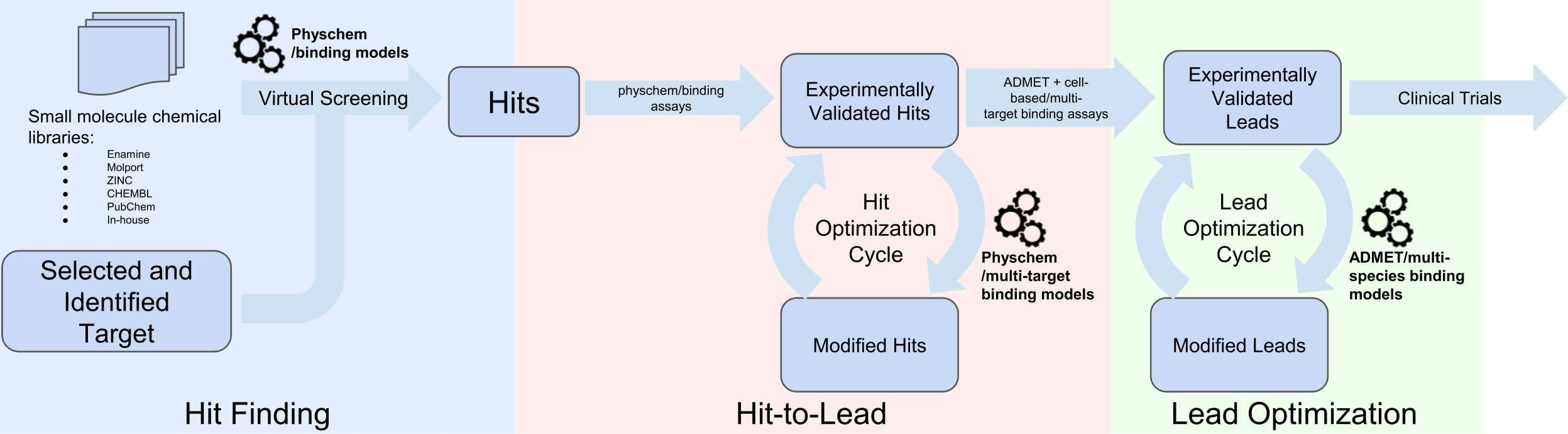
# Applications of machine learning in drug discovery

1. QSAR & ADMET modeling based on deep learning

Review and perspectives :

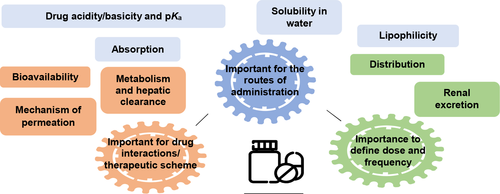
* Jiang, D., Wu, Z., Hsieh, CY. *et al.* Could graph neural networks learn better molecular representation for drug discovery? A comparison study of descriptor-based and graph-based models. *J Cheminform* 13, 12 (**2021**). https://doi.org/10.1186/s13321-020-00479-8
* [Recent Advances in the Prediction of Pharmacokinetics Properties in Drug Design Studies: A Review](https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/cmdc.202100542). S. Q. Pantaleão, P. O. Fernandes, J. E. Gonçalves, V. G. Maltarollo, K. M. Honorio, *ChemMedChem* **2022**, *17*, e202100542.
* Dara S, Dhamercherla S, Jadav SS, Babu CM, Ahsan MJ. Machine Learning in Drug Discovery: A Review. Artif Intell Rev. **2022**;55(3):1947-1999. doi: 10.1007/s10462-021-10058-4. Epub 2021 Aug 11. PMID: 34393317; PMCID: PMC8356896.
* Pillai N, Dasgupta A, Sudsakorn S, Fretland J, Mavroudis PD. Machine Learning guided early drug discovery of small molecules. Drug Discov Today. 2022 Aug;27(8):2209-2215. doi: 10.1016/j.drudis.2022.03.017. Epub **2022** Mar 29. PMID: 35364270.
* Nikolai Schapin, Maciej Majewski, Alejandro Varela-Rial, Carlos Arroniz, Gianni De Fabritiis,
* Machine learning small molecule properties in drug discovery, Artificial Intelligence Chemistry, **2023**, <https://doi.org/10.1016/j.aichem.2023.100020>.



