Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Gold-Catalyzed Domino Reactions of Alkynol and *p*-Quinone Methides: Divergent Synthesis of Fused- and Spiro-ketals

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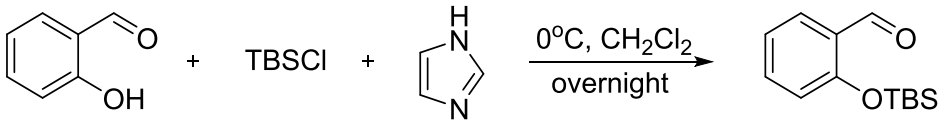
1. General Information

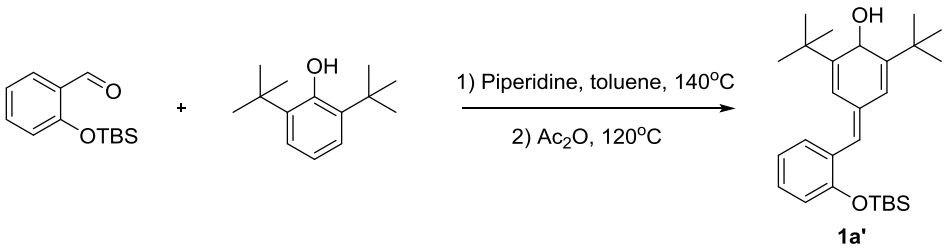
Unless otherwise noted, analytic grade solvents were used for the chromatography, and all the reagents were obtained commercially and used without further purification. Reactions were monitored by TLC. All NMR spectra were recorded on Bruker-500 MHz spectrometer. The chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz respectively. HRMS were measured on the Q-TOF6510 instruments.

2. Preparation of Starting Materials

1 was prepared according to reported procedures[1]



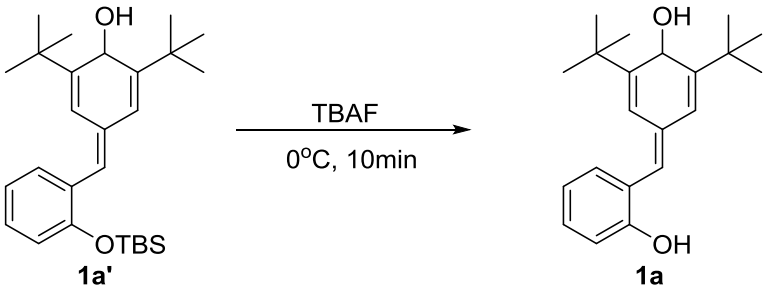
A solution of 2-hydroxybenzaldehyde (10.0 mmol, 1.05 mL) and 1-H-imidazole (20.0 mmol, 1.37 g) in CH_2Cl_2 (40 mL) was placed into a 100mL reaction vial, which was sealed at 0 ^oC. Then, TBSCl (1.2 equiv, 1.80 g) was added by dropwise slowly. The reaction mixture was stirred overtime. After that, a saturated $NaHCO_3$ solution was added dropwise to quench the reaction. The resulting solution was extracted with acetic ester (3×30 mL). Then the combined organic phases were washed with brine and dried over anhydrous Na_2SO_4, resulting in a white viscous liquid and used directly in the next step without purification.



1a'

A solution of phenols (2.2 mmol, 453 mg) and aldehydes (2.0 mmol, 472 mg) in toluene (10 mL) was placed in a Dean-Stark apparatus which was heated to reflux. Piperidine (2.0 equiv, 341 mg) was added by dropwise slowly. Then, the temperature was raised to 140 ^oC and stirred for 12 h. After that, the reaction mixture was cooled to 120 ^oC and acetic anhydride (2.0 equiv, 408 mg) was added by dropwise. The

stirring was continued for 30 min and the solution was poured on ice-water and extracted with ethyl acetate (3 × 20 mL). The organic phases were combined, washed with brine and dried over anhydrous Na_2SO_4. Then the solvent was evaporated under reduced pressure and the corresponding products **1a'** (551 mg, 65% yield) were obtained after flash column chromatography (pentane/ ethyl acetate = 18:1).



To a solution of **1a'** (1 mmol, 424 mg) in THF (10 mL) at 0 °C was added tetrabutylammonium fluoride trihydrate (TBAF 1.1 equiv, 1.1 mL). The reaction mixture was stirred for 10 min and a saturated NH_4Cl solution was added by dropwise to quench the reaction. The resulting solution was extracted with ethyl acetate (3 × 20 mL). Then the combined organic phases were washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed to give the crude product which was purified by flash column chromatography (pentane/ ethyl acetate = 36:1) to afford the desired compound **1a** (254 mg, 82% yield).

2 was prepared according to reported procedures[2]

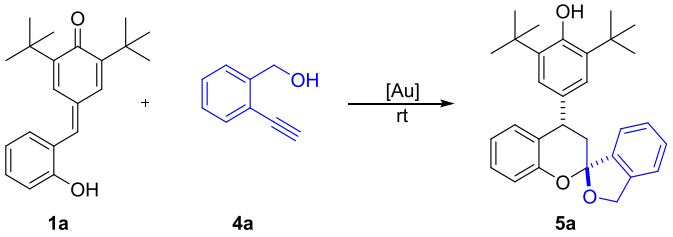
4 was prepared according to reported procedures[3]

(1) S. Liu, X. Lan, K. Chen, W. Hao, G. Li, S. Tu, and B. Jiang, *Org. Lett.* 2017, **19**, 3831−3834.

(2) N. C. Lobera, M. T. Quiros, W. W. Brennessel, M. L. Neidig, E. Buñuel and D. J. Cardenas´, *Org. Lett.* 2019, **21**, 6552−6556

(3) a) J. W. Wang, and Z. H. Xu. *Org. Lett.* 2017, **19**, 2526. b) H. Wang, and Z. H.Xu *Org. Lett.* 2014, **16**, 22.

3. Optimization of Au Catalyzed Domino Reaction to Spiroketals



1a **4a** **5a**

Entry[a]	[Au]-catalyst (mol%)	Solvent	Yield [%][b]
1	XphosAuNTf$_2$ (5)	DCE	85
2	PPh$_3$AuNTf$_2$ (5)	DCE	87
3	JohnphosAuNTf$_2$ (5)	DCE	93
4	(^{t}Bu$_2$PhO)$_3$PAuNTf$_2$ (5)	DCE	85
5	JohnphosAuNTf$_2$ (5)	toluene	83
6	JohnphosAuNTf$_2$ (5)	CH$_3$CN	72
7	JohnphosAuNTf$_2$ (5)	1,4-dioxane	90
8	**JohnphosAuNTf$_2$ (5)**	**THF**	**95 (87)**
9	JohnphosAuNTf$_2$ (1)	THF	86
10	JohnphosAuNTf$_2$ (3)	THF	87

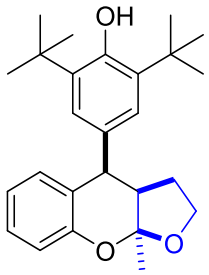
[a]Reaction conditions: 1a (0.1 mmol) and 4a (0.12 mmol) in THF (1 mL), room temperature, 12h. [b]Determined by ^{1}H NMR analysis of the crude reaction mixtures.

4. Preparation and Characterization of Compound 3 and 5.

To a mixture of alkynyl *p*-Quinone Methides **1** (0.1 mmol), alcohol **2** (0.15 mmol), JohnphosAuNTf$_2$ (0.01 mmol, 5 mol %), H$_2$O (0.2mmol, 2 equiv), 1 mL THF was added. The reaction system was stirred at room temperature for 12 hours. After the reaction was completed (determined by TLC analysis), the reaction mixture was filtered and evaporated under reduced pressure, and purified by column chromatography (silica gel, Petroleum ether/ EtOAc: 200/1 to 60/1) to afford the desired product **3**.

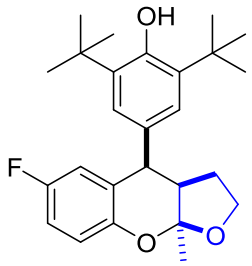
To a mixture of alkynyl *p*-Quinone Methides **1** (0.1 mmol), alcohol **4** (0.12 mmol), JohnphosAuNTf$_2$ (0.01 mmol, 5 mol %), 1 mL THF was added. The reaction system was stirred at room temperature for 12 hours. After the reaction was completed

(determined by TLC analysis), the reaction mixture was filtered and evaporated under reduced pressure, and purified by column chromatography (silica gel, Petroleum ether/ EtOAc: 200/1 to 100/1) to afford the desired product **5**.



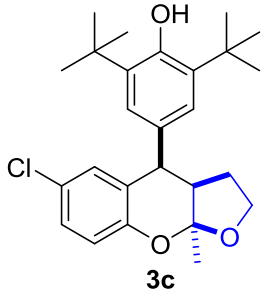
3a

Yield: 90%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.15 (ddd, *J* = 8.0, 4.4, 0.6 Hz, 1H), 7.01 (s, *J* = 4.7 Hz, 2H), 6.90 – 6.86 (m, 2H), 6.84 – 6.78 (m, 1H), 5.16 (s, 1H), 4.31 (d, *J* = 5.1 Hz, 1H), 4.07 (td, *J* = 11.1, 9.4, 3.0 Hz, 1H), 3.91 – 3.84 (m, 1H), 2.46 (ddd, *J* = 12.0, 7.8, 5.2 Hz, 1H), 1.97 (tt, *J* = 11.9, 9.3 Hz, 1H), 1.73 (m, *J* = 7.3, 6.0, 2.6 Hz, 1H), 1.68 (s, 3H), 1.43 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.43, 152.66, 135.88, 131.73, 129.09, 127.91, 124.84, 122.94, 120.41, 116.79, 107.47, 66.84, 48.35, 42.79, 34.39, 30.43, 26.48, 23.18. HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_3$ [M+Na^+] 417.2400, found 417.2395.



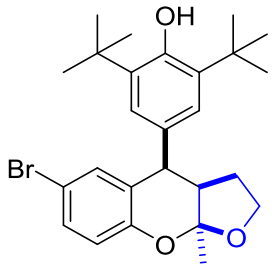
3b

Yield: 80%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.98 (s, 2H), 6.83 (m, *J* = 6.9, 3.1 Hz, 2H), 6.62 – 6.56 (m, 1H), 5.18 (s, 1H), 4.25 (d, *J* = 5.1 Hz, 1H), 4.04 (td, *J* = 9.2, 2.6 Hz, 1H), 3.86 (m, *J* = 12.5, 4.8 Hz, 1H), 2.49 – 2.41 (ddd, 1H), 1.93 (tt, *J* = 11.8, 9.3 Hz, 1H), 1.77 – 1.71 (m, 1H), 1.66 (s, 3H), 1.43 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.97, 156.09, 152.87, 149.37, 136.07, 135.95, 130.94, 125.62, 124.91, 124.85, 124.78, 117.73, 117.67, 115.12, 114.93, 114.68, 114.49, 108.46, 107.77, 66.88, 48.10, 42.98, 34.39, 30.39, 26.60, 23.15. HRMS (ESI, m/z) calcd for $C_{26}H_{33}FO_3$ [M+Na^+] 435.2306, found 435.2300.



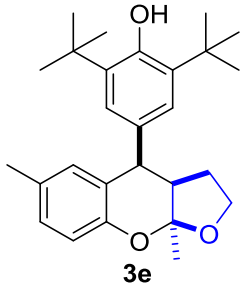
3c

Yield: 75%. ^{1}H NMR (500 MHz, $CDCl_3$) δ7.09 (ddd, *J* = 8.7, 2.6, 0.8 Hz, 1H), 6.97 (s, 2H), 6.87 (dd, *J* = 2.5, 1.1 Hz, 1H), 6.81 (d, *J* = 8.7 Hz, 1H), 5.19 (s, 1H), 4.25 (d, *J* = 5.1 Hz, 1H), 4.05 (td, *J* = 8.9, 2.0 Hz, 1H), 3.84 (m, *J* = 1.6 Hz, 1H), 2.42 (ddd, *J* = 8.8, 3.5 Hz, 1H), 2.32 – 2.25 (m, 1H), 1.92 (tt, *J* = 6.8, 5.0, 2.2 Hz, 1H), 1.76 – 1.69 (m, 1H), 1.66 (s, 3H), 1.43 (s, 18H), ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.89, 152.08, 136.07, 130.85, 128.66, 127.96, 125.22, 124.81, 124.73, 118.22, 107.80, 66.91, 48.08, 42.76, 34.41, 30.41, 26.45, 23.09. HRMS (ESI, m/z) calcd for $C_{26}H_{33}ClO_3$ [M+Na^+] 451.2010, found 451.2005.



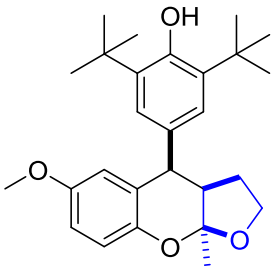
3d

Yield: 76%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (ddd, *J* = 8.7, 2.4, 0.8 Hz, 1H), 7.02 (dd, *J* = 2.3, 1.0 Hz, 1H), 6.97 (s, 2H), 6.76 (d, *J* = 8.6 Hz, 1H), 5.19 (s, 1H), 4.26 (d, *J* = 5.1 Hz, 1H), 4.08 – 4.03 (m, 1H), 3.88 – 3.81 (m, 1H), 2.44 (ddd, *J* = 12.0, 7.8, 5.2 Hz, 1H), 1.91 (ddd, *J* = 18.8, 10.7, 6.0 Hz, 1H), 1.75 – 1.68 (m, 1H), 1.69 – 1.63 (m, 3H), 1.44 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.90, 152.63, 136.08, 131.62, 130.87, 130.83, 125.27, 124.72, 118.73, 112.52, 107.77, 66.90, 48.10, 42.68, 34.42, 30.42, 26.41, 23.08. HRMS (ESI, m/z) calcd for $C_{26}H_{33}BrO_3$ [M+Na^+] 495.1505, found 495.1491.



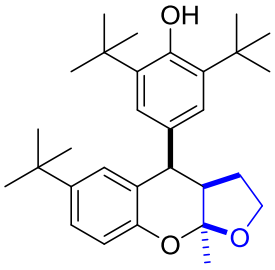
3e

Yield: 78%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.00 (s, 2H), 6.94 (dd, *J* = 8.2, 1.9 Hz, 1H), 6.78 (d, *J* = 8.2 Hz, 1H), 6.71 (s, 1H), 5.16 (s, 1H), 4.27 (d, *J* = 5.1 Hz, 1H), 4.04 (td, *J* = 8.8, 1.9 Hz, 1H), 3.86 – 3.81 (m, 1H), 2.43 (ddd, *J* = 11.9, 7.8, 5.3 Hz, 1H), 2.18 (s, 3H), 1.93 (tt, *J* = 11.9, 9.3 Hz, 1H), 1.71 – 1.66 (m, 1H), 1.66 (s, 3H), 1.43 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.61, 151.24, 135.81, 131.77, 129.62, 129.29, 128.52, 124.85, 122.54, 116.57, 107.29, 66.79, 48.52, 42.76, 34.40, 30.46, 26.53, 23.12, 20.63. HRMS (ESI, m/z) calcd for $C_{27}H_{36}O_3$ [M+Na^+] 431.2557, found 431.2545.



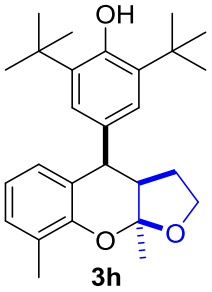
3f

Yield: 80%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.01 (s, 2H), 6.82 (d, *J* = 8.8 Hz, 1H), 6.72 (ddd, *J* = 8.8, 3.0, 0.6 Hz, 1H), 6.43 (dd, *J* = 2.9, 0.9 Hz, 1H), 5.16 (s, 1H), 4.26 (d, *J* = 5.0 Hz, 1H), 4.02 (td, *J* = 9.1, 2.7 Hz, 1H), 3.89 – 3.80 (m, 1H), 3.64 (s, 3H), 2.47 (ddd, *J* = 11.7, 7.9, 5.1 Hz, 1H), 1.93 (tt, *J* = 11.8, 9.2 Hz, 1H), 1.74 (ddd, *J* = 12.4, 7.7, 3.8 Hz, 1H), 1.66 (s, 3H), 1.43 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.54, 152.69, 147.48, 135.89, 131.32, 125.71, 124.41, 117.37, 114.05, 113.61, 107.58, 66.84, 55.77, 48.46, 43.10, 34.39, 30.44, 26.69, 23.28. HRMS (ESI, m/z) calcd for $C_{27}H_{36}O_4$ [M+Na^+] 447.2506, found 447.2506.



3g

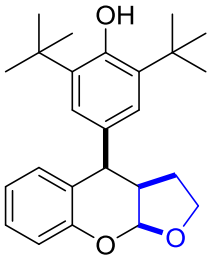
Yield: 85%. ^{1}H NMR (500 MHz, CDCl3) δ 7.18 – 7.14 (m, 1H), 6.99 (s, 2H), 6.91 (d, *J* = 1.3 Hz, 1H), 6.81 (d, *J* = 8.5 Hz, 1H), 5.14 (s, 1H), 4.31 (d, *J* = 5.2 Hz, 1H), 4.04 (td, *J* = 9.5, 2.4 Hz, 1H), 3.85 (m, *J* = 16.5, 5.8 Hz, 1H), 2.43 (ddd, *J* = 12.8, 7.8, 5.4 Hz, 1H), 1.94 – 1.86 (m, 1H), 1.66 (s, *J* = 9.7 Hz, 3H), 1.65 – 1.61 (m, 1H), 1.42 (s, *J* = 7.3 Hz, 18H), 1.18 (d, *J* = 3.8 Hz, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.52, 151.15, 142.86, 135.77, 131.91, 126.28, 124.84, 124.64, 121.49, 116.04, 107.02, 66.70, 48.62, 42.70, 34.39, 31.55, 30.45, 26.28, 23.12. HRMS (ESI, m/z) calcd for $C_{30}H_{42}O_3$ [M+Na^+] 473.3026, found 473.3029.



3h

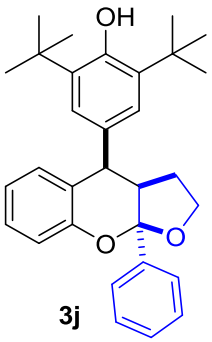
Yield: 78%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.01 (s, *J* = 5.7 Hz, 3H), 6.71 (d, *J* = 6.4 Hz, 2H), 5.14 (s, 1H), 4.27 (d, *J* = 5.0 Hz, 1H), 4.02 – 3.97 (td, 1H), 3.86 (m, *J* = 7.3 Hz, 1H), 2.47 (ddd, *J* = 11.4, 8.1, 5.1 Hz, 1H), 2.25 (s, 3H), 1.93 (tt, *J* = 11.6, 9.2 Hz, 1H), 1.77 – 1.70 (m, 1H), 1.68 (s, 3H), 1.43 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ

152.58, 151.72, 135.79, 131.89, 129.02, 126.54, 125.75, 125.07, 122.94, 119.72, 107.68, 66.73, 48.33, 43.05, 34.39, 30.44, 26.59, 23.51, 16.39. HRMS (ESI, m/z) calcd for $C_{27}H_{36}O_3$ [M+Na$^+$] 431.2557, found 431.2544.



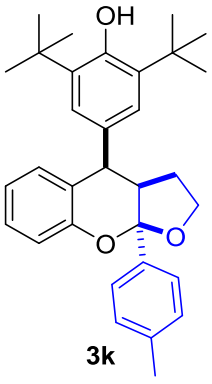
3i

Yield: 92%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.15 (m, *J* = 3.1, 2.5, 2.1 Hz, 1H), 7.03 (s, 2H), 6.90 (s, *J* = 2.7 Hz, 1H), 6.88 – 6.81 (m, 2H), 5.84 (d, *J* = 4.7 Hz, 1H), 5.17 (s, 1H), 4.40 (d, *J* = 4.6 Hz, 1H), 4.14 – 4.10 (m, 1H), 3.88 (dd, *J* = 12.8, 4.8 Hz, 1H), 2.81 – 2.74 (m, 1H), 1.89 (dq, *J* = 11.7, 9.3 Hz, 1H), 1.79 (ddd, *J* = 7.3, 5.9, 2.6 Hz, 1H), 1.43 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.41, 152.73, 135.92, 131.05, 128.56, 127.91, 125.82, 124.30, 120.87, 116.67, 102.05, 68.54, 45.48, 42.20, 34.39, 30.41, 25.17. HRMS (ESI, m/z) calcd for $C_{25}H_{32}O_3$ [M+H$^+$] 381.2424, found 381.2421.



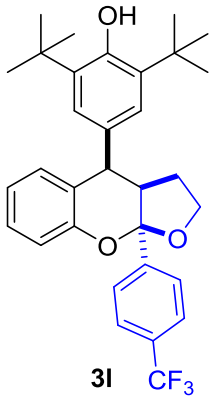
3j

Yield: 87%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 7.6, 1.8 Hz, 2H), 7.38 – 7.36 (m, 2H), 7.24 – 7.20 (m, 1H), 7.15 – 7.10 (m, 1H), 7.05 (t, *J* = 7.0 Hz, 2H), 6.91 (s, 2H), 6.84 (t, *J* = 3.8 Hz, 1H), 5.14 (s, 1H), 4.30 – 4.24 (td, 1H), 4.16 – 4.11 (m, 1H), 4.07 (d, *J* = 4.8 Hz, 1H), 2.75 (ddd, *J* = 12.3, 7.7, 4.9 Hz, 1H), 2.19 (ddd, *J* = 11.9, 7.5, 2.7 Hz, 1H), 1.98 – 1.89 (m, 1H), 1.39 (s, 18H). HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_3$ [M+H$^+$] 457.2737, found 457.2734.



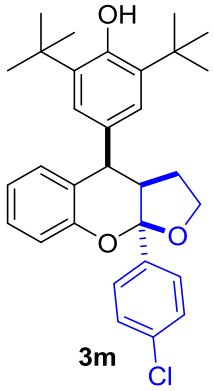
3k

Yield: 67%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.9 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.04 (d, *J* = 8.1 Hz, 1H), 6.92 (s, 2H), 6.84 (d, *J* = 7.7 Hz, 3H), 5.13 (s, 1H), 4.26 (dd, *J* = 12.9, 4.8 Hz, 1H), 4.14 (m, *J* = 10.2, 6.2 Hz, 1H), 4.08 (d, *J* = 4.5 Hz, 1H), 2.78 – 2.68 (m, 1H), 2.36 (s, 3H), 2.20 (m, *J* = 10.1 Hz, 1H), 1.96 – 1.86 (m, 1H), 1.39 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.01, 152.66, 138.26, 137.81, 135.81, 131.60, 129.08, 128.38, 125.96, 124.78, 123.11, 121.34, 120.57, 116.32, 108.32, 67.78, 50.59, 41.65, 34.38, 30.44, 26.81, 21.25. HRMS (ESI, m/z) calcd for $C_{32}H_{38}O_3$ $[M+H]^+$ 471.2894, found 471.2885.



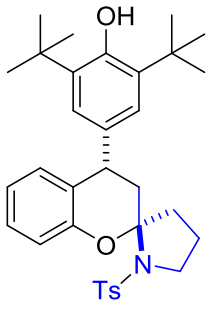
3l

Yield: 78%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 – 7.61 (m, 4H), 7.24 – 7.21 (m, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 6.91 (s, 2H), 6.90 – 6.86 (m, 2H), 5.16 (s, 1H), 4.28 (td, *J* = 9.4, 2.3 Hz, 1H), 4.17 (dt, *J* = 16.4, 8.2 Hz, 1H), 4.04 (d, *J* = 4.7 Hz, 1H), 2.72 (ddd, *J* = 12.3, 7.7, 4.9 Hz, 1H), 2.27 – 2.09 (m, 1H), 1.97 (dtd, *J* = 10.0, 7.5, 2.3 Hz, 1H), 1.40 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.66, 152.81, 144.96, 135.94, 130.99, 130.87, 130.62, 129.26, 128.36, 126.59, 125.77, 125.44, 125.41, 125.38, 125.20, 123.04, 123.00, 121.03, 116.35, 107.70, 68.17, 51.00, 41.48, 34.38, 30.40, 26.88. HRMS (ESI, m/z) calcd for $C_{32}H_{35}F_3O_3$ $[M+Na^+]$ 547.2431, found 547.2428.



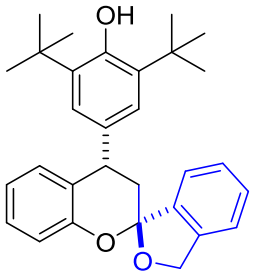
3m

Yield: 78%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.44 (m, 2H), 7.36 – 7.31 (m, 2H), 7.25 – 7.19 (m, 1H), 7.04 (d, *J* = 7.9 Hz, 1H), 6.90 (s, 2H), 6.86 (m, *J* = 4.3, 2.1 Hz, 2H), 5.15 (s, 1H), 4.26 (td, *J* = 9.5, 2.4 Hz, 1H), 4.14 (dt, *J* = 16.3, 8.1 Hz, 1H), 4.03 (d, *J* = 4.8 Hz, 1H), 2.68 (ddd, *J* = 12.2, 7.7, 4.8 Hz, 1H), 2.16 (ddd, *J* = 18.9, 10.8, 6.0 Hz, 1H), 2.02 – 1.85 (m, 1H), 1.40 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.75, 152.76, 139.54, 135.91, 134.48, 131.15, 129.22, 128.59, 128.27, 127.59, 125.78, 123.00, 120.87, 116.29, 107.87, 67.97, 50.93, 41.52, 34.38, 30.41, 26.76. HRMS (ESI, m/z) calcd for $C_{31}H_{35}ClO_3$ $[M+Na^+]$ 513.2167, found 513.2147.



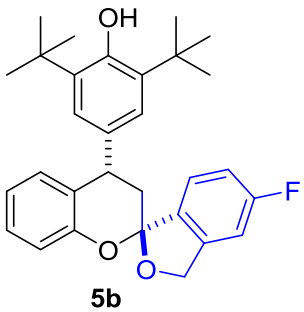
3n

Yield: 61%. 1H NMR (500 MHz, CDCl3) δ 7.90 (d, J = 8.3 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.12 – 7.06 (m, 1H), 7.01 (s, 2H), 6.78 (dd, J = 3.5, 2.2 Hz, 2H), 6.59 (d, J = 8.0 Hz, 1H), 5.15 (s, 1H), 4.01 (dd, J = 13.2, 5.1 Hz, 1H), 3.62 (dd, J = 8.7, 5.2 Hz, 2H), 3.38 (t, J = 13.4 Hz, 1H), 2.47 (s, 3H), 2.29 (ddd, J = 12.6, 6.8, 2.6 Hz, 1H), 2.21 (dd, J = 13.5, 5.2 Hz, 1H), 2.07 – 1.99 (m, 1H), 1.95 – 1.80 (m, 2H), 1.44 (s, 18H). 13C NMR (126 MHz, CDCl3) δ 153.43, 152.63, 143.13, 137.31, 136.00, 133.52, 129.52, 129.05, 128.50, 127.56, 125.59, 125.19, 120.38, 116.66, 96.97, 49.97, 42.50, 40.25, 38.66, 34.40, 30.42, 30.31, 21.59, 20.79. HRMS (ESI, m/z) calcd for $C_{33}H_{41}NO_4S$ [M+Na^+] 470.2649, found 470.2637.



5a

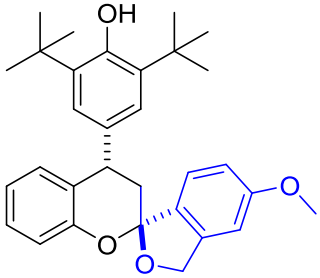
Yield: 87%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 – 7.34 (m, 4H), 7.21 – 7.12 (m, 3H), 6.91 (dd, *J* = 18.1, 7.5 Hz, 3H), 5.39 (d, *J* = 12.7 Hz, 1H), 5.19 (s, 1H), 5.17 (d, *J* = 12.7 Hz, 1H), 4.55 (dd, *J* = 13.2, 5.4 Hz, 1H), 2.70 (t, *J* = 13.2 Hz, 1H), 2.42 (dd, *J* = 13.1, 5.4 Hz, 1H), 1.49 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.29, 152.59, 140.12, 139.93, 136.08, 134.32, 129.55, 129.46, 127.97, 127.64, 126.22, 125.40, 122.12, 121.38, 120.92, 116.98, 108.70, 71.83, 39.96, 38.91, 34.50, 30.51. HRMS (ESI, m/z) calcd for $C_{30}H_{34}O_3$ [M+Na^+] 465.2400, found 465.2396.



5b

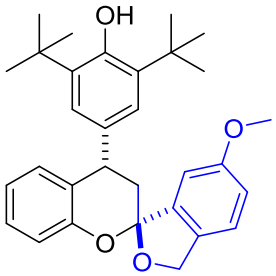
Yield: 82%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (dd, *J* = 8.3, 4.8 Hz, 1H), 7.18 – 7.00 (m, 5H), 6.90 – 6.80 (m, 3H), 5.31 (d, *J* = 13.3 Hz, 1H), 5.15 (s, 1H), 5.09 (d, *J* = 13.1 Hz, 1H), 4.47 (dd, *J* = 13.2, 5.4 Hz, 1H), 2.60 (t, *J* = 13.2 Hz, 1H), 2.36 (dd, *J* = 13.1,

5.5 Hz, 1H), 1.44 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.82, 162.85, 153.09, 152.58, 142.55, 142.48, 136.07, 135.75, 134.11, 129.42, 127.64, 126.08, 125.32, 123.66, 123.59, 121.00, 116.87, 115.38, 115.20, 108.69, 108.50, 108.19, 71.28, 71.26, 40.01, 38.86, 34.45, 30.43. HRMS (ESI, m/z) calcd for $C_{30}H_{33}FO_3$ [M+K^+] 499.2045, found 499.2048.



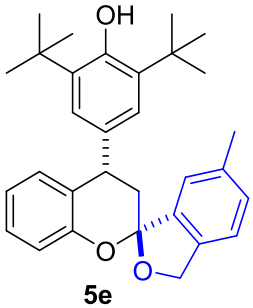
5c

Yield: 86%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.3 Hz, 1H), 7.10 (t, *J* = 5.4 Hz, 3H), 6.96 – 6.80 (m, 5H), 5.32 (d, *J* = 12.8 Hz, 1H), 5.15 (d, *J* = 1.0 Hz, 1H), 5.08 (d, *J* = 12.8 Hz, 1H), 4.48 (dd, *J* = 13.2, 5.2 Hz, 1H), 3.86 (s, 3H), 2.69 – 2.54 (m, 1H), 2.43 – 2.29 (m, 1H), 1.45 (d, *J* = 1.0 Hz, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.11, 153.33, 152.52, 141.95, 136.02, 134.33, 132.39, 129.40, 127.56, 126.14, 125.35, 122.96, 120.80, 116.92, 114.31, 108.49, 106.22, 71.58, 55.63, 40.06, 38.98, 34.45, 30.45. HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_4$ [M+H^+] 473.2686, found 473.2683.



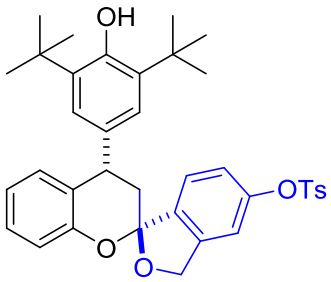
5d

Yield: 80%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 (d, *J* = 8.3 Hz, 1H), 7.16 – 7.08 (m, 3H), 6.99 (dd, *J* = 8.3, 1.8 Hz, 1H), 6.95 (s, 1H), 6.90 – 6.81 (m, 3H), 5.30 (d, *J* = 12.1 Hz, 1H), 5.15 (s, 1H), 5.07 (d, *J* = 12.1 Hz, 1H), 4.49 (dd, *J* = 13.2, 5.3 Hz, 1H), 3.84 (s, 3H), 2.61 (t, *J* = 13.2 Hz, 1H), 2.38 (dd, *J* = 13.1, 5.4 Hz, 1H), 1.45 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.98, 153.23, 152.54, 141.29, 136.05, 134.29, 131.89, 129.43, 127.61, 126.13, 125.34, 122.14, 120.89, 116.95, 116.65, 108.58, 106.56, 71.55, 55.66, 39.98, 38.85, 34.46, 30.45. HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_4$ [M+Na^+] 495.2506, found 495.2467.



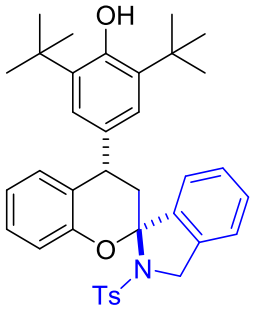
5e

Yield: 84%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 – 7.20 (m, 3H), 7.08 (s, 3H), 6.83 (dd, *J* = 7.6, 5.6 Hz, 3H), 5.30 (d, *J* = 12.5 Hz, 1H), 5.12 (s, 1H), 5.07 (d, *J* = 12.5 Hz, 1H), 4.47 (dd, *J* = 13.2, 5.4 Hz, 1H), 2.62 (t, *J* = 13.2 Hz, 1H), 2.40 (s, 3H), 2.34 (dd, *J* = 13.1, 5.5 Hz, 1H), 1.43 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.25, 152.51, 140.10, 137.84, 137.17, 136.00, 134.33, 130.45, 129.41, 127.56, 126.18, 125.33, 122.48, 121.06, 120.83, 116.93, 108.61, 71.70, 39.93, 38.85, 34.44, 30.45, 21.36. HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_3$ [M+Na^+] 479.2557, found 479.2565.



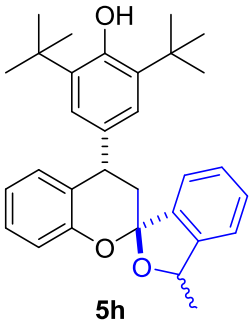
5f

Yield: 88%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.2 Hz, 2H), 7.32 (t, *J* = 7.8 Hz, 3H), 7.15 – 7.08 (m, 1H), 7.05 (s, 3H), 6.91 (dd, *J* = 8.3, 1.0 Hz, 1H), 6.87 – 6.75 (m, 3H), 5.25 (d, *J* = 13.1 Hz, 1H), 5.14 (s, 1H), 5.03 (d, *J* = 13.1 Hz, 1H), 4.44 (dd, *J* = 13.1, 5.3 Hz, 1H), 2.54 (t, *J* = 13.2 Hz, 1H), 2.45 (s, 3H), 2.31 (dd, *J* = 13.1, 5.4 Hz, 1H), 1.42 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.97, 152.59, 150.60, 145.60, 142.06, 138.66, 136.08, 134.00, 132.34, 129.90, 129.43, 128.57, 127.67, 126.05, 125.28, 123.24, 122.12, 121.08, 116.83, 115.89, 108.12, 71.25, 39.97, 38.75, 34.44, 30.42, 21.77. HRMS (ESI, m/z) calcd for $C_{37}H_{40}O_6S$ [M+Na^+] 635.2438, found 635.2413.



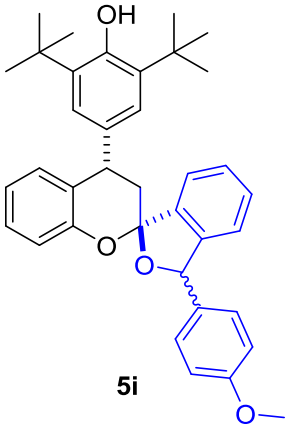
5g

Yield: 79%. ^{1}H NMR (500 MHz, CDCl3) δ 7.97 (d, *J* = 8.3 Hz, 2H), 7.37 – 7.34 (m, 1H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.28 – 7.23 (m, 3H), 7.15 – 7.11 (m, 1H), 7.06 (s, 2H), 6.91 (d, *J* = 7.4 Hz, 1H), 6.88 – 6.83 (m, 1H), 6.65 (dd, *J* = 8.2, 0.9 Hz, 1H), 5.14 (d, *J* = 4.5 Hz, 1H), 4.84 (d, *J* = 13.5 Hz, 1H), 4.67 (d, *J* = 13.5 Hz, 1H), 4.45 (dd, *J* = 13.0, 5.7 Hz, 1H), 3.74 (t, *J* = 13.5 Hz, 1H), 2.46 (dd, *J* = 14.0, 5.8 Hz, 1H), 2.43 (s, 3H), 1.43 (s, 18H). ^{13}C NMR (126 MHz, CDCl3) δ 153.55, 152.66, 143.41, 141.66, 137.42, 136.05, 134.45, 133.79, 129.70, 129.35, 129.15, 128.46, 128.29, 128.18, 127.99, 125.34, 125.19, 123.21, 122.68, 120.88, 116.76, 98.18, 53.08, 41.94, 40.67, 34.42, 30.44, 21.59. HRMS (ESI, m/z) calcd for $C_{37}H_{41}NO_4S$ [M+Na^+] 618.2649, found 618.2633.



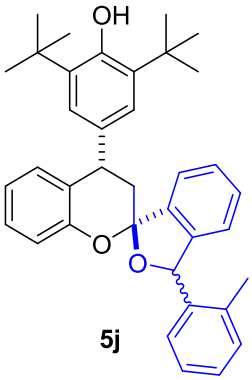
5h

Yield: 86%. ^{1}H NMR (500 MHz, CDCl3) δ 7.41 (m, *J* = 19.6, 10.9, 4.1 Hz, 3H), 7.29 – 7.23 (m, 1H), 7.09 (s, 3H), 6.87 – 6.78 (m, 3H), 5.56-5.38 (m, *J* = 6.4 Hz, 1H) 5.13 (d, *J* = 3.2 Hz, 1H), 4.55 – 4.41 (m, 1H), 2.63 (dt, *J* = 44.0, 13.2 Hz, 1H), 2.31 (ddd, *J* = 13.3, 9.1, 5.4 Hz, 1H), 1.57 (dd, *J* = 20.9, 6.5 Hz, 3H), 1.43 (d, *J* = 4.1 Hz, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.30, 152.53, 144.67, 144.57, 140.18, 139.81, 136.00, 134.37, 134.24, 129.61, 129.56, 129.46, 129.36, 128.06, 128.03, 127.55, 127.49, 126.30, 126.23, 125.38, 122.12, 121.92, 121.25, 121.15, 120.79, 120.69, 116.94, 116.88, 107.97, 107.46, 79.83, 78.48, 40.32, 40.11, 38.97, 38.64, 34.47, 30.47, 23.63, 21.16.HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_3$ [M+Na$^+$] 479.2557, found 479.2565.



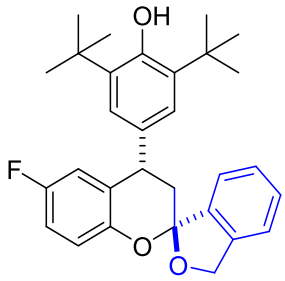
5i

Yield: 94%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.2 Hz, 1H), 7.44 – 7.33 (m, 3H), 7.22 (s, 1H), 7.17 – 7.00 (m, 4H), 6.92 – 6.74 (m, 5H), 6.36-6.20 (s, 1H), 5.13 (d, *J* = 5.5 Hz, 1H), 4.51 (dd, *J* = 13.2, 5.3 Hz, 1H), 3.78 (d, *J* = 17.0 Hz, 3H), 2.72 (dt, *J* = 61.5, 13.2 Hz, 1H), 2.44 (ddd, *J* = 55.8, 13.1, 5.3 Hz, 1H), 1.43 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.79, 159.46, 153.25, 153.18, 152.56, 143.91, 143.23, 140.31, 139.42, 136.03, 134.12, 133.82, 132.57, 129.83, 129.78, 129.36, 129.10, 128.51, 128.26, 127.55, 127.50, 126.42, 125.40, 122.60, 122.34, 122.17, 121.76, 120.81, 116.85, 116.79, 114.01, 113.91, 108.37, 107.95, 85.61, 84.28, 55.32, 55.29, 40.49, 39.87, 38.98, 38.42, 34.47, 30.46. HRMS (ESI, m/z) calcd for $C_{37}H_{40}O_4$ [M+H$^+$] 549.2999, found 549.2994.



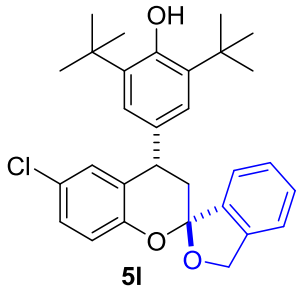
5j

Yield: 95%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (dt, *J* = 8.3, 4.9 Hz, 1H), 7.42 – 7.33 (m, 2H), 7.22 – 7.08 (m, 7H), 7.03 (d, *J* = 7.3 Hz, 1H), 6.88 (t, *J* = 8.4 Hz, 1H), 6.81 (d, *J* = 5.0 Hz, 2H), 6.66-6.58 (s, 1H), 5.14 (d, *J* = 7.8 Hz, 1H), 4.52 (dd, *J* = 13.2, 5.0 Hz, 1H), 2.79-2.65 (t, *J* = 13.2 Hz, 1H), 2.58 – 2.32 (m, 4H), 1.44 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.29, 153.17, 152.59, 152.55, 143.63, 142.87, 140.36, 139.84, 139.29, 137.88, 136.43, 136.05, 136.02, 134.97, 134.09, 134.06, 130.86, 130.35, 129.84, 129.78, 129.34, 129.27, 128.29, 128.26, 128.22, 128.19, 127.83, 127.55, 127.50, 126.53, 126.46, 126.39, 126.27, 125.40, 122.40, 122.30, 122.15, 121.88, 120.81, 116.86, 116.80, 108.47, 107.95, 82.41, 81.93, 40.65, 39.39, 39.02, 38.45, 34.48, 30.47, 19.69, 19.55. HRMS (ESI, m/z) calcd for $C_{37}H_{40}O_3$ [M+H$^+$] 533.3050, found 533.3043.



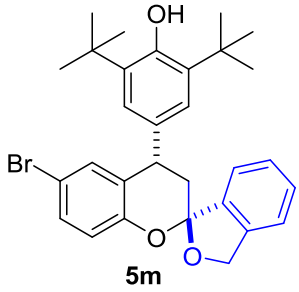
5k

Yield: 68%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 – 7.31 (m, 4H), 7.07 (s, 2H), 6.79 (ddd, *J* = 13.9, 8.7, 4.0 Hz, 2H), 6.57 (dd, *J* = 9.4, 2.6 Hz, 1H), 5.34 (d, *J* = 12.7 Hz, 1H), 5.17 (s, 1H), 5.12 (d, *J* = 12.7 Hz, 1H), 4.45 (dd, *J* = 13.2, 5.4 Hz, 1H), 2.61 (t, *J* = 13.2 Hz, 1H), 2.36 (dd, *J* = 13.2, 5.5 Hz, 1H), 1.44 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.17, 156.28, 152.75, 149.24, 140.00, 139.62, 136.21, 133.53, 129.61, 127.96, 127.71, 127.65, 125.23, 122.03, 121.36, 117.91, 117.84, 115.41, 115.23, 114.45, 114.26, 108.66, 71.84, 39.41, 39.10, 34.44, 30.40. HRMS (ESI, m/z) calcd for $C_{30}H_{33}FO_3$ [M+Na$^+$] 483.2306, found 483.2301.



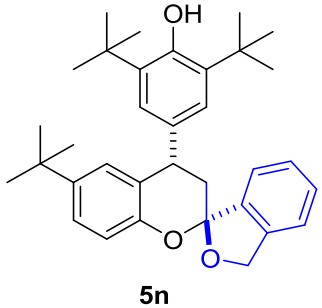
5l

Yield: 76%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 – 7.32 (m, 4H), 7.11 – 7.04 (m, 3H), 6.86 (dd, *J* = 2.5, 1.0 Hz, 1H), 6.76 (d, *J* = 8.7 Hz, 1H), 5.33 (d, *J* = 12.8 Hz, 1H), 5.17 (s, 1H), 5.12 (d, *J* = 12.7 Hz, 1H), 4.44 (dd, *J* = 13.2, 5.5 Hz, 1H), 2.60 (t, *J* = 13.2 Hz, 1H), 2.35 (dd, *J* = 13.2, 5.5 Hz, 1H), 1.44 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.77, 151.95, 140.01, 139.47, 136.23, 133.42, 129.65, 128.95, 127.97, 127.94, 127.63, 125.71, 125.22, 122.02, 121.36, 118.42, 108.73, 71.88, 39.61, 38.91, 34.46, 30.41. HRMS (ESI, m/z) calcd for $C_{30}H_{33}ClO_3$ [M+Na$^+$] 499.2010, found 499.1984.



5m

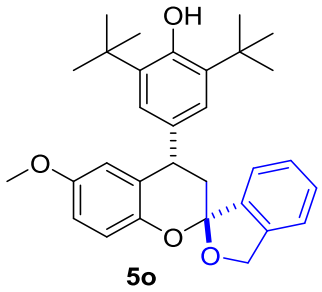
Yield: 82%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.31 (m, 4H), 7.24 – 7.18 (m, 1H), 7.06 (s, 2H), 7.04 – 6.99 (m, 1H), 6.72 (d, *J* = 8.7 Hz, 1H), 5.33 (d, *J* = 12.7 Hz, 1H), 5.18 (s, 1H), 5.12 (d, *J* = 12.7 Hz, 1H), 4.46 (dd, *J* = 13.2, 5.5 Hz, 1H), 2.59 (t, *J* = 13.2 Hz, 1H), 2.35 (dd, *J* = 13.2, 5.5 Hz, 1H), 1.45 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.78, 152.51, 140.01, 139.44, 136.23, 133.42, 131.90, 130.54, 129.67, 128.44, 127.98, 125.22, 122.02, 121.37, 118.93, 113.16, 108.71, 71.90, 39.70, 38.87, 34.47, 30.42. HRMS (ESI, m/z) calcd for $C_{30}H_{33}BrO_3$ [M+Na$^+$] 543.1505, found 543.1497.



