

**Supporting information****Second generation steroidal 4-aminoquinolines are potent, dual-target inhibitors of the botulinum neurotoxin serotype A metalloprotease and *P. falciparum***

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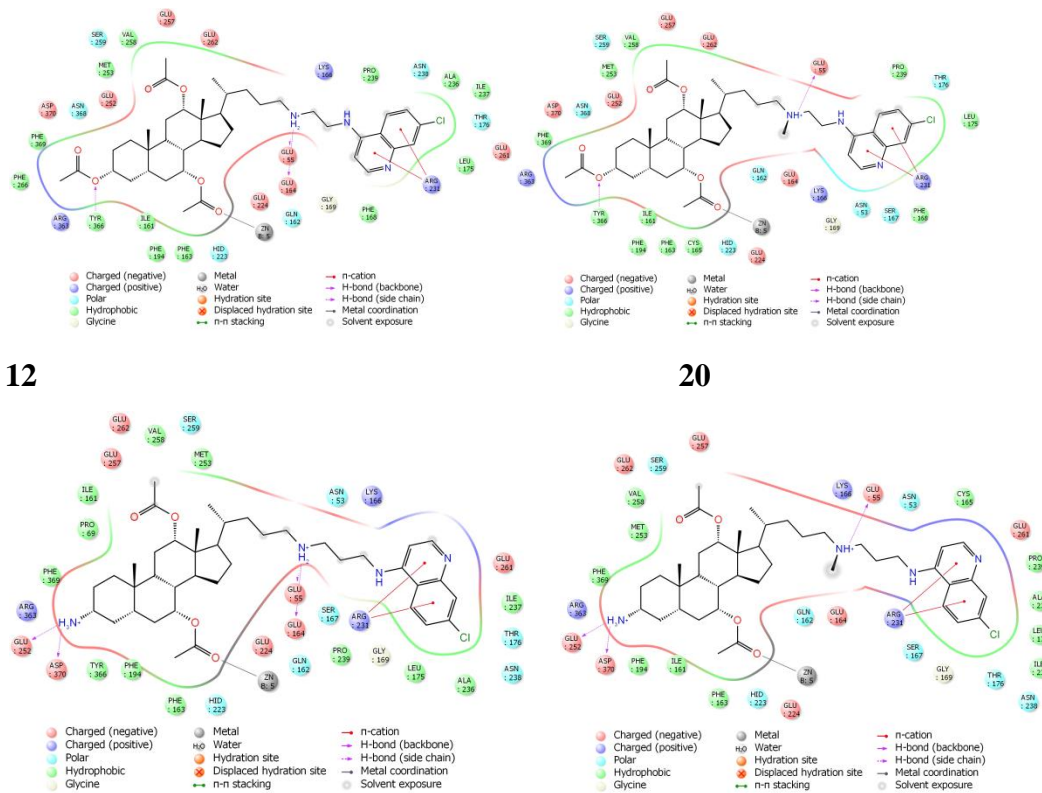
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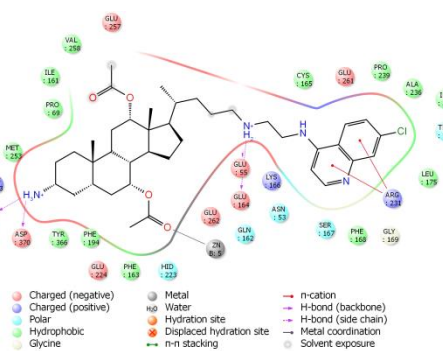
**Table 1S. In vitro inhibitory activities of tested compounds against BoNT/A LC**

Compound	% Inhibition (10 μM)
10	72.95
62	97.09
63	99.00

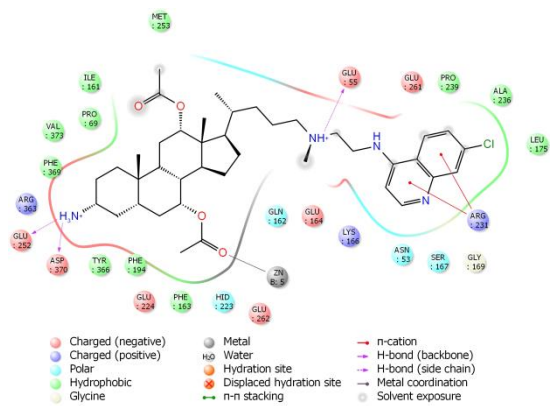
## Ligand interaction diagrams



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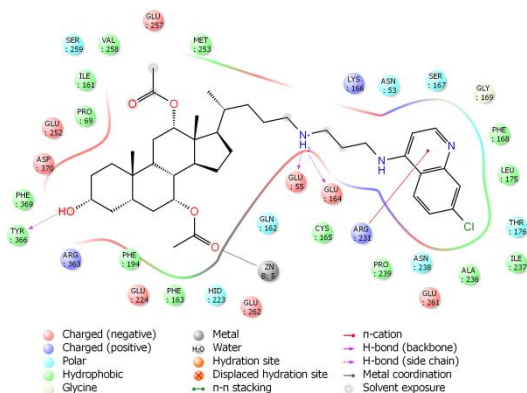
55



52

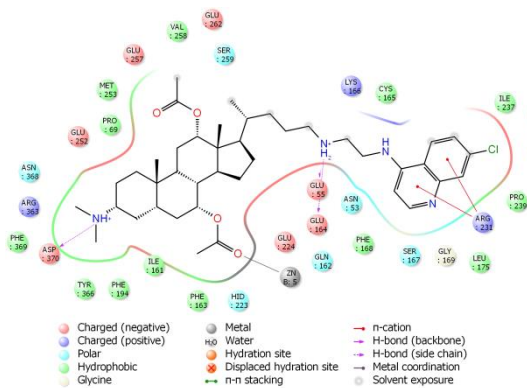
**Figure S1.** Ligand interaction diagrams for derivatives **12** (a), **20** (b), **53** (c) and **55** (d), (e) **52**, (f) **54**.

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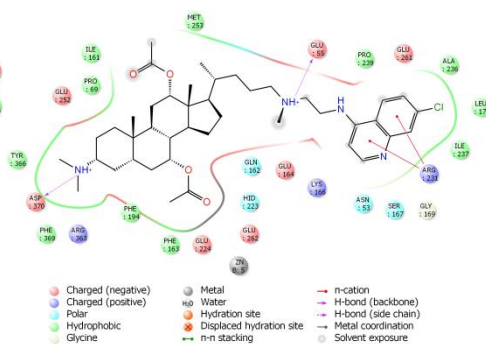


17

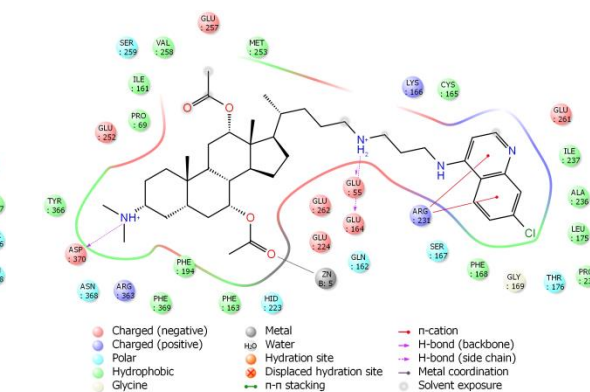
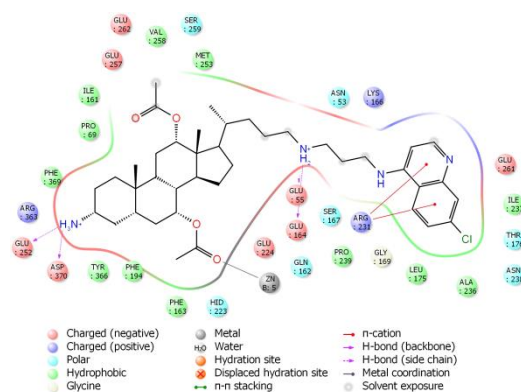
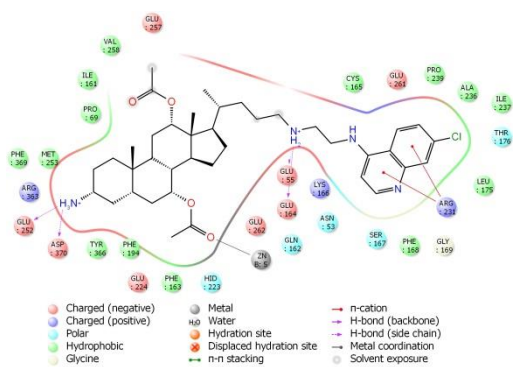
**Figure S2.** Ligand interaction diagrams for derivative **17**.



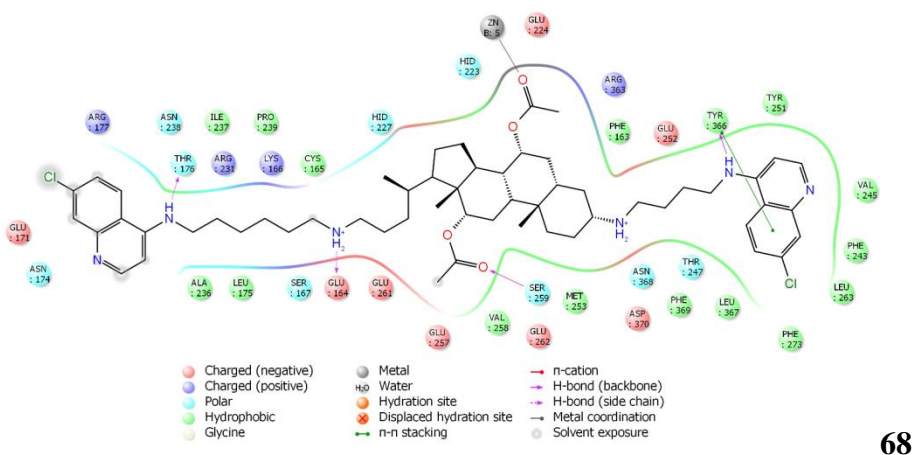
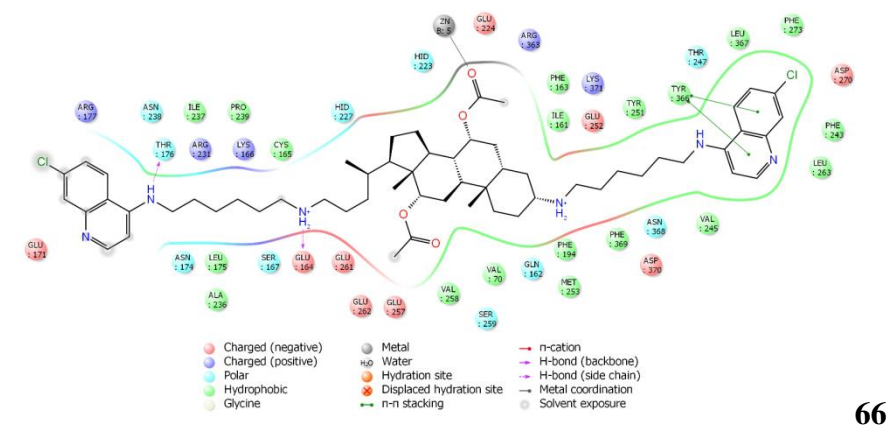
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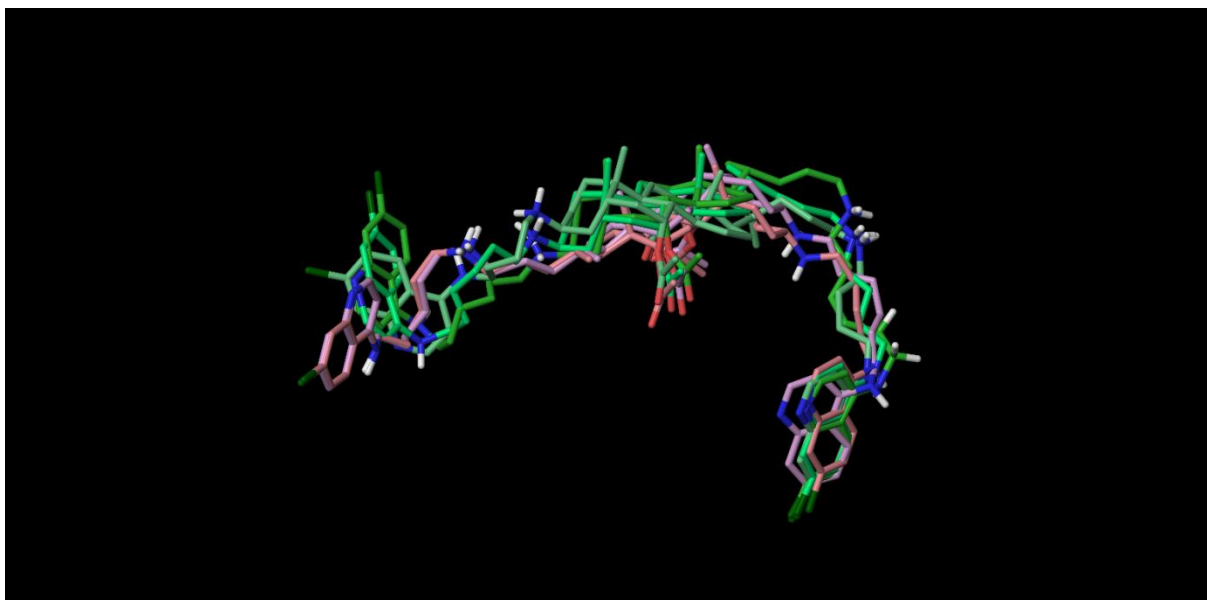
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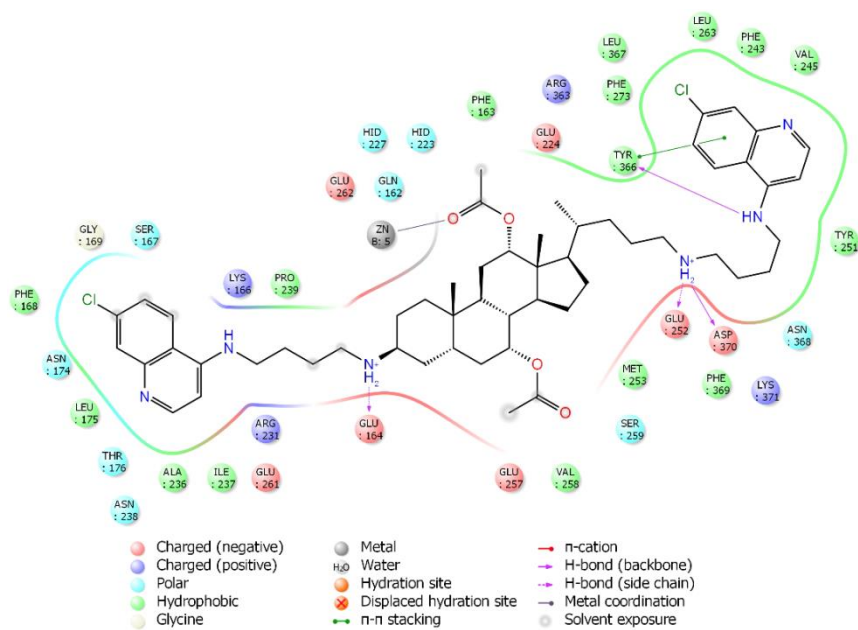
**Figure S3.** Ligand interaction diagrams for derivatives, **50**, **56** or **52**, **53**, and **51**.

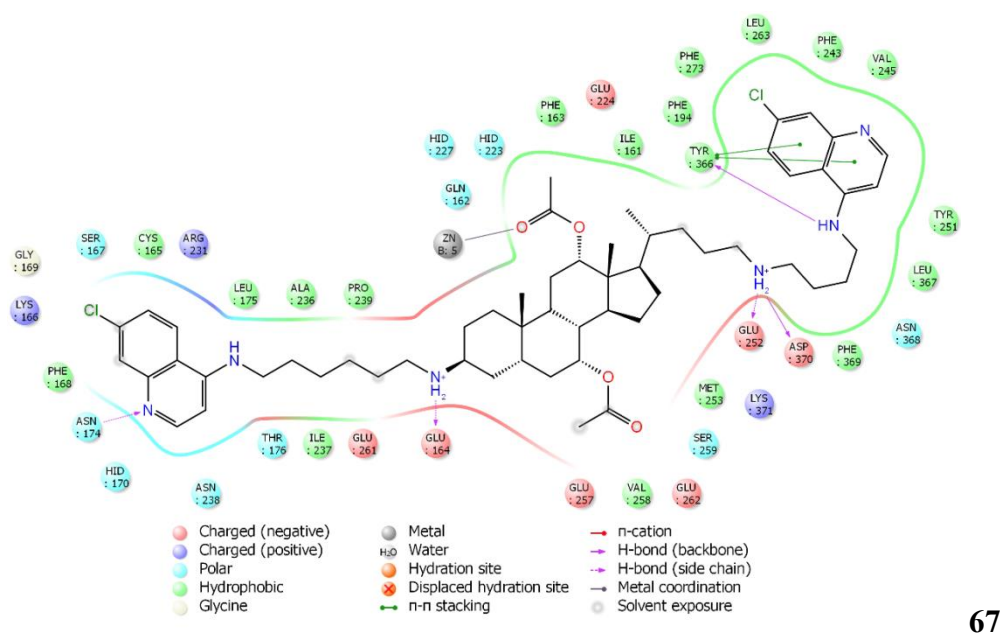
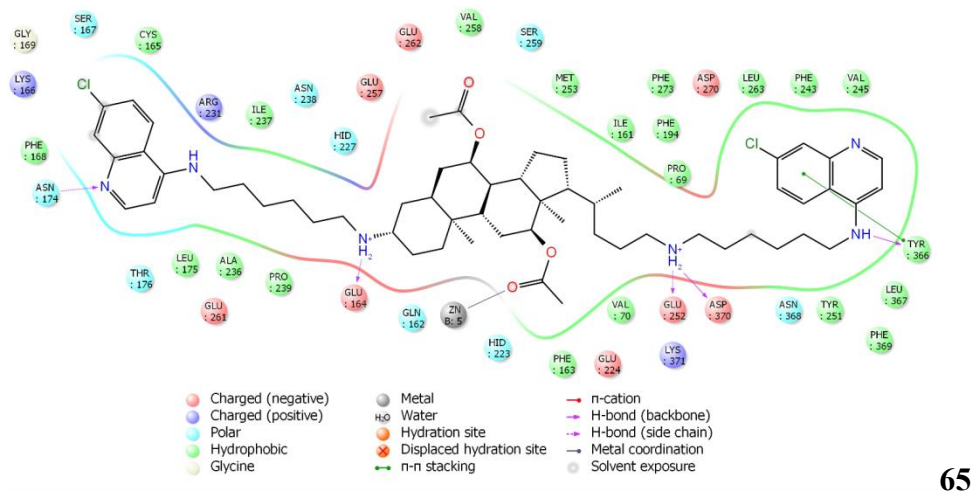


**Figure S4.** Ligand interaction diagrams for derivatives (a) **66** (b) **68**.



**Figure S5.** Overlapped docked structures of  $\alpha$ - and  $\beta$ -series of bis-ACQ derivatives.  $\alpha$ -Series (**66** and **68**) is in pink,  $\beta$ -series (**64**, **65** and **67**) is in green).





**Figure S6.** Ligand interaction diagrams for derivatives (a) **64**, (b) **65** and (c) **67**.

## Chemistry

### Synthesis

***N*-(3 $\alpha$ ,7 $\alpha$ ,12 $\alpha$ -Triacetoxy-5 $\beta$ -cholan-24-yl)-*N'*-(7'-chloroquinolin-4'-yl)-propane-1,3-diamine (**13**).** Compound **13** was obtained according to procedure described for **12**, using **11** (1.9 g, 3.65 mmol) and ACQ3 (1.99 g, 8.44 mmol). Yield 1.18g (44 %). Colorless foam softens at 91-95 °C.  $[\alpha]_D^{20} = +0.106$  ( $c = 2.0 \times 10^{-3}$  g/mL, DCM). IR (ATR): 2936w, 2866w,

1727s, 1610s, 1579s, 1535w, 1446w, 1365m, 1330w, 1232s, 1136w, 1021m, 964w, 938w, 882w, 820w, 803w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 8.46 (*d*,  $J = 5.5$ , H-C(2')), 7.906 (*d*,  $J = 2.0$ , H-C(8')), 7.76 (*d*,  $J = 9.0$ , H-C(5')), 7.34, (*dd*,  $J_1 = 2.5$ ,  $J_2 = 9.0$ , H-C(6')), 6.29 (*d*,  $J = 5.5$ , H-C(3')), 5.11-5.10 (*m*, H-C(12)), 4.91-4.89 (*m*, H-C(7)), 4.62-4.40 (*m*, H-C(3)), 3.395 (*t*,  $J = 6.0$ , 2H-C(9')), 2.99-2.92 (*m*, 2H-C(11')), 2.82-2.62 (*m*, 2H-N, 2H-C(24)), 2.12 (*s*,  $\text{CH}_3\text{COO}$ ), 2.06 (*s*,  $\text{CH}_3\text{COO}$ ), 2.03 (*s*,  $\text{CH}_3\text{COO}$ ), 0.92 (*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.85 (*d*,  $J = 6.5$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.73 (*s*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 170.54, 170.50, 170.39, 151.53, 150.76, 148.50, 134.87, 127.96, 124.82, 122.26, 117.45, 98.22, 75.43, 74.01, 70.61, 50.38, 49.28, 47.39, 45.04, 43.79, 43.55, 40.88, 37.69, 34.86, 34.57, 34.25, 33.24, 31.19, 28.98, 27.28, 26.87, 26.81, 26.09, 25.61, 22.74, 22.52, 21.48, 21.45, 21.39, 17.87, 12.23.

(+)ESI-HRMS ( $m/z$ ):  $[\text{M} + \text{H}]^+$  738.4226 (error -2.40 ppm). Combustion analysis for ( $\text{C}_{42}\text{H}_{60}\text{ClN}_3\text{O}_6 \times 1.5\text{H}_2\text{O}$ ): calculated C 65.91, H 8.30, N 5.49; found C 66.12, H 7.92, N 5.49.

HPLC purity: Method A: RT 2.092, area 98.69 %; method B: RT 8.698, area 95.46 %.

***N*-(3 $\alpha$ ,7 $\alpha$ ,12 $\alpha$ -Triacetoxy-5 $\beta$ -cholan-24-yl)-*N'*-(7'-chloroquinolin-4'-yl)-butane-1,4-diamine (14).** Alcohol **11** (2.11 g, 4.08 mmol) was dissolved in DCM (440 mL), PCC (1.32 g, 6.11 mmol) was added and mixture was stirred at r.t. for 6 h. Reaction mixture was filtered through short column of  $\text{SiO}_2$  (eluent DCM/EA = 9/1). Crude aldehyde was dissolved in dry MeOH (40 mL), ACQ4 (1.01 g; 4.06 mmol) was added and mixture was stirred overnight at r.t. followed by  $\text{NaBH}_4$  (307 mg, 8.12 mmol) added in one portion. After 5h solvent was removed under reduced pressure and the product was purified by column chromatography (dry flash,  $\text{SiO}_2$ , eluent EA/Hex gradient 1/1  $\rightarrow$  EA, EA/MeOH gradient 95/5  $\rightarrow$  1/1, MeOH). Yield 2.16 g (71%). Colorless foam softens at 80-83  $^\circ\text{C}$ .  $[\alpha]_{\text{D}}^{20} = +0.116$  ( $c = 1.4 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3396w, 3304w, 2936s, 2866m, 1730s, 1610w, 1579s, 1536s, 1448w, 1370m, 1331w, 1245s, 1133w, 1068w, 1023w, 965w, 886w, 807w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (500 MHz,

CDCl<sub>3</sub>, δ): 8.70 (*d*, *J* = 5.2 H-C(2')), 8.12 (*d*, *J* = 2.1, H-C(8')), 7.93 (*d*, *J* = 8.8, H-C(5')), 7.50, (*dd*, *J*<sub>1</sub> = 8.9, *J*<sub>2</sub> = 2.1, H-C(6')), 6.55 (*d*, *J* = 5.2, H-C(3')), 6.28 (*bs*, H-N), 5.28 (*bs*, H-C(12)), 5.13-5.08 (*m*, H-C(7)), 4.82-4.73 (*m*, H-C(3)), 3.49 (*t*, *J* = 6.6, 2H-C(9')), 2.91 (*t*, *J* = 6.7, 2H-C(12')), 2.85-2.73 (*m*, 2H-C(24)), 2.31 (*s*, CH<sub>3</sub>COO), 2.27 (*s*, CH<sub>3</sub>COO), 2.24 (*s*, CH<sub>3</sub>COO), 1.11 (*s*, CH<sub>3</sub>-C(10)), 1.02 (*d*, *J* = 6.4, CH<sub>3</sub>-C(20)), 0.91 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, δ): 170.49, 170.33, 151.98, 150.00, 149.08, 134.68, 128.58, 124.88, 121.47, 117.30, 98.80, 75.40, 74.04, 70.67, 50.40, 49.03, 47.55, 44.99, 43.36, 43.11, 40.89, 37.71, 34.92, 34.65, 34.28, 33.32, 31.22, 28.86, 27.63, 27.25, 27.14, 26.84, 26.33, 26.20, 25.53, 22.77, 22.51, 21.55, 21.44, 21.39, 17.87, 12.19. (+)ESI-HRMS (*m/z*): [M + 2H]<sup>2+</sup> 376.72256 (error -2.85 ppm), [M + H]<sup>+</sup> 752.43999 (error -4.73 ppm); Combustion analysis for (C<sub>43</sub>H<sub>62</sub>ClN<sub>3</sub>O<sub>6</sub>×3H<sub>2</sub>O): calculated C 64.04, H 8.50, N 5.21; found C 64.43, H 8.27, N 5.13. HPLC purity: Method A: RT 1.900, area 98.59 %; method C: RT 10.694, area 99.15%.

***N*-(3*α*,7*α*,12*α*-Triacetoxy-5*β*-cholan-24-yl)-*N'*-(7'-chloroquinolin-4'-yl)-hexane-1,6-diamine (15).** Aldehyde was obtained according to procedure described for **14**, using **11** (1.30 g, 2.49 mmol) and PCC (807 mg, 3.74 mmol). Reductive amination was performed using ACQ6 (614 mg, 2.21 mmol) and NaBH<sub>4</sub> (170 mg, 4.50 mmol). Crude product was purified by column chromatography (dry flash, SiO<sub>2</sub>, eluent EA/Hex gradient 1/1 → 8/2, EA, EA/MeOH gradient 9/1 → 1/9, MeOH). Yield 814 mg (42%). colorless foam softens at 74-76 °C. [α]<sub>D</sub><sup>20</sup> = +0.089 (c = 1.3×10<sup>-3</sup> g/mL, DCM). IR (KBr): 2931w, 2862w, 1728s, 1609w, 1577s, 1536w, 1447m, 1367m, 1330w, 1235s, 1133w, 1070w, 1021m, 964w, 938w, 886w, 849w, 805w cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, δ): 8.52 (*d*, *J* = 5.4 H-C(2')), 7.95 (*d*, *J* = 2.2, H-C(8')), 7.69 (*d*, *J* = 9.0, H-C(5')), 7.35, (*dd*, *J*<sub>1</sub> = 2.1, *J*<sub>2</sub> = 8.9, H-C(6')), 6.40 (*d*, *J* = 5.4, H-C(3')), 5.12 (*bs*, H-N, exchangeable with D<sub>2</sub>O), 5.08 (*bs*, H-C(12)), 4.91-4.90 (*m*, H-C(7)), 4.60-4.50 (*m*, H-C(3)), 3.40-3.20 (*m*, 2H-C(9')), 2.70-2.50 (*m*, 2H-C(14') and 2H-C(24)),



2.13 (*s*, CH<sub>3</sub>COO), 2.08 (*s*, CH<sub>3</sub>COO), 2.07 (*s*, CH<sub>3</sub>COO), 0.91 (*s*, CH<sub>3</sub>-C(10)), 0.82 (*d*, *J* = 6.5, CH<sub>3</sub>-C(20)), 0.71 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, δ): 170.49, 170.35, 151.99, 149.71, 149.09, 134.78, 128.77, 125.18, 120.91, 117.10, 99.00, 75.43, 74.06, 70.69, 50.27, 49.61, 47.46, 44.98, 43.36, 43.11, 40.91, 37.72, 34.83, 34.67, 34.58, 34.30, 33.26, 31.24, 29.59, 28.86, 28.70, 27.23, 26.99, 26.94, 26.86, 26.06, 25.54, 22.78, 22.52, 21.57, 21.45, 21.40, 17.87, 12.18. (+)ESI-HRMS (*m/z*):[M + 2H]<sup>2+</sup> 390.7382 (error -2.89 ppm), ; [M + H]<sup>+</sup> 780.4713 (error -3.76 ppm); Combustion analysis for (C<sub>45</sub>H<sub>66</sub>ClN<sub>3</sub>O<sub>6</sub>×1.5H<sub>2</sub>O): calculated C 66.93, H 8.61, N 5.20; found C 66.59, H 8.31, N 5.13. HPLC purity: Method A: RT 1.971, area 99.39 %; method C: RT 11.700, area 95.41 %.

***N*-(3α-Hydroxy-7α,12α-diacetoxy-5β-cholan-24-yl)-*N'*-(7'-chloroquinolin-4'-yl)-**

**propane-1,3-diamine (17).** Alcohol **17** was obtained according to procedure described for **16**, using **13** (727 mg, 0.24 mmol) and anh. K<sub>2</sub>CO<sub>3</sub> (241 mg, 0.43 mmol). Yield 626 mg (91%). Colorless foam softens at 110-114 °C. [ $\alpha$ ]<sub>D</sub><sup>20</sup> = +0.114 (*c* = 2.0×10<sup>-3</sup> g/mL, DCM). IR (ATR): 3249w, 2930m, 2863m, 1714m, 1610s, 1577s, 1540m, 1433m, 1372s, 1330w, 1240s, 1138w, 1114w, 1073m, 1019m, 966w, 902w, 853w, 803w cm<sup>-1</sup>. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>, δ): 8.47 (*d*, *J* = 5.6, H-C(2')), 7.92 (*d*, *J* = 2.2, H-C(8')), 7.80 (*bs*, H-N), 7.73 (*d*, *J* = 9.0, H-C(5')), 7.32 (*dd*, *J*<sub>1</sub> = 2.0, *J*<sub>2</sub> = 8.7, H-C(6')), 6.30 (*d*, *J* = 5.6, H-C(3')), 5.11 (*bs*, H-C(12)), 4.95-4.85 (*m*, H-C(7)), 3.60-3.35 (*m*, H-C(3) and 2H-C(9')), 2.96-2.86 (*m*, 2H-C(11')), 2.70-2.58 (*m*, 2H-C(24)), 2.11 (*s*, CH<sub>3</sub>COO), 2.04 (*s*, CH<sub>3</sub>COO), 0.91 (*s*, CH<sub>3</sub>-C(10)), 0.86 (*d*, *J* = 6.2, CH<sub>3</sub>-C(20)), 0.73 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>, δ): 170.69, 151.94, 150.59, 148.94, 134.64, 128.29, 124.70, 122.12, 117.51, 98.21, 75.43, 71.50, 70.77, 50.49, 49.42, 47.50, 44.99, 43.88, 43.43, 40.95, 38.58, 37.67, 34.92, 34.80, 34.18, 33.30, 31.26, 30.41, 28.93, 27.24, 27.15, 26.57, 25.53, 22.69, 22.49, 21.52, 21.38, 17.85, 12.17. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, δ): 8.27 (*d*, *J* = 5.6, H-C(2')), 7.77-7.73 (*m*, H-C(8') and H-C(5')), 7.24

(*dd*,  $J_1 = 8.9$ ,  $J_2 = 2.1$ , H-C(6')), 6.25 (*d*,  $J = 5.6$ , H-C(3')), 5.00 (*bs*, H-C(12)), 4.81-4.77 (*m*, H-C(7)), 3.75 (*bs*, H-N, exchangeable with D<sub>2</sub>O), 3.39-3.31 (*m*, H-C(3)), 3.31-3.35 (*m*, 2H-C(9')), 2.71 (*t*,  $J = 6.3$ , 2H-C(11')), 2.55-2.44 (*m*, 2H-C(24)), 2.01 (*s*, CH<sub>3</sub>COO), 1.97 (*s*, CH<sub>3</sub>COO), 0.90 (*s*, CH<sub>3</sub>-C(10)), 0.74 (*d*,  $J = 6.4$ , CH<sub>3</sub>-C(20)), 0.64 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, δ): 170.02, 170.85, 151.11, 150.72, 148.18, 134.90, 127.05, 124.83, 122.13, 117.19, 98.08, 75.51, 70.98, 70.87, 50.11, 49.22, 49.05, 48.88, 48.71, 48.54, 48.37, 47.98, 47.45, 44.83, 43.17, 42.08, 40.75, 38.12, 37.51, 34.79, 34.61, 34.00, 33.11, 31.07, 29.94, 28.70, 27.29, 27.05, 26.25, 25.26, 22.52, 22.24, 21.13, 20.96, 17.59. (+)ESI-HRMS (*m/z*): [M + H]<sup>+</sup> 696.4133 (error -0.71 ppm). Combustion analysis for (C<sub>40</sub>H<sub>58</sub>ClN<sub>3</sub>O<sub>5</sub>×2H<sub>2</sub>O): calculated C 65.60, H 8.53, N 5.74; found C 65.95, H 8.20, N 5.85. HPLC purity: Method B: RT 8.583, area 95.71 %; method C: RT 13.187, area 95.02 %.

***N*-(3α-Hydroxy-7α,12α-diacetoxy-5β-cholan-24-yl)-*N'*-(7'-chloroquinolin-4'-yl)-butane-1,4-diamine (18).** Alcohol **18** was obtained according to procedure described for **16**, using **14** (2.21 g, 0.24 mmol) and anh. K<sub>2</sub>CO<sub>3</sub> (673 mg, 4.87 mmol). Product was isolated after column chromatography purification (Biotage SP1 flash, RP-column, eluent gradient MeOH/H<sub>2</sub>O 7:3 → MeOH, NH-column eluent gradient EA → EA/MeOH 8:2). Yield 1.67 g (80 %). colorless foam softens at 101-103 °C.  $[\alpha]_D^{20} = +0.064$  ( $c = 1.4 \times 10^{-3}$  g/mL, DCM). IR (ATR): 3303m, 3059w, 29.36s, 2866m, 1726s, 1610w, 1581s, 1540w, 1450w, 1374m, 1332w, 1250s, 1138w, 1076m, 1021m, 967w, 900w, 852w, 808w cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, δ): 8.51 (*d*,  $J = 5.5$ , H-C(2')), 7.94 (*d*,  $J = 2.1$ , H-C(8')), 7.71 (*d*,  $J = 8.9$ , H-C(5')), 7.33, (*dd*,  $J_1 = 8.9$ ,  $J_2 = 2.1$ , H-C(6')), 6.37 (*d*,  $J = 5.5$ , H-C(3')), 6.01 (*bs*, H-N, exchangeable with D<sub>2</sub>O), 5.11-5.07 (*m*, H-C(12)), 4.92-4.88 (*m*, H-C(7)), 3.55-3.46 (*m*, H-C(3)), 3.30 (*t*,  $J = 6.4$ , 2H-C(9')), 2.70 (*t*,  $J = 6.8$ , 2H-C(12')), 2.64-2.52 (*m*, 2H-C(24)), 2.11 (*s*, CH<sub>3</sub>COO), 2.07 (*s*, CH<sub>3</sub>COO), 0.90 (*s*, CH<sub>3</sub>-C(10)), 0.83 (*d*,  $J = 6.6$ , CH<sub>3</sub>-C(20)), 0.72 (*s*, CH<sub>3</sub>-C(13)).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 170.64, 170.61, 152.05, 149.99, 149.15, 134.71, 128.70, 124.94, 121.37, 117.31, 98.85, 75.47, 71.65, 70.84, 50.54, 49.14, 47.56, 45.02, 43.41, 43.21, 38.69, 37.76, 34.98, 34.85, 34.27, 33.37, 31.36, 30.49, 28.96, 27.87, 37.30, 36.55, 26.30, 25.56, 22.80, 22.55, 21.62, 21.45, 17.92, 12.22. (+)ESI-HRMS ( $m/z$ ):  $[\text{M} + \text{Na}]^+$  732.4113 (error -0.09 ppm). Combustion analysis for  $(\text{C}_{41}\text{H}_{60}\text{ClN}_3\text{O}_5 \times 0.5\text{H}_2\text{O})$ : calculated C 68.45, H 8.55, N 5.84; found C 65.22, H 8.35, N 5.62. HPLC purity: Method A: RT 1.879, area 99.04 %; method D: RT 5.495, area 97.05 %.

***N*-(3 $\alpha$ -Hydroxy-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholan-24-yl)-N'-(7'-chloroquinolin-4'-yl)-hexane-1,6-diamine (19).** Alcohol **19** was obtained according to procedure described for **16**, using **15** (204.9 mg, 0.26 mmol) and anh.  $\text{K}_2\text{CO}_3$  (64 mg, 0.46 mmol). Yield 180 mg (92%), colorless foam softens at 98-101 °C.  $[\alpha]_{\text{D}}^{20} = +0.074$  ( $c = 1.6 \times 10^{-3}$  g/mL, DCM). IR (ATR): 3302m, 306w, 2933s, 2863m, 1725s, 1609w, 1581s, 1540w, 1450m, 1373m, 1332w, 1250s, 1140w, 1076m, 1022m, 966w, 939w, 899w, 852w, 809w, 736m  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 8.50 (*d*,  $J = 5.6$ , H-C(2')), 7.94 (*d*,  $J = 1.6$ , H-C(8')), 7.76 (*d*,  $J = 9.0$ , H-C(5')), 7.40-7.30, (*m*, H-C(6')), 6.38 (*d*,  $J = 5.6$ , H-C(3')), 5.37 (*bs*, H-N, exchangeable with  $\text{D}_2\text{O}$ ), 5.07 (*bs*, H-C(12)), 4.89 (*bs*, H-C(7)), 3.60-3.20 (*m*, H-C(3) and 2H-C(9')), 2.50-2.80 (*m*, 2H-C(14') and 2H-C(24)), 2.10 (*s*,  $\text{CH}_3\text{COO}$ ), 2.07 (*s*,  $\text{CH}_3\text{COO}$ ), 0.90 (*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.80 (*d*,  $J = 6.2$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.70 (*s*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 170.69, 151.81, 149.85, 148.92, 134.86, 128.47, 125.20, 121.15, 117.07, 98.90, 75.45, 71.39, 70.85, 49.98, 49.29, 47.43, 44.96, 43.34, 42.92, 40.97, 38.58, 37.69, 34.81, 34.21, 33.16, 31.30, 30.40, 29.22, 28.88, 28.53, 27.20, 26.84, 25.77, 25.49, 22.74, 22.49, 21.58, 21.40, 17.79, 12.13.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 8.52 (*d*,  $J = 5.5$ , H-C(2')), 7.95 (*d*,  $J = 2.1$ , H-C(8')), 7.73 (*d*,  $J = 9.2$ , H-C(5')), 7.35, (*dd*,  $J_1 = 8.9$ ,  $J_2 = 2.1$ , H-C(6')), 6.40 (*d*,  $J = 5.3$ , H-C(3')), 5.20 (*bs*, H-N, exchangeable with  $\text{D}_2\text{O}$ ), 5.08 (*bs*, H-C(12)), 4.92-4.86 (*m*, H-C(7)), 3.55-3.45 (*m*,

H-C(3)), 3.34-3.24 (*m*, 2H-C(9')), 2.50-2.80 (*m*, 2H-C(14') and 2H-C(24)), 2.11 (*s*, CH<sub>3</sub>COO), 2.07 (*s*, CH<sub>3</sub>COO), 0.90 (*s*, CH<sub>3</sub>-C(10)), 0.81 (*d*, *J* = 6.4, CH<sub>3</sub>-C(20)), 0.70 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, δ): 170.61, 151.83, 149.85, 148.96, 134.82, 128.55, 125.16, 121.14, 117.12, 98.93, 75.44, 71.54, 70.82, 49.82, 49.10, 47.48, 44.98, 43.36, 43.03, 41.01, 38.68, 37.72, 34.83, 34.24, 33.16, 31.34, 30.48, 28.91, 28.56, 27.23, 26.81, 25.52, 22.76, 22.51, 26.60, 21.43, 17.81, 12.17. (+)ESI-HRMS (*m/z*): [M + 2H]<sup>2+</sup> 369.7326 (error -3.80 ppm). Combustion analysis for (C<sub>43</sub>H<sub>64</sub>ClN<sub>3</sub>O<sub>5</sub>×0.5H<sub>2</sub>O): calculated C 69.10, H 8.77, N 5.62; found C 68.85, H 8.95, N 5.40. HPLC purity: Method A: RT 1.869, area 99.39 %; method C: RT=11.500, area 95.59 %.

***N*-Methyl-*N*-(3*α*,7*α*,12*α*-triacetoxy-5*β*-cholan-24-yl)-*N'*-(7'-chloroquinolin-4'-yl)-**

**propane-1,3-diamine (21).** Compound **21** was obtained according to procedure described for **20**, using **13** (303 mg, 0.41 mmol. Yield 254 mg (83%), colorless foam softens at 76-80 °C. [ $\alpha$ ]<sub>D</sub><sup>20</sup> = +0.103 (*c* = 1.2×10<sup>-3</sup> g/mL, DCM). IR (KBr): 3404w, 2945m, 2869w, 2797w, 1734s, 1611w, 1582s, 1538w, 1451w, 1375m, 1331w, 1248s, 1138s, 1072w, 1025w, 965w, 938w, 889w, 849w, 806w cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, δ): 8.49 (*d*, *J* = 5.4, H-C(2')), 7.94 (*d*, *J* = 1.9, H-C(8')), 7.90 (bs, H-N, exchangeable with D<sub>2</sub>O), 7.66 (*d*, *J* = 9.0, H-C(5')), 7.34 (*dd*, *J*<sub>1</sub> = 9.0, *J*<sub>2</sub> = 2.1, H-C(6')), 6.31 (*d*, *J* = 5.4, H-C(3')), 5.06 (*s*, H-C(12)), 4.90-4.87 (*m*, H-C(7)), 4.60-4.53 (*m*, H-C(3)), 3.39 (*bs*, 2H-C(9')), 2.64, (*t*, *J* = 5.1, 2H-C(11')), 2.44-2.40 (*m*, 2H-C(24)), 2.37 (*s*, CH<sub>3</sub>-N), 2.07 (*s*, CH<sub>3</sub>COO), 2.06 (*s*, CH<sub>3</sub>COO), 2.05 (*s*, CH<sub>3</sub>COO), 0.90 (*s*, CH<sub>3</sub>-C(10)), 0.78 (*d*, *J* = 6.4, CH<sub>3</sub>-C(20)), 0.68 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, δ): 170.53, 170.46, 170.38, 151.78, 150.74, 148.81, 134.73, 128.24, 124.85, 121.98, 117.54, 98.29, 75.37, 74.03, 70.62, 58.78, 57.57, 47.71, 45.01, 44.16, 43.39, 42.06, 40.89, 37.69, 35.03, 34.61, 34.57, 34.26, 33.63, 31.19, 29.65, 28.91, 27.19, 26.82, 25.56, 24.18, 23.90, 22.72, 22.52, 21.55, 21.45, 21.33, 17.87, 12.19. (+)ESI-HRMS (*m/z*):

$[M + H]^+$  752.43936 (error -0.84 ppm). Combustion analysis for ( $C_{43}H_{62}ClN_3O_6 \times 1.5H_2O$ ): calculated C 66.26, H 8.41, N 5.39; found C 66.54, H 8.25, N 5.41. HPLC purity: Method A: RT 2.032, area 99.46 %; method B: RT 8.689, area 96.92 %.

***N*-(3-Oxo-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholan-24-yl)-*N'*-(7'-chloroquinolin-4'-yl)-propane-1,3-diamine (23).** Ketone **30** was obtained according to procedure described for **22**, using **17** (416 mg, 0.59 mmol) and IBX (822 mg, 2.94 mmol). Yield 366 mg (88%), colorless foam softens at 100-105 °C.  $[\alpha]_D^{20} = +0.149$  ( $c = 2.0 \times 10^{-3}$  g/mL, DCM). IR (ATR): 3409m, 2948m, 2869w, 1733s, 1719sm, 1653w, 1642w, 1612w, 1582s, 1541m, 1445m, 1376s, 1332w, 1244s, 1215m, 1138w, 1078w, 1024w, 964w, 901w, 852w, 807w  $cm^{-1}$ .  $^1H$  NMR (200 MHz,  $CDCl_3$ ,  $\delta$ ): 8.49 (*d*,  $J = 5.1$ , H-C(2')), 7.92 (*d*,  $J = 1.7$ , H-C(8')), 7.84 (*bs*, H-N), 7.73 (*d*,  $J = 8.4$ , H-C(5')), 7.36-7.25, (*m*, H-C(6')), 6.31 (*d*,  $J = 5.1$ , H-C(3')), 5.16 (*bs*, H-C(12)), 5.05-4.95 (*m*, H-C(7)), 3.39 (*bs*, 2H-C(9')), 3.10-2.84 (*m*, H $\alpha$ -C(4) and 2H-C(11')), 2.72-2.56 (*m*, 2H-C(24)), 2.11 (*s*,  $CH_3COO$ ), 2.03 (*s*,  $CH_3COO$ ), 1.03 (*s*,  $CH_3-C(10)$ ), 0.87 (*d*,  $J = 6.7$ ,  $CH_3-C(20)$ ), 0.78 (*s*,  $CH_3-C(13)$ ).  $^{13}C$  NMR (50 MHz,  $CDCl_3$ ,  $\delta$ ): 212.02, 170.37, 170.09, 151.98, 150.45, 148.95, 134.35, 128.25, 127.85, 124.45, 122.12, 117.46, 98.12, 75.14, 70.39, 50.40, 49.38, 47.40, 44.92, 44.39, 43.85, 43.19, 42.02, 37.53, 36.47, 35.96, 35.27, 34.81, 34.20, 33.19, 30.70, 29.64, 27.06, 26.46, 25.69, 22.60, 21.47, 21.25, 21.18, 17.75, 12.11.  $^1H$  NMR (500 MHz,  $CDCl_3$ ,  $\delta$ ): 8.47 (*d*,  $J = 5.5$ , H-C(2')), 7.90 (*d*,  $J = 2.1$ , H-C(8')), 7.77 (*bs*, H-N, exchangeable with  $D_2O$ ), 7.70 (*d*,  $J = 8.9$ , H-C(5')), 7.30, (*dd*,  $J_1 = 8.8$ ,  $J_2 = 2.2$ , H-C(6')), 6.29 (*d*,  $J = 5.5$ , H-C(3')), 5.14 (*bs*, H-C(12)), 5.00-4.95 (*m*, H-C(7)), 3.37 (*bs*, 2H-C(9')), 2.99 (*dd*,  $J_1 = 15.1$ ,  $J_2 = 14$ , H $\alpha$ -C(4)), 2.93-2.87 (*m*, 2H-C(11')), 2.69-2.57 (*m*, 2H-C(24)), 2.09 (*s*,  $CH_3COO$ ), 2.01 (*s*,  $CH_3COO$ ), 1.00 (*s*,  $CH_3-C(10)$ ), 0.86 (*d*,  $J = 6.6$ ,  $CH_3-C(20)$ ), 0.76 (*s*,  $CH_3-C(13)$ ).  $^{13}C$  NMR (125 MHz,  $CDCl_3$ ,  $\delta$ ): 212.01, 170.39, 170.13, 152.14, 150.50, 149.14, 134.46, 128.53, 124.57, 122.07, 117.57, 98.26, 75.26, 70.51, 50.55,

49.62, 47.56, 45.07, 44.51, 44.11, 43.34, 42.15, 37.70, 36.58, 36.10, 34.98, 34.35, 33.35, 30.86, 29.81, 27.24, 26.68, 25.84, 22.74, 21.61, 21.36, 21.29, 17.92, 12.25. (+)ESI-HRMS ( $m/z$ ):  $[M + 2H]^{2+}$  347.7032 (error + 1.58 ppm),  $[M + H]^+$  694.3964 (error -2.48 ppm); Combustion analysis for ( $C_{40}H_{56}ClN_3O_5 \times H_2O$ ): calculated C 67.44, H 8.21, N 5.90; found C 67.78, H 8.00, N 5.82. HPLC purity: Method C: RT=13.105, area 95.15%; method D: RT 5.414, area 95.21%.

***N*-(3-Oxo-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholan-24-yl)-*N'*-(7'-chloroquinolin-4'-yl)-butane-1,4-diamine (24).** Ketone **24** was obtained according to procedure described for **22**, using **18** (1.35 g, 1.91 mmol) and IBX (2.58 g, 9.13 mmol). Yield 1.26 g (93%), colorless foam softens at 91-92 °C.  $[\alpha]_D^{20} = +0.069$  ( $c = 1.8 \times 10^{-3}$  g/mL, DCM). IR (ATR): 3405m, 2948m, 2870w, 1732s, 1667w, 1612w, 1581s, 1539w, 1449w, 1374m, 1332w, 1245s, 1136w, 1078w, 1025m, 966w, 901w, 851w, 810w  $cm^{-1}$ .  $^1H$  NMR (500 MHz,  $CDCl_3$ ,  $\delta$ ): 8.52 (*d*,  $J = 5.5$ , H-C(2')), 7.94 (*d*,  $J = 2.1$ , H-C(8')), 7.70 (*d*,  $J = 8.9$ , H-C(5')), 7.32, (*dd*,  $J_1 = 8.8$ ,  $J_2 = 2.2$ , H-C(6')), 6.37 (*d*,  $J = 5.5$ , H-C(3')), 6.02 (*bs*, H-N, exchangeable with  $D_2O$ ), 5.14 (*bs*, H-C(12)), 5.02-4.97 (*m*, H-C(7)), 3.34-3.27 (*m*, 2H-C(9')), 3.03-2.93 (*m*, H $\alpha$ -C(4)), 2.70, (*t*,  $J = 6.6$ , 2H-C(12')), 2.65-2.53 (*m*, H-N and 2H-C(24)), 2.10 (*s*,  $CH_3COO$ ), 2.06 (*s*,  $CH_3COO$ ), 1.02 (*s*,  $CH_3-C(10)$ ), 0.84 (*d*,  $J = 6.6$ ,  $CH_3-C(20)$ ), 0.76 (*s*,  $CH_3-C(13)$ ).  $^{13}C$  NMR (125 MHz,  $CDCl_3$ ,  $\delta$ ): 212.06, 170.40, 170.13, 152.11, 149.95, 149.21, 134.66, 128.76, 124.89, 121.35, 117.32, 98.86, 75.28, 70.58, 50.56, 49.19, 47.60, 45.06, 44.55, 43.26, 43.22, 42.14, 37.74, 36.60, 36.11, 34.98, 34.38, 33.37, 30.91, 29.80, 27.91, 27.24, 26.61, 26.31, 25.81, 22.80, 21.62, 21.44, 21.31, 17.94, 12.25. (+)ESI-HRMS ( $m/z$ ):  $[M + Na]^+$  730.3964 (error +0.86 ppm). Combustion analysis for ( $C_{41}H_{58}ClN_3O_5 \times 0.5H_2O$ ): calculated C 68.64, H 8.29, N 5.86; found C 68.39, H 8.41, N 5.63. HPLC purity: Method A: RT 1.872, Area 99.17 %; method C: RT 12.077, area 95.14 %.

***N*-(3-Oxo-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholan-24-yl)-*N'*-(7'-chloroquinolin-4'-yl)-hexane-1,6-diamine (25).** Ketone **32** was obtained according to procedure described for **22**, using **19** (349 mg, 0.47 mmol) and IBX (632 mg, 2.26 mmol). Yield 283 mg (81%), colorless foam softens at 85-90 °C.  $[\alpha]_D^{20} = +0.042$  ( $c = 1.5 \times 10^{-3}$  g/mL, DCM). IR (ATR): 3314w, 2938s, 2867m, 1733s, 1611w, 1583s, 1539w, 1451w, 1376m, 1333w, 1250s, 1216w, 1136w, 1027w, 852w, 811w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 8.52 (*d*,  $J = 5.35$ , H-C(2')), 7.95 (*d*,  $J = 2.2$ , H-C(8')), 7.66 (*d*,  $J = 9.0$ , H-C(5')), 7.35 (*dd*,  $J_1 = 8.8$ ,  $J_2 = 2.2$ , H-C(6')), 6.40 (*d*,  $J = 5.5$ , H-C(3')), 5.15-5.11 (*m*, H-C(12)), 5.03 (*bs*, H-N, exchangeable with  $\text{D}_2\text{O}$ ), 5.01-4.98 (*m*, H-C(7)), 3.35-3.27 (*m*, 2H-C(9')), 2.98 (*dd*,  $J_1 = 15.1$ ,  $J_2 = 13.8$ , H $\alpha$ -C(4)), 2.64-2.48, (*m*, 2H-C(14') and 2H-C(24)), 2.10 (*s*,  $\text{CH}_3\text{COO}$ ), 2.06 (*s*,  $\text{CH}_3\text{COO}$ ), 1.01 (*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.83 (*d*,  $J = 6.6$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.76 (*s*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 212.09, 170.41, 170.14, 152.01, 149.65, 149.10, 134.77, 128.81, 125.20, 120.80, 117.07, 99.03, 75.29, 70.57, 50.56, 49.93, 47.45, 45.01, 44.53, 43.24, 43.15, 42.13, 37.73, 36.58, 36.09, 34.85, 34.36, 33.29, 30.90, 30.03, 29.78, 28.78, 27.19, 27.09, 27.03, 26.44, 25.79, 22.79, 21.60, 21.43, 21.30, 17.90, 12.21. (+)ESI-HRMS ( $m/z$ ):  $[\text{M} + \text{H}]^+$  736.4416 (error -4.79 ppm). Combustion analysis for ( $\text{C}_{43}\text{H}_{62}\text{ClN}_3\text{O}_5$ ): calculated C 70.13, H 8.49, N 5.71; found C 69.83, H 8.19, N 5.73. HPLC purity: Method A: RT 1.810, area 99.47 %; method C: RT=12.061, area 97.17 %.

**Methyl 3 $\alpha$ -amino-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholanoate (26).** Amine **26** was synthesized according to procedures described in ref. **Error! Bookmark not defined.**

**Methyl 3 $\alpha$ -acetamido-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholate (27).** Into stirred solution of **26** (238 mg, 0.47 mmol) and  $\text{Et}_3\text{N}$  (130  $\mu\text{L}$ , 0.94 mmol) in DCM (3 mL),  $\text{Ac}_2\text{O}$  (67  $\mu\text{L}$ , 0.705 mmol) was added. Mixture was stirred at r.t. for 1.5 h, diluted with DCM (25 mL), washed with

brine (2×10 mL) and dried over anh. Na<sub>2</sub>SO<sub>4</sub>. Solution was filtered off and solvent was removed under reduced pressure. Into remained oil, heptane was added and evaporated to dryness to remove traces of AcOH and Ac<sub>2</sub>O. Crude product was purified by column chromatography (dry flash, SiO<sub>2</sub>, EA). Yield 197.2 mg (76.6%). Mp = 164-167 °C (acetone/hexane).  $[\alpha]_D^{20} = +0.122$  (c = 1.52×10<sup>-3</sup> g/mL, DCM). IR (KBr): 3396m, 2953m, 2871m, 1736s, 1653m, 1541m, 1438m, 1377m, 1248s, 1174w, 1024m, 967w, cm<sup>-1</sup>. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>, δ): 5.81 (*d*, *J* = 7.2, N-H), 5.39 (*d*, *J* = 8.0, H-N), 5.09 (*bs*, H-C(12)), 4.91 (*bs*, H-C(7)), 4.14 (*bs*, H-C(3)), 3.66 (*s*, CO<sub>2</sub>CH<sub>3</sub>), 2.126 (*s*, CH<sub>3</sub>COO), 2.12 (*s*, CH<sub>3</sub>COO), 2.08 (*s*, CH<sub>3</sub>COO), 2.07 (*s*, CH<sub>3</sub>COO), 1.97 (*bs*, CH<sub>3</sub>CONH), 0.95 (*s*, CH<sub>3</sub>-C(10)), 0.92 (*s*, CH<sub>3</sub>-C(10)), 0.81 (*d*, *J* = 6.2, CH<sub>3</sub>-C(20)), 0.73 (*bs*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>, δ): 174.52, 170.49, 170.38, 170.31, 170.17, 169.38, 169.15, 75.42, 75.25, 70.76, 70.61, 51.46, 49.58, 47.23, 44.96, 44.90, 43.35, 43.26, 41.37, 37.60, 36.91, 36.09, 35.34, 34.58, 34.50, 34.20, 32.63, 31.48, 31.21, 30.77, 30.64, 28.84, 28.9, 28.04, 27.08, 25.49, 24.62, 23.54, 23.09, 22.69, 22.54, 21.58, 21.50, 21.32, 21.25, 17.39, 14.02, 12.13. (+)ESI-HRMS (*m/z*): [M + K]<sup>+</sup> 586.31366 (error -0.68 ppm). Combustion analysis for (C<sub>31</sub>H<sub>49</sub>NO<sub>7</sub>×0.5 H<sub>2</sub>O): calculated C 66.88, H 9.05, N 2.52; found C 66.99, H 8.77, N 2.40.

**Methyl 3α-methanesulfonamido-7α,12α-diacetoxy-5β-cholanoate (28).** Compound **28** was obtained according to procedure described for **27**, using **26** (250 mg, 0.494 mmol), methanesulfonylchloride (50 μL, 0.646 mmol). Yield 257 mg (89%), colorless foam softens at 92-100 °C.  $[\alpha]_D^{20} = +0.10$  (c = 1.2×10<sup>-3</sup> g/mL, DCM). IR (KBr): 3530w, 3284w, 2953m, 2872w, 173s, 1441m, 1379m, 1319m, 1249s, 1152m, 1082w, 1024m, 968w, cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, δ): 5.10-5.07 (*m*, H-C(12)), 4.93-4.89 (*m*, H-C(7)), 4.32 (*d*, *J* = 7, N-H, exchangeable with D<sub>2</sub>O), 3.66 (*s*, CO<sub>2</sub>CH<sub>3</sub>), 3.19-3.09 (*m*, H-C(3)), 2.94 (*s*, CH<sub>3</sub>-SO<sub>2</sub>NH), 2.38-2.30 (*m*, 1H), 2.26-2.16 (*m*, 1H), 2.13 (*s*, CH<sub>3</sub>COO), 2.08 (*s*, CH<sub>3</sub>COO), 0.92 (*s*, CH<sub>3</sub>-



C(10)), 0.81 (*d*,  $J = 6.5$ , CH<sub>3</sub>-C(20)), 0.73 (*bs*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, δ): 174.49, 170.43, 170.23, 75.33, 70.66, 54.02, 51.50, 47.34, 45.03, 43.31, 41.89, 41.61, 37.69, 37.37, 35.42, 34.58, 34.08, 31.20, 30.86, 30.73, 29.41, 28.80, 27.13, 25.45, 22.77, 22.61, 21.59, 21.35, 17.48, 12.19. (+)ESI-HRMS (*m/z*): [M + NH<sub>4</sub>]<sup>+</sup> 601.3501 (error -2.69 ppm), [M + Na]<sup>+</sup> 606.30589 (error -2.0 ppm). Combustion analysis for (C<sub>30</sub>H<sub>49</sub>NO<sub>8</sub>S × H<sub>2</sub>O): calculated C 59.87, H 8.54, N 2.33; found C 59.90, H 8.48, N 2.37.

**Methyl 3α-*N*-*tert*-butylcarbamate-7α,12α-diacetoxydiacetoxy-5β-cholanoate (29).**

Compound **29** was obtained according to procedure described for **27**, using **26** (6.04 g, 11.94 mmol) and Boc<sub>2</sub>O (3.91 g, 17.91 mmol). Yield of crude product 7.00 g (97%). Analytical sample was obtained after column purification (dry-flash, SiO<sub>2</sub>, eluent Hex / EA). Colorless foam softens at 84-86 °C.  $[\alpha]_{\text{D}}^{20} = +0.061$  ( $c = 1.1 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3444s, 2954m, 2872w, 1736s, 1517m, 1451w, 1378m, 1246s, 1172m, 1067w, 1024m, 966w cm<sup>-1</sup>. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>, δ): 5.12-5.06 (*m*, H-C(12)), 4.94-4.86 (*m*, H-C(7)), 4.36 (*bs*, H-N-Boc), 3.66 (*s*, CO<sub>2</sub>CH<sub>3</sub>), 3.34-3.20 (*m*, H-C(3)), 2.12 (*s*, CH<sub>3</sub>COO), 2.08 (*s*, CH<sub>3</sub>COO), 1.44 (*s*, (CH<sub>3</sub>)<sub>3</sub>C-N(Boc)), 0.91 (*s*, CH<sub>3</sub>-C(10)), 0.81 (*d*,  $J = 6.0$ , CH<sub>3</sub>-C(20)), 0.72 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>, δ): 174.56, 170.44, 170.31, 155.16, 79.22, 75.40, 70.83, 51.49, 50.84, 47.30, 45.01, 43.34, 41.50, 37.65, 36.36, 35.45, 34.56, 34.21, 31.25, 30.83, 30.72, 28.81, 28.37, 27.13, 25.46, 22.76, 22.67, 21.60, 21.34, 17.44, 12.15. (+)ESI-HRMS (*m/z*): [M + Na]<sup>+</sup> 628.3820 (error -1.45 ppm). Combustion analysis for (C<sub>34</sub>H<sub>55</sub>NO<sub>8</sub> × 0.5 H<sub>2</sub>O): calculated C 66.42, H 9.18, N 2.28; found C 66.65, H 8.88, N 2.27.

**3α-Acetamido-7α,12α-diacetoxy-5β-cholanoic acid (30).** Methyl ester **27** (200 mg, 0.365 mmol) was hydrolyzed at 80 °C with NaOH (22 mg, 0.55 mmol) in *i*-PrOH / H<sub>2</sub>O mixture (8 mL, 3:1 v / v). After 2 h reaction was cooled and poured onto ice / water / HCl. The mixture was extracted with DCM (4×20 mL). Combined organic layers were washed once with brine,

dried over anh.  $\text{Na}_2\text{SO}_4$ , filtered and solvent was removed under reduced pressure. Yield: 176 mg (90 %), colorless foam softness at 134-138 °C.  $[\alpha]_{\text{D}}^{20} = +0.112$  ( $c = 1.0 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3440m, 2952m, 2871m, 1733s, 1647m, 1552w, 1443w, 1378m, 1249s, 1122w, 1024w, 968w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 5.41 (*d*,  $J = 7.8$ , H-N), 5.09 (*bs*, H-C(12)), 4.91 (*bs*, H-C(7)), 3.65 (*bs*, H-C(3)), 2.13 (*s*,  $\text{CH}_3\text{COO}$ ), 2.09 (*s*,  $\text{CH}_3\text{COO}$ ), 1.88 (*s*,  $\text{CH}_3\text{CONH}$ ), 0.92 (*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.82 (*d*,  $J = 5.8$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.73 (*s*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 178.67, 170.42, 170.29, 169.57, 75.47, 70.83, 49.71, 47.29, 45.01, 43.37, 41.39, 37.64, 36.05, 35.36, 34.47, 34.23, 31.23, 30.74, 30.54, 28.86, 28.02, 27.09, 25.51, 23.49, 22.71, 21.61, 21.34, 17.43, 12.16. (+)ESI-HRMS ( $m/z$ ):  $[\text{M} + \text{H}]^+$  534.34219 (error -0.63 ppm). Combustion analysis for ( $\text{C}_{30}\text{H}_{47}\text{NO}_8 \times 1.5 \text{H}_2\text{O}$ ): calculated C 64.26, H 8.99, N 2.50; found C 64.55, H 8.72, N 2.47.

**3 $\alpha$ -Methanesulfonamido-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholanoic acid (31).** Cholanoic acid **31** was obtained according to procedure described for **30**, using **27** (204 mg, 0.349 mmol). Yield 188 mg (94%), colorless foam softens at 108-117 °C.  $[\alpha]_{\text{D}}^{20} = +0.034$  ( $c = 1.0 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3525w, 3280m, 2932s, 2872m, 1732s, 1444m, 1379s, 1317m, 1250s, 1151m, 1082m, 1024m, 967w, 759w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 5.09 (*bs*, H-C(12)), 4.93-4.90 (*m*, H-C(7)), 4.50 (*d*,  $J = 7.5$ , N-H, exchangeable with  $\text{D}_2\text{O}$ ), 3.19-3.09 (*m*, H-C(3)), 2.97 (*s*,  $\text{CH}_3\text{-SO}_2\text{NH}$ ), 2.42-2.34 (*m*, 1H), 2.28-2.20 (*m*, 1H), 2.13 (*s*,  $\text{CH}_3\text{COO}$ ), 2.09 (*s*,  $\text{CH}_3\text{COO}$ ), 0.92 (*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.82 (*d*,  $J = 6.5$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.73 (*bs*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 170.46, 170.30, 75.34, 70.69, 53.99, 47.33, 45.04, 43.31, 41.89, 41.60, 37.69, 37.33, 35.42, 34.54, 34.07, 31.18, 30.72, 30.52, 29.39, 28.79, 27.14, 25.44, 22.77, 22.60, 21.58, 21.35, 17.47, 12.20. (+)ESI-HRMS ( $m/z$ ):  $[\text{M} + \text{K}]^+$  608.26569 (error +0.49 ppm). Combustion analysis for ( $\text{C}_{29}\text{H}_{47}\text{NO}_8\text{S} \times 0.5 \text{H}_2\text{O}$ ): calculated C 60.18, H 8.36, N 2.42; found C 59.91, H 8.45, N 2.38.

**3 $\alpha$ -N-tert-Butylcarbamate-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholanoic acid (32). Methyl ester 29**

(7.20 g, 11.89 mmol) was hydrolyzed at 80 °C with NaOH (710 mg, 17.75 mmol) in *i*-PrOH / H<sub>2</sub>O mixture (290 mL, 3:1 v / v). After 4 h the reaction mixture was cooled and poured onto ice cold water and neutralized with diluted HCl (1:1, v/v) to pH 7 and DCM was added (150 mL). Layers were separated, water layer was extracted with CH<sub>2</sub>Cl<sub>2</sub> (3× 20 mL) and combined organic layers were washed with water, brine, dried over anh. Na<sub>2</sub>SO<sub>4</sub> and evaporated to dryness. Yield 6.90 g (98%) of crude product. Analytical sample obtained upon column chromatography (dry-flash, SiO<sub>2</sub>, eluent Hex /EA). Colorless foam softens at 197-202 °C.  $[\alpha]_D^{20} = +0.110$  (c = 1.55×10<sup>-3</sup> g/mL, DCM). IR (KBr): 3411w, 3260w, 2954m, 2870w, 1732s, 1712m, 1681m, 1505m, 1451w, 1378m, 1315w, 1284m, 1245m, 1173m, 1126w, 1072w, 1033w, 1000w, 969w, 889,w, 858w, cm<sup>-1</sup>. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>,  $\delta$ ): 5.09 (*bs*, H-C(12)), 4.90-4.70 (*m*, H-C(7)), 3.26 (*bs*, H-C(3)), 2.12 (*s*, CH<sub>3</sub>COO), 2.08 (*s*, CH<sub>3</sub>COO), 1.45 (*s*, (CH<sub>3</sub>)<sub>3</sub>C-N(Boc)), 0.91(*s*, CH<sub>3</sub>-C(10)), 0.82 (*d*, *J* = 5.8, CH<sub>3</sub>-C(20)), 0.73 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>,  $\delta$ ): 170.46, 75.42, 70.85, 51.02, 47.34, 45.01, 43.34, 41.50, 37.67, 36.31, 35.43, 34.54, 34.20, 31.23, 30.57, 28.79, 28.37, 27.15, 25.44, 22.76, 22.65, 21.58, 21.32, 17.44, 12.15. (+)ESI-HRMS (*m/z*):[M + Na]<sup>+</sup> 614.3663 (error - 0.97 ppm). Combustion analysis (C<sub>33</sub>H<sub>53</sub>NO<sub>8</sub>): Calculated C 66.98, H 9.03, N 2.37; found C 67.33, H 9.07, N 2.33.

**3 $\alpha$ -Acetamido-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholan-24-ol (33). Mixture of 30 (200 mg, 0.37**

mmol), Et<sub>3</sub>N (51  $\mu$ L, 0.37 mmol), and ClCO<sub>2</sub>Et (35  $\mu$ L, 0.37 mmol) in DCM (10 mL) were stirred at r.t. After 3 h reaction mixture was evaporated to dryness, residue was dissolved in DCM/THF mixture (20 mL, 3:1 v/v), NaBH<sub>4</sub> (56 mg, 1.48 mmol) was added, and after 15 min of intensive stirring MeOH (4 mL) was added in one portion, and stirring was continued. After 90 min mixture was poured onto ice / brine / HCl and left for 1 h. Mixture was

extracted with  $\text{CH}_2\text{Cl}_2$  (6×20 mL), and organic layer was washed once with brine, dried over anh.  $\text{Na}_2\text{SO}_4$ , and filtered. The solvent was removed under reduced pressure and product was isolated after column chromatography (dry flash,  $\text{SiO}_2$ , eluent Hex/EA gradient 9/1 → EA and EA/MeOH 95/5). Yield 124 mg (63.5 %), colorless foam softness at 129-131 °C.  $[\alpha]_{\text{D}}^{20} = +0.056$  ( $c = 1.0 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3443s, 2946s, 2869m, 1734s, 1650s, 1553m, 1444w, 1378s, 1248s, 1115w, 1023w, 968.7w,  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 5.45 (d,  $J = 7.8$ , H-N), 5.10 (*bs*, H-C(12)), 4.96-4.88 (*m*, H-C(7)), 3.70-3.52 (*m*, H-C(3) and 2H-C(24)), 2.13 (*s*,  $\text{CH}_3\text{COO}$ ), 2.08 (*s*,  $\text{CH}_3\text{COO}$ ), 1.97 (*s*,  $\text{CH}_3\text{CONH}$ ), 0.92(*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.82 (*d*,  $J = 6.2$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.73 (*s*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 170.38, 170.22, 169.29, 75.52, 70.79, 63.22, 49.60, 47.40, 44.92, 43.32, 41.35, 37.58, 36.03, 35.32, 34.63, 34.18, 31.52, 31.19, 28.97, 28.82, 28.00, 27.13, 25.47, 23.49, 22.67, 21.58, 21.32, 17.34, 12.11. (+)ESI-HRMS ( $m/z$ ): $[\text{M} + \text{K}]^+$  558.31923 (error +0.15 ppm). Combustion analysis ( $\text{C}_{30}\text{H}_{49}\text{NO}_6 \times 0.5\text{H}_2\text{O}$ ): calculated C 68.15, H 9.53, N 2.65; found C 68.15, H 9.77, N 2.58.

**3 $\alpha$ -Sulfonamido-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholan-24-ol (34).** Alcohol **34** was obtained according to procedure described for **33**, using **31** (155 mg, 0.272 mmol). The product was isolated after column chromatography (dry flash,  $\text{SiO}_2$ , eluent DCM/MeOH gradient 9/1 → 1/1 and Lobar Lichroprep A,  $\text{SiO}_2$ , DCM/EA=65/35). Yield 81.9 mg (54%). Colorless foam softens at 96-98 °C.  $[\alpha]_{\text{D}}^{20} = +0.090$  ( $c = 1.4 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3442m, 2946m, 2871w, 1733s, 1631w, 1448w, 1379m, 1318m, 1248s, 1150m, 1079w, 1023m, 972w, 896w, 759w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 5.10 (*bs*, H-C(12)), 4.94-4.88 (*m*, H-C(7)), 4.46 (*d*,  $J = 7.4$ , N-H), 3.68-3.54 (*m*, 2H-C(24)), 3.24-3.02 (*m*, H-C(3)), 2.97 (*s*,  $\text{CH}_3\text{-SO}_2\text{NH}$ ), 2.16 (*s*,  $\text{CH}_3\text{COO}$ ), 2.09 (*s*,  $\text{CH}_3\text{COO}$ ), 0.92 (*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.83 (*d*,  $J = 6.2$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.73 (*bs*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 170.57, 170.37, 75.40, 70.68, 63.34, 53.97, 47.43, 44.94, 43.26, 41.82, 41.57, 37.64, 37.27, 35.38, 34.70, 34.03, 31.54, 31.15,

29.33, 29.06, 28.75, 27.17, 25.40, 22.72, 22.56, 21.56, 21.34, 17.79, 12.15. (+)ESI-HRMS

( $m/z$ ):  $[M + NH_4]^+$  573.3575 (error +1.25 ppm). Combustion analysis for ( $C_{29}H_{49}NO_7S \times 0.5 H_2O$ ): calculated C 61.67, H 8.92, N 2.48, S 5.68 found C 61.55, H 8.79, N 2.55, S 5.92.

**3 $\alpha$ -N-tert-Butylcarbamate-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholan-24-ol (35).** Compound **35** was obtained according to procedure described for **33**, using **32** (7.00 g, 11.82 mmol). When reduction was completed, the solvent was removed under reduced pressure, and the residue was dissolved in DCM and transferred to separatory funnel. Water was added and pH was adjusted to pH 1 with diluted HCl. Layers was separated, water layer was extracted with DCM (3 $\times$ 50 mL), combined organic layer was washed with sat. NaHCO<sub>3</sub> and brine, and dried over anh. Na<sub>2</sub>SO<sub>4</sub>. After filtration solvent was removed under reduced pressure, the product was isolated after column chromatography (dry flash, SiO<sub>2</sub>, eluent Hex/EA gradient 8/2 to 1/1). Yield 5.20 g (76 %), colorless foam softens at 104-107 °C.  $[\alpha]_D^{20} = +0.084$  ( $c = 1.25 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3444m, 2940m, 2870m, 2357w, 1735s, 1716s, 1521m, 1451w, 1378m, 1248s, 1172m, 1062m, 1024m, 999w, 966w, 894w, 853w cm<sup>-1</sup>. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>,  $\delta$ ): 5.12-5.06 (*m*, H-C(12)), 4.94-4.86 (*m*, H-C(7)), 4.38 (*bs*, H-N-Boc), 3.68-3.54 (*m*, 2H-C(24)), 3.25 (*bs*, H-O), 2.12 (*s*, CH<sub>3</sub>COO), 2.08 (*s*, CH<sub>3</sub>COO), 1.44 (*s*, (CH<sub>3</sub>)<sub>3</sub>C-N(Boc)), 0.91 (*s*, CH<sub>3</sub>-C(10)), 0.83 (*d*,  $J = 6.4$ , CH<sub>3</sub>-C(20)), 0.73 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>,  $\delta$ ): 170.50, 170.37, 155.18, 79.24, 75.49, 70.88, 63.38, 50.82, 47.45, 44.96, 43.34, 41.50, 37.65, 36.36, 35.45, 34.72, 34.21, 31.57, 31.26, 29.08, 28.81, 28.37, 27.20, 25.46, 22.67, 21.61, 21.36, 17.81, 12.16. (+)ESI-HRMS ( $m/z$ ):  $[M + Na]^+$  600.3871 (error +4.85 ppm). Combustion analysis (C<sub>33</sub>H<sub>55</sub>NO<sub>7</sub>): Calculated C 68.60, H 9.59, N 2.42; found C 68.73, H 9.19, N 2.39.

**24-N-[(7-Chloroquinoline-4-yl)amino]propylamino-3 $\alpha$ -acetamido-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane (37).** Compound **37** was obtained according to procedure described for **36**, using alcohol **33** (134 mg, 0.26 mmol). Yield 75 mg (39%), colorless foam softens at 108-112 °C.  $[\alpha]_D^{20} = +0.085$  ( $c = 1.5 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3296m, 3067w, 2937s, 2867s, 1731s, 1653m, 1612m, 1583s, 1542m, 1449m, 1376s, 1331w, 1249s, 1137w, 1077w, 1023m, 968w, 899w, 878w, 852w, 806w, 768w, 733w,  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 8.49 (*d*,  $J = 5.4$ , H-C(2')), 7.92 (*d*,  $J = 2.1$ , H-C(8')), 7.89 (*bs*, H-N,, exchangeable with  $\text{D}_2\text{O}$ ), 7.75 (*d*,  $J = 9.0$ , H-C(5')), 7.36 (*dd*,  $J_1 = 8.9$ ,  $J_2 = 2.2$ , H-C(6')), 6.31 (*d*,  $J = 5.4$ , H-C(3')), 5.36 (*d*,  $J = 8.0$ , H-N), 5.11 (*bs*, H-C(12)), 4.93-4.88 (*m*, H-C(7)), 3.68-3.58 (*bs*, H-C(3)), 3.44-3.35 (*m*, 2H-C(9')), 2.98-2.88 (*m*, 2H-C(11')), 2.72-2.59 (*m*, 2H-C(24)), 2.08 (*s*,  $\text{CH}_3\text{COO}$ ), 2.00 (*s*,  $\text{CH}_3\text{COO}$ ), 1.98 (*s*,  $\text{CH}_3\text{CONH}$ ), 0.92 (*bs*,  $\text{CH}_3\text{-C}(10)$ ), 0.85 (*d*,  $J = 6.6$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.74 (*bs*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 170.35, 170.24, 169.19, 152.11, 150.60, 149.07, 134.49, 128.45, 124.62, 122.24, 117.63, 98.29, 75.57, 70.75, 50.55, 49.63, 47.37, 45.07, 44.15, 43.69, 41.45, 37.68, 36.08, 35.42, 34.88, 34.23, 33.33, 31.27, 29.09, 28.12, 27.32, 27.19, 26.31, 25.68, 23.63, 22.76, 21.53, 21.37, 17.92, 12.26. (+)ESI-HRMS ( $m/z$ ):  $[\text{M} + \text{H}]^+$  737.43954 (error -1.06 ppm). Combustion analysis ( $\text{C}_{42}\text{H}_{61}\text{ClN}_4\text{O}_5 \times 2\text{H}_2\text{O}$ ): calculated C 65.22, H 8.47, N 7.24; found C 64.73, H 8.33, N 7.34. HPLC purity: Method A: RT 1.792, area 99.09 %; method C: RT=13.145, area 95.23 %.

**24-N-[(7-Chloroquinoline-4-yl)amino]ethylamino-3 $\alpha$ -methanesulfonamido-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane (38).** Compound **38** was obtained according to procedure described for **36**, using alcohol **34** (503 mg, 0.9 mmol). Column chromatography (flash SP RP column MeOH/ $\text{H}_2\text{O}$  gradient 65:35  $\rightarrow$  9:1, dry flash,  $\text{SiO}_2$ , EA, EA/MeOH gradient 9:1  $\rightarrow$  6:4, EA/MeOH/ $\text{NH}_3 = 18:0.4:0.4 \rightarrow 9:2:2$ , flash chromatography (Biotage SP1 RP column MeOH/ $\text{H}_2\text{O}$  gradient 65:35  $\rightarrow$  9:1). Yield 248 mg (36%). Colorless foam softens at 108-110

$^{\circ}\text{C}$ .  $[\alpha]_{\text{D}}^{20} = +0.151$  ( $c = 1.8 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3289w, 2938m, 2868w, 1729s, 1612w, 1582s, 1538w, 1451w, 1377m, 1318m, 1250s, 1147m, 1080w, 1023w, 968w, 880w, 808w, 763w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 8.51 (*d*,  $J = 5.1$ , H-C(2')), 7.94 (*d*,  $J = 2.2$ , H-C(8')), 7.74 (*d*,  $J = 9.0$ , H-C(5')), 7.35 (*dd*,  $J_1 = 8.7$ ,  $J_2 = 2.0$ , H-C(6')), 6.38 (*d*,  $J = 5.1$ , H-C(3')), 5.99 (*bs*, H-N, exchangeable with  $\text{D}_2\text{O}$ ), 5.09 (*bs*, H-C(12)), 4.95-4.85 (*m*, H-C(7)), 4.52 (*d*,  $J = 7.4$ , N-H, exchangeable with  $\text{D}_2\text{O}$ ), 3.40-3.30 (*m*, 2H-C(9')), 3.25-2.95 (*m*, H-C(3) and 2H-C(10')), 2.96 (*s*,  $\text{CH}_3\text{-SO}_2\text{N}$ ), 2.60-2.55 (*m*, 2H-C(24)), 2.10 (*s*,  $\text{CH}_3\text{COO}$ ), 2.07 (*s*,  $\text{CH}_3\text{COO}$ ), 1.99 (*bs*, H-N, exchangeable with  $\text{D}_2\text{O}$ ), 0.92 (*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.82 (*d*,  $J = 6.7$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.71 (*bs*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (50 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 170.49, 170.29, 151.96, 149.92, 134.83, 128.53, 125.19, 121.37, 117.33, 99.10, 75.36, 70.65, 53.97, 49.67, 47.58, 47.38, 44.97, 43.28, 41.84, 41.55, 37.62, 37.31, 35.38, 34.91, 34.01, 33.21, 31.15, 29.35, 28.79, 27.24, 26.55, 25.42, 22.73, 22.56, 21.54, 21.30, 17.85, 12.15.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 8.53 (*d*,  $J = 5.3$ , H-C(2')), 7.96 (*d*,  $J = 2.1$ , H-C(8')), 7.70 (*d*,  $J = 8.9$ , H-C(5')), 7.36 (*dd*,  $J_1 = 8.9$ ,  $J_2 = 2.1$ , H-C(6')), 6.40 (*d*,  $J = 5.3$ , H-C(3')), 5.86 (*bs*, H-N, exchangeable with  $\text{D}_2\text{O}$ ), 5.09 (*bs*, H-C(12)), 4.95-4.85 (*m*, H-C(7)), 4.26 (*d*,  $J = 7.3$ , N-H, exchangeable with  $\text{D}_2\text{O}$ ), 3.40-3.30 (*m*, 2H-C(9')), 3.25-2.95 (*m*, H-C(3)), 3.06-2.99 (*m*, 2H-C(10')), 2.97 (*s*,  $\text{CH}_3\text{-SO}_2\text{N}$ ), 2.68-2.56 (*m*, 2H-C(24)), 2.10 (*s*,  $\text{CH}_3\text{COO}$ ), 2.07 (*s*,  $\text{CH}_3\text{COO}$ ), 0.92 (*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.83 (*d*,  $J = 6.4$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.71 (*bs*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 170.41, 170.19, 152.14, 149.85, 149.19, 134.79, 128.83, 125.20, 121.18, 117.38, 99.24, 75.40, 70.68, 54.05, 49.71, 47.67, 47.49, 45.04, 43.36, 41.97, 41.93, 41.62, 37.71, 37.43, 35.44, 34.98, 34.10, 33.32, 31.22, 29.44, 28.86, 27.32, 26.80, 25.50, 22.80, 21.59, 21.37, 17.93, 12.23. (+)ESI-HRMS ( $m/z$ ):  $[\text{M} + \text{H}]^+$  759.39211 (error +0.60 ppm). Combustion analysis for ( $\text{C}_{40}\text{H}_{59}\text{ClN}_4\text{O}_6\text{S} \times 2 \text{H}_2\text{O}$ ): calculated C 60.40, H 7.98, N 7.04, S 4.03 found C 60.39, H 7.84, N 7.20, S 3.95. HPLC purity: Method A: RT 1.884, area 98.92 %; method C: RT 10.467, area 98.11 %.

**24-N-[(7-Chloroquinoline-4-yl)amino]proylamino-3 $\alpha$ -methanesulfonamido-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane (39).** Compound **39** was obtained according to procedure described for **36**, using alcohol **34** (496 mg, 0.89 mmol). Column chromatography (dry flash, SiO<sub>2</sub>, EA, EA/MeOH gradient 9:1  $\rightarrow$  6:4, EA/MeOH/NH<sub>3</sub> = 18:0.4:0.4  $\rightarrow$  18:1.4:1.4, flash chromatography Biotage SP1RP column MeOH/H<sub>2</sub>O gradient 75:25  $\rightarrow$  9:1). Yield 221 mg (32 %). Colorless foam softens at 102-105 °C.  $[\alpha]_D^{20} = +0.058$  ( $c = 1.0 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3404m, 3298m, 2936m, 2868m, 1728m, 1611w, 1583s, 1539w, 1449m, 1377m, 1319m, 1249s, 1147m, 1080w, 1023w, 694w, 900w, 880w, 852w, 807w, 762w cm<sup>-1</sup>. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>,  $\delta$ ): 8.49 (*d*,  $J = 5.1$ , H-C(2')), 7.95-7.85 (*m*, H-C(8') and N-H, exchangeable with D<sub>2</sub>O), 7.74 (*d*,  $J = 9.0$ , H-C(5')), 7.34 (*dd*,  $J_1 = 9.0$ ,  $J_2 = 2.2$ , H-C(6')), 6.31 (*d*,  $J = 5.6$ , H-C(3')), 5.11 (*bs*, H-C(12)), 4.95-4.84 (*m*, H-C(7)), 4.48 (*d*,  $J = 7.3$ , N-H, exchangeable with D<sub>2</sub>O), 3.38 (*bs*, 2H-C(9')), 3.14 (*bs*, H-C(3)), 3.00-2.85 (*m*, CH<sub>3</sub>-SO<sub>2</sub>N and 2H-C(11')), 2.63 (*bs*, 2H-C(24)), 2.10 (*s*, CH<sub>3</sub>COO), 2.02 (*s*, CH<sub>3</sub>COO), 0.92 (*s*, CH<sub>3</sub>-C(10)), 0.86 (*d*,  $J = 6.2$ , CH<sub>3</sub>-C(20)), 0.74 (*bs*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>,  $\delta$ ): 170.55, 170.37, 152.16, 150.57, 149.12, 134.50, 128.49, 124.59, 122.19, 117.60, 98.25, 75.40, 70.59, 53.99, 50.55, 49.65, 47.40, 44.99, 44.15, 43.46, 41.92, 41.55, 37.60, 37.24, 35.36, 34.89, 34.54, 34.01, 33.29, 31.14, 29.32, 28.90, 28.37, 27.26, 27.17, 26.48, 25.51, 22.69, 22.60, 21.49, 21.34, 17.86, 12.20. (+)ESI-HRMS ( $m/z$ ): [M + H]<sup>+</sup> 773.40793 (error +0.81 ppm). Combustion analysis for (C<sub>41</sub>H<sub>61</sub>ClN<sub>4</sub>O<sub>6</sub>S  $\times$  1.5 H<sub>2</sub>O): calculated C 61.52, H 8.06, N 7.00, S 4.01 found C 61.45, H 8.07, N 7.06, S 3.60. HPLC purity: Method A: RT 1.773, area 98.86 %; method B: RT 1.843, area 98.21 %.

**24-N-Methyl-N-[(7-chloroquinoline-4-yl)amino]propylamino-3 $\alpha$ -methanesulfonamide-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane (43).** Compound **43** was obtained according to procedure described for **42**, using amine **39** (100 mg, 0.13 mmol). Yield 72 mg (71%), colorless foam



softness at 80-85 °C.  $[\alpha]_D^{20} = +0.085$  ( $c = 2.0 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3065w, 2947m, 2869m, 2800w, 1731s, 1610w, 1582s, 1539w, 1448w, 1376s, 1320m, 1246s, 1148m, 1080w, 1023w, 971w, 939w, 899w, 850w, 808w, 764w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 8.50 (*d*,  $J = 5.5$ , H-C(2')), 7.95 (*d*,  $J = 2.1$ , H-C(8')), 7.82 (*bs*, H-N, exchangeable with  $\text{D}_2\text{O}$ ), 7.69 (*d*,  $J = 8.8$ , H-C(5')), 7.34 (*dd*,  $J_1 = 8.8$ ,  $J_2 = 2.1$ , H-C(6')), 6.31 (*d*,  $J = 5.5$ , H-C(3')), 5.06 (*bs*, H-C(12)), 4.91-4.88 (*m*, H-C(7)), 4.39 (*bs*, H-N, exchangeable with  $\text{D}_2\text{O}$ ), 3.42-3.35 (*m*, 2H-C(9')), 3.19-3.10 (*m*, H-C(3)), 2.97 (*s*,  $\text{CH}_3\text{-N}$ ), 2.70-2.61 (*m*, 2H-C(11')), 2.43 (*t*,  $J = 7.6$ , 2H-C(24)), 2.38 (*s*,  $\text{CH}_3\text{-SO}_2\text{N}$ ), 2.06 (*s*,  $\text{CH}_3\text{COO}$ ), 2.05 (*s*,  $\text{CH}_3\text{COO}$ ), 0.91 (*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.78 (*d*,  $J = 6.4$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.68 (*s*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 170.41, 170.26, 151.78, 150.78, 148.80, 134.74, 128.19, 124.88, 122.02, 117.55, 98.31, 75.34, 70.62, 58.71, 57.34, 54.02, 47.73, 45.02, 44.04, 43.35, 42.00, 41.97, 41.62, 37.66, 37.34, 35.42, 35.05, 34.06, 33.62, 31.18, 29.39, 28.89, 27.18, 25.50, 24.23, 23.82, 22.72, 22.61, 21.57, 21.31, 17.88, 12.20. (+)ESI-HRMS ( $m/z$ ):  $[\text{M} + \text{H}]^+$  787.42335 (error +0.50 ppm). Combustion analysis for ( $\text{C}_{42}\text{H}_{63}\text{ClN}_4\text{O}_6\text{S} \times 2\text{H}_2\text{O}$ ): calculated C 61.26, H 8.20, N 6.80, S 3.89. Found C 60.91, H 8.08, N 6.80, S 3.98. HPLC purity: Method A: RT 1.879, area 99.37 %; method B: RT 1.866, area 99.37 %.

**24-N-Methyl-N-[(7-chloroquinoline-4-yl)amino]propylamino-3 $\alpha$ -N'-tert-**

**butylcarbamate-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane (45).** Into stirred solution of **41** (1.38 g, 1.73 mmol) and formaldehyde (37 %, 581  $\mu\text{L}$ , 20.9 mmol) in DCM (85 mL),  $\text{NaBH}(\text{OAc})_3$  (3.65 g, 17.2 mmol) was added in 3 equal portions in 8 h intervals. Upon completion of the reaction, the reaction mixture was suspended in DCM/ $\text{H}_2\text{O}$  mixture, pH was adjusted to pH 12 with 0.5 M NaOH and transferred to separatory funnel and worked-up in usual manner. Product was isolated after flash column chromatography purification (Biotage SP1, NH column, eluent EA/Hex gradient 6/4  $\rightarrow$  EA, Biotage SP1, RP column, eluent MeOH/ $\text{H}_2\text{O}$

gradient 75/25 → MeOH and RP column MeOH/H<sub>2</sub>O = 95/5). Yield 880.1 mg (63 %). **45**: Colorless foam softens at 108-110 °C.  $[\alpha]_D^{20} = +0.042$  ( $c = 1.6 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3674w, 3430s, 2946m, 2867m, 2800w, 1731s, 1613m, 1581s, 1535m, 1456m, 1372m, 1331w, 1244s, 1170m, 1066w, 1024m, 966w, 850w, 806w, 768w cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, δ): 8.49 (*d*,  $J = 4.5$ , H-C(2')), 7.93 (*s*, H-C(8')), 7.86 (*s*, H-N-Boc, exchangeable with D<sub>2</sub>O), 7.62 (*d*,  $J = 8.8$ , H-C(5')), 7.32 (*d*,  $J = 8.6$ , H-C(6')), 6.31 (*d*,  $J = 4.9$ , H-C(3')), 5.06 (*s*, H-C(12)), 4.88 (*s*, H-C(7)), 3.38 (*bs*, 2H-C(9')), 3.27 (*bs*, H-C(3)), 2.61 (*bs*, 2H-C(11')), 2.45-2.31 (*m*, 2H-C(24) and CH<sub>3</sub>-N), 2.05 (*s*, 2xCH<sub>3</sub>COO), 1.44 (*s*, (CH<sub>3</sub>)<sub>3</sub>C-N(Boc)), 0.90 (*s*, CH<sub>3</sub>-C(10)), 0.77 (*d*,  $J = 5.8$ , CH<sub>3</sub>-C(20)), 0.68 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, δ): 170.37, 170.32, 152.06, 150.65, 149.09, 134.59, 128.49, 124.78, 121.90, 117.61, 98.34, 79.18, 75.42, 70.80, 58.93, 57.74, 47.78, 45.01, 44.37, 43.36, 42.23, 41.54, 37.68, 36.38, 35.48, 35.09, 34.65, 34.23, 33.70, 31.27, 30.97, 28.88, 28.41, 27.21, 25.52, 24.28, 24.11, 22.75, 22.70, 21.62, 21.32, 17.90, 12.19. (+)ESI-HRMS ( $m/z$ ):  $[M + H]^+$  809.4978 (error -0.49 ppm). Combustion analysis for C<sub>46</sub>H<sub>69</sub>ClN<sub>4</sub>O<sub>6</sub>: Calculated C 68.25, H 8.59, N 6.92; found C 68.02, H 8.63, N 6.75. HPLC purity: Method C: RT 7.896, area 96.46; method D: RT 5.553, area 96.83 %.

**24-N-Fmoc-N-[(7-Chloroquinoline-4-yl)amino]ethylamino-3 $\alpha$ -N'-tert-butylcarbamate-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane (46)**. Mixture of **40** (ST10) (1.07 g, 1.36 mmol) and Fmoc-Su (460 mg, 1.36 mmol) in 32 mL DCM was stirred for 4 h at r.t. Solvent was evaporated under reduced pressure and product was isolated after flash column chromatography purification (Biotage SP1, SiO<sub>2</sub> column, eluent EA/Hex gradient 9/1 → EA). Yield 1.00 g (74 %).

