Poster Presentation

MS67.P31

A New Look at Organic Hydrates: Chemistry, Crystal Structure and Bioactivity

M. Oliveira¹, P. Wood², M. Hickey¹, O. Almarsson³, J. Alvarez¹, N. Feeder², P. Galek², D. Moustakas¹

Alkermes, Inc., Waltham, USA, ²Cambridge Crystallographic Data Centre, Cambridge, UK, ³Moderna Therapeutics, Cambridge, USA

Crystalline organic hydrates in the Cambridge Structural Database have been surveyed to better understand water coordination environments and hydration likelihood. Particular emphasis has been paid to the subsets of bioactive organic hydrates and five classes of compound that are important in terms of pharmaceutical activity. Bioactive compounds are found to exhibit a greater hydration likelihood than general small organic compounds, but the distribution of environments remains the same, with the most common by far being where water accepts once and donates twice (DDA, 49.8%).

Keywords: Hydrates, water coordination, bioactive