

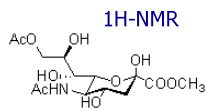
Supplementary Data

Elucidation of several neglected reactions in the GC-MS identification of sialic acids as heptafluorobutyrate calls for an urgent reassessment of previous claims

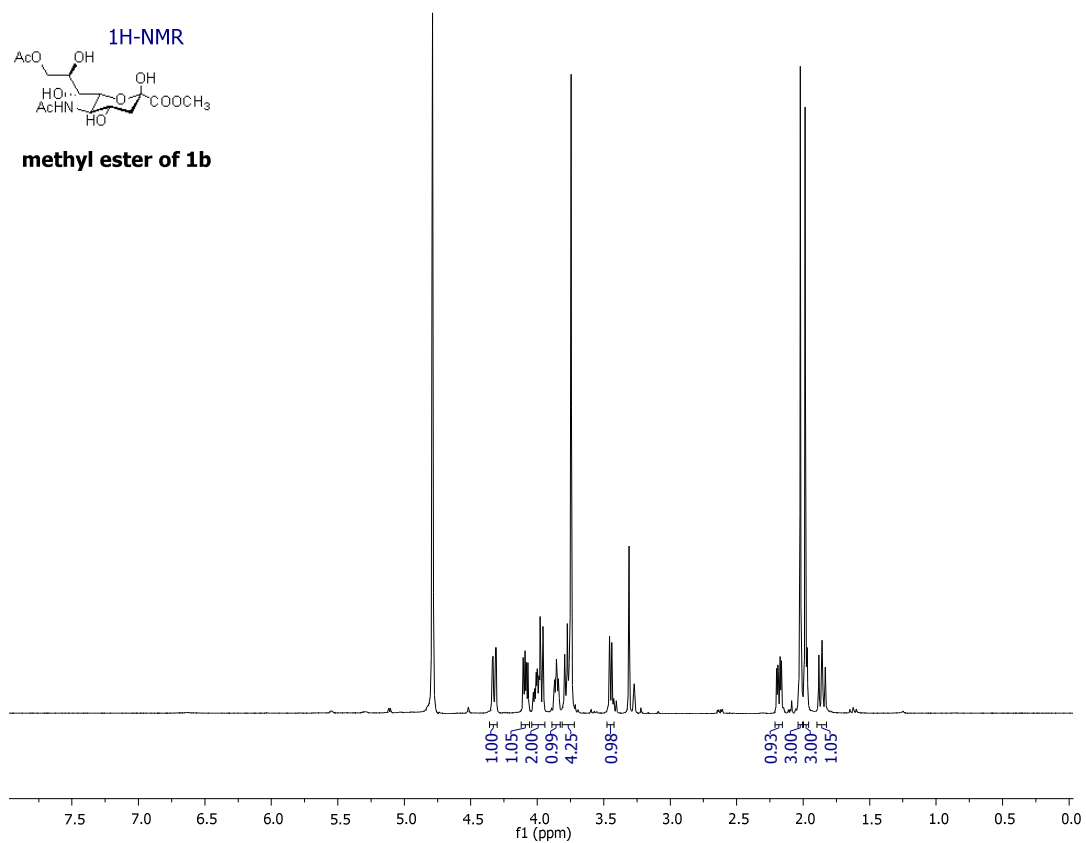
Paola Rota*, Luigi Anastasia, Pietro Allevi

Department of Biomedical, Surgical and Dental Sciences, University of Milan, via Saldini 50, I-20133 Milan, Italy; corresponding author: Paola Rota; Telephone: +39 02 50316047; Fax: +39 02 50316040; E-mail: paola.rota@unimi.it

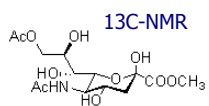
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methyl ester of 1b



175.1
173.1
171.7



methyl ester of 1b

96.7

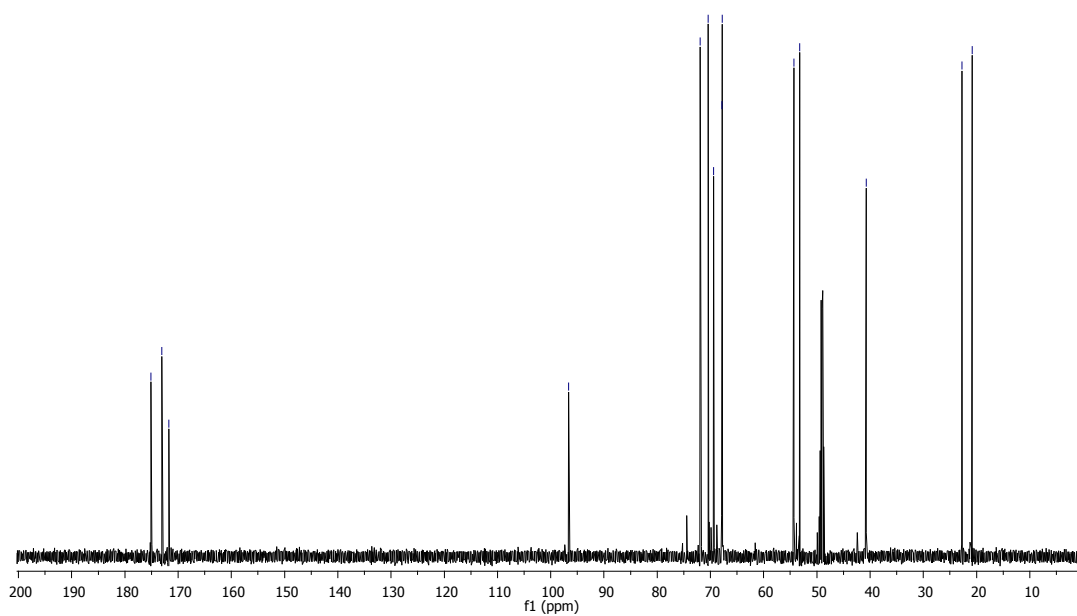
71.9
70.4
69.4

67.8
67.8

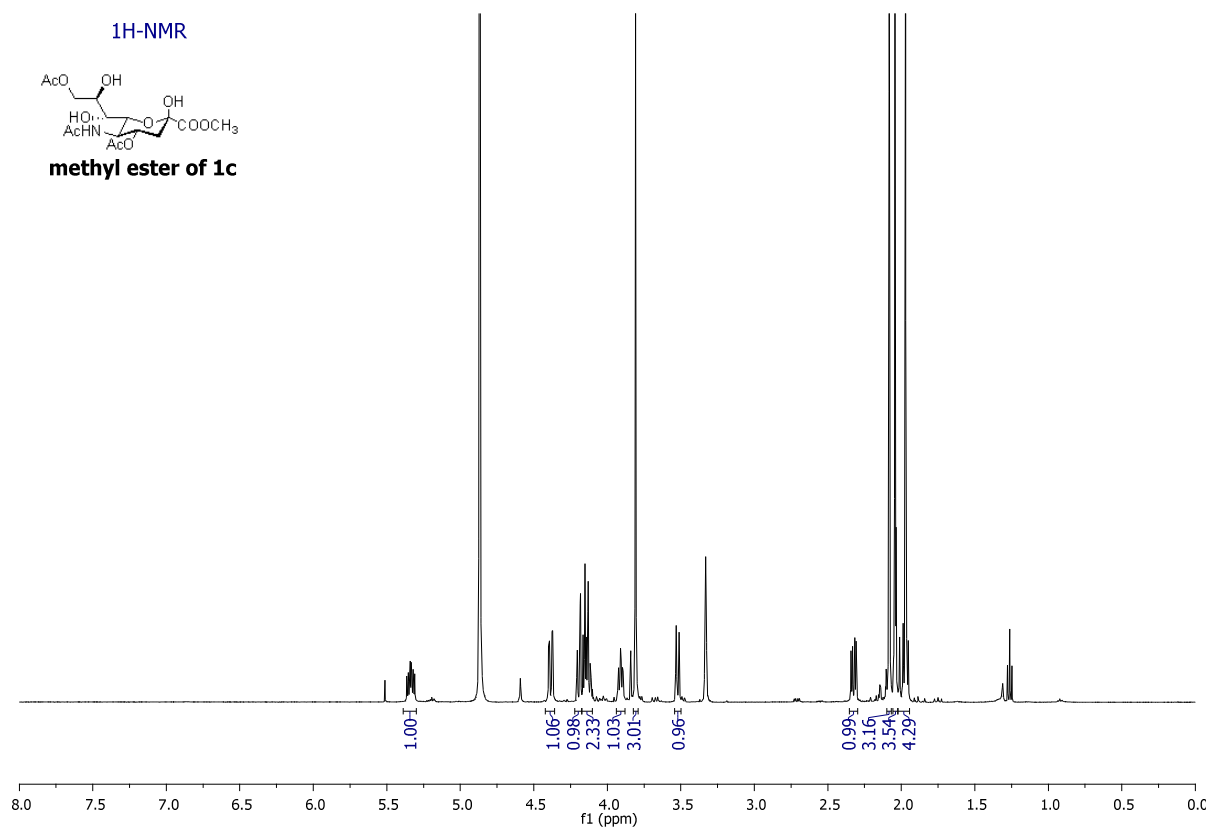
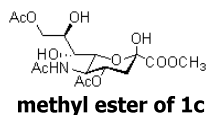
54.3
53.2

40.7

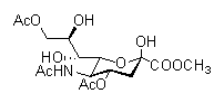
22.7
20.8



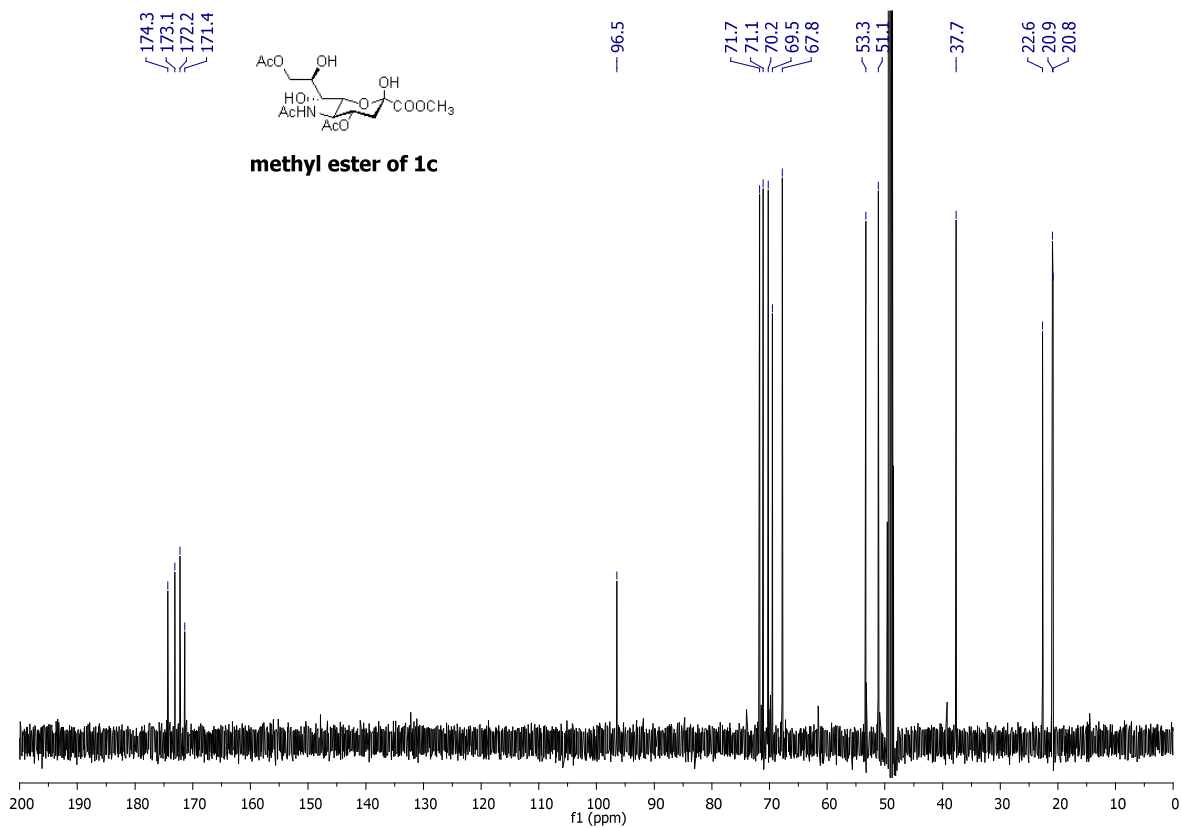
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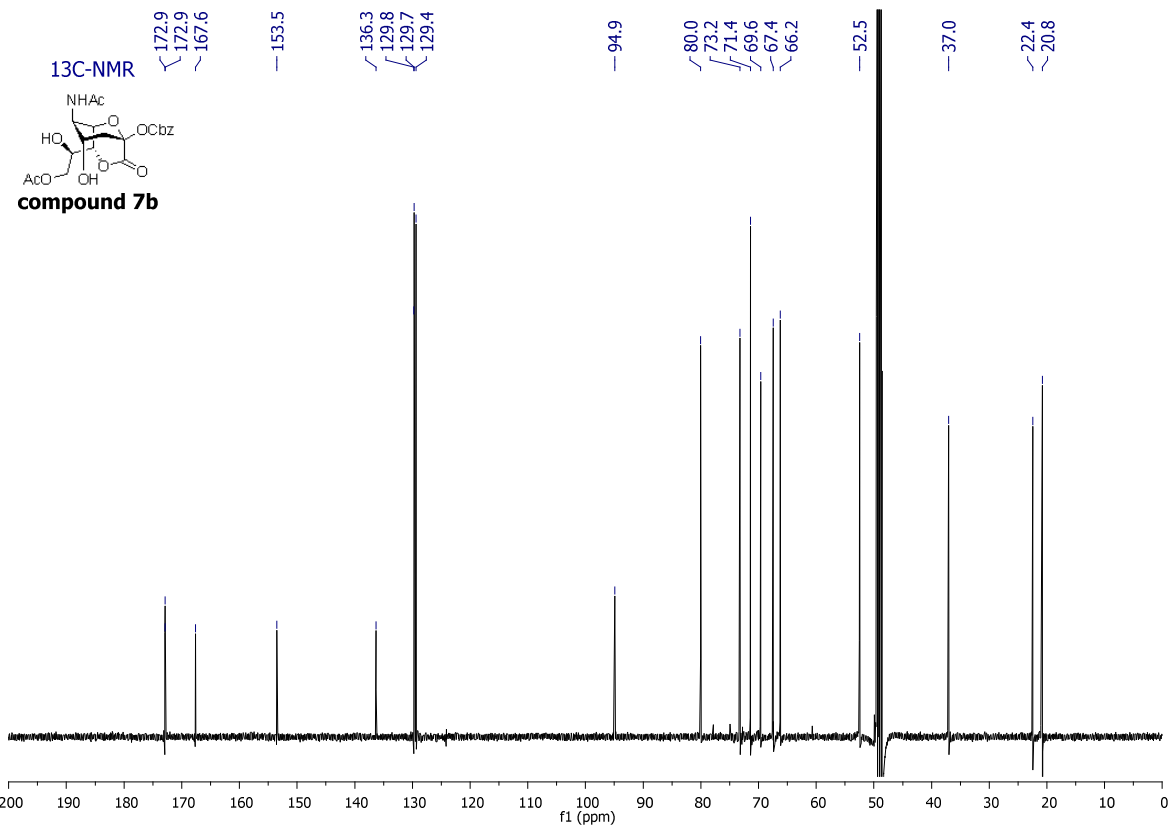
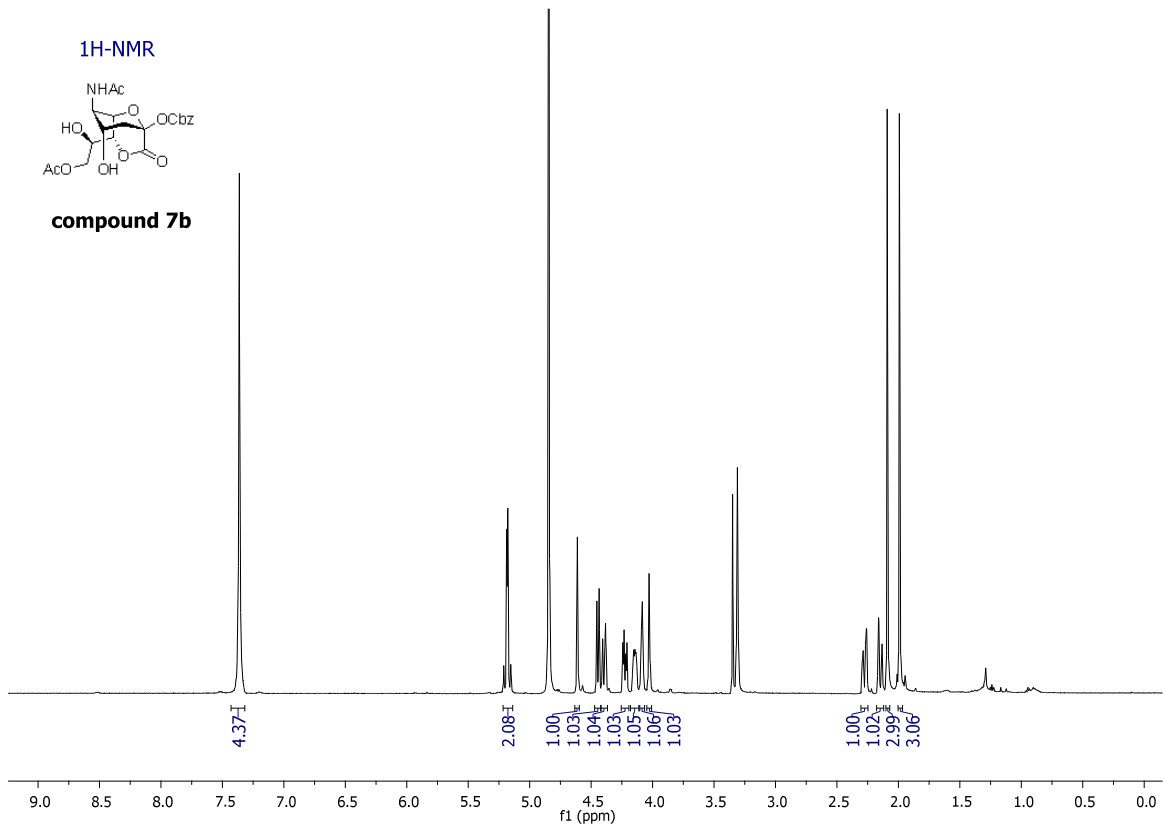
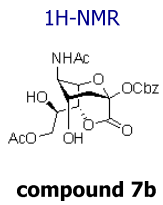


