

## Supporting Information

### Design and Synthesis of Novel Quinolinone-3-aminoamides and their $\alpha$ -Lipoic Acid Adducts as Antioxidant and Antiinflammatory Agents.

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#### Full experimental details and analytical and spectroscopic data for compounds **5**, **8**, **10**.

##### Additional $^1\text{H}$ NMR and IR Spectroscopic Data

#### *N*-ethylamino-1,2-dihydro-4-hydroxy-1-methyl-2-oxo-3-quinolinecarboxamide (**5**).

Prepared from quinolinone **3** and 1,2-ethylenediamine. Yield 50% (Method A) and 71% (Method B), orange solid, mp 167-169°C.  $^1\text{H}$  NMR ( $\text{CDCl}_3/\text{CF}_3\text{COOD}$ ):  $\delta$  10.62 (br s, 0.4H, CONH), 8.24 (dd, 1H,  $J_{5,6} = 8.1$  Hz,  $J_{5,7} = 1.2$  Hz, 5-H), 7.81 (pseudotriplet, 1H, 7-H), 7.48-7.7.36 (m, 2H, 6-H, 8-H), 3.83 (br s, 2H,  $\text{NH-CH}_2$ -), 3.69 (s, 3H, N- $\text{CH}_3$ ), 3.46 (br s, 2H,  $\text{-CH}_2\text{NH}_2$ ).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3/\text{CF}_3\text{COOD}$ ):  $\delta$  172.7 (9-C), 172.6 (4-C), 163.1 (2-C), 139.5 (8a-C), 135.3 (C-7), 126.0 (5-C), 124.2 (6-C), 116.7 (8-C), 115.1 (4a-C), 112.9 (3-C), 41.7 (10-C), 37.6 (11-C), 30.2 (N- $\text{CH}_3$ ).

$^1\text{H}$  NMR ( $\text{CDCl}_3/\text{CD}_3\text{OD}$ ):  $\delta$  10.45 (br s, 1H, CONH), 8.19 (d, 1H,  $J_{5,6} = 8.1$  Hz, 5-H), 7.67 (pseudotriplet, 1H, 7-H), 7.37-7.29 (m, 2H, 6-H, 8-H), 3.66 (s, 3H, N- $\text{CH}_3$ ), 3.49 (pseudotriplet, 2H,  $\text{NH-CH}_2$ -), 2.91 (pseudotriplet, 2H,  $\text{-CH}_2\text{NH}_2$ ).

IR(KBr/ $\text{cm}^{-1}$ ): 1633, 1588, 1532.

Anal. ( $\text{C}_{13}\text{H}_{15}\text{N}_3\text{O}_3$ ) C, H, N.

#### *N*-ethylamino-1,2-dihydro-4-hydroxy-2-oxo-1-phenyl-3-quinolinecarboxamide (**6**). $^1\text{H}$

NMR ( $\text{CDCl}_3/\text{CD}_3\text{OD}$ ):  $\delta$  10.30 (br s, 1H, CONH), 8.22 (d, 1H,  $J_{5,6} = 8.1$  Hz, 5-H), 7.63-7.54

(m, 2H), 7.45 (pseudotriplet, 1H), 7.29-7.25 (m, 4H), 6.62 (d, 1H,  $J = 8.7$  Hz), 3.52 (br s, 2H, NH-CH<sub>2</sub>-), 2.94 (pseudotriplet, 2H, -CH<sub>2</sub>NH<sub>2</sub>).

IR(KBr/cm<sup>-1</sup>): 1634, 1601, 1532.

***N*-hexylamino-1,2-dihydro-4-hydroxy-1-methyl-2-oxo-3-quinolinecarboxamide (7).**

IR(KBr/cm<sup>-1</sup>): 1627, 1542.

***N*-hexylamino-1,2-dihydro-4-hydroxy-2-oxo-1-phenyl-3-quinolinecarboxamide (8).**

Prepared from quinolinone **4** and 1,6-hexamethylenediamine. Yield 46% (Method A) and 74% (Method B), white solid, mp 183-185°C. <sup>1</sup>H NMR (CDCl<sub>3</sub>/CD<sub>3</sub>OD):  $\delta$  10.10 (br s, 1H, CONH), 8.25 (d, 1H,  $J_{5,6} = 8.4$  Hz, 5-H), 7.62-7.55 (m, 2H), 7.45 (pseudotriplet, 1H), 7.29-7.26 (m, 4H), 6.63 (d, 1H,  $J = 8.7$  Hz), 3.49-3.37 (m, 2H, NH-CH<sub>2</sub>-), 2.66 (pseudotriplet, 2H, -CH<sub>2</sub>NH<sub>2</sub>), 1.59-1.18 (m, 8H, -(CH<sub>2</sub>)<sub>4</sub>-).

IR(KBr/cm<sup>-1</sup>): 1614, 1552.

Anal. (C<sub>22</sub>H<sub>25</sub>N<sub>3</sub>O<sub>3</sub>) C, H, N.

