

Contents class Wintersemester 2017/18 (Modern Applications of NMR Spectroscopy)

**Structure Elucidation in Organic and Inorganic Chemistry: Methods and Examples.**

*This class introduces modern NMR experiments for structure elucidation/verification of organic and inorganic molecules. Methods are demonstrated by their application to example molecules*

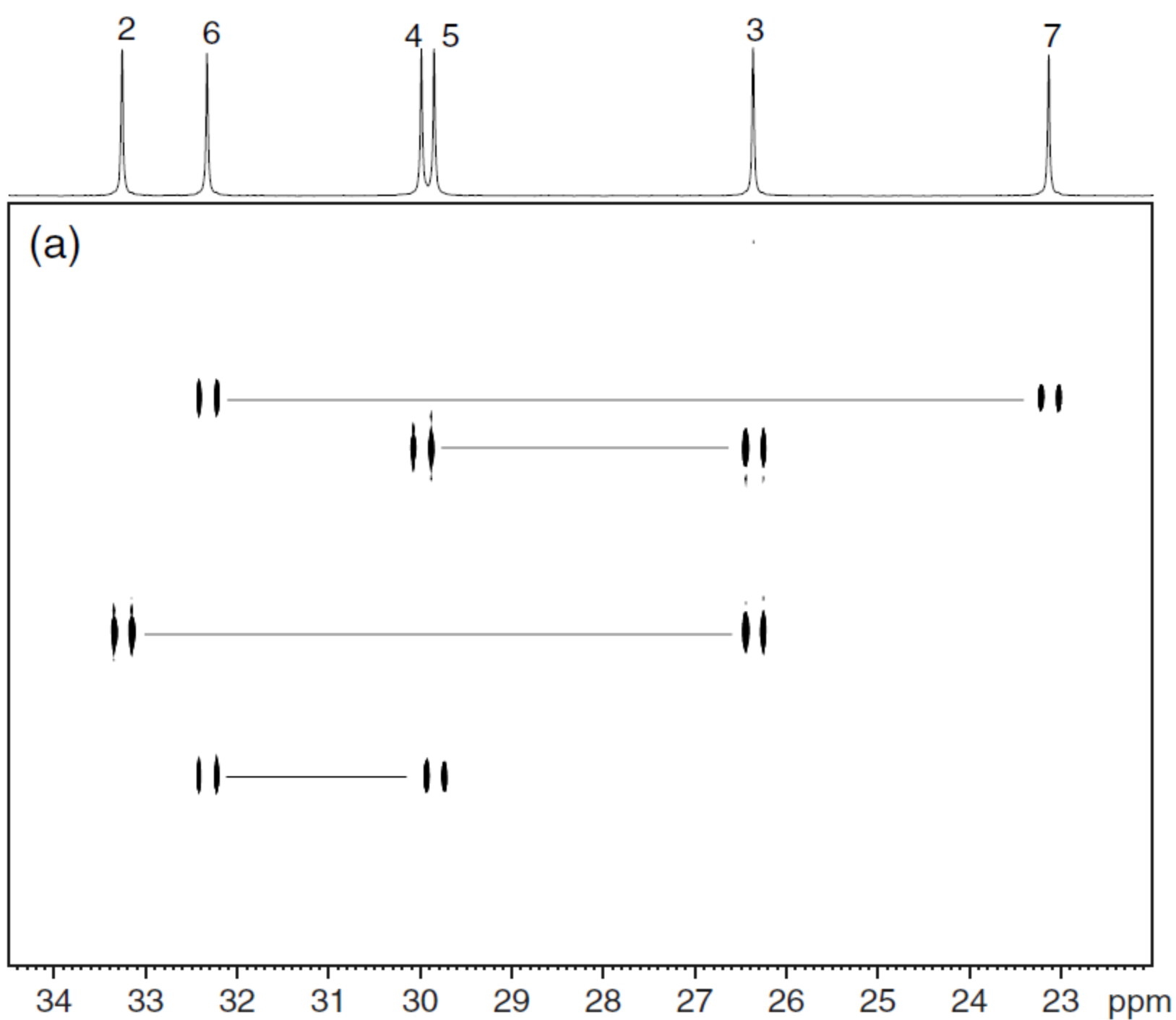
Class 1 – Dec. 6<sup>th</sup>

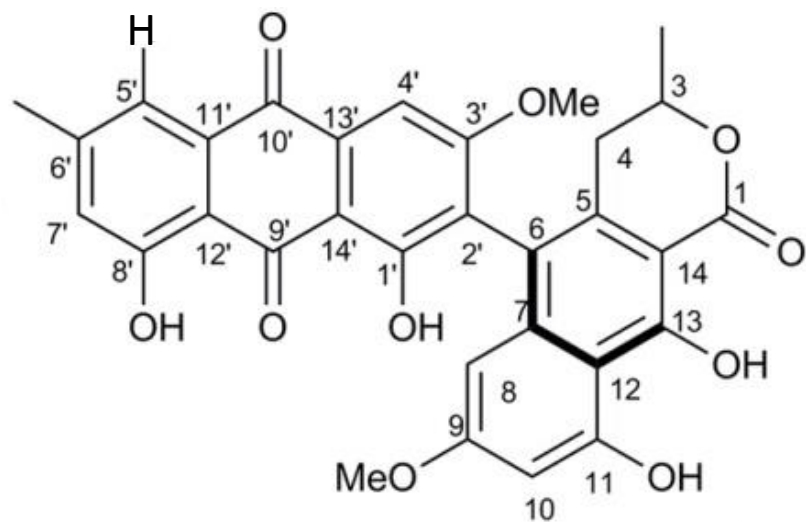
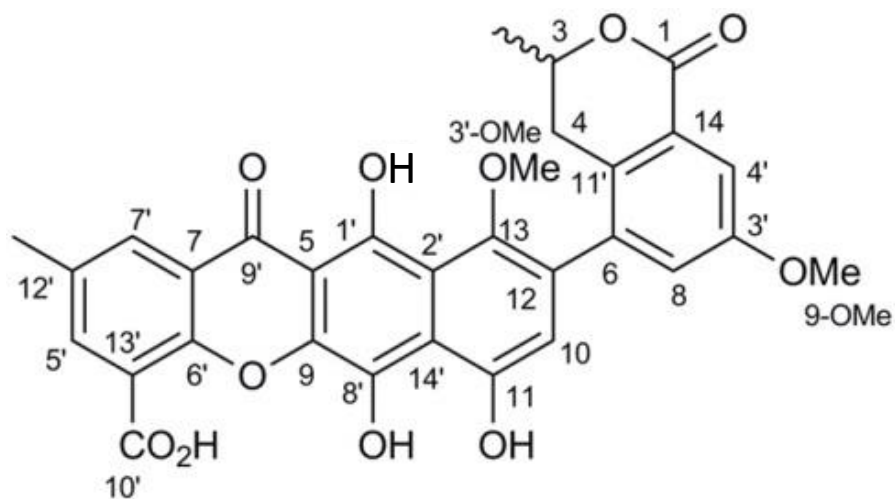
What the class will be about: Showing specific examples for structure elucidation, thereby detailing on advanced/less common NMR experiments.

INADEQUATE: One example from natural compounds chemistry, one from metabolite research

References:

- Buddrus, *Magn. Reson. Chem.* **2002**, *40*, 3 (general reading in INADEQUATE)
- Nuzillard, *J. Nat. Prod.* **2015**, *78*, 597 (structure revision)
- Pedras, *Phytochem.* **2016**, *132*, 26 (metabolic precursors in biosynthesis)





Revised structure

12.413  
12.031

9.800

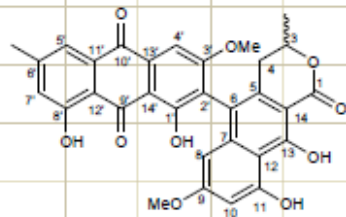
7.702  
7.698  
7.574  
7.260 CDCl<sub>3</sub>  
7.133  
7.131  
7.128  
7.125  
6.587  
6.579  
6.151  
6.143

