

# Cimipronidine: A cyclic guanidine alkaloid from

## *Cimicifuga racemosa* (L.) Nutt.<sup>§</sup>

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# Supplementary Data

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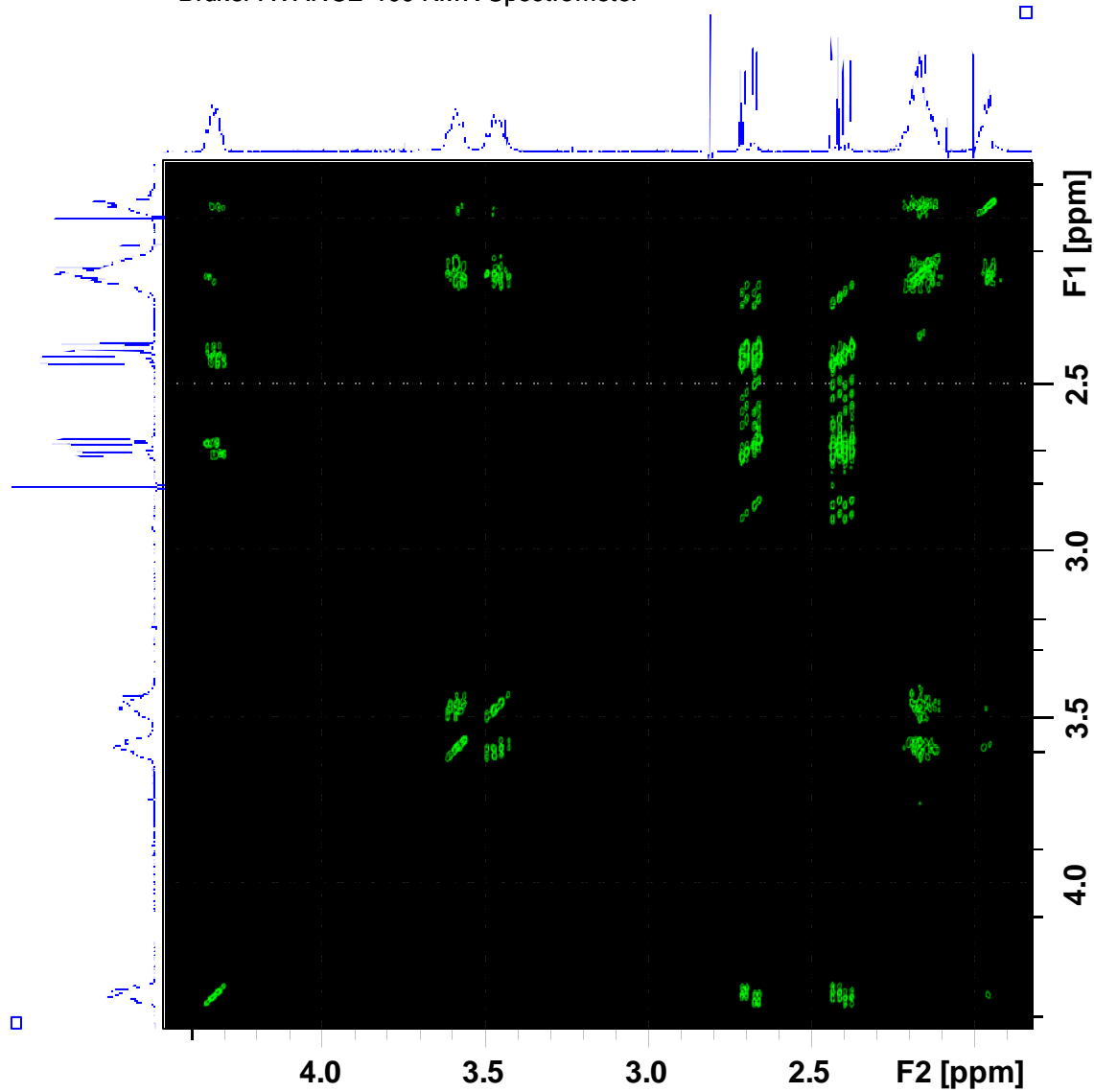
‡ Program for Collaborative Research in the Pharmaceutical Sciences

