

## Synthesis and characterisation of lanthanide-hydroporphyrin dyads

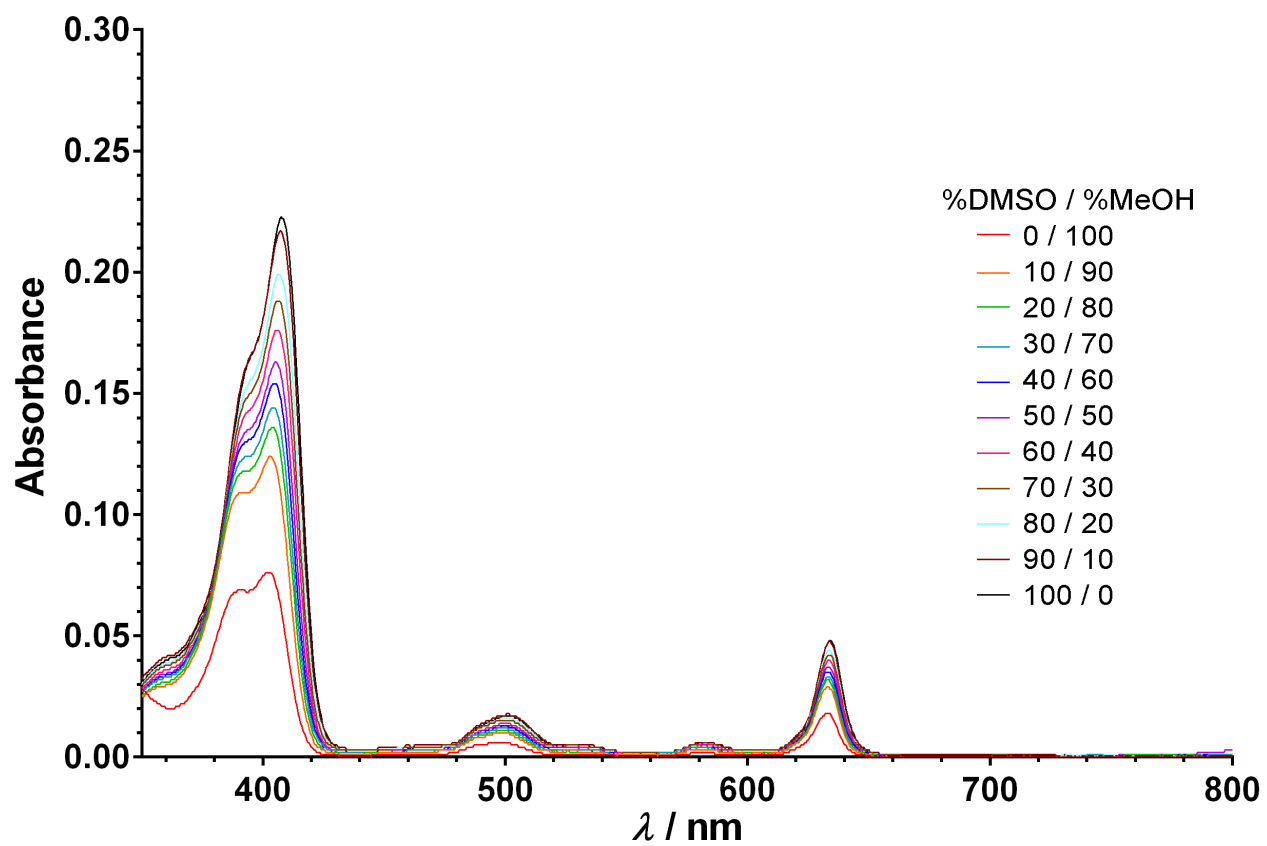
Ruisheng Xiong, Julien Andres, Kira Scheffler and K. Eszter Borbas\*

Department of Chemistry - BMC, Uppsala University, SE-75123, Uppsala, Sweden

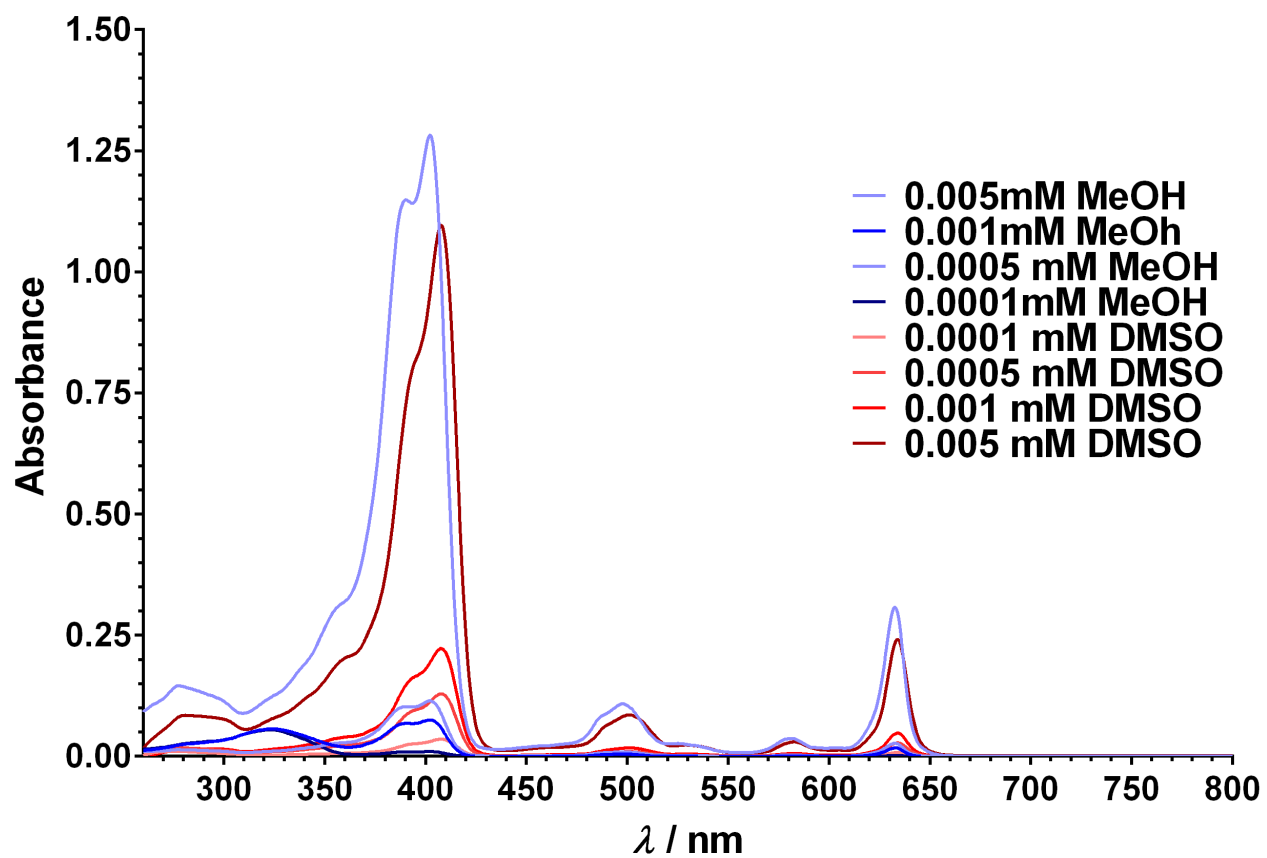
[eszter.borbas@kemi.uu.se](mailto:eszter.borbas@kemi.uu.se)

### Table of contents

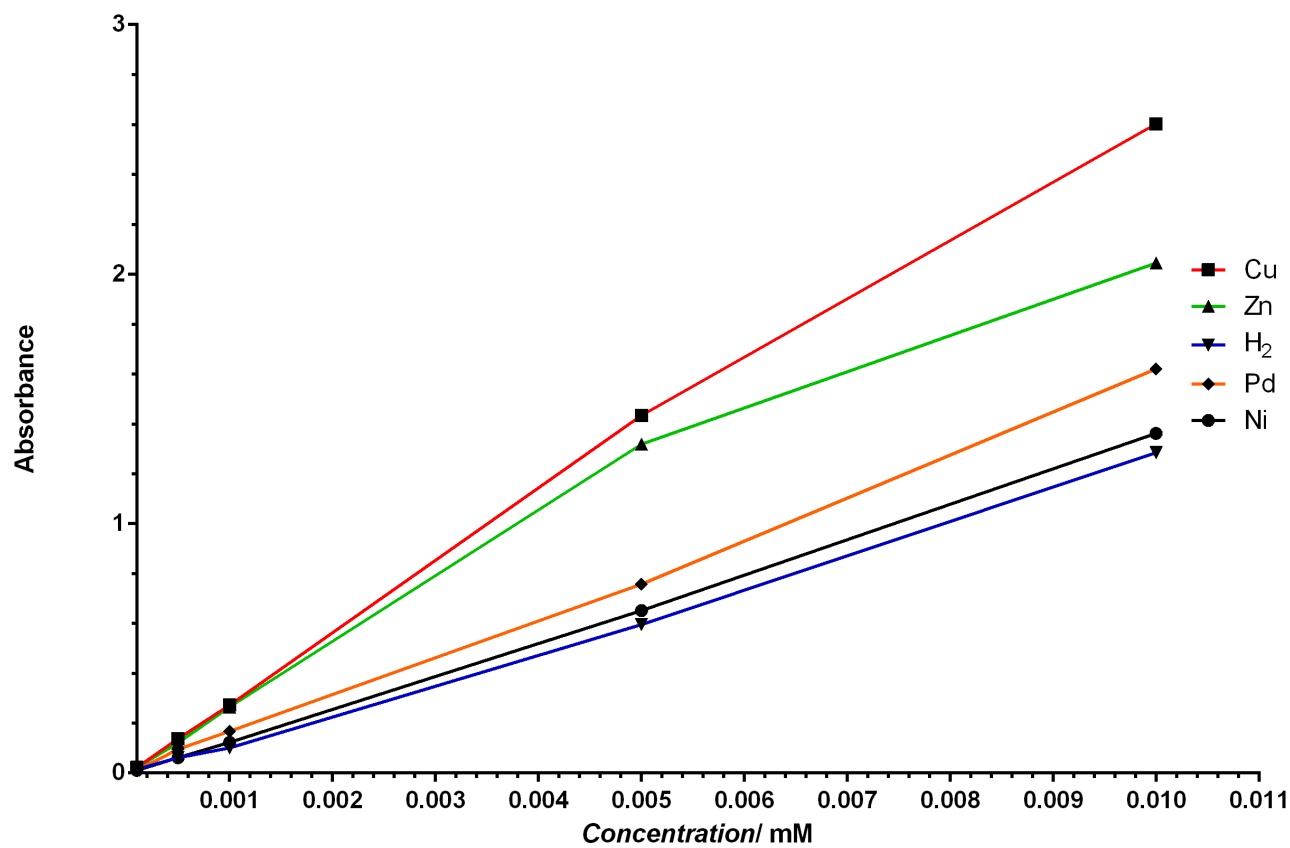
Figures S1–S4	S2
Additional photophysical discussion	S6
$^1\text{H}$ and $^{13}\text{C}$ NMR spectra of new compounds	S7



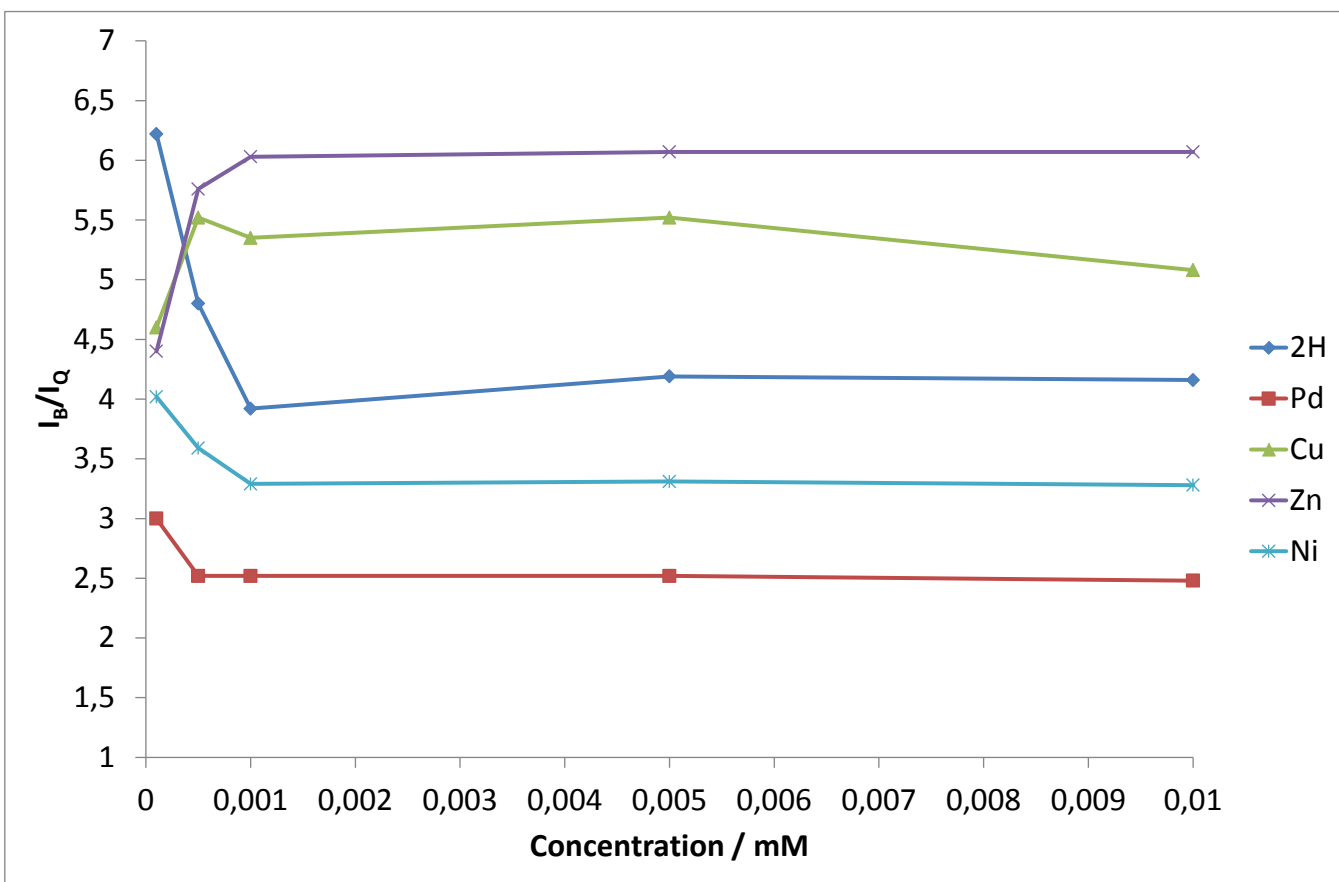
**Figure S1.** Absorption spectra of free base chlorin reference compound 7, 1 μM in solvent mixtures containing different ratios of DMSO/MeOH.



**Figure S2.** Absorption spectra of free base chlorin reference compound 7 in DMSO and in MeOH at different concentrations.



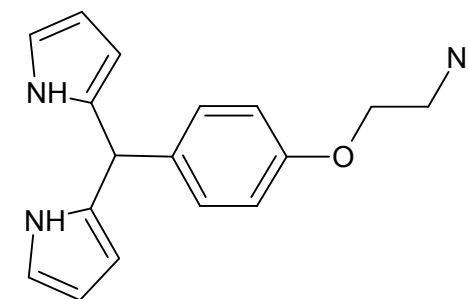
**Figure S3.** Linearity of the Beer-Lambert law for 6–8.



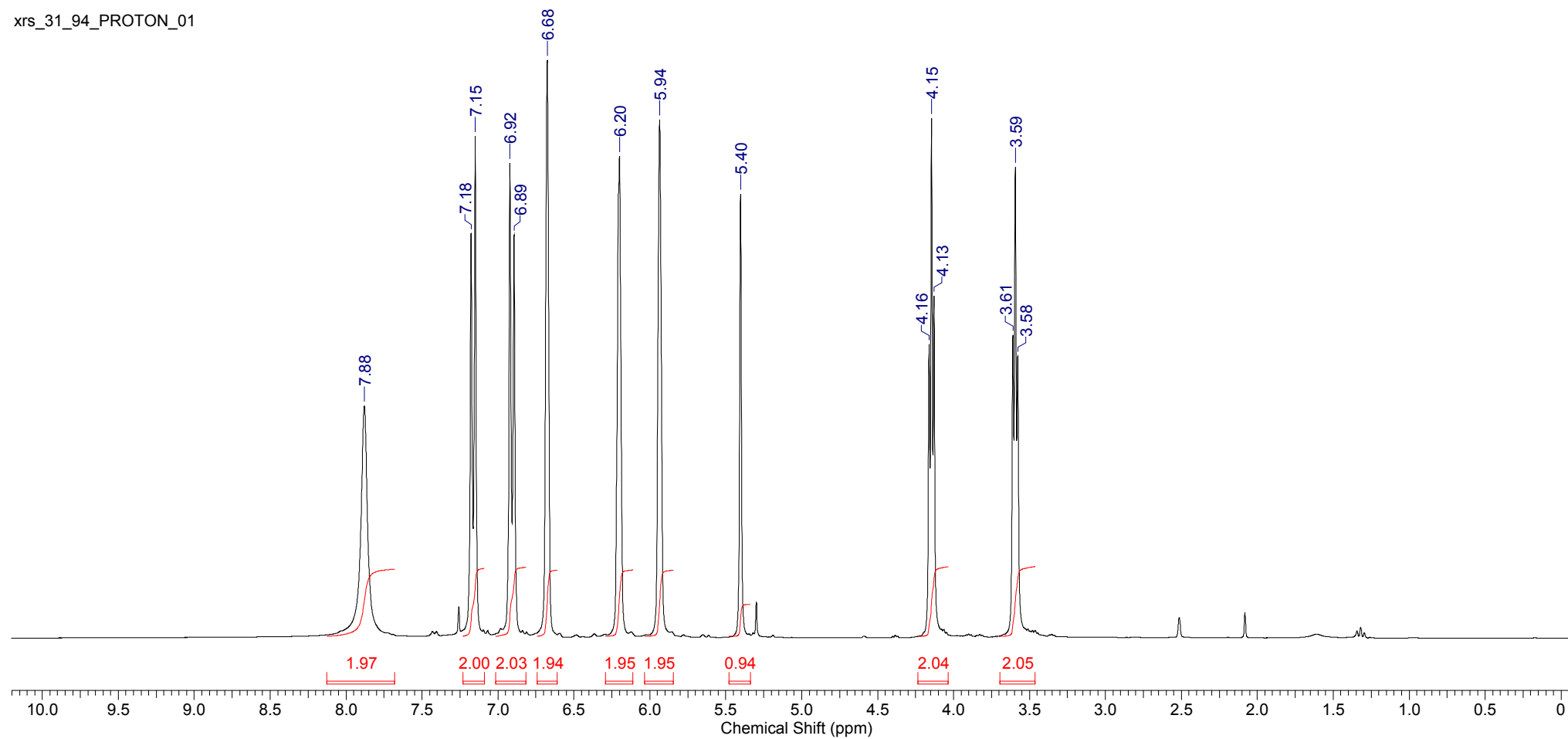
**Figure S4.** Dependence of  $I_B/I_Q$ -ratio on chlorin concentration.

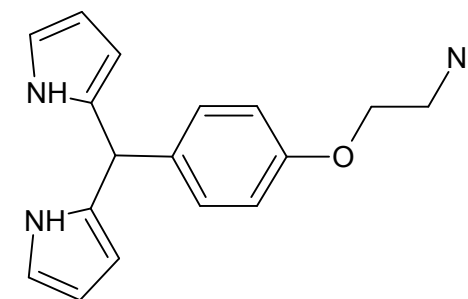
### **Choosing the quantum yield standard**

Due to the high Stokes shift upon excitation in the Soret band, finding fluorescence standards with known quantum yields were not straightforward. Cresyl violet, which is a classical red emitting fluorescence standard for quantum yield determinations was not suitable for the whole series of **6–8**, as the Q-band shifts too far away from the Cresyl violet absorption to be used with every complex. Furthermore, Cresyl violet has an extinction coefficient at the Soret band location that is 20–100 times lower, making it difficult to get equal absorbances of the reference and of the chlorins in this spectral range. A porphyrin standard circumvents this issue since it belongs to the same molecule family and hence displays similar photophysical properties (i.e. high extinction Soret band, large Stokes shift). In addition, the same concentration range can be used with the TPP standard by choosing the excitation wavelengths where the absorbances of the chlorin samples cross the one of the TPP standard, thus ensuring a same amount of absorbed quanta providing that the monochromatic excitation peak is kept at a minimal bandwidth (closed slits in the excitation monochromator).

