PREDICTIVE SCIENCES AND HIGH THROUGHPUT SCREENING COMBINED FOR EFFICIENT FORMULATION DEVELOPMENTS

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The applied predictive formulation sciences, Hansen Solubility Parameters (HSP) and Hydrophilic Lipophilic Difference – Net Average Curvature (HLD-NAC) are very powerful to find matching ingredients, resulting in improved stability and efficacy of end-products. These models are applicable to solutions, dispersions and emulsions, which basically includes all types of formulated products. Although they have been applied for many years, there is still a limited use in formulation developments and ingredients thereof. The equations of these sciences require (practical) parameters of the ingredients and once generated, compatible ingredients can be predicted to develop and optimize specific formulations. The ingredient data generated from these models is predictive and sustainable: you can use them over and over, allowing to move away from trial-and-error and improve digitalization into product developments. A very efficient way to enhance the properties and reduce complexity, time and cost in the development of formulations or ingredients. When combined with High Throughput (HT) screening for automated, parallel and small-scale preparation of samples and end-products, further efficiency can be achieved. The predictive sciences and the required ingredient parameters will be explained via practical applications to showcase how this can lead to efficient product developments, even making incompatible ingredients compatible with the rest of the formulation. Also, how to further increase efficiency by means of HT screening will be explained and why this is needed to fill up the ingredient database for these predictive sciences.

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