

Para aminosalicilic acid in the treatment of manganese toxicity. Complexation of Mn^{2+} with 4-amino-2-hydroxybenzoic acid and its N-acetylated metabolite.

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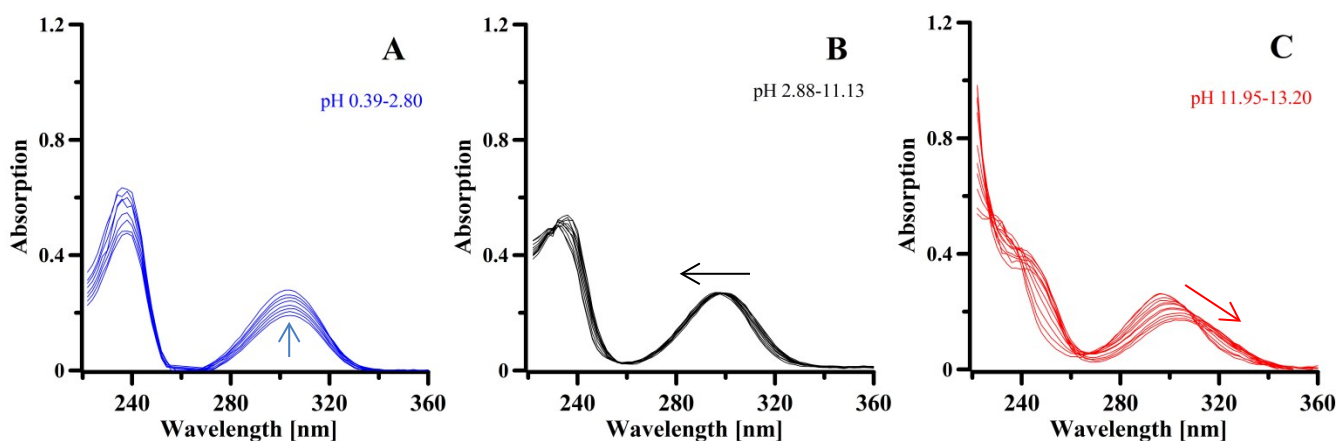
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Electronic Supplementary Material



