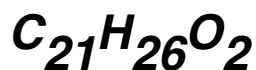


Molecular formula

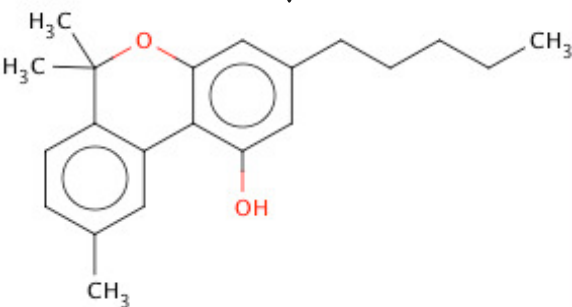


### Constitutional Descriptors

Atom count  
Bond count

...

Labeled graph

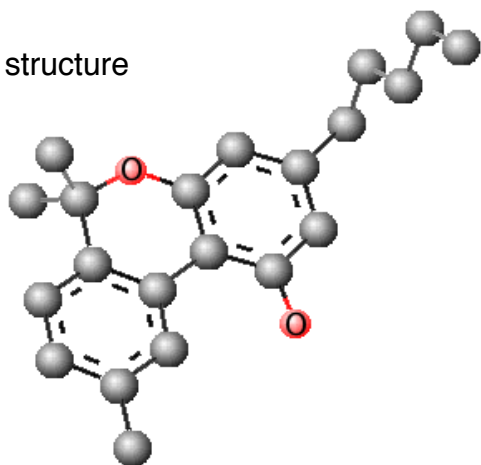


### Topological Descriptors

Longest chain  
Number of rings  
Graph invariants  
BCUT

...

3D structure

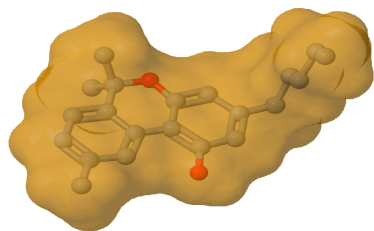


### Geometric Descriptors

Moments of inertia  
3D Autocorrelation  
WHIM  
Number of rings

...

Surface



### Hybrid Descriptors

CPSA  
Electrotopological indices  
Shape descriptors  
Zernike moments

...