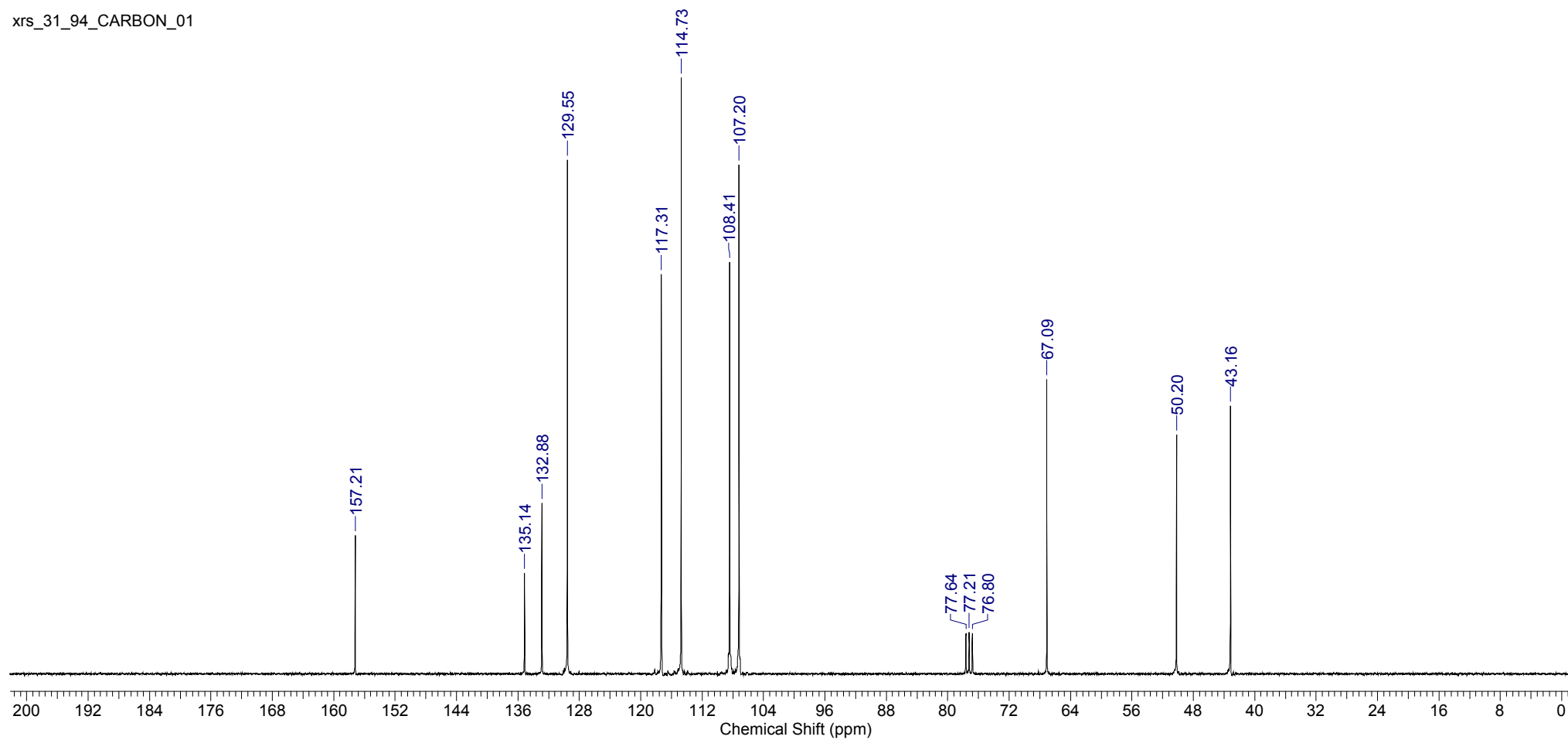


xrs\_31\_94\_PROTON\_01

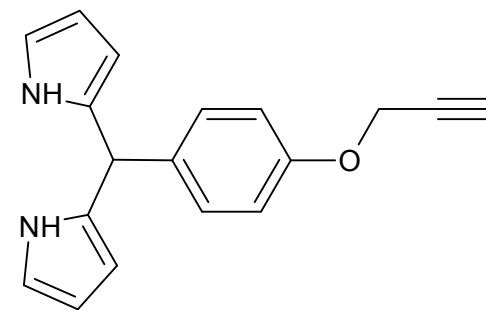




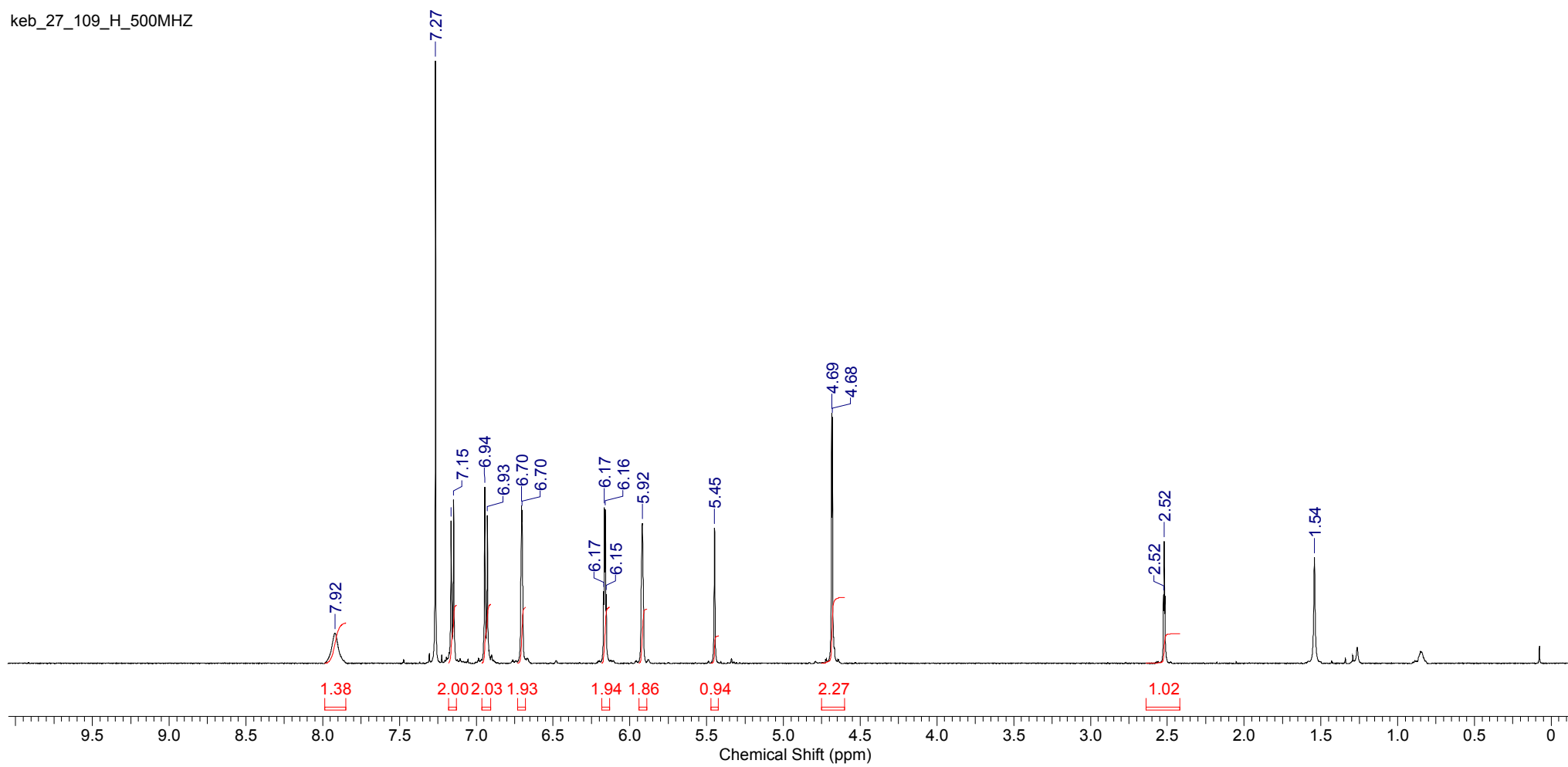
xrs\_31\_94\_CARBON\_01







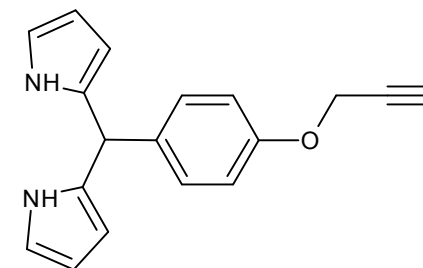
keb\_27\_109\_H\_500MHZ



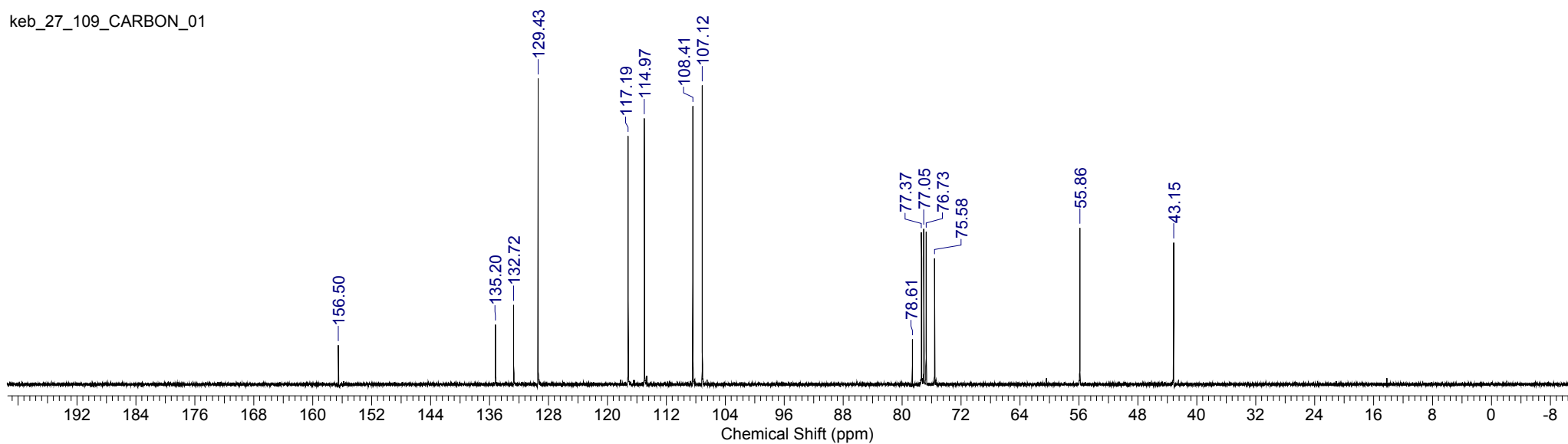
This report was created by ACD/NMR Processor Academic Edition. For more information go to [www.acdlabs.com/nmrproc/](http://www.acdlabs.com/nmrproc/)

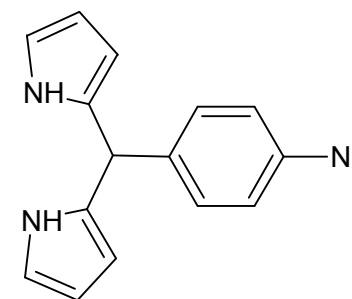
2014/ 6/ 19 19: 16: 40

<b>Formula</b> C <sub>16</sub> H <sub>16</sub> NO <sub>2</sub>	<b>FW</b> 276.3324		
<b>Acquisition Time (sec)</b> 1.3107	<b>Date</b> Jun 19 2014	<b>Date Stamp</b> Jun 19 2014	
<b>File Name</b> E:\UJ_PHD_Spectra\NMR\keb_27_109_20140619_01\keb_27_109_CARBON_01.fid\fid		<b>Frequency (MHz)</b> 100.58	
<b>Nucleus</b> 13C	<b>Number of Transients</b> 512	<b>Original Points Count</b> 32768	<b>Points Count</b> 32768
<b>Pulse Sequence</b> s2pul	<b>Receiver Gain</b> 30.00	<b>Solvent</b> CHLOROFORM-d	<b>Spectrum Offset (Hz)</b> 11063.0342
<b>Spectrum Type</b> STANDARD	<b>Sweep Width (Hz)</b> 25000.00	<b>Temperature (degree C)</b> 25.000	

