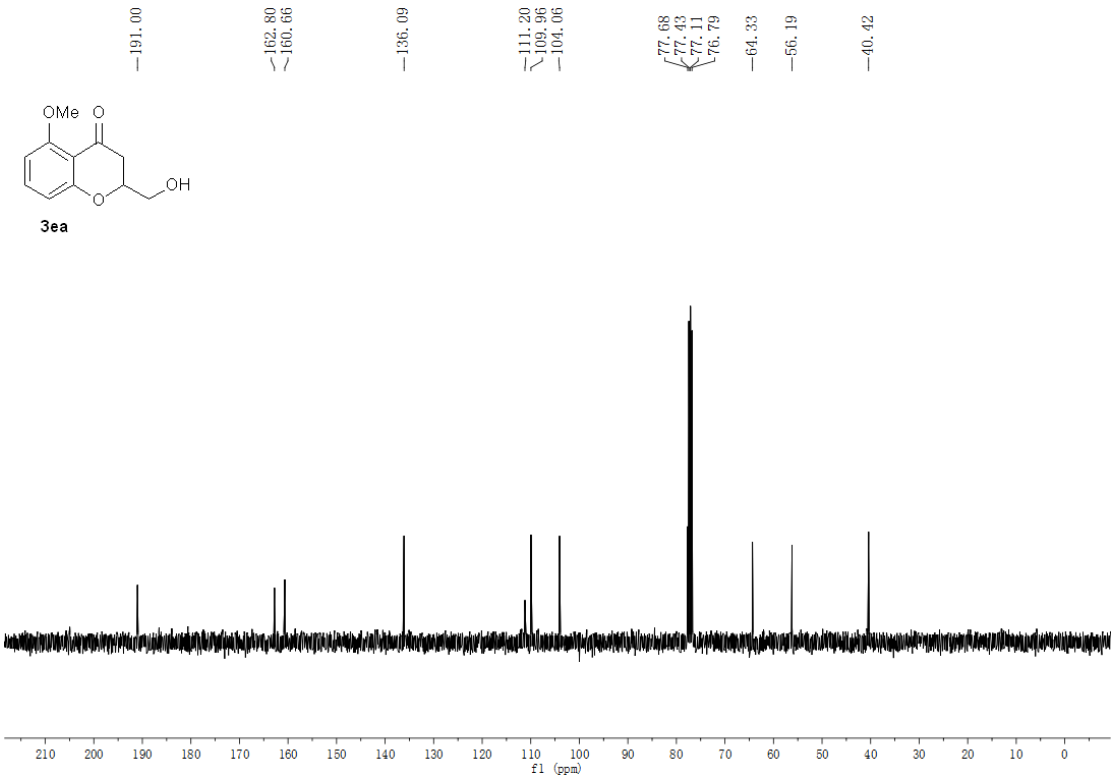
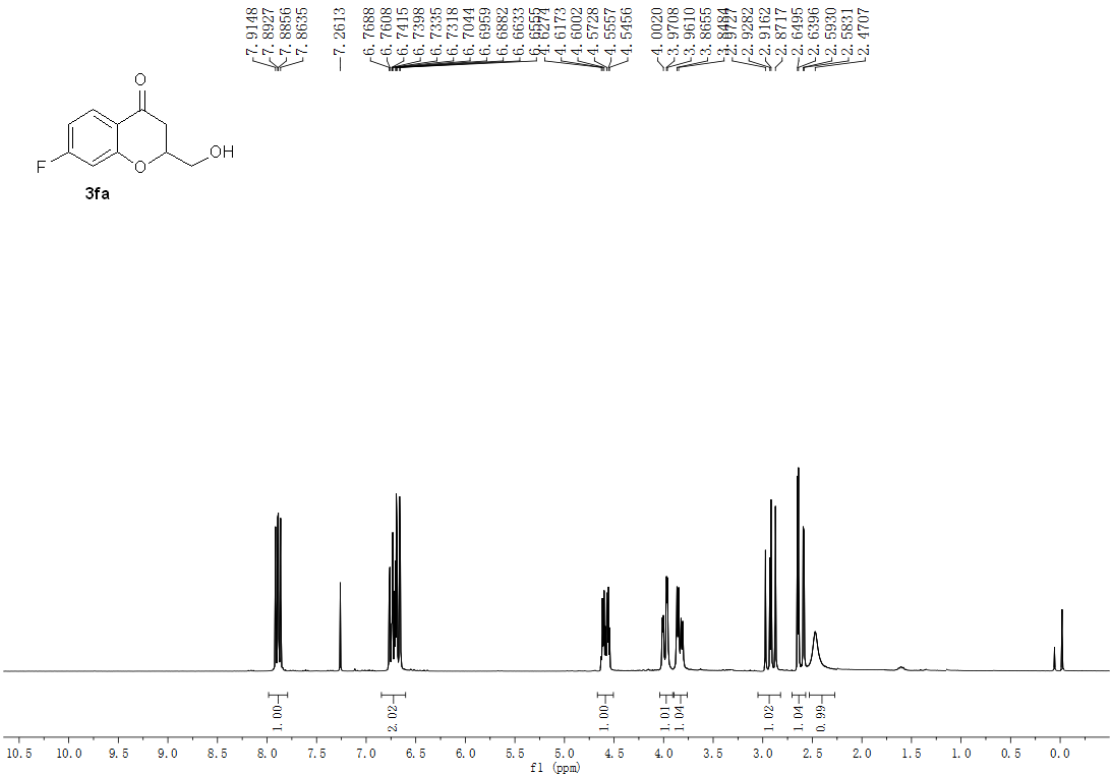
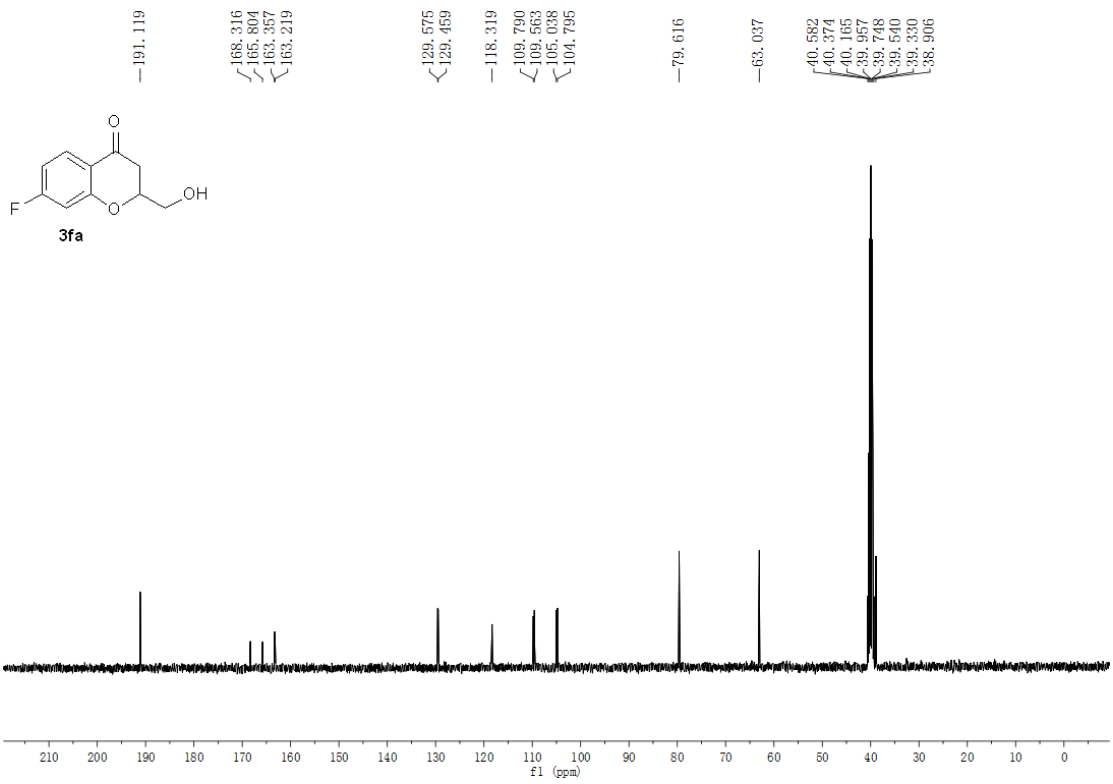
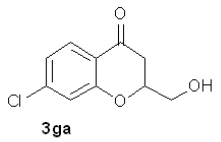
6.5606
6.5093
6.4886
4.5332
4.5257
4.5123
4.4923
4.4790
4.4714
3.9098
3.9028
3.8828
3.8254
2.8777
2.8699
2.8366
2.6035
2.5846
2.5773
2.5435
2.5363
1.00
1.00
1.00
1.00
0.99
3.00
1.02
1.04
0.96
1.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

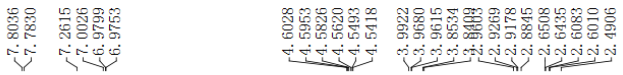

191.00
162.80
160.66
136.09
111.20
109.96
104.06
77.68
77.43
77.11
76.79
64.33
56.19
40.42
OMe
O
OH
3ea
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

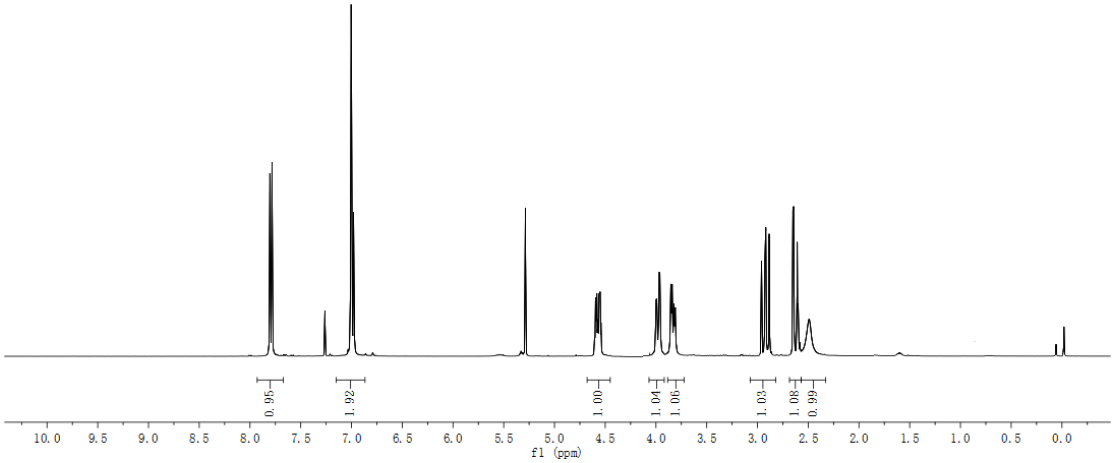

7.9148
7.8927
7.8856
7.8635
7.2613
6.7688
6.7608
6.7415
6.7398
6.7335
6.7318
6.7044
6.6959
6.6882
6.6633
4.6173
4.6002
4.5728
4.5557
4.5456
4.0020
3.9708
3.9610
3.8655
2.9727
2.9282
2.9162
2.8717
2.6495
2.6396
2.5930
2.5831
2.4707
O
F
OH
3fa
1.00
2.02
1.00
1.01
1.04
1.02
1.04
0.99
f1 (ppm)


191.119
168.316
165.804
163.357
163.219
129.575
129.459
118.319
109.790
109.563
105.038
104.795
79.616
63.037
40.582
40.374
40.165
39.957
39.748
39.540
39.330
38.906
O
F
OH
3fa
f1 (ppm)

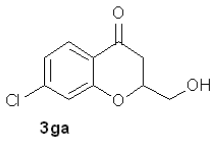

O
Cl
O
OH

3ga

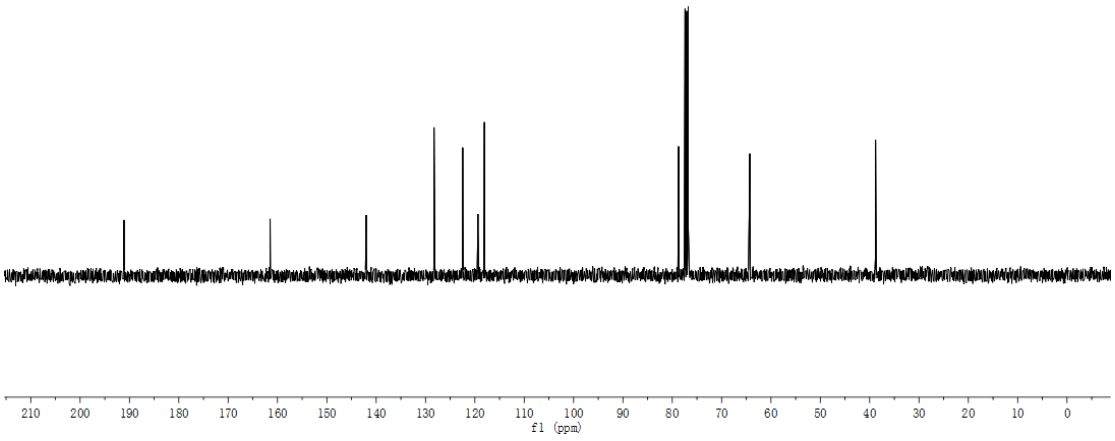

7.8036
7.7830
7.2615
7.0026
6.9799
6.9753
4.6028
4.5953
4.5826
4.5620
4.5493
4.5418
3.9922
3.9680
3.9615
3.8534
2.9269
2.9178
2.8845
2.6508
2.6435
2.6083
2.6010
2.4906

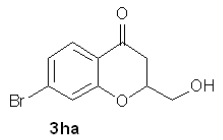

0.95
1.92
1.00
1.04
1.06
1.03
1.08
0.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


191.11
161.48
142.03
128.28
122.47
119.38
118.06
78.71
77.41
77.09
76.78
64.28
38.80

