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Cyclic analogs of desferrioxamine E siderophore for ^{68}Ga nuclear imaging: coordination chemistry and biological activity in *staphylococcus aureus.*

Autorzy

Andrzej Mular

Abraham Shanzer

Henryk Kozłowski

Isabella Hubmann

Matthias Misslinger

Julia Krzywik

Clemens Decristoforo

Elżbieta Gumienna-Kontecka

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Streszczenie

As multidrug-resistant bacteria are an emerging problem and threat to humanity, novel strategies for treatment and diagnostics are actively sought. We aim to utilize siderophores, iron-specific strong chelating agents produced by microbes, as gallium ion carriers for diagnosis, applying that Fe(III) can be successfully replaced by Ga(III) without losing biological properties of the investigated complex, which allows molecular imaging by positron emission tomography (PET). Here, we report synthesis, full solution chemistry, thermodynamic characterization, and the preliminary biological evaluation of biomimetic derivatives (FOX) of desferrioxamine E (FOXE) siderophore, radiolabeled with ^{68}Ga for possible applications in PET imaging of *S. aureus*. From a series of six biomimetic analogs, which differ from FOXE with cycle length and position of hydroxamic and amide groups, the highest Fe(III) and Ga(III) stability was determined for the most FOXE alike compounds–FOX 2-4 and FOX 2-5; we have also established the stability constant of the Ga-FOXE complex. For this purpose, spectroscopic and potentiometric titrations, together with the Fe(III)–Ga(III) competition method, were used. [^{68}Ga]Ga-FOXE derivatives uptake and microbial growth promotion studies conducted on *S. aureus* were efficient for compounds with a larger cavity, i.e., FOX 2-5, 2-6, and 3-5. Even though showing low uptake values, Fe-FOX 2-4 seems to be also a good Fe-source to support the growth of *S. aureus*. Overall, proposed derivatives may hold potential as inert and stable carrier agents for radioactive Ga(III) ions for diagnostic medical applications or interesting starting compounds for further modifications.

Słowa kluczowe

Reaction products, Ligands, Ions, Stability, Titration

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