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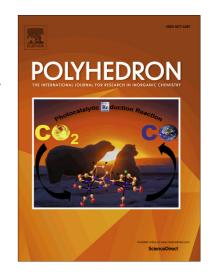
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ACCEPTED MANUSCRIPT

Evaluation of Iron(III)-N(amine)₂N(py)₂ Complexes as Potential Bioreductively Activated Carriers for Naphthoquinone-based Drugs

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Abstract

Two new iron(III) complexes, [Fe(bhnq)(L1)]NO₃·CH₃OH·2H₂O (1) and [Fe(bhnq)(L2)]ClO₄·CH₃OH (2) (L1 = N, N'-bis(pyridin-2-ylmethyl)ethylenediamine and L2 = N, N'-dimethyl-N, N'-bis(pyridin-2-ylmethyl)ethylenediamine), were investigated as potential candidates for bioreductively activated prodrugs. These complexes present a distorted octahedral structure with 2,2'-bis(3-hydroxy-1,4-naphthoquinone), (bhnq)²⁻, coordinated in a bidentate fashion to the iron(III) ion. A reversible wave associated with the Fe³⁺/Fe²⁺ couple was observed in MeCN for 1 and 2 respectively at -0.05 V and 0.01 V vs SHE. Unlike previously studied cobalt(III)-based analogs and one iron(III) platform that showed efficient bioreductive activation, complexes 1 and 2 undergo fast dissociation in aqueous buffered solutions with immediate release of the bhnq²⁻ ligand. Therefore, we conclude that the labile $3a^5$ iron(III) ion is a limited bioreducible carrier for naphthoquinone-based prodrugs when coordinated to this $[N_2N^{Py}_2]$ platform. Considerable modification of the current ligands or the meticulous selection of other alternative ligand platforms may be necessary to attain this goal.

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