

The top features were collected from the SelectFromModel of Random Forest Regressor model for Fe chelation.

Features	Bit Substructure	Section description
PubChemFP152	<chem>&gt;= 2 saturated or aromatic nitrogen-containing ring size 5</chem>	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.
PubChemFP485	<chem>N:C:C:N</chem>	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.
PubChemFP438	<chem>C(-C)(-N)(=N)</chem>	Detailed Atomic Neighborhoods - These bits test for the presence of detailed atomic neighborhood patterns, regardless of number, but where bond orders are specific, bond aromaticity matches both single and double bonds, and where "-", "=", and "#" match a single bond, double bond, and triple bond, respectively.
PubChemFP374	<chem>C(~H)(~H)(~H)</chem>	These bits test for the presence of atomic neighborhood patterns, regardless of bond order (denoted by "~") or number, but when bond aromaticity (denoted by ":") is important.
PubChemFP821	<chem>CC1C(N)CCCC1</chem>	These bits test for the presence of complex SMARTS patterns, regardless of count, but where bond orders and bond aromaticity are specific.
PubChemFP359	<chem>&gt;= 2 saturated or aromatic heteroatom-containing ring size 6</chem>	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.
PubChemFP672	<chem>O=C-C=C-[#1]</chem>	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.

Features	Bit Substructure	Section description
PubChemFP19	$\geq 2$ O	Greater than or equal to two oxygen atoms.
PubChemFP187	$\geq 2$ saturated or aromatic nitrogen-containing ring size 6	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.
PubChemFP643	[#1]-C-C-N-[#1]	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.