5n

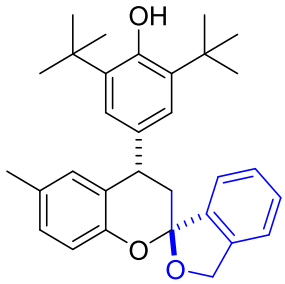
Yield: 79%.^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 – 7.30 (m, 4H), 7.15 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.09 (s, 2H), 6.93 – 6.88 (m, 1H), 6.78 (d, *J* = 8.5 Hz, 1H), 5.35 (d, *J* = 12.7 Hz, 1H), 5.13 (m, *J* = 6.3 Hz, 2H), 4.50 (dd, *J* = 13.2, 5.4 Hz, 1H), 2.58 (t, *J* = 13.2 Hz, 1H), 2.37 (dd, *J* = 13.1, 5.5 Hz, 1H), 1.43 (s, 18H), 1.18 (s, 9H). ^{13}C NMR (126

MHz, $CDCl_3$) δ 152.41, 151.08, 143.27, 140.07, 139.96, 135.92, 134.45, 129.45, 127.90, 126.55, 125.31, 124.82, 124.43, 122.06, 121.32, 116.19, 108.52, 71.75, 40.45, 38.88, 34.45, 34.12, 31.50, 30.44. HRMS (ESI, m/z) calcd for $C_{34}H_{42}O_3$ [M+Na^+] 521.3026, found 521.2989.



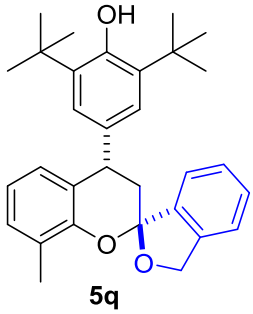
5o

Yield: 92%. ^{1}H NMR (500 MHz, CDCl3) δ 7.40 (ddd, *J* = 30.7, 17.3, 7.4 Hz, 4H), 7.10 (s, 2H), 6.79 (d, *J* = 8.8 Hz, 1H), 6.71 (dd, *J* = 8.8, 3.0 Hz, 1H), 6.43 (d, *J* = 2.8 Hz, 1H), 5.35 (d, *J* = 12.7 Hz, 1H), 5.15 (s, 1H), 5.12 (d, *J* = 12.7 Hz, 1H), 4.47 (dd, *J* = 13.2, 5.4 Hz, 1H), 3.65 (s, 3H), 2.63 (t, *J* = 13.2 Hz, 1H), 2.36 (dd, *J* = 13.1, 5.5 Hz, 1H), 1.45 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.70, 152.58, 147.45, 140.06, 139.94, 136.05, 134.02, 129.48, 127.91, 126.90, 125.32, 122.06, 121.33, 117.50, 114.50, 113.51, 108.56, 71.73, 55.80, 39.86, 39.17, 34.45, 30.46. HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_4$ [M+Na^+] 492.5206, found 495.2463.



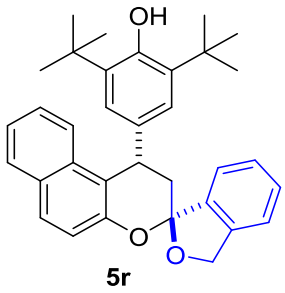
5p

Yield: 87%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (ddd, *J* = 29.4, 18.4, 7.5 Hz, 4H), 7.10 (s, 2H), 6.93 (dd, *J* = 8.2, 1.9 Hz, 1H), 6.75 (d, *J* = 8.2 Hz, 1H), 6.70 (s, 1H), 5.34 (d, *J* = 12.7 Hz, 1H), 5.15 (s, 1H), 5.12 (d, *J* = 12.7 Hz, 1H), 4.47 (dd, *J* = 13.1, 5.5 Hz, 1H), 2.62 (t, *J* = 13.2 Hz, 1H), 2.36 (dd, *J* = 13.1, 5.6 Hz, 1H), 2.19 (s, 3H), 1.45 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.48, 151.13, 140.10, 139.98, 135.96, 134.47, 130.02, 129.62, 129.45, 128.27, 127.88, 125.59, 125.34, 122.06, 121.32, 116.72, 108.55, 71.72, 40.29, 38.89, 34.46, 30.47, 20.65. HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_3$ [M+Na^+] 479.2557, found 479.2563.



5q

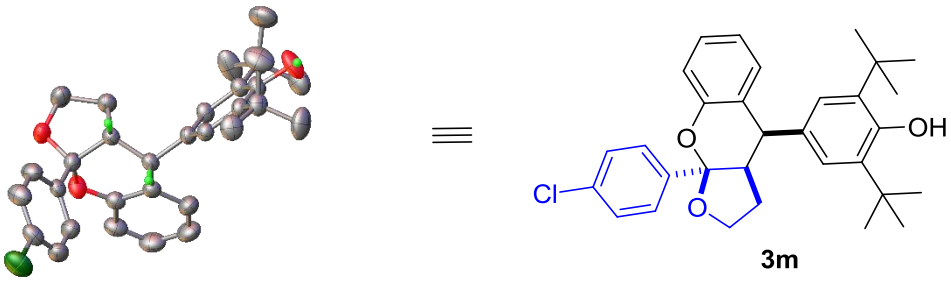
Yield: 80%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (ddd, *J* = 20.1, 13.3, 7.3 Hz, 4H), 7.10 (s, 2H), 6.99 (d, *J* = 6.6 Hz, 1H), 6.78 – 6.66 (m, 2H), 5.33 (d, *J* = 12.6 Hz, 1H), 5.14 (s, 1H), 5.11 (d, *J* = 12.7 Hz, 1H), 4.48 (dd, *J* = 13.2, 5.2 Hz, 1H), 2.63 (t, *J* = 13.2 Hz, 1H), 2.36 (dd, *J* = 13.1, 5.4 Hz, 1H), 2.13 (s, 3H), 1.45 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.47, 151.37, 140.36, 140.16, 135.93, 134.49, 129.26, 128.81, 127.73, 126.91, 125.80, 125.66, 125.39, 122.14, 121.20, 120.10, 108.45, 71.59, 39.86, 38.97, 34.45, 30.47, 16.35. HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_3$ [M+Na^+] 479.2557, found 479.2545.



5r

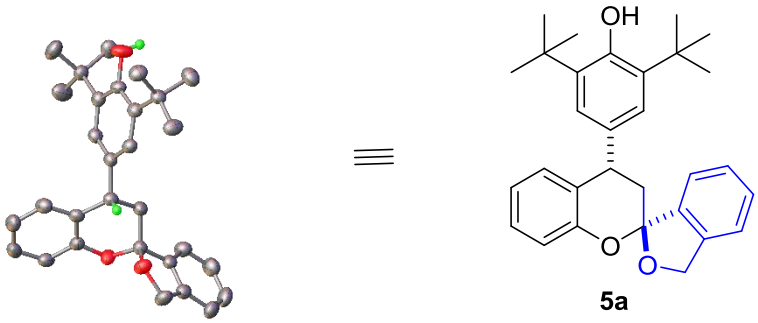
Yield: 80%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 14.3, 8.4 Hz, 2H), 7.39 (ddd, *J* = 15.5, 8.0, 5.5 Hz, 5H), 7.21 (dd, *J* = 11.0, 3.9 Hz, 1H), 7.15 – 7.07 (m, 2H), 6.91 (s, 2H), 5.28 (d, *J* = 14.0 Hz, 1H), 5.12 (d, *J* = 12.8 Hz, 1H), 5.05 (s, 1H), 4.85 (t, *J* = 9.4 Hz, 1H), 2.71 (d, *J* = 9.4 Hz, 2H), 1.31 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.06, 151.88, 144.25, 140.21, 139.69, 136.90, 136.14, 132.50, 130.17, 129.53, 128.92, 128.08, 127.91, 125.83, 125.11, 125.02, 124.15, 122.91, 122.27, 121.31, 119.39, 117.03, 108.10, 71.91, 43.18, 37.61, 34.34, 30.33. HRMS (ESI, m/z) calcd for $C_{34}H_{36}O_3$ [M+Na^+] 515.2557, found 515.2559.

5. X-ray Crystallography Data



3m

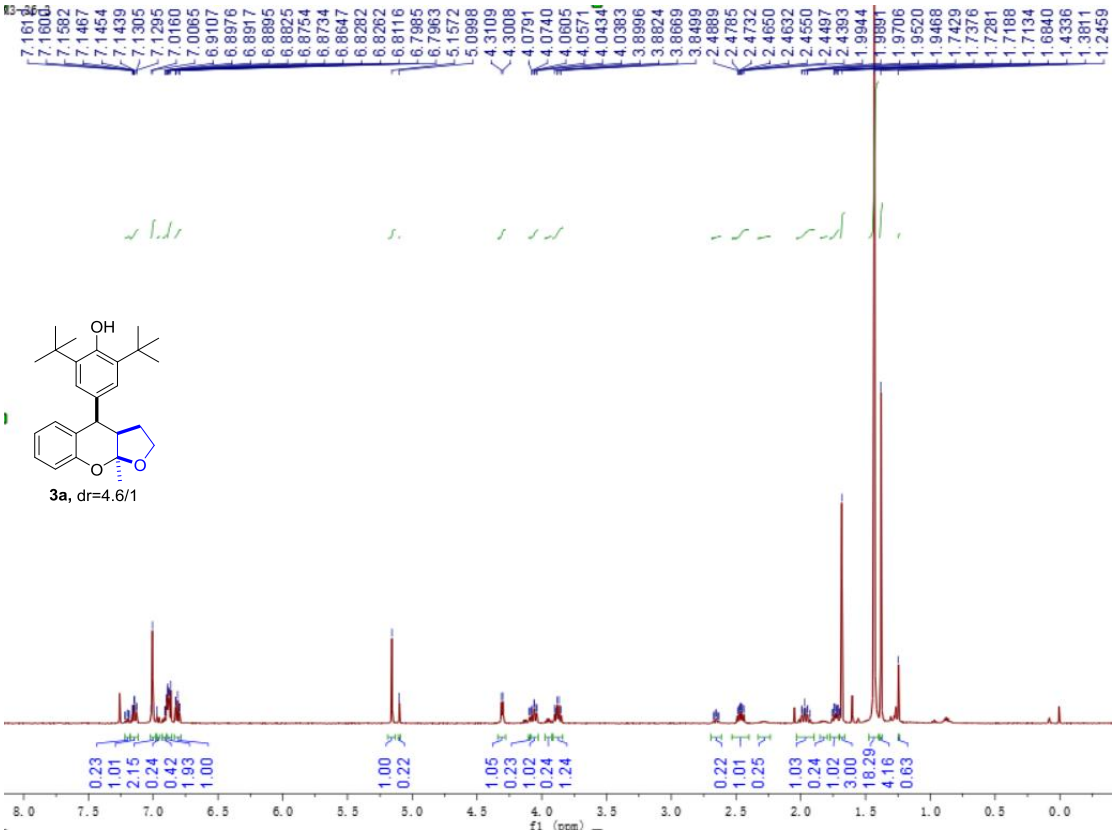
CCDC 1974774 (**3m**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

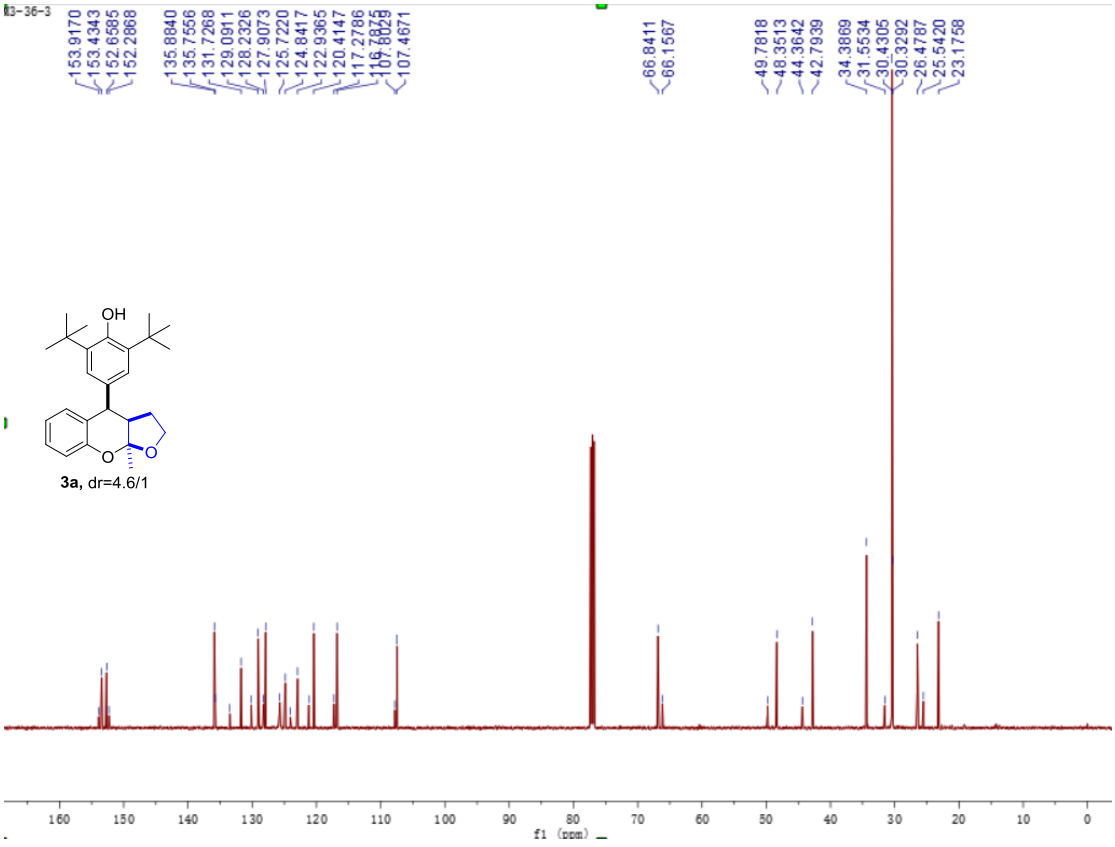


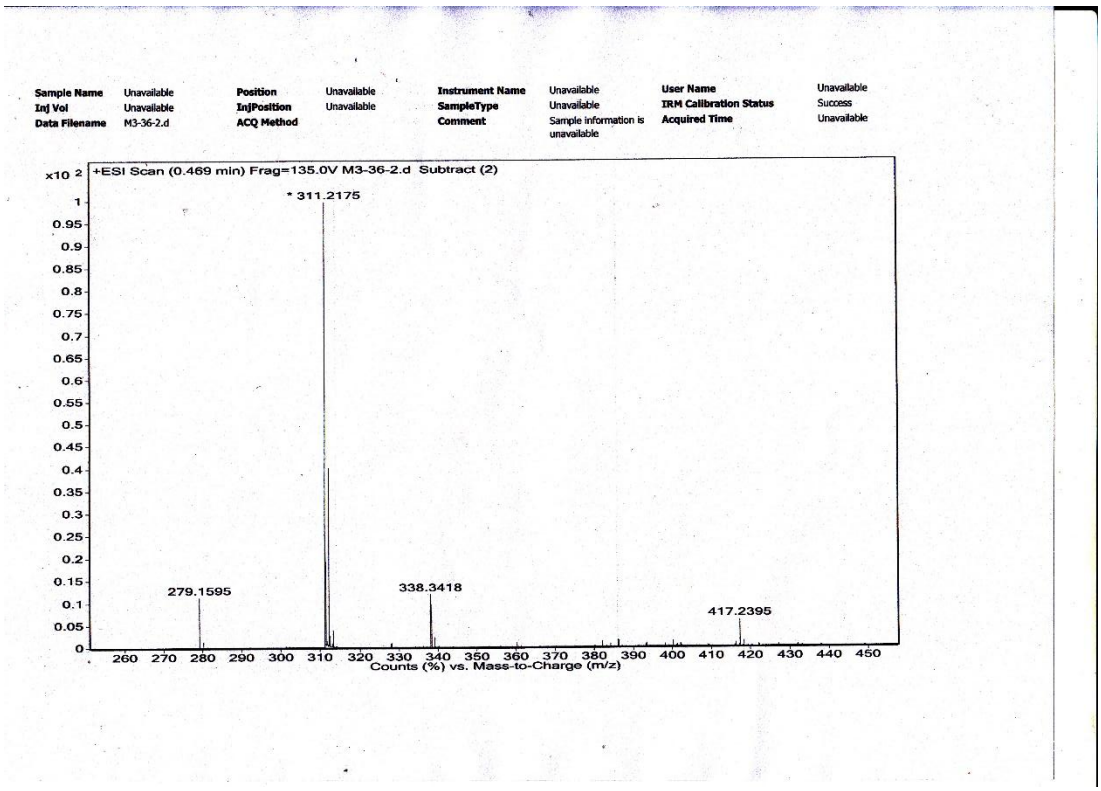
5a

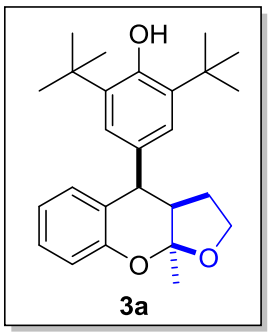
CCDC 1974775 (**5a**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

6. NMR and HRMS Spectra of All Compounds





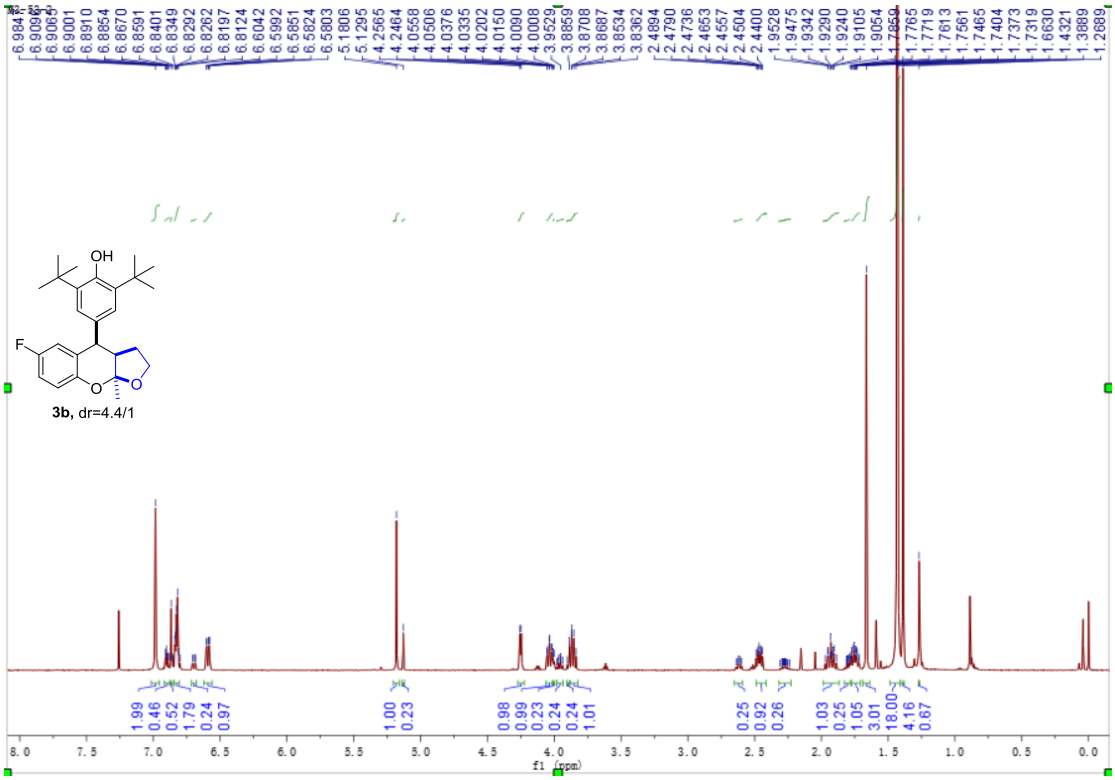


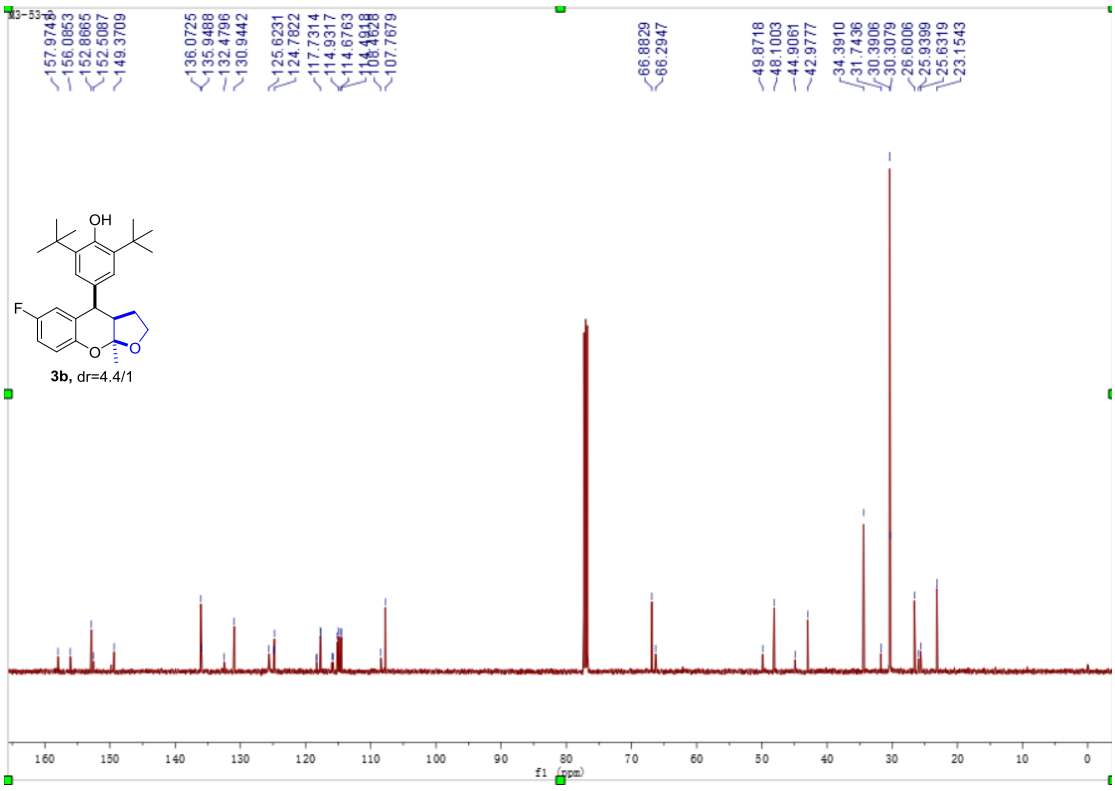


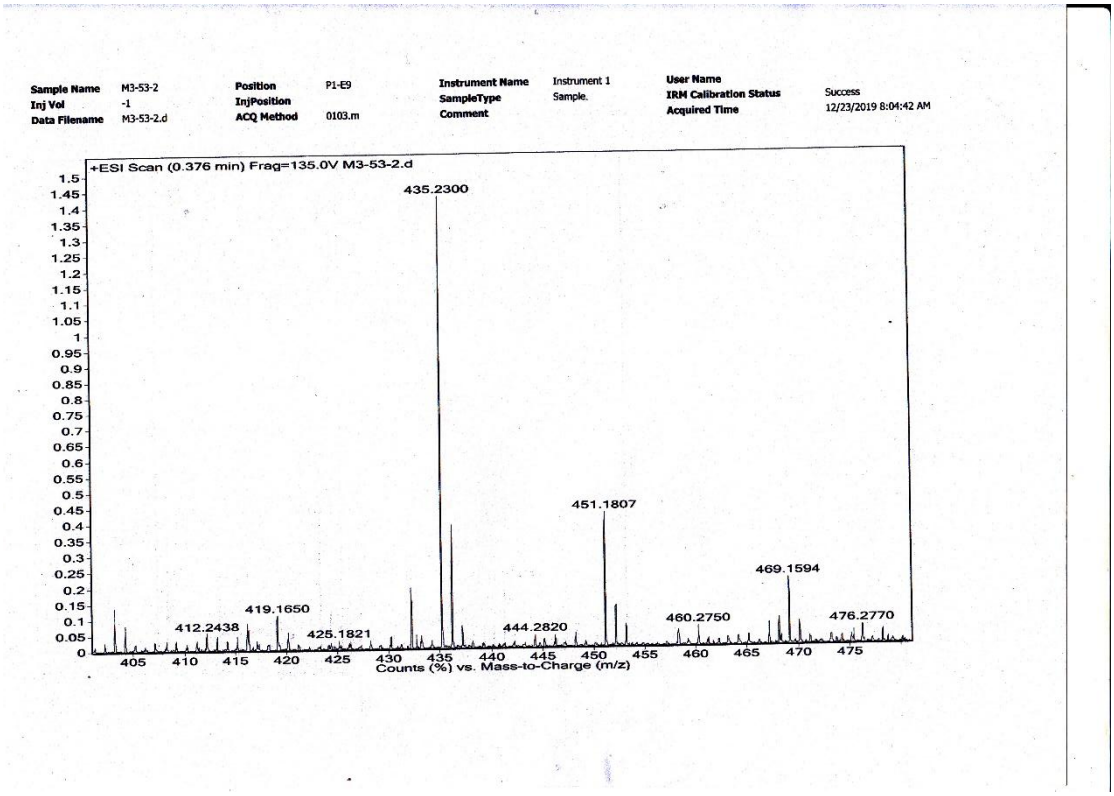
3a

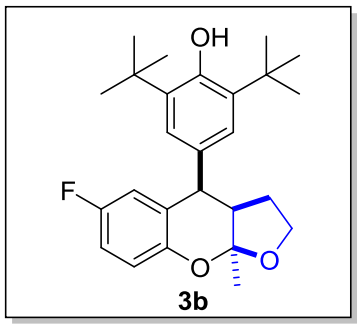
Chemical Formula: $C_{26}H_{34}O_3$
Exact Mass: 394.2508
Molecular Weight: 394.5550
m/z: 394.2508 (100.0%), 395.2541 (28.1%), 396.2575 (2.7%), 396.2575 (1.1%)
Elemental Analysis: C, 79.15; H, 8.69; O, 12.16

HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_3$ [M+Na^+] 417.2400, found 417.2395.


OH
F
O
O
3b, dr=4.4/1
f1 (ppm)


OH
F
O
O
3b, dr=4.4/1
f1 (ppm)

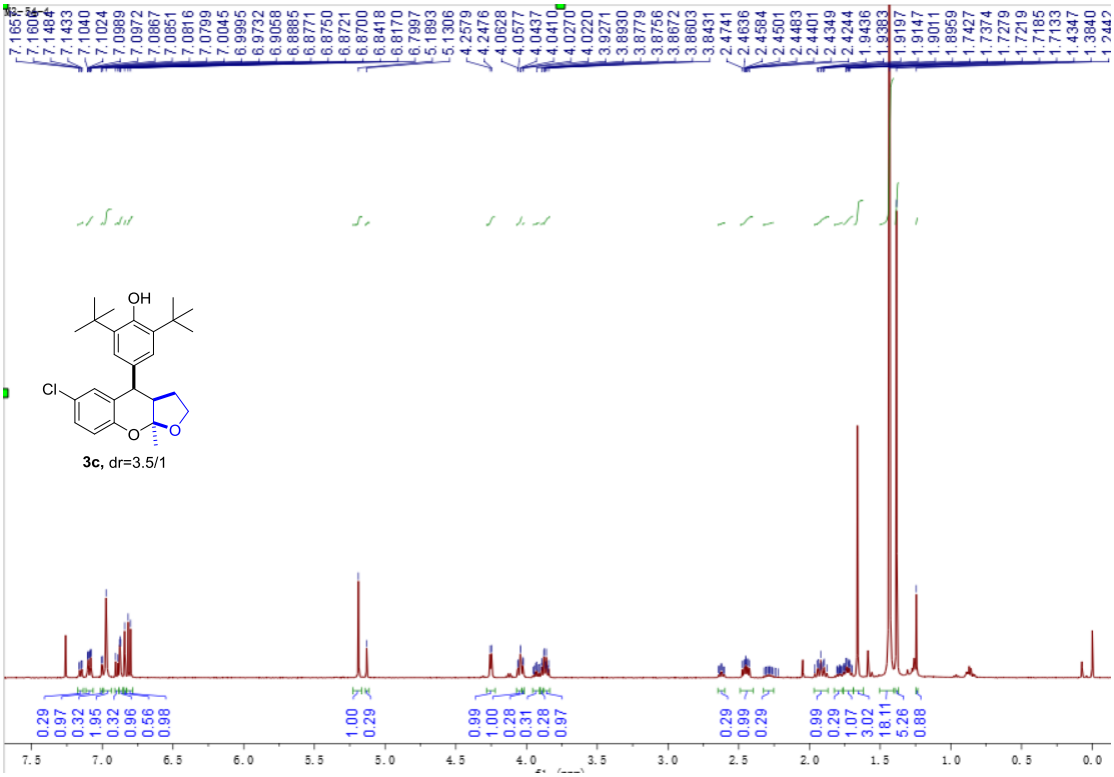


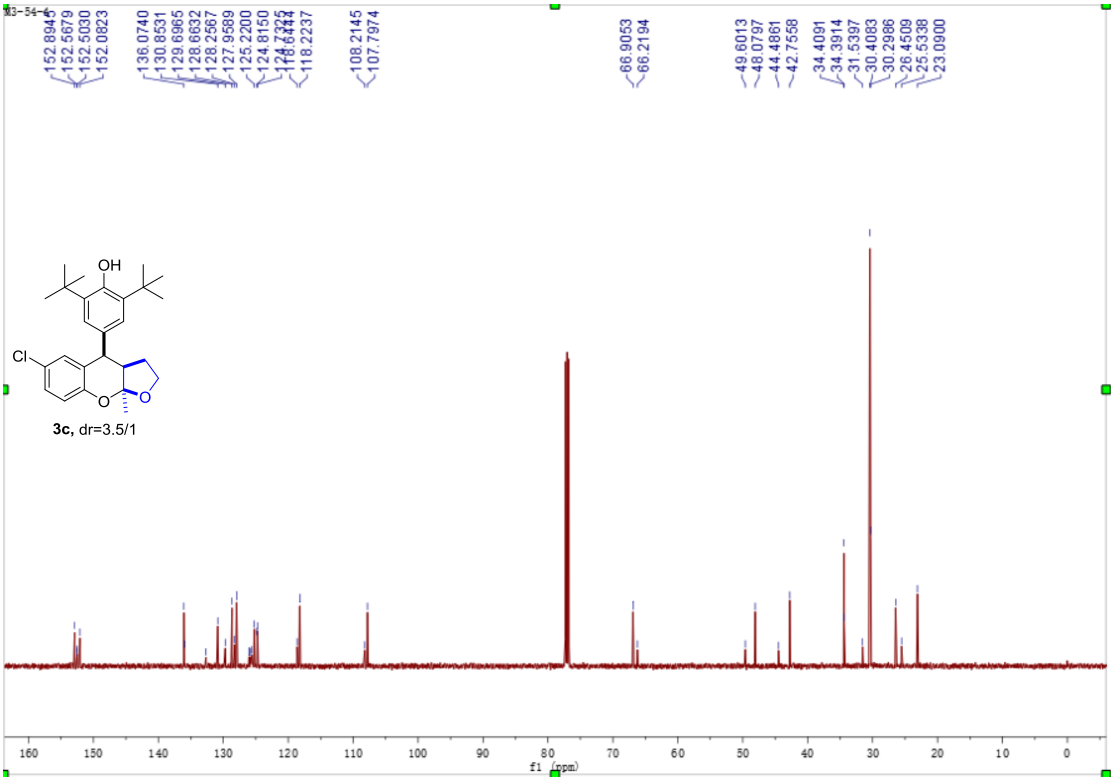


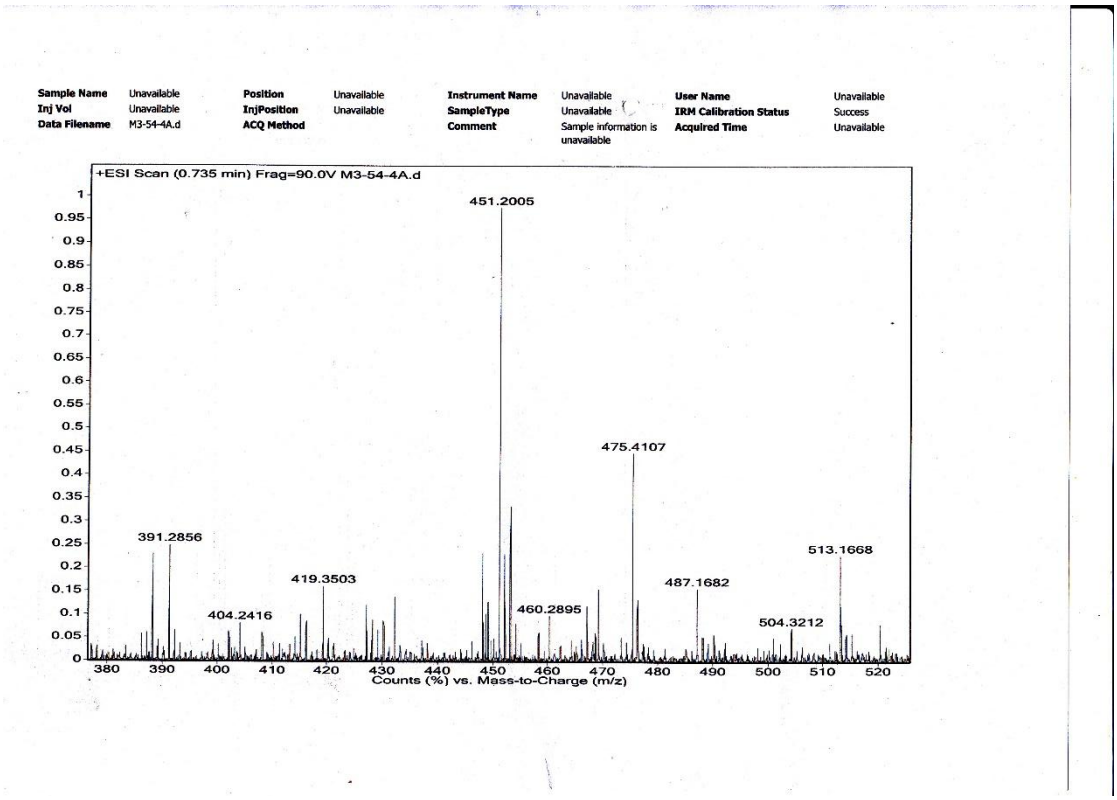
3b

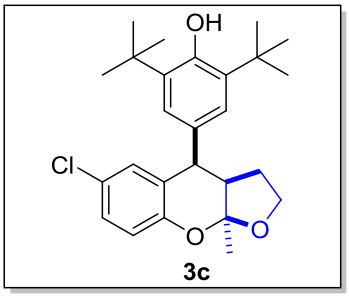
Chemical Formula: $C_{26}H_{33}FO_3$
Exact Mass: 412.2414
Molecular Weight: 412.5454
m/z: 412.2414 (100.0%), 413.2447 (28.1%), 414.2481 (2.7%), 414.2481 (1.1%)
Elemental Analysis: C, 75.70; H, 8.06; F, 4.61; O, 11.63

HRMS (ESI, m/z) calcd for $C_{26}H_{33}FO_3$ [M+Na^+] 435.2306, found 435.2300.


OH
Cl
O
O
3c, dr=3.5/1


OH
Cl
O
O
3c, dr=3.5/1
f1 (ppm)

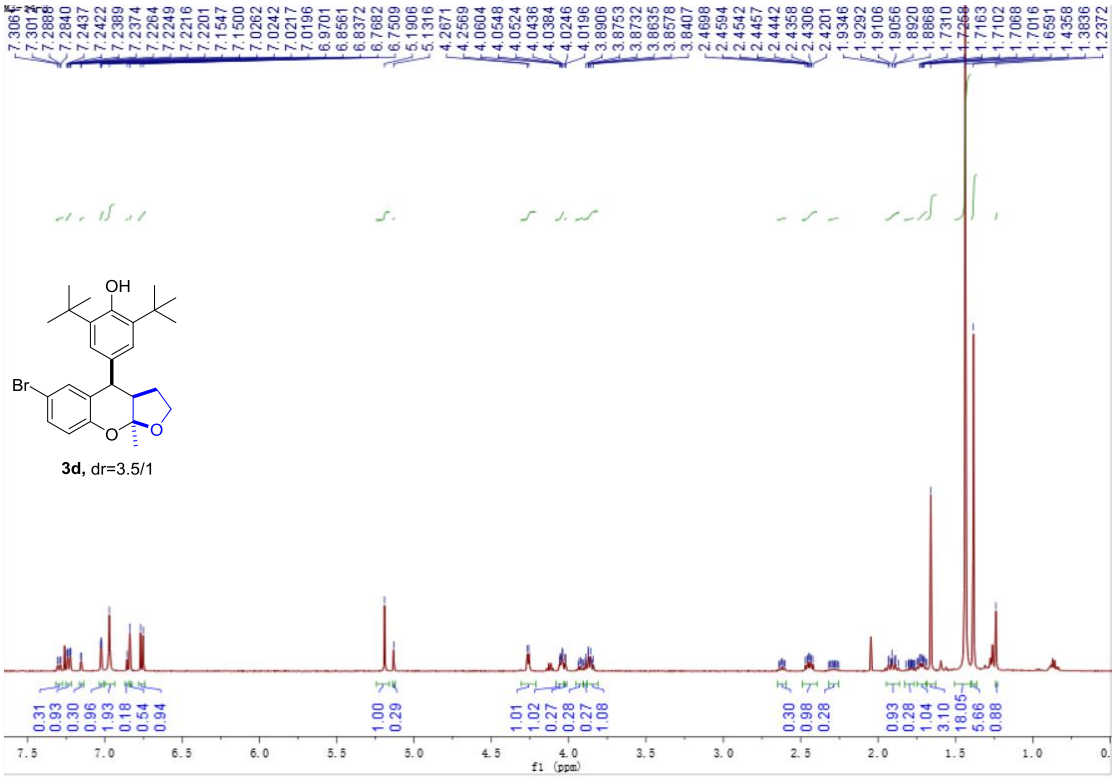




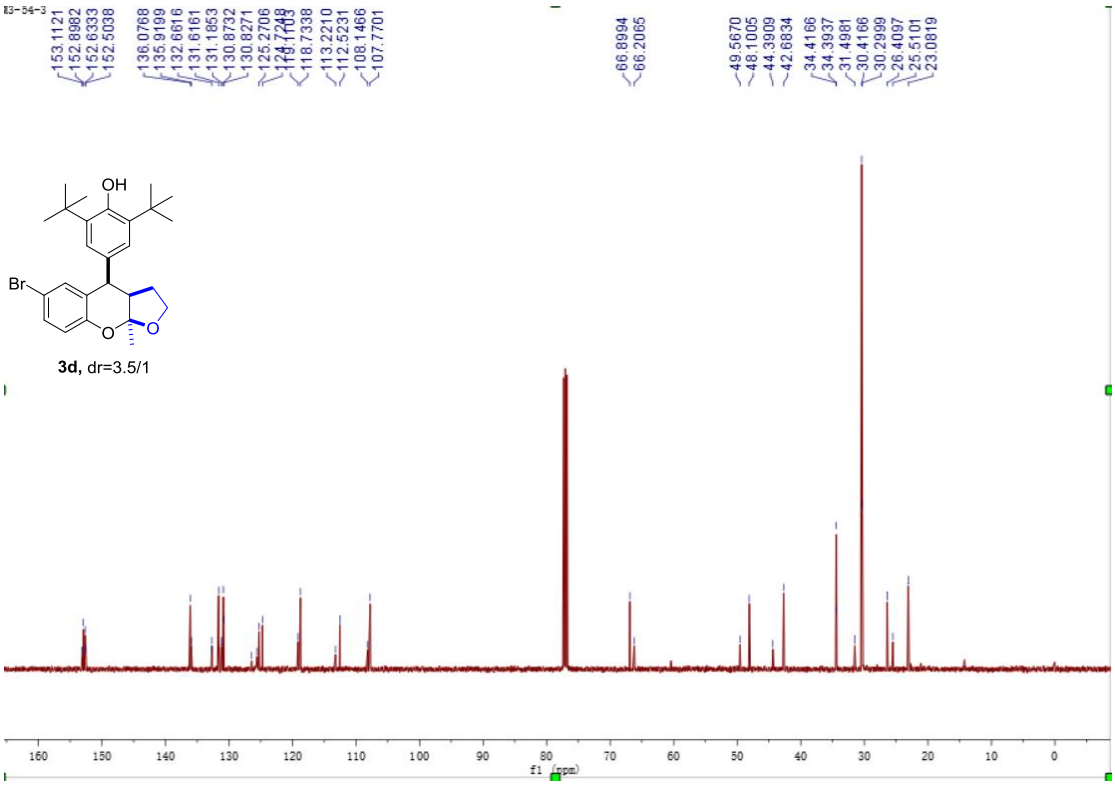
3c

Chemical Formula: $C_{26}H_{33}ClO_3$
Exact Mass: 428.2118
Molecular Weight: 428.9970
m/z: 428.2118 (100.0%), 430.2089 (32.0%), 429.2152 (28.1%), 431.2122 (9.0%), 430.2185 (2.7%), 430.2185 (1.1%)
Elemental Analysis: C, 72.79; H, 7.75; Cl, 8.26; O, 11.19

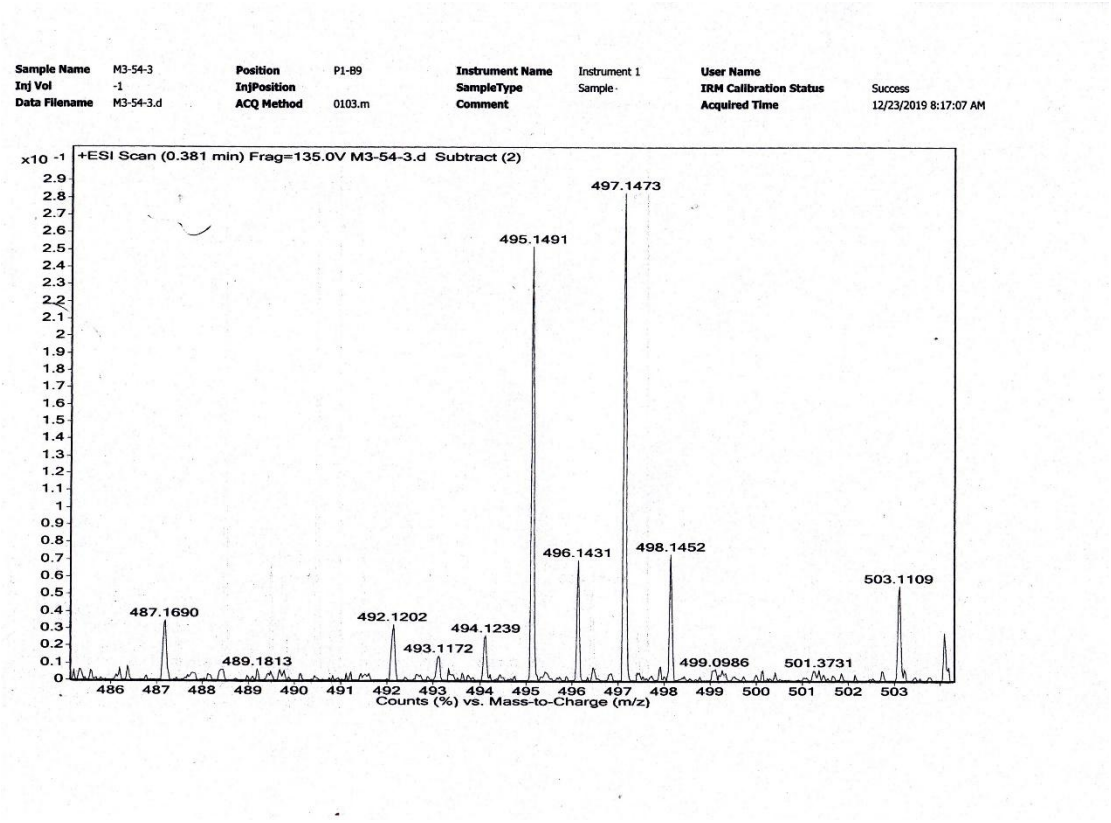
HRMS (ESI, m/z) calcd for $C_{26}H_{33}ClO_3$ [M+Na^+] 451.2010, found 451.2005.

