

Supporting Information for **B911439D**

Unprecedented cubane-type silver cluster with a novel phosphinite-functionalized *N*-heterocyclic carbene ligand

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- Crystal structure determination of **4** (Fig. S-1)
 - NMR spectra of compounds **1-4**.

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Crystal structure determination of **4**.

The two independent molecules show a very similar structure. Their overlapped structures (blue and red spheres) are shown below (Fig. S-1).

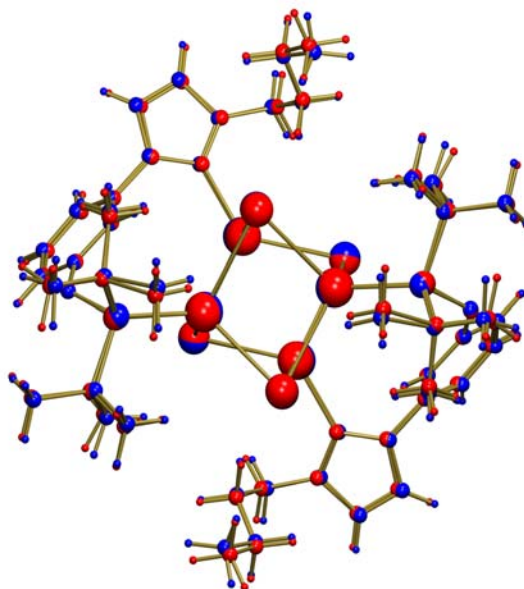
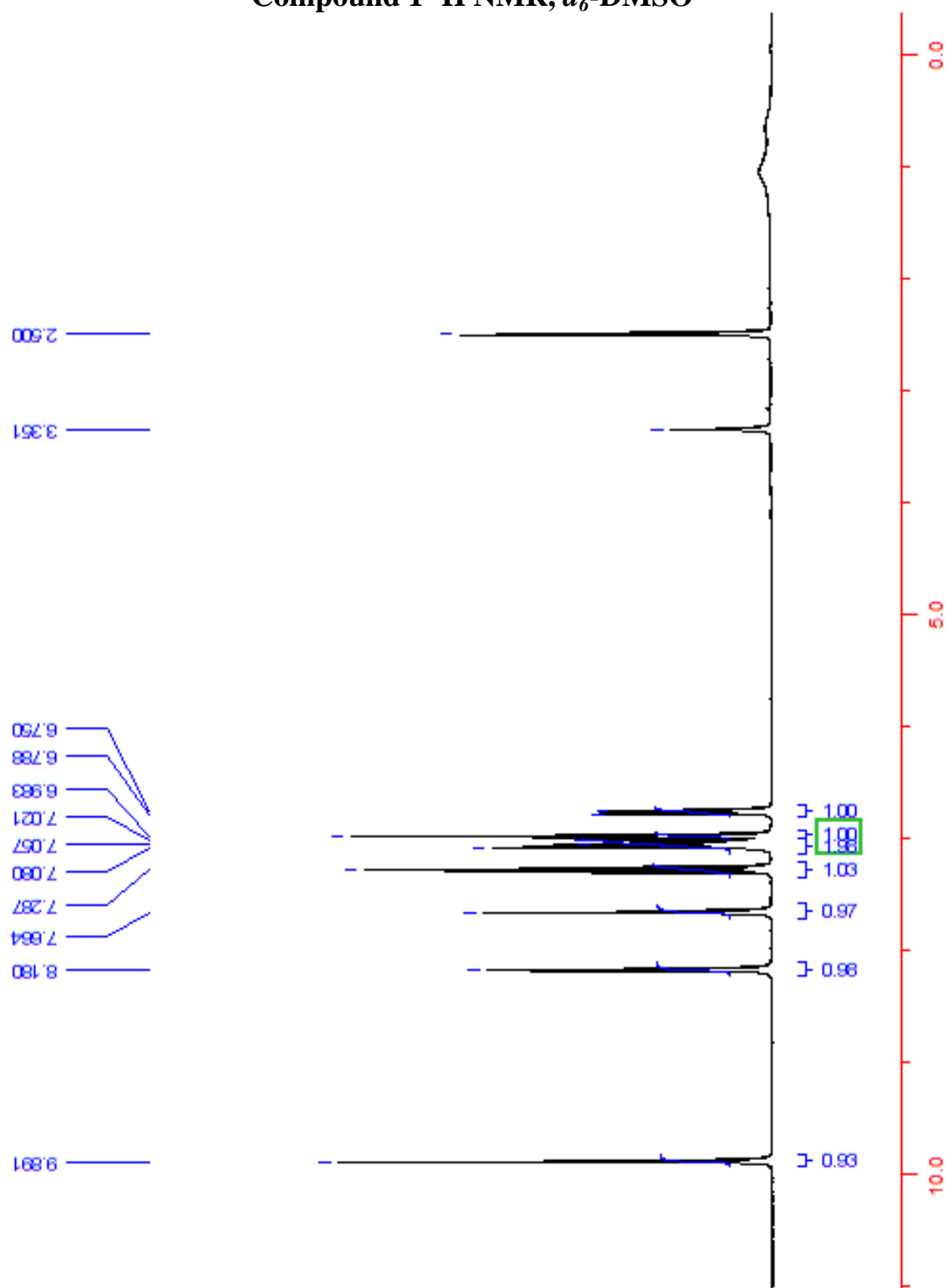


