Poster Presentation

MS67.P18

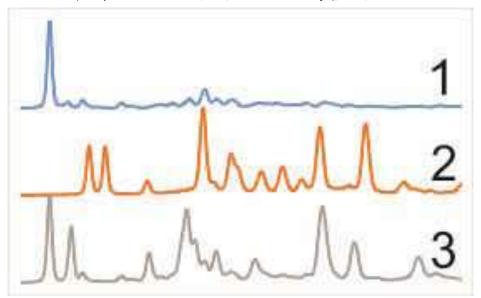
Co-crystals and inclusion compounds of leucyl-containing dipeptides

M. Ignacio¹, A. Smith¹, D. Soldatov¹

¹University of Guelph, Department of Chemistry, Guelph, Canada

Short peptides are ecologically friendly and non-toxic molecules, so they can be safely utilized in green chemistry processes or incorporated in pharmaceuticals and food additives. It has been shown that some dipeptides can form crystals that incorporate other molecules through intermolecular hydrogen bonding and van der Waals interactions[1]. The utilization of such dipeptides for solid state organic synthesis or storage and stabilization of bioactive molecules would be of great practical interest, but the principles that define the successful combinations are not clear. In order to identify what factors lead to complementary pairs of a dipeptide and a second component, a series of leucine-containing dipeptides was screened against 40 organic solvents and solids. Direct or solvent-assisted grinding was used followed by PXRD analysis. It was found that each dipeptide was able to form new phases with some of the utilized reactive and bioactive molecules. The Figure illustrates three experimental powder patterns in the 5-35 20 degree range. The dipeptide leucyl-valine (1) and the second component 5-acetylsalicylamide (2) combine to form a new crystalline phase (3). After screening was complete, a series of crystallizations was performed and several crystals comprised of both a dipeptide and another molecule have been isolated and studied. A number of structural motifs were observed, although a layered architecture with the second component included in the interlayer space prevailed.

[1] D.V. Soldatov, Nanoporous Materials (A. Sayari and M. Jaroniec, eds.; N.J.: World Scientific), 2008, 213-224.



Keywords: peptides, co-crystals, screening