Crystallization of anionic small molecules with the help of a cation screen

Ekaterina Slyshkina, Jaclyn Parris, Bernhard Spingler

University of Zurich, Zurich, Switzerland;

spingler@chem.uzh.ch

The CSD currently contains more than 1.1 million structures.[1] This impressive number is the result of at least the same number of experiments, which were for the most part all *manually* set up. There are very few reports about robots that were used to set up crystallization trials for the growth of single crystals of small molecules.[2]

Recently, we have developed an anion screen to crystallize organic [3, 4] and inorganic [5] cations of small molecules from aqueous solutions. For some of these studies [3, 5], we employed robotic systems such as the Crystal Gryphon LCP and the Rock Imager 1000, both of which are well established in protein crystallography [6, 7].

In this presentation, we would like to present our work, which resulted in a cation screen. This screen consists of 96 different aqueous solutions with almost 90 different cations, inorganic and organic ones. There exists a commercial cation screen dedicated exclusively for protein crystallography, but this screen only contains seven different inorganic cations. We will present anions that could be crystallized with the help of this screen and thereby elucidating on the possibilities and limitations of our novel cation screen.

- [1] Taylor, R. & Wood, P. A. (2019). Chem. Rev. 119, 9427.
- [2] Tyler, A. R., Ragbirsingh, R., McMonagle, C. J., Waddell, P. G., Heaps, S. E., Steed, J. W., Thaw, P., Hall, M. J. & Probert, M. R. (2020). Chem 6, 1755.
- [3] Nievergelt, P. P., Babor, M., Čejka, J. & Spingler, B. (2018). Chem. Sci. 9, 3716.
- [4] Babor, M., Nievergelt, P. P., Čejka, J., Zvoníček, V. & Spingler, B. (2019). IUCrJ 6, 145.
- [5] Alvarez, R., Nievergelt, P. P., Slyshkina, E., Müller, P., Alberto, R. & Spingler, B. (2020). Dalton Trans. 49, 9632.
- [6] Cherezov, V. (2011). Curr. Opin. Struct. Biol. 21, 559.
- [7] Broecker, J., Morizumi, T., Ou, W.-L., Klingel, V., Kuo, A., Kissick, D. J., Ishchenko, A., Lee, M.-Y., Xu, S., Makarov, O., Cherezov, V., Ogata, C. M. & Ernst, O. P. (2018). *Nat. Protoc.* 13, 260.

Keywords: single crystal growth, crystallization, salt screening

This research was funded by the University of Zurich and the R'Equip programme of the Swiss National Science Foundation (project No. 206021 164018).