

Supplementary Information

Enzyme and photoredox sequential catalysis for the synthesis of 1,3-oxazine derivatives in one pot

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1. Materials

Lipase B *candida antarctica* immobilized on Immobead 150, recombinant from yeast (CALB) was purchased from Sigma-Aldrich [52583-50 G, Lot#BCBD1758, 3766 U/g solid. 1 U corresponds to the amount of enzyme which liberates 1 μ mol butyric acid per minute at pH 7.5 and 40 °C (tributyrin as substrate)]. Ethyl *N*-aryl glycinate **1** were prepared according to the literature.^[1] Unless otherwise noted, all reagents were purchased from commercial suppliers and used without further purification.

2. General methods

Reactions were monitored by thin-layer chromatography (TLC) with Haiyang GF254 silica gel plates (Qingdao Haiyang chemical industry Co Ltd. Qingdao, China) using UV light and vanillic aldehyde as visualizing agents. Flash column chromatography was performed using 200-300 mesh silica gel at increased pressure. ¹H NMR and ¹³C NMR spectra were recorded on Bruker-AM 600 (600 MHz) (Bruker BioSpin AG Ltd., Beijing, China). Chemical shifts were reported in ppm from TMS with the solvent resonance as the internal standard. Data were reported as follows: chemical shifts (δ) in ppm, coupling constants (J) in Hz, and solvent (CDCl₃). High-resolution mass spectra were obtained by using ESI ionization sources (Varian QFT-ESI).

3. Extra information for optimization of the reaction conditions

Table S1 Screening of the enzyme loading ^a

CC1=CC=C(C=C1)NC(=O)OCC + Oc1ccc2ccccc2c1
 $\xrightarrow[\text{CALB, MeCN, rt, 48 h}]{\text{12 W fluorescent bulb, Ru(bpy)}_3\text{Cl}_2}$
CC1=CC=C(C=C1)N(Cc2cc3ccccc3oc2)C1

1a **2a** **3aa**

Entry	CALB (U)	Yield (%) ^b
1	113	58
2	151	61
3	188	62
4	226	63
5	264	57
6	301	56

^a Reaction conditions: **1a** (0.6 mmol), **2a** (0.2 mmol), MeCN (1 mL, containing 1.6% water), Ru(bpy)₃Cl₂ (1 mol%)

and CALB under irradiation of 12 W fluorescent bulb at rt for 48 h.

^b Determined by HPLC.

Table S2 Screening of the fluorescent bulb ^a

CC1=CC=C(C=C1)NC(=O)OCC + Oc1ccc2ccccc2c1
 $\xrightarrow[\text{CALB, MeCN, rt, 48 h}]{\text{fluorescent bulb, Ru(bpy)}_3\text{Cl}_2}$
CC1=CC=C(C=C1)N(Cc2cc3ccccc3oc2)C1

1a **2a** **3aa**

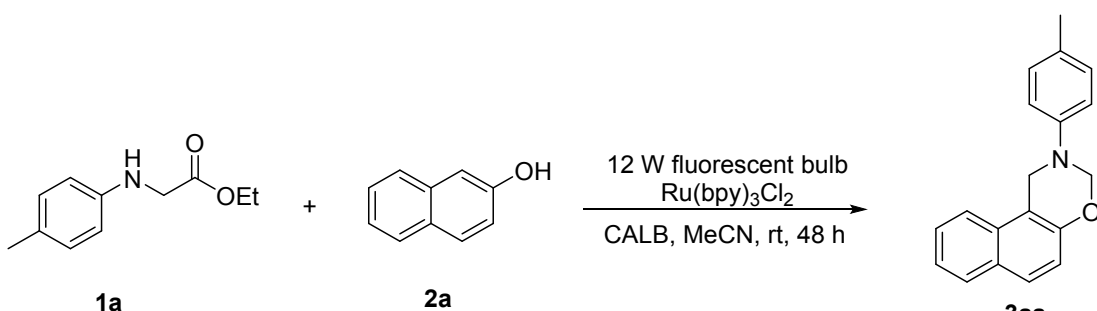
Entry	fluorescent bulb (W)	Yield (%) ^b
1	5	53
2	12	62
3	23	60
4	32	62

^a Reaction conditions: **1a** (0.6 mmol), **2a** (0.2 mmol), MeCN (1 mL, containing 1.6% water), Ru(bpy)₃Cl₂ (1 mol%)

and CALB (188 U) under irradiation of fluorescent bulb at rt for 48 h.

^b Determined by HPLC.

Table S3 Influence of water addition on the model reaction ^a



1a + **2a** $\xrightarrow[\text{CALB, MeCN, rt, 48 h}]{\text{12 W fluorescent bulb, Ru(bpy)}_3\text{Cl}_2}$ **3aa**

Entry	MeCN (mL) ^c	Water addition (mL)	Yield (%) ^b
1	1.00	0	62
2	0.975	0.025	60
3	0.950	0.050	59
4	0.925	0.075	59
5	0.900	0.100	42
6	0.850	0.150	28
7	0.800	0.200	28

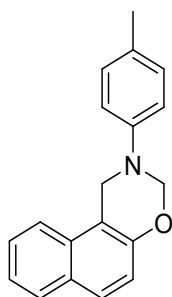
^a Reaction conditions: **1a** (0.6 mmol), **2a** (0.2 mmol), solvent (1 mL), Ru(bpy)₃Cl₂ (1 mol%) and CALB (188 U)

under irradiation of 12 W fluorescent bulb at rt for 48 h.

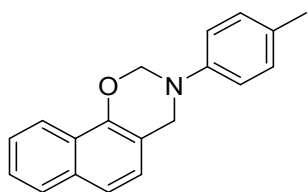
^b Determined by HPLC.

^c MeCN (containing 1.6% water).

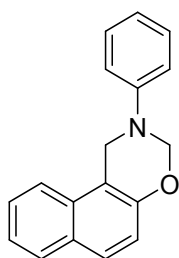
4. Characterization data of the products



2-(*p*-tolyl)-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine (3aa)^[2]: Yellowish liquid; ¹H NMR (600 MHz, CDCl₃): δ 7.82 (d, *J* = 8.1 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.68 (d, *J* = 8.9 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.11 (s, 4H), 7.09 (d, *J* = 8.9 Hz, 1H), 5.44 (s, 2H), 4.97 (s, 2H), 2.30 (s, 3H); ¹³C NMR (151 MHz, CDCl₃): δ 152.4, 146.5, 131.3, 131.3, 129.8, 129.1, 128.7, 128.2, 126.7, 123.6, 121.0, 118.9, 118.8, 112.6, 80.1, 48.3, 20.6.

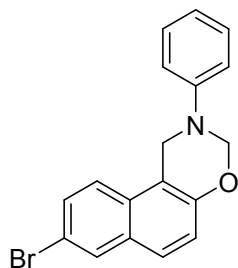


3-(*p*-tolyl)-3,4-dihydro-2*H*-naphtho[2,1-*e*][1,3]oxazine (4a)^[3]: Yellowish liquid; ¹H NMR (600 MHz, CDCl₃): δ 8.16 (d, *J* = 7.5 Hz, 1H), 7.74 - 7.79 (m, 1H), 7.43 - 7.50 (m, 2H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 1H), 7.03 - 7.12 (m, 4H), 5.53 (s, 2H), 4.73 (s, 2H), 2.28 (s, 3H); ¹³C NMR (151 MHz, CDCl₃): δ 149.7, 146.4, 133.3, 131.2, 129.8, 127.5, 126.0, 125.4, 125.1, 124.5, 121.3, 120.2, 118.9, 114.6, 80.4, 50.9, 20.5.

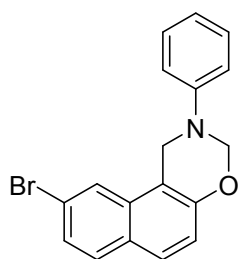


2-phenyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine (3ba)^[2]: Yellowish liquid; ¹H NMR (600 MHz, CDCl₃): δ 7.82 (d, *J* = 8.1 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.68 (d, *J* = 8.9 Hz, 1H), 7.52 - 7.58 (m, 1H), 7.39 - 7.45 (m, 1H), 7.26 - 7.36 (m, 2H), 7.20 (d, *J* = 7.8 Hz, 2H), 7.09 (d, *J* = 8.9 Hz, 1H), 6.98 (t, *J* = 7.3 Hz, 1H), 5.47 (s, 2H), 5.00 (s, 2H); ¹³C NMR (151 MHz, CDCl₃): δ 152.4,

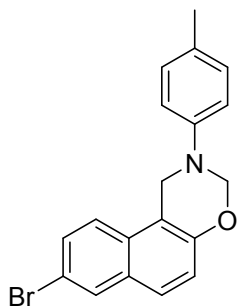
148.8, 131.3, 129.3, 129.1, 128.7, 128.3, 126.7, 123.7, 121.6, 120.9, 118.8, 118.6, 112.5, 79.6, 48.2.



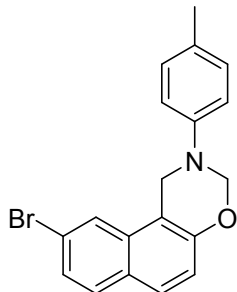
8-bromo-2-phenyl-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine (3bb): Yellowish liquid; ^1H NMR (600 MHz, CDCl_3): δ 7.94 (s, 1H), 7.44 - 7.69 (m, 3H), 7.31 (t, $J = 7.9$ Hz, 2H), 7.18 (d, $J = 8.0$ Hz, 2H), 7.09 (d, $J = 9.0$ Hz, 1H), 6.99 (t, $J = 7.3$ Hz, 1H), 5.45 (s, 2H), 4.95 (s, 2H); ^{13}C NMR (151 MHz, CDCl_3): δ 152.65, 148.59, 130.65, 130.26, 129.87, 129.78, 129.35, 127.40, 122.64, 121.81, 119.98, 118.59, 117.30, 112.80, 79.64, 48.05. HRMS (ESI) m/z 340.0338 ($\text{M} + \text{H}^+$), Cal. $\text{C}_{18}\text{H}_{15}\text{BrNO}$, 340.0332.



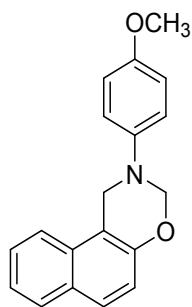
9-bromo-2-phenyl-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine (3bc): White solid; m.p. 110.0-111.8 $^{\circ}\text{C}$; ^1H NMR (600 MHz, CDCl_3): δ 7.86 (s, 1H), 7.63 (dd, $J = 17.0, 8.8$ Hz, 2H), 7.47 (dd, $J = 8.6, 1.4$ Hz, 1H), 7.31 (t, $J = 7.9$ Hz, 2H), 7.19 (d, $J = 8.0$ Hz, 2H), 7.08 (d, $J = 8.9$ Hz, 1H), 6.99 (t, $J = 7.3$ Hz, 1H), 5.45 (s, 2H), 4.91 (s, 2H); ^{13}C NMR (151 MHz, CDCl_3): δ 153.2, 148.5, 132.6, 130.3, 129.4, 128.2, 127.5, 127.0, 123.4, 121.8, 121.3, 119.3, 118.6, 111.9, 79.6, 48.1. HRMS (ESI) m/z 340.0336 ($\text{M} + \text{H}^+$), Cal. $\text{C}_{18}\text{H}_{15}\text{BrNO}$, 340.0332.



8-bromo-2-(*p*-tolyl)-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine (3ab): White solid; m.p. 141.4-143.3 °C; ¹H NMR (600 MHz, CDCl₃): δ 7.94 (s, 1H), 7.58 (dd, *J* = 16.3, 10.3 Hz, 3H), 7.08 (dd, *J* = 15.2, 8.1 Hz, 5H), 5.42 (s, 2H), 4.91 (s, 2H), 2.29 (s, 3H); ¹³C NMR (151 MHz, CDCl₃): δ 152.6, 146.3, 131.5, 130.6, 130.2, 129.9, 129.8, 127.3, 122.7, 112.0, 119.0, 117.2, 112.8, 80.1, 48.2, 20.5. HRMS (ESI) *m/z* 354.0492 (*M* + *H*⁺), Cal. C₁₉H₁₇BrNO, 354.0488.

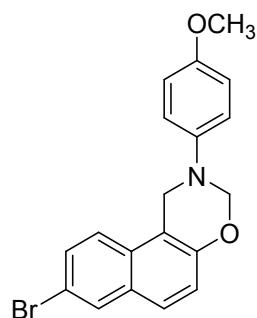


9-bromo-2-(*p*-tolyl)-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine (3ac): White solid; m.p. 128.4-129.4 °C; ¹H NMR (600 MHz, CDCl₃): δ 7.85 (s, 1H), 7.63 (dd, *J* = 18.7, 8.8 Hz, 2H), 7.47 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.06 - 7.11 (m, 5H), 5.42 (s, 2H), 4.88 (s, 2H), 2.30 (s, 3H); ¹³C NMR (151 MHz, CDCl₃): δ 153.2, 146.2, 132.6, 131.5, 130.3, 129.9, 128.2, 127.4, 127.0, 123.4, 121.2, 119.3, 118.9, 111.9, 80.1, 48.3, 20.5. HRMS (ESI) *m/z* 354.0492 (*M* + *H*⁺), Cal. C₁₉H₁₇BrNO, 354.0488.



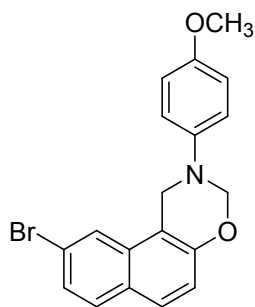
2-(4-methoxyphenyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine (3da)^[2]: Yellowish liquid;

¹H NMR (600 MHz, CDCl₃): δ 7.82 (d, J = 8.1 Hz, 1H), 7.70 (dd, J = 12.6, 8.8 Hz, 2H), 7.54 (dd, J = 11.2, 4.1 Hz, 1H), 7.41 (t, J = 7.4 Hz, 1H), 7.14 (d, J = 9.0 Hz, 2H), 7.09 (d, J = 8.9 Hz, 1H), 6.84 (d, J = 9.0 Hz, 2H), 5.39 (s, 2H), 4.92 (s, 2H), 3.77 (s, 3H); ¹³C NMR (151 MHz, CDCl₃): δ 155.2, 152.4, 142.8, 131.3, 129.1, 128.7, 128.2, 126.7, 123.6, 121.1, 120.9, 118.8, 114.6, 112.6, 80.9, 55.5, 48.8.

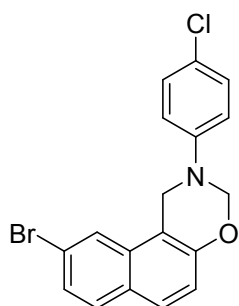


8-bromo-2-(4-methoxyphenyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine (3db): White solid;

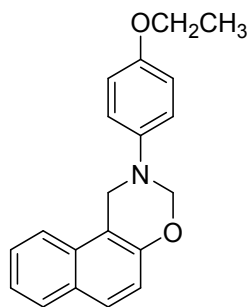
m.p. 160.2-161.0 °C; ¹H NMR (600 MHz, CDCl₃): δ 7.94 (s, 1H), 7.46 - 7.68 (m, 3H), 7.12 (d, J = 8.2 Hz, 2H), 7.08 (d, J = 8.9 Hz, 1H), 6.84 (d, J = 8.1 Hz, 2H), 5.37 (s, 2H), 4.86 (s, 2H), 3.76 (s, 3H); ¹³C NMR (151 MHz, CDCl₃): δ 155.3, 152.6, 142.6, 130.6, 130.3, 129.8, 127.3, 123.0, 121.1, 120.0, 117.2, 114.6, 112.8, 80.9, 55.5, 48.7. HRMS (ESI) m/z 370.0442 (M + H⁺), Cal. C₁₉H₁₇BrNO₂, 370.0437.



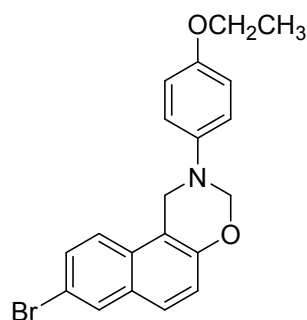
9-bromo-2-(4-methoxyphenyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine (3dc): White solid; m.p. 114.6-115.7 °C; ^1H NMR (600 MHz, CDCl_3): δ 7.83 (s, 1H), 7.63 (dd, J = 15.5, 8.8 Hz, 2H), 7.46 (dd, J = 8.6, 1.5 Hz, 1H), 7.12 (d, J = 8.9 Hz, 2H), 7.07 (d, J = 8.9 Hz, 1H), 6.84 (d, J = 8.9 Hz, 2H), 5.37 (s, 2H), 4.83 (s, 2H), 3.76 (s, 3H); ^{13}C NMR (151 MHz, CDCl_3): δ 155.3, 153.1, 142.5, 132.6, 130.3, 128.1, 127.4, 126.9, 123.5, 121.1, 119.3, 114.6, 111.8, 80.8, 55.5, 48.7. HRMS (ESI) m/z 370.0442 ($\text{M} + \text{H}^+$), Cal. $\text{C}_{19}\text{H}_{17}\text{BrNO}_2$, 370.0437.



