

## Supporting Information

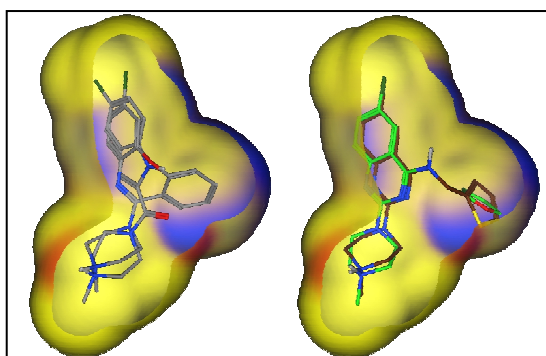
### The discovery of quinazolines as histamine H<sub>4</sub> receptor ligands using a scaffold hopping approach

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Experimental details for compounds **7**, **19-22**, **26-29**, **32-33**, **35-39**, **41-64**.

***N*-benzyl-6-chloro-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (7)**

Synthesized from 2,4,6-trichloroquinazoline and benzylamine according to general method A. Yield: 512 mg (54%). Mp 124.6-126.9°C; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ (ppm) 7.44-7.31 (m, 8H), 5.63 (s, 1H), 4.76 (d, *J*= 5.3 Hz, 2H), 3.89 (t, *J*= 5.0 Hz, 4H), 2.44, (t, *J*= 5.0 Hz, 4H), 2.31 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 158.90, 158.87, 150.74, 138.55, 132.83, 128.43, 127.55, 127.20, 126.96, 125.39, 120.65, 111.05, 54.96, 46.09, 44.91, 43.71; MS (ESI) *m/z* 368 (M+H)<sup>+</sup>.

**7-chloroquinazolin-2,4(1*H*,3*H*)-dione (19)**

Prepared according to general method D from 2-amino-4-chlorobenzoic acid ( 4.25 g, 24.8 mmol) and urea ( 15.0 g, 248 mmol). Yield: 2.87 g (59%) of a beige powder. <sup>1</sup>H-NMR (DMSO- $\delta_6$ ) δ (ppm) 11.40 (br s, 1H), 11.24 (br s, 1H), 7.86 (d, *J*= 8.4 Hz, 1H), 7.22-7.15 (m, 2H).

**6-chloro-8-methylquinazolin-2,4(1*H*,3*H*)-dione (20)**

Prepared according to general method D from 2-amino-3-methyl-5-chlorobenzoic acid (4.0 g, 21.6 mmol) and urea (12.93 g, 216 mmol). Yield: 3.79 g (83%) of a yellow powder. <sup>1</sup>H-NMR (DMSO- $\delta_6$ ) δ (ppm) 7.60 (s, 1H), 7.44 (s, 1H), 2.28 (s, 3H).

**6-fluoroquinazolin-2,4(1*H*,3*H*)-dione (21)**

Prepared according to general method D from 2-amino-5-fluorobenzoic acid (1.0 g, 6.45 mmol) and urea (3.87 g, 64.5 mmol). Yield: 968 mg (83%) of a white solid. <sup>1</sup>H-NMR (DMSO- $\delta_6$ ) δ (ppm) 11.29 (br s, 2H), 7.59-7.47 (m, 2H), 7.20-7.14 (m, 1H).

**5-methylquinazolin-2,4(1*H*,3*H*)-dione (22)**

Prepared according to general method D from 2-amino-6-methylbenzoic acid (3.75 g, 24.8 mmol) and urea (248 g, mmol). Yield: 1.94 g (44%) of a white powder. <sup>1</sup>H-NMR (DMSO- $\delta_6$ ) δ (ppm) 11.02 (br s, 2H), 7.42 (t, *J*= 7.8 Hz, 1H), 6.98 (d, *J*= 8.1 Hz, 1H), 6.91 (d, *J*= 7.4 Hz, 1H), 2.62 (s, 3H).

### **2,4,6-trichloro-8-methylquinazoline (26)**

Prepared according to general method E from 6-chloro-8-methylquinazolin-2,4(1*H*,3*H*)-dione (1.00 g, 4.76 mmol). Yield: 414 mg (35%). <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm); <sup>13</sup>C-NMR (CDCl<sub>3</sub>) δ (ppm) 8.01 (s, 1H), 7.72 (s, 1H), 2.69 (s, 3H); 162.83, 154.25, 150.12, 139.15, 136.48, 134.46, 122.88, 122.23, 17.13.

### **2,4-dichloro-6-fluoroquinazoline (27)**

Prepared according to general method E from 6-fluoroquinazolin-2,4(1*H*,3*H*)-dione (500 mg, 3.01 mmol). Yield: 470 mg (72%). <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 7.97-69 (m, 3H).

### **2,4-dichloro-5-methylquinazoline (28)**

Prepared according to general method E from 5-methylquinazolin-2,4(1*H*,3*H*)-dione (960 mg, 5.44 mmol). Yield: 1.07 g (90%). <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 7.77-7.67 (m, 2H), 7.43-7.38 (m, 1H), 2.92 (s, 3H); <sup>13</sup>C-NMR (CDCl<sub>3</sub>) δ (ppm) 162.89, 154.33, 153.94, 136.84, 135.08, 132.13, 126.73, 121.89, 24.83

### **2-(4-methylpiperazin-1-yl)quinazolin-4-amine (29)**

Synthesized from 2,4,6-trichloroquinazoline and saturated ammonia in EtOH according to general method A. After work-up the compound was purified by recrystallisation from EtOAc. Yield 162 mg (55%) of beige crystals. Mp 181.6-183.3°C; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.57-7.43 (m, 3H), 7.10-7.02 (m, 1H), 5.31 (s, 1H), 3.89 (t, *J*= 5.1 Hz, 4H), 2.45 (t, *J*= 5.1 Hz, 4H), 2.31 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 161.45, 158.81, 152.58, 133.01, 125.78, 121.60, 121.02, 109.63, 55.02, 46.12, 43.65; MS (ESI) *m/z* 244 (M+H)<sup>+</sup>.

### **4-(benzyloxy)-2-(4-methylpiperazin-1-yl)quinazoline (32)**

Synthesized from 2,4,6-trichloroquinazoline and benzylamine according to general method B. Yield 163 mg (32 %) of a yellow solid. Mp 88.0-89.0°C; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.94 (dd, *J*= 0.9 Hz, *J*= 8.1 Hz, 1H), 7.61-7.06 (m, 8H), 5.52 (s, 2H), 3.94 (t, *J*= 5.0 Hz, 4H), 2.48 (t, *J*= 5.1 Hz, 4H), 2.33 (s, 3H); MS (ESI) *m/z* 335 (M+H)<sup>+</sup>.

### **2-(4-methylpiperazin-1-yl)-*N*-phenylquinazolin-4-amine (33)**

Synthesized from 2,4,6-trichloroquinazoline and aniline according to general method A. Yield 165 mg (34%) of a beige solid. Mp 135.3-138.7°C; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.68-7.51 (m, 4H), 7.47-7.24 (m, 3H), 7.14-7.07 (m, 2H), 3.91 (t, *J*= 4.9 Hz, 4H), 2.46 (t, *J*= 5.0 Hz, 4H), 2.31 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 158.49, 157.32, 152.65, 138.55, 132.75, 128.70, 126.19, 123.56, 121.32, 121.01, 120.27, 110.25, 55.01, 46.13, 43.82; MS (ESI) *m/z* 320 (M+H)<sup>+</sup>.

#### **2-(4-methylpiperazin-1-yl)-*N*-phenethylquinazolin-4-amine (35)**

Synthesized from 2,4-dichloroquinazoline and phenethylamine according to general method A. Yield: 370 mg (71 %) of a yellow solid. Mp 92.5-95.2°C; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.52-7.42 (m, 2H), 7.36-7.01 (m, 6H), 7.04-6.96 (m, 1H), 5.57 (m, 1H), 3.94 (t, *J*= 5.0 Hz, 4H), 3.82 (q, *J*= 7.0 Hz, 2H), 2.98 (t, *J*= 7.0 Hz, 2H), 2.48 (t, *J*= 5.1 Hz, 4H), 2.33 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 159.50, 158.80, 151.99, 139.02, 132.32, 128.68, 128.56, 126.40, 125.76, 120.79, 120.33, 110.30, 55.07, 46.15, 43.71, 42.17, 35.18; MS (ESI) *m/z* 348 (M+H)<sup>+</sup>.

#### **6-chloro-2-(4-methylpiperazin-1-yl)-*N*-phenylethylquinazolin-4-amine (36)**

Synthesized from 2,4,6-trichloroquinazoline and phenethylamine according to general method A. Yield 232 mg (71%). Mp 136.6-138.8°C; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.38-7.19 (m, 8H), 5.42 (app br t, 1H), 3.94-3.89 (m, 4H), 3.80 (q, *J*= 6.9 Hz, 2 H), 2.97 (t, *J*= 7.1 Hz, 2H), 2.46 (t, *J*=5.1 Hz, 4H), 2.32 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 158.80, 159.70, 150.70, 138.81, 132.80, 128.62, 128.60, 127.34, 126.48, 125.45, 119.86, 110.83, 54.99, 46.10, 43.62, 42.30, 35.10; MS (ESI) *m/z* 382 (M+H)<sup>+</sup>.

#### **6-chloro-*N*-isopropyl-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (37)**

Synthesized from 2,4,6-trichloroquinazoline and isopropylamine according to general method A. Yield: 227 mg (83%). Mp 187.8-189.8°C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 7.42-7.31 (m, 3H), 5.13 (d, *J*= 6.6 Hz, 1H), 4.39 (sp, *J*= 6.6 Hz, 1H), 3.88 (t, *J*= 4.9 Hz, 4H), 2.45 (t, *J*= 5.0 Hz, 4H), 2.31 (s, 3H), 1.29 (d, *J*= 6.5 Hz, 6H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 158.88, 157.98, 150.69, 132.63, 127.34, 125.31, 119.89, 110.82, 55.00, 46.12, 43.59, 42.68, 22.35; MS (ESI) *m/z* 320 (M+H)<sup>+</sup>.

**6-chloro-*N,N*-dimethyl-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (38)**

Synthesized from 2,4,6-trichloroquinazoline and *N,N*-dimethylamine according to general method A. A solution of *N,N*-dimethylamine in EtOH (33%) was used and stirring was continued for 24 hours. Yield: 301 mg (77%) of a yellow solid. Mp 89.8-92.8°C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 7.75-7.74 (m, 1H), 7.39-7.38 (m, 2H), 3.88 (t, *J*= 5.1 Hz, 4H), 3.23 (s, 6H), 2.45 (t, *J*= 5.1 Hz, 4H), 2.32 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 163.67, 158.14, 152.94, 132.32, 127.32, 124.69, 124.26, 112.08, 55.02, 46.16, 43.69, 41.54; MS (ESI) *m/z* 306 (M+H)<sup>+</sup>.

**6-chloro-*N*-cyclohexyl-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (39)**

Synthesized from 2,4,6-trichloroquinazoline and cyclohexylamine according to general method A. Yield: 115 mg (36%). Mp 148.9-152.0°C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 7.41-7.30 (m, 3H), 5.49 (m, 1H), 3.88 (t, *J*= 4.9 Hz, 4H), 3.37 (t, *J*= 6.1 Hz, 2H), 2.44 (t, *J*= 5.0 Hz, 4H), 2.30 (s, 3H), 1.79-1.63 (m, 6H), 1.25-0.95 (m, 5H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 158.95, 158.88, 150.71, 132.68, 127.36, 125.33, 119.84, 110.88, 55.01, 47.30, 46.14, 43.62, 37.64, 31.04, 26.25, 25.26; MS (ESI) *m/z* 374 (M+H)<sup>+</sup>.

**7-chloro-*N*-methyl-2-(4-methylpiperazin-1-yl)-quinazolin-4-amine (41)**

Prepared according to general method E from 2,4,7-trichloroquinazoline (300 mg, 1.28 mmol) and methylamine (0.23 ml, 40% w/w in water). Yield: 219 mg (59%). <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 7.39 (d, *J*= 2.0, 1H), 7.30 (d, *J*= 8.6 Hz, 1H), 6.93 (dd, *J*= 2.1 Hz, *J*= 8.6 Hz, 1H), 5.47 (br s, 1H), 3.91 (t, *J*= 5.0 Hz, 4H), 4.81 (d, *J*= 4.8 Hz, 3H), 2.44 (t, *J*= 5.1 Hz, 4H); <sup>13</sup>C-NMR (CDCl<sub>3</sub>) δ (ppm) 159.98, 159.22, 153.02, 138.10, 124.81, 121.76, 121.08, 108.78, 55.03, 46.14, 43.58, 27.90.

**5-methyl-*N*-methyl-2-(4-methylpiperazin-1-yl)-quinazolin-4-amine (42)**

Prepared according to general method E from 2,4-dichloro-5-methylquinazoline (208 mg, 0.89 mmol) and methylamine (0.25 ml, 33% w/w in water). Yield: 196 mg (74%). <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 7.29-7.27 (m, 2H), 6.75 (m, 1H), 5.82 (br s, 1H), 3.88 (t, *J*= 4.5 Hz, 4H), 3.04 (d, *J*= 4.4 Hz, 3H), 2.69 (s, 3H), 2.45 (t, *J*= 4.3 Hz, 4H), 2.30 (s, 3H); <sup>13</sup>C-

NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 161.80, 158.10, 153.82, 132.51, 131.33, 124.38, 124.28, 110.98, 55.09, 46.17, 43.63, 28.52, 23.96.

***N*-(4-aminobenzyl)-6-chloro-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (43)**

Synthesized from 2,4,6-trichloroquinazoline and 4-aminobenzylamine according to general method A. Yield: 245 mg (74%) Mp 145.9-148.5°C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 7.37-7.32 (m, 3H), 7.15 (d, *J*= 8.4 Hz, 2H), 6.65 (d, *J*= 8.4 Hz, 2H), 5.47 (m, 1H), 4.60 (d, *J*=5.0 Hz, 2H), 3.91 (t, *J*=5.0 Hz, 4H), 2.45 (t, *J*= 5.0 Hz, 4H), 2.31 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 158.53, 158.40, 150.34, 147.34, 132.21, 128.40, 126.68, 126.11, 123.71, 121.87, 113.36, 111.11, 54.38, 45.67, 43.36, 43.09; MS (ESI) *m/z* 383 (M+H)<sup>+</sup>.

***N*-(4-methoxybenzyl)-6-chloro-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (44)**

Synthesized from 2,4,6-trichloroquinazoline and 4-methoxybenzylalcohol according to general method A. Yield: 202 mg (59%). <sup>1</sup>H-NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 7.35-7.19 (m, 5H), 6.82 (d, *J*= 7.7 Hz, 2H), 5.61 (m, 1H), 4.62 (d, *J*= 5.0 Hz, 2H), 3.86 (t, *J*= 4.5 Hz, 4H), 3.74 (s, 3H), 2.41 (t, *J*= 4.6 Hz, 4H), 2.27 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 158.95, 158.73, 158.55, 150.67, 132.83, 130.20, 129.16, 127.25, 125.49, 120.02, 113.95, 110.74, 55.14, 54.92, 46.04, 44.64, 43.58; MS (ESI) *m/z* 398 (M+H)<sup>+</sup>.

***N*-(4-fluorobenzyl)-6-chloro-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (45)**

Synthesized from 2,4,6-trichloroquinazoline and 4-fluorobenzylamine according to general method A. Purification was done by trituration with a small amount of ether. Yield: 315 mg (95%). Mp 127.4-131.5°C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>)  $\delta$  (ppm); 7.40-7.19 (m, 5H), 7.01-6.92 (m, 2H), 5.68 (m, 1H), 4.67 (d, *J*= 5.4 Hz, 2H), 3.84 (t, *J*= 4.8 Hz, 4H), 2.39 (t, *J*= 5.1 Hz, 4H), 2.27 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 164.44, 159.56, 158.68, 158.63, 150.65, 134.19, 134.13, 132.94, 129.40, 129.24, 127.20, 125.61, 120.21, 115.55, 115.12, 110.78, 54.87, 46.00, 44.34, 43.56; MS (ESI) *m/z* 386 (M+H)<sup>+</sup>.

***N*-(6-chloro-2-(4-methylpiperazin-1-yl)quinazolin-4-ylamino)methylbenzotrile (46)**

Synthesized from 2,4,6-trichloroquinazoline and 4-cyanobenzylamine according to general method A. Yield: 252 mg (75%). Mp 127.4-131.5°C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 7.60 (d, *J*= 8.4 Hz, 2H), 7.47-7.35 (m, 5H), 5.85 (m, 1H), 4.82 (d, *J*= 5.7 Hz, 2H), 3.80 (t, *J*= 5.0 Hz, 4H), 2.38 (t, *J*= 5.0 Hz, 4H), 2.29 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 158.63, 158.16, 150.36, 145.53, 132.50, 131.97, 127.87, 126.80, 123.94, 121.82, 118.70, 110.88, 109.13, 54.22, 45.60, 43.53, 43.04; MS (ESI) *m/z* 393 (M+H)<sup>+</sup>.

**6-chloro-*N*-(3,4-difluorobenzyl)-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (47)**

Synthesized from 2,4,6-trichloroquinazoline and 3,4-difluorobenzylamine according to general method A. Yield: 294 mg (85%). Mp 127.4-131.5°C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm); 7.49 (d, *J*= 1.6 Hz, 1H), 7.44-7.33 (m, 2H), 7.19-7.03 (m, 3H), 5.97 (m, 1H), 4.68 (d, *J*= 5.6 Hz, 2H), 3.85 (t, *J*= 5.0 Hz, 4H), 2.43 (t, *J*= 5.0 Hz, 4H), 2.30 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 158.59, 158.47, 150.71, 135.46, 133.12, 127.36, 125.78, 123.51, 123.43, 123.38, 123.31, 119.99, 117.41, 117.07, 116.69, 116.35, 110.57, 54.82, 45.98, 44.09, 44.06, 43.55; MS (ESI) *m/z* 404 (M+H)<sup>+</sup>.