174.3
173.1
172.2
171.4

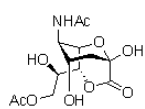


methyl ester of 1c

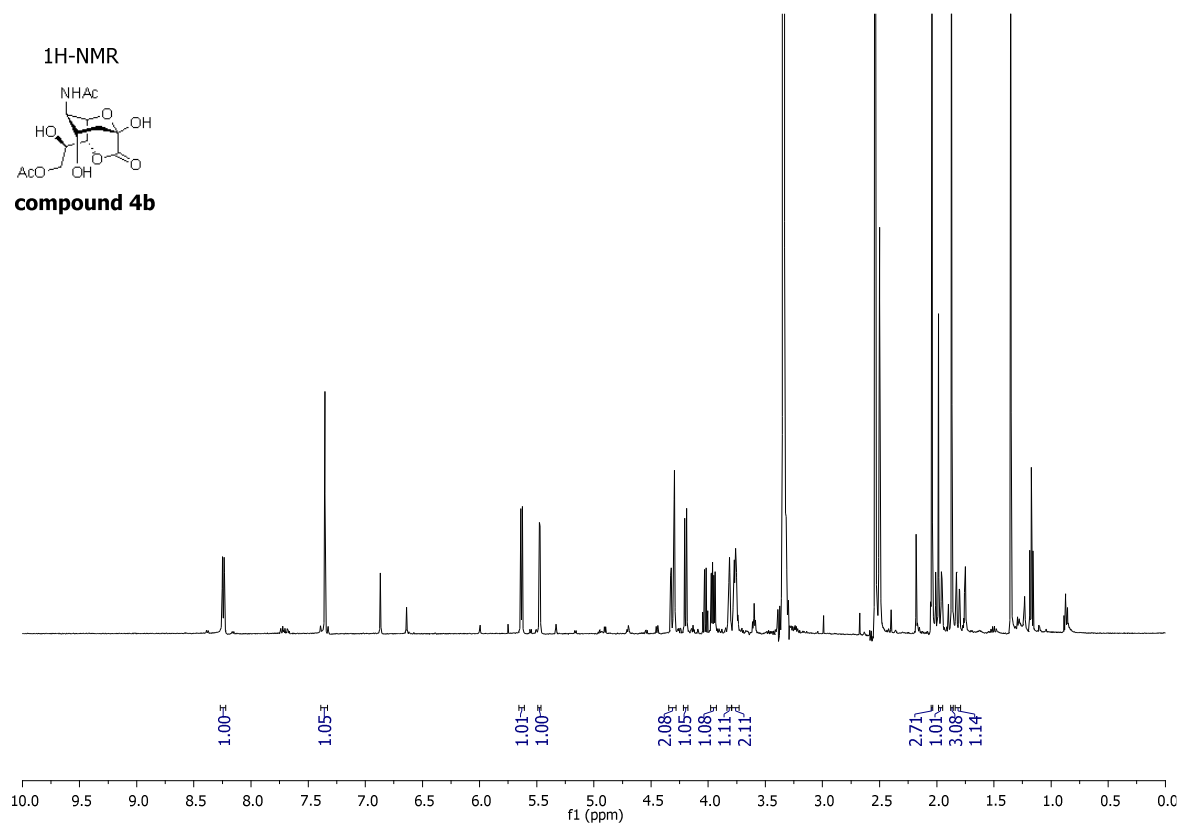




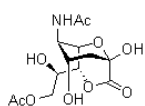
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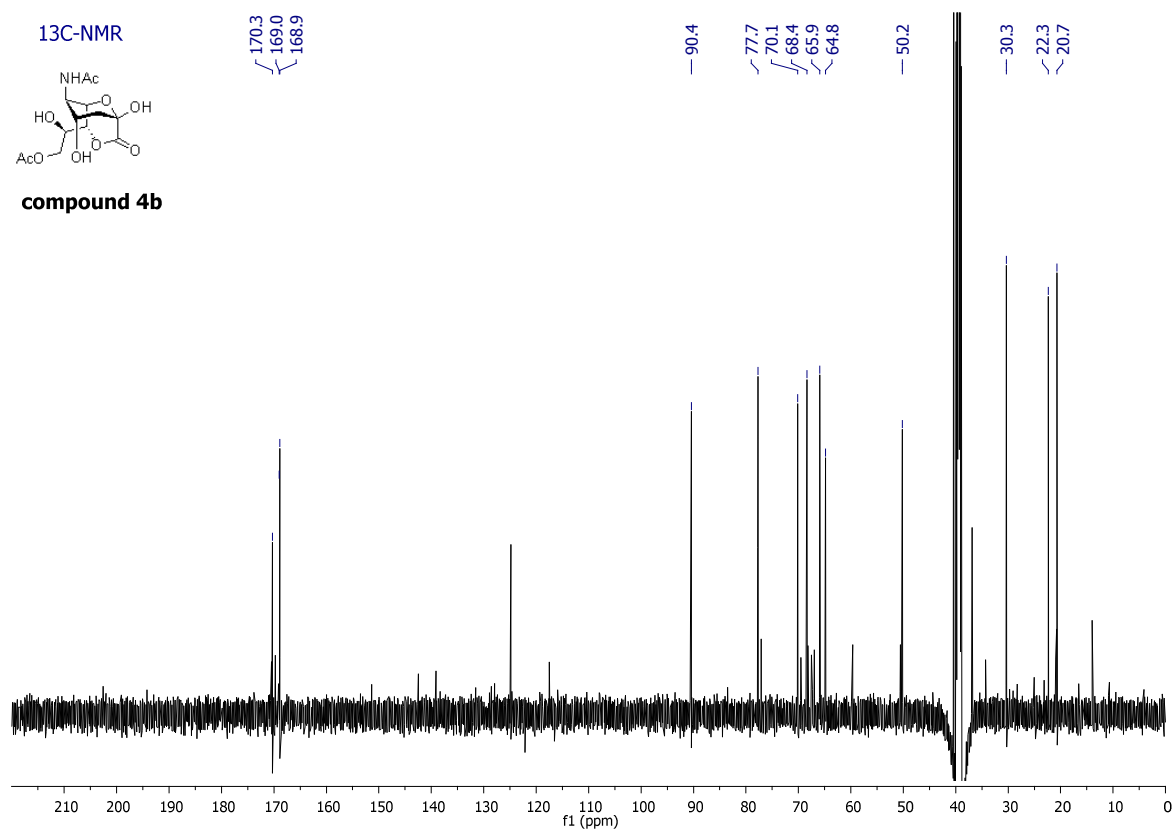
compound 4b



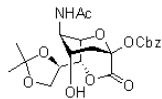
13C-NMR



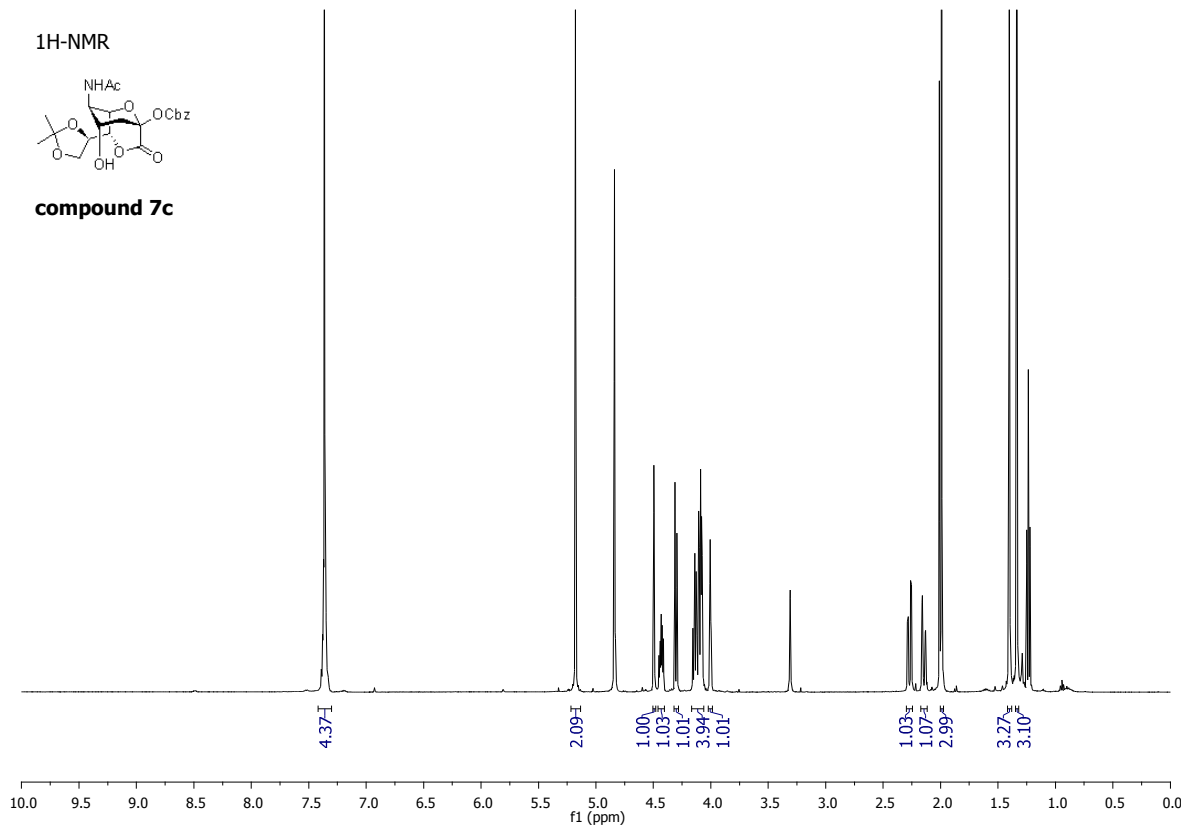
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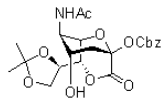
¹H-NMR



