simultaneous explorations of computationally and experimentally generated solid form landscapes for understanding the structural basis of phase transitions in anhydrate/hydrate systems.

[1] Braun, DE et al., Cryst. Growth Des. Submitted.

[2] Braun, DE et al., Mol. Pharmaceutics, 13, 1012−1029, 2016.

Keywords: hydrate, polytypism, screening

MS32-O2 Selection of Solid State Forms for New Chemical Entities: Challenges, Opportunities and Lessons

Christoph Saal[1]

1. Merckgroup, Darmstadt, Germany

email: christoph.saal@merckgroup.com

Over the last decades, selection of solid-state forms – including pharmaceutical salts, polymorphs and co-crystals - has become a crucial step at the transition from research to development. Respective solid-state forms represent efficient ways of optimizing physico-chemical parameters of pharmaceutical research compounds. Clearly, in this context solubility and bioavailability play a key role as pharmaceutical industry has to develop more and more low-soluble new chemical entities. However, these are not the only parameters to be considered, as behavior of a solid-state form with regard to manufacturability, processability and stability also have to be considered. In the end, the selection of a salt form is based on a manifold of different aspects, which have to be carefully balanced. The lecture gives an introduction into solid state form selection based on scientific knowledge. Experiences gained by several specific examples where selection of a suitable solid-state form has been challenging – and even sometimes surprising properties of solid state forms became crucial - are discussed.

Keywords: Abstract_ECM_CS