Colorless foam softens at 63-68 °C.  $[\alpha]_D^{20} = +0.036$  ( $c = 1.5 \times 10^{-3}$  g/mL, DCM). IR (ATR): 3351w, 2936m, 2867m, 1704s, 1611w, 1582m, 1522w, 1452m, 1371m, 1239s, 1169m, 1067m, 1022w, 880w, 814w, 741w cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, δ): 8.33 (*bs*, H-C(2')),

7.90-7.10 (*m*, Ar), 6.21 (*bs*, H-C(3')), 5.01 (*bs*, H-C(12)), 4.88 (*bs*, H-C(7)), 3.75-3.55 (*m*, H-C(3) and 2H-C(9')), 3.30 (*bs*, 2H-C(10')), 2.95-2.80 (*m*, 2H-C(24)), 2.07 (*s*, CH<sub>3</sub>COO), 2.05 (*s*, CH<sub>3</sub>COO), 1.43 (*s*, (CH<sub>3</sub>)<sub>3</sub>C-N(Boc)), (*s*, CH<sub>3</sub>-C(10)), 0.68 (*d*, *J* = 5.85, CH<sub>3</sub>-C(20)), 0.60 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>, δ): 174.15, 170.36, 158.57, 152.47, 148.10, 143.57, 141.36, 137.08, 127.78, 127.03, 126.51, 124.54, 122.57, 120.02, 116.18, 97.54, 75.38, 70.81, 50.80, 47.80, 47.23, 44.99, 43.30, 41.48, 37.65, 36.34, 34.89, 34.21, 32.59, 31.26, 28.77, 28.37, 27.26, 25.42, 22.65, 21.61, 21.38, 19.19, 17.79, 12.20. (+)ESI-HRMS (*m/z*): [M + Na]<sup>+</sup> 1025.51865 (error +2.04 ppm). Combustion analysis for C<sub>44</sub>H<sub>64</sub>ClN<sub>4</sub>O<sub>8</sub>·H<sub>2</sub>O: Calculated C 66.19, H 8.33, N 7.02; found C 65.86, H 5.42, N 6.96.

**24-N-Fmoc-N-[(7-Chloroquinoline-4-yl)amino]propylamino-3α-N'-tert-butylcarbamate-7α,12α-diacetoxy-5β-cholane (47).** Compound **47** was obtained according to procedure described for **46** using **41** (2.24 g, 2.81 mmol) and Fmoc-Su (947.9 mg, 2.81 mmol). Product was isolated after column chromatography purification [dry flash, SiO<sub>2</sub>, eluent EA, EA/MeOH gradient 95/5 → 8/2, flash chromatography (Biotage SP1, RP column, eluent MeOH/H<sub>2</sub>O gradient 9/1 to 95/5, SiO<sub>2</sub> column, eluent EA/Hex gradient 9/1 → EA)]. Yield 2.45 g (86 %). Colorless foam softens at 112-116 °C. [α]<sub>D</sub><sup>20</sup> = + 0.060 (*c* = 1.8×10<sup>-3</sup> g/mL, DCM). IR (KBr): 3394m, 3066w, 2934m, 2868m, 1731s, 1706s, 1611m, 1580s, 1534m, 1479m, 1450m, 1426m, 1372m, 1244s, 1170m, 1135m, 1102w, 1066w, 1024m, 1000w, 966w, 939w, 881w, 851w, 808w cm<sup>-1</sup>. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>, δ): 8.49 (*d*, *J* = 5.4, H-C(2')), 8.0-7.2 (*m*, Ar), 6.48 (*bs*, H-N-Boc, exchangeable with D<sub>2</sub>O), 6.34 (*d*, *J* = 5.4, H-C(3')), 5.09 (*bs*, H-C(12)), 4.91 (*bs*, H-C(7)), 4.65 (*d*, *J* = 5.6, CH<sub>2</sub>CH (Fmoc)), 4.23 (*t*, *J* = 5.6, CH<sub>2</sub>CH(Fmoc)), 3.50-2.80 (*m*, 2H-C(9'), 2H-C(11'), 2H-C(24) and H-C(3)), 2.37 (*s*, H-N, exchangeable with D<sub>2</sub>O), 2.11 (*s*, CH<sub>3</sub>COO), 2.05 (*s*, CH<sub>3</sub>COO), 1.45 (*s*, (CH<sub>3</sub>)<sub>3</sub>C-N(Boc)), 0.91 (*s*, CH<sub>3</sub>-C(10)), 0.75 (*d*, *J* = 6.0 CH<sub>3</sub>-C(20)), 0.71 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR

(50 MHz, CDCl<sub>3</sub>,  $\delta$ ): 170.37, 170.29, 157.17, 155.15, 151.85, 149.85, 149.19, 143.86, 141.38, 134.83, 128.42, 127.67, 127.03, 125.23, 124.59, 121.85, 119.93, 98.21, 79.20, 75.38, 70.79, 66.86, 50.75, 47.45, 44.96, 43.86, 43.32, 41.44, 38.62, 37.60, 36.31, 35.40, 34.78, 34.16, 32.59, 31.23, 28.79, 28.35, 27.22, 26.06, 25.44, 25.11, 22.62, 21.58, 21.34, 17.73, 14.11, 12.16. (+)ESI-HRMS ( $m/z$ ): [M + H]<sup>+</sup> 1017.5503 (error +1.39 ppm). Combustion analysis for C<sub>44</sub>H<sub>66</sub>ClN<sub>4</sub>O<sub>8</sub>×H<sub>2</sub>O: Calculated C 68.03, H 8.37, N 7.05; found C 67.86, H 8.42, N 7.96.

**24-N-Fmoc-N-[(7-Chloroquinoline-4-yl)amino]ethylamino-3 $\alpha$ -amino-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane (48).** Compound **46** (946 mg, 0.94 mmol) was stirred at r.t. in DCM/ TFA mixture (13 mL, 3:1, v/v) for 4 h. Solvent was removed under reduced pressure; the residue was transferred as DCM solution to separatory funnel and worked-up in usual manner. Crude product 817 mg was forwarded to the next reaction step without additional purification.

**24-N-Fmoc-N-[(7-Chloroquinoline-4-yl)amino]propylamino-3 $\alpha$ -amino-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane (49).** Compound **47** (1.26 g, 1.24 mmol) was stirred at r.t. in DCM/ TFA mixture (20 mL, 1:1, v/v) for 95 min. Solvent was removed under reduced pressure, and the residue was transferred as DCM solution to separatory funnel and worked-up in usual manner. Product was isolated after column chromatography purification. Yield 1.10 g (96 %). Colorless foam softens at 88-91 °C.  $[\alpha]_D^{20} = +0.025$  (c = 1.6×10<sup>-3</sup> g/mL, DCM). IR (KBr): 3409m, 3065w, 2942m, 2864m, 1728s, 1610m, 1581s, 1538m, 1449m, 1427m, 1376m, 1330m, 1244s, 1136m, 1077m, 1024m, 964w, 897w, 850w cm<sup>-1</sup>. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>,  $\delta$ ): 8.48 (*d*, *J* = 5.3, H-C(2')), 8.00-7.20 (*m*, Ar), 6.48 (*bs*, H-N, exchangeable with D<sub>2</sub>O), 6.29 (*m*, H-C(3')), 5.07 (*bs*, H-C(12)), 4.89 (*bs*, H-C(7)), 4.64 (*d*, *J* = 5.6, CH<sub>2</sub>CH-C(Fmoc)), 4.23 (*t*, *J* = 5.6, CH<sub>2</sub>CH(Fmoc)), 3.40-2.80 (*m*, 2H-C(9'), 2H-C(11') and 2H-C(24)), 2.70-

2.50 (*m*, H-N and H-C(3)), 2.12 (*s*, CH<sub>3</sub>COO), 2.07 (*s*, CH<sub>3</sub>COO), 0.90 (*s*, CH<sub>3</sub>-C(10)), 0.78-0.64 (*m*, CH<sub>3</sub>-C(20) and CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>, δ): 223.59, 170.66, 151.85, 150.58, 149.19, 143.88, 141.40, 134.85, 128.69, 128.36, 127.67, 127.03, 125.25, 124.59, 122.15, 120.95, 119.93, 119.68, 117.55, 107.73, 98.21, 75.43, 70.85, 66.88, 51.58, 50.47, 49.43, 47.77, 47.49, 44.99, 43.92, 43.34, 41.42, 39.31, 37.70, 35.43, 34.81, 34.32, 33.28, 32.63, 31.37, 28.92, 27.24, 26.48, 25.53, 22.72, 21.61, 21.45, 17.71, 12.18. (+)ESI-HRMS (*m/z*): [M + H]<sup>+</sup> 917.4978 (error -0.93 ppm). Combustion analysis for C<sub>55</sub>H<sub>69</sub>ClN<sub>4</sub>O<sub>6</sub>×H<sub>2</sub>O: Calculated C 70.60, H 7.65, N 5.99; found C 70.48, H 7.42, N 6.01.

**24-N-[(7-Chloroquinoline-4-yl)amino]propylamino-3α-N',N'-dimethylamino-7α,12α-**

**diacetoxy-5β-cholane (51).** To a stirred mixture of **49** (589 mg, 0.64 mmol) and formaldehyde (37%, 0.3 mL, 4.04 mmol) in dry methanol (20 mL) at r.t. was added a suspension of anhydrous ZnCl<sub>2</sub> (87 mg, 0.64 mmol) and NaBH<sub>3</sub>CN (81 mg, 1.28 mmol) in dry methanol (20 mL). After 24 h of stirring at r.t. the solvent was removed under reduced pressure, and the residue was transferred into separatory funnel as DCM solution, water was added and pH was adjusted to pH 12 with 0.1 M NaOH. Then, the layers were separated, water layer was extracted with DCM (2×15 mL), combined organic layers were washed with sat. NaHCO<sub>3</sub> and brine and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. Solution was filtered off, solvent removed under reduced pressure and crude product (584 mg) was dissolved in solution of piperidine in DCM (20 %, 25 mL). After stirring at r.t. the solvent was removed under reduced pressure, transferred to separatory funnel as DCM solution and worked-up in a usual manner. After column chromatography [dry flash, SiO<sub>2</sub>, eluent MeOH, MeOH/NH<sub>3</sub> gradient 99/1 → 94/6, flash chromatography (Biotage SP1, SiO<sub>2</sub> column, eluent MeOH/NH<sub>3</sub> gradient 98/2 → 95/5, and N-H column, eluent EA/ether = 9/1, EA, gradient EA/MeOH 95/5 → 9/1)] **51** (130.7 mg, 28 %) and **57** (26.3 mg, 6 %) was isolated. **51**: colorless foam softens at 78-82

°C.  $[\alpha]_D^{20} = +0.140$  ( $c = 1.8 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3426s, 2936m, 2868m, 1730m, 1613m, 1582s, 1451m, 1376m, 1331w, 1244s, 1163w, 1140w, 1070w, 1026m, 966w, 899w, 877w, 851w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 8.48 (*d*,  $J = 5.5$ , H-C(2')), 7.93 (*d*,  $J = 2.2$ , H-C(8')), 7.83 (*d*,  $J = 9.0$ , H-C(5')), 7.32 (*dd*,  $J_1 = 8.9$ ,  $J_2 = 2.1$ , H-C(6')), 6.30 (*d*,  $J = 5.5$ , H-C(3')), 5.09 (*bs*, H-C(12)), 4.93 (*bs*, H-N, exchangeable with  $\text{D}_2\text{O}$ ), 4.92-4.87 (*m*, H-C(7)), 3.41 (*t*,  $J = 5.9$ , 2H-C(9')), 2.95 (*t*,  $J = 5.7$ , 2H-C(11')), 2.75-2.61 (*m*, 2H-C(24)), 2.35 (*s*, 2 $\text{CH}_3$ -N), 2.23-2.13 (*m*, H-C(3)), 2.10 (*s*,  $\text{CH}_3\text{COO}$ ), 2.07 (*s*,  $\text{CH}_3\text{COO}$ ), 0.91 (*s*,  $\text{CH}_3$ -C(10)), 0.83 (*d*,  $J = 6.5$ ,  $\text{CH}_3$ -C(20)), 0.71 (*s*,  $\text{CH}_3$ -C(13)).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 170.53, 170.48, 151.51, 150.71, 148.53, 134.90, 127.95, 124.94, 122.29, 117.48, 98.26, 75.40, 70.82, 64.71, 50.00, 48.53, 47.66, 45.04, 43.32, 43.14, 41.65, 41.04, 37.73, 35.54, 34.99, 34.38, 33.26, 32.61, 31.47, 28.86, 27.28, 26.54, 25.93, 25.42, 23.19, 23.06, 22.77, 22.65, 21.54, 21.34, 17.86, 12.21. (+)ESI-HRMS ( $m/z$ ):  $[\text{M} + \text{H}]^+$  723.4611 (error -1.19 ppm). Combustion analysis for  $\text{C}_{42}\text{H}_{63}\text{ClN}_4\text{O}_4$ : Calculated C 69.73, H 8.78, N 7.74; found C 70.12, H 8.98, N 7.68. HPLC purity: Method A: RT 1.804, area 97.63 %; method C: RT 12.462, area 95.41 %.

**24-N-[(7-Chloroquinoline-4-yl)amino]propylamino-3 $\alpha$ -amino-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -**

**cholane (53).** Compound **41** (260 mg, 0.326 mmol) was stirred at r.t. in DCM/ TFA mixture (5 mL, 1:1, v/v) for 90 min. Solvent was removed under reduced pressure, and the residue was transferred as DCM solution to separatory funnel and worked-up in a usual manner.

Yield 187 mg (82 %). Colorless foam softens at 79–82 °C.  $[\alpha]_D^{20} = +0.084$  ( $c = 1.4 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3410m, 2940m, 2866m, 1730m, 1611m, 1582s, 1542m, 1450m, 1377m, 1332w, 1244s, 1138w, 1079w, 1026w, 965w, 898w, 852w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ,  $\delta$ ): 8.48 (*d*,  $J = 5.3$ , H-C(2')), 7.93 (*d*,  $J = 1.9$ , H-C(8')), 7.82 (*bs*, H-N, exchangeable with  $\text{D}_2\text{O}$ ), 7.73 (*d*,  $J = 9.0$ , H-C(5')), 7.31 (*dd*,  $J_1 = 8.8$ ,  $J_2 = 2.1$ , H-C(6')), 6.29 (*d*,  $J = 5.4$ ,

H-C(3')), 5.10 (*bs*, H-C(12)), 4.92-4.85 (*m*, H-C(7)), 3.38 (*t*,  $J = 5.7$ , 2H-C(9')), 2.97-2.87 (*m*, 2H-C(11')), 2.75-2.55 (*m*, 2H-C(24) and H-C(3)), 2.11 (*s*, CH<sub>3</sub>COO), 2.04 (*s*, CH<sub>3</sub>COO), 0.90 (*s*, CH<sub>3</sub>-C(10)), 0.85 (*d*,  $J = 6.6$ , CH<sub>3</sub>-C(20)), 0.73 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>,  $\delta$ ): 170.64, 151.98, 150.60, 148.90, 134.64, 128.25, 124.69, 122.15, 117.52, 98.21, 75.49, 70.85, 51.64, 50.49, 49.42, 47.54, 45.03, 43.91, 43.46, 41.49, 39.41, 37.73, 35.51, 34.96, 34.31, 33.33, 31.38, 31.18, 29.01, 27.28, 27.13, 26.54, 25.59, 22.76, 21.57, 21.44, 17.87, 12.21. (+)ESI-HRMS ( $m/z$ ): [M + H]<sup>+</sup> 695.4280 (error -2.49 ppm). Combustion analysis for C<sub>40</sub>H<sub>59</sub>ClN<sub>4</sub>O<sub>4</sub>×0.5H<sub>2</sub>O: Calculated C 68.21, H 8.59, N 7.95; found C 68.01, H 8.54, N 7.64. HPLC purity: Method C: RT 11.493, area 97.92%; method D: RT 5.137, area 97.997 %.

**24-N-Methyl-N-[(7-chloroquinoline-4-yl)amino]propylamino-3 $\alpha$ -amino-7 $\alpha$ ,12 $\alpha$ -**

**diacetoxy-5 $\beta$ -cholane (55).** Compound **45** (133 mg, 0.164 mmol) was stirred at r.t. in DCM/TFA mixture (2.5 mL, 1:1, v/v) 3 h. Solvent was removed under reduced pressure, and the residue was transferred as DCM solution into separatory funnel and worked-up in a usual manner. Product was isolated after column chromatography (dry flash, SiO<sub>2</sub>, eluent EA, EA/MeOH gradient 9/1  $\rightarrow$  7/3, gradient EA/MeOH/NH<sub>3</sub> 18 / 0.2 / 0.2  $\rightarrow$  18 / 1.4 / 1.4). Yield 41 mg (35 %). Colorless foam softens at 75-77 °C.  $[\alpha]_D^{20} = +0.090$  ( $c = 2.0 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3408m, 2939s, 2865m, 1731m, 1611m, 1582s, 1542m, 1452m, 1377m, 1332m, 1243s, 1158w, 1137m, 1026m, 966w, 898w, 850w, 807w cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>,  $\delta$ ): 8.50 (*d*,  $J = 5.5$ , H-C(2')), 7.94 (*d*,  $J = 2$ , H-C(8')), 7.82 (*bs*, 2H-N, exchangeable with D<sub>2</sub>O), 7.70 (*d*,  $J = 8.9$ , H-C(5')), 7.33 (*dd*,  $J_1 = 8.9$ ,  $J_2 = 2.2$ , H-C(6')), 6.31 (*d*,  $J = 5.5$ , H-C(3')), 5.06 (*s*, H-C(12)), 4.87 (*d*,  $J = 2.6$ , H-C(7)), 3.38 (*t*,  $J = 5.7$ , 2H-C(9')), 2.81 (*bs*, 2H-N, exchangeable with D<sub>2</sub>O), 2.70-2.57 (*m*, 2H-C(11') and H-C(3)), 2.48-2.40 (*m*, 2H-C(24)), 2.38 (*s*, CH<sub>3</sub>-N), 2.08 (*s*, CH<sub>3</sub>COO), 2.07 (*s*, CH<sub>3</sub>COO), 0.90 (*s*, CH<sub>3</sub>-C(10)), 0.78 (*d*,

$J = 6.5$ , CH<sub>3</sub>-C(20)), 0.68 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>,  $\delta$ ): 170.64, 151.74, 150.80, 148.76, 134.79, 128.16, 124.93, 122.02, 117.55, 98.29, 75.45, 70.86, 58.63, 57.30, 51.57, 47.81, 45.05, 43.96, 43.38, 41.89, 41.89, 39.11, 37.76, 35.50, 35.09, 34.36, 33.63, 31.40, 30.92, 28.98, 27.23, 25.58, 24.20, 23.77, 22.79, 22.67, 21.63, 21.42, 17.87, 12.21. (+)ESI-HRMS ( $m/z$ ):[M +H]<sup>+</sup> 709.4454 (error -0.68 ppm). Combustion analysis for C<sub>41</sub>H<sub>61</sub>ClN<sub>4</sub>O<sub>4</sub>: Calculated C 67.70, H 8.73, N 7.70; found C 67.65, H 8.83, N 7.60. HPLC purity: Method A: RT 2.240, area 96.94 %; method B: RT 1.792, area 98.41 %.

**24-N-Methyl-N-[(7-chloroquinoline-4-yl)amino]propylamino-3 $\alpha$ -N',N'-dimethylamino-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane (57).** Mixture of **55** (453.8 mg, 0.64 mmol) and formaldehyde (37 %, 0.48 mL, 6.43 mmol) in 3 mL of CH<sub>3</sub>CN was stirred at r.t. for 20 min. Then, NaBH<sub>3</sub>CN (122 mg, 1.94 mmol) was added and which was after 30 min followed by glac. AcOH (0.7 mL, pH = 6). After 72 h the solvent was removed under reduced pressure, and the obtained crude was transferred into separatory funnel as DCM solution, water was added and pH was adjusted to pH 12 with 0.1 M NaOH and the reaction mixture was further worked-up in usual manner. Product was isolated after column chromatography [dry flash, SiO<sub>2</sub>, eluent EA, EA/MeOH gradient 9/1  $\rightarrow$  1/1, EA/MeOH/NH<sub>3</sub> gradient 18/ 0.2 / 0.2  $\rightarrow$  18/ 3.4 / 3.4), flash chromatography (Biotage SP1 RP column, eluent MeOH/H<sub>2</sub>O gradient 7/3  $\rightarrow$  MeOH and NH column, eluent EA/Hex gradient 7/3  $\rightarrow$  EA)]. Yield 59 mg (13 %). Colorless foam softens at 73-76 °C.  $[\alpha]_D^{20} = +0.049$  ( $c = 1.8 \times 10^{-3}$  g/mL, DCM). IR (KBr): 3431s, 2925m, 2868m, 1731m, 1613m, 1582s, 1452m, 1379m, 1244m, 1125m, 1028m, 607m cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>,  $\delta$ ): 8.50 (*d*,  $J = 5.2$ , H-C(2')), 7.93 (*d*,  $J = 2.0$ , H-C(8')), 7.82 (*bs*, H-N, exchangeable with D<sub>2</sub>O), 7.64 (*d*,  $J = 8.9$ , H-C(5')), 7.32 (*dd*,  $J_1 = 8.9$ ,  $J_2 = 2.1$ , H-C(6')), 6.31 (*d*,  $J = 5.4$ , H-C(3')), 5.06 (*bs*, H-C(12)), 4.88 (*d*,  $J = 2.5$ , H-C(7)), 3.42-3.35 (*m*, 2H-C(9')), 2.63 (*t*,  $J = 5.5$ , 2H-C(11')), 2.41 (*t*,  $J = 6.5$ , 2H-C(24)), 2.37 (*s*, CH<sub>3</sub>-N), 2.31 (*s*, (CH<sub>3</sub>)<sub>2</sub>N-C(3)), 2.07 (*s*, CH<sub>3</sub>COO), 2.06 (*s*, CH<sub>3</sub>COO), 0.90 (*s*, CH<sub>3</sub>-C(10)), 0.78 (*d*,  $J = 6.6$ ,



CH<sub>3</sub>-C(20)), 0.68 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, δ): 170.60, 170.56, 152.00, 150.68, 149.04, 134.65, 128.45, 124.83, 121.91, 117.60, 98.34, 75.44, 70.88, 64.97, 58.82, 57.64, 47.85, 45.04, 44.24, 43.29, 42.09, 41.74, 41.68, 37.74, 35.66, 35.14, 34.41, 33.68, 32.22, 31.53, 28.89, 27.22, 25.44, 24.27, 24.03, 23.59, 22.76, 22.71, 21.63, 21.37, 17.88, 12.20. (+)ESI-HRMS (*m/z*): [M + H]<sup>+</sup> 737.4767 (error -0.43 ppm). Combustion analysis for C<sub>43</sub>H<sub>65</sub>ClN<sub>4</sub>O<sub>4</sub>: Calculated C 70.03, H 8.88, N 7.60; found C 69.82, H 8.60, N 7.63.

Higher yields were obtained when **57** was prepared starting from **51** (59 mg, 0.08 mmol) according to procedure described for **56**. Column purification: dry-flash, SiO<sub>2</sub> column, eluent EA/MeOH gradient 9:1 → 3:7, MeOH, eluent MeOH/NH<sub>3</sub> conc. gradient 3.9:0.1 → 3.5:0.5; flash Biotage SP1, NH column, eluent EA/hexane gradient 8:2 → EA. Yield 58 mg (93%). HPLC purity: Method C: RT 9.682, area 95.17 %; method D: RT 5.092, area 98.86 %.

***N,N*-di(3*α*-Amino-7*α*,12*α*-diacetoxy-5*β*-cholan-24-yl)-*N'*-(7'-chloroquinoline-4'-yl)-1,3-propanediamine (61).** Compound **61** was obtained according to procedure described for **60** using **59** (656 mg, 0.484 mmol). After 5 h the solvent was removed under reduced pressure, and the residue was transferred as DCM solution to separatory funnel and worked-up in a usual manner. Product was isolated after column chromatography procedure (dry flash, SiO<sub>2</sub>, eluent EA, EA/MeOH gradient 9/1 → 7/3 and EA/MeOH/NH<sub>3</sub> gradient 18 / 0.2 / 0.2 → 18 / 1.7 / 1.7). Yield 511 mg (91 %). Colorless foam softens at 113-117 °C. [α]<sub>D</sub><sup>20</sup> = +0.065 (c = 2.1 × 10<sup>-3</sup> g/mL, DCM). IR (KBr): 3752w, 3402m, 2948m, 2856m, 1731s, 1668s, 1613m, 1581s, 1540w, 1452m, 1379s, 1245s, 1137w, 1024m, 965w, 851w cm<sup>-1</sup>. <sup>1</sup>H NMR (200 MHz, CDCl<sub>3</sub>, δ): 8.49 (*d*, *J* = 5,1, H-C(2')), 7.92 (*d*, *J* = 1.7, H-C(8')), 7.80 (*bs*, H-N, exchangeable with D<sub>2</sub>O), 7.68 (*d*, *J* = 9.0, H-C(5')), 7.33 (*dd*, *J*<sub>1</sub> = 9.0, *J*<sub>2</sub> = 1.7, H-C(6')), 6.32 (*d*, *J* = 5.6, H-C(3')), 5.73 (*bs*, 2 × NH<sub>2</sub>, exchangeable with D<sub>2</sub>O), 5.06 (*bs*, 2 × H-C(12)), 4.87 (*bs*, 2 × H-C(7)), 3.36 (*bs*, 2H-C(9')), 2.72-2.36 (*m*, 2H-C(11'), 2 × H-C(3) and 2 × 2H-C(24)), 2.07 (*s*, CH<sub>3</sub>COO), 2.05 (*s*, CH<sub>3</sub>COO), 2.02 (*s*, CH<sub>3</sub>COO), 0.90 (*s*, 2 × CH<sub>3</sub>-C(10)), 0.75 (*d*, *J* = 6.2,

2×CH<sub>3</sub>-C(20)), 0.67 (*s*, 2×CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (50 MHz, CDCl<sub>3</sub>, δ): 172.77, 170.69, 170.53, 170.49, 152.07, 150.54, 149.06, 134.57, 128.42, 124.61, 122.03, 117.49, 98.37, 75.42, 70.85, 54.90, 54.22, 51.56, 47.83, 44.96, 44.45, 43.30, 41.41, 39.29, 37.64, 35.42, 35.03, 34.85, 34.27, 33.65, 31.34, 31.06, 28.92, 28.13, 27.15, 25.49, 24.38, 23.58, 23.00, 22.73, 22.56, 21.60, 21.38, 17.75, 12.13. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, δ): 8.50 (*d*, *J* = 5.3, H-C(2')), 7.93 (*d*, *J* = 2.1, H-C(8')), 7.74-7.63 (*m*, H-N, exchangeable with D<sub>2</sub>O and H-C(5')), 7.33 (*dd*, *J*<sub>1</sub> = 8.8, *J*<sub>2</sub> = 2.2, H-C(6')), 6.31 (*d*, *J* = 5.5, H-C(3')), 5.05 (*bs*, 2×H-C(12)), 4.87 (*bs*, 2×H-C(7)), 3.36 (*bs*, 2H-C(9')), 2.72-2.54 (*m*, 2H-C(11')), 2×H-C(3), 2.52-2.40 (*m*, 2×2H-C(24)), 2.06 (*s*, CH<sub>3</sub>COO), 2.05 (*s*, CH<sub>3</sub>COO), 2.02 (*s*, CH<sub>3</sub>COO), 0.90 (*s*, 2×CH<sub>3</sub>-C(10)), 0.75 (*d*, *J* = 6.0, 2×CH<sub>3</sub>-C(20)), 0.67 (*s*, 2×CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, δ): 170.64, 170.60, 152.14, 150.50, 149.17, 134.58, 128.58, 124.63, 121.96, 117.54, 98.43, 75.46, 70.89, 54.96, 55.30, 53.39, 51.66, 47.91, 45.04, 44.48, 43.38, 41.52, 39.51, 37.74, 35.53, 35.11, 34.36, 33.74, 31.43, 31.27, 29.66, 28.99, 27.22, 25.58, 24.54, 23.66, 22.80, 22.76, 21.65, 21.42, 21.26, 17.85, 12.20. (+)ESI-HRMS (*m/z*): [M + H]<sup>+</sup> 1154.7660 (error +1.22 ppm). Combustion analysis for C<sub>68</sub>H<sub>104</sub>ClN<sub>5</sub>O<sub>8</sub>×H<sub>2</sub>O: Calculated C 69.62, H 9.11, N 5.97; found C 69.39, H 9.27, N 5.91. HPLC purity: Method C: RT = 10.553, area 95.61 %; method D: RT 5.288, area 95.46 %.

***N,N'*-{4'-[(7-Chloroquinoline-4-yl)amino]propyl}-7 $\alpha$ ,12 $\alpha$ -diacetoxy-3,24-diamine (63**, mixture of diastereoisomers). Compound **63** was obtained according to procedure described for **62** using **23** (852 mg, 1.23 mmol), ACQ3 (579 mg, 2.46 mmol) and NaBH<sub>3</sub>CN (107 mg, 1.71 mmol). Column chromatography dry flash, SiO<sub>2</sub>, eluent gradient EtOAc → EtOAc/MeOH = 1:9 → MeOH, gradient EtOAc/MeOH/NH<sub>3</sub> = 18:1:1 → EtOAc/MeOH/NH<sub>3</sub> = 9:1:1, flash chromatography Biotage SP1 RP, gradient MeOH/H<sub>2</sub>O = 8:2 → 9:1. Yield 286 mg, 26 %. Colorless solid, [ $\alpha$ ]<sub>D</sub><sup>20</sup> = +0.041 (*c* = 1.1×10<sup>-3</sup> g/mL, DCM). IR (KBr): 3405m, 2930s, 2863w, 1728m, 1610w, 1582s, 1538w, 1450w, 1372w, 1331w, 1246m, 1170w,

1137w, 1077w, 1023w, 963w, 900w, 878w, 852w, 805w, 766w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ ,  $\delta$ ): 8.34 (*d*,  $J = 5.7$ ,  $2\times\text{H-C}(2')$ ), 8.10-8.02 (*m*,  $2\times\text{H-C}(5')$ ), 7.79-7.76 (*m*,  $2\times\text{H-C}(8')$ ), 7.41-7.34 (*m*,  $2\times\text{H-C}(6')$ ), 6.54-6.48 (*m*,  $2\times\text{H-C}(3')$ ), 5.08-5.02 (*bs*,  $\text{H-C}(12)$ ), 4.85 (*bs*,  $\text{H-C}(7)$  covered with methanol signal), 3.41 (*t*,  $J = 6.7$ ,  $2\times\text{H-C}(9')$ ), 2.84 (*bs*,  $\text{H}\alpha\text{-C}(3)$ ), 2.81-2.65 (*m*,  $2\times\text{H-C}(11')$ ), 2.75-2.50 (*m*,  $2\text{H-C}(24)$ ), 2.06 (*s*,  $\text{CH}_3\text{COO}$ ), 2.02 (*s*,  $\text{CH}_3\text{COO}$ ), 0.92 (*s*,  $\text{CH}_3\text{-C}(10)$ , one isomer), 0.88 (*s*,  $\text{CH}_3\text{-C}(10)$ , second isomer), 0.85-0.78 (*m*,  $\text{CH}_3\text{-C}(20)$ ), 0.73 (*s*,  $\text{CH}_3\text{-C}(13)$  one isomer), 0.72 (*s*,  $\text{CH}_3\text{-C}(13)$ , second isomer).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ,  $\delta$ ): 172.37, 152.86, 152.82, 152.64, 149.86, 136.44, 127.83, 126.12, 124.44, 118.96, 99.79, 77.35, 72.86, 54.15, 51.38, 46.41, 46.37, 44.88, 42.89, 42.57, 39.09, 37.24, 36.39, 34.61, 34.17, 32.33, 31.20, 29.97, 29.27, 29.03, 28.42, 27.00, 26.80, 25.40, 23.995, 23.95, 23.26, 21.59, 21.37, 18.58, 12.71 (+)ESI-HRMS ( $m/z$ ):  $[\text{M} + 2\text{H}]^{2+}$  457.24877 (error -0.62 ppm),  $[\text{M} + \text{H}]^+$  913.49058 (error -0.28 ppm). Combustion analysis  $\text{C}_{52}\text{H}_{70}\text{Cl}_2\text{N}_6\text{O}_4 \times \text{H}_2\text{O}$ : Calculated C 67.01, H 7.79, N 9.02; found C 66.95, H 7.99, N 9.07. HPLC purity: Method C: RT1 5.533, RT2 8.731, area 95.07 %; method D: RT1 5.495, RT2 5.495, area 99.55 %.

***N,N'*-{4'-[(7-Chloroquinoline-4-yl)amino]butyl}-7 $\alpha$ ,12 $\alpha$ -diacetoxy-3 $\beta$ ,24-diamine (64).**

Compound **64** was obtained according to procedure described for **62**, using **24** (150 mg, 0.21 mmol), ACQ4 (105 mg, 0.42 mmol) and  $\text{NaBH}_3\text{CN}$  (22 mg, 0.34 mmol). Column chromatography dry flash,  $\text{SiO}_2$ , gradient  $\text{EtOAc} \rightarrow \text{EtOAc/MeOH} = 3:7 \rightarrow \text{MeOH} \rightarrow \text{EtOAc/MeOH/NH}_3 = 18:1:1$ , flash chromatography Biotage SP1 NH column, eluent  $\text{EtOAc/MeOH}$  and  $\text{DCM/MeOH}$ . Yield 16 mg (8%) **64** and 10 mg (5%) of unresolvable mixture of epimers. **64**: Colorless solid,  $[\alpha]_{\text{D}}^{20} = +0.046$  ( $c = 1.6 \times 10^{-3}$  g/mL, MeOH). IR (film): 3898w, 3738w, 3670w, 3646w, 3612w, 3304m, 2942m, 2868w, 2280w, 1721m, 1610w, 1582s, 1540w, 1451w, 1371m, 1332w, 1247m, 1136w, 1078w, 1024w, 900w, 878w,

851w, 806w, 731w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ ,  $\delta$ ): 8.35-8.30 (*m*,  $2\times\text{H-C}(2')$ ), 8.12-8.05 (*m*,  $2\times\text{H-C}(8')$ ), 7.79-7.74 (*m*,  $2\times\text{H-C}(5')$ ), 7.41-7.35 (*m*,  $2\times\text{H-C}(6')$ ), 6.53-6.47 (*m*,  $2\times\text{H-C}(3')$ ), 5.06 (*bs*,  $\text{H-C}(12)$ ), 4.86 (*bs*,  $\text{H-C}(7)$ , covered with  $\text{CD}_3\text{OD}$ ), 3.40-3.34 (*m*,  $2\times\text{H-C}(9')$ ), 2.84 (*bs*,  $\text{H}\alpha\text{-C}(3)$ ), 2.67-2.62 (*m*,  $2\text{H-C}(12')$ ), 2.61-2.56 (*m*,  $2\text{H-C}(12')$ ), 2.55-2.45 (*m*,  $2\text{H-C}(24)$ ), 2.07 (*s*,  $\text{CH}_3\text{COO}$ ), 2.03 (*s*,  $\text{CH}_3\text{COO}$ ), 0.93 (*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.82 (*d*,  $J = 6.6$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.72 (*s*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ,  $\delta$ ): 172.40, 172.36, 152.84, 152.59, 149.86, 136.42, 127.78, 126.07, 124.46, 118.93, 99.79, 77.33, 72.85, 54.07, 51.19, 50.37, 48.03, 46.36, 44.84, 43.98, 43.93, 39.09, 37.18, 36.37, 35.97, 34.57, 34.03, 32.33, 31.15, 29.96, 28.44, 28.25, 28.00, 27.45, 27.28, 26.83, 26.78, 25.24, 23.97, 23.26, 21.59, 21.38, 18.56, 12.71. (+)ESI-HRMS ( $m/z$ ):  $[\text{M} + 2\text{H}]^{2+}$  471.26355 (error -2.46 ppm),  $[\text{M} + \text{H}]^+$  941.51879 (error -3.55 ppm). Combustion analysis  $\text{C}_{54}\text{H}_{74}\text{Cl}_2\text{N}_6\text{O}_4 \times \text{H}_2\text{O}$ : Calculated C 67.55, H 7.98, N 8.75; found C 67.25, H 7.89, N 8.53. HPLC purity: Method C: RT 8.807, area 97.79 %; method D: RT 5.135, area 99.23 %.

***N,N'*-{4'-[(7-Chloroquinoline-4-yl)amino]hexyl}-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane-3 $\beta$ ,24-diamine (65) and *N,N'*-{4'-[(7-chloroquinoline-4-yl)amino]hexyl}-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane-3 $\alpha$ ,24-diamine (66)}**. Compounds were obtained according to procedure described for **62**, using **25** (200 mg, 0.27 mmol), ACQ6 (151 mg, 0.54 mmol) and  $\text{NaBH}_3\text{CN}$  (60 mg, 0.95 mmol). Column chromatography: dry flash,  $\text{SiO}_2$ , eluent EA, gradient EA/MeOH 95/5  $\rightarrow$  2/8, MeOH, gradient EA/MeOH/ $\text{NH}_3$  18/1/1  $\rightarrow$  9/1/1; Lobar RP column, eluent MeOH/ $\text{H}_2\text{O}$  9/1 and MeOH; flash chromatography Biotage SP1RP column, eluent gradient EA/MeOH/ $\text{NH}_3$  8/1/1  $\rightarrow$  9/1/1; preparative TLC  $\text{SiO}_2$ , eluent EA/MeOH/ $\text{NH}_3$ =9/1/1. Yields 7 mg (2.5%) **65** ( $\beta$  epimer) and 6 mg (2.3%) **66** ( $\alpha$  epimer). **65**: Colorless solid,  $[\alpha]_{\text{D}}^{20} = +0.080$  ( $c = 1.8 \times 10^{-3}$  g/mL, MeOH). IR (film): 3313w, 2927m, 2856w, 1724w, 1610w, 1581s, 1539w, 1452w, 1371w, 1332w, 1249m, 1136w, 1080w, 1023w, 901w, 879w, 851w,

807w, 766w, 736w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ ,  $\delta$ ): 8.35-8.31 (*m*,  $2\times\text{H-C}(2')$ ), 8.11-8.06 (*m*,  $2\times\text{H-C}(5')$ ), 7.76- (*d*,  $J = 2.2$ ,  $2\times\text{H-C}(8')$ ), 7.37 (*dd*,  $J_1 = 9.0$ ,  $J_2 = 2.1$ ,  $2\times\text{H-C}(6')$ ), 6.50-6.45 (*m*,  $2\times\text{H-C}(3')$ ), 5.07 (*bs*,  $\text{H-C}(12)$ ), 4.86 (*bs*,  $\text{H-C}(7)$ , covered with MeOH), 3.38-3.30 (*m*,  $2\times 2\text{H-C}(9')$ ), 2.79 (*bs*,  $\text{H-C}(3)$ ), 2.60-2.42 (*m*,  $2\times 2\text{H-C}(14')$  and  $2\text{H-C}(24)$ ), 2.08 (*s*,  $\text{CH}_3\text{COO}$ ), 2.03 (*s*,  $\text{CH}_3\text{COO}$ ), 0.92 (*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.83 (*d*,  $J = 6.5$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.74 (*s*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ,  $\delta$ ): 172.28, 172.22, 152.73, 152.43, 149.74, 136.24, 127.63, 125.90, 124.32, 118.79, 99.60, 77.20, 72.73, 53.75, 51.24, 50.61, 48.03, 46.22, 44.70, 43.94, 38.96, 37.06, 36.27, 35.82, 34.50, 34.05, 33.07, 32.21, 32.15, 31.01, 30.77, 30.49, 30.38, 30.10, 29.82, 29.32, 29.30, 28.31, 28.19, 28.10, 26.83, 26.65, 25.07, 23.84, 23.74, 23.12, 21.45, 21.24, 18.44, 14.45, 12.57. (+)ESI-HRMS ( $m/z$ ):  $[\text{M} + \text{H}]^+$  997.5854 (error +0.62 ppm). Combustion analysis  $\text{C}_{58}\text{H}_{82}\text{Cl}_2\text{N}_6\text{O}_4 \times \text{H}_2\text{O}$ : Calculated C 68.55, H 8.33, N 8.27; found C 68.27, H 8.49, N 8.53. HPLC purity: Method C: RT 11.422, area 97.88 %; method D: RT 5.150, area 99.24.

**66:** Colorless solid,  $[\alpha]_{\text{D}}^{20} = +0.122$  ( $c = 3.9 \times 10^{-3}$  g/mL, MeOH). IR (film): 3303w, 3061w, 2928s, 2856m, 1726m, 1610w, 1580s, 1538w, 1452w, 1372w, 1332w, 1250m, 1136w, 1079w, 1023w, 879w, 851w, 807w, 766w, 737w  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_3\text{OD}$ ,  $\delta$ ): 8.36-8.31 (*m*,  $2\times\text{H-C}(2')$ ), 8.09 (*d*,  $J = 9.1$ ,  $2\times\text{H-C}(5')$ ), 7.77 (*d*,  $J = 2.0$ ,  $2\times\text{H-C}(8')$ ), 7.38 (*dd*,  $J_1 = 9.0$ ,  $J_2 = 2.1$ ,  $2\times\text{H-C}(6')$ ), 6.51 (*d*,  $J = 5.8$ ,  $2\times\text{H-C}(3')$ ), 5.06 (*bs*,  $\text{H-C}(12)$ ), 4.87 (*bs*,  $\text{H-C}(7)$ ), 3.36 (*t*,  $J = 7.0$ ,  $2\times 2\text{H-C}(9')$ ), 2.60-2.45 (*m*,  $2\times 2\text{H-C}(14')$  and  $2\text{H-C}(24)$ ), 2.36-2.30 (*m*,  $\text{H-C}(3)$ ), 2.06 (*s*,  $\text{CH}_3\text{COO}$ ), 2.04 (*s*,  $\text{CH}_3\text{COO}$ ), 0.94 (*s*,  $\text{CH}_3\text{-C}(10)$ ), 0.83 (*d*,  $J = 6.6$ ,  $\text{CH}_3\text{-C}(20)$ ), 0.76 (*s*,  $\text{CH}_3\text{-C}(13)$ ).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CD}_3\text{OD}$ ,  $\delta$ ): 172.42, 172.30, 152.76, 152.45, 149.76, 136.28, 127.62, 125.91, 124.32, 118.80, 99.61, 77.17, 72.64, 59.35, 51.13, 50.51, 47.76, 46.24, 44.76, 43.92, 43.88, 42.80, 39.02, 37.10, 36.51, 36.26, 35.86, 34.45, 32.46, 30.48, 30.28, 30.20, 30.09, 29.29, 29.24, 28.31, 28.14, 28.06, 26.66, 26.46, 23.83, 23.14, 21.48, 21.23, 18.41, 12.54. (+)ESI-HRMS ( $m/z$ ):  $[\text{M} + 2\text{H}]^{2+}$  499.2938 (error -4.31

ppm)  $[M + H]^+$  997.5824 (error -2.30 ppm). Combustion analysis  $C_{58}H_{82}Cl_2N_6O_4 \times H_2O$ :

Calculated C 68.55, H 8.33, N 8.27; found C 68.60, H 8.30, N 8.35. HPLC purity: Method

C: RT 9.878, area 99.98 %; method D: RT 5.208, area 96.76 %.

**3 $\beta$ -N-{6'-[(7-Chloroquinoline-4-yl)amino]hexyl}-24-N'-{4'-[(7-chloroquinolin-4-yl)amino]butyl}-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane-3,24-diamine (67) and**

**3 $\alpha$ -N-{6'-[(7-chloroquinoline-4-yl)amino]hexyl}-24-N'-{4'-[(7-chloroquinoline-4-yl)amino]butyl}-7 $\alpha$ ,12 $\alpha$ -diacetoxy-5 $\beta$ -cholane-3,24-diamine (68).** Compounds were

obtained according to procedure described for **62**, using **24** (200 mg, 0.28 mmol), ACQ6

(157 mg, 0.56 mmol) and NaBH<sub>3</sub>CN (27 mg, 0.42 mmol). Column chromatography: dry

flash, SiO<sub>2</sub>, gradient EtOAc  $\rightarrow$  EtOAc/MeOH = 2:8, MeOH, gradient EtOAc/MeOH/NH<sub>3</sub> =

18:1:1  $\rightarrow$  9:1:1; flash chromatography (Biotage SP1 RP column, gradient MeOH/H<sub>2</sub>O = 9:1

$\rightarrow$  MeOH; preparative TLC, SiO<sub>2</sub>, eluent EtOAc/MeOH/NH<sub>3</sub> = 9:1:1). Yields 14.4 mg (5%)

**67** and 4.2 mg (2%) **68**. Compound **67**: Colorless solid,  $[\alpha]_D^{20} = +0.020$  ( $c = 1.8 \times 10^{-3}$  g/mL,

MeOH). IR (film): 3297m, 2932m, 2861w, 1724m, 1610w, 1581s, 1539w, 1451w, 1371w,

1332w, 1250m, 1167w, 1136w, 1079w, 1023w, 901w, 879w, 851w, 807w, 736w cm<sup>-1</sup>. <sup>1</sup>H

NMR (500 MHz, CD<sub>3</sub>OD,  $\delta$ ): 8.35-8.32 (*m*, H-C(2') and H-C(2'')), 8.10-8.07 (*m*, H-C(8')

and H-C(8'')), 7.78-7.75 (*m*, H-C(5') and H-C(5'')), 7.40-7.35 (*m*, H-C(6') and H-C(6'')),

6.52-6.47 (*m*, H-C(3') and H-C(3'')), 5.06 (*bs*, H-C(12)), 4.85 (*bs*, H-C(7), covered with

MeOH), 3.40-3.32 (*m*, 2H-C(9') and 2H-C(9'')), 2.83 (*bs*, Ha-C(3)), 2.68-2.61 (*m*, 2H-

C(12'')), 2.58-2.46 (*m*, 2H-C(12') and 2H-C(24)), 2.08 (*s*, CH<sub>3</sub>COO), 2.03 (*s*, CH<sub>3</sub>COO),

0.92 (*s*, CH<sub>3</sub>-C(10)), 0.83 (*d*,  $J = 6.6$ , CH<sub>3</sub>-C(20)), 0.73 (*s*, CH<sub>3</sub>-C(13)). <sup>13</sup>C NMR (125 MHz,

CD<sub>3</sub>OD,  $\delta$ ): 170.85, 170.80, 151.32, 151.28, 151.03, 151.00, 148.31, 134.85, 126.23, 126.21,

124.52, 124.49, 122.90, 117.38, 98.24, 98.19, 75.76, 71.28, 52.50, 49.64, 48.82, 46.56, 44.81,

43.28, 42.51, 42.37, 37.54, 35.62, 34.82, 34.39, 33.02, 32.40, 30.76, 29.57, 28.84, 28.42,

27.90, 26.89, 26.83, 26.66, 26.45 25.72, 25.28, 25.23, 23.50, 22.42, 21.67, 20.03, 19.82, 17.00, 11.15. (+)ESI-HRMS ( $m/z$ ): $[M + H]^+$  969.55129 (error -2.22 ppm). Combustion analysis  $C_{56}H_{78}Cl_2N_6O_4 \times 0.5H_2O$ : Calculated C 68.69, H 8.13, N 8.58; found C 68.57, H 8.29, N 8.45. HPLC purity: Method C: RT 8.674, area 95.27 %; method D: RT 5.072, area 99.21 %.

**68**: Colorless solid,  $[\alpha]_D^{20} = +0.013$  ( $c = 8.0 \times 10^{-4}$  g/mL, MeOH). IR (film): 3300m, 2927s, 2856w, 1728m, 1670w, 1610w, 1580s, 1540w, 1452w, 1372w, 1332w, 1246m, 1134w, 1078w, 1024w, 964w, 939w, 880w, 850w, 805w, 732w  $cm^{-1}$ .  $^1H$  NMR (500 MHz,  $CD_3OD$ ,  $\delta$ ): 8.37-8.30 (*m*, H-C(2') and H-C(2'')), 8.12-8.07 (*m*, H-C(8') and H-C(8'')), 7.79-7.75 (*m*, H-C(5') and H-C(5'')), 7.42-7.36 (*m*, H-C(6') and H-C(6'')), 6.54-6.48 (*m*, H-C(3') and H-C(3'')), 5.06 (*bs*, H-C(12)), 4.87 (*bs*, H-C(7)), 3.42-3.34 (*m*, 2H-C(9') and 2H-C(9'')), 2.70-2.63 (*m*, 2H-C(12'')), 2.63-2.48 (*m*, 2H-C(14') and 2H-C(24)), 2.42-2.34 (*m*, H $\beta$ -C(3)), 2.06 (*s*,  $CH_3COO$ ), 2.04 (*s*,  $CH_3COO$ ), 0.94 (*s*,  $CH_3-C(10)$ ), 0.82 (*d*,  $J = 6.4$ ,  $CH_3-C(20)$ ), 0.74 (*s*,  $CH_3-C(13)$ ).  $^{13}C$  NMR (125 MHz,  $CD_3OD$ ,  $\delta$ ): 172.38, 172.28, 152.76, 152.73, 152.46, 152.43, 149.74, 136.29, 127.63, 125.95, 125.92, 124.31, 118.81, 99.66, 99.60, 77.14, 72.60, 59.33, 50.97, 50.15, 49.62, 47.61, 46.25, 44.74, 43.86, 43.75, 42.75, 39.00, 36.80, 36.43, 36.22, 35.83, 34.39, 32.43, 32.14, 30.28, 30.22, 30.09, 29.23, 28.30, 28.11, 28.01, 27.89, 27.72, 27.10, 26.56, 26.47, 23.82, 23.11, 21.48, 21.23, 18.38, 12.54. (+)ESI-HRMS ( $m/z$ ): $[M + 2H]^{2+}$  485.28020 (error -0.32 ppm),  $[M + H]^+$  969.55344 (error 0.65 ppm). Combustion analysis  $C_{56}H_{78}Cl_2N_6O_4 \times 0.5H_2O$ : Calculated C 68.69, H 8.13, N 8.58; found C 68.51, H 8.21, N 8.77. HPLC purity: method C: RT 8.846, area 99.18 %; method D: RT 5.181, area 96.31 %.

**HPLC analyses for purity**

Compounds were analyzed for purity (HPLC) using a Waters 1525 HPLC dual pump system equipped with an Alltech, Select degasser system, and dual  $\lambda$  2487 UV-VIS detector. For data processing, Empower software was used (methods A and B). Methods C and D: Agilent Technologies 1260 Liquid Chromatograph equipped with Quat Pump (G1311B), Injector (G1329B) 1260 ALS, TCC 1260 ( G1316A) and Detector 1260 DAD VL+ (G1315C). For data processing, LC OpenLab CDS ChemStation software was used.

**Method A:** Octadecylsilica was used as the stationary phase (Symmetry C18 analytical column, 4.6 mm  $\times$  150 mm, 5  $\mu$ m, series no. 021336278136 37). Compounds were dissolved in mixture containing 0.2% HCOOH/CH<sub>3</sub>OH 1/1 [% , v/v] final concentrations were 0.1-0.5 mg/mL and injection volume was 10 $\mu$ l. Eluent was made from the following solvents: 0.2% formic acid in water (A) and methanol (B). The analysis were performed at the UV max of the compounds (at 340 nm) to maximize selectivity.

Compounds **12, 52, 16, 22, 23**, were eluted using gradient protocol: 0 - 2 min 98 %A, 2 - 7 min 98 %A  $\rightarrow$  2 %A, 7-9 min 2 %A, 9-16 min 2 %A  $\rightarrow$  98 %A.

Compounds **36, 40, 60, 41, 21, 37, 38, 39, 42, 43, 13, 62, 51, 50, 44, 54, 56, 55, 15, 19, 25, 14, 18, 24** were eluted using gradient protocol: 0-3 min 10 %A, 3-6 min 10 %A  $\rightarrow$  90 %A, 6-9 min 90 %A, 9-12 min 90 %A  $\rightarrow$  10 %A, 12-13 min 10 % A.

Compound **17** was eluted using gradient protocol: 0 - 2 min 95 %A, 2 - 7 min 95 %A  $\rightarrow$  5 %A, 7-9 min 5 %A, 9-16 min 5 %A  $\rightarrow$  95 %A.

Compounds **66, 65**, were eluted using gradient protocol: 0-3 min 20 %A, 3-6 min 20 %A  $\rightarrow$  80 %A, 6-9 min 80 %A, 9-12 min 80 %A  $\rightarrow$  20 %A, 12-13 min 20 % A.

Compounds **61, 57, 20** were eluted using gradient protocol: : 0-3 min 6 %A, 3-6 min 6 %A  $\rightarrow$  94 %A, 6-9 min 94 %A, 9-12 min 94 %A  $\rightarrow$  6 %A, 12-13 min 6 % A.

**Method B:** Octadecylsilica was used as the stationary phase (Nucleosil C18 analytical column, 4 mm  $\times$  150 mm, 5  $\mu$ m). Compounds were dissolved in mixture containing 0.2%



HCOOH/CH<sub>3</sub>OH 1/1 [% , v/v], final concentrations were 0.1-0.5 mg/mL and injection volume was 10µL. Eluent was made from the following solvents: 0.2 % formic acid in water (A) and methanol (B). The analysis were performed at the UV max of the compounds (at 340 nm) to maximize selectivity.

Compounds **12, 40, 52, 16, 22, 20, 21, 13, 17, 50** were eluted using gradient protocol: 0 - 2 min 98 %A, 2 - 7 min 98 %A→ 2 %A, 7-9 min 2 %A, 9-16 min 2 %A→ 98 %A.

Compounds **60, 53, 37, 38, 39, 42, 43, 62, 59, 44, 54, 56, 15, 19, 25, 14, 18, 24** were eluted using gradient protocol: 0-3 min 10 %A, 3-6 min 10 %A→ 90 %A, 6-9 min 90 %A, 9-12 min 90 %A→ 10 %A, 12-13 min 10 % A.

Compounds **51, 55** were eluted using gradient protocol: 0 - 3 min 6 %A, 3 - 6 min 6 %A→ 94 %A, 6-9 min 94 %A, 9-12 min 94 %A→ 6 %A, 12-13 min 6 %A.

Compounds **36, 41, 23, 57**, were eluted using gradient protocol: 0 - 3 min 2 %A, 3 - 6 min 2 %A→ 98 %A, 6-9 min 98 %A, 9-12 min 98 %A→ 2 %A, 12-13 min 2 %A.

Compounds **66, 65**, were eluted using gradient protocol: 0-3 min 20 %A, 3-6 min 20 %A→ 80 %A, 6-9 min 80 %A, 9-12 min 80 %A→ 20 %A, 12-13 min 20 % A.

Compound **61** was eluted using gradient protocol: 0-3 min 4 %A, 3-6 min 4 %A→ 96 %A, 6-9 min 96 %A, 9-12 min 96 %A→ 4 %A, 12-13 min 4 % A.

**Method C:** Zorbax Eclipse Plus C18 4.6 \_ 150mm, 1.8µ, S.N. USWKY01594 was used as the stationary phase. Eluent was made from the following solvents: 0.2% formic acid in water (A) and methanol (B). The analysis were performed at the UV max of the compounds (at 330 nm or 254 nm for compound **63**) to maximize selectivity. Compounds were dissolved in methanol, final concentrations were ~ 1mg/mL. Flow rate was 0.5mL/min.

Compounds were eluted using gradient protocol: 0 - 1 min 95%A, 1 - 6 min 95%A→ 5%A, 6 - 11 min 5%A, 11 – 15 min 5%A→ 95%A, 15 – 20 min 95%A.

Compounds **45** and **57** were eluted using gradient protocol: 0 - 1 min 95%A, 1 - 6 min 95%A→ 0%A, 6 - 11 min 0%A, 11 – 15 min 0%A→ 95%A, 15 – 20 min 95%A.

**Method D:** Poroshell 120 EC-C18, 4.6 \_ 50mm, 2.7 $\mu$ , S.N. USCFU07797 was used as the stationary phase. Eluent was made from the following solvents: 0.2% formic acid in water (A) and methanol (B). The analysis were performed at the UV max of the compounds (at 330 nm or 254 nm for compound **66**) to maximize selectivity. Compounds were dissolved in methanol, final concentrations were ~ 1mg/mL. Flow rate was 0.5mL/min. Compounds were eluted using gradient protocol: 0 - 1 min 95%A, 1 - 3 min 95%A $\rightarrow$  0%A, 3 - 10 min 0%A, 10 - 12 min 0%A $\rightarrow$  95%A, 12 - 15 min 95%A.

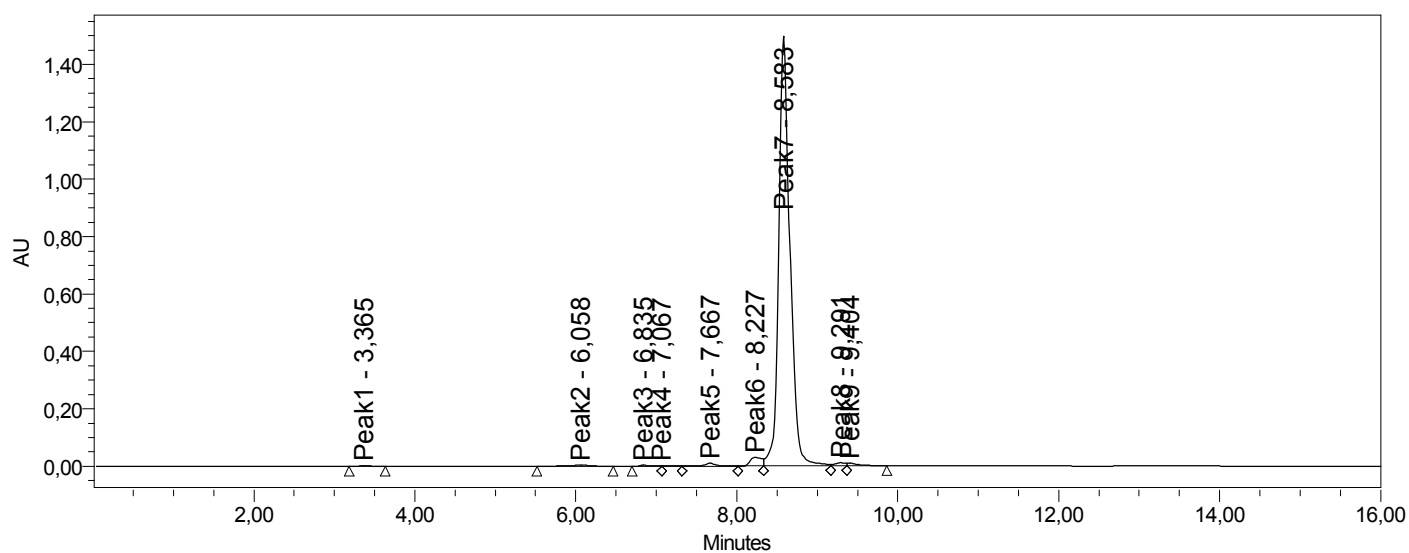


Reported by User: System

Project Name: Organskajedinjenja

### SAMPLE INFORMATION

Sample Name: DO152Á Compound 12	Acquired By: System
Sample Type: Unknown	Date Acquired: 4.6.2012 14:09:40
Vial: 5	Acq. Method Set: 98225434005_MS
Injection #: 1	Date Processed: 4.6.2012 15:28:18
Injection Volume: 10,00 ul	Processing Method: do152 11
Run Time: 16,0 Minutes	Channel Name: 2487Channel 2
Sample Set Name:	Proc. Chnl. Descr.:



	Peak Name	RT	Area	% Area	Height
1	Peak1	3,365	17300	0,11	1699
2	Peak2	6,058	86364	0,56	4728
3	Peak3	6,835	45929	0,30	3843
4	Peak4	7,067	16655	0,11	1982
5	Peak5	7,667	116557	0,75	10064
6	Peak6	8,227	305824	1,98	29779
7	Peak7	8,583	14675122	95,04	1489514
8	Peak8	9,291	94072	0,61	9950
9	Peak9	9,404	83317	0,54	8496



Method A

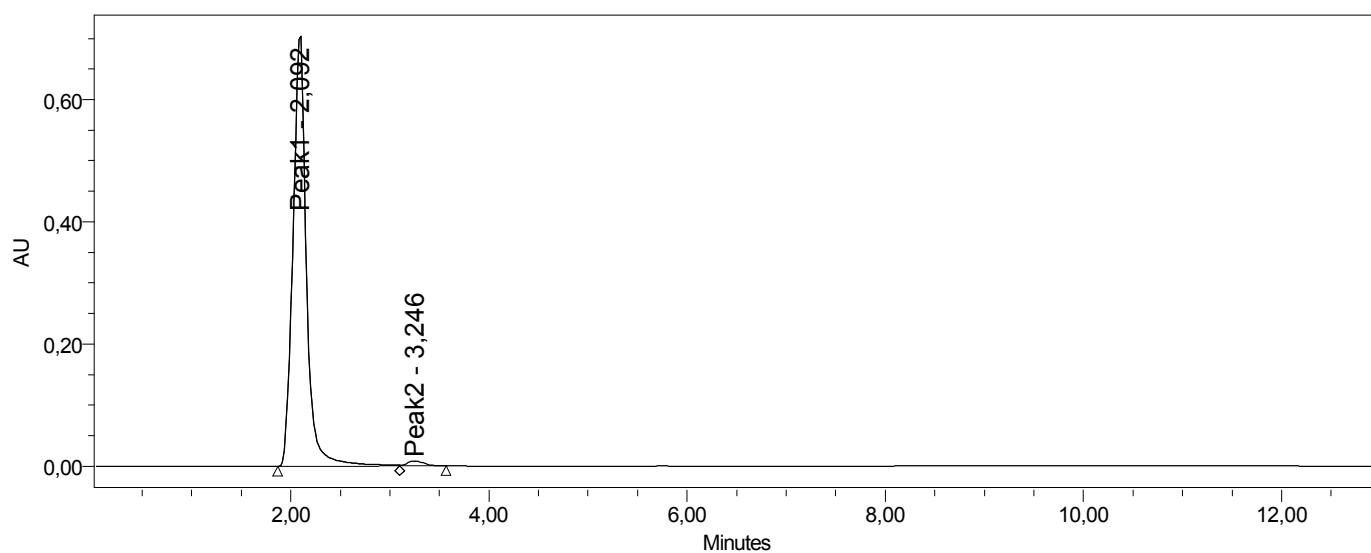
## Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

## SAMPLE INFORMATION

Sample Name:	DR06	Compound 13	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	18.7.2012 11:17:59
Vial:	1		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	18.7.2012 11:40:54
Injection Volume:	10,00 ul		Processing Method:	DR06
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



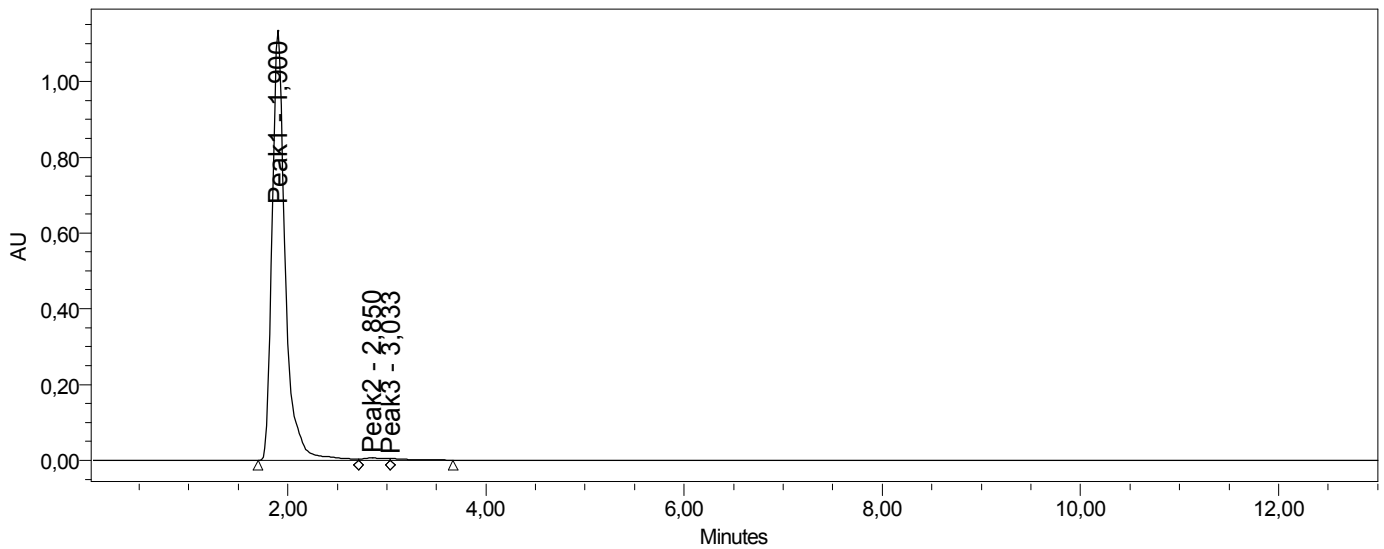
	Peak Name	RT	Area	% Area	Height
1	Peak1	2,092	6660900	98,69	706478
2	Peak2	3,246	88276	1,31	7570

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	DOZS11 Compound 14	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	19.7.2012 11:37:31
Vial:	4	Acq. Method Set:	10902543400513m_MS
Injection #:	1	Date Processed:	19.7.2012 11:52:21
Injection Volume:	10,00 ul	Processing Method:	DOZS11
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



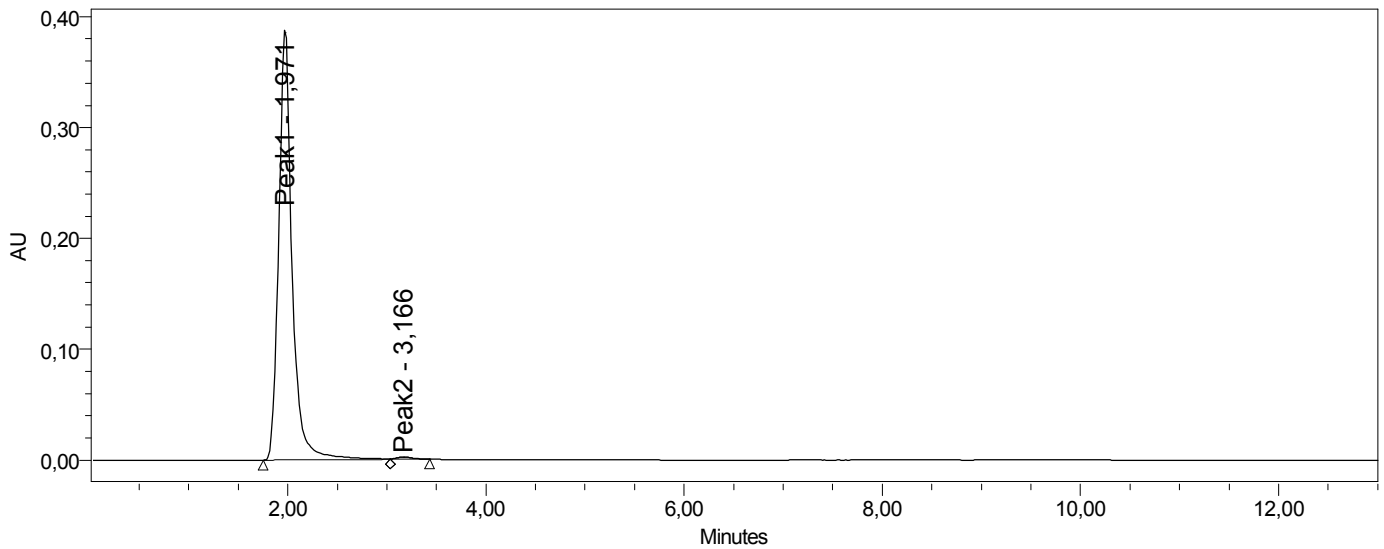
	Peak Name	RT	Area	% Area	Height
1	Peak1	1,900	10480061	98,59	1131248
2	Peak2	2,850	94128	0,89	6179
3	Peak3	3,033	55912	0,53	4825

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

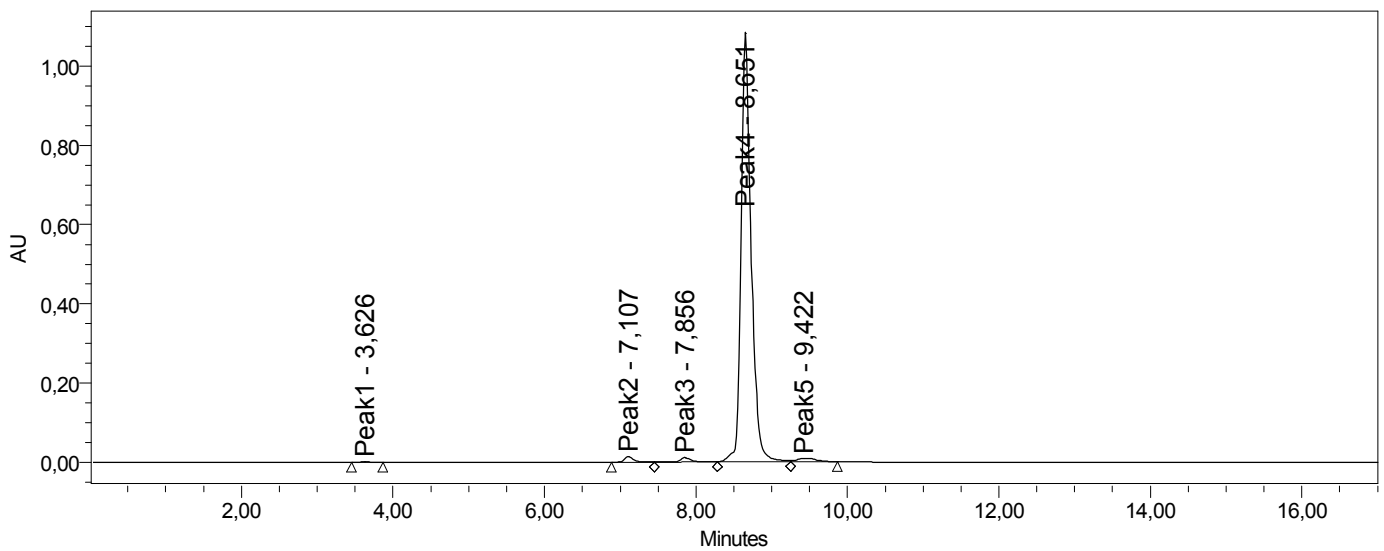
Sample Name:	DOJK06 Compound 15	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	19.7.2012 10:55:50
Vial:	1	Acq. Method Set:	10902543400513m_MS
Injection #:	1	Date Processed:	19.7.2012 11:12:06
Injection Volume:	10,00 ul	Processing Method:	DOJK06
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,971	3633586	99,39	387128
2	Peak2	3,166	22169	0,61	2037

SAMPLE INFORMATION

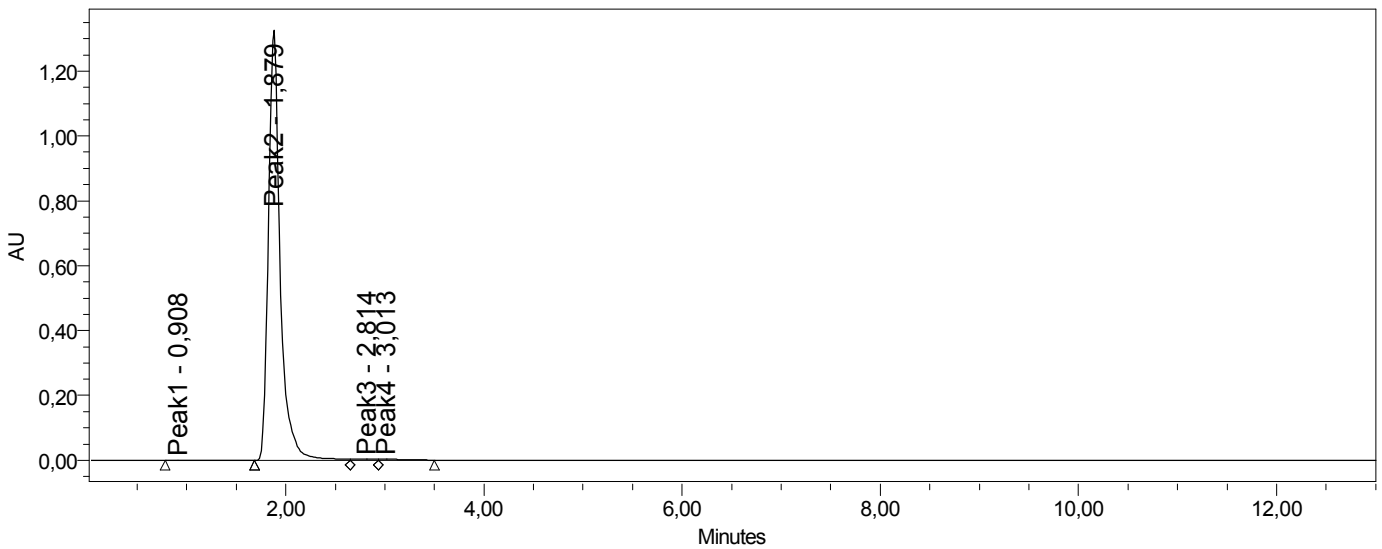
Sample Name:	DO183 Compound 16	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5.6.2012 11:07:08
Vial:	2	Acq. Method Set:	98225434005_MS
Injection #:	1	Date Processed:	5.6.2012 11:28:53
Injection Volume:	10,00 ul	Processing Method:	DO183 2
Run Time:	17,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	3,626	9572	0,09	931
2	Peak2	7,107	112946	1,08	14450
3	Peak3	7,856	120199	1,15	11172
4	Peak4	8,651	10042346	96,19	1075678
5	Peak5	9,422	155045	1,49	8483

SAMPLE INFORMATION

Sample Name:	DOZS12 Compound 18	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	19.7.2012 11:51:18
Vial:	5	Acq. Method Set:	10902543400513m_MS
Injection #:	1	Date Processed:	19.7.2012 12:21:59
Injection Volume:	10,00 ul	Processing Method:	DOZS12
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,908	6572	0,06	272
2	Peak2	1,879	10985407	99,04	1324027
3	Peak3	2,814	49573	0,45	3150
4	Peak4	3,013	50386	0,45	3601

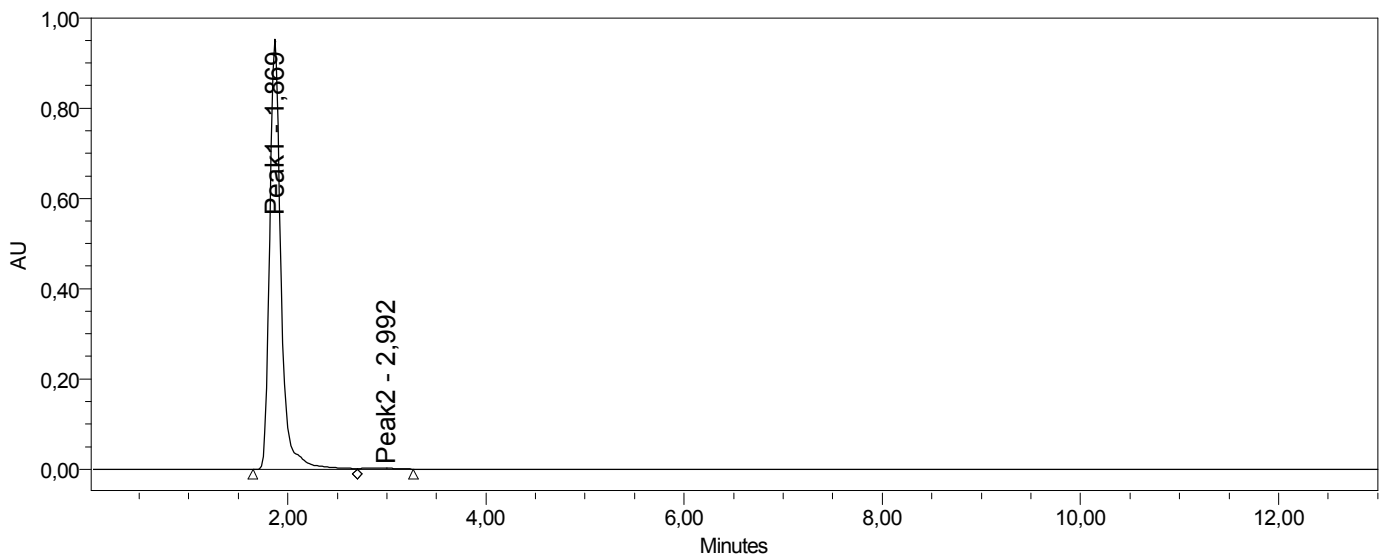


Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	DOJK07	Compound 19	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	19.7.2012 11:23:36
Vial:	3		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	19.7.2012 11:38:53
Injection Volume:	10,00 ul		Processing Method:	DOJK07
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



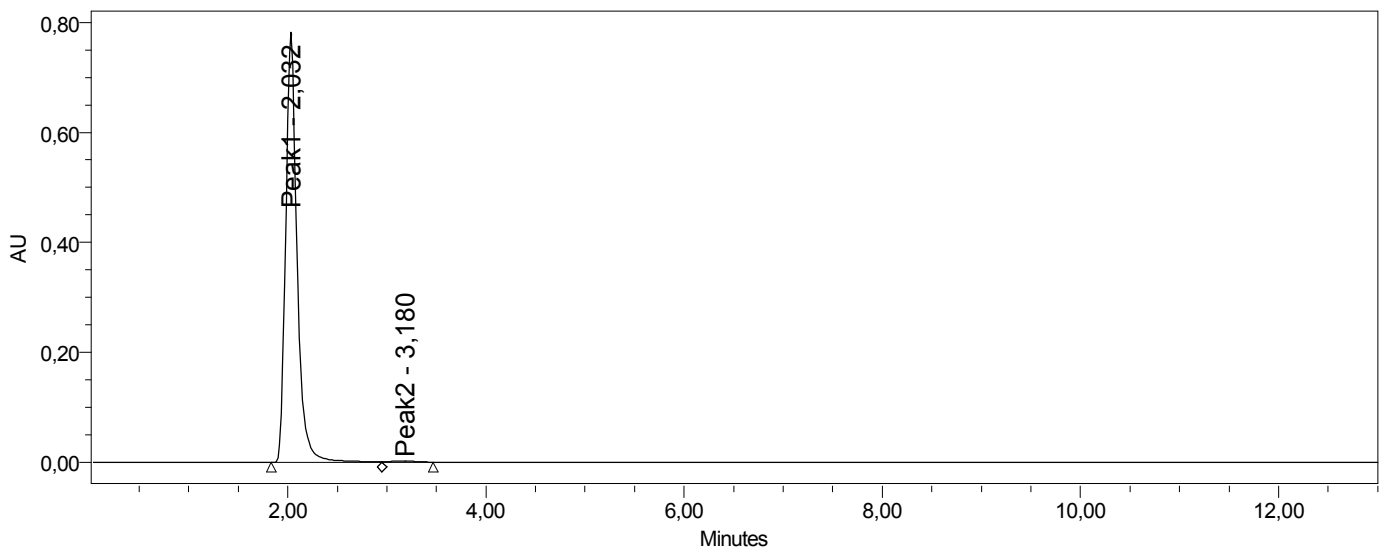
	Peak Name	RT	Area	% Area	Height
1	Peak1	1,869	7549586	99,39	948295
2	Peak2	2,992	45965	0,61	2058

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

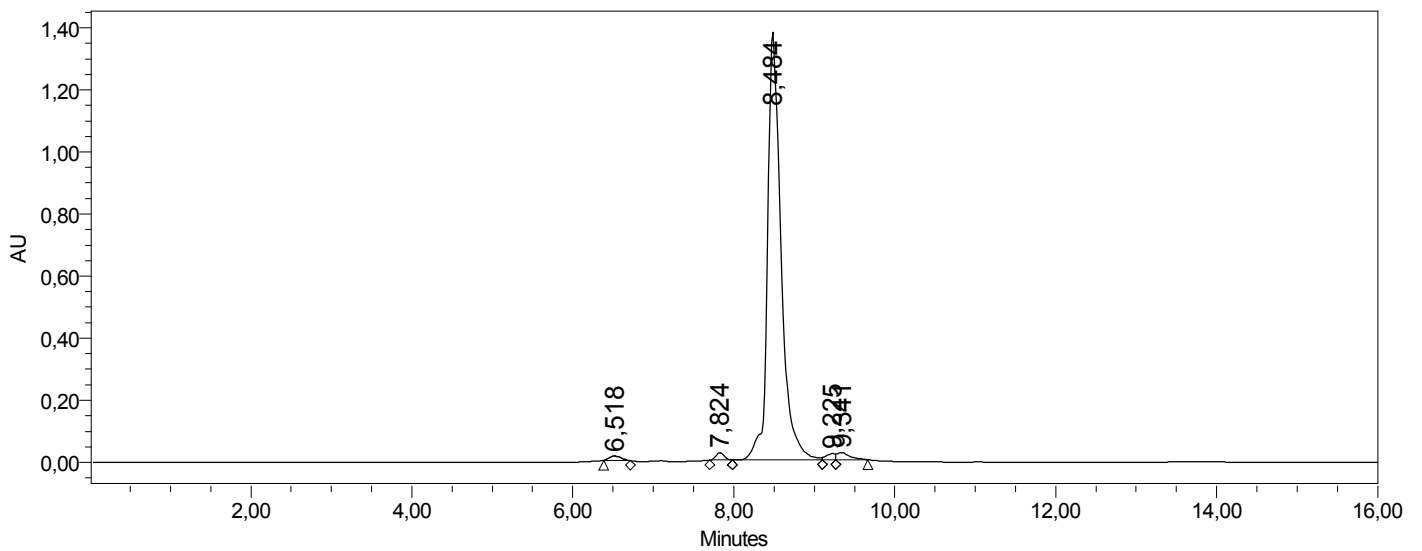
Sample Name:	DO193	Compound 21	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	18.7.2012 14:26:02
Vial:	13		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	18.7.2012 14:41:14
Injection Volume:	10,00 ul		Processing Method:	DO193
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,032	6247539	99,46	777700
2	Peak2	3,180	34076	0,54	2146

SAMPLE INFORMATION

Sample Name:	DO184	Compound 22	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	5.6.2012 12:14:01
Vial:	5		Acq. Method Set:	98225434005_MS
Injection #:	1		Date Processed:	5.6.2012 13:27:27
Injection Volume:	10,00 ul		Processing Method:	proba4rtr
Run Time:	16,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



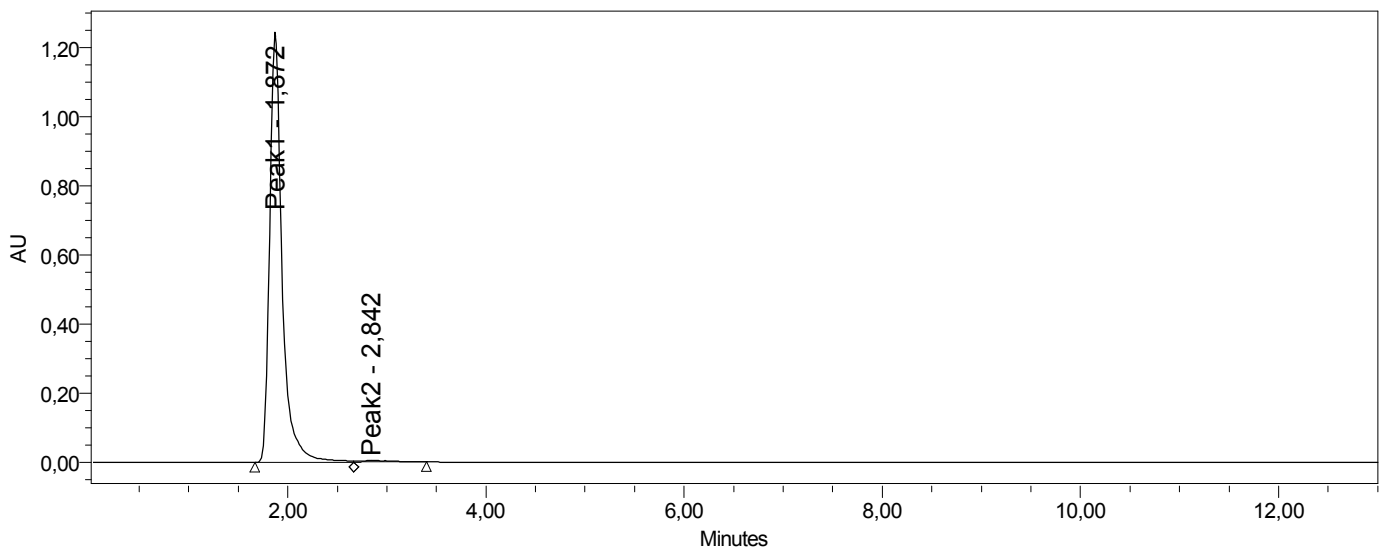
	RT	Area	% Area	Height
1	6,518	136102	0,81	13769
2	7,824	168970	1,00	24317
3	8,484	16157420	95,76	1371249
4	9,225	156009	0,92	19973
5	9,341	254034	1,51	22655

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	DOZS13 Compound 24	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	19.7.2012 12:05:11
Vial:	6	Acq. Method Set:	10902543400513m_MS
Injection #:	1	Date Processed:	19.7.2012 12:23:11
Injection Volume:	10,00 ul	Processing Method:	DOZS13
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



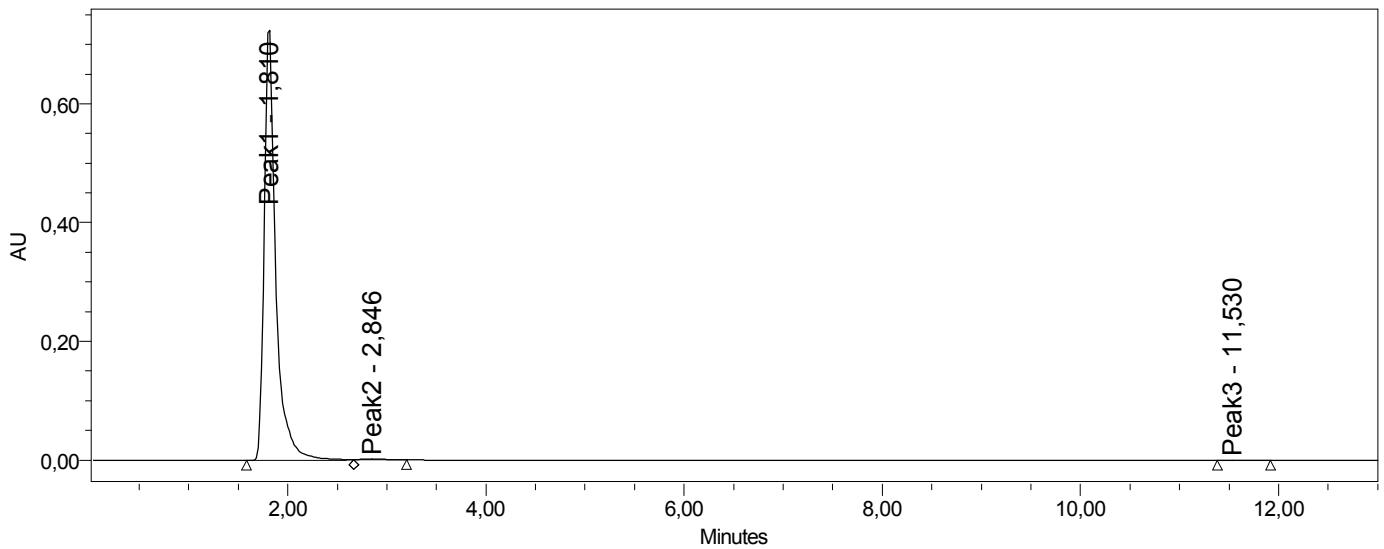
	Peak Name	RT	Area	% Area	Height
1	Peak1	1,872	10842029	99,17	1243086
2	Peak2	2,842	90494	0,83	3733

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	DOJK08	Compound 25	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	19.7.2012 11:09:47
Vial:	2		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	19.7.2012 11:24:59
Injection Volume:	10,00 ul		Processing Method:	DOJK08
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,810	5905692	99,47	725594
2	Peak2	2,846	27517	0,46	1637
3	Peak3	11,530	3833	0,06	407

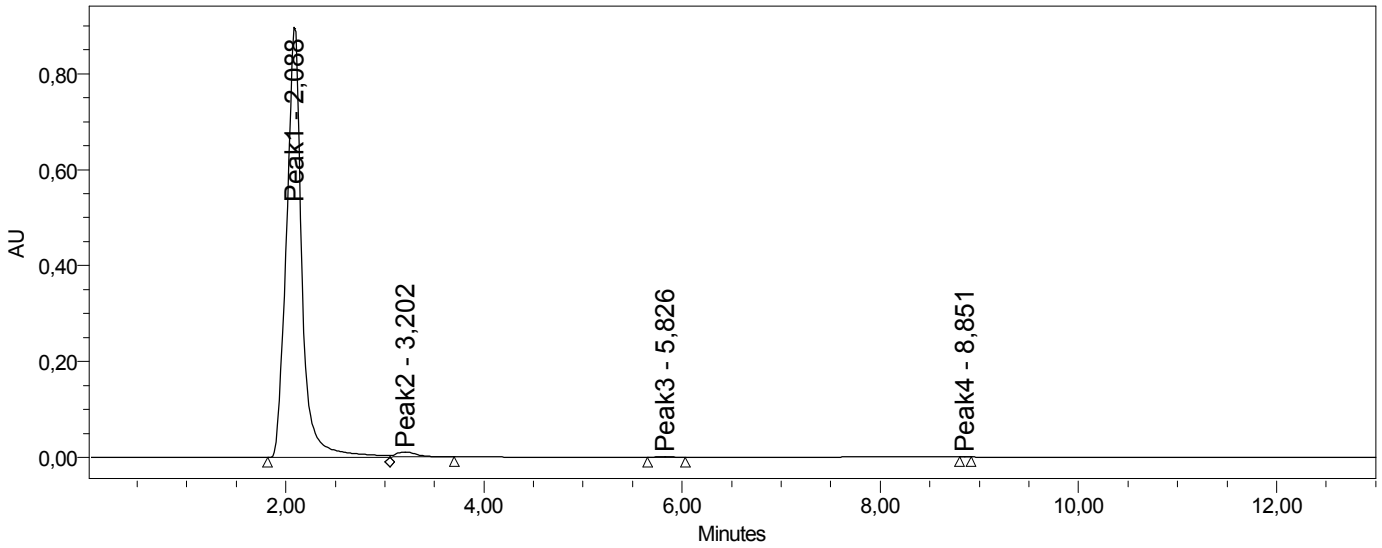


Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	DO174 Compound 36	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	18.7.2012 11:45:33
Vial:	2	Acq. Method Set:	10902543400513m_MS
Injection #:	1	Date Processed:	18.7.2012 12:00:12
Injection Volume:	10,00 ul	Processing Method:	DO174
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



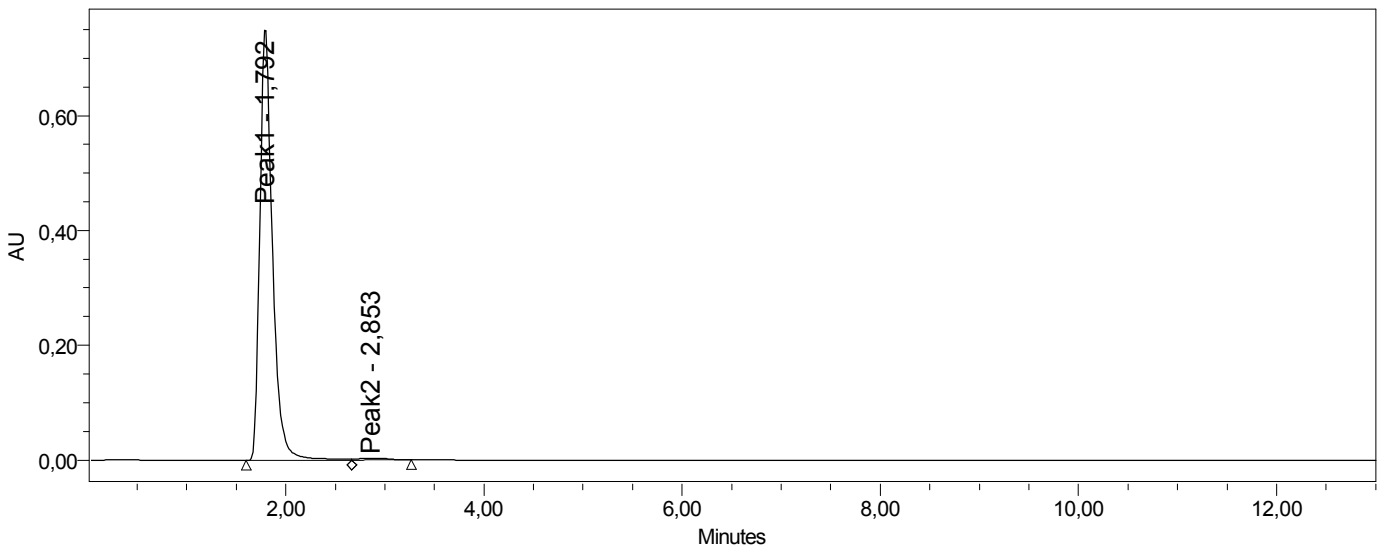
	Peak Name	RT	Area	% Area	Height
1	Peak1	2,088	9692935	98,43	896550
2	Peak2	3,202	148240	1,51	10323
3	Peak3	5,826	5674	0,06	501
4	Peak4	8,851	928	0,01	331

