



## Supporting Information

for

### **Using UHPLC–MS profiling for the discovery of new sponge-derived metabolites and anthelmintic screening of the NatureBank bromotyrosine library**

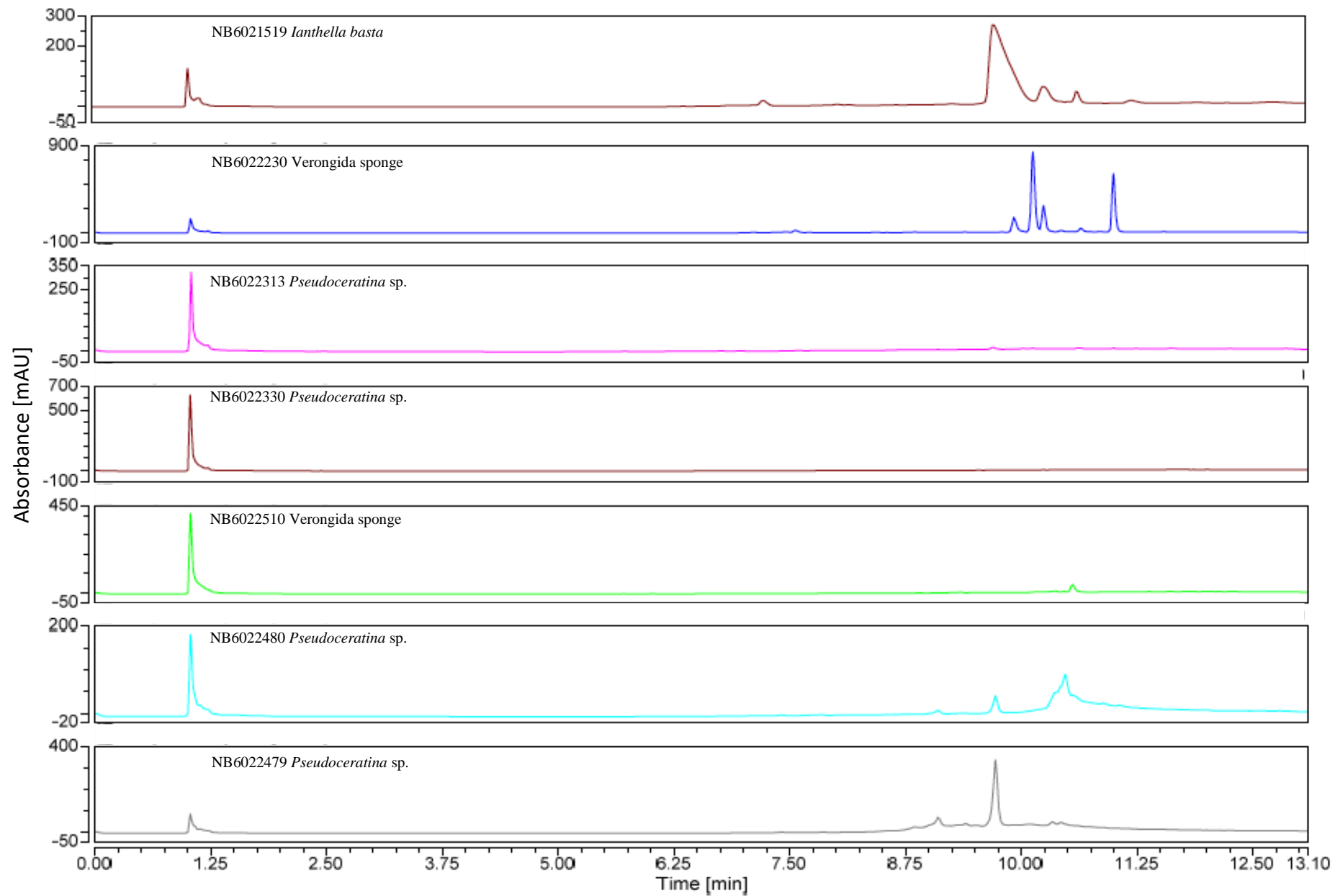
Sasha Hayes, Aya C. Taki, Kah Yean Lum, Joseph J. Byrne, Merrick G. Ekins, Robin B. Gasser and Rohan A. Davis

*Beilstein J. Org. Chem.* **2022**, *18*, 1544–1552. [doi:10.3762/bjoc.18.164](https://doi.org/10.3762/bjoc.18.164)

