

SUMMARY

MARIA CURIE-SKŁODOWSKA UNIVERSITY
Faculty of Chemistry
Department of Crystallography, Analytical Laboratory

Lublin – 2019

THE ROLE OF QUERCETIN MOLECULES IN SUPRAMOLECULAR CHEMISTRY

Author: mgr inż. Urszula Maciołek
Doctoral supervisor: prof. dr hab. Anna E. Koziół
Auxiliary supervisor: dr Ewaryst Mendyk

In the present doctoral dissertation, synthesis methods were devised as well as eight new co-crystals in the solid state and one quercetin complex were obtained using a mechanochemical method. As a result of the carried out analyses, it was established that both neutral molecules and salts with an organic cation or anion used as co-formers. The following were successfully used as co-formers: 4-(1-benzofuran-2-yl)pyridine, 4-(5-ethyl-1-benzofuran-2-yl)pyridine, 1,10-phenanthroline, o-dianisidine, caffeine, pyridine-3-sulphonic acid, naproxen sodium salt, diclofenac sodium salt and ketamine hydrochloride. In the newly obtained multicomponent phases, the crystals demonstrate different chemical compositions. For the obtained crystals, micrographs (optical microscopy and SEM) were made, the chemical composition was established, the crystalline structures were solved, the spectra (IR and Raman) were interpreted and the thermal stability was determined. It has been shown that quercetin is a polymorphic supramolecular synthon capable of changing the conformation, and the directionality of the intermolecular hydrogen bonds formed with its participation is variable.

The research also included the development of conditions and the synthesis of the new quercetin-5'-sulphonic acid complexes with sodium and potassium cations and their solvates as well as ammonium salt. A total of eight new crystalline phases were obtained and it was shown that neutral O-donor ligands in the coordination sphere and outside the metal cations sphere in QSA⁻ complexes are easily interchangeable with inert solvent molecules (Ace, DMSO, EtOH) by means of a solvothermal synthesis. For the obtained crystalline complexes, their morphology was determined, structures were established, IR and Raman spectra as well as thermal analysis were performed. For three of the synthesized new complexes, calculations of topological charge distribution in the crystal were performed. The quercetin-5'-sulphonic anion has been found to be a ligand with variable coordination properties. Based on numerous research methods, the relations between the structure of molecules and crystal lattices and physicochemical properties were demonstrated.

The obtained compounds are interesting not only from the point of view of supramolecular chemistry. For selected compounds, research on anticancer activity (against cancerous colon cells) was performed. In vitro studies have shown that some compounds have a high potential based on the ability to induce apoptosis in relation to cancer cells. The obtained results suggest that they possess application potential for use as supportive substances or substances involved in cancer therapy.