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	DO194	Compound 37	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	18.7.2012 12:17:23
Vial:	4		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	18.7.2012 12:32:47
Injection Volume:	10,00 ul		Processing Method:	DO194
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



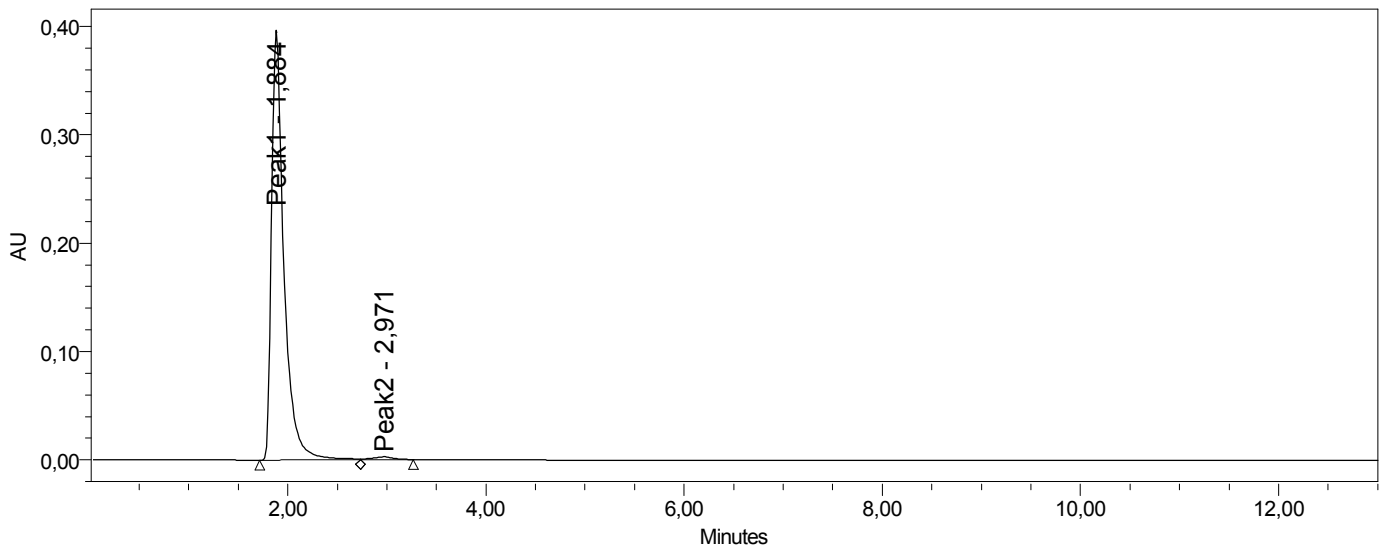
	Peak Name	RT	Area	% Area	Height
1	Peak1	1,792	6673440	99,09	755512
2	Peak2	2,853	61429	0,91	3057

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	DO195	Compound 38	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	18.7.2012 12:45:01
Vial:	6		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	18.7.2012 13:00:17
Injection Volume:	10,00 ul		Processing Method:	DO195
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,884	3446210	98,92	395282
2	Peak2	2,971	37663	1,08	2613

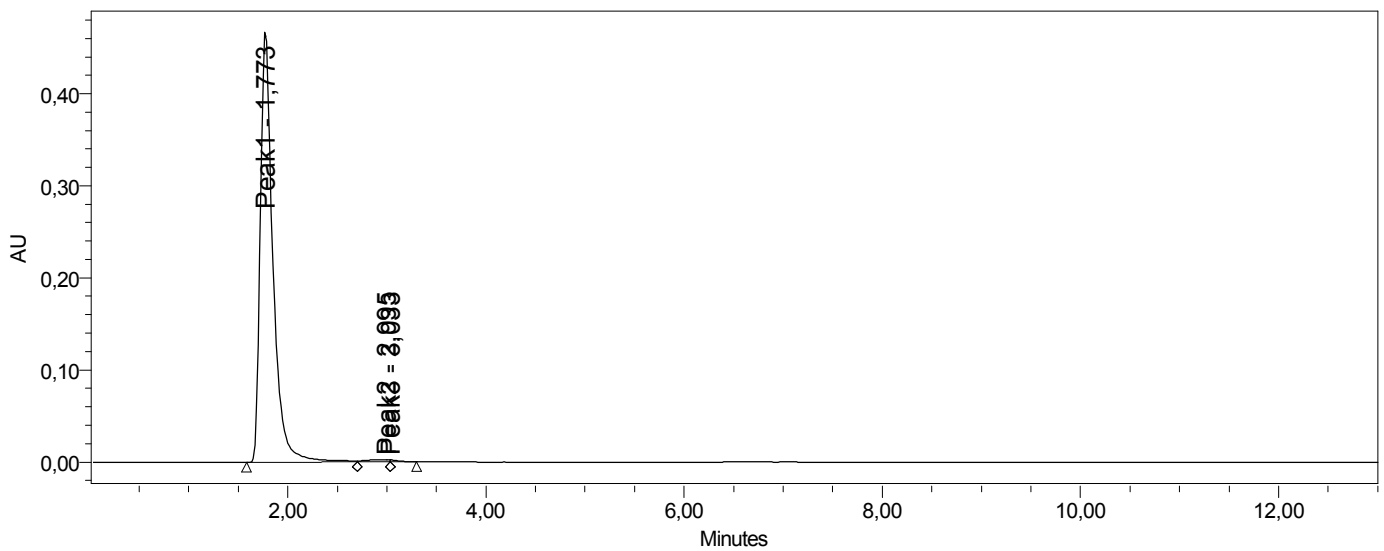


Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	DO196	Compound 39	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	18.7.2012 13:13:54
Vial:	8		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	18.7.2012 13:29:01
Injection Volume:	10,00 ul		Processing Method:	DO196
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



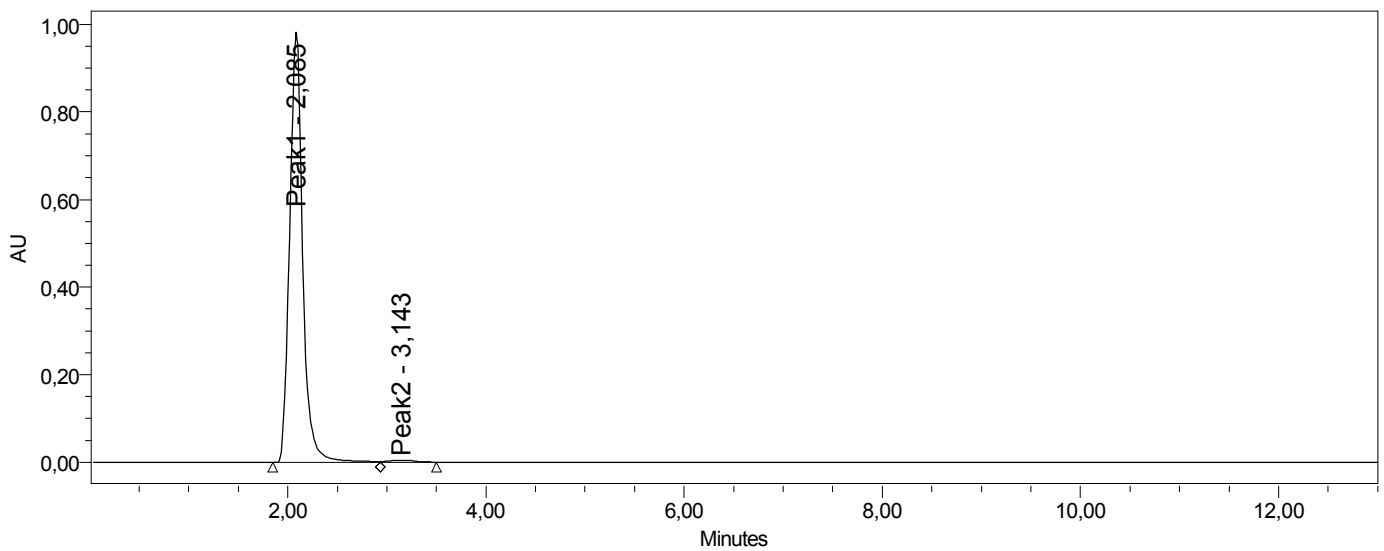
	Peak Name	RT	Area	% Area	Height
1	Peak1	1,773	4160601	98,86	468149
2	Peak2	2,995	37246	0,88	2336
3	Peak3	3,033	10807	0,26	2117

Reported by User: System

Project Name: Organskajedinjenja

## SAMPLE INFORMATION

Sample Name:	DO179 Compound 40	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	18.7.2012 12:02:53
Vial:	3	Acq. Method Set:	10902543400513m_MS
Injection #:	1	Date Processed:	18.7.2012 12:18:41
Injection Volume:	10,00 ul	Processing Method:	DO179
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



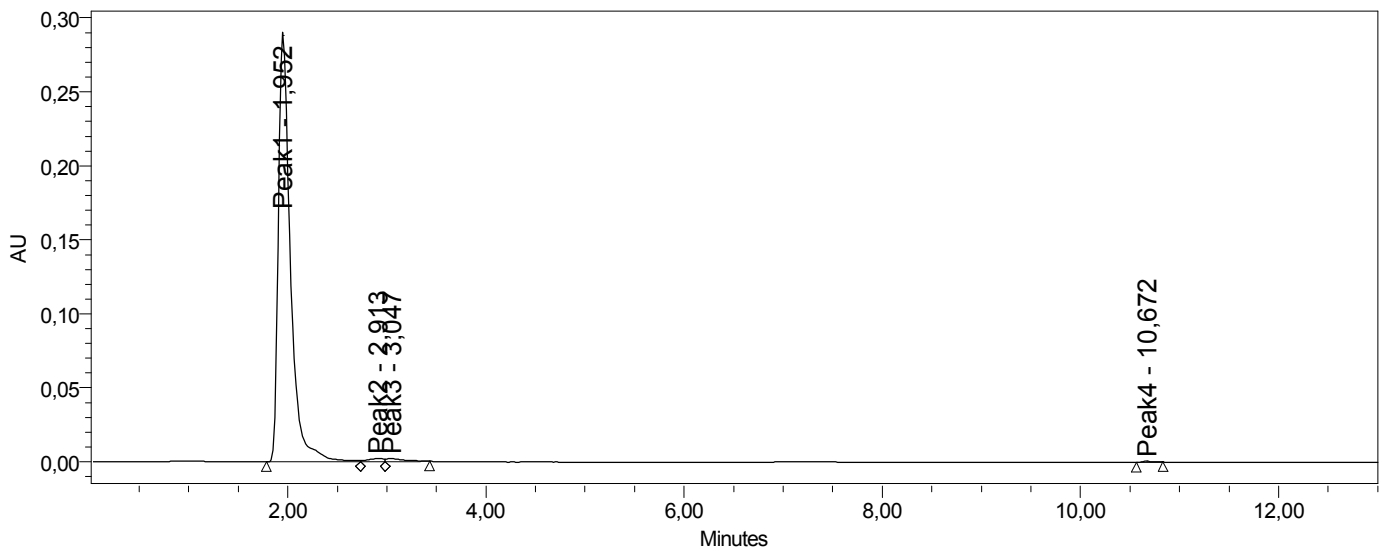
	Peak Name	RT	Area	% Area	Height
1	Peak1	2,085	8971779	99,22	978169
2	Peak2	3,143	70514	0,78	3959

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	DO191	Compound 41	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	18.7.2012 12:31:11
Vial:	5		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	18.7.2012 12:46:25
Injection Volume:	10,00 ul		Processing Method:	DO191
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



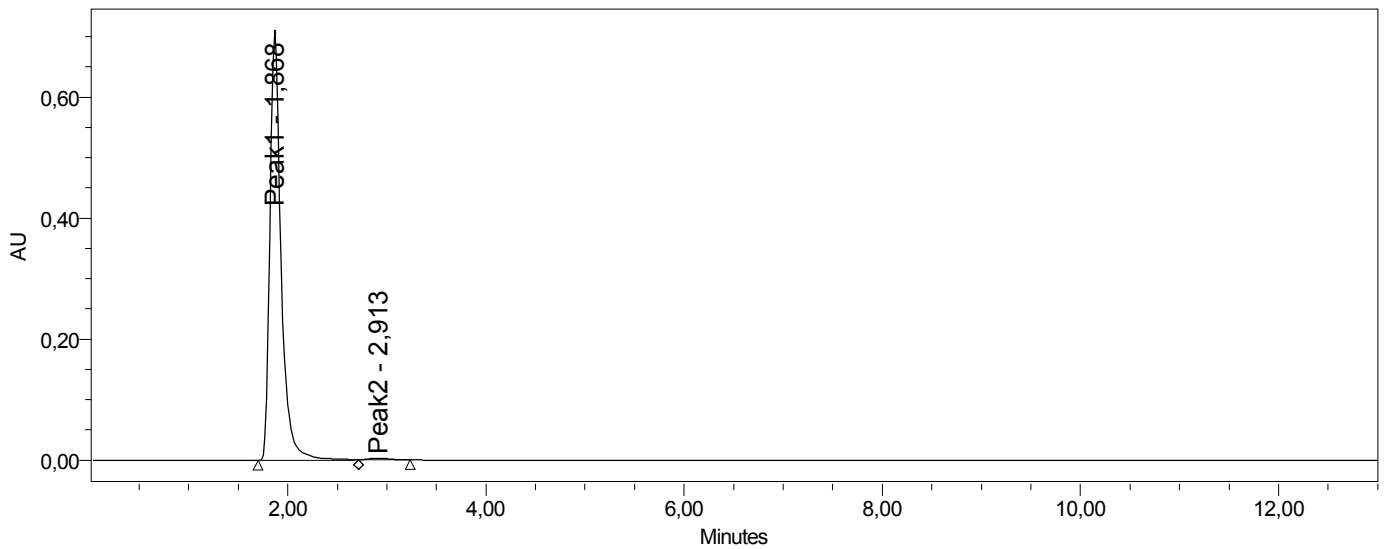
	Peak Name	RT	Area	% Area	Height
1	Peak1	1,952	2469475	98,07	289267
2	Peak2	2,913	21184	0,84	1876
3	Peak3	3,047	23458	0,93	1833
4	Peak4	10,672	4055	0,16	620

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	DO197	Compound 42	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	18.7.2012 12:58:57
Vial:	7		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	18.7.2012 13:14:53
Injection Volume:	10,00 ul		Processing Method:	DO197
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



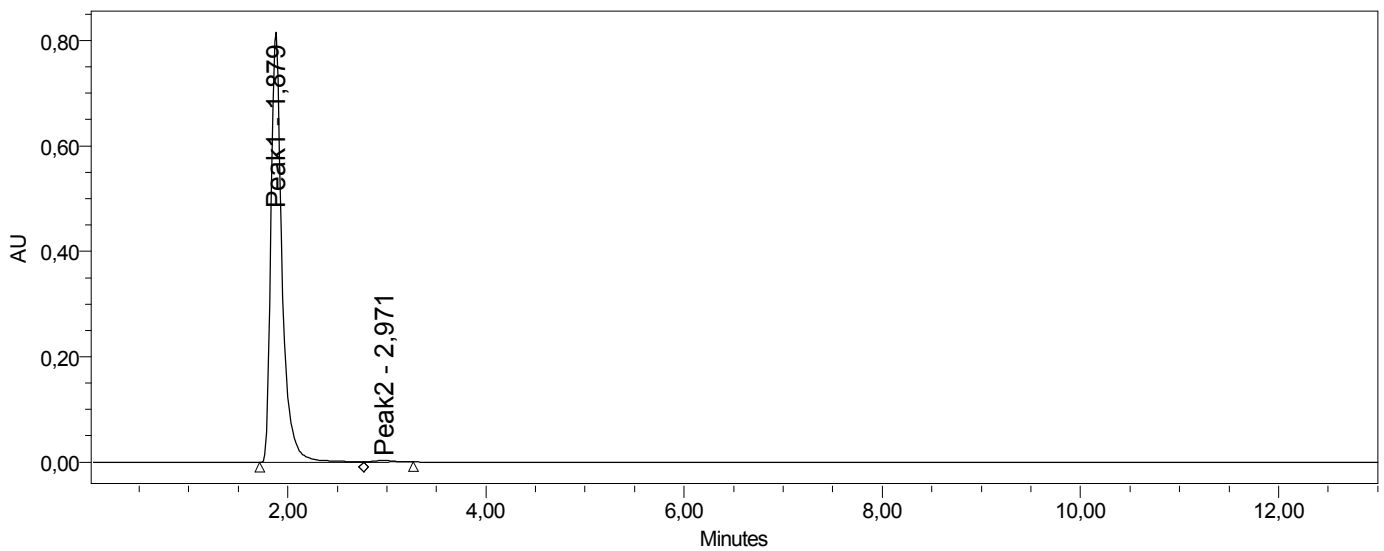
	Peak Name	RT	Area	% Area	Height
1	Peak1	1,868	5571036	99,31	706487
2	Peak2	2,913	38854	0,69	2378

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

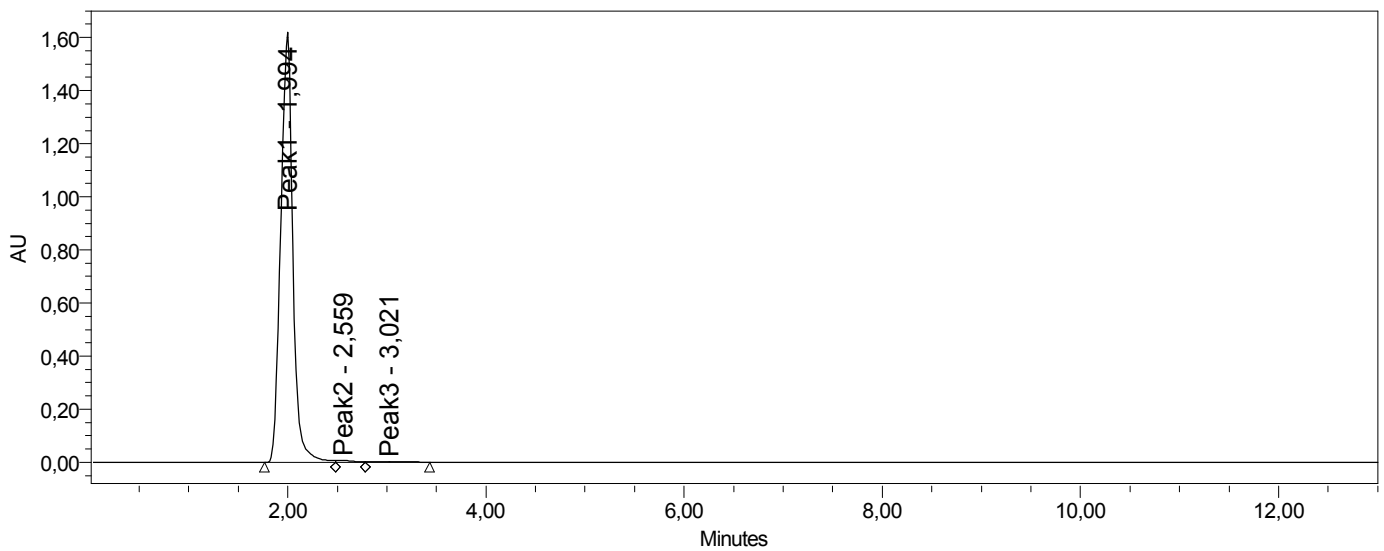
Sample Name:	DO199 Compound 43	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	18.7.2012 13:27:44
Vial:	9	Acq. Method Set:	10902543400513m_MS
Injection #:	1	Date Processed:	18.7.2012 13:42:47
Injection Volume:	10,00 ul	Processing Method:	DO199
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,879	6377676	99,37	814645
2	Peak2	2,971	40401	0,63	3137

SAMPLE INFORMATION

Sample Name:	ST11	Compound 44	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	18.7.2012 13:41:34
Vial:	10		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	18.7.2012 13:56:46
Injection Volume:	10,00 ul		Processing Method:	ST11
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



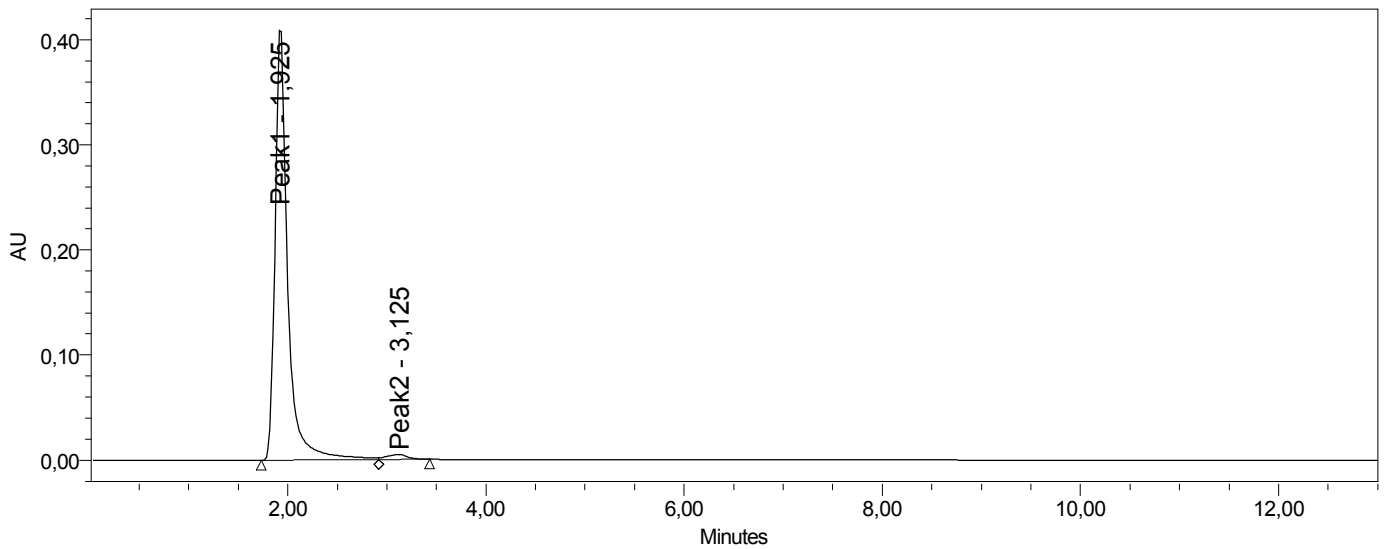
	Peak Name	RT	Area	% Area	Height
1	Peak1	1,994	13768996	99,12	1618399
2	Peak2	2,559	74020	0,53	6674
3	Peak3	3,021	48607	0,35	2175

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

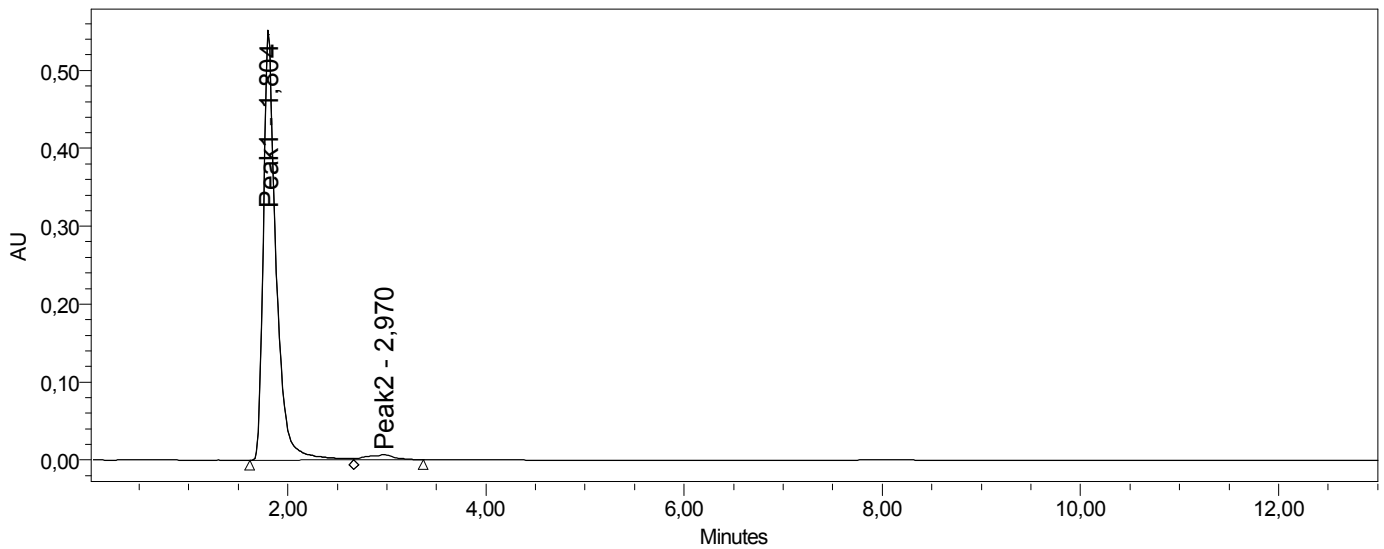
Sample Name:	MV78 Compound 50	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	19.7.2012 14:28:45
Vial:	18	Acq. Method Set:	10902543400513m_MS
Injection #:	1	Date Processed:	19.7.2012 14:45:14
Injection Volume:	10,00 ul	Processing Method:	MV78
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,925	3625124	98,15	411540
2	Peak2	3,125	68261	1,85	4922

SAMPLE INFORMATION

Sample Name:	MV61	Compound 51	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	18.7.2012 14:40:13
Vial:	14		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	18.7.2012 14:55:42
Injection Volume:	10,00 ul		Processing Method:	MV61
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,804	4925314	97,63	550272
2	Peak2	2,970	119351	2,37	6371

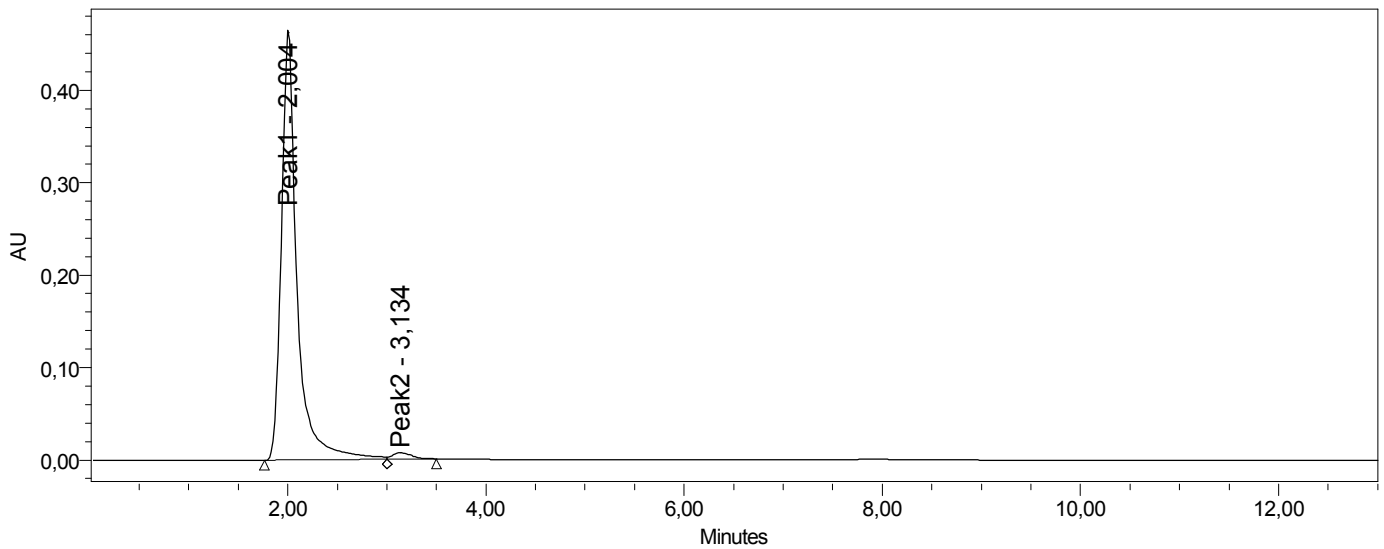


Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

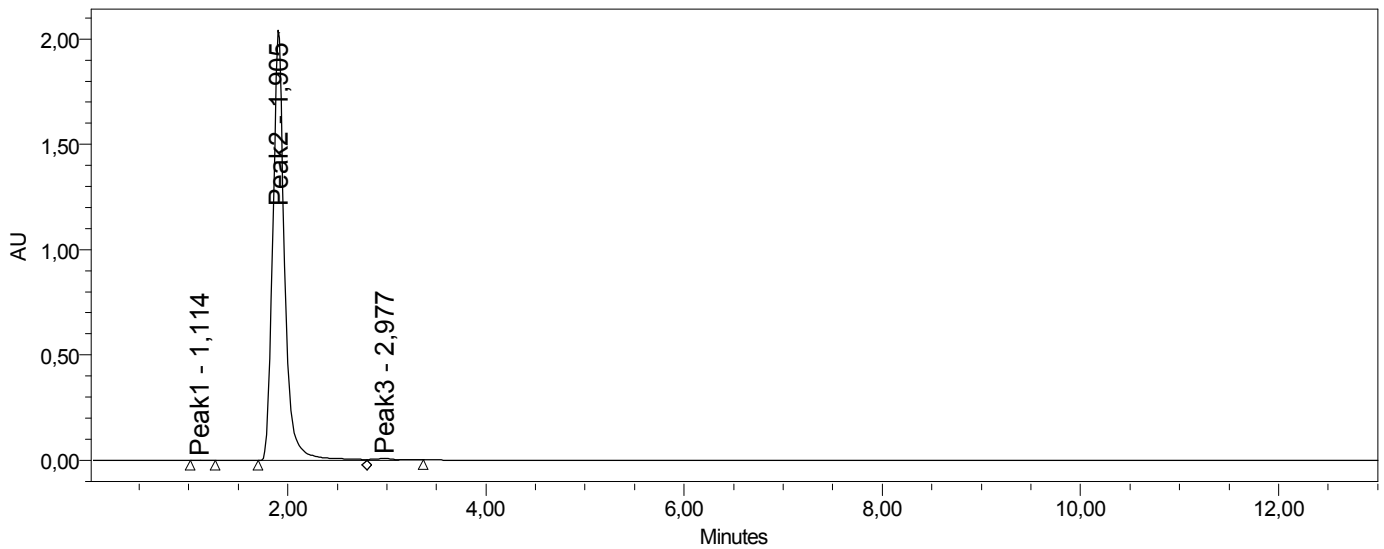
Sample Name:	DO181	Compound 52	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	26.7.2012 11:50:45
Vial:	2		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	26.7.2012 12:11:51
Injection Volume:	10,00 ul		Processing Method:	DO181
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,004	5081751	98,23	464041
2	Peak2	3,134	91549	1,77	6875

SAMPLE INFORMATION

Sample Name:	ST13	Compound 54	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	18.7.2012 13:55:19
Vial:	11		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	18.7.2012 14:27:55
Injection Volume:	10,00 ul		Processing Method:	ST13
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



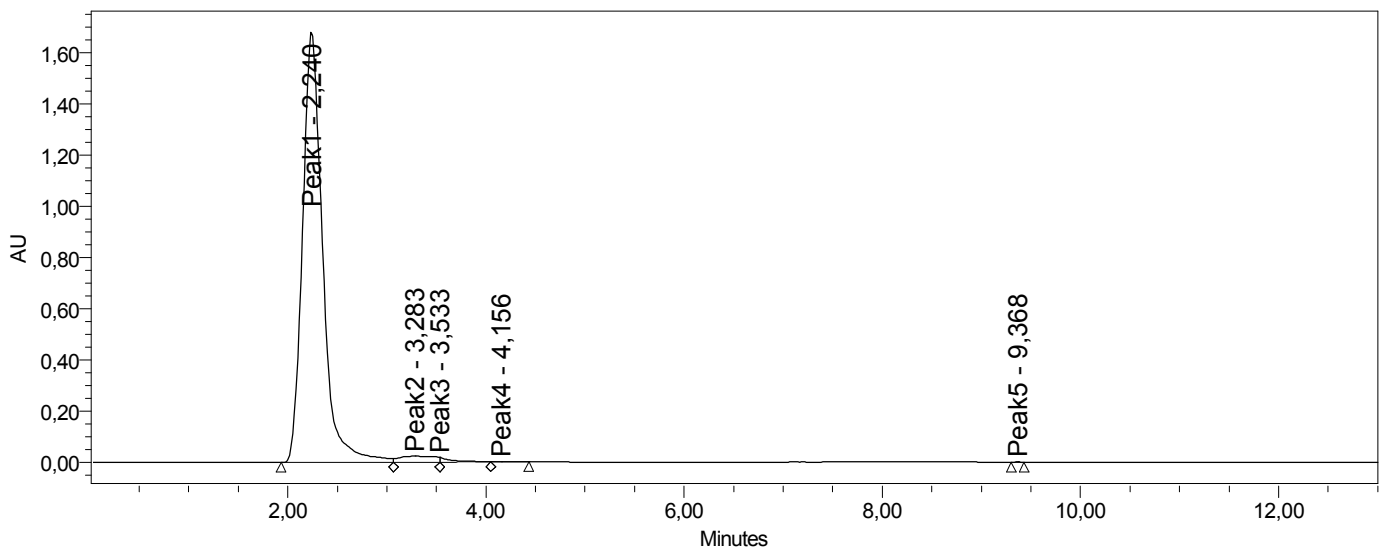
	Peak Name	RT	Area	% Area	Height
1	Peak1	1,114	2682	0,02	389
2	Peak2	1,905	16841376	99,44	2040094
3	Peak3	2,977	92952	0,55	7056

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	MV29	Compound 55	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	17.8.2012 13:24:21
Vial:	14		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	17.8.2012 13:38:46
Injection Volume:	10,00 ul		Processing Method:	MV29
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



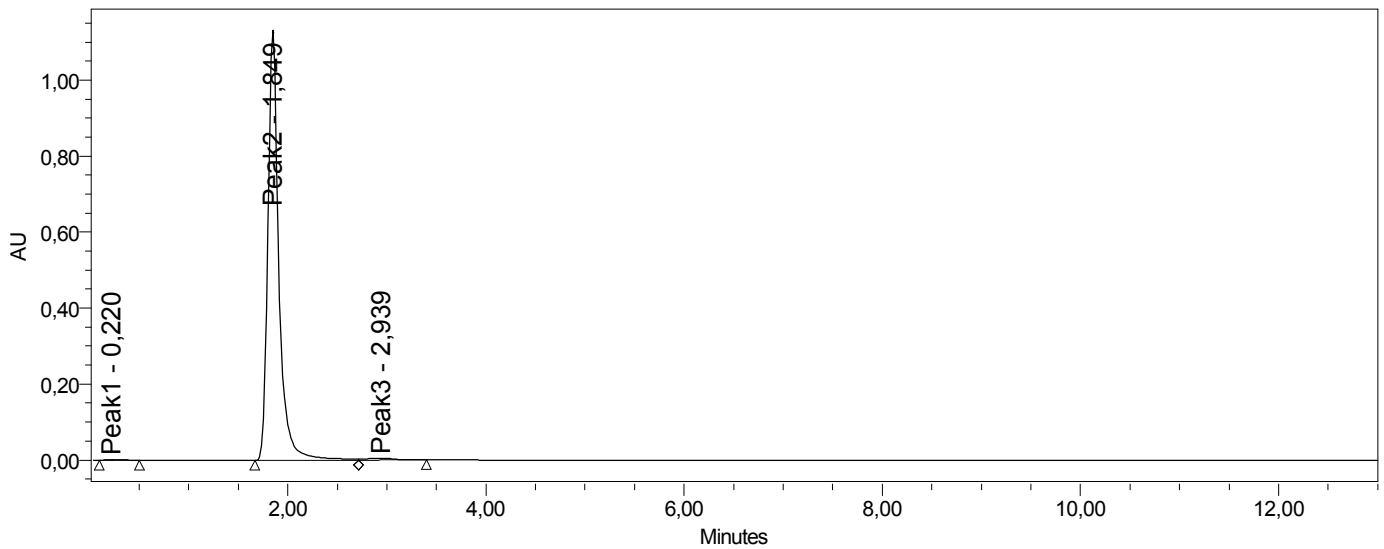
	Peak Name	RT	Area	% Area	Height
1	Peak1	2,240	23588920	96,94	1682321
2	Peak2	3,283	572035	2,35	23420
3	Peak3	3,533	149199	0,61	17852
4	Peak4	4,156	19466	0,08	1481
5	Peak5	9,368	4506	0,02	1650

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	ST14 Compound 56	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	18.7.2012 14:09:13
Vial:	12	Acq. Method Set:	10902543400513m_MS
Injection #:	1	Date Processed:	18.7.2012 14:29:31
Injection Volume:	10,00 ul	Processing Method:	ST14
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



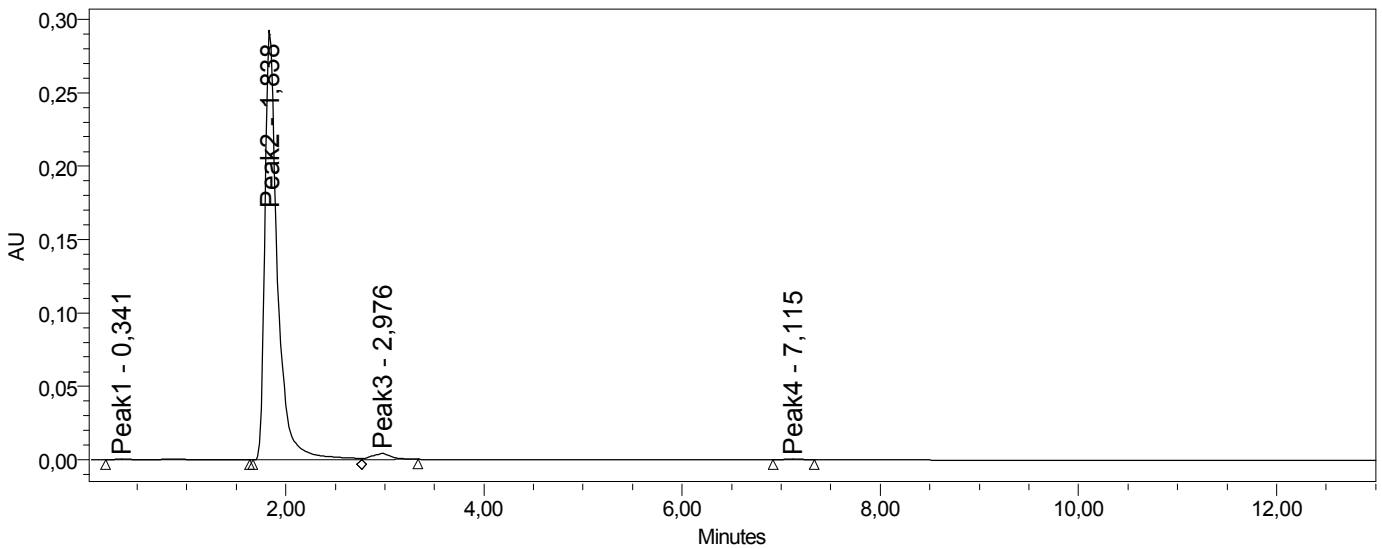
	Peak Name	RT	Area	% Area	Height
1	Peak1	0,220	13715	0,16	1463
2	Peak2	1,849	8707139	98,82	1121724
3	Peak3	2,939	89964	1,02	5042

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

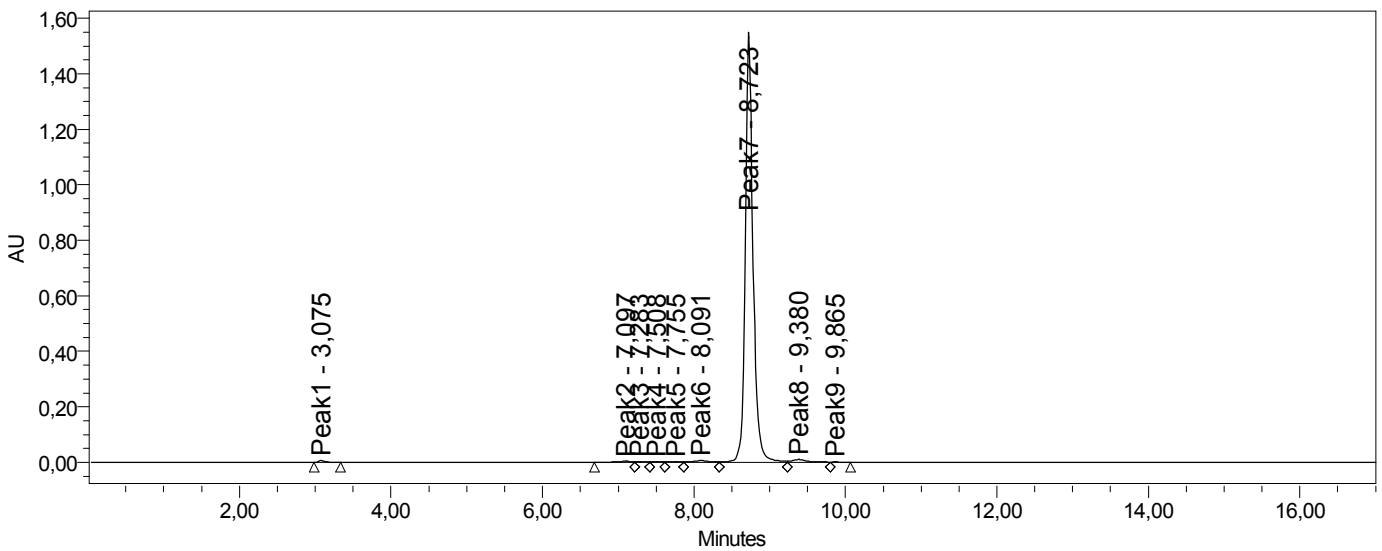
Sample Name:	DO180 Compound 60	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	18.7.2012 14:54:03
Vial:	15	Acq. Method Set:	10902543400513m_MS
Injection #:	1	Date Processed:	18.7.2012 15:09:12
Injection Volume:	10,00 ul	Processing Method:	DO180
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,341	15198	0,57	398
2	Peak2	1,838	2593563	97,10	292198
3	Peak3	2,976	55470	2,08	4070
4	Peak4	7,115	6766	0,25	595

SAMPLE INFORMATION

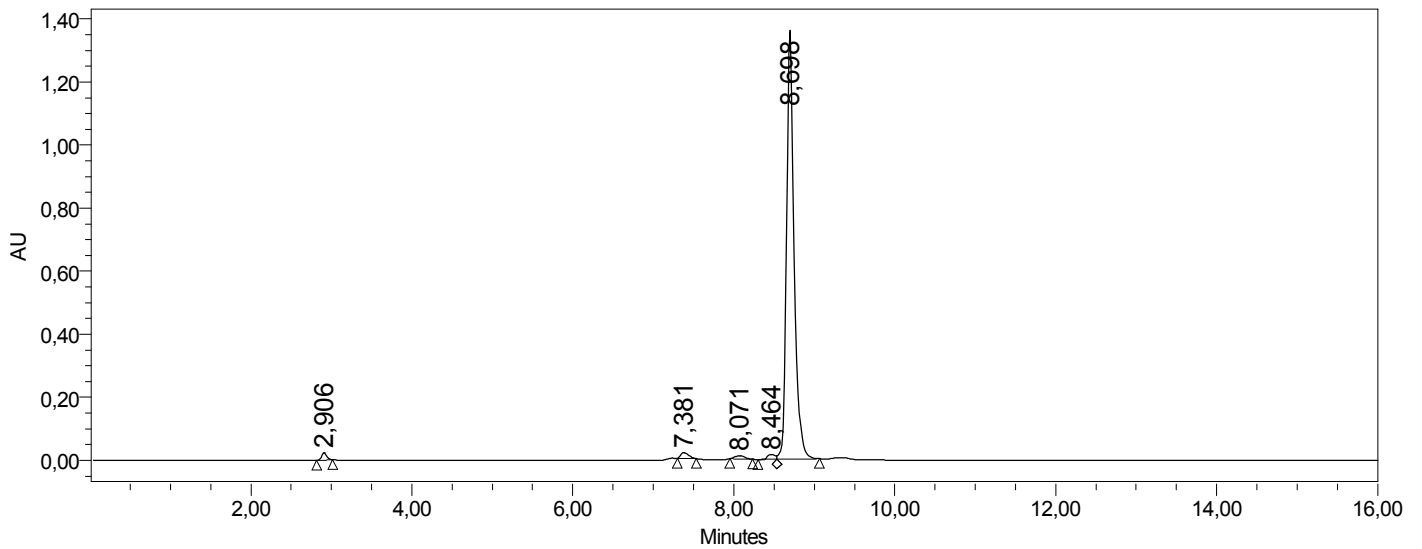
Sample Name:	DO152 6 Compound 12	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	23.5.2012 15:47:45
Vial:	10	Acq. Method Set:	98225434005_MS
Injection #:	1	Date Processed:	9.7.2012 13:20:04
Injection Volume:	10,00 ul	Processing Method:	DO152 10
Run Time:	17,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	3,075	35790	0,31	5733
2	Peak2	7,097	50713	0,43	4047
3	Peak3	7,283	19393	0,17	1991
4	Peak4	7,508	17530	0,15	1693
5	Peak5	7,755	20545	0,18	1582
6	Peak6	8,091	85555	0,73	5876
7	Peak7	8,723	11308508	96,87	1546669
8	Peak8	9,380	129209	1,11	9796
9	Peak9	9,865	6393	0,05	782

SAMPLE INFORMATION

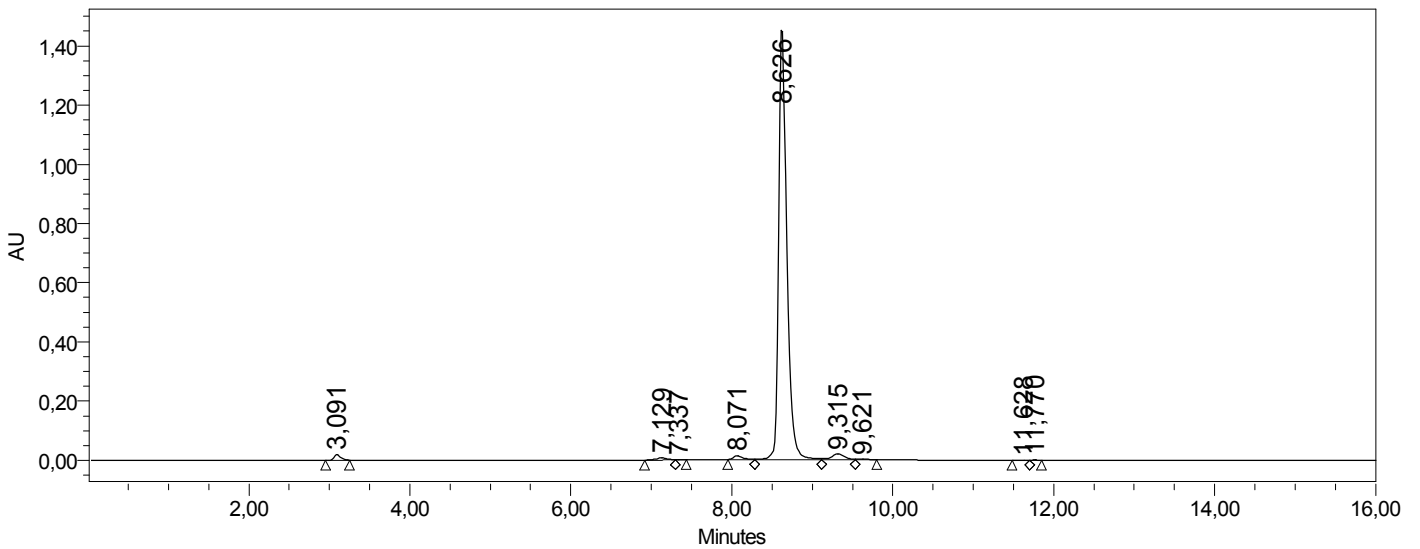
Sample Name:	DR06 Compound 13	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	9.7.2012 13:33:29
Vial:	8	Acq. Method Set:	98225434005_MS
Injection #:	1	Date Processed:	9.7.2012 13:57:51
Injection Volume:	10,00 ul	Processing Method:	DR06 8
Run Time:	16,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	RT	Area	% Area	Height
1	2,906	103254	1,12	22809
2	7,381	123863	1,35	18673
3	8,071	87062	0,95	10796
4	8,464	102613	1,12	15942
5	8,698	8763478	95,46	1347666

SAMPLE INFORMATION

Sample Name:	DO183	Compound 16	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	9.7.2012 11:41:35
Vial:	2		Acq. Method Set:	98225434005_MS
Injection #:	1		Date Processed:	9.7.2012 12:08:43
Injection Volume:	10,00 ul		Processing Method:	DO183 2
Run Time:	16,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	

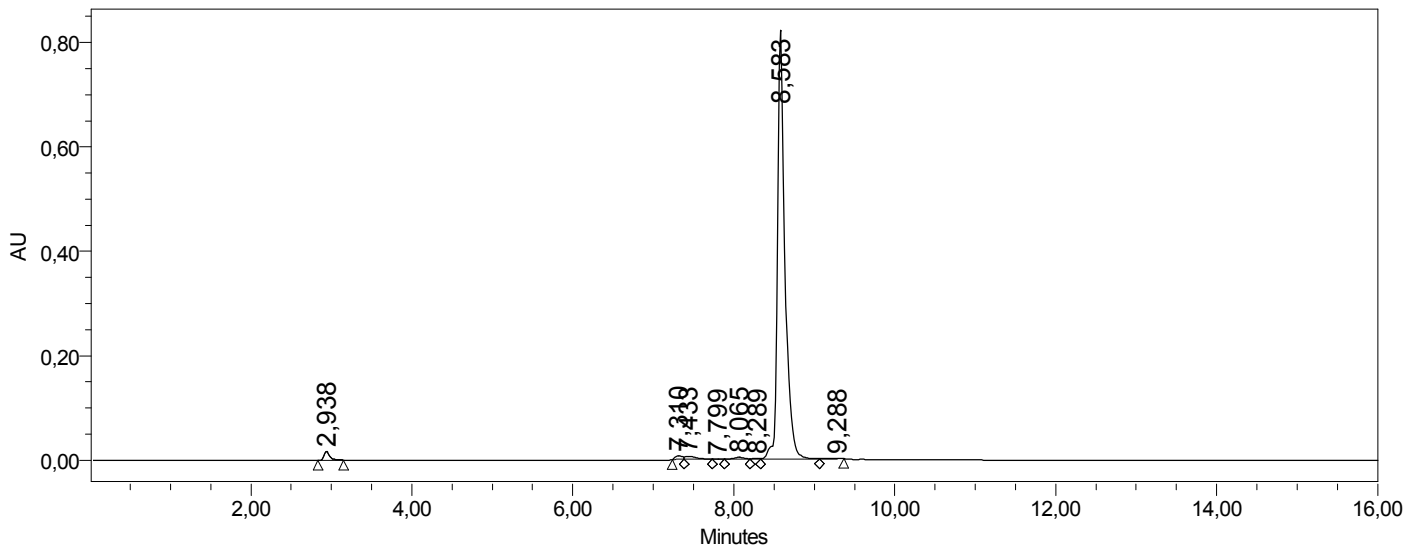


	RT	Area	% Area	Height
1	3,091	109050	1,02	19219
2	7,129	72970	0,68	8040
3	7,337	6525	0,06	1407
4	8,071	93936	0,88	12458
5	8,626	10133114	95,11	1466196
6	9,315	211542	1,99	19259
7	9,621	19960	0,19	2303
8	11,628	3066	0,03	378
9	11,770	3986	0,04	1008



SAMPLE INFORMATION

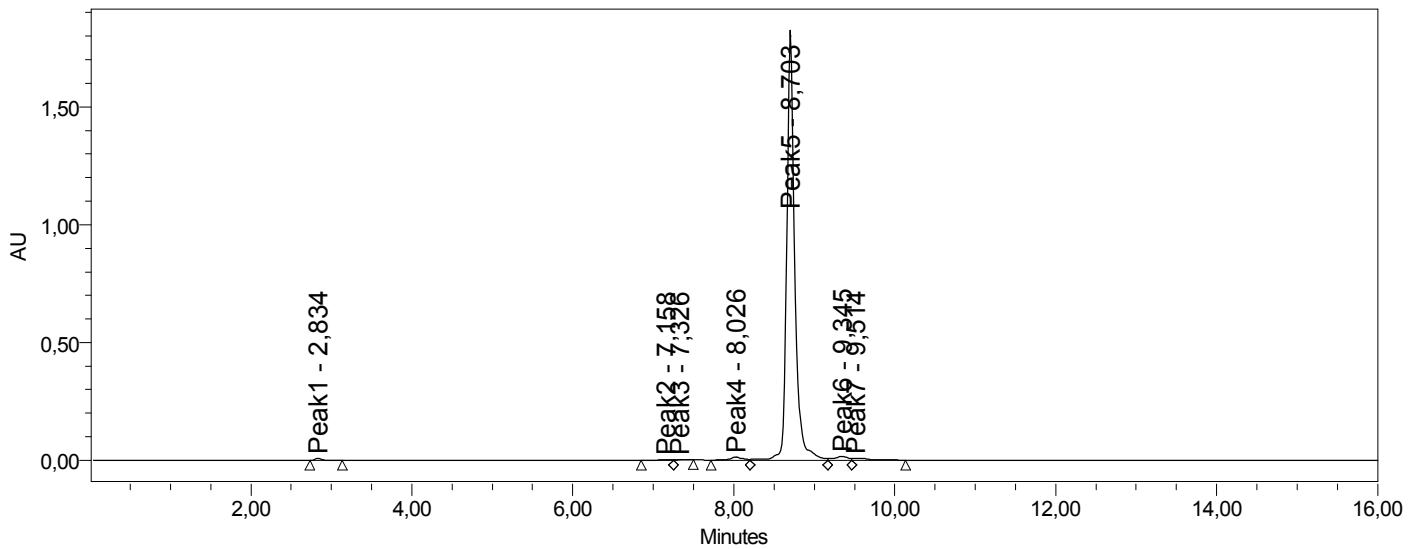
Sample Name:	DR07	Compound 17	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	10.7.2012 10:58:51
Vial:	1		Acq. Method Set:	98225434005_MS
Injection #:	1		Date Processed:	10.7.2012 11:16:50
Injection Volume:	10,00 ul		Processing Method:	DR07
Run Time:	16,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



	RT	Area	% Area	Height
1	2,938	85244	1,52	16912
2	7,310	44674	0,80	7242
3	7,433	58121	1,04	5810
4	7,799	988	0,02	199
5	8,065	29315	0,52	3413
6	8,289	9291	0,17	1746
7	8,583	5353520	95,71	810755
8	9,288	12465	0,22	1433

SAMPLE INFORMATION

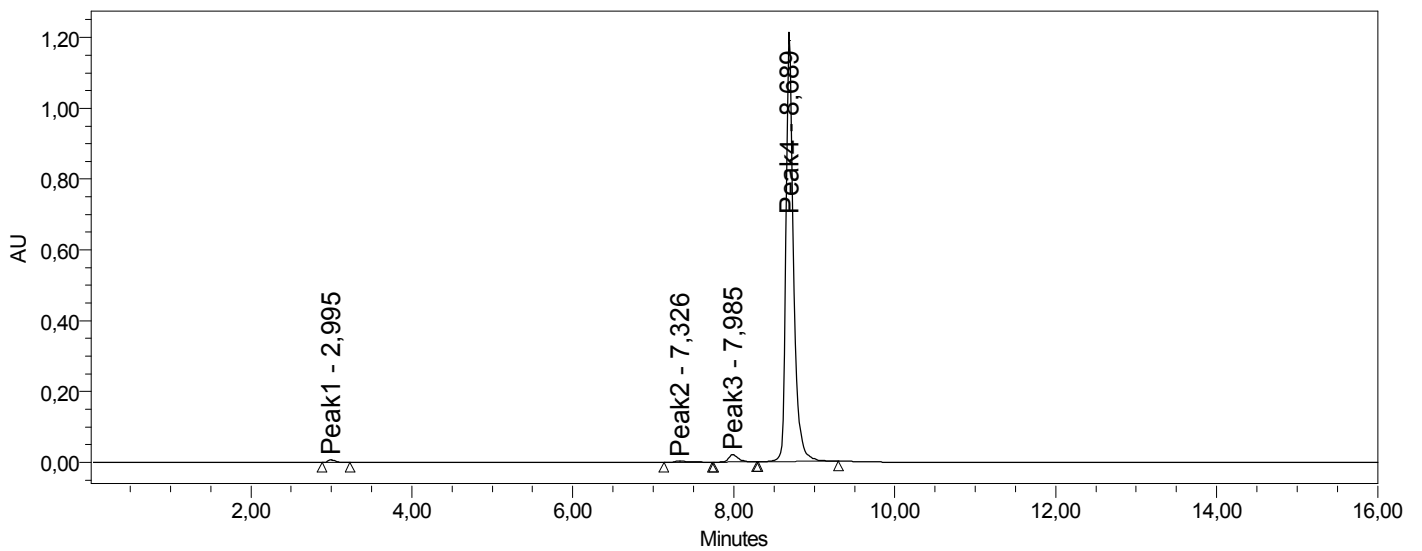
Sample Name:	DO186	Compound 20	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	10.7.2012 14:55:44
Vial:	12		Acq. Method Set:	98225434005_MS
Injection #:	1		Date Processed:	10.7.2012 15:15:03
Injection Volume:	10,00 ul		Processing Method:	DO186
Run Time:	16,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,834	47150	0,36	8747
2	Peak2	7,158	20178	0,16	2104
3	Peak3	7,326	15664	0,12	2069
4	Peak4	8,026	125759	0,97	13255
5	Peak5	8,703	12449570	96,21	1803552
6	Peak6	9,345	178880	1,38	15269
7	Peak7	9,514	102965	0,80	6955

SAMPLE INFORMATION

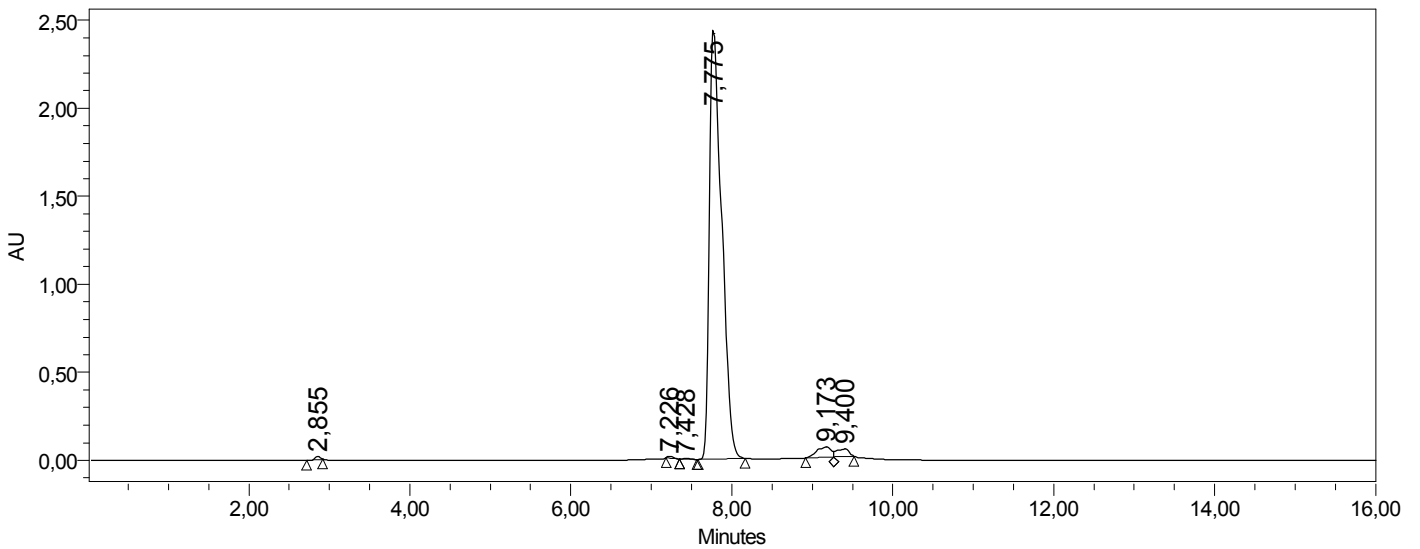
Sample Name:	DO193	Compound 21	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	10.7.2012 15:34:31
Vial:	14		Acq. Method Set:	98225434005_MS
Injection #:	1		Date Processed:	10.7.2012 15:52:12
Injection Volume:	10,00 ul		Processing Method:	DO193
Run Time:	16,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,995	41857	0,52	7322
2	Peak2	7,326	36546	0,46	3048
3	Peak3	7,985	167544	2,10	21556
4	Peak4	8,689	7750627	96,92	1204189

SAMPLE INFORMATION

Sample Name:	DO184	Compound 22	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	9.7.2012 12:17:50
Vial:	4		Acq. Method Set:	98225434005_MS
Injection #:	1		Date Processed:	9.7.2012 13:06:45
Injection Volume:	10,00 ul		Processing Method:	DO184 4
Run Time:	16,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



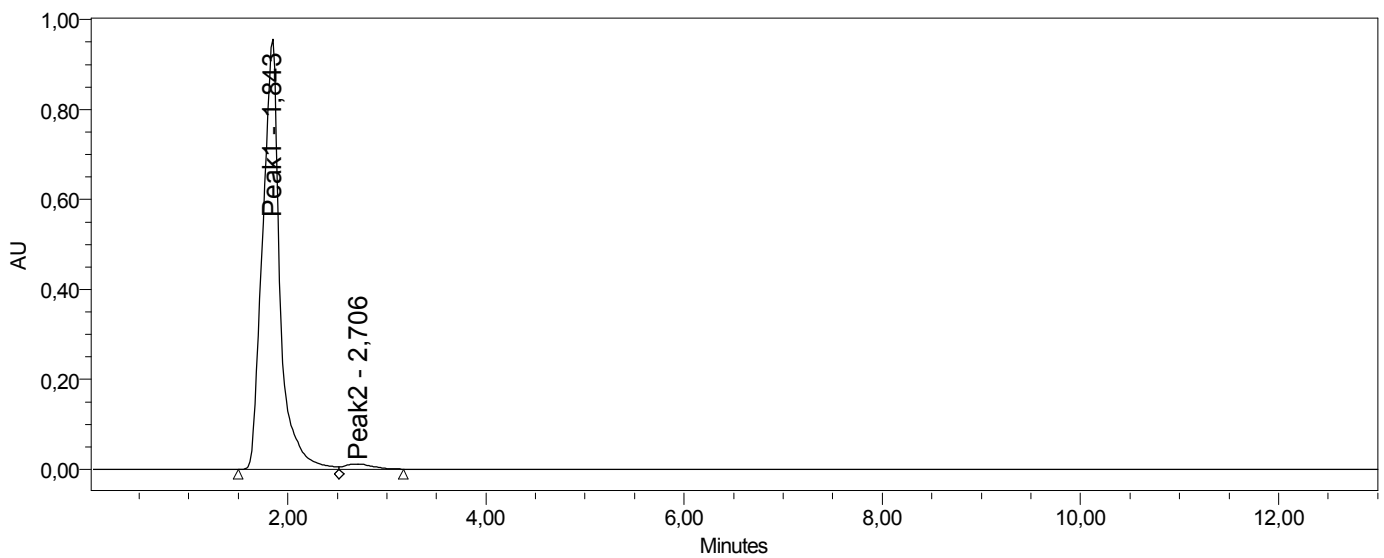
	RT	Area	% Area	Height
1	2,855	78731	0,29	19420
2	7,226	47556	0,18	10140
3	7,428	25503	0,09	4210
4	7,775	25737693	95,05	2457603
5	9,173	720071	2,66	57546
6	9,400	469672	1,73	42467

Reported by User: System

Project Name: Organskajedinjenja

**SAMPLE INFORMATION**

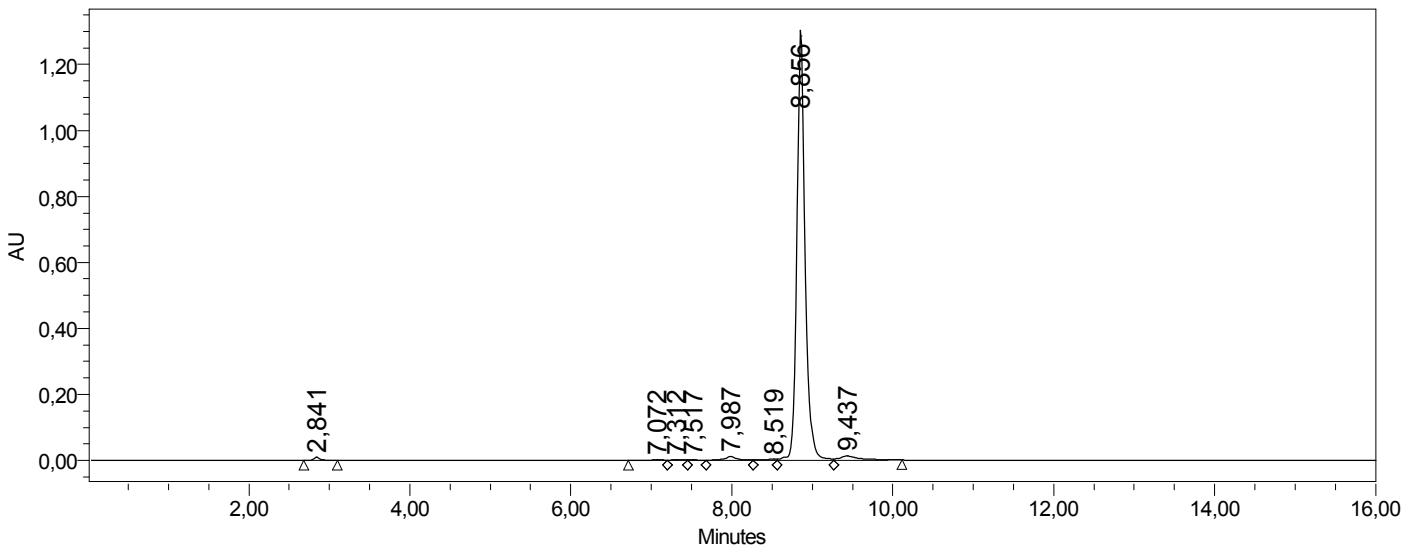
Sample Name:	DO196	<b>Compound 39</b>	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	11.7.2012 13:23:10
Vial:	9		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	11.7.2012 13:49:49
Injection Volume:	10,00 ul		Processing Method:	Do196
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,843	11643932	98,21	958195
2	Peak2	2,706	212803	1,79	11120

SAMPLE INFORMATION

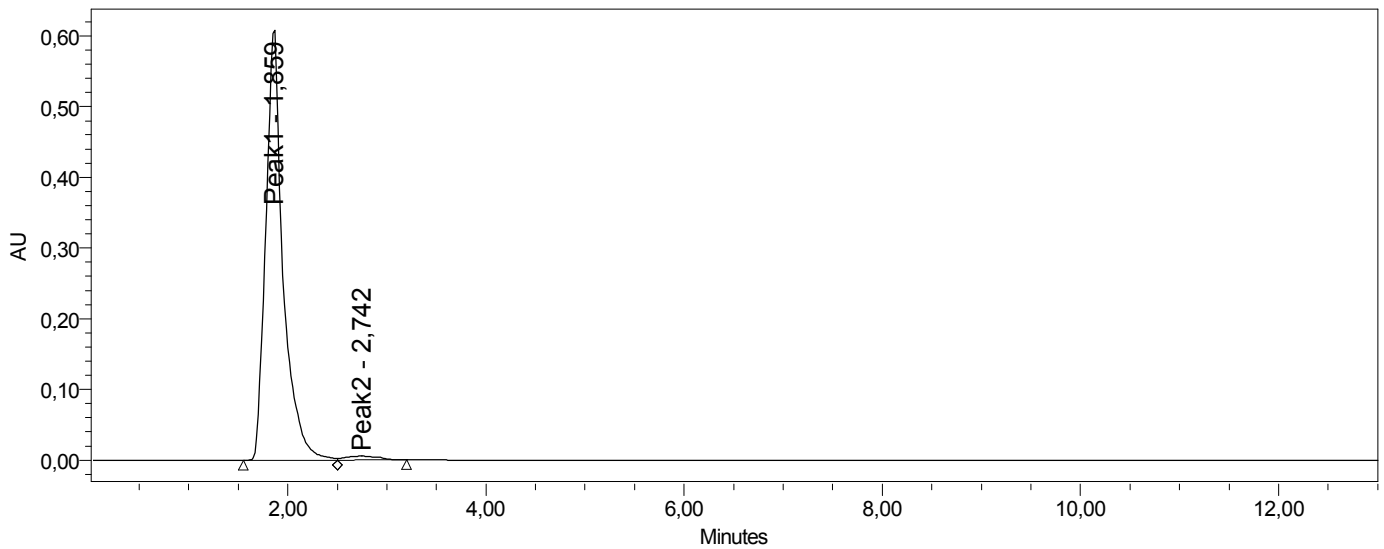
Sample Name:	DO179 Compound 40	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	10.7.2012 12:27:16
Vial:	5	Acq. Method Set:	98225434005_MS
Injection #:	1	Date Processed:	10.7.2012 12:45:56
Injection Volume:	10,00 ul	Processing Method:	DO179
Run Time:	16,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	RT	Area	% Area	Height
1	2,841	50248	0,53	8937
2	7,072	20870	0,22	2116
3	7,312	18966	0,20	1942
4	7,517	9047	0,10	859
5	7,987	118230	1,24	12090
6	8,519	33517	0,35	3359
7	8,856	9054210	95,25	1298066
8	9,437	201127	2,12	12718

SAMPLE INFORMATION

Sample Name:	DO197 Compound 42	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	11.7.2012 13:59:42
Vial:	11	Acq. Method Set:	10902543400513m_MS
Injection #:	1	Date Processed:	11.7.2012 14:16:19
Injection Volume:	10,00 ul	Processing Method:	DO197
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,859	7406062	98,31	609527
2	Peak2	2,742	127100	1,69	5603

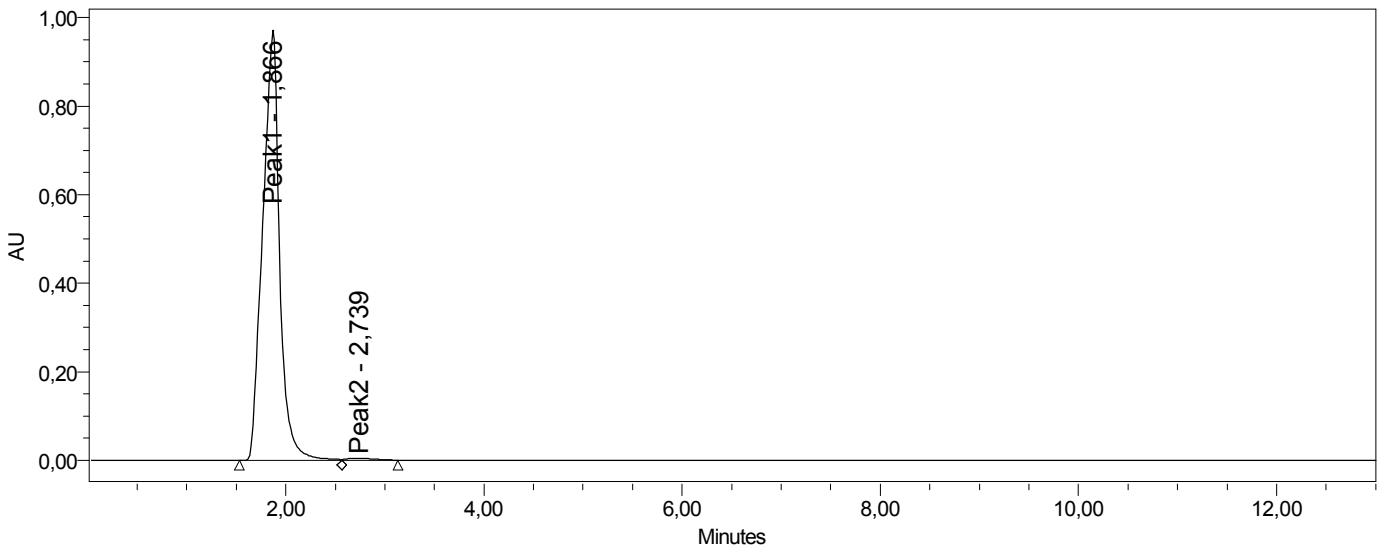


Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	DO199	Compound 43	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	11.7.2012 13:07:43
Vial:	8		Acq. Method Set:	10902543400513m_MS
Injection #:	1		Date Processed:	22.8.2012 9:38:17
Injection Volume:	10,00 ul		Processing Method:	DO199
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	

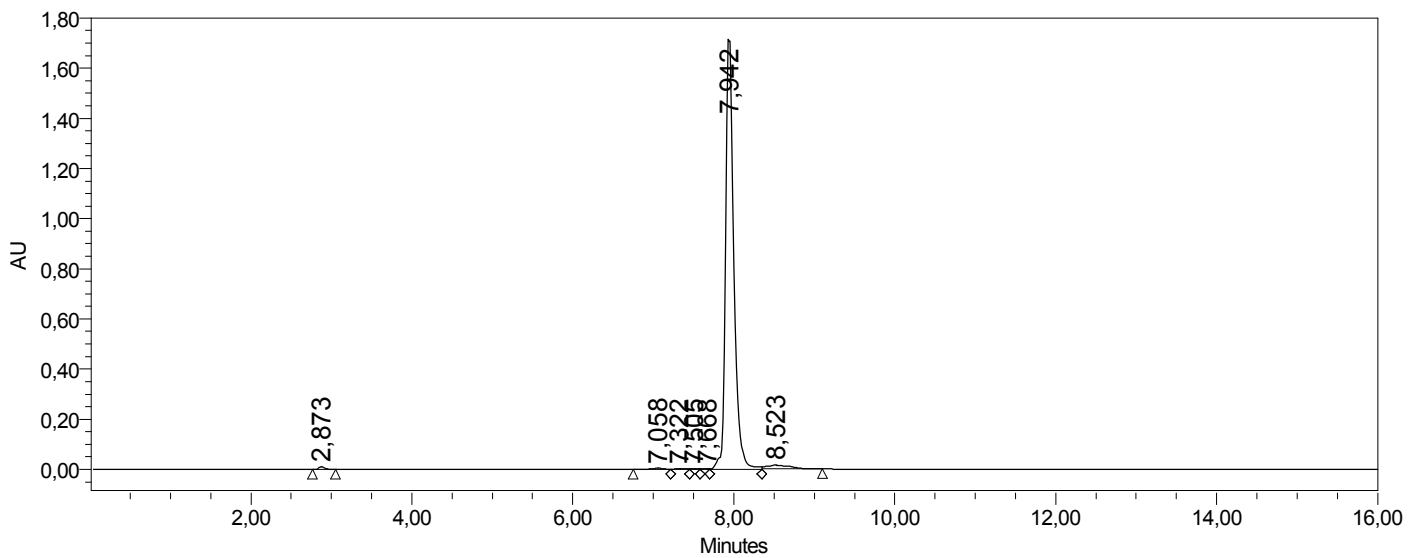


	Peak Name	RT	Area	% Area	Height
1	Peak1	1,866	11502563	99,37	969345
2	Peak2	2,739	72644	0,63	4037



SAMPLE INFORMATION

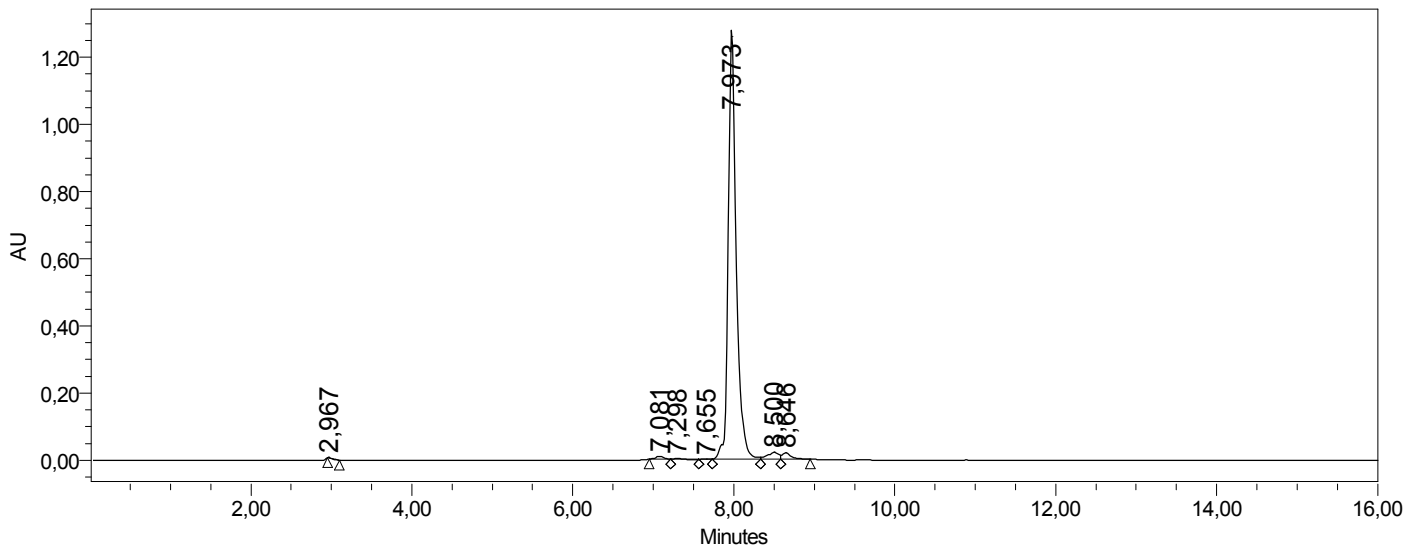
Sample Name:	NV78 Compound 50	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	10.7.2012 15:13:58
Vial:	13	Acq. Method Set:	98225434005_MS
Injection #:	1	Date Processed:	10.7.2012 15:35:48
Injection Volume:	10,00 ul	Processing Method:	MV78
Run Time:	16,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	RT	Area	% Area	Height
1	2,873	47104	0,38	9512
2	7,058	37378	0,30	4081
3	7,322	21853	0,18	2906
4	7,505	6308	0,05	912
5	7,668	8073	0,07	1486
6	7,942	11897269	96,45	1728281
7	8,523	317314	2,57	15479

SAMPLE INFORMATION

Sample Name:	DO181 Compound 52	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	10.7.2012 12:10:12
Vial:	4	Acq. Method Set:	98225434005_MS
Injection #:	1	Date Processed:	10.7.2012 12:34:01
Injection Volume:	10,00 ul	Processing Method:	DO181
Run Time:	16,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



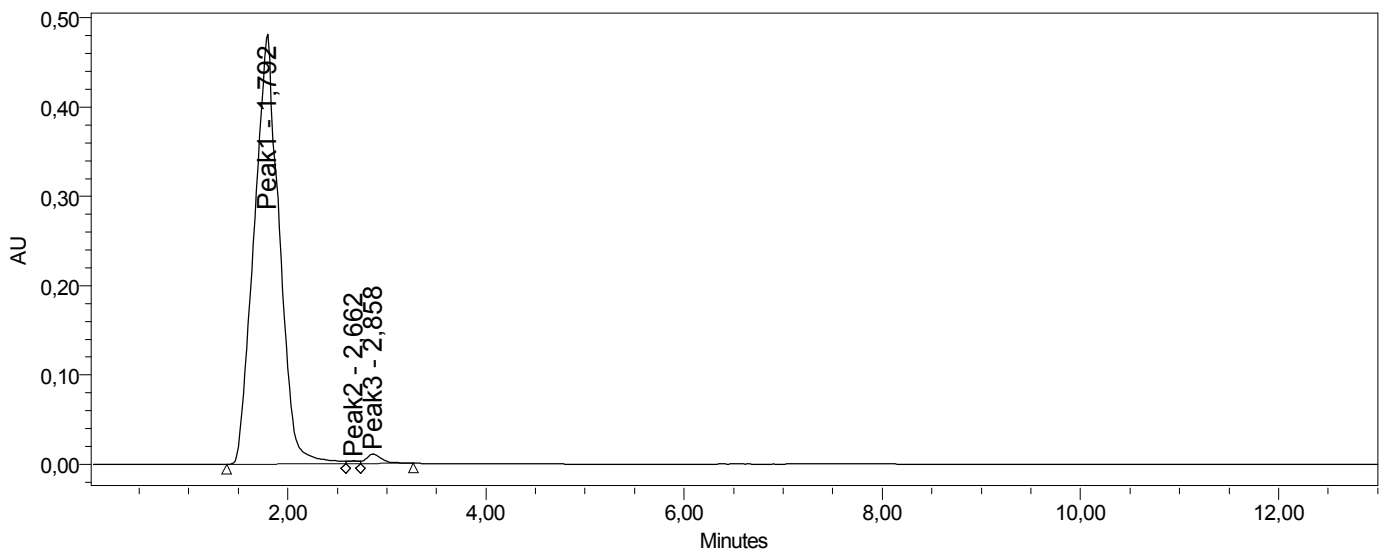
	RT	Area	% Area	Height
1	2,967	9899	0,11	1955
2	7,081	60180	0,66	8892
3	7,298	18844	0,21	2095
4	7,655	7613	0,08	1125
5	7,973	8694118	95,08	1275092
6	8,500	203211	2,22	20936
7	8,646	149925	1,64	18766

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	MV29	Compound 55	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	8.8.2012 10:34:01
Vial:	3		Acq. Method Set:	6942543400513m_MS
Injection #:	1		Date Processed:	8.8.2012 10:48:19
Injection Volume:	10,00 ul		Processing Method:	MV29k2
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



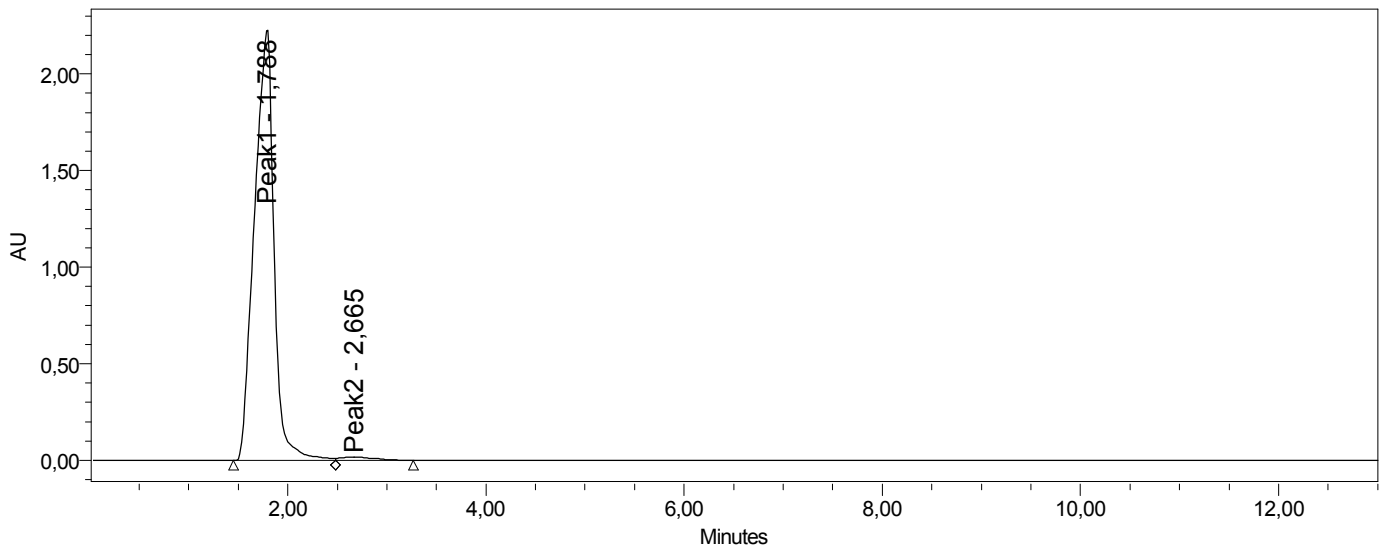
	Peak Name	RT	Area	% Area	Height
1	Peak1	1,792	8498337	98,41	482280
2	Peak2	2,662	23495	0,27	2952
3	Peak3	2,858	114002	1,32	10699

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	JK05 Compound 62	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	13.7.2012 14:03:35
Vial:	16	Acq. Method Set:	10902543400513m_MS
Injection #:	1	Date Processed:	13.7.2012 14:18:46
Injection Volume:	10,00 ul	Processing Method:	JK05
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



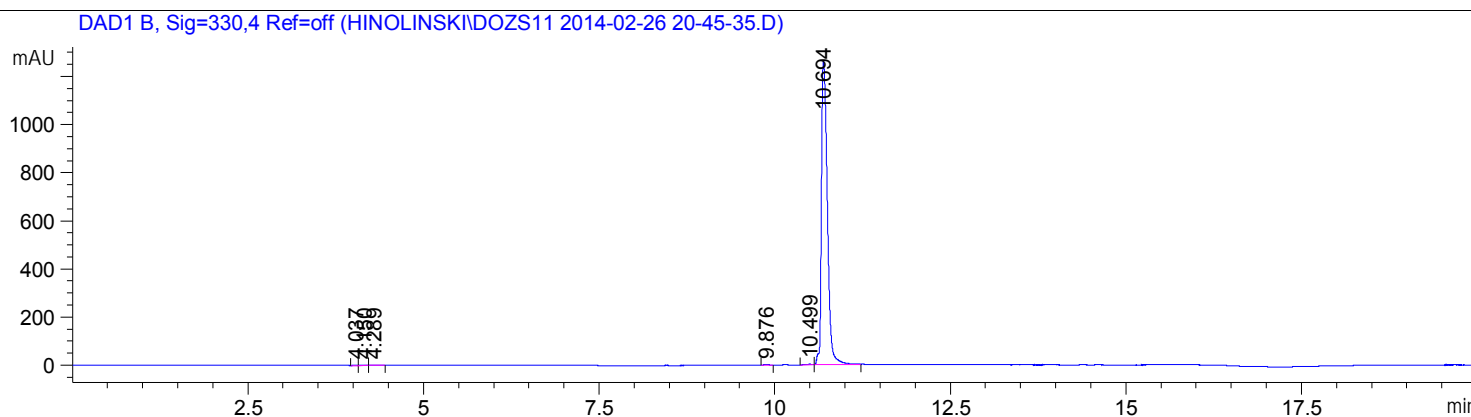
	Peak Name	RT	Area	% Area	Height
1	Peak1	1,788	30564596	98,83	2254359
2	Peak2	2,665	362651	1,17	16434

```

=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location  : Vial 84
Injection Date  : 2/26/2014 8:46:43 PM
                                           Inj Volume : 3.000 µl

Acq. Method     : C:\CHEM32\1\METHODS\METODA 7.M
Last changed    : 2/26/2014 8:44:29 PM by SYSTEM
                 (modified after loading)

Analysis Method  : C:\CHEM32\1\METHODS\PRANJE.M
Last changed    : 9/18/2013 2:53:53 PM by SYSTEM
=====
  
```



Fraction Information

No Fractions found.

