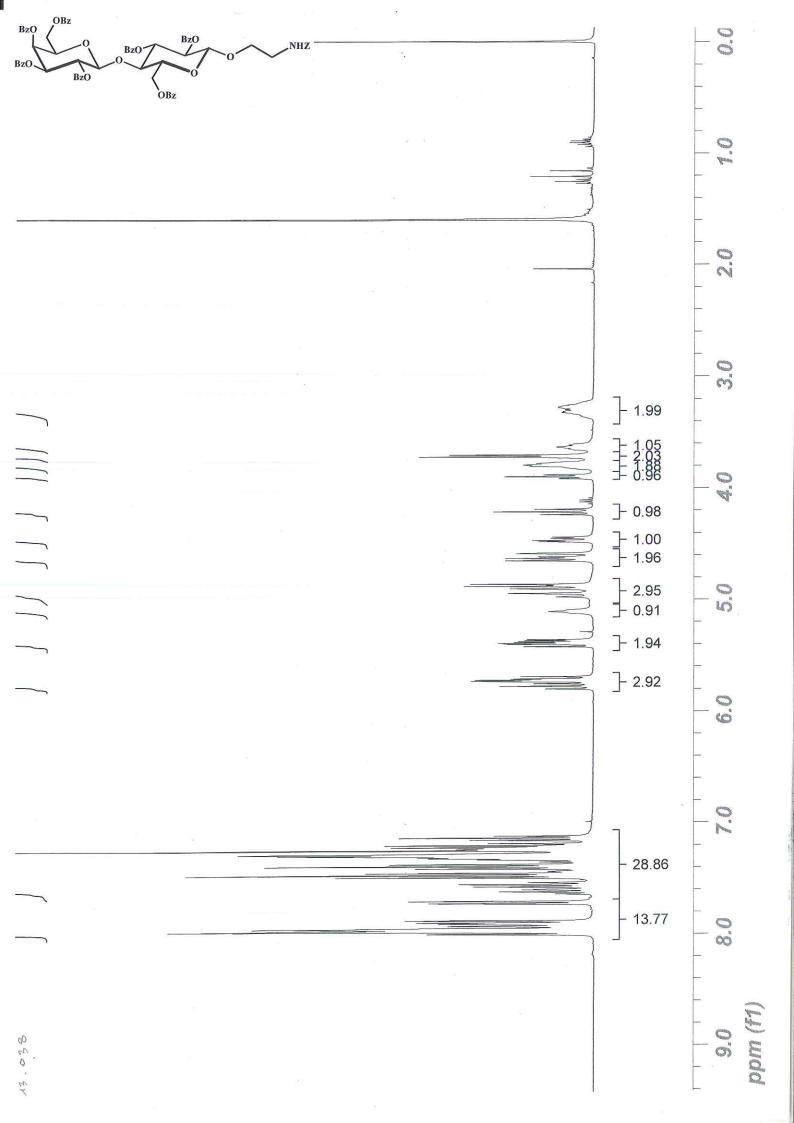
Electronic Supplementary Material (ESI) for ChemComm. This journal is © The Royal Society of Chemistry 2020 0.0 BzO BzO, • BzO BzO NHZ BzO OBz 1.0 2.0 3.0]- 2.06]- 1.00]- 1.03]- 1.02 4.0]- 1.06]- 3.09]- 2.11]- 3.03]- 0.91]- 2.08 5.0 - 1.05 - 2.03 6.0]- 1.00 7.0 - 32.37 12.46 8.0 9.0) widd 420.51



Fédération de Recherche Physique et Chimie du Vivant (FR2708 : CBM/ICOA) HRMS Plate-forme de Spectrométrie de Masse Haute Résolution

