Title

UiO-66(Zr) as drug delivery system for non-steroidal anti-inflammatory drugs

Abstract

The toxicity for the human body of non-steroidal anti-inflammatory drugs (NSAIDs) overdoses is a consequence of their low water solubility, high doses, and facile accessibility to the population. New drug delivery systems (DDS) are necessary to overcome the bioavailability and toxicity related to NSAIDs. In this context, UiO-66(Zr) metal-organic framework (MOF) shows high porosity, stability, and load capacity, thus being a promising DDS. However, the adsorption and release capability for different NSAIDs is scarcely described. In this work, the biocompatible UiO-66(Zr) MOF was used to study the adsorption and release conditions of ibuprofen, naproxen, and diclofenac using a theoretical and experimental approximation. DFT results showed that the MOF-drug interaction was due to an intermolecular hydrogen bond between protons of the groups in the defect sites, ($\mu 3 - OH$, and $- OH2$) and a lone pair of oxygen carboxyl functional group of the NSAIDs. Also, the experimental results suggest that the solvent where the drug is dissolved affects the adsorption process. The adsorption kinetics are similar between the drugs, but the maximum load capacity differs for each drug. The release kinetics assay showed a solvent dependence kinetics whose maximum liberation capacity is affected by the interaction between the drug and the material. Finally, the biological assays show that none of the systems studied are cytotoxic for HMVEC. Additionally, the wound healing assay suggests that the UiO-66(Zr) material has potential application on the wound healing process. However, further studies should be done.

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Drug delivery systems; Drug release; Molecular modelling; UiO-66@NSAID

Index Keywords

Adsorption; Anti-Inflammatory Agents, Non-Steroidal; Cell Survival; Diclofenac; Drug Carriers; Drug Delivery Systems; Drug Liberation; Humans; Ibuprofen; Metal-Organic Frameworks; Naproxen; Phthalic Acids; Biochemistry; Biocompatibility; Controlled drug delivery; Drug dosage; Drug interactions; Hydrogen bonds; Kinetics; Organometallics; Targeted drug delivery; Toxicity; diclofenac; ibuprofen; metal organic framework; naproxen; nonsteroid antiinflammatory agent; oxygen; proton; solvent; zirconium; diclofenac; drug carrier; ibuprofen; metal organic framework; naproxen; nonsteroid antiinflammatory agent; phthalic acid derivative; UiO-66; Drug release; Drug-delivery systems; High dose; High porosity; Human bodies; Low water; Metalorganic frameworks (MOFs); Non-steroidal anti-inflammatory drugs; UiO-66@non-steroidal anti-inflammatory drug; Water solubilities; adsorption; adsorption kinetics; Article; bioavailability; controlled study; desorption; drug

adsorption; drug delivery system; drug distribution; drug release; electric potential; high performance liquid chromatography; human; human cell; hydrogen bond; isotherm; kinetics; pH; porosity; release assay; scanning electron microscopy; thermostability; water solubility; wound healing; wound healing assay; X ray diffraction; cell survival; chemistry; drug effect; Adsorption

Chemicals/CAS

diclofenac, 15307-79-6, 15307-86-5; ibuprofen, 15687-27-1, 79261-49-7, 31121-93-4, 527688-20-6; naproxen, 22204-53-1, 26159-34-2, 26159-31-9; oxygen, 7782-44-7; proton, 12408-02-5, 12586-59-3; zirconium, 14940-68-2, 7440-67-7; Anti-Inflammatory Agents, Non-Steroidal, ; Diclofenac, ; Drug Carriers, ; Ibuprofen, ; Metal-Organic Frameworks, ; Naproxen, ; Phthalic Acids, ; UiO-66,

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