

## Common chemical descriptors for QSAR/QSPR analysis

Chemical descriptors	Based on	Examples
Theoretical descriptors		
0D	Molecular formula	Molecular weights, atom counts, bond counts
1D	Chemical graph	Fragment counts, functional group counts
2D	Structural topology	Weiner index, Balaban index, Randic index, BCUTS
3D	Structural geometry	WHIM, autocorrelation, 3D-MORSE, GETAWAY
4D	Chemical conformation	Volsurf, GRID, Raptor
Experimental descriptors		
Hydrophobic parameters	Hydrophobicity	Partition coefficients (logP), hydrophobic substituent constant ( $\pi$ )
Electronic parameters	Electronic properties	Acid dissociation constant, Hammett constant
Steric parameters	Steric properties	Taft steric constant, Charton's constant