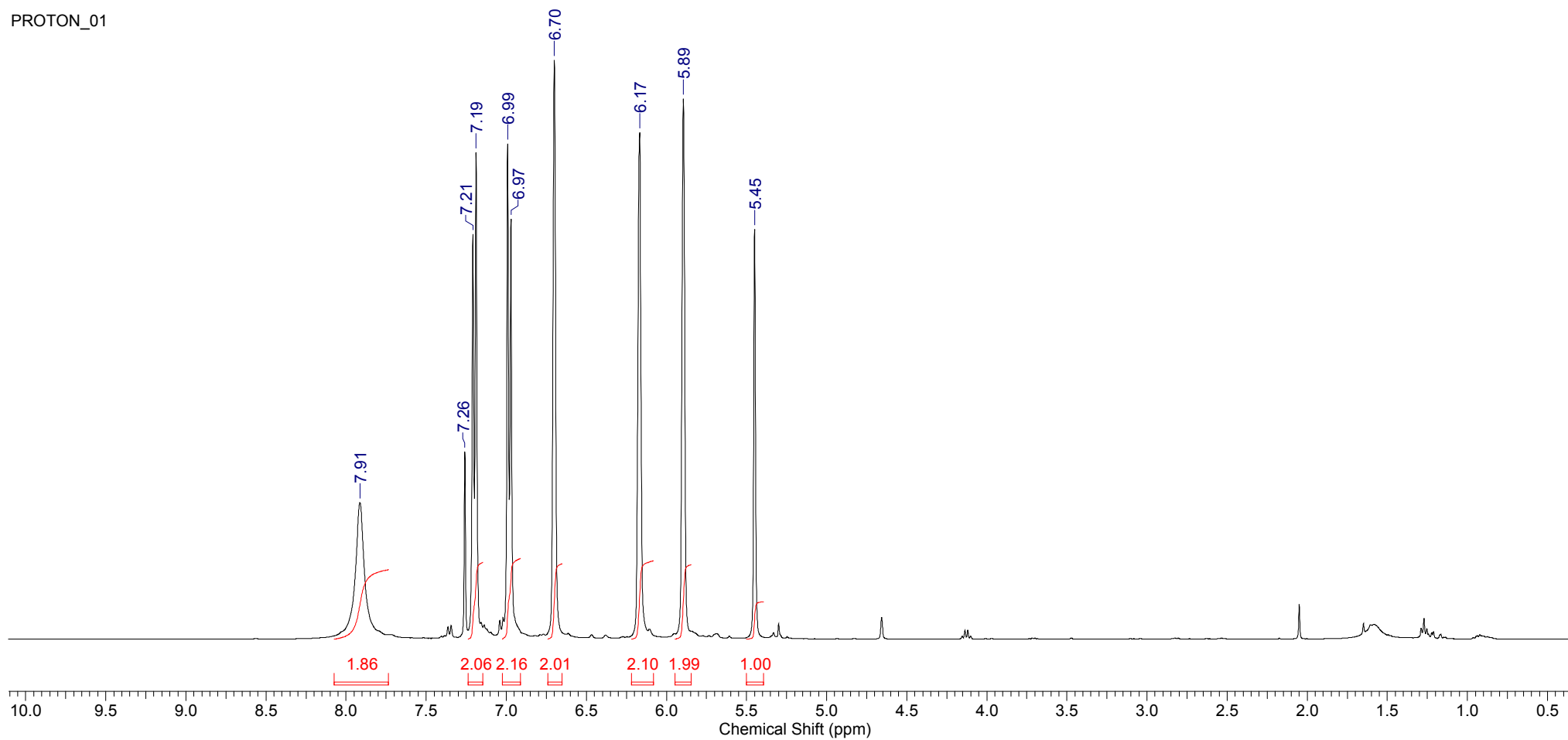


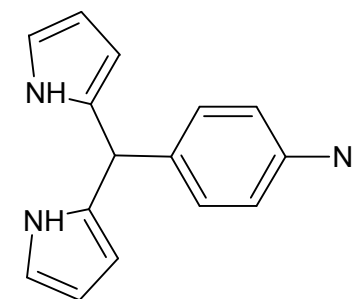
keb\_27\_109\_CARBON\_01



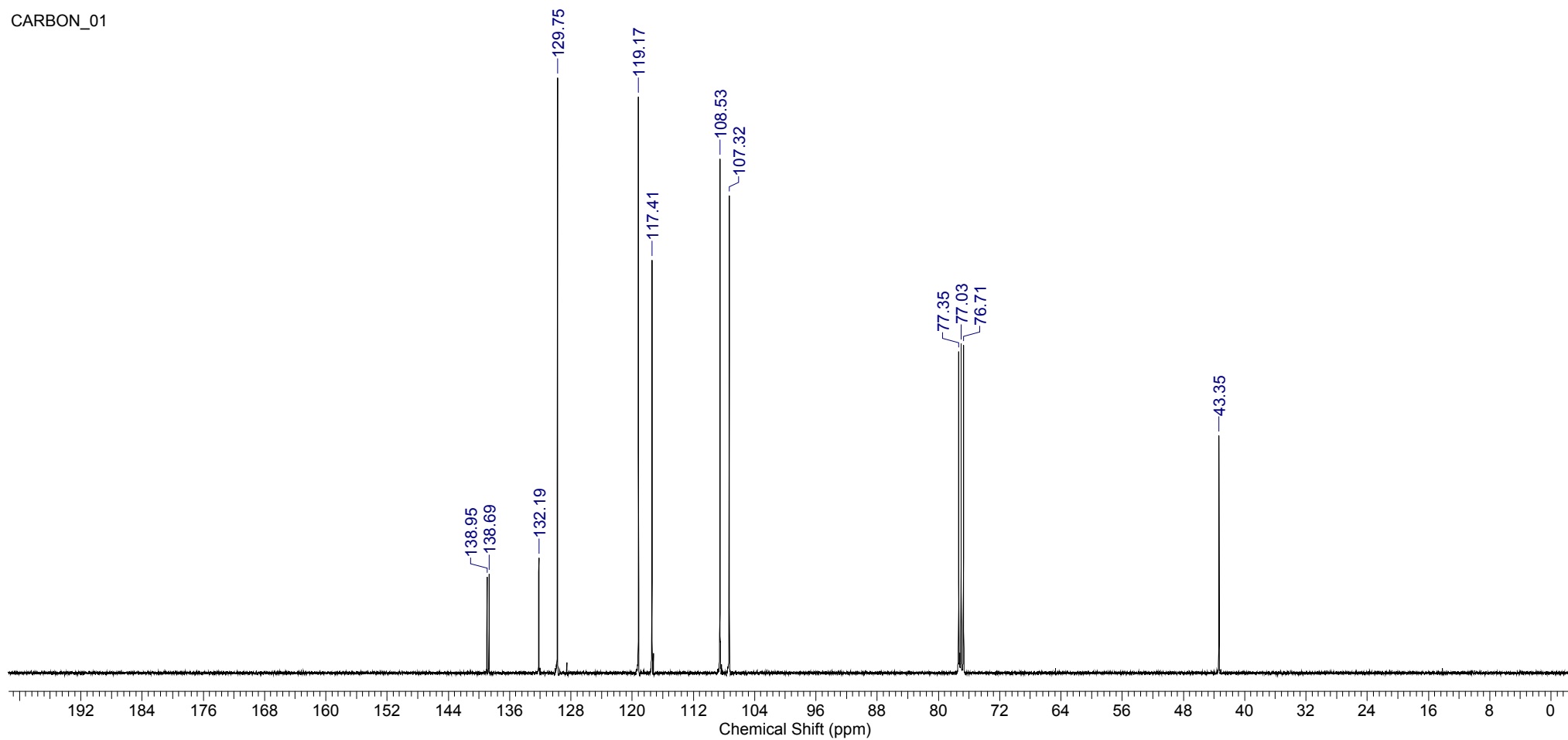


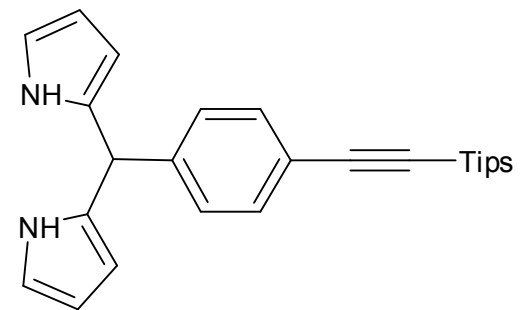
PROTON\_01



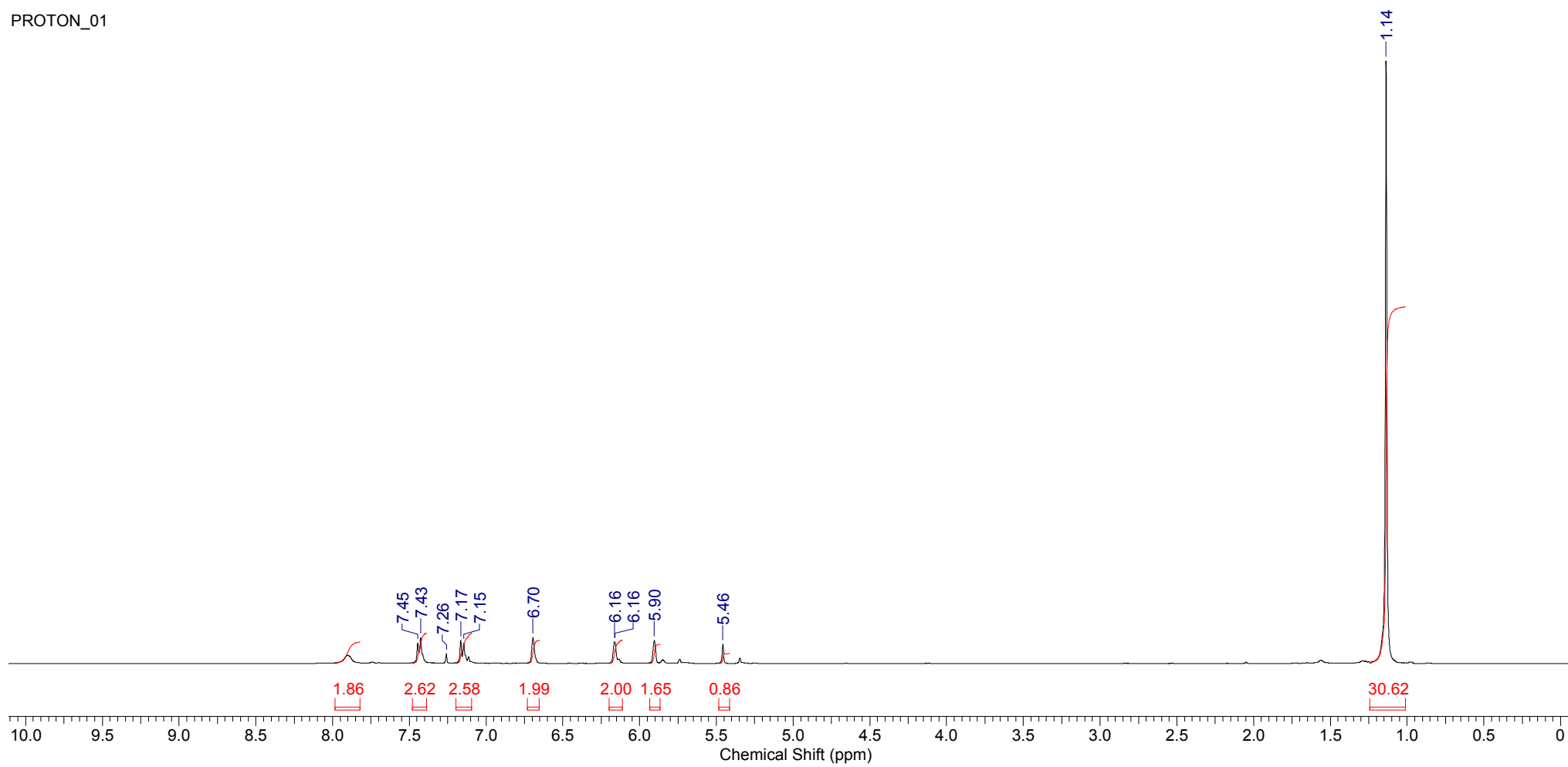


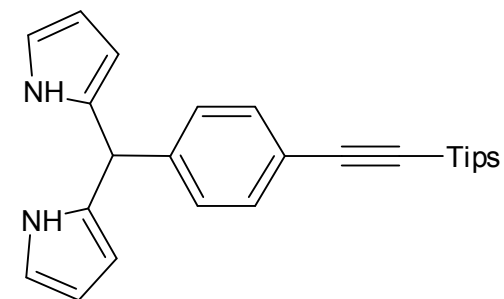
CARBON\_01



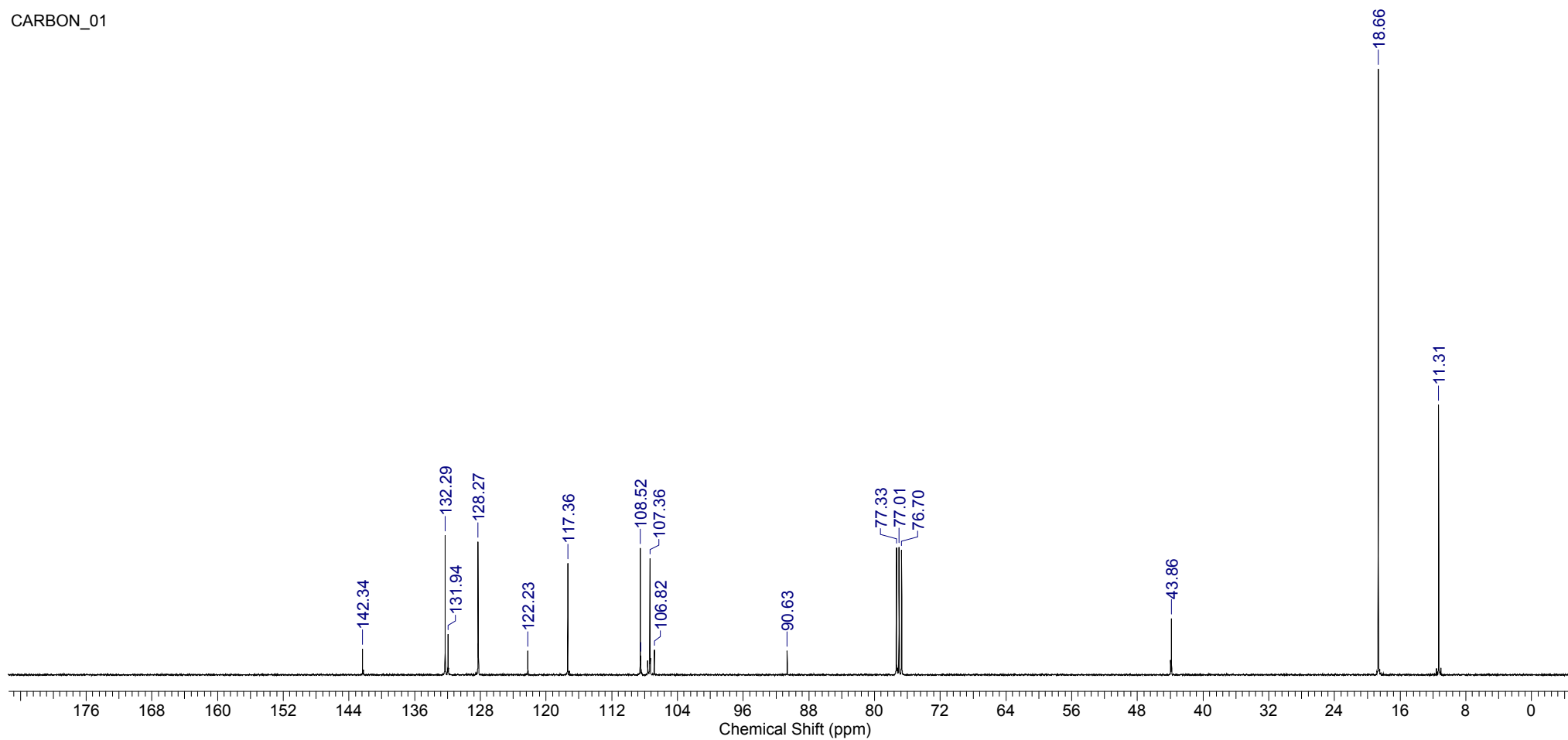


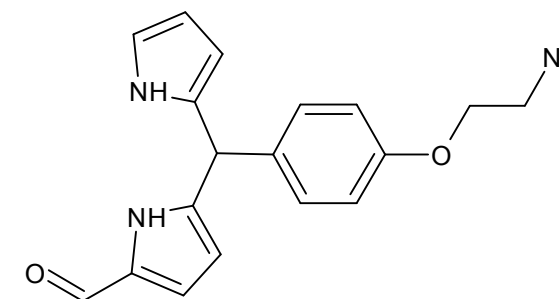
PROTON\_01



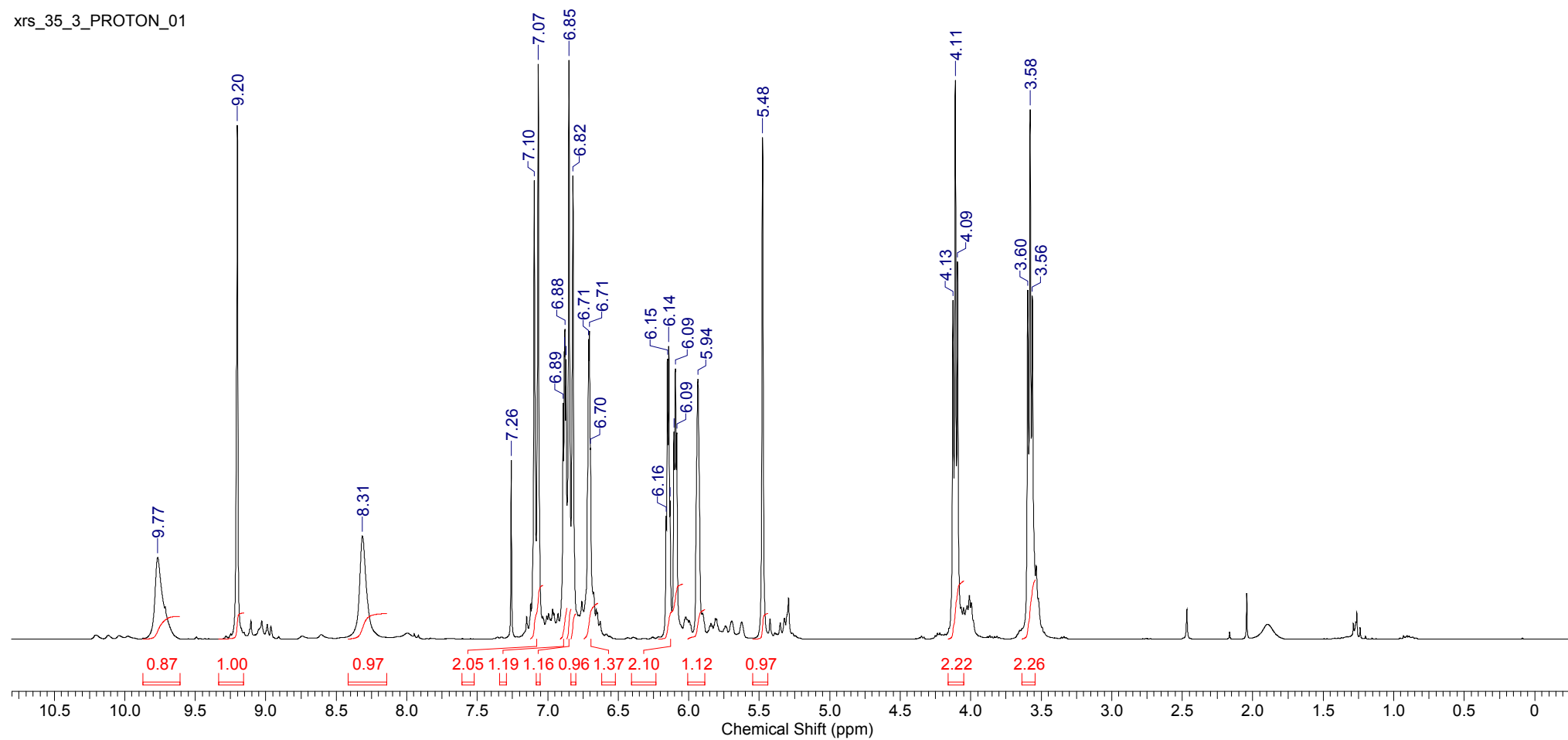


CARBON\_01

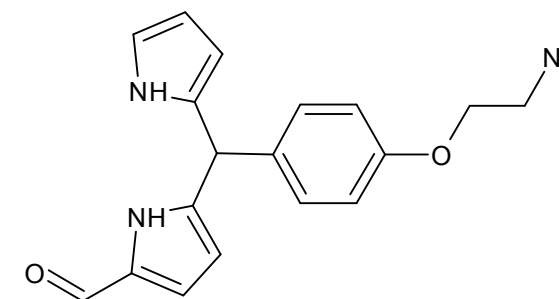




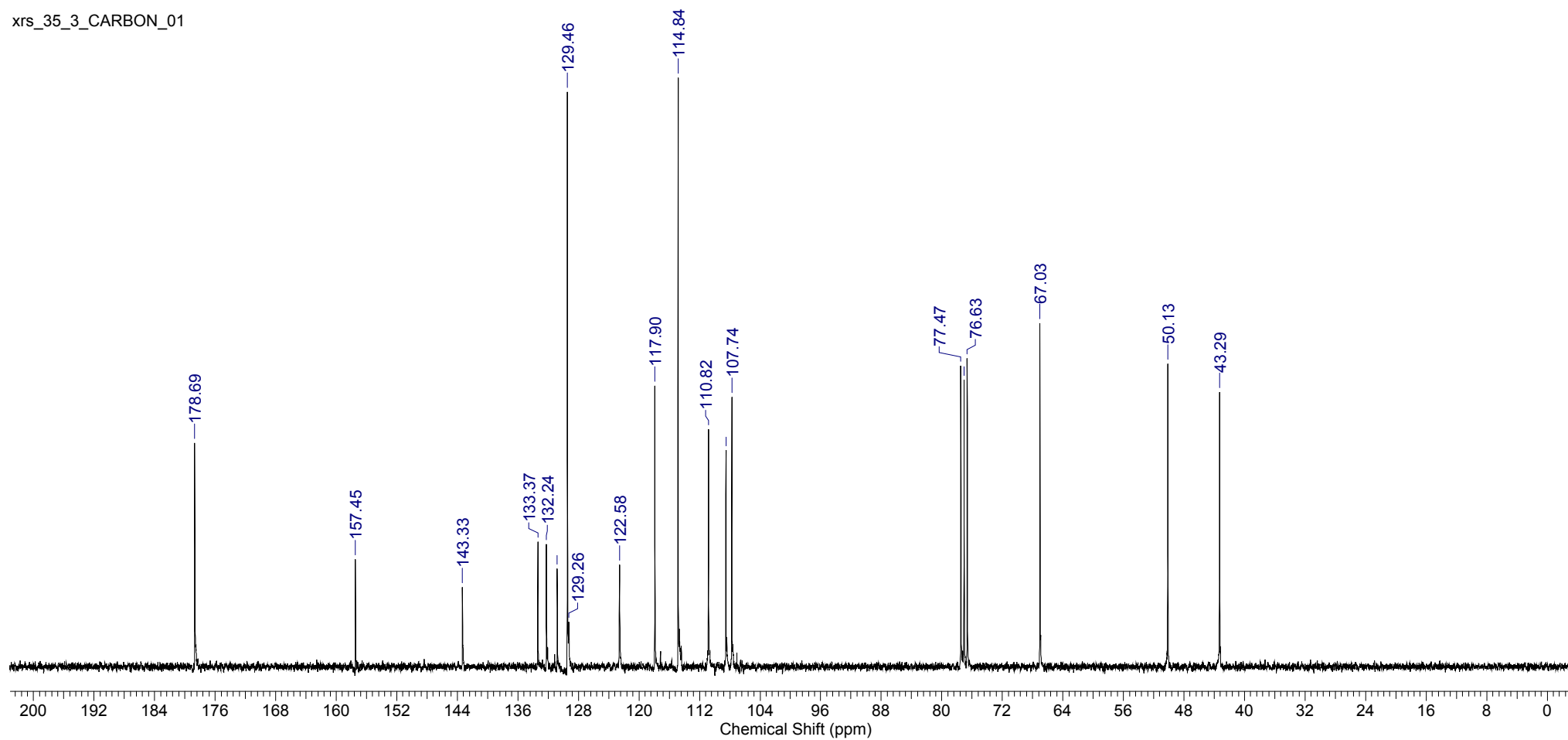
xrs\_35\_3\_PROTON\_01



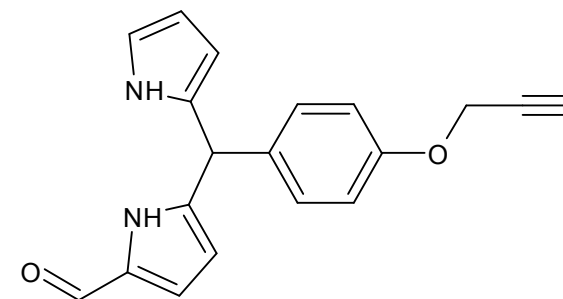
E:\UJ\_PHD Spectral NMR xrs\_35\_3\_30Apr2014\_01\xrs\_35\_3\_PROTON\_01



