One-Pot Efficient Multicomponent Synthesis of Carbazolyl Furan-2(5H)-one and Tetrahydropyrimididine Derivatives

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<th>page number</th>
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<td>NMR spectra, LCMS and CHN analysis of 4a-t and 6a-j</td>
<td>S3-S91</td>
</tr>
</tbody>
</table>
Element Name | Element % | Ret. Time
--- | --- | ---
Nitrogen | 8.58 | 0.78
Carbon | 66.72 | 1.16
Hydrogen | 4.85 | 3.74
Method filename: \texttt{E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_exa}
Sample ID: SRM-140 (43)
Analysis type: Unknown
Chromatogram filename: \texttt{UNK-09092010-33.dat}
Sample weight: 1.006

![Chemical Structure](image)

**Element Name** | **Element %** | **Ret. Time**
--- | --- | ---
Nitrogen | 6.21 | 0.74
Carbon | 70.65 | 1.15
Hydrogen | 5.11 | 3.87

\texttt{S7}
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM138
Inj. Volume: 5,000
Data Name: C:\LCMSsolution\User\Data\SRM138-APCI-POS1.qid
Method Name: C:\LCMSsolution\User\Methods\esi.qm

[Image of chromatogram]

LC Chromatogram

[Image of MS spectrum]

MS Spectrum

Line#1 R.Time:0.626(Scan#; 38) Positive
Mass/Peak:374 Base/Peak:475.25(8324550)
Raw Mode: Single 6.626x29
BG Mode: Peak Start 0.527(32)

[Image of MS peak table]

MS Peak Table
Peak# R.Time I.Time F.Time Area Height A/H Mark %Total Name
1 0.626 0.527 0.743 6320663 1130273 6.04 100.00

Base m/z Base Int.
475.25 8324550

OPERATOR
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: F:\Program Files\Thermo Finnigan\Eager 300 for EA\1112\DATA\Sys_data_exa
Sample ID: SRM-138 (# 36)
Analysis type: Unknown
Chromatogram filename: UNK-09092010-26.dat
Sample weight: 1.215

Element Name | Element % | Ret. Time
--------------|-----------|---------
Nitrogen      | 5.85      | 0.78    
Carbon        | 68.11     | 1.17    
Hydrogen      | 4.91      | 3.68    

4c
| ppm | 1.06 | 1.08 | 1.10 | 1.431 | 1.44 | 1.46 | 4.08 | 4.09 | 4.11 | 4.13 | 4.32 | 4.34 | 4.36 | 4.37 | 6.03 | 7.23 | 7.25 | 7.27 | 7.31 | 7.33 | 7.35 | 7.37 | 7.40 | 7.42 | 7.48 | 8.071 | 8.415 |
|-----|------|------|------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 0   | 1.06 | 1.08 | 1.10 | 1.431 | 1.44 | 1.46 | 4.08 | 4.09 | 4.11 | 4.13 | 4.32 | 4.34 | 4.36 | 4.37 | 6.03 | 7.23 | 7.25 | 7.27 | 7.31 | 7.33 | 7.35 | 7.37 | 7.40 | 7.42 | 7.48 | 8.071 | 8.415 |
| 1   | 1.06 | 1.08 | 1.10 | 1.431 | 1.44 | 1.46 | 4.08 | 4.09 | 4.11 | 4.13 | 4.32 | 4.34 | 4.36 | 4.37 | 6.03 | 7.23 | 7.25 | 7.27 | 7.31 | 7.33 | 7.35 | 7.37 | 7.40 | 7.42 | 7.48 | 8.071 | 8.415 |
| 2   | 1.06 | 1.08 | 1.10 | 1.431 | 1.44 | 1.46 | 4.08 | 4.09 | 4.11 | 4.13 | 4.32 | 4.34 | 4.36 | 4.37 | 6.03 | 7.23 | 7.25 | 7.27 | 7.31 | 7.33 | 7.35 | 7.37 | 7.40 | 7.42 | 7.48 | 8.071 | 8.415 |
| 3   | 1.06 | 1.08 | 1.10 | 1.431 | 1.44 | 1.46 | 4.08 | 4.09 | 4.11 | 4.13 | 4.32 | 4.34 | 4.36 | 4.37 | 6.03 | 7.23 | 7.25 | 7.27 | 7.31 | 7.33 | 7.35 | 7.37 | 7.40 | 7.42 | 7.48 | 8.071 | 8.415 |
| 4   | 1.06 | 1.08 | 1.10 | 1.431 | 1.44 | 1.46 | 4.08 | 4.09 | 4.11 | 4.13 | 4.32 | 4.34 | 4.36 | 4.37 | 6.03 | 7.23 | 7.25 | 7.27 | 7.31 | 7.33 | 7.35 | 7.37 | 7.40 | 7.42 | 7.48 | 8.071 | 8.415 |

