Supplementary information

The iPPI-DB initiative: A community-centered database of Protein-Protein Interaction modulators

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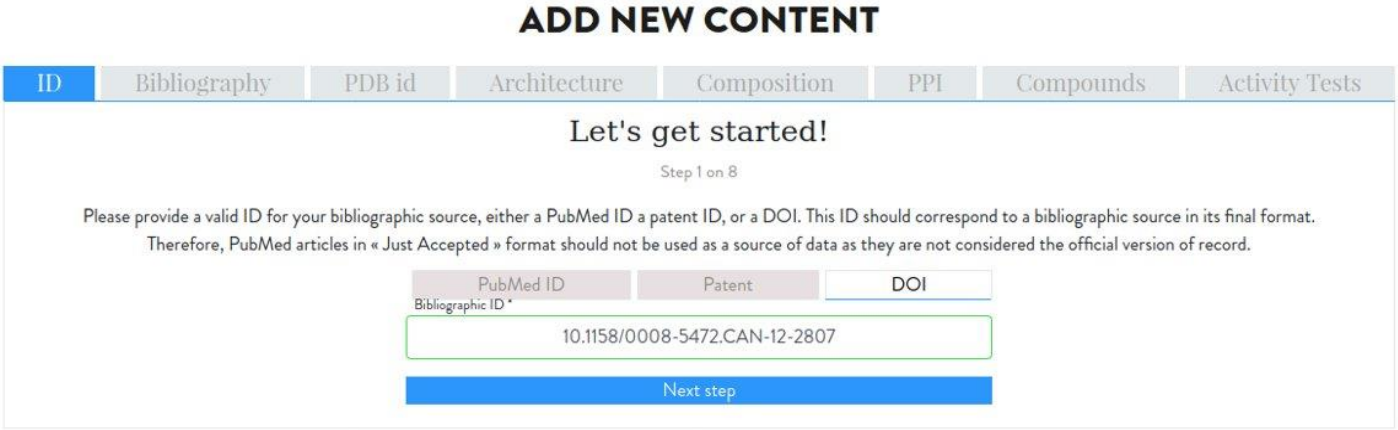
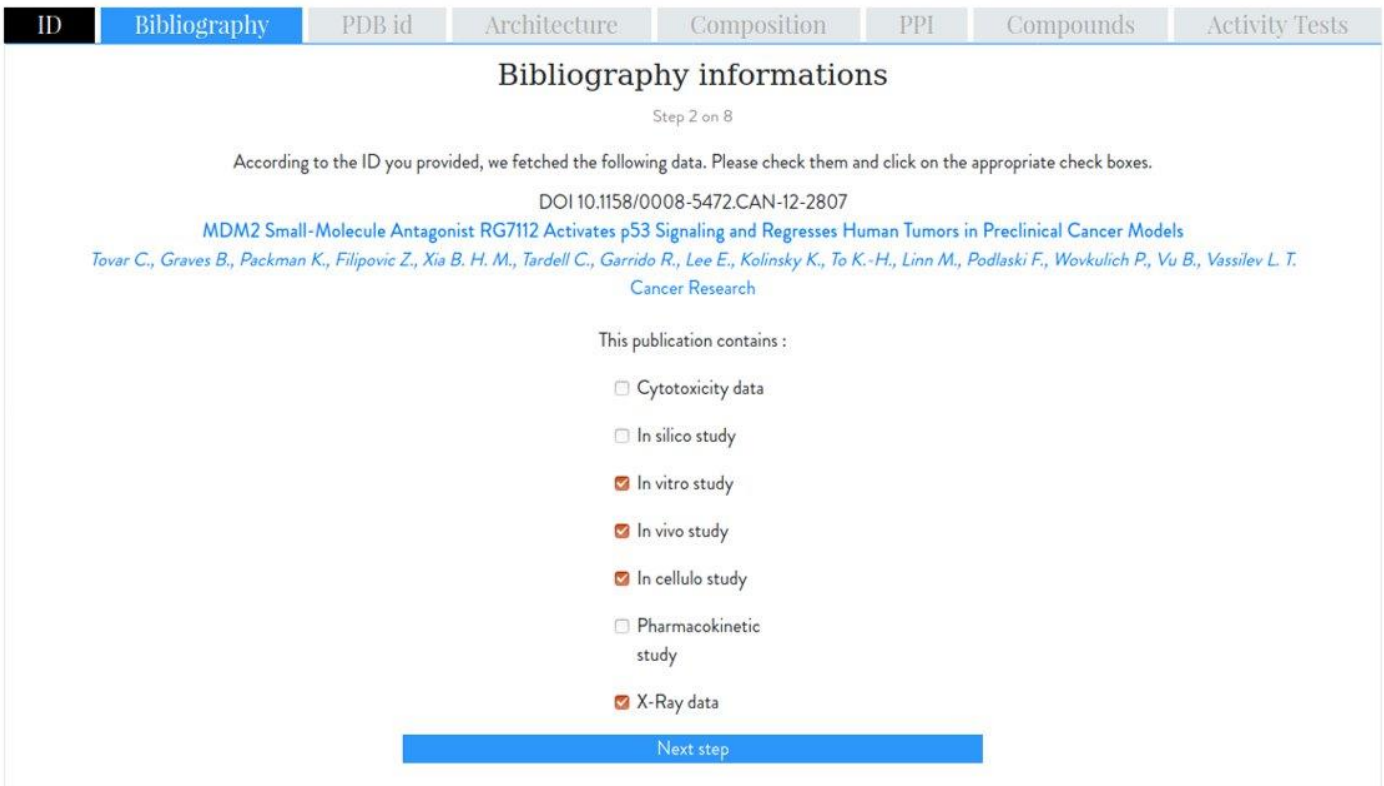
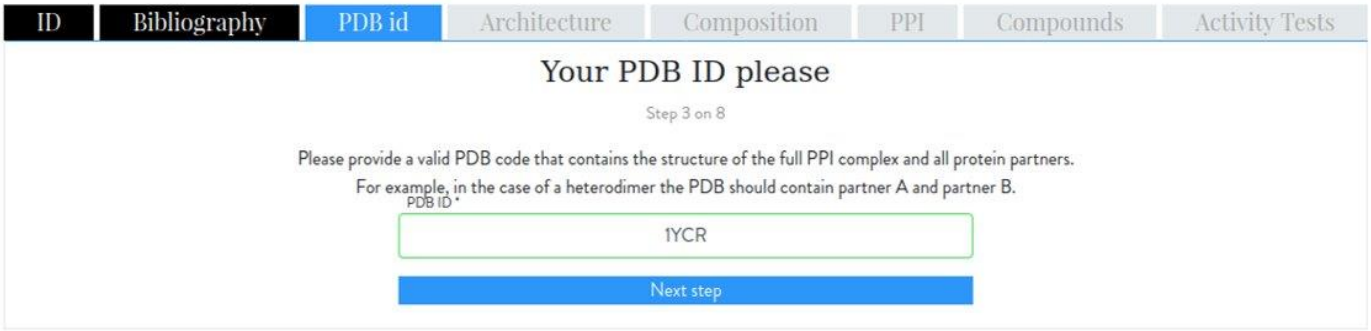


