Crystal engineering is a rapidly expanding area of solid-state chemical research. It has applications in materials science, molecular biology or pharmaceutical science. This leads to the growing interest in designing and preparing molecular crystals and understanding crystal packing. The work in this field is focused on predicting variable hydrogen bond patterns (homosynthons and heterosynthons) involved in the crystals. The small molecules such as aminopyridines or aminopyrimidines, with nitrogen atoms and amine groups, may be used as a model for understanding for example the purine or pyrimidine bases. We already know the strong recognition pattern of the carboxylic acid group with amine group ($R_2^2(8)$ heterosynthon), which is a popular synthon for crystal design and is present in different crystal structures.

In my work I present studies on the hydrogen bonded network formed between two sulfonic acids (5-sulfoisophthalic acid (5SIP) and L-cysteic acid (CSA)) and different aromatic amines (aminopyridines, aminopyrimidines, amino-1,3,5-triazines and purine and pyrimidine bases). The determination of the fifteen new crystal structures shows that the compounds crystallize in the monoclinic, triclinic or orthorhombic space groups. Moreover the spectroscopic measurements (IR, Raman) have also been made for them and their molecular organization have been analyzed. I have studied the possibility of creating a heterosynthon N-H···O/O-H···N for sulfonate and carboxylic groups and I also checked how the position of the amine group changes the motifs and the supramolecular networks. The growing number of the nitrogen atoms and the amine groups has a huge impact on the motifs and the supramolecular networks. In the presence of smaller amines molecule 5SIP or CSA acid anions form homomotifs which are extended into one-dimensional ribbon or chain and the situation changes when bigger amines appear. What is more, in the case of water used as a solvent, I also noticed that it became involved in creation the supramolecular motifs and chains – in the end it is a molecule that “likes” hydrogen bonds.

Futhermore I observed that the conditions of crystallization such as temperature, solvent, the type and molar ratio of the substrates or the synthesis method had a significant impact on the receiving novel three-dimensional, supramolecular networks. My research increases knowledge about the possibilities of creating organic structures by 5-sulfoisophthalic acid and L-cysteic acid with aromatic amines.