The top features were collected from SelectFromModel of RandomForestRegressor model for HDAC.

Features	Bit Substructure	Section description
PubChemFP338	C(~C)(~C)(~H)(~N)	Simple atom nearest neighbors - These bits test for the presence of atomic nearest neighbor patterns, regardless of bond order (denoted by "~") or number, but when the aromaticity of the bond (denoted by ":") is important.
PubChemFP656	C-C-N-C-C	These bits test for the presence of single SMARTS patterns, regardless of number, but if the bond order is specific and the aromaticity of the bond corresponds to both single and double bonds.
PubChemFP397	N(~C)(:C)(:C)	Simple atom nearest neighbors - These bits test for the presence of atomic nearest neighbor patterns, regardless of bond order (denoted by "~") or number, but when the aromaticity of the bond (denoted by ":") is important.
PubChemFP489	N-C-S-C	These bits test for the presence of single SMARTS patterns, regardless of number, but if the bond order is specific and the aromaticity of the bond corresponds to both single and double bonds.
PubChemFP349	C(~C)(~H)(~S)	Simple atom nearest neighbors - These bits test for the presence of atomic nearest neighbor patterns, regardless of bond order (denoted by "~") or number, but when the aromaticity of the bond (denoted by ":") is important.
PubChemFP116	>= 1 saturated or aromatic carbon-only ring size 3	Rings in a canonical Extended Smallest Set of Smallest Rings (ESSSR) - These bits test for the presence or number of the described chemical ring system. An ESSSR ring is one that does not have three consecutive atoms in common with any other ring in the chemical structure. For example, naphthalene has three ESSSR rings (two phenyl fragments and the 10-membered shell), while biphenyl has only two ESSSR rings.
PubChemFP335	C(~C)(~C)(~C)(~H)	Simple atom nearest neighbors - These bits test for the presence of atomic nearest neighbor patterns, regardless of bond order (denoted by "~") or number, but when the aromaticity of the bond (denoted by ":") is important.
PubChemFP517	N-N-C-N	These bits test for the presence of single SMARTS patterns, regardless of number, but if the bond order is specific and the

Features	Bit Substructure	Section description
		aromaticity of the bond corresponds to both single and double bonds.
PubChemFP791	NC1CCC(N)CC1	Complex SMARTS patterns - These bits test for the presence of complex SMARTS patterns, regardless of number, but where the bond order and aromaticity of the bond are specific.
PubChemFP645	O=C-N-C-C	These bits test for the presence of single SMARTS patterns, regardless of number, but if the bond order is specific and the aromaticity of the bond corresponds to both single and double bonds.