

## Supplementary Material

### ON WATER REACTIVITY AND REGIOSELECTIVITY OF QUINONES IN C-N COUPLING WITH AMINES

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## 1. General Information

Melting points were determined on a hot-stage apparatus and are uncorrected. The IR spectra were recorded on a FT-IR Bruker IFS 55 spectrophotometer from KBr discs; wave numbers are reported in  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were obtained from a Bruker DRX-300 spectrometer (300 and 75 MHz respectively) in  $\text{CDCl}_3$ . Chemical shifts were recorded in ppm ( $\delta$ ) relative to TMS as an internal standard. J-values are given in Hz. Electron impact (IE) high resolution mass spectra were recorded on a Thermo Finnigan model MAT 95XP Mass Spectrometer and Maldi-TOF (TOF) high-resolution mass spectrum were recorded on a Waters LCT Premier XE Mass Spectrometer.

## 2. Synthetic General Procedure

The reaction of quinone **I** with amine **IV<sub>a</sub>** was carried out using condition b. The reactions of quinones **I** and **II** with amines **IV<sub>a</sub>** and **V<sub>a</sub>** were carried out using conditions A and B, described below. The reactions of quinone **II** with amines **IV<sub>b</sub>** to **IV<sub>g</sub>** and **V<sub>b</sub>** to **V<sub>n</sub>** were carried out using conditions B. The synthesis of compounds **II**,<sup>1</sup> **VIII-IX**, **XI**,<sup>2</sup> **XVI-XIX**<sup>3</sup> have been previously described.

A) Dissolving reactants in methylene chloride and stirring at room temperature overnight.

B) Using water as the reaction medium and stirring at room temperature overnight.

## 3. Characterization of Compound and NMR spectra

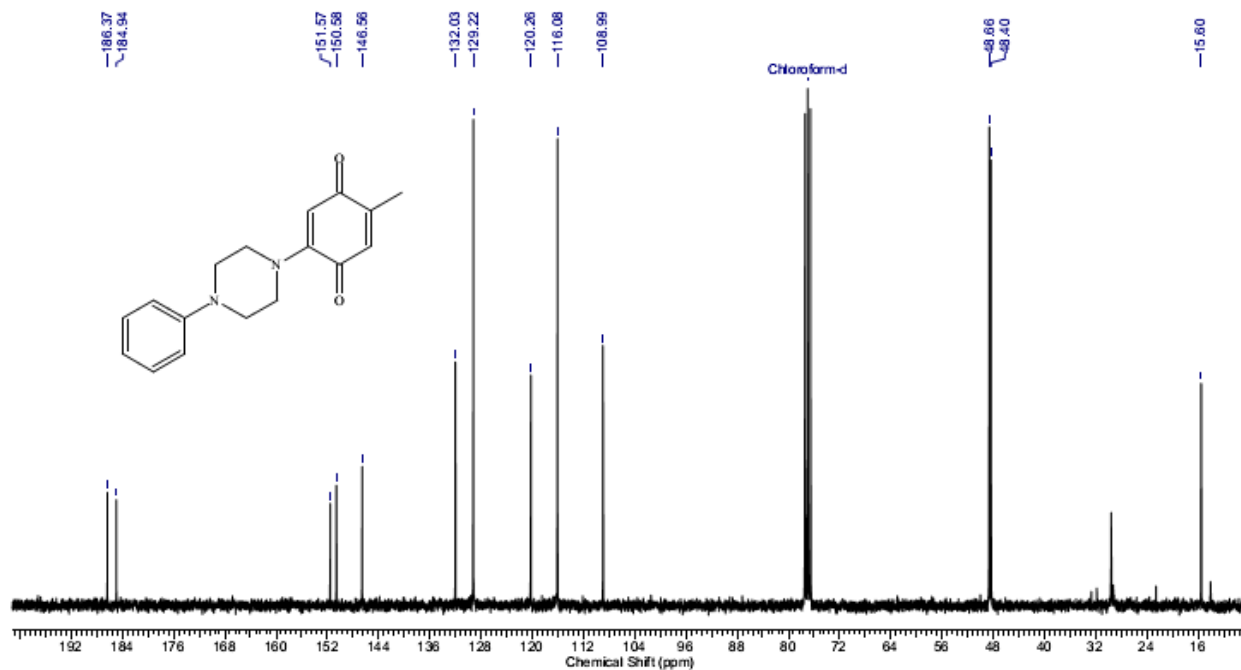
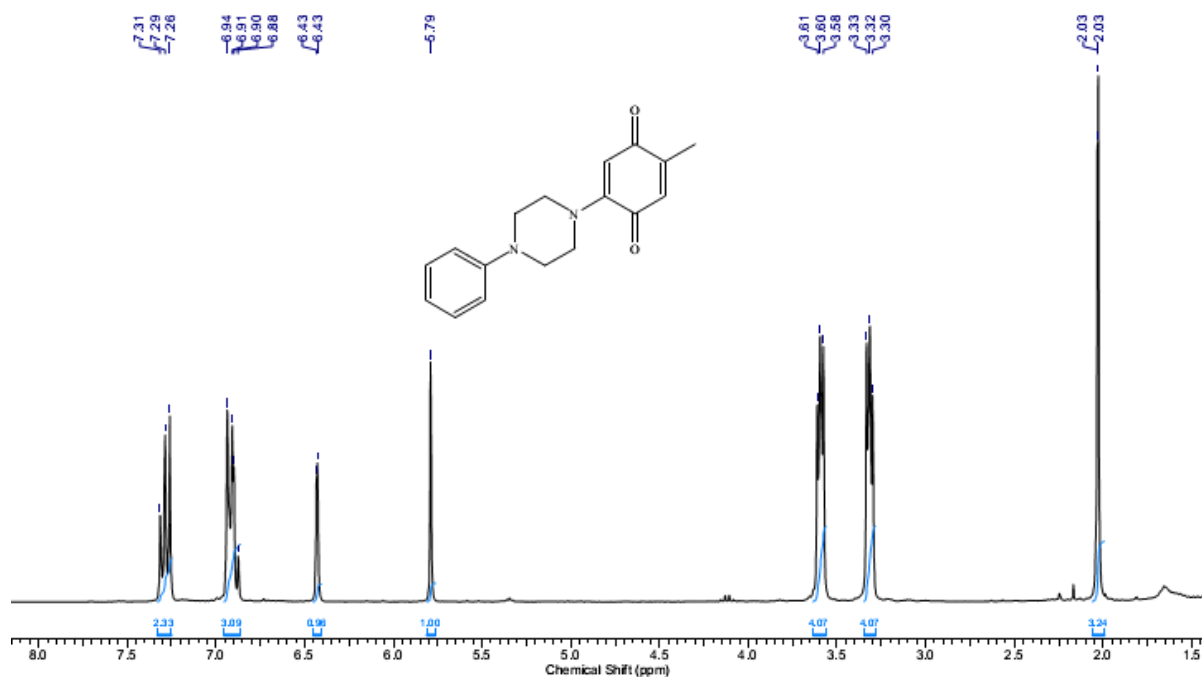
### 2-Methyl-5-(4-phenyl-piperazin-1-yl)-[1,4]benzoquinone (VI)

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[1] R. Araya-Maturana, B.K. Cassels, T. Delgado-Castro, J.A.Valderrama, B.E. Weiss-López, *Tetrahedron* **1999**, 55, 637.

[2] S.C. Srivastava, U. Hornemann, *Angew. Chem.* **1976**, 88, 87.

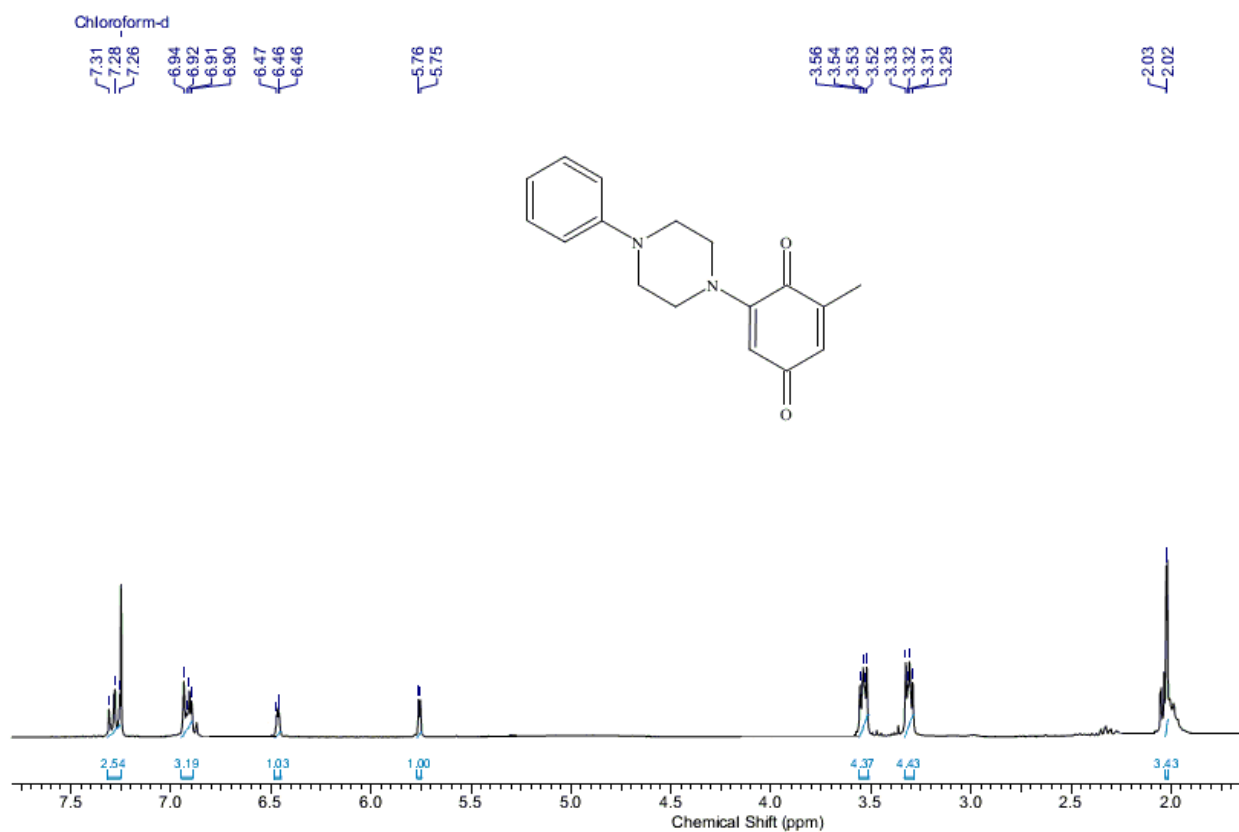
[3] J.A. Valderrama, J.A. Ibacache, V. arancibia, J. Rodriguez, C. Theoduloz, *Bioorg. Med. Chem.* 2009, 2894.

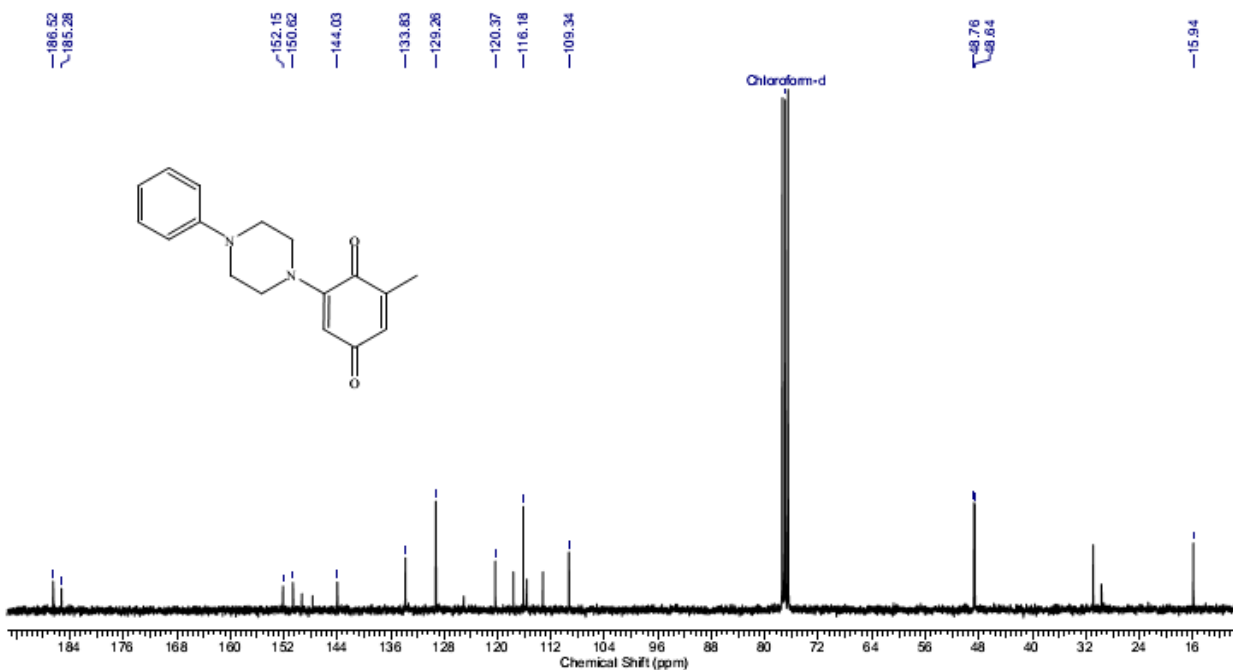


Red powder; mp 107-109 °C;  $\nu_{\max}$ (KBr)/cm<sup>-1</sup> 762(C-H<sub>ar</sub>), 1024(C-N), 1643(C=O); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 2.03 (d, 3H,  $J$  = 1.3 Hz), 3.32 (t, 4H,  $J$  = 5.3 Hz), 3.60 (t, 4H,  $J$  = 5.4 Hz), 5.79 (s, 1H), 6.43 (d, 1H,  $J$  = 1.5 Hz), 6.89 (d, 1H,  $J$  = 7.3 Hz), 6.93 (d, 2H,  $J$  = 8.5 Hz), 7.29 (t, 2H,  $J$  = 7.9 Hz), <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 15.60, 48.40, 48.66, 108.99, 116.08, 120.26,

129.22, 132.03, 146.56, 150.58, 151.57, 184.94, 186.37; m/z (TOF) calcd. for  $C_{17}H_{18}N_2O_2H^+$  283.1447, found 283.1441.

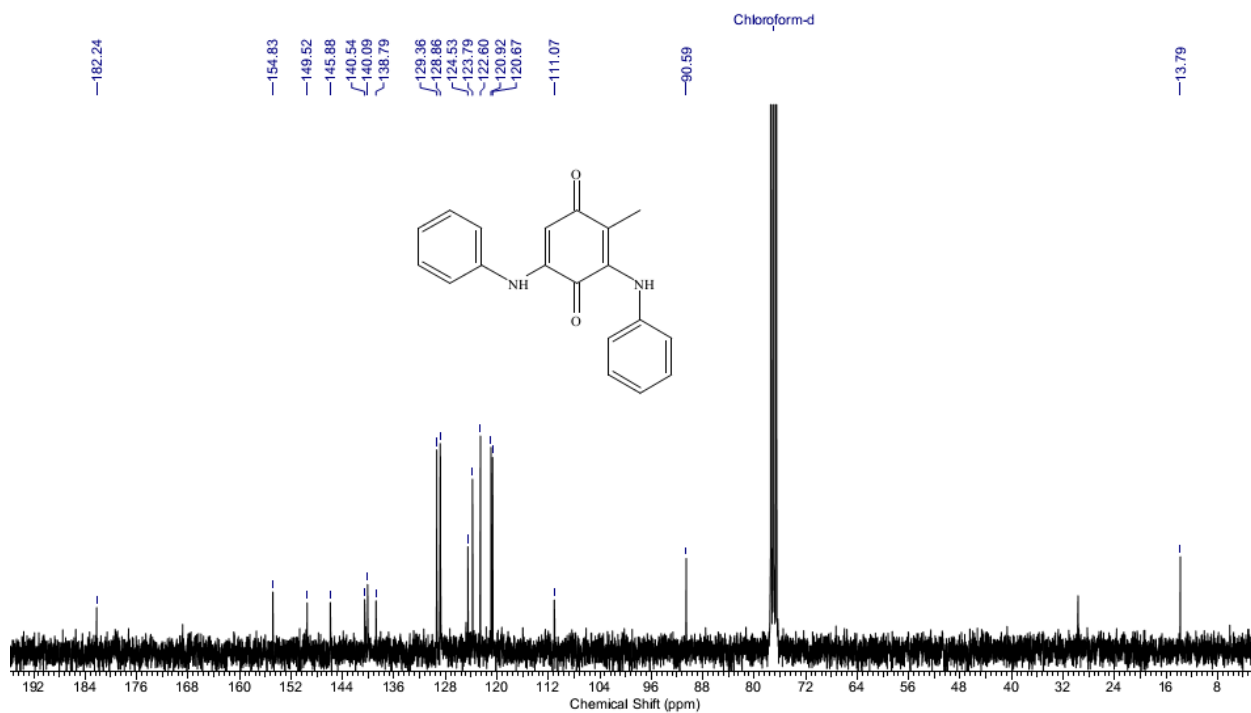
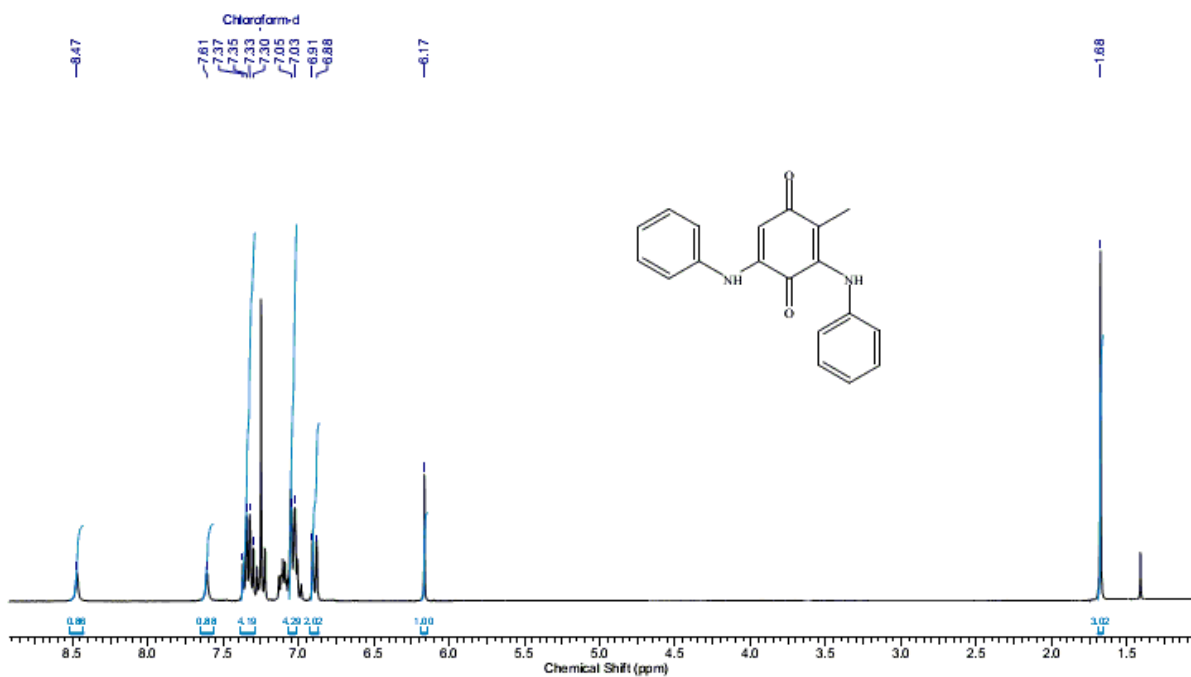
## 2-Methyl-6-(4-phenyl-piperazin-1-yl)-[1,4]benzoquinone (VII)





Red powder; mp 65-67 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  747(C-H<sub>ar</sub>), 1024(C-N), 1645(C=O);  $^1\text{H}$  NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta\text{H}$  2.03 (d, 3H,  $J = 1.6$  Hz); 3.31 (q, 4H,  $J = 5.0$  Hz, 7.1 Hz); 3.53 (q, 4H,  $J = 5.0$  Hz, 6.9 Hz); 5.76 (d, 1H,  $J = 2.5$  Hz); 6.47 (q, 1H,  $J = 7.3$  Hz, 9.8 Hz); 6.92 (m, 3H); 7.28 (q, 2H,  $J = 7.5$  Hz, 8.9 Hz);  $^{13}\text{C}$  NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta\text{C}$  15.94, 48.64, 48.76, 109.34, 116.18, 120.37, 129.26, 133.83, 144.03, 150.6, 152.15, 185.28, 186.52;  $m/z$  (TOF) calcd. for C<sub>17</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>H<sup>+</sup> 283.1447, found 283.1444.

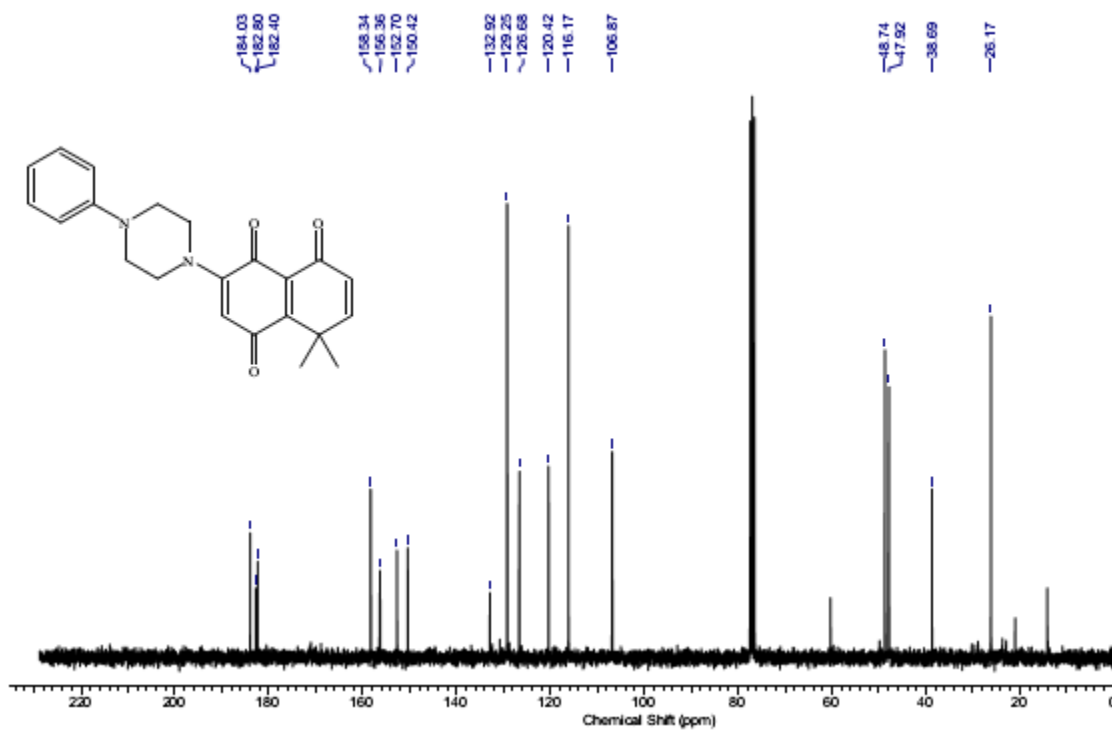
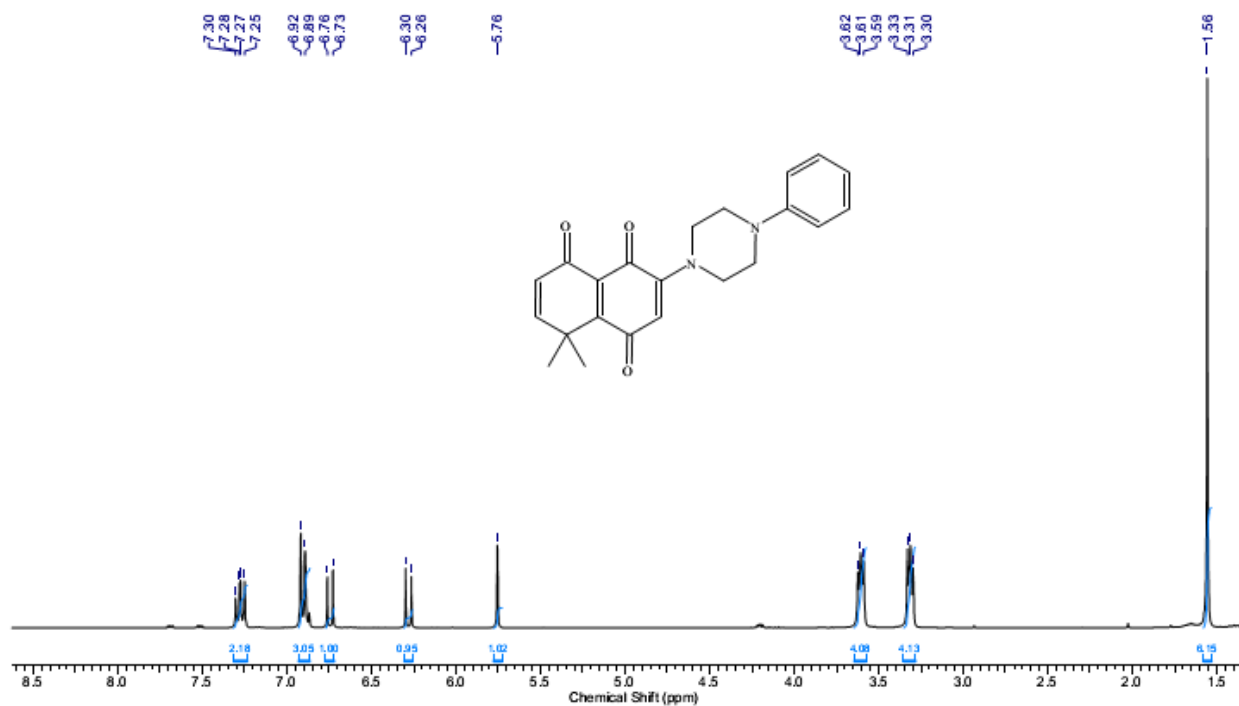
### 3,5-Dianilino-2-methylbenzo-1,4-quinone (X)



Red powder; mp 123-125 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  751(C-H<sub>ar</sub>), 1573(C=O), 3438(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 2.04 (s, 3H,  $J = 1.2$  Hz), 6.17 (s, 1H), 6.90 (dd, 2H,  $J = 1.1$  Hz, 8.4 Hz), 7.04 (m, 4H), 7.34 (m, 4H), 7.61 (s, 1H), 8.47 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 13.79, 90.59, 111.07, 120.67, 120.92, 122.60, 123.79, 124.53, 128.75, 128.86, 129.36, 138.79, 140.09, 140.54, 145.88, 149.52, 154.83, 182.24; m/z (TOF) calcd. for C<sub>19</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>H<sup>+</sup> 305.1290, found 305.1293.

