MS32-P02 | EFFICIENT RECOGNITION OF STEROIDS BY PLANAR AROMATIC MOLECULES: A NOVEL BIOMOLECULAR RECOGNITION MOTIF AND ITS POTENTIAL APPLICATIONS

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Traditionally, functional groups attached to the backbone of steroid molecules were seen as the key factors in their molecular recognition and, consequently, their physiological function. However, a systematic study of the cocrystals of steroids with electron-rich, planar aromatic molecules (arenes) by our group has recently revealed the α···π interaction: a previously undescribed interaction mode of steroids involving the α-face of a steroid and the π-electron system of aromatic molecules. Progesterone was found to reliably engage in α···π interaction with various arenes, whereas other steroids studied so far suggest a strong dependence of this interaction on the fine structural details of the steroid backbone. This mimics the steroid behavior in the biological systems, where small structural differences give rise to significantly different biological functions.

We set out to pursue the cocrystallization of progesterone with a variety of polyaromatic hydrocarbons and heterocycles using the mechanochemical solid-state screening methods developed in our group. Furthermore, we sought to expand the set of steroid cocrystal formers towards biologically and pharmaceutically relevant adrenosterone (a weak androgen), cholest-4-en-3-one (metabolite of cholesterol), exemestane (anticancer drug) and levonorgestrel (used in birth control), all of which exhibit a degree of structural similarity with progesterone. Finally, we investigated the possibility of combining the α···π interaction with known interactions such as hydrogen and halogen bonding to engineer increasingly complex molecular solids.

This presentation will outline our initial findings, which confirm the reliability of the α···π interactions and establish its applicability to steroid molecules beyond progesterone.