Modified amino acids targeting the polyamine biosynthetic pathway: A case study of DFMO in the fighting against

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Introduction: Targeting the polyamine biosynthetic pathway by inhibiting ornithine decarboxylase is a powerful approach in the fight against diverse viruses, including SARS-CoV-2 [1]. Difluoromethylornithine (DFMO) is the best-known inhibitor of ornithine decarboxylase and a broad-spectrum unique therapeutical agent. Nevertheless, its pharmacokinetic profile is not perfect, especially when large doses are required in antiviral treatment. But in fact, recent studies revealed that DFMO analogues can be promising drugs either in current or next viral outbreaks.

Purpose: This presentation will focus on a holistic investigation onf the first insight into the supramolecular structure of DFMO and its analogues, supplemented by a comprehensive, qualitative and quantitative survey of non-covalent interactions via Hirshfeld surface, molecular electrostatic potential, enrichment ratio and energy frameworks analysis visualizing 3-D topology.

Conclusion: In the light of the drug discovery, supramolecular studies of amino acids, essential constituents of proteins, are of prime importance. Notably, the same amino-carboxy synthons are observed in the bio-system containing DFMO. Synthon concept is promising in future design of idealized effective drugs.

Biography:

Joanna works at the university in Poland. The most important article is "A global review on short peptides", last: "The first supramolecular insight into DFMO system: A new antiviral perspective". She is a member of the European Peptide Society. She was awarded a verified certificate from HarvardUniversity.

Publication of speakers:

1. 1. Novel biologically important supramolecular synthons in short peptides
2. The First Insight Into the Supramolecular System of D,L-α-Difluoromethylornithine: A New Antiviral Perspective
3. Short Peptides: On the Trail of Future Stem Cell-Based Regenerative Therapies.

Full name of webinars, dates,

Webinar on Nano materials. March 30, 2021

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