Supporting information

Rh(III)-catalyzed C-H/C-C bond annulation of enaminones with iodonium ylides to form isocoumarins

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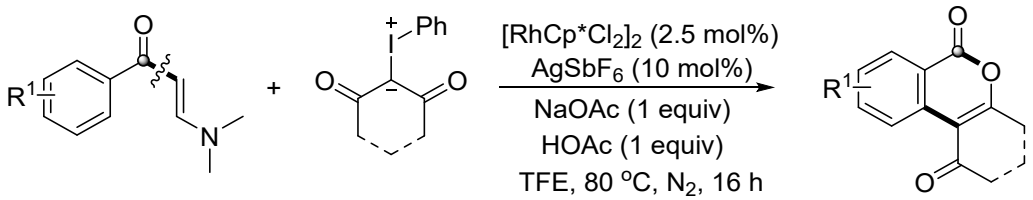
1. General Information

All chemicals were analytically pure and used directly after purchased. All solvents were used without any particular precautions to extrude moisture. ^{1}H NMR spectra were recorded on 400 MHz spectrometer, and ^{13}C NMR spectra were recorded on a 100 MHz spectrometer. All spectra were referenced to the solvent peaks (^{1}H: residual $CDCl_3$ = 7.26 ppm, ^{13}C: $CDCl_3$ = 77.00 ppm). High-resolution mass spectra (HRMS) were equipped with an ESI source and a TOF detector. Column chromatography was performed on silica gel (70-230 mesh ASTM) using the reported eluents. Thin-layer chromatography (TLC) was carried out on 4×15 cm plates with a layer thickness of 0.2 mm (silica gel 60 F254). enaminones[1] and aryl iodonium ylide [2] were synthesized according to the previously reported procedure.

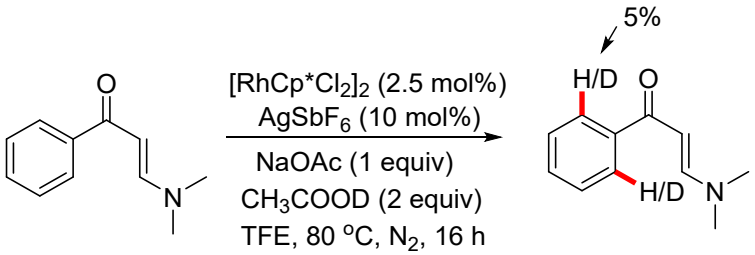
2. Typical procedure for synthesis of 3



To a tube equipped with magnetic stir bar, enaminone (**1**, 0.20 mmol), iodonium ylides (**2**, 0.30 mmol), $[RhCp^*Cl_2]_2$ (2.5 mol %), $AgSbF_6$ (10 mol%), NaOAc (1 equiv.) and HOAc (1 equiv.) in TFE (2.0 mL) were added and stirred at 80 °C for 16 h under N_2 atmosphere. After removal of the solvent under reduced pressure, purification was performed by flash column chromatography on silica gel with petroleum ether/ethyl acetate (gradient mixture ratio from 10:1 to 1:1) as eluent to afford the corresponding products.

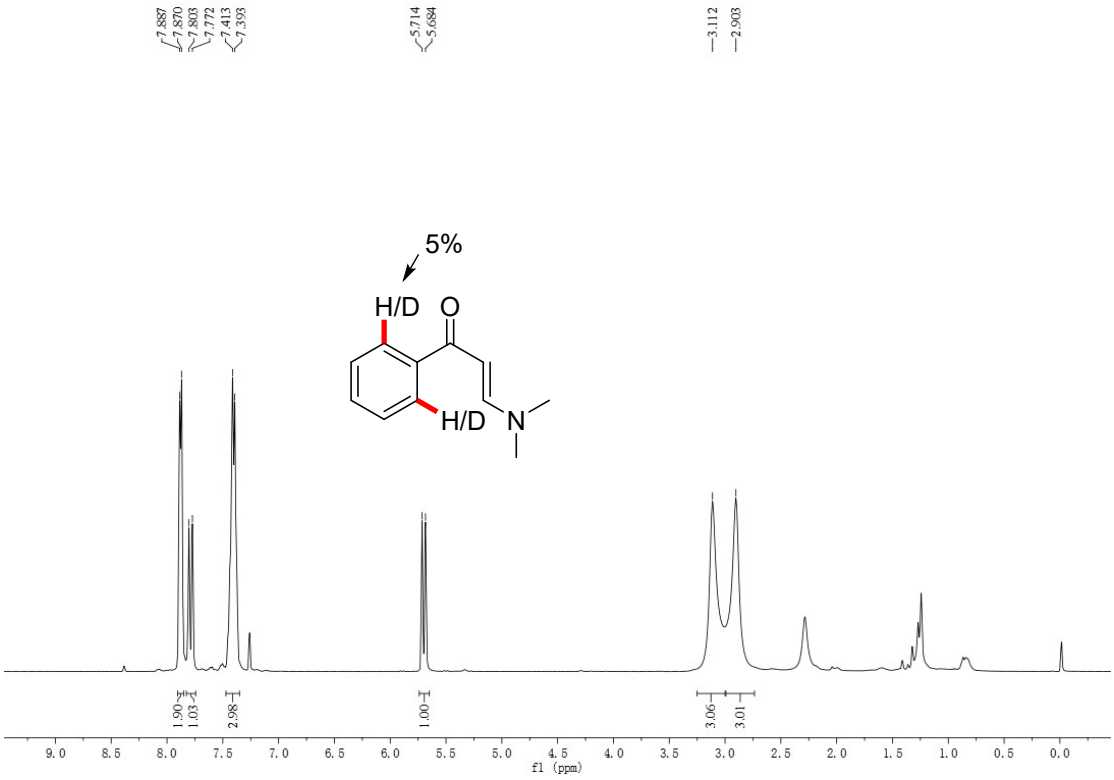
3. Mechanism Experiments

(1) H/D exchange

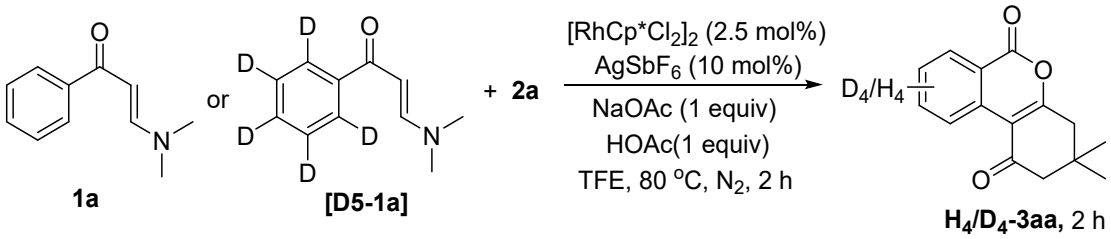


To a tube equipped with magnetic stir bar, enaminone (**1a**, 0.20 mmol), $[RhCp^*Cl_2]_2$ (2.5 mol %), $AgSbF_6$ (10 mol%), NaOAc (1 equiv.) and CH_3COOD (0.40 mmol, 2 equiv.) in TFE (2.0 mL) were added and stirred at 80 °C for 16 h under N_2 atmosphere. After removal of the solvent under reduced pressure, purification was performed by flash column chromatography on silica gel with petroleum ether/ethyl acetate (gradient

mixture ratio from 10:1 to 1:1) as eluent to afford the corresponding products.



(2) General procedure for estimation of the KIE:



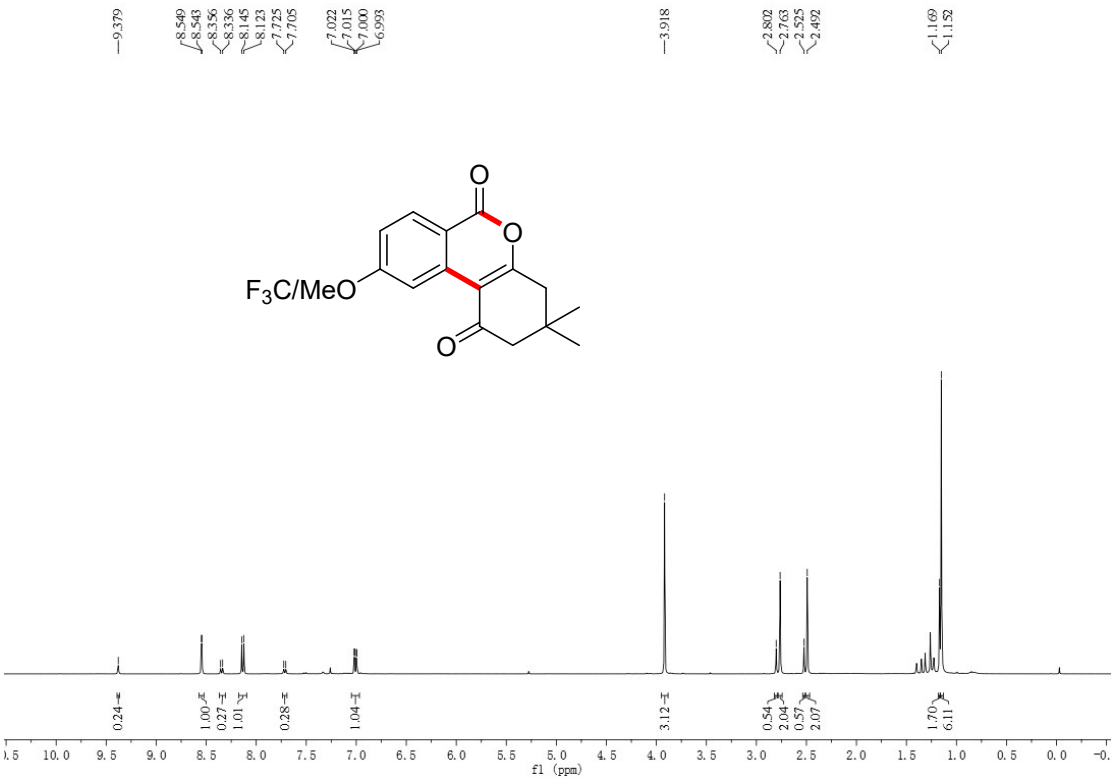
1a **[D5-1a]** **H_4/D_4-3aa,** 2 h

To two separated tube charged with enaminones (**1a**, 0.20 mmol) or **D_5-1a** (0.20 mmol), iodonium ylide (**2a**, 0.3 mmol), $[RhCp^*Cl_2]_2$ (2.5 mol %), $AgSbF_6$ (10 mol%), NaOAc (1 equiv.) and HOAc (1 equiv.) in TFE(2.0 mL) were added and stirred at 80 °C for 2 h under N_2 atmosphere. After removal of the solvent under reduced pressure, purification was performed by flash column chromatography on silica gel with petroleum ether/ethyl acetate (gradient mixture ratio from 20:1 to 4:1) as eluent to afford the corresponding products.

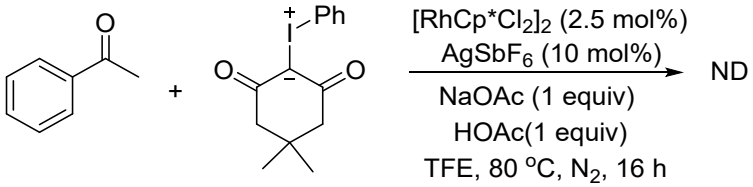
(3) Intermolecular competition reaction with differently substituted enaminones

A suspension of enaminone **1e** (41.0 mg, 0.2 mmol) and **1k** (48.6 mg, 0.2 mmol), (4,4-dimethyl-2,6-dimethylenecyclohexylidene)(phenyl)-λ^3-iodane **2a** (68.4 mg, 0.2

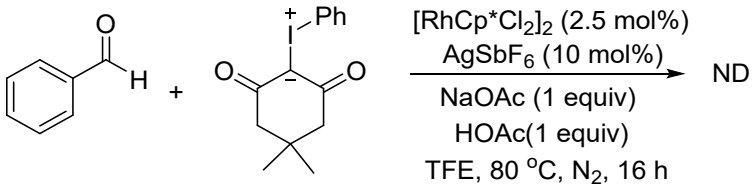
mmol), [RhCp*Cl_2]$_2$ (2.5 mol %), $AgSbF_6$ (10 mol%), NaOAc (1 equiv.) and HOAc (1 equiv.) in TFE(2.0 mL) were added and stirred at 80 °C for 16 h under N_2 atmosphere. After removal of the solvent under reduced pressure, purification was performed by flash column chromatography on silica gel with petroleum ether/ethyl acetate (gradient mixture ratio from 20:1 to 4:1) as eluent to afford the corresponding products **3ea** and **3ka** at a ratio of 1:0.25.



(4) Control experiments

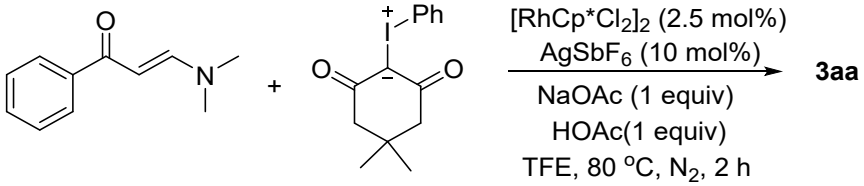


To a tube equipped with magnetic stir bar, acetophenone (0.20 mmol), iodonium ylides (**2a**, 0.30 mmol), [RhCp*Cl_2]$_2$ (2.5 mol %), $AgSbF_6$ (10 mol%), NaOAc (1 equiv.) and HOAc (1 equiv.) in TFE (2.0 mL) were added and stirred at 80 °C for 16 h under N_2 atmosphere.

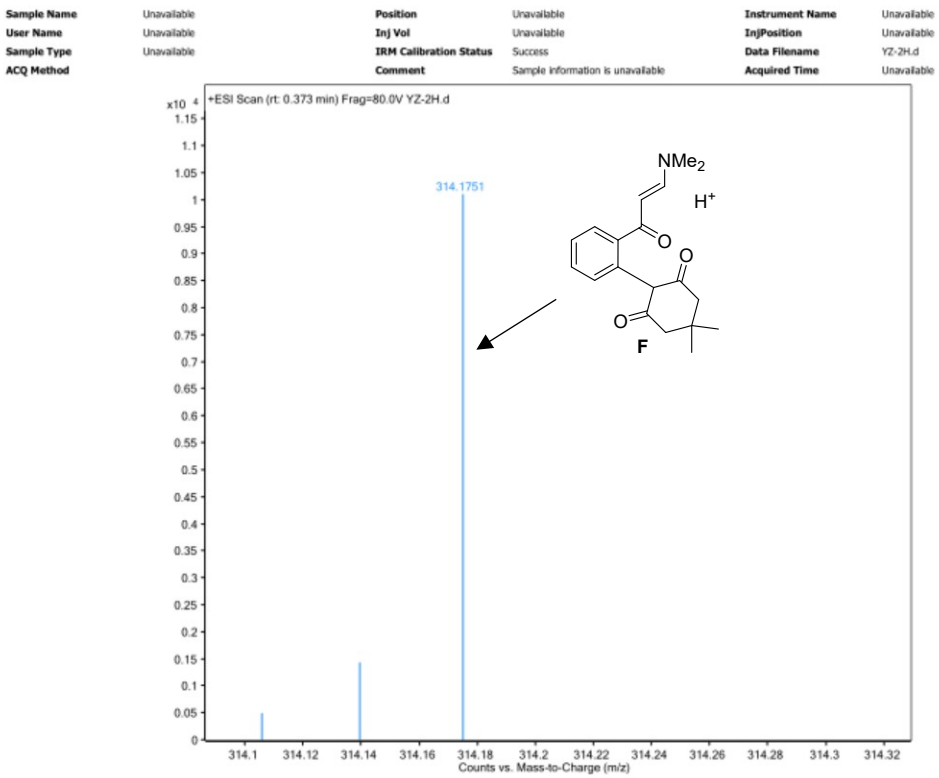


To a tube equipped with magnetic stir bar, benzaldehyde (0.20 mmol), iodonium ylides (**2a**, 0.30 mmol), $[RhCp^*Cl_2]_2$ (2.5 mol %), $AgSbF_6$ (10 mol%), NaOAc (1 equiv.) and HOAc (1 equiv.) in TFE (2.0 mL) were added and stirred at 80 °C for 16 h under N_2 atmosphere.

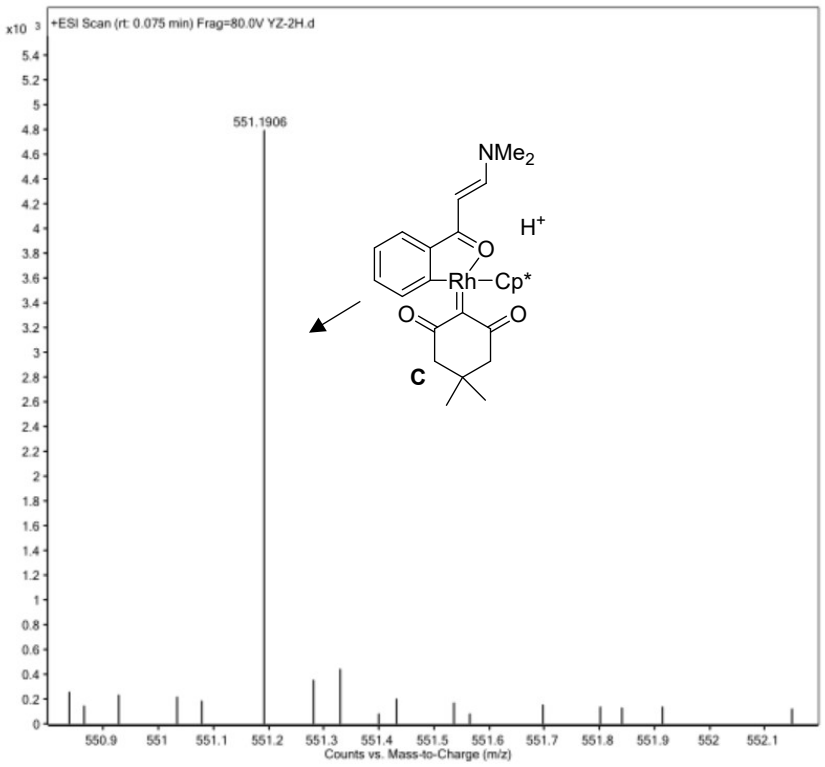
(5) **Intermediate detection**



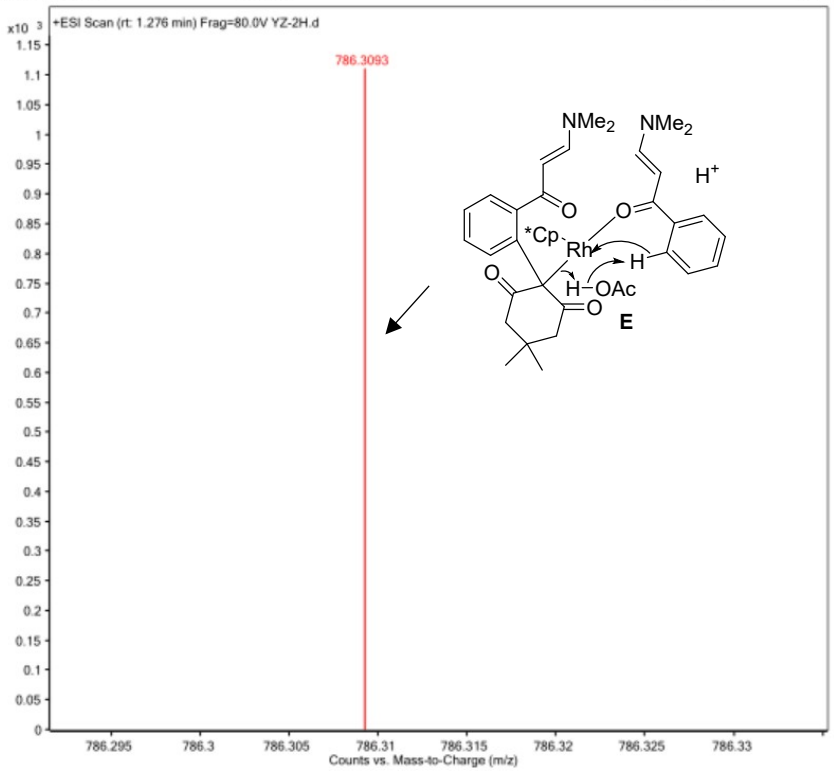
To a tube equipped with magnetic stir bar, enaminone (**1a**, 0.20 mmol), iodonium ylides (**2a**, 0.30 mmol), $[RhCp^*Cl_2]_2$ (2.5 mol %), $AgSbF_6$ (10 mol%), NaOAc (1 equiv.) and HOAc (1 equiv.) in TFE (2.0 mL) were added and stirred at 80 °C for 2 h under N_2 atmosphere. Then we detected the reaction mixture by HRMS.



Sample Name	Sample34	**Position**	P1-D7	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	YZ-2H.d
ACQ Method	shui20jiachun80 3min.m	**Comment**		**Acquired Time**	10/27/2022 6:14:17 PM

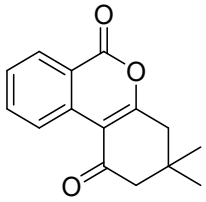


Sample Name	Sample34	**Position**	P1-D7	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	YZ-2H.d
ACQ Method	shui20jiachun80 3min.m	**Comment**		**Acquired Time**	10/27/2022 6:14:17 PM



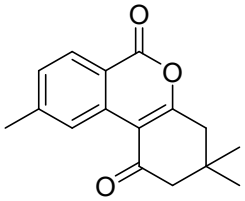
4. Characterization of compounds 3

3,3-Dimethyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3aa)[3]



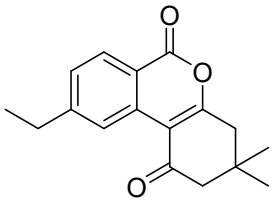
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 38.7 mg, 80% yield, pale yellow solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.03 (d, *J* = 8.3 Hz, 1H), 8.27 (d, *J* = 7.9 Hz, 1H), 7.78 (t, *J* = 8.2 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 1H), 2.79 (s, 2H), 2.51 (s, 2H), 1.17 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.89, 167.91, 160.67, 135.59, 133.80, 129.53, 128.35, 125.77, 119.71, 110.52, 52.80, 42.49, 31.91, 28.10.

3,3,9-Trimethyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ba)



silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 48.1 mg, 94% yield, pale yellow solid. m.p. 142-144 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.81 (s, 1H), 8.12 (d, *J* = 8.1 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 2.76 (s, 2H), 2.49 (s, 2H), 2.48 (s, 3H), 1.15 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.98, 168.02, 160.63, 146.88, 133.72, 129.52, 129.46, 125.73, 117.15, 110.40, 52.82, 42.48, 31.84, 28.04, 22.41. **HRMS (ESI)**: Calcd for $C_{16}H_{16}O_3$ $[M+H]^+$: 257.1172; found: 257.1171

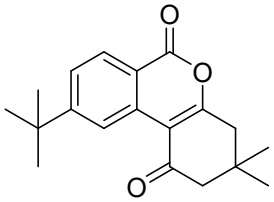
9-Ethyl-3,3-dimethyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ca)



silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 51.3 mg, 95% yield, yellow solid. m.p. 100-102 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.86 (s, 1H), 8.16 (d, *J* = 8.1 Hz, 1H), 7.34 (d, *J* = 9.4 Hz, 1H), 2.81 – 2.73 (m, 4H), 2.49 (s, 2H), 1.27 (t, *J* = 7.6 Hz, 3H), 1.15 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 197.02, 167.99, 160.64, 152.98, 133.88, 129.61, 128.40, 124.72, 117.36, 110.49, 52.84, 42.48, 31.85, 29.61, 28.05, 15.13. **HRMS (ESI)**: Calcd for $C_{17}H_{18}O_3$ $[M+H]^+$: 271.1329; found: 271.1329

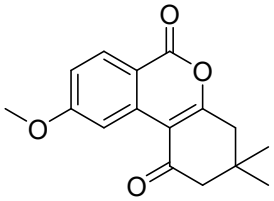
9-(Tert-butyl)-3,3-dimethyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione

(3da)



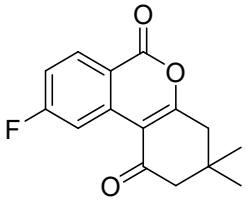
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 49.5 mg, 83% yield, white solid. m.p. 160-162 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.11 (s, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 2.77 (s, 2H), 2.50 (s, 2H), 1.37 (s, 9H), 1.16 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 197.13, 167.98, 160.60, 159.72, 133.74, 129.30, 126.01, 122.34, 117.13, 110.67, 52.92, 42.52, 35.72, 31.89, 30.97, 28.07. **HRMS (ESI)**: Calcd for $C_{19}H_{22}O_3$ $[M+H]^+$: 299.1642; found: 299.1639

9-Methoxy-3,3-dimethyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ea)



silica gel column chromatography (petroleum ether/ethyl acetate = 2:1), 52.2 mg, 96% yield, pale yellow solid. m.p. 124-126 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.54 (d, *J* = 2.3 Hz, 1H), 8.13 (d, *J* = 8.9 Hz, 1H), 7.01 (dd, *J* = 8.9, 2.4 Hz, 1H), 3.92 (s, 3H), 2.76 (s, 2H), 2.49 (s, 2H), 1.15 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 197.12, 168.87, 165.34, 160.27, 136.16, 131.53, 116.92, 112.47, 110.20, 107.87, 55.64, 52.79, 42.53, 31.82, 28.04. **HRMS (ESI)**: Calcd for $C_{16}H_{16}O_4$ $[M+H]^+$: 273.1121; found: 273.1120

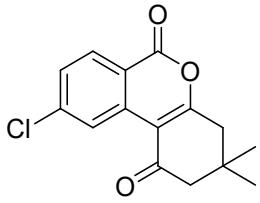
9-Fluoro-3,3-dimethyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3fa)



silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 45.8 mg, 88% yield, yellow solid. m.p. 119-121 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.75 (dd, *J* = 11.3, 2.4 Hz, 1H), 8.26 (dd, *J* = 8.8, 5.9 Hz, 1H), 7.19 (td, *J* = 8.6, 2.5 Hz, 1H), 2.78 (s, 2H), 2.51 (s, 2H), 1.16 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.49, 169.13, 167.18 (d, $J_{C\text{-}F}$ = 256.1 Hz), 159.66, 136.47 (d, $J_{C\text{-}F}$ = 12.3 Hz), 132.62 (d, $J_{C\text{-}F}$ = 10.6 Hz), 116.56 (d, $J_{C\text{-}F}$ = 23.6 Hz), 116.14 (d, $J_{C\text{-}F}$ = 2.3 Hz), 112.34 (d, $J_{C\text{-}F}$ = 26.2 Hz), 109.89 (d, $J_{C\text{-}F}$

