Supporting Information

Oxidation of Disulfides to Taurine and Sulfanilic Acid Derivatives

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$^1$H and $^{13}$C NMR spectra and LC/MS data for compounds 1-2, 5 and 9-26
Compound 1:
Sample Name: NF-267_60/40  
Polarity/Scan Types: Positive Q1 MS  
Acq. Date: Thursday, March 12, 2015  
Scan Mode(s): Start: 150.0, Stop: 800.0, Step: 0.1  
Acq. File: 2015-03-12.wiff

**TIC of +Q1 from Sample 4 (NF-267_60/40) of 2015-03-12.wiff (Turbo Spray)**  
Max. 5.0e7 cps

**+Q1: 7.164 to 7.761 min from Sample 4 (NF-267_60/40) of 2015-03-12.wiff (Turbo Sprays)**  
Max. 3.1e8 cps

**XIC of +Q1: 360.950 to 381.450 Da from Sample 4 (NF-267_60/40) of 2015-03-12.wiff (T...**  
Max. 2.1e7 cps

**TWC of DAD Spectral Data: fro...**  
Max. 6.3e4 mAU  
**DAD Spectral Data: 7.213 to ...**  
Max. 1944.9 mAU  
**XWC of DAD Spectral Data: 200.0 to 400.0 nm from Sample 4 (NF-267_60/40) of 2015...**  
Max. 6.2e4 mAU

**Peak Lists for "XWC of DAD Spectral Data: 200.0 to 400.0 nm from Sample 4 (NF-267_60/40) of 2015-03-12"**

<table>
<thead>
<tr>
<th>Time (min)</th>
<th>Area (mAU x min)</th>
<th>% Area</th>
<th>Height (mAU)</th>
<th>% Height</th>
<th>Width (min)</th>
<th>Baseline Type</th>
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<tbody>
<tr>
<td>1</td>
<td>0.4335</td>
<td>5713.3436</td>
<td>0.5128</td>
<td>2191.1430</td>
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<td>0.5326</td>
<td>5171.9053</td>
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<td>0.4400</td>
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<td>4</td>
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<td>1996.4140</td>
<td>0.1791</td>
<td>209.6971</td>
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<tr>
<td>5</td>
<td>7.3371</td>
<td>1.0871e6</td>
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<tr>
<td>6</td>
<td>10.2100</td>
<td>8000.0298</td>
<td>0.7269</td>
<td>349.1331</td>
<td>0.5445</td>
<td>0.8400</td>
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</tbody>
</table>

LC Pump Device: Agilent 1100 binary pump
Compound 2:
Compound 5:
Sample Name: NF-205_60/40
Polarity/Scan Type: Positive Q1 MS
Acq. Date: Monday, October 20, 2014
Scan Mass(es): Start: 180.0, Stop: 800.0, Step: 0.1

**TIC of +Q1 from Sample 1 (NF-205_60/40) of 2014-10-20.wiff (Turbo Spray)**
Max. 1.9e7 cps.

**+Q1: 12.221 to 12.747 min from Sample 1 (NF-205_60/40) of 2014-10-20.wiff (Turbo Sp...**
Max. 1.2e6 cps.

**XIC of +Q1: 554.849 to 535.349 Da from Sample 1 (NF-205_60/40) of 2014-10-20.wiff (T...**
Max. 9.2e6 cps.

**TWC of DAD Spectral Data: fr...**
Max. 7.8e4 mAU.

**DAD Spectral Data: 12.083 to ...**
Max. 641.6 mAU.

**XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 1 (NF-205_60/40) of 2014...**
Max. 6.4 e4 mAU.

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Peak List for 'XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 1 (NF-205_60/40) of 2014-10-20.wiff'

