BIBLIOGRAPHY

[1]   K. Sachdev and M. K. Gupta, "A comprehensive review of computational techniques for the prediction of drug side effects," *Drug Dev Res*, vol. 81, no. 6, pp. 650–670, Sep. 2020, doi: 10.1002/DDR.21669.

[2]   M. J. Jahid and J. Ruan, "An ensemble approach for drug side effect prediction," *Proceedings - 2013 IEEE International Conference on Bioinformatics and Biomedicine, IEEE BIBM 2013*, pp. 440–445, 2013, doi: 10.1109/BIBM.2013.6732532.

[3]   "Learning Objectives", Accessed: Jan. 21, 2023. [Online]. Available: www.nccmerp.org/about-medication-errors.

[4]   L. C. Huang, X. Wu, and J. Y. Chen, "Predicting adverse side effects of drugs," *BMC Genomics*, vol. 12, no. SUPPL. 5, pp. 1–10, Dec. 2011, doi: 10.1186/1471-2164-12-S5-S11/FIGURES/5.

[5]   J. J. Coleman and S. K. Pontefract, "Adverse drug reactions," *Clinical Medicine*, vol. 16, no. 5, p. 481, Oct. 2016, doi: 10.7861/CLINMEDICINE.16-5-481.

[6]   L. C. Huang, X. Wu, and J. Y. Chen, "Predicting adverse drug reaction profiles by integrating protein interaction networks with drug structures," *Proteomics*, vol. 13, no. 2, pp. 313–324, Jan. 2013, doi: 10.1002/PMIC.201200337.

[7]   B. Shaker, S. Ahmad, J. Lee, C. Jung, and D. Na, "In silico methods and tools for drug discovery," *Comput Biol Med*, vol. 137, p. 104851, Oct. 2021, doi: 10.1016/J.COMPBIOMED.2021.104851.

[8]   S. R. Kazmi, R. Jun, M. S. Yu, C. Jung, and D. Na, "In silico approaches and tools for the prediction of drug metabolism and fate: A review," *Comput Biol Med*, vol. 106, pp. 54–64, Mar. 2019, doi: 10.1016/J.COMPBIOMED.2019.01.008.

[9]   O. C. Uner, R. G. Cinbis, O. Tastan, and A. E. Cicek, "DeepSide: A Deep Learning Framework for Drug Side Effect Prediction," *bioRxiv*, p. 843029, Nov. 2019, doi: 10.1101/843029.

[10]   S. Muttakin, T. E. Moxon, and O. Gouseti, "In vivo, in vitro, and in silico studies of the GI tract," *Interdisciplinary Approaches to Food Digestion*, pp. 29–67, Jan. 2019, doi: 10.1007/978-3-030-03901-1_3/COVER.

[11]   A. Cortés-Cabrera, G. M. Morris, P. W. Finn, A. Morreale, and F. Gago, "Comparison of ultra-fast 2D and 3D ligand and target descriptors for side effect prediction and network analysis in polypharmacology," *Br J Pharmacol*, vol. 170, no. 3, pp. 557–567, Oct. 2013, doi: 10.1111/BPH.12294.

[12]   S. Vilar, N. P. Tatonetti, and G. Hripcsak, "3D Pharmacophoric Similarity improves Multi Adverse Drug Event Identification in Pharmacovigilance," *Scientific Reports 2015 5:1*, vol. 5, no. 1, pp. 1–9, Mar. 2015, doi: 10.1038/srep08809.

[13]   S. Vilar, T. Lorberbaum, G. Hripcsak, and N. P. Tatonetti, "Improving Detection of Arrhythmia Drug-Drug Interactions in Pharmacovigilance Data through the Implementation of Similarity-Based Modeling," *PLoS One*, vol. 10, no. 6, p. e0129974, Jun. 2015, doi: 10.1371/JOURNAL.PONE.0129974.

[14]   Danishuddin and A. U. Khan, "Descriptors and their selection methods in QSAR analysis: paradigm for drug design," *Drug Discov Today*, vol. 21, no. 8, pp. 1291–1302, Aug. 2016, doi: 10.1016/J.DRUDIS.2016.06.013.

[15]   V. Prachayasittikul *et al.*, "Large-scale classification of P-glycoprotein inhibitors using SMILES-based descriptors," *http://dx.doi.org/10.1080/1062936X.2016.1264468*, vol. 28, no. 1, pp. 1–16, Jan. 2017, doi: 10.1080/1062936X.2016.1264468.