Area Percent Report

```

Sorted By       : Signal
Multiplier      : 1.0000
Dilution        : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

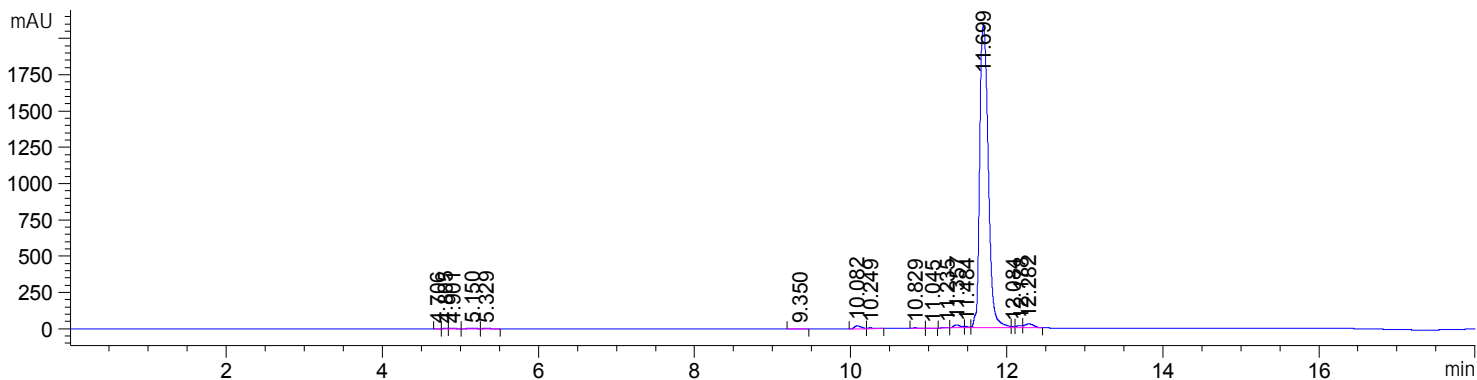
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.037	BV	0.0563	8.69776	2.10002	0.1166
2	4.150	VV	0.0837	17.49445	2.59416	0.2346
3	4.289	VB	0.0951	13.40362	1.67149	0.1797
4	9.876	VB	0.0708	8.55184	1.57636	0.1147
5	10.499	BV	0.0819	15.50056	2.38157	0.2078
6	10.694	VB	0.0931	7394.27734	1258.24707	99.1466

Totals : 7457.92557 1268.57067

\*\*\* End of Report \*\*\*

```
=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location : Vial 22
Injection Date  : 2/20/2014 10:29:16 AM
                                           Inj Volume : 7.500 µl
Acq. Method     : C:\CHEM32\1\METHODS\METODA 7.M
Last changed    : 2/20/2014 10:40:45 AM by SYSTEM
                  (modified after loading)
Analysis Method  : C:\CHEM32\1\METHODS\METODA 7.M
Last changed    : 2/19/2014 3:10:21 PM by SYSTEM
=====
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\DOJK06 2014-02-20 10-28-03.D)



```
=====
Fraction Information
=====
```

No Fractions found.

```
=====
Area Percent Report
=====
```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Sample Name: JK06

Signal 2: DAD1 B, Sig=330,4 Ref=off

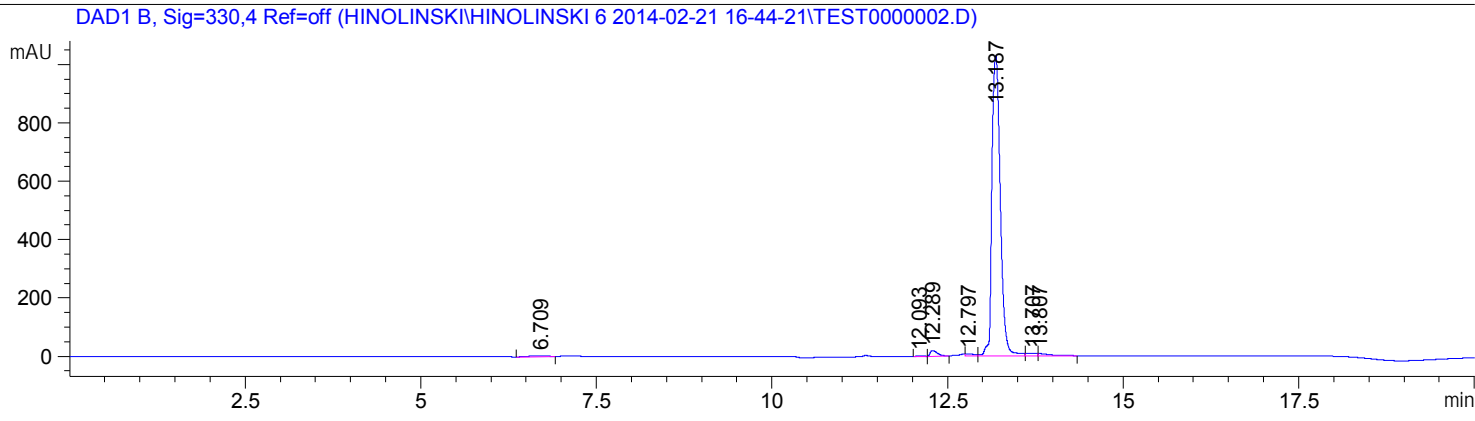
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.706	VV	0.0622	7.23272	1.42613	0.0431
2	4.805	VV	0.0586	11.70099	2.67164	0.0697
3	4.901	VB	0.0796	16.67839	2.55658	0.0993
4	5.150	BV	0.1040	21.87318	2.49038	0.1302
5	5.329	VB	0.0821	8.87225	1.28471	0.0528
6	9.350	BB	0.0972	8.60202	1.04878	0.0512
7	10.082	BV	0.0886	117.61160	20.00121	0.7003
8	10.249	VB	0.0790	29.08188	4.84406	0.1732
9	10.829	BB	0.0717	17.86604	3.67498	0.1064
10	11.045	BB	0.0681	6.03111	1.08016	0.0359
11	11.235	BB	0.0989	9.60299	1.17490	0.0572
12	11.357	BV	0.0998	125.79803	19.11553	0.7491
13	11.484	VV	0.0573	36.52851	7.92797	0.2175
14	11.699	VV	0.1215	1.60226e4	2087.60083	95.4097
15	12.084	VV	0.0322	28.99114	11.18867	0.1726
16	12.178	VV	0.0750	91.37415	16.79968	0.5441
17	12.282	VB	0.1138	233.03242	28.66618	1.3876

Totals : 1.67935e4 2213.55241

=====  
\*\*\* End of Report \*\*\*

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    2
Acq. Instrument : HPLC-Solaja                 Location  : Vial 34
Injection Date  : 2/21/2014 5:11:54 PM      Inj       :    1
                                                Inj Volume: 5.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 6 2014-02-21 16-44-21\METODA 7.M (
                : Sequence Method)
Last changed    : 2/21/2014 4:44:22 PM by SYSTEM
  
```



=====  
 Fraction Information  
 =====

No Fractions found.

=====  
 Area Percent Report  
 =====

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs  
 Signal 2: DAD1 B, Sig=330,4 Ref=off

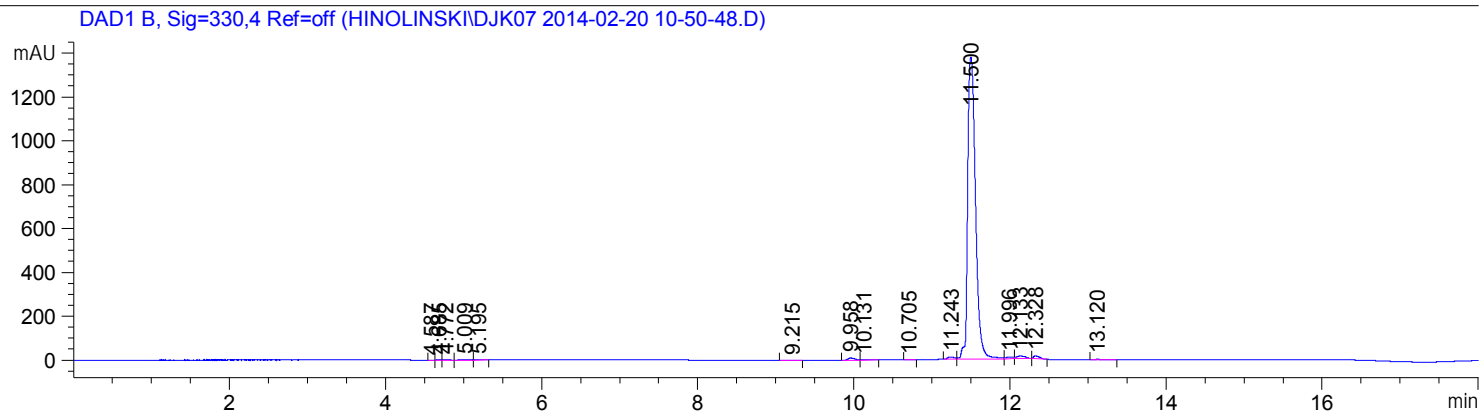
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.709	BV	0.2344	86.05817	4.32957	0.9602
2	12.093	BB	0.0762	10.51504	1.72388	0.1173
3	12.289	BB	0.1046	128.86201	18.88998	1.4378
4	12.797	VV	0.1066	58.68514	7.01316	0.6548
5	13.187	VV	0.1327	8516.03027	1027.66528	95.0174
6	13.707	VV	0.1197	83.13605	8.24247	0.9276
7	13.807	VB	0.1299	79.31776	7.23449	0.8850

Totals : 8962.60445 1075.09886

=====  
 \*\*\* End of Report \*\*\*



=====  
Acq. Operator : SYSTEM  
Acq. Instrument : HPLC-Solaja Location : Vial 23  
Injection Date : 2/20/2014 10:52:04 AM Inj Volume : 7.500 µl  
Acq. Method : C:\CHEM32\1\METHODS\METODA 7.M  
Last changed : 2/20/2014 10:40:45 AM by SYSTEM  
(modified after loading)  
Analysis Method : C:\CHEM32\1\METHODS\METODA 7.M  
Last changed : 2/19/2014 3:10:21 PM by SYSTEM



=====  
Fraction Information  
=====

No Fractions found.  
=====

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.587	VV	0.0565	5.81544	1.26840	0.0579
2	4.685	VV	0.0570	10.07004	2.35113	0.1003
3	4.772	VB	0.0755	13.99395	2.28411	0.1394
4	5.009	BV	0.0940	18.05120	2.28976	0.1798
5	5.195	VB	0.0733	6.31388	1.07773	0.0629
6	9.215	BB	0.0933	8.41399	1.06941	0.0838
7	9.958	BV	0.0852	60.36195	10.32249	0.6011
8	10.131	VB	0.0784	19.00268	3.04076	0.1892
9	10.705	BB	0.0549	7.22036	1.57765	0.0719
10	11.243	BV	0.0928	65.36218	10.68954	0.6509
11	11.500	VV	0.1098	9598.78711	1377.40308	95.5881
12	11.996	VV	0.0862	52.47046	7.92991	0.5225
13	12.133	VB	0.1115	97.59934	12.04516	0.9719
14	12.328	BB	0.0739	68.86954	13.51773	0.6858
15	13.120	VB	0.0855	9.48490	1.32480	0.0945

Totals : 1.00418e4 1448.19166

=====  
\*\*\* End of Report \*\*\*

Sample Name: D0186

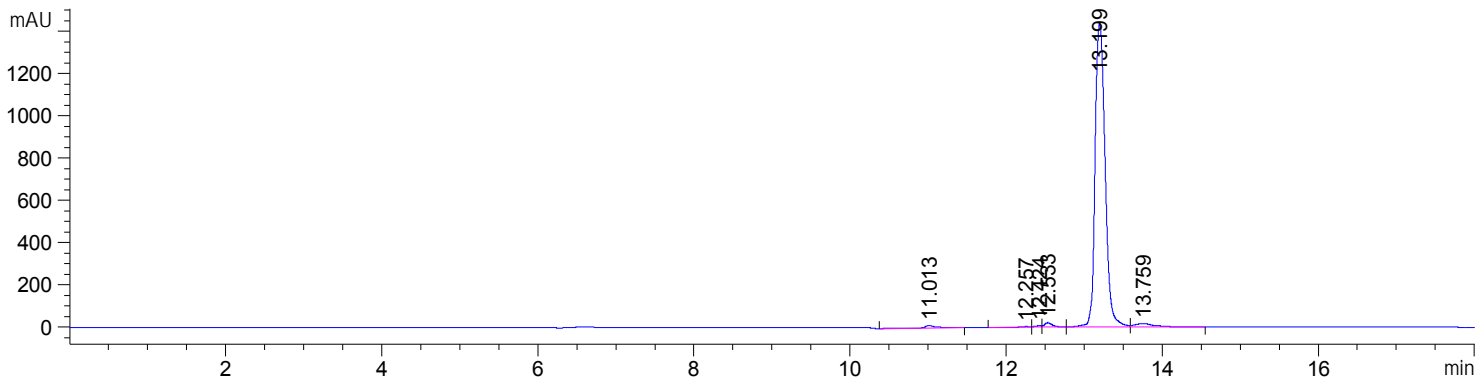
## Compound 20 Method C

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    2
Acq. Instrument : HPLC-Solaja                 Location  : Vial 32
Injection Date  : 2/21/2014 4:12:30 PM      Inj       :    1
                                                Inj Volume: 2.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 5 2014-02-21 15-47-00\METODA 7.M (
                : Sequence Method)
Last changed    : 2/21/2014 3:47:00 PM by SYSTEM
=====

```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\HINOLINSKI 5 2014-02-21 15-47-00\TEST000002.D)



```

=====
Fraction Information
=====

```

```

=====
No Fractions found.
=====

```

```

=====
Area Percent Report
=====

```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.013	BB	0.1744	166.23553	12.12893	1.2392
2	12.257	BV	0.1204	30.58098	3.05293	0.2280
3	12.424	VV	0.0728	34.70166	5.97099	0.2587
4	12.533	VB	0.1054	135.93785	20.10739	1.0133
5	13.199	BV	0.1423	1.27679e4	1434.42065	95.1766
6	13.759	VB	0.2141	279.60245	15.94336	2.0843

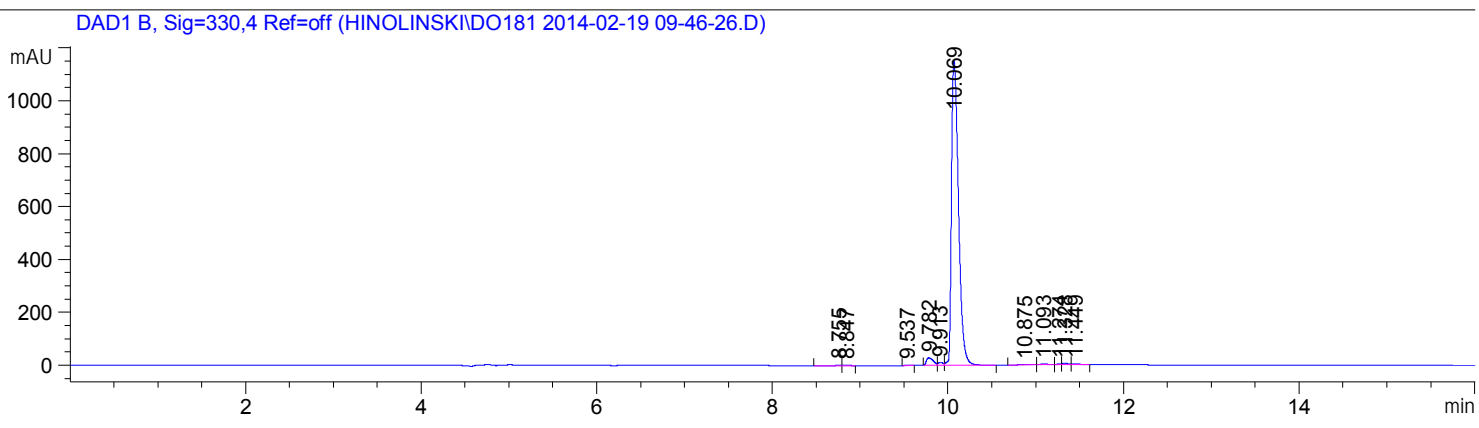
```
Totals :                1.34150e4  1491.62425
```

```

=====
*** End of Report ***

```

```
=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location : Vial 41
Injection Date  : 2/19/2014 9:47:39 AM
                                           Inj Volume : 5.000 µl
Acq. Method    : C:\CHEM32\1\METHODS\METODA 7.M
Last changed   : 2/19/2014 9:23:40 AM by SYSTEM
                 (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M
Last changed   : 9/18/2013 2:53:53 PM by SYSTEM
=====
```



```
=====
Fraction Information
=====
```

No Fractions found.

```
=====
Area Percent Report
=====
```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

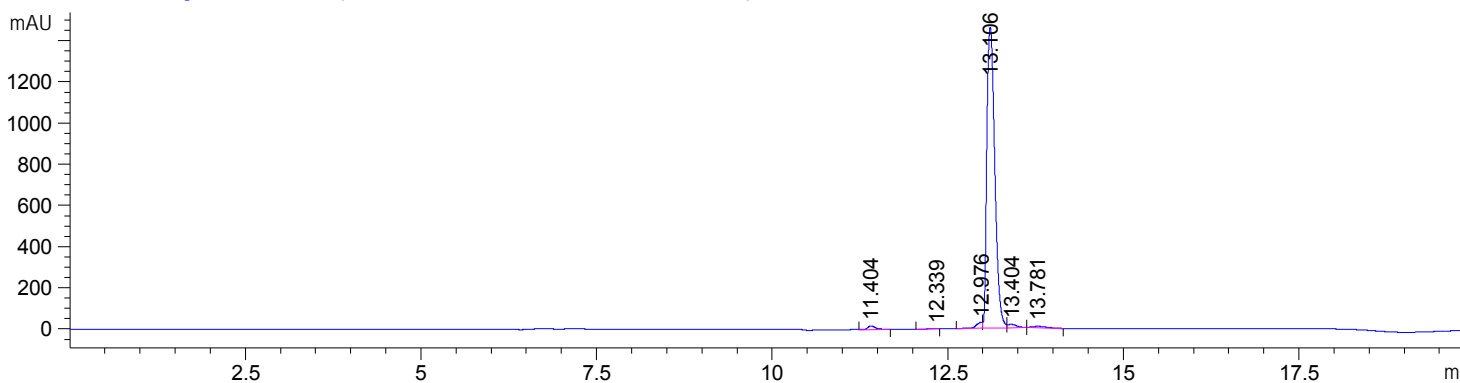
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.755	BV	0.0843	14.75049	2.19836	0.2204
2	8.847	VV	0.0769	20.37475	3.47413	0.3045
3	9.537	BB	0.0551	6.45124	1.40293	0.0964
4	9.782	BV	0.0844	145.50365	27.66089	2.1743
5	9.913	VV	0.0616	38.97849	9.16115	0.5825
6	10.069	VB	0.0866	6363.96094	1149.05420	95.0962
7	10.875	BV	0.1022	18.90684	2.29344	0.2825
8	11.093	VB	0.0766	20.12285	3.34847	0.3007
9	11.274	BV	0.0460	12.53524	4.30000	0.1873
10	11.328	VV	0.0701	28.63871	5.56271	0.4279
11	11.449	VB	0.0730	21.90523	3.65288	0.3273

Totals : 6692.12843 1212.10918

=====  
\*\*\* End of Report \*\*\*

=====  
Acq. Operator : SYSTEM  
Acq. Instrument : HPLC-Solaja Location : Vial 8  
Injection Date : 2/21/2014 11:08:40 AM Inj Volume : 5.000 µl  
Acq. Method : C:\CHEM32\1\METHODS\METODA 7.M  
Last changed : 2/21/2014 11:07:18 AM by SYSTEM  
(modified after loading)  
Analysis Method : C:\CHEM32\1\METHODS\METODA 7.M  
Last changed : 2/20/2014 2:58:40 PM by SYSTEM

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\DR09 2014-02-21 11-07-25.D)



=====  
Fraction Information  
=====

No Fractions found.  
=====

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 2: DAD1 B, Sig=330,4 Ref=off

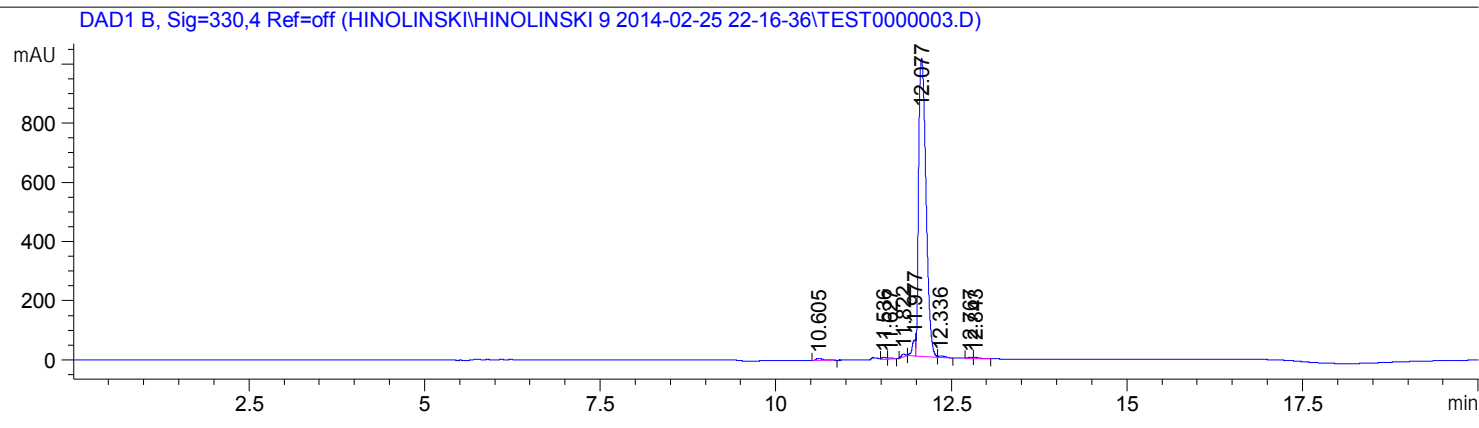
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.404	VB	0.1187	147.29094	17.85912	1.2157
2	12.339	BV	0.1197	13.35825	1.34118	0.1103
3	12.976	BV	0.0856	179.39629	28.23582	1.4807
4	13.106	VV	0.1261	1.15281e4	1460.27515	95.1511
5	13.404	VB	0.1080	145.85057	16.12716	1.2038
6	13.781	BB	0.1663	101.57732	7.25804	0.8384

Totals : 1.21156e4 1531.09648

=====  
\*\*\* End of Report \*\*\*

```

=====
Acq. Operator   : SYSTEM                               Seq. Line :    3
Acq. Instrument : HPLC-Solaja                          Location  : Vial 56
Injection Date  : 2/25/2014 11:10:31 PM              Inj       :    1
                                                    Inj Volume: 5.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 9 2014-02-25 22-16-36\METODA 24.M (
                  Sequence Method)
Last changed    : 2/25/2014 10:16:36 PM by SYSTEM
  
```



=====  
 Fraction Information  
 =====

No Fractions found.

=====  
 Area Percent Report  
 =====

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.605	BB	0.0891	45.47674	6.88395	0.5932
2	11.536	VV	0.0668	29.65431	6.04188	0.3868
3	11.627	VB	0.0629	16.13100	3.49195	0.2104
4	11.822	BB	0.0673	34.05287	8.48385	0.4442
5	11.977	BV	0.0524	176.41385	52.86920	2.3010
6	12.077	VV	0.1161	7294.38867	1006.11627	95.1406
7	12.336	VB	0.0988	33.36090	4.30850	0.4351
8	12.767	VV	0.0660	17.46827	3.28944	0.2278
9	12.843	VB	0.0731	20.00685	3.30386	0.2609

Totals :                                    7666.95346 1094.78890

=====  
 \*\*\* End of Report \*\*\*

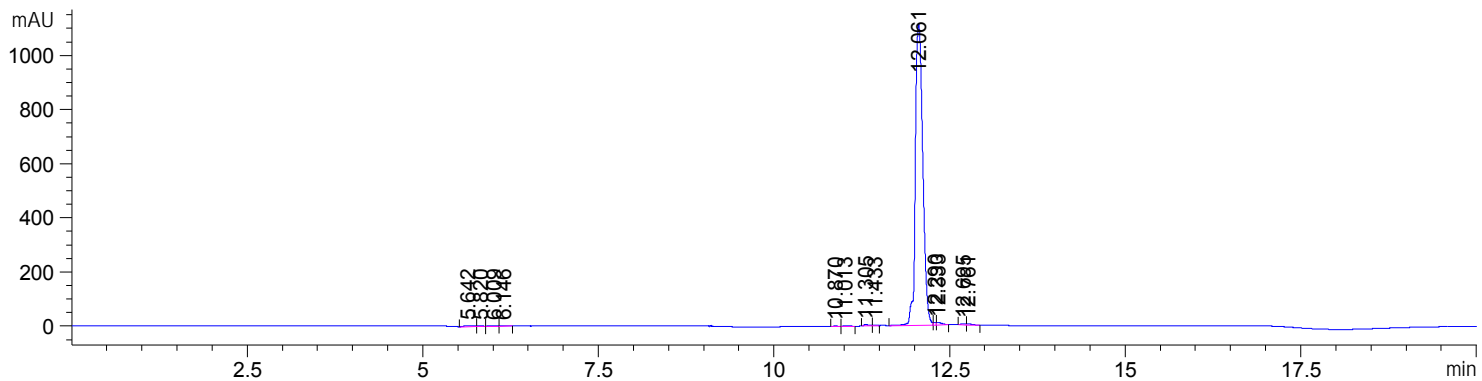
Sample Name: DOJK08

Compound 25

Method C

```
=====
Acq. Operator   : SYSTEM                      Seq. Line :    6
Acq. Instrument : HPLC-Solaja                 Location  : Vial 62
Injection Date  : 2/26/2014 12:29:28 AM      Inj       :    1
                                                    Inj Volume: 5.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 9 2014-02-25 22-16-36\METHODA 24.M (
                : Sequence Method)
Last changed    : 2/25/2014 10:16:36 PM by SYSTEM
=====
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\HINOLINSKI 9 2014-02-25 22-16-36\TEST0000006.D)



```
=====
Fraction Information
=====
```

```
No Fractions found.
=====
```

```
Area Percent Report
=====
```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```



Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.642	BV	0.1278	36.26812	3.36398	0.4312
2	5.820	VV	0.0748	17.15714	2.88639	0.2040
3	6.009	VV	0.0977	18.80373	2.28020	0.2236
4	6.146	VB	0.0826	10.56242	1.62935	0.1256
5	10.870	BV	0.0627	6.37159	1.22561	0.0758
6	11.013	VB	0.0773	8.66594	1.35110	0.1030
7	11.305	BV	0.0777	25.77197	4.61158	0.3064
8	11.433	VB	0.0484	6.06162	1.55901	0.0721
9	12.061	BV	0.1168	8172.54492	1110.94275	97.1698
10	12.290	VV	0.0395	25.65238	9.06508	0.3050
11	12.333	VB	0.0672	44.77309	8.68314	0.5323
12	12.695	VV	0.0728	18.50238	3.46563	0.2200
13	12.761	VB	0.0638	19.44583	3.67121	0.2312

Totals : 8410.58114 1154.73502

=====  
\*\*\* End of Report \*\*\*

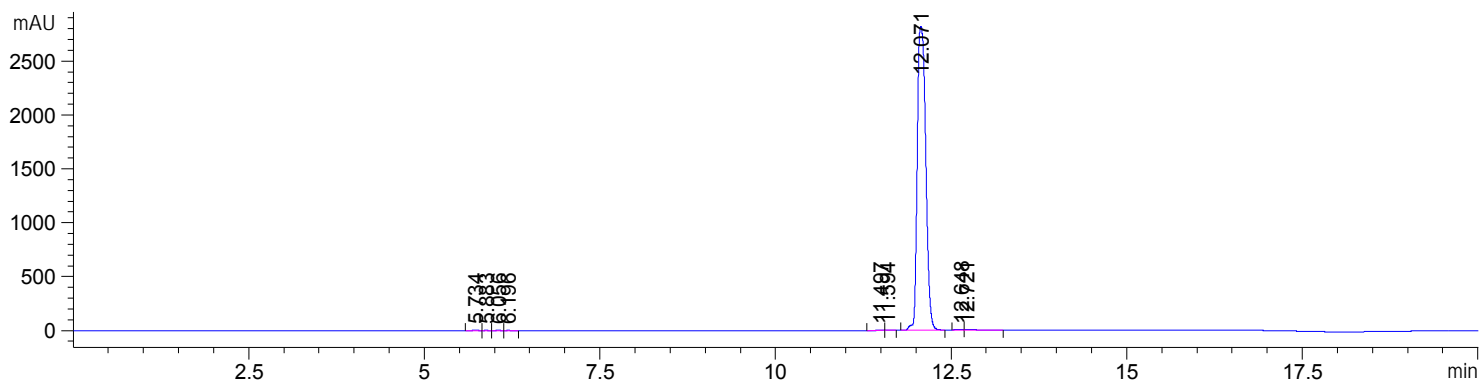
Sample Name: D0174

## Compound 36

## Method C

```
=====
Acq. Operator   : SYSTEM                      Seq. Line :    4
Acq. Instrument : HPLC-Solaja                 Location  : Vial 57
Injection Date  : 2/25/2014 11:36:51 PM      Inj       :    1
                                                Inj Volume: 5.000 µl
Method         : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 9 2014-02-25 22-16-36\METODA 24.M (
                Sequence Method)
Last changed    : 2/25/2014 10:16:36 PM by SYSTEM
=====
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\HINOLINSKI 9 2014-02-25 22-16-36\TEST0000004.D)



```
=====
Fraction Information
=====
```

```
No Fractions found.
=====
```

```
Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 2: DAD1 B, Si g=330, 4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.734	BV	0.1247	34.74579	3.31755	0.1456
2	5.883	VV	0.0804	18.31310	2.99248	0.0767
3	6.056	VV	0.0919	18.64886	2.44772	0.0782
4	6.196	VB	0.0860	11.68477	1.71578	0.0490
5	11.497	BV	0.0852	13.33289	2.02765	0.0559
6	11.594	VB	0.0664	7.07617	1.34354	0.0297
7	12.071	BV	0.1012	2.36822e4	2813.83350	99.2431
8	12.648	BV	0.0889	30.85190	4.19247	0.1293
9	12.721	VB	0.1278	45.96009	4.45875	0.1926

Totals : 2.38628e4 2836.32944

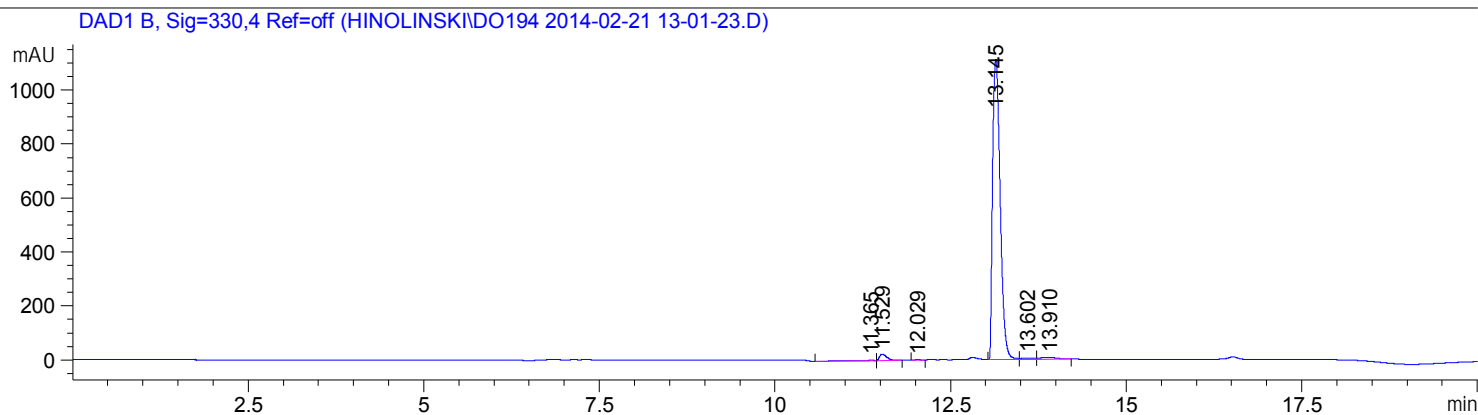
=====  
\*\*\* End of Report \*\*\*

```

=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location : Vial 11
Injection Date  : 2/21/2014 1:02:35 PM
                                           Inj Volume : 5.000 µl

Acq. Method    : C:\CHEM32\1\METHODS\METODA 7.M
Last changed   : 2/21/2014 12:38:38 PM by SYSTEM
                 (modified after loading)

Analysis Method : C:\CHEM32\1\METHODS\METODA 7.M
Last changed   : 2/20/2014 2:58:40 PM by SYSTEM
  
```



=====  
 Fraction Information  
 =====

No Fractions found.

=====  
 Area Percent Report  
 =====

```

Sorted By       : Signal
Multiplier      : 1.0000
Dilution        : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.365	BV	0.4126	66.33316	1.88258	0.7592
2	11.529	VB	0.1153	174.55154	23.47076	1.9979
3	12.029	BV	0.0710	12.85775	2.20732	0.1472
4	13.145	BV	0.1209	8320.55859	1111.08850	95.2343
5	13.602	VV	0.1422	54.91820	4.55336	0.6286
6	13.910	VB	0.1828	107.71581	6.92975	1.2329

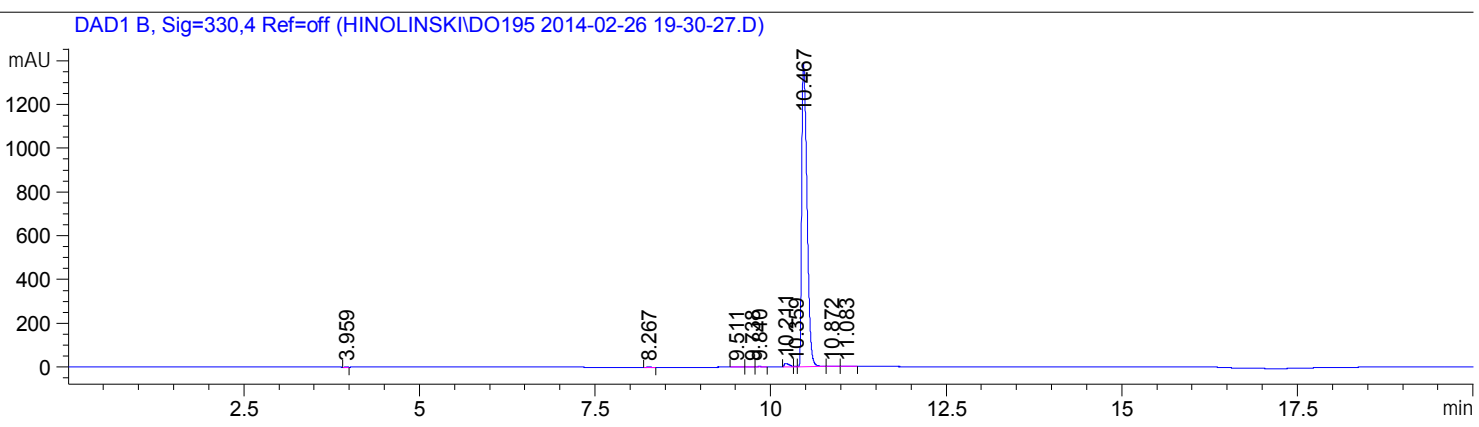
Totals :                                      8736.93505 1150.13227

=====  
 \*\*\* End of Report \*\*\*

```
=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja                    Location : Vial 83
Injection Date  : 2/26/2014 7:31:34 PM
                                                 Inj Volume : 2.000 µl

Acq. Method     : C:\CHEM32\1\METHODS\METODA 7.M
Last changed    : 2/26/2014 7:30:08 PM by SYSTEM
                                                 (modified after loading)

Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M
Last changed    : 9/18/2013 2:53:53 PM by SYSTEM
=====
```



=====  
Fraction Information  
=====

No Fractions found.  
=====

=====  
Area Percent Report  
=====

Sorted By            :        Signal  
Multiplier          :        1.0000  
Dilution             :        1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.959	BB	0.0469	6.22457	2.17706	0.0841
2	8.267	BB	0.0549	5.25604	1.15871	0.0710
3	9.511	BV	0.0824	9.35642	1.36666	0.1264
4	9.738	VV	0.0776	8.47712	1.40132	0.1145
5	9.840	VB	0.0681	9.86576	1.86846	0.1333
6	10.211	VV	0.0689	77.25272	15.55775	1.0438
7	10.359	VV	0.0350	5.75576	2.31383	0.0778
8	10.467	VB	0.0842	7261.27490	1384.18518	98.1114
9	10.872	BV	0.0778	7.18719	1.09850	0.0971
10	11.083	VB	0.0744	10.40300	1.68820	0.1406

Totals : 7401.05349 1412.81568

=====  
\*\*\* End of Report \*\*\*

Sample Name: D0191 **Compound 41**

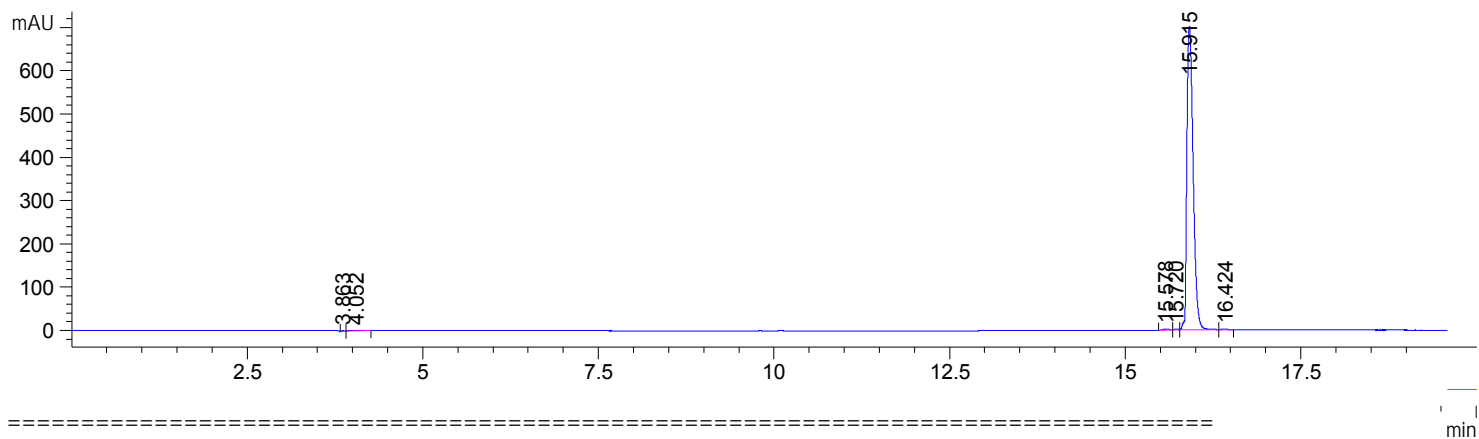
**Method C**

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    2
Acq. Instrument : HPLC-Solaja                 Location  : Vial 72
Injection Date  : 2/24/2014 8:40:01 PM      Inj       :    1
                                           Inj Volume: 2.000 µl

Acq. Method     : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 8 2014-02-24 20-12-39\METODA 8.M
Last changed    : 2/24/2014 8:34:12 PM by SYSTEM
Analysis Method : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 8 2014-02-24 20-12-39\METODA 8.M (
                  Sequence Method)
Last changed    : 2/24/2014 8:12:39 PM by SYSTEM
Method Info     : BENZOTIAZOLI
    
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\HINOLINSKI 8 2014-02-24 20-12-39\TEST000002.D)



Fraction Information

No Fractions found.

Area Percent Report

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.863	BV	0.0390	5.16061	1.79463	0.1172
2	4.052	VB	0.1515	25.32899	1.98973	0.5754
3	15.578	BV	0.0753	14.38167	2.58968	0.3267
4	15.720	VV	0.0629	8.63869	1.81897	0.1962
5	15.915	VV	0.0982	4340.81494	701.01807	98.6065
6	16.424	VB	0.0900	7.83396	1.05020	0.1780

Totals : 4402.15886 710.26128

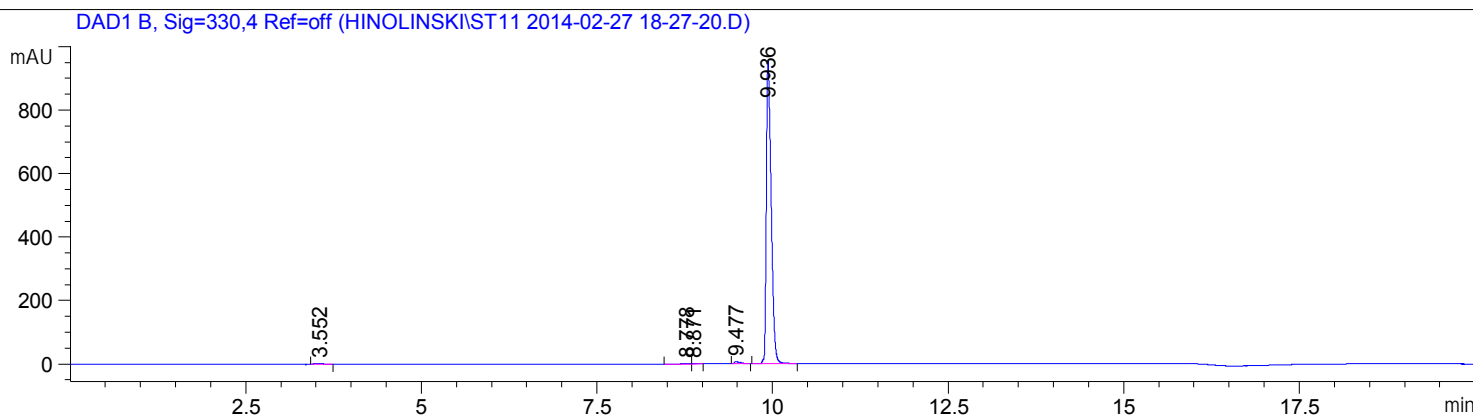
\*\*\* End of Report \*\*\*

```

=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja                      Location  : Vial 77
Injection Date  : 2/27/2014 6:28:38 PM
                                           Inj Volume: 2.000 µl

Acq. Method     : C:\CHEM32\1\METHODS\METODA 24.M
Last changed    : 2/27/2014 6:25:04 PM by SYSTEM
                  (modified after loading)

Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M
Last changed    : 9/18/2013 2:53:53 PM by SYSTEM
  
```



=====  
 Fraction Information  
 =====

No Fractions found.

=====  
 Area Percent Report  
 =====

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

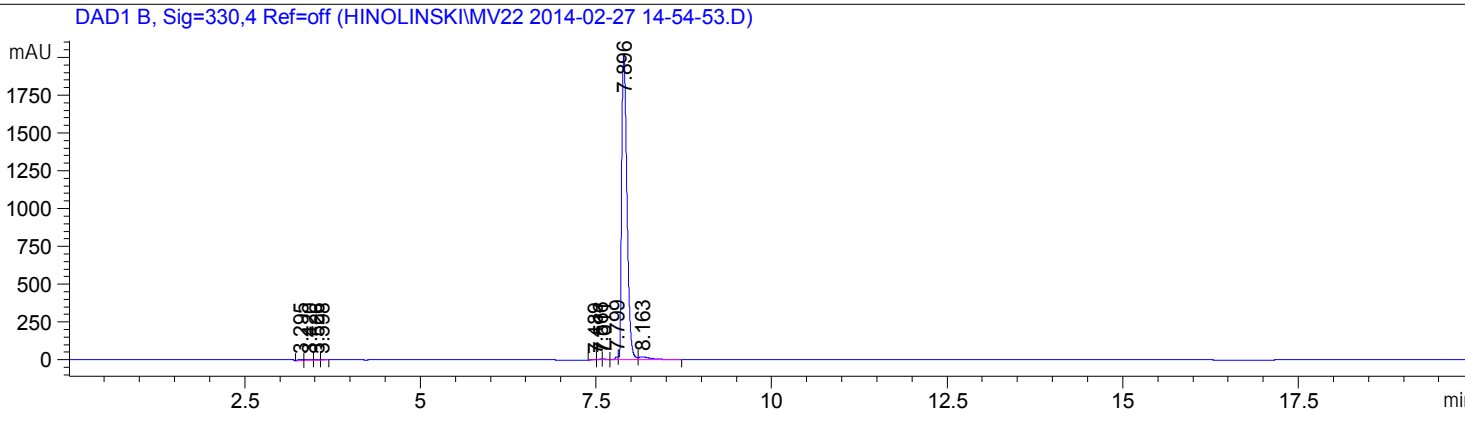
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.552	VB	0.1360	21.57221	1.88557	0.4633
2	8.778	BV	0.1134	17.16291	1.80479	0.3686
3	8.871	VB	0.0537	5.04941	1.16190	0.1085
4	9.477	BB	0.0811	39.85469	6.67863	0.8560
5	9.936	BB	0.0760	4572.14014	952.83606	98.2035

Totals :                      4655.77936    964.36694

=====  
 \*\*\* End of Report \*\*\*



=====  
Acq. Operator : SYSTEM  
Acq. Instrument : HPLC-Solaja Location : Vial 71  
Injection Date : 2/27/2014 2:55:59 PM Inj Volume : 5.000 µl  
Acq. Method : C:\CHEM32\1\METHODS\METODA 24.M  
Last changed : 2/27/2014 2:39:03 PM by SYSTEM  
(modified after loading)  
Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M  
Last changed : 9/18/2013 2:53:53 PM by SYSTEM



=====  
Fraction Information  
=====

No Fractions found.  
=====

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.295	BV	0.0700	29.83358	5.94979	0.2733
2	3.420	VV	0.0820	38.07766	5.55012	0.3488
3	3.526	VV	0.0681	21.82052	3.97027	0.1999
4	3.598	VB	0.0514	10.97804	2.56818	0.1006
5	7.489	BV	0.0448	7.40382	2.35009	0.0678
6	7.566	VV	0.0491	13.15521	3.87252	0.1205
7	7.611	VB	0.0540	13.90615	3.49097	0.1274
8	7.799	BV	0.0436	46.89835	16.77225	0.4296
9	7.896	VV	0.0826	1.05308e4	2010.04443	96.4580
10	8.163	VB	0.1538	204.62837	17.77680	1.8743

Totals : 1.09175e4 2072.34543

=====  
\*\*\* End of Report \*\*\*

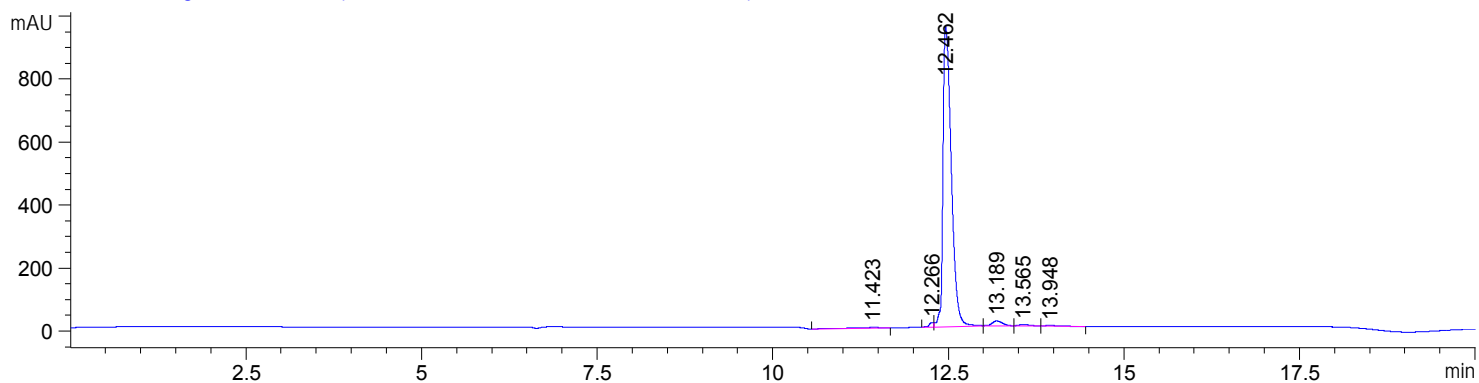
```

=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location : Vial 7
Injection Date  : 2/21/2014 10:43:28 AM
                                           Inj Volume : 1.500 µl

Acq. Method     : C:\CHEM32\1\METHODS\METODA 7.M
Last changed    : 2/21/2014 10:54:24 AM by SYSTEM
                  (modified after loading)

Analysis Method : C:\CHEM32\1\METHODS\METODA 7.M
Last changed    : 2/20/2014 2:58:40 PM by SYSTEM
  
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\MV61 2014-02-21 10-42-11.D)



=====  
 Fraction Information  
 =====

No Fractions found.  
 =====

=====  
 Area Percent Report  
 =====

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 2: DAD1 B, Sig=330,4 Ref=off

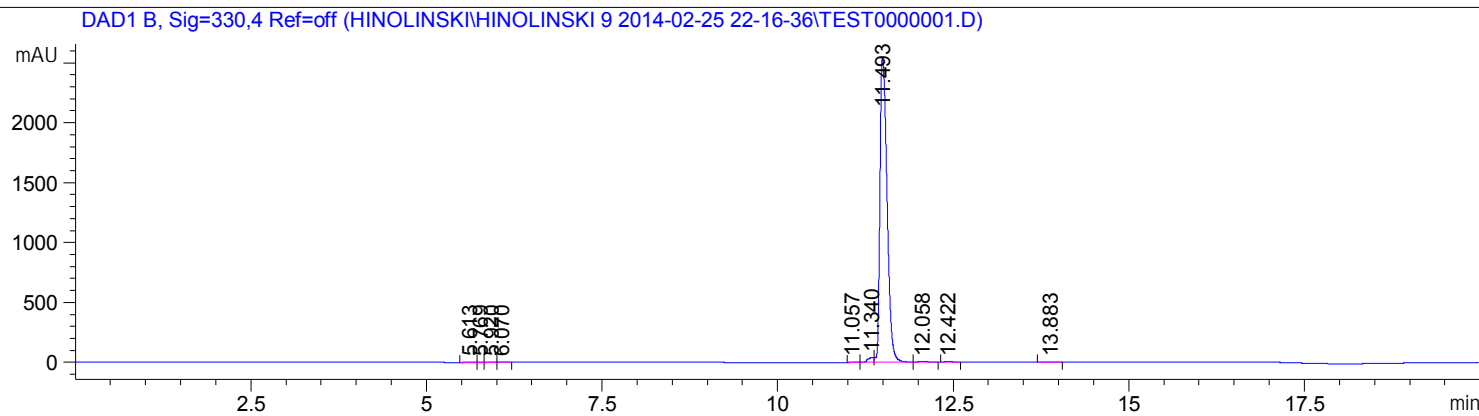
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.423	BB	0.3545	80.20527	2.68111	0.9768
2	12.266	BV	0.0686	60.87838	13.25480	0.7414
3	12.462	VB	0.1281	7834.17725	950.83105	95.4108
4	13.189	BV	0.1326	150.77586	15.01812	1.8363
5	13.565	VV	0.1404	53.32525	4.54446	0.6494
6	13.948	VB	0.1795	31.63280	2.07948	0.3852

Totals : 8210.99481 988.40904

=====  
 \*\*\* End of Report \*\*\*

```

=====
Acq. Operator   : SYSTEM                               Seq. Line :    1
Acq. Instrument : HPLC-Solaja                          Location  : Vial 54
Injection Date  : 2/25/2014 10:17:54 PM              Inj       :    1
                                                    Inj Volume: 5.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 9 2014-02-25 22-16-36\METODA 24.M (
                  Sequence Method)
Last changed    : 2/25/2014 10:16:36 PM by SYSTEM
=====
  
```



=====  
 Fraction Information  
 =====

No Fractions found.

=====  
 Area Percent Report  
 =====

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.613	BV	0.1217	24.77264	2.42405	0.1356
2	5.769	VV	0.0628	8.54417	1.63935	0.0468
3	5.920	VV	0.0901	12.88919	1.72560	0.0706
4	6.070	VB	0.0762	7.49557	1.18722	0.0410
5	11.057	BV	0.0866	16.42900	2.51783	0.0899
6	11.340	VV	0.0815	238.29944	40.27359	1.3044
7	11.493	VV	0.1109	1.78894e4	2532.88477	97.9245
8	12.058	VB	0.1252	40.66521	3.84978	0.2226
9	12.422	BB	0.0971	16.75681	2.08881	0.0917
10	13.883	BB	0.0769	13.31058	2.17637	0.0729

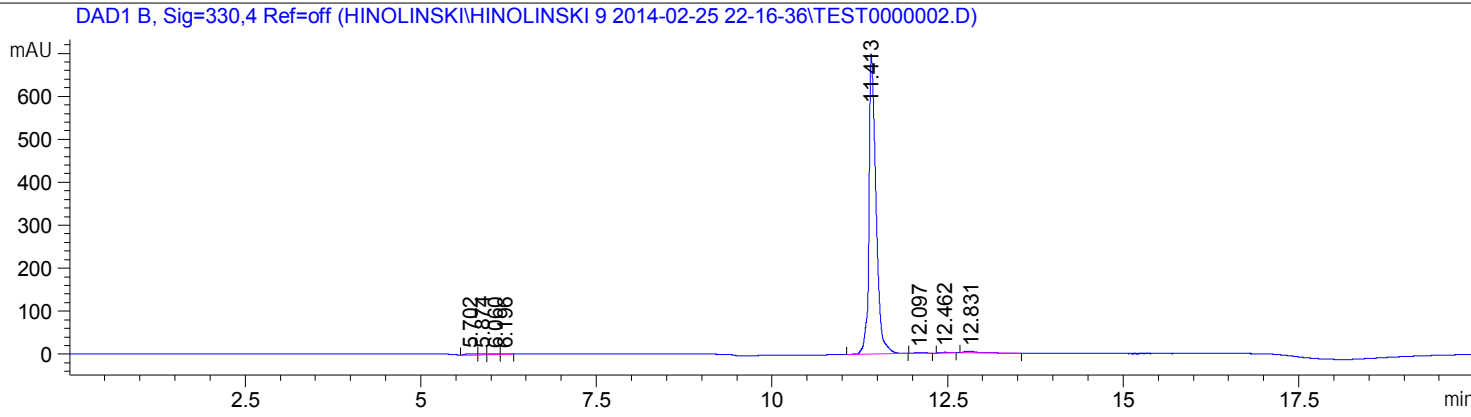
Totals :                      1.82685e4 2590.76737

=====  
 \*\*\* End of Report \*\*\*

Sample Name: ST13 **Compound 54** **Method C**

```

=====
Acq. Operator   : SYSTEM                               Seq. Line :    2
Acq. Instrument : HPLC-Solaja                          Location  : Vial 55
Injection Date  : 2/25/2014 10:44:13 PM                Inj       :    1
                                                    Inj Volume: 5.000 µl
Method          : C:\CHEM32\1\DATA\HI NOLINSKI \HI NOLINSKI 9 2014-02-25 22-16-36\METODA 24.M (
                Sequence Method)
Last changed    : 2/25/2014 10:16:36 PM by SYSTEM
=====
    
```



Fraction Information

No Fractions found.

Area Percent Report

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.702	BV	0.1296	36.57756	3.35749	0.7252
2	5.874	VV	0.0715	18.11462	3.03915	0.3592
3	6.060	VV	0.0989	19.11790	2.32680	0.3791
4	6.196	VB	0.0833	11.05497	1.65761	0.2192
5	11.413	BB	0.1077	4883.66016	697.03918	96.8300
6	12.097	BB	0.0941	13.61810	1.71603	0.2700
7	12.462	BB	0.0969	11.65178	1.43263	0.2310
8	12.831	BB	0.1806	49.74744	3.30498	0.9864

Totals : 5043.54253 713.87387

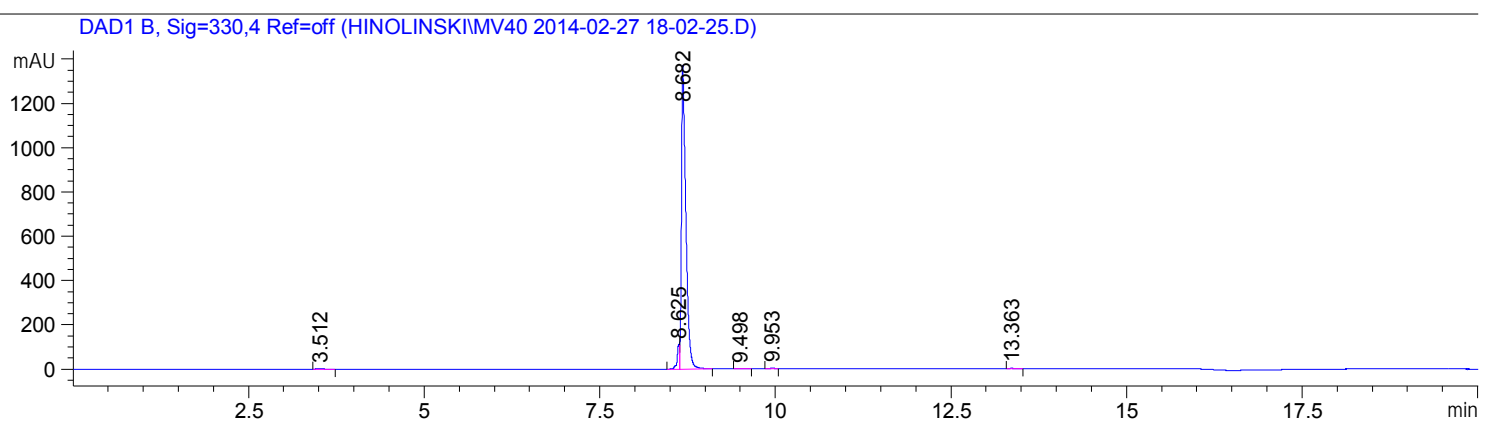
\*\*\* End of Report \*\*\*

```

=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja                      Location  : Vial 72
Injection Date  : 2/27/2014 6:03:31 PM
                                                    Inj Volume: 1.500 µl

Acq. Method     : C:\CHEM32\1\METHODS\METODA 24.M
Last changed    : 2/27/2014 6:02:10 PM by SYSTEM
                  (modified after loading)

Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M
Last changed    : 9/18/2013 2:53:53 PM by SYSTEM
  
```



=====  
 Fraction Information  
 =====

No Fractions found.

=====  
 Area Percent Report  
 =====

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

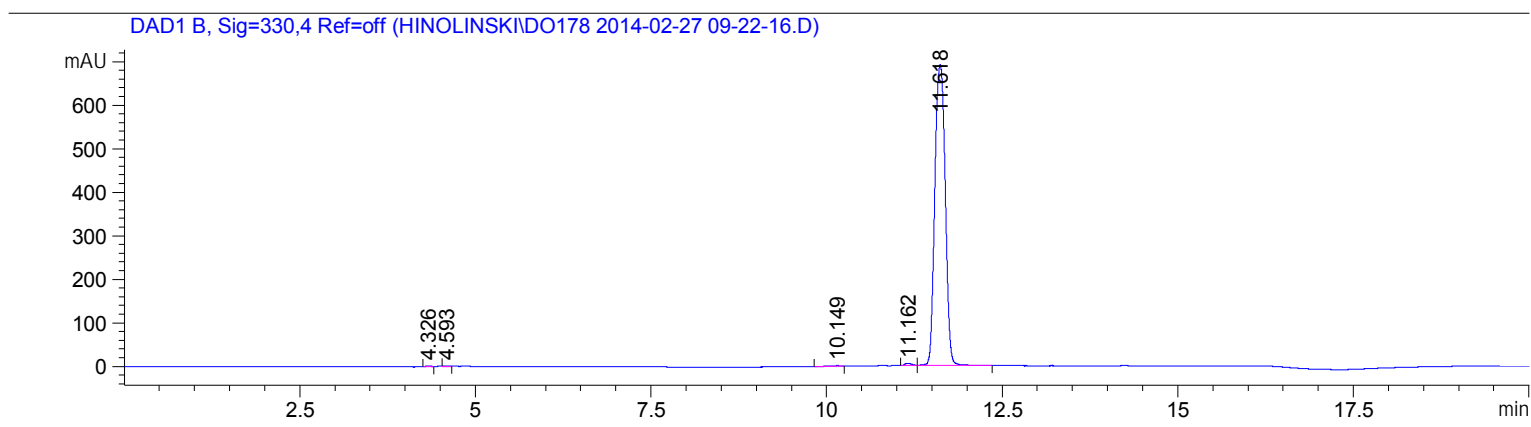
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.512	VB	0.1292	21.04389	1.93720	0.3362
2	8.625	BV	0.0336	252.08754	112.73808	4.0278
3	8.682	VV	0.0602	5956.11426	1370.96179	95.1661
4	9.498	BB	0.0684	6.69030	1.27198	0.1069
5	9.953	BV	0.0697	12.64812	2.45145	0.2021
6	13.363	BB	0.0622	10.06762	2.31454	0.1609

Total s : 6258.65173 1491.67503

=====  
 \*\*\* End of Report \*\*\*

```
=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location : Vial 87
Injection Date  : 2/27/2014 9:23:31 AM
                                           Inj Volume : 10.000 µl
Acq. Method    : C:\CHEM32\1\METHODS\METODA 24.M
Last changed   : 2/27/2014 8:32:34 AM by SYSTEM
                 (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M
Last changed   : 9/18/2013 2:53:53 PM by SYSTEM
=====
```



```
=====
Fraction Information
=====
```

No Fractions found.

```
=====
Area Percent Report
=====
```

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Sample Name: D0178

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.326	BB	0.0662	8.77658	1.64607	0.1219
2	4.593	VV	0.0619	6.46930	1.28189	0.0899
3	10.149	BB	0.0979	10.87971	1.32378	0.1511
4	11.162	BV	0.0861	34.76116	4.88114	0.4829
5	11.618	VB	0.1665	7137.80811	691.08551	99.1542

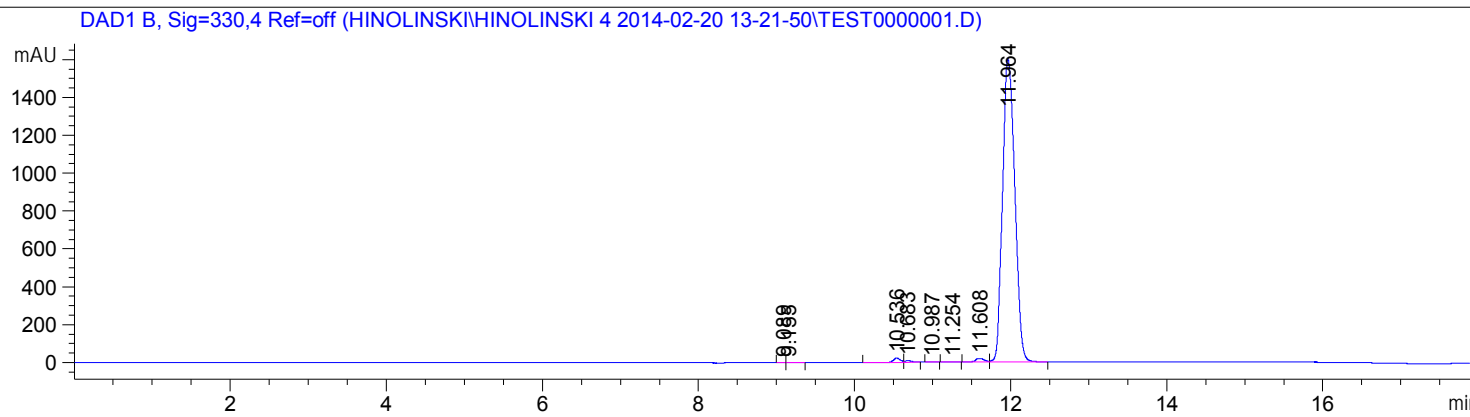
Totals :                               7198.69486   700.21840

=====  
\*\*\* End of Report \*\*\*



```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    1
Acq. Instrument : HPLC-Solaja                 Location  : Vial 1
Injection Date  : 2/20/2014 1:23:06 PM       Inj       :    1
                                                    Inj Volume: 10.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 4 2014-02-20 13-21-50\METODA 7.M (
                : Sequence Method)
Last changed    : 2/20/2014 1:21:50 PM by SYSTEM
  
```



Fraction Information

No Fractions found.

Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

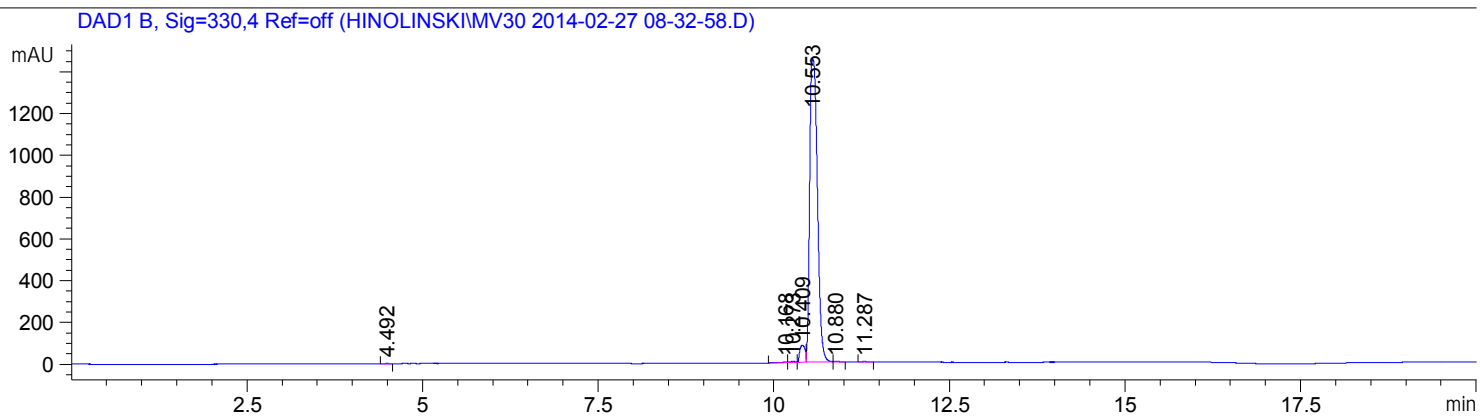
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.089	VV	0.0618	8.54477	1.70955	0.0479
2	9.155	VB	0.0707	12.71255	2.15816	0.0712
3	10.536	BV	0.0908	141.91032	23.05680	0.7949
4	10.683	VB	0.0870	51.84019	8.33943	0.2904
5	10.987	BB	0.0560	5.44765	1.17759	0.0305
6	11.254	BB	0.0884	9.70442	1.36534	0.0544
7	11.608	BV	0.1009	139.59642	18.31508	0.7819
8	11.964	VB	0.1659	1.74833e4	1601.37720	97.9289

Totals : 1.78530e4 1657.49914

\*\*\* End of Report \*\*\*

```

=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location : Vial 85
Injection Date  : 2/27/2014 8:34:10 AM
                                           Inj Volume : 10.000 µl
Acq. Method     : C:\CHEM32\1\METHODS\METODA 24.M
Last changed    : 2/27/2014 8:32:34 AM by SYSTEM
                  (modified after loading)
Analysis Method  : C:\CHEM32\1\METHODS\PRANJE.M
  
```



=====  
 Fraction Information  
 =====

No Fractions found.  
 =====

=====  
 Area Percent Report  
 =====

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.492	BB	0.0673	6.42647	1.17558	0.0556
2	10.168	BV	0.0933	18.56855	2.46612	0.1606
3	10.273	VV	0.0830	26.76161	4.24795	0.2314
4	10.409	VV	0.0862	426.93210	82.11183	3.6917
5	10.553	VB	0.1210	1.10575e4	1449.50037	95.6142
6	10.880	BB	0.0677	10.34705	1.97354	0.0895
7	11.287	BB	0.0784	18.17168	2.83167	0.1571

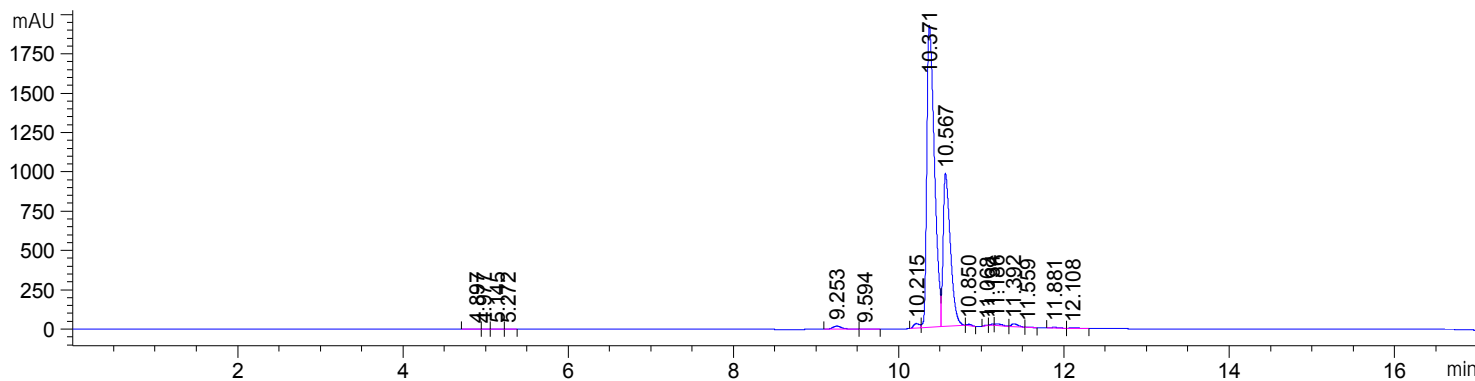
Totals :                    1.15647e4  1544.30705

=====  
 \*\*\* End of Report \*\*\*

=====

Acq. Operator	: SYSTEM	Seq. Line	: 1
Acq. Instrument	: HPLC-Solaja	Location	: Vial 21
Injection Date	: 2/19/2014 2:20:00 PM	Inj	: 1
		Inj Volume	: 5.000 µl
Method	: C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 2 2014-02-19 14-18-46\METODA 7.M (Sequence Method)		
Last changed	: 2/19/2014 2:18:46 PM by SYSTEM		

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\HINOLINSKI 2 2014-02-19 14-18-46\TEST000001.D)



=====  
Fraction Information  
=====

No Fractions found.  
=====

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.897	BV	0.1073	24.18136	2.84077	0.1276
2	4.977	VB	0.0554	8.57369	2.20271	0.0452
3	5.145	BV	0.0819	20.64248	3.01480	0.1089
4	5.272	VB	0.0673	7.01048	1.28158	0.0370
5	9.253	BV	0.1219	176.33762	21.35053	0.9307
6	9.594	VB	0.0936	9.36458	1.19286	0.0494
7	10.215	BV	0.0802	150.01939	29.57986	0.7918
8	10.371	VV	0.0992	1.23132e4	1922.30261	64.9853
9	10.567	VB	0.0940	5926.94336	974.06238	31.2806
10	10.850	BB	0.0654	37.13902	9.33766	0.1960
11	11.068	BB	0.0502	7.29534	2.17178	0.0385
12	11.134	BV	0.0427	21.07627	7.75579	0.1112
13	11.186	VB	0.0798	69.94500	11.52516	0.3691
14	11.392	BV	0.0884	96.42045	17.19282	0.5089
15	11.559	VB	0.0803	16.61453	2.84007	0.0877
16	11.881	BB	0.0897	36.33640	5.28650	0.1918
17	12.108	BB	0.0912	26.56188	3.88792	0.1402

Totals : 1.89477e4 3017.82580

=====  
\*\*\* End of Report \*\*\*



Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.598	BV	0.0737	140.26274	27.65811	0.7675
2	8.344	BB	0.0408	103.46177	39.16729	0.5662
3	8.533	VV	0.0752	1.39331e4	2867.69385	76.2442
4	8.731	VB	0.0612	3441.26855	783.84924	18.8312
5	9.005	VB	0.0527	106.27769	29.41607	0.5816
6	9.261	BV	0.0698	364.46271	86.19911	1.9944
7	9.370	VB	0.0553	150.82022	39.68163	0.8253
8	9.477	BB	0.0490	34.65574	10.37789	0.1896

Totals : 1.82743e4 3884.04320

=====  
\*\*\* End of Report \*\*\*



Sample Name: DOJK09-G

## Compound 65

## Method C

```

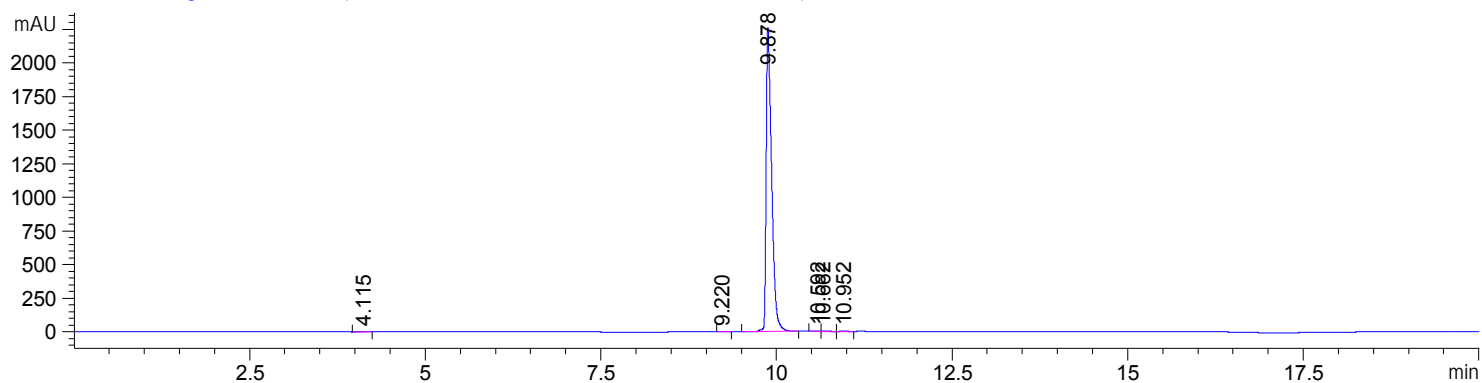
=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location  : Vial 82
Injection Date  : 2/26/2014 7:59:02 PM
                                           Inj Volume : 1.000 µl

Acq. Method     : C:\CHEM32\1\METHODS\METODA 7.M
Last changed    : 2/26/2014 7:52:38 PM by SYSTEM
                 (modified after loading)

Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M
Last changed    : 9/18/2013 2:53:53 PM by SYSTEM
=====

```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\DOJK09-G 2014-02-26 19-57-56.D)



```

=====
Fraction Information
=====

```

```

=====
No Fractions found.
=====

```

```

=====
Area Percent Report
=====

```

```

Sorted By           :      Signal
Multiplier          :      1.0000
Dilution            :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.115	BB	0.1399	15.96979	1.36559	0.1294
2	9.220	BB	0.0590	9.45455	1.98570	0.0766
3	9.878	BB	0.0843	1.22533e4	2258.72559	99.2982
4	10.592	VV	0.0887	27.94959	4.17232	0.2265
5	10.662	VB	0.0714	20.14357	3.76592	0.1632
6	10.952	BB	0.0733	13.08130	2.17050	0.1060

```
Totals :                1.23399e4  2272.18561
```

```

=====
*** End of Report ***

```

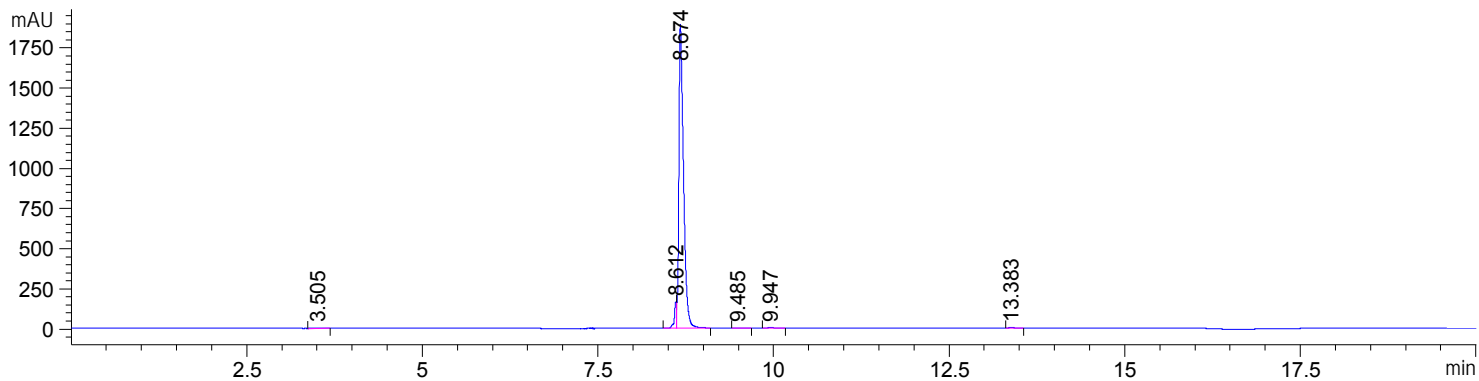




```

=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location  : Vial 72
Injection Date  : 2/27/2014 5:41:07 PM
                                           Inj Volume : 2.000 µl
Acq. Method     : C:\CHEM32\1\METHODS\METODA 24.M
Last changed    : 2/27/2014 5:39:53 PM by SYSTEM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M
Last changed    : 9/18/2013 2:53:53 PM by SYSTEM
  
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\DOZS15 2014-02-27 17-39-59.D)



=====  
 Fraction Information  
 =====

No Fractions found.  
 =====

=====  
 Area Percent Report  
 =====

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.505	VB	0.1397	21.50900	1.85658	0.2362
2	8.612	BV	0.0337	369.45660	164.55032	4.0564
3	8.674	VV	0.0710	8677.65723	1891.88940	95.2748
4	9.485	BB	0.0673	7.12599	1.29212	0.0782
5	9.947	BB	0.0775	14.55247	2.55314	0.1598
6	13.383	BB	0.0620	17.73038	4.05211	0.1947

Totals : 9108.03167 2066.19368

=====  
 \*\*\* End of Report \*\*\*



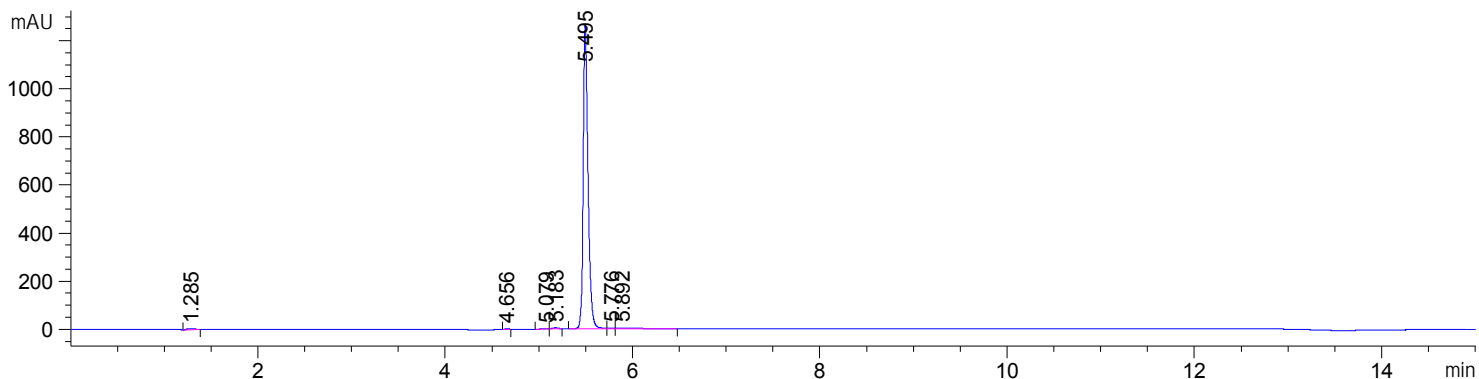
```

=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location : Vial 5
Injection Date  : 2/28/2014 10:30:04 AM
                                           Inj Volume : 2.000 µl

Acq. Method     : C:\CHEM32\1\METHODS\METODA 25.M
Last changed    : 2/28/2014 10:28:47 AM by SYSTEM
                  (modified after loading)

Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M
Last changed    : 9/18/2013 2:53:53 PM by SYSTEM
  
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\DOZS12 2014-02-28 10-28-51.D)



=====  
 Fraction Information  
 =====

No Fractions found.  
 =====

=====  
 Area Percent Report  
 =====

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.285	BB	0.0764	30.82211	5.10553	0.6626
2	4.656	BV	0.0422	12.17721	4.09883	0.2618
3	5.079	BV	0.0544	11.05448	2.69109	0.2376
4	5.183	VV	0.0616	22.25791	4.98515	0.4785
5	5.495	BV	0.0538	4514.38184	1260.92078	97.0470
6	5.776	VV	0.0597	14.55320	3.22330	0.3129
7	5.892	VB	0.1987	46.50219	2.79328	0.9997

Totals :                      4651.74893 1283.81795

=====  
 \*\*\* End of Report \*\*\*

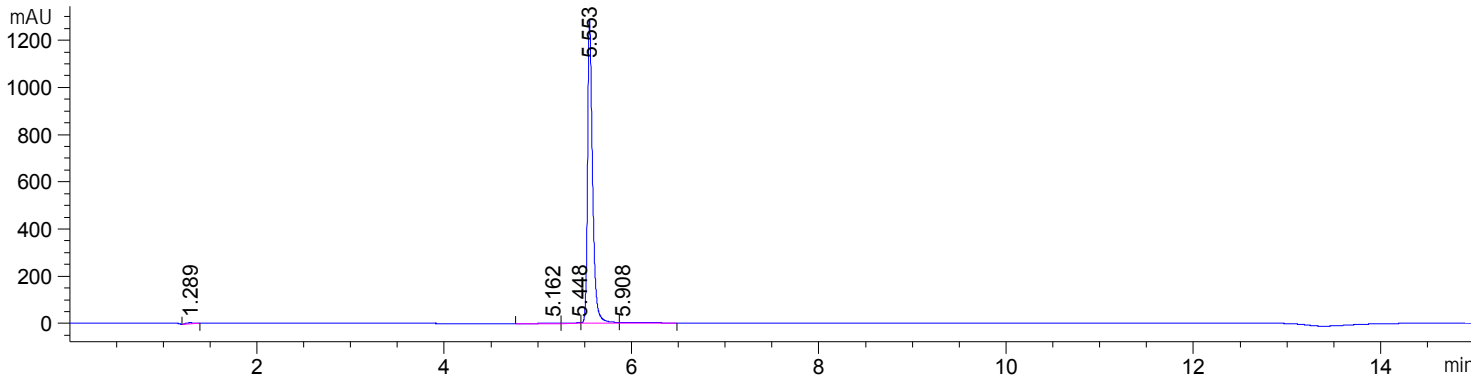


Sample Name: MV22      Compound 45      Method D

```

=====
Acq. Operator   : SYSTEM                               Seq. Line :    9
Acq. Instrument : HPLC-Solaja                          Location  : Vial 71
Injection Date  : 2/27/2014 11:56:36 PM                Inj       :    1
                                                    Inj Volume: 2.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\METODA 25.M (
                  Sequence Method)
Last changed    : 2/27/2014 9:05:38 PM by SYSTEM
    
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\TEST000009.D)



Fraction Information

No Fractions found.

Area Percent Report

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
    
```

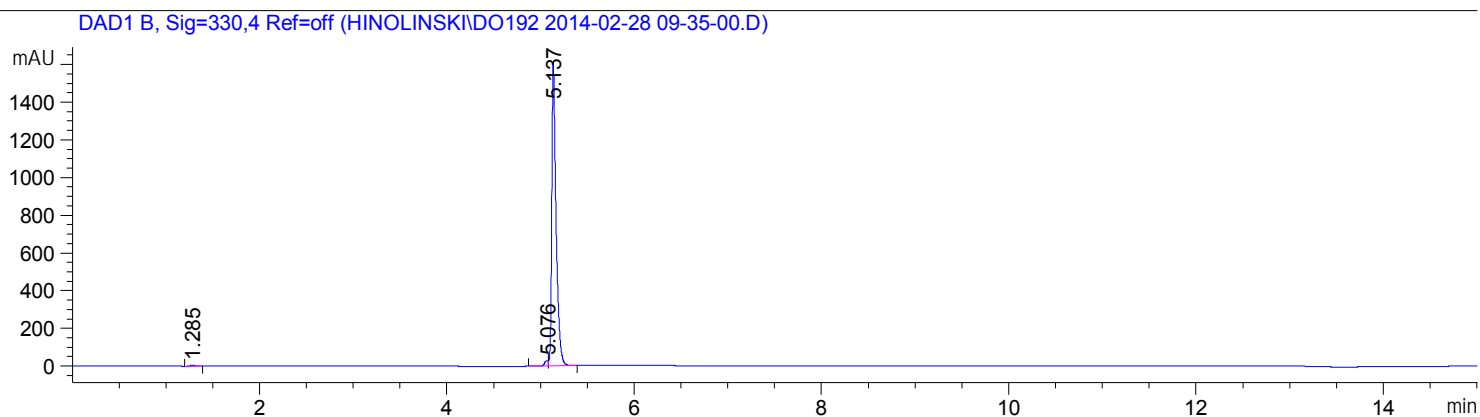
Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.289	BB	0.0772	32.15473	5.23525	0.6476
2	5.162	BV	0.1235	31.88377	3.17802	0.6421
3	5.448	VV	0.0875	29.10960	4.27066	0.5862
4	5.553	VV	0.0558	4808.14307	1280.33252	96.8295
5	5.908	VB	0.2011	64.28740	3.75680	1.2947

Totals :                      4965.57857 1296.77325

\*\*\* End of Report \*\*\*

=====  
Acq. Operator : SYSTEM  
Acq. Instrument : HPLC-Solaja Location : Vial 54  
Injection Date : 2/28/2014 9:36:13 AM Inj Volume : 2.000 µl  
Acq. Method : C:\CHEM32\1\METHODS\METODA 25.M  
Last changed : 2/28/2014 9:12:27 AM by SYSTEM  
(modified after loading)  
Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M  
Last changed : 9/18/2013 2:53:53 PM by SYSTEM  
(modified after loading)



=====  
Fraction Information  
=====

No Fractions found.  
=====

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.285	BB	0.0900	31.90867	5.24447	0.6086
2	5.076	BV	0.0408	73.09942	28.11178	1.3943
3	5.137	VB	0.0457	5137.63428	1611.56714	97.9970

Totals : 5242.64236 1644.92340

=====  
\*\*\* End of Report \*\*\*

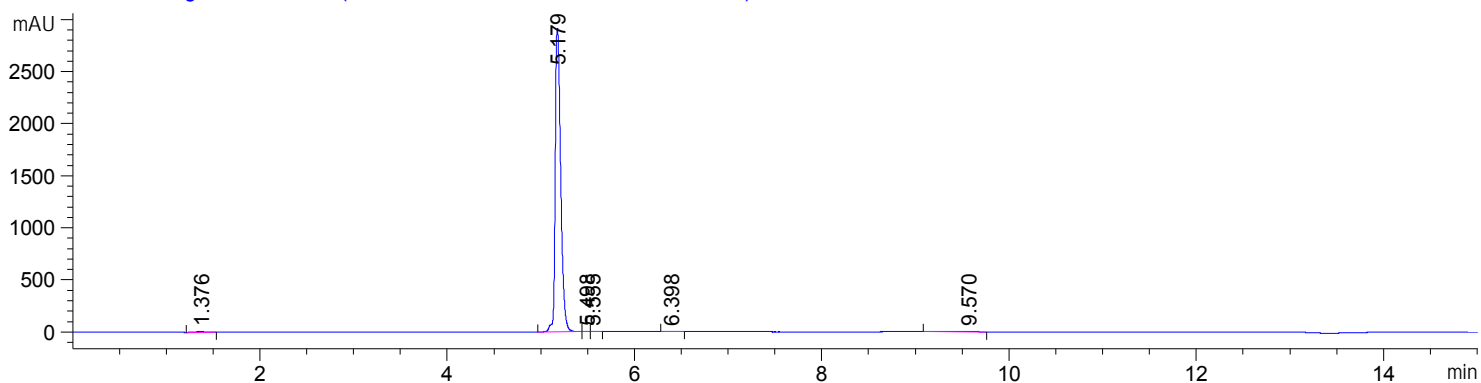
Sample Name: ST14 Compound 56

```

=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location : Vial 54
Injection Date  : 2/27/2014 8:30:42 PM
                                           Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\METHODS\METODA 24.M
Last changed    : 2/27/2014 8:33:45 PM by SYSTEM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M
Last changed    : 9/18/2013 2:53:53 PM by SYSTEM
=====

```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\UVFI 2014-02-27 20-29-26.D)



```

=====
Fraction Information
=====

```

```

=====
No Fractions found.
=====

```

```

=====
Area Percent Report
=====

```

```

Sorted By       : Signal
Multiplier      : 1.0000
Dilution        : 1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.376	BB	0.1502	70.69771	5.77826	0.5856
2	5.179	VV	0.0552	1.19118e4	2914.95850	98.6723
3	5.498	VV	0.0564	12.32152	2.88321	0.1021
4	5.555	VB	0.0545	10.09038	2.22248	0.0836
5	6.398	VB	0.0602	16.21222	3.36451	0.1343
6	9.570	BB	0.2250	50.95580	2.66631	0.4221

```
Totals :                1.20721e4  2931.87327
```

```

=====
*** End of Report ***

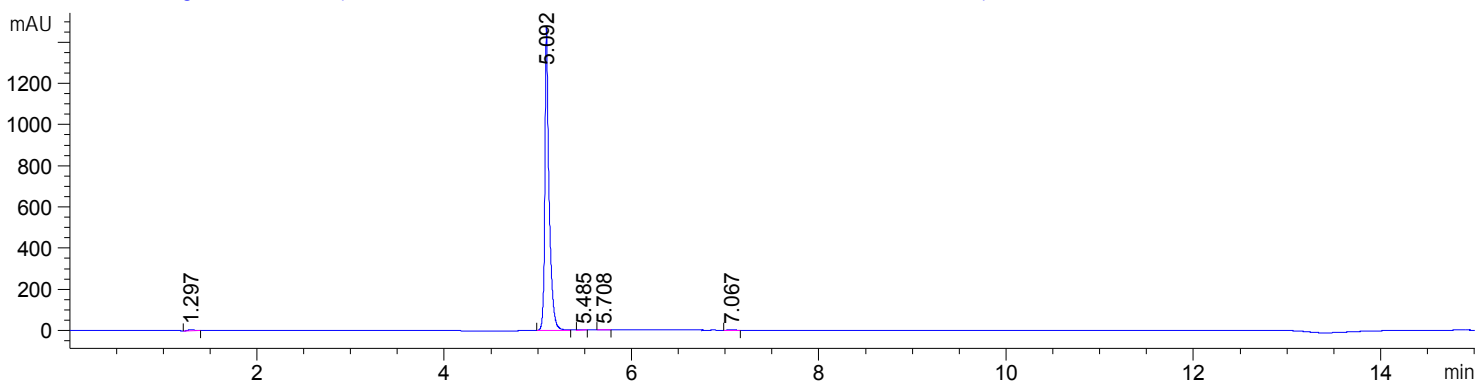
```



```

=====
Acq. Operator   : SYSTEM                               Seq. Line :    2
Acq. Instrument : HPLC-Solaja                          Location  : Vial 72
Injection Date  : 2/27/2014 9:28:04 PM                Inj       :    1
                                                    Inj Volume: 2.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\METODA 25.M (
                  Sequence Method)
Last changed    : 2/27/2014 9:05:38 PM by SYSTEM
  
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\TEST000002.D)



Fraction Information

No Fractions found.

Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.297	BB	0.0766	30.77659	5.15579	0.6570
2	5.092	BV	0.0443	4631.22754	1468.61035	98.8594
3	5.485	VV	0.0625	8.02072	1.55961	0.1712
4	5.708	VV	0.0625	8.42438	1.72487	0.1798
5	7.067	BB	0.0536	6.20943	1.68097	0.1325

Totals : 4684.65866 1478.73159

\*\*\* End of Report \*\*\*

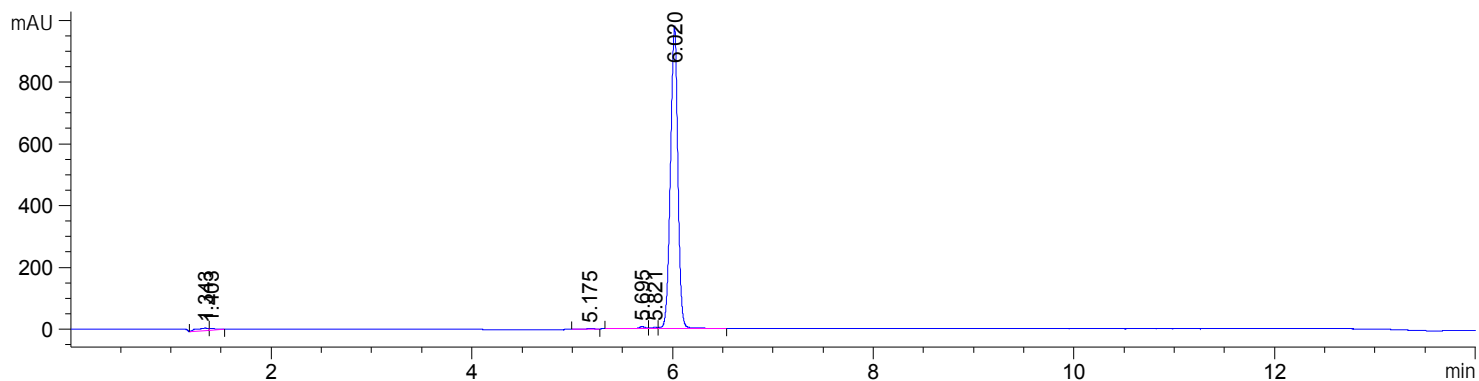
Sample Name: D0178 Compound 58 Method D

```

=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location : Vial 87
Injection Date  : 2/28/2014 8:55:56 AM
                                           Inj Volume : 7.500 µl
Acq. Method     : C:\CHEM32\1\METHODS\METODA 25.M
Last changed    : 2/28/2014 8:54:30 AM by SYSTEM
                  (modified after loading)
Analysis Method  : C:\CHEM32\1\METHODS\PRANJE.M
Last changed    : 9/18/2013 2:53:53 PM by SYSTEM
=====

```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\DO178 2014-02-28 08-54-42.D)



```

=====
Fraction Information
=====

```

```

=====
No Fractions found.
=====

```

```

=====
Area Percent Report
=====

```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.343	BV	0.1169	67.87621	7.51195	1.3109
2	1.403	VB	0.0573	23.39939	5.42418	0.4519
3	5.175	BV	0.0677	8.89435	1.59157	0.1718
4	5.695	BV	0.0760	43.59182	7.58748	0.8419
5	5.821	VV	0.0586	18.57452	3.96548	0.3587
6	6.020	VB	0.0793	5015.60059	977.76709	96.8648

```
Totals :                5177.93688 1003.84776
```

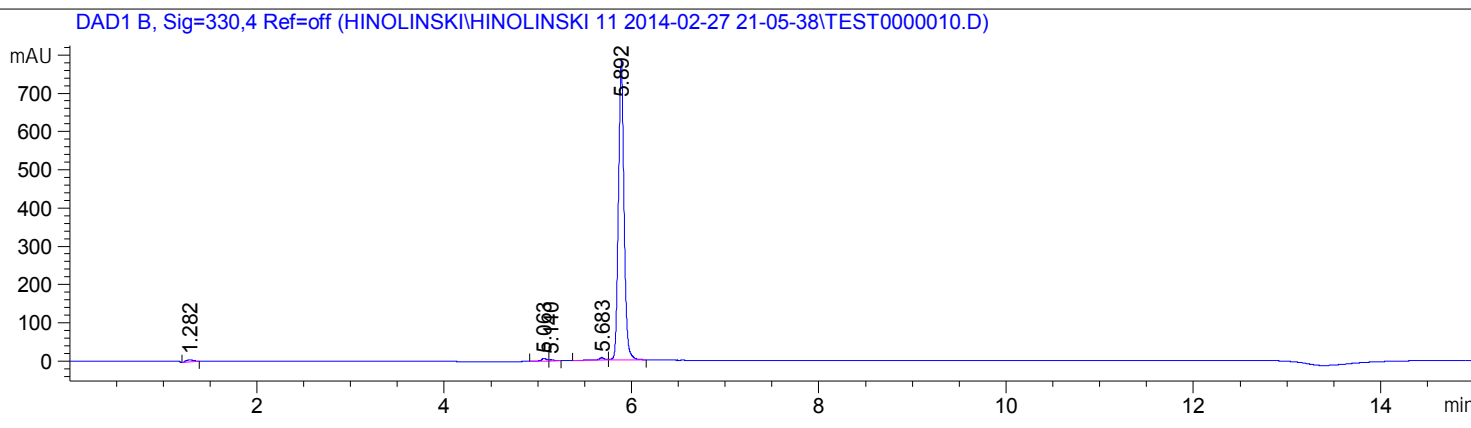
```

=====
*** End of Report ***

```

```

=====
Acq. Operator   : SYSTEM                               Seq. Line :   10
Acq. Instrument : HPLC-Solaja                          Location  : Vial 61
Injection Date  : 2/28/2014 12:17:50 AM                Inj       :    1
                                                    Inj Volume: 2.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\METODA 25.M (
                  Sequence Method)
Last changed    : 2/27/2014 9:05:38 PM by SYSTEM
  
```



Fraction Information

No Fractions found.