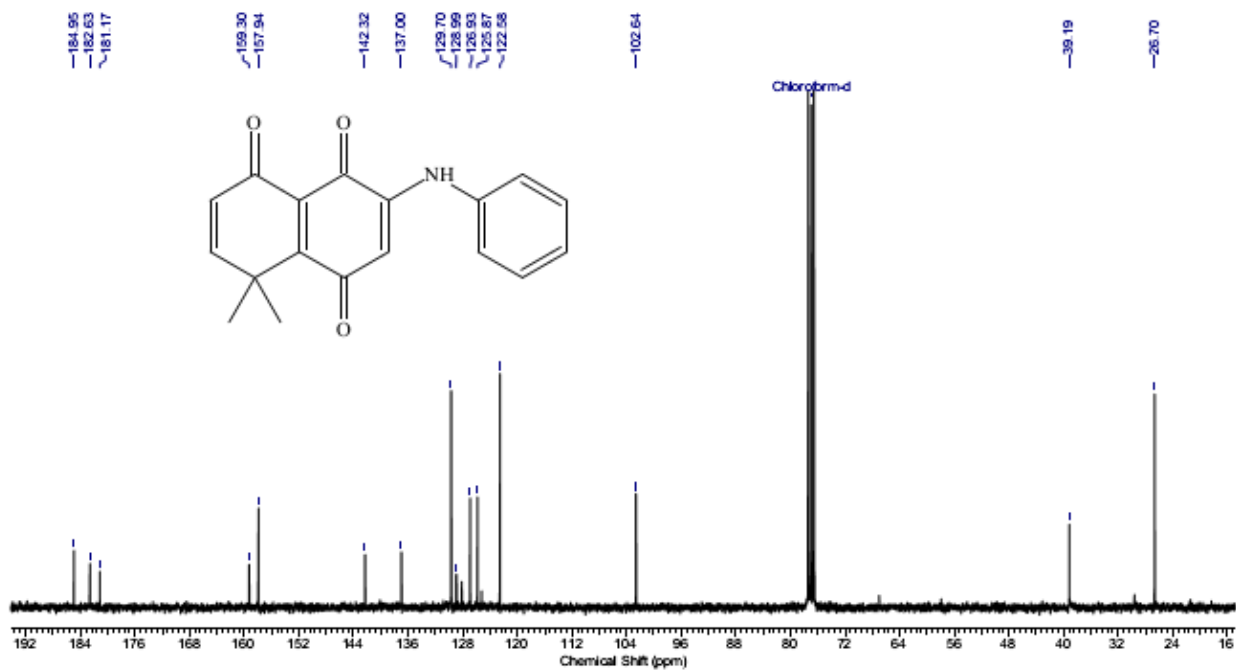
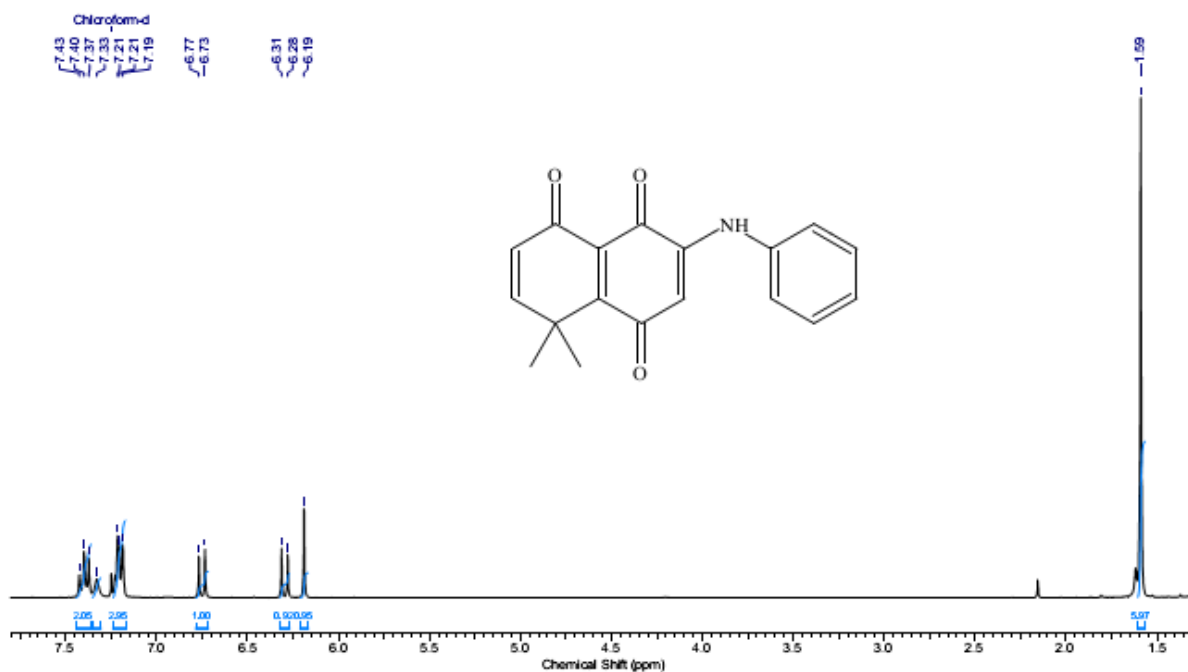


# 8,8-Dimethyl-3-(4-phenylpiperazin-1-yl)naphthalene-1,4,5(8H)-trione (XII)



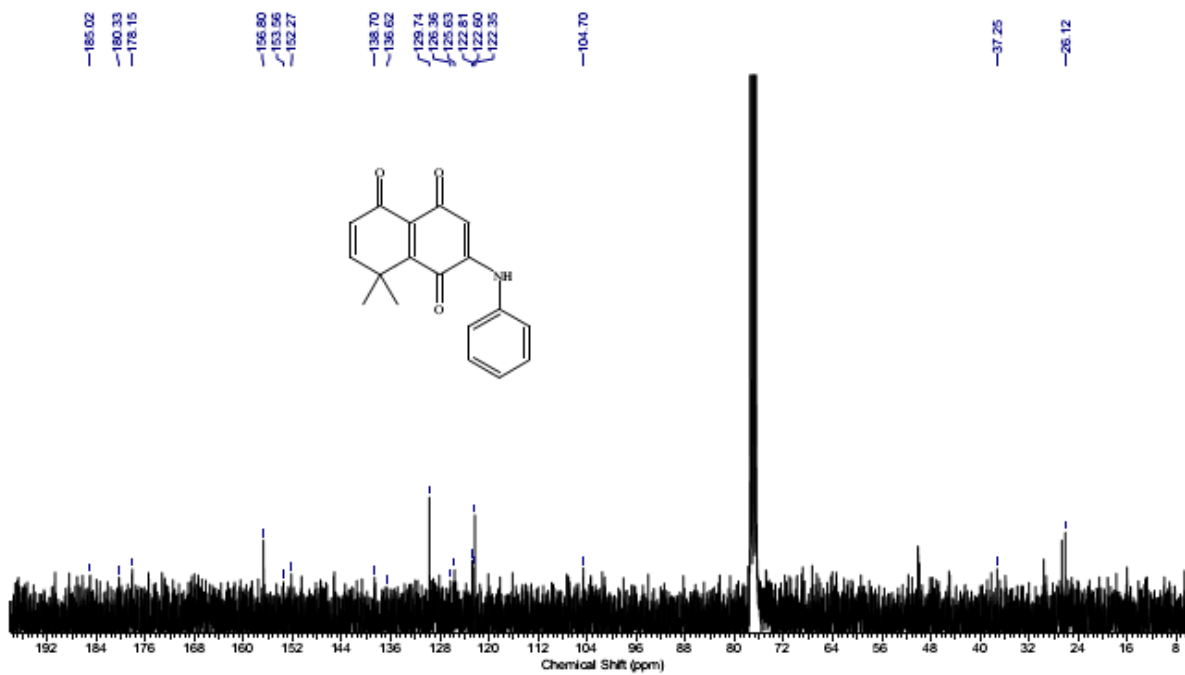
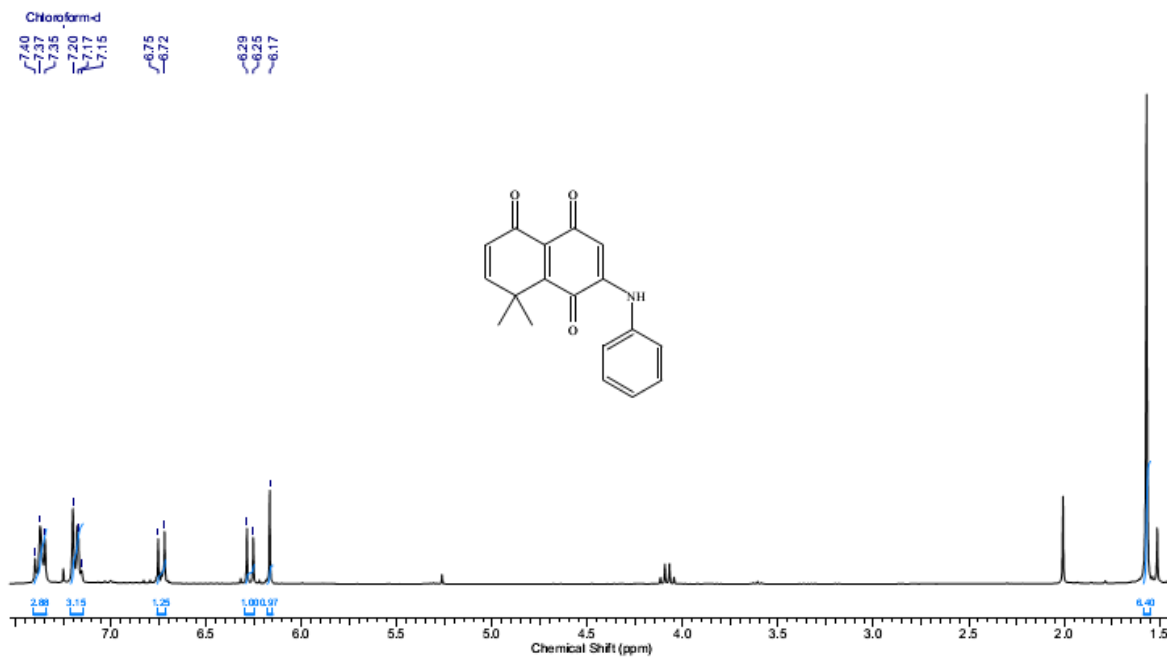
Red powder; mp 144-145 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  748(C-H<sub>ar</sub>), 1233(C-N), 1694(C=O); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.50 (s, 6H), 3.26 (t, 4H,  $J = 4.9$ ), 3.55 (t, 4H,  $J = 5.3$ ), 5.70 (s, 1H), 6.23 (d, 1H,  $J = 10.2$  Hz), 6.69 (d, 1H,  $J = 10.2$  Hz), 6.85 (t, 3H,  $J = 7.4$  Hz), 7.22 (q, 2H,  $J = 7.3$  Hz,  $J = 9.1$  Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.17, 38.69, 47.92, 48.74, 106.87, 116.17, 120.42, 126.68, 129.25, 132.92, 150.42, 152.70, 156.36, 158.34, 182.80, 184.03;  $m/z$  (TOF) calcd. for C<sub>22</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub>Na<sup>+</sup> 385.1528, found 385.1526. Regiochemistry of compound 12 was assigned by 2D-NMR (HMBC, HSQC).

### 3-Anilino-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XIV)



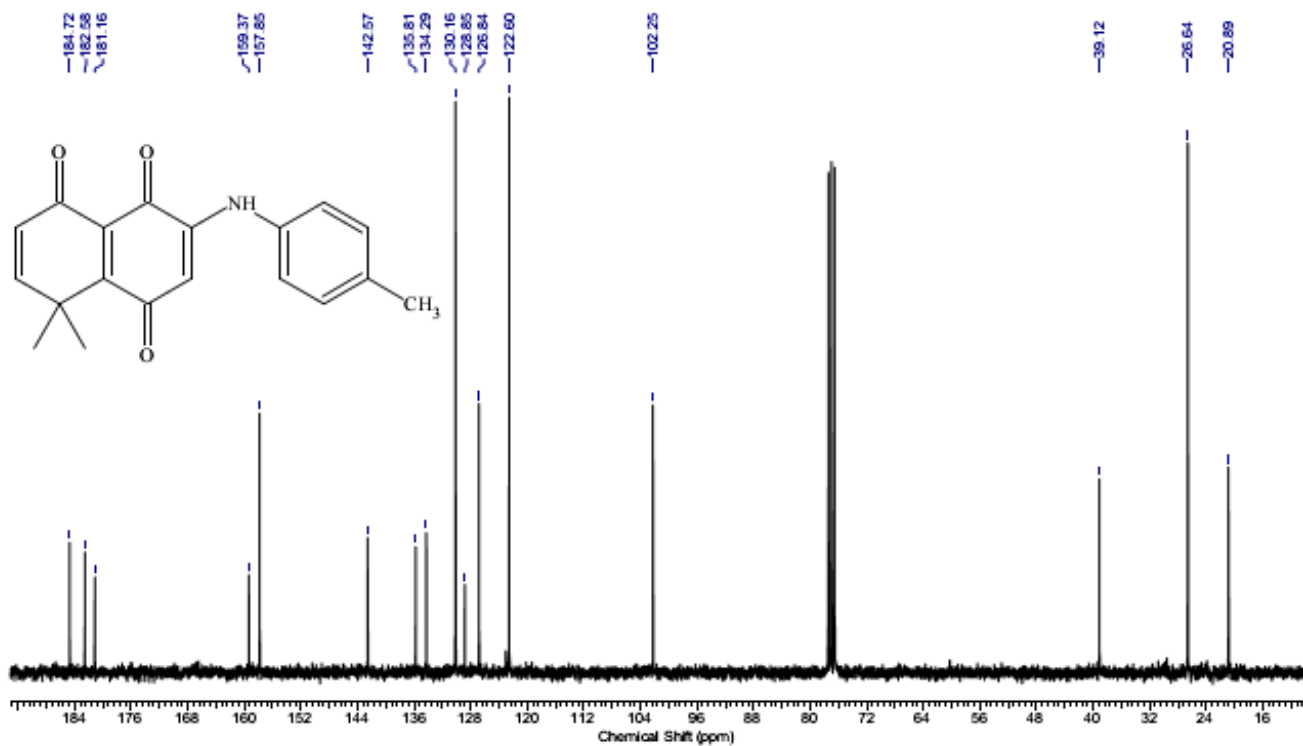
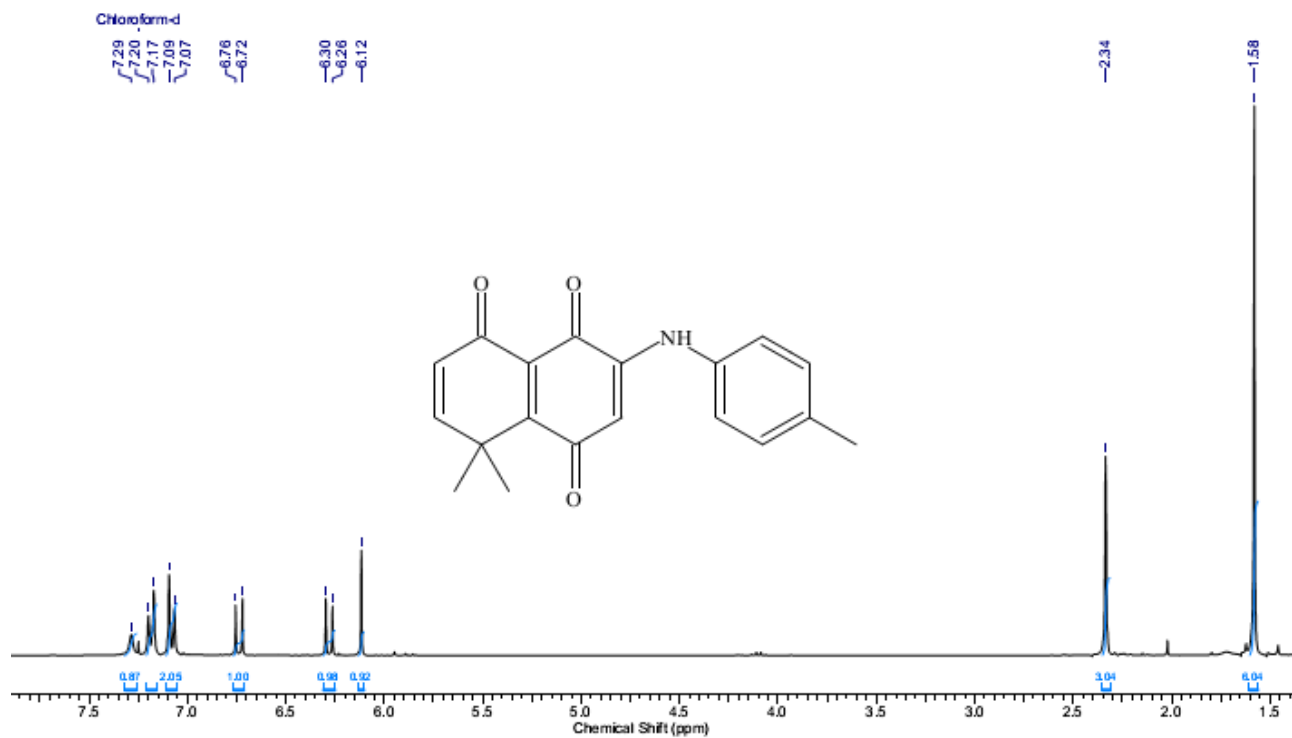
Red powder; mp 158-160 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  832(C-H<sub>ar</sub>), 1699(C=O), 3250(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.59 (s, 6H), 6.19 (s, 1H), 6.30 (d, 1H,  $J = 10.0$  Hz), 6.76 (d, 1H,  $J = 10.1$  Hz), 7.21 (q, 3H,  $J = 6.4$  Hz, 8.3 Hz), 7.33 (s, 1H), 7.40 (t, 2H,  $J = 8.1$  Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.70, 30.19, 102.64, 122.58, 125.87, 126.93, 128.99, 129.70, 137.00, 142.32, 157.94, 159.30, 181.17, 182.63, 184.95; m/z (TOF) calcd. for C<sub>18</sub>H<sub>15</sub>NO<sub>3</sub>Na<sup>+</sup> 316.0950, found 316.0965. Regiochemistry of compound **14** was assigned by 2D-NMR (HMBC, HSQC).

## 2-Anilino-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XV)



Red powder; mp 129-131 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  762(C-H<sub>ar</sub>), 1690(C=O), 3314(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.57 (s, 6H), 6.17 (s, 1H), 6.35 (d, 1H,  $J = 10.1$  Hz), 6.75 (d, 1H,  $J = 10.1$  Hz), 7.19 (m, 3H), 7.33 (s, 1H), 7.40 (t, 2H,  $J = 7.9$  Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.12, 37.25, 104.70, 122.35, 122.60, 122.81, 125.63, 126.36, 129.74, 136.62, 138.70, 152.27, 153.56, 156.80, 178.15, 180.33, 185.02; m/z (TOF) calcd. for C<sub>18</sub>H<sub>15</sub>NO<sub>3</sub>H<sup>+</sup> 294.1127, found 294.1130.

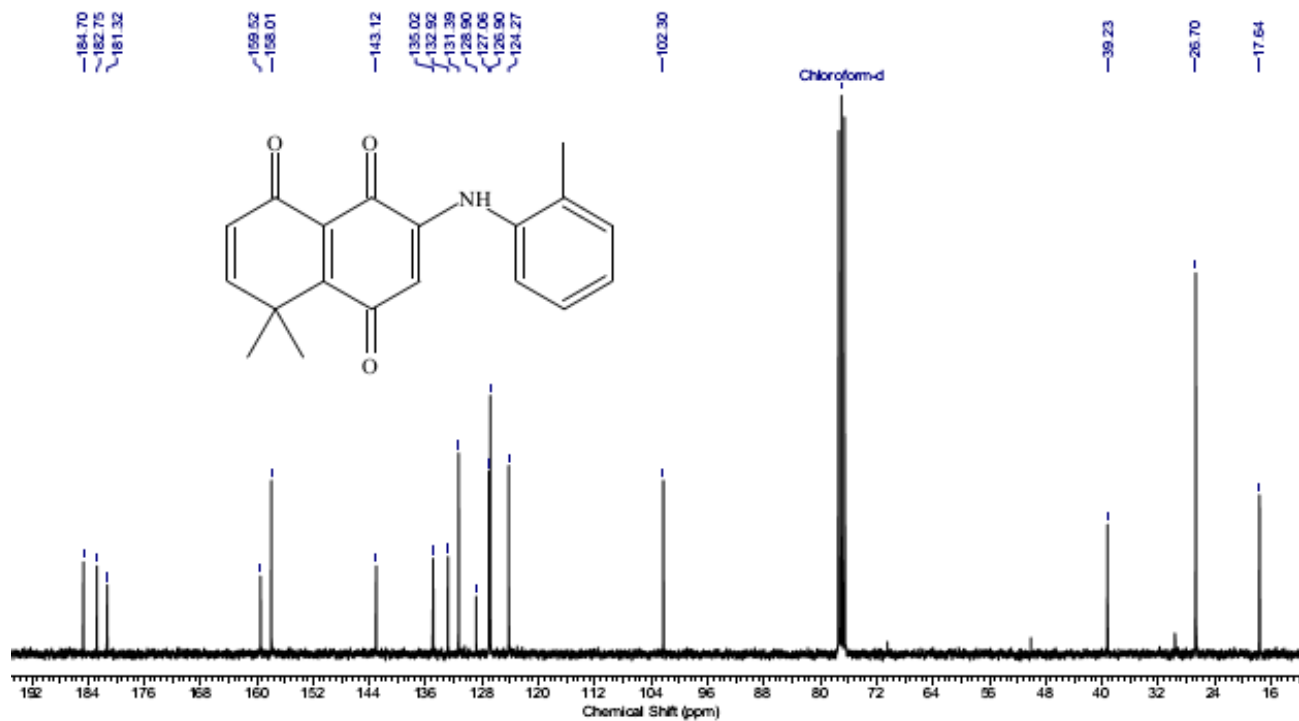
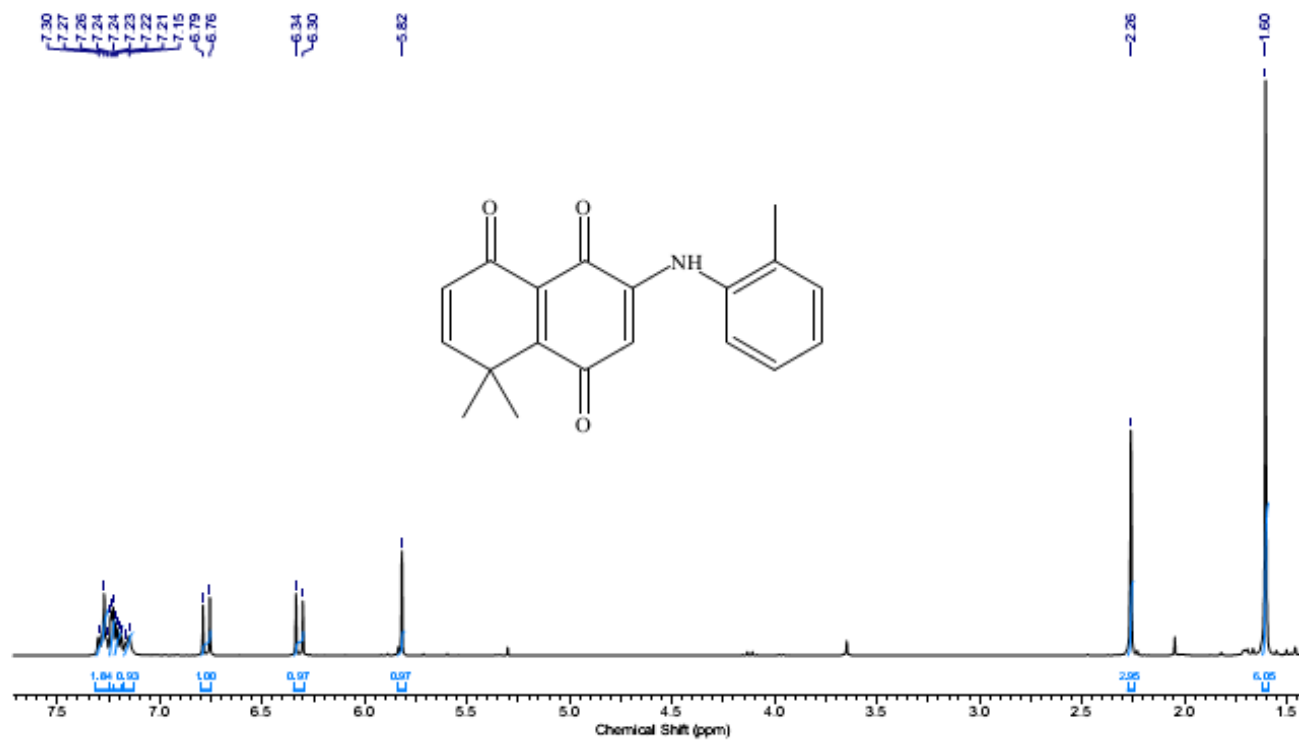
### 3-(p-Toluidino)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXa)



Red powder; mp 152-153 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  781(C-H<sub>ar</sub>), 1601(C=O), 3243(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.58 (s, 6H), 2.34 (s, 3H), 6.12 (s, 1H), 6.28 (d, 1H, *J* = 10.2 Hz), 6.74 (d, 1H, *J* = 10.2 Hz), 7.08 (d, 2H, *J* = 8.3 Hz), 7.19 (d, 2H, *J* = 8.2 Hz), 7.29 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 20.89, 26.64, 39.12, 102.25, 122.60, 126.84, 130.16, 134.29, 135.81, 142.57, 157.85, 159.37, 181.16, 182.58, 184.72; *m/z* (TOF) calcd. for C<sub>19</sub>H<sub>17</sub>NO<sub>3</sub>Na<sup>+</sup> 330.1105, found 330.1107.

