Supporting Information

Compound 1a

ESI-MS of 1a

HR-MS of 1a

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra
Card Serial Number: M153320
Sample Serial Number: 1a
Operator: HUAQIN                Date: 2015/11/16
Operation Mode: MALDI-FT_DHB

Elemental composition search on mass 527.21

<table>
<thead>
<tr>
<th>m/z</th>
<th>Theo. Mass</th>
<th>Delta (ppm)</th>
<th>RDB equiv.</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>527.2080</td>
<td>527.2078</td>
<td>0.50</td>
<td>22.5</td>
<td>C_{33}H_{27}O_{3}N_{4}</td>
</tr>
<tr>
<td>527.2091</td>
<td>527.2091</td>
<td>-2.05</td>
<td>22.0</td>
<td>C_{35}H_{29}O_{4}N</td>
</tr>
<tr>
<td>527.2104</td>
<td>527.2104</td>
<td>-4.59</td>
<td>27.0</td>
<td>C_{36}H_{25}N_{5}</td>
</tr>
</tbody>
</table>
$^1$H NMR of 1a

$^{13}$C NMR of 1a
### ESI-MS of 1b

**M153315 #3 RT: 0.14 AV: 1 NL: 2.61E5**

T: FTMS + p MALDI Full ms [100.00-1000.00]

![ESI-MS graph](image)

### HR-MS of 1b

**National Center for Organic Mass Spectrometry in Shanghai**

**Shanghai Institute of Organic Chemistry**

**Chinese Academic of Sciences**

**High Resolution MS DATA REPORT**

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number: M153316

Sample Serial Number: 1b

Operator: HUAQIN                Date: 2015/11/16

Operation Mode: MALDI-FT_DHB

**Elemental composition search on mass 541.22**

<table>
<thead>
<tr>
<th>m/z</th>
<th>Theo. Mass 541.2234</th>
<th>Delta (ppm)</th>
<th>RDB equiv.</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>541.2234</td>
<td>541.2234</td>
<td>-0.03</td>
<td>22.5</td>
<td>C_{34}H_{29}O_{3}N_{4}</td>
</tr>
<tr>
<td>541.2248</td>
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<td>-2.51</td>
<td>22.0</td>
<td>C_{36}H_{31}O_{4}N</td>
</tr>
<tr>
<td>541.2261</td>
<td>541.2261</td>
<td>-4.98</td>
<td>27.0</td>
<td>C_{37}H_{27}N_{5}</td>
</tr>
</tbody>
</table>
$^1$H NMR of 1b

$^{13}$C NMR of 1b
Compound 1c

ESI-MS of 1c

HR-MS of 1c

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra
Card Serial Number: M153314
Sample Serial Number: 1c
Operator: HUAQIN                Date: 2015/11/16
Operation Mode: MALDI-FT_DHB

Elemental composition search on mass 555.24

<table>
<thead>
<tr>
<th>m/z</th>
<th>Theo.</th>
<th>Delta (ppm)</th>
<th>RDB equiv.</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>555.2392</td>
<td>555.2391</td>
<td>0.17</td>
<td>22.5</td>
<td>C₃₅ H₃₁ O₃ N₄</td>
</tr>
<tr>
<td>555.2404</td>
<td>555.2391</td>
<td>-2.25</td>
<td>22.0</td>
<td>C₃₇ H₃₃ O₄ N</td>
</tr>
<tr>
<td>555.2417</td>
<td>555.2391</td>
<td>-4.66</td>
<td>27.0</td>
<td>C₃₈ H₂₉ N₅</td>
</tr>
</tbody>
</table>
$^1$H NMR of 1c

$^{13}$C NMR of 1c
ESI-MS of 1d

HR-MS of 1d

Instrument: Thermo Fisher Scientific LTQ FT Ultra
Card Serial Number: M153322
Sample Serial Number: 1d
Operator: HUAQIN                Date: 2015/11/16
Operation Mode: MALDI-FT_DHB
Elemental composition search on mass 528.20

