

| Asset# | Relationship | Settings | InputName (user choice) | InputID, node normalized | OutputID | UI | Expected Result / Suggested Comparator | MolePro | | | | | |
|----------|------------------------------------|----------|-------------------------|-----------------------------|----------------------------|--|--|---|--|--|--|--|--|
| Asset:1 | Treats | Inferred | alcoholic hepatitis | MONDO:0001505 | PUBCHEM.COMPOUND:107526 | (2r,3s,4r,5r)-2,3,4,5,6-pentahydroxyhexanal | D(+)-Glucose | gestrose | | | | | |
| Asset:2 | Treats | Inferred | alcoholic hepatitis | MONDO:0001505 | PUBCHEM.COMPOUND:11547499 | 2-(4-chloro-3-(3-(1-hydroxycycloheptyl)propyl)-2-hydroxypropyl)-5-hydroxy-1,4-dihydroquinoline | CE-224535 | | | | | | |
| Asset:3 | Treats | Inferred | alcoholic hepatitis | MONDO:0001505 | Drugbank:db00260 | Drugbank:db00260 | Cycloserine | levycycloserine | | | | | |
| Asset:4 | Treats | Inferred | alcoholic hepatitis | MONDO:0001505 | PUBCHEM.COMPOUND:2833 | N-(1,2,3,10-tetramethoxy-9-oxo-5,6,7,9-tetrahydro-2H-benzocyclohept-5-yl)colchicine | Colchicine | colchicine | | | | | |
| Asset:5 | Treats | Inferred | alcoholic hepatitis | MONDO:0001505 | Drugbank:db03708 | Drugbank:db03708 | Adenosine 5'-phosphosulfate | adenosine phosphosulfate | | | | | |
| Asset:6 | Treats | Inferred | alcoholic hepatitis | MONDO:0001505 | PUBCHEM.COMPOUND:49863538 | Unk-n(meso3h)dab(meso3h)-unk-dab(meso3) | colistimethate | COLISTIMETHATE | | | | | |
| Asset:7 | Treats | Inferred | alcoholic hepatitis | MONDO:0001505 | PUBCHEM.COMPOUND:6473881 | (1aR,7aS,10aS,10bS)-1a,5-dimethyl-8-methylparthenolide | parthenolide | parthenolide | | | | | |
| Asset:8 | Treats | Inferred | Peptic Ulcer Perforat | MONDO:0004260 | PUBCHEM.COMPOUND:16133850 | Forteo | Teriparatide | teriparatide | | | | | |
| Asset:9 | Treats | Inferred | Peptic Ulcer Perforat | MONDO:0004260 | PUBCHEM.COMPOUND:11583880 | 5-Cholesten-3beta-25-diol-3-sulfate | Larsucosterol | LARSUCOSTEROL | | | | | |
| Asset:10 | Treats | Inferred | Peptic Ulcer Perforat | MONDO:0004260 | PUBCHEM.COMPOUND:10954115 | (2S,3R,4S,5S)-2,3,4,5,6-pentahydroxyhexane | L-Glucose | levoglucose | | | | | |
| Asset:11 | Treats | Inferred | Peptic Ulcer Perforat | MONDO:0004260 | PUBCHEM.COMPOUND:7847 | Acrolein | propenal | acrolein | | | | | |
| Asset:12 | Treats | Inferred | Gastroesophageal Rf | MONDO:0007186 | PUBCHEM.COMPOUND:441347 | Reglan | Metoclopramide | metoclopramide hydrochloride | | | | | |
| Asset:13 | Treats | Inferred | Gastroesophageal Rf | MONDO:0007186 | PUBCHEM.COMPOUND:5039 | Zantac | Ranitidine | ranitidine | | | | | |
| Asset:14 | Treats | Inferred | Gastroesophageal Rf | MONDO:0007186 | PUBCHEM.COMPOUND:4513 | Axid Ar | Nizatidine | nizatidine | | | | | |
| Asset:15 | Treats | Inferred | Gastroesophageal Rf | MONDO:0007186 | PUBCHEM.COMPOUND:6336690 | Gaviscon | Aluminum hydroxide; magnesium hydroxide | Gaviscon | | | | | |
| Asset:16 | Treats | Inferred | Gastroesophageal Rf | MONDO:0007186 | PUBCHEM.COMPOUND:174 | 1,2-ethanediol | Ethylene Glycol | macrogol | | | | | |
| Asset:17 | Treats | Inferred | Gastroesophageal Rf | MONDO:0007186 | PUBCHEM.COMPOUND:56842000 | Talcid | Hydrotalcite | Hydrotalcite | | | | | |
| Asset:18 | Treats | Inferred | Gastroesophageal Rf | MONDO:0007186 | PUBCHEM.COMPOUND:135398738 | Dbc-dome | Dacarbazine | dacarbazine | | | | | |
| Asset:19 | Treats | Inferred | Cowden Disease | MONDO:0016063 | PUBCHEM.COMPOUND:5352062 | Istodax | Romidepsin | romidepsin | | | | | |
| Asset:20 | Treats | Inferred | Cowden Disease | MONDO:0016063 | PUBCHEM.COMPOUND:47289 | 4-(N-Nitrosomethylamino)-1-(3-pyridyl)-1-butanol | NNK | 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanol | | | | | |
| Asset:21 | Treats | Inferred | Cowden Disease | MONDO:0016063 | PUBCHEM.COMPOUND:24963252 | (1r)-2,3-dihydroxypropyl-6-fluoro-5-(2-fluorophenyl)-1,4-dihydroquinoline | TAK-733 | TAK-733 | | | | | |
| Asset:22 | Treats | Inferred | Cowden Disease | MONDO:0016063 | PUBCHEM.COMPOUND:44369251 | CHEMBL:154012 | N-[1-[8-(3-Amino-propylamino)-octyl]-4-(4-hydroxy-phenyl)-ethyl]-3-phenyl-propionamide | NA | | | | | |
| Asset:23 | Treats | Inferred | Cowden Disease | MONDO:0016063 | PUBCHEM.COMPOUND:11405964 | Chembl.compound.chembl218473 | 2-(2-chlorobenzyl)-3-hydroxy-7,8,9-trifluoro-1,2,3,4-tetrahydroquinoline | NA | | | | | |
| Asset:24 | decreases activity or abundance of | Inferred | Lapirudin | PUBCHEM.COMPOUND:CHEMBL:204 | CHEMBL:204 | UNIPROT:KB:P00734 | Thrombin | THROMBIN | | | | | |
| Asset:25 | Treats | Inferred | Bethlem Myopathy | MONDO:0008029 | PUBCHEM.COMPOUND:75007581 | 5,6,8,13,17,23,24,27,31,35-Decamethyl-10,20-dihydroxy-1,3-bis(2-hydroxyethyl)ammonium chloride | Collagenase (Pubchem synonym) | NA | | | | | |