Area Percent Report

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

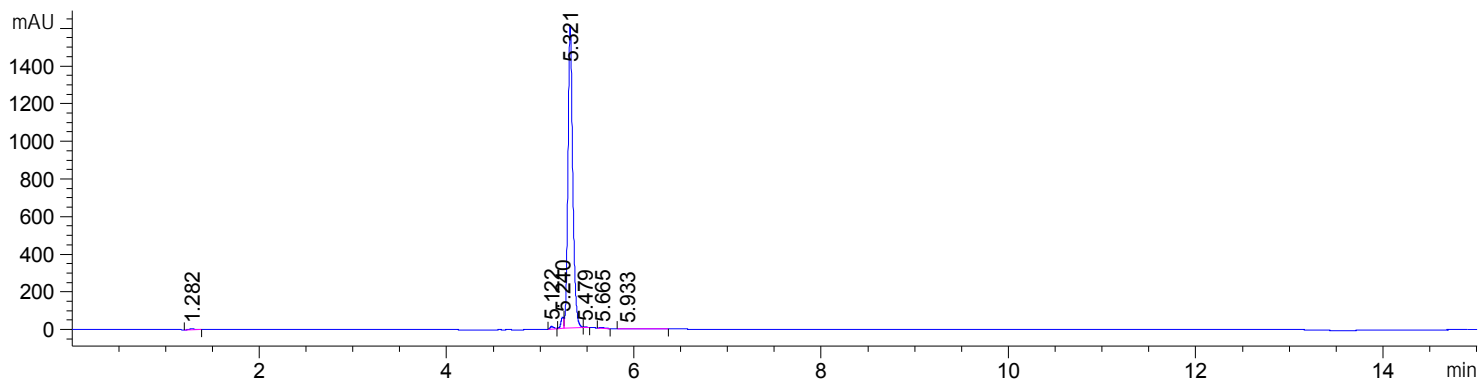
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.282	BB	0.0879	31.53892	5.34119	0.9388
2	5.063	BV	0.0566	26.59043	6.95812	0.7915
3	5.140	VB	0.0493	11.97652	3.34003	0.3565
4	5.683	BV	0.0710	36.46378	6.86361	1.0854
5	5.892	VB	0.0655	3252.84106	782.67798	96.8277

Totals :                      3359.41072    805.18092

\*\*\* End of Report \*\*\*

=====  
Acq. Operator : SYSTEM  
Acq. Instrument : HPLC-Solaja Location : Vial 53  
Injection Date : 2/28/2014 10:54:17 AM Inj Volume : 2.000 µl  
Acq. Method : C:\CHEM32\1\METHODS\METODA 25.M  
Last changed : 2/28/2014 10:28:47 AM by SYSTEM  
(modified after loading)  
Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M  
Last changed : 9/18/2013 2:53:53 PM by SYSTEM

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\DO180 2014-02-28 10-53-04.D)



=====  
Fraction Information  
=====

No Fractions found.  
=====

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 2: DAD1 B, Sig=330,4 Ref=off

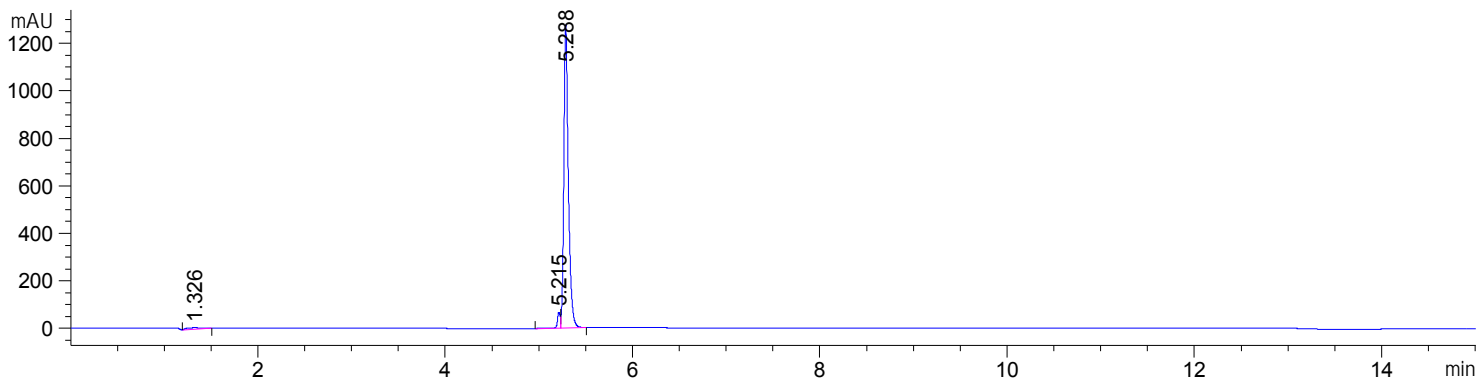
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.282	BB	0.0746	31.32107	5.21197	0.5260
2	5.122	BB	0.0346	30.97727	13.10603	0.5202
3	5.240	BV	0.0324	123.60563	59.16384	2.0758
4	5.321	VV	0.0536	5735.92188	1607.23230	96.3262
5	5.479	VB	0.0357	10.29071	4.26195	0.1728
6	5.665	BB	0.0448	11.20796	3.41772	0.1882
7	5.933	VB	0.1189	11.36069	1.14377	0.1908

Totals : 5954.68520 1693.53758

=====  
\*\*\* End of Report \*\*\*

=====  
Acq. Operator : SYSTEM  
Acq. Instrument : HPLC-Solaja Location : Vial 85  
Injection Date : 2/28/2014 10:02:20 AM Inj Volume : 5.000 µl  
Acq. Method : C:\CHEM32\1\METHODS\METODA 25.M  
Last changed : 2/28/2014 10:01:03 AM by SYSTEM  
(modified after loading)  
Analysis Method : C:\CHEM32\1\METHODS\PRANJE.M  
Last changed : 9/18/2013 2:53:53 PM by SYSTEM  
=====

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\MV30 2014-02-28 10-01-10.D)



=====  
Fraction Information  
=====

No Fractions found.  
=====

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.326	BB	0.1329	70.05448	6.49267	1.5604
2	5.215	BV	0.0298	133.64371	66.92734	2.9768
3	5.288	VB	0.0492	4285.82715	1276.07971	95.4628

Totals : 4489.52534 1349.49972

=====  
\*\*\* End of Report \*\*\*  
=====

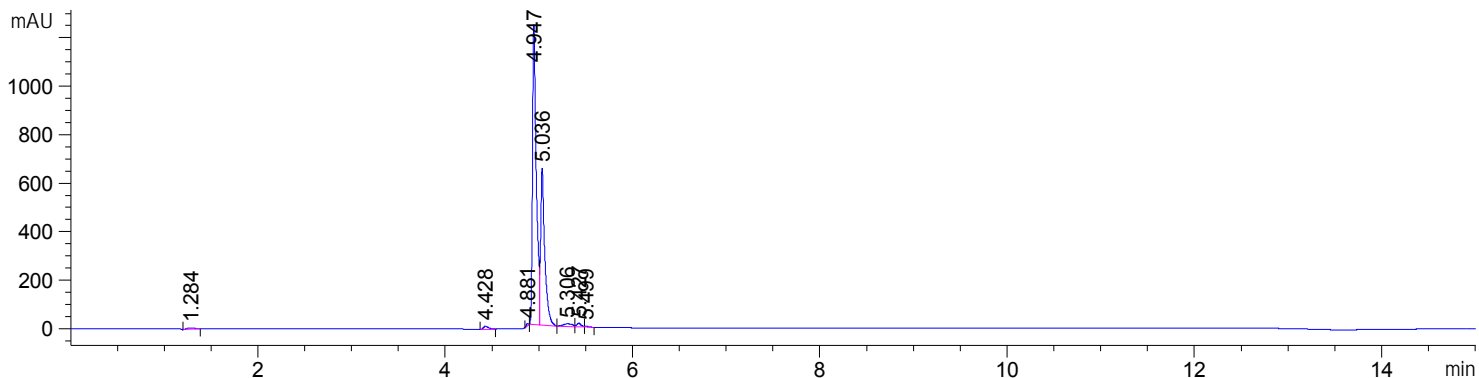
```

=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location : Vial 21
Injection Date  : 2/28/2014 9:17:02 AM
                                           Inj Volume : 2.000 µl

Acq. Method     : C:\CHEM32\1\METHODS\METODA 25.M
Last changed    : 2/28/2014 9:12:27 AM by SYSTEM
                  (modified after loading)

Analysis Method  : C:\CHEM32\1\METHODS\PRANJE.M
Last changed    : 9/18/2013 2:53:53 PM by SYSTEM
  
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\JK05 2014-02-28 09-15-51.D)



Fraction Information

No Fractions found.

Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
se Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.284	BB	0.0762	30.68703	5.20760	0.5389
2	4.428	BV	0.0558	44.56494	12.14464	0.7826
3	4.881	BB	0.0273	14.29690	8.65168	0.2511
4	4.947	BV	0.0402	3469.44141	1236.32007	60.9227
5	5.036	VB	0.0435	2001.60938	647.83722	35.1479
6	5.306	BV	0.0763	75.77526	12.75458	1.3306
7	5.427	VV	0.0473	48.33295	14.92499	0.8487
8	5.499	VB	0.0419	10.11355	3.37761	0.1776

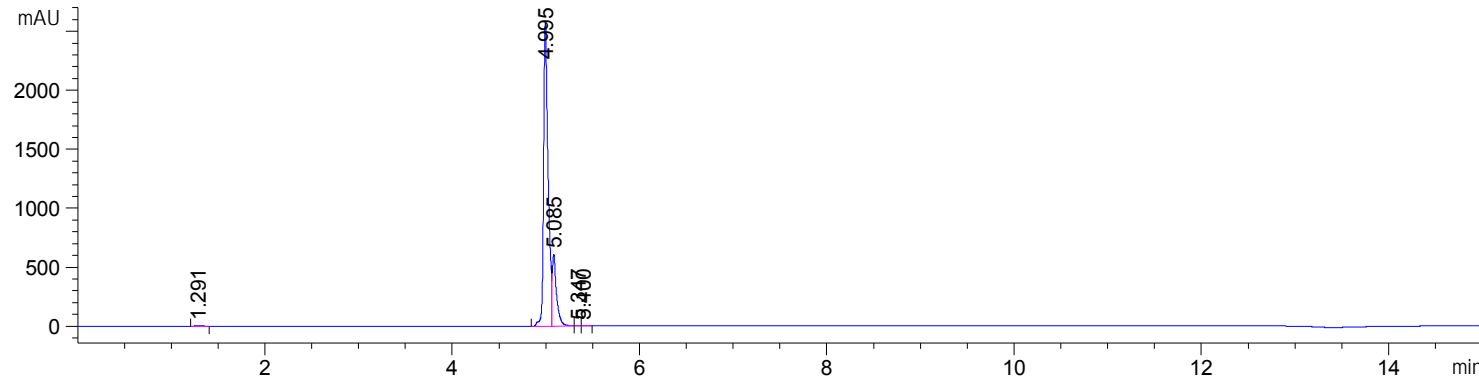
Totals : 5694.82140 1941.21838

\*\*\* End of Report \*\*\*

```

=====
Acq. Operator   : SYSTEM                               Seq. Line :    5
Acq. Instrument : HPLC-Solaja                          Location  : Vial 74
Injection Date  : 2/27/2014 10:31:48 PM              Inj       :    1
                                                    Inj Volume: 2.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\METODA 25.M (
                  Sequence Method)
Last changed    : 2/27/2014 9:05:38 PM by SYSTEM
  
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\TEST000005.D)



Fraction Information

No Fractions found.

Area Percent Report

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.291	BB	0.0761	33.34475	5.36028	0.3144
2	4.995	BV	0.0488	8674.29395	2574.86401	81.7809
3	5.085	VV	0.0431	1884.24561	608.60223	17.7646
4	5.347	VV	0.0493	8.57778	2.23154	0.0809
5	5.400	VB	0.0514	6.29111	1.60006	0.0593

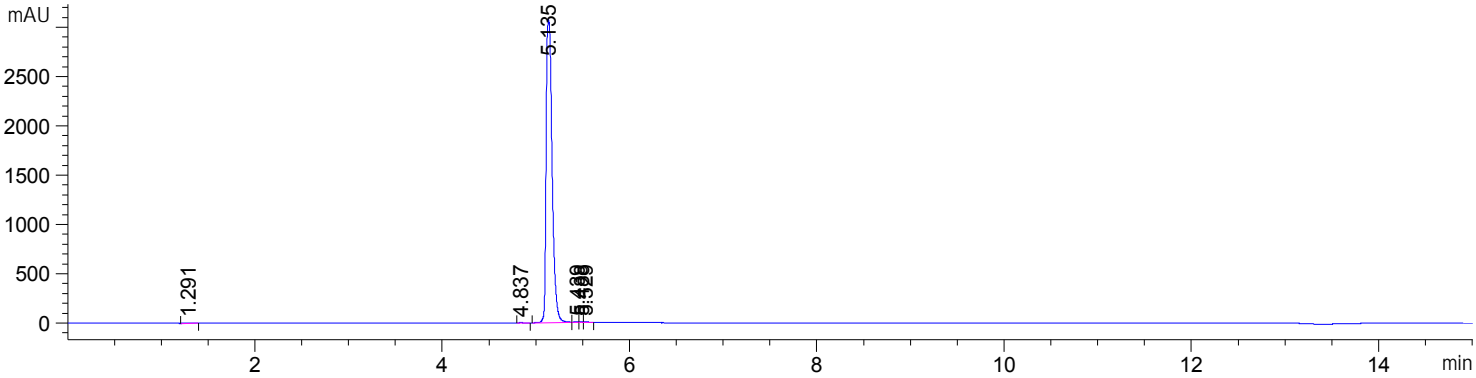
Totals :                      1.06068e4   3192.65812

\*\*\* End of Report \*\*\*

```

=====
Acq. Operator   : SYSTEM                               Seq. Line :    6
Acq. Instrument : HPLC-Solaja                          Location  : Vial 73
Injection Date  : 2/27/2014 10:53:00 PM                Inj       :    1
                                                    Inj Volume: 2.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\METODA 25.M (
                  Sequence Method)
Last changed    : 2/27/2014 9:05:38 PM by SYSTEM
  
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\TEST000006.D)



=====  
 Fraction Information  
 =====

No Fractions found.

=====  
 Area Percent Report  
 =====

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.291	BB	0.0843	32.10134	5.14675	0.2346
2	4.837	BB	0.0448	16.26962	5.09167	0.1189
3	5.135	BB	0.0545	1.35803e4	3076.87012	99.2306
4	5.439	BV	0.0365	14.59687	5.77229	0.1067
5	5.488	VV	0.0364	16.51150	6.66786	0.1206
6	5.529	VB	0.0421	25.82304	8.83148	0.1887

Totals :                      1.36856e4   3108.38018

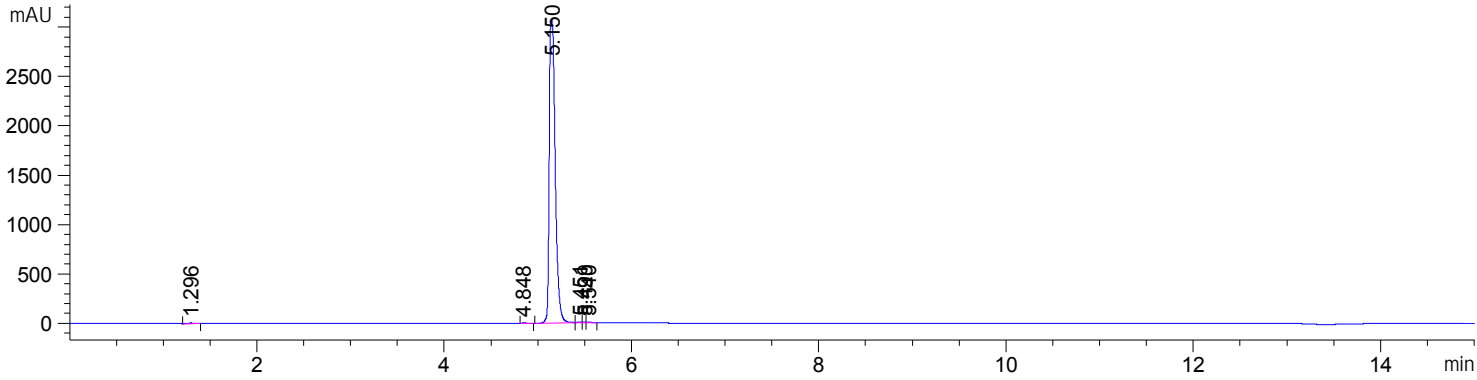
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 \*\*\* End of Report \*\*\*



```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    3
Acq. Instrument : HPLC-Solaja                 Location  : Vial 73
Injection Date  : 2/27/2014 9:49:14 PM      Inj       :    1
                                           Inj Volume: 2.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\METODA 25.M (
                  Sequence Method)
Last changed    : 2/27/2014 9:05:38 PM by SYSTEM
  
```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\TEST000003.D)



Fraction Information

No Fractions found.

Area Percent Report

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 2: DAD1 B, Sig=330,4 Ref=off

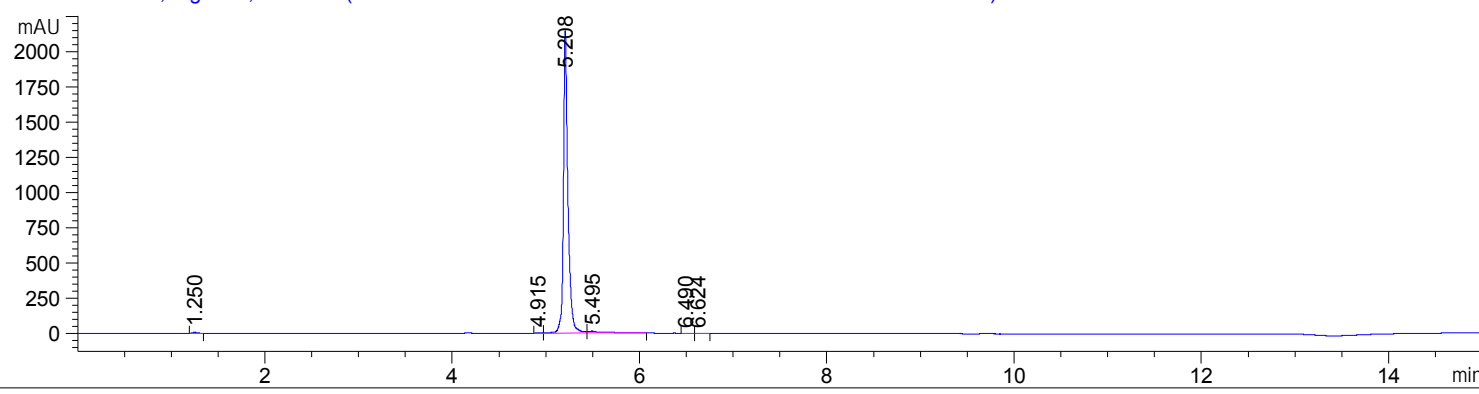
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.296	BB	0.0732	31.22255	5.15455	0.2272
2	4.848	BB	0.0475	16.73750	5.07316	0.1218
3	5.150	BB	0.0543	1.36351e4	3073.64551	99.2389
4	5.451	BV	0.0366	14.51578	5.71865	0.1056
5	5.499	VV	0.0346	16.28599	6.64245	0.1185
6	5.540	VB	0.0420	25.80930	8.72343	0.1878

Totals : 1.37397e4 3104.95775

\*\*\* End of Report \*\*\*

```

=====
Acq. Operator   : SYSTEM                               Seq. Line :    4
Acq. Instrument : HPLC-Solaja                          Location  : Vial 63
Injection Date  : 2/27/2014 10:10:30 PM                Inj       :    1
                                                    Inj Volume: 2.000 µl
Method          : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\METODA 25.M (
                  Sequence Method)
Last changed    : 2/27/2014 9:05:38 PM by SYSTEM
DAD1 A, Sig=254,4 Ref=off (HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\TEST000004.D)
  
```



Fraction Information

No Fractions found.

Area Percent Report

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

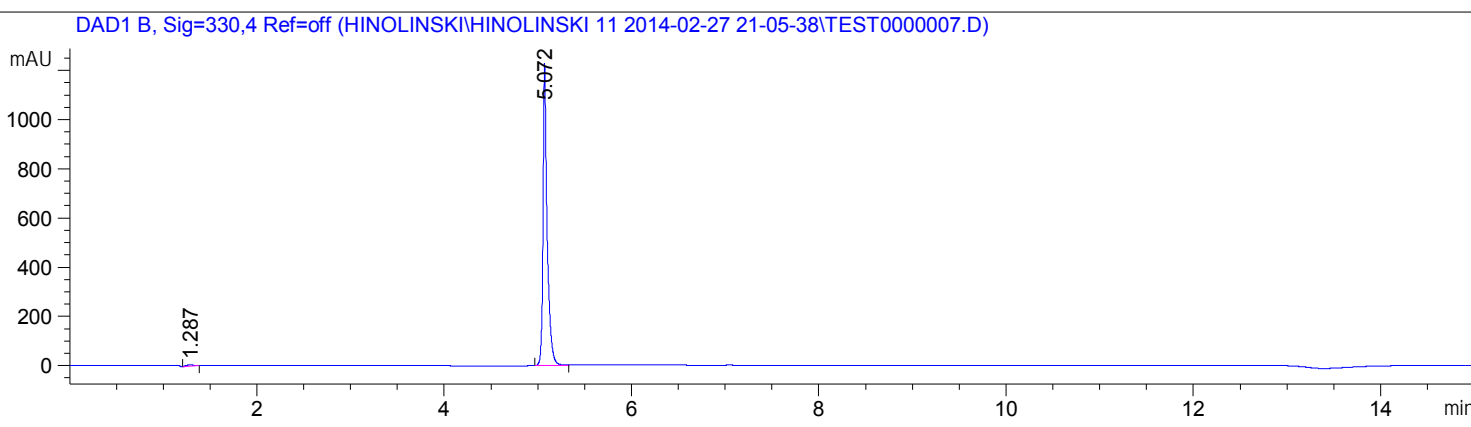
Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.250	BB	0.0775	38.33717	8.06219	0.5200
2	4.915	BV	0.0549	6.66064	1.65775	0.0903
3	5.208	VV	0.0468	7133.92041	2146.30713	96.7591
4	5.495	VB	0.1583	182.20453	14.23526	2.4713
5	6.490	VV	0.0705	6.17663	1.08386	0.0838
6	6.624	VB	0.0591	5.56605	1.24736	0.0755

Totals : 7372.86544 2172.59354

\*\*\* End of Report \*\*\*

=====  
Acq. Operator : SYSTEM Seq. Line : 7  
Acq. Instrument : HPLC-Solaja Location : Vial 72  
Injection Date : 2/27/2014 11:14:09 PM Inj : 1  
Inj Volume : 2.000 µl  
Method : C:\CHEM32\1\DATA\HINOLINSKI\HINOLINSKI 11 2014-02-27 21-05-38\METODA 25.M ( Sequence Method)  
Last changed : 2/27/2014 9:05:38 PM by SYSTEM



=====  
Fraction Information  
=====

No Fractions found.

=====  
Area Percent Report  
=====

Sorted By : Signal  
Multiplier : 1.0000  
Dilution : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.287	BB	0.0899	30.25244	5.05081	0.7935
2	5.072	BV	0.0435	3782.41846	1227.06824	99.2065

Totals : 3812.67089 1232.11905

=====  
\*\*\* End of Report \*\*\*

```

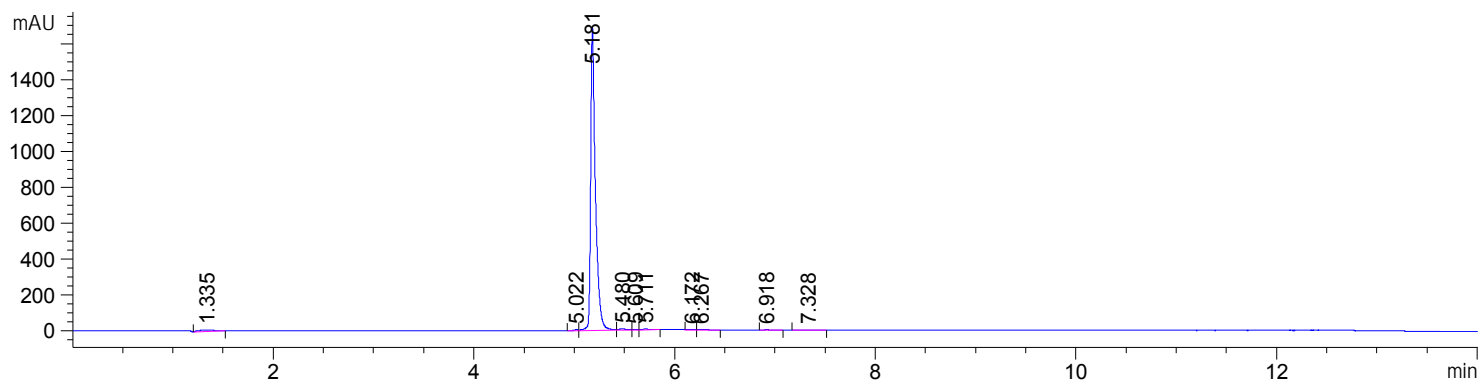
=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC-Solaja           Location : Vial 75
Injection Date  : 2/28/2014 8:35:00 AM
                                           Inj Volume : 5.000 µl

Acq. Method     : C:\CHEM32\1\METHODS\METODA 25.M
Last changed    : 2/28/2014 8:35:51 AM by SYSTEM
                  (modified after loading)

Analysis Method  : C:\CHEM32\1\METHODS\PRANJE.M
Last changed    : 9/18/2013 2:53:53 PM by SYSTEM
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```

DAD1 B, Sig=330,4 Ref=off (HINOLINSKI\DOZS18 2014-02-28 08-33-43.D)



```

=====
Fraction Information
=====

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=====
No Fractions found.
=====

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```

=====
Area Percent Report
=====

```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 2: DAD1 B, Sig=330,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.335	BB	0.1327	75.52184	7.03539	1.3104
2	5.022	BV	0.0386	11.59436	4.34548	0.2012
3	5.181	VV	0.0463	5550.89209	1691.44263	96.3123
4	5.480	VV	0.0821	41.15622	6.85275	0.7141
5	5.609	VV	0.0464	9.74525	2.67977	0.1691
6	5.711	VB	0.0670	24.94572	4.93526	0.4328
7	6.172	VV	0.0567	5.22887	1.11552	0.0907
8	6.267	VB	0.0753	18.34690	3.25498	0.3183
9	6.918	BB	0.0556	13.23581	3.66509	0.2297
10	7.328	BB	0.0749	12.76073	2.17729	0.2214

```
Totals :                5763.42779 1727.50416
```

```

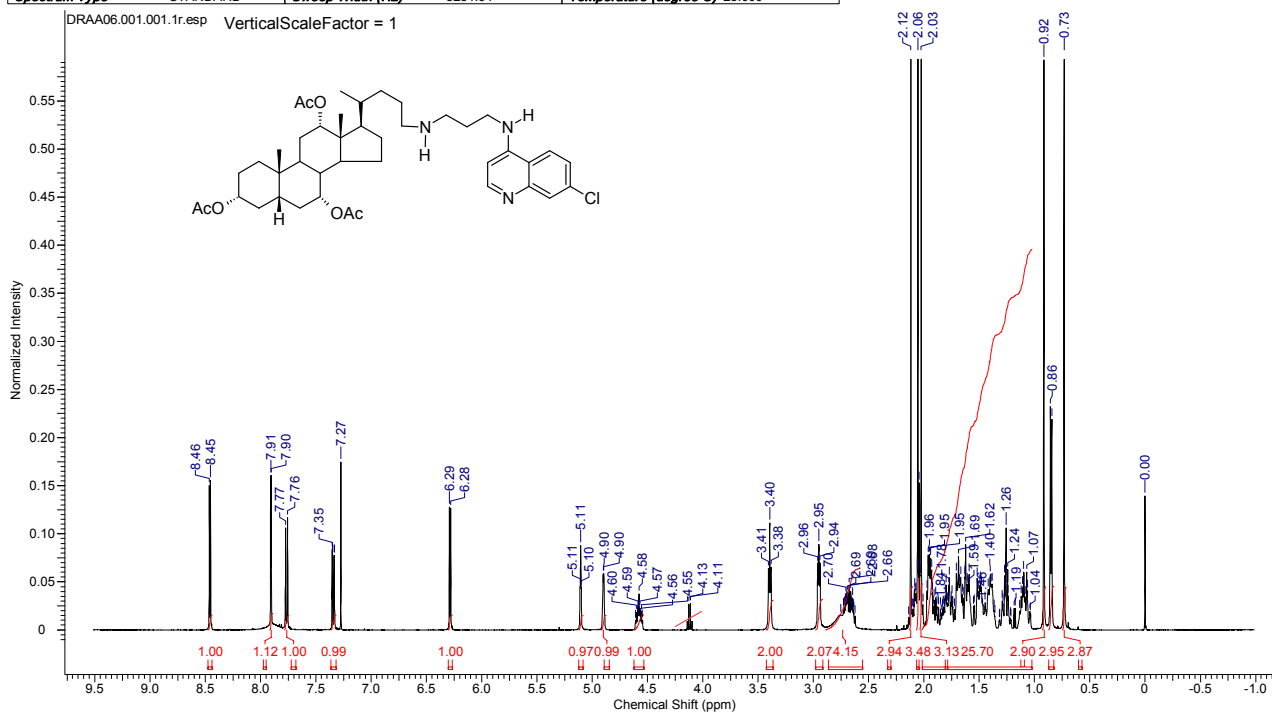
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*** End of Report ***

```

**Compound 13 (DR06):**  $^1\text{H}$  NMR spectrum (500 MHz). HPLC purity: method A: RT 2.092, area 98.69 %; method B: RT 8.698, area 95.46 %.

2/26/2014 11:33:48 AM

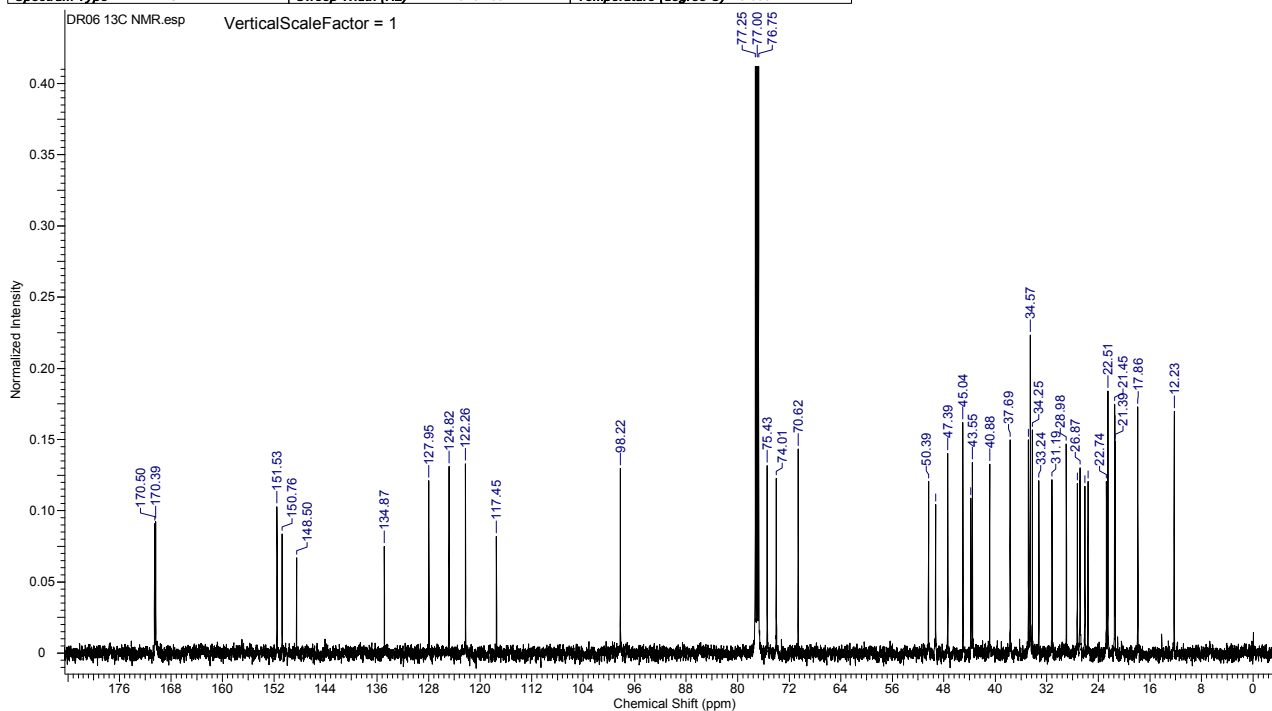
Number of Nuclei 0 H's					
Acquisition Time (sec)	3.1195	Date	22 May 2009 10:53:20	Date Stamp	22 May 2009 10:53:20
File Name	C:\Users\Dejan\Openical\Documents\Radovi\Aminohinoliniski\DO152\i\ostali\Recenzija\Spektri NMR_Ostalo\DR06\DR06\1\pdata\111r				
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16
Original Points Count	16384	Owner	nmsu	Points Count	32768
Receiver Gain	80.60	SW(cyclical) (Hz)	5252.10	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	5251.94	Temperature (degree C)	25.000
				Pulse Sequence	zg30
				Spectrum Offset (Hz)	2132.0439



**Compound 13 (DR06):**  $^{13}\text{C}$  NMR spectrum (125 MHz).

2/26/2014 11:38:43 AM

Number of Nuclei 0 C's					
Acquisition Time (sec)	0.5505	Date	22 May 2009 11:06:08	Date Stamp	22 May 2009 11:06:08
File Name	C:\Users\Dejan\Openical\Documents\Radovi\Aminohinoliniski\DO152\i\ostali\Recenzija\Spektri NMR_Ostalo\DR06\DR06\2\pdata\111r				
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	516
Original Points Count	16384	Owner	nmsu	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000
				Pulse Sequence	zgpg30
				Spectrum Offset (Hz)	13830.7002

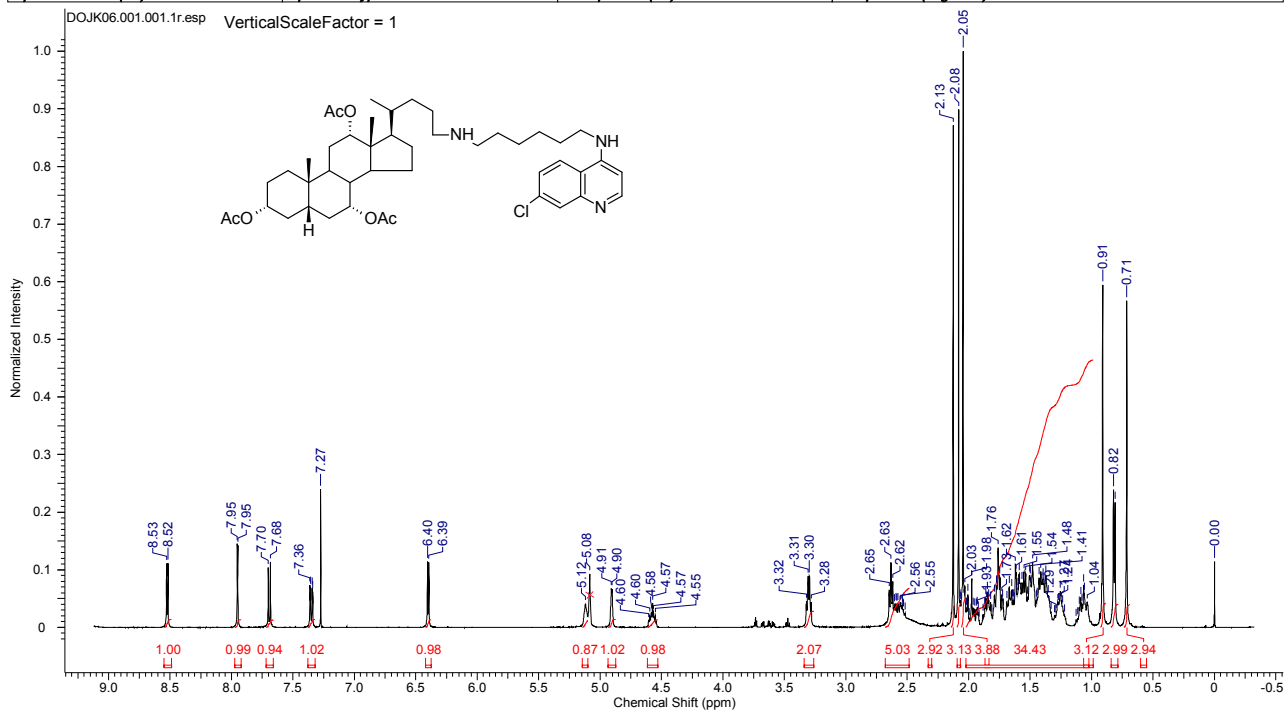




**Compound 15 (DOJK06):**  $^1\text{H}$  NMR spectrum (500 MHz). HPLC purity: method A: RT 1.971, area 99.39 %; method C: RT 11.700, area 95.41 %.

2/26/2014 3:48:05 PM

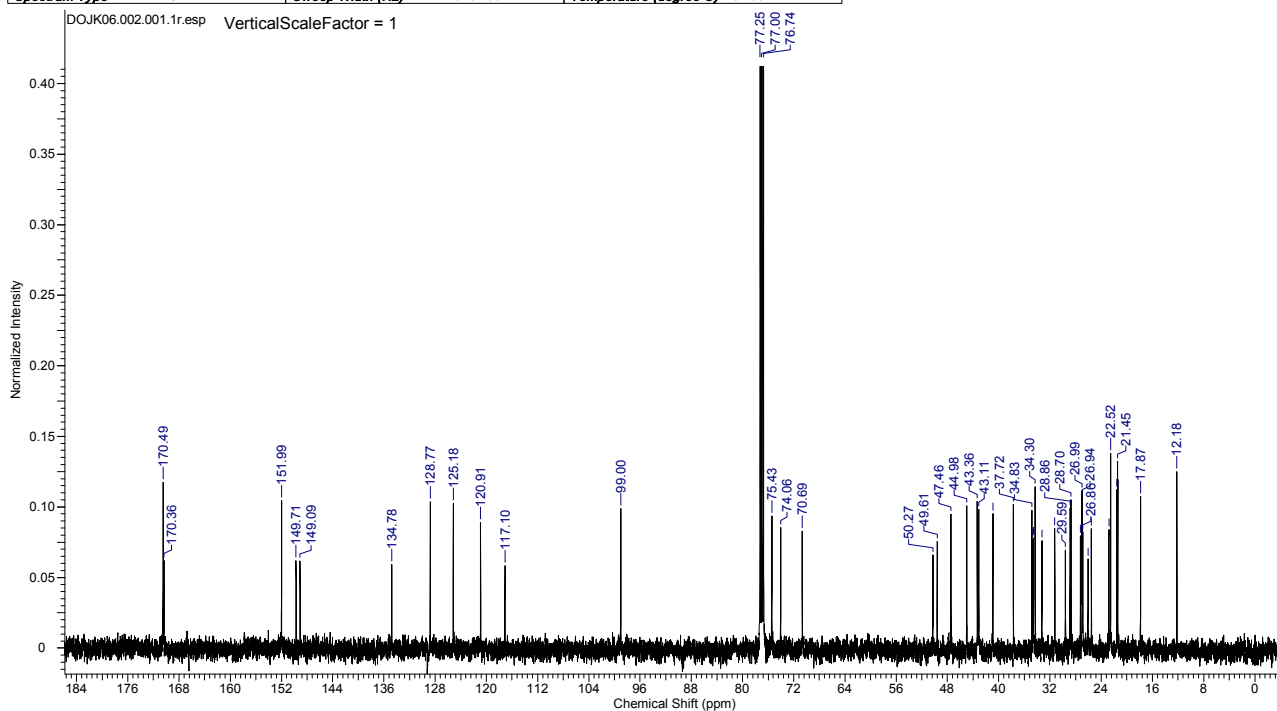
Number of Nuclei 0 H's					
Acquisition Time (sec)	3.4669	Date	22 Mar 2011 15:58:08	Date Stamp	22 Mar 2011 15:58:08
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DOJK06.1\pdata\111r				
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16
Original Points Count	16384	Owner	nmrsu	Points Count	32768
Receiver Gain	101.00	SW(cyclical) (Hz)	4725.90	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2200.9209	Spectrum Type	STANDARD	Sweep Width (Hz)	4725.75
				Temperature (degree C)	25.000



**Compound 15 (DOJK06):**  $^{13}\text{C}$  NMR spectrum (125 MHz).

2/26/2014 3:50:16 PM

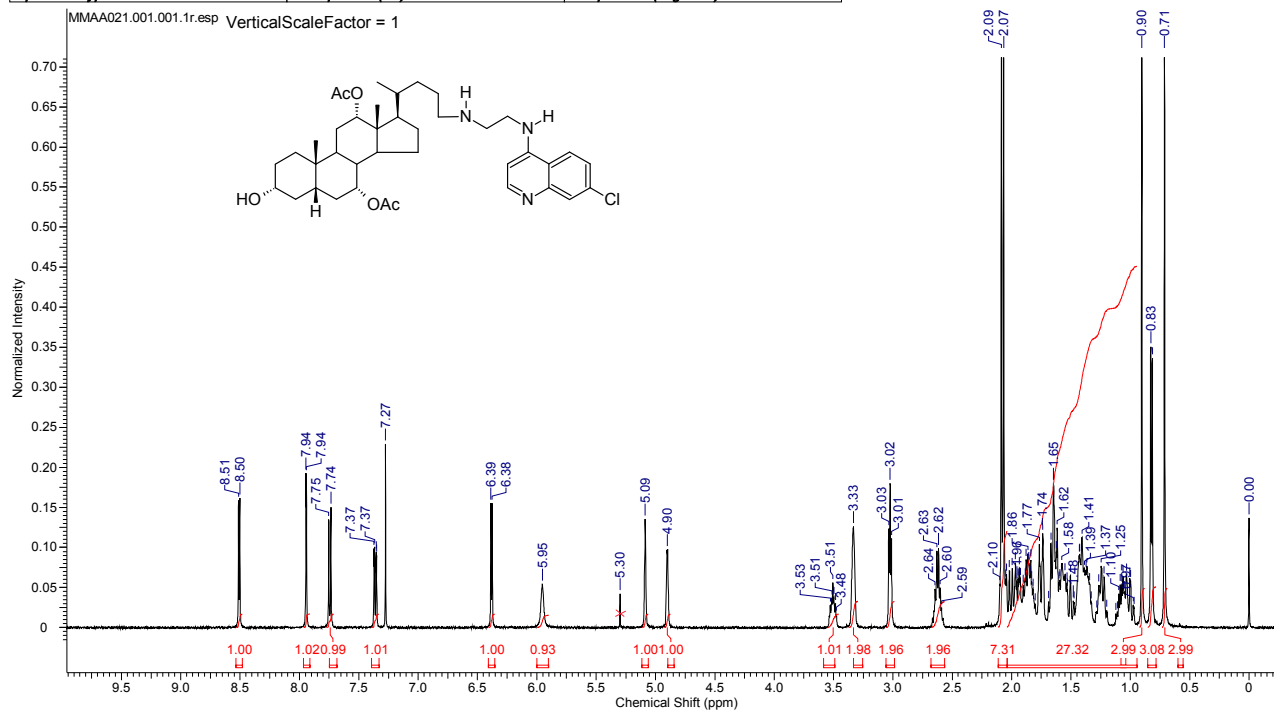
Number of Nuclei 0 C's					
Acquisition Time (sec)	0.5505	Date	22 Mar 2011 16:00:16	Date Stamp	22 Mar 2011 16:00:16
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DOJK06.2\pdata\111r				
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	269
Original Points Count	16384	Owner	nmrsu	Points Count	32768
Receiver Gain	724.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.200
				Spectrum Offset (Hz)	13831.0020



**Compound 16 (DO183):  $^1\text{H}$  NMR spectrum (500 MHz).** HPLC purity: method A: RT 8.651, area 96.19 %; method B: RT 8.626, area 95.11 %

2/26/2014 3:53:39 PM

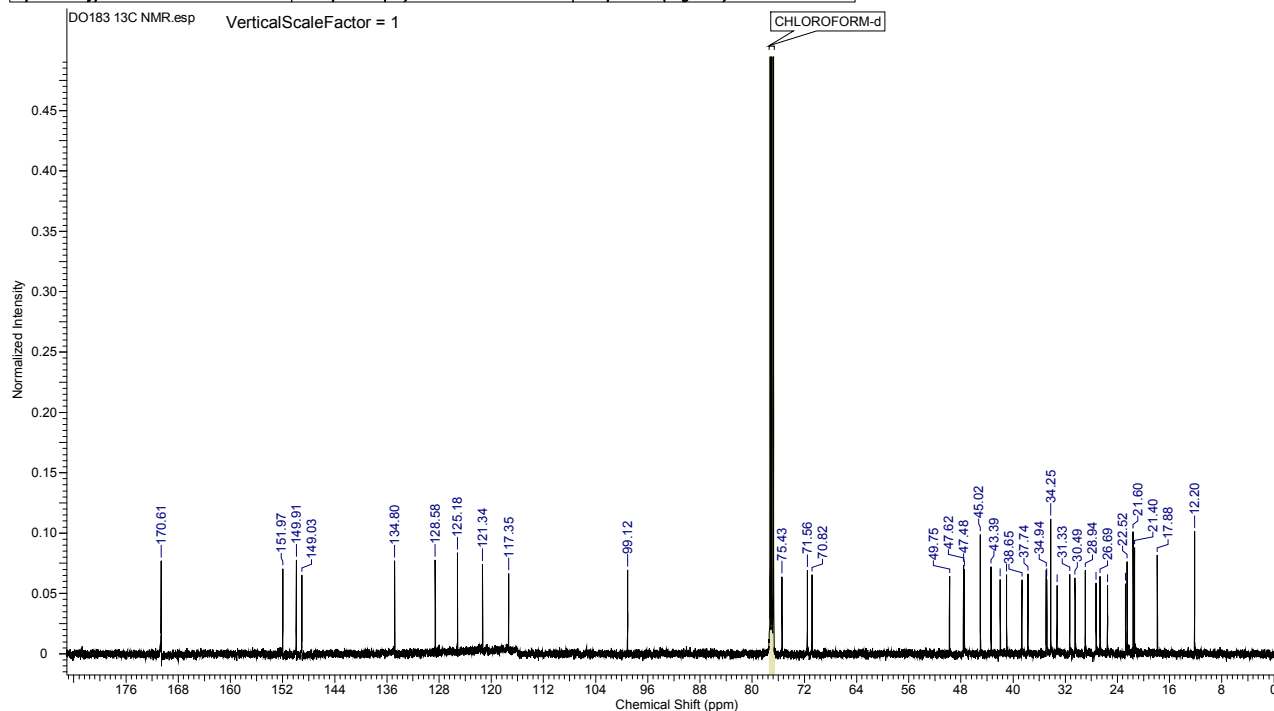
Number of Nuclei 0 H's							
Acquisition Time (sec)	2.7525	Date	28 Apr 2008 10:40:32				
File Name	C:\Users\Dejan Osenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO183\MMAA02111\pdata\11r		Date Stamp	28 Apr 2008 10:40:32			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	1	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	16384	Pulse Sequence	zq30
Receiver Gain	45.20	SW(cyclical) (Hz)	5952.38	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2502.6123
Spectrum Type	STANDARD	Sweep Width (Hz)	5952.02	Temperature (degree C)	24.900		



**Compound 16 (DO183):  $^{13}\text{C}$  NMR spectrum (125 MHz).**

3/2/2014 11:51:50 AM

Number of Nuclei 0 C's							
Acquisition Time (sec)	1.1010	Date	28 Apr 2008 10:51:12				
File Name	C:\Users\Dejan Osenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO183\MMAA02112\pdata\21r		Date Stamp	28 Apr 2008 10:51:12			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	2611	Origin	spect
Original Points Count	32768	Owner	nmsru	Points Count	32768	Pulse Sequence	zpgg30
Receiver Gain	203.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	13831.6260
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000		

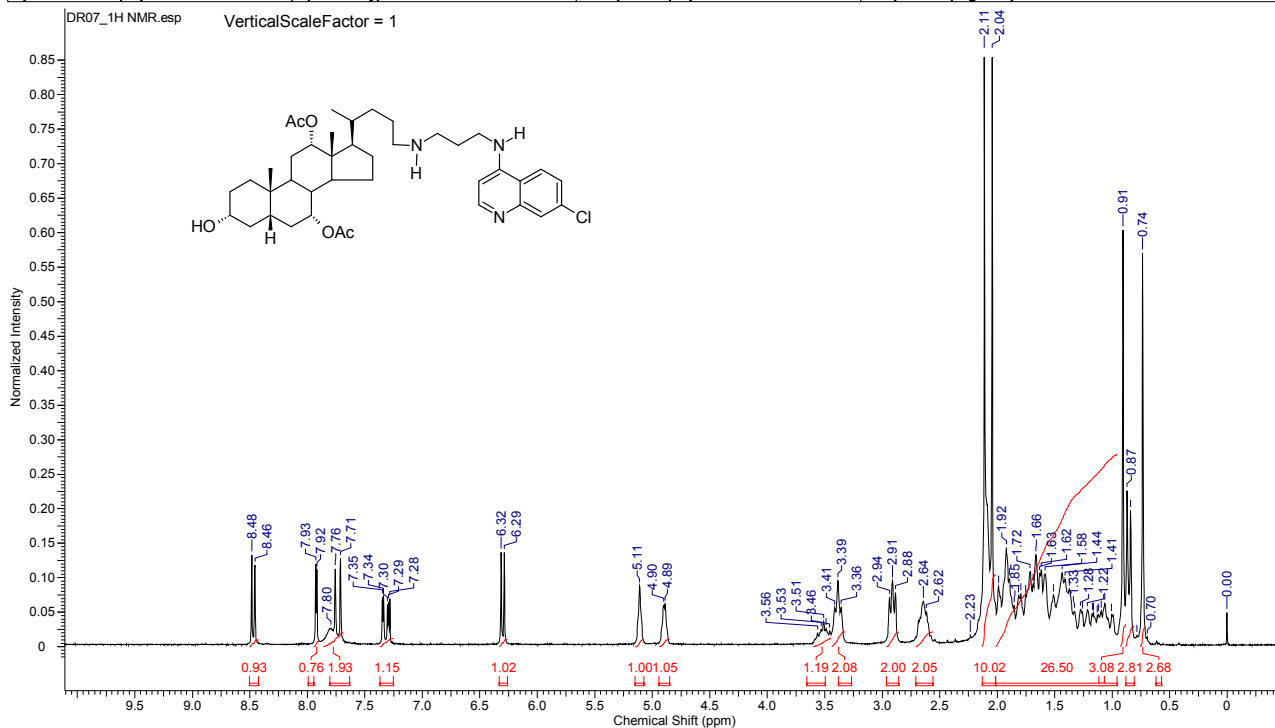




**Compound 17 (DR07):  $^1\text{H}$  NMR spectrum (200 MHz):** HPLC purity: method B: RT 8.583, area 95.71 %; method C: RT 13.187, area 95.02 %.

2/25/2014 11:26:24 AM

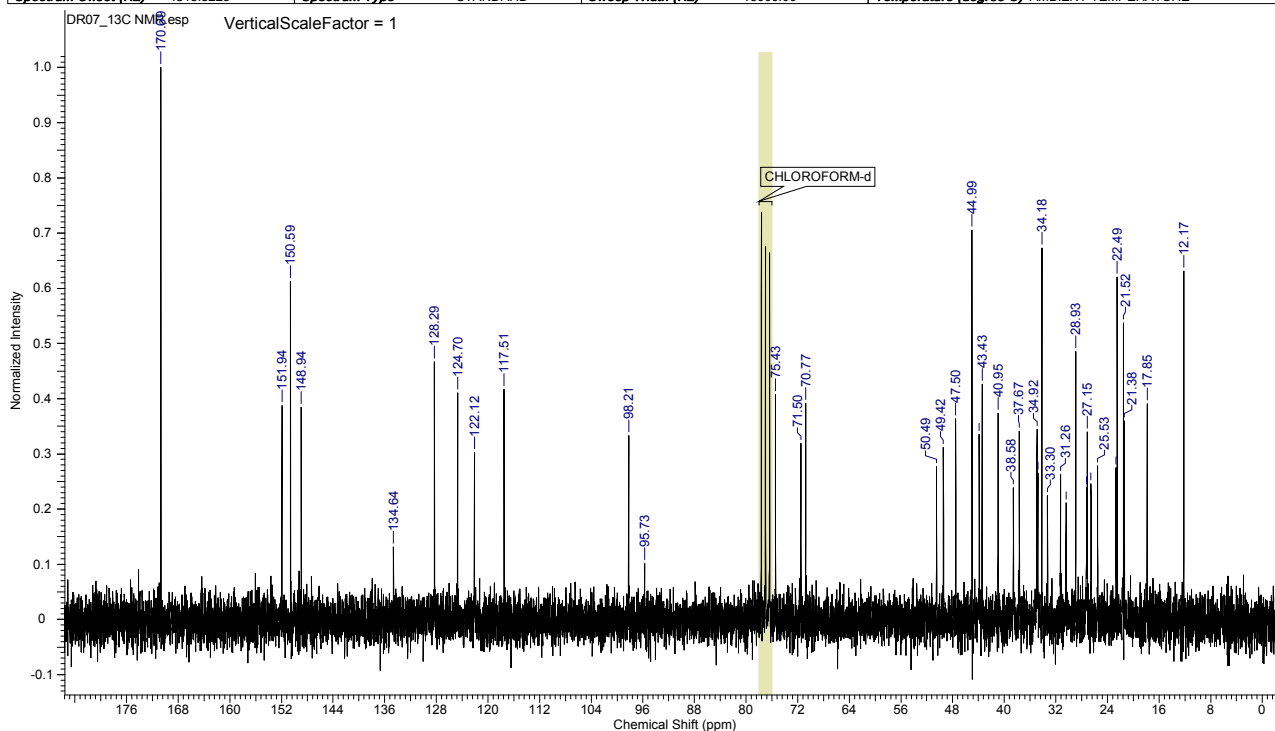
Number of Nuclei 0 H's					
Acquisition Time (sec)	1.4400	Comment	DRAA007	Date	May 25 09
File Name	C:\Users\Dejan Oспенica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzijal\Spektri NMR_Staril200 MHz\DR07\hdraa007.fid\fid				
Frequency (MHz)	199.97	Nucleus	$^1\text{H}$	Number of Transients	32
Points Count	8192	Pulse Sequence	s2pul	Receiver Gain	5.00
Spectrum Offset (Hz)	1687.8647	Spectrum Type	STANDARD	Sweep Width (Hz)	4600.00
				Solvent	CHLOROFORM-d
				Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 17 (DR07):  $^{13}\text{C}$  NMR spectrum (50 MHz)**

3/2/2014 12:02:21 PM

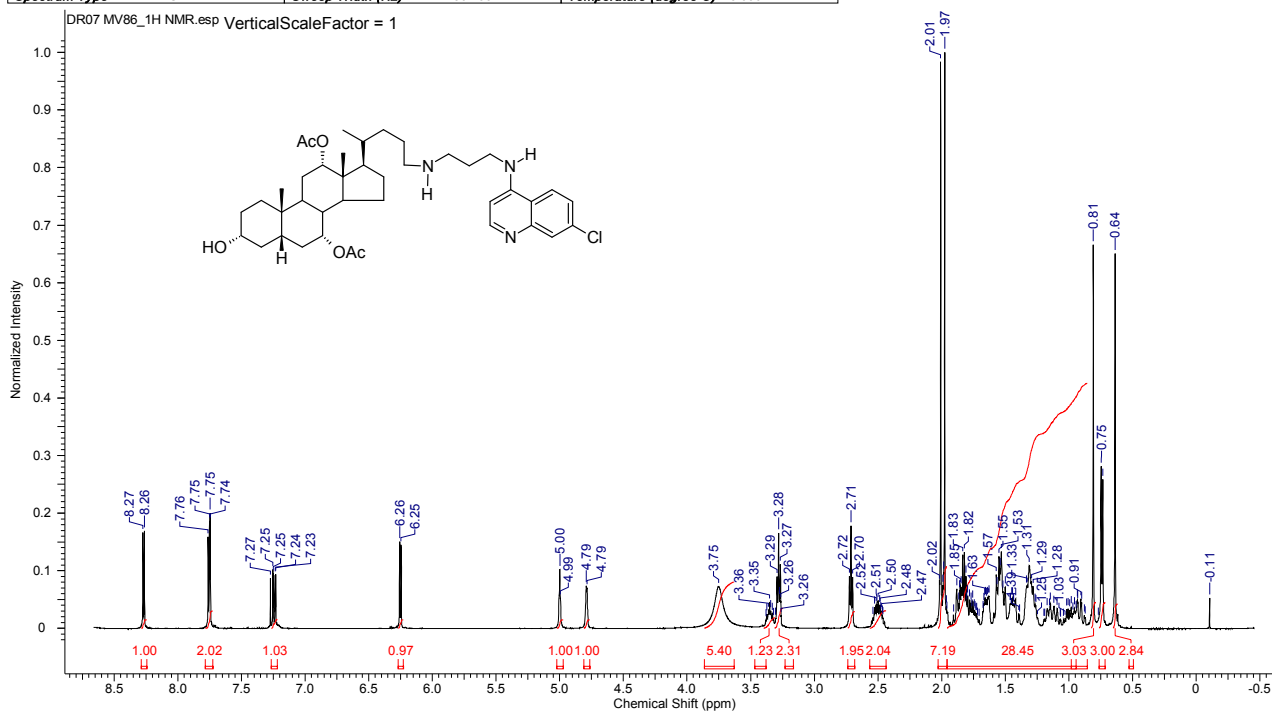
Number of Nuclei 0 C's					
Acquisition Time (sec)	1.0667	Comment	DRAA007	Date	May 25 09
File Name	C:\Users\Dejan Oспенica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzijal\Spektri NMR_Staril200 MHz\DR07\cdraa007.fid\fid				
Frequency (MHz)	50.29	Nucleus	$^{13}\text{C}$	Number of Transients	803
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	25.00
Spectrum Offset (Hz)	4813.8223	Spectrum Type	STANDARD	Sweep Width (Hz)	15000.00
				Solvent	CHLOROFORM-d
				Temperature (degree C)	AMBIENT TEMPERATURE



Compound 17 (DR07): <sup>1</sup>H NMR spectrum (500 MHz)

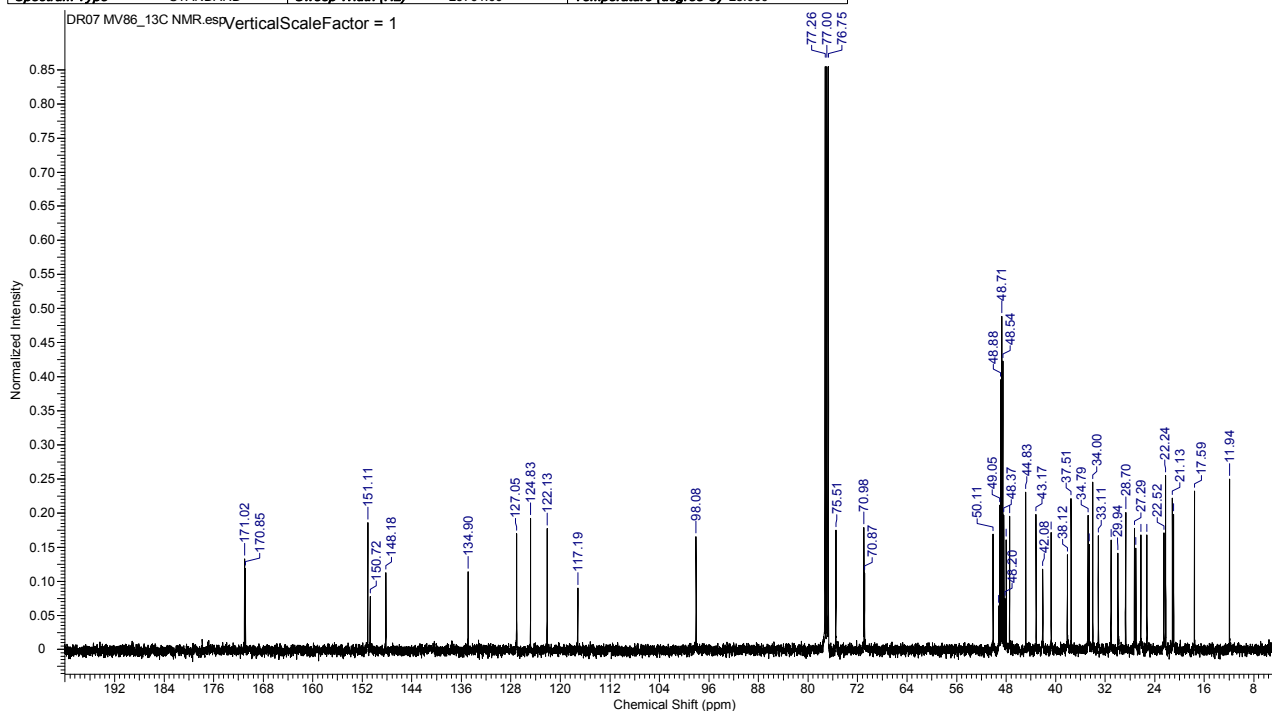
2/25/2014 11:37:54 AM

Number of Nuclei 0 H's							
Acquisition Time (sec)	3.5914	Date	22 Mar 2011 16:23:44				
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinolinski\DO152 i ostali\Recenzija\Spektri NMR_ Stari\500 MHz\MV861\data\11r		Date Stamp	22 Mar 2011 16:23:44			
Frequency (MHz)	500.26	Nucleus	<sup>1</sup> H	Number of Transients	13	Origin	spect
Original Points Count	16384	Owner	nmrsu	Points Count	32768	Pulse Sequence	zq30
Receiver Gain	101.00	SW(cyclical) (Hz)	4562.04	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2052.5569
Spectrum Type	STANDARD	Sweep Width (Hz)	4561.90	Temperature (degree C)	25.000		

Compound 17 (DR07): <sup>13</sup>C NMR spectrum (125 MHz)

2/25/2014 11:38:55 AM

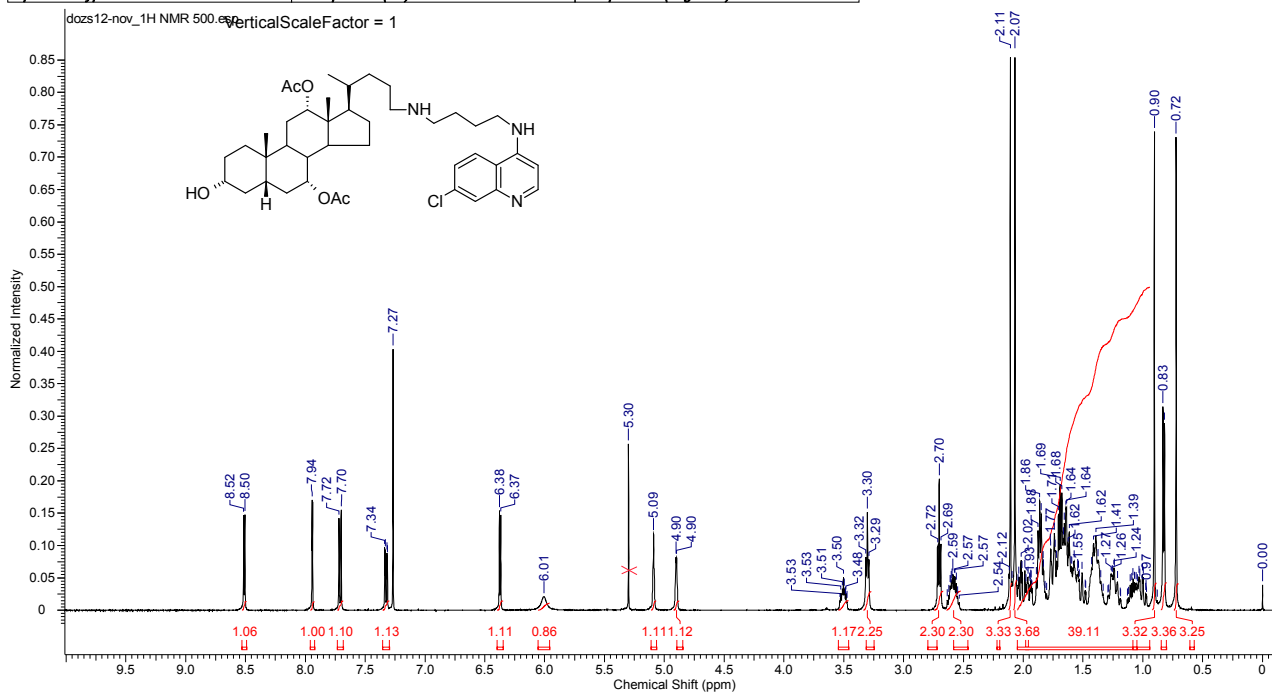
Number of Nuclei 0 C's							
Acquisition Time (sec)	0.5505	Date	22 Mar 2011 16:28:00				
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinolinski\DO152 i ostali\Recenzija\Spektri NMR_ Stari\500 MHz\MV862\data\11r		Date Stamp	22 Mar 2011 16:28:00			
Frequency (MHz)	125.79	Nucleus	<sup>13</sup> C	Number of Transients	293	Origin	spect
Original Points Count	16384	Owner	nmrsu	Points Count	32768	Pulse Sequence	zpgp30
Receiver Gain	724.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	13819.6709
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000		



**Compound 18 (DOZS12):  $^1\text{H}$  NMR spectrum (500 MHz):** HPLC purity: method A: RT 1.879, area 99.04 %; method D: RT 5.495, area 97.05 %.

2/25/2014 11:51:41 AM

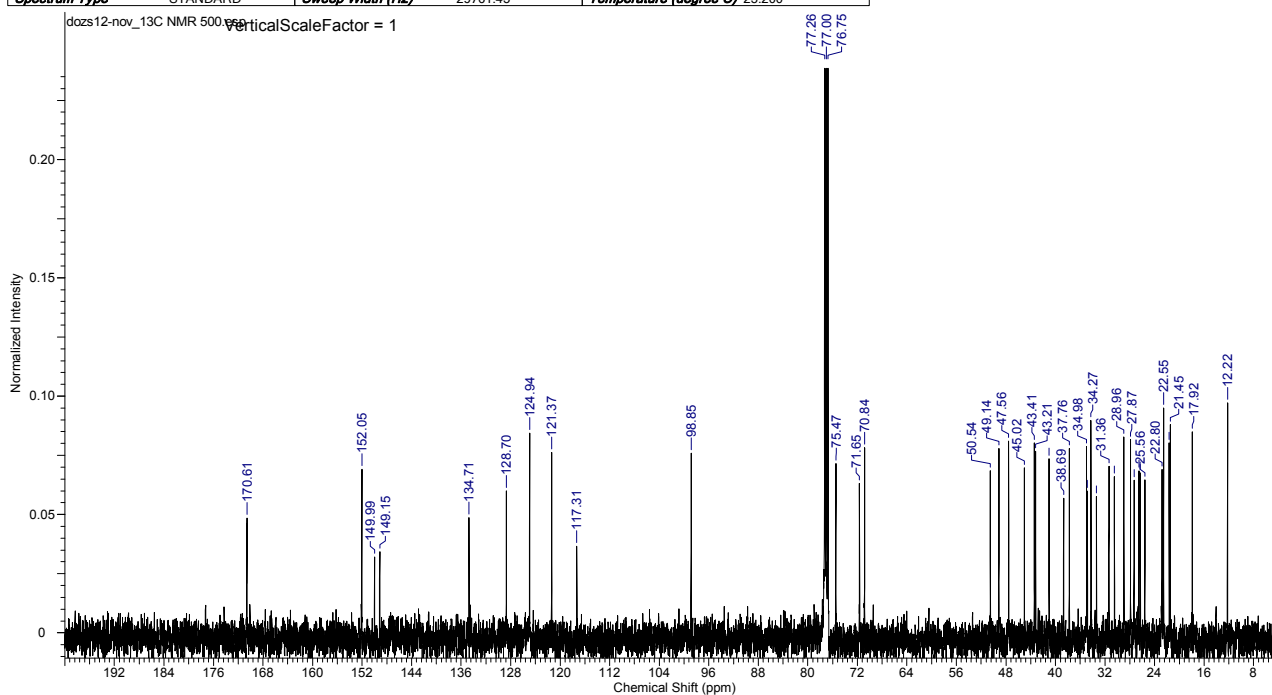
Number of Nuclei 0 H's				
Acquisition Time (sec)	2.1823	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	
Date Stamp	22 Feb 2014 10:40:16		Date	22 Feb 2014 10:40:16
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR novidozs12-nov\1\1\data\1\1r			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	
Original Points Count	16384	Owner	nmrsu	
Receiver Gain	362.00	SW(cyclical) (Hz)	7507.51	
Spectrum Type	STANDARD	Sweep Width (Hz)	7507.28	
		Number of Transients	22	
		Points Count	32768	
		Solvent	CHLOROFORM-d	
		Temperature (degree C)	24.900	
		Origin	spect	
		Pulse Sequence	zg30	
		Spectrum Offset (Hz)	3490.9019	



**Compound 18 (DOZS12):  $^{13}\text{C}$  NMR spectrum (125 MHz):**

2/25/2014 11:59:00 AM

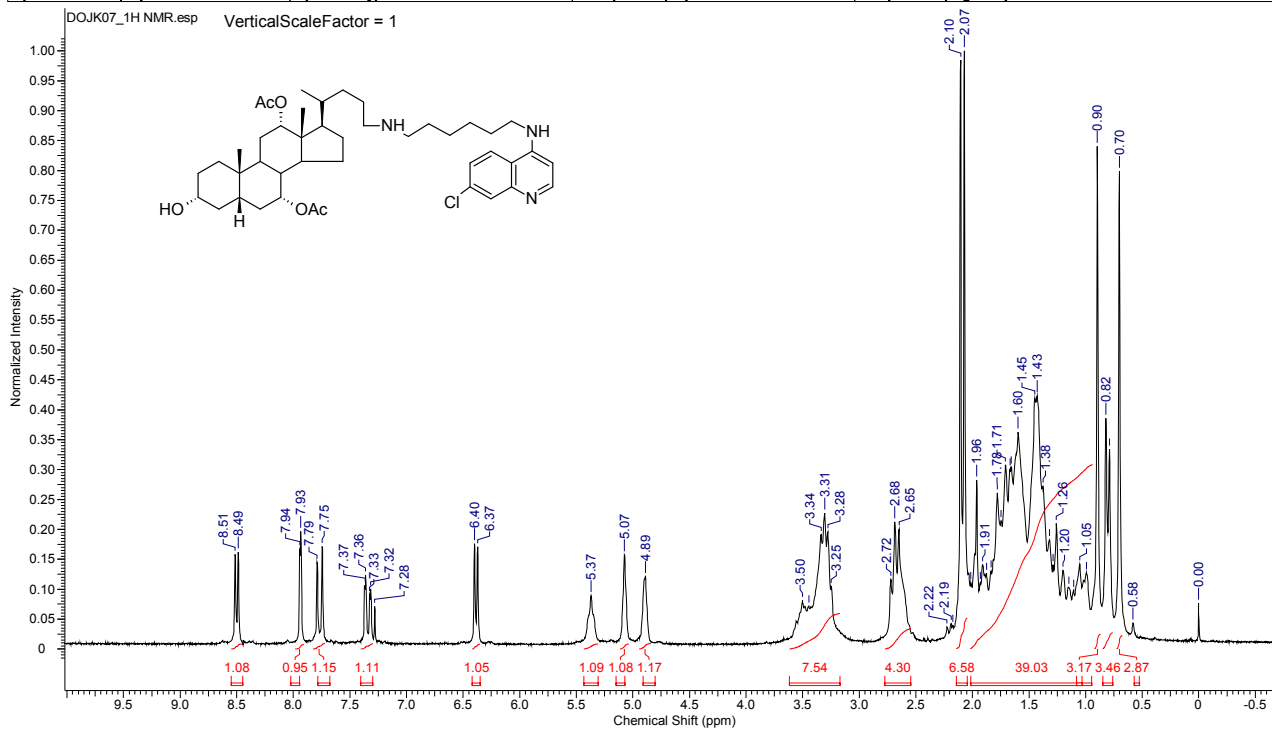
Number of Nuclei 0 C's				
Acquisition Time (sec)	0.5505	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	
Date Stamp	22 Feb 2014 10:29:36		Date	22 Feb 2014 10:29:36
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR novidozs12-nov\2\2\data\1\1r			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	
Original Points Count	16384	Owner	nmrsu	
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.45	
		Number of Transients	283	
		Points Count	65536	
		Solvent	CHLOROFORM-d	
		Temperature (degree C)	25.200	
		Origin	spect	
		Pulse Sequence	zgpg30	
		Spectrum Offset (Hz)	13832.3740	



**Compound 19 (DOJK07):**  $^1\text{H}$  NMR spectrum (200 MHz): HPLC purity: method A: RT 1.869, area 99.39 %; method C: RT=11.500, area 95.59 %.

2/25/2014 12:03:22 PM

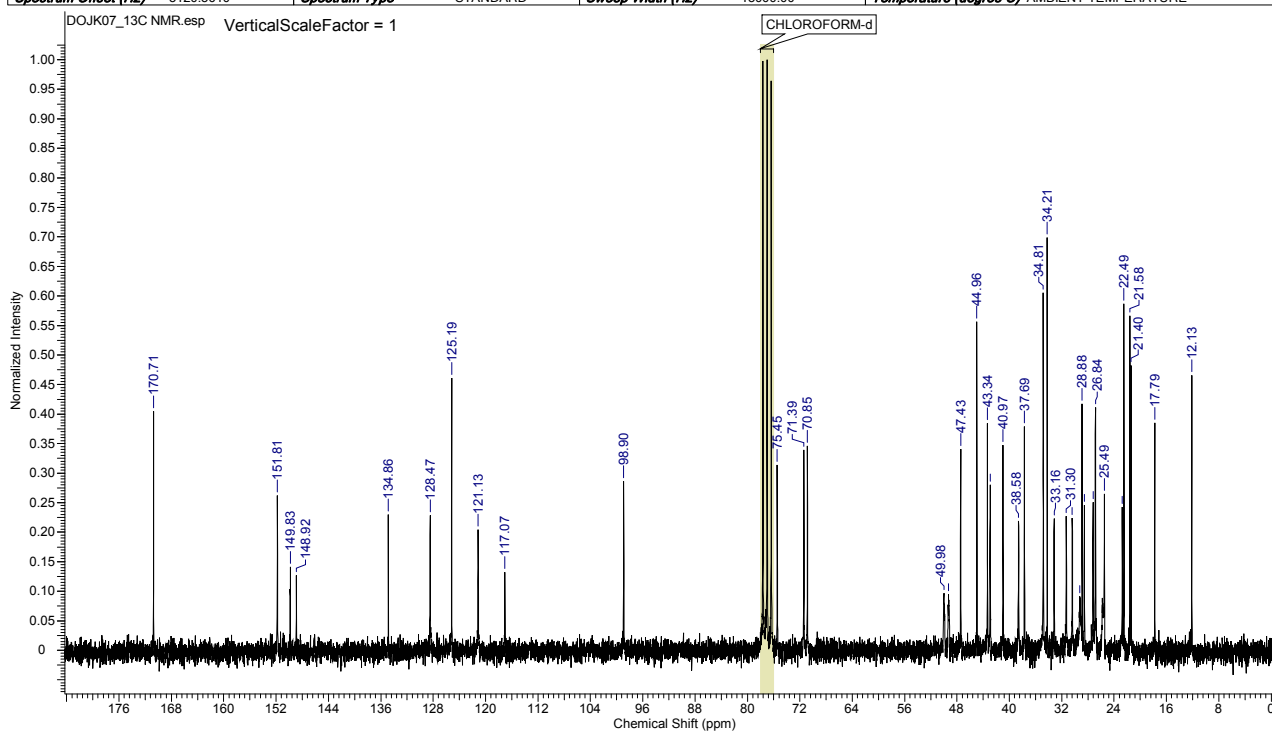
Number of Nuclei 0 H's					
Acquisition Time (sec)	1.3913	Comment	dojk07	Date	Apr 5 11
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR_Stan\200 MHz\DOJK07\hdojk07.fid.fid				
Frequency (MHz)	199.97	Nucleus	$^1\text{H}$	Number of Transients	66
Points Count	8192	Pulse Sequence	s2pul	Receiver Gain	9.00
Spectrum Offset (Hz)	1687.8647	Spectrum Type	STANDARD	Sweep Width (Hz)	4600.00
				Solvent	CHLOROFORM-d
				Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 19 (DOJK07):**  $^{13}\text{C}$  NMR spectrum (50 MHz):

2/27/2014 5:22:32 PM

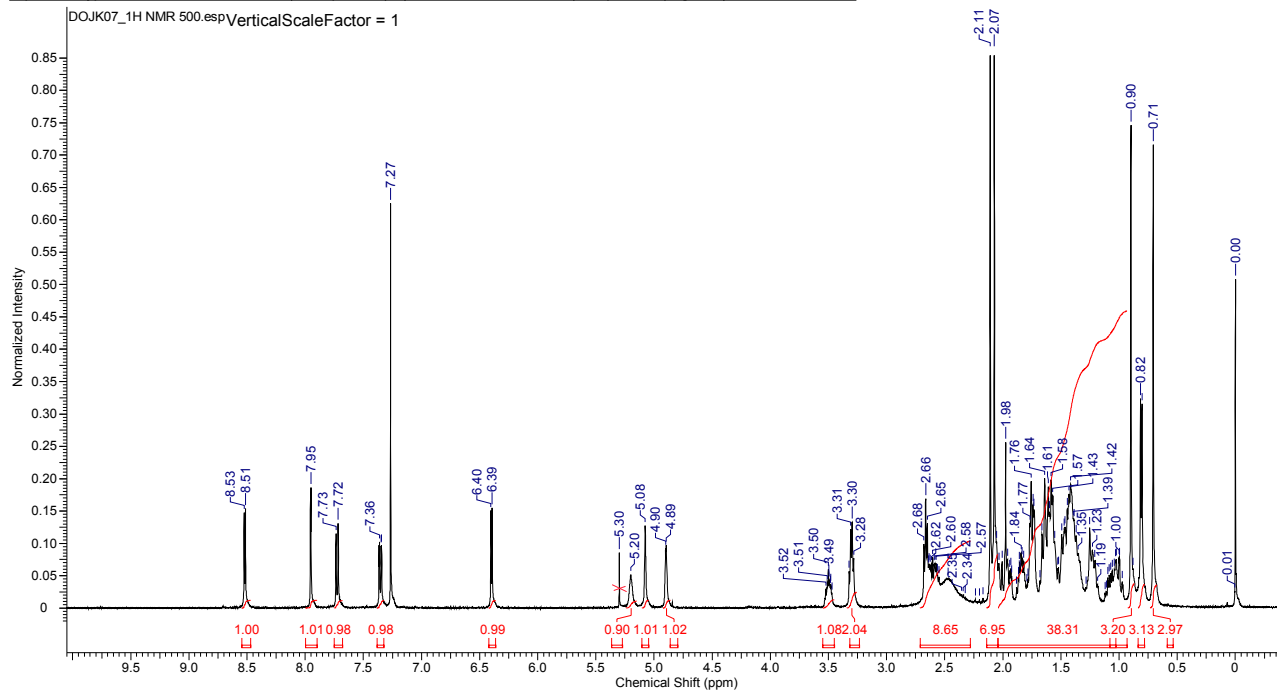
Number of Nuclei 0 C's					
Acquisition Time (sec)	1.0667	Comment	dojk07	Date	Apr 5 11
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR_Stan\200 MHz\DOJK07\hdojk07.fid.fid				
Frequency (MHz)	50.29	Nucleus	$^{13}\text{C}$	Number of Transients	17116
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	25.00
Spectrum Offset (Hz)	5120.5610	Spectrum Type	STANDARD	Sweep Width (Hz)	15000.00
				Solvent	CHLOROFORM-d
				Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 19 (DOJK07): <sup>1</sup>H NMR spectrum (500 MHz):**

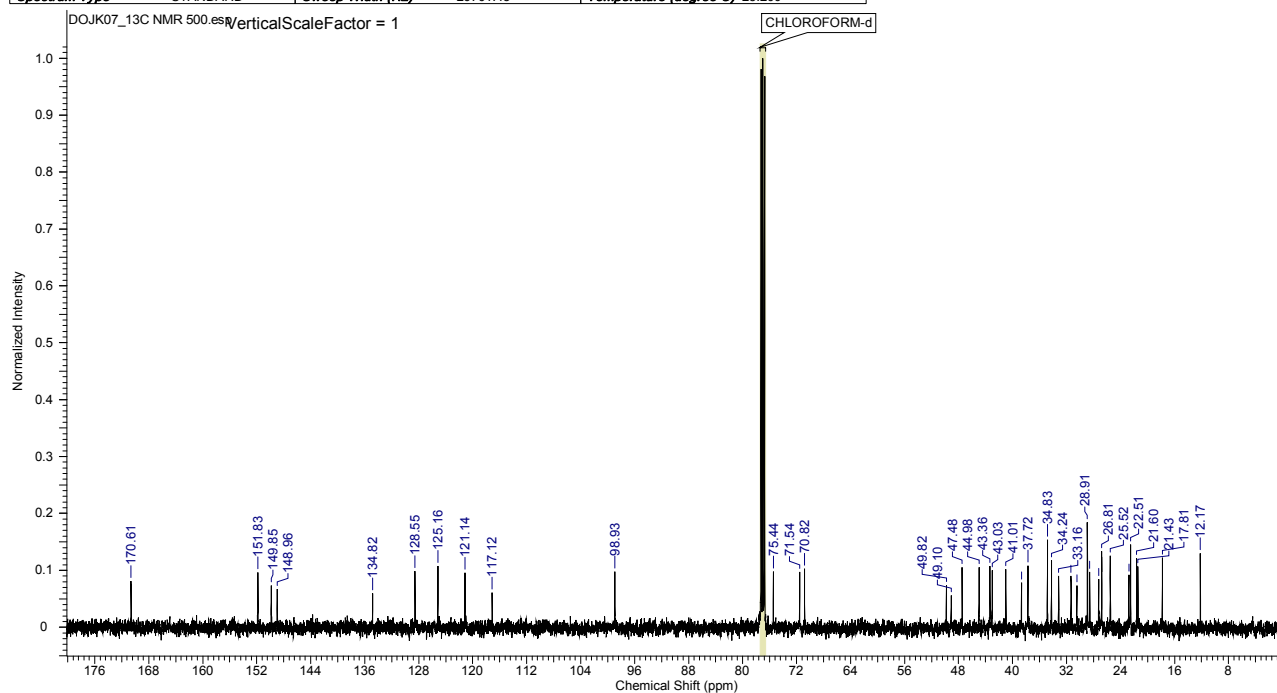
2/25/2014 12:06:27 PM

Number of Nuclei 0 H's					
Acquisition Time (sec)	2.1823	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	Date	19 Feb 2014 10:44:32
Date Stamp	19 Feb 2014 10:44:32				
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR novidojk07\1\pdata\111r				
Frequency (MHz)	500.26	Nucleus	1H	Number of Transients	16
Original Points Count	16384	Owner	nmrsu	Points Count	32768
Receiver Gain	362.00	SW(cyclical) (Hz)	7507.51	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	7507.28	Temperature (degree C)	27.000
				Origin	spect
				Pulse Sequence	zg30
				Spectrum Offset (Hz)	3489.7109

**Compound 19 (DOJK07): <sup>13</sup>C NMR spectrum (125 MHz):**

2/27/2014 5:20:33 PM

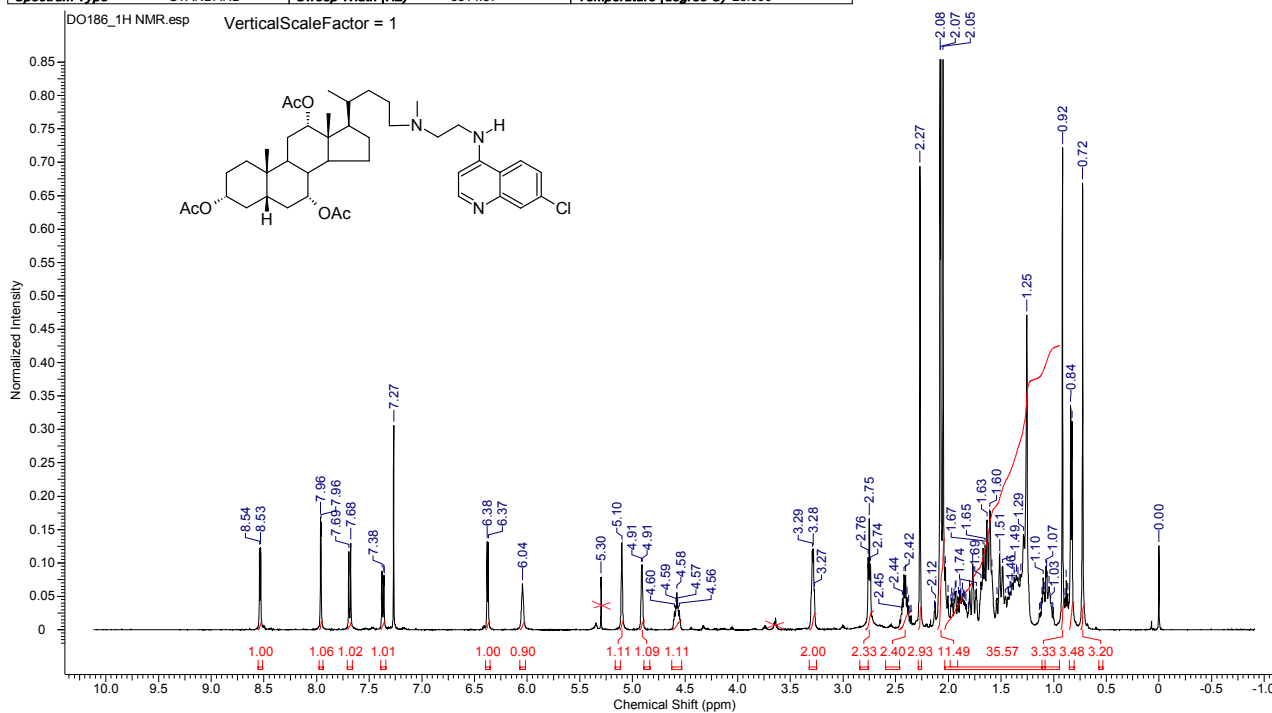
Number of Nuclei 0 C's					
Acquisition Time (sec)	0.5505	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	Date	20 Feb 2014 10:29:36
Date Stamp	20 Feb 2014 10:29:36				
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR novidojk07\2\pdata\111r				
Frequency (MHz)	125.79	Nucleus	13C	Number of Transients	100
Original Points Count	16384	Owner	nmrsu	Points Count	65536
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.45	Temperature (degree C)	25.200
				Origin	spect
				Pulse Sequence	zgpg30
				Spectrum Offset (Hz)	13830.0361



**Compound 20 (DO186):  $^1\text{H}$  NMR spectrum (500 MHz):** HPLC purity: method B: RT 8.703, area 96,21 %; method C: RT 13.199, area 95.18 %.

2/25/2014 12:10:29 PM

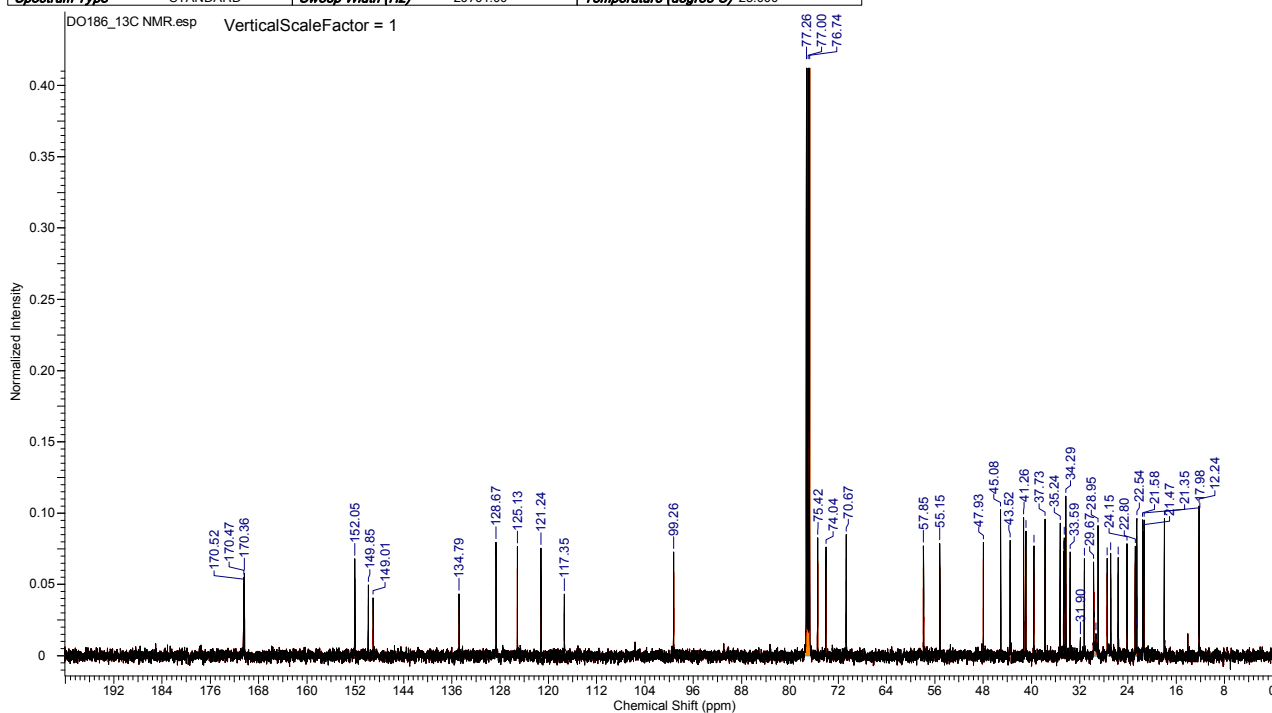
Number of Nuclei 0 H's				
Acquisition Time (sec)	2.9710	Date	19 Feb 2009 11:05:52	
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinoliniski\DO152\i ostali\Recenzija\Spektri NMR_Star\500 MHz\DO186\DOAA074a1\pdata\11r		Date Stamp	19 Feb 2009 11:05:52
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	
Original Points Count	16384	Owner	nmrsu	
Receiver Gain	114.00	SW(cyclical) (Hz)	5514.71	
Spectrum Type	STANDARD	Sweep Width (Hz)	5514.37	
		Temperature (degree C)	25.000	
		Number of Transients	16	
		Points Count	16384	
		Solvent	CHLOROFORM-d	
		Spectrum Offset (Hz)	2304.3628	
		Pulse Sequence	zg30	



**Compound 20 (DO186):  $^{13}\text{C}$  NMR spectrum (125 MHz):**

2/25/2014 12:12:29 PM

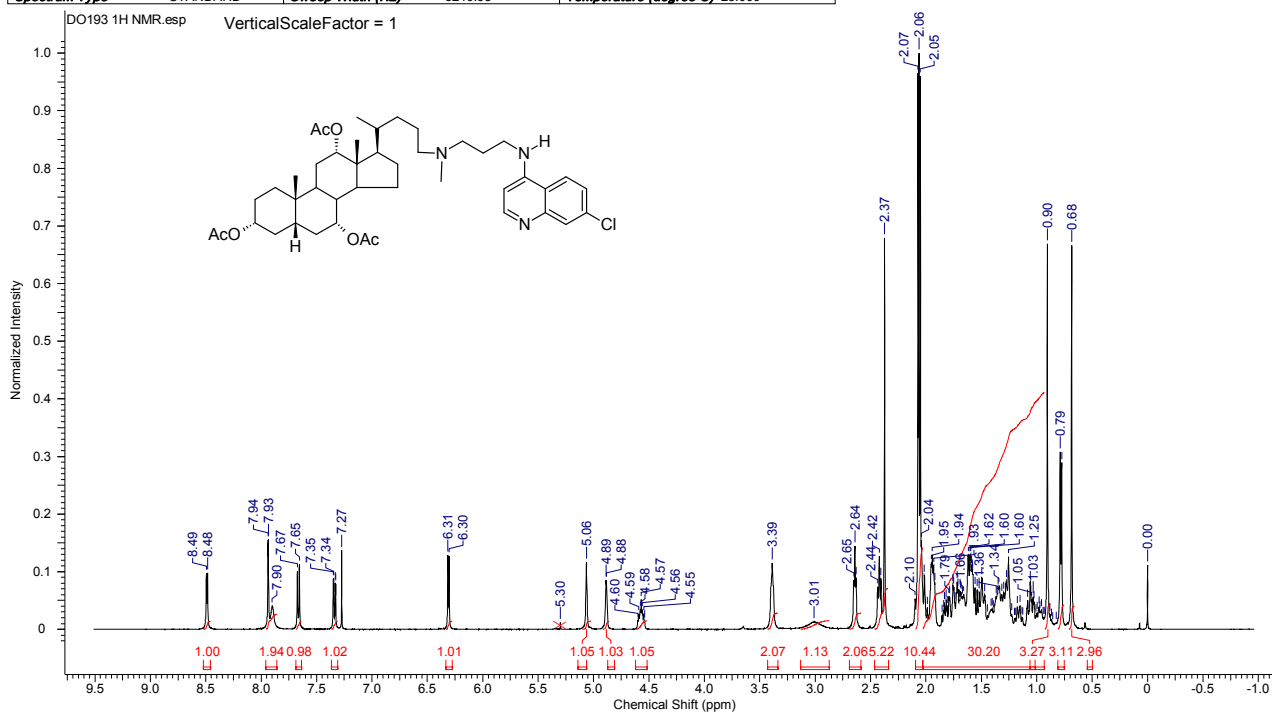
Number of Nuclei 0 C's				
Acquisition Time (sec)	1.1010	Date	19 Feb 2009 11:16:32	
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinoliniski\DO152\i ostali\Recenzija\Spektri NMR_Star\500 MHz\DO186\DOAA074a2\pdata\11r		Date Stamp	19 Feb 2009 11:16:32
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	
Original Points Count	32768	Owner	nmrsu	
Receiver Gain	812.00	SW(cyclical) (Hz)	29761.90	
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	
		Temperature (degree C)	25.000	
		Number of Transients	643	
		Points Count	32768	
		Solvent	CHLOROFORM-d	
		Spectrum Offset (Hz)	13833.8828	
		Pulse Sequence	zpgq30	



**Compound 21(DO193):**  $^1\text{H}$  NMR spectrum (500 MHz): HPLC purity: method A: RT 2.032, area 99.46 %; method B: RT 8.689, area 96.92 %.

