

Table S1: List of IDs and other information retrieved from each database.

Database	Compound Information	Gene Information	Pathway Information
KEGG	<ul style="list-style-type: none">• ID (prefix “C”)• Synonyms• Other IDs (ChEBI, CAS)	<ul style="list-style-type: none">• ID (prefix “hsa”)• Other IDs (UniProt, KEGG, Ensembl, HUGO name)	<ul style="list-style-type: none">• ID (prefix ”map” and “hsa”)• Name
HMDB	<ul style="list-style-type: none">• ID (prefix “HMDB”)• Synonyms• Other IDs (ChEBI,DrugBank, ChemSpider, KEGG,BioCyc, PubChem compound, CAS)	<ul style="list-style-type: none">• ID (UniProt)• Other IDs (HUGO name)	<ul style="list-style-type: none">• ID (SMPDB id)• Name• Ontologies (biofluid type, cellular location, origins, tissue location)
Reactome	<ul style="list-style-type: none">• ID (ChEBI ID)	<ul style="list-style-type: none">• ID (UniProt)	<ul style="list-style-type: none">• ID (prefix “R-HSA-”)• Name
WikiPathways	<ul style="list-style-type: none">• ID• Other IDs (HMDB, KEGG, PubChem compound, ChEBI, CAS, ChemSpider)	<ul style="list-style-type: none">• ID• Other IDs (UniProt, Entrez, Ensembl)	<ul style="list-style-type: none">• ID (prefix “WP”)• Name• Category (e.g. Metabolism)