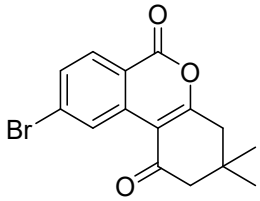
= 3.1 Hz), 52.54, 42.45, 31.86, 28.06. **^{19}F NMR (376 MHz, $CDCl_3$)** δ -98.88. **HRMS (ESI)**: Calcd for $C_{15}H_{13}FO_3$ $[M+H]^+$: 261.0921; found: 261.0921

9-Chloro-3,3-dimethyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ga)



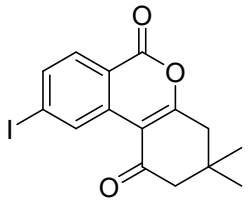
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 40.3 mg, 73% yield, white solid. m.p. 157-159 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.07 (d, *J* = 1.8 Hz, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 7.45 (dd, *J* = 8.5, 1.9 Hz, 1H), 2.78 (s, 2H), 2.51 (s, 2H), 1.16 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.43, 169.06, 159.83, 142.65, 134.99, 130.95, 128.86, 125.65, 117.96, 109.65, 52.58, 42.49, 31.86, 28.06. **HRMS (ESI)**: Calcd for $C_{15}H_{13}ClO_3$ $[M+H]^+$: 277.0626; found: 277.0624

9-Bromo-3,3-dimethyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ha)



silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 49.3 mg, 77% yield, white solid. m.p. 167-169 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.23 (d, *J* = 1.6 Hz, 1H), 8.06 (d, *J* = 8.5 Hz, 1H), 7.61 (dd, *J* = 8.5, 1.8 Hz, 1H), 2.78 (s, 2H), 2.50 (s, 2H), 1.16 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.40, 169.02, 159.97, 134.98, 131.75, 131.61, 130.87, 128.66, 118.32, 109.51, 52.57, 42.49, 31.85, 28.05. **HRMS (ESI)**: Calcd for $C_{15}H_{13}BrO_3$ $[M+H]^+$: 321.0121; found: 321.0210

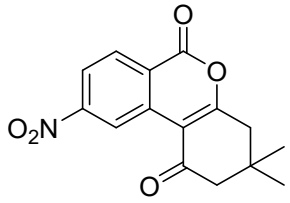
9-Iodo-3,3-dimethyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ia)



silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 55.2 mg, 75% yield, white solid. m.p. 178-180 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.42 (s, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.81 (dd, *J* = 8.4, 1.0 Hz, 1H), 2.77 (s, 2H), 2.49 (s, 2H), 1.15 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.35, 168.83, 160.16, 137.54, 134.68, 134.58,

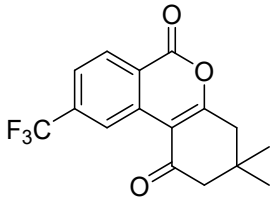
130.43, 118.72, 109.23, 104.87, 52.55, 42.46, 31.81, 28.03. **HRMS (ESI)**: Calcd for $C_{15}H_{13}IO_3$ $[M+H]^+$: 368.9982; found: 368.9981

3,3-Dimethyl-9-nitro-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ja)



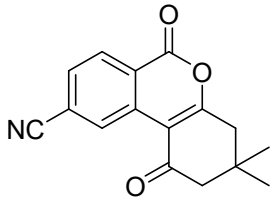
silica gel column chromatography (petroleum ether/ethyl acetate = 2:1), 28.1 mg, 49% yield, yellow solid. m.p. 167-169 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.92 (d, *J* = 1.8 Hz, 1H), 8.43 (d, *J* = 8.7 Hz, 1H), 8.28 (dd, *J* = 8.7, 2.0 Hz, 1H), 2.84 (s, 2H), 2.56 (s, 2H), 1.20 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.06, 169.67, 158.95, 152.10, 135.11, 131.21, 123.76, 122.39, 121.38, 109.64, 52.40, 42.45, 31.96, 28.08. Calcd for $C_{15}H_{13}NO_5$ $[M+Na]^+$: 310.0686; found: 310.0682

3,3-Dimethyl-9-(trifluoromethyl)-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ka)



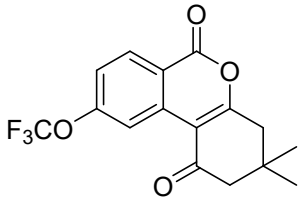
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 52.1 mg, 84% yield, white solid. m.p. 175-177 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.39 (s, 1H), 8.36 (d, *J* = 8.3 Hz, 1H), 7.72 (d, *J* = 8.3 Hz, 1H), 2.81 (s, 2H), 2.53 (s, 2H), 1.18 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.44, 169.07, 159.50, 136.75 (q, $J_{C\text{-}F}$ = 32.7 Hz), 134.30, 130.28, 124.66 (q, $J_{C\text{-}F}$ = 3.4 Hz), 123.78 (q, $J_{C\text{-}F}$ = 248.1 Hz), 123.26 (q, $J_{C\text{-}F}$ = 4.1 Hz), 122.15, 109.83, 52.55, 42.45, 31.91, 28.04. **^{19}F NMR (376 MHz, $CDCl_3$)** δ -63.39. **HRMS (ESI)**: Calcd for $C_{16}H_{13}F_3O_3$ $[M+Na]^+$: 333.0709; found: 333.0707

3,3-Dimethyl-1,6-dioxo-2,3,4,6-tetrahydro-1*H*-benzo[c]chromene-9-carbonitrile (3la)



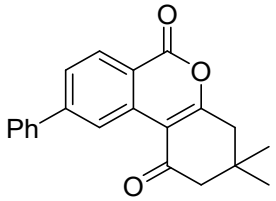
silica gel column chromatography (petroleum ether/ethyl acetate = 2:1), 27.2 mg, 51% yield, white solid. m.p. 144-146 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.45 (d, *J* = 0.9 Hz, 1H), 8.35 (d, *J* = 8.2 Hz, 1H), 7.74 (dd, *J* = 8.2, 1.4 Hz, 1H), 2.82 (s, 2H), 2.54 (s, 2H), 1.18 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.29, 169.49, 159.13, 134.29, 130.68, 130.26, 130.26, 122.44, 118.97, 117.59, 109.29, 52.45, 42.46, 31.93, 28.06. **HRMS (ESI)**: Calcd for $C_{16}H_{13}NO_3$ $[M+Na]^+$: 290.0788; found: 290.0785

3,3-Dimethyl-9-(trifluoromethoxy)-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ma)



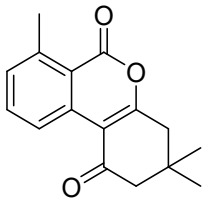
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 43.7 mg, 67% yield, yellow solid. m.p. 99-101 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.97 (s, 1H), 8.30 (d, *J* = 8.8 Hz, 1H), 7.33 (d, *J* = 8.8 Hz, 1H), 2.80 (s, 2H), 2.52 (s, 2H), 1.17 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.46, 169.29, 159.51, 154.54, 135.96, 131.99, 120.23, 120.20 (q, $J_{C\text{-}F}$ = 259.8 Hz), 117.78, 116.90, 109.78, 52.55, 42.49, 31.90, 28.06. **^{19}F NMR (376 MHz, $CDCl_3$)** δ -57.41. **HRMS (ESI)**: Calcd for $C_{16}H_{13}F_3O_4$ $[M+H]^+$: 327.0839; found: 327.0842

3,3-Dimethyl-9-phenyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3na)



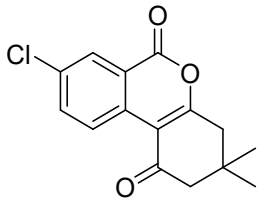
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 55.4 mg, 87% yield, pale yellow solid. m.p. 158-160 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.33 (s, 1H), 8.31 (d, *J* = 8.3 Hz, 1H), 7.75 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.71 (d, *J* = 7.3 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 2H), 7.42 (t, *J* = 7.2 Hz, 1H), 2.80 (s, 2H), 2.53 (s, 2H), 1.18 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.96, 168.31, 160.58, 148.18, 139.52, 134.26, 130.09, 128.97, 128.66, 127.54, 127.11, 124.07, 118.30, 110.54, 52.85, 42.54, 31.91, 28.10. **HRMS (ESI)**: Calcd for $C_{21}H_{18}O_3$ $[M+H]^+$: 319.1329; found: 319.1328

3,3,7-Trimethyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3oa)



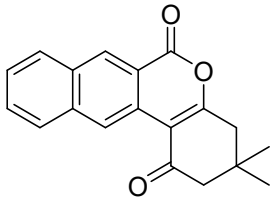
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 19.5 mg, 38% yield, white solid. m.p. 127-129 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.94 (d, *J* = 8.3 Hz, 1H), 7.62 (t, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 7.4 Hz, 1H), 2.79 (s, 3H), 2.76 (s, 2H), 2.50 (s, 2H), 1.16 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.82, 167.86, 159.71, 143.36, 135.29, 134.78, 131.40, 123.57, 118.15, 110.55, 53.07, 42.46, 31.81, 28.10, 23.73. **HRMS (ESI)**: Calcd for $C_{16}H_{16}O_3$ $[M+H]^+$: 257.1172; found: 257.1169

8-Chloro-3,3-dimethyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3pa)



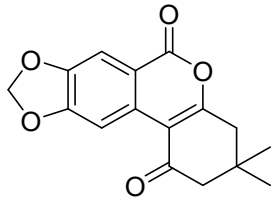
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 11.6 mg, 21% yield, white solid. m.p. 170-172 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.03 (d, *J* = 8.9 Hz, 1H), 8.24 (d, *J* = 2.4 Hz, 1H), 7.72 (dd, *J* = 8.9, 2.4 Hz, 1H), 2.80 (s, 2H), 2.52 (s, 2H), 1.18 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.66, 168.05, 159.58, 135.79, 134.40, 132.23, 128.90, 127.62, 121.22, 110.12, 52.69, 42.45, 31.95, 28.12. **HRMS (ESI)**: Calcd for $C_{15}H_{13}ClO_3$ $[M+H]^+$: 277.0626; found: 277.0624

3,3-Dimethyl-3,4-dihydro-1*H*-naphtho[2,3-c]chromene-1,6(2*H*)-dione (3qa)



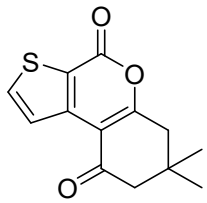
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 43.2 mg, 74% yield, white solid. m.p. 181-183 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.48 (s, 1H), 8.86 (s, 1H), 7.97 (t, *J* = 9.1 Hz, 2H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 2.80 (s, 2H), 2.55 (s, 2H), 1.19 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 197.24, 166.76, 160.90, 136.79, 131.90, 131.67, 129.45, 129.15, 128.92, 127.68, 127.14, 125.30, 117.92, 110.51, 52.84, 42.50, 31.90, 28.14. **HRMS (ESI)**: Calcd for $C_{19}H_{16}O_3$ $[M+H]^+$: 293.1172; found: 293.1169

3,3-Dimethyl-3,4-dihydro-1*H*-[1,3]dioxolo[4',5':4,5]benzo[1,2-c]chromene-1,6(2*H*)-dione (3ra)



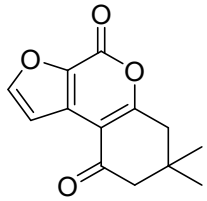
silica gel column chromatography (petroleum ether/ethyl acetate = 2:1), 30.9 mg, 54% yield, yellow solid. m.p. 163-165 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.95 (d, *J* = 8.4 Hz, 1H), 7.00 (d, *J* = 8.4 Hz, 1H), 6.14 (s, 2H), 2.73 (s, 2H), 2.53 (s, 2H), 1.16 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 193.90, 165.82, 160.03, 154.13, 142.26, 126.93, 115.33, 114.58, 111.05, 109.61, 102.04, 52.31, 42.31, 32.45, 28.29. **HRMS (ESI)**: Calcd for $C_{16}H_{14}O_5$ $[M+H]^+$: 287.0914; found: 287.0911

7,7-Dimethyl-7,8-dihydro-4*H*-thieno[2,3-c]chromene-4,9(6*H*)-dione (3sa)



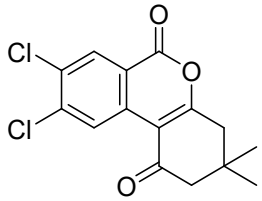
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 42.2 mg, 85% yield, white solid. m.p. 125-127 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.18 (d, *J* = 5.2 Hz, 1H), 7.89 (d, *J* = 5.2 Hz, 1H), 2.80 (s, 2H), 2.48 (s, 2H), 1.16 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 194.99, 169.29, 156.70, 143.41, 137.69, 125.94, 122.75, 111.32, 51.43, 41.71, 32.35, 28.15. **HRMS (ESI)**: Calcd for $C_{13}H_{12}O_3S$ $[M+H]^+$: 249.0580; found: 249.0576

7,7-Dimethyl-7,8-dihydro-4*H*-furo[2,3-c]chromene-4,9(6*H*)-dione (3ta)



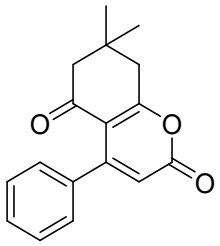
silica gel column chromatography (petroleum ether/ethyl acetate = 2:1), 17.2 mg, 37% yield, white solid. m.p. 148-150 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.85 (d, *J* = 1.0 Hz, 1H), 7.37 (d, *J* = 1.0 Hz, 1H), 2.78 (s, 2H), 2.47 (s, 2H), 1.17 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 195.02, 168.98, 151.34, 136.82, 132.47, 110.12, 109.10, 99.95, 50.97, 41.60, 32.85, 28.24. **HRMS (ESI)**: Calcd for $C_{13}H_{12}O_4$ $[M+H]^+$: 233.0808; found: 233.0807

8,9-Dichloro-3,3-dimethyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ua)



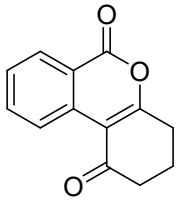
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 18.6 mg, 30% yield, yellow solid. m.p. 163-165 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.24 (s, 1H), 8.32 (s, 1H), 2.79 (s, 2H), 2.52 (s, 2H), 1.18 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.30, 169.07, 158.91, 141.00, 132.96, 132.92, 130.81, 127.87, 119.34, 109.31, 52.51, 42.49, 31.93, 28.09. **HRMS (ESI)**: Calcd for $C_{15}H_{12}Cl_2O_3$ $[M+H]^+$: 311.0236; found: 311.0235

7,7-Dimethyl-4-phenyl-7,8-dihydro-2*H*-chromene-2,5(6*H*)-dione (3va)



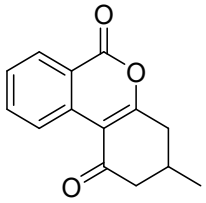
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 29.5 mg, 55% yield, yellow liquid. m.p. 110-112 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.43 – 7.35 (m, 3H), 7.22 – 7.14 (m, 2H), 6.08 (s, 1H), 2.81 (s, 2H), 2.42 (s, 2H), 1.16 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 193.31, 173.37, 159.77, 156.35, 136.99, 128.88, 127.87, 127.07, 114.15, 113.18, 52.21, 42.71, 32.01, 28.15. **HRMS (ESI)**: Calcd for $C_{17}H_{16}O_3$ $[M+H]^+$: 269.1172; found: 269.1172

3,4-Dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ab)[3]



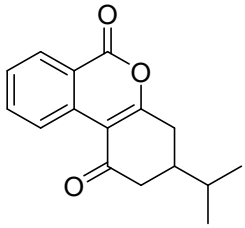
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 31.3 mg, 73% yield, pale yellow solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.01 (d, *J* = 8.2 Hz, 1H), 8.24 (d, *J* = 7.8 Hz, 1H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 2.92 (t, *J* = 5.5 Hz, 2H), 2.64 (t, *J* = 5.9 Hz, 2H), 2.26 – 2.04 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.83, 169.40, 160.37, 135.54, 133.95, 129.47, 128.33, 125.95, 119.78, 111.49, 38.87, 28.90, 19.92.

3-Methyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ac) [3]



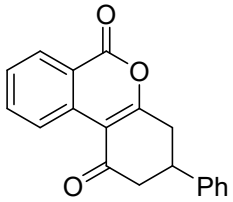
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 36.9 mg, 81% yield, yellow solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.02 (d, *J* = 8.3 Hz, 1H), 8.24 (d, *J* = 7.9 Hz, 1H), 7.76 (t, *J* = 7.7 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 2.92 (d, *J* = 18.4 Hz, 1H), 2.80 – 2.56 (m, 2H), 2.52 – 2.26 (m, 2H), 1.17 (d, *J* = 5.6 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.83, 168.84, 160.45, 135.54, 133.86, 129.48, 128.33, 125.82, 119.71, 111.04, 47.07, 36.76, 27.62, 20.71.

3-Isopropyl-3,4-dihydro-1H-benzo[c]chromene-1,6(2*H*)-dione (3ad)[4]



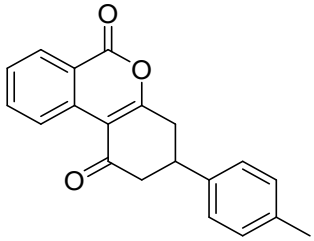
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 40.9 mg, 80% yield, white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.99 (d, *J* = 8.3 Hz, 1H), 8.22 (d, *J* = 7.9 Hz, 1H), 7.75 (t, *J* = 8.3 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 2.88 (dd, *J* = 18.2, 4.6 Hz, 1H), 2.76 - 2.63 (m, 2H), 2.36 (dd, *J* = 15.8, 13.3 Hz, 1H), 2.04 (qd, *J* = 11.1, 4.5 Hz, 1H), 1.67 (dq, *J* = 13.4, 6.7 Hz, 1H), 0.98 (d, *J* = 6.7 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 197.20, 169.42, 160.40, 135.50, 133.80, 129.44, 128.28, 125.73, 119.62, 110.98, 43.02, 38.69, 32.72, 31.73, 19.41, 19.35.

3-Phenyl-3,4-dihydro-1*H*-benzo[c]chromene-1,6(2*H*)-dione (3ae) [3]



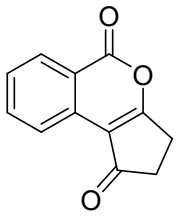
silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 48.1 mg, 83% yield, yellow solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.08 (d, *J* = 8.2 Hz, 1H), 8.29 (d, *J* = 7.9 Hz, 1H), 7.81 (t, *J* = 7.7 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.39 (t, *J* = 7.2 Hz, 2H), 7.30 (d, *J* = 7.1 Hz, 3H), 3.56 (s, 1H), 3.27 – 3.00 (m, 2H), 3.03 – 2.76 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 195.99, 168.55, 160.34, 141.36, 135.69, 133.75, 129.61, 129.00, 128.54, 127.47, 126.53, 125.92, 119.78, 111.29, 45.84, 37.91, 36.30.

3-(*p*-tolyl)-3,4-dihydro-1H-benzo[c]chromene-1,6(2H)-dione (3af)[5]



silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 31.0 mg, 51% yield, white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.08 (d, *J* = 8.3 Hz, 1H), 8.29 (d, *J* = 7.9 Hz, 1H), 7.80 (t, *J* = 8.4 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 3.60 – 3.45 (m, 1H), 3.20 – 3.08 (m, 2H), 2.98 – 2.78 (m, 2H), 2.36 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 196.13, 168.63, 160.37, 138.39, 137.15, 135.67, 133.77, 129.62, 129.59, 128.50, 126.39, 125.91, 119.76, 111.25, 45.96, 37.55, 36.43, 21.00.

2,3-Dihydrocyclopenta[c]isochromene-1,5-dione (3ag) [3]



silica gel column chromatography (petroleum ether/ethyl acetate = 4:1), 23.6 mg, 59% yield, white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.48 (d, *J* = 7.8 Hz, 1H), 8.26 (d, *J* = 7.9 Hz, 1H), 7.80 (t, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 3.02 (s, 2H), 2.75 (d, *J* = 3.7 Hz, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 200.32, 180.41, 161.05, 135.83, 131.84, 130.39, 129.04, 123.21, 118.57, 114.51, 34.56, 25.76.

5. References

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(2) Moriarty, R. M.; Tyagi, S.; Ivanov, D.; Constantinescu, M. *J. Am. Chem. Soc.* **2008**, *130*, 7564

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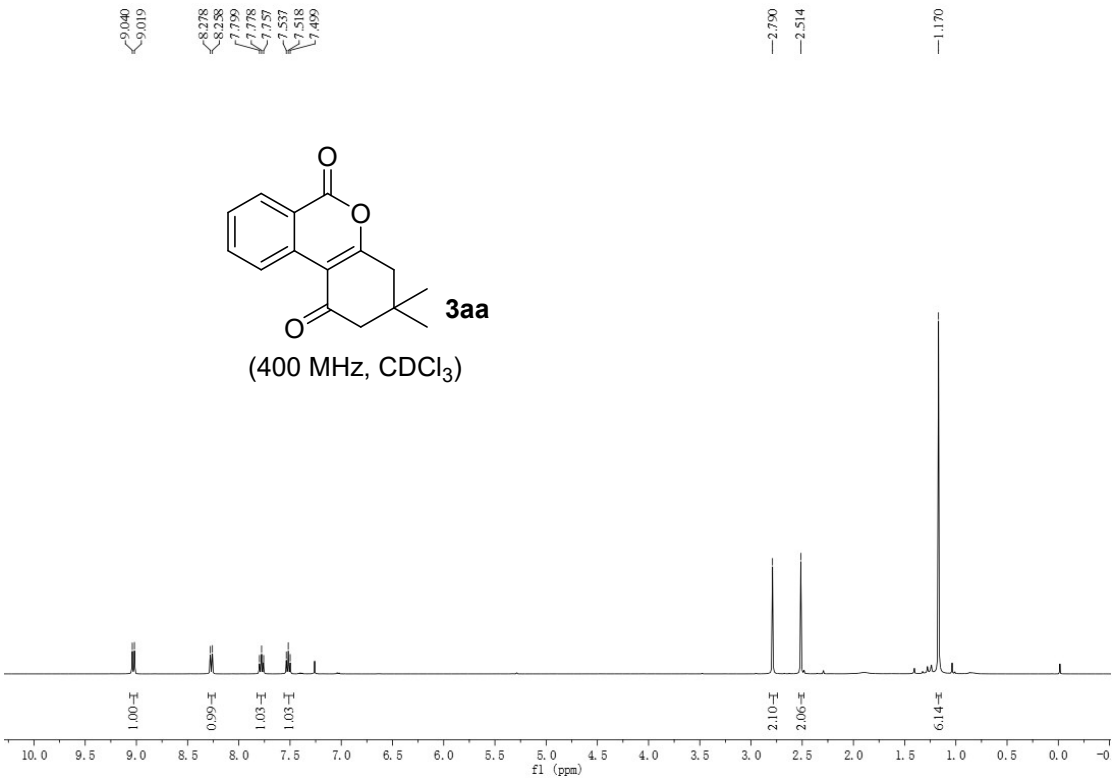
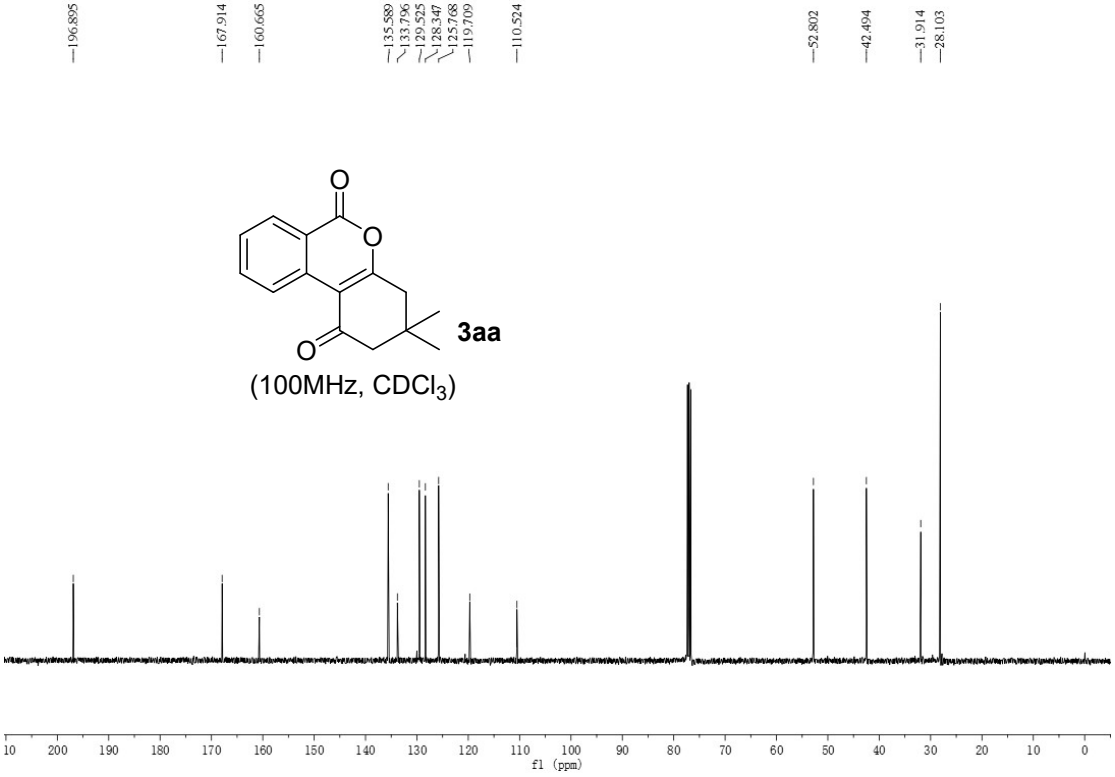
(5) S. Kumar, S. Nunewar, V. Kanchupalli, *Asian J. Org. Chem.* **2021**, *11*, e202100689

