

C8953
NMR strukturní analýza
seminář

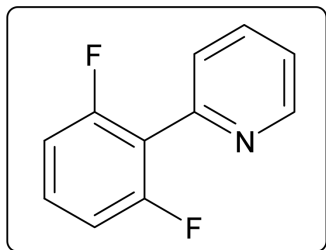
Heteronuclear correlations

Jan Novotný

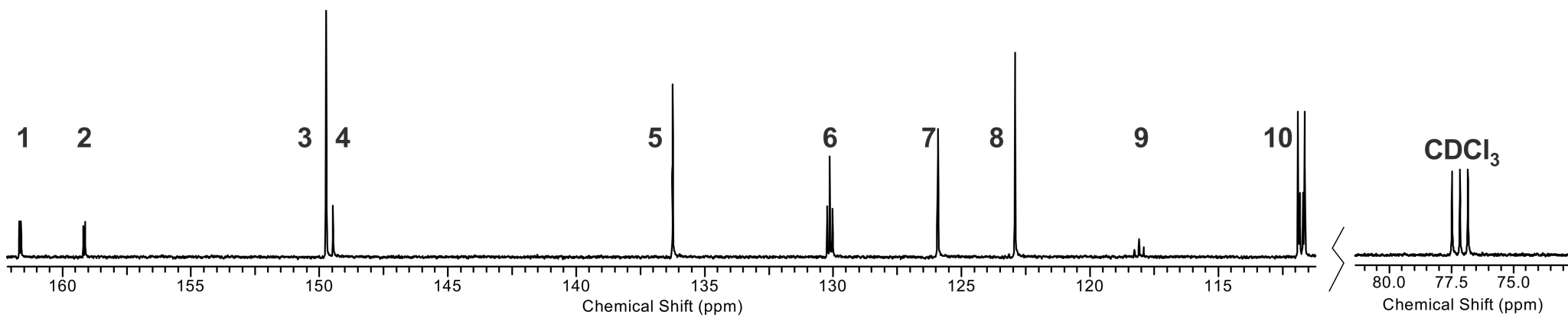
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1D ^{13}C NMR