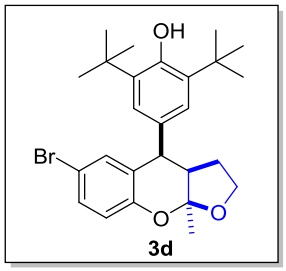


3d, dr=3.5/1



3d, dr=3.5/1

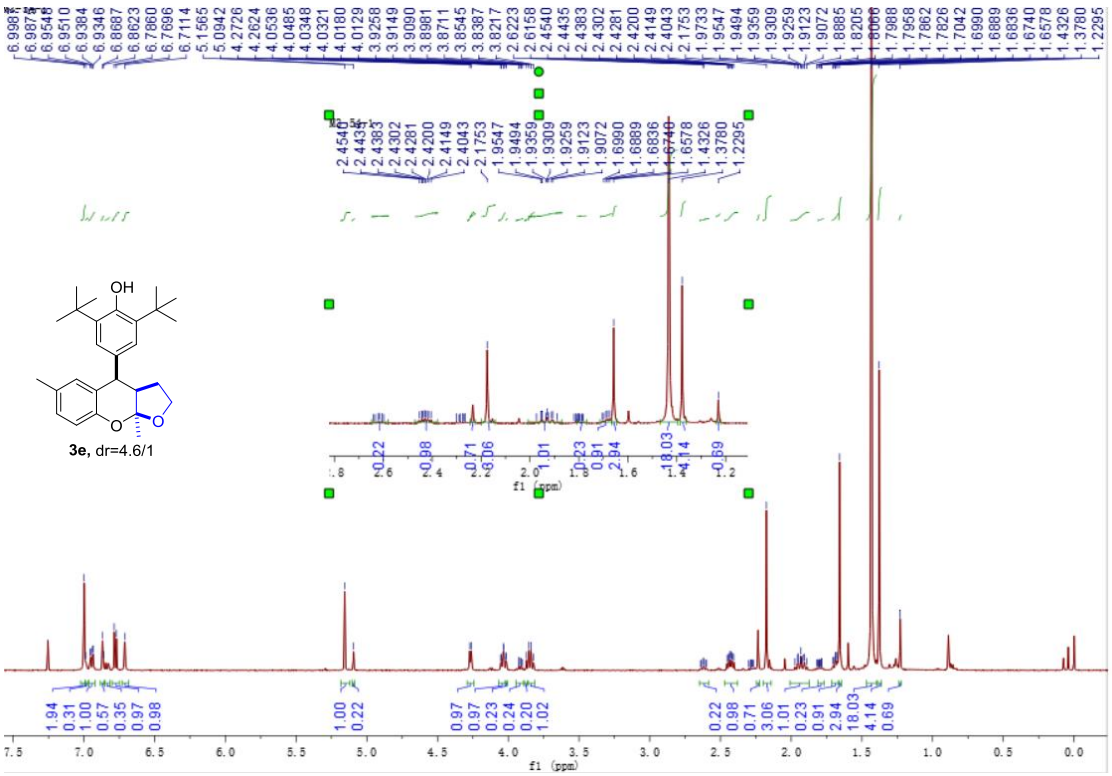


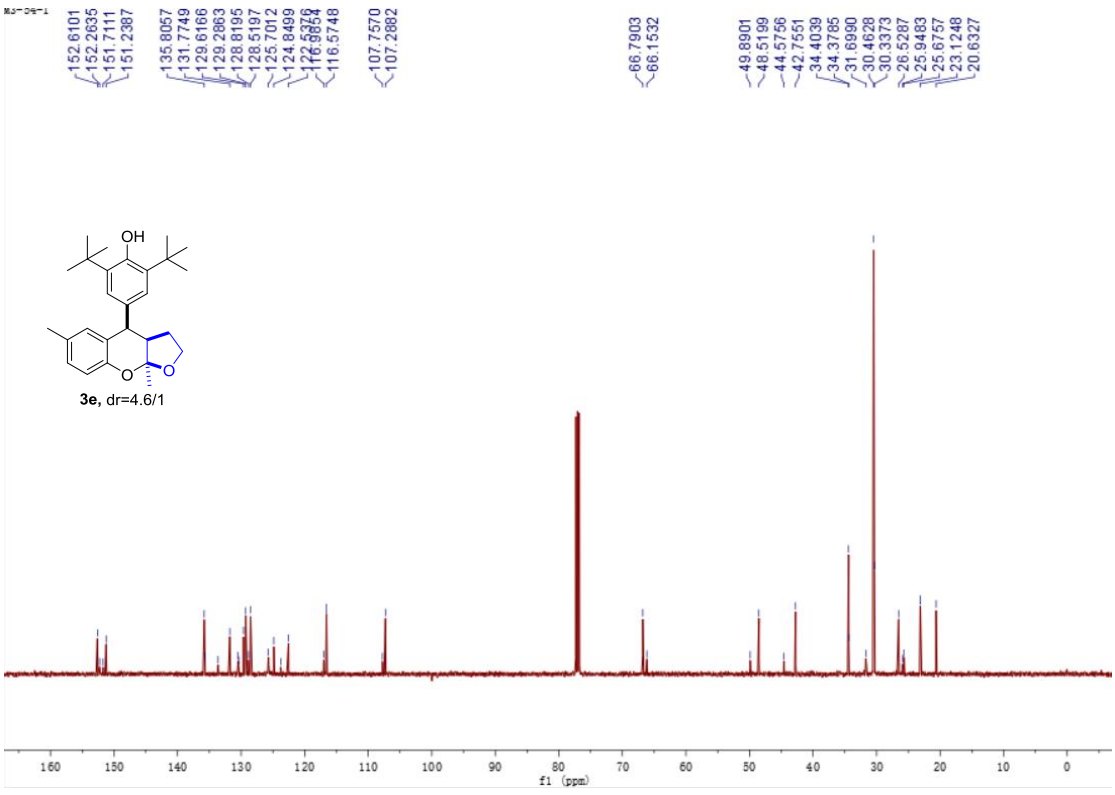


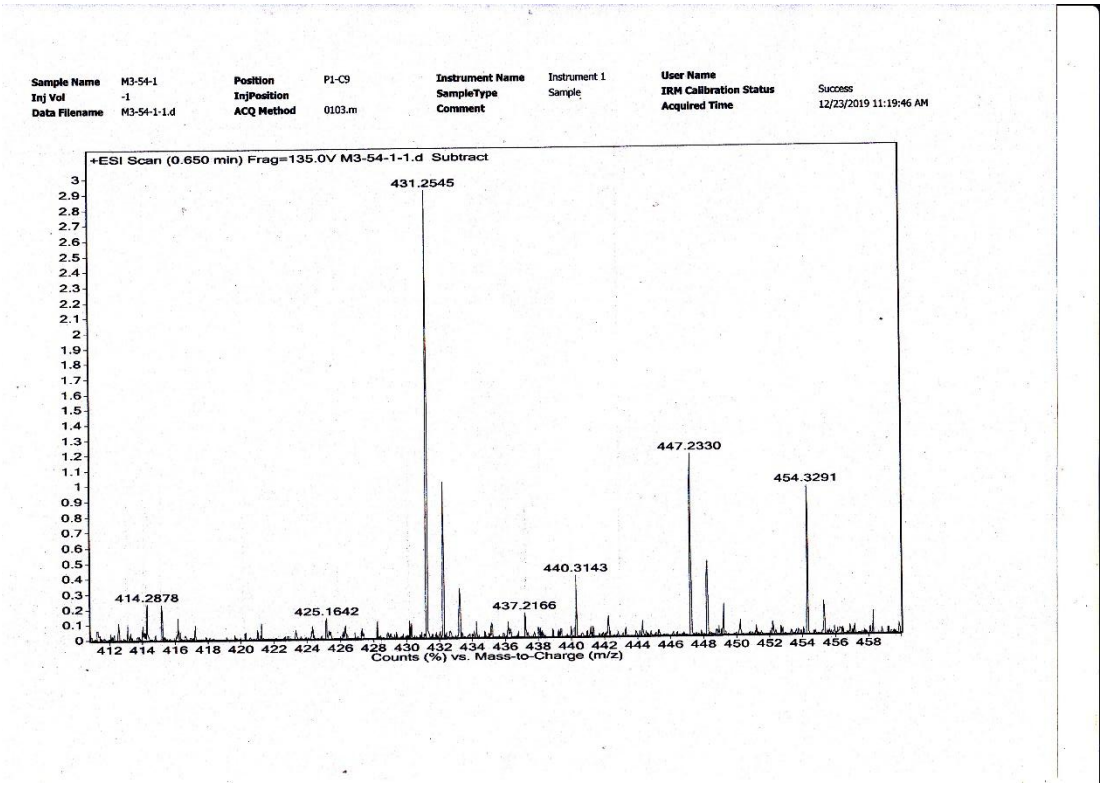
3d

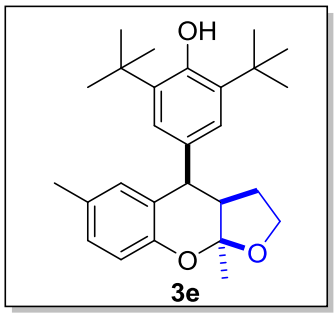
Chemical Formula: $C_{26}H_{33}BrO_3$
Exact Mass: 472.1613
Molecular Weight: 473.4510
m/z: 472.1613 (100.0%), 474.1593 (97.3%), 473.1647 (28.1%), 475.1626 (27.4%), 476.1660 (3.7%), 474.1680 (2.1%), 474.1680 (1.1%)
Elemental Analysis: C, 65.96; H, 7.03; Br, 16.88; O, 10.14

HRMS (ESI, m/z) calcd for $C_{26}H_{33}BrO_3$ [M+Na^+] 495.1505, found 495.1491.


OH
3e, dr=4.6/1
f1 (ppm)


OH
3e, dr=4.6/1
f1 (ppm)

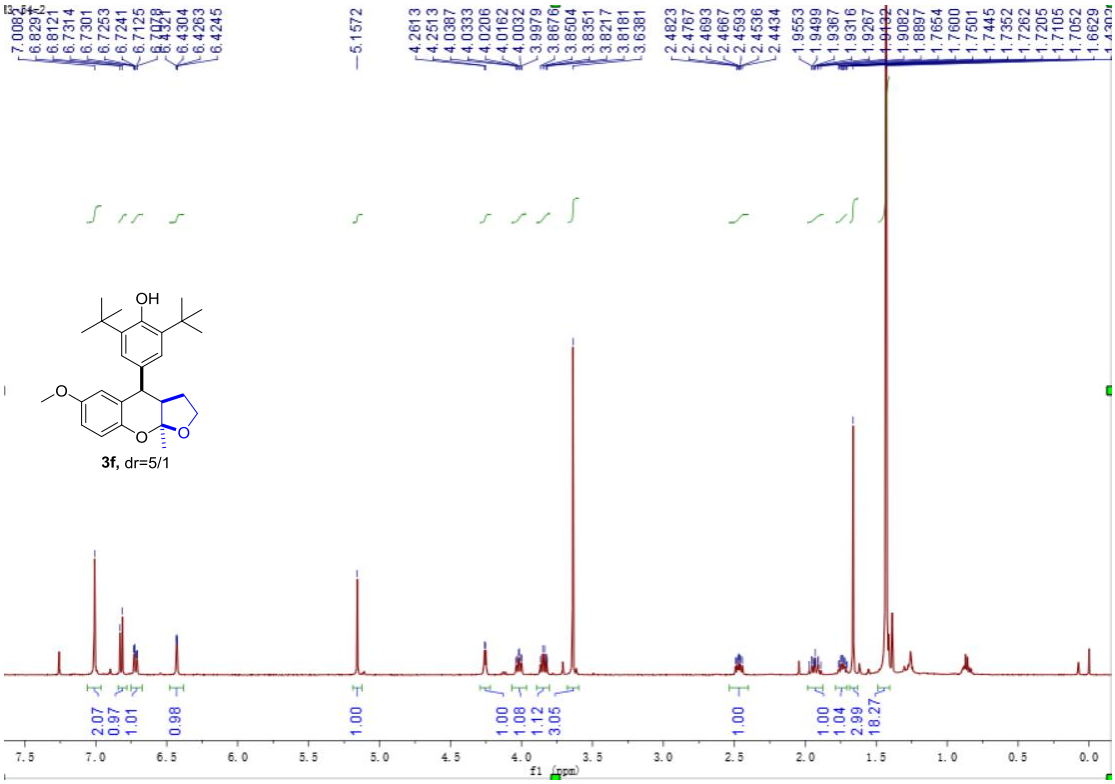




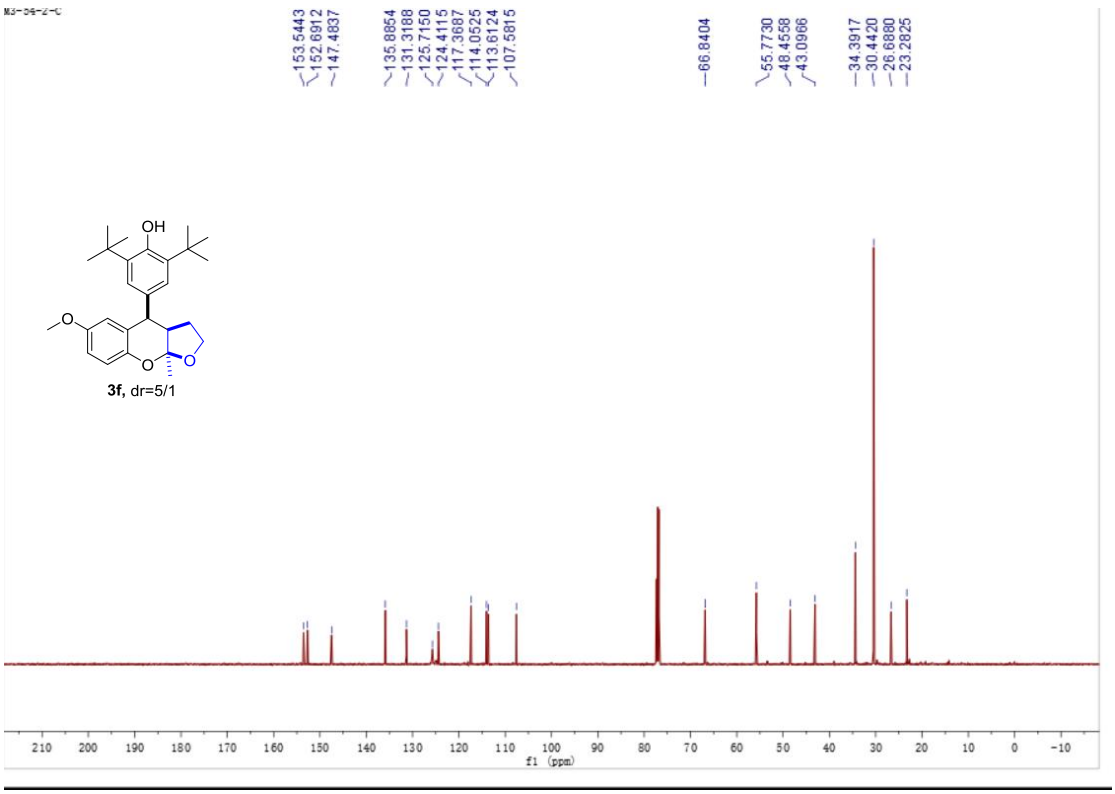
3e

Chemical Formula: $C_{27}H_{36}O_3$
Exact Mass: 408.2664
Molecular Weight: 408.5820
m/z: 408.2664 (100.0%), 409.2698 (29.2%), 410.2732 (2.7%), 410.2732 (1.4%)
Elemental Analysis: C, 79.37; H, 8.88; O, 11.75

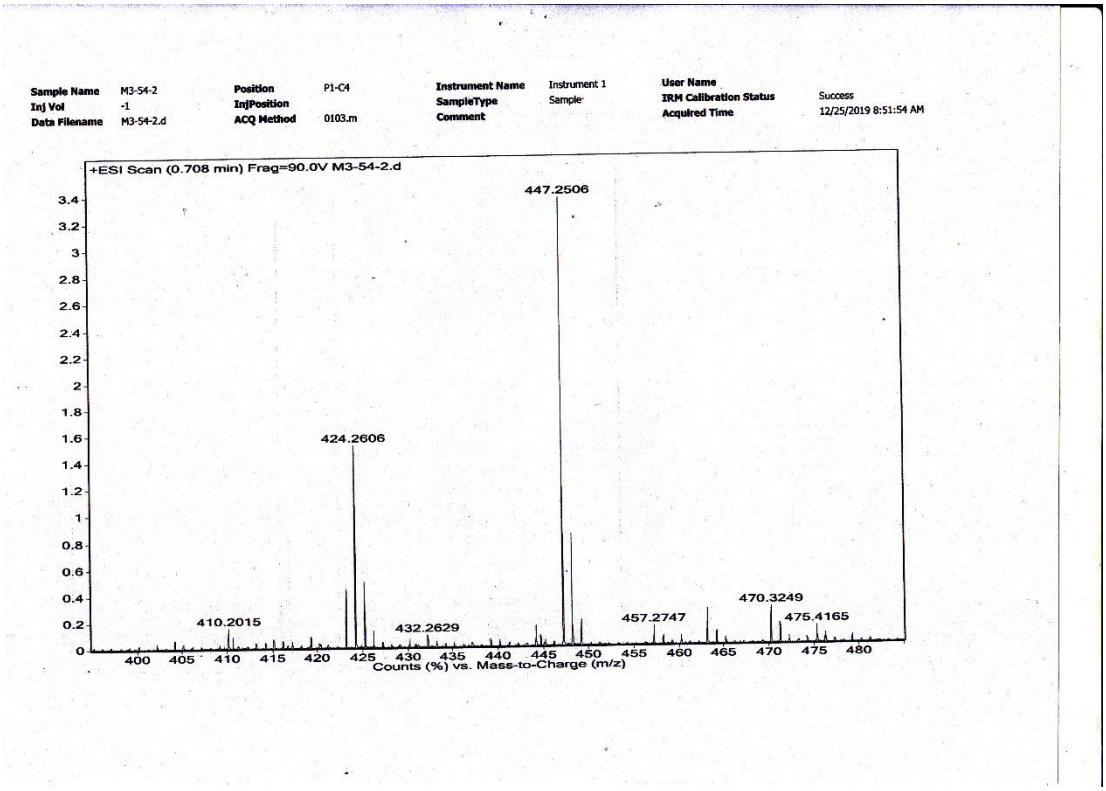
HRMS (ESI, m/z) calcd for $C_{27}H_{36}O_3$ $[M+Na^+]$ 431.2557, found 431.2545.

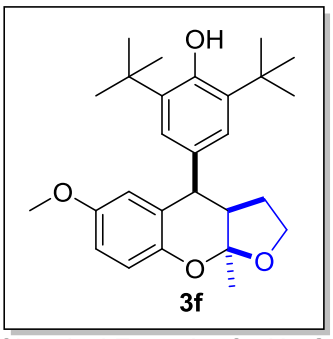


3f, dr=5/1



3f, dr=5/1

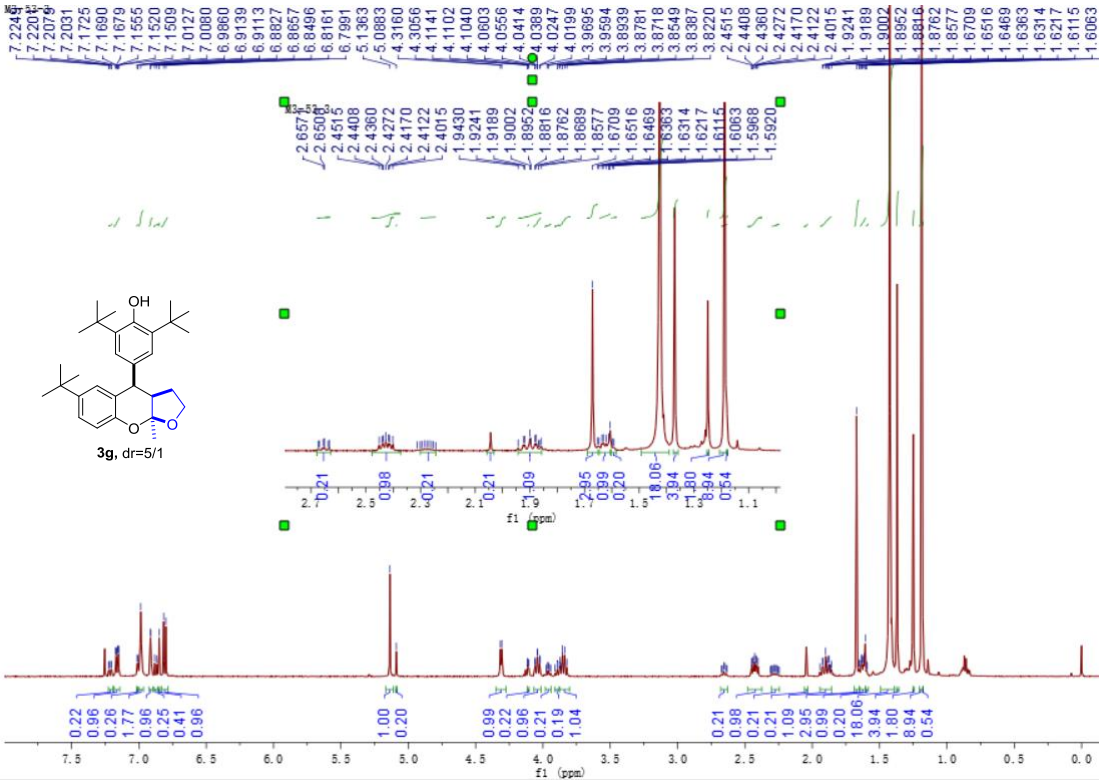


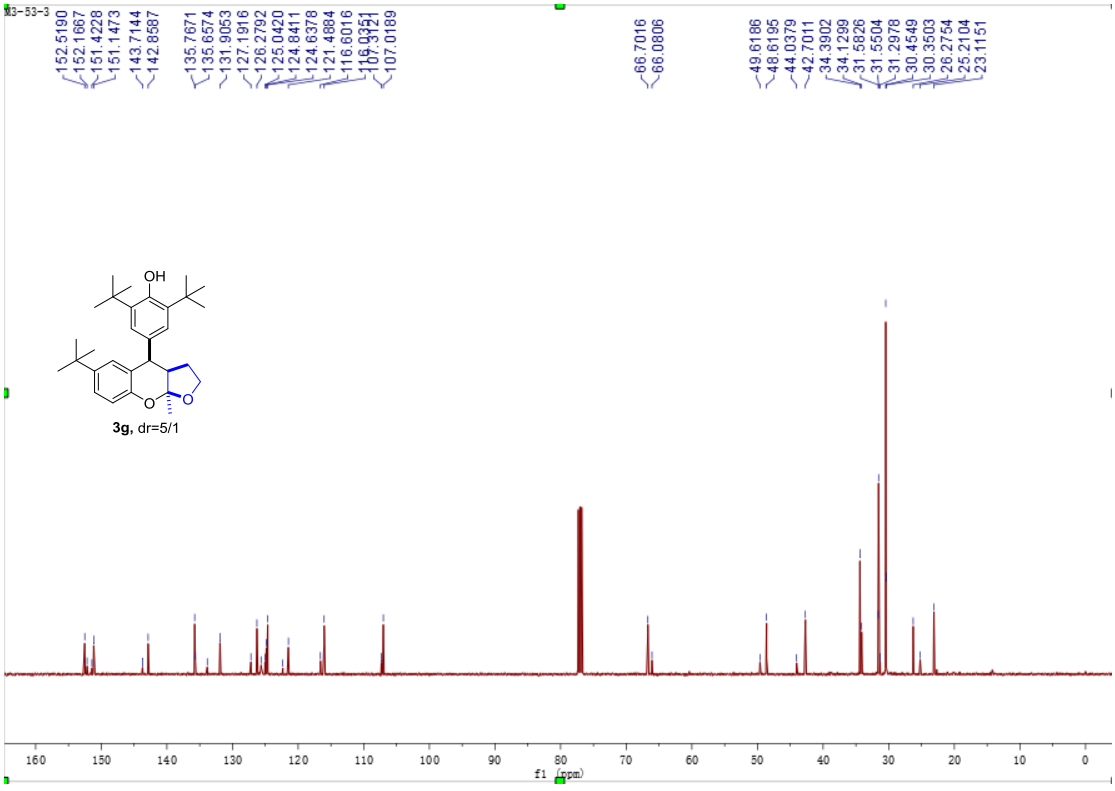


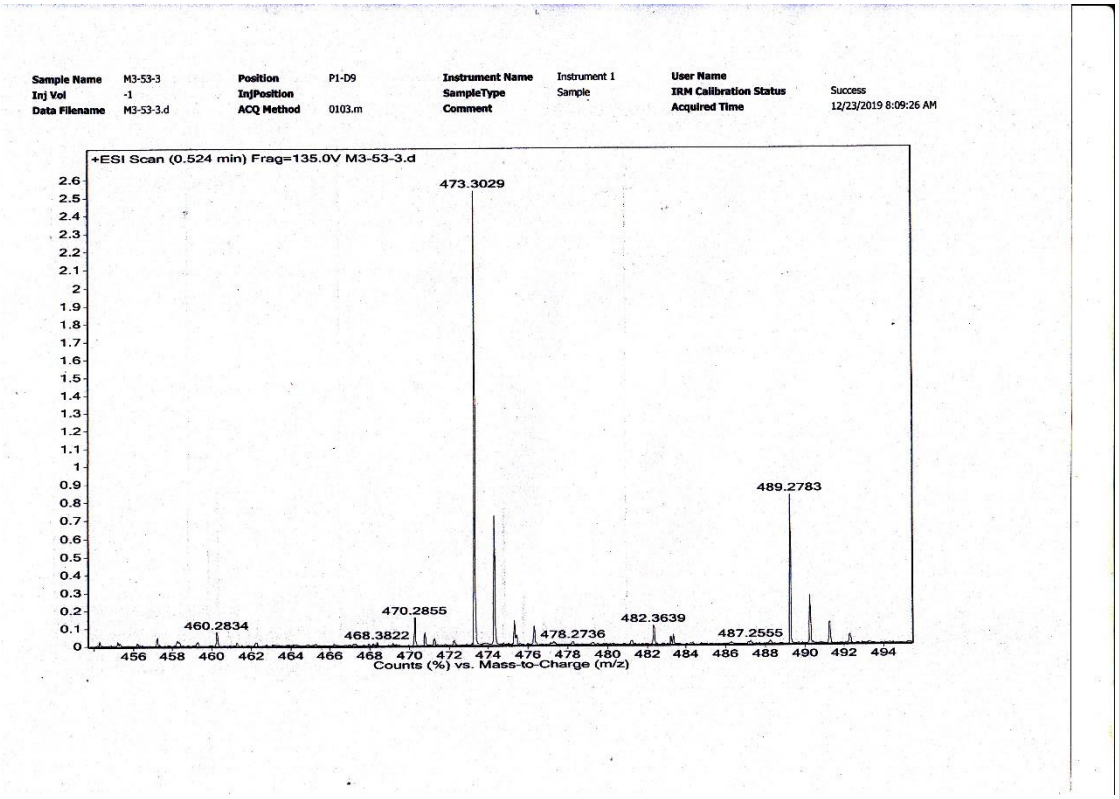
3f

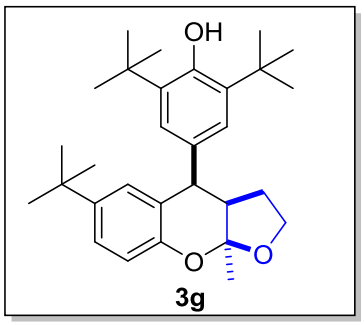
Chemical Formula: $C_{27}H_{36}O_4$
Exact Mass: 424.2614
Molecular Weight: 424.5810
m/z: 424.2614 (100.0%), 425.2647 (29.2%), 426.2681 (2.7%), 426.2681 (1.4%)
Elemental Analysis: C, 76.38; H, 8.55; O, 15.07

HRMS (ESI, m/z) calcd for $C_{27}H_{36}O_4$ [M+Na^+] 447.2506, found 447.2506.


OH
O
O
3g, dr=5/1


OH
O
O
3g, dr=5/1

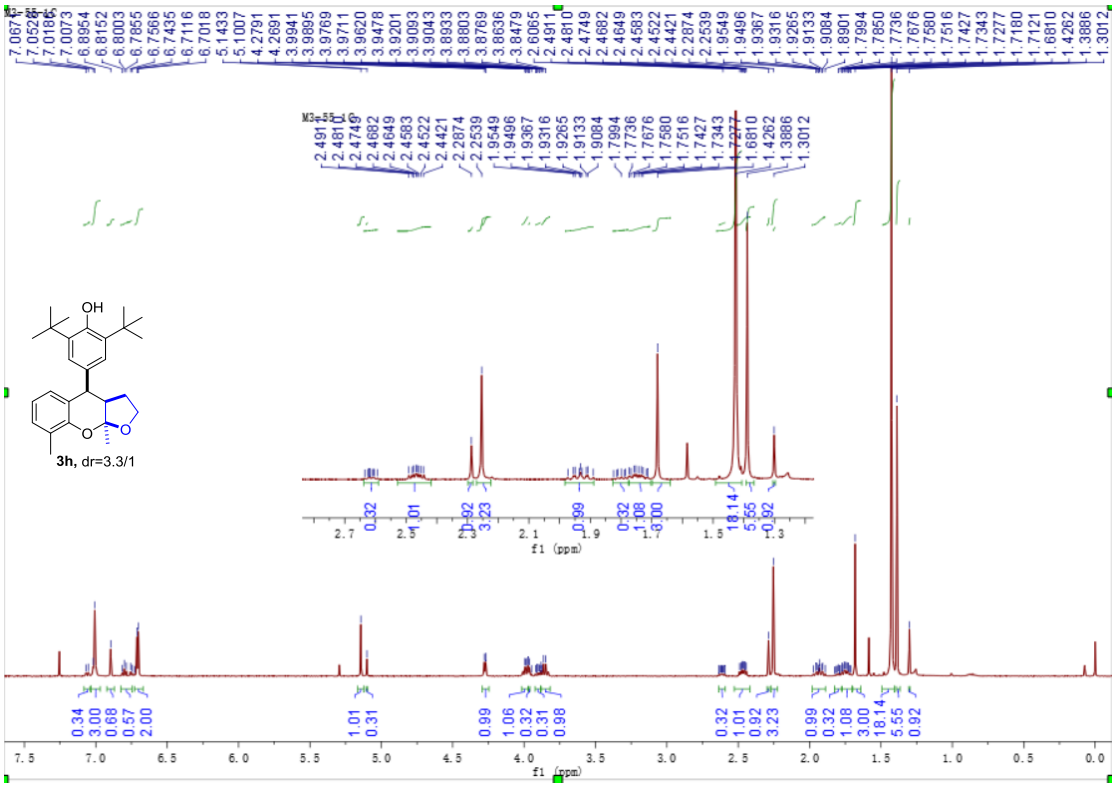


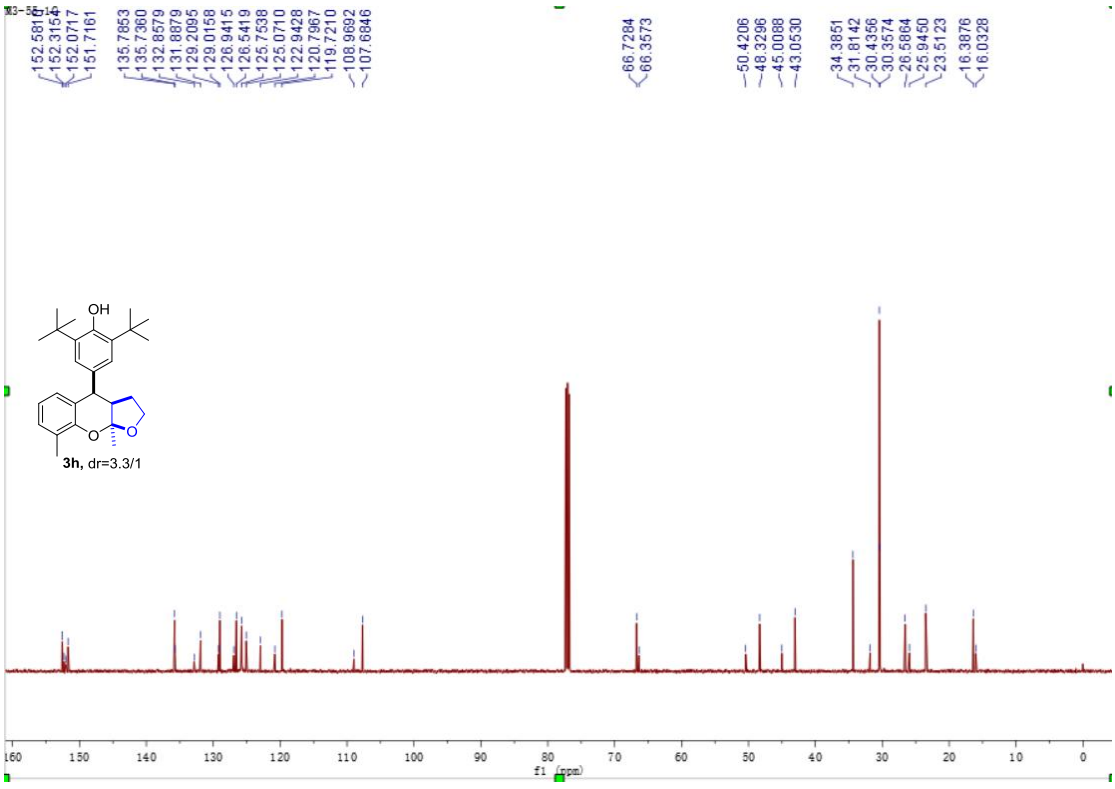


3g

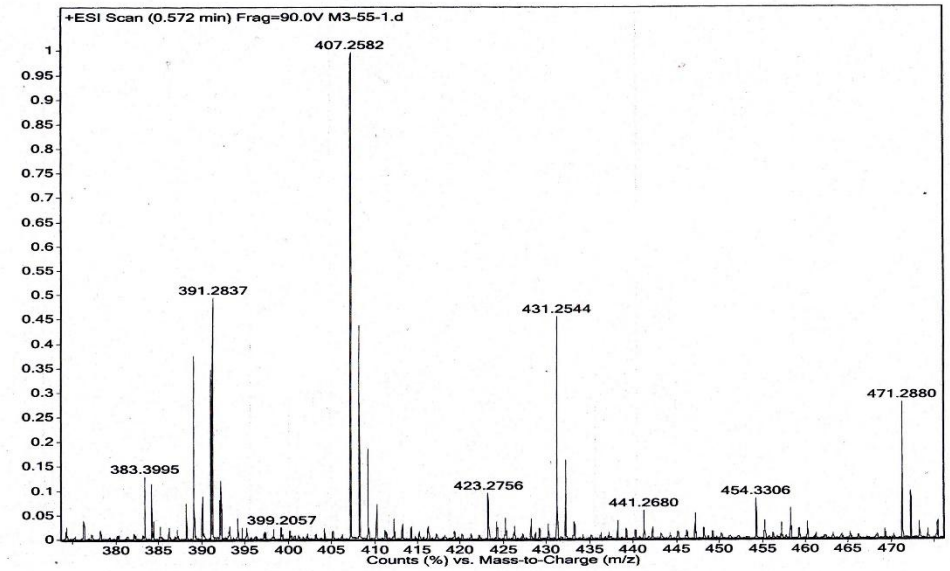
Chemical Formula: $C_{30}H_{42}O_3$
Exact Mass: 450.3134
Molecular Weight: 450.6630
m/z: 450.3134 (100.0%), 451.3168 (32.4%), 452.3201 (2.7%), 452.3201 (2.4%)
Elemental Analysis: C, 79.96; H, 9.39; O, 10.65

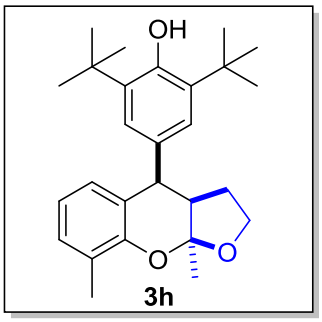
HRMS (ESI, m/z) calcd for $C_{30}H_{42}O_3$ [M+Na^+] 473.3026, found 473.3029.


OH
3h, dr=3.3/1
f1 (ppm)


OH
3h, dr=3.3/1
f1 (ppm)

Sample Name	M3-55-1	**Position**	P1-F4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	M3-55-1.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	12/25/2019 8:43:47 AM

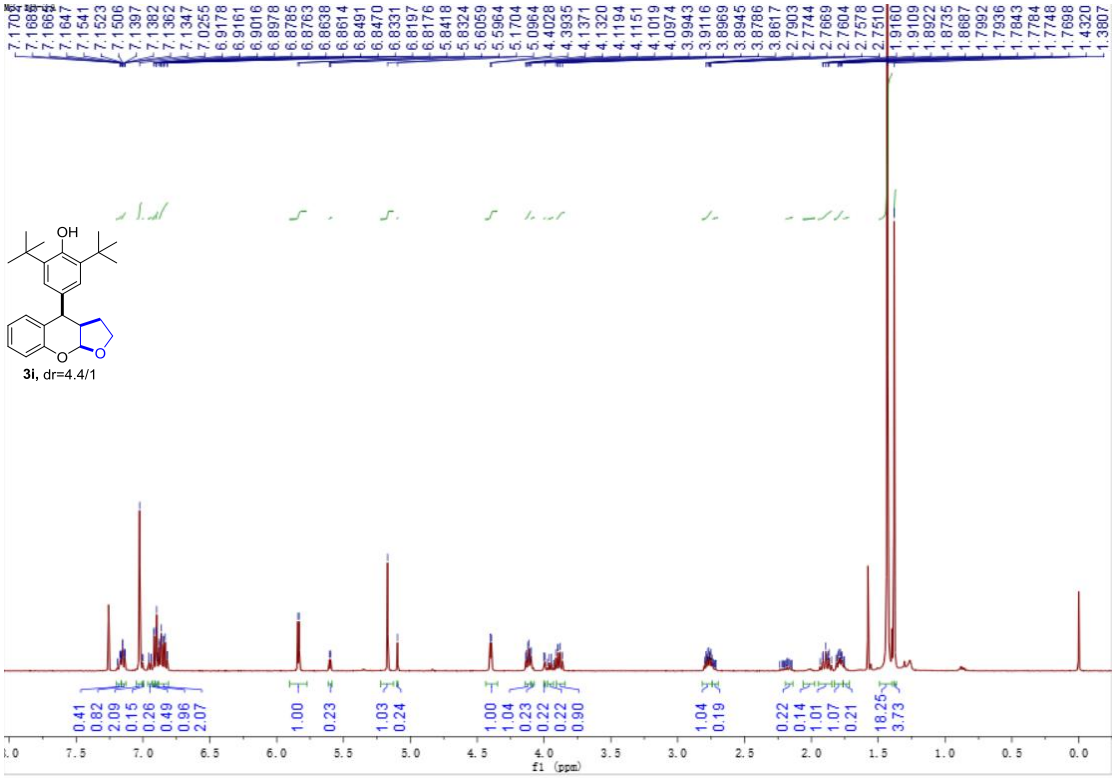


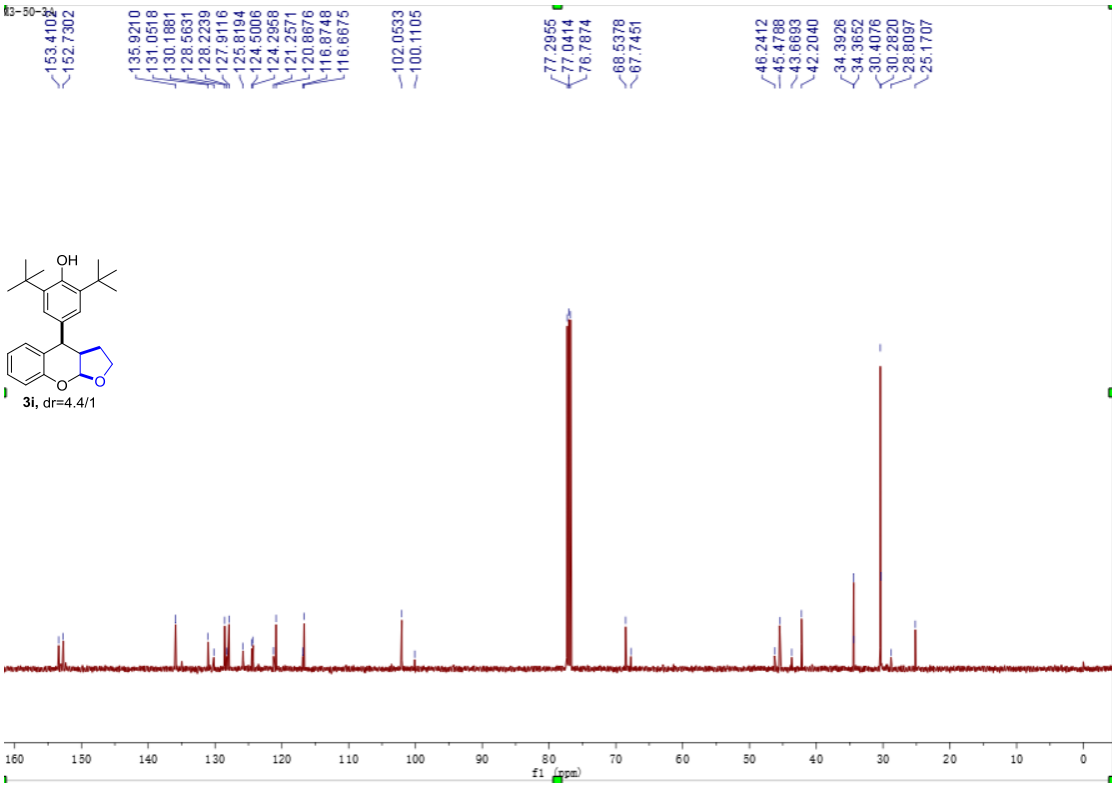


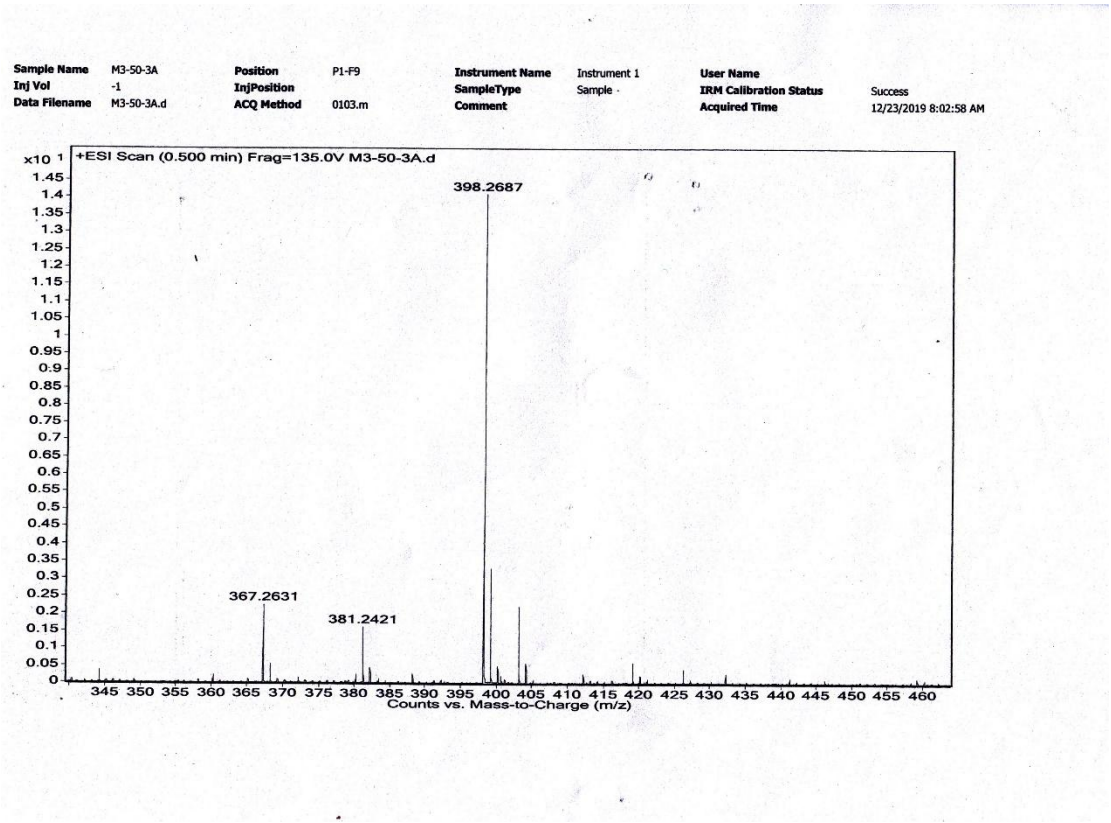
3h

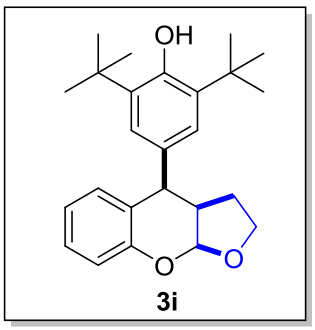
Chemical Formula: $C_{27}H_{36}O_3$
Exact Mass: 408.2664
Molecular Weight: 408.5820
m/z: 408.2664 (100.0%), 409.2698 (29.2%), 410.2732 (2.7%), 410.2732 (1.4%)
Elemental Analysis: C, 79.37; H, 8.88; O, 11.75

HRMS (ESI, m/z) calcd for $C_{27}H_{36}O_3$ [M+Na^+] 431.2557, found 431.2544.