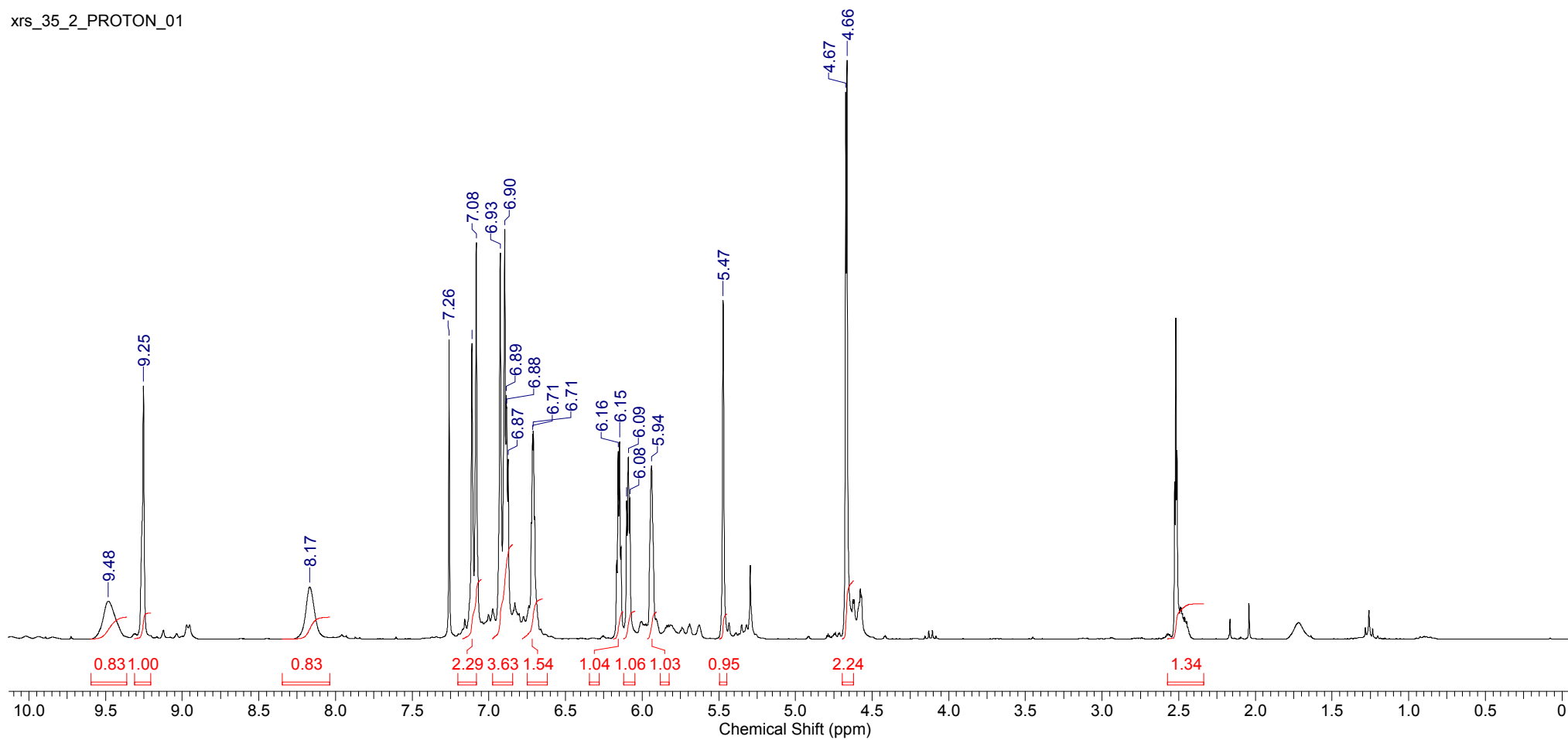
xrs\_35\_3\_CARBON\_01

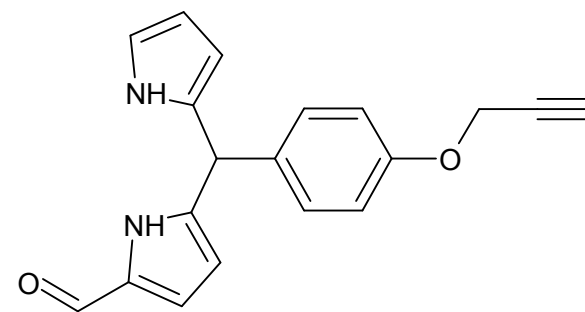




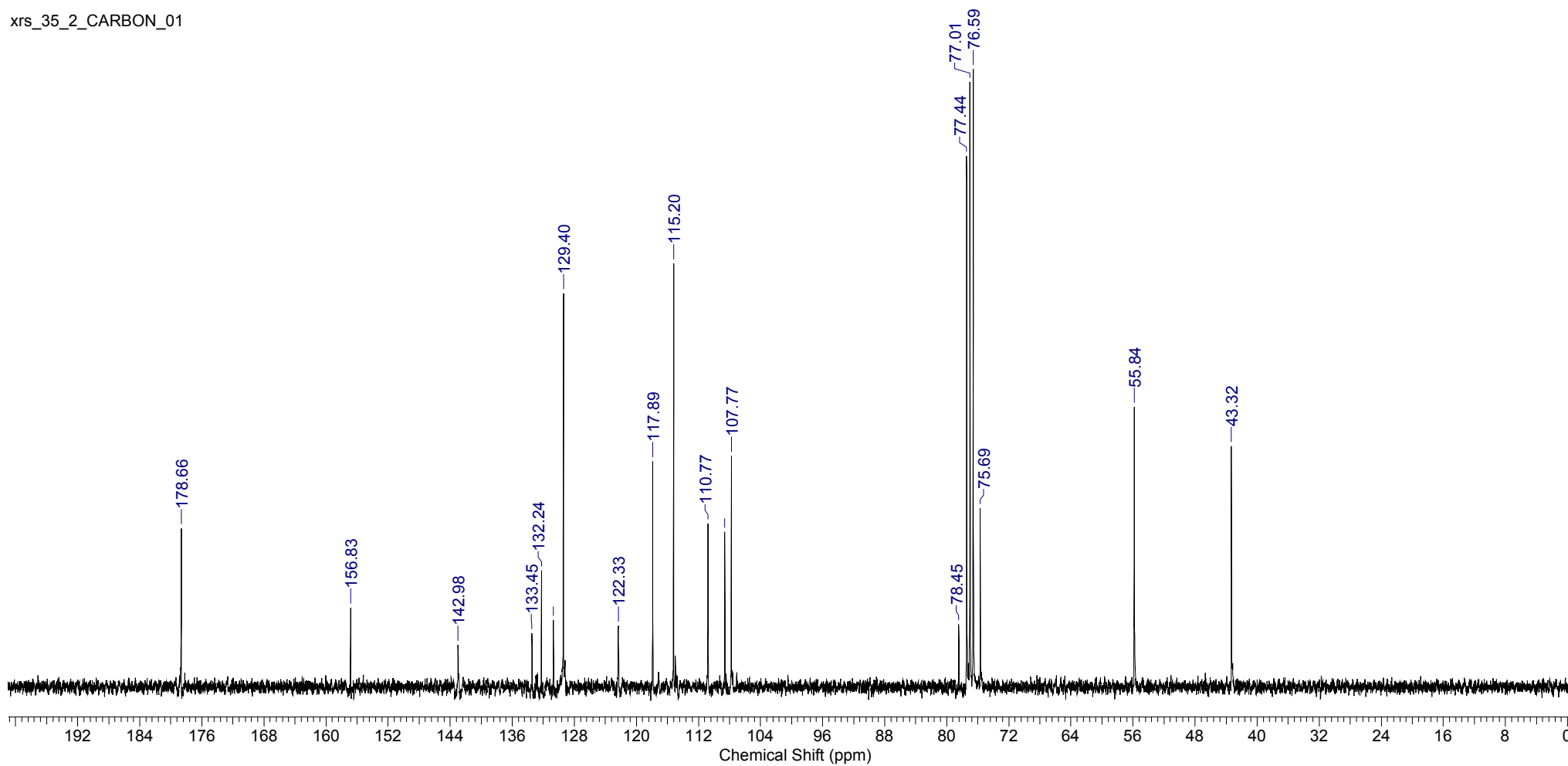


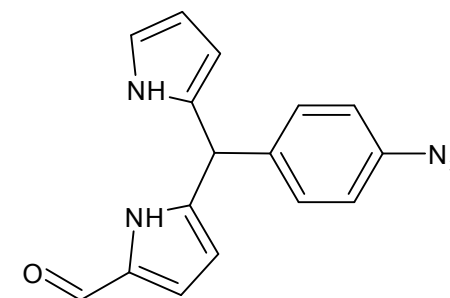
xrs\_35\_2\_PROTON\_01



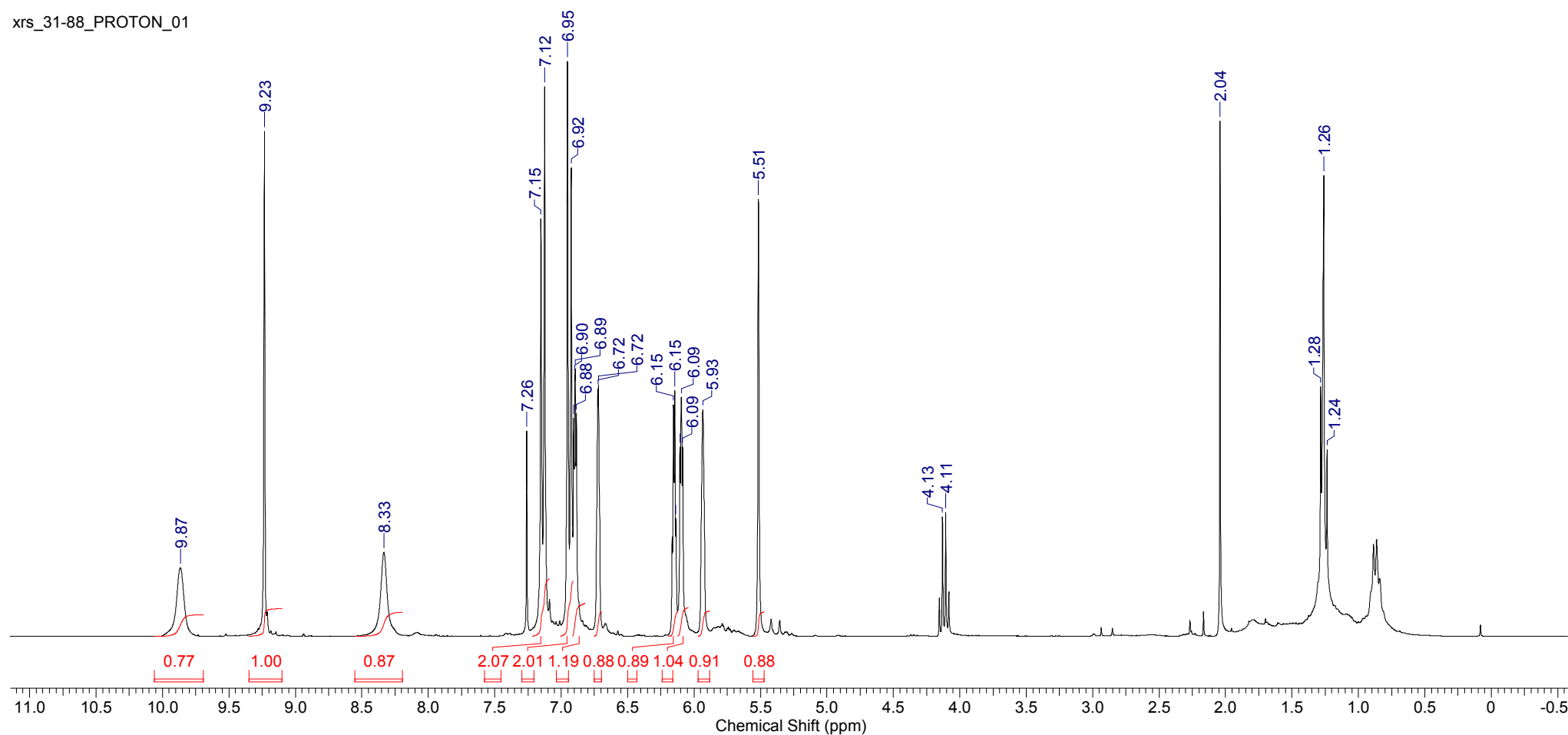


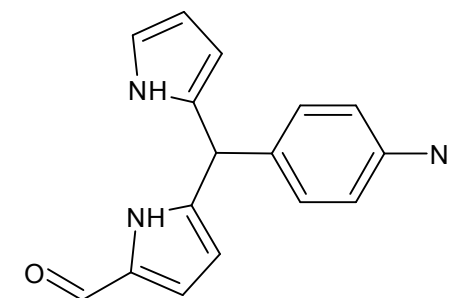
xrs\_35\_2\_CARBON\_01



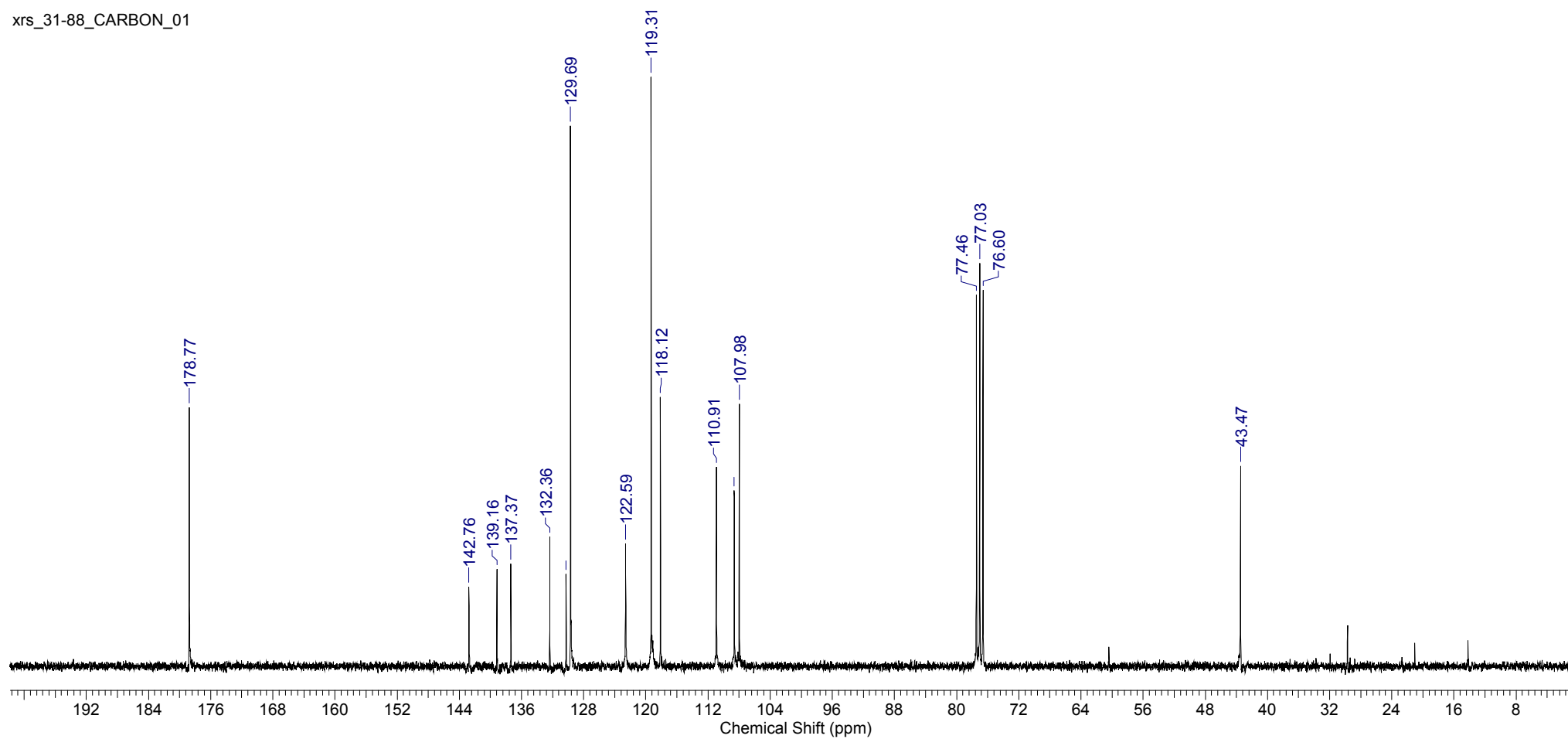


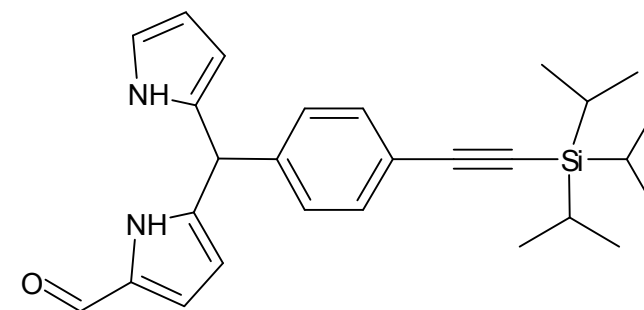
xrs\_31-88\_PROTON\_01



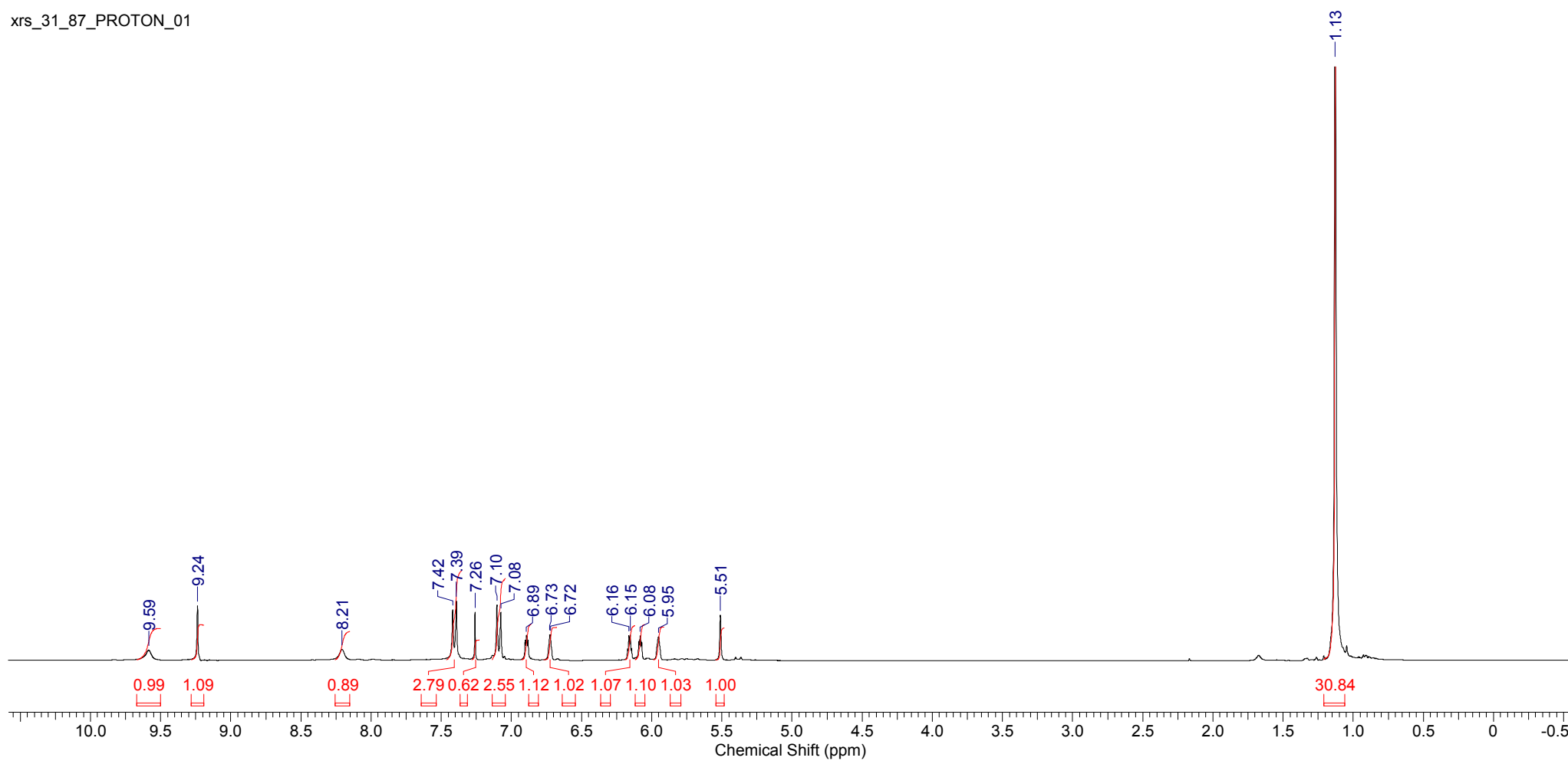


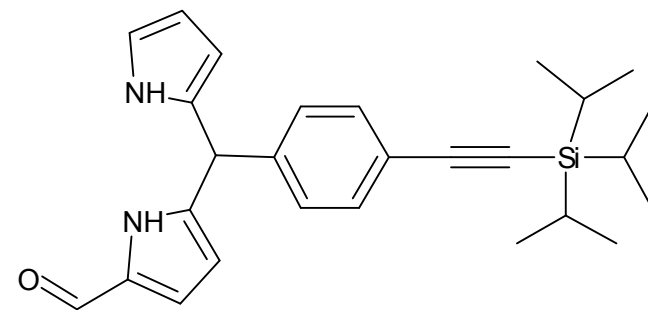
xrs\_31-88\_CARBON\_01



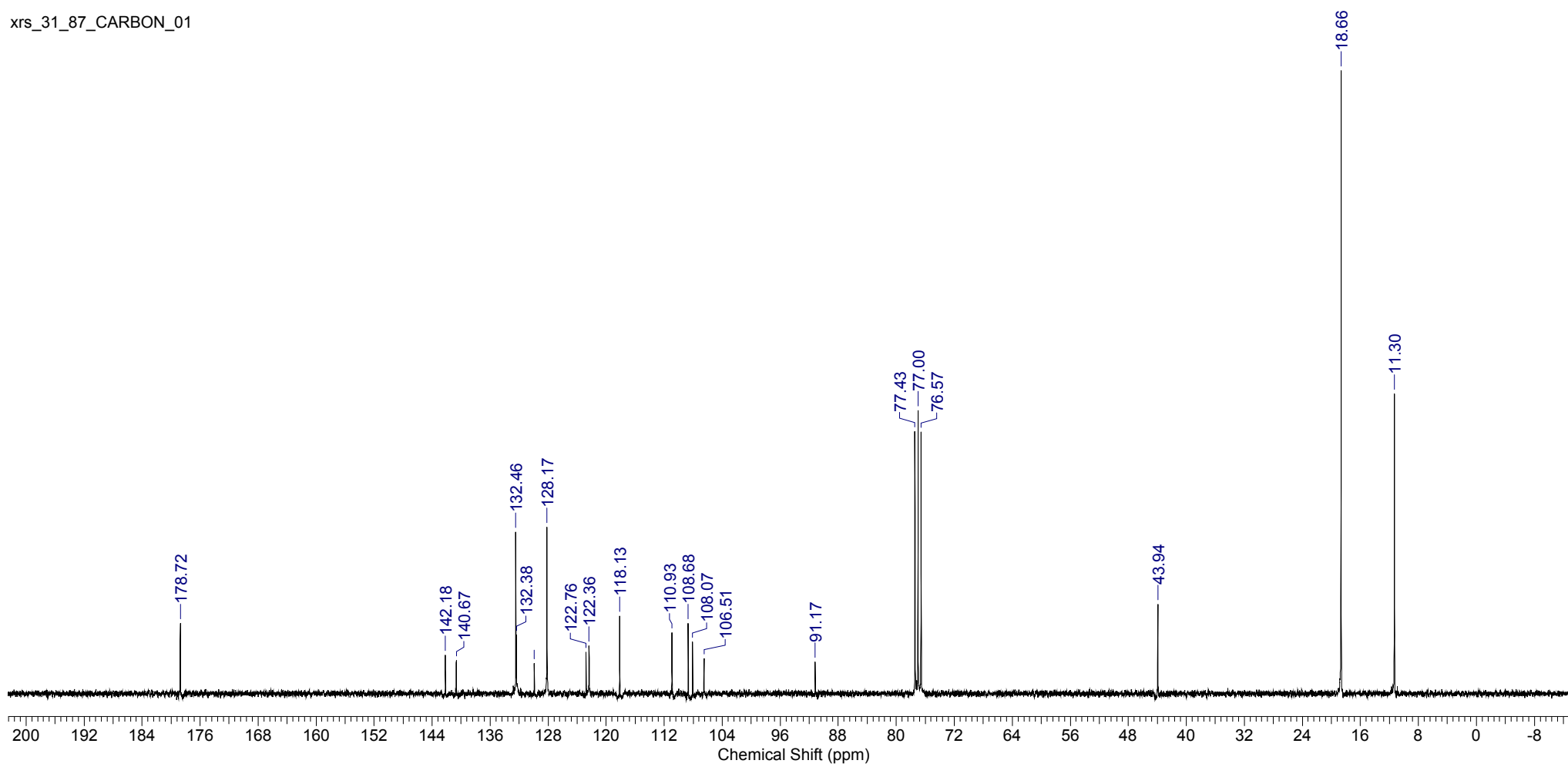


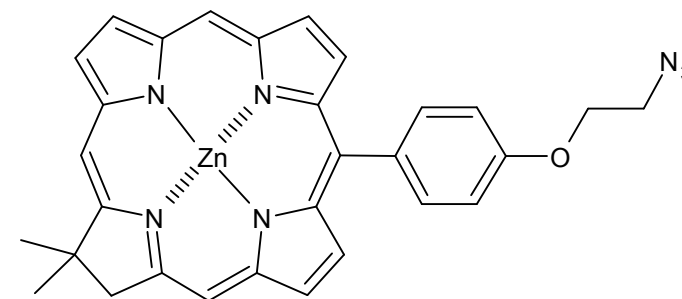
xrs\_31\_87\_PROTON\_01



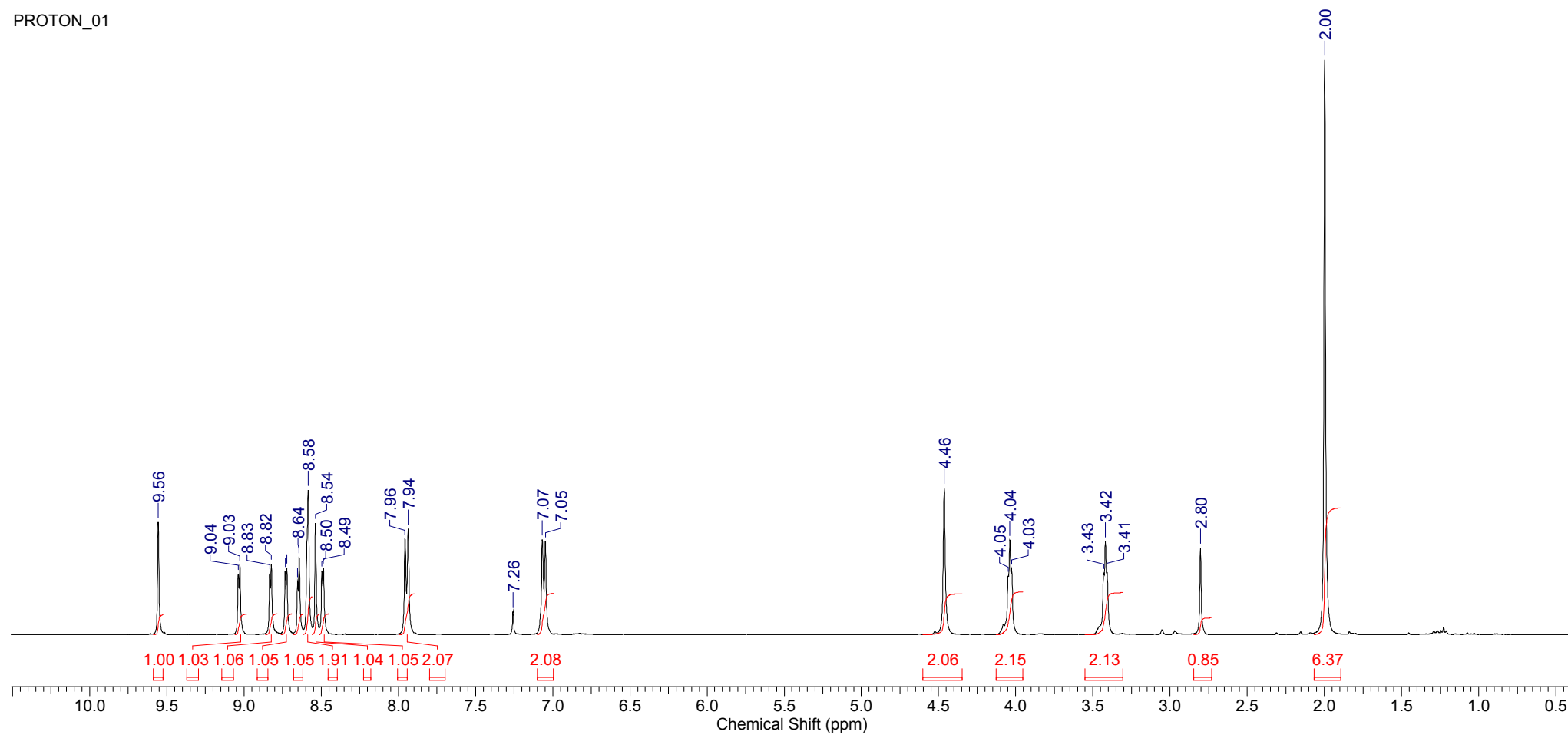


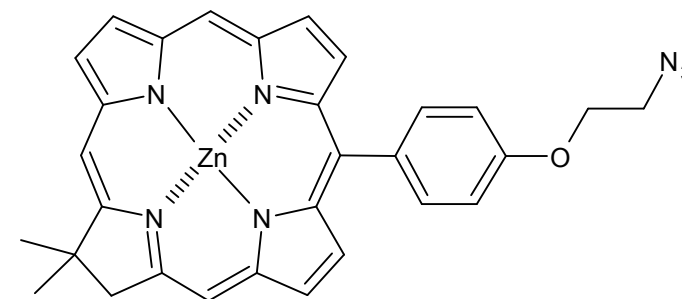
xrs\_31\_87\_CARBON\_01



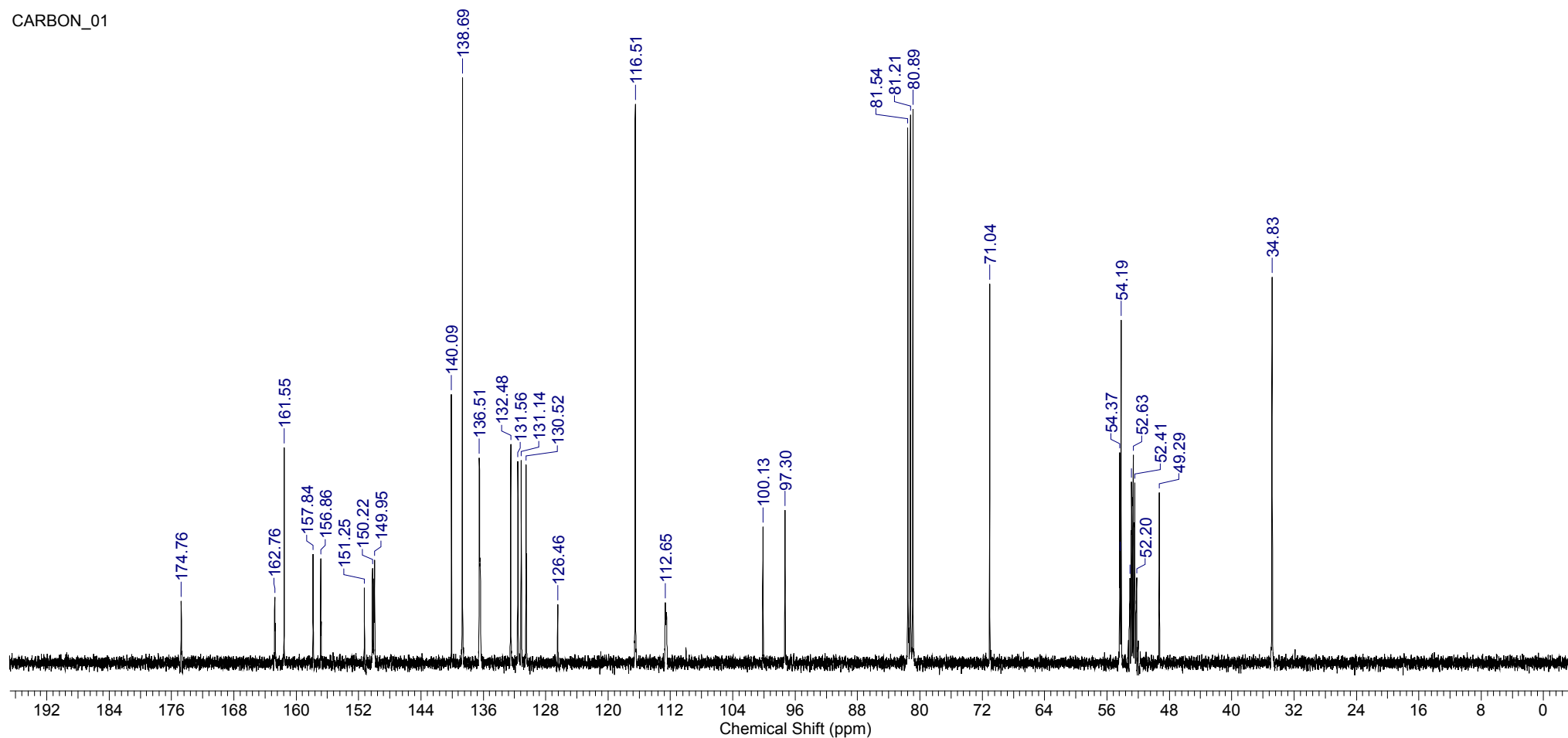


PROTON\_01

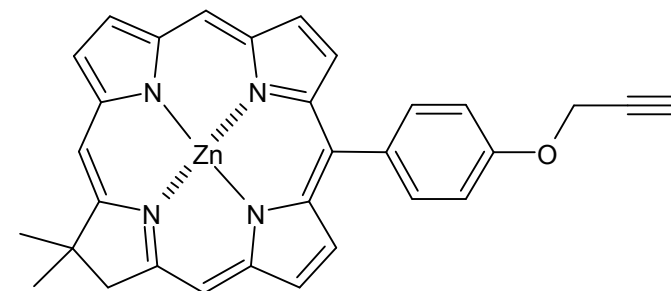




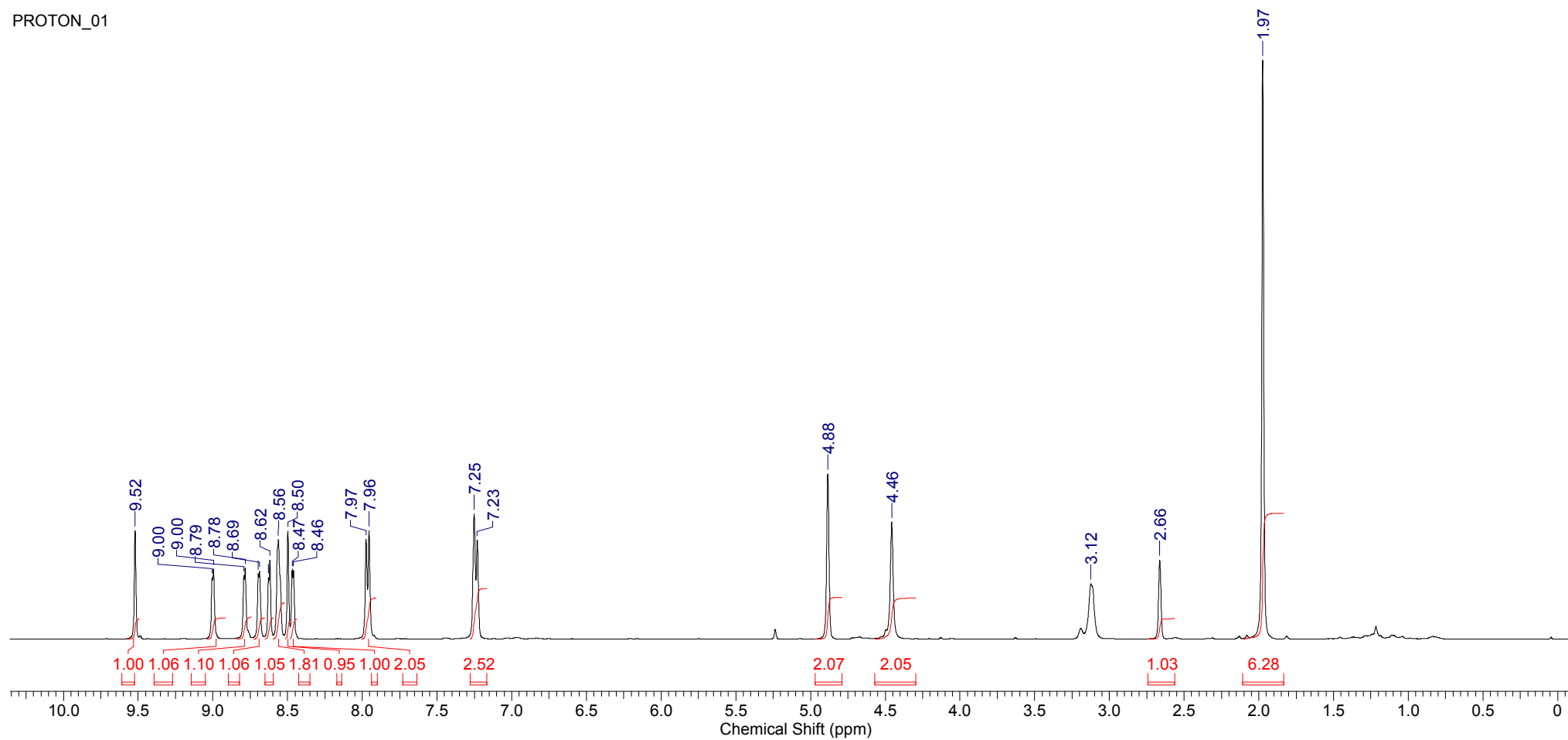
CARBON\_01

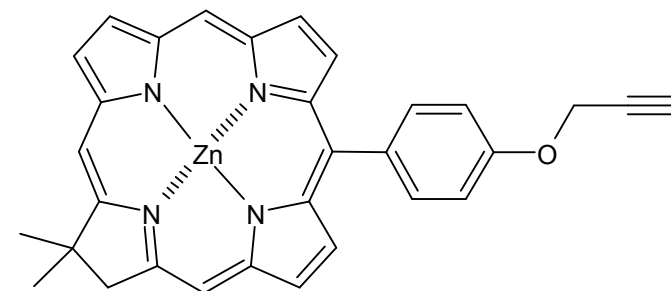




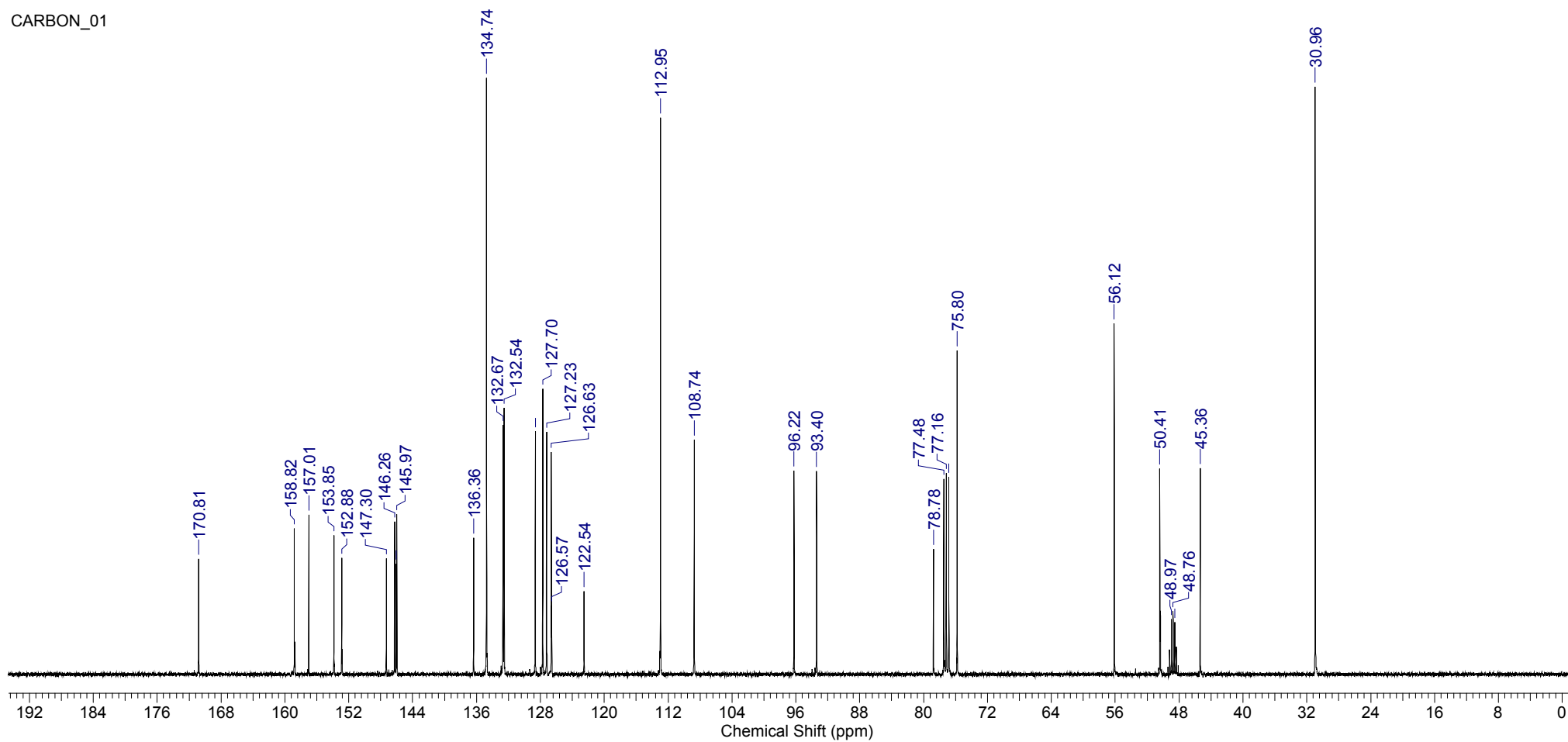


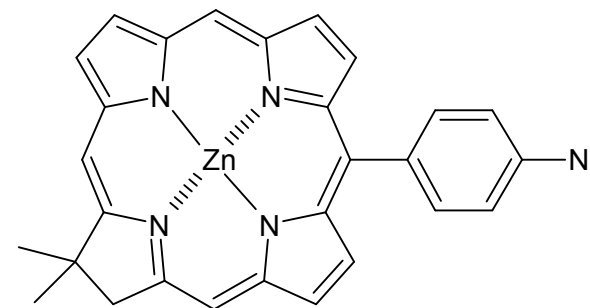
PROTON\_01



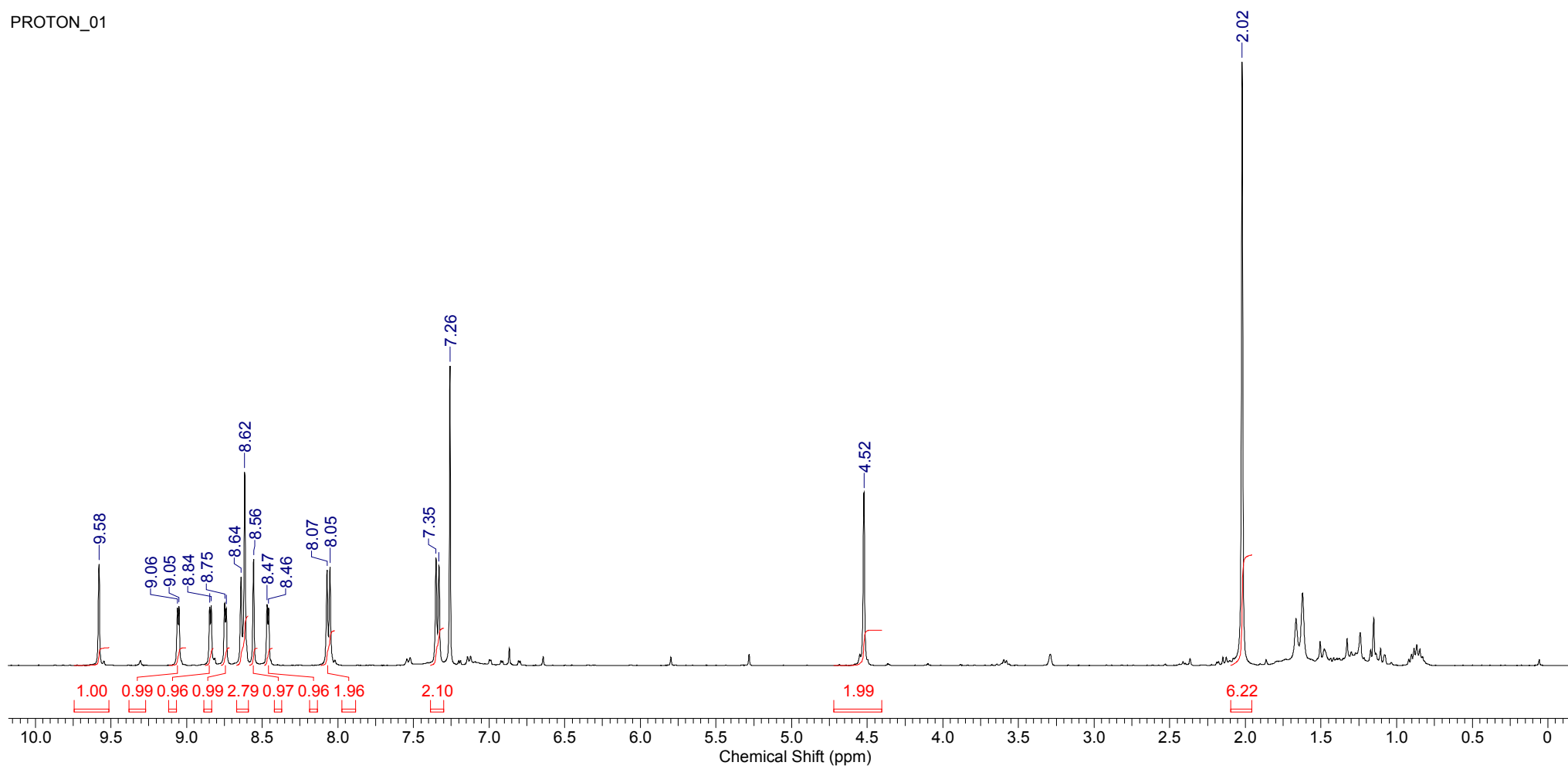


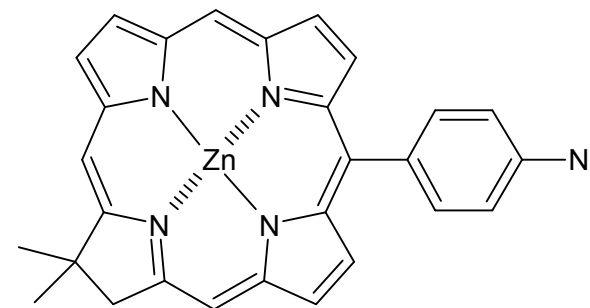
CARBON\_01