**2-(6-chloro-2-(4-methylpiperazin-1-yl)quinazolin-4-ylamino)ethanol (48)**

Synthesized from 2,4,6-trichloroquinazoline and 2-aminoethanol according to general method A. The compound was purified by recrystallisation from EtOAc. Yield: 207 mg (75 %) of a white fluffy solid. Mp 188.7-190.3°C; <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) δ (ppm) 8.14 (d, *J*= 2.3 Hz, 1H), 7.48 (dd, *J*= 2.2 Hz, *J*= 8.9 Hz, 1H), 7.25 (d, *J*= 8.9 Hz, 1H), 4.76 (t, *J*= 5.4 Hz, 1H), 3.75 (app br s, 4H), 3.63-3.51 (m, 4H), 2.33 (t, *J*= 4.6 Hz, 4H), 2.19 (s, 3H); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>) δ (ppm) 159.94, 158.40, 132.18, 126.67, 123.67, 121.89, 111.09, 58.68, 54.36, 45.36, 43.15, 43.04; MS (ESI) *m/z* 322 (M+H)<sup>+</sup>.

**ethyl 2-(6-chloro-2-(4-methylpiperazin-1-yl)quinazolin-4-ylamino)acetate (49)**

Synthesized from 2,4,6-trichloroquinazoline and ethyl 2-aminoacetate according to general method A. The compound was purified by recrystallisation from EtOAc. Yield: 150 mg (42%) of a white fluffy solid. Mp 108.5-109.7°C; <sup>1</sup>H-NMR (DMSO- *d*<sub>6</sub>) δ (ppm) 8.65 (m, 1H), 8.12 (d, *J*= 2.3 Hz, 1H), 7.52 (dd, *J*= 2.3 Hz, *J*= 9.0 Hz, 1H), 7.27 (d, *J*= 9.0 Hz, 1H), 4.14-4.03 (m, 4H), 3.69 (m, 4H), 3.33-3.31 (m, 2H), 2.29 (m, 4H), 2.18 (s,

3H), 1.16 (t,  $J= 7.1$  Hz, 3H);  $^{13}\text{C}$  NMR (DMSO-  $\delta_6$ )  $\delta$  (ppm) 169.86, 158.83, 157.94, 150.26, 132.60, 126.80, 123.97, 121.86, 110.73, 60.04, 54.29, 45.62, 42.91, 13.91; MS (ESI)  $m/z$  364 (M+H) $^+$ .

**6-chloro-*N*-(furan-2-ylmethyl)-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (50)**

Synthesized from 2,4,6-trichloroquinazoline and furan-2-ylmethanamine according to general method A. Yield: 270 mg (77 %) of a light brown solid. Mp 156.5-158.8°C;  $^1\text{H}$ -NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 7.42-7.32 (m, 4H), 6.32 (d,  $J= 1.8$  Hz, 1H), 6.27 (d,  $J= 1.8$  Hz, 1H), 5.67 (m, 1H), 4.73 (d,  $J= 5.1$  Hz, 2H), 3.90-3.88 (m, 4H), 2.45 (t,  $J= 4.9$  Hz, 4H), 2.31 (s, 3H);  $^{13}\text{C}$  NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 158.62, 158.41, 151.21, 150.79, 142.12, 132.95, 127.33, 125.54, 120.04, 110.71, 110.37, 107.61, 54.99, 46.13, 43.64, 38.04; MS (ESI)  $m/z$  358 (M+H) $^+$ .

***N*-(furan-2-ylmethyl)-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (51)**

Prepared according to general method E from 2,4-dichloroquinazoline (200 mg, 1.01 mmol) and furfurylamine (89  $\mu\text{l}$ , 1.01 mmol). Yield: 205 mg (63%).  $^1\text{H}$ -NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 7.52-7.39 (m, 3H), 7.35-7.34 (m, 1H), 7.05-6.97 (m, 1H), 5.75 (m, 1H), 4.74 (d,  $J= 5.2$  Hz, 2H), 3.91 (t,  $J= 5.0$  Hz, 4H), 2.45 (t,  $J= 5.0$  Hz, 4H), 2.30 (s, 3H);  $^{13}\text{C}$ -NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 159.22, 158.58, 152.08, 151.59, 141.98, 132.47, 125.72, 120.86, 110.34, 110.19, 107.42, 55.02, 46.13, 43.68, 37.96.

**6-fluoro-*N*-(furan-2-ylmethyl)-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (52)**

Prepared according to general method E from 2,4-dichloro-6-fluoroquinazoline (200 mg, 0.92 mmol) and furfurylamine (80  $\mu\text{l}$ , 0.92 mmol). Yield: 225 mg (72%).  $^1\text{H}$ -NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 7.45-7.20 (m, 3H), 7.09 (dd,  $J= 8.9$  Hz,  $J= 2.7$  Hz, 1H), 6.34-6.26 (m, 2H), 5.55 (m, 1H), 4.74 (d,  $J= 5.2$  Hz, 2H), 3.89 (t,  $J=5.0$  Hz, 4H), 2.46 (t,  $J= 5.1$  Hz, 4H), 2.32 (s, 3H);  $^{13}\text{C}$ -NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 159.33, 158.90, 158.82, 158.42, 154.53, 151.30, 149.04, 142.10, 127.85, 127.70, 121.91, 121.43, 110.36, 109.81, 109.65, 107.56, 105.24, 104.79, 55.00, 46.14, 43.71, 38.06.

**6-chloro-8-methyl-N-(furan-2-ylmethyl)-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (53)**

Prepared according to general method E from 2,4,6-trichloro-8-methylquinazoline (200 mg, 0.81 mmol) and furfurylamine (72  $\mu$ l, 0.81 mmol). Yield: 244 mg (82%).  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ )  $\delta$  (ppm) 7.35 (s, 1H), 7.29-7.22 (m, 3H), 6.31-6.25 (m, 2H), 5.56 (m, 1H), 4.72 (d,  $J$ = 5.2 Hz, 2H), 3.92 (t,  $J$ = 4.83 Hz, 4H), 2.48-2.43 (m, 7H), 2.32 (s, 3H);  $^{13}\text{C-NMR}$  ( $\text{CDCl}_3$ )  $\delta$  (ppm) 158.86, 157.84, 151.46, 149.66, 142.02, 136.26, 132.51, 124.91, 117.39, 110.35, 110.05, 107.47, 54.93, 46.07, 43.54, 38.09, 17.34.

**6-chloro-N-(furan-3-ylmethyl)-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (54)**

Synthesized from 2,4,6-trichloroquinazoline and furan-3-ylmethanamine according to general method A. Yield: 174 mg (87%). Mp 133.5-138.5 $^\circ\text{C}$ ;  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ )  $\delta$  (ppm) 7.42-7.31 (m, 5H), 6.41 (s, 1H), 5.53 (m, 1H), 4.57 (d,  $J$ = 5.2 Hz, 2H), 3.90 (t,  $J$ =5.0 Hz, 4H), 2.44 (t,  $J$ = 5.0 Hz, 4H), 2.30 (s, 3H);  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ )  $\delta$  (ppm) 158.68, 158.57, 150.73, 143.44, 140.26, 132.93, 127.36, 125.56, 122.07, 119.95, 110.69, 110.29, 54.96, 46.08, 43.59, 35.95; MS (ESI)  $m/z$  358 (M+H) $^+$ .

**6-chloro-2-(4-methylpiperazin-1-yl)-N-(thiophen-2-ylmethyl)quinazolin-4-amine (55)**

Synthesized from 2,4,6-trichloroquinazoline and thiophen-2-ylmethanamine according to general method A. Yield: 246 mg (77%). Mp 153.8-155.7 $^\circ\text{C}$ ;  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ )  $\delta$  (ppm) 7.43-7.33 (m, 3H), 7.20 (d,  $J$ = 1.2 Hz, 1H), 7.04-6.93 (m, 2H), 5.66 (m, 1H), 4.92 (d, 5.4 Hz, 2H), 3.94 (t,  $J$ = 5.0 Hz, 4H), 2.46 (t,  $J$ = 5.1 Hz, 4H), 2.32 (s, 3H);  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ )  $\delta$  (ppm) 158.55, 158.27, 150.84, 140.84, 132.97, 127.35, 126.55, 126.13, 125.53, 125.33, 119.97, 110.62, 55.01, 46.13, 43.67, 39.77; MS (ESI)  $m/z$  374 (M+H) $^+$ .

**6-chloro-(4-methylpiperazin-1-yl)-N-(thiophen-3-ylmethyl)quinazolin-4-amine (56)**

Synthesized from 2,4,6-trichloroquinazoline and thiophen-3-ylmethanamine according to general method A. Yield: 211 mg (66%). Mp 144.0-146.0 $^\circ\text{C}$ ;  $^1\text{H-NMR}$  ( $\text{CDCl}_3$ )  $\delta$  (ppm) 7.43-7.23 (m, 5H), 7.09 (d,  $J$ = 5.0 Hz, 1H), 5.59 (m, 1H), 4.75 (d,  $J$ = 5.3 Hz, 2H), 3.90 (t,  $J$ = 5.0 Hz, 4H), 2.45 (t,  $J$ = 5.0 Hz, 4H), 2.31 (s, 3H);  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ )  $\delta$  (ppm)

158.68, 158.54, 150.73, 138.97, 132.95, 127.33, 126.40, 125.61, 122.50, 120.01, 54.93, 46.04, 43.57, 40.26; MS (ESI)  $m/z$  424 (M+H)<sup>+</sup>.

**6-chloro-2-(4-methylpiperazin-1-yl)-N-(2-(thiophen-2-yl)ethyl)quinazolin-4-amine (57)**

Synthesized from 2,4,6-trichloroquinazoline and 2-(thiophen-2-yl)ethanamine according to general method A. Yield: 246 mg (77%) of a brown oil. <sup>1</sup>H-NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 7.42-7.32 (m, 3H), 7.17 (d,  $J$ = 4.0 Hz, 1H), 6.95 (t,  $J$ = 4.3 Hz, 1H), 6.83 (d,  $J$ = 3.1 Hz, 1H), 5.55 (m, 1H), 3.93-3.77 (m, 6H), 3.19 (t,  $J$ = 6.7 Hz, 2H), 2.46 (t,  $J$ = 5.0 Hz, 4H), 2.32 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 158.76, 158.62, 150.76, 141.18, 132.87, 127.37, 127.01, 125.49, 125.27, 123.96, 119.89, 110.82, 55.01, 46.14, 43.65, 42.50, 29.18; MS (ESI)  $m/z$  388 (M+H)<sup>+</sup>.

**6-chloro-N-((5-methylfuran-2-yl)methyl)-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (58)**

Synthesized from 2,4,6-trichloroquinazoline and (5-methylfuran-2-yl)methanamine according to general method A. Yield: 330 mg (100%). Mp 109.2-114.7°C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 7.41-7.32 (m, 3H), 6.15 (d,  $J$ = 2.9 Hz, 1H), 5.90 (m, 1H), 5.60 (m, 1H), 4.66 (d,  $J$ = 5.0 Hz, 2H), 3.91 (t,  $J$ = 5.0 Hz, 4H), 2.45 (t,  $J$ = 5.0 Hz, 4H), 2.31 (s, 3H), 2.26 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 158.66, 158.40, 151.94, 150.73, 149.26, 132.89, 127.27, 125.50, 120.13, 110.80, 108.60, 106.20, 54.98, 46.09, 43.62, 38.16, 13.44; MS (ESI)  $m/z$  372 (M+H)<sup>+</sup>.

**6-chloro-2-(4-methylpiperazin-1-yl)-N-((4-methylthiophen-2-yl)methyl)quinazolin-4-amine (59)**

Synthesized from 2,4,6-trichloroquinazoline and (4-methylthiophen-2-yl)methanamine according to general method A. Yield: 238 mg (71%). Mp 126.4-127.8°C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 7.44-7.33 (m, 3H), 6.83 (s, 1H), 6.78-6.77 (m, 1H), 5.70 (m, 1H), 5.40 (d,  $J$ =5.4 Hz, 2H), 3.93 (t,  $J$ = 5.1 Hz, 4H), 2.46 (t,  $J$ = 5.1 Hz, 4H), 2.32 (s, 3H), 2.21 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>)  $\delta$  (ppm) 158.61, 158.31, 150.84, 140.61, 137.28, 132.96, 128.52,

127.24, 125.54, 120.39, 120.05, 110.69, 55.03, 46.14, 43.69, 39.93, 15.52; MS (ESI) m/z 388 (M+H)<sup>+</sup>.

**6-chloro-2-(4-methylpiperazin-1-yl)-N-((3-methylthiophen-2-yl)methyl)quinazolin-4-amine (60)**

Synthesized from 2,4,6-trichloroquinazoline and (3-methylthiophen-2-yl)methanamine according to general method A. Yield: 257 mg (77%). Mp 172.8-174.4°C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 7.39-7.29 (m, 3H), 7.15 (d, *J*= 5.1 Hz, 1H), 6.78 (d, *J*= 5.1 Hz, 1H), 5.23 (m, 1H), 4.79 (d, *J*= 5.0 Hz, 2H), 3.90 (t, *J*= 5.0 Hz, 4H), 2.43 (t, *J*= 5.0 Hz, 4H), 2.28 (s, 3H), 2.21 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 158.63, 158.28, 150.79, 135.20, 133.38, 132.95, 129.97, 127.34, 125.53, 123.56, 120.00, 110.65, 55.02, 46.13, 43.67, 37.79, 13.63; MS (ESI) m/z 388 (M+H)<sup>+</sup>.

**6-chloro-N-((5-methyl-1,2,4-oxadiazol-3-yl)methyl)-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (61)**

Synthesized from 2,4,6-trichloroquinazoline and (3-methyl-1,2,4-oxadiazol-5-yl)methanamine according to general method A. Yield: 55 mg (17%). <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 7.47 (d, *J*=1.1 Hz, 1H), 7.40-7.26 (m, 2H), 6.53 (m, 1H), 4.86 (d, *J*= 5.4 Hz, 2H), 3.81 (t, *J*= 4.9 Hz, 4H), 2.43 (t, *J*= 5.1 Hz, 4H), 2.38 (s, 3H), 2.31 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 176.65, 166.99, 158.30, 158.09, 150.81, 133.29, 127.36, 125.78, 120.11, 110.33, 54.85, 46.07, 43.54, 37.41, 11.36; MS (ESI) m/z 374 (M+H)<sup>+</sup>.

**6-chloro-(4-methylpiperazin-1-yl)-N-(thiazol-2-ylmethyl)quinazolin-4-amine (62)**

Synthesized from 2,4,6-trichloroquinazoline and thiazol-2-ylmethanamine according to general method A. Yield: 215 mg (67%). Mp 186.5-187.4 °C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 7.72 (d, *J*= 3.3 Hz, 1H), 7.49-7.33 (m, 3H), 7.27 (d, *J*=3.4 Hz, 1H), 6.31 (m, 1H), 5.06 (d, *J*= 5.5 Hz, 2H), 3.90 (t, *J*= 5.0 Hz, 4H), 2.44 ( *J*= 5.1 Hz, 4H), 2.31 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 167.36, 158.36, 150.84, 141.96, 133.18, 127.35, 125.76, 120.22, 119.45, 110.64, 54.95, 46.07, 43.61, 42.41, 30.80; MS (ESI) m/z 375 (M+H)<sup>+</sup>.

**6-chloro-(4-methylpiperazin-1-yl)-N-(thiazol-5-ylmethyl)quinazolin-4-amine (63)**

Synthesized from 2,4,6-trichloroquinazoline and thiazol-5-ylmethanamine according to general method A. Yield: 217 mg (67%). Mp 226.3-228.6°C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 8.79 (d, *J*= 2.0 Hz, 1H), 7.47 (d, *J*=1.9 Hz, 1H), 7.41-7.24 (m, 3H), 6.33 (m, 1H), 4.89 (d, *J*= 5.2 Hz, 2H), 3.89 (t, *J*= 5.0 Hz, 4H), 2.44 (t, *J*= 5.1 Hz, 4H), 2.31 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 158.65, 158.57, 153.87, 153.17, 150.70, 132.88, 127.24, 125.52, 120.26, 114.92, 110.81, 54.99, 46.13, 43.63, 40.91; MS (ESI) *m/z* 375 (M+H)<sup>+</sup>.

***N*-(benzo[*b*]thiophen-2-ylmethyl)-6-chloro-2-(4-methylpiperazin-1-yl)quinazolin-4-amine (64)**

Synthesized from 2,4,6-trichloroquinazoline and benzo[*b*]thiophen-2-ylmethanamine according to general method A. The compound was purified by recrystallisation from EtOAc. Yield: 62 mg (17%). Mp 193-9-194.4°C; <sup>1</sup>H-NMR (CDCl<sub>3</sub>) δ (ppm) 7.77-7.67 (m, 2H), 7.44-7.26 (m, 6H), 5.78 (m, 1H), 5.00 (d, *J*= 5.4 Hz, 2H), 3.93 (t, *J*= 5.0 Hz, 4H), 2.45 (t, *J*= 5.0 Hz, 4H), 2.31 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ (ppm) 158.56, 158.42, 150.91, 141.96, 139.73, 139.17, 133.10, 127.40, 125.68, 124.28, 124.21, 123.15, 122.36, 122.21, 120.02, 110.63, 54.99, 46.11, 43.71, 40.63; MS (ESI) *m/z* 374 (M+H)<sup>+</sup>.

Purity data for compounds **5**, **7**, **11** and **29-64** as determined by LCMS.

