List of ten best papers

1. Modi, S. R.; Dantuluri, A. K.; Perumalla, S. R.; Sun, C. C.; Bansal, A. K. Effect of crystal habit on intrinsic dissolution behavior of celecoxib due to differential wettability. **Crystal Growth Design,**2014: 14, 5283-5292 (Cited by 9; Citation / year = 4.5)

It has been speculated that the differential surface contribution of crystal facets in different crystal habits may affect pharmaceutical performance, however, convincing experimental evidence has been lacking in the scientific literature. We established a molecule-centered approach towards crystal habit modification of a BCS class II drug, celecoxib (CEL) and its effect on solubility, dissolution behavior, oral bioavailability and overall pharmaceutical product performance.

2. Gupta P, Kakumanu V K and Bansal A K. Stability and solubility of celecoxib–PVP amorphous dispersions: a molecular perspective. **Pharmaceutical Research,** 2004: 21(10), 1762-1769 (Cited by 125; Citation / year = 10.4)

This paper unveiled the molecular events responsible for stabilization, recrystallization and performance of ASDs. A novel inverse relationship was established between enthalpy relaxation and solubility advantage from ASD.

3. Kaushal A M, Gupta P and Bansal A K. Amorphous drug delivery systems: Molecular aspects, design, and performance. **Critical Review in Therapeutic Drug Carrier System,** 2004:21(3), 133–193 (Cited by 182; Citation / year = 15.2)

Fundamental understanding of thermodynamic and kinetic factors governing physical stability of amorphous state remains one of the areas of interest for pharmaceutical industry. This critical review captures the deep scientific understanding of this topic. This has implications in development of amorphous solid dispersions with enhanced aqueous solubility and oral bioavailability.

4. Shete, Ganesh, Pawar, Yogesh, Thanki, Kaushik, Jain, Sanyog and Bansal, AK. Oral bioavailability and pharmacodynamic activity of hesperetin nanocrystals generated using a novel bottom-up technology. **Molecular Pharmaceutics** 2015 Apr 6;12(4):1158-70. doi: 10.1021/mp5008647 (Cited by 5)

Our laboratory has patented and out-licensed to industry-partner, a novel 'bottom-up' spray drying based process for the generation of nanocrystalline solid dispersion (NSD) of drugs called as 'NanoCrySP technology'. NanoCrySP is a spray drying based method to generate solid

particles containing drug nanocrystals and small molecule excipients. Latter act as a crystallization inducing agent and encourage nucleation of drug crystals.

5. Kaushal A, Chakraborti A K and Bansal A K. FTIR Studies on differential intermolecular association in crystalline and amorphous states of structurally related non-steroidal anti-inflammatory drugs. **Molecular Pharmaceutics**, 2008:5(6), 937–945 (Cited by 39; Citation / year = 5.6)

Differential intermolecular interactions in crystalline and amorphous form are critical for selection of stabilization strategies of amorphous form. FTIR studies were carried out, using four structurally similar COX-2 inhibitors, to obtain insights into intermolecular interactions in crystalline and amorphous states. Self aggregation tendency explained differential intermolecular interactions between different drugs. Hydrogen bond strength of similar groups in crystalline state was grossly different while they were similar in the amorphous state, due to removal of constraints posed by crystal packing.

6. Thakur PS, Thakore SD, and Bansal AK. Role of Surface Characteristics of Mannitol in Crystallization of Fenofibrate during Spray Drying. **Journal of Pharmaceutical Sciences,** 109(2), Feb 2020, Pages 1105-1114

This study investigates the role of surface characteristics of mannitol on crystallization kinetics of amorphous fenofibrate. Crystallization kinetics of amorphous fenofibrate was assessed on 2 surfaces of mannitol having different porosity, roughness, and polarity. Fenofibrate showed faster crystallization in the presence of rougher surface (t_{ind} < 1 min) compared with smooth surface (t_{ind} = 49.28 min). This was attributed to higher porosity (75%) and surface polarity (~1.25-fold) of rough surface as compared with smooth surface. Polar nature provided primitive sites for faster crystallization of amorphous fenofibrate.