#### Diagram

The diagram shows various peaks and chemical shifts with associated intensities. The peaks are labeled with their respective chemical shifts in ppm. The diagram includes a spectrum with peaks ranging from 1.06 to 8.415 ppm, with detailed annotations for each peak's intensity. The chemical structure is also shown, indicating bonds and atomic labels such as N, NH, and other functional groups.
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM139
Inj. Volume: 5.000
Data Name: C:\LCMS\solution\User\Data\SRM139-APCI-POS1.qld
Method Name: C:\LCMS\solution\User\Method\esi.qbm

![Chemical Structure](image)

**LC Chromatogram**

![Chromatogram](image)

**MS Spectrum**

![Spectrum](image)

Operator:

S12
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM121
Inj. Volume: 5.000
Data Name: C:\LCMSsolution\User\Data\SRM121-APCI-NEG1.qld
Method Name: C:\LCMSsolution\User\Methods\esi.qml

**LC Chromatogram**

Ch(254.0nm)*1.00

**MS Spectrum**

Mass Peaks: 330 Base Peak: 349.33(17/19)
Re: Mode: Single 0.866(49)
RI: Mode: Peak Start 0.922(36)

OPERATOR
Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_e
Sample ID: SRM-121 (#12)
Analysis type: Unk
Chromatogram filename: UNK-20012011-2.dat
Sample weight: 1.112

Element | Name  | Element % | Ret. Time |
---------|-------|-----------|-----------|
Nitrogen | 6.41  | 0.77      | 9.77      |
Carbon   | 73.48 | 1.17      | 1.17      |
Hydrogen | 5.45  | 3.69      | 3.69      |

4e
LCMS-2010A DATA REPORT
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User: Admin
Sample: SRM-134
Inj. Volume: 5.000
Data Name: C:\LCMSsolution\User\Data\SRM-134-APCI-POS1.qld
Method Name: C:\LCMSsolution\User\Method\esi.qlm

![Chemical Structure](image)

**LC Chromatogram**

![Chromatogram Graph]

**MS Spectrum**

![MS Spectrum Graph]

**MS Peak Table**

<table>
<thead>
<tr>
<th>Peak</th>
<th>R.Time</th>
<th>Intensity</th>
<th>Area</th>
<th>Height</th>
<th>A.H.</th>
<th>Mark</th>
<th>%Total</th>
<th>Name</th>
<th>Base m/z</th>
<th>Base Int.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.300</td>
<td>0.973</td>
<td>1216</td>
<td>1100</td>
<td>0.06</td>
<td>0.00</td>
<td>100.00</td>
<td>210.10</td>
<td>3282072</td>
<td></td>
</tr>
</tbody>
</table>

OPERATOR
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_exa
Sample ID: SRM-135 (# 104)
Analysis type: Unknown
Chromatogram filename: UNK-18082010-24.dat
Sample weight: 1.315

<table>
<thead>
<tr>
<th>Element</th>
<th>Name</th>
<th>Element %</th>
<th>Ret. Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td></td>
<td>5.86</td>
<td>0.77</td>
</tr>
<tr>
<td>Carbon</td>
<td></td>
<td>71.32</td>
<td>1.13</td>
</tr>
<tr>
<td>Hydrogen</td>
<td></td>
<td>5.62</td>
<td>3.74</td>
</tr>
</tbody>
</table>

[Chemical structure image]

