Classes, Referred Ontologies and Prefixes

Class Name	Reused?	Referred Ontology	IRI	Prefix
Algorithm	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://purl.obolibrary.org/obo/IAO_0000064	IAO:0000064
Genetic_Algorithm	y	http://www.biomodels.net/kisao/KISAO_FULL#	http://www.biomodels.net/kisao/KISAO#KISAO_0000506	KISAO:0000506
Monte_Carlo	y	http://www.ebi.ac.uk/swo/swo.owl	http://www.ebi.ac.uk/swo/algorithm/SWO_4000008	SWO:4000008
Supervised_Learning	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://purl.enanomapper.org/onto/ENM_8000002	ENM:8000002
Trial_and_Error	n			
Assay_method	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0003028	BAO:0003028
in_vitro	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0020008	BAO:0020008
in_vivo	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0020009	BAO:0020009
bioassay	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0000015	BAO:0000015
in_silico	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0020007	BAO:0020007
QSAR_descriptor	y	http://semanticchemistry.github.io/semanticchemistry/ontology/cheminf.owl	http://semanticscience.org/resource/CHEMINF_000064	CHEMINF:000064
linear_QSAR	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0002306	BAO:0002306
non-linear_dimensional_QSAR	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0002309	BAO:0002309
three_dimensional_QSAR	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0002312	BAO:0002312
two_dimensional_QSAR	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0002316	BAO:0002316
Biological_Activity	y	http://biomodels.net/SBO/	http://biomodels.net/SBO/SBO_0000412	SBO:0000412
EC50	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0000188	BAO:0000188
IC50	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0000190	BAO:0000190
pKi	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0190004	BAO:0190004
pIC50	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0000199	BAO:0000199
Biological_Target	y	http://purl.obolibrary.org/obo/ero	http://purl.obolibrary.org/obo/ERO_0001536	ERO:0001536
Chemical_Descriptor	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000123	CHEMINF:000123
acidic_group_count	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000293	CHEMINF:000293
aromatic_atom_count	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000232	CHEMINF:000232
atom_count	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000263	CHEMINF:000263
basic_group_count	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000294	CHEMINF:000294
BBB	y	http://purl.obolibrary.org/obo/ncit.owl	http://purl.obolibrary.org/obo/NCIT_C13194	NCIT:C13194
Finger_Prints	n			
Highest_Occupied_Molecular_Orbital_Energy	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000291	CHEMINF:000291
hydrogen_bond_acceptors	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000245	CHEMINF:000245
hydrogen_bond_acceptors_count (using_Lipinski's_definition)	n			
hydrogen_bond_donors	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000244	CHEMINF:000244
hydrogen_bond_donnors_count (using_Lipinski's_definition)	n			
lipinski	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000312	CHEMINF:000312
Lowest_Unoccupied_Molecular_Orbital_Energy	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000292	CHEMINF:000292
molar_refractivity	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000001	CHEMINF:000001
Molecular_mass	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000088	CHEMINF:000088
partition_coefficient	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000496	CHEMINF:000496
plane_polarized_light_method	y	http://purl.obolibrary.org/obo/fix.owl	http://purl.obolibrary.org/obo/FIX_0000130	FIX:0000130
polar_surface_area_descriptor	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000307	CHEMINF:000307
AlogP_descriptor	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000295	CHEMINF:000295
heavy_atom_count	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000300	CHEMINF:000300
atomic QSAR descriptor	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000112	CHEMINF:000112
Moreau-Broto_autocorrelation (first_ionization_potential)_descriptors	n			
Moreau-Broto_autocorrelation (mass)_descriptors	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_001531	CHEMINF:001531
Moreau-Broto_autocorrelation (polarizability)_descriptors	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_001532	CHEMINF:001532

