1. Bioinformatics and Computational Biology of Molecular Structure, Function and Evolution

Regular Papers:

B252 "Enhancing Gene Cluster Identification and Classification in Bacterial Genomes Through Synonym Replacement and Deep Learning"

Zhihua Du, Ningyu Zhong, and Jianqiang Li

B322 "Combinative Bio-feature Proteins Generation via Pre-trained Protein Large Language Models"

Xin Sun and Yuhao Wu

B497 "Hierarchical Molecular Structure Network Based on Co-attention Mechanism for Drug-Drug Interaction Prediction"

Yue Luo and Lei Deng

B500 "ADiffGDA: Exploring Gene-Drug Associations via Adaptive Graph Diffusion Networks"

Che Zhang, Yanhao Fan, Xiaowen Hu, Yurong Qian, and Lei Deng

B512 "Knowledge-guided Protein Complex Identification with Fuzzy-based Graph Representation Learning"

Yue Yang, Guodong Li, Dongxu Li, Pengwei Hu, and Lun Hu

B609 "CodonT5: A Multi-task Codon Language Model to Perform Generative Codon Optimization"

Ashley Babjac and Scott Emrich

B646 "ViDTA: Enhanced Drug-Target Affinity Prediction via Virtual Graph Nodes and Attention-based Feature Fusion"

Minghui Li, Zikang Guo, Yang Wu, Peijin Guo, Yao Shi, Shengshan Hu, Wei Wan, and Shengqing Hu

B658 "FEATURE-pHLA: Physico-chemical features efficiently predict peptide-HLA binding affinity"

Hamda Alhosani, Raghvendra Mall, Ankita Singh, and Filippo Castiglione

B714 "GP-nano: a geometric graph network for nanobody polyreactivity prediction"

Xiaolong Zhou, Qianmu Yuan, Shuangjia Zheng, Yu Wang, and Yuedong Yang

B717 "FibGrid: Characterizing Anatomical Pathways in Hypergrid for Direct Tract Segmentation"

Yu Xie, Yazhe Zhai, Yifei He, Jiahao Yu, Jiaolong Qin, and Ye Wu

B907 "SVPS, pairwise whole genome alignment-based structural variant identification"

Malcolm Todd, Lingling Jin, and Ian McQuillan

B971 "MEMO-stab: Sequence-based Annotation of Mutation Effect on Transmembrane Protein Stability with Protein Language Model-Driven Machine Learning"

Zhe Liu, Yihang Bao, Wenhao Li, Weihao Li, Weidi Wang, and Guan Ning Lin

B1019 "Efficient Antibody Structure Refinement Using Energy-Guided SE(3) Flow Matching"

Jiying Zhang, Zijing Liu, Shengyuan Bai, He Cao, Yu Li, and Lei Zhang

B1244 "Secondary Structure-Guided Novel Protein Sequence Generation with Latent Graph Diffusion"

Yutong Hu, Yang Tan, Andi Han, Lirong Zheng, Liang Hong, and Bingxin Zhou

B1246 "SCOP: A Sequence-Structure Contrast-Aware Framework for Protein Function Prediction"

Runze Ma, Chengxin He, Huiru Zheng, Xinye Wang, Haiying Wang, Yidan Zhang, and Lei Duan

B1297 "TADClam: overlapped and hierarchical topologically associating domains detection with community affiliation model"

Zhao Ling, Shi Ying Li, Qiu Shi Liang, and Shuai Cheng Li

B1341 "TDLM: A Diffusion Language Model for TCR Sequence Exploration and Generation"

Haoyan Wang, Yuhang Yang, Yifei Huang, Tianyi Zang, and Yadong liu

B1404 "ComLMEss: Combining multiple protein language models enables accurate essential protein prediction"

Xu Liu, Yiming Li, Fuhao Zhang, Ruiqing Zheng, Fei Guo, Min Li, and Min Zeng

B1477 "PocketLG: Protein Binding Pocket Identification Using Protein Language Model and Graph Transformer"

Li Zhang, Heng Chang, Zehua Sun, Wenjie Li, Li Zhu, and Han Wang

B1536 "Developing H5N1 Avian Influenza Mutation and Evolution Feature Analysis and Web Service"

Ming Xiao, Qichen Shang, Qiaozhen Zhang, Yi Xiao, Jun Yu, and Le Zhang

B1562 "RBP-Former: Joint Prediction of RNA-protein Binding Sites on Full-length RNA Transcripts for Multiple RBPs"