***N*-o-phenylamino-1,2-dihydro-4-hydroxy-1-methyl-2-oxo-3-quinolinecarboxamide (9).**

IR(KBr/cm<sup>-1</sup>): 3399, 3335, 3017, 1642, 1563.

***N*-o-phenylamino-1,2-dihydro-4-hydroxy-2-oxo-1-phenyl-3-quinolinecarboxamide**

**(10).** Prepared from quinolinone **4** and 1,2-phenylenediamine, according to Method B. Yield 85%, light green solid, mp 229-231°C. <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  16.81 (s, 1H, OH), 11.88 (s, 1H, CONH), 8.27 (dd, 1H,  $J_{5,6} = 8.1$ ,  $J_{5,7} = 1.5$  Hz, 5-H), 7.67-7.57 (m, 3H), 7.52-7.46 (m, 1H), 7.40 (dd, 1H,  $J = 8.1$ , 1.8 Hz), 7.33-7.28 (m, 3H), 7.06 (pseudotriplet, 1H), 6.82-6.78 (m, 2H), 6.67 (d, 1H,  $J = 8.7$  Hz), 3.82 (br s, 2H, -NH<sub>2</sub>). <sup>13</sup>C NMR (CDCl<sub>3</sub>):  $\delta$  173.1 (4-C), 169.7

(CONH), 163.3 (2-C), 141.0, 140.7 (8a-C), 137.1, 133.7 (7-C), 130.5, 129.4, 129.1, 127.4, 125.6, 125.3 (5-C), 122.9 (6-C), 122.8, 119.1, 117.3, 116.2 (4a-C), 116.0 (8-C), 97.2 (3-C).

IR(KBr/cm<sup>-1</sup>): 3399, 3065, 1634, 1563.

Anal. (C<sub>22</sub>H<sub>17</sub>N<sub>3</sub>O<sub>3</sub>) C, H, N.

***N*-p-phenylamino-1,2-dihydro-4-hydroxy-1-methyl-2-oxo-3-quinolinecarboxamide**

**(11)**. IR(KBr/cm<sup>-1</sup>): 3404, 3336, 3070, 1645, 1589, 1560.

***N*-p-phenylamino-1,2-dihydro-4-hydroxy-2-oxo-1-phenyl-3-quinolinecarboxamide**

**(12)**. IR(KBr/cm<sup>-1</sup>): 3481, 3382, 3051, 1635, 1601, 1559.

***N*-(1,2-dihydro-4-hydroxy-1-methyl-2-oxo-3-quinolinecarbonyl)-N'-(1,2-dithiolane-3-pentanoyl)-ethylenediamine (14)**. IR(KBr/cm<sup>-1</sup>): 3292, 3195, 3083, 1634, 1547.

***N*-(1,2-dihydro-4-hydroxy-2-oxo-1-phenyl-3-quinolinecarbonyl)-N'-(1,2-dithiolane-3-pentanoyl)-ethylenediamine (15)**. IR(KBr/cm<sup>-1</sup>): 3326, 3237, 3063, 1644, 1557.

***N*-(1,2-dihydro-4-hydroxy-1-methyl-2-oxo-3-quinolinecarbonyl)-N'-(1,2-dithiolane-3-pentanoyl)-hexamethylenediamine (16)**. IR(KBr/cm<sup>-1</sup>): 3287, 3088, 1635, 1566.

***N*-(1,2-dihydro-4-hydroxy-2-oxo-1-phenyl-3-quinolinecarbonyl)-N'-(1,2-dithiolane-3-pentanoyl)-hexamethylenediamine (17)**. IR(KBr/cm<sup>-1</sup>): 3299, 3070, 1643, 1560.

**Combustion Analysis Data for all new Compounds**

<b>Compd</b>	<b>Calcd</b>				<b>Found</b>			
	<b>C</b>	<b>H</b>	<b>N</b>	<b>S</b>	<b>C</b>	<b>H</b>	<b>N</b>	<b>S</b>
<b>5</b>	59.76	5.79	16.08		59.51	5.58	16.65	
<b>6</b>	66.86	5.30	13.00		66.91	5.06	12.84	
<b>7</b>	64.33	7.30	13.24		64.21	7.72	12.92	
<b>8</b>	69.64	6.64	11.07		69.34	6.83	11.03	
<b>9</b>	66.01	4.89	13.58		66.32	4.62	13.67	
<b>10</b>	71.15	4.61	11.31		71.04	5.02	11.06	
<b>11</b>	66.01	4.89	13.58		65.72	4.61	13.03	
<b>12</b>	71.15	4.61	11.31		71.29	4.48	11.00	
<b>14</b>	56.10	6.05	9.35	14.26	56.48	6.57	9.24	13.97
<b>15</b>	61.03	5.71	8.21	12.53	59.99	5.44	8.02	12.53
<b>16</b>	59.38	6.98	8.31	12.68	59.83	6.89	8.97	12.85
<b>17</b>	63.46	6.57	7.40	11.30	63.15	6.58	7.74	11.57
<b>18</b>	64.38	5.22	7.51	11.46	63.99	5.43	7.86	11.09