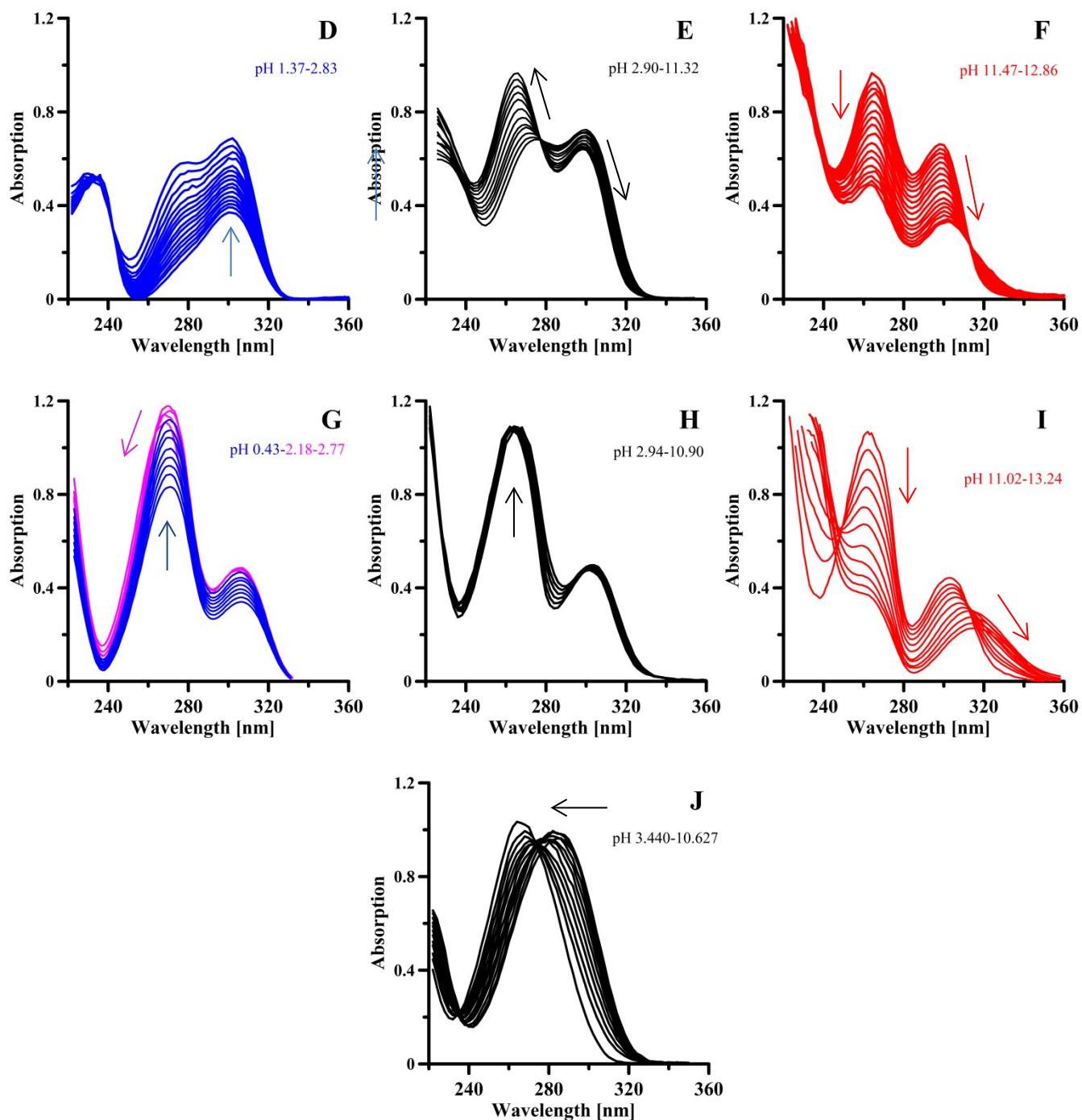


Figure S1. UV spectra of SAL (A-C), PAS (D-F), Ac-PAS (G-I) and 4-aminobenzoic acid (J). The concentration of the ligands was 0.5 mM, at 0.1 M NaCl ionic strength, 25 °C and 0.2 cm optical path length.

