

Principal Component Analysis in Drug-Excipient Interactions

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Abstract : Studies about the interaction between active pharmaceutical ingredients (API) and excipients are so important in the pre-formulation stage of development of all dosage forms. Analytical techniques such as differential scanning calorimetry (DSC), Thermal gravimetry (TG), and Fourier transform infrared spectroscopy (FTIR) are commonly used tools for investigating regarding compatibility and incompatibility of APIs with excipients. Sometimes the interpretation of data obtained from these techniques is difficult because of severe overlapping of API spectrum with excipients in their mixtures. Principal component analysis (PCA) as a powerful factor analytical method is used in these situations to resolve data matrices acquired from these analytical techniques. Binary mixtures of API and interested excipients are considered and produced. Peaks of FTIR, DSC, or TG of pure API and excipient and their mixtures at different mole ratios will construct the rows of the data matrix. By applying PCA on the data matrix, the number of principal components (PCs) is determined so that it contains the total variance of the data matrix. By plotting PCs or factors obtained from the score of the matrix in two-dimensional spaces if the pure API and its mixture with the excipient at the high amount of API and the 1:1 mixture form a separate cluster and the other cluster comprise of the pure excipient and its blend with the API at the high amount of excipient. This confirms the existence of compatibility between API and the interested excipient. Otherwise, the incompatibility will overcome a mixture of API and excipient.

Keywords : API, compatibility, DSC, TG, interactions

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