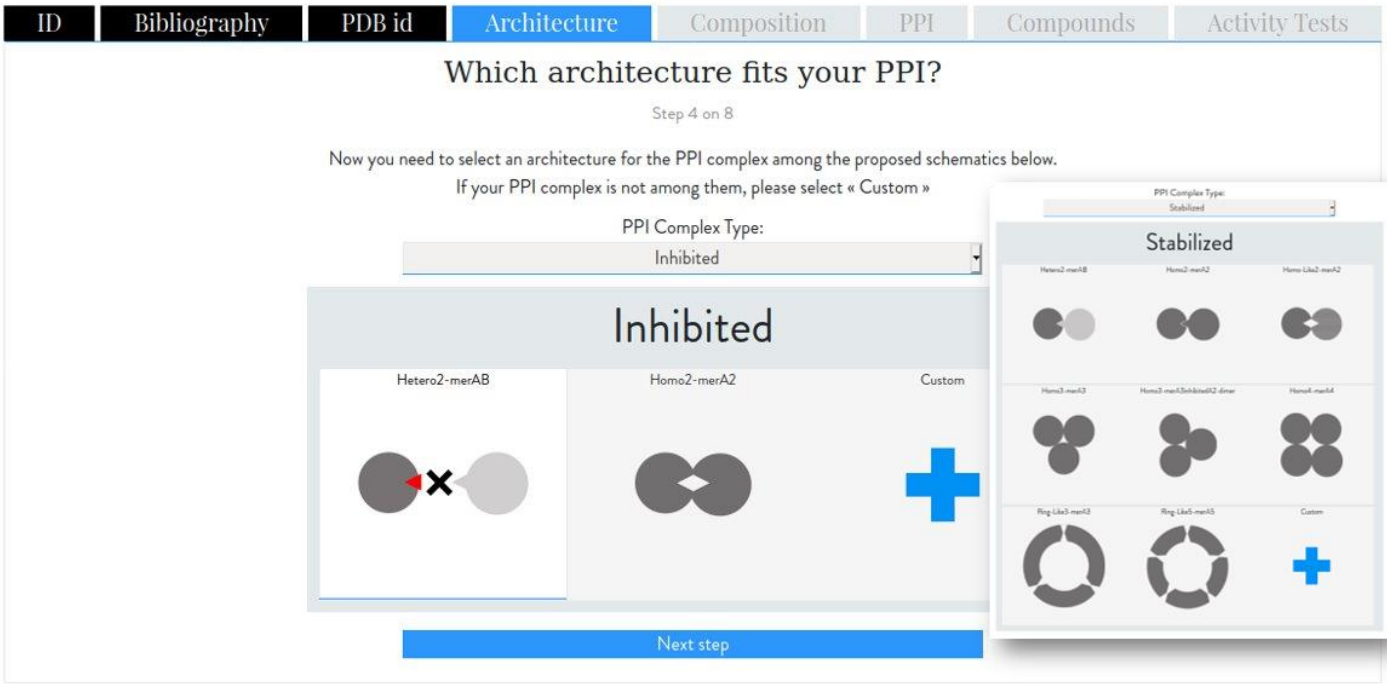
Step 1: Enter the ID of the bibliographic source, such as PubMed ID, patent ID or DOI. The website will automatically fetch the information (title, author...).