§ UIC/NIH Center for Botanical Dietary Supplements Research

± Department of Medicinal Chemistry and Pharmacognosy

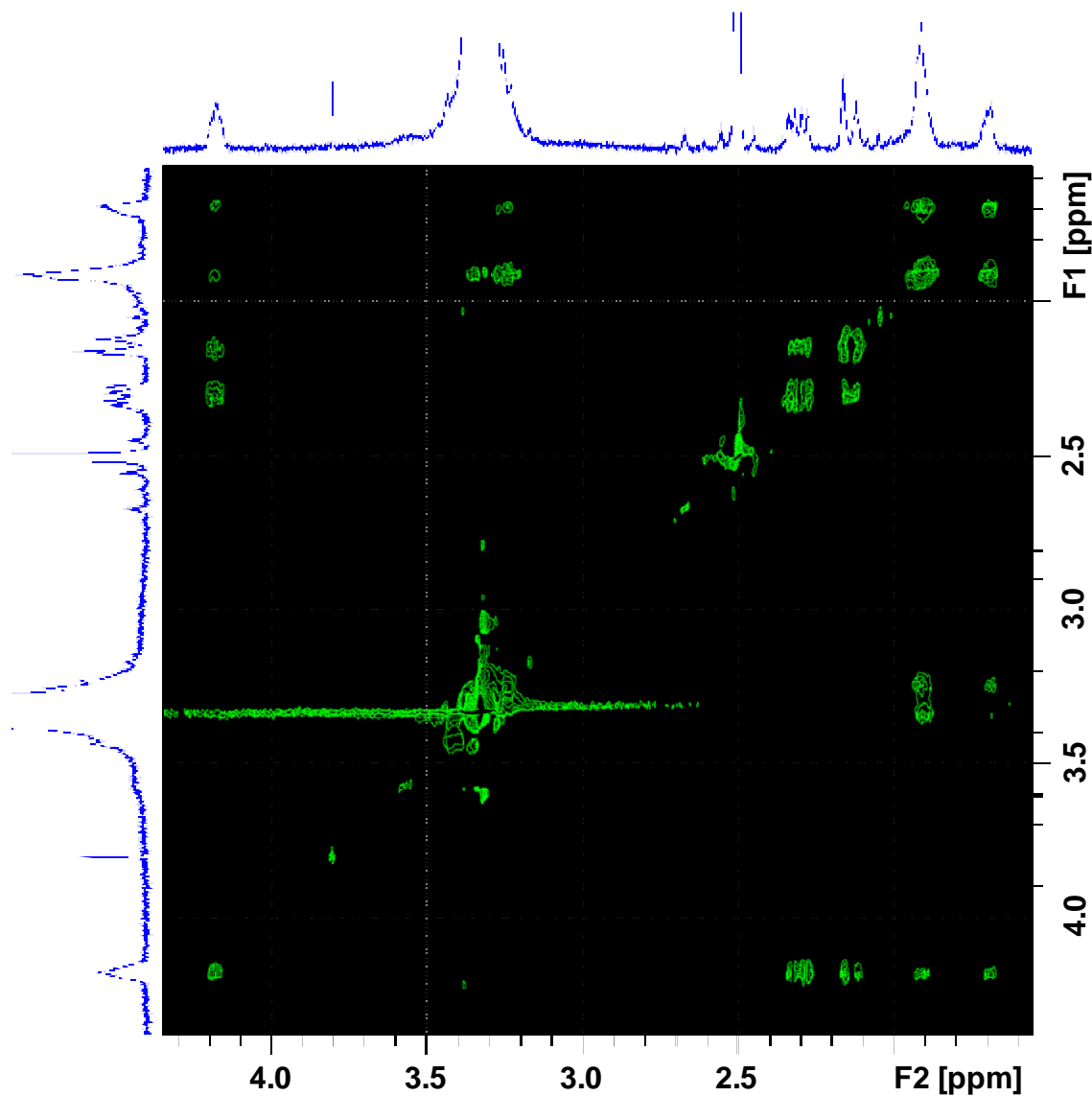
|| Institute for Tuberculosis Research

Sample: Cimipronidine (1)  
Solvent: D2O  
Standard 2-D Gradient Enhanced COSY  
H-H Correlation Experiment  
Bruker AVANCE-400 NMR Spectrometer