2/26/2014 4:32:33 PM

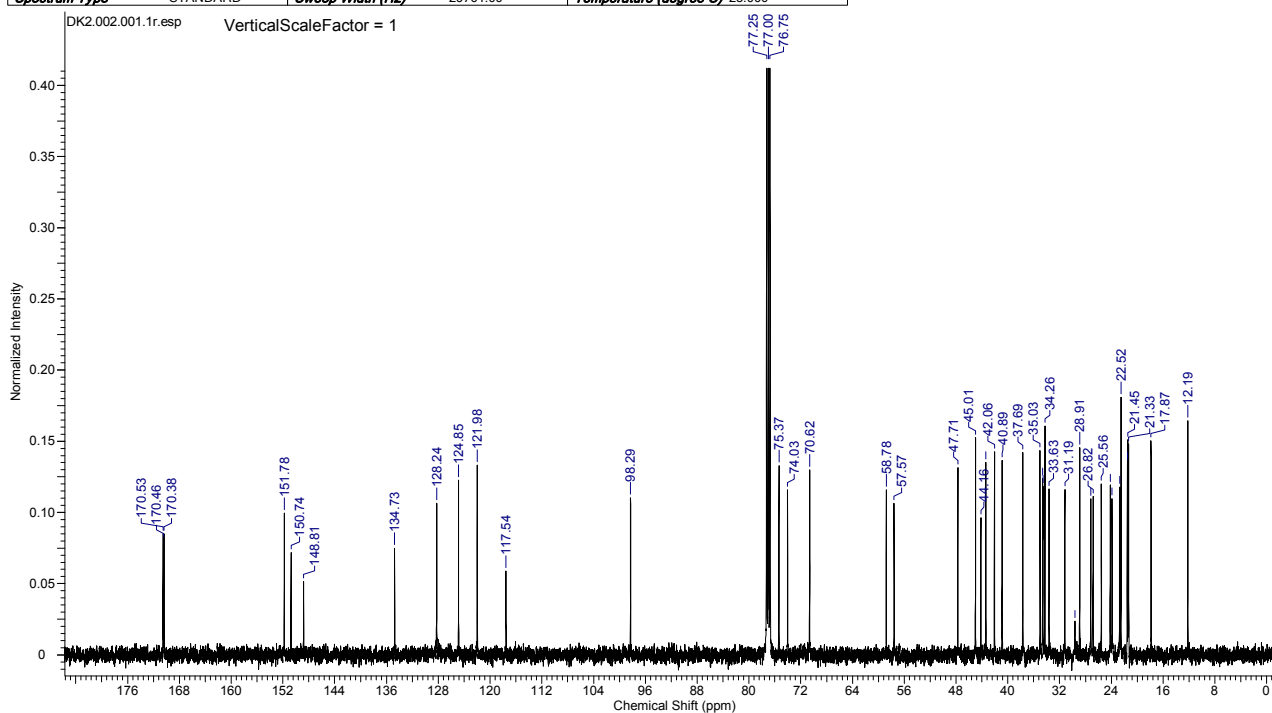
Number of Nuclei 0 H's							
Acquisition Time (sec)	3.1261	Date	02 Sep 2009 12:20:48				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO193\DK2\1\data\1\1r		Date Stamp	02 Sep 2009 12:20:48			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	71.80	SW(cyclical) (Hz)	5241.09	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2138.4419
Spectrum Type	STANDARD	Sweep Width (Hz)	5240.93	Temperature (degree C)	25.000		



**Compound 21(DO193):**  $^{13}\text{C}$  NMR spectrum (125MHz):

2/26/2014 4:34:17 PM

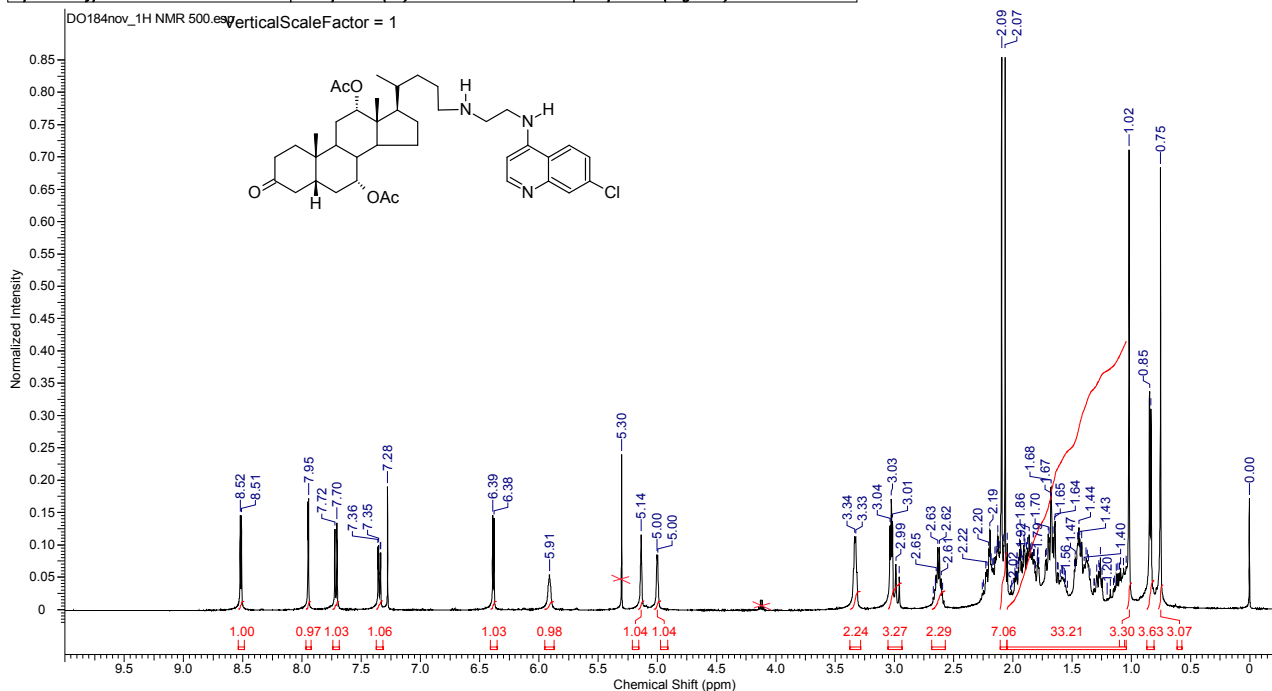
Number of Nuclei 0 C's							
Acquisition Time (sec)	0.5505	Date	02 Sep 2009 11:25:20				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO193\DK2\2\data\1\1r		Date Stamp	02 Sep 2009 11:25:20			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	587	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	1820.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	13830.7754
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000		



**Compound 22(DO184):  $^1\text{H}$  NMR spectrum (500 MHz):** HPLC purity: method A: RT 8.484, area 95.76 %; method B: RT 7.775, area 95.05 %; **method C: RT 10.069, area 95.10 %.**

2/25/2014 12:26:00 PM

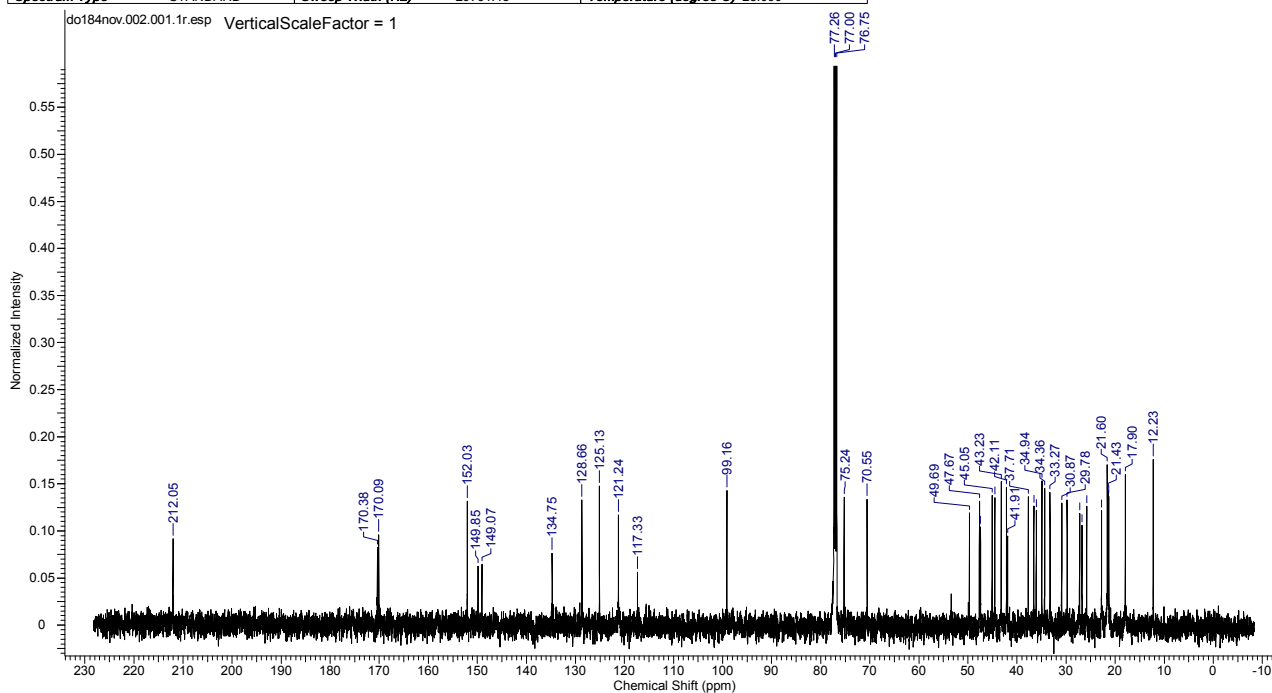
Number of Nuclei 0 H's			
Acquisition Time (sec)	2.1823	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118
Date Stamp	21 Feb 2014 10:06:08	Date	21 Feb 2014 10:06:08
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR novido184nov1\pdata\111r		
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$
Original Points Count	16384	Owner	nmsru
Receiver Gain	362.00	SW(cyclical) (Hz)	7507.51
Spectrum Type	STANDARD	Sweep Width (Hz)	7507.28
		Solvent	CHLOROFORM-d
		Temperature (degree C)	24.800
		Number of Transients	14
		Points Count	32768
		Origin	spect
		Pulse Sequence	zg30
		Spectrum Offset (Hz)	3495.1990



**Compound 22(DO184):  $^{13}\text{C}$  NMR spectrum (125 MHz):**

2/25/2014 12:27:53 PM

Number of Nuclei 0 C's			
Acquisition Time (sec)	0.5505	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118
Date Stamp	21 Feb 2014 10:06:08	Date	21 Feb 2014 10:06:08
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR novido184nov2\pdata\111r		
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$
Original Points Count	16384	Owner	nmsru
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.45
		Solvent	CHLOROFORM-d
		Temperature (degree C)	25.000
		Number of Transients	174
		Points Count	65536
		Origin	spect
		Pulse Sequence	zpgp30
		Spectrum Offset (Hz)	13829.1396

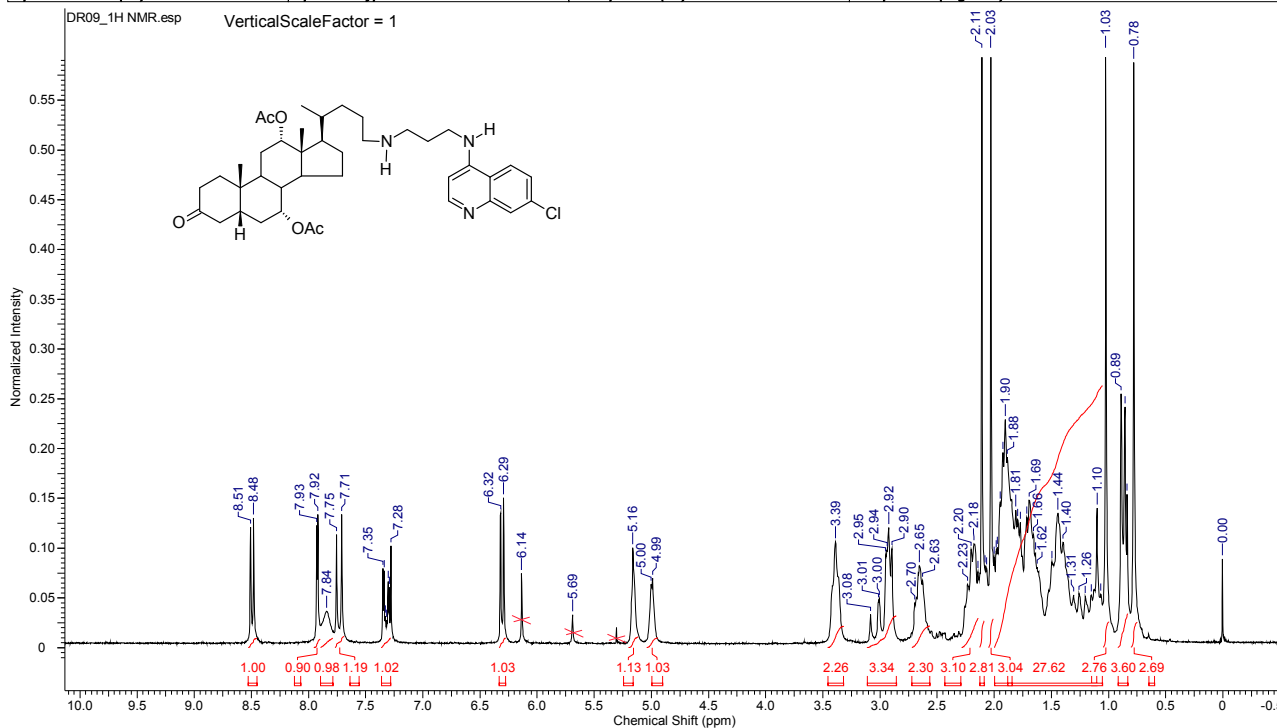




**Compound 23(DR09):** <sup>1</sup>H NMR spectrum (200 MHz): HPLC purity: method C: RT=13.105, area 95.15 %; method D: RT 5.414, area 95.21 %.

2/25/2014 12:32:13 PM

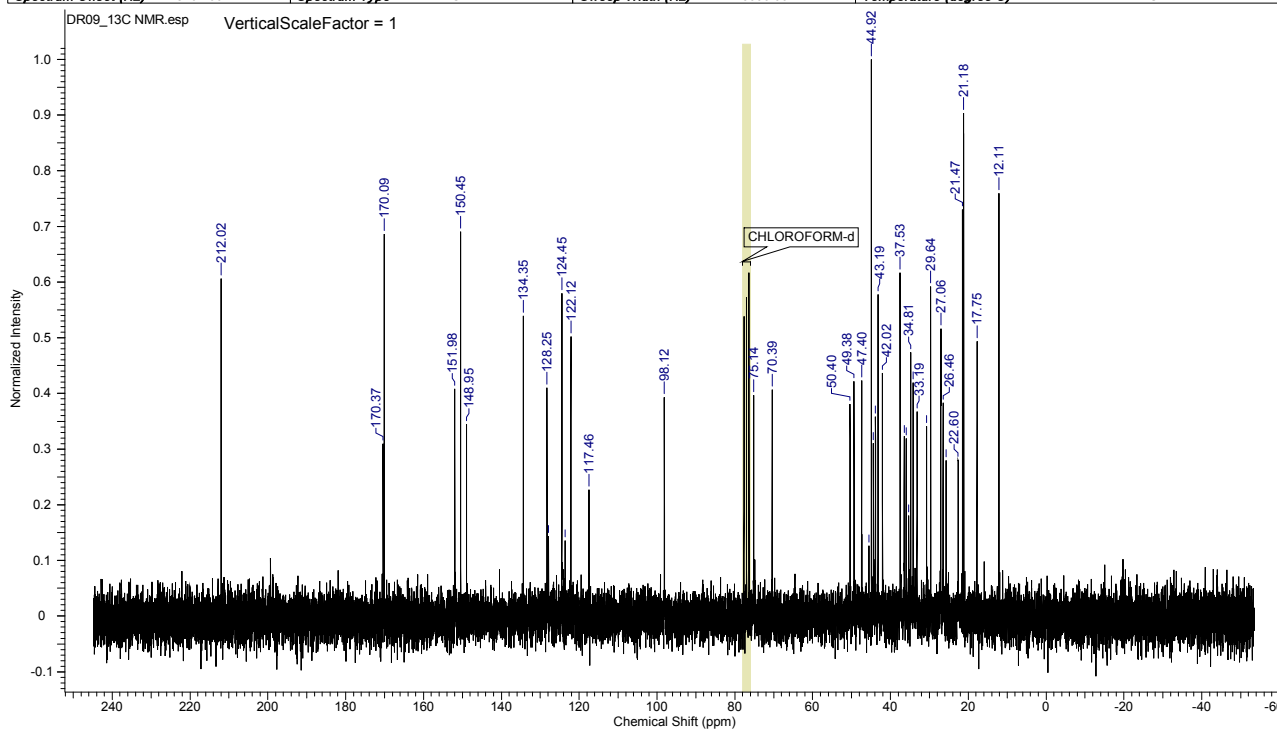
Number of Nuclei 0 H's					
Acquisition Time (sec)	1.3913	Comment	DR09	Date	Jun 1 09
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinolinski\DO152 i ostali\Recenzija\Spektri NMR_Star\200 MHz\DR09\hdr09.fid.fid				
Frequency (MHz)	199.97	Nucleus	<sup>1</sup> H	Number of Transients	104
Points Count	8192	Pulse Sequence	s2pul	Receiver Gain	7.00
Spectrum Offset (Hz)	1687.3032	Spectrum Type	STANDARD	Sweep Width (Hz)	4600.00
				Solvent	CHLOROFORM-d
				Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 23(DR09):** <sup>13</sup>C NMR spectrum (50 MHz):

2/27/2014 6:17:05 PM

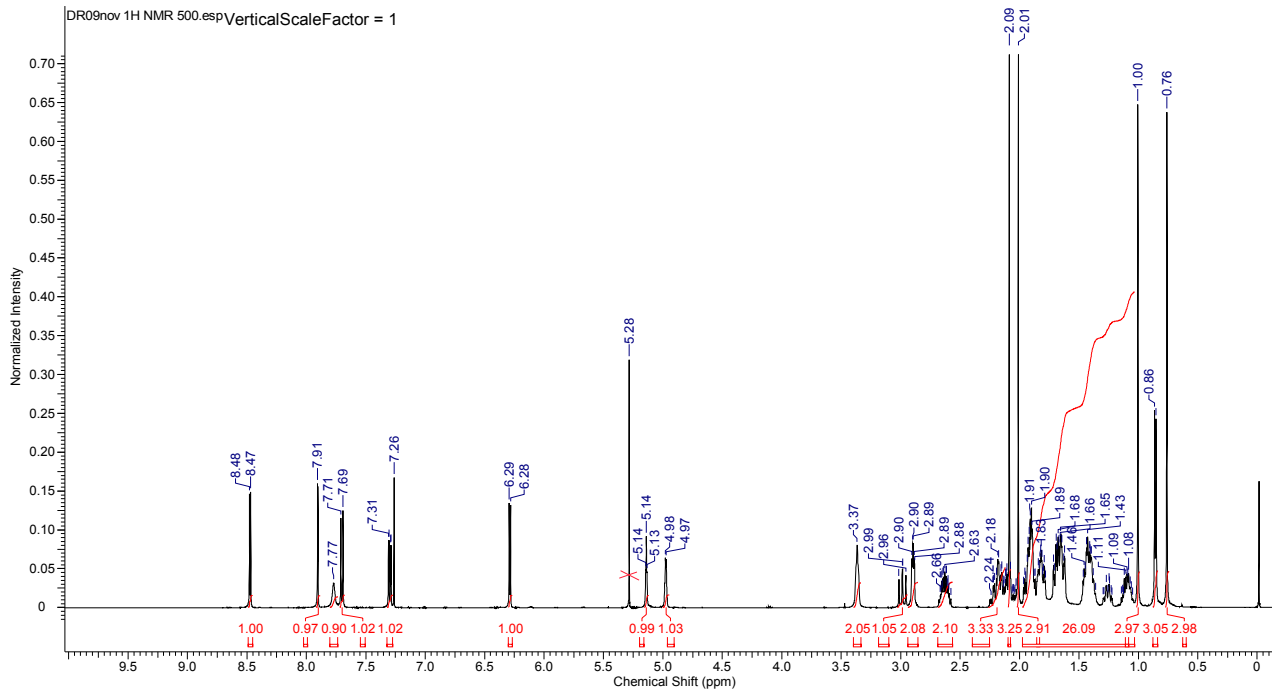
Number of Nuclei 0 C's					
Acquisition Time (sec)	1.0667	Comment	DR09	Date	Jun 1 09
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinolinski\DO152 i ostali\Recenzija\Spektri NMR_Star\200 MHz\DR09\cdr09.fid.fid				
Frequency (MHz)	50.29	Nucleus	<sup>13</sup> C	Number of Transients	330
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	25.00
Spectrum Offset (Hz)	4810.1602	Spectrum Type	STANDARD	Sweep Width (Hz)	15000.00
				Solvent	CHLOROFORM-d
				Temperature (degree C)	AMBIENT TEMPERATURE



Compound 23(DR09): <sup>1</sup>H NMR spectrum (500 MHz):

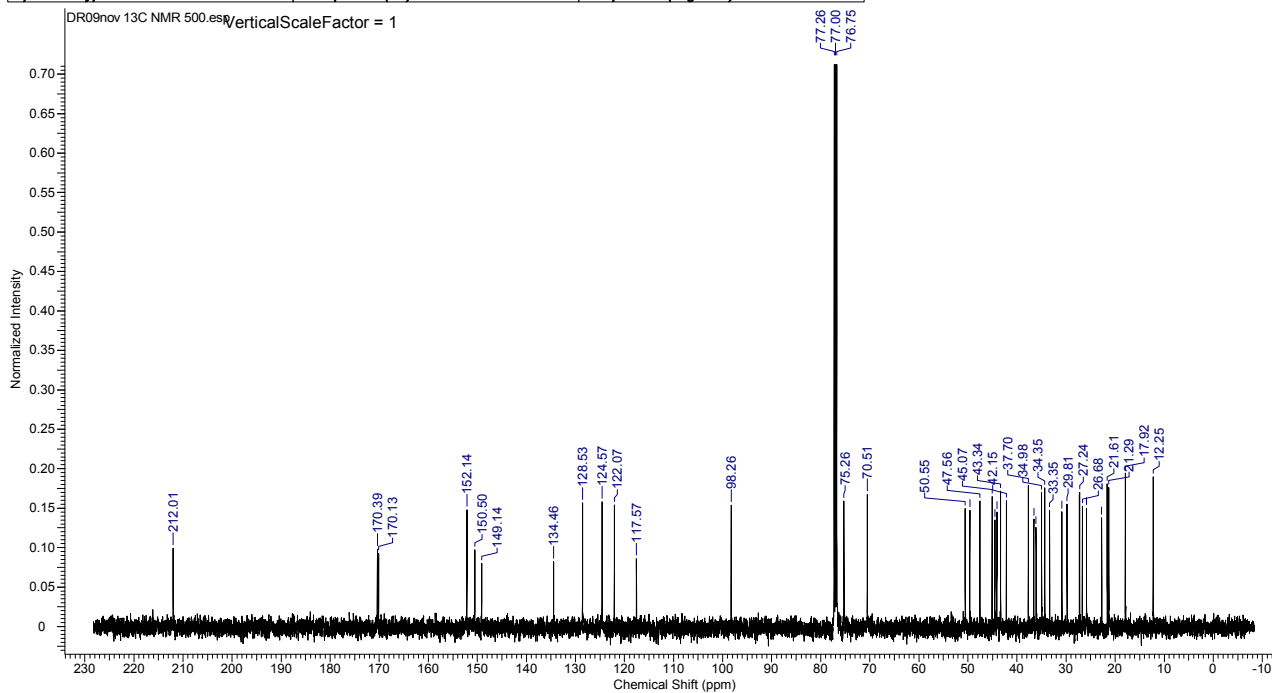
2/25/2014 12:36:09 PM

Number of Nuclei 0 H's					
Acquisition Time (sec)	2.1823	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	Date	21 Feb 2014 09:21:20
Date Stamp	21 Feb 2014 09:21:20				
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR nov\dr09nov\1\pdata\11r				
Frequency (MHz)	500.26	Nucleus	<sup>1</sup> H	Number of Transients	14
Original Points Count	16384	Owner	nmrsu	Points Count	32768
Receiver Gain	71.80	SW(cyclical) (Hz)	7507.51	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	7507.28	Temperature (degree C)	25.000
				Origin	spect
				Pulse Sequence	zg30
				Spectrum Offset (Hz)	3489.0959

Compound 23(DR09): <sup>13</sup>C NMR spectrum (125 MHz):

2/25/2014 12:37:03 PM

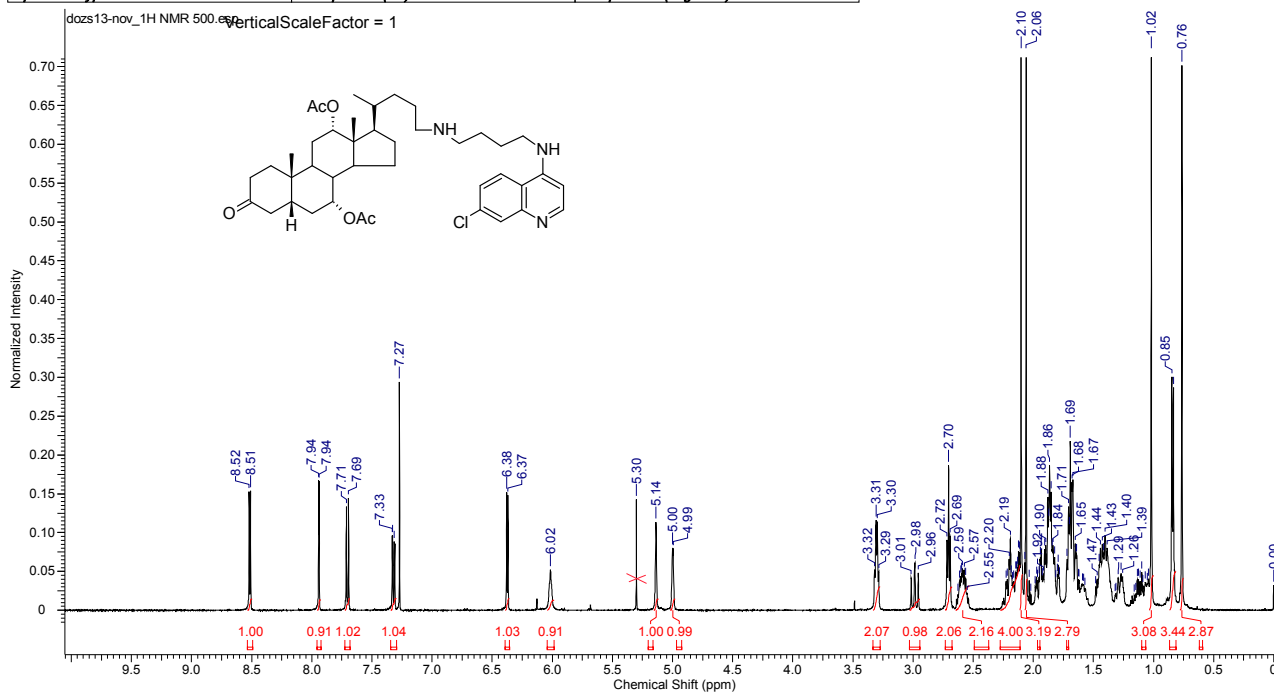
Number of Nuclei 0 C's					
Acquisition Time (sec)	0.5505	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	Date	21 Feb 2014 09:23:28
Date Stamp	21 Feb 2014 09:23:28				
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR nov\dr09nov\2\pdata\11r				
Frequency (MHz)	125.79	Nucleus	<sup>13</sup> C	Number of Transients	88
Original Points Count	16384	Owner	nmrsu	Points Count	65536
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.45	Temperature (degree C)	25.200
				Origin	spect
				Pulse Sequence	zpgg30
				Spectrum Offset (Hz)	13829.1035



**Compound 24(DOZS13):**  $^1\text{H}$  NMR spectrum (500 MHz): HPLC purity: method A: RT 1.872, area 99.17 %; method C: RT 12.077, area 95.14 %.

2/25/2014 1:26:52 PM

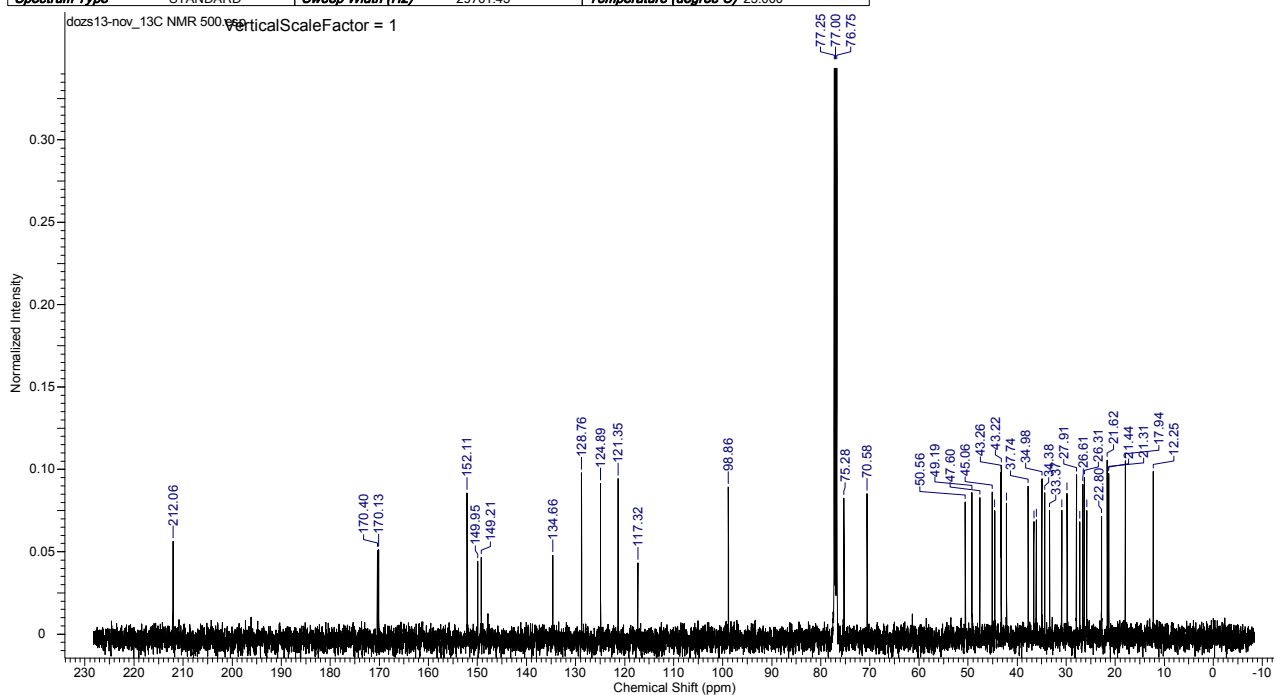
Number of Nuclei 0 H's					
Acquisition Time (sec)	2.1823	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	Date	22 Feb 2014 10:21:04
Date Stamp	22 Feb 2014 10:21:04				
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR novidozs13-nov1\pdata\11r				
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	14
Original Points Count	16384	Owner	nmrsu	Points Count	32768
Receiver Gain	362.00	SW(cyclical) (Hz)	7507.51	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	7507.28	Temperature (degree C)	24.800
				Spectrum Offset (Hz)	3491.4070



**Compound 24(DOZS13):**  $^{13}\text{C}$  NMR spectrum (125 MHz):

2/25/2014 12:42:27 PM

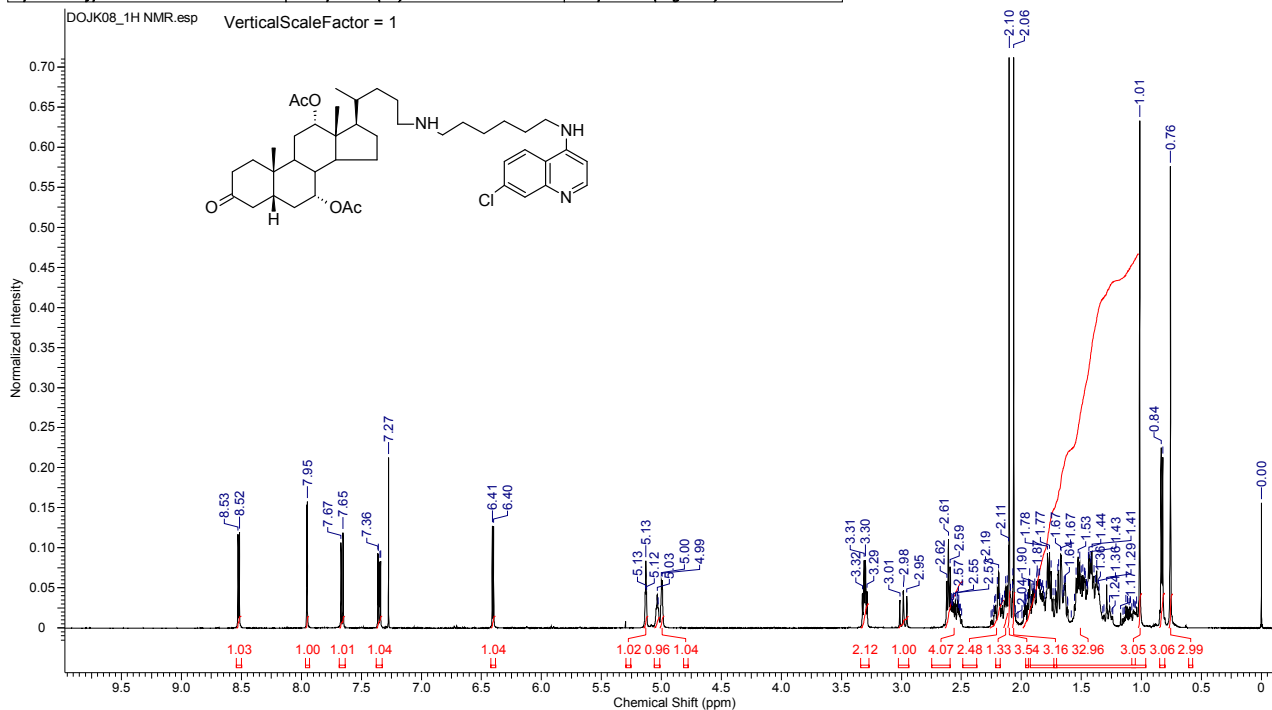
Number of Nuclei 0 C's					
Acquisition Time (sec)	0.5505	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	Date	22 Feb 2014 10:12:32
Date Stamp	22 Feb 2014 10:12:32				
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR novidozs13-nov2\pdata\11r				
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	265
Original Points Count	16384	Owner	nmrsu	Points Count	65536
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.45	Temperature (degree C)	25.000
				Spectrum Offset (Hz)	13831.5049



**Compound 25(DOJK08):**  $^1\text{H}$  NMR spectrum (500 MHz): HPLC purity: method A: RT 1.810, area 99.47 %; method C: RT=12.061, area 97.17 %.

2/25/2014 12:45:40 PM

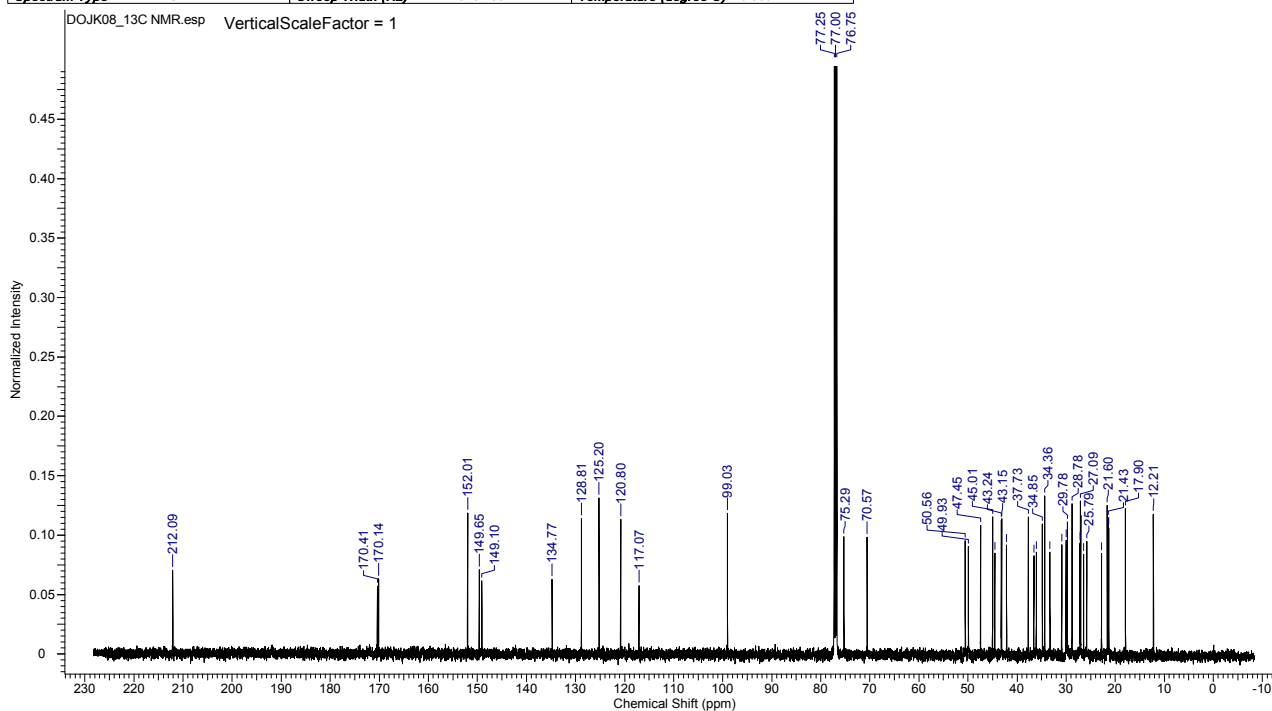
Number of Nuclei 0 H's				
Acquisition Time (sec)	2.7263	Date	02 Jun 2011 09:00:16	
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_ Stari\500 MHz\DOJKET1\1\pdata\111r		Date Stamp	02 Jun 2011 09:00:16
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	
Original Points Count	16384	Owner	nmsru	
Receiver Gain	256.00	SW(cyclical) (Hz)	6009.62	
Spectrum Type	STANDARD	Sweep Width (Hz)	6009.43	
		Points Count	32768	
		Solvent	CHLOROFORM-d	
		Temperature (degree C)	25.000	
		Origin	spect	
		Pulse Sequence	zg30	
		Spectrum Offset (Hz)	2562.5410	



**Compound 25(DOJK08):**  $^{13}\text{C}$  NMR spectrum (125 MHz):

2/25/2014 12:47:16 PM

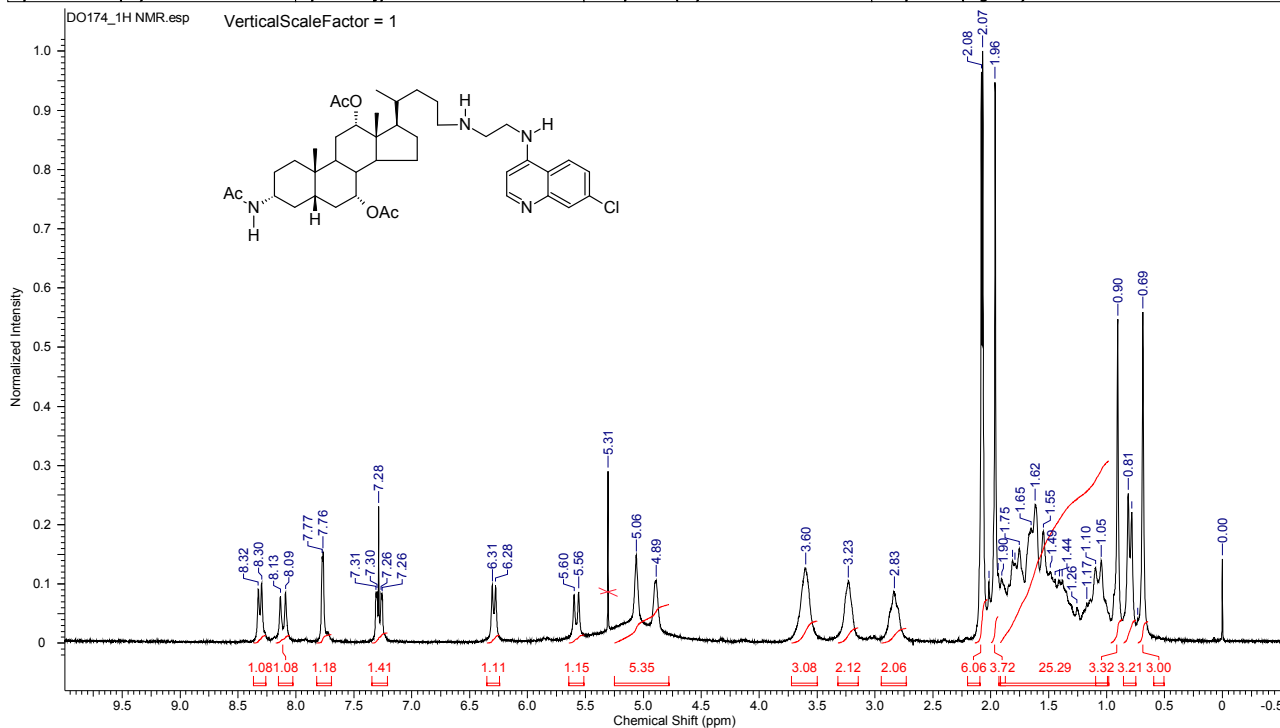
Number of Nuclei 0 C's				
Acquisition Time (sec)	0.5505	Date	02 Jun 2011 09:04:32	
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_ Stari\500 MHz\DOJKET1\6\pdata\111r		Date Stamp	02 Jun 2011 09:04:32
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	
Original Points Count	16384	Owner	nmsru	
Receiver Gain	1030.00	SW(cyclical) (Hz)	29761.90	
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	
		Points Count	703	
		Solvent	CHLOROFORM-d	
		Temperature (degree C)	25.000	
		Origin	spect	
		Pulse Sequence	zgpg30	
		Spectrum Offset (Hz)	13830.7256	



**Compound 36(DO174):**  $^1\text{H}$  NMR spectrum (200 MHz): HPLC purity: method A: RT 2.088, area 98.43 %; method C: RT 12.072, area 99.24 %.

2/25/2014 1:03:56 PM

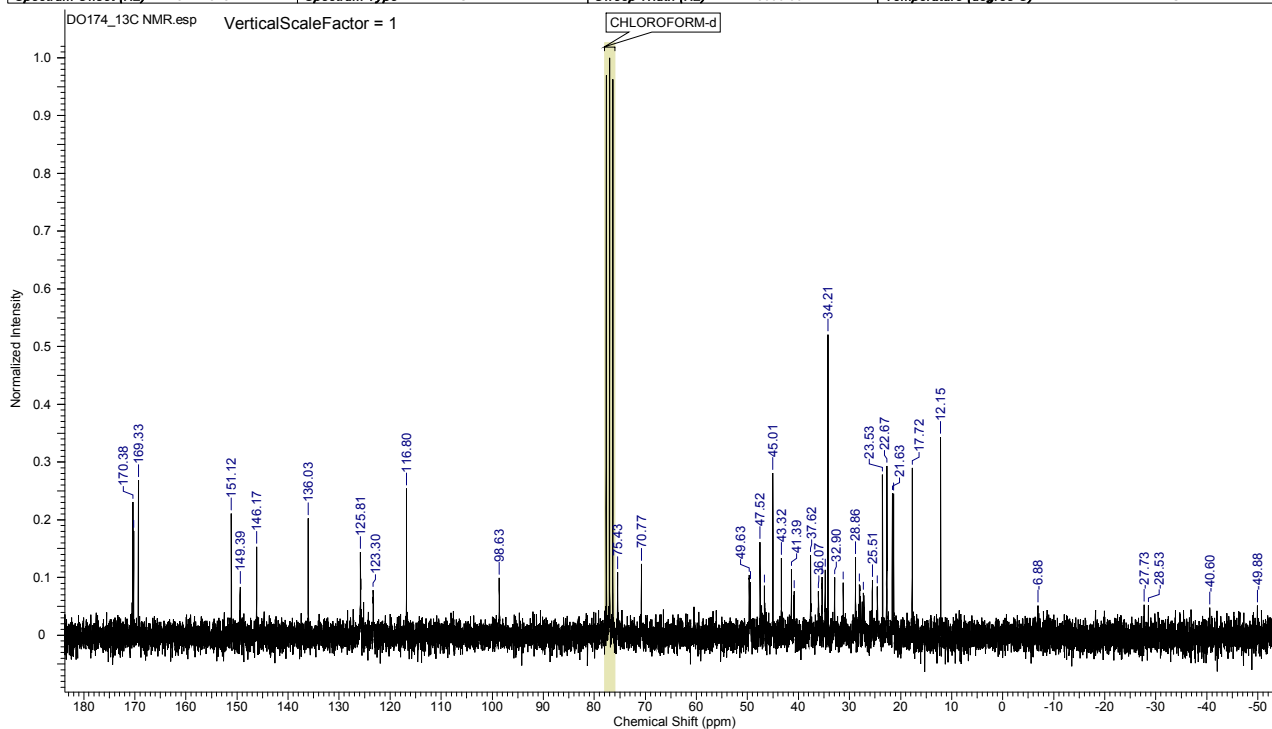
Number of Nuclei 0 H's							
Acquisition Time (sec)	3.4763	Comment	DOAA032cd6	Date	Jul 16 07	Date Stamp	Jul 16 07
File Name	C:\Users\Dejan Opseica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Star1200 MHz\DO174\doaa032cd6.fid\fid						
Frequency (MHz)	199.97	Nucleus	$^1\text{H}$	Number of Transients	32	Original Points Count	10448
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	6.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	1103.7272	Spectrum Type	STANDARD	Sweep Width (Hz)	3005.46	Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 36(DO174):**  $^{13}\text{C}$  NMR spectrum (50 MHz):

2/28/2014 11:33:13 AM

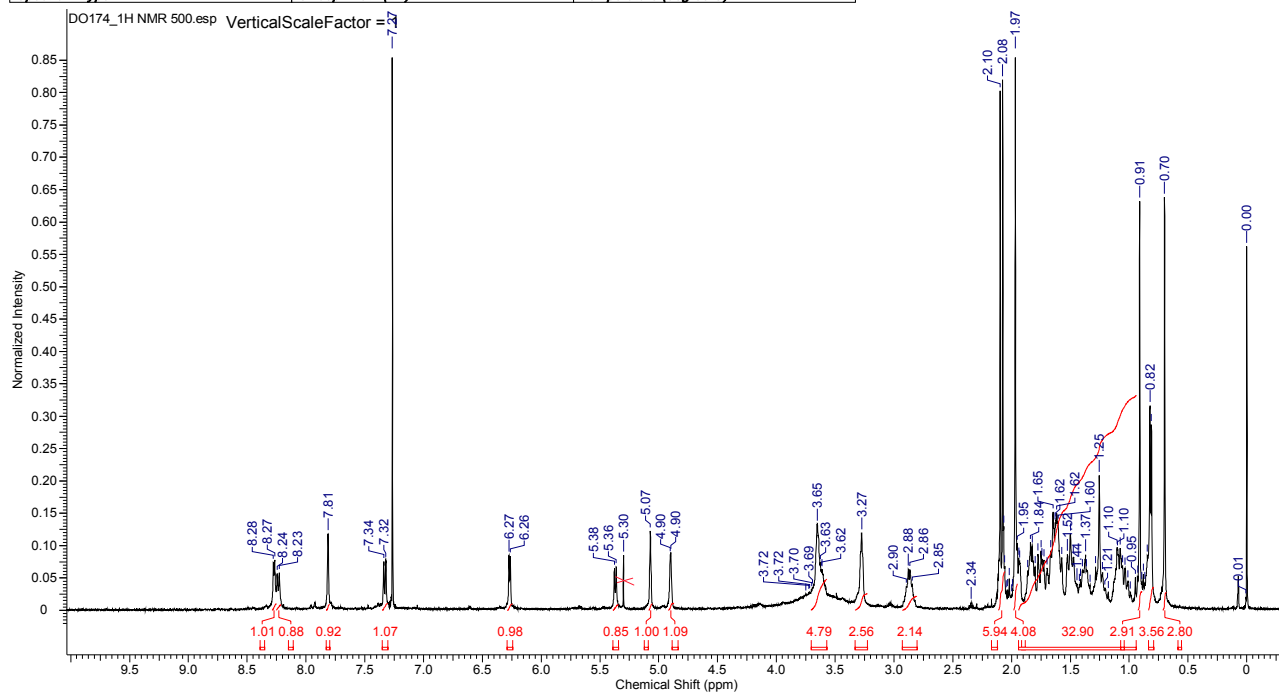
Number of Nuclei 0 C's							
Acquisition Time (sec)	1.0667	Comment	DOAA032cd6	Date	Jul 16 07	Date Stamp	Jul 16 07
File Name	C:\Users\Dejan Opseica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Star1200 MHz\DO174\doaa032cd6.fid\fid						
Frequency (MHz)	50.29	Nucleus	$^{13}\text{C}$	Number of Transients	3399	Original Points Count	16000
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	25.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	4814.7378	Spectrum Type	STANDARD	Sweep Width (Hz)	15000.00	Temperature (degree C)	AMBIENT TEMPERATURE



Compound 36 (DO174):  $^1\text{H}$  NMR spectrum (500 MHz):

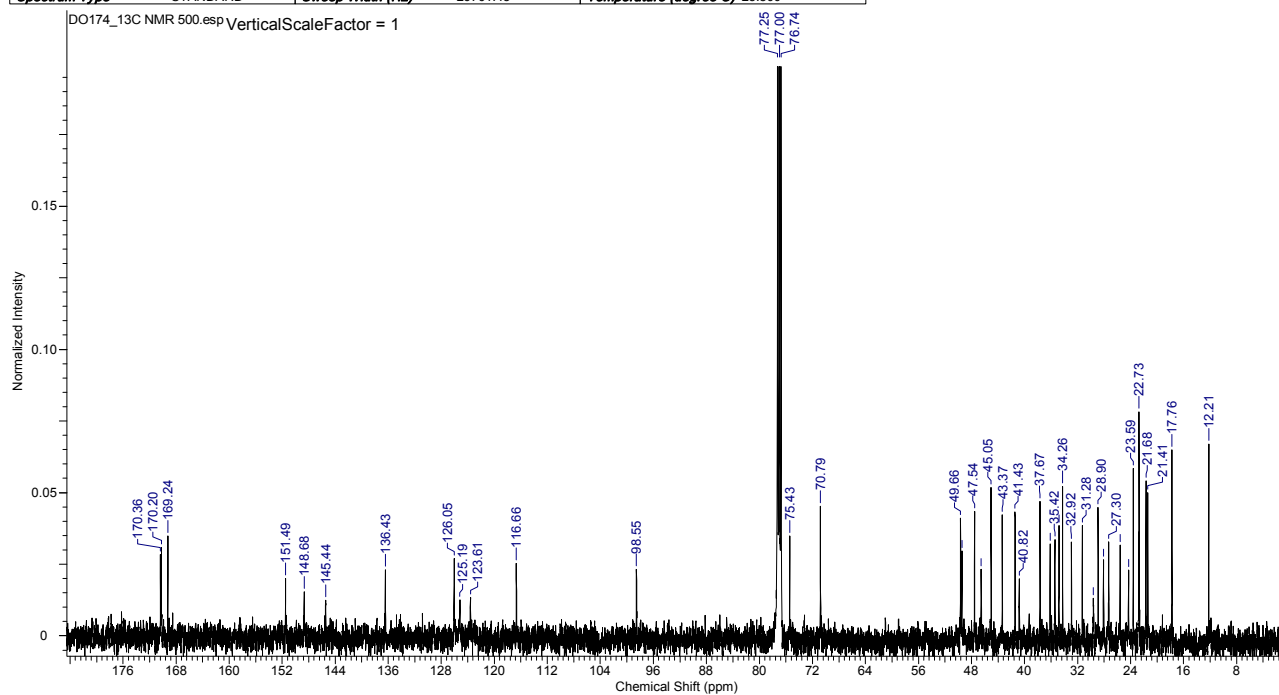
2/25/2014 1:10:23 PM

Number of Nuclei 0 H's					
Acquisition Time (sec)	2.1823	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	Date	19 Feb 2014 10:55:12
Date Stamp	19 Feb 2014 10:55:12				
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR nov\do174\1\data\111r				
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16
Original Points Count	16384	Owner	nmsu	Points Count	32768
Receiver Gain	362.00	SW(cyclical) (Hz)	7507.51	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	7507.28	Temperature (degree C)	25.000
				Origin	spect
				Pulse Sequence	zg30
				Spectrum Offset (Hz)	3489.8513

Compound 36 (DO174):  $^{13}\text{C}$  NMR spectrum (125 MHz):

2/25/2014 1:11:26 PM

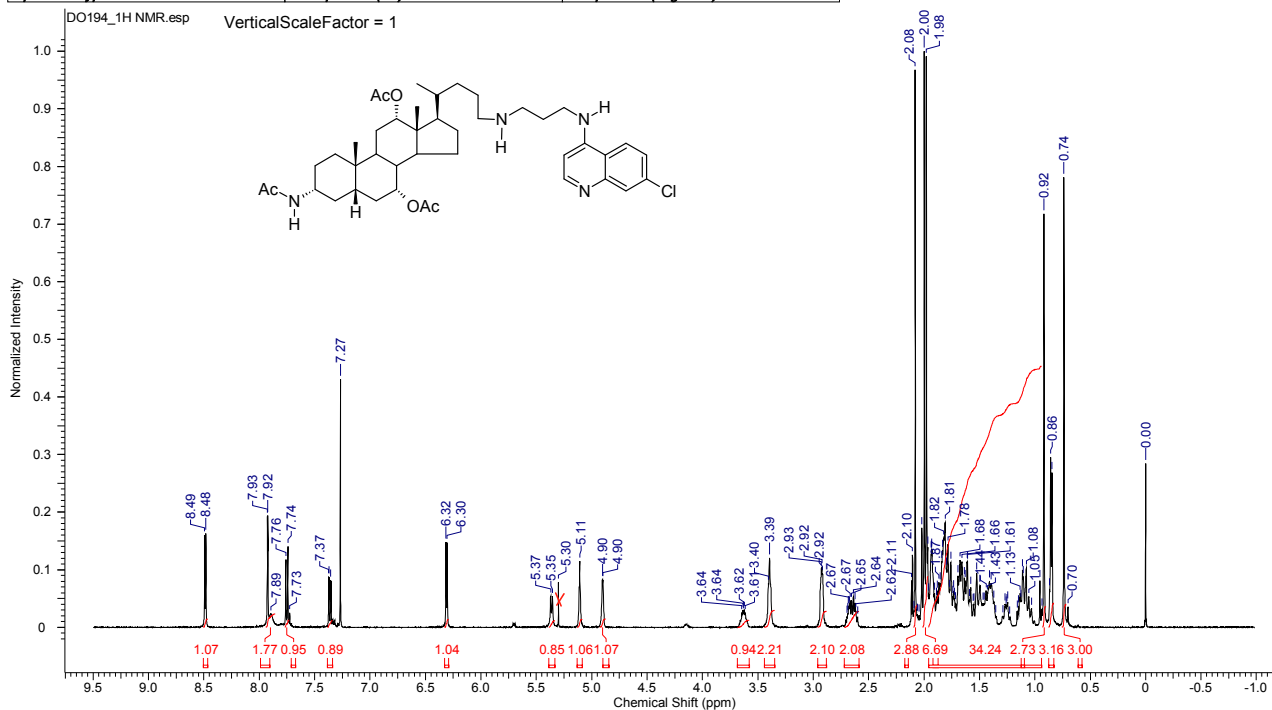
Number of Nuclei 0 C's					
Acquisition Time (sec)	0.5505	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	Date	20 Feb 2014 09:53:20
Date Stamp	20 Feb 2014 09:53:20				
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR nov\do174\2\data\111r				
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	700
Original Points Count	16384	Owner	nmsu	Points Count	65536
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.45	Temperature (degree C)	25.300
				Origin	spect
				Pulse Sequence	zgpg30
				Spectrum Offset (Hz)	13830.8887



**Compound 37 (DO194):  $^1\text{H}$  NMR spectrum (500 MHz):** HPLC purity: method A: RT 1.792, area 99.09 %; method C: RT=13.145, area 95.23 %.

2/28/2014 12:10:35 PM

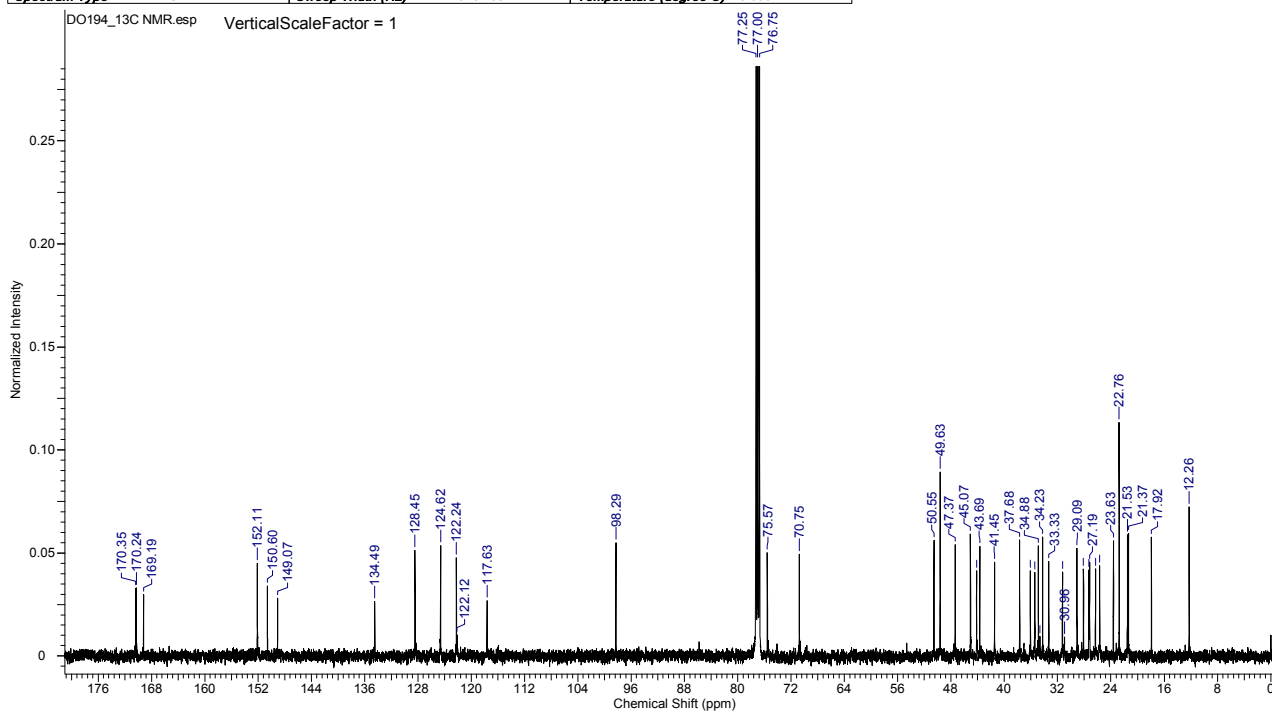
Number of Nuclei 0 H's							
Acquisition Time (sec)	3.1261	Date	18 Sep 2009 13:22:40				
File Name	C:\Users\Dejan Osenica\Documents\Radovi\Aminohinolinski\DO152 i ostali\Recenzija\Spektri NMR_Star\500 MHz\DO194\1\data\1\1r		Date Stamp	18 Sep 2009 13:22:40			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	32768	Pulse Sequence	zq30
Receiver Gain	181.00	SW(cyclical) (Hz)	5241.09	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2129.9771
Spectrum Type	STANDARD	Sweep Width (Hz)	5240.93	Temperature (degree C)	25.000		



**Compound 37 (DO194):  $^{13}\text{C}$  NMR spectrum (125 MHz):**

2/25/2014 1:31:33 PM

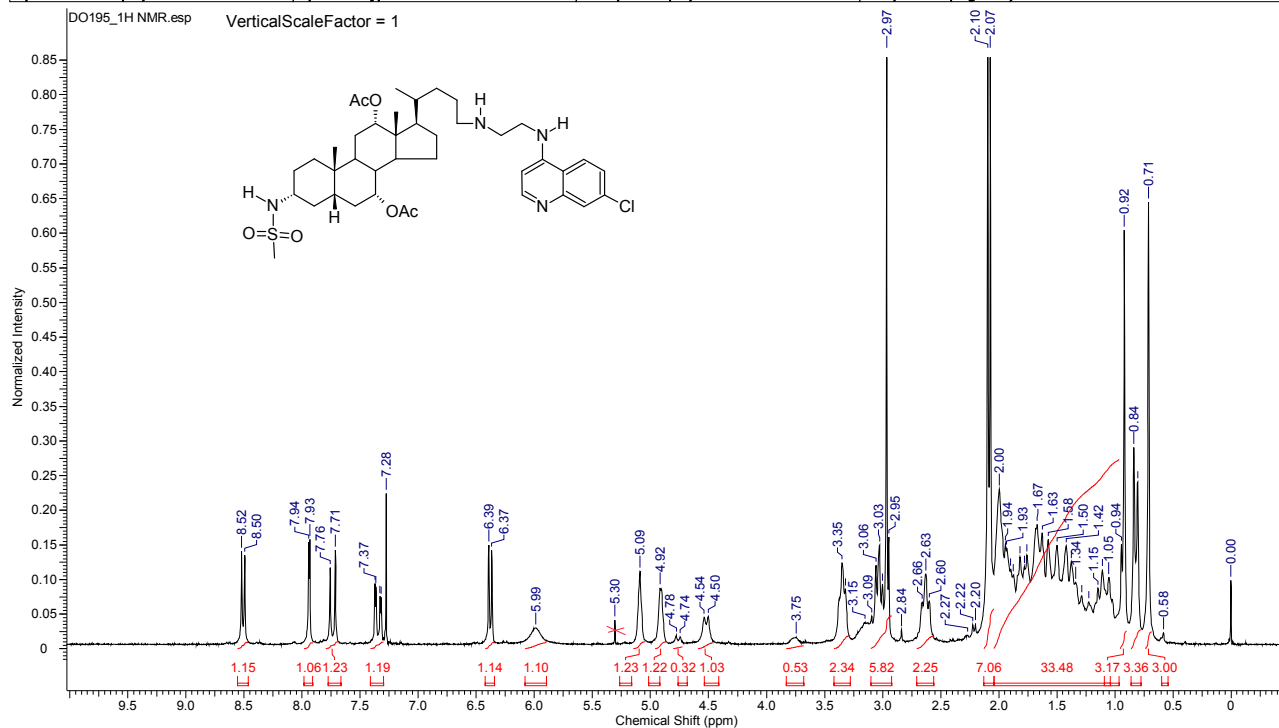
Number of Nuclei 0 C's							
Acquisition Time (sec)	0.5505	Date	18 Sep 2009 13:26:56				
File Name	C:\Users\Dejan Osenica\Documents\Radovi\Aminohinolinski\DO152 i ostali\Recenzija\Spektri NMR_Star\500 MHz\DO194\2\data\1\1r		Date Stamp	18 Sep 2009 13:26:56			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	1815	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	32768	Pulse Sequence	zqpg30
Receiver Gain	1030.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	13832.5488
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000		



**Compound 38 (DO195):  $^1\text{H}$  NMR spectrum (200 MHz):** HPLC purity: method A: RT 1.884, area 98.92 %; method C: RT 10.467, area 98.11 %.

2/25/2014 1:34:49 PM

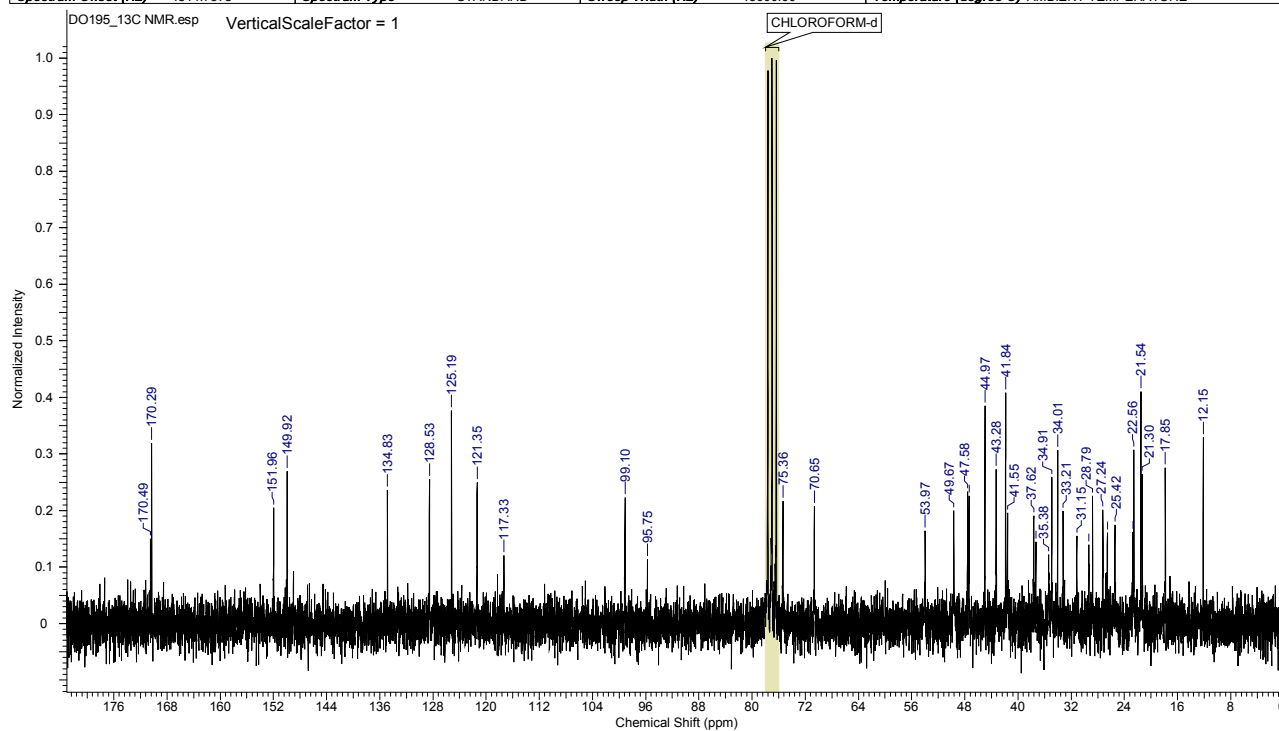
Number of Nuclei 0 H's					
Acquisition Time (sec)	1.3913	Comment	DO195	Date	Oct 28 09
File Name	C:\Users\Dejan\Openical\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR_Star1\200 MHz\DO195\hdo195.fid\fid				
Frequency (MHz)	199.97	Nucleus	$^1\text{H}$	Number of Transients	128
Points Count	8192	Pulse Sequence	s2pul	Receiver Gain	11.00
Spectrum Offset (Hz)	1686.7415	Spectrum Type	STANDARD	Sweep Width (Hz)	4600.00
				Solvent	CHLOROFORM-d
				Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 38 (DO195):  $^{13}\text{C}$  NMR spectrum (50 MHz):**

2/28/2014 12:30:31 PM

Number of Nuclei 0 C's					
Acquisition Time (sec)	1.0667	Comment	DO195	Date	Oct 28 09
File Name	C:\Users\Dejan\Openical\Documents\Radovi\Aminohinoliniski\DO152\ostali\Recenzija\Spektri NMR_Star1\200 MHz\DO195\cdo195.fid\fid				
Frequency (MHz)	50.29	Nucleus	$^{13}\text{C}$	Number of Transients	2797
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	25.00
Spectrum Offset (Hz)	4814.7378	Spectrum Type	STANDARD	Sweep Width (Hz)	15000.00
				Solvent	CHLOROFORM-d
				Temperature (degree C)	AMBIENT TEMPERATURE

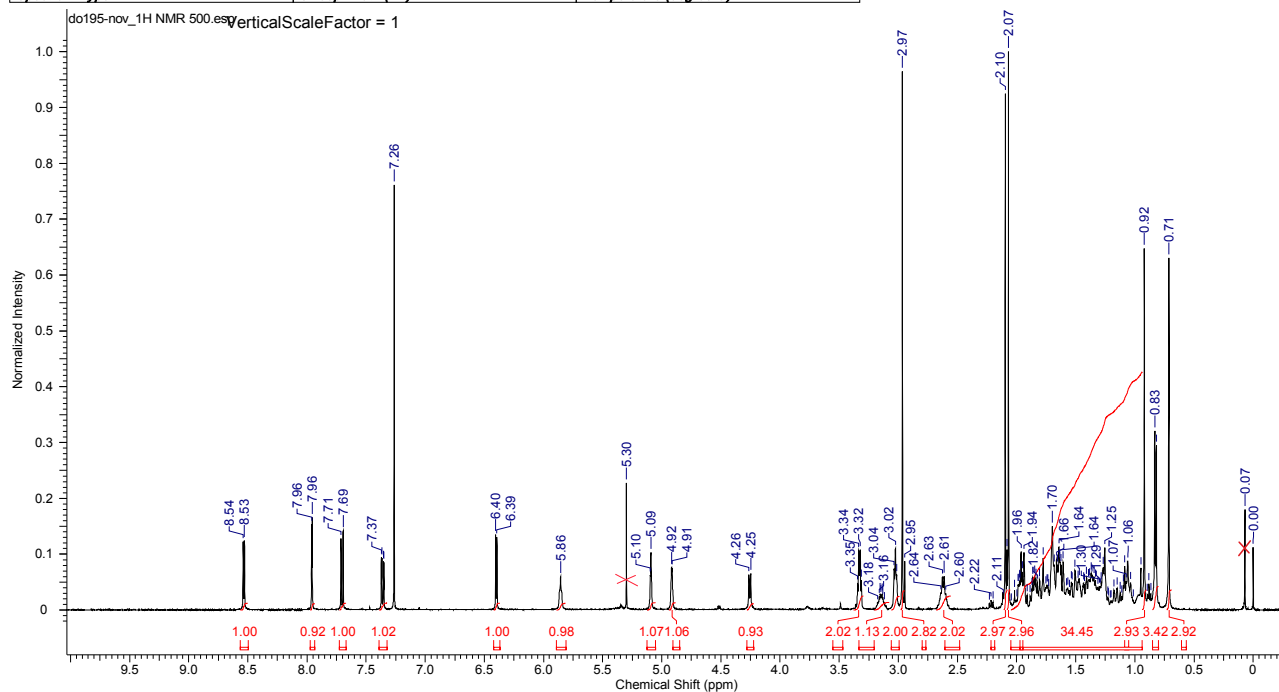




Compound 38 (DO195): <sup>1</sup>H NMR spectrum (500 MHz):

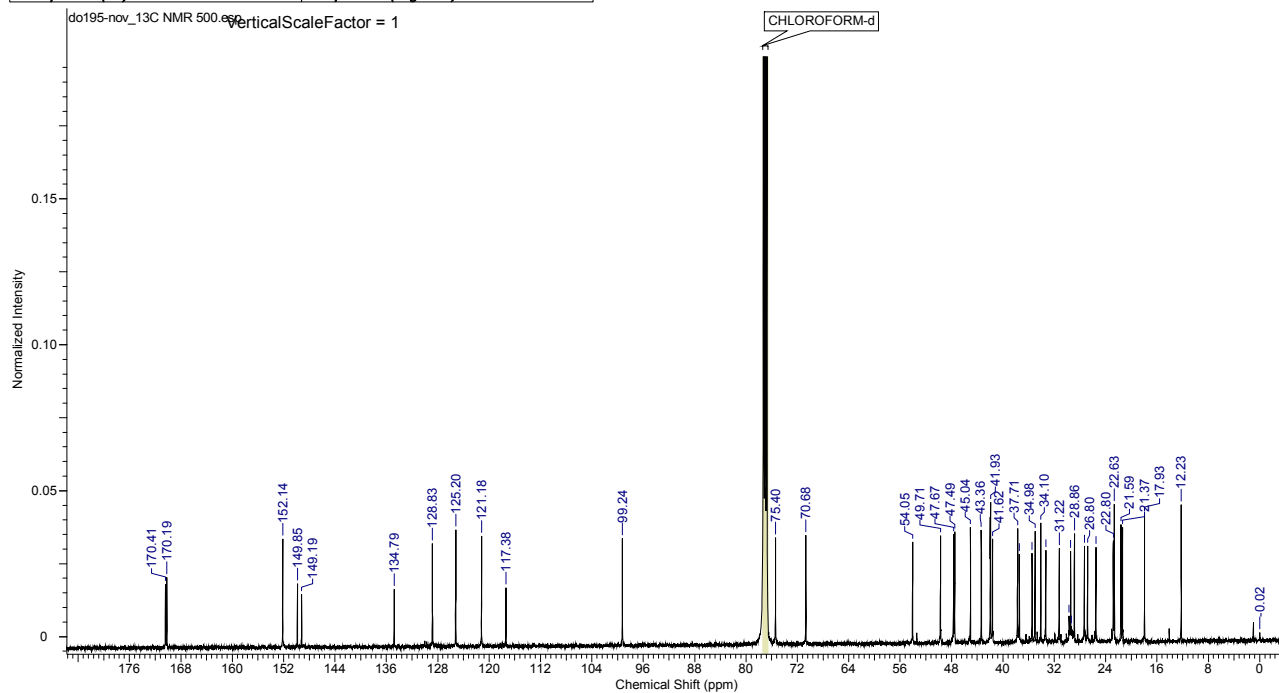
2/25/2014 1:38:48 PM

Number of Nuclei 0 H's			
Acquisition Time (sec)	2.1823	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118
Date Stamp	22 Feb 2014 10:53:04		
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR nov\do195-nov\1\pdata\1\1r		
Frequency (MHz)	500.26	Nucleus	<sup>1</sup> H
Original Points Count	16384	Owner	nmsu
Receiver Gain	362.00	Points Count	32768
Spectrum Type	STANDARD	Solvent	CHLOROFORM-d
		Sweep Width (Hz)	7507.51
		Temperature (degree C)	25.000
		Spectrum Offset (Hz)	3488.3303

Compound 38 (DO195): <sup>13</sup>C NMR spectrum (125 MHz):

2/28/2014 12:52:01 PM

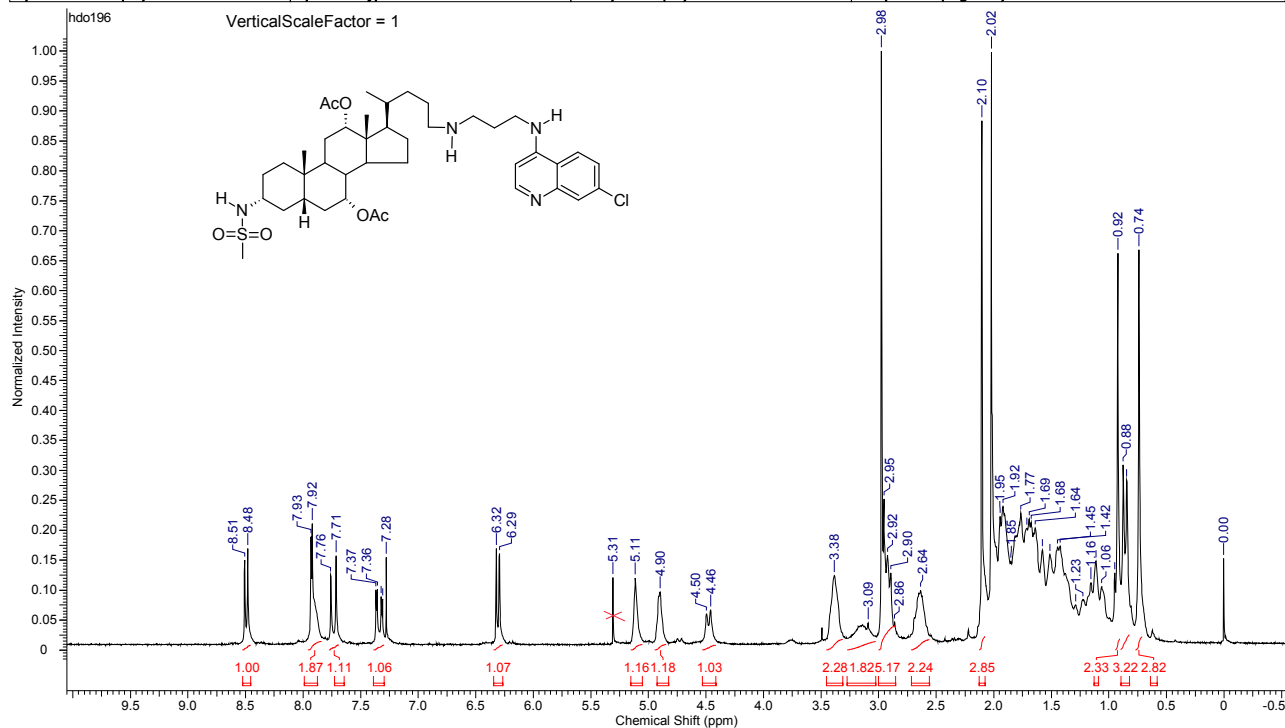
Number of Nuclei 0 C's			
Acquisition Time (sec)	0.5505	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118
Date Stamp	22 Feb 2014 10:57:20		
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR nov\do195-nov\2\pdata\1\1r		
Frequency (MHz)	125.79	Nucleus	<sup>13</sup> C
Owner	nmsu	Points Count	65536
SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Temperature (degree C)	25.100
		Spectrum Offset (Hz)	13833.2148
		Original Points Count	16384
		Receiver Gain	2050.00



**Compound 39 (DO196):  $^1\text{H}$  NMR spectrum (200 MHz):** HPLC purity: method A: RT 1.773, area 98.86 %; method B: RT 1.843, area 98.21 %.

2/26/2014 4:51:59 PM

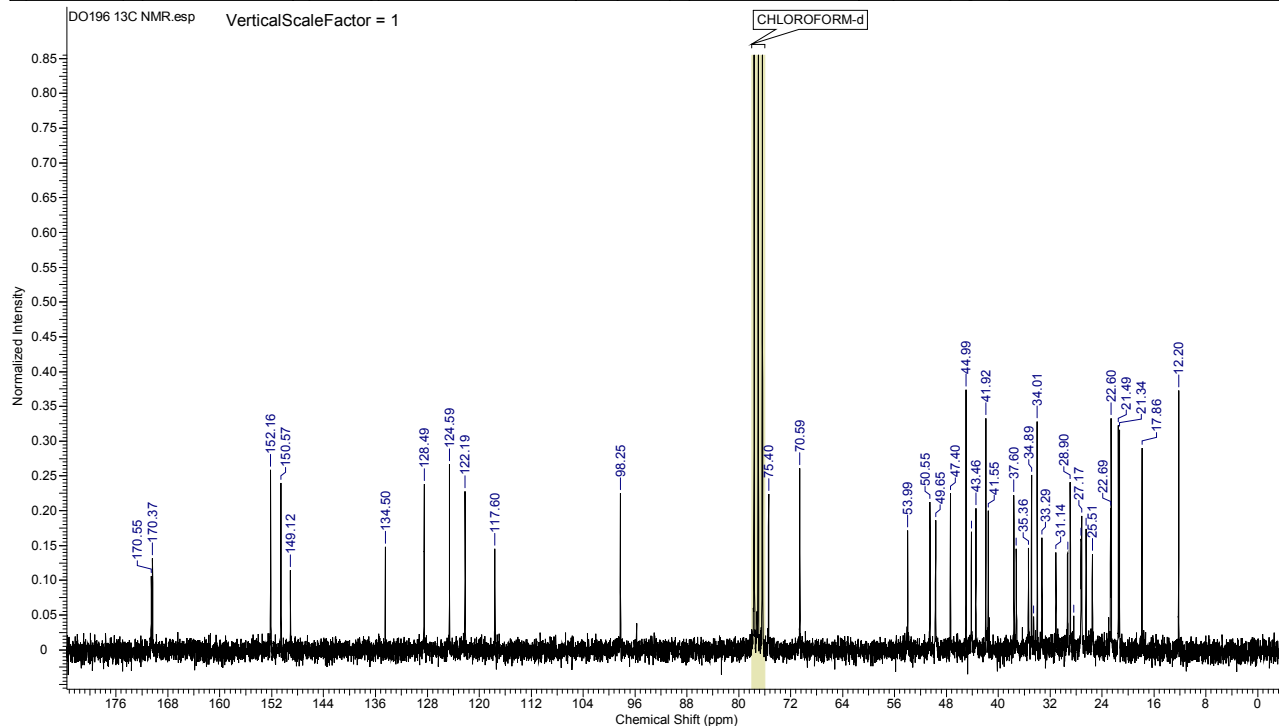
Number of Nuclei 0 H's							
Acquisition Time (sec)	1.3913	Comment	DO196	Date	Dec 17 09	Date Stamp	Dec 17 09
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO196\hdo196.fid\fid						
Frequency (MHz)	199.97	Nucleus	$^1\text{H}$	Number of Transients	128	Original Points Count	6400
Points Count	8192	Pulse Sequence	s2pul	Receiver Gain	11.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	1686.7415	Spectrum Type	STANDARD	Sweep Width (Hz)	4600.00	Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 39 (DO196):  $^{13}\text{C}$  NMR spectrum (50 MHz):**

2/28/2014 12:59:50 PM

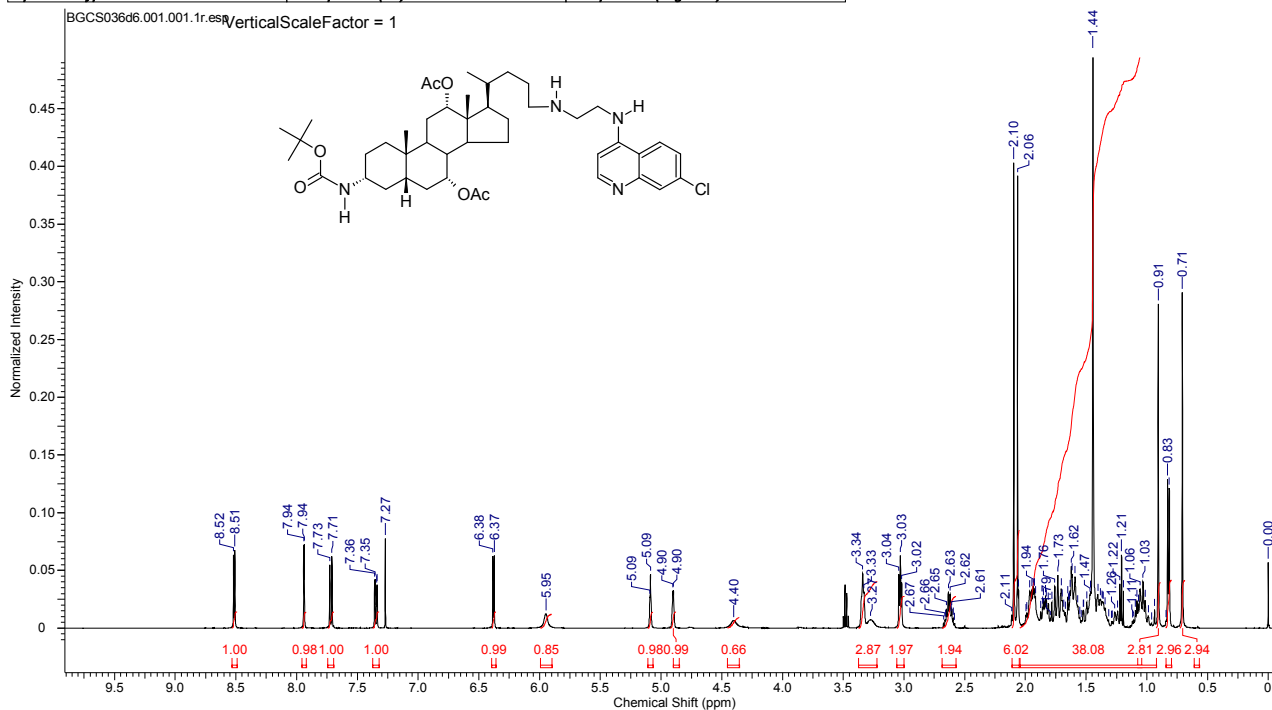
Number of Nuclei 0 C's							
Acquisition Time (sec)	1.0667	Comment	DO196	Date	Dec 17 09	Date Stamp	Dec 17 09
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO196\cdo196.fid\fid						
Frequency (MHz)	50.29	Nucleus	$^{13}\text{C}$	Number of Transients	16400	Original Points Count	16000
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	25.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	4814.7378	Spectrum Type	STANDARD	Sweep Width (Hz)	15000.00	Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 40 (DO179):  $^1\text{H}$  NMR spectrum (500 MHz):** HPLC purity: method A: RT 2.085, area 99.22 %; method B: RT 8.856, area 95.25 %.

2/26/2014 6:46:29 PM

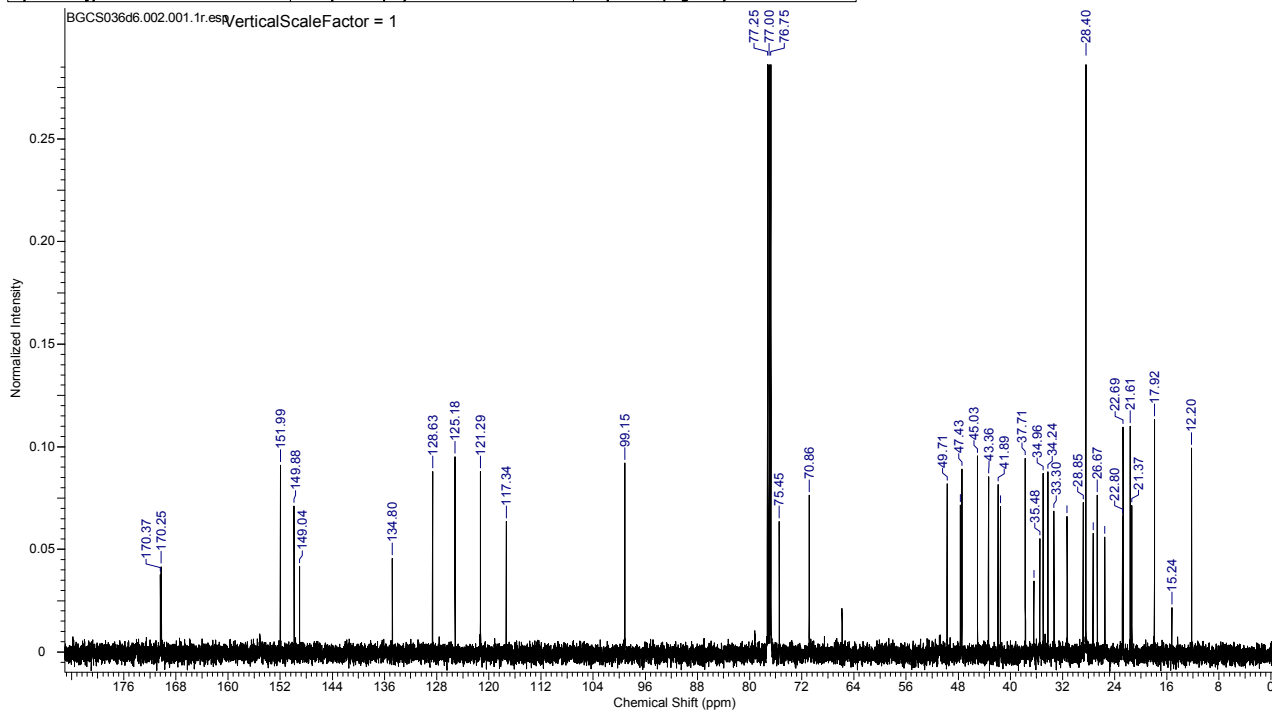
Number of Nuclei 0 H's				
Acquisition Time (sec)	2.7263	Date	03 Mar 2008 14:13:36	
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO179\BGCS036d6\1\pdata\1\1r		Date Stamp	03 Mar 2008 14:13:36
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	
Original Points Count	16384	Owner	nmsu	
Receiver Gain	114.00	SW(cyclical) (Hz)	6009.62	
Spectrum Type	STANDARD	Sweep Width (Hz)	6009.25	
		Points Count	16384	
		Solvent	CHLOROFORM-d	
		Temperature (degree C)	25.000	
		Pulse Sequence	zg30	
		Spectrum Offset (Hz)	2554.9321	



**Compound 40 (DO179):  $^{13}\text{C}$  NMR spectrum (125 MHz):**

2/26/2014 6:47:45 PM

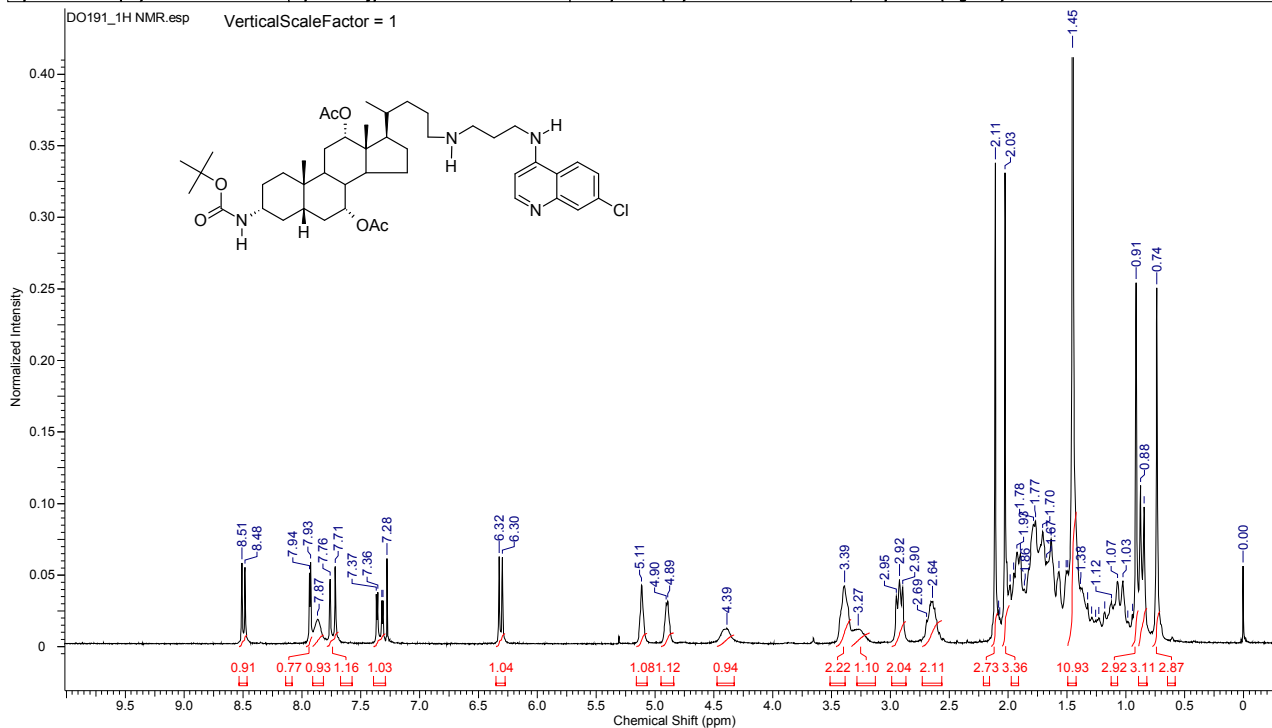
Number of Nuclei 0 C's				
Acquisition Time (sec)	1.1010	Date	03 Mar 2008 14:22:08	
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO179\BGCS036d6\2\pdata\1\1r		Date Stamp	03 Mar 2008 14:22:08
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	
Original Points Count	32768	Owner	nmsu	
Receiver Gain	1030.00	SW(cyclical) (Hz)	29761.90	
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	
		Number of Transients	536	
		Solvent	CHLOROFORM-d	
		Temperature (degree C)	25.000	
		Pulse Sequence	zgpg30	
		Spectrum Offset (Hz)	13833.4551	



**Compound 41 (DO191):  $^1\text{H}$  NMR spectrum (200 MHz):** HPLC purity: method A: RT 1.952, area 98.07 %; method C: RT 15.915, area 98.61 %.