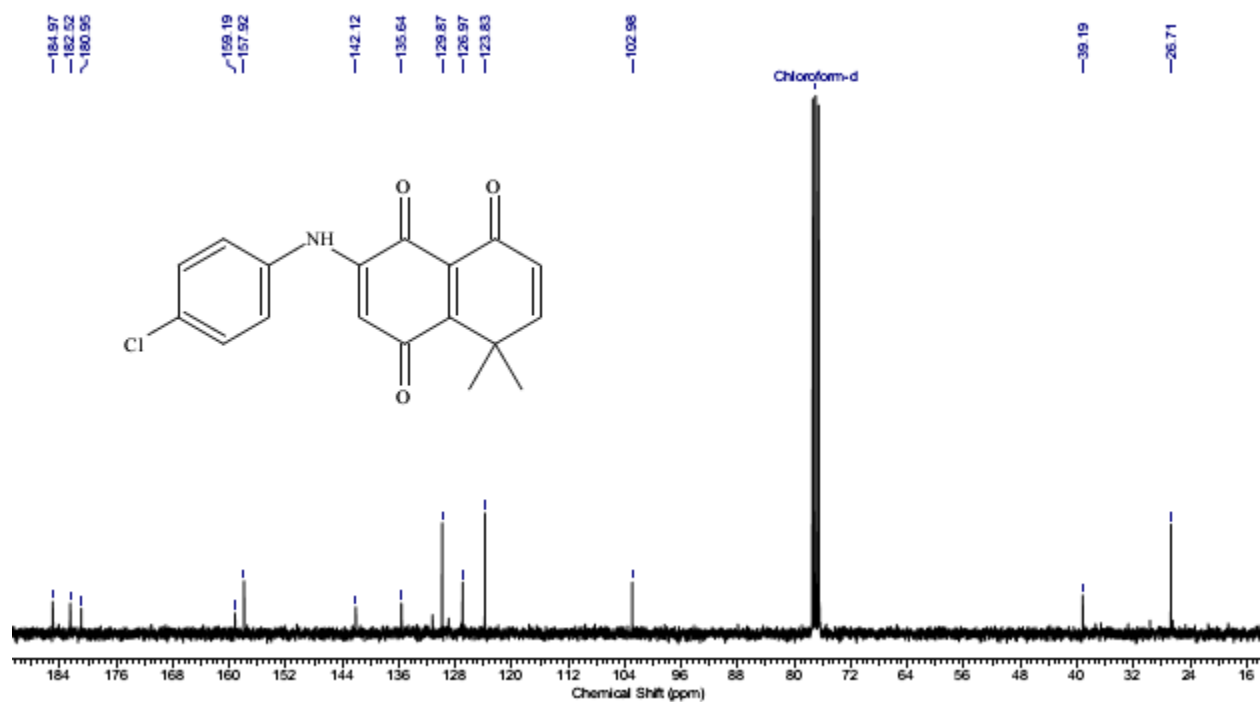
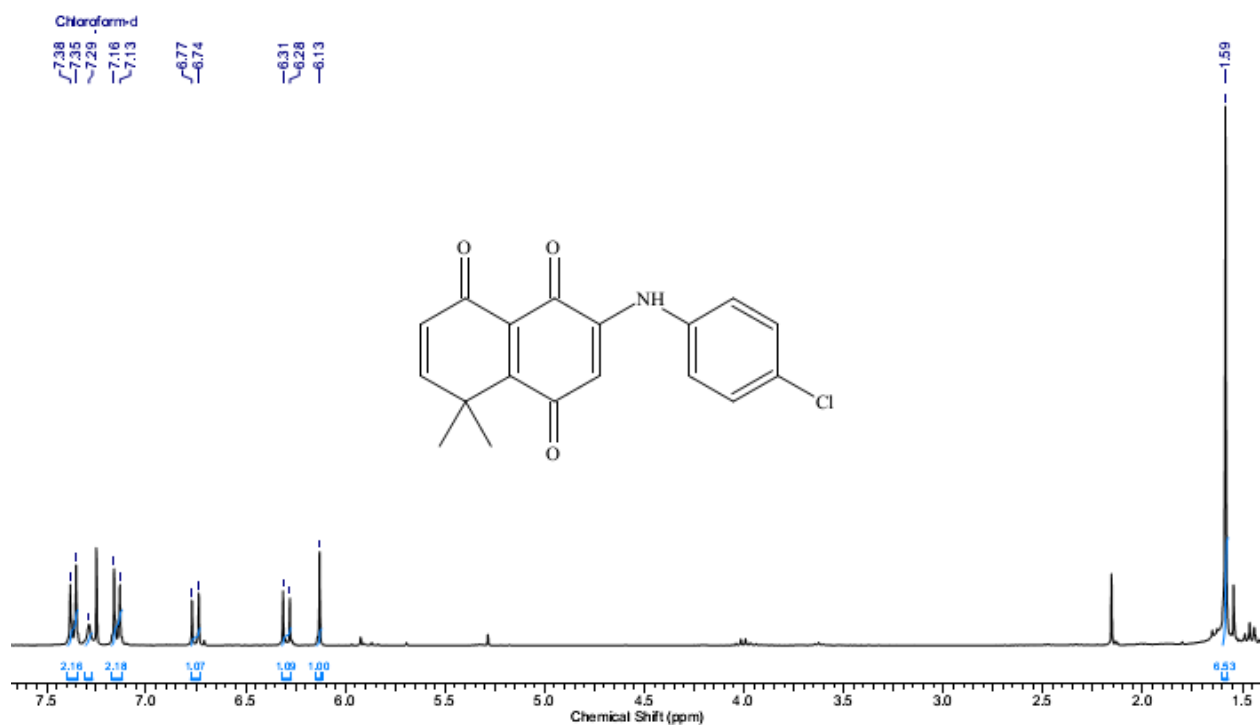


### 3-(o-Toluidino)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXb)



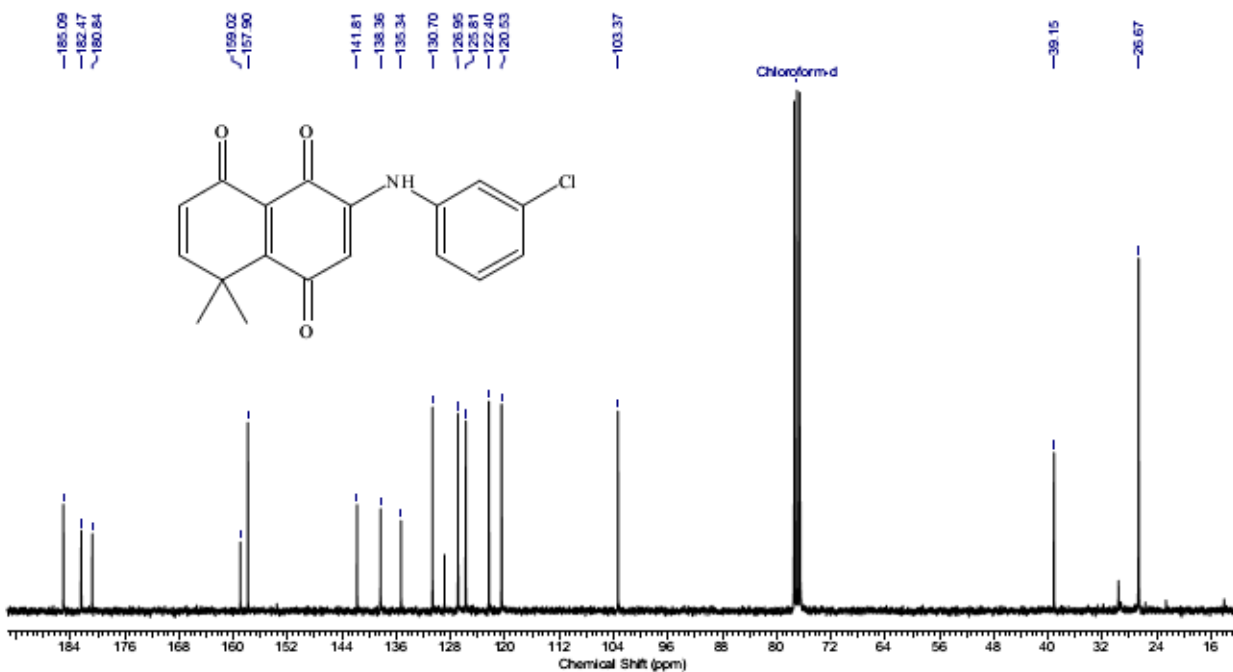
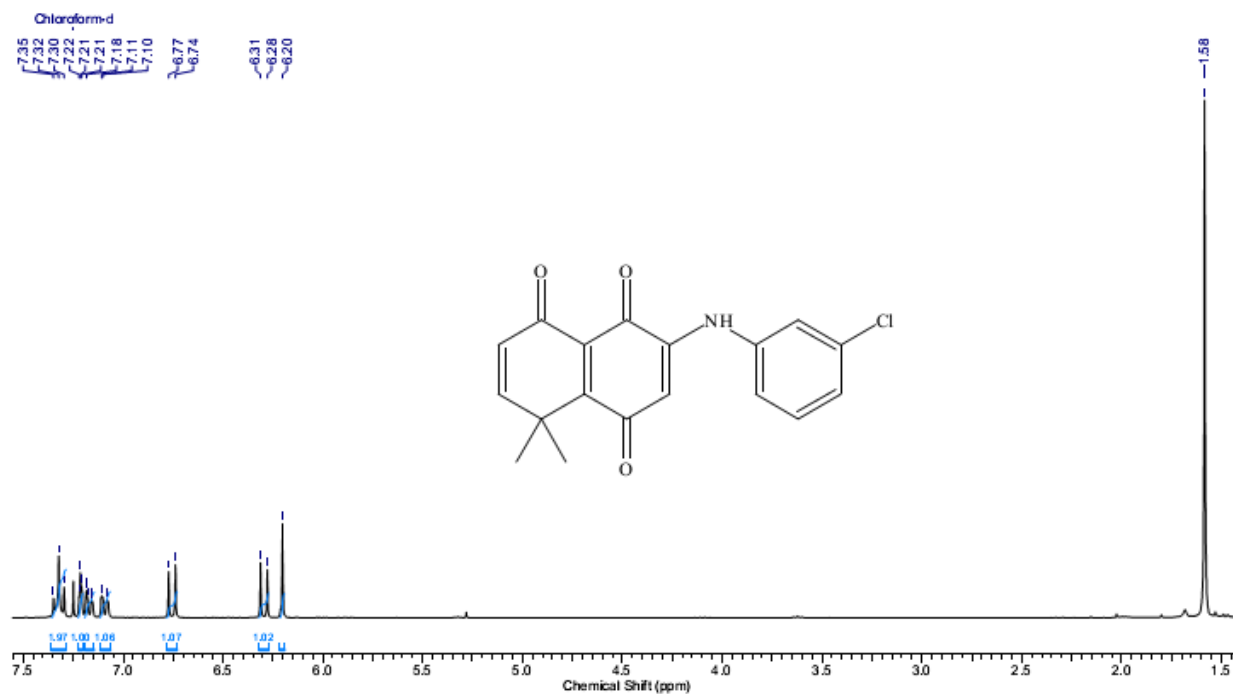
Red powder; mp 145-147 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  834(C-H<sub>ar</sub>), 1610(C=O), 3318(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.60 (s, 6H); 2.26 (s, 3H); 5.82 (s, 1H); 6.32 (d, 1H, *J* = 10.1 Hz); 6.78 (d, 1H, *J* = 10.1 Hz); 7.16 (t, 1H, *J* = 3.8 Hz); 7.21 (dd, 1H, *J* = 2.2 Hz, 6.7 Hz); 7.24 (t, 1H, *J* = 1.9 Hz); 7.28 (m, 2H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 17.64, 26.70, 39.23, 102.30, 124.27, 126.90, 127.06, 128.90, 131.39, 132.92, 135.02, 143.12, 158.01, 159.52, 181.32, 182.75, 182.75, 184.70. *m/z* (IE) calcd. for C<sub>19</sub>H<sub>17</sub>NO<sub>3</sub> 307.12084, found 307.12063.

### 3-(p-Chlorophenylamino)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXc)



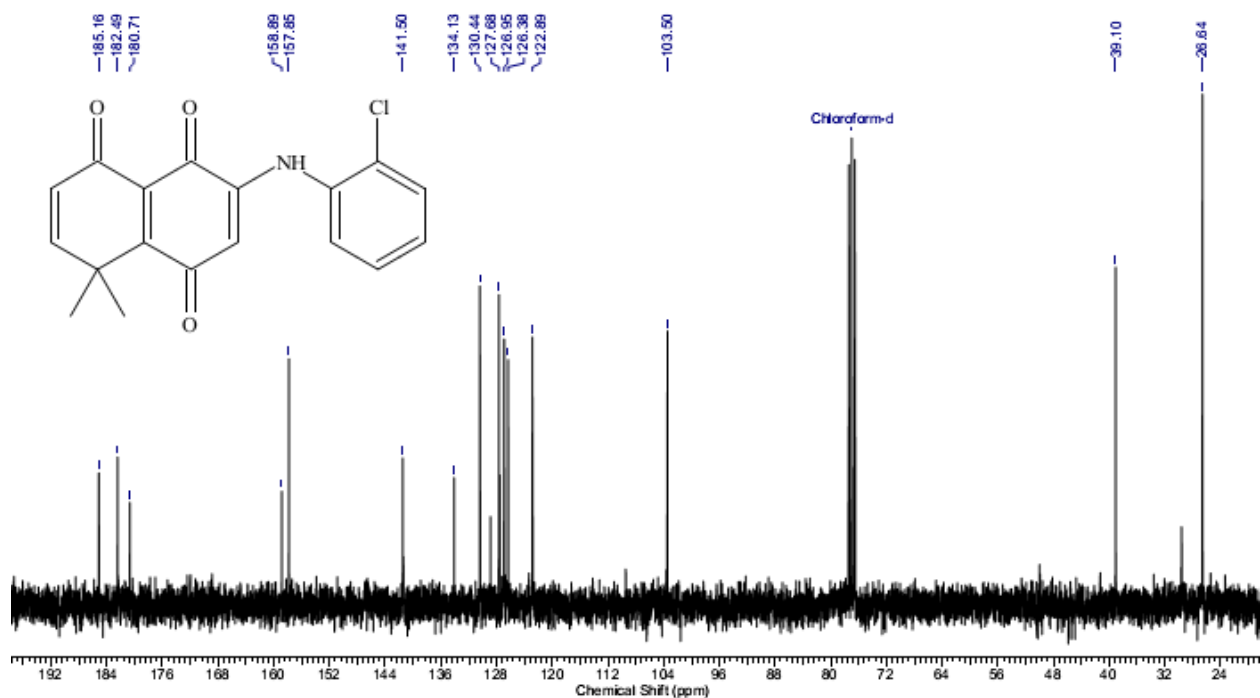
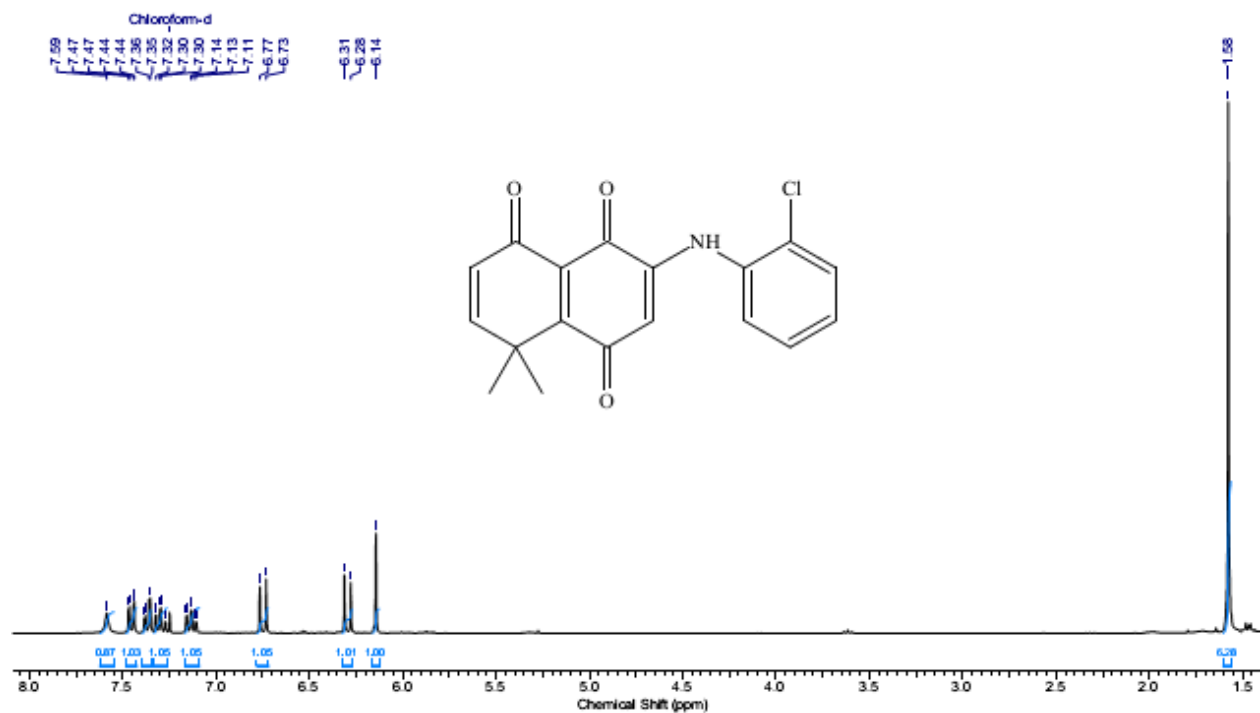
Red powder; mp 151-153 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  827(C-H<sub>ar</sub>), 1697(C=O), 3261(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.59 (s, 6H), 6.13 (s, 1H), 6.30 (d, 1H,  $J = 10.1$  Hz), 6.75 (d, 1H,  $J = 10.1$  Hz), 7.14 (d, 2H,  $J = 8.8$  Hz), 7.29 (s, 1H), 7.56 (d, 2H,  $J = 8.8$  Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.71, 39.19, 102.98, 123.83, 126.97, 135.64, 142.12, 157.92, 159.19, 180.95, 182.52, 184.97; m/z (IE) calcd. for C<sub>18</sub>H<sub>14</sub>ClNO<sub>3</sub> 327.0662, found 327.0664.

### 3-(m-Chlorophenylamino)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXd)



Red powder; mp 130-131 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  684(C-H<sub>ar</sub>), 1694(C=O), 3245(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.58 (s, 6H), 6.20 (s, 1H), 6.30 (d, 1H,  $J = 10.1$  Hz), 6.76 (d, 1H,  $J = 10.1$  Hz), 7.09 (dd, 1H,  $J = 1.1$  Hz, 8.1 Hz), 7.17 (dd, 1H,  $J = 1.8$  Hz,  $J = 7.1$  Hz), 7.21 (t, 1H,  $J = 1.9$  Hz), 7.32 (t, 2H,  $J = 8.1$  Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.67, 39.15, 103.37, 120.53, 122.40, 125.81, 122.40, 125.81, 126.95, 130.70, 135.34, 138.36, 141.81, 157.90, 159.02, 180.84, 182.47, 185.09; m/z (IE) calcd. for C<sub>18</sub>H<sub>14</sub>ClNO<sub>3</sub> 327.0662, found 327.0660.

