Supporting information

Synthesis and aromatisation of cyclic enediyne-containing amino acids

Jasper Kaiser, Bart C. J. van Esseveldt, Margot J. A. Segers, Floris L. van Delft, Jan M. M. Smits, Sam Butterworth and Floris P. J. T. Rutjes

* Institute for Molecules and Materials, Radboud University Nijmegen, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands. Fax: +31 24 365 3393; Tel: +31 24 365 3202; E-mail: F.Rutjes@science.ru.nl
‡ AstraZeneca R&D, Alderley Park, Macclesfield, Cheshire SK10 4TG, United Kingdom.

Contents

\(^{13}\)C-NMR and / or \(^{1}\)H-NMR spectra of compounds 14-19, 23-26, 28, 29, 31-36.
75 MHz
CDCl3

HN
COOCH₃

14

OH
300 MHz
CDCl₃

16

HN

COOCH₃

O

Ms

Ts

H

N

300 MHz
CDCl₃
75 MHz
CDCl₃

TsHN

CO₂Me

17
75 MHz
CDCl₃

18

HN
COOCH₃

HN
Ts

170.374
143.575
136.956
132.126
131.969
129.576
127.952
127.315
127.153
126.202
124.941
93.826
86.470
83.009
80.109
77.000
61.865
54.325
52.818
31.070
24.886
21.469
16.325

135.0
130.0
125.0

125.0
130.0
135.0

ppm (t1)

ppm (t1)
300MHz
CDCl3

N-Ts

COOCH₃

19
75 MHz
CDCl₃

HN
COOCH₃

OH

Ts

HN

COOCH₃

23
300 MHz
CDCl3

HN

COOCH₃

Ts

OH

25
300 MHz
CDCl₃

[Chemical structure image]

26

ppm (t1)
$75 \text{ MHz}$
$\text{CDCl}_3$

$\text{TsHN}$
$\text{CO}_2\text{Me}$

Diagram of a molecular structure labeled as 28.
300 MHz
CDCl₃

TsHN
CO₂Me

28
75 MHz
CDCl3

N-Ts

COOCH₃

29
75 MHz
CDCl3

[Chemical structure image]

32
300 MHz
CDCl3

TsHN

COOCH₃

32
75 MHz
CDCl3

![Chemical Structure](image)

| ppm (t1) | 171.694 | 143.589 | 137.838 | 129.730 | 126.973 | 122.629 | 120.096 | 99.377 | 90.955 | 86.716 | 81.791 | 77.000 | 57.104 | 52.227 | 41.850 | 32.966 | 21.518 | 19.055 |
|----------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|

33
<table>
<thead>
<tr>
<th>ppm (t1)</th>
<th>171.631</th>
<th>143.561</th>
<th>137.686</th>
<th>129.682</th>
<th>128.221</th>
<th>127.509</th>
<th>127.095</th>
<th>126.889</th>
<th>125.956</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 MHz</td>
<td>CDCl3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

![NCO2Me](image)

34
300 MHz
CDCl₃

CO₂Me

34
75 MHz
CDCl₃

35

NTs
COOCH₃
400 MHz
CDCl₃

36

7.786 7.754 7.730 7.704
7.786 7.754 7.730 7.704
7.786 7.754 7.730 7.704
7.786 7.754 7.730 7.704
7.786 7.754 7.730 7.704
7.786 7.754 7.730 7.704


1.00 1.04 1.05 1.01 2.03 2.05
1.00 1.04 1.05 1.01 2.03 2.05
1.00 1.04 1.05 1.01 2.03 2.05
1.00 1.04 1.05 1.01 2.03 2.05
1.00 1.04 1.05 1.01 2.03 2.05
1.00 1.04 1.05 1.01 2.03 2.05

7.786 7.754 7.730 7.704
7.786 7.754 7.730 7.704
7.786 7.754 7.730 7.704
7.786 7.754 7.730 7.704
7.786 7.754 7.730 7.704
7.786 7.754 7.730 7.704

7.507 7.486 7.463 7.421
7.507 7.486 7.463 7.421
7.507 7.486 7.463 7.421
7.507 7.486 7.463 7.421
7.507 7.486 7.463 7.421
7.507 7.486 7.463 7.421