

**Efficient synthesis of naphtho[1,2-*e*][1,3]oxazine derivatives via a chemoselective reaction with the aid of low-valent titanium reagent**

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## General Experimental Methods

THF was distilled from sodium-benzophenone immediately prior to use. All reactions were conducted under N<sub>2</sub> atmosphere. Melting points are uncorrected. IR spectra were recorded on Varian F-1000 spectrometer in KBr with absorptions in cm<sup>-1</sup>. <sup>1</sup>H NMR and <sup>13</sup>C NMR were determined on Varian Inova-400 MHz spectrometer in DMSO-*d*<sub>6</sub> solution. *J* values are in Hz. Chemical shifts are expressed in ppm downfield from internal standard TMS. HRMS data were obtained using TOF-MS instrument. X-Ray diffractions were recorded on a Siemens P4 or Simart-1000 diffractometer.

### General procedure for the synthesis of **3** is represented as follows

To a solution of 2-naphthol (**1**, 14.42 g, 0.1 mol) in absolute MeOH (50 mL) was added the appropriate aromatic aldehyde (0.2 mol; for liquid aldehydes, a freshly distilled sample was used) and 25% methanolic ammonia solution (20 mL). The mixture was left to stand at ambient temperature for 2 days, during which a crystalline product (**2**) separated out. The crystals were filtered off and washed with cool MeOH (2 × 20 mL), dried and suspended in 20% HCl (200 mL). The mixture was stirred and refluxed for 3 h, and the crystalline hydrochloride of **3** that separated out was filtered off and washed with EtOAc (2 × 25 mL). The hydrochloride was suspended in H<sub>2</sub>O (30 mL), and the mixture was treated with conc. NH<sub>4</sub>OH (30 mL) and extracted with EtOAc (3 × 50 mL). After drying (Na<sub>2</sub>SO<sub>4</sub>) and evaporation, crystalline **3** was obtained, which was recrystallized from *i*-Pr<sub>2</sub>O.

### General procedure for the synthesis of **4** is represented as follows

To a solution of the appropriate amino naphthol (**3**, 1 mmol) in absolute MeOH (20 mL), an equivalent amount of aromatic aldehyde was added (for liquid aldehydes, a freshly distilled sample was used), and the mixture was left to stand at ambient temperature for 24 h. The crystalline products **4** were filtered off, washed with Et<sub>2</sub>O and recrystallized.

### General procedure for the synthesis of **5** is represented as follows

TiCl<sub>4</sub> (0.3 mL, 3 mmol) was added dropwise using a syringe to a stirred suspension

of magnesium powder (0.14 g, 6 mmol) in freshly distilled anhydrous THF (10 mL) at r.t. under a dry N<sub>2</sub> atmosphere. After completion of the addition, the mixture was refluxed for 2 h. The suspension of the low-valent titanium reagent formed was cooled to r.t. and a solution of 1,3-diaryl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazines (**4**, 1 mmol) and triphosgene (1 mmol) in THF (5 mL) was added dropwise. The reaction mixture was then refluxed for 15 min under N<sub>2</sub>. After this period, the TLC analysis of the mixture showed the reaction to be completed. The reaction mixture was quenched with 5% HCl (15 mL) and extracted with ClCH<sub>2</sub>CH<sub>2</sub>Cl (3 × 20 mL). The combined extracts were washed with water (3 × 20 mL) and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. After evaporation of the solvent under reduced pressure, the crude product **5** was purified by recrystallization from acetone.

**General procedure for the synthesis of 6 is represented as follows**

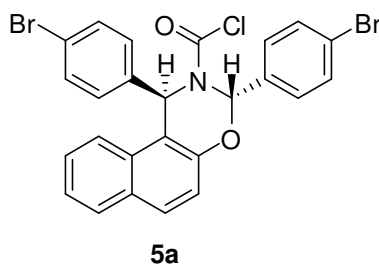
TiCl<sub>4</sub> (0.3 mL, 3 mmol) was added dropwise using a syringe to a stirred suspension of samarium powder (0.9 g, 6 mmol) in freshly distilled anhydrous THF (10 mL) at r.t. under a dry N<sub>2</sub> atmosphere. After completion of the addition, the mixture was refluxed for 2 h. The suspension of the low-valent titanium reagent formed was cooled to r.t. and a solution of 1,3-diaryl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazines (**4**, 1 mmol) and triphosgene (1 mmol) in THF (5 mL) was added dropwise. The reaction mixture was then refluxed for 15 min under N<sub>2</sub>. After this period, the TLC analysis of the mixture showed the reaction to be completed. The reaction mixture was quenched with 5% HCl (15 mL) and extracted with ClCH<sub>2</sub>CH<sub>2</sub>Cl (3 × 20 mL). The combined extracts were washed with water (3 × 20 mL) and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. After evaporation of the solvent under reduced pressure, the crude product **6** was purified by recrystallization from acetone.

**General procedure for the synthesis of 7 is represented as follows**

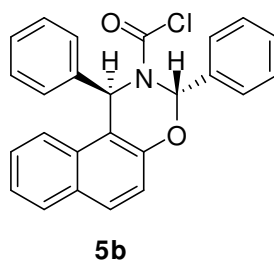
TiCl<sub>4</sub> (0.3 mL, 3 mmol) was added dropwise using a syringe to a stirred suspension of iron powder (0.17 g, 3 mmol) in freshly distilled anhydrous THF (10 mL) at r.t. under a dry N<sub>2</sub> atmosphere. After completion of the addition, the mixture was refluxed for 2 h. The suspension of the low-valent titanium reagent formed was cooled to r.t. and a solution of 1,3-diaryl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazines (**4**, 1 mmol)

and Triethyl orthoformate (1 mmol) in THF (5 mL) was added dropwise. The reaction mixture was then refluxed for 15 min under N<sub>2</sub>. After this period, the TLC analysis of the mixture showed the reaction to be completed. The reaction mixture was quenched with 5% HCl (15 mL) and extracted with ClCH<sub>2</sub>CH<sub>2</sub>Cl (3 × 20 mL). The combined extracts were washed with water (3 × 20 mL) and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. After evaporation of the solvent under reduced pressure, the crude product **7** was purified by recrystallization from acetone.

## Characterizations for compounds

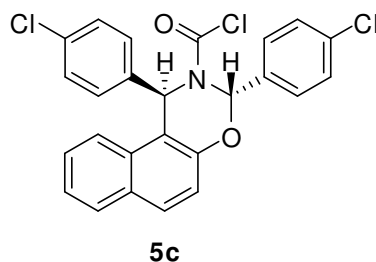


**Trans-1,3-bis(4-bromophenyl)-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbonyl chloride (5a):** m.p. 178-180 °C. IR (KBr)  $\nu$ : 1740, 1627, 1588, 1518, 1487, 1398, 1369, 1327, 1265, 1239, 1199, 1154, 1074, 1041, 1013, 969, 918, 883, 834, 817, 745  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 6.85 (s, 1H, CH), 7.15-7.20 (m, 3H, CH+ArH), 7.36-7.51 (m, 9H, ArH), 7.73 (d,  $J = 8.8$  Hz, 2H, ArH), 7.78 (d,  $J = 8.0$  Hz, 1H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 54.39, 79.28, 114.57, 117.22, 117.97, 118.09, 118.64, 119.99, 120.47, 122.81, 123.17, 123.47, 124.26, 124.62, 125.51, 126.12, 126.61, 127.27, 127.44, 134.45, 142.77. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{25}\text{H}_{16}^{79}\text{Br}_2^{35}\text{ClNO}_2$ : 554.9236, found 554.9247.

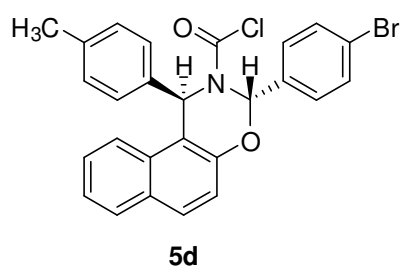


**Trans-1,3-diphenyl-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbonyl chloride (5b):** m.p. 171-173 °C. IR (KBr)  $\nu$ : 1733, 1623, 1602, 1494, 1468, 1454, 1394, 1316, 1233, 1185, 1148, 1042, 1025, 970, 927, 867, 819, 780, 757, 691  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 6.73-6.83 (m, 4H, 2CH + ArH), 6.87-6.98 (m, 7H, ArH), 7.14-7.17 (m, 2H, ArH), 7.29-7.33 (m, 1H, ArH), 7.42 (d,  $J = 9.2$  Hz, 1H, ArH), 7.57 (s, 1H, ArH), 7.80 (d,  $J = 7.6$  Hz, 1H, ArH), 7.89 (d,  $J = 9.2$  Hz, 1H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 50.34, 79.74, 106.66, 113.77, 118.83, 118.89, 119.67, 121.68, 122.48, 122.69, 123.32, 123.42, 123.57, 124.07, 124.28, 124.95, 125.08, 126.15, 126.39, 130.49, 144.76. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{25}\text{H}_{18}^{35}\text{ClNO}_2$ : 399.1026,

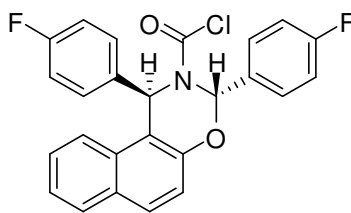
found 399.1022.



**Trans-1,3-bis(4-chlorophenyl)-1H-naphtho[1,2-e][1,3]oxazine-2(3H)-carbonyl chloride (5c):** m.p. 199-200 °C. IR (KBr)  $\nu$ : 1730, 1627, 1519, 1488, 1405, 1373, 1272, 1243, 1202, 1155, 1012, 971, 915, 884, 833, 750, 724  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 6.87 (s, 1H, CH), 7.16 (d,  $J = 8.8$  Hz, 1H, ArH), 7.28-7.31(m, 3H, CH+ ArH), 7.38-7.42 (m, 2H, ArH), 7.47-7.52 (m, 5H, ArH), 7.72-7.75 (m, 3H, ArH), 7.78 (d,  $J = 8.0$  Hz, 1H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 54.44, 80.28, 114.56, 117.23, 120.44, 122.88, 123.08, 124.31, 124.47, 124.61, 124.75, 125.20, 125.31, 125.78, 126.09, 129.74, 129.96, 130.00, 130.37, 133.92, 142.77. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{25}\text{H}_{16}^{35}\text{Cl}_3\text{NO}_2$ : 467.0247, found 467.0257.

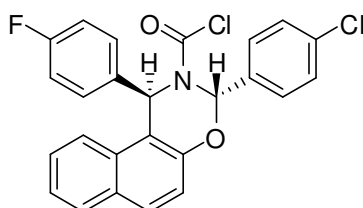


**Trans-3-(4-bromophenyl)-1-p-tolyl-1H-naphtho[1,2-e][1,3]oxazine-2(3H)-carbonyl chloride (5d):** m.p. 230-232 °C. IR (KBr)  $\nu$ : 1711, 1626, 1601, 1510, 1485, 1395, 1322, 1259, 1239, 1210, 1151, 1072, 1010, 973, 882, 818, 781, 749, 709  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 2.22 (s, 3H,  $\text{CH}_3$ ), 6.58-6.70 (m, 4H, CH+ ArH), 6.79-6.81 (m, 2H, ArH), 6.98 (d,  $J = 8.4$  Hz, 2H, ArH), 7.10 (s, 1H, CH), 7.20-7.22 (m, 1H, ArH), 7.31-7.39 (m, 3H, ArH), 7.49 (s, 1H, ArH), 7.80 (d,  $J = 3.6$  Hz, 1H, ArH), 7.88 (d,  $J = 8.8$  Hz, 1H, ArH). HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{26}\text{H}_{19}^{79}\text{Br}^{35}\text{ClNO}_2$ : 491.0288, found 491.0272.



**5e**

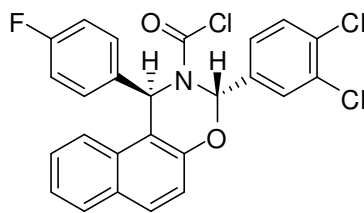
**Trans-1,3-bis(4-fluorophenyl)-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbonyl chloride (5e):** m.p. 158-160 °C. IR (KBr)  $\nu$ : 1723, 1628, 1603, 1505, 1369, 1327, 1274, 1244, 1223, 1511, 1100, 969, 914, 868, 837, 785, 737  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 6.85 (s, 1H, CH), 7.15-7.20 (m, 3H, CH+ ArH), 7.39-7.51 (m, 9H, ArH), 7.73 (d,  $J = 8.8$  Hz, 2H, ArH), 7.78 (d,  $J = 8.0$  Hz, 1H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 54.44, 80.24, 110.93, 111.06, 111.22, 111.35, 114.59, 117.32, 120.36, 123.02, 123.32, 123.43, 124.56, 125.40, 125.64, 125.75, 125.98, 131.25, 131.29, 142.71, 156.25, 156.64, 159.54, 159.93. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{25}\text{H}_{16}^{35}\text{ClF}_2\text{NO}_2$ : 435.0838, found 435.0831.



**5f**

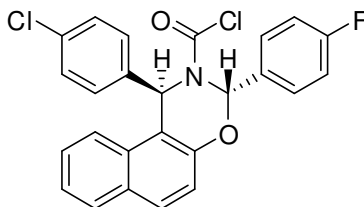
**Trans-3-(4-chlorophenyl)-1-(4-fluorophenyl)-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbonyl chloride (5f):** m.p. 178-179 °C. IR (KBr)  $\nu$ : 1754, 1624, 1604, 1507, 1491, 1466, 1375, 1341, 1280, 1236, 1154, 1090, 1047, 1012, 975, 913, 886, 841, 812, 752, 724, 707  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 6.91 (s, 1H, CH), 7.00-7.04 (m, 3H, CH+ ArH), 7.17 (d,  $J = 8.8$  Hz, 1H, ArH), 7.39-7.43 (m, 2H, ArH), 7.47-7.52 (m, 2H, ArH), 7.54-7.58 (m, 3H, ArH), 7.72-7.75 (m, 3H, ArH), 7.79 (d,  $J = 8.0$  Hz, 1H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 49.64, 79.25, 110.18, 110.46, 113.65, 118.63, 119.91, 122.71, 123.17, 123.64, 124.22, 125.04, 125.83, 125.87, 125.92, 126.13, 126.49, 129.21, 129.76, 144.42, 159.01. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{25}\text{H}_{16}^{35}\text{Cl}_2\text{FNO}_2$ : 451.0542, found 451.0560.





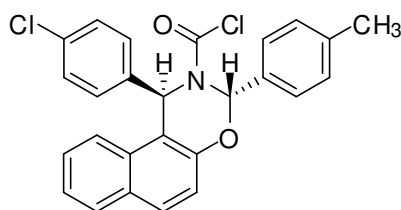
**5g**

**Trans-3-(3,4-dichlorophenyl)-1-(4-fluorophenyl)-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbonyl chloride (5g):** m.p. 200-201 °C. IR (KBr)  $\nu$ : 1717, 1626, 1602, 1505, 1468, 1403, 1335, 1245, 1229, 1245, 1205, 1155, 1096, 1031, 888, 861, 835, 735  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 6.94 (s, 1H, CH), 7.01-7.05 (m, 2H, CH+ ArH), 7.13 (d,  $J = 8.4$  Hz, 1H, ArH), 7.21 (d,  $J = 8.8$  Hz, 1H, ArH), 7.36 (d,  $J = 8.4$  Hz, 1H, ArH), 7.40-7.43 (m, 1H, ArH), 7.47-7.55 (m, 5H, ArH), 7.68 (d,  $J = 7.6$  Hz, 1H, ArH), 7.76-7.81 (m, 2H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 54.78, 79.11, 111.22, 111.51, 114.39, 117.47, 120.50, 120.59, 123.15, 123.58, 124.60, 125.68, 125.79, 126.05, 126.24, 128.48, 128.63, 131.02, 131.06, 131.59, 142.81, 156.36, 159.66. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{25}\text{H}_{15}^{35}\text{Cl}_3\text{FNO}_2$ : 485.0152, found 485.0178.



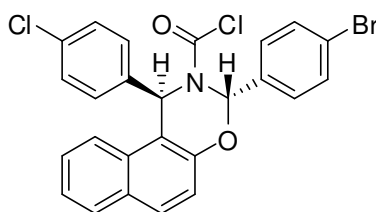
**5h**

**Trans-1-(4-chlorophenyl)-3-(4-fluorophenyl)-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbonyl chloride (5h):** m.p. 185-186 °C. IR (KBr)  $\nu$ : 1728, 1628, 1604, 1510, 1489, 1471, 1413, 1372, 1331, 1295, 1273, 1243, 1203, 1152, 970, 914, 869, 831, 790, 777, 736  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 6.89 (s, 1H, CH), 6.95-6.99 (m, 2H, CH+ ArH), 7.16 (d,  $J = 8.8$  Hz, 1H, ArH), 7.28-7.31 (m, 5H, ArH), 7.40 (t,  $J = 7.2$  Hz, 1H, ArH), 7.48-7.53 (m, 3H, ArH), 7.72-7.75 (m, 2H, ArH), 7.78 (d,  $J = 8.0$  Hz, 1H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 53.46, 80.26, 110.94, 111.23, 114.58, 117.19, 120.38, 123.04, 123.31, 123.43, 124.23, 124.44, 124.58, 125.18, 125.29, 125.75, 126.03, 129.70, 133.94, 142.74, 159.92. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{25}\text{H}_{16}^{35}\text{Cl}_2\text{FNO}_2$ : 451.0542, found 451.0544.



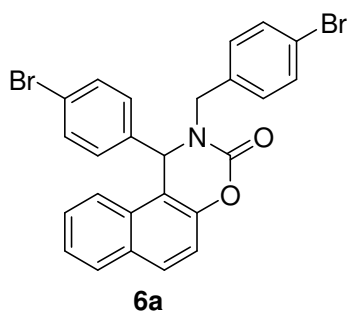
5i

**Trans-1-(4-chlorophenyl)-3-p-tolyl-1H-naphtho[1,2-*e*][1,3]oxazine-2(3*H*)-carbonyl chloride (5i):** m.p. 182-184 °C. IR (KBr)  $\nu$ : 2927, 2895, 1686, 1624, 1600, 1517, 1488, 1465, 1444, 1432, 1396, 1328, 1232, 1186, 1142, 1015, 852, 879, 818, 794, 768, 745  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 2.39 (s, 3H,  $\text{CH}_3$ ), 6.15(s, 1H, CH), 7.23-7.24 (m, 2H, CH+ ArH), 7.30-7.37 (m, 9H, ArH), 7.42-7.45 (m, 1H, ArH), 7.81-7.83 (m, 2H, ArH), 7.98 (s, 1H, ArH). HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{26}\text{H}_{19}^{35}\text{Cl}_2\text{NO}_2$ : 447.0793, found 447.0790.

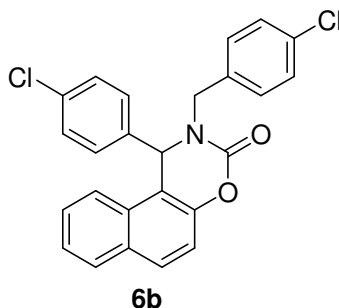


5j

**Trans-3-(4-bromophenyl)-1-(4-chlorophenyl)-1H-naphtho[1,2-*e*][1,3]oxazine-2(3*H*)-carbonyl chloride (5j):** m.p. 190-192 °C. IR (KBr)  $\nu$ : 1738, 1627, 1600, 1519, 1487, 1404, 1371, 1326, 1273, 1242, 1155, 1088, 1072, 1037, 1011, 970, 883, 800, 748, 721  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 6.88 (s, 1H, CH), 7.15-7.20 (m, 3H, CH+ ArH), 7.30 (d,  $J = 8.4$  Hz, 2H, ArH), 7.39-7.42 (m, 3H, ArH), 7.47-7.52 (m, 4H, ArH), 7.30 (d,  $J = 8.4$  Hz, 2H, ArH), 7.78 (d,  $J = 8.0$  Hz, 1H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 54.33, 80.30, 114.55, 117.22, 118.62, 120.44, 123.08, 123.15, 124.47, 124.60, 125.19, 125.29, 125.52, 125.78, 125.85, 126.09, 127.258, 129.74, 133.88, 142.77, 144.75. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{25}\text{H}_{16}^{79}\text{Br}^{35}\text{Cl}_2\text{NO}_2$ : 510.9741, found 510.9741.

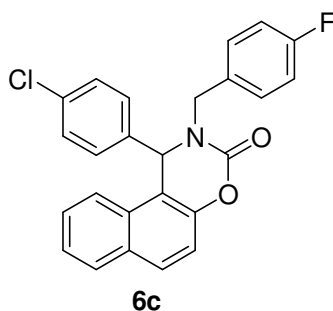


**2-(4-Bromobenzyl)-1-(4-bromophenyl)-1,2-dihydronaphtho[1,2-*e*][1,3]oxazin-3-one (6a):** m.p. 221-222 °C. IR (KBr)  $\nu$ : 1721, 1634, 1590, 1517, 1486, 1403, 1359, 1237, 1211, 1188, 1105, 1070, 1010, 951, 805, 772, 741  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 4.29 (d,  $J = 15.6$  Hz, 1H, CH), 4.80 (d,  $J = 15.6$  Hz, 1H, CH), 6.31 (s, 1H, CH), 7.26 (d,  $J = 8.4$  Hz, 2H, ArH), 7.44-7.55 (m, 9H, ArH), 7.88 (d,  $J = 8.4$  Hz, 1H, ArH), 7.97 (d,  $J = 8.0$  Hz, 1H, ArH), 8.03 (d,  $J = 8.8$  Hz, 1H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 50.35, 59.14, 115.24, 117.36, 121.15, 122.50, 123.36, 126.06, 128.35, 128.91, 129.47, 130.36, 130.39, 131.19, 131.34, 132.01, 132.77, 136.56, 140.19, 147.13, 150.39. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{25}\text{H}_{17}^{79}\text{Br}_2\text{NO}_2$ : 520.9626, found 520.9638.

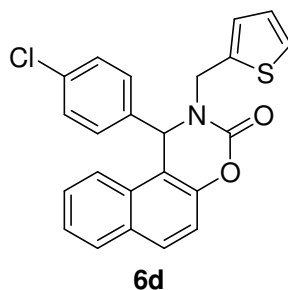


**2-(4-Chlorobenzyl)-1-(4-chlorophenyl)-1,2-dihydronaphtho[1,2-*e*][1,3]oxazin-3-one (6b):** m.p. 196-197 °C. IR (KBr)  $\nu$ : 1721, 1634, 1595, 1516, 1489, 1455, 1407, 1359, 1238, 1208, 1188, 1158, 1088, 1013, 994, 951, 805, 772, 709  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 4.31 (d,  $J = 15.6$  Hz, 1H, CH), 4.82 (d,  $J = 15.6$  Hz, 1H, CH), 6.33 (s, 1H, CH), 7.31-7.55 (m, 11H, ArH), 7.88 (d,  $J = 8.4$  Hz, 1H, ArH), 7.96 (d,  $J = 8.0$  Hz, 1H, ArH), 8.02 (d,  $J = 8.8$  Hz, 1H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 50.32, 59.07, 115.32, 117.37, 123.36, 126.05, 128.36, 128.92, 129.09, 129.47, 129.83, 130.01, 130.09, 131.19, 131.33, 132.64, 133.86, 136.15, 139.82, 147.14, 150.42. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{25}\text{H}_{17}^{35}\text{Cl}_2\text{NO}_2$ : 433.0636, found

433.0628.

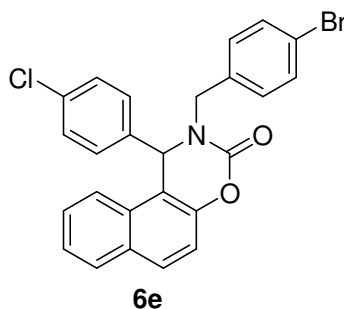


**2-(4-Fluorobenzyl)-1-(4-chlorophenyl)-1,2-dihydronaphtho[1,2-*e*][1,3]oxazin-3-one (6c):** m.p. 198-200 °C. IR (KBr)  $\nu$ : 1720, 1634, 1602, 1509, 1491, 1452, 1413, 1361, 1220, 1189, 1152, 1092, 1015, 994, 951, 851, 833, 805, 742, 733  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 3.93 (d,  $J = 15.2$  Hz, 1H, CH), 5.32 (d,  $J = 15.2$  Hz, 1H, CH), 5.70 (s, 1H, CH), 7.02-7.06 (m, 2H, ArH), 7.28-7.40 (m, 9H, ArH), 7.46-7.48 (m, 1H, ArH), 7.80-7.86 (m, 2H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 44.21, 53.51, 109.15, 111.34, 111.63, 112.39, 117.48, 120.77, 123.11, 124.19, 124.50, 124.72, 125.01, 125.22, 125.33, 126.28, 126.41, 126.48, 126.53, 130.30, 133.22, 142.31, 146.09. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{25}\text{H}_{17}^{35}\text{ClFNO}_2$ : 417.0932, found 417.0932.

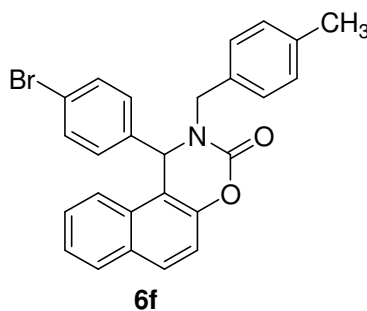


**1-(4-Chlorophenyl)-1,2-dihydro-2-((thiophen-2-yl)methyl)naphtho[1,2-*e*][1,3]oxazin-3-one (6d):** m.p. 165-167 °C. IR (KBr)  $\nu$ : 1717, 1634, 1589, 1516, 1490, 1473, 1444, 1277, 1216, 1191, 1089, 1015, 993, 886, 837, 805, 773, 744, 714  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 4.19 (d,  $J = 15.6$  Hz, 1H, CH), 5.43 (d,  $J = 15.6$  Hz, 1H, CH), 5.90 (s, 1H, CH), 6.98-7.00 (m, 1H, ArH), 7.08-7.09 (m, 1H, ArH), 7.27-7.37 (m, 6H, ArH), 7.38-7.43 (m, 2H, ArH), 7.51-7.53 (m, 1H, ArH), 7.79-7.84 (m, 2H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 39.71, 53.32, 109.11, 112.35, 117.55, 120.71, 121.73, 122.56, 123.04, 123.14, 124.21, 124.46, 124.83, 124.98, 126.19, 126.38, 130.27, 133.11, 133.21, 142.21, 145.53. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{23}\text{H}_{16}^{35}\text{ClNO}_2\text{S}$ :

405.0590, found 405.0593.

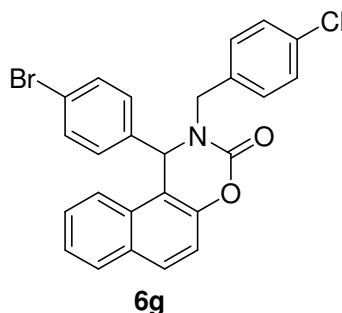


**2-(4-Bromobenzyl)-1-(4-chlorophenyl)-1,2-dihydronaphtho[1,2-*e*][1,3]oxazin-3-one (6e):** m.p. 194-196 °C. IR (KBr)  $\nu$ : 1722, 1634, 1592, 1516, 1487, 1455, 1403, 1238, 1207, 1188, 1083, 1011, 832, 805, 741  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 3.91 (d,  $J = 15.6$  Hz, 1H, CH), 5.30 (d,  $J = 15.6$  Hz, 1H, CH), 5.68 (s, 1H, CH), 7.20 (d,  $J = 8.0$  Hz, 2H, ArH), 7.28-7.41 (m, 7H, ArH), 7.45-7.49 (m, 3H, ArH), 7.80-7.86 (m, 2H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 44.28, 53.63, 109.02, 112.37, 117.47, 117.55, 120.79, 123.12, 124.15, 124.49, 124.68, 125.02, 125.12, 126.30, 126.41, 127.67, 129.77, 130.37, 133.06, 142.26, 146.07. HRMS:  $m/z$  [ $\text{M}^+$ ] calcd for  $\text{C}_{25}\text{H}_{17}^{79}\text{Br}^{35}\text{ClNO}_2$ : 477.0131, found 477.0122.

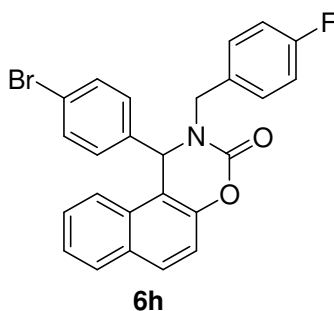


**2-(4-Methylbenzyl)-1-(4-bromophenyl)-1,2-dihydronaphtho[1,2-*e*][1,3]oxazin-3-one (6f):** m.p. 170-172 °C. IR (KBr)  $\nu$ : 1717, 1634, 1589, 1516, 1487, 1472, 1406, 1355, 1236, 1209, 1188, 1080, 1012, 994, 951, 827, 805, 772, 741, 727  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 2.34 (s, 3H,  $\text{CH}_3$ ), 3.86 (d,  $J = 15.6$  Hz, 1H, CH), 5.37 (d,  $J = 15.6$  Hz, 1H, CH), 5.71 (s, 1H, CH), 7.15-7.17 (m, 2H, ArH), 7.20-7.24 (m, 4H, ArH), 7.34-7.38 (m, 3H, ArH), 7.44-7.47 (m, 3H, ArH), 7.78-7.84 (m, 2H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) ( $\delta$ , ppm): 16.57, 44.41, 53.12, 109.15, 112.40, 117.54, 118.32, 120.64, 122.95, 123.56, 124.21, 124.42, 125.08, 125.21, 126.21, 126.34,

127.46, 127.86, 133.37, 133.81, 142.34, 146.08. HRMS:  $m/z$   $[M^+]$  calcd for  $C_{26}H_{20}^{79}BrNO_2$ : M, 457.0677, found 457.0659.

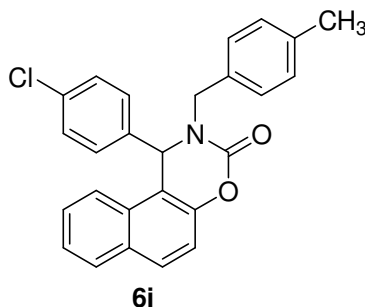


**2-(4-Chlorobenzyl)-1-(4-bromophenyl)-1,2-dihydronaphtho[1,2-*e*][1,3]oxazin-3-one (6g)**: m.p. 228-229 °C. IR (KBr)  $\nu$ : 1718, 1634, 1590, 1517, 1487, 1454, 1425, 1406, 1425, 1358, 1237, 1213, 1189, 1080, 1012, 951, 826, 805, 772, 741, 725  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $CDCl_3$ ) ( $\delta$ , ppm): 3.91 (d,  $J = 15.6$  Hz, 1H, CH), 5.32 (d,  $J = 15.6$  Hz, 1H, CH), 5.67 (s, 1H, CH), 7.20-7.24 (m, 3H, ArH), 7.31-7.48 (m, 9H, ArH), 7.70-7.75 (m, 2H, ArH).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ) ( $\delta$ , ppm): 44.23, 53.69, 108.95, 112.36, 117.45, 118.49, 120.78, 123.12, 124.13, 124.48, 124.71, 124.83, 124.97, 126.30, 126.39, 127.96, 129.22, 129.44, 133.59, 142.26, 146.04. HRMS:  $m/z$   $[M^+]$  calcd for  $C_{25}H_{17}^{79}Br^{35}ClNO_2$ : 477.0131, found 477.0135.

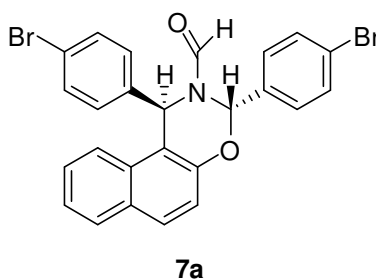


**2-(4-Fluorobenzyl)-1-(4-bromophenyl)-1,2-dihydronaphtho[1,2-*e*][1,3]oxazin-3-one (6h)**: m.p. 218-219 °C. IR (KBr)  $\nu$ : 1717, 1635, 1507, 1473, 1436, 1408, 1361, 1222, 1187, 1152, 1100, 1079, 1012, 994, 853, 832, 772, 742  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $CDCl_3$ ) ( $\delta$ , ppm): 3.93 (d,  $J = 15.2$  Hz, 1H, CH), 5.32 (d,  $J = 15.2$  Hz, 1H, CH), 5.69 (s, 1H, CH), 7.02-7.06 (m, 2H, ArH), 7.23 (d,  $J = 8.4$  Hz, 2H, ArH), 7.27-7.32 (m, 2H, ArH), 7.35-7.40 (m, 3H, ArH), 7.46-7.48 (m, 3H, ArH), 7.80-7.86 (m, 2H, ArH).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ) ( $\delta$ , ppm): 44.17, 53.53, 109.03, 111.33, 111.61, 112.37, 117.44, 118.45, 120.75, 123.09, 124.15, 124.48, 124.98, 125.19, 125.30,

126.26, 126.38, 127.94, 133.68, 142.27, 146.05, 156.34, 159.61. HRMS:  $m/z$  [ $M^+$ ] calcd for  $C_{25}H_{17}^{79}BrFNO_2$ : 461.0427, found 461.0408.

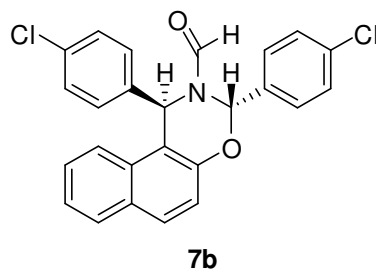


**2-(4-Methylbenzyl)-1-(4-chlorophenyl)-1,2-dihydro-naphtho[1,2-*e*][1,3]oxazin-3-one (6i):** m.p. 170-172 °C. IR (KBr)  $\nu$ : 1721, 1634, 1588, 1515, 1491, 1409, 1355, 1237, 1207, 1189, 1015, 994, 951, 885, 741, 728  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $CDCl_3$ ) ( $\delta$ , ppm): 2.36 (s, 3H,  $CH_3$ ), 3.87 (d,  $J = 15.2$  Hz, 1H, CH), 5.37 (d,  $J = 15.2$  Hz, 1H, CH), 5.74 (s, 1H, CH), 7.17-7.19 (m, 2H, ArH), 7.23 (s, 1H, ArH), 7.28-7.48 (m, 9H, ArH), 7.81-7.87 (m, 2H, ArH).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ) ( $\delta$ , ppm): 16.57, 44.40, 53.05, 109.24, 112.40, 117.56, 120.64, 122.95, 123.56, 124.23, 124.42, 124.78, 124.90, 125.21, 126.11, 126.35, 127.49, 130.16, 133.31, 133.36, 142.34, 146.09. HRMS:  $m/z$  [ $M^+$ ] calcd for  $C_{26}H_{20}^{35}ClNO_2$ : 413.1183, found 413.1189.

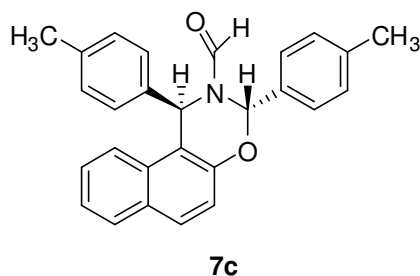


**Trans-1,3-bis(4-bromophenyl)-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbaldehyde (7a):** m.p. 238-240 °C. IR (KBr)  $\nu$ : 1681, 1624, 1599, 1515, 1487, 1432, 1344, 1327, 1232, 1141, 1070, 1009, 820, 790, 769, 740  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $DMSO-d_6$ ) ( $\delta$ , ppm): 6.39 (s, 1H, CH), 7.11 (s, 1H, CH), 7.31 (d,  $J = 8.4$  Hz, 1H, ArH), 7.37 (d,  $J = 9.2$  Hz, 1H, ArH), 7.43-7.54 (m, 6H, ArH), 7.62 (d,  $J = 8.0$  Hz, 2H, ArH), 7.73 (d,  $J = 8.0$  Hz, 2H, ArH), 7.97-8.02 (m, 3H, ArH + CHO).  $^{13}C$  NMR (100 MHz,  $DMSO-d_6$ ) ( $\delta$ , ppm): 51.04, 81.17, 104.98, 112.76, 122.27, 123.46, 123.84, 126.03, 128.07, 129.47, 130.09, 130.96, 131.01, 131.25, 131.36, 132.17, 132.53,

132.69, 140.51, 151.79, 160.68. HRMS:  $m/z$  [ $M^+$ ] Calcd for  $C_{25}H_{17}^{79}Br_2NO_2$ : 520.9626, found 520.9628.



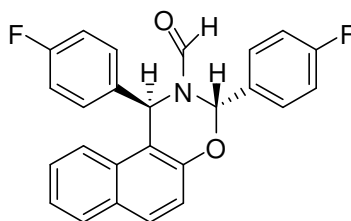
**Trans-1,3-bis(4-chlorophenyl)-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbaldehyde (7b):** m.p. 216-218 °C. IR (KBr)  $\nu$ : 1683, 1624, 1598, 1516, 1487, 1465, 1432, 1403, 1346, 1328, 1231, 1142, 1087, 1012, 853, 833, 820, 769, 755, 741, 706  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $DMSO-d_6$ ) ( $\delta$ , ppm): 6.37 (s, 1H, CH), 7.11 (s, 1H, CH), 7.33-7.36 (m, 3H, ArH), 7.41-7.46 (m, 4H, ArH), 7.49-7.52 (m, 3H, ArH), 7.55-7.58 (m, 2H, ArH), 7.93-7.98 (m, 3H, ArH + CHO).  $^{13}C$  NMR (100 MHz,  $DMSO-d_6$ ) ( $\delta$ , ppm): 50.96, 81.08, 112.75, 119.19, 123.44, 124.96, 128.02, 129.45, 129.59, 129.76, 129.80, 129.98, 130.92, 131.03, 131.31, 131.57, 133.59, 135.16, 140.09, 151.79, 160.62. HRMS:  $m/z$  [ $M^+$ ] Calcd for  $C_{25}H_{17}^{35}Cl_2NO_2$ : 433.0636, found 433.0635.