**Table 1:** Purity and retention times of the synthesised compounds determined by analytical HPLC-MS.

Cmpd	Nr	Con- dition <sup>a</sup>	Retention time (min)	Purity <sup>b</sup>	Cmpd	Nr	Con- dition <sup>a</sup>	Retention time (min)	Purity <sup>b</sup>
VUF10249	<b>5</b>	<i>II</i>	7.82	98%	VUF10553	<b>46</b>	<i>I</i>	13.07	100%
VUF10329	<b>7</b>	<i>II</i>	8.26	99%	VUF10556	<b>47</b>	<i>I</i>	13.90	98%
VUF10331	<b>11</b>	<i>II</i>	7.99	98%	VUF10455	<b>48</b>	<i>I</i>	10.76	98%
VUF10147	<b>29</b>	<i>I</i>	9.71	100%	VUF10456	<b>49</b>	<i>I</i>	12.15	98%
VUF10351	<b>30</b>	<i>I</i>	10.95	99%	VUF10457	<b>50</b>	<i>I</i>	12.97	99%
VUF10327	<b>31</b>	<i>I</i>	14.12	100%	VUF10501	<b>51</b>	<i>I</i>	11.81	100%
VUF10328	<b>32</b>	<i>I</i>	14.34	99%	VUF10500	<b>52</b>	<i>I</i>	12.29	99%
VUF10247	<b>33</b>	<i>I</i>	12.45	99%	VUF10502	<b>53</b>	<i>I</i>	14.71	99%
VUF10246	<b>34</b>	<i>I</i>	12.43	99%	VUF10499	<b>54</b>	<i>I</i>	12.93	99%
VUF10332	<b>35</b>	<i>II</i>	8.02	97%	VUF10497	<b>55</b>	<i>I</i>	13.37	98%
VUF10453	<b>36</b>	<i>I</i>	14.10	99%	VUF10507	<b>56</b>	<i>I</i>	14.45	99%
VUF10452	<b>37</b>	<i>I</i>	13.22	99%	VUF10498	<b>57</b>	<i>I</i>	13.86	98%
VUF10350	<b>38</b>	<i>I</i>	12.96	99%	VUF10503	<b>58</b>	<i>I</i>	13.48	98%
VUF10508	<b>39</b>	<i>I</i>	15.22	100%	VUF10516	<b>59</b>	<i>I</i>	13.88	98%
VUF10349	<b>40</b>	<i>I</i>	11.78	100%	VUF10515	<b>60</b>	<i>I</i>	13.85	99%
VUF10458	<b>41</b>	<i>I</i>	11.82	99%	VUF10511	<b>61</b>	<i>I</i>	11.58	100%
VUF10459	<b>42</b>	<i>I</i>	11.17	100%	VUF10520	<b>62</b>	<i>I</i>	11.79	99%
VUF10509	<b>43</b>	<i>I</i>	12.20	98%	VUF10559	<b>63</b>	<i>I</i>	11.86	99%
VUF10505	<b>44</b>	<i>I</i>	13.45	99%	VUF10510	<b>64</b>	<i>I</i>	13.37	99%
VUF10513	<b>45</b>	<i>I</i>	13.68	100%					

<sup>a</sup> The conditions can be found in the experimental section of the main article; <sup>b</sup> The purities were calculated as the percentage peak area of the analyzed compound by UV detection at 254 nm.

Purity data for compounds **66-81** as determined by LCMS.

**Table 2:** Purity, retention times and mass of the synthesised compounds determined by analytical HPLC-MS.

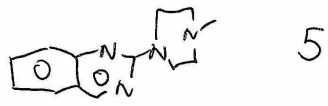
Cmpd	Con- dition <sup>a</sup>	Retention time (min)	Purity <sup>b</sup>	M+H <sup>+</sup> (m/z)
<b>66</b>	<i>III</i>	1.59	97%	318
<b>67</b>	<i>III</i>	1.78	95%	306
<b>68</b>	<i>III</i>	1.78	99%	320
<b>69</b>	<i>III</i>	1.71	97%	306
<b>70</b>	<i>III</i>	1.51	96%	278
<b>71</b>	<i>III</i>	1.52	99%	278
<b>72</b>	<i>III</i>	1.52	96%	292
<b>73<sup>c</sup></b>	<i>I</i>	13.50	97%	318
<b>74</b>	<i>III</i>	1.82	92%	360
<b>75</b>	<i>III</i>	1.72	96%	332
<b>76</b>	<i>I</i>	11.00	100%	292
<b>77</b>	<i>III</i>	1.80	97%	318
<b>78</b>	<i>III</i>	1.61	98%	320
<b>79</b>	<i>III</i>	1.60	98%	320
<b>80</b>	<i>III</i>	1.57	96%	306
<b>81</b>	<i>III</i>	1.75	97%	375

<sup>a</sup> The conditions can be found in the experimental section of the main article; <sup>b</sup> The purities were calculated as the percentage peak area of the analyzed compound by UV detection at 254 nm; <sup>c</sup> Compound **73** corresponds to compound VUF10552 of the given LCMS tracings.

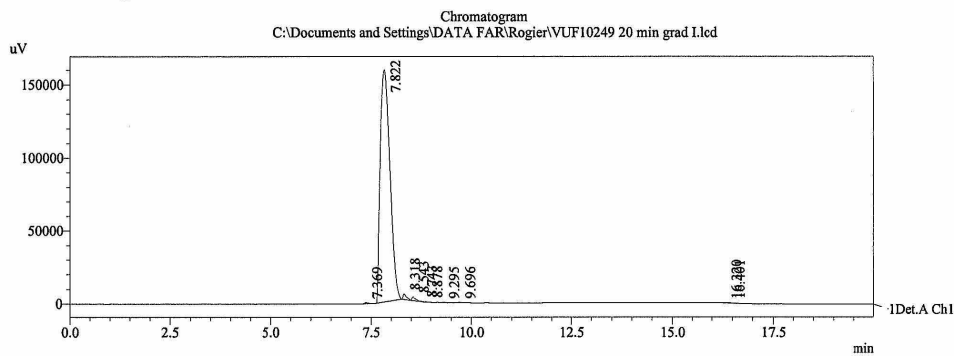
LCMS tracings for the compounds in Table 1 (S13) and Compound 72.

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 32  
 Injection Volume : 5 uL  
 Data File Name : VUF10249 20 min grad I.lcd  
 Method File Name : grad\_positivemode 20min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 6/4/2007 9:32:03 PM  
 Data Processed : 6/4/2007 9:52:08 PM



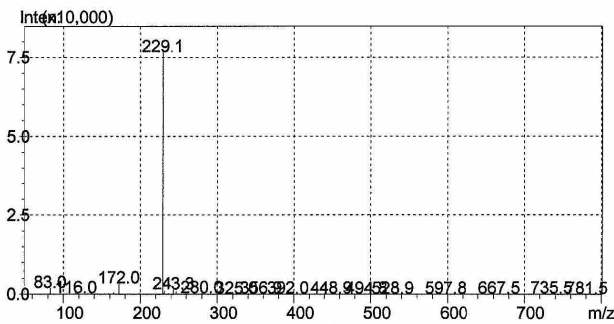
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

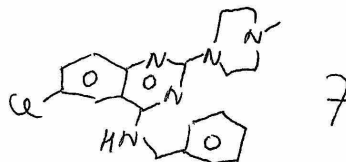
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.369	5705	815	0.208	0.486
2	7.822	2685819	158823	97.984	94.675
3	8.318	22693	3775	0.828	2.250
4	8.543	16825	2600	0.614	1.550
5	8.743	1133	302	0.041	0.180
6	8.878	1188	199	0.043	0.119
7	9.295	1823	328	0.067	0.196
8	9.696	2713	344	0.099	0.205
9	16.320	1472	234	0.054	0.139
10	16.401	1720	334	0.063	0.199
Total		2741091	167756	100.000	100.000



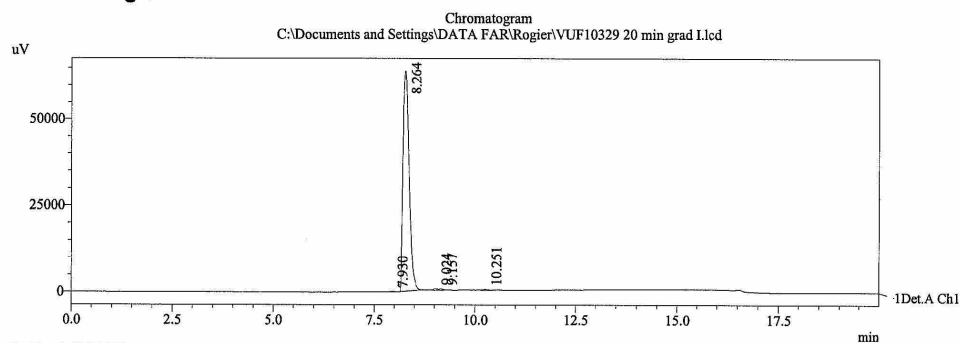
C:\Documents and Settings\DATA FAR\Rogier\VUF10249 20 min grad I.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 34  
 Injection Volume : 5 uL  
 Data File Name : VUF10329 20 min grad 1.lcd  
 Method File Name : grad\_positivemode 20min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 6/6/2007 5:35:46 AM  
 Data Processed : 6/6/2007 5:55:49 AM



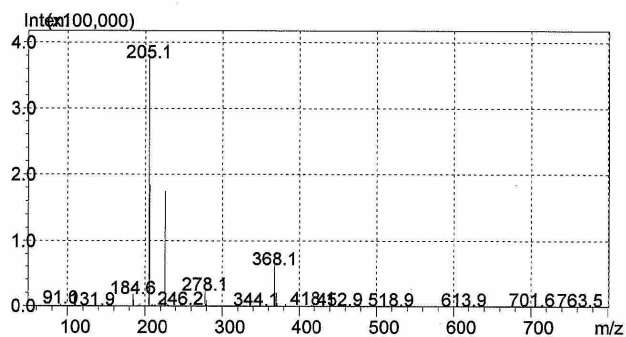
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

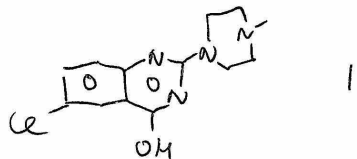
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.930	623	94	0.091	0.145
2	8.264	678350	63984	98.812	98.268
3	9.024	3085	381	0.449	0.586
4	9.157	2509	409	0.366	0.628
5	10.251	1935	244	0.282	0.374
Total		686502	65112	100.000	100.000



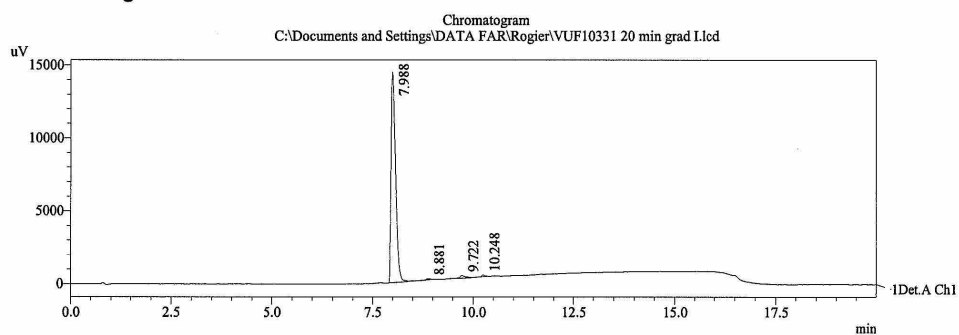
C:\Documents and Settings\DATA FAR\Rogier\VUF10329 20 min grad 1.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vail # : 31  
 Injection Volume : 5 uL  
 Data File Name : VUF10331 20 min grad I.lcd  
 Method File Name : grad\_positivemode 20min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 6/6/2007 4:28:59 AM  
 Data Processed : 6/7/2007 3:12:12 PM



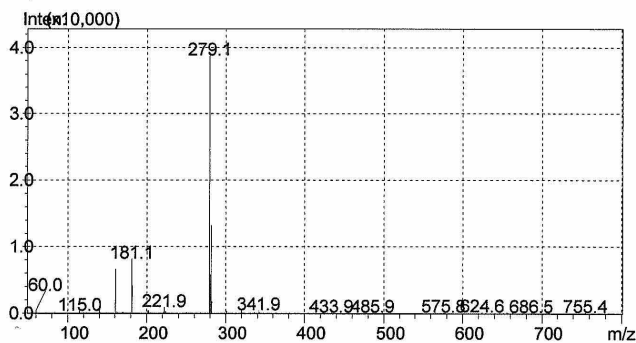
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

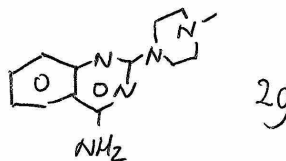
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.988	112112	14458	97.588	97.588
2	8.881	502	66	0.437	0.445
3	9.722	1688	183	1.469	1.235
4	10.248	581	108	0.505	0.732
Total		114883	14815	100.000	100.000



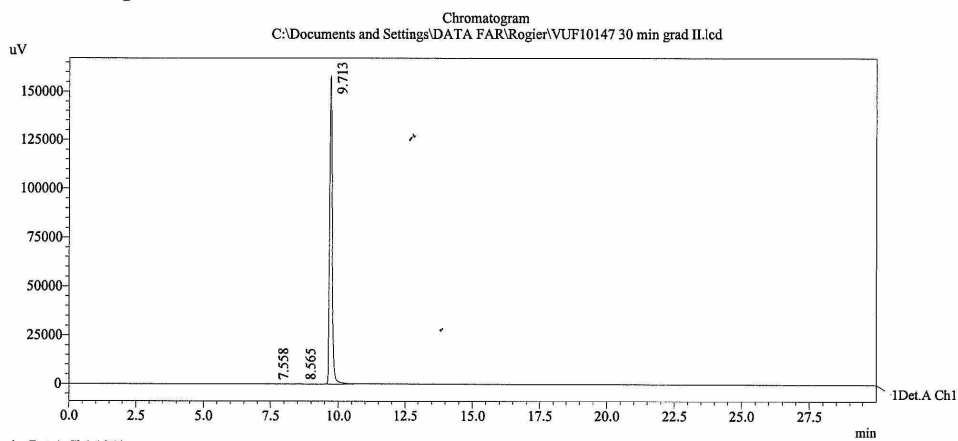
C:\Documents and Settings\DATA FAR\Rogier\VUF10331 20 min grad I.lcd

### ==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 81  
 Injection Volume : 5 uL  
 Data File Name : VUF10147 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 8:07:44 AM  
 Data Processed : 5/16/2007 9:16:06 AM

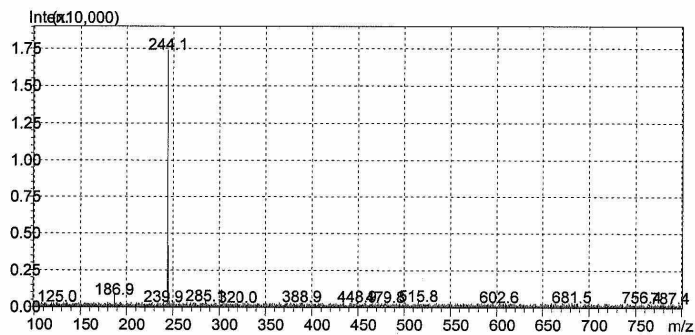


#### <Chromatogram>



PeakTable

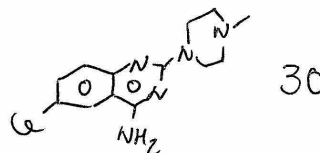
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.558	2382	233	0.224	0.147
2	8.565	1557	187	0.146	0.118
3	9.713	1060164	158292	99.630	99.735
Total		1064102	158713	100.000	100.000



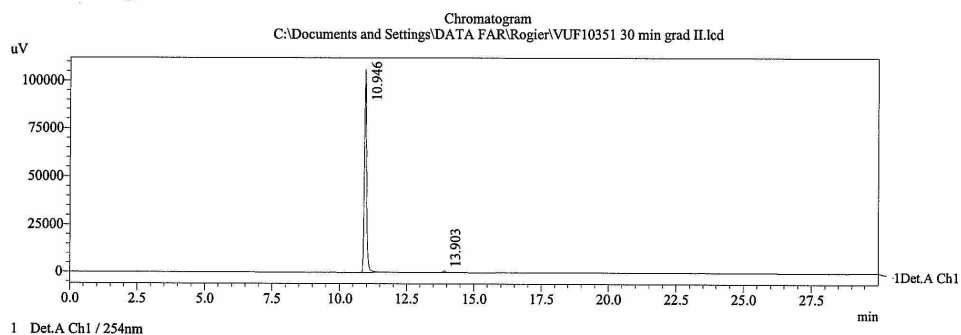
C:\Documents and Settings\DATA FAR\Rogier\VUF10147 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vail # : 68  
 Injection Volume : 5 uL  
 Data File Name : VUF10351 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 2:12:43 AM  
 Data Processed : 5/16/2007 2:42:46 AM

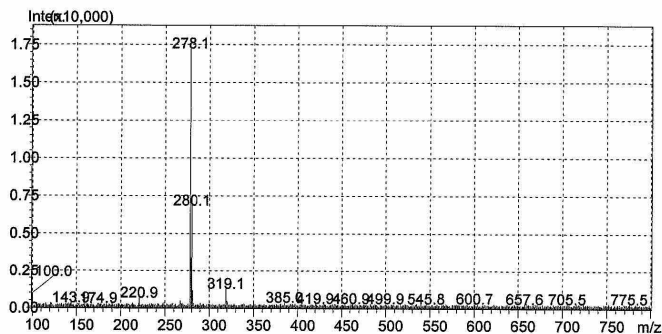


<Chromatogram>



PeakTable

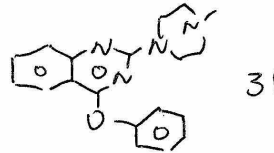
Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.946	614020	106122	98.964	99.133
2	13.903	6427	928	1.036	0.867
Total		620447	107049	100.000	100.000



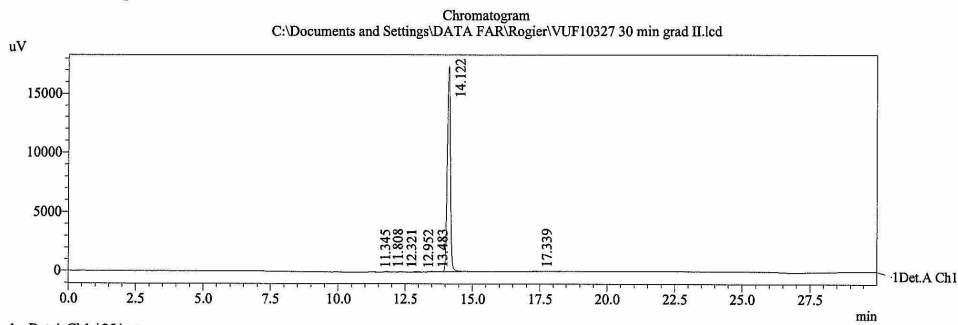
C:\Documents and Settings\DATA FAR\Rogier\VUF10351 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 77  
 Injection Volume : 5 uL  
 Data File Name : VUF10327 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 6:30:51 AM  
 Data Processed : 5/16/2007 2:29:21 PM

