

Arylthiazoline Unit as a Ferric Ion Chelating Moiety in Siderophores: The Coordination Chemistry of Anguibactin and Its Analogs

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The 2-(2-hydroxyphenyl)- and 2-(2,3-dihydroxyphenyl)thiazoline motifs appear repeatedly across microbial siderophores, yet the thermodynamic properties of their Fe(III) complexes remain fragmentarily described. Herein we present the Fe(III) coordination chemistry of anguibactin (**Ang**), the siderophore of *Vibrio anguillarum*, together with four designed analogs (**L1–L4**) that pair a phenol- or catechol-thiazoline core with an auxiliary donor group, either carboxylate or hydroxamate, analyzing the contribution of each functional group against a common scaffold. Using physicochemical analyses in MeOH/H₂O (80:20, w/w), we determined the protonation equilibria, complex stoichiometries, pH-dependent speciation, and Fe(III) affinities. At physiological pH all ligands form bis-ligand complexes in which iron is bound through the phenolate–thiazoline unit and the auxiliary donor rather than a catecholate sphere. Replacing the carboxylate by a hydroxamate unit substantially increases Fe(III) affinity. Of importance, **Ang** retains the highest affinity of the series (pFe = 28.2), exceeding that of closely related desferrithiocin and being close to other efficient siderophores, like tris(hydroxamate) ferrioxamines or pyoverdine, a peptide-based siderophore comprising dihydroxyquinoline, hydroxamate, and catecholate motifs. As **Ang** has been proposed as a thermally stable counterpart to acinetobactin – a siderophore from the multidrug-resistant pathogen *Acinetobacter baumannii*, the structure–property relationships can support the future design of arylthiazoline-based “Trojan horse” siderophore–antibiotic conjugates.

Słowa kluczowe

Aromatic compounds, Deprotonation, Hydrocarbons, Ligands, Equilibrium constant

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