OH
O
O
3i, dr=4.4/1
f1 (ppm)


OH
O
O
3i, dr=4.4/1
f1 (ppm)

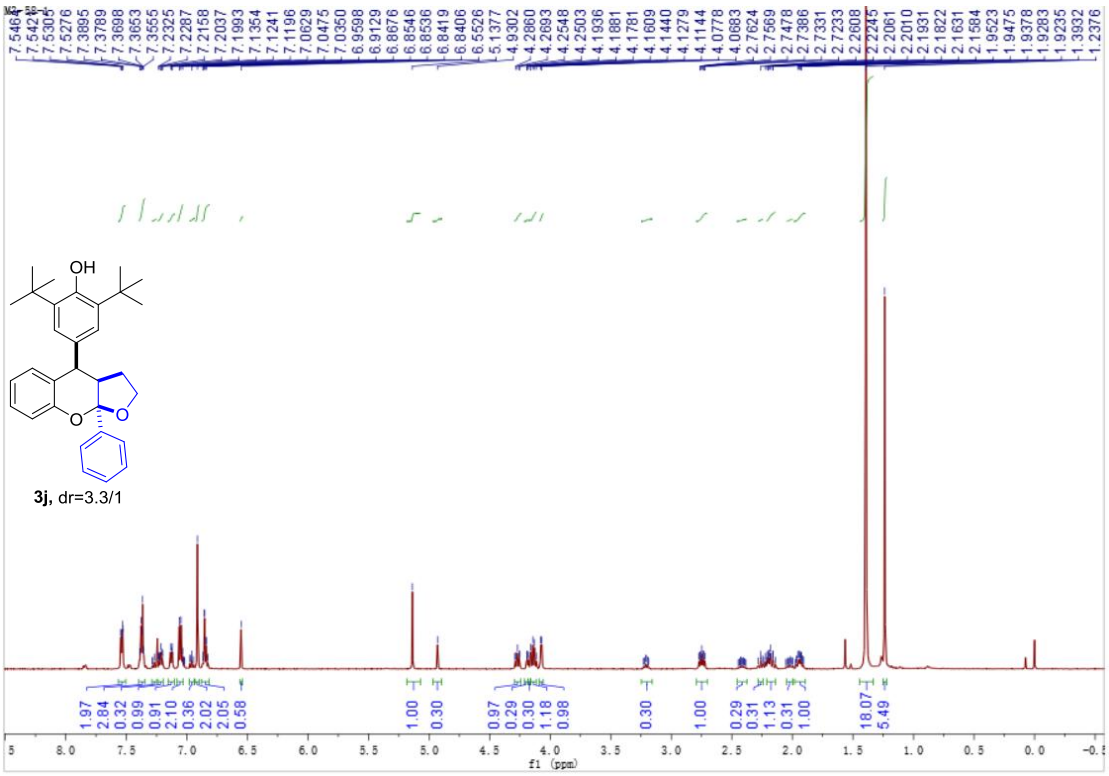


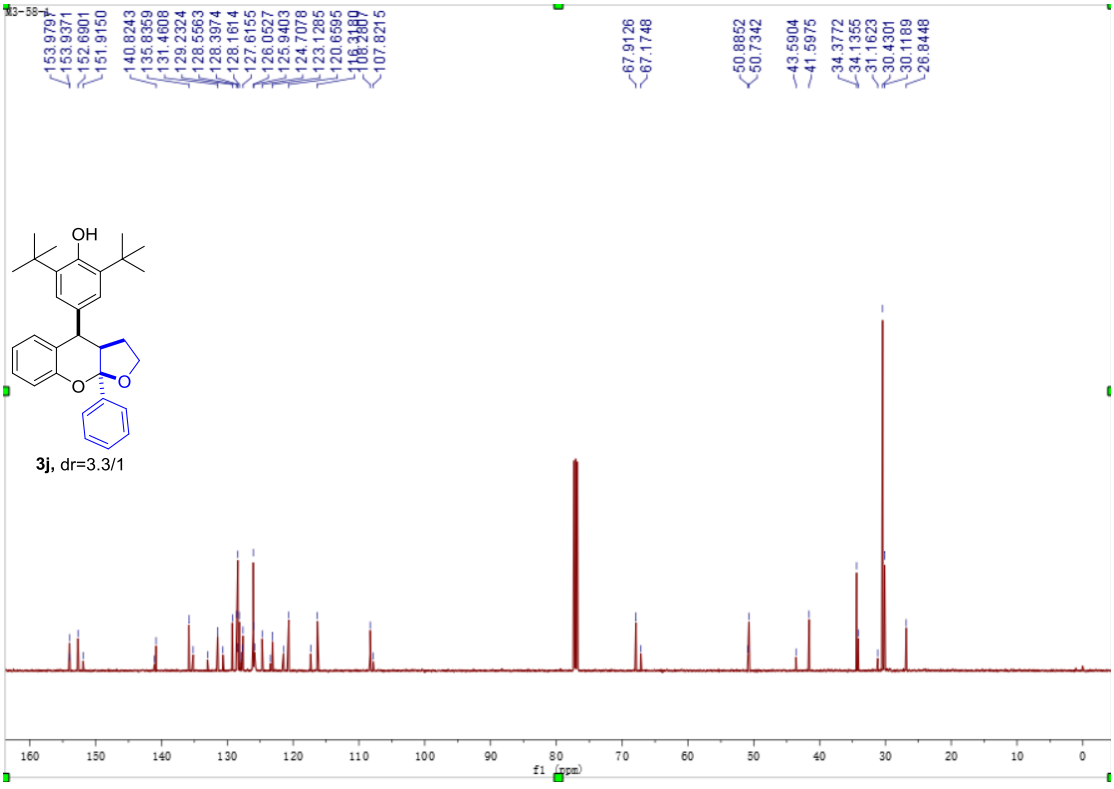


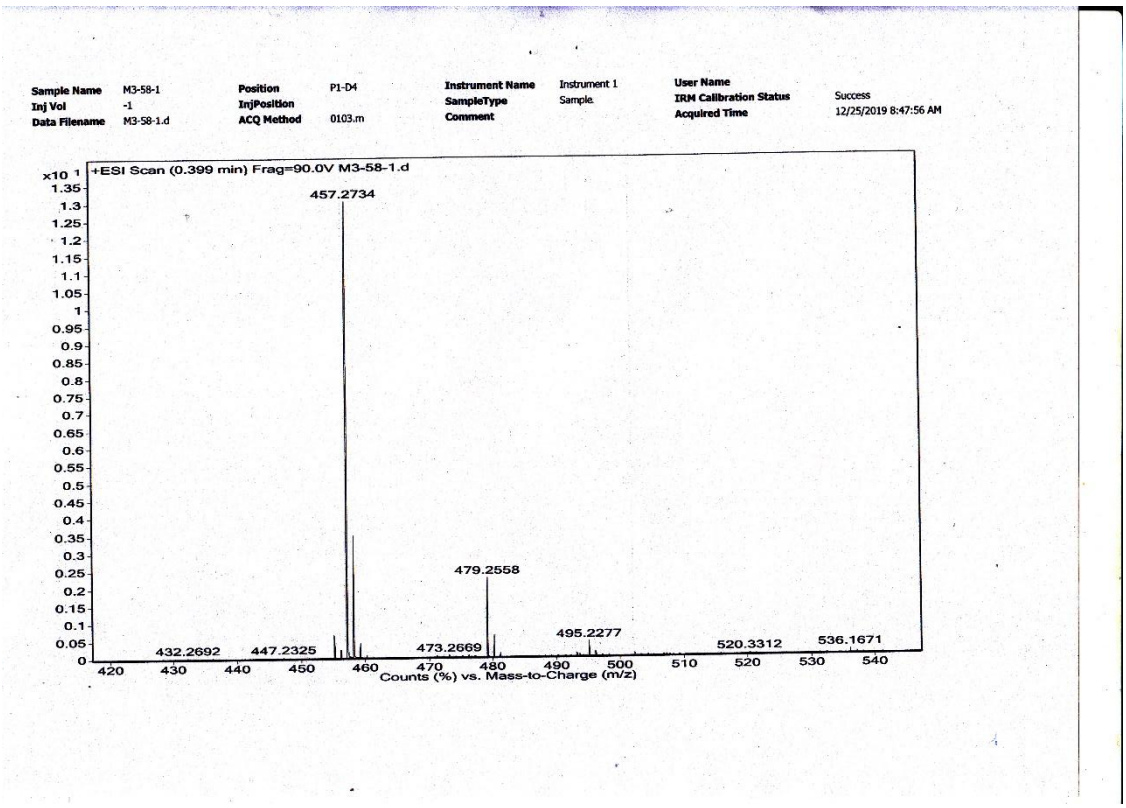
3i

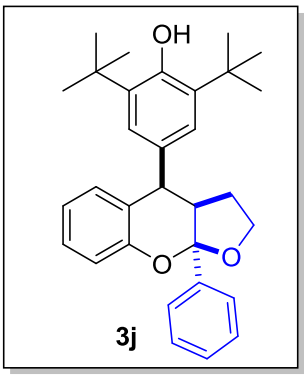
Chemical Formula: $C_{25}H_{32}O_3$
Exact Mass: 380.2351
Molecular Weight: 380.5280
m/z: 380.2351 (100.0%), 381.2385 (27.0%), 382.2419 (2.7%)
Elemental Analysis: C, 78.91; H, 8.48; O, 12.61

HRMS (ESI, m/z) calcd for $C_{25}H_{32}O_3$ $[M+H^+]$ 381.2424, found 381.2421.


OH
O
O
3j, dr=3.3/1
f1 (ppm)

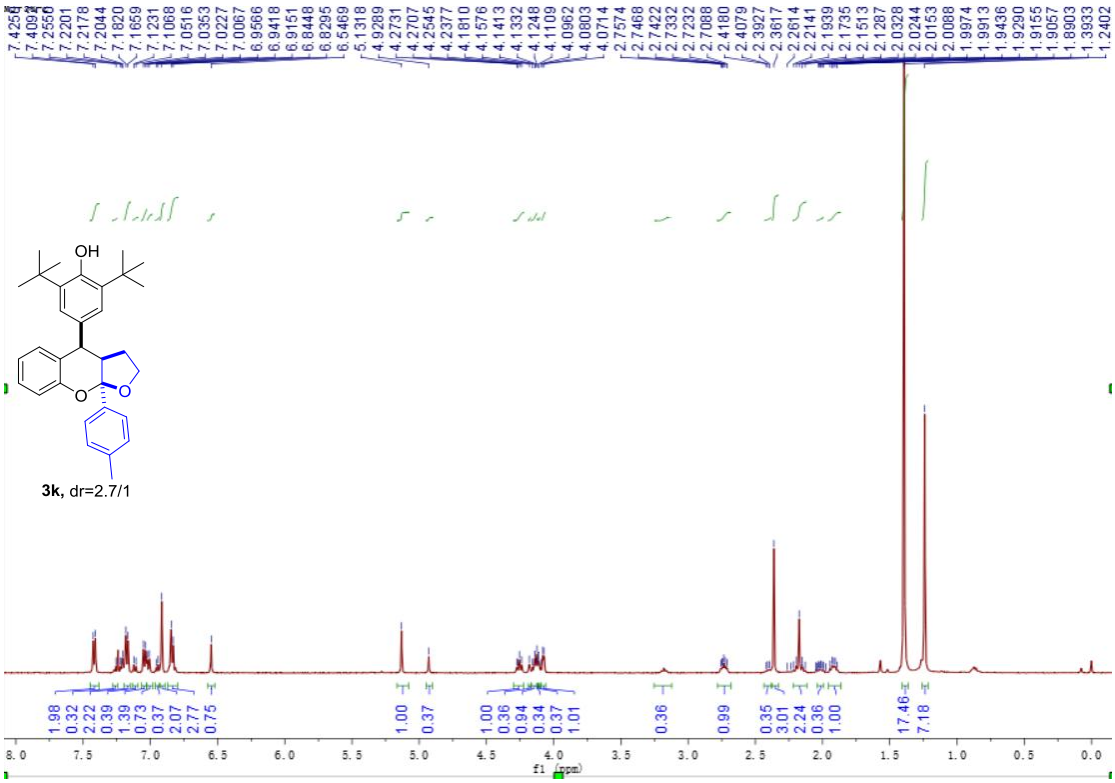

OH
O
O
3j, dr=3.3/1
f1 (ppm)

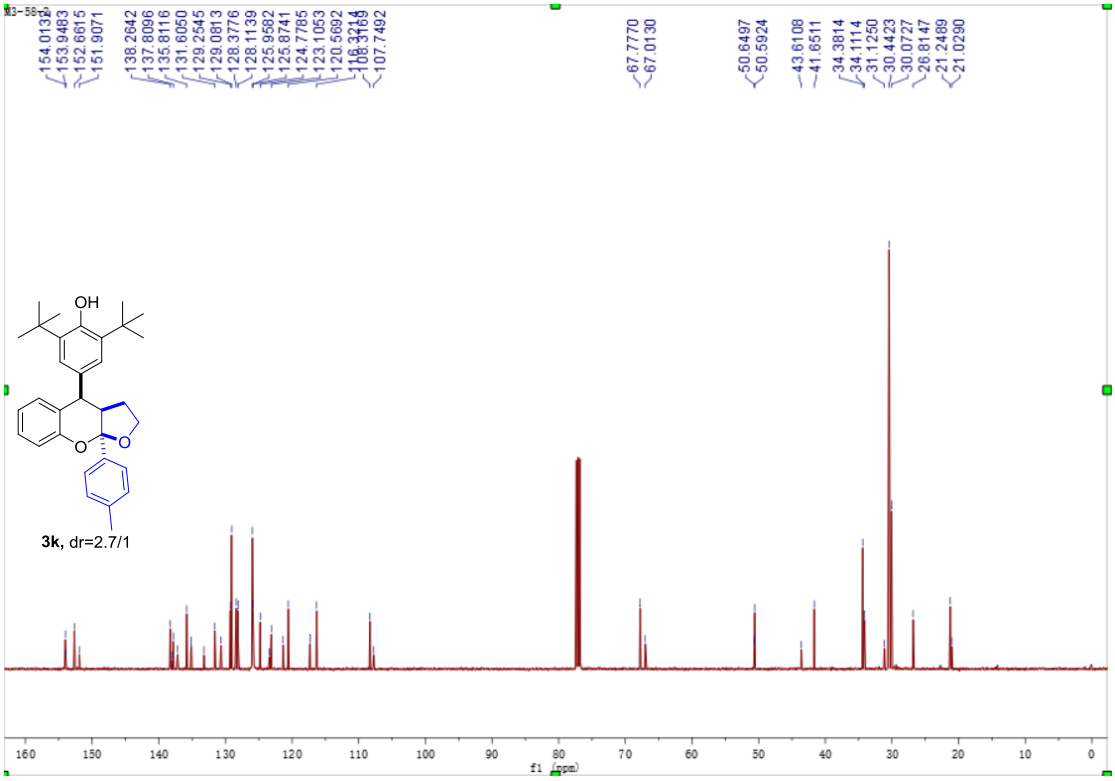


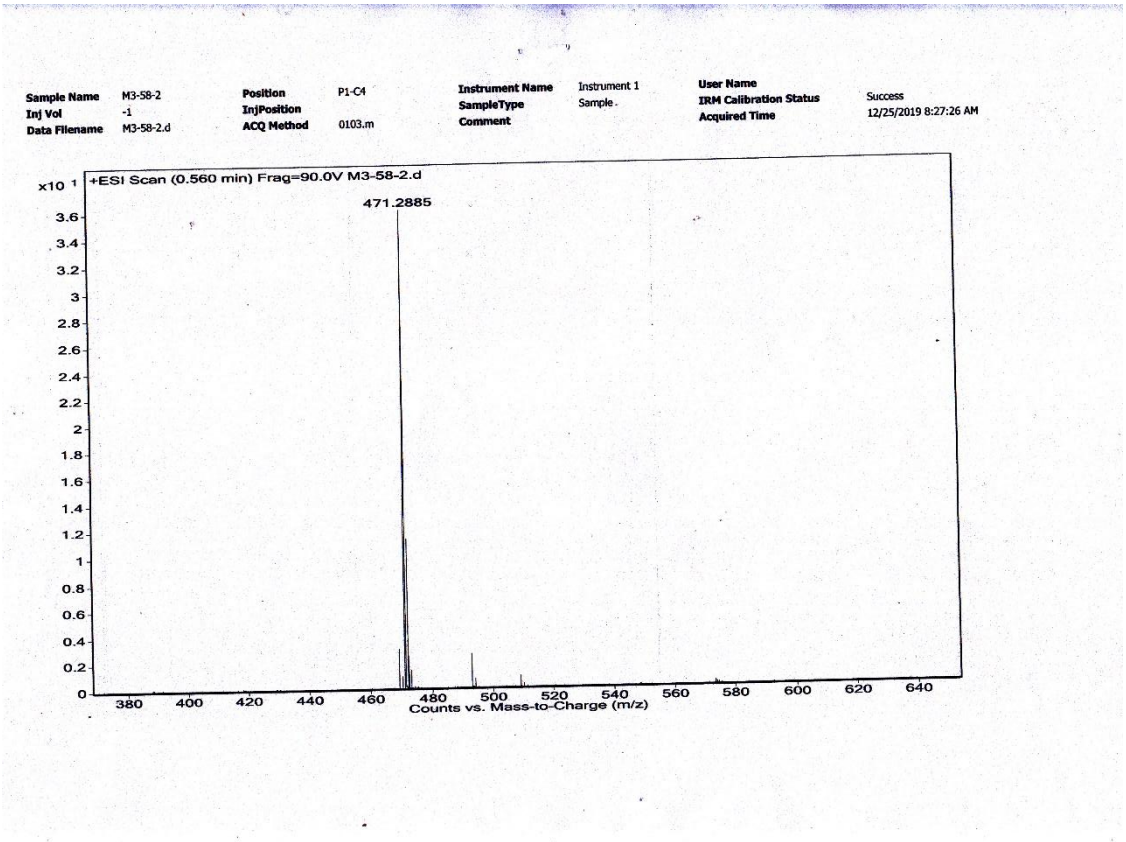


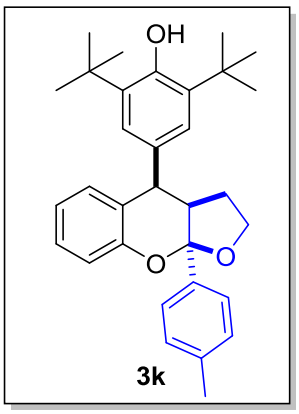
Chemical Formula: $C_{31}H_{36}O_3$
Exact Mass: 456.2664
Molecular Weight: 456.6260
m/z: 456.2664 (100.0%), 457.2698 (33.5%), 458.2732 (2.7%), 458.2732 (2.7%)
Elemental Analysis: C, 81.54; H, 7.95; O, 10.51

HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_3$ $[M+H^+]$ 457.2737, found 457.2734.


OH
3k, dr=2.7/1


OH
3k, dr=2.7/1

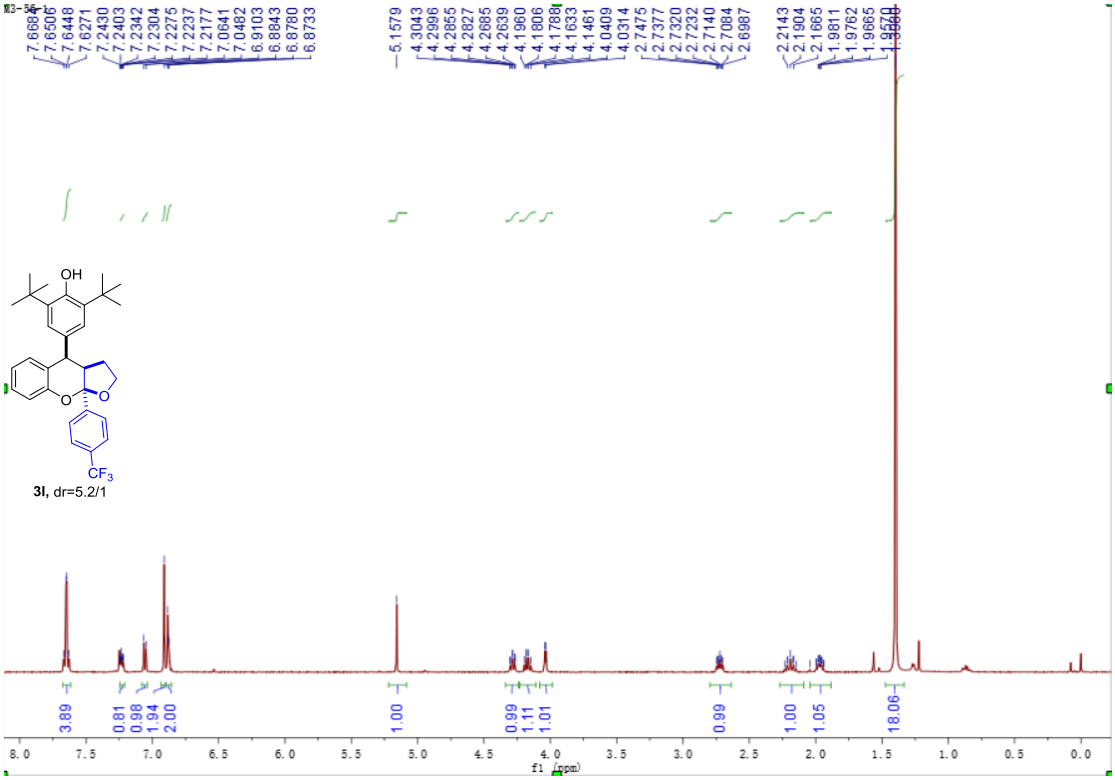


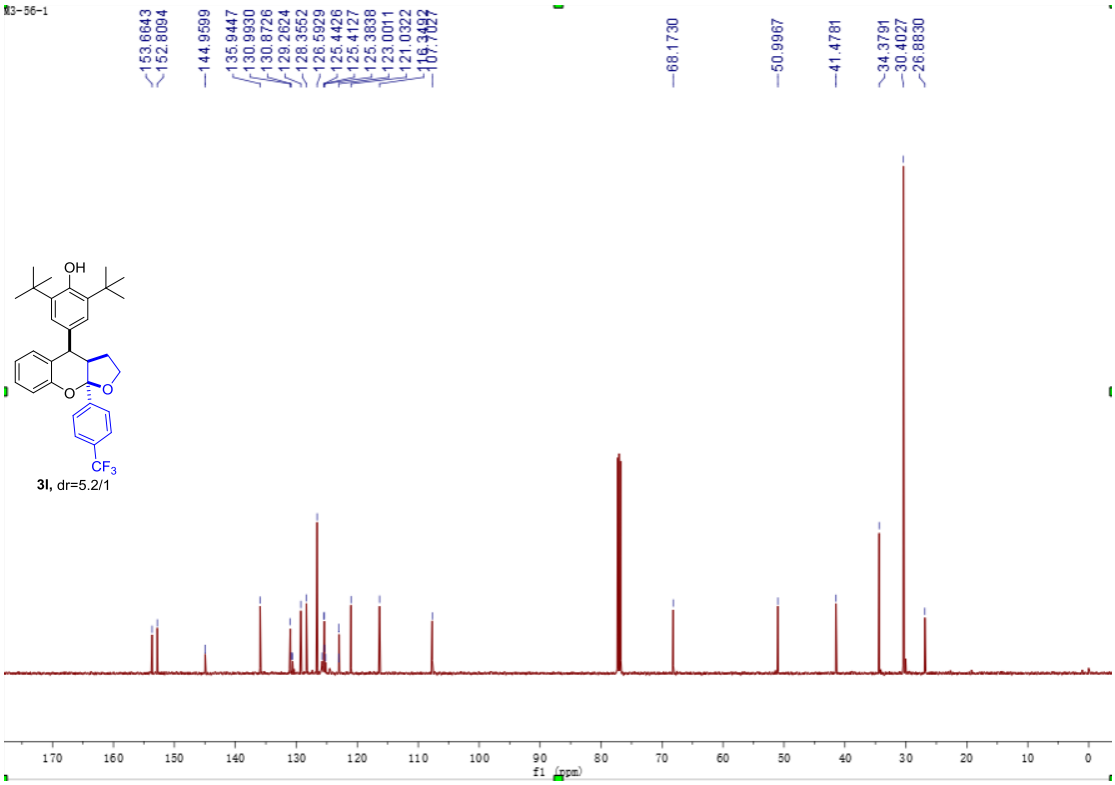


3k

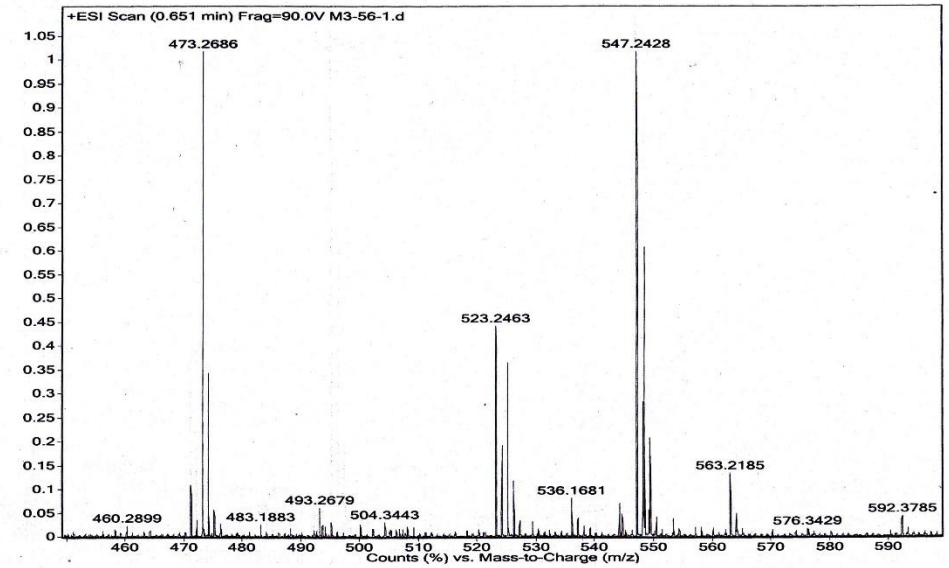
Chemical Formula: $C_{32}H_{38}O_3$
Exact Mass: 470.2821
Molecular Weight: 470.6530
m/z: 470.2821 (100.0%), 471.2854 (34.6%), 472.2888 (3.1%), 472.2888 (2.7%)
Elemental Analysis: C, 81.66; H, 8.14; O, 10.20

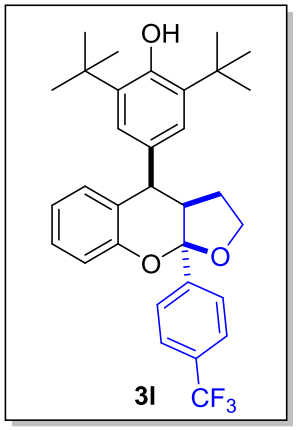
HRMS (ESI, m/z) calcd for $C_{32}H_{38}O_3$ $[M+H]^+$ 471.2894, found 471.2885.


OH
CF3
3l, dr=5.2/1
f1 (ppm)


OH
CF3
3l, dr=5.2/1
f1 (ppm)

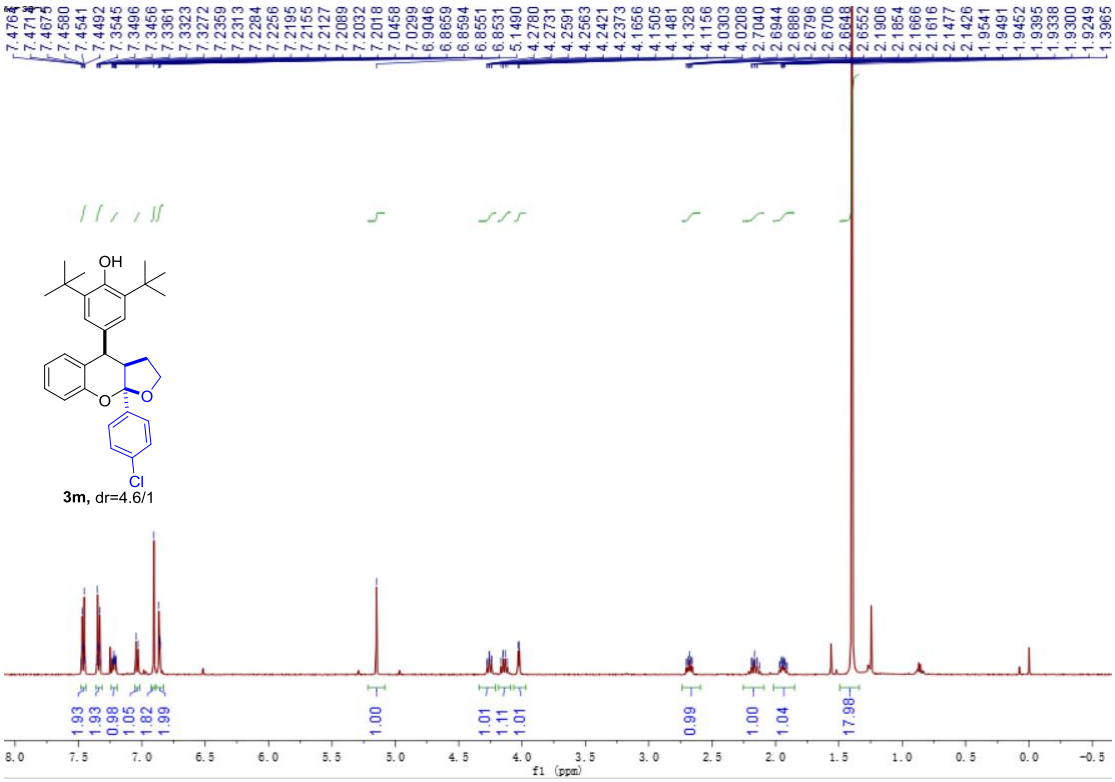
Sample Name	M3-56-1	**Position**	P1-E4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	M3-56-1.d	**ACQ Method**	0103.m	**Comment**		**Acquired Time**	12/25/2019 8:45:47 AM

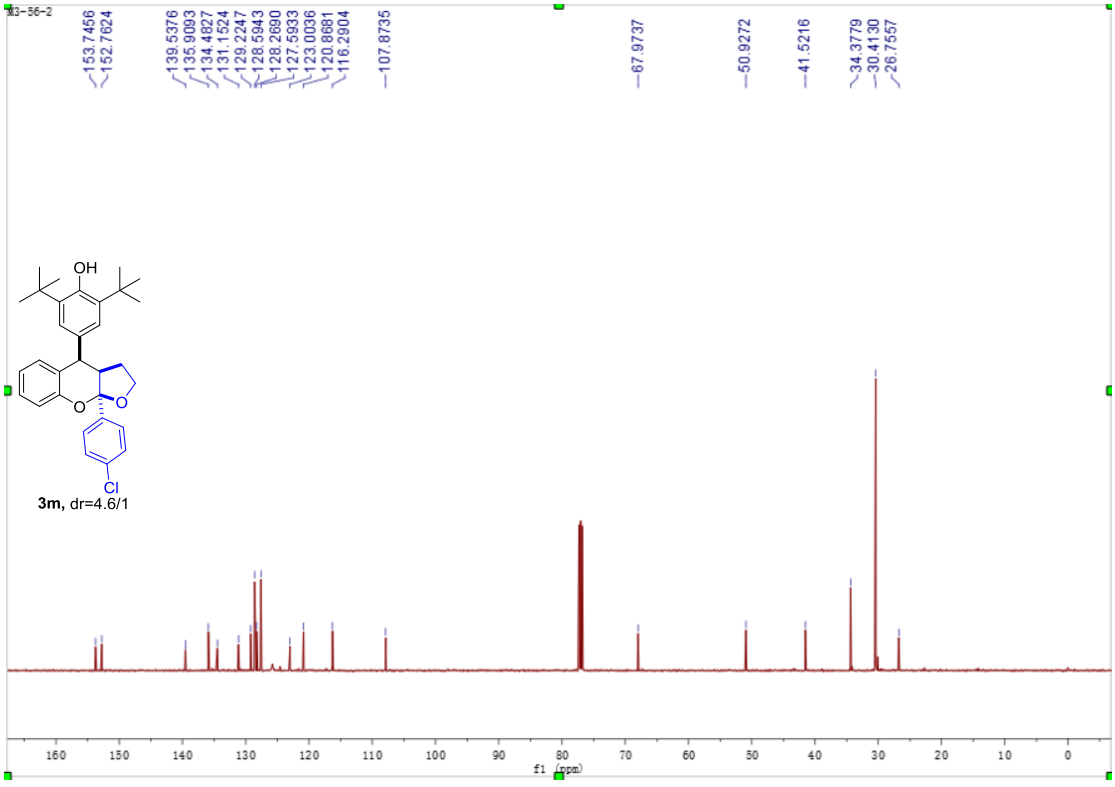


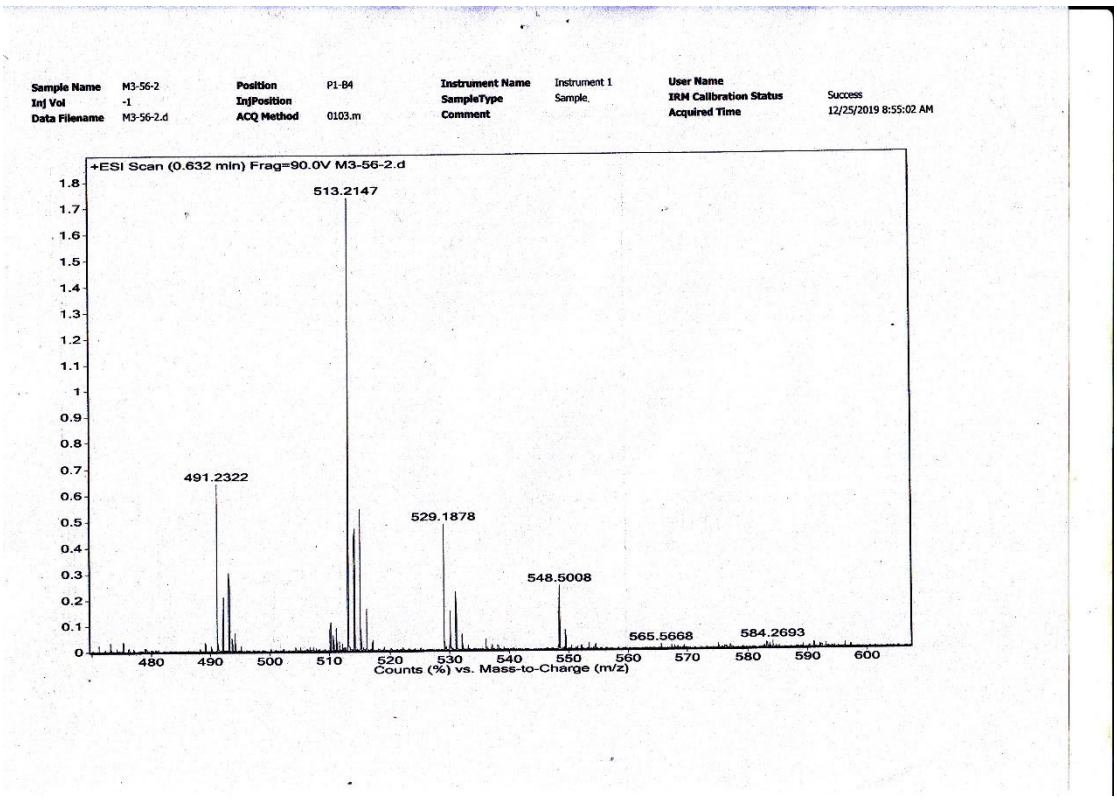


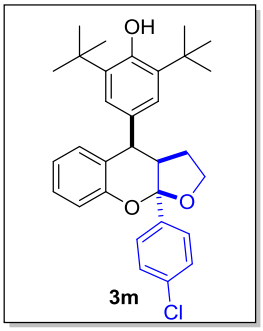
Chemical Formula: $C_{32}H_{35}F_3O_3$
Exact Mass: 524.2538
Molecular Weight: 524.6242
m/z: 524.2538 (100.0%), 525.2572 (34.6%), 526.2605 (3.1%), 526.2605 (2.7%)
Elemental Analysis: C, 73.26; H, 6.72; F, 10.86; O, 9.15

HRMS (ESI, m/z) calcd for $C_{32}H_{35}F_3O_3$ [M+Na^+] 547.2431, found 547.2428.


OH
O
O
Cl
3m, dr=4.6/1
1.93
1.93
0.98
1.05
1.82
1.99
1.00
1.01
1.11
1.01
0.99
1.00
1.04
17.98
f1 (ppm)

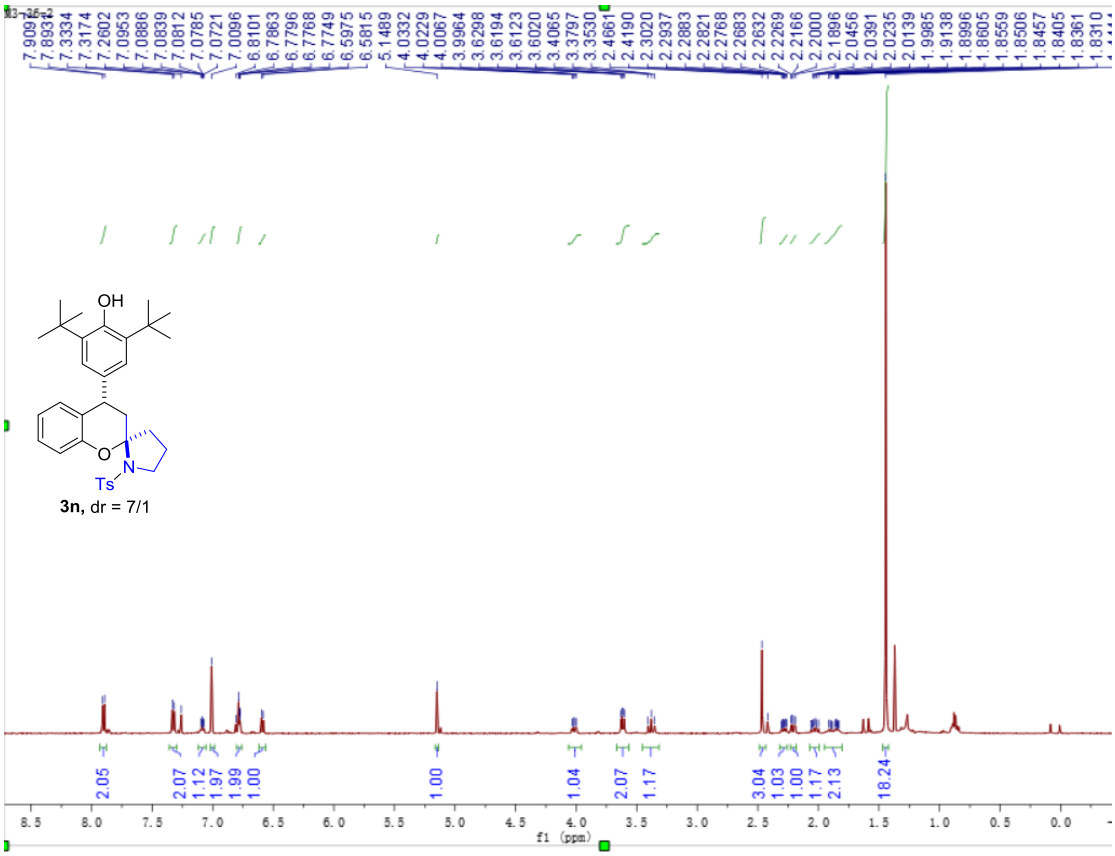

153.7456
152.7624
139.5376
135.9093
134.4827
131.1524
129.2247
128.5943
128.2690
127.5933
123.0036
120.8681
116.2904
107.8735
67.9737
50.9272
41.5216
34.3779
30.4130
26.7557
OH
O
O
Cl
3m, dr=4.6/1
f1 (ppm)



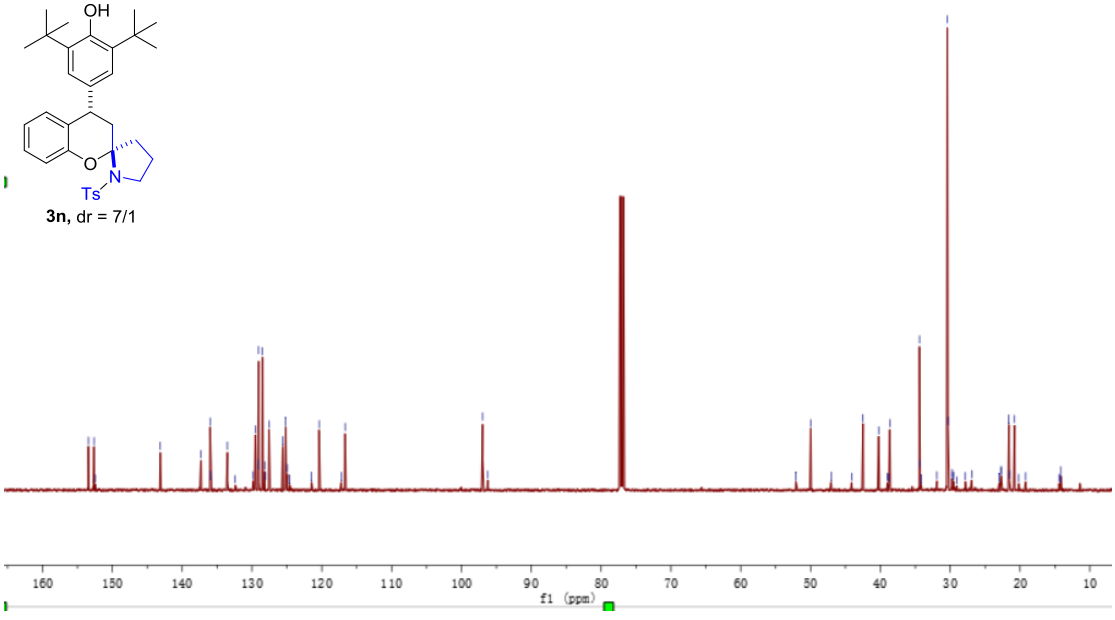


Chemical Formula: $C_{31}H_{35}ClO_3$
Exact Mass: 490.2275
Molecular Weight: 491.0680
m/z: 490.2275 (100.0%), 491.2308 (33.5%), 492.2245 (32.0%), 493.2279 (10.7%), 492.2342 (2.7%), 492.2342 (2.7%)
Elemental Analysis: C, 75.82; H, 7.18; Cl, 7.22; O, 9.77

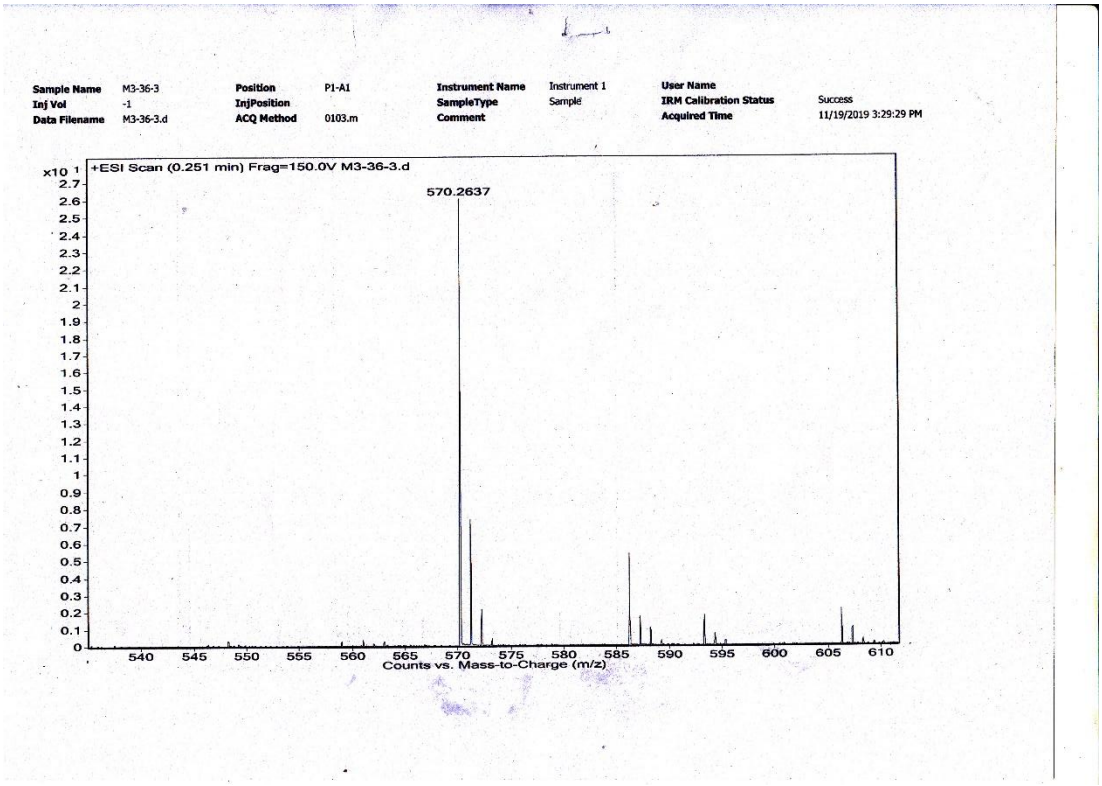
HRMS (ESI, m/z) calcd for $C_{31}H_{35}ClO_3$ [M+Na^+] 513.2167, found 513.2147.