**Trans-1,3-dip-tolyl-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbaldehyde (7c):** m.p. 217-218 °C. IR (KBr)  $\nu$ : 2914, 1674, 1623, 1599, 1508, 1447, 1432, 1398, 1311, 1233, 1139, 1080, 1016, 877, 847, 823, 777, 805, 752  $cm^{-1}$ .  $^1H$  NMR (400 MHz,  $DMSO-d_6$ ) ( $\delta$ , ppm): 2.30 (s, 3H,  $CH_3$ ), 2.35 (s, 3H,  $CH_3$ ), 6.28 (s, 1H, CH), 7.08 (s, 1H, CH), 7.18-7.22 (m, 4H, ArH), 7.29-7.33 (m, 5H, ArH), 7.37-7.43 (m, 2H, ArH), 7.46-7.48 (m, 1H, ArH), 7.88 (s, 1H, CHO), 7.91-7.96 (m, 2H, ArH).  $^{13}C$  NMR (100 MHz,  $DMSO-d_6$ ) ( $\delta$ , ppm): 21.36, 21.49, 51.26, 81.54, 113.12, 113.14, 119.15, 123.49, 124.78, 127.69, 127.82, 129.01, 129.36, 129.86, 130.16, 130.25, 130.35, 130.63, 138.15, 138.49, 140.04, 151.92, 160.36. HRMS:  $m/z$  [ $M^+$ ] Calcd for  $C_{27}H_{23}NO_2$ :

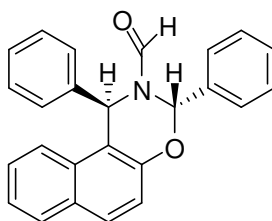


393.1729, found 393.1725.



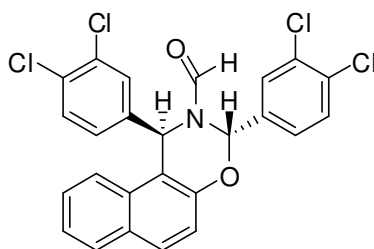
**7d**

**Trans-1,3-bis(4-fluorophenyl)-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbaldehyde (7d):** m.p. 186-187 °C. IR (KBr)  $\nu$ : 1669, 1602, 1506, 1345, 1398, 1300, 1227, 1154, 1077, 1016, 818, 769, 751  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 6.36 (s, 1H, CH), 7.13 (s, 1H, CH), 7.22 (t,  $J = 8.8$  Hz, 2H, ArH), 7.32-7.46 (m, 7H, ArH), 7.48-7.55 (m, 3H, ArH), 7.92-7.99 (m, 3H, ArH + CHO).  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 50.86, 81.04, 112.87, 116.25, 116.54, 116.83, 119.16, 123.47, 124.88, 127.94, 128.81, 128.85, 129.42, 129.92, 130.22, 130.34, 131.21, 131.33, 131.36, 137.51, 137.54, 151.83, 160.49. HRMS:  $m/z$  [ $\text{M}^+$ ] Calcd for  $\text{C}_{25}\text{H}_{17}\text{F}_2\text{NO}_2$ : M, 401.1227, found 401.1227.



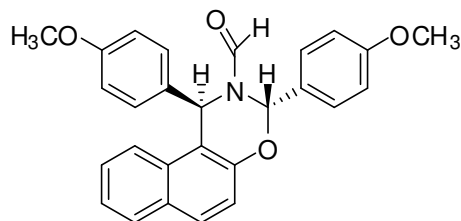
**7e**

**Trans-1,3-diphenyl-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbaldehyde (7e):** m.p. 152-154 °C. IR (KBr)  $\nu$ : 3063, 3031, 2903, 1674, 1621, 1598, 1515, 1492, 1458, 1431, 1395, 1345, 1323, 1312, 1231, 1158, 1136, 1082, 1013, 987, 922, 868, 821, 714  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 6.35 (s, 1H, CH), 7.14 (s, 1H, CH), 7.34-7.50 (m, 14H, ArH), 7.91-7.99 (m, 3H, ArH + CHO).  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 51.57, 81.58, 113.01, 119.19, 123.48, 124.83, 127.76, 127.87, 128.89, 129.10, 129.38, 129.58, 129.69, 129.88, 130.49, 130.73, 131.51, 132.59, 141.33, 151.91, 160.45. HRMS:  $m/z$  [ $\text{M}^+$ ] Calcd for  $\text{C}_{25}\text{H}_{19}\text{NO}_2$ : 365.1416, found 365.1417.



7f

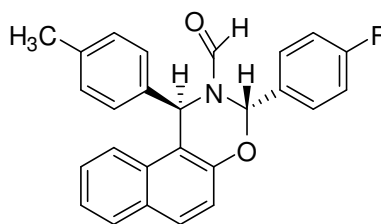
**Trans-1,3-bis(3,4-dichlorophenyl)-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbaldehyde (7f):** m.p. 229-231 °C. IR (KBr)  $\nu$ : 3064, 2910, 1676, 1624, 1599, 1560, 1515, 1468, 1423, 1326, 1226, 1129, 1079, 1022, 926, 812, 769, 751  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 6.51 (s, 1H, CH), 7.14 (s, 1H, CH), 7.32 (d,  $J = 7.6$  Hz, 1H, ArH), 7.40 (d,  $J = 8.8$  Hz, 1H, ArH), 7.45-7.58 (m, 5H, ArH), 7.65-7.68 (m, 1H, ArH), 7.78 (d,  $J = 8.4$  Hz, 1H, ArH), 7.86 (s, 1H, ArH), 7.97-8.06 (m, 3H, ArH+CHO).  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 50.59, 80.61, 112.36, 112.40, 119.23, 123.44, 125.09, 128.15, 128.42, 129.53, 129.97, 130.16, 131.10, 131.15, 131.22, 131.31, 131.71, 131.83, 132.14, 132.55, 133.28, 133.87, 141.87, 151.66, 161.07. HRMS:  $m/z$  [ $\text{M}^+$ ] Calcd for  $\text{C}_{25}\text{H}_{15}^{35}\text{Cl}_4\text{NO}_2$ : 500.9857, found 500.9847.



7g

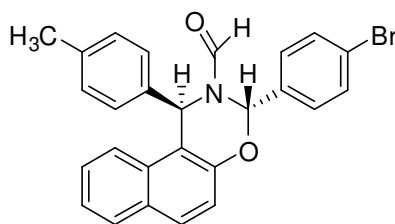
**Trans-1,3-bis(4-methoxyphenyl)-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbaldehyde (7g):** m.p. 162-164 °C. IR (KBr)  $\nu$ : 2907, 2840, 1672, 1610, 1511, 1464, 1434, 1324, 1305, 1253, 1227, 1178, 1079, 1004, 839, 819, 704  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 3.74 (s, 3H,  $\text{OCH}_3$ ), 3.79 (s, 3H,  $\text{OCH}_3$ ), 6.27 (s, 1H, CH), 6.94 (d,  $J = 8.4$  Hz, 2H, ArH), 7.04 (d,  $J = 8.8$  Hz, 2H, ArH), 7.06 (s, 1H, CH), 7.24 (d,  $J = 8.4$  Hz, 2H, ArH), 7.31 (d,  $J = 8.8$  Hz, 1H, ArH), 7.36-7.43 (m, 4H, ArH), 7.47-7.49 (m, 1H, ArH), 7.88 (s, 1H, CHO), 7.91-7.96 (m, 2H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 50.93, 55.72, 55.92, 81.38, 113.16, 114.88, 1153.09, 119.18, 123.51, 124.31, 124.77, 127.85, 129.38, 129.84, 130.35, 130.59, 130.67, 131.49, 133.51, 151.92, 159.60, 160.32, 160.86. HRMS:  $m/z$  [ $\text{M}^+$ ] Calcd for  $\text{C}_{27}\text{H}_{23}\text{NO}_4$ :

425.1627, found 425.1628.



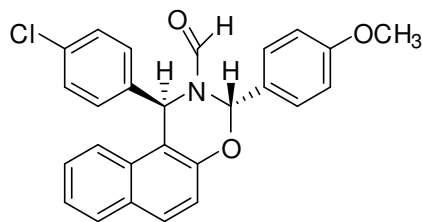
7h

**Trans-3-(4-fluorophenyl)-1-p-tolyl-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbaldehyde (7h):** m.p. 178-180 °C. IR (KBr)  $\nu$ : 3052, 2918, 1673, 1621, 1598, 1513, 1453, 1434, 1396, 1416, 1321, 1226, 1160, 1100, 1002, 855, 808, 759, 739  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 2.30 (s, 3H,  $\text{CH}_3$ ), 6.34 (s, 1H, CH), 7.08 (s, 1H, CH), 7.20 (s, 4H, ArH), 7.32-7.34 (m, 3H, ArH), 7.38-7.42 (m, 2H, ArH), 7.47-7.50 (m, 3H, ArH), 7.89-7.97 (m, 3H, ArH+ CHO). HRMS:  $m/z$  [ $\text{M}^+$ ] Calcd for  $\text{C}_{26}\text{H}_{20}\text{FNO}_2$ : 397.1478, found 397.1477.



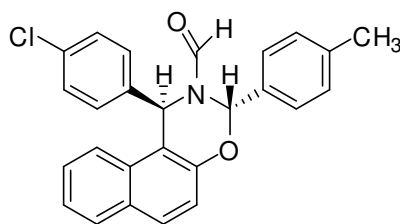
7i

**Trans-3-(4-bromophenyl)-1-p-tolyl-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbaldehyde (7i):** m.p. 233-235 °C. IR (KBr)  $\nu$ : 1676, 1623, 1597, 1507, 1467, 1489, 1448, 1432, 1396, 1344, 1303, 1274, 1231, 1140, 1073, 1010, 876, 847, 825, 807, 778, 753, 704  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 2.29 (s, 3H,  $\text{CH}_3$ ), 6.31 (s, 1H, CH), 7.08 (s, 1H, CH), 7.20 (s, 4H, ArH), 7.31-7.34 (m, 1H, ArH), 7.38-7.40 (m, 4H, ArH), 7.46-7.47 (m, 1H, ArH), 7.68-7.70 (m, 2H, ArH), 7.91-7.97 (m, 3H, ArH + CHO).  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 21.40, 51.33, 81.04, 104.98, 113.27, 119.14, 123.52, 123.79, 124.90, 127.92, 129.04, 129.40, 130.00, 130.19, 130.71, 131.47, 132.13, 132.73, 133.19, 138.32, 151.69, 160.51. HRMS:  $m/z$  [ $\text{M}^+$ ] Calcd for  $\text{C}_{26}\text{H}_{20}^{79}\text{BrNO}_2$ : 457.0677, found 457.0675.



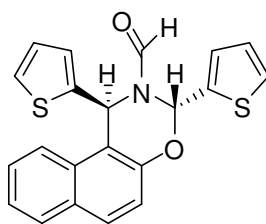
7j

**Trans-1-(4-chlorophenyl)-3-(4-methoxyphenyl)-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbaldehyde (7j):** m.p. 179-181 °C. IR (KBr)  $\nu$ : 1676, 1614, 1598, 1515, 1461, 1488, 1433, 1396, 1305, 1252, 1229, 1174, 1139, 1016, 1004, 875, 827, 809, 773  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 3.79 (s, 3H,  $\text{OCH}_3$ ), 6.28 (s, 1H, CH), 7.04 (d,  $J = 8.8$  Hz, 2H, ArH), 7.09 (s, 1H, CH), 7.32-7.46 (m, 10H, ArH), 7.91-7.98 (m, 3H, ArH+ CHO). HRMS:  $m/z$  [ $\text{M}^+$ ] Calcd for  $\text{C}_{26}\text{H}_{20}^{35}\text{ClNO}_3$ : 429.1132, found 429.1138.



7k

**Trans-1-(4-chlorophenyl)-3-*p*-tolyl-1H-naphtho[1,2-*e*][1,3]oxazine-2(3H)-carbaldehyde (7k):** m.p. 176-178 °C. IR (KBr)  $\nu$ : 1685, 1624, 1599, 1517, 1488, 1444, 1432, 1396, 1345, 1328, 1233, 1185, 1142, 1077, 1015, 852, 818, 768, 745  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 2.35 (s, 3H,  $\text{CH}_3$ ), 6.30 (s, 1H, CH), 7.09 (s, 1H, CH), 7.30-7.35 (m, 7H, ArH), 7.39-7.49 (m, 5H, ArH), 7.90 (s, 1H, CHO), 7.93-7.98 (m, 2H, ArH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ) ( $\delta$ , ppm): 21.53, 50.91, 81.65, 112.66, 119.29, 123.43, 124.95, 127.84, 128.04, 129.47, 129.62, 129.69, 129.91, 130.28, 131.02, 131.12, 131.14, 133.56, 140.12, 151.99, 160.55. HRMS:  $m/z$  [ $\text{M}^+$ ] Calcd for  $\text{C}_{26}\text{H}_{20}^{35}\text{ClNO}_2$ : 413.1183, found 413.1181.



7l

**Trans-1,3-di(thiophen-2-yl)-1*H*-naphtho[1,2-*e*][1,3]oxazine-2(3*H*)-carbaldehyde (71):** m.p. 159-161 °C. IR (KBr)  $\nu$ : 1665, 1623, 1597, 1515, 1453, 1428, 1396, 1369, 1320, 1223, 1133, 1081, 1005, 915, 855, 819, 745, 713  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) ( $\delta$ , ppm): 6.78 (s, 1H, CH), 6.91-6.99 (m, 2H, CH+ ArH), 7.17-7.20 (m, 2H, ArH), 7.29 (d,  $J = 8.8$  Hz, 1H, ArH), 7.36 (d,  $J = 2.0$  Hz, 1H, ArH), 7.40-7.49 (m, 2H, ArH), 7.58 (d,  $J = 3.2$  Hz, 1H, ArH), 7.64 (d,  $J = 3.2$  Hz, 1H, ArH), 7.82 (d,  $J = 5.2$  Hz, 1H, ArH), 7.95 (t,  $J = 9.2$  Hz, 2H, ArH), 8.01 (s, 1H, CHO). HRMS:  $m/z$  [ $\text{M}^+$ ] Calcd for  $\text{C}_{21}\text{H}_{15}\text{NO}_2\text{S}_2$ : M, 377.0544, found 377.0544.

## Crystal structures of compounds

### Crystal data for 5c

$C_{25}H_{16}Cl_3NO_2$ ;  $M = 468.74$ , colourless block crystals,  $0.28 \times 0.20 \times 0.17$  mm, monoclinic, space group  $P2_1/c$ ,  $a = 12.4435(12)$  Å,  $b = 11.3232(9)$  Å,  $c = 15.7047(19)$  Å,  $\alpha = 90^\circ$ ,  $\beta = 100.9270(10)^\circ$ ,  $\gamma = 90^\circ$ ,  $V = 2172.7(4)$  Å<sup>3</sup>,  $Z = 4$ ,  $D_c = 1.443$  g·cm<sup>-3</sup>,  $F(000) = 960$ ,  $\mu$  (MoK $\alpha$ ) =  $0.445$  mm<sup>-1</sup>. Intensity data were collected on a diffractometer with graphite monochromated MoK $\alpha$  radiation ( $\lambda = 0.71073$  Å) using  $\omega$  scan mode with  $1.92^\circ < \theta < 25.01^\circ$ . 3824 unique reflections were measured and 2266 reflections with  $I > 2\sigma(I)$  were used in the refinement. The structure was solved by direct methods and expanded using Fourier techniques. The final cycle of full-matrix least squares technique to  $R = 0.0426$  and  $wR = 0.0783$ .

### Crystal data for 6i

$C_{26}H_{20}ClNO_2$ ;  $M = 413.88$ , colourless block crystals,  $0.38 \times 0.30 \times 0.12$  mm, monoclinic, space group  $P2_1/c$ ,  $a = 15.1846(18)$  Å,  $b = 8.1074(10)$  Å,  $c = 16.585(2)$  Å,  $\alpha = 90^\circ$ ,  $\beta = 95.3460(10)^\circ$ ,  $\gamma = 90^\circ$ ,  $V = 2032.9(4)$  Å<sup>3</sup>,  $Z = 4$ ,  $D_c = 1.352$  g·cm<sup>-3</sup>,  $F(000) = 864$ ,  $\mu$  (MoK $\alpha$ ) =  $0.211$  mm<sup>-1</sup>. Intensity data were collected on a diffractometer with graphite monochromated MoK $\alpha$  radiation ( $\lambda = 0.71073$  Å) using  $\omega$  scan mode with  $1.35^\circ < \theta < 25.01^\circ$ . 3573 unique reflections were measured and 1583 reflections with  $I > 2\sigma(I)$  were used in the refinement. The structure was solved by direct methods and expanded using Fourier techniques. The final cycle of full-matrix least squares technique to  $R = 0.0489$  and  $wR = 0.1014$ .

### Crystal data for 7b

$C_{25}H_{17}Cl_2NO_2$ ;  $M = 434.30$ , colourless block crystals,  $0.46 \times 0.40 \times 0.28$  mm, Triclinic, space group  $P -1$ ,  $a = 7.555(2)$  Å,  $b = 12.330(4)$  Å,  $c = 12.404(4)$  Å,  $\alpha = 111.777(5)^\circ$ ,  $\beta = 97.341(4)^\circ$ ,  $\gamma = 101.905(4)^\circ$ ,  $V = 1023.1(5)$  Å<sup>3</sup>,  $Z = 2$ ,  $D_c = 1.410$  g·cm<sup>-3</sup>,  $F(000) = 448$ ,  $\mu$  (MoK $\alpha$ ) =  $0.340$  mm<sup>-1</sup>. Intensity data were collected on a diffractometer with graphite monochromated MoK $\alpha$  radiation ( $\lambda = 0.71070$  Å) using  $\omega$  scan mode with  $3.08^\circ < \theta < 26.35^\circ$ . 3700 unique reflections were measured and 2888 reflections with  $I > 2\sigma(I)$  were used in the refinement. The structure was solved

by direct methods and expanded using Fourier techniques. The final cycle of full-matrix least squares technique to  $R = 0.0501$  and  $wR = 0.1079$ .

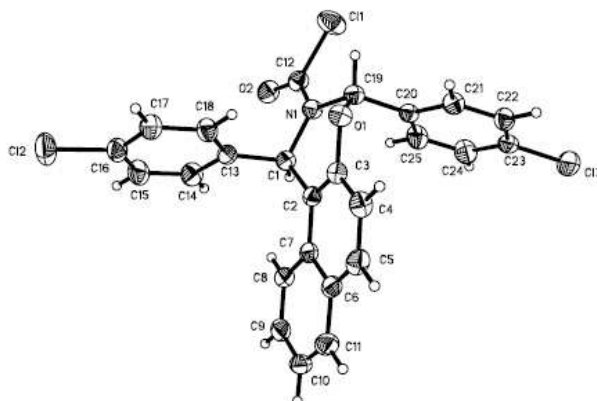


FIGURE 1. ORTEP plot of the molecular structure of compound **5c** in crystal

**TABLE 1** Bond lengths (Å) for **5c**

Bond	Bond Lengths	Bond	Bond Lengths	Bond	Bond Lengths
Cl(1)-C(12)	1.782(3)	C(2)-C(7)	1.421(4)	C(14)-C(15)	1.385(4)
Cl(2)-C(16)	1.740(3)	C(3)-C(4)	1.397(4)	C(15)-C(16)	1.366(5)
Cl(3)-C(23)	1.733(3)	C(4)-C(5)	1.353(4)	C(16)-C(17)	1.372(4)
N(1)-C(12)	1.336(4)	C(5)-C(6)	1.410(4)	C(17)-C(18)	1.379(4)
N(1)-C(19)	1.470(3)	C(6)-C(11)	1.408(4)	C(19)-C(20)	1.516(4)
N(1)-C(1)	1.489(3)	C(6)-C(7)	1.422(4)	C(20)-C(25)	1.374(4)
O(1)-C(3)	1.385(3)	C(7)-C(8)	1.414(4)	C(20)-C(21)	1.383(4)
O(1)-C(19)	1.419(3)	C(8)-C(9)	1.369(4)	C(21)-C(22)	1.374(4)
O(2)-C(12)	1.194(3)	C(9)-C(10)	1.392(5)	C(22)-C(23)	1.370(4)
C(1)-C(2)	1.521(4)	C(10)-C(11)	1.353(5)	C(23)-C(24)	1.361(4)
C(1)-C(13)	1.527(4)	C(13)-C(18)	1.381(4)	C(24)-C(25)	1.383(4)
C(2)-C(3)	1.365(4)	C(13)-C(14)	1.385(4)		

**TABLE 2** Bond angles (°) for **5c**

Angles	(°)	Angles	(°)
C(1)-N(1)-C(4)	124.6(4)	C(14)-C(9)-C(10)	122.0(5)
C(1)-N(2)-C(2)	125.4(4)	C(14)-C(9)-N(2)	119.6(4)
C(1)-N(2)-C(9)	118.5(4)	C(10)-C(9)-N(2)	118.4(5)
C(2)-N(2)-C(9)	116.2(4)	C(9)-C(14)-C(13)	119.7(5)
C(2)-N(3)-C(15)	128(4)	C(20)-C(15)-C(16)	117(8)
C(2)-N(3)-C(15')	127(10)	C(20)-C(15)-N(3)	122(6)
C(15)-N(3)-C(15')	15(10)	C(16)-C(15)-N(3)	121(5)
N(1)-C(1)-N(2)	116.9(4)	C(17)-C(16)-C(15)	121(5)
N(1)-C(1)-S(1)	118.9(4)	C(20')-C(15')-N(3)	124(10)

N(2)-C(1)-S(1)	124.2(3)	C(16')-C(15')-N(3)	116(10)
N(3)-C(2)-N(2)	115.2(4)	C(18')-C(17')-Cl(1')	123(10)
N(3)-C(2)-C(3)	130.6(5)	C(16')-C(17')-Cl(1')	117(10)
N(2)-C(2)-C(3)	114.3(4)	C(17')-C(18')-C(19')	120(10)
C(4)-C(3)-C(2)	119.1(4)	C(17')-C(18')-C(21')	120(10)
C(8)-C(3)-C(2)	123.6(5)	C(19')-C(18')-C(21')	120(10)
C(3)-C(4)-N(1)	119.4(4)	C(20')-C(19')-C(18')	120(10)
N(1)-C(4)-C(5)	118.5(5)	C(15')-C(20')-C(19')	120(10)
C(7)-C(8)-C(3)	120.6(5)		

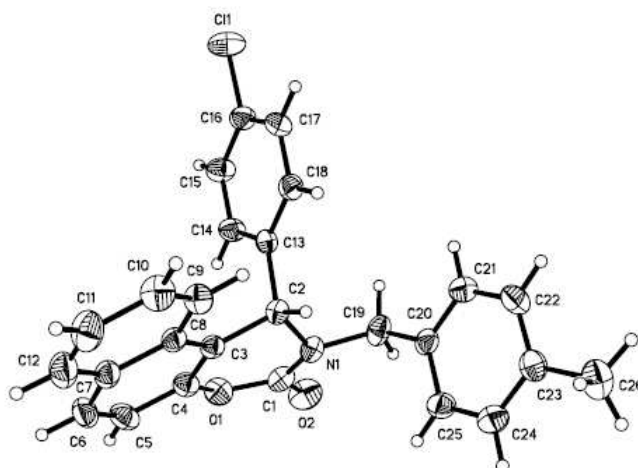


FIGURE 2. ORTEP plot of the molecular structure of compound **6i** in crystal

**TABLE 3** Bond lengths (Å) for **6i**

Bond	Bond Lengths	Bond	Bond Lengths	Bond	Bond Lengths
Cl(1)-C(16)	1.729(3)	C(5)-C(6)	1.353(4)	C(16)-C(17)	1.377(4)
N(1)-C(1)	1.352(4)	C(6)-C(7)	1.407(4)	C(17)-C(18)	1.376(4)
N(1)-C(19)	1.464(3)	C(7)-C(12)	1.401(4)	C(19)-C(20)	1.501(4)
N(1)-C(2)	1.474(3)	C(7)-C(8)	1.418(4)	C(20)-C(25)	1.374(4)
O(1)-C(1)	1.358(3)	C(8)-C(9)	1.404(4)	C(20)-C(21)	1.376(4)
O(1)-C(4)	1.392(3)	C(9)-C(10)	1.365(4)	C(21)-C(22)	1.374(4)
O(2)-C(1)	1.206(3)	C(10)-C(11)	1.401(5)	C(22)-C(23)	1.369(4)
C(2)-C(3)	1.497(4)	C(11)-C(12)	1.354(5)	C(23)-C(24)	1.379(4)
C(2)-C(13)	1.514(4)	C(13)-C(18)	1.379(4)	C(23)-C(26)	1.504(4)
C(3)-C(4)	1.361(4)	C(13)-C(14)	1.385(4)	C(24)-C(25)	1.377(4)
C(3)-C(8)	1.426(4)	C(14)-C(15)	1.379(4)		
C(4)-C(5)	1.399(4)	C(15)-C(16)	1.365(4)		

**TABLE 4** Bond angles (°) for **6i**

Angles	(°)	Angles	(°)
C(1)-N(1)-C(19)	117.3(3)	C(9)-C(10)-C(11)	119.7(3)



C(1)-N(1)-C(2)	123.0(2)	C(12)-C(11)-C(10)	120.7(3)
C(19)-N(1)-C(2)	115.3(2)	C(11)-C(12)-C(7)	120.7(3)
C(1)-O(1)-C(4)	120.7(2)	C(18)-C(13)-C(14)	117.8(3)
O(2)-C(1)-N(1)	124.8(3)	C(18)-C(13)-C(2)	121.8(3)
O(2)-C(1)-O(1)	118.1(3)	C(14)-C(13)-C(2)	120.4(3)
N(1)-C(1)-O(1)	117.1(3)	C(15)-C(14)-C(13)	121.8(3)
N(1)-C(2)-C(3)	108.8(2)	C(16)-C(15)-C(14)	119.2(3)
N(1)-C(2)-C(13)	112.2(2)	C(15)-C(16)-C(17)	120.3(3)
C(3)-C(2)-C(13)	112.0(2)	C(15)-C(16)-Cl(1)	119.2(3)
C(4)-C(3)-C(8)	118.5(3)	C(17)-C(16)-Cl(1)	120.5(3)
C(4)-C(3)-C(2)	118.5(3)	C(18)-C(17)-C(16)	120.0(3)
C(8)-C(3)-C(2)	123.0(3)	C(17)-C(18)-C(13)	120.9(3)
C(3)-C(4)-O(1)	121.4(3)	N(1)-C(19)-C(20)	113.9(2)
C(3)-C(4)-C(5)	123.4(3)	C(25)-C(20)-C(21)	117.1(3)
O(1)-C(4)-C(5)	115.2(3)	C(25)-C(20)-C(19)	121.6(3)
C(6)-C(5)-C(4)	118.5(3)	C(21)-C(20)-C(19)	121.2(3)
C(5)-C(6)-C(7)	121.7(3)	C(22)-C(21)-C(20)	121.2(3)
C(12)-C(7)-C(6)	121.4(3)	C(23)-C(22)-C(21)	122.0(3)
C(12)-C(7)-C(8)	119.4(3)	C(22)-C(23)-C(24)	116.9(3)
C(6)-C(7)-C(8)	119.2(3)	C(22)-C(23)-C(26)	121.4(3)
C(9)-C(8)-C(7)	118.2(3)	C(24)-C(23)-C(26)	121.7(3)
C(9)-C(8)-C(3)	123.0(3)	C(25)-C(24)-C(23)	121.2(3)
C(7)-C(8)-C(3)	118.8(3)	C(20)-C(25)-C(24)	121.6(3)
C(10)-C(9)-C(8)	121.3(3)		

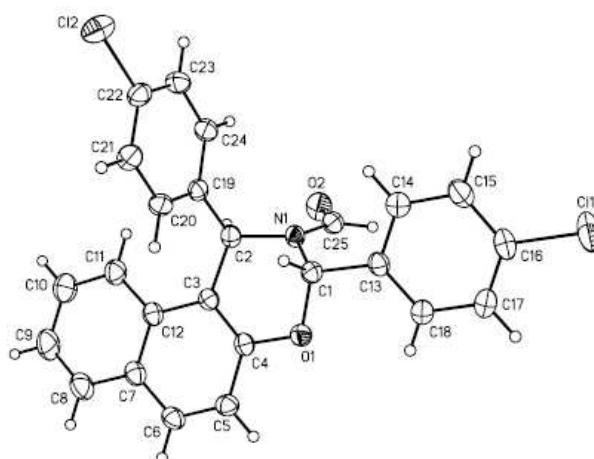


FIGURE 3. ORTEP plot of the molecular structure of compound **7b** in crystal

**Table 5.** Selected bond lengths (Å) for **7b**

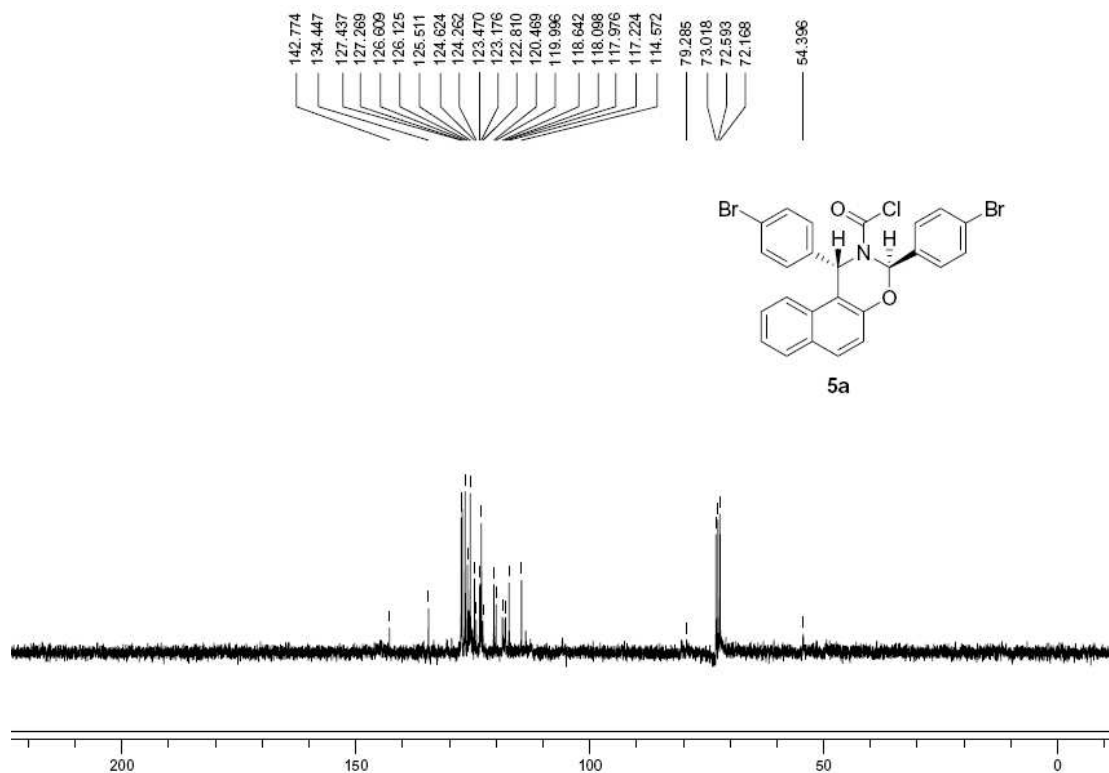
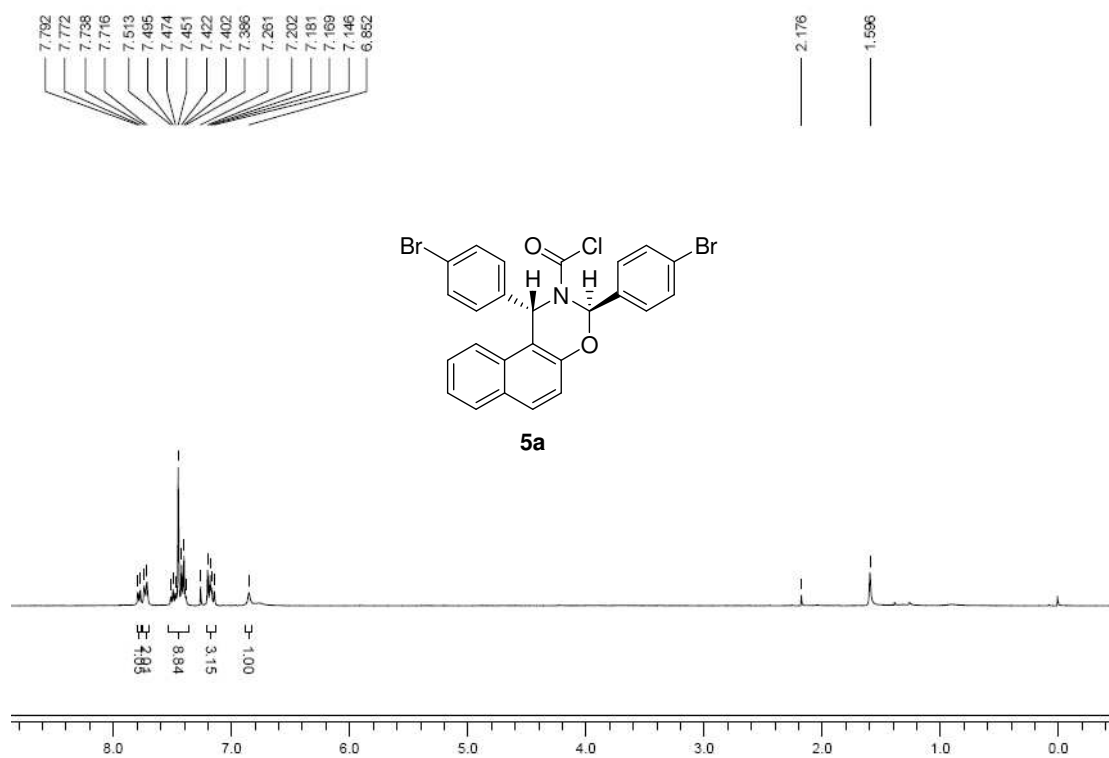
Bond	Bond Lengths	Bond	Bond Lengths	Bond	Bond Lengths
Cl(1)-C(16)	1.740(2)	C(3)-C(12)	1.432(3)	C(14)-C(15)	1.372(3)

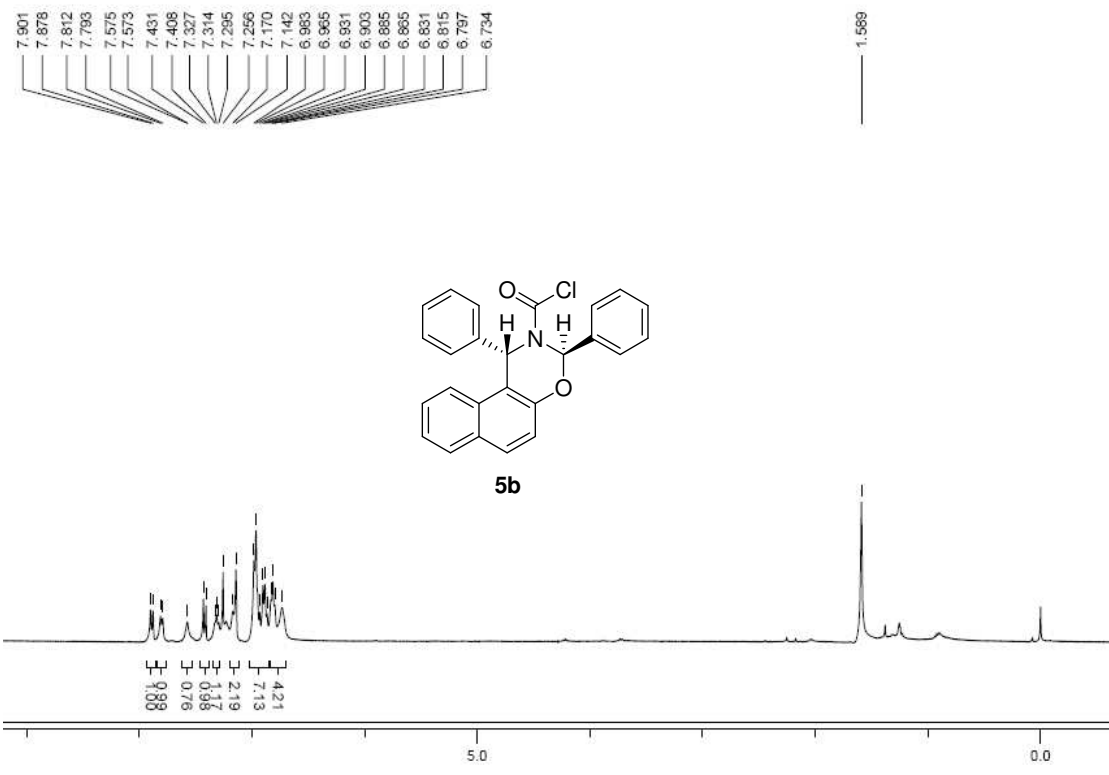
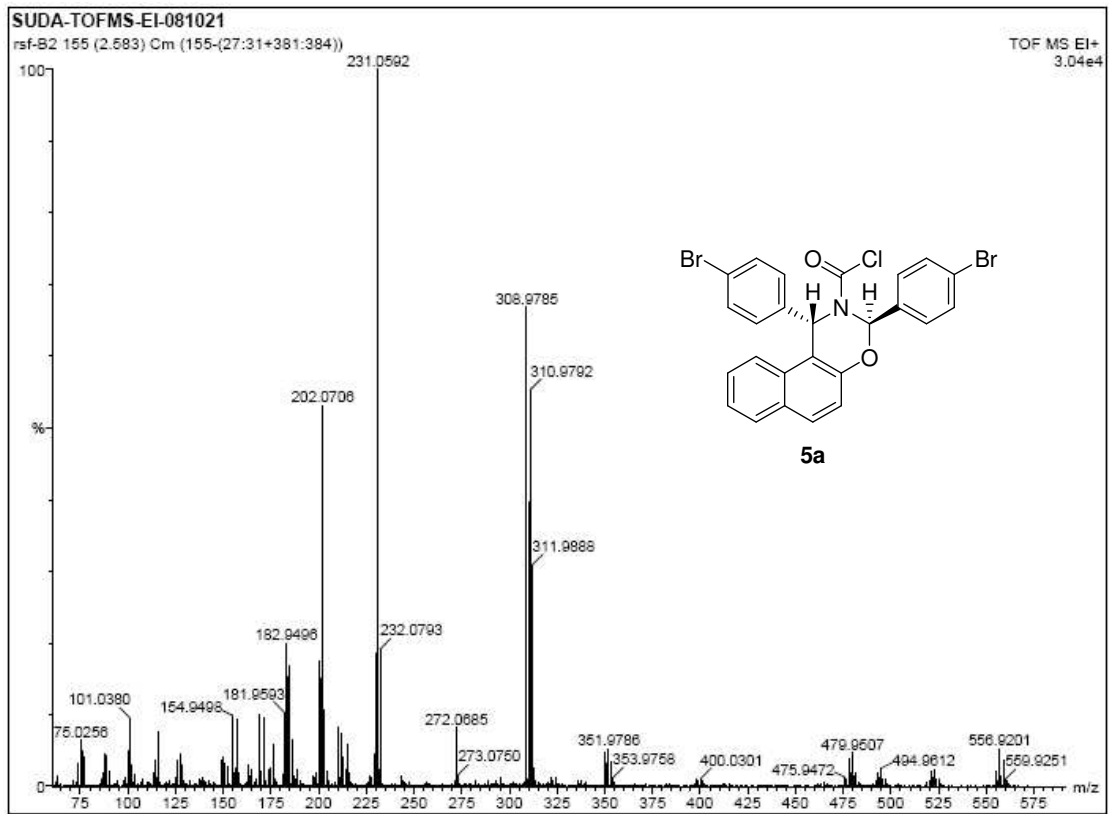
Cl(2)-C(22)	1.744(2)	C(4)-C(5)	1.411(3)	C(15)-C(16)	1.376(4)
O(1)-C(4)	1.381(2)	C(5)-C(6)	1.356(3)	C(16)-C(17)	1.369(3)
O(1)-C(1)	1.431(2)	C(6)-C(7)	1.409(3)	C(17)-C(18)	1.386(3)
O(2)-C(25)	1.210(3)	C(7)-C(8)	1.410(3)	C(19)-C(20)	1.378(3)
N(1)-C(25)	1.351(3)	C(7)-C(12)	1.423(3)	C(19)-C(24)	1.387(3)
N(1)-C(1)	1.441(3)	C(8)-C(9)	1.355(4)	C(20)-C(21)	1.383(3)
N(1)-C(2)	1.469(3)	C(9)-C(10)	1.391(4)	C(21)-C(22)	1.375(3)
C(1)-C(13)	1.510(3)	C(10)-C(11)	1.364(3)	C(22)-C(23)	1.374(3)
C(2)-C(3)	1.517(3)	C(11)-C(12)	1.419(3)	C(23)-C(24)	1.377(3)
C(2)-C(19)	1.522(3)	C(13)-C(18)	1.376(3)		
C(3)-C(4)	1.368(3)	C(13)-C(14)	1.389(3)		

