

SUPPORTING INFORMATION

Targeted Isolation of Monoterpene Indole Alkaloids from *Palicourea sessilis*

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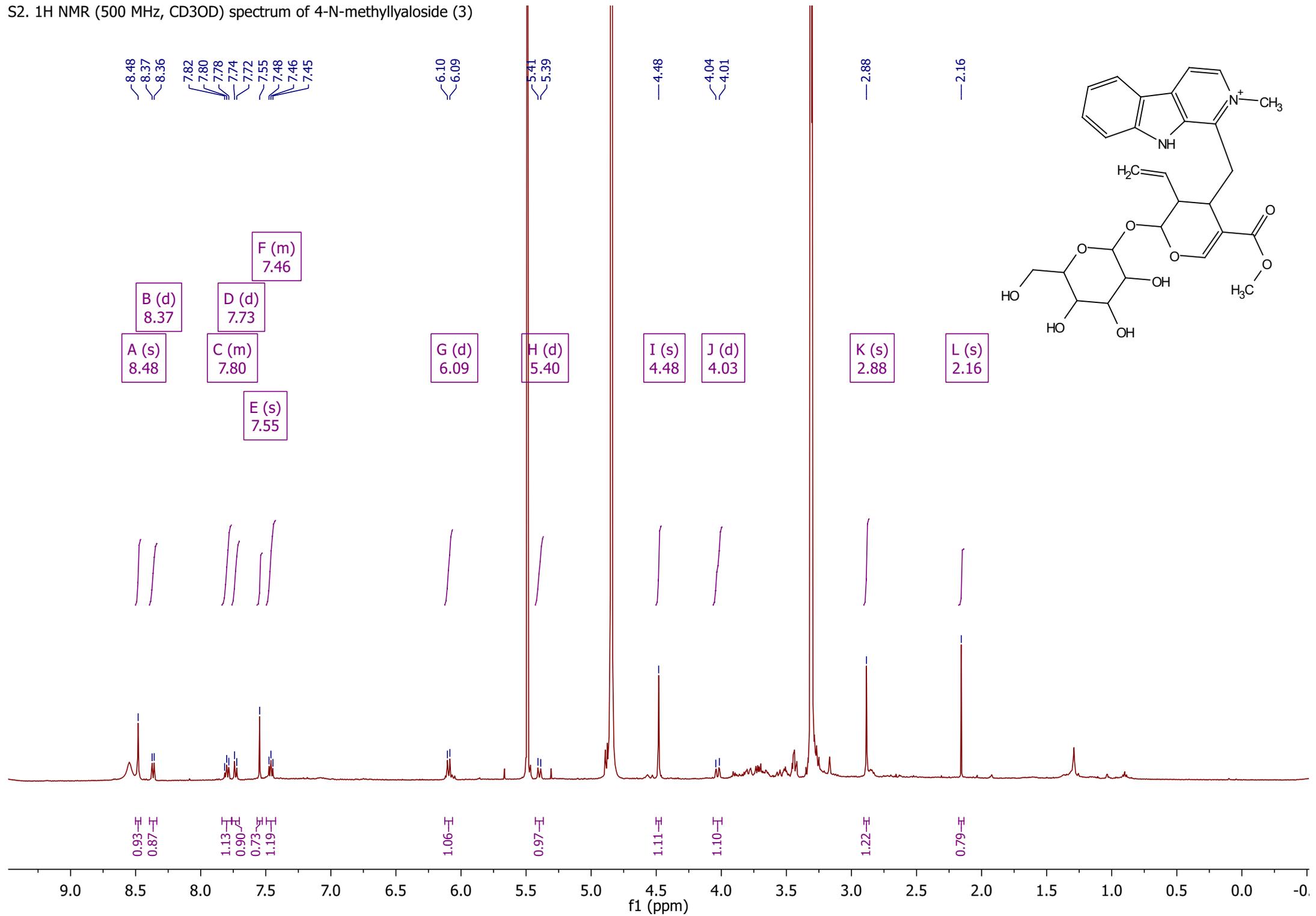
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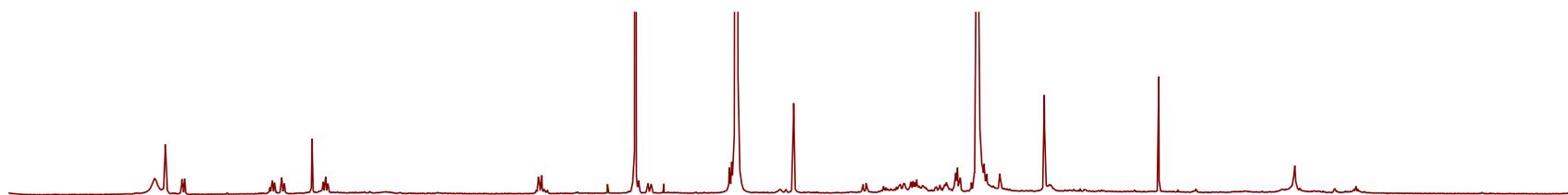
[∇] *Herbarium Dr. Roberto Miguel Klein, Department of Natural Sciences, Universidade Regional de Blumenau - FURB, Blumenau/SC, Brazil*

[°] Both authors contributed equally to this work.

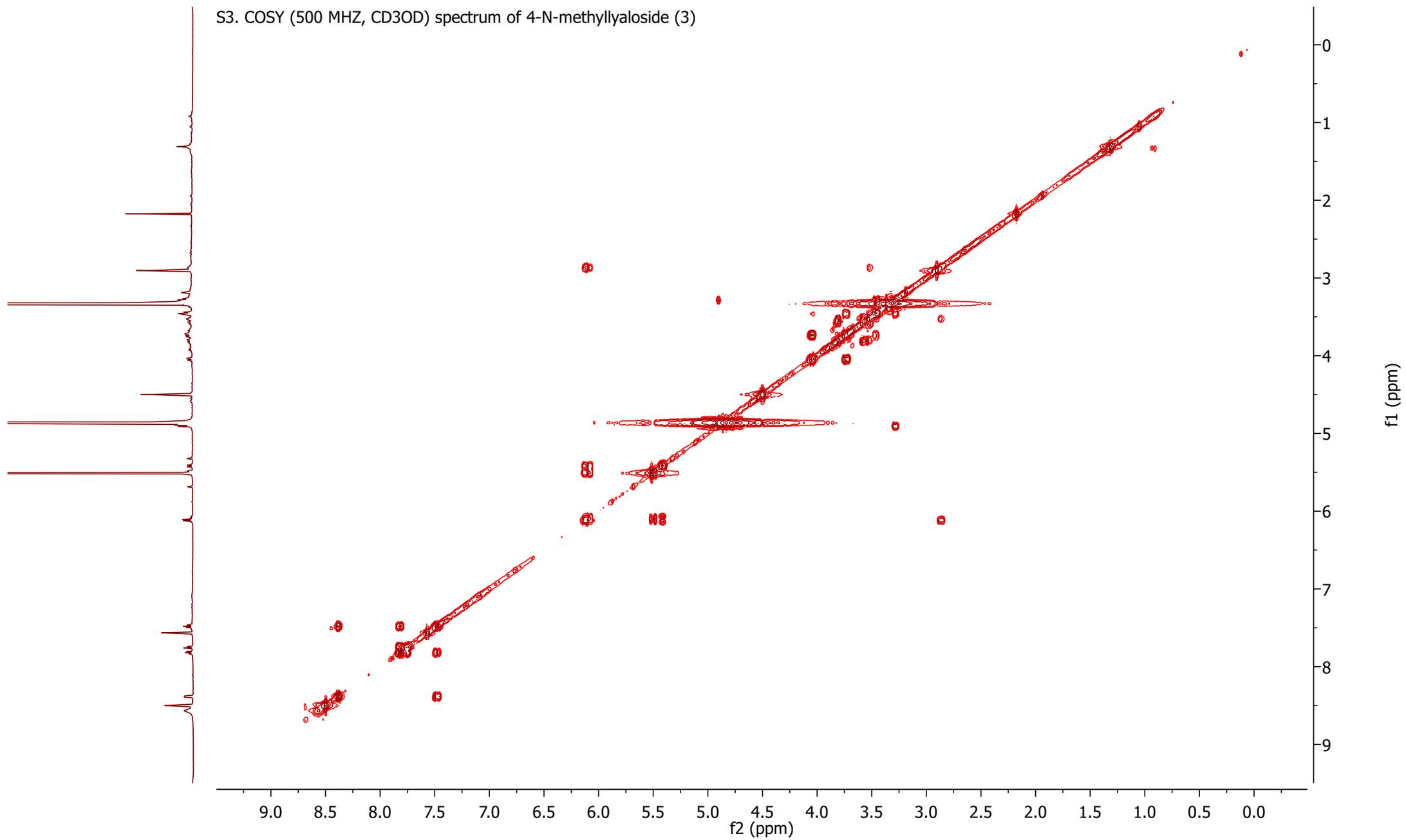
Figure S1. Cluster A related to the monoterpene indole alkaloids within the whole alkaloid extract of *P. sessilis*. The depicted structures correspond to the first hits obtained when querying an *in silico*-generated spectrometric database of metabolites previously isolated from the Rubiaceae family. Alphanumerical codes correspond to the CRC codes, which are the *Dictionary of Natural Products* unique identifiers (see text for name of the compounds). The size of the nodes is relative to the intensities of precursor ions observed.