6. Copies of ^{1} H, ^{13}C, and ^{19}F NMR of products


9.040
9.019
8.278
8.258
7.799
7.778
7.757
7.537
7.518
7.499
2.790
2.514
1.170
3aa
(400 MHz, CDCl3)
1.00
0.99
1.03
1.03
2.10
2.06
6.14
f1 (ppm)


196.895
167.914
160.665
135.589
133.796
129.525
128.347
125.768
119.709
110.524
52.802
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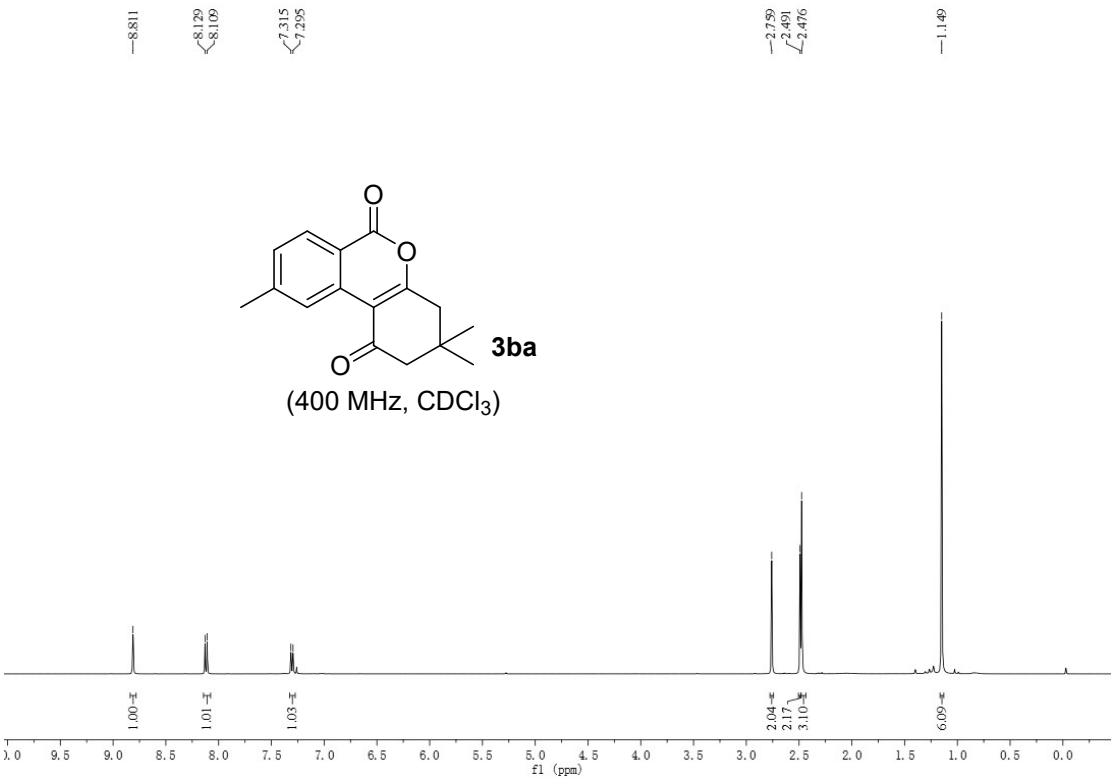
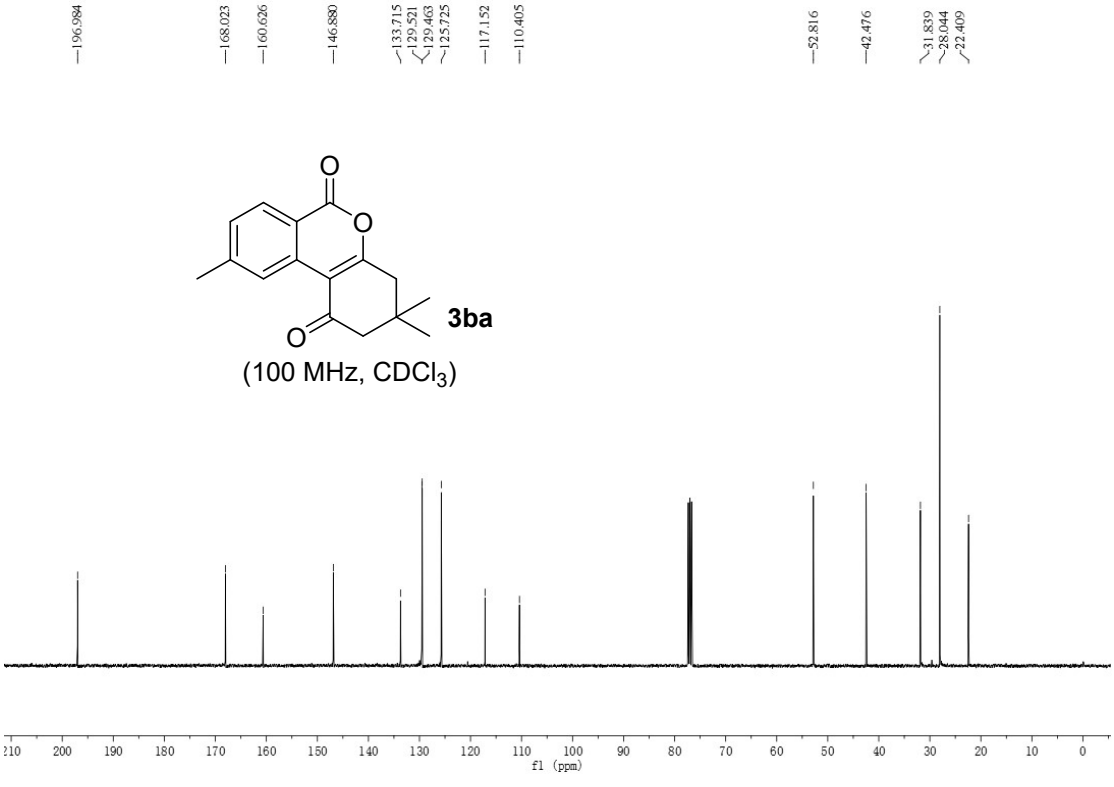
31.914
28.103
3aa
(100MHz, CDCl3)
f1 (ppm)



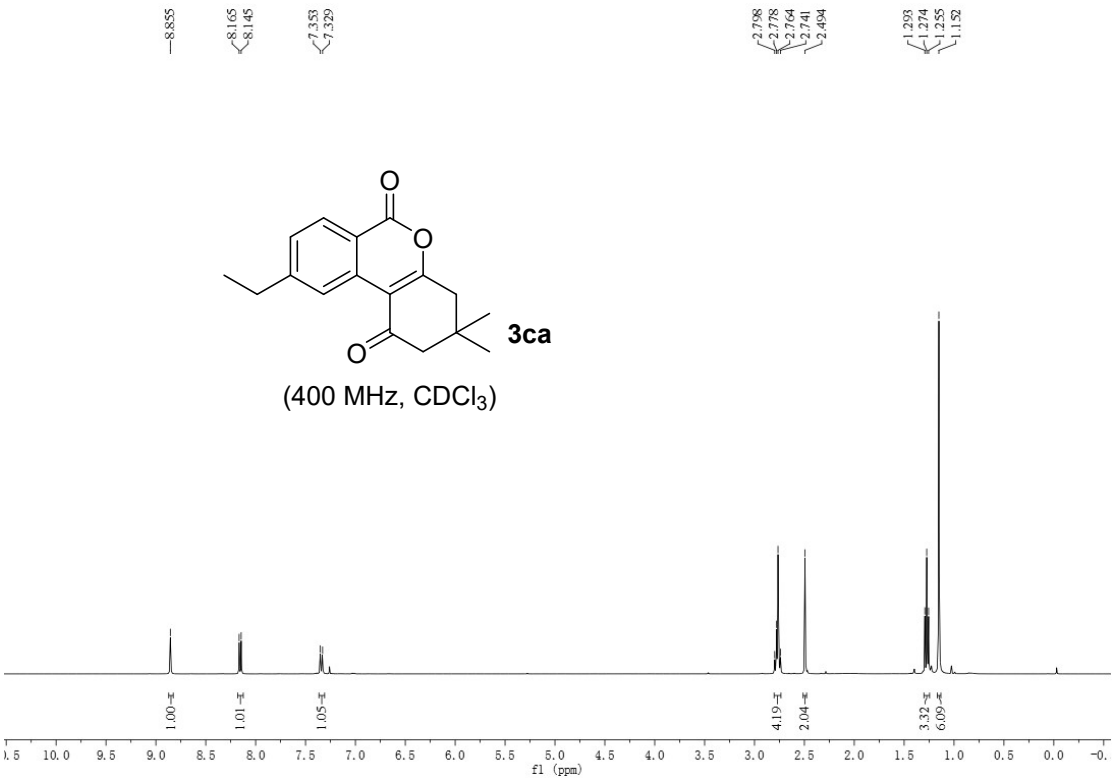
3ba

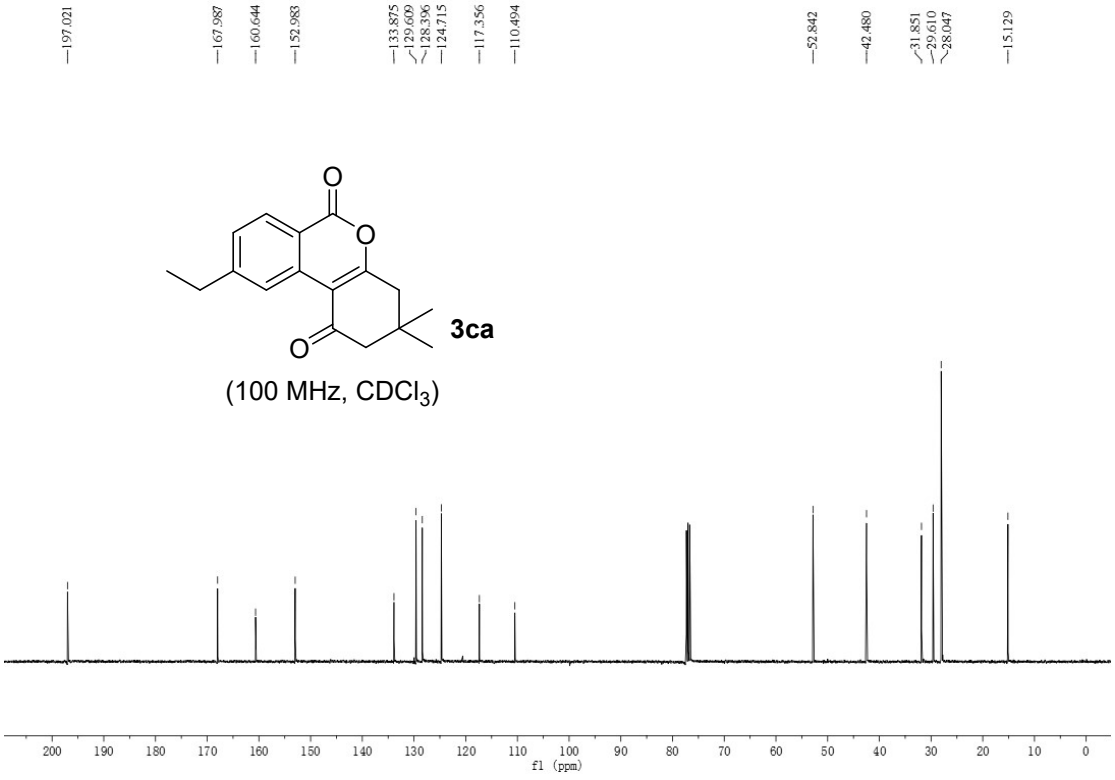
(400 MHz, $CDCl_3$)

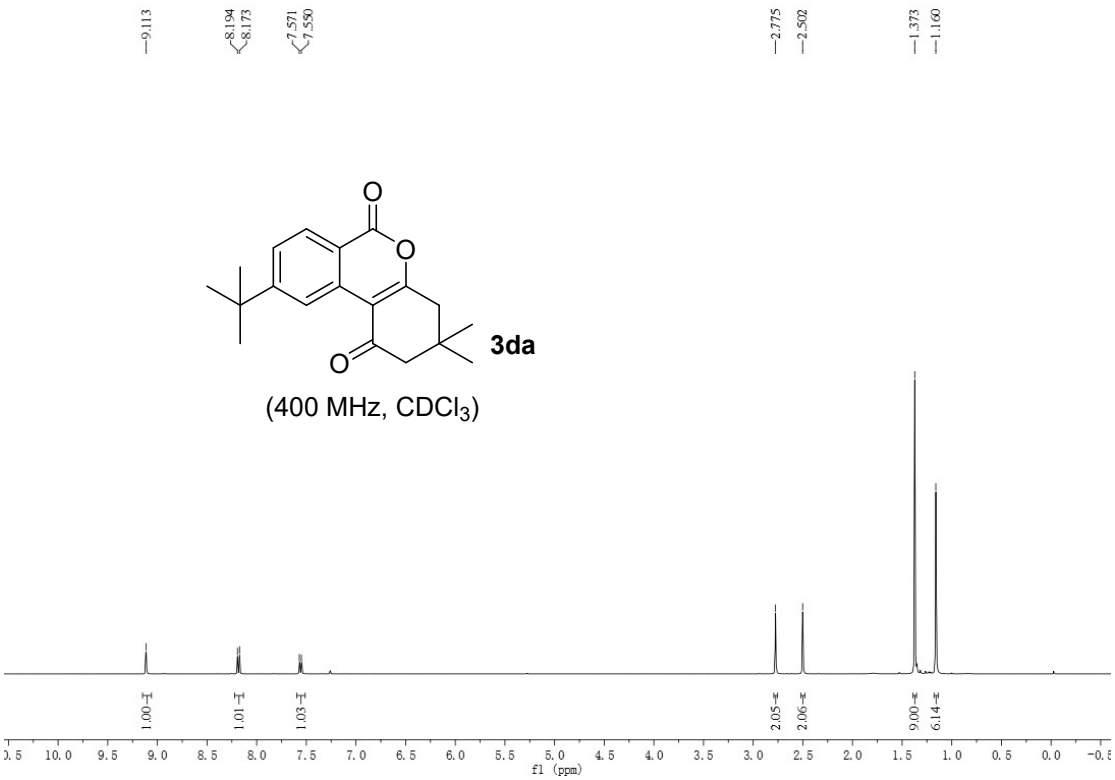


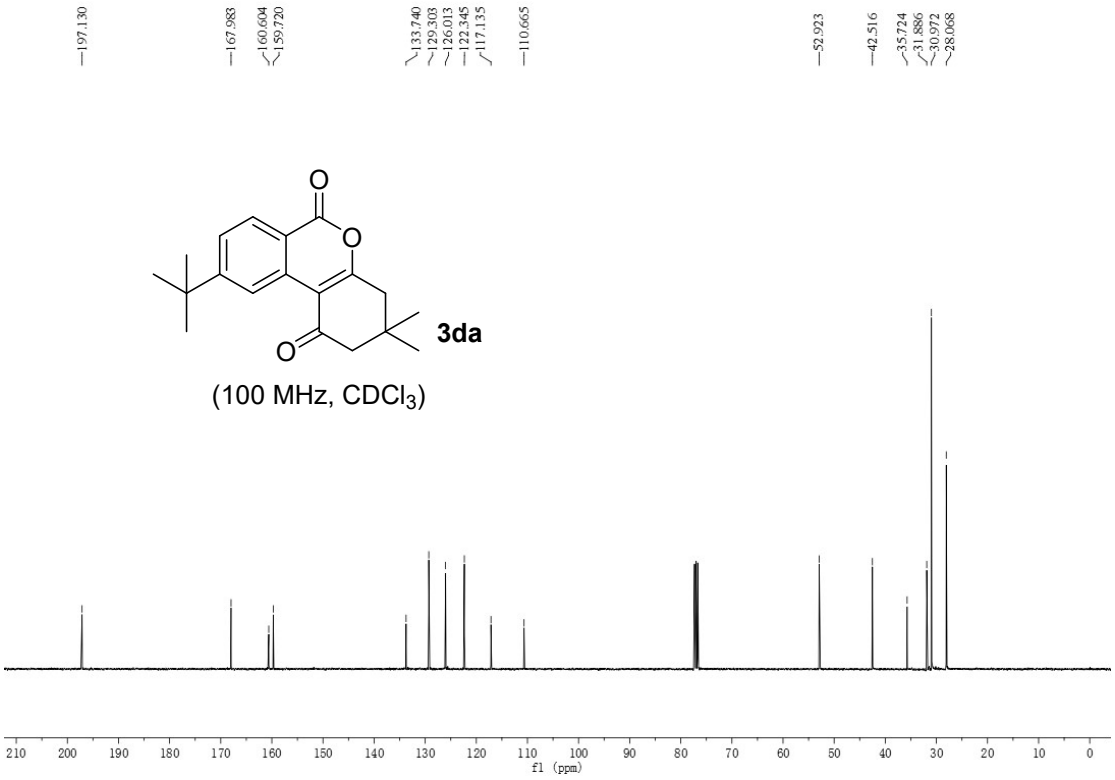
3ba

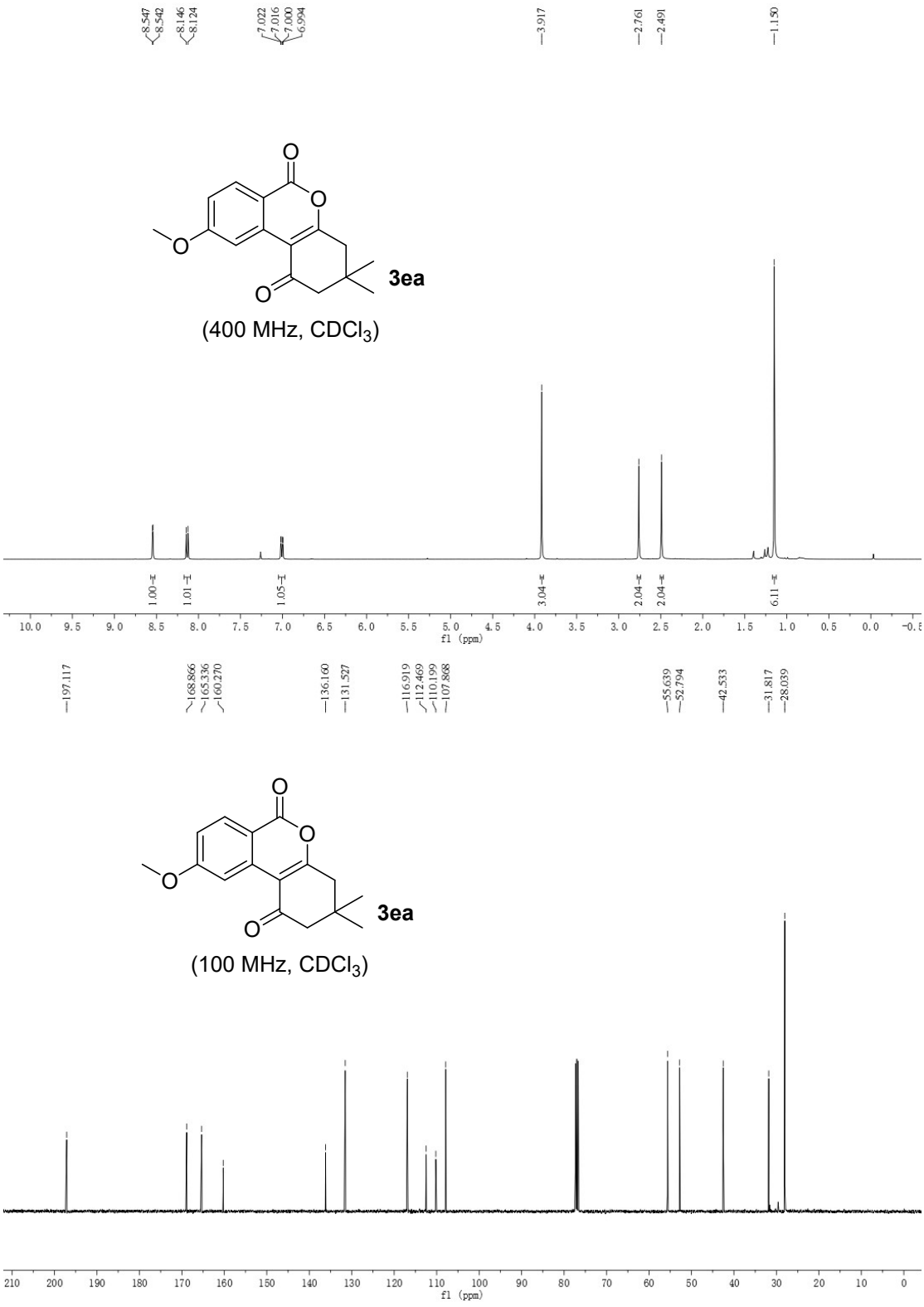
(100 MHz, $CDCl_3$)

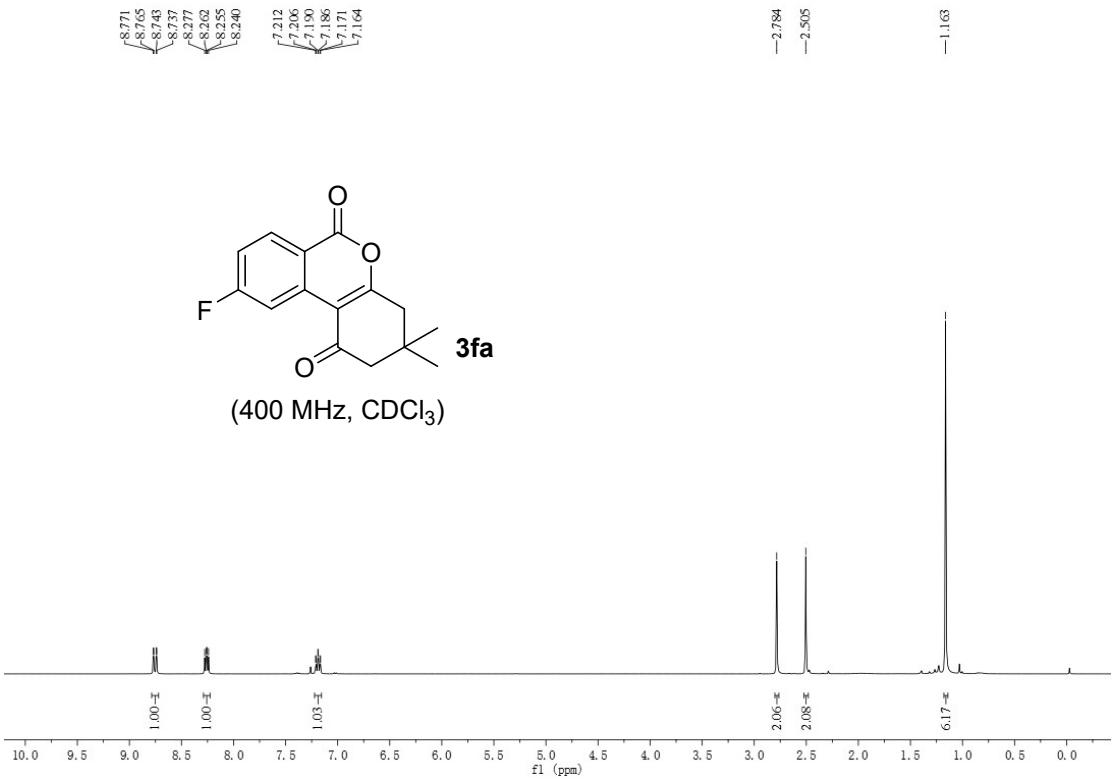

8.855
8.165
8.145
7.353
7.329
2.798
2.778
2.764
2.741
2.494
1.293
1.274
1.255
1.152
3ca
(400 MHz, CDCl3)
1.00
1.01
1.05
4.19
2.04
3.32
6.09
f1 (ppm)


197.021
167.987
160.644
152.983
133.875
129.609
128.396
124.715
117.356
110.494
52.842
42.480
31.851
29.610
28.047
15.129
3ca
(100 MHz, CDCl3)
f1 (ppm)

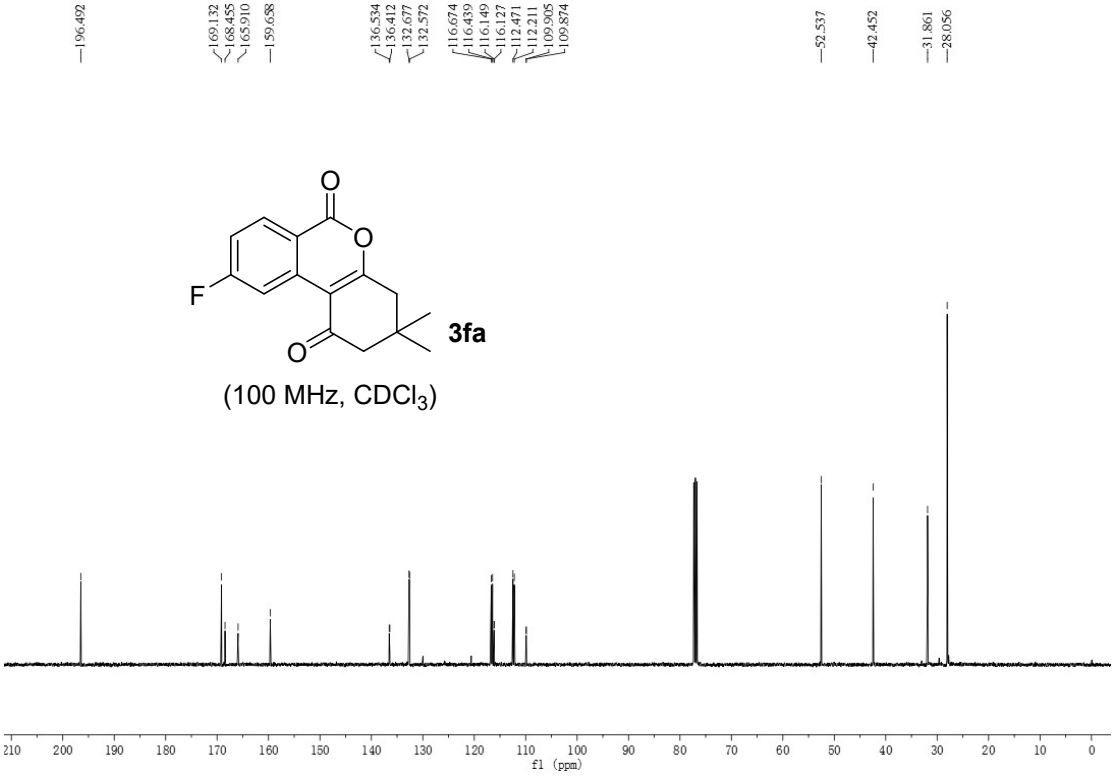

9.113
8.194
8.173
7.571
7.550
2.775
2.502
1.373
1.160
3da
(400 MHz, CDCl3)
1.00
1.01
1.03
2.05
2.06
9.00
6.14
f1 (ppm)