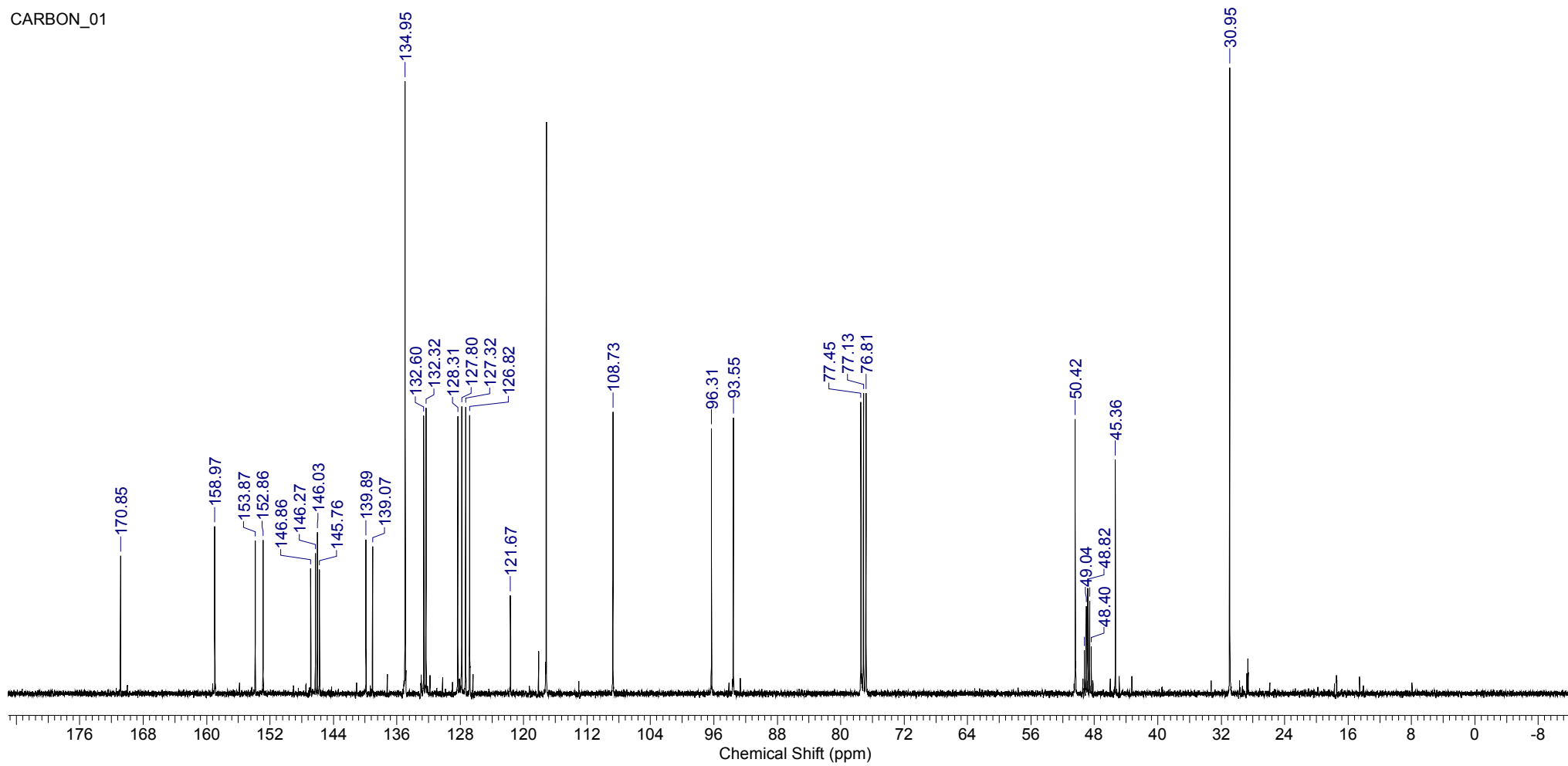


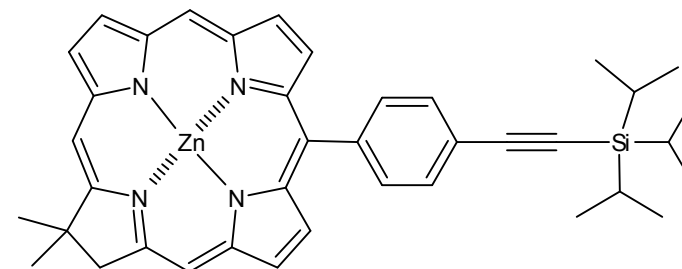
PROTON\_01



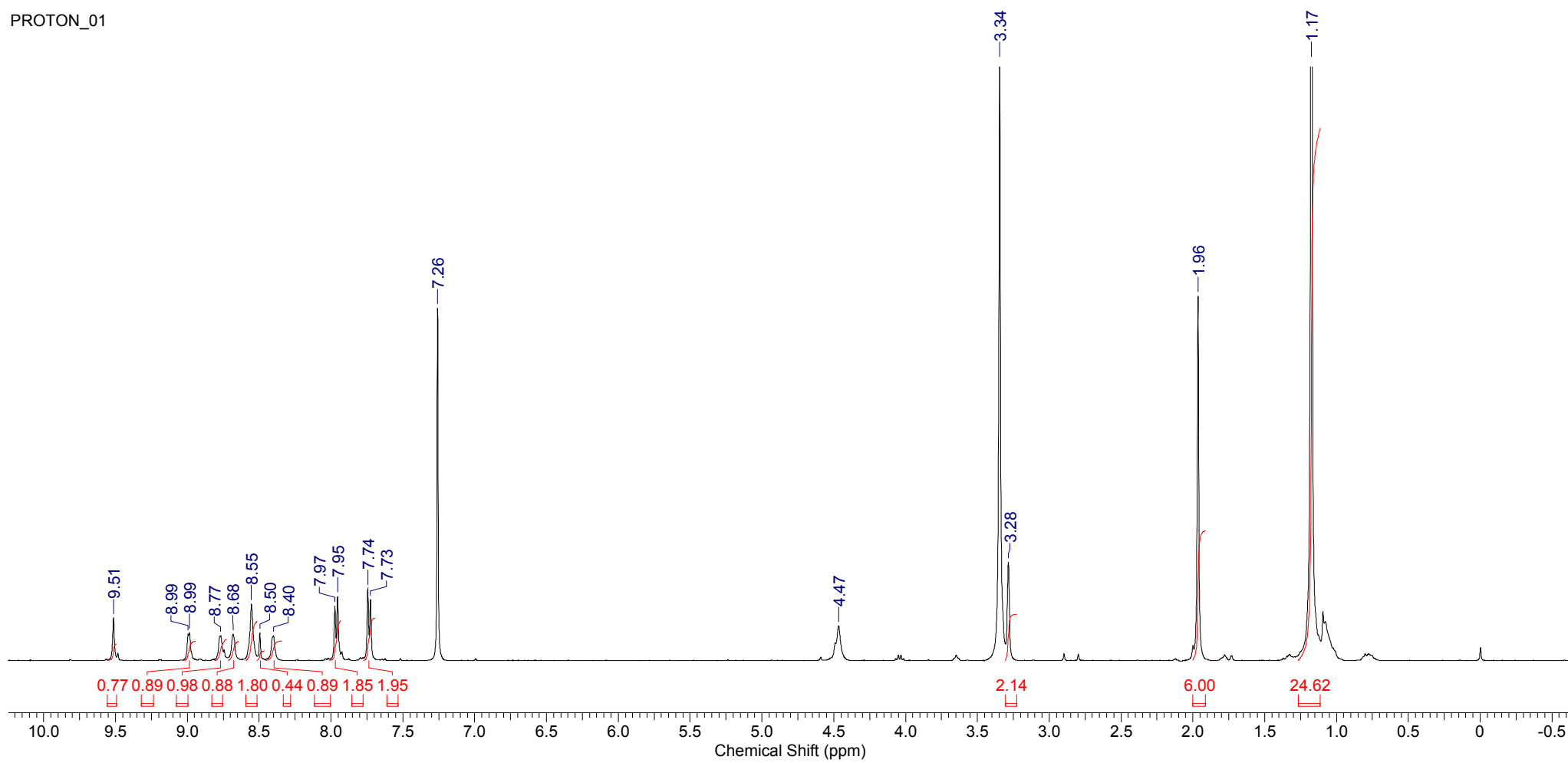


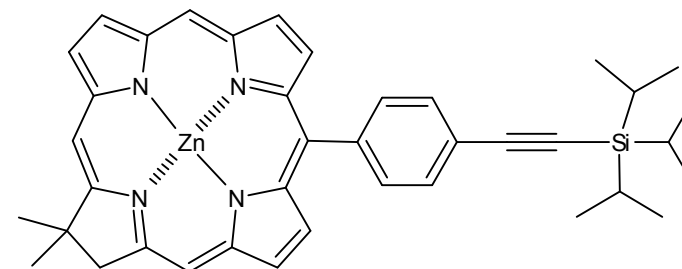
CARBON\_01



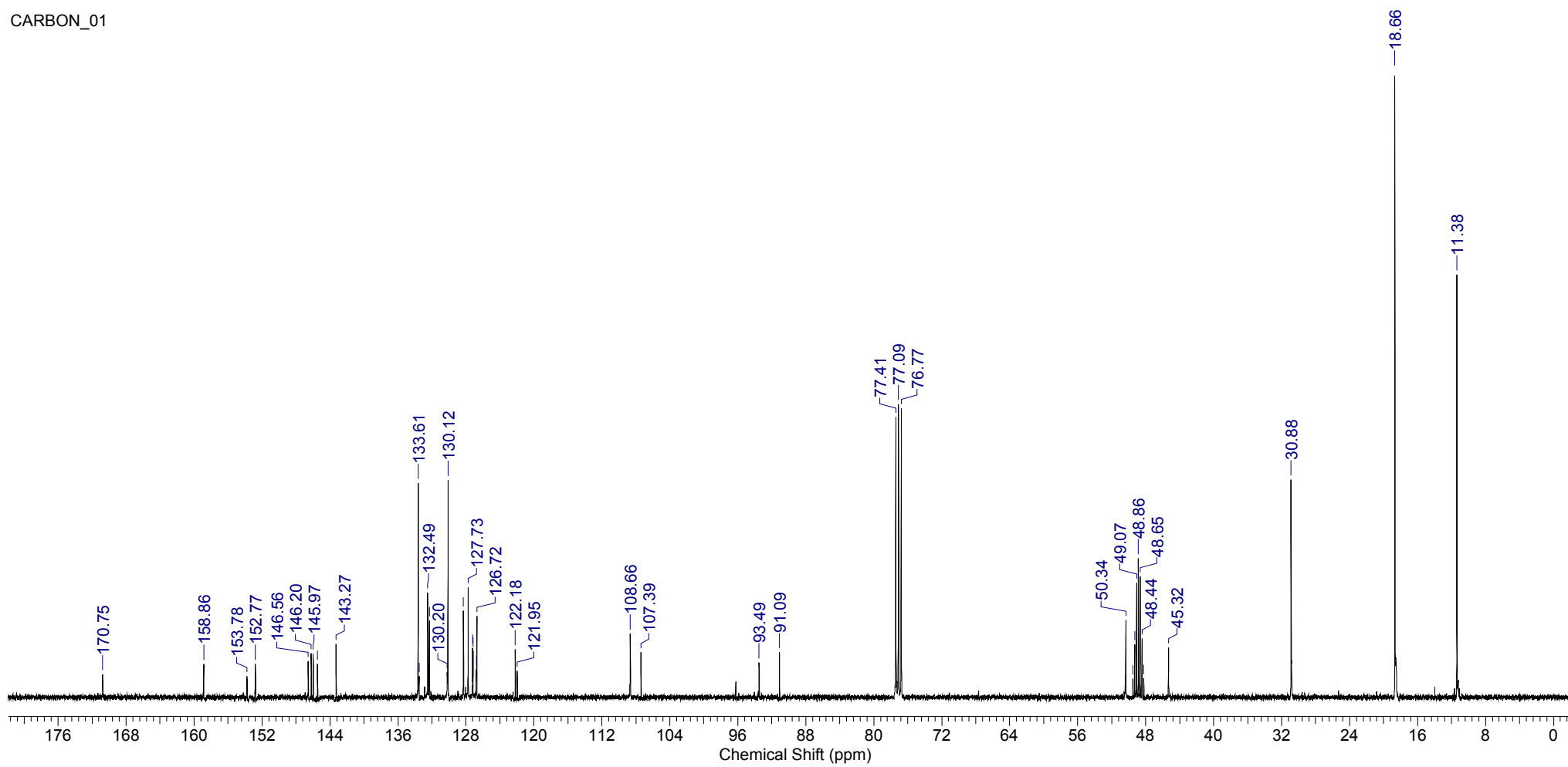


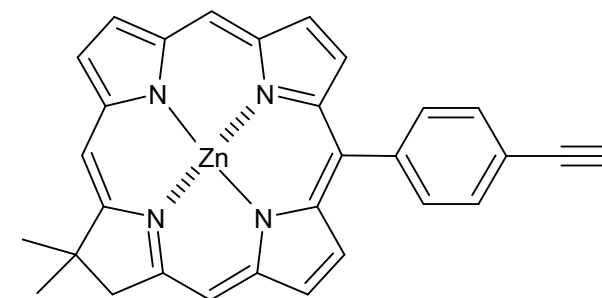
PROTON\_01



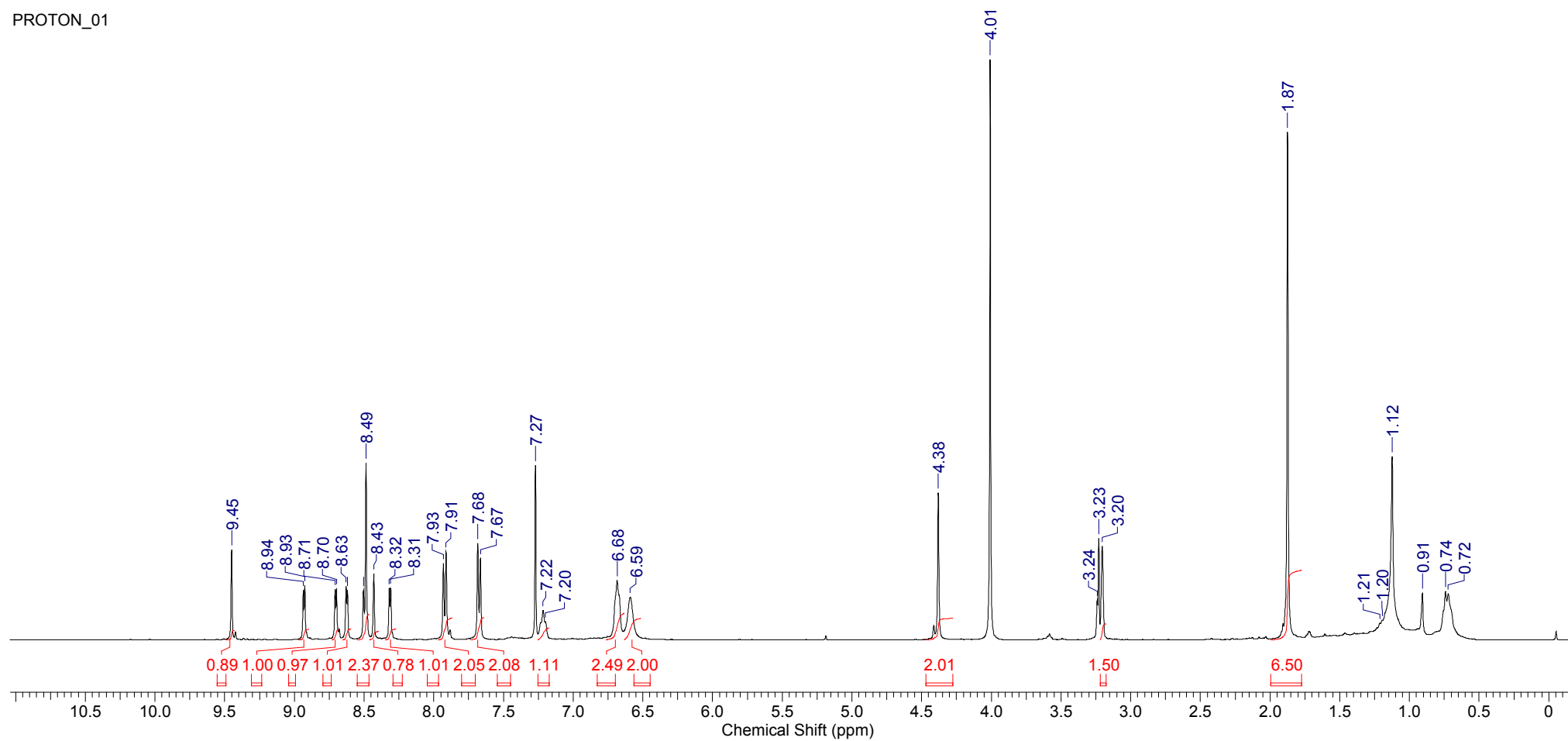


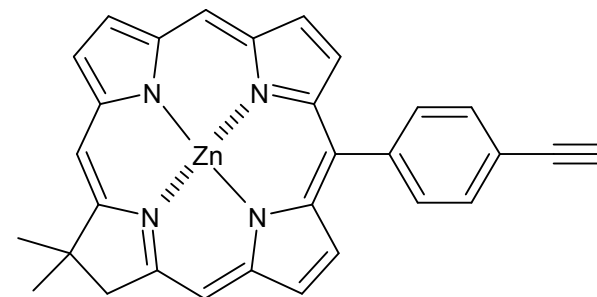
CARBON\_01



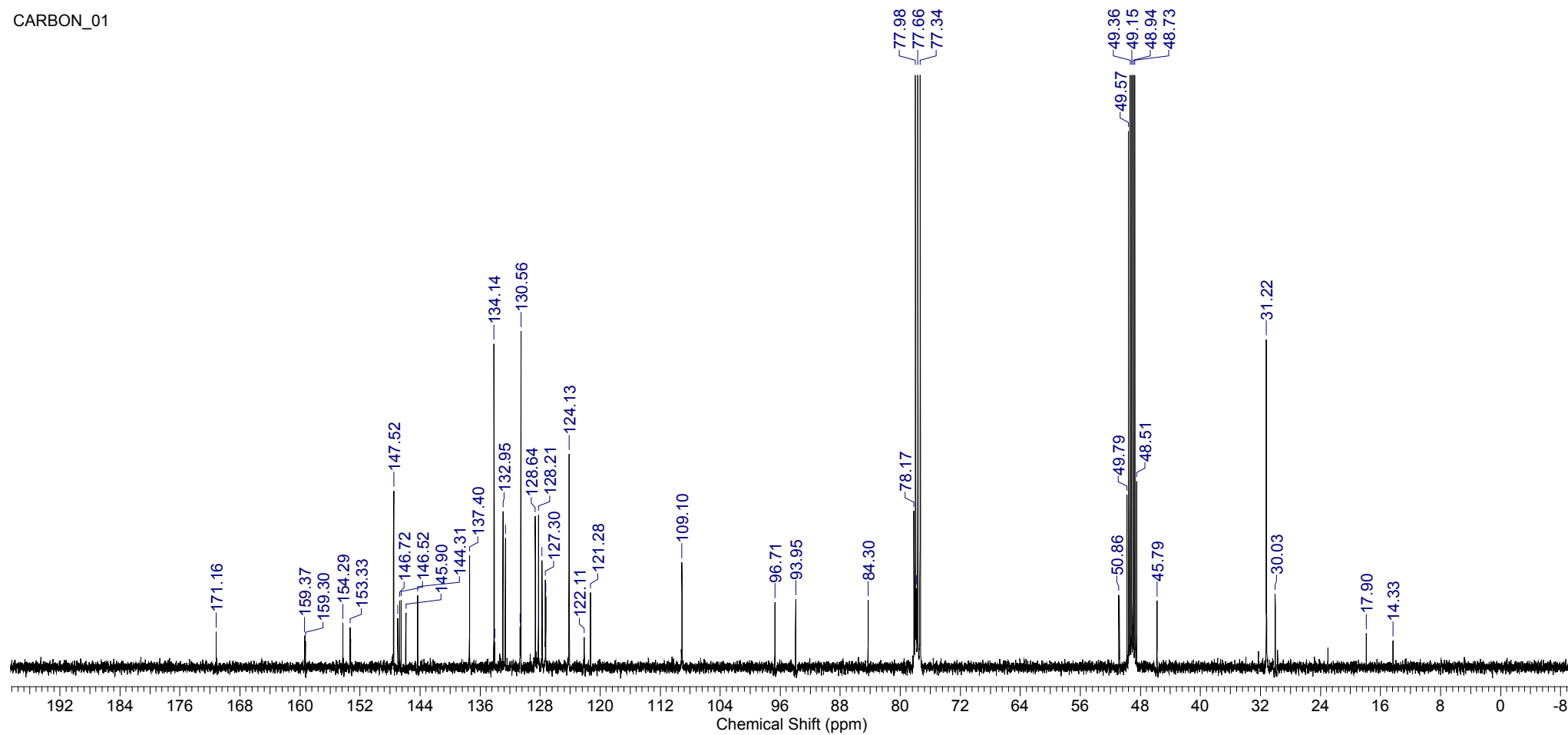


PROTON\_01

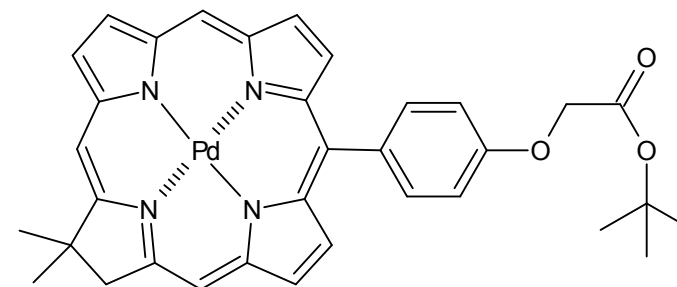




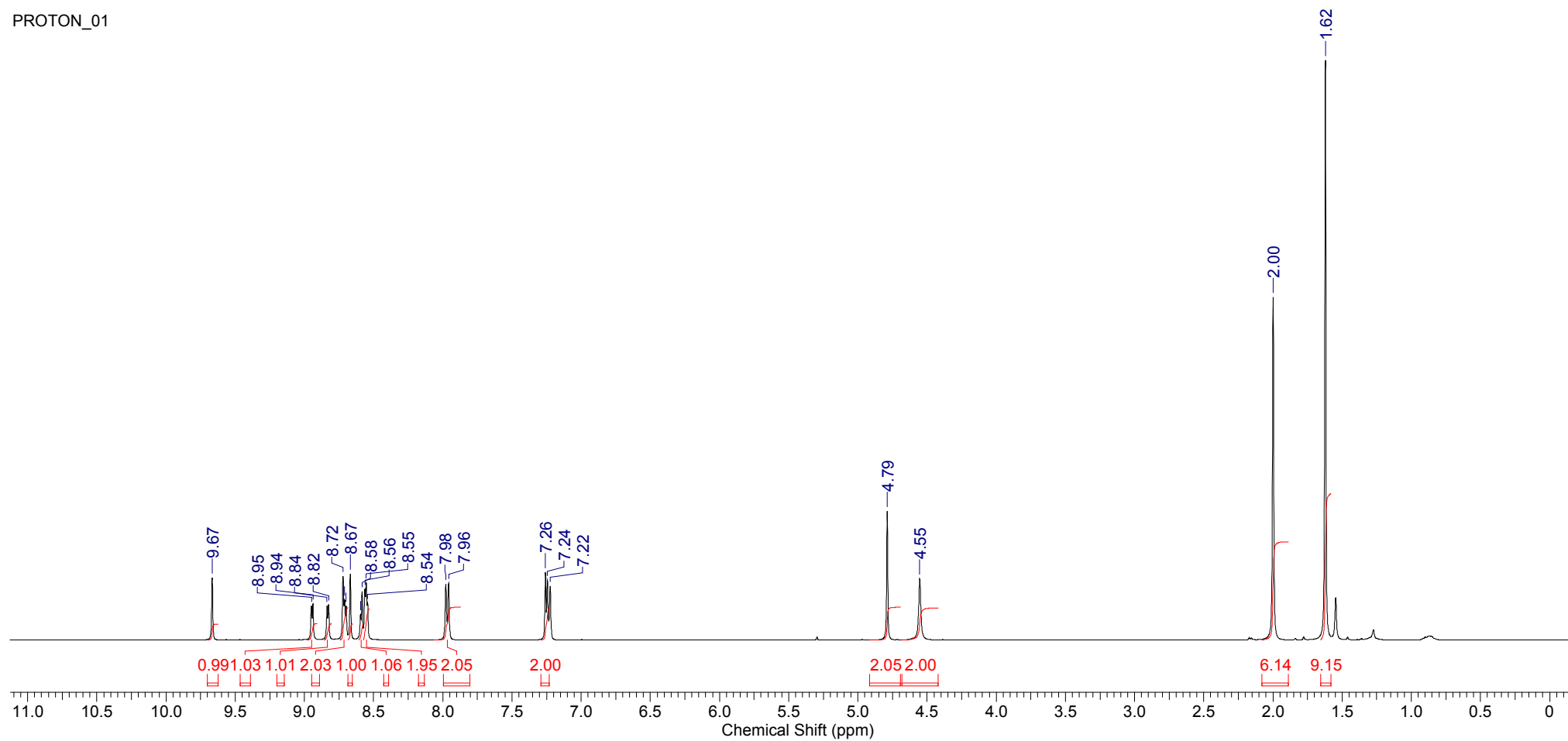
CARBON\_01

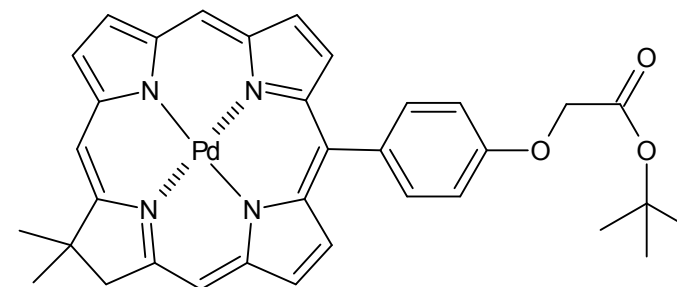




