Poster Presentation

MS59.P09

Serotonin in different compounds: crystallographic and computational insight

D. Rychkov[1,2], E. Boldyreva[1,2], V. Kovalskii[3], S. Hunter[4], C. Pulham[4], C. Morrison[4]

[1]Novosibirsk State University, REC-008, Novosibirsk, Russia, [2]Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia, [3]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia, [4]The University of Edinburgh, School of Chemistry and Centre for Science at Extreme Conditions, Edinburgh, Scotland, UK

Biologically active substances are in the focus of pharmaceutical and chemical research. Serotonin, one of the most common neurotransmitters, is widely studied in relation to its effect on humans from cellular to neurological levels. Although serotonin plays a key role in some biological processes, its chemistry and crystallography are not sufficiently understood. The aim of the present study was to crystallize serotonin adipate and creatinine sulfate monohydrate, determine their crystal structures, and analyze them in a comparison with other previously known serotonin crystal structures. Special attention was paid to the interrelation between the molecular conformation and crystalline environment. This issue was addressed using crystallographic and computational chemistry (DFT-D, MD) approaches. In our research was shown that the crystal structure of the creatinine sulfate complex significantly differs from what was previously determined. The conformation of serotonin in the new structure differs from serotonin conformations in all other known complexes, as well as from the most stable conformation, predicted by the adiabatic conformational analysis using quantum chemical calculations (DFT, MP) in different phases. This work has explicitly shown the influence of different interactions on serotonin molecular conformation in the crystalline state, described from a crystallographic and theoretical point of view. It has been previously demonstrated that salt formation in the presence of different anions produces variation in pharmacological, therapeutic and physic-chemical properties. This study has shown that alterations of the anion affects the molecular geometry of the bioactive substance and invite further investigation to rationalize the geometry changes. The work was supported by the RFBR Grants №14-03-31866, 13-03-92704, Russian Ministry of Science and Education and RAS, Siberian Supercomputer Center SB RAS Integration Grant №130, Edinburgh Compute and Data Facility

Keywords: serotonin, diffraction, DFT