[16]   A. P. Toropova, A. A. Toropov, and E. Benfenati, "A quasi-QSPR modelling for the photocatalytic decolourization rate constants and cellular viability (CV%) of nanoparticles by CORAL," *http://dx.doi.org/10.1080/1062936X.2014.984327*, vol. 26,

no. 1, pp. 29–40, Jan. 2015, doi: 10.1080/1062936X.2014.984327.

[17]   G. B. Goh, N. O. Hodas, C. Siegel, and A. Vishnu, "SMILES2Vec: An Interpretable
        General-Purpose Deep Neural Network for Predicting Chemical Properties," vol. 8, p.
        pages, Dec. 2017, doi: 10.48550/arxiv.1712.02034.

[18]   S. S. Hu, P. Chen, P. Gu, and B. Wang, "A Deep Learning-Based Chemical System for
        QSAR Prediction," *IEEE J Biomed Health Inform*, vol. 24, no. 10, pp. 3020–3028, Oct.
        2020, doi: 10.1109/JBHI.2020.2977009.

[19]   G. Gini, F. Zanoli, A. Gamba, G. Raitano, and E. Benfenati, "Could deep learning in
        neural networks improve the QSAR models?,"
        https://doi.org/10.1080/1062936X.2019.1650827, vol. 30, no. 9, pp. 617–642, Sep.
        2019, doi: 10.1080/1062936X.2019.1650827.

[20]   B. Jang, M. Kim, G. Harerimana, S. U. Kang, and J. W. Kim, "Bi-LSTM Model to Increase
        Accuracy in Text Classification: Combining Word2vec CNN and Attention
        Mechanism," *Applied Sciences 2020, Vol. 10, Page 5841*, vol. 10, no. 17, p. 5841, Aug.
        2020, doi: 10.3390/APP10175841.

[21]   S. N. M. Yousoff, A. Baharin, and A. Abdullah, "A review on optimization algorithm for
        deep learning method in bioinformatics field," *IECBES 2016 - IEEE-EMBS Conference
        on Biomedical Engineering and Sciences*, pp. 707–711, 2016, doi:
        10.1109/IECBES.2016.7843542.

[22]   A. Nainwal, Y. Kumar, and B. Jha, "Arrhythmia classification based on improved
        monarch butterfly optimization algorithm," *Journal of King Saud University -
        Computer and Information Sciences*, vol. 34, no. 8, pp. 5100–5109, Sep. 2022, doi:
        10.1016/J.JKSUCI.2022.01.002.

[23]   G. B. Goh, N. Hodas, C. Siegel, and A. Vishnu, "SMILES2vec: Predicting Chemical
        Properties from Text Representations." Jun. 04, 2018.

[24]   A. Danchin, "In vivo, in vitro and in silico: an open space for the development of
        microbe-based applications of synthetic biology," *Microb Biotechnol*, vol. 15, no. 1, p.
        42, Jan. 2022, doi: 10.1111/1751-7915.13937.

[25]   L. David, A. Thakkar, R. Mercado, and O. Engkvist, "Molecular representations in AI-
        driven drug discovery: a review and practical guide," *Journal of Cheminformatics 2020
        12:1*, vol. 12, no. 1, pp. 1–22, Sep. 2020, doi: 10.1186/S13321-020-00460-5.

[26]   G. B. Goh PNNL, N. Hodas PNNL, C. Siegel PNNL, and A. Vishnu PNNL, "SMILES2Vec:
        An Interpretable General-Purpose Deep Neural Network for Predicting Chemical
        Properties," vol. 8, p. pages, Dec. 2017, doi: 10.48550/arxiv.1712.02034.

[27]   G. Vrbančič, L. Brezočnik, U. Mlakar, D. Fister, and I. Fister Jr., "NiaPy: Python
        microframework for building nature-inspired algorithms," *J Open Source Softw*, vol. 3,
        no. 23, p. 613, Mar. 2018, doi: 10.21105/JOSS.00613.

[28]   Y. Feng, S. Deb, G. G. Wang, and A. H. Alavi, "Monarch butterfly optimization: A
        comprehensive review," *Expert Syst Appl*, vol. 168, p. 114418, Apr. 2021, doi:
        10.1016/J.ESWA.2020.114418.

[29]   G. B. Goh PNNL, N. Hodas PNNL, C. Siegel PNNL, and A. Vishnu PNNL, "SMILES2Vec:
        An Interpretable General-Purpose Deep Neural Network for Predicting Chemical
        Properties," vol. 8, p. pages, Dec. 2017, doi: 10.475/123.