Yichong Li, Xiaojian Liu, Fan Cheng, Xiaoyong Pan, and Yang Yang

B1576 "Directed Evolution of Proteins via Bayesian Optimization in Embedding Space"

Matouš Soldát and Jiří Kléma

B1586 "GATBind: Accurate protein-RNA binding sites prediction via graph attention networks with pre-trained language model"

Siyuan Shen, Shangqian Wu, Jie Chen, Zhijian Huang, and Lei Deng

B1852 "Integrating Biological Language Processing and Memory Attention Model for Protein-DNA Binding Residue Prediction"

Shixuan Guan, Xiucai Ye, and Tetsuya Sakurai

Short Papers:

B220 "PICNIC: refinement of AlphaFold2 tertiary structure predictions using deep 3D residual neural networks"

Ross Stewart, Chenguang Zhao, Tong Liu, and Zheng Wang

B257 "AREDCI: Assessing Reproducibility and Differential Chromatin Interactions for ChIA-PET Sequencing Data"

Jialiang Sun, Zhihan Ruan, Chaoyang Yan, and Jian Liu

B294 "ProtSolM: Protein Solubility Prediction with Multi-modal Features"

Yang Tan, Jia Zheng, Liang Hong, and Bingxin Zhou

B371 "A Vectorization Method Induced By Maximal Margin Classification For Persistent Diagrams"

An Wu, Yu Pan, Fuqi Zhou, Jinghui Yan, and Chuanlu Liu

B374 "Protein Representation Learning with Sequence Information Embedding: Does it Always Lead to a Better Performance?"

Yang Tan, Lirong Zheng, Bozitao Zhong, Liang Hong, and Bingxin Zhou

B576 "Prediction of miRNA family based on class-incremental learning"

Yajun Liu, Lulu Qiu, Aimin Li, Rong Fei, Junhuai Li, and Fang-Xiang Wu

B585 "LMDTA: Molecular Pre-trained and Interaction Fine-tuned Attention Neural Network for Drug-Target Affinity Prediction"

Minjie Hu, Kuo Yang, Kuan Xu, and Xuezhong Zhou

B633 "Partition, Predict and Assemble: Targeting Long RNA Secondary Structure Prediction"

Xiaoya Fan, Yuming CUI, Zheng Zhao, Zengyou He, Qi Zhao, and Zhong Wang

B864 "M2oE: Multimodal Collaborative Expert Peptide Model"

Zengzhu Guo and Zhiqi Ma

B899 "GPU Acceleration of Conformational Stability Computation for CD4+ T-cell Epitope Prediction"

Jiarui Li, Samuel Landry, and Ramgopal Mettu

B972 "Predicting Psychosis Progression in Clinical High-Risk Individuals Using Peripheral Transcriptomic and Epigenomic Profiles: A Machine Learning Approach"

Zhe Liu, Weidi Wang, Mingxia Zhai, An Gu, Shunying Yu, and Guan Ning Lin

B1024 "IEARACDA: Predicting circRNA-disease associations based on information enhancement and arctangent rank approximation"

Shanchen Pang, Zheqi Song, Tiyao Liu, Wenhao Wu, Yuanyuan Zhang, and Shudong Wang

B1126 "DrugEL: Ensemble Learning Model for Identification of Druggable Proteins"

Md. Mamun Ali, Kawsar Ahmed, Francis Bui, and Fang-Xiang Wu

B1255 "DISHIC: An Effective Tool for Differential Interaction Analysis in Single-Cell Hi-C Data" Yichao Zhao, Ruiqing Zheng, Li Tang, Pengzhen Jia, and Min Li

B1380 "Predicting Antibody Stability pH Values from Amino Acid Sequences: Leveraging Protein Language Models for Formulation Optimization"

Takuya Tsutaoka, Noriji Kato, Toru Nishino, Yuangzhong Li, and Masahito Ohue

B1397 "SLP-T5: A New Method for Predicting Protein Sub-chloroplast Localization Based on Text-to-Text Transfer Transformer"

Ge Kong, Jiao Wang, Yuanhao Fan, and Juan Wang

B1620 "multiTAD: an Attention-Based Deep Learning Model for Identifying TAD Boundaries through Multi-Size Feature Integration"