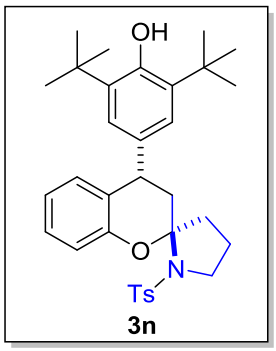


3n, dr = 7/1



3n, dr = 7/1

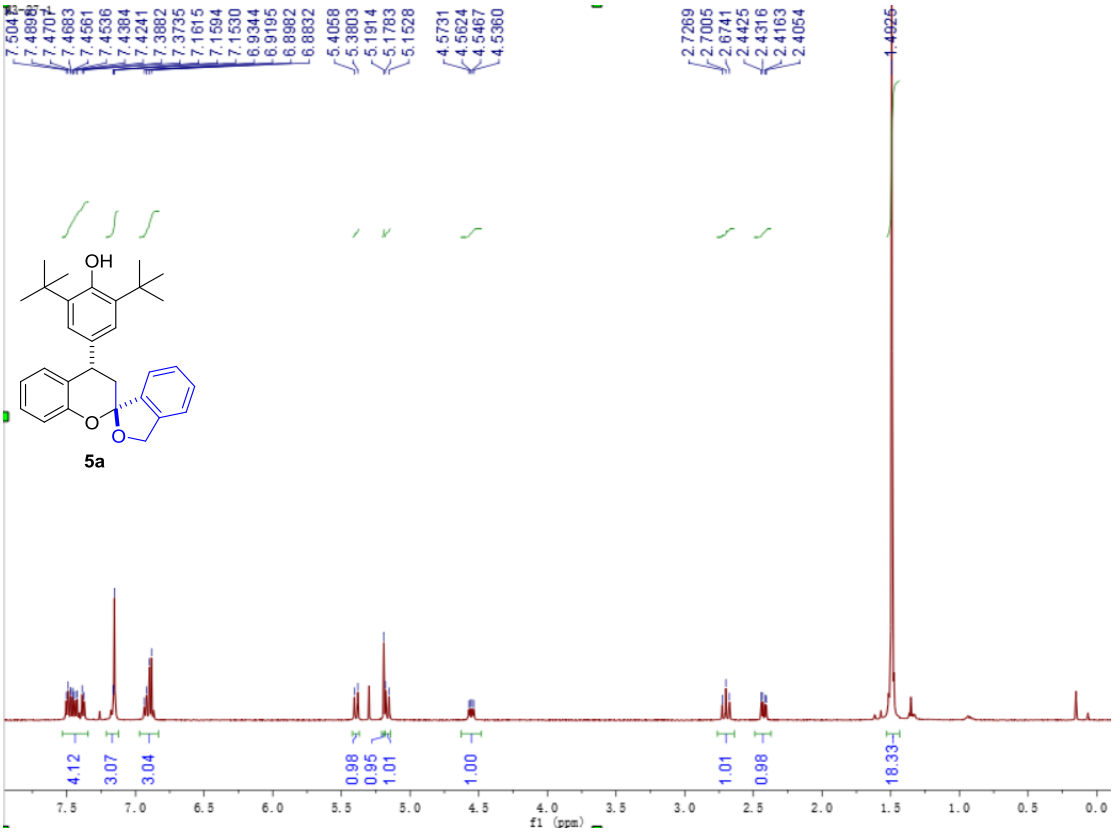


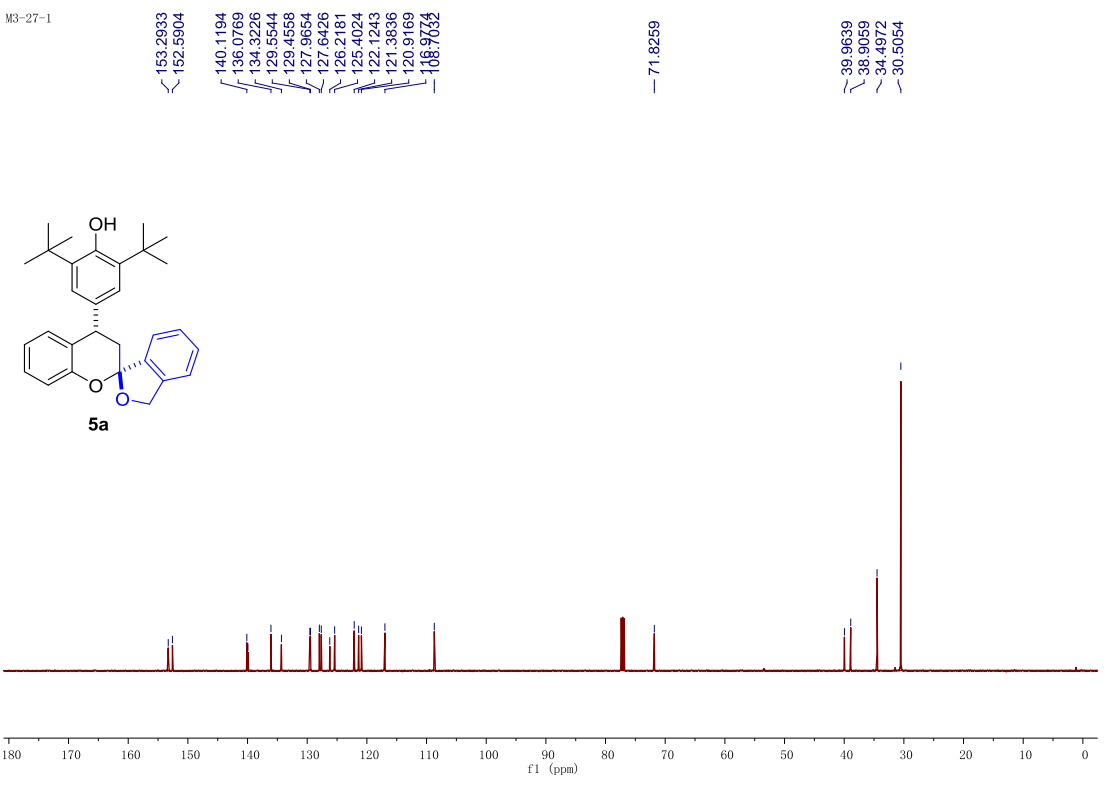


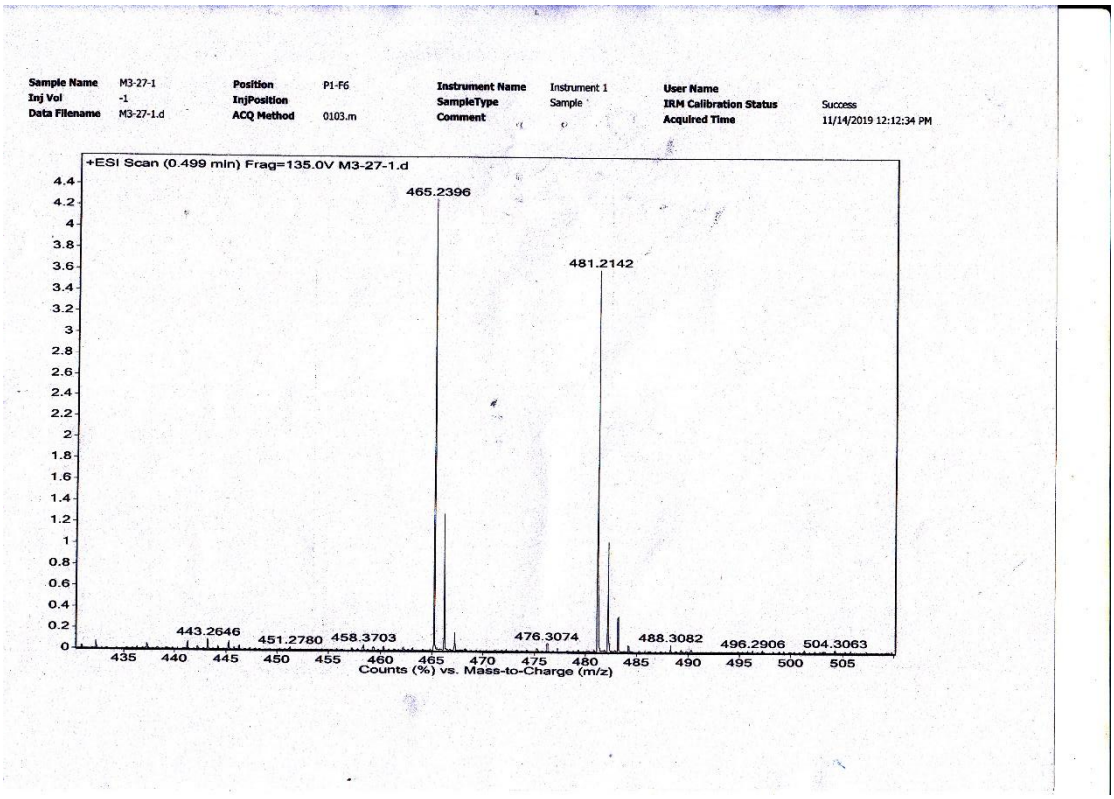
3n

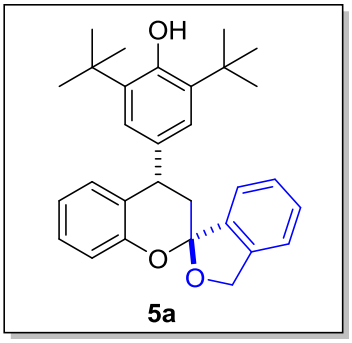
Chemical Formula: $C_{33}H_{41}NO_4S$
Exact Mass: 547.2756
Molecular Weight: 547.7540
m/z: 547.2756 (100.0%), 548.2790 (35.7%), 549.2823 (6.2%), 549.2714 (4.5%), 550.2748 (1.6%)
Elemental Analysis: C, 72.36; H, 7.54; N, 2.56; O, 11.68; S, 5.85

HRMS (ESI, m/z) calcd for $C_{33}H_{41}NO_4S$ [M+Na^+] 470.2649, found 470.2637.


7.5041
7.4898
7.4707
7.4683
7.4561
7.4536
7.4384
7.4241
7.3882
7.3735
7.1615
7.1594
7.1530
6.9344
6.9195
6.8982
6.8832
5.4058
5.3803
5.1914
5.1783
5.1528
4.5731
4.5624
4.5467
4.5360
2.7269
2.7005
2.6741
2.4425
2.4316
2.4163
2.4054
1.4925
OH
O
O
5a
4.12
3.07
3.04
0.98
0.95
1.01
1.00
1.01
0.98
18.33
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)


M3-27-1
153.2933
152.5904
140.1194
136.0769
134.3226
129.5544
129.4558
127.9654
127.6426
126.2181
125.4024
122.1243
121.3836
120.9169
71.8259
39.9639
38.9059
34.4972
30.5054
OH
O
O
5a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

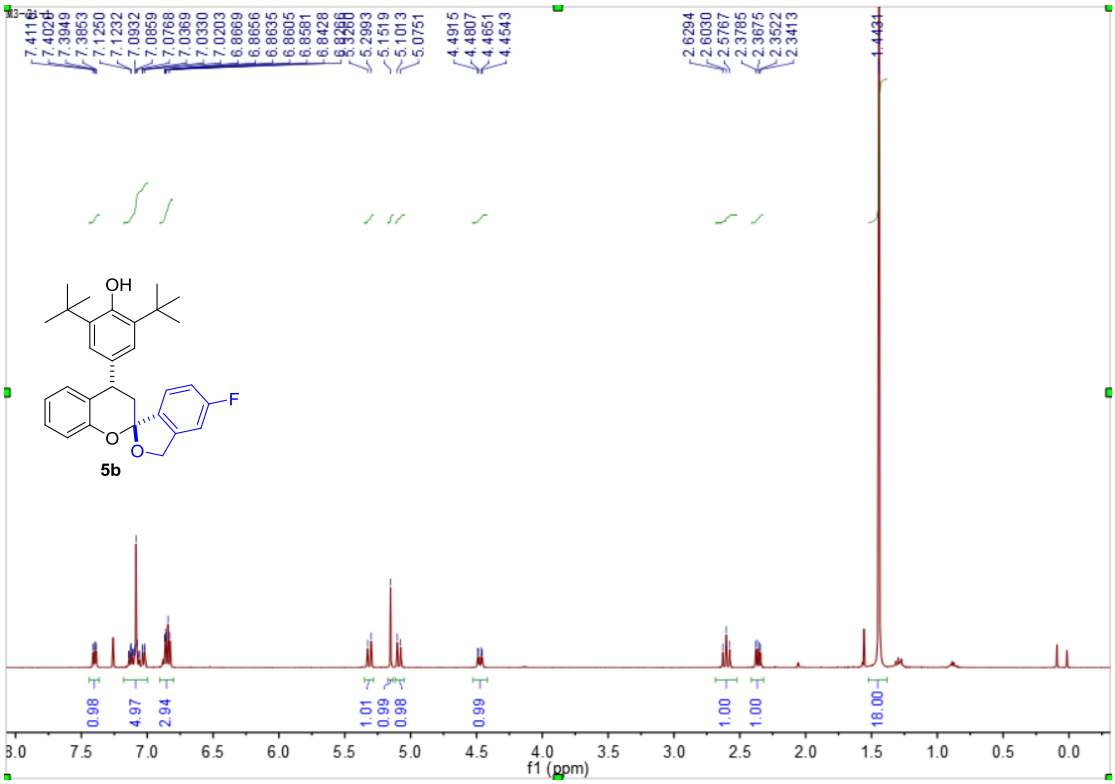


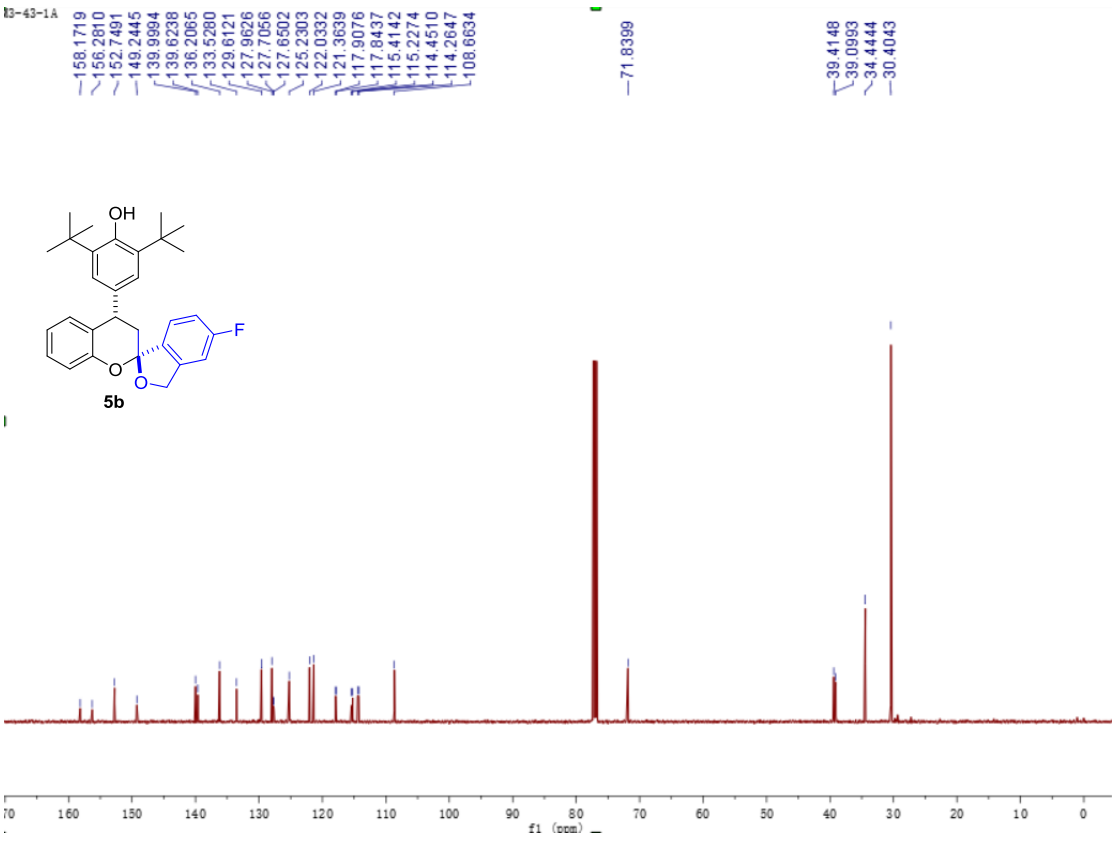


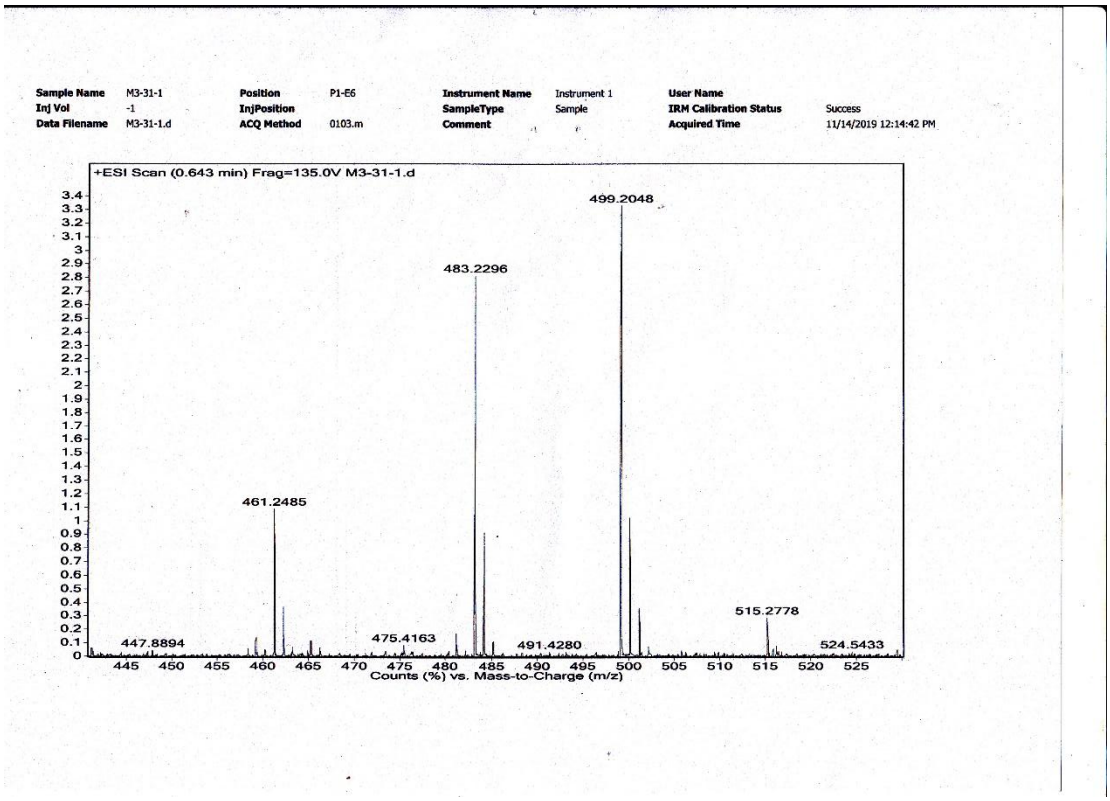
5a

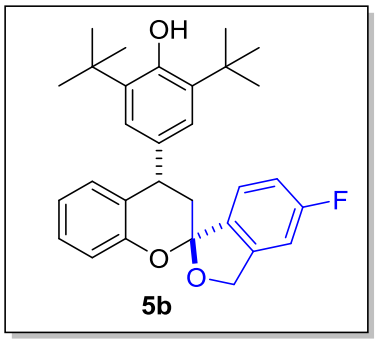
Chemical Formula: $C_{30}H_{34}O_3$
Exact Mass: 442.2508
Molecular Weight: 442.5990
m/z: 442.2508 (100.0%), 443.2541 (32.4%), 444.2575 (2.7%), 444.2575 (2.4%)
Elemental Analysis: C, 81.41; H, 7.74; O, 10.84

HRMS (ESI, m/z) calcd for $C_{30}H_{34}O_3$ [M+Na^+] 465.2400, found 465.2396.


OH
F
O
O
5b
7.4116
7.4026
7.3949
7.3853
7.1250
7.1232
7.0932
7.0859
7.0768
7.0369
7.0330
7.0203
6.8669
6.8656
6.8635
6.8605
6.8581
6.8428
5.2993
5.1519
5.1013
5.0751
4.4915
4.4807
4.4651
4.4543
2.6294
2.6030
2.5767
2.3785
2.3675
2.3522
2.3413
1.4431
0.98
4.97
2.94
1.01
0.99
0.98
0.99
1.00
1.00
18.00
f1 (ppm)


158.1719
156.2810
152.7491
149.2445
139.9994
139.6238
136.2065
133.5280
129.6121
127.9626
127.7056
127.6502
125.2303
122.0332
121.3639
117.9076
117.8437
115.4142
115.2274
114.4510
114.2647
108.8634
71.8399
39.4148
39.0993
34.4444
30.4043
f1 (ppm)

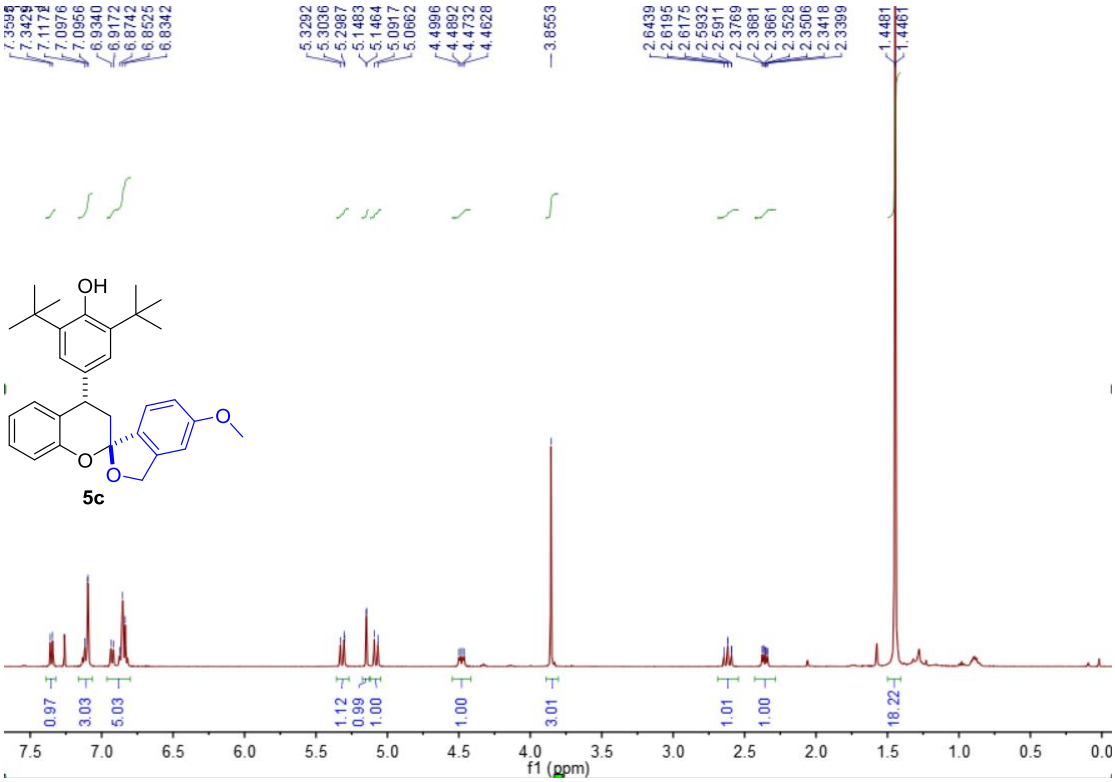




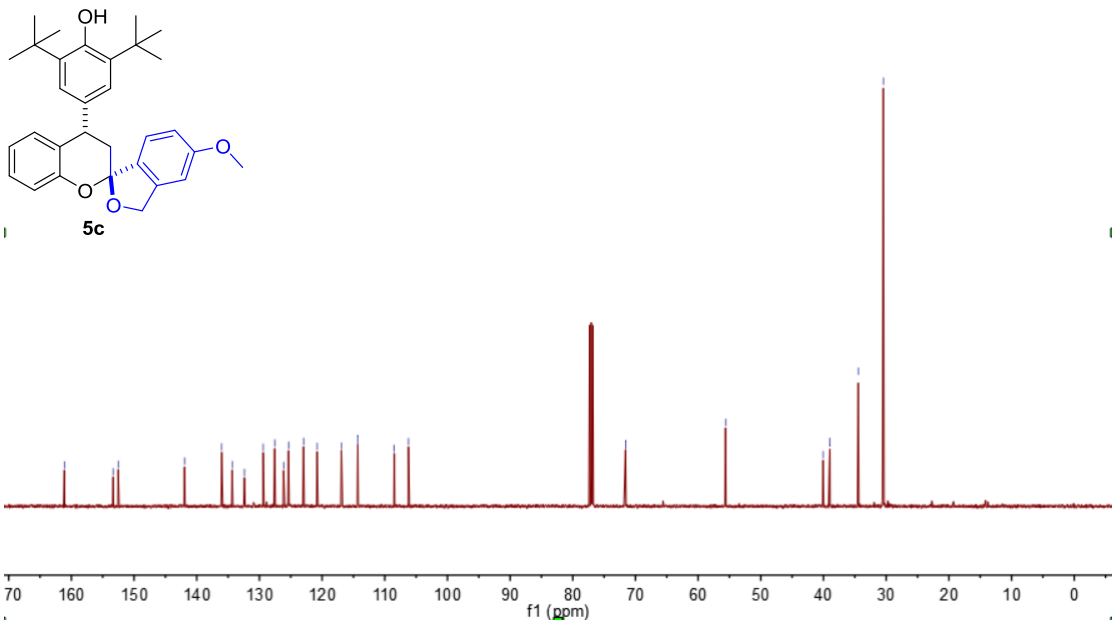
5b

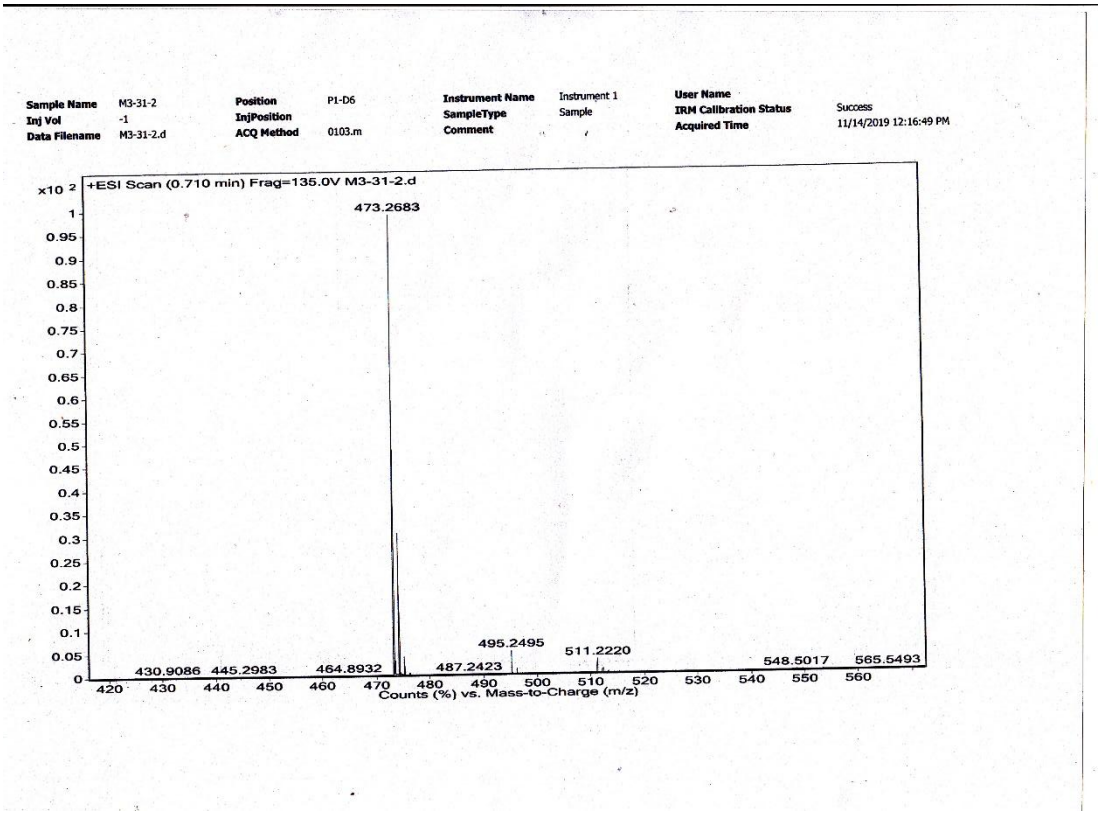
Chemical Formula: $C_{30}H_{33}FO_3$
Exact Mass: 460.2414
Molecular Weight: 460.5894
m/z: 460.2414 (100.0%), 461.2447 (32.4%), 462.2481 (2.7%), 462.2481 (2.4%)
Elemental Analysis: C, 78.23; H, 7.22; F, 4.12; O, 10.42

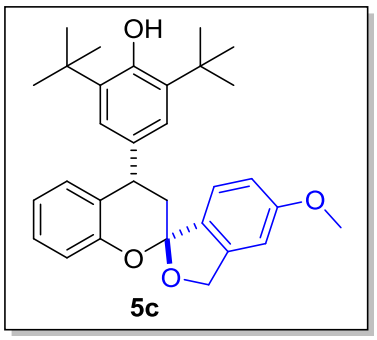
HRMS (ESI, m/z) calcd for $C_{30}H_{33}FO_3$ [M+K^+] 499.2045, found 499.2048.


OH
O
O
5c
f1 (ppm)


f1 (ppm)


OH
O
O
5c
f1 (ppm)

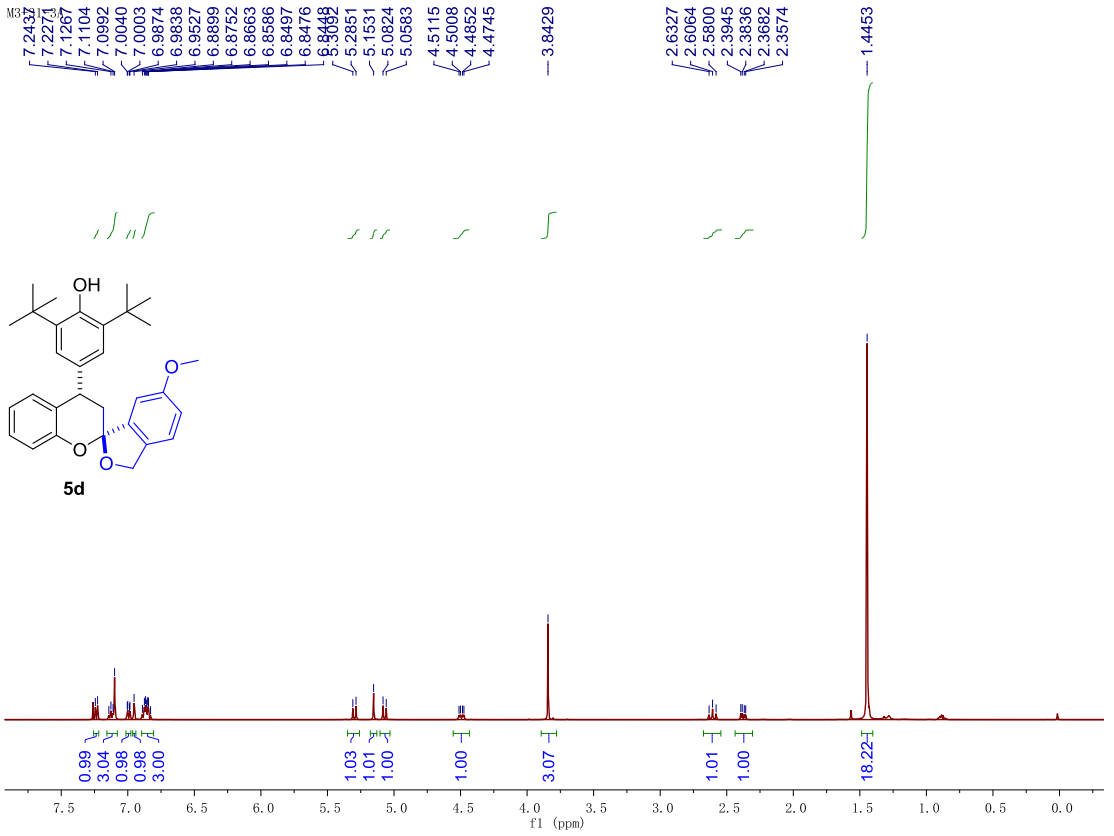


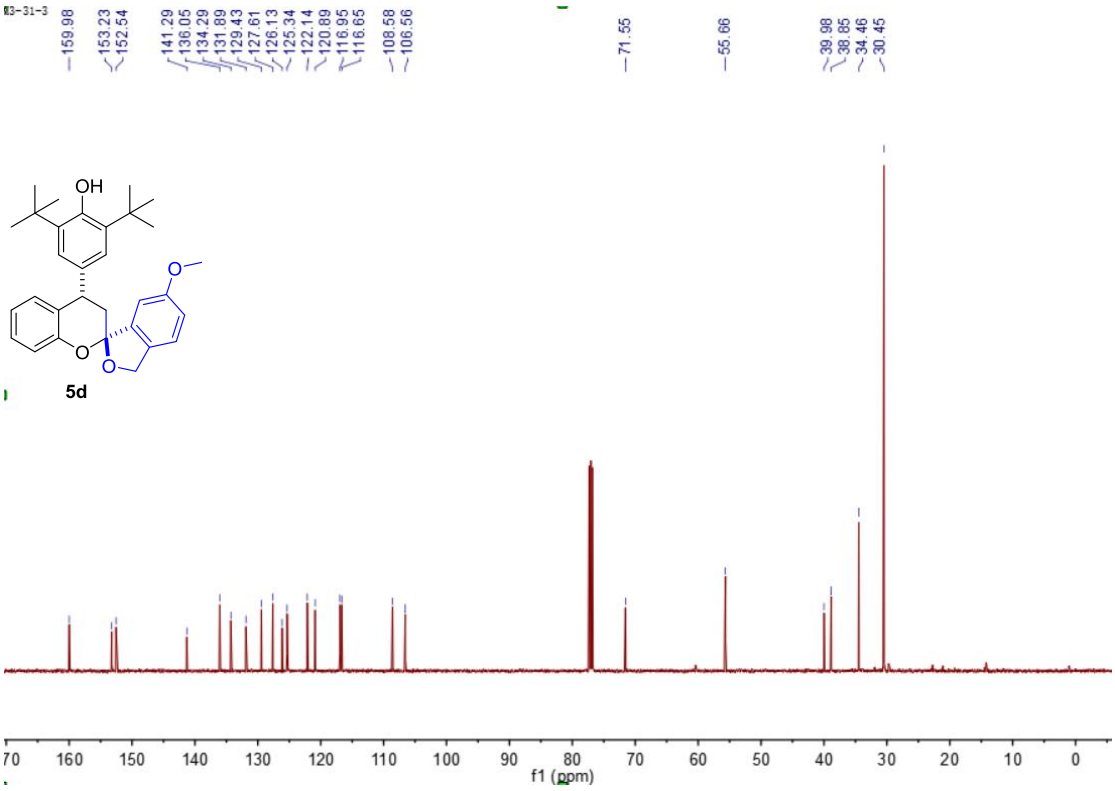


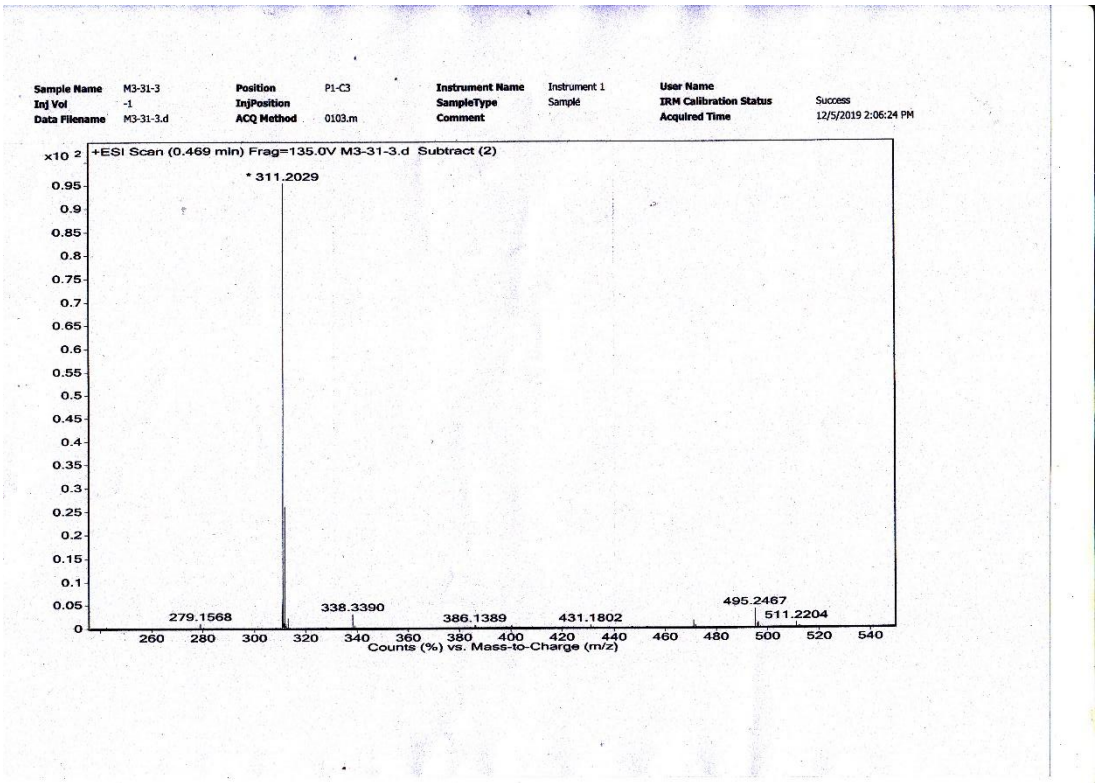
5c

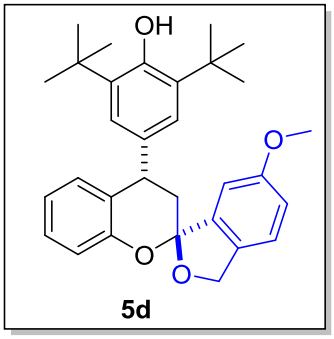
Chemical Formula: $C_{31}H_{36}O_4$
Exact Mass: 472.2614
Molecular Weight: 472.6250
m/z: 472.2614 (100.0%), 473.2647 (33.5%), 474.2681 (2.7%), 474.2681 (2.7%)
Elemental Analysis: C, 78.78; H, 7.68; O, 13.54

HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_4$ $[M+H^+]$ 473.2686, found 473.2683.


7.2432
7.2274
7.1267
7.1104
7.0992
7.0040
7.0003
6.9874
6.9838
6.9527
6.8899
6.8752
6.8663
6.8586
6.8497
6.8476
5.2851
5.1531
5.0824
5.0583
4.5115
4.5008
4.4852
4.4745
3.8429
2.6327
2.6064
2.5800
2.3945
2.3836
2.3682
2.3574
1.4453
OH
O
O
5d
0.99
3.04
0.98
0.98
3.00
1.03
1.01
1.00
1.00
3.07
1.01
1.00
18.22
f1 (ppm)


M3-31-3
159.98
153.23
152.54
141.29
136.05
134.29
131.89
129.43
127.61
126.13
125.34
122.14
120.89
116.95
116.65
108.58
106.56
71.55
55.66
39.98
38.85
34.46
30.45
OH
O
O
5d
f1 (ppm)

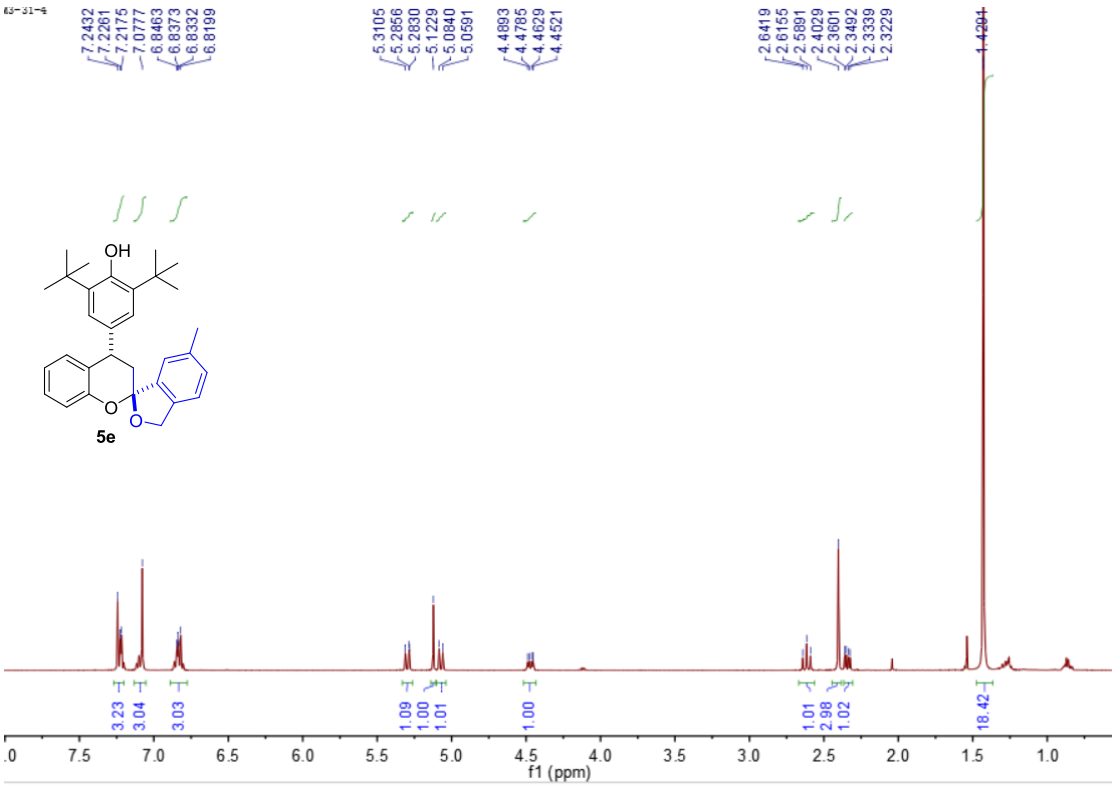


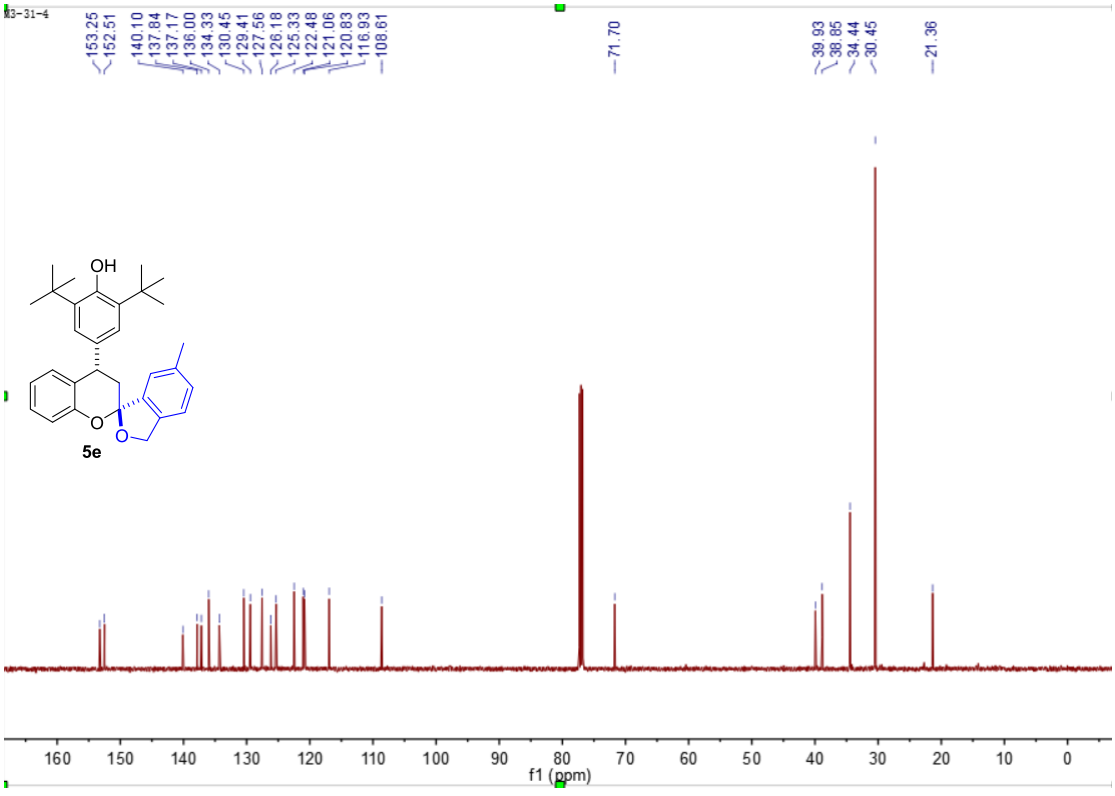


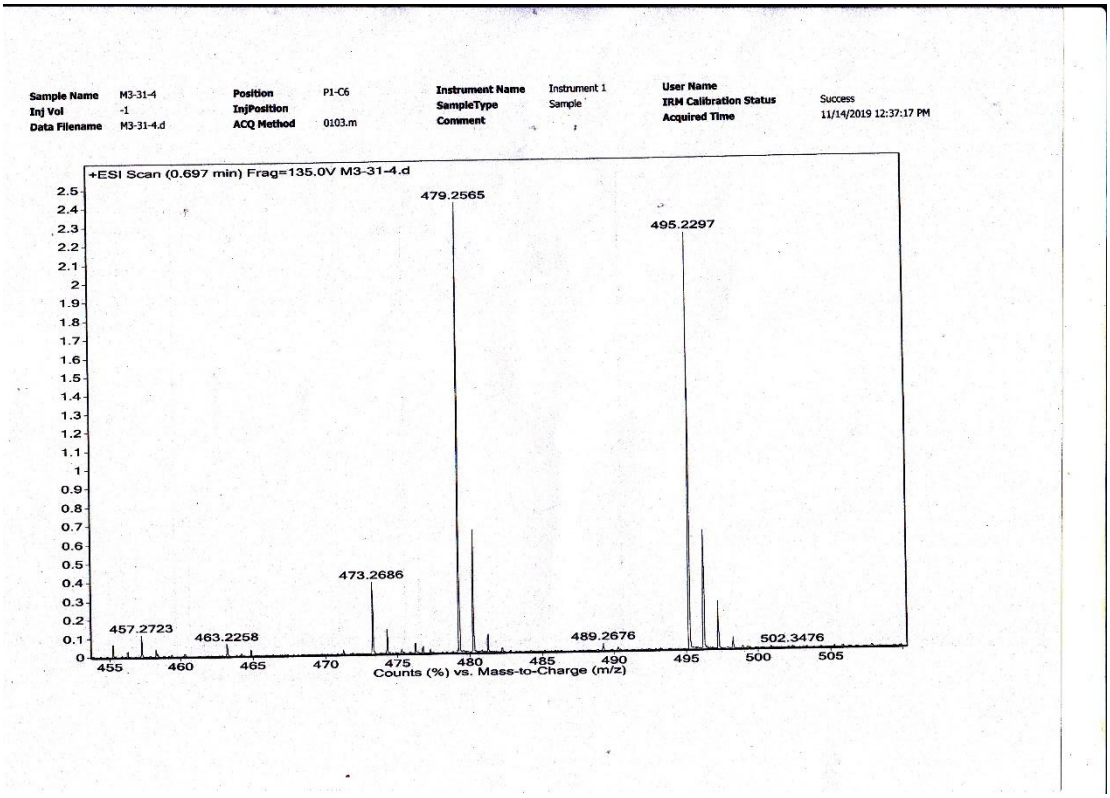
5d

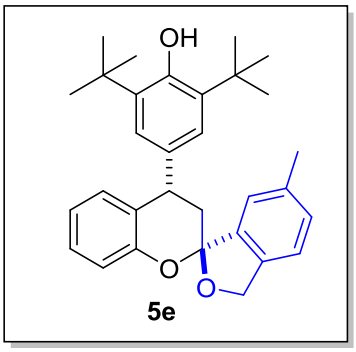
Chemical Formula: $C_{31}H_{36}O_4$
Exact Mass: 472.2614
Molecular Weight: 472.6250
m/z: 472.2614 (100.0%), 473.2647 (33.5%), 474.2681 (2.7%), 474.2681 (2.7%)
Elemental Analysis: C, 78.78; H, 7.68; O, 13.54

HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_4$ [M+Na^+] 495.2506, found 495.2467.