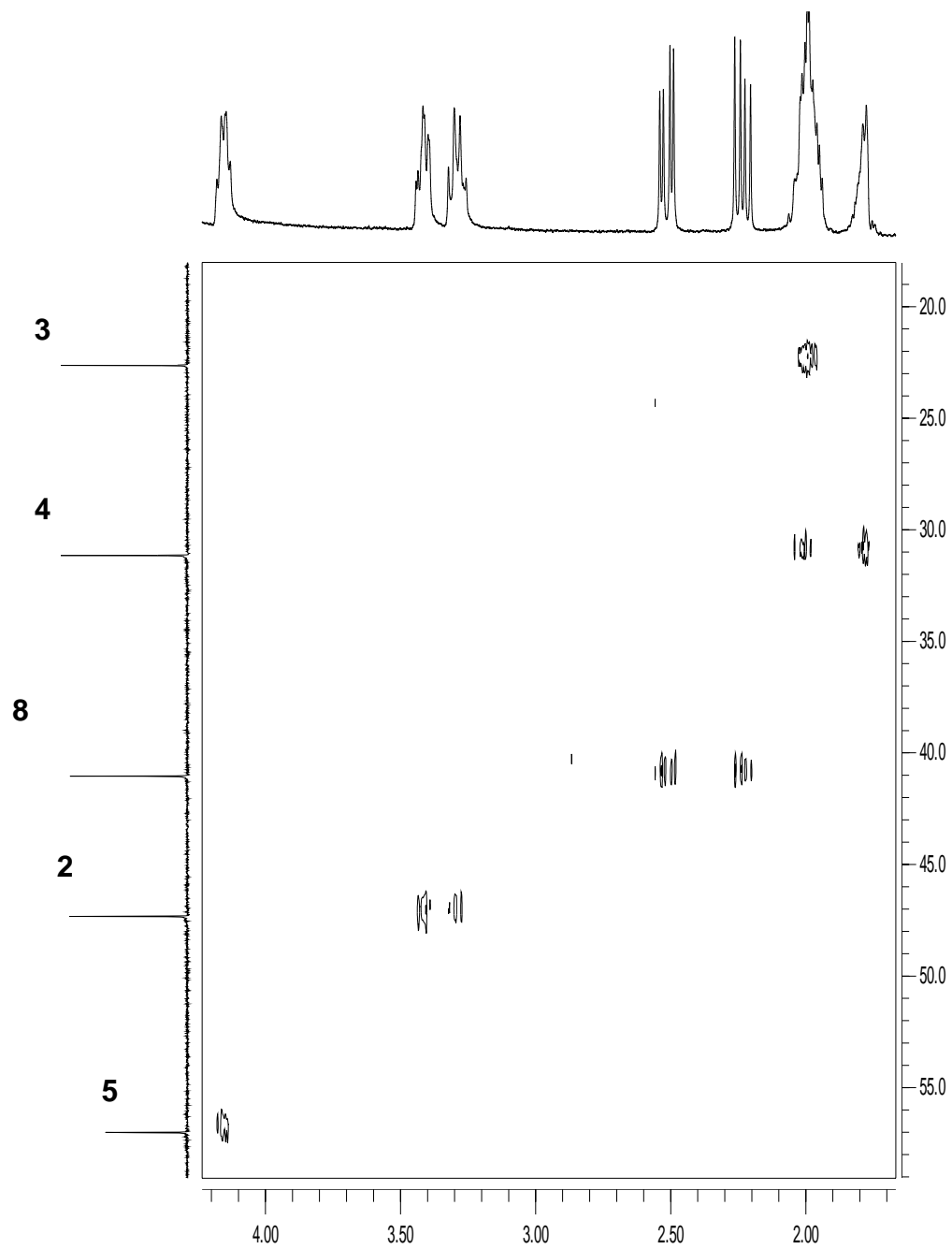


S1.  $^1\text{H}$ - $^1\text{H}$  COSY of **1** in D<sub>2</sub>O (400 MHz)