Xue Wang, Li Tang, Hanyu Luo, Yajing Deng, and Min Li

B1746 "Prediction of single-stranded DNA binding proteins with protein language model"

Siwen Wu, Jinbo Xu, and Jun-tao Guo

B1811 "MFN: Explainable DNA triple helix Stabilized Design based on mCGR and flow network"

Xiaoru Wen, Lijun Sun, Lei Xie, Yanfen Zheng, Ben Cao, and Bin Wang

2. Computational Systems Biology

Regular Papers:

B387 "SMCL-MDR: Predicting miRNA-Drug Resistance using Self-Attention Mechanism and Contrastive Learning"

Jipu Jiang, Guihua Duan, and Cheng Yan

B518 "TSEML: A task-specific embedding-based method for few-shot classification of cancer molecular subtypes"

Ran Su, Rui Shi, Hui Cui, Ping Xuan, Xikang Feng, and Qiangguo Jin

B534 "NeuroSparse: An Unsupervised Framework for Inferring Brain Connectivity in Autism Diagnosis"

Shuqi Yang, Lijuan Zhang, Qing Lan, Qiujie Ma, huan Huang, Jiaqing Miao, Shiyu Mou, Dezhong Yao, Cheng Luo, and Ying Tan

B653 "scEAGC: an efficient anchor graph clustering for single-cell transcriptomics and proteomics data"

Qiaoming Liu, Yadong Wang, and Guohua Wang

B785 "Hypergraph-based Self-supervised Multi-channel Network for Drug-target Interaction Prediction"

Xiaoting Zeng, Yu Liang, Peng Yang, Weilin Chen, and Baiying Lei

B905 "Gene-Metabolite Association Prediction with Interactive Knowledge Transfer Enhanced Graph for Metabolite Production"

KEXUAN XIN, QINGYUN WANG, JUNYU CHEN, PENGFEI YU, HUIMIN ZHAO, and HENG JI

B1316 "Control backbone detection in omnigenic disease neighborhood targeting core module"

Yuxuan Cai, Bingbo Wang, and Junru Zheng

B1371 "EPI-RMDL: Prediction of Enhancer-Promoter Interactions Based on RoFormer Mechanism and Deep Learning"

Mengyun Song, Jie Wen, Yabin Kuang, and Minzhu Xie

B1409 "Integrating topology and biological information to predict essential proteins via Shannon entropy"

Yan Liu, Zhong Wang, Zengyou He, Hexin Zhang, and Jing Qin

B1415 "Network embedding for detecting protein complexes in attributed networks"

Xiangmao Meng, Keming Wang, Ju Xiang, and Wenkang Wang

B1416 "Essential protein discovery on weighted PPI networks via statistical information fusion"

Yan Liu, Ye Yuan, Zhong Wang, Zengyou He, Hexin Zhang, Hongwei Wu, and Ya-Dong Wang

B1449 "A Mixed Integer Linear Program for Post-translational Modification Characterization"

Shengzhi Lai, Peize Zhao, Ning Li, and Weichuan Yu

B1456 "MFF-LncLoc: Subcellular Localization Prediction of IncRNAs Based on Multi-Feature Fusion Using Transformers"

Ziyu Fan, Ying Jiang, Shuning Yang, and Lei Deng

B1459 "LSNSCDA: Unraveling CircRNA—Drug Sensitivity via Local Smoothing Graph Neural Network and Credible Negative Samples"

Ziyu Fan, Yuanpeng Zhang, Yahan Li, Zeyu Zhong, and Lei Deng

B1461 "A Heterogeneous Network-based Contrastive Learning Approach for Predicting Drug-Target Interaction"

Junwei Hu, Michael Bewong, Selasi Kwashie, Wen Zhang, Vincent M. Nofong, Guangsheng Wu, and Zaiwen Feng

B1498 "Iterative Glycan Structure Generation by Component Localization and Classification from Mass Spectra"

Defeng Li, Zizheng Nie, Yanmin Liu, Xiaojun Cai, Yong Zhang, and Xuefeng Cui

B1499 "CRISPR-DBA: a deep learning framework for uncertainty quantification of CRISPR off-target activities"

Xinzhe Cao and Peter Minary

B1502 "Prior-guided longitudinal metabolomic analysis"

Kowshika Sarker, Ruoqing Zhu, Hannah Diane Holscher, and ChengXiang Zhai

B1508 "IntNet: A novel framework using reconstructed mutation samples and a biologically informed neural network for pathway analysis"