* Dias, A.L., Bustillo, L. & Rodrigues, T. Limitations of representation learning in small molecule property prediction. *Nat Commun* 14, 6394 (**2023**). <https://doi.org/10.1038/s41467-023-41967-3>

#### Cheng Fang, Ye Wang, Richard Grater, Sudarshan Kapadnis, Cheryl Black, Patrick Trapa, and Simone Sciabola. Prospective Validation of Machine Learning Algorithms for Absorption, Distribution, Metabolism, and Excretion Prediction: An Industrial Perspective. Journal of Chemical Information and Modeling **2023** 63 (11), 3263-3274. DOI: 10.1021/acs.jcim.3c00160

* Tropsha, A., Isayev, O., Varnek, A. *et al.* Integrating QSAR modelling and deep learning in drug discovery: the emergence of deep QSAR. *Nat Rev Drug Discov* **23**, 141–155 (**2024**). <https://doi.org/10.1038/s41573-023-00832-0>



#### <https://books.rsc.org/books/edited-volume/2061/chapter-abstract/6377890/Machine-Learning-in-Drug-Design?redirectedFrom=fulltext>

QSAR modeling :

* Vukovic, K.; Gadaleta, D.; Benfenati, E. Methodology of aiQSAR: a group-specific approach to QSAR modelling. *J. Cheminform* **2019**, *11* (1), 27,  DOI: 10.1186/s13321-019-0350-y
* Kwon, S., Bae, H., Jo, J. *et al.* Comprehensive ensemble in QSAR prediction for drug discovery. *BMC Bioinformatics* **20**, 521 (**2019**). https://doi.org/10.1186/s12859-019-3135-4
* Li, X., Fourches, D. Inductive transfer learning for molecular activity prediction: *Next*-*Gen QSAR Models with MolPMoFiT*. *J Cheminform* 12, 27 (**2020**). <https://doi.org/10.1186/s13321-020-00430-x>
* Yang, ZY., Fu, L., Lu, AP. *et al.* Semi-automated workflow for molecular pair analysis and QSAR-assisted transformation space expansion. *J Cheminform* 13, 86 (**2021**). <https://doi.org/10.1186/s13321-021-00564-6>
* Integrating Expert Knowledge with Deep Learning Improves QSAR Models for CADD Modeling. Yunchao (Lance) Liu, Rocco Moretti, Yu Wang, Bobby Bodenheimer, Tyler Derr, Jens Meiler. bioRxiv **2023**.04.17.537185; https://doi.org/10.1101/2023.04.17.537185
* Vishakha Gautam, Rahul Gupta, Deepti Gupta, Anubhav Ruhela, Aayushi Mittal, Sanjay Kumar Mohanty, Sakshi Arora, Ria Gupta, Chandan Saini, Debarka Sengupta, Natarajan Arul Murugan, Gaurav Ahuja, deepGraphh: AI-driven web service for graph-based quantitative structure–activity relationship analysis, Briefings in Bioinformatics, Volume 23, Issue 5, September 2022, bbac288, <https://doi.org/10.1093/bib/bbac288>
* Zhifeng Gao and Xiaohong Ji and Guojiang Zhao and Hongshuai Wang and Hang Zheng and Guolin Ke and Linfeng Zhang. Uni-QSAR: an Auto-ML Tool for Molecular Property Prediction. **2023**, 2304.12239, arXiv, <https://doi.org/10.48550/arXiv.2304.12239>
* Mervin L, Voronov A, Kabeshov M, Engkvist O. Qptuna: an automated QSAR modelling platform for molecular property prediction in drug design. ChemRxiv. **2024**; doi:10.26434/chemrxiv-2024-2rlk7 This content is a preprint and has not been peer-reviewed.

Permeability:

#### Ning-Ning Wang, Jie Dong, Yin-Hua Deng, Min-Feng Zhu, Ming Wen, Zhi-Jiang Yao, Ai-Ping Lu, Jian-Bing Wang, and Dong-Sheng Cao. ADME Properties Evaluation in Drug Discovery: Prediction of Caco-2 Cell Permeability Using a Combination of NSGA-II and Boosting. Journal of Chemical Information and Modeling ****2016**** 56 (4), 763-773 DOI: 10.1021/acs.jcim.5b00642

* Chi, C.-T.; Lee, M.-H.; Weng, C.-F.; Leong, M.K. In Silico Prediction of PAMPA Effective Permeability Using a Two-QSAR Approach. Int. J. Mol. Sci. **2019**, 20, 3170. https://doi.org/10.3390/ijms20133170
* Wang Y, Chen X. QSPR model for Caco-2 cell permeability prediction using a combination of HQPSO and dual-RBF neural network. RSC Adv. **2020** Nov 26;10(70):42938-42952. doi: 10.1039/d0ra08209k. PMID: 35514900; PMCID: PMC9058322
* Roy, D., Dutta, D., Wishart, D.S. *et al.* Predicting PAMPA permeability using the 3D-RISM-KH theory: are we there yet?. *J Comput Aided Mol Des* **35**, 261–269 (**2021**). https://doi.org/10.1007/s10822-020-00364-4
* Falcón-Cano G, Molina C, Cabrera-Pérez MÁ. Reliable Prediction of Caco-2 Permeability by Supervised Recursive Machine Learning Approaches. Pharmaceutics. **2022** Sep 21;14(10):1998. doi: 10.3390/pharmaceutics14101998. PMID: 36297432; PMCID: PMC9610902.
* Gousiadou C, Doganis P, Sarimveis H. Development of artificial neural network models to predict the PAMPA effective permeability of new, orally administered drugs active against the coronavirus SARS-CoV-2. Netw Model Anal Health Inform Bioinform. **2023**;12(1):16. doi: 10.1007/s13721-023-00410-9. Epub **2023** Feb 6. PMID: 36778642; PMCID: PMC9901841.

BBB prediction:

#### The Blood–Brain Barrier (BBB) Score. Mayuri Gupta, Hyeok Jun Lee, Christopher J. Barden, and Donald F. Weaver Journal of Medicinal Chemistry ****2019**** 62 (21), 9824-9836 DOI: 10.1021/acs.jmedchem.9b01220

* Liu L, Zhang L, Feng H, Li S, Liu M, Zhao J, Liu H. Prediction of the Blood-Brain Barrier (BBB) Permeability of Chemicals Based on Machine-Learning and Ensemble Methods. Chem Res Toxicol. **2021** Jun 21;34(6):1456-1467. doi: 10.1021/acs.chemrestox.0c00343. Epub 2021 May 28. PMID: 34047182.
* Tong X, Wang D, Ding X, et al. Blood-brain barrier penetration prediction enhanced by uncertainty estimation. Journal of Cheminformatics. **2022** Jul;14(1):44. DOI: 10.1186/s13321-022-00619-2. PMID: 35799215; PMCID: PMC9264551.
* Kumar R, Sharma A, Alexiou A, Bilgrami AL, Kamal MA, Ashraf GM. DeePred-BBB: A Blood Brain Barrier Permeability Prediction Model With Improved Accuracy. Front Neurosci. 2022 May 3;16:858126. doi: 10.3389/fnins.**2022**.858126. PMID: 35592264; PMCID: PMC9112838
* Shaker B, Yu MS, Song JS, Ahn S, Ryu JY, Oh KS, Na D. LightBBB: computational prediction model of blood-brain-barrier penetration based on LightGBM. Bioinformatics. **2021** May 23;37(8):1135-1139. doi: 10.1093/bioinformatics/btaa918. PMID: 33112379
* Shaker B, Lee J, Lee Y, Yu MS, Lee HM, Lee E, Kang HC, Oh KS, Kim HW, Na D. A machine learning-based quantitative model (LogBB\_Pred) to predict the blood-brain barrier permeability (logBB value) of drug compounds. Bioinformatics. **2023** Oct 3;39(10):btad577. doi: 10.1093/bioinformatics/btad577. PMID: 37713469; PMCID: PMC10560102
* DeepGRID: Deep Learning Using GRID Descriptors for BBB Prediction. Loriano Storchi, Gabriele Cruciani, and Simon Cross. Journal of Chemical Information and Modeling **2023** 63 (17), 5496-5512 . DOI: 10.1021/acs.jcim.3c00768

