SYNTHESIS AND LUMINESCENCE OF SOLUBLE *meso*-UNSUBSTITUTED TETRABENZO- AND TETRANAPHTHO [2,3]PORPHYRINS

SUPPORTING INFORMATION

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Materials and Methods

All solvents were purified according to the standard procedures. *Selecto* silica gel or neutral aluminum oxide (Brockmann I, ~150 mesh) was used for column chromatography. All starting materials and reagents were obtained from standard commercial suppliers. Analytical TCL's were run on commercial Riedel-de Haën plates coated with silica gel $60F_{264}$ (0.2-mm thickness).

Static fluorescence and phosphorescence measurements were performed on SPEX Fluorolog-2 spectrofluorometer (Jobin-Yvon Horiba, Inc.), equipped with an infra-red enhanced R2658P PMT (Hamamatsu). Phosphorescence lifetimes were measured using an in-house constructed frequency domain phosphorometer.[1] Solutions for phosphorescence measurements were purged with Ar. The absorbances of the samples at the wavelengths used for excitation were kept below 0.05 OD. The quantum yields were obtained by computing the integrals of the corrected emission spectra and referencing them to the fluorescence quantum yield of ZnTPP in deoxygenated benzene (ϕ_{fluor}=0.033).[2] The spectra were normalized by the optical density of the samples at the excitation wavelengths, relative photon intensity of the source and quantum efficiency of the detector throughout the emission range.

Phosphorescence oxygen quenching constants (K_q) were determined as described previously.[3]

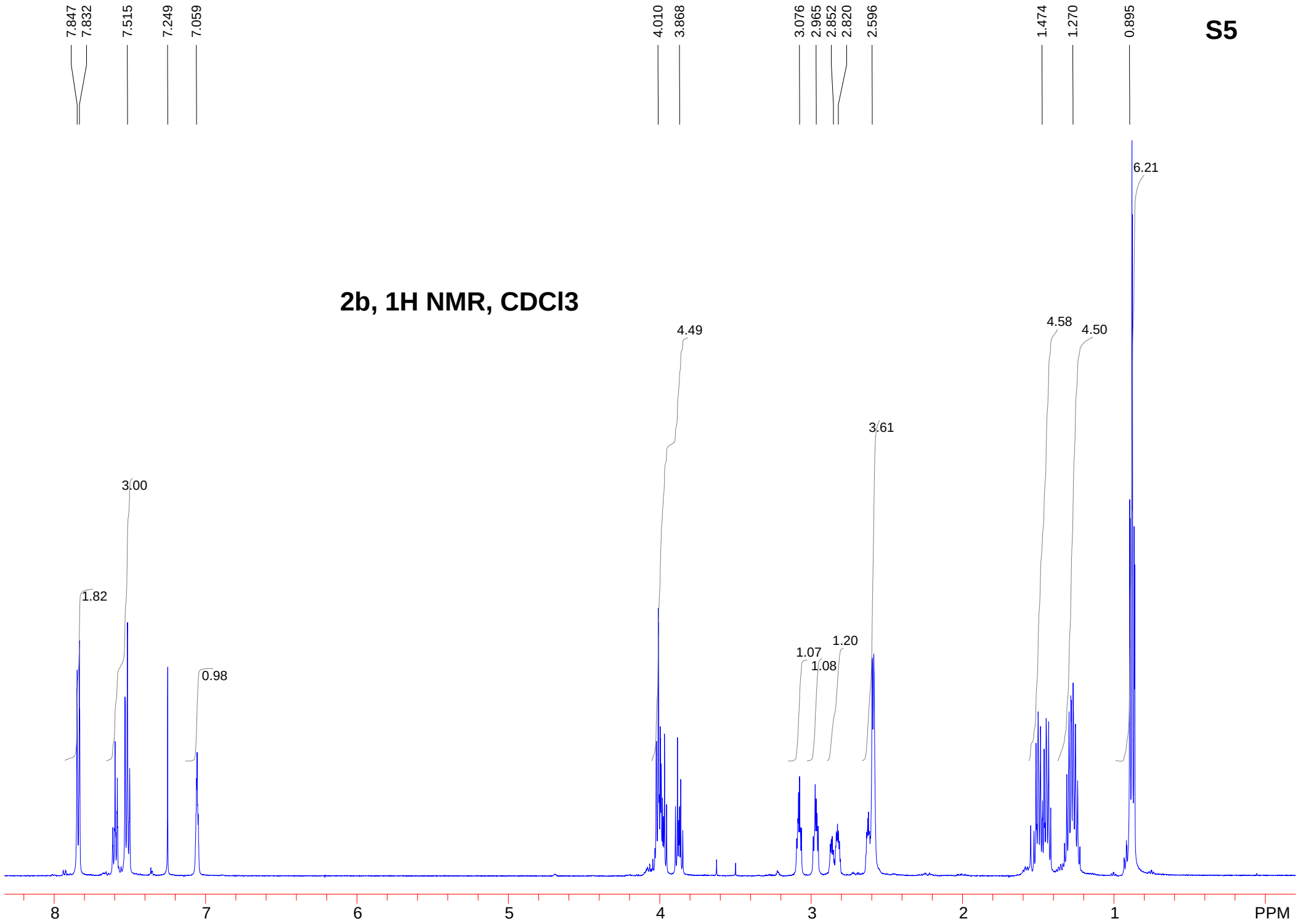
References and Notes

(1) Vinogradov, S. A.; Fernandez-Seara, M. A.; Dugan, B. W.; Wilson, D. F. *Rev. Sci. Instrum.* **2001**, *72*, 3396.

(2) Quimby, D. J.; Longo, F. R. *J. Am. Chem. Soc.* **1975**, *97*, 5111.

(3) Rozhkov, V.V.; Wilson, D.F.; Vinogradov, S.A. *Macromolecules* **2002**, *35*, 1991.

NMR spectra



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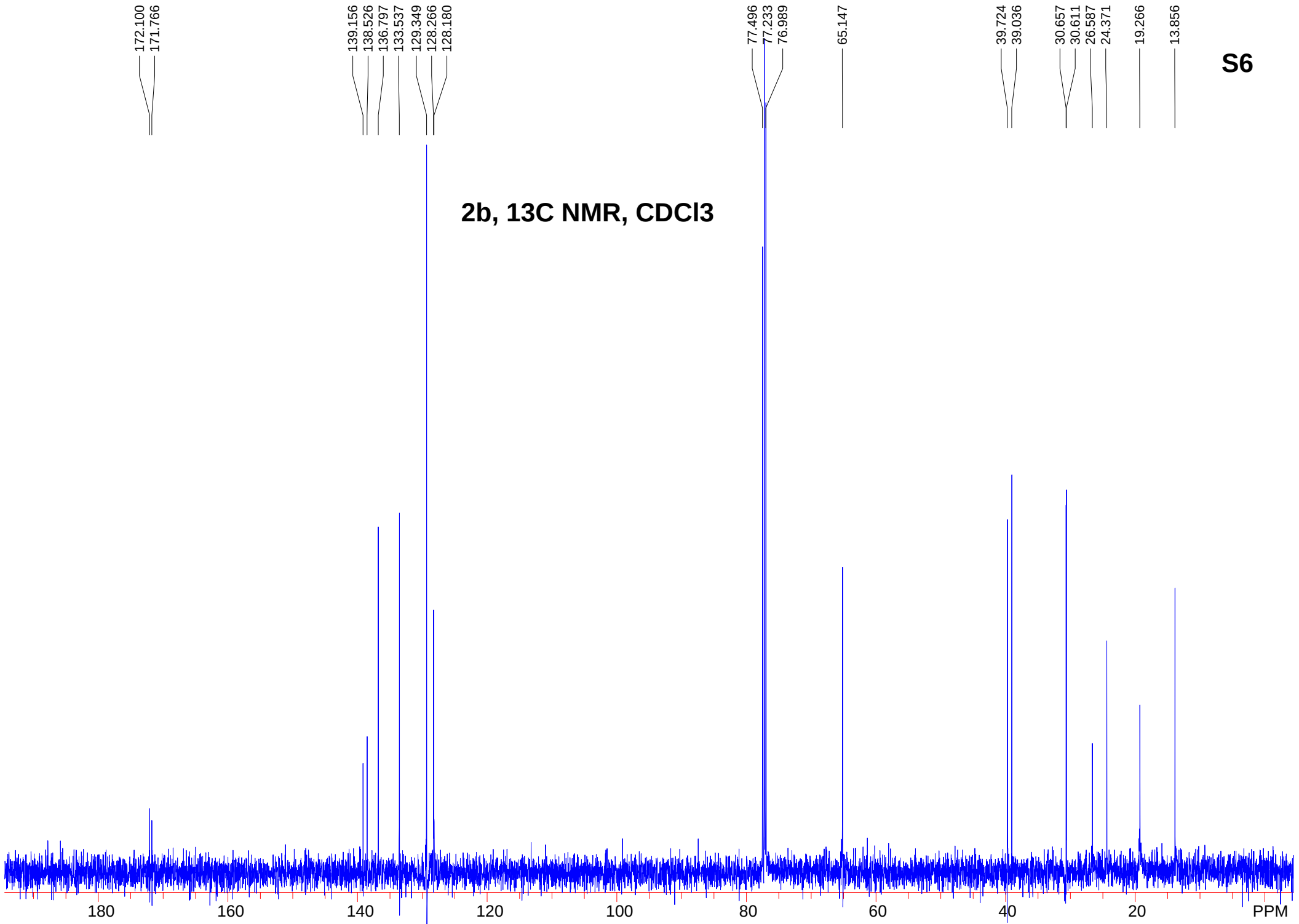

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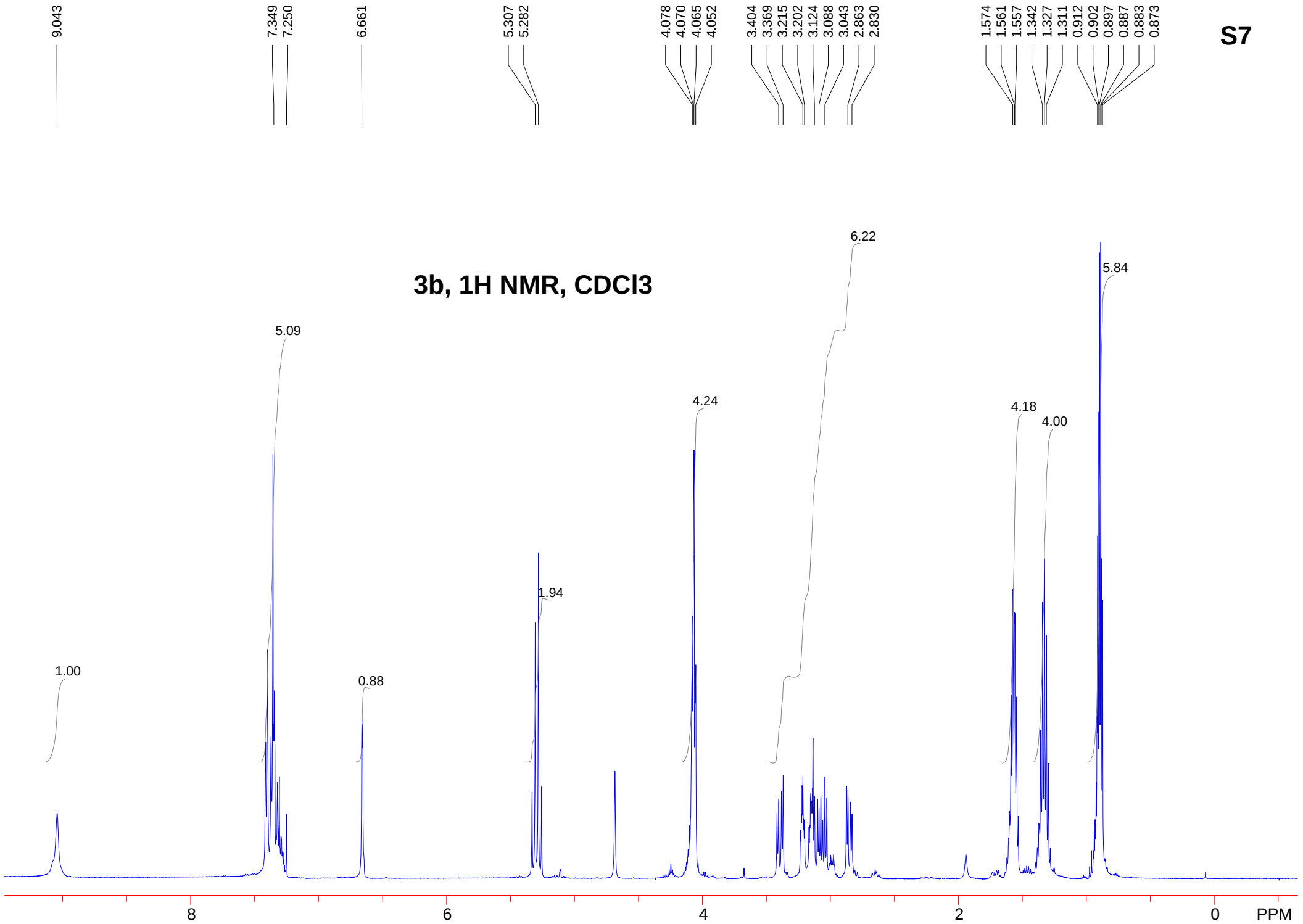

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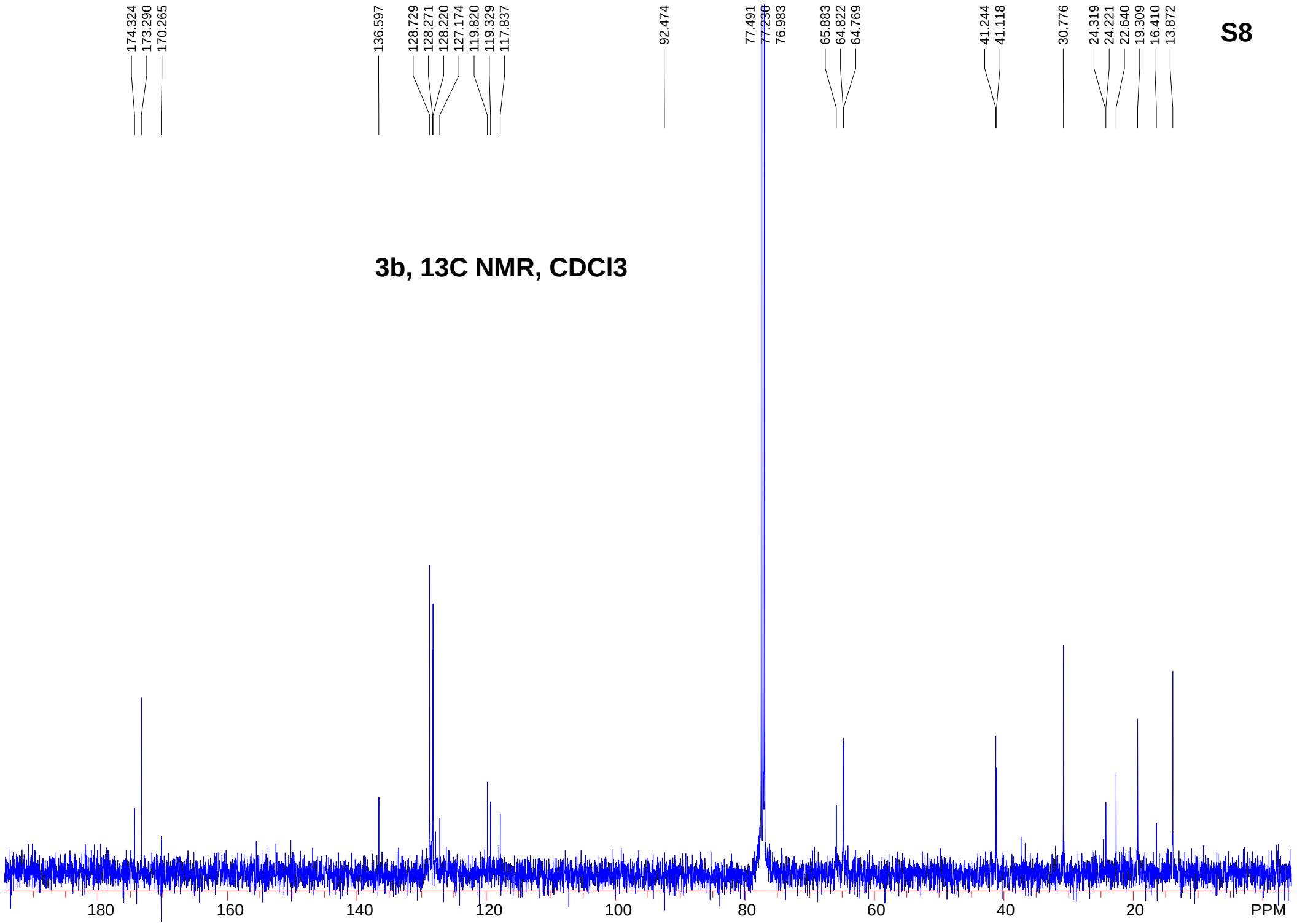

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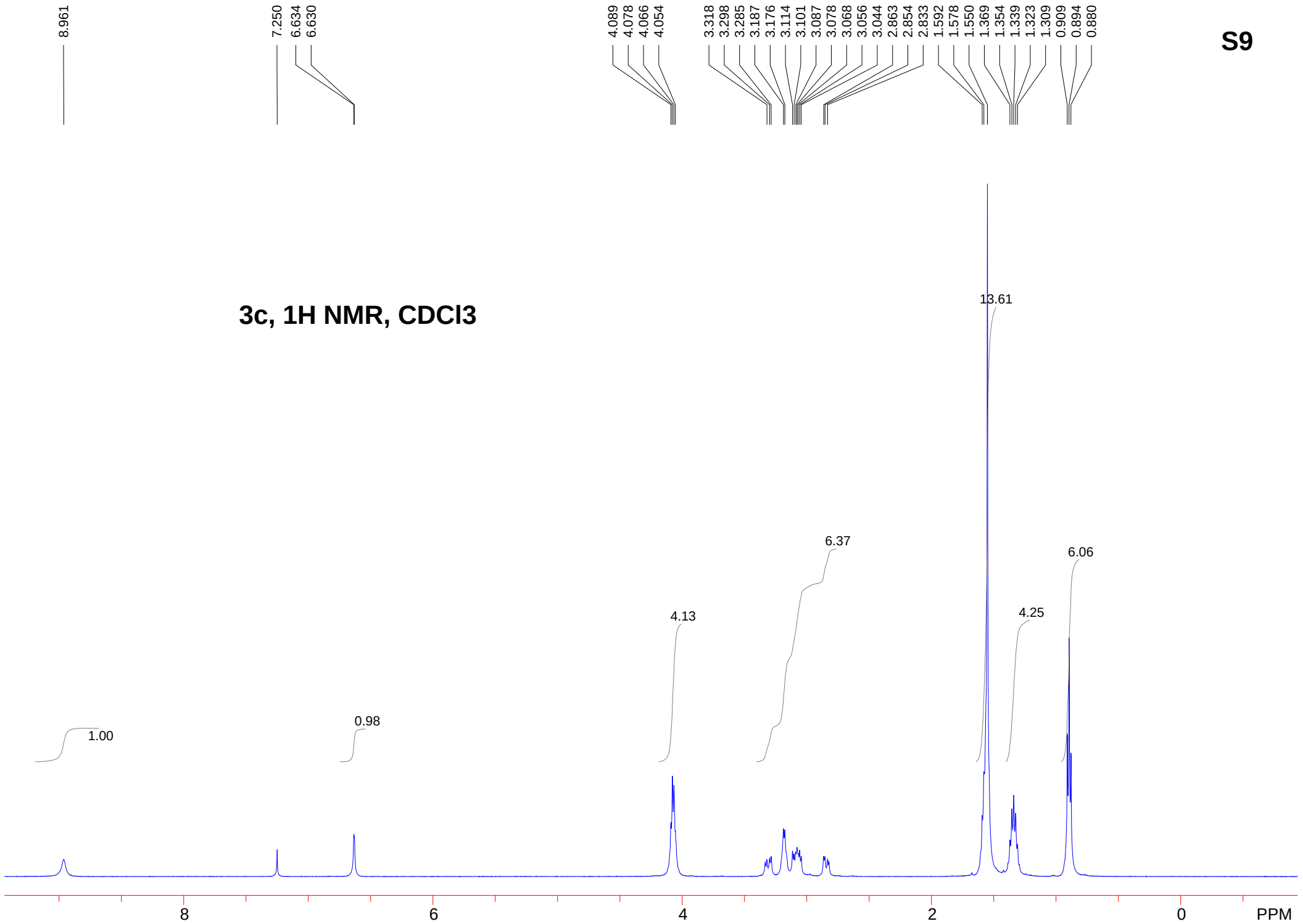