<table>
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<tr>
<th>Time (min)</th>
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<th>% Height</th>
<th>Width (min)</th>
<th>Baseline Type</th>
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<td>4.1805e4</td>
<td>6.8404</td>
<td>3384.9330</td>
<td>5.0568</td>
<td>0.5133</td>
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<tr>
<td>2</td>
<td>12.2627</td>
<td>5.6935e5</td>
<td>93.1596</td>
<td>6.3554e4</td>
<td>94.9432</td>
<td>0.9867</td>
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</table>

LC Pump Device: Agilent 1100 binary pump

10
Compound 9:
Compound 10:

![Chemical Structure of Compound 10]
Sample Name: NF-185  Polarity/Scan Type: Positive Q1 MS
Acq. Date: Tuesday, September 10, 2014 Scan Mass(es): Start: 200.0, Step: 1206.0, Step: 0.1
Acq. File: 2014-09-29.wiff

1. TIC of +Q1: from Sample 8 (NF-185) of 2014-09-29.wiff (Turbo Spray)
   Max. 6.0e6 cps.

   Max. 2.7e5 cps.

3. XIC of +Q1: 780.150 to 780.650 Da from Sample 8 (NF-185) of 2014-09-29.wiff (Turbo Spray).
   Max. 2.2e6 cps.

4. TIC of DAD Spectral Data: fr...
   Max. 1.2e5 mAU.

5. DAD Spectral Data: 13.792 to...
   Max. 1.3124 mAU.

6. XIC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 8 (NF-185) of 2014-09-29...
   Max. 1.0e5 mAU.

Peak List for "XIC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 8 (NF-185) of 2014-09-29.wiff"

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<th>Time (min)</th>
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<th>Width (min)</th>
<th>Baseline Type</th>
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<td>0.4719</td>
<td>0.0021</td>
<td>839.5170</td>
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<td>1.976</td>
<td>0.5133</td>
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<tr>
<td>3</td>
<td>13.4001</td>
<td>0.3585</td>
<td>616.0710</td>
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<td>0.1333</td>
<td>Valley</td>
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<tr>
<td>4</td>
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<td>397.078</td>
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<td>0.1867</td>
<td>Valley</td>
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<tr>
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<td>13.8728</td>
<td>0.0168</td>
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<td>0.7133</td>
<td>0.2867</td>
<td>Base to Base</td>
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<tr>
<td>6</td>
<td>14.5556</td>
<td>0.0011</td>
<td>1460.3955</td>
<td>1.3564</td>
<td>0.2867</td>
<td>Base to Base</td>
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</tbody>
</table>

LC Pump Device: Agilent 1100 binary pump
Compound 11:
Compound 12:
Sample Name: NF-203HPLC_60/40  Polarity/Scan Type: Positive Q1 MS
Acq. Date: Thursday, October 30, 2014  Scan Mass(es): Start: 200.0, Stop: 1260.0, Step: 0.1

**TIC of +Q1: from Sample 2 (NF-203HPLC_60/40) of 2014-10-30.wiff**
Max. 8.4e6 cps

**+Q1: 11.191 to 11.612 min from Sample 2 (NF-203HPLC_60/40) of 2014-10-30.wiff**
Max. 2.4e5 cps

**XIC of +Q1: 792.049 to 792.549 Da from Sample 2 (NF-203HPLC_60/40) of 2014-10-30.wiff**
Max. 2.9e6 cps

**TIC of DAD Spectral Data:**
Max. 1.0e6 mAU

**DAD Spectral Data:**
Max. 866.2 mAU

**XIC of DAD Spectral Data: 200.0 to 400.0 nm from Sample 2 (NF-203HPLC_60/40) of 2014-10-30.wiff**
Max. 1.0e5 mAU

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### Peak List for "XIC of DAD Spectral Data: 200.0 to 400.0 nm from Sample 2 (NF-203HPLC_60/40) of 2014-10-30.wiff"

