

## Supplementary Materials

### **NMR-Based Structural Insights on Folic Acid and its Interactions with Copper(II) ions**

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## Table S1

[illegible]

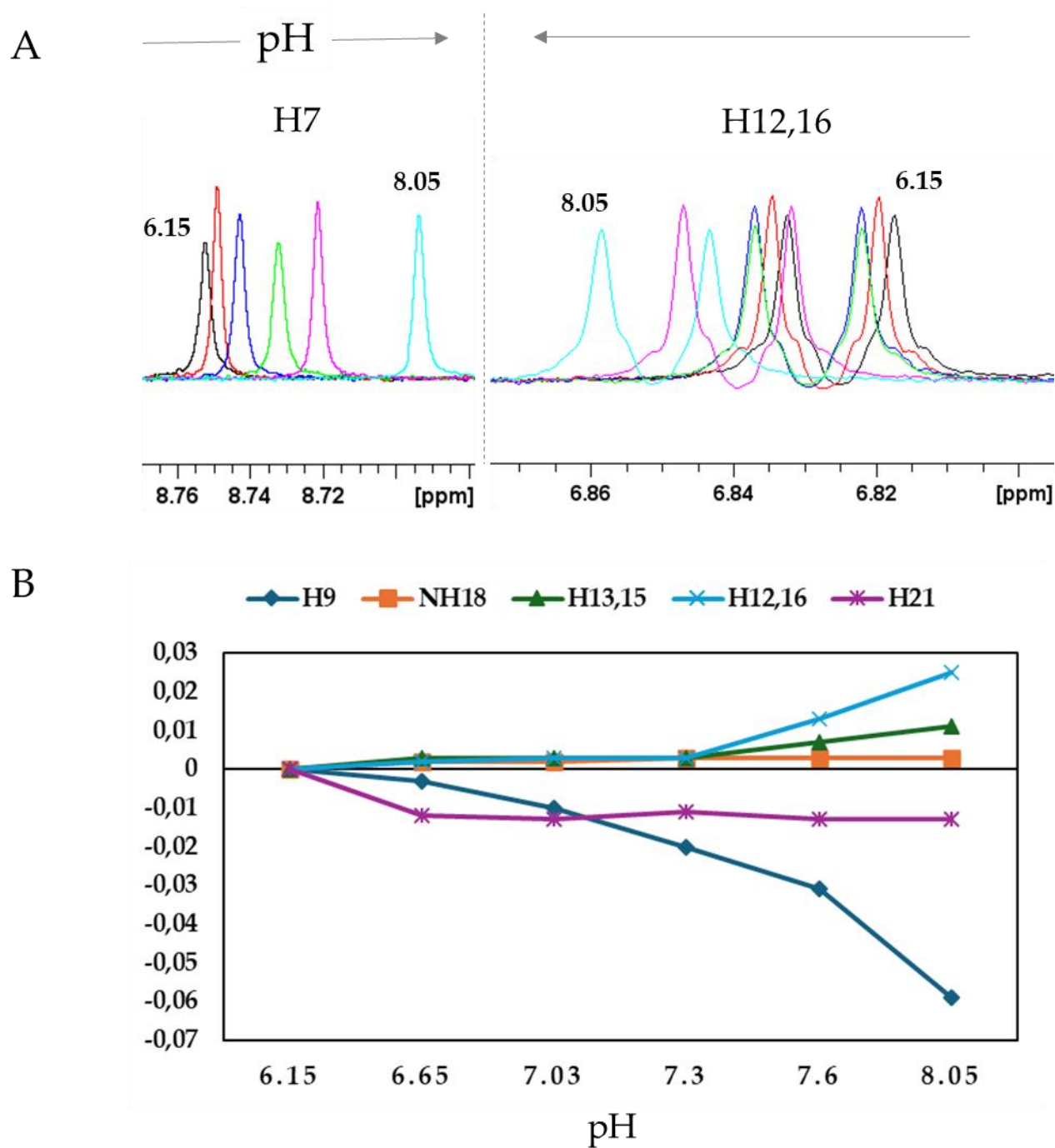


Figure S1. pH dependence of proton chemical shift of FA 0.5 mM: A. Superimposition of  $^1\text{H}$  NMR signals of H7 and H12,16 at different pH values starting from 6.15 to 8.05; B. Chemical shift variations of FA protons at different pH values.