Solubility:

* Boobier, S., Hose, D.R.J., Blacker, A.J. *et al.* Machine learning with physicochemical relationships: solubility prediction in organic solvents and water. *Nat Commun* **11**, 5753 (**2020**). https://doi.org/10.1038/s41467-020-19594-z
* SolTranNet–A Machine Learning Tool for Fast Aqueous Solubility Prediction. Paul G. Francoeur and David R. Koes. Journal of Chemical Information and Modeling **2021** 61 (6), 2530-2536 . DOI: 10.1021/acs.jcim.1c00331
* Ye, Z., Ouyang, D. Prediction of small-molecule compound solubility in organic solvents by machine learning algorithms. *J Cheminform* 13, 98 (**2021**). https://doi.org/10.1186/s13321-021-00575-3
* Novel Solubility Prediction Models: Molecular Fingerprints and Physicochemical Features vs Graph Convolutional Neural Networks. Sumin Lee, Myeonghun Lee, Ki-Won Gyak, Sung Dug Kim, Mi-Jeong Kim, and Kyoungmin Min. ACS Omega **2022** 7 (14), 12268-12277 . DOI: 10.1021/acsomega.2c00697
* ALipSol: An Attention-Driven Mixture-of-Experts Model for Lipophilicity and Solubility Prediction. Jialu Wu, Junmei Wang, Zhenxing Wu, Shengyu Zhang, Yafeng Deng, Yu Kang, Dongsheng Cao, Chang-Yu Hsieh, and Tingjun Hou. Journal of Chemical Information and Modeling **2022** 62 (23), 5975-5987 . DOI: 10.1021/acs.jcim.2c01290
* Prediction of the Aqueous Solubility of Compounds Based on Light Gradient Boosting Machines with Molecular Fingerprints and the Cuckoo Search Algorithm. Mengshan Li, Huijie Chen, Hang Zhang, Ming Zeng, Bingsheng Chen, and Lixin Guan. ACS Omega **2022** 7 (46), 42027-42035 . DOI: 10.1021/acsomega.2c03885

#### Evaluation of Deep Learning Architectures for Aqueous Solubility Prediction. Gihan Panapitiya, Michael Girard, Aaron Hollas, Jonathan Sepulveda, Vijayakumar Murugesan, Wei Wang, and Emily Saldanha. ACS Omega ****2022**** 7 (18), 15695-15710 . DOI: 10.1021/acsomega.2c00642

* Ryu, Seongok and Sumin Lee. “Accurate, reliable and interpretable solubility prediction of druglike molecules with attention pooling and Bayesian learning.” ArXiv abs/2210.07145 (**2022**): n. pag.

#### Attention-Based Graph Neural Network for Molecular Solubility Prediction. Waqar Ahmad, Hilal Tayara, and Kil To Chong. ACS Omega ****2023**** 8 (3), 3236-3244 DOI: 10.1021/acsomega.2c06702

* Liu J, Lei X, Ji C, Pan Y. Fragment-pair based drug molecule solubility prediction through attention mechanism. Front Pharmacol. **2023** Oct 10;14:1255181. doi: 10.3389/fphar.2023.1255181. PMID: 37881183; PMCID: PMC10595153

CYP prediction / metabolic stability:

* Priyanka Banerjee, Mathias Dunkel, Emanuel Kemmler, Robert Preissner, SuperCYPsPred—a web server for the prediction of cytochrome activity, Nucleic Acids Research, Volume 48, Issue W1, 02 July **2020**, Pages W580–W585, <https://doi.org/10.1093/nar/gkaa166>
* David S Wishart, Siyang Tian, Dana Allen, Eponine Oler, Harrison Peters, Vicki W Lui, Vasuk Gautam, Yannick Djoumbou-Feunang, Russell Greiner, Thomas O Metz, BioTransformer 3.0—a web server for accurately predicting metabolic transformation products, Nucleic Acids Research, Volume 50, Issue W1, 5 July **2022,** Pages W115–W123, https://doi.org/10.1093/nar/gkac313
* Jae Yong Ryu, Jeong Hyun Lee, Byung Ho Lee, Jin Sook Song, Sunjoo Ahn, Kwang-Seok Oh, PredMS: a random forest model for predicting metabolic stability of drug candidates in human liver microsomes, Bioinformatics, Volume 38, Issue 2, January **2022**, Pages 364–368, <https://doi.org/10.1093/bioinformatics/btab547>
* Ai D, Cai H, Wei J, Zhao D, Chen Y, Wang L. DEEPCYPs: A deep learning platform for enhanced cytochrome P450 activity prediction. Front Pharmacol. **2023** Apr 10;14:1099093. doi: 10.3389/fphar.2023.1099093. PMID: 37101544; PMCID: PMC10123292.
* Bing-Xue Du, Yahui Long, Xiaoli Li, Min Wu, Jian-Yu Shi, CMMS-GCL: cross-modality metabolic stability prediction with graph contrastive learning, Bioinformatics, Volume 39, Issue 8, August **2023**, btad503, https://doi.org/10.1093/bioinformatics/btad503
* Chen Z, Zhang L, Zhang P, Guo H, Zhang R, Li L, Li X. Prediction of Cytochrome P450 Inhibition Using a Deep Learning Approach and Substructure Pattern Recognition. J Chem Inf Model. **2023** Oct 21. doi: 10.1021/acs.jcim.3c01396. Epub ahead of print. PMID: 37864562.

Toxicity prediction:

* Wu, K.; Wei, G.-W. Quantitative toxicity prediction using topology based multitask deep neural networks. *J. Chem. Inf. Model.* **2018**, *58* (2), 520– 531,  DOI: 10.1021/acs.jcim.7b00558
* Karim, A.; Mishra, A.; Newton, M. A. H.; Sattar, A. Efficient Toxicity Prediction via Simple Features Using Shallow Neural Networks and Decision Trees. *Acs Omega* **2019**, *4* (1), 1874– 1888,  DOI: 10.1021/acsomega.8b03173
* Gadaleta, D.; Vuković, K.; Toma, C.; Lavado, G. J.; Karmaus, A. L.; Mansouri, K.; Kleinstreuer, N. C.; Benfenati, E.; Roncaglioni, A. SAR and QSAR modeling of a large collection of LD50 rat acute oral toxicity data. *J. Cheminformatics* **2019**, *11* (1), 1– 16,  DOI: 10.1186/s13321-019-0383-2
* Chen, J. R.; Cheong, H. H.; Siu, S. W. I. BESTox: A Convolutional Neural Network Regression Model Based on Binary-Encoded SMILES for Acute Oral Toxicity Prediction of Chemical Compounds. *Lect N Bioinformat* **2020**, *12099*, 155– 166,  DOI: 10.1007/978-3-030-42266-0\_12
* Ryu, J. Y.; Lee, M. Y.; Lee, J. H.; Lee, B. H.; Oh, K. S. DeepHIT: a deep learning framework for prediction of hERG-induced cardiotoxicity. *Bioinformatics* **2020**, *36* (10), 3049– 3055,  DOI: 10.1093/bioinformatics/btaa075
* Jain, S.; Siramshetty, V. B.; Alves, V. M.; Muratov, E. N.; Kleinstreuer, N.; Tropsha, A.; Nicklaus, M. C.; Simeonov, A.; Zakharov, A. V. Large-Scale Modeling of Multispecies Acute Toxicity End Points Using Consensus of Multitask Deep Learning Methods. *J. Chem. Inf. Model.* **2021**, *61* (2), 653– 663,  DOI: 10.1021/acs.jcim.0c01164
* Karim, A.; Riahi, V.; Mishra, A.; Newton, M. A. H.; Dehzangi, A.; Balle, T.; Sattar, A. Quantitative Toxicity Prediction via Meta Ensembling of Multitask Deep Learning Models. *Acs Omega* **2021**, *6* (18), 12306– 12317,  DOI: 10.1021/acsomega.1c01247
* Chu, C. S.; Simpson, J. D.; O’Neill, P. M.; Berry, N. G. Machine learning–Predicting Ames mutagenicity of small molecules. *Journal of Molecular Graphics and Modelling* **2021**, *109*, 108011,  DOI: 10.1016/j.jmgm.2021.108011
* Chen, J., Si, YW., Un, CW. *et al.* Chemical toxicity prediction based on semi-supervised learning and graph convolutional neural network. *J Cheminform* **13**, 93 (**2021**). https://doi.org/10.1186/s13321-021-00570-8
* Chemical representation learning for toxicity prediction. Born, Jannis and Markert, Greta and Janakarajan, Nikita and Kimber, Talia B. and Volkamer, Andrea and Martínez, María Rodríguez and Manica, Matteo. ***Digital Discovery***, **2023**, **2**, 674-691.DOI: 10.1039/D2DD00099G