100 MHz, CDCl_3



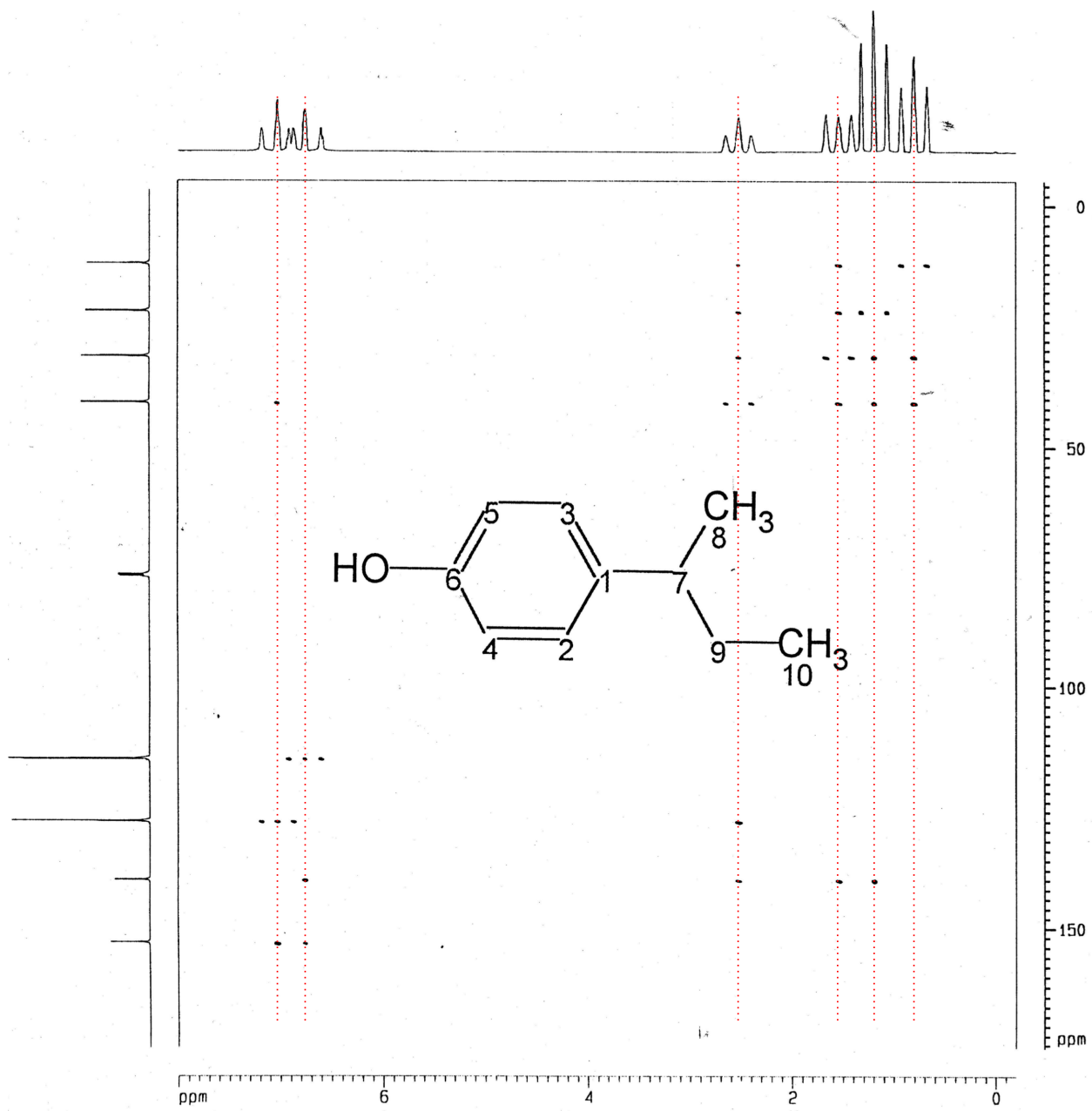
Polarization transfer

- ▶ bigger population difference of ^1H nucleus is transferred via J-coupling to less sensitive nucleus X (^{13}C , ^{15}N)
- ▶ fundamental building block of heteronuclear correlation experiments: in 2D-HX experiment each crosspeak manifests interaction of H and X nucleus coupled through bonds
- ▶ **Task: Draw the evolution of magnetization during basic INEPT pulse sequence. Consider C-H interacting pair.**

Practical notes $^1\text{H-X}$ HSQC

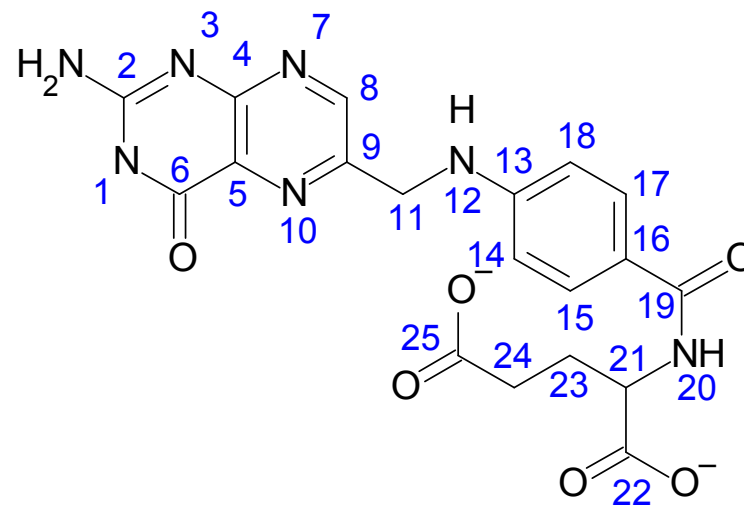
- ▶ resolution of overlaps
- ▶ routine experiments to control biomolecular sample
- ▶ easy identification of geminal protons
- ▶ indirect determination of protons bonded to NMR inactive heteroatom
- ▶ heteronuclear correlation \Rightarrow no diagonal crosspeak, no symmetry
- ▶ X decoupled during acquisition \Rightarrow singlet crosspeak

