SMCC crosslinker, 1H-NMR Analysis, solvent: DMSO-d6

MedKoo Cat#: 610311
Name: SMCC crosslinker
CAS#: 64987-85-5
Chemical Formula: C16H18N2O6
Exact Mass: 334.1165
Molecular Weight: 334.328
SMCC crosslinker, HPLC Analysis

Column: Inertil ODS-3, 5um 4.6*150mm
Mobile phase: Solvent A: H2O(0.05%H3PO4) Solvent B: ACN(0.05%H3PO4)
Temperature: 40 °C
Flow rate: 1mL/min
Run time: 3min gradient(50%B), 15min gradient (50%-95%B), 5min(95%), then 7min @(50%B)
Detector: UV
Wavelength: 220/254 nm
User name: ZJB E-005

Sample description: in ACN
Injection Volume: 4 uL

PeakTable

<table>
<thead>
<tr>
<th>Peak#</th>
<th>Ret. Time</th>
<th>Area</th>
<th>Area %</th>
<th>Theoretical Plate</th>
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<tbody>
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<td>0.162</td>
<td>1212.892</td>
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<td>3.656</td>
<td>3194511</td>
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<td>0.018</td>
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Molecular Weight: 334.328
SMCC crosslinker, LCMS Analysis

Column
Mobile Phase: Solvent A: H2O:FA=99.95:0.05  Solvent B: MeCN
Temperature: 30°C
Flow rate: 0.8 mL/min.
Run time: 3 min @ 40%B, and then 15 min (40-80%B), then 5 min 80%B
Detector: UV
Wavelength: 254/263nm
Scan: Positive/Negative
User name: SZJ
Sample description: 1 mg/ml in MeCN
Data Filename: 101-B.lcd
Method Filename: positive-negative 3min-2.lcm
Vial #: 1-102
Injection Volume: 3 uL

Peak Table

<table>
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<th>Area%</th>
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</tbody>
</table>

MS Chromatogram

MS Spectrum

Peak#: 1  R.Time: 0.845 (Scan#: 72)
Mass Peaks: 494
Spectrum Mode: Averaged 0.825-0.875 (70-74)
BG Mode: Calc Segment 1 - Event 2

Peak#: 1  R.Time: 0.855 (Scan#: 71)
Mass Peaks: 620
Spectrum Mode: Averaged 0.817-0.867 (69-73)
BG Mode: Calc Segment 1 - Event 1