ADMET prediction:

* Peng, Y. Z.; Lin, Y. M.; Jing, X. Y.; Zhang, H.; Huang, Y. R.; Luo, G. S. Enhanced Graph Isomorphism Network for Molecular ADMET Properties Prediction. *Ieee Access* **2020**, *8*, 168344– 168360,  DOI: 10.1109/ACCESS.2020.3022850
* Guoli Xiong, Zhenxing Wu, Jiacai Yi, Li Fu, Zhijiang Yang, Changyu Hsieh, Mingzhu Yin, Xiangxiang Zeng, Chengkun Wu, Aiping Lu, Xiang Chen, Tingjun Hou, Dongsheng Cao, ADMETlab 2.0: an integrated online platform for accurate and comprehensive predictions of ADMET properties, Nucleic Acids Research, Volume 49, Issue W1, 2 July **2021**, Pages W5–W14, <https://doi.org/10.1093/nar/gkab255>
* Venkatraman, V. FP-ADMET: a compendium of fingerprint-based ADMET prediction models. *J. Cheminformatics* **2021**, *13* (1), 34583740  DOI: 10.1186/s13321-021-00557-5
* Yu Wei, Shanshan Li, Zhonglin Li, Ziwei Wan, Jianping Lin, Interpretable-ADMET: a web service for ADMET prediction and optimization based on deep neural representation, Bioinformatics, Volume 38, Issue 10, May **2022**, Pages 2863–2871, <https://doi.org/10.1093/bioinformatics/btac192>
* Tevosyan A, Khondkaryan L, Khachatrian H, Tadevosyan G, Apresyan L, Babayan N, Stopper H, Navoyan Z. Improving VAE based molecular representations for compound property prediction. J Cheminform. **2022** Oct 14;14(1):69. doi: 10.1186/s13321-022-00648-x. PMID: 36242073; PMCID: PMC9569108
* Bhatia AS, Saggi MK, Kais S. Quantum Machine Learning Predicting ADME-Tox Properties in Drug Discovery. J Chem Inf Model. **2023** Nov 13;63(21):6476-6486. doi:10.1021/acs.jcim.3c01079. Epub 2023 Aug 21. PMID: 37603536.
* Fralish, Z., Chen, A., Skaluba, P. *et al.* DeepDelta: predicting ADMET improvements of molecular derivatives with deep learning. *J Cheminform* **15**, 101 (**2023**). https://doi.org/10.1186/s13321-023-00769-x
* Improved GNNs for Log D7.4 Prediction by Transferring Knowledge from Low-Fidelity Data. Yan-Jing Duan, Li Fu, Xiao-Chen Zhang, Teng-Zhi Long, Yuan-Hang He, Zhao-Qian Liu, Ai-Ping Lu, Ya-Feng Deng, Chang-Yu Hsieh, Ting-Jun Hou, and Dong-Sheng Cao. Journal of Chemical Information and Modeling **2023** 63 (8), 2345-2359 . DOI: 10.1021/acs.jcim.2c01564
* ADMET-AI: A machine learning ADMET platform for evaluation of large-scale chemical libraries. Kyle Swanson, Parker Walther, Jeremy Leitz, Souhrid Mukherjee, Joseph C. Wu, Rabindra V. Shivnaraine, James Zou. bioRxiv **2023**.12.28.573531; doi: https://doi.org/10.1101/2023.12.28.573531
* Prediction of Small-Molecule Developability Using Large-Scale In Silico ADMET Models. Maximilian Beckers, Noé Sturm, Finton Sirockin, Nikolas Fechner, and Nikolaus Stiefl. Journal of Medicinal Chemistry **2023** 66 (20), 14047-14060. DOI: 10.1021/acs.jmedchem.3c01083
* Yi, J., Shi, S., Fu, L. *et al.* OptADMET: a web-based tool for substructure modifications to improve ADMET properties of lead compounds. *Nat Protoc* (**2024**). https://doi.org/10.1038/s41596-023-00942-4
* Walter M, Borghardt JM, Humbeck L, Skalic M. Multi-task ADME/PK Prediction at Industrial Scale: Leveraging Large and Diverse Experimental Datasets. ChemRxiv. **2024**; doi:10.26434/chemrxiv-2024-pf4w9 This content is a preprint and has not been peer-reviewed.

PK prediction:

* Prediction of Oral Pharmacokinetics Using a Combination of In Silico Descriptors and In Vitro ADME Properties. Yohei Kosugi and Natalie Hosea. Molecular Pharmaceutics **2021** 18 (3), 1071-1079 . DOI: 10.1021/acs.molpharmaceut.0c01009
* Iwata H, Matsuo T, Mamada H, Motomura T, Matsushita M, Fujiwara T, Maeda K, Handa K. Predicting Total Drug Clearance and Volumes of Distribution Using the Machine Learning-Mediated Multimodal Method through the Imputation of Various Nonclinical Data. J Chem Inf Model. 2022 Sep 12;62(17):4057-4065. doi: 10.1021/acs.jcim.2c00318. Epub **2022** Aug 22. PMID: 35993595; PMCID: PMC9472274
* Wei-Chun Chou, Zhoumeng Lin, Machine learning and artificial intelligence in physiologically based pharmacokinetic modeling, Toxicological Sciences, Volume 191, Issue 1, January **2023**, Pages 1–14, https://doi.org/10.1093/toxsci/kfac101
* Sherwin S. S. Ng and Yunpeng Lu. Evaluating the Use of Graph Neural Networks and Transfer Learning for Oral Bioavailability Prediction. Journal of Chemical Information and Modeling **2023** 63 (16), 5035-5044. DOI: 10.1021/acs.jcim.3c00554
* Rath M, Wellnitz J, Martin H-J, Melo-Filho C, Hochuli J, Martins da Silva G, et al. Novel Pharmacokinetics Profiler (PhaKinPro): Model Development, Validation, and Implementation as a Web-Tool for Triaging Compounds with Undesired PK Profiles. ChemRxiv. **2023**; doi:10.26434/chemrxiv-2023-rnc4l This content is a preprint and has not been peer-reviewed.
* Stoyanova R, Katzberger PM, Komissarov L, Khadhraoui A, Sach-Peltason L, Groebke Zbinden K, Schindler T, Manevski N. Computational Predictions of Nonclinical Pharmacokinetics at the Drug Design Stage. J Chem Inf Model. **2023** Jan 23;63(2):442-458. doi: 10.1021/acs.jcim.2c01134. Epub **2023** Jan 3. PMID: 36595708
* Guo W, Dong Y, Hao GF. Transfer learning empowers accurate pharmacokinetics prediction of small samples. Drug Discov Today. **2024** Mar 8:103946. doi: 10.1016/j.drudis.**2024**.103946. Epub ahead of print. PMID: 38460571.
* Andrea Gruber, Florian Führer, Stephan Menz, Holger Diedam, Andreas H. Göller, Sebastian Schneckener. Prediction of Human Pharmacokinetics From Chemical Structure: Combining Mechanistic Modeling with Machine Learning. Journal of Pharmaceutical Sciences, **2024**, <https://doi.org/10.1016/j.xphs.2023.10.035>.
* PKSmart: An Open-Source Computational Model to Predict in vivo Pharmacokinetics of Small Molecules. Srijit Seal, Maria-Anna Trapotsi, Vigneshwari Subramanian, Ola Spjuth, Nigel Greene, Andreas Bender. bioRxiv 2024.02.02.578658; doi: https://doi.org/10.1101/2024.02.02.578658