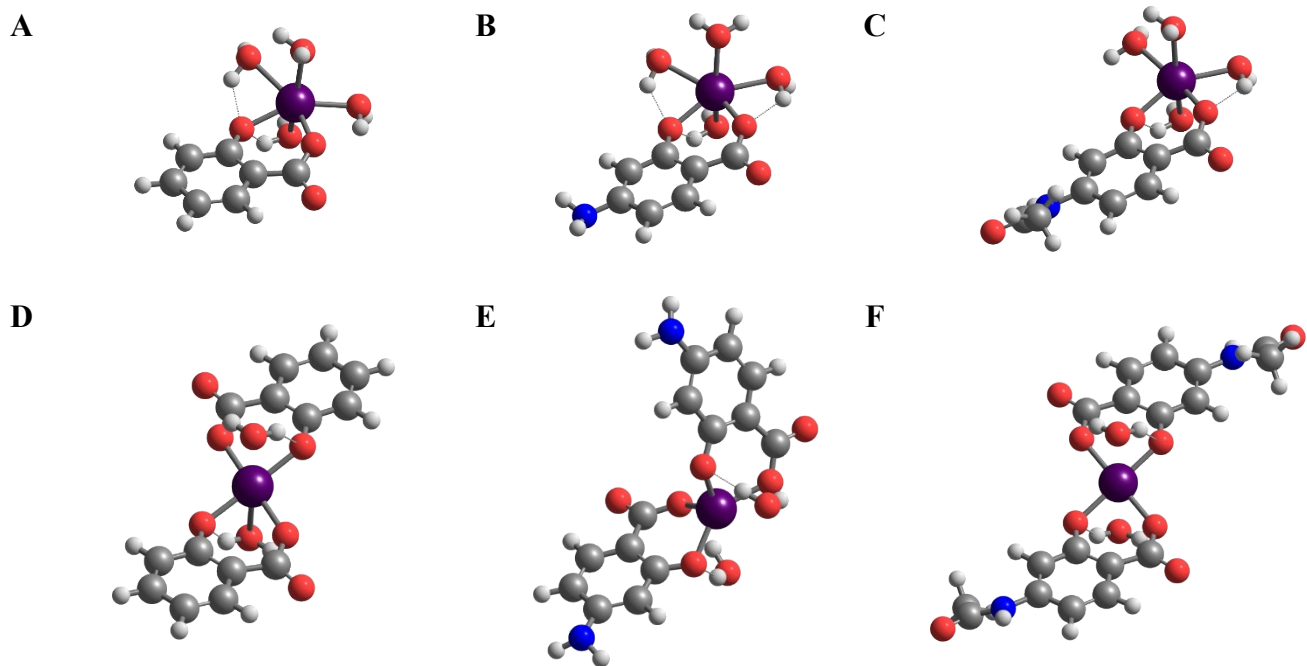
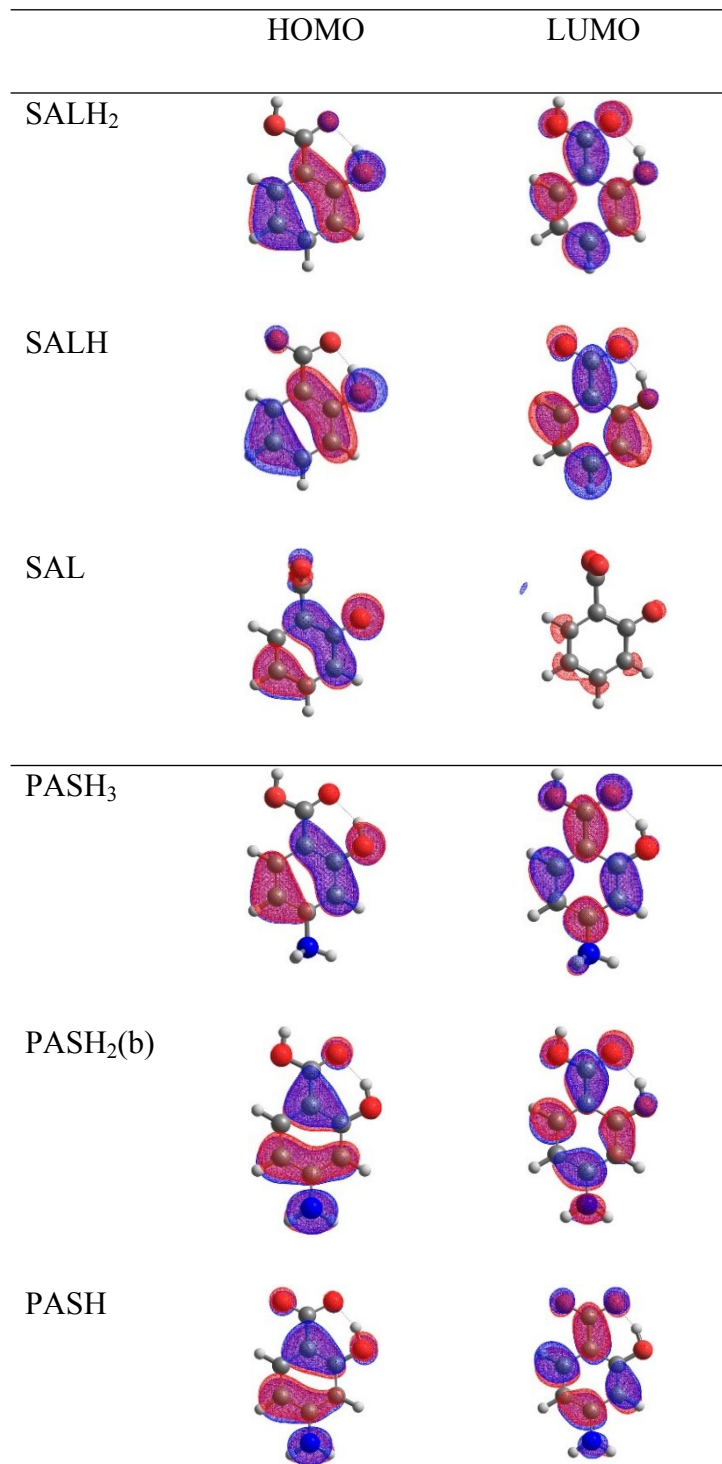