<table>
<thead>
<tr>
<th>Time (min)</th>
<th>Area (mAU x min)</th>
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<th>Height (mAU)</th>
<th>% Height</th>
<th>Width (min)</th>
<th>Baseline Type</th>
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<tbody>
<tr>
<td>1</td>
<td>11.3041 9.8355e5</td>
<td>99.5614</td>
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<td>99.1625</td>
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<tr>
<td>2</td>
<td>12.0439 4332.5589</td>
<td>0.4386</td>
<td>896.2970</td>
<td>0.8374</td>
<td>0.2200</td>
<td>Base to Base</td>
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</tbody>
</table>

LC Pump Device: Agilent 1100 Binary pump
Compound 13:
Compound 14:
Compound 15:

![Chemical structure of Compound 15 with NMR spectrum]
Sample Name: NF-271_90/10  Polarity/Scan Type: Positive Q1 MS
Acq. Date: Wednesday, March 18, 2015  Scan Mass(es): Start: 100.0, Stop: 500.0, Step: 0.1
Acq. File: 2015-03-18.wiff

TIC of +Q1: from Sample 1 (NF-271_90/10) of 2015-03-18.wiff (Turbo Spray)
Max. 6.5e7 cps

+Q1: 0.461 to 0.670 min from Sample 1 (NF-271_90/10) of 2015-03-18.wiff (Turbo Spra...
Max. 6.2e5 cps

+Q1: 0.887 to 3.223 min from Sample 1 (NF-271_90/10) of 2015-03-18.wiff (Turbo Spra...
Max. 1.1e6 cps

XIC of +Q1: 229.850 to 230.350 Da from Sample 1 (NF-271_90/10) of 2015-03-18.wiff (T...
Max. 1.7e7 cps

WFC of DAD Spectral Data: from...
Max. 2.4e4 mAU

DAD Spectral Data: 1.027 to 2....
Max. 656.8 mAU

XWC of DAD Spectral Data: 200.0 to 400.0 nm from Sample 1 (NF-271_90/10) of 2015...
Max. 2.4e4 mAU

Peak List for "XWC of DAD Spectral Data: 200.0 to 400.0 nm from Sample 1 (NF-271_90/10) of 2015-03-18.wiff"

<table>
<thead>
<tr>
<th>Time (min)</th>
<th>Area (mAU x min)</th>
<th>% Area</th>
<th>Height (mAU)</th>
<th>% Height</th>
<th>Width (min)</th>
<th>Baseline Type</th>
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<tbody>
<tr>
<td>1</td>
<td>0.4850</td>
<td>4.1901e4</td>
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<td>1.2363</td>
<td>1.0033e6</td>
<td>95.9910</td>
<td>2.0719e4</td>
<td>90.3720</td>
<td>2.6067</td>
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</tbody>
</table>

LC Pump Device: Agilent 1100 binary pump
Compound 16:
Compound 17:

\[
\begin{align*}
\text{HN} & \qquad \text{SO}_3\text{H} \\
\end{align*}
\]
**Sample Name:** NF197  
**Polarity/Scan Type:** Positive Q1 MS  
**Acq. Date:** Friday, November 21, 2014  
**Scan Mass(es):** Start: 150.0, Stop: 800.0, Step: 0.1  
**Acq. File:** 2014-11-21.wiff

**TIC of +Q1: from Sample 5 (NF197) of 2014-11-21.wiff (Turbo Spray)**  
Max. 7.6e6 cps

**+Q1: 1.874 to 3.524 min from Sample 5 (NF197) of 2014-11-21.wiff (Turbo Spray)**  
Max. 1.9e5 cps

**+Q1: 0.585 to 1.089 min from Sample 5 (NF197) of 2014-11-21.wiff (Turbo Spray)**  
Max. 1.6e5 cps

**XIC of +Q1: 244.949 to 245.449 Da from Sample 5 (NF197) of 2014-11-21.wiff (Turbo Spr...**  
Max. 2.4e6 cps

**TWC of DAD Spectral Data: fr...**  
Max. 8.564 mAU

**DAD Spectral Data: 1.807 to 3....**  
Max. 530.6 mAU

**XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 5 (NF197) of 2014-11-21....**  
Max. 6.8e4 mAU

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**Peak List for "XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 5 (NF197) of 2014-11-21.wiff"**