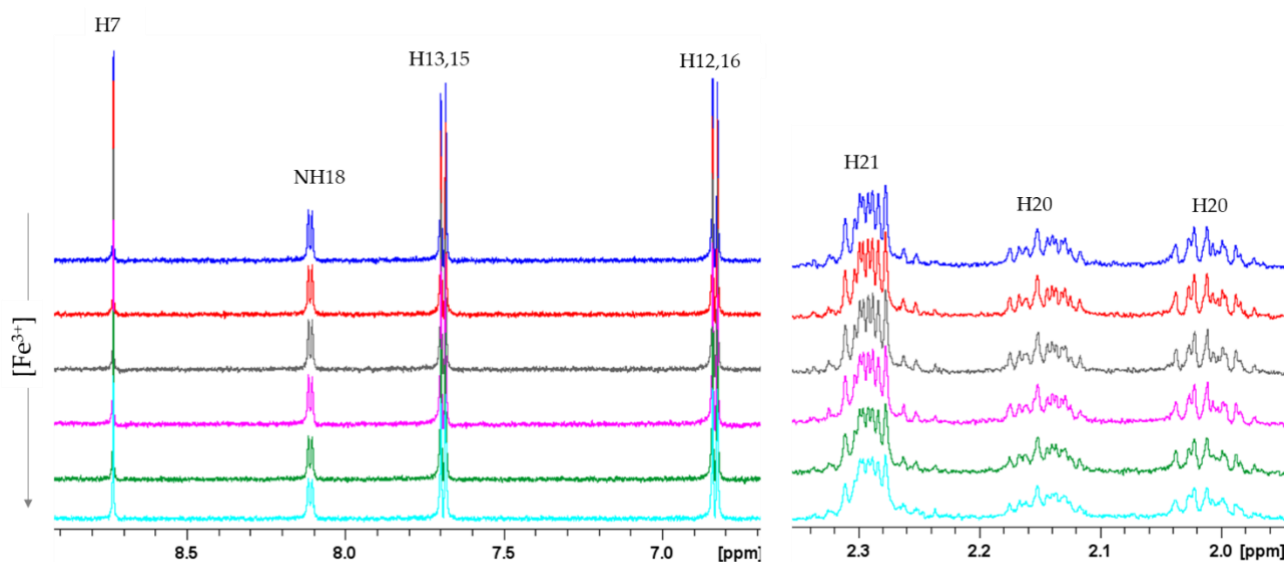


Figure S2.  $^1\text{H}$  NMR spectra of FA 0.5 mM in phosphate buffer 20 mM (pH 7.35) and  $T=298$  K in absence and in presence of  $\text{Fe}^{3+}$  ions.  $\text{Fe}^{3+} = 0$  eqs (blue);  $\text{Fe}^{3+} = 0.02$  eqs (red);  $\text{Fe}^{3+} = 0.04$  eqs (gray);  $\text{Fe}^{3+} = 0.08$  eqs (magenta);  $\text{Fe}^{3+} = 0.12$  eqs (green);  $\text{Fe}^{3+} = 0.20$  eqs (light blue).