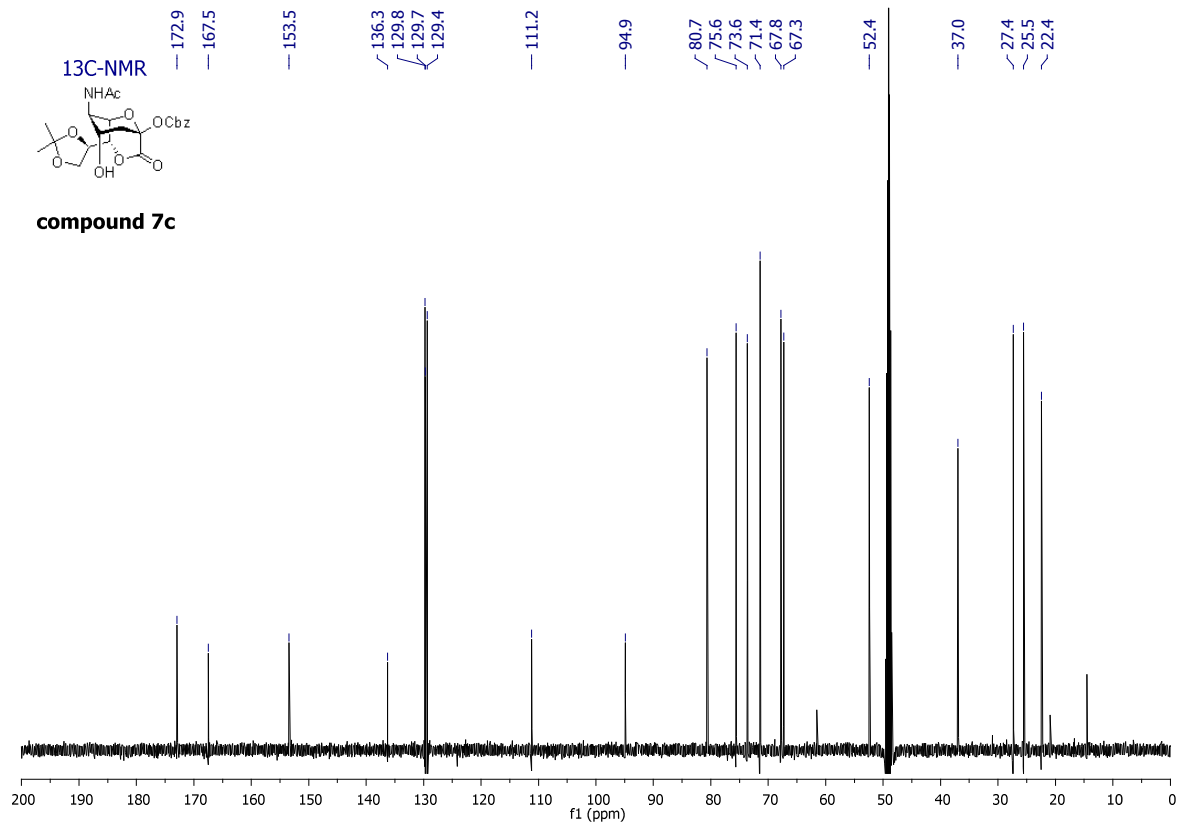
compound 7c



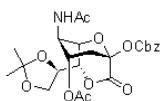
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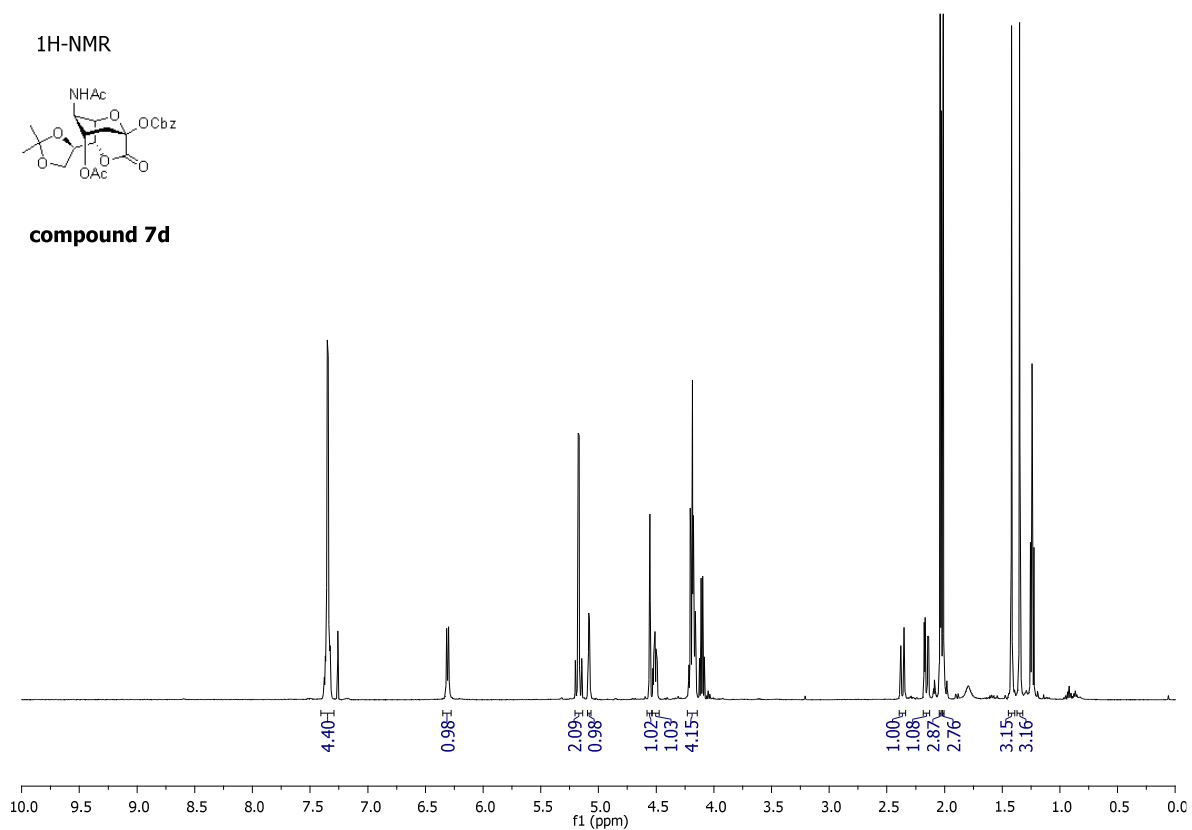
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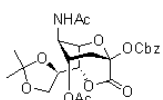
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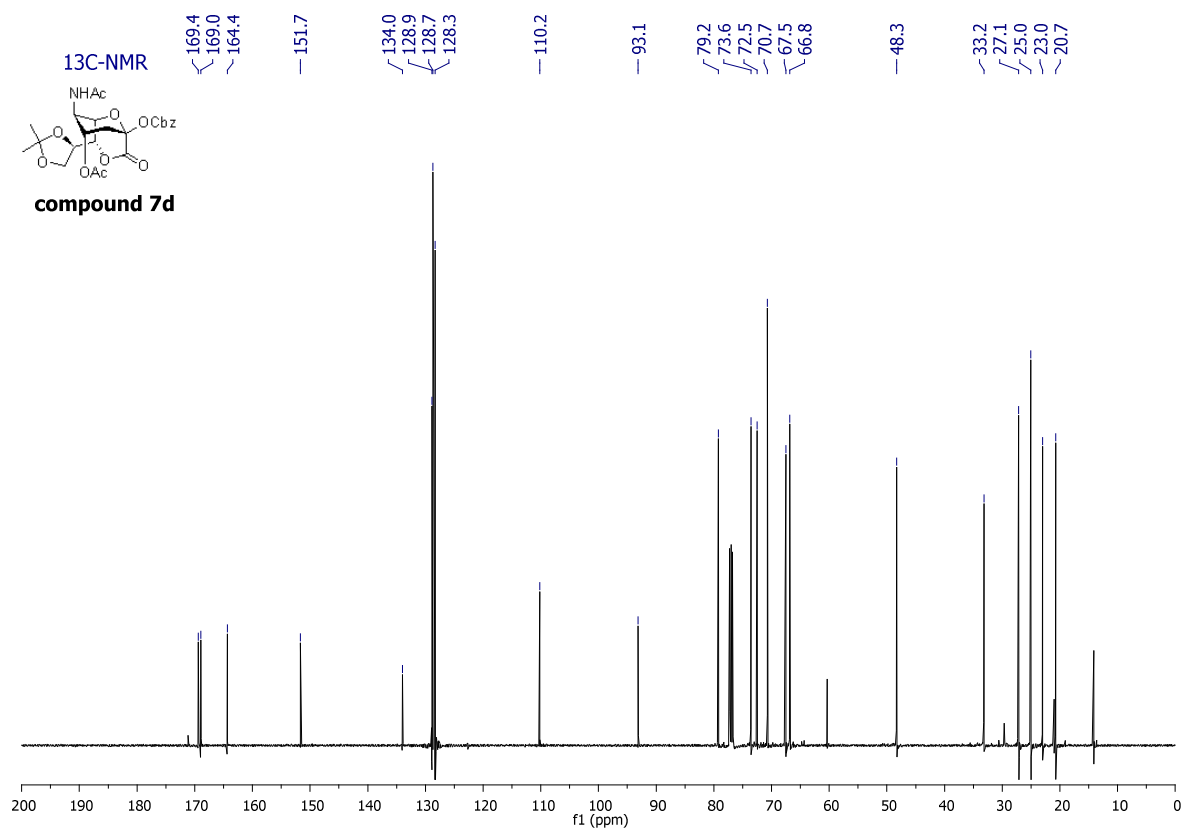
compound 7d



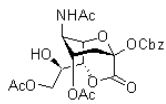
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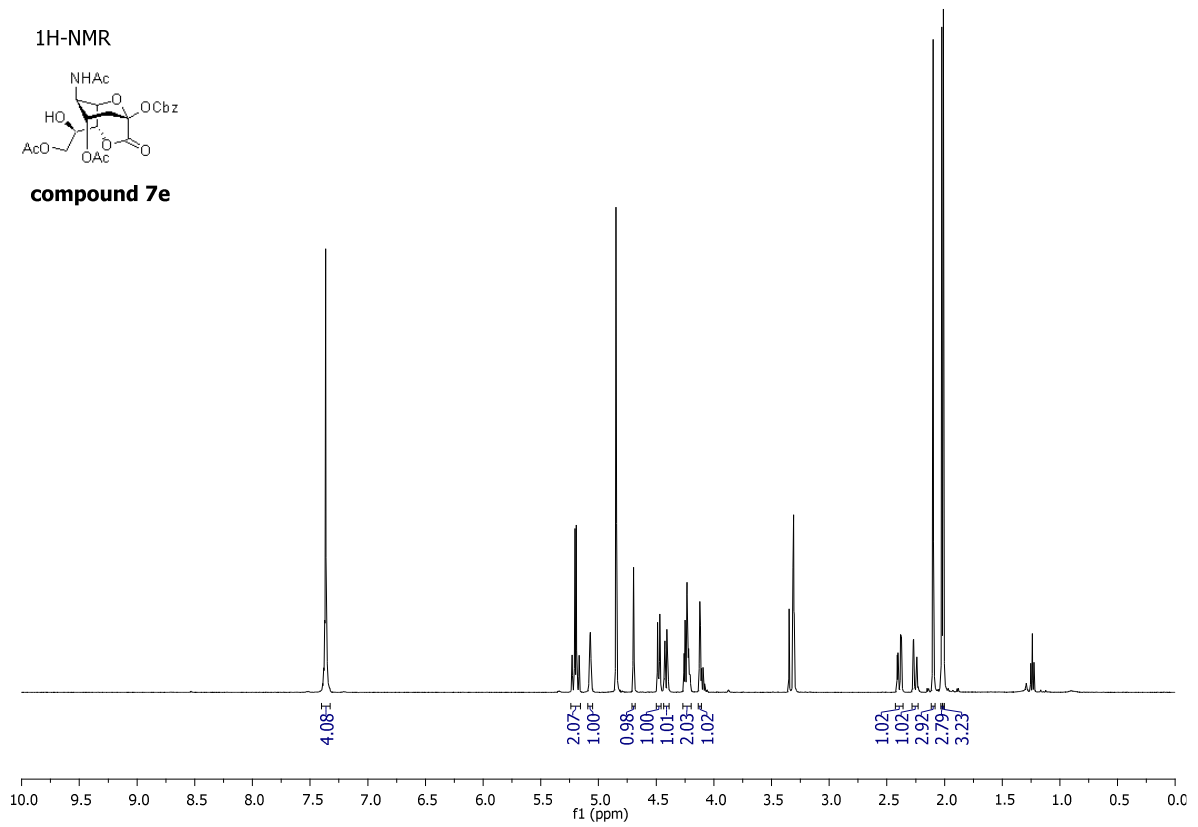
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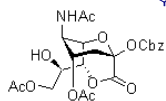
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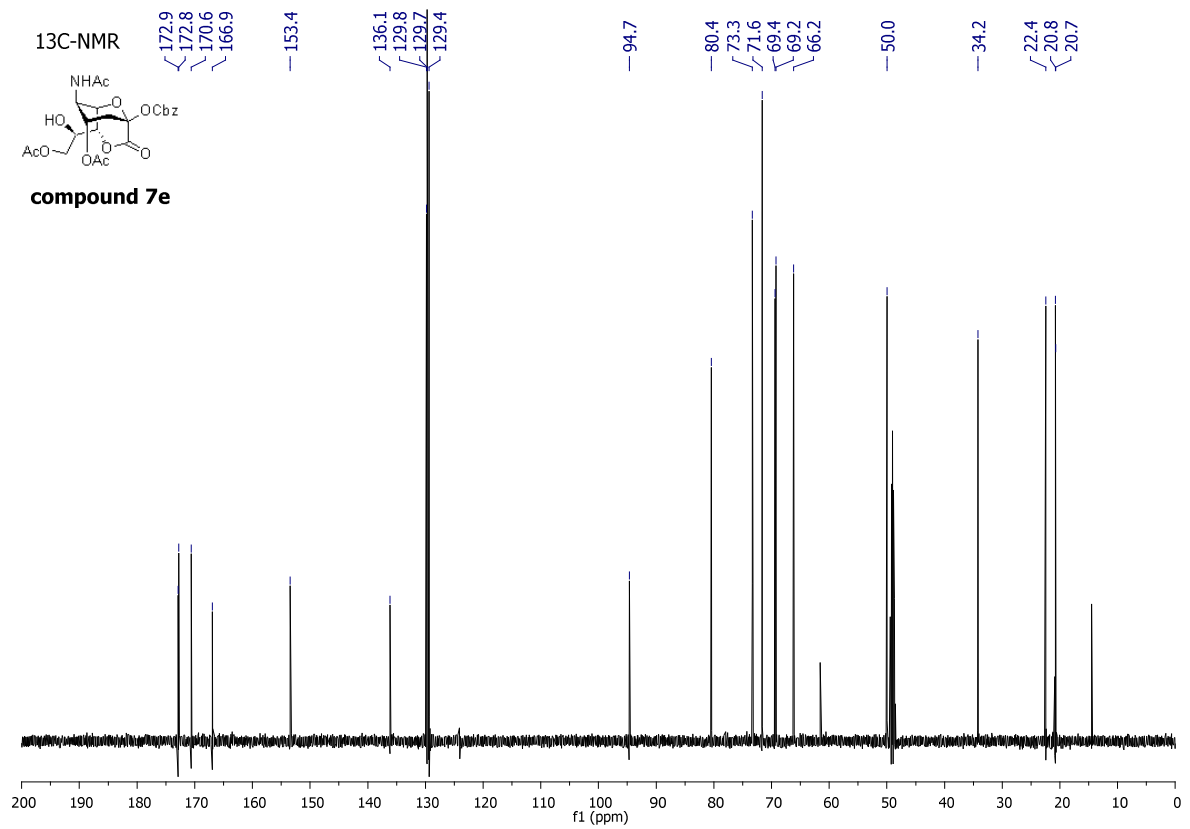
compound 7e