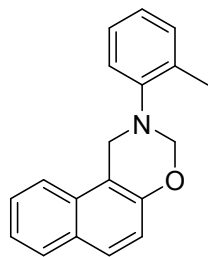
9-bromo-2-(4-chlorophenyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine (3ec): White solid; m.p. 129.3-129.8 °C; ^1H NMR (600 MHz, CDCl_3): δ 7.84 (s, 1H), 7.65 (dd, J = 15.0, 8.7 Hz, 2H), 7.48 (d, J = 8.6 Hz, 1H), 7.24 (d, J = 7.1 Hz, 2H), 7.10 (d, J = 7.1 Hz, 2H), 7.07 (d, J = 8.2 Hz, 1H), 5.41 (s, 2H), 4.88 (s, 2H); ^{13}C NMR (151 MHz, CDCl_3): δ 153.0, 147.2, 132.5, 130.3, 129.3, 128.4, 127.5, 127.1, 126.9, 123.4, 121.4, 119.9, 119.2, 111.5, 79.5, 48.3. HRMS (ESI) m/z 373.9945 ($\text{M} + \text{H}^+$), Cal. $\text{C}_{18}\text{H}_{14}\text{BrClNO}$, 373.9942.



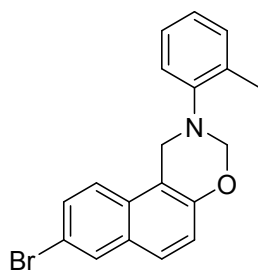
2-(4-ethoxyphenyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine (3fa)^[2]: Yellowish liquid; ¹H NMR (600 MHz, CDCl₃): δ 7.75 (d, J = 8.1 Hz, 1H), 7.63 (dd, J = 12.7, 8.7 Hz, 2H), 7.47 (t, J = 7.6 Hz, 1H), 7.34 (t, J = 7.5 Hz, 1H), 7.07 (d, J = 9.0 Hz, 2H), 7.03 (d, J = 8.9 Hz, 1H), 6.77 (d, J = 9.0 Hz, 2H), 5.32 (s, 2H), 4.85 (s, 2H), 3.92 (q, J = 7.0 Hz, 2H), 1.34 (t, J = 7.0 Hz, 3H); ¹³C NMR (151 MHz, CDCl₃): δ 154.5, 152.4, 142.6, 131.3, 129.1, 128.7, 128.2, 126.6, 123.6, 121.1, 120.9, 118.8, 115.3, 112.6, 80.8, 63.8, 48.8, 14.9.



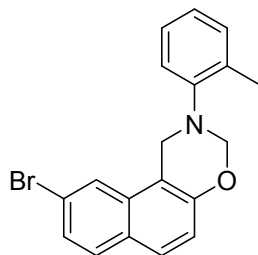
8-bromo-2-(4-ethoxyphenyl)-2,3-dihydro-1H-naphtho[1,2-e][1,3]oxazine (3fb): White solid; m.p. 108.8-110.4 °C; ¹H NMR (600 MHz, CDCl₃): δ 7.94 (s, 1H), 7.51 - 7.61 (m, 3H), 7.09 (t, J = 9.6 Hz, 3H), 6.82 (d, J = 8.8 Hz, 2H), 5.36 (s, 2H), 4.86 (s, 2H), 3.98 (q, J = 6.9 Hz, 2H), 1.39 (t, J = 7.0 Hz, 3H); ¹³C NMR (151 MHz, CDCl₃): δ 154.6, 152.6, 142.4, 130.6, 130.3, 129.8, 127.3, 122.7, 121.1, 120.0, 117.2, 115.3, 112.8, 80.9, 77.2, 77.0, 76.8, 63.8, 48.7, 14.9. HRMS (ESI) m/z 384.0598 (M + H⁺), Cal. C₂₀H₁₉BrNO₂, 384.0594.



2-(*o*-tolyl)-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine (3ca)^[2]: Yellowish liquid; ¹H NMR (600 MHz, CDCl₃): δ 7.84 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.9 Hz, 1H), 7.67 (d, *J* = 8.3 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.4 Hz, 1H), 7.28 (t, *J* = 8.6 Hz, 2H), 7.16 (d, *J* = 8.9 Hz, 1H), 7.05 - 7.10 (m, 2H), 5.30 (s, 2H), 4.82 (s, 2H), 2.52 (s, 3H); ¹³C NMR (151 MHz, CDCl₃): δ 152.4, 148.7, 132.5, 131.3, 131.2, 129.1, 128.7, 128.2, 126.8, 126.6, 124.4, 123.6, 122.0, 121.0, 118.9, 112.8, 80.9, 48.9, 18.4.



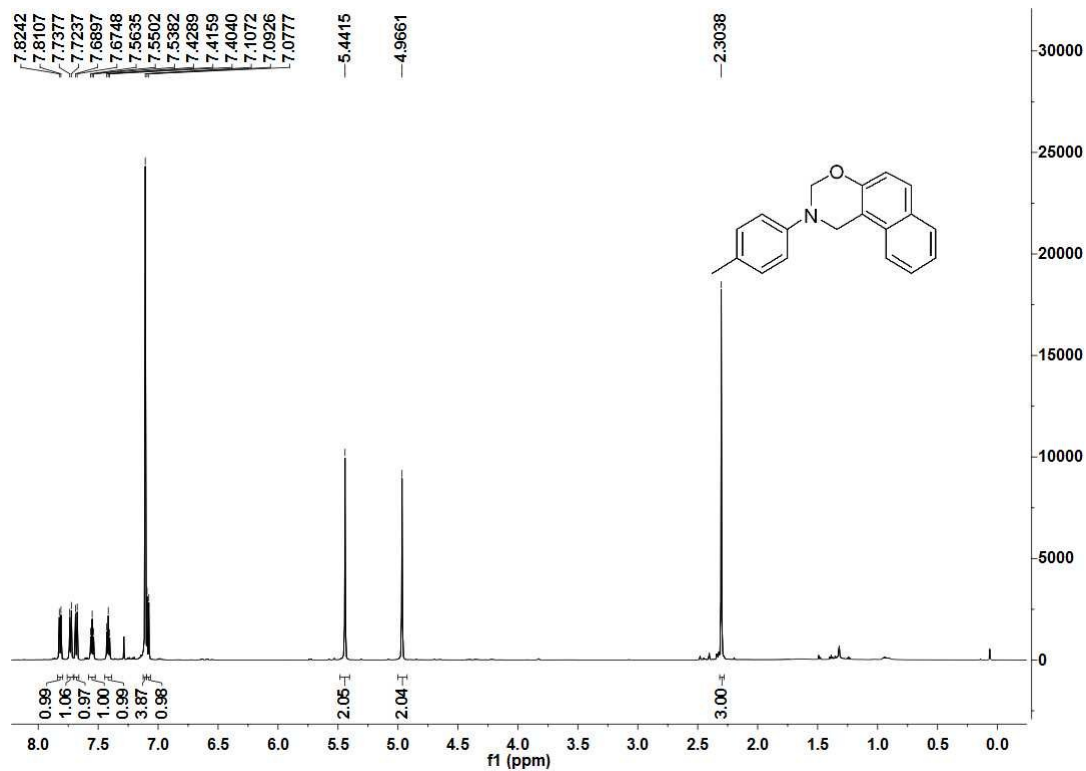
8-bromo-2-(*o*-tolyl)-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine (3cb): White solid; m.p. 137.0-138.1 °C; ¹H NMR (600 MHz, CDCl₃): δ 7.97 (s, 1H), 7.54 - 7.65 (m, 2H), 7.51 (d, *J* = 8.7 Hz, 1H), 7.27 (s, 2H), 7.13 - 7.19 (m, 1H), 7.05 - 7.13 (m, 2H), 5.30 (s, 2H), 4.77 (s, 2H), 2.52 (s, 3H); ¹³C NMR (151 MHz, CDCl₃): δ 152.7, 148.5, 132.6, 131.3, 130.7, 130.3, 129.8, 127.3, 126.8, 124.6, 122.7, 121.9, 120.1, 117.2, 113.0, 81.0, 48.7, 18.4. HRMS (ESI) *m/z* 354.0493 (*M* + *H*⁺), Cal. C₁₉H₁₇BrNO, 354.0488.



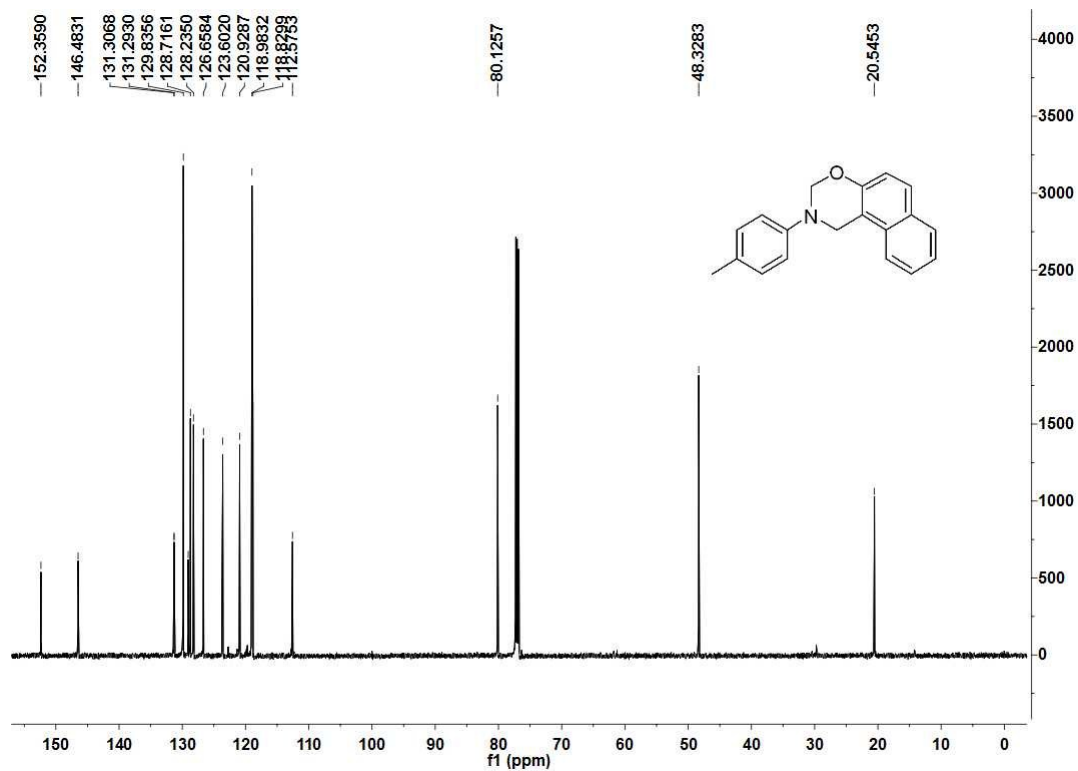
9-bromo-2-(*o*-tolyl)-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine (3cc): White solid; m.p. 96.1-97.7 °C; ^1H NMR (600 MHz, CDCl_3): δ 7.72 (s, 1H), 7.59 (dd, J = 8.8, 2.8 Hz, 2H), 7.40 (dd, J = 8.6, 1.4 Hz, 1H), 7.19 (dd, J = 4.9, 3.1 Hz, 2H), 7.07 (d, J = 8.9 Hz, 1H), 6.97 - 7.04 (m, 2H), 5.22 (s, 2H), 4.66 (s, 2H), 2.44 (s, 3H); ^{13}C NMR (151 MHz, CDCl_3): δ 153.2, 148.5, 132.6, 132.5, 131.2, 130.3, 128.1, 127.5, 126.9, 126.8, 124.6, 123.5, 121.9, 121.2, 119.4, 112.0, 81.0, 48.6, 18.4. HRMS (ESI) m/z 354.0490 ($\text{M} + \text{H}^+$), Cal. $\text{C}_{19}\text{H}_{17}\text{BrNO}$, 354.0488.

5. ^1H NMR and ^{13}C NMR spectra of the products.