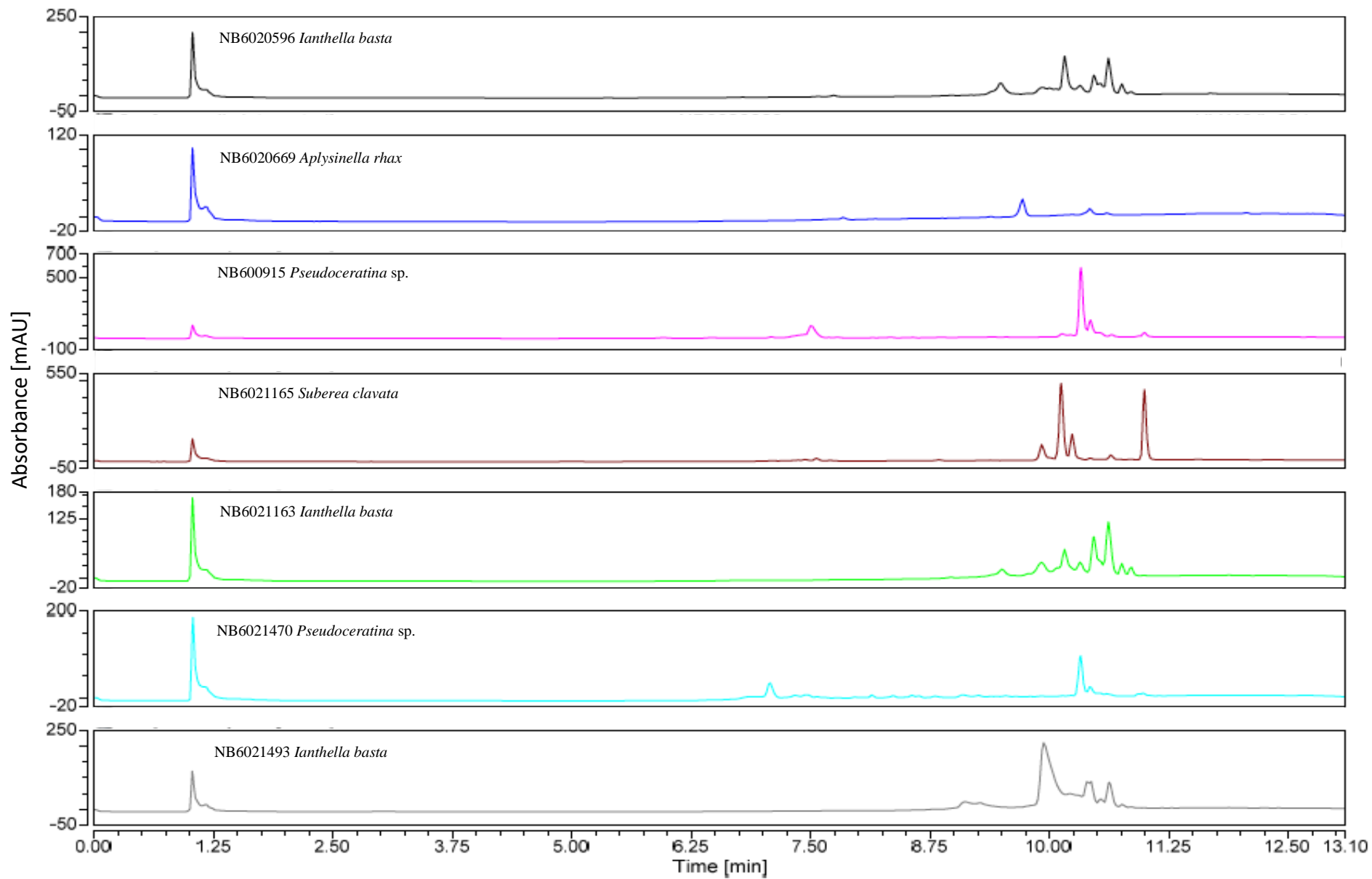
### **UHPLC–UV chromatograms, characterisation data and copies of spectra for 5-debromopurealidin H (1)**