Test asset sheet for chemical names contains preferred names instead of long chemical names or brand names

To access MolePro endpoint to get the preferred compound name you can use the [swagger API](#) and the `post_compound_by_id`. In the brackets between the quotes insert 1 ID with the CURIE such that : `:_prefix_:_id_`.
 A list of prefixes to use given the source name is provided below:

| source name | prefix |
|------------------|----------------------|
| pubchem | CID: |
| chembl | ChEMBL: |
| drugbank | DrugBank: |
| hmdb | HMDB: |
| inchikey | <none> |
| inchi | <none> |
| smiles | <none> |
| chebi | CHEBI: |
| chebi-retired | CHEBI: |
| mesh | MESH: |
| unii | UNII: |
| kegg | KEGG.COMPOUND: |
| kegg-drug | KEGG.DRUG: |
| kegg-glycan | KEGG.GLYCAN: |
| gtopdb | GTOPDB: |
| chembank | ChemBank: |
| drugcentral | DrugCentral: |
| cas | CAS: |
| mychem_info | <none> |
| bindingdb | BINDINGDB: |
| pdb | PDB.LIGAND: |
| lipidmaps | LIPIDMAPS: |
| bigg | BIGG.METABOLITE: |
| secondary_hmdb | HMDB: |
| drugstore | DrugStore: |
| xchem | XChem: |
| cansar | canSAR: |
| nci_thesaurus | NCIT: |
| pubchem-retired | CID: |
| pubchem-sid | SID: |
| lincs | LINCS.SMALLMOLECULE: |
| pharmgkb | PHARMGKB.CHEMICAL: |
| comptox | comptox: |
| unii | UNII: |
| entrez | NCBIGene: |
| hgnc | HGNC: |
| mim | OMIM: |
| ensembl | ENSEMBL: |
| mygene_info | <none> |
| pharmgkb | PHARMGKB.GENE: |
| rxnorm | RXCUI: |
| disease_ontology | DOID: |
| hpo | HP: |
| omim | OMIM: |
| umls | UMLS: |
| nci_thesaurus | NCIT: |
| mondo | MONDO: |
| snomed | SNOMEDCT: |
| efo | EFO: |
| umls | UMLS: |
| snomed | SNOMEDCT: |
| pharmgkb | PHARMGKB.DISEASE: |
| mesh | MESH: |
| chembl | ChEMBL: |
| bigg | BIGG.REACTION: |

