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One hydrogen bond does not a separation make, or does it?-The importance of high resolution structural data

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The enantiomeric purity of a chemical entity is important in various industries, such as analytical, food, pesticide and pharmaceutical. When a compound is produced as a racemic modification typically only one of the enantiomers exhibits the required biological effect. One of the main resolution method is based on the formation of diastereomeric salts. The full understanding of the mechanism of chiral discrimination may lead us to design the 'perfect' resolving agent for a given racemic modification.
In order to understand the molecular recognition during the resolution process we have studied a series of inclusion compounds [1] and diastereomeric salt formations [2] to map the correlation between structure and the success of the enantiomeric resolution. One of our latest publications [3] discusses a series of experiments when a sugar derivative was employed to resolve racemic chiral amines. The non-bonding interactions which give rise to the structures of the diastereomeric salts were analyzed and the selectivity was explained by the formation of one additional hydrogen bond between the ion pairs. This result emphasizes the importance of high resolution structural data to obtain accurate hydrogen atom positions.

[1] a) Báthori, N. B., Nassimbeni, L. R. (2010). Cryst. Growth & Des., 10, 1782-1787. [2] a) Báthori, N. B. Nassimbeni, L. R. Oliver, C. L. (2011) Chem. Commun., 47, 2670–2672. b) Nassimbeni, L. R, Báthori, N. B., Curtin, T.-L. (2012) Cryst. Growth & Des., 12, 4144–4148. [3] Báthori, N. B. Nassimbeni, L. R. van de Streek, J. (2015) Chem. Commun., 51, 5664-5667.

Summary

The presentation aims to highlight the importance of high resolution structural data when single crystal structures are interpreted.

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