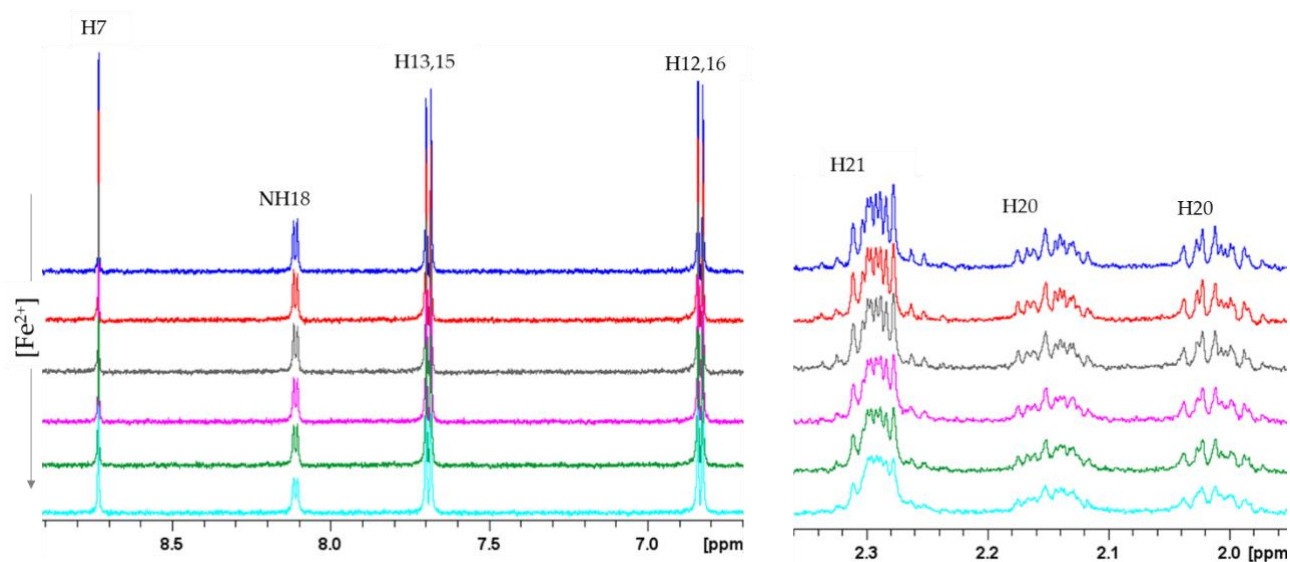


Figure S3.  $^1\text{H}$  NMR spectra of FA 0.5 mM in phosphate buffer 20 mM (pH 7.35) and  $T=298$  K in absence and in presence of  $\text{Fe}^{2+}$  ions.  $\text{Fe}^{2+} = 0$  eqs (blue);  $\text{Fe}^{2+} = 0.02$  eqs (red);  $\text{Fe}^{2+} = 0.04$  eqs (gray);  $\text{Fe}^{2+} = 0.08$  eqs (magenta);  $\text{Fe}^{2+} = 0.12$  eqs (green);  $\text{Fe}^{2+} = 0.20$  eqs (light blue).

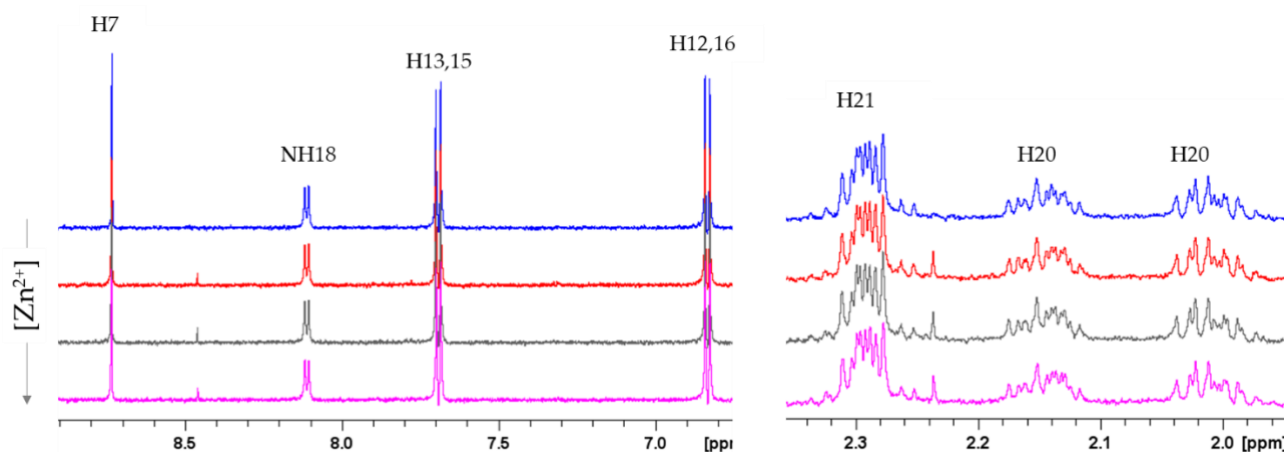


Figure S4.  $^1\text{H}$  NMR spectra of FA 0.5 mM in phosphate buffer 20 mM (pH 7.35) and  $T=298$  K in absence and in presence of  $\text{Zn}^{2+}$  ions.  $\text{Zn}^{2+} = 0$  eqs (blue);  $\text{Zn}^{2+} = 0.3$  eqs (red);  $\text{Zn}^{2+} = 0.6$  eqs (gray);  $\text{Zn}^{2+} = 0.9$  eqs (magenta).