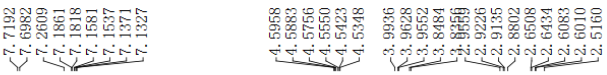

O
Cl
O
OH

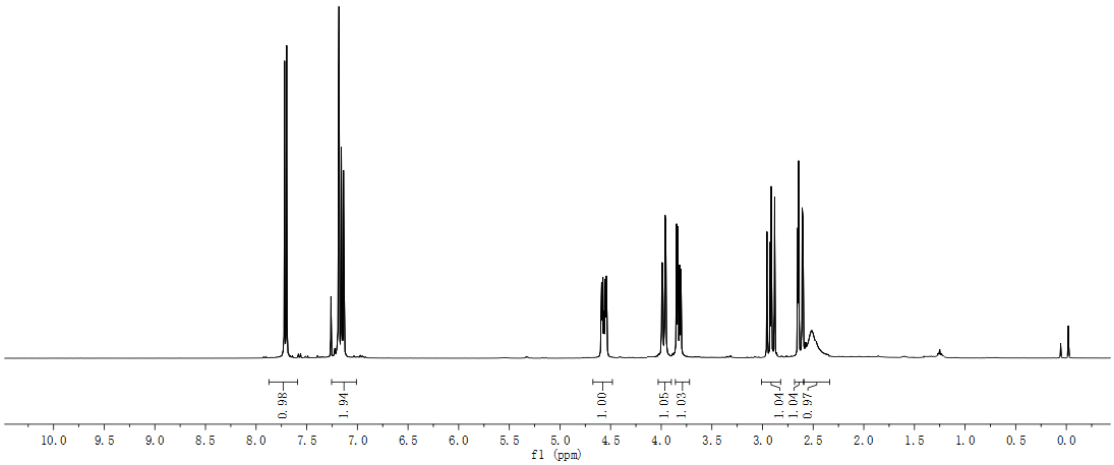
3ga

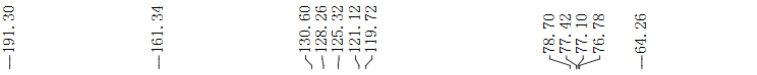

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

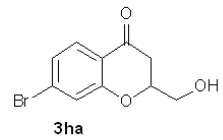

O
Br
O
OH

3ha

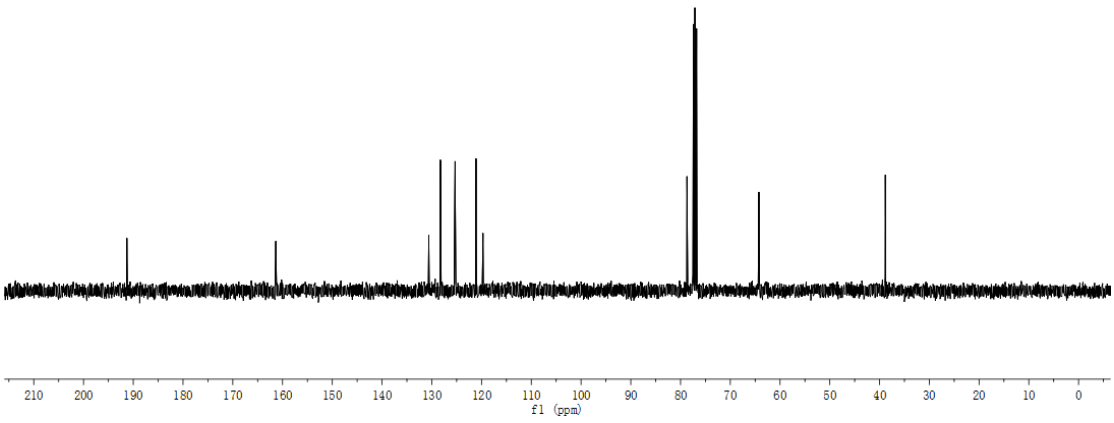

7.7192
7.6982
7.2609
7.1861
7.1818
7.1581
7.1537
7.1371
7.1327
4.5958
4.5883
4.5756
4.5550
4.5423
4.5348
3.9936
3.9628
3.9552
3.8484
2.9226
2.9135
2.8802
2.6508
2.6434
2.6083
2.6010
2.5160

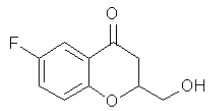

0.98
1.94
1.00
1.05
1.03
1.04
1.04
0.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


191.30
161.34
130.60
128.26
125.32
121.12
119.72
78.70
77.42
77.10
76.78
64.26
38.83

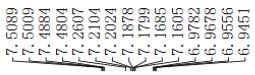

O
Br
O
OH

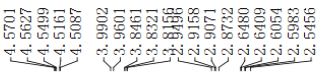
3ha

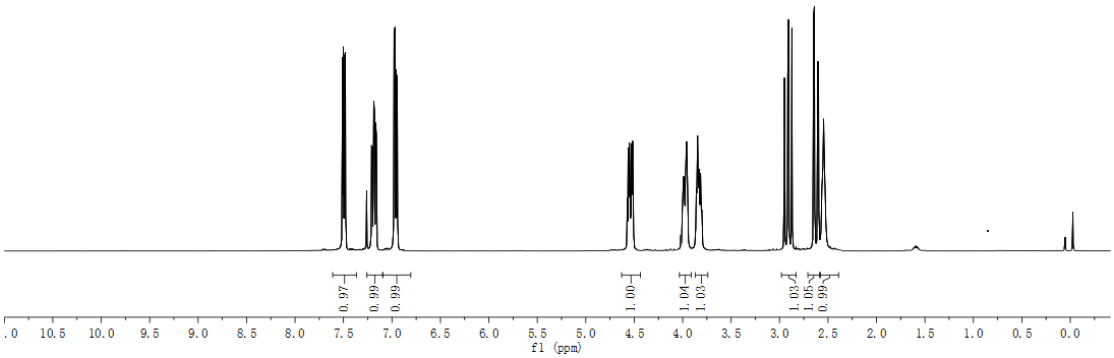

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
F
OH
O

3ia

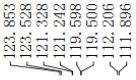

7.5089
7.5009
7.4884
7.4804
7.2607
7.2104
7.2024
7.1878
7.1799
7.1685
7.1605
6.9782
6.9678
6.9556
6.9451


4.5701
4.5627
4.5499
4.5161
4.5087
3.9902
3.9601
3.8461
3.8321
3.8156
3.8056
2.9158
2.9071
2.8732
2.6480
2.6409
2.6054
2.5983
2.5456


0.97
0.99
0.99
1.00
1.04
1.03
1.03
1.05
0.99
f1 (ppm)


191.345
191.322

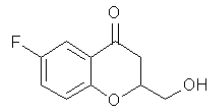
158.933
157.379
157.356
155.723


123.853
123.528
121.328
121.242
119.598
119.500
112.206
111.896

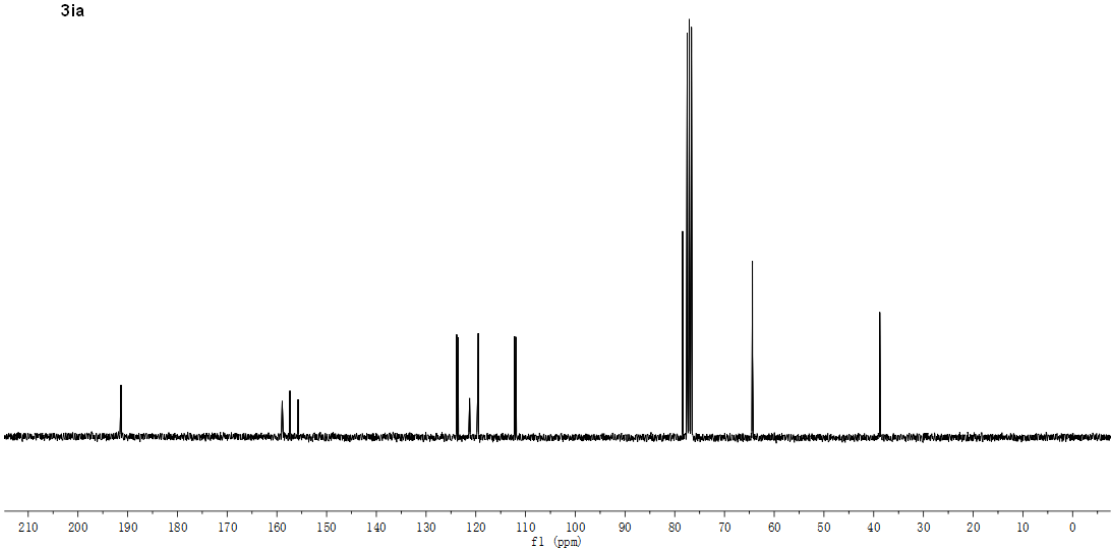

78.441
77.491
77.068
76.644

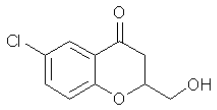

64.378


38.785


O
F
OH
O

3ia


f1 (ppm)



3ja

7.7710
7.7626
7.3750
7.3663
7.3456
7.3369
7.1997
6.9124
6.8830

4.5317
4.5226
4.5151
4.4704
4.4611
3.9527
3.9130
3.7958
3.7571
2.9229
2.8780
2.8665
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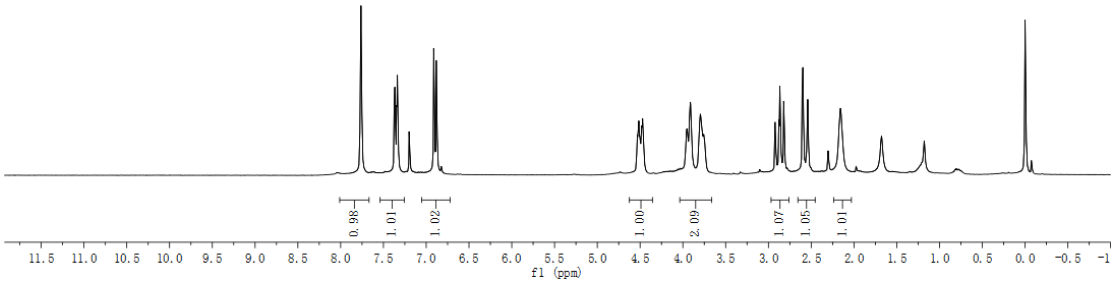
2.6067
2.5973
2.5500
2.5407
2.1574



191.48
160.26
136.04
125.63
125.58
122.05
120.65
79.20
63.10
40.59
40.38
40.17
39.96
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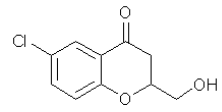
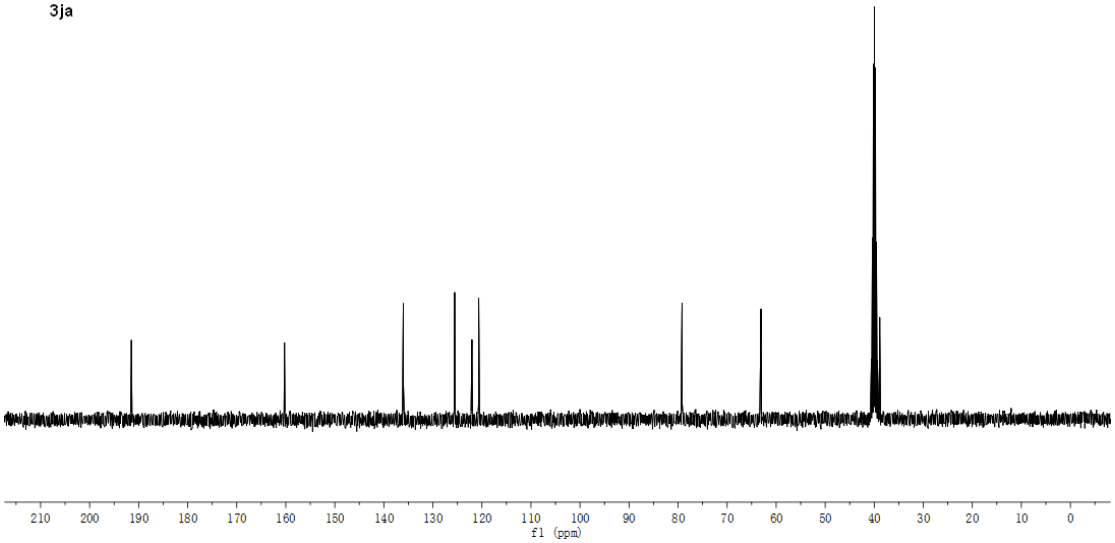
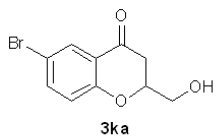
39.54
39.34
38.89



3ja





3ka

7.9748
7.9685
7.5609
7.5547
7.5389
7.5327
6.9166
6.8886
4.5806
4.5745
4.5680
4.5469
4.5410
4.5343
4.0094
3.9790
3.8539
3.8419
3.8234
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2.9337
2.9250
2.8913
2.6580
2.6509
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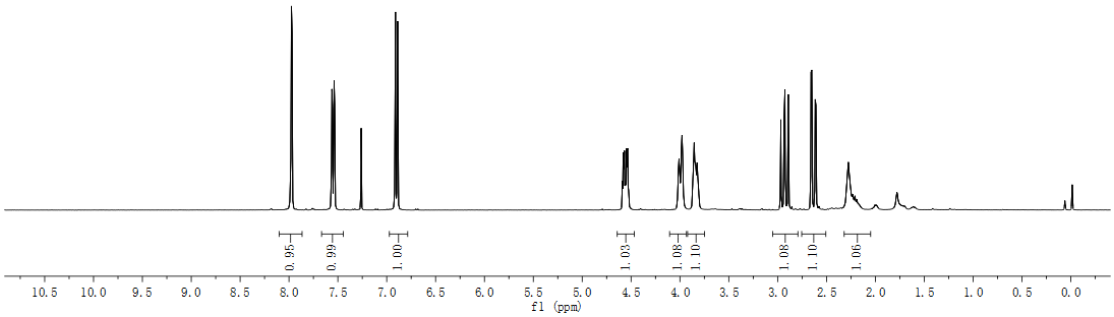
2.6084
2.2772



190.79
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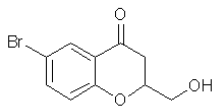
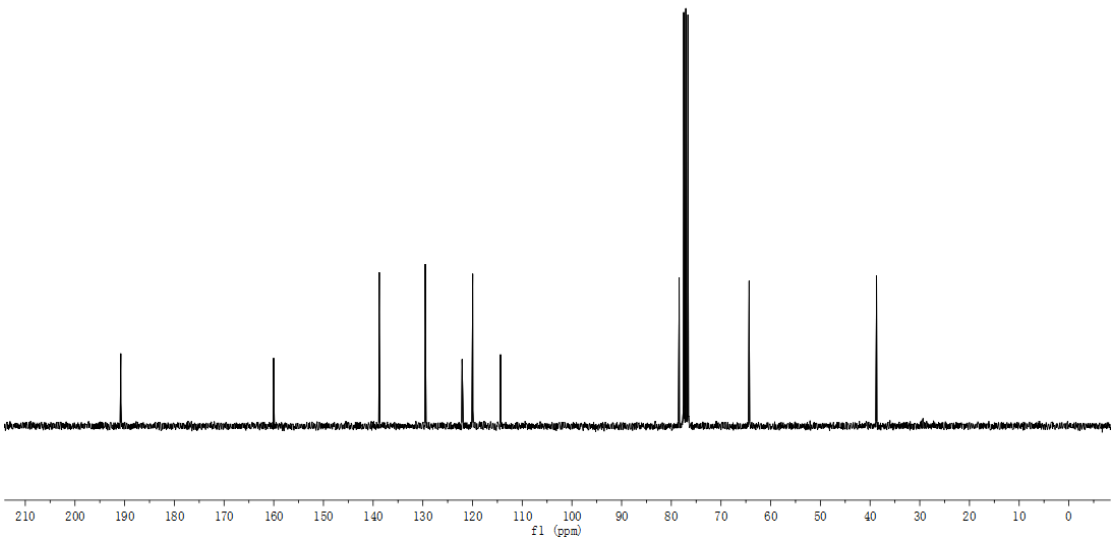
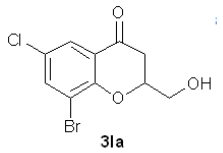
119.96
114.36
78.41
77.49
77.06
76.64
64.34
38.69



