Small molecule

IDG Field Name	Definition	Importance
Name	Canonical (trade or IUPAC) name of molecule	1
SMILES	SMILES representation as provided from the vendor (full structure with all information)	1
Vendor	Vendor or lab that supplied the compound	1
Vendor_cat	ID or catalogue number assigned to the specific supplied sample by the vendor or provider	1
PubChem_ID	PubChem identifier of small molecule	2
ChEMBL_ID	ChEMBL identifier of small molecule	2
ZINC_ID	ZINC database identifier	1
Purity	Purity of the compound in percent	1
Molecular_weight	Molecular weight of one molecule (including addends)	1
Water_solubility	Experimental water solubility of the compound in mg per ml or g per l	3
logP/hydrophobicity	Logarithm of the water/octanol partition coefficient (logP) or hydrophobicity score	3