2/25/2014 1:45:15 PM

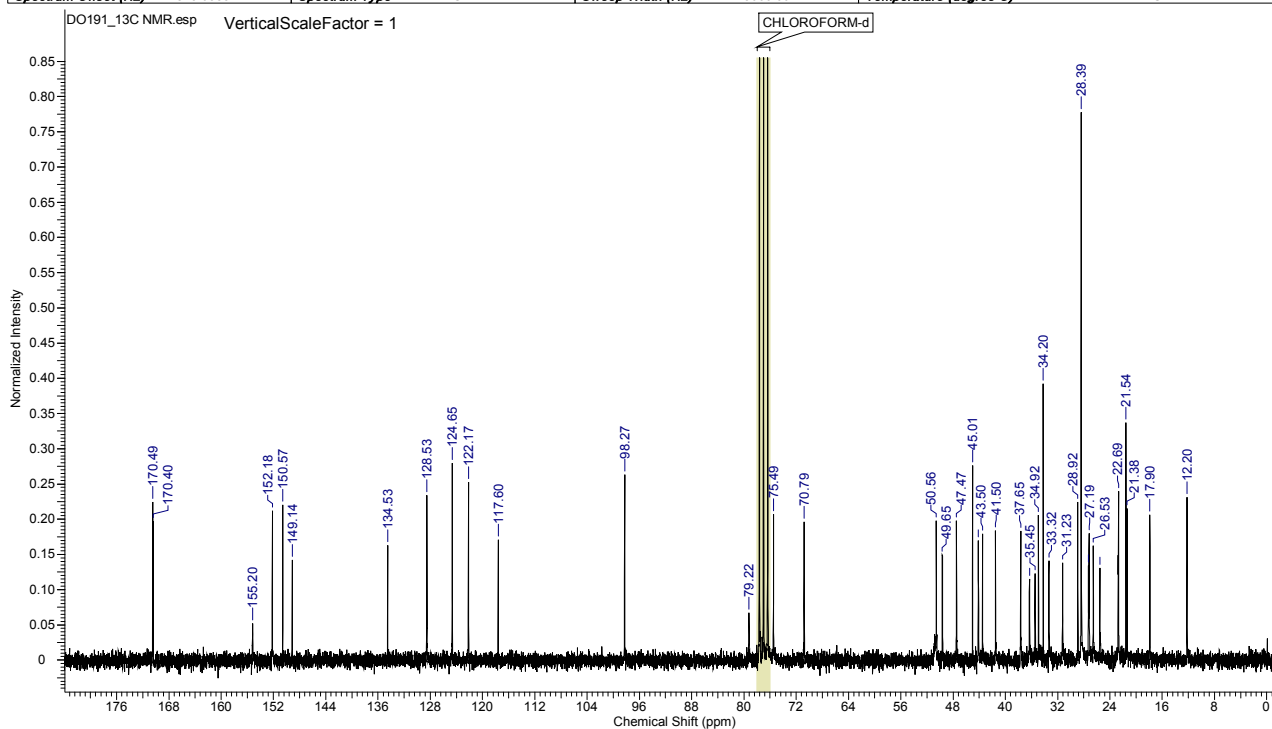
Number of Nuclei 0 H's							
Acquisition Time (sec)	1.3913	Comment	VF1	Date	Aug 22 09	Date Stamp	Aug 22 09
File Name	C:\Users\Dejan Oспенica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Star200 MHz\DO191\hv1.fid.fid						
Frequency (MHz)	199.97	Nucleus	$^1\text{H}$	Number of Transients	128	Original Points Count	6400
Points Count	8192	Pulse Sequence	s2pul	Receiver Gain	11.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	1686.7415	Spectrum Type	STANDARD	Sweep Width (Hz)	4600.00	Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 41 (DO191):  $^{13}\text{C}$  NMR spectrum (50 MHz):**

2/28/2014 1:48:21 PM

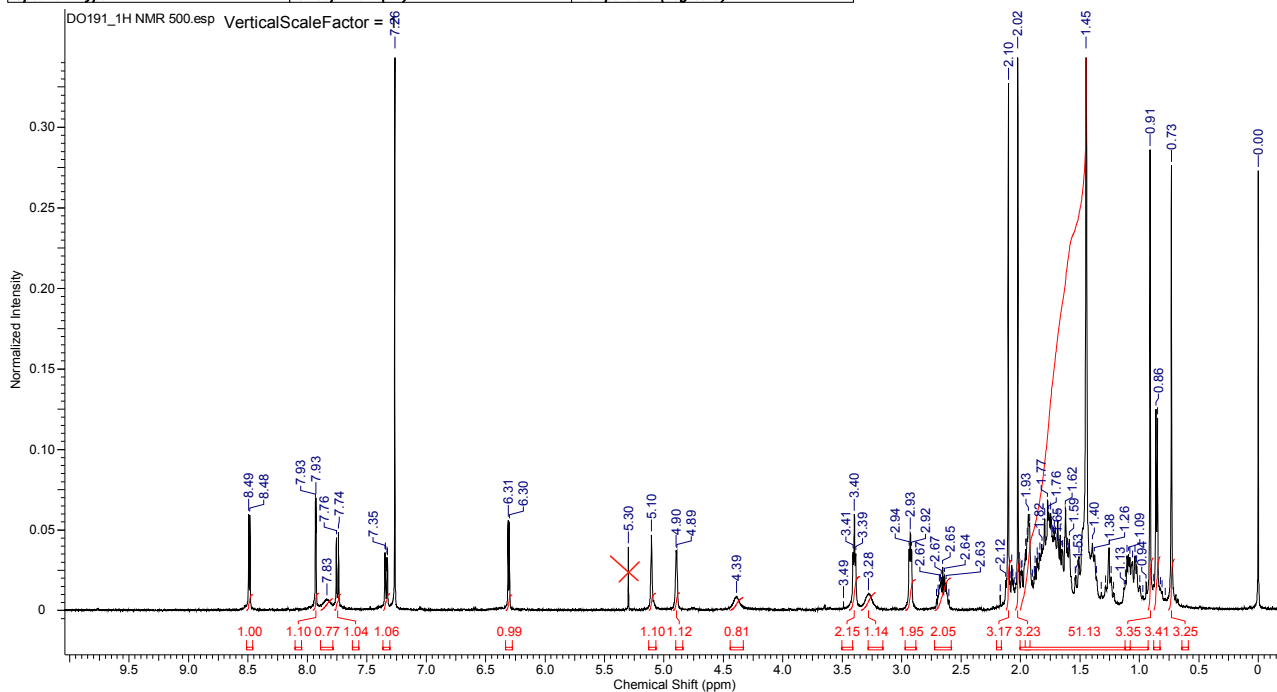
Number of Nuclei 0 C's							
Acquisition Time (sec)	1.0667	Comment	VF1	Date	Aug 22 09	Date Stamp	Aug 22 09
File Name	C:\Users\Dejan Oспенica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Star200 MHz\DO191\cv1.fid.fid						
Frequency (MHz)	50.29	Nucleus	$^{13}\text{C}$	Number of Transients	24000	Original Points Count	16000
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	25.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	4815.6533	Spectrum Type	STANDARD	Sweep Width (Hz)	15000.00	Temperature (degree C)	AMBIENT TEMPERATURE



Compound 41 (DO191):  $^1\text{H}$  NMR spectrum (500 MHz):

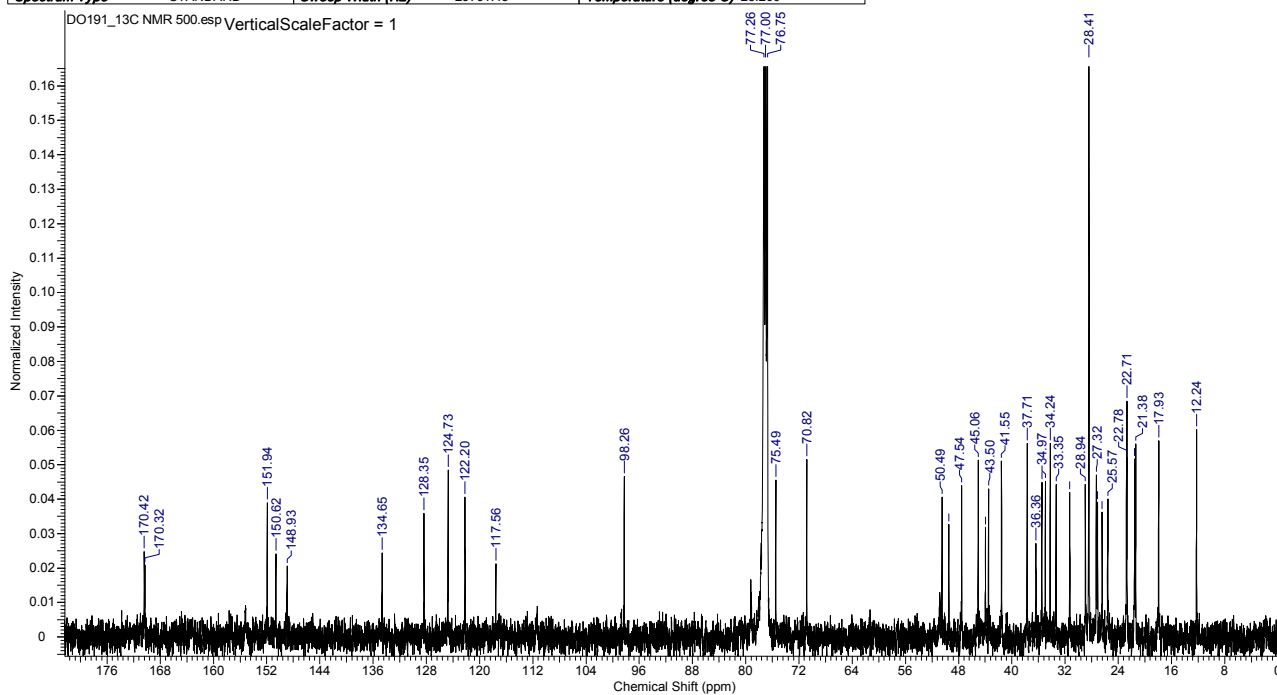
2/25/2014 1:48:04 PM

Number of Nuclei 0 H's				
Acquisition Time (sec)	2.1823	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	
Date Stamp	19 Feb 2014 10:50:56		Date	19 Feb 2014 10:50:56
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR novi\do191\1\data\111r			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	
Original Points Count	16384	Owner	nimsu	
Receiver Gain	362.00	SW(cyclical) (Hz)	7507.51	
Spectrum Type	STANDARD	Sweep Width (Hz)	7507.28	
		Solvent	CHLOROFORM-d	
		Temperature (degree C)	27.000	
		Number of Transients	16	
		Points Count	32768	
		Pulse Sequence	zg30	
		Spectrum Offset (Hz)	3489.0959	

Compound 41 (DO191):  $^{13}\text{C}$  NMR spectrum (125 MHz):

2/25/2014 1:49:22 PM

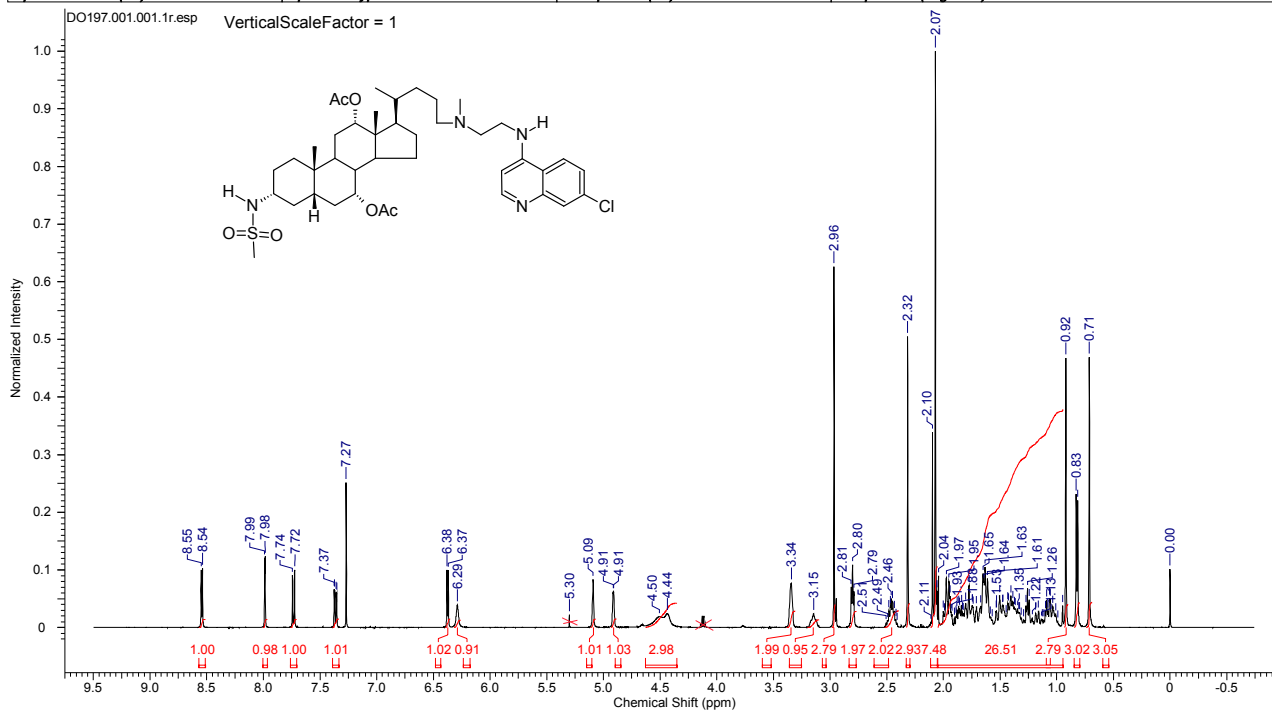
Number of Nuclei 0 C's				
Acquisition Time (sec)	0.5505	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	
Date Stamp	20 Feb 2014 15:06:56		Date	20 Feb 2014 15:06:56
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR novi\do191\2\data\111r			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	
Original Points Count	16384	Owner	nimsu	
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.45	
		Solvent	CHLOROFORM-d	
		Temperature (degree C)	25.200	
		Number of Transients	1687	
		Points Count	65536	
		Pulse Sequence	zqpg30	
		Spectrum Offset (Hz)	13832.2607	



**Compound 42 (DO197):  $^1\text{H}$  NMR spectrum (500 MHz):** HPLC purity: method A: RT 1.868, area 99.31 %; method B: RT 1.859, area 98.31 %.

2/26/2014 5:06:15 PM

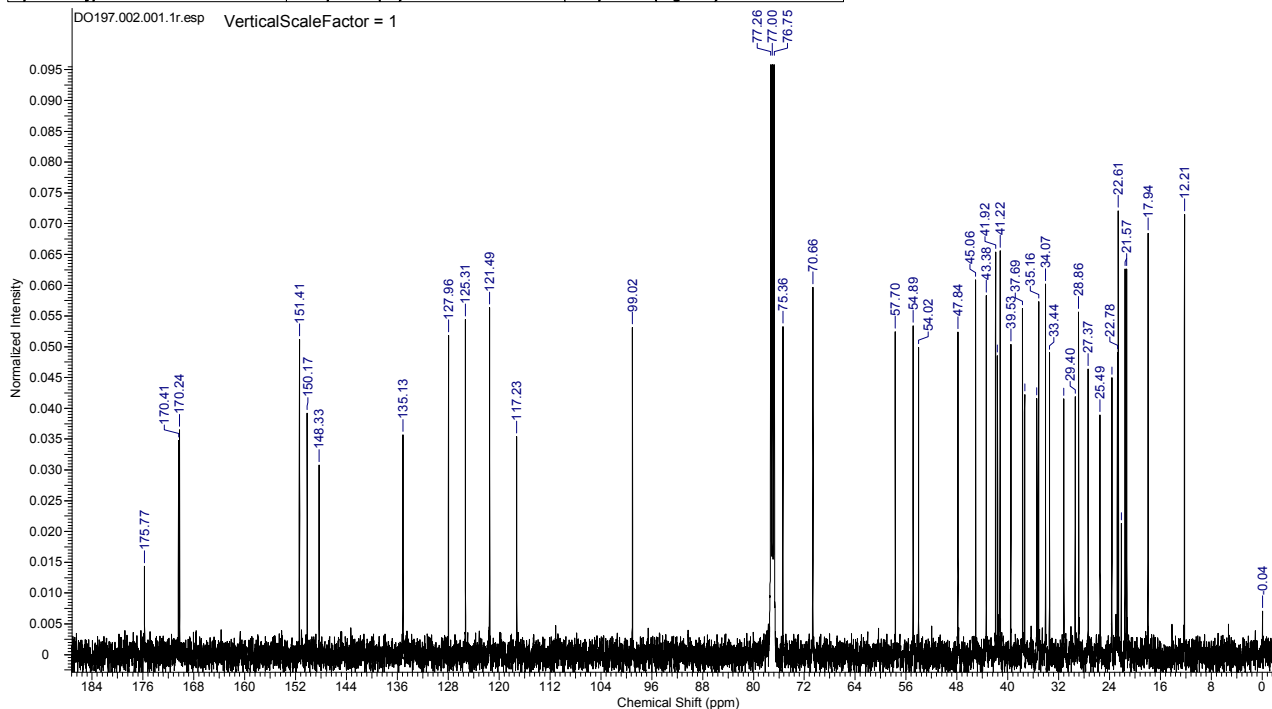
Number of Nuclei 0 H's					
Acquisition Time (sec)	3.1982	Date	04 Nov 2009 12:26:56	Date Stamp	04 Nov 2009 12:26:56
File Name	C:\Users\Dejan Oспенica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO197\1\data\1\1r				
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16
Original Points Count	16384	Owner	nmrsu	Points Count	32768
Receiver Gain	101.00	SW(cyclical) (Hz)	5122.95	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2190.0869	Spectrum Type	STANDARD	Sweep Width (Hz)	5122.79
				Temperature (degree C)	24.900



**Compound 42 (DO197):  $^{13}\text{C}$  NMR spectrum (125 MHz):**

2/26/2014 5:08:26 PM

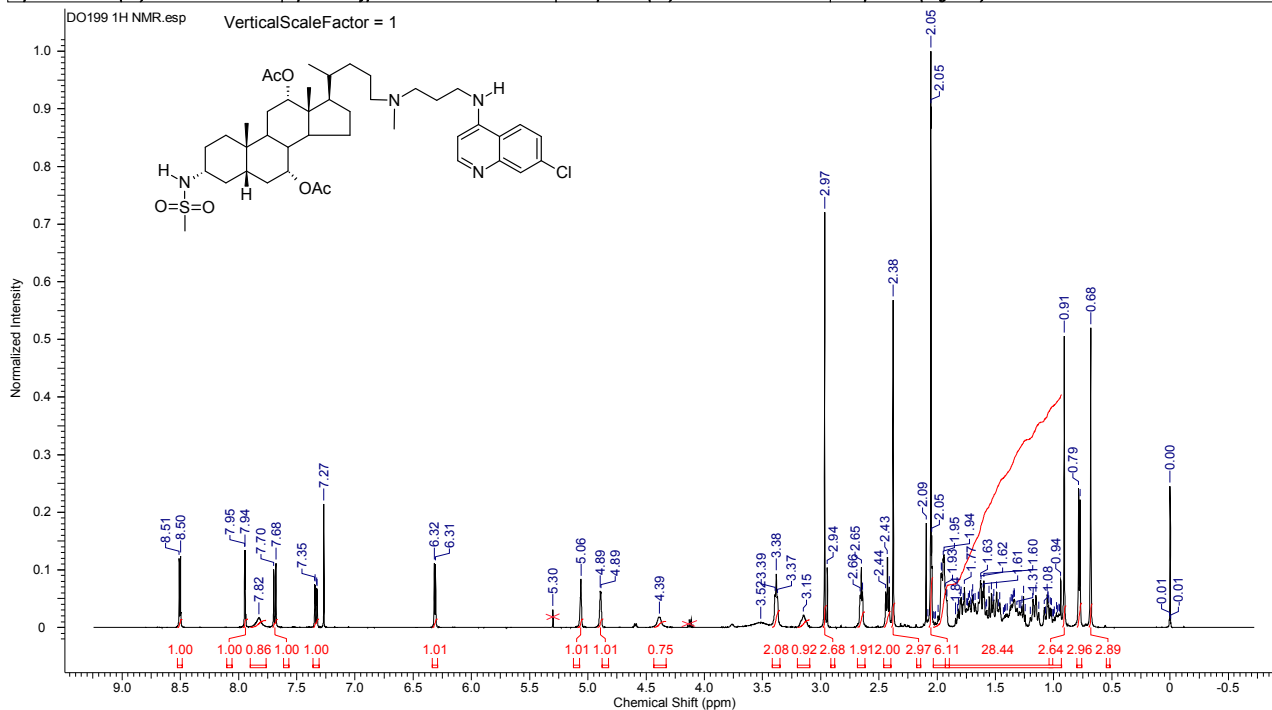
Number of Nuclei 0 C's					
Acquisition Time (sec)	0.5505	Date	04 Nov 2009 12:35:28	Date Stamp	04 Nov 2009 12:35:28
File Name	C:\Users\Dejan Oспенica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO197\2\data\1\1r				
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	1027
Original Points Count	16384	Owner	nmrsu	Points Count	32768
Receiver Gain	1440.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000
				Spectrum Offset (Hz)	13831.9326



**Compound 43 (DO199):  $^1\text{H}$  NMR spectrum (500 MHz):** HPLC purity: method A: RT 1.879, area 99.37 %; method B: RT 1.866, area 99.37 %.

2/28/2014 3:21:13 PM

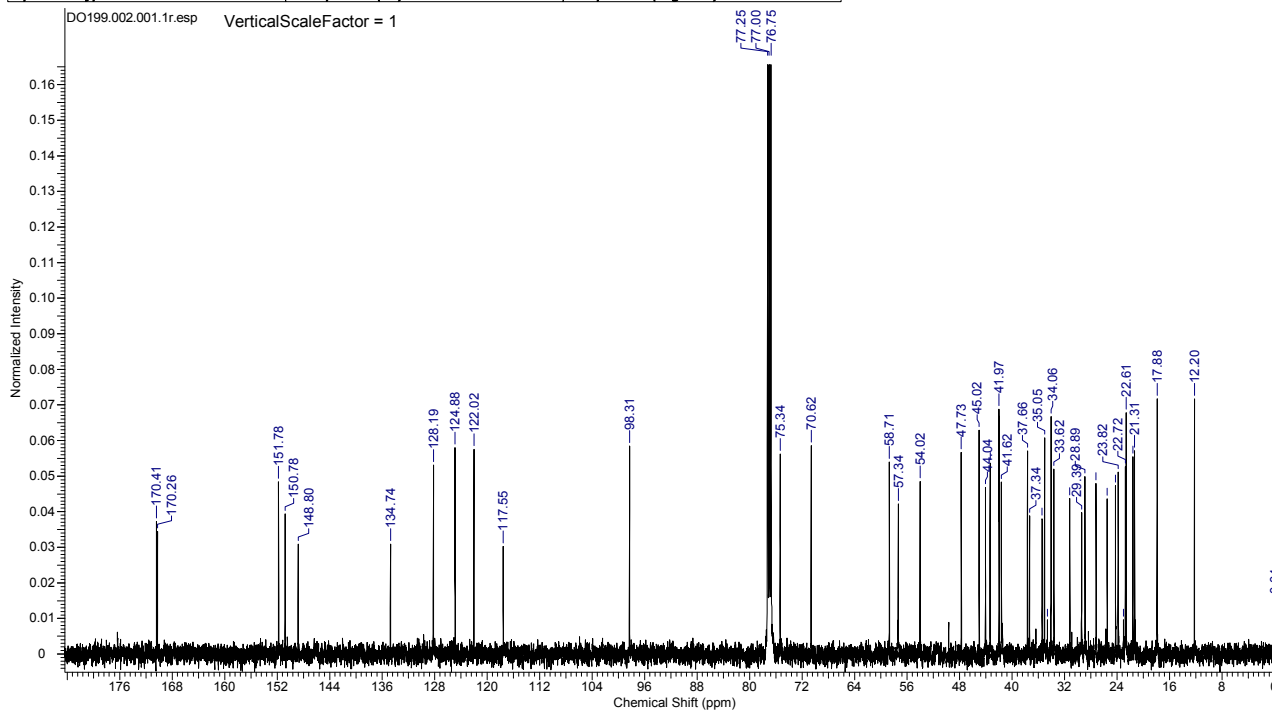
Number of Nuclei 0 H's					
Acquisition Time (sec)	3.2855	Date	11 Jan 2010 11:16:32	Date Stamp	11 Jan 2010 11:16:32
File Name	C:\Users\Dejan Oспенica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO199\1\data\11r				
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16
Original Points Count	16384	Owner	nmrsu	Points Count	16384
Receiver Gain	144.00	SW(cyclical) (Hz)	4986.70	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2131.6174	Spectrum Type	STANDARD	Sweep Width (Hz)	4986.40
				Temperature (degree C)	25.000



**Compound 43 (DO199):  $^{13}\text{C}$  NMR spectrum (125 MHz):**

2/26/2014 5:21:25 PM

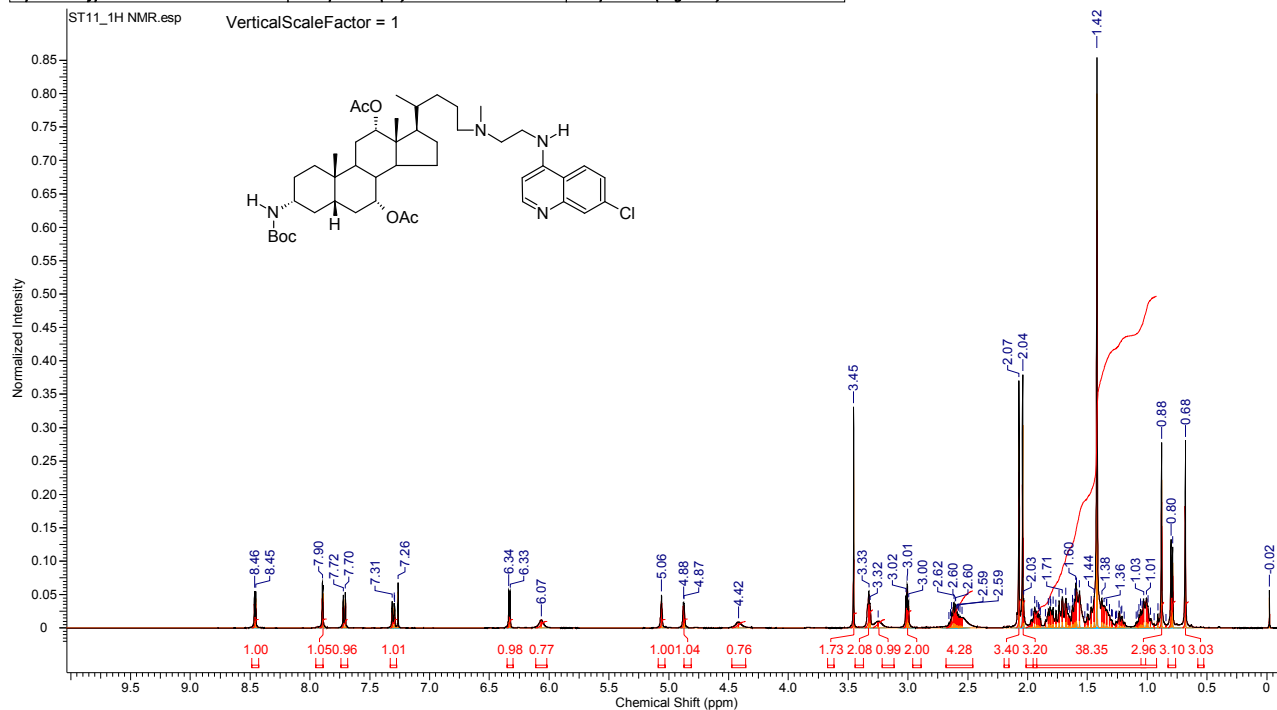
Number of Nuclei 0 C's					
Acquisition Time (sec)	0.5505	Date	11 Jan 2010 11:27:12	Date Stamp	11 Jan 2010 11:27:12
File Name	C:\Users\Dejan Oспенica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO199\2\data\11r				
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	1216
Original Points Count	16384	Owner	nmrsu	Points Count	32768
Receiver Gain	912.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000
				Spectrum Offset (Hz)	13832.2471



**Compound 44 (ST11):  $^1\text{H}$  NMR spectrum (500 MHz):** HPLC purity: method A: RT 1.994, area 99.12 %; method C: RT 9.936, area 98.20 %.

2/25/2014 2:07:18 PM

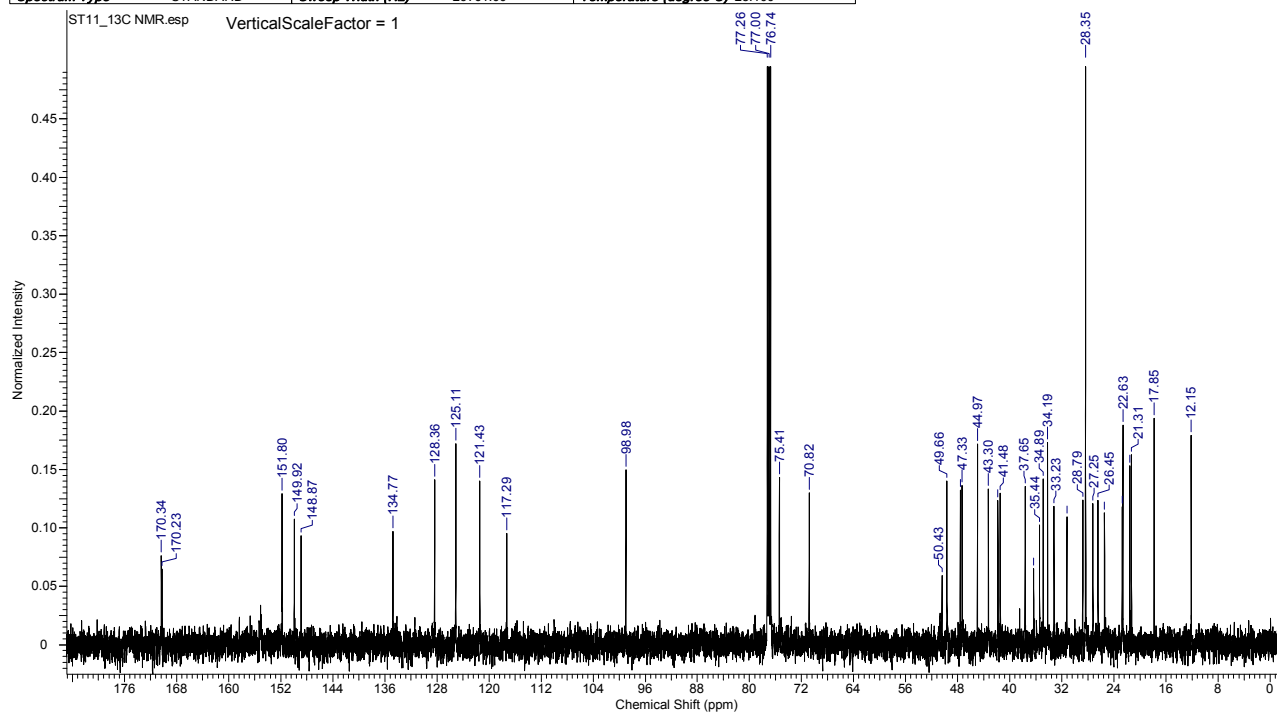
Number of Nuclei 0 H's				
Acquisition Time (sec)	2.5166	Date	19 Mar 2012 09:46:56	
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzijal\Spektri NMR_ Stari\500 MHz\KAA074-3\1\pdata\111r		Date Stamp	19 Mar 2012 09:46:56
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	
Original Points Count	16384	Owner	nmsru	
Receiver Gain	57.00	SW(cyclical) (Hz)	6510.42	
Spectrum Type	STANDARD	Sweep Width (Hz)	6510.22	
		Temperature (degree C)	25.000	
		Points Count	32768	
		Solvent	CHLOROFORM-d	
		Pulse Sequence	zg30	
		Spectrum Offset (Hz)	2753.9351	



**Compound 44 (ST11):  $^{13}\text{C}$  NMR spectrum (125 MHz):**

2/25/2014 2:08:41 PM

Number of Nuclei 0 C's				
Acquisition Time (sec)	0.5505	Date	19 Mar 2012 09:51:12	
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzijal\Spektri NMR_ Stari\500 MHz\KAA074-3\2\pdata\111r		Date Stamp	19 Mar 2012 09:51:12
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	
Original Points Count	16384	Owner	nmsru	
Receiver Gain	1030.00	SW(cyclical) (Hz)	29761.90	
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	
		Temperature (degree C)	25.100	
		Points Count	32768	
		Solvent	CHLOROFORM-d	
		Pulse Sequence	zgpg30	
		Spectrum Offset (Hz)	13827.5557	

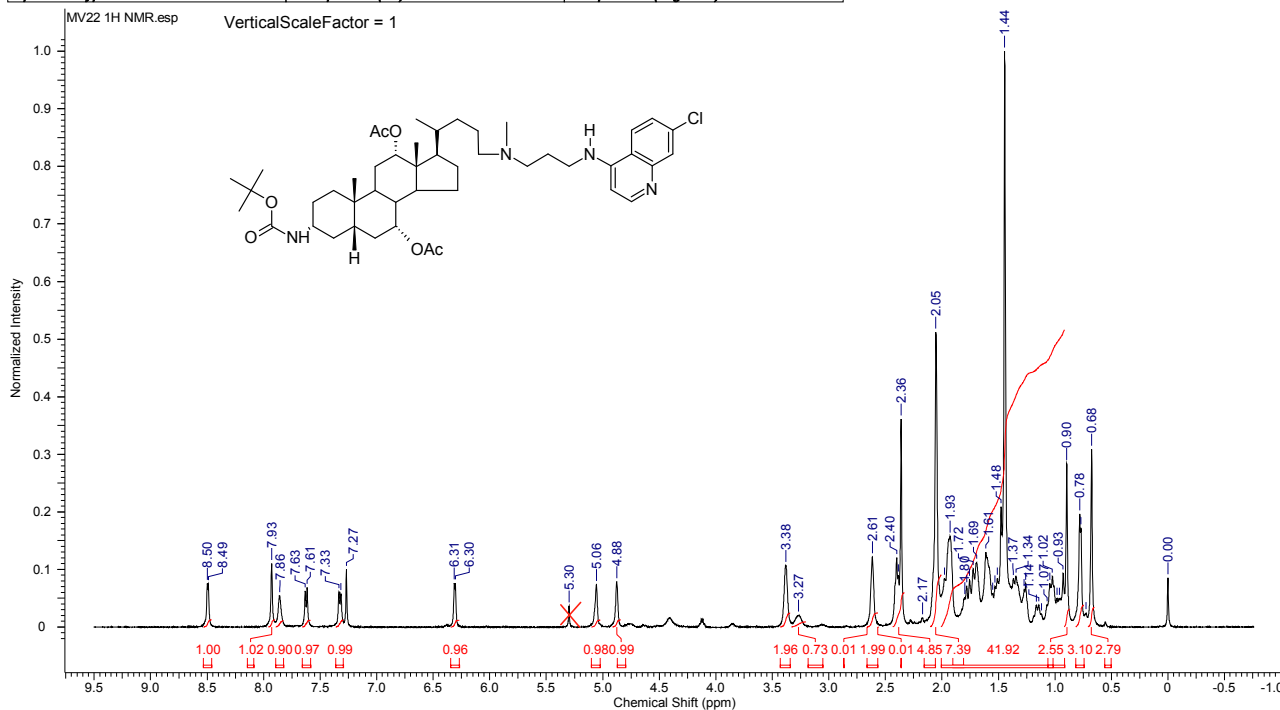




**Compound 45 (MV22):**  $^1\text{H}$  NMR spectrum (500 MHz): HPLC purity: method C: RT 7.896, area 96.46; method D: RT 5.553, area 96.83 %.

2/26/2014 7:22:00 PM

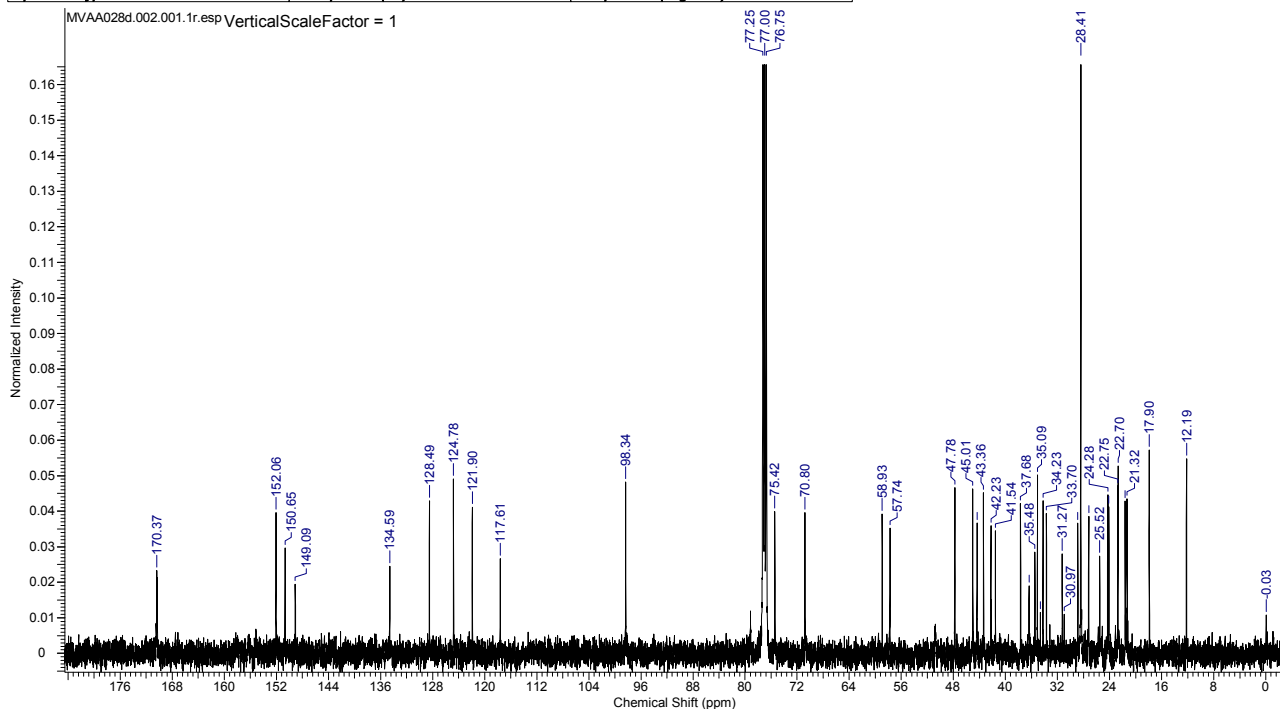
Number of Nuclei 0 H's							
Acquisition Time (sec)	3.1894	Date	10 Dec 2009 16:28:00				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\MV22\MVAA028d\1\data\11r		Date Stamp	10 Dec 2009 16:28:00			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmrsu	Points Count	32768	Pulse Sequence	zq30
Receiver Gain	144.00	SW(cyclical) (Hz)	5136.99	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2186.4534
Spectrum Type	STANDARD	Sweep Width (Hz)	5136.83	Temperature (degree C)	25.000		



**Compound 45 (MV22):**  $^{13}\text{C}$  NMR spectrum (125 MHz):

2/26/2014 5:26:36 PM

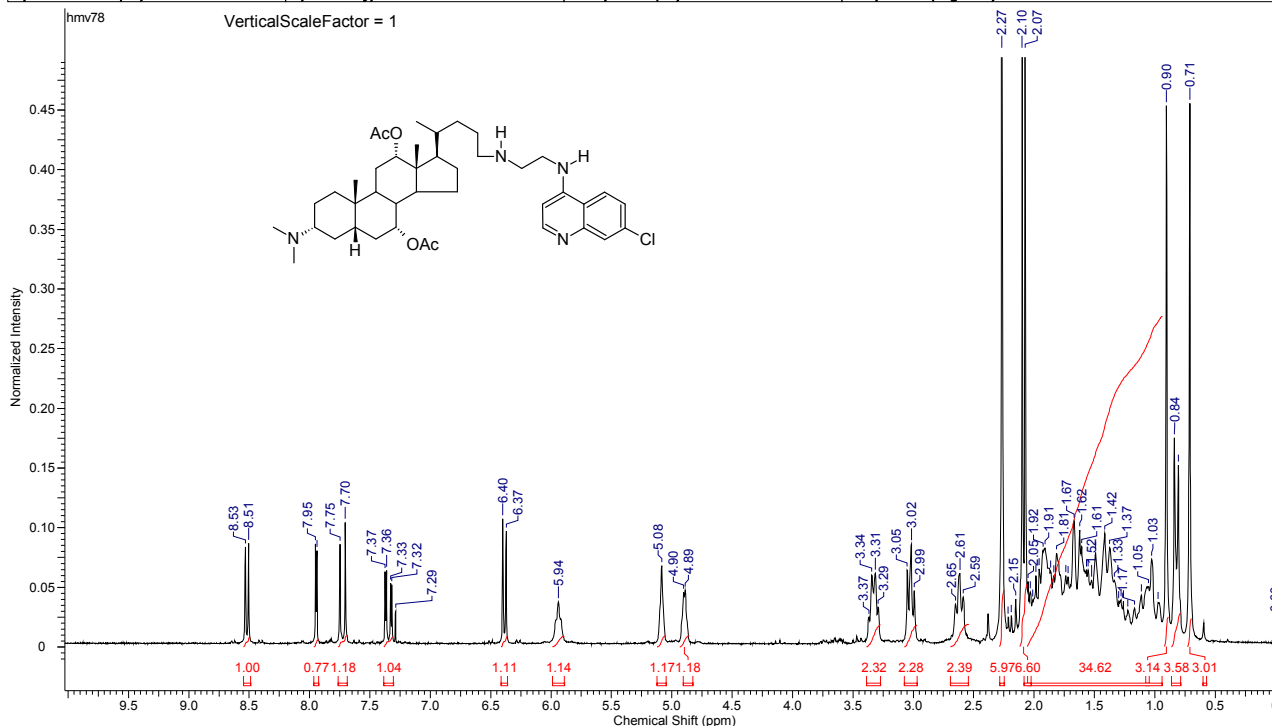
Number of Nuclei 0 C's							
Acquisition Time (sec)	0.5505	Date	10 Dec 2009 16:34:24				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\MV22\MVAA028d\2\data\11r		Date Stamp	10 Dec 2009 16:34:24			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	835	Origin	spect
Original Points Count	16384	Owner	nmrsu	Points Count	32768	Pulse Sequence	zpgg30
Receiver Gain	812.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	13832.5371
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000		



**Compound 50 (MV78):**  $^1\text{H}$  NMR spectrum (200 MHz). HPLC purity: method A: RT 1.925, area 98.15 %; method B: RT 7.942, area 96.45 %.

2/26/2014 7:26:32 PM

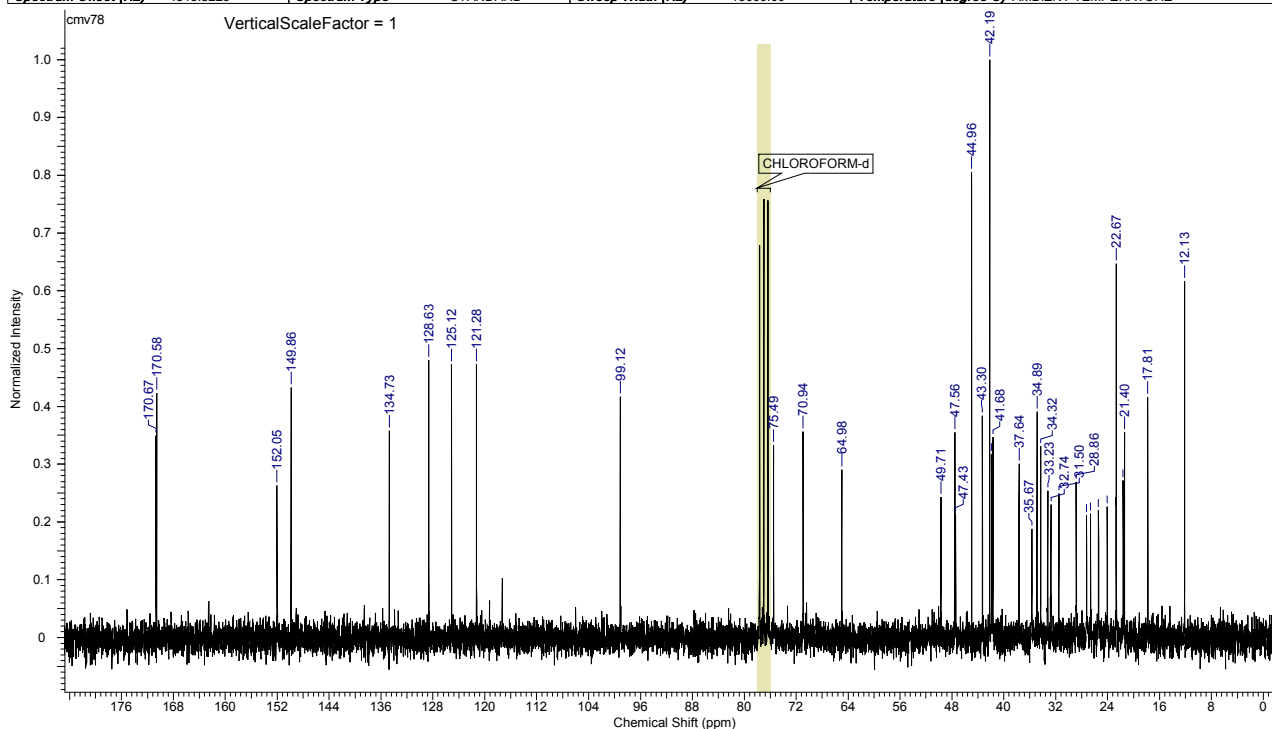
Number of Nuclei 0 H's					
Acquisition Time (sec)	1.3878	Comment	MV78	Date	Feb 11 11
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\MV78\hmv78.fid.fid				
Frequency (MHz)	199.97	Nucleus	$^1\text{H}$	Number of Transients	32
Points Count	8192	Pulse Sequence	s2pul	Receiver Gain	4.00
Spectrum Offset (Hz)	1689.5496	Spectrum Type	STANDARD	Sweep Width (Hz)	4600.00
				Solvent	CHLOROFORM-d
				Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 50 (MV78):**  $^{13}\text{C}$  NMR spectrum (50 MHz).

2/28/2014 4:13:47 PM

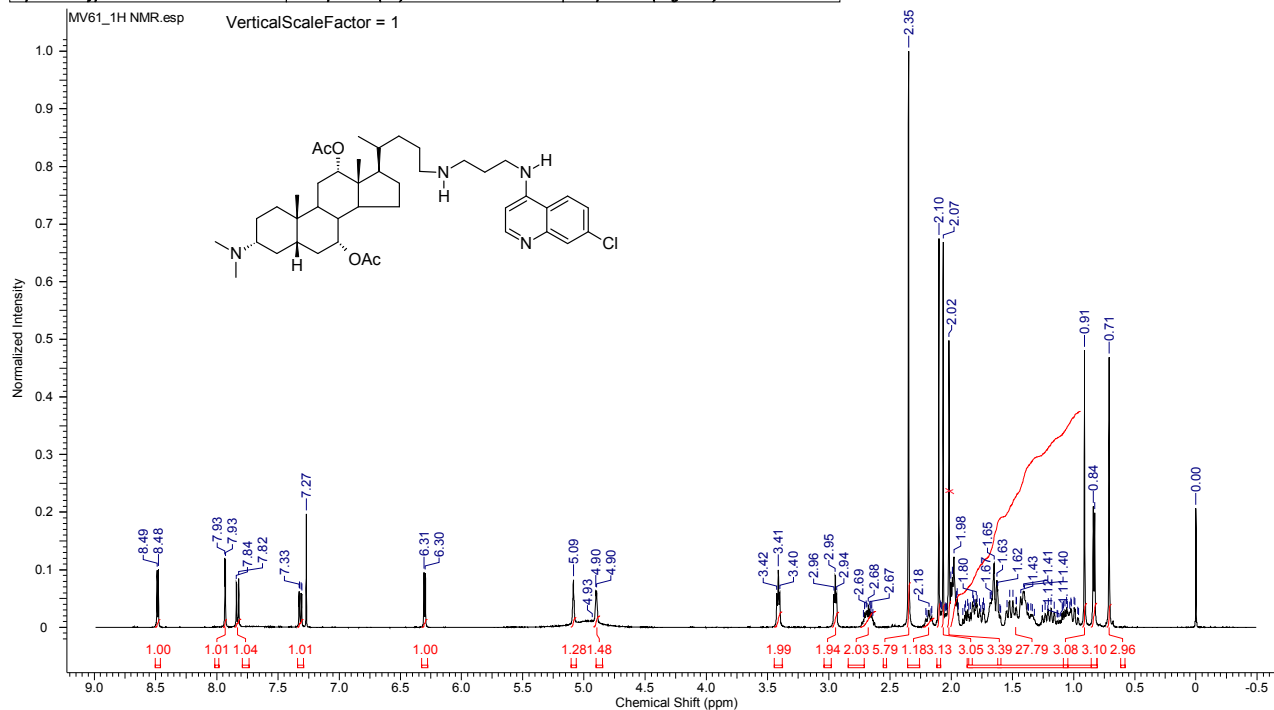
Number of Nuclei 0 C's					
Acquisition Time (sec)	1.0667	Comment	MV78	Date	Feb 11 11
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\MV78\cmv78.fid.fid				
Frequency (MHz)	50.29	Nucleus	$^{13}\text{C}$	Number of Transients	1307
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	25.00
Spectrum Offset (Hz)	4813.8223	Spectrum Type	STANDARD	Sweep Width (Hz)	15000.00
				Solvent	CHLOROFORM-d
				Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 51 (MV61):**  $^1\text{H}$  NMR spectrum (500 MHz). HPLC purity: method A: RT 1.804, area 97.63 %; method B: RT 1.922, area 98.03 %; method C: RT 12.462, area 95.41 %.

2/26/2014 7:28:52 PM

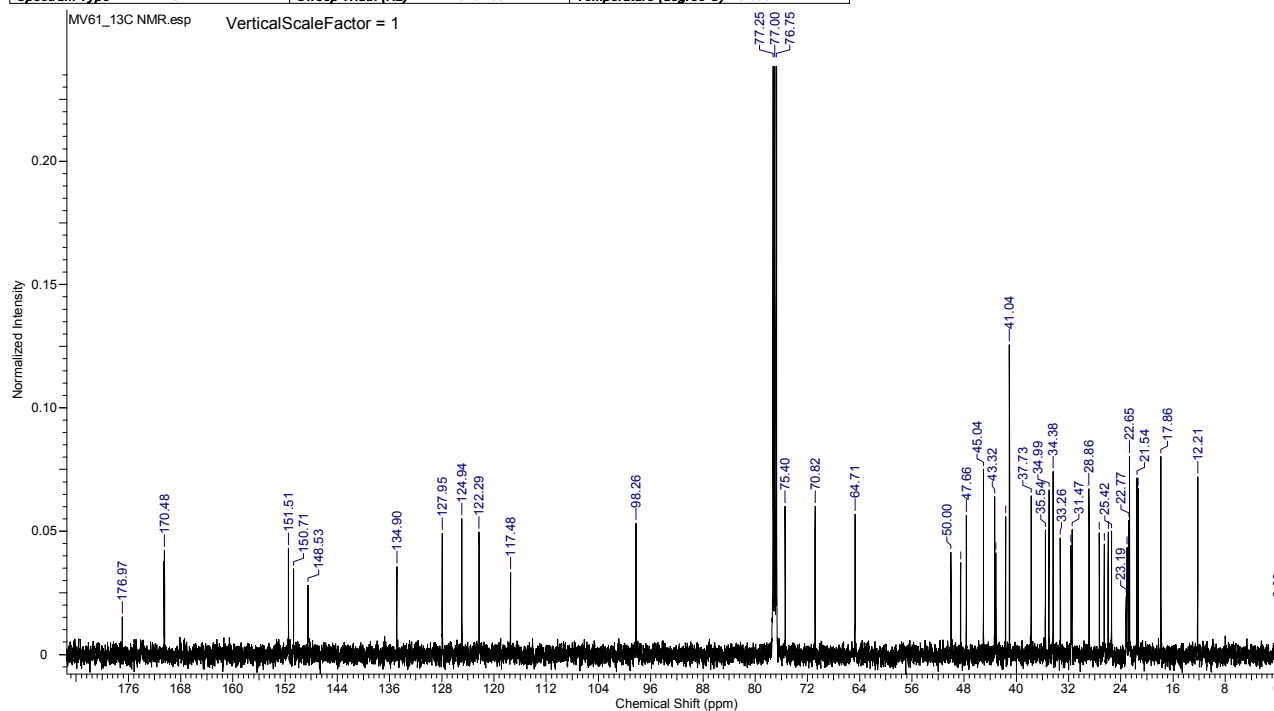
Number of Nuclei 0 H's							
Acquisition Time (sec)	3.4537	Date	15 Mar 2010 12:31:12				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Star\500 MHz\MV6111\pdata\11r		Date Stamp	15 Mar 2010 12:31:12			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmrsu	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	228.00	SW(cyclical) (Hz)	4743.83	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2125.5134
Spectrum Type	STANDARD	Sweep Width (Hz)	4743.69	Temperature (degree C)	25.000		



**Compound 51 (MV61):**  $^{13}\text{C}$  NMR spectrum (125 MHz).

2/25/2014 2:28:55 PM

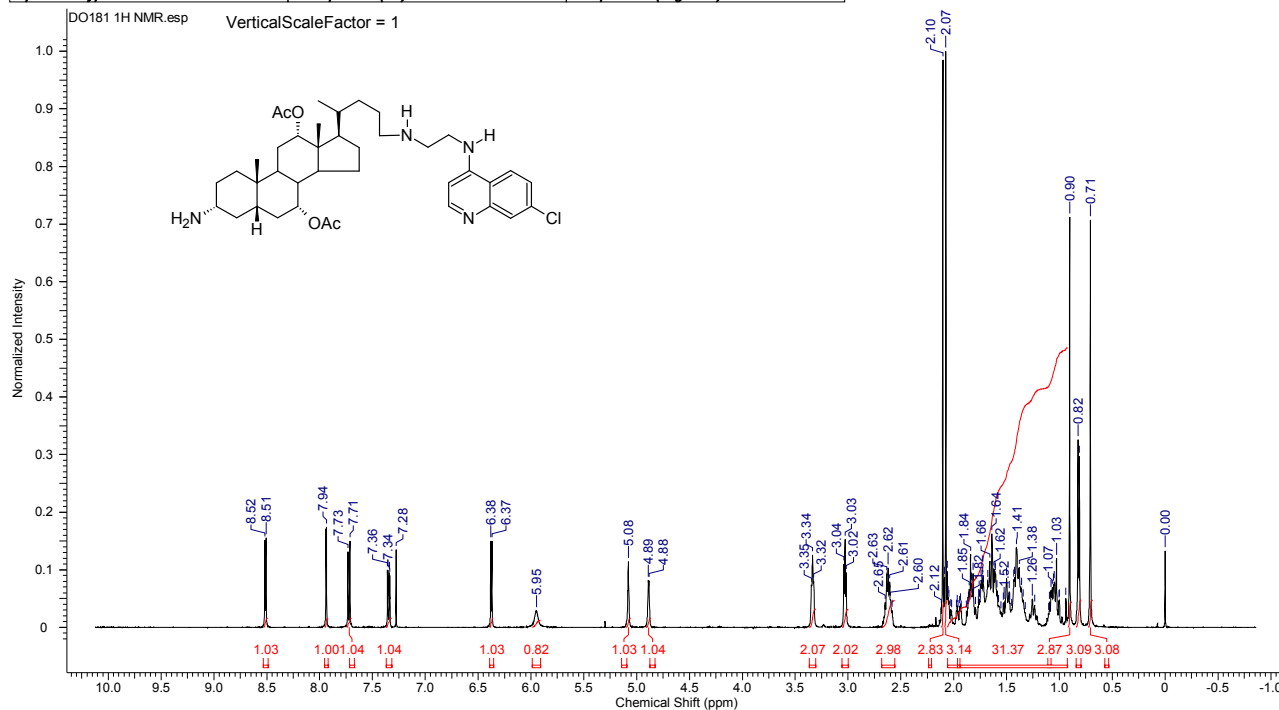
Number of Nuclei 0 C's							
Acquisition Time (sec)	0.5505	Date	15 Mar 2010 12:37:36				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Star\500 MHz\MV612\pdata\11r		Date Stamp	15 Mar 2010 12:37:36			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	825	Origin	spect
Original Points Count	16384	Owner	nmrsu	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	912.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	13832.5234
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000		



**Compound 52 (DO181):  $^1\text{H}$  NMR spectrum (500 MHz).** HPLC purity: method A: RT 2.004, area 98.23 %; method B: RT 7.973, area 95.08 %;

2/26/2014 5:47:00 PM

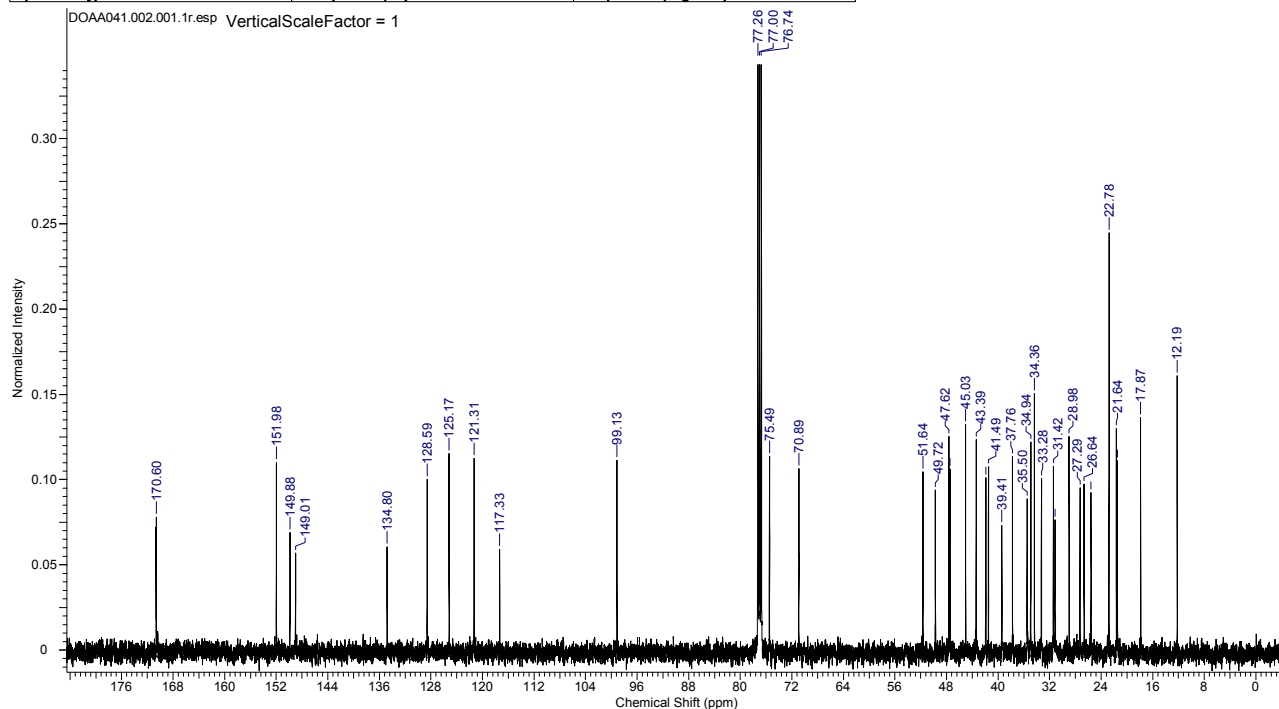
Number of Nuclei 0 H's							
Acquisition Time (sec)	2.9819	Date	20 Mar 2008 11:01:36				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO181\DOAA0411\1\data\111r		Date Stamp	20 Mar 2008 11:01:36			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	16384	Pulse Sequence	zg30
Receiver Gain	114.00	SW(cyclical) (Hz)	5494.51	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2315.4834
Spectrum Type	STANDARD	Sweep Width (Hz)	5494.17	Temperature (degree C)	25.000		



**Compound 52 (DO181):  $^{13}\text{C}$  NMR spectrum (125 MHz).**

2/26/2014 5:48:41 PM

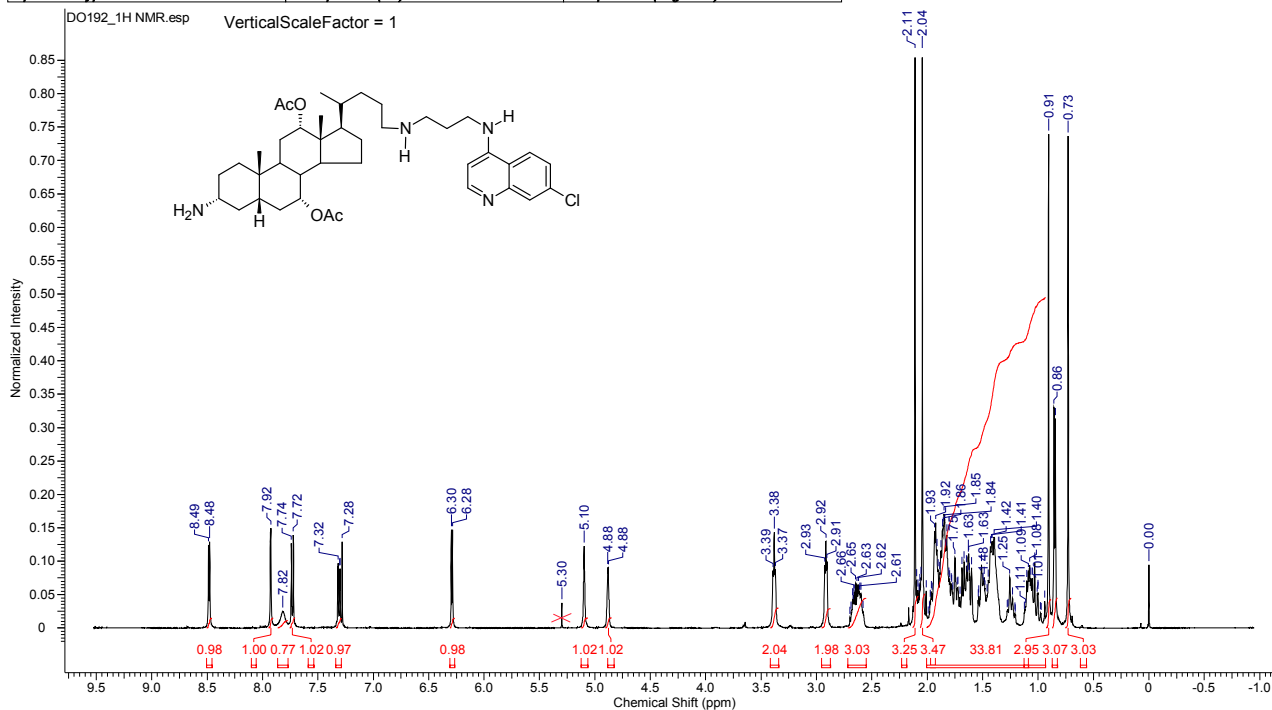
Number of Nuclei 0 C's							
Acquisition Time (sec)	1.1010	Date	20 Mar 2008 11:08:00				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO181\DOAA0412\1\data\111r		Date Stamp	20 Mar 2008 11:08:00			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	349	Origin	spect
Original Points Count	32768	Owner	nmsru	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	1030.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	13831.9209
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000		



**Compound 53 (DO192):  $^1\text{H}$  NMR spectrum (500 MHz).** HPLC purity: method C: RT 11.493, area 97.92%; method D: RT 5.137, area 97.997 %.

2/25/2014 4:25:18 PM

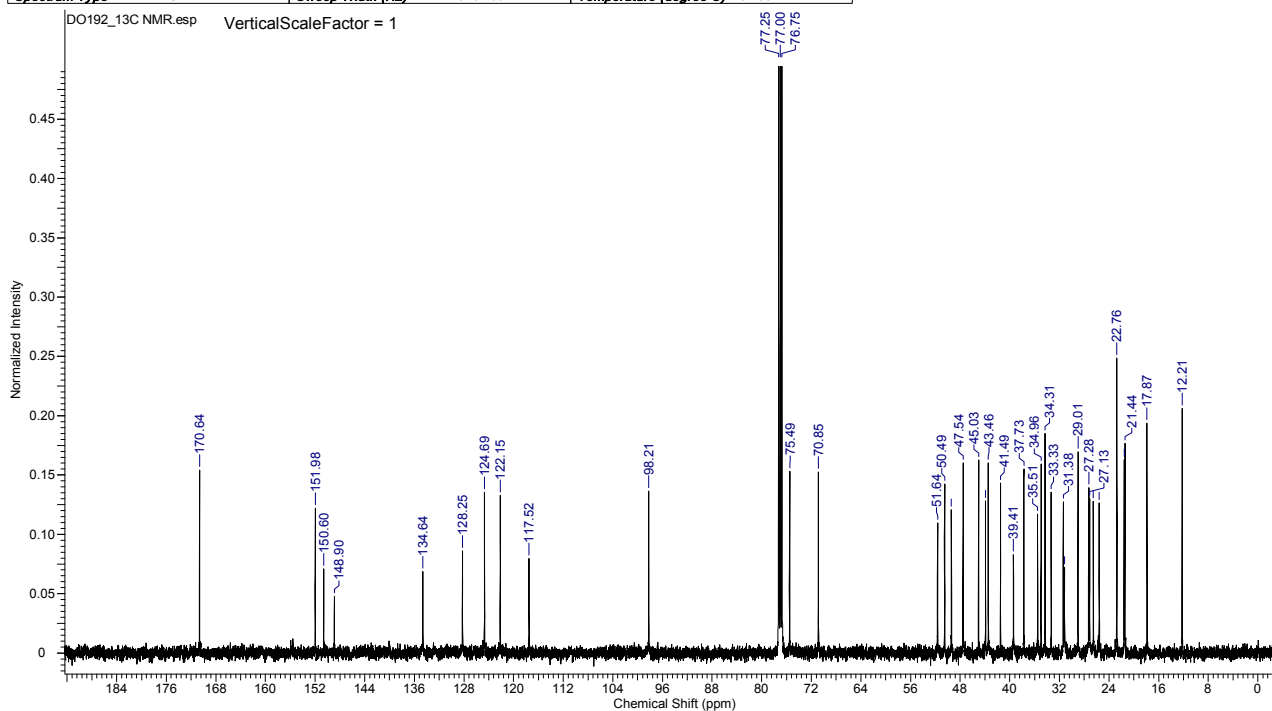
Number of Nuclei 0 H's							
Acquisition Time (sec)	3.1261	Date	26 Aug 2009 15:47:44				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Star1\500 MHz\DOAA089\1\data\11r		Date Stamp	26 Aug 2009 15:47:44			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	71.80	SW(cyclical) (Hz)	5241.09	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2144.5515
Spectrum Type	STANDARD	Sweep Width (Hz)	5240.93	Temperature (degree C)	25.000		



**Compound 53 (DO192):  $^{13}\text{C}$  NMR spectrum (125 MHz).**

2/25/2014 4:26:45 PM

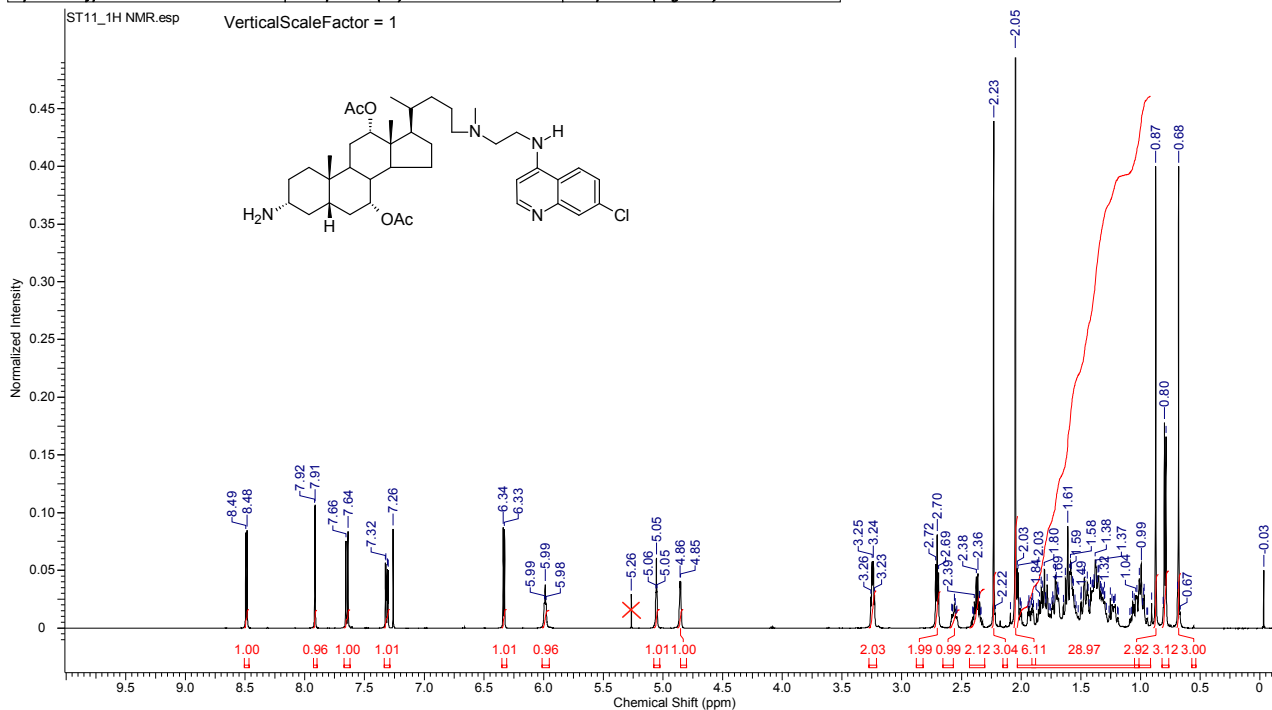
Number of Nuclei 0 C's							
Acquisition Time (sec)	0.5505	Date	26 Aug 2009 14:07:28				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Star1\500 MHz\DOAA089\2\data\11r		Date Stamp	26 Aug 2009 14:07:28			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	662	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	912.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	12571.2354
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.100		



**Compound 54 (ST13):  $^1\text{H}$  NMR spectrum (500 MHz).** HPLC purity: method A: RT 1.905, area 99.44%; method C: RT 11.413, area 96.83 %.

2/26/2014 7:30:53 PM

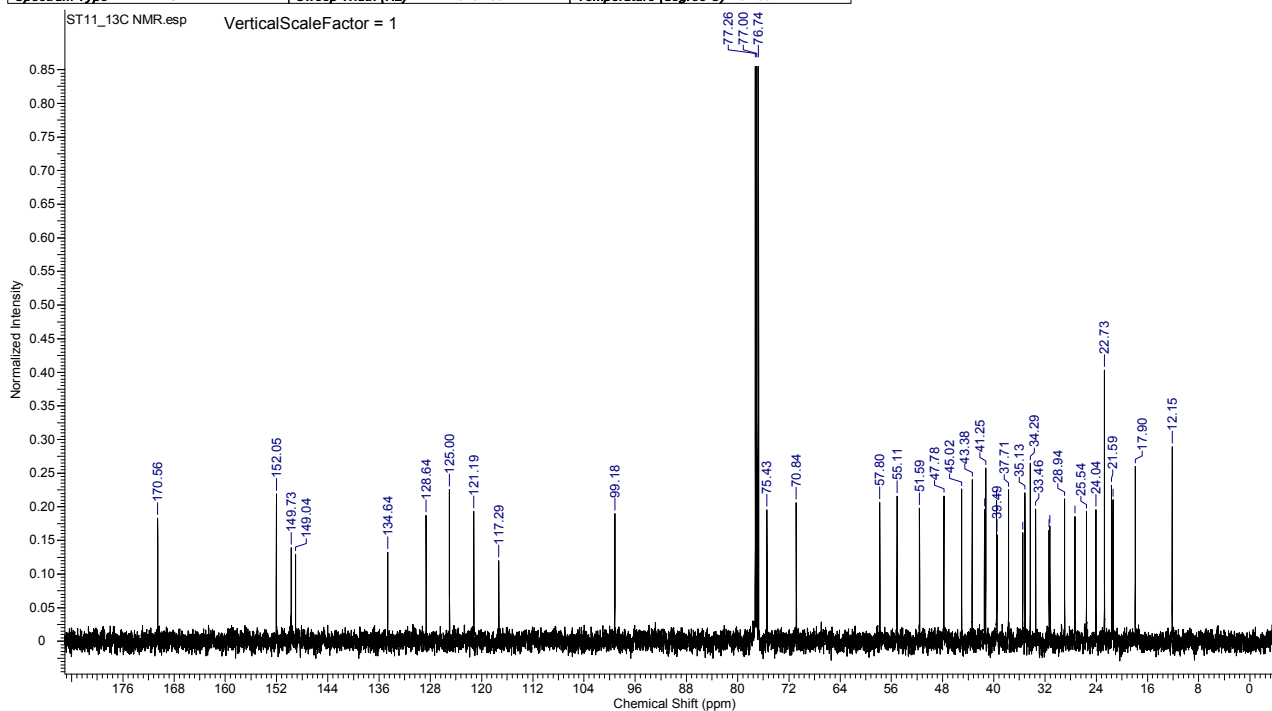
Number of Nuclei 0 H's							
Acquisition Time (sec)	2.7394	Date	29 Mar 2012 09:21:36				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_ Stari\500 MHz\UKAA0771\pdata\111r		Date Stamp	29 Mar 2012 09:21:36			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmsu	Points Count	32768	Pulse Sequence	zq30
Receiver Gain	71.80	SW(cyclical) (Hz)	5980.86	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2546.4924
Spectrum Type	STANDARD	Sweep Width (Hz)	5980.68	Temperature (degree C)	25.000		



**Compound 54 (ST13):  $^{13}\text{C}$  NMR spectrum (125 MHz).**

2/25/2014 4:39:44 PM

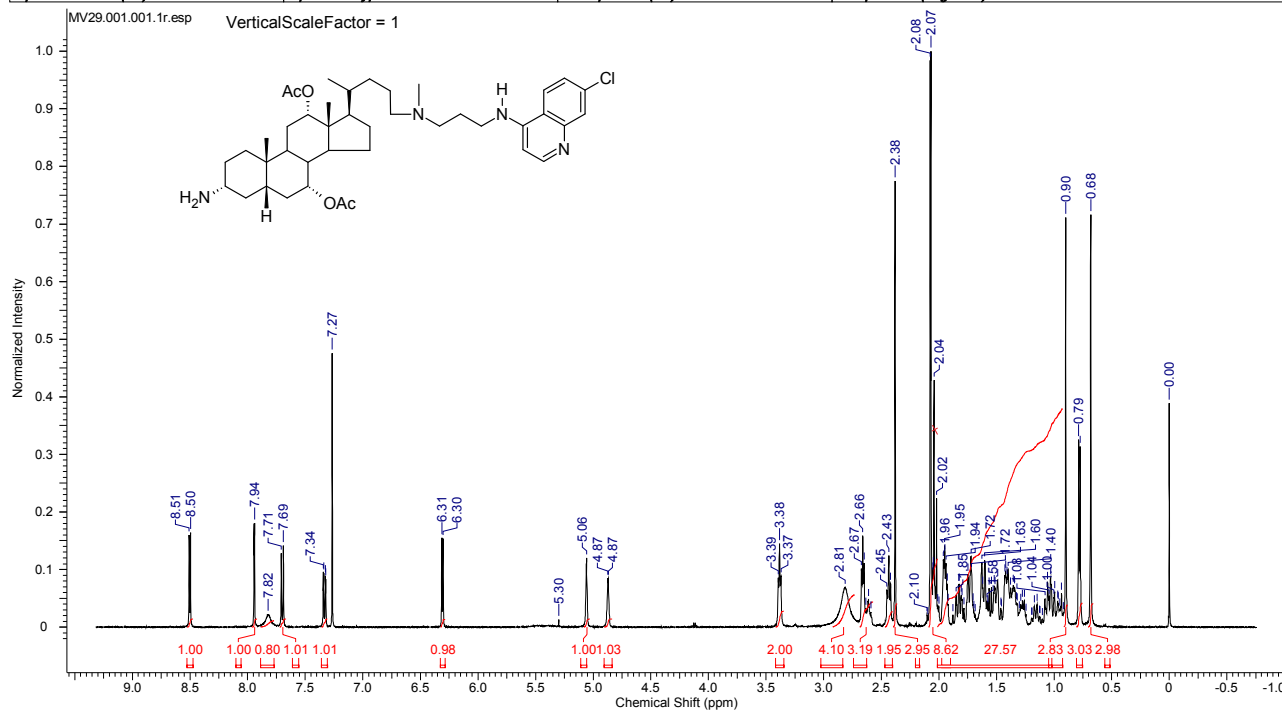
Number of Nuclei 0 C's							
Acquisition Time (sec)	0.5505	Date	29 Mar 2012 09:21:36				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_ Stari\500 MHz\UKAA0772\pdata\111r		Date Stamp	29 Mar 2012 09:21:36			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	42	Origin	spect
Original Points Count	16384	Owner	nmsu	Points Count	32768	Pulse Sequence	zqpg30
Receiver Gain	1030.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	12567.7393
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.400		



**Compound 55 (MV29):**  $^1\text{H}$  NMR spectrum (500 MHz). HPLC purity: method A: RT 2.240, area 96.94 %; method B: RT 1.792, area 98.41 %.

2/26/2014 5:53:24 PM

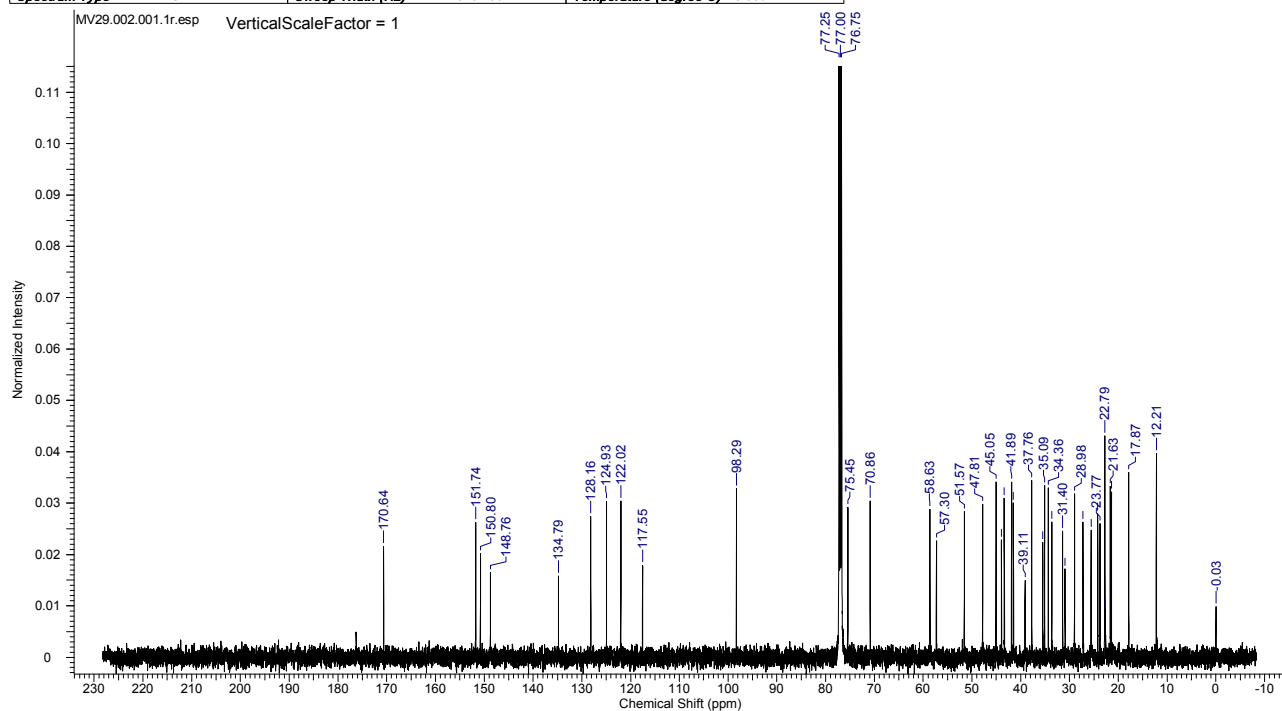
Number of Nuclei 0 H's					
Acquisition Time (sec)	3.2506	Date	18 Dec 2009 12:58:56	Date Stamp	18 Dec 2009 12:58:56
File Name	C:\Users\Dejan Oспенica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\MV29\1\data\111r				
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16
Original Points Count	16384	Owner	nmrsu	Points Count	32768
Receiver Gain	256.00	SW(cyclical) (Hz)	5040.32	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2142.3103	Spectrum Type	STANDARD	Sweep Width (Hz)	5040.17
				Temperature (degree C)	25.000



**Compound 55 (MV29):**  $^{13}\text{C}$  NMR spectrum (125 MHz).

2/26/2014 5:55:10 PM

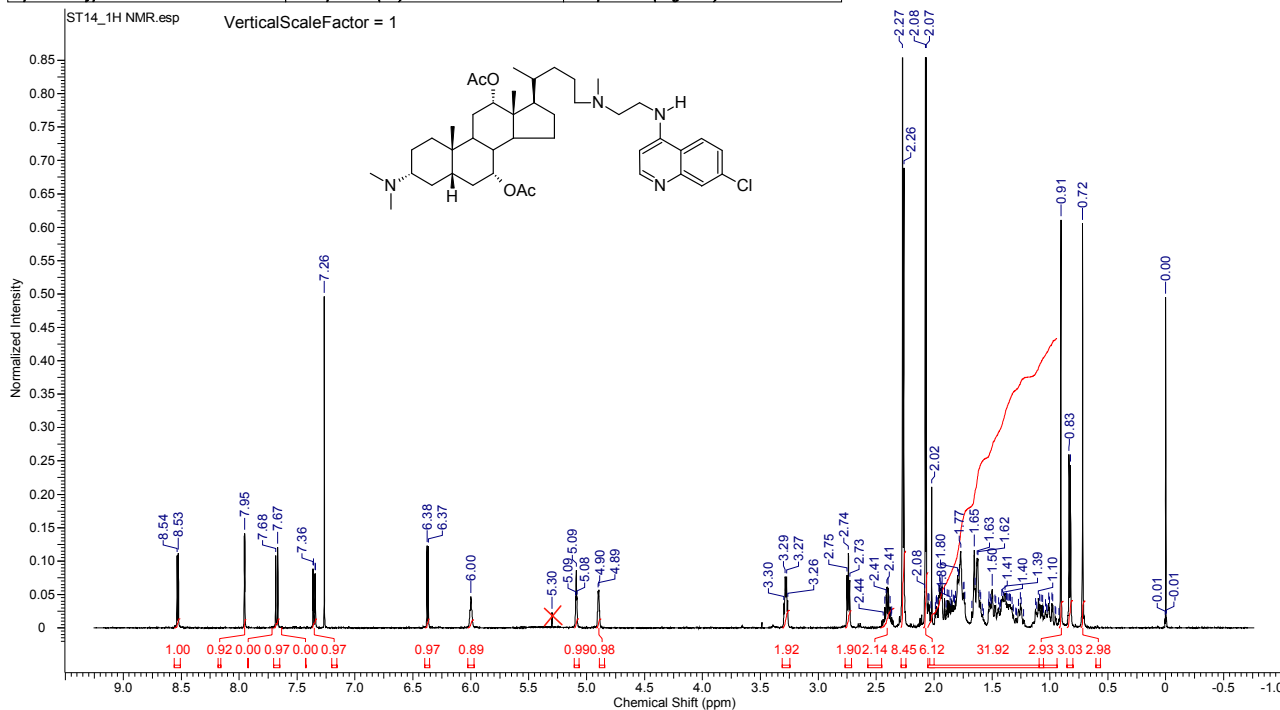
Number of Nuclei 0 C's					
Acquisition Time (sec)	0.5505	Date	18 Dec 2009 12:22:40	Date Stamp	18 Dec 2009 12:22:40
File Name	C:\Users\Dejan Oспенica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\MV29\2\data\111r				
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	2007
Original Points Count	16384	Owner	nmrsu	Points Count	32768
Receiver Gain	1030.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Spectrum Offset (Hz)	13833.4160
				Temperature (degree C)	25.000



**Compound 56 (ST14):**  $^1\text{H}$  NMR spectrum (500 MHz). HPLC purity: method A: RT 1.849, area 98.82 %; method D: RT 5.179, area 98.67 %.

2/26/2014 7:32:06 PM

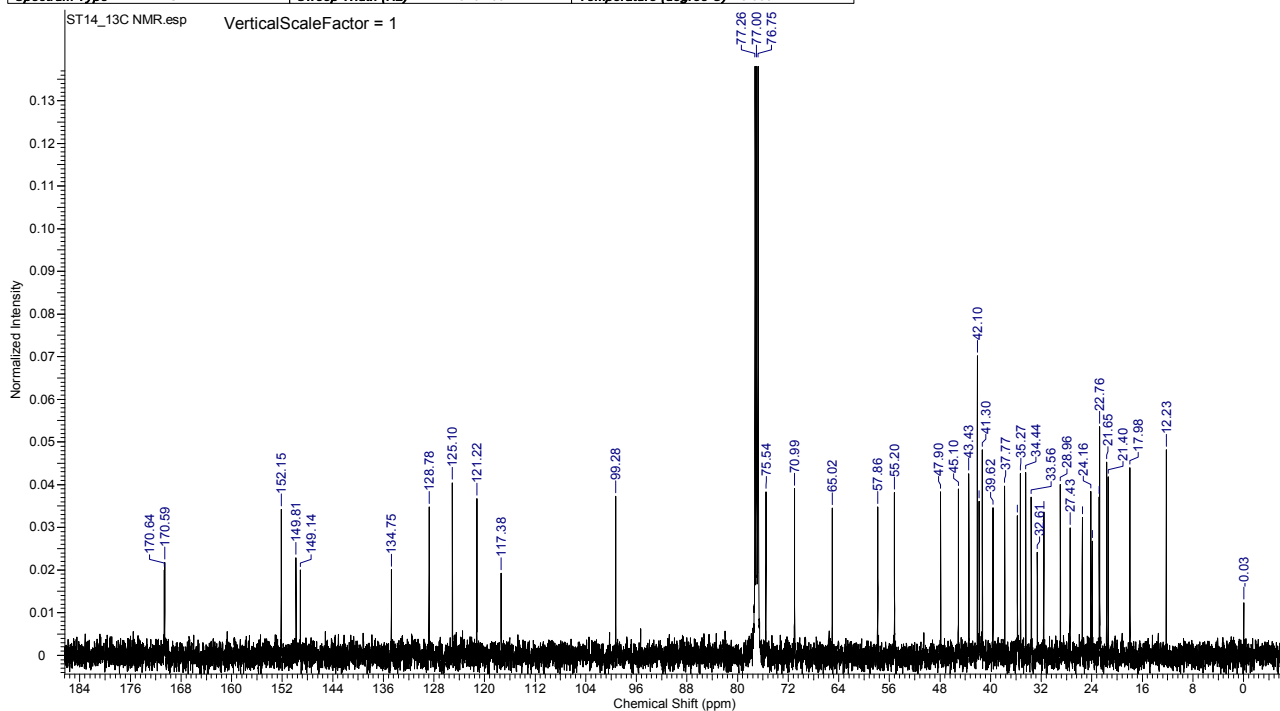
Number of Nuclei 0 H's							
Acquisition Time (sec)	3.2681	Date	21 Jun 2010 10:46:56				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Star1500 MHz\STAA0381\1\data\111r		Date Stamp	21 Jun 2010 10:46:56			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	256.00	SW(cyclical) (Hz)	5013.37	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2124.4246
Spectrum Type	STANDARD	Sweep Width (Hz)	5013.22	Temperature (degree C)	25.000		



**Compound 56 (ST14):**  $^{13}\text{C}$  NMR spectrum (125 MHz).

2/25/2014 4:44:35 PM

Number of Nuclei 0 C's							
Acquisition Time (sec)	0.5505	Date	21 Jun 2010 10:57:36				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Star1500 MHz\STAA0381\2\data\111r		Date Stamp	21 Jun 2010 10:57:36			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	1402	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	1030.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	13833.7441
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000		

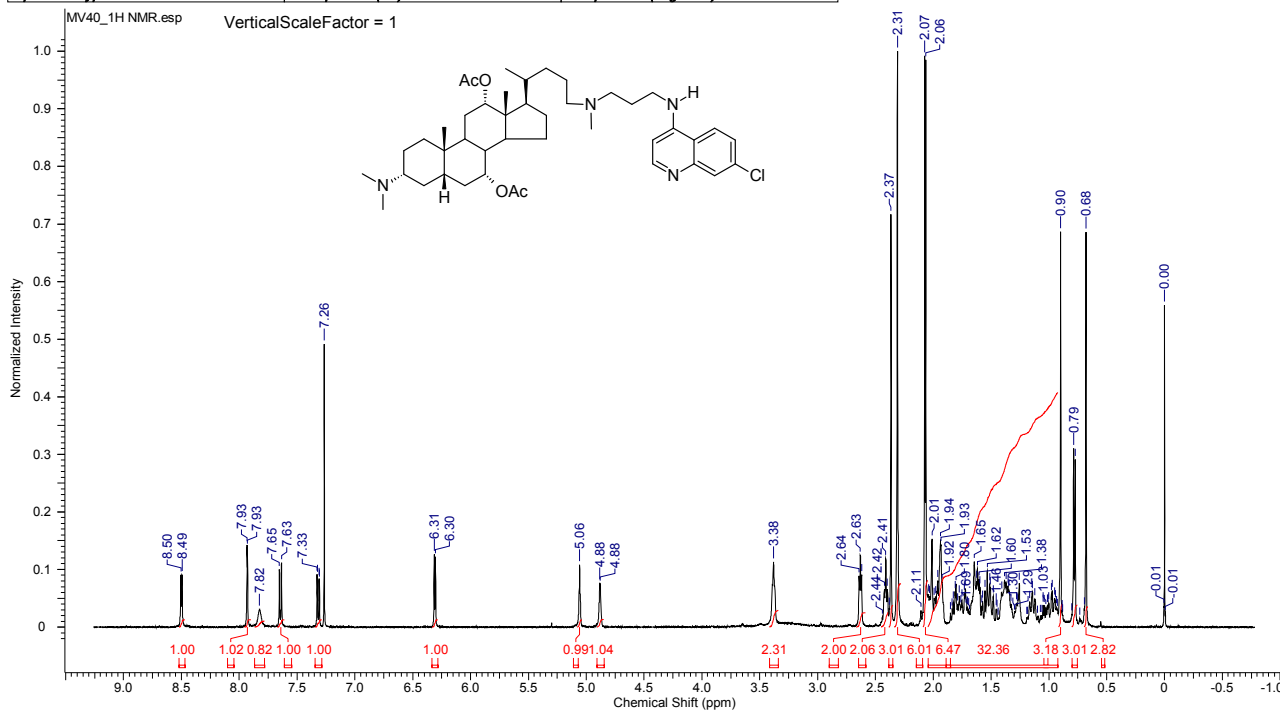




**Compound 57 (MV40):**  $^1\text{H}$  NMR spectrum (500 MHz). HPLC purity: method C: RT 9.682, area 95.17 %; method D: RT 5.092, area 98.86 %.