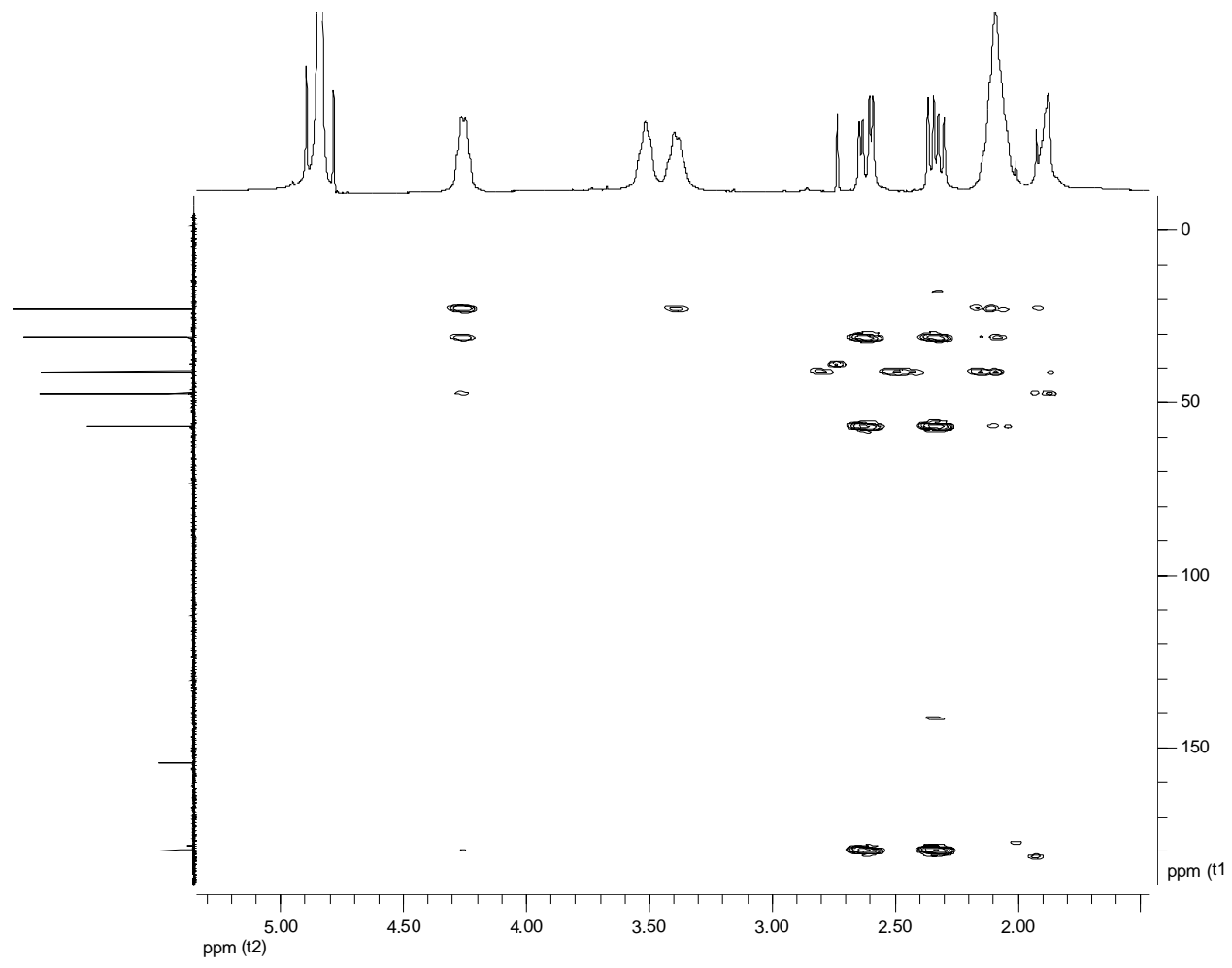
Sample: Cimipronidine (1)  
Solvent: DMSO solution / ~1 mg  
2-D TOCSY (MLEV-17, Phase Sensitive)  
Using the 'mlevph' Pulse Sequence  
H-H Correlation Experiment Mix Time(d9) 80 ms  
Bruker AVANCE-400 NMR Spectrometer  
D.Lankin