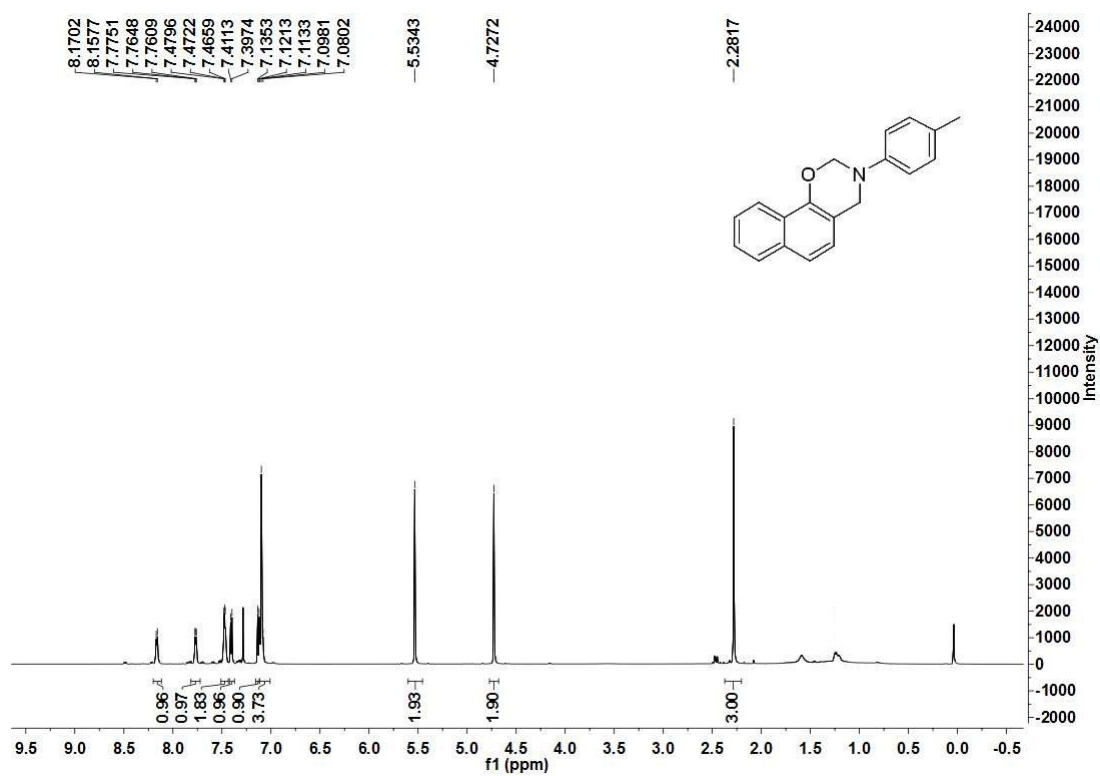
^1H NMR Spectrum (CDCl_3) of **3aa**



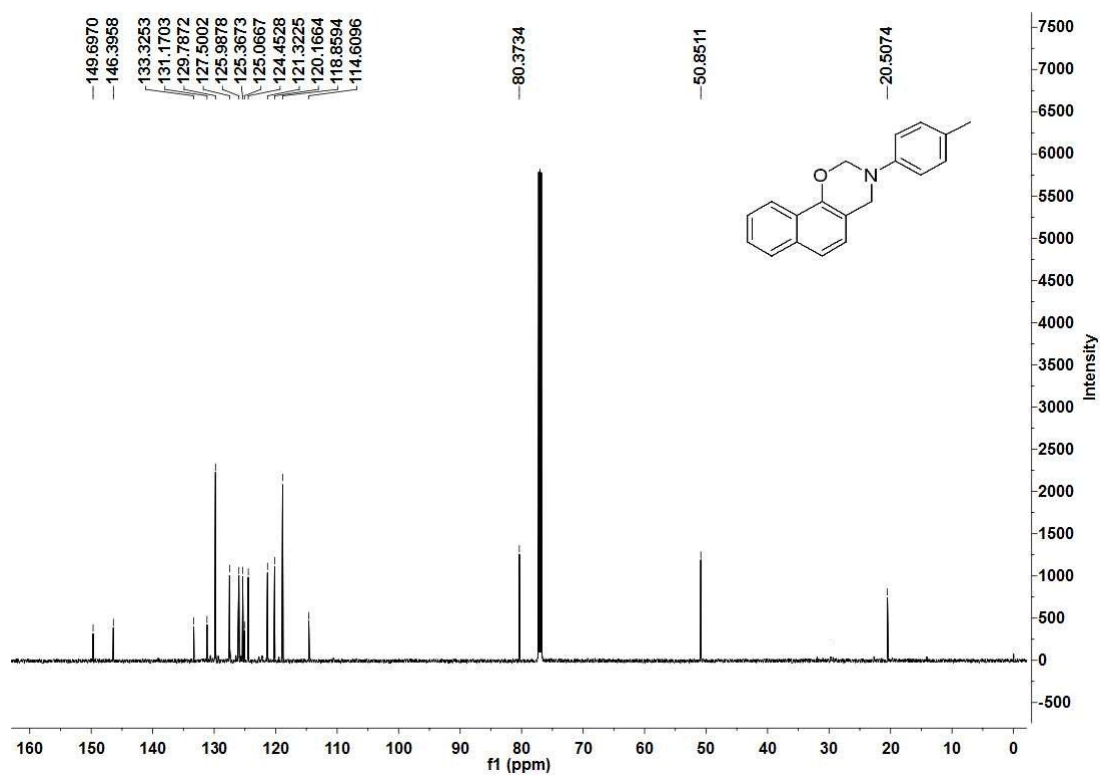
^{13}C NMR Spectrum (CDCl_3) of **3aa**



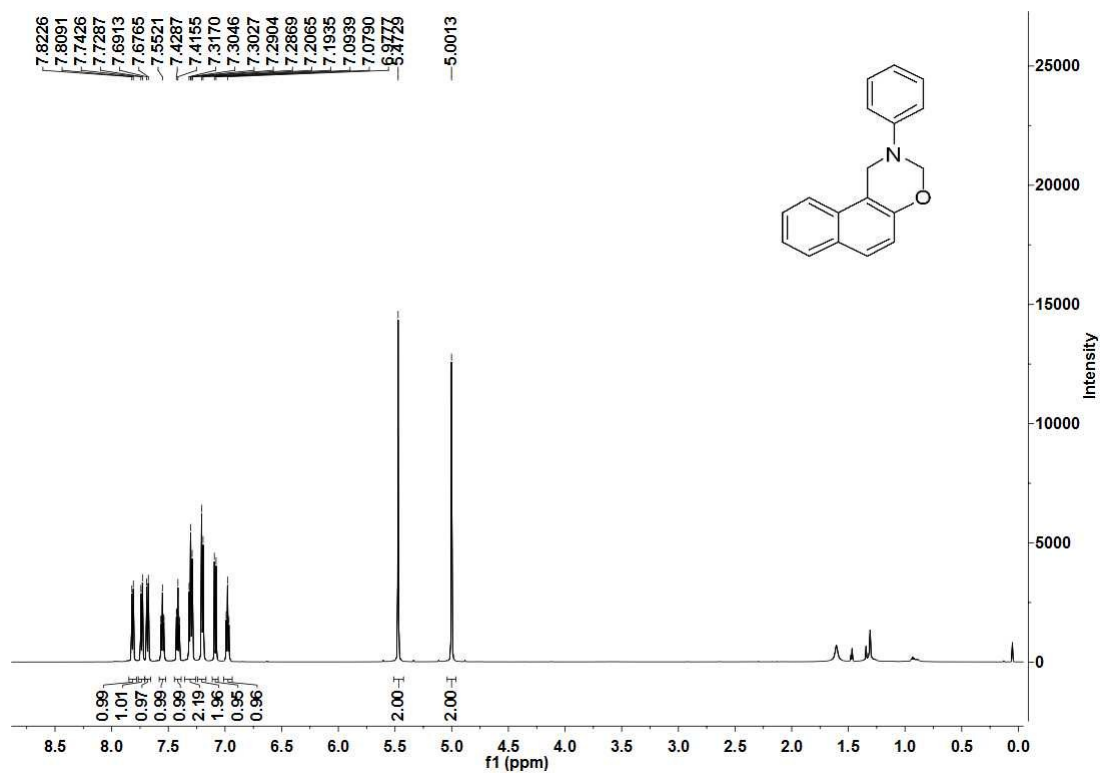
^1H NMR Spectrum (CDCl_3) of **4a**



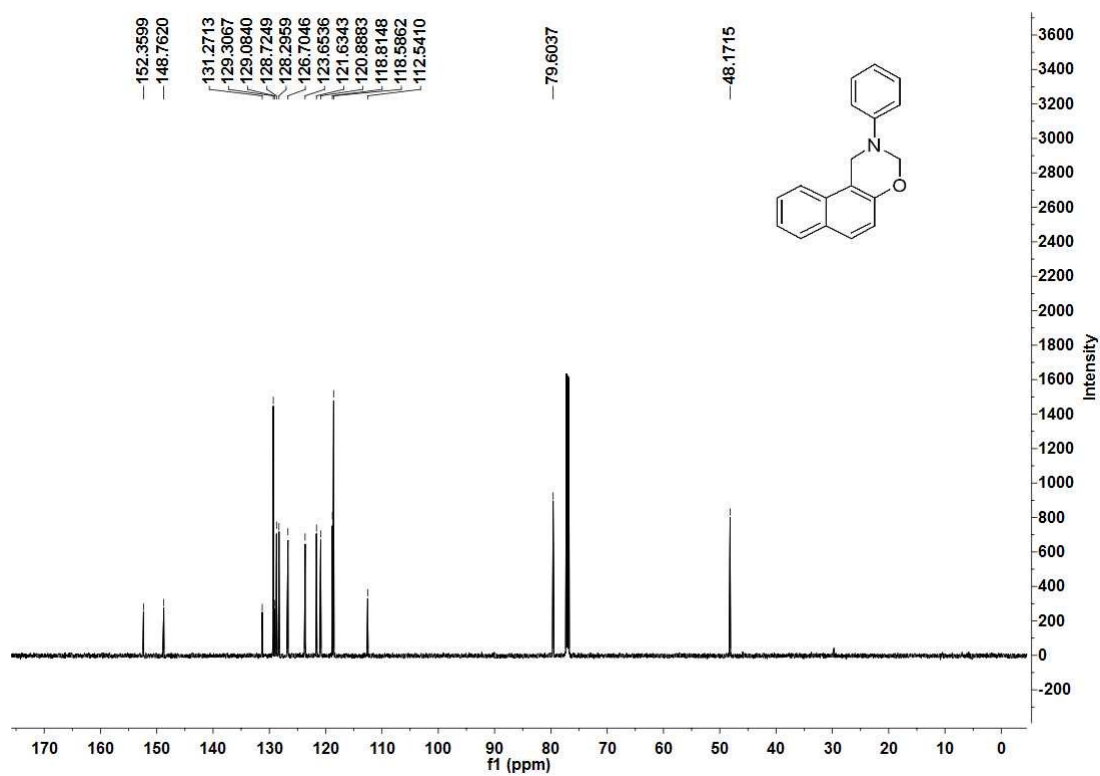
^{13}C NMR Spectrum (CDCl_3) of **4a**



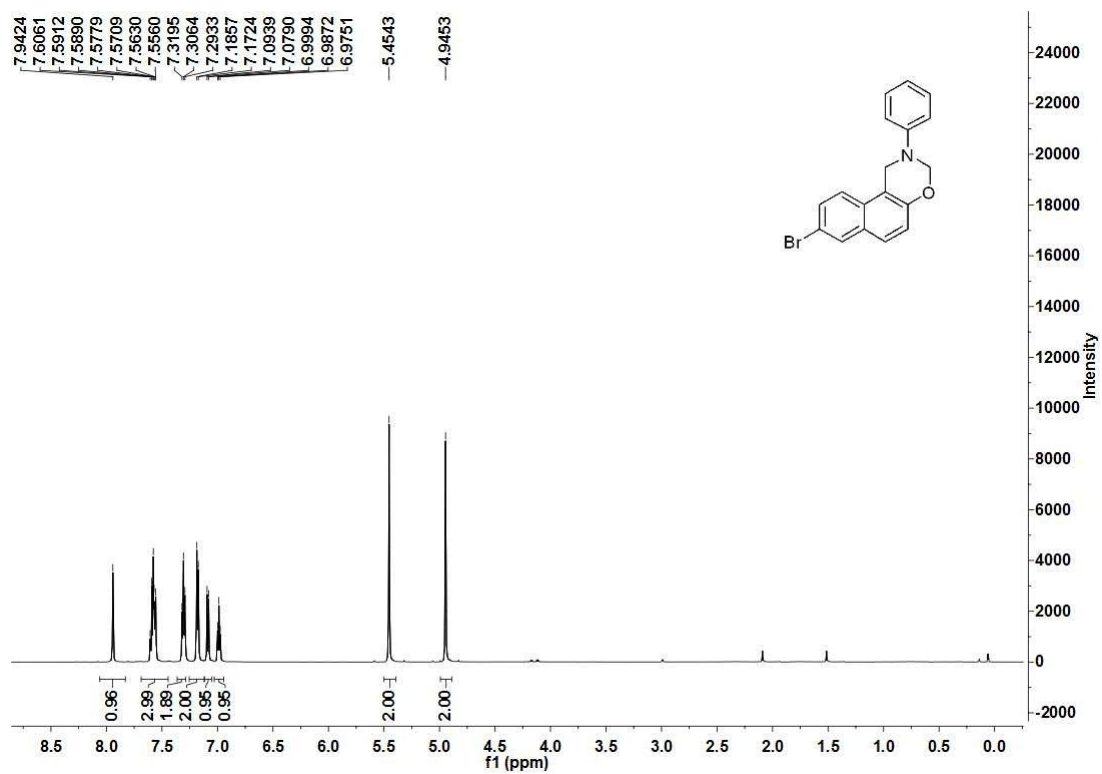
¹H NMR Spectrum (CDCl₃) of **3ba**



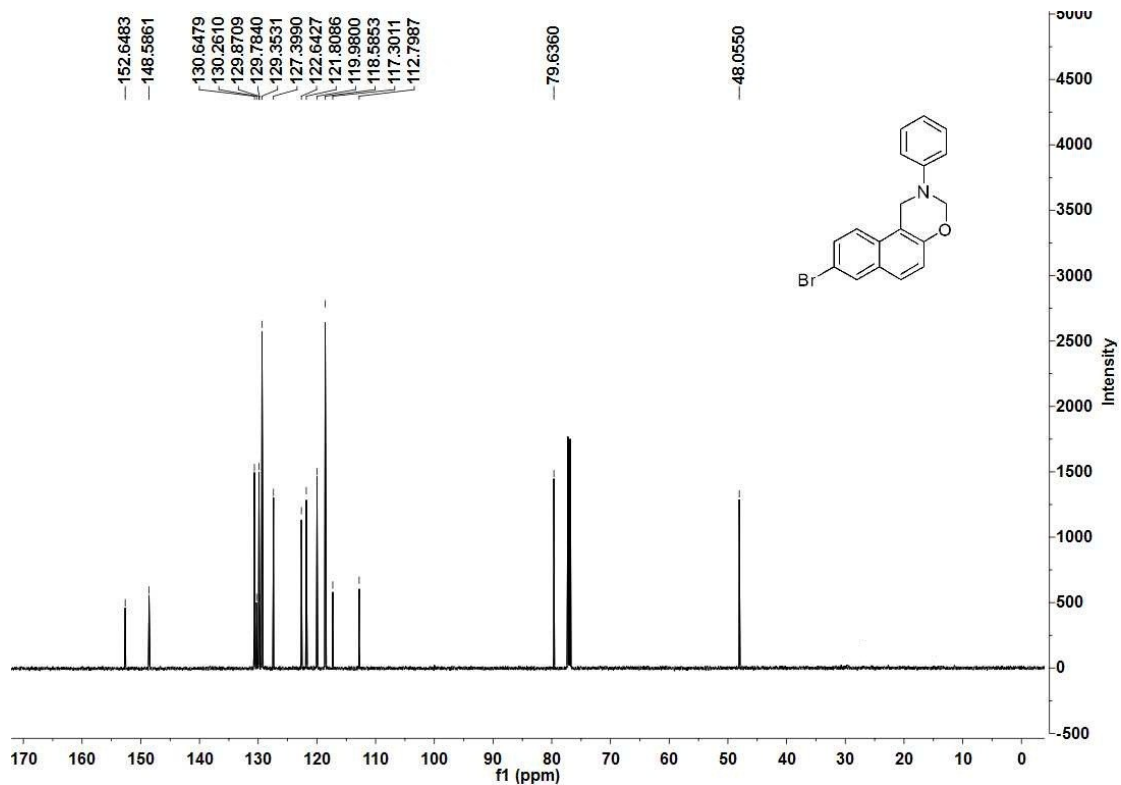
¹³C NMR Spectrum (CDCl₃) of **3ba**



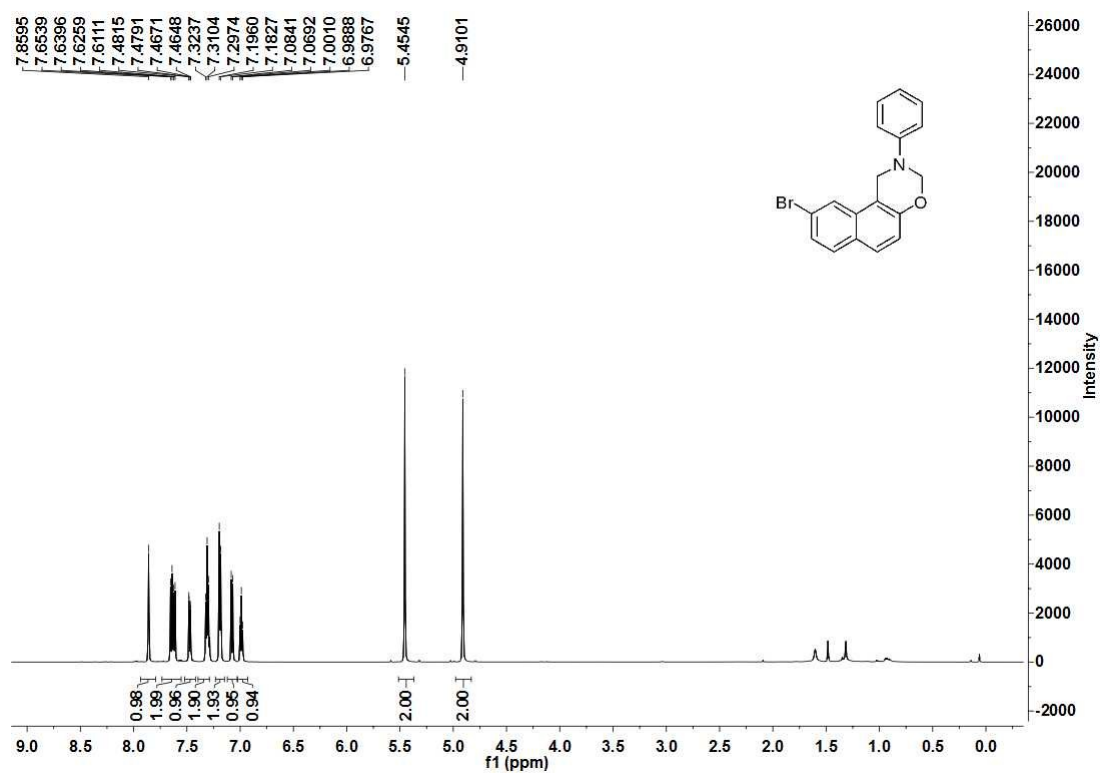
¹H NMR Spectrum (CDCl₃) of **3bb**



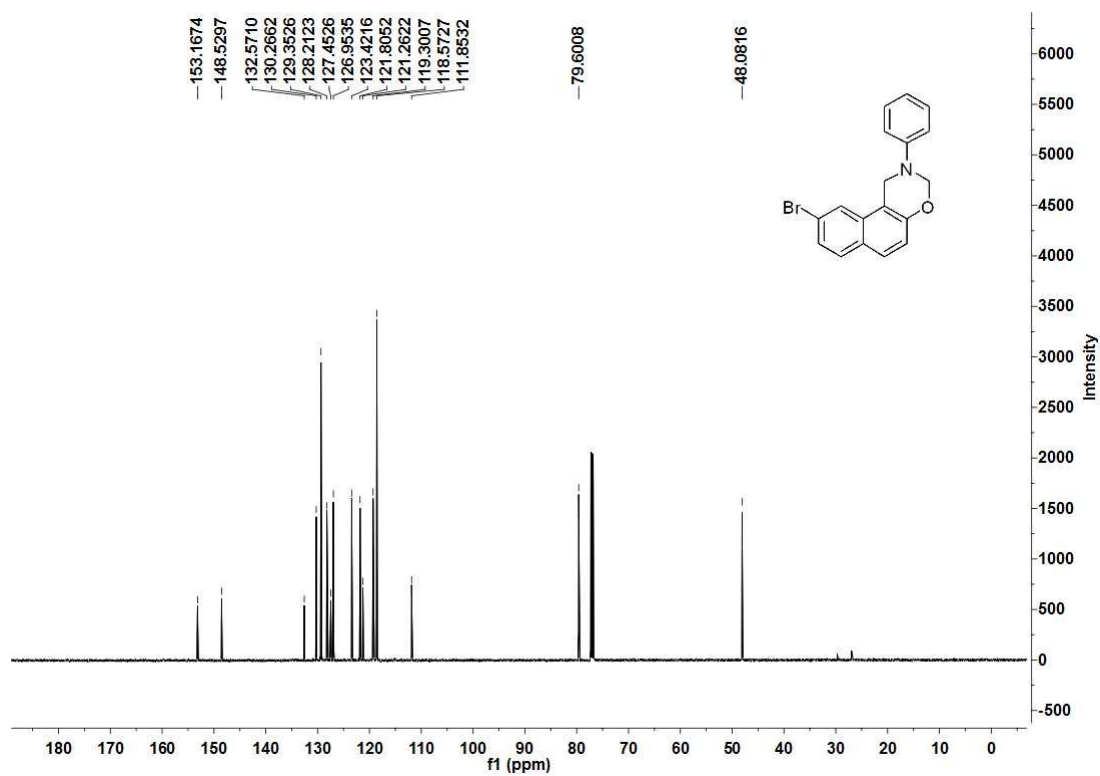
¹³C NMR Spectrum (CDCl₃) of **3bb**



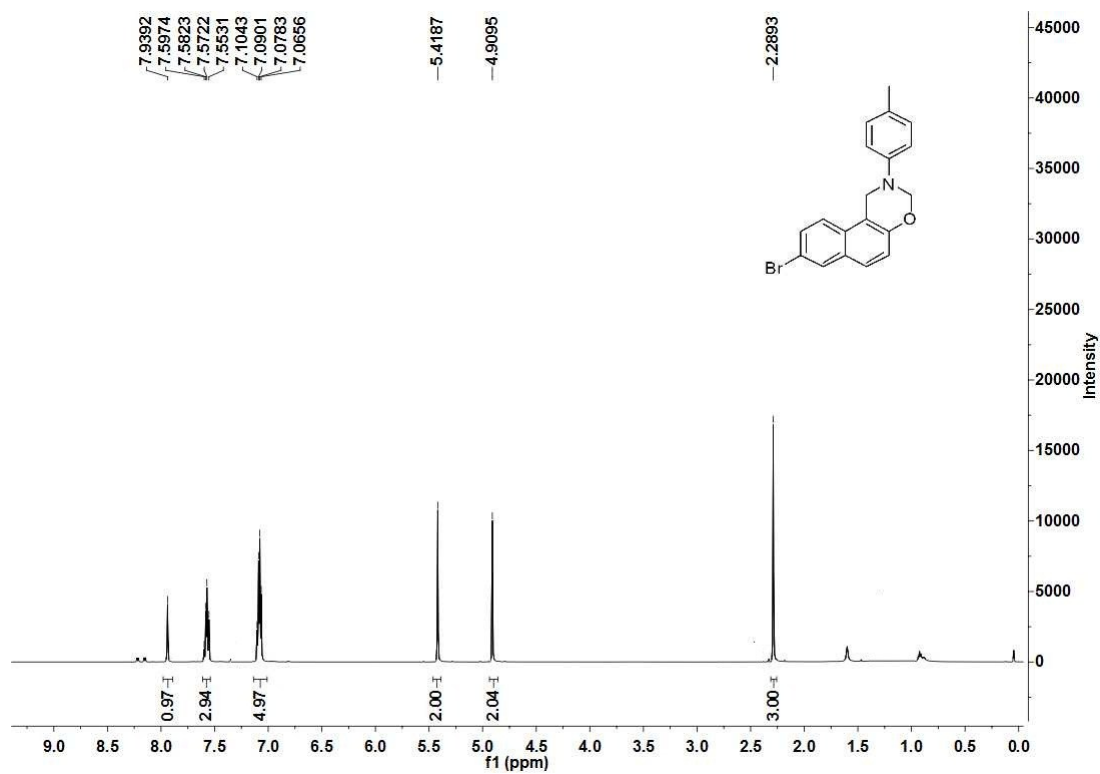
¹H NMR Spectrum (CDCl₃) of **3bc**



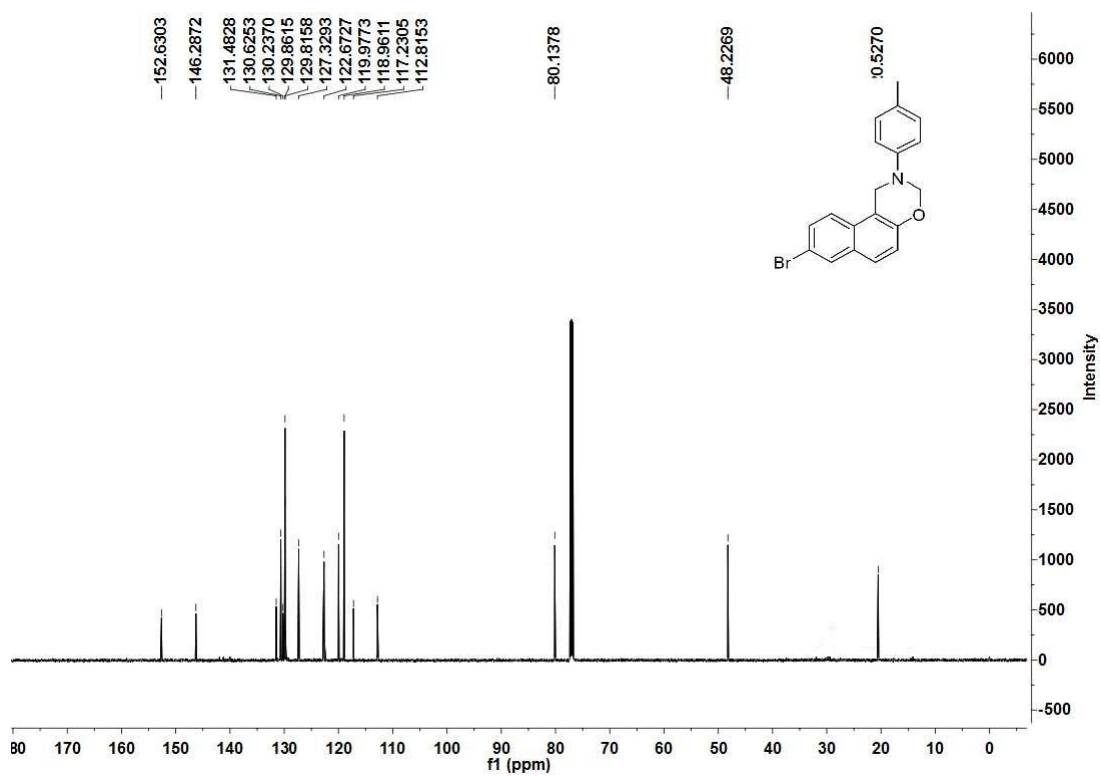