197.130
167.983
160.604
159.720
133.740
129.303
126.013
122.345
117.135
110.665
52.923
42.516
35.724
31.886
30.972
28.068
3da
(100 MHz, CDCl3)
f1 (ppm)

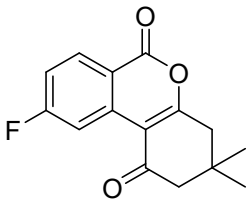

8.547
8.542
8.146
8.124
7.022
7.016
7.000
6.994
3.917
2.761
2.491
1.150
3ea
(400 MHz, CDCl3)
1.00
1.01
1.05
3.04
2.04
2.04
6.11
f1 (ppm)
197.117
168.866
165.336
160.270
136.160
131.527
116.919
112.469
110.199
107.868
55.639
52.794
42.533
31.817
28.039
3ea
(100 MHz, CDCl3)
f1 (ppm)



(400 MHz, $CDCl_3$)

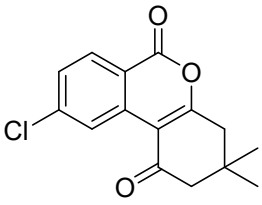


(100 MHz, $CDCl_3$)



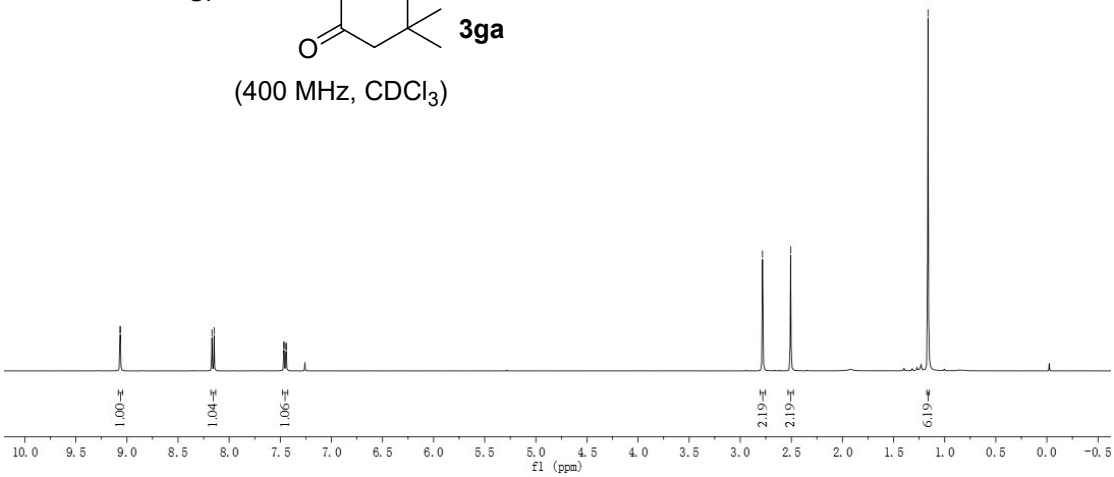
3fa

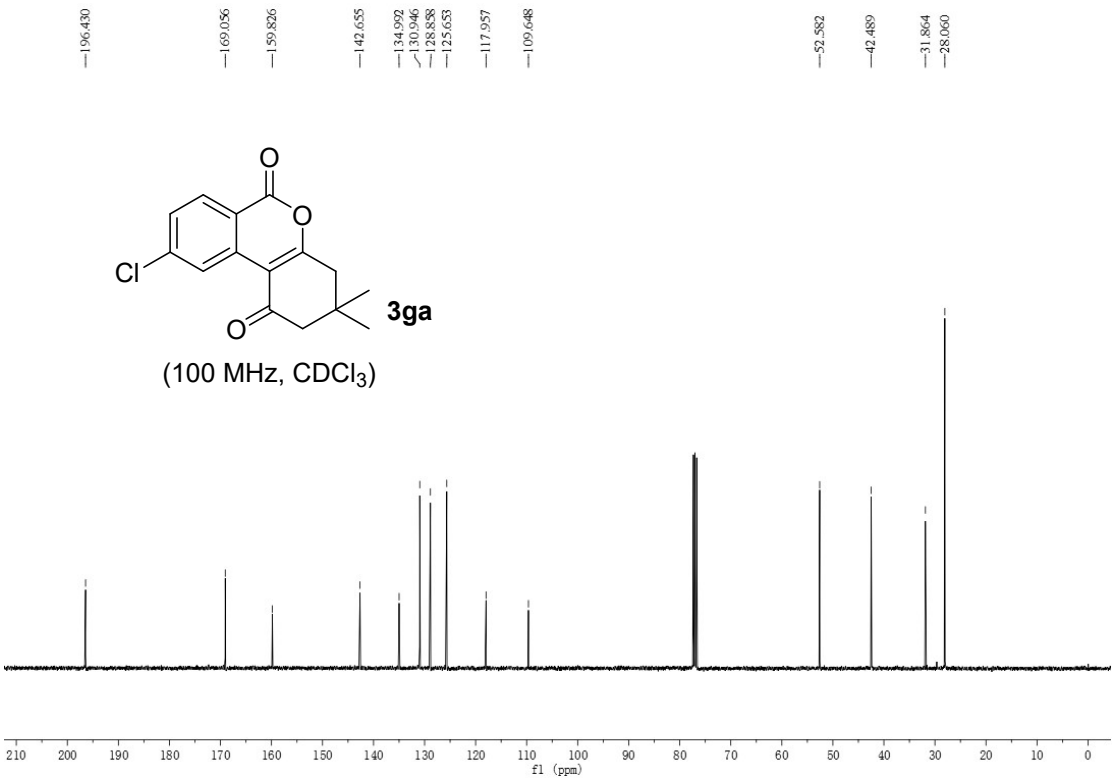
(376 MHz, $CDCl_3$)

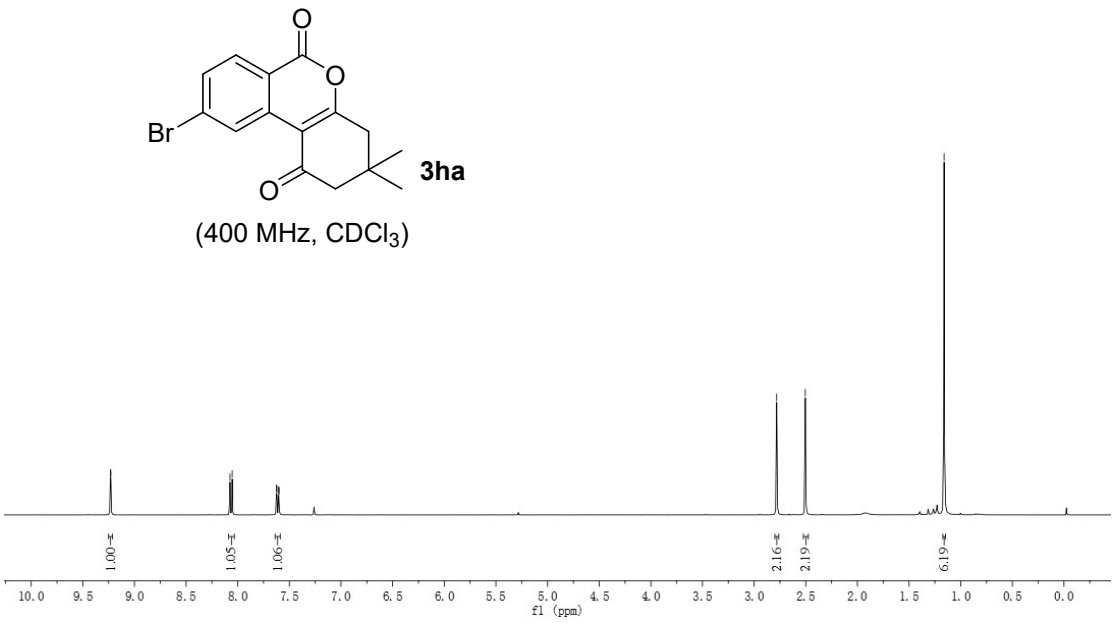


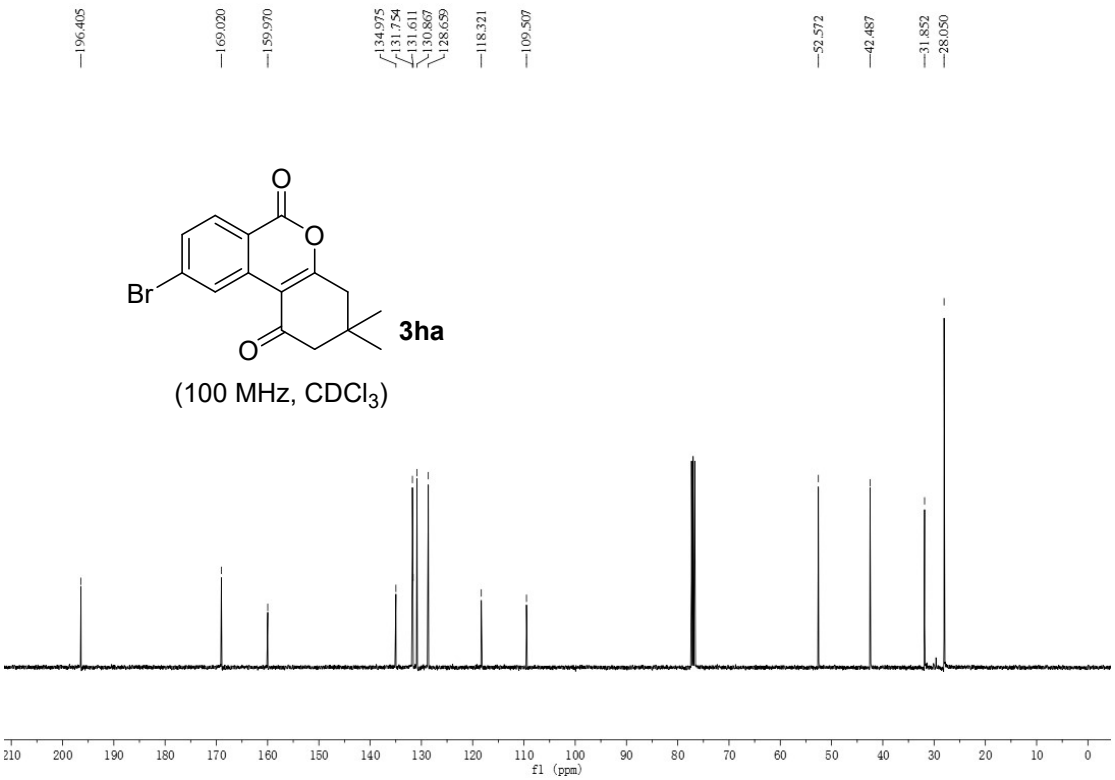
3ga

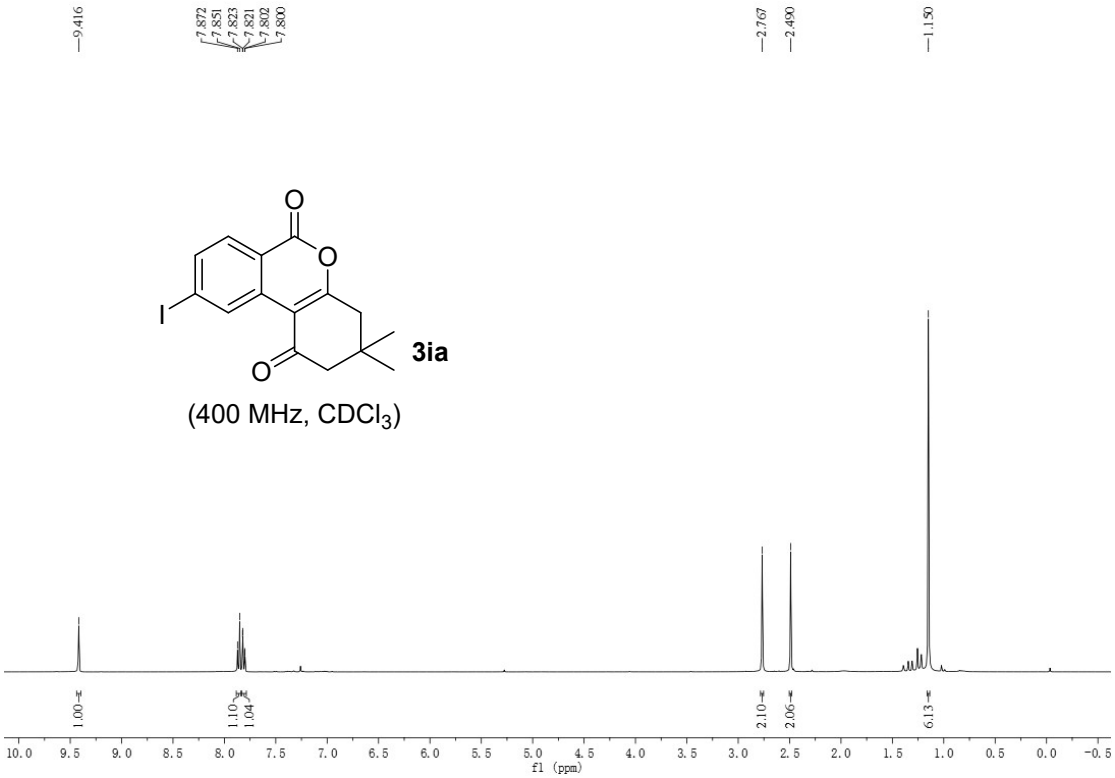
(400 MHz, $CDCl_3$)

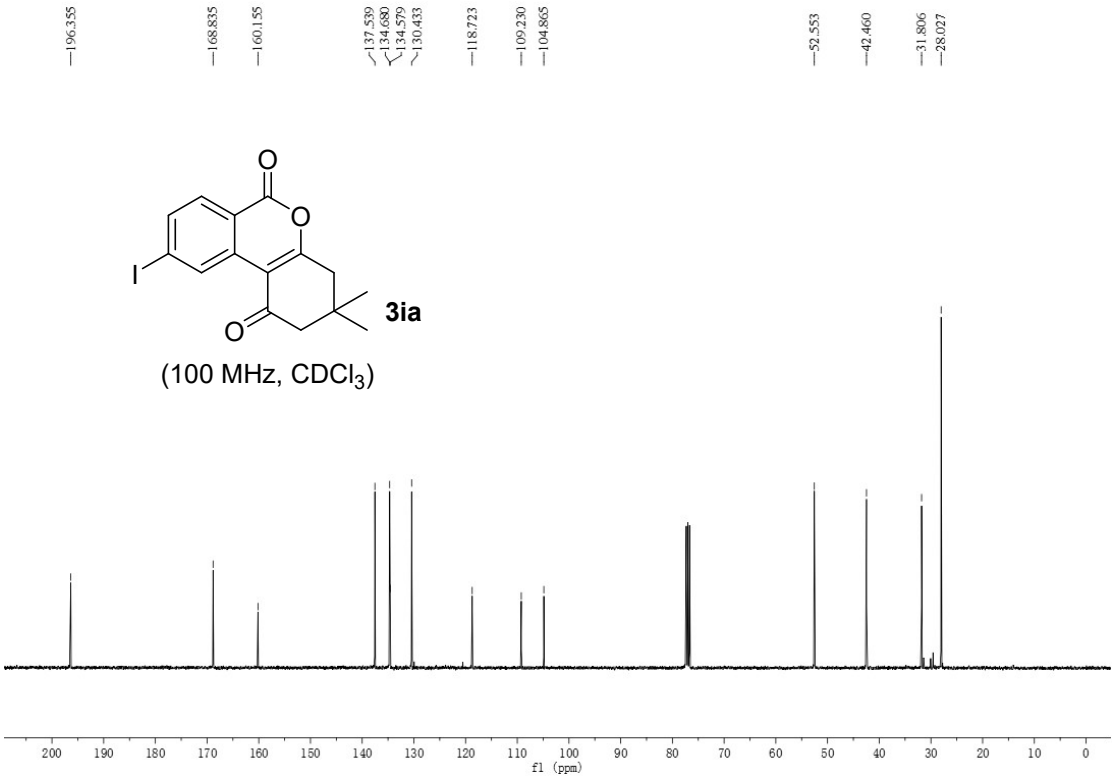


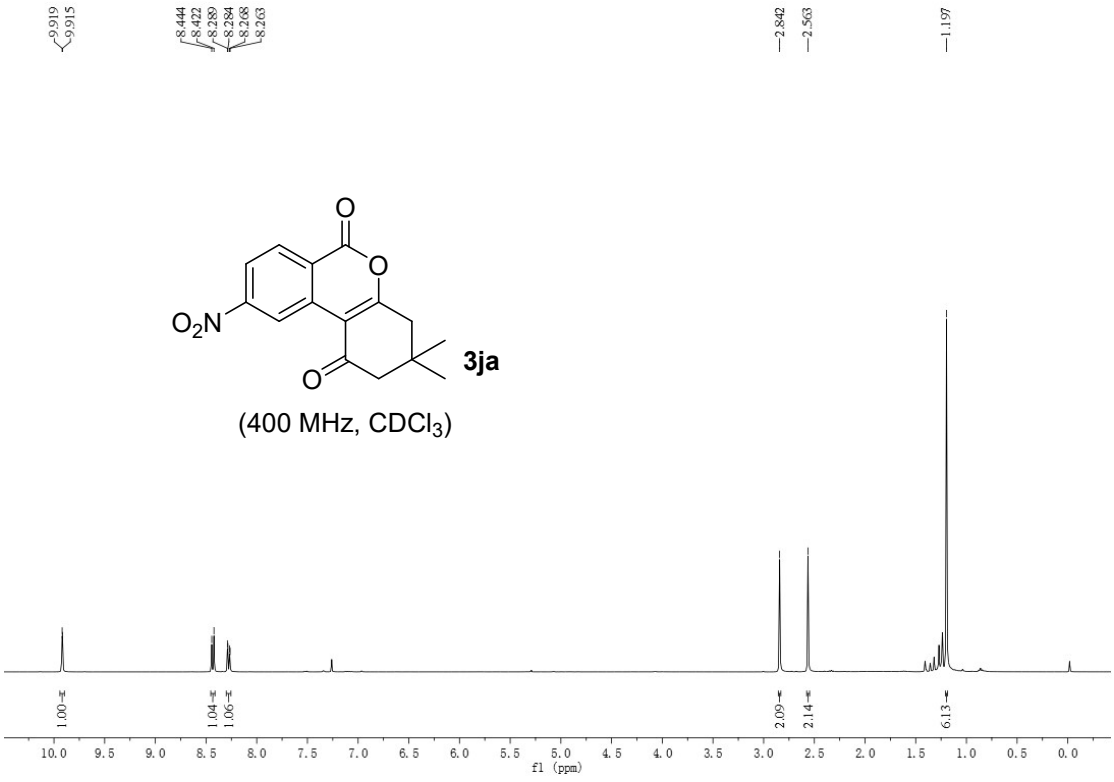

196.430
169.056
159.826
142.655
134.992
130.946
128.858
125.653
117.957
109.648
52.582
42.489
31.864
28.060
Cl
O
O
O
3ga
(100 MHz, CDCl3)
f1 (ppm)
9.233
9.229
8.075
8.054
7.625
7.620
7.604
7.599
2.782
2.504
1.160

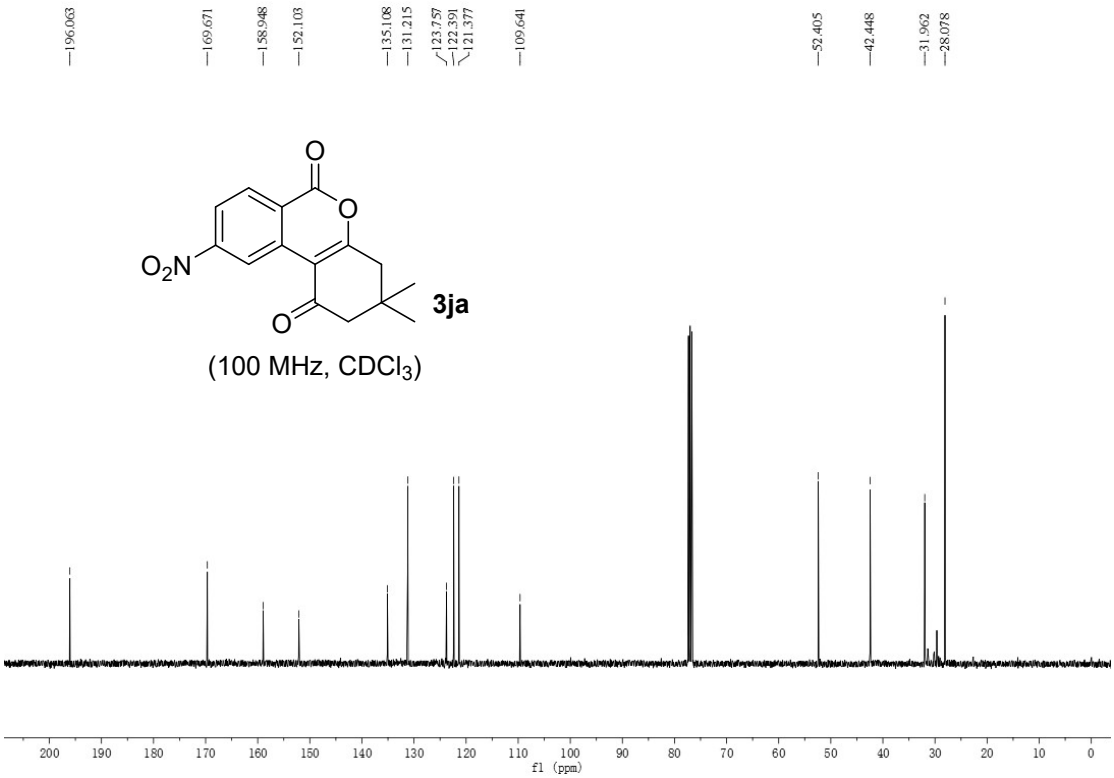

Br
O
O
O
3ha
(400 MHz, CDCl3)
f1 (ppm)
1.00
1.05
1.06
2.16
2.19
6.19

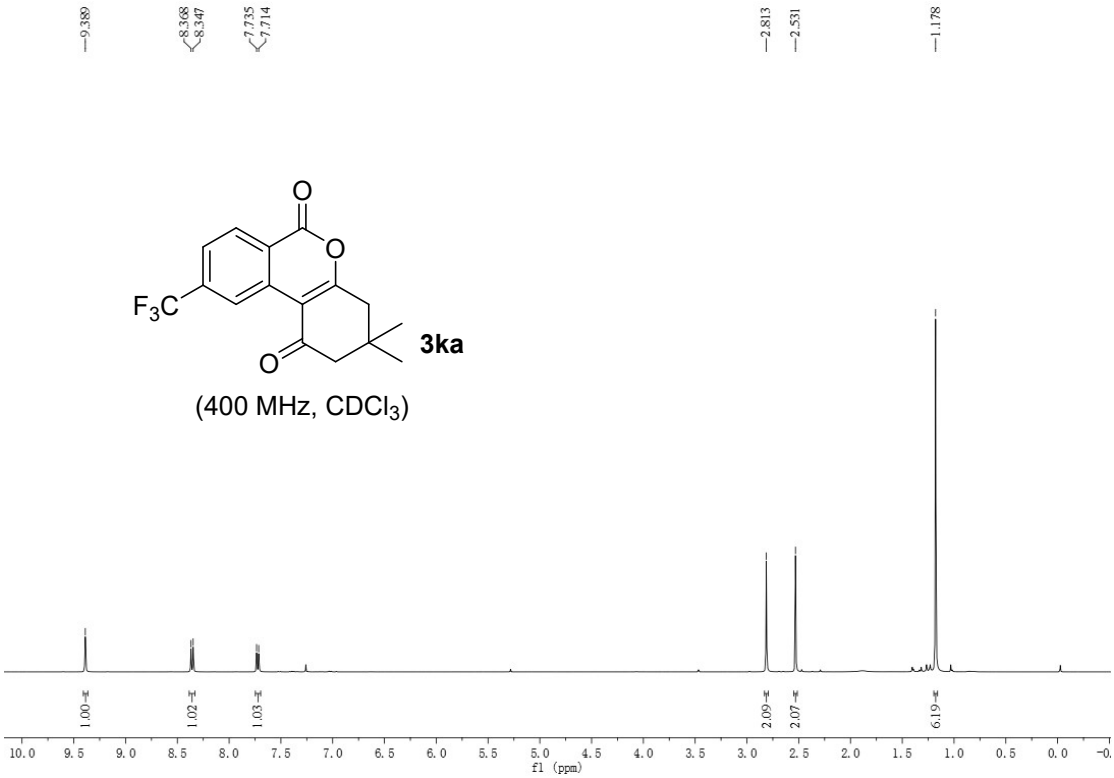

196.405
169.020
159.970
134.975
131.754
131.611
130.867
128.659
118.321
109.507
52.572
42.487
31.852
28.050
Br
O
O
O
3ha
(100 MHz, CDCl3)
f1 (ppm)