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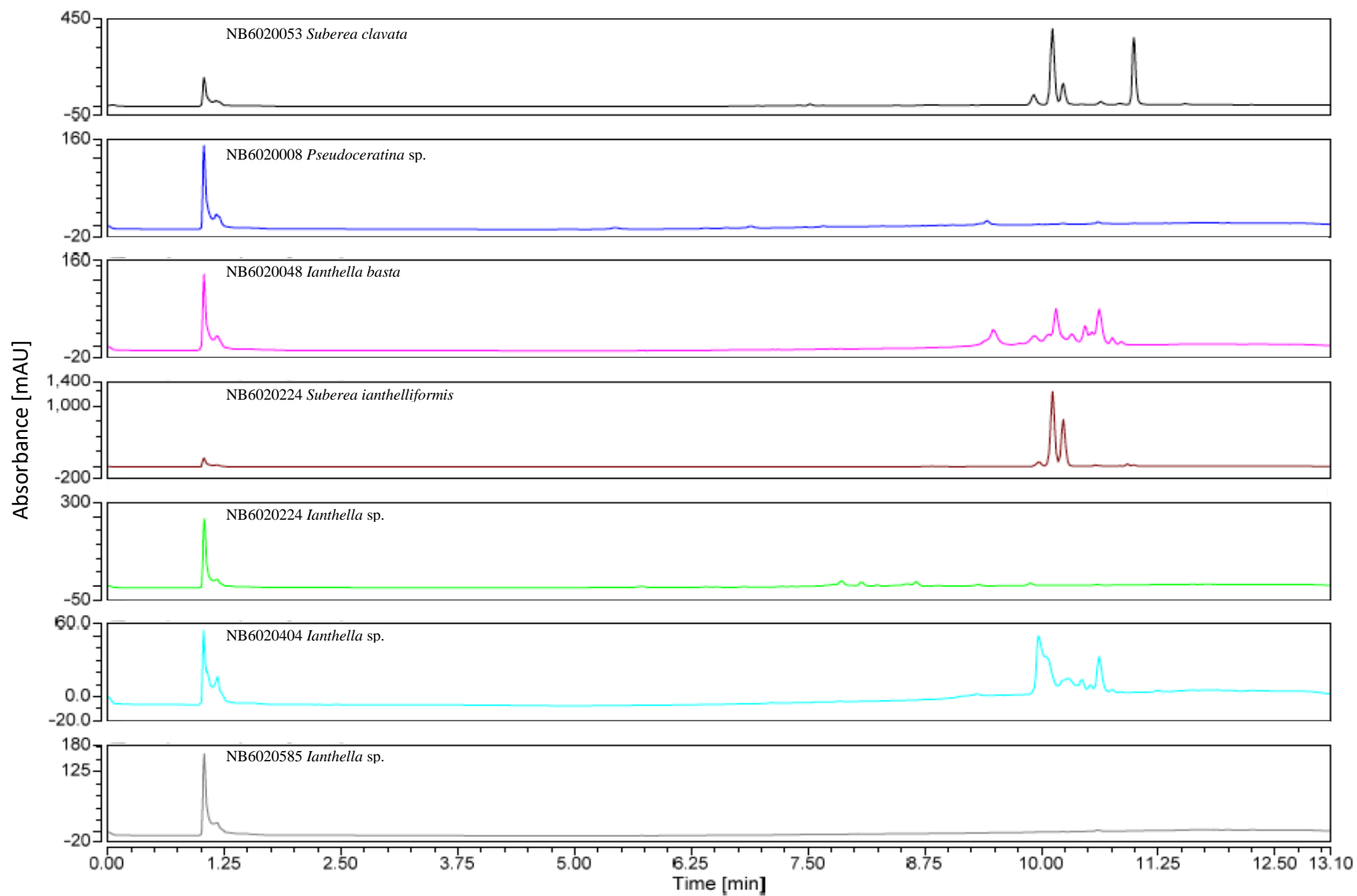
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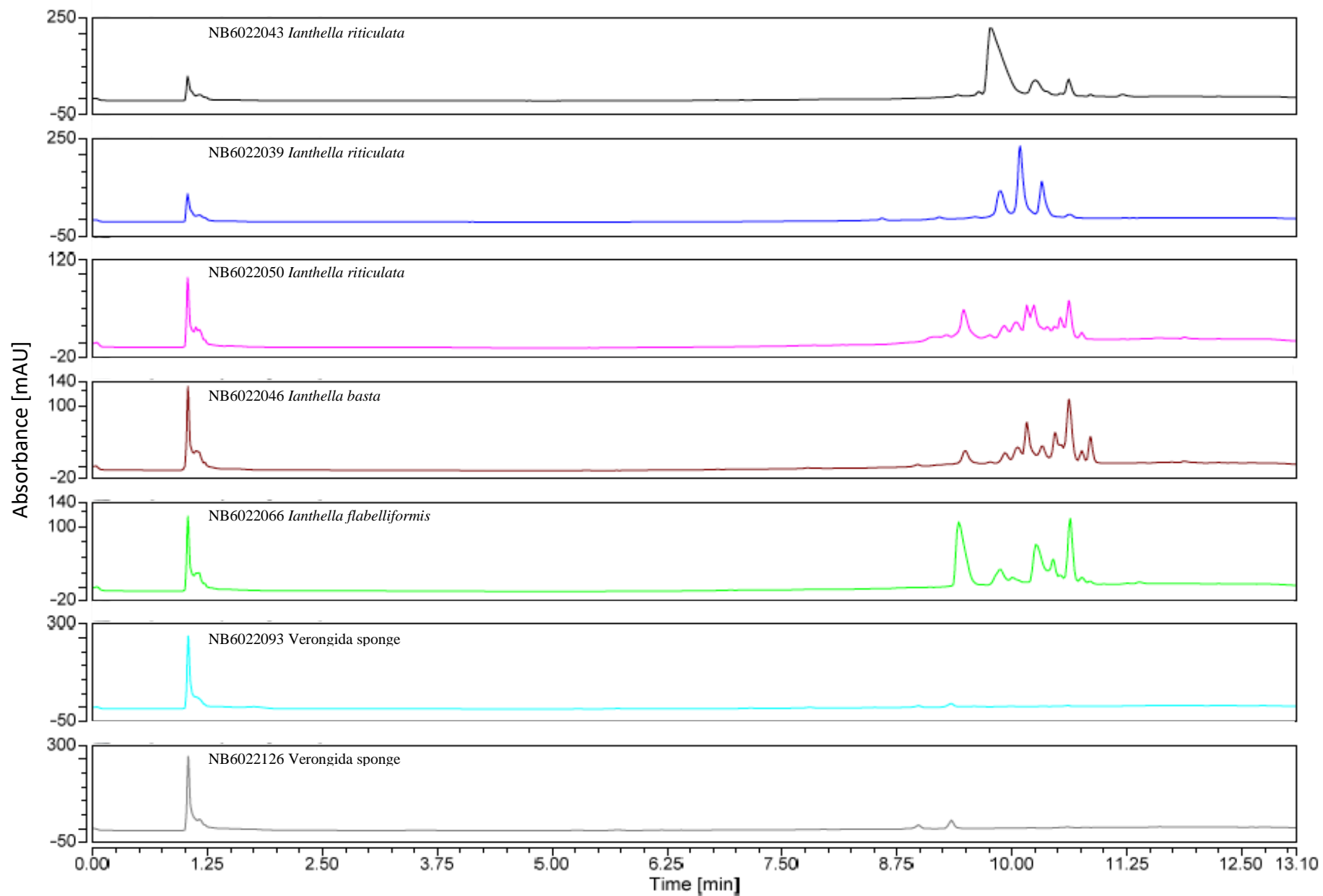
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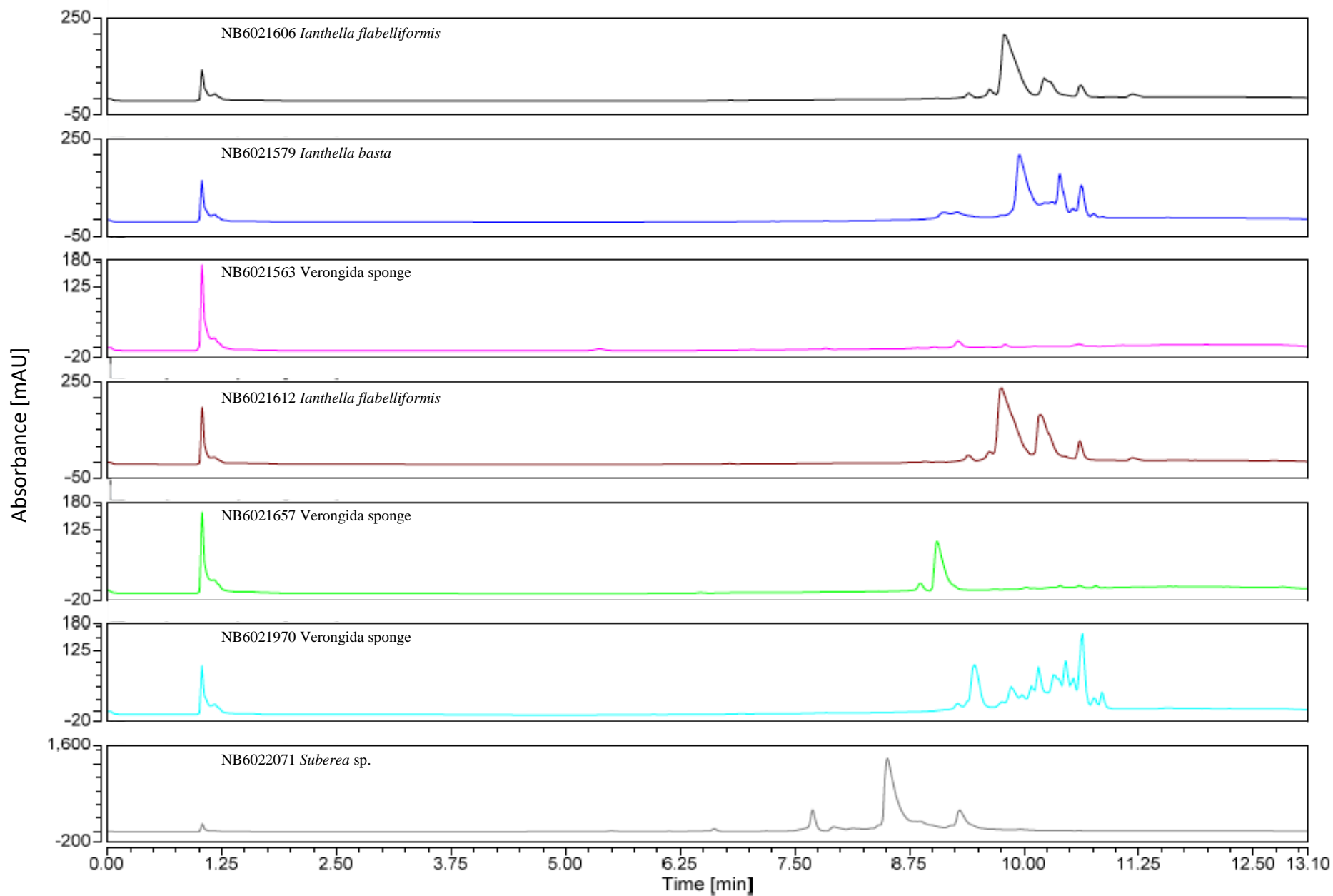
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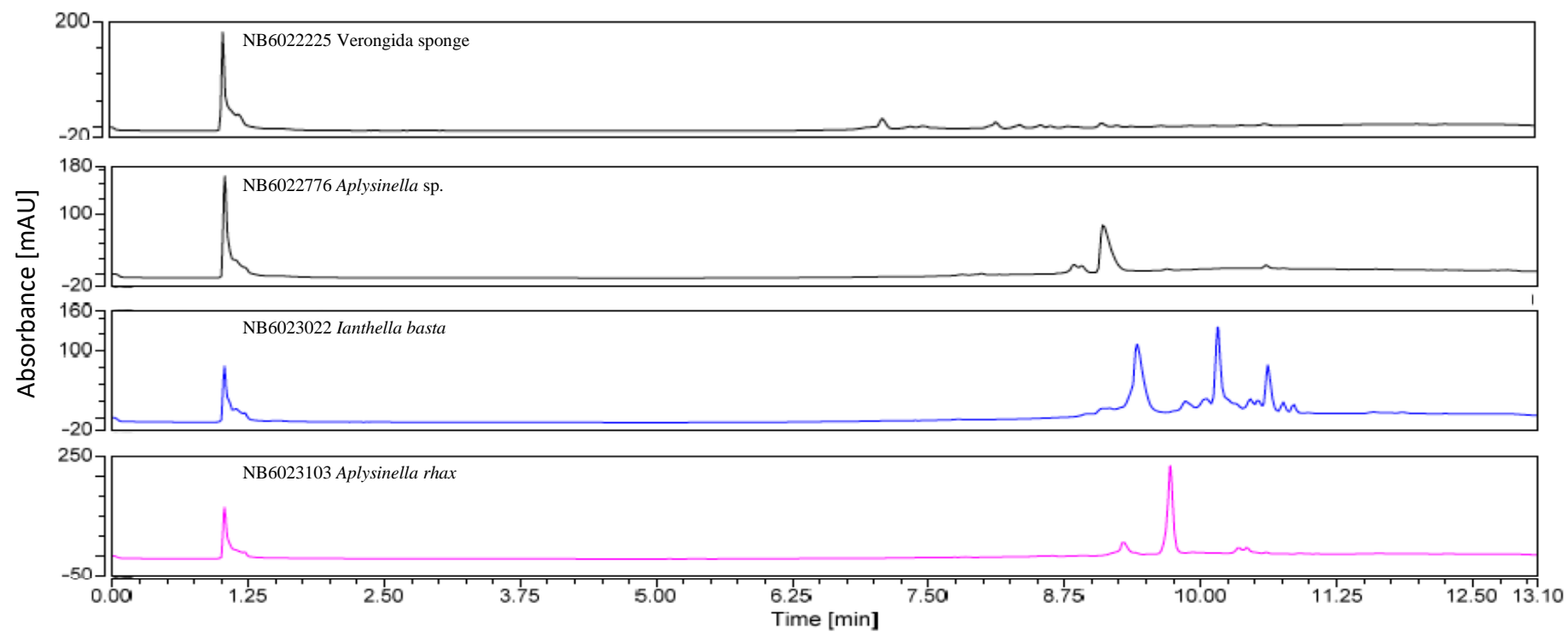
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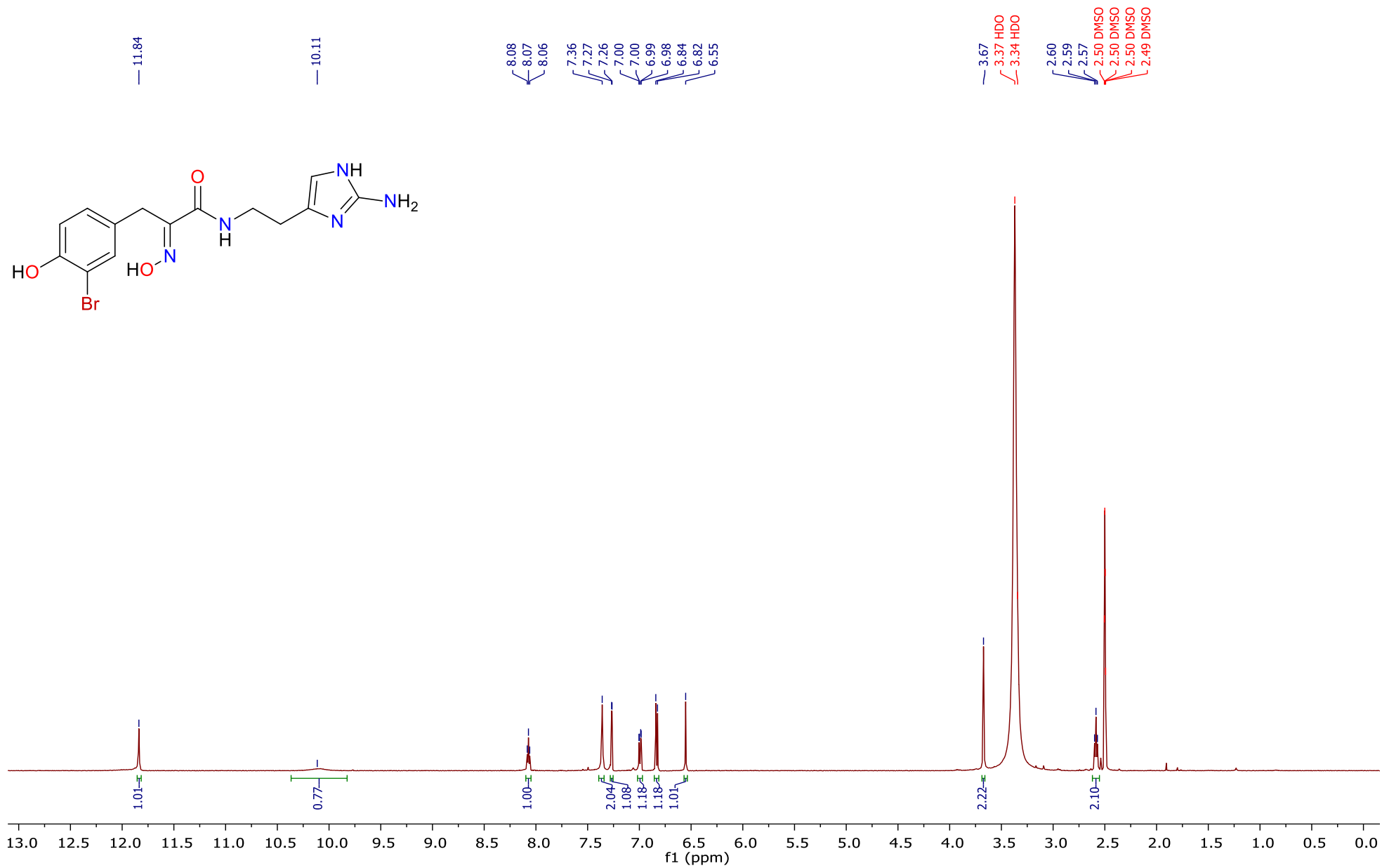