4g
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
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User: Admin
Sample: SRM-142
Inj. Volume: 5.000
Data Name: C:\LCMSsolution\User\Data\SRM-142-APCI-POS1.qld
Method Name: C:\LCMSsolution\User\Method\esi.qll

**LC Chromatogram**

Chl (254.0nm) x 1.00

**MS Spectrum**

- Time: 0.781 (Scan# 47) Positive
- MassPeaks: 448 BasePeak: 213.00 (483/185)
- RawMode: Single 0.781 (47)
- RG Mode: Peak Surt 0.577 (23)

OPERATOR
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ext.dat
Sample ID: SRM-142 (# 100)
Analysis type: Unknown
Chromatogram filename: UNK-18082910-20.dat
Sample weight: 1.115

Element Name | Element % | Ret. Time
--- | --- | ---
Nitrogen | 5.56 | 0.79
Carbon | 63.45 | 1.16
Hydrogen | 4.31 | 3.67

4h
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data.exe
Sample ID: SRM-147 (# 105)
Analysis type: Unknown
Chromatogram filename: UNK-18082010-25.dat
Sample weight: 1.096

---

Element Name  Element %  Ret. Time
---  --------  --------
Nitrogen      5.45       0.77
Carbon        62.34      1.15
Hydrogen      4.39       3.71

---

4i

---

S28
LCMS-2010A DATA REPORT
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User: Admin
Sample: SRM148
Inj. Volume: 5.000
Data Name: C:\LCMSsolution\User\Data\SRM148-APCI-NEG1.qld
Method Name: C:\LCMSsolution\User\Method\esi.qlm

LC Chromatogram

Ch1(254 nm)*1.00

mAbs

LC MS Spectrum

Line 1: E. Time: 0.811 (Scan: 49) Negative
Mins/Peaks: 311BasPeak: 599.40(1344100)
Raw Mode: Single 0.814(999)
Bid Mode: Peak Start 0.527(12)

m/z

OPERATOR
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: \Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data.exe
Sample ID: SRM-148 (# 101)
Analysis type: UnkNown
Chromatogram filename: UNK-18082010-21.dat
Sample weight: 1.209

Element Name | Element % | Ret. Time
--------------|-----------|-----------
Nitrogen      | 5.62      | 0.78      
Carbon        | 75.81     | 1.15      
Hydrogen      | 5.29      | 3.67      

4j
LCMS-2010A DATA REPORT
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User: Admin
Sample: SRM149
Inj. Volume: 5.000
Data Name: C:\LCMS\Solution\User\Data\SRM149-APCI-POS1.qld
Method Name: C:\LCMS\Solution\User\Method\esi.qml

![LC Chromatogram](image1)

![MS Spectrum](image2)

Linel: 1. Retime: 0.77 (Scan# 47), Positive Masses in 0.2-2.5, User Peak 545 (512, 577) Raw Mode: Single 0.77 (47)
DQ Mode: Peak Start 0.565 (34)

OPERATOR
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data.exe
Sample ID: SRM-145 (# 103)
Analysis type: UnkNown
Chromatogram filename: UNK-18082010-23.dat
Sample weight: 1.562

![Chemical Structure](image)

<table>
<thead>
<tr>
<th>Element</th>
<th>Element %</th>
<th>Ret. Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>5.65</td>
<td>0.88</td>
</tr>
<tr>
<td>Carbon</td>
<td>69.52</td>
<td>1.31</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.91</td>
<td>4.74</td>
</tr>
</tbody>
</table>
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM207
Inj. Volume: 5.000
Data Name: C:\LCMSsolution\User\Data\SRM207-ESI-POS1.qld
Method Name: C:\LCMSsolution\User\Method\esi.qdm

LC Chromatogram

MS Spectrum

MS Peak Table

OPERATOR
### Table

| ppm  | 0.001 | 0.971 | 0.98 | 1.00 | 1.41 | 4.00 | 4.02 | 4.03 | 4.05 | 4.32 | 4.33 | 6.29 | 7.19 | 7.21 | 7.23 | 7.24 | 7.26 | 7.29 | 7.35 | 7.38 | 7.40 | 7.42 | 7.44 | 7.45 | 7.47 | 7.94 | 8.05 | 8.07 | 8.12 | 8.40 |
|------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 180  | 170   | 160   | 150  | 140  | 130  | 120  | 110  | 100  | 90   | 80   | 70   | 60   | 50   | 40   | 30   | 20   | 10   | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    |