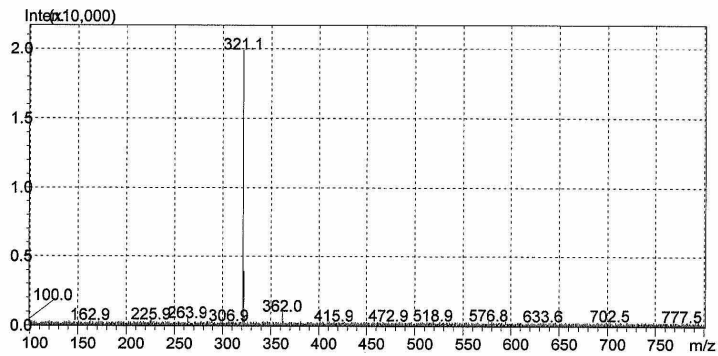


<Chromatogram>



PeakTable

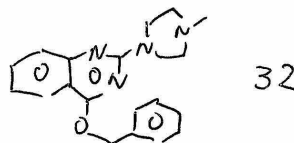
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.345	264	43	0.187	0.245
2	11.808	378	61	0.268	0.344
3	12.321	202	34	0.143	0.191
4	12.952	309	25	0.219	0.144
5	13.483	259	36	0.184	0.205
6	14.122	139192	17367	98.714	98.629
7	17.339	401	43	0.285	0.241
Total		141006	17609	100.000	100.000



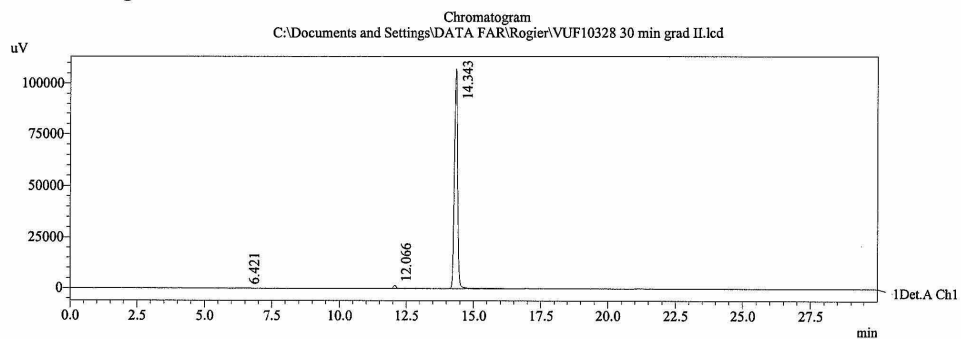
C:\Documents and Settings\DATA FAR\Rogier\VUF10327 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 78  
 Injection Volume : 5 uL  
 Data File Name : VUF10328 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 7:03:05 AM  
 Data Processed : 5/16/2007 7:33:10 AM

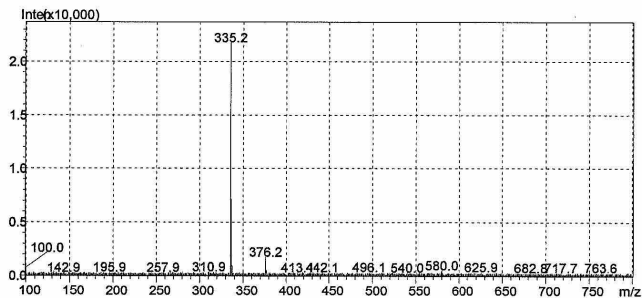


<Chromatogram>



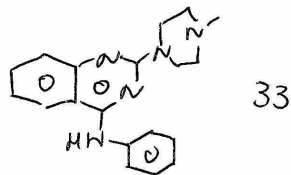
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.421	1554	89	0.172	0.082
2	12.066	11365	1581	1.261	1.452
3	14.343	888163	107200	98.566	98.466
Total		901082	108870	100.000	100.000

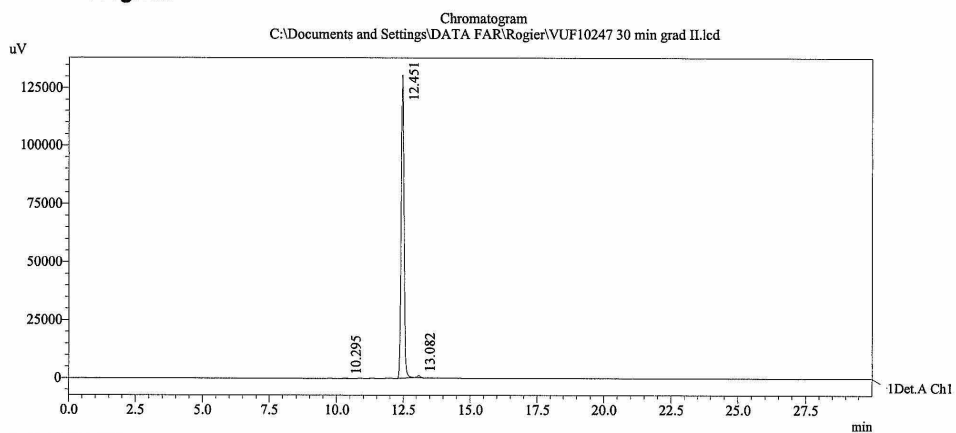


==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 82  
 Injection Volume : 5 uL  
 Data File Name : VUF10247 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 8:40:01 AM  
 Data Processed : 5/16/2007 9:10:06 AM

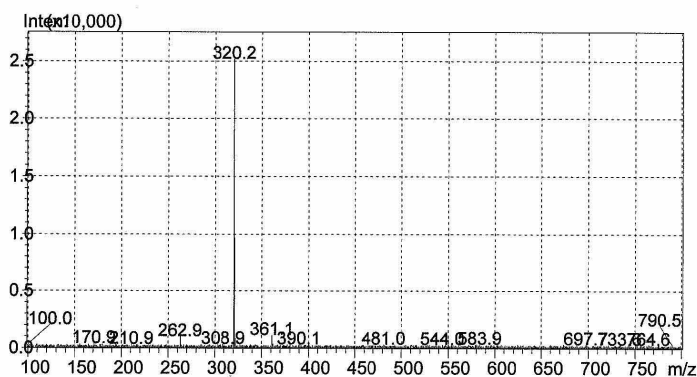


<Chromatogram>



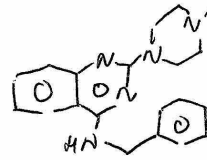
1 Det.A Ch1 / 254nm

Detector A Ch1 254nm		PeakTable			
Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.295	1165	163	0.116	0.124
2	12.451	995367	130850	99.206	99.204
3	13.082	6802	886	0.678	0.672
Total		1003334	131900	100.000	100.000



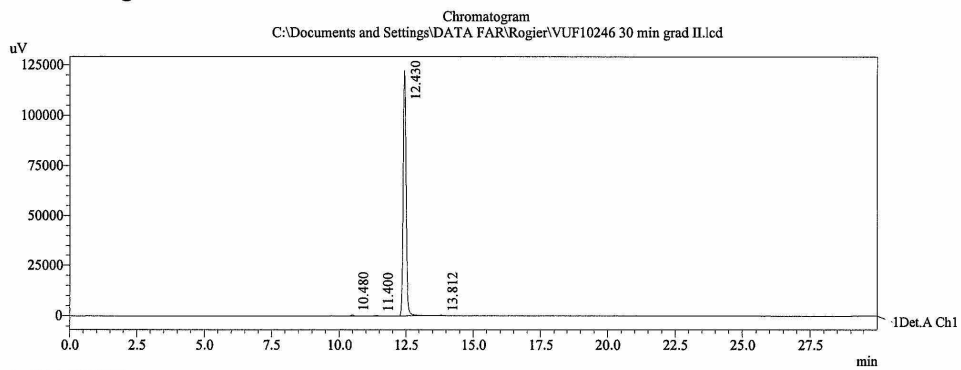
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 83  
 Injection Volume : 5 uL  
 Data File Name : VUF10246 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 9:12:20 AM  
 Data Processed : 5/16/2007 9:42:25 AM



34

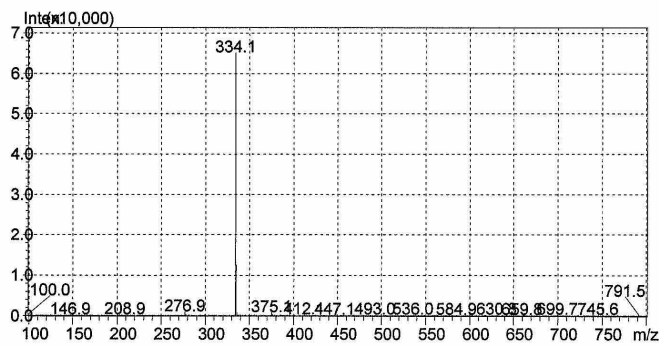
<Chromatogram>



1 Det.A Ch1 / 254nm

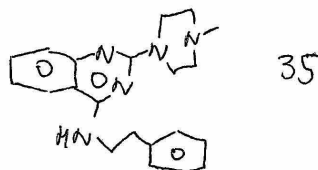
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.480	4193	637	0.434	0.516
2	11.400	2013	195	0.209	0.158
3	12.430	957517	122342	99.170	99.127
4	13.812	1803	246	0.187	0.199
Total		965527	123420	100.000	100.000

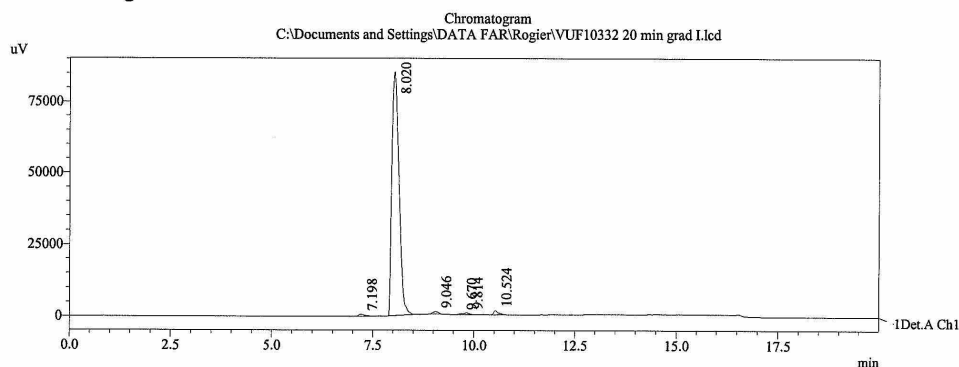


==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 10  
 Injection Volume : 5 uL  
 Data File Name : VUF10332 20 min grad 1.lcd  
 Method File Name : grad\_positivemode 20min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 6/5/2007 8:40:50 PM  
 Data Processed : 6/5/2007 9:00:54 PM



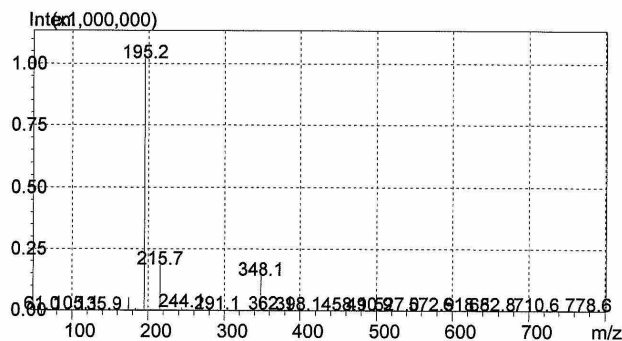
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1 Det.A Ch1 / 254nm

PeakTable

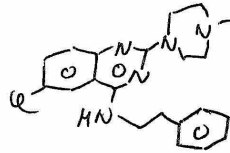
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.198	7297	684	0.673	0.766
2	8.020	1049313	85134	96.811	95.417
3	9.046	8420	881	0.777	0.988
4	9.670	2233	345	0.206	0.387
5	9.814	4931	687	0.455	0.770
6	10.524	11687	1492	1.078	1.672
Total		1083881	89223	100.000	100.000



C:\Documents and Settings\DATA FAR\Rogier\VUF10332 20 min grad 1.lcd

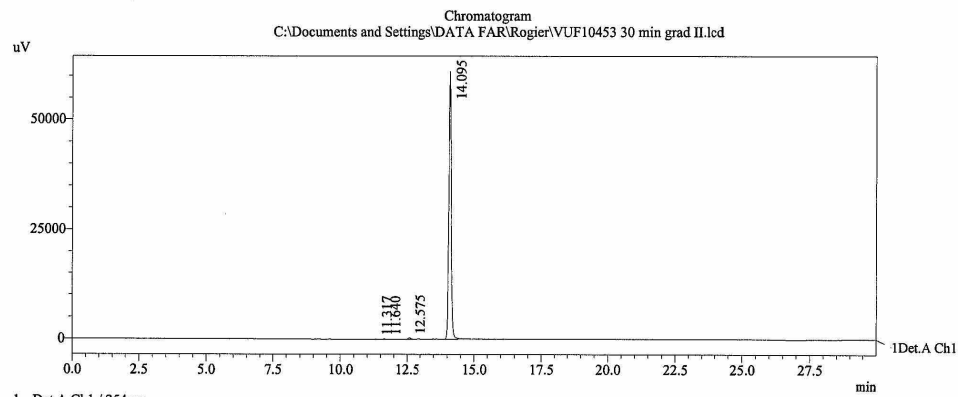
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 67  
 Injection Volume : 5 uL  
 Data File Name : VUF10453 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 1:40:29 AM  
 Data Processed : 5/16/2007 2:10:31 AM



36

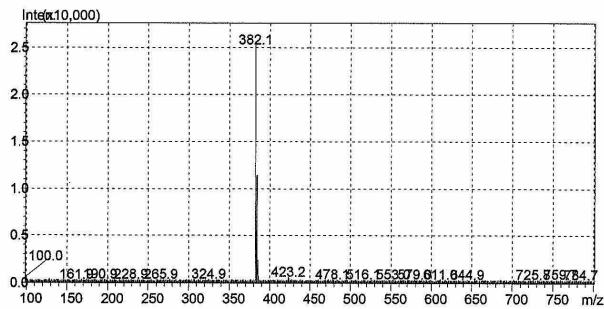
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

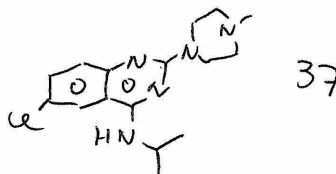
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.317	217	41	0.057	0.066
2	11.640	545	104	0.142	0.169
3	12.575	2717	384	0.710	0.623
4	14.095	379031	61064	99.091	99.142
Total		382510	61592	100.000	100.000



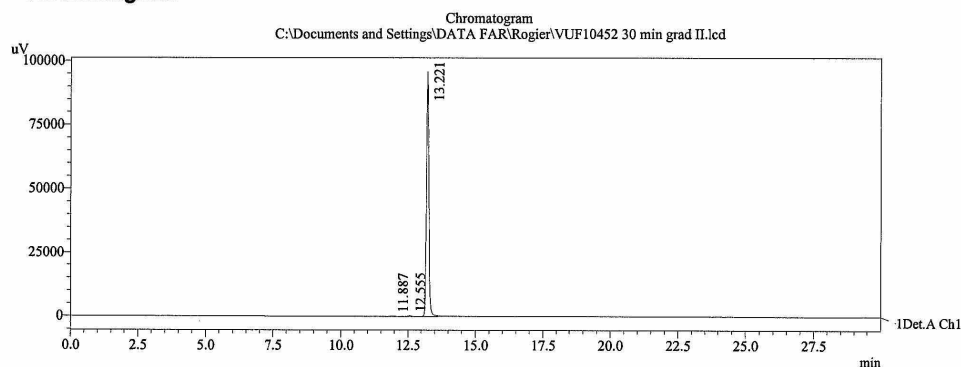
C:\Documents and Settings\DATA FAR\Rogier\VUF10453 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 66  
 Injection Volume : 5 uL  
 Data File Name : VUF10452 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 1:08:14 AM  
 Data Processed : 5/16/2007 1:38:17 AM

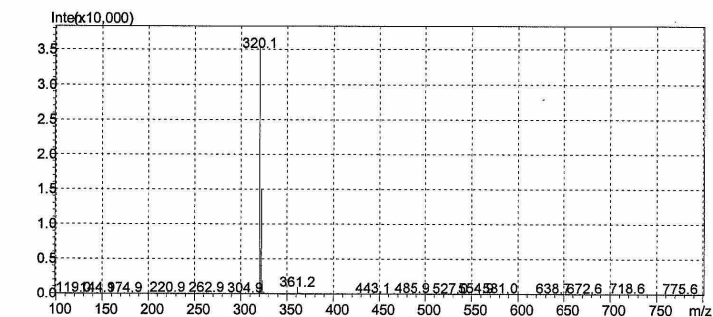


<Chromatogram>



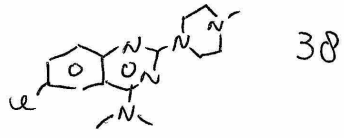
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.887	1250	143	0.209	0.148
2	12.555	2250	369	0.376	0.383
3	13.221	594128	95879	99.414	99.468
Total		597627	96392	100.000	100.000

