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Detection, analysis, and visualization of relevant scaffolds in medicinal chemistry project databases

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Analysis of structure-activity relationships within lead optimization databases requires knowledge of each of the common scaffold substructures, an understanding of how the substitution sites map to each other, and an optimal assignment of scaffolds to input molecules in the event of ambiguity. We will present algorithms for solving each of these problems, which are capable of operating using only the molecules themselves as input, as well as being able to take into account any scaffold hints which may be known beforehand. Also discussed will be methods for depicting the resulting information in a visually intuitive way, as well as compilation of the results in the form of a report, which allows structure-activity trends to be examined interactively.