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Predictive application of bioisostere transformations to identify novel high quality compound ideas

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Abstract

We will describe how the principle of bioisosterism can be applied, in combination with predictive modelling and multi-parameter optimisation, to quickly search for new, high quality compound ideas and optimisation strategies. Bioisosteres are functional groups which have similar physical or chemical characteristics and hence similar biological effects. The relationships between bioisosteres may be encoded as molecular transformations and automatically applied to new compounds to generate novel compound structures that are likely to preserve the required biological activities. *In silico* models can be applied to predict the properties of the resulting structures, such as ADME and physicochemical characteristics. These data can, in turn, be integrated using a multi-parameter optimisation approach to prioritise those ideas that are most likely to achieve a required property profile. To illustrate this, we will discuss how the BIOSTER™ database of >20,000 precedented bioisostere transformations and molecular modifications resulting from alternative analogue design techniques [1] has been integrated with the StarDrop™ software [2]. We will describe example applications in drug discovery, including lead hopping and patent protection.