S2. ¹H NMR (500 MHz, CD₃OD) spectrum of 4-N-methyllyalloside (3)

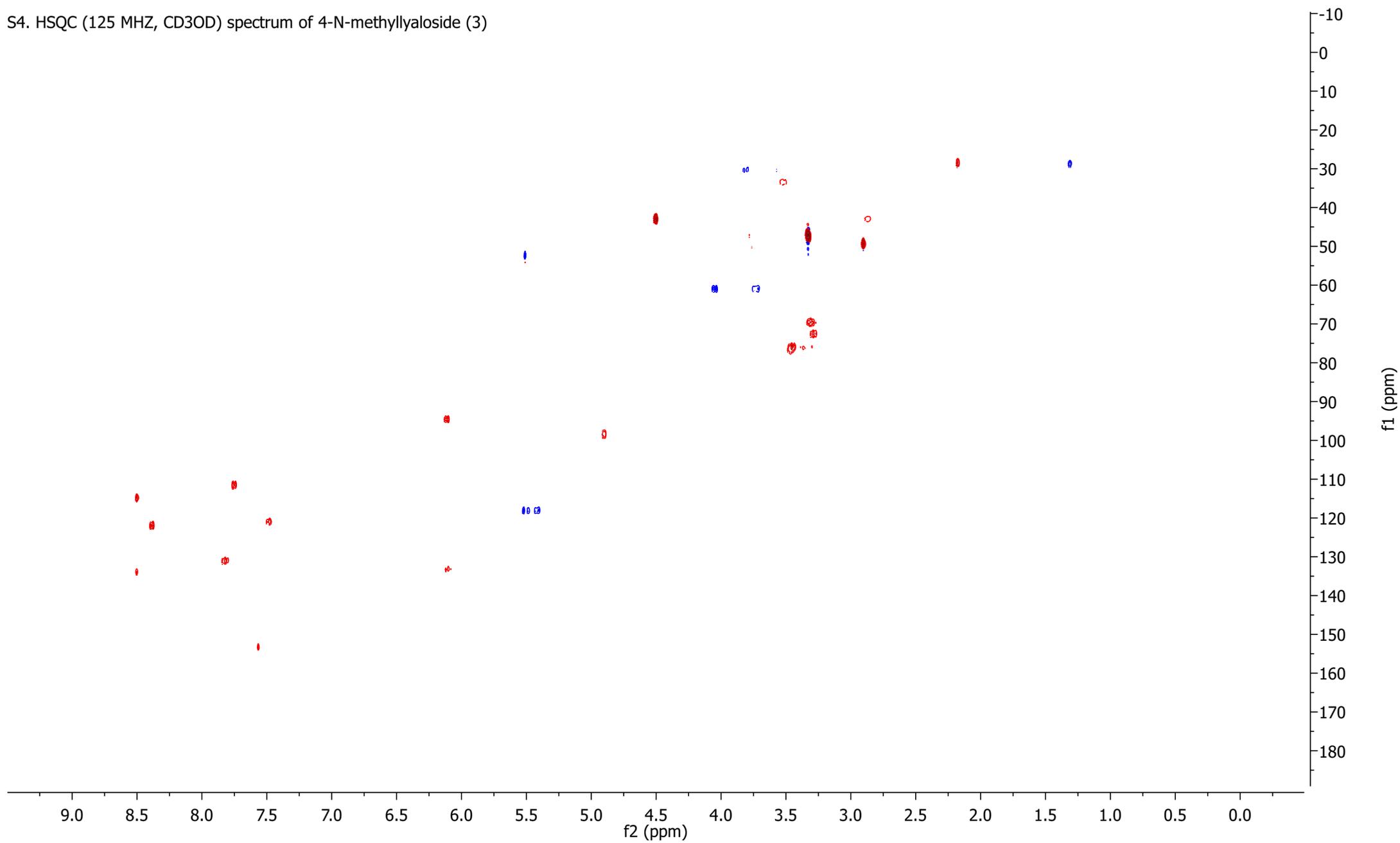




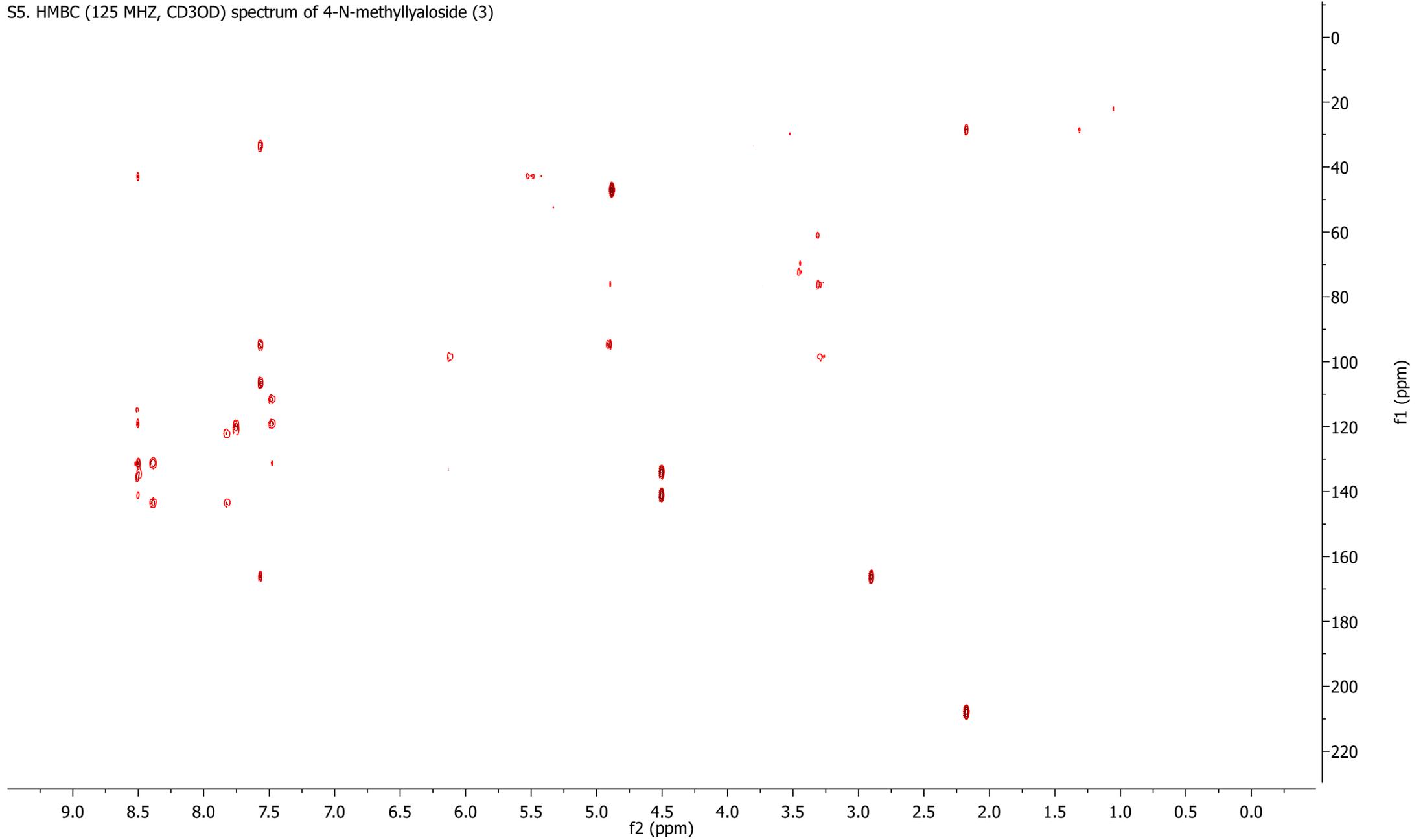
S3. COSY (500 MHz, CD3OD) spectrum of 4-N-methyllyalloside (3)