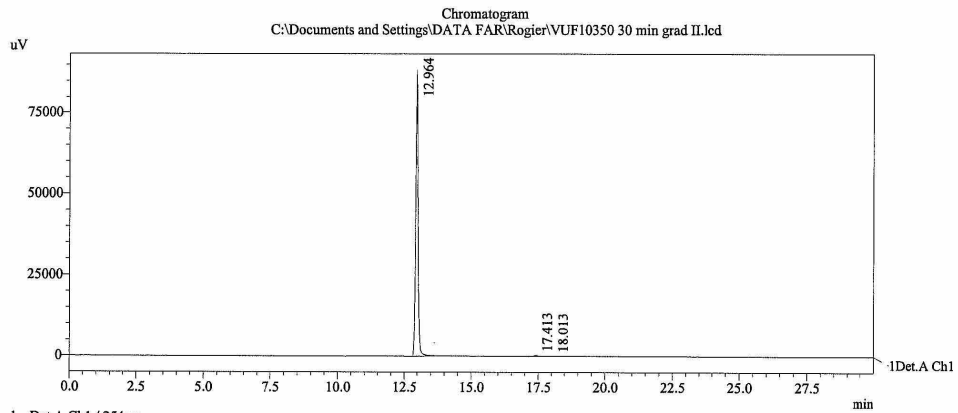


==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 65  
 Injection Volume : 5 uL  
 Data File Name : VUF10350 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.icb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 12:36:00 AM  
 Data Processed : 5/16/2007 1:06:03 AM



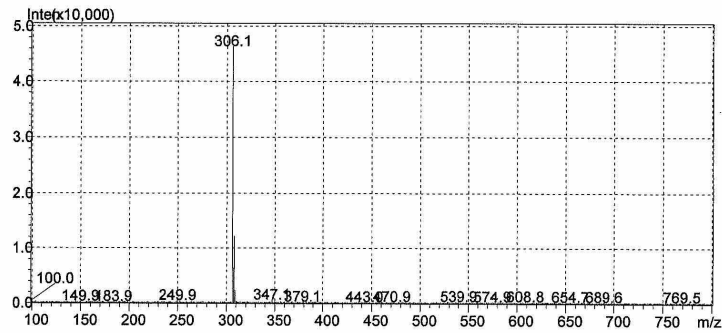
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

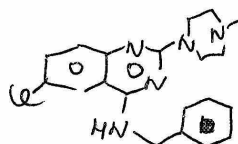
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.964	538328	88491	99.354	99.555
2	17.413	2464	296	0.455	0.333
3	18.013	1039	99	0.192	0.111
Total		541830	88886	100.000	100.000



C:\Documents and Settings\DATA FAR\Rogier\VUF10350 30 min grad II.lcd

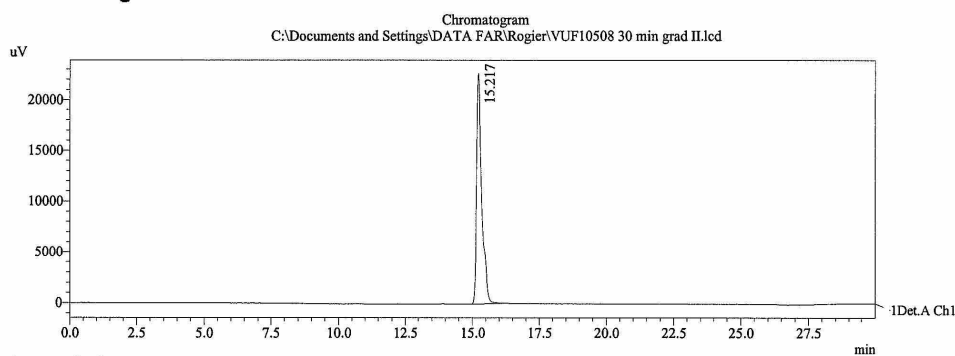
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vail # : 35  
 Injection Volume : 5 uL  
 Data File Name : VUF10508 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/22/2007 7:24:46 PM  
 Data Processed : 5/22/2007 7:54:53 PM



3g

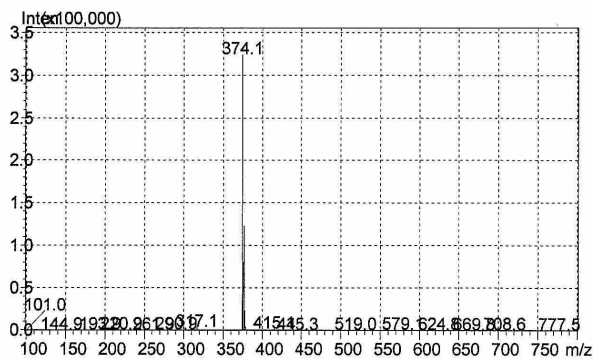
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

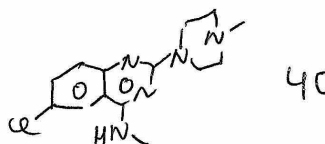
Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.217	301391	22690	100.000	100.000
Total		301391	22690	100.000	100.000



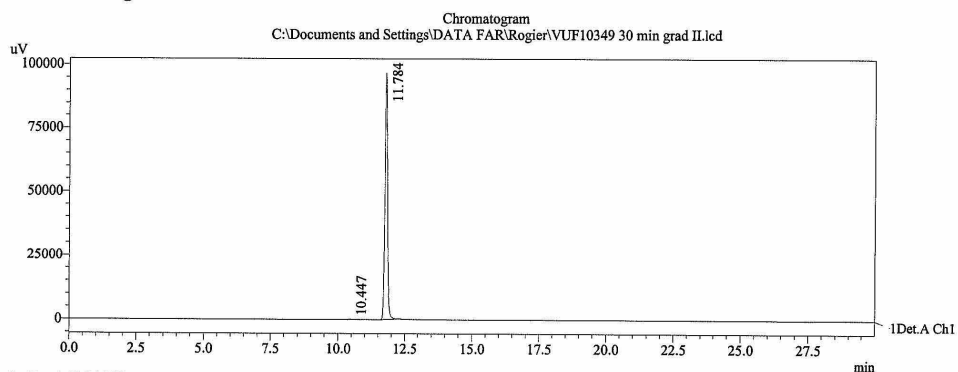
C:\Documents and Settings\DATA FAR\Rogier\VUF10508 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vail # : 76  
 Injection Volume : 5 uL  
 Data File Name : VUF10349 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 5:58:37 AM  
 Data Processed : 5/16/2007 6:28:40 AM

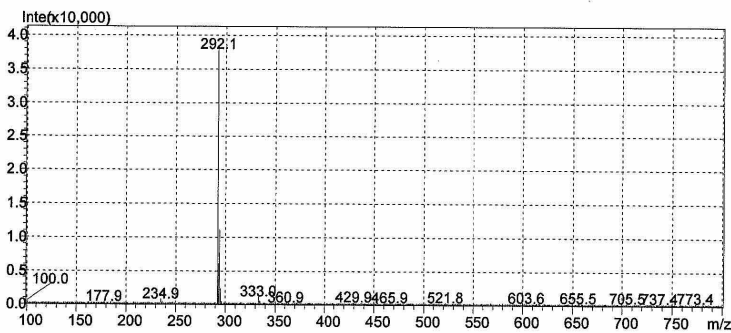


<Chromatogram>



PeakTable

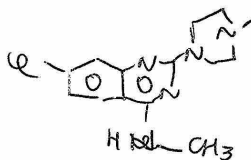
Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.447	2580	255	0.385	0.263
2	11.784	666877	96842	99.615	99.737
Total		669456	97097	100.000	100.000



C:\Documents and Settings\DATA FAR\Regier\VUF10349 30 min grad II.lcd

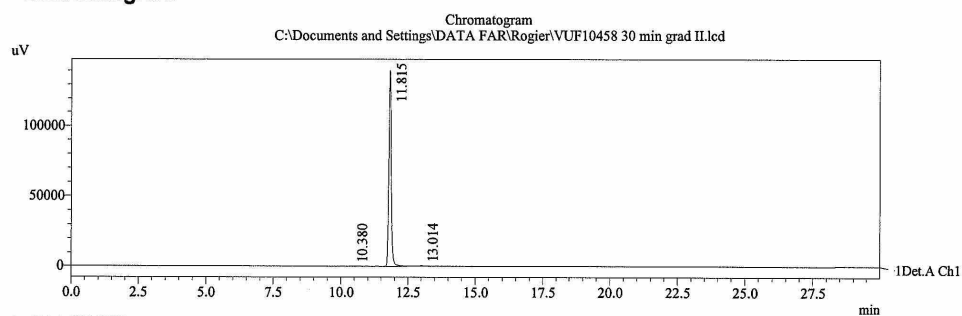
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 69  
 Injection Volume : 5 uL  
 Data File Name : VUF10458 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 2:45:01 AM  
 Data Processed : 5/16/2007 3:15:04 AM



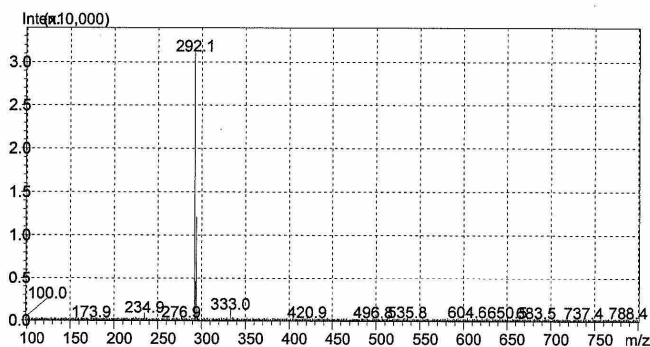
41

<Chromatogram>



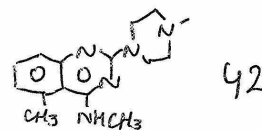
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.380	1267	183	0.143	0.130
2	11.815	880176	140313	99.492	99.549
3	13.014	3229	452	0.365	0.321
Total		884671	140949	100.000	100.000

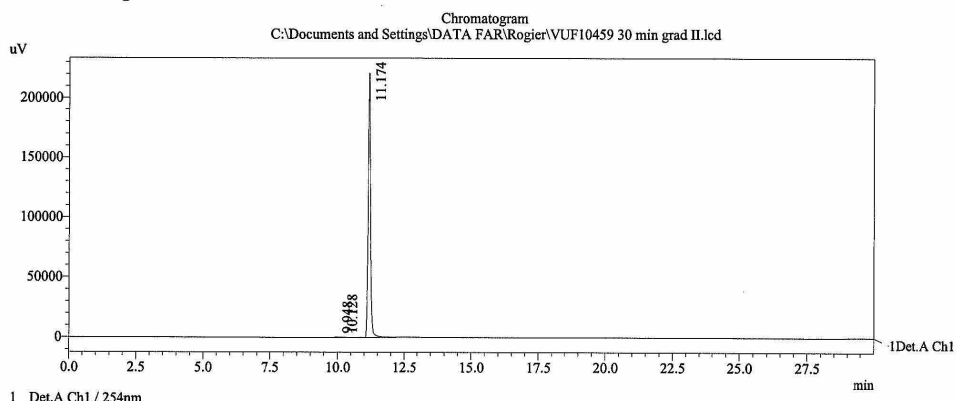


==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 71  
 Injection Volume : 5 uL  
 Data File Name : VUF10459 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 3:17:16 AM  
 Data Processed : 5/16/2007 3:47:21 AM

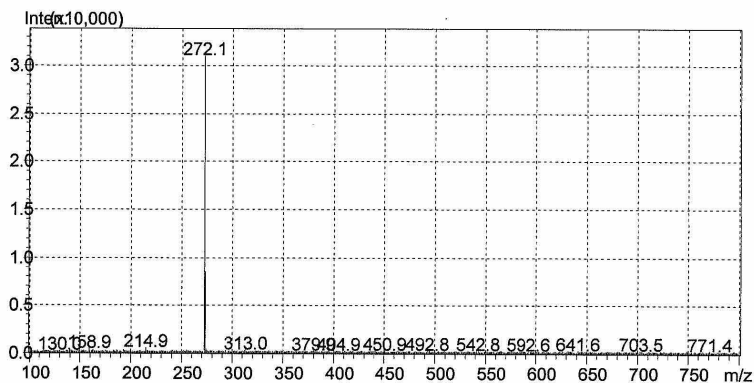


<Chromatogram>



PeakTable

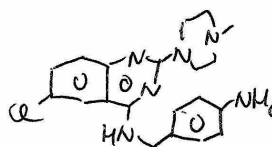
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.948	2535	403	0.186	0.182
2	10.128	1764	237	0.129	0.107
3	11.174	1358759	220912	99.685	99.711
Total		1363057	221552	100.000	100.000



C:\Documents and Settings\DATA FAR\Rogier\VUF10459 30 min grad II.lcd

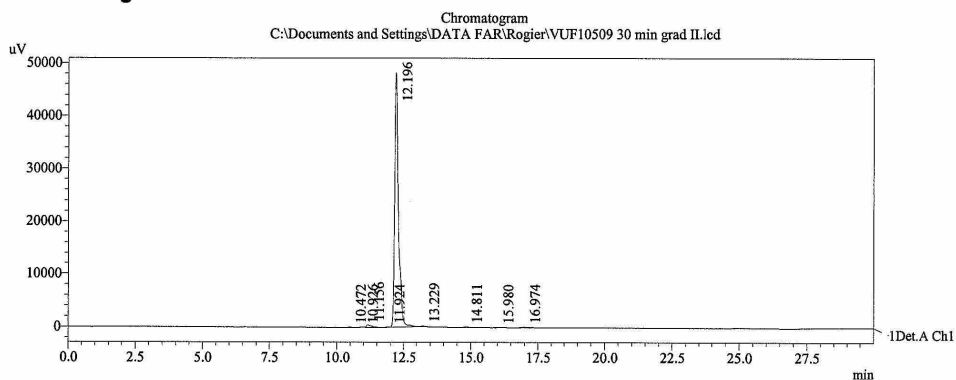
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 39  
 Injection Volume : 5 uL  
 Data File Name : VUF10509 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/22/2007 9:33:58 PM  
 Data Processed : 5/22/2007 10:04:01 PM



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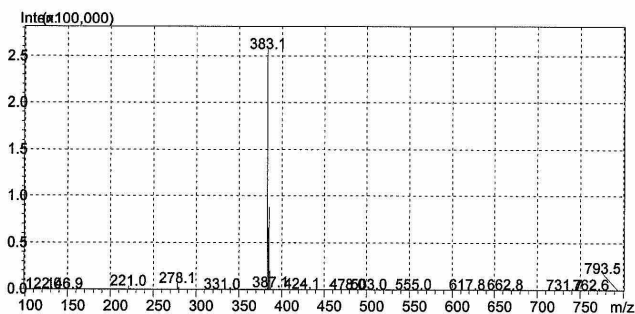
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

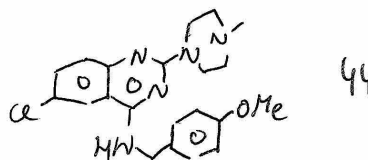
Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.472	367	60	0.076	0.121
2	10.926	507	84	0.104	0.170
3	11.156	6403	518	1.319	1.049
4	11.924	279	39	0.057	0.079
5	12.196	473488	48258	97.572	97.746
6	13.229	943	129	0.194	0.261
7	14.811	1262	122	0.260	0.247
8	15.980	266	32	0.055	0.066
9	16.974	1757	129	0.362	0.262
Total		485270	49371	100.000	100.000



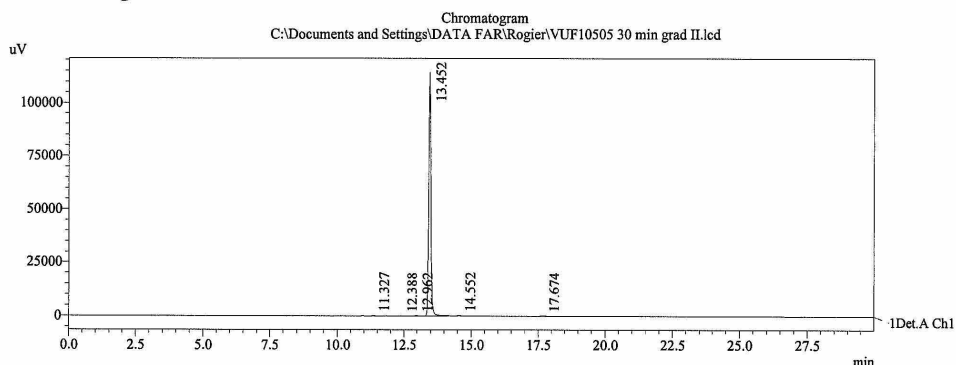
C:\Documents and Settings\DATA FAR\Rogier\VUF10509 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 55  
 Injection Volume : 5 uL  
 Data File Name : VUF10505 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/15/2007 7:45:29 PM  
 Data Processed : 5/15/2007 8:15:34 PM



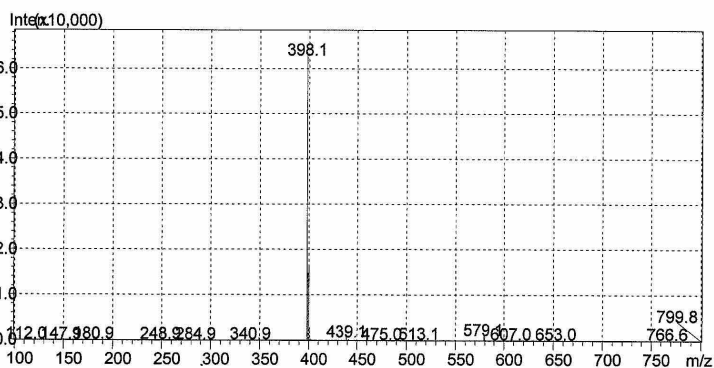
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

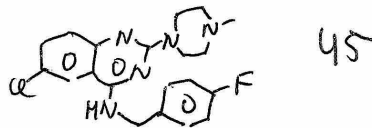
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.327	2179	412	0.335	0.356
2	12.388	1290	145	0.198	0.125
3	12.962	1730	240	0.266	0.207
4	13.452	642010	114462	98.747	98.919
5	14.552	1717	301	0.264	0.260
6	17.674	1228	154	0.189	0.133
Total		650155	115713	100.000	100.000



