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PocketGraph: graph representation of binding site volumes

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The representation of small molecules as molecular graphs [1] is a common technique in various fields of cheminformatics. This approach employs abstract descriptions of topology and properties for rapid analyses and comparison. Receptor-based methods in contrast mostly depend on more complex representations impeding simplified analysis and limiting the possibilities of property assignment. In this study we demonstrate that ligand-based methods can be applied to receptor-derived binding site analysis.

We introduce the new method PocketGraph that translates representations of binding site volumes into linear graphs and enables the application of graph-based methods to the world of protein pockets. The method uses the PocketPicker [2] algorithm for characterization of binding site volumes and employs a Growing Neural Gas [3] procedure to derive graph representations of pocket topologies.

Self-organizing map (SOM) projections revealed a limited number of pocket topologies. We argue that there is only a small set of pocket shapes realized in the known ligand-receptor complexes.

References

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