<table>
<thead>
<tr>
<th>Time (min)</th>
<th>Area (mAU x min)</th>
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<th>Height (mAU)</th>
<th>% Height</th>
<th>Width (min)</th>
<th>Baseline Type</th>
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<td>Base to Base</td>
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<tr>
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<td>4.7375e5</td>
<td>57.3007</td>
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<td>12.2238</td>
<td>Base to Base</td>
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</table>

**LC Pump Device:** Agilent 1100 binary pump

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40
Compound 18:
NF-191g: 36.5d
NF-191g in d6-MSD, 303K
auf Probe NF-192-2
Sample Name: NP-191-2-HPLC  Polarity/Scan Type: Positive Q1 MS
Acq. Date: Tuesday, November 18, 2014  Scan Mass(es): Start: 150.0, Stop: 600.0, Step: 0.1

**TIC of +Q1: from Sample 2 (NP-191-2-HPLC) of 2014-11-17.wiff (Turbo Spray)**
Max. 1.2e7 cps.

**+Q1: 0.519 to 1.007 min from Sample 2 (NP-191-2-HPLC) of 2014-11-17.wiff (Turbo Spr...**
Max. 9.1e4 cps.

**+Q1: 5.989 to 7.422 min from Sample 2 (NP-191-2-HPLC) of 2014-11-17.wiff (Turbo Spr...**
Max. 5.9e5 cps.

**XIC of +Q1: 259.650 to 259.450 Da from Sample 2 (NP-191-2-HPLC) of 2014-11-17.wiff ...**
Max. 4.0e6 cps.

**TWC of DAD Spectral Data: from 3.1e4 mAU**
Max. 3.1e4 mAU

**DAD Spectral Data: 5.847 to 7...**
Max. 9.184 mAU

**XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 2 (NP-191-2-HPLC) of 201...**
Max. 2.2e4 mAU

**Peak List for XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 2 (NP-191-2-HPLC) of 201-17.wiff**

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<th>% Height</th>
<th>Width (min)</th>
<th>Baseline Type</th>
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<tr>
<td>2</td>
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<td>2.2058e4</td>
<td>64.0793</td>
<td>3.0400 Base to Base</td>
</tr>
</tbody>
</table>

LC Pump Device: Agilent 1100 binary pump

43
Compound 19:

\[
\begin{align*}
\text{O} & \quad \text{N} & \quad \text{SO}_3\text{H} \\
\text{NH} & \quad 6' \\
\text{N} & \quad 5' \\
\text{O} & \quad 1' \\
\text{O} & \quad \text{OEt}
\end{align*}
\]
Sample Name: NF-211 HPLC  
Polarity/Scan Type: Positive Q1 MS  
Acq. Date: Friday, October 31, 2014  
Scan Mass(es): START: 190.0, STOP: 800.0, STEP: 0.1  