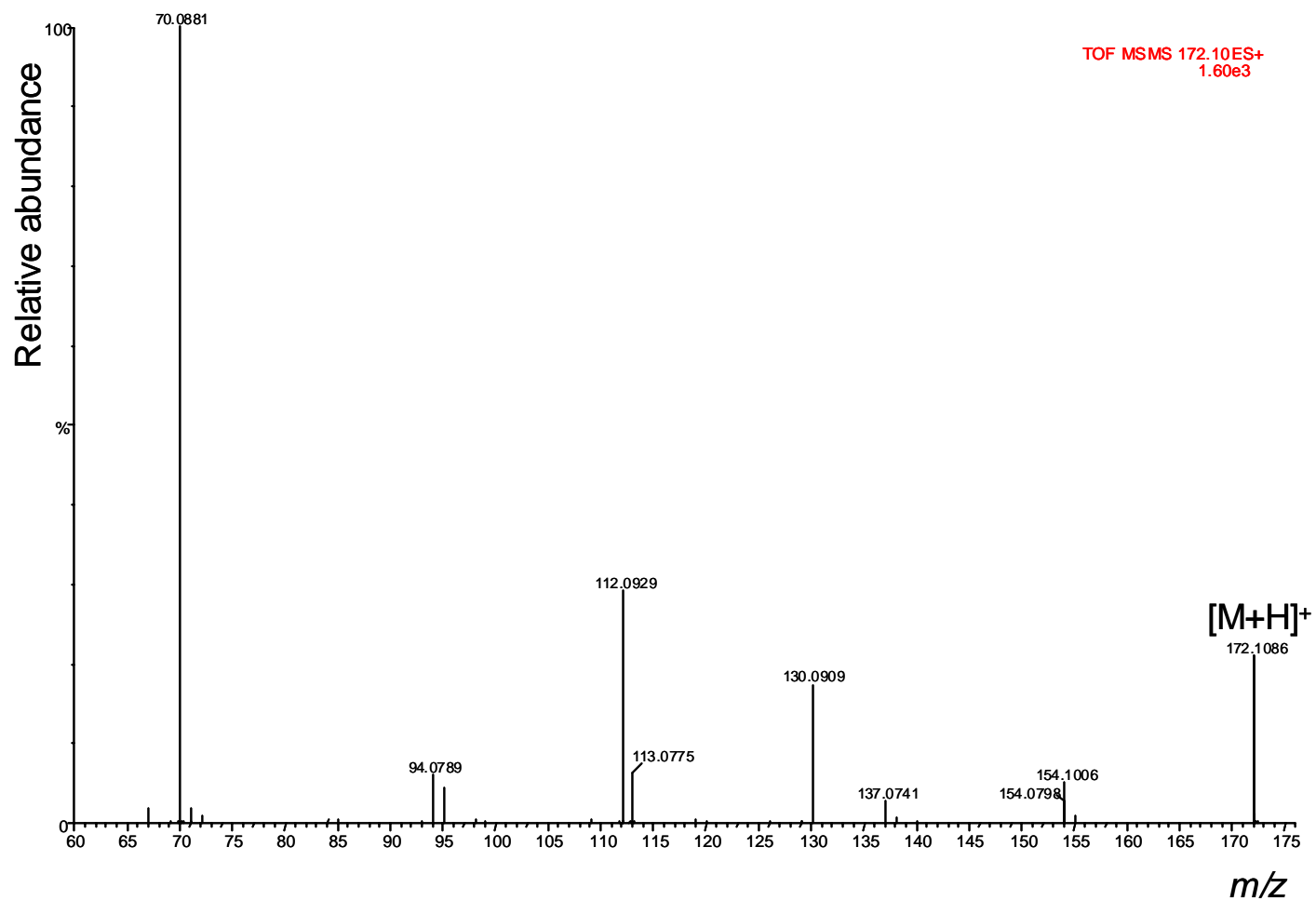
S2.  $^1\text{H}$ - $^1\text{H}$  TOCSY of 1 in  $\text{D}_2\text{O}$  (400 MHz)