4.763  
4.742  
4.737  
4.722  
4.716  
4.695  
4.574

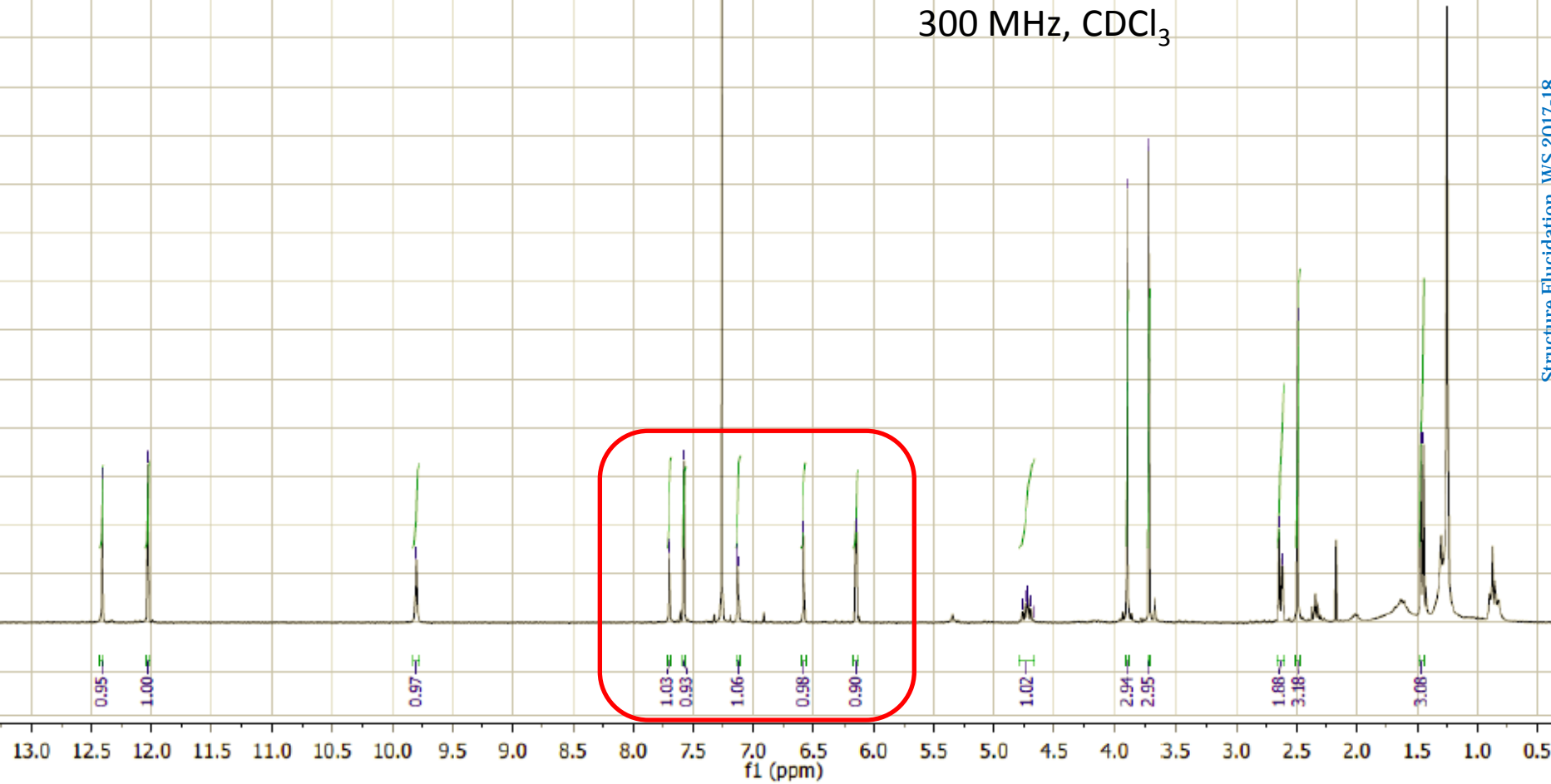
3.891  
3.714

2.643  
2.623  
