

MS42-P06 | TESTING A HOME-MADE SAMPLE HOLDER WITH FLOW-THROUGH CAPILLARY TO STUDY IN-SITU RE-SOLVATION PROCESS

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In our powder diffraction laboratory, we studied the desolvation and resolvation of solvates of a pharmaceutical substance called ibrutinib [1,2]. We have chosen its known structures of methanol, fluorobenzene and anisole solvates as suitable compounds for testing because of several reasons. First of all, their crystal structures are known and they form both the channel-making and cavity-making arrangement of the ibrutinib molecules, where particular solvents are occupying channels or cavities, respectively. The second reason was much more practice – we had enough amount of different ibrutinib solvates in our laboratory.

For in-situ study of the desolvation processes we have used a simple setup of an open capillary in Debye-Scherrer configuration. However, for the in-situ study of the resolvation processes a completely new holder was constructed. This holder can be precisely aligned to the center of the powder diffractometer by using two perpendicular micrometer position stages in *z* and *y* directions. The borosilicate-glass flow-through capillary is connected to the holder by both ends allowing liquid or gas to pass. Both connectors allows connection of e.g. PTFE tubes for liquid or gas supply to the capillary.

[1] Zvoníček, V.; Skořepová, E.; Dušek, M.; Žvátora, P.; Šoóš, M. Ibrutinib Polymorphs: Crystallographic Study. *Cryst. Growth Des.* **2018**, *18*, 1315–1326.

[2] Zvoníček, V.; Skořepová, E.; Dušek, M.; Babor, M.; Žvátora, P.; Šoóš, M. First Crystal Structures of Pharmaceutical Ibrutinib: Systematic Solvate Screening and Characterization. *Cryst. Growth Des.* **2017**, *17*, 3116–3127.

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