**Poster 12**
**Informatics meets energetics for rapid de-risking of medicines**

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**Purpose**
Computational based predictive and informatics-based tools to design and de-risk medicines have seen tremendous growth in the last decade and have been recently well-integrated within pharmaceutical research. Advanced computational tools employing first-principles electronic structure theory, molecular dynamics, data-driven modeling, and machine learning have been incorporated into workflows for both solid-state and formulation design. One of the common applications of computational tools within the pharmaceutical industry is to understand the risk of crystal polymorphism.

This poster presentation is intended to introduce advancements in computational modeling techniques employed by pharmaceutical industries to de-risk medicines and understand the risk associated with polymorphism. We further plan to discuss the integration of energetically based computational models to data-driven informatics-based approaches for rapid de-risking of medicines.

**Methods**
One of the several energetics-based tools includes Crystal Structure Predictions (CSP) which provides us with an energetically ranked landscape of tens to hundreds of structures to compare with the experimental form and identify the risk of finding a more stable structure than the observed form. The informatics-based approaches, on the other hand, allow for a rapid understanding of the potential risk of polymorphism by comparing the structures against a large dataset consisting of > 1.1M experimental structures maintained by the Cambridge Crystallographic Data Centre (CCDC). Within the informatics-based tools, some routinely used approaches include looking at the inter- and intra-molecular geometry, interaction donor-acceptor maps, and hydrogen bonding networks.

**Results**
Although quite robust, CSP calculations are computationally expensive and are triggered at a later stage in the MatSci workflow. The application of computationally inexpensive informatics-based tools to explore CSP-based landscapes remains an area of interest for the pharmaceutical industry. With the creation of the novel CSD Landscape Generator that allows for generating a solid form landscape using informatics, another opportunity to find a correlation between Informatics and CSP-based landscapes emerges. Establishing a correlation between Informatics and Energetics could allow for rapid de-risking at the earlier stages of our workflow.

**Conclusion**
Energetics-based predictive tools have been well-integrated within Material Science workflows for de-risking active pharmaceutical ingredients (API) and understanding the risk of polymorphism. In this poster we discuss some recent advancements in the crystal structure prediction (CSP) framework and propose a plan for implementation for “Informatics meets energetics” based modeling approaches for rapid de-risking & design of medicines. In this poster, we discuss the advancements in the CSP framework and propose a plan for “Informatics meets energetics”.

**Keywords:** CSP, healthchecks, derisk, design, polymorphism, computational