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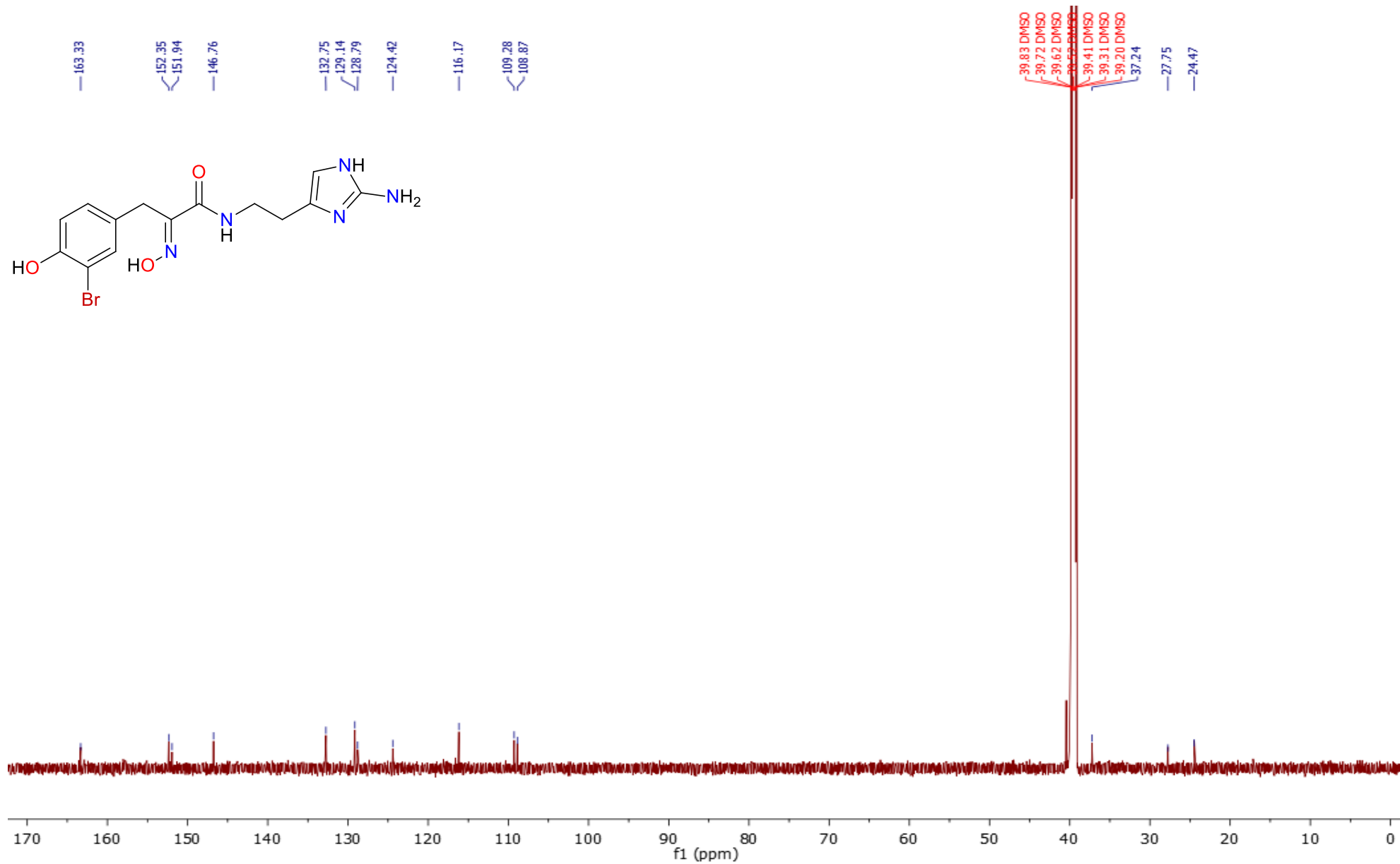