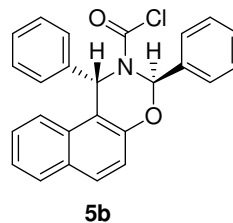
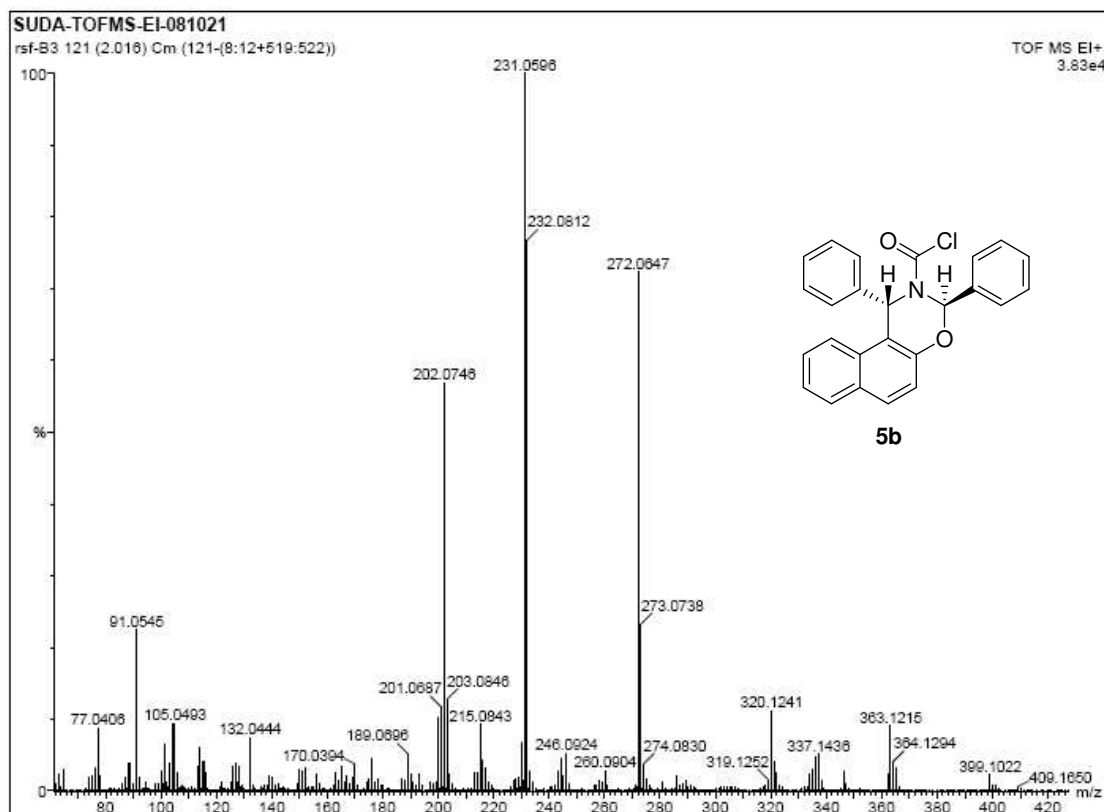
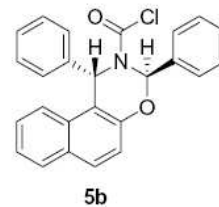
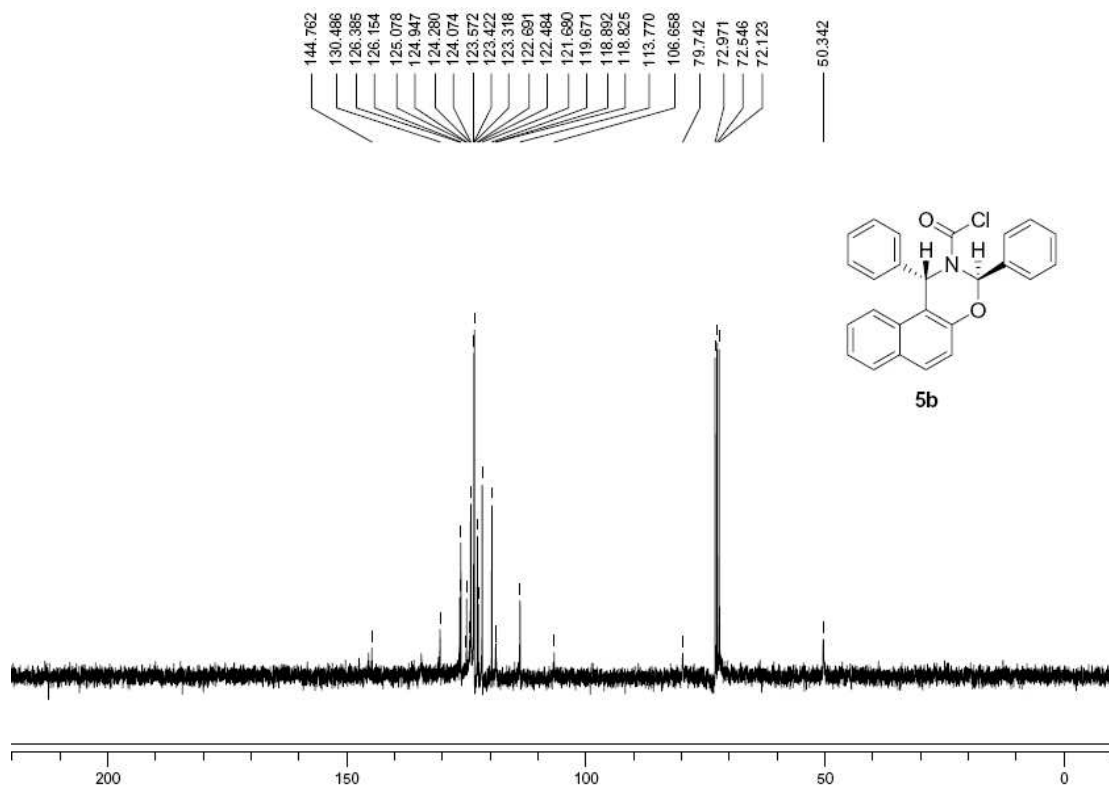
**Table 6.** Selected bond angles (°) for **7b**

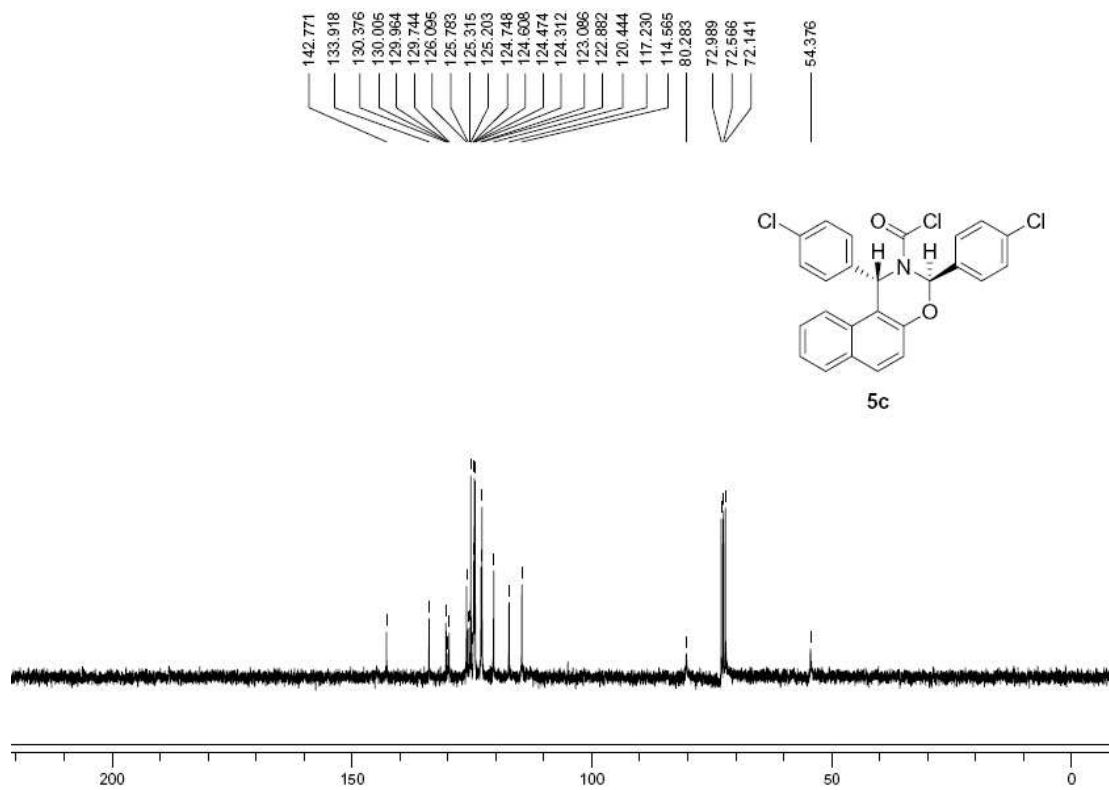
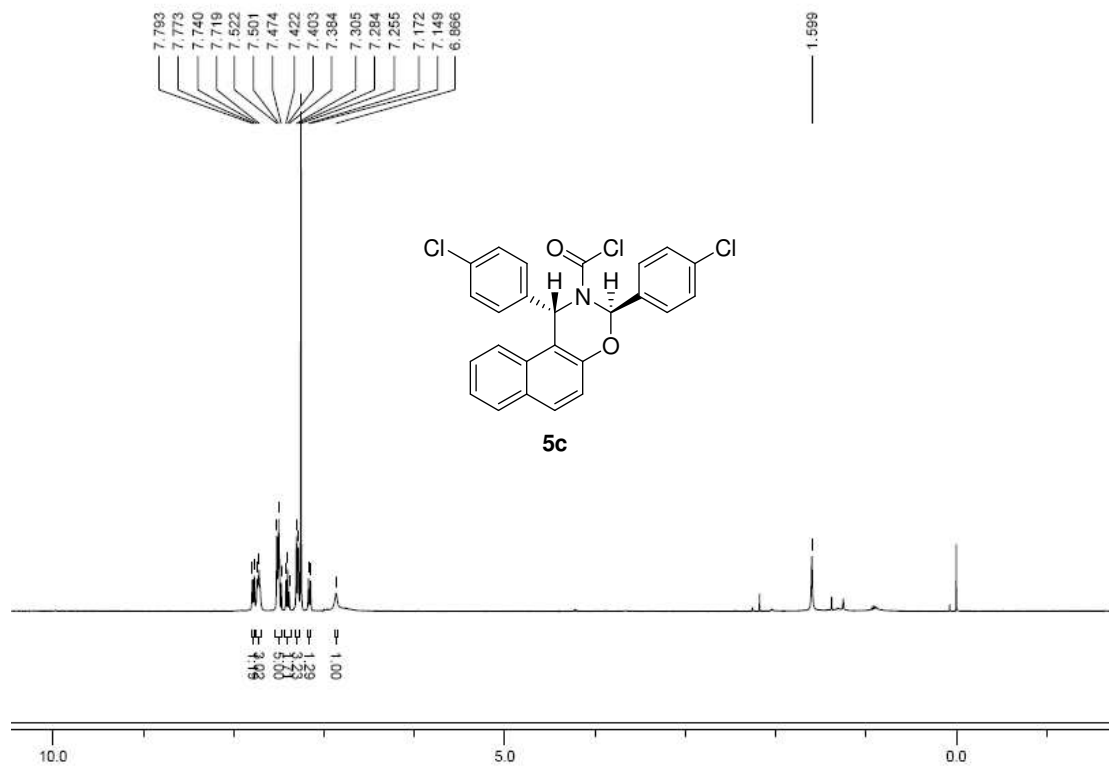
Angles	(°)	Angles	(°)
C(4)-O(1)-C(1)	112.94(15)	C(11)-C(12)-C(7)	118.0(2)
C(25)-N(1)-C(1)	122.98(18)	C(11)-C(12)-C(3)	122.9(2)
C(25)-N(1)-C(2)	120.74(18)	C(7)-C(12)-C(3)	119.1(2)
C(1)-N(1)-C(2)	112.79(16)	C(18)-C(13)-C(14)	118.7(2)
O(1)-C(1)-N(1)	109.49(16)	C(18)-C(13)-C(1)	123.11(19)
O(1)-C(1)-C(13)	109.41(16)	C(14)-C(13)-C(1)	118.11(19)
N(1)-C(1)-C(13)	115.08(17)	C(15)-C(14)-C(13)	121.1(2)
N(1)-C(2)-C(3)	107.91(16)	C(14)-C(15)-C(16)	119.1(2)
N(1)-C(2)-C(19)	109.53(16)	C(17)-C(16)-C(15)	120.9(2)
C(3)-C(2)-C(19)	115.97(17)	C(17)-C(16)-Cl(1)	119.5(2)
C(4)-C(3)-C(12)	118.90(19)	C(15)-C(16)-Cl(1)	119.57(19)
C(4)-C(3)-C(2)	120.64(18)	C(16)-C(17)-C(18)	119.5(2)
C(12)-C(3)-C(2)	120.36(18)	C(13)-C(18)-C(17)	120.5(2)
C(3)-C(4)-O(1)	123.57(18)	C(20)-C(19)-C(24)	118.5(2)
C(3)-C(4)-C(5)	121.94(19)	C(20)-C(19)-C(2)	123.25(18)
O(1)-C(4)-C(5)	114.49(18)	C(24)-C(19)-C(2)	118.21(19)
C(6)-C(5)-C(4)	119.5(2)	C(19)-C(20)-C(21)	121.4(2)
C(5)-C(6)-C(7)	121.4(2)	C(22)-C(21)-C(20)	118.7(2)
C(6)-C(7)-C(8)	122.0(2)	C(23)-C(22)-C(21)	121.1(2)
C(6)-C(7)-C(12)	119.04(19)	C(23)-C(22)-Cl(2)	119.53(17)
C(8)-C(7)-C(12)	118.9(2)	C(21)-C(22)-Cl(2)	119.40(19)
C(9)-C(8)-C(7)	121.5(2)	C(22)-C(23)-C(24)	119.5(2)
C(8)-C(9)-C(10)	119.8(2)	C(23)-C(24)-C(19)	120.8(2)
C(11)-C(10)-C(9)	121.1(3)	O(2)-C(25)-N(1)	125.2(2)
C(10)-C(11)-C(12)	120.7(2)		

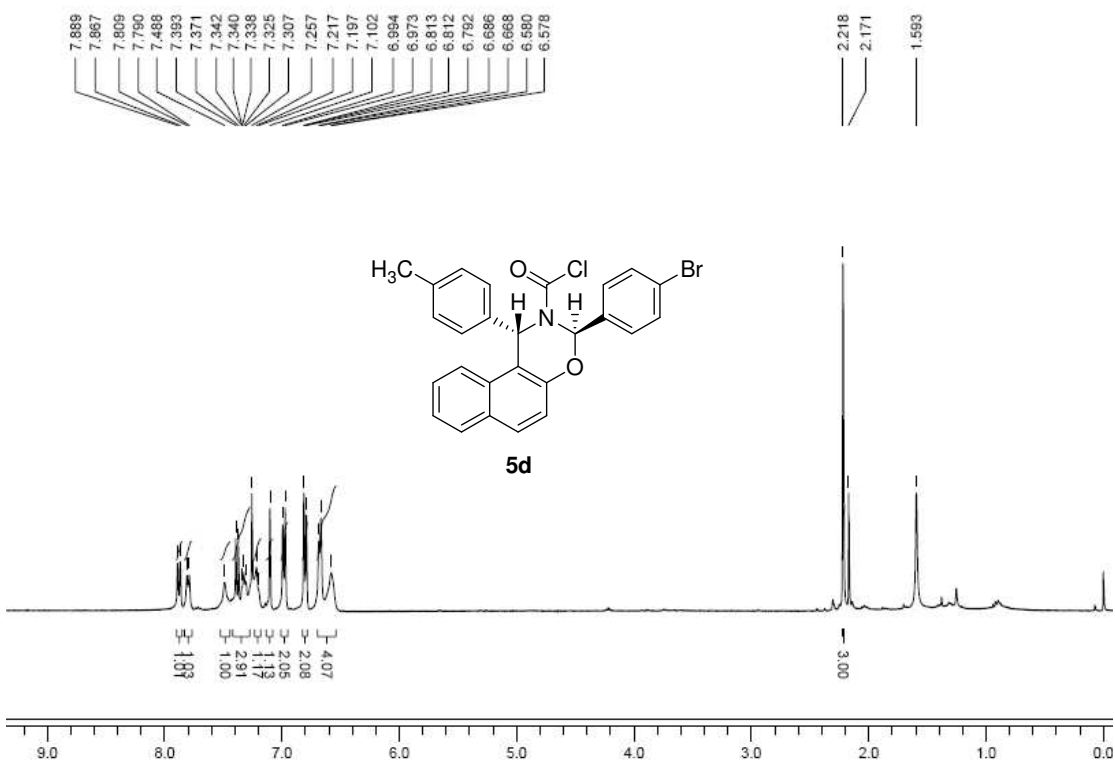
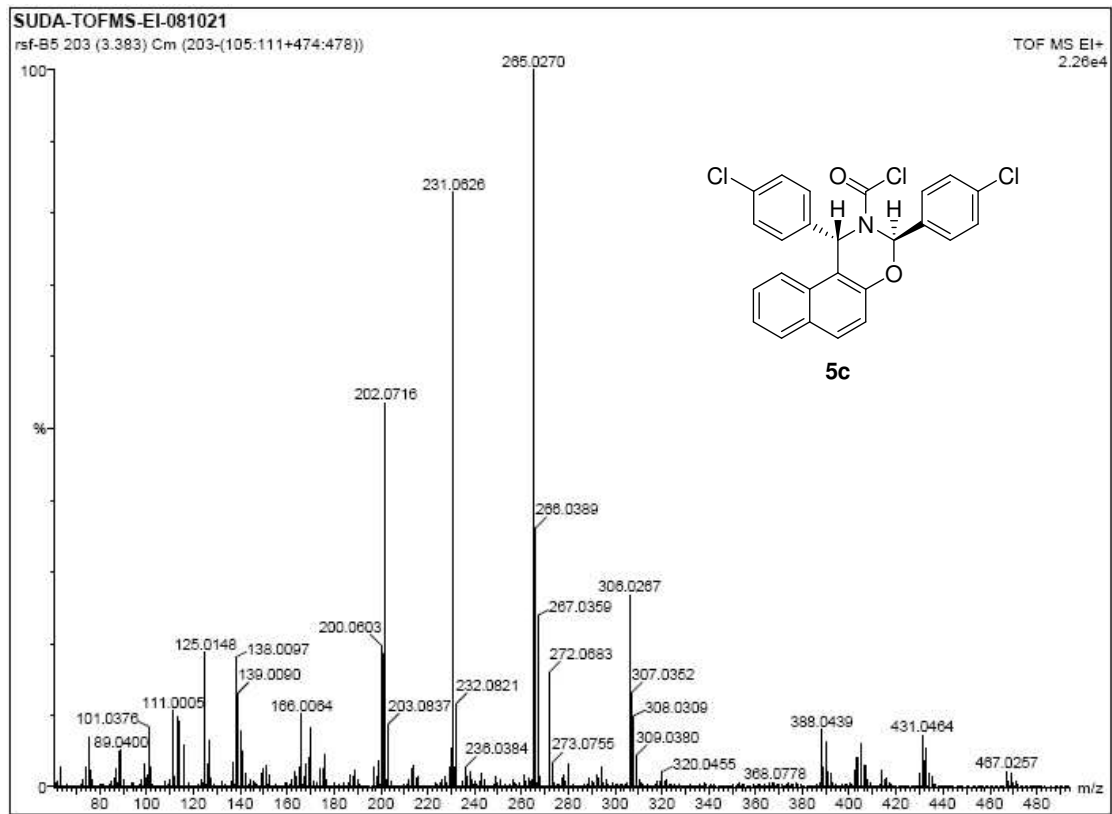
# Copies of $^1\text{H}$ NMR and HRMS of compounds

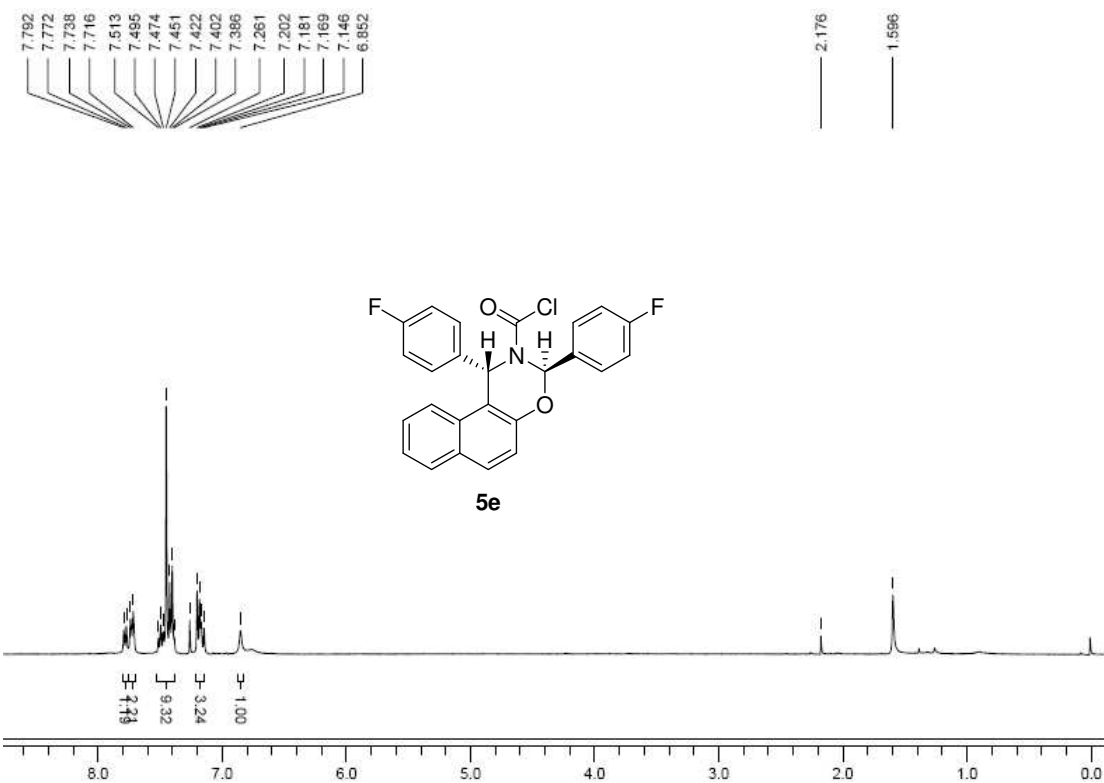
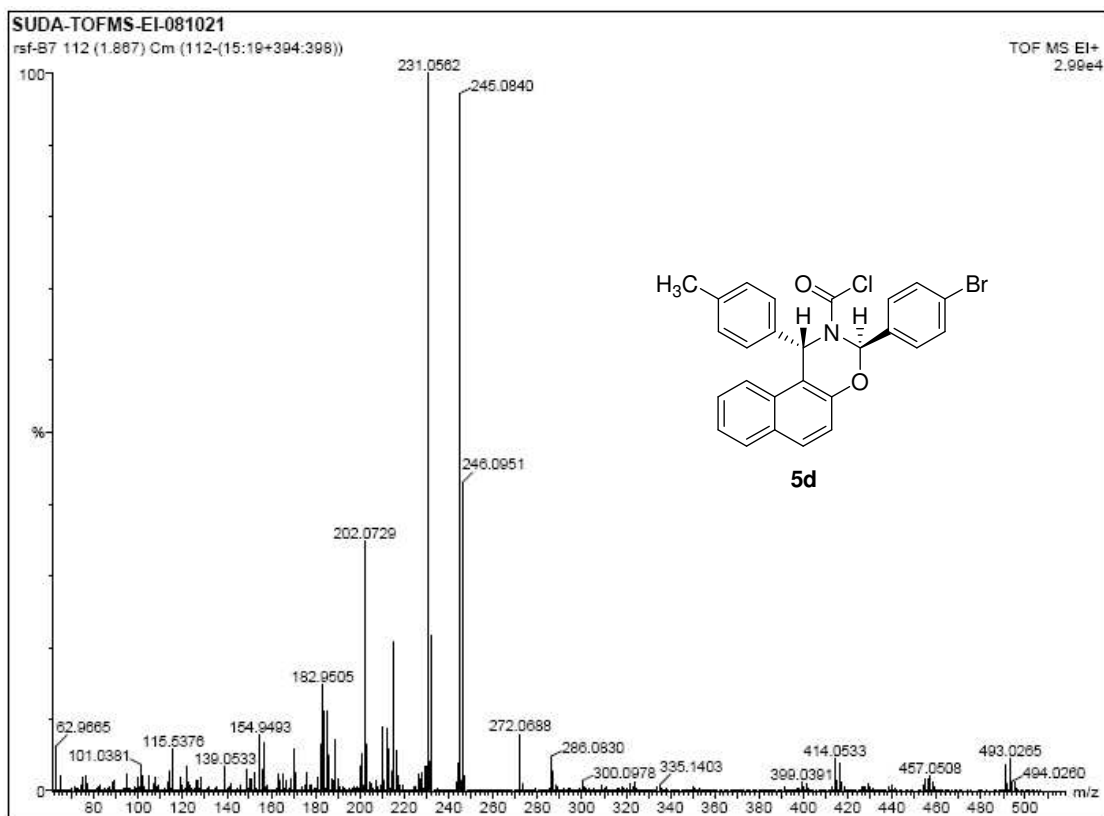




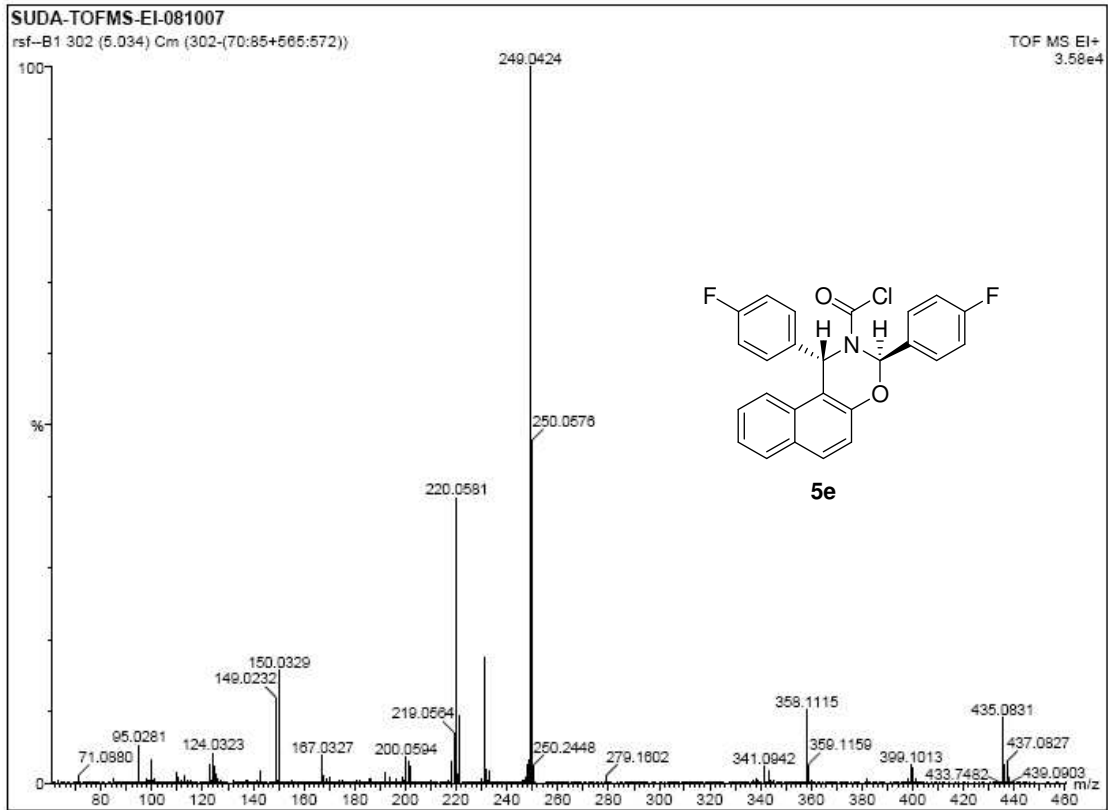
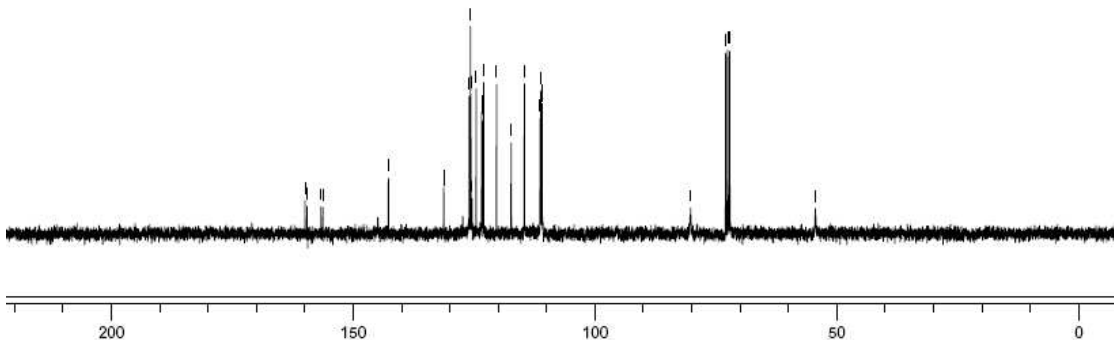
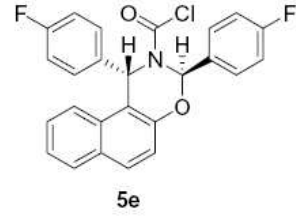
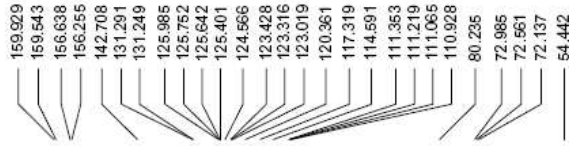


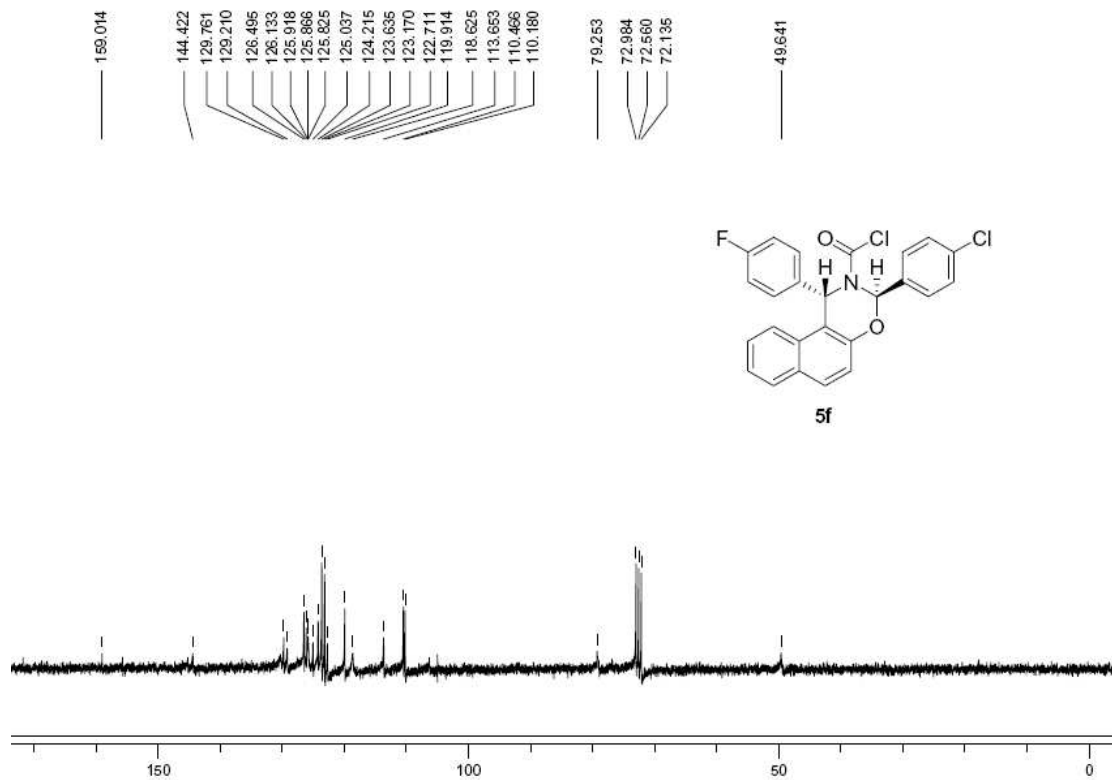
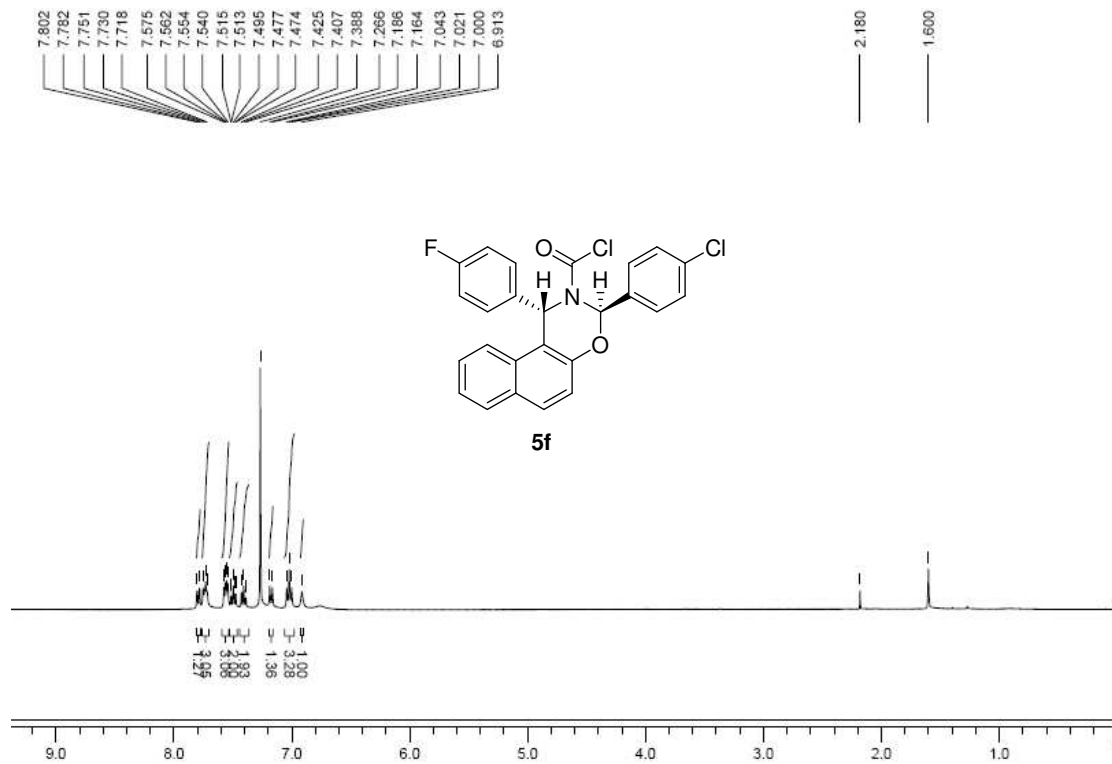