3ka



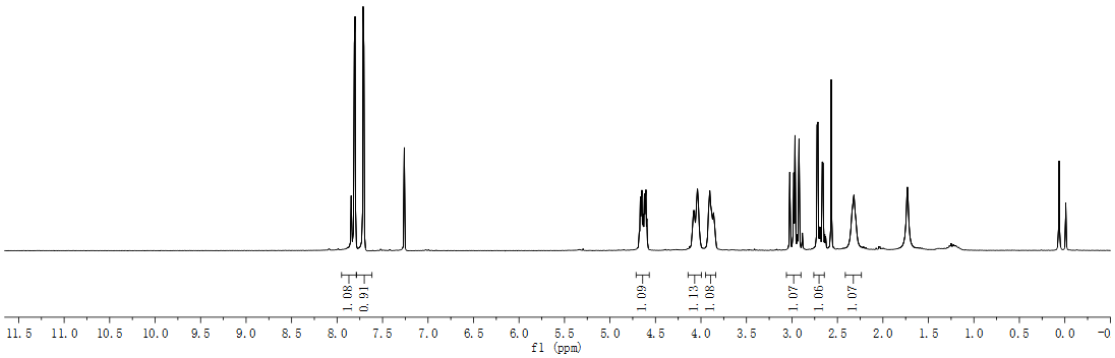


3Ia

7.8104
7.8019
7.7137
7.7052
7.2612

4.6758
4.6582
4.6488
4.6388
4.6217
4.6046
4.5948
4.0782
4.0378
3.9028
3.8616

3.0236
2.9792
2.9666
2.9223
2.7237
2.7138
2.6667
2.6568
2.3190



190.86
156.91
138.14
125.74
125.26
122.87
112.77
79.89
63.07
40.61
40.40
40.19
39.98
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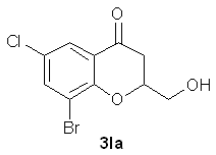
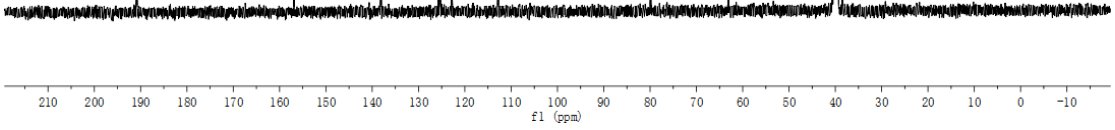
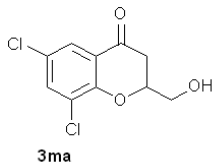
39.57
39.36
38.48

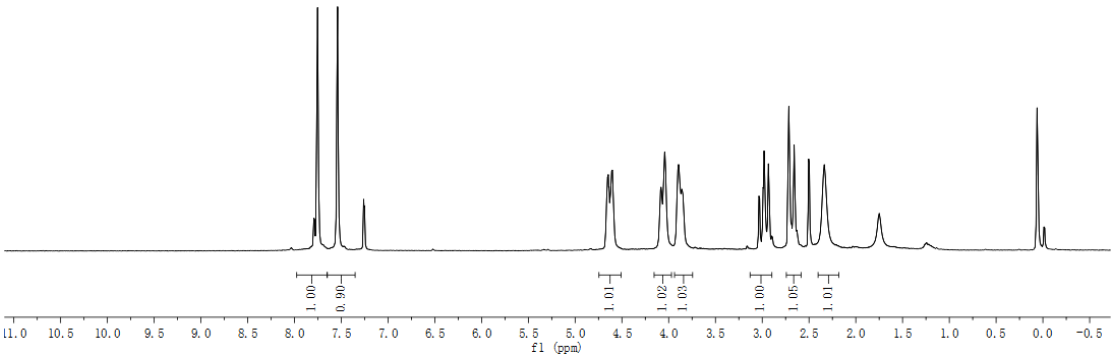


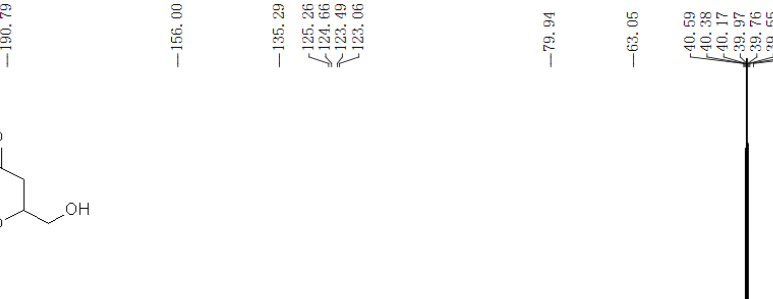
3Ia

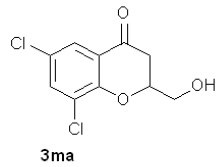




3ma

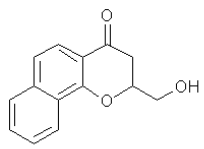






3ma

f1 (ppm)



3na

8.3119
8.2910
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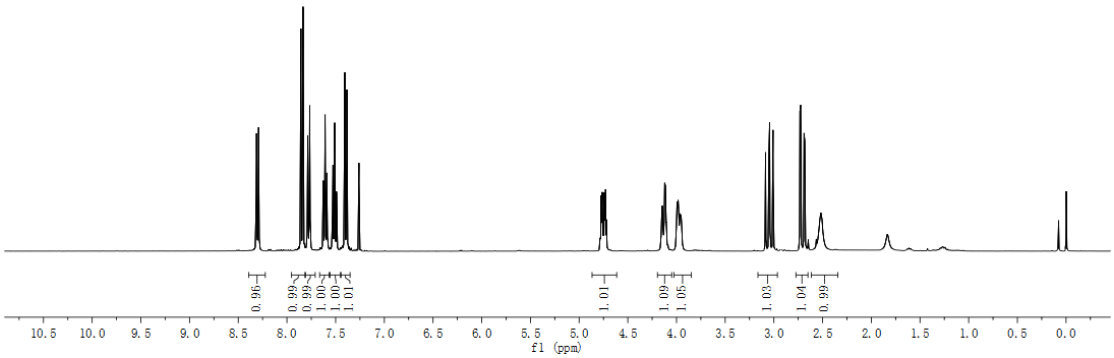

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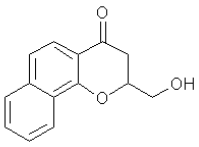
64.46
38.41



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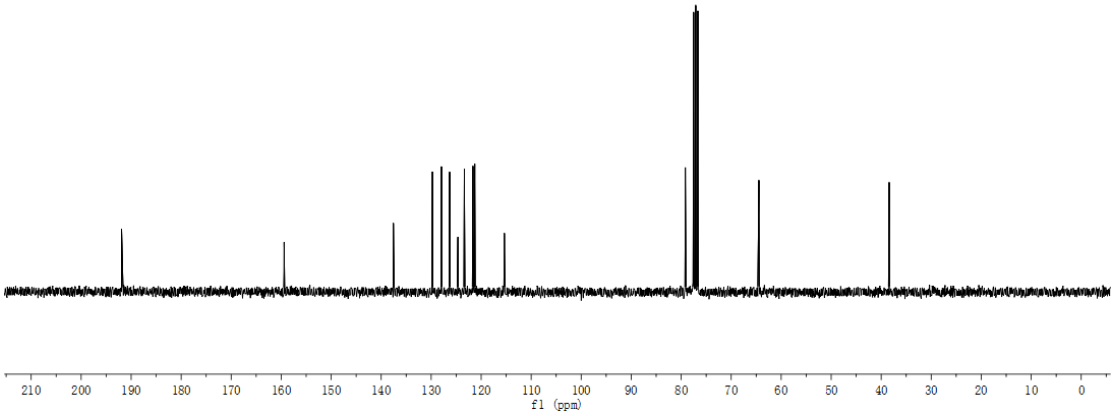

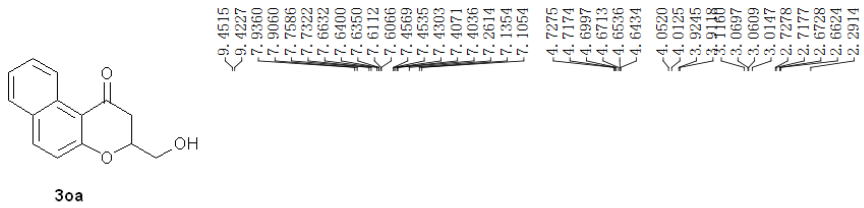
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7.6112
7.6066
7.4569
7.4535
7.4303
7.4071
7.4036
7.2614
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7.1054
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4.7174
4.6997
4.6713
4.6536
4.6434
4.0520
4.0125
3.9245
3.9118
3.1160
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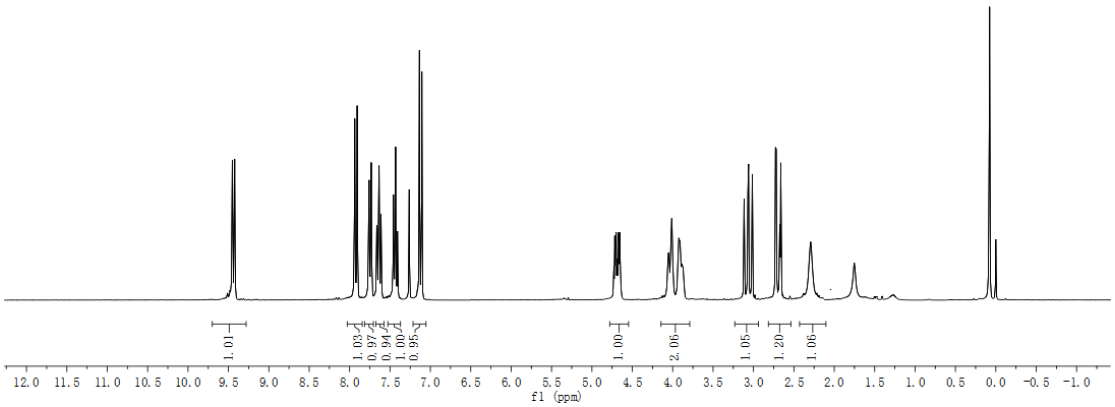
2.7278
2.7177
2.6728
2.6624
2.2914
O
OH
O