**TIC of +Q1: from Sample 1 (NF-211 HPLC) of 2014-10-31.wiff (Turbo Spray)**  
Max. 1.4e7 cps.

**+Q1: 7.492 to 8.335 min from Sample 1 (NF-211 HPLC) of 2014-10-31.wiff (Turbo Spray...**  
Max. 6.8e5 cps.

**XIC of +Q1: 316.75 to 317.25 Da from Sample 1 (NF-211 HPLC) of 2014-10-31.wiff (Tur...**  
Max. 4.5e6 cps.

**TWC of DAD Spectral Data: fr...**  
Max. 3.6e4 mAU.  
**DAD Spectral Data: 7.380 to ...**  
Max. 1153.7 mAU.

**XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 1 (NF-211 HPLC) of 2014-...**  
Max. 2.3e4 mAU.

**Peak List for "XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 1 (NF-211 HPLC) of 2014-10-31.wiff"**

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<tr>
<th>Time (min)</th>
<th>Area (mAU x min)</th>
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<th>% Height</th>
<th>Width (min)</th>
<th>Baseline Type</th>
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<td>1.6000</td>
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LC Pump Device: Agilent 1100 binary pump
Compound 20:
Compound 21:
Sample Name: NF-1H6 HPLC  
Polarity/Cron Type: Positive Q1 MS  
Acq. Date: Wednesday, November 19, 2014  
Scan Mass(es): Start: 150.0, Stop: 800.0, Step: 0.1  

**TIC of +Q1: from Sample 3 (NF-196 HPLC) of 2014-11-19.wiff (Turbo Spray), Smoothed**  
Max. 9.6e6 cps

**+Q1: 0.586 to 0.961 min from Sample 3 (NF-196 HPLC) of 2014-11-19.wiff (Turbo Spray)**  
Max. 1.5e5 cps

**+Q1: 7.270 to 8.265 min from Sample 3 (NF-196 HPLC) of 2014-11-19.wiff (Turbo Spray)**  
Max. 4.4e5 cps

**XIC of +Q1: 284.849 to 285.149 Da from Sample 3 (NF-196 HPLC) of 2014-11-19.wiff (Turbo Spray)**  
Max. 2.6e6 cps

**TWC of DAD Spectral Data: fr...**  
Max. 6.8e4 mAU

**DAD Spectral Data: 7.153 to ...**  
Max. 1085.9 mAU

**XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 3 (NF-196 HPLC) of 2014...**  
Max. 5.3e4 mAU

Peak List for "XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 3 (NF-196 HPLC) of 2014-11-19.wiff"

<table>
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<th>Time (min)</th>
<th>Area (mAU x min)</th>
<th>% Area</th>
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<th>% Height</th>
<th>Width (min)</th>
<th>Baseline Type</th>
</tr>
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<tbody>
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<td>11.556311</td>
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<td>174.2754</td>
<td>0.2117</td>
<td>Base to Base</td>
</tr>
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</table>

LC Pump Device: Agilent 1100 binary pump
Compound 22:
Compound 23:
Sample Name: NF-221 HPLC_PolarRP  Polarity/Scan Type: Positive Q1 MS
Acq. Date: Tuesday, December 22, 2014  Scan Mass(es): Start: 155.0, Stop: 800.0, Step: 0.1
Acq. File: 2014-12-02.wiff

- **TIC of Q1**: from Sample 2 (NF-221 HPLC_PolarRP) of 2014-12-02.wiff (Turbo Spray)  Max. 1.1e7 cps

- **XIC of Q1**: 1.817 to 3.600 min from Sample 2 (NF-221 HPLC_PolarRP) of 2014-12-02.wiff (Tu...  Max. 3.0e5 cps

- **XIC of Q1**: 272.850 to 273.350 Da from Sample 2 (NF-221 HPLC_PolarRP) of 2014-12-...  Max. 4.6e5 cps

- **TWC of DAD Spectral Data**: from...  Max. 2.0e4 mAU
- **DAD Spectral Data**: 1.713 to 3....  Max. 241.9 mAU

- **XWC of DAD Spectral Data**: 200.0 to 400.0 nm from Sample 2 (NF-221 HPLC_PolarRP)...  Max. 1.6e4 mAU

**Peak List for "XWC of DAD Spectral Data: 200.0 to 400.0 nm from Sample 2 (NF-221 HPLC_PolarRP) of 2014-12-02.wiff"**

<table>
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<th>% Height</th>
<th>Width (min)</th>
<th>Baseline Type</th>
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</thead>
<tbody>
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</tr>
<tr>
<td>2</td>
<td>2.9579</td>
<td>6.8718e4</td>
<td>62.5897</td>
<td>1869.2451</td>
<td>17.3857</td>
<td>1.5133</td>
</tr>
</tbody>
</table>

LC Pump Device: Agilent 1100 binary pump
Compound 24:
Sample Name: NF-198  Polarity/Scan Type: Positive Q1 MS
Acq. Date: Monday, October 06, 2014  Scan Mass(es): Start: 190.0, Stop: 800.0, Step: 0.1
Acq. File: 2014-10-06.wiff

TIC of +Q1: from Sample 4 (NF-198) of 2014-10-06.wiff (Turbo Spray)  Max. 1.1e7 cps.