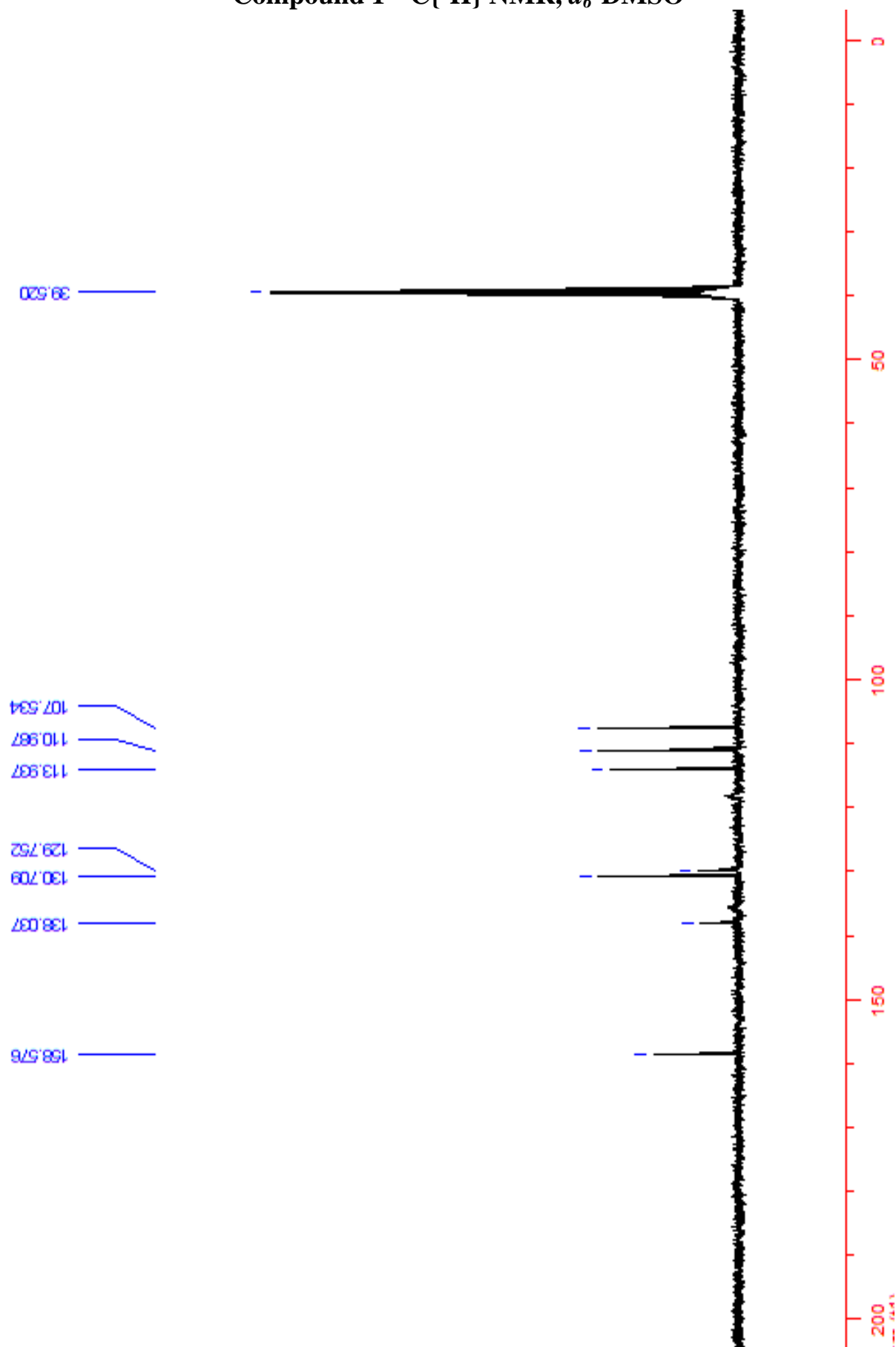
Fig. S-1. View of the overlapped structures of the two independent molecules of **4** which show a very similar structure.

NMR spectra of compounds 1-4.