<table>
<thead>
<tr>
<th>m/z</th>
<th>Theo. Mass</th>
<th>Delta (ppm)</th>
<th>RDB equiv.</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>528.2031</td>
<td>528.2030</td>
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<td>C₃₂H₂₆O₃N₅</td>
</tr>
<tr>
<td>528.2044</td>
<td>528.2044</td>
<td>-2.31</td>
<td>22.0</td>
<td>C₃₄H₂₈O₄N₂</td>
</tr>
</tbody>
</table>
$^1$H NMR of 1d

$^{13}$C NMR of 1d
ESI-MS of 1e

HR-MS of 1e

Instrument: Thermo Fisher Scientific LTQ FT Ultra
Card Serial Number: M153318
Sample Serial Number: 1e
Operator: HUAQIN Date: 2015/11/16
Operation Mode: MALDI-FT_DHB

Elemental composition search on mass 542.22

<table>
<thead>
<tr>
<th>m/z</th>
<th>Theo. Mass</th>
<th>Delta (ppm)</th>
<th>RDB equiv.</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>542.2186</td>
<td>542.2187</td>
<td>-0.21</td>
<td>22.5</td>
<td>C$<em>{33}$ H$</em>{28}$ O$_3$ N$_5$</td>
</tr>
<tr>
<td>542.2200</td>
<td>542.2200</td>
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<td>22.0</td>
<td>C$<em>{35}$ H$</em>{30}$ O$_4$ N$_2$</td>
</tr>
</tbody>
</table>
Supporting Information

$^1$H NMR of 1e

$^{13}$C NMR of 1e
ESI-MS of 1f

HR-MS of 1f

Instrument: Thermo Fisher Scientific LTQ FT Ultra
Card Serial Number: M153324
Sample Serial Number: 1f
Operator: HUAQIN                Date: 2015/11/16
Operation Mode: MALDI-FT_DHB

Elemental composition search on mass 556.23

<table>
<thead>
<tr>
<th>m/z</th>
<th>Theo. Mass</th>
<th>Delta (ppm)</th>
<th>RDB equiv.</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>556.2345</td>
<td>556.2343</td>
<td>0.24</td>
<td>22.5</td>
<td>C_34 H_30 O_3 N_5</td>
</tr>
<tr>
<td>556.2357</td>
<td>556.2357</td>
<td>-2.17</td>
<td>22.0</td>
<td>C_36 H_32 O_4 N_2</td>
</tr>
</tbody>
</table>
$^1$H NMR of 1f

$^{13}$C NMR of 1f
Compound 2a

ESI-MS of 2a

HR-MS of 2a

Instrument: Thermo Fisher Scientific LTQ FT Ultra
Card Serial Number: M153334
Sample Serial Number: 2a
Operator: HUAQIN                Date: 2015/11/16
Operation Mode: MALDI-FT_DHB

Elemental composition search on mass 527.21

<table>
<thead>
<tr>
<th>m/z</th>
<th>Theo. Mass</th>
<th>Delta (ppm)</th>
<th>RDB equiv.</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>527.2078</td>
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</tr>
<tr>
<td>527.2091</td>
<td>527.2091</td>
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<td>22.0</td>
<td>C_{35}H_{29}O_{4}N</td>
</tr>
<tr>
<td>527.2104</td>
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<td>-4.95</td>
<td>27.0</td>
<td>C_{36}H_{25}N_{5}</td>
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</table>
$^1$H NMR of 2a

$^{13}$C NMR of 2a
Supporting Information

Compound 2b

ESI-MS of 2b

HR-MS of 2b

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra
Card Serial Number: M153330
Sample Serial Number: 2b
Operator: HUAQIN                Date: 2015/11/16
Operation Mode: MALDI-FT_DHB

Elemental composition search on mass 541.22

<table>
<thead>
<tr>
<th>m/z</th>
<th>Theo. Mass</th>
<th>Delta (ppm)</th>
<th>RDB equiv.</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>541.2239</td>
<td>541.2234</td>
<td>0.91</td>
<td>22.5</td>
<td>C_{34} H_{29} O_{3} N_{4}</td>
</tr>
<tr>
<td>541.2248</td>
<td>541.2248</td>
<td>-1.57</td>
<td>22.0</td>
<td>C_{36} H_{31} O_{4} N</td>
</tr>
<tr>
<td>541.2261</td>
<td>541.2261</td>
<td>-4.04</td>
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<td>C_{37} H_{27} N_{5}</td>
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</tbody>
</table>
$^1$H NMR of 2b