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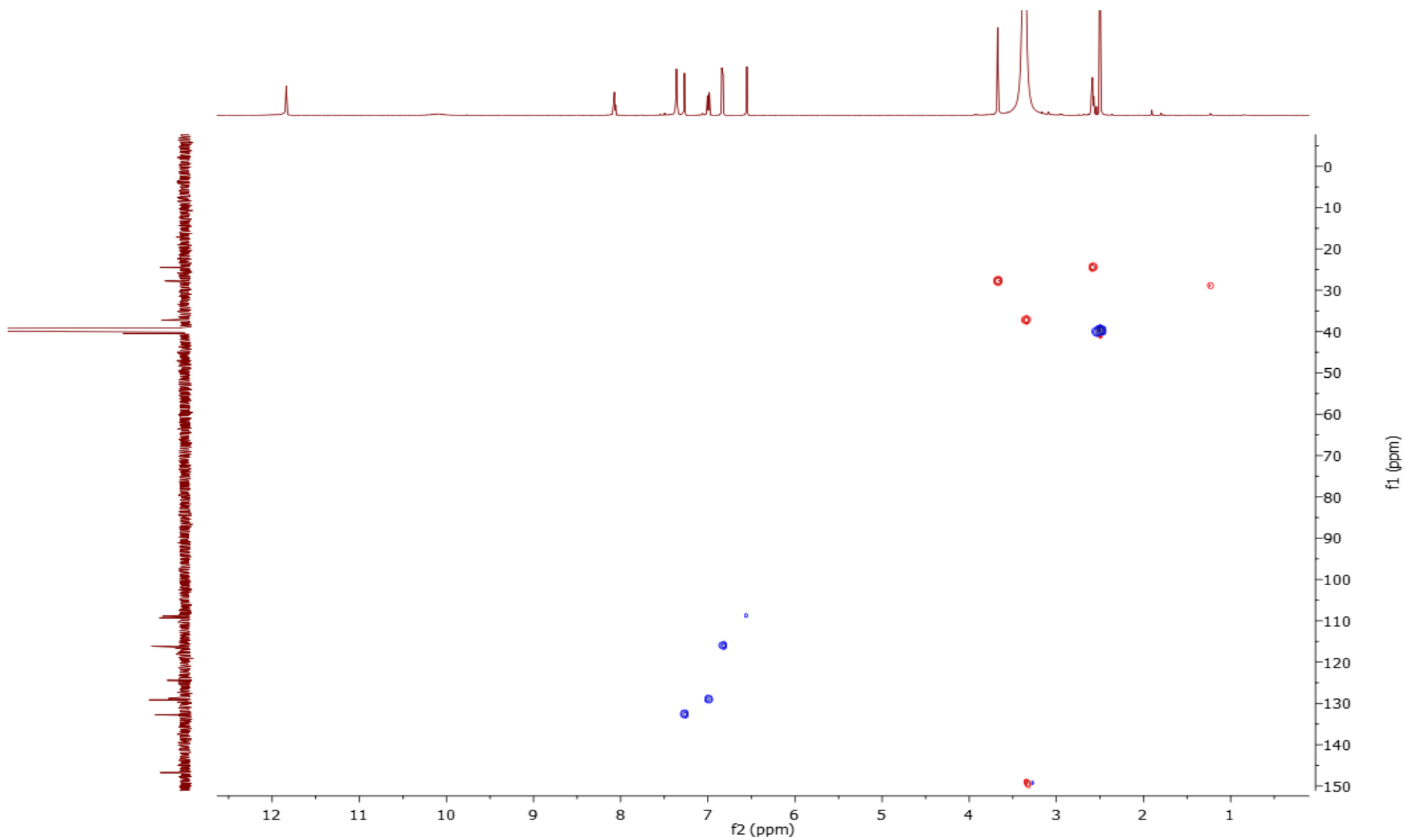