2/25/2014 4:48:20 PM

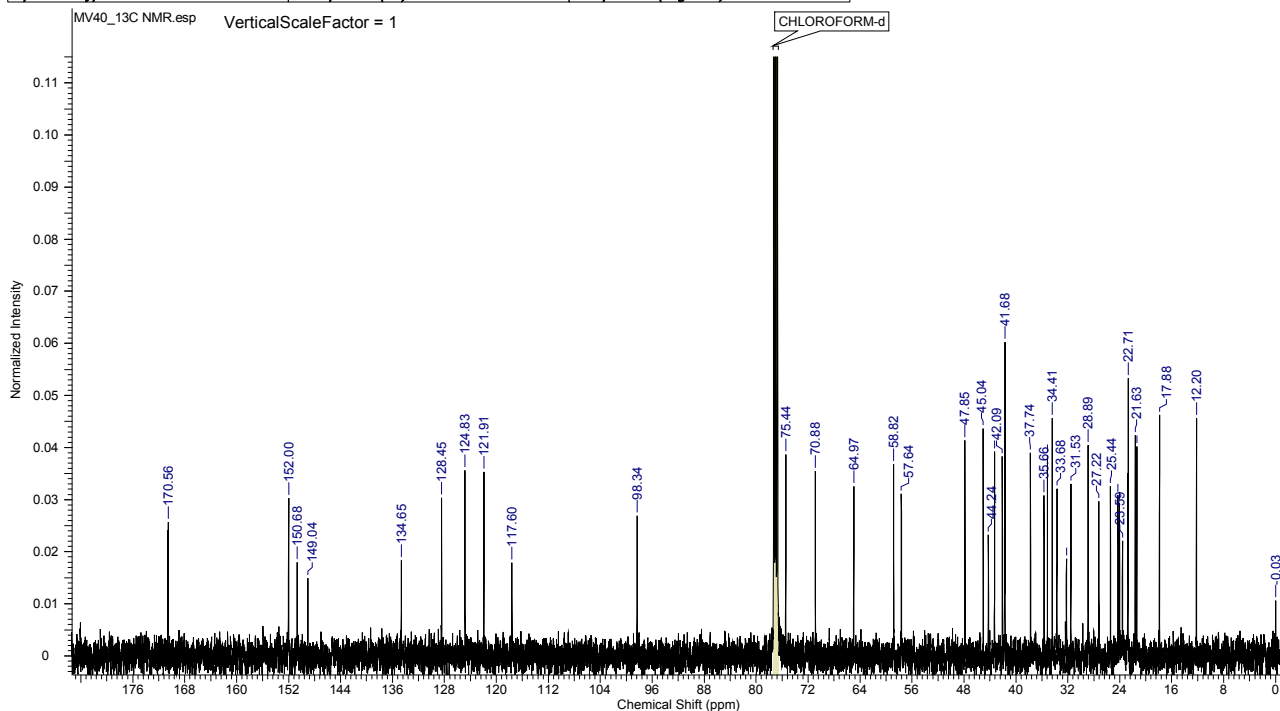
Number of Nuclei 0 H's							
Acquisition Time (sec)	3.2637	Date	15 Mar 2010 11:25:04				
File Name	C:\Users\Dejan Osenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzijal\Spektri NMR_ Stari\500 MHz\MV40\1\pdata\111r		Date Stamp	15 Mar 2010 11:25:04			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmsu	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	228.00	SW(cyclical) (Hz)	5020.08	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2122.0854
Spectrum Type	STANDARD	Sweep Width (Hz)	5019.93	Temperature (degree C)	25.000		



**Compound 57 (MV40):**  $^{13}\text{C}$  NMR spectrum (125 MHz).

3/1/2014 8:59:52 PM

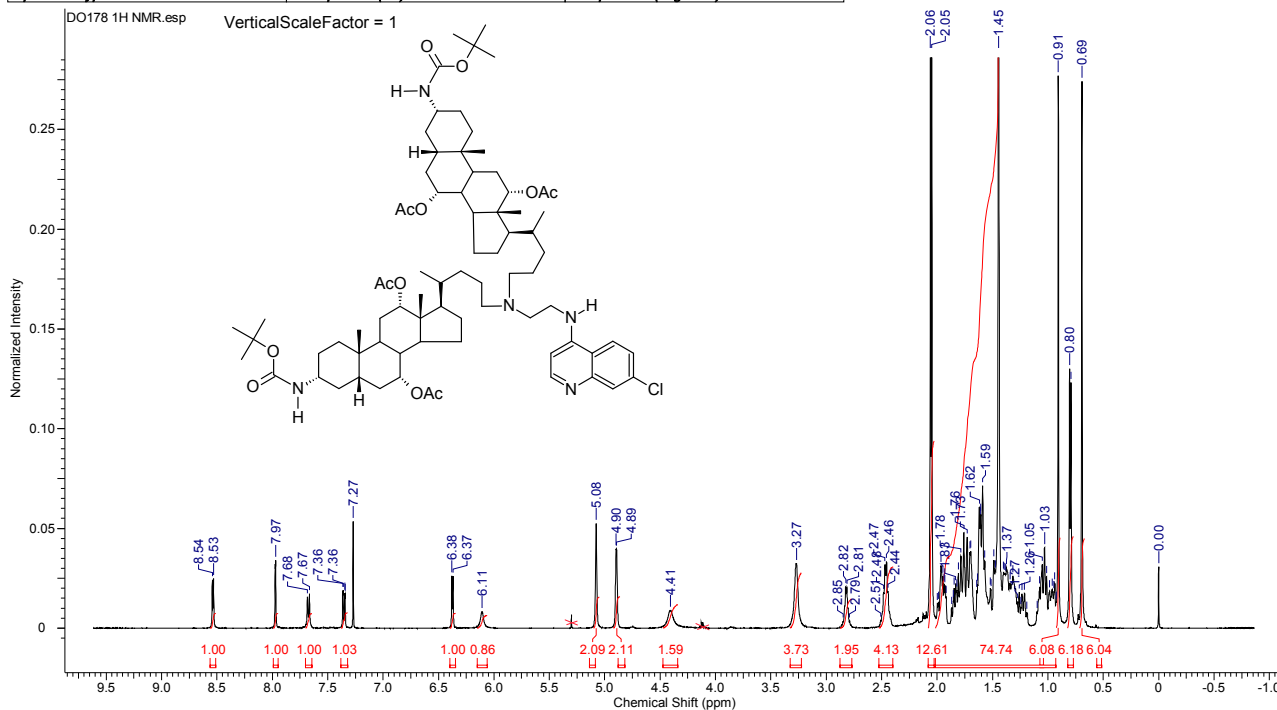
Number of Nuclei 0 C's							
Acquisition Time (sec)	0.5505	Date	15 Mar 2010 11:31:28				
File Name	C:\Users\Dejan Osenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzijal\Spektri NMR_ Stari\500 MHz\MV40\2\pdata\111r		Date Stamp	15 Mar 2010 11:31:28			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	1205	Origin	spect
Original Points Count	16384	Owner	nmsu	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	1030.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	13833.4434
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000		



**Compound 58 (DO178):  $^1\text{H}$  NMR spectrum (500 MHz). HPLC purity: method C: RT=11.618, area 99.15 %; method D: RT 6.020, area 96.86 %.**

2/26/2014 6:20:08 PM

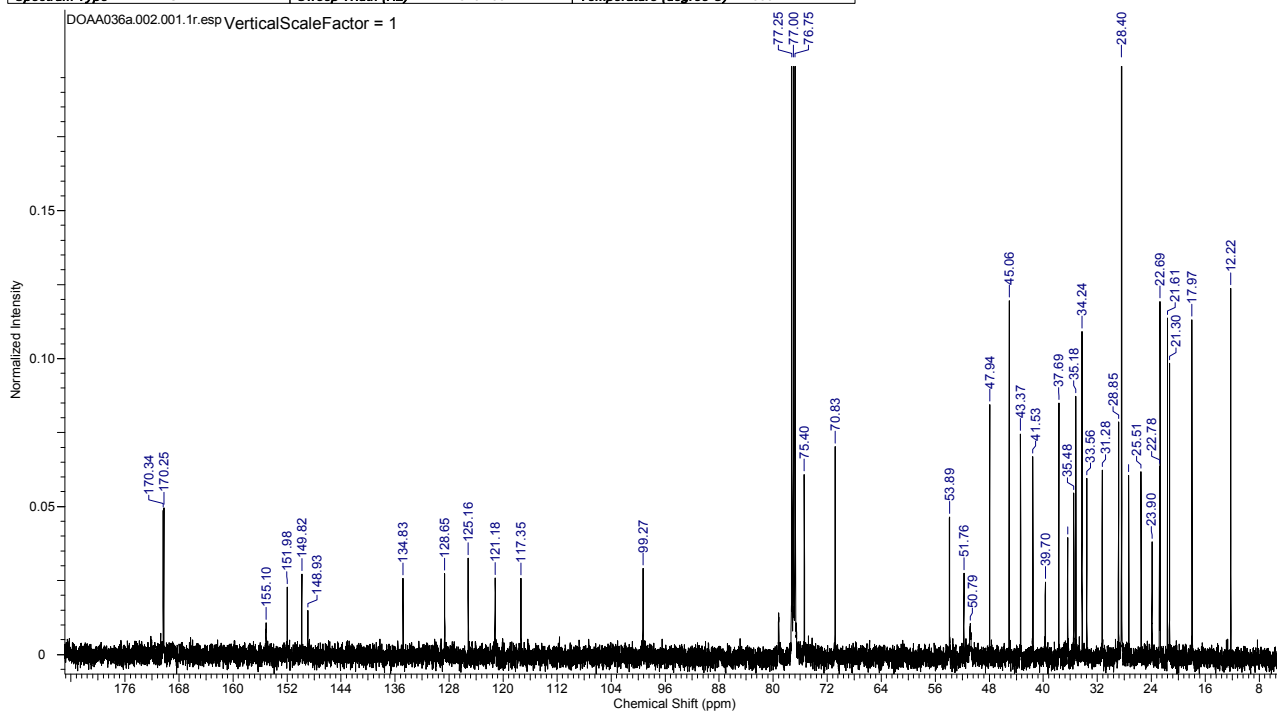
Number of Nuclei 0 H's							
Acquisition Time (sec)	3.1261	Date	04 Mar 2008 13:33:04				
File Name	C:\Users\Dejan Opšenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO178\DOAA036a\1\data\11r		Date Stamp	04 Mar 2008 13:33:04			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	16384	Pulse Sequence	zg30
Receiver Gain	114.00	SW(cyclical) (Hz)	5241.09	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2188.8513
Spectrum Type	STANDARD	Sweep Width (Hz)	5240.77	Temperature (degree C)	25.000		



**Compound 58 (DO178):  $^{13}\text{C}$  NMR spectrum (125 MHz).**

2/26/2014 6:24:23 PM

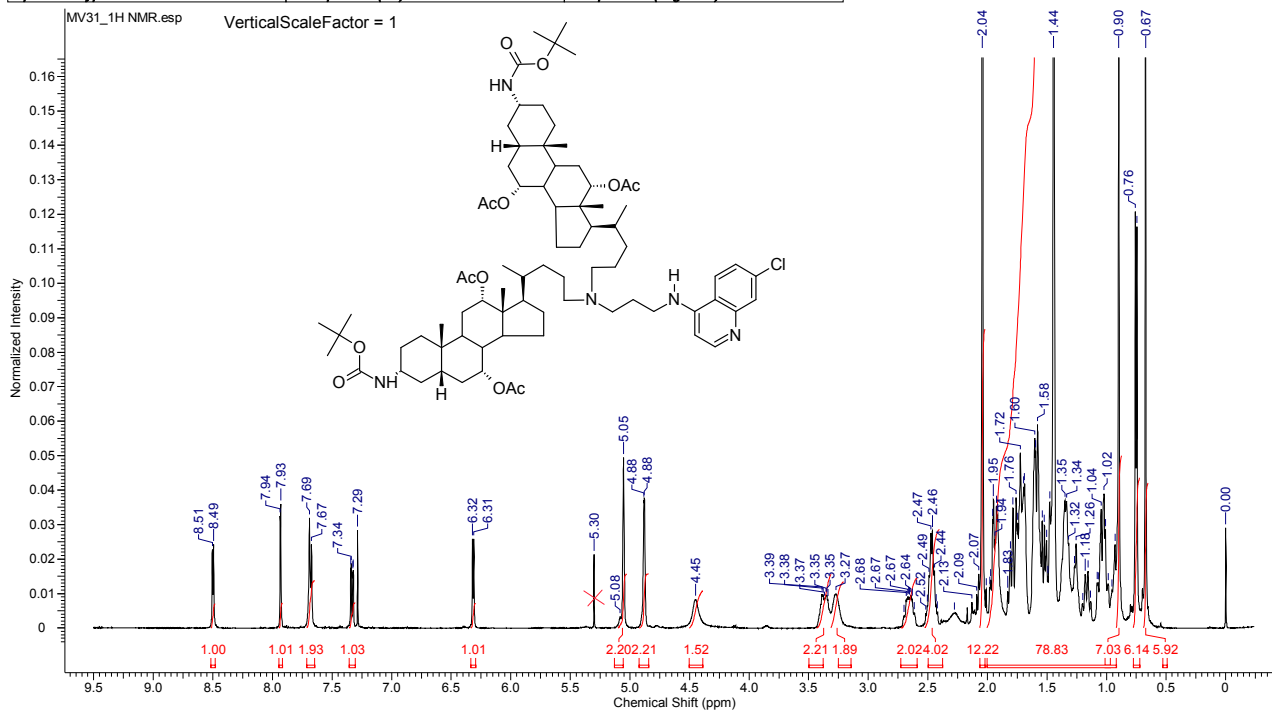
Number of Nuclei 0 C's							
Acquisition Time (sec)	1.1010	Date	04 Mar 2008 13:41:36				
File Name	C:\Users\Dejan Opšenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Ostalo\DO178\DOAA036a\2\data\11r		Date Stamp	04 Mar 2008 13:41:36			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	869	Origin	spect
Original Points Count	32768	Owner	nmsru	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	1620.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	13833.4043
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	24.900		



**Compound 59 (MV31):**  $^1\text{H}$  NMR spectrum (500 MHz). HPLC purity: method C: RT 11,964, area 97.93 %; method D: RT 5.892, area 96.83 %.

2/26/2014 7:33:28 PM

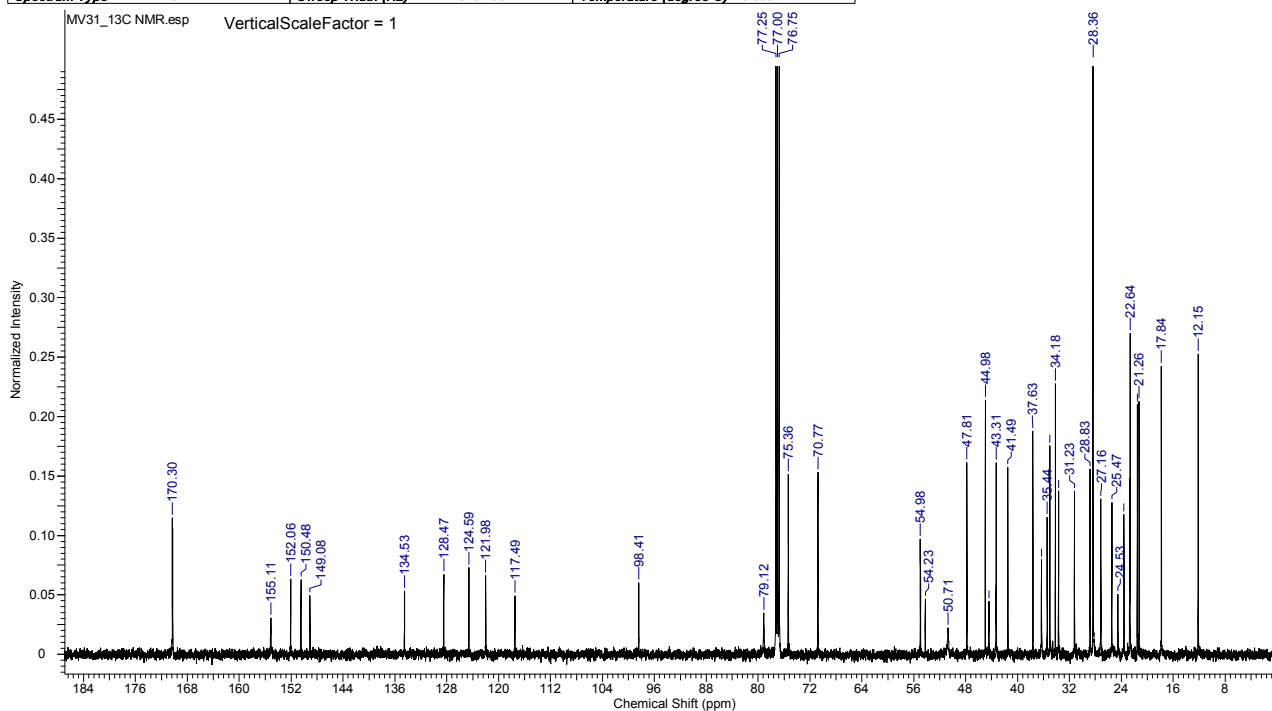
Number of Nuclei 0 H's							
Acquisition Time (sec)	3.3620	Date	11 Nov 2009 13:30:56				
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_ Stari\500 MHz\MVAA018a\1\pdata\11r		Date Stamp	11 Nov 2009 13:30:56			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmrsu	Points Count	32768	Pulse Sequence	zg30
Receiver Gain	50.80	SW(cyclical) (Hz)	4873.29	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2316.7156
Spectrum Type	STANDARD	Sweep Width (Hz)	4873.15	Temperature (degree C)	25.000		



**Compound 59 (MV31):**  $^{13}\text{C}$  NMR spectrum (125 MHz).

2/25/2014 5:06:16 PM

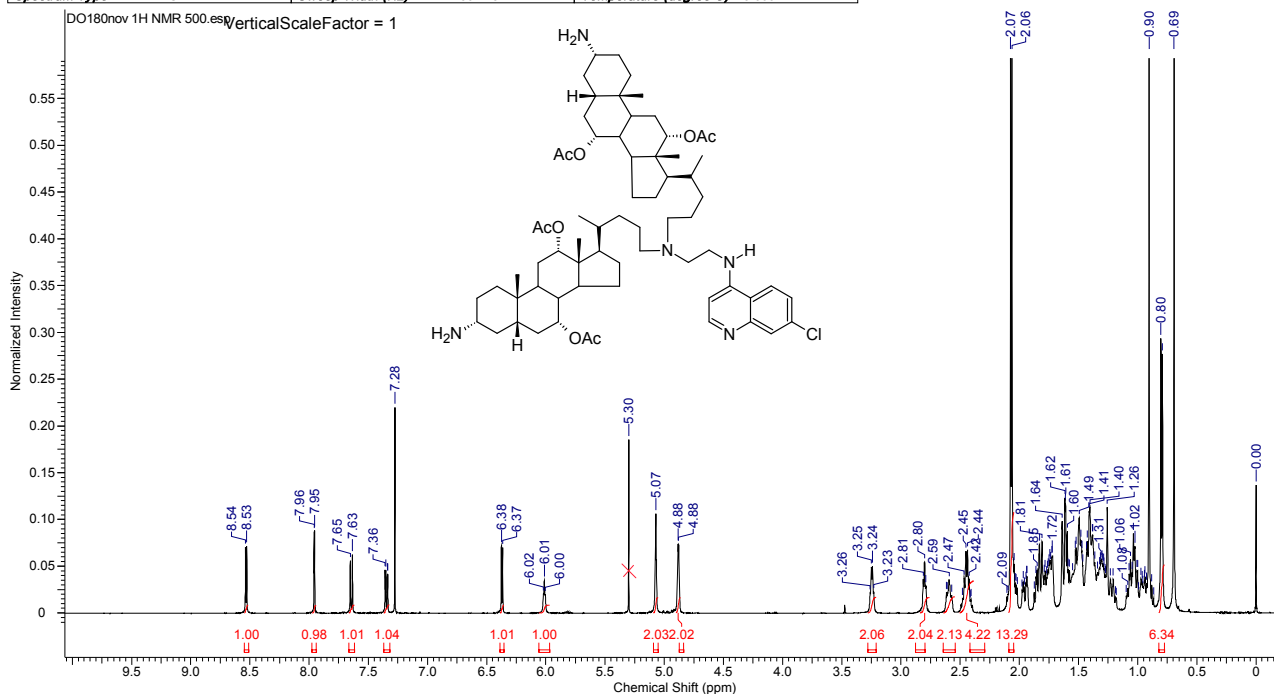
Number of Nuclei 0 C's							
Acquisition Time (sec)	0.5505	Date	11 Nov 2009 13:39:28				
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_ Stari\500 MHz\MVAA018a\2\pdata\11r		Date Stamp	11 Nov 2009 13:39:28			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	620	Origin	spect
Original Points Count	16384	Owner	nmrsu	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	13827.9844
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000		



**Compound 60 (DO180):  $^1\text{H}$  NMR spectrum (500 MHz).** HPLC purity: method A: RT 1.838, area 97.10 %; method D: RT 5.321, area 96.33 %.

3/1/2014 10:04:28 PM

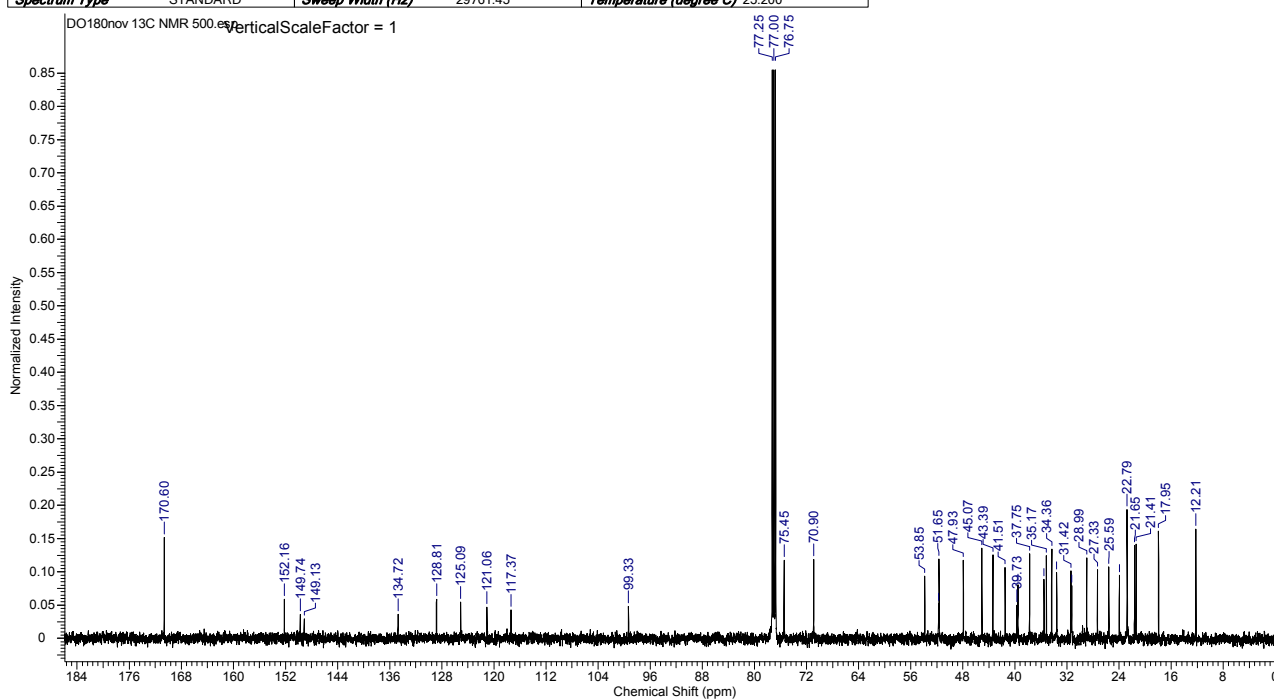
Number of Nuclei 0 H's				
Acquisition Time (sec)	2.1823	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	
Date Stamp	28 Feb 2014 09:44:48		Date	28 Feb 2014 09:44:48
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinolin\DO152\ostali\Recenzija\Spektri NMR novido180-nov11\data\111r			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	
Original Points Count	16384	Owner	nrmrsu	
Receiver Gain	101.00	SW(cyclical) (Hz)	7507.51	
Spectrum Type	STANDARD	Sweep Width (Hz)	7507.28	
		Solvent	CHLOROFORM-d	
		Temperature (degree C)	25.000	
		Number of Transients	16	
		Points Count	32768	
		Origin	spect	
		Pulse Sequence	zq30	
		Spectrum Offset (Hz)	3496.3342	



**Compound 60 (DO180):  $^{13}\text{C}$  NMR spectrum (125 MHz).**

3/1/2014 10:07:20 PM

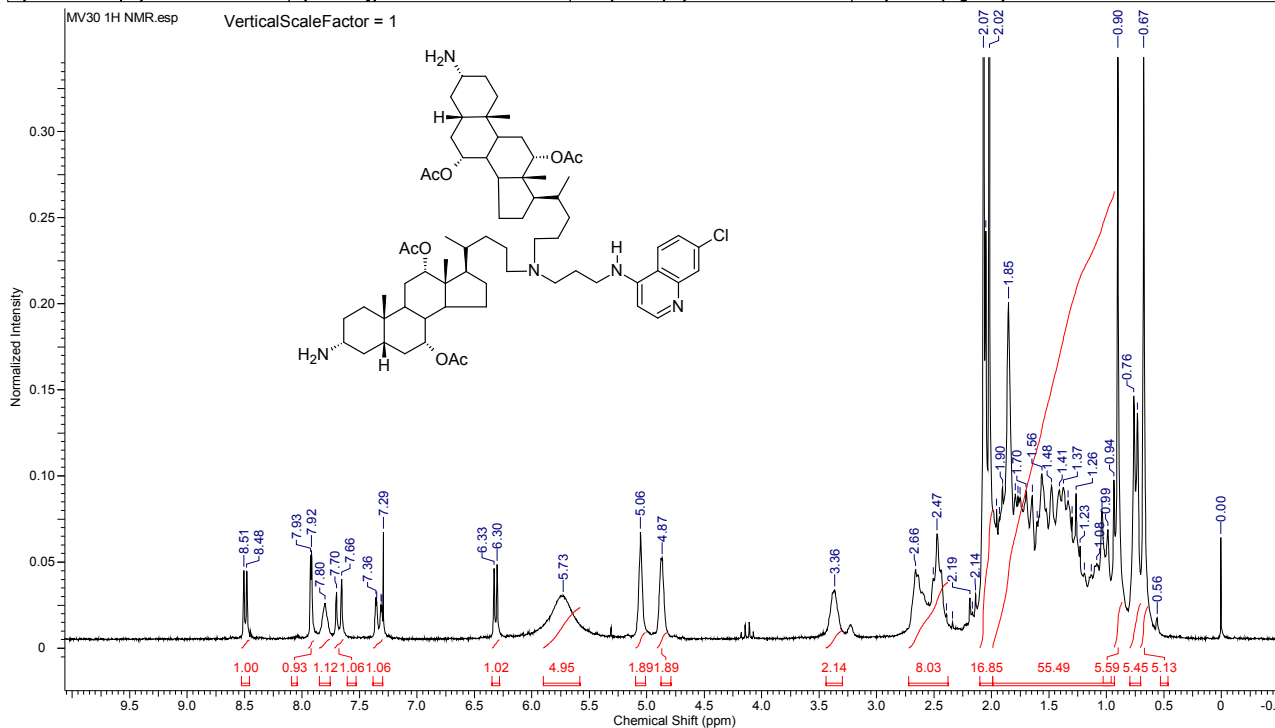
Number of Nuclei 0 C's				
Acquisition Time (sec)	0.5505	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	
Date Stamp	28 Feb 2014 09:46:56		Date	28 Feb 2014 09:46:56
File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinolin\DO152\ostali\Recenzija\Spektri NMR novido180-nov2\data\111r			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	
Original Points Count	16384	Owner	nrmrsu	
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.45	
		Solvent	CHLOROFORM-d	
		Temperature (degree C)	25.200	
		Number of Transients	176	
		Points Count	65536	
		Origin	spect	
		Pulse Sequence	zqpg30	
		Spectrum Offset (Hz)	13831.1650	



**Compound 61 (MV30):**  $^1\text{H}$  NMR spectrum (200 MHz). HPLC purity: method C: RT = 10.553, area 95.61 %; method D: RT 5.288, area 95.46 %.

2/25/2014 5:09:57 PM

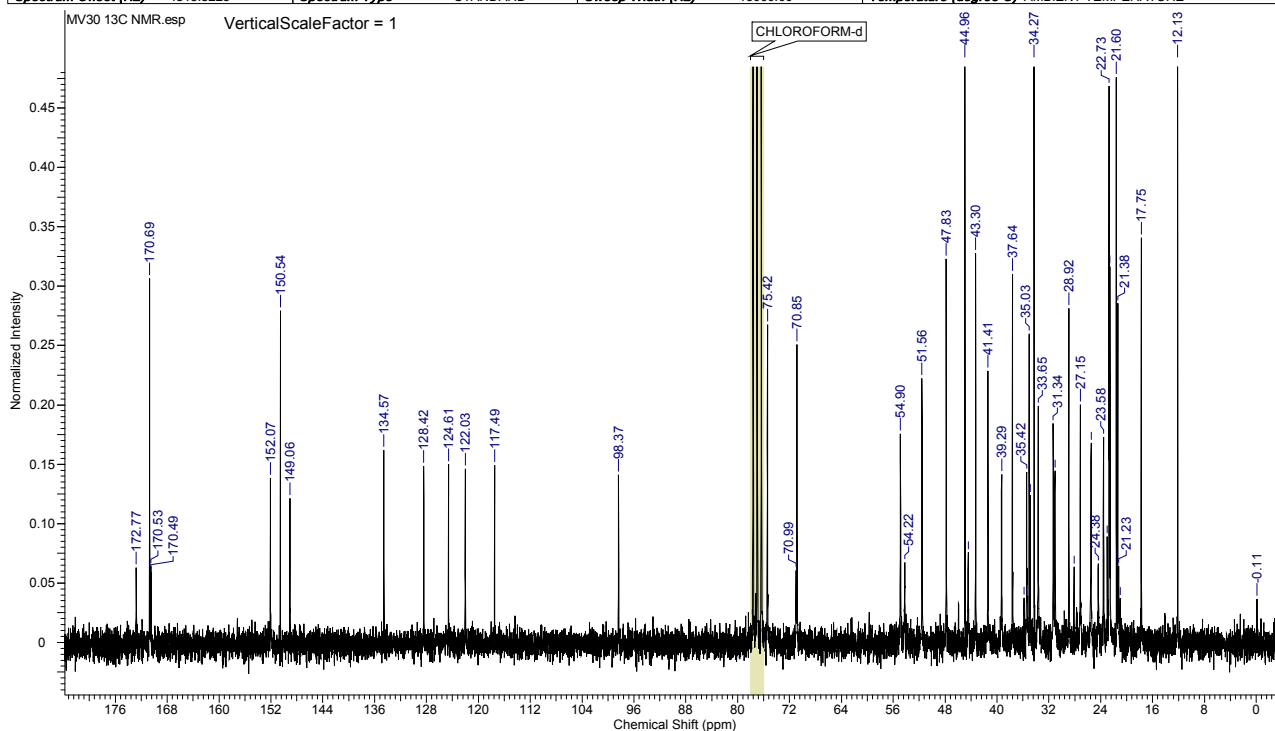
Number of Nuclei 0 H's					
Acquisition Time (sec)	1.3913	Comment	MV30	Date	Dec 15 09
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Frequency (MHz)	199.97	Nucleus	$^1\text{H}$	Number of Transients	55
Points Count	8192	Pulse Sequence	s2pul	Receiver Gain	9.00
Spectrum Offset (Hz)	1690.1111	Spectrum Type	STANDARD	Sweep Width (Hz)	4600.00
				Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 61 (MV30):**  $^{13}\text{C}$  NMR spectrum (50 MHz).

3/1/2014 10:27:11 PM

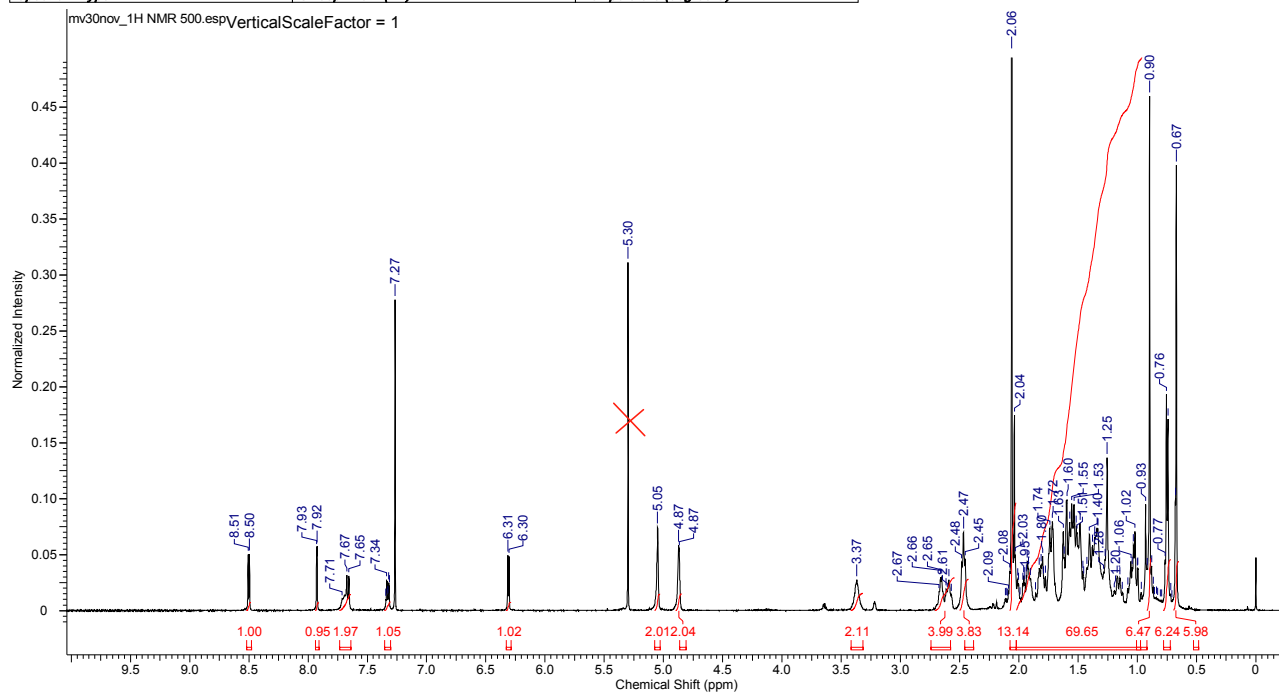
Number of Nuclei 0 C's					
Acquisition Time (sec)	1.0667	Comment	MV30	Date	Dec 15 09
File Name	C:\Users\Dejan\Openical\Documents\Radovi\Aminohinolinski\DO152\ostali\Recenzijal\Spektri NMR_Staril200 MHz\MV30\cmv30.fid\fid				
Frequency (MHz)	50.29	Nucleus	$^{13}\text{C}$	Number of Transients	17172
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	25.00
Spectrum Offset (Hz)	4813.8223	Spectrum Type	STANDARD	Sweep Width (Hz)	15000.00
				Temperature (degree C)	AMBIENT TEMPERATURE



2/25/2014 5:12:22 PM

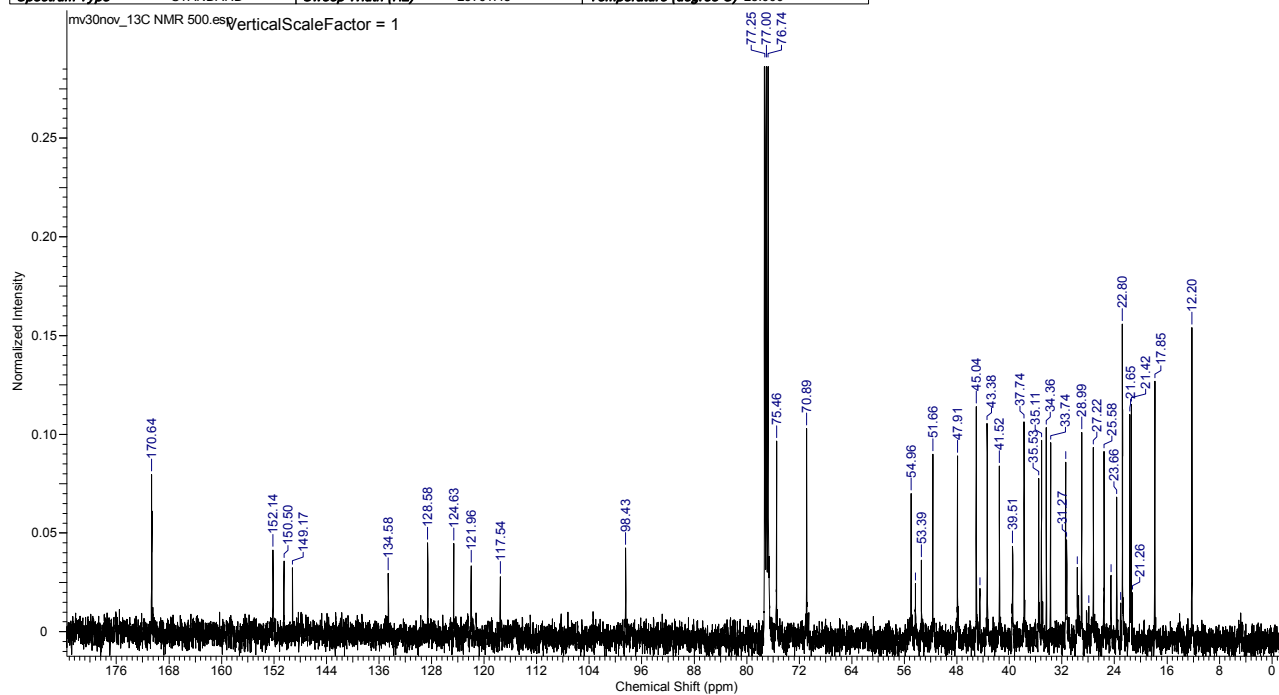
**Compound 61 (MV30): <sup>1</sup>H NMR spectrum (500 MHz).**

Number of Nuclei 0 H's				
Acquisition Time (sec)	2.1823	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	
Date Stamp	22 Feb 2014 09:59:44		Date	22 Feb 2014 09:59:44
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinolinolski\DO152\ostali\Recenzija\Spektri NMR nov\mv30nov1\pdata\111r			
Frequency (MHz)	500.26	Nucleus	<sup>1</sup> H	
Original Points Count	16384	Owner	nimsu	
Receiver Gain	362.00	SW(cyclical) (Hz)	7507.51	
Spectrum Type	STANDARD	Sweep Width (Hz)	7507.28	
		Solvent	CHLOROFORM-d	
		Temperature (degree C)	25.100	
		Number of Transients	38	
		Points Count	32768	
		Origin	spect	
		Pulse Sequence	zg30	
		Spectrum Offset (Hz)	3491.4070	

**Compound 61 (MV30): <sup>13</sup>C NMR spectrum (125 MHz).**

2/25/2014 5:13:20 PM

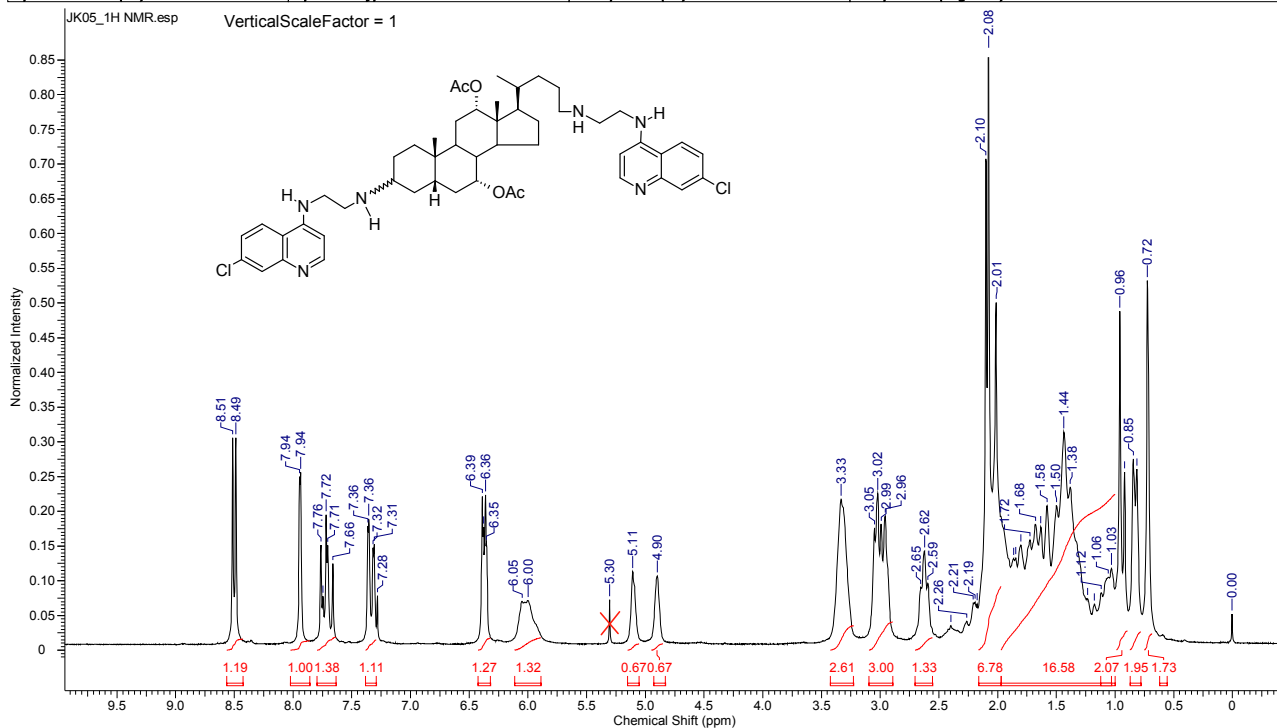
Number of Nuclei 0 C's				
Acquisition Time (sec)	0.5505	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	
Date Stamp	22 Feb 2014 09:29:52		Date	22 Feb 2014 09:29:52
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinolinolski\DO152\ostali\Recenzija\Spektri NMR nov\mv30nov2\pdata\111r			
Frequency (MHz)	125.79	Nucleus	<sup>13</sup> C	
Original Points Count	16384	Owner	nimsu	
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.45	
		Solvent	CHLOROFORM-d	
		Temperature (degree C)	25.000	
		Number of Transients	700	
		Points Count	65536	
		Origin	spect	
		Pulse Sequence	zgpg30	
		Spectrum Offset (Hz)	13831.5049	



**Compound 62 (JK05):  $^1\text{H}$  NMR spectrum (200 MHz).** HPLC purity: method B: RT 1.788, area 98.83 %; method C: RT1=10.371, RT2=10,566, area 95.15 %; method D: RT1 4.947, RT2 5.036, area 96.07 %.

2/25/2014 5:35:11 PM

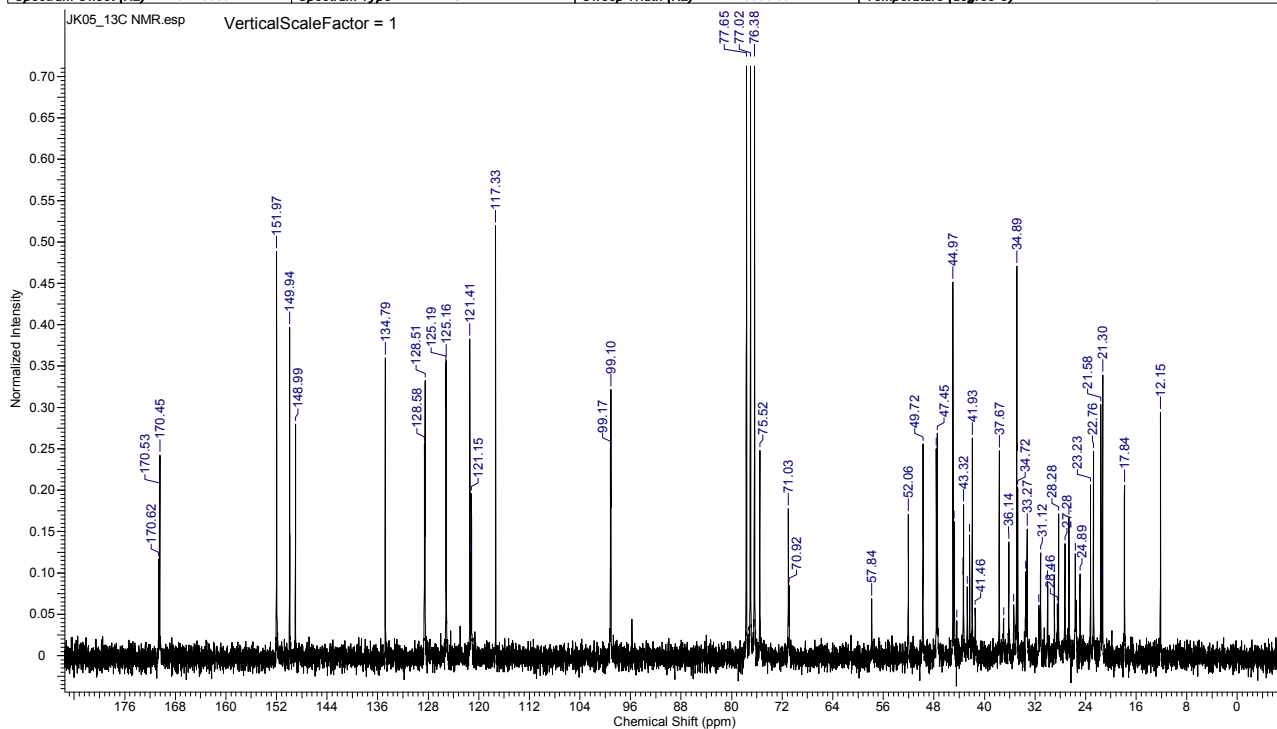
Number of Nuclei 0 H's					
Acquisition Time (sec)	1.3913	Comment	JK05	Date	Sep 29 10
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinolinski\DO152 i ostali\Recenzija\Spektri NMR_Star200 MHz\JK05\hjk05.fid.fid				
Frequency (MHz)	199.97	Nucleus	$^1\text{H}$	Number of Transients	512
Points Count	8192	Pulse Sequence	s2pul	Receiver Gain	9.00
Spectrum Offset (Hz)	1688.4263	Spectrum Type	STANDARD	Sweep Width (Hz)	4600.00
				Solvent	CHLOROFORM-d
				Temperature (degree C)	AMBIENT TEMPERATURE



**Compound 62 (JK05):  $^{13}\text{C}$  NMR spectrum (50 MHz).**

2/25/2014 5:37:17 PM

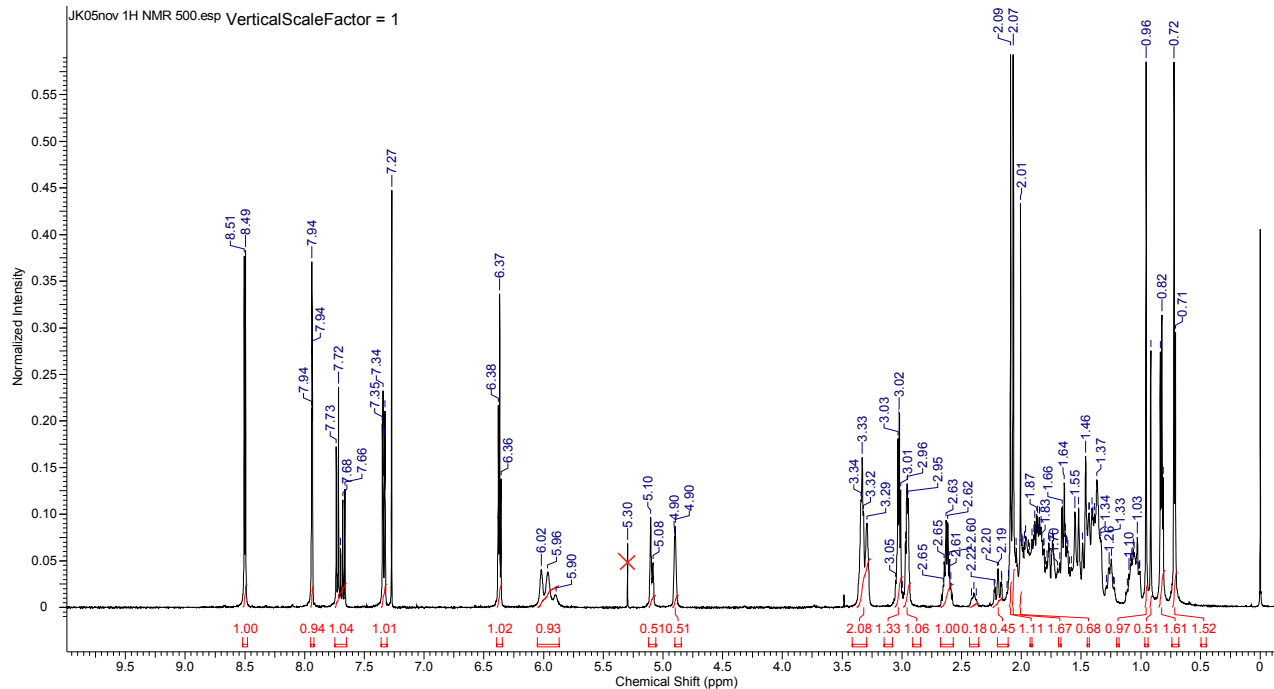
Number of Nuclei 0 C's					
Acquisition Time (sec)	1.0667	Comment	JK05	Date	Sep 29 10
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinolinski\DO152 i ostali\Recenzija\Spektri NMR_Star200 MHz\JK05\cjk05.fid.fid				
Frequency (MHz)	50.29	Nucleus	$^{13}\text{C}$	Number of Transients	16984
Points Count	16384	Pulse Sequence	s2pul	Receiver Gain	25.00
Spectrum Offset (Hz)	4814.6650	Spectrum Type	STANDARD	Sweep Width (Hz)	15000.00
				Solvent	CHLOROFORM-d
				Temperature (degree C)	AMBIENT TEMPERATURE



Compound 62 (JK05): <sup>1</sup>H NMR spectrum (500 MHz).

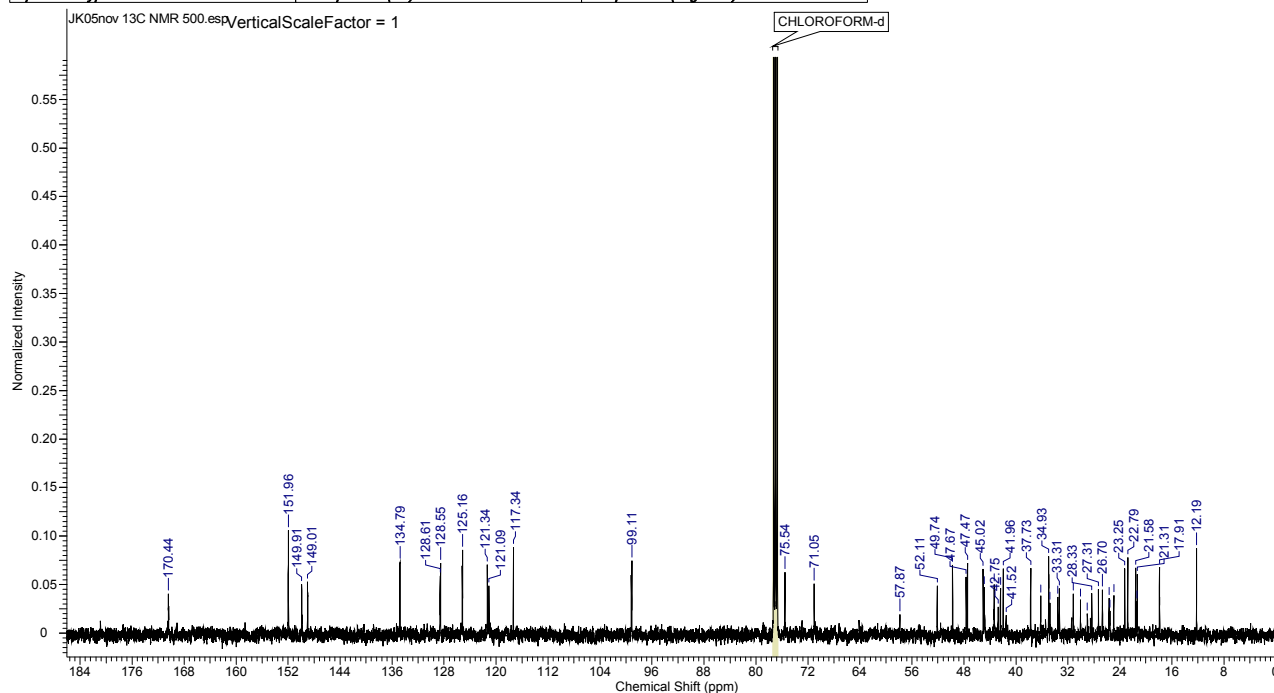
2/25/2014 5:38:33 PM

Number of Nuclei 0 H's					
Acquisition Time (sec)	2.1823	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	Date	21 Feb 2014 10:33:52
Date Stamp	21 Feb 2014 10:33:52				
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR nov\jk05nov\1\pdata\1\1r				
Frequency (MHz)	500.26	Nucleus	1H	Number of Transients	16
Original Points Count	16384	Owner	nimsu	Points Count	32768
Receiver Gain	362.00	SW(cyclical) (Hz)	7507.51	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	7507.28	Temperature (degree C)	25.000
				Spectrum Offset (Hz)	3493.8381

Compound 62 (JK05): <sup>13</sup>C NMR spectrum (125 MHz).

3/1/2014 11:39:51 PM

Number of Nuclei 0 C's					
Acquisition Time (sec)	0.5505	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118	Date	21 Feb 2014 10:12:32
Date Stamp	21 Feb 2014 10:12:32				
File Name	C:\Users\Dejan Opsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR nov\jk05nov\2\pdata\1\1r				
Frequency (MHz)	125.79	Nucleus	13C	Number of Transients	224
Original Points Count	16384	Owner	nimsu	Points Count	65536
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.45	Temperature (degree C)	25.100
				Spectrum Offset (Hz)	13830.0361

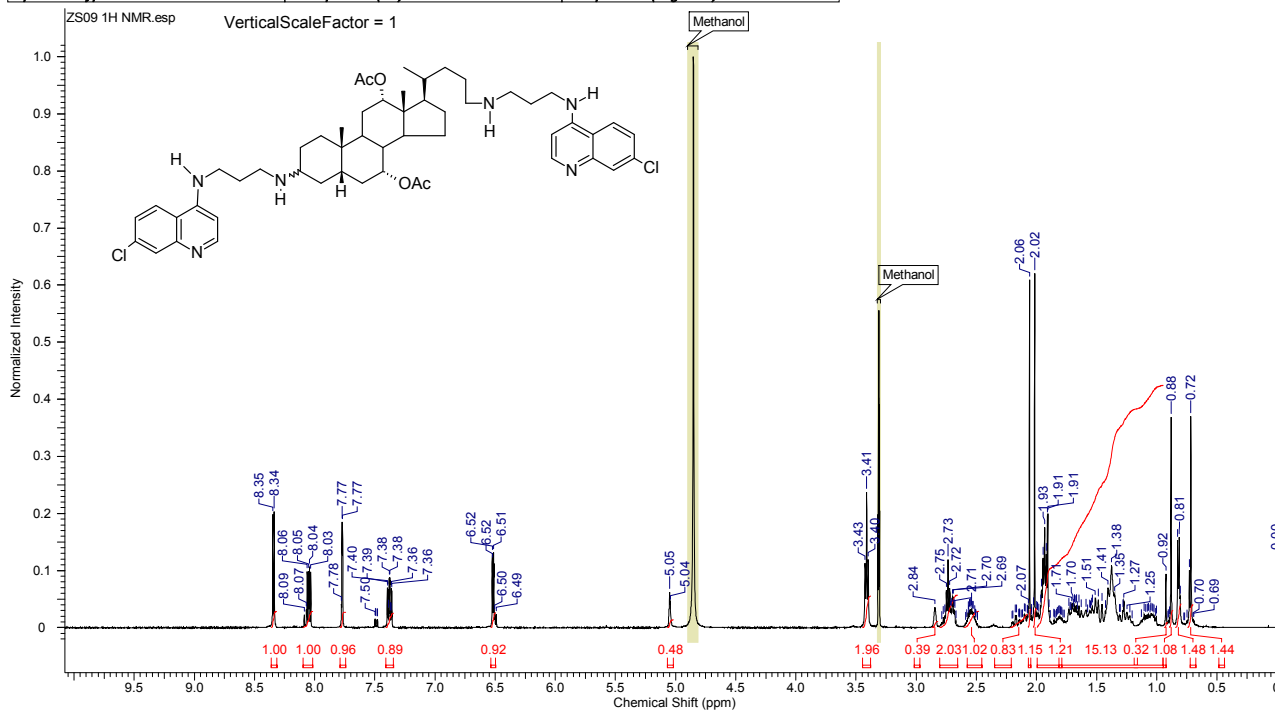




**Compound 63 (ZS09):  $^1\text{H}$  NMR spectrum (500 MHz).** HPLC purity: method C: RT1 5.533, RT2 8.731, area 95.07 %; method D: RT1 5.495, RT2 5.495, area 99.55 %.

2/26/2014 7:36:16 PM

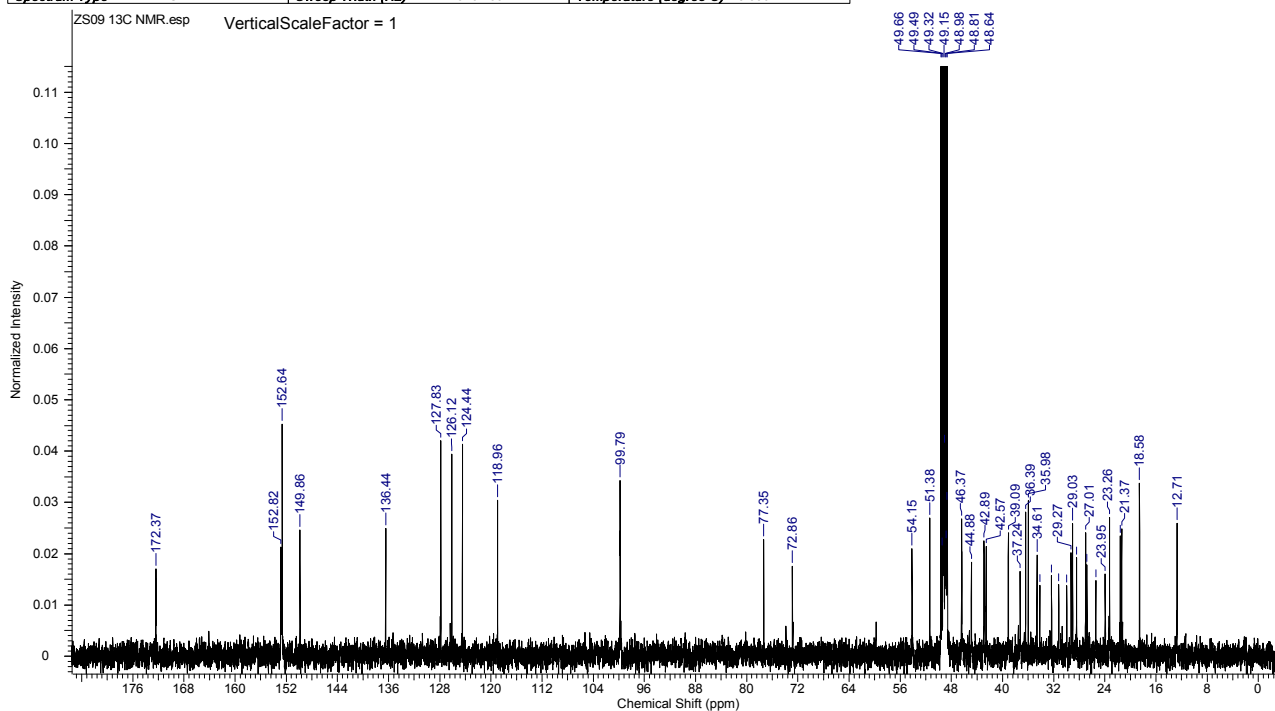
Number of Nuclei 0 H's				
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Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	
Original Points Count	16384	Owner	nmsu	
Receiver Gain	322.00	SW(cyclical) (Hz)	6188.12	
Spectrum Type	STANDARD	Sweep Width (Hz)	6187.93	
		Number of Transients	16	
		Points Count	32768	
		Solvent	METHANOL-d4	
		Temperature (degree C)	25.000	
		Origin	spect	
		Pulse Sequence	zq30	
		Spectrum Offset (Hz)	2741.7690	



**Compound 63 (ZS09):  $^{13}\text{C}$  NMR spectrum (125 MHz).**

2/25/2014 5:47:51 PM

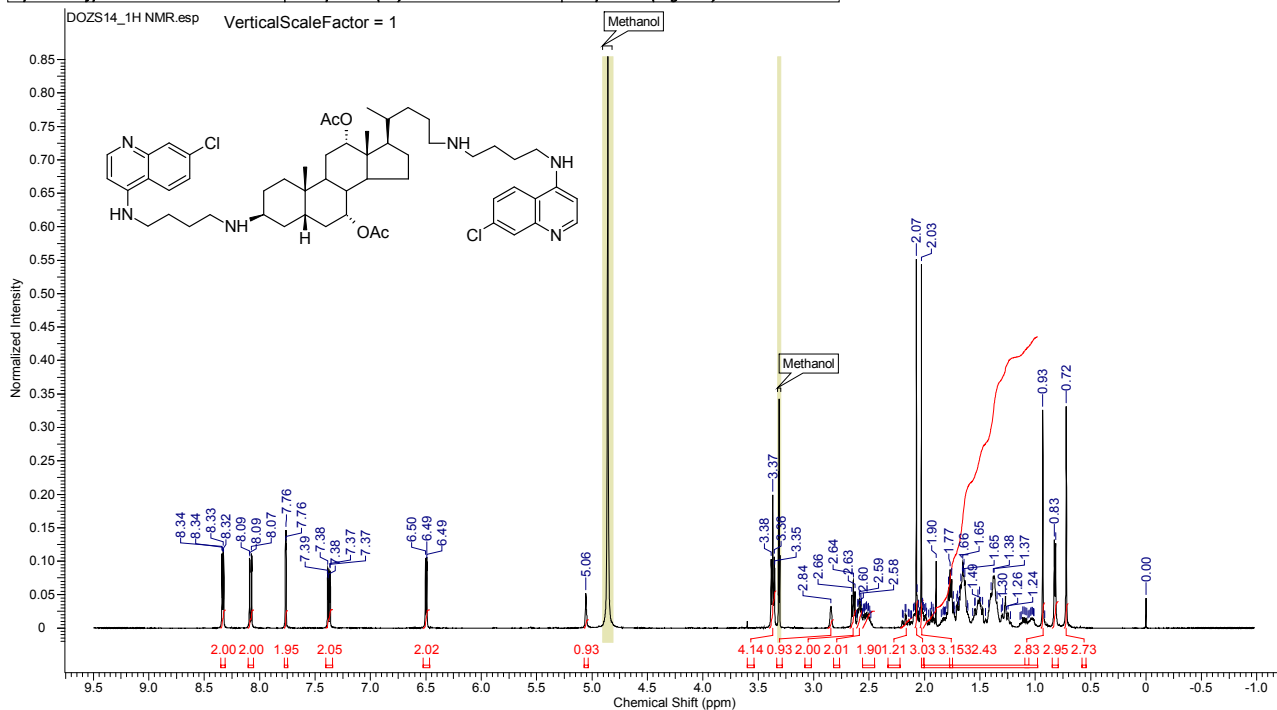
Number of Nuclei 0 C's				
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Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	
Original Points Count	16384	Owner	nmsu	
Receiver Gain	1030.00	SW(cyclical) (Hz)	29761.90	
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	
		Number of Transients	432	
		Points Count	32768	
		Solvent	METHANOL-d4	
		Temperature (degree C)	25.000	
		Origin	spect	
		Pulse Sequence	zqpg30	
		Spectrum Offset (Hz)	14030.4600	



**Compound 64 (DOZS14):  $^1\text{H}$  NMR spectrum (500 MHz).** HPLC purity: method C: RT 8.807, area 97.79 %; method D: RT 5.135, area 99.23 %.

2/26/2014 7:38:59 PM

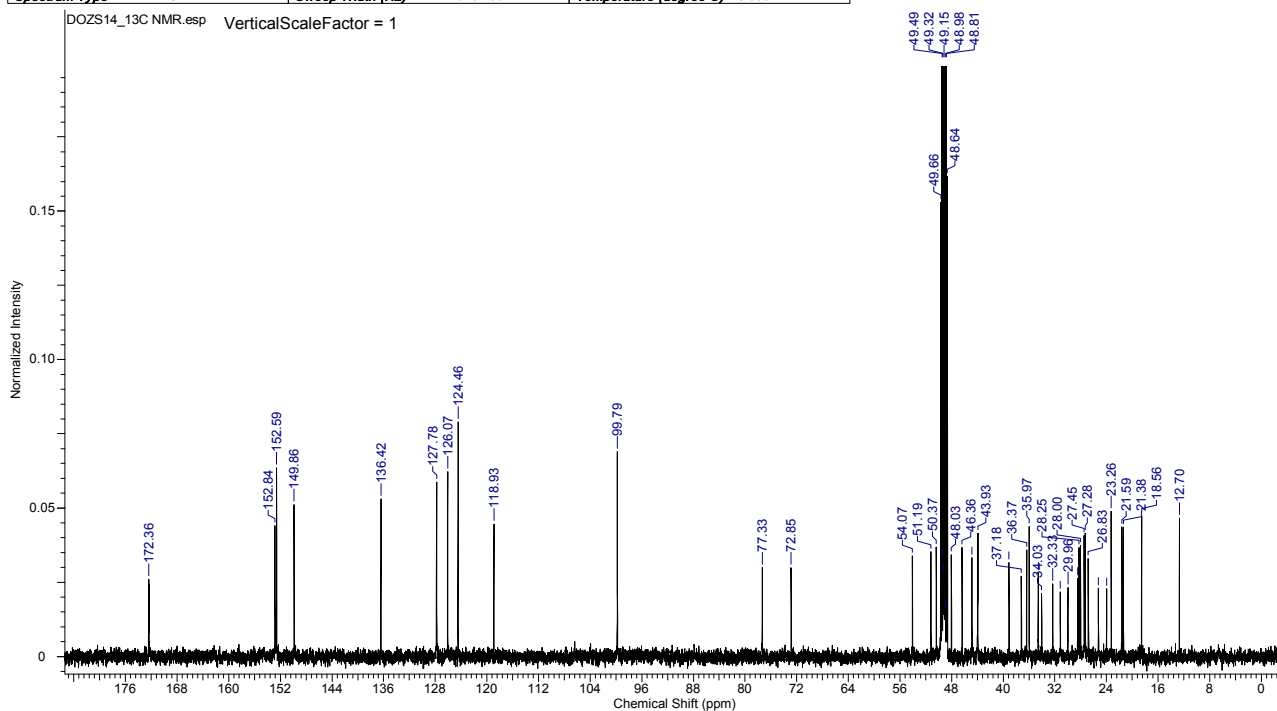
Number of Nuclei 0 H's							
Acquisition Time (sec)	3.1261	Date	20 May 2011 14:56:32				
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Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	32768	Pulse Sequence	zq30
Receiver Gain	114.00	SW(cyclical) (Hz)	5241.09	Solvent	METHANOL-d4	Spectrum Offset (Hz)	2131.7581
Spectrum Type	STANDARD	Sweep Width (Hz)	5240.93	Temperature (degree C)	25.000		



**Compound 64 (DOZS14):  $^{13}\text{C}$  NMR spectrum (125 MHz).**

2/25/2014 6:17:56 PM

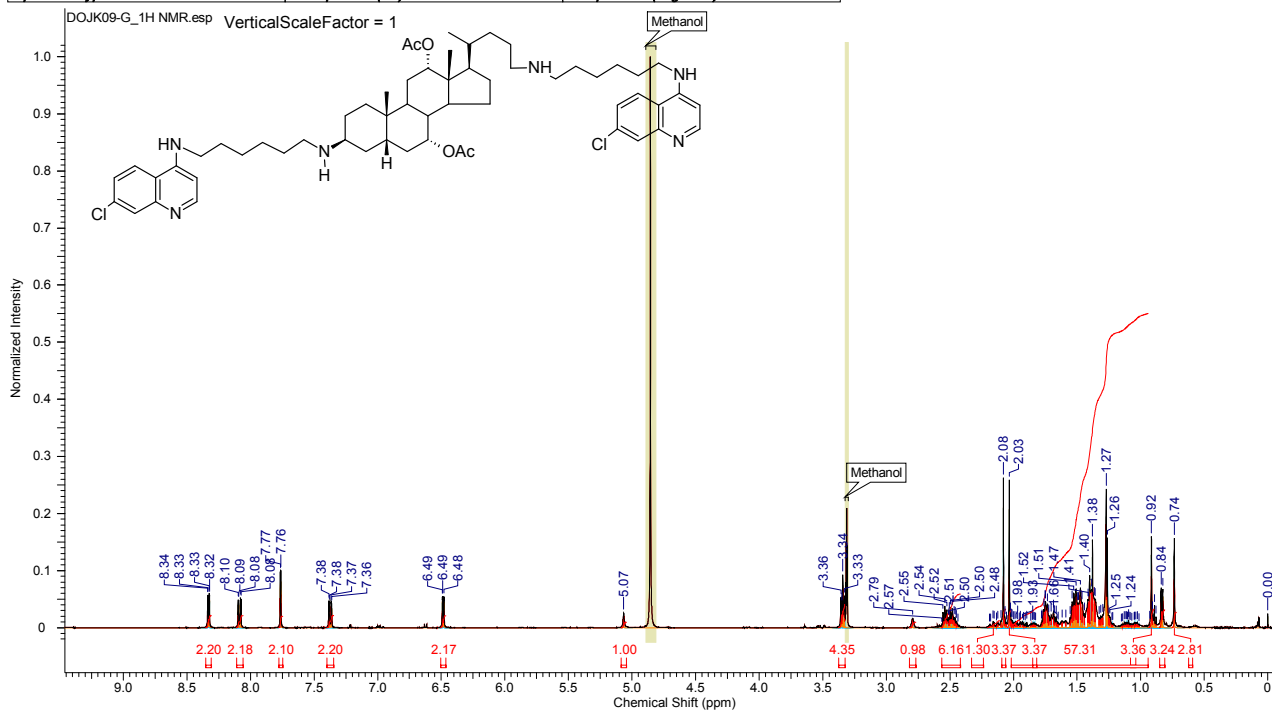
Number of Nuclei 0 C's							
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Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	605	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	32768	Pulse Sequence	zqpg30
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	METHANOL-d4	Spectrum Offset (Hz)	14029.8936
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000		



**Compound 65 (DOJK09-G): <sup>1</sup>H NMR spectrum (500 MHz).** HPLC purity: method C: RT 11.422, area 97.88 %; method D: RT 5.150, area 99.24.

2/25/2014 6:23:48 PM

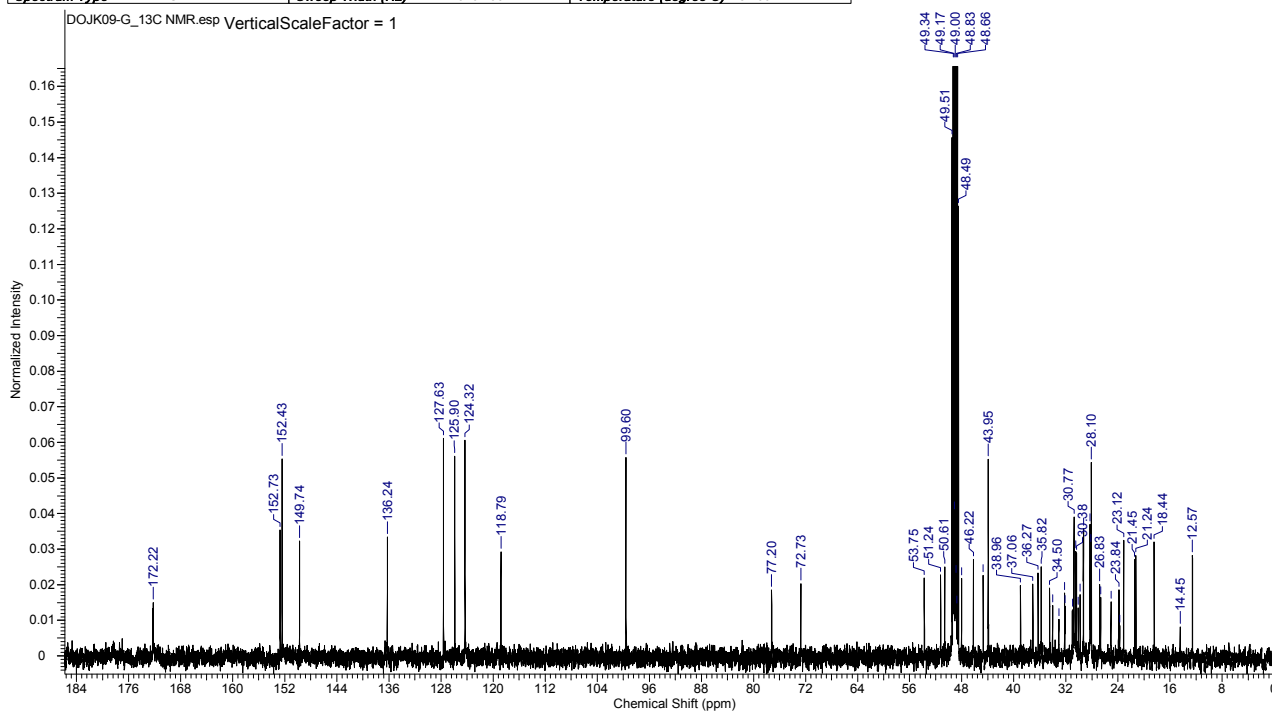
Number of Nuclei 0 H's				
Acquisition Time (sec)	2.9797	Date	02 Jun 2011 09:38:40	
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Frequency (MHz)	500.26	Nucleus	<sup>1</sup> H	
Original Points Count	16384	Owner	nmsru	
Receiver Gain	144.00	SW(cyclical) (Hz)	5498.53	
Spectrum Type	STANDARD	Sweep Width (Hz)	5498.37	
		Number of Transients	16	
		Points Count	32768	
		Solvent	METHANOL-d4	
		Temperature (degree C)	25.000	
		Origin	spect	
		Pulse Sequence	zg30	
		Spectrum Offset (Hz)	1989.5295	



**Compound 65 (DOJK09-G): <sup>13</sup>C NMR spectrum (125 MHz).**

2/25/2014 6:25:34 PM

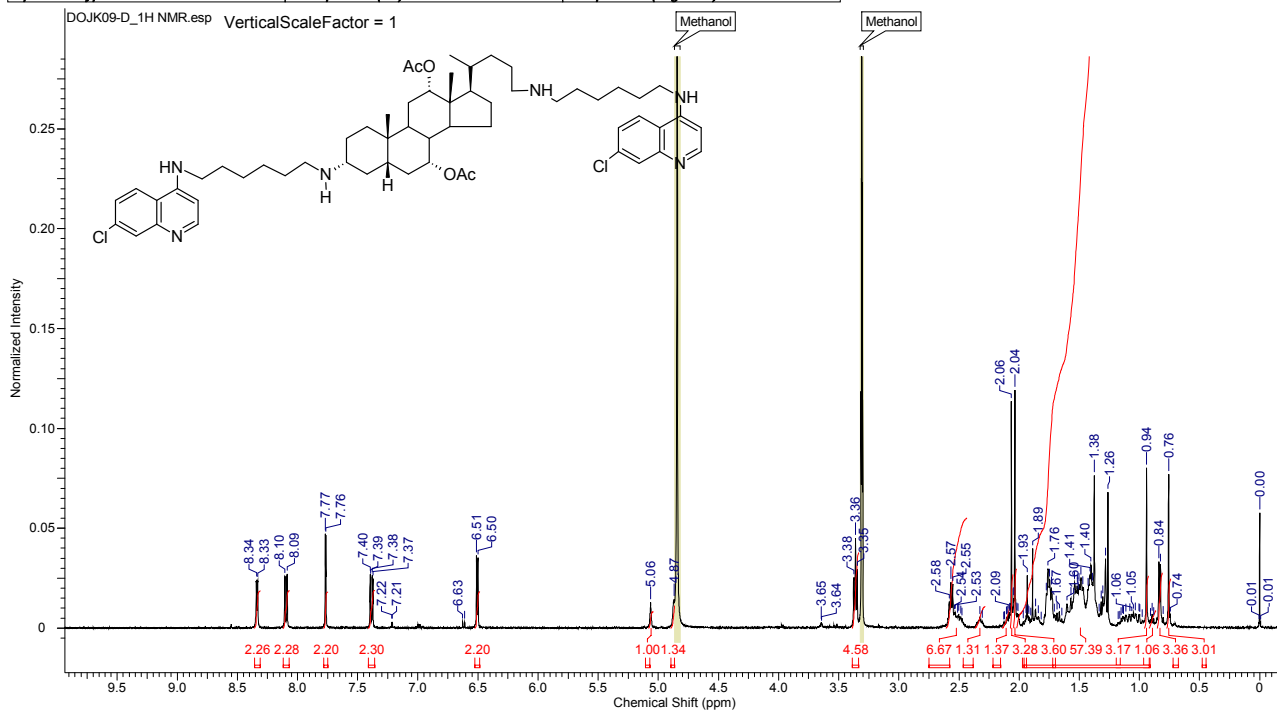
Number of Nuclei 0 C's				
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File Name	C:\Users\Dejan Ospenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_ Stari\500 MHz\DOJK09-G2\pdata\11r		Date Stamp	02 Jun 2011 09:42:56
Frequency (MHz)	125.79	Nucleus	<sup>13</sup> C	
Original Points Count	16384	Owner	nmsru	
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	
		Number of Transients	760	
		Points Count	32768	
		Solvent	METHANOL-d4	
		Temperature (degree C)	25.100	
		Origin	spect	
		Pulse Sequence	zgpg30	
		Spectrum Offset (Hz)	14011.5469	



**Compound 66 (DOJK09-D):**  $^1\text{H}$  NMR spectrum (500 MHz). HPLC purity: method C: RT 9.878, area 99.98 % ; method D: RT 5.208, area 96.76 %.

2/25/2014 6:27:19 PM

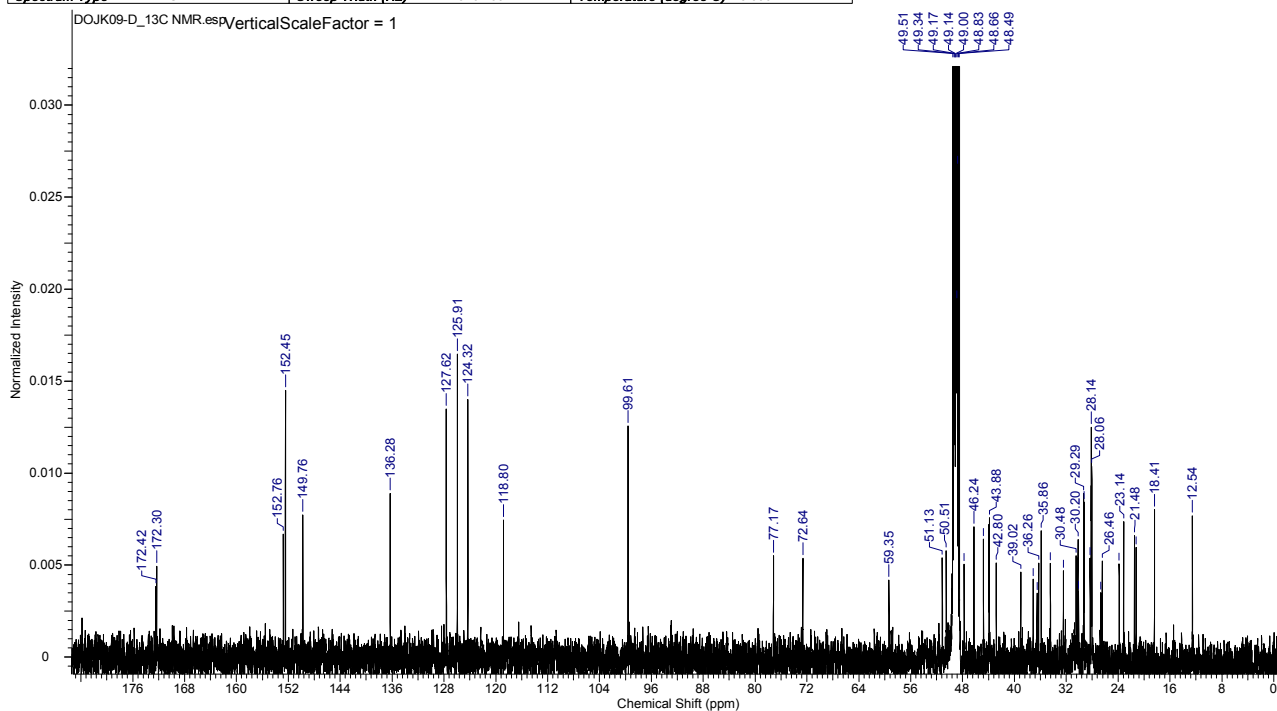
Number of Nuclei 0 H's					
Acquisition Time (sec)	2.7394	Date	08 Jun 2011 09:17:20	Date Stamp	08 Jun 2011 09:17:20
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Star500 MHz\DOJK09-D\1\pdata\11r			Origin	spect
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	32
Original Points Count	16384	Owner	nmsu	Points Count	32768
Receiver Gain	256.00	SW(cyclical) (Hz)	5980.86	Solvent	METHANOL-d4
Spectrum Type	STANDARD	Sweep Width (Hz)	5980.68	Temperature (degree C)	25.000
				Pulse Sequence	zg30
				Spectrum Offset (Hz)	2501.1787



**Compound 66 (DOJK09-D):**  $^{13}\text{C}$  NMR spectrum (125 MHz).

2/25/2014 6:29:08 PM

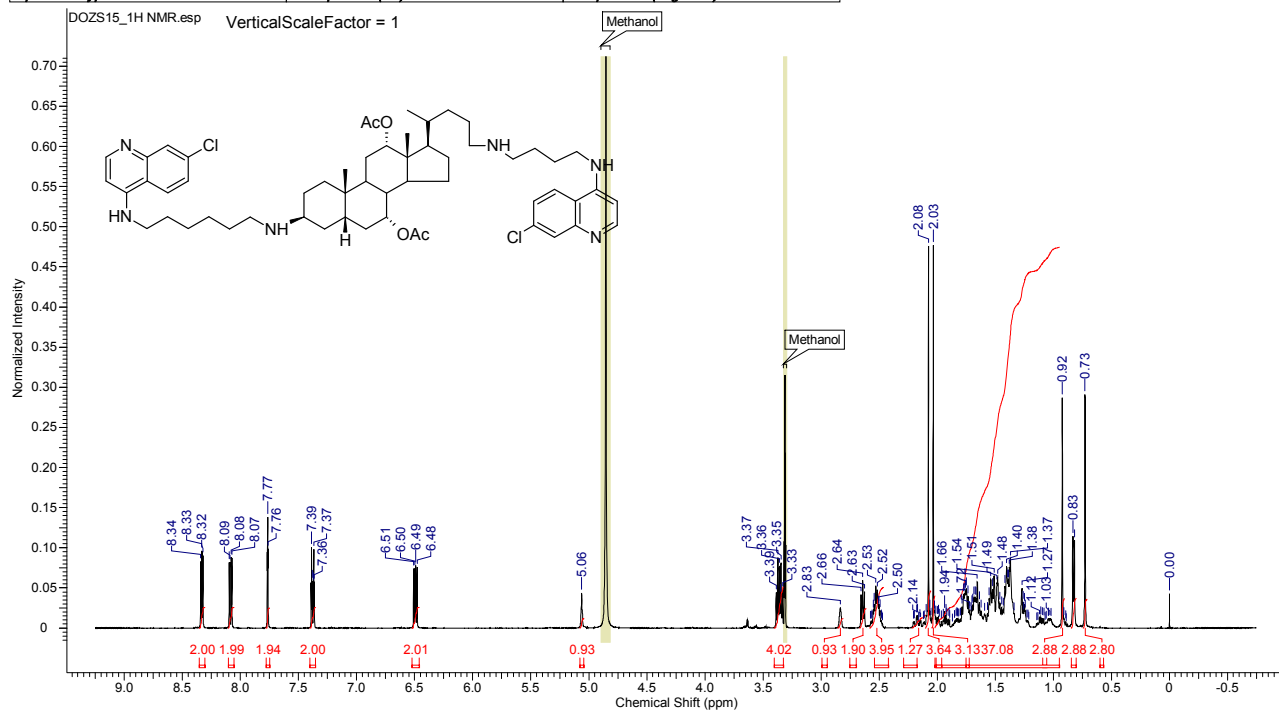
Number of Nuclei 0 C's					
Acquisition Time (sec)	0.5505	Date	08 Jun 2011 09:53:36	Date Stamp	08 Jun 2011 09:53:36
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_Star500 MHz\DOJK09-D\6\pdata\11r			Origin	spect
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	2159
Original Points Count	16384	Owner	nmsu	Points Count	32768
Receiver Gain	1030.00	SW(cyclical) (Hz)	29761.90	Solvent	METHANOL-d4
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000
				Pulse Sequence	zgpg30
				Spectrum Offset (Hz)	14013.2061



**Compound 67 (DOZS15):**  $^1\text{H}$  NMR spectrum (500 MHz). HPLC purity: method C: RT 8.674, area 95.27 %; method D: RT 5.072, area 99.21 %.

2/26/2014 7:40:26 PM

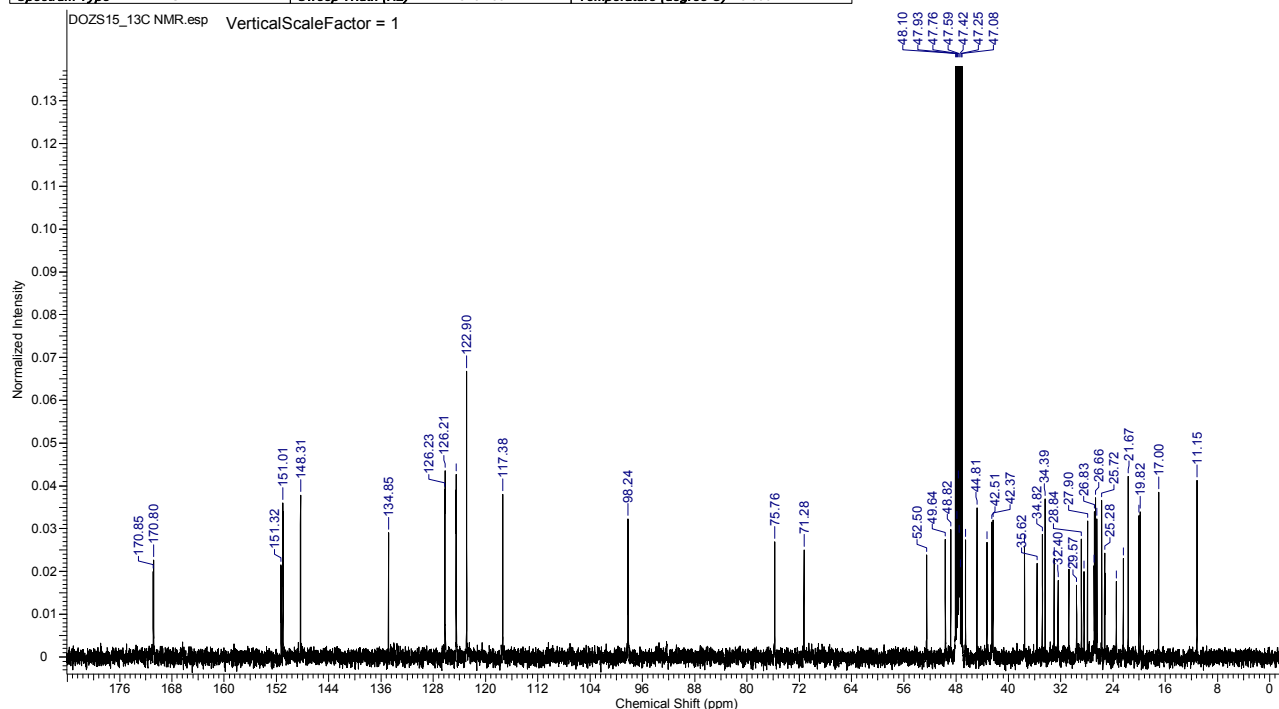
Number of Nuclei 0 H's							
Acquisition Time (sec)	3.2768	Date	27 May 2011 11:57:20				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_ Stari\500 MHz\DOZS15\1\data\11r		Date Stamp	27 May 2011 11:57:20			
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$	Number of Transients	16	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	32768	Pulse Sequence	zq30
Receiver Gain	90.50	SW(cyclical) (Hz)	5000.00	Solvent	METHANOL-d4	Spectrum Offset (Hz)	2126.2390
Spectrum Type	STANDARD	Sweep Width (Hz)	4999.85	Temperature (degree C)	25.000		



**Compound 67 (DOZS15):**  $^{13}\text{C}$  NMR spectrum (125 MHz).

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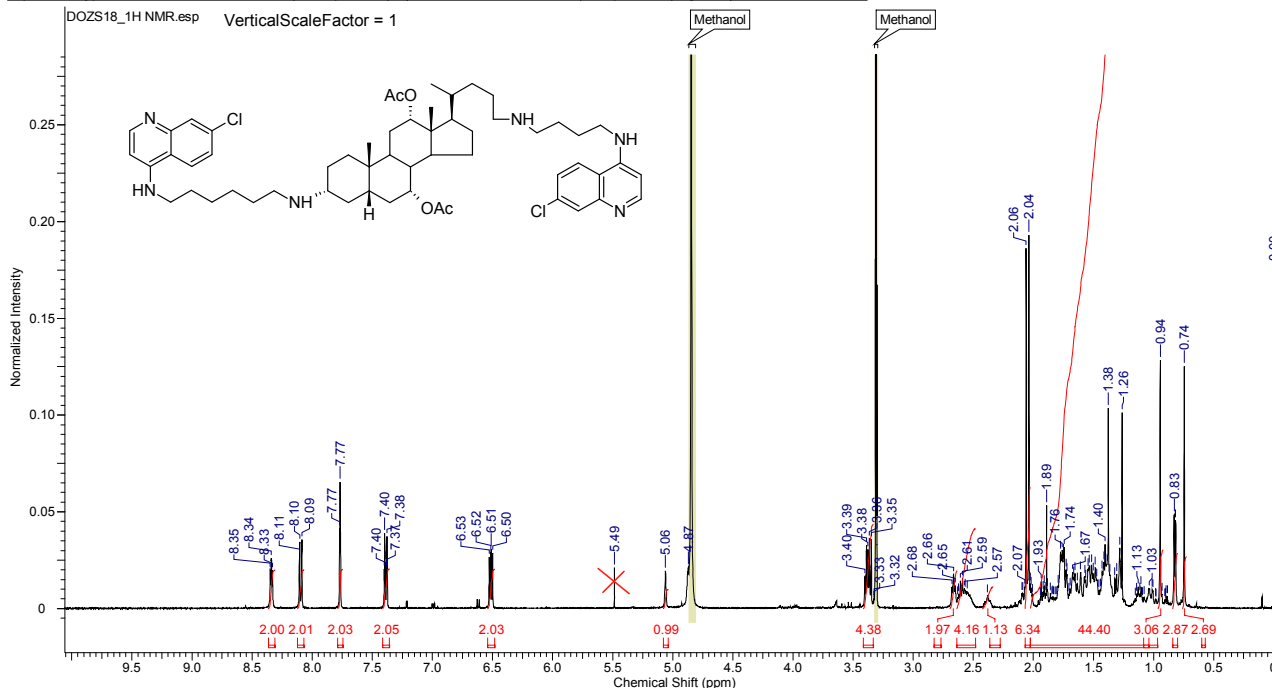
Number of Nuclei 0 C's							
Acquisition Time (sec)	0.5505	Date	27 May 2011 12:03:44				
File Name	C:\Users\Dejan Ovsenica\Documents\Radovi\Aminohinoliniski\DO152 i ostali\Recenzija\Spektri NMR_ Stari\500 MHz\DOZS15\2\data\11r		Date Stamp	27 May 2011 12:03:44			
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$	Number of Transients	716	Origin	spect
Original Points Count	16384	Owner	nmsru	Points Count	32768	Pulse Sequence	zqpg30
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	METHANOL-d4	Spectrum Offset (Hz)	13833.8447
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	25.000		



**Compound 68 (DOZS18):  $^1\text{H}$  NMR spectrum (500 MHz). HPLC purity: method C: RT 8.846, area 99.18 %; method D: RT 5.181, area 96.31 %.**

2/26/2014 7:41:43 PM

Number of Nuclei 0 H's			
Acquisition Time (sec)	2.7394	Comment	5 mm BBO BB-1H/D Z-GRD Z8007/0118
Date Stamp	06 Jun 2011 09:25:52	Date	06 Jun 2011 09:25:52
File Name	C:\Users\Dejan\Openical\Documents\Radovi\Aminohinoliniski\DO152\i ostali\Recenzija\Spektri NMR_Star500 MHz\DOZS15B\10\pdata1\11r		
Frequency (MHz)	500.26	Nucleus	$^1\text{H}$
Original Points Count	16384	Owner	nmsru
Receiver Gain	256.00	SW(cyclical) (Hz)	5980.86
Spectrum Type	STANDARD	Sweep Width (Hz)	5980.68
		Solvent	METHANOL-d4
		Temperature (degree C)	24.900
		Number of Transients	33
		Points Count	32768
		Origin	spect
		Pulse Sequence	zg30
		Spectrum Offset (Hz)	2508.4824



**Compound 68 (DOZS18):  $^{13}\text{C}$  NMR spectrum (125 MHz).**

2/25/2014 6:35:14 PM

Number of Nuclei 0 C's			
Acquisition Time (sec)	0.5505	Date	06 Jun 2011 09:49:20
Date Stamp	06 Jun 2011 09:49:20	Date Stamp	06 Jun 2011 09:49:20
File Name	C:\Users\Dejan\Openical\Documents\Radovi\Aminohinoliniski\DO152\i ostali\Recenzija\Spektri NMR_Star500 MHz\DOZS15B\6\pdata1\11r		
Frequency (MHz)	125.79	Nucleus	$^{13}\text{C}$
Original Points Count	16384	Owner	nmsru
Receiver Gain	1030.00	SW(cyclical) (Hz)	29761.90
Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00
		Solvent	METHANOL-d4
		Temperature (degree C)	25.000
		Number of Transients	2406
		Points Count	32768
		Origin	spect
		Pulse Sequence	zgpg30
		Spectrum Offset (Hz)	14012.9160