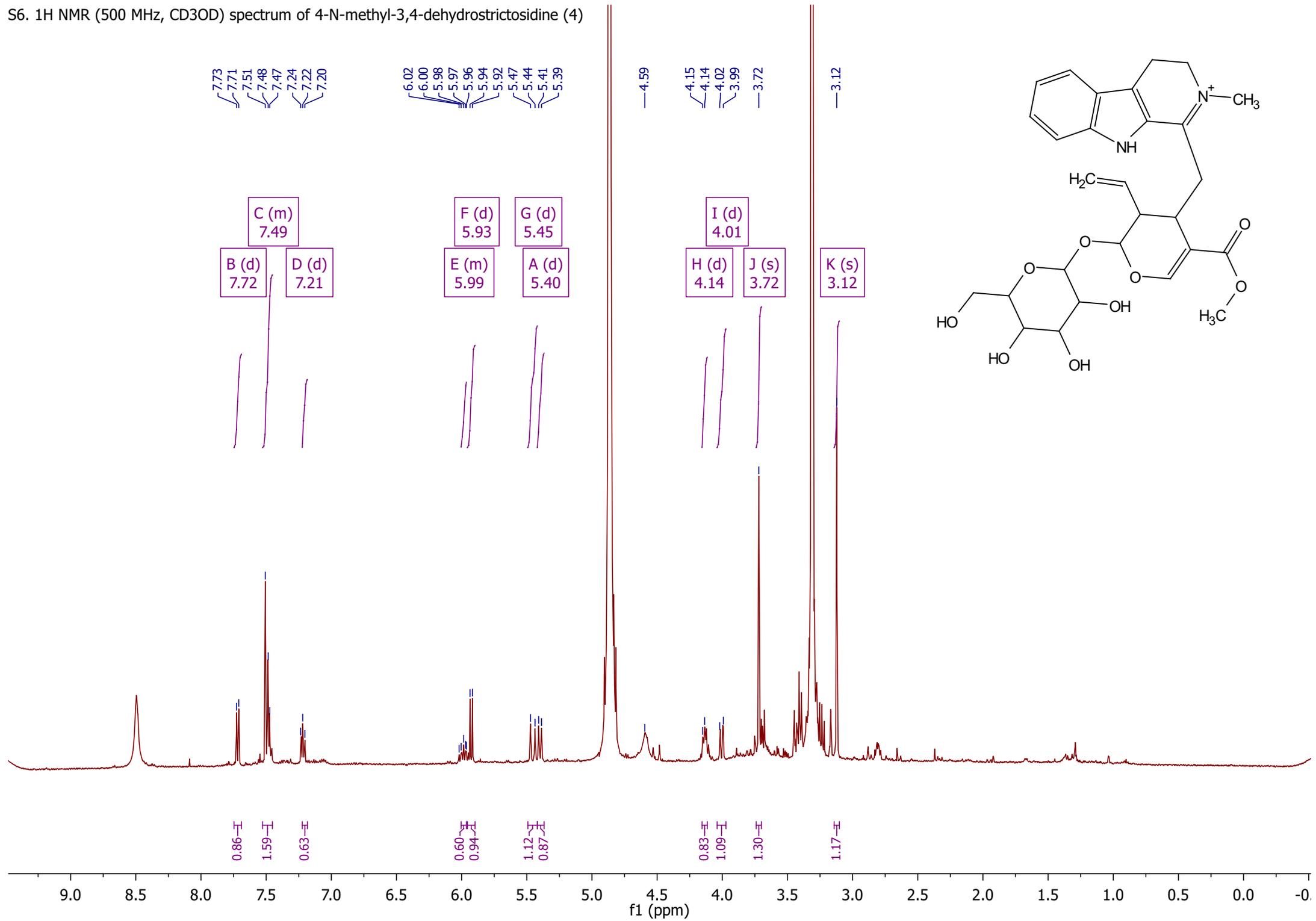
S4. HSQC (125 MHz, CD3OD) spectrum of 4-N-methyllyaloside (3)



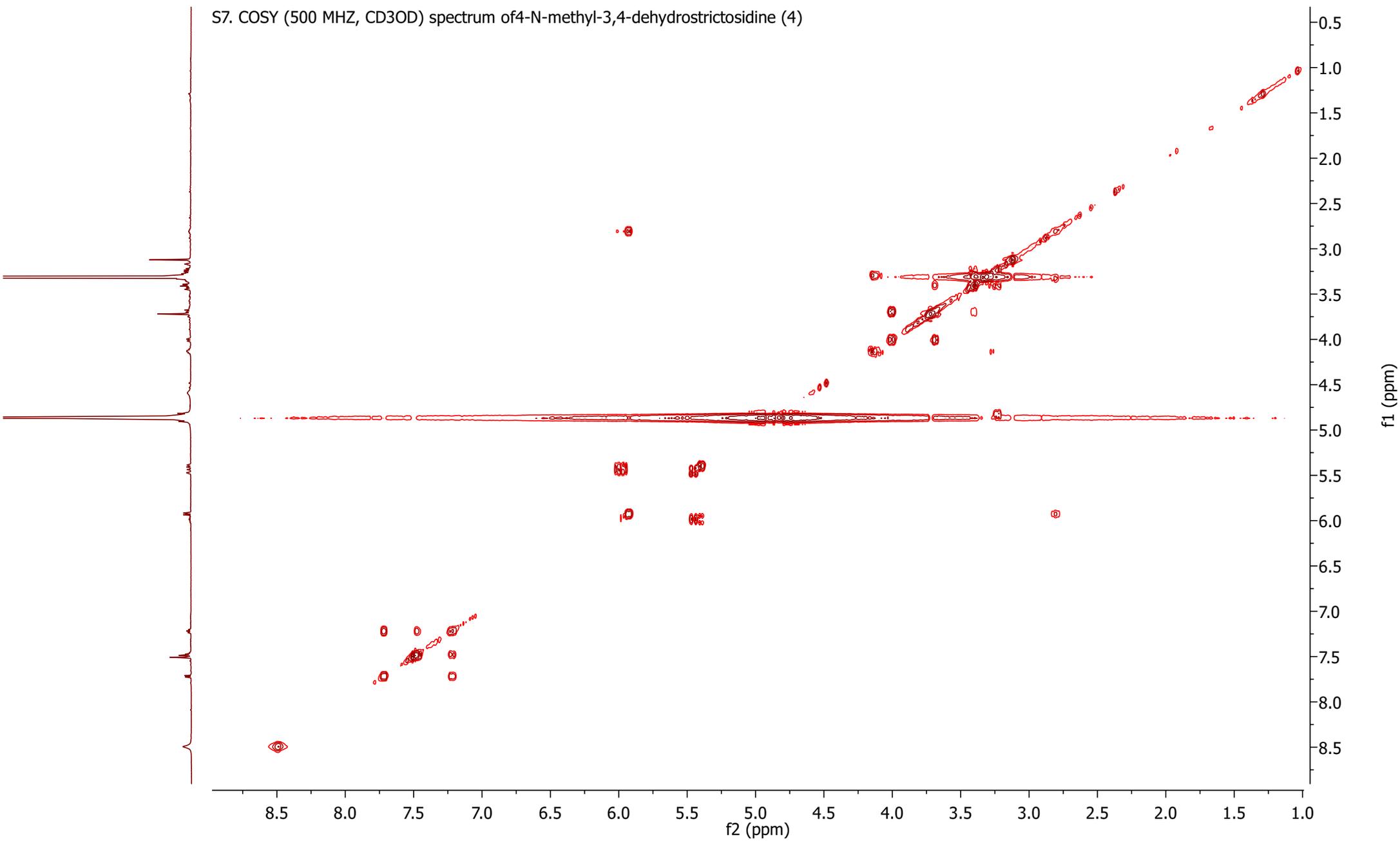
S5. HMBC (125 MHz, CD3OD) spectrum of 4-N-methyllyalloside (3)