OH
O
O
5e
7.2432
7.2261
7.2175
7.0777
6.8463
6.8373
6.8332
6.8199
5.3105
5.2856
5.2830
5.1229
5.0840
5.0591
4.4893
4.4785
4.4629
4.4521
2.6419
2.6155
2.5891
2.4029
2.3601
2.3492
2.3339
2.3229
1.4284
3.23
3.04
3.03
1.09
1.00
1.01
1.00
1.01
2.98
1.02
18.42
f1 (ppm)


OH
O
O
5e
153.25
152.51
140.10
137.84
137.17
136.00
134.33
130.45
129.41
127.56
126.18
125.33
122.48
121.06
120.83
116.93
108.61
71.70
39.93
38.85
34.44
30.45
21.36
f1 (ppm)

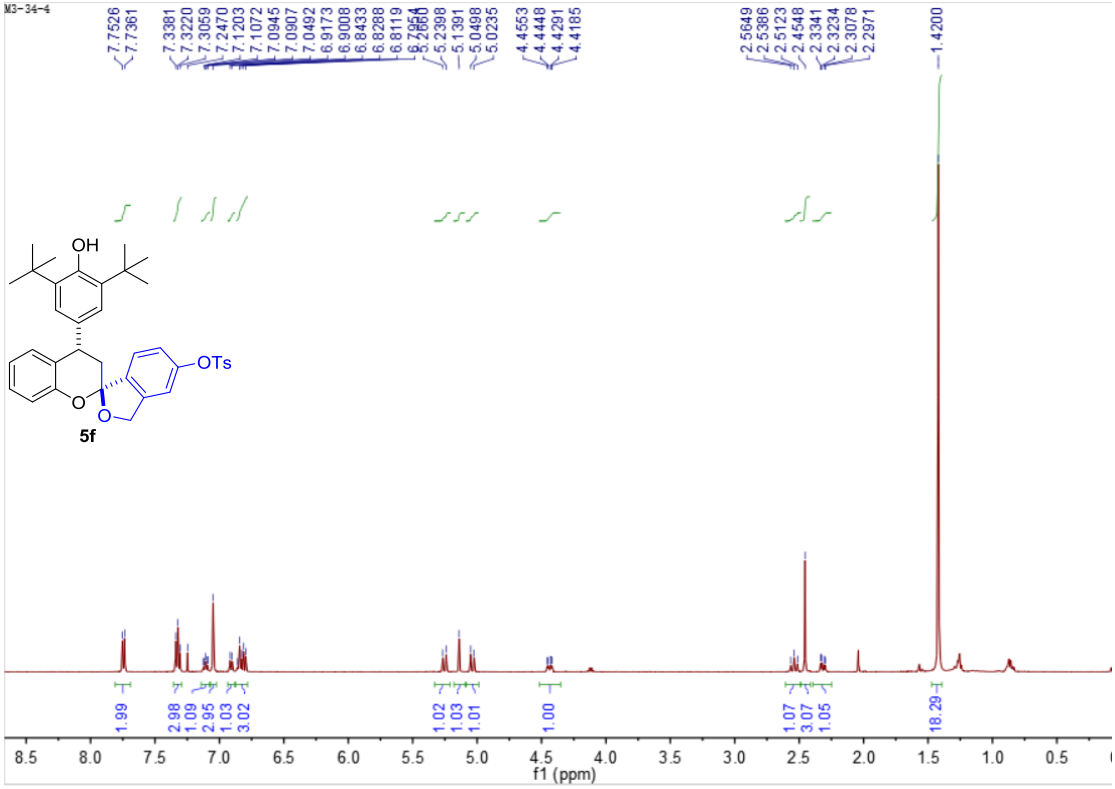


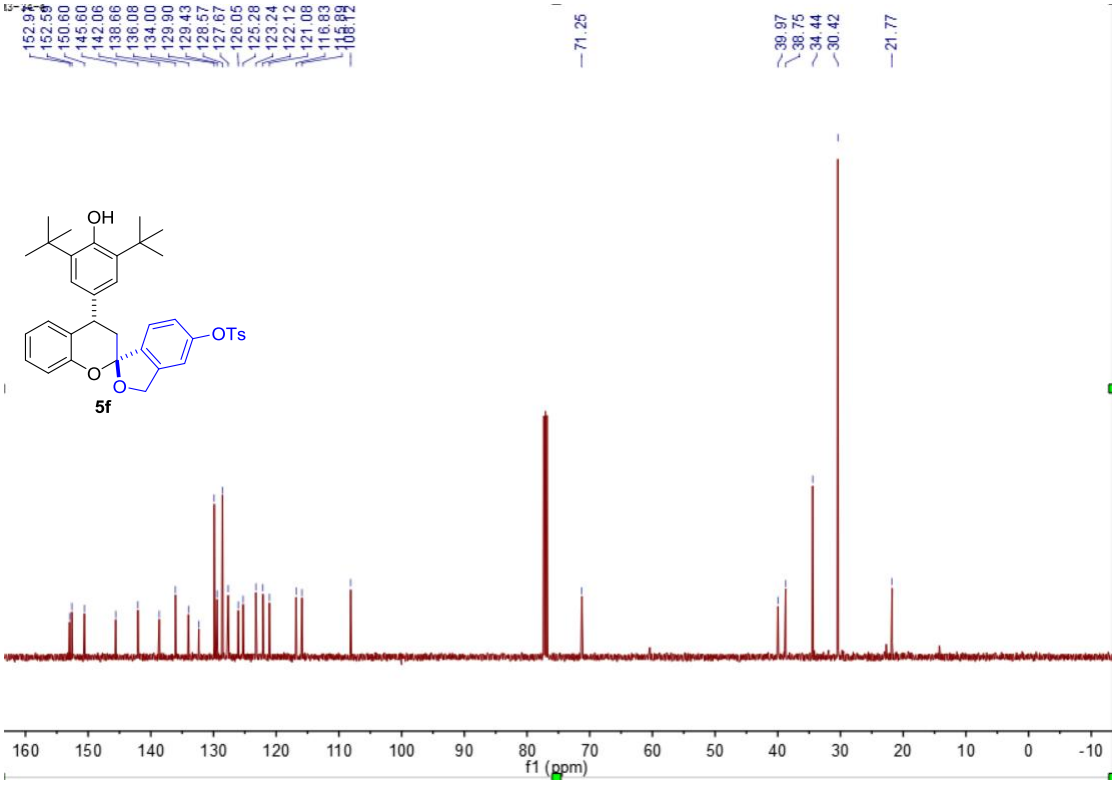


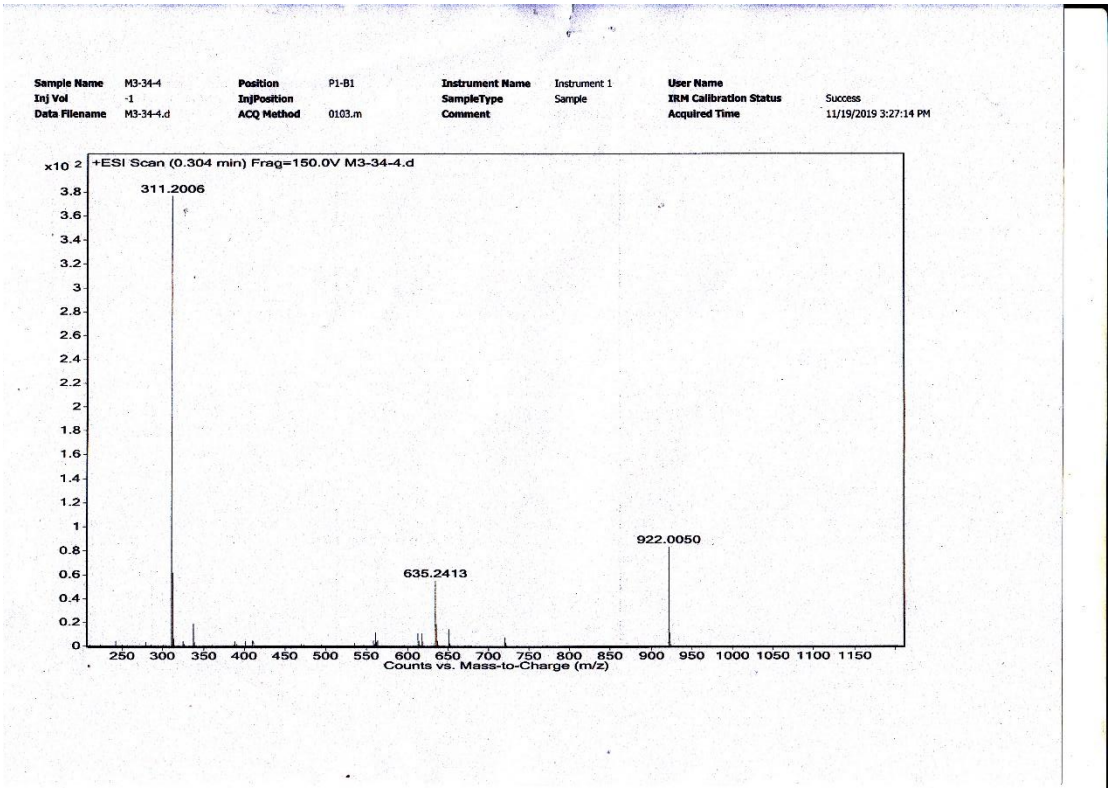
5e

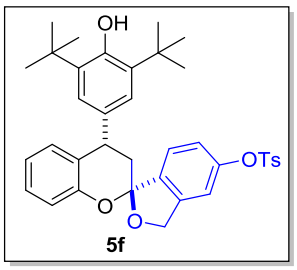
Chemical Formula: $C_{31}H_{36}O_3$
Exact Mass: 456.2664
Molecular Weight: 456.6260
m/z: 456.2664 (100.0%), 457.2698 (33.5%), 458.2732 (2.7%), 458.2732 (2.7%)
Elemental Analysis: C, 81.54; H, 7.95; O, 10.51

HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_3$ $[M+Na^+]$ 479.2557, found 479.2565.


M3-34-4
OH
OTs
O
O
5f
f1 (ppm)


OH
OTs
O
O
5f
f1 (ppm)

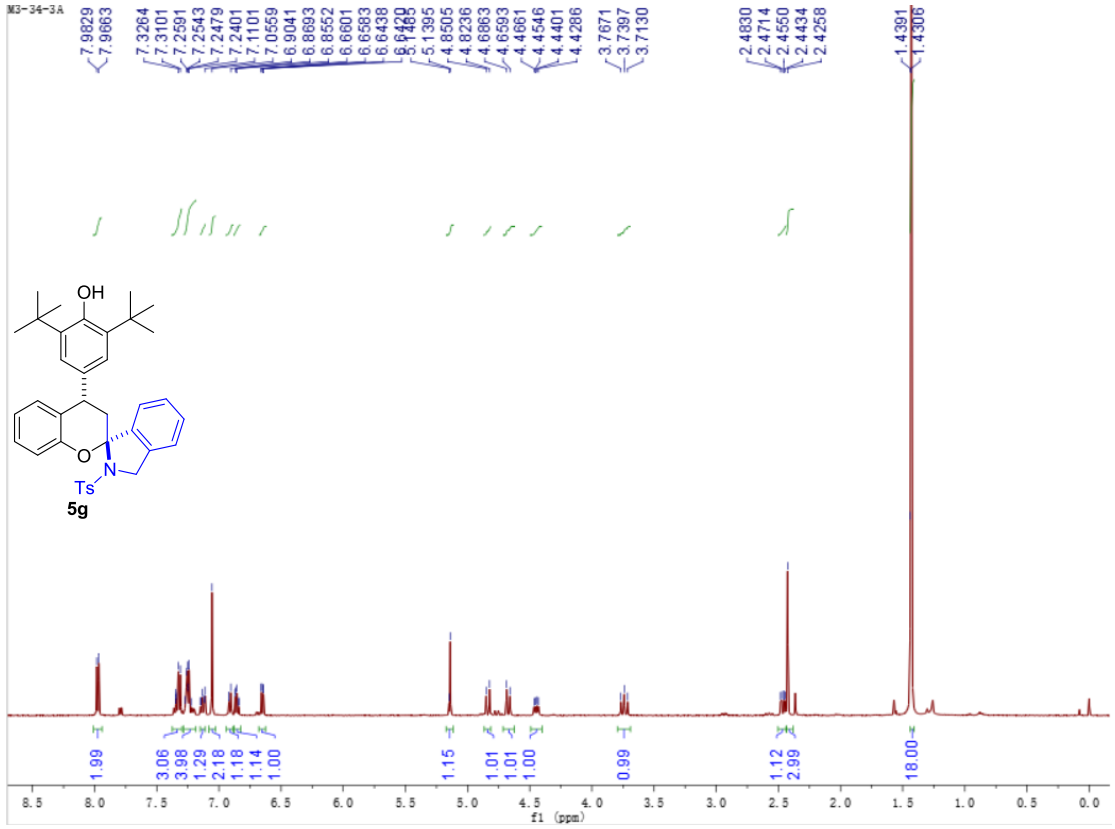


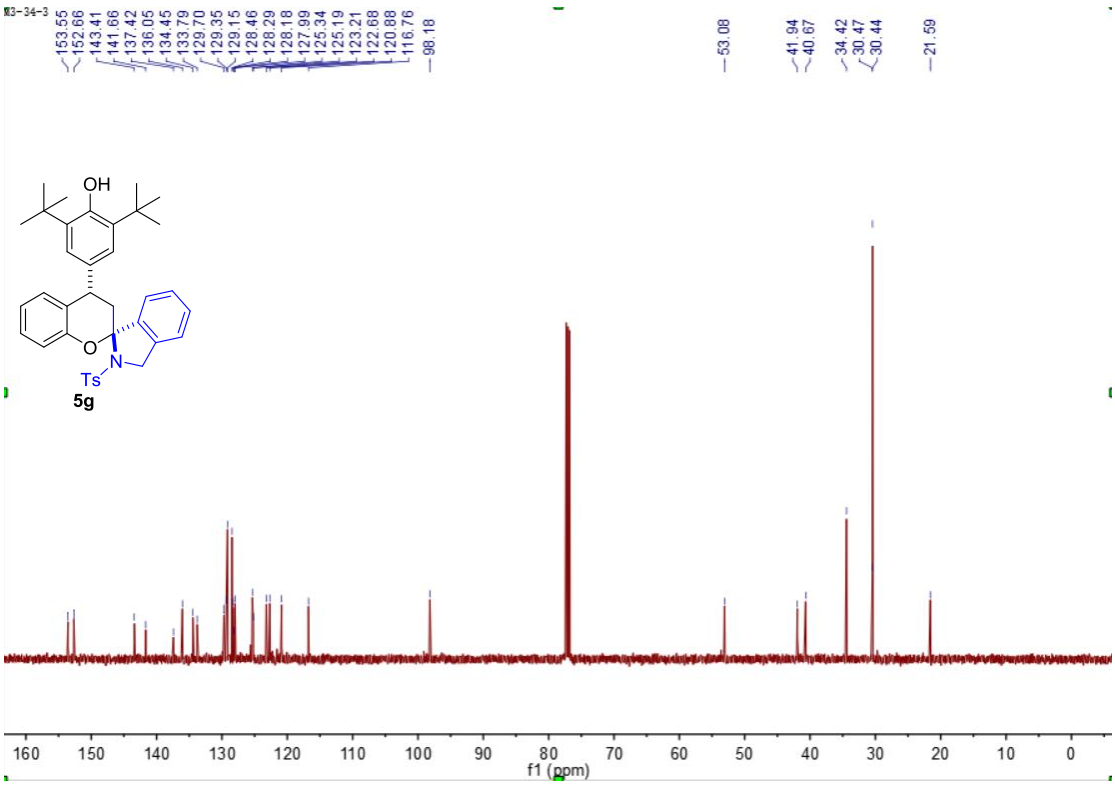


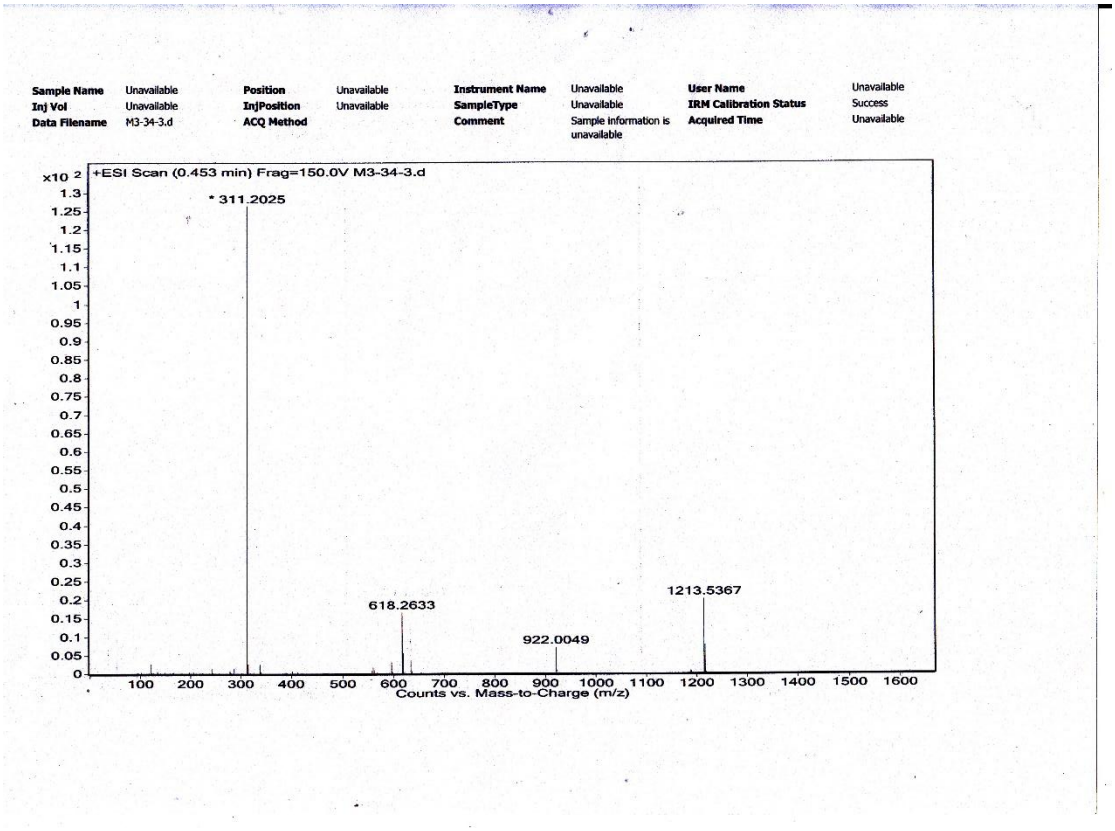
5f

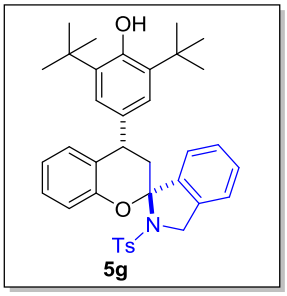
Chemical Formula: $C_{37}H_{40}O_6S$
Exact Mass: 612.2546
Molecular Weight: 612.7810
m/z: 612.2546 (100.0%), 613.2579 (40.0%), 614.2613 (5.1%), 614.2504 (4.5%), 614.2613 (2.7%), 615.2537 (1.8%), 614.2588 (1.2%)
Elemental Analysis: C, 72.52; H, 6.58; O, 15.67; S, 5.23

HRMS (ESI, m/z) calcd for $C_{37}H_{40}O_6S$ [M+Na^+] 635.2438, found 635.2413.


M3-34-3A
OH
Ts
5g
f1 (ppm)


M3-34-3
OH
Ts
5g
f1 (ppm)

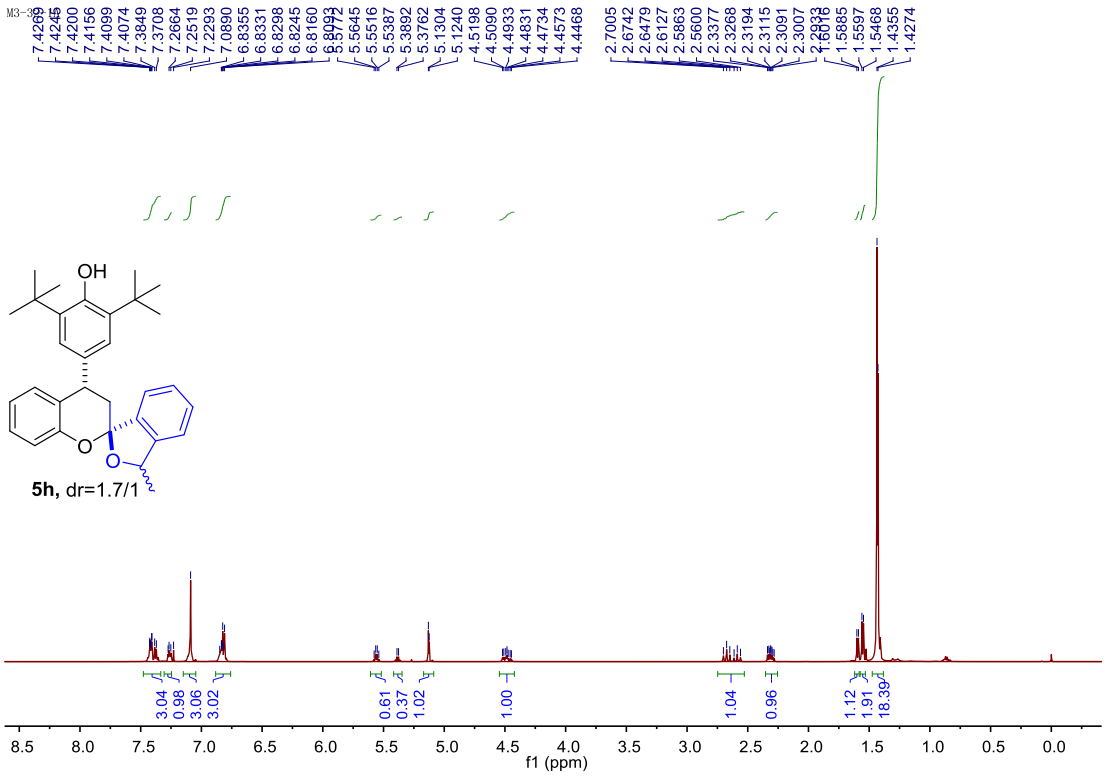


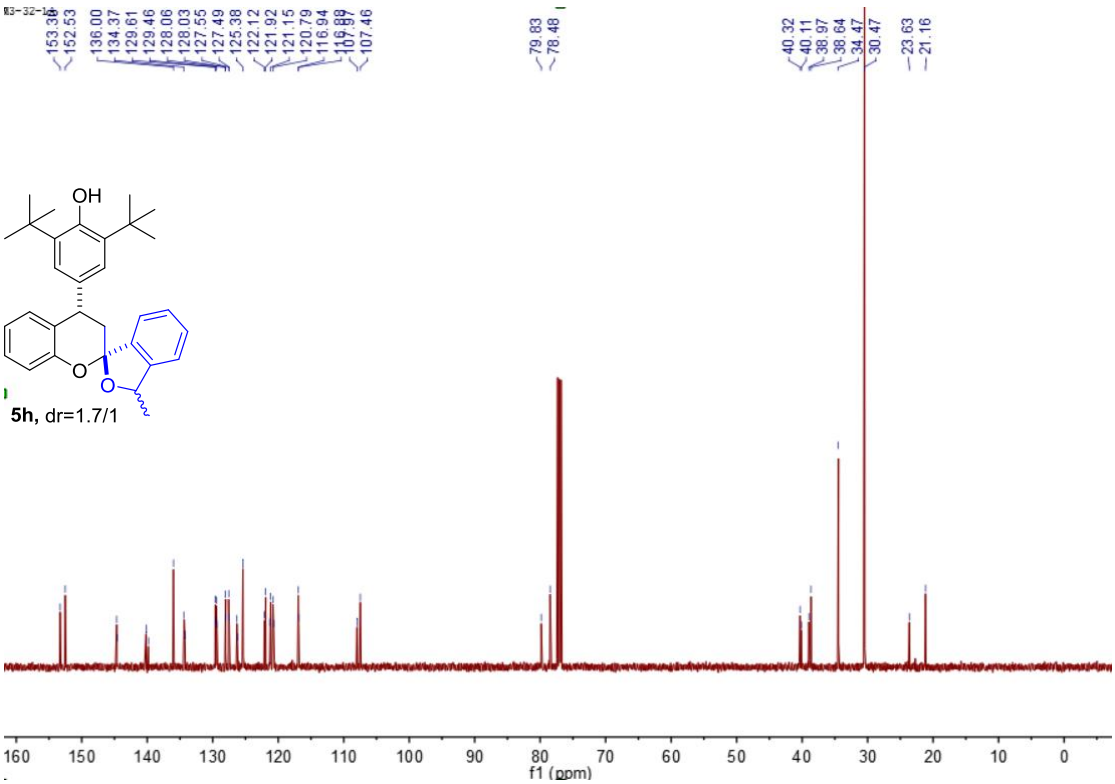


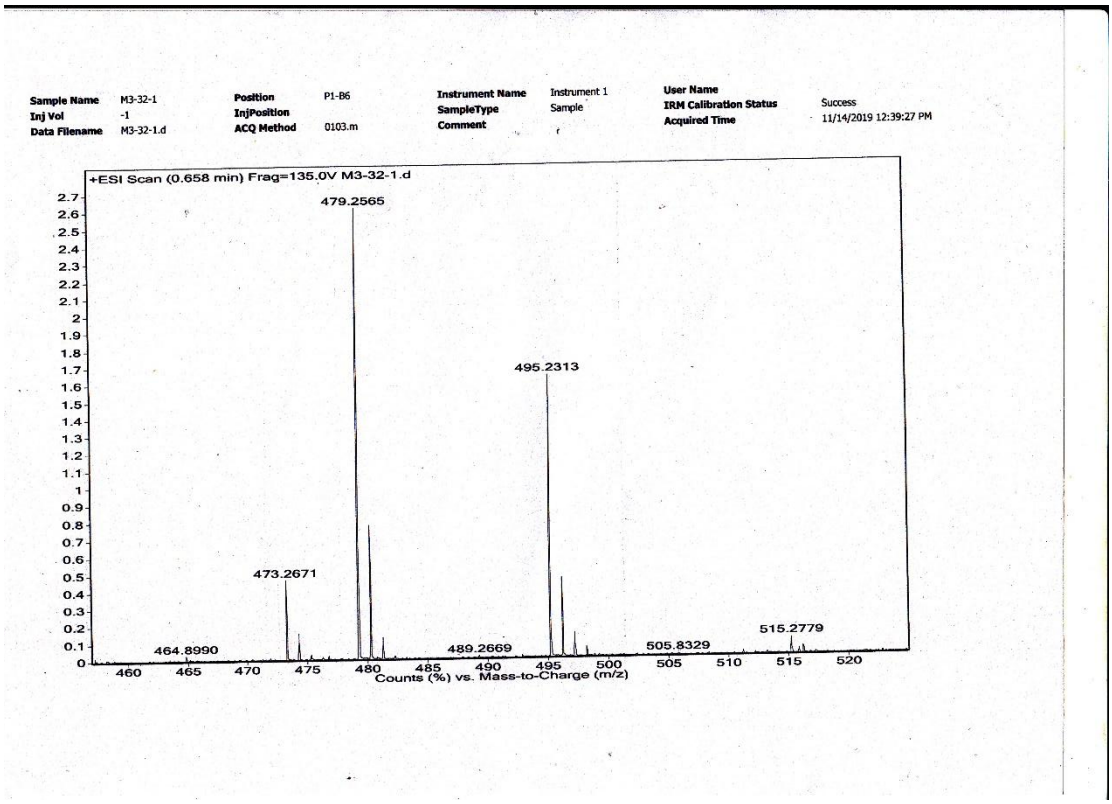
5g

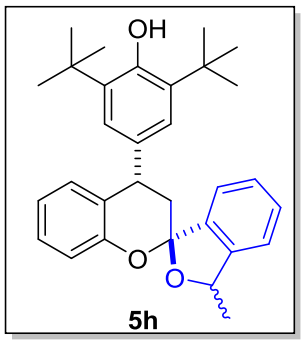
Chemical Formula: $C_{37}H_{41}NO_4S$
Exact Mass: 595.2756
Molecular Weight: 595.7980
m/z: 595.2756 (100.0%), 596.2790 (40.0%), 597.2823 (5.1%), 597.2714 (4.5%), 597.2823 (2.7%), 598.2748 (1.8%)
Elemental Analysis: C, 74.59; H, 6.94; N, 2.35; O, 10.74; S, 5.38

HRMS (ESI, m/z) calcd for $C_{37}H_{41}NO_4S$ [M+Na^+] 618.2649, found 618.2633.


OH
O
O
5h, dr=1.7/1
f1 (ppm)

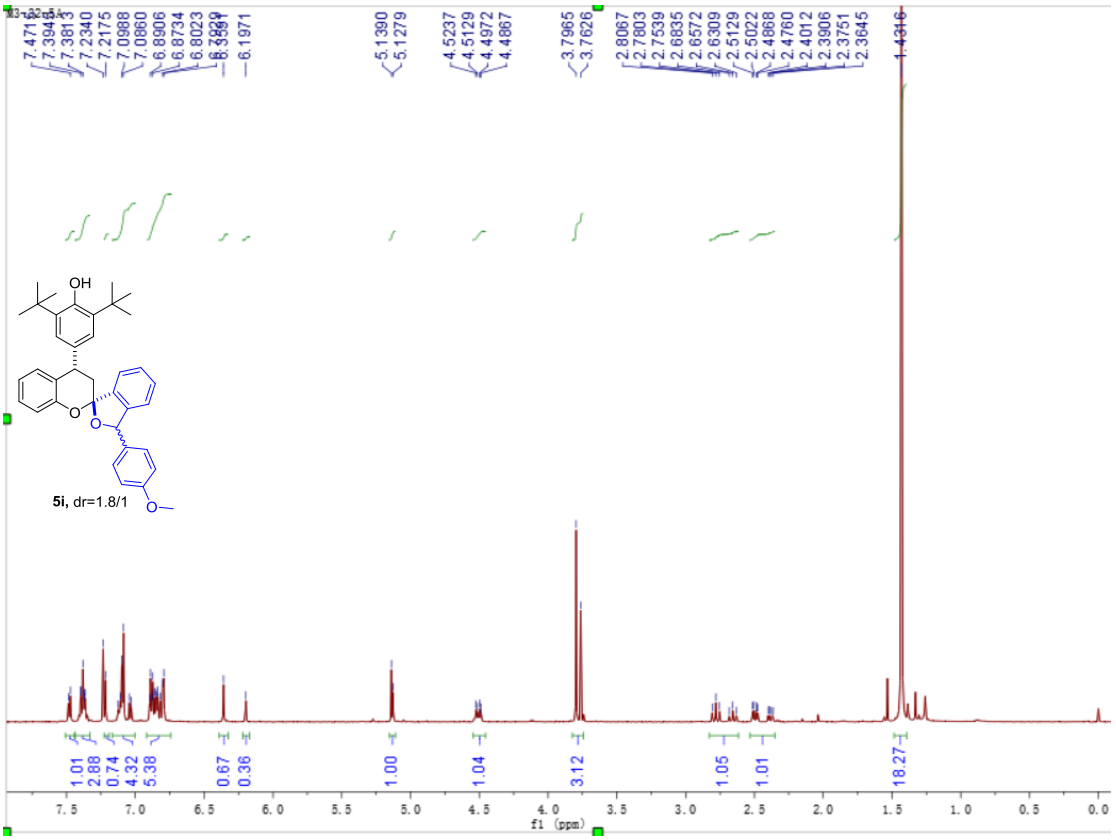

OH
O
O
5h, dr=1.7/1
f1 (ppm)

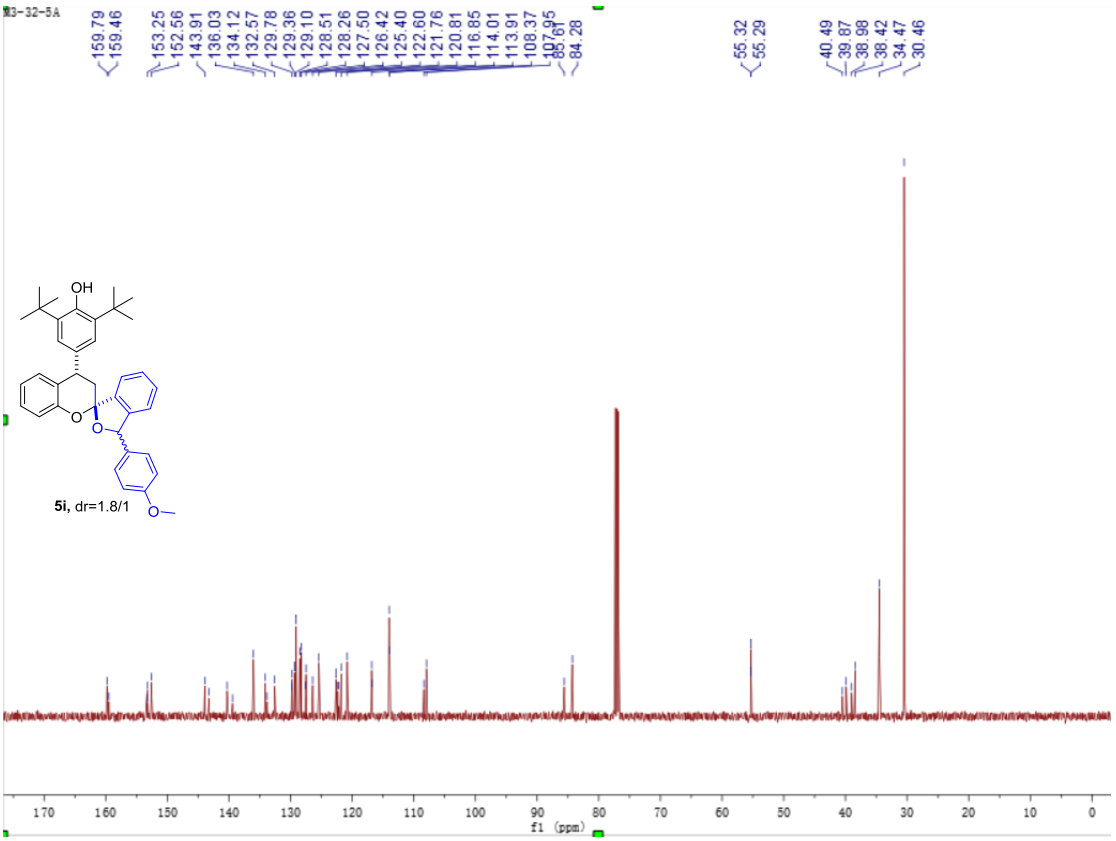


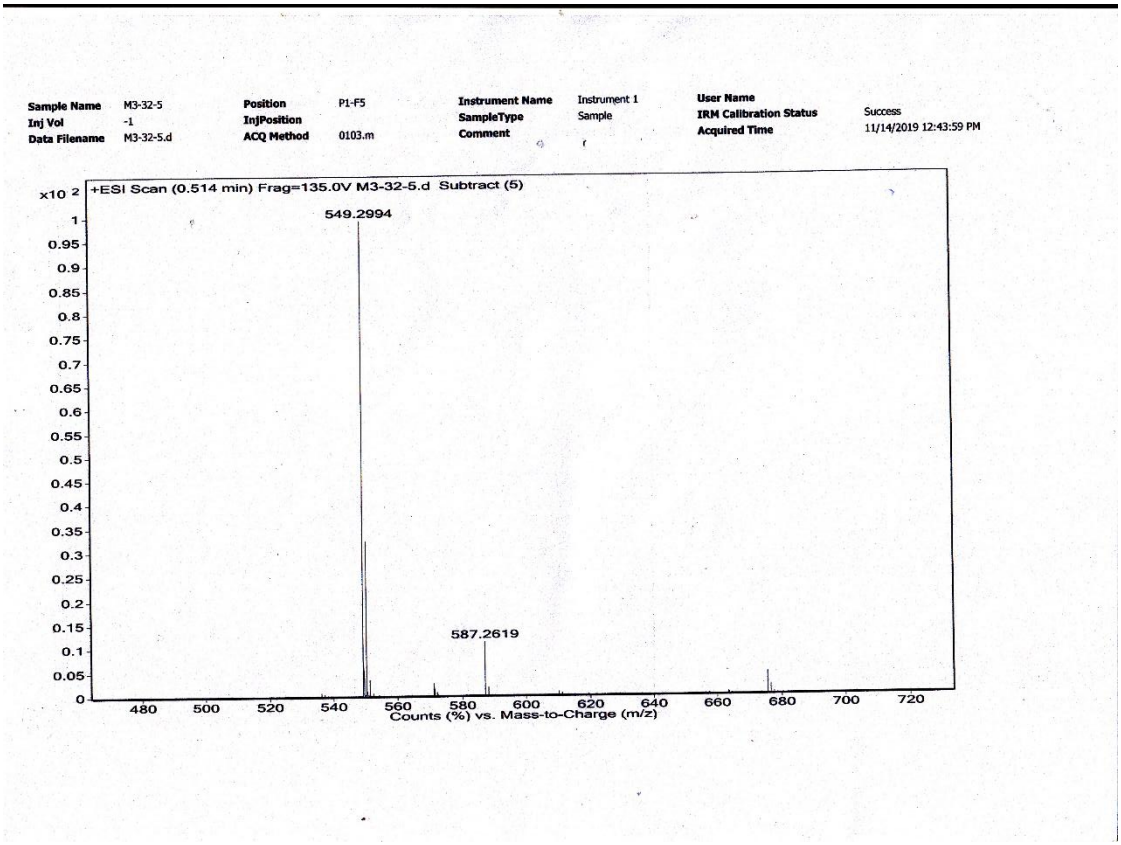


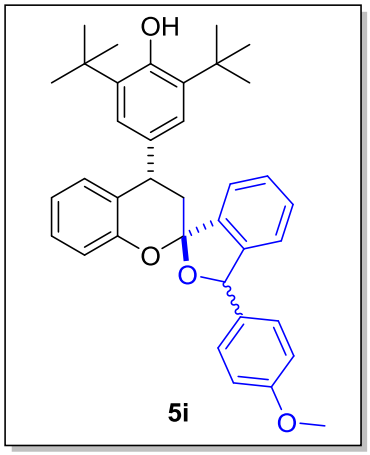
Chemical Formula: $C_{31}H_{36}O_3$
Exact Mass: 456.2664
Molecular Weight: 456.6260
m/z: 456.2664 (100.0%), 457.2698 (33.5%), 458.2732 (2.7%), 458.2732 (2.7%)
Elemental Analysis: C, 81.54; H, 7.95; O, 10.51

HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_3$ [M+Na^+] 479.2557, found 479.2565.


7.4716
7.3945
7.3813
7.2340
7.2175
7.0988
7.0860
6.8906
6.8734
6.8023
6.1971
5.1390
5.1279
4.5237
4.5129
4.4972
4.4867
3.7965
3.7626
2.8067
2.7803
2.7539
2.6835
2.6572
2.6309
2.5129
2.5022
2.4868
2.4760
2.4012
2.3906
2.3751
2.3645
1.4816
OH
O
O
5i, dr=1.8/1
1.01
2.88
0.74
4.32
5.38
0.67
0.36
1.00
1.04
3.12
1.05
1.01
18.27
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)

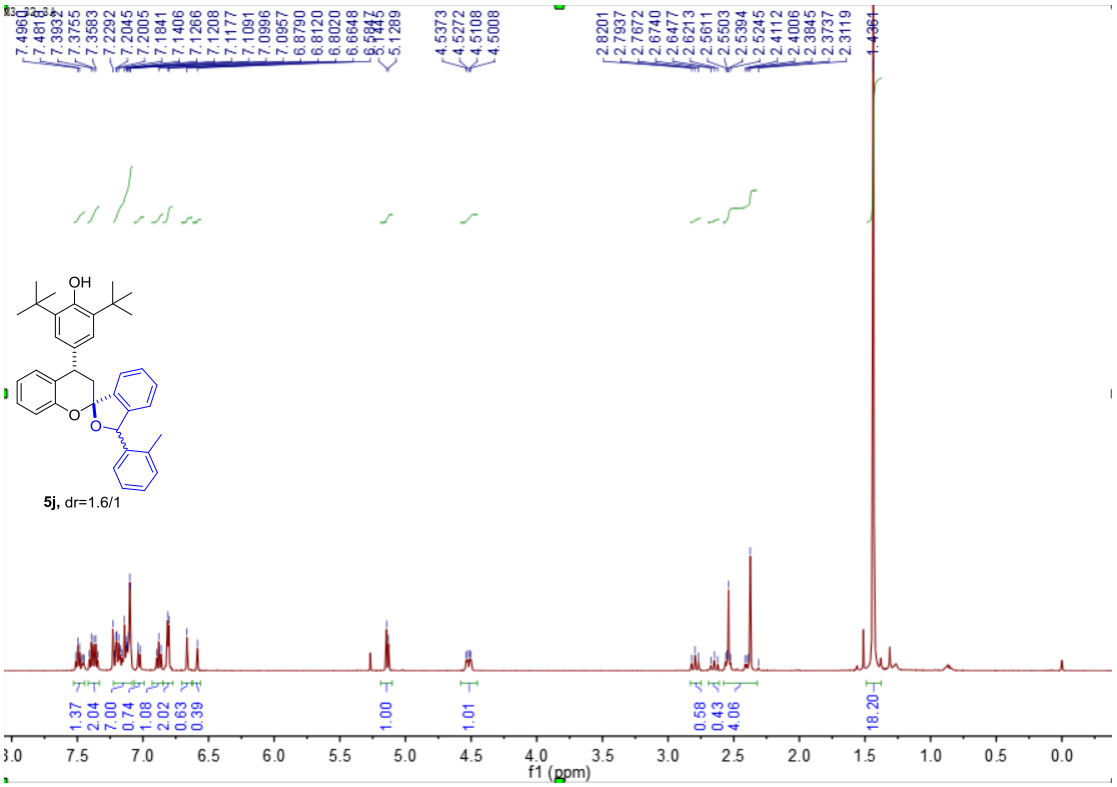

M3-32-5A
159.79
159.46
153.25
152.56
143.91
136.03
134.12
132.57
129.78
129.36
129.10
128.51
128.26
127.50
126.42
125.40
122.60
121.76
120.81
116.85
114.01
113.91
108.37
84.28
55.32
55.29
40.49
39.87
38.98
38.42
34.47
30.46
OH
O
O
5i, dr=1.8/1
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

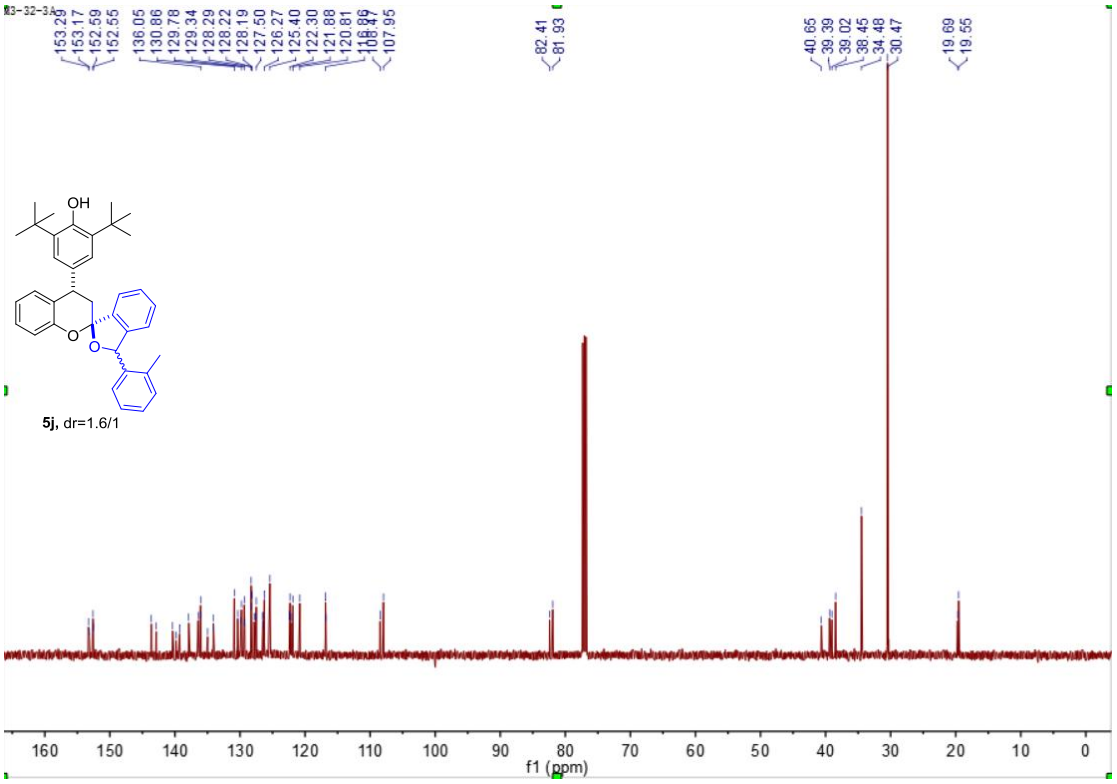


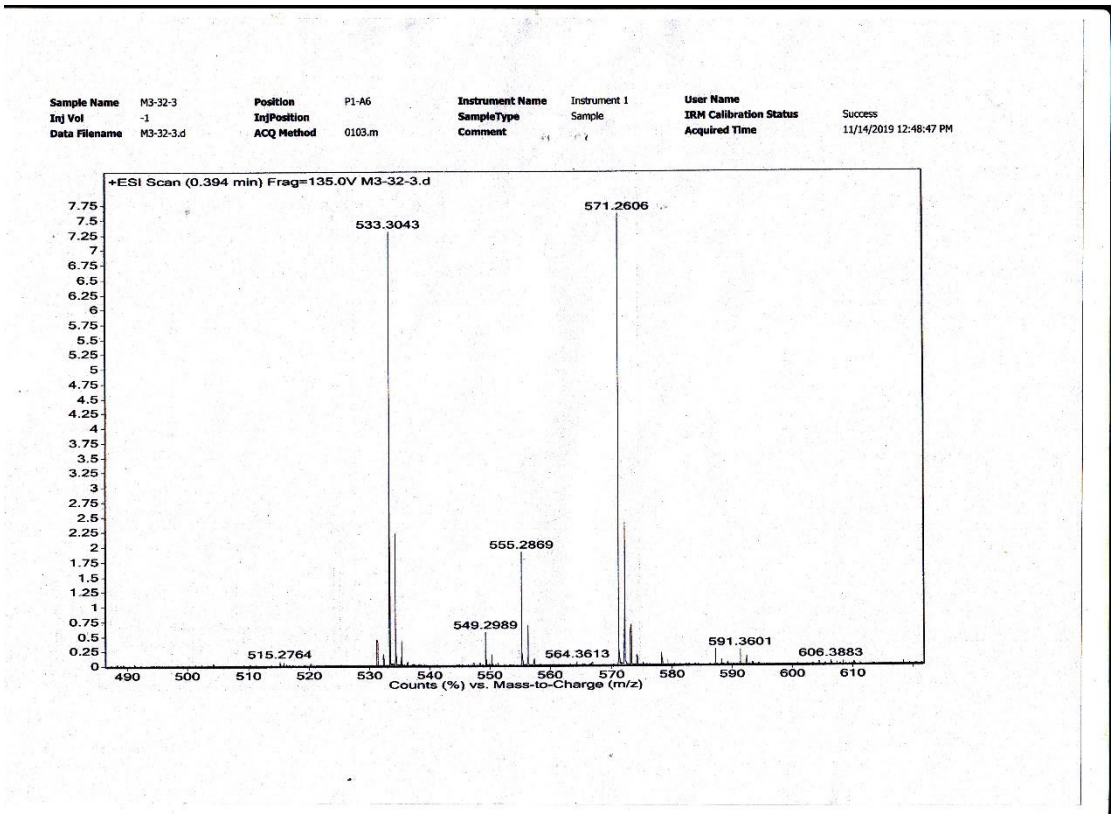


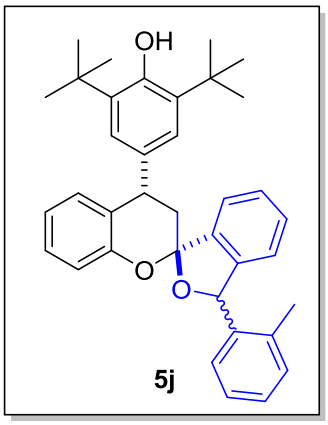
Chemical Formula: $C_{37}H_{40}O_4$
Exact Mass: 548.2927
Molecular Weight: 548.7230
m/z: 548.2927 (100.0%), 549.2960 (40.0%), 550.2994 (5.1%), 550.2994 (2.7%)
Elemental Analysis: C, 80.99; H, 7.35; O, 11.66

HRMS (ESI, m/z) calcd for $C_{37}H_{40}O_4$ $[M+H^+]$ 549.2999, found 549.2994.