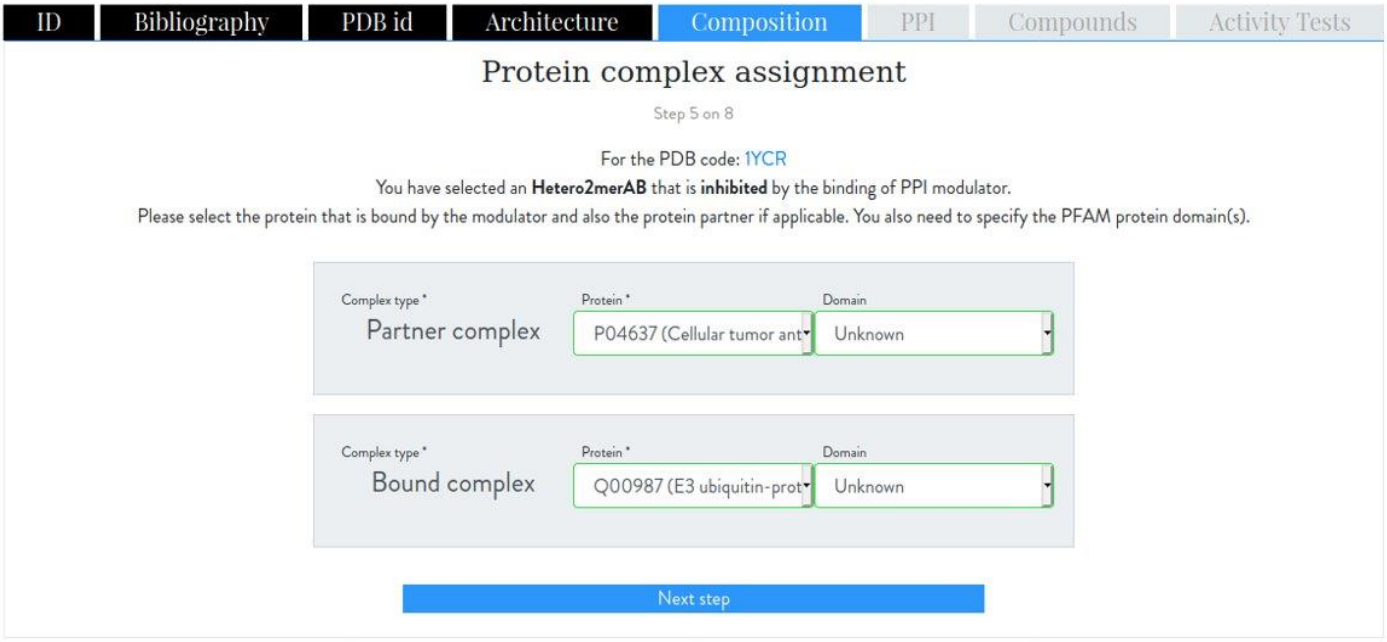
Step 2: Select the studies carried out within the publication.