¹³C NMR Spectrum (CDCl₃) of **3bc**



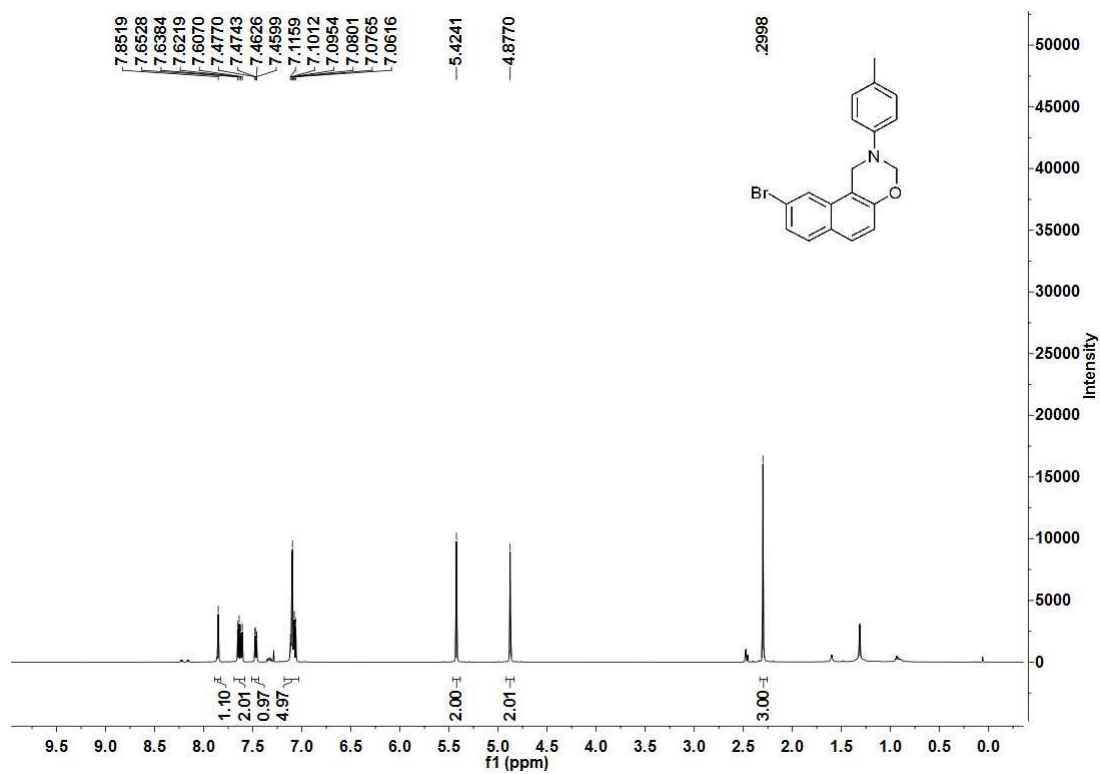
^1H NMR Spectrum (CDCl_3) of **3ab**



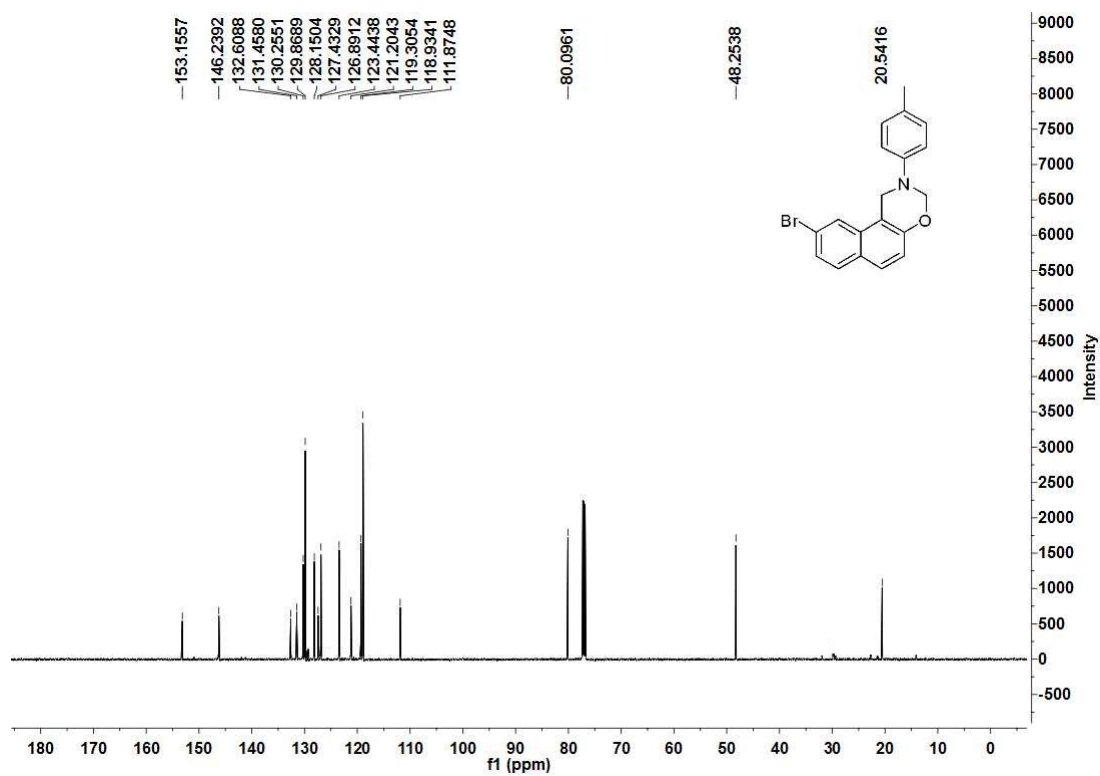
^{13}C NMR Spectrum (CDCl_3) of **3ab**



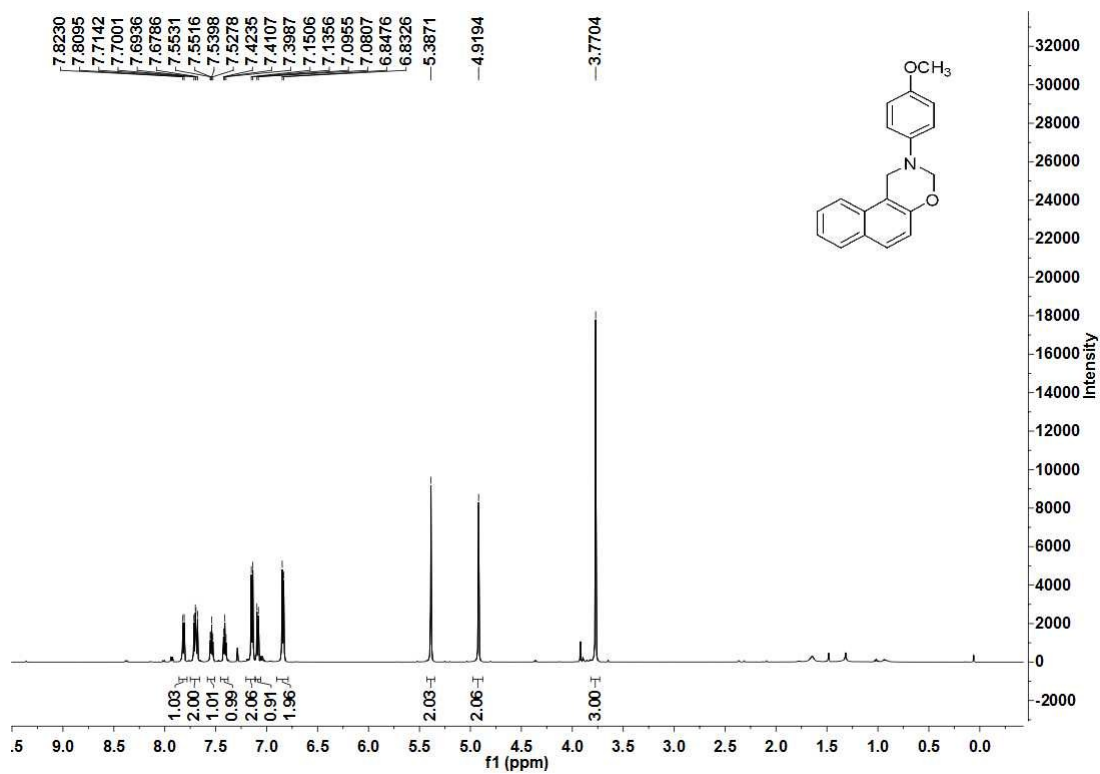
^1H NMR Spectrum (CDCl_3) of **3ac**



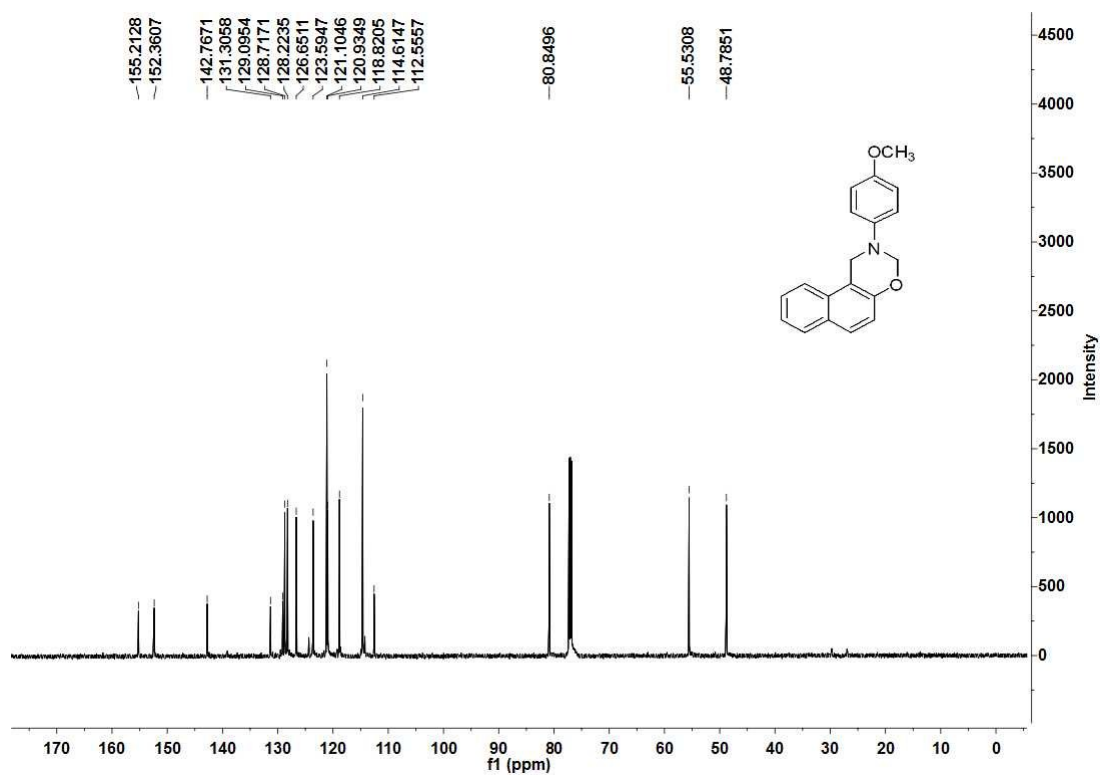
^{13}C NMR Spectrum (CDCl_3) of **3ac**



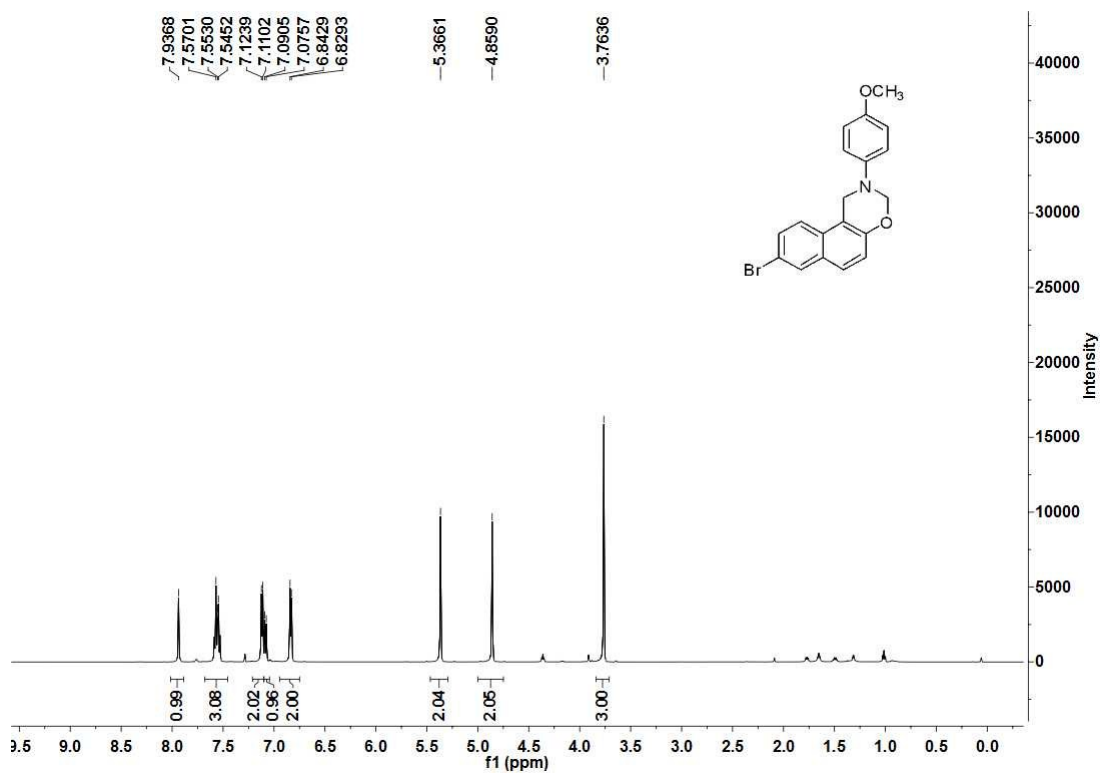
¹H NMR Spectrum (CDCl₃) of **3da**



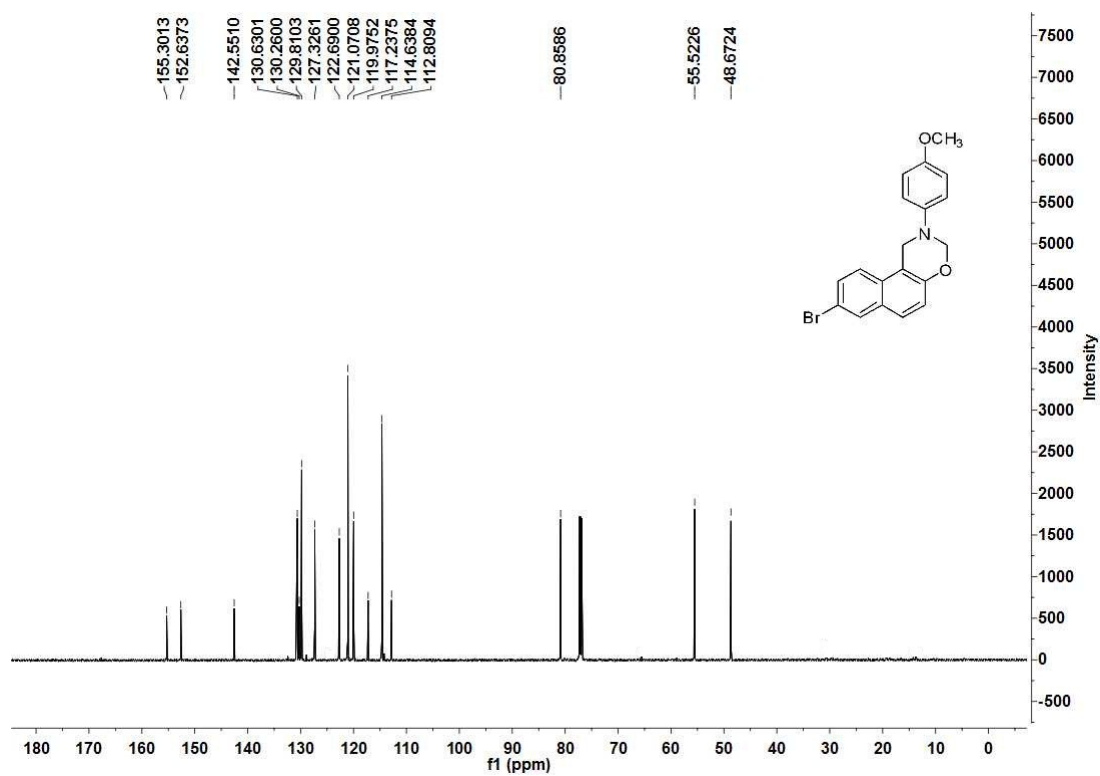
¹³C NMR Spectrum (CDCl₃) of **3da**



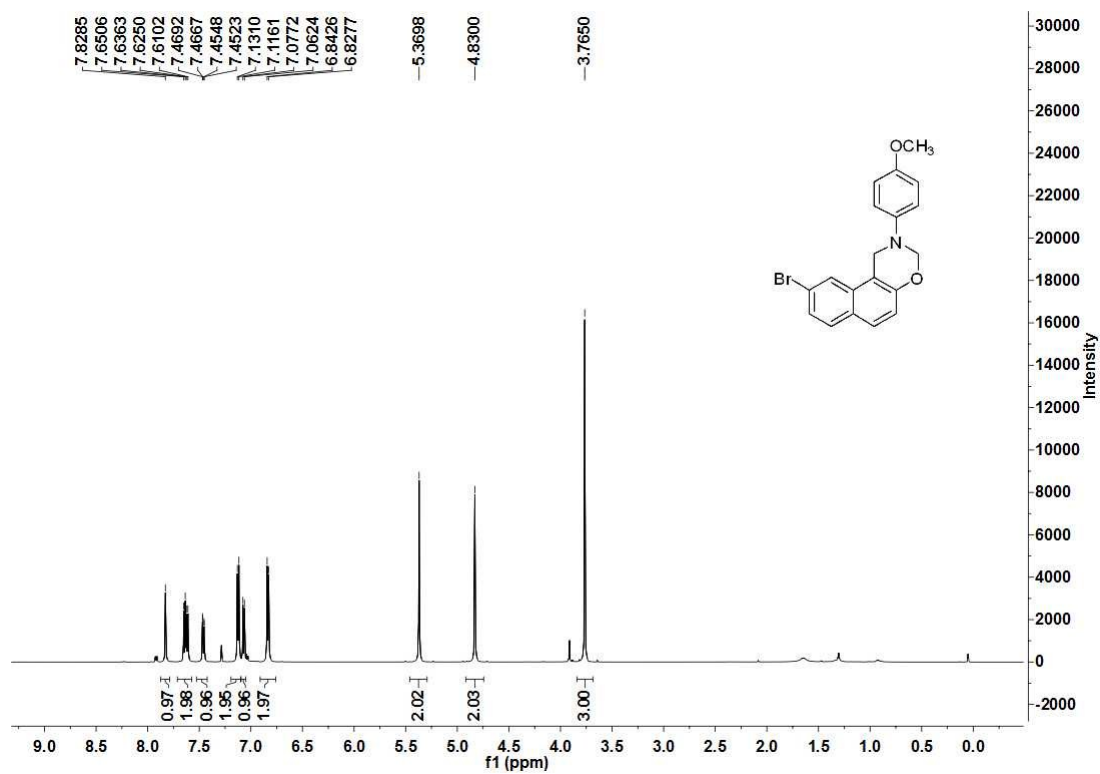
¹H NMR Spectrum (CDCl₃) of **3db**



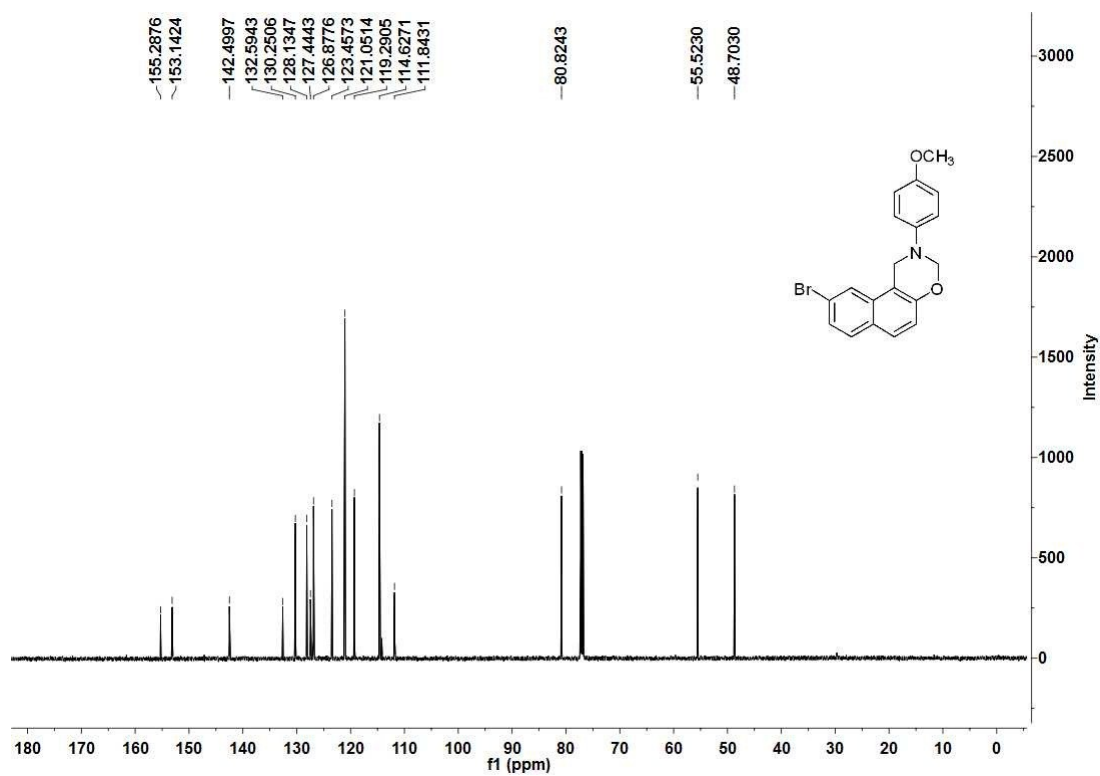
¹³C NMR Spectrum (CDCl₃) of **3db**



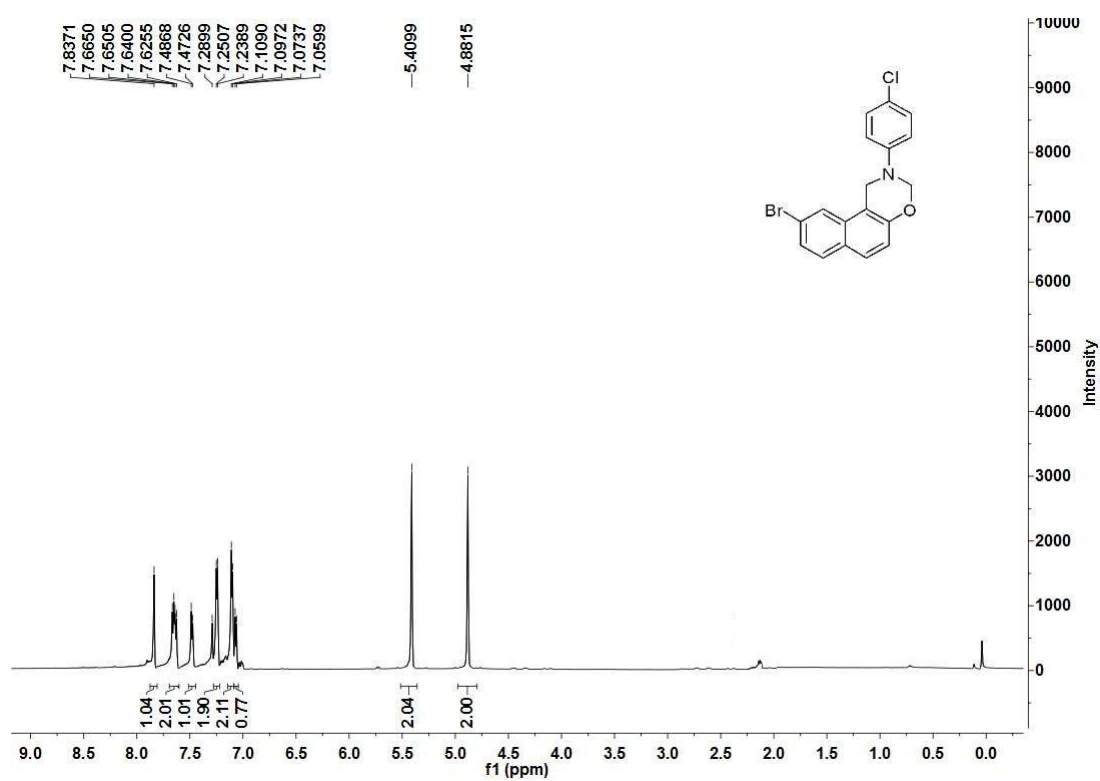
^1H NMR Spectrum (CDCl_3) of **3dc**