[30]   H. Askr, E. Elgeldawi, H. Aboul Ella, Y. A. M. M. Elshaier, M. M. Gomaa, and A. E.
        Hassanien, "Deep learning in drug discovery: an integrative review and future
        challenges," *Artif Intell Rev*, vol. 56, no. 7, pp. 5975–6037, Jul. 2023, doi:
        10.1007/S10462-022-10306-1/FIGURES/6.

[31]   B. Fan, W. Fan, C. Smith, and H. "Skip" Garner, "Adverse drug event detection and
        extraction from open data: A deep learning approach," *Inf Process Manag*, vol. 57,
        no. 1, p. 102131, Jan. 2020, doi: 10.1016/J.IPM.2019.102131.

[32]   X. Zeng, S. Zhu, X. Liu, Y. Zhou, R. Nussinov, and F. Cheng, "deepDR: a network-based

deep learning approach to in silico drug repositioning," *Bioinformatics*, vol. 35, no. 24, pp. 5191–5198, Dec. 2019, doi: 10.1093/BIOINFORMATICS/BTZ418.

[33]   F. Noor and H. ElBoghdadi, "Neural Nets Distributed On Microcontrollers Using Metaheuristic Parallel Optimization Algorithm," *SSRN Electronic Journal*, Oct. 2020, doi: 10.2139/SSRN.3761765.

[34]   S. Sarv Ahrabi and A. Momenzadeh, "Metaheuristics and Pontryagin's minimum principle for optimal therapeutic protocols in cancer immunotherapy: a case study and methods comparison," *J Math Biol*, vol. 81, no. 2, pp. 691–723, Aug. 2020, doi: 10.1007/S00285-020-01525-7/FIGURES/9.

[35]   G. A. Pinheiro, J. Mucelini, M. D. Soares, R. C. Prati, J. L. F. Da Silva, and M. G. Quiles, "Machine Learning Prediction of Nine Molecular Properties Based on the SMILES Representation of the QM9 Quantum-Chemistry Dataset," *Journal of Physical Chemistry A*, vol. 124, no. 47, pp. 9854–9866, Nov. 2020, doi: 10.1021/ACS.JPCA.0C05969/SUPPL_FILE/JP0C05969_SI_001.PDF.

[36]   A. L. Nazarova and A. Nakano, "VLA-SMILES: Variable-Length-Array SMILES Descriptors in Neural Network-Based QSAR Modeling," *Mach Learn Knowl Extr*, vol. 4, no. 3, pp. 715–737, Sep. 2022, doi: 10.3390/MAKE4030034/S1.

[37]   C. Li, J. Feng, S. Liu, and J. Yao, "A Novel Molecular Representation Learning for Molecular Property Prediction with a Multiple SMILES-Based Augmentation," *Comput Intell Neurosci*, vol. 2022, 2022, doi: 10.1155/2022/8464452.

[38]   Z. Zhou, S. Kearnes, L. Li, R. N. Zare, and P. Riley, "Optimization of Molecules via Deep Reinforcement Learning," *Scientific Reports 2019 9:1*, vol. 9, no. 1, pp. 1–10, Jul. 2019, doi: 10.1038/s41598-019-47148-x.

[39]   A. Mahdaddi, S. Meshoul, and M. Belguidoum, "EA-based hyperparameter optimization of hybrid deep learning models for effective drug-target interactions prediction," *Expert Syst Appl*, vol. 185, p. 115525, Dec. 2021, doi: 10.1016/J.ESWA.2021.115525.

[40]   R. Winter, F. Montanari, A. Steffen, H. Briem, F. Noé, and D. A. Clevert, "Efficient multi-objective molecular optimization in a continuous latent space," *Chem Sci*, vol. 10, no. 34, pp. 8016–8024, Aug. 2019, doi: 10.1039/C9SC01928F.

[41]   Y. Kwon and J. Lee, "MolFinder: an evolutionary algorithm for the global optimization of molecular properties and the extensive exploration of chemical space using SMILES," *J Cheminform*, vol. 13, no. 1, pp. 1–14, Dec. 2021, doi: 10.1186/S13321-021-00501-7/FIGURES/7.

[42]   Y. F. Zhang *et al.*, "SPVec: A Word2vec-Inspired Feature Representation Method for Drug-Target Interaction Prediction," *Front Chem*, vol. 7, p. 504142, Jan. 2020, doi: 10.3389/FCHEM.2019.00895/BIBTEX.

[43]   M. Campillos, M. Kuhn, A. C. Gavin, L. J. Jensen, and P. Bork, "Drug target identification using side-effect similarity," *Science*, vol. 321, no. 5886, pp. 263–266, Jul. 2008, doi: 10.1126/SCIENCE.1158140.

