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# Applications of chemography in natural products

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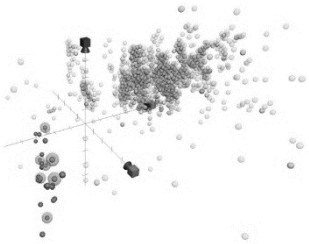
The concept of chemography, navigating chemical space, have over the last decade been applied to a number of studies of natural products.
It has been demonstrated that the concept of proximity in the ChemGPS-NP eight-dimensional chemical property space can be interpreted as a molecular similarity [2], and hence a proxy for the expected biological activity of a particular compound [1].
Combined with methods to define volumes from asymmetric 'clouds' of compound representations, and estimating if a specific compound representation is included in that volume, this provide us with a way of predicting biological activity for a compound – or indicating that an observed activity might be a result of a novel mode of action [3,4].
The basis of an efficient exploration of these possibilities, will be the definition of high-quality reference sets for different biological activities, effectively acting as placeholders.
In this study examples of these applications are demonstrated and discussed.



ChemGPS-NP-based analysis for a series of briarane-type diterpenoids active in an inhibition assay of COX-2, as well as previously studied 2,592 COX-2 (light green) inhibitors from the ChEMBL database.

## References

[1] Buonfiglio R et al. *J Chem Inf Mod.* 2015; 55:2375-2390.
[2] Rosén J et al. *J Med Chem* 2009; 52:1953-1962.
[3] Xu J-H et al. *Marine Drugs* 2018; 16:75-83.
[4] Yang L et al. *Molecules* 2017; 22:1392-1408.