+Q1: 8.112 to 9.669 min from Sample 4 (NF-198) of 2014-10-06.wiff (Turbo Spray)  Max. 4.5e6 cps.

XIC of +Q1: 320.850 to 321.350 Da from Sample 4 (NF-198) of 2014-10-06.wiff (Turbo S...  Max. 4.6e6 cps.

TWC of DAD Spectral Data: fr...  Max. 3.8e4 mAU.

DAD Spectral Data: 8.533 to ...  Max. 1034.3 mAU.

XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 4 (NF-198) of 2014-10-06...  Max. 3.1e4 mAU.

Peak List for "XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 4 (NF-198) of 2014-10-06.wiff"

<table>
<thead>
<tr>
<th>Time (min)</th>
<th>Area (mAU x min)</th>
<th>% Area</th>
<th>Height (mAU)</th>
<th>% Height</th>
<th>Width (min)</th>
<th>Baseline Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0969e4</td>
<td>1.1045</td>
<td>15222630</td>
<td>4.6000</td>
<td>0.3933</td>
<td>Base to Base</td>
</tr>
<tr>
<td>2</td>
<td>9.7300e5</td>
<td>98.8585</td>
<td>3.1570e4</td>
<td>95.4000</td>
<td>3.6267</td>
<td>Base to Base</td>
</tr>
</tbody>
</table>

LC Pump Device: Agilent 1100 binary pump
Compound 25:
Sample Name: NF-91HPLC_PolarRP  Polarity/Scan Type: Positive Q1 MS,
Acq. Date: Tuesday, February 26, 2013  Scan Mass(es): Start: 150.0, Stop: 800.0, Step: 0.1

**TIC from Sample 1 (NF-91HPLC_PolarRP) of 2013-02-26.wiff (Turbo Spray)**
Max. 1.5e8 cps.

**+Q1: Exp 1, 2.545 to 3.299 min from Sample 1 (NF-91HPLC_PolarRP) of 2013-02-26.wiff**
Max. 2.0e6 cps.

**-Q1: Exp 2, 2.585 to 3.279 min from Sample 1 (NF-91HPLC_PolarRP) of 2013-02-26.wiff**
Max. 1.2e5 cps.

**XIC of -Q1: Exp 2, 286.850 to 287.350 Da from Sample 1 (NF-91HPLC_PolarRP) of 2013-0...**
Max. 1.1e6 cps.

**TWC of DAD Spectral Data: from...**
Max. 1.0e4 mAU.

**DAD Spectral Data: 2.420 to 2.9...**
Max. 147.8 mAU.

**XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 1 (NF-91HPLC_PolarRP)...**
Max. 1.1e4 mAU.

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Peak List for "XWC of DAD Spectral Data: 220.0 to 400.0 nm from Sample 1 (NF-91HPLC_PolarRP) of 2013-02-29.wiff"

<table>
<thead>
<tr>
<th>Time (min)</th>
<th>Area (mAU x min)</th>
<th>% Area</th>
<th>Height (mAU)</th>
<th>% Height</th>
<th>Width (min)</th>
<th>Baseline Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.8602</td>
<td>100.0000</td>
<td>4386.4337</td>
<td>100.0000</td>
<td>0.5600</td>
<td>Base to Base</td>
</tr>
</tbody>
</table>

LC Pump Device: Agilent 1100 binary pump
Compound 26: