I. In Silico Tools for Pharmacokinetic and Toxicological Predictions

1. ADMET LAB 2.0 (ADMETlab 2.0 is an integrated online platform foe accurate and comprehensive predictions of ADMET properties) https://admetmesh.scbdd.com/
2. SwissADME (Website to compute physiochemical descriptors and to predict ADME parameters, pharmacokinetic properties, drug-like nature and medicinal chemistry friendliness of one or multiple small molecules to support drug discovery.)
   http://www.swissadme.ch/
1. PreADMET (web-based application for predicting ADME data and building drug-like library using in silico method.) https://preadmet.webservice.bmdrc.org/
2. PkCSM (Software for predicition of pharmacokinetic properties) http://biosig.unimelb.edu.au/pkcsm/prediction
3. vNN-ADMET (online platform to predict absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties and to build new models based on variable nearest neighbor (vNN) methodology) https://vnnadmet.bhsai.org/vnnadmet/login.xhtml
4. SMARTcyp - prediction of interaction at metabolism level, uses a specialized algorithm that involves a reactivity descriptor and an accessibility descriptor. https://smartcyp.sund.ku.dk/mol_to_som
5. MetaPred – A webserver for predicition of Cytochrome P450 isoform responsible for metabolising a drug molecule. http://crdd.osdd.net/raghava/metapred/help.php
6. SuperCYP https://bio.tools/supercyp
7. Stimulation Plus Software - develops absorption, distribution, metabolism, excretion, and toxicity (ADMET) modeling and simulation software for Pharmaceutical biotechnology industry. https://www.simulations-plus.com/software/admetpredictor/
8. AdmetSAR - A comprehensive source and free tool for evaluating chemical ADMET properties. http://lmmd.ecust.edu.cn/admetsar2
9. Percepta Platform - is a portfolio of software applications and a technology ecosystem for predicting and managing physicochemical, ADME/Tox, and other molecular property data. https://www.acdlabs.com/products/percepta-platform/
10. VirtualToxLab – is one of the *in-silico* tool for predicting toxic potential of existing and hypothetical compounds. https://pharma.unibas.ch/de/research/research-groups/computational-pharmacy-2155/research/virtualtoxlab/
11. CASEUltra - CASE Ultra is being used by the pharma industry to screen drug candidates for potential toxicity at all stages of drug discovery.
    http://www.multicase.com/case-ultra

1. Derek Nexus – Derek Nexus is one of the knowledge-based toxicology software which gives predictions for a variety of endpoints. https://www.lhasalimited.org/products/derek-nexus.htm
1. Meteor Nexus - It is one of the knowledge base software which helps to predict the metabolic fate of chemicals. https://www.lhasalimited.org/products/meteor-nexus.htm
2. PASS Online – Pass online predicts over 4000 kinds of biological activity, including pharmacological effects, mechanisms of action, toxic and adverse effects, interaction with metabolic enzymes and transporters, influence on gene expression, etc. http://www.way2drug.com/PASSOnline/