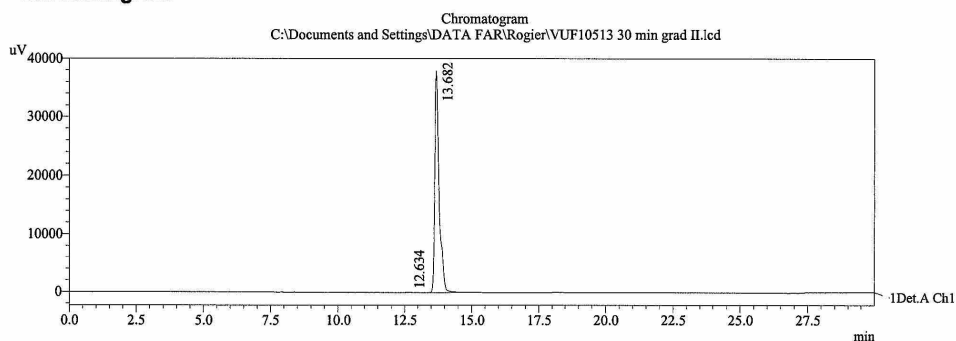
C:\Documents and Settings\DATA FAR\Rogier\VUF10505 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vail # : 42  
 Injection Volume : 5 uL  
 Data File Name : VUF10513 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/22/2007 11:10:52 PM  
 Data Processed : 5/22/2007 11:40:56 PM

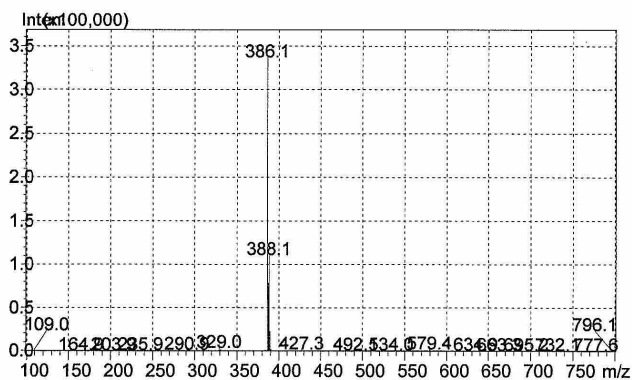


<Chromatogram>



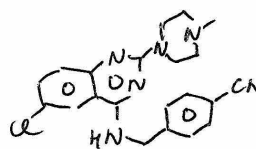
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.634	1145	93	0.269	0.244
2	13.682	424614	38002	99.731	99.756
Total		425759	38095	100.000	100.000



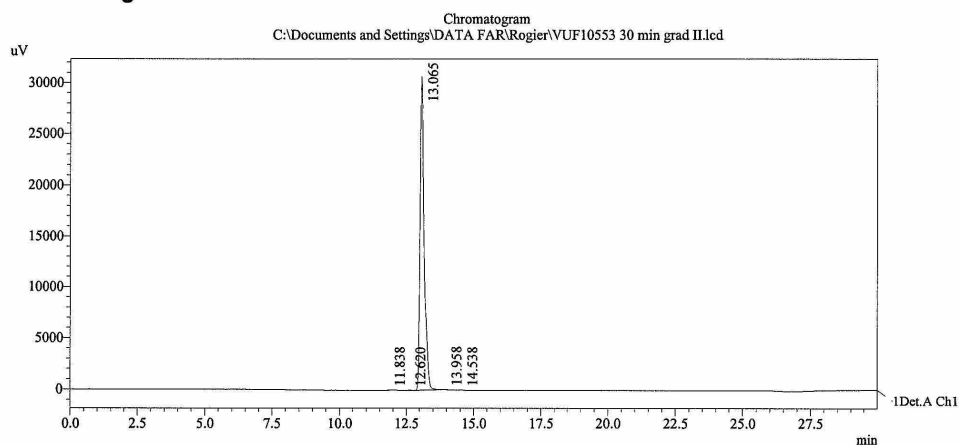
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 38  
 Injection Volume : 5 uL  
 Data File Name : VUF10553 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultL.CMS.lcr  
 Data Acquired : 5/22/2007 9:01:36 PM  
 Data Processed : 5/22/2007 9:31:40 PM



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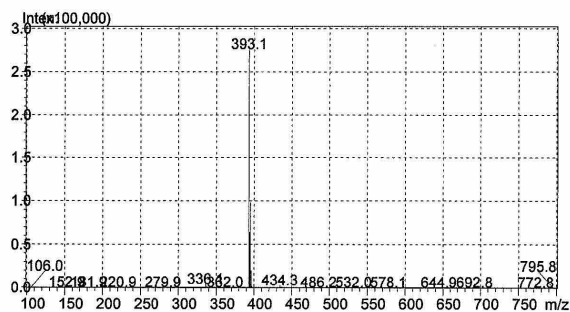
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

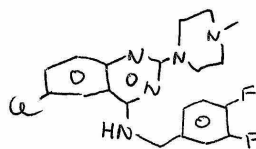
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.838	228	33	0.071	0.107
2	12.620	351	34	0.109	0.110
3	13.065	321962	30688	99.635	99.547
4	13.958	438	51	0.136	0.167
5	14.538	161	21	0.050	0.069
Total		323140	30828	100.000	100.000



C:\Documents and Settings\DATA FAR\Rogier\VUF10553 30 min grad II.lcd

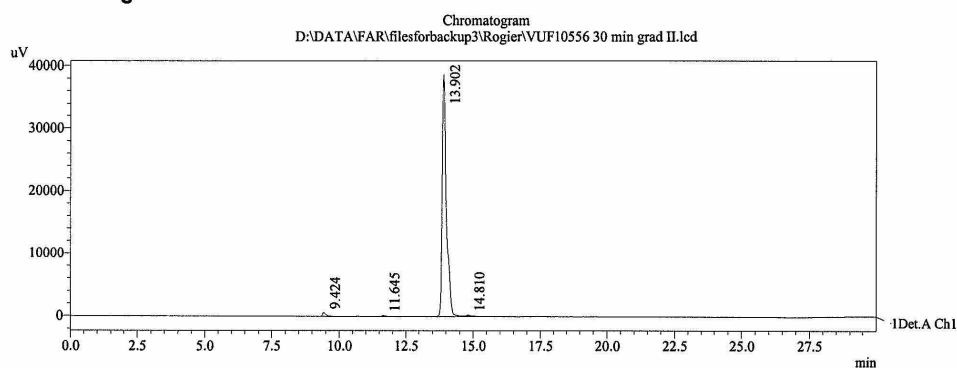
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 34  
 Injection Volume : 5 uL  
 Data File Name : VUF10556 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultL.CMS.lcr  
 Data Acquired : 5/22/2007 6:52:30 PM  
 Data Processed : 5/22/2007 7:22:35 PM



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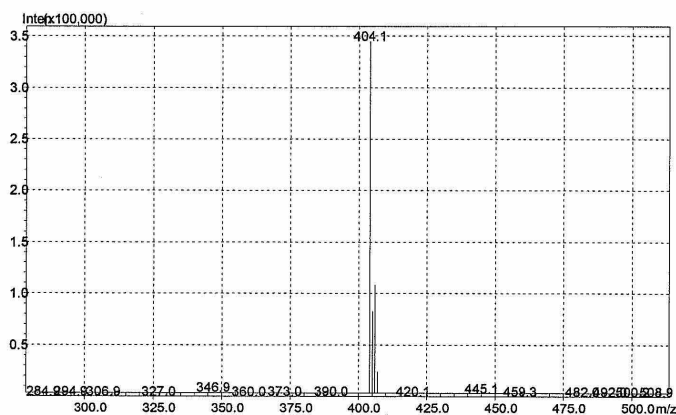
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

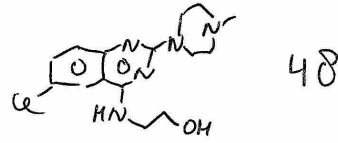
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.424	5764	601	1.337	1.514
2	11.645	1710	206	0.397	0.520
3	13.902	421638	38672	97.806	97.476
4	14.810	1983	194	0.460	0.490
Total		431094	39673	100.000	100.000



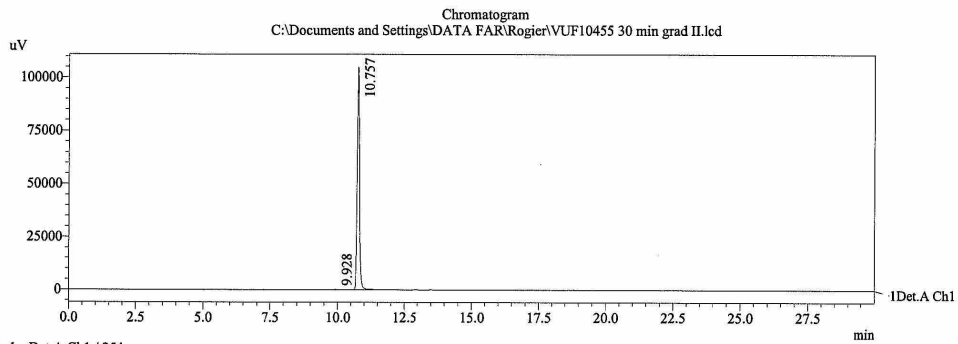
D:\DATA\FAR\filesforbackup3\Rogier\VUF10556 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 72  
 Injection Volume : 5 uL  
 Data File Name : VUF10455 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 3:49:34 AM  
 Data Processed : 5/16/2007 4:19:36 AM

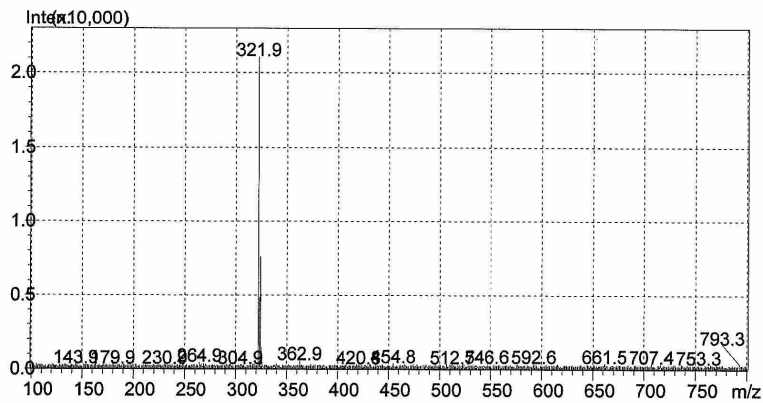


<Chromatogram>



PeakTable

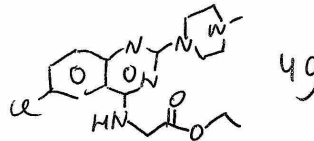
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.928	1528	234	0.246	0.222
2	10.757	618220	105032	99.754	99.778
Total		619748	105266	100.000	100.000



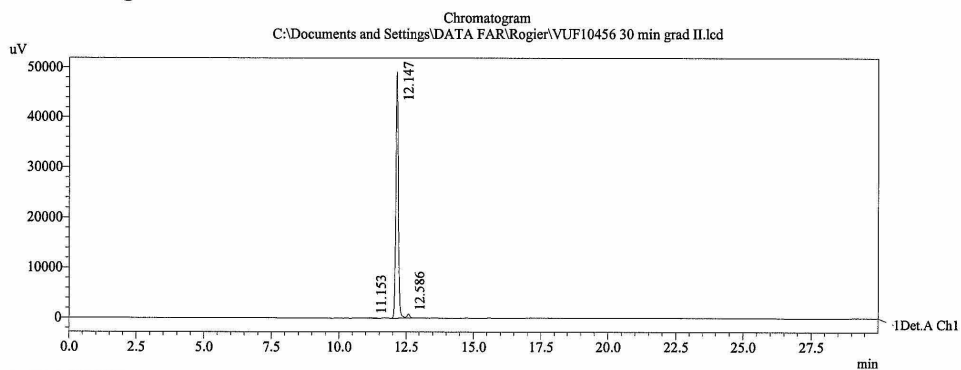
C:\Documents and Settings\FAR\Regier\VUF10455 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 74  
 Injection Volume : 5 uL  
 Data File Name : VUF10456 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 4:54:06 AM  
 Data Processed : 5/16/2007 5:24:11 AM

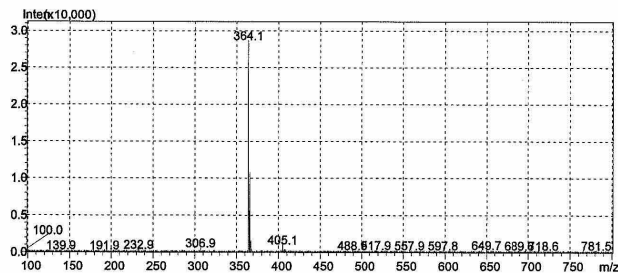


<Chromatogram>



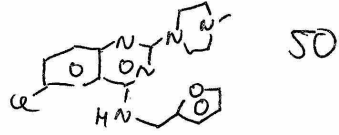
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.153	1388	130	0.428	0.260
2	12.147	316542	49228	97.728	98.194
3	12.586	5971	775	1.843	1.546
Total		323901	50133	100.000	100.000

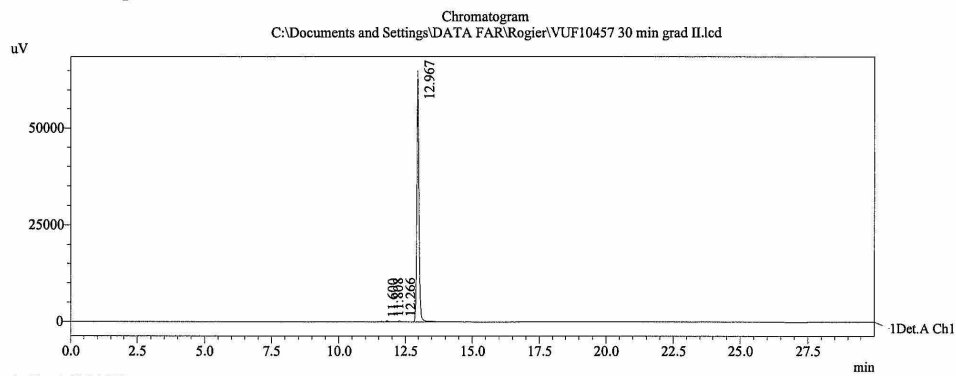


==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 59  
 Injection Volume : 5 uL  
 Data File Name : VUF10457 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/15/2007 9:54:35 PM  
 Data Processed : 5/15/2007 10:24:40 PM



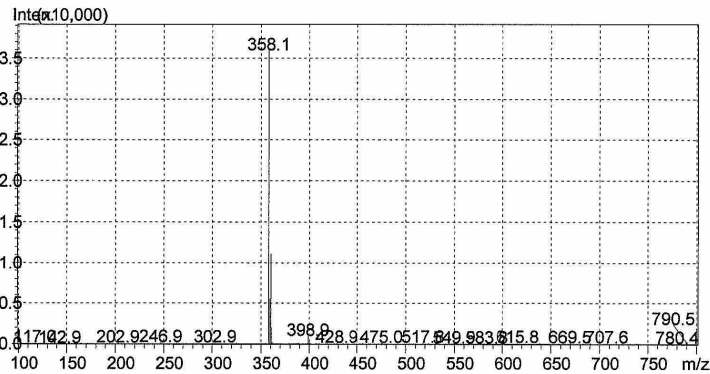
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

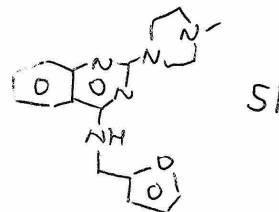
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.600	1130	202	0.311	0.306
2	11.808	2326	302	0.639	0.458
3	12.266	2163	377	0.594	0.571
4	12.967	358204	65083	98.456	98.666
Total		363822	65963	100.000	100.000



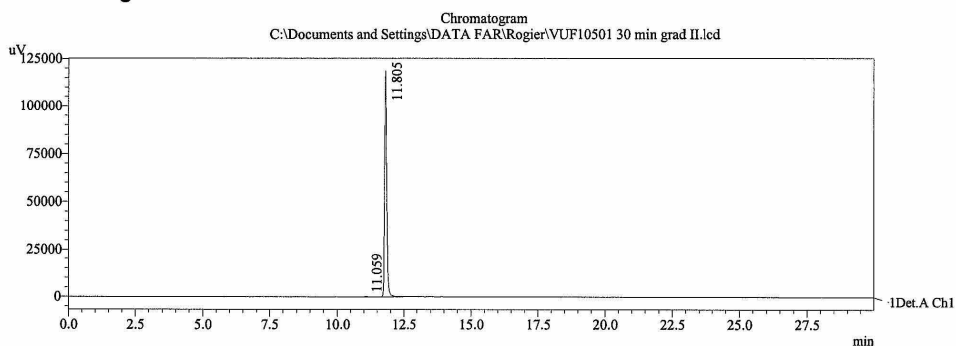
C:\Documents and Settings\DATA FAR\Rogier\VUF10457 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vail # : 58  
 Injection Volume : 5 uL  
 Data File Name : VUF10501 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/15/2007 9:22:16 PM  
 Data Processed : 5/15/2007 9:52:20 PM

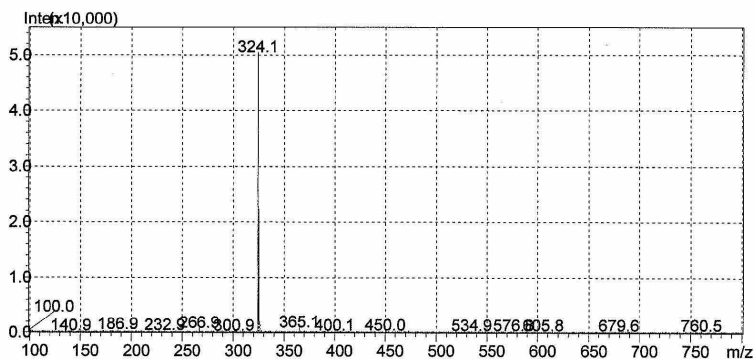


<Chromatogram>



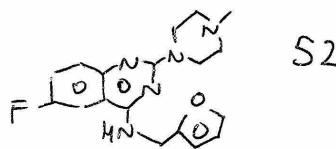
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.059	2915	497	0.455	0.417
2	11.805	638316	118644	99.545	99.583
Total		641231	119141	100.000	100.000