2.617  
2.492

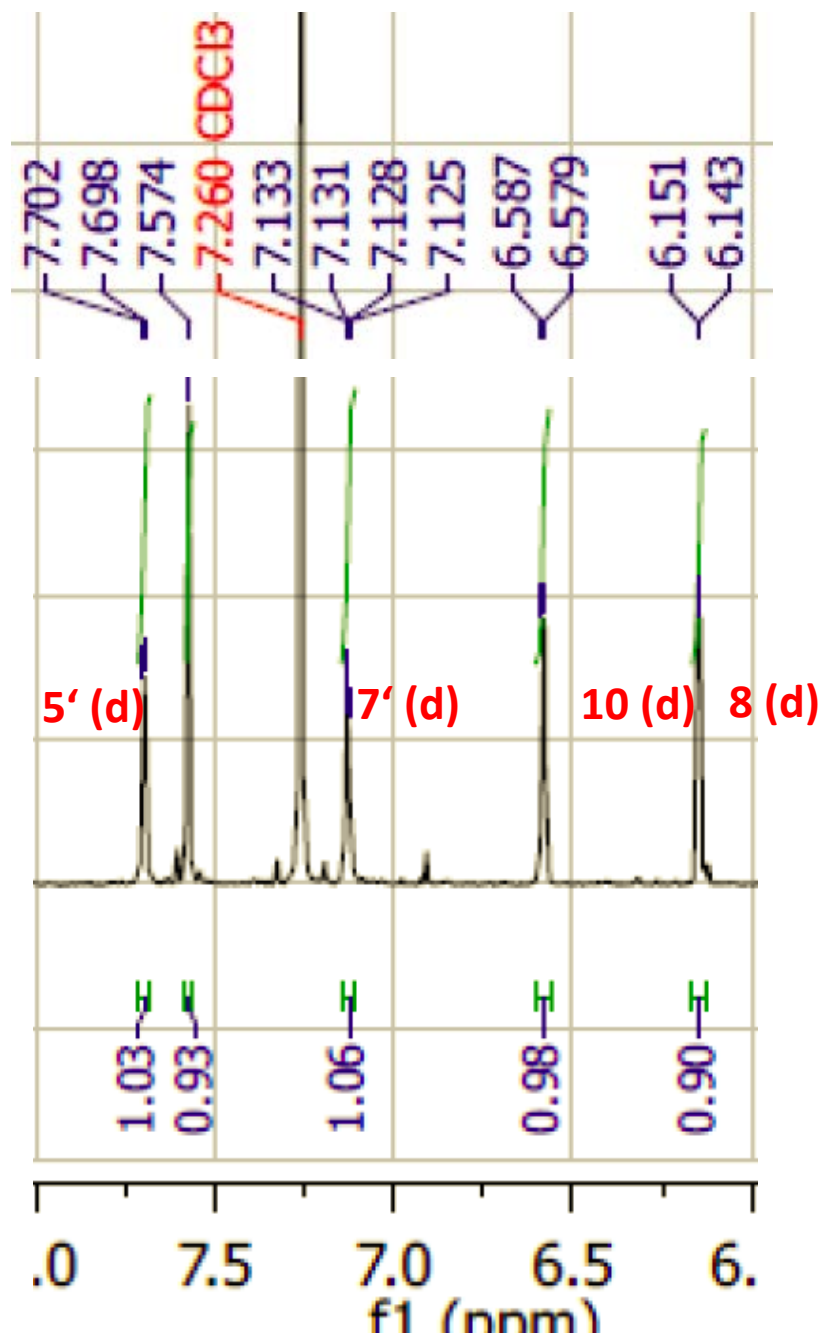
1.467  
1.446

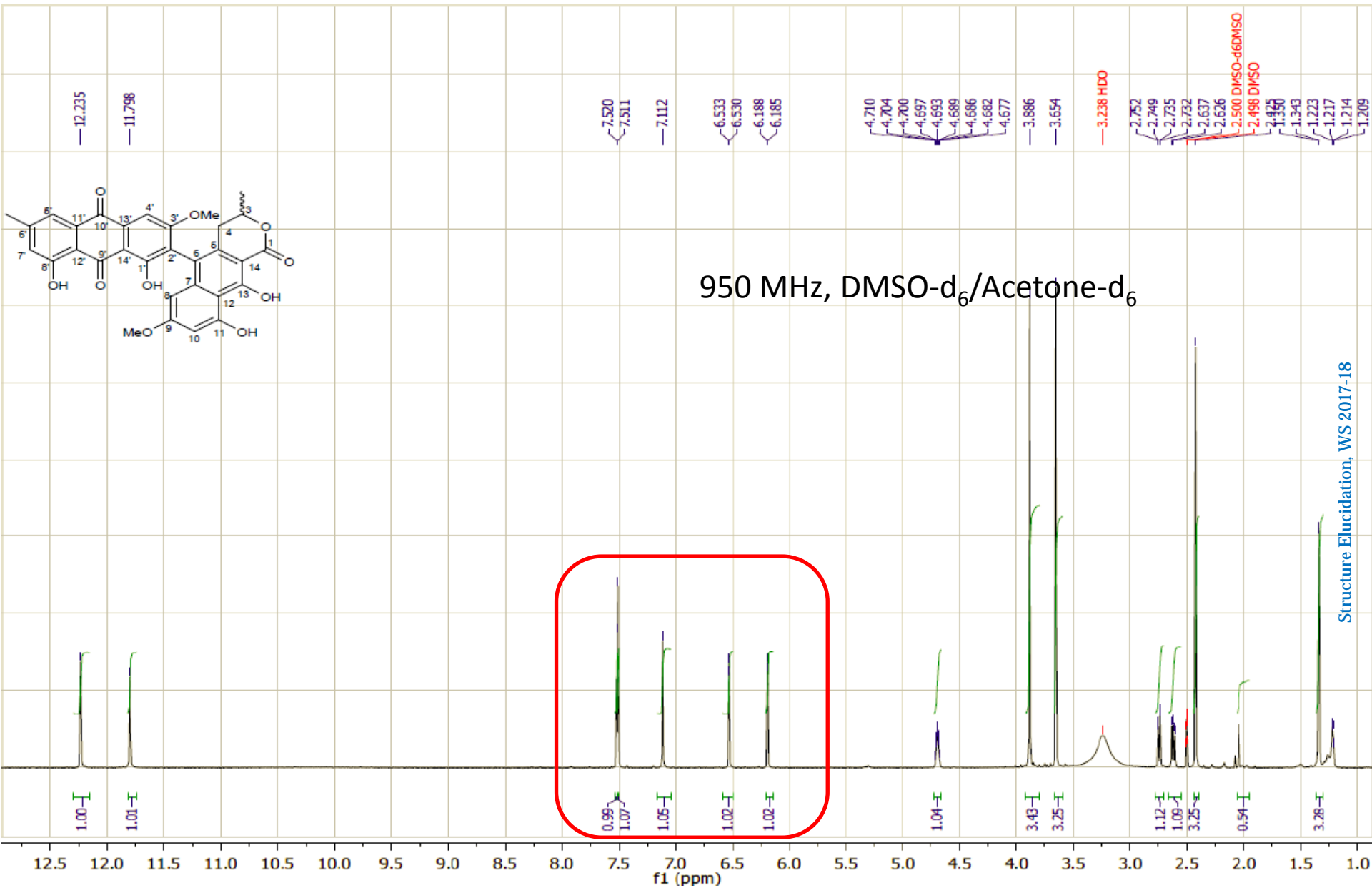