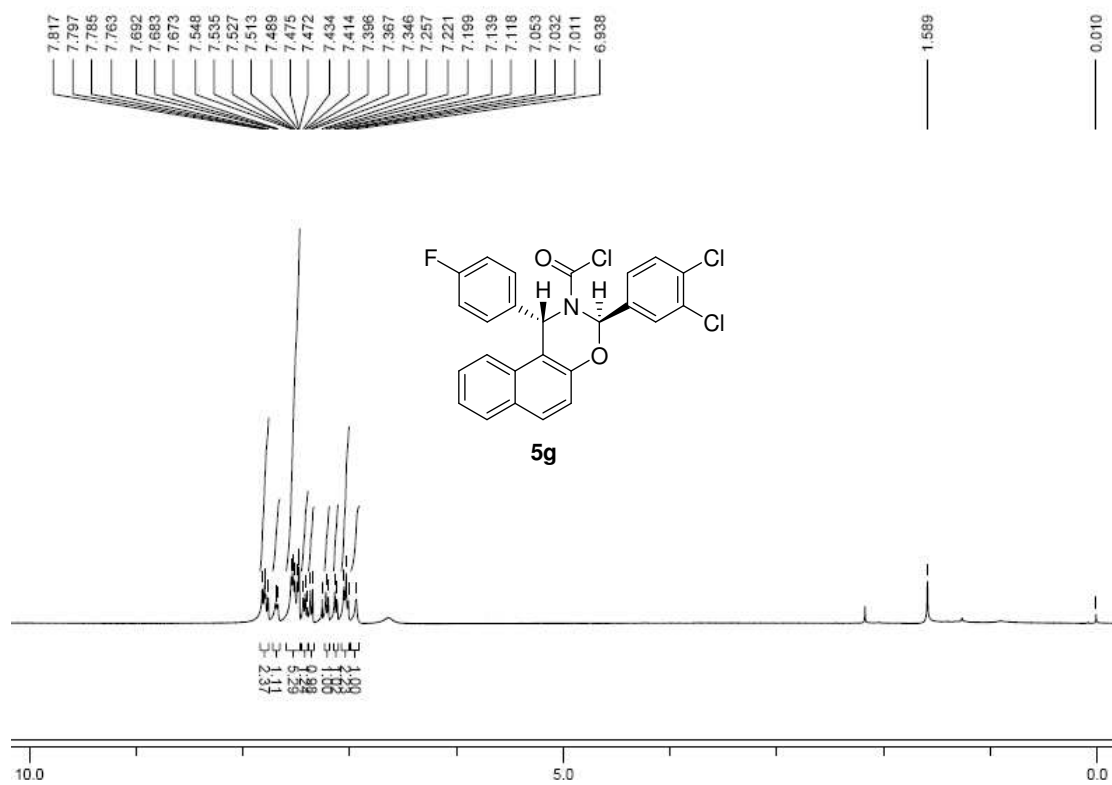
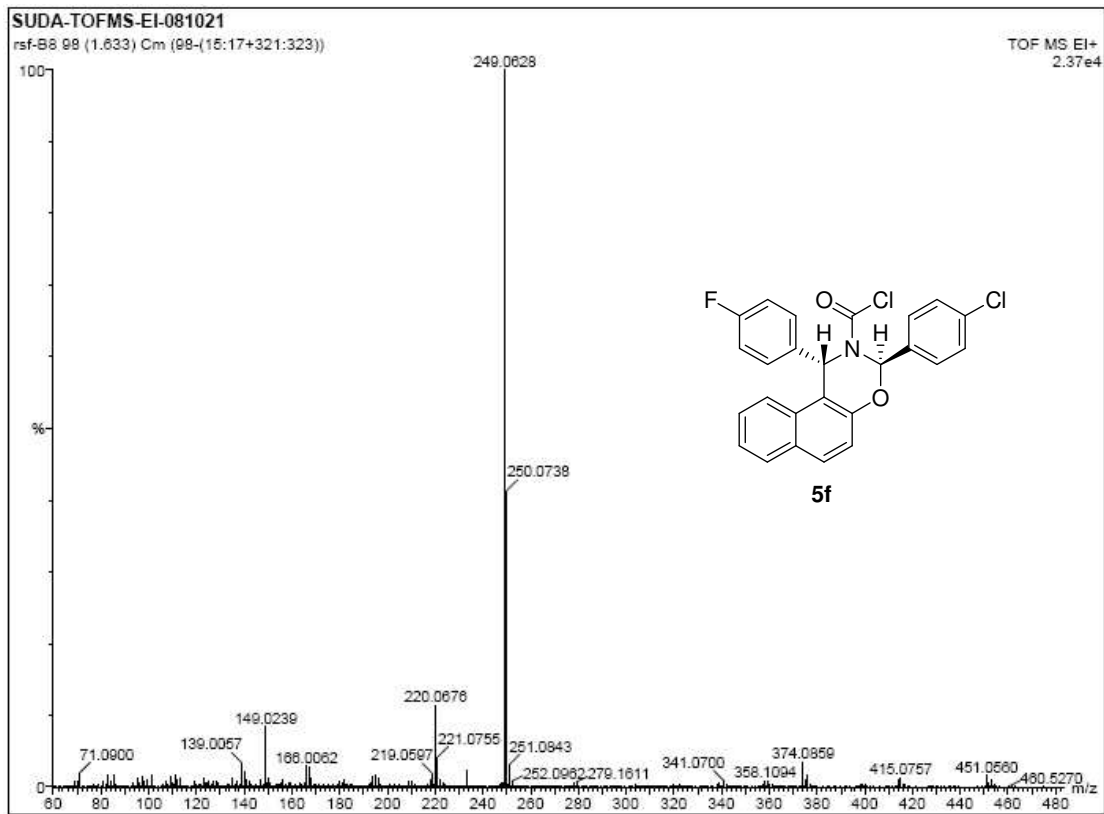


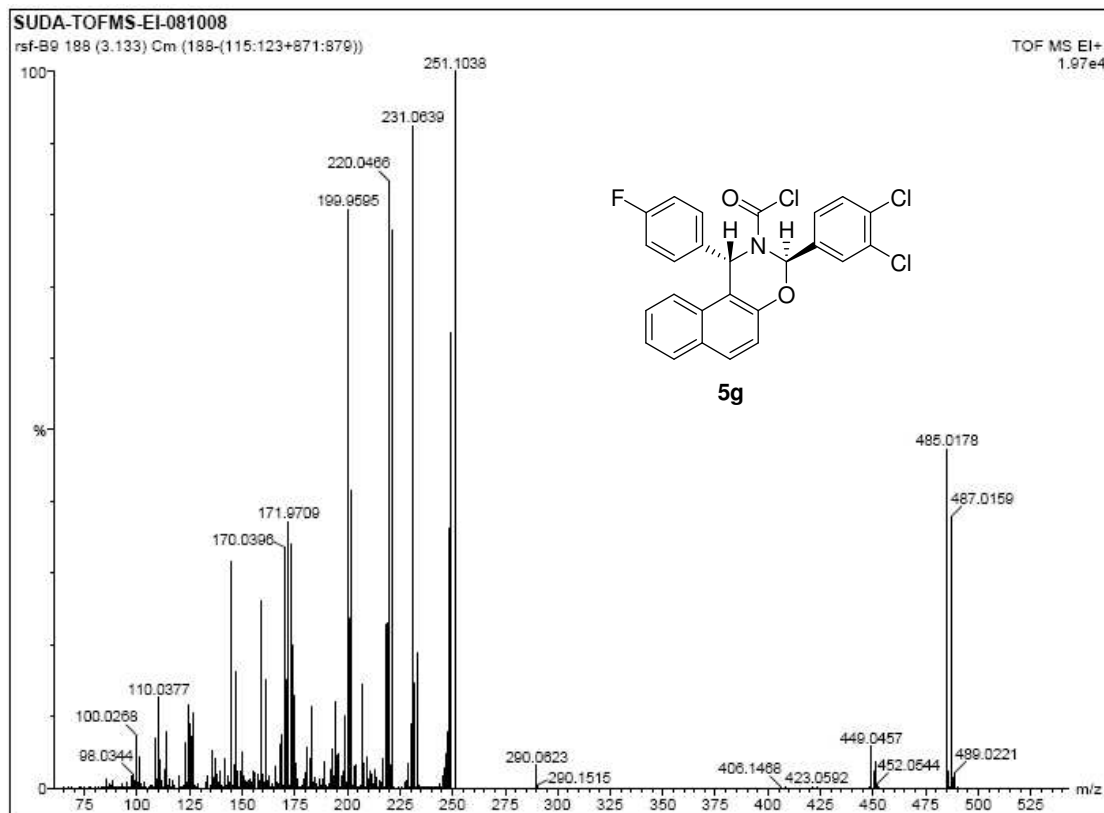
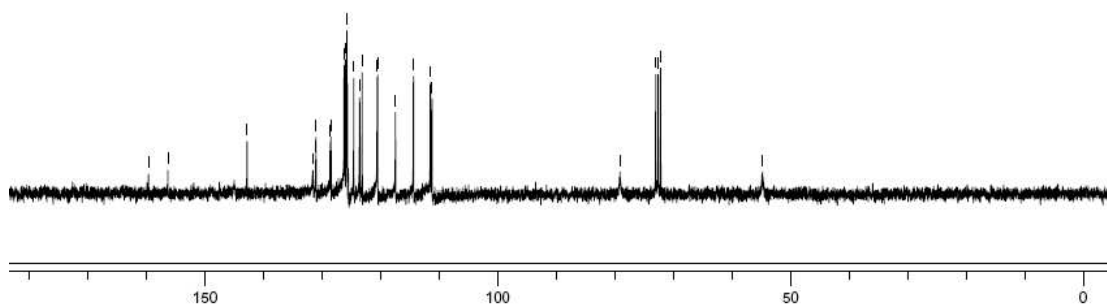
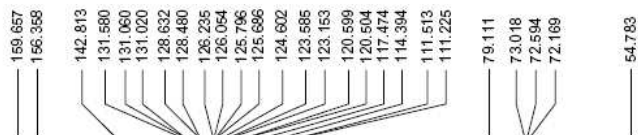


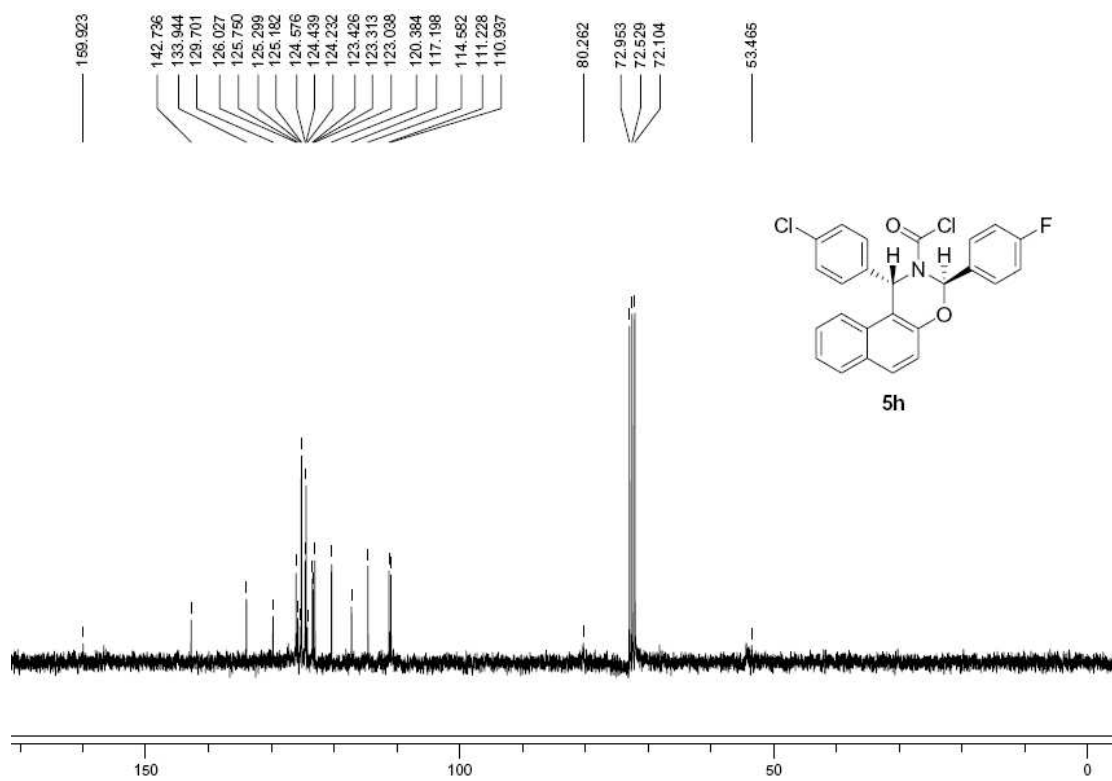
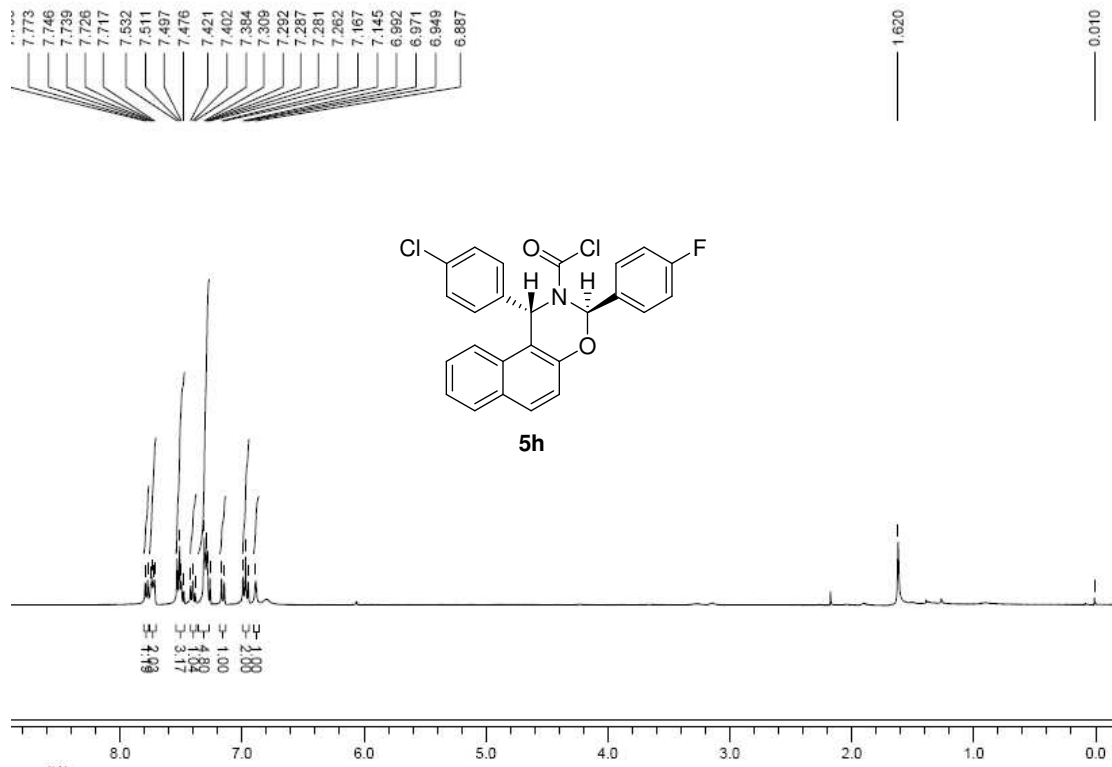


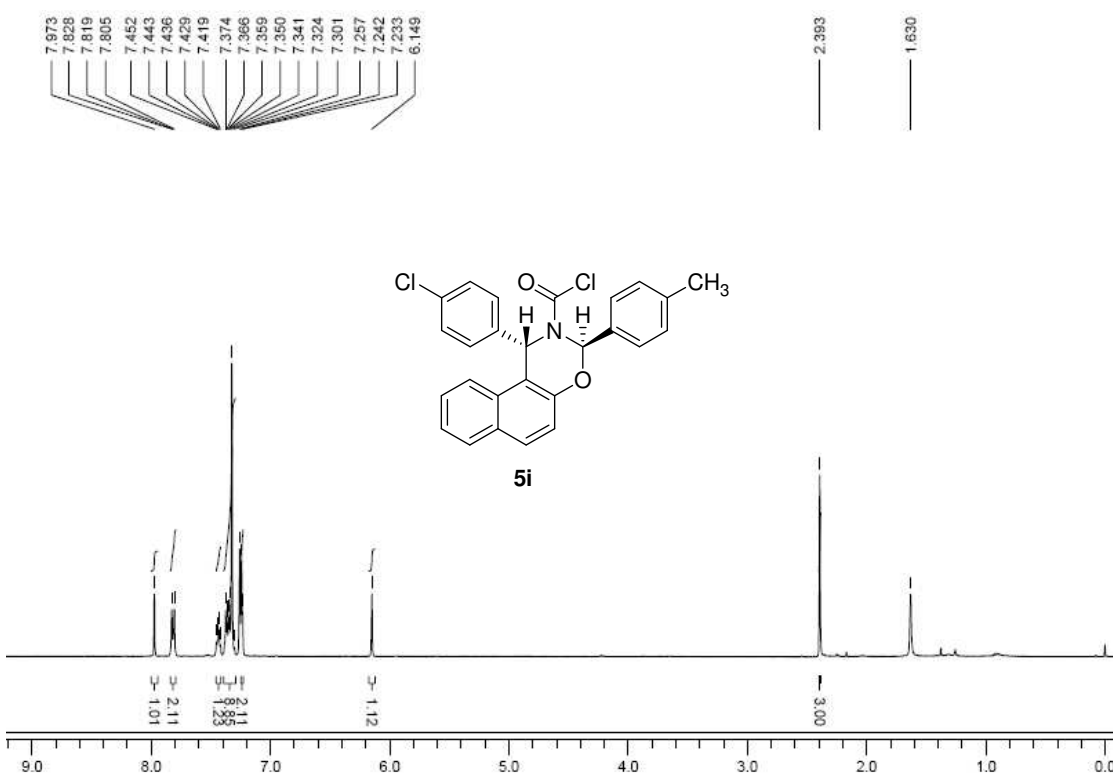
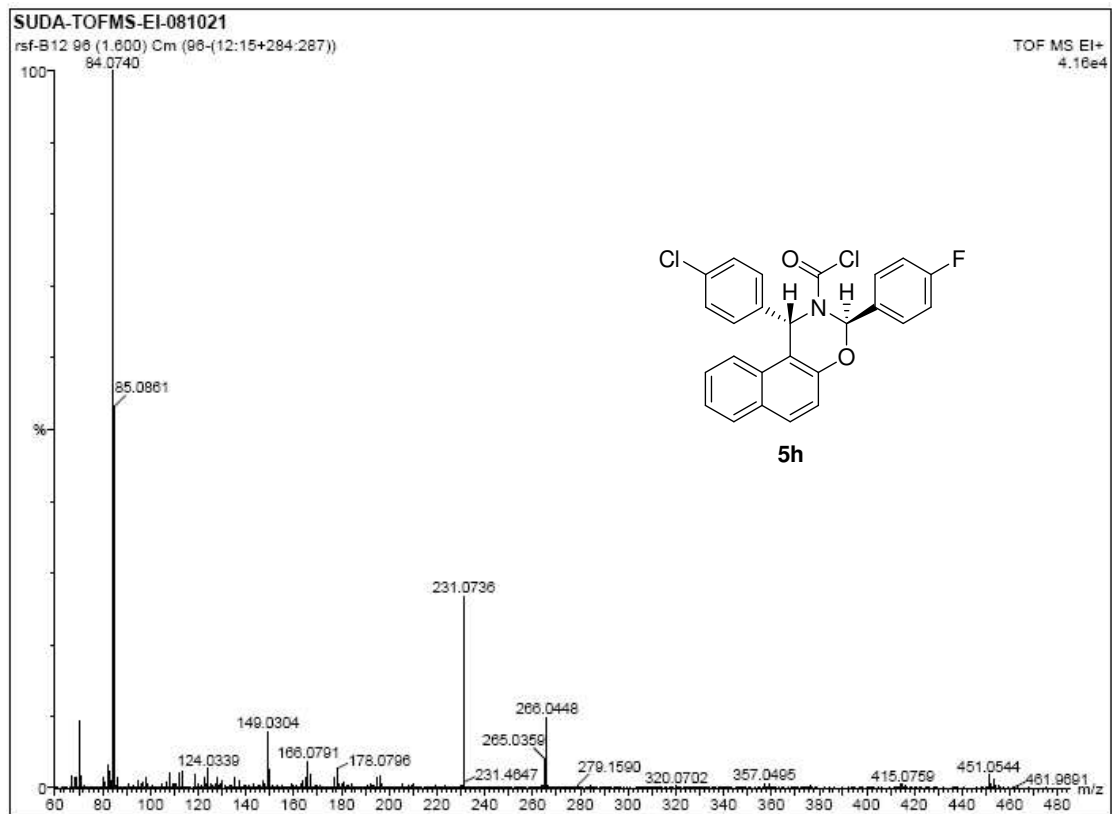


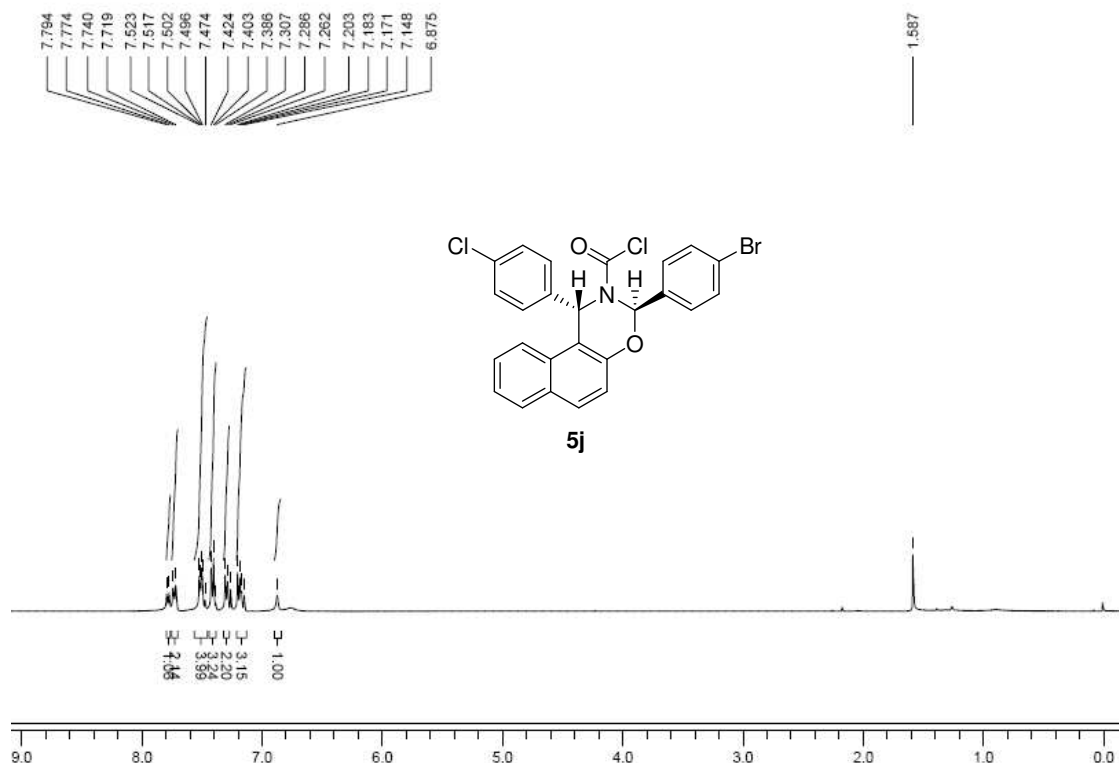
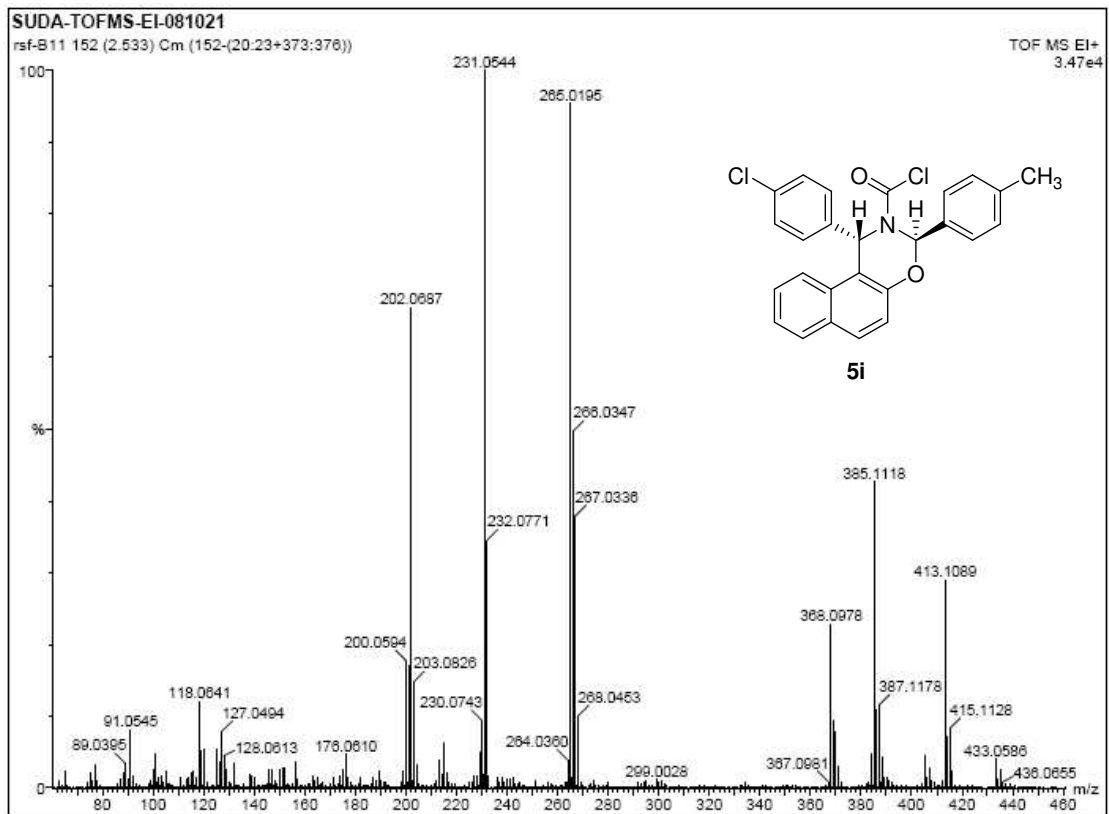


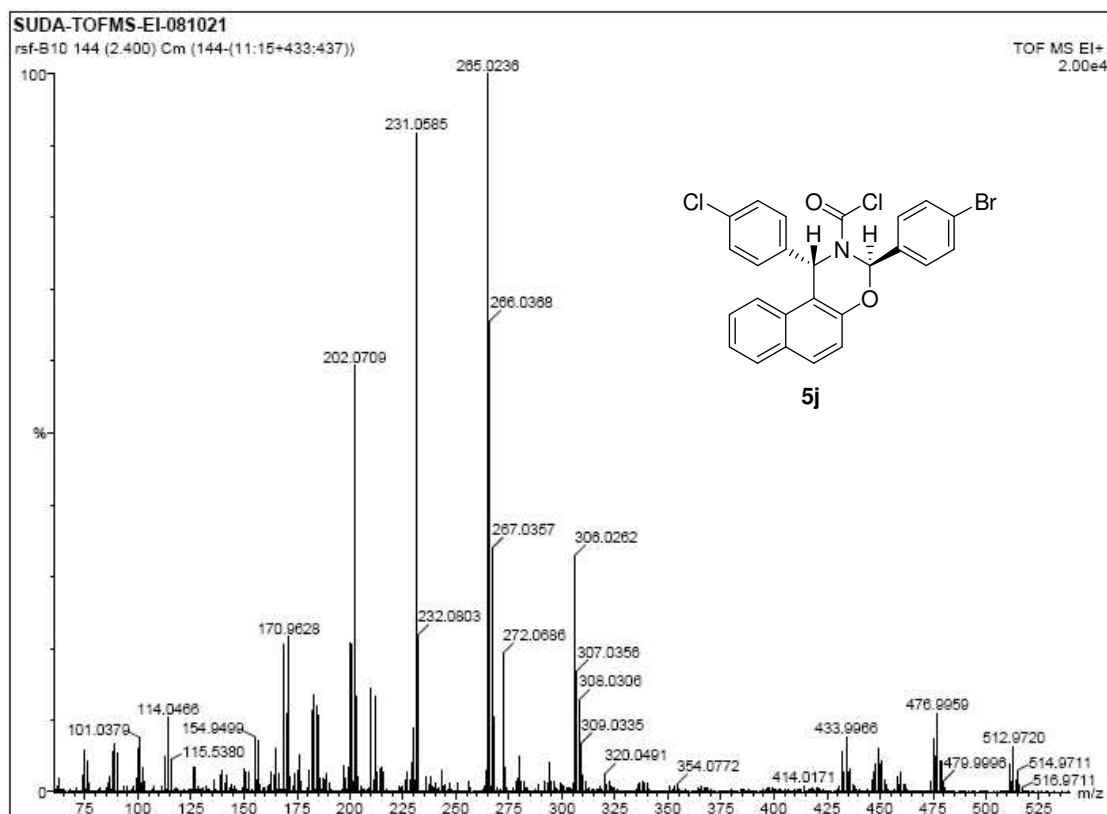
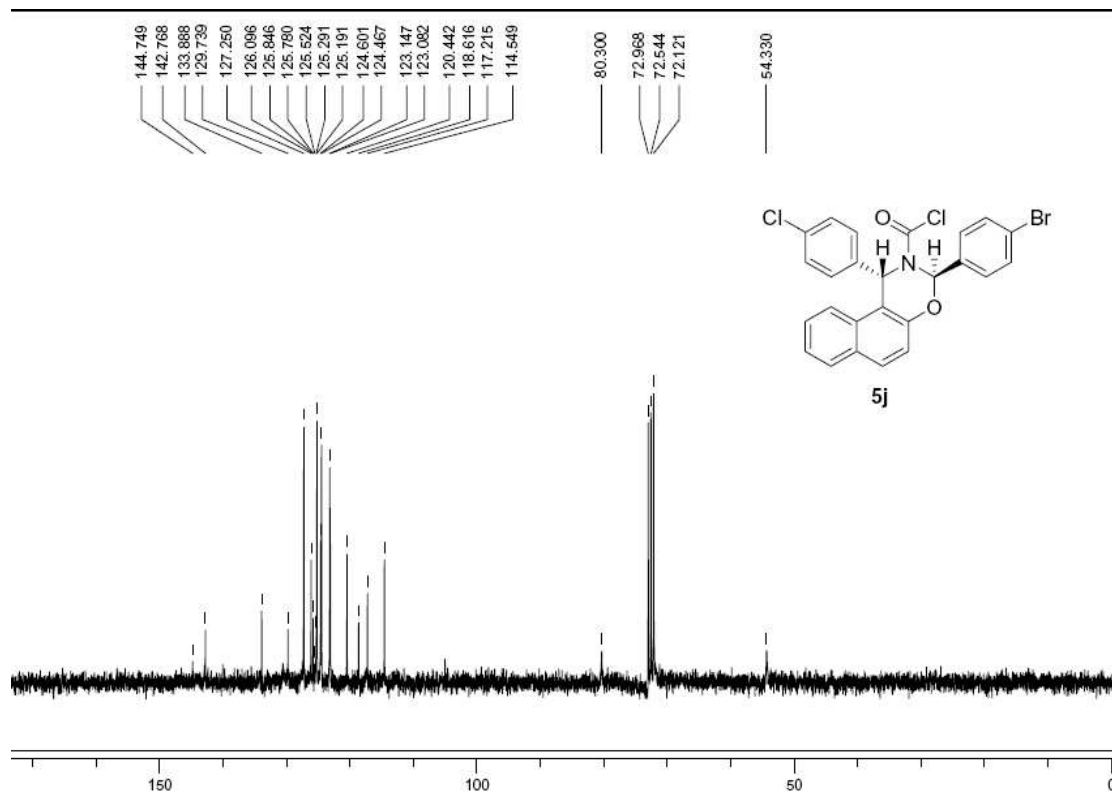




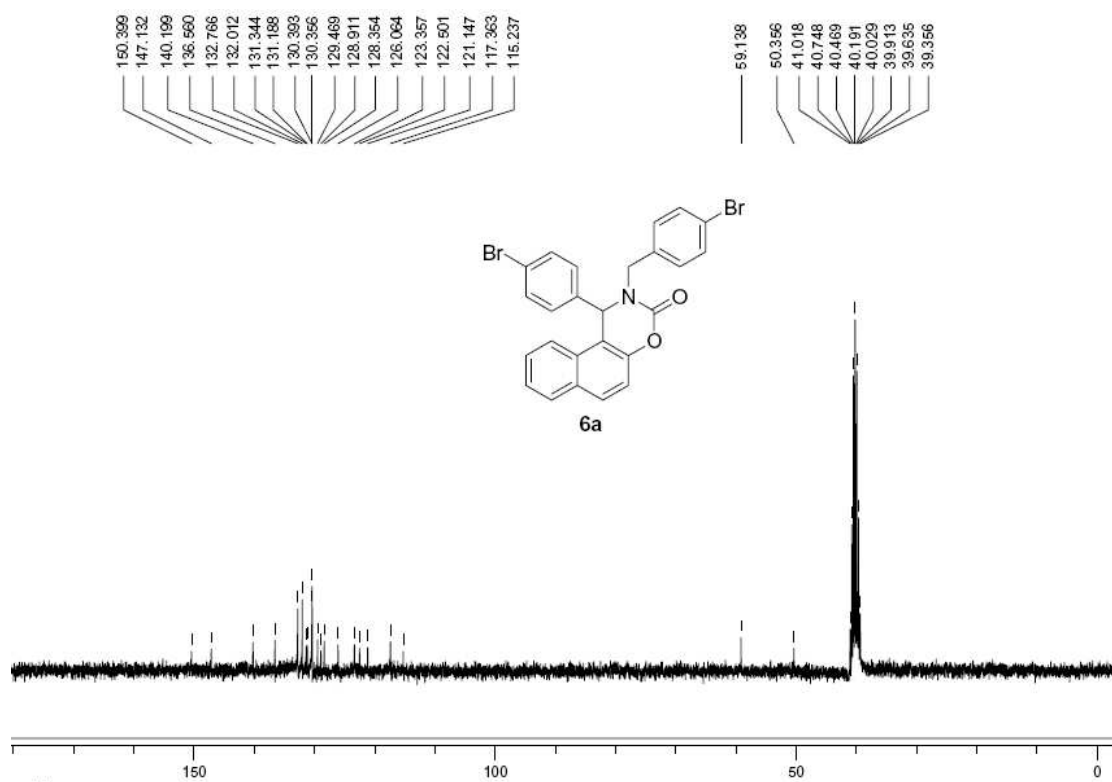
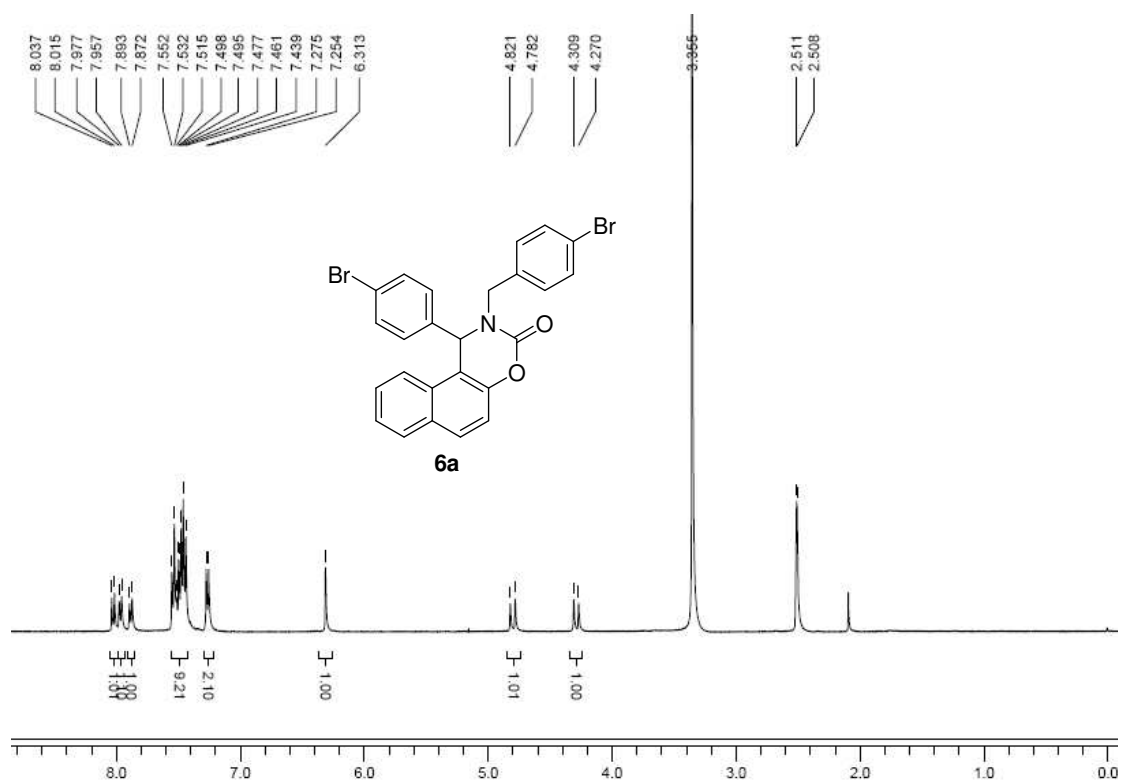