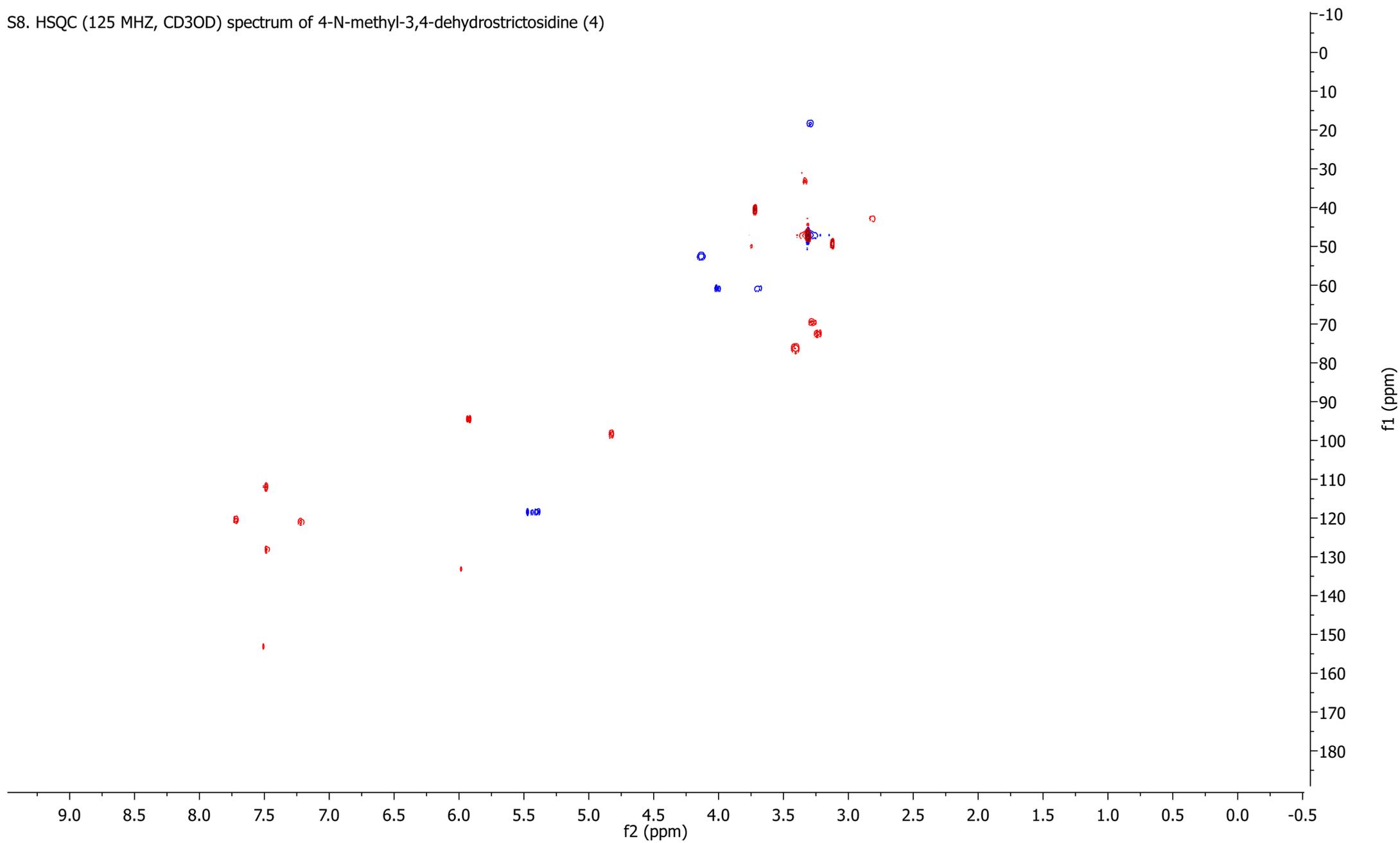
S6. ¹H NMR (500 MHz, CD₃OD) spectrum of 4-N-methyl-3,4-dehydrostrictosidine (4)



