Functional group switching: harnessing the power of bioisosterism strategies in drug design

Colin Bournez[1], Alain Valery[1], Christophe Salome[1], Quentin Lefebvre[1] and Thomas Fessard[1]

[1]*SpiroChem AG, Rosental area, WRO-1047-3 | Mattenstrasse 22 4058 Basel, Switzerland*

The replacement of specific atom(s) or functional group(s) during a drug design/optimization project represents a significant strategic approach. It can serve diverse objectives for the molecule such as the optimization of its physico-chemical properties, the augmentation of its activity, or the improvement of its synthetic accessibility, among others. The concept of bioisosteric replacement is the substitution of functional groups in a molecule with alternative groups possessing comparable biological properties (Figure 1). This can provide novel SAR hypotheses and the access to unexplored chemical spaces that are unencumbered by intellectual property limitations. In this poster, we present our scaffold switching capabilities at SpiroChem, facilitating the seamless replacement of virtually any motif in a molecule while preserving its essential characteristics. Furthermore, we present recent illustrative examples highlighting the impact of such replacements on the overall properties of the molecules [1,2].

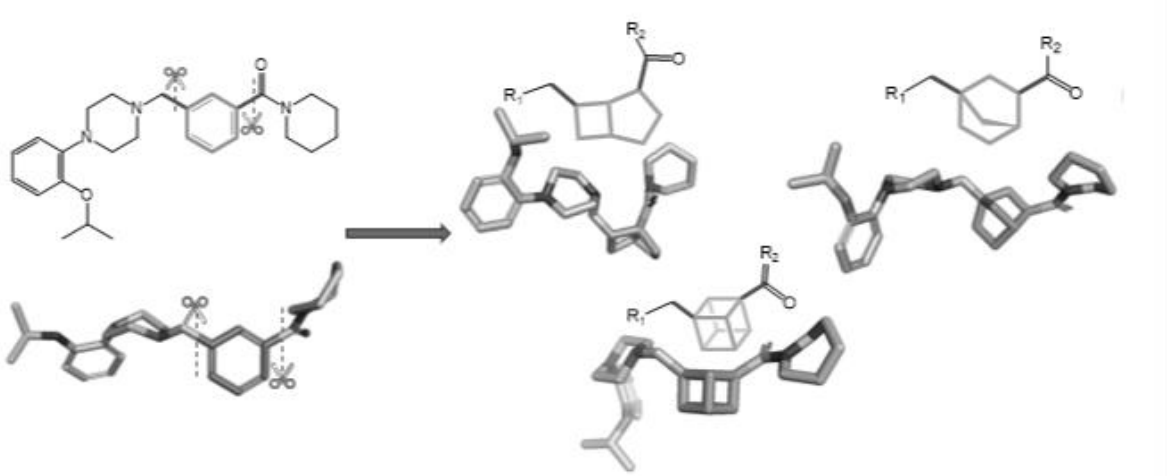

Figure 1. Various example of switching core of a molecule

Bibliography :

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