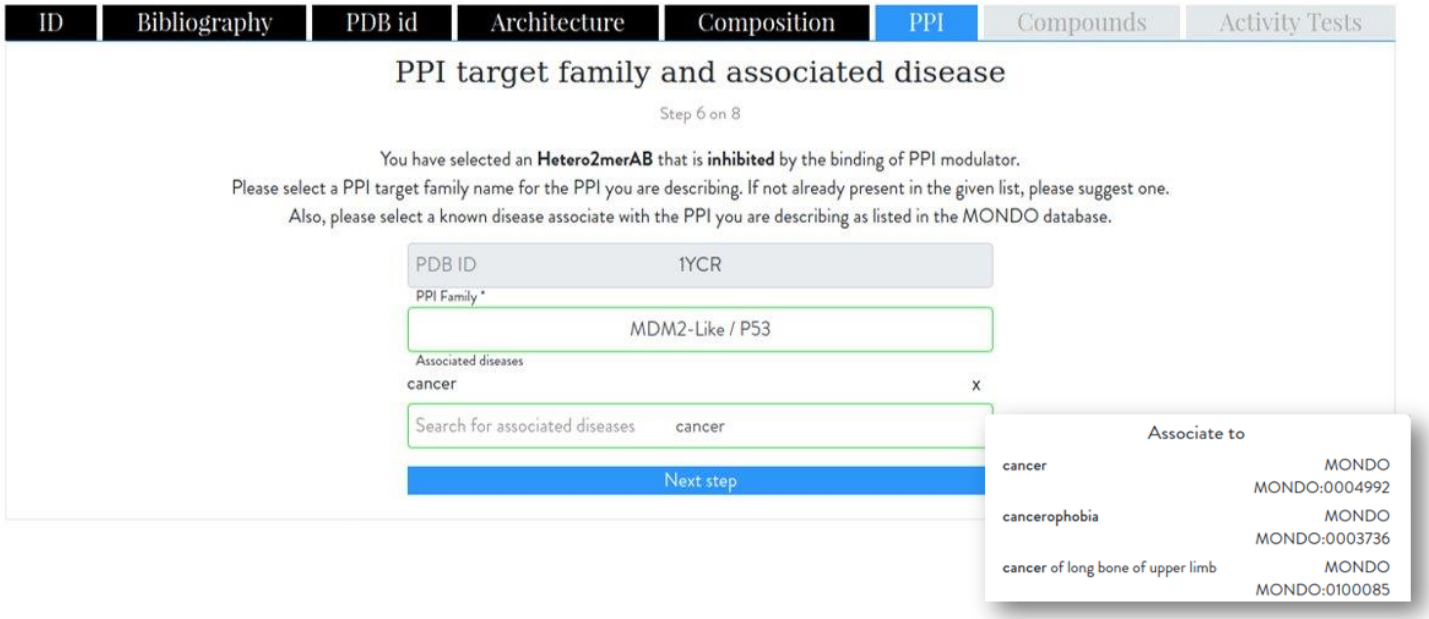
Step 3: Enter the PDB ID containing the struture of the protein-protein interaction.