Figure S2. Minimum energy geometries of the MnL and $[\text{MnL}_2]^{2-}$ species with no extra explicit water molecules added. Optimizations performed at the B3LYP/6-31G(d,p)/SDD level of theory in the CPCM solvation model (solvent: water). A) $[\text{Mn}(\text{H}_2\text{O})_4(\text{SAL})]$; B) $[\text{Mn}(\text{H}_2\text{O})_4(\text{PAS})]$; C) $[\text{Mn}(\text{H}_2\text{O})_4(\text{AcPAS})]$; D) $[\text{Mn}(\text{H}_2\text{O})_2(\text{SAL})_2]^{2-}$; E) $[\text{Mn}(\text{H}_2\text{O})_2(\text{PAS})_2]^{2-}$; F) $[\text{Mn}(\text{H}_2\text{O})_2(\text{AcPAS})_2]^{2-}$.



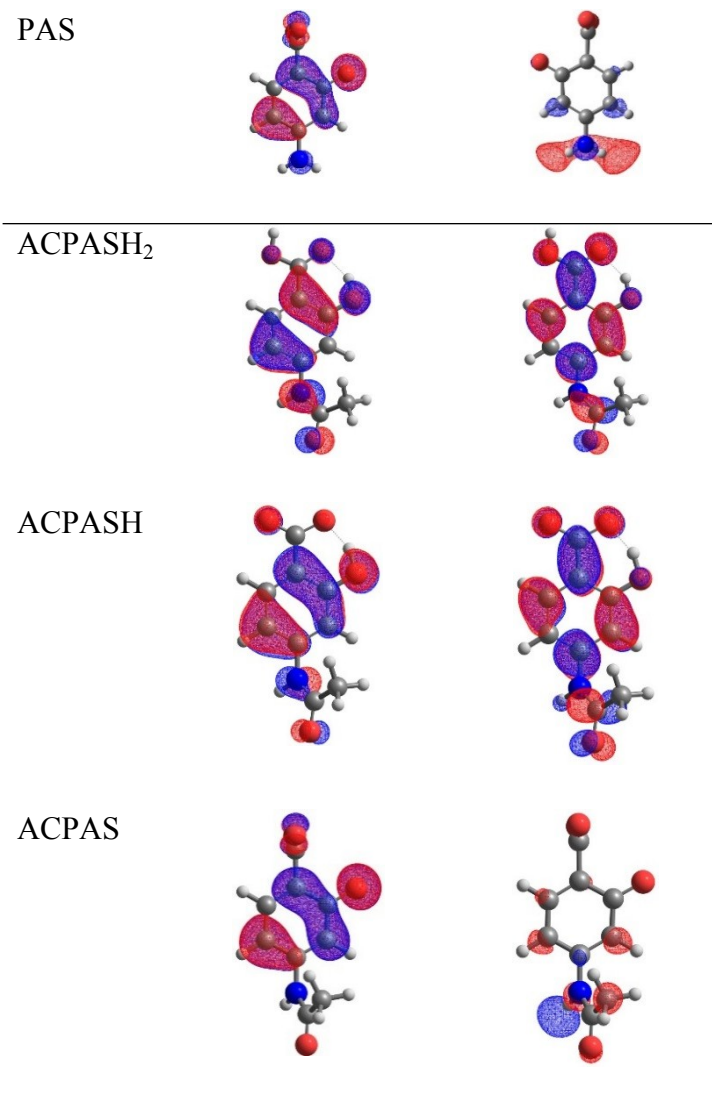


Figure S3. Plots of the HOMO LUMO orbitals of the various protonated forms of the salicylic acid derivatives.