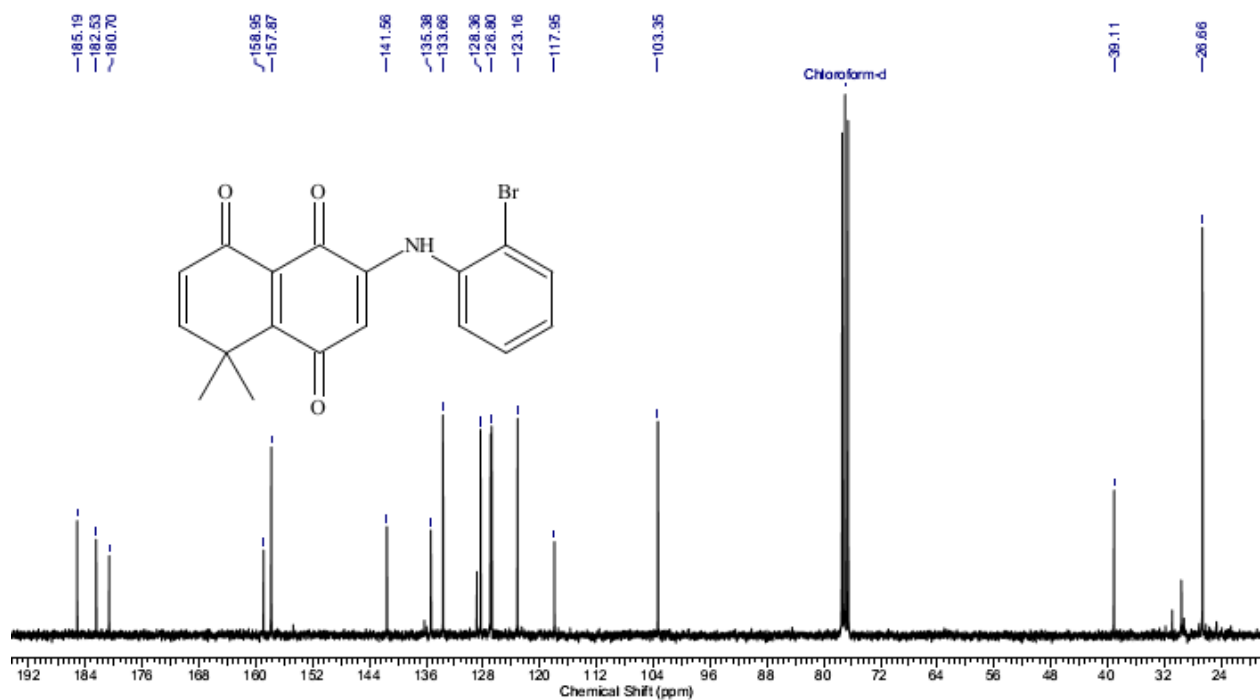
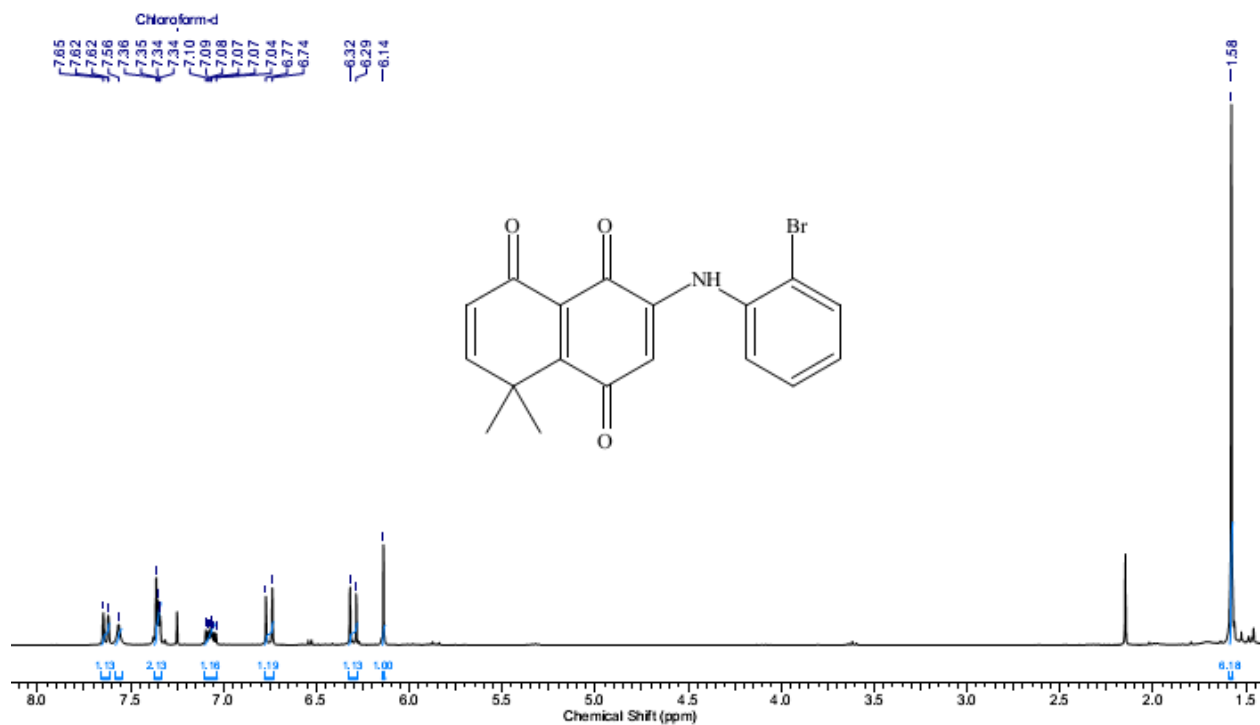
### 3-(o-Chlorophenylamino)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXe)



Red powder; mp 101-103 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  690(C-H<sub>ar</sub>), 1682(C=O), 3115(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.58 (s, 6H), 6.14 (s, 1H), 6.30 (d, 1H, *J* = 10.2 Hz), 6.75 (d, 1H, *J* = 10.1 Hz), 7.14 (td, 1H, *J* = 1.6 Hz, 7.6 Hz), 7.30 (td, 1H, *J* = 1.3 Hz, 8.2 Hz), 7.37 (dd, 1H, *J* = 1.6 Hz, 8.0 Hz), 7.46 (dd, 1H, *J* = 1.3 Hz, 7.9 Hz), 7.59 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.64, 39.10, 103.50, 122.89, 126.38, 126.95, 127.68, 130.44, 134.13, 141.50, 157.85, 158.89, 180.71, 182.49, 185.16; *m/z* (TOF) calcd. for C<sub>18</sub>H<sub>14</sub>ClNO<sub>3</sub>H<sup>+</sup> 328.0740 found 328.0737.

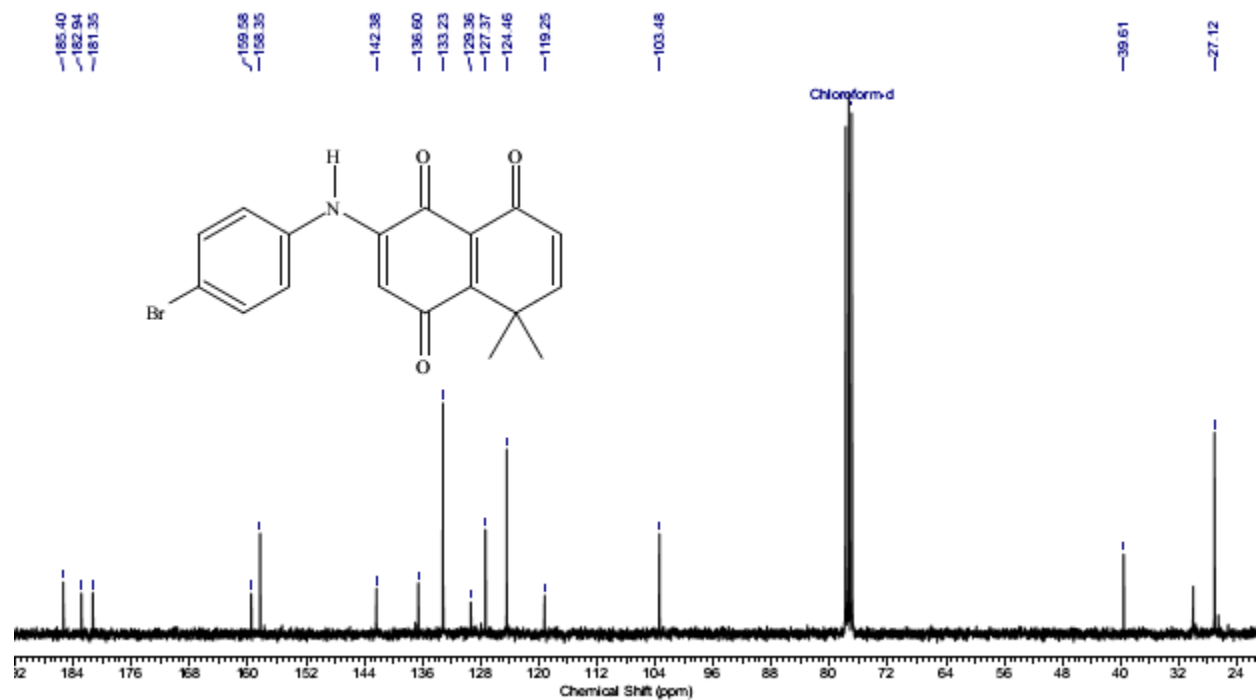
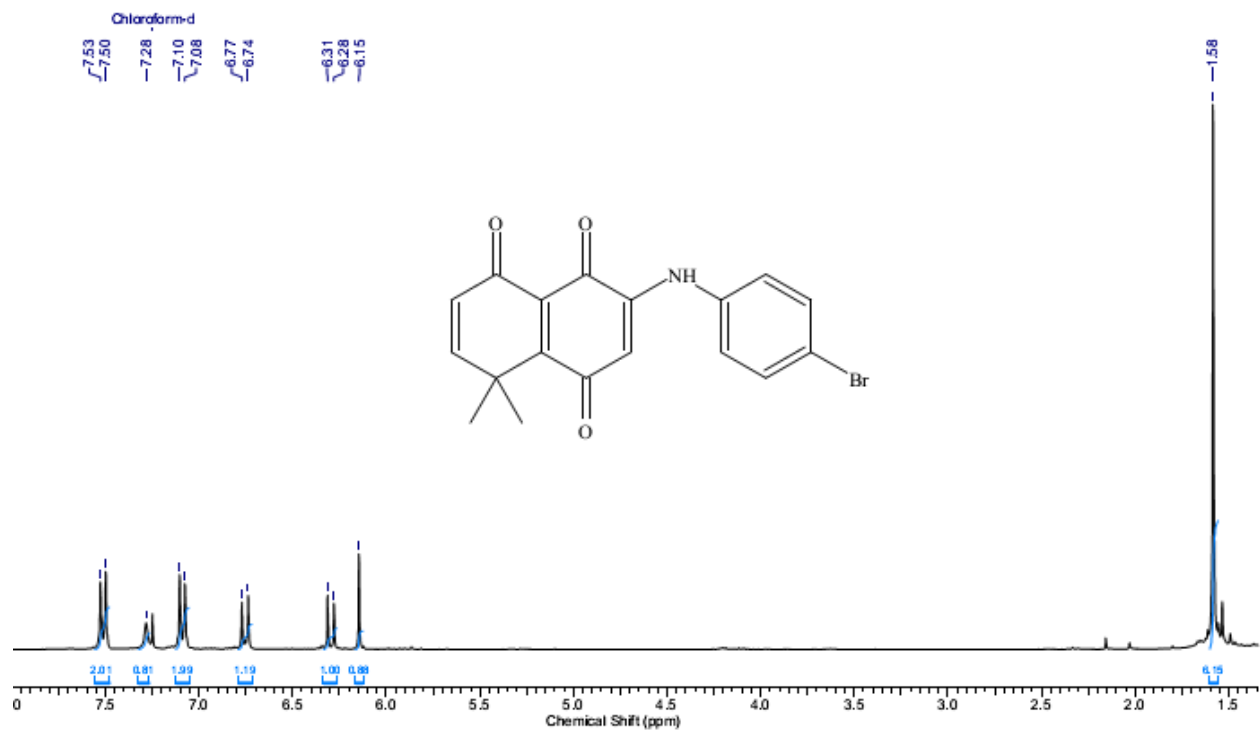


### 3-(o-Bromophenylamino)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXf)



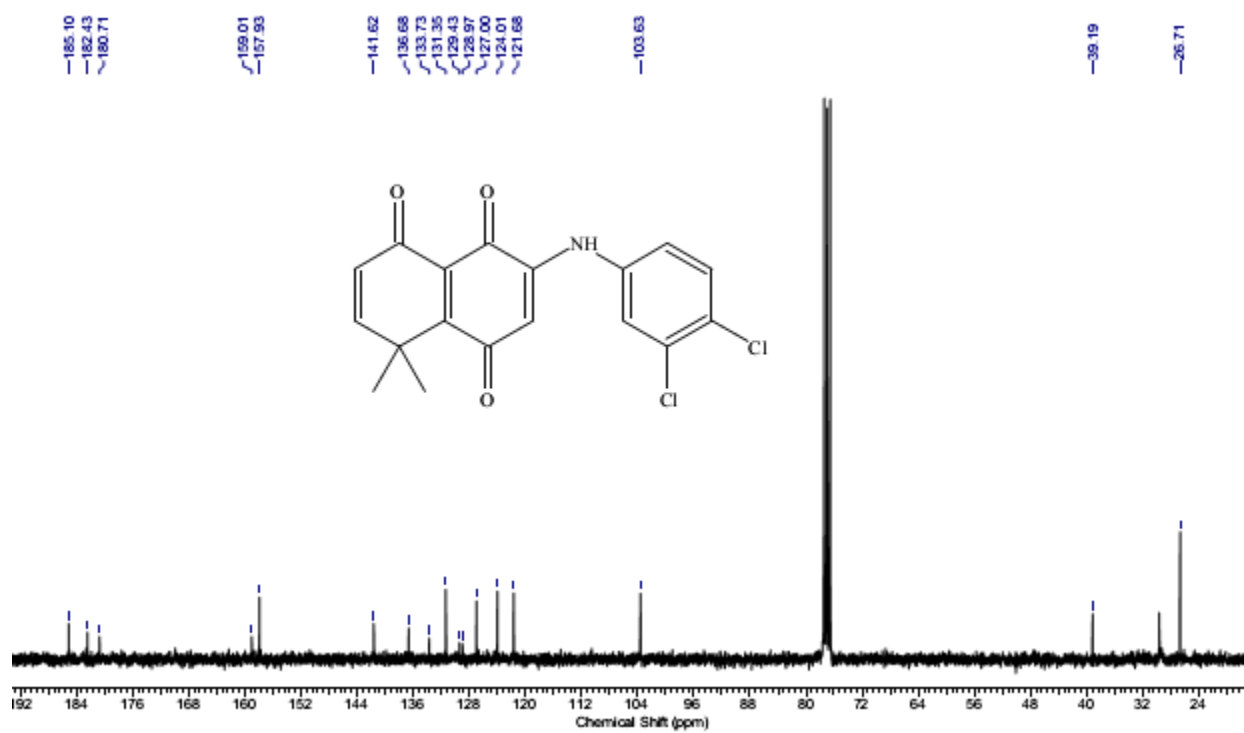
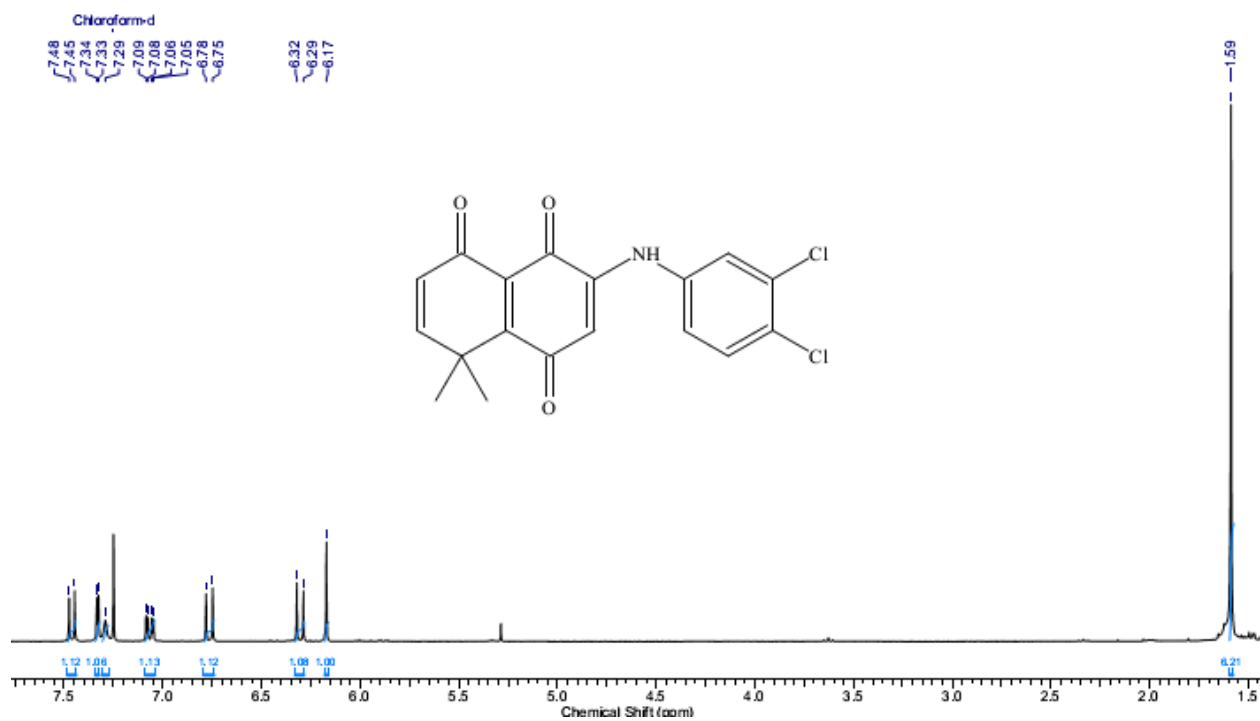
Red powder; mp 97-99 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  762(C-H<sub>ar</sub>), 1689(C=O), 3301(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.58 (s, 6H), 6.14 (s, 1H), 6.31 (d, 1H,  $J = 10.1$  Hz), 6.76 (d, 1H,  $J = 10.1$  Hz), 7.07 (m, 1H,  $J = 3.1$  Hz, 6.0 Hz, 8.3 Hz), 7.35 (t, 2H,  $J = 3.4$ ), 7.56 (s, 1H), 7.64 (d, 1H,  $J = 8.5$  Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 17.64, 26.70, 39.23, 102.30, 124.27, 126.90, 127.06, 128.90, 131.39, 132.92, 135.02, 143.12, 158.01, 159.52, 181.32, 182.75, 184.70; m/z (IE) calcd. for C<sub>18</sub>H<sub>14</sub>BrNO<sub>3</sub> 371.0157, found 371.0146.

### 3-(p-Bromophenylamino)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXg)



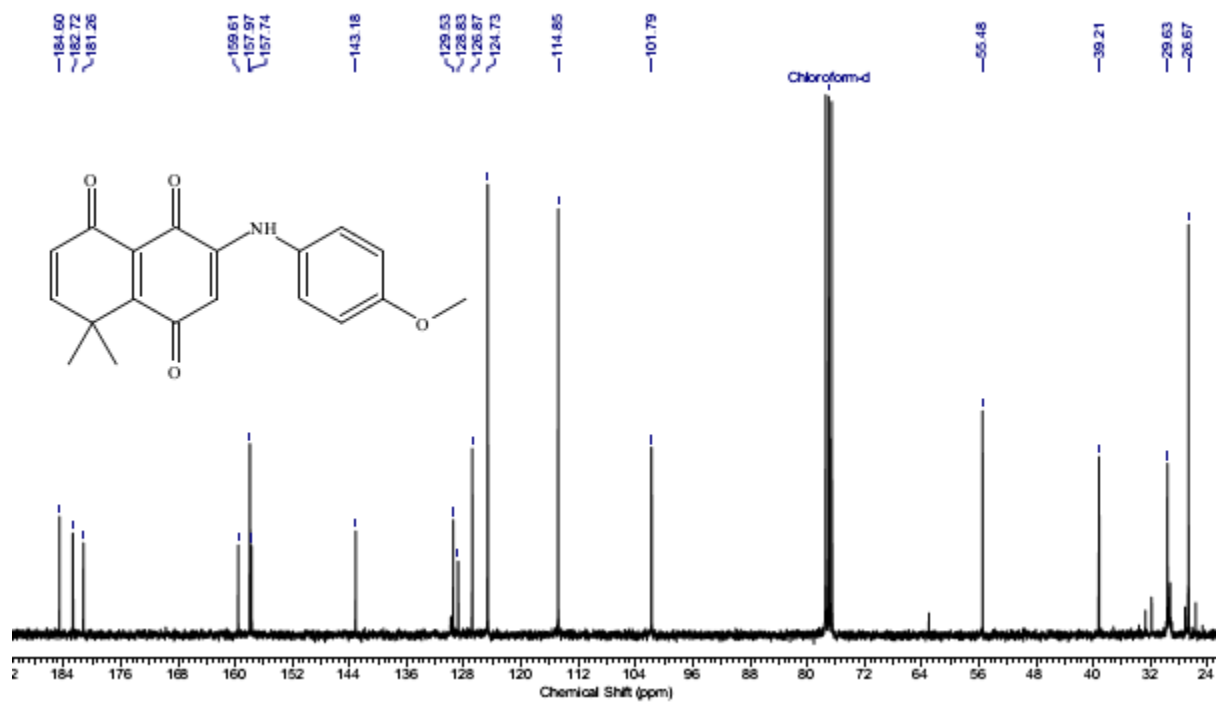
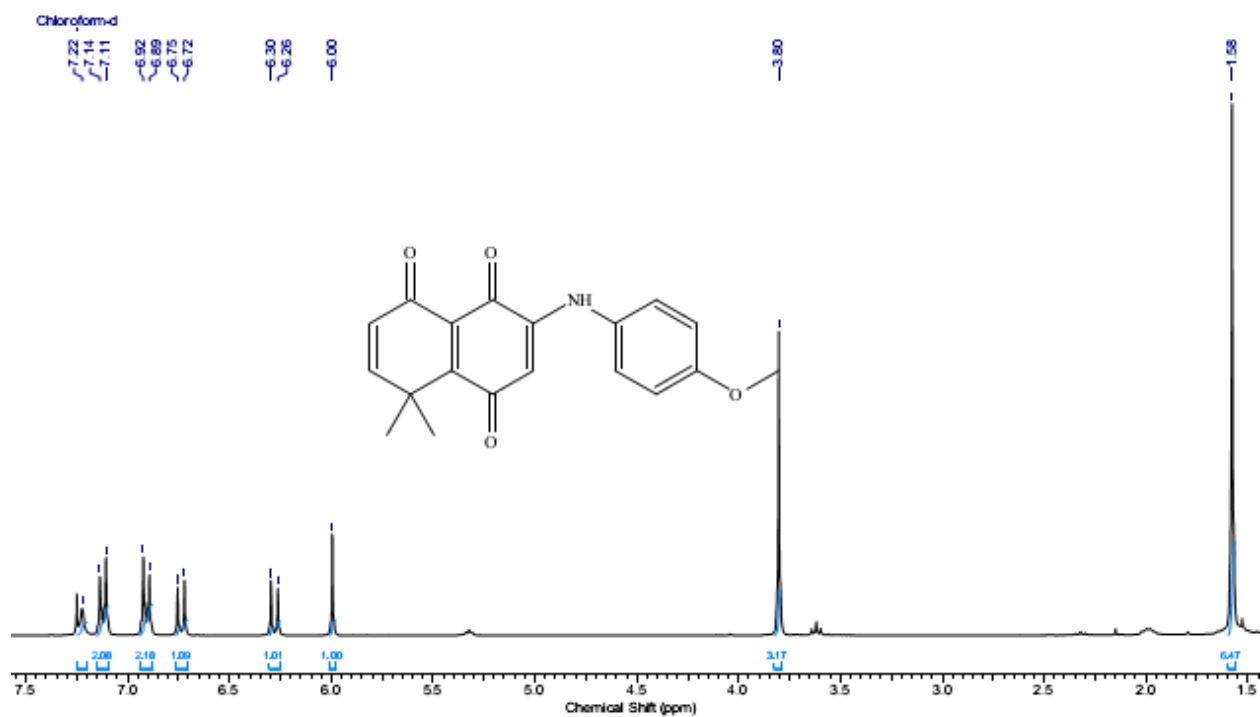
Red powder; mp 168-170 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  818(C-H<sub>ar</sub>), 1678(C=O), 3298(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.58 (s, 6H), 6.15 (s, 1H), 6.29 (d, 1H,  $J = 10.1$  Hz), 6.76 (d, 1H,  $J = 10.1$  Hz), 7.09 (d, 2H,  $J = 8.6$  Hz), 7.28 (s, 1H), 7.52 (d, 2H,  $J = 8.8$  Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 27.12, 39.61, 103.48, 119.25, 124.46, 127.37, 129.36, 133.23, 136.60, 142.38, 158.35, 159.58, 181.35, 182.94, 185.40; m/z (TOF) calcd. for C<sub>18</sub>H<sub>14</sub>NO<sub>3</sub>BrNa<sup>+</sup> 394.0055, found 394.0049.

### 3-(3,4-Dichlorophenylamino)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXg)



Red powder; mp 175–177 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  833(C-H<sub>ar</sub>), 1695(C=O), 3440(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.59 (s, 6H), 6.17 (s, 1H), 6.31 (d, 1H,  $J = 10.2$  Hz), 6.77 (d, 1H,  $J = 10.0$  Hz), 7.07 (dd, 1H,  $J = 2.6$  Hz, 8.6 Hz), 7.29 (s, 1H), 7.34 (d, 1H,  $J = 2.6$  Hz), 7.47 (d, 1H,  $J = 8.6$  Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.71, 39.19, 103.62, 121.68, 124.01, 127.00, 129.42, 131.34, 133.73, 136.67, 141.62, 157.93, 159.01, 180.70, 182.42, 185.09;  $m/z$  (IE) calcd. for C<sub>18</sub>H<sub>13</sub>Cl<sub>2</sub>NO<sub>3</sub> 361.0272, found 361.02666.

