

Zirconium-Based Metal–Organic Frameworks as Acriflavine Cargos in the Battle against Coronaviruses—A Theoretical and Experimental Approach

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Streszczenie

In this study, we present a complementary approach for obtaining an effective drug, based on acriflavine (ACF) and zirconium-based metal–organic frameworks (MOFs), against SARS-CoV-2. The experimental results showed that acriflavine inhibits the interaction between viral receptor-binding domain (RBD) of spike protein and angiotensin converting enzyme-2 (ACE2) host receptor driving viral cell entry. The prepared ACF@MOF composites exhibited low (MOF-808 and UiO-66) and high (UiO-67 and NU-1000) ACF loadings. The drug release profiles from prepared composites showed different release kinetics depending on the local pore environment. The long-term ACF release with the effective antiviral ACF concentration was observed for all studied ACF@MOF composites. The density functional theory (DFT) calculations allowed us to determine that π – π stacking together with electrostatic interaction plays an important role in acriflavine adsorption and release from ACF@MOF composites. The molecular docking results have shown that acriflavine interacts with several possible binding sites within the RBD and binding site at the RBD/ACE2 interface. The cytotoxicity and ecotoxicity results have confirmed that the prepared ACF@MOF composites may be considered potentially safe for living organisms. The complementary experimental and theoretical results presented in this study have confirmed that the ACF@MOF composites may be considered a potential candidate for the COVID-19 treatment, which makes them good candidates for clinical trials.

Słowa kluczowe

metal–organic frameworks, acriflavine, SARS-CoV-2, drug delivery, density functional theory calculations

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Angielski

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