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Abstract	:	Understanding the synthonic and surface energy properties of a drug molecule is essential for optimising the performance of formulated products, particularly in the pharmaceutical industry. However, gaining this insight often requires costly trial-and-error experiments. In this study, advanced surface analysis tools were introduced that provided visualisation and topological information based on crystallographic data. By using functional group analysis, roughness calculations, and statistical interaction data, direct comparisons of crystal surfaces were enabled. Molecular modelling simulations were conducted utilising Material Studio 7.0 software to evaluate the suitability of lactose (as an excipient) and aspirin (as an active pharmaceutical ingredient, API) crystals for the selective laser sintering (SLS) 3D-printing process. The study also examined each crystal's morphology, lattice energy convergence, and contributions, such as interatomic and intermolecular interactions. These simulations offered preliminary insights into the potential compatibility of the selected compounds. Surface analysis of the aspirin and lactose crystal facets ranked their stability from strongest to weakest. For aspirin, the ranking was (1 0 0), (0 1 1), and (0 0 2), while for lactose, the order was (0 2 0), (0 0 1), and (0 1 1), indicating greater stability in the lactose facets. Theoretically, crystal faces with higher attachment and slice energies grow more rapidly and hold less morphological importance (MI), resulting in smaller surface areas. The stability of lactose monohydrate crystals may be linked to the presence of water molecules in their structure, which enhance the binding between the two substances...see more.