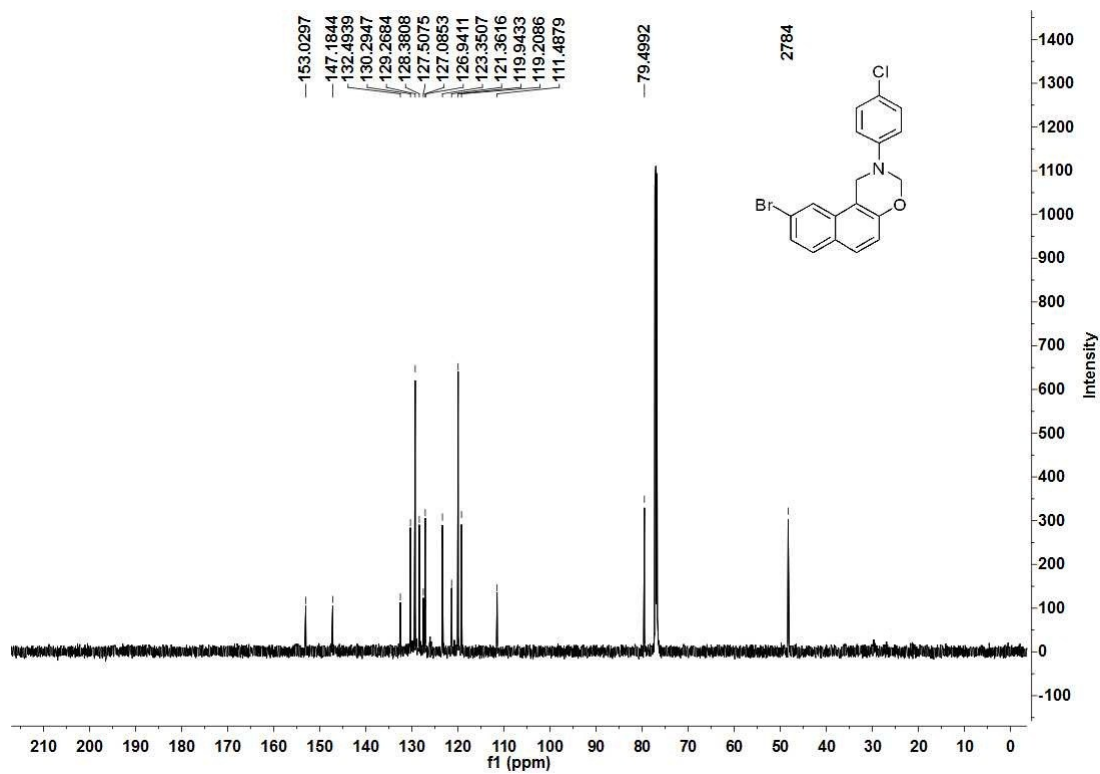
^{13}C NMR Spectrum (CDCl_3) of **3dc**



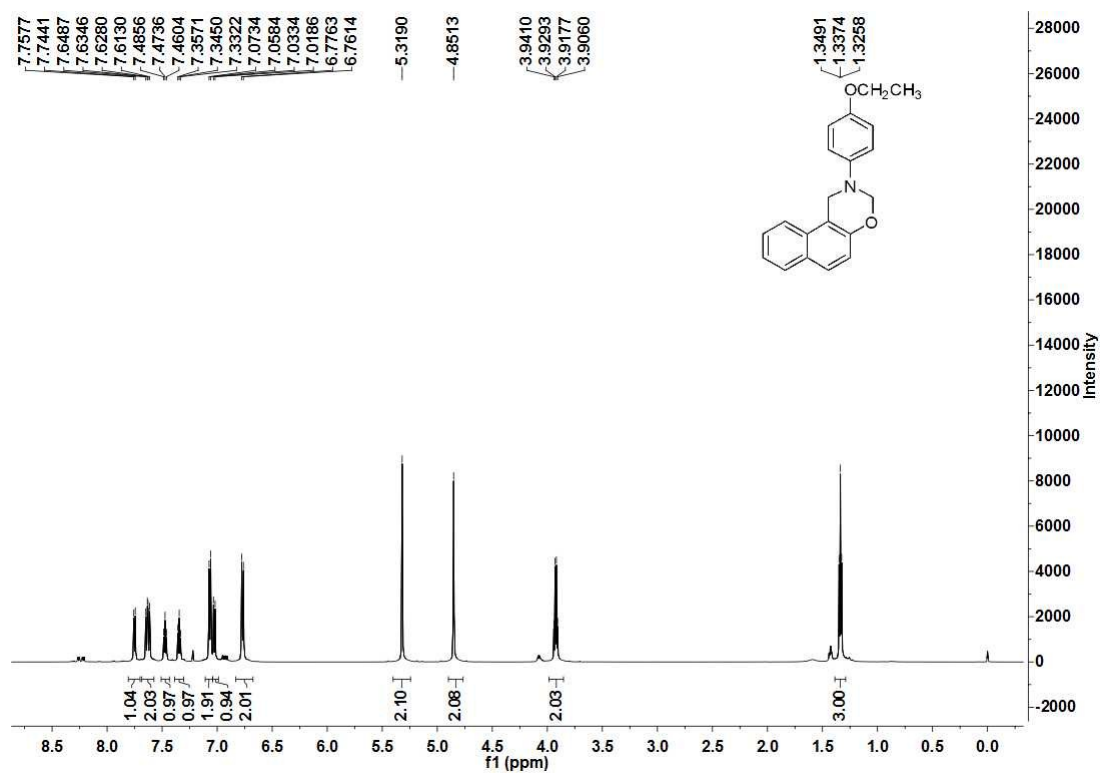
¹H NMR Spectrum (CDCl₃) of **3ec**



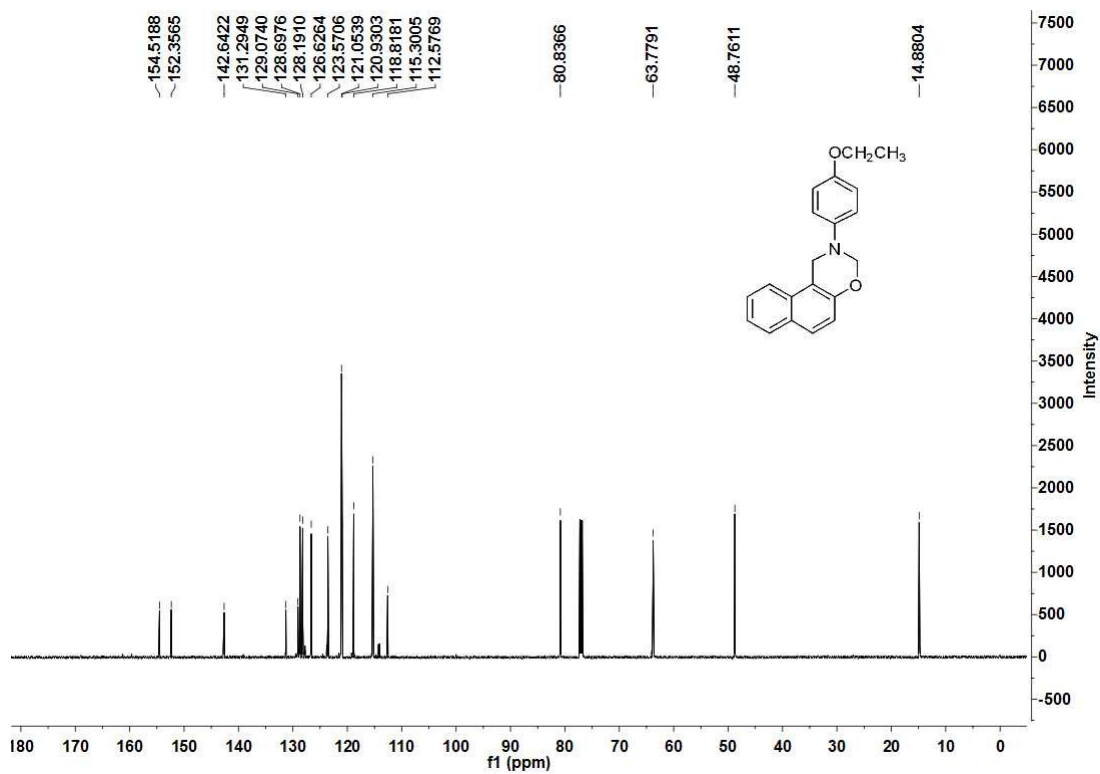
¹³C NMR Spectrum (CDCl₃) of **3aa**



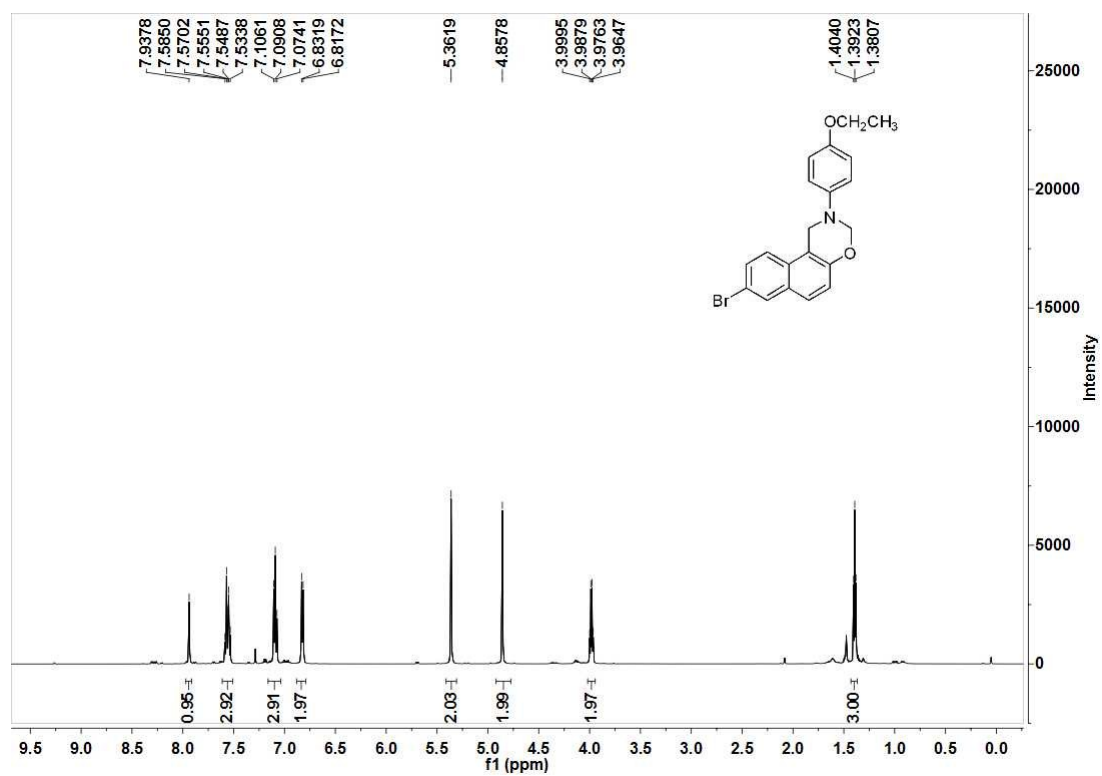
^1H NMR Spectrum (CDCl_3) of **3fa**



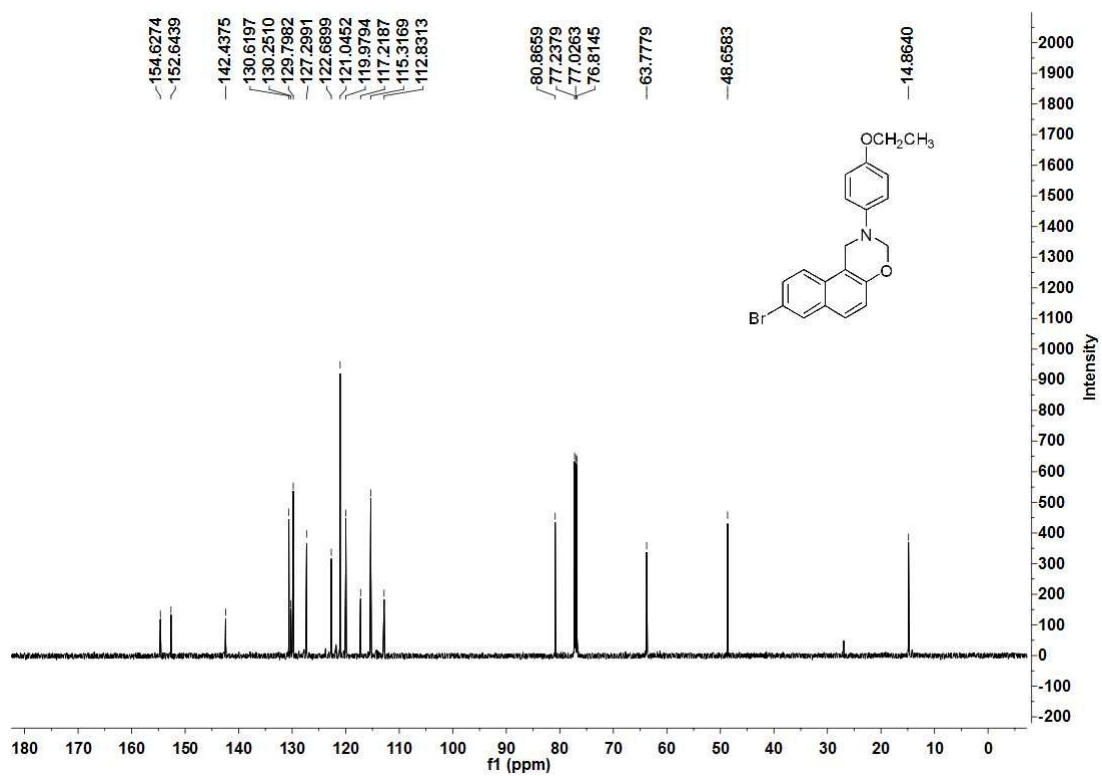
^{13}C NMR Spectrum (CDCl_3) of **3fa**



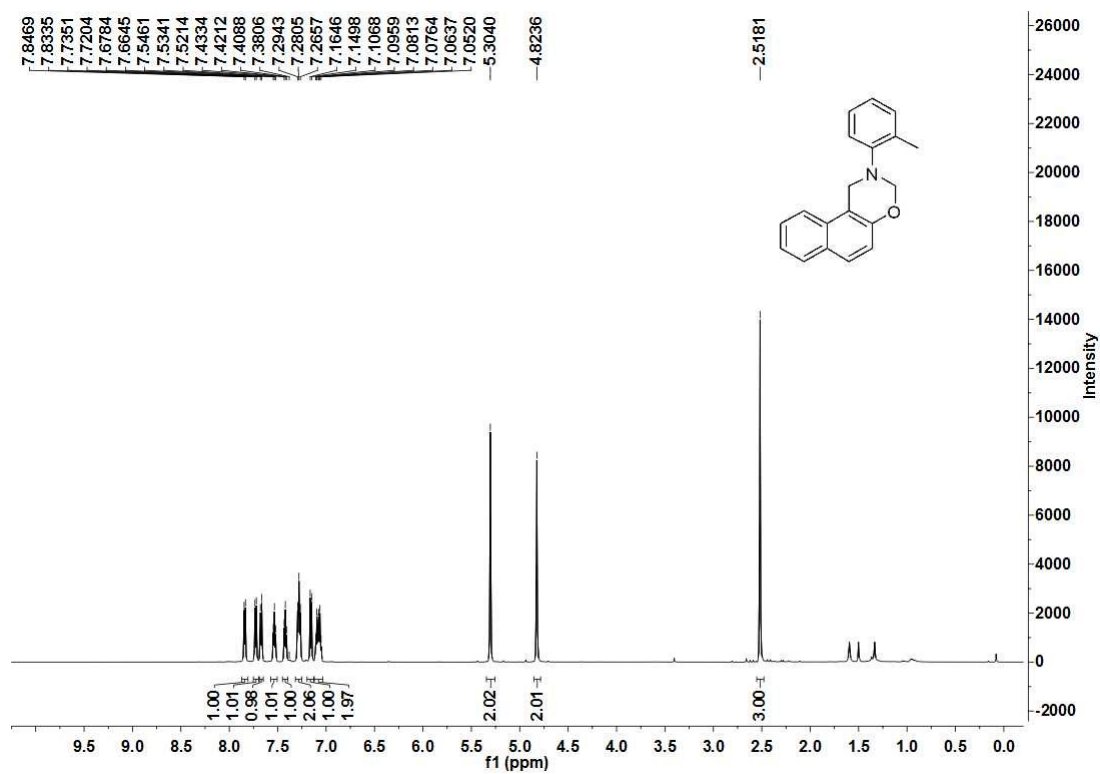
¹H NMR Spectrum (CDCl₃) of **3fb**



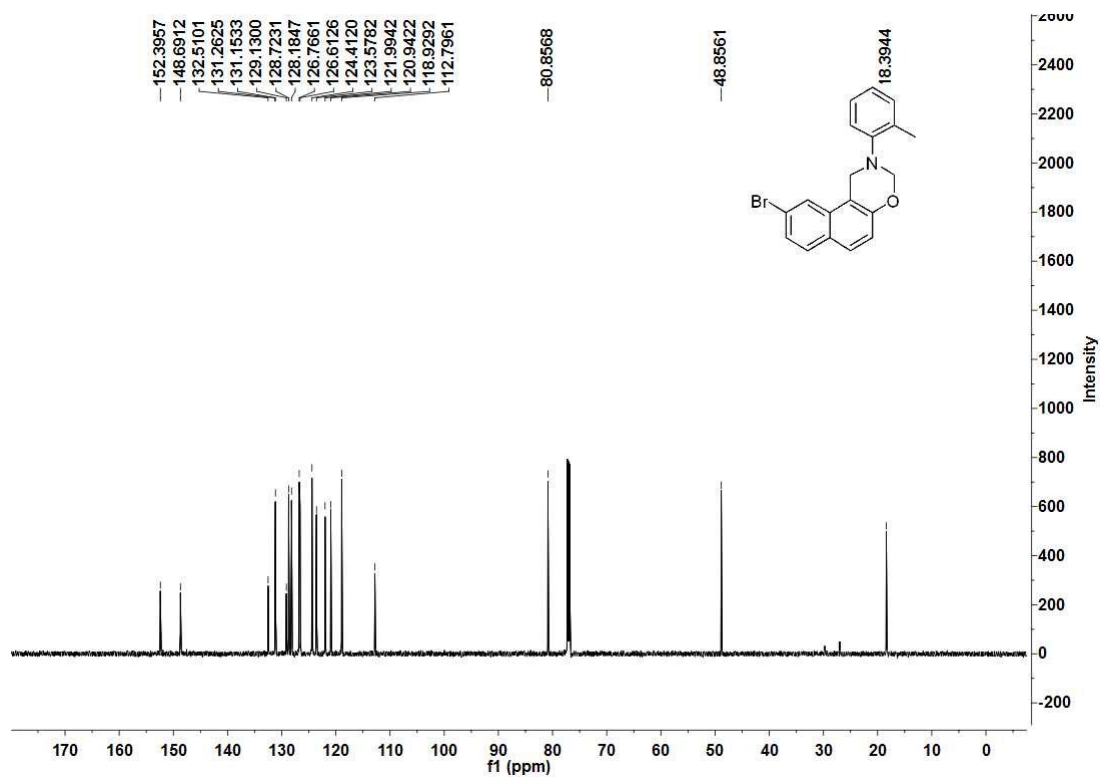
¹³C NMR Spectrum (CDCl₃) of **3fb**



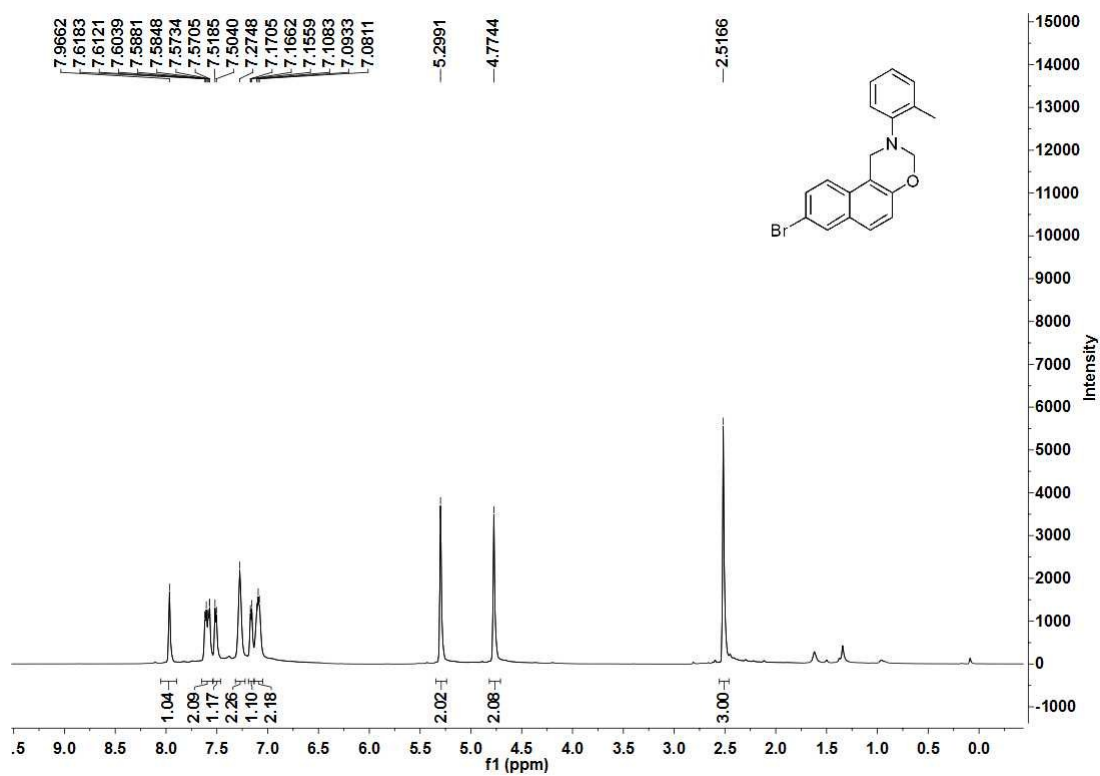
¹H NMR Spectrum (CDCl₃) of **3ca**



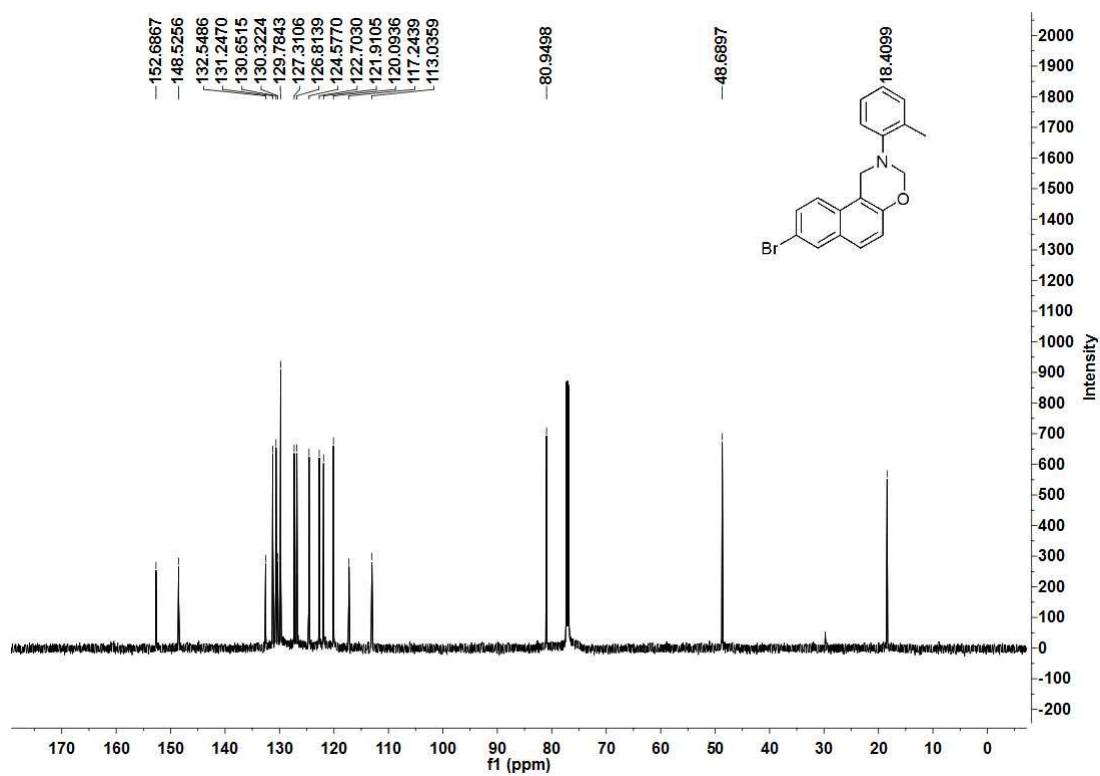
¹³C NMR Spectrum (CDCl₃) of **3ca**



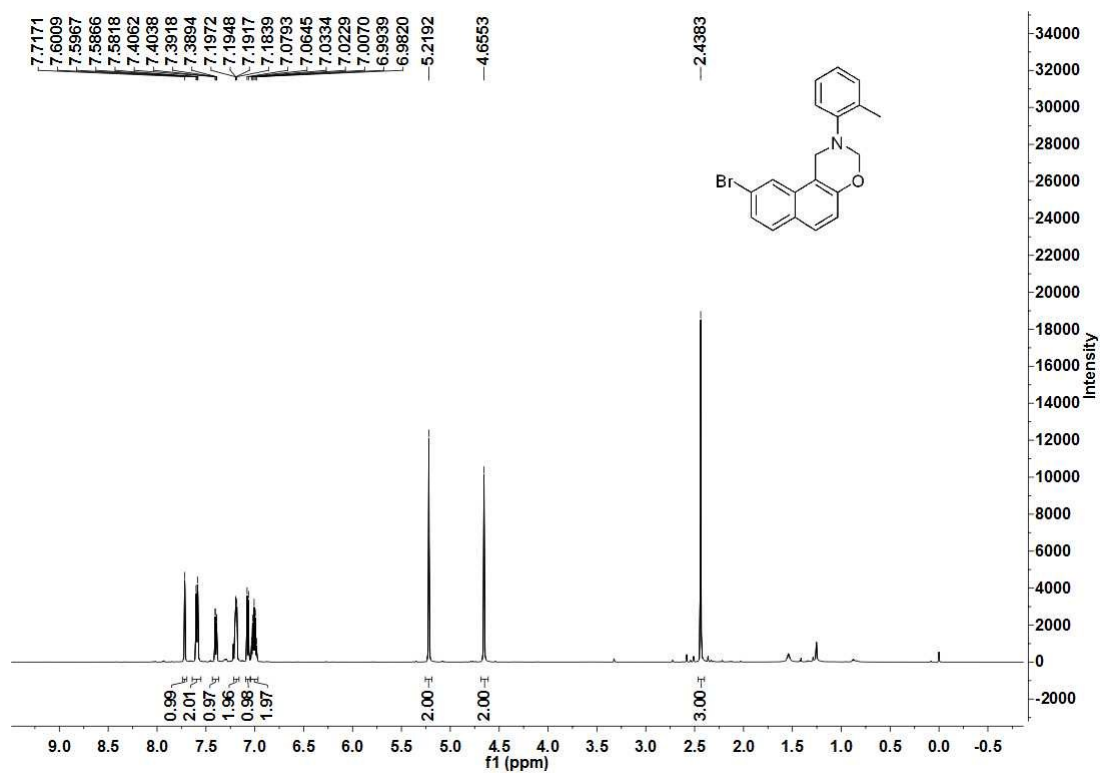