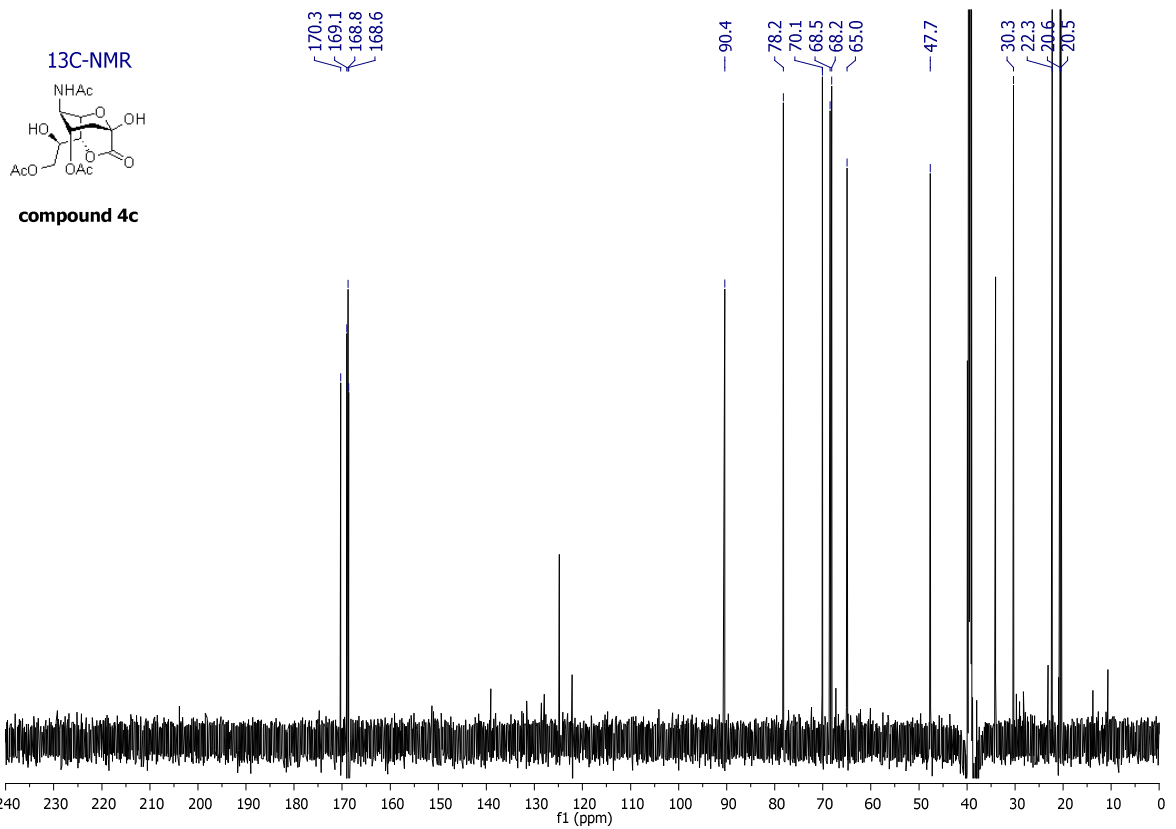
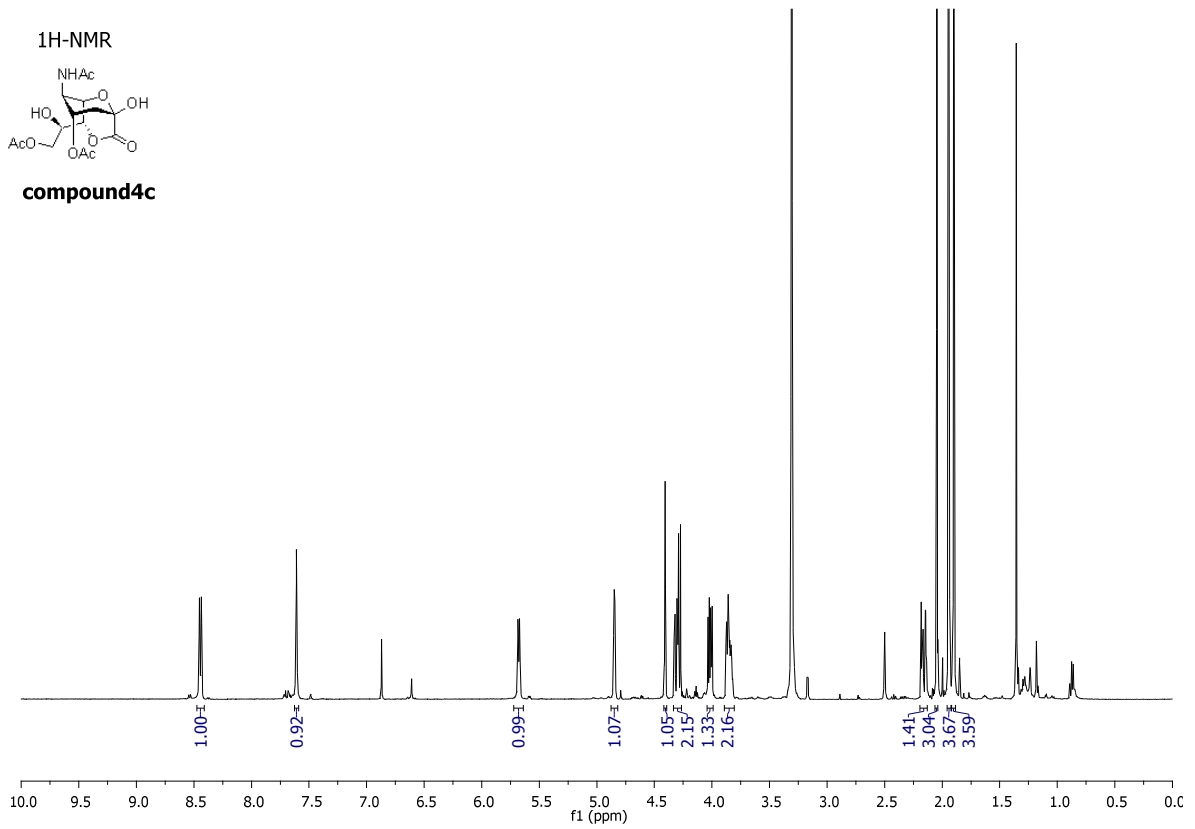
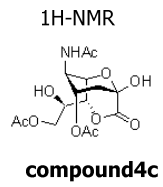


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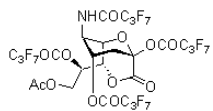


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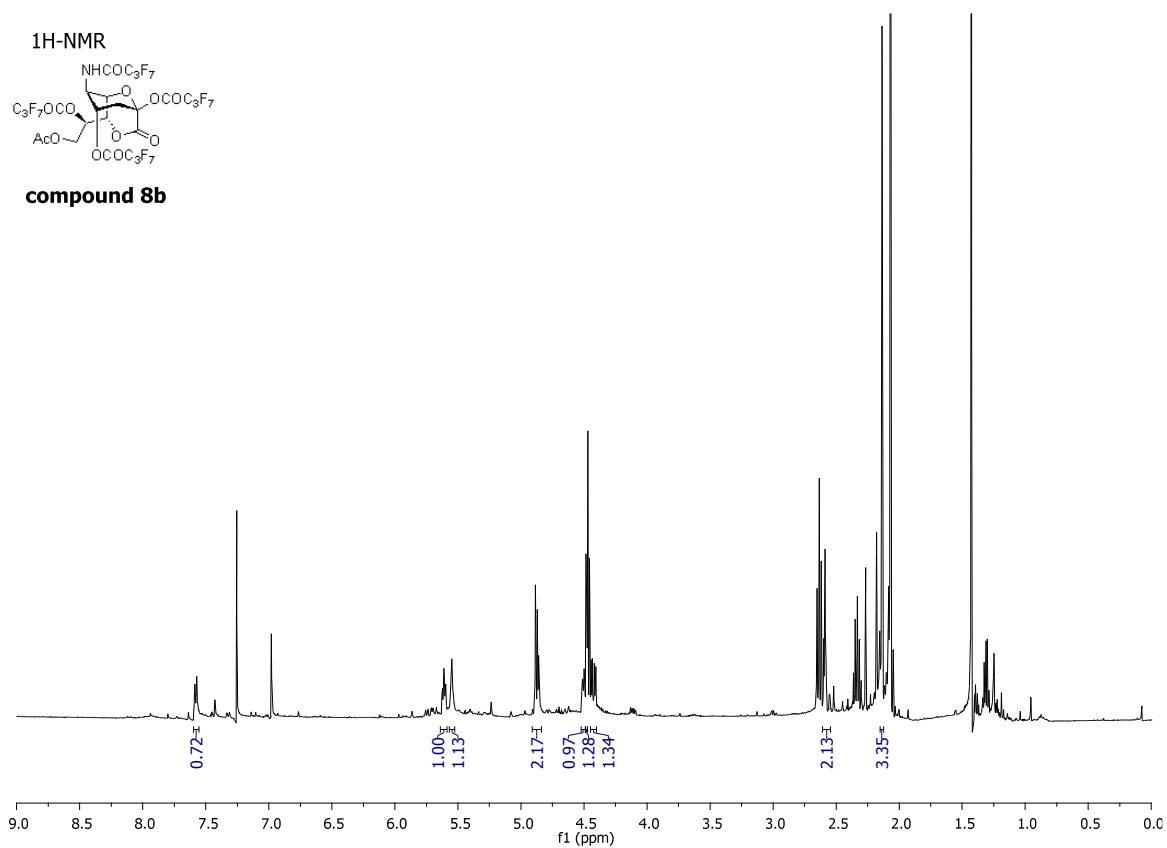




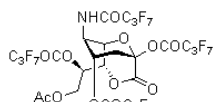
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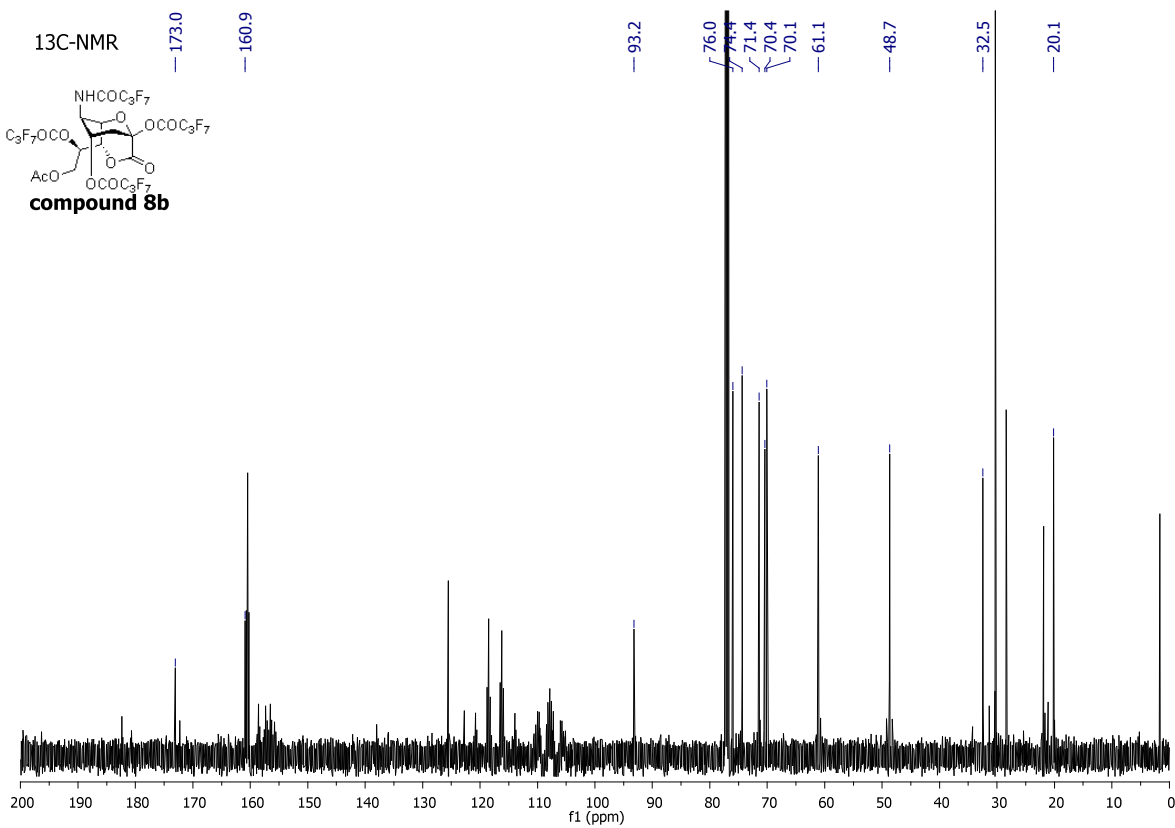
compound 8b



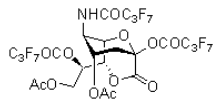
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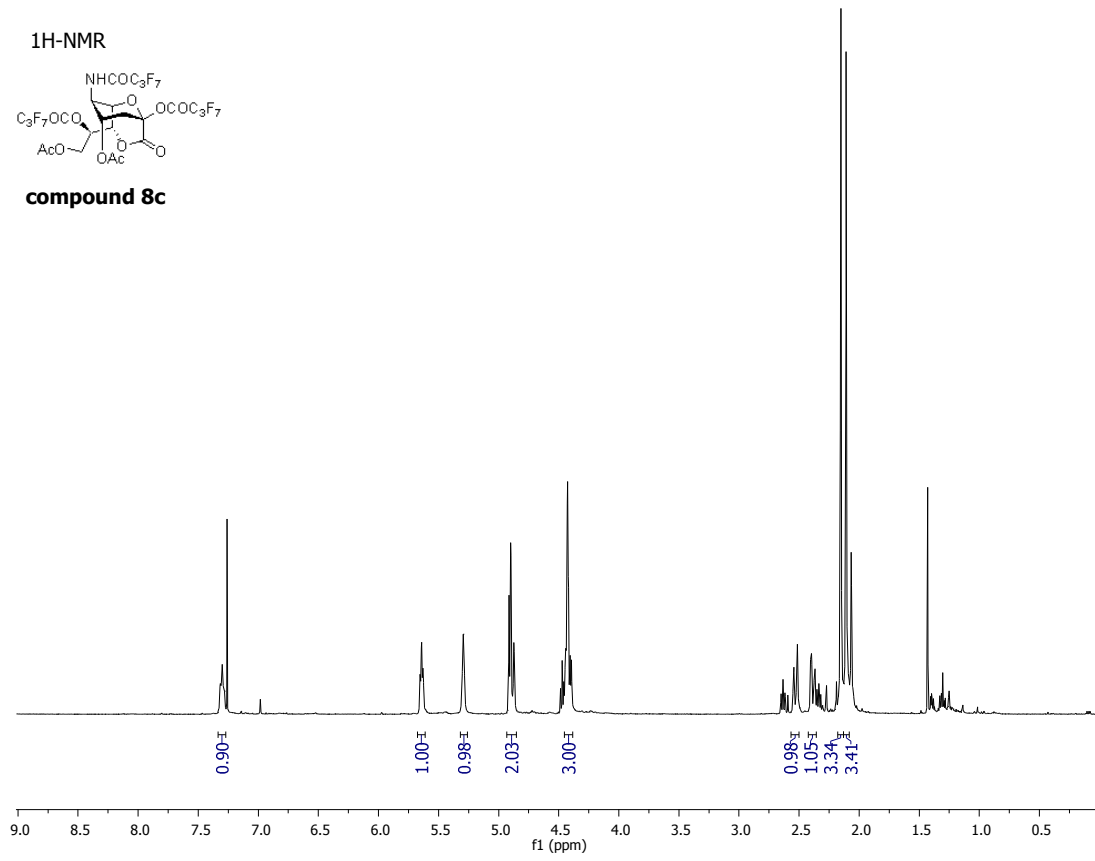
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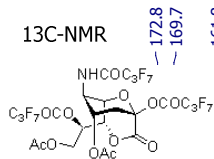
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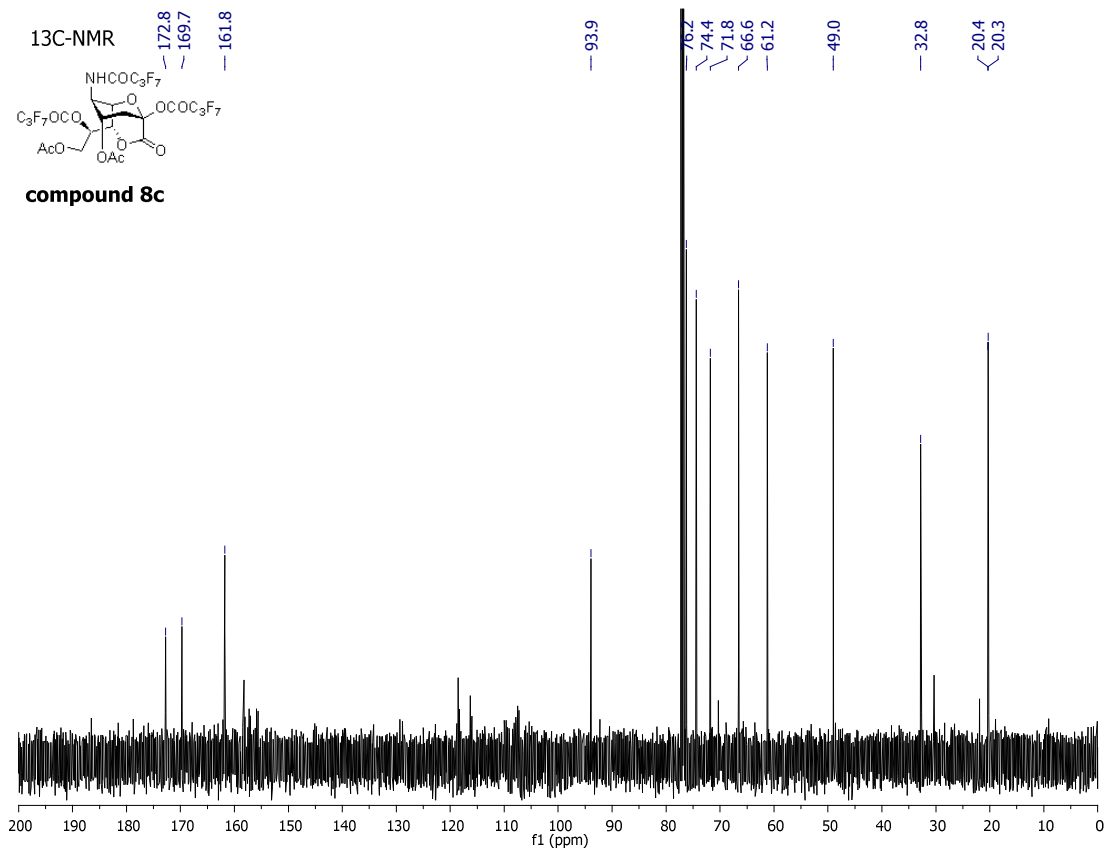
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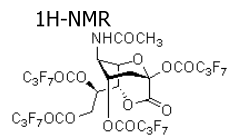


¹³C-NMR

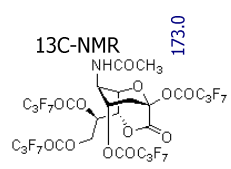
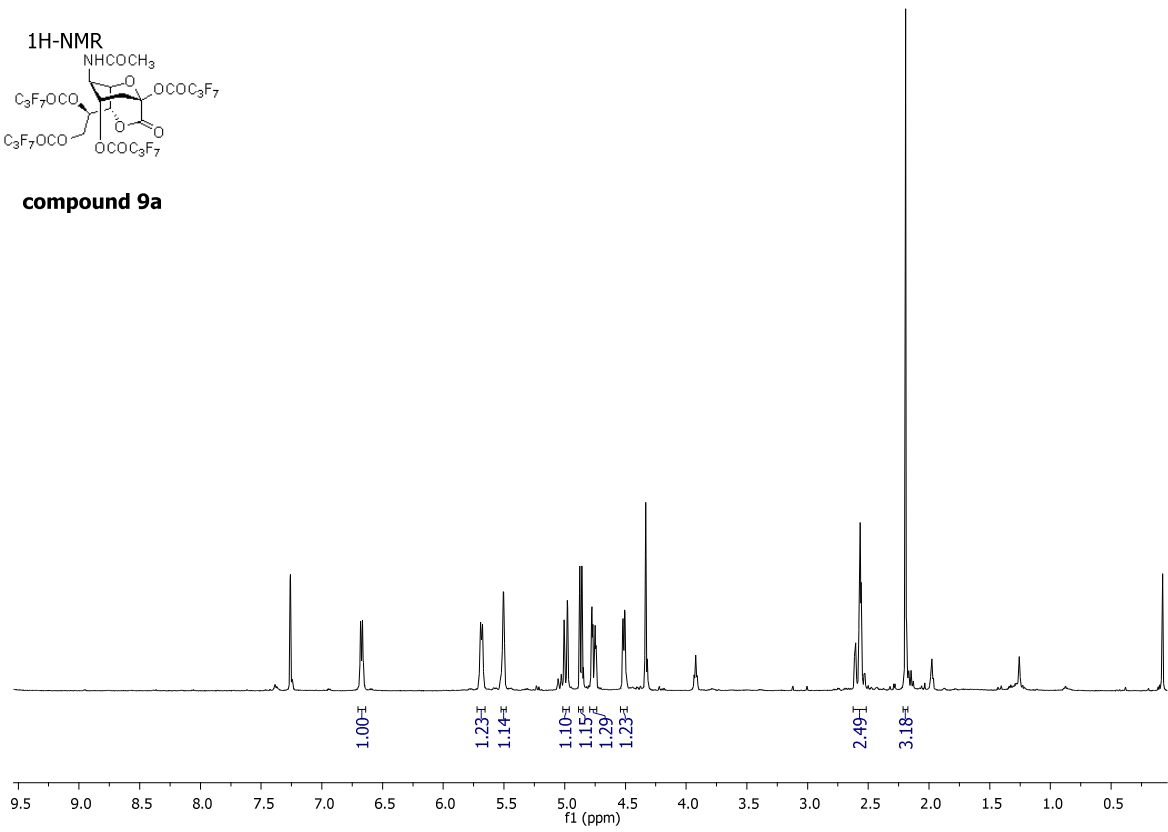


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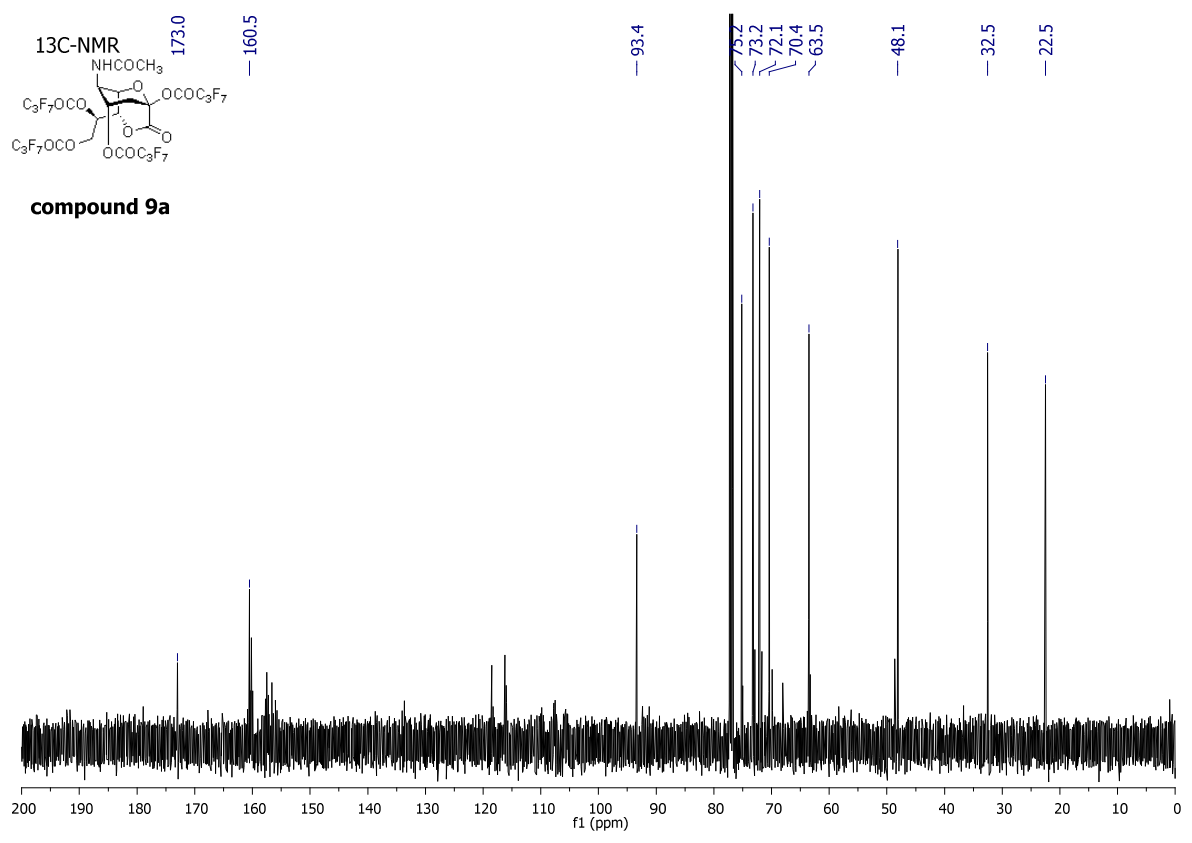




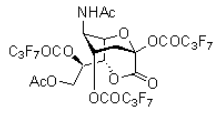
compound 9a



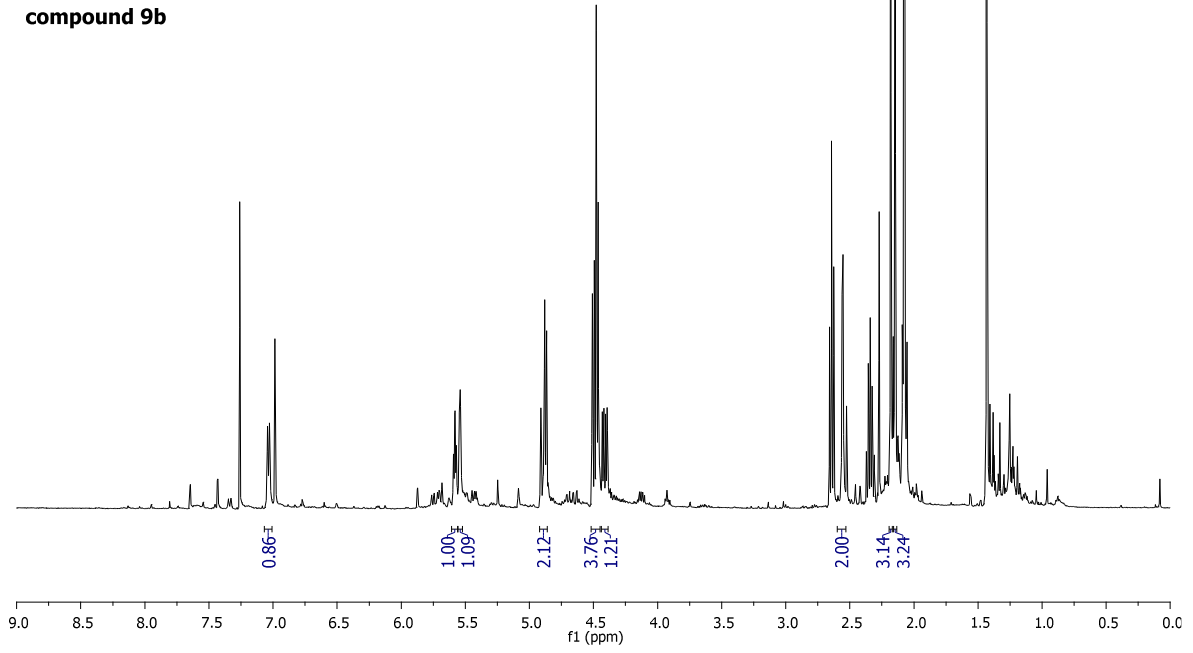
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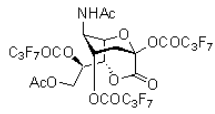
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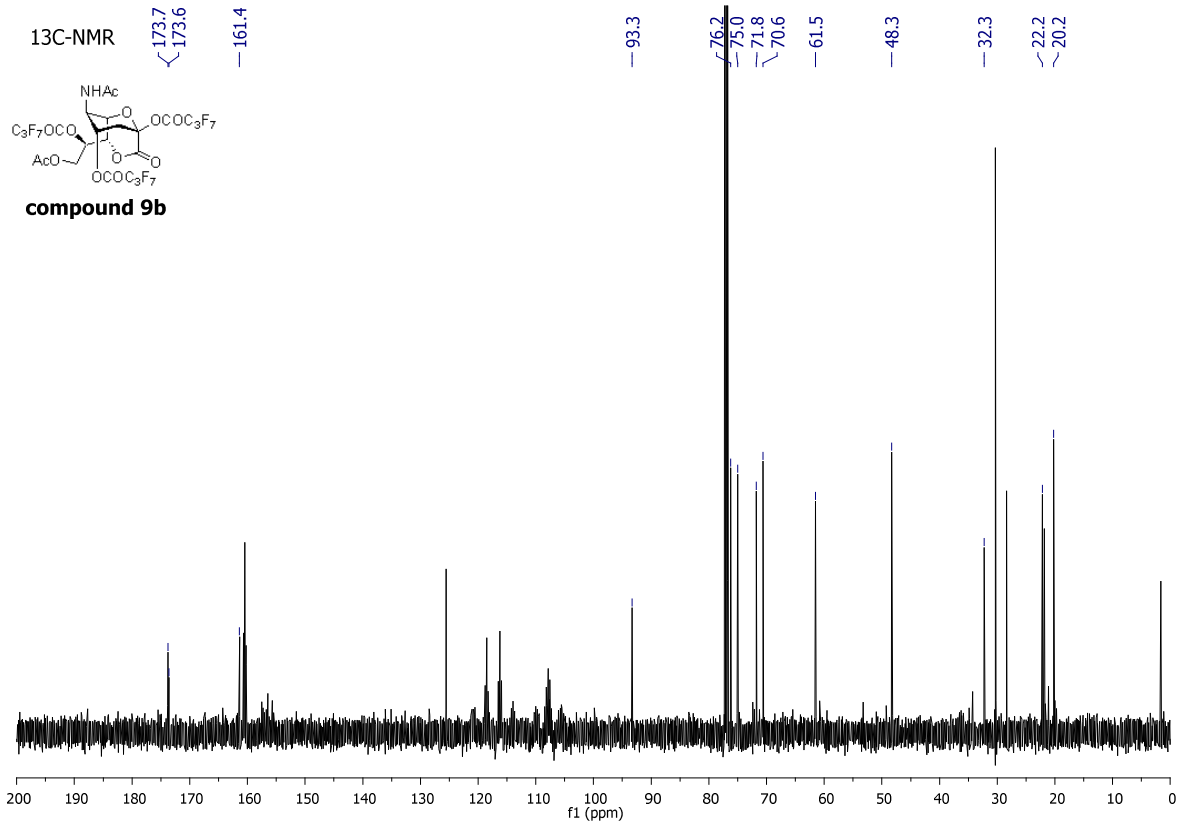
compound 9b



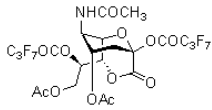
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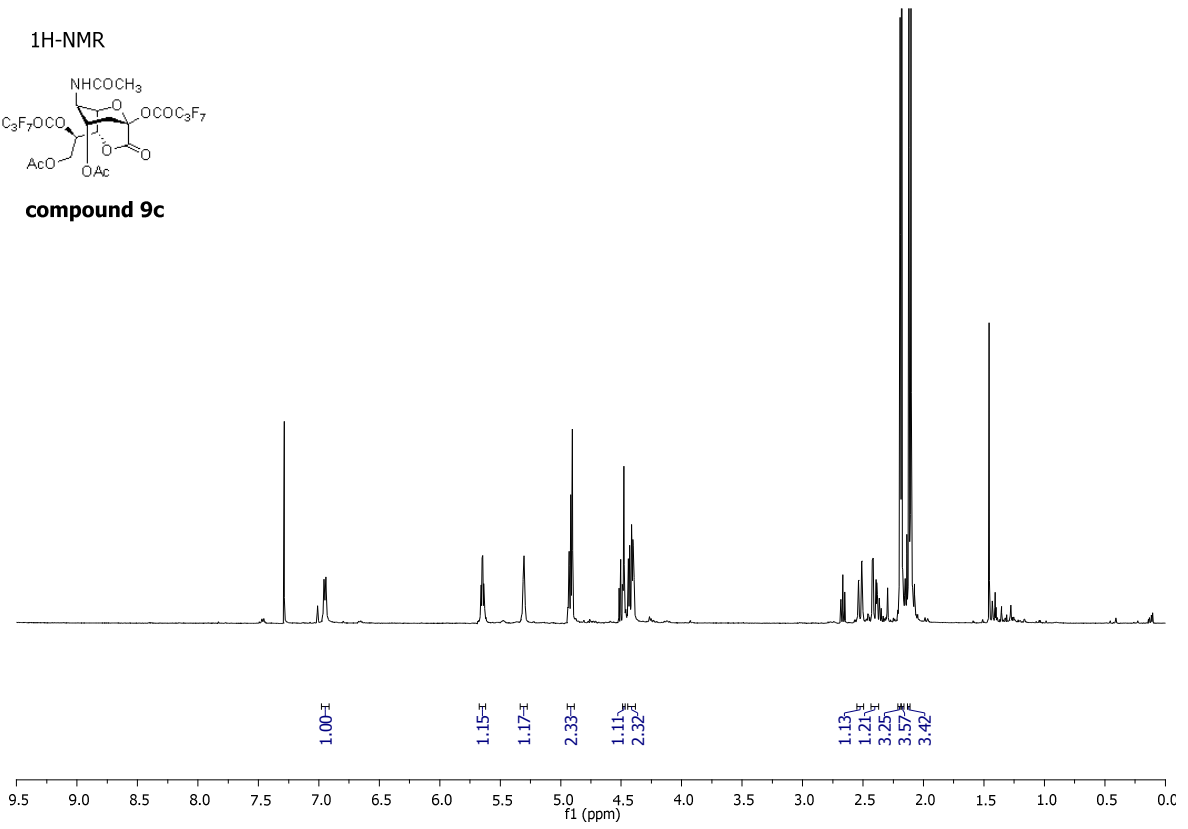
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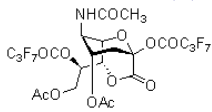
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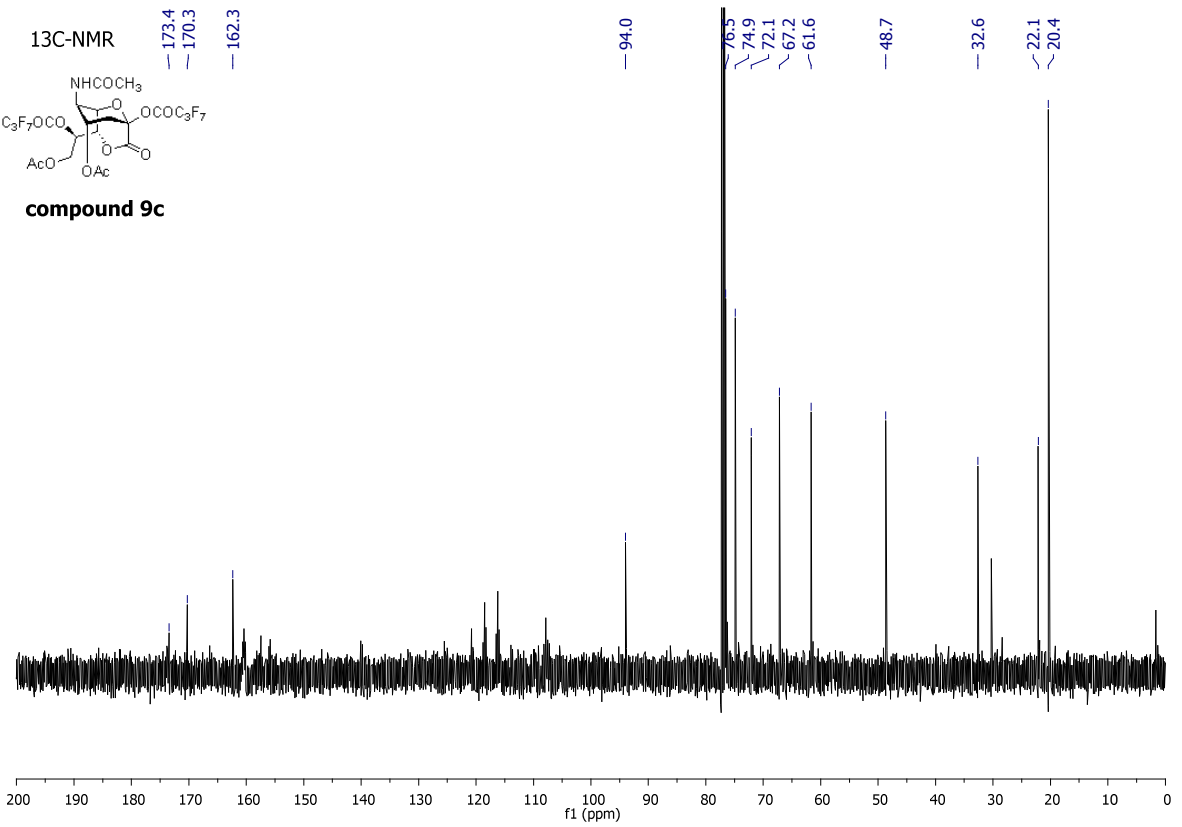
compound 9c



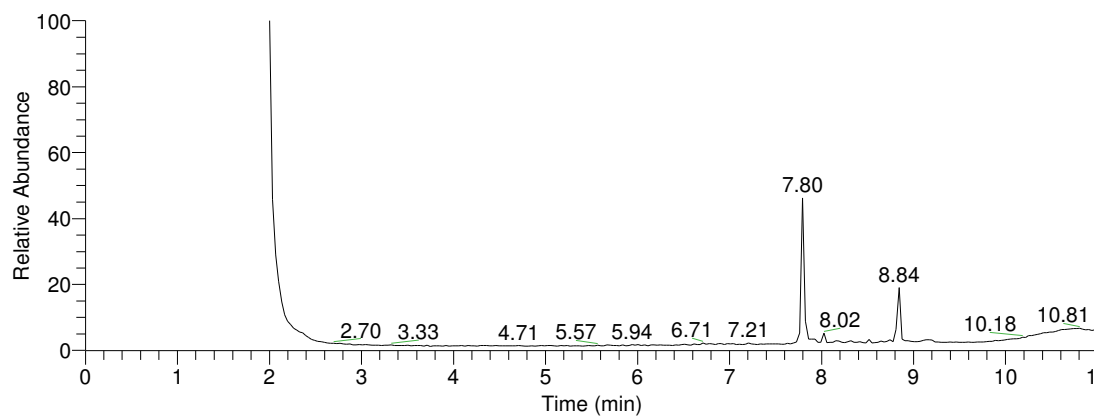
13C-NMR



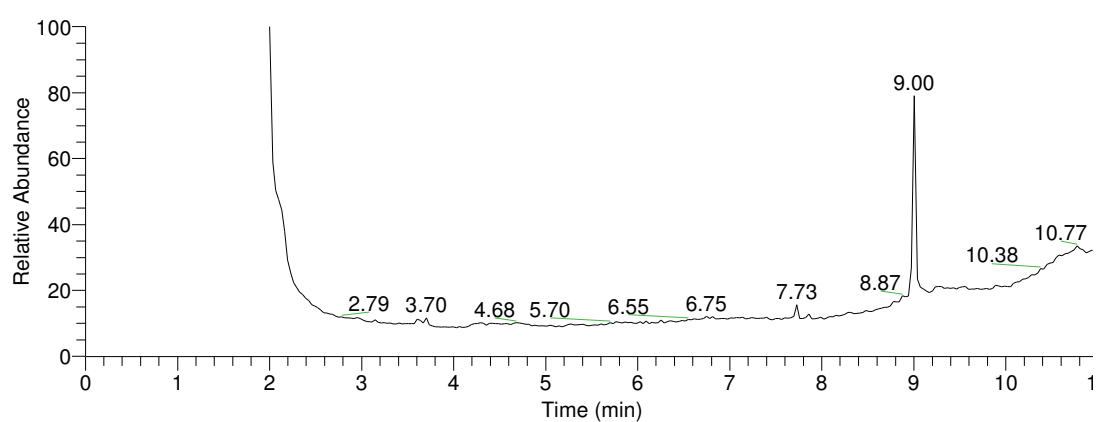
compound 9c



A)



B)



C)