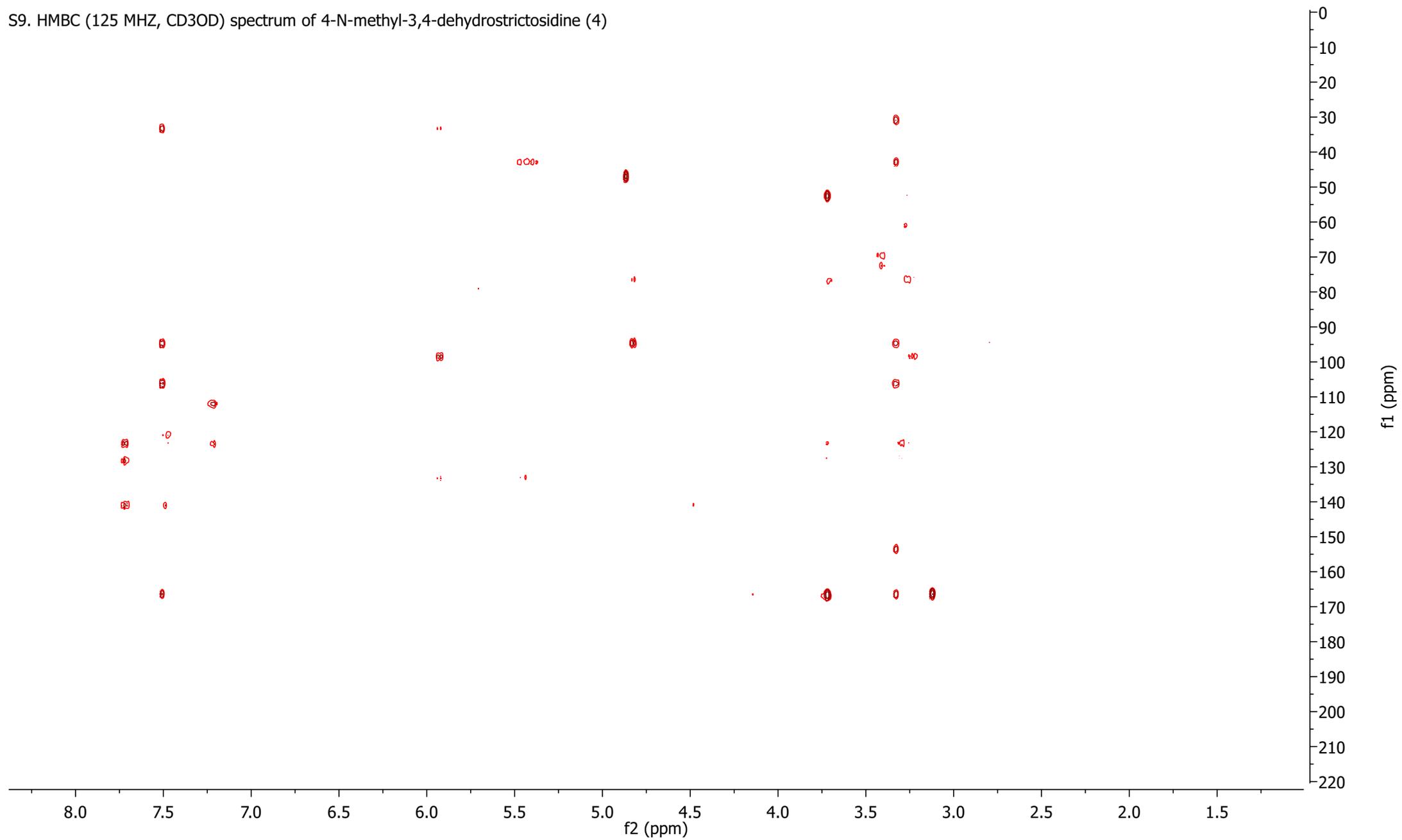
S7. COSY (500 MHz, CD3OD) spectrum of 4-N-methyl-3,4-dehydrostrictosidine (4)



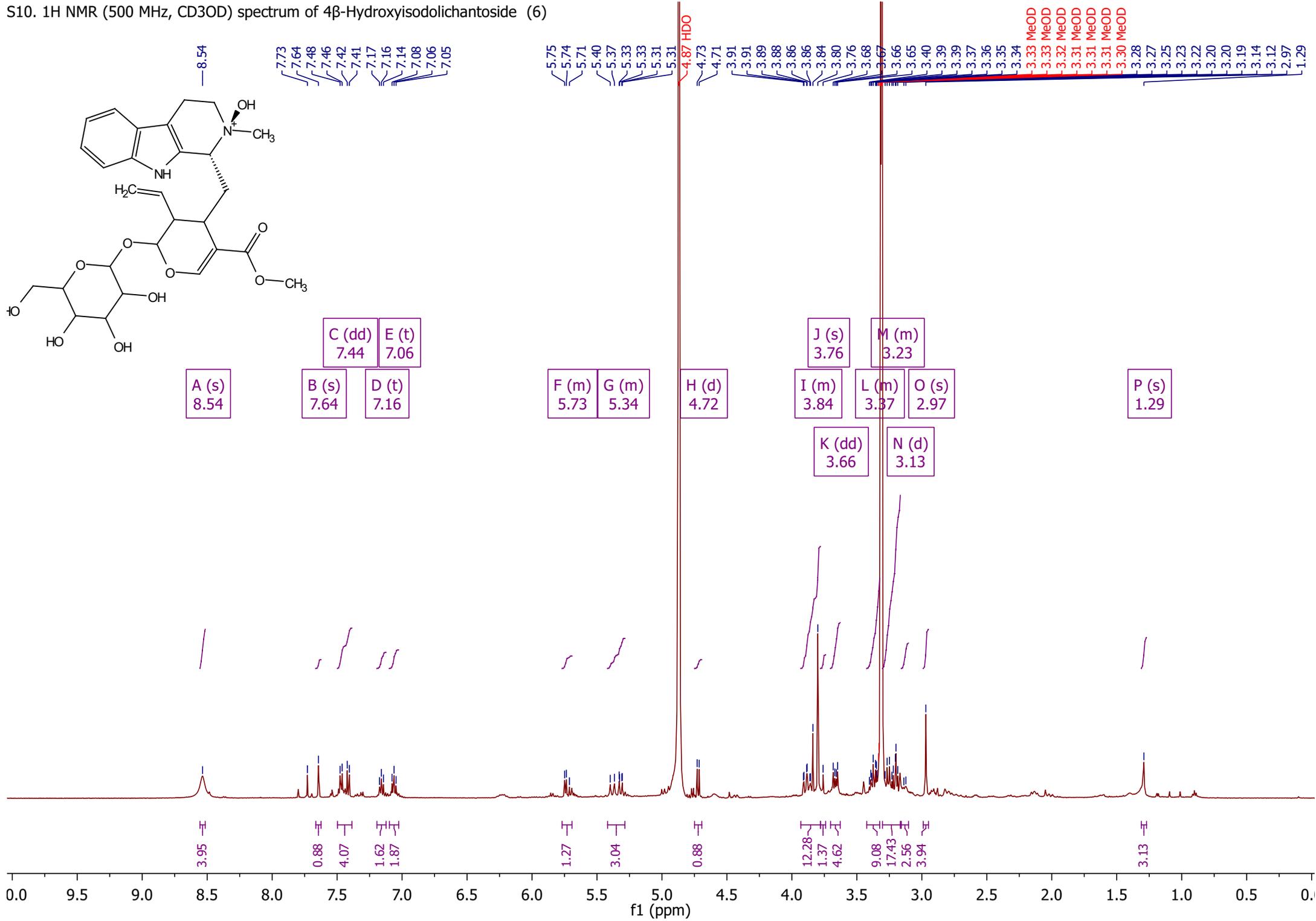
S8. HSQC (125 MHz, CD3OD) spectrum of 4-N-methyl-3,4-dehydrostrictosidine (4)