### Organic Compound

\[ \text{Compound: } 4n \]

- NH
- O
- N

### Mass Spectra

- 37.712: 6.23 3.07
- 14.017: 1.421 1.410 1.004 0.988 0.971
- 13.922: 0.001
- 13.868: 0.001

### Chemical Analysis

- Peak Analysis
  - 167.125
  - 164.546
  - 140.592
  - 140.400
  - 139.198
  - 138.111
  - 129.559
  - 126.547
  - 125.989
  - 124.981
  - 122.998
  - 122.935
  - 122.797
  - 122.715
  - 122.644
  - 120.687
  - 120.585
  - 120.307
  - 119.155
  - 118.897
  - 115.989
  - 113.223
  - 108.682
  - 108.510
  - 108.292
  - 91.725
  - 77.426
  - 77.109
  - 60.501

### Molecular Structure

- Chemical structure of compound 4n

---

*Note: The image contains a detailed chemical analysis and mass spectrometry data for a compound identified as 4n.*
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM136
Inj. Volume: 5.000
Data Name: C:\LCM\Solution\User\Data\SRM136-APCI-POS1.qld
Method Name: C:\LCM\Solution\User\Method\est.qml

mAbs

250
200
150
100
50
0

Chromaogram

min

MS Spectrum

Line#: 1  R Time: 0.559(Scan#: 46)  Positive
MassPeaks: 469  BasePeak: 210.10(141.4751)
Ramp Mode: Single 0.3996(6)
BG Mode: Peak Start 0.527(22)

OPERATOR
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: E:\Program Files\Thermo Fisher\Eager 300 for EA1112\DATA\Sys_data_exa
Sample ID: SRM-136 (# 21)
Analysis type: Unknown
Chromatogram filename: UNK-09092010-11.dat
Sample weight: 1.019

![Chemical Structure Image]

Element | Name   | %   | Ret. Time |
---------|--------|-----|-----------|
        | Nitrogen| 7.45 | 0.89      |
        | Carbon  | 75.42| 1.39      |
        | Hydrogen| 5.66 | 4.72      |
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SRM-219 (#11)
Analysis type: Unknown
Chromatogram filename: UNK-20012011-1.dat
Sample weight: 1.136

<table>
<thead>
<tr>
<th>Element Name</th>
<th>Element %</th>
<th>Ret. Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>10.21</td>
<td>0.77</td>
</tr>
<tr>
<td>Carbon</td>
<td>67.18</td>
<td>1.18</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.85</td>
<td>3.69</td>
</tr>
</tbody>
</table>
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM210
Inj. Volume: 5.000
Data Name: C:\LCMSolution\User\Data\SRM210-APCI-POS1.qd
Method Name: C:\LCMSolution\User\Method\esi.qm

LC Chromatogram

MS Spectrum

MS Peak Table

OPERATOR

S46
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method file name: I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data.exe
Sample ID: SRM-206 (# 73)
Analysis type: Unknown
Chromatogram file name: UNK-17012011-3.dat
Sample weight: 1.106

<table>
<thead>
<tr>
<th>Element Name</th>
<th>Element %</th>
<th>Ret. Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>8.79</td>
<td>0.76</td>
</tr>
<tr>
<td>Carbon</td>
<td>66.55</td>
<td>1.18</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.41</td>
<td>3.74</td>
</tr>
</tbody>
</table>
Method filename:  I:\Program Files\Thermo Firmigan\Eager 300 for EA1112\DATA\Sys_data.exe
Sample ID:  SRM-155 (# 55)
Analysis type:  Unknw
Chromatogram filename:  UNK-24112010-5.dat
Sample weight:  1.132

---

Element Name | Element % | Ret. Time
---|---|---
Nitrogen | 3.83 | 0.89
Carbon | 66.31 | 1.40
Hydrogen | 4.52 | 4.72