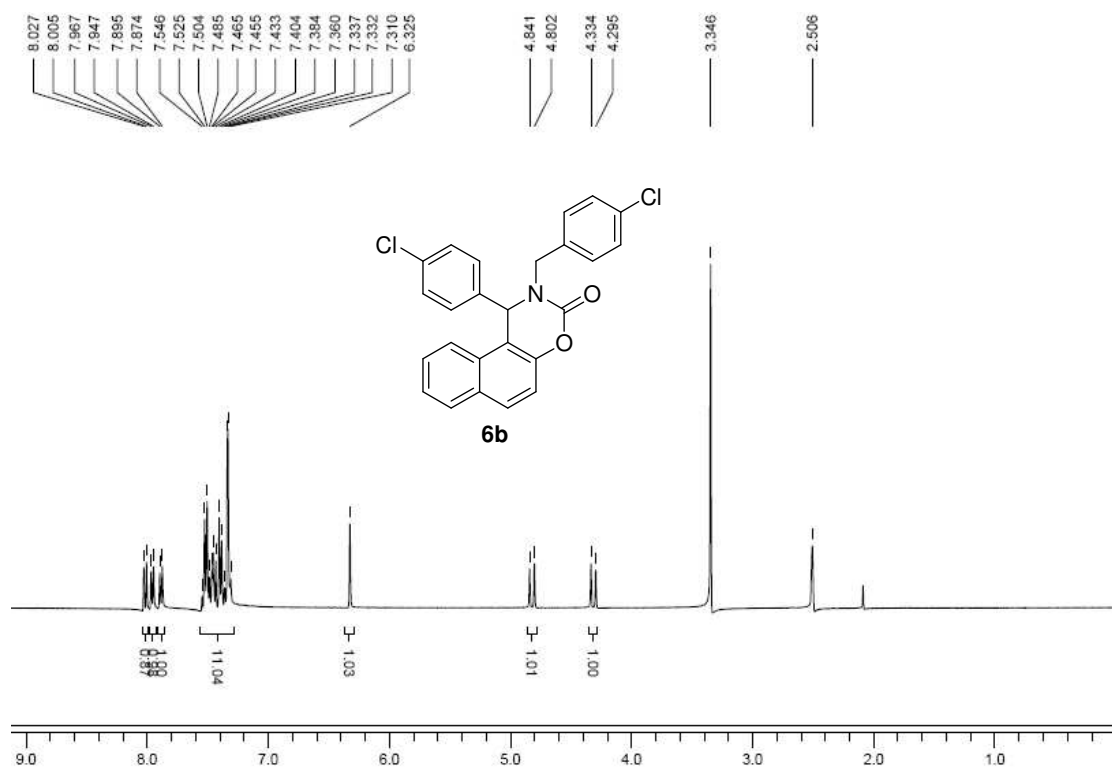
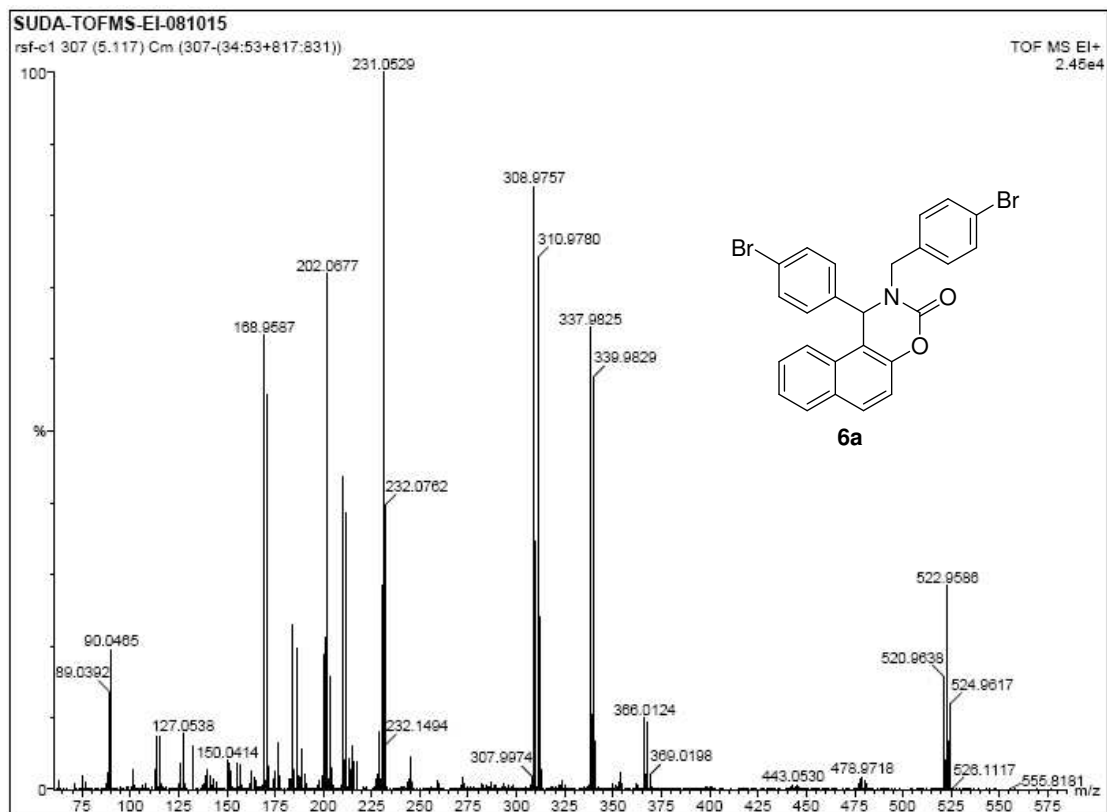


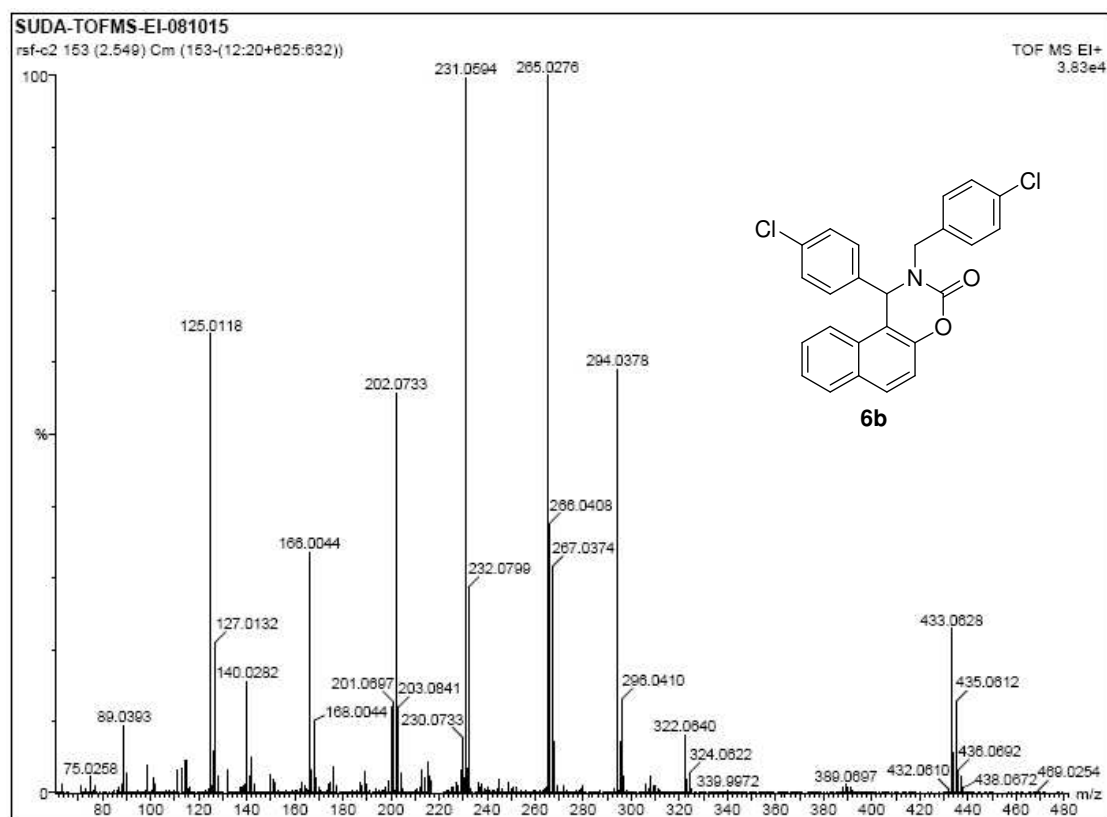
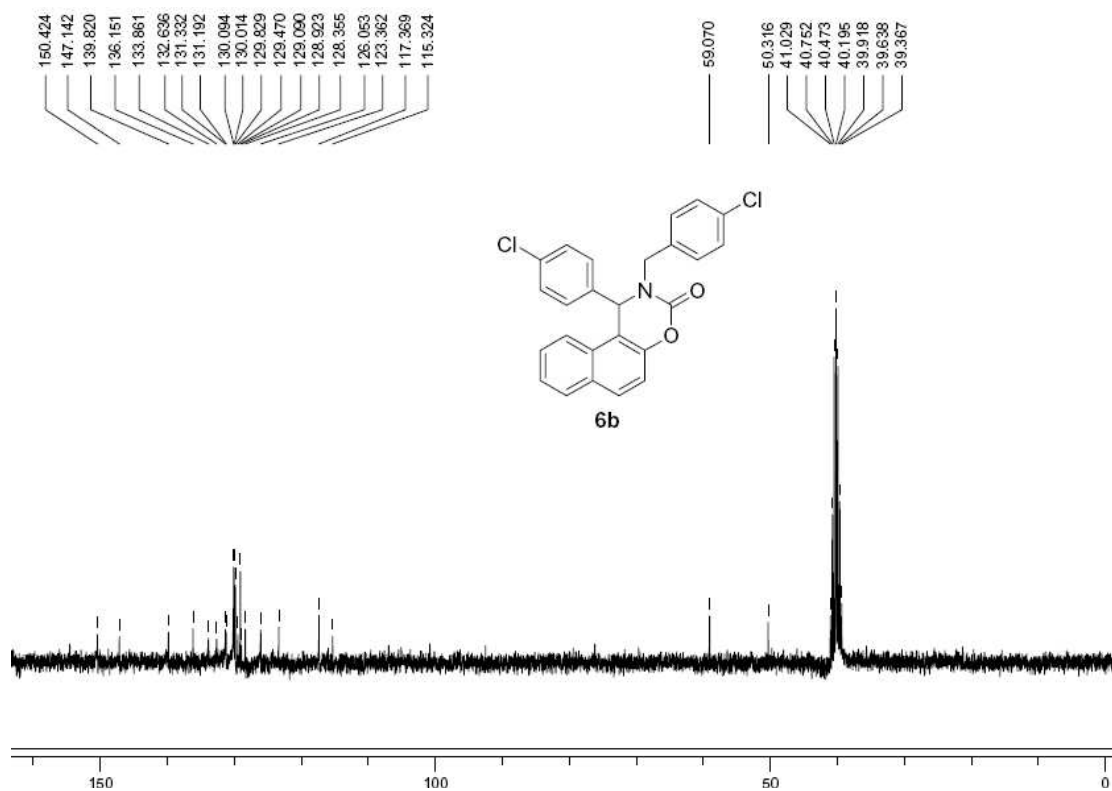


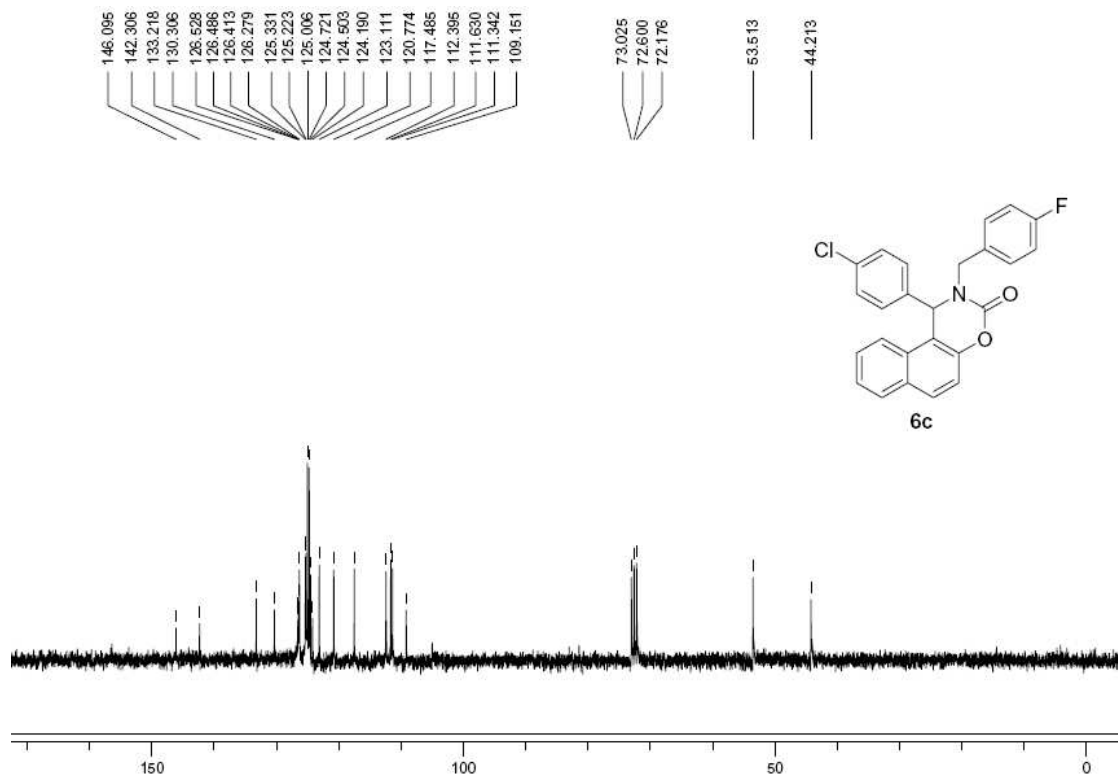
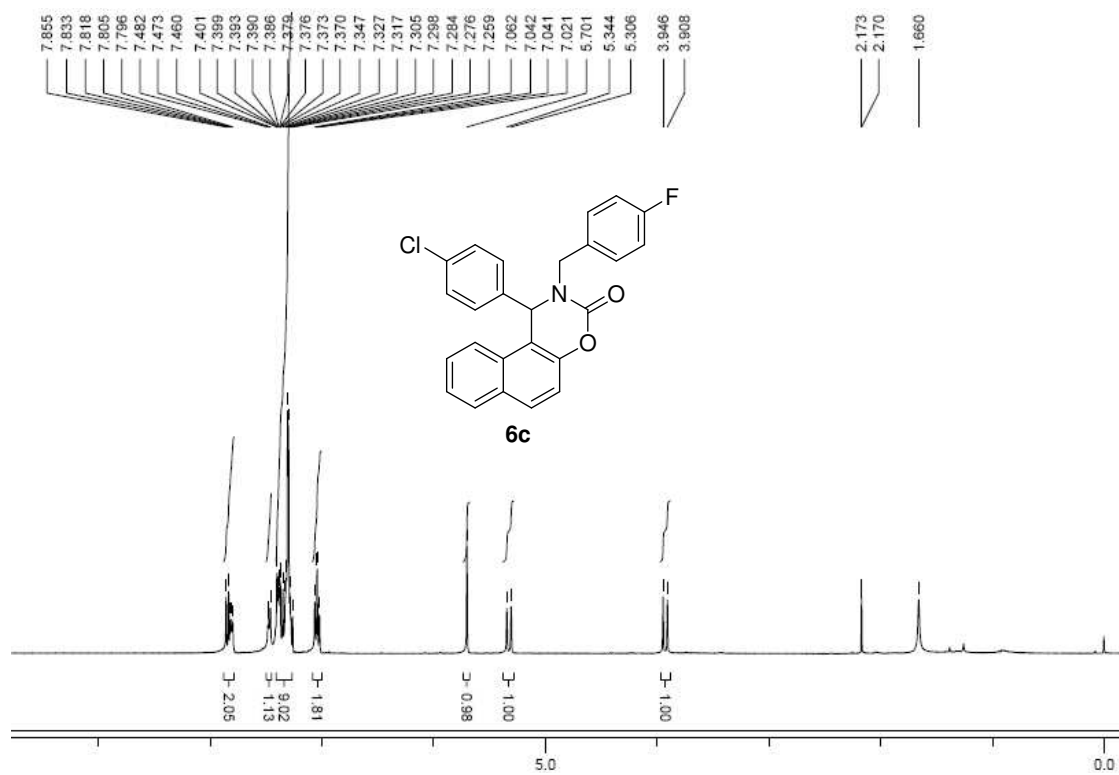


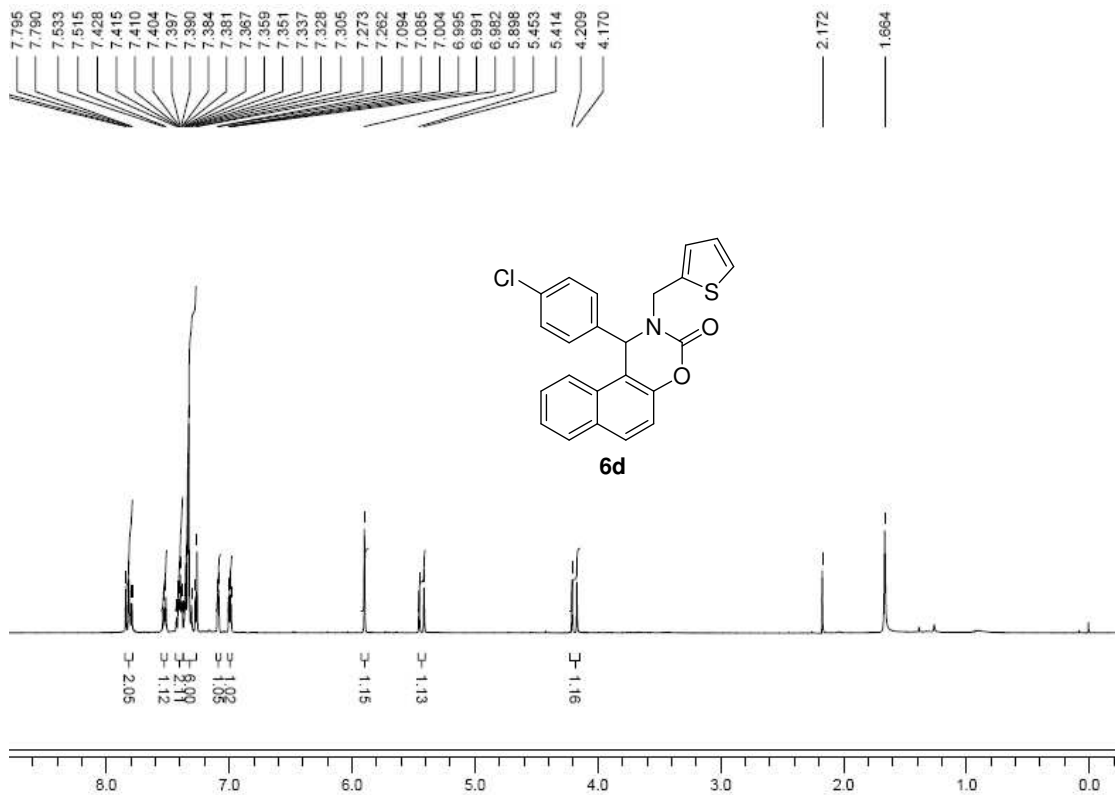
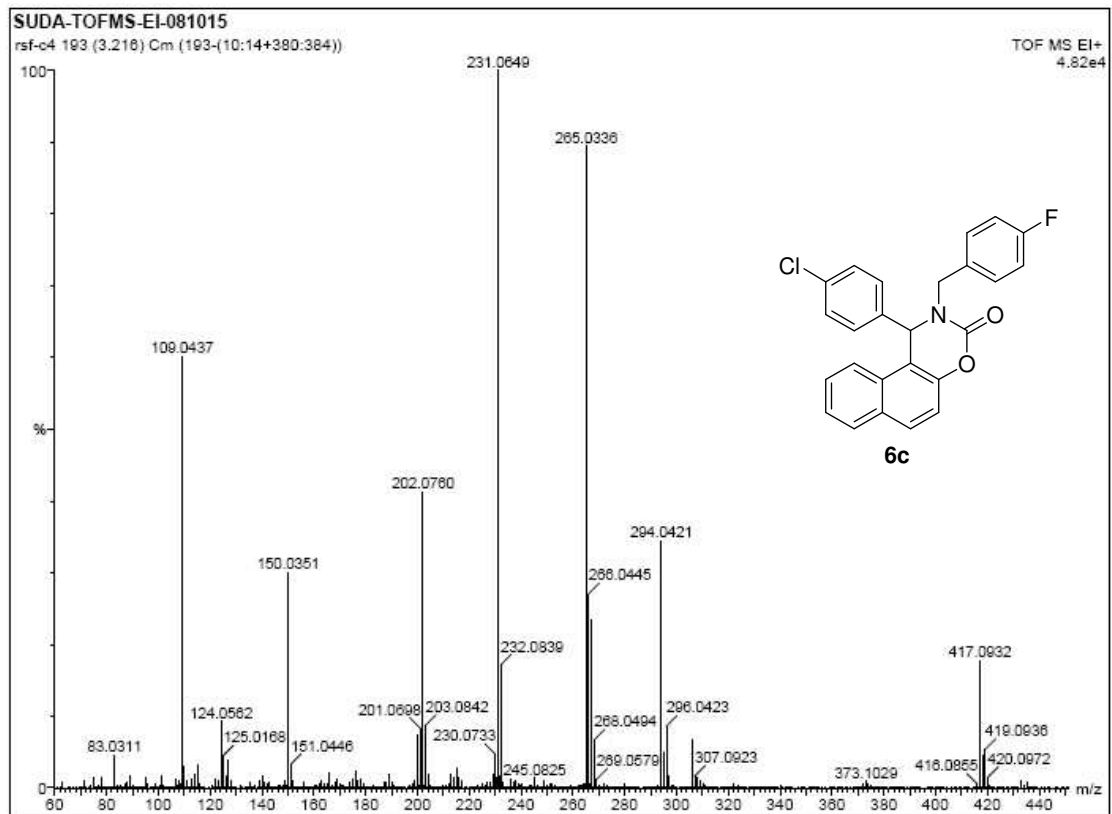


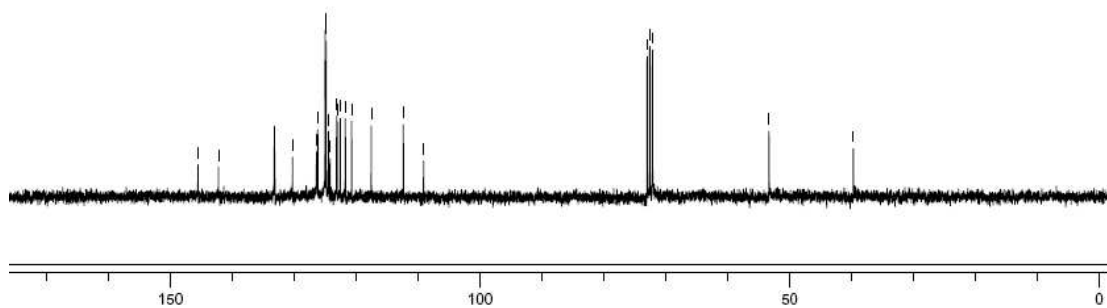
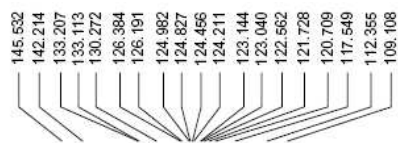






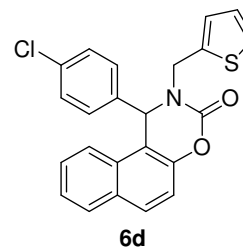
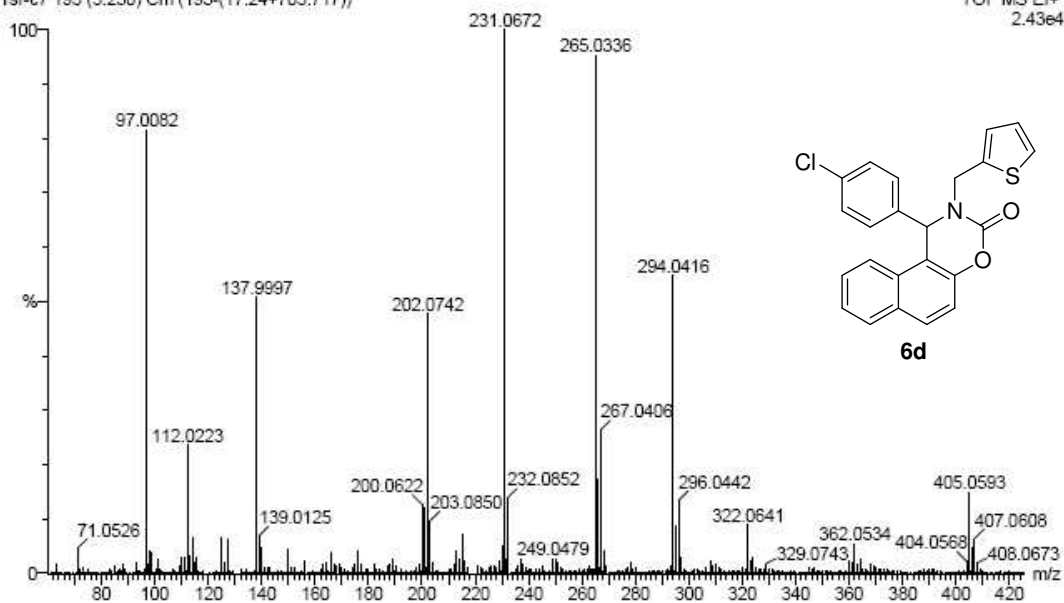




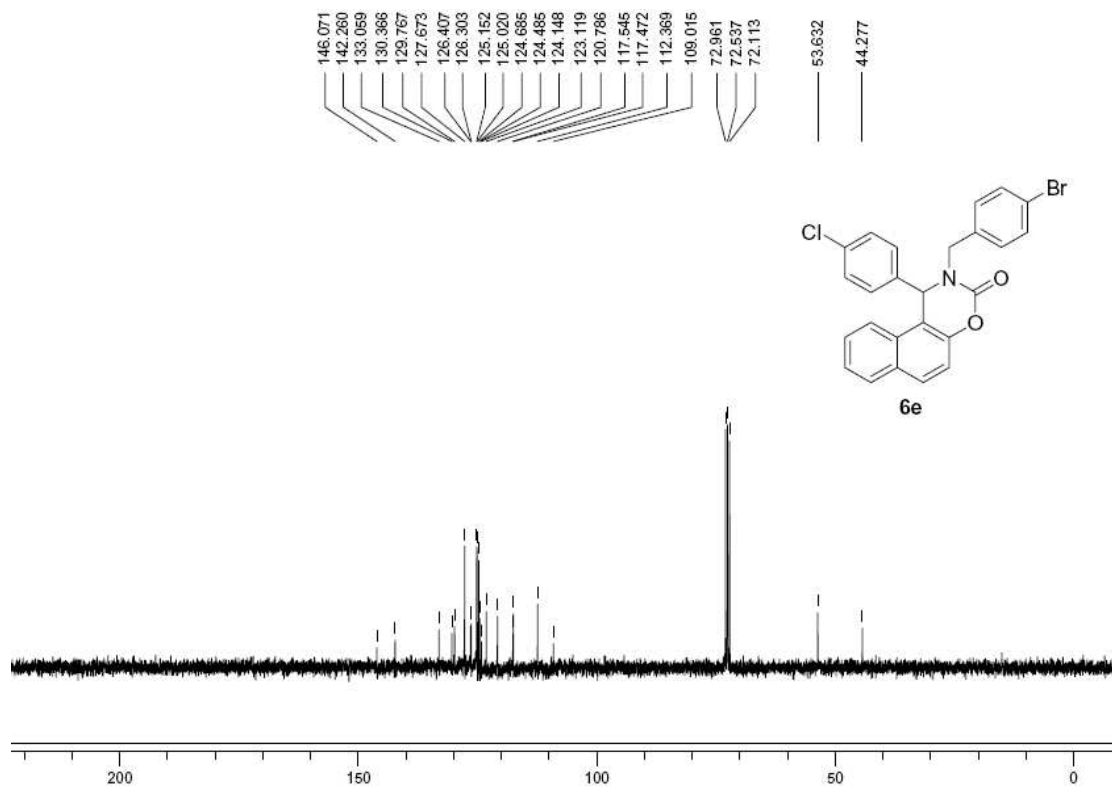
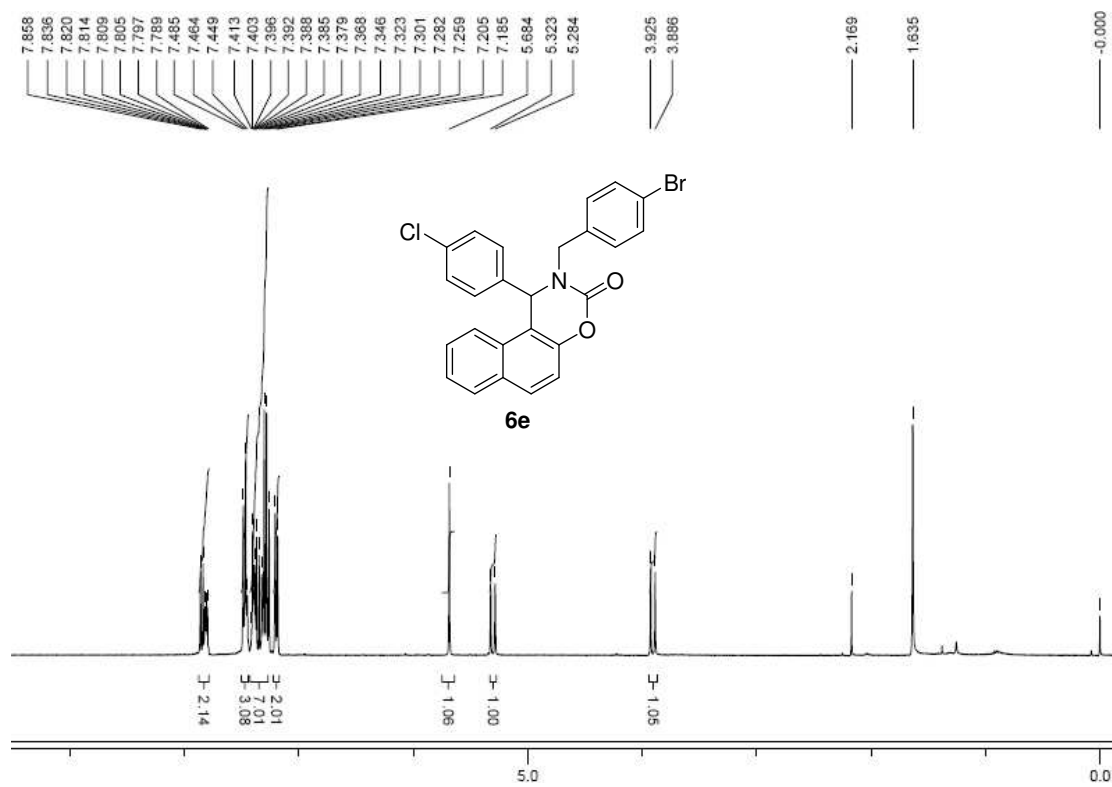


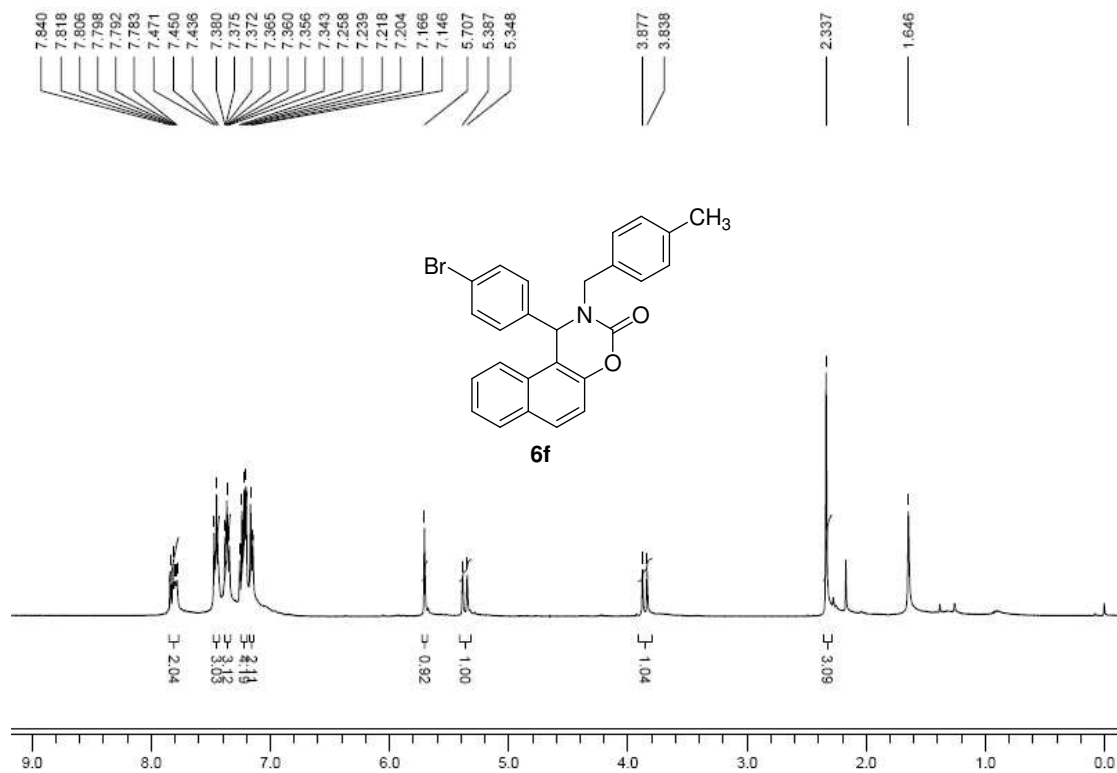
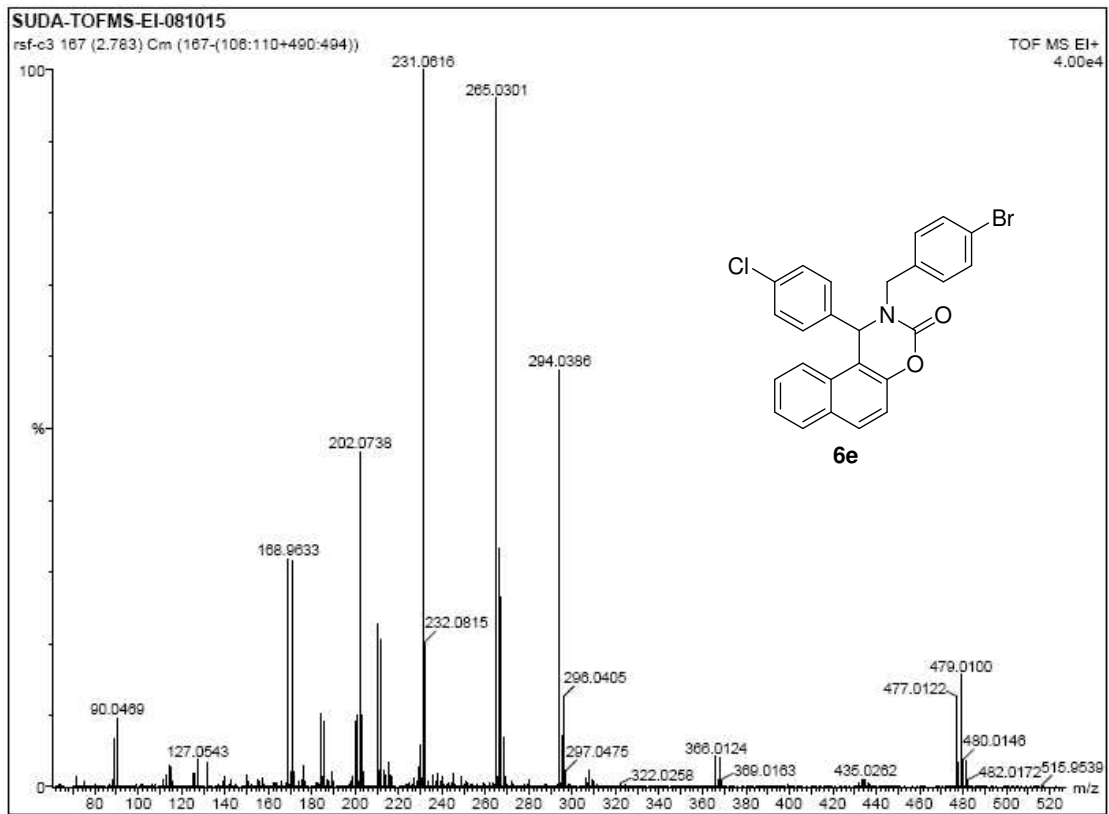
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rsf-c7 195 (3.250) Cm (195-(17.24+705.717))

TOF MS EI+  
2.43e4

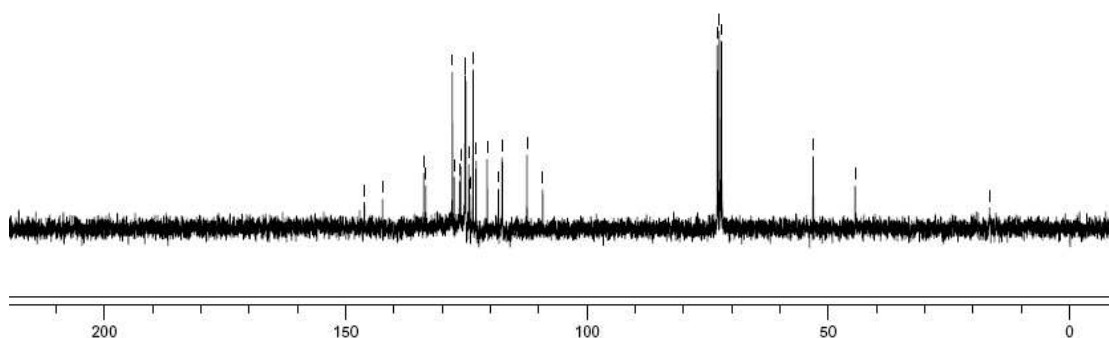
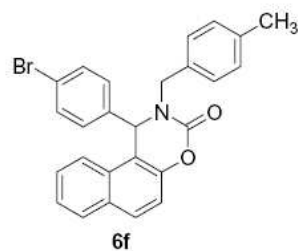
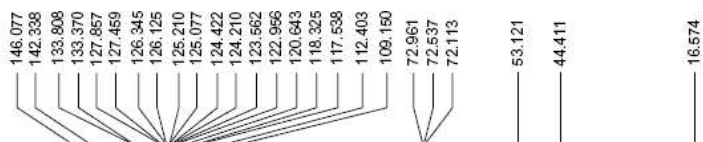


Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
405.0593	14.68	405.0590	0.3	0.7	16.0	1	S C23 H16 N O2 S 35Cl
407.0608	6.20	407.0561	4.7	11.6	16.0	1	C23 H16 N O2 S 37Cl



