[MS25-P18] New structure of serotonin salt – comparison and conformational analysis of all known serotonin complexes.

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Biologically active substances are in the focus of biological, pharmaceutical and chemical research. Serotonin, one of the most common neurotransmitters, is widely studied in relation to its effect on humans at all levels -from cellular to neurological[1–3]. Although serotonin plays a key role in some biological processes, its chemistry and crystallography are not sufficiently studied. Serotonin adipate has been used in medical formulations in Russia and Eastern Europe as an analogue of serotonin creatinine sulfate monohydrate, but the crystal structure of the adipate salt remained unknown. On the other hand, the structure of well-known serotonin creatinine sulfate monohydrate was determined in earlier 1965[4] and data is insufficient for full-fledged analysis. The aim of the present study was to crystallize serotonin adipate and creatinine sulfate monohydrate, determine its crystal structure and analyze it in comparison with other previously known crystal structures of serotonin. Special attention was paid to the interrelation between the molecular conformation and crystalline environment. In our research was shown that the crystal structure of creatinine sulfate complex significantly differs from what was previously determined. Moreover, 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[5][6]. This work has explicitly shown the influence of different interactions on serotonin molecular conformation in the crystalline state. Three main conclusions can be made: i) crystalline environment defines the conformation of the serotonin molecules

ii) "flat" (thermodynamically unfavourable) conformations can be stabilized in the crystalline state if hydrogen bonds are the only intermolecular interactions iii) additional stacking and donor-acceptor interactions change molecular conformation dramatically, such that the molecules are no longer flat, in accordance with current experimental data It has been previously demonstrated that salt formation in the presence of different anions produces variation in pharmacological, therapeutic and physico-chemical properties[7], [8]. This study has shown that alteration of the anion affects the molecular geometry of the biologically active substance. It is feasible to hypothesis that it is this phenomenon that contributes to the aforementioned observations of variation in biological and physical properties

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