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Poster presentation

MolWind – mapping molecule spaces to geospatial worlds

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Visualizing molecular contexts represented by bioactive compounds, genes, proteins etc. and their relationships remains a challenging task. Mapping of structural spaces to geospatial layers can provide unique ways of intuitive navigation in complex data sets and therefore improve data analysis. We have implemented a server called Molwind which communicates with NASA's geo browser "World Wind" [1] by dynamically generating molecule layers and tiles from a set of chemical structures that have been hierarchically partitioned before. For the organization of chemical datasets we have chosen a combination of Murcko fragmentation [2], ring extraction and iterative substructure searches resulting in a hierarchy of fragments which grow larger with increasing levels or depth.

Our server enables scientists to interactively browse chemical compound spaces by changing between different levels of structural detail while maintaining relationships between similar (neighbouring) compound classes. Conceptually, it allows arbitrarily layered datasets to be served to the World Wind client and can therefore be easily extended to visualize e.g. protein families or pathway modules. The already existing functionality and extendibility of NASA's World Wind system sets an excellent basis for leveraging the interactivity offered by modern geospatial browsers in the area of research data exploration.

References

1. **NASA World Wind** [http://worldwind.arc.nasa.gov/]
2. Murcko MA: **The Properties of Known Drugs – 1.** *Molecular Frameworks* . Bemis GW, *J Med Chem*, 1996, **39**: 2887.