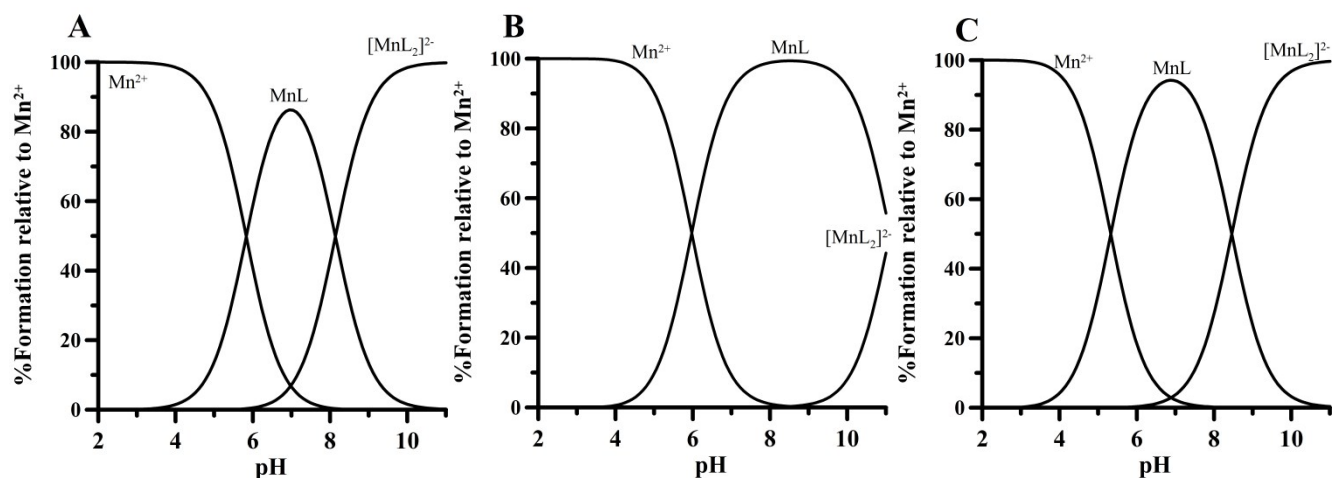


Figure S4. Speciation plots of manganese complexes with SAL (A), PAS (B) and Ac-PAS (C) calculated using the stability constants in Table 2. Ligand concentration was 0.5mM and a 1:5 metal to ligand ratio was used.