^1H - ^{13}C HMBC + ^1H - ^{13}C HSQC

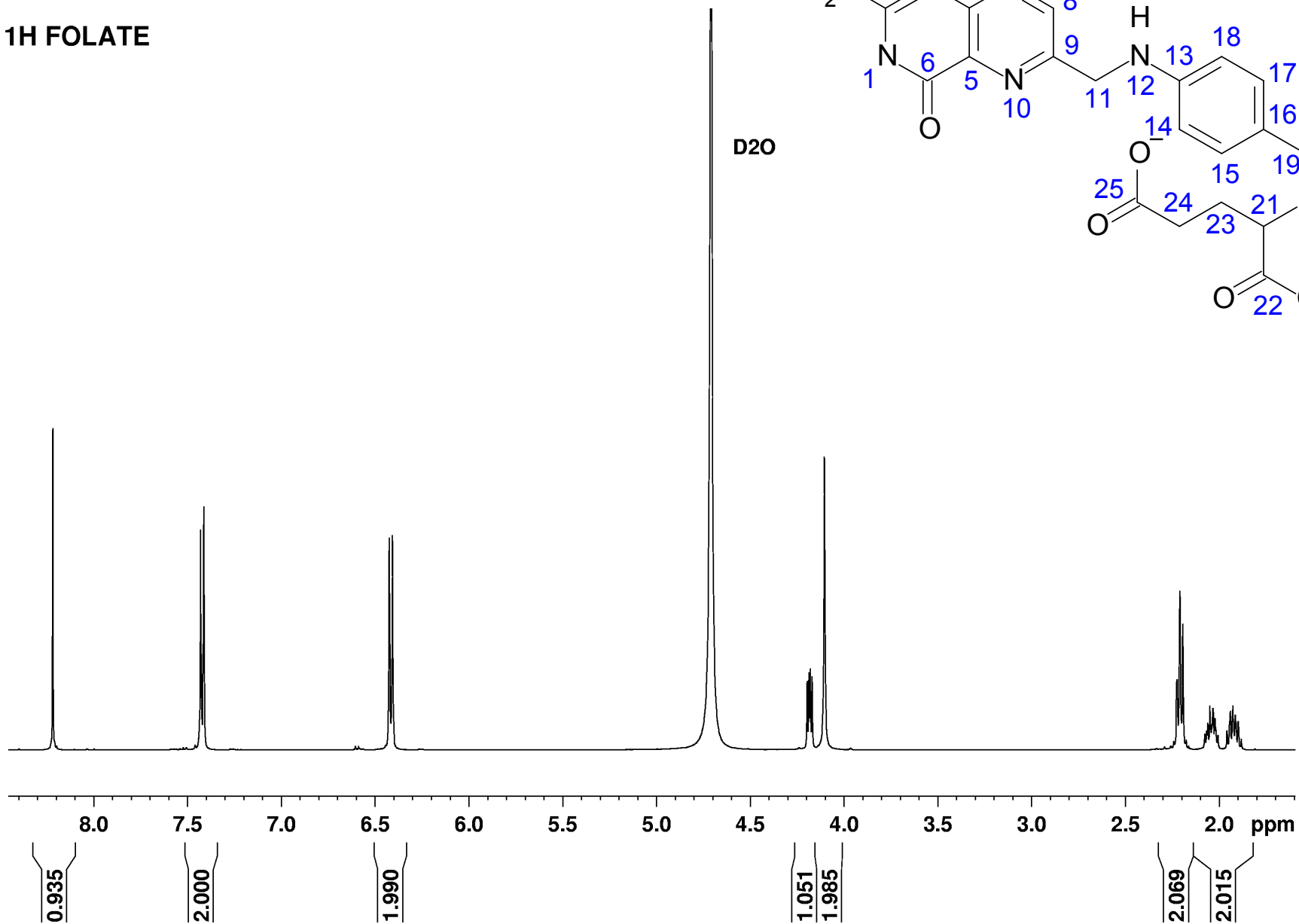


Folic Acid: ^1H 1D