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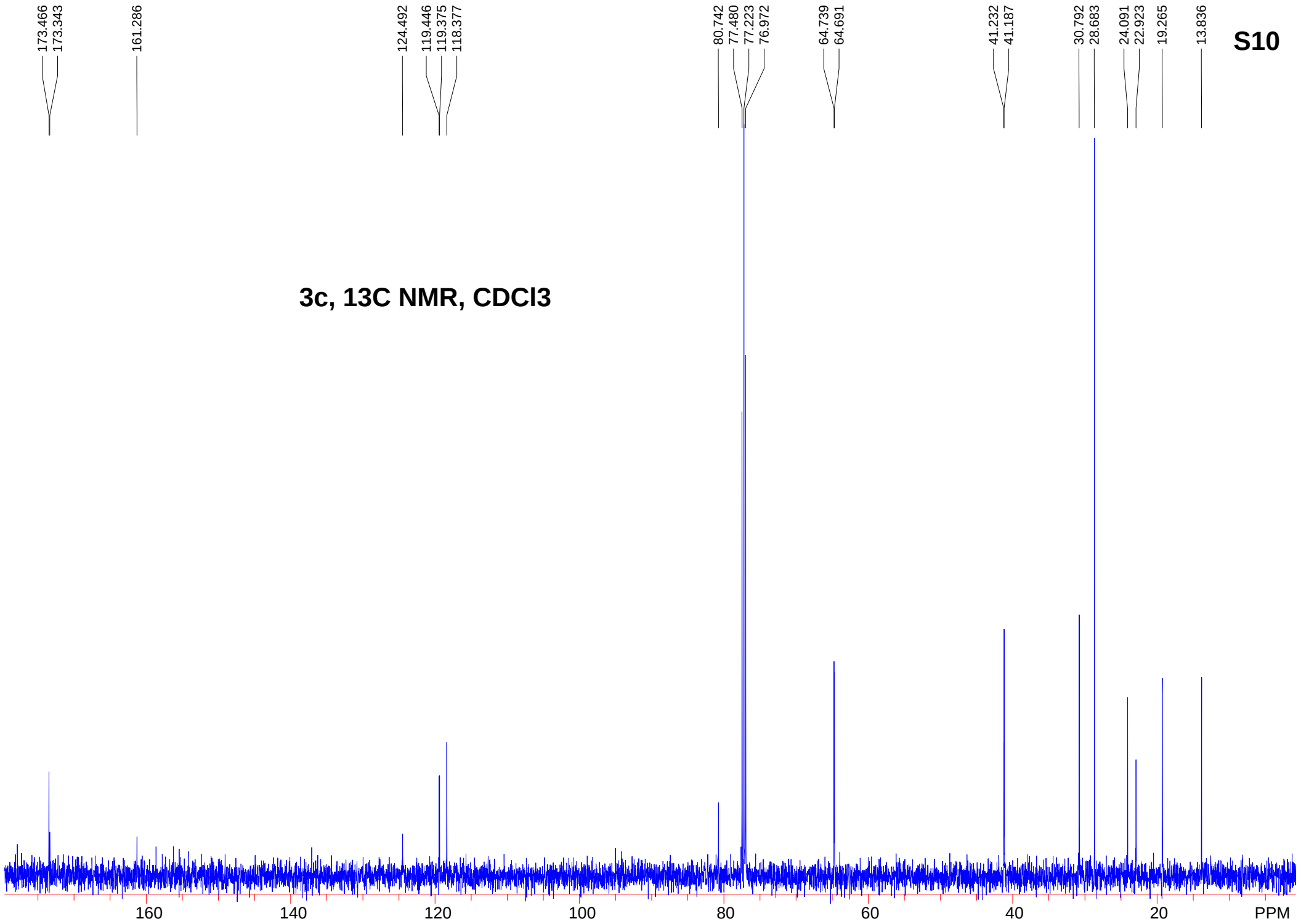

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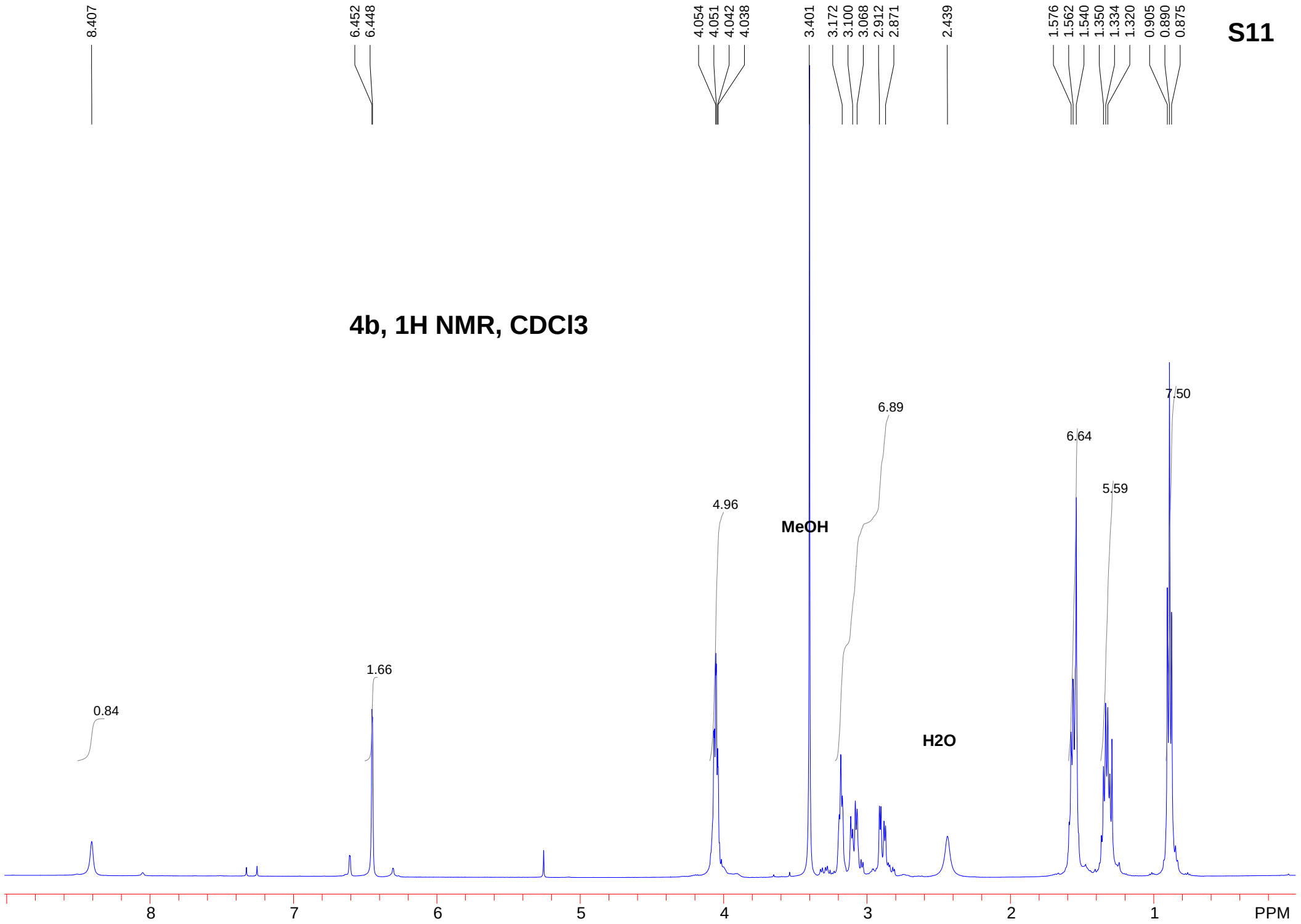

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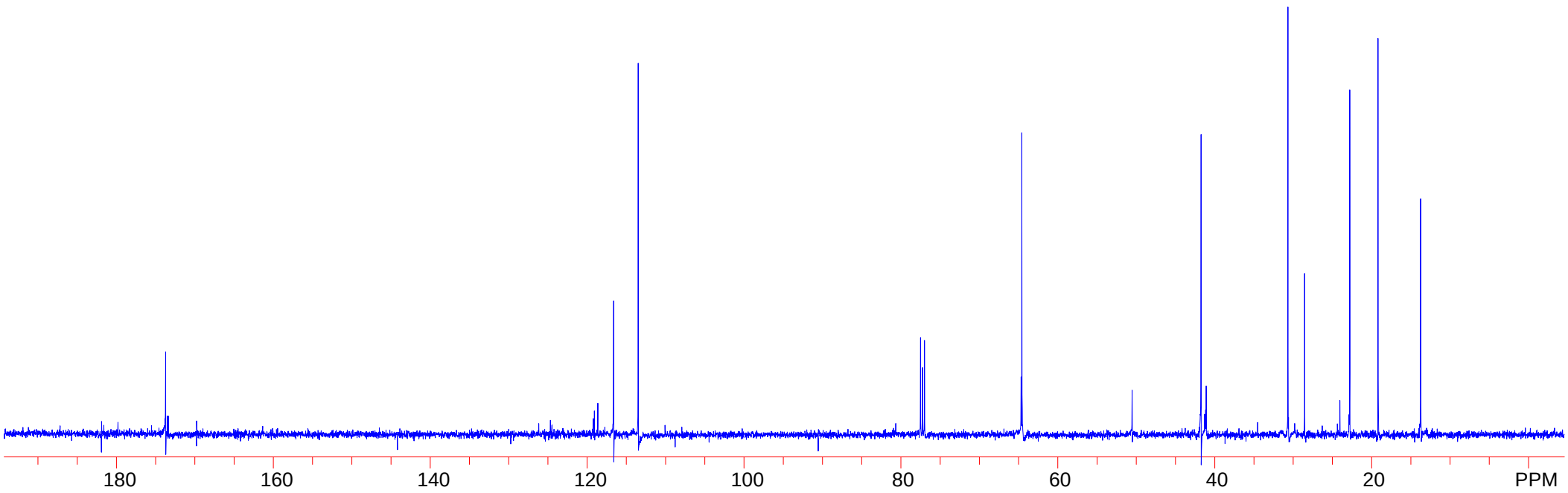
4b, 13C NMR, CDCl3



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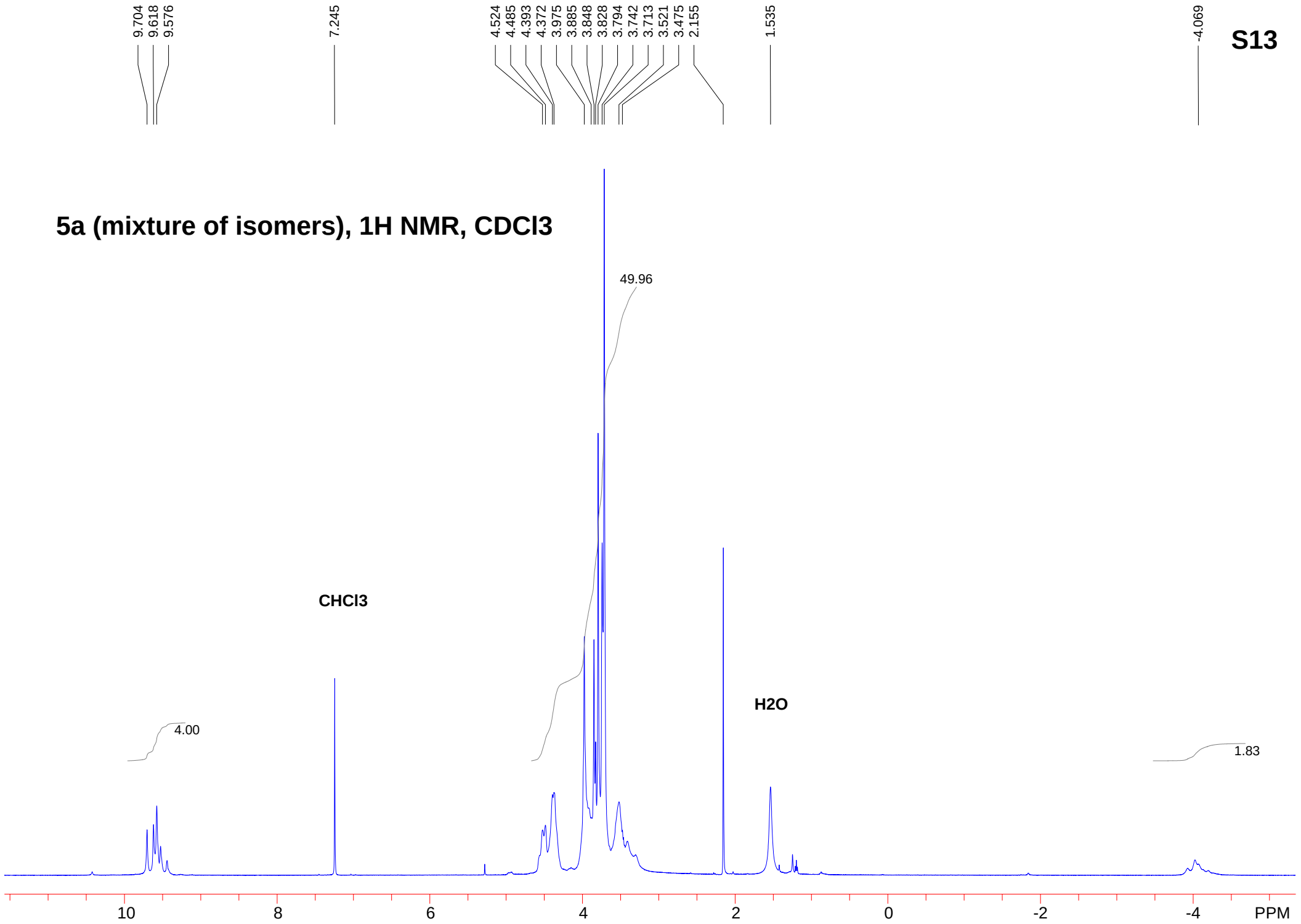

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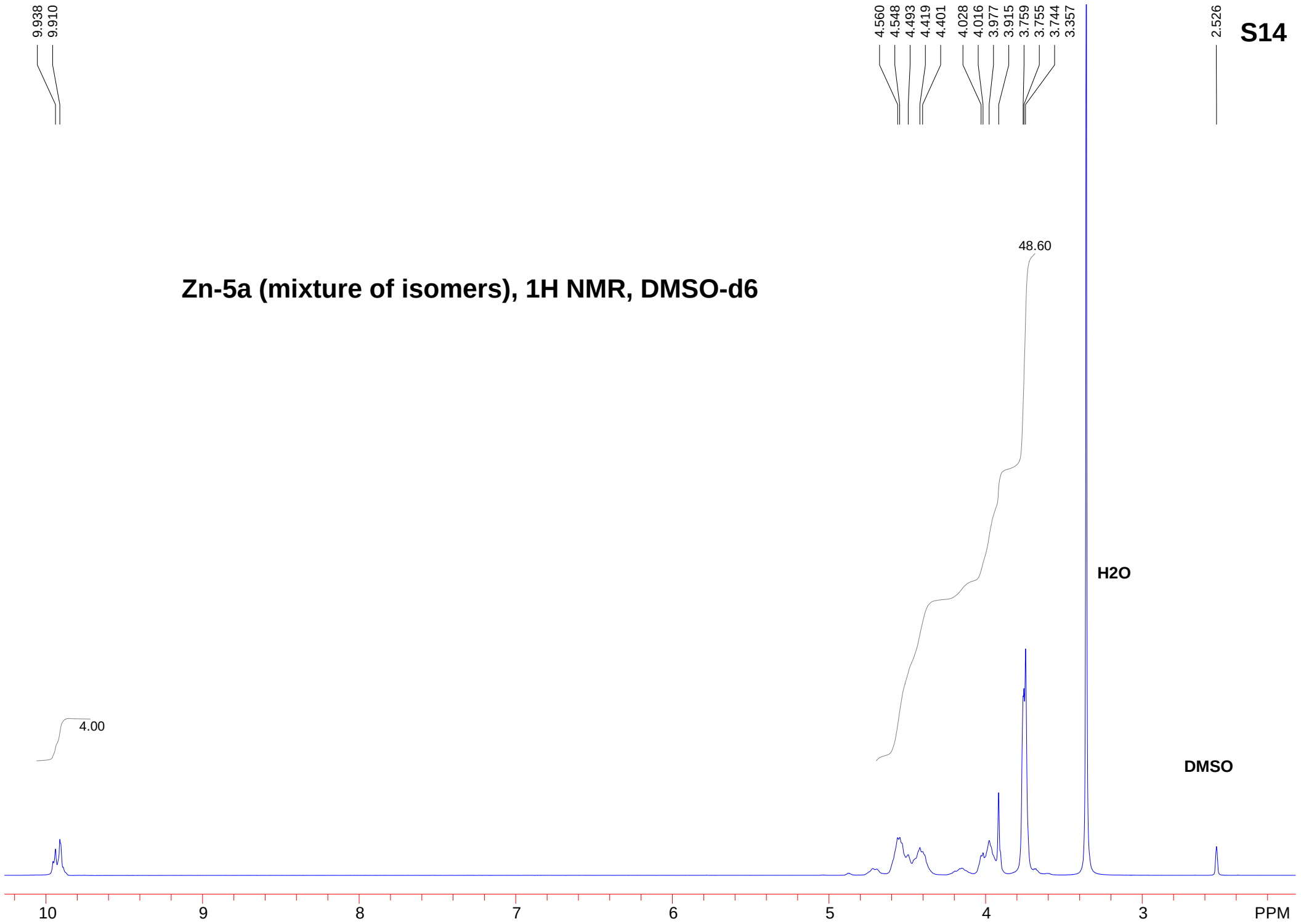