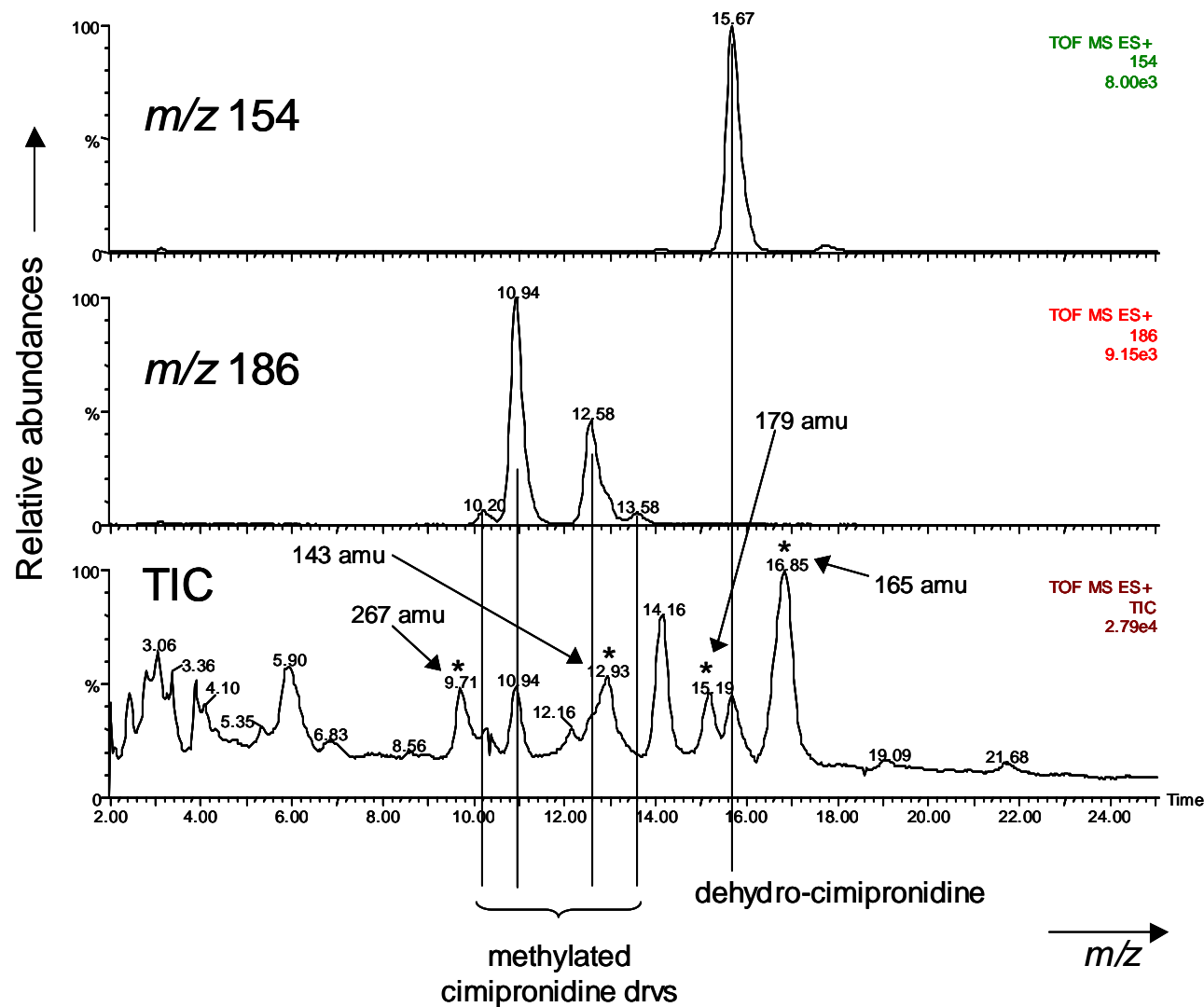
**S3.** HSQC of **1** in  $\text{D}_2\text{O}$  (500 MHz)



**S4.** HMBC (8.5 Hz) of **1** in D<sub>2</sub>O (500 MHz)



**S 5.** Positive ion electrospray high resolution tandem mass spectrum of **1**. The precursor ion of  $m/z$  172.1086 was used as a lock mass.



**S 6.** Positive ion electrospray LC-MS of a 5-HT<sub>7</sub> active fraction containing **1** and its analogues. Based on their protonated molecules and MS-MS fragmentation pattern, at least four methylated ( $m/z$  186) and one dehydrated ( $m/z$  154) cimipronidine (**1**) analogue are contained in the active fraction. Compounds with no obvious structural correlation are marked with \*