Analysis Info Acquisition Date 12/09/2012 15:59:11 Sample Name JCJ.13.037 X005057CYC.d Laboratory Analysis Name 255552.00 Method Instrument / Ser# maXis Positif.m 086 **Acquisition Parameter** Set Nebulizer 0.6 Bar Positive Ion Polarity Source Type ESI 200 °C Focus Not active Set Capillary 4500 V Set Dry Heater 7.0 l/min Scan Begin Set End Plate Offset -500 V Set Dry Gas 50 m/z 3000 m/z Set Collision Cell RF 1000.0 Vpp Set Divert Valve Waste Scan End +MS, 0.34-0.38min #20-22, Background Subtracted Intens. x10⁵ 0.8 1+ 1248.3865 0.6 0.4 1+ 0.2 1053.2962 475.1385579.1657 0.0 1000 1200 200 600 800 m/z 400 Intens. 1248,3865 +MS, 0.34-0.38min #20-22, Background Subtracted x104 1 +1249.3899 4 3 1+ 1250,3935 2 1+ 1+ 1252,3979 1 1251.3954 ×109 1248,3860 C71H62NO20, 1248.3865 1 +1249.3893 4 3 1+ 1250.3924 2 1+ 1251.3953 1 1+ 1252.3982 0 1252 1248 1249 1250 1251 1253 1254 1255 m/z e^{Conf} rdb N-Rule Ion Formula err [ppm] mSigma Meas. m/z # m/z C34H27O9 579.164959 -1.3 24.2 21.5 579.165713 even ok 1 8.2 1053.296427 0.3 37.5 1053.296162 ok 1 C61H49O17 even C63H170NO7 1053.297183 1.0 15.2 -20.5 ok 2 even 1053.295913 -0.2 68.3 55.5 3 C74H41N2O6 even ok 1248.386455 C71H62NO20 1248.385970 -0.4 14.2 41.5 even ok 1 1248.386726 28.1 2 C73H183N2O10 0.2 -16.5 even ok 3 C85H179O3 1248.384876 -1.389.8 -3.5 even ok C71H65N2O20 1265.412519 -0.3 11.1 40.5 ok 1265.412862 even 1 0.3 24.5 1265.413276 -17.5 ok 1 C73H186N3O10 even C85H182NO3 1265.411425 -1.1 86.1 -4.5 even ok 1 1270.367914 C71H61NNaO20 -0.3 31.8 41.5 ok - 1270.368237 even 1 C73H182N2NaO10 1270.368671 0.3 23.8 -16.5 even ok 1 1270.366820 50.8 ok C85H178NaO3 -1.1 -3.5 even 1

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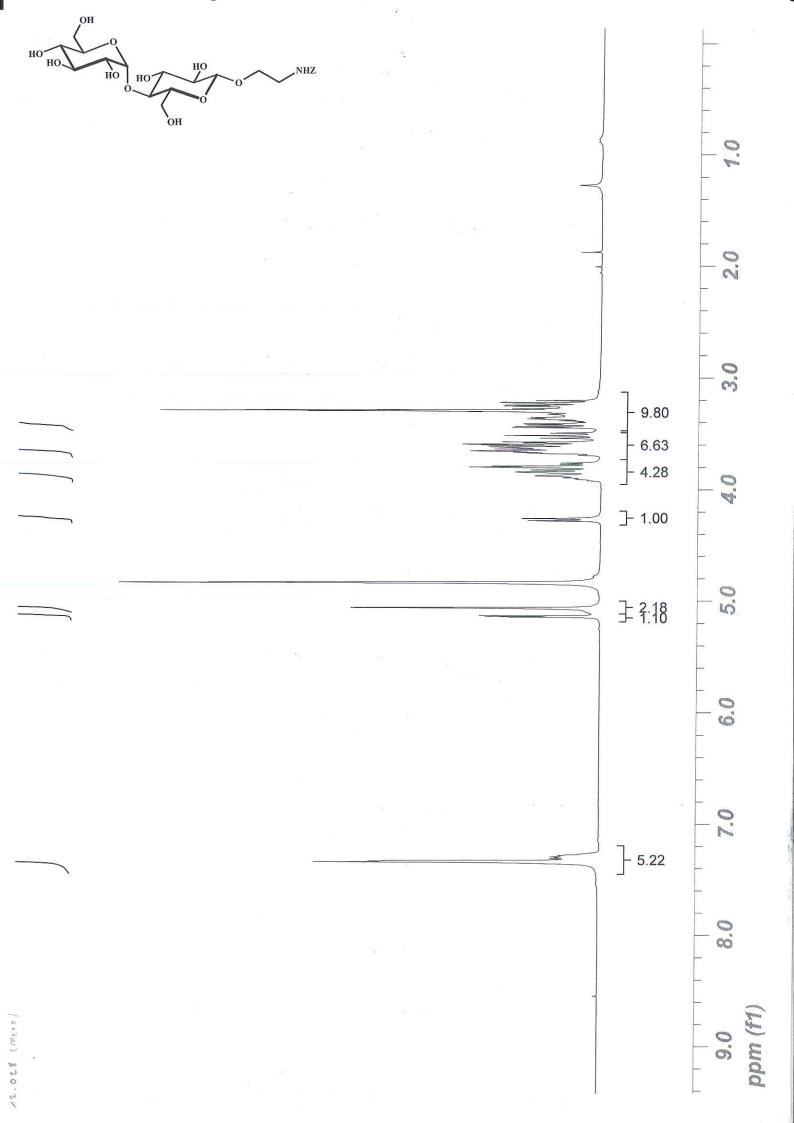