3oa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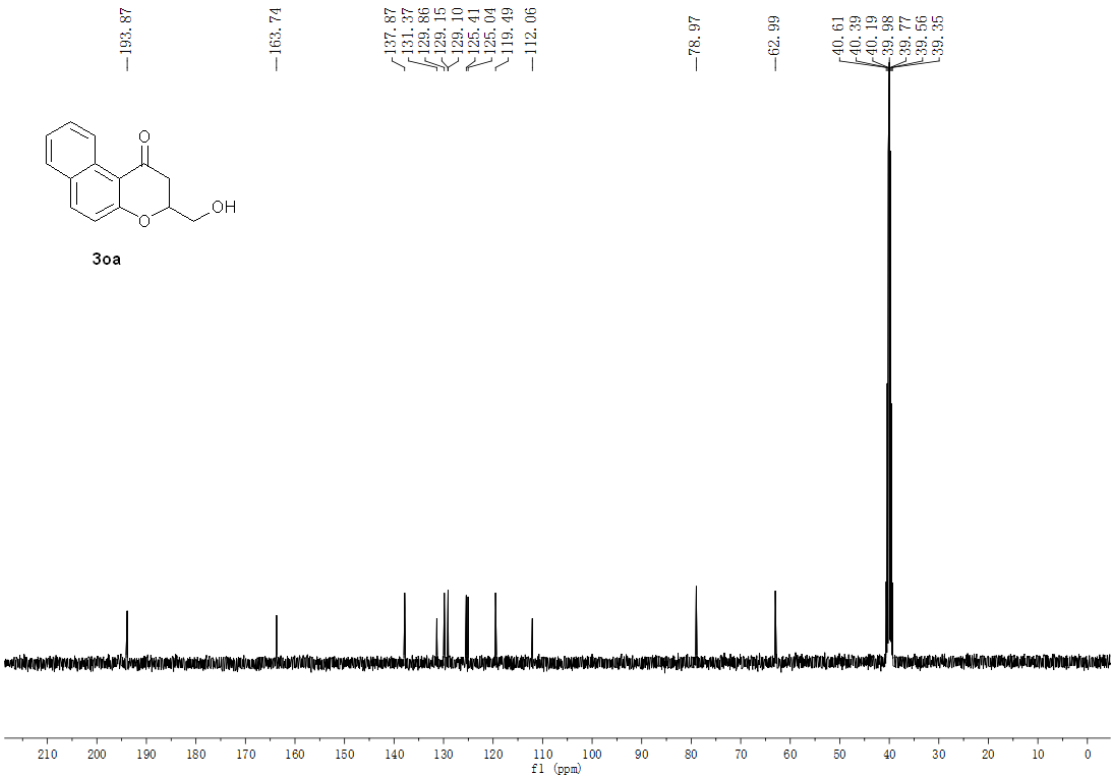
1.03
0.97
0.94
1.00
0.95
1.00
2.06
1.05
1.20
1.06
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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129.15
129.10
125.41
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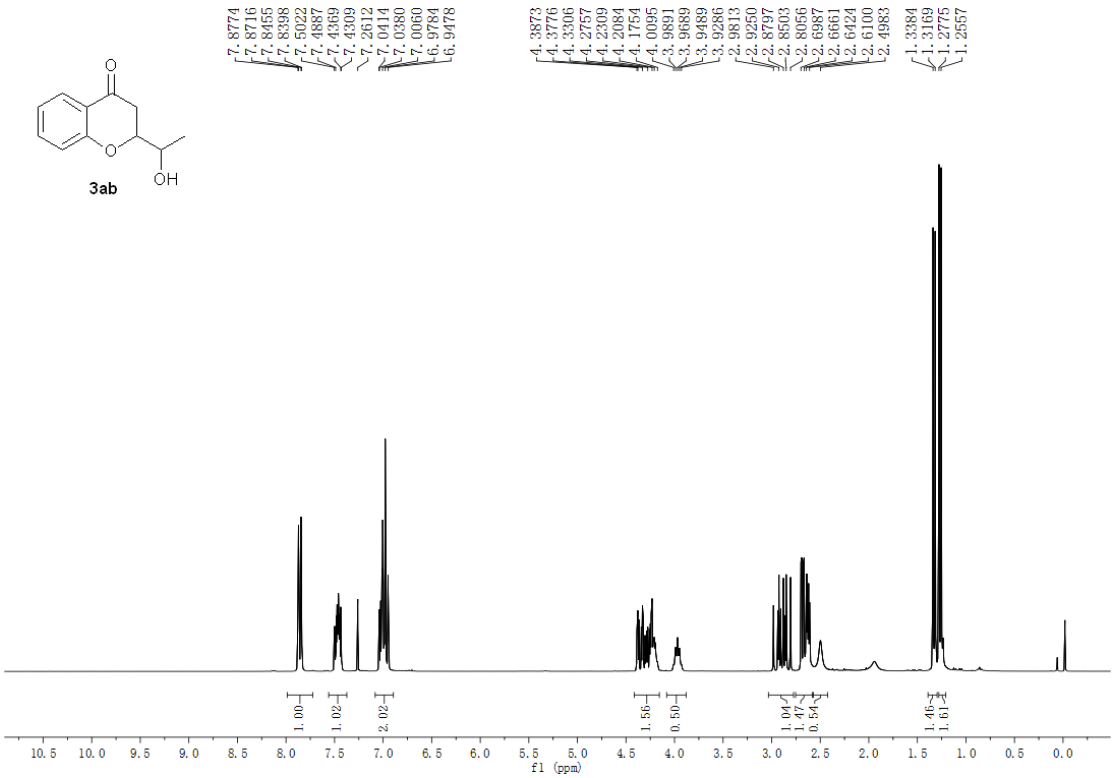
119.49
112.06
78.97
62.99
40.61
40.39
40.19
39.98
39.77
39.56
39.35
O
OH
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3oa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6.9478
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4.3306
4.2757
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4.2084
4.1754
4.0095
3.9891
3.9689
3.9489
3.9286
2.9813
2.9250
2.8797
2.8503
2.8056
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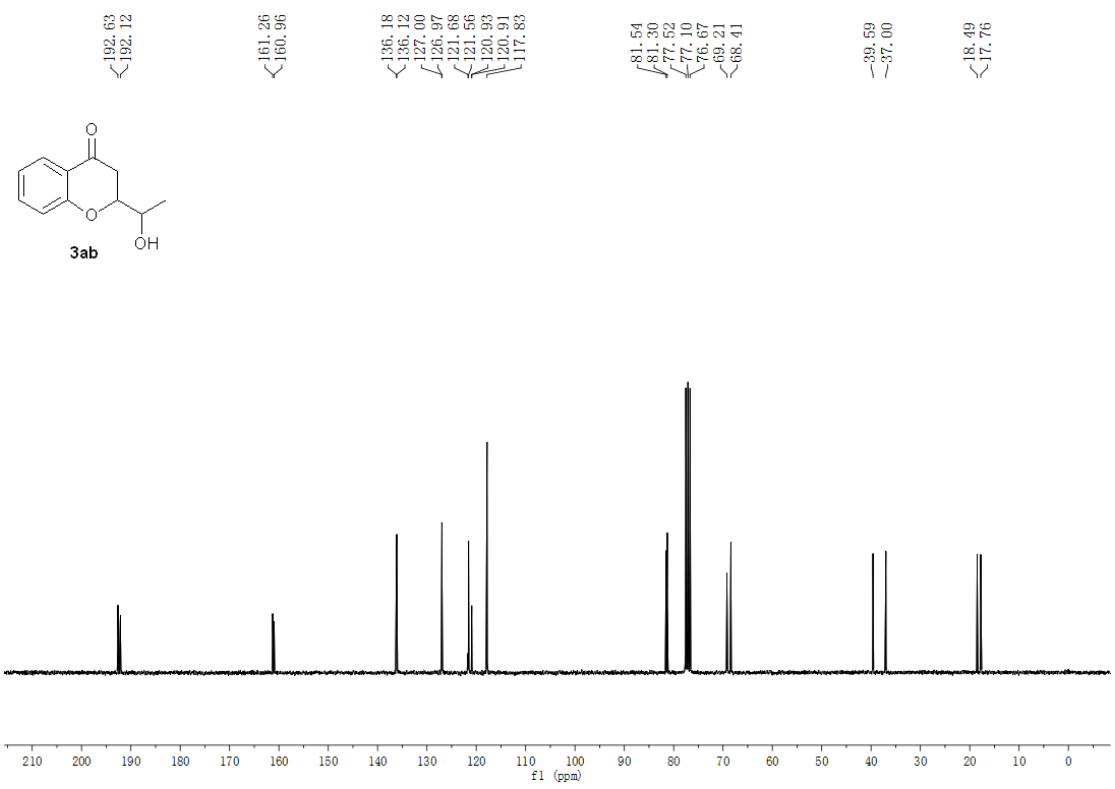
1.3384
1.3169
1.2775
1.2557
O
O
OH
3ab
1.00
1.02
2.02
1.56
0.50
1.04
1.47
0.54
1.46
1.61
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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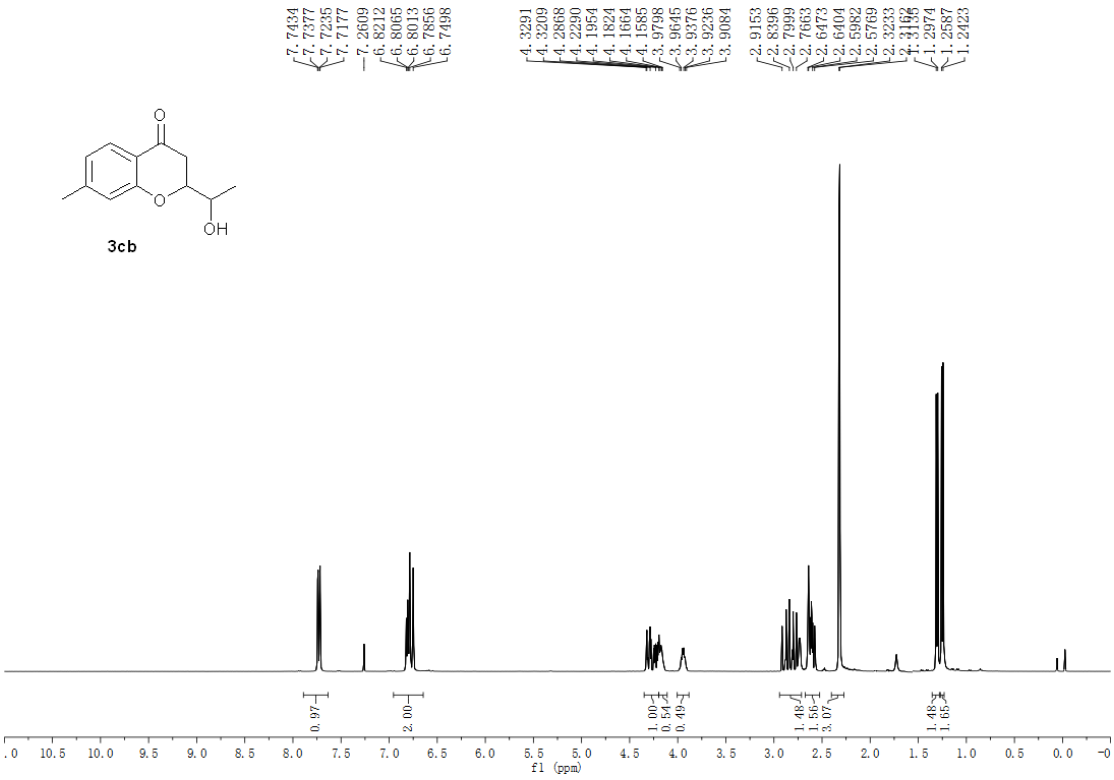
120.91
117.83
81.54
81.30
77.52
77.10
76.67
69.21
68.41
39.59
37.00
18.49
17.76
O
O
OH
3ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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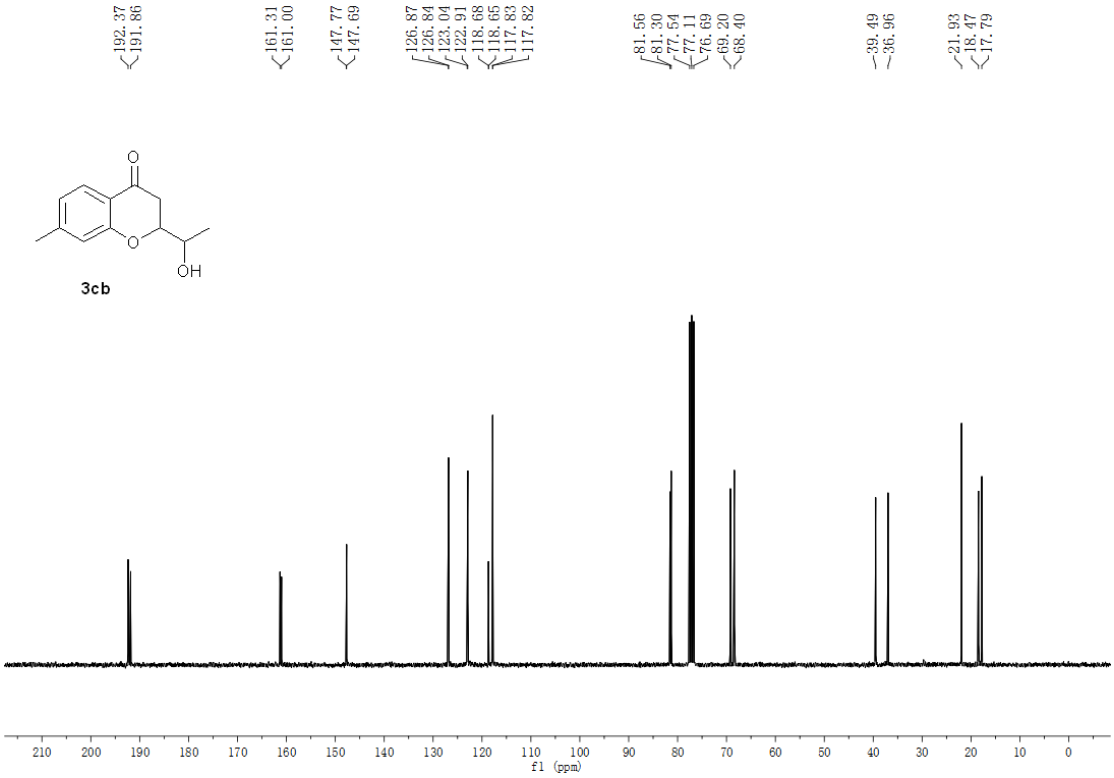
7.7235
7.7177
7.2609
6.8212
6.8065
6.8013
6.7856
6.7498
4.3291
4.3209
4.2868
4.2290
4.1954
4.1824
4.1664
4.1585
3.9798
3.9645
3.9376
3.9236
3.9084
2.9153
2.8396
2.7999
2.7663
2.6473
2.6404
2.5982
2.5769
2.3233
1.2974
1.2587
1.2423
O
O
OH
3cb
0.97
2.00
1.00
0.54
0.49
1.46
1.56
3.07
1.48
1.65
f1 (ppm)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161.31
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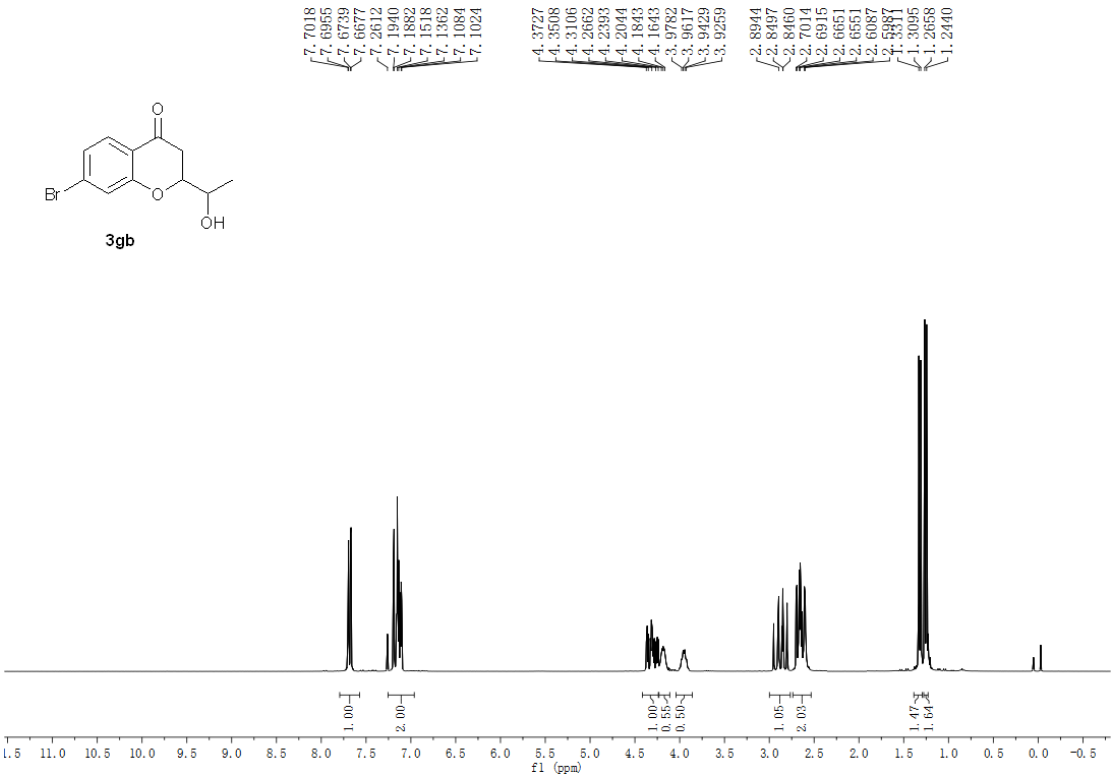
147.69
126.87
126.84
123.04
122.91
118.68
118.65
117.83
117.82
81.56
81.30
77.54
77.11
76.69
69.20
68.40
39.49
36.96
21.93
18.47
17.79
O
O
OH
3cb
f1 (ppm)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7.1940
7.1882
7.1518
7.1362
7.1084
7.1024
4.3727
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4.3106
4.2662
4.2393
4.2044
4.1843
4.1643
3.9782
3.9617
3.9429
3.9259
2.8944
2.8497
2.8460
2.7014
2.6915
2.6651
2.6551
2.6087
2.5987
1.3511
1.3095
1.2658
1.2440
Br
O
OH
3gb
