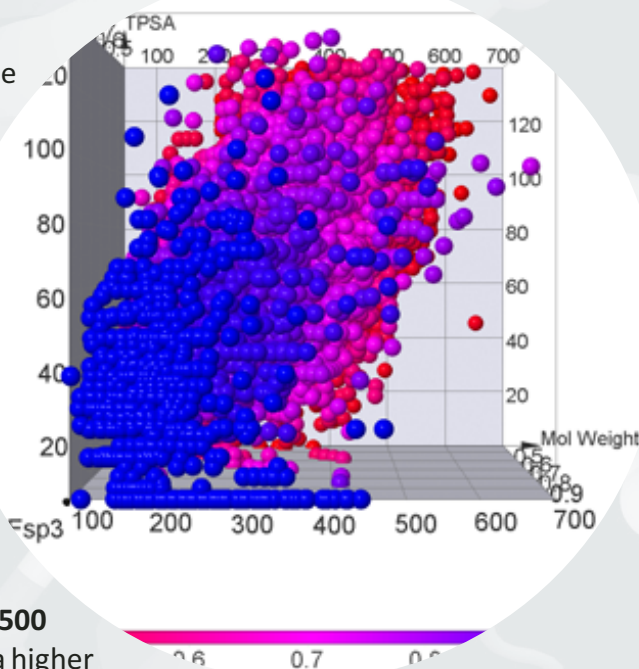


## Fsp3 Compound Library

Scientific community studying medical chemicals has become increasingly aware of the value of the physical and structural properties of molecules. It is now known that the molecules which follow Lipinski's rule of five are more likely to appear biologically active. Other thresholds for properties were also proposed, for example, topological polar surface area and rotatable bonds number. Following the work of Frank Lovering et al. "Escape from Flatland: Increasing Saturation as an Approach to Improving Clinical Success", which discovers saturation of chemical compounds as the measure of the likelihood of compounds to be biologically active, we created a library which comprises known thresholds of medical compounds and also contains highly saturated compounds.

Reaxense's **Fsp3-enriched Compound Library** comprises **34,500 small molecules** of non-flat drug-like screening compounds with a higher potential for biological activity.



### Features:

- **34,500  $sp^3$ -enriched compounds**
- **High diversity over the library**
- **Purity >90%; spectral data available**
- **TPSA (Topological Polar Surface Area) < 140**
- **Rotatable bonds count  $\leq 10$**
- **Fsp3 > 0.4**
- **Lipinski's rule of five compliant (one restriction can be violated)**

# Selection Criteria:

Parameter	Value
Fsp3	> 0.4
Number of Hydrogen Bond Acceptors (HBA)*	≤ 10
Number of Hydrogen Bond Donors (HBD)*	≤ 5
Number of Rotatable Bonds (RB)	≤ 10
Topological Polar Surface Area (TPSA)	<140
Molecular Weight (MW)*	200 - 500
Octanol-water Partition Coefficient (cLogP)*	≤ 5

\*One of these criteria can be violated

## Structure examples:

