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### Molecular identification in metabolomics using infrared ion spectroscopy

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## Supporting information

### Molecular identification in metabolomics using infrared ion spectroscopy

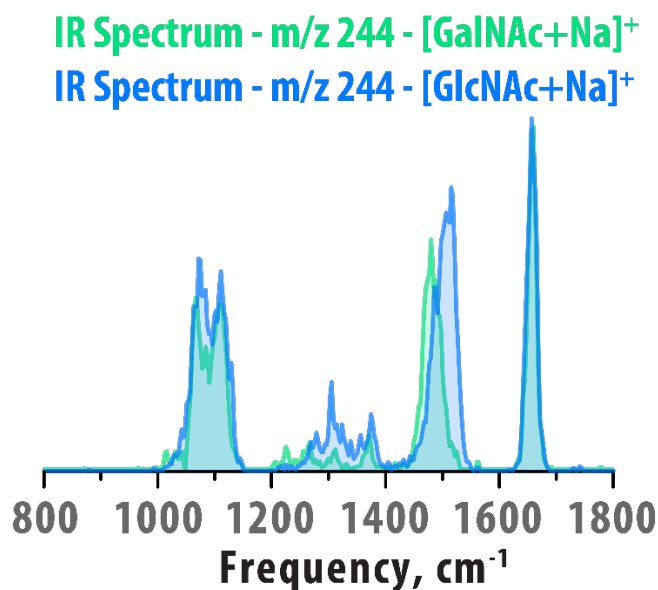
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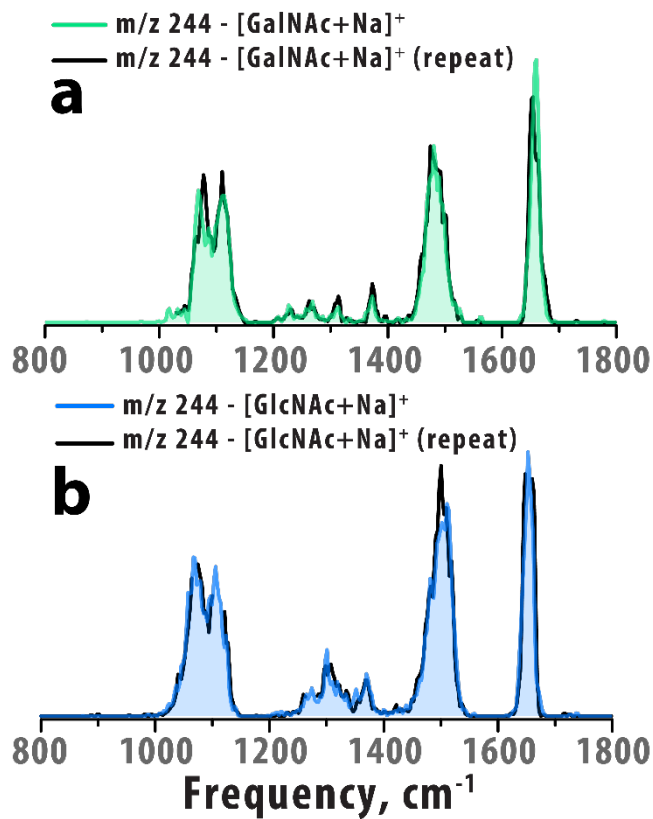
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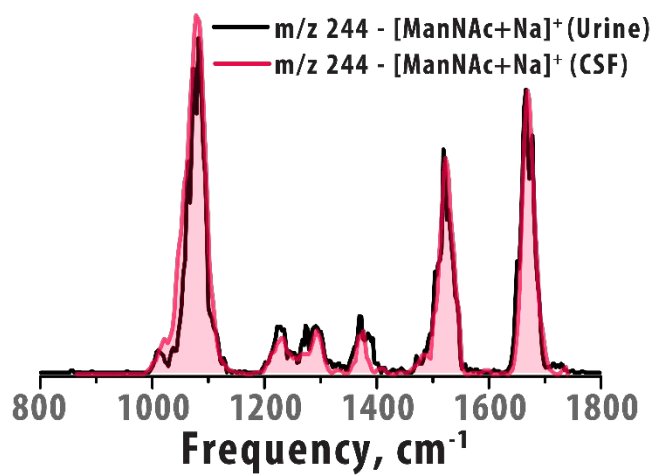
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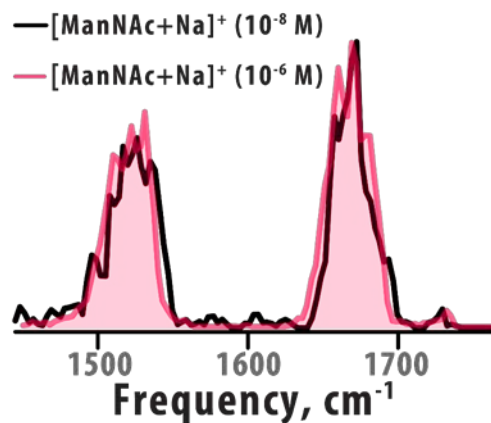
**Figure S1** | IR spectra of GalNAc and GlcNAc reference model compounds illustrating that each of the three N-acetylhexosamines are distinguishable from one another on the basis of the IR spectra.



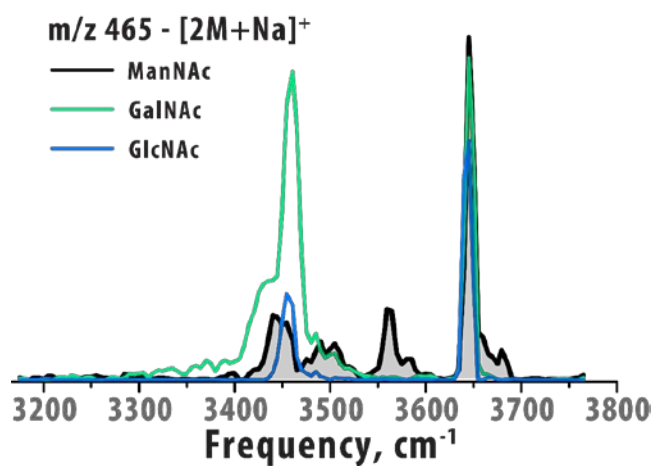
**Figure S2** | Panels (a) and (b) present duplicate IR spectra measured for the GalNAc and GlcNAc reference model compounds, respectively, demonstrating the reproducibility of the distinctive features of their IR spectra in both cases.



**Figure S3** | The IR spectrum of ManNAc measured after direct infusion +ESI of a diluted urine sample (black) and a cerebrospinal fluid sample (CSF, red).



**Figure S4** | Partial IR spectrum of the ManNAc reference compound measured at 10<sup>-8</sup> M (black) and at 10<sup>-6</sup> M (red), demonstrating that IR spectra are largely concentration independent over a wide range.



**Figure S5** | IR spectra of [2M+Na]<sup>+</sup> ions from the three N-acetylhexosamines discussed in Figure 1 generated using an OPO IR source in the 3200-3800 cm<sup>-1</sup> region. The [2M+Na]<sup>+</sup> dimer complex ions were selected because the [M+Na]<sup>+</sup> monomer ions did not show sufficient fragmentation after irradiation with the relatively low-power OPO output (<15 mJ pulse energy).