

List of 12 sets of fingerprint descriptors calculated from the PaDEL-Descriptor software.

Fingerprint	Number	Description
2D Atom Pairs	780	Presence/absence of atom pairs for different topological distances.
2D Atom Pairs Count	780	Number of frequency of atom pairs for different topological distances.
E-state	79	Electrotopological state atom types
CDK	1,024	Fingerprint with a length of 1,024 and search depth of 8.
CDK Extended	1,024	Extends the fingerprint with additional bits describing ring features.
CDK Graph Only	1,024	A special version that considers only the connectivity and not the bond order.
Klekota-Roth	4,860	Presence/absence of SMARTS patterns for functional groups.
Klekota-Roth Count	4,860	Frequency counting of SMARTS patterns for functional groups.
MACCS	166	Binary representation of chemical features defined by MACCS keys.
PubChem	881	Binary representation of substructures, as defined by PubChem.
Substructure	307	Presence/absence of chemical substructures.
Substructure Count	307	Frequency count of chemical substructures.