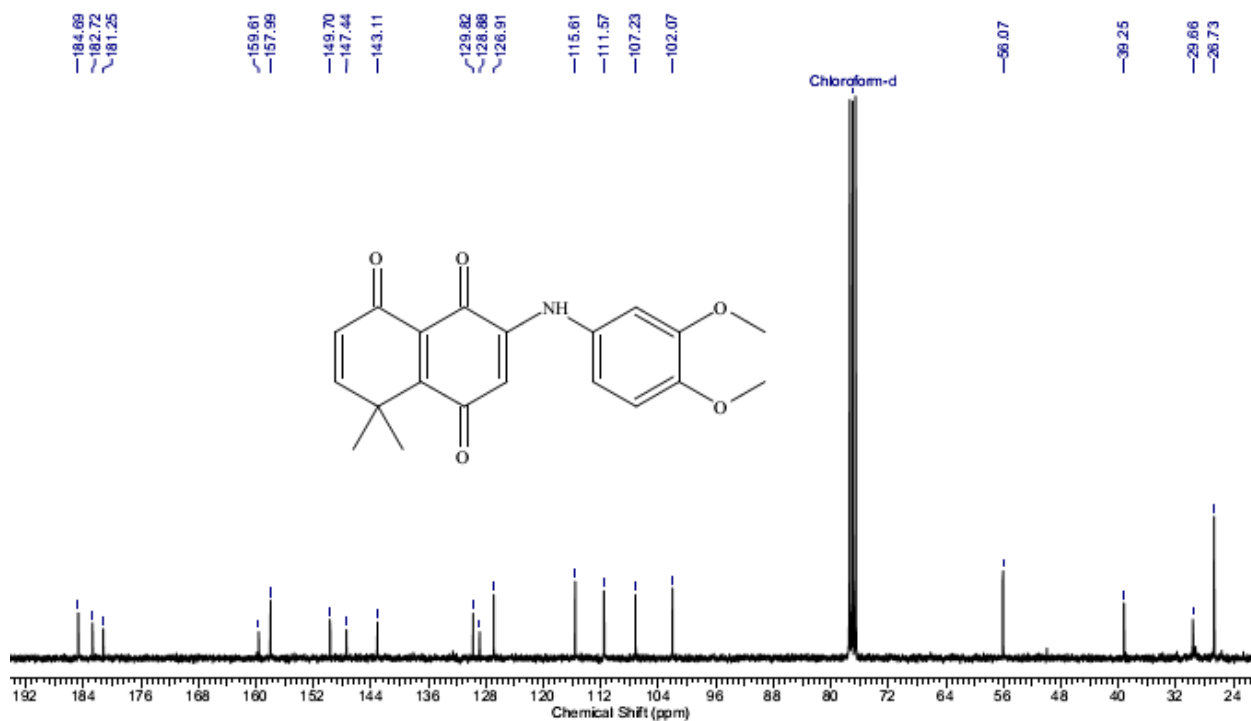
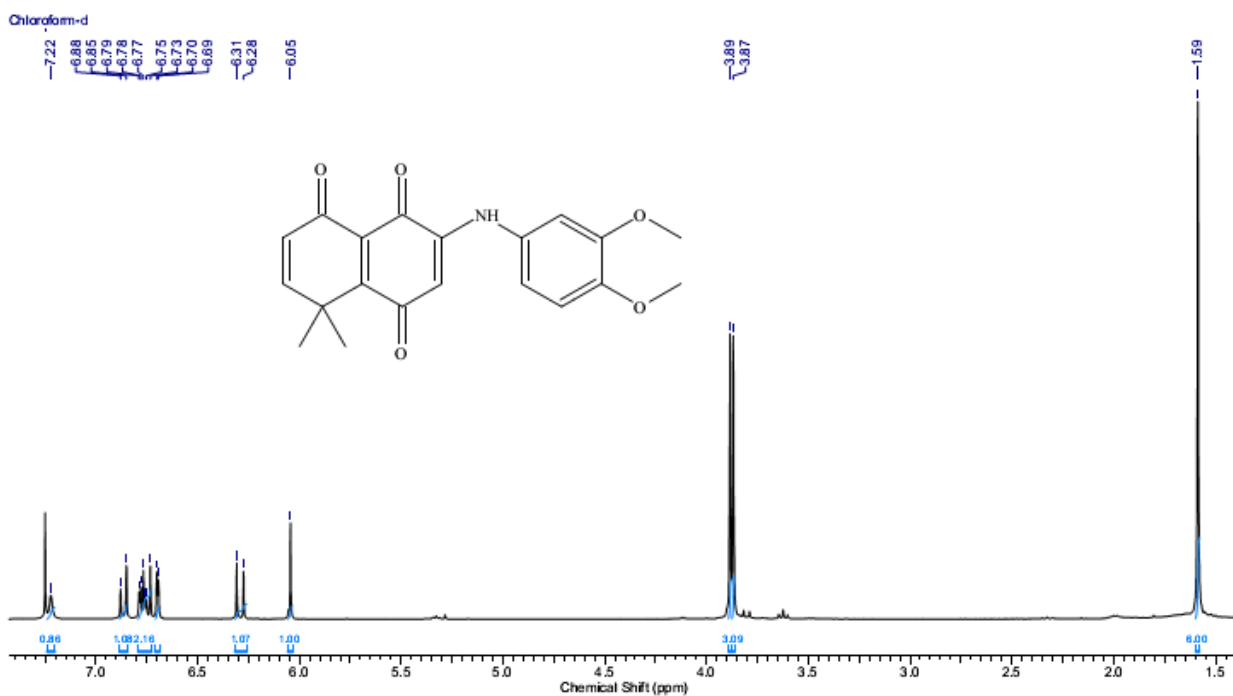
### 3-(p-Methoxyphenylamino)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXh)



Red powder; mp 145-147 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  821(C-H<sub>ar</sub>), 1609(C=O), 3316(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.58 (s, 6H), 3.80 (s, 3H), 6.00 (s, 1H), 6.28 (d, 1H,  $J = 10.1$  Hz), 6.74 (d, 1H,  $J = 10.1$  Hz), 6.91 (d, 2H,  $J = 8.9$  Hz), 7.13 (d, 2H,  $J = 8.9$  Hz), 7.22 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.67, 29.63, 39.21, 55.48, 101.79, 114.85, 124.73, 126.87, 128.83, 129.53, 143.18, 157.74, 157.97, 159.61, 181.26, 182.72, 184.60; m/z (TOF) calcd. for C<sub>19</sub>H<sub>17</sub>NO<sub>4</sub>H<sup>+</sup> 324.1236, found 324.1232.

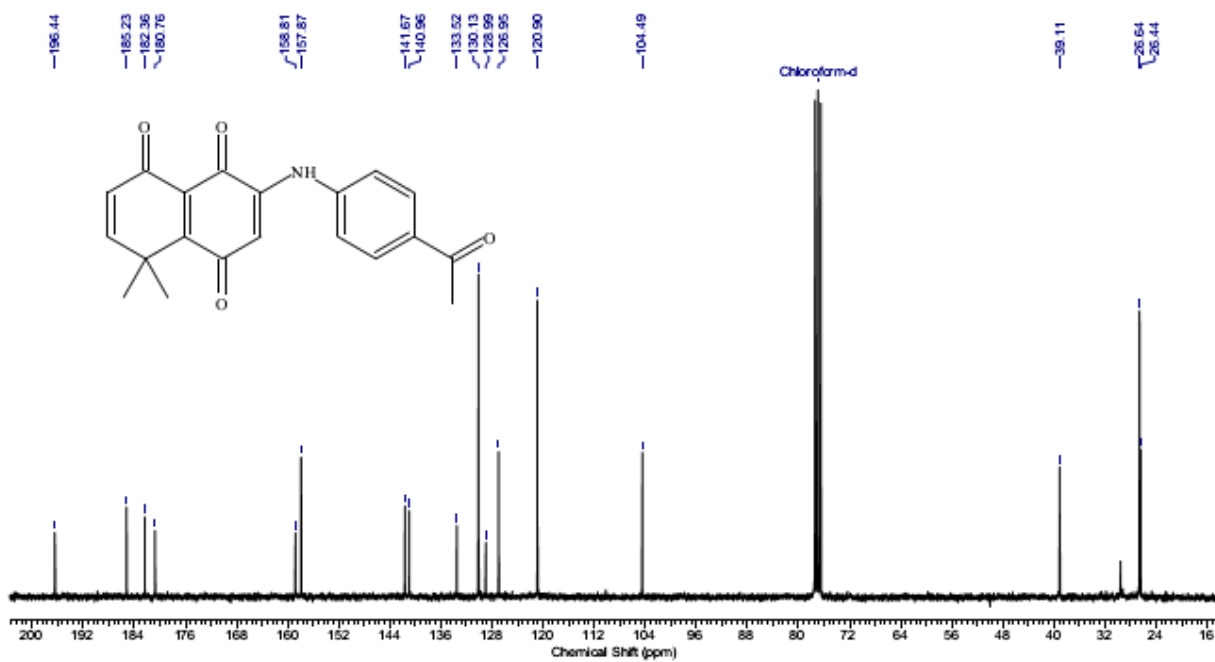
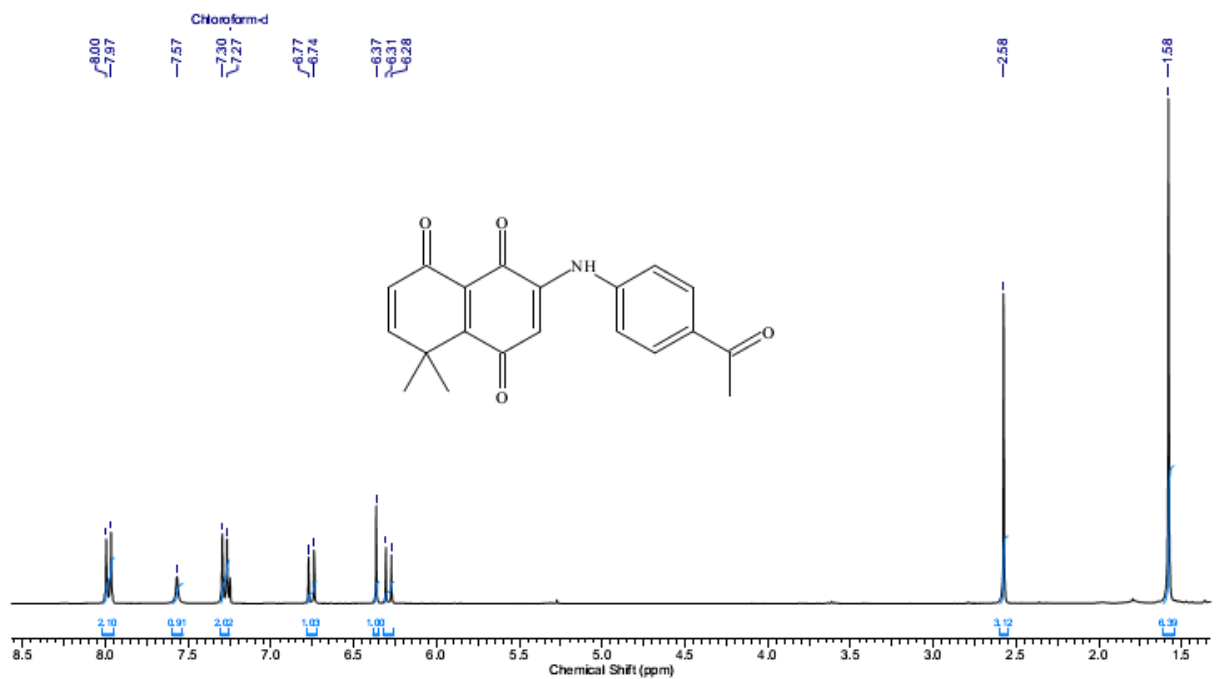


**3-(3,4-Dimethoxyphenylamino)-8,8-dimethylnaphthalene-1,4,5(8H)-trione  
(XXi)**



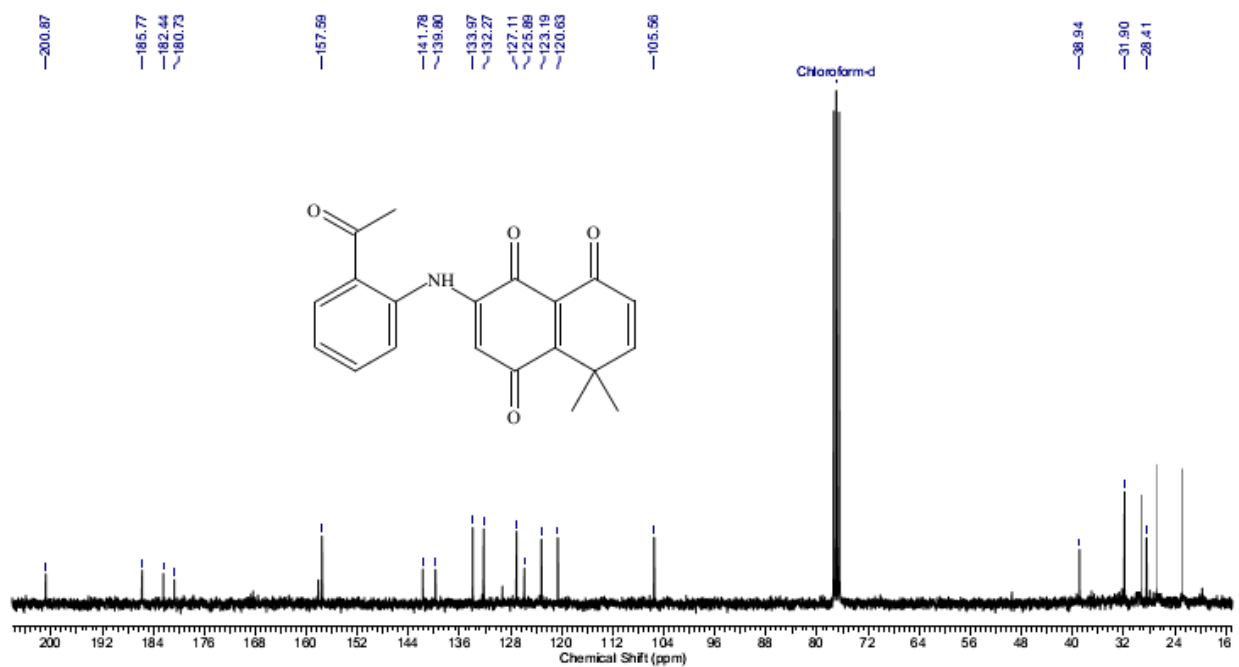
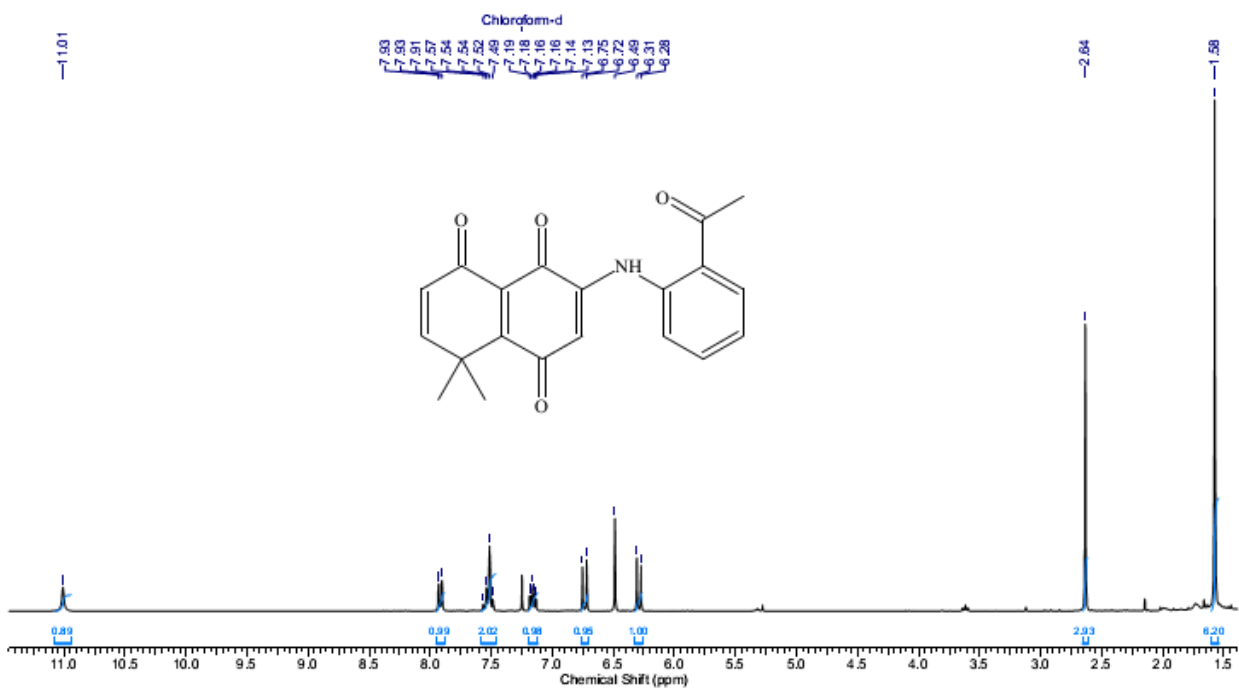
Red powder; mp 129-131 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  827(C-H<sub>ar</sub>), 1628(C=O), 3329(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.59 (s, 6H), 3.87 (s, 3H), 3.89 (s, 3H), 6.05 (s, 1H), 6.30 (d, 1H,  $J = 10.1$  Hz), 6.70 (d, 1H,  $J = 2.3$  Hz), 6.75 (d, 1H,  $J = 10.1$  Hz), 6.77 (dd, 1H,  $J = 5.6$  Hz, 10.1 Hz), 6.87 (d, 1H,  $J = 8.5$  Hz), 7.22 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.73, 29.66, 39.25, 56.07, 102.07, 107.23, 111.57, 115.61, 126.91, 128.88, 129.82, 143.11, 147.44, 149.70, 157.99, 159.61, 181.25, 182.72, 184.69;  $m/z$  (IE) calcd. for C<sub>20</sub>H<sub>19</sub>NO<sub>5</sub> 353.1263, found 353.12736.

### 3-(p-Acetylphenylamino)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXj)



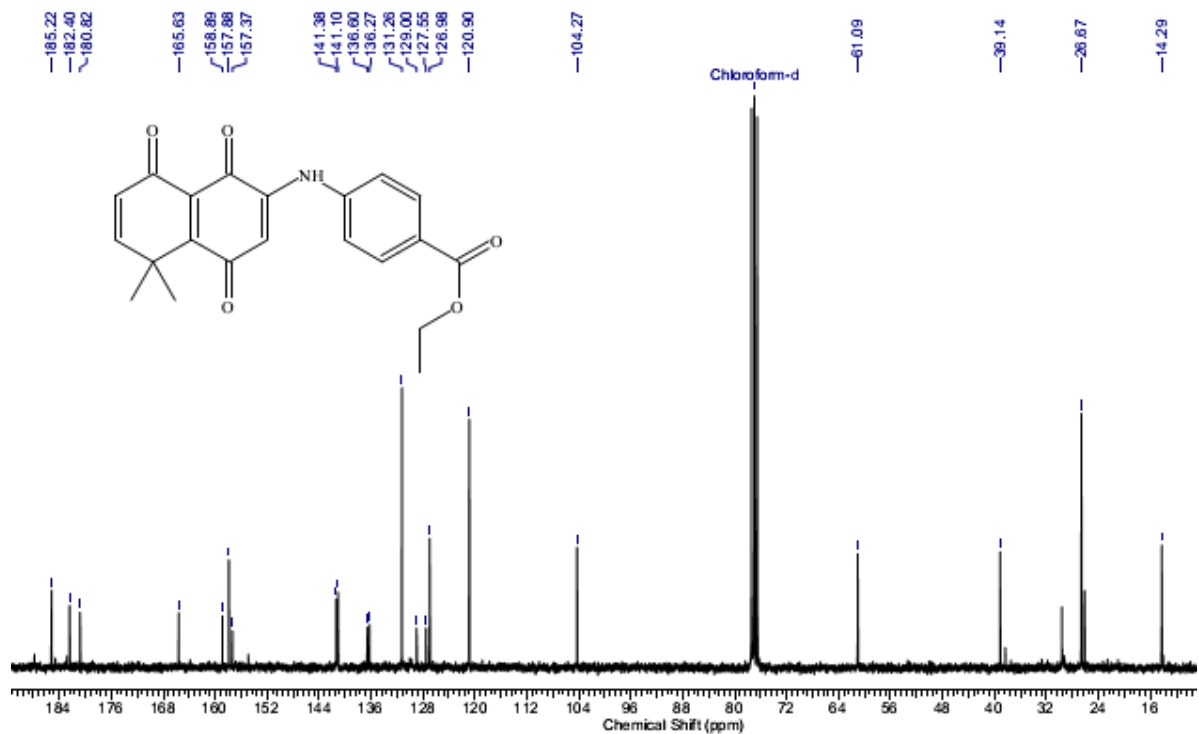
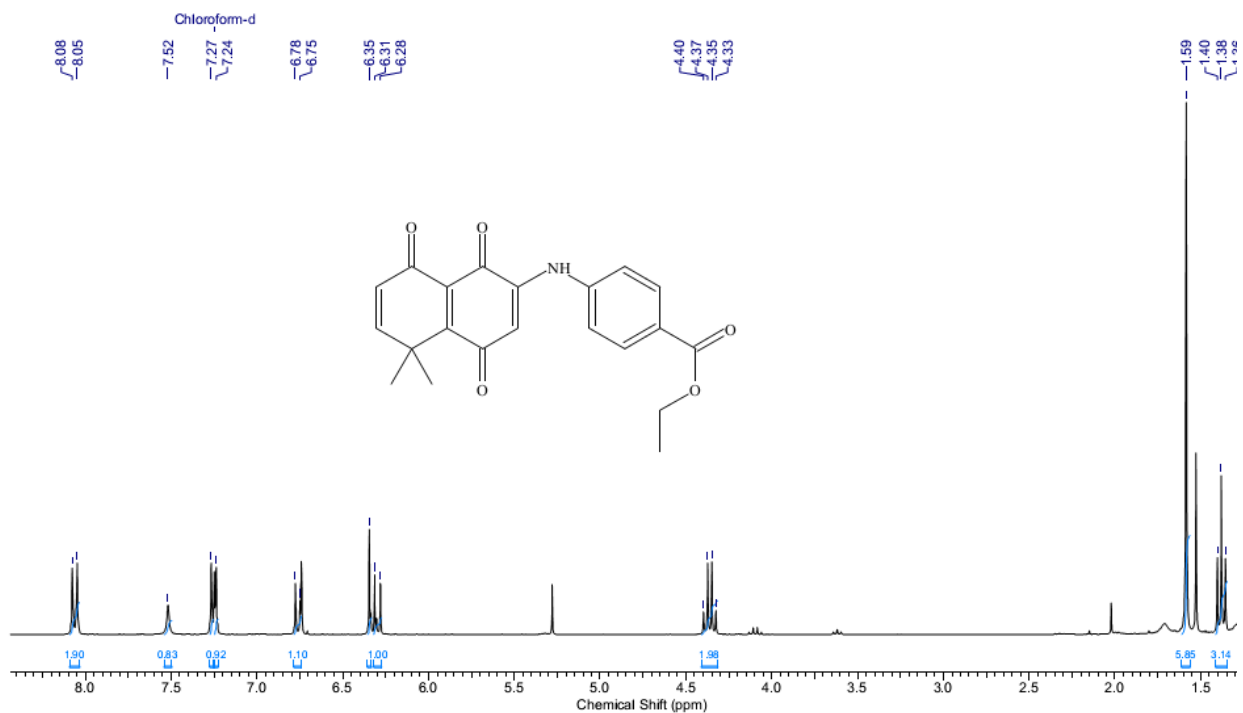
Red powder; mp 195-196 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  827 (C-H<sub>ar</sub>), 1693(C=O), 3425(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.58 (s, 6H), 2.58 (s, 3H), 6.30 (d, 1H, *J* = 10.0 Hz), 6.37 (s, 1H), 6.76 (d, 1H, *J* = 10.0 Hz), 7.29 (d, 2H, *J* = 8.6 Hz), 7.57 (s, 1H), 7.99 (d, 2H, *J* = 8.6 Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.44, 26.64, 39.11, 104.49, 120.90, 126.95, 128.99, 130.13, 133.52, 140.96, 141.67, 157.87, 158.81, 180.76, 182.36, 185.23, 196.44; m/z (TOF) calcd. for C<sub>20</sub>H<sub>17</sub>NO<sub>4</sub>H<sup>+</sup> 336.1236 found 336.1231.

### 3-(o-Acetylphenylamino)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXk)



Red powder; mp 160-162 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  751(C-H<sub>ar</sub>), 1698(C=O), 3410(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.58 (s, 6H), 2.64 (s, 3H), 6.30 (d, 1H, *J* = 10.0 Hz), 6.49 (s, 1H), 6.74 (d, 1H, *J* = 10.1 Hz), 7.16 (td, 1H, *J* = 1.8 Hz, 6.7 Hz), 7.53 (q, 2H, *J* = 6.6 Hz, 8.1 Hz), 7.92 (dd, 1H, *J* = 1.0 Hz, 8.5 Hz), 11.10 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 29.34, 31.90, 38.94, 105.56, 120.63, 123.19, 125.89, 127.11, 132.27, 133.97, 139.80, 147.78, 157.59, 180.73, 182.44, 185.77, 200.87; *m/z* (TOF) calcd. for C<sub>20</sub>H<sub>17</sub>NO<sub>4</sub>H<sup>+</sup> 336.1236 found 336.1241.