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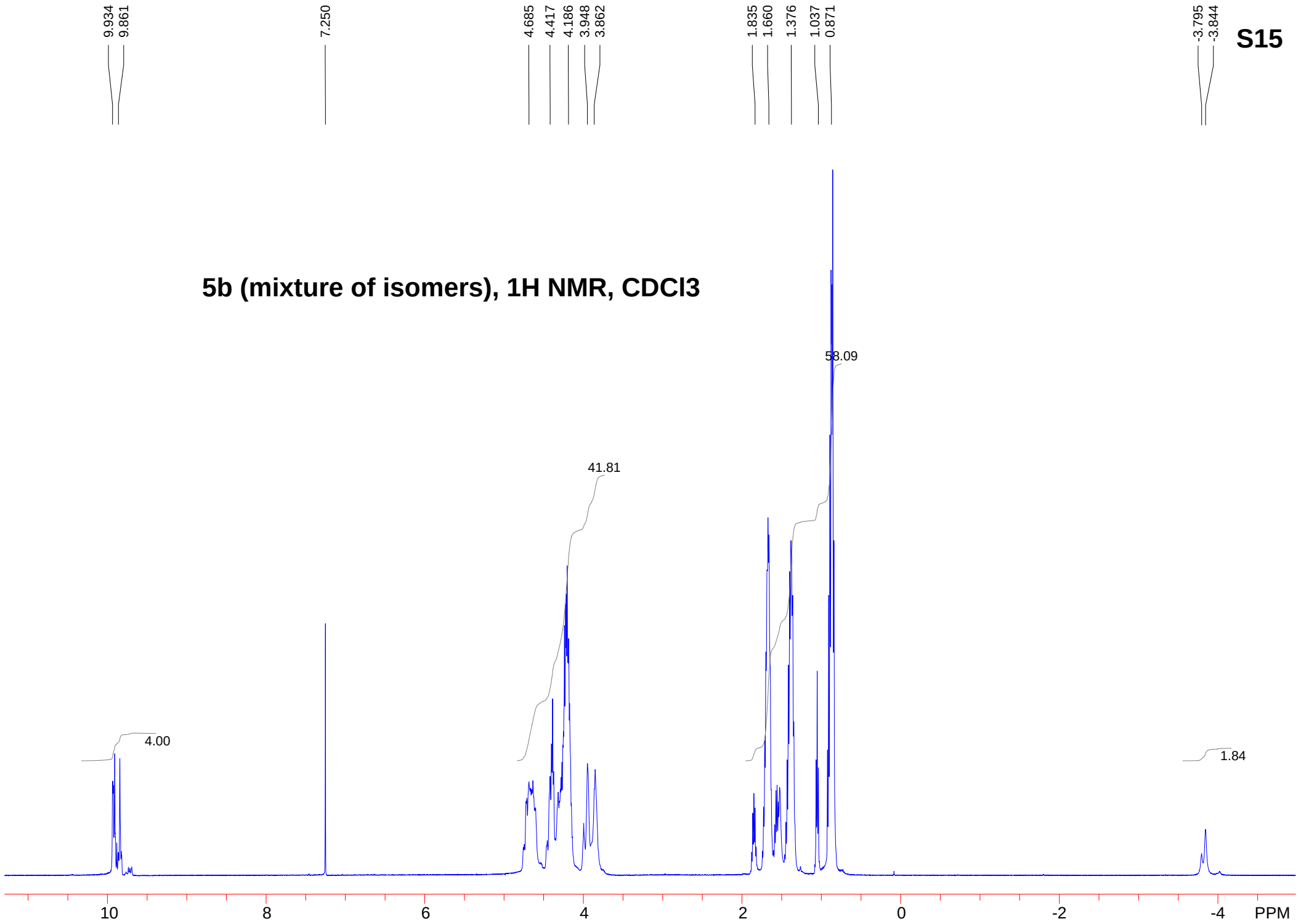

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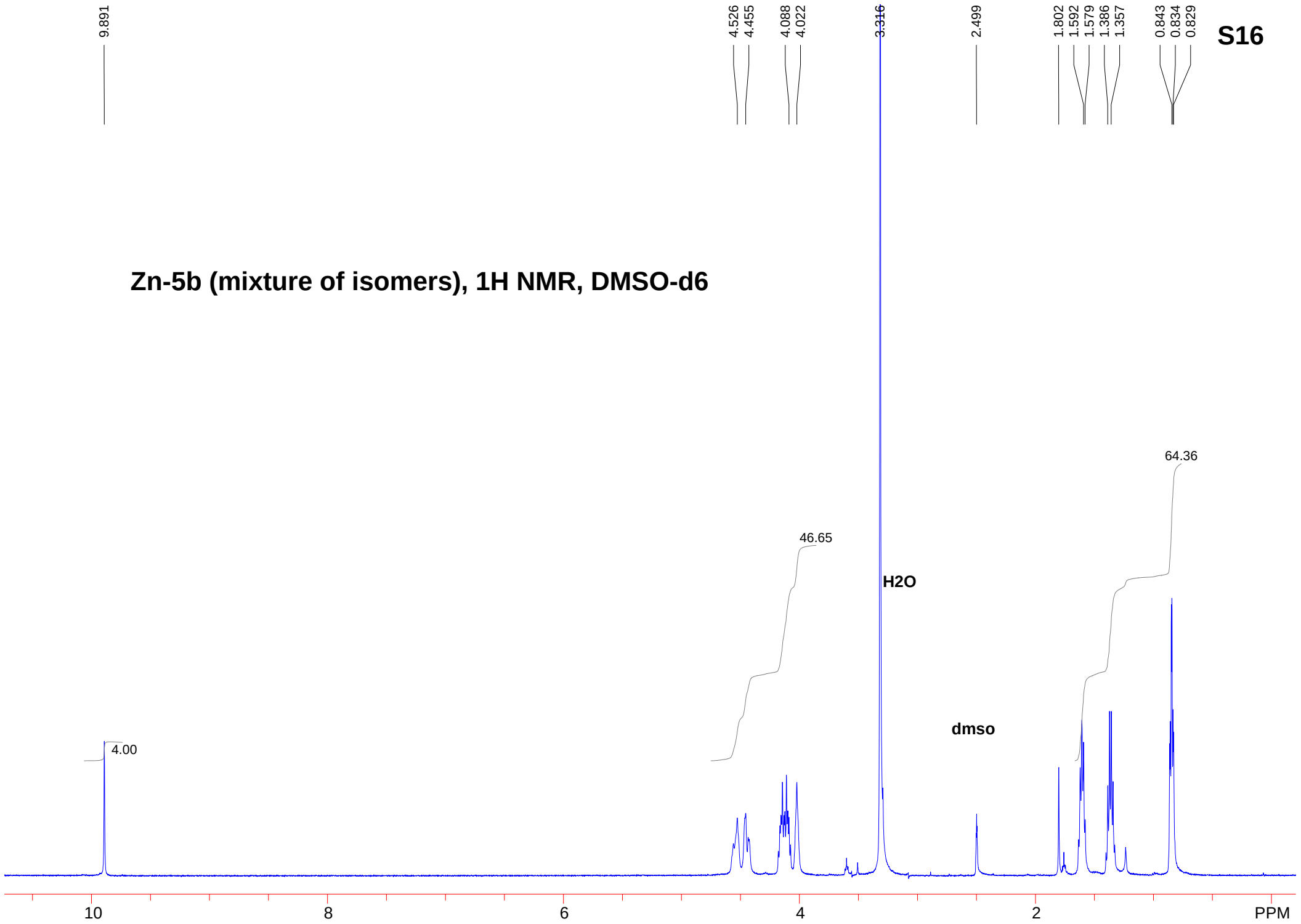
Zn-5b (mixture of isomers), 1H NMR, DMSO-d6



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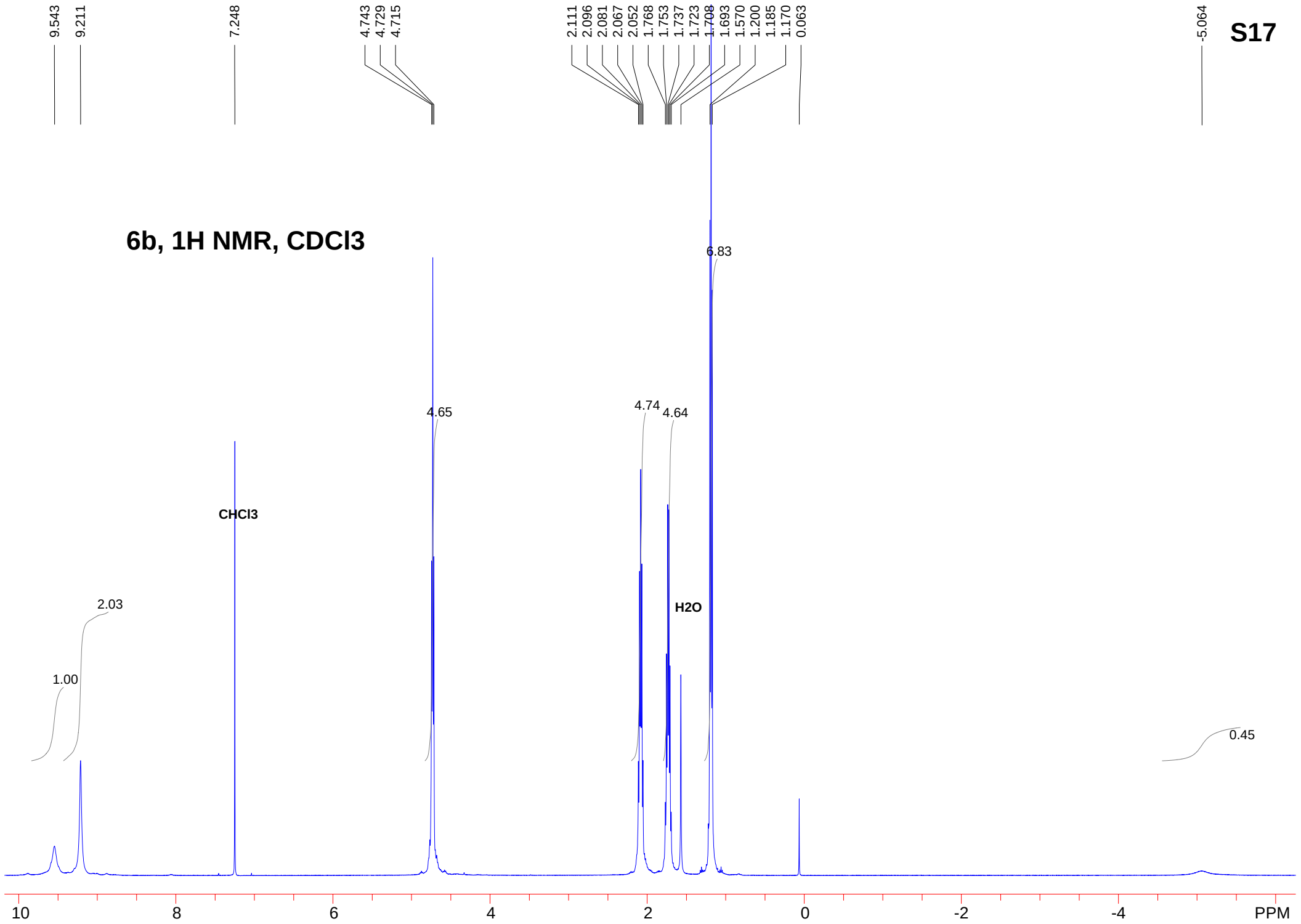

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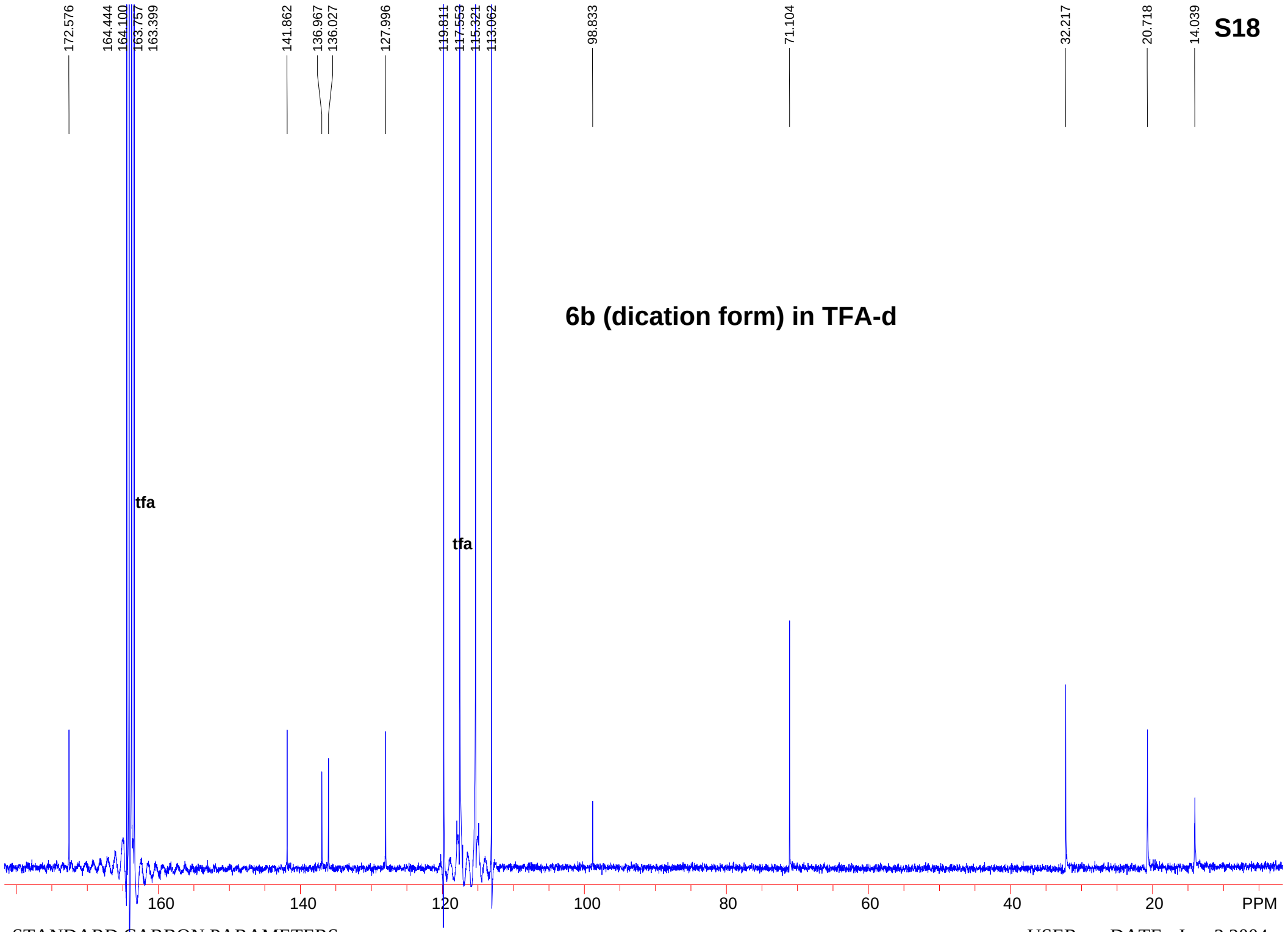

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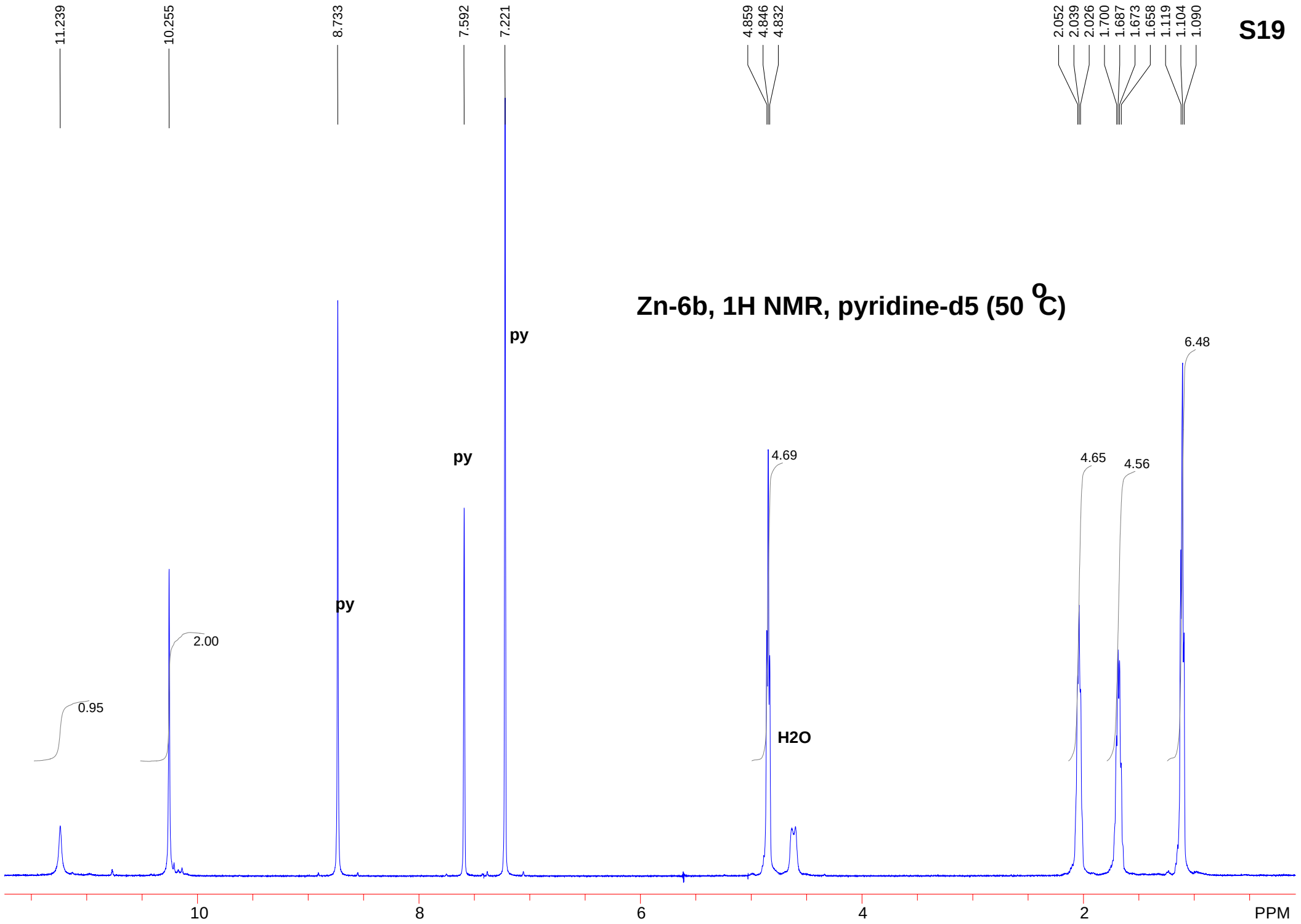

