

TABLE V. Classes, subclasses and properties of ontoqsar ontology.

Class	Subclasses	Properties
Inhibitor	Drug	Drug phase Inhibitor ID
Biological Target	-	Biological target name PDB Family
Diagnosis	Tumor Size	Disease name (Diagnostic property) Phase (Tumor size property) Aggressiveness (Tumor size property)
Functional Groups	Benzene Phenols Amide Amine Aldehyde Carboxylic Acid Ether Alcohol Ketones Hydrocarbon Ester	-
Pharmacorific group	-	Group name
Chemical descriptor	HOMO LUMO HBA HBD Basic groups Log P PSA Aromatic groups Molecular mass Number of atoms Lipinski's rule APOL ALOG P (Molar Refractivity) Acid groups Fingerprints	Yes / No (Lipinski Rule property) Descriptor ID PubChem dataset (Fingerprints property)
Pharmacokinetics	Metabolism Absorption Distribution Toxicity Excretion	-
Biological Activity	IC <sub>50</sub> EC <sub>50</sub> pKI	-
Publication	-	DOI Date Journal title Authors Title
Assay Method	<i>in vivo</i> <i>in vitro</i> <i>in silico</i>	Technique name Organism ( <i>In vivo</i> property) Temperature ( <i>In vitro</i> property) Cell lineage ( <i>In vitro</i> property)
Quantum Calculation	<i>Ab Initio</i> <i>Hartree-Fock</i> <i>Semi-empirical</i> <i>Pi electron</i> <i>Valence electron</i>	-
QSAR	2D-QSAR 3D-QSAR Linear QSAR Non linear QSAR	Software name

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Statistical Validation	Internal validation	-
	Split validation	
	Cross validation	
	Statistical regression	
	Y scrambling	
Algorithm	Genetic algorithms	-
	Monte Carlo	
	Reinforcement learning	
	Trial and error	