A serendipitous formation of a cysteine-bridged disaccharide

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1. <sup>1</sup>H, <sup>13</sup>C, COSY, HMQC spectra of bridged disaccharides 6 and 7

2. High resolution mass spectra of bridged disaccharides 6 and 7

## Instruments and spectra

<sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on Varian Gemini 400 at ambient temperature, in CDCl<sub>3</sub>. The splitting patterns are reported as follows: singlet (s), doublet (d), triplet (t), doublet of doublets (dd), multiplet (m) and broad singlet (br s). High resolution mass spectra were obtained on a Waters Synapt G2 mass spectrometer in the positive mode.

Figure 1: <sup>1</sup>H NMR spectrum of compound 6











Figure 6: <sup>13</sup>C NMR spectrum of compound 7









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Single Mass Analysis Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron Ions 449 formula(e) evaluated with 68 results within limits (all results (up to 1000) for each mass) Elements Used:	•
Mare Cale Mare mDa DDM DBE Bormula LETT LETT Norm Eli-Conf % C H N O S	×
Mass         Cat. Mass         Initial         PMI         Doc         Portugat         PMI         PMI	
824.2296       -2.8       -3.4       1.5.       C30       140.630       62.75       27.6.       10.600       20       46       3       23       1         824.2296       -2.8       -3.4       1.5.       C30       140.800       62.77       0.19       34       42       5       17       1         824.2392       -3.4       -4.1       -1.5       C21       H50       N3       228       1       10       142       5       17       1         824.2224       4.4       5.3       2.3.       C40       H12       N 0.65       273.0       11.253       0.00       10       42       1       16         824.2230       6.5       7.9       3.5       C20       H46       N5 025       275.6       13.060       0.00       23       46       5       25       1         824.2337       -6.9       -8.4       20.5       C39       H42       N 0.05       277.1       1.029       0.00       39       42       3       15       1         824.2342       -7.4       -9.0       2.5       C26       10.00       26       50       1       26       1         824.2189 <td>8</td>	8
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7/0 7/5 780 786 790 795 800 805 810 815 820 825 830 835 840 845 850 855 860 865 870 875 880 885 890 895 900 905 910 915 920 925 930 935 940 94 For Help, press F1	950
GMN-025F MN_TUT_120207_2b 88 (0.403) Cm (88:97-11:16) 1: <sup>1</sup>	OF MS ES+
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Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0	
Element prediction: Off Number of isotope peaks used for i-FIT = 3	
Monoisotopic Mass, Even Electron Ions	
1315 formula(e) evaluated with 189 results within limits (all results (up to 1000) for each mass) Elements Used:	
Mass Calc. Mass mDa PPM DBE Formula I-FIT I-FIT Norm Fit Conf % C H N O S	
767.2030 0.7 0.9 33.5 C47 H31 N2 09 111.3 5.206 0.55 47 31 2 9 767.2045 40.8 1.0 41.5 C56 H31 02 S 113.4 7.251 0.07 56 31 2 1	
767.2028 0.9 1.2 6.5 C26 H43 N2 022 5 110.8 4.730 0.88 26 43 2 22 1 767.2028 1.6 21 25 C29 H43 N2 022 5 110.8 4.730 0.88 26 43 2 22 1	
767.2013 2.6 3.4 46.5 C29 H27 02 112.5 6.337 0.18 59 27 2	
767.2003 2.6 5.4 28.5 CH H35 R2 09 5 112.5 5.391 5.17 14 35 2 9 1 767.2010 2.7 3.5 19.5 C3 H39 015 5 111.1 4.990 0.68 38 39 15 1	
767.2005 3.2 4.2 37.5 C51 H31 N2 O4 5 113.3 7.140 0.08 51 31 2 4 1	
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666.1486 683.1262 708.1888 760.3112	
684.1226 725.1985 742.2170	814 2014 849,2182 855.2077
621.1341 644.1264 665.1565 693.1494 732.6994 743.2242 770.1964 786.2392	5.1566 839.1853 856.2128
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437.1118	900 2425
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δ <sup>φ</sup>	
	895.1969
271.0812	
257.0485 332.1058 455.1418	896.2008
456.0855	
170.0532	911.1721
139.0393 212.0646 272.0844 272.0844 272.0844 377.0901 419.3161 515.1242 542.1404 674.1371 707.1863 1813.1956	912.1748
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