SalTox-v1.0.

Overview: The software provides a native interface for toxicity prediction towards salmon species, enabling users to obtain toxicity predictions based on the developed q-RASAR model.

System requirement for using the software

1. The user must download and install Python on their system before running the software.

2. There is a 'dependencies' file. Run one time that file in Python.

Input file specifications

The tool takes an input file having .xlsx extension containing the required set of descriptors for the query or the external set compounds to compute the median lethal toxicity of salmon species in terms of pLC_{50}.

The query or the external set file should contain the compound number (No.) in the first column and the descriptors in the subsequent columns. **The user needs to maintain the same order of descriptors as shown in the figure.** The two-dimensional (2D) descriptors can be computed using alvaDesc software and the RASAR descriptors can be computed from RASAR-Desc-Calc-v3.0.3 software [1] with the optimized hyper-parameters being **Gaussian kernel setting with the number of similar training compounds = 10 and σ = 2.**

No.	NsssCH	B02[S-S]	B03[N-O]	LOGP99	SD similarity(GK)	sm2(GK)[Banerjee-Roy similarity coefficient 2]
6	0	1	0	3.560179975	0.388991894	1.094936372
11	1	0	0	5.205899909	0.007099755	-0.005757834
19	1	0	1	3.7685	0.191715726	-0.172658069
27	2	0	0	5.152000062	0.034311931	-0.009689839
30	0	0	0	3.050399914	0.004711994	0.002229657
32	2	0	1	3.04230006	0.135464333	-0.183283849
36	0	0	0	3.258499935	0.004974554	-0.001973026
40	1	0	1	3.164120018	0.205697059	-0.357293434
42	0	0	0	4.685300022	0.015104309	0.010604833
48	0	0	0	5.988619976	0.045316832	0.043347932
50	1	0	0	2.905700013	0.013943681	-0.000694213

Output file

An excel **(.xlsx)** sheet named "**Predictions.xlsx**" is generated representing the predicted values of pLC_{50}, as shown in the following figure.

IDs	Predictions
6	6.127036205
11	6.284763541
19	5.921983046
27	6.558634675
30	5.031038009
32	6.125011634
36	5.112346317
40	5.429350028
42	5.694107835
48	6.194715686
50	5.314862536
51	4.629338596

Reference

1. https://sites.google.com/jadavpuruniversity.in/dtc-lab-software/home