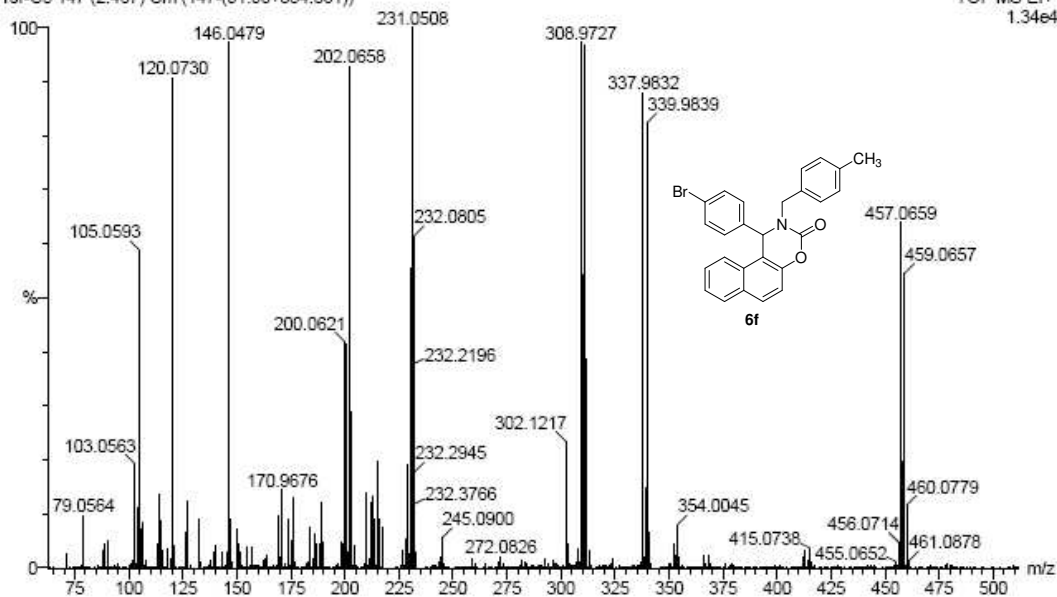






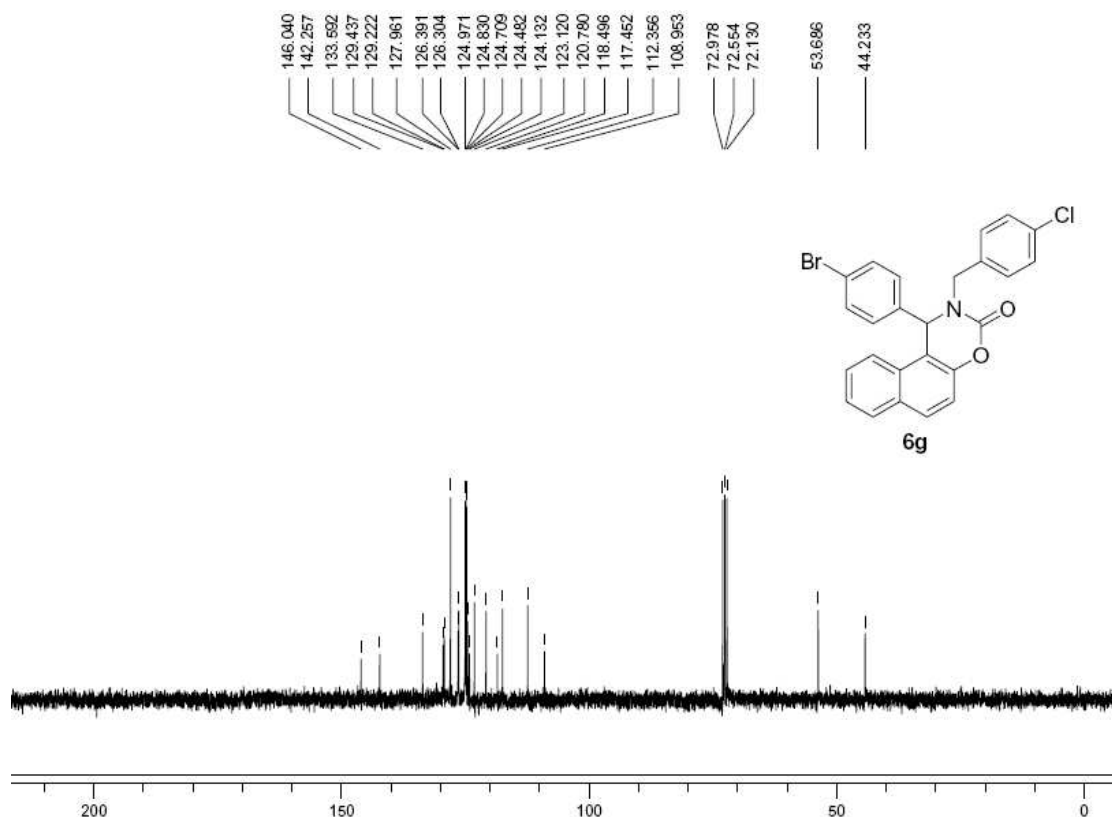
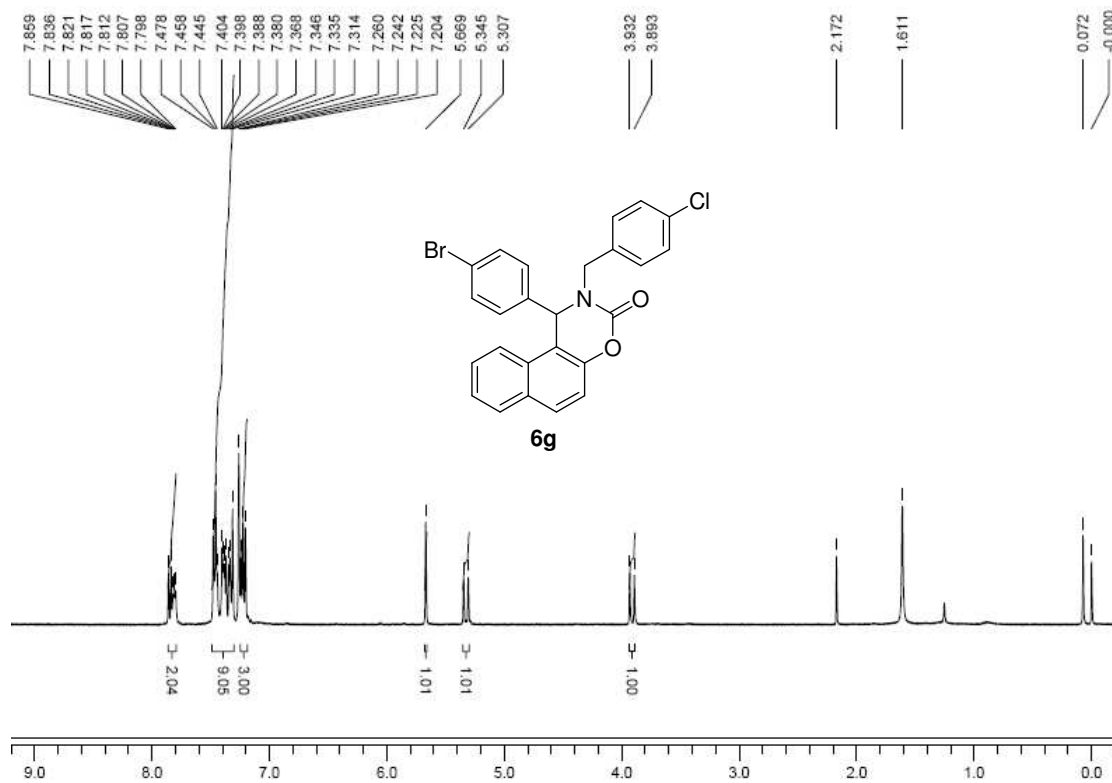
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rsf-C5 147 (2.467) Cm (147-(91:96+354:361))

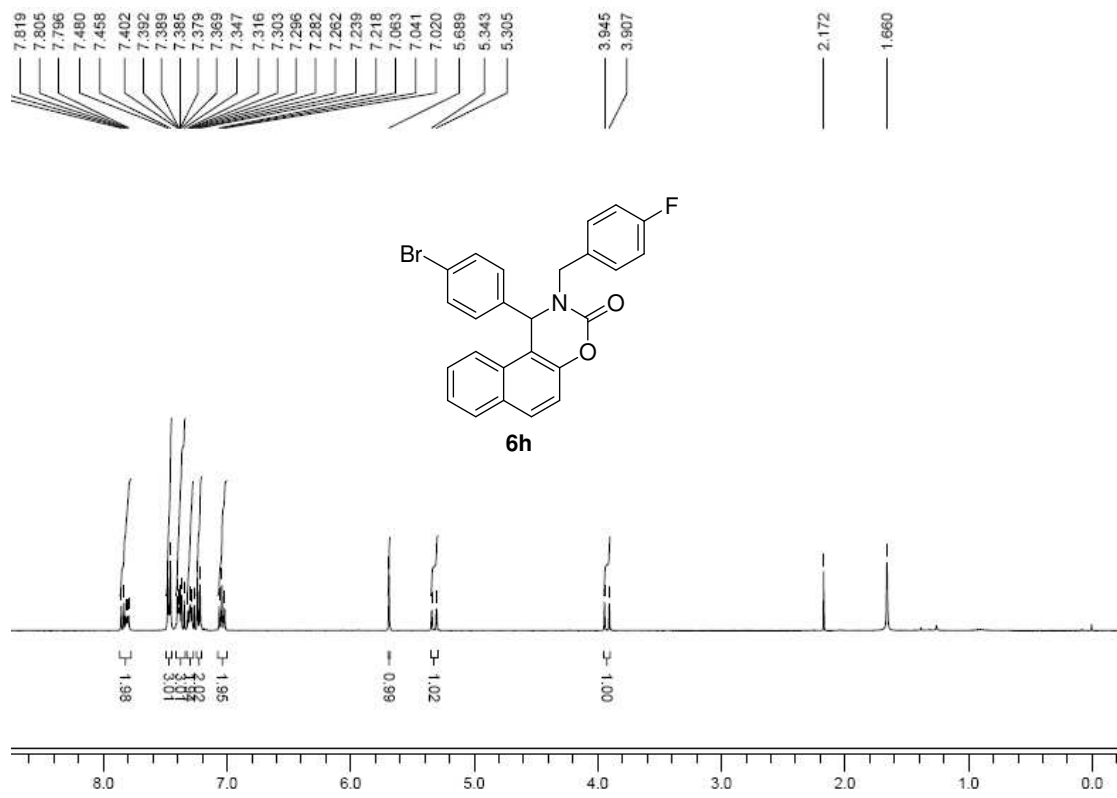
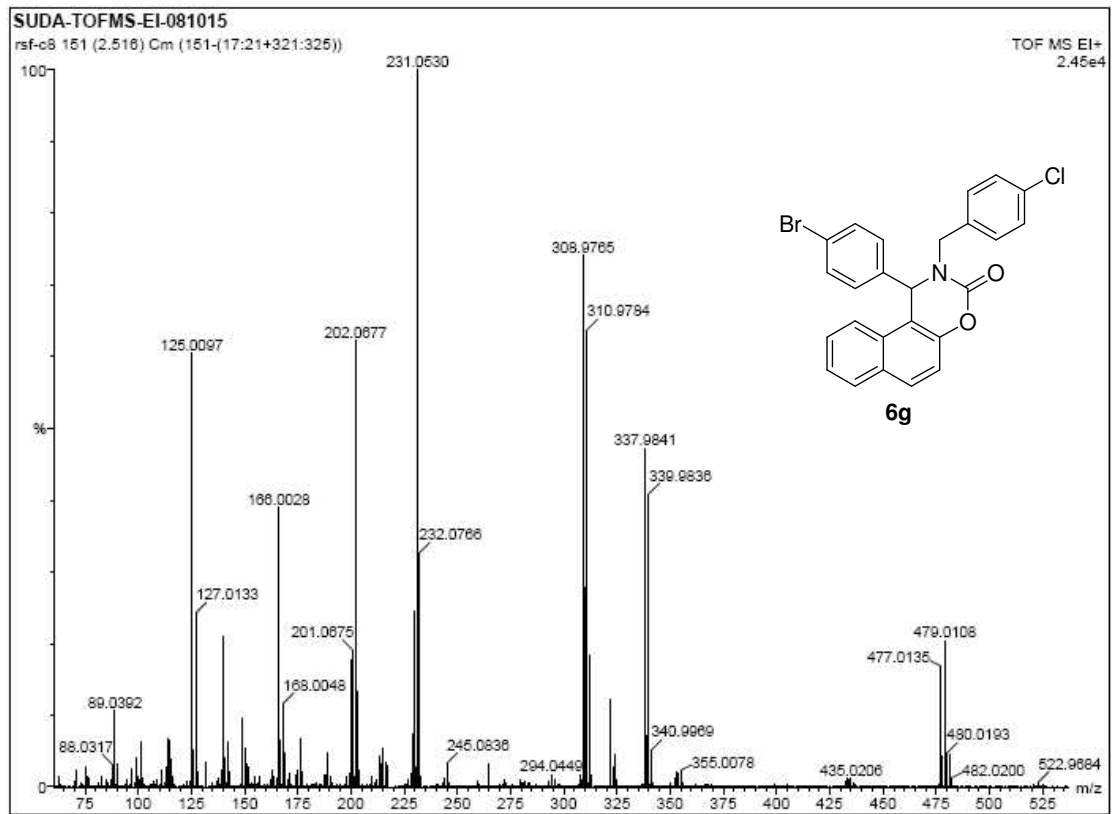
TOF MS EI+  
1.34e4

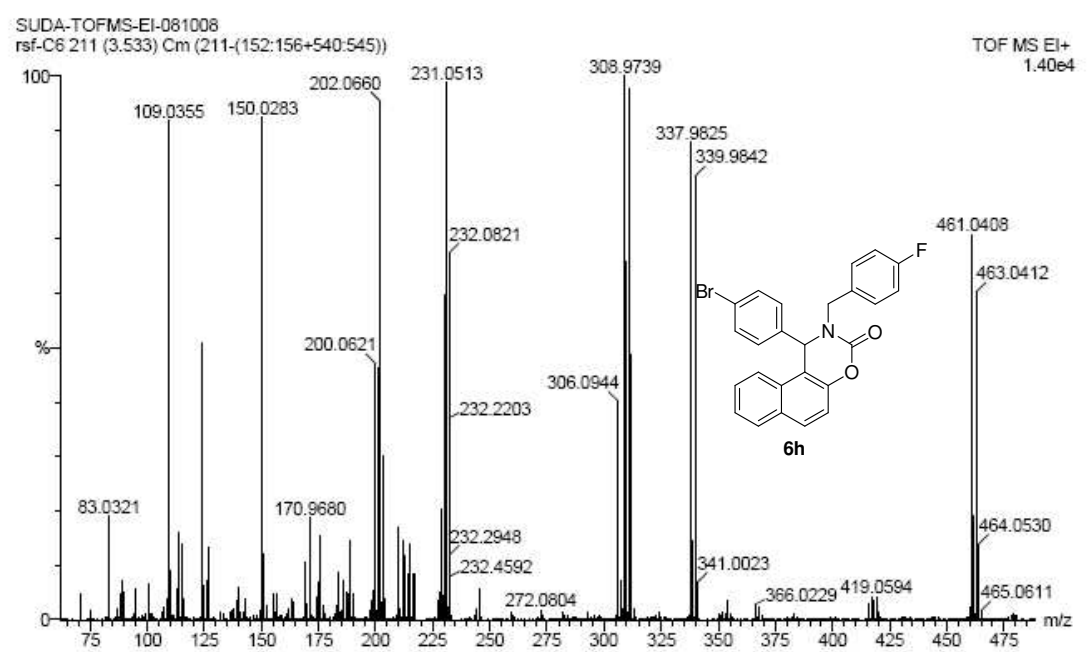
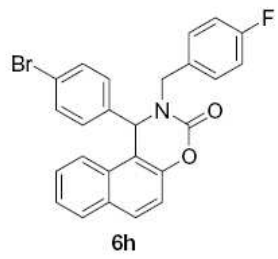
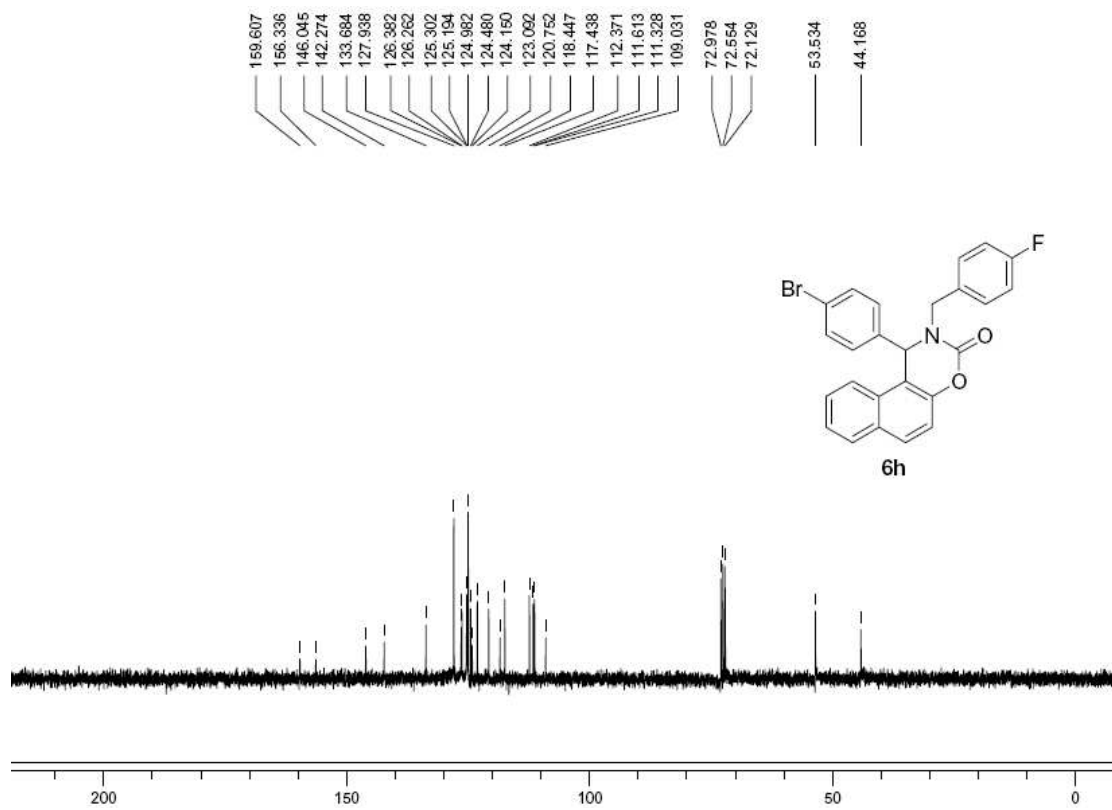


Minimum: 10.00  
Maximum: 100.00

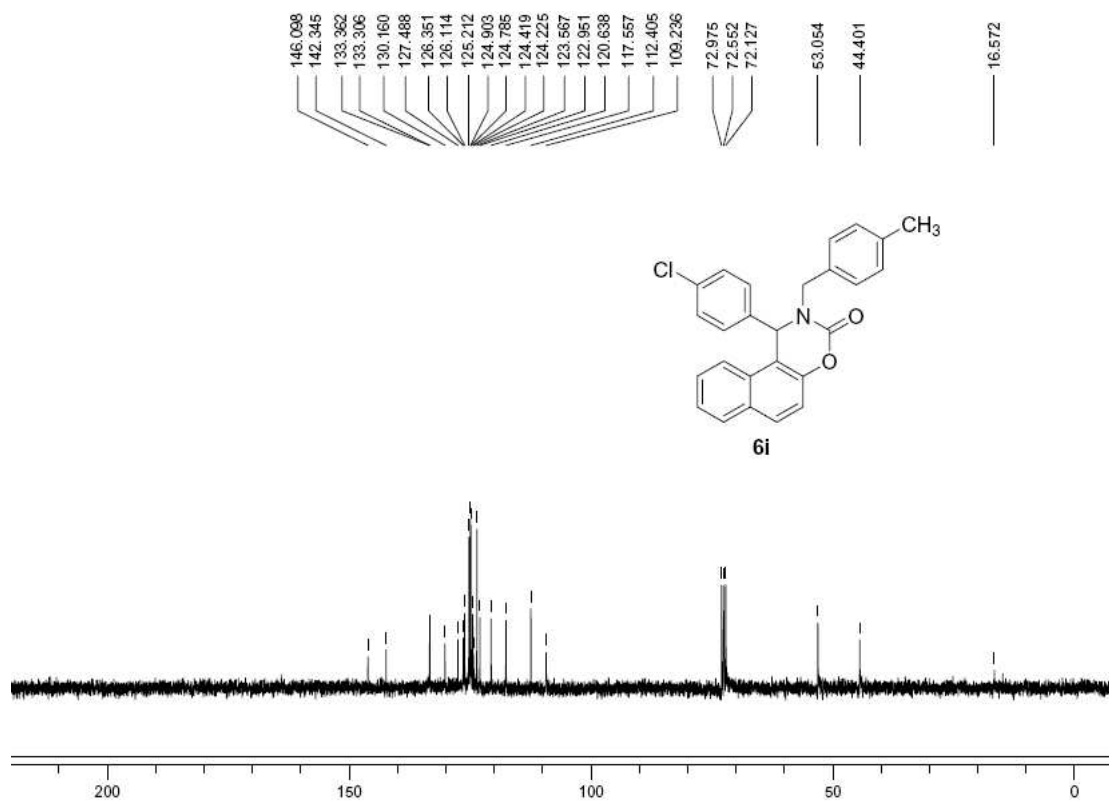
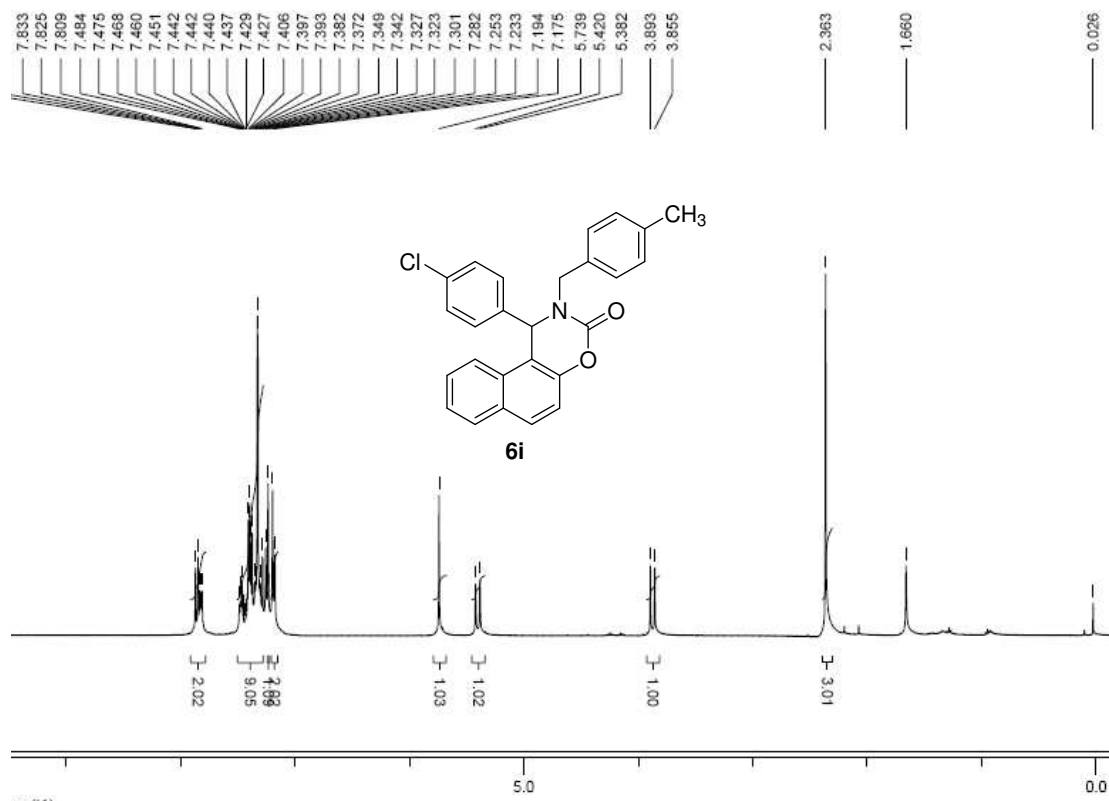
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
		339.9796	4.3	12.6	13.5	2	C17 H9 N O2 81Br
		339.9888	-4.9	-14.3	17.0	1	C21 H9 79Br
457.0659	63.99	457.0677	-1.8	-4.0	17.0	1	C26 H20 N O2 79Br
459.0657	54.37	459.0657	0.0	0.0	17.0	1	C26 H20 N O2 81Br

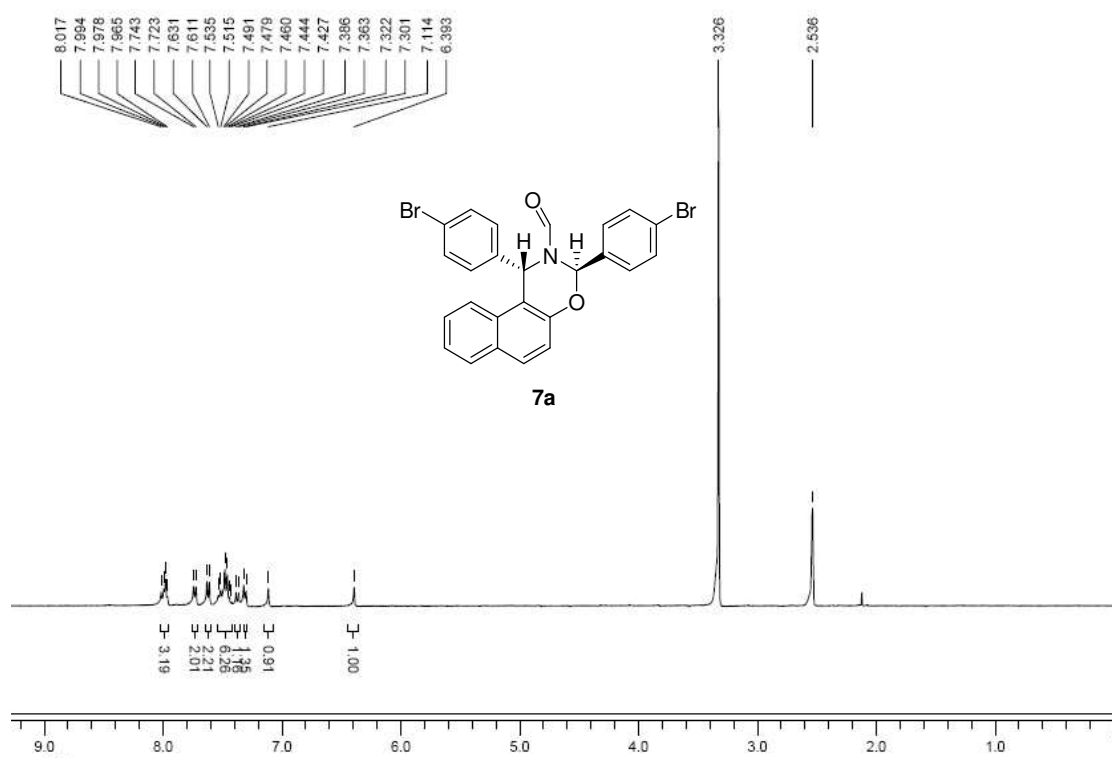
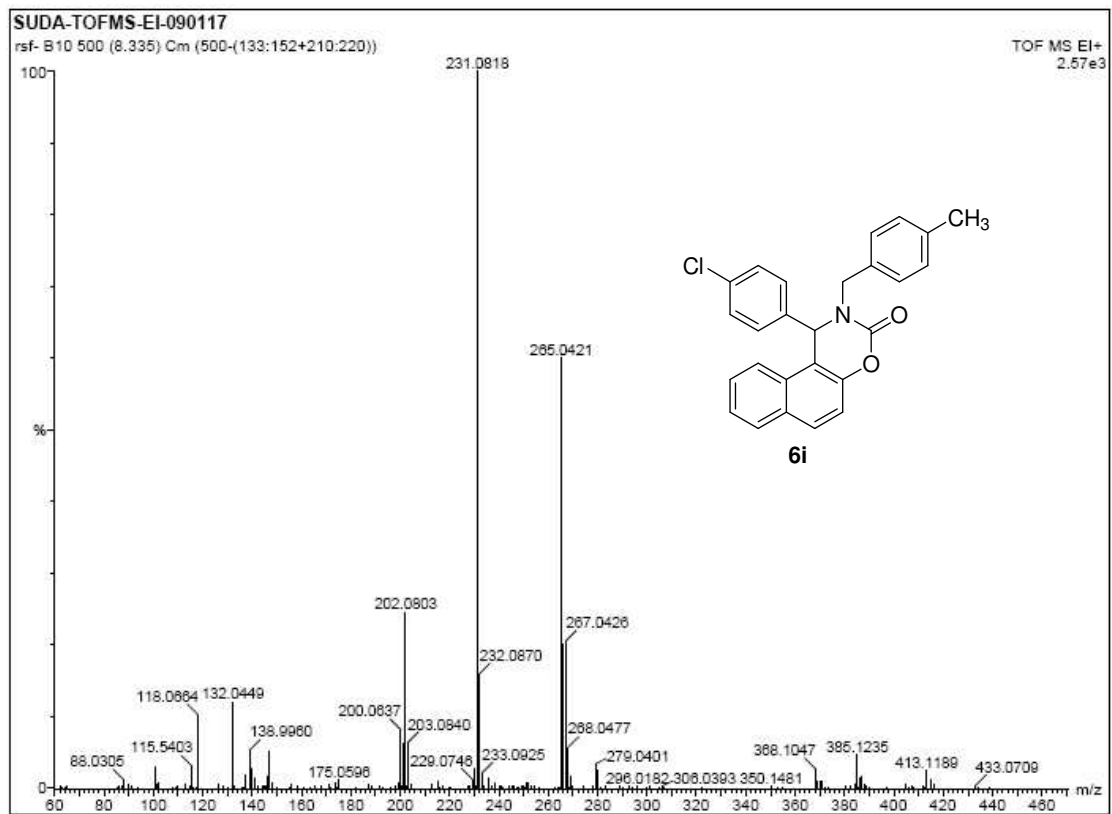


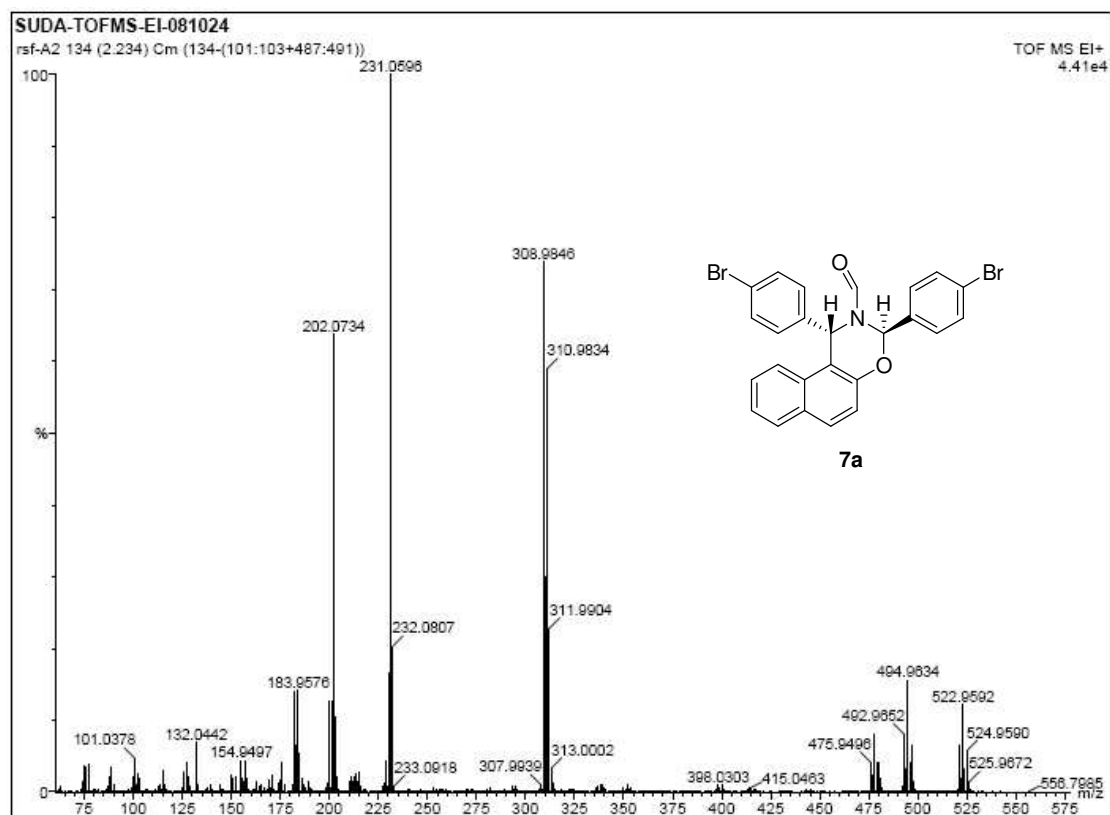
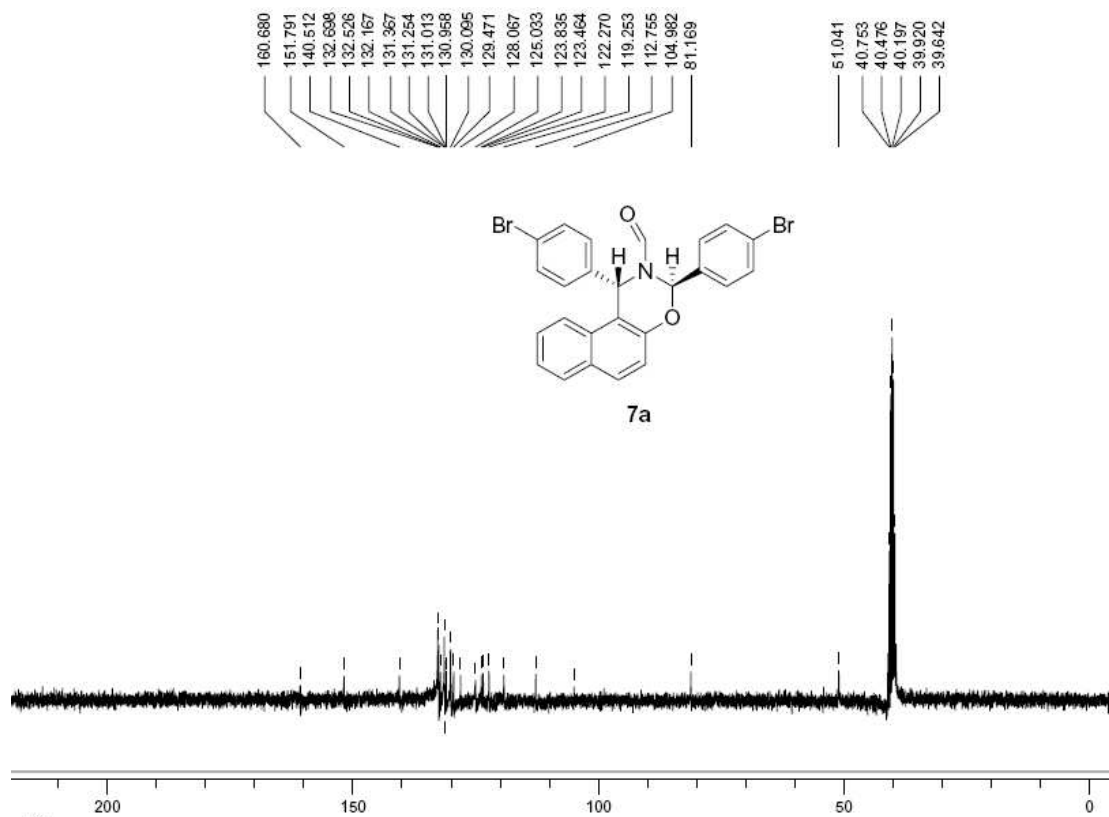


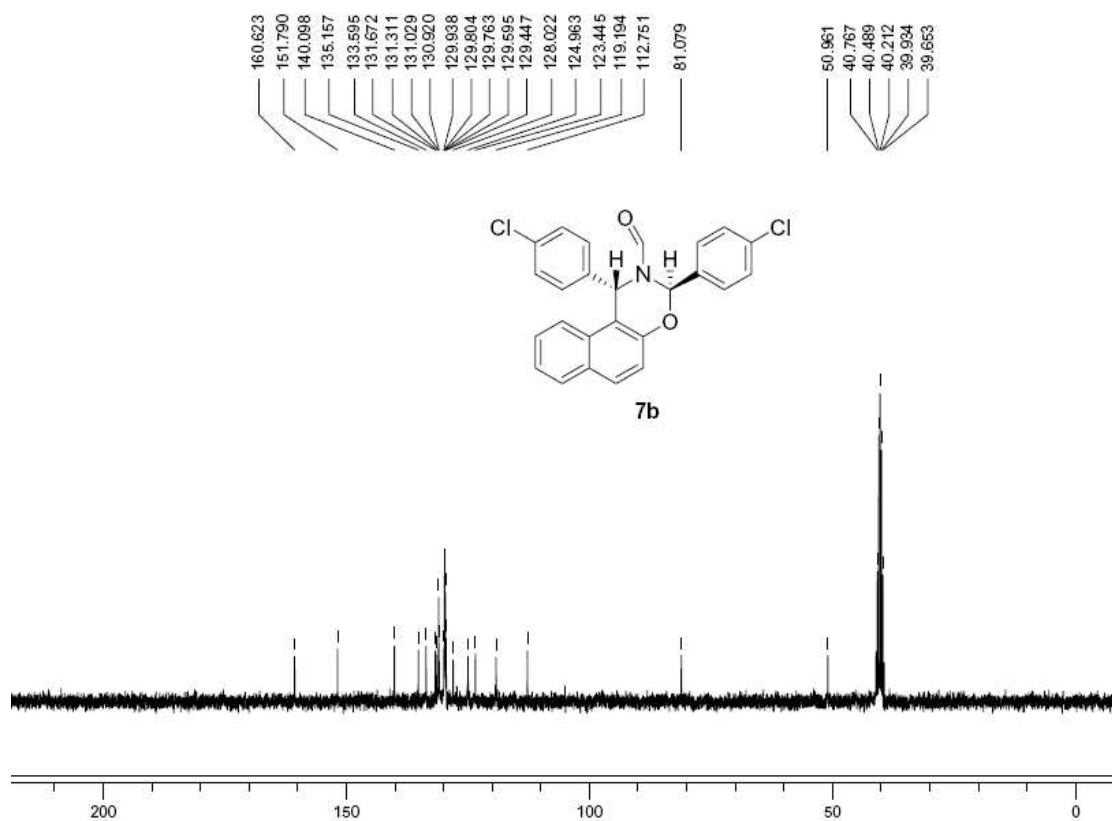
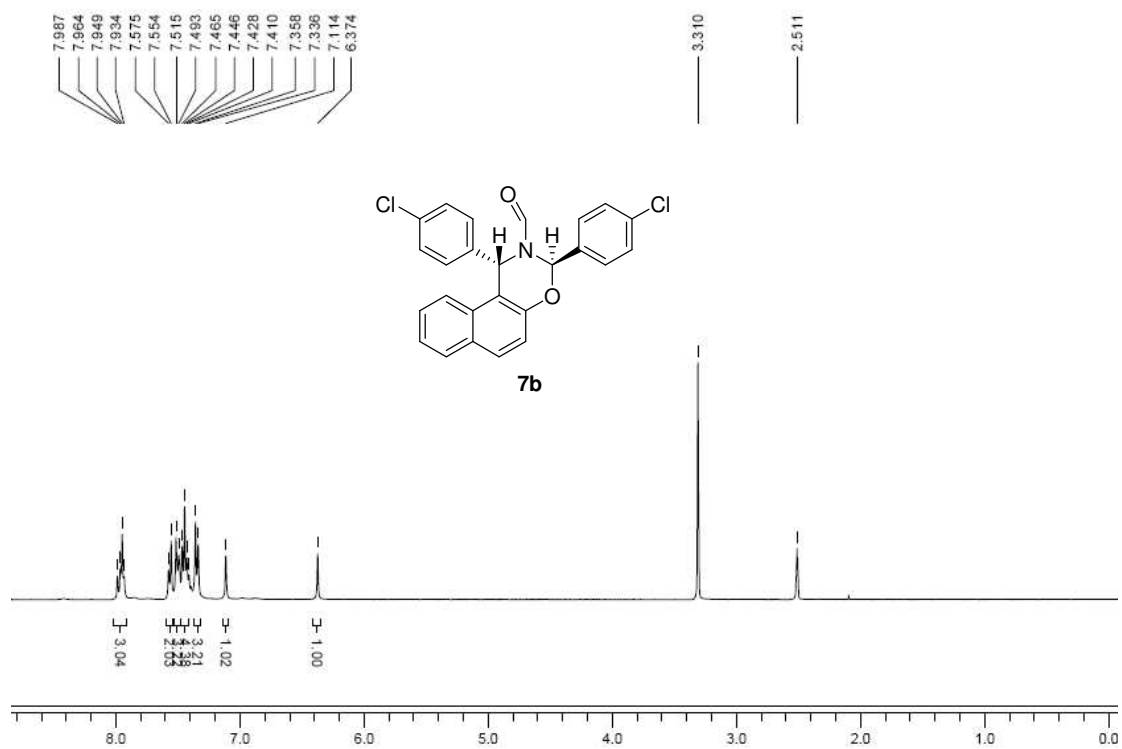


Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
339.9842	81.48	339.9888	-4.6	-13.4	17.0	1	C21 H9 79Br
		339.9796	4.6	13.5	13.5	2	C17 H9 N
461.0408	70.81	461.0427	-1.9	-4.1	17.0	1	O2 81Br
							C25 H17 N
463.0412	60.12	463.0406	0.6	1.2	17.0	1	O2 F 79Br
							C25 H17 N
							O2 F 81Br

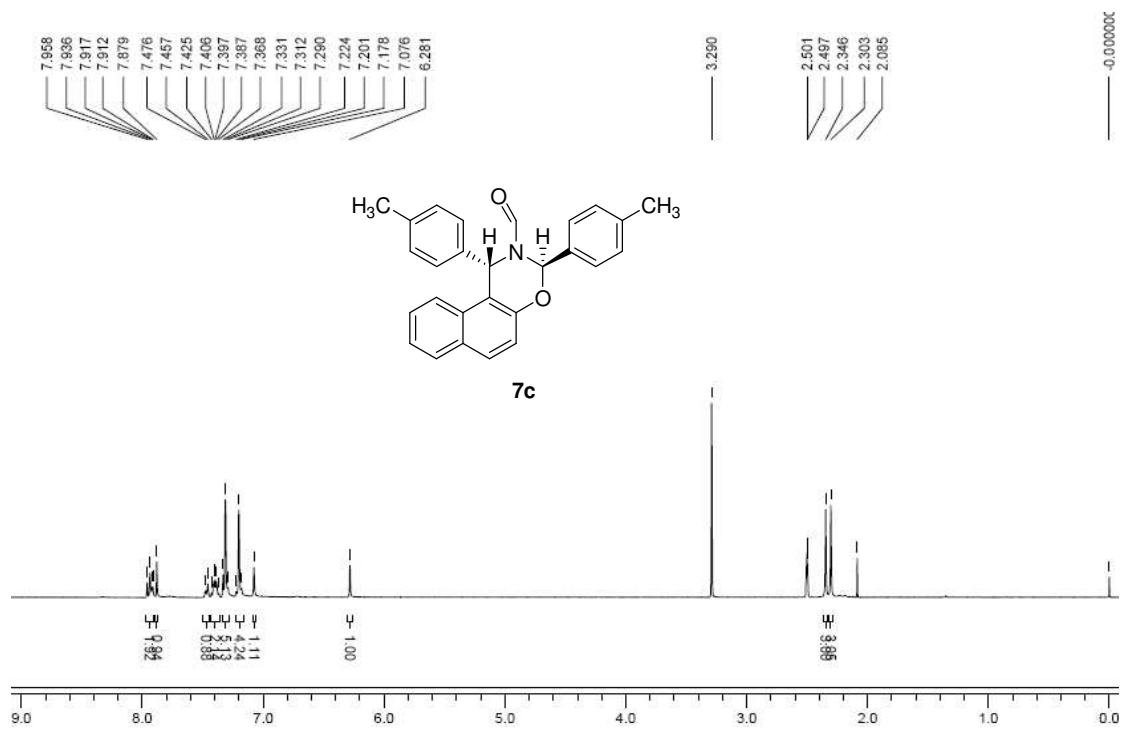
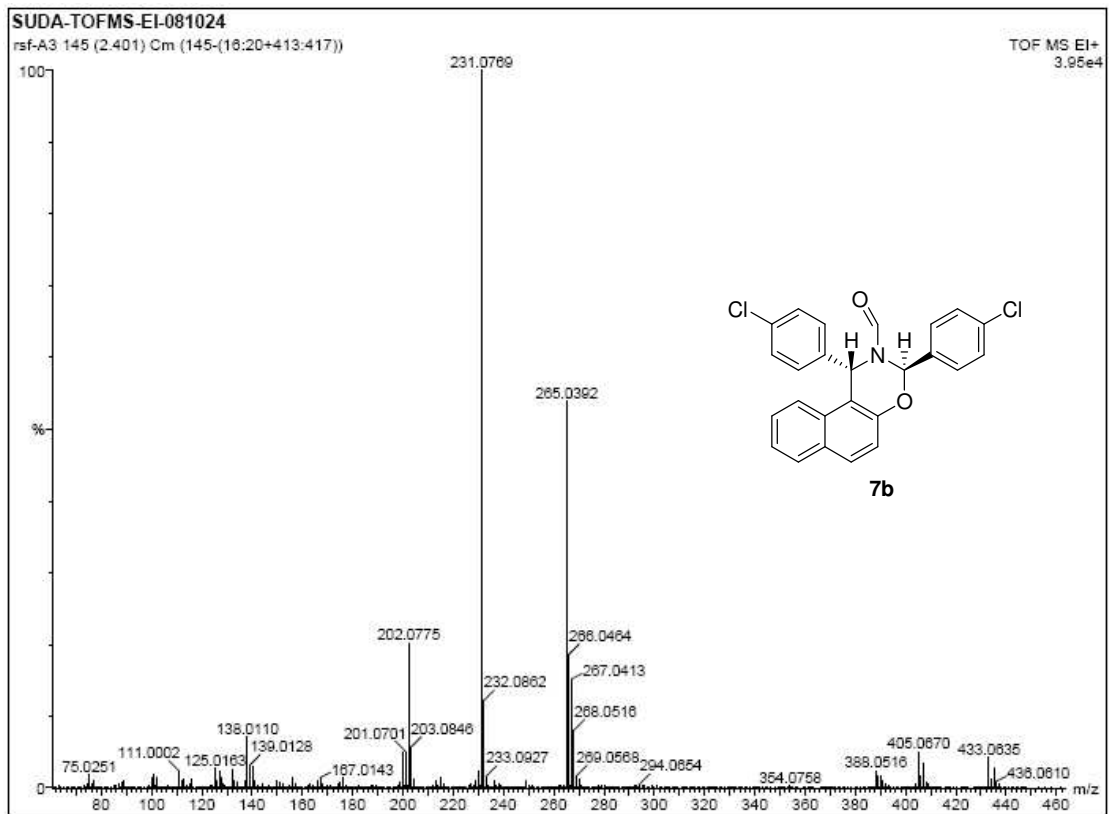


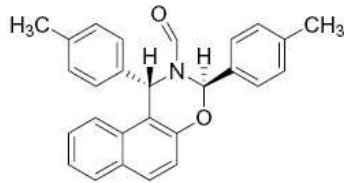
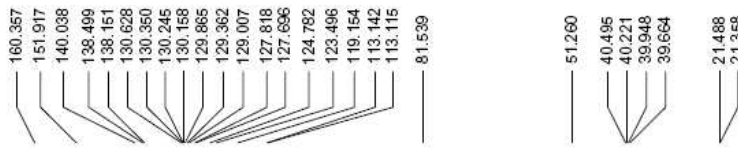




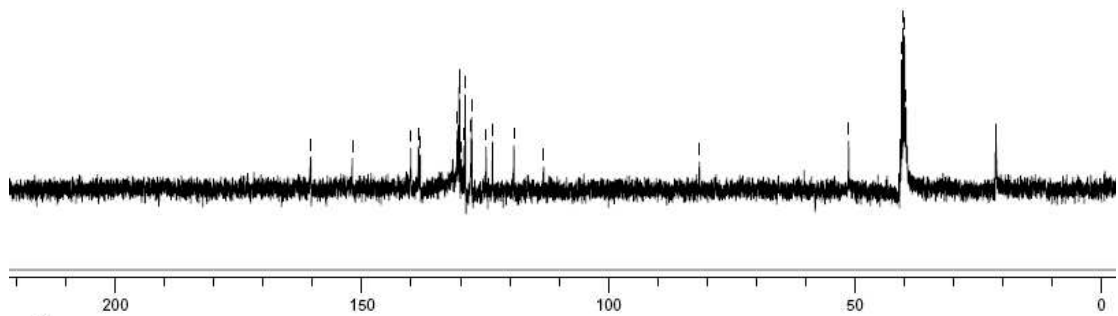






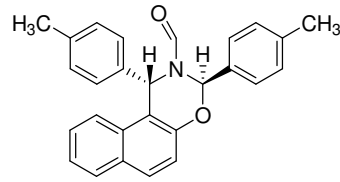
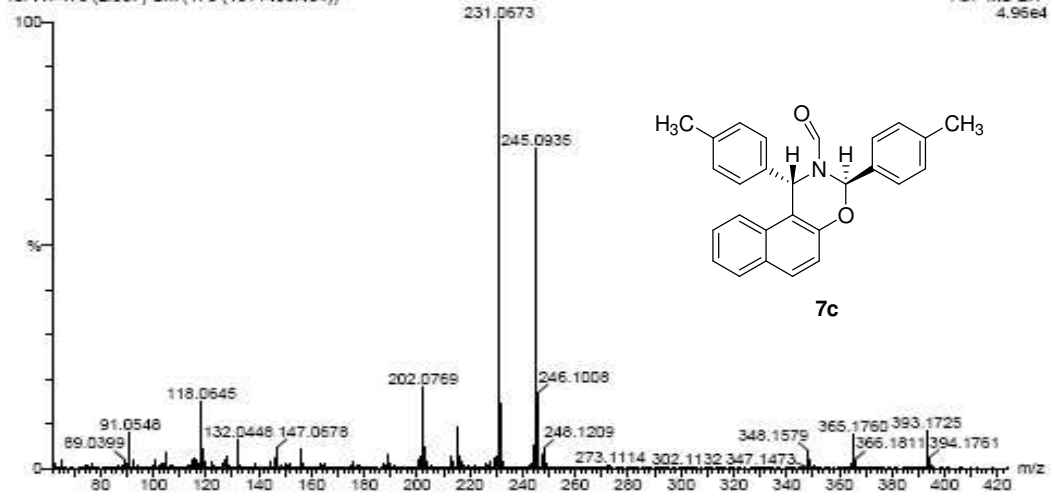


7c



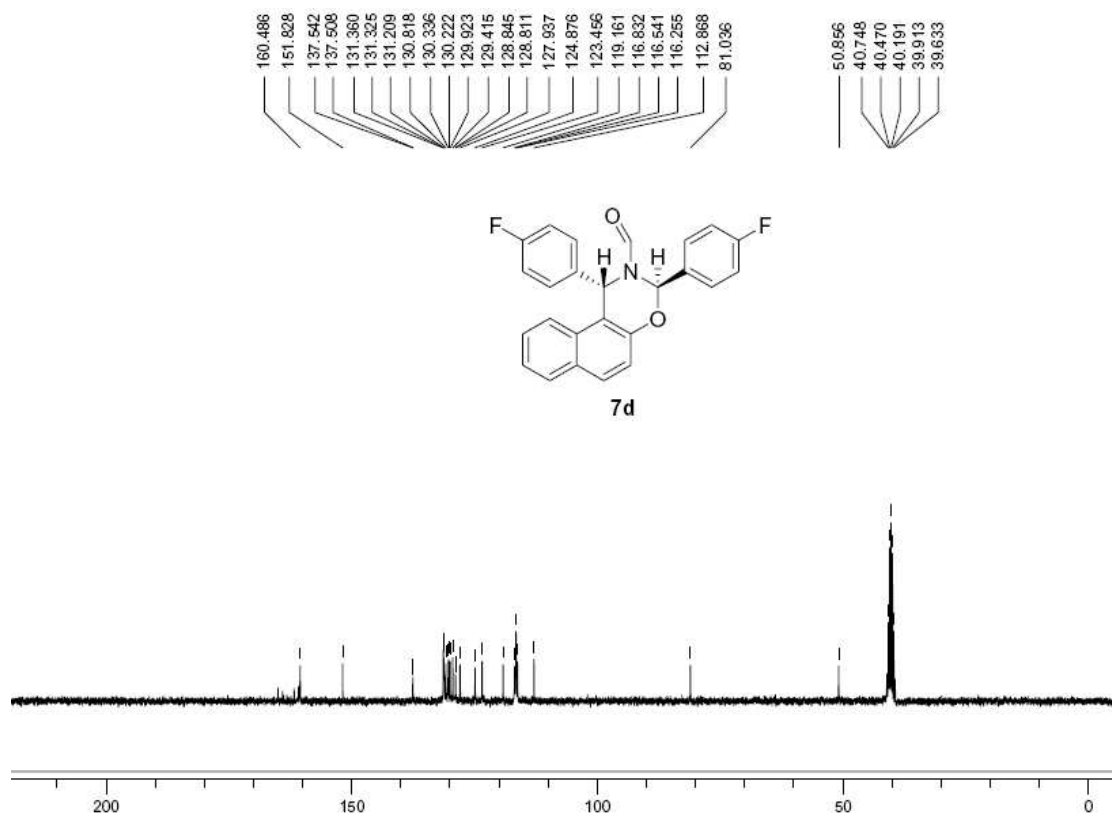
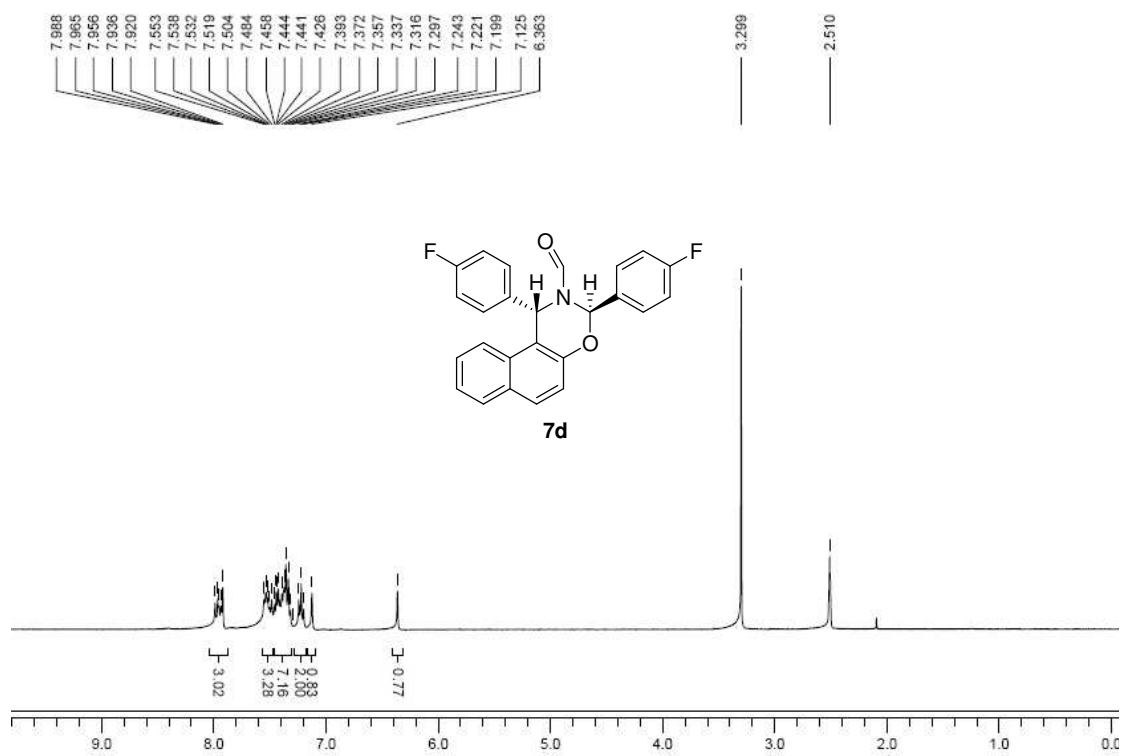
SUDA-TOFMS-EI-061024  
ref-A1 178 (2.967) Cm (178-(131+433:434))

TOF MS EI+  
4.96e4



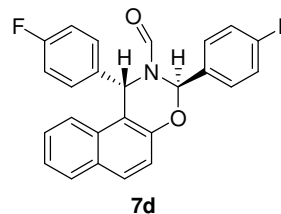
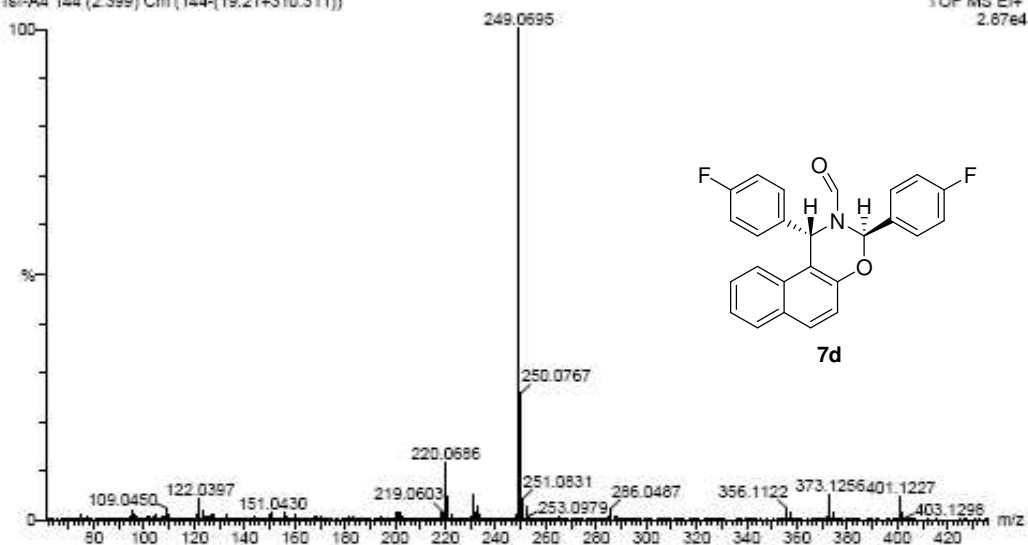
7c

Mass	RA	Calc. Mass	mDa	PFM	DBE	Score	Formula
91.0548	7.93	91.0548	0.0	0.3	4.5	1	C7 H7
105.0696	3.44	105.0704	-0.8	-7.9	4.5	1	C8 H9
118.0645	14.73	118.0657	-1.2	-9.9	5.5	1	C8 H8 N
132.0448	6.32	132.0449	-0.1	-1.1	6.5	1	C8 H6 N O
147.0678	4.63	147.0684	-0.6	-4.2	6.0	1	C9 H9 N O
156.0571	4.13	156.0575	-0.4	-2.7	8.0	1	C11 H6 O
189.0695	3.00	189.0704	-0.9	-4.9	11.5	1	C15 H9
202.0769	17.98	202.0789	-1.4	-6.7	12.0	1	C16 H10
203.0840	4.55	203.0861	-2.1	-10.2	11.5	1	C16 H11
215.0860	9.04	215.0861	-1.1	-5.0	12.5	1	C17 H11
231.0673	100.00	231.0684	-1.1	-4.8	13.0	1	C16 H9 N
232.0848	14.29	232.0888	-4.0	-17.9	12.0	1	C17 H12 O
244.0886	4.96	244.0888	-0.2	-0.9	13.0	1	C18 H12 O
245.0935	71.36	245.0966	-3.1	-12.6	12.5	1	C18 H13 O
246.1008	16.85	246.1045	-3.7	-14.9	12.0	1	C18 H14 O
247.1096	3.14	247.1129	-2.7	-10.9	11.5	1	C18 H15 O
248.1209	4.27	248.1201	0.8	9.2	11.0	1	C18 H16 O
365.1760	7.32	365.1780	-2.0	-5.4	16.0	1	C26 H23 N
393.1725	8.19	393.1729	-0.4	-1.0	17.0	1	C27 H23 N

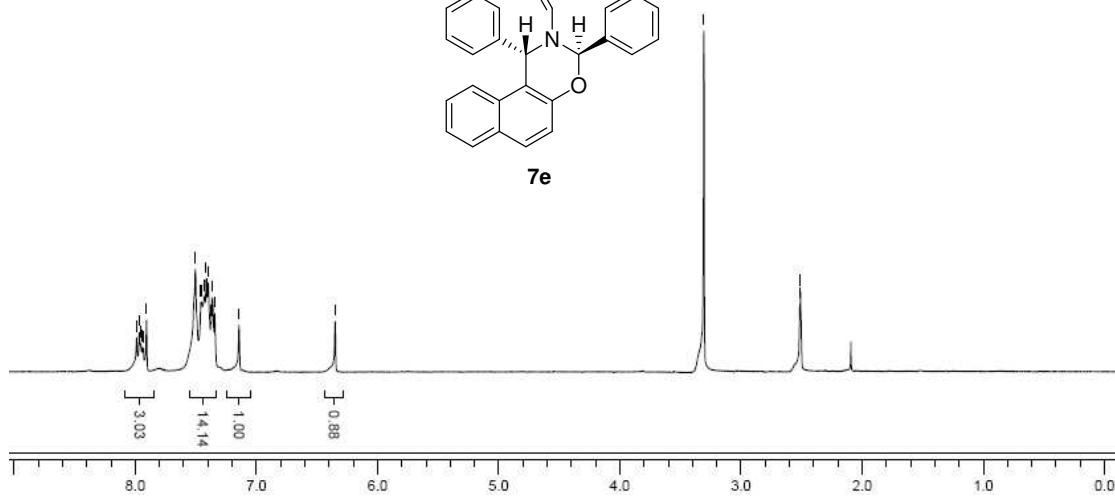
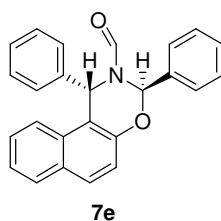
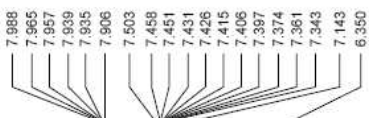


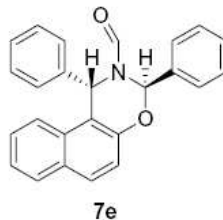
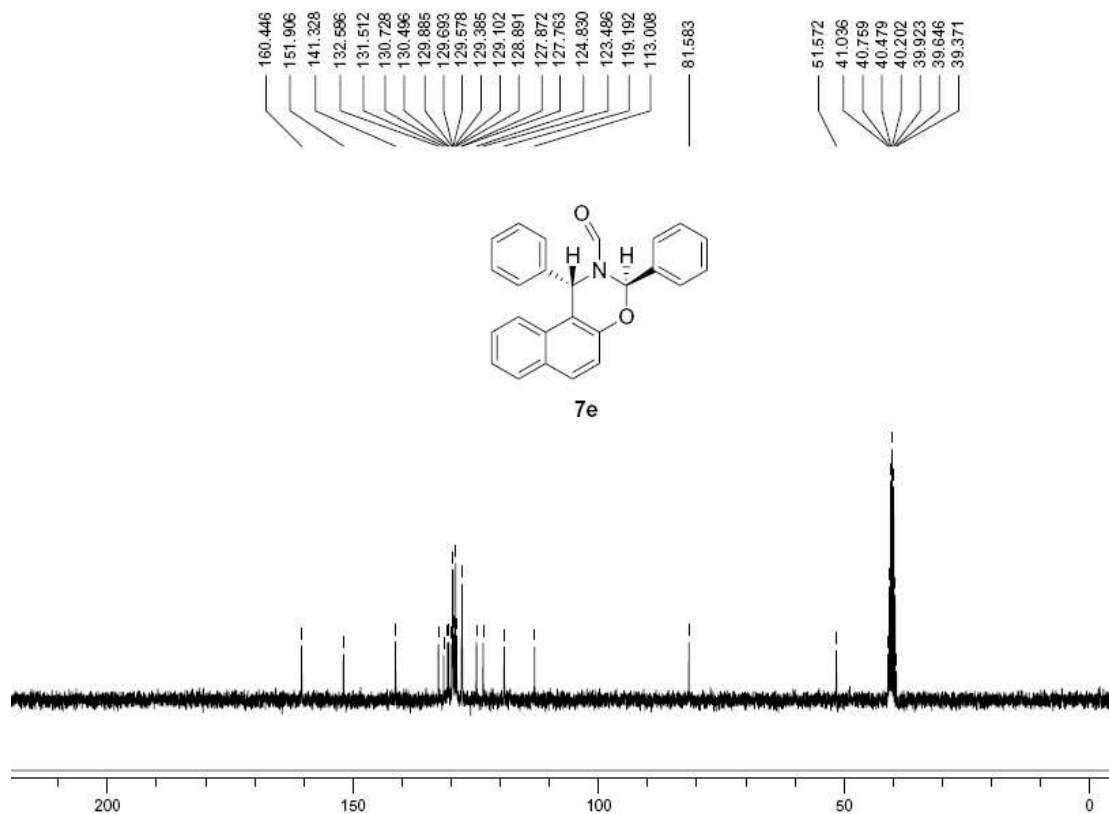
SUDA-TOFMS-EI-081024  
 ref-A4 144 (2.399) Cm (144-(19:21+310:311))

TOF MS EI+  
 2.87e4



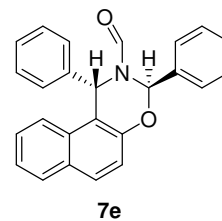
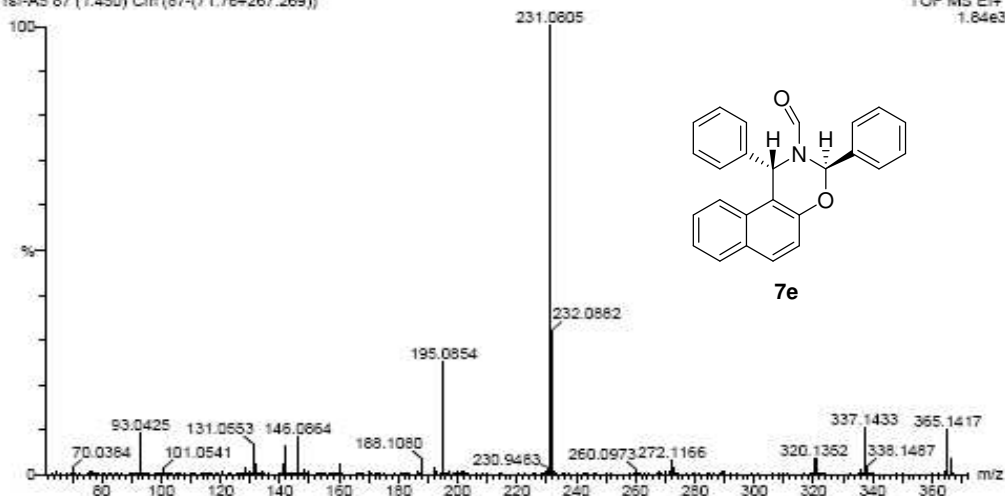
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
251.0891	4.24	251.0861	-3.0	-11.9	15.5	1	C20 H11
		251.0872	-4.1	-16.4	11.5	2	C17 H12 O F
373.1256	5.09	373.1278	-2.2	-6.0	16.0	1	C24 H17 N O F2
401.1227	4.69	401.1227	0.0	-0.1	17.0	1	C28 H17 N O2 F2



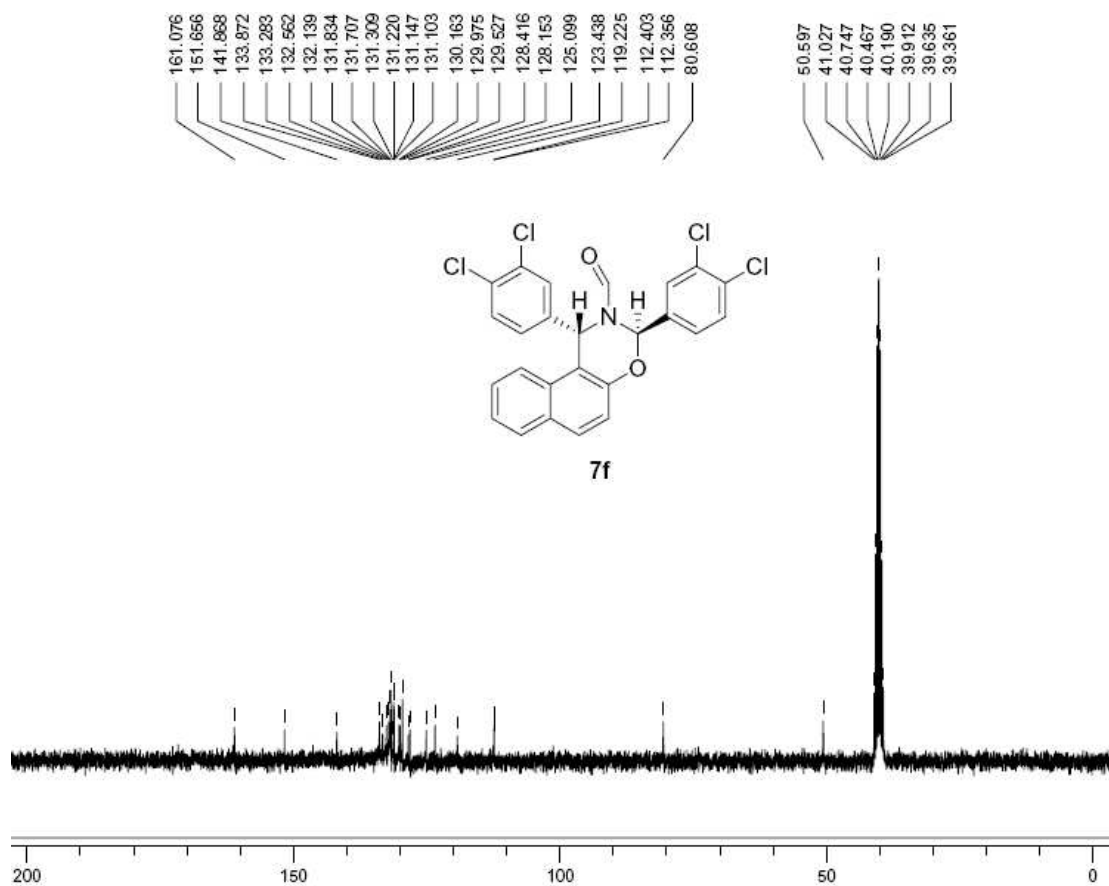
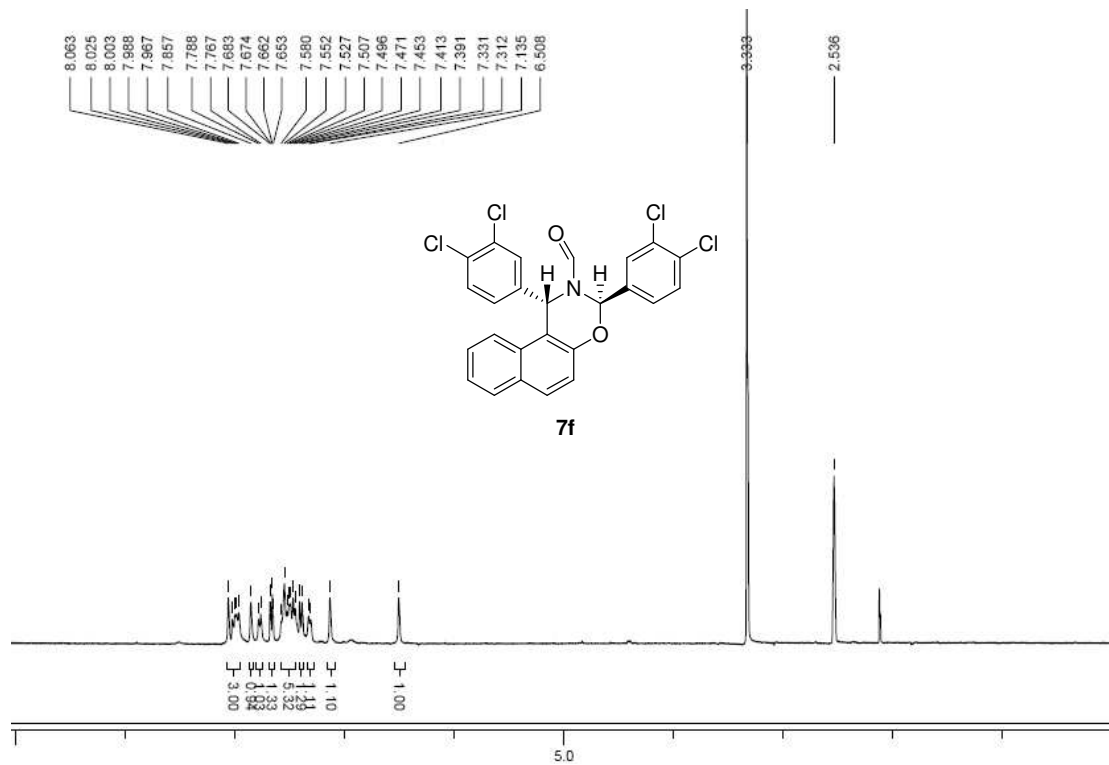


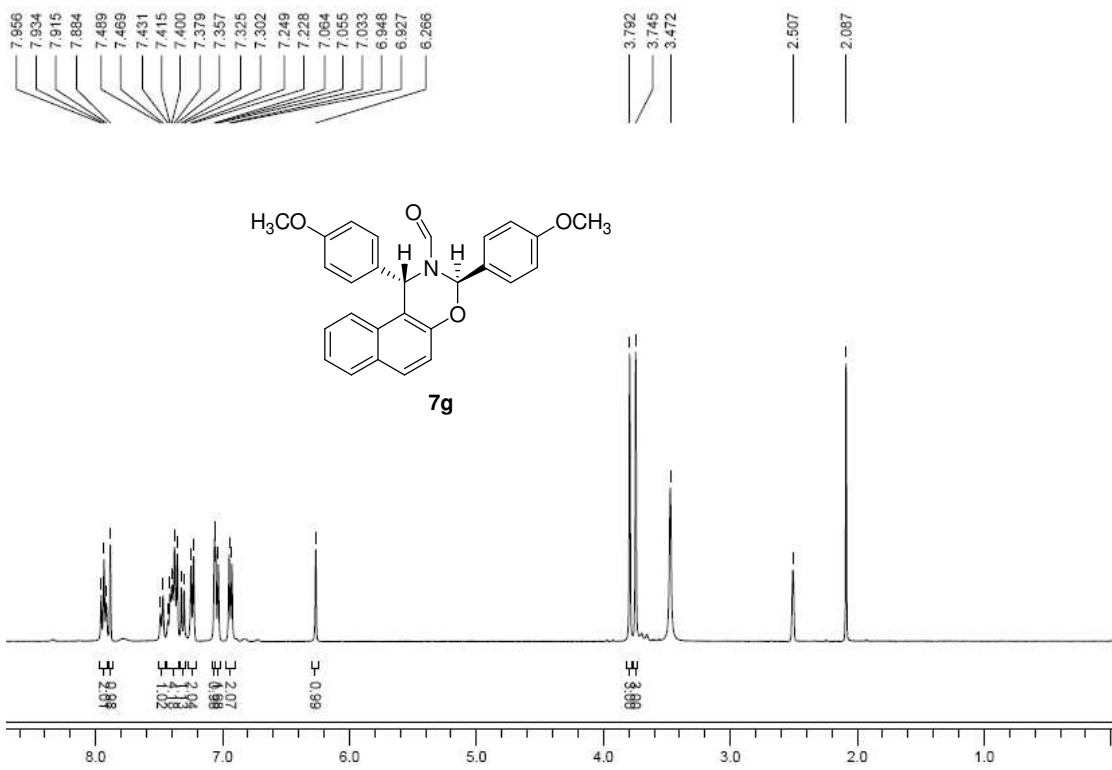
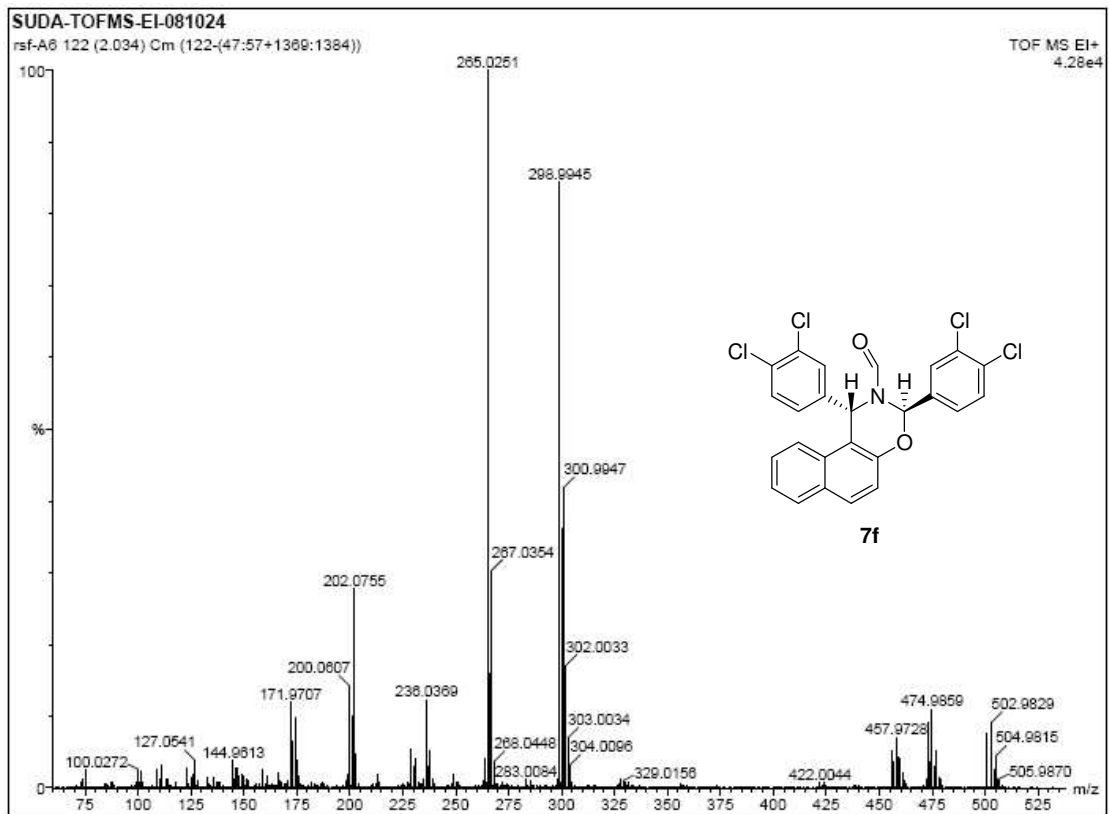
SUDA-TOFMS-EI-061024  
rsf-A5 67 (1.450) Cm (67-(71.76+267.269))