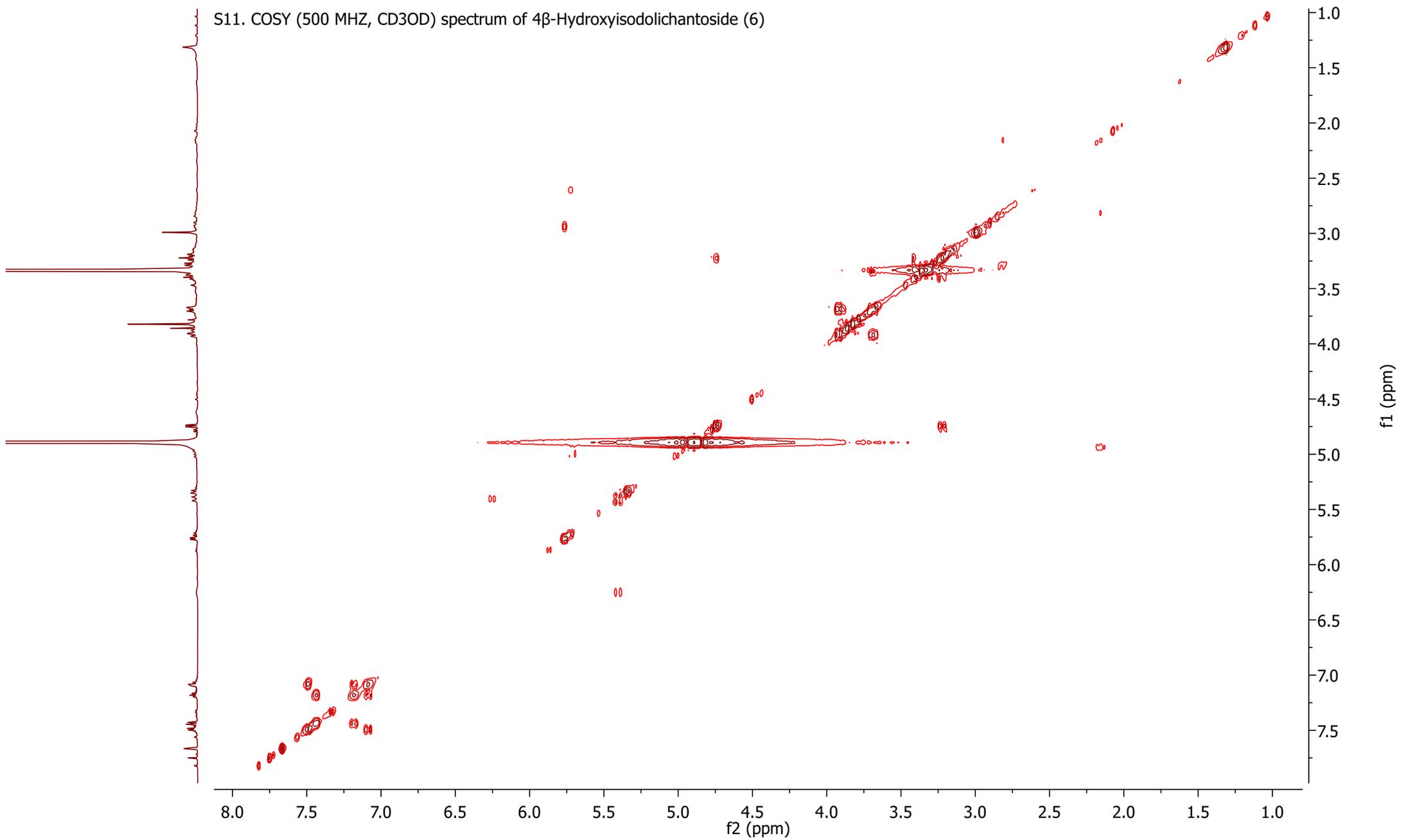
S9. HMBC (125 MHz, CD3OD) spectrum of 4-N-methyl-3,4-dehydrostrictosidine (4)



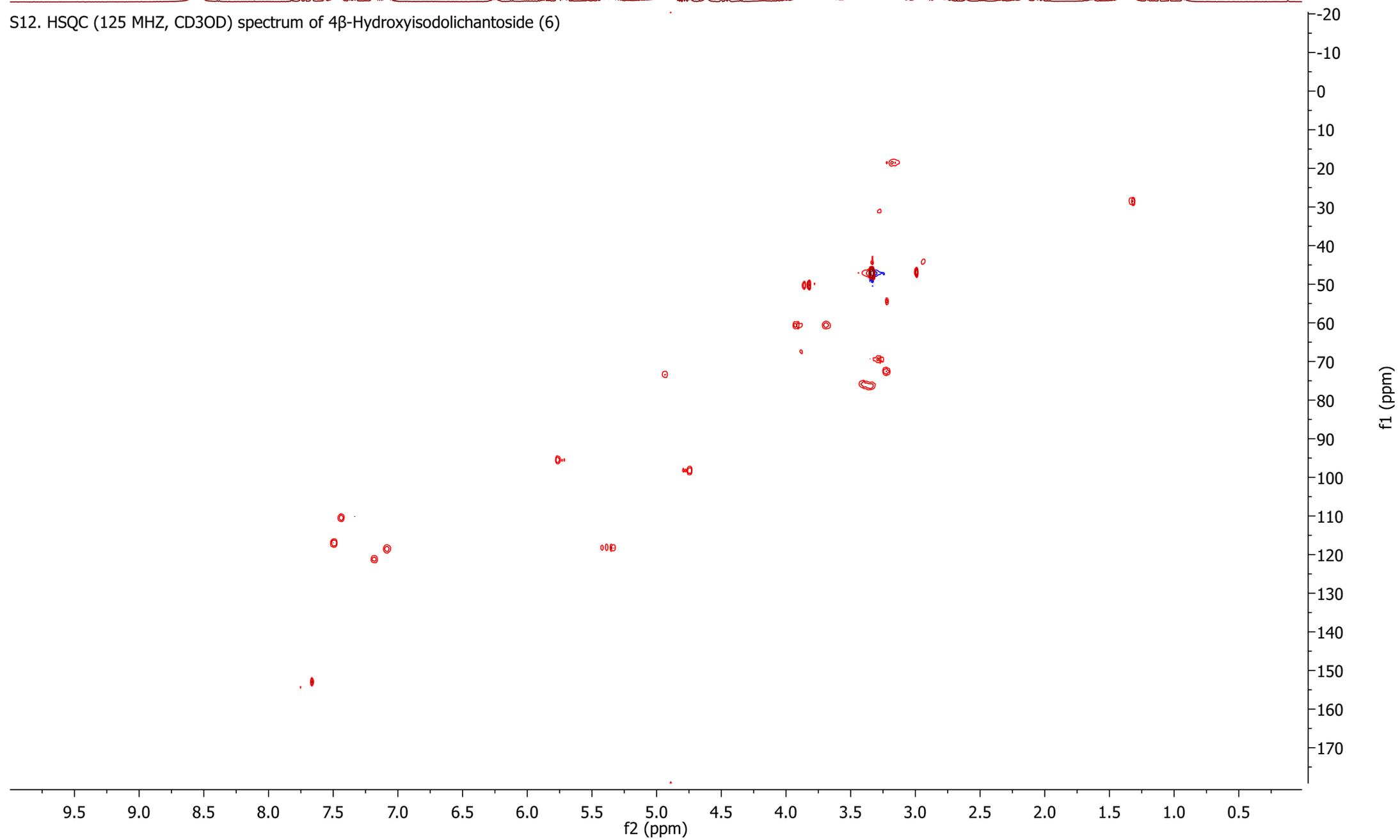
S10. 1H NMR (500 MHz, CD3OD) spectrum of 4β-Hydroxyisodolichantoside (6)