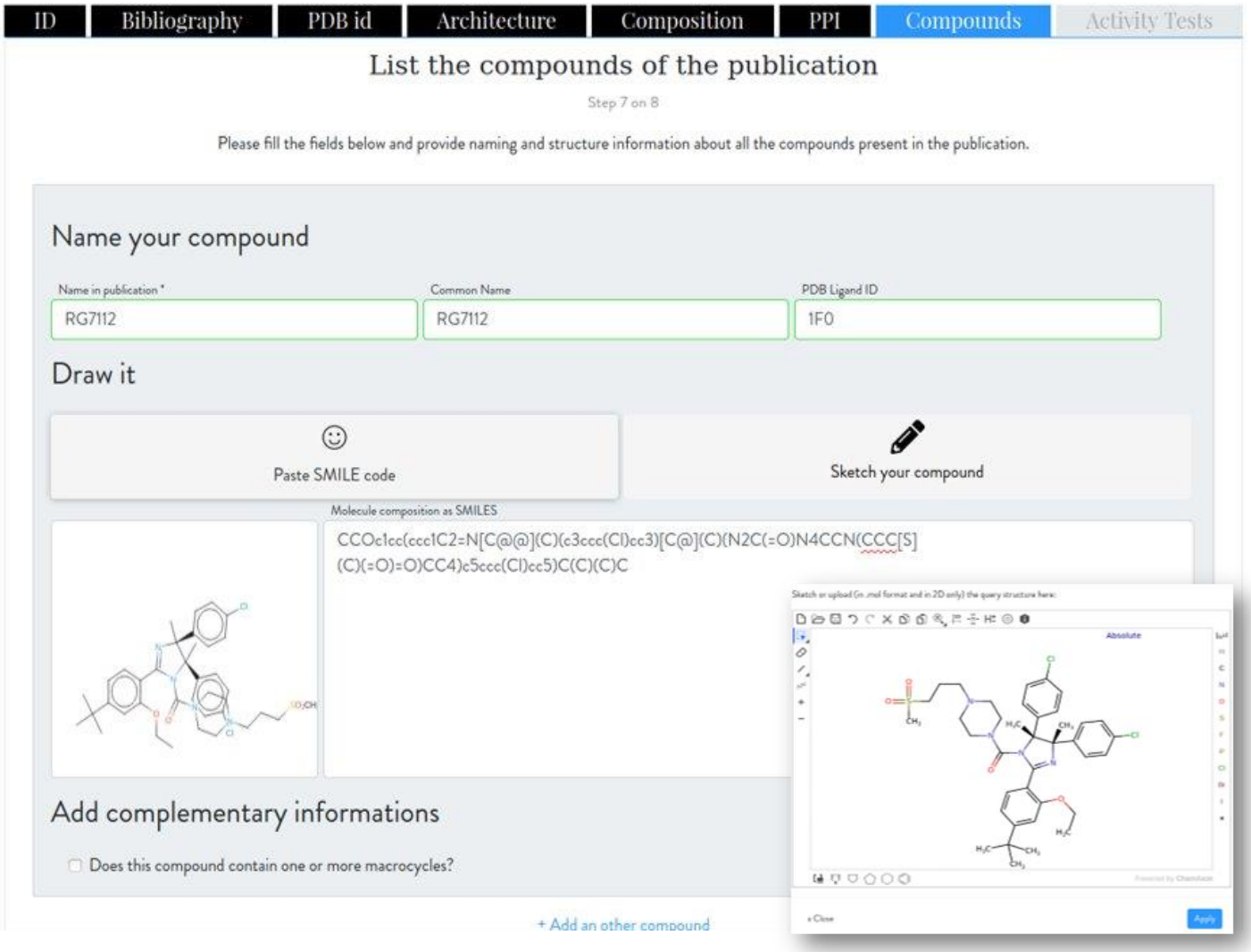
Step 4: Select the mode of action of the compounds acting on the interaction between "Inhibited" or "Stabilized" and the type of structural architecture of the target