| | |
|-----------------|----------------------|
| metanetx | METANETX.REACTION: |
| seed | SEED.REACTION: |
| rhea | RHEA: |
| biocyc | MetaCyc: |
| ec | EC: |
| kegg | KEGG.REACTION: |
| chembl | ChEMBL: |
| uniprot | UniProtKB: |
| ensembl | ENSEMBL: |
| lincs | LINCS.PROTEIN: |
| go | GO: |
| go | GO: |
| go | GO: |
| go | GO: |
| kegg | KEGG.PATHWAY: |
| reactome | REACT: |
| msigdb | MSigDB: |
| smpdb | SMPDB: |
| wikipathways | WIKIPATHWAYS: |
| chembl | CHEMBL.TARGET: |
| chembl | CHEMBL.DOCUMENT: |
| ncbi_taxon | NCBITaxon: |
| clo | CLO: |
| efo | EFO: |
| cellosaurus | CELLOSAURUS: |
| lincs | LINCS.CELL: |
| cell_ontology | CL: |
| pubchem | CID: |
| chembl | ChEMBL: |
| drugbank | DrugBank: |
| hmdb | HMDB: |
| inchikey | <none> |
| inchi | <none> |
| smiles | <none> |
| chebi | CHEBI: |
| chebi-retired | CHEBI: |
| mesh | MESH: |
| unii | UNII: |
| kegg | KEGG.COMPOUND: |
| kegg-drug | KEGG.DRUG: |
| kegg-glycan | KEGG.GLYCAN: |
| gtopdb | GTOPDB: |
| chembank | ChemBank: |
| drugcentral | DrugCentral: |
| cas | CAS: |
| mychem_info | <none> |
| bindingdb | BINDINGDB: |
| pdb | PDB.LIGAND: |
| lipidmaps | LIPIDMAPS: |
| bigg | BIGG.METABOLITE: |
| secondary_hmdb | HMDB: |
| drugstore | DrugStore: |
| xchem | XChem: |
| cansar | canSAR: |
| nci_thesaurus | NCIT: |
| pubchem-retired | CID: |
| pubchem-sid | SID: |
| lincs | LINCS.SMALLMOLECULE: |
| pharmgkb | PHARMGKB.CHEMICAL: |

| | | |
|-----------------|----------------------|--|
| pubchem | CID: | |
| chembl | ChEMBL: | |
| drugbank | DrugBank: | |
| hmdb | HMDB: | |
| inchikey | <none> | |
| inchi | <none> | |
| smiles | <none> | |
| chebi | CHEBI: | |
| chebi-retired | CHEBI: | |
| mesh | MESH: | |
| unii | UNII: | |
| kegg | KEGG.COMPOUND: | |
| kegg-drug | KEGG.DRUG: | |
| kegg-glycan | KEGG.GLYCAN: | |
| gtopdb | GTOPDB: | |
| chembank | ChemBank: | |
| drugcentral | DrugCentral: | |
| cas | CAS: | |
| mychem_info | <none> | |
| bindingdb | BINDINGDB: | |
| pdb | PDB.LIGAND: | |
| lipidmaps | LIPIDMAPS: | |
| bigg | BIGG.METABOLITE: | |
| secondary_hmdb | HMDB: | |
| drugstore | DrugStore: | |
| xchem | XChem: | |
| cansar | canSAR: | |
| nci_thesaurus | NCIT: | |
| pubchem-retired | CID: | |
| pubchem-sid | SID: | |
| lincs | LINCS.SMALLMOLECULE: | |
| pharmgkb | PHARMGKB.CHEMICAL: | |
| pubchem | CID: | |
| chembl | ChEMBL: | |
| drugbank | DrugBank: | |
| hmdb | HMDB: | |
| inchikey | <none> | |
| inchi | <none> | |
| smiles | <none> | |
| chebi | CHEBI: | |
| chebi-retired | CHEBI: | |
| mesh | MESH: | |
| unii | UNII: | |
| kegg | KEGG.COMPOUND: | |
| kegg-drug | KEGG.DRUG: | |
| kegg-glycan | KEGG.GLYCAN: | |
| gtopdb | GTOPDB: | |
| chembank | ChemBank: | |
| drugcentral | DrugCentral: | |
| cas | CAS: | |
| mychem_info | <none> | |
| bindingdb | BINDINGDB: | |
| pdb | PDB.LIGAND: | |
| lipidmaps | LIPIDMAPS: | |
| bigg | BIGG.METABOLITE: | |
| secondary_hmdb | HMDB: | |
| drugstore | DrugStore: | |
| xchem | XChem: | |
| cansar | canSAR: | |
| nci_thesaurus | NCIT: | |
| pubchem-retired | CID: | |
| pubchem-sid | SID: | |
| lincs | LINCS.SMALLMOLECULE: | |
| pharmgkb | PHARMGKB.CHEMICAL: | |

| | | |
|-------------|----------------|--|
| pubchem | CID: | |
| chembl | ChEMBL: | |
| kegg | KEGG.COMPOUND: | |
| pubchem-sid | SID: | |
| pubchem | CID: | |
| chembl | ChEMBL: | |
| kegg | KEGG.COMPOUND: | |
| pubchem-sid | SID: | |