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HRMS

Analysis Info Sample Name Analysis Name Method	JCJ.13.038 X005058CYC.d Positif.m				Labor			255552.00
Acquisition Para Source Type Focus Scan Begin Scan End	ESI Not active 50 m/z 3000 m/z	Set End Pla	lon Polarity Set Capillary Set End Plate Offset Set Collision Cell RF		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve		ater B	086 0.6 Bar 200 °C 7.0 I/min Waste
Intens. ×105 2.0 1.5 1.0					+MS, 0.	34-0.39min -		kground Subtracted 1+ 8.3869
0.5		1+ 475.1387579.1649		L	1053,29		69	
	200	400	600	800		1000	1200	m/z
x10 ⁵ 1.00 0.75 0.50 0.25	1248,386	1+ 1249.3904	1+ 1250.3931	1+ 1251.3955 人	1- 1252.	÷	. 20 20, 044	kground Subtracted
0.00 ×103 1.25 1.00 0.75	1248,386	0 1+ 1249.3893					C71	H62NO20, 1248.3865
0.50 0.25			1+ 1250.3924	1+ 1251.3953 ∧	1- 1252,			
0.00	1248	1249 12	50	1251	1252	1253	125	j4 m/z
Meas. m 670.22759 1248.38690 1265.41348	01 1 C37H36NO1 07 1 C71H62NO2 2 C73H183N20 3 C85H179O3	1 670.228283 0 1248.385970 010 1248.386720 1248.384870 1248.384870 20 1265.412519 010 1265.413270	7 -(6 -(6 -(6 -(m] mSigma 1.0 10.1 0.8 8.9 0.1 23.4 1.6 84.5 0.8 4.7 0.2 19.0 1.6 79.5	rdb 20.5 41.5 -16.5 -3.5 40.5 -17.5 -4.5	e Conf even even even even even even even	N-Rule ok ok ok ok ok ok	19