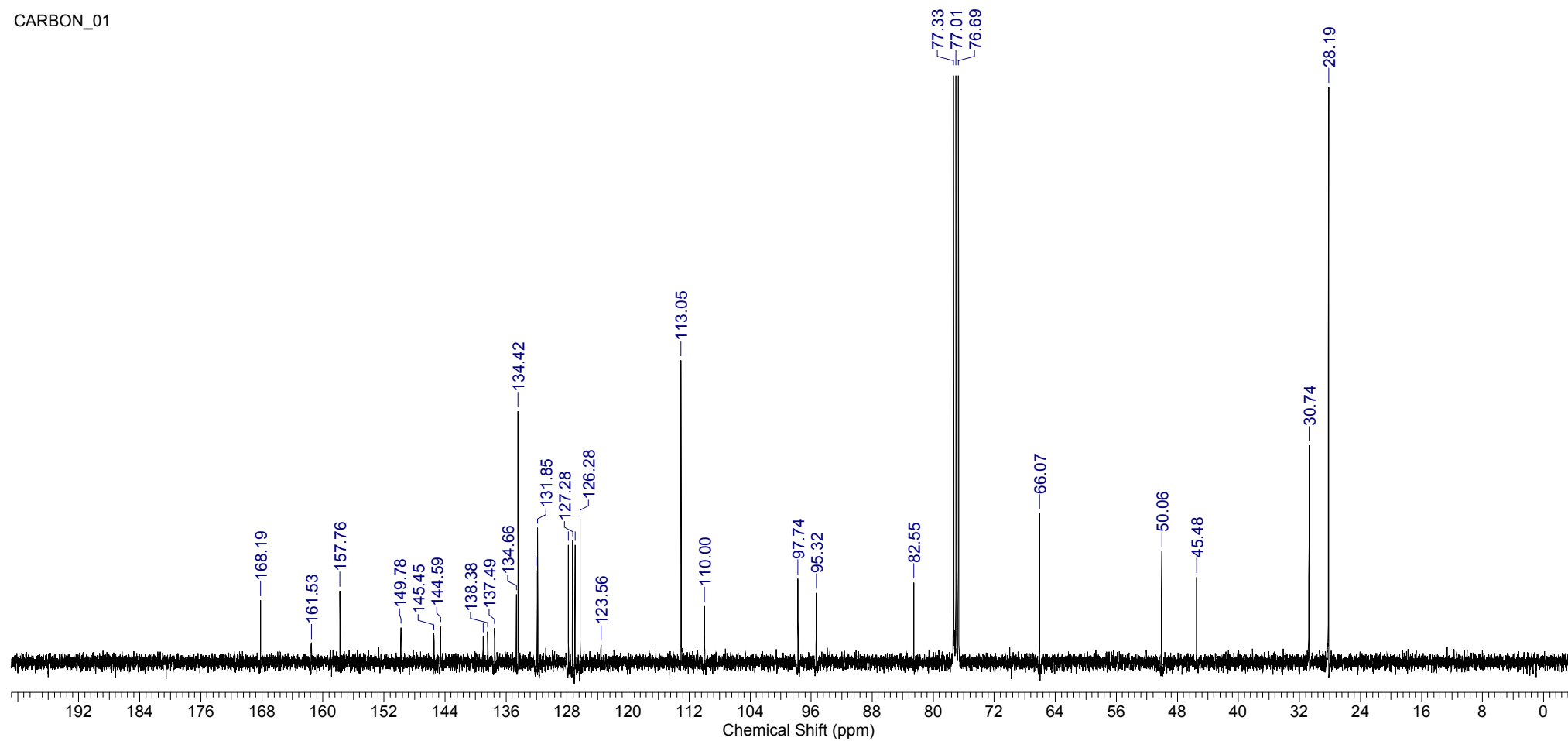


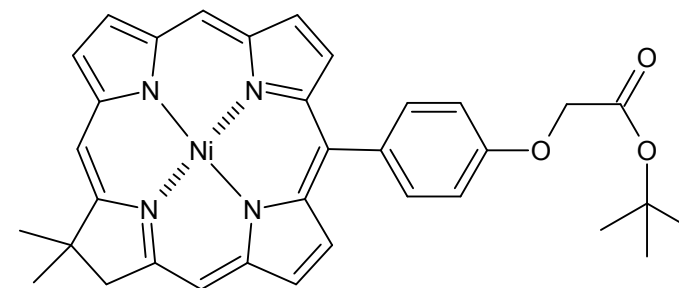
PROTON\_01



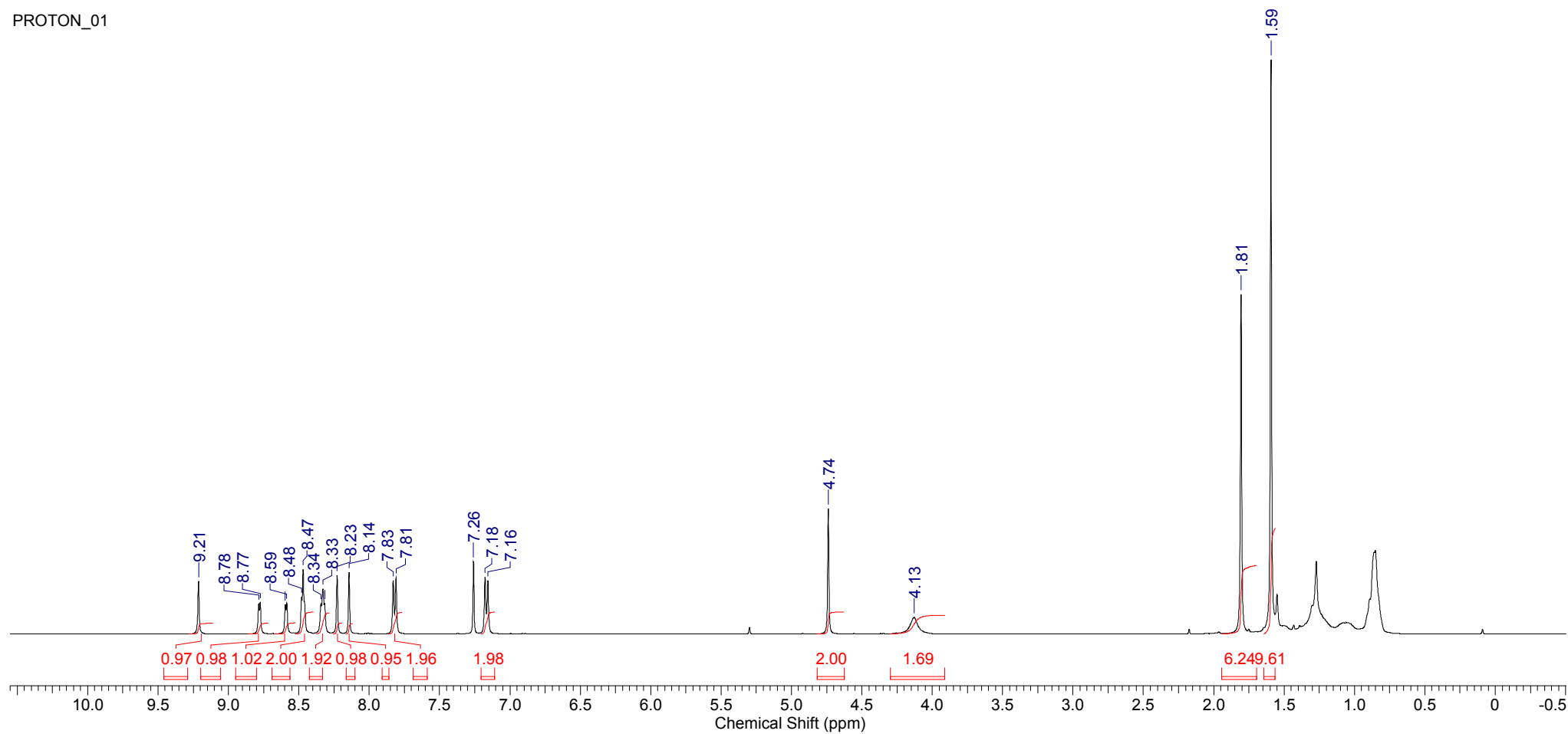


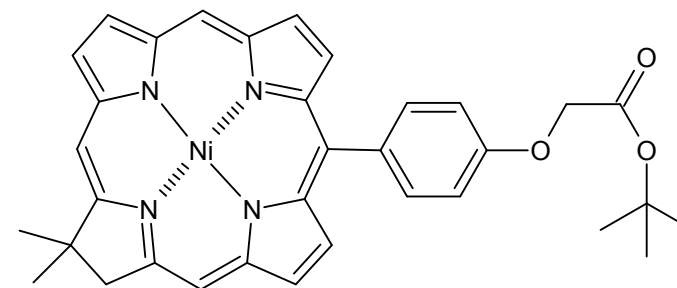
CARBON\_01



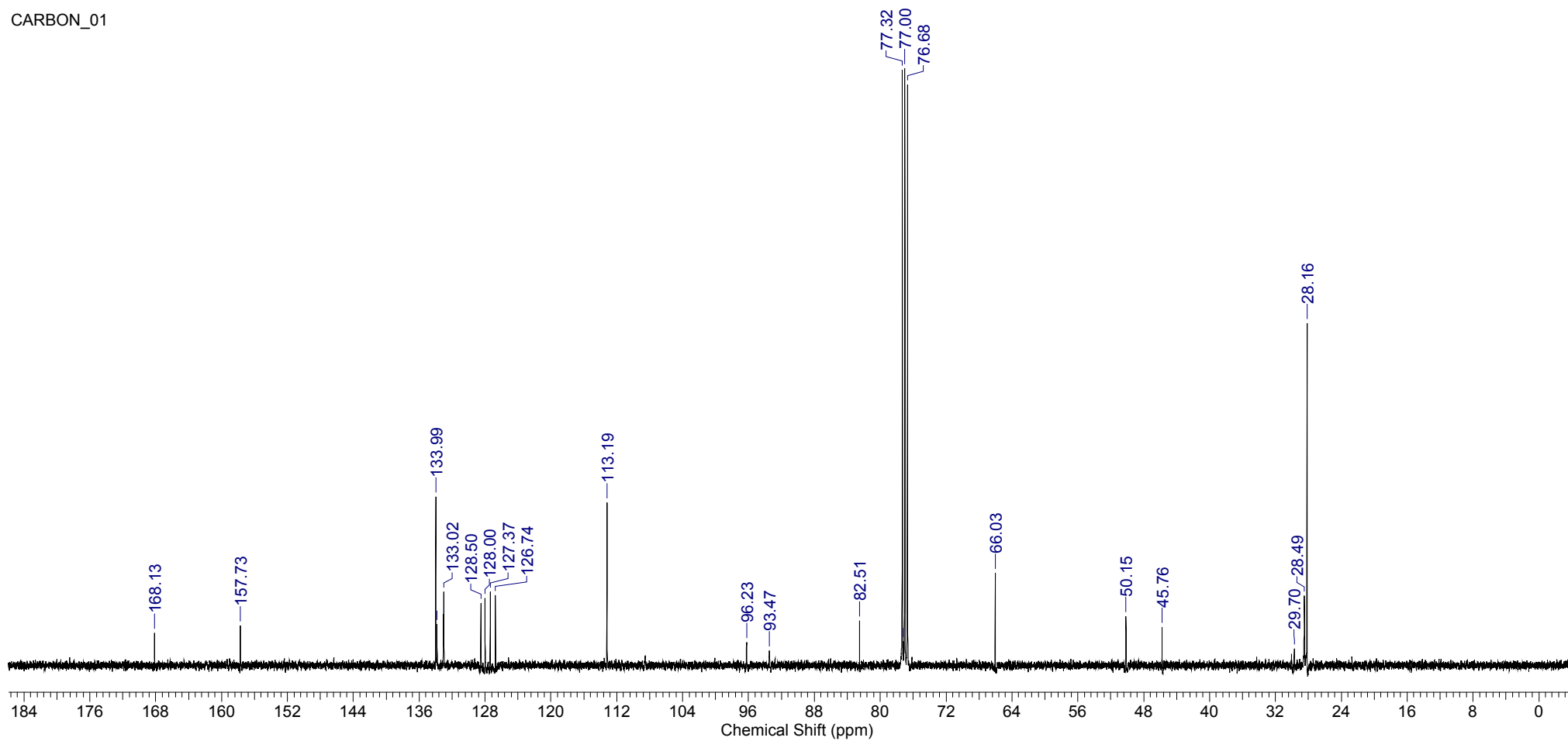


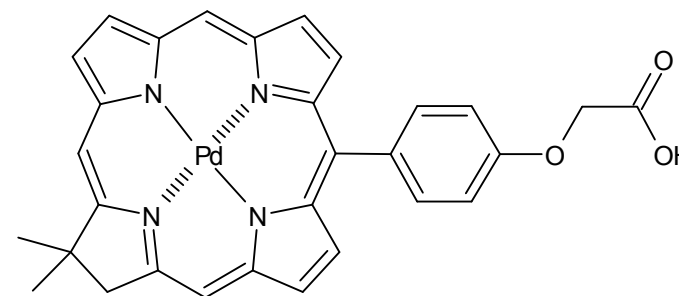
PROTON\_01



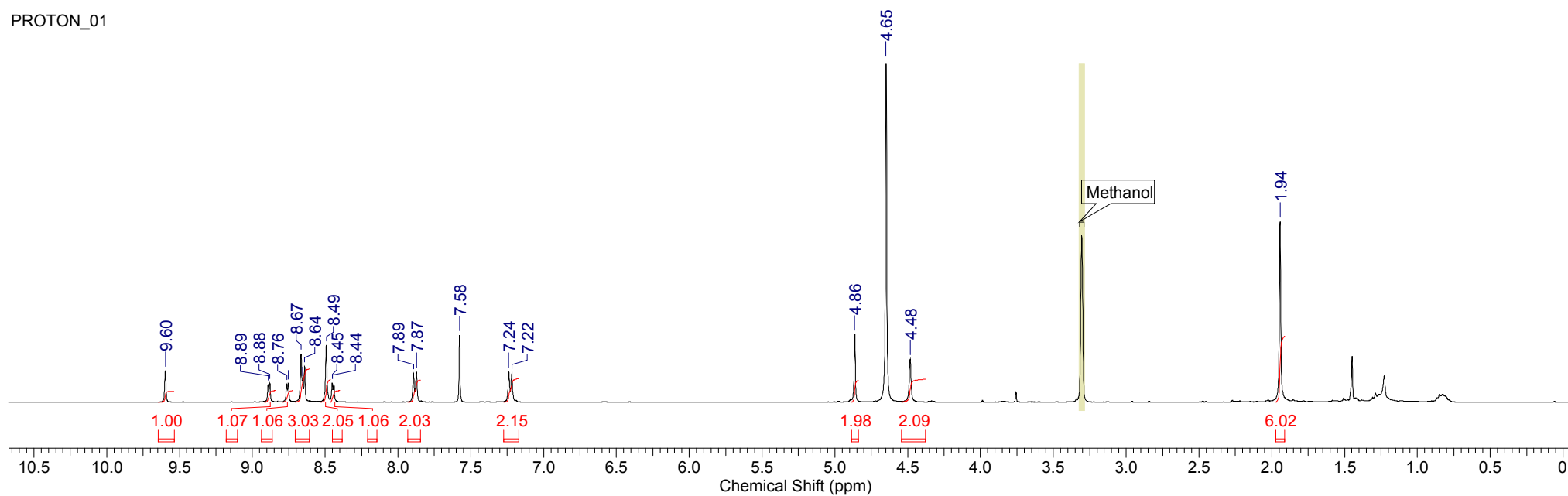


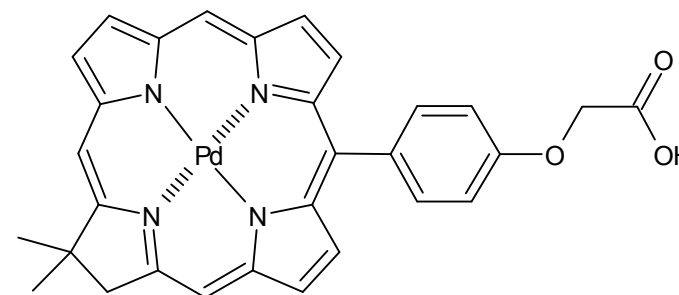
CARBON\_01



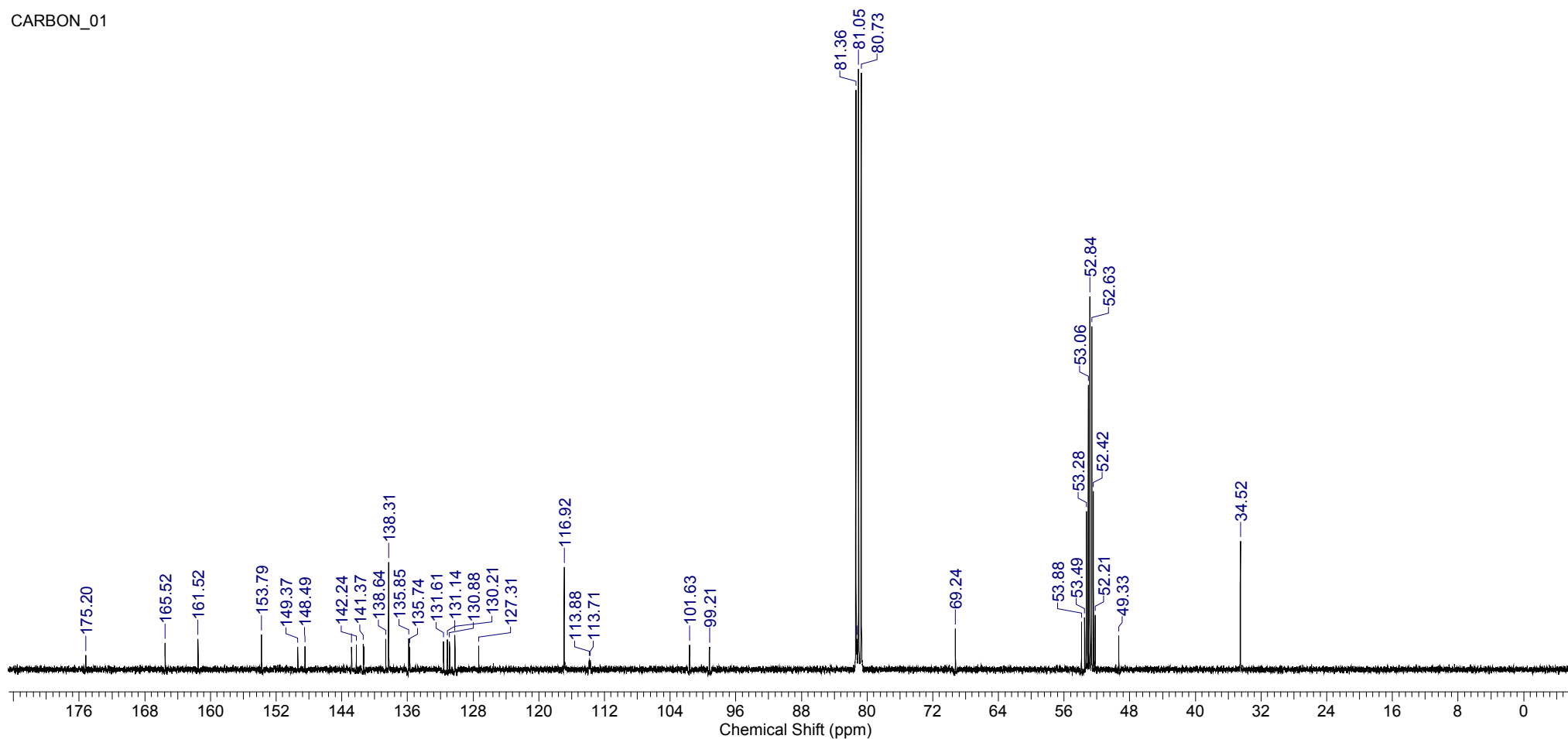


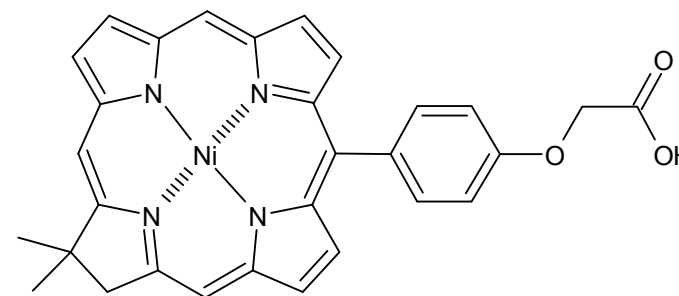
PROTON\_01



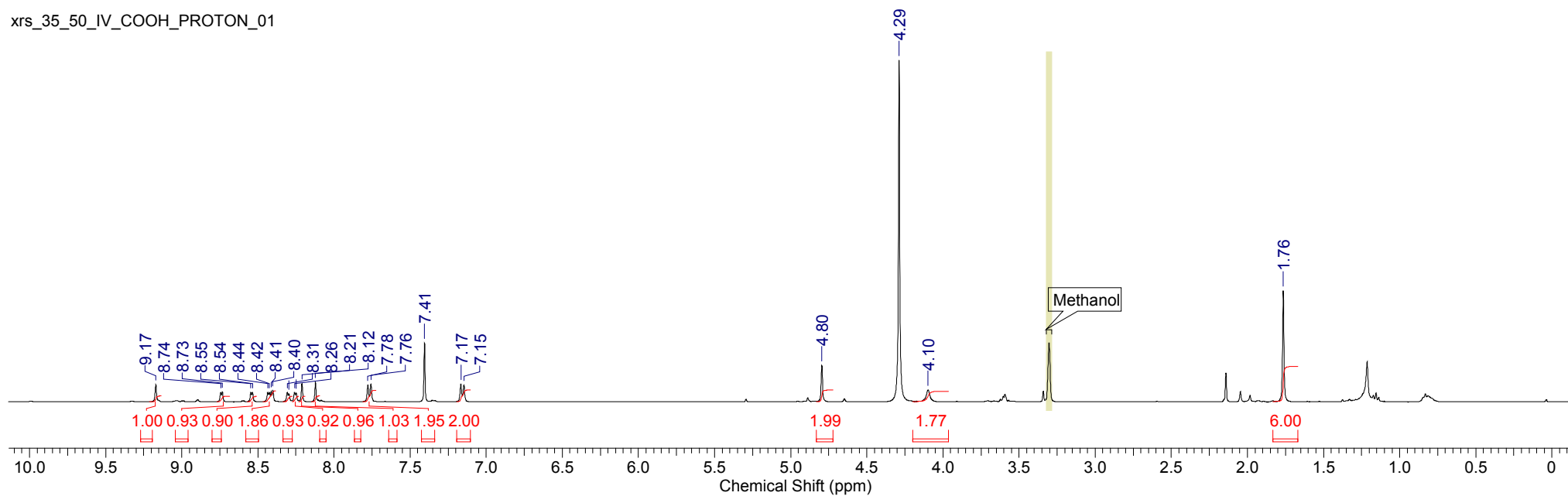


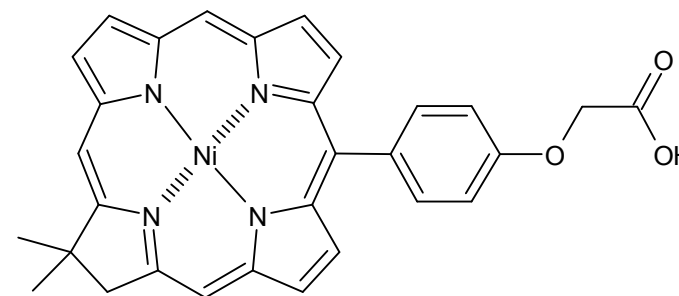