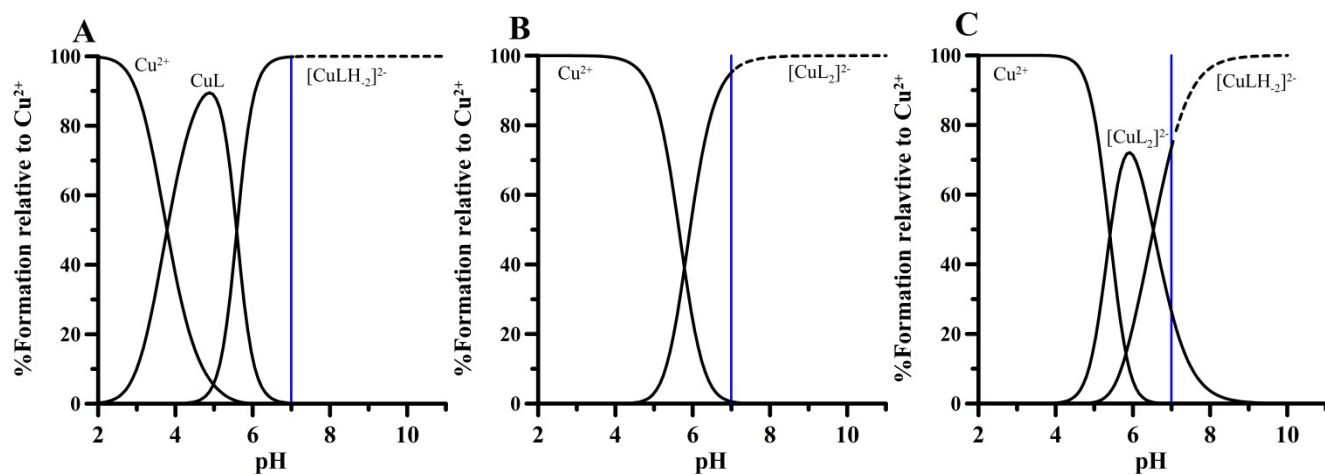


Figure S5. Speciation plots of copper complexes with SAL (A), PAS (B) and Ac-PAS (C) calculated using the stability constants in Table 6. Ligand concentration was 0.5 mM. A 1:5 metal to ligand ratio and 0.1 M NaCl ionic strength were used. The pH of complex precipitation is marked with the blue line.

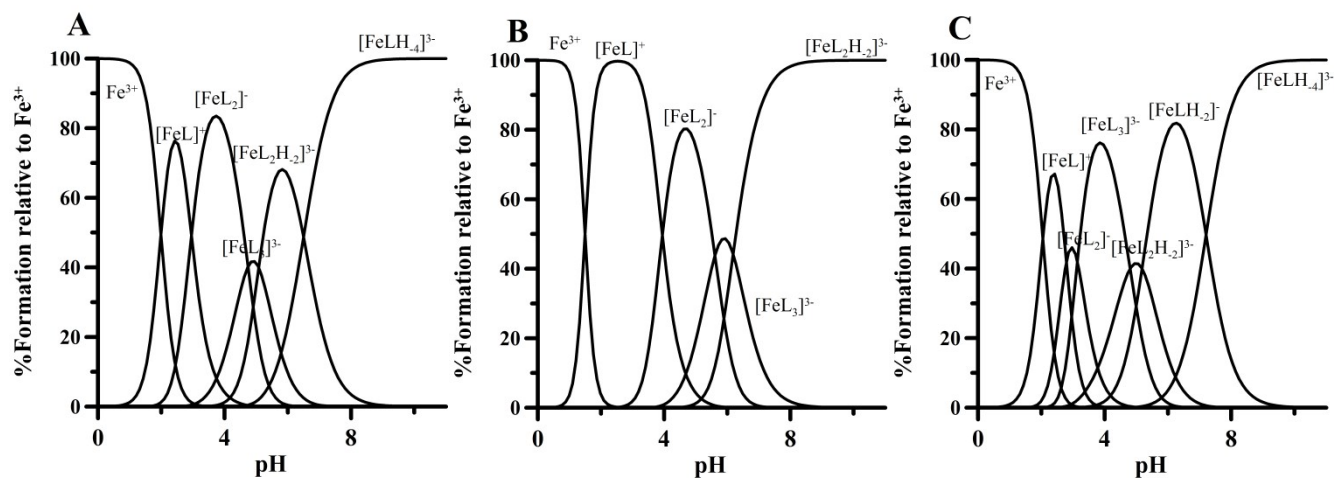


Figure S6. Speciation plots relative of iron and SAL (A), PAS (B) and Ac-PAS (C) complexes calculated using the stability constants in Table 6. Ligand concentration were 0.5 mM and a 1:5 metal to ligand ratio, 0.1 M NaCl ionic strength were used. The pH of complex precipitation is marked with the blue line.