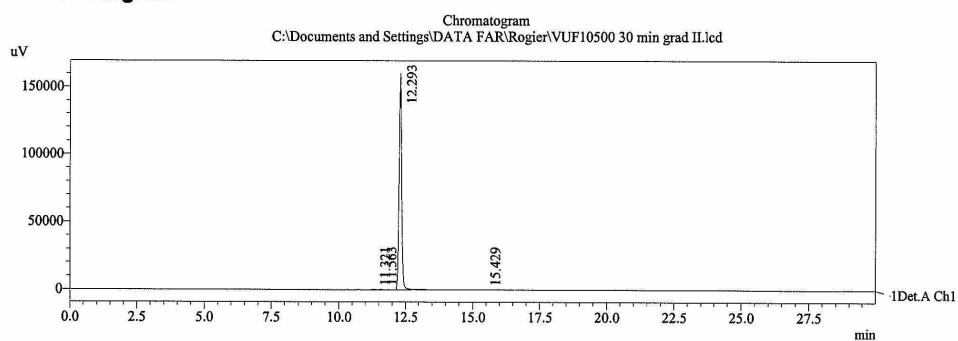


==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vail # : 75  
 Injection Volume : 5 uL  
 Data File Name : VUF10500 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 5:26:23 AM  
 Data Processed : 5/16/2007 5:56:26 AM

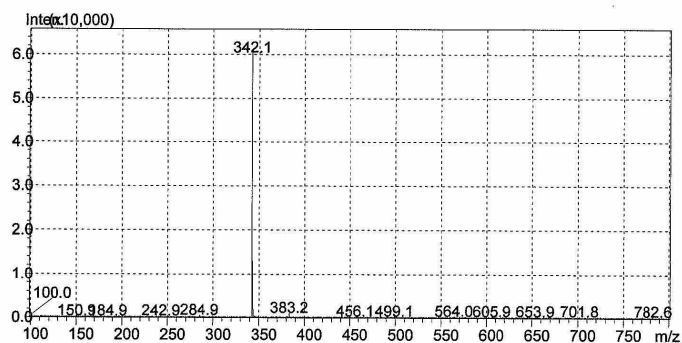


<Chromatogram>



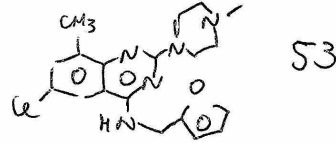
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.321	2534	315	0.235	0.195
2	11.563	2974	475	0.275	0.294
3	12.293	1072430	160501	99.294	99.343
4	15.429	2123	271	0.197	0.168
Total		1080060	161562	100.000	100.000

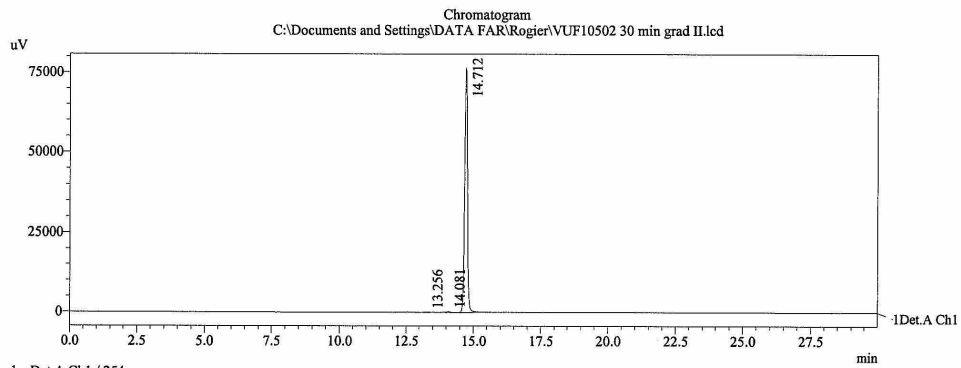


==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 73  
 Injection Volume : 5 uL  
 Data File Name : VUF10502 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 4:21:49 AM  
 Data Processed : 5/16/2007 4:51:52 AM



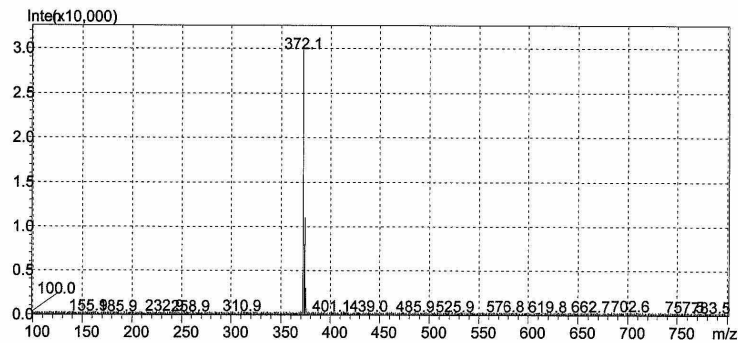
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

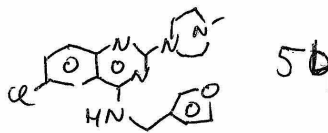
Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.256	1015	108	0.185	0.140
2	14.081	1925	278	0.351	0.362
3	14.712	545040	76537	99.464	99.498
Total		547980	76923	100.000	100.000



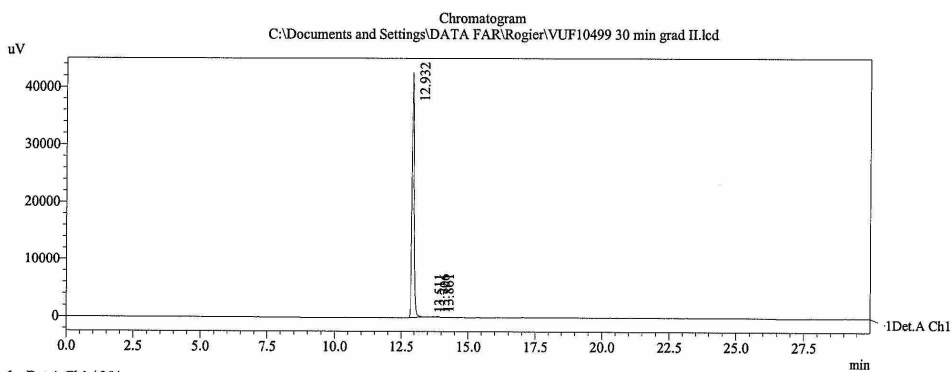
C:\Documents and Settings\DATA FAR\Rogier\VUF10502 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 62  
 Injection Volume : 5 uL  
 Data File Name : VUF10499 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/15/2007 10:59:10 PM  
 Data Processed : 5/15/2007 11:29:14 PM



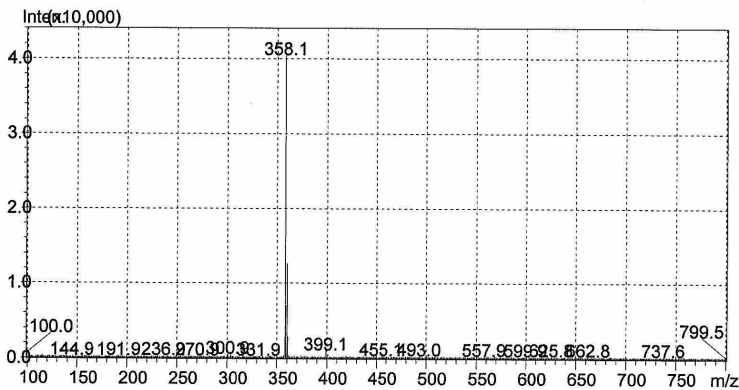
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

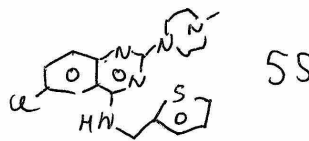
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.932	238079	42648	99.354	99.298
2	13.511	255	58	0.106	0.136
3	13.706	371	88	0.155	0.205
4	13.861	923	155	0.385	0.362
Total		239628	42950	100.000	100.000



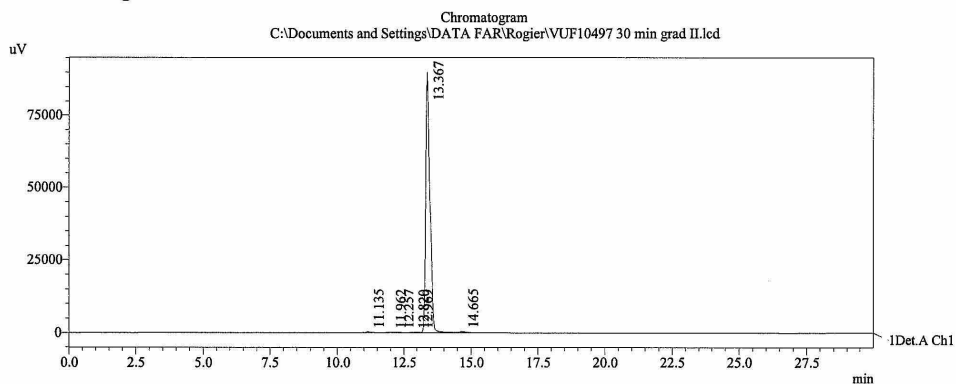
C:\Documents and Settings\FAR\Rogier\VUF10499 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 33  
 Injection Volume : 5 uL  
 Data File Name : VUF10497 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/22/2007 1:16:03 PM  
 Data Processed : 5/22/2007 1:46:09 PM



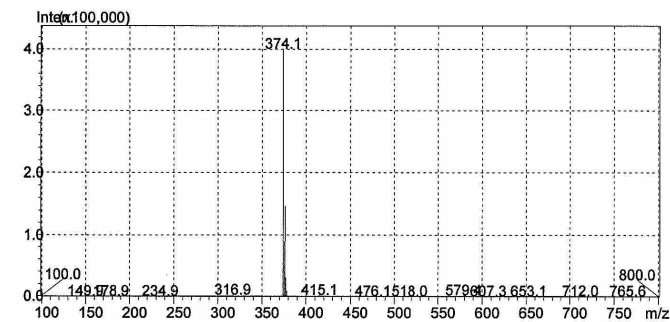
<Chromatogram>



Detector A Ch1 254nm

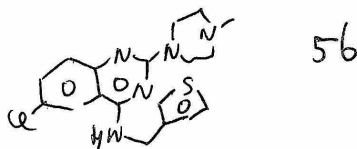
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.135	3038	321	0.302	0.351
2	11.962	3213	187	0.320	0.204
3	12.257	2133	190	0.212	0.208
4	12.820	1315	132	0.131	0.144
5	12.969	2165	215	0.215	0.235
6	13.367	988070	90056	98.337	98.449
7	14.665	4844	374	0.482	0.409
Total		1004778	91474	100.000	100.000

PeakTable

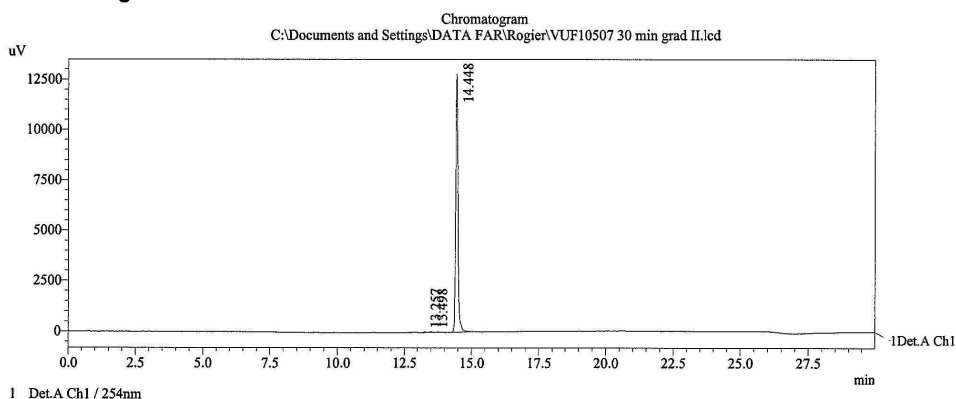


==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 52  
 Injection Volume : 8 uL  
 Data File Name : VUF10507 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/15/2007 6:08:36 PM  
 Data Processed : 5/15/2007 6:38:41 PM



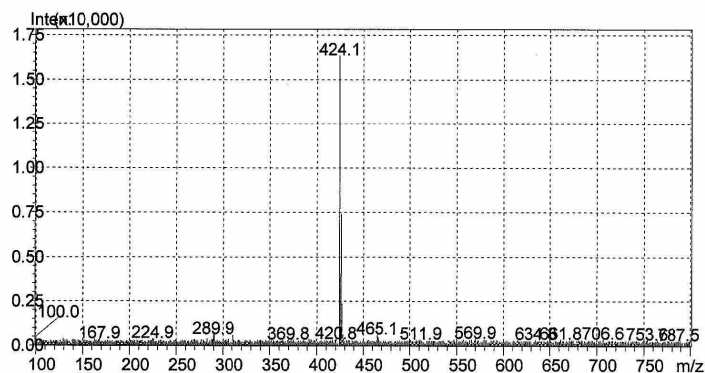
<Chromatogram>



I Det.A Ch1 / 254nm

PeakTable

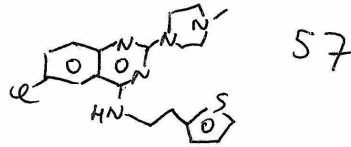
Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.257	213	39	0.287	0.305
2	13.498	186	32	0.251	0.247
3	14.448	73803	12801	99.462	99.448
Total		74203	12872	100.000	100.000



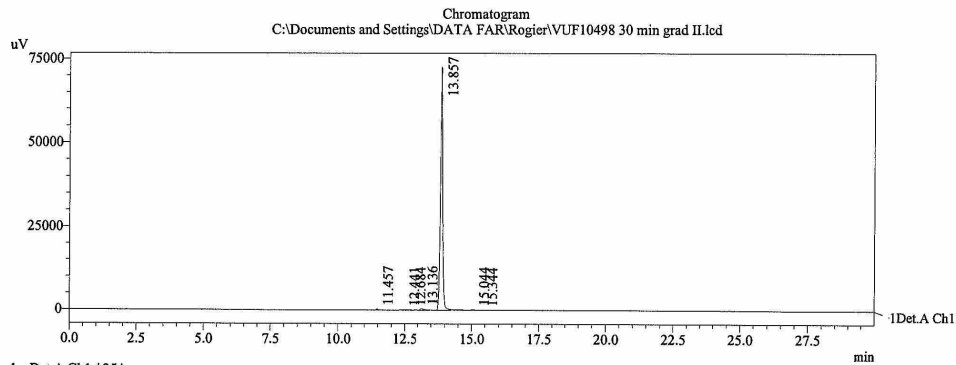
C:\Documents and Settings\DATA FAR\Rogier\VUF10507 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 63  
 Injection Volume : 5 uL  
 Data File Name : VUF10498 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/15/2007 11:31:26 PM  
 Data Processed : 5/16/2007 12:01:31 AM

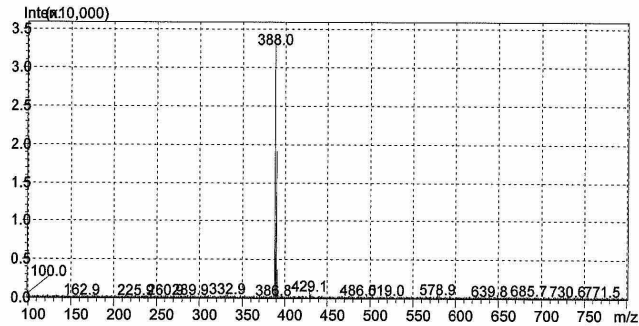


<Chromatogram>



1 Det.A Ch1 / 254nm

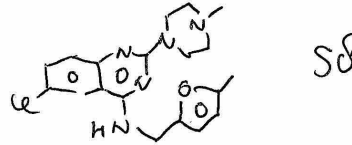
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.457	1896	357	0.428	0.482
2	12.441	1186	128	0.268	0.172
3	12.684	1178	196	0.266	0.264
4	13.136	4600	467	1.038	0.630
5	13.857	432505	72649	97.645	98.102
6	15.044	1344	226	0.303	0.305
7	15.344	229	34	0.052	0.045
Total		442936	74054	100.000	100.000



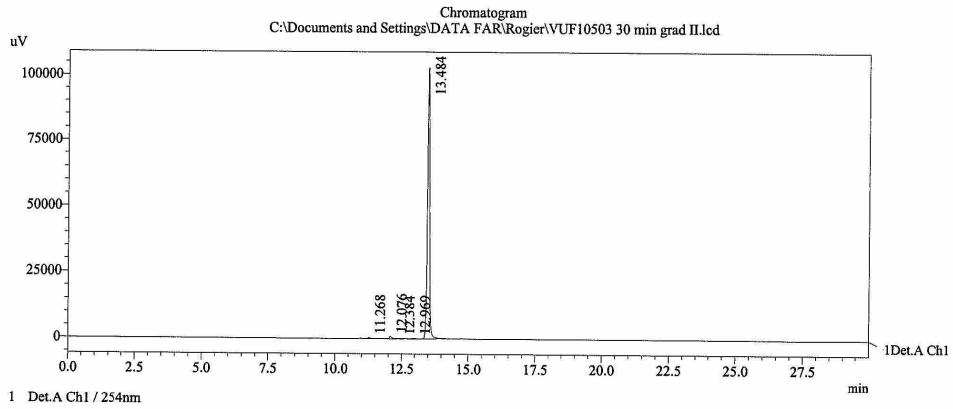
C:\Documents and Settings\FAR\Roger\WUF10498 30 min grad II.lcd

==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vail # : 61  
 Injection Volume : 5 uL  
 Data File Name : VUF10503 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/15/2007 10:26:53 PM  
 Data Processed : 5/15/2007 10:56:57 PM