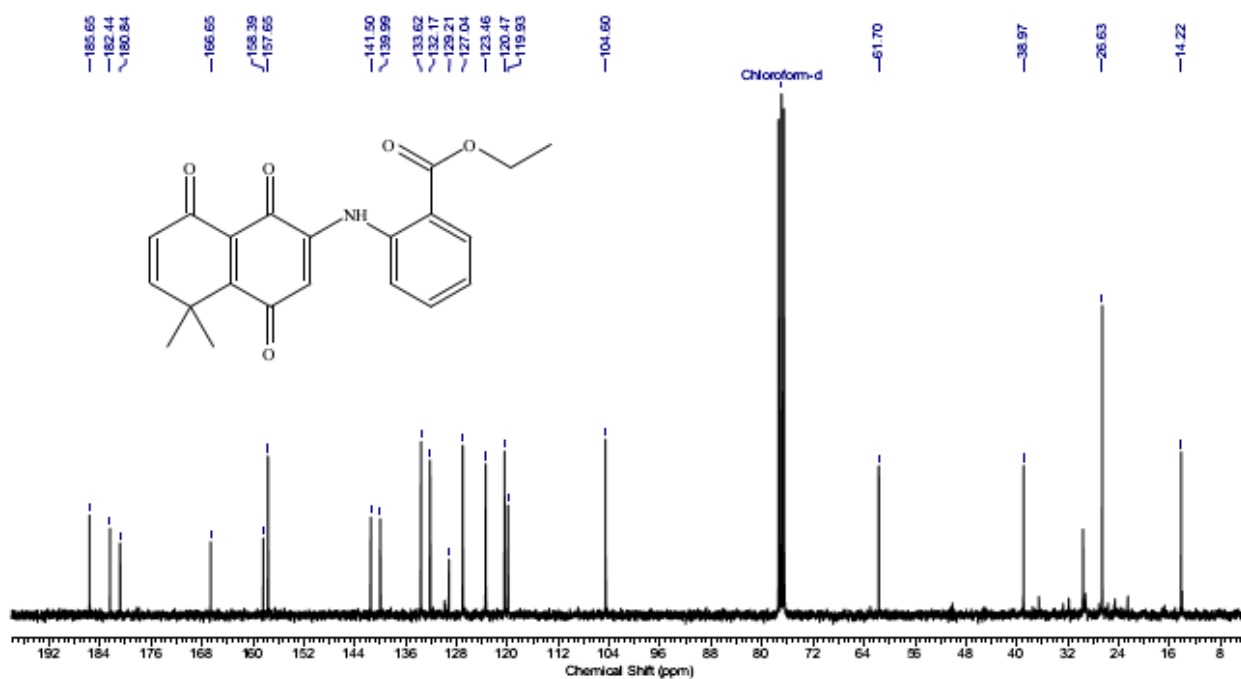
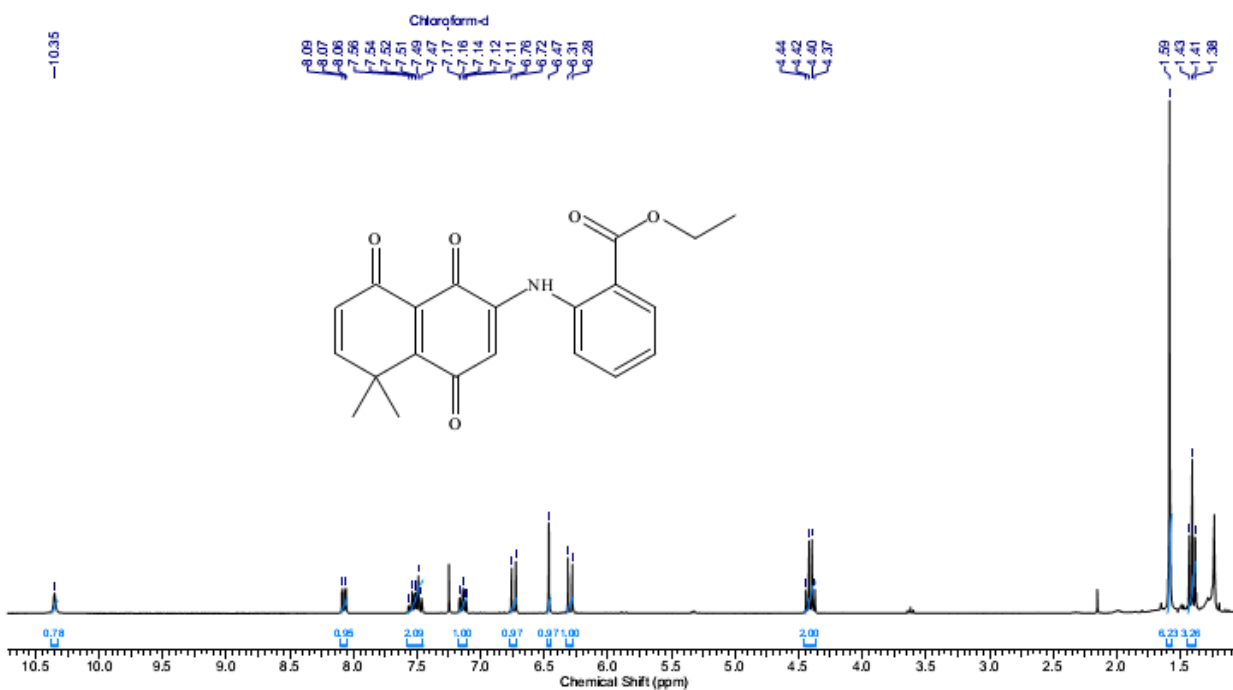
**Ethyl 4-(5,5-dimethyl-1,4,8-trioxo-1,4,5,8-tetrahydronaphthalen-2-ylamino)benzoate (XXI)**



Red powder; mp 160-162 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  836(C-H<sub>ar</sub>), 1698(C=O), 3410(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.38 (t, 3H,  $J = 7.1$  Hz), 1.59 (s, 6H), 4.36 (q, 2H,  $J = 7.1$  Hz), 6.39 (d, 1H,  $J = 10.1$  Hz), 6.35 (s, 1H), 6.77 (d, 1H,  $J = 10.2$  Hz), 7.26 (d, 2H,  $J = 8.7$  Hz), 7.52 (s, 1H), 8.07 (d, 2H,  $J = 8.7$  Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 14.29, 26.67, 39.14, 61.09, 104.27, 120.90, 126.98, 127.55, 129.00, 131.26, 136.27, 136.60, 141.10, 141.38, 157.37, 157.88, 158.89, 165.63, 180.82, 182.40, 185.22; m/z (TOF) calcd. for C<sub>21</sub>H<sub>19</sub>NO<sub>5</sub>H<sup>+</sup> 366.1341 found 366.1331.

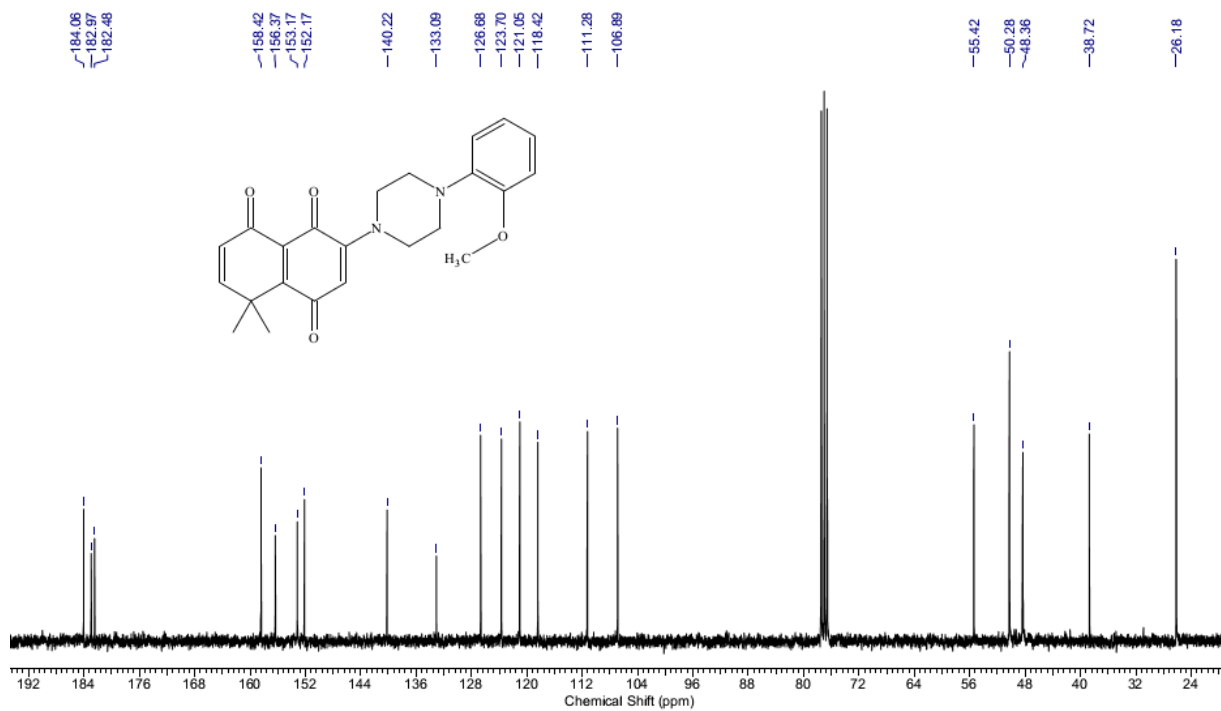
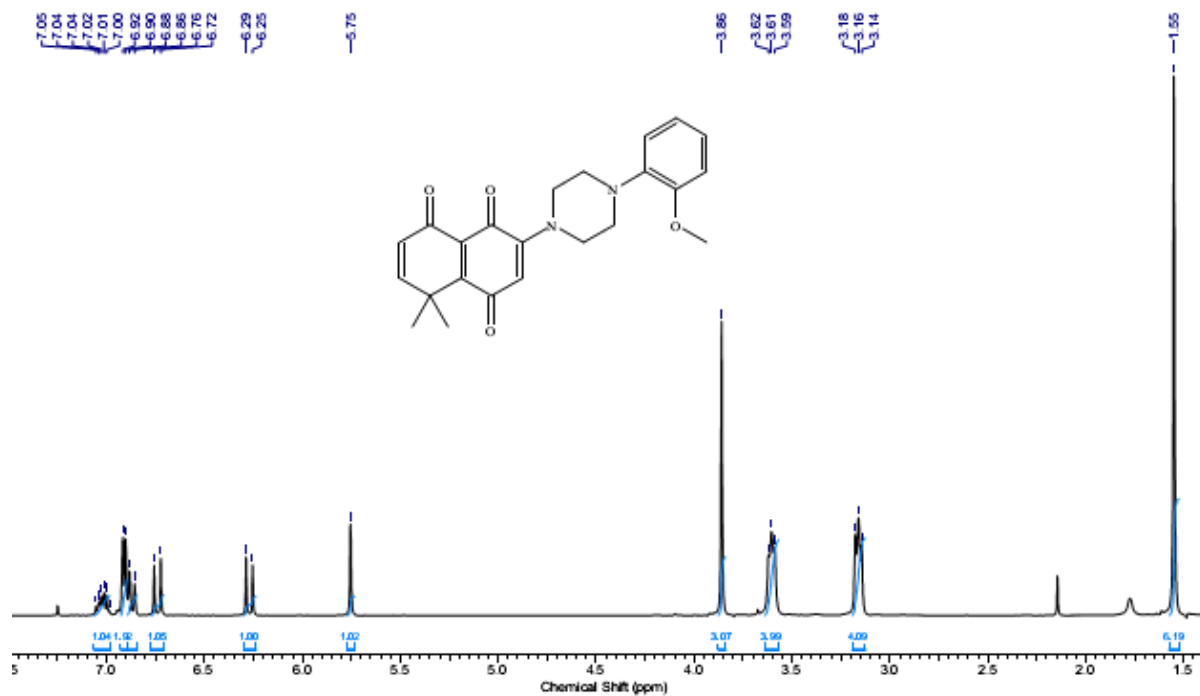


**Ethyl 2-(5,5-dimethyl-1,4,8-trioxo-1,4,5,8-tetrahydronaphthalen-2-ylamino)benzoate (XXm)**



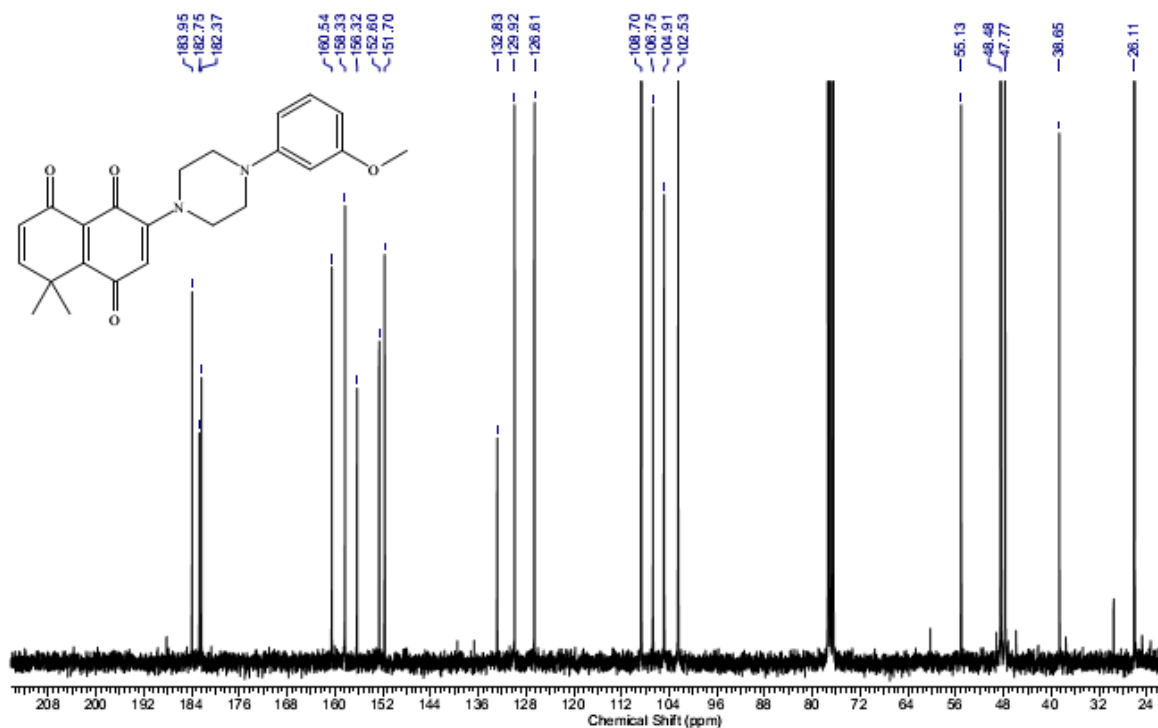
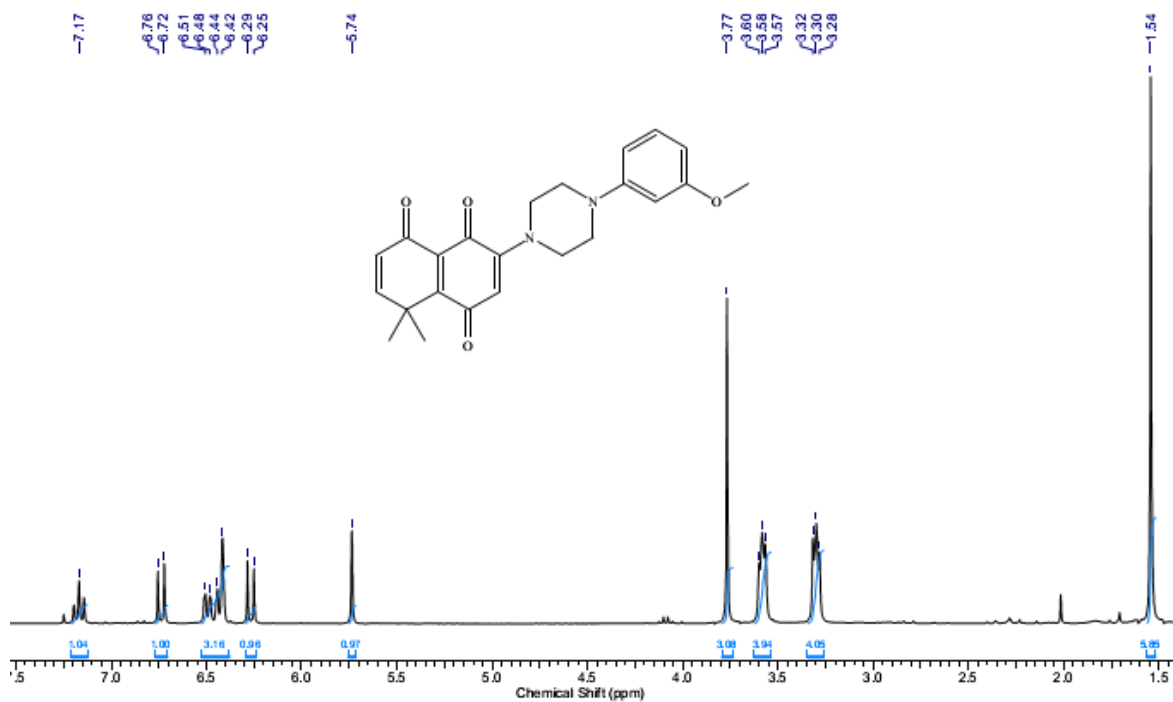
Red powder; mp 115-117 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  758(C-H<sub>ar</sub>), 1703(C=O), 3435(N-H); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.41 (t, 3H,  $J = 7.1$  Hz), 1.59 (s, 6H); 6.23 (s, 6H), 4.41 (q, 2H,  $J = 7.1$  Hz), 6.30 (d, 1H,  $J = 10.0$  Hz), 6.47 (s, 1H), 6.74 (d, 1H,  $J = 10.1$  Hz), 7.14 (dt, 1H,  $J = 1.4$  Hz, 7.1 Hz), 7.51 (m, 2H), 8.07 (dd, 1H,  $J = 1.4$  Hz, 7.8 Hz), 10.35 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 14.22, 26.63, 38.97, 61.70, 104.60, 119.93, 120.47, 123.46, 127.04, 129.21, 132.17, 133.62, 139.99, 141.50, 157.65, 158.39, 166.65, 180.84, 182.44, 185.65; m/z (TOF) calcd. for C<sub>21</sub>H<sub>19</sub>NO<sub>5</sub> 365.1263 C<sub>21</sub>H<sub>19</sub>NO<sub>5</sub> 365.12632, found 365.12632

**3-(4-(2-Methoxyphenyl)piperazin-1-yl)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXIa)**



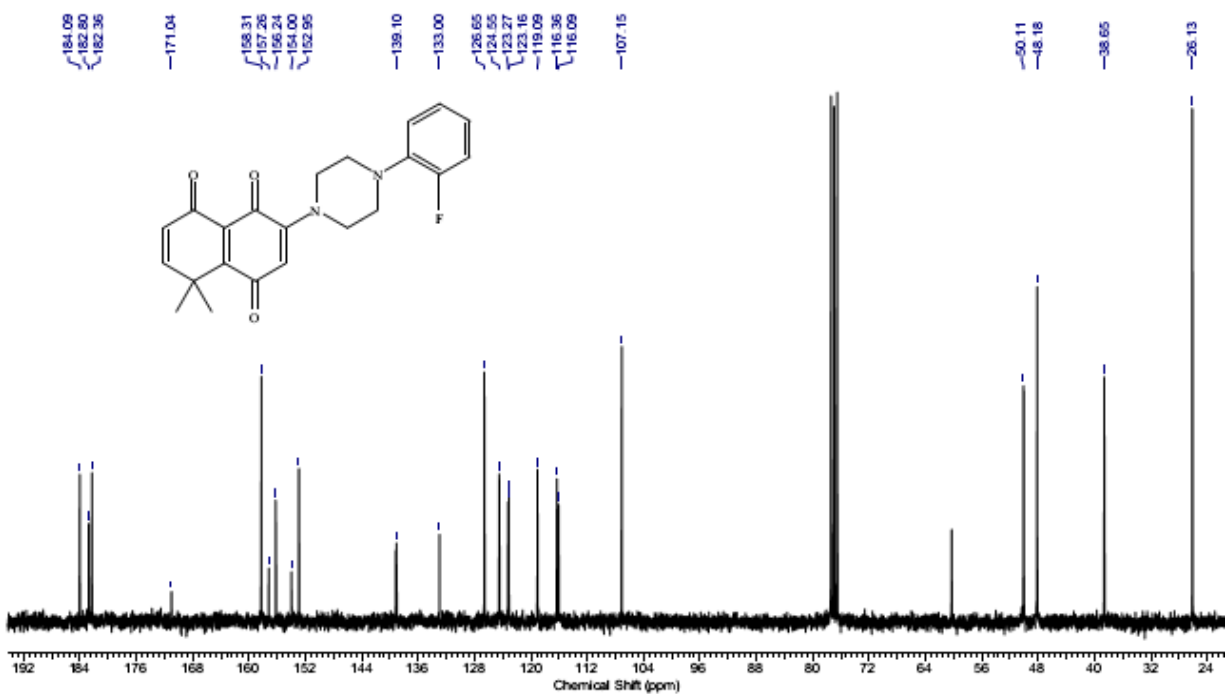
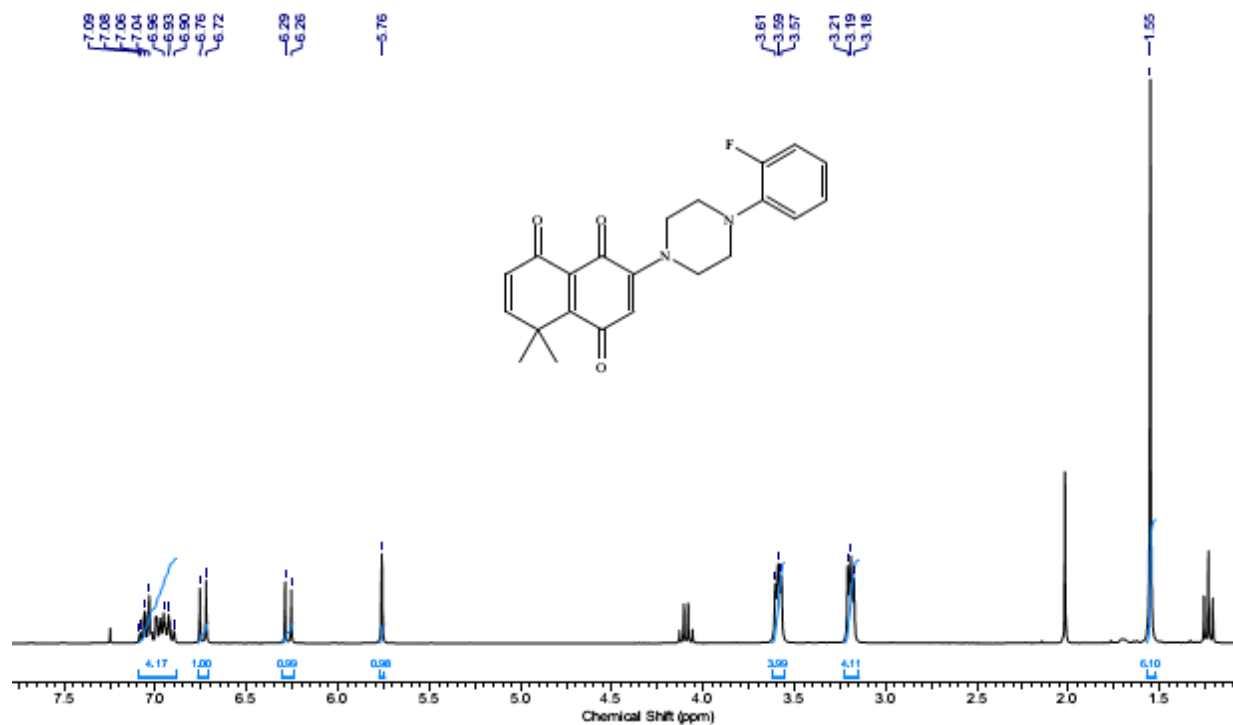
Red powder; mp 138-139 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  757(C-H<sub>ar</sub>), 1219(C-N), 1699(C=O); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.55 (s, 6H); 3.16 (t, 4H, *J* = 4.8 Hz); 3.61 (t, 4H, *J* = 4.8 Hz); 3.86 (s, 3H); 5.75 (s, 1H); 6.27 (d, 1H, *J* = 10.1 Hz); 6.75 (d, 1H, *J* = 10.1 Hz); 6.87 (d, 1H, *J* = 8.0 Hz); 6.91 (d, 2H, *J* = 4.2 Hz); 7.03 (m, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.18, 38.72, 48.36, 50.28, 55.42, 106.89, 111.28, 118.42, 121.05, 123.70, 126.68, 133.09, 140.22, 152.17, 153.17, 156.37, 158.42, 182.48, 182.97, 184.06; *m/z* (TOF) calcd. for C<sub>23</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>Na<sup>+</sup> 415.1634, found 415.1636.