1H FOLATE

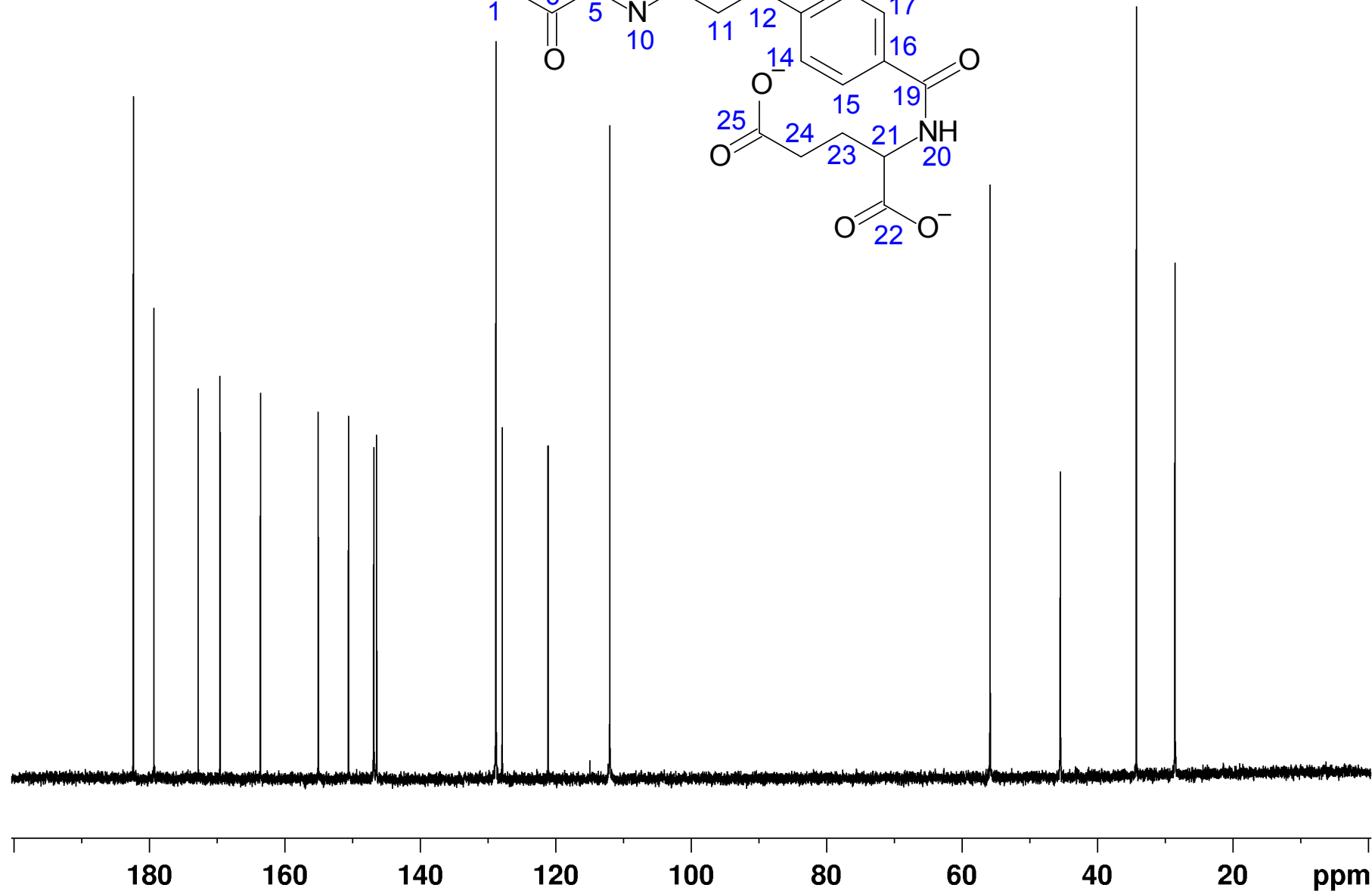
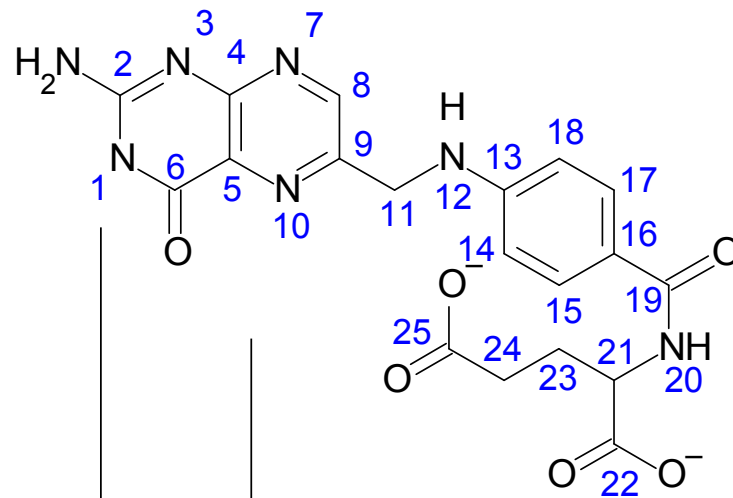


