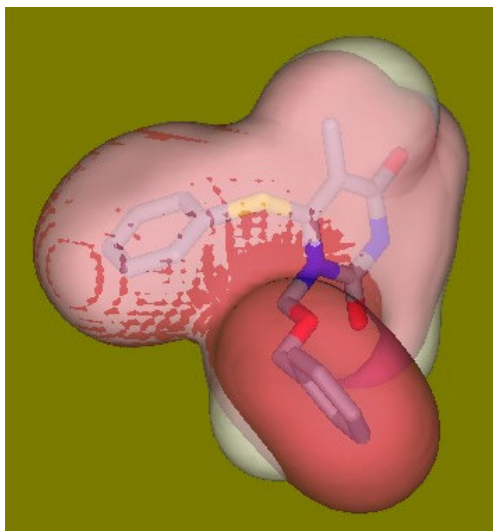


Shape Module



The *Shape Module* utilizes the *Shape Toolkit* from OpenEye Scientific Software to generate Tanimoto, Tversky, and Ochai (1-Cosine) 3D shape similarities between conformers of input datasets, such as hits from an HTS screen. MXN similarity searching can be performed, or compounds can be clustered either asymmetrically or symmetrically by shape utilizing the *Grouping Module*. Resulting clusters can be visualized via *VIDA* from OpenEye Scientific Software. Shape centroids can be extracted and lead hopping hitlists obtained which display both the 2D and 3D similarity scores. 2D similarity scores are generated from the 320 “drug like” MDL Keys in the *Fingerprint Module*. Hitlist statistics are also included.

System Architecture: Linux Red Hat 7.x, Irix 6.5, Win 2000

Software Requirements: *Shape toolkit*, (optional: *Omega*, *VIDA*, and *OEChem*) OpenEye Scientific Software, business@eyesopen.com.

Mesa Module Requirements: *Fingerprint Module* or binary fingerprint input (for lead hopping), *Grouping Module* (for shape clustering)

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