**3-(4-(3-Methoxyphenyl)piperazin-1-yl)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXIb)**



Red powder; mp 133-135 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  754(C-H<sub>ar</sub>), 1209(C-N), 1695(C=O); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.54 (s, 6H); 3.30 (t, 4H,  $J = 4.8$  Hz); 3.58 (t, 4H,  $J = 5.3$  Hz); 3.77 (s, 3H); 5.74 (s, 1H); 6.27 (d, 1H,  $J = 10.1$  Hz); 6.47 (m, 3H); 6.74 (d, 1H,  $J = 10.1$  Hz); 7.17 (t, 1H,  $J = 7.96$  Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.11; 38.65; 47.77; 48.48; 55.13; 102.53; 104.91; 106.75; 108.70; 126.61; 129.92; 132.83; 151.70; 152.60; 156.32; 158.33; 160.54; 182.37; 182.75; 183.95. m/z (TOF) calcd. for C<sub>23</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>Na<sup>+</sup> 415.1634, found 415.1643.

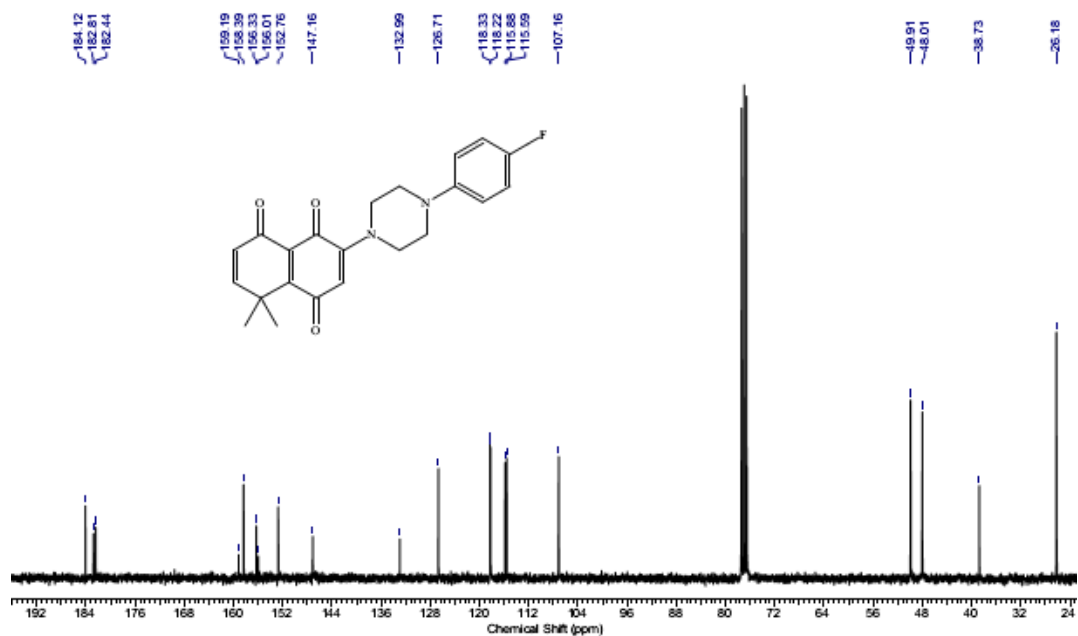
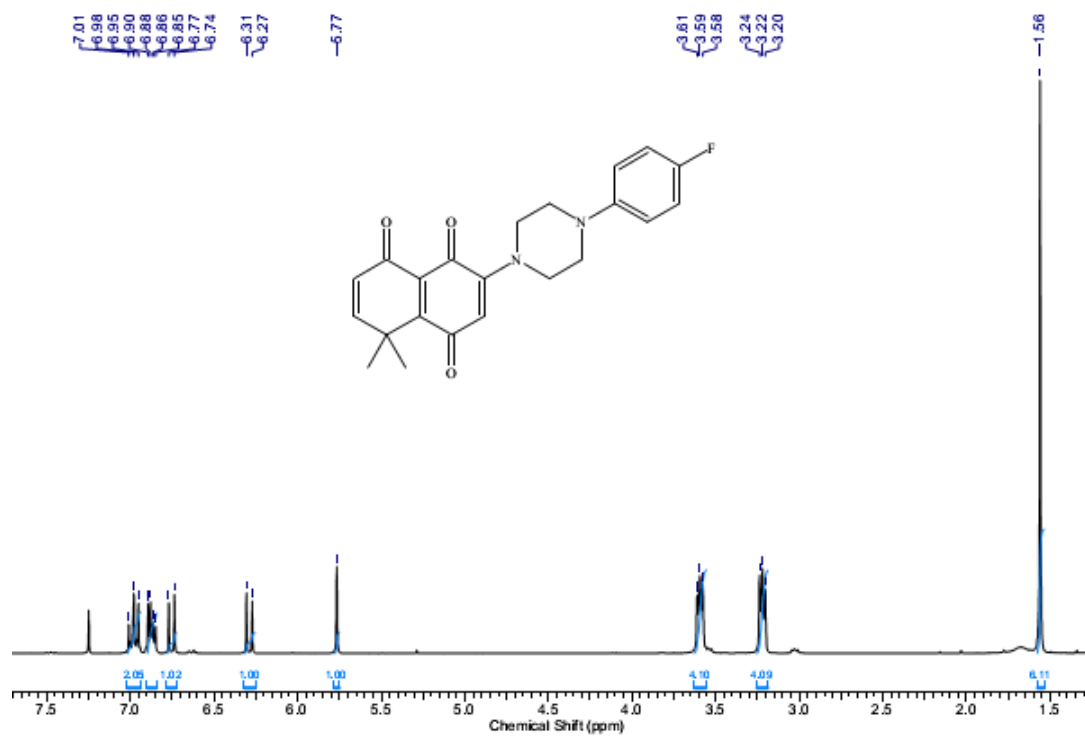
**3-(4-(2-Fluorophenyl)piperazin-1-yl)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXIc)**



Red powder; mp 106-107 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  758(C-H<sub>ar</sub>), 1232(C-N), 1700(C=O); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.55 (s, 6H); 3.19 (t, 4H,  $J = 4.8$  Hz); 3.59 (t, 4H,  $J = 5.1$  Hz); 5.76 (s, 1H); 6.28 (d, 1H,  $J = 10.1$  Hz); 6.74 (d, 1H,  $J = 10.2$  Hz); 7.00 (m, 4H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.13; 38.65; 49.18; 50.09; 107.15; 116.09; 116.36; 119.11; 123.21; 124.53; 126.65; 133.00; 139.11; 152.95; 154.00; 156.24; 157.26; 158.31; 171.04; 182.36; 182.80; 184.09; m/z (TOF) calcd. for C<sub>22</sub>H<sub>21</sub>N<sub>2</sub>O<sub>3</sub>FNa<sup>+</sup> 403.1434, found 403.1435.

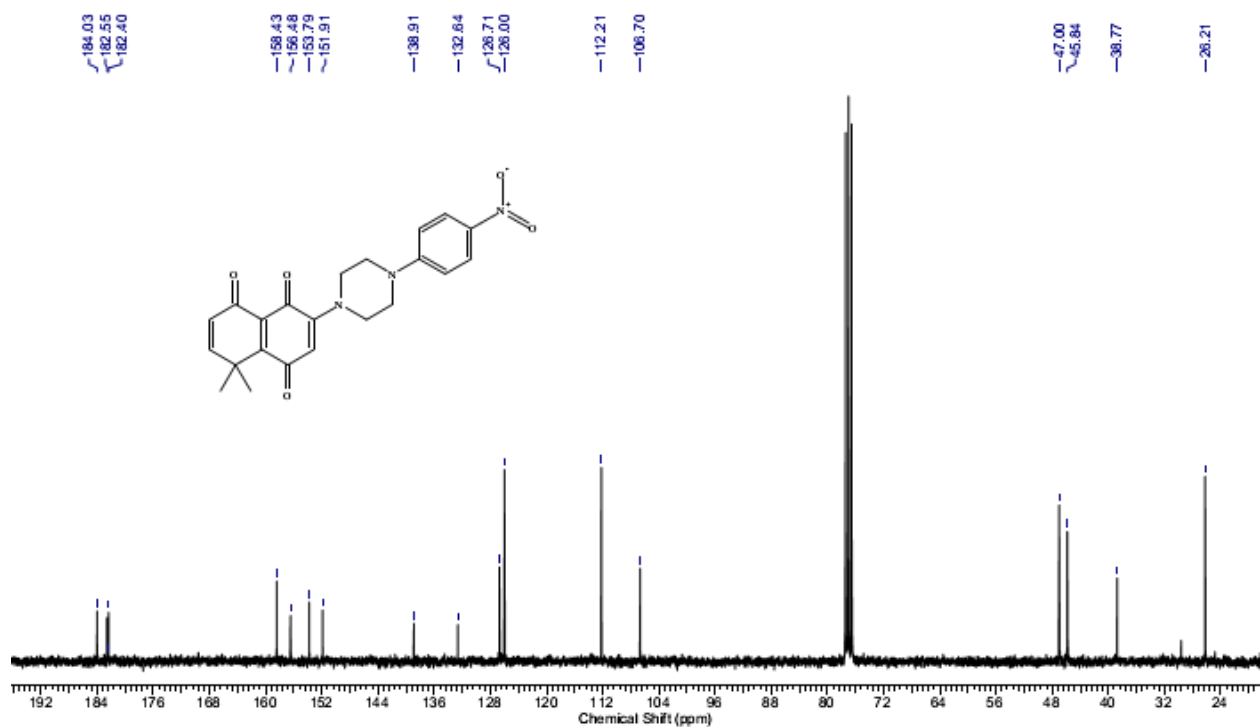
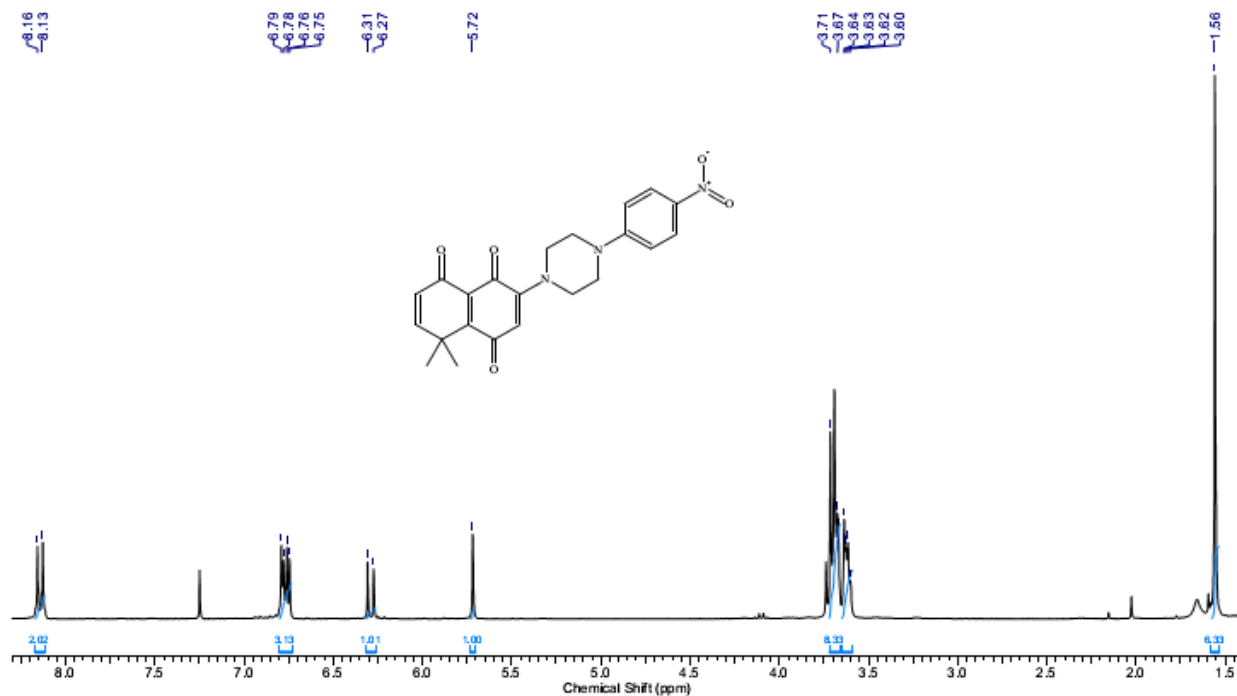


**3-(4-(4-Fluorophenyl)piperazin-1-yl)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXId)**



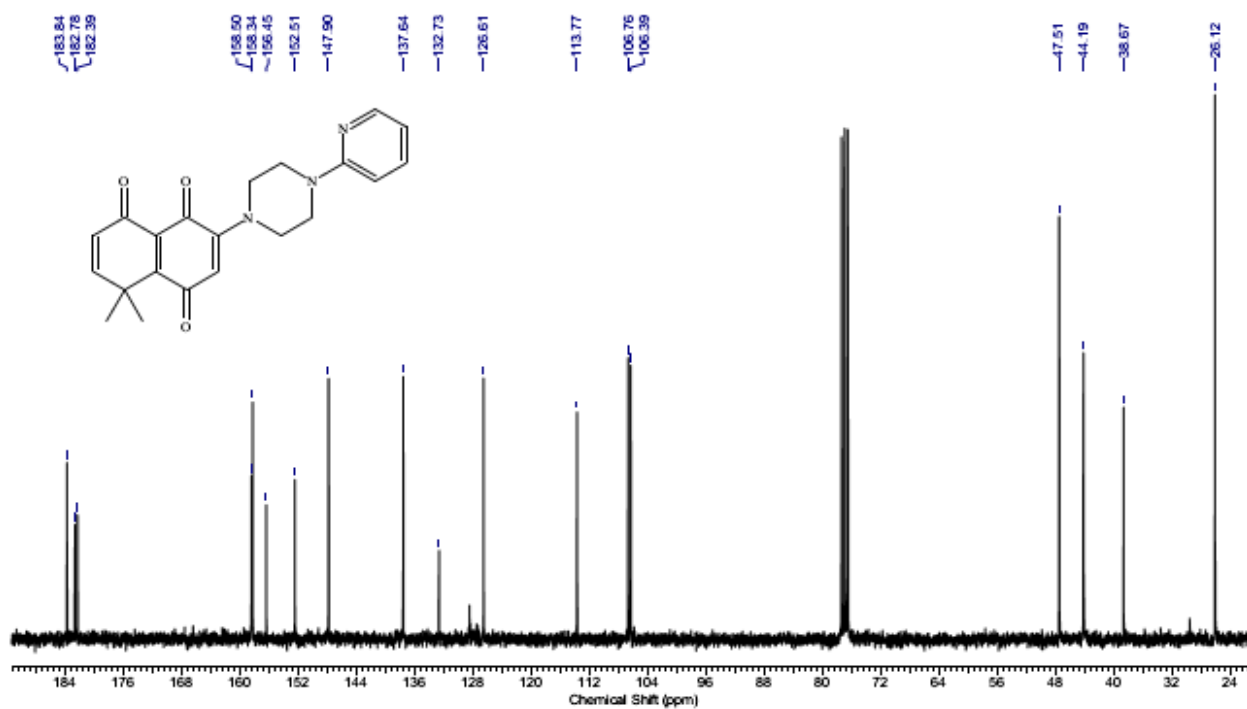
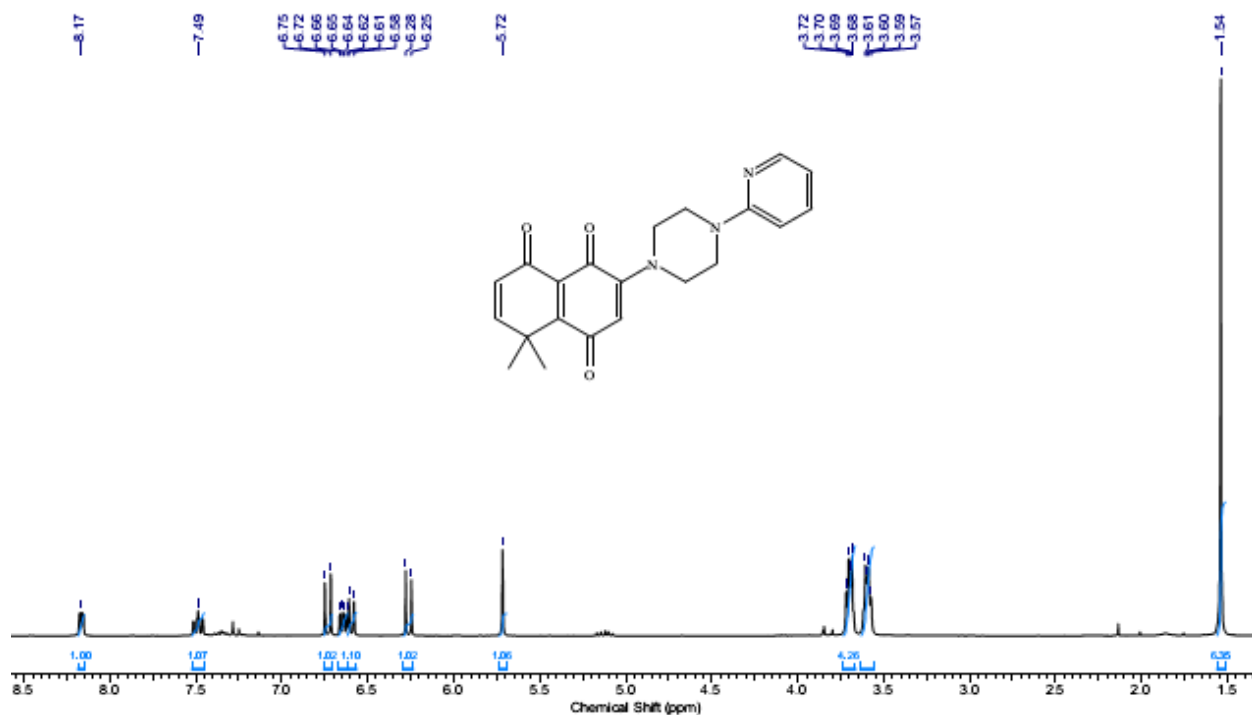
Red powder; mp 170-172 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  828(C-H<sub>ar</sub>), 1207(C-N), 1695(C=O); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.56 (s, 6H); 3.22 (t, 4H,  $J = 4.9$  Hz); 3.59 (t, 4H,  $J = 5.3$  Hz); 5.77 (s, 1H); 6.29 (d, 1H,  $J = 10.1$  Hz); 6.76 (d, 1H,  $J = 10.1$  Hz); 6.88 (m, 2H); 6.98 (m, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.18; 38.73; 48.01; 49.91; 107.16; 115.59; 115.88; 118.27; 126.71; 132.99; 147.18; 152.76; 156.01; 156.33; 158.39; 159.19; 182.44; 182.81; 184.12; m/z (TOF) calcd. for C<sub>22</sub>H<sub>21</sub>N<sub>2</sub>O<sub>3</sub>FNa<sup>+</sup> 403.1434, found 403.1444.

**3-(4-(4-Nitrophenyl)piperazin-1-yl)-8,8-dimethylnaphthalene-1,4,5(8H)-trione  
(XXIe)**



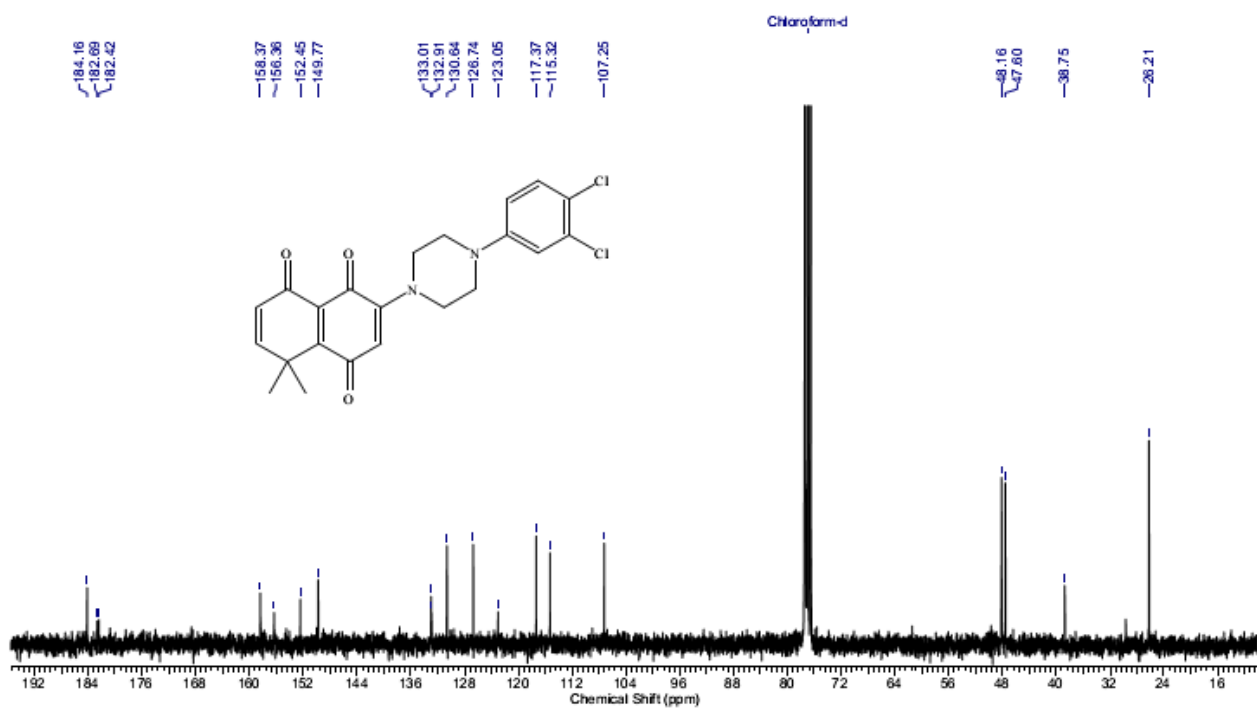
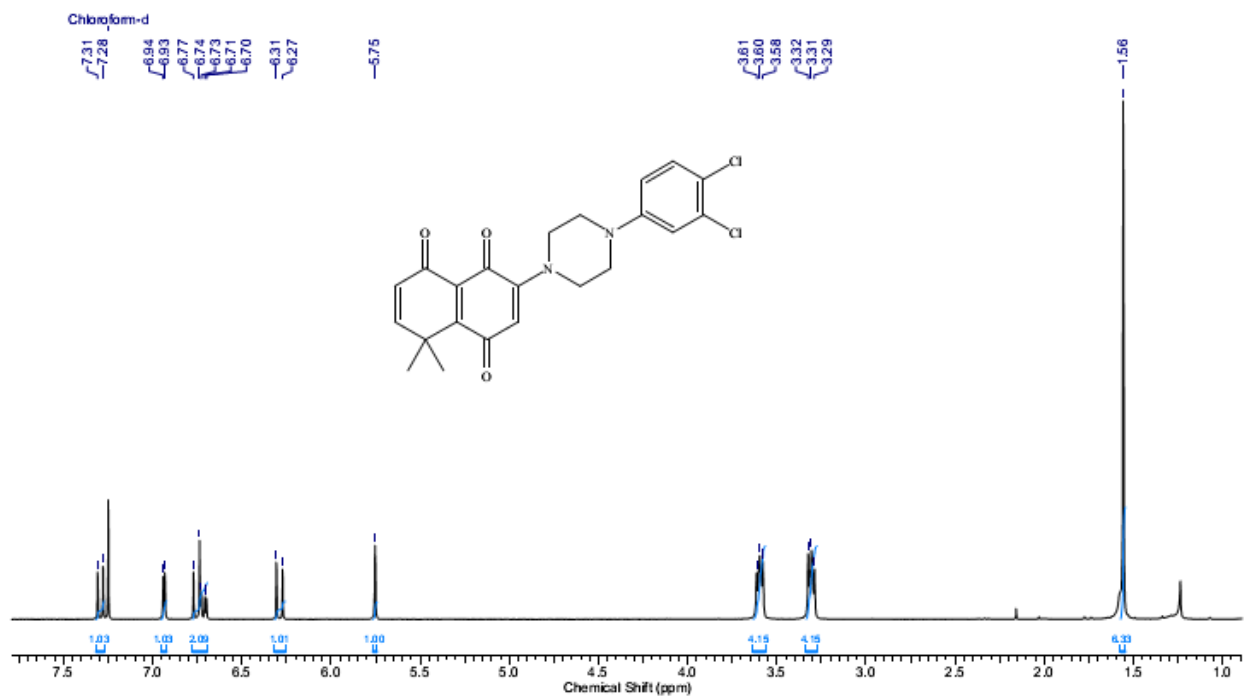
Red powder; mp 180-182 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  818(C-H<sub>ar</sub>), 1230(C-N), 1296(N-O), 1563(N-O), 1701(C=O); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.56 (s, 6H); 3.62 (m, 4H); 3.69 (m, 4H); 5.72 (s, 1H); 6.29 (d, 1H,  $J = 10.2$  Hz); 6.77 (m, 3H); 8.15 (d, 2H,  $J = 9.34$  Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.21; 38.77; 45.84; 47.00; 106.70; 112.21; 126.00; 126.71; 132.64; 138.91; 153.79; 156.48; 158.43; 182.40; 182.55; 184.03;  $m/z$  (TOF) calcd. for C<sub>22</sub>H<sub>21</sub>N<sub>3</sub>O<sub>5</sub>Na<sup>+</sup> 430.1379, found 430.1374.