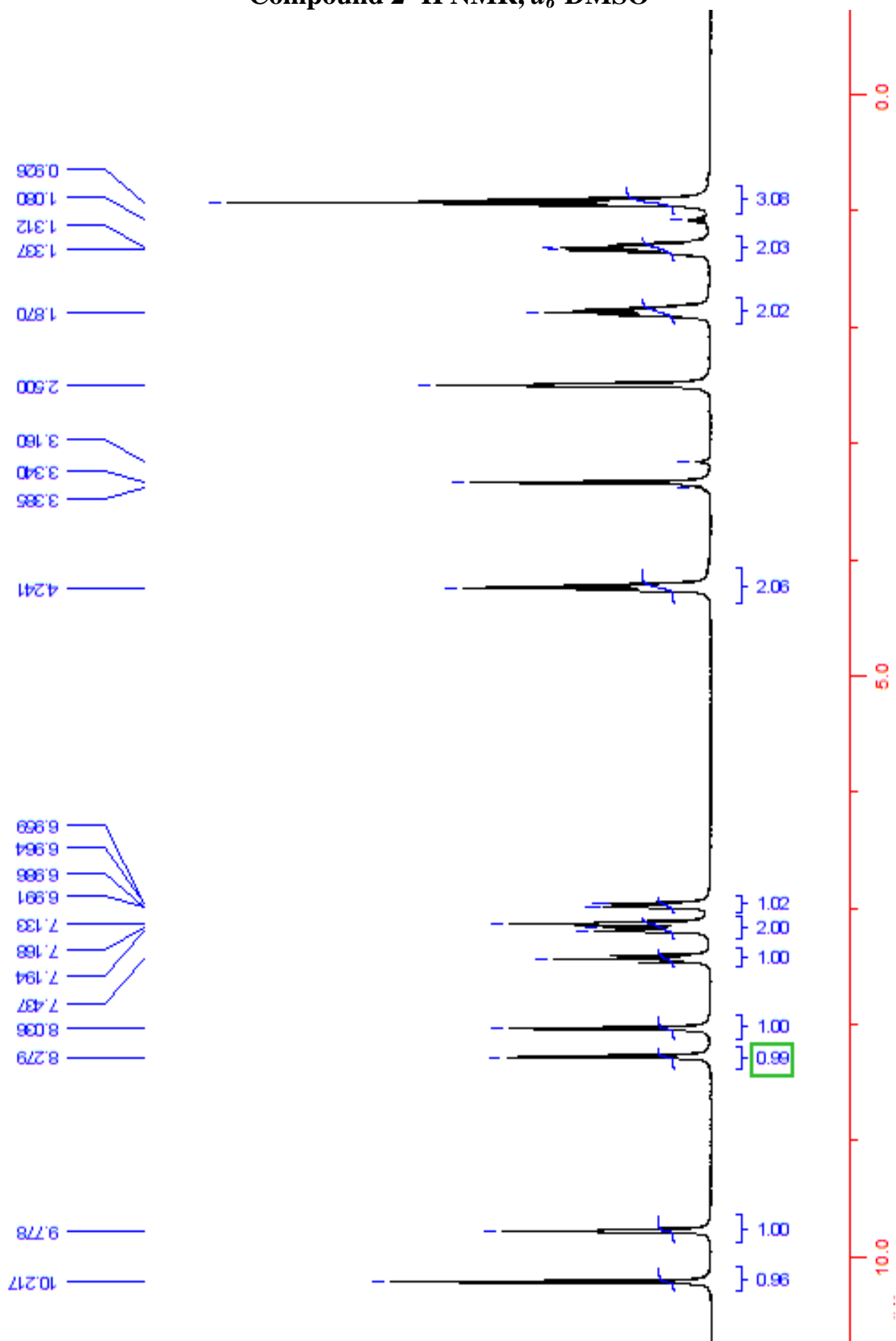
Compound 1 ^1H NMR, d_6 -DMSO



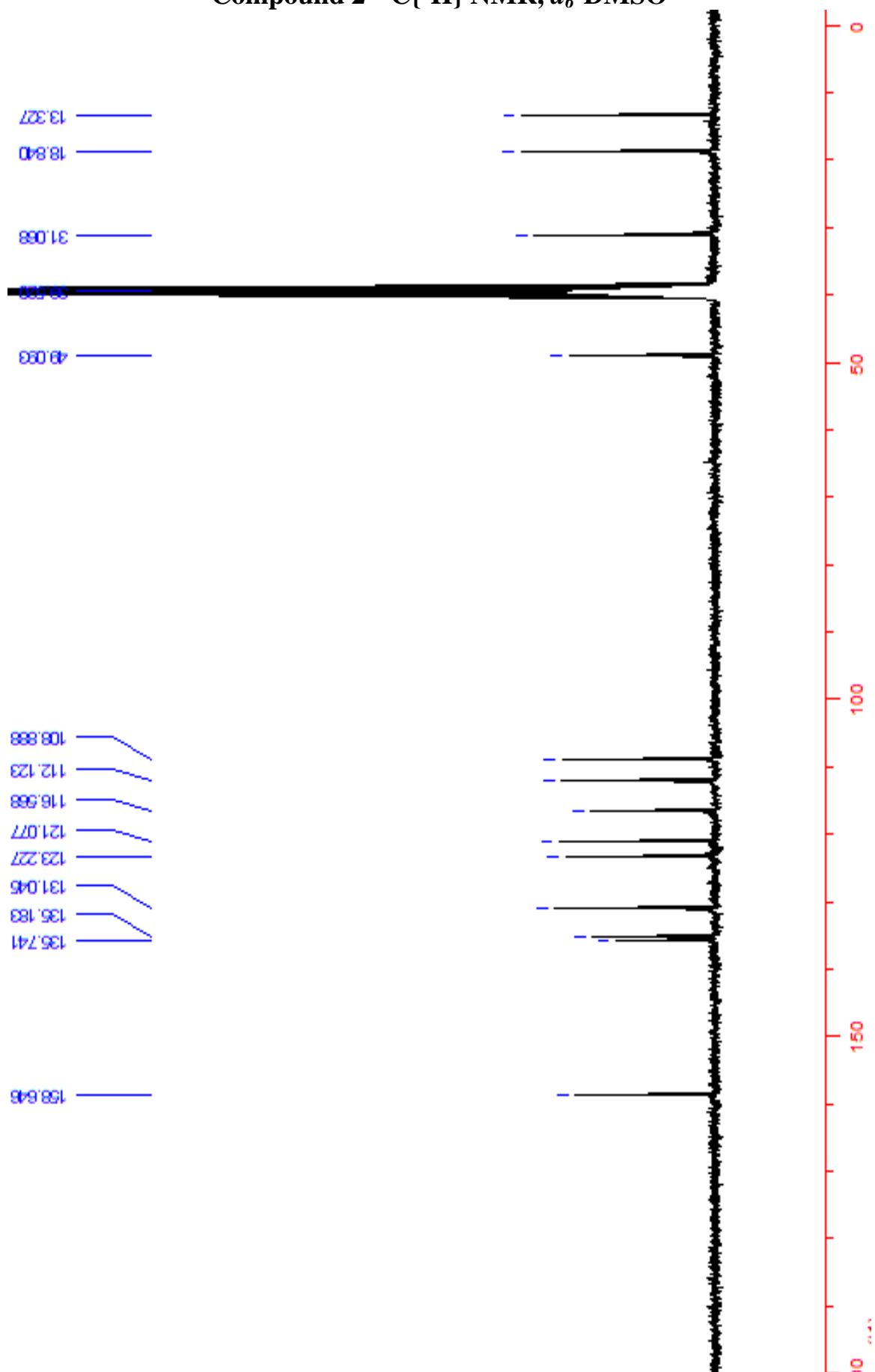
Compound 1 $^{13}\text{C}\{^1\text{H}\}$ NMR, d_6 -DMSO



