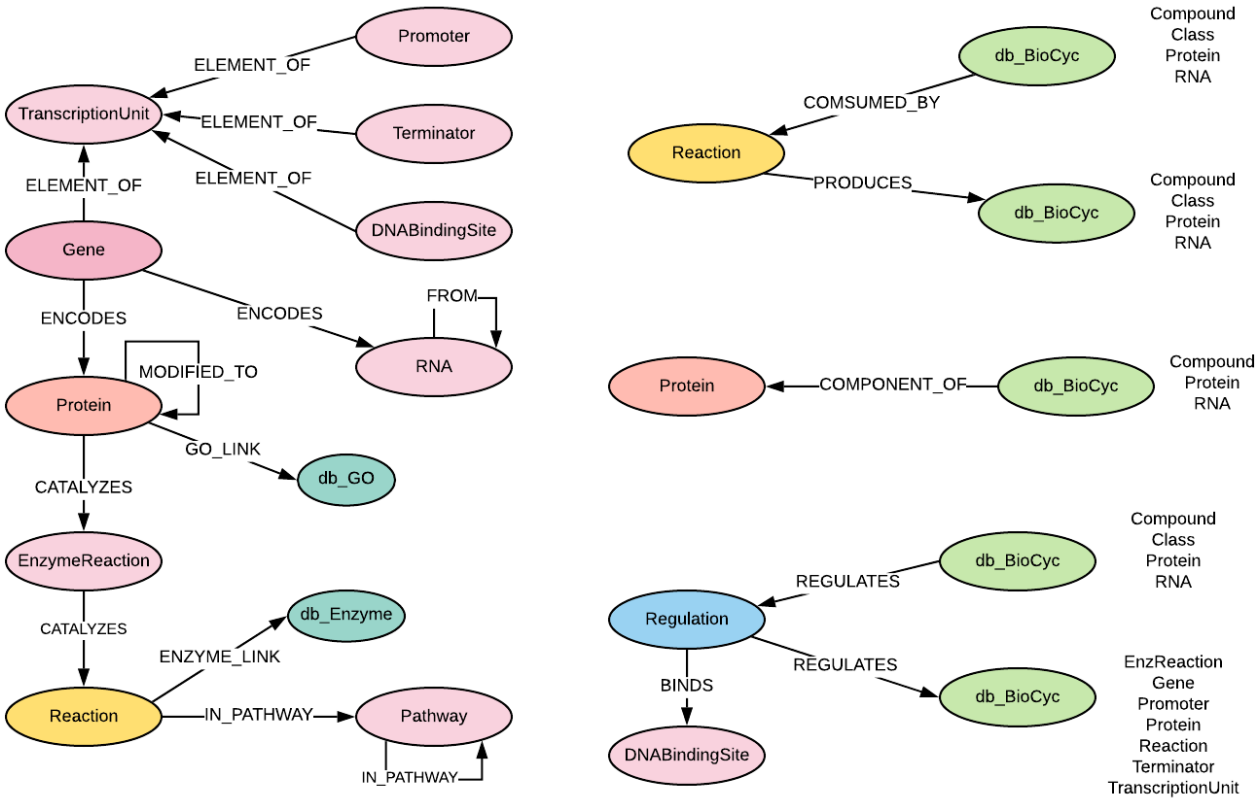
BioCyc Spec for Knowledge Graph

The BioCyc database collection is an assortment of organism specific Pathway/ Genome Databases (PGDBs). They provide reference to genome and metabolic pathway information for thousands of organisms. Currently we loaded the following databases:

- EcoCyc: for E. coli strain K-12 MG1655 with tax_id 511145
- HumanCyc: for Homo sapiens with tax_id 9606
- YeastCyc: for Saccharomyces cerevisiae S288C with tax_id 559292
- PseudomonasCyc: for Pseudomonas putida with tax_id 160488

In Lifelike graph database, each node in BioCyc was labeled as db_BioCyc, and nodes for each biocyc database was labeled as additional database name, such as db_EcoCyc, db_HumanCyc. Therefore for any EcoCyc, there are 3 labels: db_BioCyc, db_EcoCyc and the entity name (e.g. Gene, Protein)

Graph database schema for BioCyc



Node labels and attributes:

id has the same value for biocyc_id, and displayName and pathways attributes were added post-loading for annotation

Node Label	Attribute
Class	abbrev_name

Node Label	Attribute
Class	biocyc_id
Class	data_source
Class	displayName
Class	id
Class	inchi_key
Class	name
Class	synonyms
Compound	abbrev_name
Compound	biocyc_id
Compound	data_source
Compound	displayName
Compound	id
Compound	inchi_key
Compound	name
DNABindingSite	abs_center_pos
DNABindingSite	biocyc_id
DNABindingSite	description
DNABindingSite	displayName
DNABindingSite	id
DNABindingSite	site_length
EnzReaction	biocyc_id
EnzReaction	description
EnzReaction	displayName
EnzReaction	genes
EnzReaction	id
EnzReaction	name
Gene	accession
Gene	biocyc_id
Gene	description
Gene	displayName