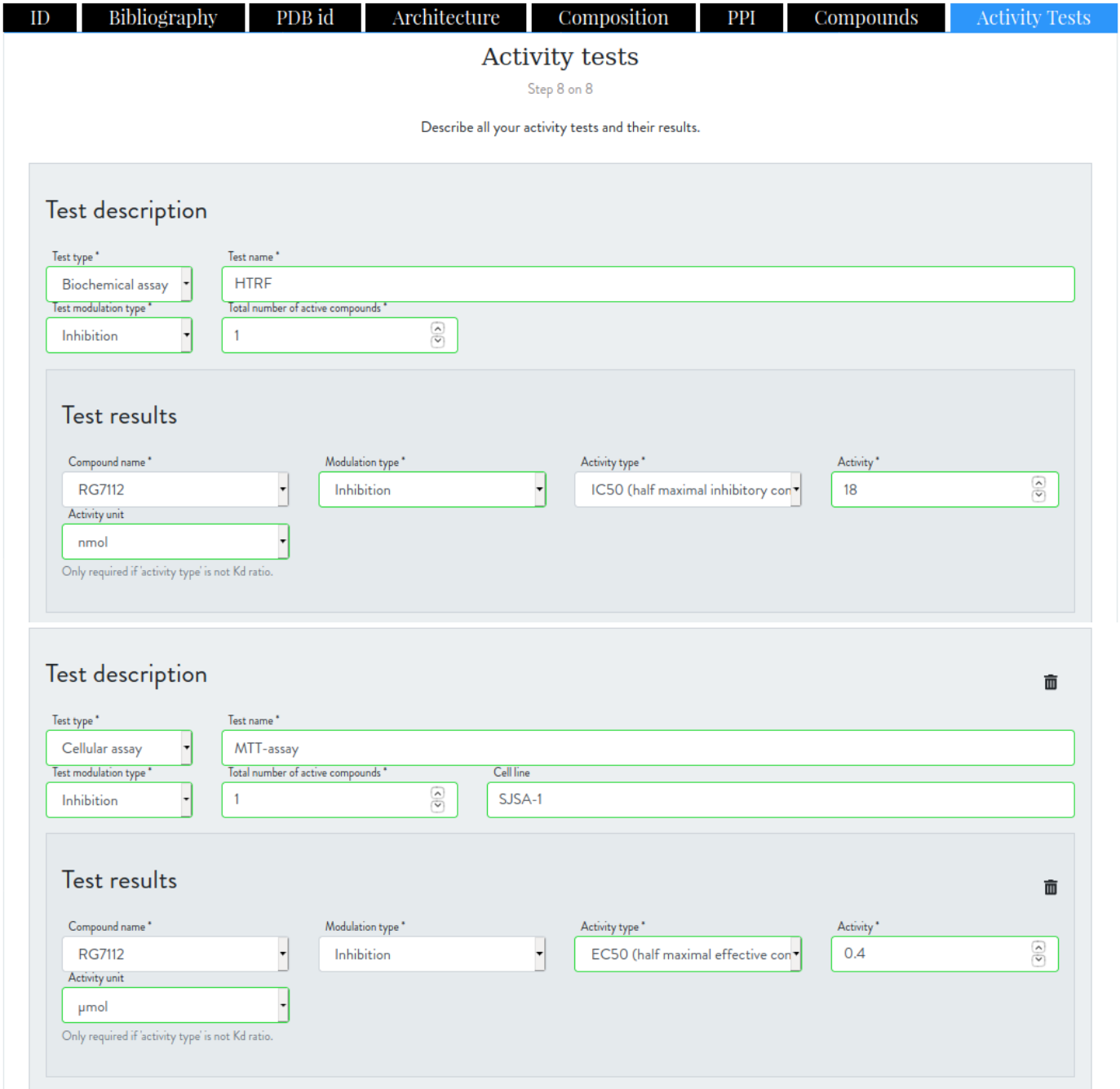
Step 5: Choose the protein that is bound by the compound (bound) and the protein that is displaced by the compound (partner)



