Artificial neural networks for co-crystal prediction

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A significant amount of attention has been given to the design and synthesis of cocrystals by both industry and academia because of its potential to change a molecule's physicochemical properties. Yet, difficulties arise when searching for adequate combinations of molecules (or coformers) to form cocrystals, hampering the efficient exploration of the target's solid-state landscape.

Here we present the application of a data-driven cocrystal prediction method, based on two types of artificial neural network models and cocrystal data present in the Cambridge Structural Database [1]. The models accept pairs of coformers and predict whether a cocrystal is likely to form. By combining the output of multiple models of both types, our approach shows to have excellent performance on the proposed cocrystal training and validation sets, and has an estimated accuracy of 80% for molecules for which previous cocrystallization data is unavailable [2].

[1] Devogelaer, JJ, Meekes H, Tinnemans P, Vlieg E, de Gelder R. Cocrystal prediction by artificial neural networks, Angew. Chem. Int. Ed. 2020, 59, 21711-21718.
[2] Devogelaer, Charpentier MD, Tijink A, Dupray V, Coquerel G., Johnston K. JJ, Meekes H, Tinnemans P, Vlieg E, ter Horst JH, de Gelder R., Cryst. Growth Des. 2021, 21, 3428-3437