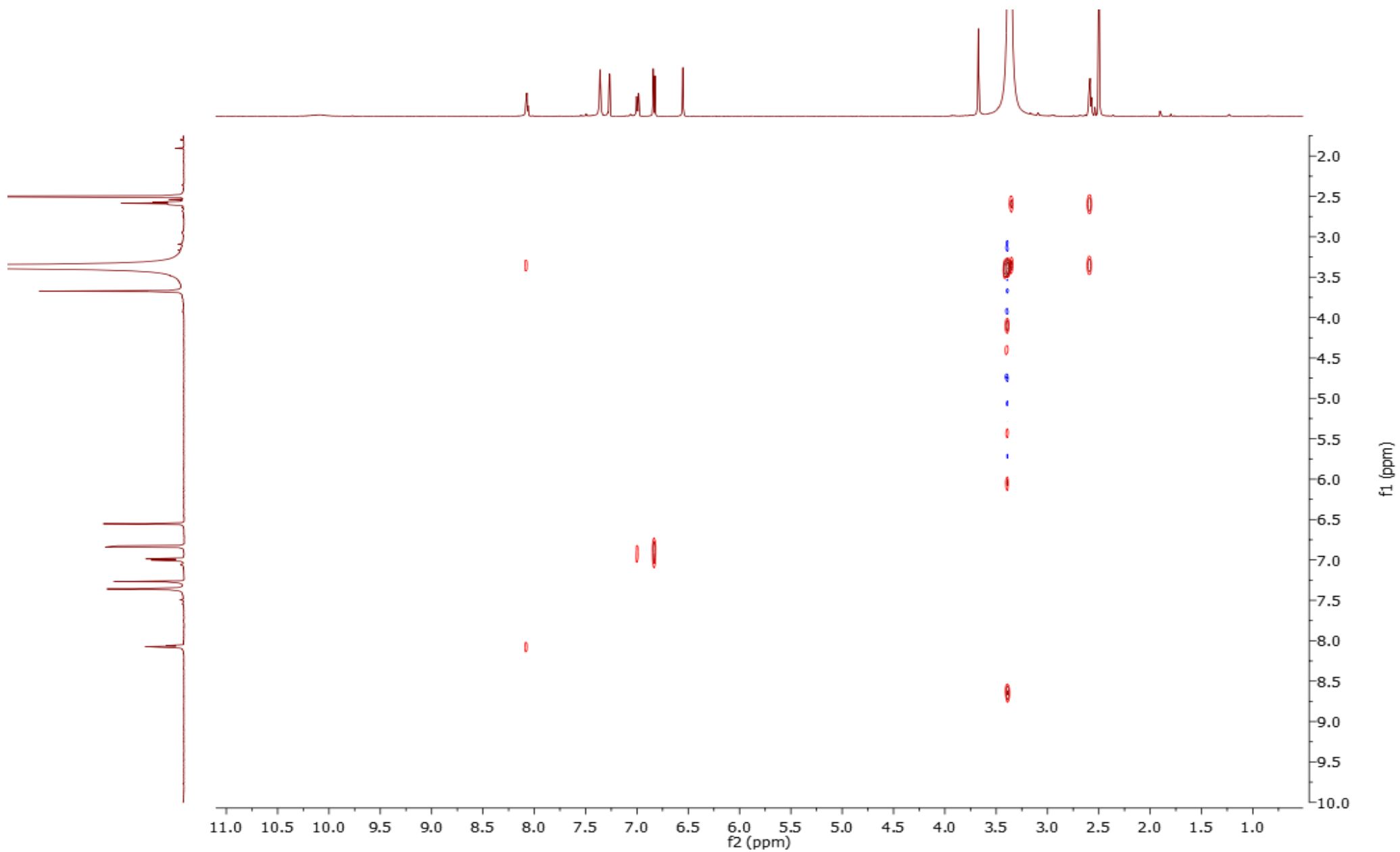
**Figure S2:** <sup>1</sup>H NMR (800 MHz) spectrum of 5-debromopurealidin H (1) in DMSO-*d*<sub>6</sub>