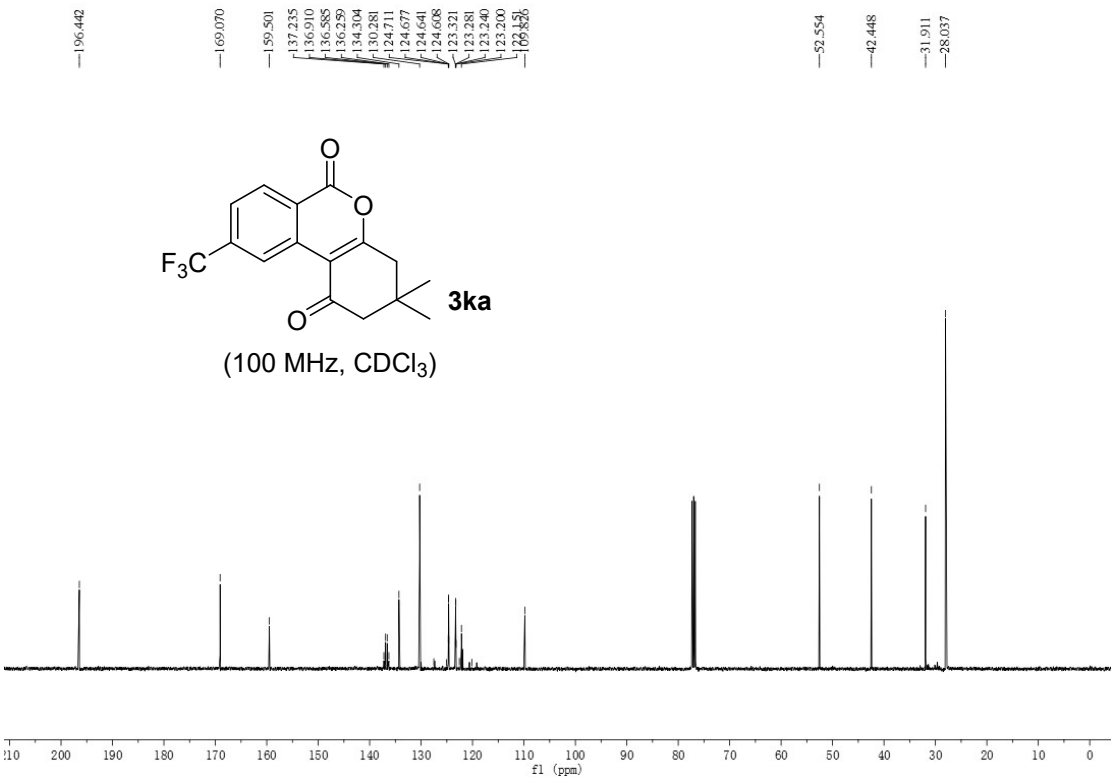

9.416
7.872
7.851
7.823
7.821
7.802
7.800
2.767
2.490
1.150
1.00
1.10
1.04
2.10
2.06
6.13
I
O
O
O
3ia
(400 MHz, CDCl3)
f1 (ppm)


196.355
168.835
160.155
137.539
134.680
134.579
130.433
118.723
109.230
104.865
52.553
42.460
31.806
28.027
O
O
I
O
3ia
(100 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

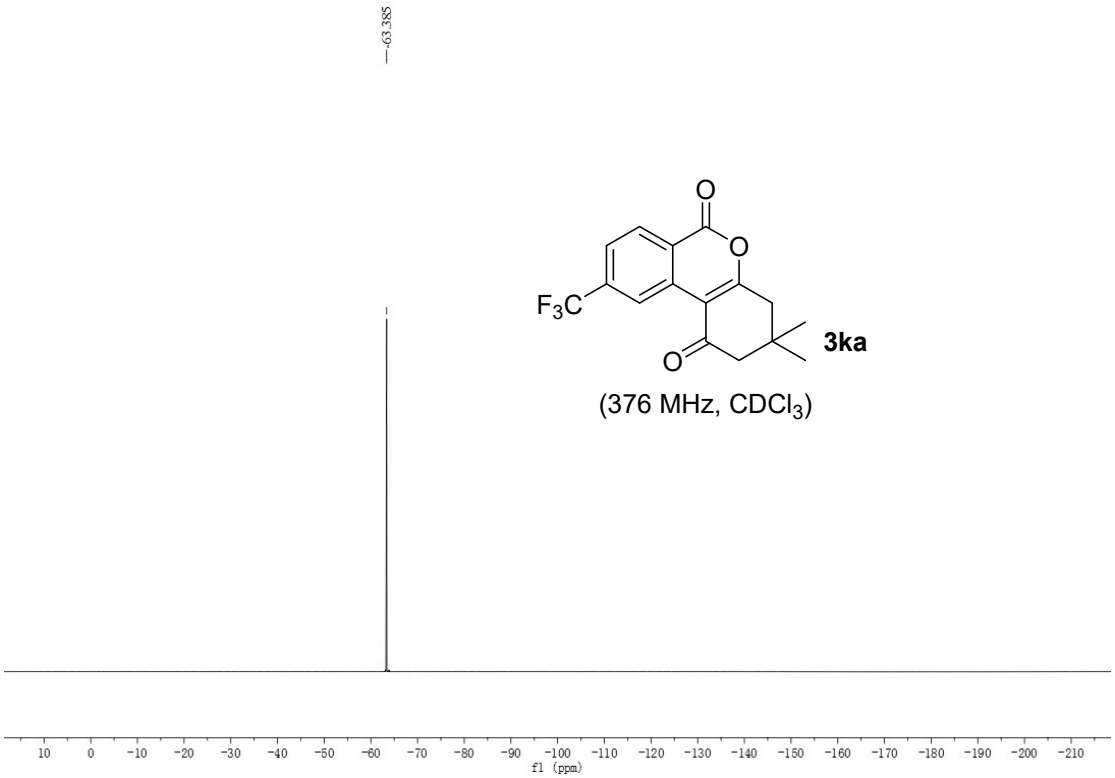

9.919
9.915
8.444
8.422
8.289
8.284
8.268
8.263
2.842
2.563
1.197
O
O
O2N
O
3ja
(400 MHz, CDCl3)
1.00
1.04
1.06
2.09
2.14
6.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


196.063
169.671
158.948
152.103
135.108
131.215
123.757
122.391
121.377
109.641
52.405
42.448
31.962
28.078
O
O
O2N
O
3ja
(100 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

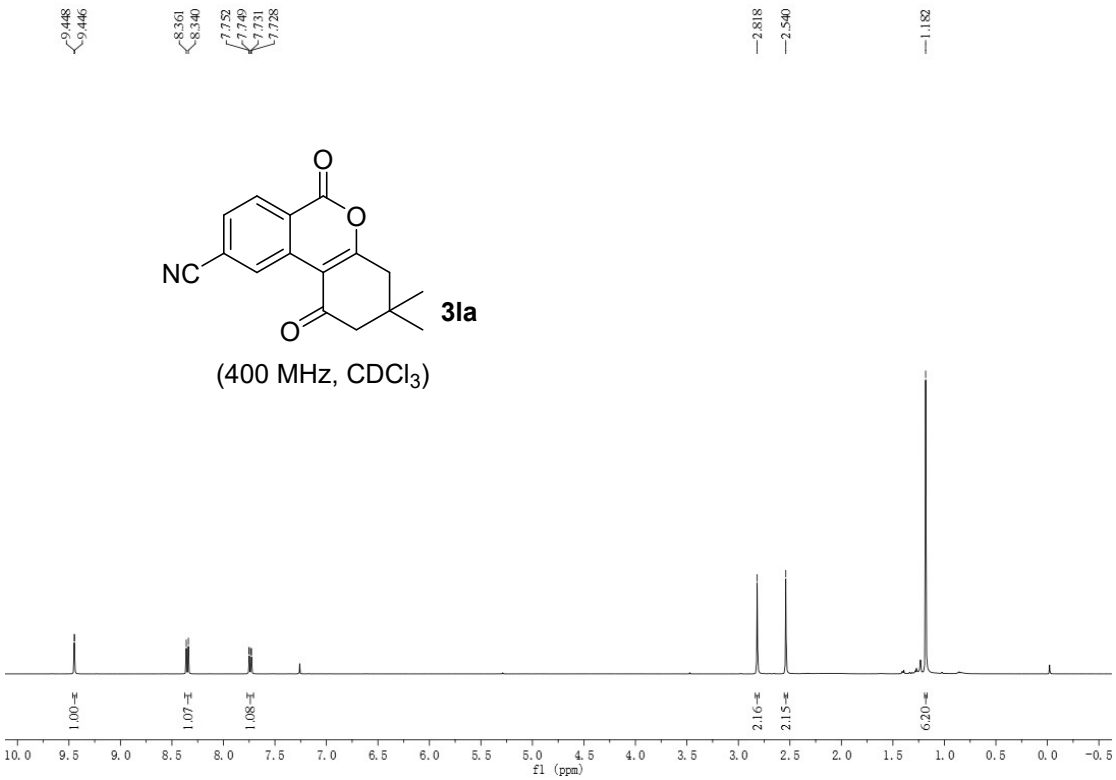

9.389
8.368
8.347
7.735
7.714
2.813
2.531
1.178
O
O
F3C
O
3ka
(400 MHz, CDCl3)
1.00
1.02
1.03
2.09
2.07
6.19
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

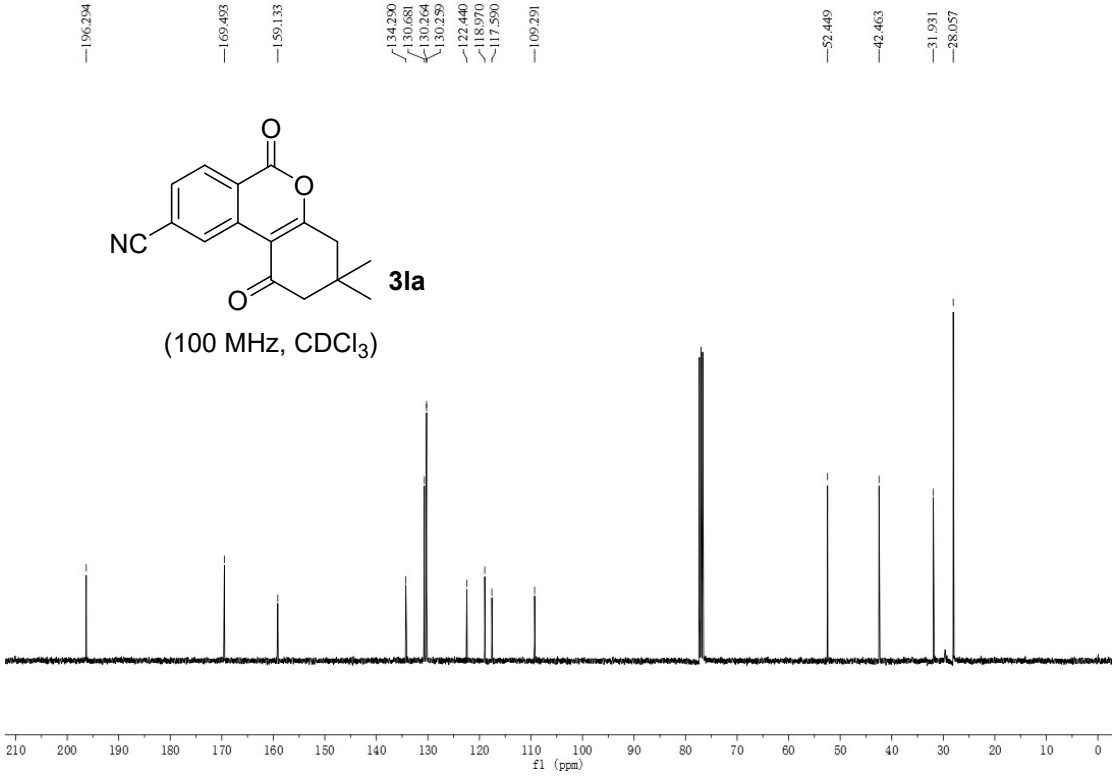


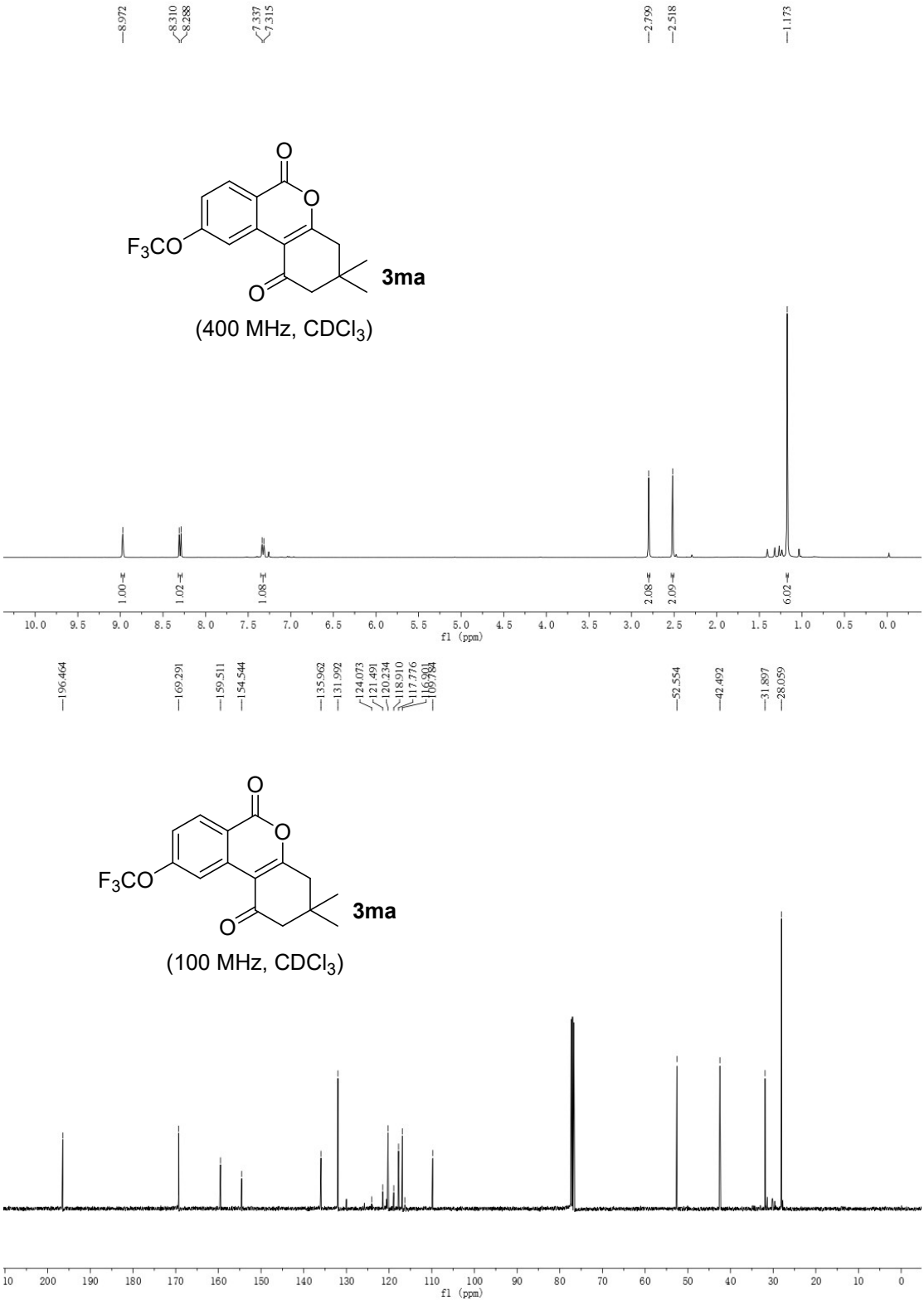
(100 MHz, $CDCl_3$)

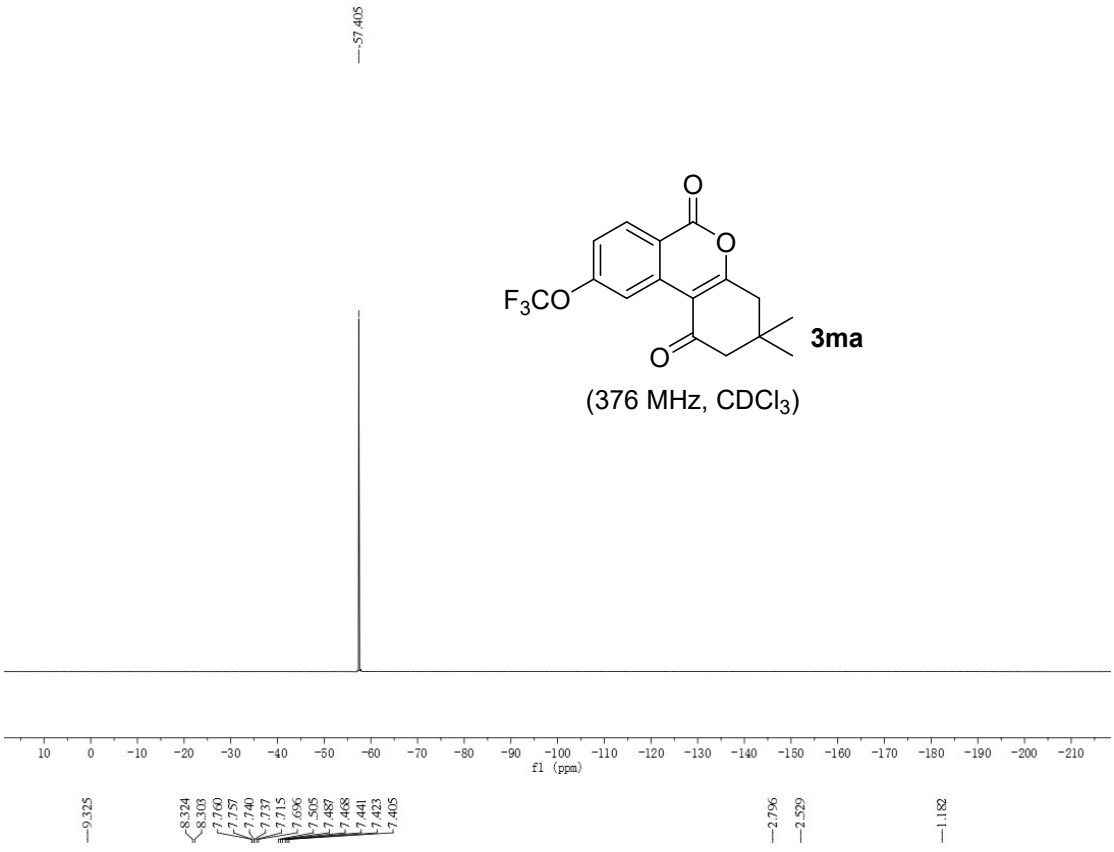


(376 MHz, $CDCl_3$)


9.448
9.446
8.361
8.340
7.752
7.749
7.731
7.728
2.818
2.540
1.182
NC
3la
(400 MHz, CDCl3)
1.00
1.07
1.08
2.16
2.15
6.20
f1 (ppm)

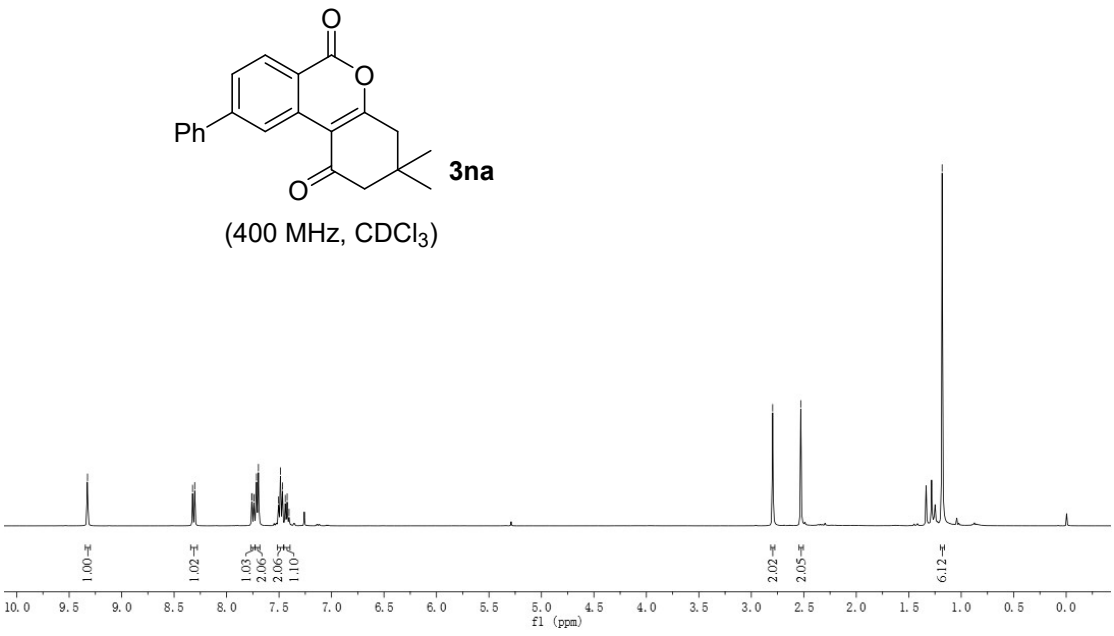

196.294
169.493
159.133
134.290
130.681
130.264
130.259
122.440
118.970
117.590
109.291
52.449
42.463
31.931
28.057
NC
3la
(100 MHz, CDCl3)
f1 (ppm)


8.972
8.310
8.288
7.337
7.315
2.799
2.518
1.173
O
O
F3CO
O
3ma
(400 MHz, CDCl3)
1.00
1.02
1.08
2.08
2.09
6.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
196.464
169.291
159.511
154.544
135.962
131.992
124.073
121.491
120.234
118.910
117.776
52.554
42.492
31.897
28.059
O
O
F3CO
O
3ma
(100 MHz, CDCl3)
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



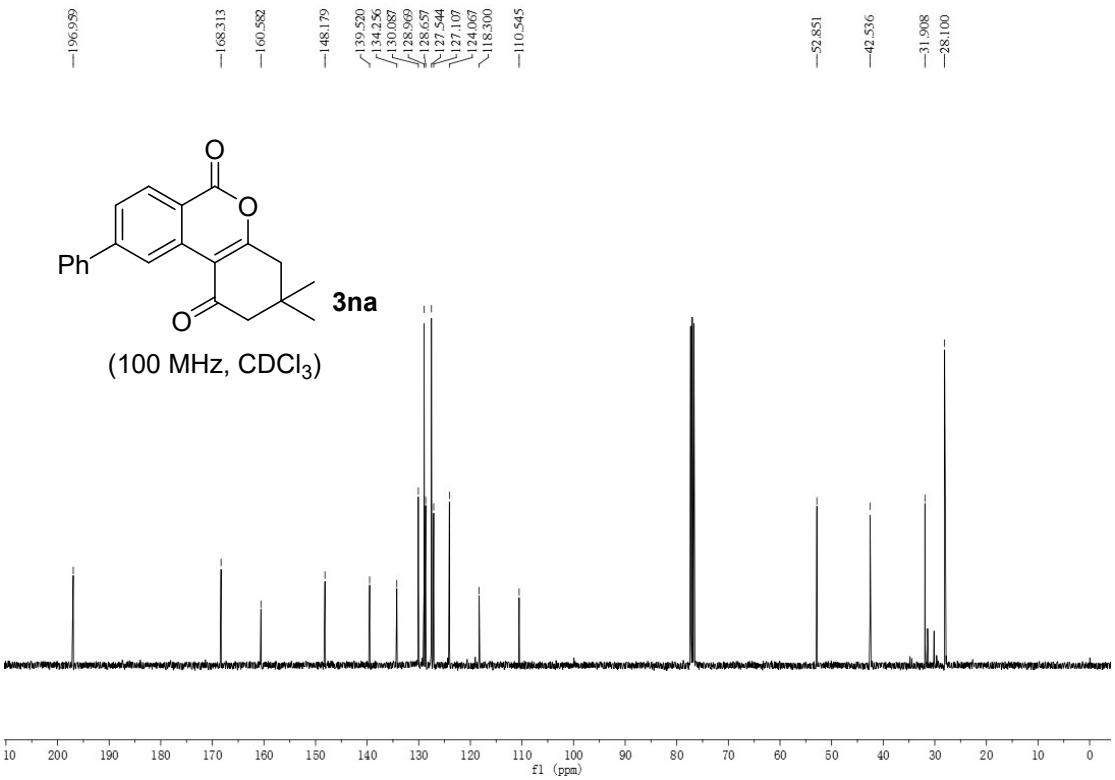
3ma

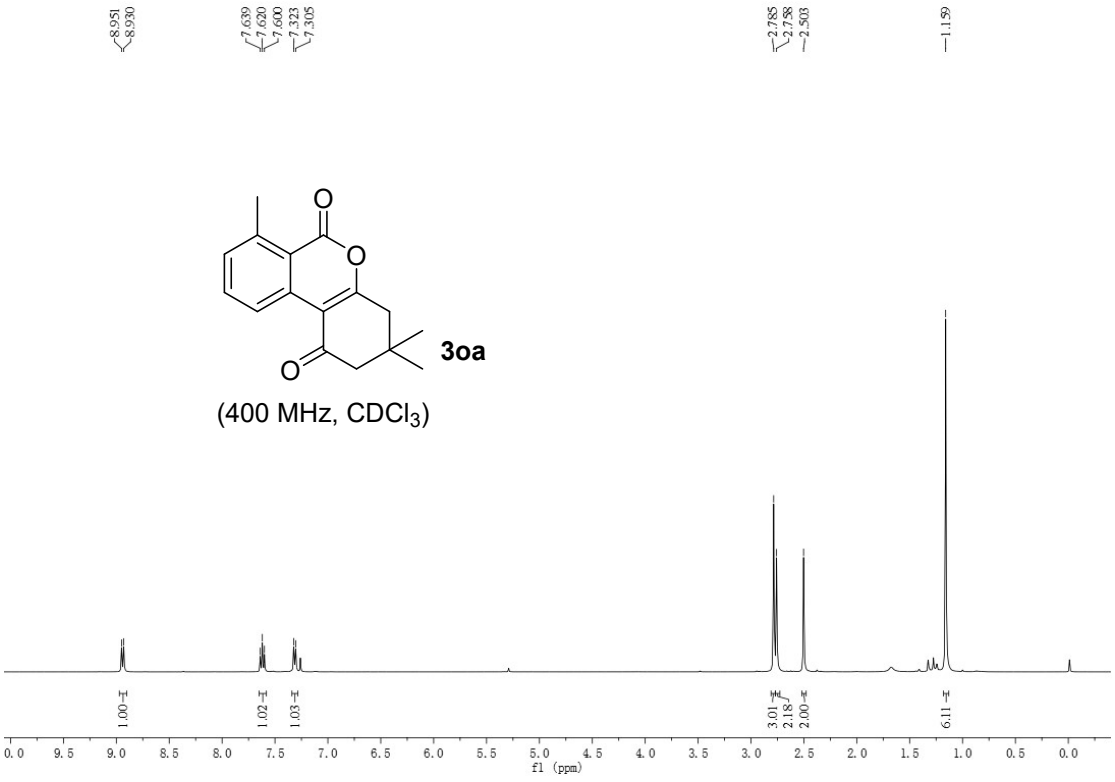
(376 MHz, $CDCl_3$)