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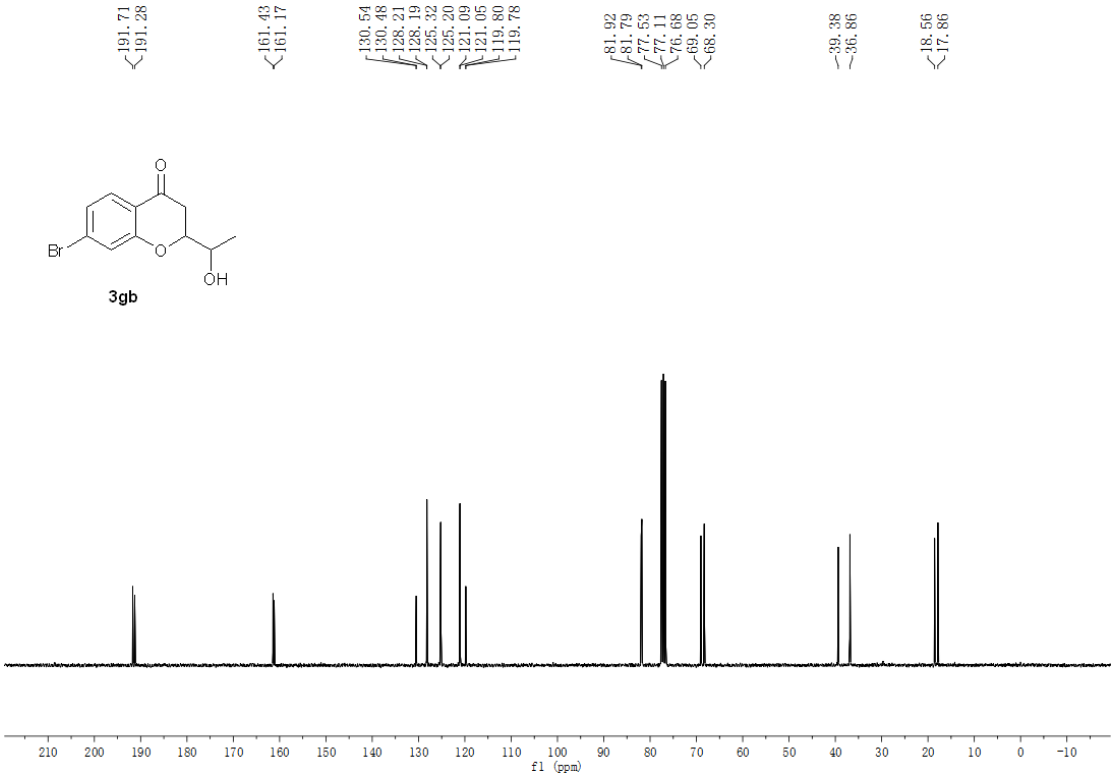
2.00
1.00
0.55
0.50
1.05
2.03
1.47
1.64
f1 (ppm)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130.48
128.21
128.19
125.32
125.20
121.09
121.05
119.80
119.78
81.92
81.79
77.53
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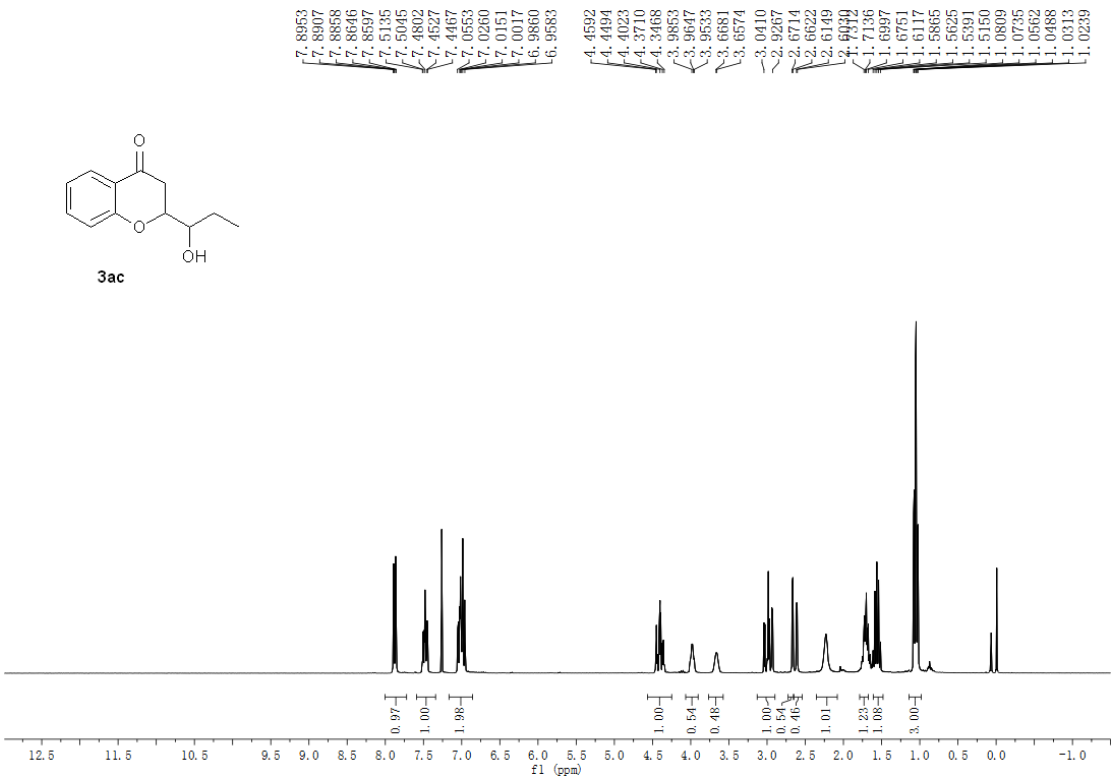
76.68
69.05
68.30
39.38
36.86
18.56
17.86
Br
O
OH
3gb
f1 (ppm)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7.4527
7.4467
7.0553
7.0260
7.0151
7.0017
6.9860
6.9583
4.4592
4.4494
4.4023
4.3710
4.3468
3.9853
3.9647
3.9533
3.6681
3.6574
3.0410
2.9267
2.6714
2.6622
2.6149
1.7136
1.6997
1.6751
1.6117
1.5865
1.5625
1.5391
1.5150
1.0809
1.0735
1.0562
1.0488
1.0313
1.0239
O
O
OH
3ac
0.97
1.00
1.98
1.00
0.54
0.48
1.00
0.54
0.46
1.01
1.23
1.08
3.00
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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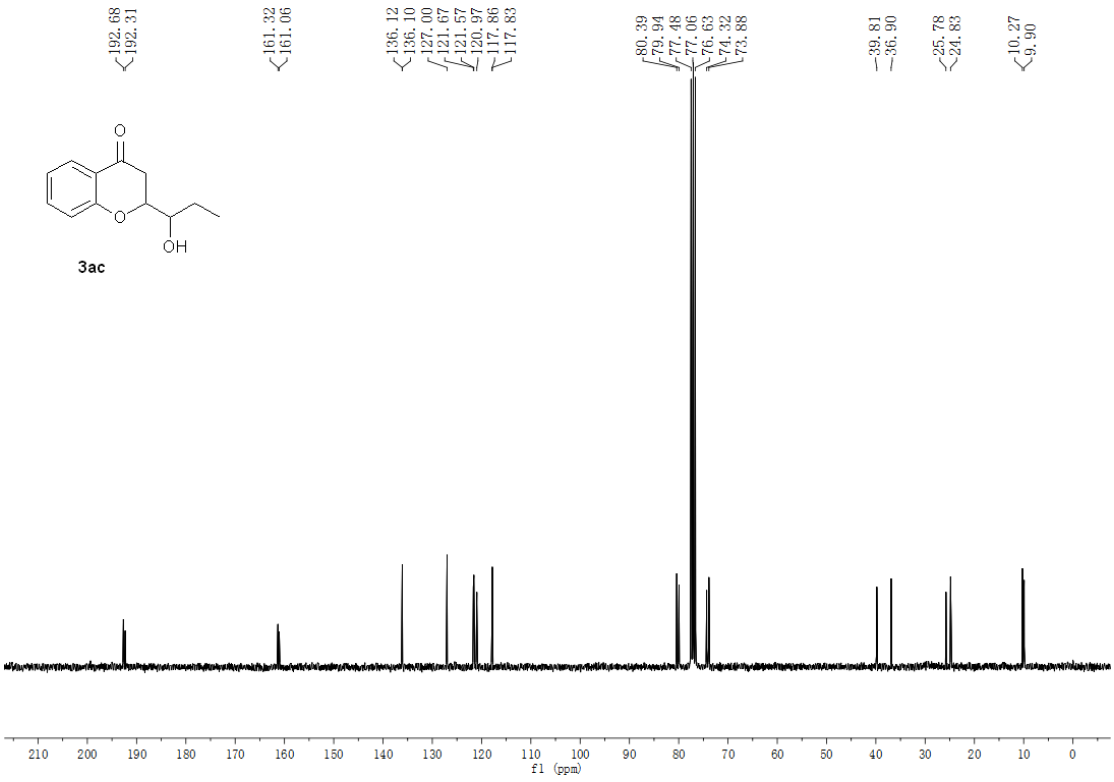
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-1.0
f1 (ppm)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136.10
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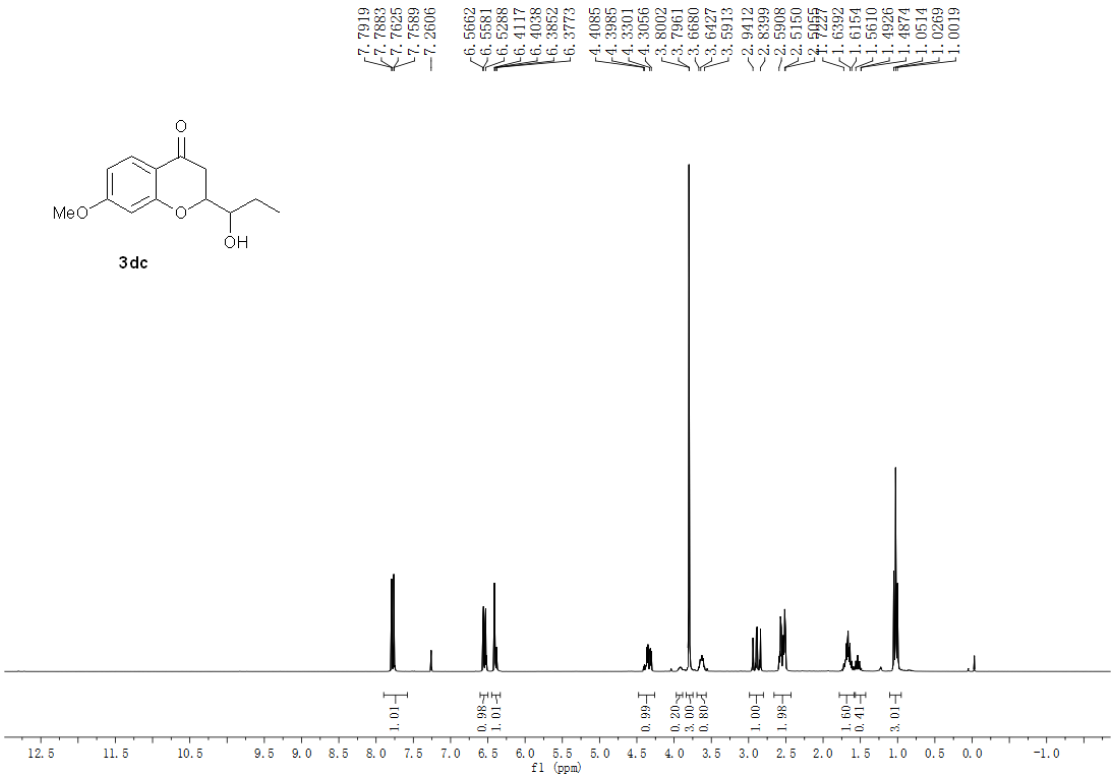
121.67
121.57
120.97
117.86
117.83
80.39
79.94
77.48
77.06
76.63
74.32
73.88
39.81
36.90
25.78
24.83
10.27
9.90
O
O
OH
3ac
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.3773
4.4085
4.3985
4.3301
4.3056
3.8002
3.7961
3.6680
3.6427
3.5913
2.9412
2.8399
2.5908
2.5150
2.5065
1.6392
1.6154
1.5610
1.4926
1.4874
1.0514
1.0269
1.0019
MeO
O
OH
3dc
1.01
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1.01
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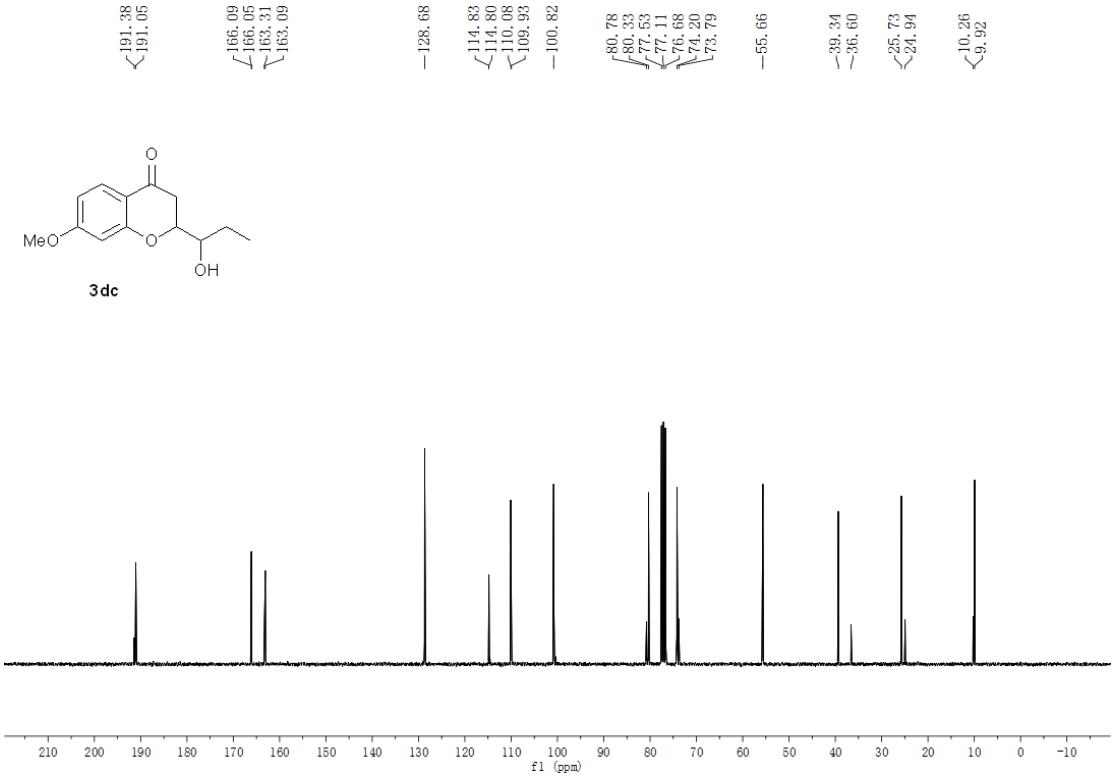
0.20
3.00
0.80
1.00
1.98
1.60
0.41
3.01
f1 (ppm)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110.08
109.93
100.82
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80.33
77.53
77.11
76.68
74.20
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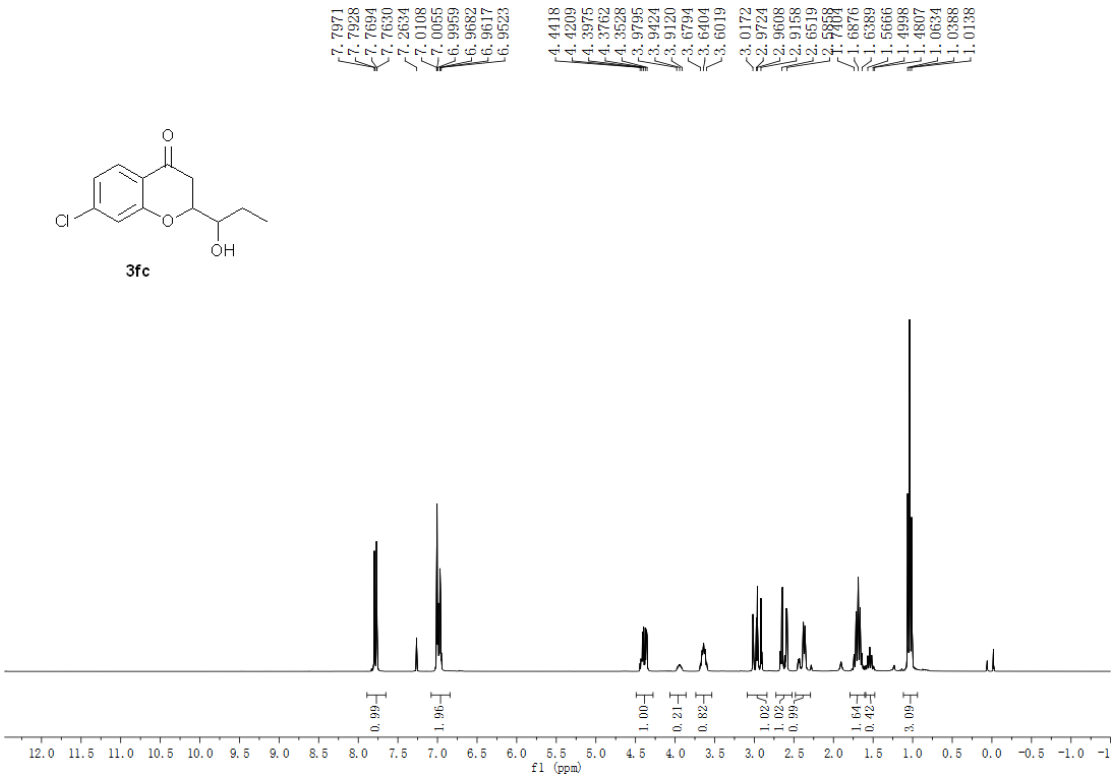
36.60
25.73
24.94
10.26
9.92
MeO
O
OH
3dc
f1 (ppm)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7.0055
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6.9523
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4.4209
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4.3762