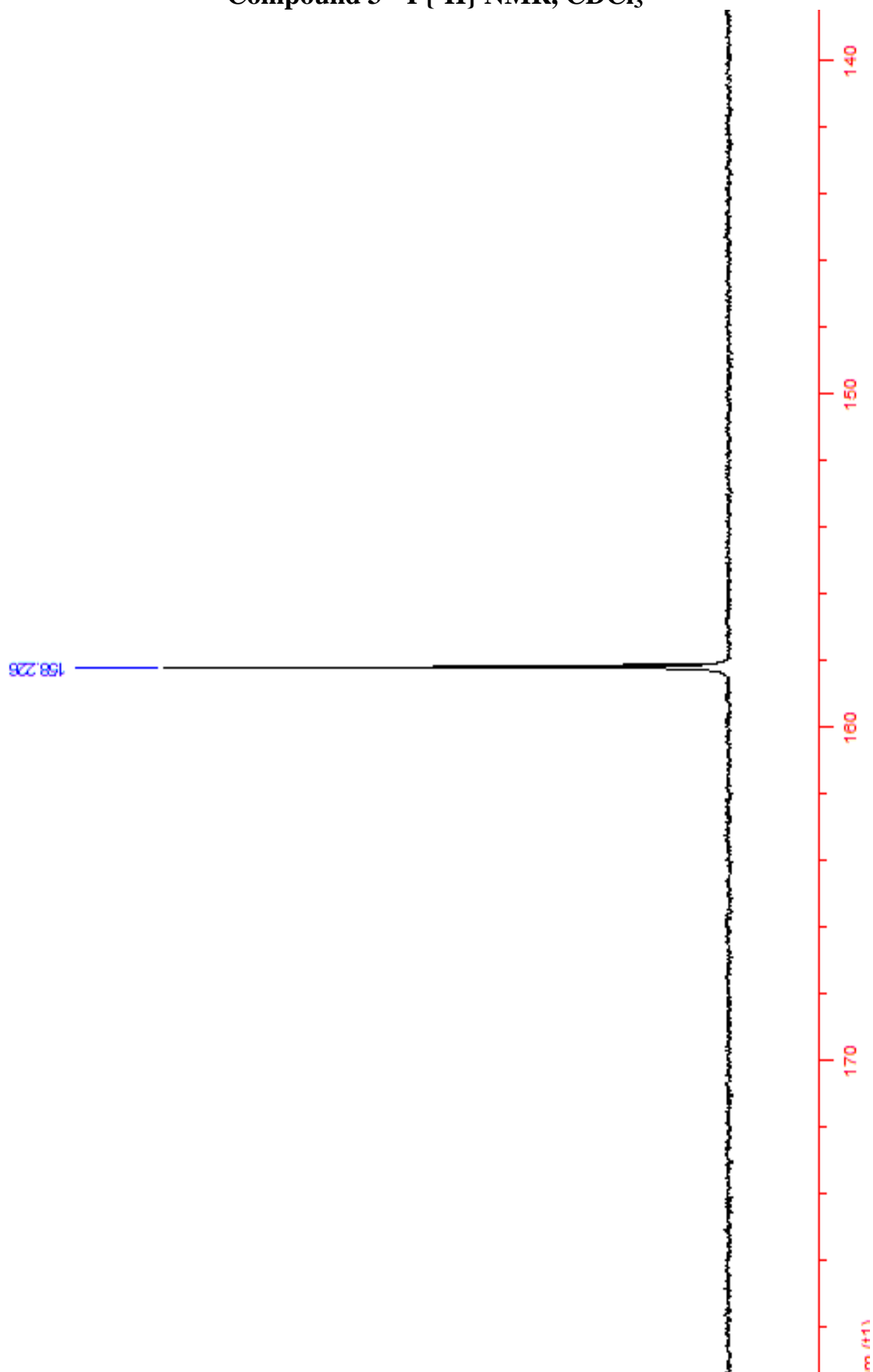
Compound 2 ^1H NMR, d_6 -DMSO