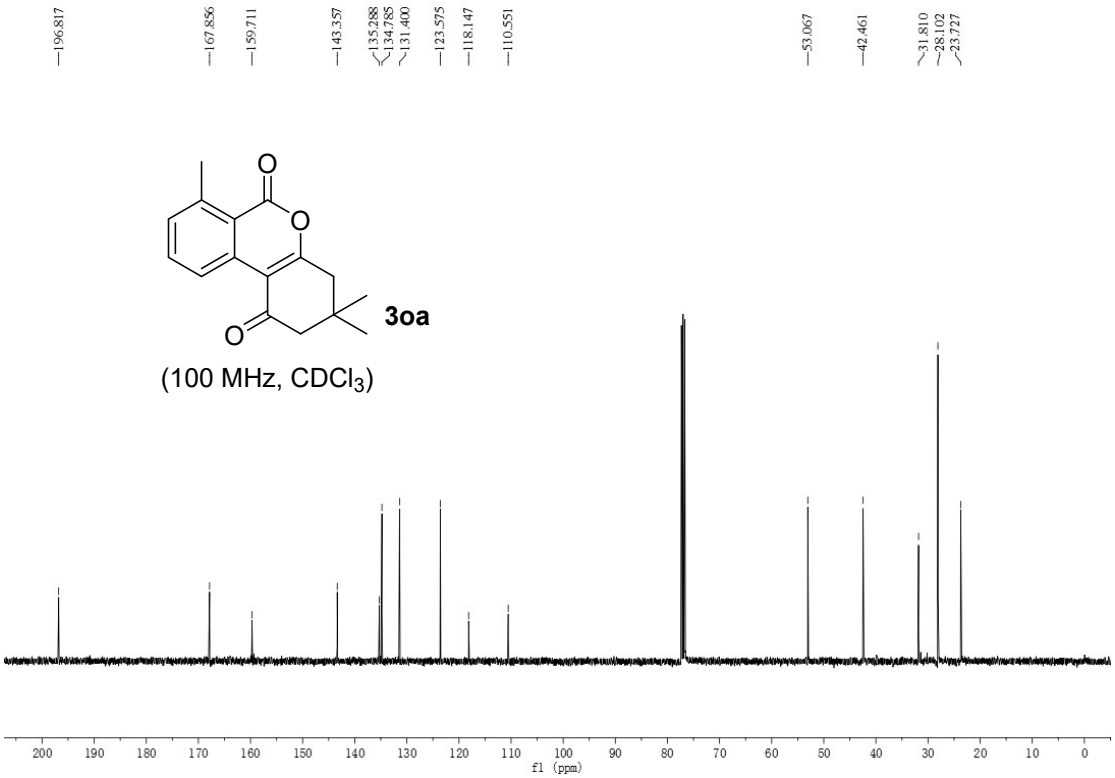


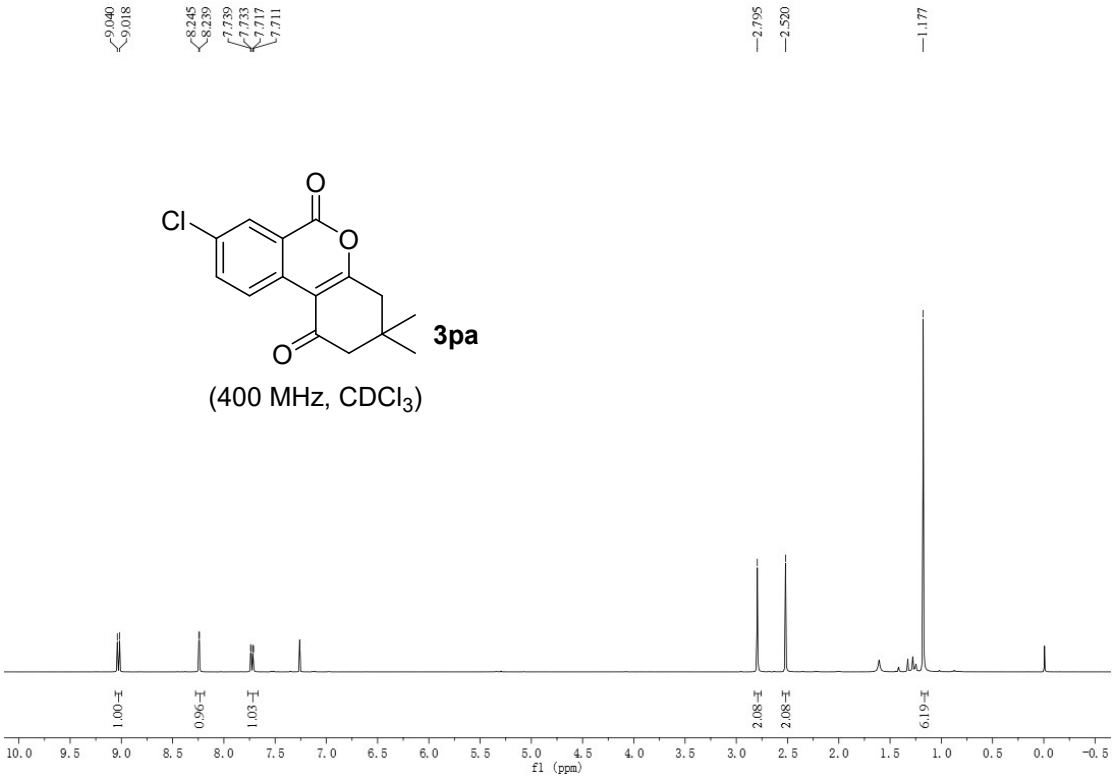
3na

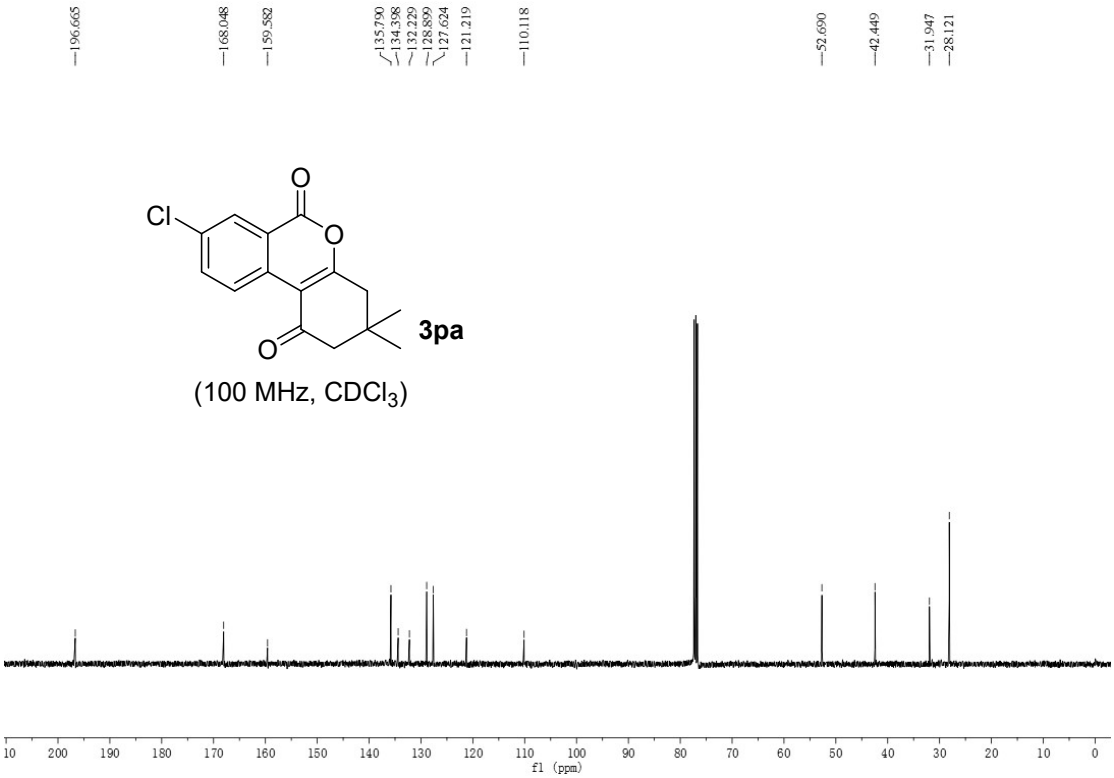
(400 MHz, $CDCl_3$)


196.959
168.313
160.582
148.179
139.520
134.256
130.087
128.969
128.657
127.544
127.107
124.067
118.300
110.545
52.851
42.536
31.908
28.100
O
O
Ph
O
3na
(100 MHz, CDCl3)
f1 (ppm)


8.951
8.930
7.639
7.620
7.600
7.323
7.305
2.785
2.758
2.503
1.159
O
O
O
3oa
(400 MHz, CDCl3)
1.00
1.02
1.03
3.01
2.18
2.00
6.11
f1 (ppm)


196.817
167.856
159.711
143.357
135.288
134.785
131.400
123.575
118.147
110.551
53.067
42.461
31.810
28.102
23.727
3oa
(100 MHz, CDCl3)
f1 (ppm)


9.040
9.018
8.245
8.239
7.739
7.733
7.717
7.711
2.795
2.520
1.177
Cl
3pa
(400 MHz, CDCl3)
1.00
0.96
1.03
2.08
2.08
6.19
f1 (ppm)


196.665
168.048
159.582
135.790
134.398
132.229
128.899
127.624
121.219
110.118
52.690
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31.947
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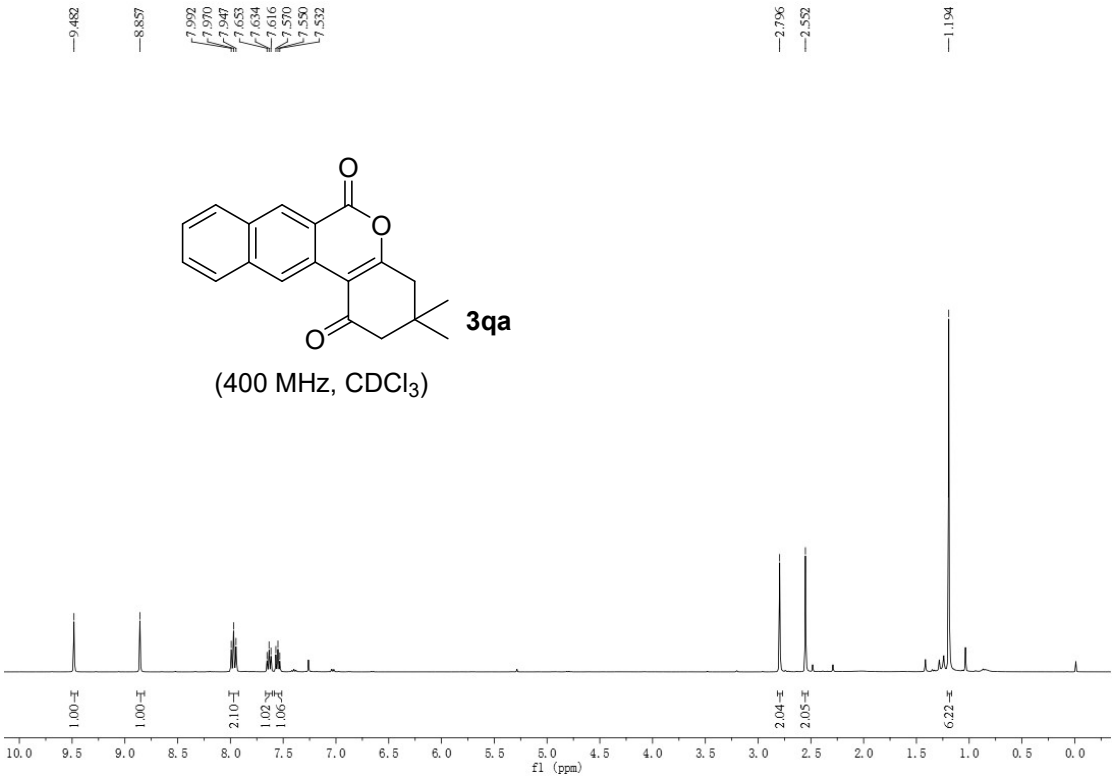
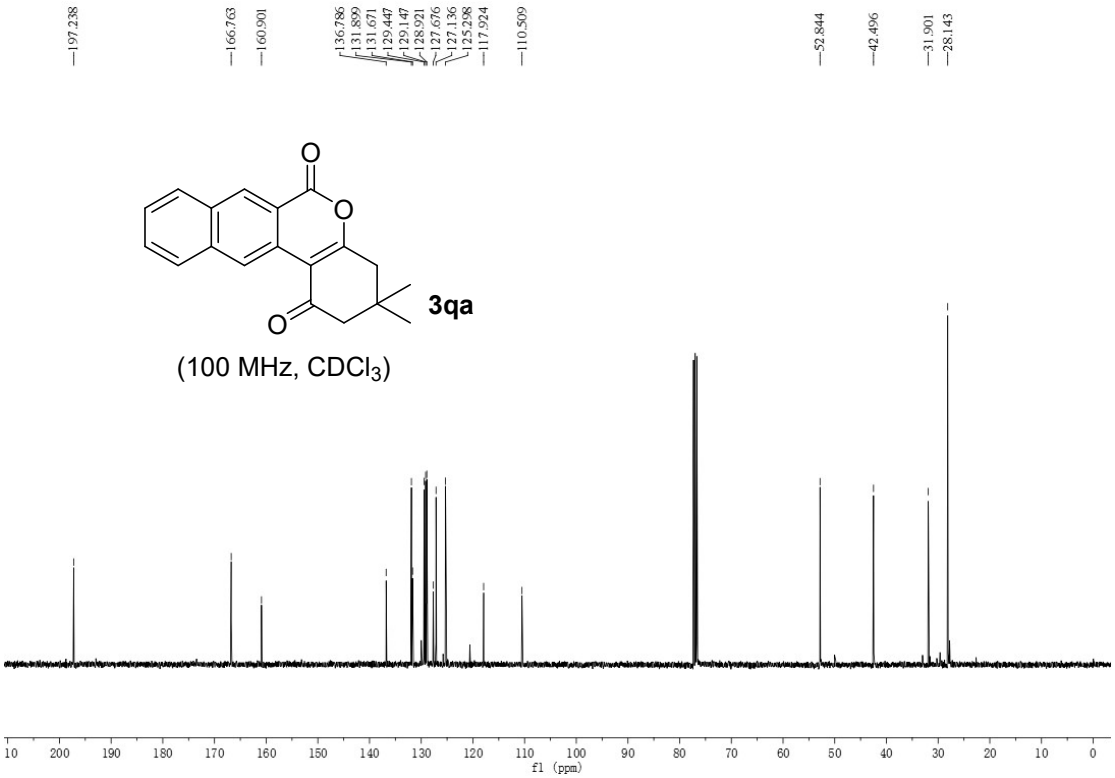
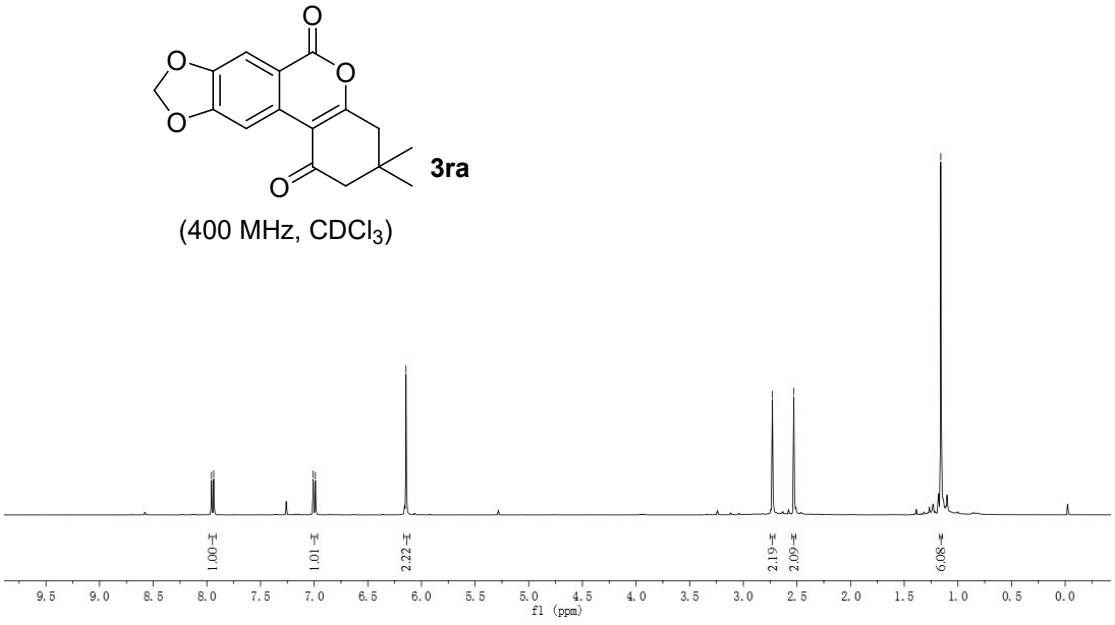
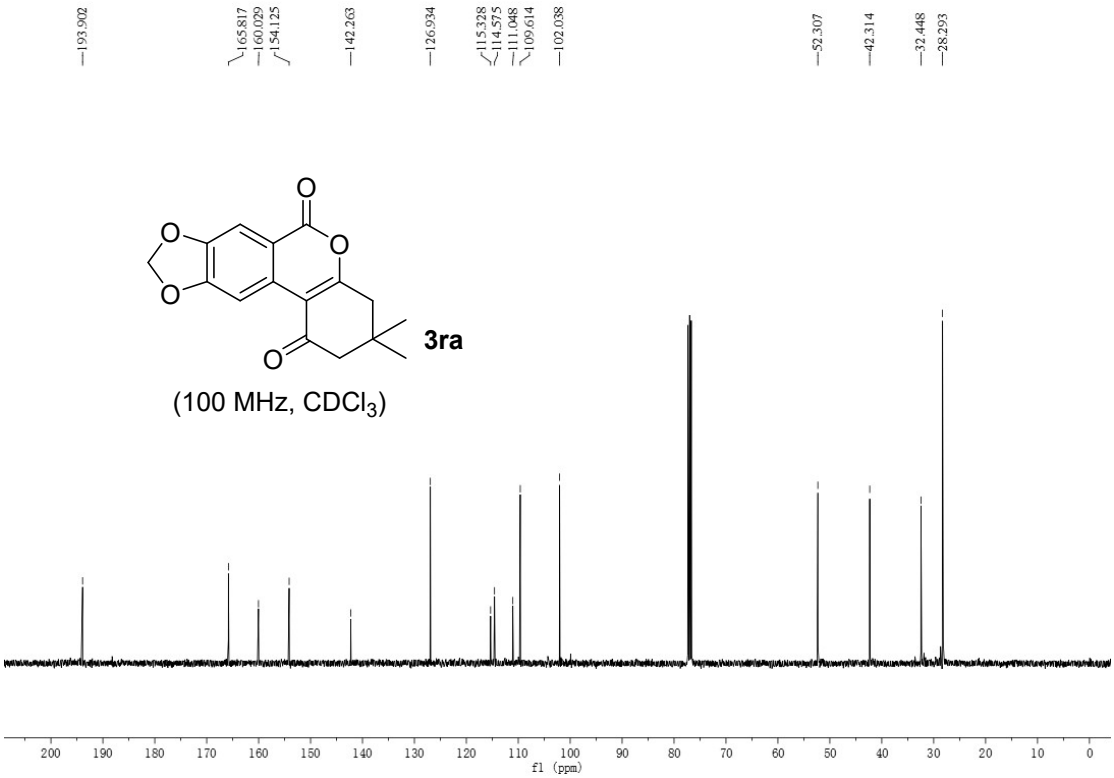
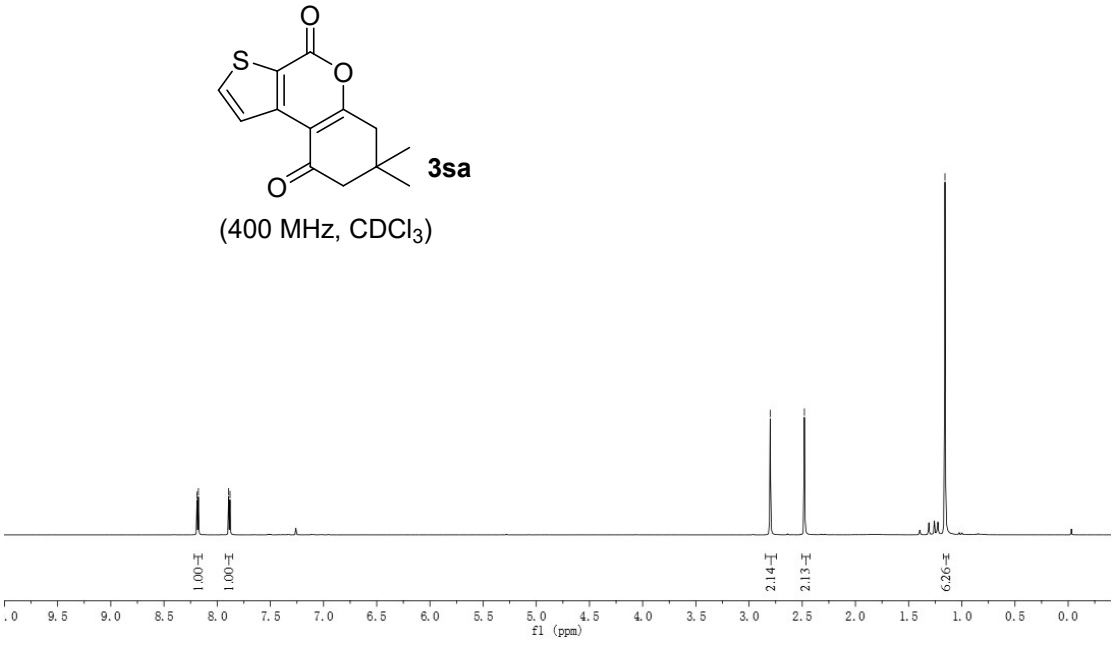
Cl
O
O
O
3pa
(100 MHz, CDCl3)
f1 (ppm)

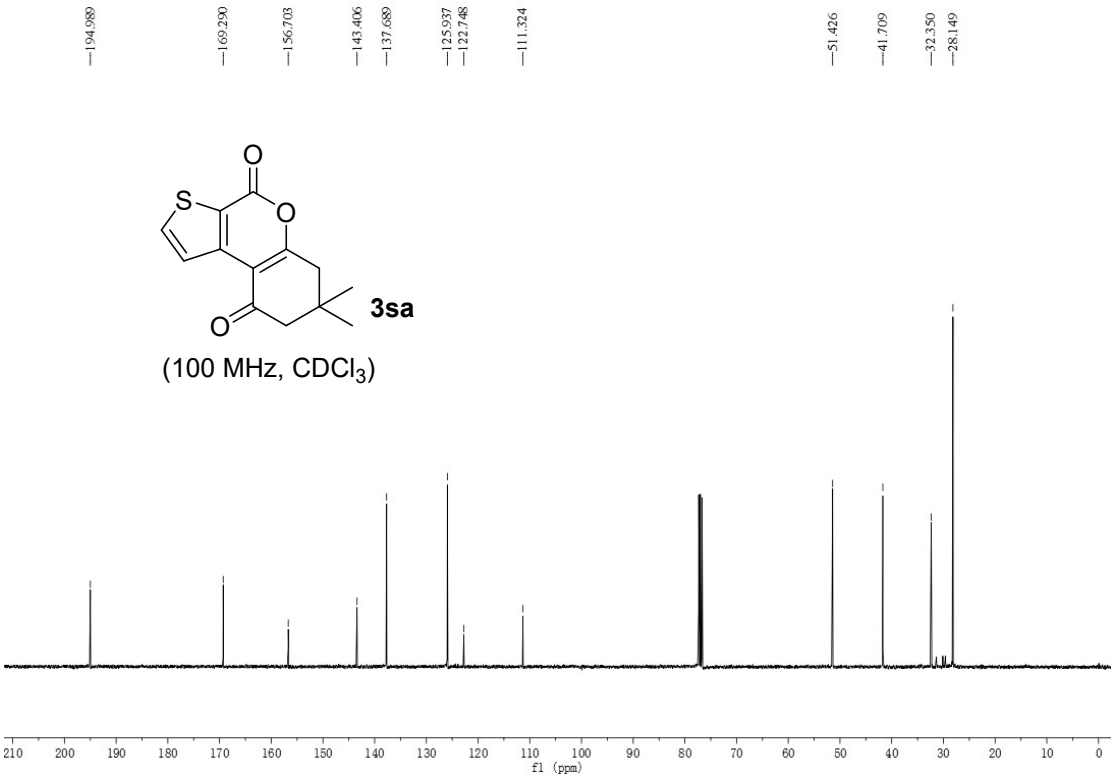

9.482
8.857
7.992
7.970
7.947
7.653
7.634
7.616
7.570
7.550
7.532
2.796
2.552
1.194
O
O
O
3qa
(400 MHz, CDCl3)
1.00
1.00
2.10
1.02
1.06
2.04
2.05
6.22
f1 (ppm)