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3.6404
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2.6519
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1.6389
1.5666
1.4998
1.4807
1.0634
1.0388
1.0138
O
Cl
O
OH
3fc
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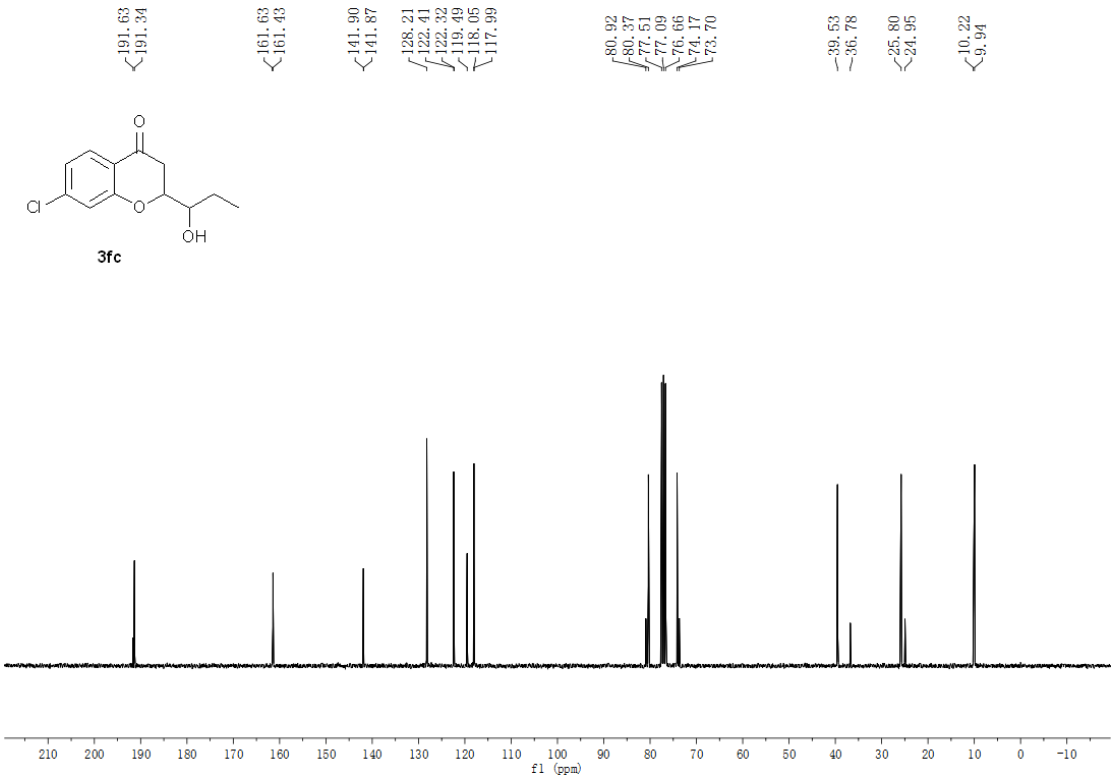
0.21
0.82
1.02
1.02
0.99
1.64
0.42
3.09
f1 (ppm)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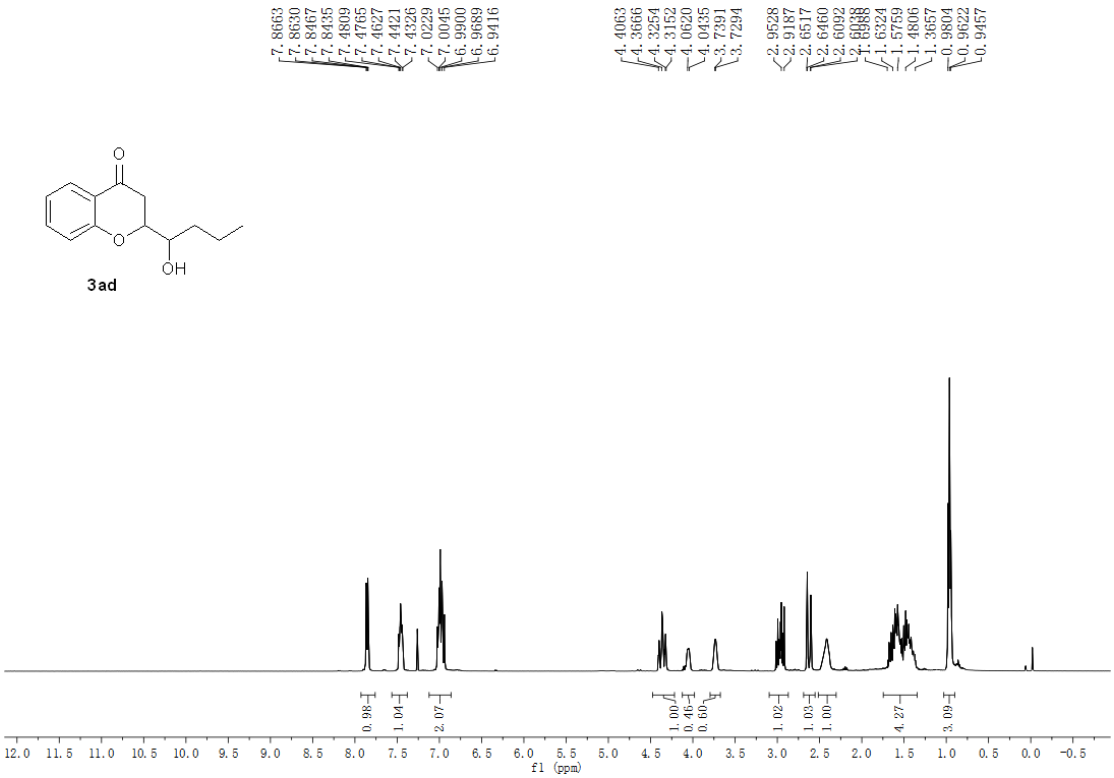
141.87
128.21
122.41
122.32
119.49
118.05
117.99
80.92
80.37
77.51
77.09
76.66
74.17
73.70
39.53
36.78
25.80
24.95
10.22
9.94
O
Cl
O
OH
3fc
f1 (ppm)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7.0045
6.9900
6.9689
6.9416
4.4063
4.3666
4.3254
4.3152
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4.0435
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1.4806
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0.9457
O
O
OH
3ad
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1.03
1.00
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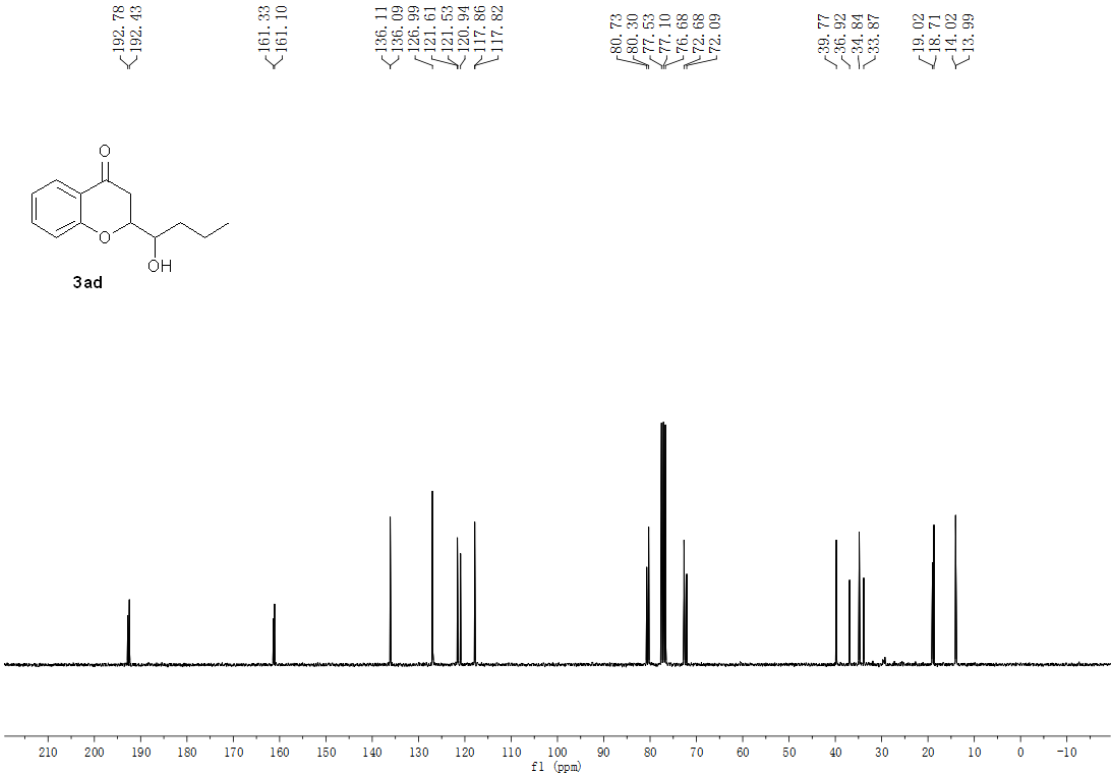
3.09
f1 (ppm)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136.09
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121.53
120.94
117.86
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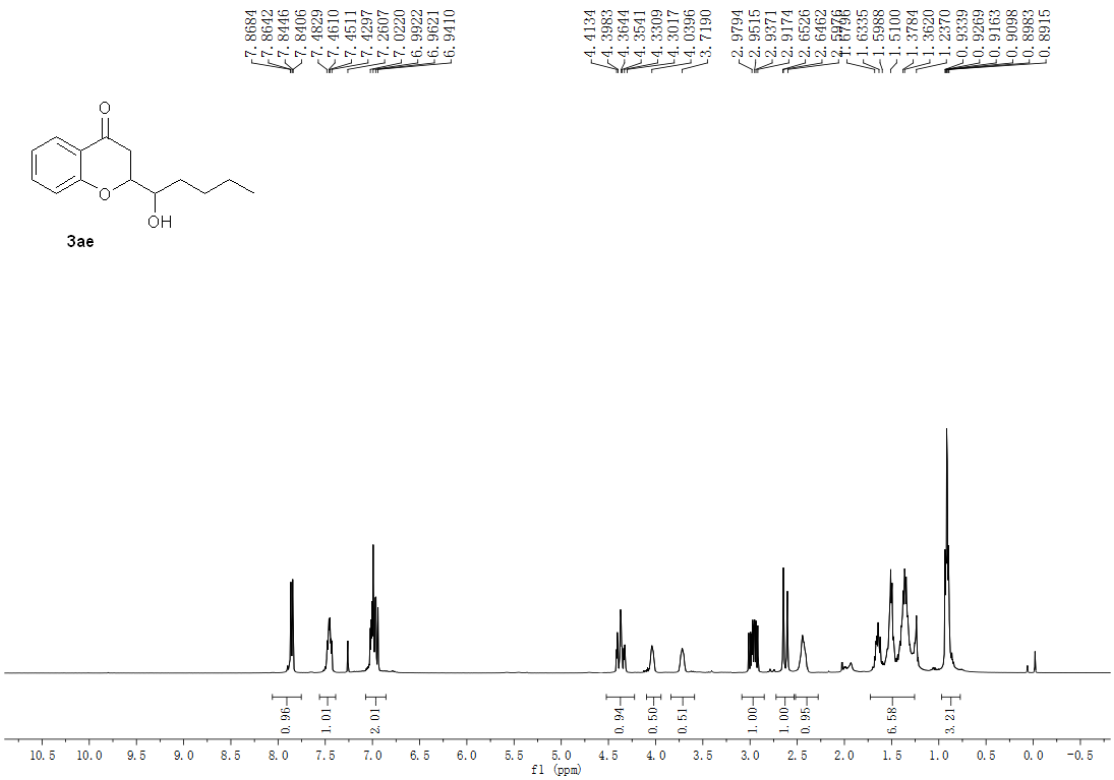
80.73
80.30
77.53
77.10
76.68
72.68
72.09
39.77
36.92
34.84
33.87
19.02
18.71
14.02
13.99
O
O
OH
3ad
f1 (ppm)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6.9621
6.9410
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4.3983
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4.3017
4.0396
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1.3784
1.3620
1.2370
0.9339
0.9269
0.9163
0.9098
0.8983
0.8915
O
O
OH
3ae
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0.94
0.50
0.51
1.00
1.00
0.95
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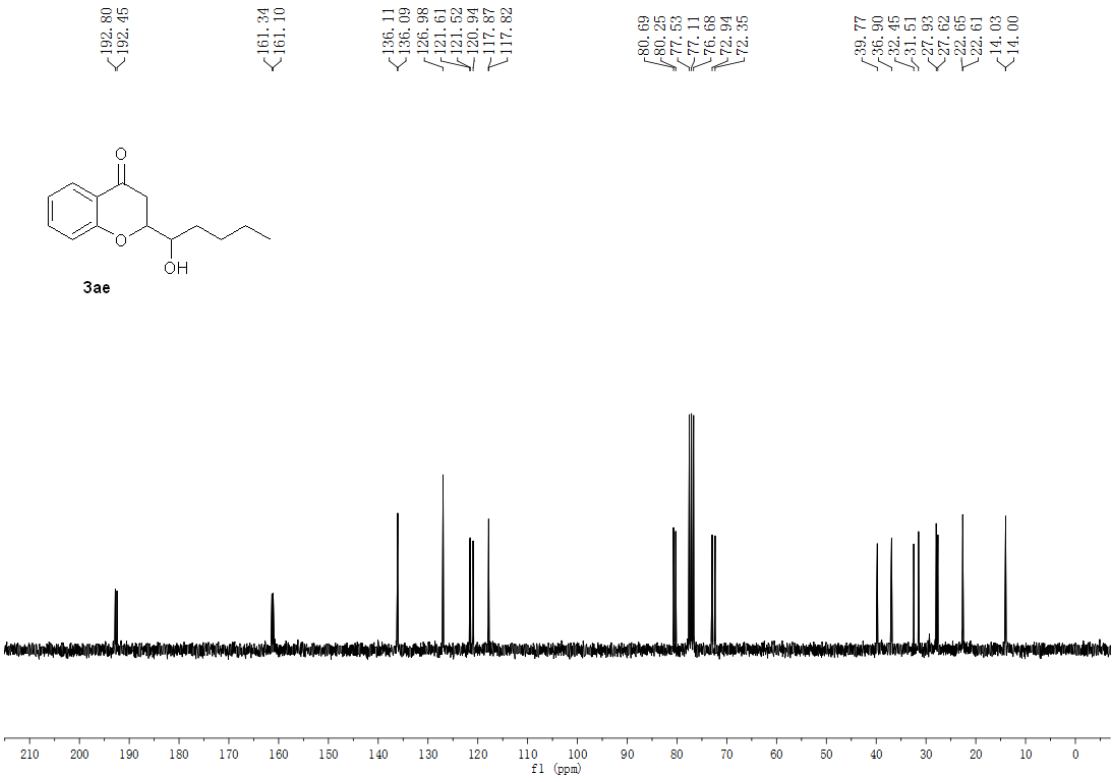
3.21
f1 (ppm)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121.61
121.52
120.94
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117.82
80.69
80.25
77.53
77.11
76.68
72.94
72.35
39.77
36.90
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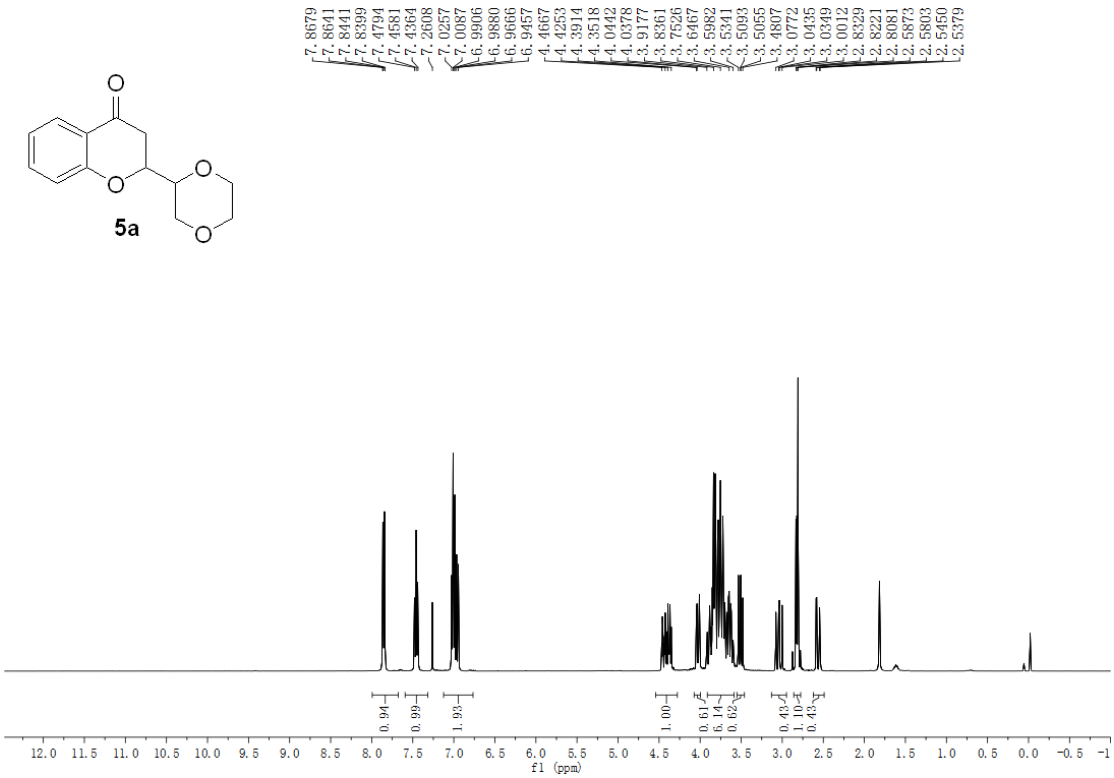
31.51
27.93
27.62
22.65
22.61