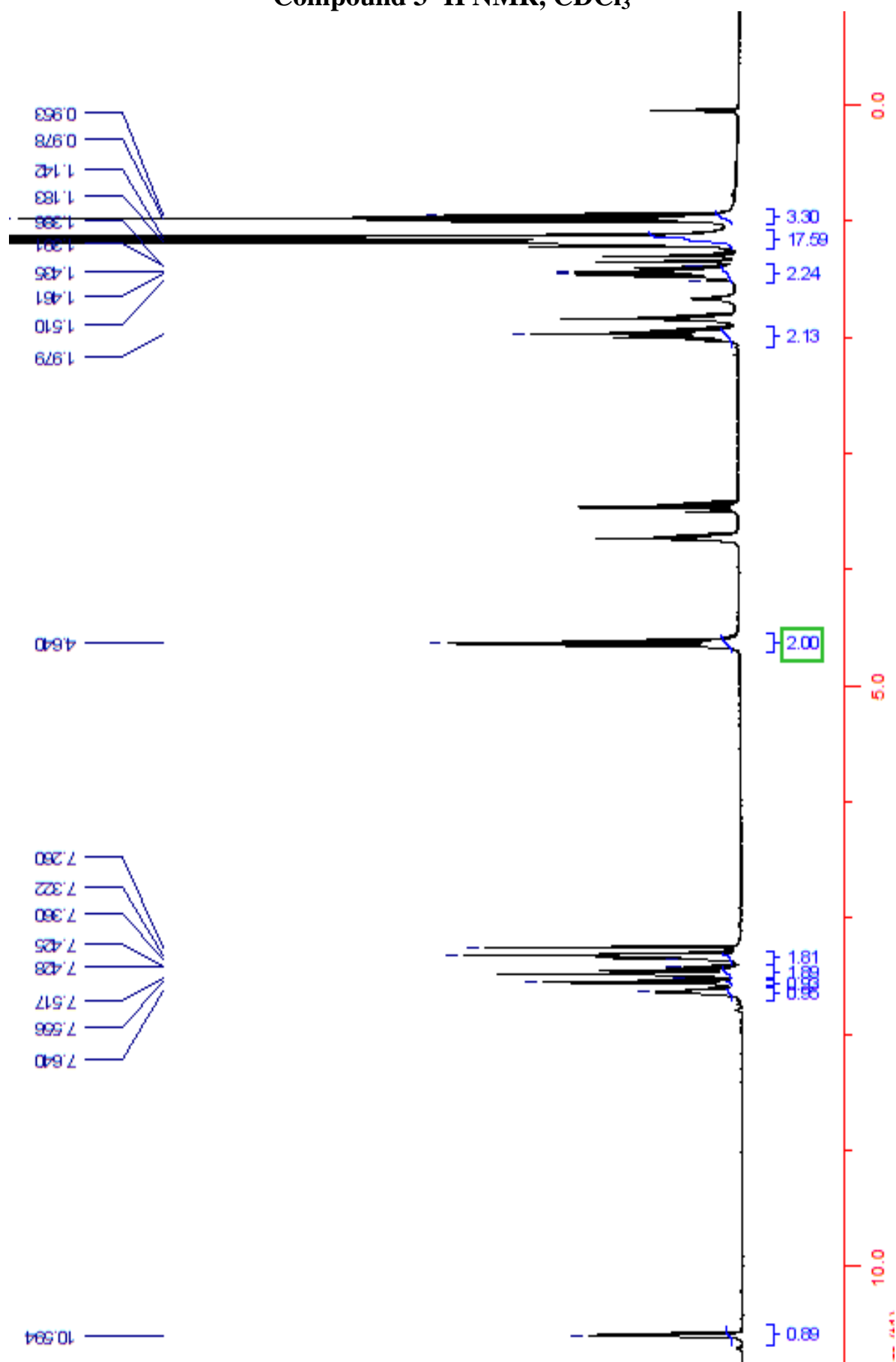
Compound 2 $^{13}\text{C}\{^1\text{H}\}$ NMR, d_6 -DMSO