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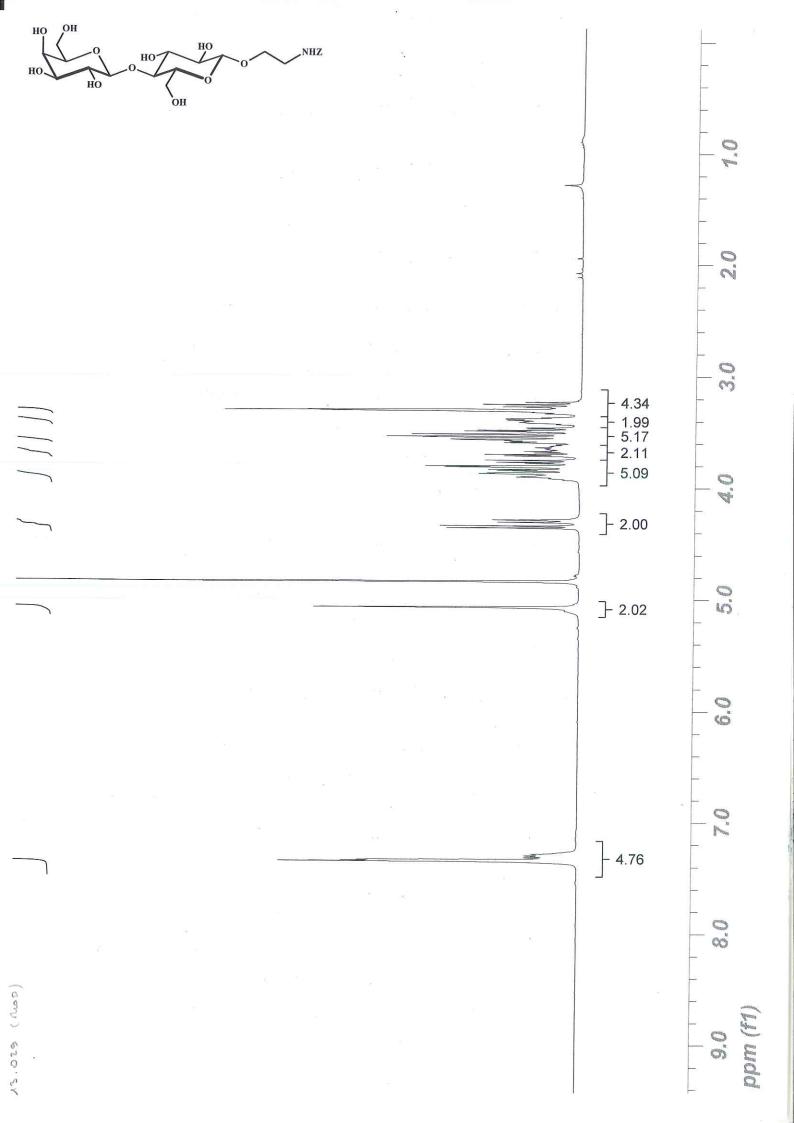
Fédération de Recherche Physique et Chimie du Vivant (FR2708 : CBM/ICOA) Plate-forme de Spectrométrie de Masse Haute Résolution

Analysis Info Acquisition Date 20/06/2012 13:24:05 Sample Name JCJ13.028 Analysis Name X004321CYC.d Laboratory Method Positif.m Instrument / Ser# maXis 255552.00 086 **Acquisition Parameter** Source Type ESI Ion Polarity Positive Set Nebulizer 0.6 Bar Focus Not active Set Capillary 4500 V 200 °C Set Dry Heater Set End Plate Offset Scan Begin 7.0 l/min 50 m/z -500 V Set Dry Gas 3000 m/z Scan End Set Collision Cell RF 1000.0 Vpp Set Divert Valve Waste Intens. +MS, 0.07-0.87min #4-51, -Peak Bkgrnd x105 1+ 520.2018 1.0 1+ 196.0972 0.5 1+ 152.1072 358.1494 0.0 100 200 300 400 500 600 m/z Intens. 1, x10⁴ 520.2018 +MS, 0.07-0.87min #4-51, -Peak Bkgrnd 6 4 1+ 521,2050 2 1 +522.2069 ×104 1. 520,2025 C22H34NO13, 520.2030 6 4 1+ 521.2058 2 1 +522.2080 0 520 519 521 522 523 524 m/z mSigma Meas. m/z # Ion Formula m/z err [ppm] rdb e^COnf N-Rule 196.097168 C10H14NO3 1 196.096820 -1.8 0.5 4.5 even ok 358.149369 1 C16H24NO8 358.149643 0.8 2.2 5.5 even ok 520.201820 C22H34NO13 520.202467 1.2 3.1 6.5 1 even ok 542.183153 C22H33NNaO13 2.3 29.0 1 542.184411 6.5 even ok

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> cyril.colas@univ-orleans.fr +33 (0)2 38 49 46 61