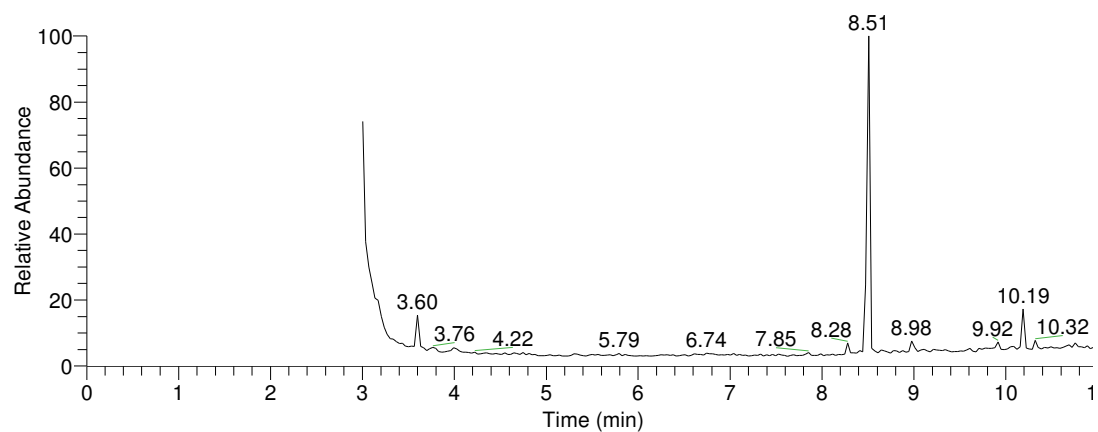
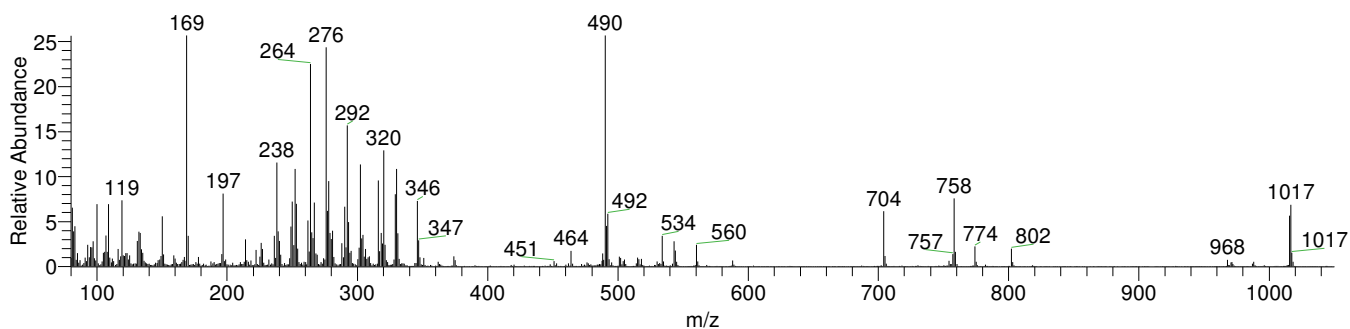
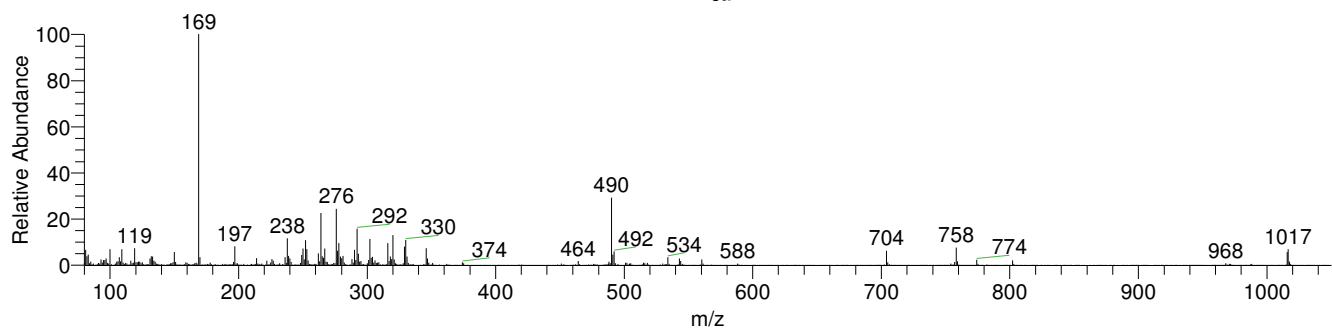
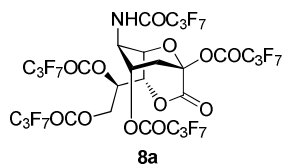
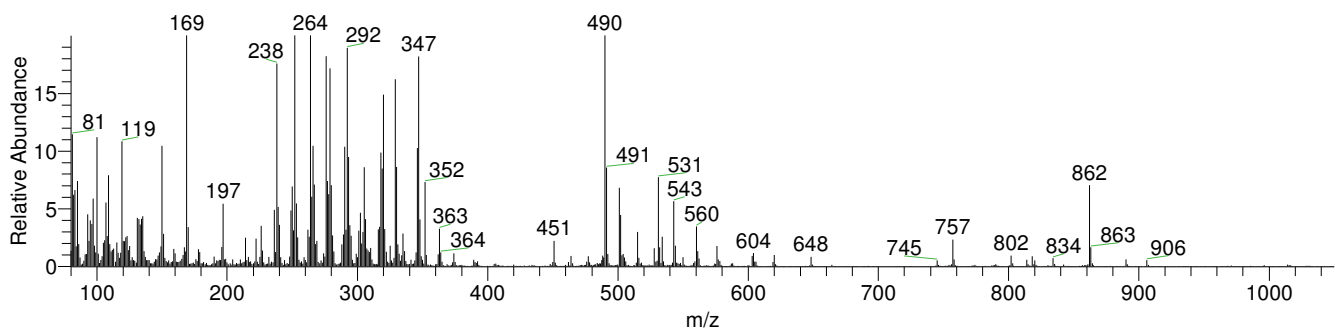
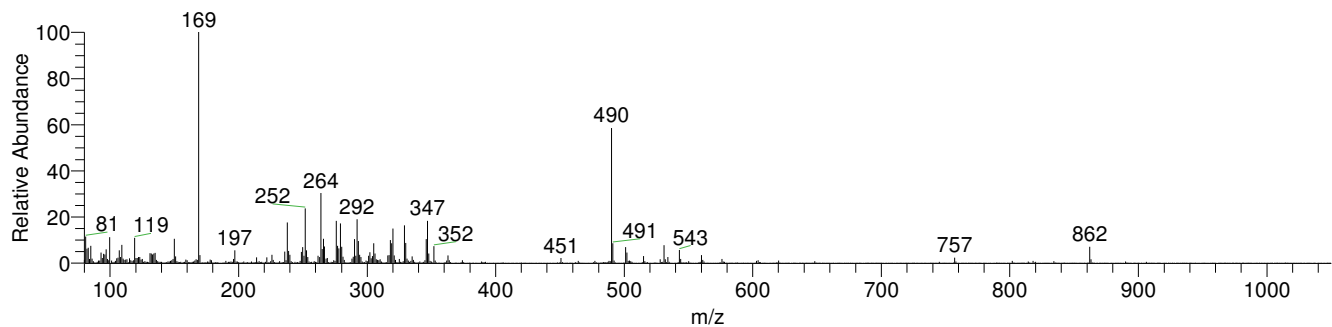
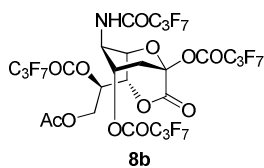


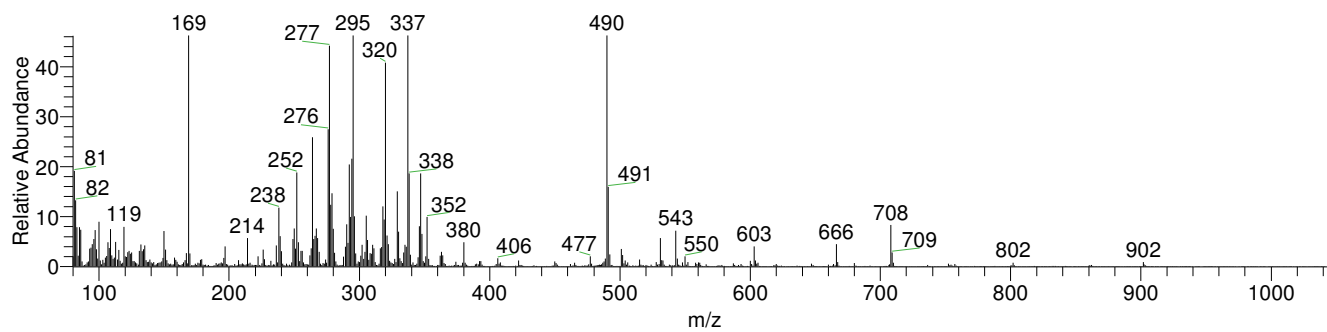
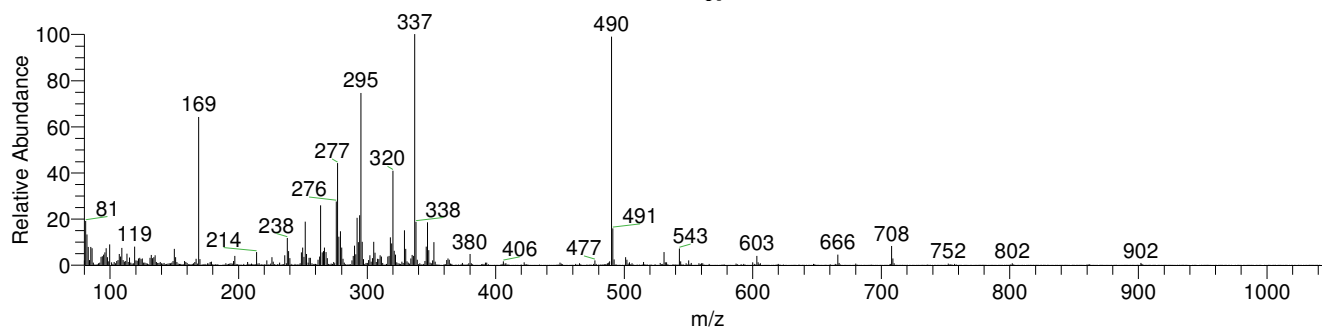
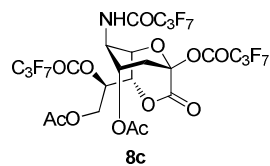
Fig. 1S. Total ion chromatograms of products obtained by HFBA derivatization (HFBA, MeCN, 150°C, 5 min) of (A) methyl ester of acid **1a**, (B) methyl ester of acid **1b** and (C) methyl ester of acid **1c**.



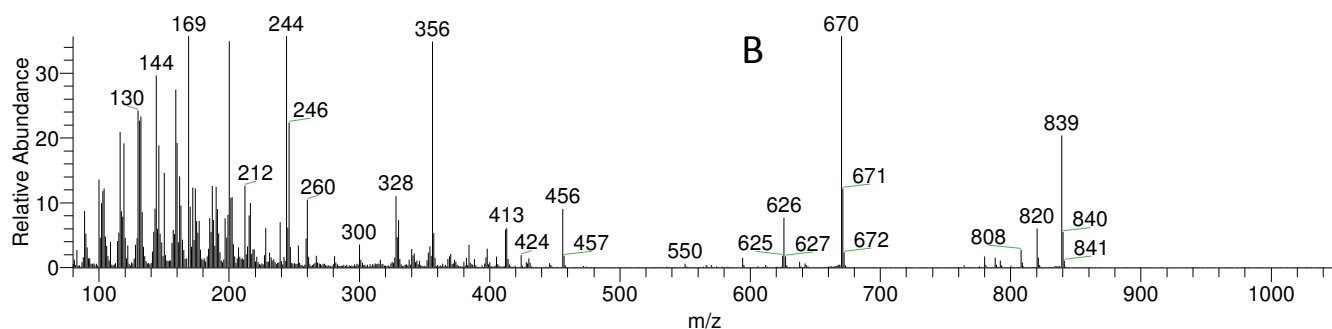
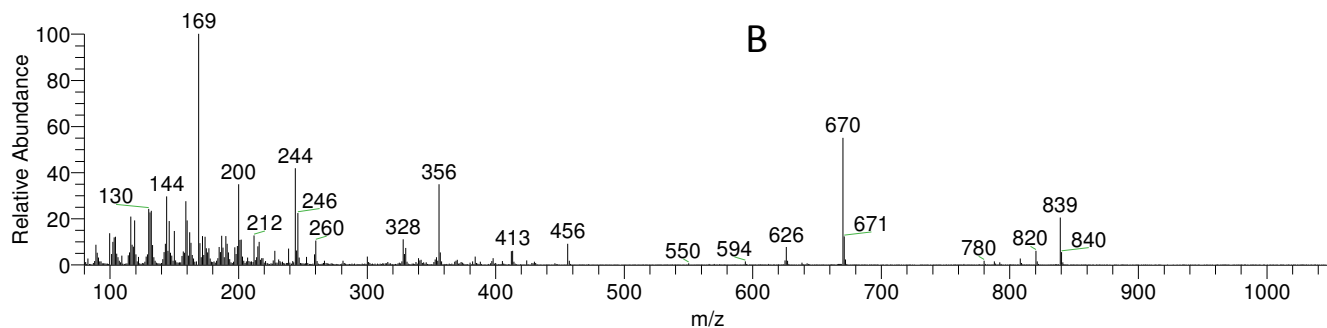
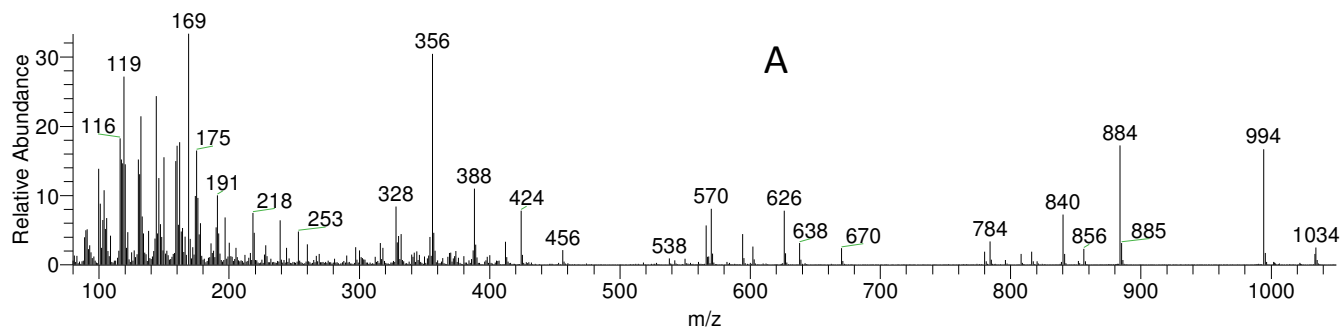
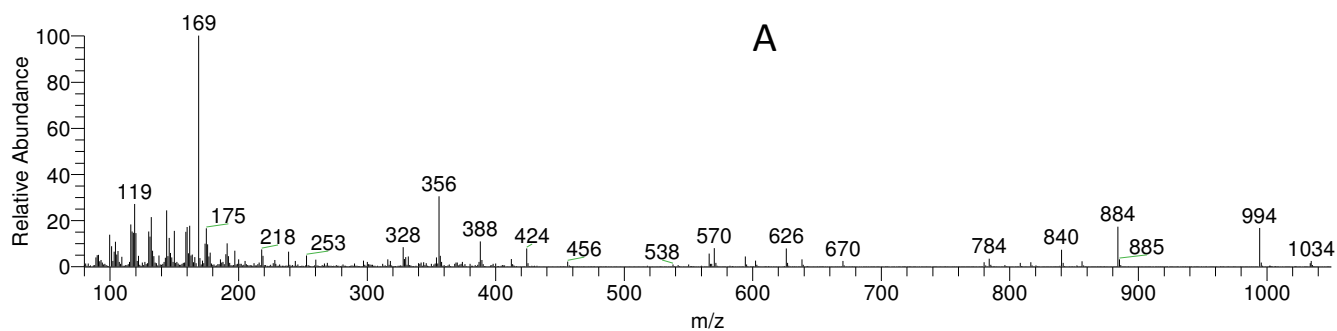
EI mass spectrum of lactone **8a** obtained by derivatization (HFBA, MeCN, 150 °C, 5 min) of the corresponding acid **1a** or of the lactone **4a**



