Supporting Information

for

A facile synthetic route to benzimidazolium salts bearing bulky aromatic N-substituents

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NMR and HRMS–ESI analyses
NMR analyses
1-Cl
1-Cl
2-Cl
3-Cl
3-Cl
4-Cl

Diagram of a molecular structure with labeled PPM values.
HRMS–ESI analyses
1-Cl = BIMes
2-Cl = BIPr
3-Cl = BPh
4-Cl = BPy
HR-ESI-MS (Bruker maXis)

Analysis Info
Analysis Name: D:\Data\Service\6404alhres.d
Method: tune_low_modified_09_01_14_pos.m
Sample Name: BIMes
Comment: Solvent: MeOH
Client: Grieco

Acquisition Date: 6/20/2014 9:40:15 AM
Operator: ust
Instrument: maXis
ID: 255552.00033

Acquisition Parameter
Source Type: ESI
Scan Begin: 50 m/z
Scan End: 3000 m/z
Ion Polarity: Positive
Set Capillary: 1500 V
Set End Plate Offset: -500 V
Set Nebulizer: 0.5 Bar
Set Dry Heater: 180 °C
Set Dry Gas: 4.0 l/min

Intens. x10^5:

m/z

<MS, 0.1-0.3 min #8-17>
HR-ESI-MS (Bruker maXis)

Analysis Info
Analysis Name: D:\Data\Service\6404althres.d
Method: tune_low_modified_09_01_14_pos.m
Sample Name: BIMes
Comment: Solvent: MeOH
Client: Grieco

Acquisition Date: 6/20/2014 9:40:15 AM
Operator: ust
Instrument: maXis
Instrument ID: 255552.00033

Acquisition Parameter
Source Type: ESI
Scan Begin: 50 m/z
Scan End: 3000 m/z
Ion Polarity: Positive
Set Capillary: 1500 V
Set End Plate Offset: -500 V
Set Nebulizer: 0.5 Bar
Set Dry Heater: 180 °C
Set Dry Gas: 4.0 l/min

Int.

3.0

2.5

2.0

1.5

1.0

0.5

0.0

measured pattern

CaH2N2, M, 355.21688

355.21644

356.21985

357.2307

+MS, 0.1-0.3 mm i.e 48-17

calculated pattern

355.21686 1+

356.22010 1+

357.2225 1+

354 355 356 357 358 m/z

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HR-ESI-MS (Bruker maXis)

Analysis Info
Analysis Name: D:\Data\Service\6403alhres.d
Method: tune_low_modified_08_01_14_pos.m
Sample Name: BIPr
Comment: Solvent: MeOH
Client: Gileco

Acquisition Info
Acquisition Date: 6/20/2014 9:24:26 AM
Operator: ust
Instrument: maXis
255552.000033

Acquisition Parameter
Source Type: ESI
Ion Polarity: Positive
Scan Begin: 50 m/z
Set Capillary: 1500 V
Scan End: 3000 m/z
Set End Plate Offset: -500 V
Set Nebulizer: 0.5 Bar
Set Dry Heater: 160 °C
Set Dry Gas: 4.0 l/min

Graph:
Intens. x10^5
25
20
15
10
5
0
0.0 100 200 300 400 500 600 700 800 m/z

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## HR-ESI-MS (Bruker maXis)

<table>
<thead>
<tr>
<th>Meas. m/z</th>
<th>#</th>
<th>Ion Formula</th>
<th>m/z</th>
<th>err [ppm]</th>
<th>mSigma</th>
<th># mSigma</th>
<th>Score</th>
<th>rdb</th>
<th>e⁻ Conf</th>
<th>N-Rule</th>
</tr>
</thead>
<tbody>
<tr>
<td>439.31042</td>
<td>1</td>
<td>C31H39N2</td>
<td>439.31078</td>
<td>0.82</td>
<td>13.8</td>
<td>1</td>
<td>100.00</td>
<td>13.5</td>
<td>even</td>
<td>ok</td>
</tr>
<tr>
<td>439.31128</td>
<td>2</td>
<td>C16H35N14O</td>
<td>439.31128</td>
<td>1.96</td>
<td>83.9</td>
<td>2</td>
<td>9.22</td>
<td>6.5</td>
<td>even</td>
<td>ok</td>
</tr>
<tr>
<td>439.30994</td>
<td>3</td>
<td>C15H39N10O5</td>
<td>439.30994</td>
<td>-1.00</td>
<td>96.9</td>
<td>3</td>
<td>8.35</td>
<td>1.5</td>
<td>even</td>
<td>ok</td>
</tr>
</tbody>
</table>
HR-ESI-MS (Bruker maXis)

Analysis Info
Analysis Name: D:\Data\Service\6403alhres.d
Method: tune_low_modified_09_01_14_pos.m
Sample Name: BIPr
Comment: Solvent: MeOH
Client: Grieco

Acquisition Parameter
Source Type: ESI
Scan Begin: 50 m/z
Scan End: 3000 m/z
Ion Polarity: Positive
Set Capillary: 1500 V
Set End Plate Offset: -500 V
Set Nebulizer: 0.5 Bar
Set Dry Heater: 180 °C
Set Dry Gas: 4.0 l/min

measured pattern

C₅H₃N₂, m/z 439.31078

calculated pattern

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HR-ESI-MS (Bruker maXis)

Analysis Info
Analysis Name: D:\Data\Service6513alhres.d
Method: tune_low_modified_09_01_14_pos.m
Sample Name: BPh
Comment: Solvent: MeOH/H2O 1:1
Client: Grieco

Acquisition Parameter
Source Type: ESI
Scan Begin: 50 m/z
Scan End: 3000 m/z
Ion Polarity: Positive
Set Capillary: 1000 V
Set End Plate Offset: -500 V
Set Nebulizer: 0.5 Bar
Set Dry Heater: 180 °C
Set Dry Gas: 4.0 l/min

 Acquisition Date: 7/7/2014 5:02:28 PM
Operator: ust
Instrument: maXis
255552.00033

Intens. x10^5
50 100 150 200 250 300 350 400 450 500 m/z

+MS, 0.1-0.3 min 48:17

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HR-ESI-MS (Bruker maXis)

Analysis Info
Analysis Name: D:\Data\Service\0513allres.d
Method: tune_low_modified_06_01_14_pos.m
Sample Name: BPh
Comment: Solvent: MeOH/H2O 1:1
Client: Grieo

Acquisition Date: 7/7/2014 5:02:28 PM
Operator: ust
Instrument: maXis 255552.00033

Acquisition Parameter
Source Type: ESI
Scan Begin: 50 m/z
Scan End: 3000 m/z
Ion Polarity: Positive
Set Capillary: 1000 V
Set End Plate Offset: -500 V
Set Nebulizer: 0.5 Bar
Set Dry Heater: 180 °C
Set Dry Gas: 4.0 l/min

Intensities
measured pattern
calculated pattern

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