# SC3

## Crystal Modeling And Polymorphism

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Modeling of pharmaceutical compounds in order to deduce the crystal structure from measured X-ray data or pure in silico modeling to predict different possible polymorphic forms is a well known technique.
Less commonly known are modeling techniques which are applied when the crystal structure is already known. A wide field of application in the pharmaceutical development process is known and they often deliver significant impact for a successful product development.
Identification and quantification of compounds are main topics for polymorphism research. Modeling is applied by the well known fingerprinting by simulation of powder X-ray data and in the field of method development. Precise simulations of X-ray experiments give valuable information about possible pathways for establishing methods for quantification of mixtures of different polymorphic forms. As virtually all important parameters of the experiment can be taken into account the development can be done much faster and the result can be predicted well precise before in lab experiments take place.[1]
Morphology prediction is another applied technique in the development of a drug substance. Materials behave mechanically different upon change in morphology, e.g. due to crystallization and/or different polymorphic forms. Processes like milling depend on the processibility of a given compound. This technique is often applied for trouble shooting when the compound shows unfavorable properties like stickiness or electrostatic charging of the particles. The technique is discussed with the example of Glycopyrronium bromide.[2]

1. Poster presentation at PPXRD-4, Barcelona (2005)
2. J. J. Guy, T. A. Hamor, J. Chem. Soc., Perkin Trans.2 (1973)