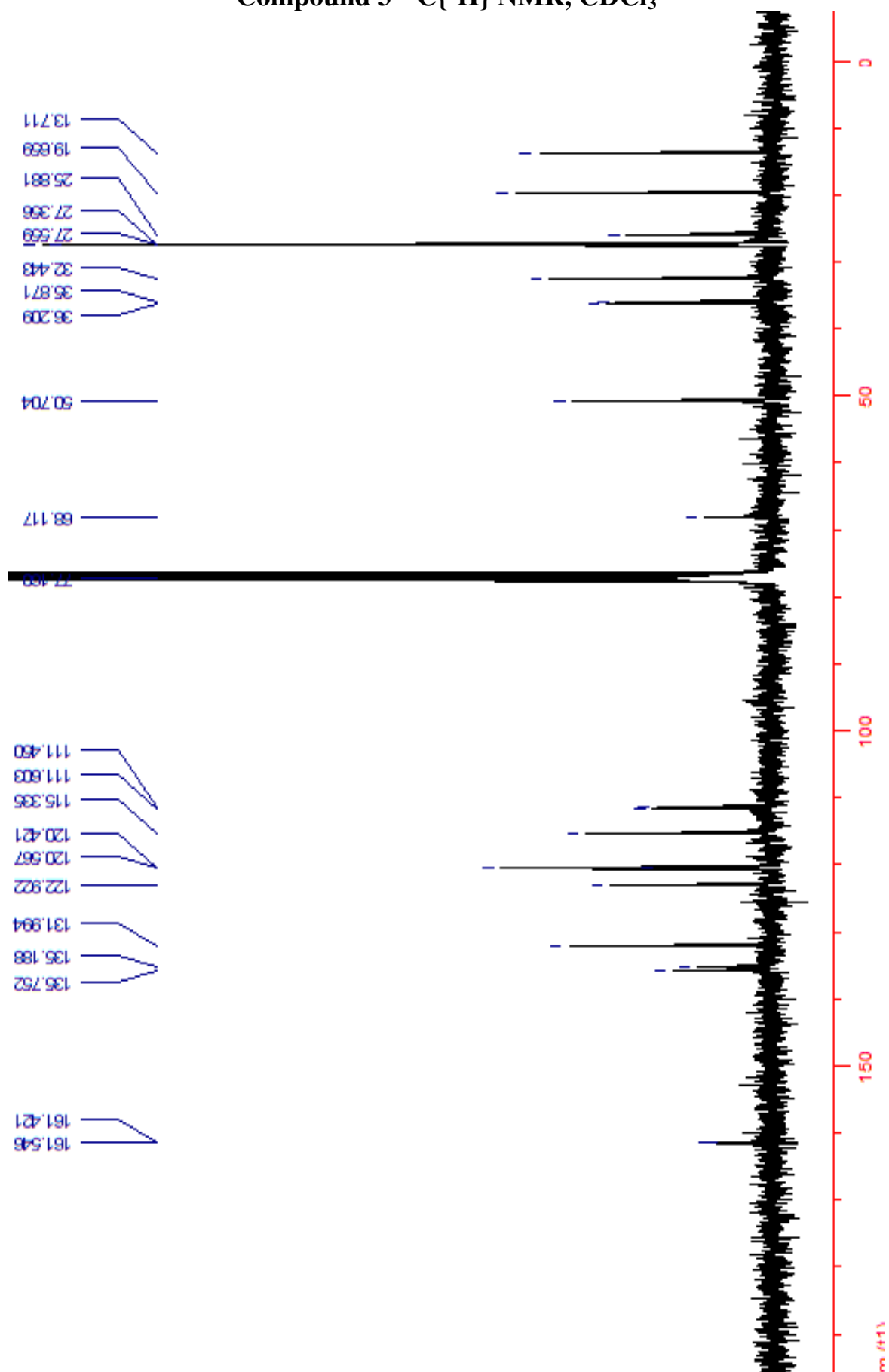
Compound 3 $^{31}\text{P}\{^1\text{H}\}$ NMR, CDCl_3