14.03
14.00
O
O
OH
3ae
f1 (ppm)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6.9880
6.9666
6.9457
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4.0442
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3.9177
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3.5055
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3.0772
3.0435
3.0349
3.0012
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2.8221
2.8081
2.5873
2.5803
2.5450
2.5379
5a
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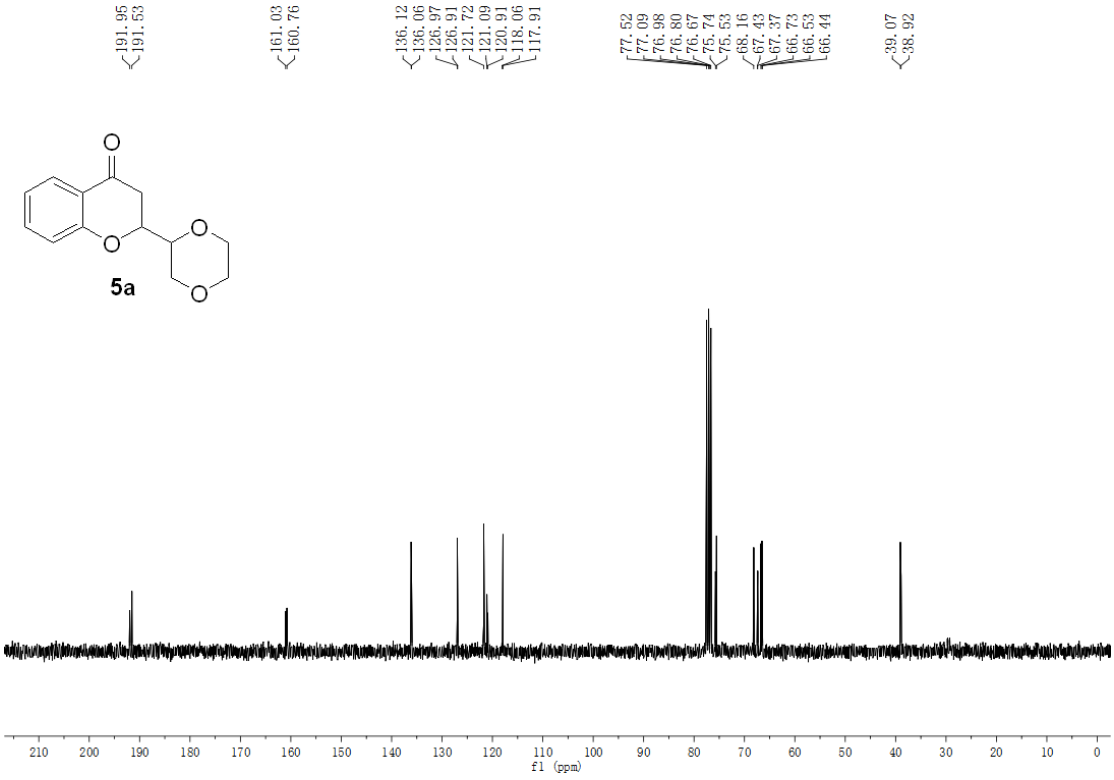
1.00
0.61
6.14
0.62
0.43
1.10
0.43
f1 (ppm)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191.53
161.03
160.76
136.12
136.06
126.97
126.91
121.72
121.09
120.91
118.06
117.91
77.52
77.09
76.98
76.80
76.67
75.74
75.53
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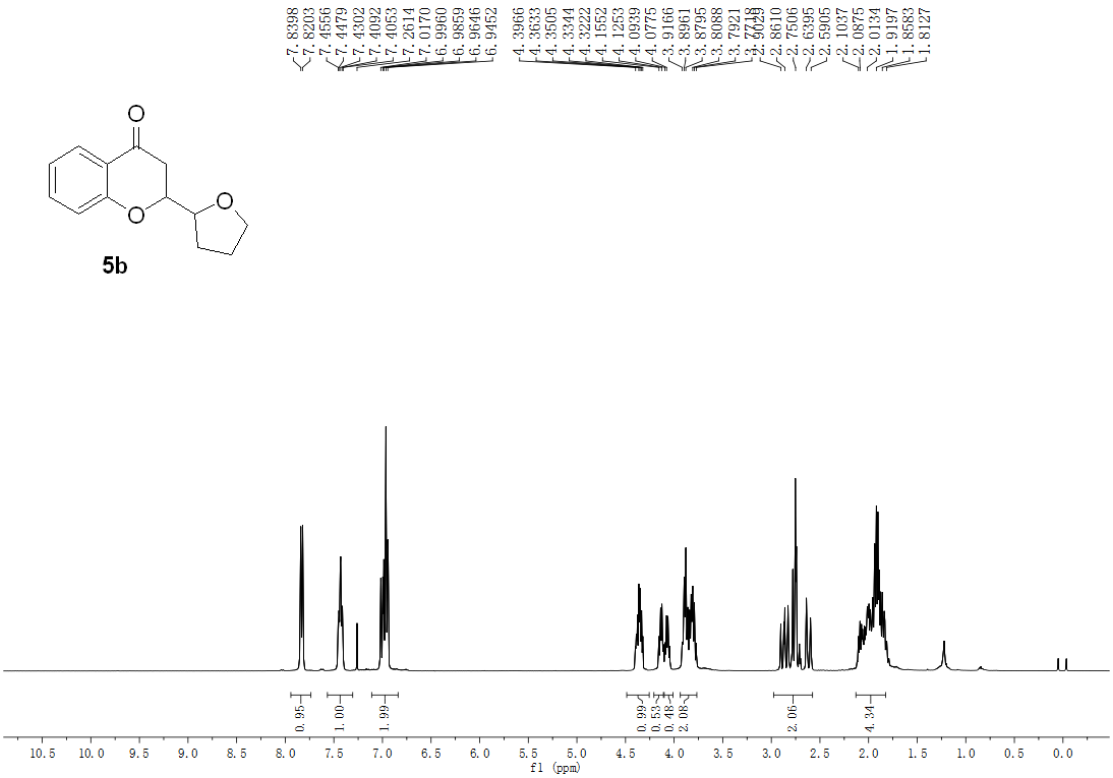
67.43
67.37
66.73
66.53
66.44
39.07
38.92
5a
f1 (ppm)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6.9859
6.9646
6.9452
4.3966
4.3633
4.3505
4.3344
4.3222
4.1552
4.1253
4.0939
4.0775
3.9166
3.8961
3.8795
3.8088
3.7921
2.9029
2.8610
2.7506
2.6395
2.5905
2.1037
2.0875
2.0134
1.9197
1.8583
1.8127
5b
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1.00
1.99
0.99
0.53
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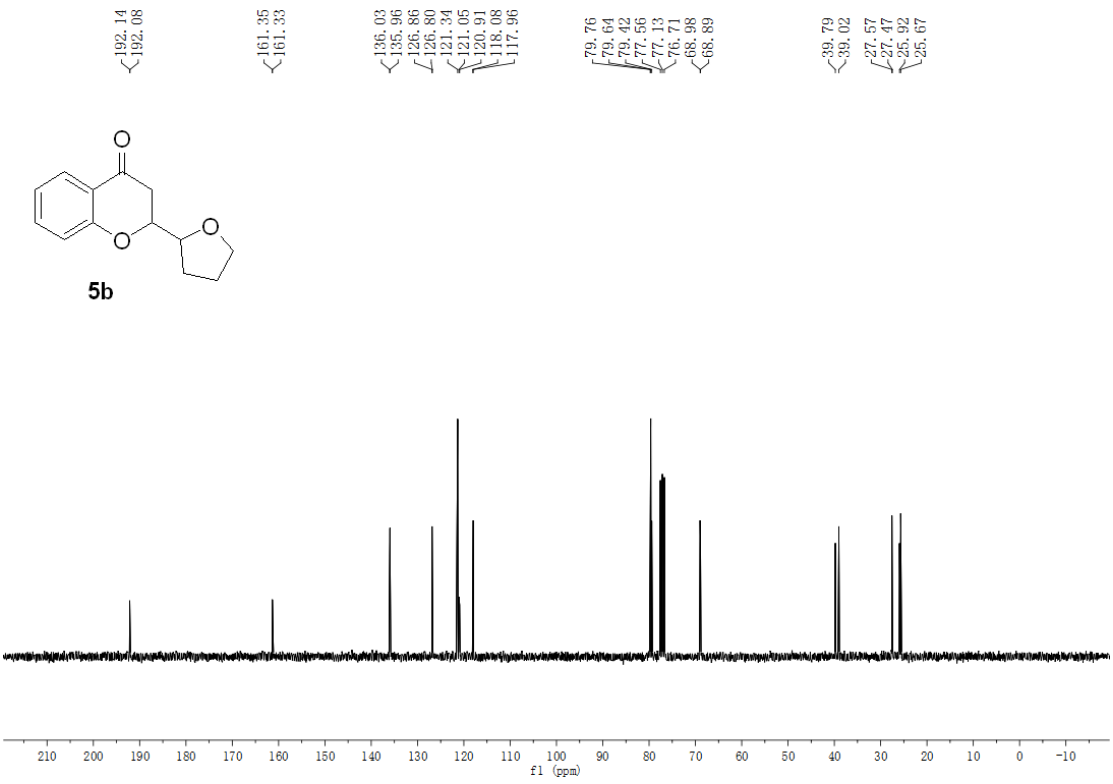
2.08
2.06
4.34
f1 (ppm)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192.08
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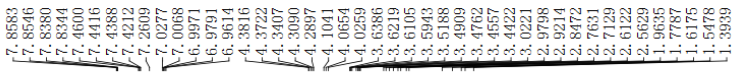
161.33
136.03
135.96
126.86
126.80
121.34
121.05
120.91
118.08
117.96
79.76
79.64
79.42
77.56
77.13
76.71
68.98
68.89
39.79
39.02
27.57
27.47
25.92
25.67
5b
f1 (ppm)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7.4600
7.4416
7.4388
7.4212
7.2609
7.0277
7.0068
6.9971
6.9791
6.9614
4.3816
4.3722
4.3407
4.3090
4.2897
4.1041
4.0654
4.0259
3.6386
3.6219
3.6105
3.5943
3.5188
3.4909
3.4762
3.4557
3.4422
3.0221
2.9798
2.9214
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2.7129
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2.5629
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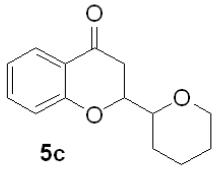
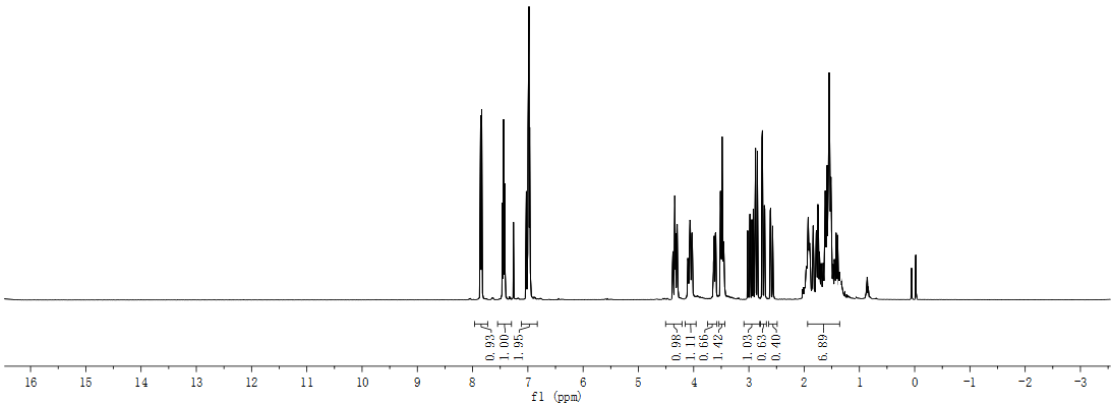
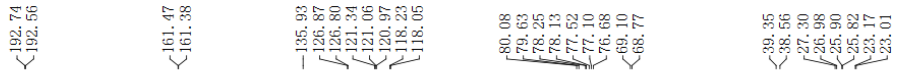
1.5478
1.3939