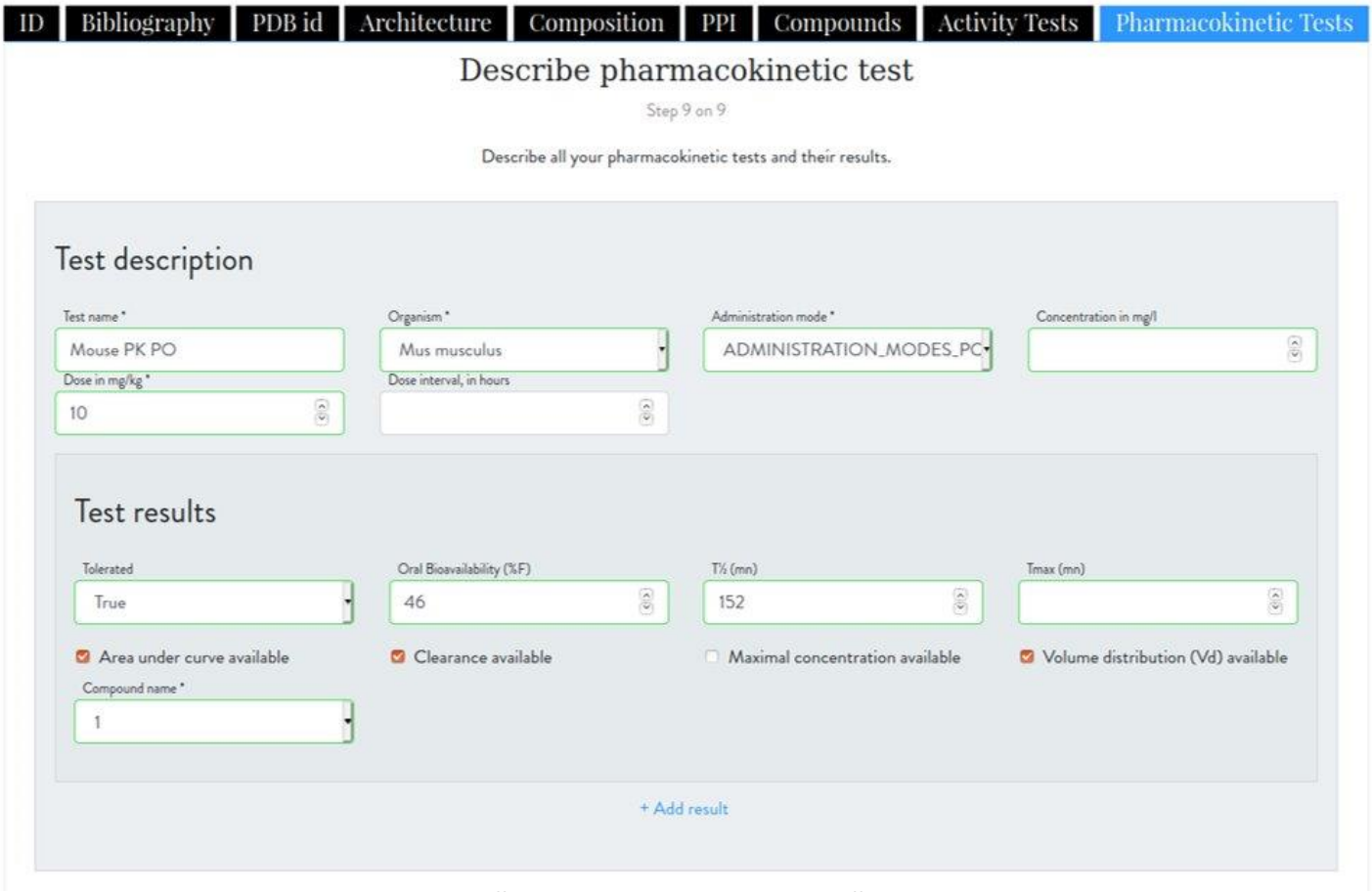
Step 6: Select/Create the PPI family in the dropdown list, then the known associated diseases. The associated diseases list is built from the Mondo Disease Ontology.



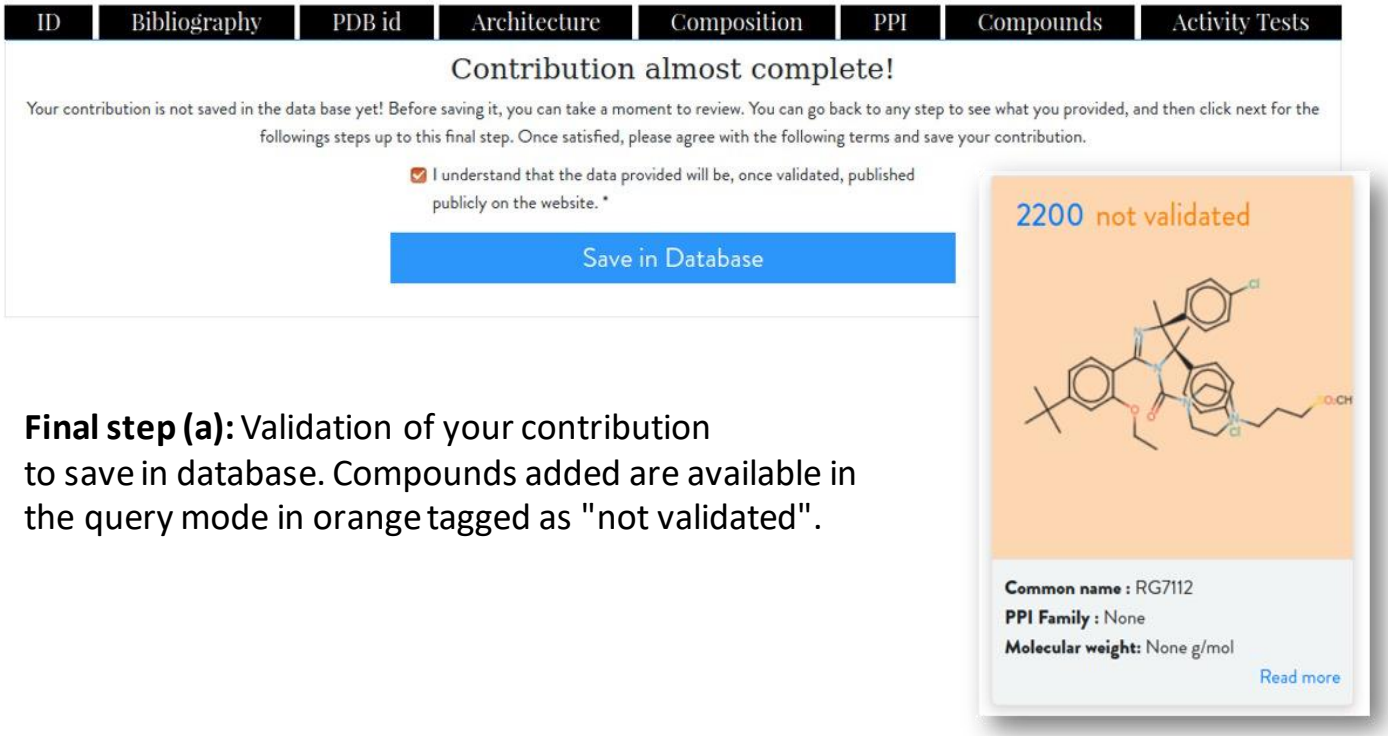
Step 7: Fill the form describing the compounds according to their name in the publication, their common name, their 3-character PDB ID if any. The compound can be directly built from the SMILES code, drawn using MarvinSketch from ChemAxon, or by pasting a IUPAC code into the MarvinSketch window.