Node Label	Attribute
Gene	id
Gene	left_end_position
Gene	name
Gene	pathways
Gene	right_end_position
Gene	strand
Pathway	biocyc_id
Pathway	displayName
Pathway	genes
Pathway	id
Pathway	name
Promoter	biocyc_id
Promoter	description
Promoter	displayName
Promoter	genes
Promoter	id
Promoter	name
Promoter	pos_1
Promoter	strand
Protein	abbrev_name
Protein	biocyc_id
Protein	description
Protein	displayName
Protein	genes
Protein	id
Protein	molecular_weight_kd
Protein	name
Protein	pi
RNA	abbrev_name
RNA	biocyc_id

Node Label	Attribute
RNA	description
RNA	displayName
RNA	genes
RNA	id
RNA	location
RNA	name
Reaction	biocyc_id
Reaction	description
Reaction	displayName
Reaction	ec_number
Reaction	id
Reaction	name
Regulation	biocyc_id
Regulation	displayName
Regulation	id
Regulation	mechanism
Regulation	mode
Regulation	type
Terminator	biocyc_id
Terminator	description
Terminator	genes
Terminator	id
Terminator	left_end_position
Terminator	right_end_position
TranscriptionUnit	biocyc_id
TranscriptionUnit	description
TranscriptionUnit	displayName
TranscriptionUnit	genes
TranscriptionUnit	id
TranscriptionUnit	name

Node outgoing relationships

StartNode	Relationship	EndNode	Cardinality
Class	CHEBI_LINK	Chemical	1
Class	COMPONENT_OF	Protein	+
Class	CONSUMED_BY	Reaction	+
Class	HAS_SYNONYM	Synonym	+
Class	REGULATES	Regulation	+
Class	TYPE_OF	Class	+
Compound	CHEBI_LINK	Chemical	1
Compound	COMPONENT_OF	Protein	+
Compound	CONSUMED_BY	Reaction	+
Compound	HAS_SYNONYM	Synonym	+
Compound	REGULATES	Regulation	+
Compound	TYPE_OF	Class	+
DNABindingSite	ELEMENT_OF	TranscriptionUnit	1
EnzReaction	CATALYZES	Reaction	1
EnzReaction	HAS_SYNONYM	Synonym	+
Gene	ELEMENT_OF	TranscriptionUnit	1
Gene	ENCODES	Protein	1
Gene	ENCODES	RNA	1
Gene	HAS_SYNONYM	Synonym	+
Gene	IS	db_NCBI Gene	1
Pathway	HAS_SYNONYM	Synonym	+
Pathway	IN_PATHWAY	Pathway	1
Pathway	TYPE_OF	Class	+
Promoter	ELEMENT_OF	TranscriptionUnit	1
Promoter	HAS_SYNONYM	Synonym	+
Protein	CATALYZES	EnzReaction	+
Protein	COMPONENT_OF	Protein	+
Protein	CONSUMED_BY	Reaction	+

StartNode	Relationship	EndNode	Cardinality
Protein	GO_LINK	db_GO	+
Protein	HAS_SYNONYM	Synonym	+
Protein	MODIFIED_TO	Protein	+
Protein	REGULATES	Regulation	+
Protein	TYPE_OF	Class	+
RNA	COMPONENT_OF	Protein	+
RNA	CONSUMED_BY	Reaction	+
RNA	HAS_SYNONYM	Synonym	+
RNA	MODIFIED_TO	RNA	+
RNA	REGULATES	Regulation	+
RNA	TYPE_OF	Class	+
Reaction	ENZYME_LINK	EC_Number	+
Reaction	HAS_SYNONYM	Synonym	+
Reaction	IN_PATHWAY	Pathway	+
Reaction	PRODUCES	Class	+
Reaction	PRODUCES	Compound	+
Reaction	PRODUCES	Protein	+
Reaction	TYPE_OF	Class	+
Regulation	BINDS	DNABindingSite	1
Regulation	REGULATES	EnzReaction	1
Regulation	REGULATES	Gene	1
Regulation	REGULATES	Promoter	1
Regulation	REGULATES	Protein	1
Regulation	REGULATES	Reaction	1
Regulation	REGULATES	Terminator	1
Regulation	REGULATES	TranscriptionUnit	1
Regulation	TYPE_OF	Class	+
Terminator	ELEMENT_OF	TranscriptionUnit	1
TranscriptionUnit	HAS_SYNONYM	Synonym	+