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Physicochemical characterization of crystalline supramolecular systems containing established drugs and new drug candidates

Mino R Caira
University of Cape Town, South Africa

Crystalline supramolecular systems containing drug molecules, for example drug solvates, co-crystals and inclusion compounds, are enjoying increasing attention as they represent new multi-component forms whose pharmaceutically relevant properties (e.g. aqueous solubility, stability, developability) may be significantly more favourable than those of the untreated drug. In the case of established drugs, this could translate into extended patent life, while for new drug leads early intervention in generating such 'supramolecular derivatives' could facilitate the selection of the most promising contenders for further development. Physicochemical characterization of these multi-component crystalline phases to establish their stoichiometric composition, thermodynamic stabilities and structural nature at the molecular level is essential but can often pose more challenges than those encountered when dealing with single-component systems (e.g. polymorphically pure drugs). Such challenges may be associated with included solvent (e.g. content variability and structural disorder) and with difficulties in unequivocal assignment of the nature of heteromolecular interactions (e.g. distinguishing co-crystals and salts). This presentation will focus on the use of thermal analysis and X-ray diffraction methods on both powders and single crystals as fundamental techniques used to address these issues. Their application to supramolecular systems such as co-crystals of active pharmaceutical ingredients and cyclodextrin inclusion complexes of bioactive molecules will be illustrated. Closely related topics to be highlighted are the ubiquitous occurrence of crystal polymorphism for the systems in question and the limits of the utility of powder X-ray diffraction in phase identification.

Biography

Mino R Caira has directed the Centre for Supramolecular Chemistry Research at the University of Cape Town (UCT) since 2005. He retired as Professor of Physical Chemistry in 2014 and was subsequently appointed as a Senior Scholar in the Department of Chemistry at UCT. His expertise is in the area of solid-state chemistry of drug polymorphs and novel multi-component systems containing active pharmaceutical ingredients. He has published over 300 papers in international journals and since 2009 has served on the Editorial Advisory Board of the *Journal of Pharmaceutical Sciences*.

mino.caira@uct.ac.za

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