[44]   S. Kim, D. Jin, and H. Lee, "Predicting Drug-Target Interactions Using Drug-Drug Interactions," *PLoS One*, vol. 8, no. 11, p. e80129, Nov. 2013, doi: 10.1371/JOURNAL.PONE.0080129.

[45]   Y. Yamanishi, M. Kotera, M. Kanehisa, and S. Goto, "Drug-target interaction prediction from chemical, genomic and pharmacological data in an integrated framework," *Bioinformatics*, vol. 26, no. 12, pp. i246–i254, Jun. 2010, doi: 10.1093/BIOINFORMATICS/BTQ176.

[46]   L. N. Cueni and M. Detmar, "The Lymphatic System in Health and Disease," *https://home.liebertpub.com/lrb*, vol. 6, no. 3–4, pp. 109–122, Dec. 2008, doi: 10.1089/LRB.2008.1008.

[47]   I. Tai-Nagara *et al.*, "Blood and lymphatic systems are segregated by the FLCN tumor

suppressor," *Nature Communications 2020 11:1*, vol. 11, no. 1, pp. 1–12, Dec. 2020, doi: 10.1038/s41467-020-20156-6.

[48] Y. Xie, T. R. Bagby, M. S. Cohen, and M. L. Forrest, "Drug delivery to the lymphatic system: importance in future cancer diagnosis and therapies," *http://dx.doi.org/10.1517/17425240903085128*, vol. 6, no. 8, pp. 785–792, Aug. 2009, doi: 10.1517/17425240903085128.

[49] I. Cascorbi, "Drug Interactions—Principles, Examples and Clinical Consequences," *Dtsch Arztebl Int*, vol. 109, no. 33–34, p. 546, Aug. 2012, doi: 10.3238/ARZTEBL.2012.0546.

[50] A. M. Veselinovic, J. B. Veselinovic, J. V. Zivkovic, and G. M. Nikolic, "Application of SMILES Notation Based Optimal Descriptors in Drug Discovery and Design".

[51] H. Junaedi, "PENGGAMBARAN RANTAI KARBON DENGAN MENGGUNAKAN SIMPILIED MOLECULAR INPUT LINE SYSTEM (SMILES)".

[52] J. Arús-Pous *et al.*, "SMILES-based deep generative scaffold decorator for de-novo drug design," *J Cheminform*, vol. 12, no. 1, pp. 1–18, May 2020, doi: 10.1186/S13321-020-00441-8/FIGURES/12.

[53] D. Weininger, "SMILES, a Chemical Language and Information System: 1: Introduction to Methodology and Encoding Rules," *J Chem Inf Comput Sci*, vol. 28, no. 1, pp. 31–36, Feb. 1988, doi: 10.1021/CI00057A005/ASSET/CI00057A005.FP.PNG_V03.

[54] N. K. Manaswi, "RNN and LSTM," *Deep Learning with Applications Using Python*, pp. 115–126, 2018, doi: 10.1007/978-1-4842-3516-4_9.

[55] Y. Yu, X. Si, C. Hu, and J. Zhang, "A Review of Recurrent Neural Networks: LSTM Cells and Network Architectures," *Neural Comput*, vol. 31, no. 7, pp. 1235–1270, Jul. 2019, doi: 10.1162/NECO_A_01199.

[56] A. Khan and A. Sarfaraz, "RNN-LSTM-GRU based language transformation," *Soft comput*, vol. 23, no. 24, pp. 13007–13024, Dec. 2019, doi: 10.1007/S00500-019-04281-Z/FIGURES/15.

[57] C. B. Vennerød, A. Kjærran, and E. S. Bugge, "Long Short-term Memory RNN," May 2021, Accessed: Aug. 30, 2023. [Online]. Available: https://arxiv.org/abs/2105.06756v1

[58] K. Smagulova and A. P. James, "A survey on LSTM memristive neural network architectures and applications," *The European Physical Journal Special Topics 2019 228:10*, vol. 228, no. 10, pp. 2313–2324, Oct. 2019, doi: 10.1140/EPJST/E2019-900046-X.

[59] G. G. Wang, S. Deb, and Z. Cui, "Monarch butterfly optimization," *Neural Comput Appl*, vol. 31, no. 7, pp. 1995–2014, Jul. 2019, doi: 10.1007/S00521-015-1923-Y/TABLES/7.

[60] M. Kuhn, I. Letunic, L. J. Jensen, and P. Bork, "The SIDER database of drugs and side effects," *Nucleic Acids Res*, vol. 44, no. D1, pp. D1075–D1079, Jan. 2016, doi: 10.1093/NAR/GKV1075.