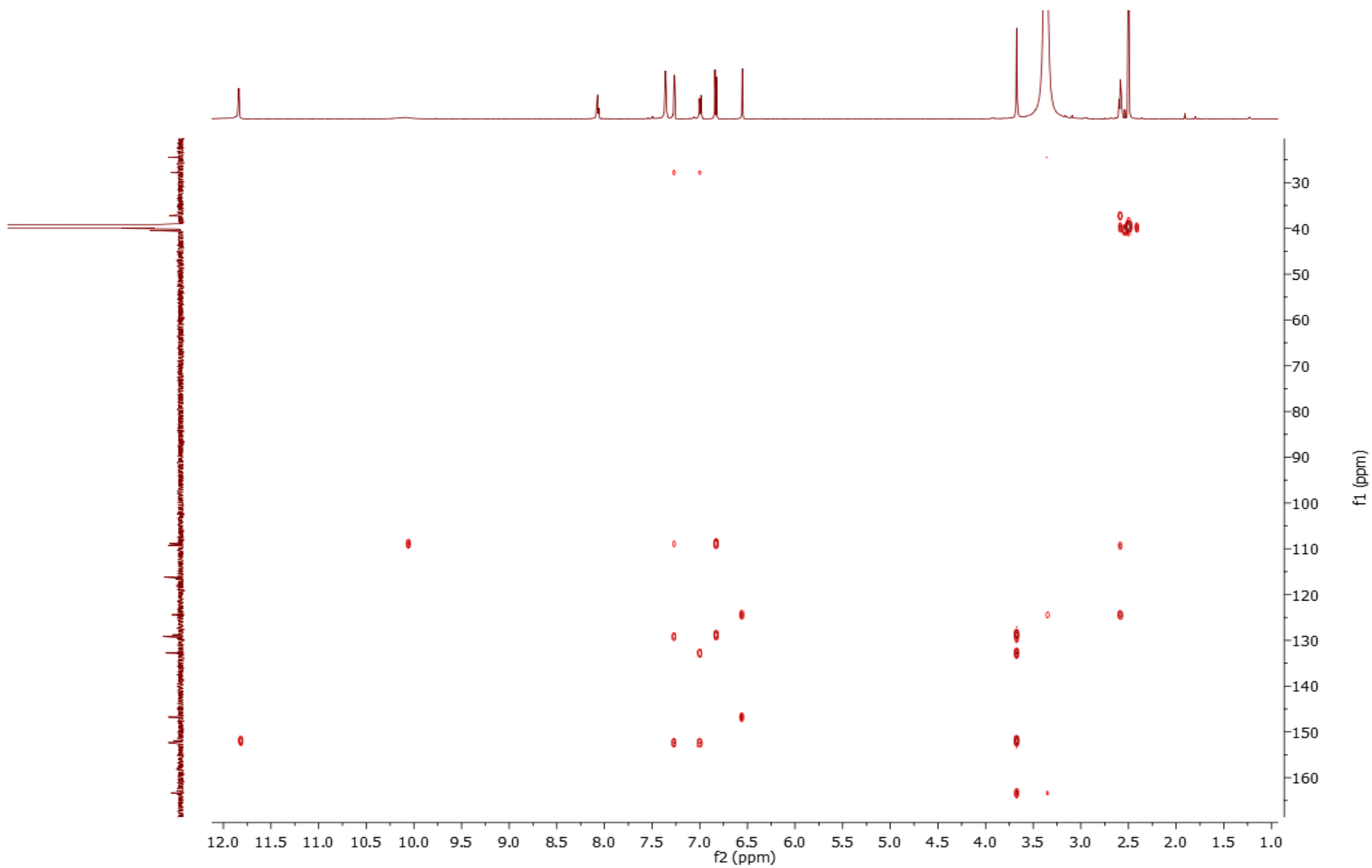
**Figure S3:**  $^{13}\text{C}$  NMR (200 MHz) spectrum of 5-debromopurealidin H (**1**) in  $\text{DMSO-}d_6$