**3-(4-(Pyridin-2-yl)piperazin-1-yl)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXIf)**



Red powder; mp 141-143 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  772(C-H<sub>ar</sub>), 1238(C-N), 1696(C=O); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.54 (s, 6H); 3.59 (q, 4H,  $J = 4.2$  Hz, 7.5 Hz); 3.70 (t, 4H,  $J = 4.2$  Hz, 7.5 Hz); 5.72 (s, 1H); 6.27 (d, 1H,  $J = 10.3$  Hz); 6.60 (d, 1H,  $J = 8.6$  Hz); 6.64 (q, 1H,  $J = 5.5$  Hz, 7.1 Hz); 6.74 (d, 1H,  $J = 10.2$  Hz); 7.49 (m, 1H), 8.17 (dd, 1H,  $J = 1.1$  Hz, 4.8 Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.12; 38.67; 44.19; 47.51; 106.39; 106.76; 113.77; 126.61; 132.73; 137.64; 147.90; 152.51; 156.45; 158.34; 158.50; 182.39; 182.78; 183.84; m/z (TOF) calcd. for C<sub>21</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>H<sup>+</sup> 364.1661, found 364.1669.

### 3-(4-(3,4-Dichlorophenyl)piperazin-1-yl)-8,8-dimethylnaphthalene-1,4,5(8H)-trione (XXIg)



Red powder; mp 142-144 °C;  $\nu_{\max}(\text{KBr})/\text{cm}^{-1}$  662(C-H<sub>ar</sub>), 1228(C-N), 1695(C=O); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$ H 1.56 (s, 6H); 3.31 (t, 4H, J = 4.9 Hz); 3.60 (t, 4H, J = 4.9 Hz); 5.75 (s, 1H); 6.29 (d, 1H, J = 10.1 Hz); 6.74 (m, 2H); 6.94 (d, 1H, J = 2.9 Hz); 7.30 (d, 1H, J = 8.9 Hz); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$ C 26.21; 38.75; 47.60; 48.16; 107.25; 115.32; 117.37; 123.05; 126.74; 130.64; 132.91; 133.01; 149.77; 152.45; 156.36; 158.37; 182.42; 182.69; 184.16; m/z (TOF) calcd. for C<sub>22</sub>H<sub>20</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>3</sub>H<sup>+</sup> 431.0930 found 431.0929.



### B3LYP/6-31G (d,p) calculated structure and absolute energies.

#### Compound I

E(RB3LYP)= -420.78305054 au

C	0.14935400	1.66751800	0.00033500
C	1.40077700	1.18450500	0.00016500
C	1.65313200	-0.28062400	-0.00098000
C	0.47467200	-1.17703700	-0.00033900
C	-0.79190900	-0.71508900	-0.00009600
C	-1.03042900	0.76540600	0.00011300
O	2.79577900	-0.72522200	0.00040700
O	-2.16823800	1.22074200	-0.00043700
C	-2.00932000	-1.58962400	0.00036000
H	-2.63460500	-1.37731200	-0.87296600
H	-2.63090100	-1.38131800	0.87735000
H	-1.73757900	-2.64716000	-0.00243500
H	-0.07332600	2.73042500	0.00072500
H	2.28030700	1.82143000	0.00054100
H	0.69811600	-2.24056400	-0.00031100

#### Compound Ia

E(B3LYP)= -573.64701080 au

C	0.37849900	2.07384600	-0.06998100
C	-0.95090300	2.05750500	0.10396000
C	-1.69143500	0.77115700	0.11449400
C	-0.92814900	-0.47602700	-0.08817300
C	0.41033600	-0.48429400	-0.27028900
C	1.15110000	0.81737800	-0.24255800
O	2.37487600	0.87054000	-0.34975200
O	-2.91279500	0.76549700	0.28115000
C	1.20907500	-1.72949700	-0.50574300
H	0.58460400	-2.61773000	-0.39316200
H	2.06821600	-1.79090600	0.17076600
H	1.62765300	-1.72388900	-1.51955900
H	0.96285500	2.98887700	-0.07912900
H	-1.54202100	2.95701600	0.24586400
H	-1.52269400	-1.38742800	-0.08479800
O	4.28944000	-1.14060700	0.61670900
H	3.83052600	-0.43965800	0.12683700
H	4.38054600	-0.77458700	1.50525400
O	-3.75097600	-2.02242800	0.21319700
H	-3.70116400	-1.05911000	0.34144100
H	-4.16401400	-2.11700300	-0.65420200

## Compound II

E(B3LYP)= -688.93352418 au

C	-2.18292200	1.79350800	-0.09333400
C	-1.04870000	2.50213000	-0.15072600
C	0.27530000	1.84874300	-0.06176300
C	0.33634500	0.34273200	0.00407100
C	-0.82505200	-0.37036600	-0.00066200
C	-2.15680600	0.32307100	0.10430500
H	-3.16907600	2.24742700	-0.11344300
H	-1.02561000	3.58394300	-0.24014600
C	-0.81868800	-1.87269500	-0.10812100
C	0.49167800	-2.51911300	0.06016300
H	0.48316400	-3.60446100	0.08125300
C	1.62451100	-1.80984900	0.11736100
C	1.71422900	-0.30961000	0.04816400
O	-3.18555900	-0.26076100	0.40456800
O	1.28700400	2.54401300	-0.06955400
O	-1.82332000	-2.51900700	-0.36512100
C	2.53726200	0.04405000	-1.22652700
H	3.50150200	-0.47315000	-1.19281200
H	2.01240000	-0.27877900	-2.13032100
H	2.71881100	1.11737600	-1.27989500
C	2.48918400	0.16269000	1.31518300
H	1.93229000	-0.08098300	2.22469800
H	2.66727500	1.23682400	1.27976100
H	3.45403900	-0.35227000	1.36138100
H	2.58214200	-2.32164500	0.20170200

## Compound IIa

E(B3LYP)= -841.79970691 au

C	0.56269300	-2.34040300	-0.49053800
C	1.64405300	-1.59296800	-0.22987000
C	1.54138100	-0.12604700	-0.08537400
C	0.18601500	0.52403000	-0.13528700
C	-0.90719800	-0.26951400	-0.29694300
C	-0.76291800	-1.71297300	-0.69472300
H	0.61508400	-3.41184200	-0.65749400
H	2.65091300	-1.99419400	-0.13961900
C	-2.28861700	0.27832400	-0.11602500
C	-2.41347000	1.73767200	-0.16100300
H	-3.42278300	2.13635000	-0.18110600
C	-1.33024600	2.52129200	-0.07170600
C	0.09017600	2.03542800	0.03477600
O	-1.64887400	-2.31067500	-1.28527500

O	2.56240400	0.54008800	0.10820300
O	-3.25305000	-0.44461600	0.12456500
C	0.62374100	2.47660900	1.43055700
H	0.50391500	3.55876500	1.54385100
H	0.06529000	1.98611300	2.23270900
H	1.68130000	2.23042600	1.52668600
C	0.90487900	2.74981900	-1.08542200
H	0.54368800	2.45880500	-2.07617300
H	1.96366300	2.50639200	-1.00545900
H	0.78562000	3.83334400	-0.98619700
H	-1.44723800	3.60333600	-0.03719900
H	-2.61624800	-1.91137400	1.26064300
O	-1.94838900	-2.42406700	1.75054000
H	-2.08336700	-3.32426400	1.42808300
H	4.26694100	-0.50596000	0.15248500
O	4.83639700	-1.29277400	0.20205700
H	5.00237900	-1.39715100	1.14741700

### Compound IIb

E(B3LYP)= -918.23365777 au

C	0.12882900	3.00617300	-0.19251500
C	1.40184300	2.62725500	-0.02480900
C	1.77652800	1.20071000	0.11092700
C	0.71081100	0.15025500	-0.04384800
C	-0.56423900	0.55325500	-0.30301400
C	-0.95649500	1.99807700	-0.19969600
H	-0.18266700	4.04499100	-0.24006800
H	2.22565900	3.33000400	0.05271300
C	-1.62582200	-0.43145200	-0.68205400
C	-1.33749200	-1.83394800	-0.38711200
H	-2.15821300	-2.53523900	-0.49720400
C	-0.09644400	-2.22213900	-0.06846600
C	1.09923600	-1.31853500	0.07279400
O	-2.11495300	2.35909200	-0.04330800
O	2.95594700	0.92310800	0.31593900
O	-2.63621200	-0.07506300	-1.28954000
C	2.12151200	-1.73110400	-1.02964600
H	2.26543300	-2.81569700	-0.99650200
H	1.74434900	-1.47406100	-2.02410600
H	3.09466000	-1.26592100	-0.86939300
C	1.70717500	-1.59382500	1.48193400
H	0.99803200	-1.32468800	2.26977000
H	2.63298100	-1.03738400	1.62071900
H	1.93154700	-2.66072900	1.57367400
H	0.11308700	-3.27837300	0.09100100
H	-3.10441600	0.90494700	1.27027000
O	-2.98415100	0.07932600	1.76114900
H	-3.64196100	-0.51731100	1.35671400

H	-5.54936000	-1.09215300	-0.10556400
O	-4.66567700	-1.46976500	-0.01514000
H	-4.12888900	-1.02949600	-0.70319200
H	4.67746400	-0.08232400	0.23473800
O	5.34059400	-0.72595400	-0.05401500
H	5.72524900	-0.32084300	-0.84122400

### Compound III

E(RB3LYP)= -857.66934114 au

C	1.58127800	0.11430700	-0.01924700
C	0.26761300	-0.39433400	0.09091100
C	-0.81193500	0.48882800	0.13198800
C	-0.54389300	1.87225300	0.07569700
C	1.75413000	1.51703900	-0.07902100
C	2.73134300	-0.82869500	-0.07582900
C	0.02205600	-1.87256700	0.18408100
C	1.19221500	-2.76887700	0.10189200
H	0.97657400	-3.83171900	0.15445500
C	2.43733800	-2.28458500	-0.01452500
H	3.31066200	-2.92800300	-0.06659400
O	-1.10450400	-2.32919400	0.33407100
O	3.89995100	-0.46595300	-0.17399900
C	3.09204100	2.19578400	-0.19883700
H	3.74783200	1.93539800	0.63656900
H	3.62202800	1.87622500	-1.10036200
H	2.92825500	3.27361100	-0.22334000
C	-1.65637600	2.88556200	0.13012300
H	-2.37522400	2.71921300	-0.68009300
H	-2.20834200	2.80178300	1.07171800
H	-1.23851000	3.88801700	0.03947900
N	0.70070800	2.34936500	-0.02865000
C	-2.24210200	0.03501100	0.27644700
O	-2.76253700	-0.31688300	-0.91266200
O	-2.86147700	0.08775200	1.31514900
C	-4.11148600	-0.81838800	-0.86169800
H	-4.78037900	-0.08228500	-0.41041000
H	-4.14183700	-1.74020900	-0.27631900
H	-4.39081400	-1.01138300	-1.89691700

### Compound IIIa

E(RB3LYP)= -1010.53200258 au

C	-1.31661500	-0.05441800	-0.28000500
C	0.07243500	0.09659500	-0.05612800
C	0.87284700	-1.03423400	0.10286000

C	0.25351500	-2.30177600	0.04375400
C	-1.84704900	-1.36544700	-0.34475100
C	-2.15858400	1.15689000	-0.44980300
C	0.68721100	1.46042400	0.02492300
C	-0.17644300	2.63335000	-0.20237100
H	0.32240400	3.59927000	-0.16055200
C	-1.49108600	2.48222900	-0.42378300
H	-2.15279800	3.32893200	-0.58018500
O	1.88236000	1.60096700	0.28378500
O	-3.37922300	1.12235300	-0.61195700
C	-3.29463500	-1.68233000	-0.59715500
H	-3.93539300	-1.29992400	0.20469100
H	-3.64728500	-1.21366400	-1.52055500
H	-3.39745100	-2.76577400	-0.66644200
C	1.04849100	-3.56661200	0.22713300
H	1.85534600	-3.63010000	-0.51169700
H	1.51598500	-3.58791000	1.21668800
H	0.39014300	-4.42772600	0.11527600
N	-1.05546400	-2.44021500	-0.18118000
C	2.35458700	-0.97036900	0.37374800
O	3.05025900	-0.83054400	-0.76794300
O	2.84384400	-1.13081100	1.46906900
C	4.47751200	-0.72232700	-0.60406500
H	4.87330300	-1.59733000	-0.08400000
H	4.71898400	0.17630200	-0.03195900
H	4.88302300	-0.65545000	-1.61283700
H	2.51583300	3.50052000	0.25167900
O	2.41788800	4.46764300	0.22708600
H	2.47363900	4.72863200	1.15498500
H	-4.86322300	0.67480300	0.65639400
O	-5.42341200	0.20983400	1.29685700
H	-6.19109600	-0.05645300	0.77545900

### Compound IV<sub>a</sub>

E(B3LYP)= -287.61650370 au

C	-0.00420700	0.93948400	0.00000000
C	-0.00376700	0.22122000	1.20813300
C	-0.00376700	-1.17145400	1.20227100
C	-0.00328600	-1.88137900	0.00000000
C	-0.00376700	-1.17145400	-1.20227100
C	-0.00376700	0.22122000	-1.20813300
N	-0.06261100	2.33598700	0.00000000
H	-0.00794700	0.76292000	-2.15112700
H	-0.00159300	-1.70508800	-2.14884900
H	-0.00161200	-2.96665200	0.00000000
H	-0.00159300	-1.70508800	2.14884900

H	-0.00794700	0.76292000	2.15112700
H	0.29717000	2.77662600	-0.83576700
H	0.29717000	2.77662600	0.83576700

### Compound IV<sub>a1</sub>

E(B3LYP)= -364.04607930 au

C	0.42577100	0.29183300	0.00000000
C	0.42402700	-0.41922700	1.20869400
C	0.42402700	-1.81270300	1.20341700
C	0.42424900	-2.52007400	0.00000000
C	0.42402700	-1.81270300	-1.20341700
C	0.42402700	-0.41922700	-1.20869400
N	0.36420800	1.70300400	0.00000000
H	0.41994800	0.12343100	-2.15085300
H	0.42588200	-2.34721400	-2.14907200
H	0.42593400	-3.60532100	0.00000000
H	0.42588200	-2.34721400	2.14907200
H	0.41994800	0.12343100	2.15085300
H	0.76652500	2.12514700	-0.82926700
H	0.76652500	2.12514700	0.82926700
H	-1.40841500	2.68011700	0.00000000
O	-2.14196000	3.32293500	0.00000000
H	-2.93276800	2.77057700	0.00000000

### Compound V<sub>a</sub>

E(B3LYP)= -499.00103432

C	-0.84687400	0.00293800	-0.05996200
C	-1.56735600	-1.16075400	0.26511300
C	-2.96357100	-1.15415200	0.28768700
C	-3.67838400	0.00710300	0.00522900
C	-2.97187900	1.17014200	-0.31413600
C	-1.58222200	1.16974800	-0.35380900
N	0.56369800	0.02567300	-0.14198900
H	-1.05783200	2.07389400	-0.64541400
H	-3.50834900	2.08493100	-0.55107200
H	-4.76362800	0.00870000	0.02844700
H	-3.49085400	-2.06949800	0.54275000
H	-1.04432800	-2.07537500	0.51787100
C	1.26130300	1.08141400	0.60675300
C	1.27523500	-1.24905500	-0.07249100
C	2.71262000	-1.07491000	-0.56561800
N	3.38247900	-0.05182500	0.23479800
C	2.69563800	1.23224800	0.10489100
H	4.35190000	0.03887500	-0.05612500

H	2.66552400	1.60226100	-0.93711000
H	3.21472300	1.97945800	0.71520800
H	2.68094200	-0.82680500	-1.64285000
H	3.24745400	-2.02435800	-0.45336800
H	0.76448200	-1.97225900	-0.71431400
H	1.29529900	-1.65511800	0.95471100
H	1.28314900	0.84304900	1.68439600
H	0.73121700	2.02697700	0.48526300

### Compound **V<sub>a1</sub>**

E(B3LYP)= -575.43516228 au

C	-1.20876900	-0.11321800	0.13652200
C	-1.76524600	1.16983900	0.28034000
C	-3.13770200	1.37360000	0.12216400
C	-3.98535600	0.31587000	-0.19767500
C	-3.44041900	-0.96246100	-0.34804100
C	-2.07739800	-1.17785400	-0.17690200
N	0.16857600	-0.37243300	0.33550500
H	-1.68169500	-2.18557600	-0.25552800
H	-4.08518700	-1.80453200	-0.58435400
H	-5.05089700	0.47992900	-0.32419300
H	-3.53865400	2.37675300	0.23890300
H	-1.13009200	2.01994700	0.49914100
C	0.87273100	-1.06242000	-0.75207300
C	0.98647100	0.69647800	0.91473400
C	2.31490600	0.12323800	1.40923900
N	3.01305700	-0.52598200	0.28926600
C	2.20314300	-1.62356600	-0.25518300
H	3.91387600	-0.87961200	0.60160600
H	2.00046500	-2.40396800	0.49797700
H	2.74224200	-2.08466400	-1.08965400
H	2.11999900	-0.58024100	2.23603900
H	2.94076300	0.93734500	1.78757300
H	0.45017500	1.12739100	1.76436400
H	1.20281200	1.49735300	0.18922300
H	1.06672700	-0.37130200	-1.59184600
H	0.25443800	-1.87730600	-1.13125300
O	3.22350100	1.86757000	-1.35720000
H	3.26096200	0.99547600	-0.90915800
H	2.90045500	1.66430800	-2.24339000

### Compound **VIII**

E(B3LYP)= -707.21384648 au

C	0.87726600	-0.86726100	-0.15598200
C	0.46082800	0.42194500	0.01227000
C	1.48958800	1.52790000	0.14106900
C	2.90740900	1.16022700	0.13799400
C	3.31424900	-0.11665400	-0.00400000
C	2.28891200	-1.21311800	-0.18037400
O	1.11416100	2.69378800	0.24063000
O	2.67721600	-2.37066400	-0.34669500
C	4.75021700	-0.53708000	-0.01416800
H	4.98664200	-1.05762000	-0.94765100
H	4.94054900	-1.25853600	0.78722600
H	5.41869500	0.31832800	0.10412900
H	0.19293000	-1.69097400	-0.30612800
H	3.60473700	1.98542300	0.25096400
N	-0.80248500	0.92560200	0.05212200
H	-0.79714100	1.94269400	0.07573200
C	-2.05658800	0.29542700	0.03310800
C	-3.14954500	1.04104600	-0.44092000
C	-2.27060900	-1.00765500	0.50835700
C	-4.42585800	0.48875600	-0.45435400
H	-2.98592300	2.05152900	-0.80594300
C	-3.55421300	-1.55215600	0.48184200
H	-1.45372400	-1.57840400	0.92999500
C	-4.63586600	-0.81561900	-0.00061700
H	-5.25813000	1.07858000	-0.82655600
H	-3.70629400	-2.56077900	0.85444300
H	-5.63070400	-1.24899200	-0.01789700

### Compound VIIIa

E(B3LYP)= -860.08303829 au

C	0.77569400	-0.61561500	-0.30570100
C	0.05246700	0.51540100	-0.02728300
C	0.79372500	1.82481400	0.15517600
C	2.25461100	1.80985200	0.07992400
C	2.96024000	0.69003600	-0.17995400
C	2.21746900	-0.60867900	-0.38900300
O	0.18374000	2.87647100	0.35571000
O	2.85349300	-1.64461200	-0.63177900
C	4.44969500	0.66189000	-0.29948000
H	4.73738800	0.39692200	-1.32395700
H	4.88474700	-0.11700200	0.33666300
H	4.88429700	1.63306000	-0.05331300
H	0.30341200	-1.57028200	-0.49127200
H	2.73382600	2.77344600	0.22581500
N	-1.29412500	0.63532000	0.09084800
H	-1.65556300	1.59163200	0.14578200
C	-2.29415800	-0.35727300	0.04489500



C	-3.55457800	0.02497600	-0.44628900
C	-2.10668500	-1.66344600	0.52239700
C	-4.59819400	-0.89441500	-0.48105600
H	-3.69748600	1.04378700	-0.79270200
C	-3.16060000	-2.57540400	0.47588500
H	-1.16077400	-1.95722000	0.95935100
C	-4.40611100	-2.20239900	-0.02947200
H	-5.56540800	-0.58756900	-0.86788200
H	-3.00418000	-3.58311200	0.84915100
H	-5.21997500	-2.91972600	-0.06446600
H	-1.66021500	3.56240600	0.15287800
O	-2.59885000	3.30859500	0.13840800
H	-2.90267400	3.47171300	1.04086400
H	4.59625800	-2.25202900	-0.02992100
O	5.37262500	-2.39106900	0.54028000
H	4.99572000	-2.78678000	1.33589100

### Compound IX

E(B3LYP)= -707.21210249 au

C	-0.75325400	1.21595300	-0.17729100
C	-0.55125600	-0.12454500	-0.02196000
C	-1.73704400	-1.06050300	0.08105900
C	-3.10855500	-0.49388000	0.07112000
C	-3.25306300	0.83749700	-0.06255200
C	-2.09915000	1.76989100	-0.21118600
O	-1.54366000	-2.27038300	0.16613000
O	-2.31435300	2.97389700	-0.36273500
H	0.05589700	1.92190000	-0.30585400
N	0.62115400	-0.81858700	0.02329000
H	0.46623800	-1.82305800	0.02261400
C	1.95474000	-0.37943500	0.02829400
C	2.93086800	-1.25495600	-0.47693500
C	2.35310100	0.85693500	0.55954900
C	4.27414200	-0.89392800	-0.46518800
H	2.62520800	-2.21409200	-0.88638700
C	3.70204000	1.21044900	0.55702500
H	1.62431300	1.52097600	1.00565600
C	4.66853100	0.34554200	0.04410500
H	5.01444100	-1.58195600	-0.86238300
H	3.99617800	2.16946600	0.97301600
H	5.71589300	0.62988200	0.04564700
H	-4.23211700	1.30872800	-0.08112500
C	-4.24232700	-1.46856900	0.20413100
H	-4.21567800	-2.20673100	-0.60405100
H	-4.16224600	-2.03268900	1.13922800
H	-5.20472900	-0.95313300	0.18242900

## Compound IXa

E(B3LYP)= -860.08312887 au

C	-0.84882200	1.12639200	-0.20437200
C	-0.60661500	-0.21233500	-0.03831300
C	-1.77646300	-1.16689200	0.06360200
C	-3.16077600	-0.62606600	0.01916600
C	-3.33432900	0.70084800	-0.11940700
C	-2.19400200	1.64814600	-0.22964300
O	-1.59790400	-2.37906700	0.18146800
O	-2.44215100	2.86187800	-0.33568400
H	-0.06179900	1.85674100	-0.31539500
N	0.59843800	-0.83707800	0.03358200
H	0.56279200	-1.85812300	0.04519700
C	1.90851900	-0.31790100	0.01271600
C	2.92491800	-1.21345800	-0.37283700
C	2.25286200	0.99014900	0.39193500
C	4.25211300	-0.80155500	-0.39610700
H	2.65398800	-2.22736900	-0.65088500
C	3.58997600	1.38731700	0.35647100
H	1.51014200	1.70023200	0.72746300
C	4.59441700	0.50500000	-0.03803000
H	5.02187300	-1.50433200	-0.70124500
H	3.83945100	2.40371900	0.64548900
H	5.63019500	0.82863800	-0.06468100
H	-4.32276900	1.15058700	-0.15597900
C	-4.27823200	-1.62228600	0.13022600
H	-4.22325800	-2.36007900	-0.67685500
H	-4.20872200	-2.18382100	1.06760900
H	-5.24864400	-1.12356200	0.08776900
O	0.81586300	-3.86211500	0.04642600
H	-0.14598400	-3.72892700	0.02121100
H	0.99925800	-4.09363300	0.96622900
H	-0.82962100	3.91077900	-0.13431600
H	-0.05468300	4.39460900	1.08399300
O	0.06760600	4.16804400	0.15365000