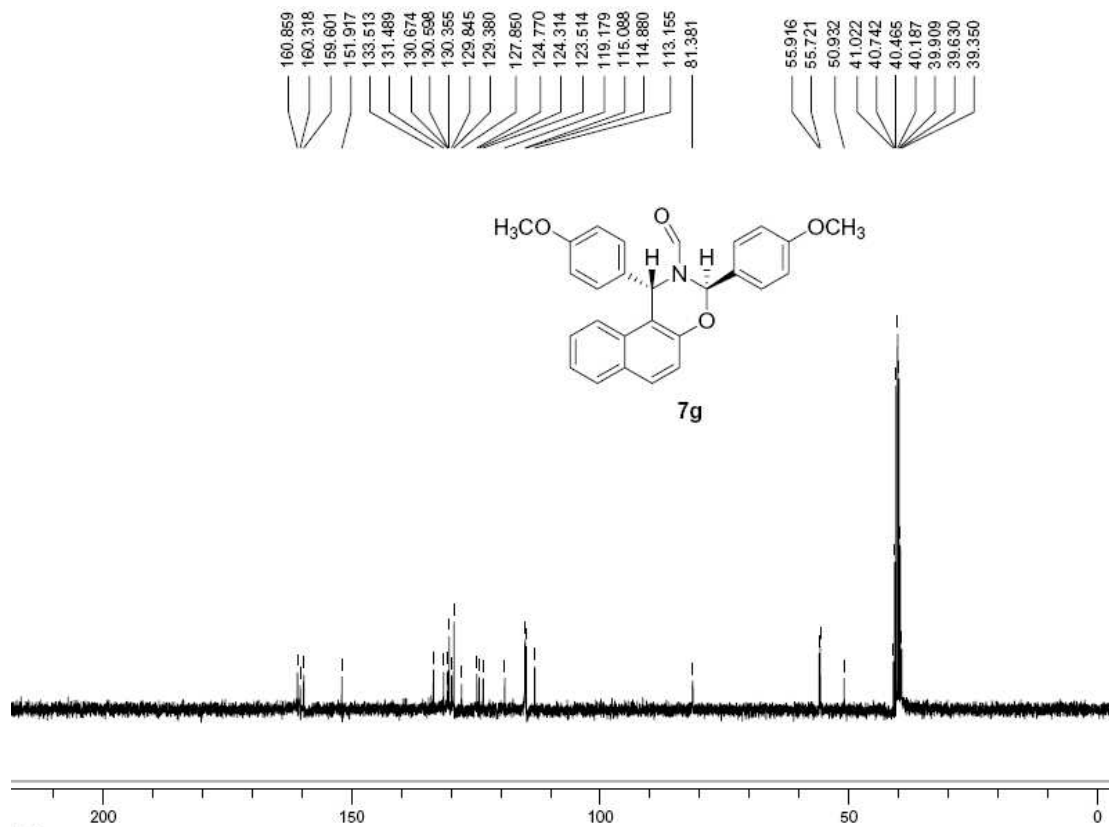
TOF MS EI+  
1.64e3



Mass	RA	Calc. Mass	mDa	PFM	DBE	Score	Formula
70.0384	1.37	70.0419	-3.5	-49.5	2.0	1	C4 H6 O
141.0710	2.23	141.0704	0.6	4.1	7.5	1	C11 H9
142.0778	6.22	142.0783	-0.8	-5.3	7.0	1	C11 H10
188.1080	3.25	188.1075	0.5	2.4	6.5	1	C12 H14 N O
195.0854	25.17	195.0810	4.4	22.6	9.5	1	C14 H11 O
231.0805	100.00	231.0810	-0.5	-2.1	12.5	1	C17 H11 O
232.0862	32.08	232.0886	-0.6	-2.7	12.0	1	C17 H12 O
272.1166	3.04	272.1201	-3.5	-12.9	13.0	1	C20 H16 O
273.1158	1.32	273.1154	0.4	1.6	13.0	1	C19 H15 N O
336.1358	1.07	336.1388	-3.0	-9.0	16.5	1	C24 H18 N O
337.1433	10.19	337.1467	-3.4	-10.0	16.0	1	C24 H19 N O
365.1417	9.84	365.1416	0.1	0.3	17.0	1	C25 H19 N O2

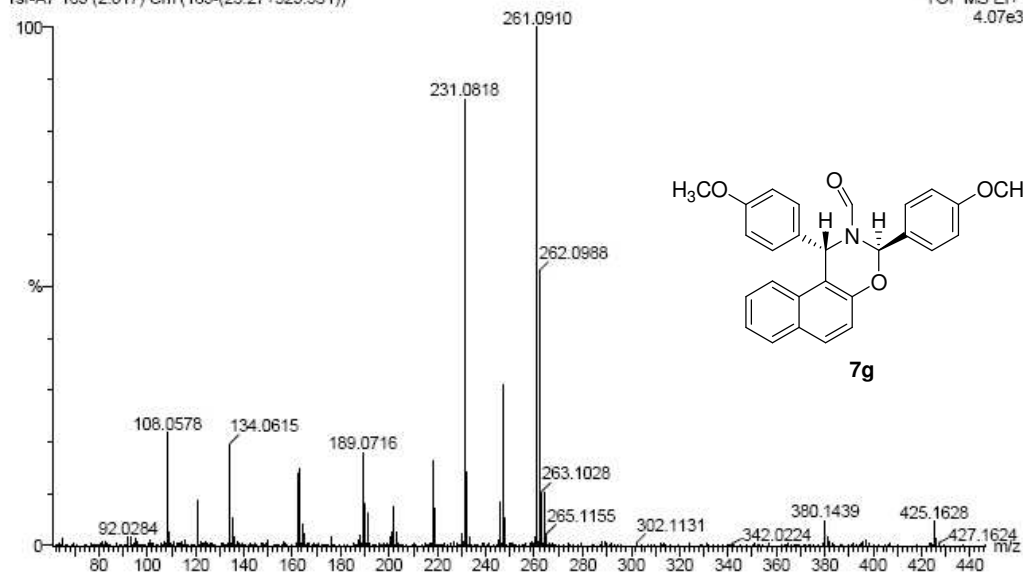






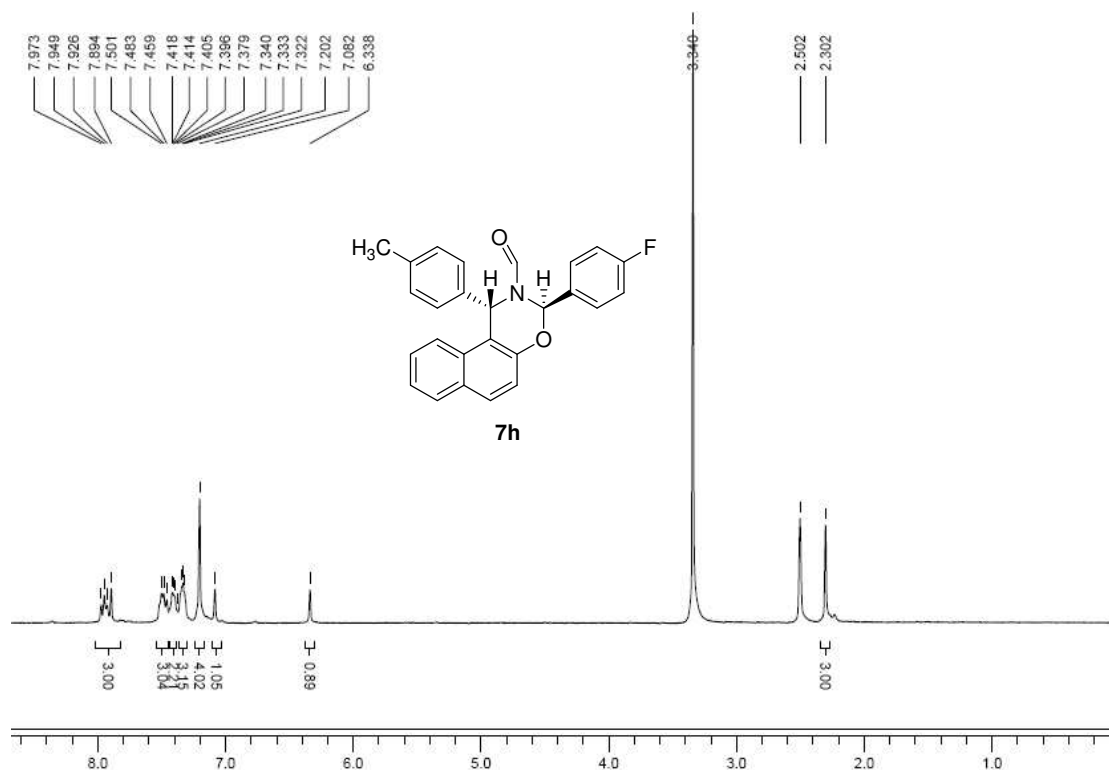
SUDA-TOFMS-EI-081024  
rsf-A7 169 (2.817) Cm (169-(23:27+329:331))

TOF MS EI+  
4.07e3

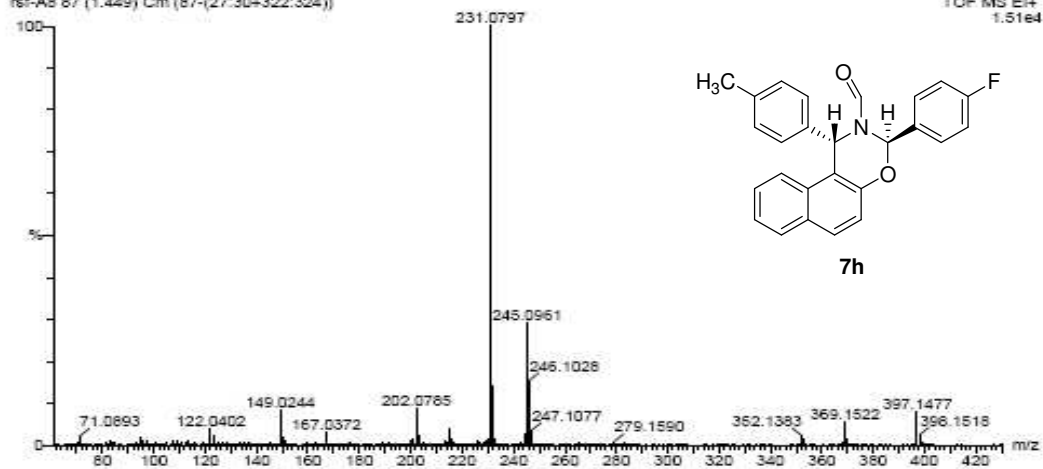


Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
262.0988	52.75	262.0994	-0.6	-2.2	12.0	1	C18 H14 O2
263.1028	10.22	263.1072	-4.4	-16.7	11.5	1	C18 H15 O2
264.1154	10.13	264.1150	0.4	1.4	11.0	1	C18 H16 O2
380.1439	4.71	380.1412	2.7	7.0	17.0	1	C26 H20 O3
425.1628	4.49	425.1627	0.1	0.2	17.0	1	C27 H23 N O4

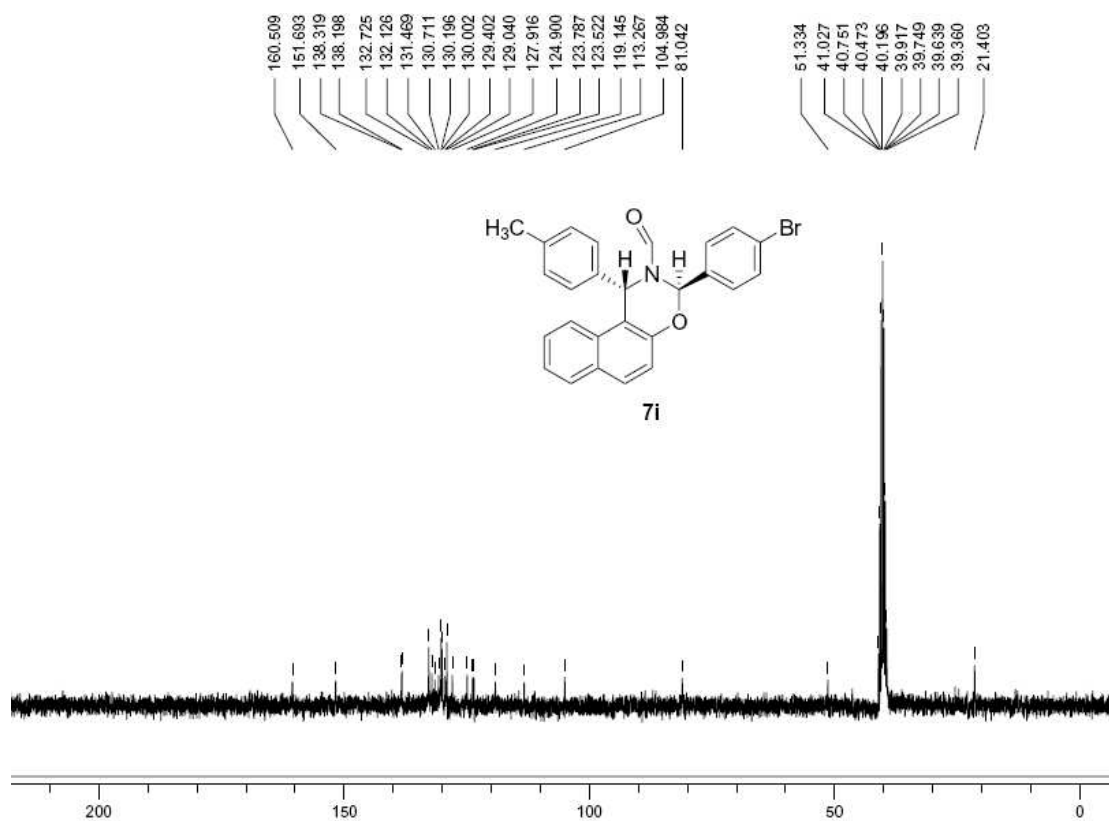
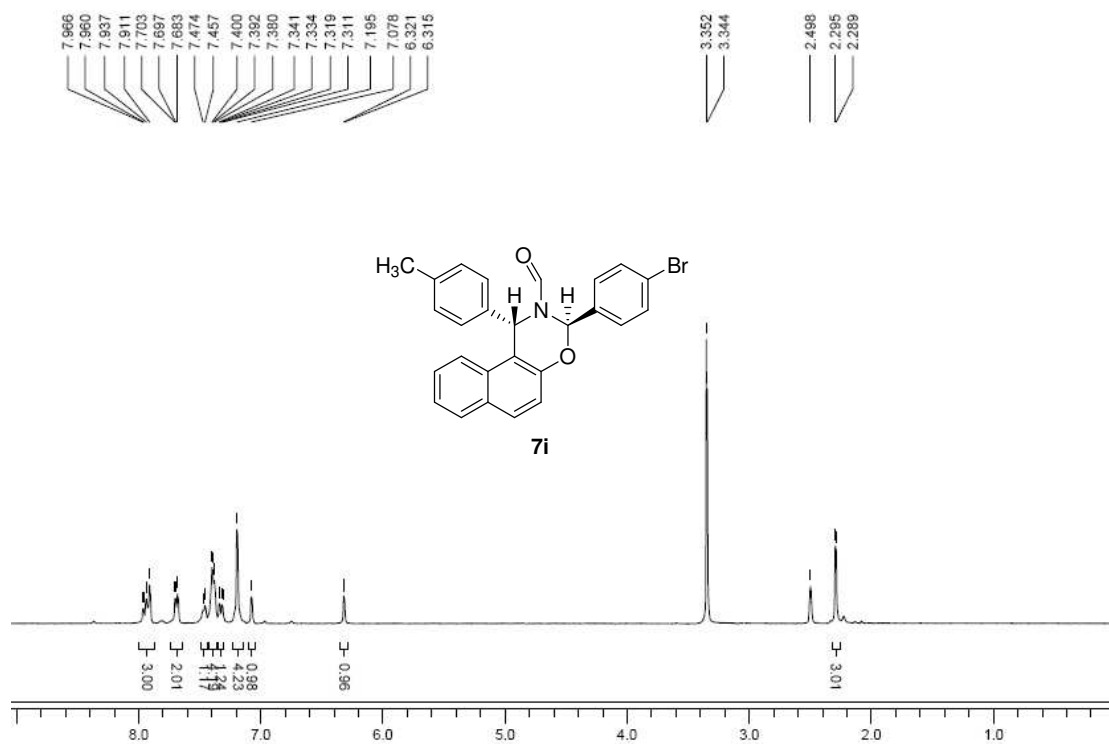




SUDA-TOFMS-EI-081024  
ref-A8 67 (1.449) Cm (67-(27:30+322:324))

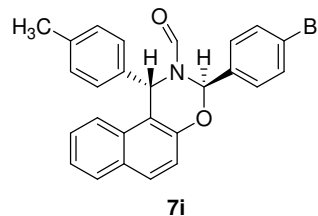
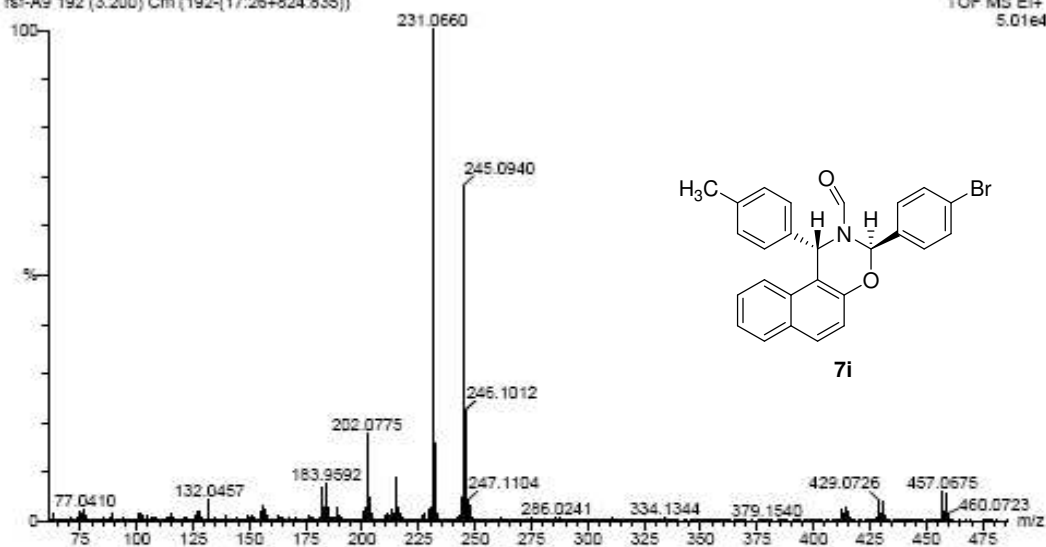


Mass	RA	Calc. Mass	mDa	PFM	DBE	Score	Formula
149.0244	8.41	149.0265	-2.1	-14.4	11.0	1	C11 H8 N
		149.0277	-3.3	-22.1	7.0	2	C8 H4 N O
202.0785	8.84	202.0789	0.2	1.2	12.0	1	F
		202.0794	-0.9	-4.4	8.0	2	C13 H11 O
231.0797	100.00	231.0810	-1.3	-5.6	12.5	2	F
		231.0821	-2.4	-10.5	8.5	1	C17 H11 O
232.0866	14.18	232.0888	-2.2	-9.5	12.0	2	F
		232.0900	-3.4	-14.5	8.0	1	C14 H12 O
245.0961	29.13	245.0966	-0.5	-2.2	12.5	1	F
		245.0978	-1.7	-6.9	8.5	2	C15 H13 O
246.1028	16.25	246.1045	-1.7	-6.8	12.0	1	F
		246.1056	-2.8	-11.4	8.0	2	C15 H14 O
369.1522	5.59	369.1529	-0.7	-1.9	16.0	1	F
							C25 H20 N
397.1477	8.06	397.1478	-0.1	-0.3	17.0	1	O
							C26 H20 N
							O2 F

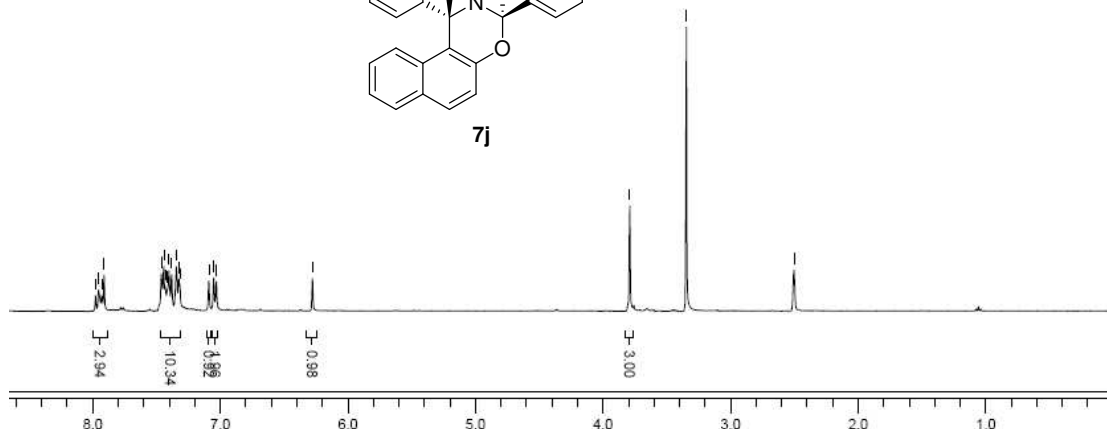
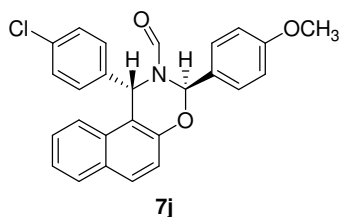


SUDA-TOFMS-EI-061024  
 ref-A9 192 (3.200) Cm (192-(17:26+824.835))

TOF MS EI+  
 5.01e4



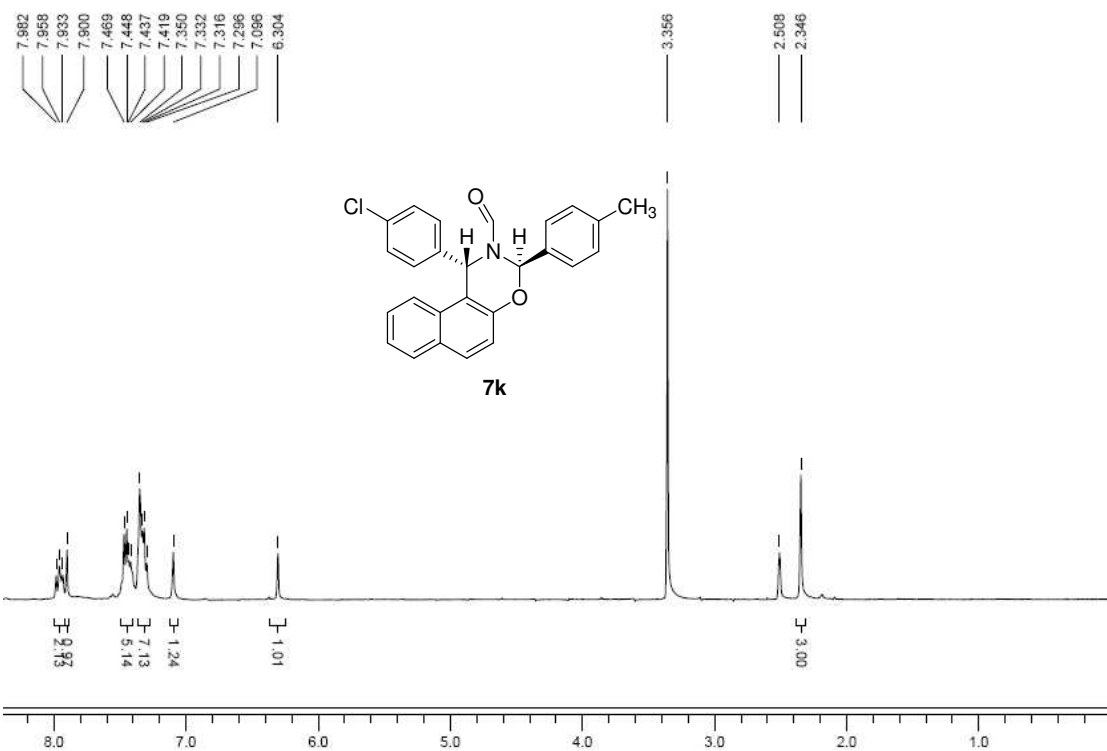
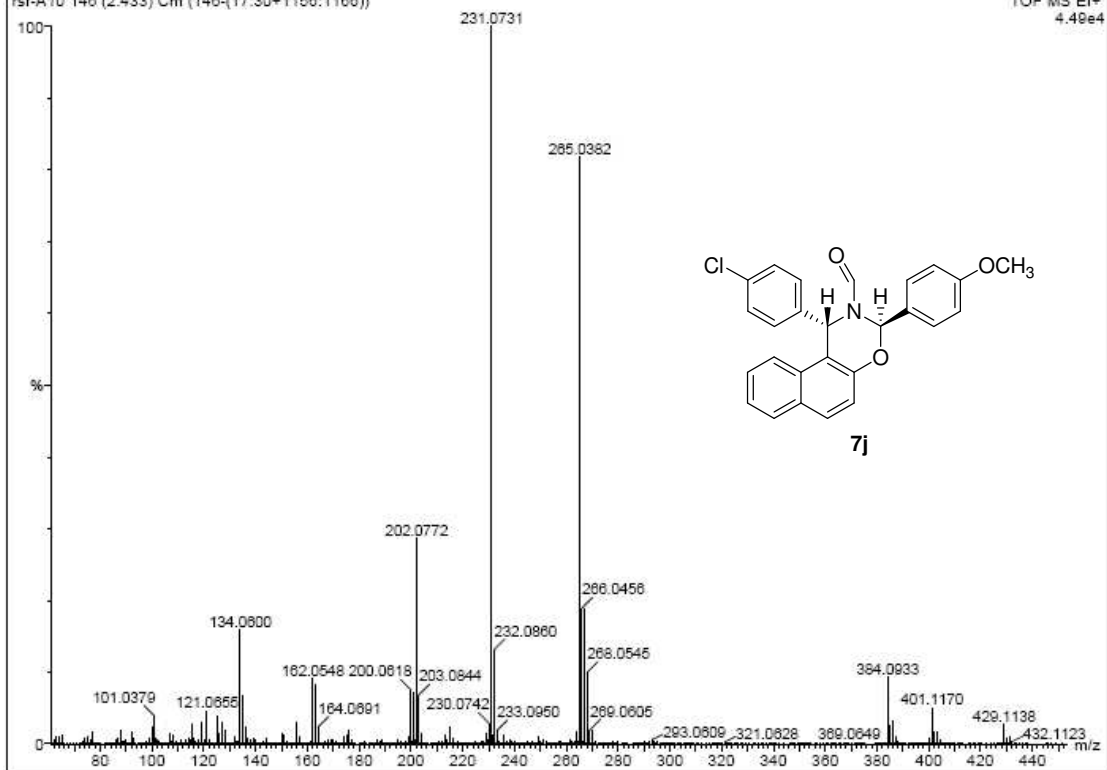
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
431.0714	3.85	431.0708	0.6	1.4	16.0	1	C26 H20 N O 81Br
457.0675	5.64	457.0677	-0.2	-0.5	17.0	1	C26 H20 N O2 79Br
459.0656	5.24	459.0657	-0.1	-0.2	17.0	1	C26 H20 N O2 81Br

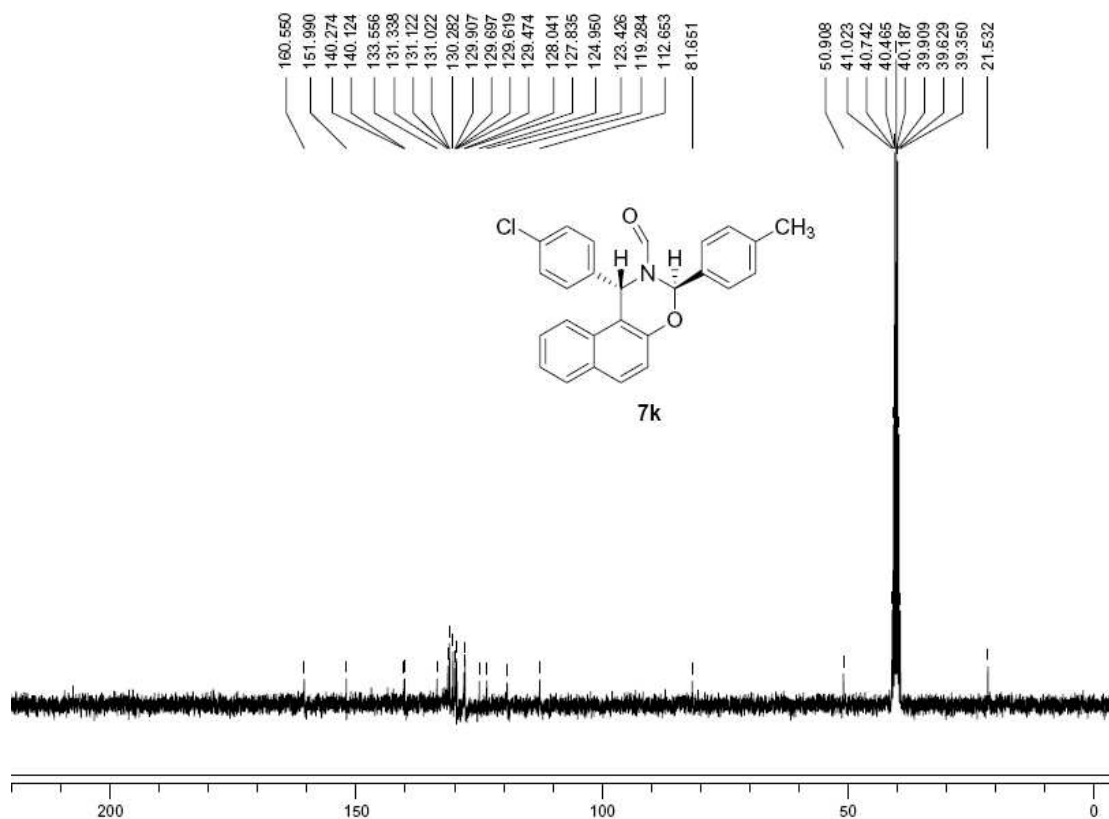


SUDA-TOFMS-EI-081024

rsf-A10 146 (2.433) Cm (146-(17.30+1158:1168))

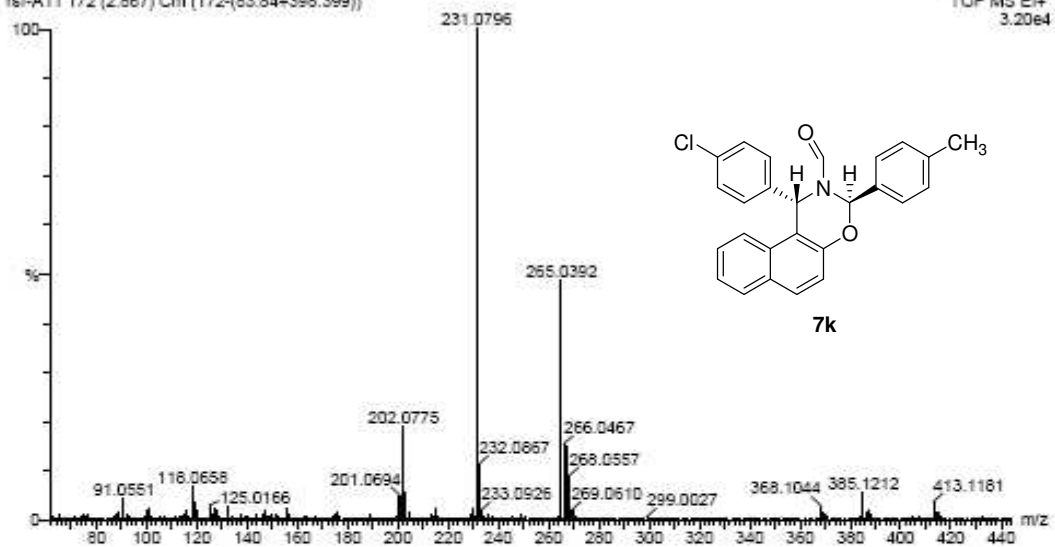
TOF MS EI+  
4.49e4



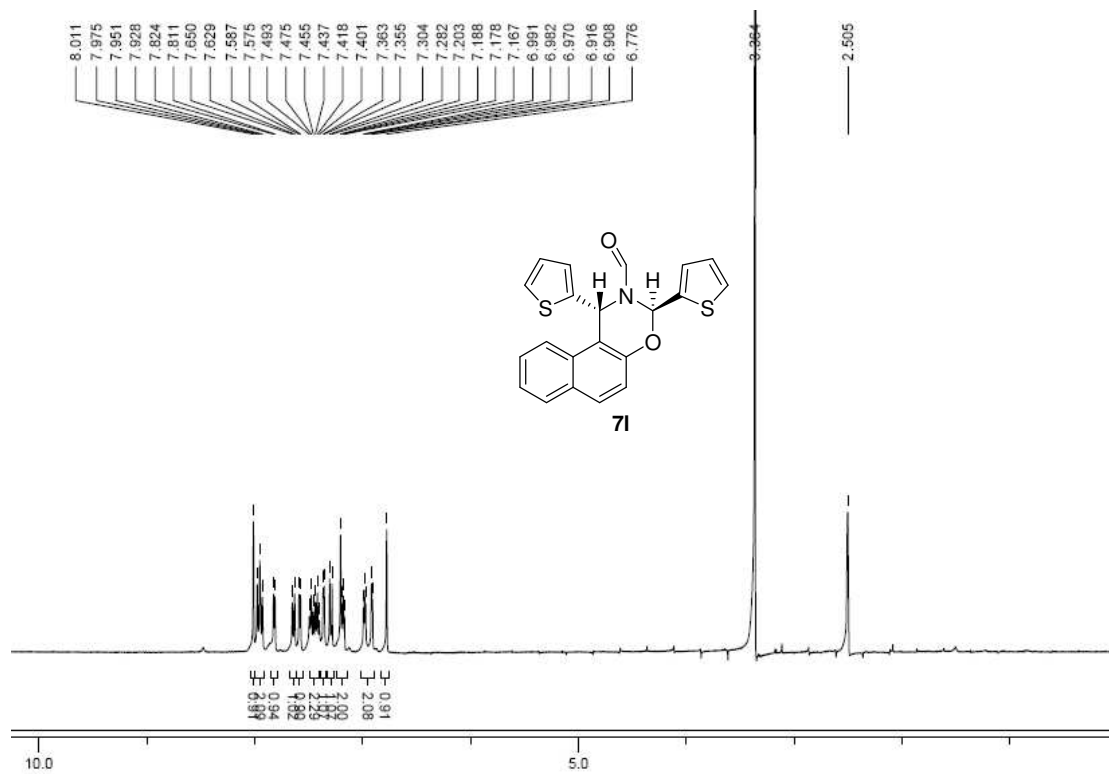


SUDA-TOFMS-EI-061024  
rsf-A11 172 (2.867) Cm (172-(83.84+398.399))

TOF MS EI+  
3.20e4



Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
	Minimum: 1.22						
	Maximum: 100.00						
		369.1046	3.2	8.6	16.5	2	C25 H18 O
		35C1					
385.1212	5.35	385.1232	-2.1	-5.6	16.0	1	C25 H20 N
		385.1172	3.9	10.1	16.5	2	O 35C1
		C26 H20 O					
		37C1					
387.1199	1.90	387.1204	-0.5	-1.3	16.0	1	C25 H20 N
							O 37C1
413.1181	3.46	413.1182	-0.2	-0.4	17.0	1	C26 H20 N
							O2 35C1
415.1159	1.23	415.1153	0.6	1.4	17.0	1	C26 H20 N
							O2 37C1



SUDA-TOFMS-EI-081024  
 ref-A12 136 (2.267) Cm (136-(10:12+215:216))

TOF MS EI+  
 4.29e4



Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
Minimum:	2.98					-1.5	
Maximum:	100.00					50.0	
221.0430	3.44	209.0391	3.0	14.2	15.5	1	C17 H5
		209.0459	-3.8	-16.0	5.5	3	C11 H13 S2
		221.0426	0.5	2.3	11.5	1	C15 H9 S
		221.0459	-2.9	-13.0	6.5	3	C12 H13 S2
		221.0391	3.9	17.5	16.5	2	C18 H5
237.0284	100.00	237.0232	0.2	0.8	7.0	2	C11 H11 N O 32
		237.0246	3.6	15.0	12.0	1	C14 H7 N O 3
238.0432	77.96	238.0419	1.3	5.6	16.0	1	C18 H6 O
		238.0452	-2.0	-8.6	11.0	2	C15 H10 O S
239.0466	7.71	239.0439	2.7	11.5	6.0	2	C11 H13 N O 32
		239.0497	-3.1	-12.9	15.5	1	C16 H7 O
		240.0575	-0.6	-2.6	15.0	1	C18 H5 O
		240.0609	-4.0	-16.6	10.0	2	C15 H12 O S
377.0544	2.99	377.0544	0.0	-0.1	15.0	1	C21 H15 N O2 S2