$^{13}$C NMR of 2b
Supporting Information

ESI-MS of 2c

HR-MS of 2c

Instrument: Thermo Fisher Scientific LTQ FT Ultra
Card Serial Number: M153328
Sample Serial Number: 2c
Operator: HUAQIN                Date: 2015/11/16
Operation Mode: MALDI-FT_DHB

Elemental composition search on mass 555.24

<table>
<thead>
<tr>
<th>m/z</th>
<th>Theo. Mass</th>
<th>Delta (ppm)</th>
<th>RDB equiv.</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>555.2396</td>
<td>555.2391</td>
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<td>22.5</td>
<td>C\textsubscript{35} H\textsubscript{31} O\textsubscript{3} N\textsubscript{4}</td>
</tr>
<tr>
<td>555.2404</td>
<td>555.2404</td>
<td>-1.44</td>
<td>22.0</td>
<td>C\textsubscript{37} H\textsubscript{33} O\textsubscript{4} N</td>
</tr>
<tr>
<td>555.2417</td>
<td>555.2417</td>
<td>-3.85</td>
<td>27.0</td>
<td>C\textsubscript{38} H\textsubscript{29} N\textsubscript{5}</td>
</tr>
</tbody>
</table>
$^1$H NMR of $2c$

$^{13}$C NMR of $2c$
### Compound 2d

**ESI-MS of 2d**

![ESI-MS graph]

**HR-MS of 2d**

**National Center for Organic Mass Spectrometry in Shanghai**

**Shanghai Institute of Organic Chemistry**

**Chinese Academic of Sciences**

**High Resolution MS DATA REPORT**

**Instrument:** Thermo Fisher Scientific LTQ FT Ultra

**Card Serial Number:** M153336

**Sample Serial Number:** 2d

**Operator:** HUAQIN

**Date:** 2015/11/16

**Operation Mode:** MALDI-FT_DHB

**Elemental composition search on mass 528.20**

<table>
<thead>
<tr>
<th>m/z</th>
<th>Theo. Mass</th>
<th>Delta (ppm)</th>
<th>RDB equiv.</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>528.2038</td>
<td>528.2044</td>
<td>-1.15</td>
<td>22.0</td>
<td>C_{34}H_{28}O_{4}N_{2}</td>
</tr>
<tr>
<td>528.2030</td>
<td>528.2030</td>
<td>1.39</td>
<td>22.5</td>
<td>C_{32}H_{26}O_{3}N_{5}</td>
</tr>
</tbody>
</table>

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$^1$H NMR of 2d

$^{13}$C NMR of 2d
Supporting Information

ESI-MS of 2e

<table>
<thead>
<tr>
<th>Resolved Mass (m/z)</th>
<th>Isotopic Peaks</th>
<th>Calculated Mass</th>
<th>Delta (ppm)</th>
<th>RDB equiv.</th>
<th>Elemental Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>542.2190</td>
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<td>542.2200</td>
<td>0.63</td>
<td>22.5</td>
<td>C_{33}H_{28}O_{3}N_{5}</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-1.84</td>
<td>22.0</td>
<td>C_{35}H_{30}O_{4}N_{2}</td>
</tr>
</tbody>
</table>
$^1$H NMR of 2e

$^{13}$C NMR of 2e
Supporting Information

**Compound 2f**

**ESI-MS of 2f**

M153325 #3  RT: 0.15  AV: 1  NL: 5.13E4
T: FTMS + p MALDI Full ms [100.00-1000.00]

**HR-MS of 2f**

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra
Card Serial Number: M153326
Sample Serial Number: 2f
Operator: HUAQIN                Date: 2015/11/16
Operation Mode: MALDI-FT_DHB

**Elemental composition search on mass 556.23**

<table>
<thead>
<tr>
<th>m/z</th>
<th>Theo. Mass</th>
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<th>Composition</th>
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</thead>
<tbody>
<tr>
<td>556.2349</td>
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<td>1.01</td>
<td>22.5</td>
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<td>C_{36}H_{32}O_{4}N_{2}</td>
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</tbody>
</table>
$^1$H NMR of 2f

$^{13}$C NMR of 2f