¹H NMR Spectrum (CDCl₃) of **3cb**



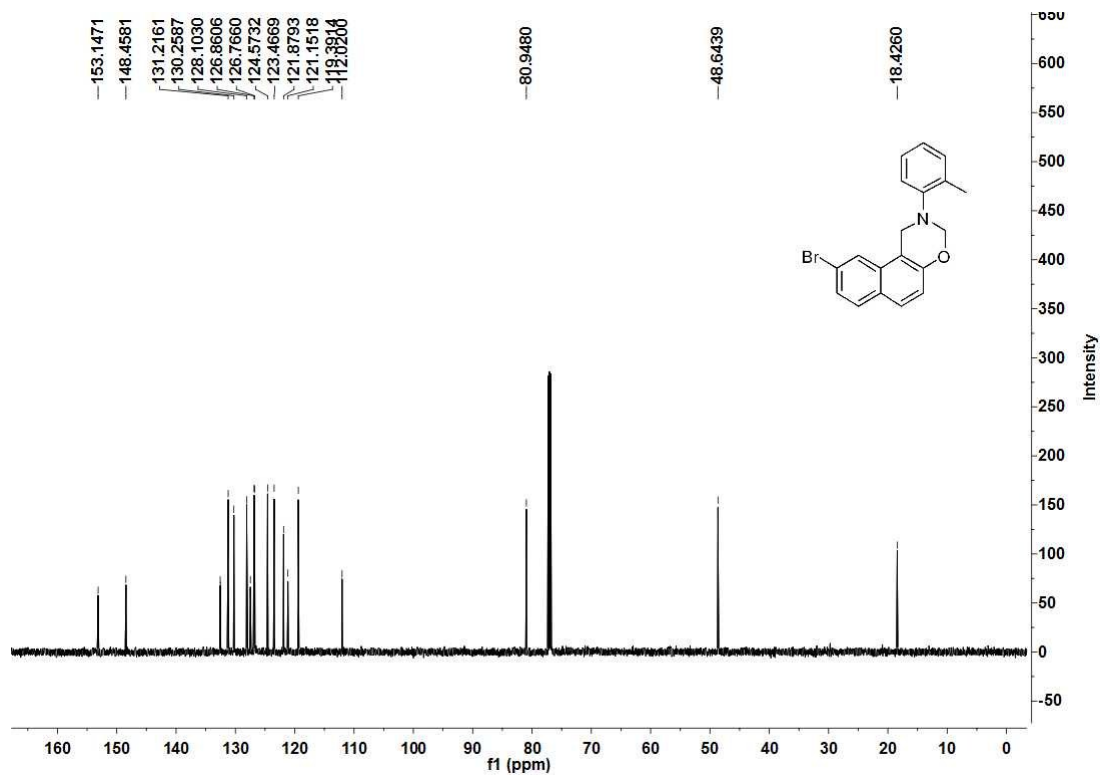
¹³C NMR Spectrum (CDCl₃) of **3cb**



^1H NMR Spectrum (CDCl_3) of **3cc**



^{13}C NMR Spectrum (CDCl_3) of **3cc**

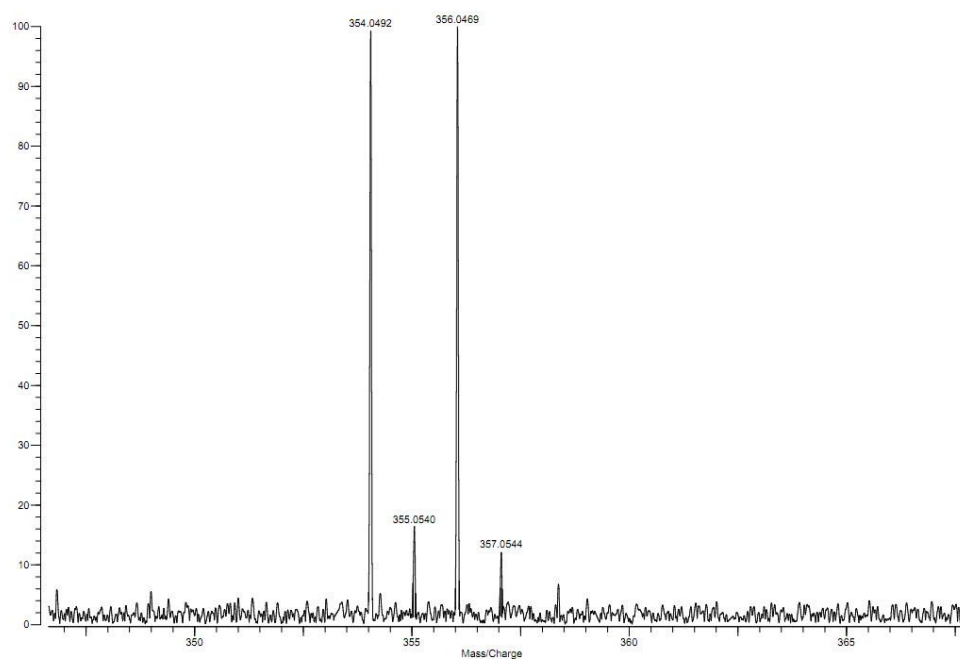


6. HRMS spectra of new compounds.

Varian QFT-ESI
File: ZGY-A3-6_ESI.trans

Mode: Positive
Scans: 2

Date: 14-SEP-2016
Time: 11:20:23
Scale: 28.4366

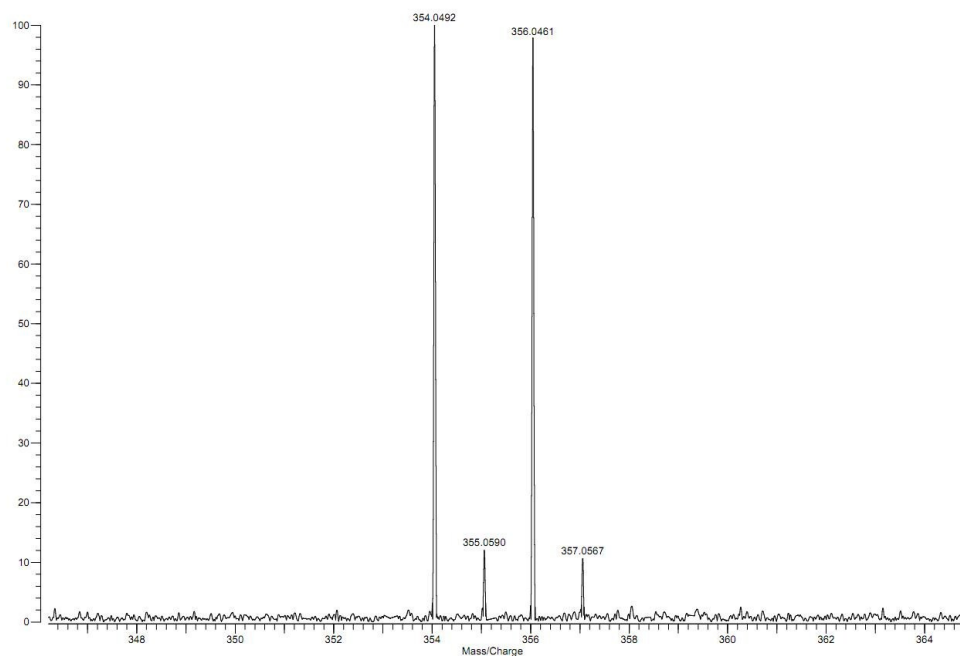


3ac

Varian QFT-ESI
File: ZGY-A3-1_ESI.trans

Mode: Positive
Scans: 1

Date: 30-AUG-2016
Time: 19:18:40
Scale: 17.5774

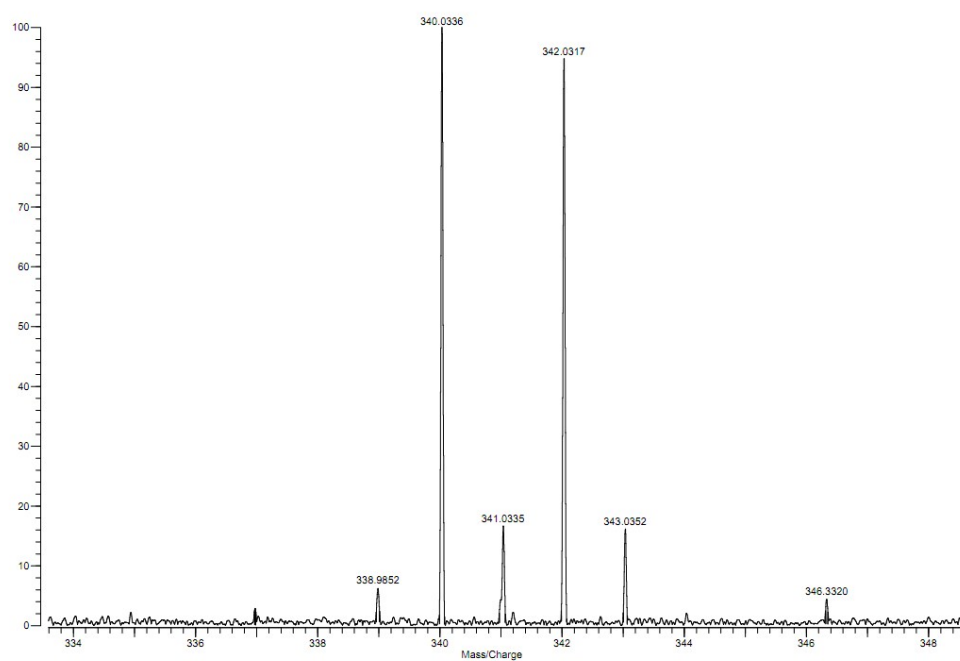


3bc

Varian QFT-ESI
File: ZGY-A3-3_ESI.trans

Mode: Positive
Scans: 1

Date: 31-JUL-2016
Time: 13:01:18
Scale: 13.7623

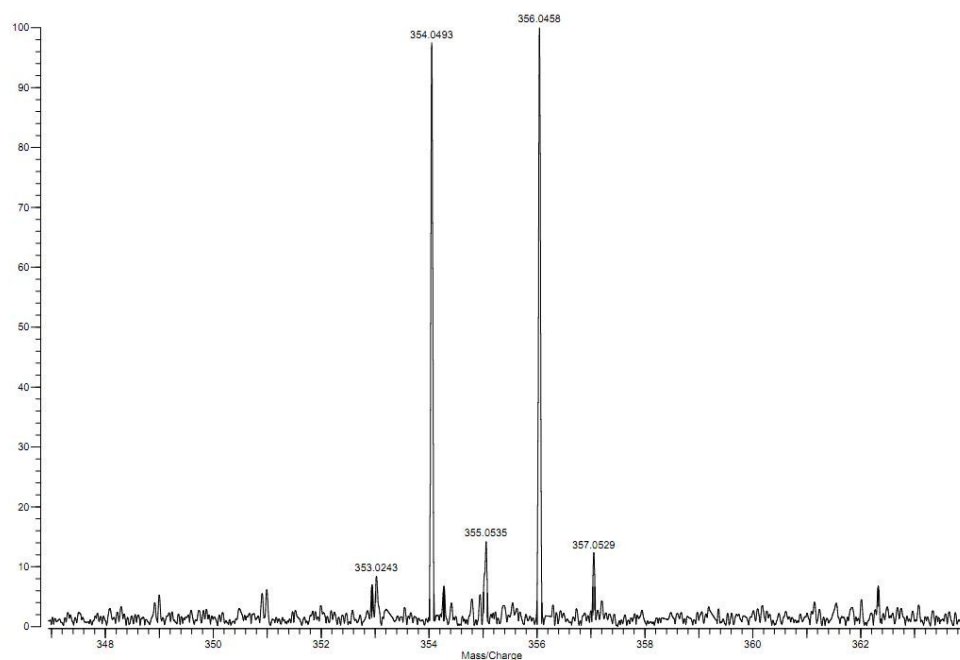


