

Entity	Qualifiers	Preferred Ontologies	Value	Comments	DOPE		
model	bqbiol.hasTaxon					Organism/Cell Annotation	Taxonomy/Cells/tissues
model	bqbiol.hasTaxon						
model	bqbiol.occursIn						
model	bqbiol.occursIn						
model	bqbiol.hasProperty	NCI Thesaurus OBO Edition	https://identifiers.org/NCIT:C45329	Active		Property Annotation; Modelling Approach, Biological Processes, Model relevance	Biological properties of the model e.g., QSAR
model	bqbiol.hasProperty	NCI Thesaurus OBO Edition NCIT	https://identifiers.org/NCIT:C154407	Inactive			
model	bqbiol.hasProperty	Bioinformatics Concept EDAM	https://identifiers.org/bptl/edam:topic_0154	Small molecules			
model	bqbiol.hasProperty	BioAssay Ontology BAO	https://identifiers.org/BAO:0002305	QSAR			
model	bqbiol.hasProperty						
model	bqbiol.hasProperty						
model	bqbiol.hasProperty			Metabolism			
model	bqbiol.hasProperty			Infectious disease			
model	bqbiol.hasProperty			Permeability			
model	bqbiol.hasProperty			ADME			
model	bqbiol.hasProperty	Bioinformatics Concept EDAM	https://identifiers.org/bptl/edam:topic_3336	Drug discovery		Property Annotation; Modelling Approach, Biological Processes, Model relevance	Standard Metadata following FAIR principles e.g ML, AI and Model relevance i.e., drug discovery. This is a constant metadata in all annotations
model	bqmodel.hasProperty	Bioinformatics Concept EDAM	https://identifiers.org/bptl/edam:topic_3474	Machine learning			
model	bqmodel.hasProperty	NCI Thesaurus OBO Edition	https://identifiers.org/NCIT:C16309	Artificial Intelligence			
model	bqmodel.hasProperty	NCI Thesaurus OBO Edition	https://identifiers.org/NCIT:C78542	Support vector machine	Optimization-Algorithm		
model	bqmodel.hasProperty	STATO: the statistical methods ontology	https://identifiers.org/STATO:0000549	Random forest (RF)	Optimization-Algorithm		
model	bqmodel.hasProperty	STATO: the statistical methods ontology	https://identifiers.org/STATO:0000031	Binary classification model	Optimization-Algorithm		
model	bqmodel.hasProperty						
model	bqmodel.hasProperty	STATO: the statistical methods ontology	https://identifiers.org/STATO:0000274	AUC-ROC	Evaluation-Performance Measure		
model	bqmodel.hasProperty	STATO: the statistical methods ontology	https://identifiers.org/STATO:0000415	Accuracy	Evaluation-Performance Measure		
model	bqmodel.hasProperty	Model Card Ontology MCRO	https://identifiers.org/MCRO:0000009	F1-measure (F1)	Evaluation-Performance Measure		
model	bqmodel.hasProperty					Evaluation Metric e.g AUROC	
model	bqmodel.hasProperty	Ontology for Biomedical Investigations OBI	https://identifiers.org/obi:OBI_0200032	X-fold cross validation	Evaluation-Method		
model	bqmodel.hasProperty					Model description e.g., Ersilia Implementation	
model	bqmodel.isDescribedBy			Web Application	Model-Executable form		
model	bqmodel.isDescribedBy	GitHub Repository		Source Code	Model-Source code		
model	bqmodel.isDescribedBy	Ersilia Model Hub		Ersilia Incorporation URL	Model-Executable form		
model	bqmodel.isDescribedBy	PubMed Identification Number PMID		PubMed URL		Functional Annotation; Model function	Data; Input and Experimental
model	bqbiol.hasInput	Chemical information ontology (cheminf)	https://identifiers.org/CHEMINE:000018	Smiles descriptors	Data-Input		
model	bqbiol.hasDataset				Data-Source		
model	bqbiol.hasDataset				Data-Source		
model	bqbiol.hasOutput				Model-Output; Classification	Model Output	
model	bqbiol.hasOutput				Model-Output; Classification		