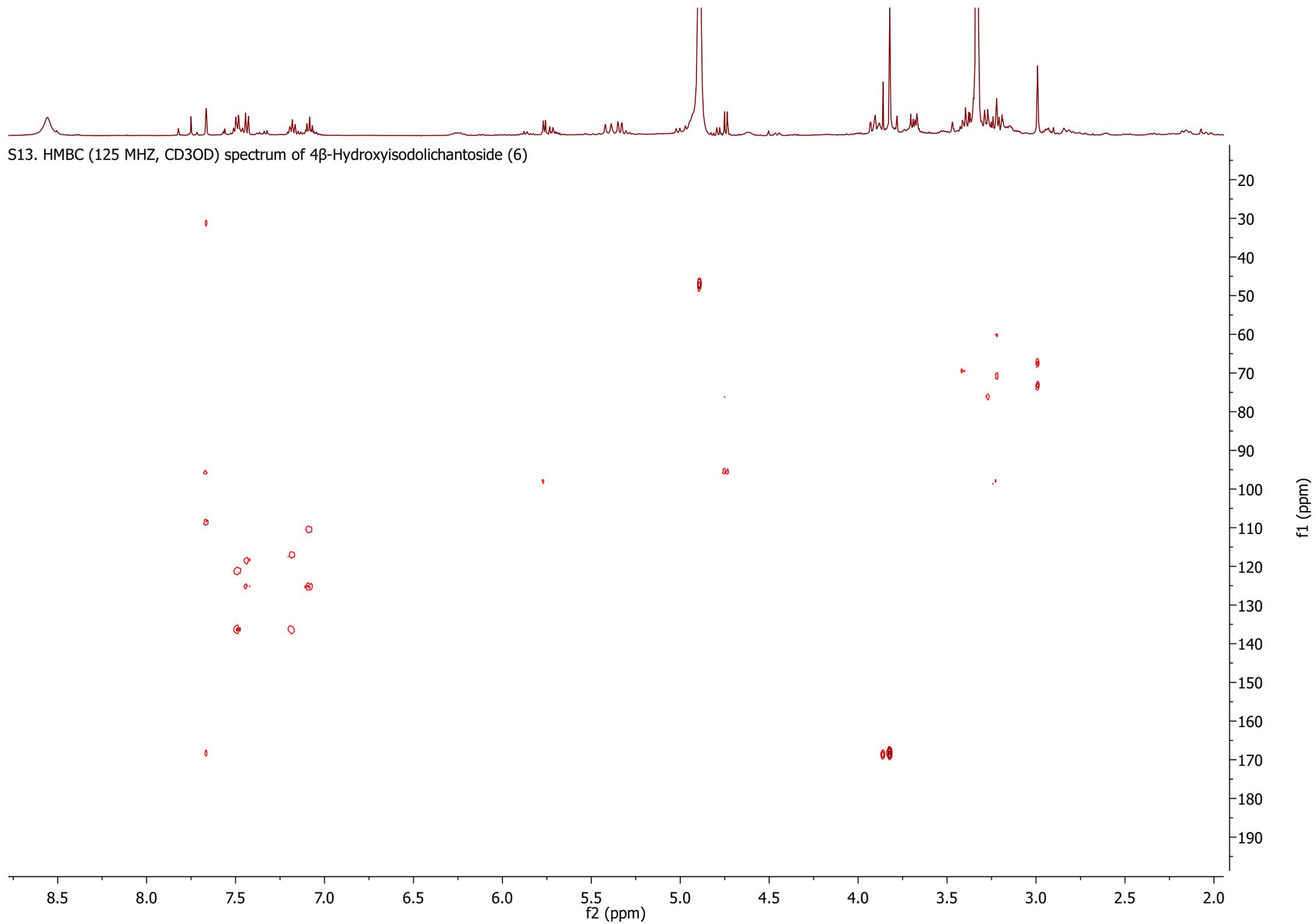
S11. COSY (500 MHz, CD3OD) spectrum of 4 β -Hydroxyisodolichantoside (6)



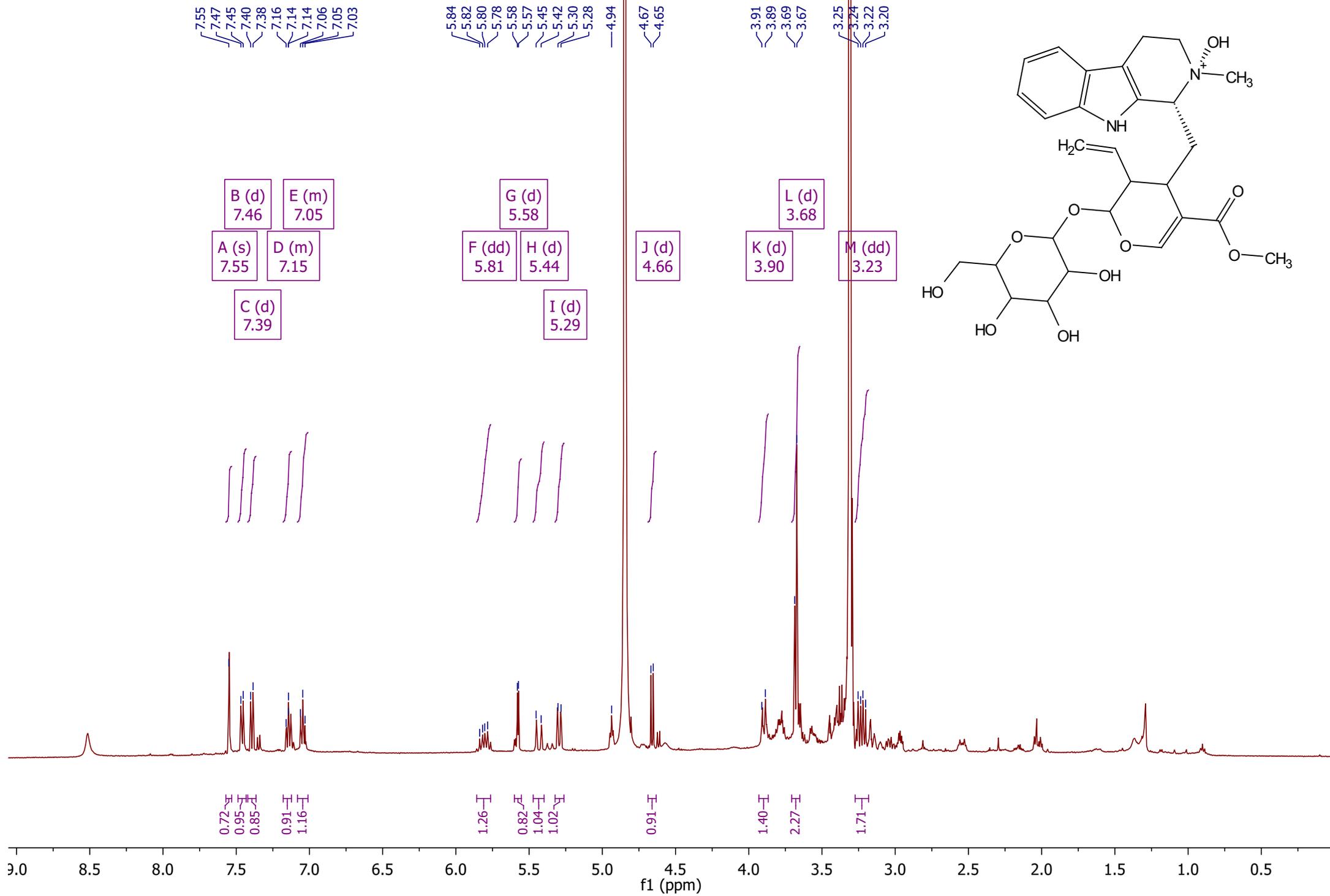
S12. HSQC (125 MHz, CD3OD) spectrum of 4 β -Hydroxyisodolichantoside (6)

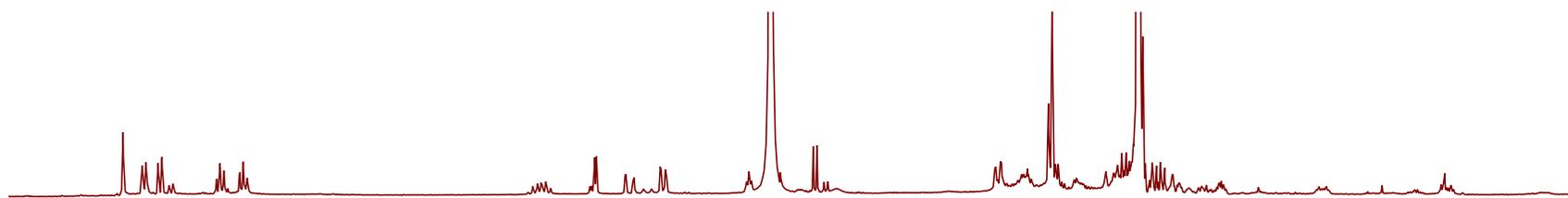


S13. HMBC (125 MHz, CD3OD) spectrum of 4 β -Hydroxyisodolichantoside (6)

