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Carbon-based nanostructures for single-molecule investigations

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We present a universal approach for the generation of multifunctional nanomaterials that employ molecular building blocks assembled on carbon nanotube (CNTs) electrodes. We will demonstrate single-molecule control in the formation of nano-hybrids via the in-solution assembly of classes of molecular materials (organic, inorganic, and biological with promising attributes) to DNA wrapped CNTs. We have linked in solution metallic single-walled CNTs (SWCNTs) with different conjugated molecular wires, and measured the molecular conductance in these molecular transport junctions, highlighting the potential of an all-carbon based approach for solution-processable molecular electronics (see image). Additionally, we produced organic-inorganic heterostructures consisting of single quantum dots (QDs) univocally linked at the terminal ends of individual SWCNTs. Monofunctionalized SWCNT-QD heterostructures were obtained and photo physical investigations at the single nanohybrid level showed evidence of electronic coupling. Studies in this context are critical in the design of novel QD-based optoelectronic and light-energy conversion devices. Finally, we will demonstrate site-specific assembly of single proteins on individual SWCNTs. As a proof of concept, we investigated different CNT-protein configurations and obtained evidence of site-specific coupling between SWCNTs and specific proteins of interest. Notably, only the right bioengineered system exhibited the expected direct protein-nanotube communication, paving the way to selective electrical addressability of proteins via the use of carbon nano electrodes.

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Physicochemical and mechanical evaluation of a novel theophylline and 4-aminobenzoic acid pharmaceutical co-crystals

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Statement of the Problem: Pharmaceutical cocrystals are solids that are crystalline materials comprise of two or more components held together by non-covalent forces. In recent years co-crystals are being studied intensively due to the potential for improved pharmaceutical properties such as increased solubility, bioavailability, chemical stability and hygroscopicity of active pharmaceutical ingredients. A crystalline particle is characterized by definite crystal habit which relates to the external structure (such as shape and size) and crystal lattice describes the internal structures. Change in crystal forms has significant effect on drug particle mechanical properties (particle strength, flowability, miscibility and tableting) dissolution rate and stability. To enhance understanding of co-crystallization process on mechanical properties of Theophylline (active pharmaceutical ingredient) in the present study the impact of crystal structure and its relationship with powder compaction has been investigated.

Methodology: Novel theophylline and 4-aminobenzoic acid pharmaceutical co-crystals at molar ratio of 1:1 were synthesized by solvent evaporation and mechano-chemical synthesis techniques. Co-crystals were mainly characterized by powder X-ray diffraction (PXRPD), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FTIR) and single crystal X-ray diffraction. Theophylline cocrystals were also subjected to powder flow, powder compaction and relative humidity stability testing studies.

Findings & Significance: The molecular structure of the novel theophylline and 4-aminobenzoic acid pharmaceutical cocrystal was further confirmed using single crystal X-ray diffraction analysis. Finally crystal structure and its relationship can be considered for improving mechanical properties of API.

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