Title of the poster: Resolution of a triazol-containing compound through co-crystallisation

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Triazoles are a special class of heterocyclic compounds with a broad spectrum of biological activities such as antimicrobial, cytotoxic, antihistaminic, anti-inflammatory or anticancer[1], consequently very interesting for pharmaceutical companies. Moreover, in those industries, 50% of the marketed drug compounds contain a chiral center[2], essential to their functioning. Where one enantiomer has the desired pharmacological effect, the other might be inactive or have adverse effects (e.g. Thalidomide). In spite of important advances in asymmetric synthesis, the most prominent way to chiral drugs still involves formation of a racemic compound followed by its resolution by a physical process.

Thus, the goal of this project is to use co-crystallization to resolve a previously synthetized triazol-containing compound by the formation of a pair of diastereoisomers. To do so, a library of chiral co-formers was screened to find the most suitable one. Once the right co-crystal was found, a ternary diagram was made to identify the right condition to get the co-crystal pure and consequently resolve the synthetized compound.

[1] Sathish Kumar, S.; Kavitha, H. P. Mini-Rev. Org. Chem. 2013,10(1), 40-65.

[2] Springuel G., Robeyns K., Norberg B., Wouters J. , Leyssens T. Cryst. Growth Des. 2014, 14(8), 3996-3404. 'Cocrystal formation between Chiral Compounds: How cocrystals differ from salts?'