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Exploring 3-hydroxy-4-pyridinone chelators synthetic versatility to attain tailor made low toxicity chromogenic reagents for iron speciation in water samples

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Considering the recognized importance of the role of iron in aquatic systems, reliable and real-time methods for iron speciation in natural waters are essential. In this scenario, a collaboration between a synthesis and an analytical chemistry group was established to explore possible alternative chromogenic reagents for the determination of iron.

Chelators of the 3-hydroxy-4-pyridinone (3,4-HPO) class are hard ligands bearing oxygen coordinating atoms thus showing a high capacity to trap iron(III) and a moderate affinity for iron(II). The ligands are bidentate, but using the appropriate anchors it is possible to synthesize hexadentate ligands thus providing chelators that can form FeL_3 or FeL complexes. Furthermore, 3,4-HPO's structure enables tailoring of hydrophilic/lipophilic balance of ligands and complexes by simply introducing proper substituents on the endocyclic nitrogen atom. The latter modifications on the ligand structure do not significantly change their stability constants towards iron.

Sequential injection was chosen as automation tool due to its proven efficiency in water monitoring. The versatility of flow procedures for sample handling and the facilitated handling of solid materials for pre-concentration and/or sample clean-up enabled the methods application to different types of waters. The relative merits of these compounds and associated analytical methods will be discussed in this paper.

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