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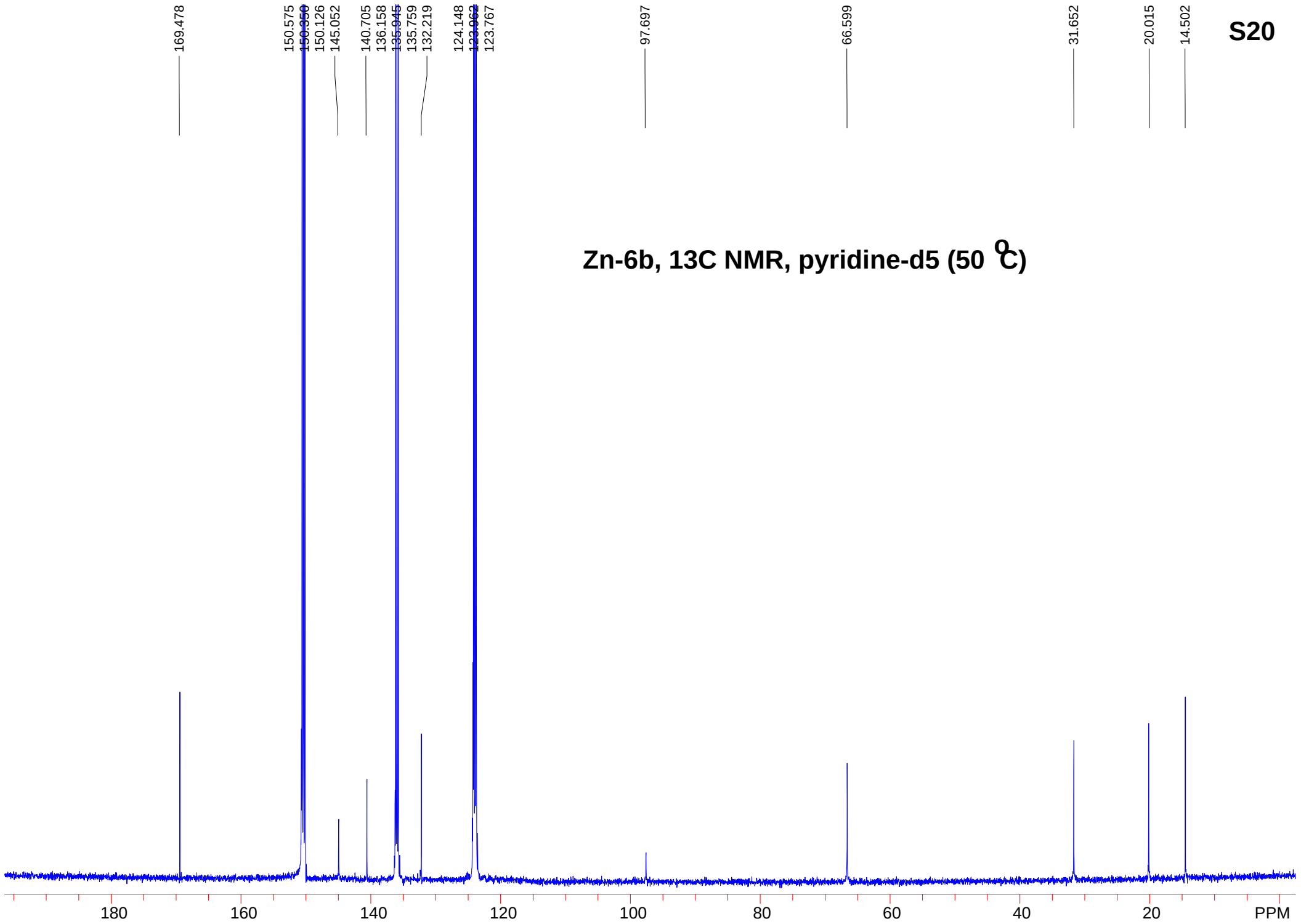

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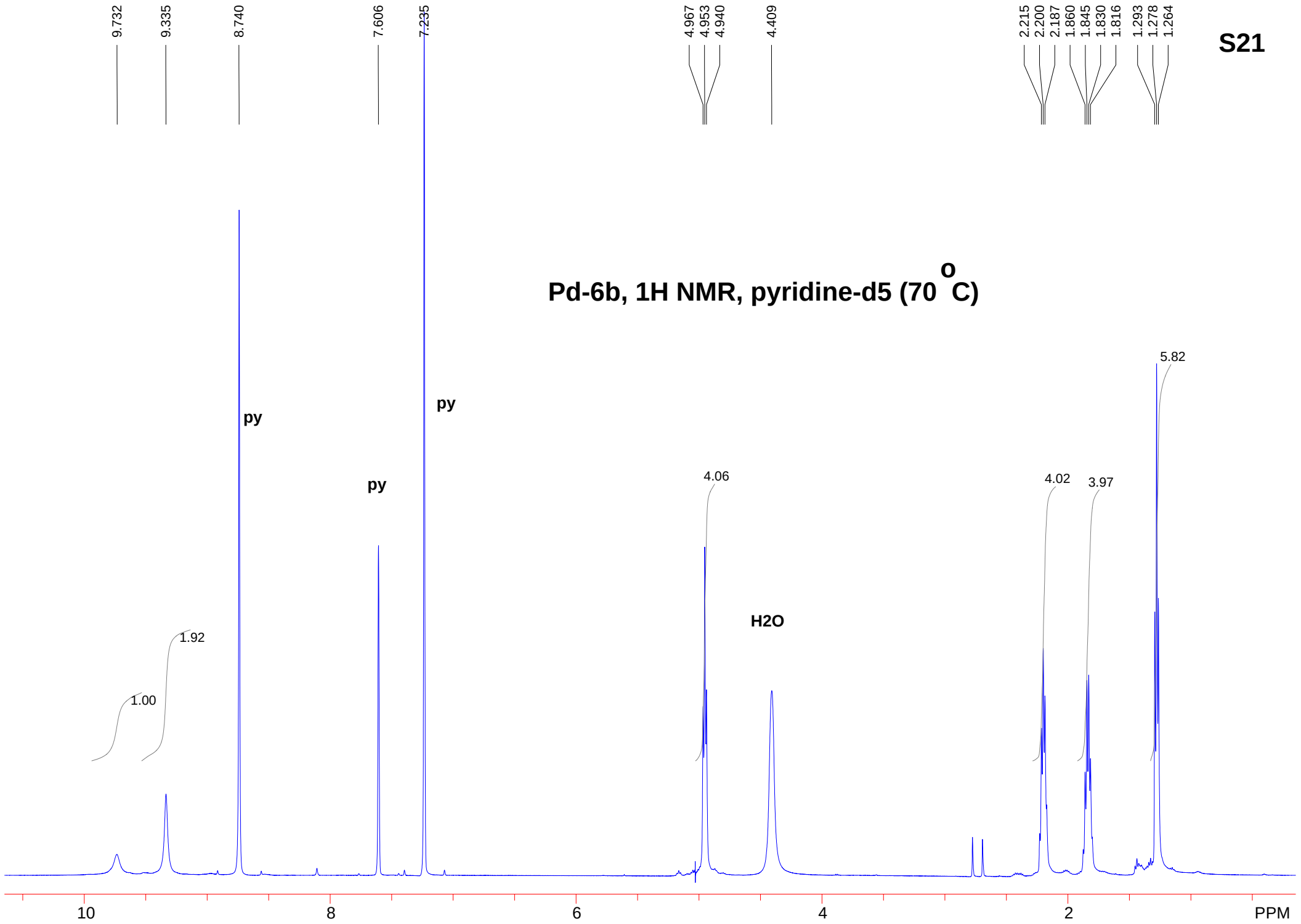

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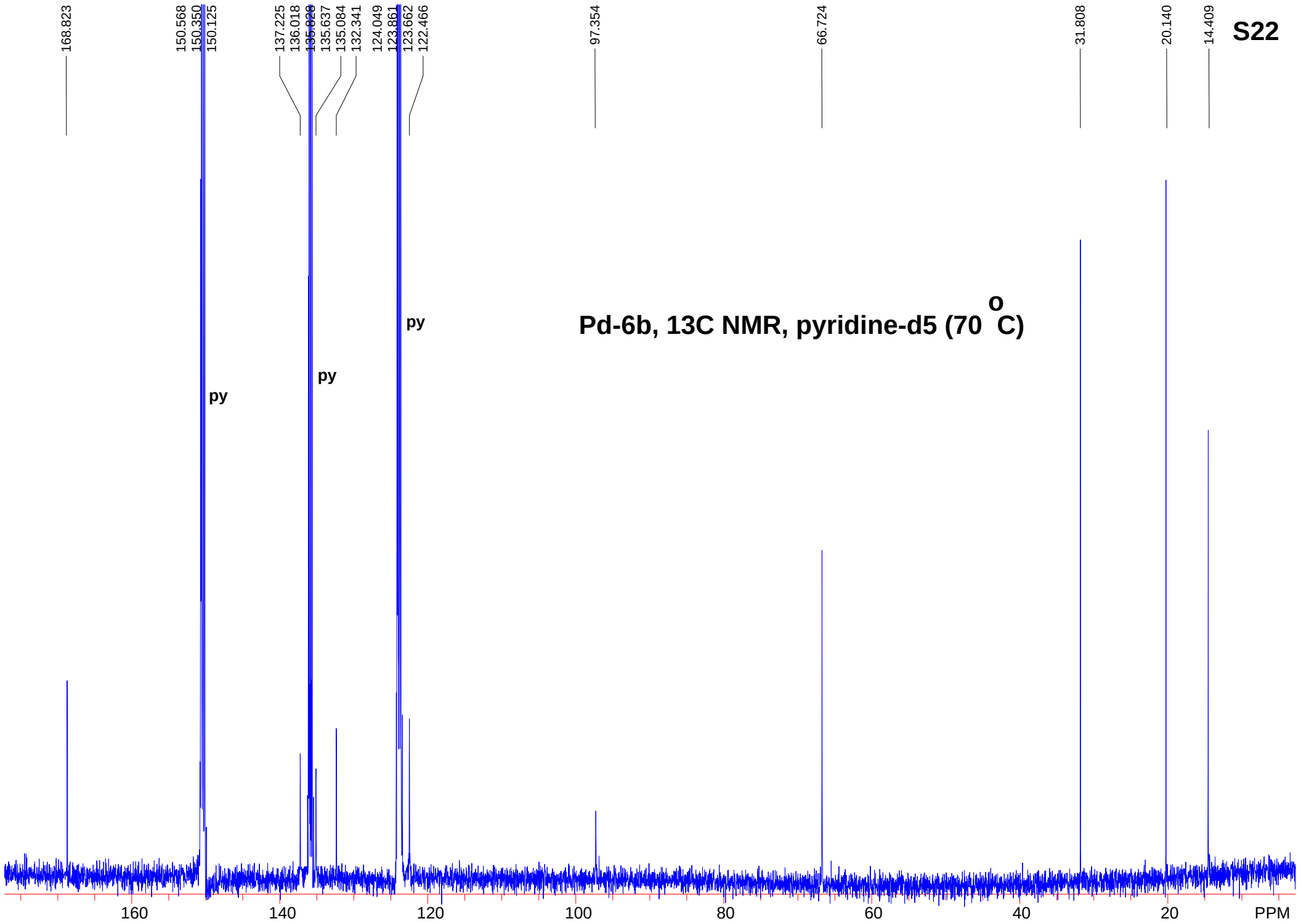

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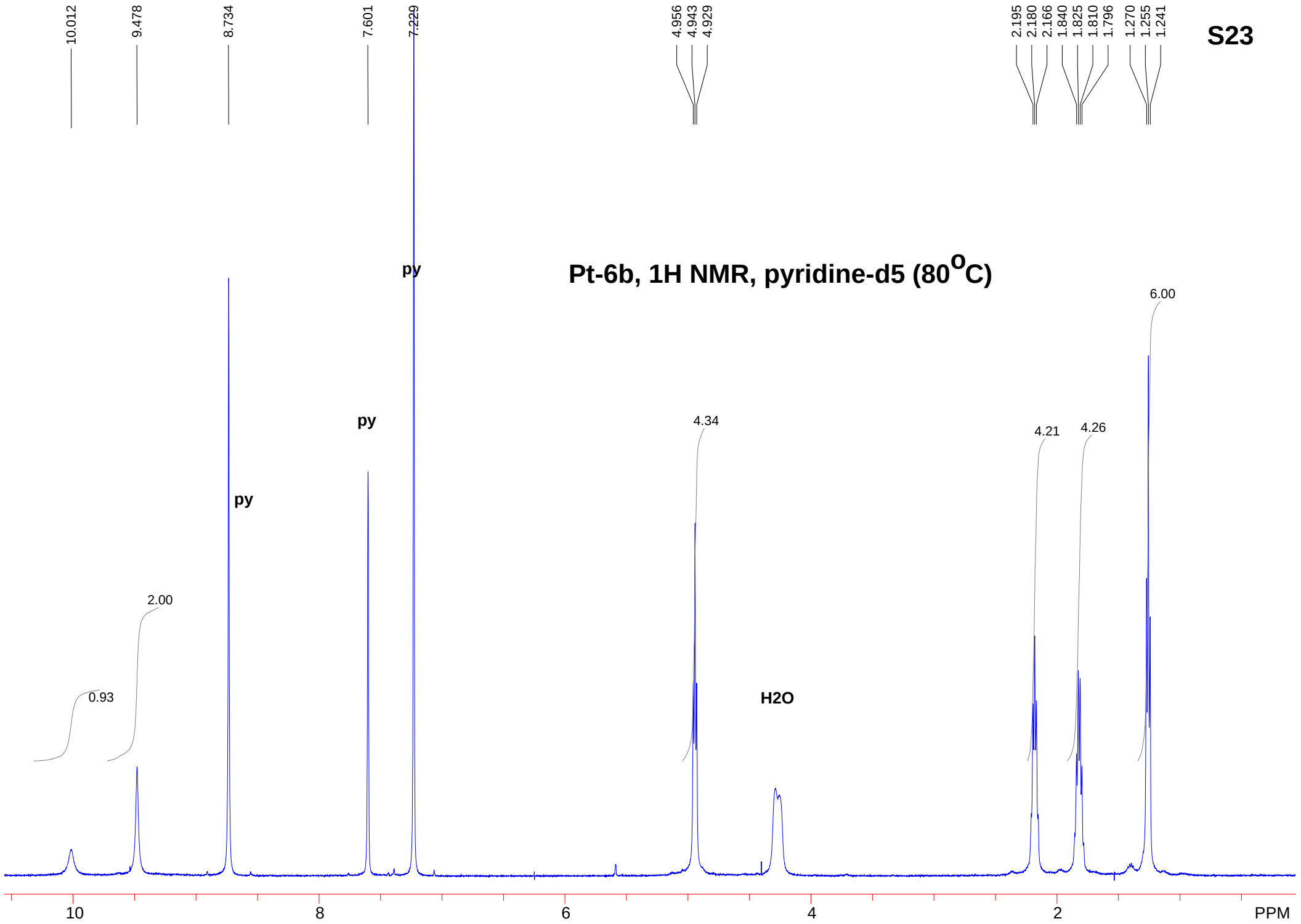

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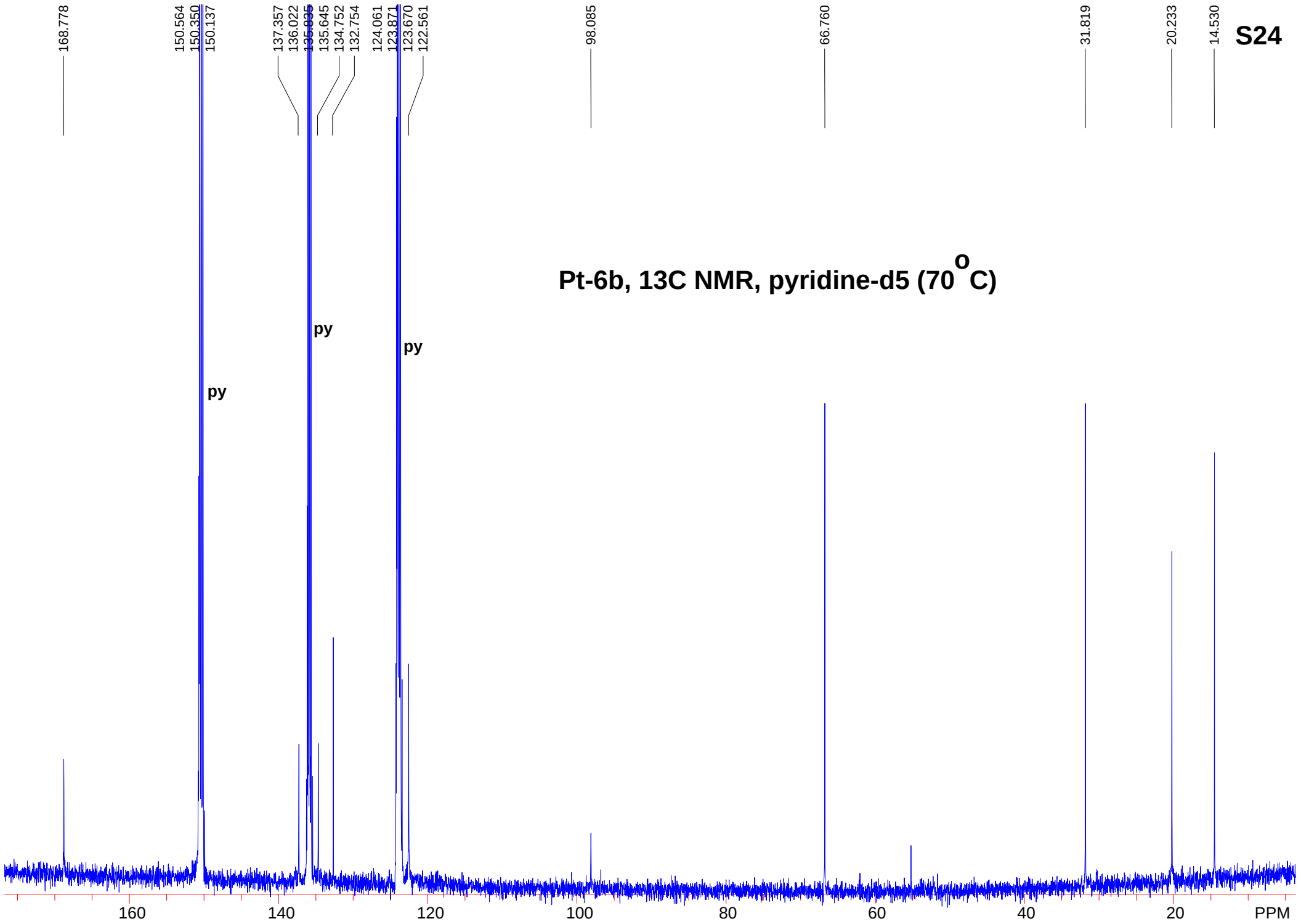

