Supporting Information

Peptidal benzotriazolide-mediated acylation of nitrile-activated methylene groups

Sandhyamayee Sahu, a Iryna O. Lebedyeva, a Siva S. Panda, a Alan R. Katritzky * a,b

a Center for Heterocyclic Compounds, Department of Chemistry, University of Florida, Gainesville, Florida, USA 32611-7200

b Chemistry Department, King Abdulaziz University, Jeddah, Saudi Arabia, 21589

Fax: +1-352-392-9199

E-mail: katritzky@chem.ufl.edu

Table of content

1H, 13CNMR spectra, CHN/HRMS, HPLC of compound 8a, 10a, 7a-f, 9a,b, 11a,b and 12a-c
S2-S69
EAGER 200 Stripchart

Sample Ident. : 15 Bocgly38t Filename : 274915

EAGER 200 Peak Integration Report

Instrument name : Instrument #1 Bline drift (fV) : .1
Company Name : U of Florida Operator Ident. : KOU
Sample Ident. : 15 Bocgly38t Filename : 274915
Sample Weight : 2.132 Calc.method: using 'K. Factors'

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<th>No.</th>
<th>Type</th>
<th>Start</th>
<th>End</th>
<th>Ret Time</th>
<th>Height</th>
<th>Area</th>
<th>Area %</th>
<th>Name</th>
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</thead>
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<td>63</td>
<td>99</td>
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<td>90170</td>
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EAGER 200 Unk Report

Instrument name : Instrument #1 Bline drift (fV) : .1
Company Name : U of Florida Operator Ident. : KOU
Sample Ident. : 15 Bocgly38t Filename : 274915
Sample Weight : 2.132 Calc.method: using 'K. Factors'

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Theoretical [M+Na]- = 413.1544
HPLC data of compound 7a
HPLC data of compound 7b
HPLC data of compound 7c

Chromatogram
zero C:\LabSolutions\Data\Sandhya\7c1.lcd

mV

5.180 11.575

7c
HPLC data of compound 7d
HPLC data of compound 7e
HPLC data of compound 7f
HPLC data of compound 9a
Theoretical [M+Na]+ = 427.1377

[M+H+2Na]+ = 449.1196

ESI scan at 2.27702724 m/z corona flow = 18.00 V 180°C 5.00e-5 L/min
HPLC data of compound 9b
HPLC data of compound 11a
M+H = 585.1726
Theoretical [M+H]^+ = 563.1901
HPLC data of compound 11b
HPLC data of compound 12a
HPLC data of compound 12b

Chromatogram
MeOH C:\LabSolutions\Data\Sandhya'2054_12b1.lcd

Det. A Ch1

1 Det. A Ch1 / 254nm
HPLC data of compound 12c

Chromatogram
MeOH C:\LabSolutions\Data\Sandhya\2054_12c1.led
det A Ch1

1 Det.A Ch1 / 254nm