Class		URL 1	URL 2	Prefix
Moreau-Broto_autocorrelation (van_der_Waals_volumes)_descriptors	n			
bond_count	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000233	CHEMINF:000233
rotatable bond count	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000254	CHEMINF:000254
Atom-type H E-State	n			
Sum of atom-type H E-State: -OH	n			
Sum of atom-type H E-State: =NH	n			
Sum of atom-type H E-State: -SH2	n			
Sum of atom-type H E-State: -NH2	n			
Minimum E-States for (strong) Hydrogen Bond donors	n			
Minimum E-States for (strong) Hydrogen Bond acceptors	n			
cycle_count	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000380	CHEMINF:000380
cycle_count_containing_heteroatoms	n			
zagreb_index	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000046	CHEMINF:000046
Diagnosis	y	http://purl.obolibrary.org/obo/ncit.owl	http://purl.obolibrary.org/obo/NCIT_C15220	NCIT:C15220
tumor_size	y	http://purl.obolibrary.org/obo/ncit.owl	http://purl.obolibrary.org/obo/NCIT_C120284	NCIT:C120284
Functional_Group_Descriptor	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://semanticscience.org/resource/CHEMINF_000068	CHEMINF:000068
alcohol	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_30879	CHEBI:30879
aldehyde	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_17478	CHEBI:17478
amide	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_32988	CHEBI:32988
amine	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_32952	CHEBI:32952
benzene	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_16716	CHEBI:16716
carboxylic_acid	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_33575	CHEBI:33575
ester	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_35701	CHEBI:35701
ether	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_25698	CHEBI:25698
hydrocarbon	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_24632	CHEBI:24632
ketone	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_17087	CHEBI:17087
phenols	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_33853	CHEBI:33853
Inhibitor	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_35222	CHEBI:35222
drug	y	http://purl.obolibrary.org/obo/chebi.owl	http://purl.obolibrary.org/obo/CHEBI_23888	CHEBI:23888
Pharmacokinetics	y	http://purl.obolibrary.org/obo/ncit.owl	http://purl.obolibrary.org/obo/NCIT_C15299	NCIT:C15299
Absorption	y	http://purl.obolibrary.org/obo/rex.owl	http://purl.obolibrary.org/obo/REX_0000188	REX:0000188
Excretion	y	http://purl.obolibrary.org/obo/ncit.owl	http://purl.obolibrary.org/obo/NCIT_C94618	NCIT:C94618
Metabolism	y	http://purl.obolibrary.org/obo/go.owl	http://purl.obolibrary.org/obo/GO_0008152	GO:0008152
Tissue_Distribution	y	http://purl.obolibrary.org/obo/omit.owl	http://purl.obolibrary.org/obo/OMIT_0014860	OMIT:0014860
Toxicity	y	http://purl.obolibrary.org/obo/ncit.owl	http://purl.obolibrary.org/obo/NCIT_C27990	NCIT:C27990
Pharmacophoric_Group	n			
publication	y	http://purl.obolibrary.org/obo/iao.owl	http://purl.obolibrary.org/obo/IAO_0000311	IAO:0000311
Quantum_Chemistry_Computational_Method	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0002317	BAO:0002317
ab_initio_quantum_chemistry_Computational_method	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0002318	BAO:0002318
hartree-fock_method	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0002319	BAO:0002319
pi-electron_computational_method	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0002327	BAO:0002327
semi-empirical_quantum_chemistry_method	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0002326	BAO:0002326
valence_electron_computational_method	y	http://www.bioassayontology.org/bao/bao_complete.owl	http://www.bioassayontology.org/bao#BAO_0002329	BAO:0002329
Charges	n			
Abs. máx (eV)	n			
Abs. máx (nM)	n			
Osc. Force	n			
Transition	n			
Contribution	n			
Dipole	n			

E solv. Water	n			
Free E	n			
Zero E	n			
Validation	y	http://purl.obolibrary.org/obo/obi.owl	http://purl.obolibrary.org/obo/OBI_0302911	OBI:0302911
cross-validation_information	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://purl.enanomapper.org/onto/ENM_8000116	ENM:8000116
external_validation	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://purl.enanomapper.org/onto/ENM_8000112	ENM:8000112
internal_validation	n			
regression_statistics	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://purl.enanomapper.org/onto/ENM_8000117	ENM:8000117
split_validation	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://purl.enanomapper.org/onto/ENM_8000113	ENM:8000113
y_scrambling	y	http://purl.enanomapper.net/onto/enanomapper.owl	http://purl.enanomapper.org/onto/ENM_8000118	ENM:8000118