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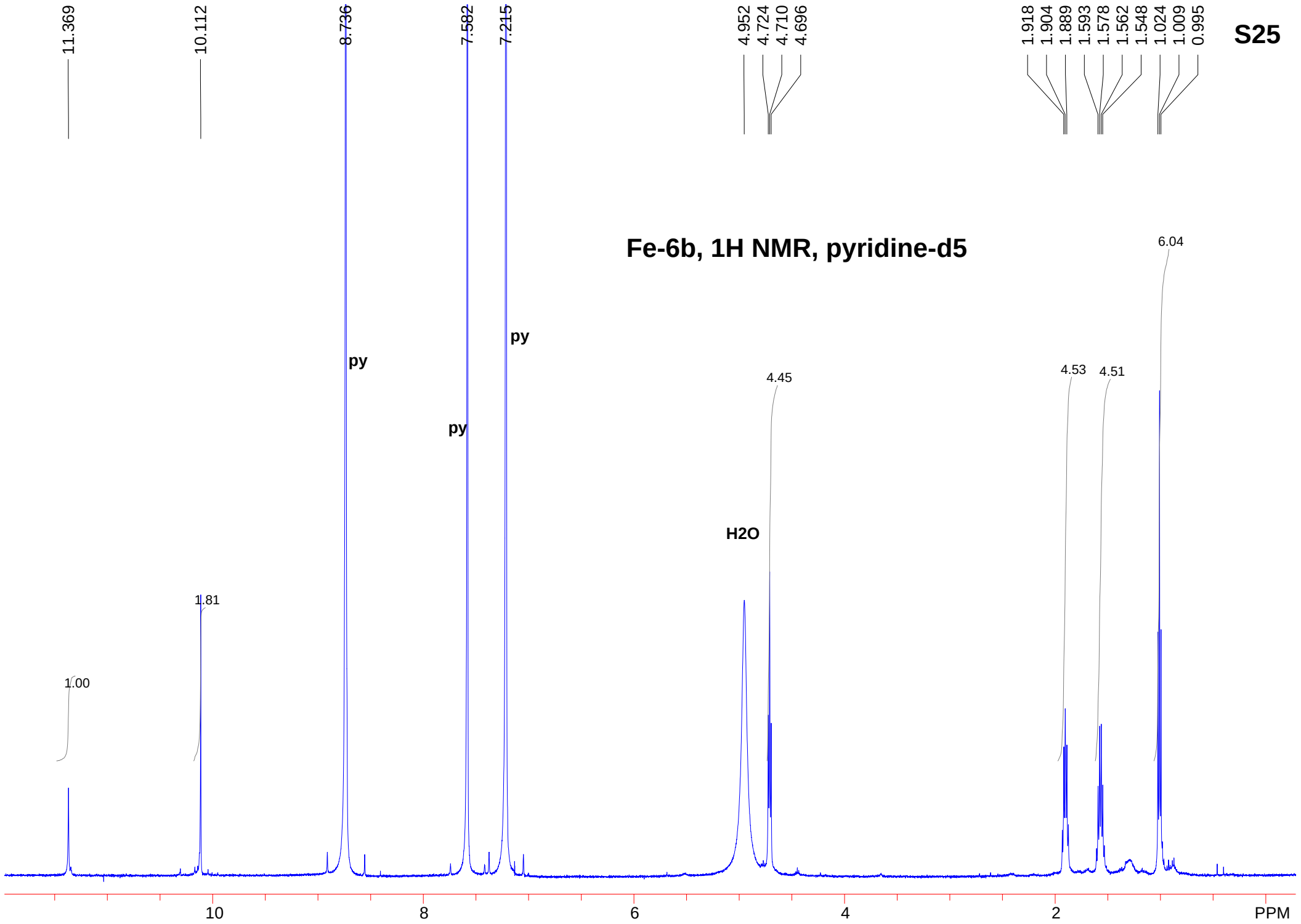

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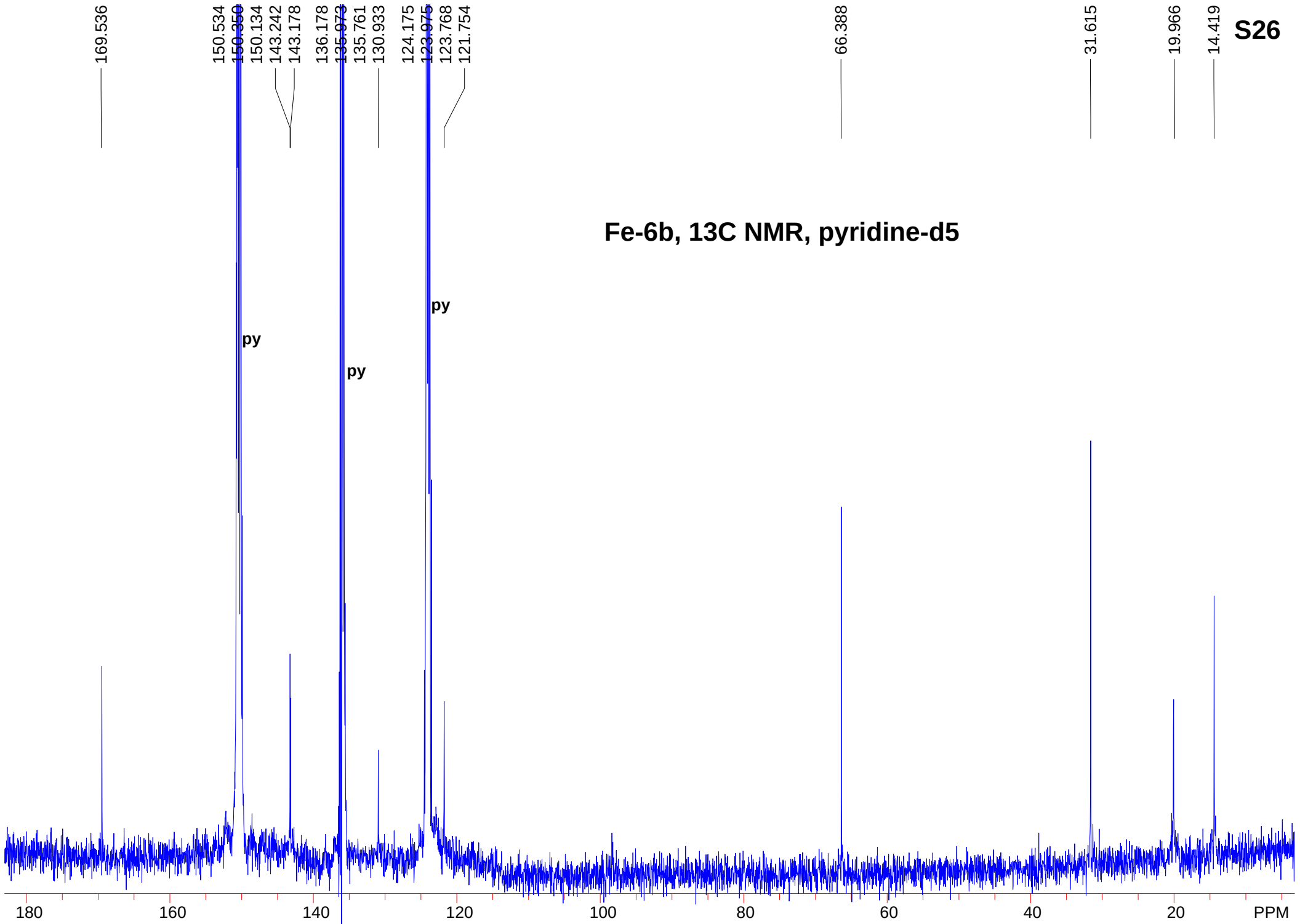

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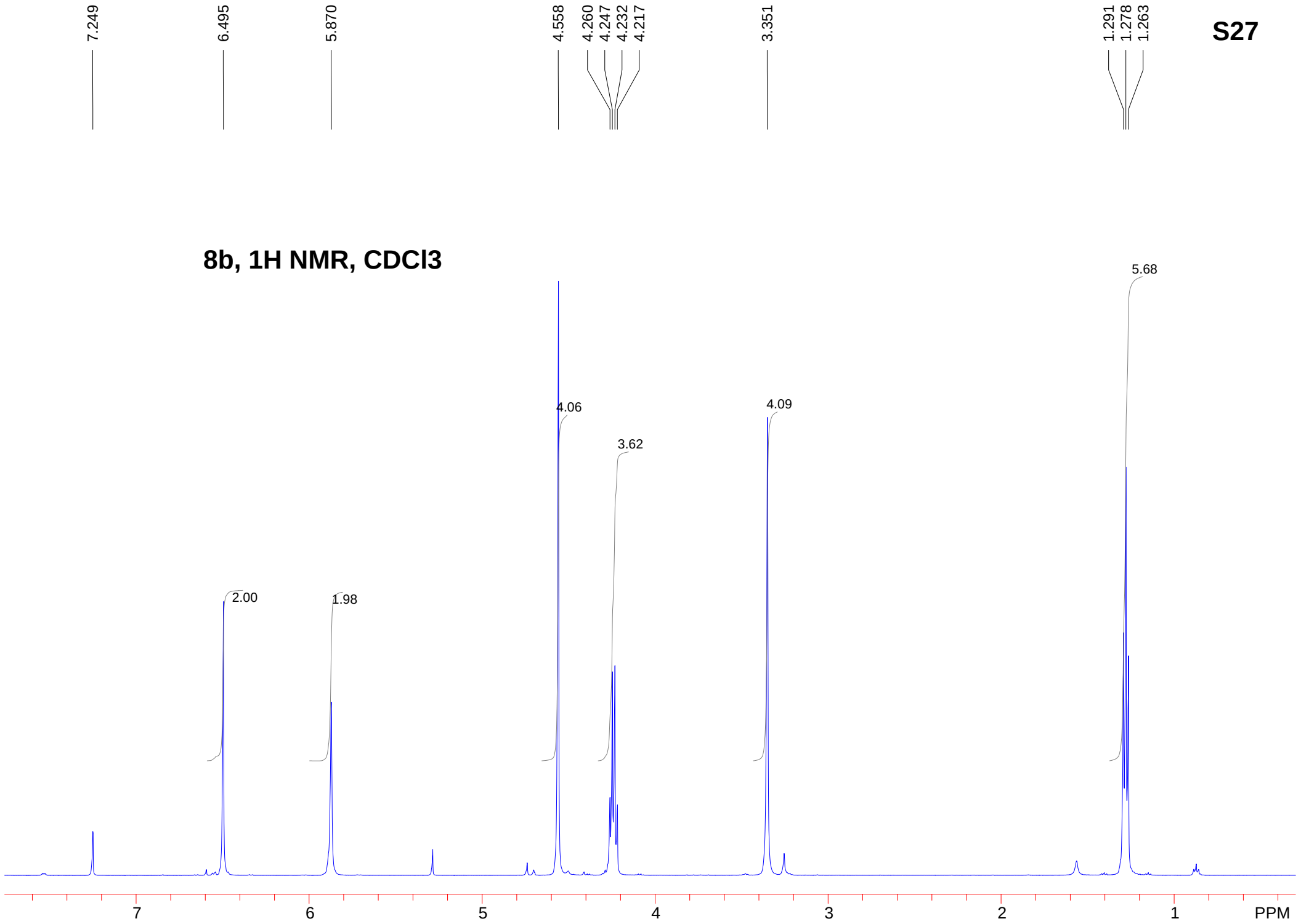

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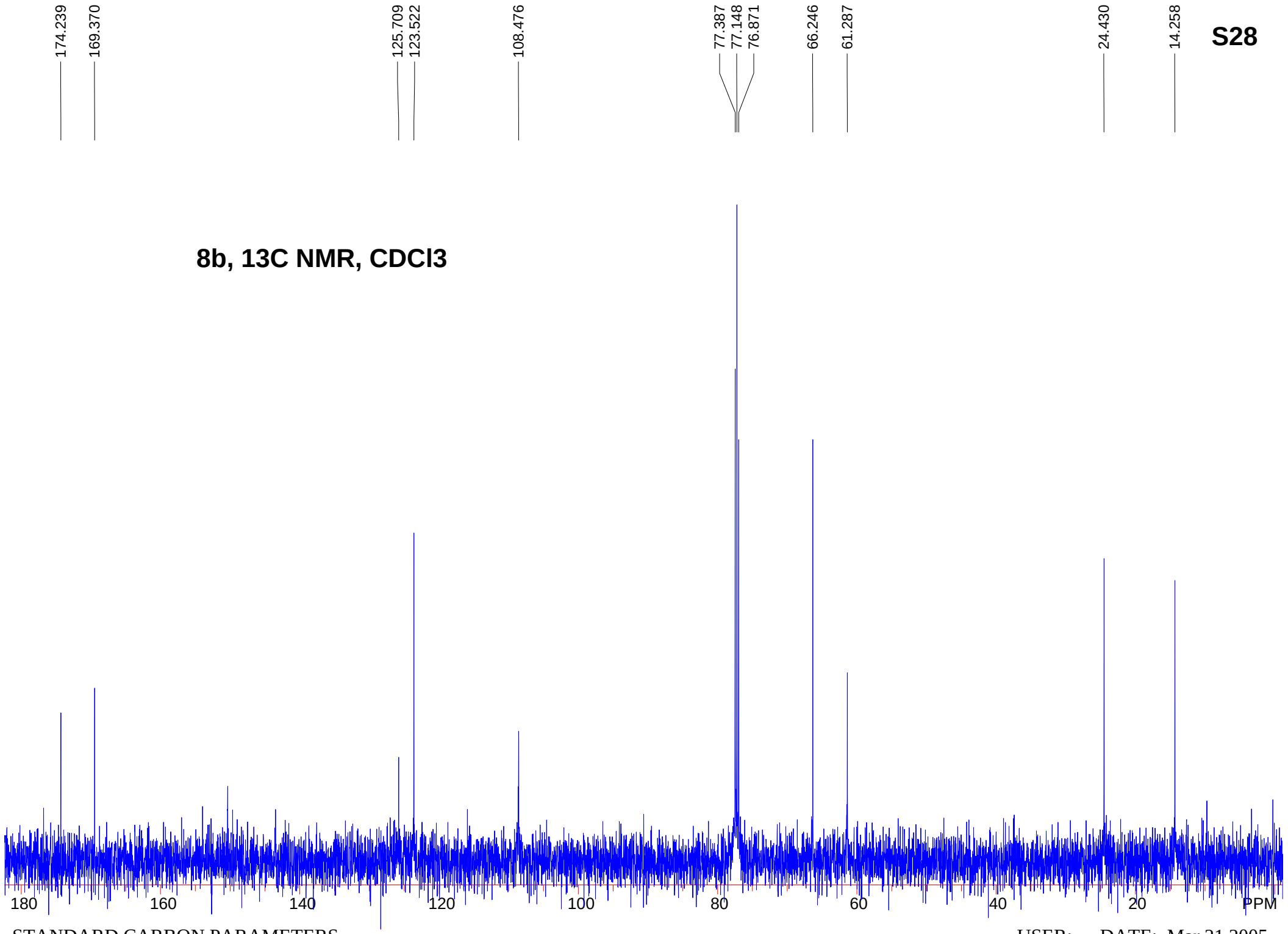

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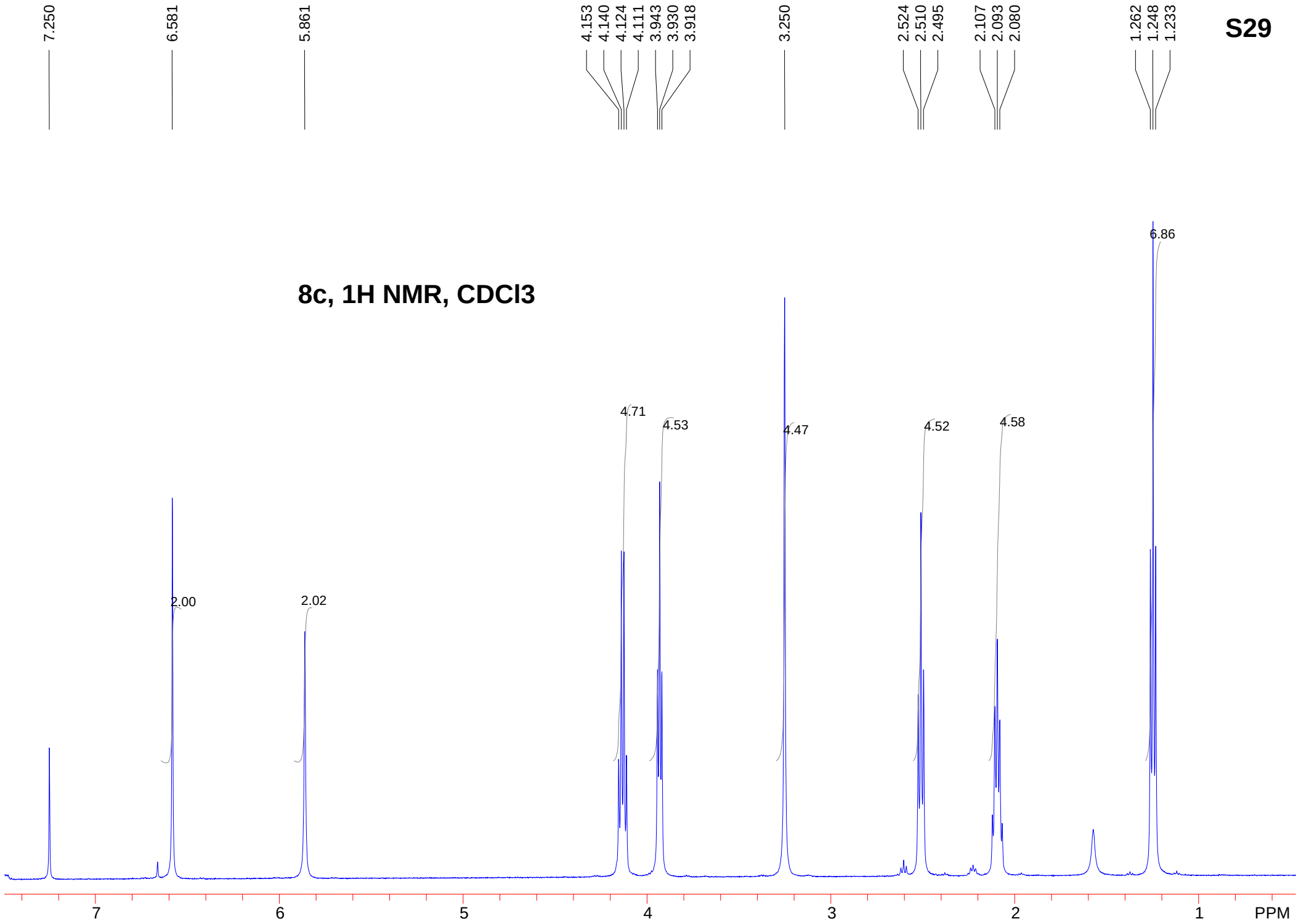

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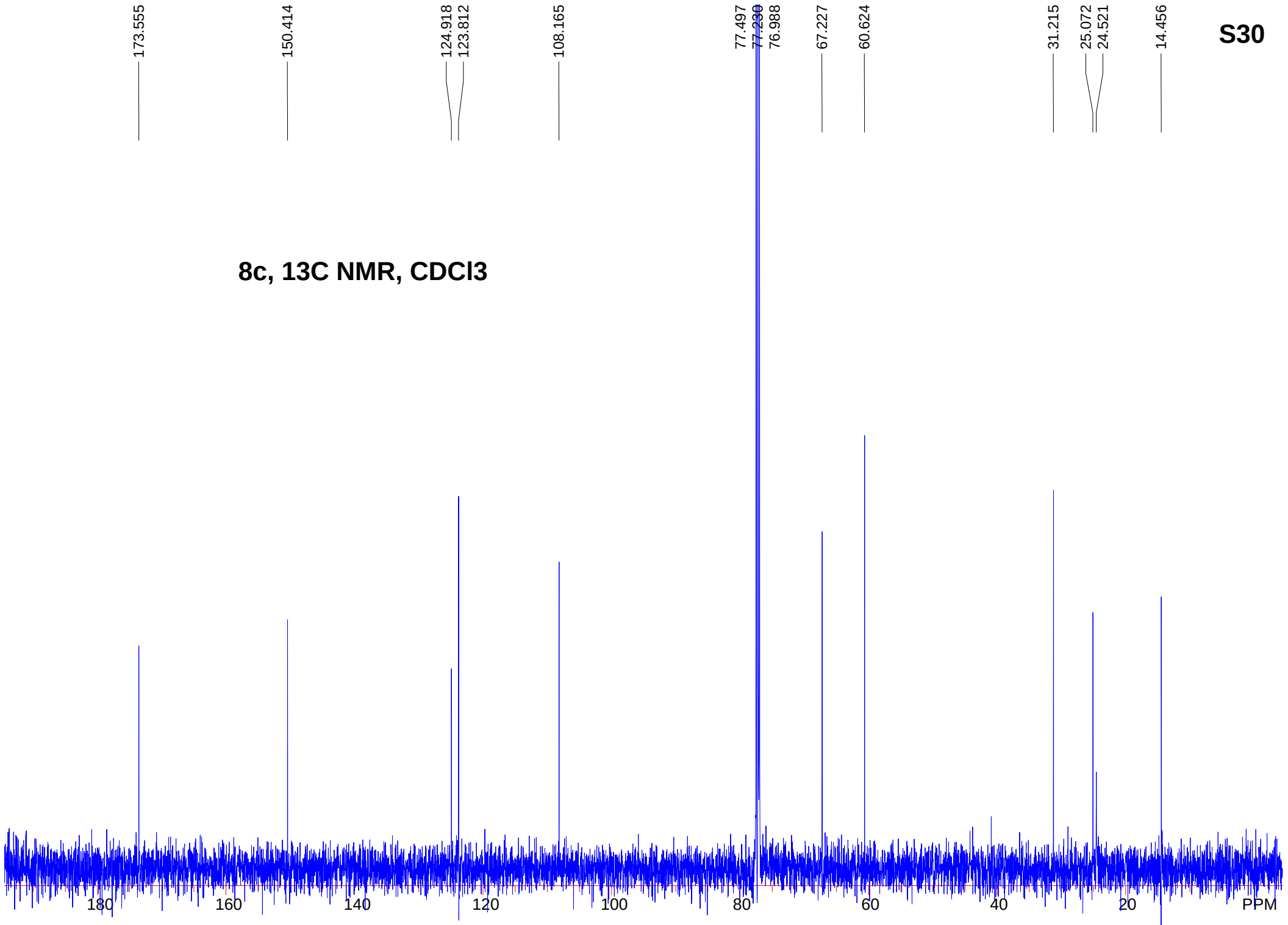