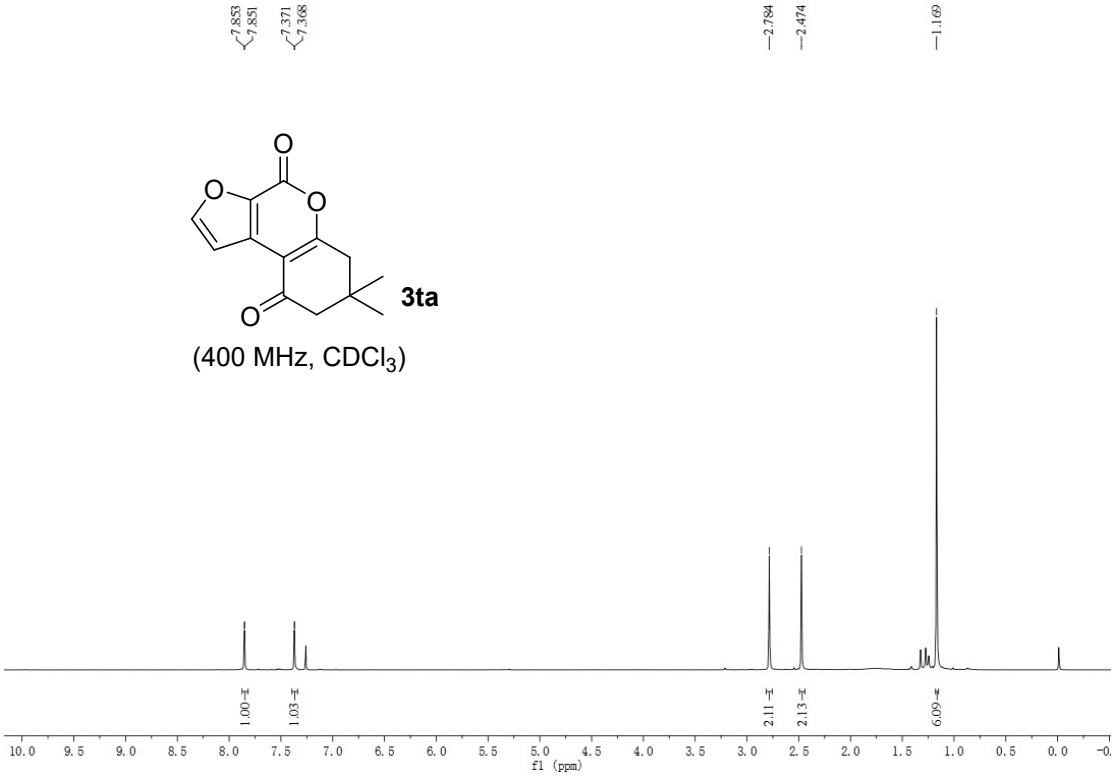

197.238
166.763
160.901
136.786
131.899
131.671
129.447
129.147
128.921
127.676
127.136
125.298
117.924
110.509
52.844
42.496
31.901
28.143
3qa
(100 MHz, CDCl3)
f1 (ppm)
7.957
7.936
7.009
6.988
6.144
2.729
2.530
1.159

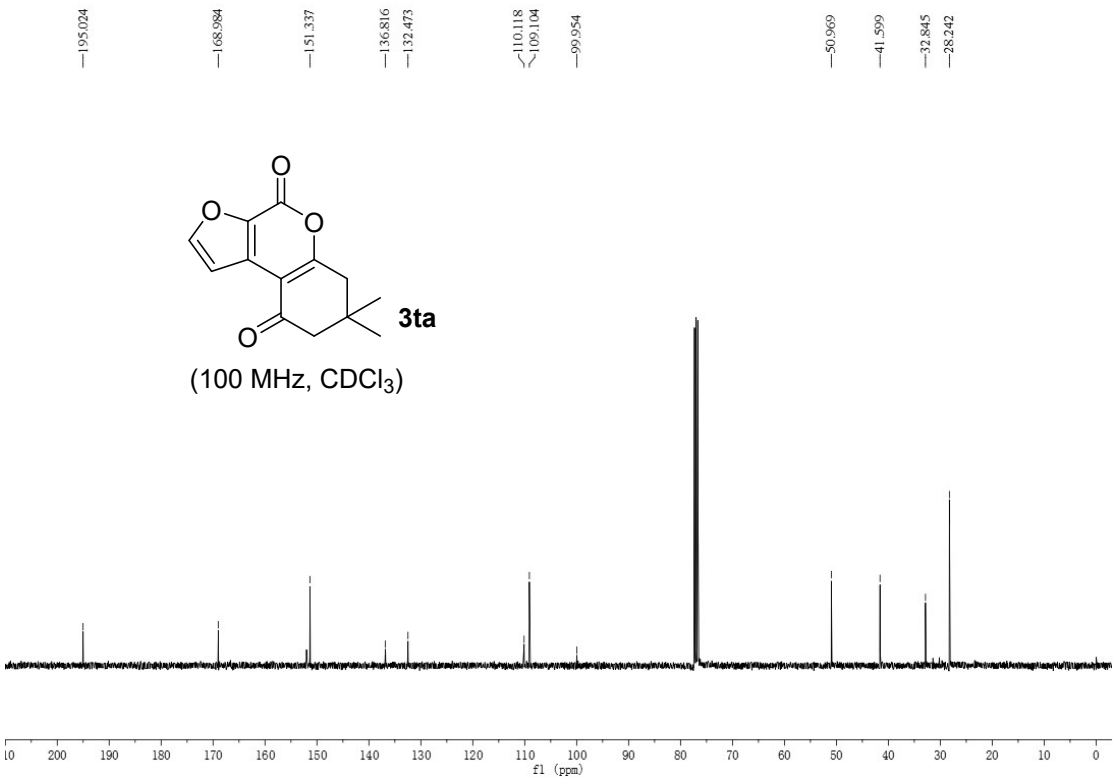

3ra
(400 MHz, CDCl3)
1.00
1.01
2.22
2.19
2.09
6.08
f1 (ppm)

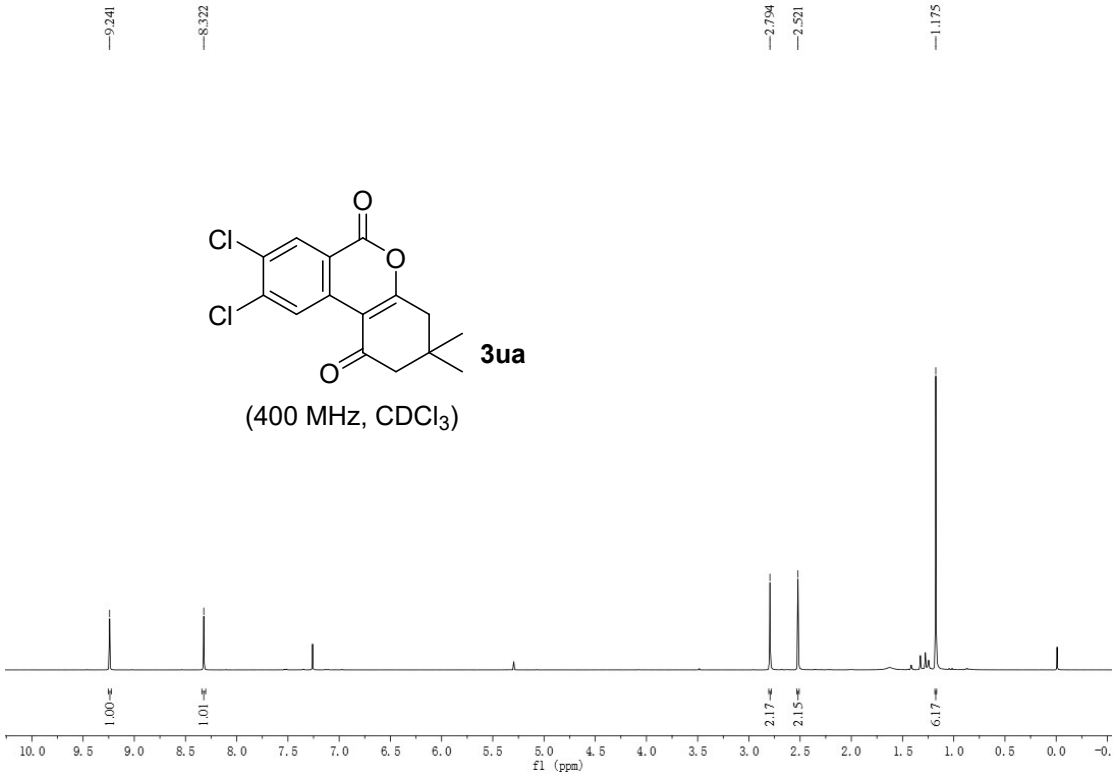

193.902
165.817
160.029
154.125
142.263
126.934
115.328
114.575
111.048
109.614
102.038
52.307
42.314
32.448
28.293
O
O
O
O
O
3ra
(100 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
8.189
8.177
7.892
7.879
2.801
2.480
1.158

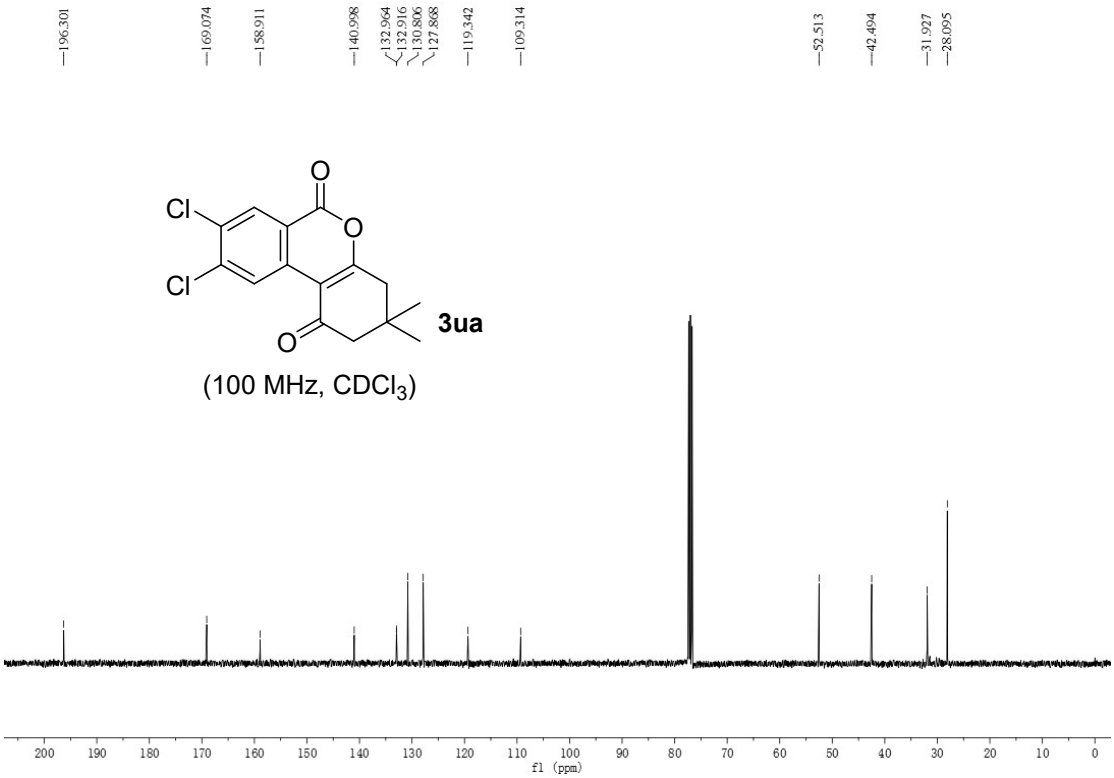

O
S
O
O
3sa
(400 MHz, CDCl3)
1.00
1.00
2.14
2.13
6.26
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

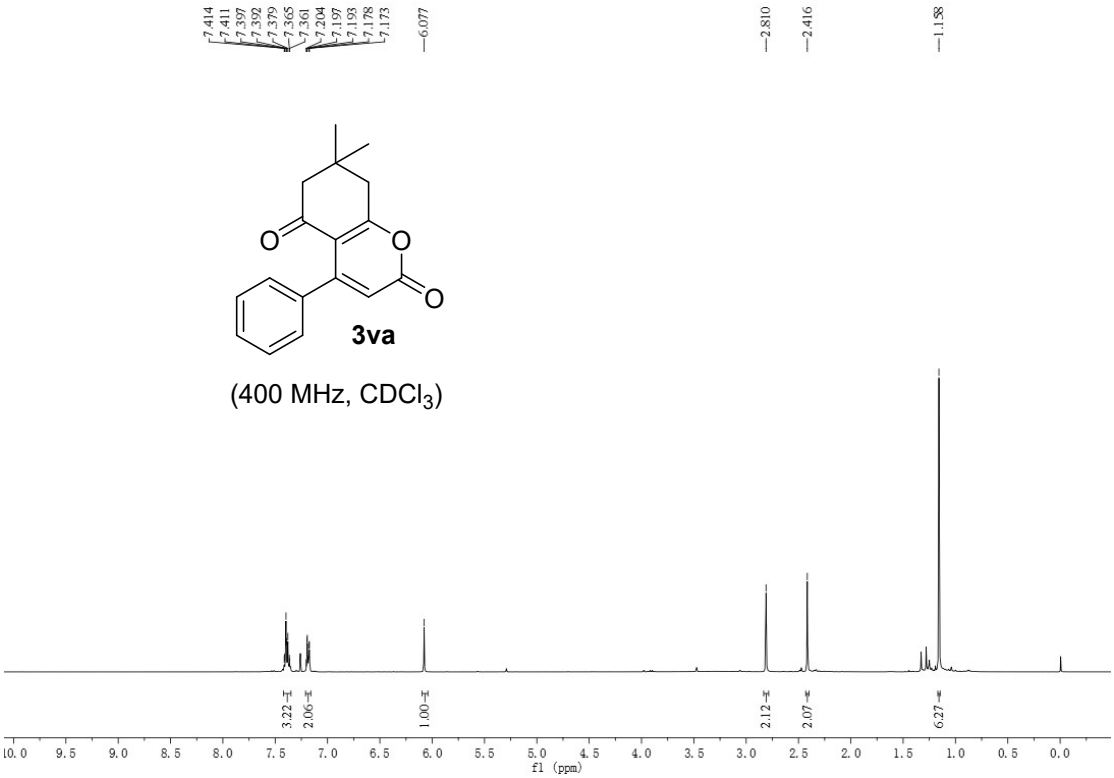

194.989
169.290
156.703
143.406
137.689
125.937
122.748
111.324
51.426
41.709
32.350
28.149
O
S
O
O
3sa
(100 MHz, CDCl3)
f1 (ppm)

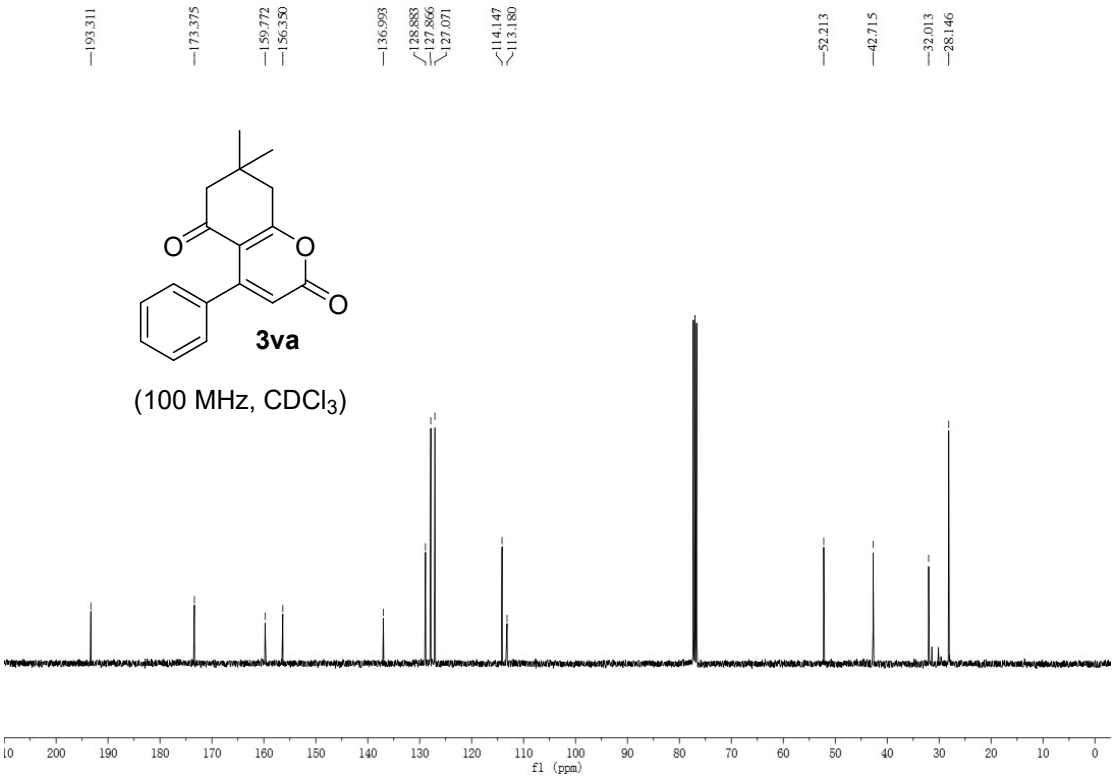

7.853
7.851
7.371
7.368
2.784
2.474
1.169
O
O
O
O
3ta
(400 MHz, CDCl3)
1.00
1.03
2.11
2.13
6.09
f1 (ppm)

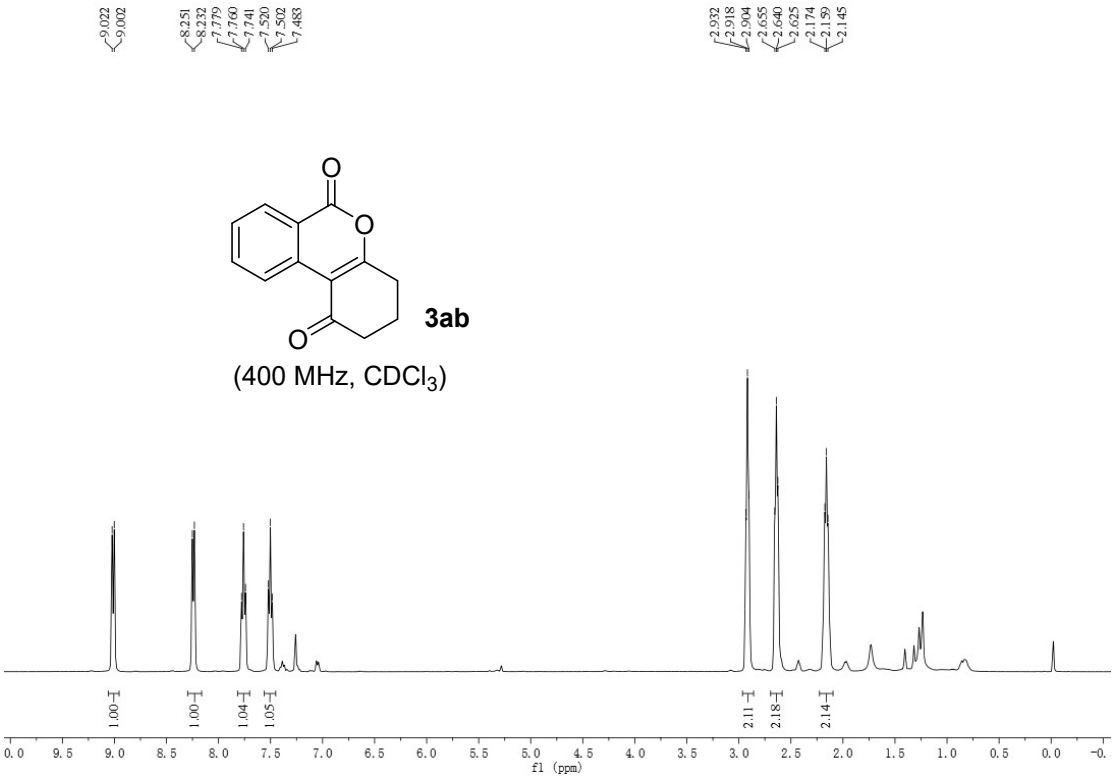

195.024
168.984
151.337
136.816
132.473
110.118
109.104
99.954
50.969
41.599
32.845
28.242
O
O
O
O
3ta
(100 MHz, CDCl3)
f1 (ppm)

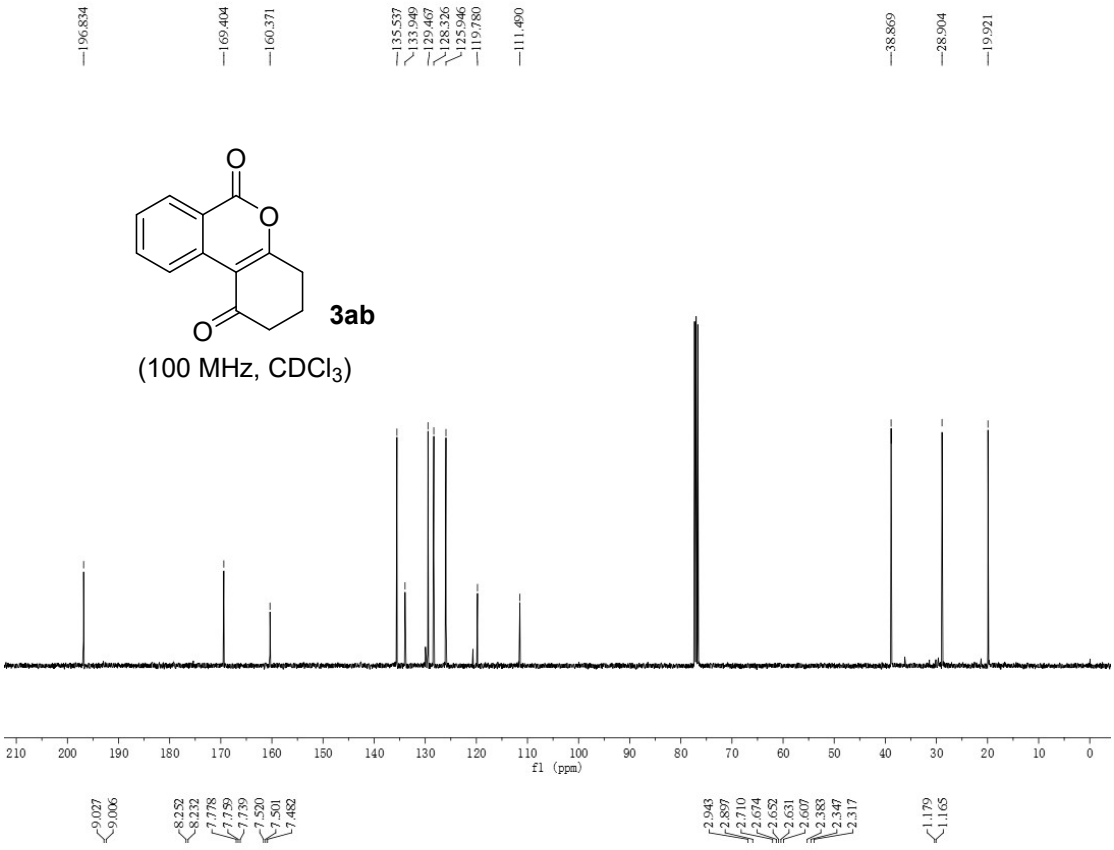

9.241
8.322
2.794
2.521
1.175
Cl
Cl
O
O
O
3ua
(400 MHz, CDCl3)
1.00
1.01
2.17
2.15
6.17
f1 (ppm)

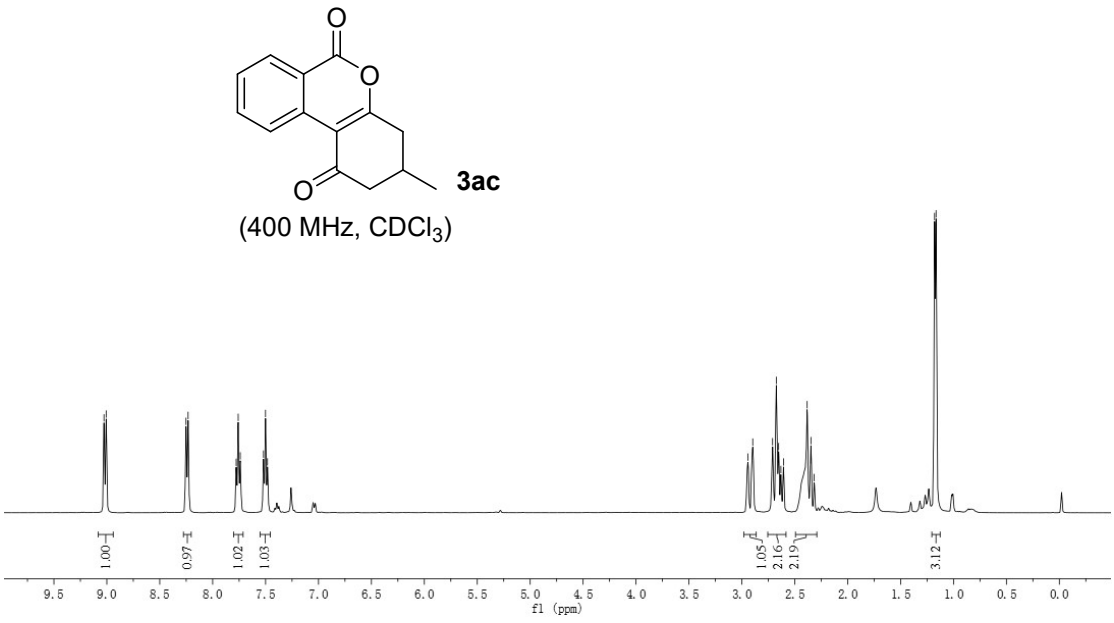

196.301
169.074
158.911
140.998
132.964
132.916
130.806
127.868
119.342
109.314
52.513
42.494
31.927
28.095
Cl
Cl
O
O
O
3ua
(100 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

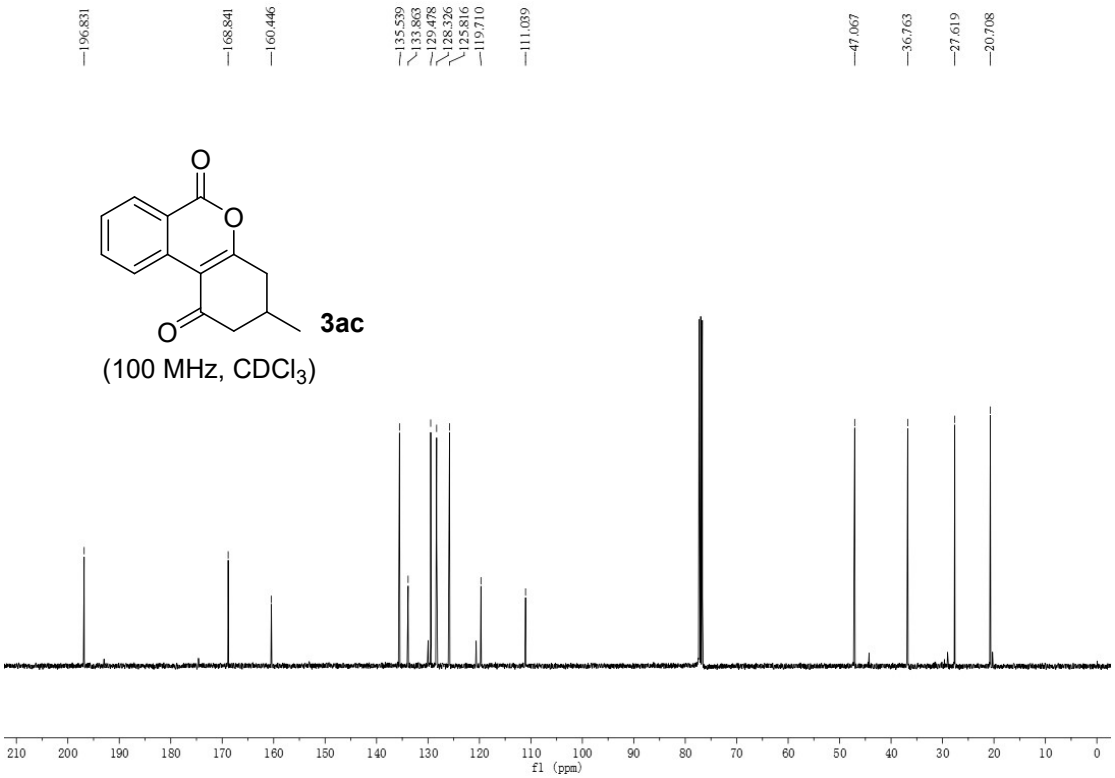

7.414
7.411
7.397
7.392
7.379
7.365
7.361
7.204
7.197
7.193
7.178
7.173
6.077
2.810
2.416
1.588
O
O
O
3va
(400 MHz, CDCl3)
3.22
2.06
1.00
2.12
2.07
6.27
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