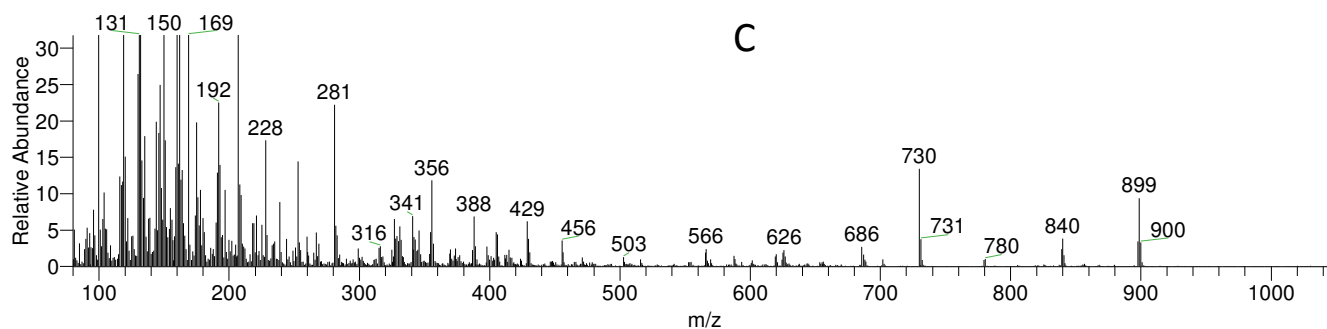
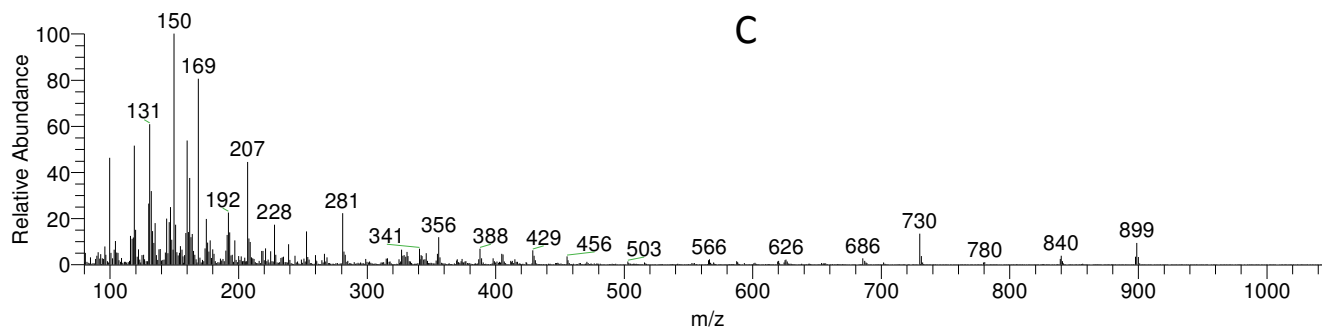
EI mass spectrum of lactone **8b** obtained by derivatization (HFBA, MeCN, 150 °C, 5 min) of the corresponding acid **1b** or of the lactone **4b**



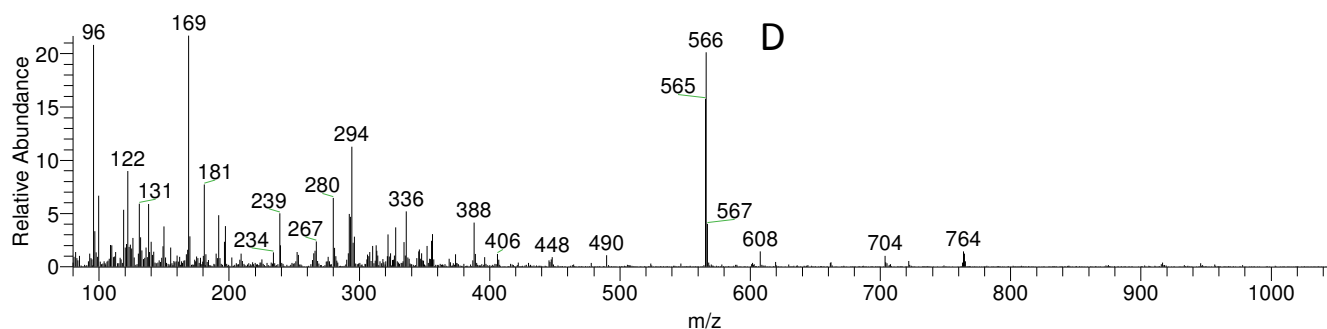
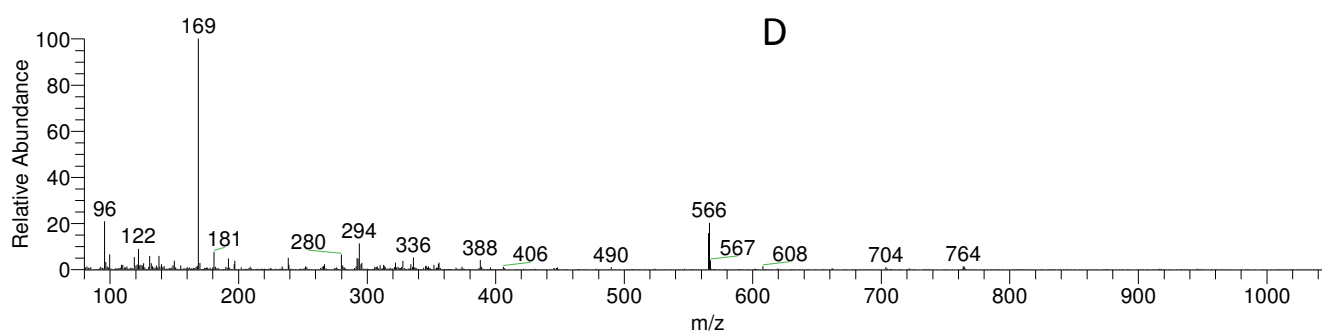
EI mass spectrum of lactone **8c** obtained by derivatization (HFBA, MeCN, 150 °C, 5 min) of the corresponding acid **1c** or of the lactone **4c**.



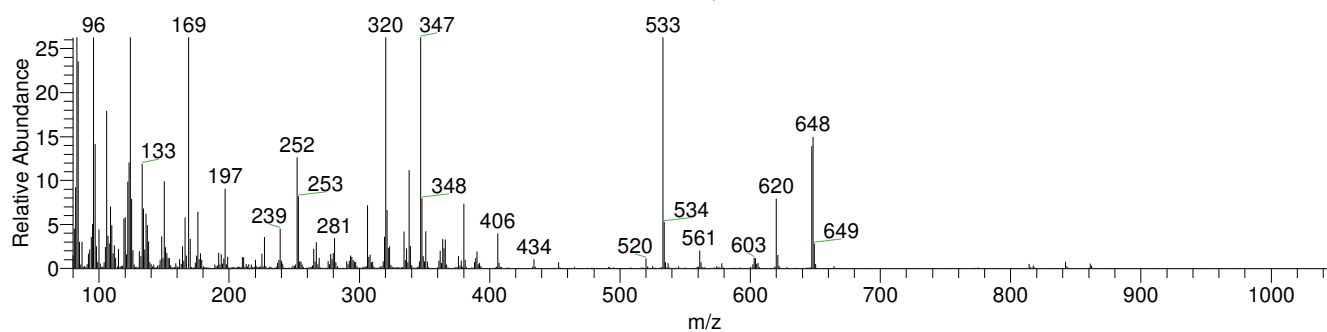
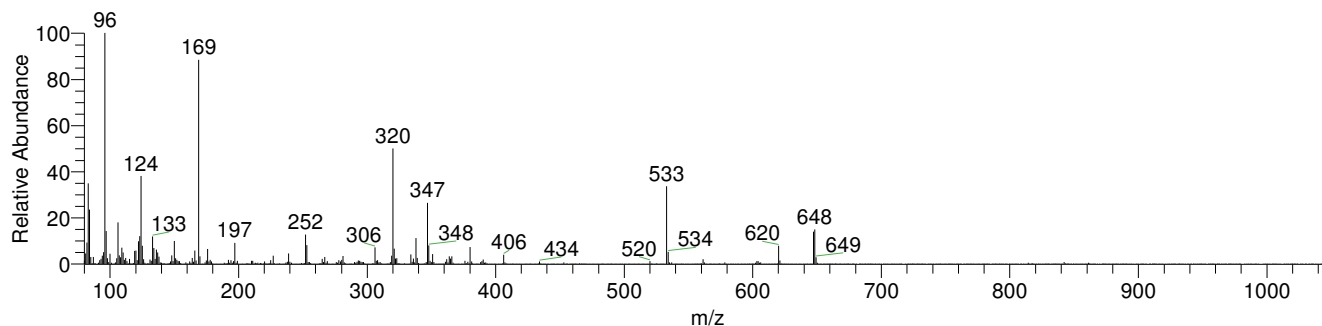
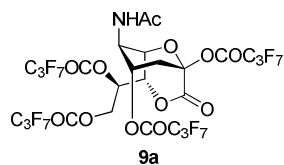
EI mass spectra obtained after derivatization (HFBA, MeCN, 150 °C, 5 min) of the methyl ester of sialic acid **1a**. A and B represent the mass spectra of peaks at 7.85 and 8.86 min of derivative of methyl ester of **1a**



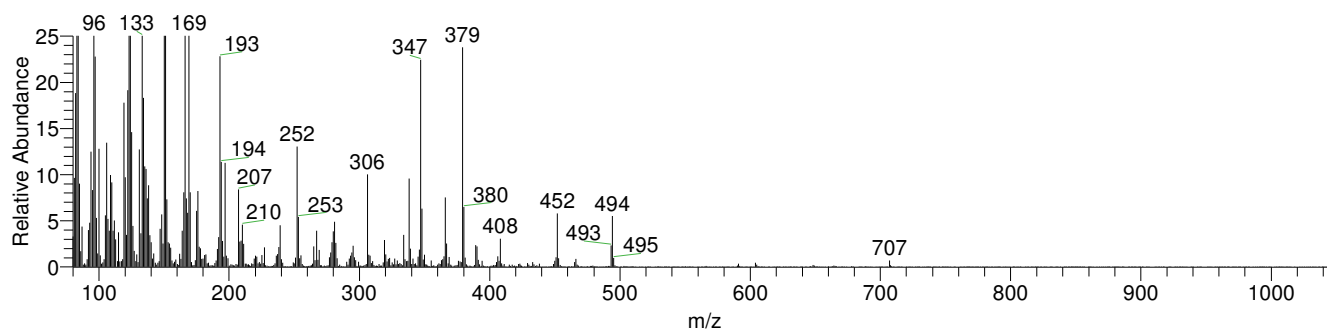
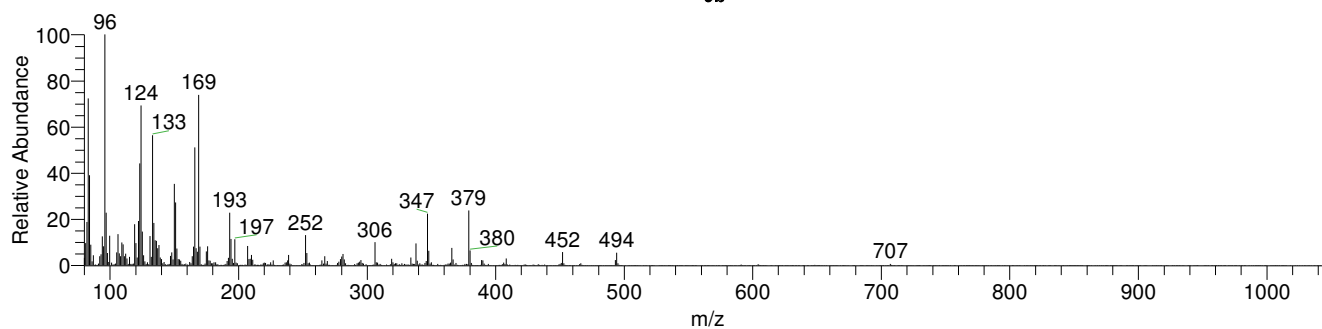
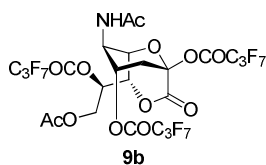
EI mass spectra obtained after derivatization (HFBA, MeCN, 150 °C, 5 min) of the methyl ester of sialic acid **1b**. C represent the mass spectrum of peak at 9.00 min of derivative of methyl ester of **1b**.



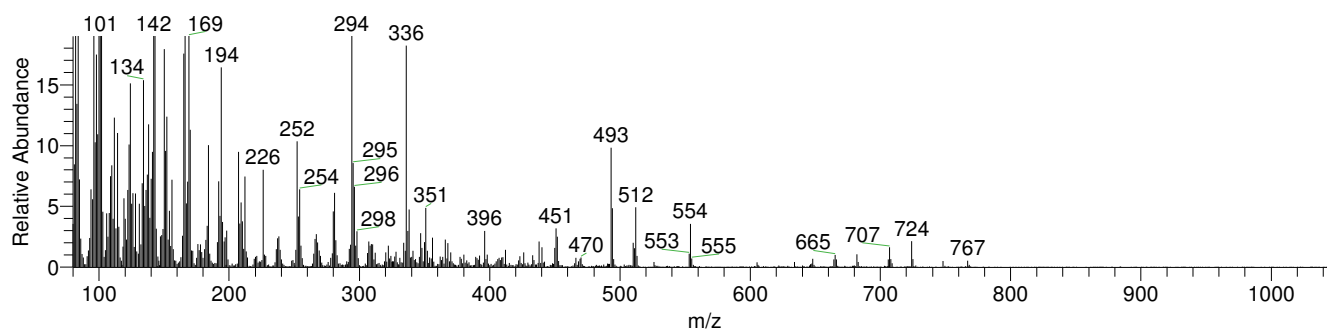
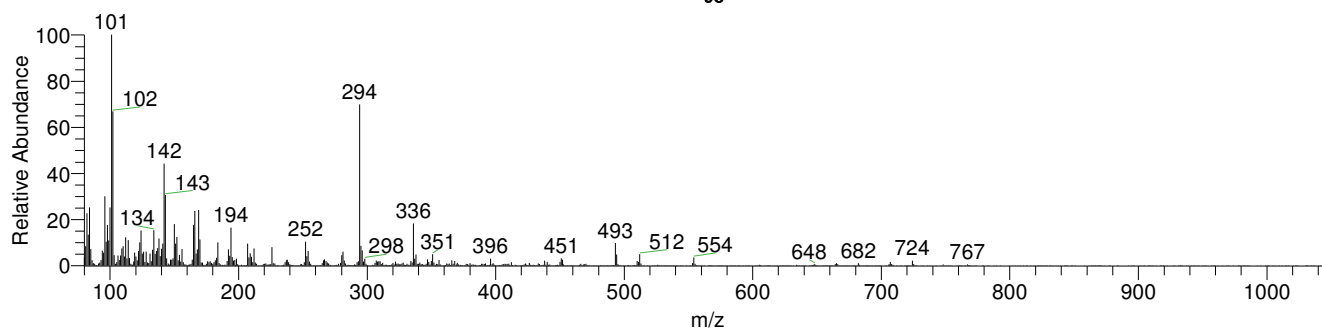
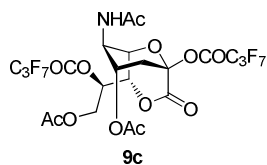
EI mass spectra obtained after derivatization (HFBA, MeCN, 150 °C, 5 min) of the methyl ester of sialic acid **1c**. D represent the mass spectrum of peak at 8.51 min of derivative of methyl ester of **1c**.



EI mass spectra of lactone **9a** obtained by derivatization with HFBA at 23°C the acids **1a** and the lactones **4a**.



EI mass spectra of lactone **9b** obtained by derivatization with HFBA at 23°C the acids **1b** and the lactones **4b**.



EI mass spectra of lactone **9c** obtained by derivatization with HFBA at 23°C the acids **1c** and the lactones **4c**.