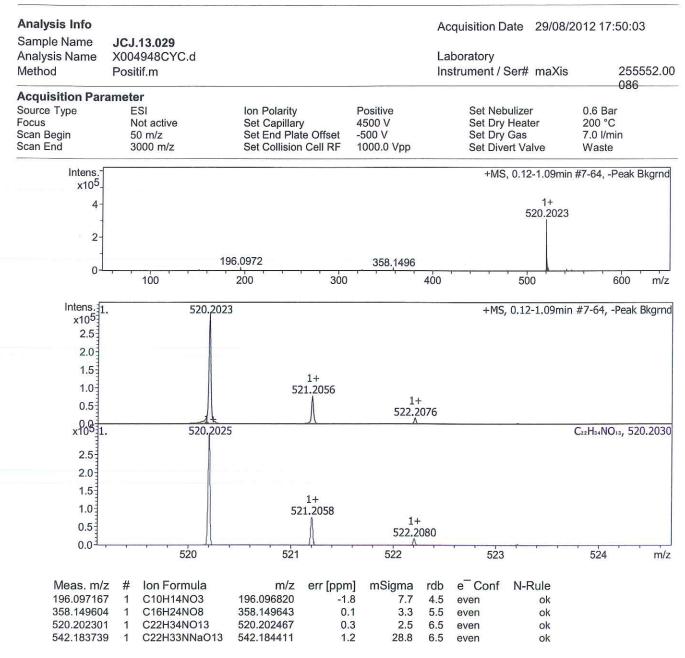
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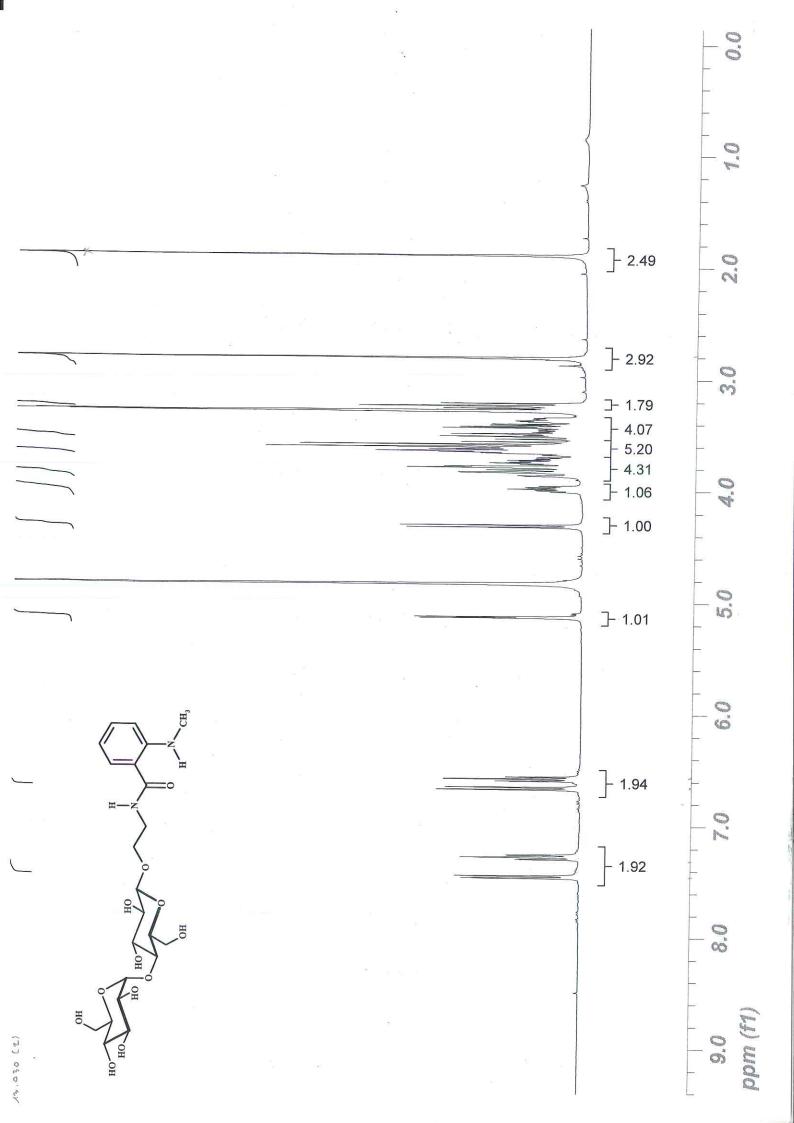