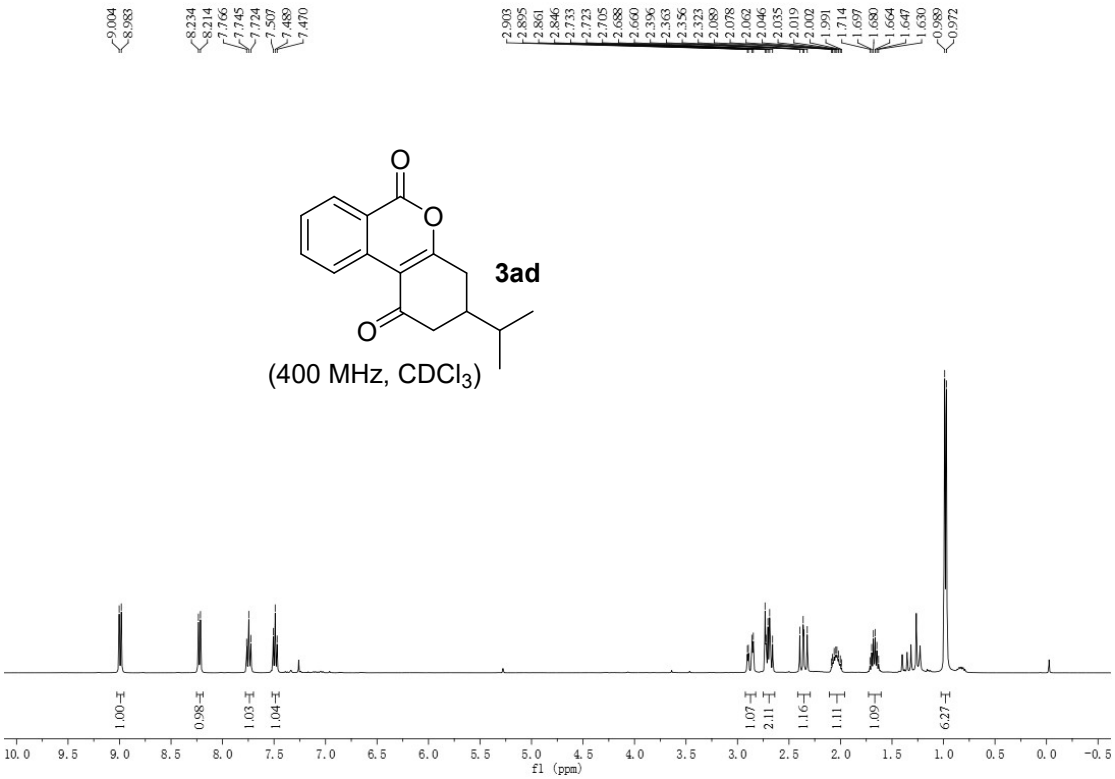

193.311
173.375
159.772
156.350
136.993
128.883
127.866
127.071
114.147
113.180
52.213
42.715
32.013
28.146
O
O
O
O
3va
(100 MHz, CDCl3)
f1 (ppm)

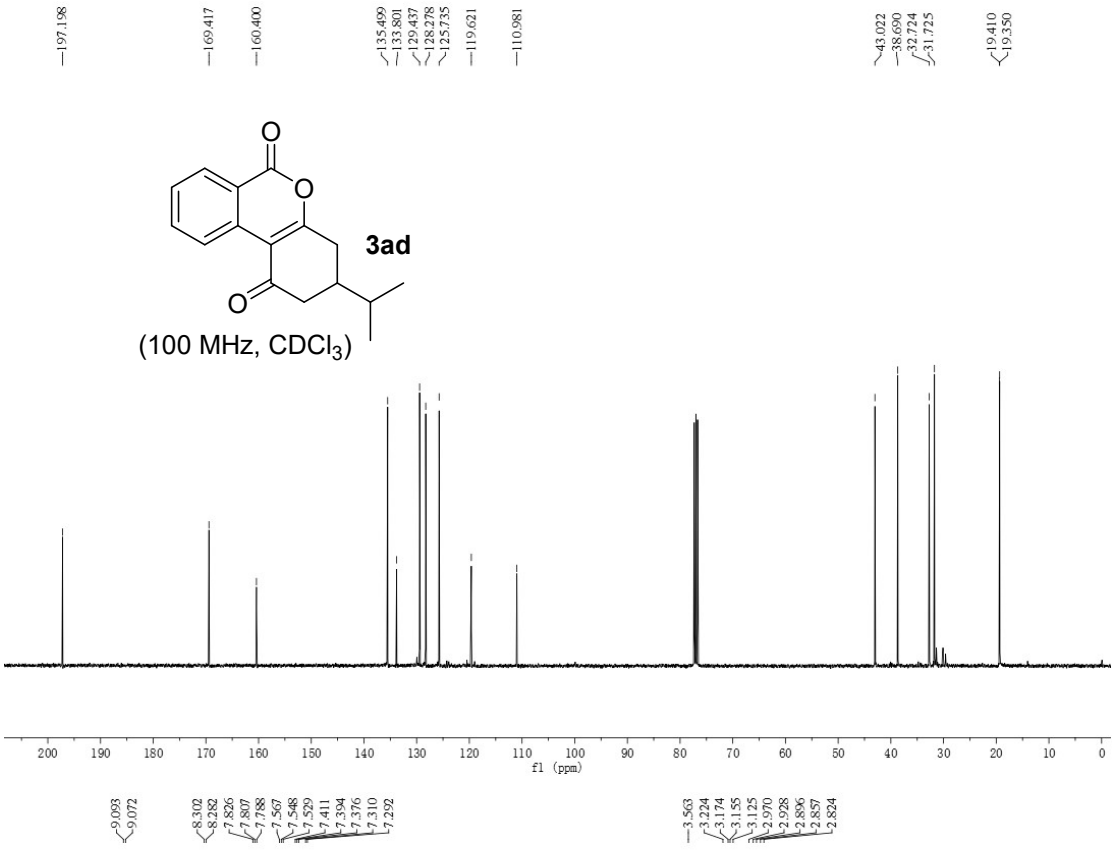

9.022
9.002
8.251
8.232
7.779
7.760
7.741
7.520
7.502
7.483
2.932
2.918
2.904
2.655
2.640
2.625
2.174
2.159
2.145
O
O
O
3ab
(400 MHz, CDCl3)
1.00
1.00
1.04
1.05
2.11
2.18
2.14
f1 (ppm)

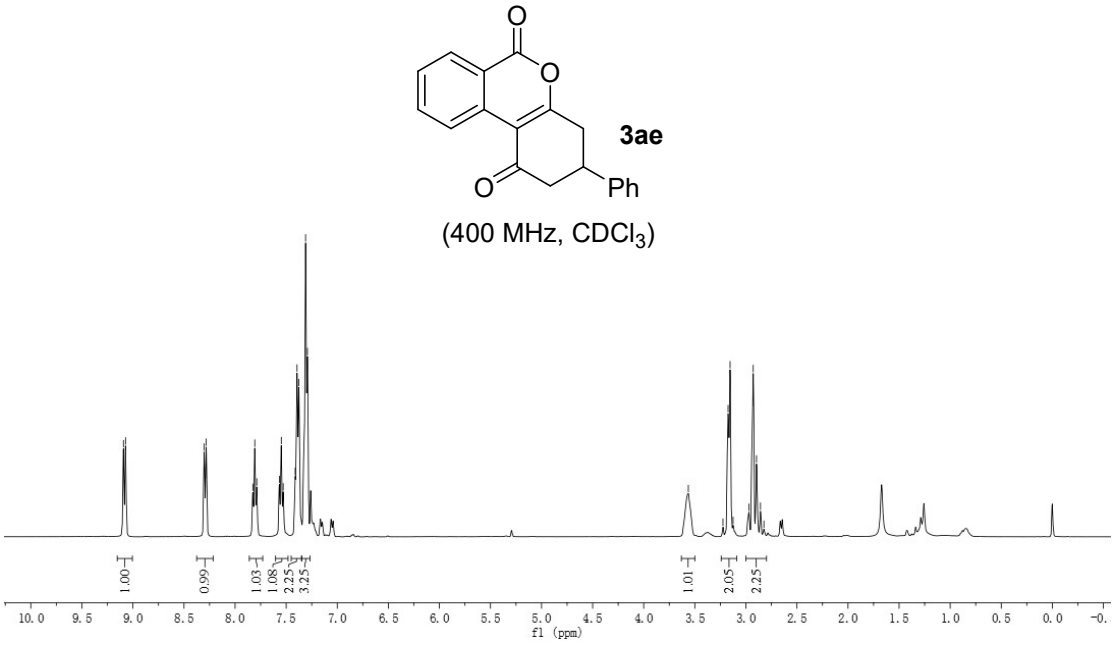

196.834
169.404
160.371
135.537
133.949
129.467
128.326
125.946
119.780
111.490
38.869
28.904
19.921
3ab
(100 MHz, CDCl3)
f1 (ppm)

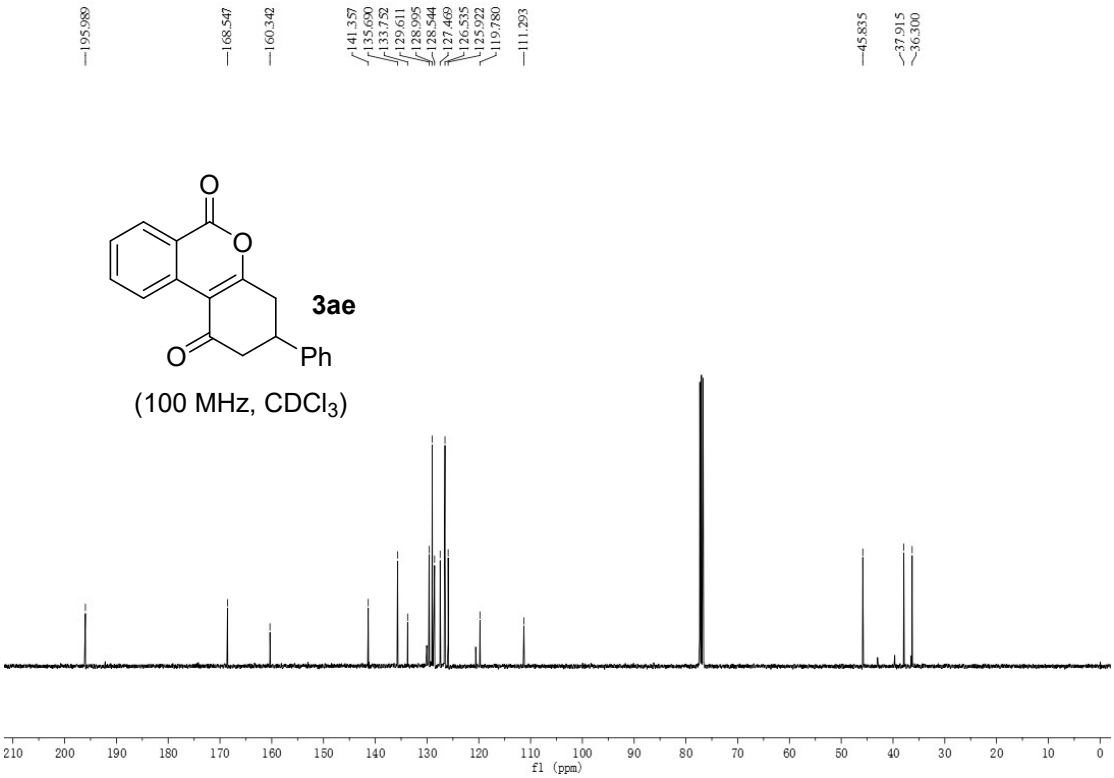

3ac
(400 MHz, CDCl3)
f1 (ppm)

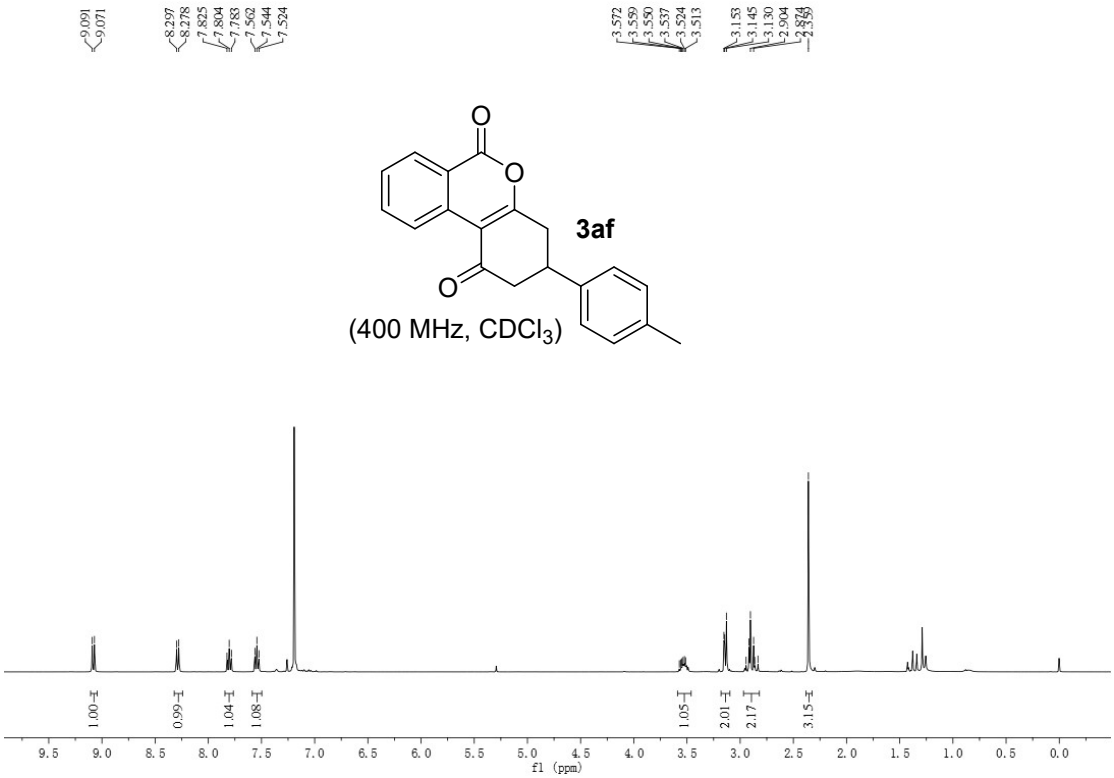

196.831
168.841
160.446
135.539
133.863
129.478
128.326
125.816
119.710
111.039
47.067
36.763
27.619
20.708
3ac
(100 MHz, CDCl3)
f1 (ppm)

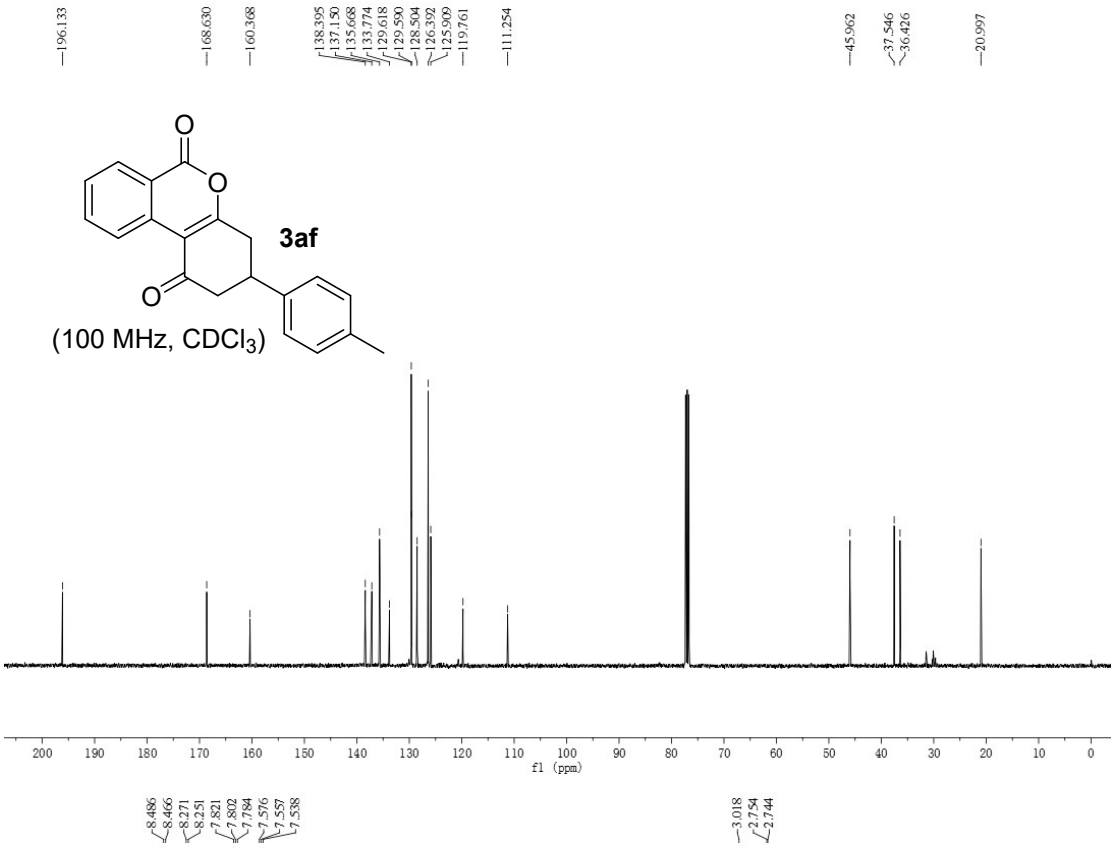

9.004
8.983
8.234
8.214
7.766
7.745
7.724
7.507
7.489
7.470
2.903
2.895
2.861
2.846
2.733
2.723
2.705
2.688
2.660
2.396
2.363
2.356
2.323
2.089
2.078
2.062
2.046
2.035
2.019
2.002
1.991
1.714
1.697
1.680
1.664
1.647
1.630
0.989
0.972
3ad
(400 MHz, CDCl3)
1.00
0.98
1.03
1.04
1.07
2.11
1.16
1.11
1.09
6.27
f1 (ppm)

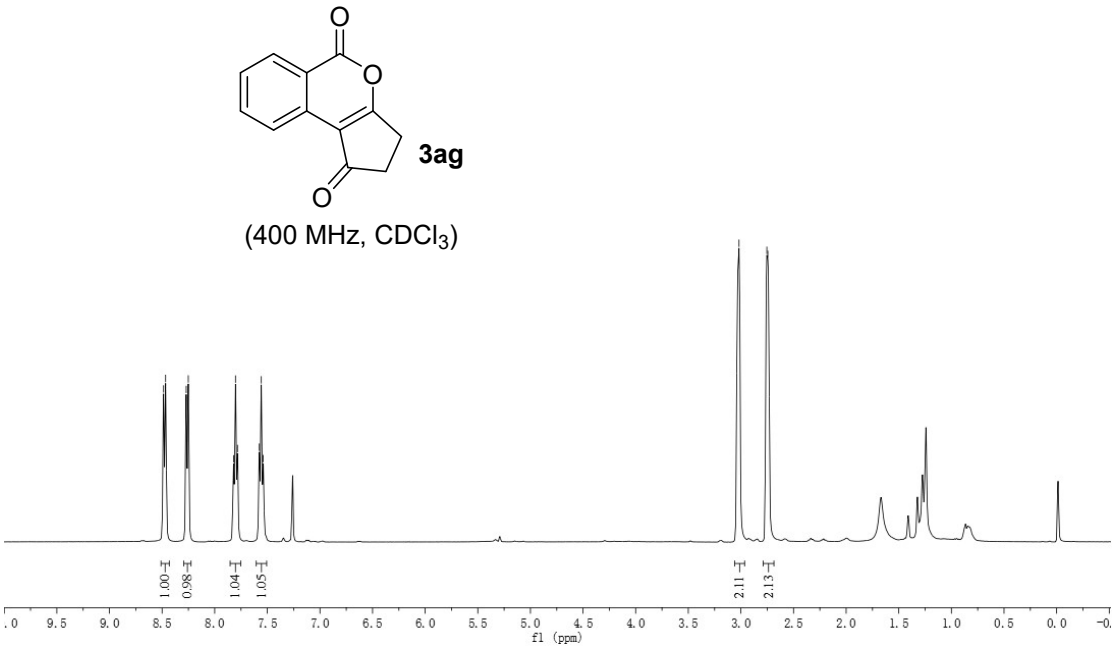

197.198
169.417
160.400
135.499
133.801
129.437
128.278
125.735
119.621
110.981
43.022
38.690
32.724
31.725
19.410
19.350
3ad
(100 MHz, CDCl3)
f1 (ppm)
9.093
9.072
8.302
8.282
7.826
7.807
7.788
7.567
7.548
7.529
7.411
7.394
7.376
7.310
7.292
3.563
3.224
3.174
3.155
3.125
2.970
2.928
2.896
2.857
2.824

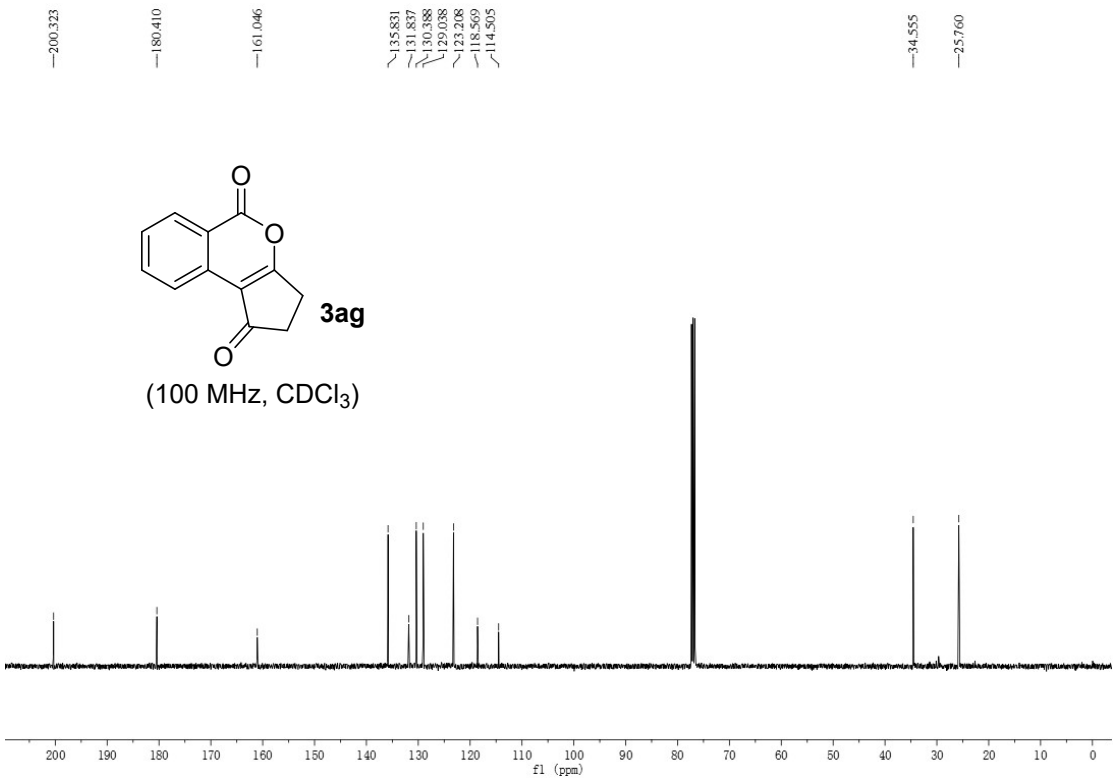

3ae
Ph
(400 MHz, CDCl3)
1.00
0.99
1.03
1.08
2.25
3.25
1.01
2.05
2.25
f1 (ppm)


195.989
168.547
160.342
141.357
135.690
133.752
129.611
128.995
128.544
127.469
126.535
125.922
119.780
111.293
45.835
37.915
36.300
O
O
O
Ph
3ae
(100 MHz, CDCl3)
f1 (ppm)


9.091
9.071
8.297
8.278
7.825
7.804
7.783
7.562
7.544
7.524
3.572
3.559
3.550
3.537
3.524
3.513
3.153
3.145
3.130
2.904
2.874
2.859
O
O
O
3af
(400 MHz, CDCl3)
1.00
0.99
1.04
1.08
1.05
2.01
2.17
3.15
f1 (ppm)


196.133
168.630
160.368
138.395
137.150
135.668
133.774
129.618
129.590
128.504
126.392
125.909
119.761
111.254
45.962
37.546
36.426
20.997
3af
(100 MHz, CDCl3)
f1 (ppm)
8.486
8.466
8.271
8.251
7.821
7.802
7.784
7.576
7.557
7.538
3.018
2.754
2.744


3ag
(400 MHz, CDCl3)
f1 (ppm)
1.00
0.98
1.04
1.05
2.11
2.13


200.323
180.410
161.046
135.831
131.837
130.388
129.038
123.208
118.569
114.505
34.555
25.760
O
O
O
3ag
(100 MHz, CDCl3)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)