7. Dynaneshwar K, PV Bharatam, CM Nagaraja, G Dubey, DP Kale, B Ugale and Bansal AK. Molecular basis of water sorption behavior of rivaroxaban-malonic acid cocrystal. **Molecular Pharmaceutics**, 2019, 16(7), 2980-2981

The present study aims to investigate the molecular basis of water sorption behavior of rivaroxaban-malonic acid cocrystal (RIV-MAL). It was hypothesized, that the amount of water sorbed by a crystalline solid is governed by the surface molecular environment of different crystal facets and their relative abundance to crystal surface. The study highlights that the amount of water sorbed by the cocrystalis governed by the surface molecular environment and additionally by the strength of hydrogen bonding. This investigation has implications on designing materials with a desired moisture-sorption property.

8. Phadke C, Sharma J, Sharma K, Bansal AK. Effect of variability of physical properties of povidone K30 on crystallization and drug-polymer miscibility of celecoxib-povidone K30 amorphous solid dispersion. **Molecular Pharmaceutics** 2019, 16(10), 4139-4148

In the present study, we have investigated the variability in physical properties of povidone K30 (PVP K30) and its impact on crystallization and drug–polymer miscibility of celecoxib–PVP K30 (CLB–PVP K30) amorphous solid dispersions (ASDs).The % crystallization showed correlation to particle size distribution (PSD) (weak positive), glass transition (T_g) (weak positive), drug–polymer miscibility (moderate negative), true density, and porosity (moderate positive) and hygroscopicity (strong positive). Miscibility showed correlation between T_g (weak positive), hygroscopicity (weak negative), PSD (moderate negative), and true density and porosity (strong negative). The study suggests PSD, hygroscopicity, true density, and porosity of PVP K30 as the functionality related characteristics for its intended functionality of physical stability when it is used as a stabilizer in ASDs.

9. Sheokand S, Sharma J and Bansal AK. Effect of surfactants on the molecular mobility and crystallization kinetics of hesperetin. **CrystEngComm**, 2019, 21, 3788-3797

This work compares the effects of the incorporation of surfactants, SLS and DOSS on the crystallization kinetics of hesperetin along with mannitol. The molecular dynamics of amorphous hesperetin in the presence of excipients and their isothermal crystallization kinetics were studied using dielectric relaxation spectroscopy (DRS) and modulated differential scanning calorimetry (mDSC) techniques, respectively. Addition of a combination of SLS–DOSS yielded an approximately 11-fold decrease in α-relaxation times when compared with pure amorphous hesperetin. Secondly, the combination of SLS and DOSS promoted the nucleation of hesperetin while their crystal growth was hindered. This study illustrated the relationship between the crystallite size of hesperetin NCSDs and the type of excipient/surface modifier(s).

10. Sheokand S, Modi SR and Bansal AK. Quantification of low levels of amorphous content in crystalline celecoxib using dynamic vapor sorption (DVS), **European Journal of Pharmaceutics and Biopharmaceutics**2016 May;102:77-86.

A minor amount of amorphous phase, especially present on the surface of crystalline pharmaceutical actives, can have a significant impact on their processing and performance. Despite the presence of sophisticated analytical tools, detection and quantification of low levels of amorphous content pose significant challenges owing to issues of sensitivity, suitability, limit of detection and limit of quantitation. Current study encompasses the quantification of amorphous content in the crystalline form of celecoxib (CLB) using a dynamic vapor sorption (DVS) based method. It was able to detect the presence of amorphous phase in a predominantly crystalline phase at concentrations as low as 0.3% w/w. The limit of quantitation was found to

be 0.9% w/w. Moreover, the influence of mechanical processing on the amorphous content in crystalline CLB was also investigated.