D2O

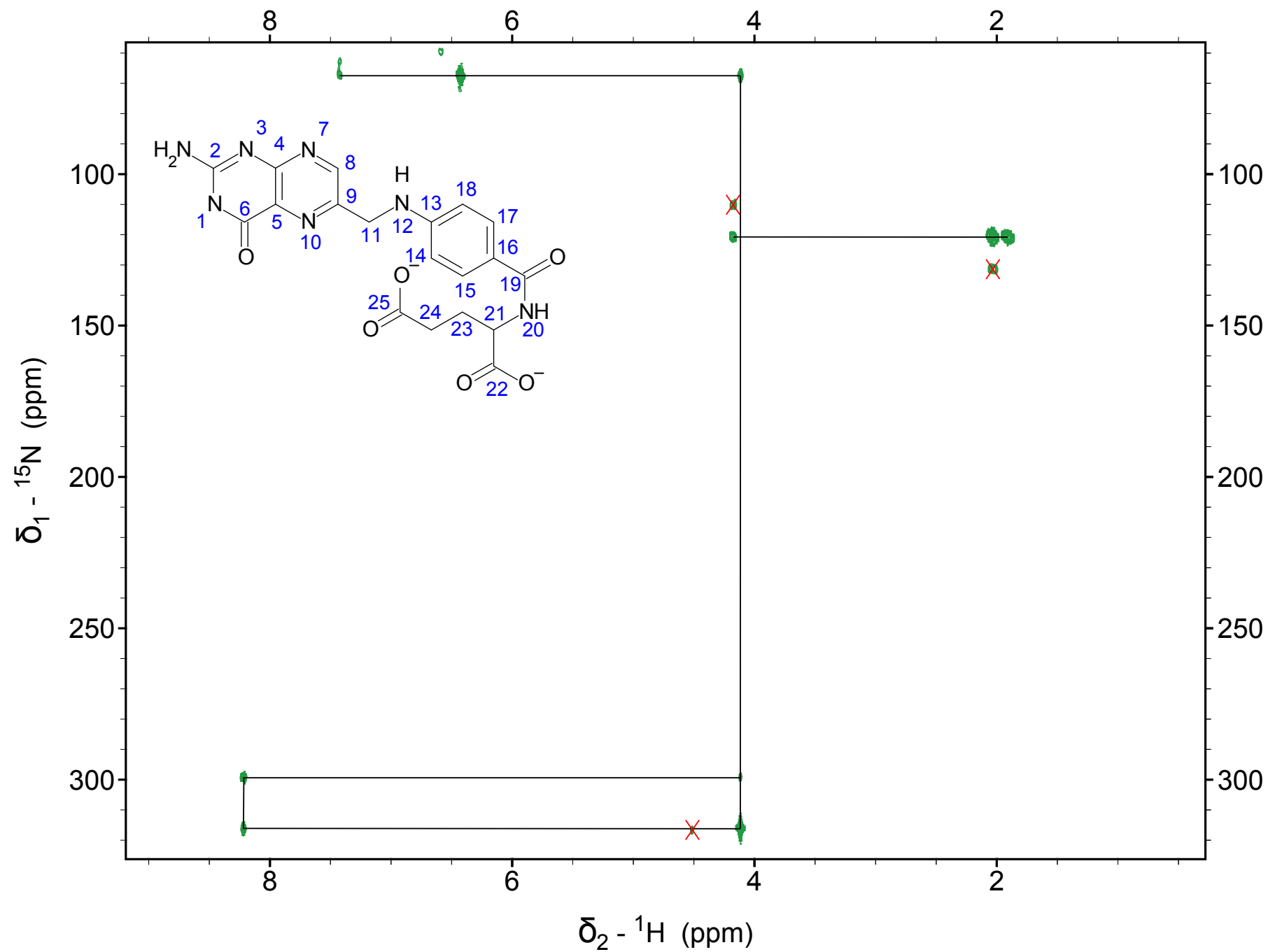


Folic Acid: ^{13}C 1D

^{13}C FOLATE



Folic Acid: ^1H - ^{15}N HMBC



Folic Acid: ^1H - ^{13}C HMBC

