

SUPPORTING INFORMATION

Hydrolyzable Tannins of Tamaricaceous Plants VII¹⁾: Structures and Cytotoxicities of Oligomeric Ellagitannins from Cultured Tissues of *Tamarix tetrandra* and Leaves of *Tamarix nilotica*

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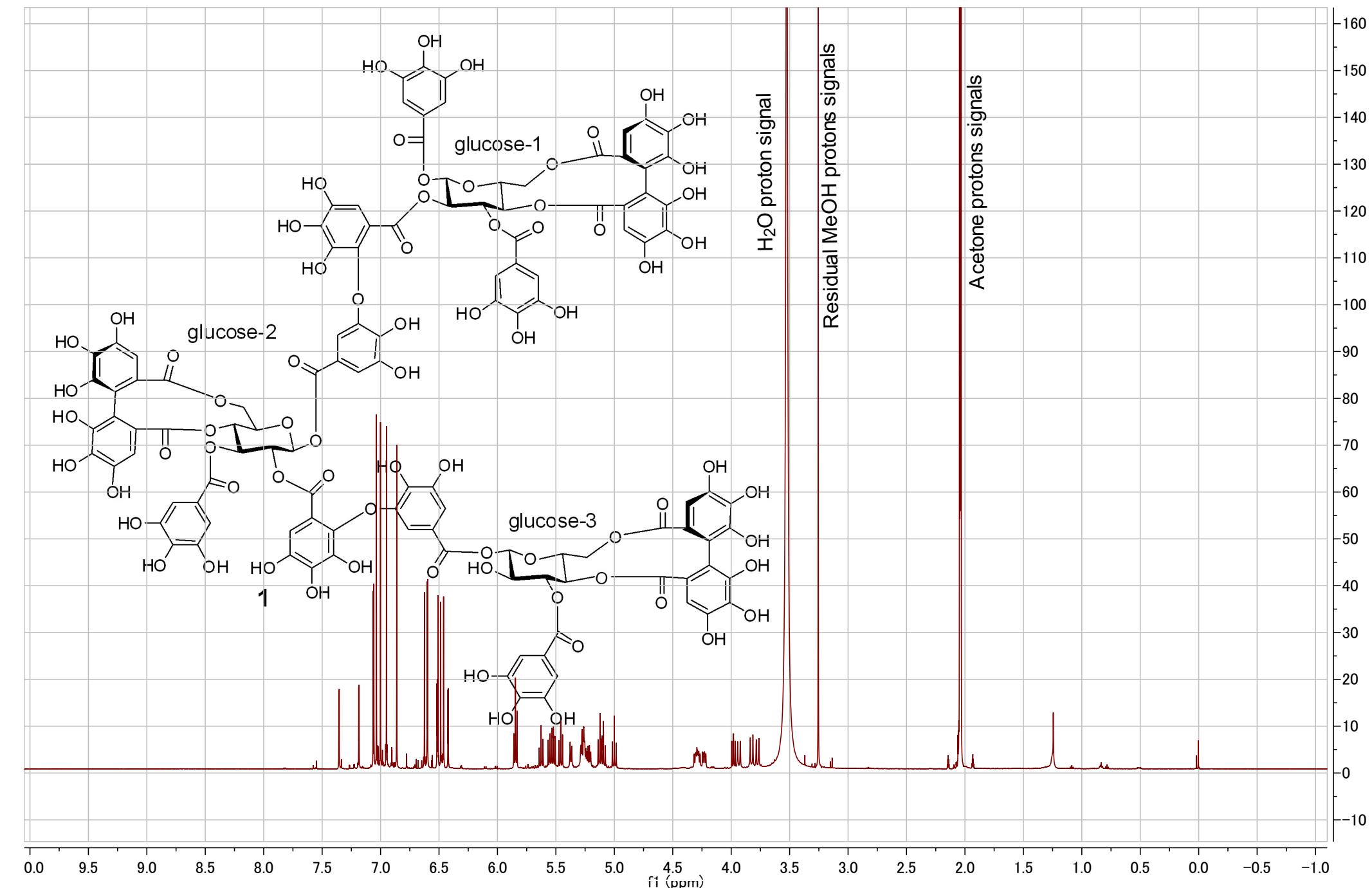
Division of Pharmacology, Department of Diagnostic and Therapeutic Sciences, School of
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College of Pharmaceutical Sciences, Matsuyama University, Bunkyo-cho, Matsuyama 790-
8578, Japan.

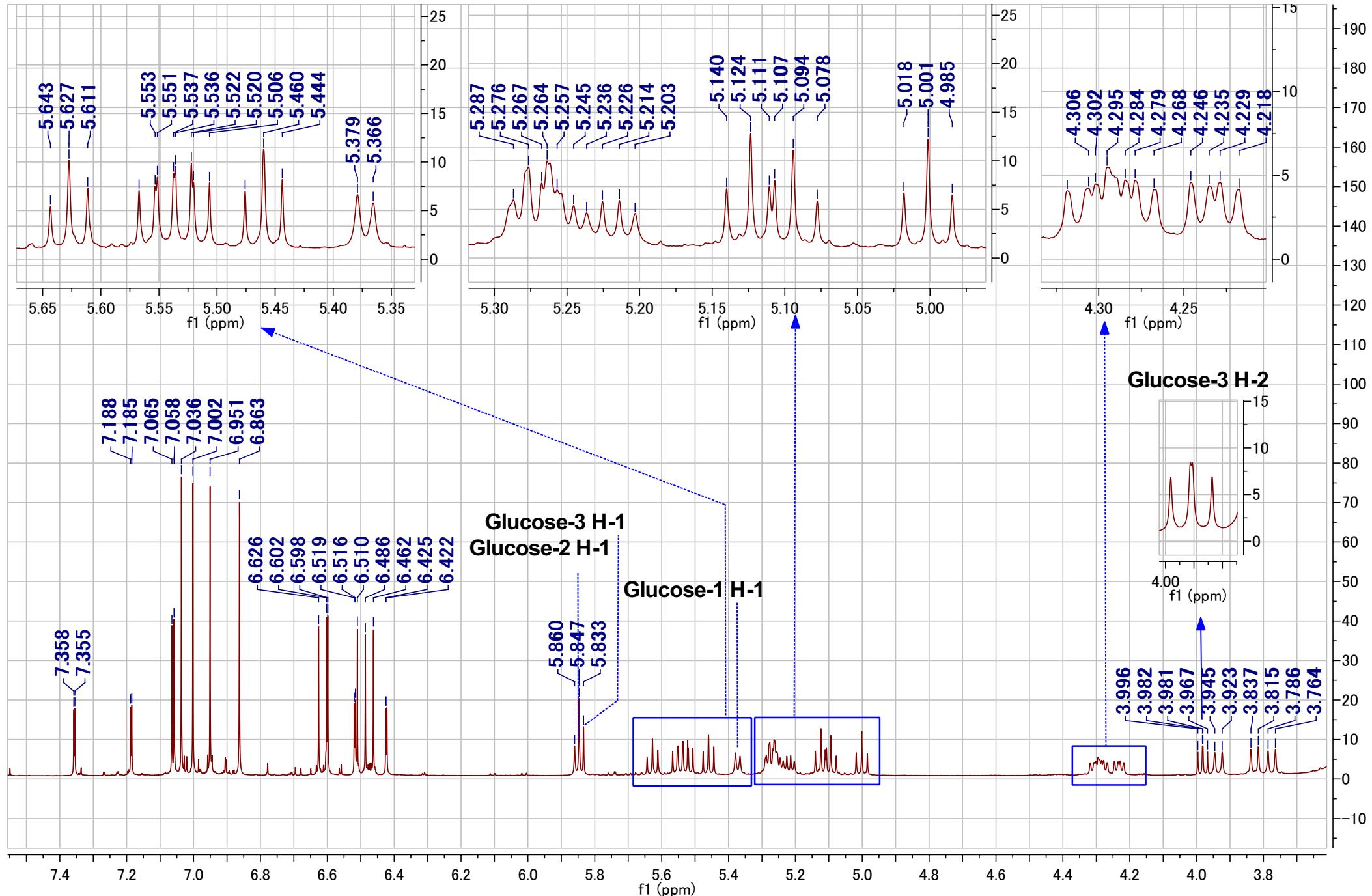
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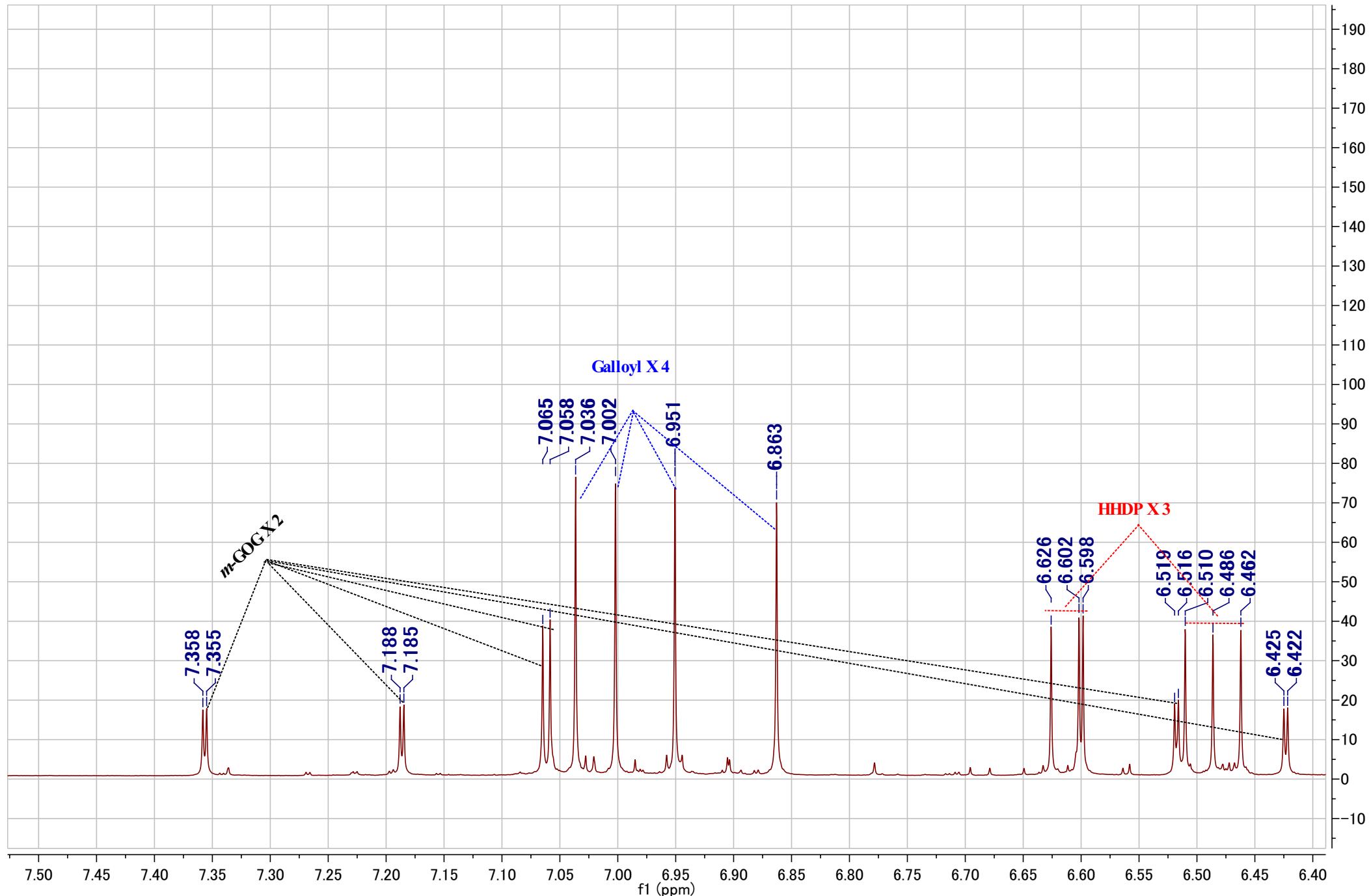
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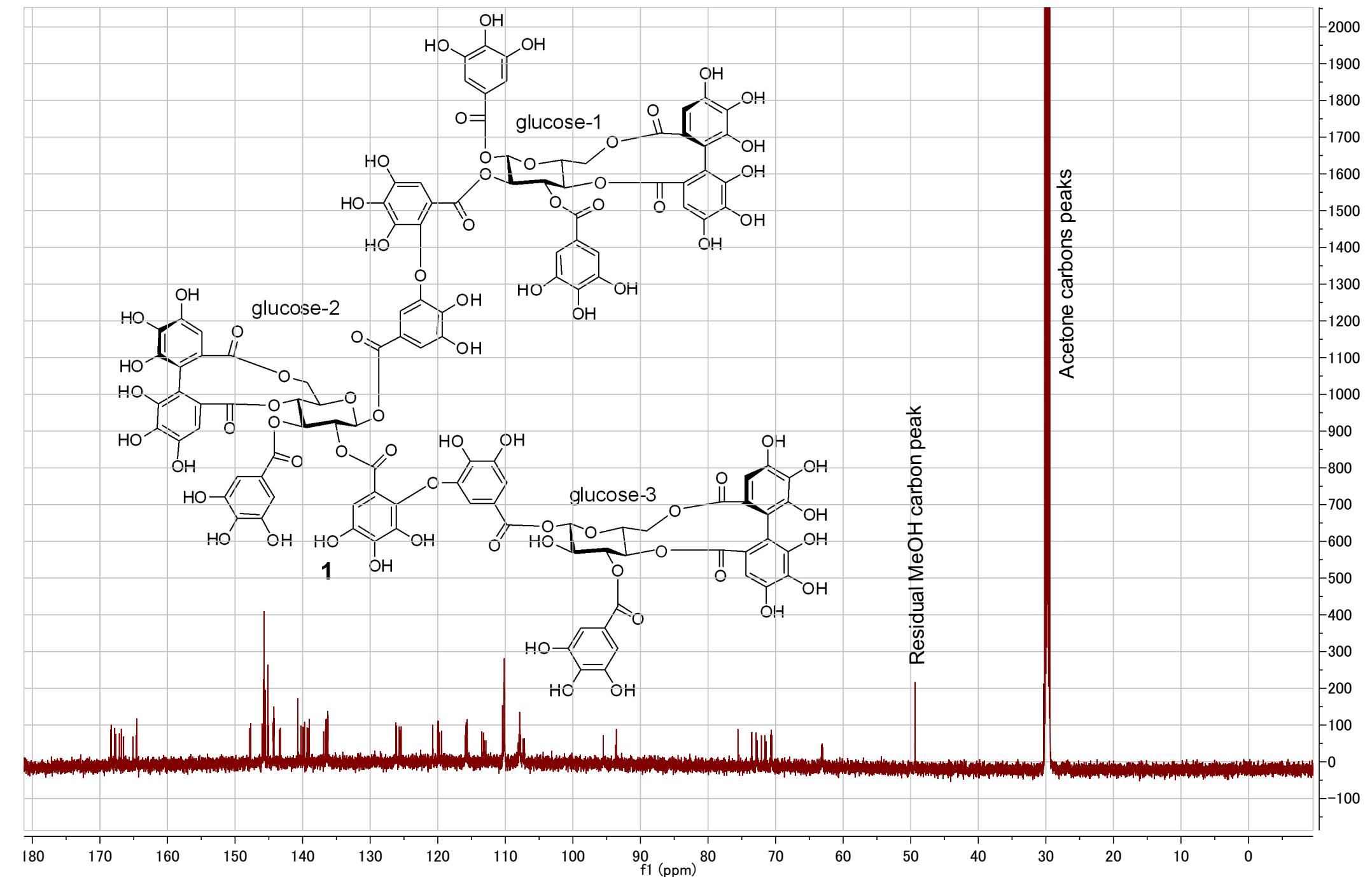
S1. ^1H NMR [600 MHz, (acetone- d_6 – D_2O , 9:1), 27 °C] spectrum of the new compound **1**



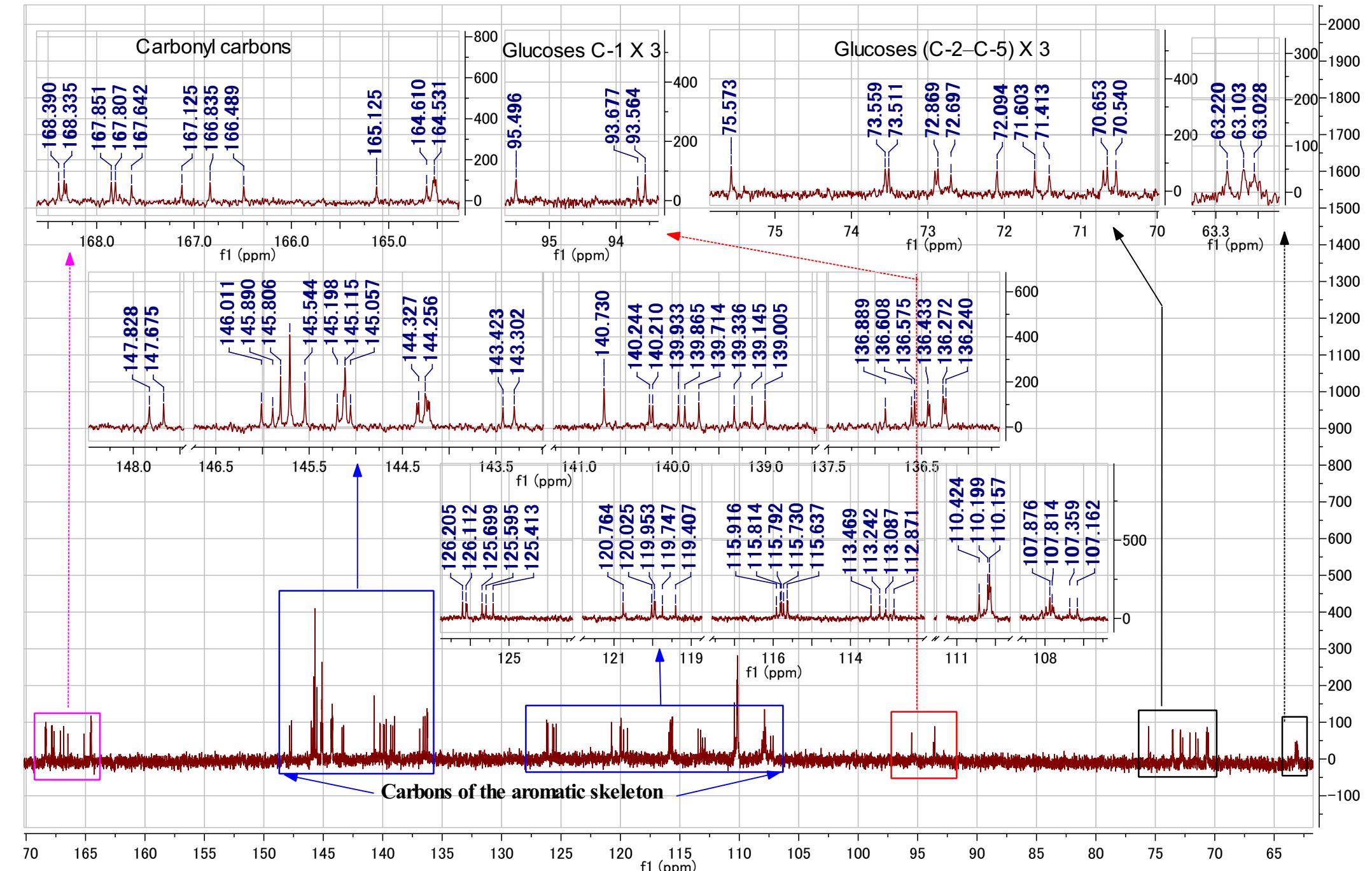
S2. Expanded aliphatic protons region of the ^1H NMR (600 MHz, acetone-d₆ – D₂O, 9:1, 27 °C] spectrum of the new compound 1



S3. Expanded aromatic protons region of ^1H NMR (600 MHz, acetone- d_6 – D_2O , 9:1, 27 °C] spectrum of the new compound 1



S4. ^{13}C NMR [151 MHz, (acetone- d_6 -D₂O, 9:1), 27 °C] spectrum of the new compound **1**



S5. Expanded ^{13}C NMR [151 MHz, (acetone- d_6 -D₂O, 9:1), 27 °C] spectrum of the new compound **1**

Display Report

Analysis Info

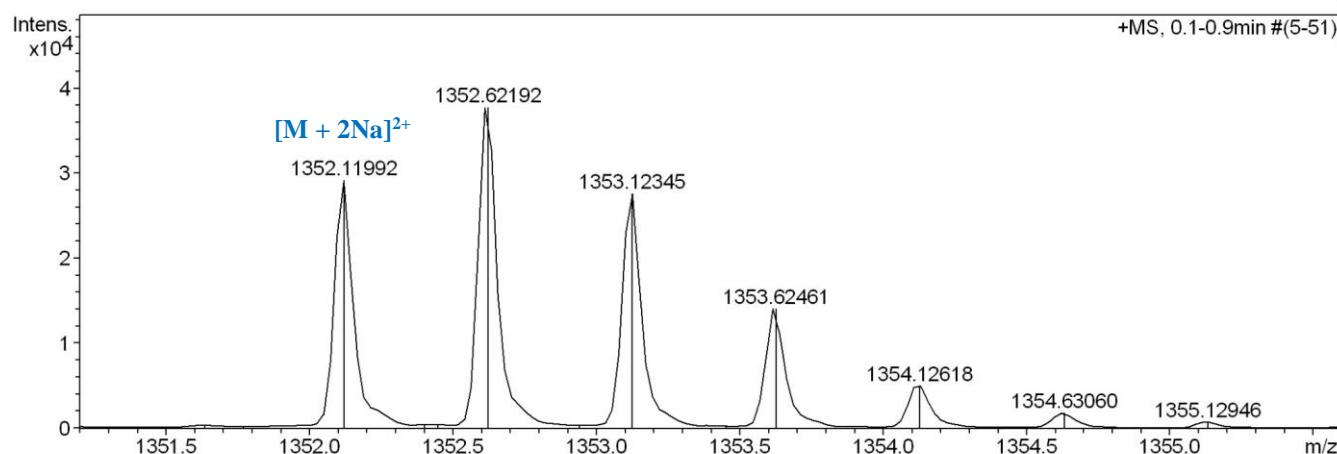
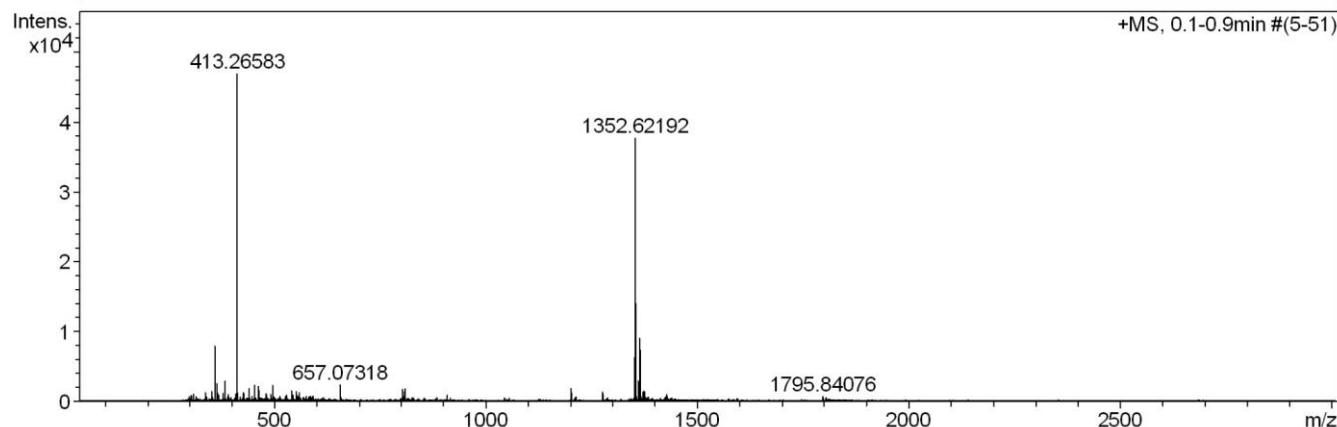
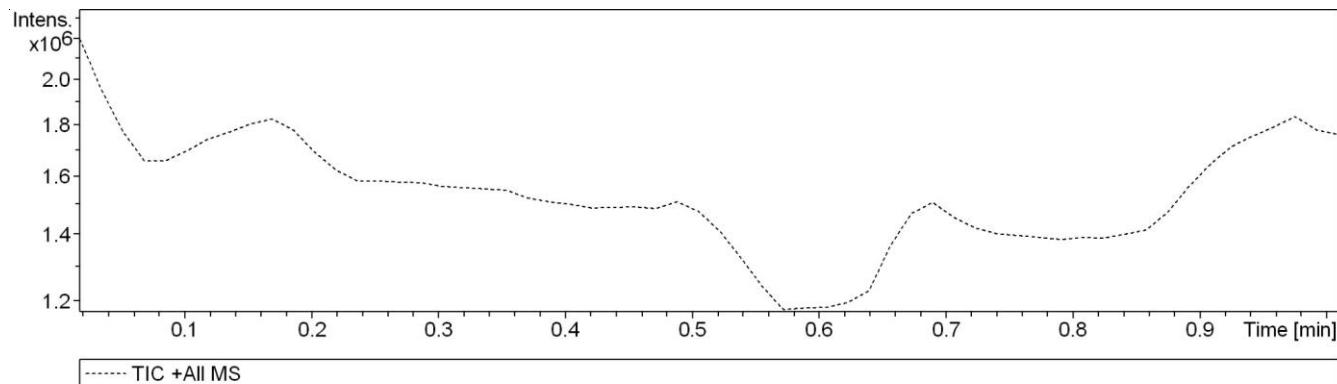
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Method 20100316_esi_pos_wide.m
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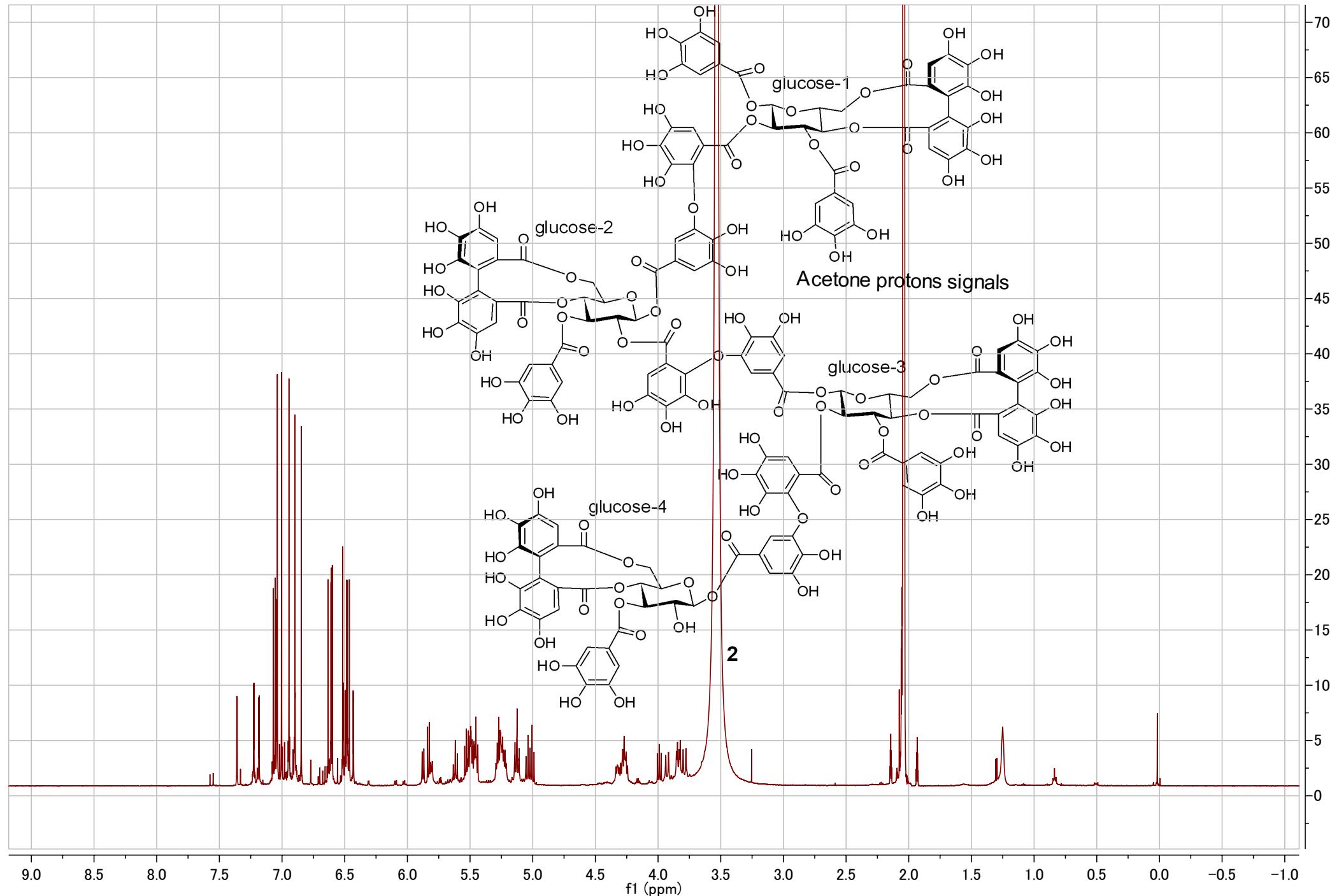
Operator bdal
 Instrument micrOTOF-Q 33

Acquisition Parameter

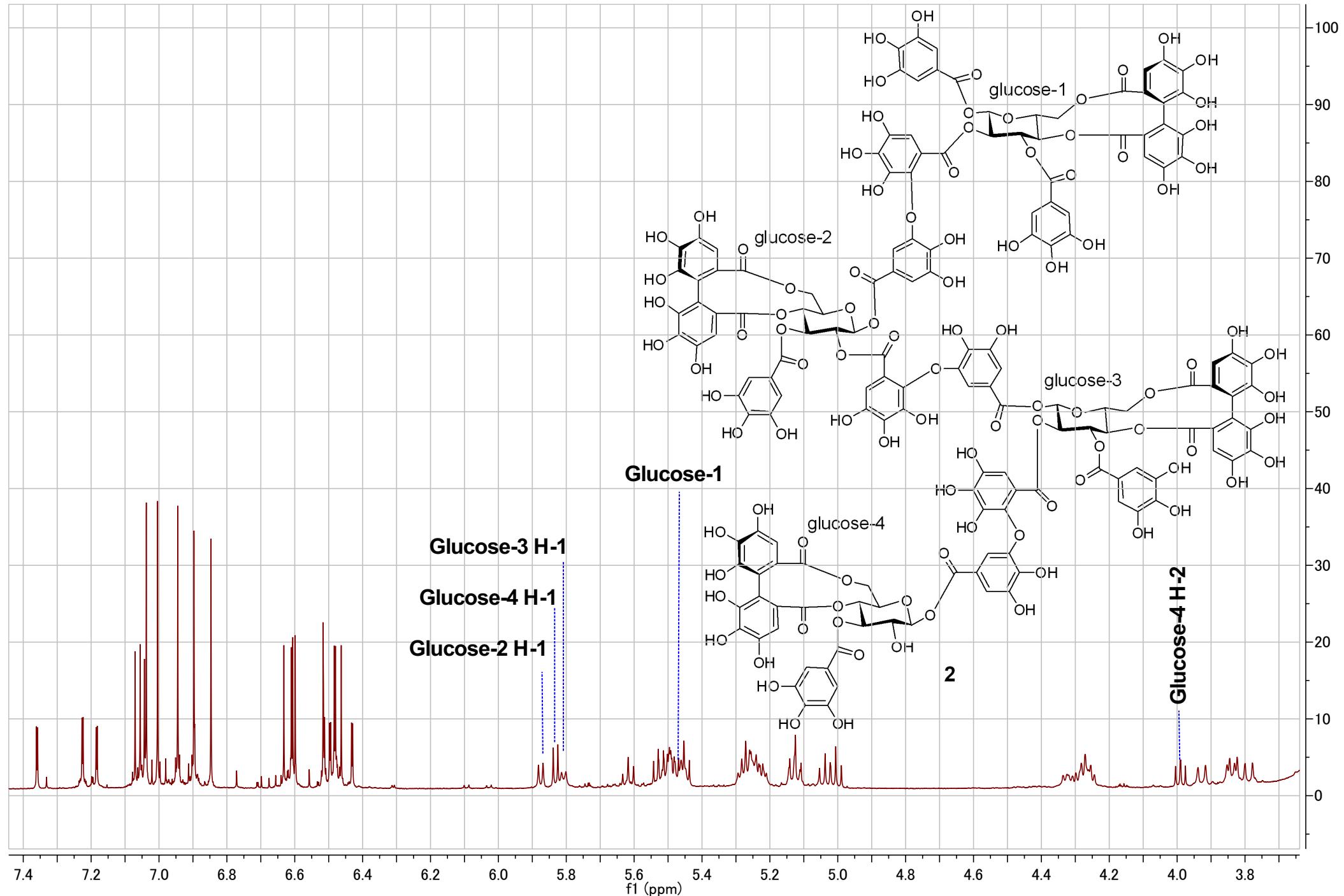
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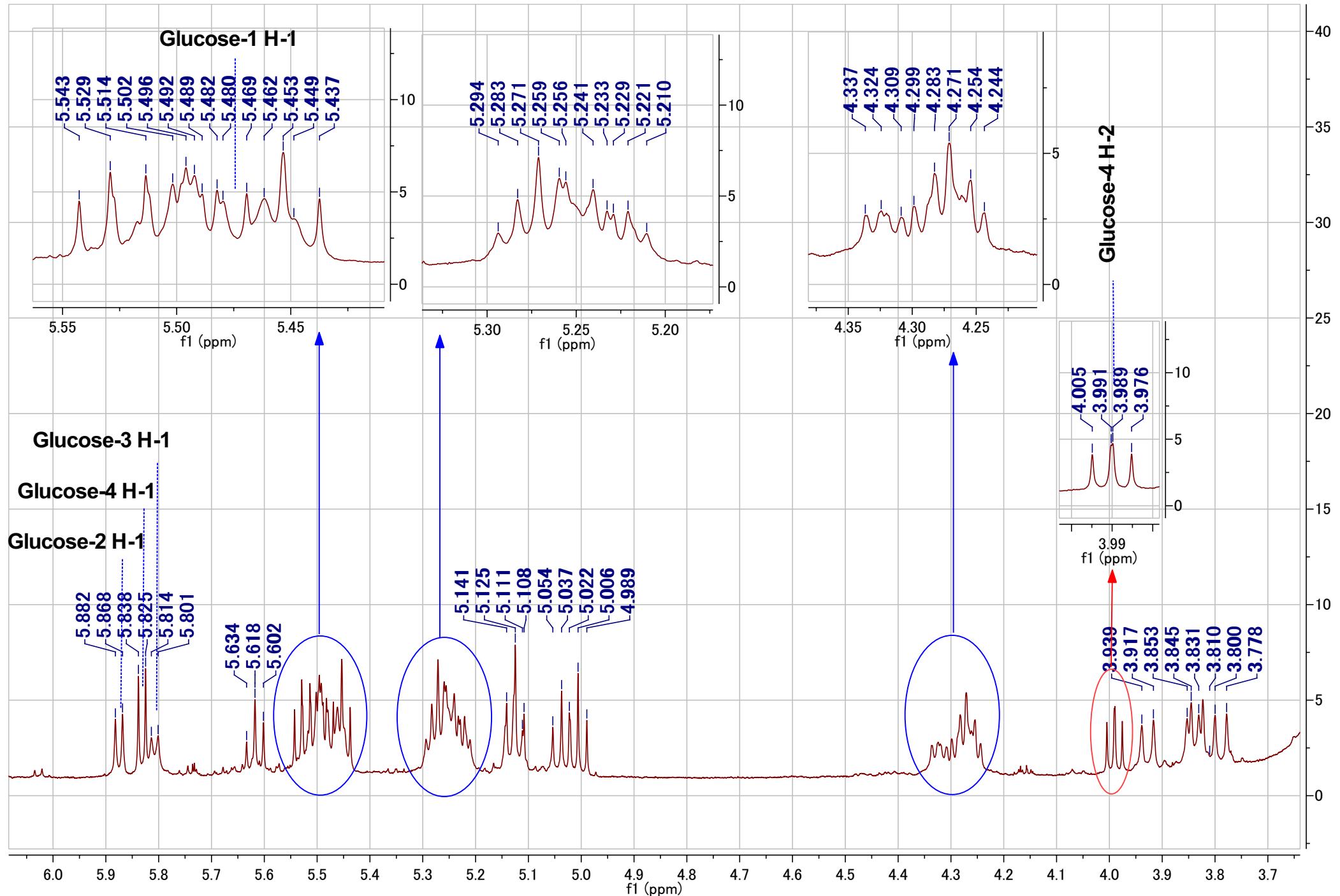
S6. (+)-HR-ESIMS spectrum of the new compound **1**



S7. ^1H NMR [600 MHz, (acetone- d_6 -D₂O, 9:1), 27 °C] spectrum of the new compound 2

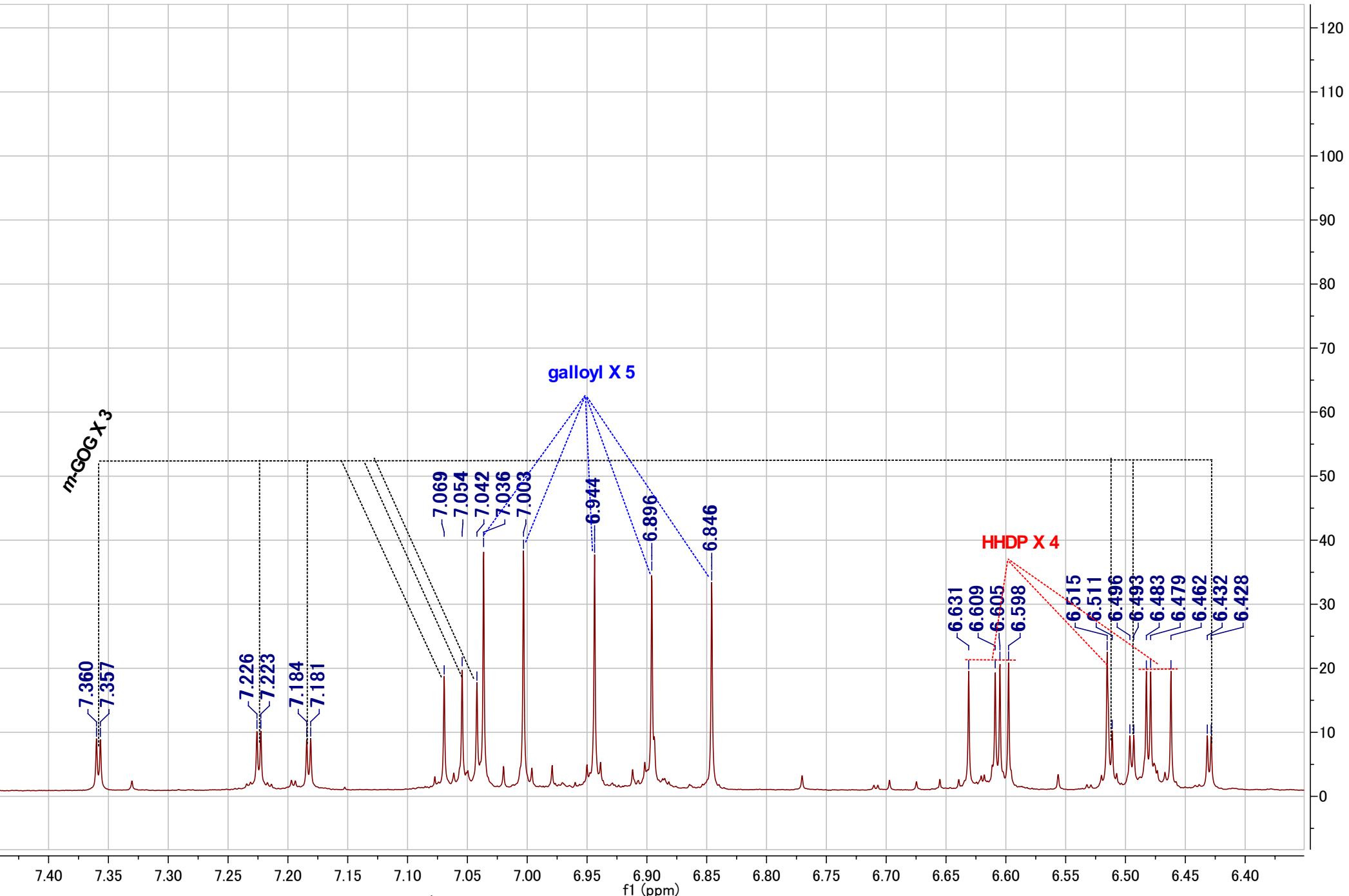


S8. Expanded ^1H NMR [600 MHz, (acetone- d_6 –D₂O, 9:1), 27 °C] spectrum of the new compound 2

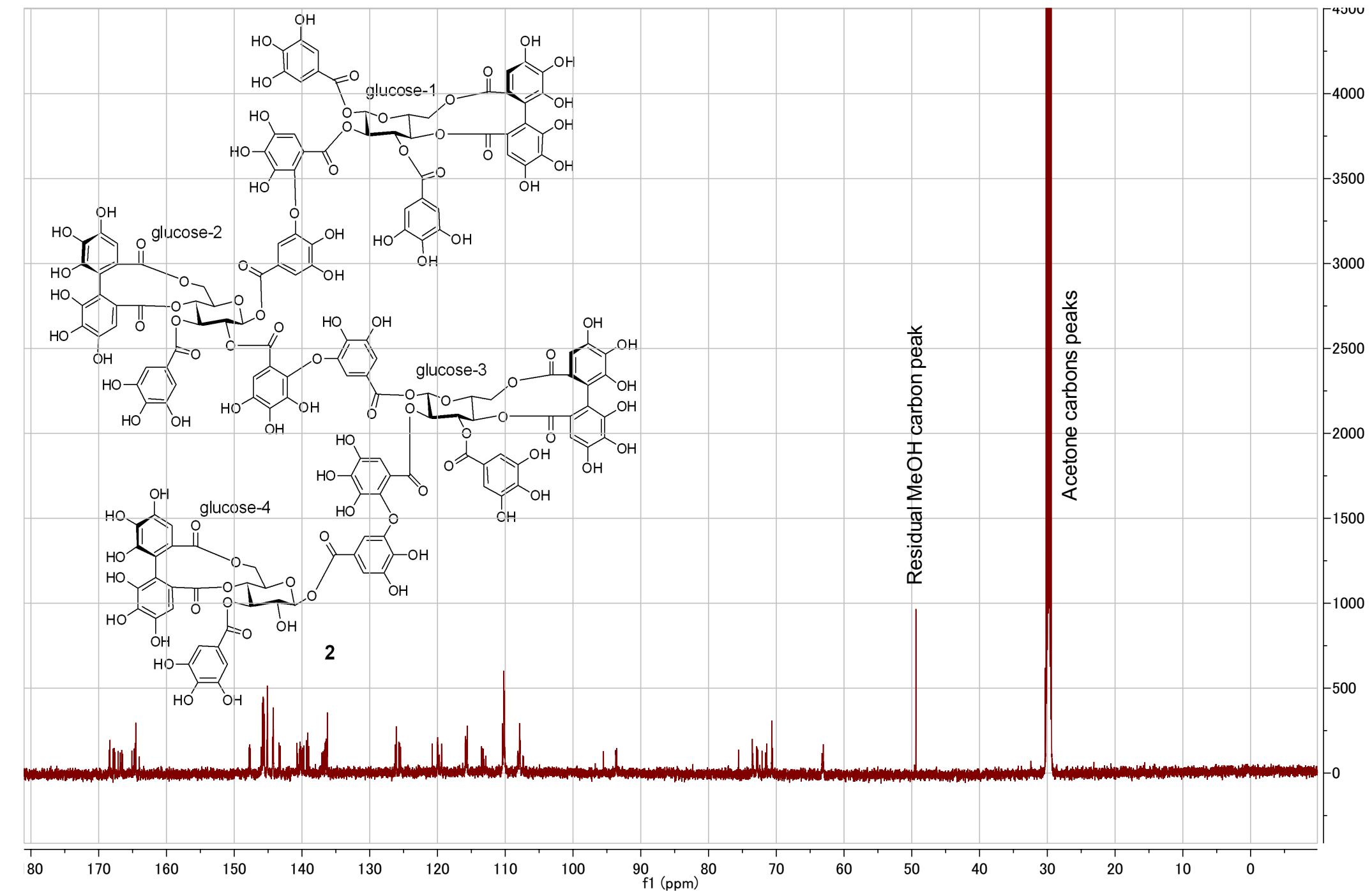


S9. Expanded aliphatic protons region of the ^1H NMR [600 MHz, (acetone- d_6 – D_2O , 9:1), 27 °C] spectrum of the new compound 2

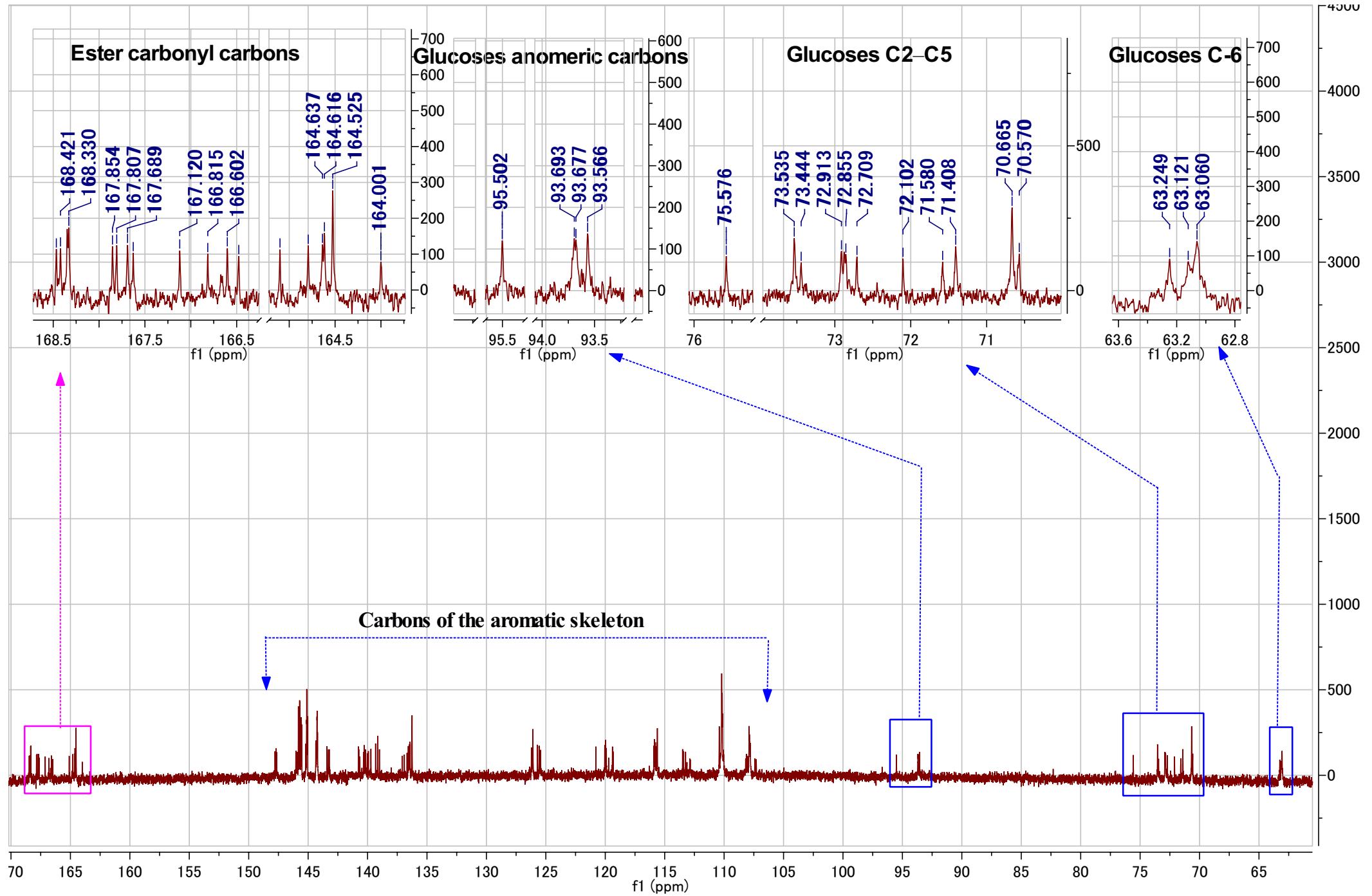
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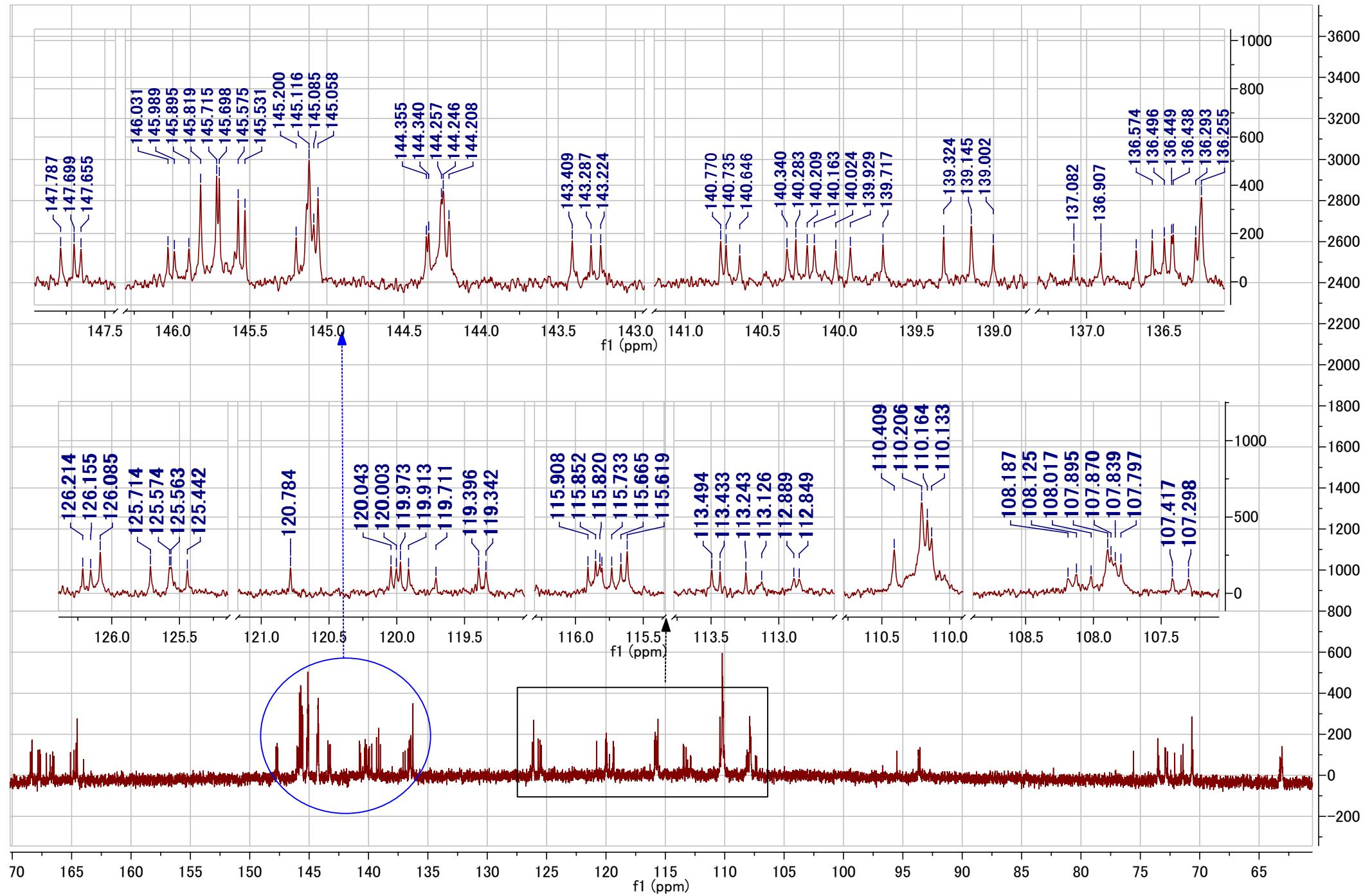
S10. Expanded aromatic protons region of ¹H NMR [600 MHz, (acetone-*d*₆-D₂O, 9:1), 27 °C] spectrum of the new compound 2



S11. ^{13}C NMR [151 MHz, (acetone- d_6 -D₂O, 9:1), 27 °C] spectrum of the new compound 2



S12. Expanded aliphatic and carbonyl carbons region of the ^{13}C NMR [151 MHz (acetone- d_6 –D₂O, 9:1), 27 °C] spectrum of the new compound 2



S13. Expanded aromatic carbons region of the ^{13}C NMR [151 MHz, (acetone- d_6 -D₂O, 9:1), 27 °C] spectrum of the new compound 2

Display Report

Analysis Info

Analysis Name **Nilotinib Q1 (2)**

Method 20100316_esi_pos_high.m

Sample Name

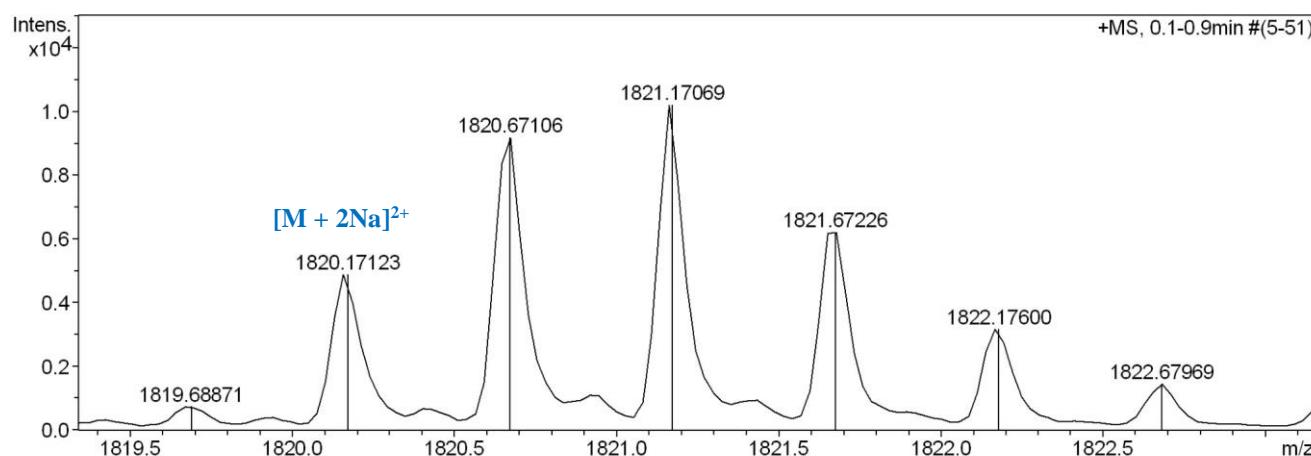
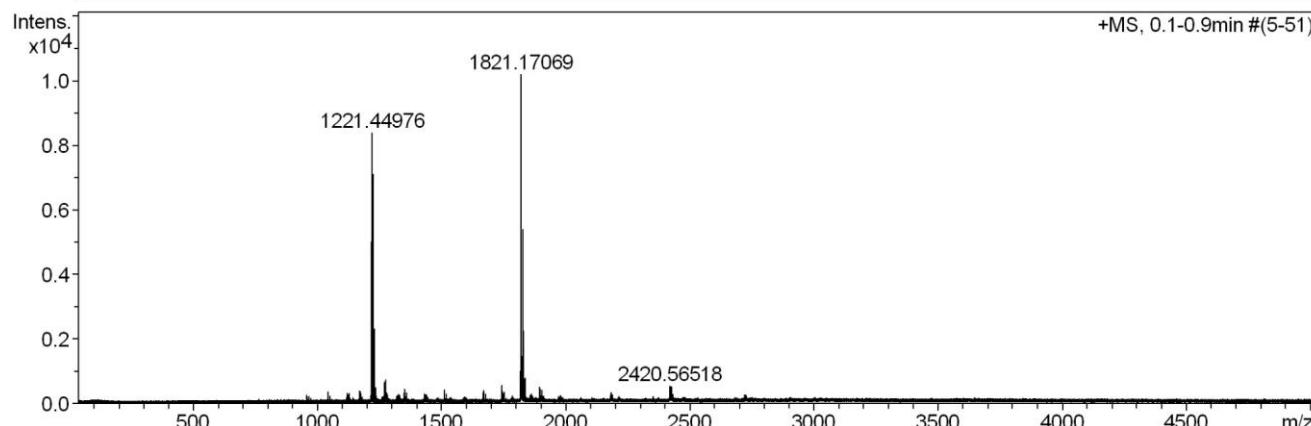
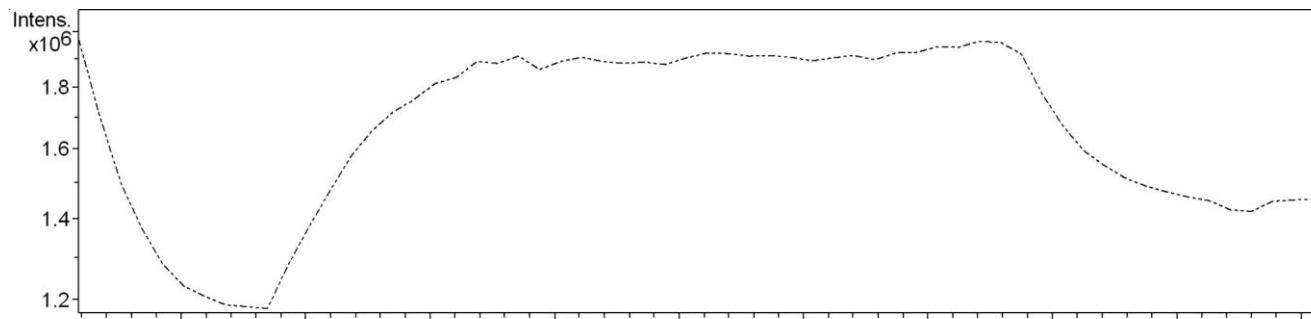
Operator
Instrument

bdal
micrOTOF-Q 33

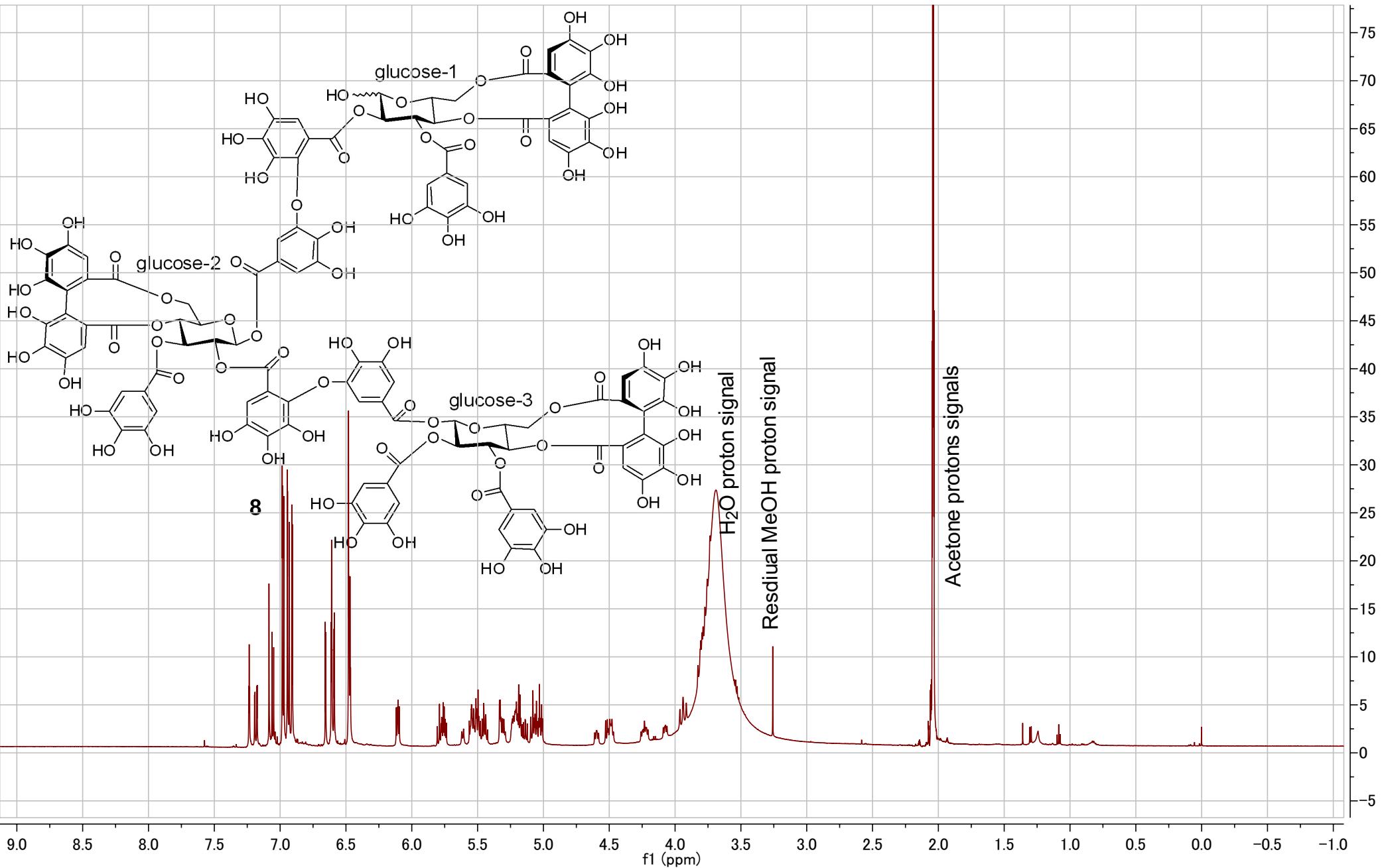
Comment

Acquisition Parameter

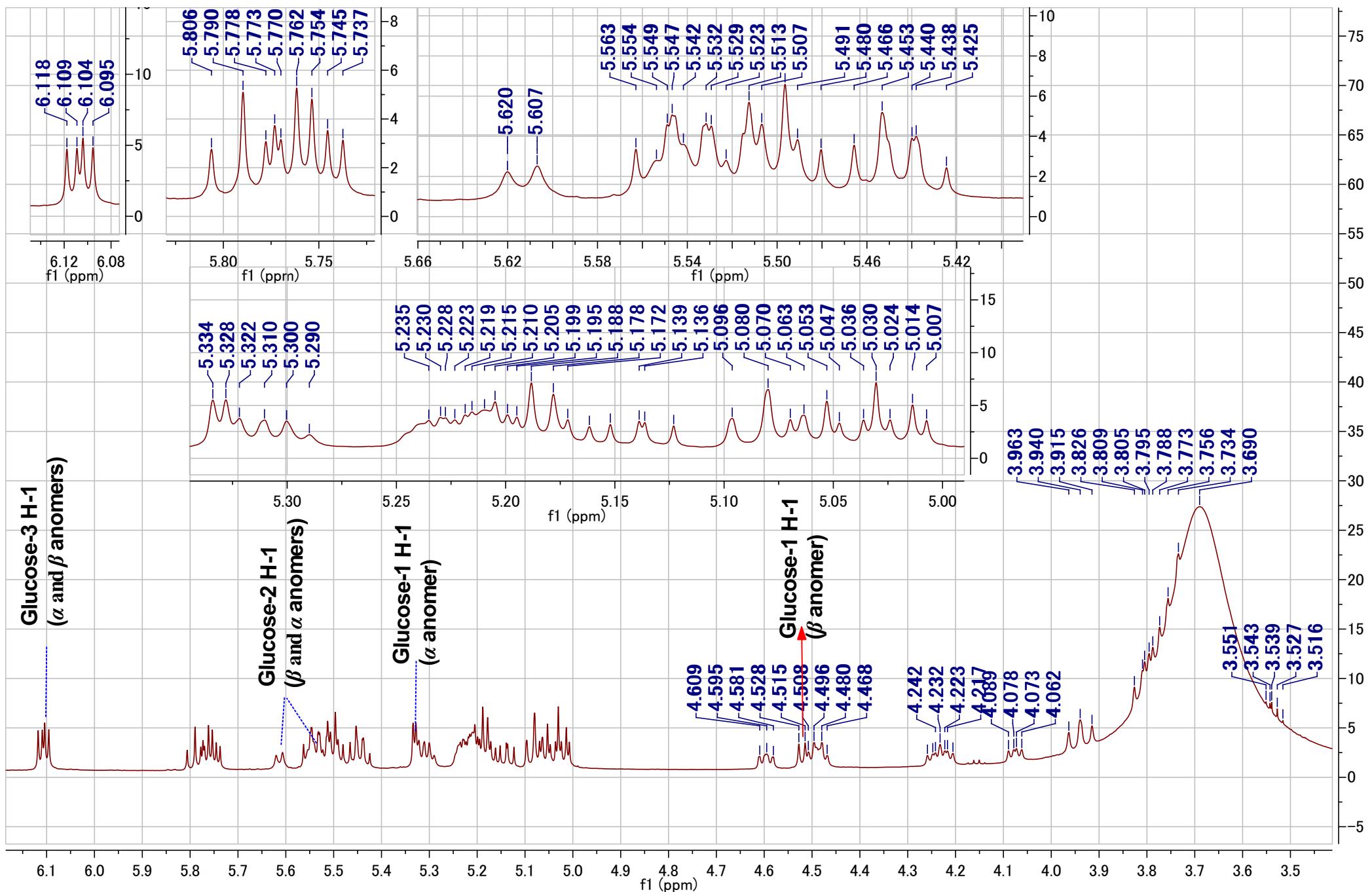
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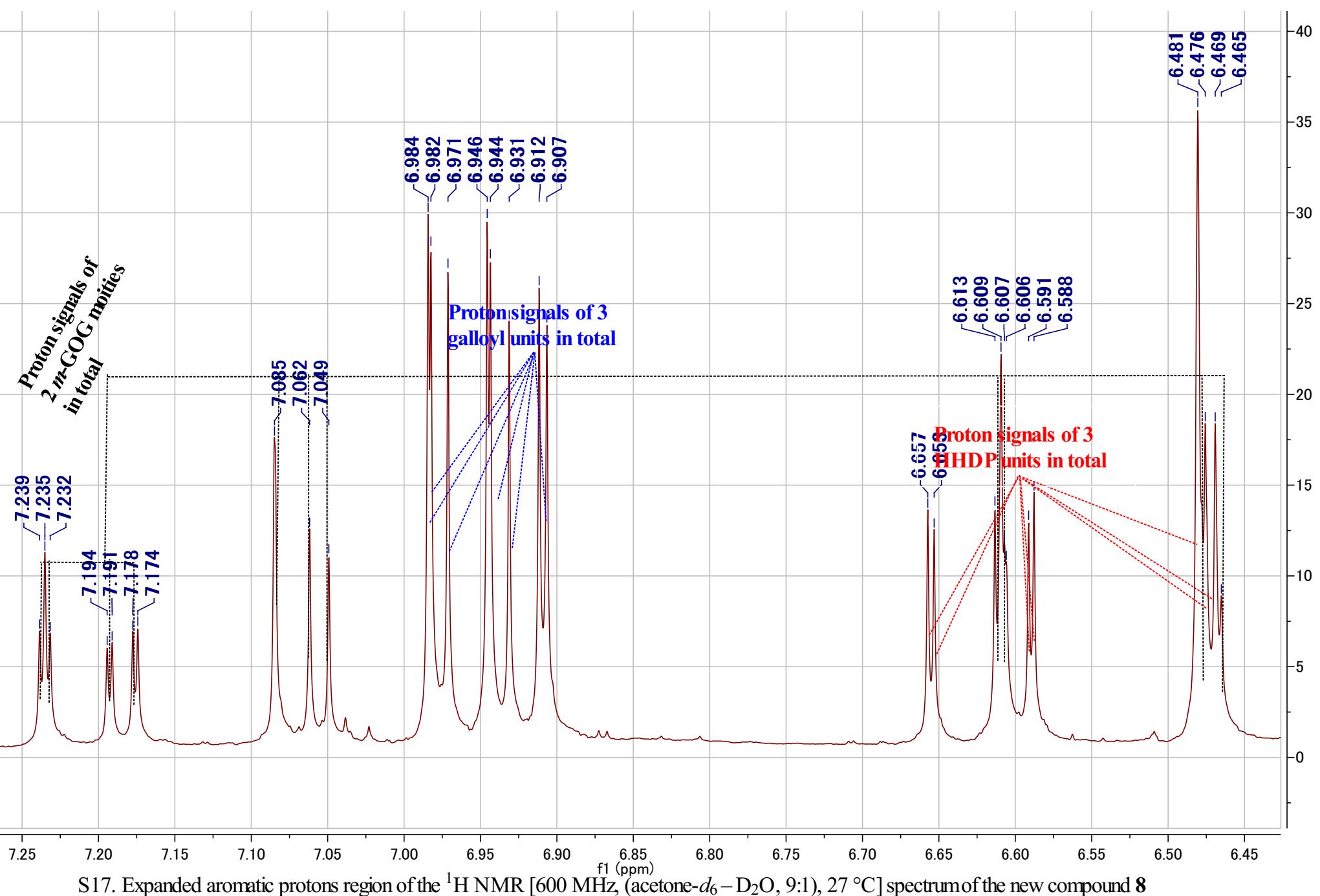
S14. (+)-HR-ESIMS spectrum of the new compound 2



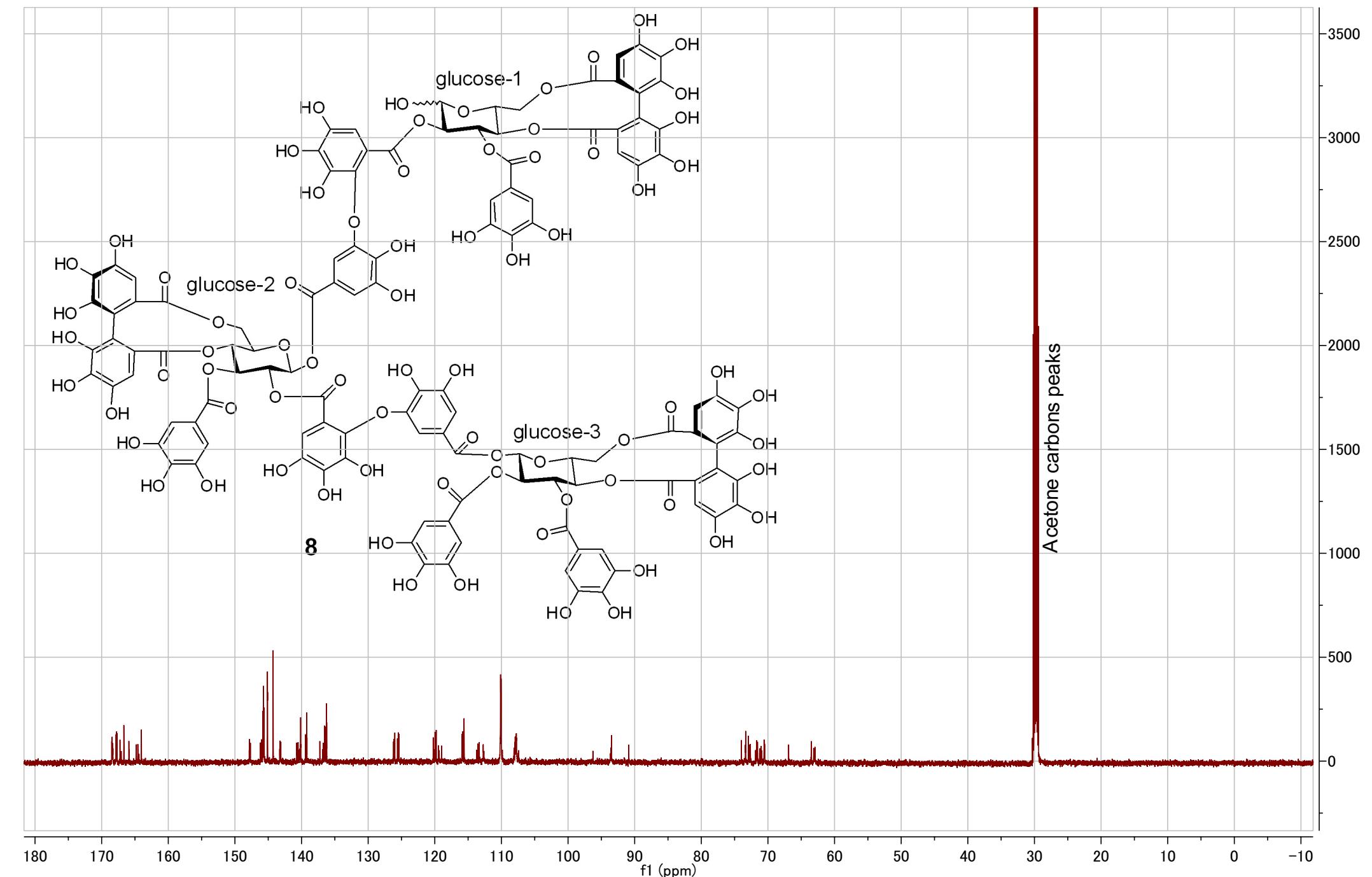
S15. ^1H NMR [600 MHz, (acetone- d_6 -D₂O, 9:1), 27 °C] spectrum of the new compound **8**



S16. Expanded aliphatic protons region of the ^1H NMR [600 MHz, ($\text{acetone-d}_6 - \text{D}_2\text{O}$, 9:1), 27 °C] spectrum of the new compound **8**

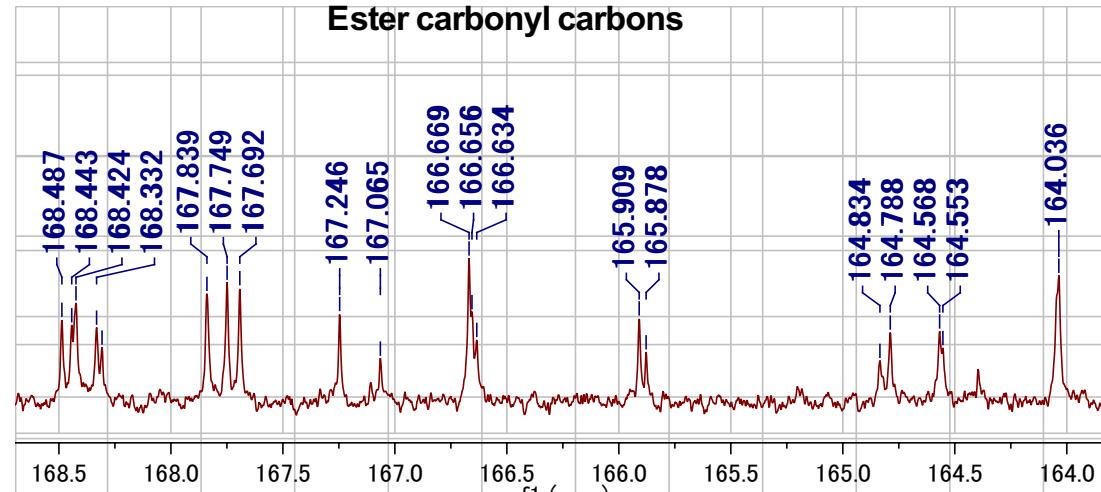


S17. Expanded aromatic protons region of the ^1H NMR [600 MHz, (acetone- d_6 – D_2O , 9:1), 27 °C] spectrum of the new compound **8**

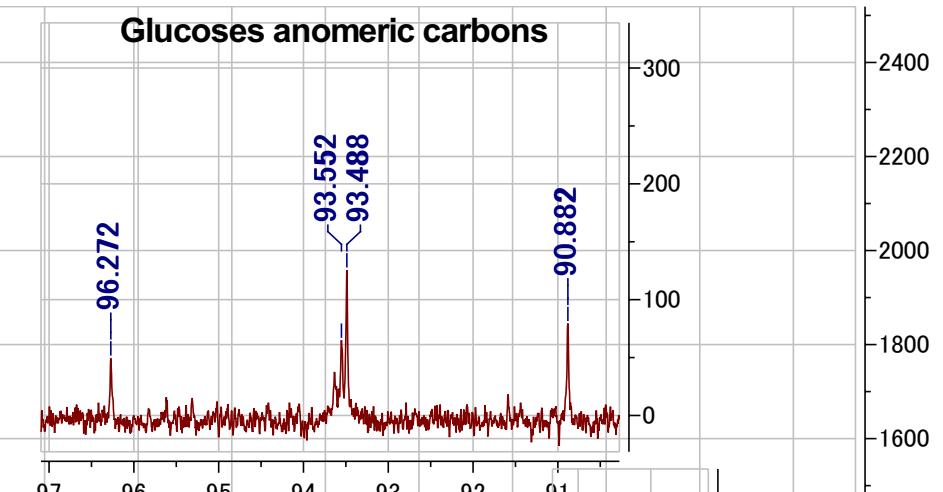


S18. ^{13}C NMR [151 MHz, (acetone- d_6 -D₂O, 9:1), 27 °C] spectrum of the new compound **8**

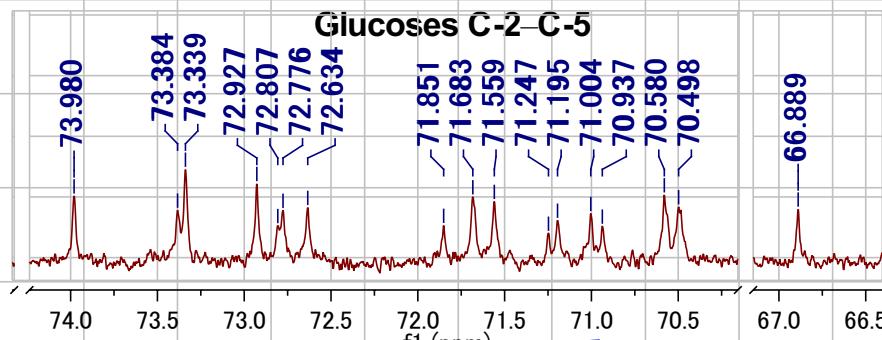
Ester carbonyl carbons



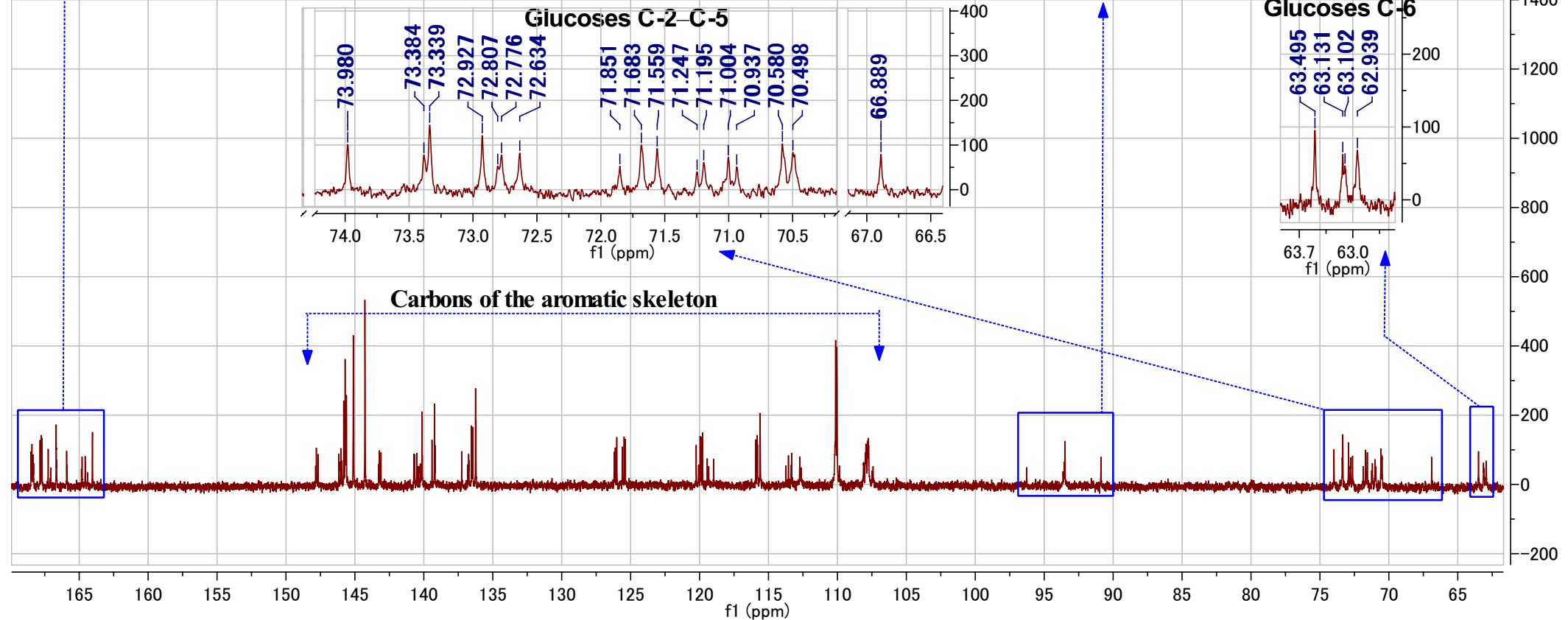
Glucoses anomeric carbons



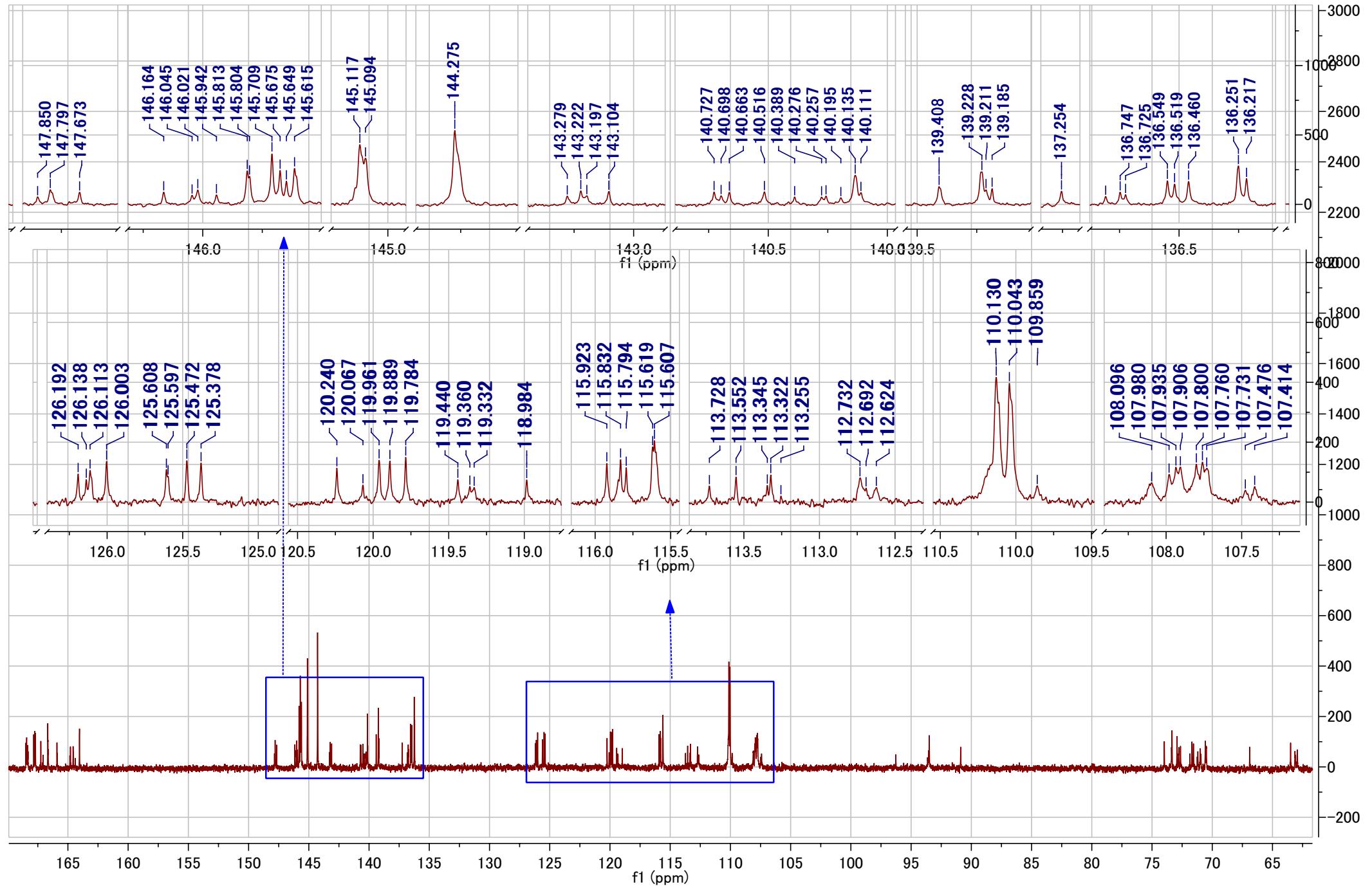
Glucoses C-2-C-5



Carbons of the aromatic skeleton



S19. Expanded aliphatic and carbonyl carbons regions of the ^{13}C NMR [151 MHz, (acetone- d_6 – D_2O , 9:1), 27 °C] spectrum of the new compound 8



S20. Expanded aromatic carbons region of the ^{13}C NMR [151 MHz, (acetone- d_6 – D₂O, 9:1), 27 °C] spectrum of the new compound 8

Display Report

Analysis Info

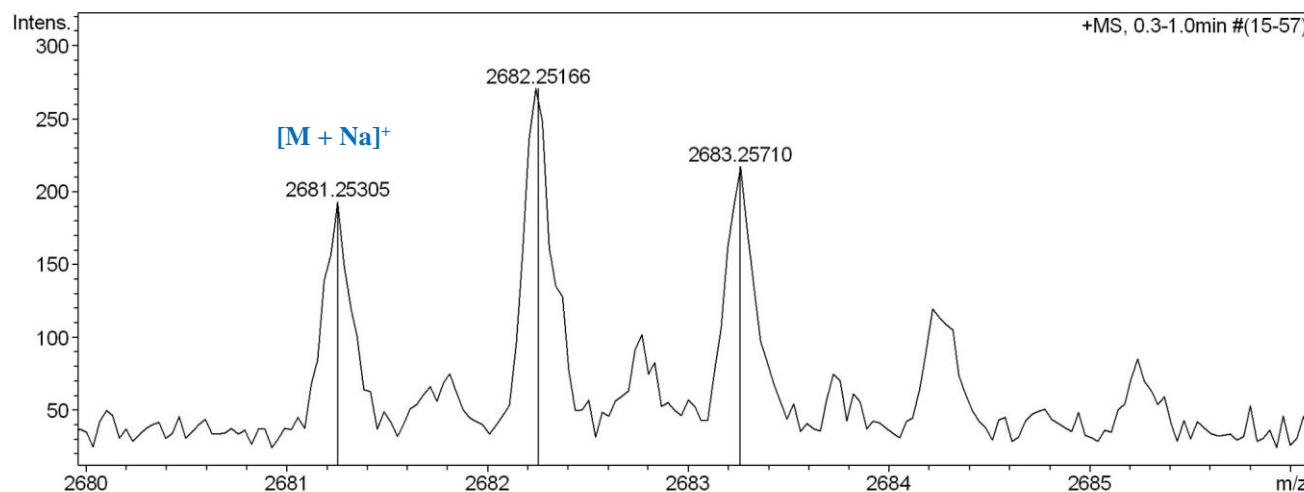
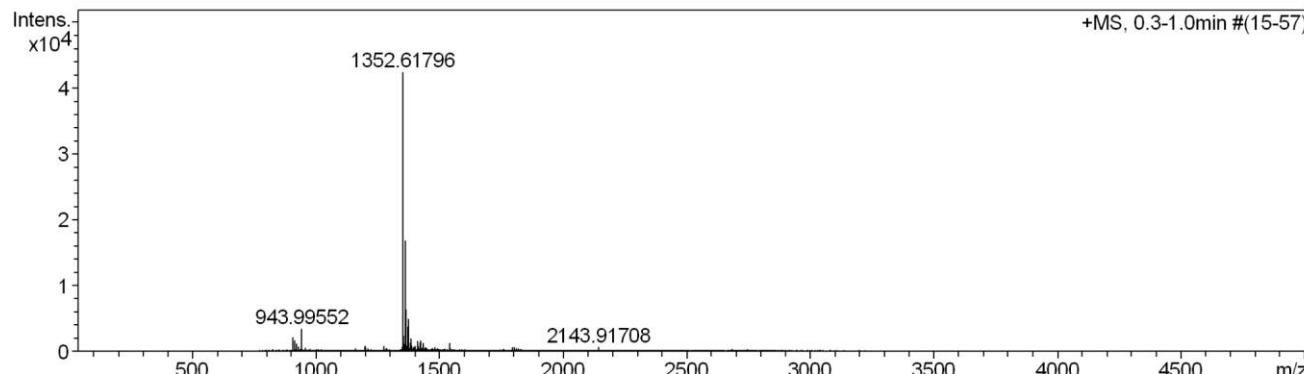
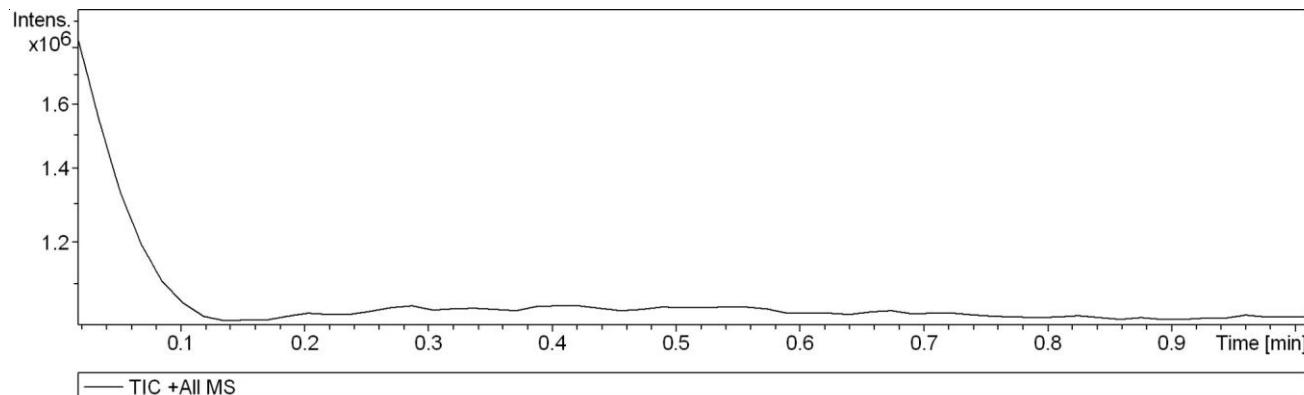
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Method 20100316_esi_pos_high.m
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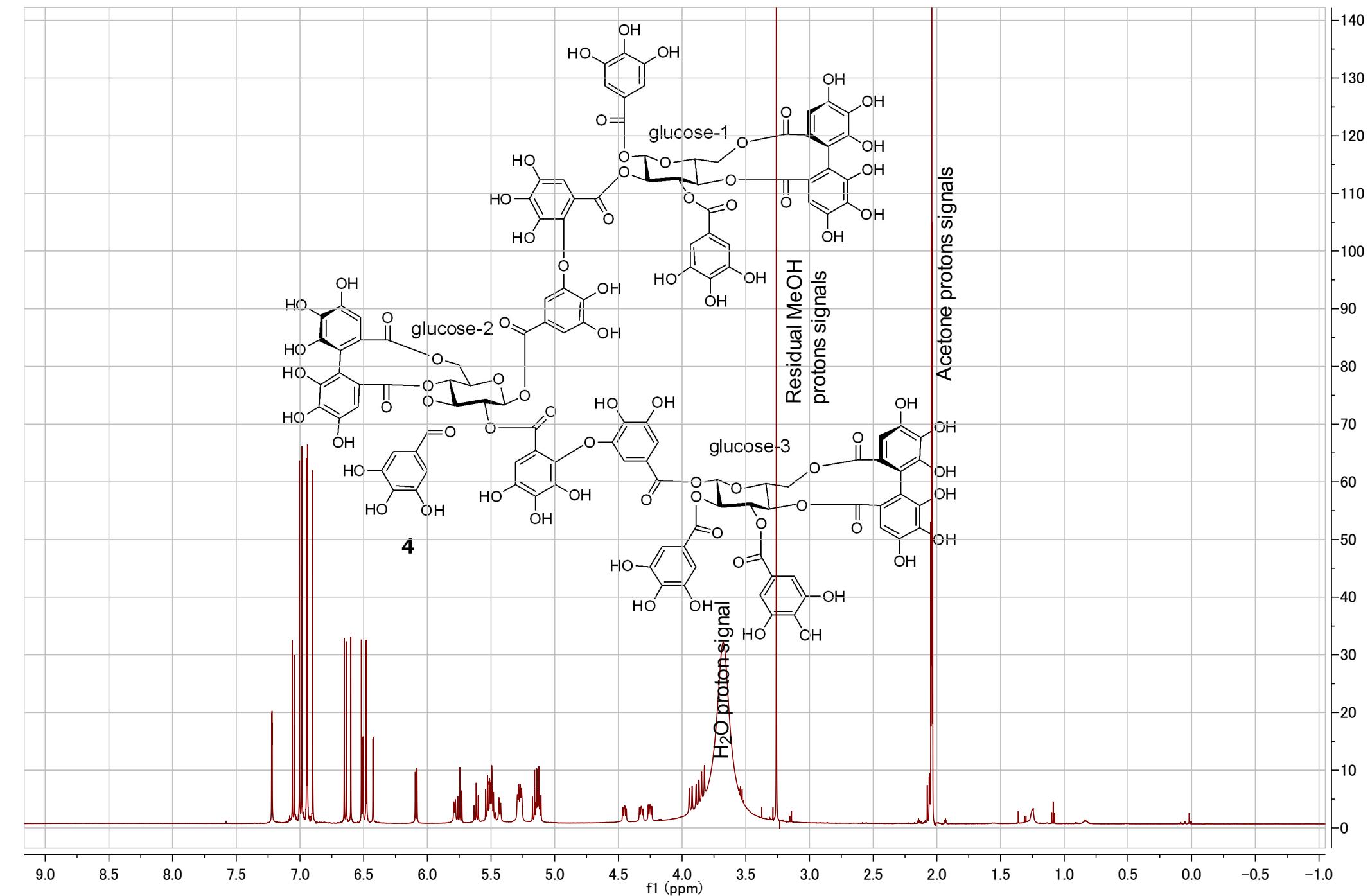
Operator bdal
 Instrument micrOTOF-Q 33

Acquisition Parameter

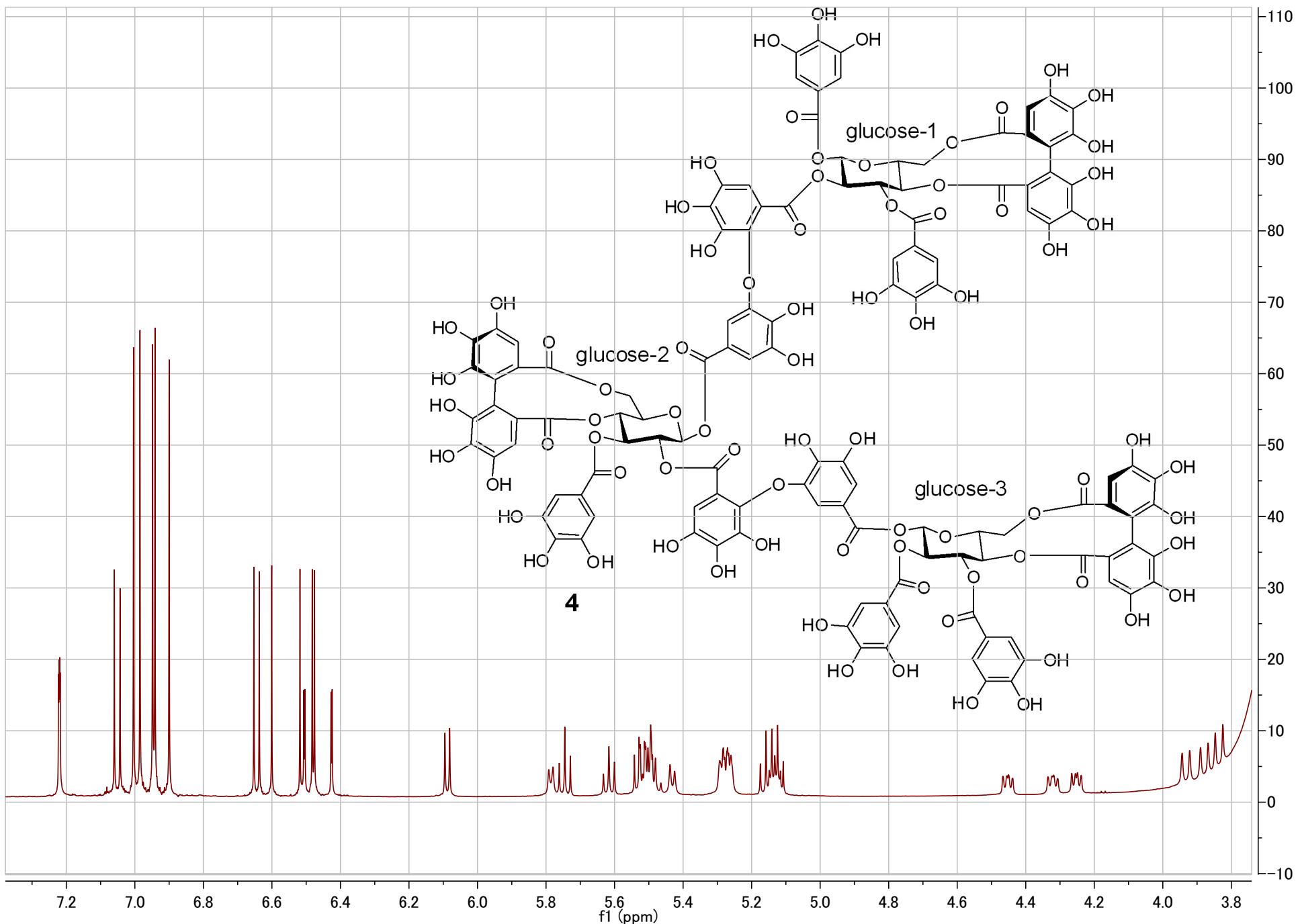
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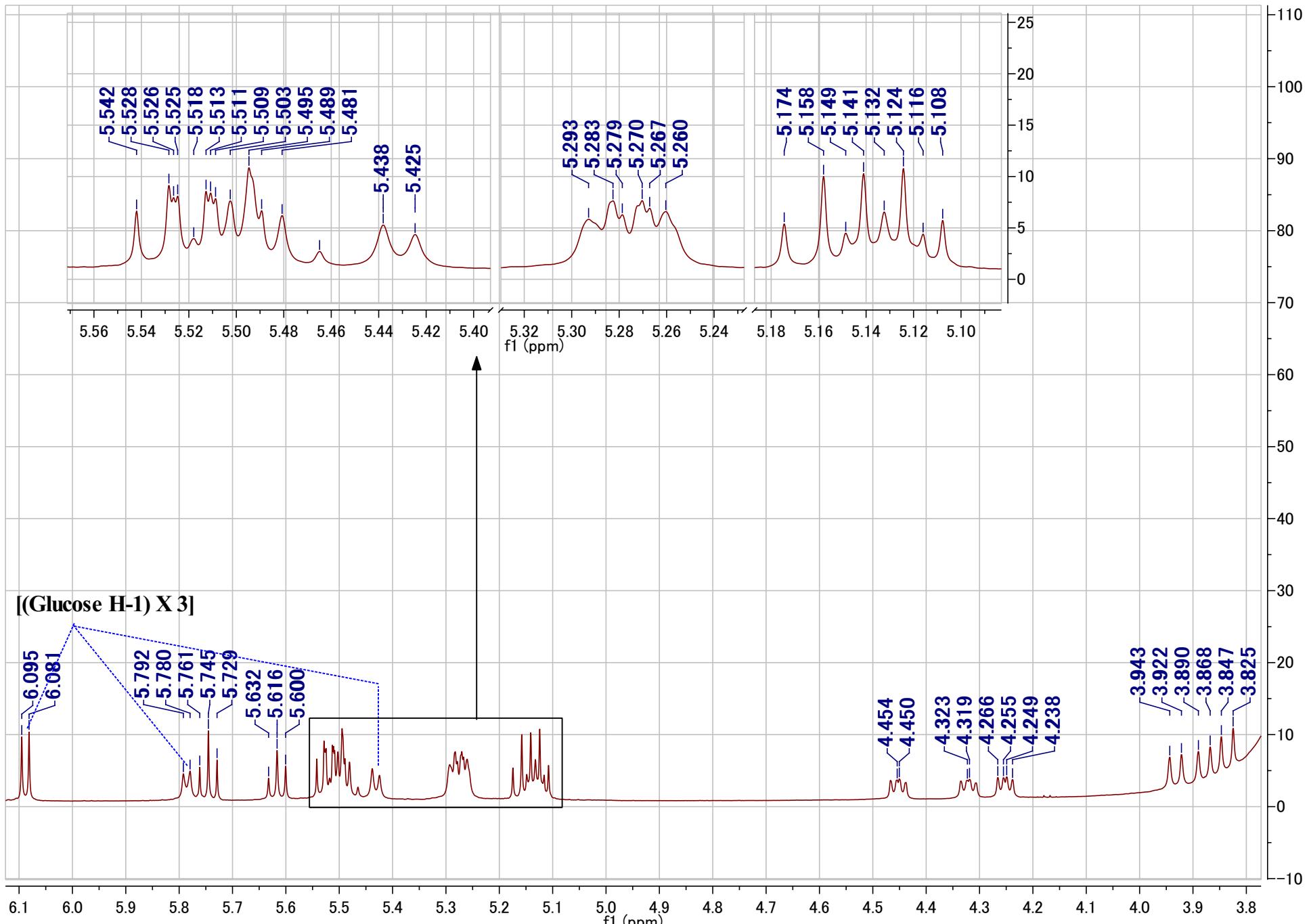
S21. (+)-HR-ESIMS spectrum of the new compound **8**



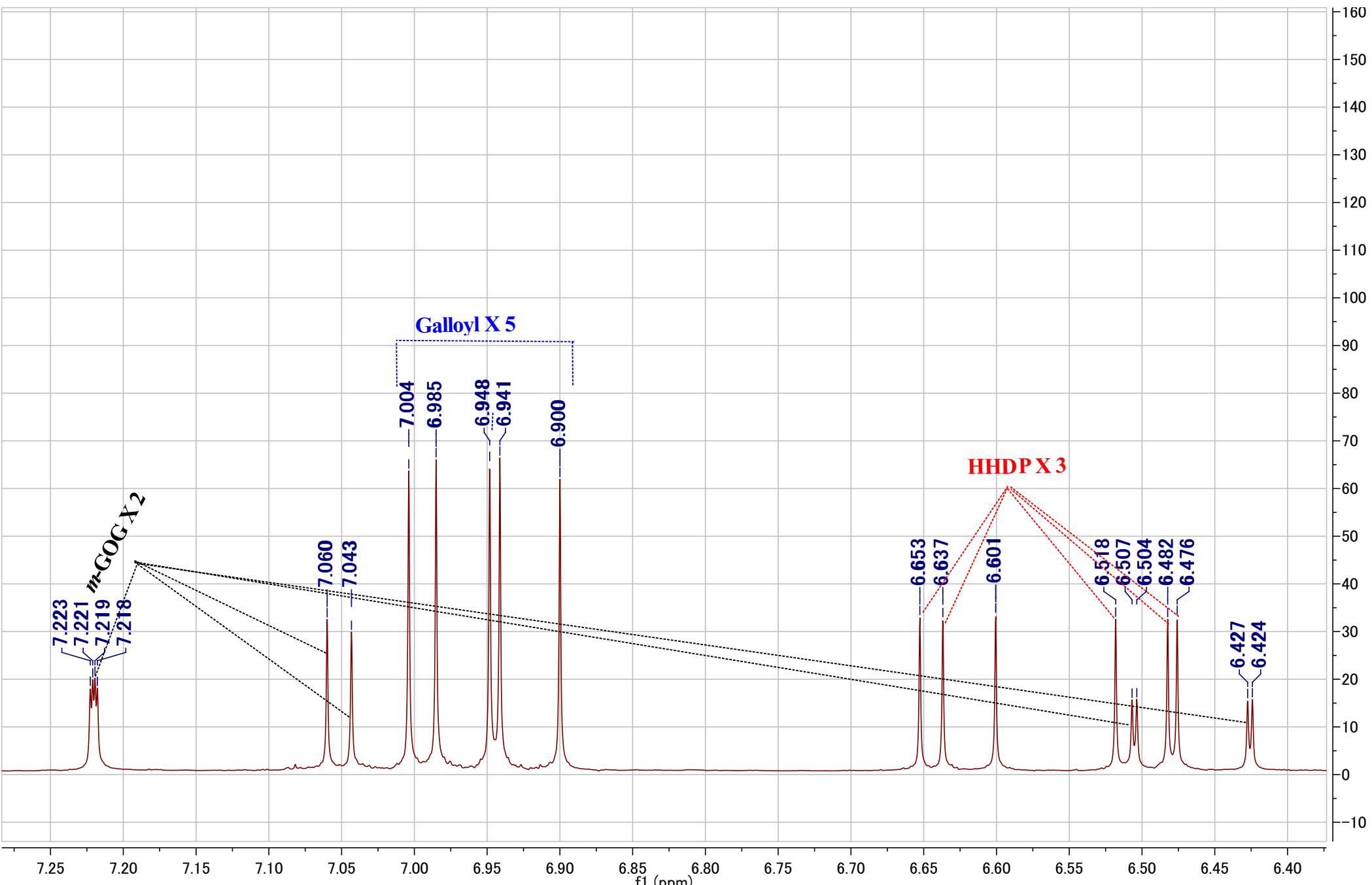
S22. ^1H NMR [600 MHz, (acetone- d_6 – D_2O , 9:1), 27 °C] spectrum of the known compound hirtellin T1 (4)



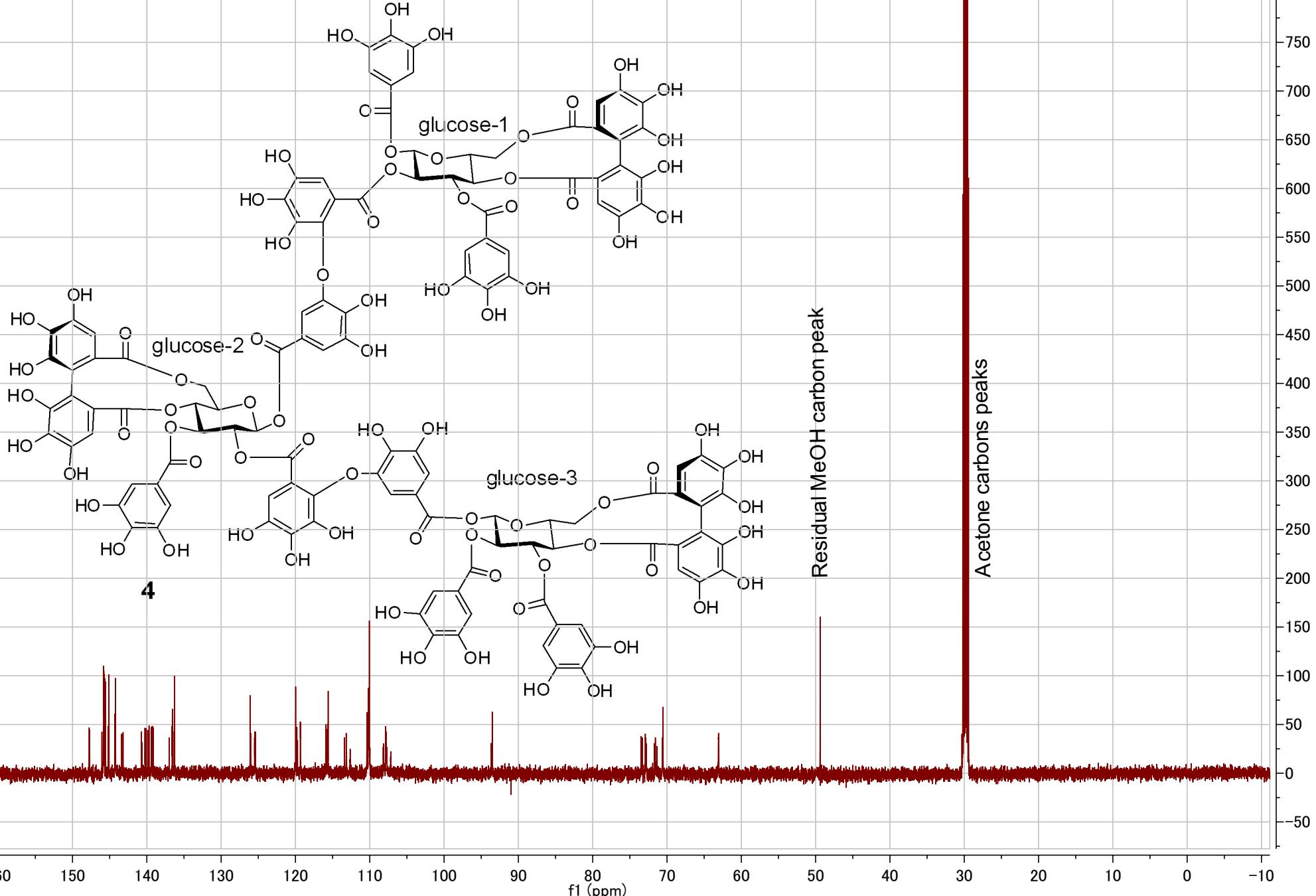
S23. Expanded ^1H NMR [600 MHz, (acetone- d_6 –D₂O, 9:1), 27 °C] spectrum of the known compound hirtellin T1 (**4**)



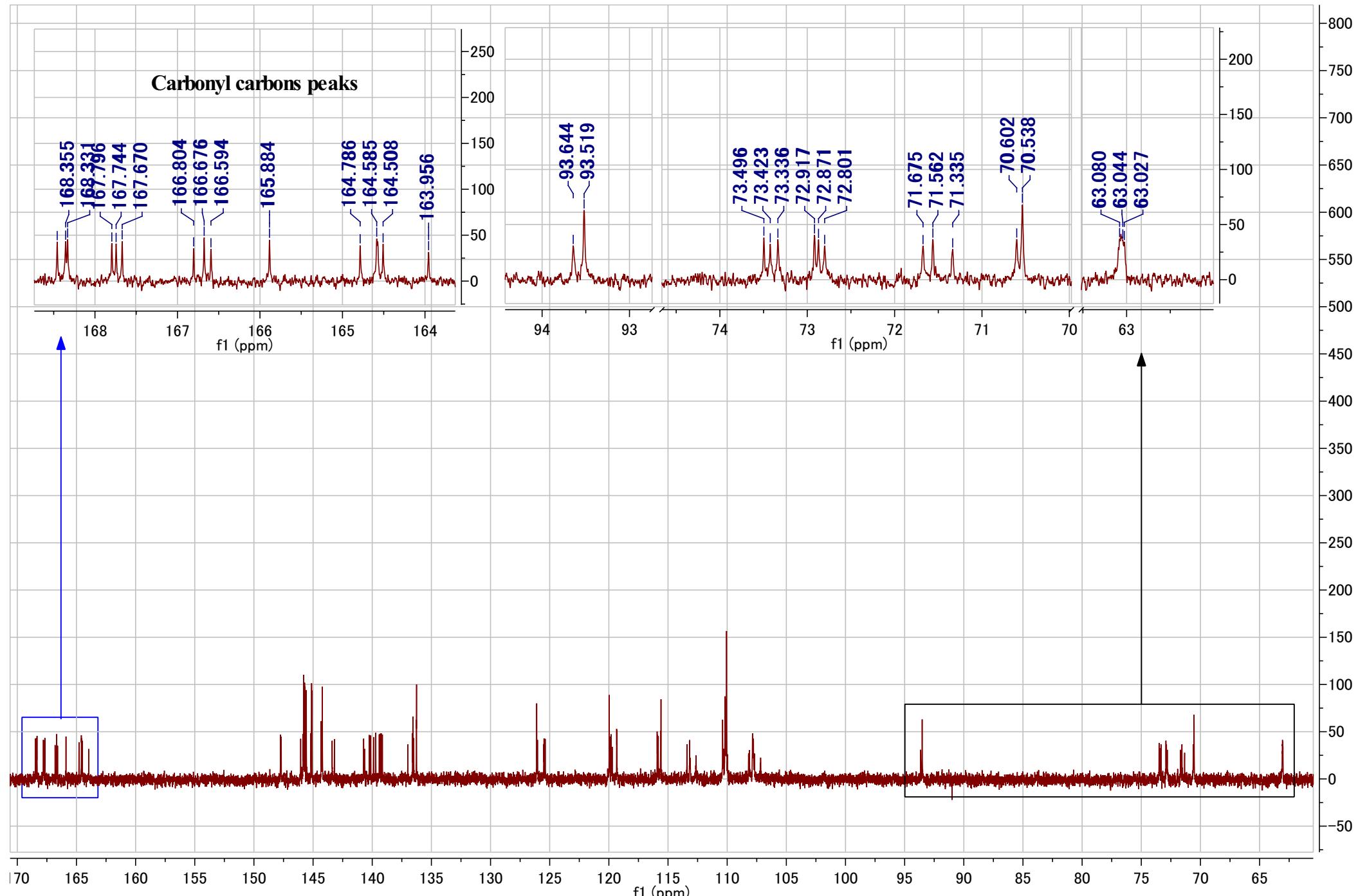
S24. Expanded aliphatic protons region of ^1H NMR [600 MHz, (acetone- d_6 – D_2O , 9:1), 27 °C] spectrum of the known compound hirtellin T1 (4)



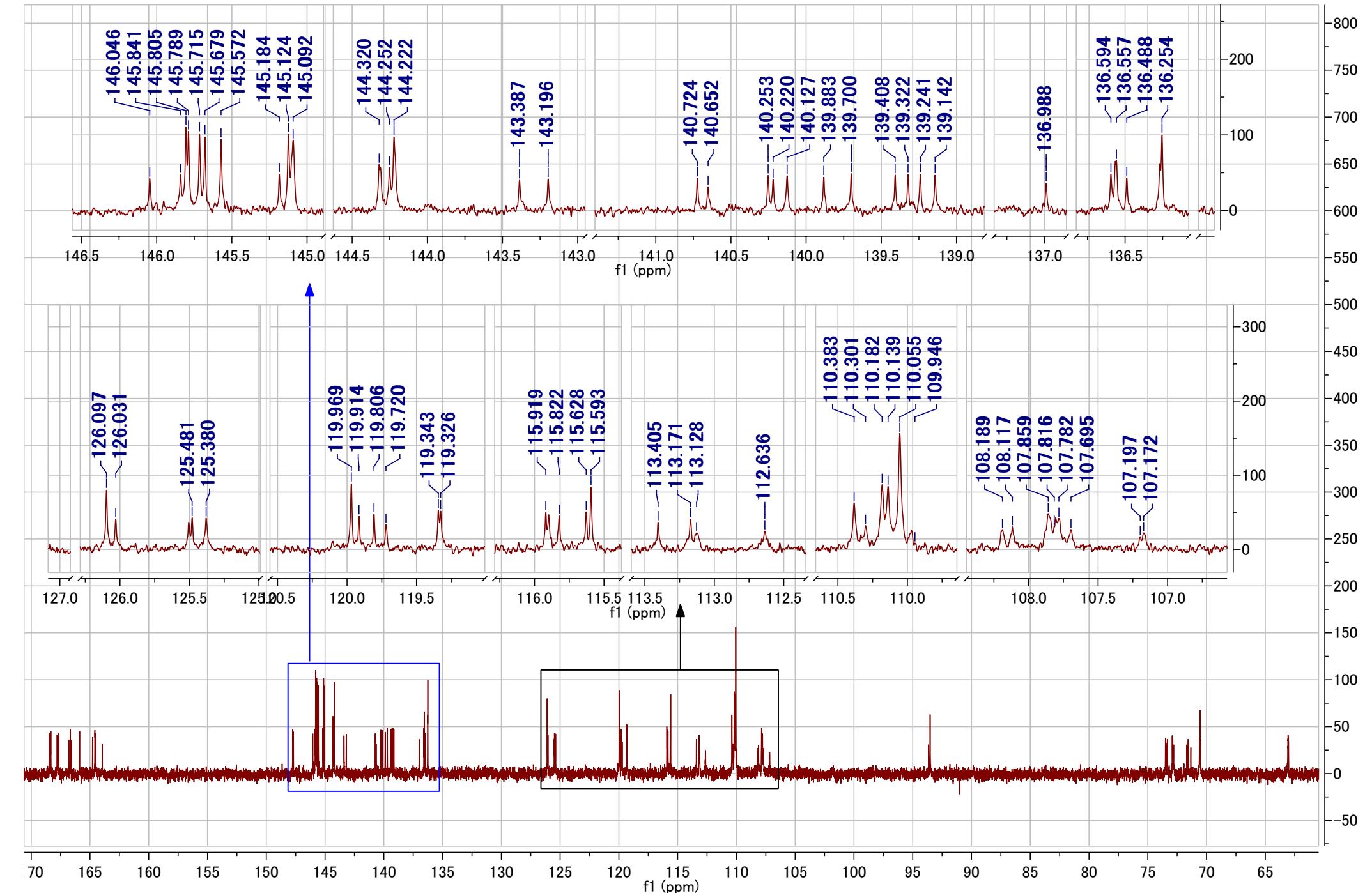
S25. Expanded aromatic protons region of ^1H NMR [600 MHz, (acetone- d_6 –D₂O, 9:1), 27 °C] spectrum of the known compound hirtellin T1 (**4**)



S26. ^{13}C NMR [151 MHz, (acetone- d_6 – D_2O , 9:1), 27 °C] spectrum of the known compound hirtellin T1 (4)



S27. Expanded aliphatic and carbonyl carbons regions of the ^{13}C NMR [151 MHz, (acetone- d_6 -D₂O, 9:1), 27 °C] spectrum of hirtellin T1 (**4**)



S28. Expanded aromatic carbons region of the ^{13}C NMR [151 MHz, (acetone- d_6 – D_2O , 9:1), 27 °C] spectrum of hirtellin T1 (4)

Display Report

Analysis Info

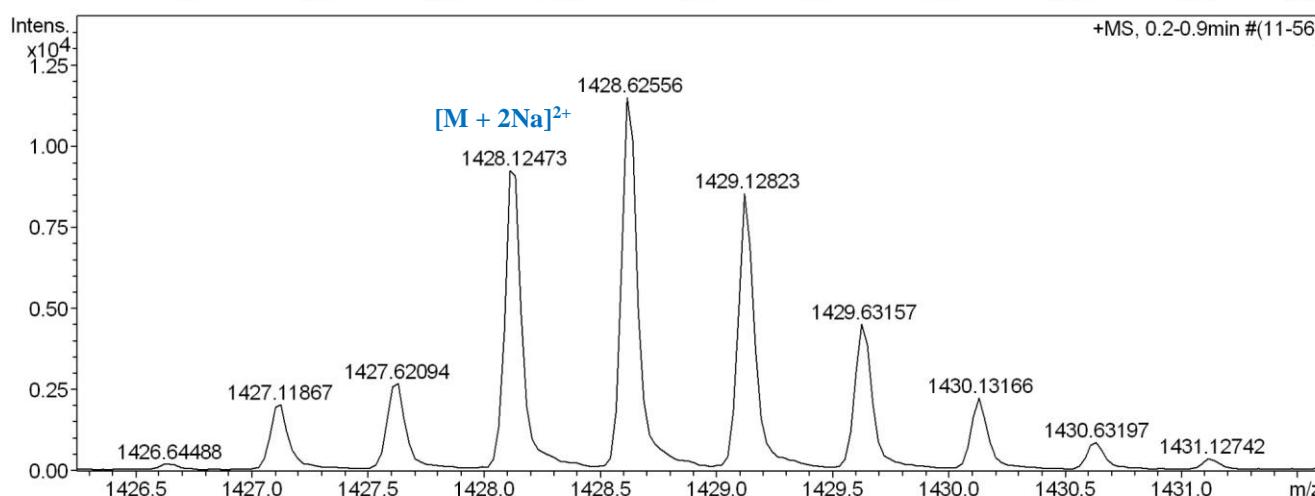
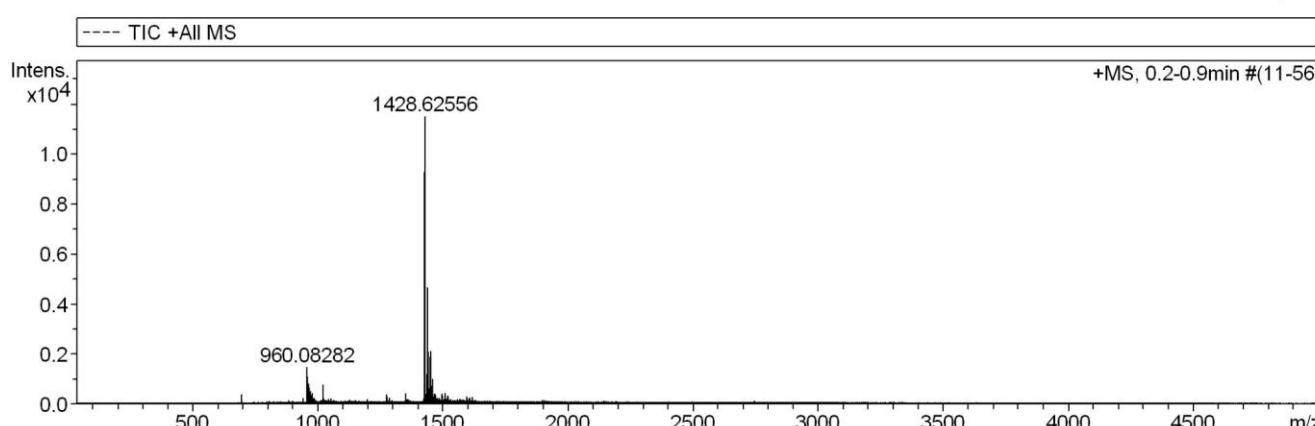
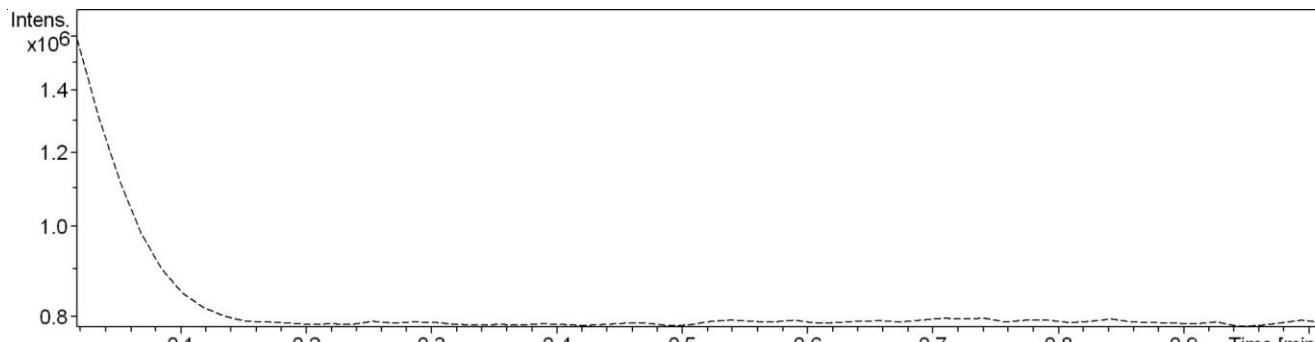
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Method 20100316_esi_pos_high.m
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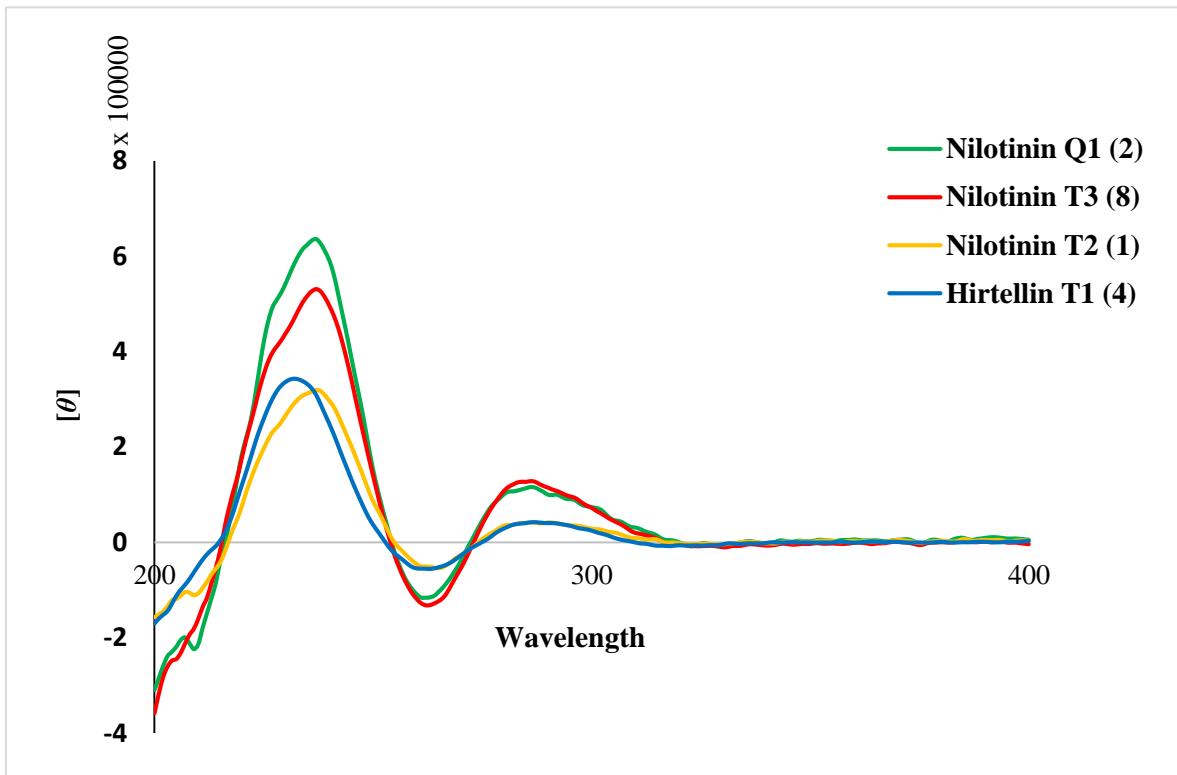
Operator bdal
 Instrument micrOTOF-Q 33

Acquisition Parameter

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Scan End	5000 m/z	Set Collision Cell RF	1300.0 Vpp	Set Divert Valve	Source



S29. (+)-HR-ESIMS spectrum of hirtellin T1 (**4**)



S30. ECD spectra of the new ellagittannins **1**, **2** and **8** in comparison with that of the known one hirtellin T1 (**4**)