

## MS32-P07 | INTERMOLECULAR HEAD-TO-HEAD INTERACTIONS OF CARBONYL AND THIOCARBONYL GROUPS

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In this study, we report unusual head-to-head carbonyl–carbonyl and thiocarbonyl–thiocarbonyl interactions explored for crystalline  $\beta$ -hydroxyketones and drug thiamazole, respectively. Three studied  $\beta$ -hydroxyketones display an ability to form dimensionally different crystal formative motifs ranging from 1D to 3D. Despite the structural differences, primarily in intermolecular interactions, the studied ketones are arranged by the same bicyclic hydrogen-bonded twelve-membered supramolecular synthon, where the  $C=O\cdots O=C$  contact plays a key role. Thiamazole molecules form an analogous  $C=S\cdots S=C$  contact, but observed outside the cyclic  $N-H\cdots S$  bonded supramolecular synthon. These unusual interactions along with all the others that are present in the crystal structures, for instance, classical H-bonds, were investigated by means of quantum-topological analysis of the calculated and experimental electron densities.

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