OH
O
O
5j, dr=1.6/1
f1 (ppm)

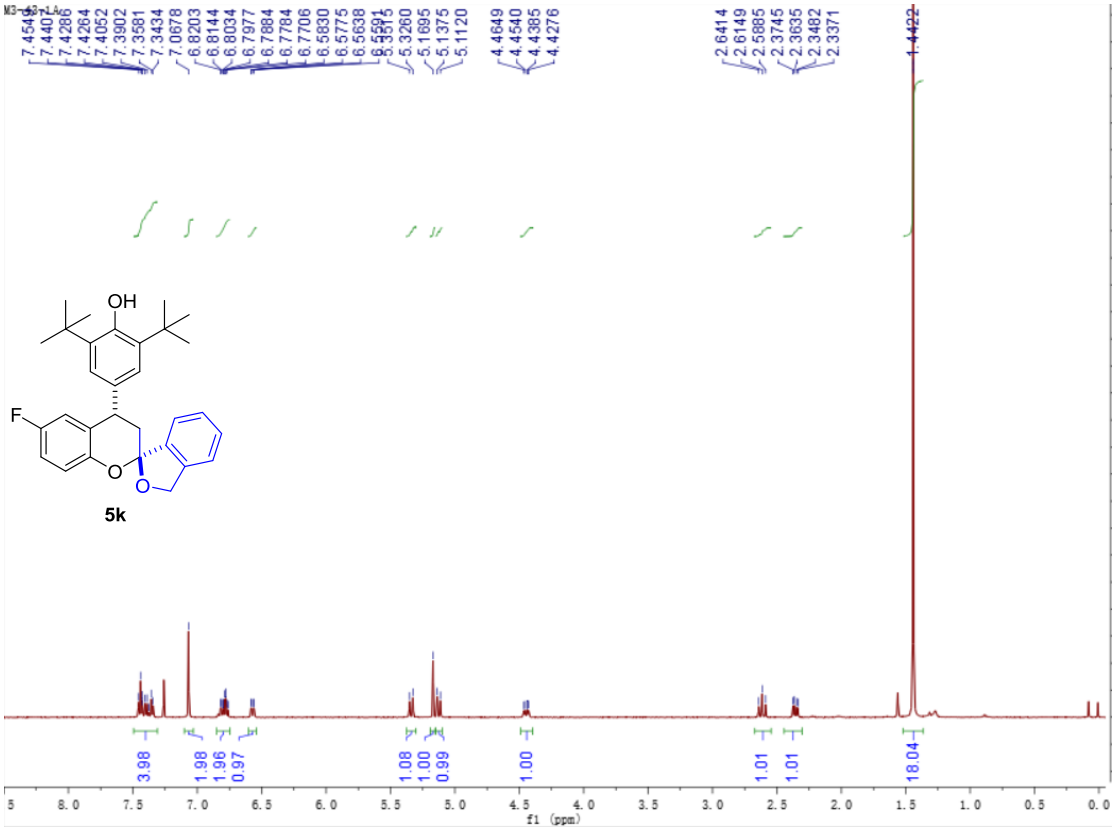

OH
O
O
5j, dr=1.6/1
f1 (ppm)

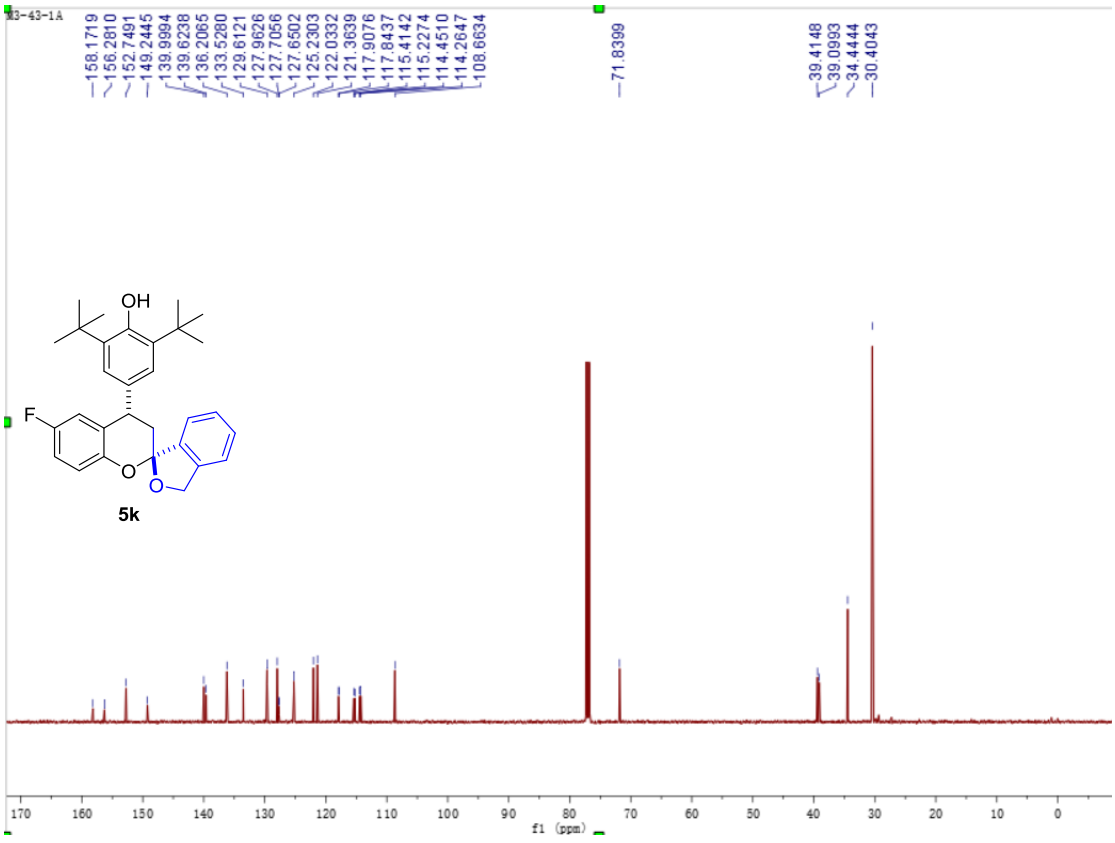


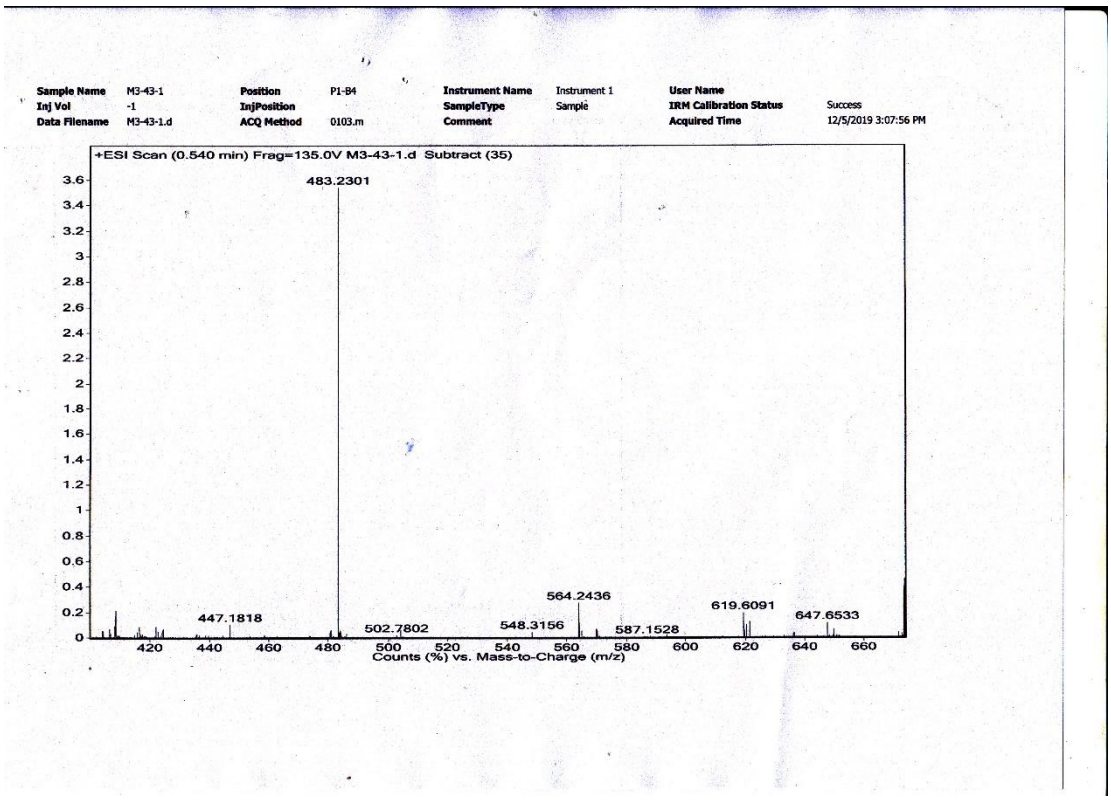


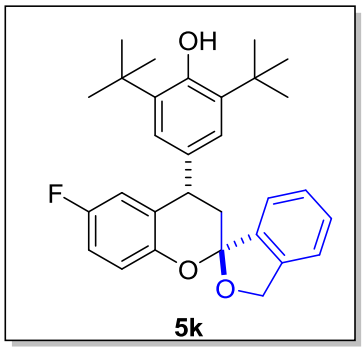
Chemical Formula: $C_{37}H_{40}O_3$
Exact Mass: 532.2977
Molecular Weight: 532.7240
m/z: 532.2977 (100.0%), 533.3011 (40.0%), 534.3045 (5.1%), 534.3045 (2.7%)
Elemental Analysis: C, 83.42; H, 7.57; O, 9.01

HRMS (ESI, m/z) calcd for $C_{37}H_{40}O_3$ [M+H$^+$] 533.3050, found 533.3043.


OH
F
O
O
5k
7.4541
7.4401
7.4286
7.4264
7.4052
7.3902
7.3581
7.3434
7.0678
6.8203
6.8144
6.8034
6.7977
6.7884
6.7784
6.7706
6.5830
6.5775
6.5638
6.5591
5.3260
5.1695
5.1375
5.1120
4.4649
4.4540
4.4385
4.4276
2.6414
2.6149
2.5885
2.3745
2.3635
2.3482
2.3371
1.4422
3.98
1.98
1.96
0.97
1.08
1.00
0.99
1.00
1.01
1.01
18.04
f1 (ppm)


M3-43-1A
158.1719
156.2810
152.7491
149.2445
139.9994
139.6238
136.2065
133.5280
129.6121
127.9626
127.7056
127.6502
125.2303
122.0332
121.3639
117.9076
117.8437
115.4142
115.2274
114.4510
114.2647
108.6634
71.8399
39.4148
39.0993
34.4444
30.4043
OH
F
O
O
5k
f1 (ppm)

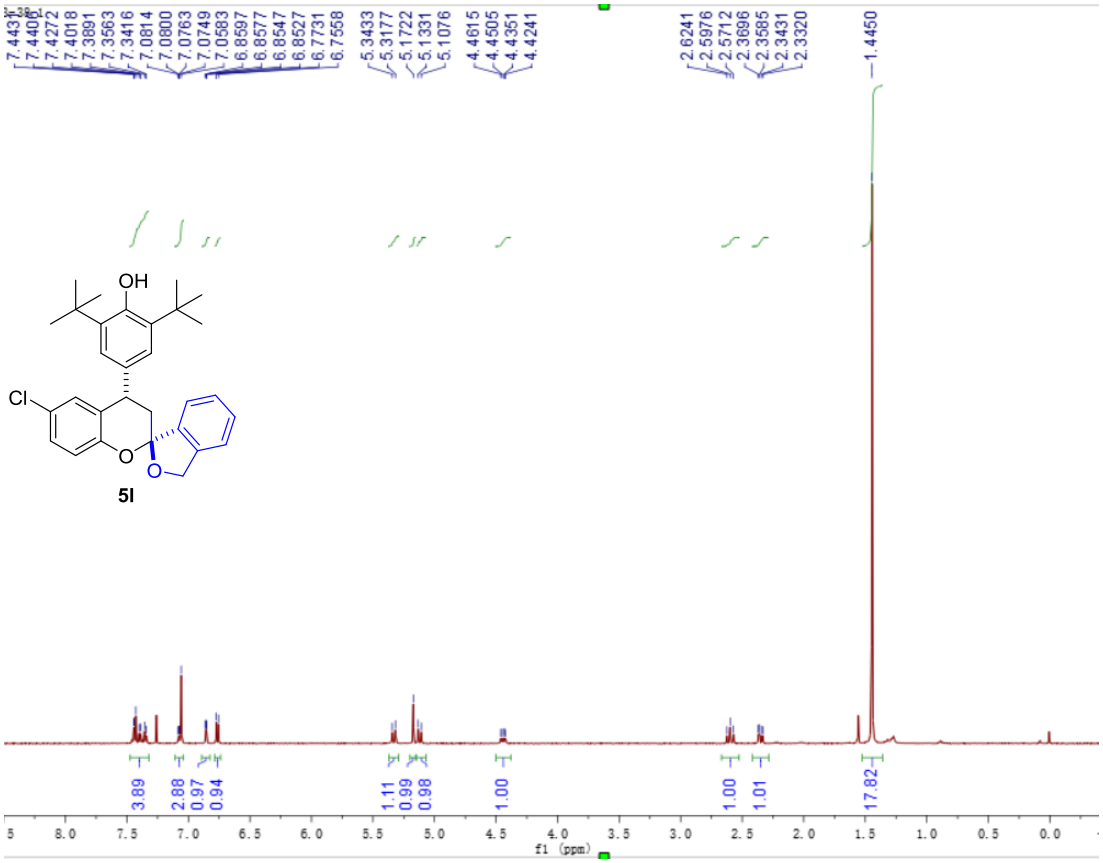


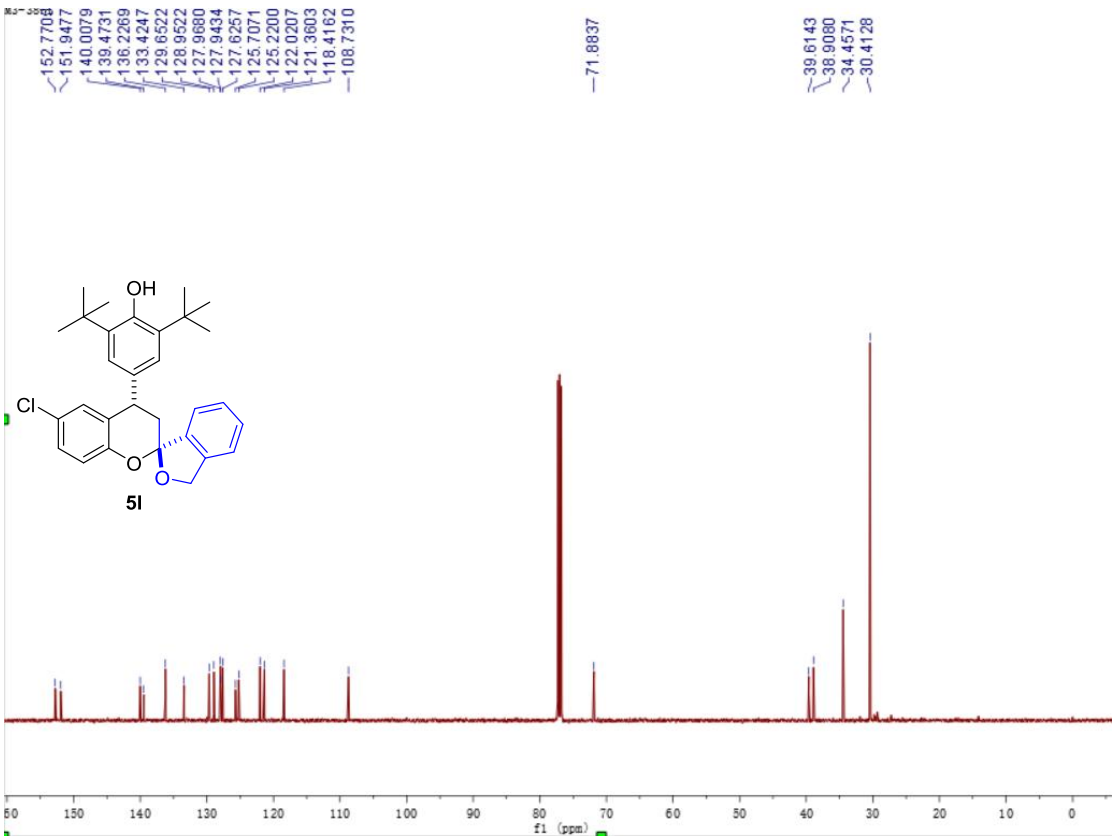


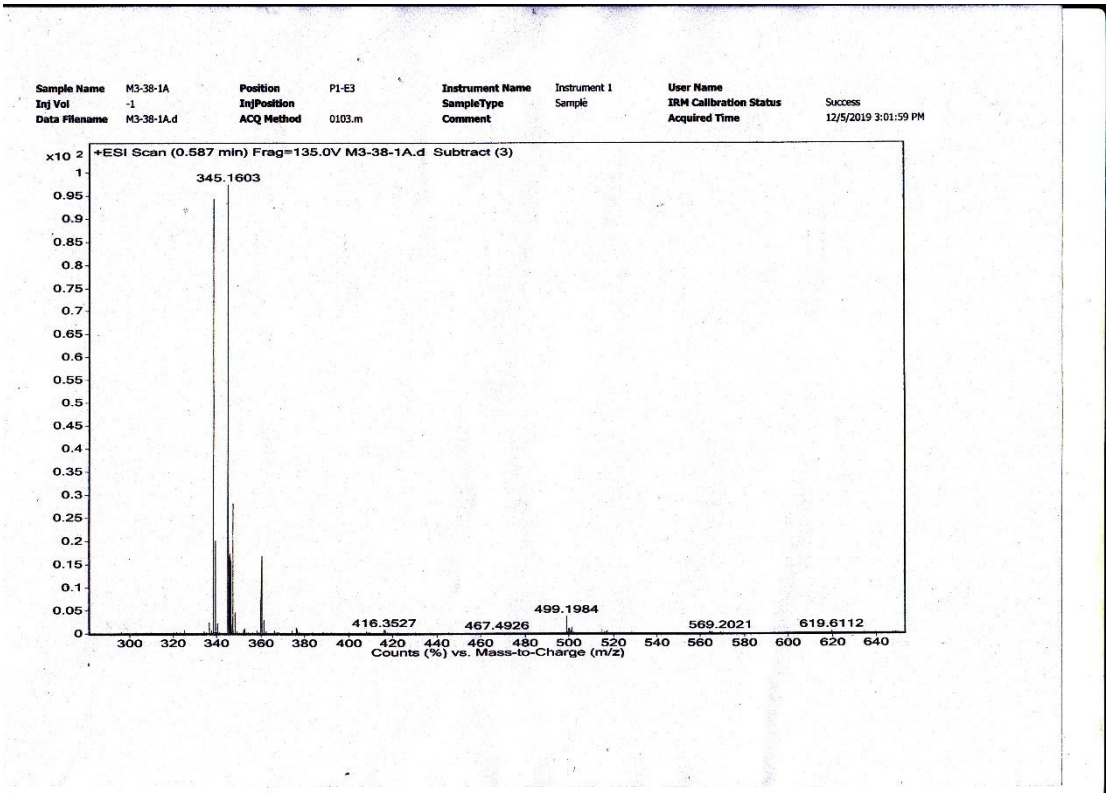
5k

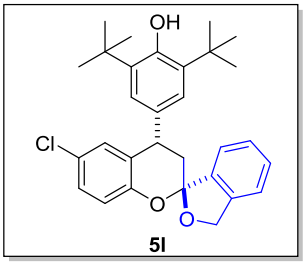
Chemical Formula: $C_{30}H_{33}FO_3$
Exact Mass: 460.2414
Molecular Weight: 460.5894
m/z: 460.2414 (100.0%), 461.2447 (32.4%), 462.2481 (2.7%), 462.2481 (2.4%)
Elemental Analysis: C, 78.23; H, 7.22; F, 4.12; O, 10.42

HRMS (ESI, m/z) calcd for $C_{30}H_{33}FO_3$ [M+Na^+] 483.2306, found 483.2301.


7.4431
7.4400
7.4272
7.4018
7.3891
7.3563
7.3416
7.0814
7.0800
7.0763
7.0749
7.0583
6.8597
6.8577
6.8547
6.8527
6.7731
6.7558
5.3433
5.3177
5.1722
5.1331
5.1076
4.4615
4.4505
4.4351
4.4241
2.6241
2.5976
2.5712
2.3696
2.3585
2.3431
2.3320
1.4450
OH
Cl
O
O
5l
3.89
2.88
0.97
0.94
1.11
0.99
0.98
1.00
1.00
1.01
17.82
f1 (ppm)


152.7708
151.9477
140.0079
139.4731
136.2269
133.4247
129.6522
128.9522
127.9680
127.9434
127.6257
125.7071
125.2200
122.0207
121.3603
118.4162
108.7310
71.8837
39.6143
38.9080
34.4571
30.4128
OH
Cl
O
O
5l
f1 (ppm)

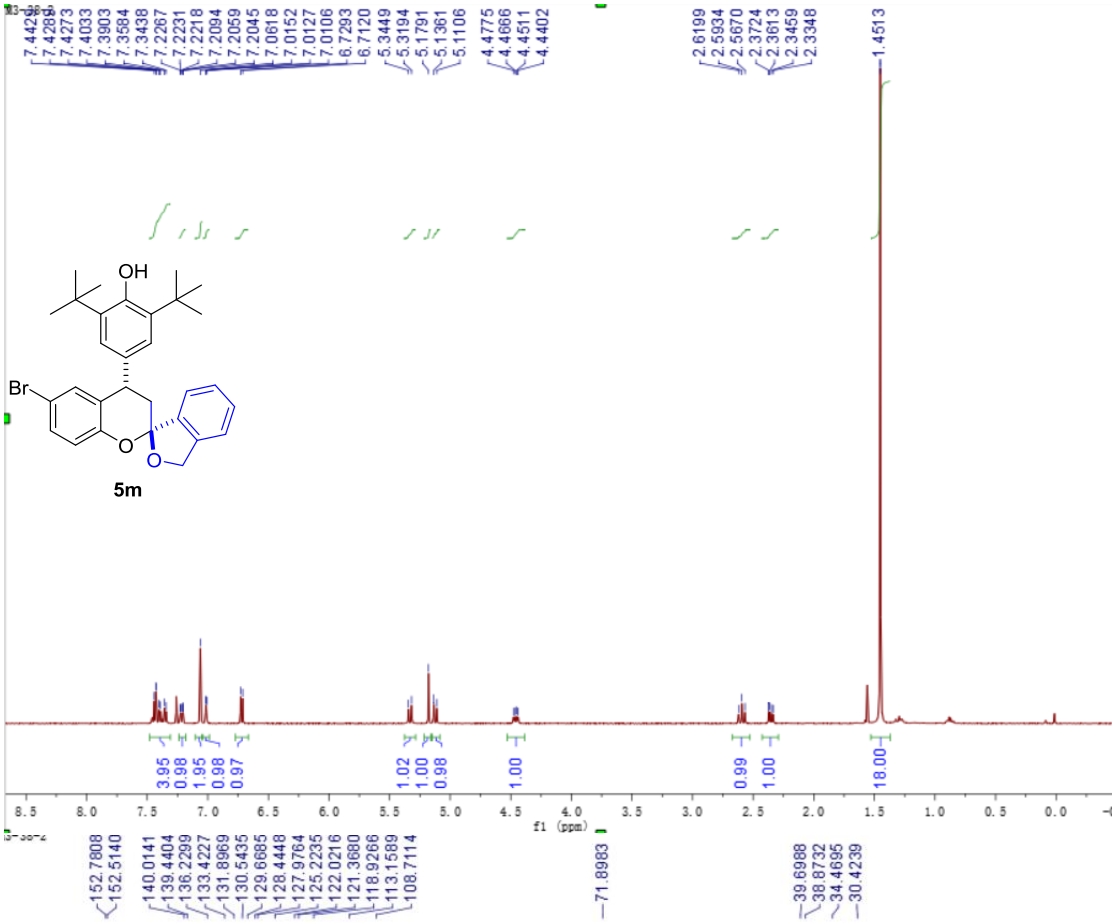


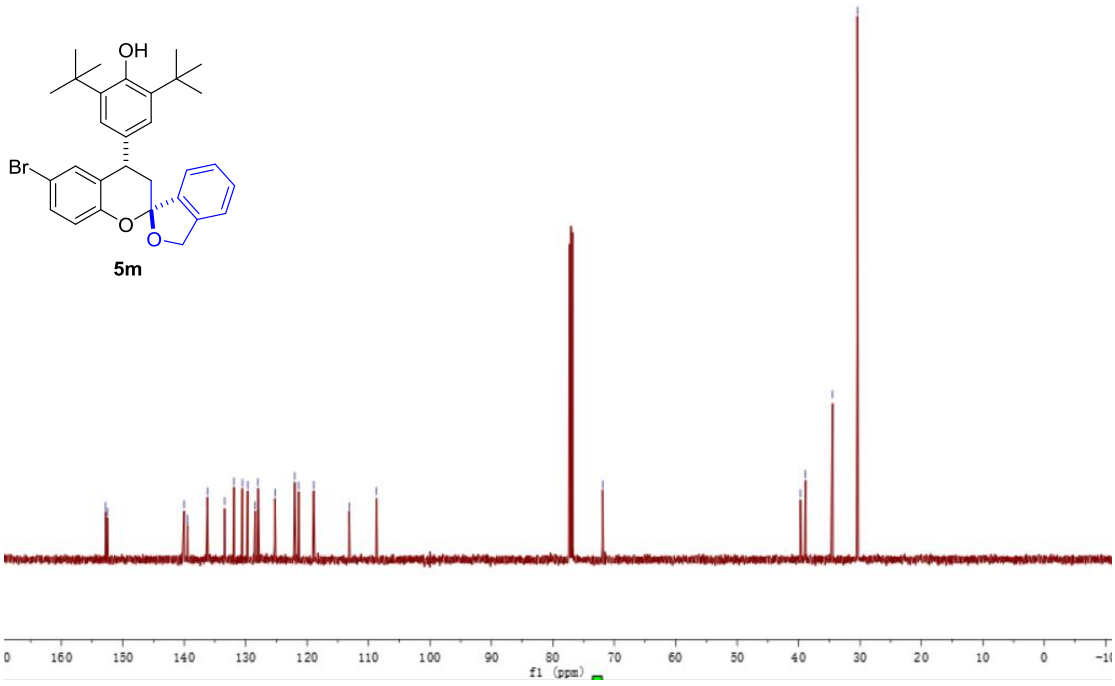


5l

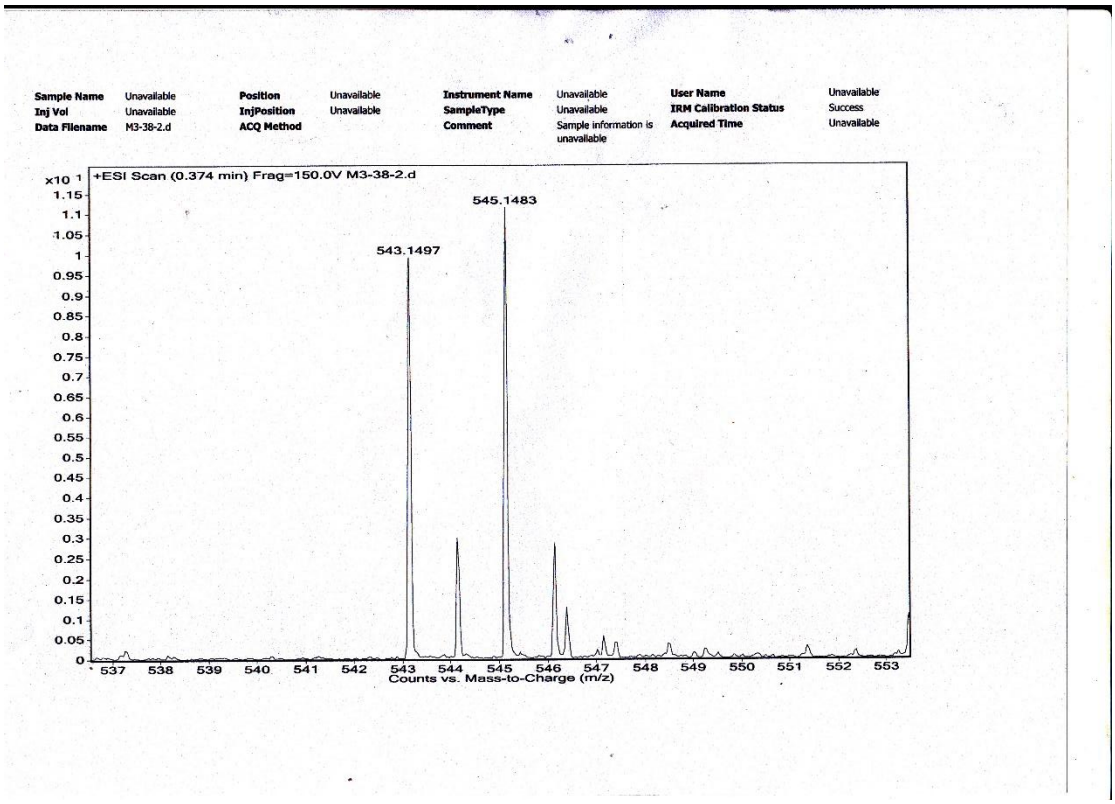
Chemical Formula: $C_{30}H_{33}ClO_3$
Exact Mass: 476.2118
Molecular Weight: 477.0410
m/z: 476.2118 (100.0%), 477.2152 (32.4%), 478.2089 (32.0%), 479.2122 (10.4%), 478.2185 (2.7%), 478.2185 (2.4%)
Elemental Analysis: C, 75.53; H, 6.97; Cl, 7.43; O, 10.06

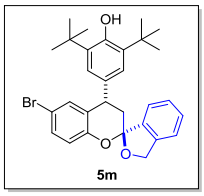
HRMS (ESI, m/z) calcd for $C_{30}H_{33}ClO_3$ $[M+Na^+]$ 499.2010, found 499.1984.


OH
Br
O
O
5m
7.4421
7.4284
7.4273
7.4033
7.3903
7.3584
7.3438
7.2267
7.2231
7.2218
7.2094
7.2059
7.2045
7.0618
7.0152
7.0127
7.0106
6.7293
6.7120
5.3449
5.3194
5.1791
5.1361
5.1106
4.4775
4.4666
4.4511
4.4402
2.6199
2.5934
2.5670
2.3724
2.3613
2.3459
2.3348
1.4513
3.95
0.98
1.95
0.98
0.97
1.02
1.00
0.98
1.00
0.99
1.00
18.00
f1 (ppm)


152.7808
152.5140
140.0141
139.4404
136.2299
133.4227
131.8969
130.5435
129.6685
128.4448
127.9764
125.2235
122.0216
121.3680
118.9266
113.1589
108.7114
71.8983
39.6988
38.8732
34.4695
30.4239
f1 (ppm)

OH
Br
O
O
5m

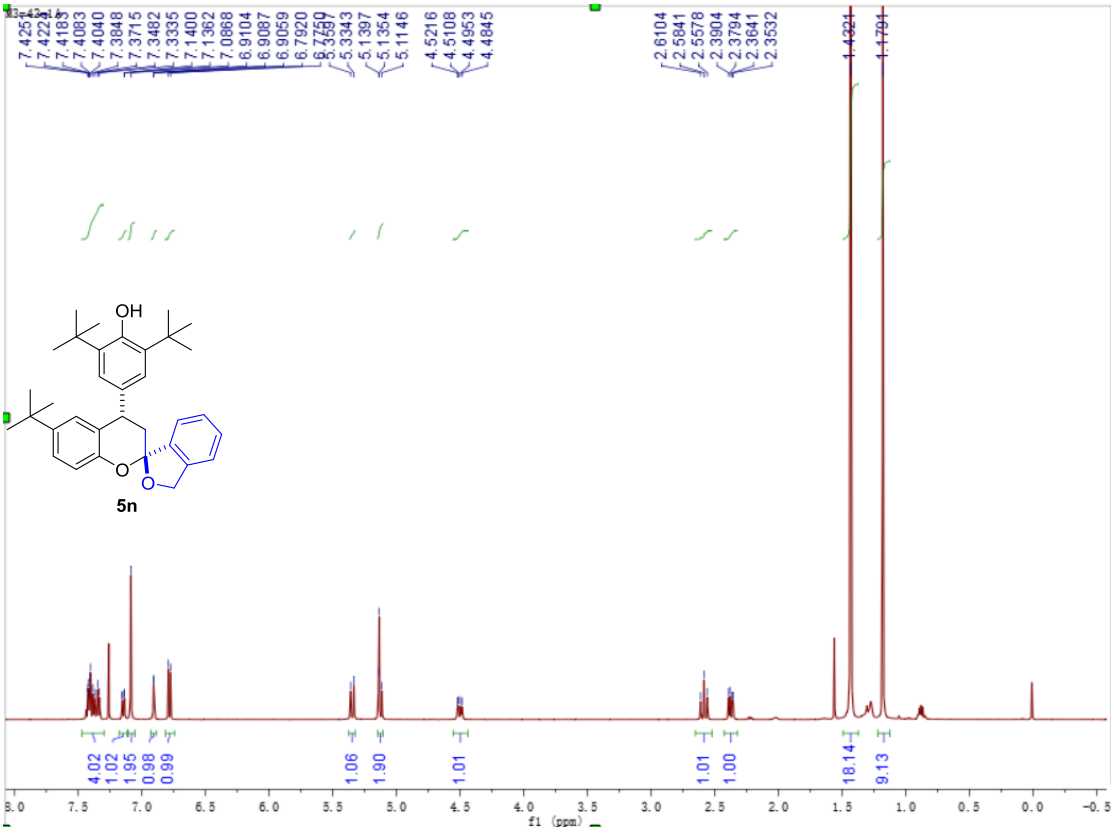


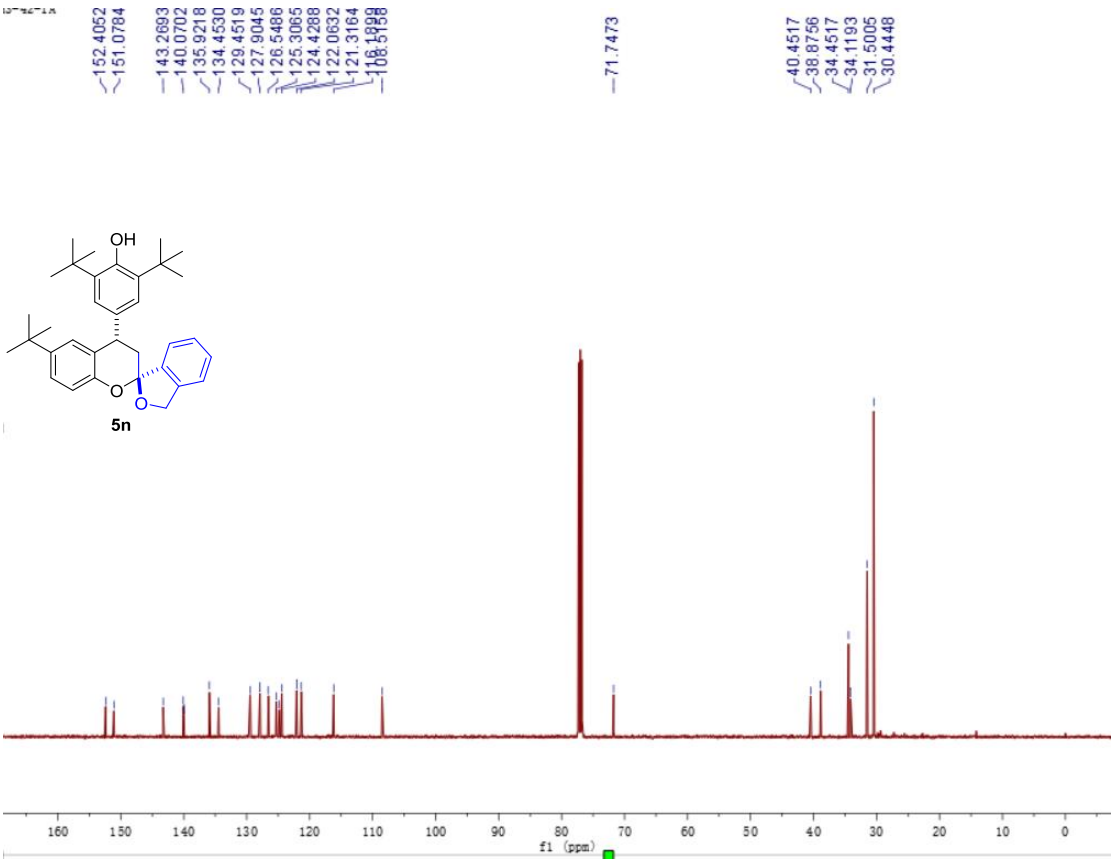


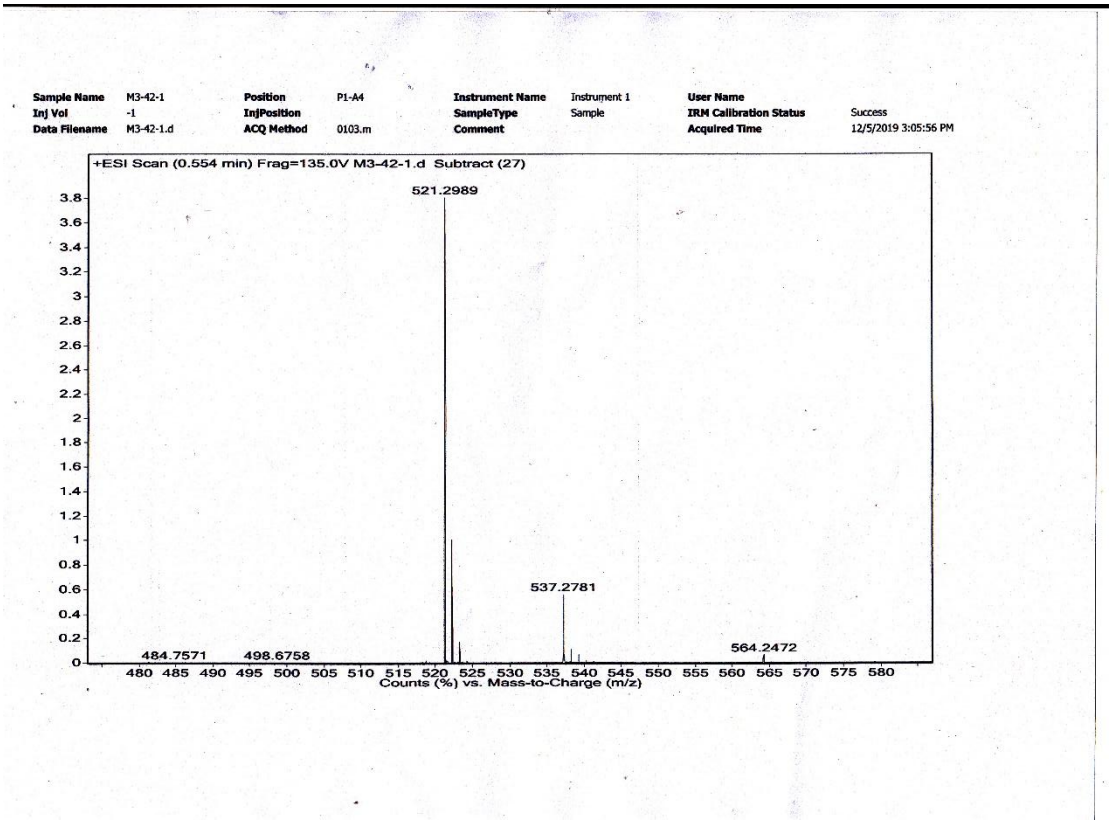
5m

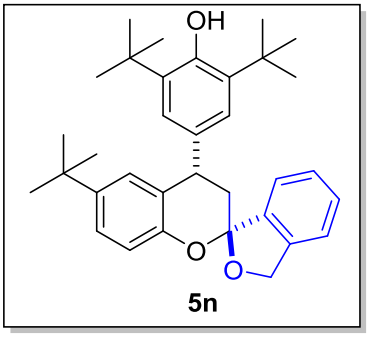
Chemical Formula: $C_{30}H_{33}BrO_3$
Exact Mass: 520.1613
Molecular Weight: 521.4950
m/z: 520.1613 (100.0%), 522.1593 (97.3%), 523.1626 (31.6%), 521.1647 (16.2%), 521.1647 (16.2%), 522.1680 (3.9%), 524.1660 (3.8%), 522.1680 (1.2%), 524.1660 (1.2%)
Elemental Analysis: C, 69.10; H, 6.38; Br, 15.32; O, 9.20

HRMS (ESI, m/z) calcd for $C_{30}H_{33}BrO_3$ [M+Na^+] 543.1505, found 543.1497.


