

Supplementary Material

List of selected papers after abstract screening:

- [1] A. Bolatchiev, V. Baturin, E. Shchetinin, and E. Bolatchieva, "Novel Antimicrobial Peptides Designed Using a Recurrent Neural Network Reduce Mortality in Experimental Sepsis," *Antibiotics*, vol. 11, no. 3, 2022, doi: 10.3390/antibiotics11030411.
- [2] K. Bouhedjar, A. Boukelia, A. Khorief Nacereddine, A. Boucheham, A. Belaidi, and A. Djerourou, "A natural language processing approach based on embedding deep learning from heterogeneous compounds for quantitative structure-activity relationship modeling," *Chem. Biol. Drug Des.*, vol. 96, no. 3, pp. 961–972, 2020, doi: 10.1111/cbdd.13742.
- [3] D. V. Bozhko *et al.*, "Artificial intelligence-driven phenotyping of zebrafish psychoactive drug responses," *Prog. Neuropsychopharmacol. Biol. Psychiatry*, vol. 112, 2022, doi: 10.1016/j.pnpbp.2021.110405.
- [4] B. Chiovini *et al.*, "Theoretical design, synthesis, and in vitro neurobiological applications of a highly efficient two-photon caged GABA validated on an epileptic case," *ACS Omega*, vol. 6, no. 23, pp. 15029–15045, 2021, doi: 10.1021/acsomega.1c01164.
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- [6] P. Das *et al.*, "Accelerated antimicrobial discovery via deep generative models and molecular dynamics simulations," *Nat. Biomed. Eng.*, vol. 5, no. 6, pp. 613–623, 2021, doi: 10.1038/s41551-021-00689-x.
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