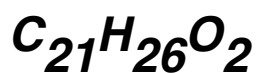


Molecular formula

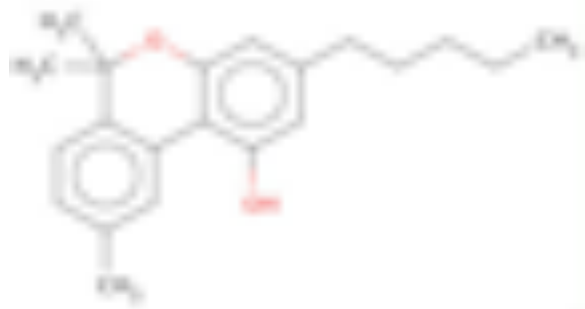


Constitutional Descriptors

Atom count
Bond count

...

Labeled graph

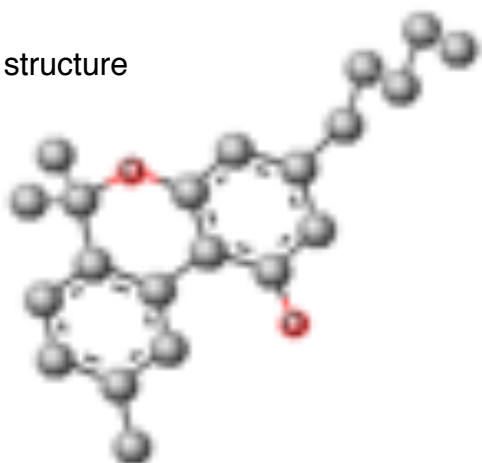


Topological Descriptors

Longest chain
Number of rings
Graph invariants
BCUT

...

3D structure

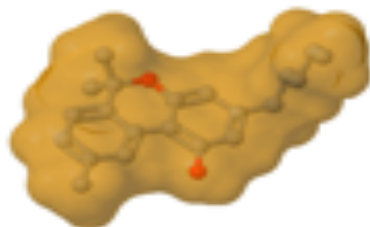


Geometric Descriptors

Moments of inertia
3D Autocorrelation
WHIM
Number of rings

...

Surface



Hybrid Descriptors

CPSA
Electrotopological indices
Shape descriptors
Zernike moments

...