---

4g
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM165
Inj. Volume: 5.000
Data Name: G:\LCMSsolution\User\Data\SRM165-APCI-POS1.qld
Method Name: C:\LCMSsolution\User\Method\JAY-4-APCI.qld

**LC Chromatogram**

<table>
<thead>
<tr>
<th>R Time</th>
<th>Area</th>
<th>Height</th>
<th>A/H Mark</th>
<th>%Total Name</th>
<th>Base m/z</th>
<th>Base Int.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.682</td>
<td>18842.398</td>
<td>148997</td>
<td>12.64</td>
<td>100.00</td>
<td>548.65</td>
<td>653495</td>
</tr>
</tbody>
</table>

**MS Spectrum**

**MS Peak Table**
**FLASH EA 1112 SERIES CHN REPORT**

**SCHOOL OF CHEMISTRY**

**UNIVERSITY OF HYDERABAD**

<table>
<thead>
<tr>
<th>Element Name</th>
<th>Element %</th>
<th>Ret. Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>7.72</td>
<td>0.89</td>
</tr>
<tr>
<td>Carbon</td>
<td>70.09</td>
<td>1.39</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.55</td>
<td>4.72</td>
</tr>
</tbody>
</table>
FLASH EA 1112 SERIES CHN REPORT  
SCHOOL OF CHEMISTRY  
UNIVERSITY OF HYDERABAD

Method filename: I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_exa
Sample ID: SRM-174 (# 126)
Analysis type: UnkNown
Chromatogram filename: UNK-29112010-26.dat
Sample weight: 1.122

![Chemical Structure]

<table>
<thead>
<tr>
<th>Element Name</th>
<th>Element %</th>
<th>Ret. Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>8.15</td>
<td>0.74</td>
</tr>
<tr>
<td>Carbon</td>
<td>62.28</td>
<td>1.16</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.31</td>
<td>3.88</td>
</tr>
</tbody>
</table>

4s
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM200
Inj. Volume: 5.000
Data Name: C:\LCMSsolution\User\Data\SRM200-ESI-NEG2.qld
Method Name: C:\LCMSsolution\User\Method\esi.qlm

LC Chromatogram

MS Spectrum

Linel: R.Time=0.778(Ion1:37) Negative
Mass/Peak: 373, Base Peak: 373.20(D25699)
Raw Mode: Single, 0.776(47)
BG Mode: Peak Start 0, 560(34)

OPERATOR
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM123
Inj. Volume: 5.000
Data Name: C:\LCMSSolution\User\Data\SRM123-ESI-POS1.qld
Method Name: C:\LCMSSolution\User\Method\esi.qml

LC Chromatogram

MS Spectrum

Line 1: R.Time: 0.758 (Scan: 45) Positive
Msim: Peaks: 469 Base/Peak: 457.60 (933.3169)
Raw Mode: Single 0.758(46)
BG Mode: Peak Start 3.510(31)

OPERATOR

S63
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: \Program Files\Thermo Finnigan\Eagar 300 for EA1112\DATA\Sys_data_exa
Sample ID: SRM-123 (# 119)
Analysis type: Unknown
Chromatogram filename: UNK-29112010-19.dat
Sample weight: 1.315

![Chemical Structure](image)

<table>
<thead>
<tr>
<th>Element Name</th>
<th>Element %</th>
<th>Ret. Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>9.15</td>
<td>0.74</td>
</tr>
<tr>
<td>Carbon</td>
<td>74.32</td>
<td>1.12</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.18</td>
<td>3.88</td>
</tr>
</tbody>
</table>
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM176
Inj. Volume: 5.000
Data Name: E:\PROGRAM\LCMSDATA\SRM176-APCI-POS1.qld
Method Name: C:\LCMSsolutionUser\Method\JAY-4-APCI.qlm

LC Chromatogram

MS Spectrum

Operator

6b
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data.exe
Sample ID: SRM-198 (H 72)
Analysis type: UnkNown
Chromatogram filename: UNK-17012011-2.dat
Sample weight: 1.205

![Chemical structure](Image)

<table>
<thead>
<tr>
<th>Element</th>
<th>Name</th>
<th>Element %</th>
<th>Ret. Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>9.89</td>
<td>0.77</td>
<td></td>
</tr>
<tr>
<td>Carbon</td>
<td>73.25</td>
<td>1.17</td>
<td></td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.36</td>
<td>3.77</td>
<td></td>
</tr>
</tbody>
</table>

S76
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM161
Inj. Volume: 5.000
Data Name: C:LCMSolution\UserData\SRM161-APCI-NEG1.qld
Method Name: C:LCMSolution\User\Methods\esi.qml

LC Chromatogram

MS Spectrum

[Graph of MS Spectrum]

MS Peak Table

<table>
<thead>
<tr>
<th>Peak#</th>
<th>R.Time</th>
<th>T.Time</th>
<th>F.Time</th>
<th>Area</th>
<th>Height</th>
<th>A/H Mark</th>
<th>%Total</th>
<th>Name</th>
<th>Base m/z</th>
<th>Base Int</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.319</td>
<td>1.027</td>
<td>1.663</td>
<td>27197339</td>
<td>1515413</td>
<td>17.38</td>
<td>100.00</td>
<td>737.65</td>
<td>796233</td>
<td></td>
</tr>
</tbody>
</table>

OPERATOR
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data.exe
Sample ID: SRM-161 (# 56)
Analysis type: Unknown
Chromatogram filename: UNK-24112010-6.dat
Sample weight: 1.142

<table>
<thead>
<tr>
<th>Element Name</th>
<th>Element %</th>
<th>Ret. Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>7.51</td>
<td>0.89</td>
</tr>
<tr>
<td>Carbon</td>
<td>78.12</td>
<td>1.39</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.65</td>
<td>4.72</td>
</tr>
</tbody>
</table>
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_exa
Sample ID: SRM-172 (54)
Analysis type: UnKown
Chromatogram filename: UNK-24112010-4.dat
Sample weight: 1.128

<table>
<thead>
<tr>
<th>Element Name</th>
<th>Element %</th>
<th>Ret. Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>8.31</td>
<td>0.89</td>
</tr>
<tr>
<td>Carbon</td>
<td>66.38</td>
<td>1.41</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>3.36</td>
<td>4.72</td>
</tr>
</tbody>
</table>

---

6g

S82
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM178
Inj. Volume: 5.000
Data Name: C:\LCMSsolution\User\Data\SRM178-ESI-POS1.qld
Method Name: C:\LCMSsolution\User\Methods\esi.qlm

mAbs
0 500 1000

LC Chromatogram

Ch(t254.0nm)x1.00

min

MS Spectrum

Line#: 1 R.Time: 0.721 (Scan#: 44) Positive
Mass/Peak: 603 BasePeak: 399.40 (2524911)
Ratio Mode: Single 0.72144
Auto Mode: Peak Scan 0.227 (22)

OPERATOR
FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: I:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data.exe
Sample ID: SRM-179 (# 75)
Analysis type: Unknown
Chromatogram filename: UNK-17012011-5.dat
Sample weight: 1.341

<table>
<thead>
<tr>
<th>Element Name</th>
<th>Element %</th>
<th>Ret. Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>7.36</td>
<td>0.88</td>
</tr>
<tr>
<td>Carbon</td>
<td>59.15</td>
<td>1.36</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.61</td>
<td>4.75</td>
</tr>
</tbody>
</table>

6i

56.13
44.63
33.12
21.62
10.11
-1.39
0.0
2.4
4.8
(min)
7.2
9.6
12.0
LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User: Admin
Sample: SRM192
Inj. Volume: 2.000
Data Name: C:\LCMSSolution\User\Data\SRM192-ESI-POSTI.qld
Method Name: C:\LCMSSolution\User\Method\esi.qlm

LC Chromatogram

MS Spectrum

Line#1: R.Time: 0.746 (Scan#45) Positive
Mass/Peak: 672, Base/Peak: 615.56 (2290.57)
Raw Mode: Single 5.746 (45)
DG Mode: Peak Start: 0.527 (32)

OPERATOR
Element Name | Element % | Ret. Time
---|---|---
Nitrogen | 7.45 | 0.77
Carbon | 58.16 | 1.16
Hydrogen | 4.37 | 3.75