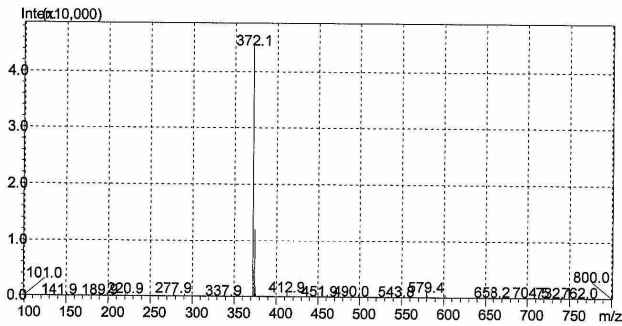


<Chromatogram>



PeakTable

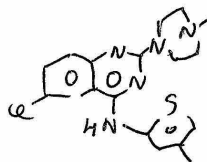
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.268	2561	439	0.425	0.419
2	12.076	5649	882	0.938	0.841
3	12.384	1452	170	0.241	0.162
4	12.969	1787	198	0.297	0.189
5	13.484	591044	103183	98.100	98.389
Total		602493	104873	100.000	100.000



C:\Documents and Settings\DATA FAR\Rogier\VUF10503 30 min grad II.lcd

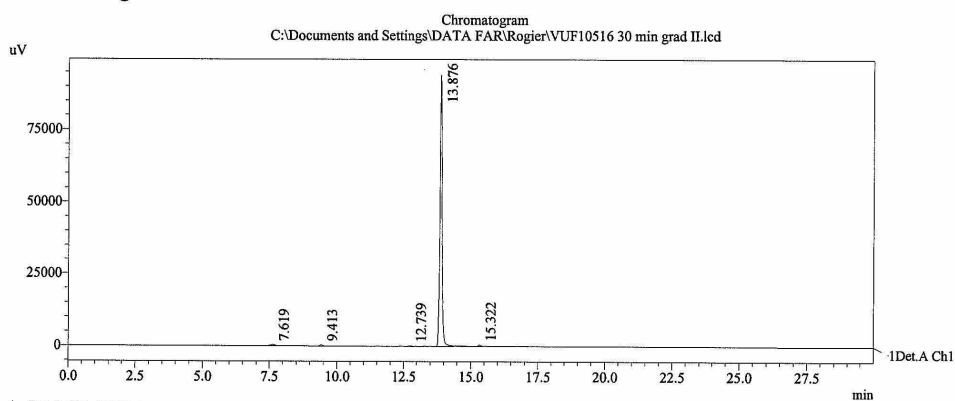
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 57  
 Injection Volume : 8 uL  
 Data File Name : VUF10516 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/15/2007 8:50:00 PM  
 Data Processed : 5/15/2007 9:20:04 PM



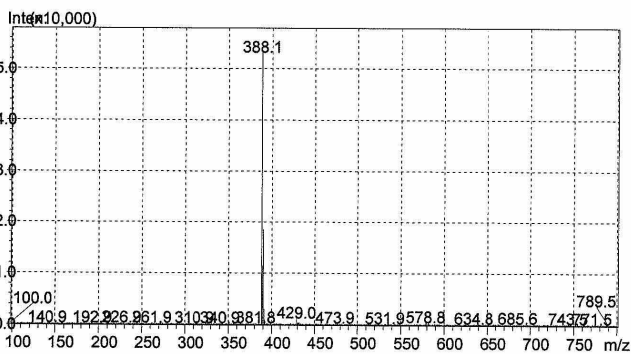
Sg

<Chromatogram>



PeakTable

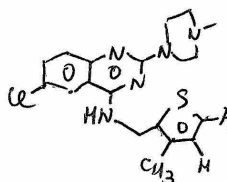
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.619	5510	438	0.988	0.457
2	9.413	2620	464	0.470	0.483
3	12.739	1901	283	0.341	0.295
4	13.876	544308	94212	97.588	98.207
5	15.322	3425	535	0.614	0.557
Total		557764	95932	100.000	100.000



C:\Documents and Settings\DATA FAR\Rogier\VUF10516 30 min grad II.lcd

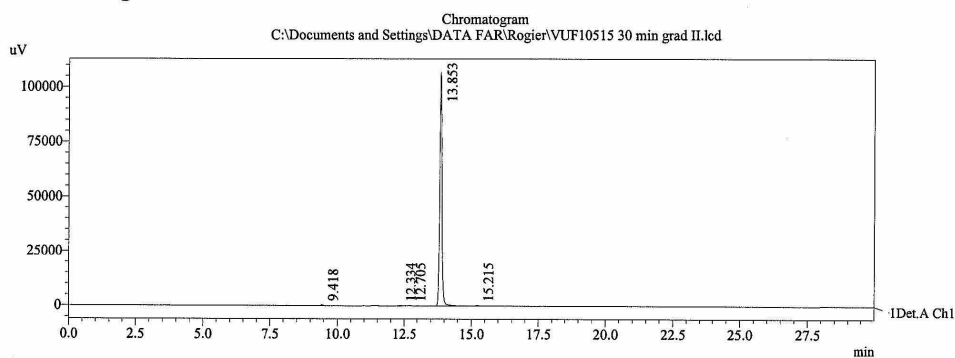
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 56  
 Injection Volume : 5 uL  
 Data File Name : VUF10515 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/15/2007 8:17:45 PM  
 Data Processed : 5/15/2007 8:47:48 PM



60

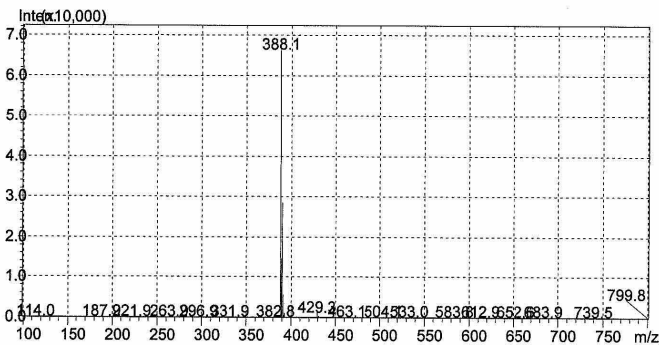
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

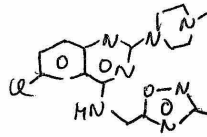
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.418	2320	445	0.374	0.411
2	12.334	1725	272	0.278	0.251
3	12.705	1792	250	0.289	0.231
4	13.853	612298	106955	98.742	98.825
5	15.215	1962	306	0.316	0.283
Total		620096	108227	100.000	100.000



C:\Documents and Settings\DATA FAR\Regier\VUF10515 30 min grad II.lcd

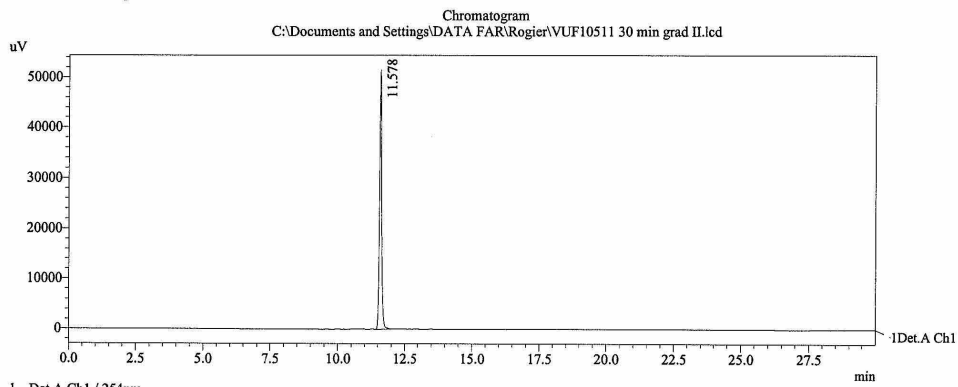
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 64  
 Injection Volume : 5 uL  
 Data File Name : VUF10511 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/16/2007 12:03:44 AM  
 Data Processed : 5/16/2007 12:33:48 AM



61

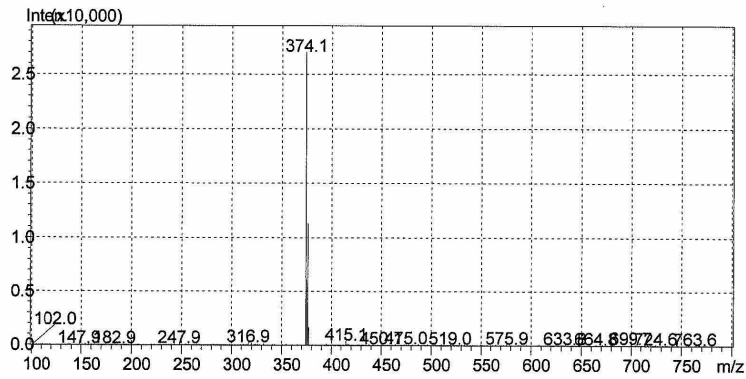
<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.578	283211	51541	100.000	100.000
Total		283211	51541	100.000	100.000

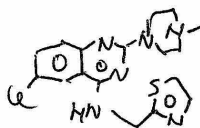


C:\Documents and Settings\FAR\Rogier\VUF10511 30 min grad II.lcd

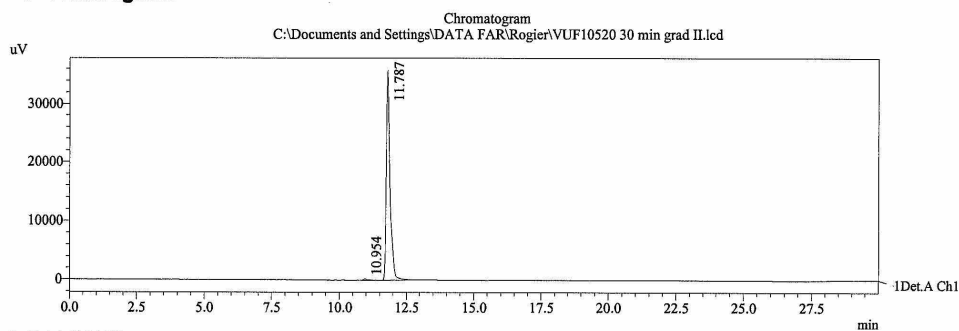
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 40  
 Injection Volume : 5 uL  
 Data File Name : VUF10520 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/22/2007 10:06:15 PM  
 Data Processed : 5/22/2007 10:36:20 PM

62

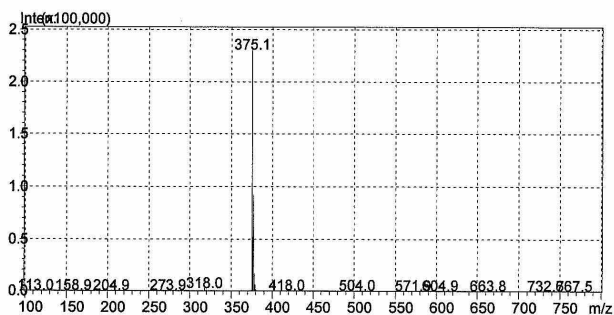


<Chromatogram>



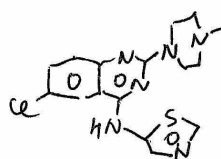
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.954	2232	241	0.638	0.665
2	11.787	347394	35929	99.362	99.335
Total		349626	36169	100.000	100.000



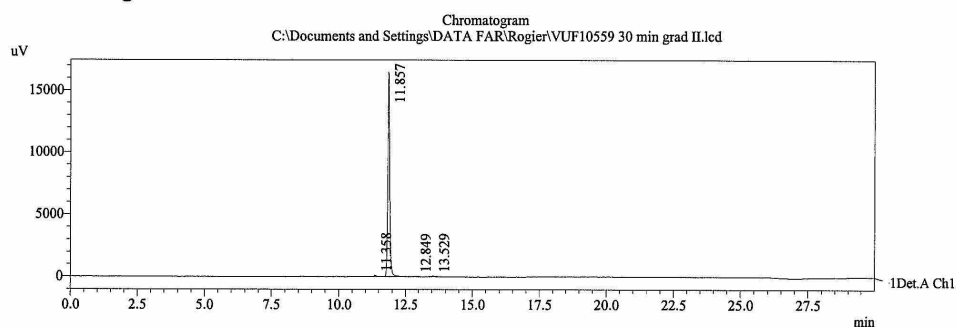
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 51  
 Injection Volume : 8 uL  
 Data File Name : VUF10559 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/15/2007 5:36:20 PM  
 Data Processed : 5/15/2007 6:06:22 PM



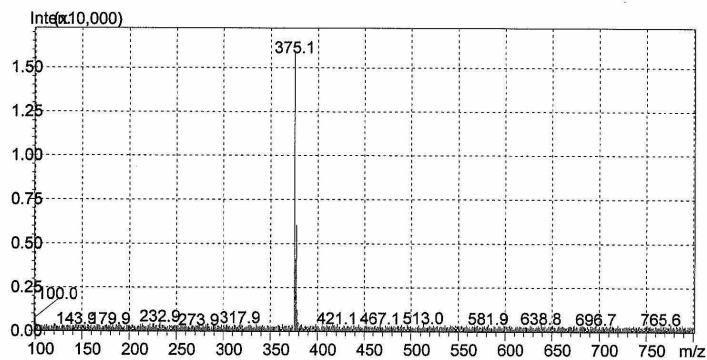
63

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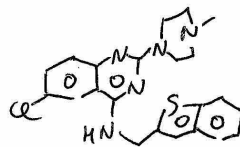
PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.358	405	101	0.483	0.608
2	11.857	82662	16500	98.702	98.889
3	12.849	235	32	0.281	0.191
4	13.529	447	52	0.534	0.313
Total		83748	16685	100.000	100.000



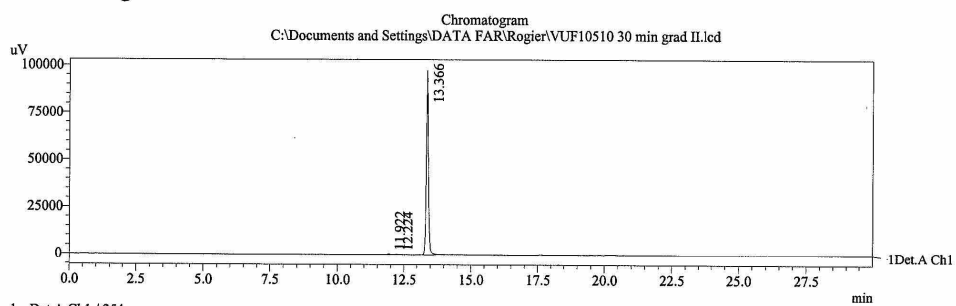
==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name :  
 Sample ID :  
 Vial # : 53  
 Injection Volume : 5 uL  
 Data File Name : VUF10510 30 min grad II.lcd  
 Method File Name : grad\_positivemode 30min 1.8ml\_min.lcm  
 Batch File Name : 28030701.lcb  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 5/15/2007 6:40:55 PM  
 Data Processed : 5/15/2007 7:11:00 PM



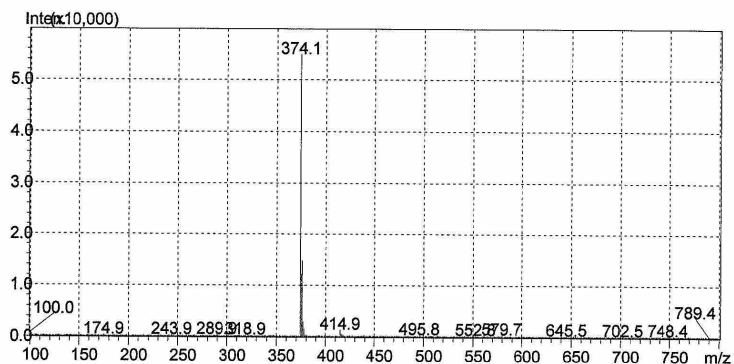
64

<Chromatogram>



PeakTable

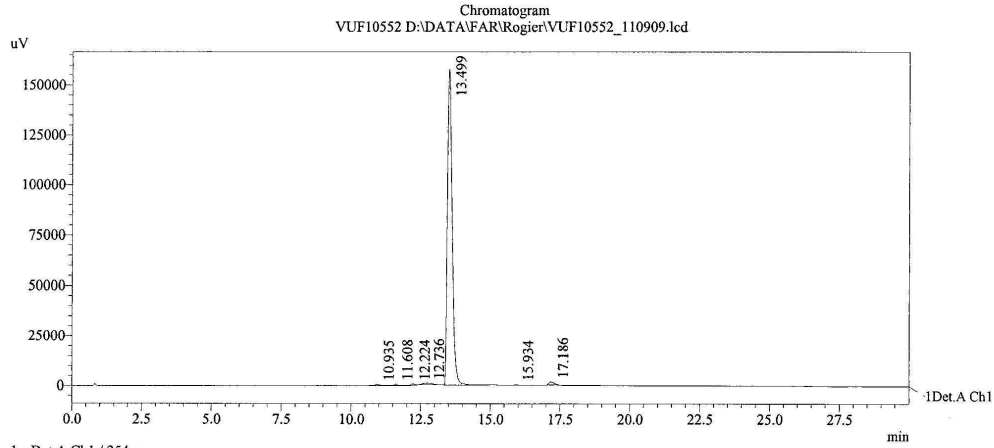
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.922	3460	567	0.639	0.575
2	12.224	1914	277	0.354	0.281
3	13.366	535920	97678	99.007	99.144
Total		541294	98522	100.000	100.000



==== Shimadzu LCMSsolution Analysis Report ====

Acquired by : Admin  
 Sample Name : VUF10552  
 Sample ID : ESI positive ion mode  
 Vial # : 31  
 Injection Volume : 20 uL  
 Data File Name : VUF10552\_110909.lcd  
 Method File Name : grad\_positivemode 30min 2.0ml\_min.lcm  
 Batch File Name :  
 Report File Name : DefaultLCMS.lcr  
 Data Acquired : 9/11/2008 1:22:32 PM  
 Data Processed : 9/11/2008 1:52:35 PM

<Chromatogram>



1 Det.A Ch1 / 254nm

PeakTable

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.935	4558	481	0.237	0.297
2	11.608	5190	710	0.269	0.439
3	12.224	5672	658	0.294	0.407
4	12.736	21425	889	1.112	0.550
5	13.499	1868191	157284	96.981	97.238
6	15.934	1733	247	0.090	0.153
7	17.186	19583	1483	1.017	0.917
Total		1926352	161753	100.000	100.000