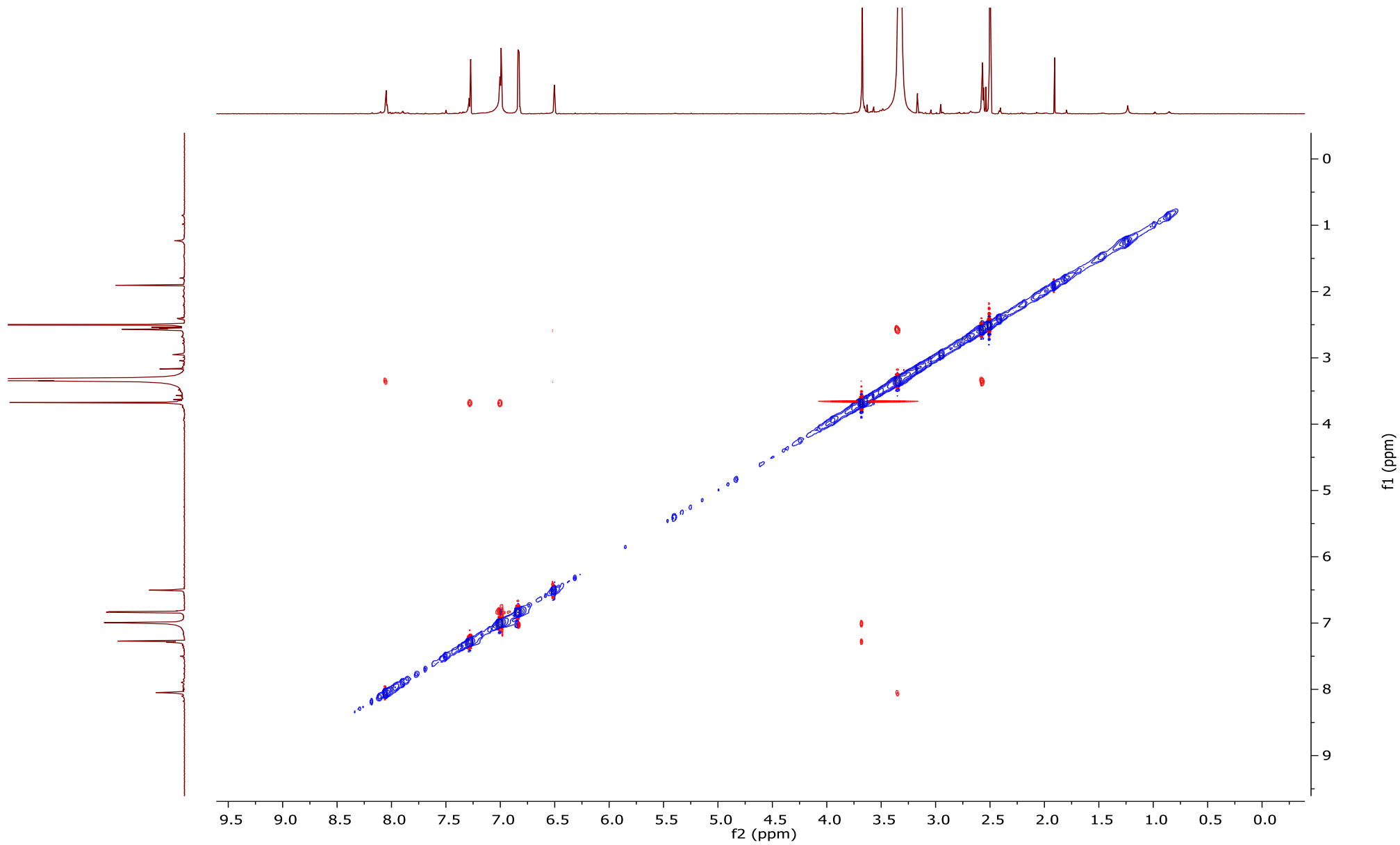
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**Figure S6:** HMBC spectrum of 5-debromopurealidin H (1) in DMSO-*d*<sub>6</sub>



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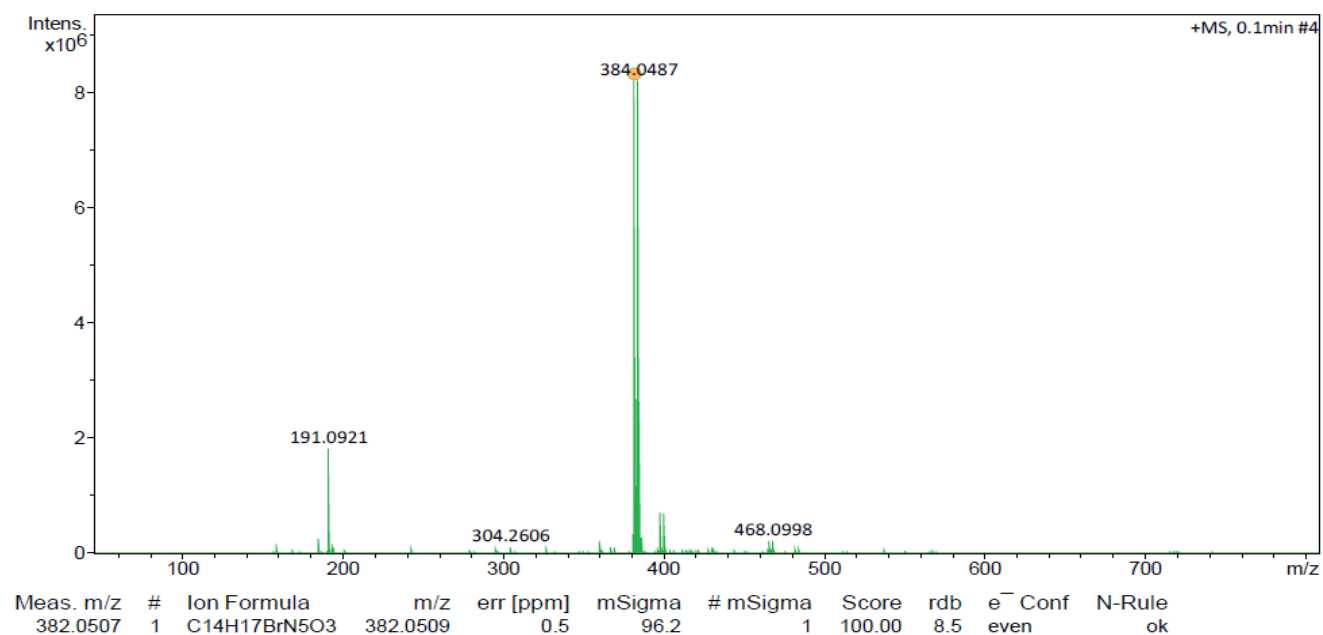
## High Resolution Mass Spectrum

### Analysis Info

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 Method DirectInfusion\_2018\_pos.m  
 Sample Name NBC110  
 Comment

Acquisition Date 5/8/2020 10:30:32 AM  
 Instrument maXis II ETD 1823391.22321

### +MS, 0.1min #4



**Figure S8:** HRESIMS of 5-debromopurealidin H (1)