IDG Metadata Specifications for:

Chemical tool

Importance 1: Required, 2: Required if available, 3: Optional

IDG Field Name	Definition	Importance
Gene	Gene that the resource is related to	1
Title	Name/title of the dataset	1
Provider_institution	Institution where work was performed	1
Description	Paragraph description of the dataset	1
PI	Principle investigator of the dataset	1
Authors	Person(s) who performed corresponding experiments	1
Assay_ID	Assay(s) associated with the data (BAO IDs)	2
Data_Format	Data file format(s) - MS, txt, HDF5, etc.	1
Data_Repository	Repository where the data has been released	1
Data_Link	Link to external data repository containing key dataset metadata	1
Endpoint	Data endpoint format (log2 expression, fold change, etc.)	1
Endpoint_detection	Physical entity/method to calculate endpoint - fluorescence intensity, mass spec, etc.	1
Activity	On target activity as published in IDG approved repository	1
External_ID	External ID (PubChem, CheBI, ZINC, etc.) corresponding to the canonical representation	1
External_ID_registration_system	Repository corresponding to the external ID	1
Ligand_type	Mode of action towards given gene	1
Link_to_the_supporting_data	External link to the data deposited in public repository/location	1
Name	Canonical (trade or IUPAC) name of molecule	1
Chemical_tool_page	Link to ChEBI where the chemical tool is registered	1
Repository_page_link	Link to the vendor for the physical sample	1
Selectivity	Selectivity against similar genes as reported to ChEBI	1
Canonical_SMILES	Canonical SMILES of molecule	1