3cb

Varian QFT-ESI
File: ZGY-A3-10(2)_ESI.trans

Mode: Positive
Scans: 3

Date: 14-SEP-2016
Time: 08:55:10
Scale: 19.9980

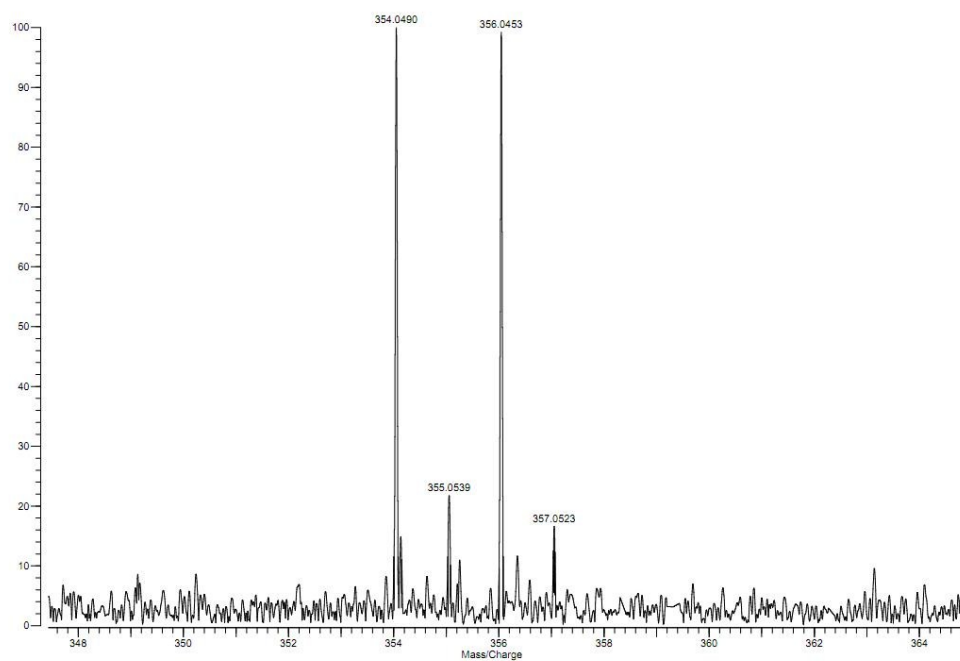


3cc

Varian QFT-ESI
File: ZGY-A3-2_ESI.trans

Mode: Positive
Scans: 10

Date: 31-JUL-2016
Time: 13:20:05
Scale: 20.8378

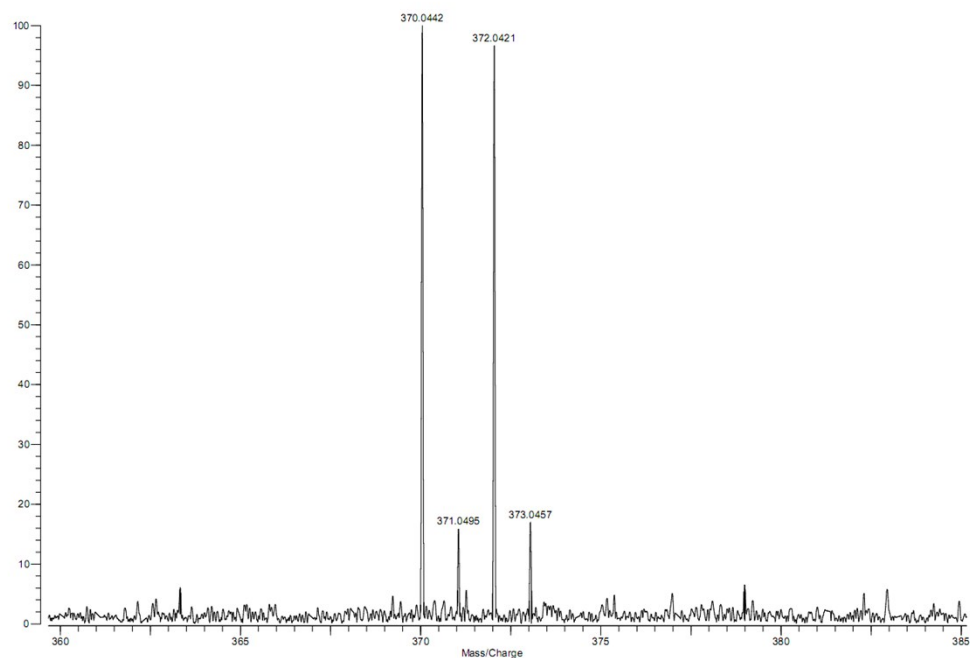


3db

Varian QFT-ESI
File: ZGY-A3-6_ESI.trans

Mode: Positive
Scans: 3

Date: 14-SEP-2016
Time: 11:56:39
Scale: 20.3547

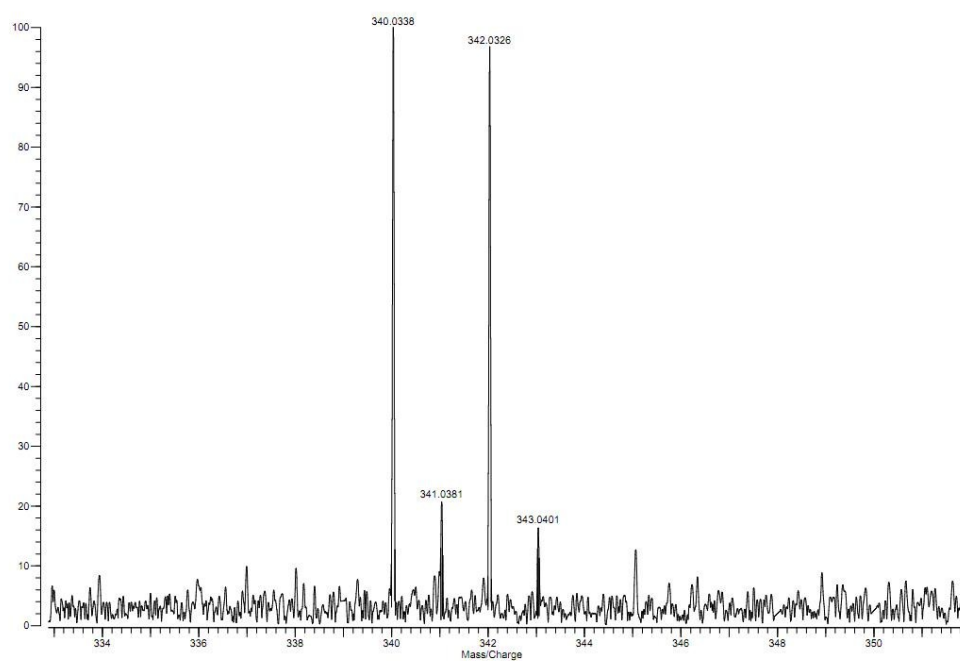


3bb

Varian QFT-ESI
File: ZGY-A3-7_ESI.trans

Mode: Positive
Scans: 1

Date: 14-SEP-2016
Time: 09:44:24
Scale: 71.1879

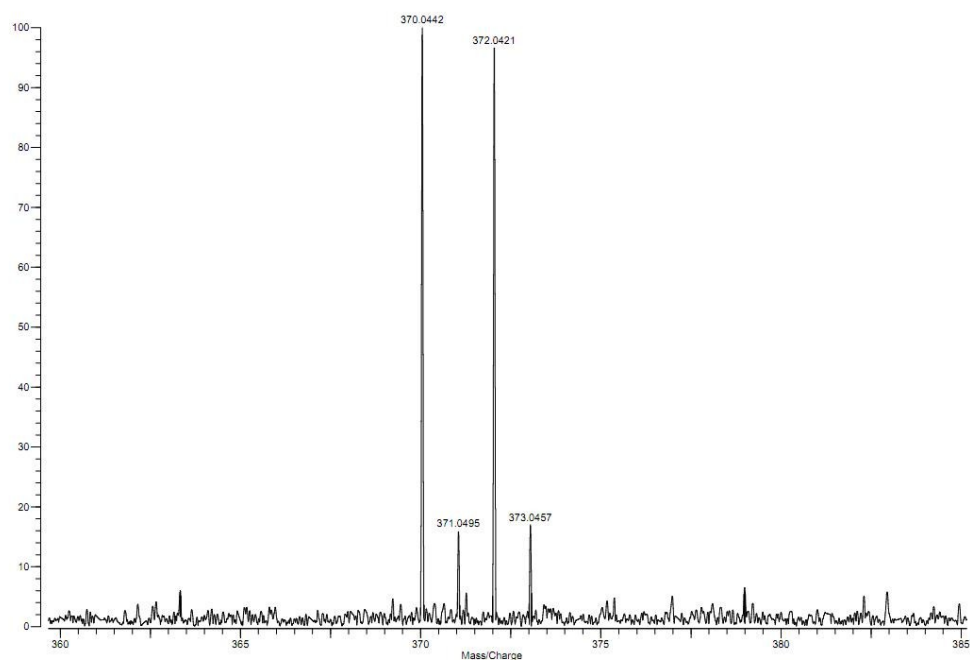


3dc

Varian QFT-ESI
File: ZGY-A3-5_ESI.trans

Mode: Positive
Scans: 1

Date: 31-JUL-2016