OH
O
O
5n
7.4251
7.4221
7.4183
7.4083
7.4040
7.3848
7.3715
7.3482
7.3335
7.1400
7.1362
7.0868
6.9104
6.9087
6.9059
6.7920
6.7750
5.3597
5.3343
5.1397
5.1354
5.1146
4.5216
4.5108
4.4953
4.4845
2.6104
2.5841
2.5578
2.3904
2.3794
2.3641
2.3532
1.4321
1.4194
4.02
1.02
1.95
0.98
0.99
1.06
1.90
1.01
1.01
1.00
18.14
9.13
f1 (ppm)


OH
O
O
5n
152.4052
151.0784
143.2693
140.0702
135.9218
134.4530
129.4519
127.9045
126.5486
125.3065
124.4288
122.0632
121.3164
71.7473
40.4517
38.8756
34.4517
34.1193
31.5005
30.4448
f1 (ppm)

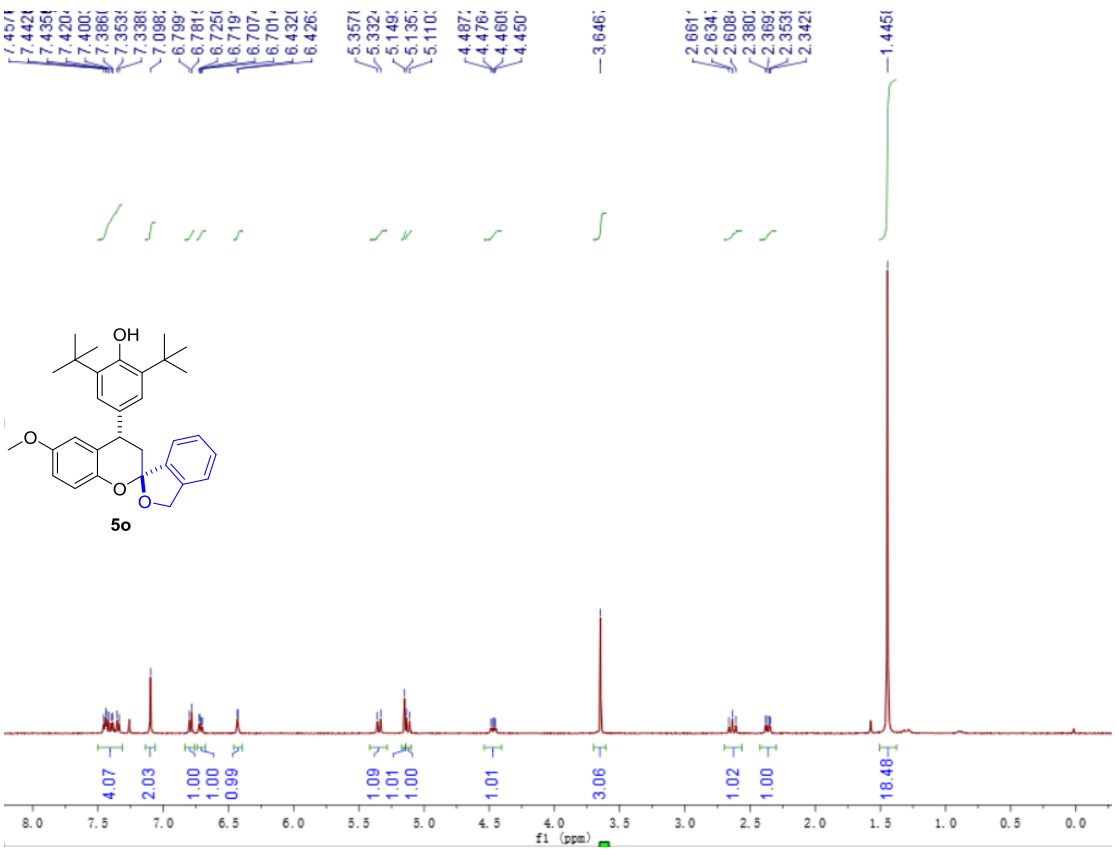


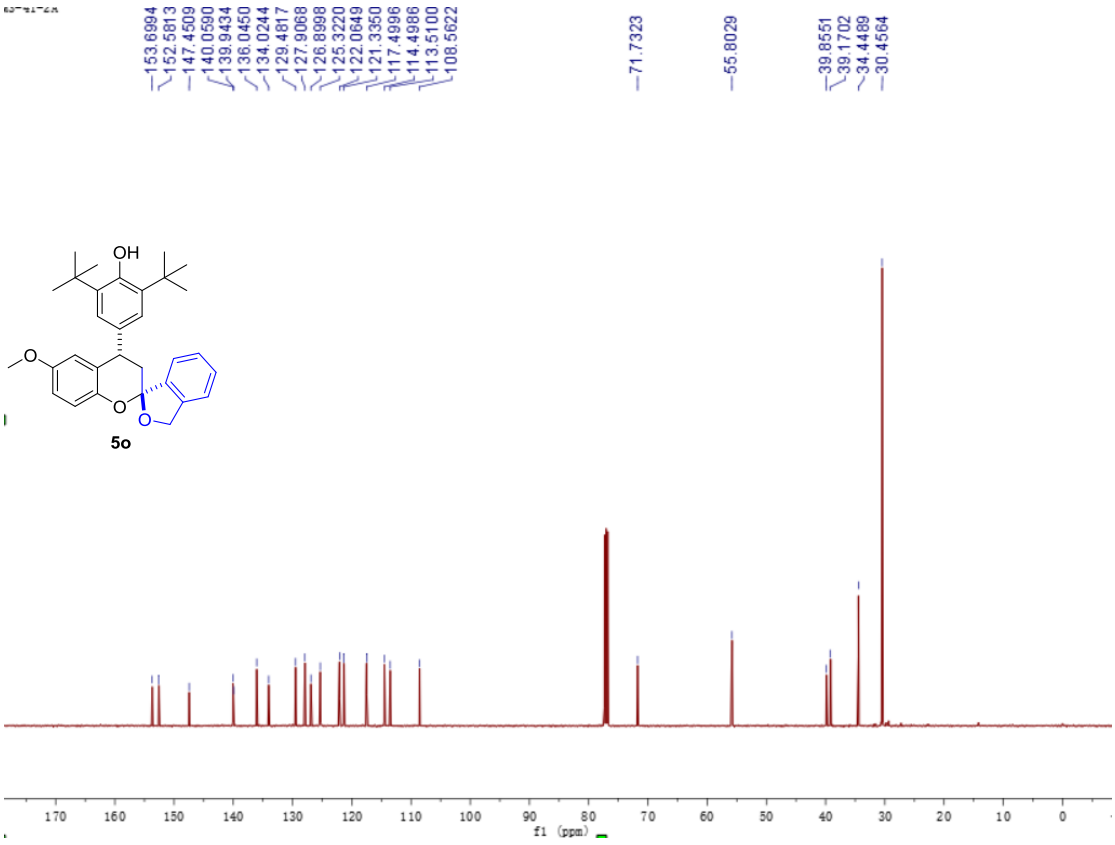


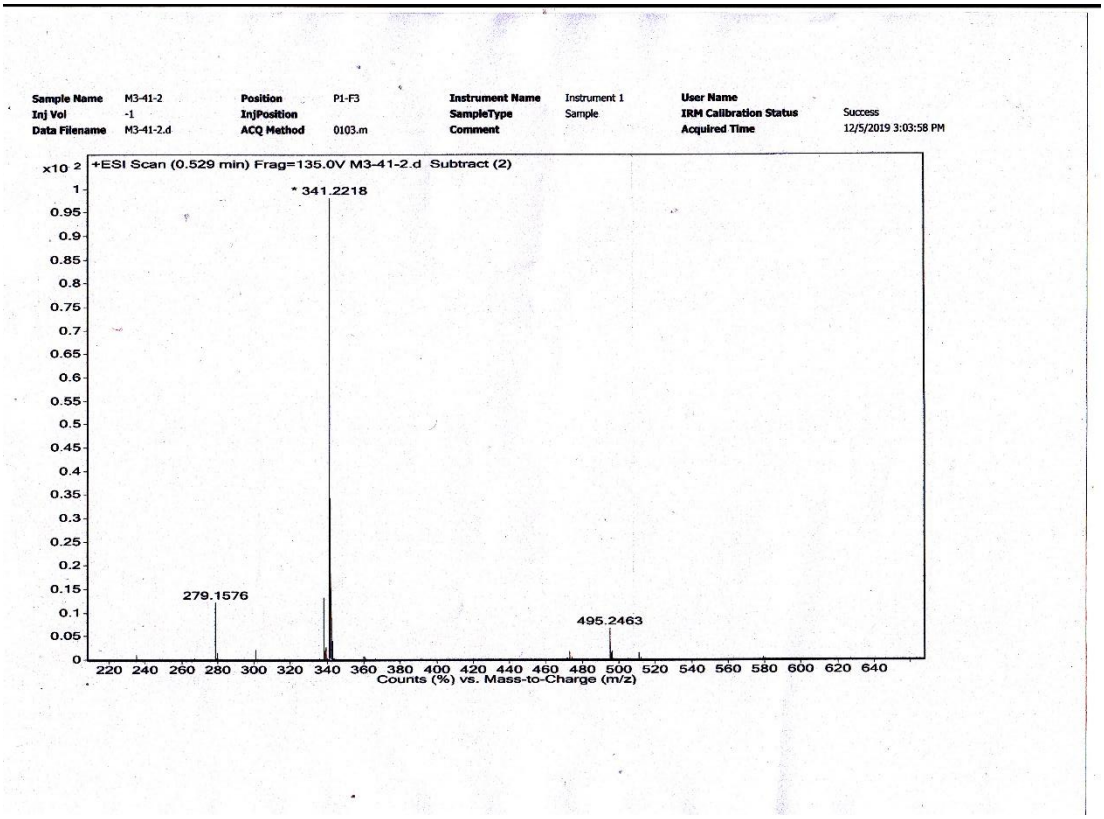
5n

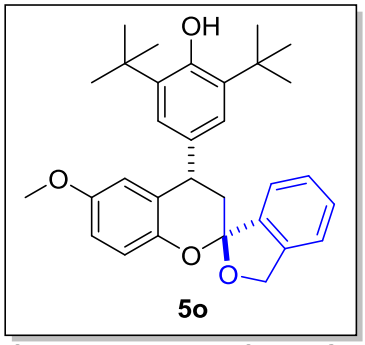
Chemical Formula: $C_{34}H_{42}O_3$
Exact Mass: 498.3134
Molecular Weight: 498.7070
m/z: 498.3134 (100.0%), 499.3168 (36.8%), 500.3201 (3.9%), 500.3201 (2.7%)
Elemental Analysis: C, 81.89; H, 8.49; O, 9.62

HRMS (ESI, m/z) calcd for $C_{34}H_{42}O_3$ [M+Na^+] 521.3026, found 521.2989.


OH
O
O
O
5o
4.07
2.03
1.00
1.00
0.99
1.09
1.01
1.00
1.01
3.06
1.02
1.00
18.48
f1 (ppm)


153.6994
152.5813
147.4509
140.0590
139.9434
136.0450
134.0244
129.4817
127.9068
126.8998
125.3220
122.0649
121.3350
117.4996
114.4986
113.5100
108.5622
71.7323
55.8029
39.8551
39.1702
34.4489
30.4564
OH
O
O
O
5o
f1 (ppm)

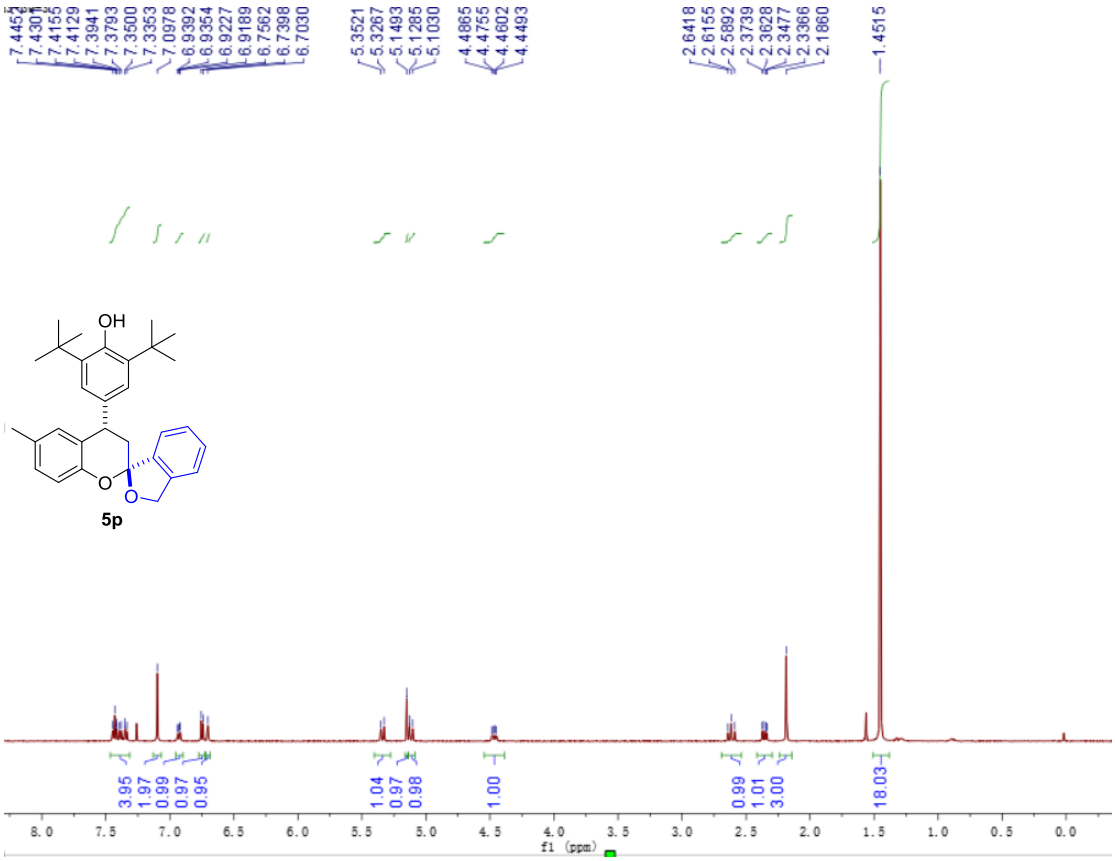




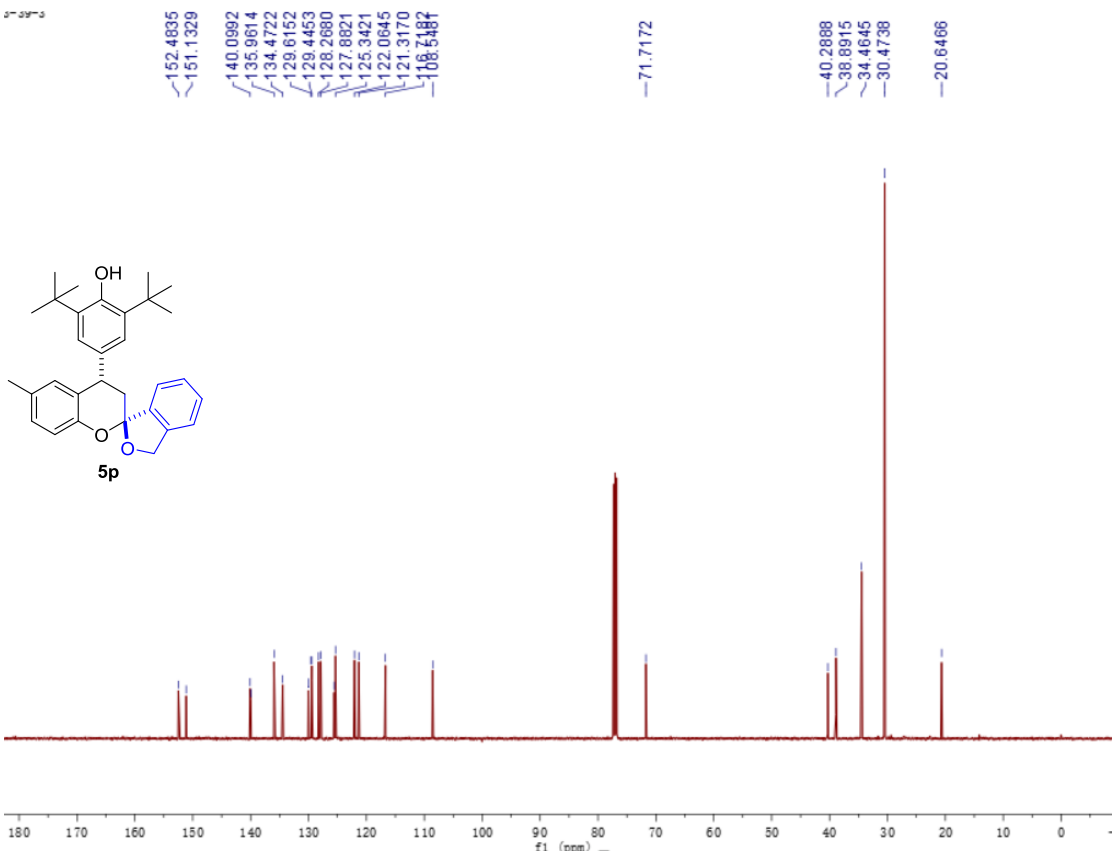
5o

Chemical Formula: $C_{31}H_{36}O_4$
Exact Mass: 472.2614
Molecular Weight: 472.6250
m/z: 472.2614 (100.0%), 473.2647 (33.5%), 474.2681 (2.7%), 474.2681 (2.7%)
Elemental Analysis: C, 78.78; H, 7.68; O, 13.54

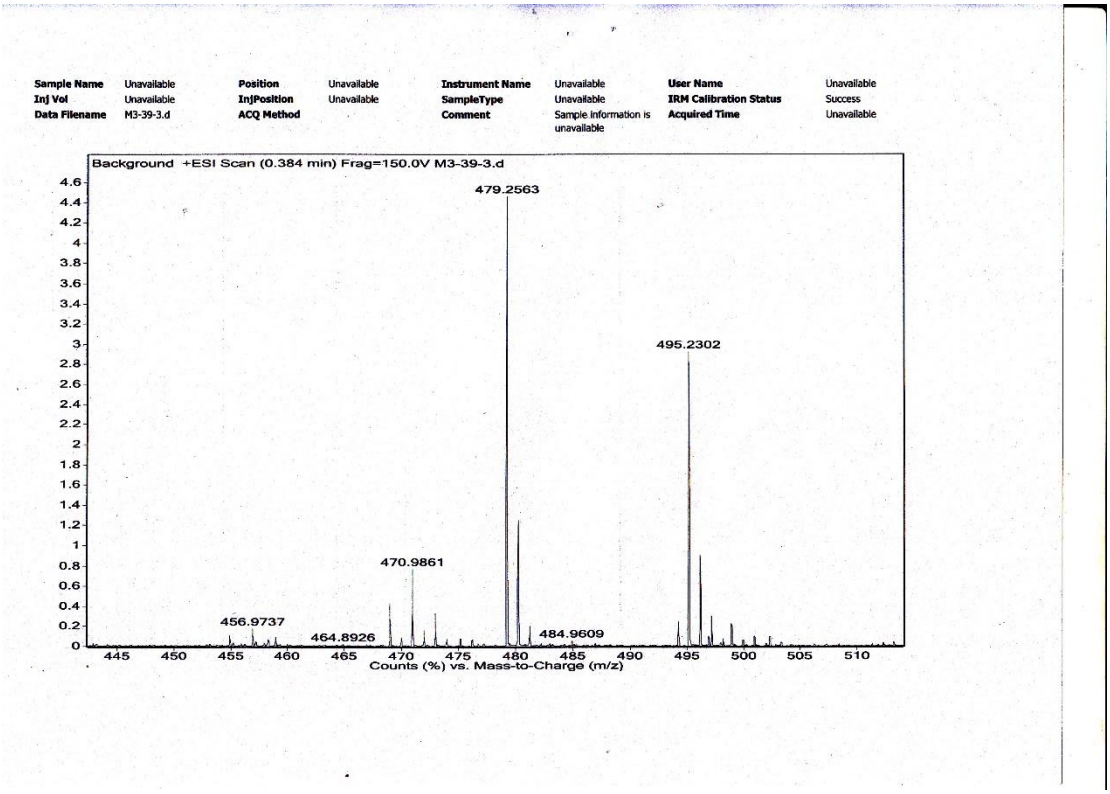
HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_4$ [M+Na^+] 492.5206, found 495.2463.

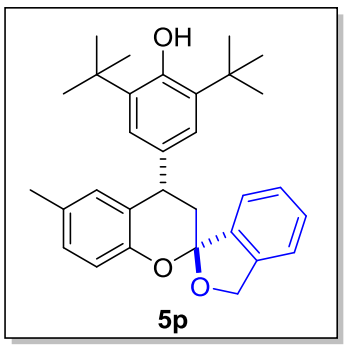

7.4452
7.4301
7.4155
7.4129
7.3941
7.3793
7.3500
7.3353
7.0978
6.9392
6.9354
6.9227
6.9189
6.7562
6.7398
6.7030
5.3521
5.3267
5.1493
5.1285
5.1030
4.4865
4.4755
4.4602
4.4493
2.6418
2.6155
2.5892
2.3739
2.3628
2.3477
2.3366
2.1860
1.4515
OH
O
O
3.95
1.97
0.99
0.97
0.95
1.04
0.97
0.98
1.00
0.99
1.01
3.00
18.03
f1 (ppm)

5p


152.4835
151.1329
140.0992
135.9614
134.4722
129.6152
129.4453
128.2680
127.8821
125.3421
122.0645
121.3170
71.7172
40.2888
38.8915
34.4645
30.4738
20.6466
OH
O
O
f1 (ppm)

5p

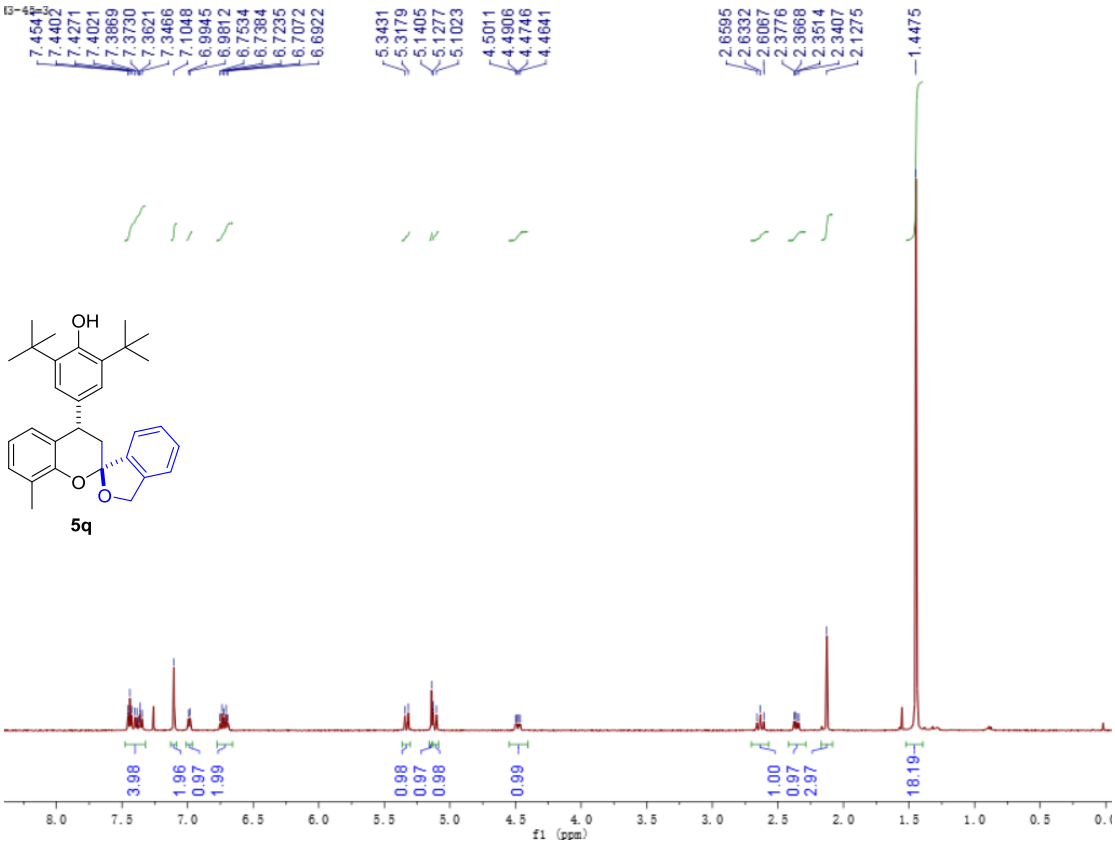


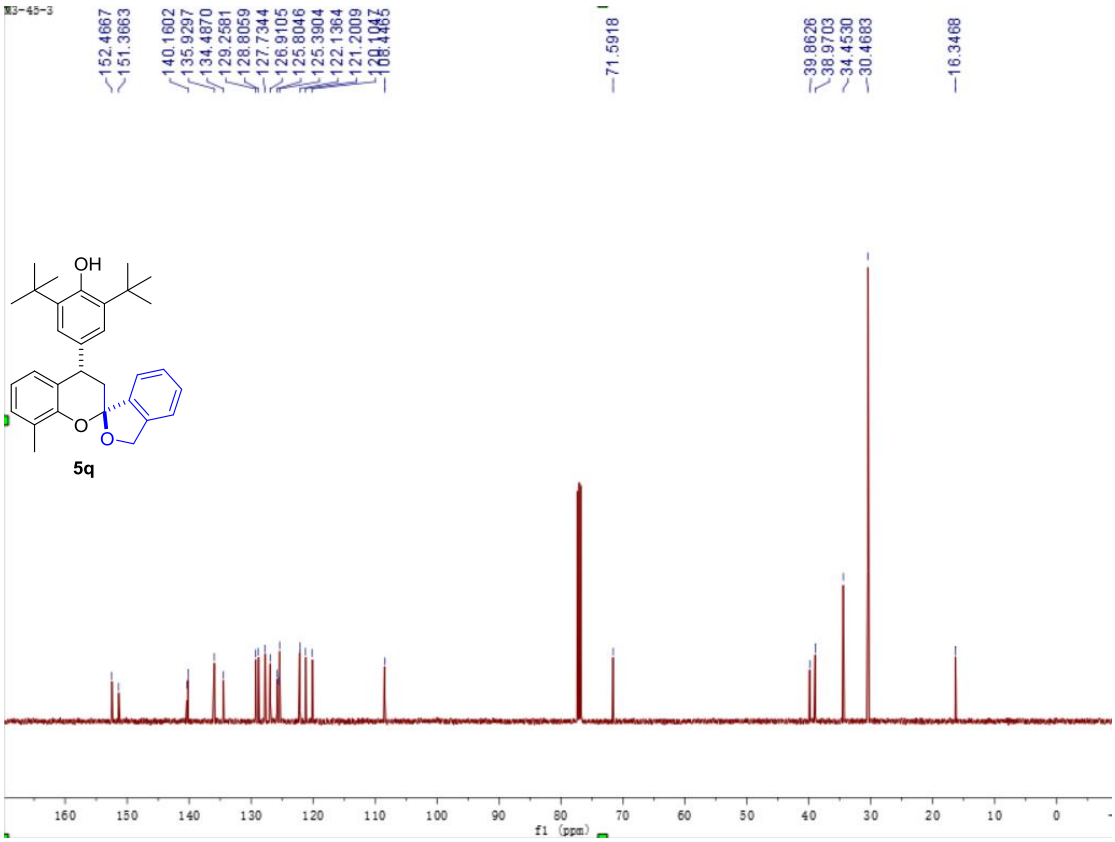


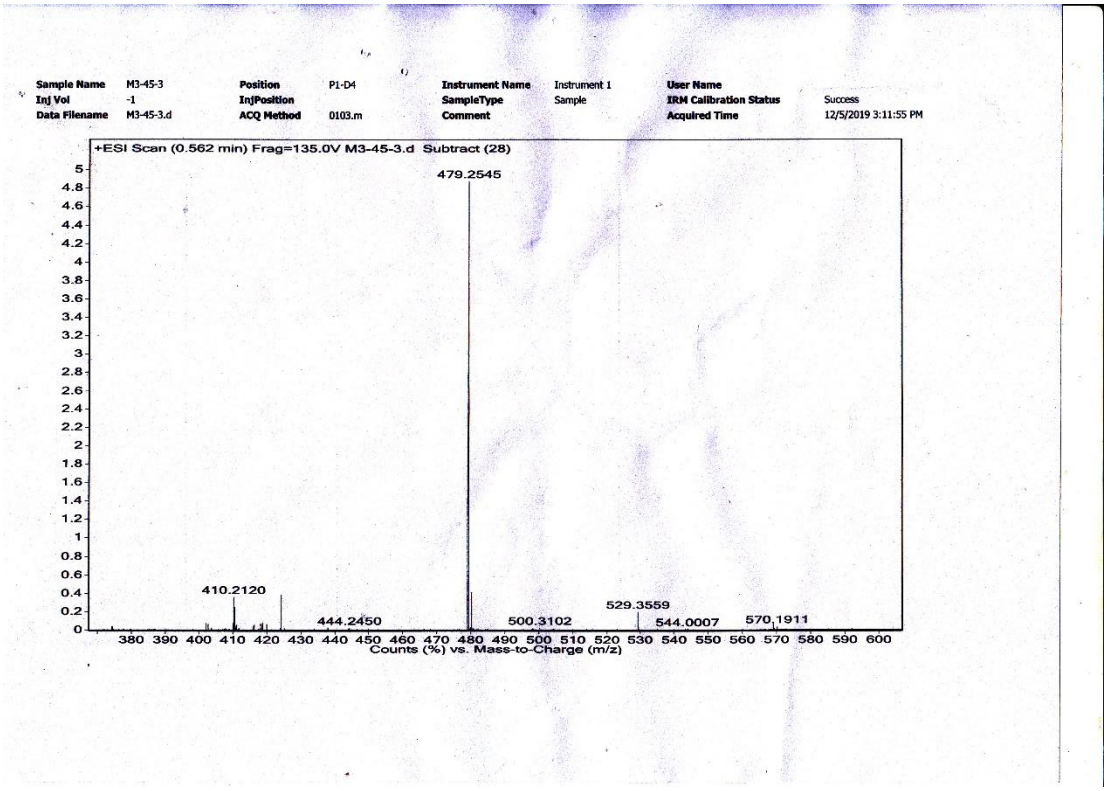
5p

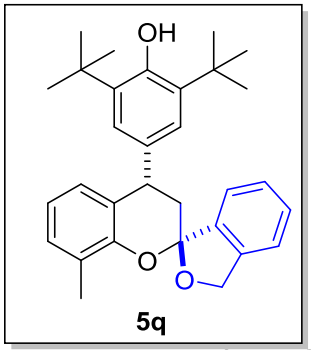
Chemical Formula: $C_{31}H_{36}O_3$
Exact Mass: 456.2664
Molecular Weight: 456.6260
m/z: 456.2664 (100.0%), 457.2698 (33.5%), 458.2732 (2.7%), 458.2732 (2.7%)
Elemental Analysis: C, 81.54; H, 7.95; O, 10.51

HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_3$ [M+Na^+] 479.2557, found 479.2563.


7.4541
7.4402
7.4271
7.4021
7.3869
7.3730
7.3621
7.3466
7.1048
6.9945
6.9812
6.7534
6.7384
6.7235
6.7072
6.6922
5.3431
5.3179
5.1405
5.1277
5.1023
4.5011
4.4906
4.4746
4.4641
2.6595
2.6332
2.6067
2.3776
2.3668
2.3514
2.3407
2.1275
1.4475
OH
O
O
5q
3.98
1.96
0.97
1.99
0.98
0.97
0.98
0.99
1.00
0.97
2.97
18.19
f1 (ppm)


M3-45-3
152.4667
151.3663
140.1602
135.9297
134.4870
129.2581
128.8059
127.7344
126.9105
125.8046
125.3904
122.1364
121.2009
71.5918
39.8626
38.9703
34.4530
30.4683
16.3468
OH
O
O
5q
f1 (ppm)

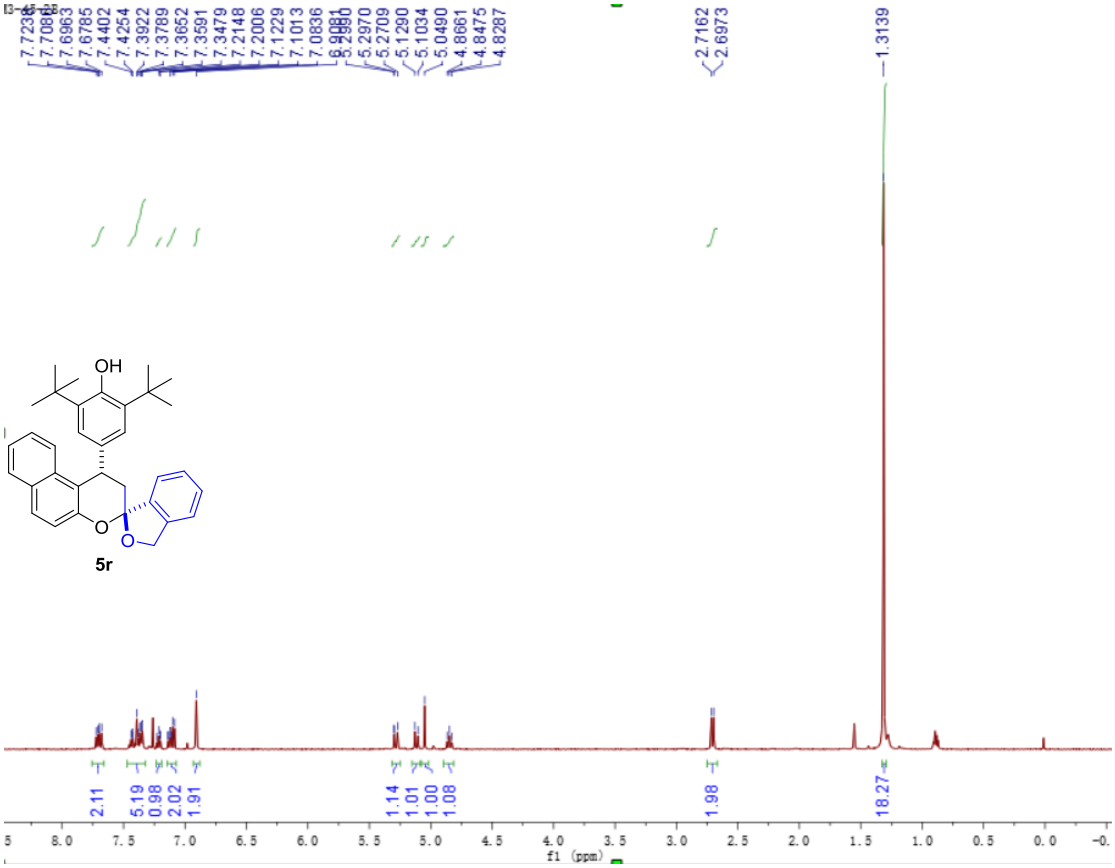


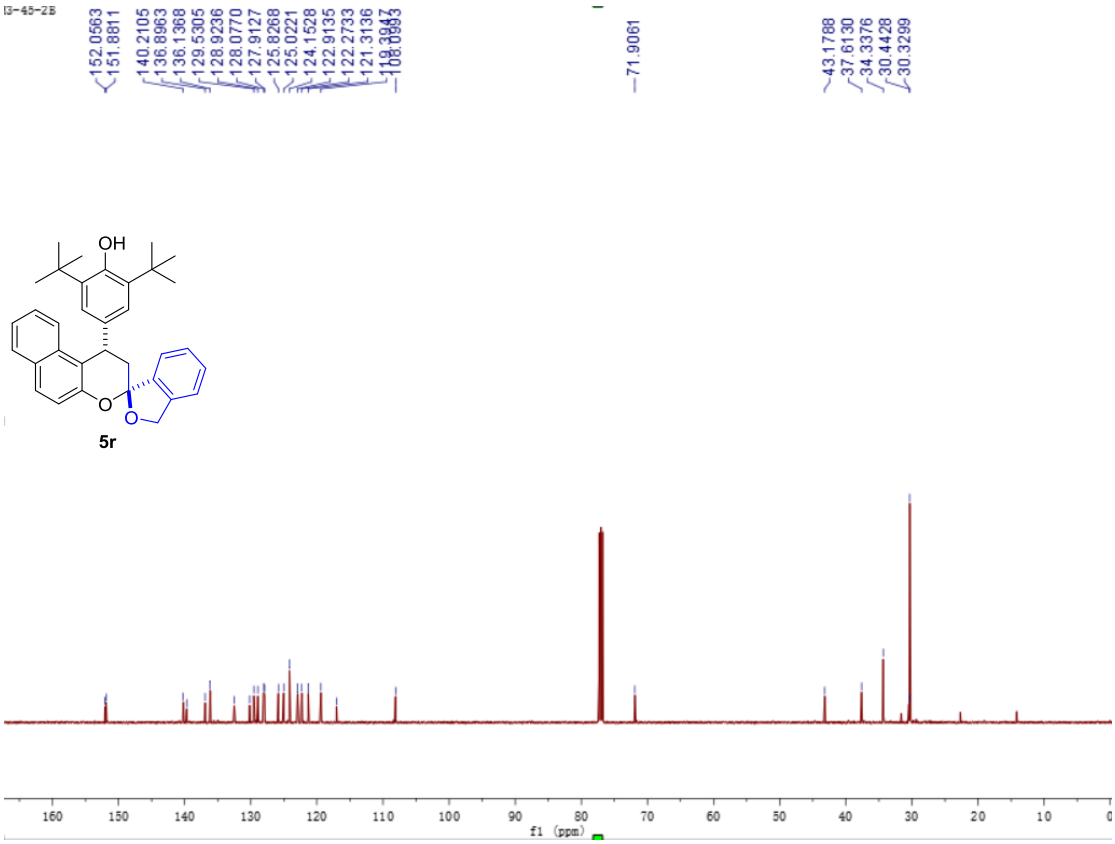


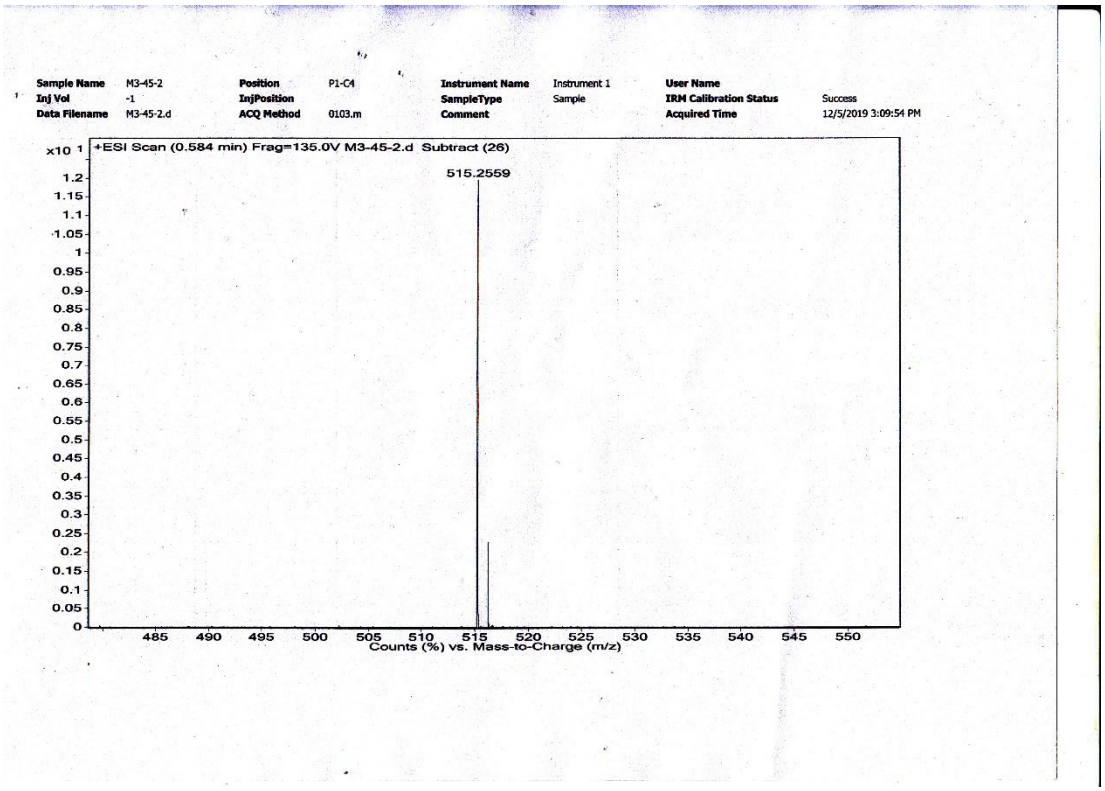
5q

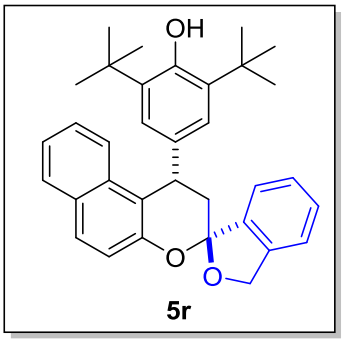
Chemical Formula: $C_{31}H_{36}O_3$
Exact Mass: 456.2664
Molecular Weight: 456.6260
m/z: 456.2664 (100.0%), 457.2698 (33.5%), 458.2732 (2.7%), 458.2732 (2.7%)
Elemental Analysis: C, 81.54; H, 7.95; O, 10.51

HRMS (ESI, m/z) calcd for $C_{31}H_{36}O_3$ [M+Na^+] 479.2557, found 479.2545.


7.7238
7.7088
7.6963
7.6785
7.4402
7.4254
7.3922
7.3789
7.3652
7.3591
7.3479
7.2148
7.2006
7.1229
7.1013
7.0836
6.9081
6.8980
5.2970
5.2709
5.1290
5.1034
5.0490
4.8661
4.8475
4.8287
2.7162
2.6973
1.3139
OH
O
O
5r
2.11
5.19
0.98
2.02
1.91
1.14
1.01
1.00
1.08
1.98
18.27
f1 (ppm)


152.0563
151.8811
140.2105
136.8963
136.1368
129.5305
128.9236
128.0770
127.9127
125.8268
125.0221
124.1528
122.9135
122.2733
121.3136
71.9061
43.1788
37.6130
34.3376
30.4428
30.3299
OH
O
O
5r
f1 (ppm)

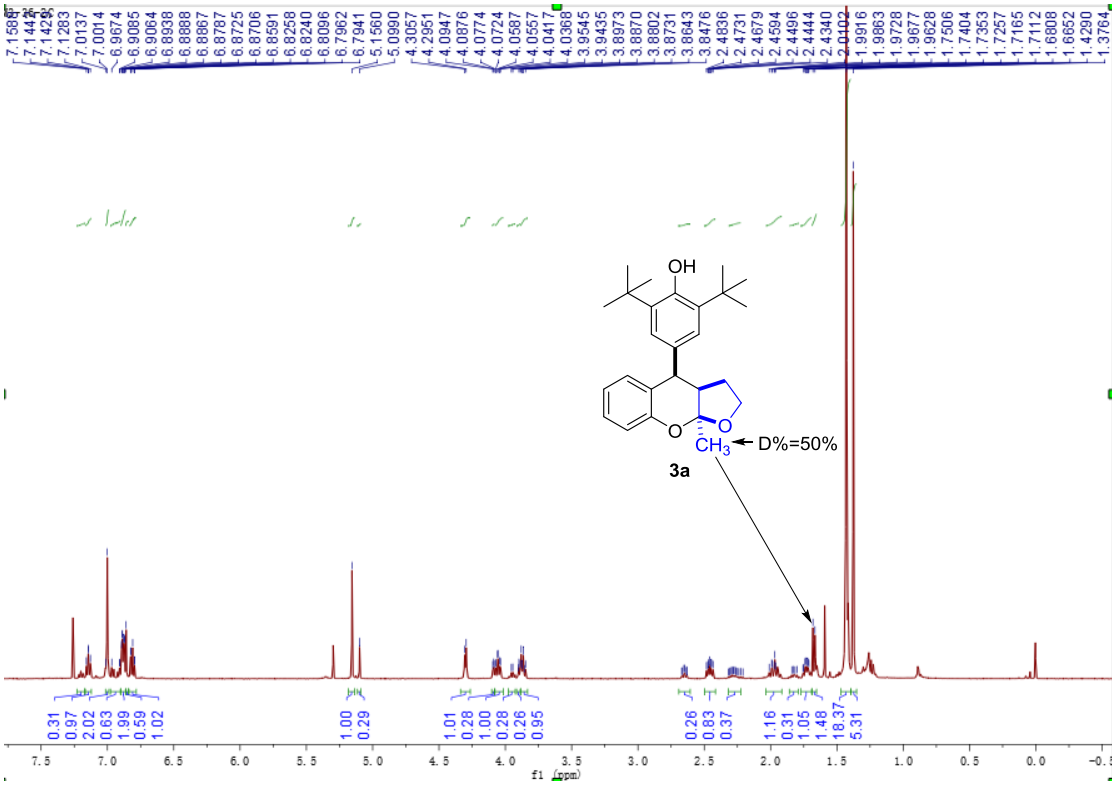




5r

Chemical Formula: $C_{34}H_{36}O_3$
Exact Mass: 492.2664
Molecular Weight: 492.6590
m/z: 492.2664 (100.0%), 493.2698 (36.8%), 494.2732 (3.9%), 494.2732 (2.7%)
Elemental Analysis: C, 82.89; H, 7.37; O, 9.74

HRMS (ESI, m/z) calcd for $C_{34}H_{36}O_3$ [M+Na^+] 515.2557, found 515.2559.


OH
O
O
CH3
D%=50%
3a
f1 (ppm)