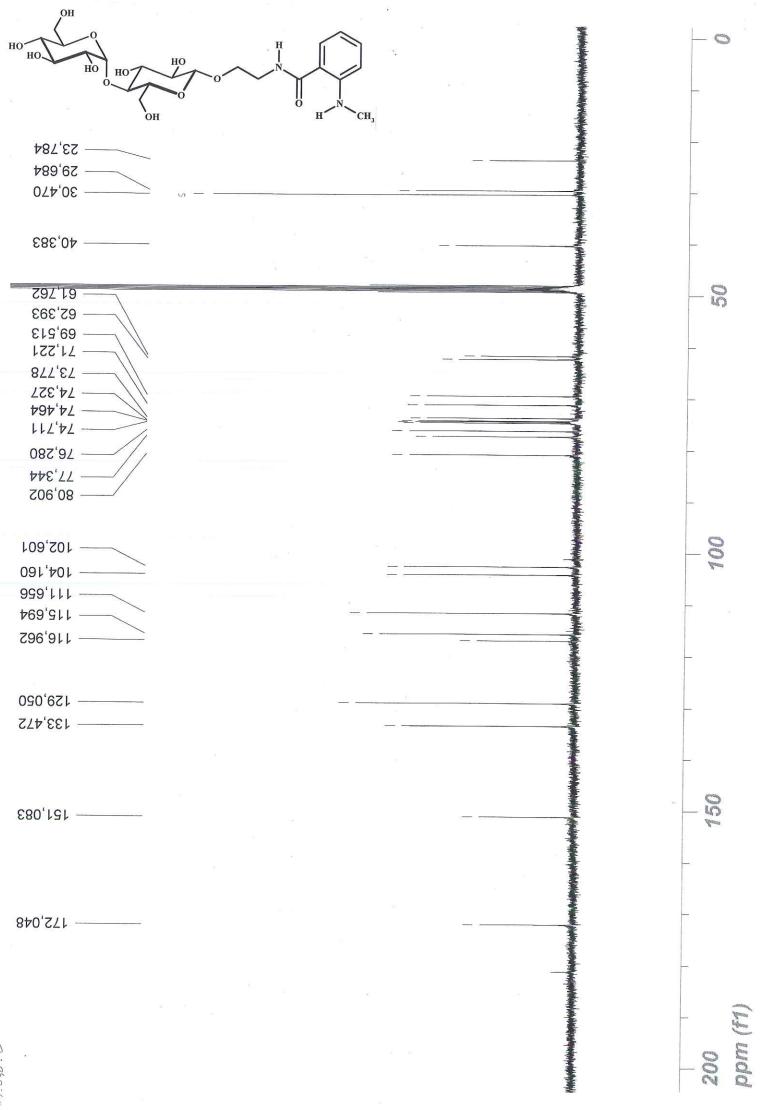
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HRMS



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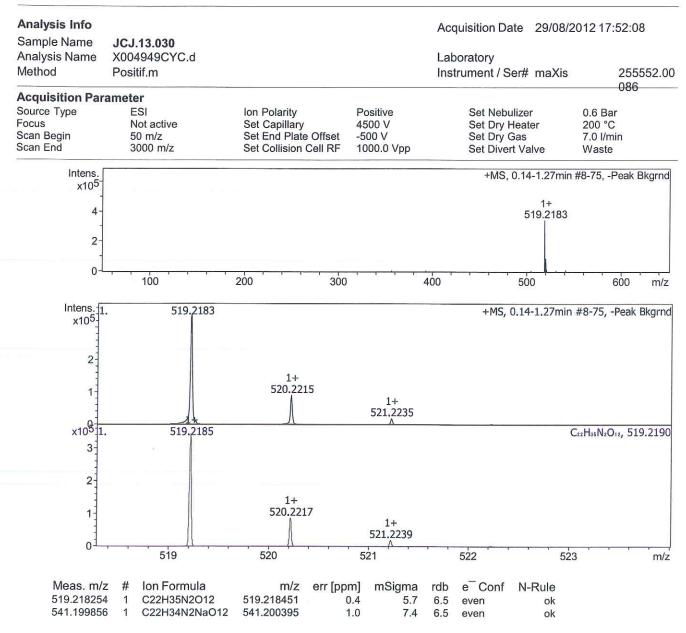