300 MHz, CDCl<sub>3</sub>

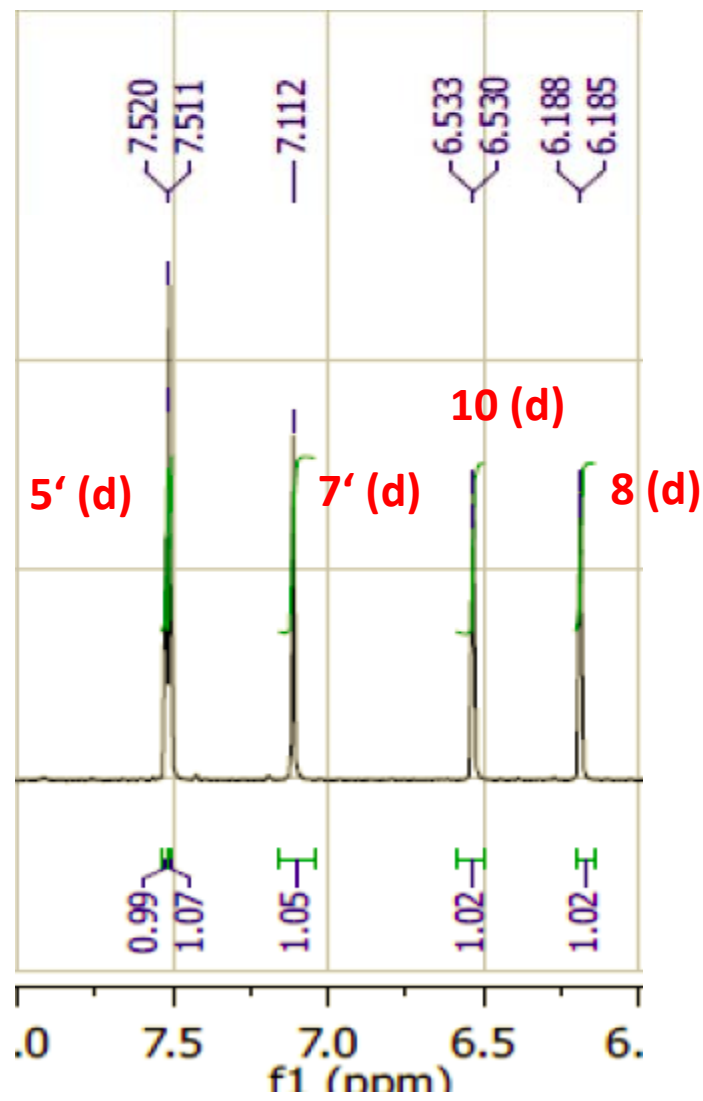


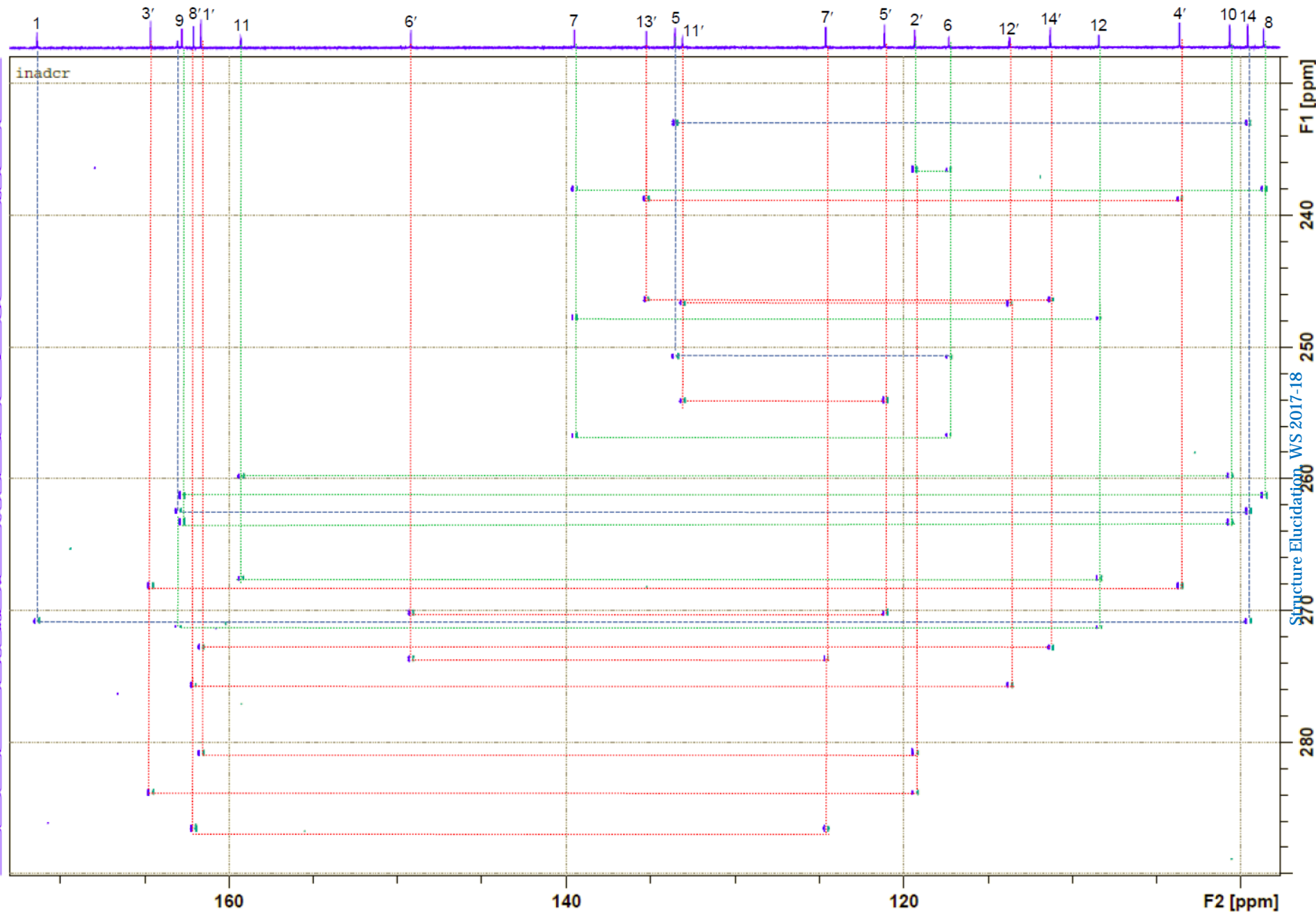
300 MHz, CDCl<sub>3</sub>





950 MHz, DMSO-d<sub>6</sub>/Acetone-d<sub>6</sub>





INADEQUATE, 950 MHz, DMSO-d<sub>6</sub>/Acetone-d<sub>6</sub>



