

Article

# In Silico Analysis of the $\text{Ga}^{3+}/\text{Fe}^{3+}$ Competition for Binding the Iron-Scavenging Siderophores of *P. aeruginosa*—Implementation of Three Gallium-Based Complexes in the “Trojan Horse” Antibacterial Strategy

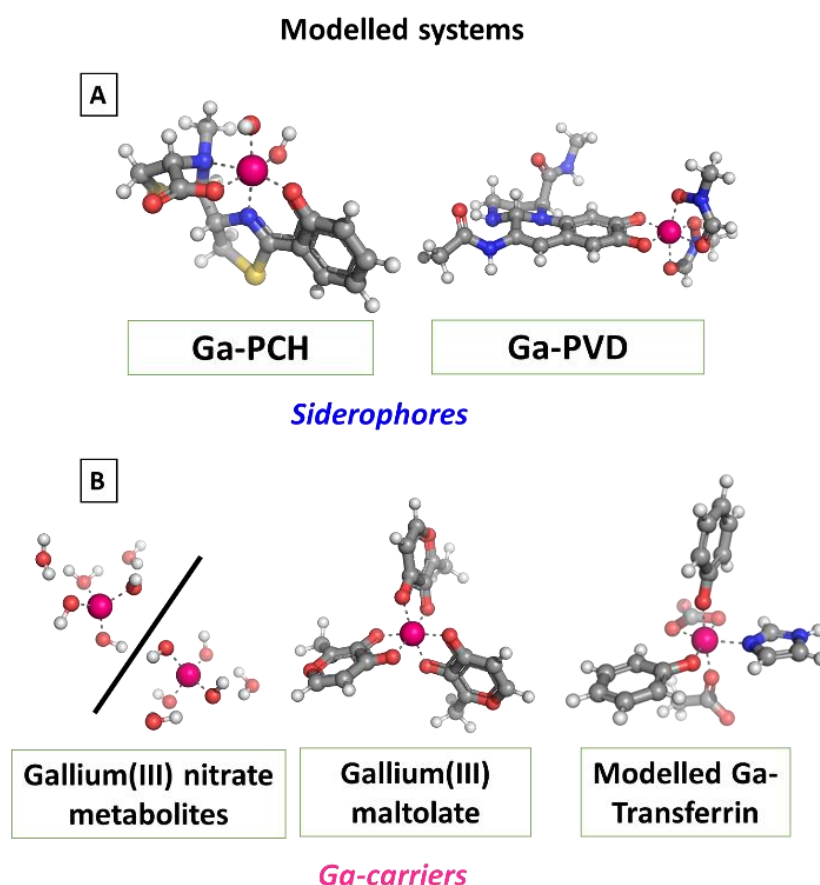
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**Figure S1.** (A) B3LYP/6-31+G(3d,p) optimized structures of Ga complex with pyochelin (whole molecule) and pyoverdine (a simplified model); (B) B3LYP/6-31+G(3d,p) optimized structures of gallium(III) nitrate metabolites, gallium(III) maltolate, and a simplified model used for the Ga-transferrin complex.