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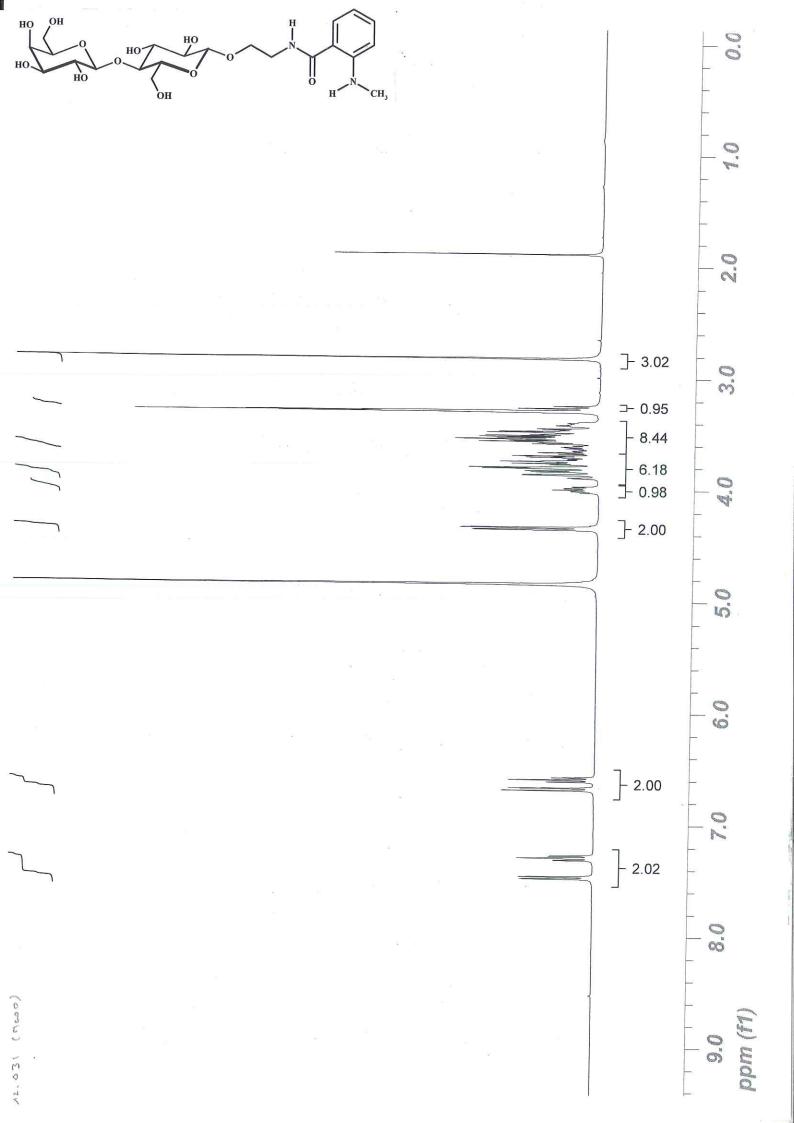
HRMS