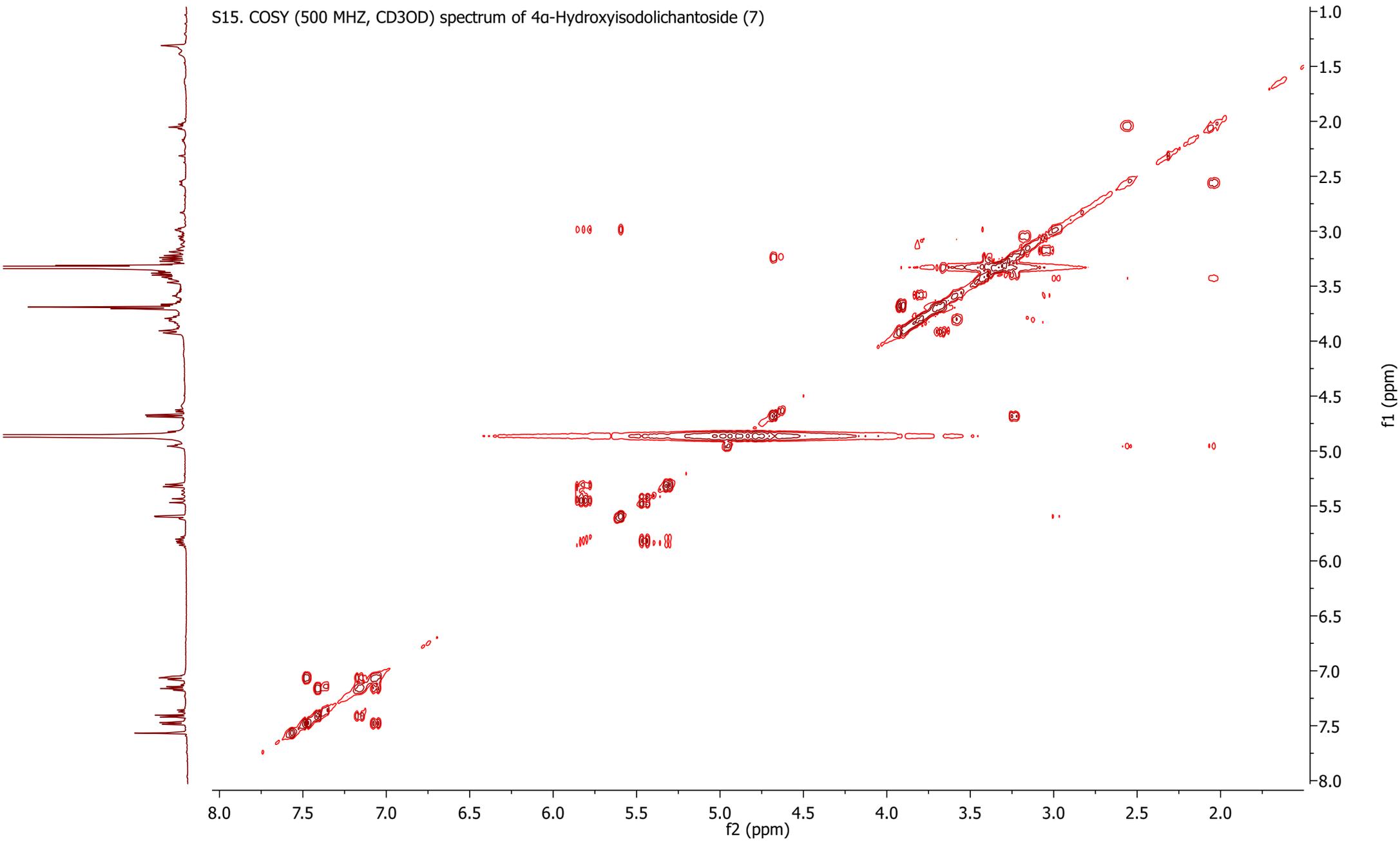


S14. ¹H NMR (500 MHz, CD₃OD) spectrum of 4a-Hydroxyisodolichantoside (7)

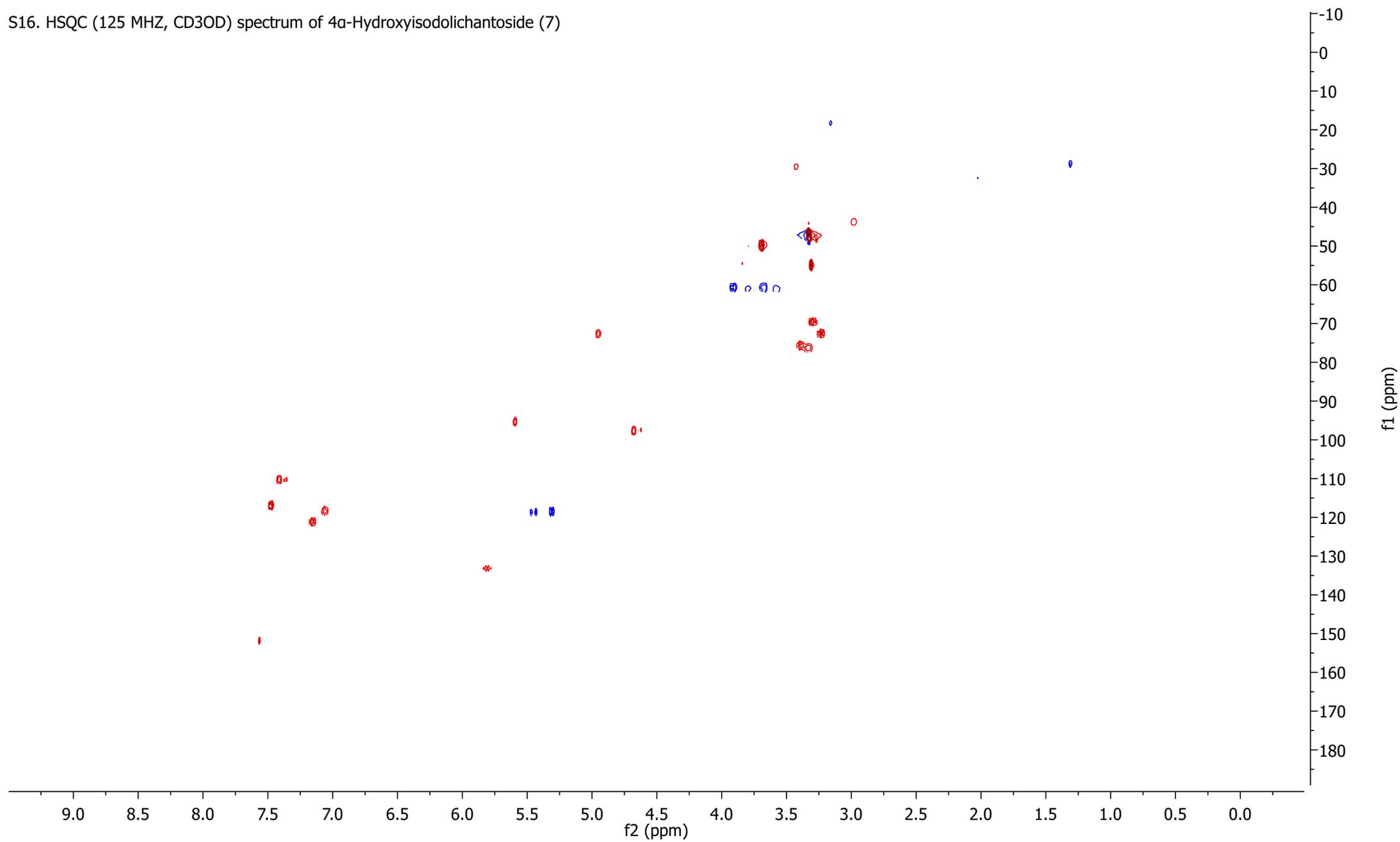




S15. COSY (500 MHz, CD₃OD) spectrum of 4α-Hydroxyisodolichantoside (7)



S16. HSQC (125 MHz, CD3OD) spectrum of 4 α -Hydroxyisodolichantoside (7)



S17. HMBC (125 MHz, CD3OD) spectrum of 4 α -Hydroxyisodolichantoside (7)