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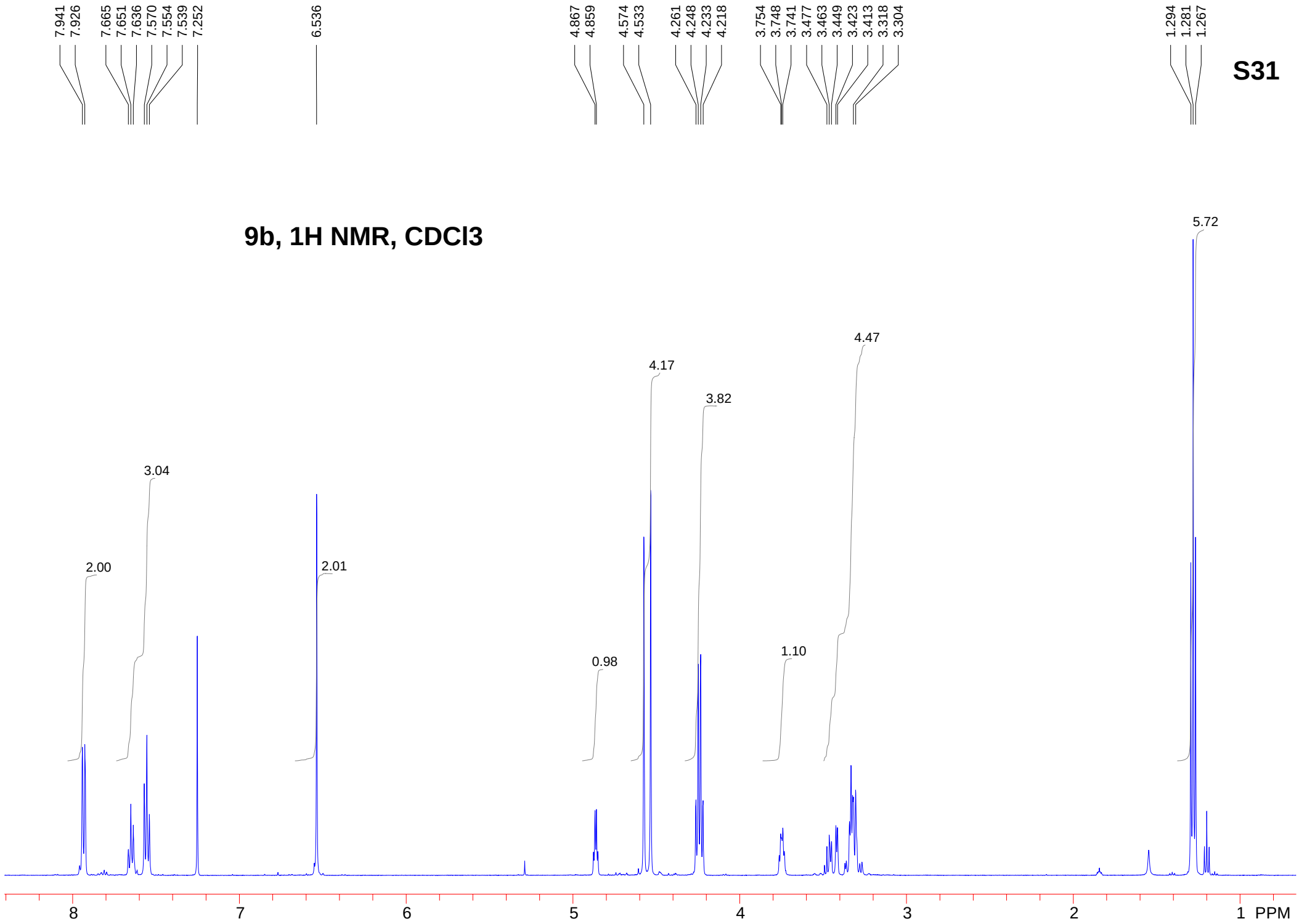

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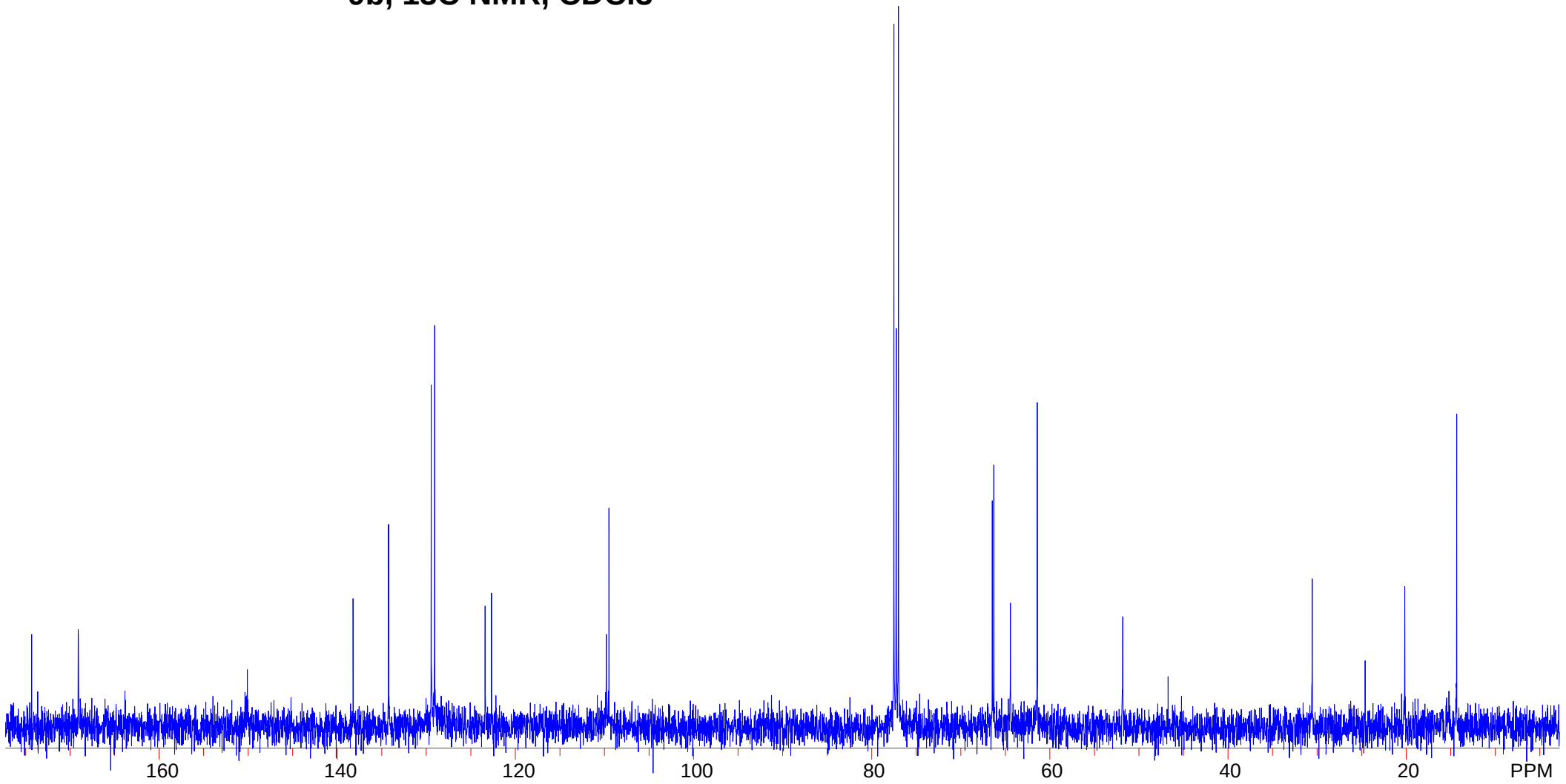
9b, 13C NMR, CDCl3



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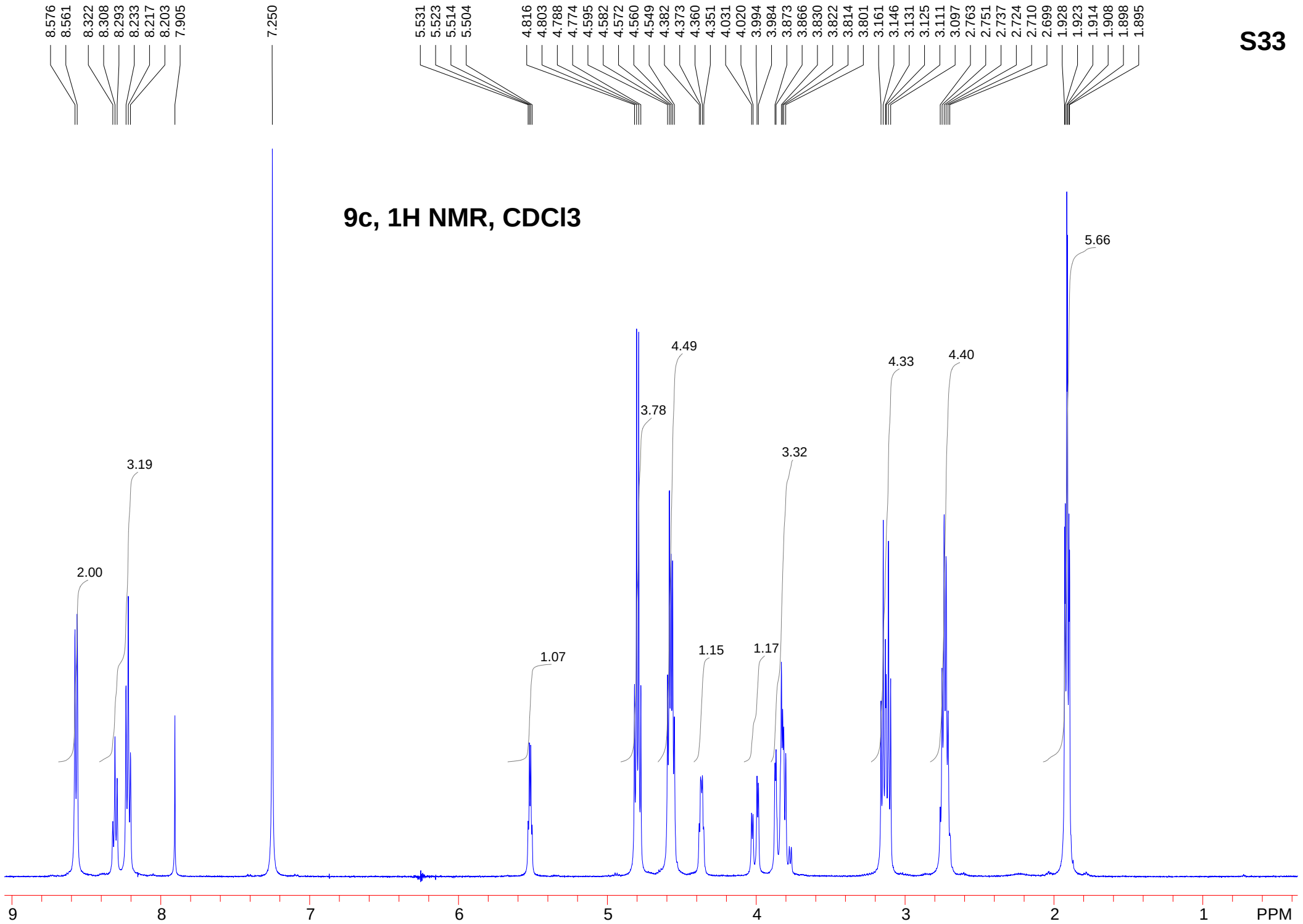

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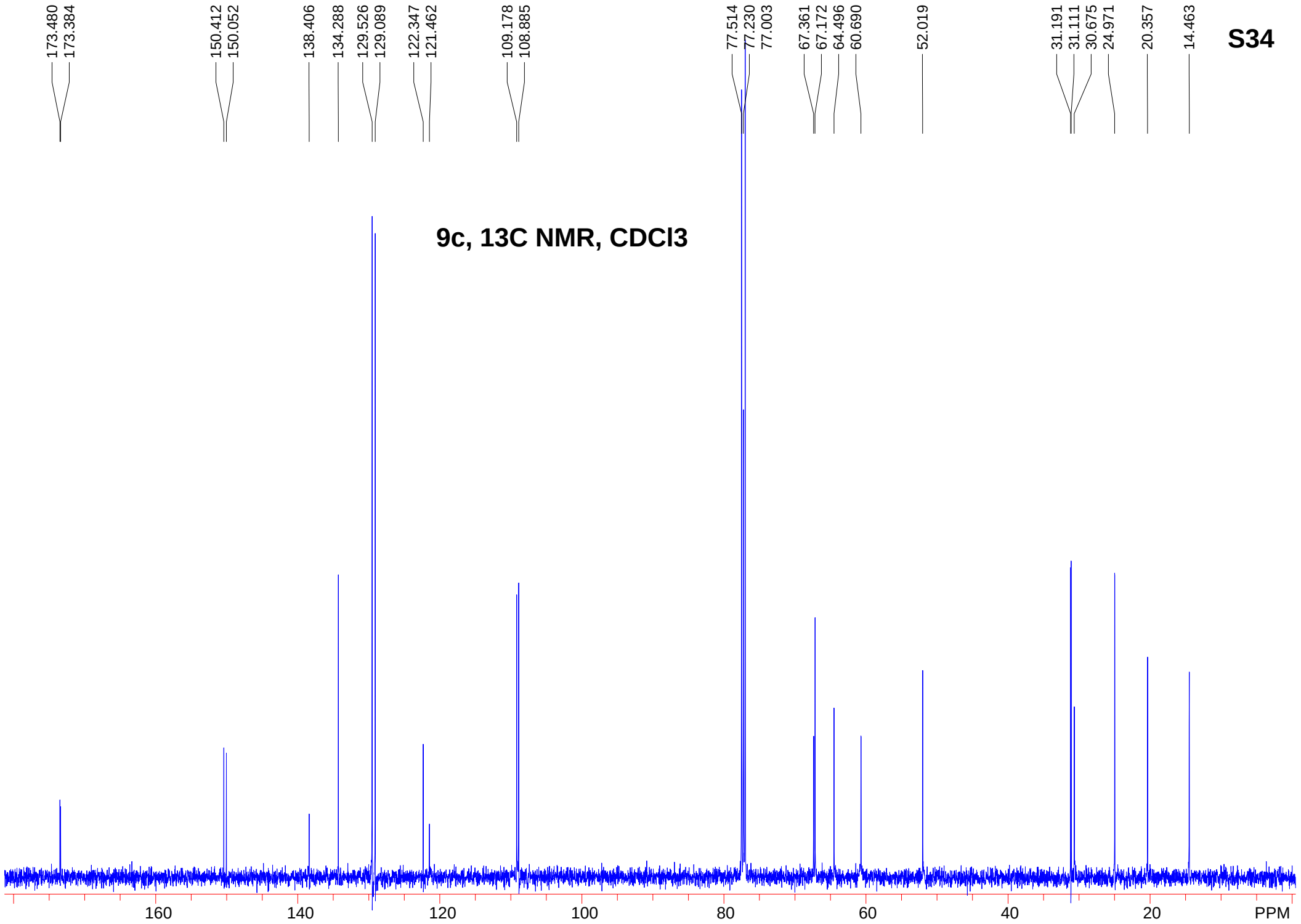
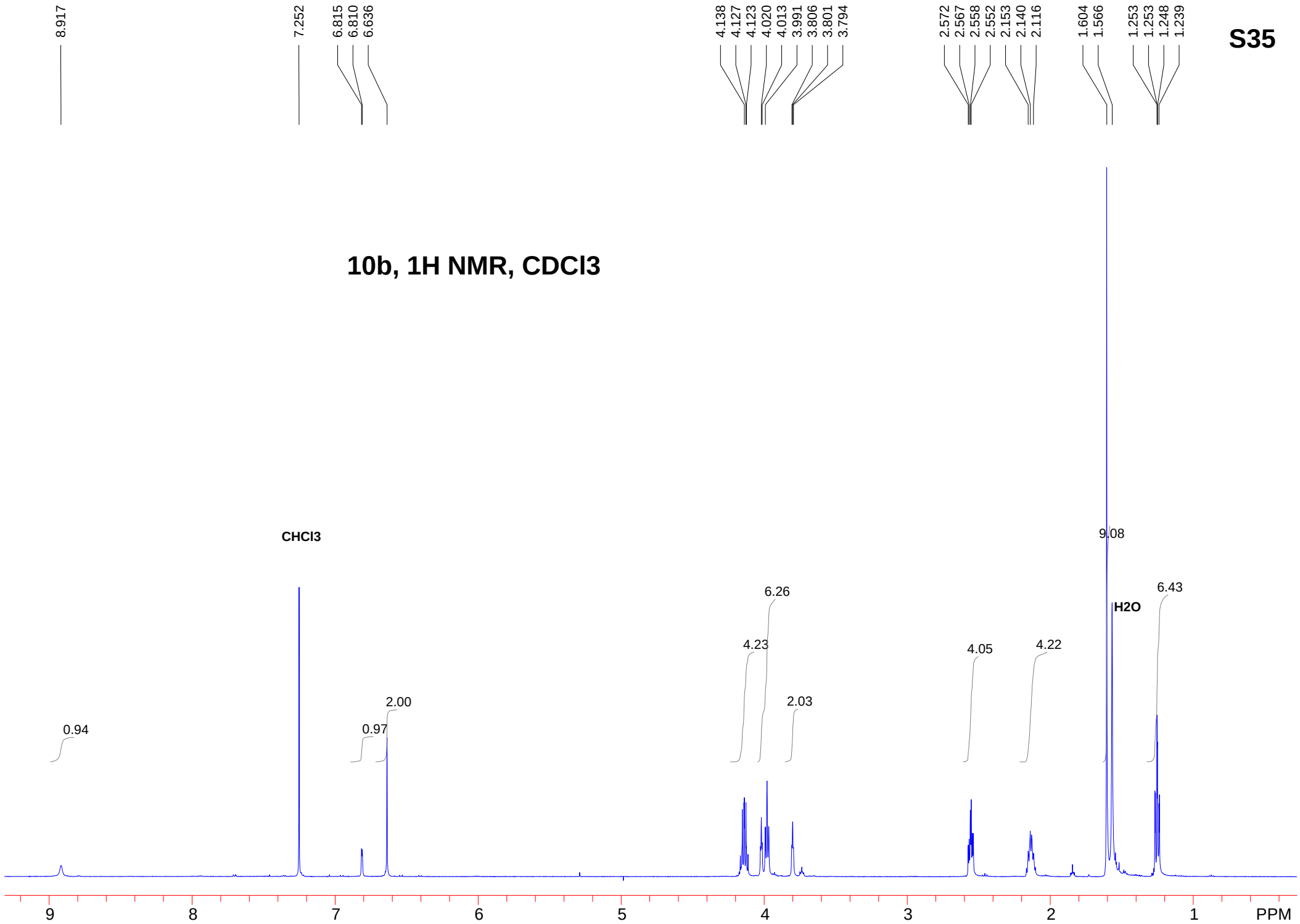