Step 8: Describe activity tests and their results. First, choose the test type: "Biochemical assay" or "Cellular assay". Select the test name, the modulation type (Inhibition, Binding or Stabilization), the number of active compounds and the cell line for the "Cellular assay". Second, fill the activity for each compound (IC50, EC50, Kd, Ki, Kd ratio), which can be declined in different unit (M, mM, µM, nM, pM).



Step 9: In the case you choose "Pharmacokinetic study" at step 2, a supplementary step appears to fill the data related to these studies. The same is true for cytotoxic assays.



Final step (a): Validation of your contribution to save in database. Compounds added are available in the query mode in orange tagged as "not validated".

CONTRIBUTION 75 - THIS CONTRIBUTION HAS NOT BEEN VALIDATED BY A CURATOR YET, DATA MIGHT BE INCOMPLETE OR INACCURATE

Bibliography

MDM2 Small-Molecule Antagonist RG7112 Activates p53 Signaling and Regresses Human Tumors in Preclinical Cancer Models
Tovar C., Graves B., Packman K., Filipovic Z., Xia B. H. M., Tardell C., Garrido R., Lee E., Kolinsky K., To K.-H., Linn M., Podlaski F., Wovkulich P., Vu B., Vassilev L. T.
Cancer Research (2013) DOI - 10.1158/0008-5472.CAN-12-2807

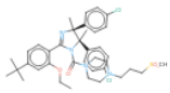
Contains : X-Ray Data, In Vitro Study, In Cellulo Study, In Vivo Study

PPI Architecture

PDB code of the PPI: 1YCR
PPI family: MDM2-Like / P53
Total number of pockets in the complex: 1
PPI name: MDM2 / P53
PPI symmetry: AS (asymmetric)
Diseases: cancer (MONDO:0004992)

Complex type	Protein	Domain
Partner	P04637	unknown
Bound	Q00987	unknown

Compounds

Compound Name In The Publication	Chemical structure	Iupac Name	Pdb Ligand Id	iPPI-DB ID
RG7112			1F0	2200

Tests

Test Activity Description - MTT-assay

Protein Domain Bound Complex: MDM2 Q00987-unknow (1)
Test Type: Cellular assay
Total Number Of Active Compounds: 1
Is Primary: False
Test Modulation Type: Inhibition
Cell Line: SJSA-1

Compound	Modulation type	Activity type	Activity
RG7112	Inhibition	pEC50	6.40

Test Activity Description - HTRF

Protein Domain Bound Complex: MDM2 Q00987-unknow (1)
Test Type: Biochemical assay
Total Number Of Active Compounds: 1
Is Primary: False
Test Modulation Type: Inhibition
Cell Line: None

Compound	Modulation type	Activity type	Activity
RG7112	Inhibition	pIC50	7.74

Final step (b): The final page summarizing all information about your contribution.