O
O
O

5c


0.93
1.00
1.95
0.98
1.11
0.66
1.42
1.03
0.63
0.40
6.89
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)


192.74
192.56
161.47
161.38
135.93
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126.80
121.34
121.06
120.97
118.23
118.05
80.08
79.63
78.25
78.13
77.52
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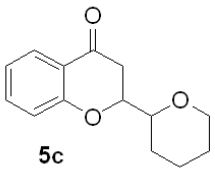
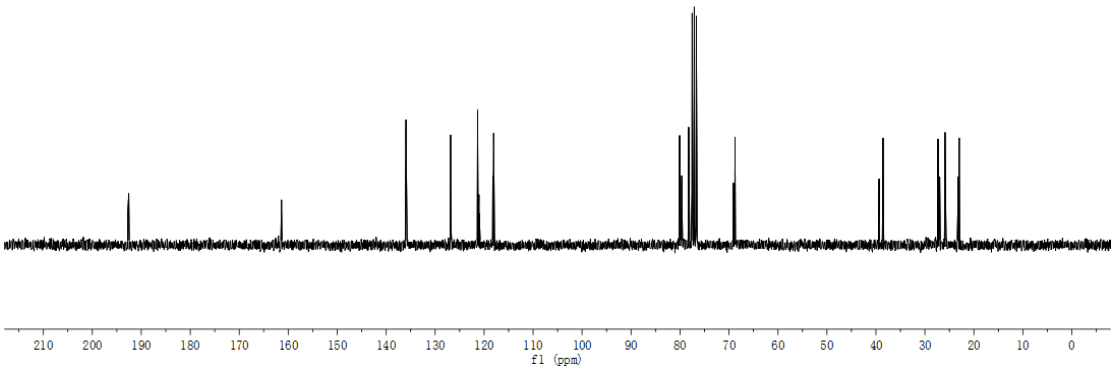
23.01


O
O
O

5c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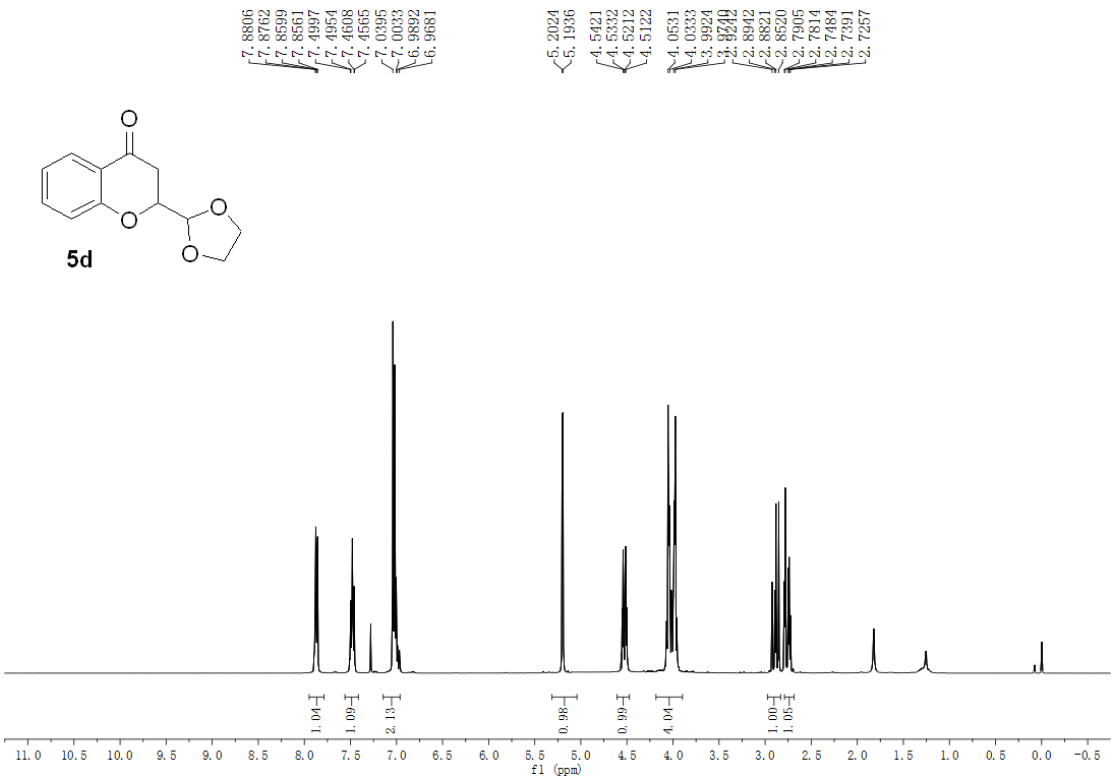
f1 (ppm)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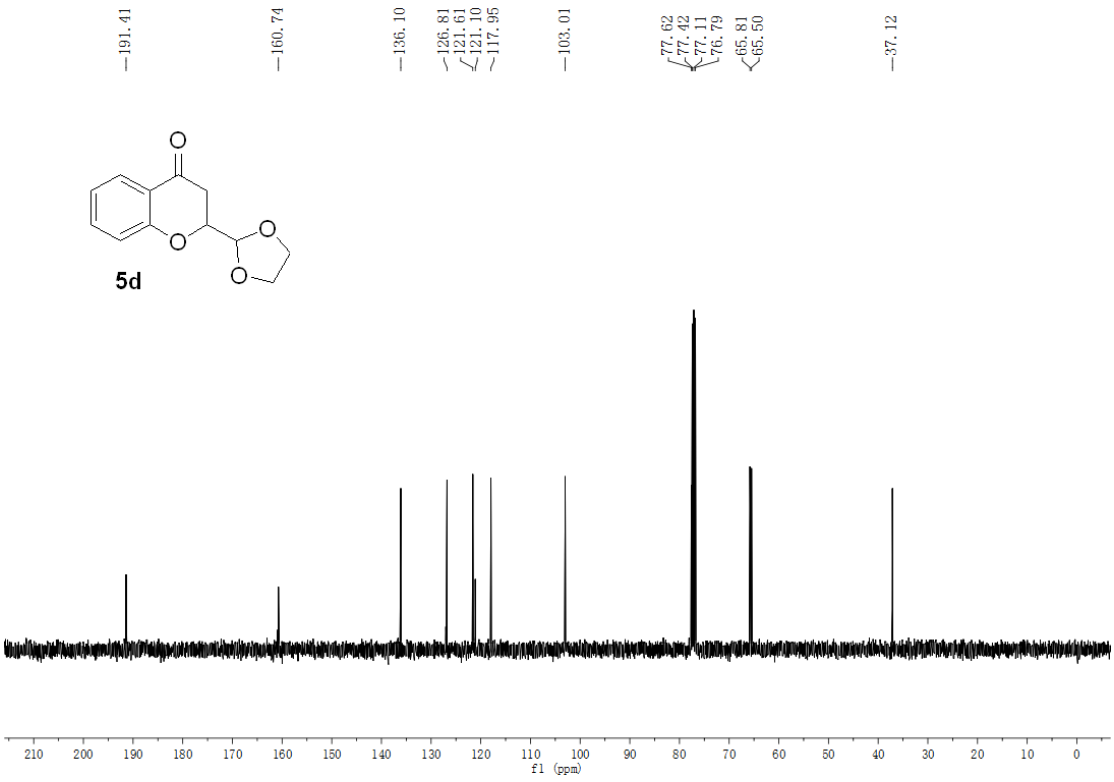
7.8561
7.4997
7.4954
7.4608
7.4565
7.0395
7.0033
6.9892
6.9681
5.2024
5.1936
4.5421
4.5332
4.5212
4.5122
4.0531
4.0333
3.9924
2.9242
2.8942
2.8821
2.8520
2.7905
2.7814
2.7484
2.7391
2.7257
5d
1.04
1.09
2.13
0.98
0.99
4.04
1.00
1.05
f1 (ppm)


191.41
160.74
136.10
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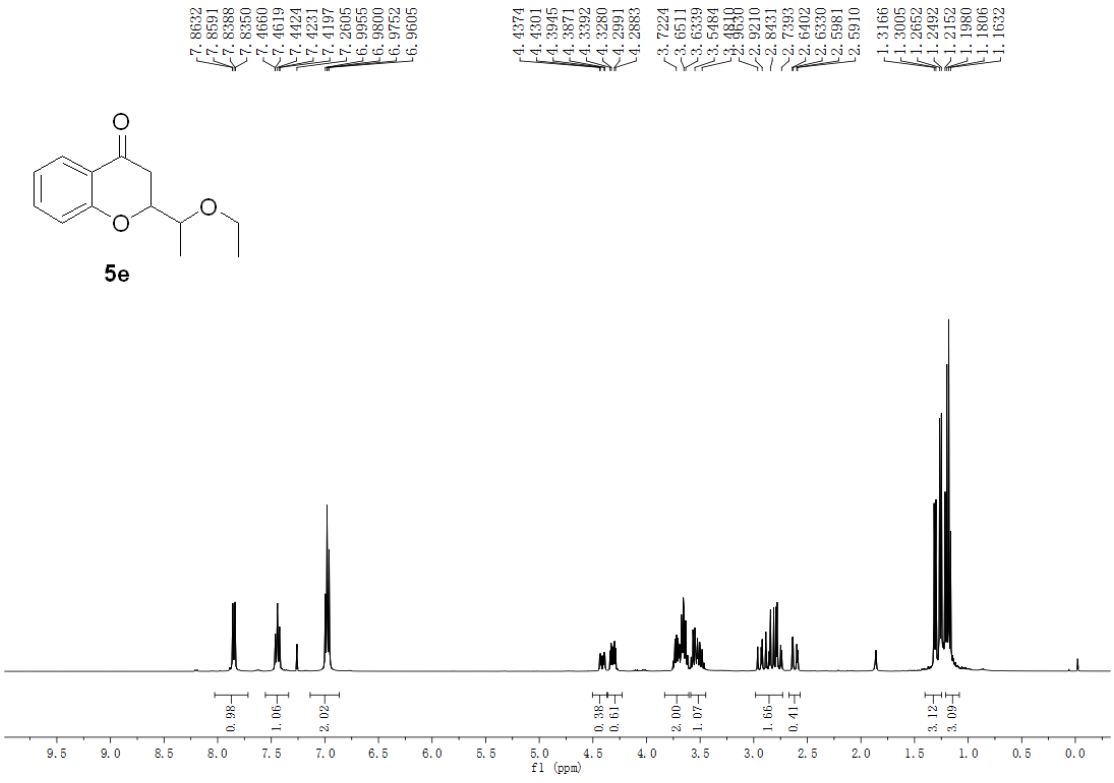
121.61
121.10
117.95
103.01
77.62
77.42
77.11
76.79
65.81
65.50
37.12
5d
f1 (ppm)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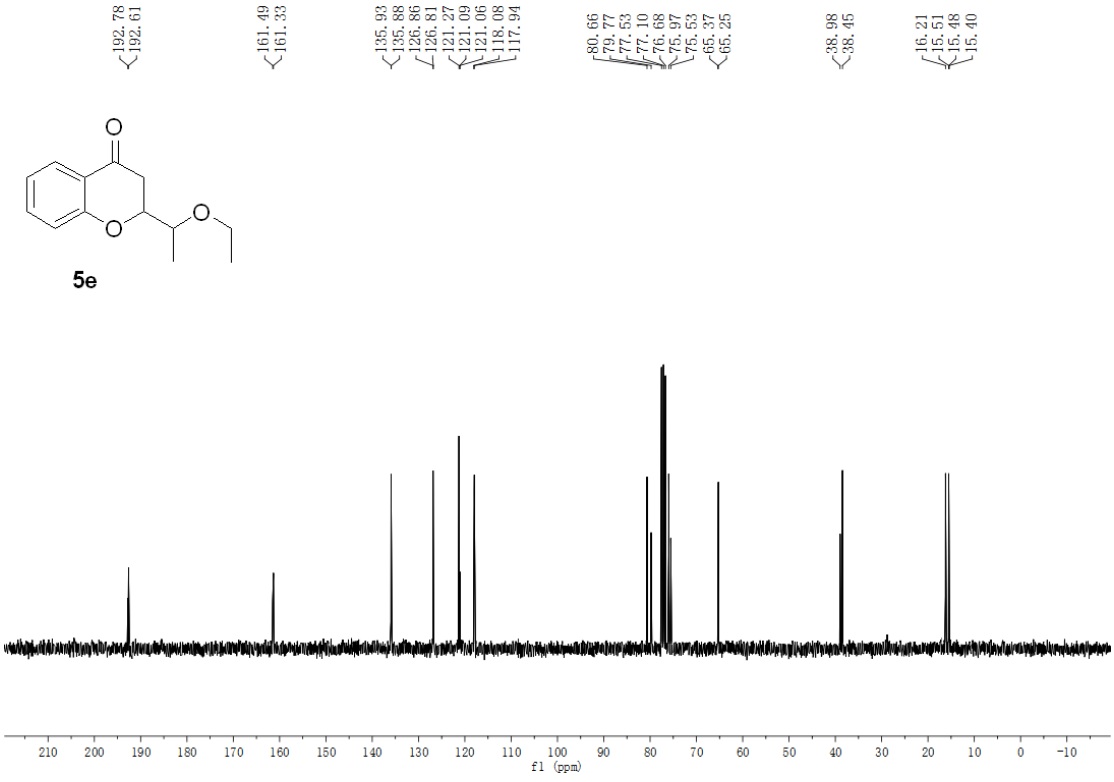
7.8591
7.8388
7.8350
7.4660
7.4619
7.4424
7.4231
7.4197
7.2605
6.9955
6.9800
6.9752
6.9605
4.4374
4.4301
4.3945
4.3871
4.3392
4.3280
4.2991
4.2883
3.7224
3.6511
3.6339
3.5484
2.9210
2.8431
2.7393
2.6402
2.6330
2.5981
2.5910
1.3166
1.3005
1.2652
1.2492
1.2152
1.1980
1.1806
1.1632
5e
0.98
1.06
2.02
0.38
0.61
2.00
1.07
1.66
0.41
3.12
3.09
f1 (ppm)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192.61
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161.33
135.93
135.88
126.86
126.81
121.27
121.09
121.06
118.08
117.94
80.66
79.77
77.53
77.10
76.68
75.97
75.53
65.37
65.25
38.98
38.45
16.21
15.51
15.48
15.40
5e
f1 (ppm)