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Systematic computational SAR analysis

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In medicinal chemistry, the exploration of structure-activity relationships (SARs) plays a fundamental role in hit-to-lead projects and lead optimization programs. Typically, SARs are explored on a case-by-case basis and comparative or large-scale SAR analyses are rarely reported.

We aim at a systematic computational exploration of global and local SAR characteristics of compound data sets. Only few attempts have been made thus far to qualitatively evaluate global SAR features, for example, through the introduction of Structure-Activity Similarity Maps [1] or 2D/3D Similarity Correlation Graphs [2]. In addition, global and local SAR characteristics have also been quantitatively assessed by means of the SAR [3] and SALI [4] function, respectively.

Here compound-based SARI scoring and annotated molecular network representations are introduced that make it possible to systematically relate global and local SAR features to each other and identify key compounds that are SAR determinants.

References

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