CARBON\_01



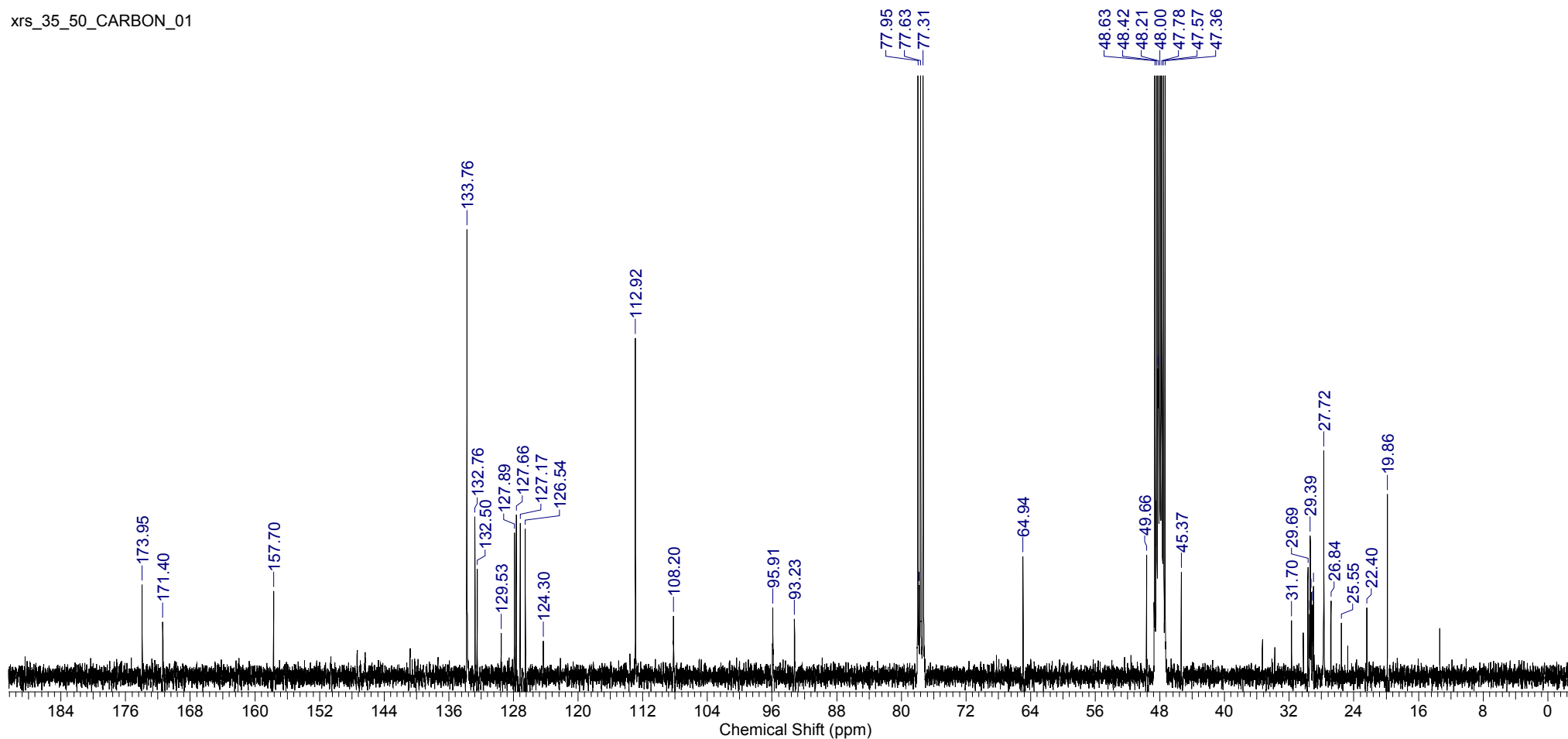


xrs\_35\_50\_IV\_COOH\_PROTON\_01

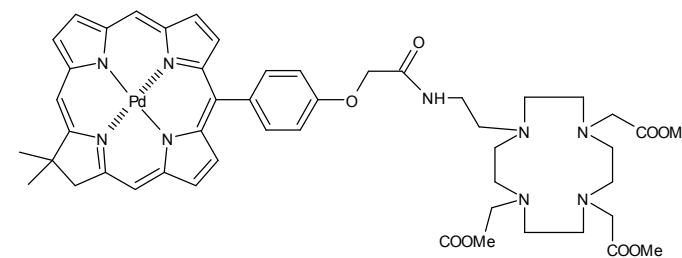




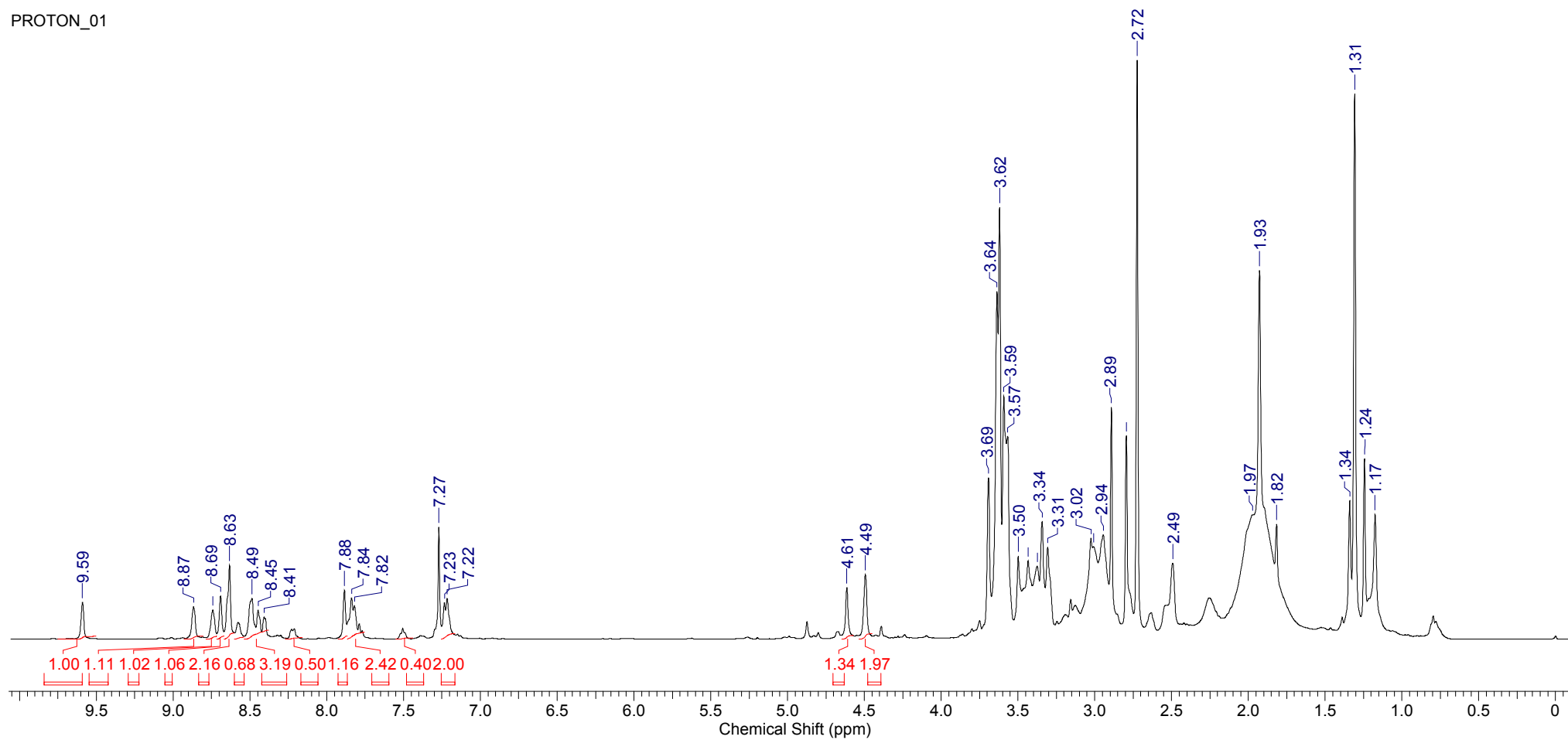
xrs\_35\_50\_CARBON\_01

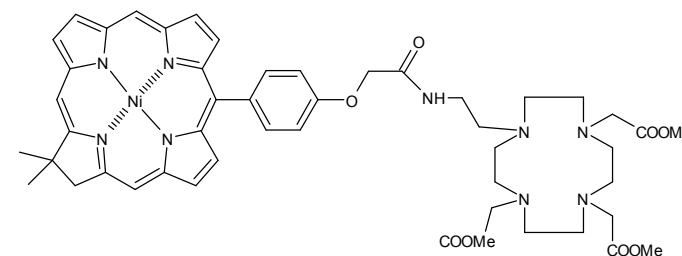




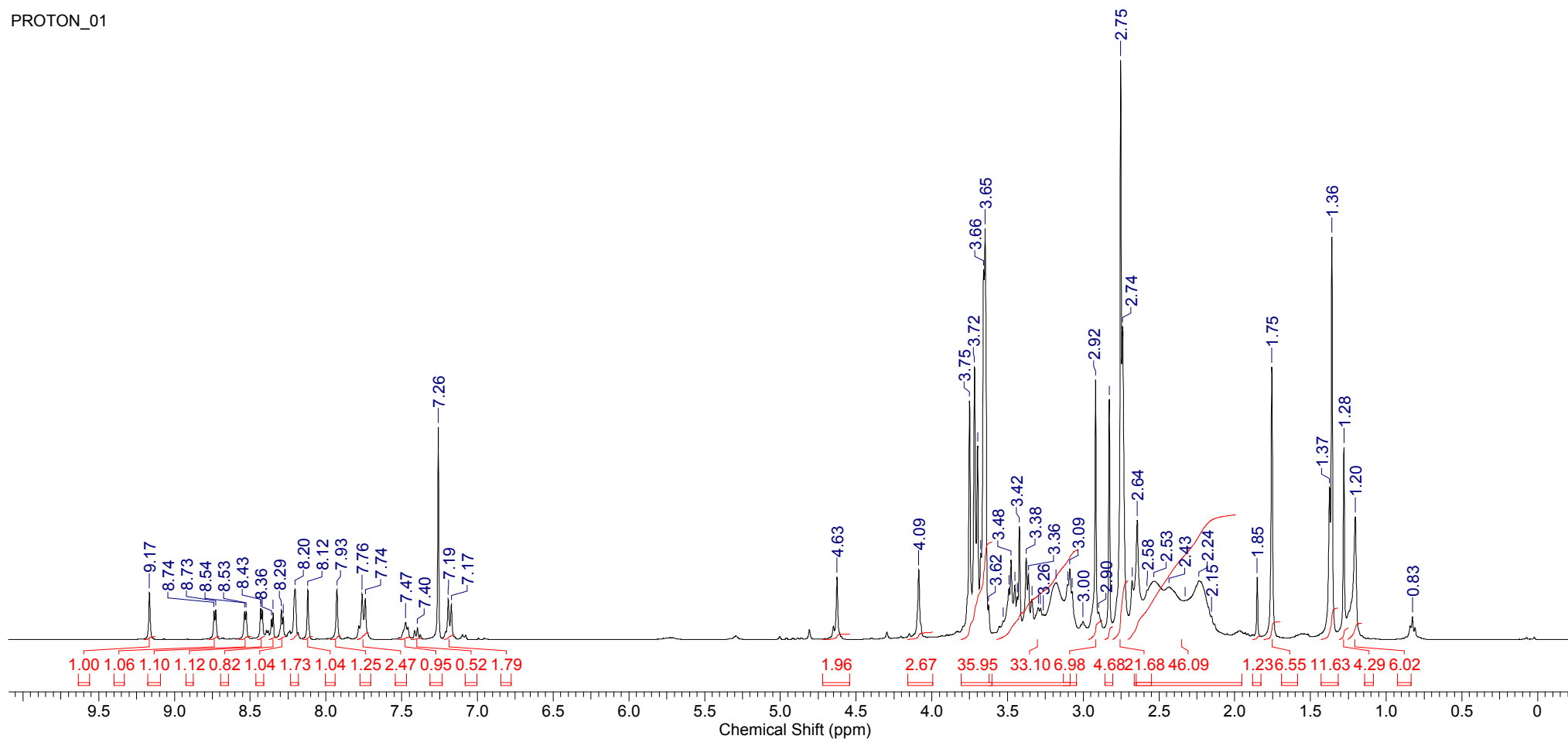


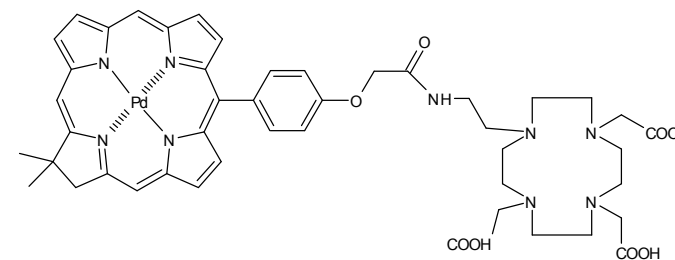
PROTON\_01



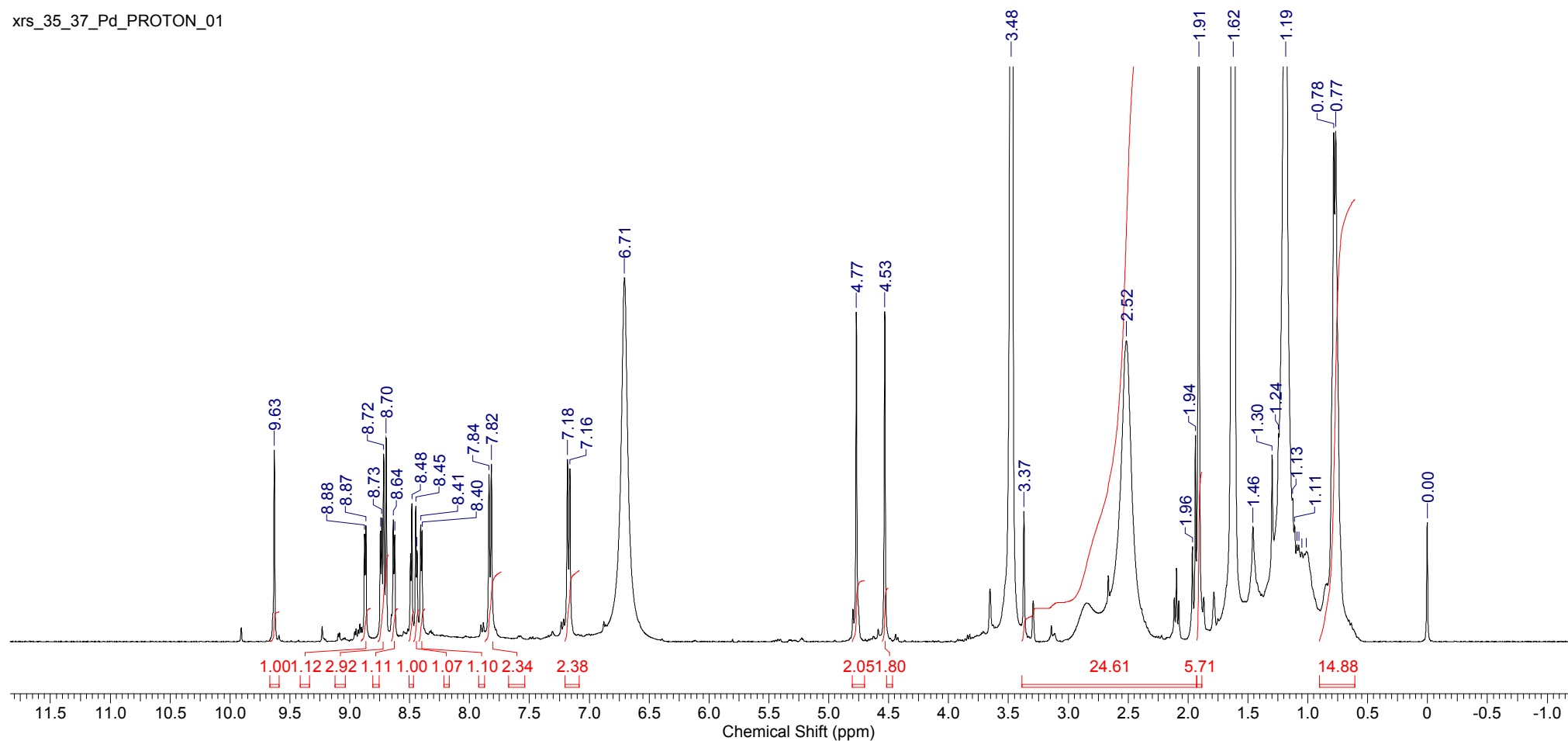


PROTON\_01

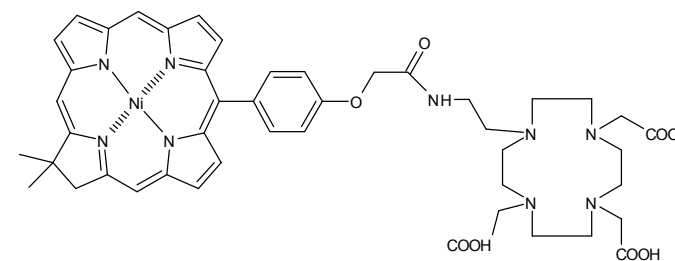




xrs\_35\_37\_Pd\_PROTON\_01



E:\UJ\_PHD Spectral NMR xrs\_35\_37\_Pd\_20140604\_01\xrs\_35\_37\_Pd\_PROTON\_01



xrs\_35\_37\_Ni\_PROTON\_01