Time: 12:44:23
Scale: 30.5957

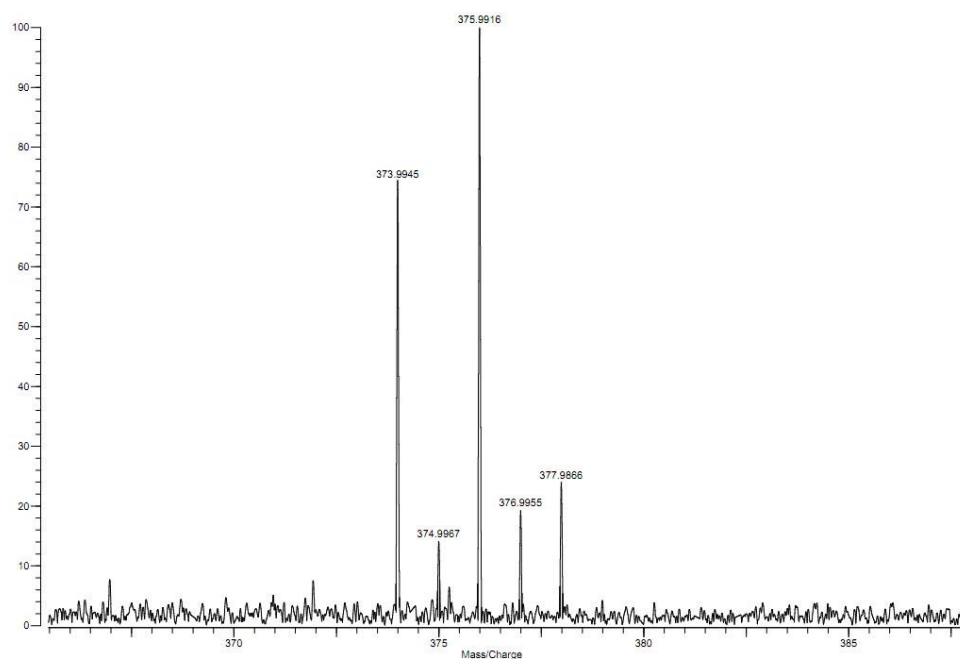


3ec

Varian QFT-ESI
File: ZGY-A3-4(3)_ESI.trans

Mode: Positive
Scans: 2

Date: 14-SEP-2016
Time: 11:39:57
Scale: 29.0129

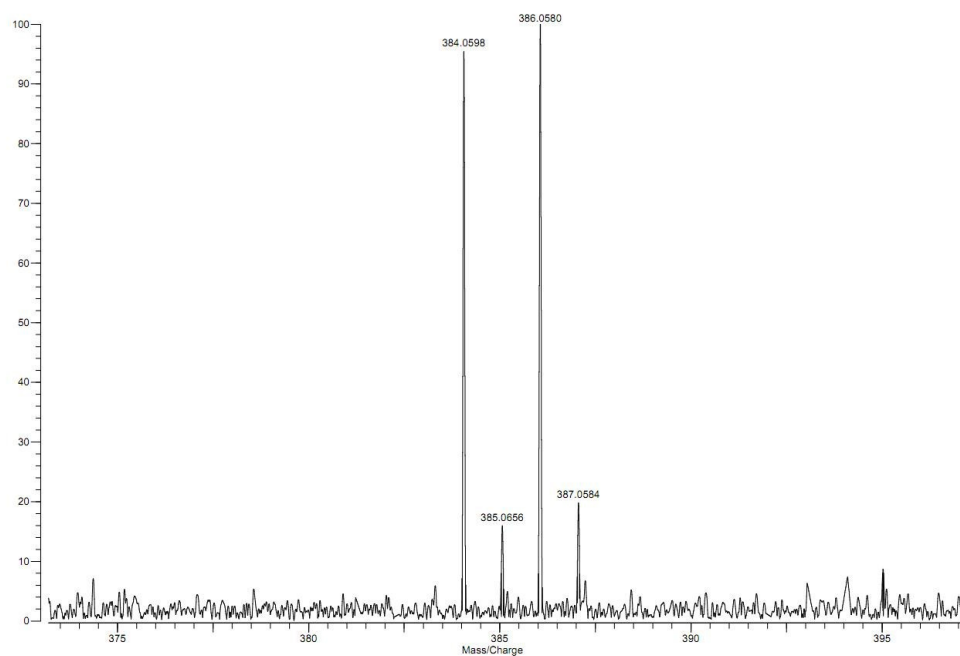


3fb

Varian QFT-ESI
File: ZGY-A3-9_ESI.trans

Mode: Positive
Scans: 1

Date: 14-SEP-2016
Time: 09:07:08
Scale: 41.9537



7. References.

- [1] N. S. Rai, B. Kalluraya, B. Lingappa, S. Shenoy, V. G. Puranic, *European Journal of Medicinal Chemistry.*; **2008**, *43*, 1715-1720.
- [2] A. H. Kategaonkar, S. S. Sonar, K. F. Shelke, B. B. Shingate, M. S. Shingare, *ACG.Org. Commun.*; **2010**, *3*, 1-7.
- [3] V. D. Dhakane, S. S. Gholap, U. P. Deshmukh, H. V. Chavan, B. P. Bandgar, *C. R. Chimie.*; **2014**, *17*, 431–436.