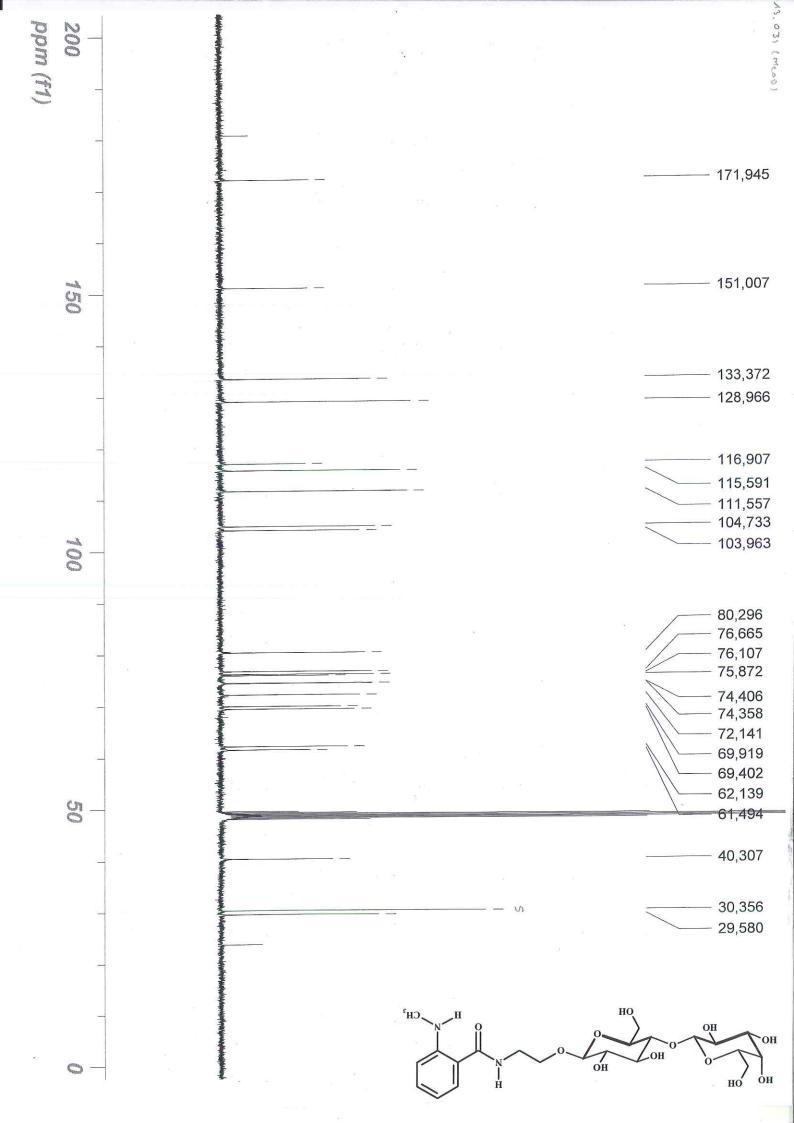


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Fédération de Recherche Physique et Chimie du Vivant (FR2708 : CBM/ICOA) HRMS Plate-forme de Spectrométrie de Masse Haute Résolution

Acquisition Date 29/08/2012 17:54:13 Analysis Info Sample Name JCJ.13.031 Laboratory X004950CYC.d Analysis Name Instrument / Ser# maXis 255552.00 Method Positif.m 086 **Acquisition Parameter** 0.6 Bar 200 °C Set Nebulizer Source Type Ion Polarity Positive ESI Set Capillary 4500 V Set Dry Heater Not active Focus -500 V 7.0 l/min Set End Plate Offset Set Dry Gas Scan Begin 50 m/z Waste 1000.0 Vpp Set Divert Valve Scan End 3000 m/z Set Collision Cell RF +MS, 0.10-1.01min #5-59, -Peak Bkgrnd Intens. x105 3-1+ 519.2182 2 1-299.2936 357.1657 0 500 600 m/z 200 300 400 100 Intens. 1. x10⁵ +MS, 0.10-1.01min #5-59, -Peak Bkgrnd 519,2182 1.5 1.0 1+ 520.2213 0.5 1+ 521.2233 ×103 C22H35N2O12, 519.2190 519.2185 1. 2.0 1.5 1.0 1+ 520.2217 0.5 1+ 521.2239 0.0 522 523 m/z 521 519 5<u>2</u>0 e^COnf N-Rule rdb Meas. m/z # Ion Formula m/z err [ppm] mSigma 3.8 6.5 ok 519.218451 0.5 even C22H35N2O12 519.218216 1 C22H34N2NaO12 541.200395 1.2 29.8 6.5 even ok 541.199739 1

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