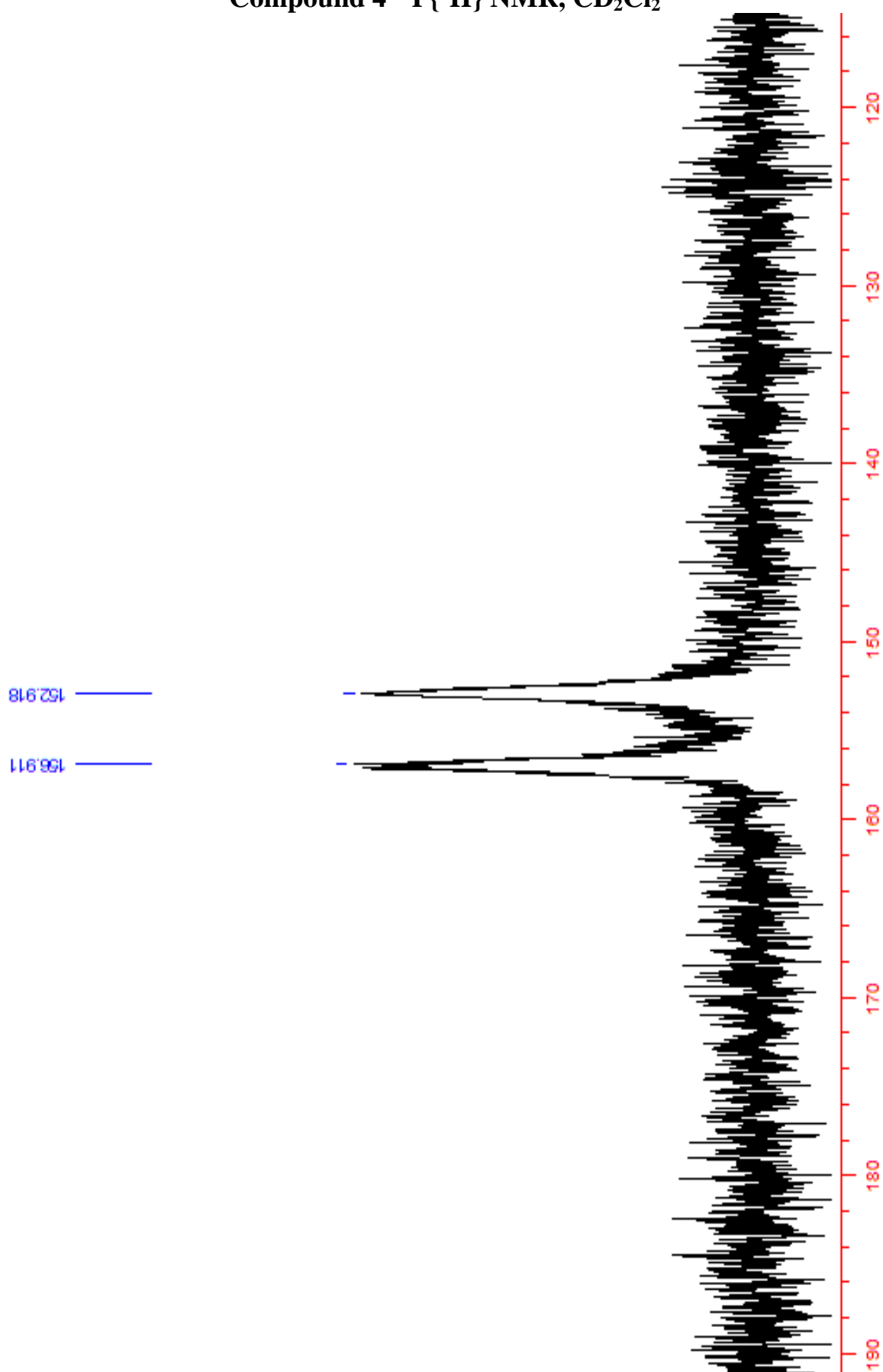
Compound 3 ^1H NMR, CDCl_3



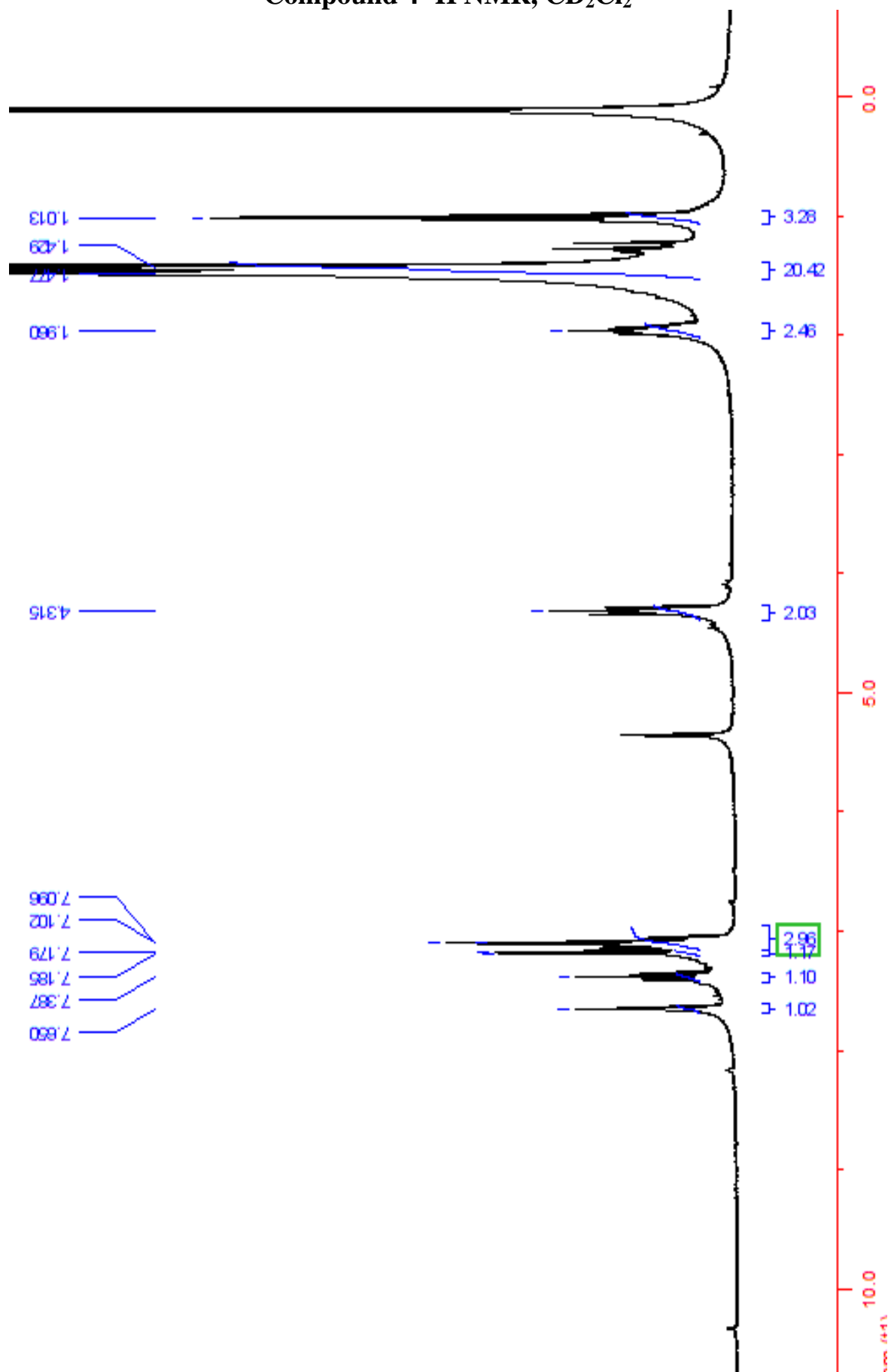
Compound 3 $^{13}\text{C}\{^1\text{H}\}$ NMR, CDCl_3



Compound 4 $^{31}\text{P}\{^1\text{H}\}$ NMR, CD_2Cl_2



Compound 4 ^1H NMR, CD_2Cl_2



Compound 4 $^{13}\text{C}\{^1\text{H}\}$ NMR, CD_2Cl_2