STANDARD CARBON PARAMETERS USER: -- DATE: Dec 20 2004

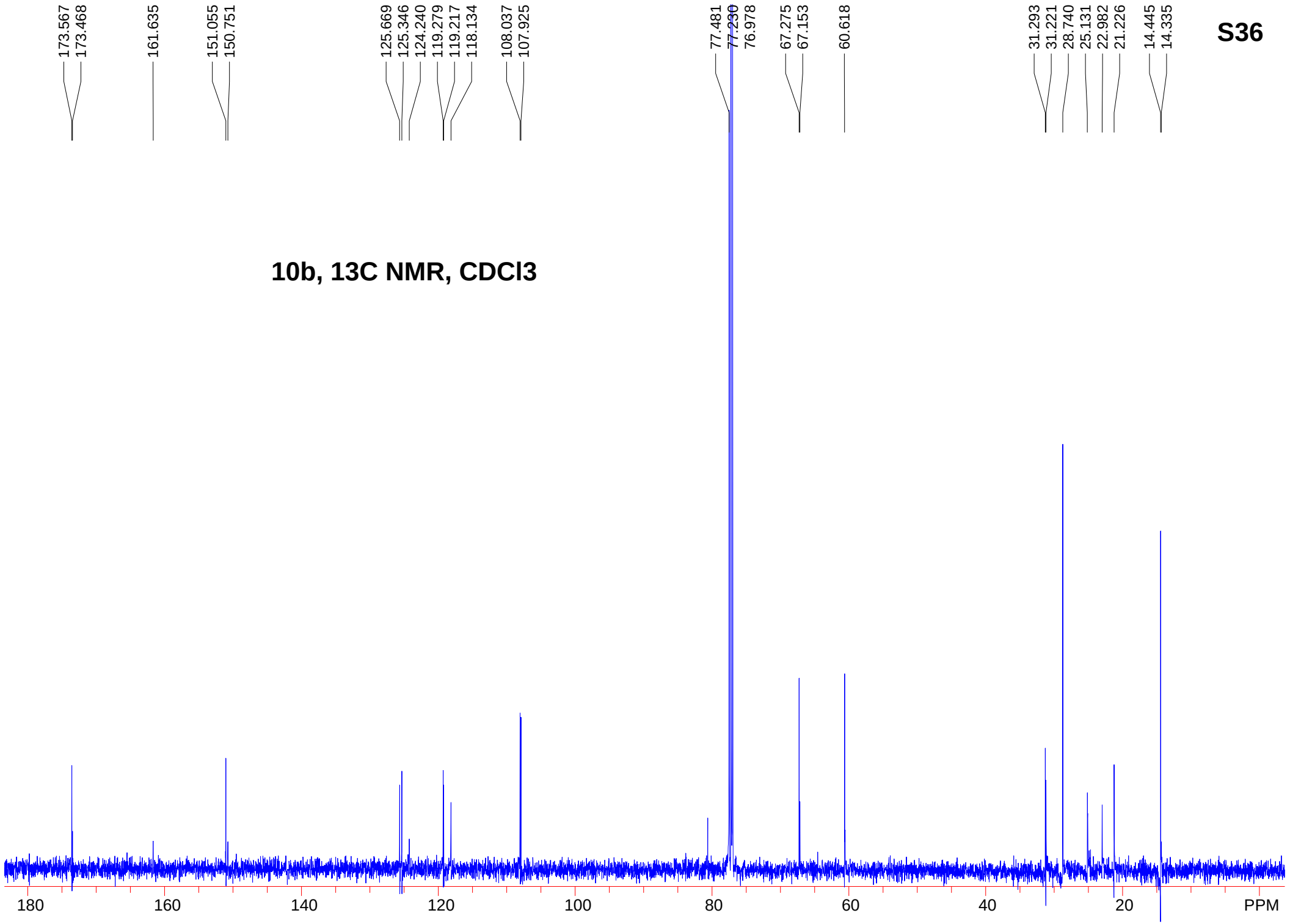
F1: 125.695	F2: 499.836	SW1: 25000		OF1: 11945.6		PTS1d: 8192
EX: s2pul		PW: 13.0 usec	PD: 2.0 sec	NA: 896	LB: 0.0	WinNuts - $of74_13C.fid



STANDARD PROTON PARAMETERS USER: -- DATE: Sep 16 2004

F1: 499.842	F2: 499.842	SW1: 20000		OF1: 2491.9		PTS1d: 32768
EX: s2pul		PW: 5.5 usec	PD: 0.0 sec	NA: 66	LB: 0.0	WinNuts - $of79_1c.fid

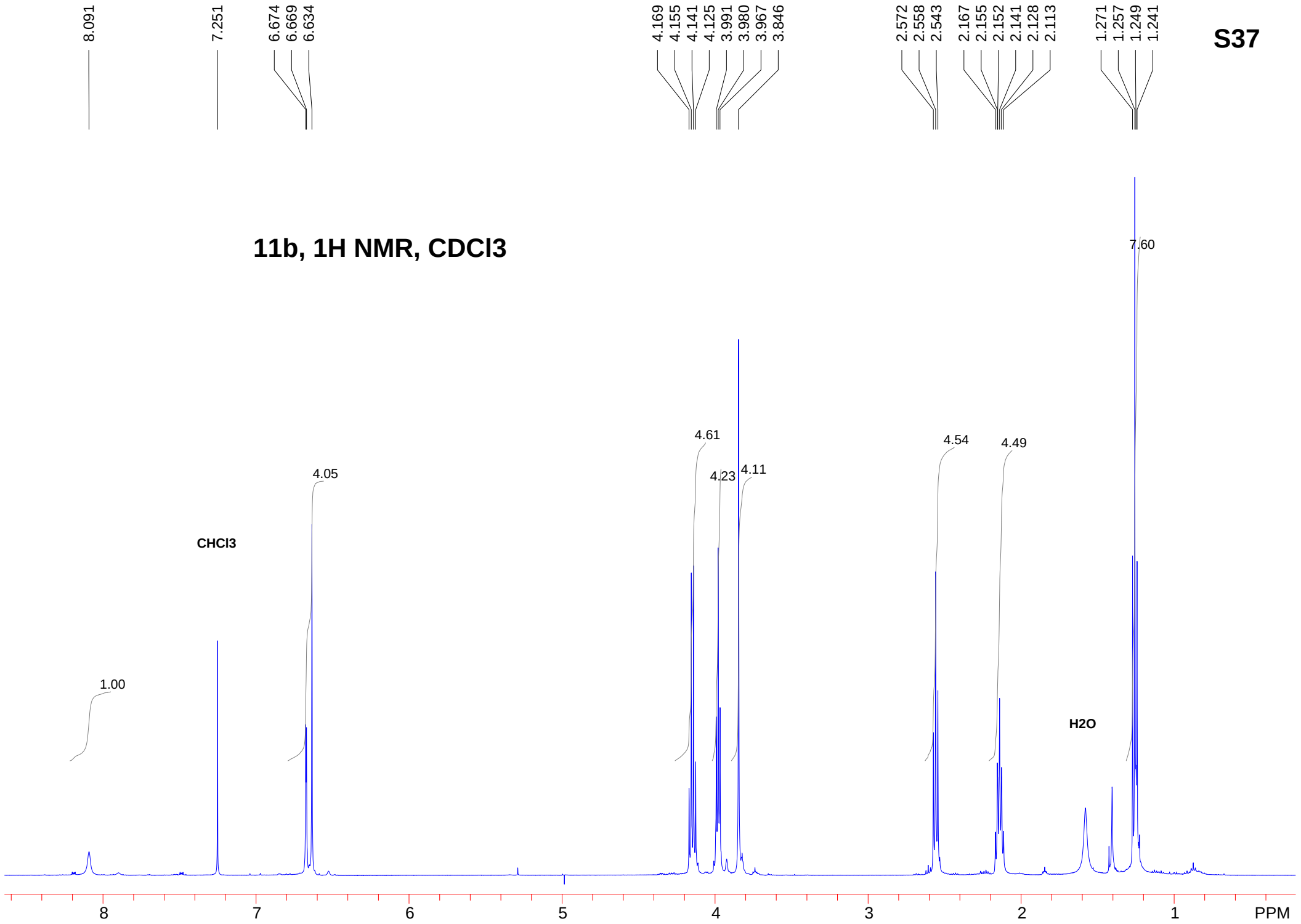
10b, 13C NMR, CDCl3



STANDARD CARBON PARAMETERS

USER: -- DATE: Sep 23 2004

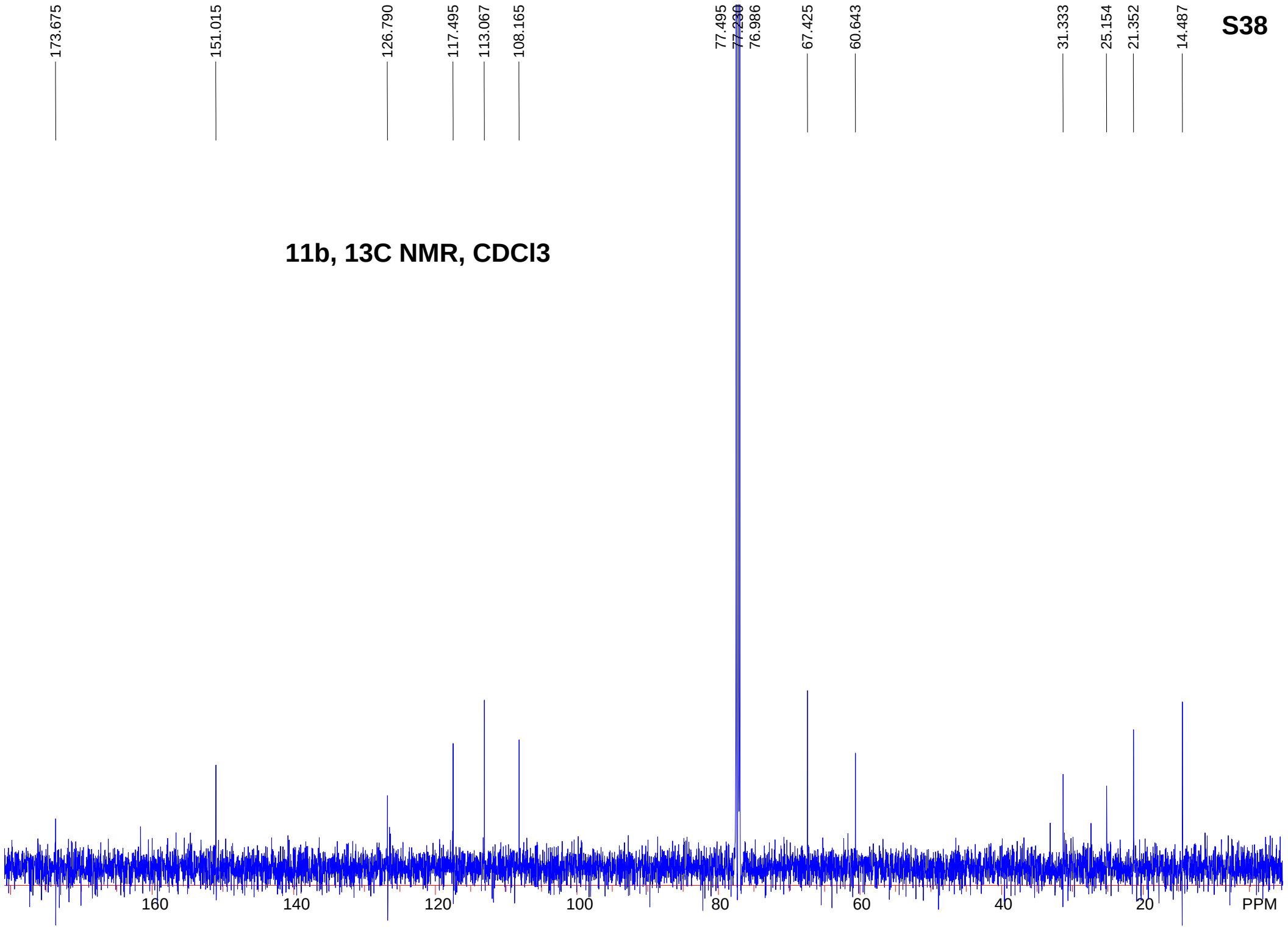
F1: 125.697	F2: 499.842	SW1: 25000		OF1: 11940.4		PTS1d: 8192
EX: s2pul		PW: 13.0 usec	PD: 2.0 sec	NA: 2302	LB: 0.0	WinNuts - $of79c_13C.fid



STANDARD PROTON PARAMETERS USER: -- DATE: Sep 16 2004

F1: 499.842	F2: 499.842	SW1: 20000		OF1: 2491.9		PTS1d: 32768
EX: s2pul		PW: 5.5 usec	PD: 0.0 sec	NA: 66	LB: 0.0	WinNuts - $of80.fid

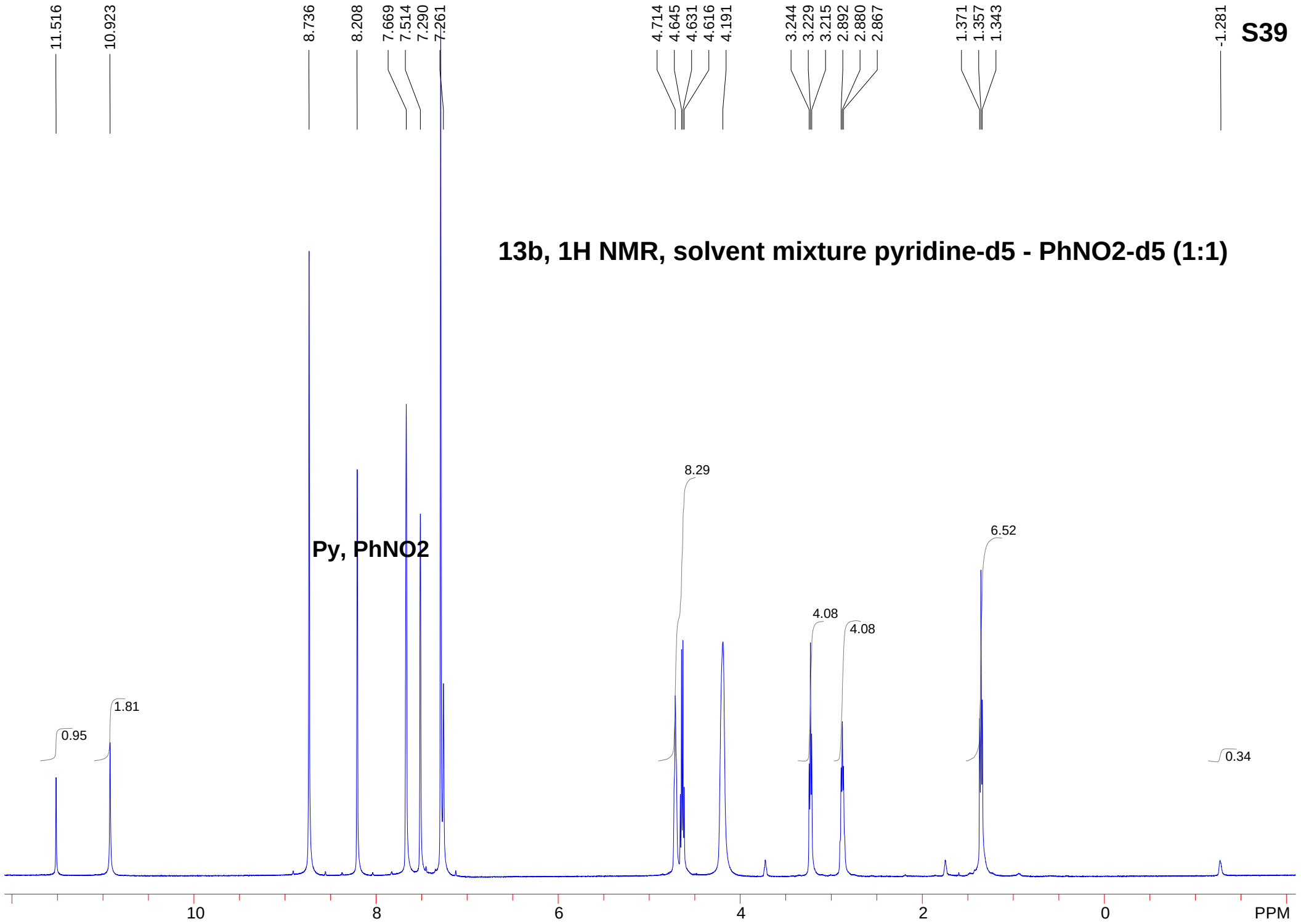
11b, 13C NMR, CDCl3



STANDARD CARBON PARAMETERS

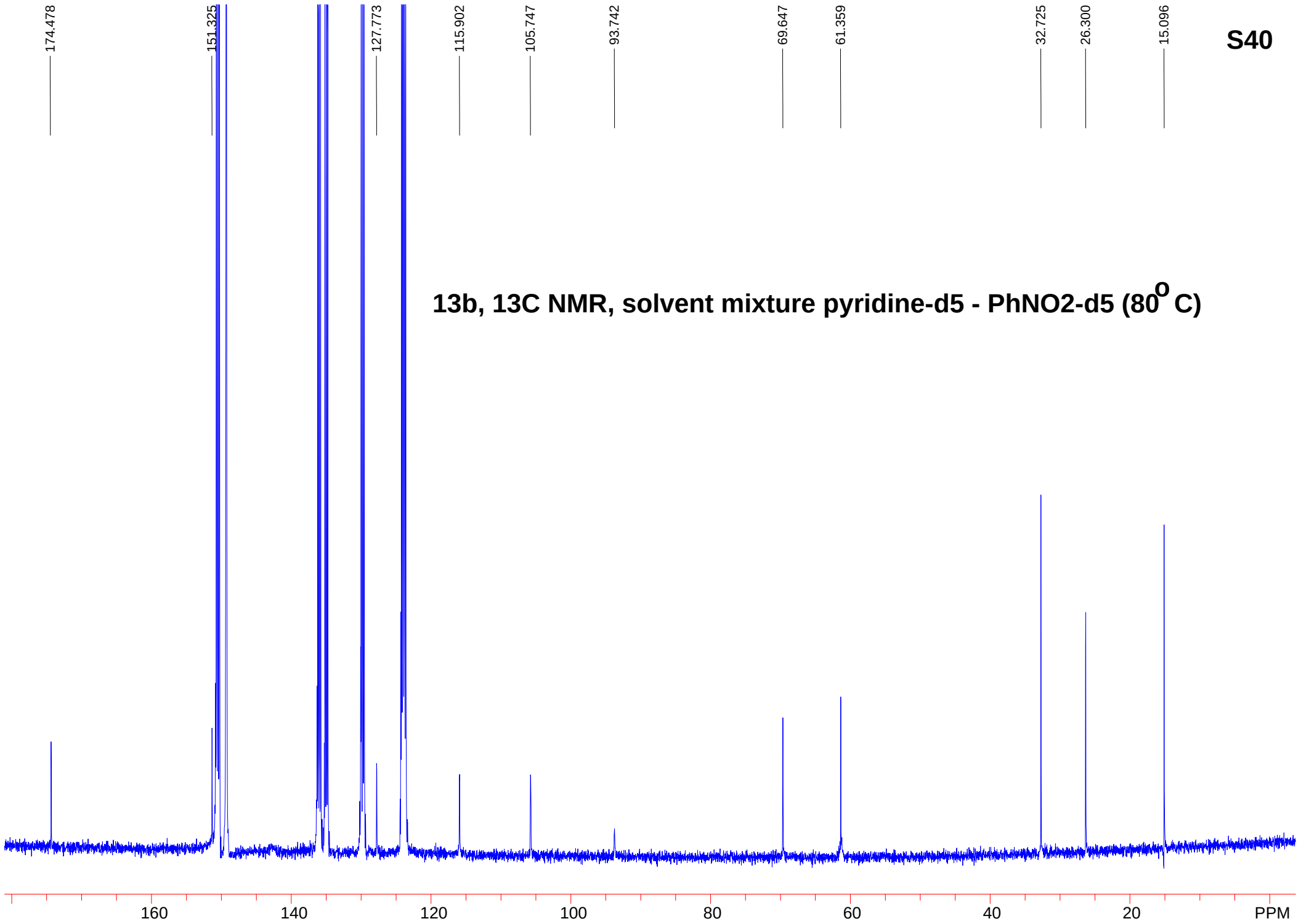
USER: -- DATE: Sep 16 2004

F1: 125.697	F2: 499.842	SW1: 25000		OF1: 11943.3		PTS1d: 8192
EX: s2pul		PW: 13.0 usec	PD: 2.0 sec	NA: 2050	LB: 0.0	WinNuts - $of80_13C.fid



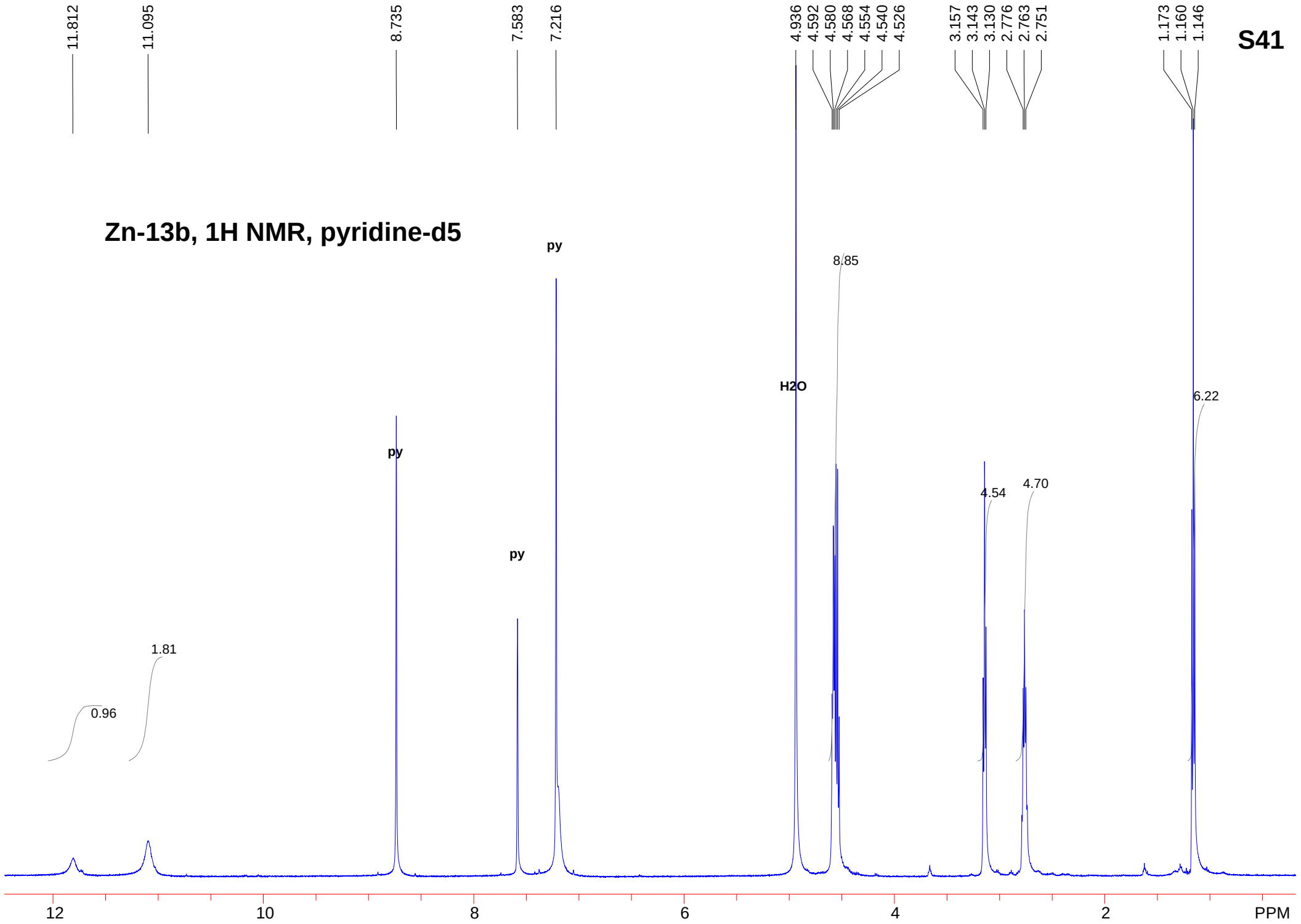
STANDARD 1H OBSERVE USER: -- DATE: Apr 14 2005

F1: 499.835	F2: 499.836	SW1: 8000		OF1: 2808.9		PTS1d: 16384
EX: s2pul		PW: 11.0 usec	PD: 1.0 sec	NA: 160	LB: 0.0	WinNuts - $of1i.fid



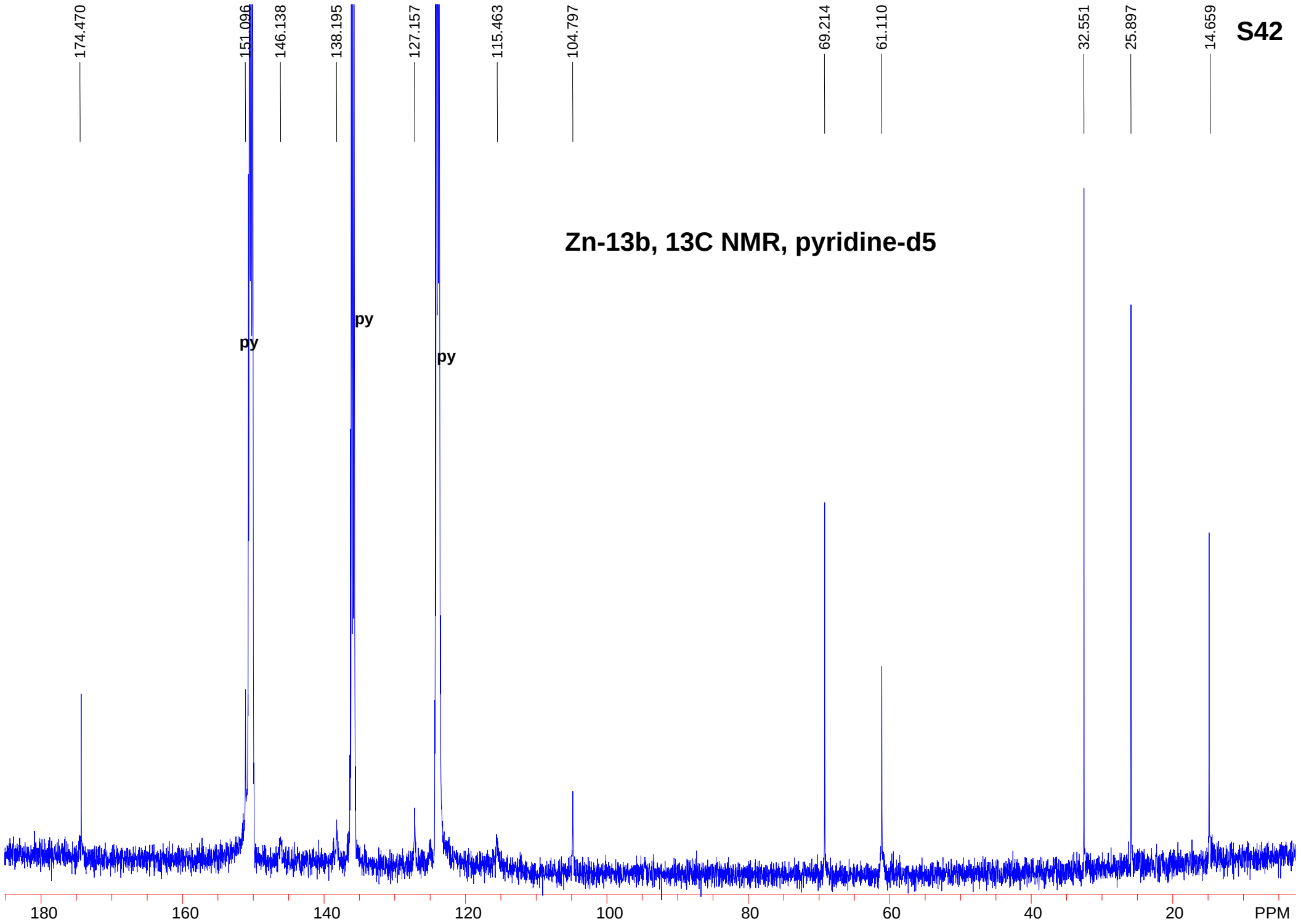
STANDARD CARBON PARAMETERS USER: -- DATE: Apr 15 2005

F1: 125.695	F2: 499.836	SW1: 25000		OF1: 12035.8		PTS1d: 8192
EX: s2pul		PW: 13.0 usec	PD: 2.0 sec	NA: 16928	LB: 0.0	WinNuts - $of1i_13C.fid



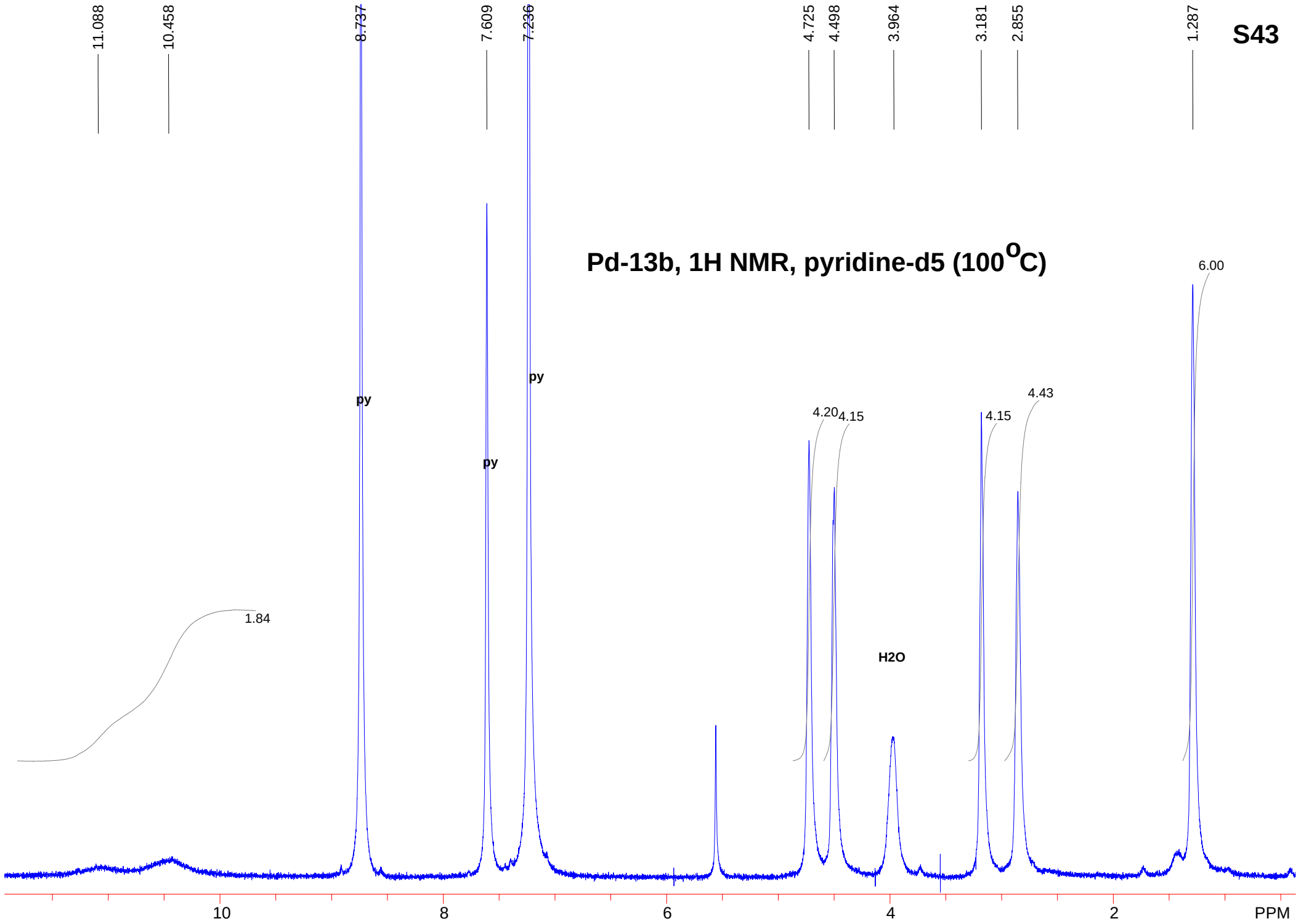
STANDARD 1H OBSERVE USER: -- DATE: Apr 12 2005

F1: 499.835	F2: 499.836	SW1: 8000		OF1: 2807.4		PTS1d: 16384
EX: s2pul		PW: 11.0 usec	PD: 1.0 sec	NA: 8	LB: 0.0	WinNuts - $of_2i.fid



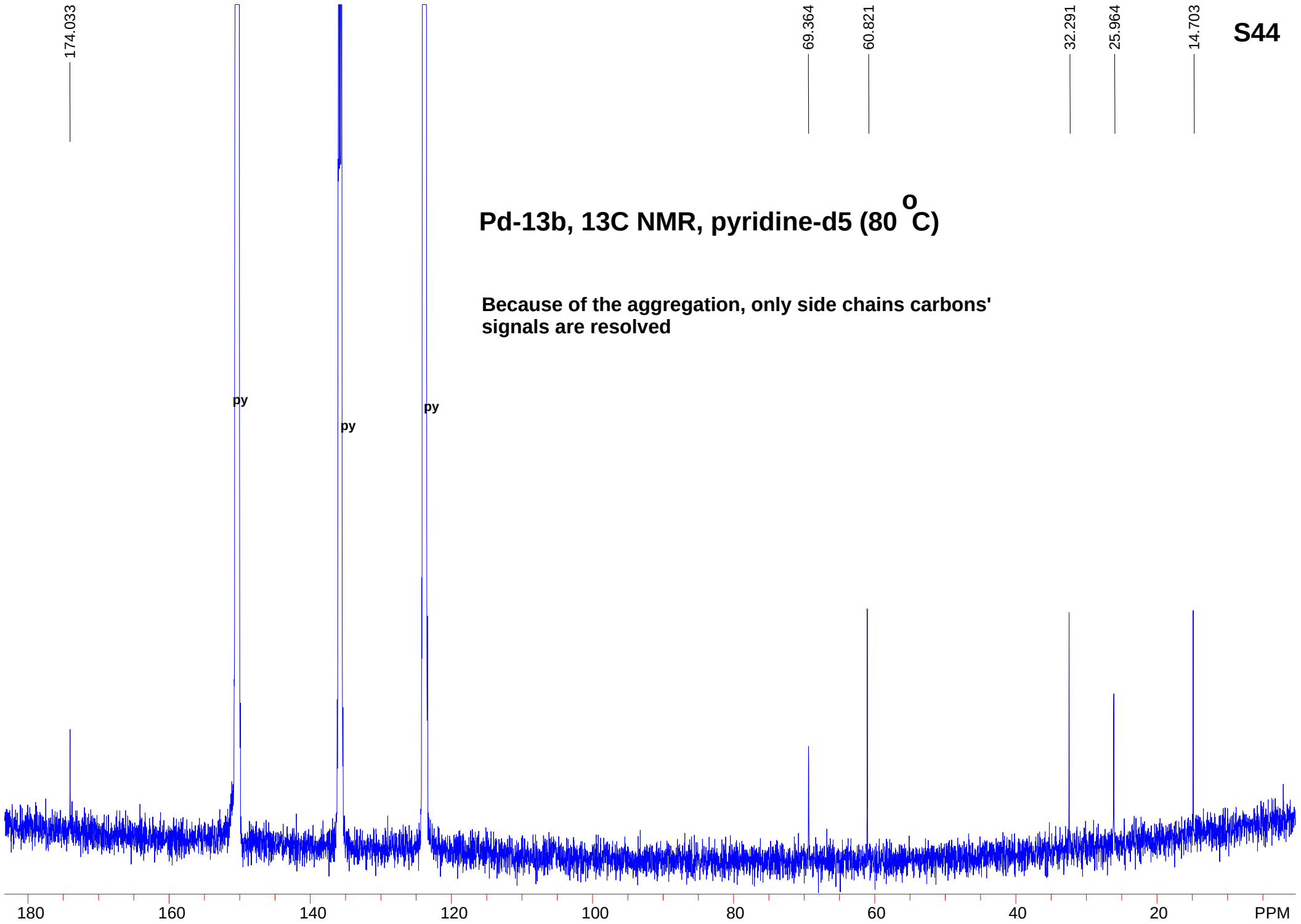
STANDARD CARBON PARAMETERS USER: -- DATE: Apr 12 2005

F1: 125.695	F2: 499.836	SW1: 25000		OF1: 12187.7		PTS1d: 8192
EX: s2pul		PW: 13.0 usec	PD: 2.0 sec	NA: 15168	LB: 0.0	WinNuts - $of2i_13C.fid



STANDARD 1H OBSERVE USER: -- DATE: Jul 26 2005

F1: 499.835	F2: 499.836	SW1: 8000		OF1: 2065.4		PTS1d: 16384
EX: s2pul		PW: 11.0 usec	PD: 1.0 sec	NA: 64	LB: 0.0	WinNuts - $13bPd_100.fid



Pd-13b, 13C NMR, pyridine-d5 (80 ^{o}C)

Because of the aggregation, only side chains carbons' signals are resolved

STANDARD CARBON PARAMETERS USER: -- DATE: Jul 26 2005

F1: 125.695	F2: 499.836	SW1: 25000		OF1: 12003.6		PTS1d: 8192	
EX: s2pul		PW: 13.0 usec	PD: 2.0 sec	NA: 14976	LB: 0.0		WinNuts - $13bPd_13C.fid