Li Zhou, Jie Li, and Weilong Tan

B1510 "Heterogeneous network impulsive dynamics for identifying disease-associated genes"

Ju Xiang, Shengkai Chen, Lin-Cong-Hua Wang, Xiangmao Meng, and Min Li

B1566 "Module-level Gene-drug Interaction Identification via Hierarchical Optimal Transport"

Ye Liu, Xiaojie Wang, Hongshan Pu, Jiazhou Chen, and Hongmin Cai

B1780 "KGM4DTI: A Depression Knowledge Graph-Driven Multi-semantic Multi-view Computational Framework for Drug-Target Interaction Prediction"

Xu Tian, Peifu Han, Xue Li, Hongzhen Ding, Wei He, Fengrui Jing, Shuang Wang, Xun Wang, and Tao Song

Short Papers:

B404 "TTCNet: Transformer and Tubular Convolution Feature Attention Network for OCTA vessel segmentation"

Chengzhang Zhu, Zhangzheng Yang, Yalong Xiao, Tao Wu, Beiji Zou, and Haoze Zhou

B694 "DCOAT: Dynamic core-attachment based protein complex detection"

Yaoran Chen, Difu Feng, Yuanyuan Zhu, Guojing Li, Ming Zhong, Tieyun Qian, and Juan Liu

B879 "MuSCaKDE - Multi-Scale modeling of Carbamoylated collagen: Kernel Density Estimation applied from all atom to rigid body simulation"

Zara Msoili, Stéphanie Baud, and Hua Wong

B908 "SiRPipe: a data mining pipeline to improve ab initio prediction of bacterial small RNAs"

Fabio Reinoso Vilca and Fabio Ribeiro Cerqueira

B1102 "scCADE: A Superior Tool for Predicting Perturbation Responses in Single-Cell Gene Expression Using Contrastive Learning and Attention Mechanisms"

Jingfeng Ou, Jiawei Li, Zhiliang Xia, Shurui Dai, Yulian Ding, Yan Guo, Limin Jiang, and Jijun Tang

B1142 "AEG-PPIS: A Dual-Branch Protein-protein Interaction Site Predictor Based on Augmented Graph Attention Network and Equivariant Graph Neural Network"

Huanhuan Dai, Haonan Song, Tongyu Han, Qing Yang, Xiangyu Meng, and Xun Wang

B1158 "MHANDTI: Drug-Target Interaction Prediction Model Based on Heterogeneous Graph Multi-Hop Attention Networks"

Chen Zhang, Jiaqi Sun, Linlin Xing, Longbo Zhang, Hongzhen Cai, and Maozu Guo

B1243 "MMDDI-MGPFF: Multi-Modal Drug Representation Learning with Molecular Graph and Pharmacological Feature Fusion for Drug-Drug Interaction Event Prediction"

Guishen Wang, Zhitong Guo, Guilin You, Ming Xu, Chen Cao, and Xiaowen Hu

B1373 "Q-TetoFormer: A New Gene Regulatory Network Prediction Method Based on Quantum Computing and Transformer"

Hanmo Wang

B1666 "NeDRex-Web: An Interactive Web Tool for Drug Repurposing by Exploring Heterogeneous Molecular Networks"

Andreas Maier, Elisa Anastasi, Olga Zolotareva, James Skelton, Maria Elkjaer, Ana Casas, Cristian Nogales, Harald Schmidt, Tim Kacprowski, David Blumenthal, Anil Wipat, Sepideh Sadegh, and Jan Baumbach

B1768 "Boundary-Guided Learning for Gene Expression Prediction in Spatial Transcriptomics"

Mingcheng Qu, Yuncong Wu, Donglin Di, Anyang Su, Tonghua Su, Yang Song, and Lei Fan

B1790 "Impact of Extracellular Vesicles Derived from Human Placenta Cells on Neural Progenitor Cell Transcriptome Dynamics"

Pallav Singh, Jessica Kinkade, Mohit Verma, Teka Khan, Toshihiko Ezashi, Nathan Bivens, R. Michael Roberts, Cheryl Rosenfeld, and Trupti Joshi

B1810 "Mondrian Abstraction and Language Model Embeddings for Differential Pathway Analysis"

Fuad Al Abir and Jake Chen

B1813 "Inferring Gene Regulatory Network Based on scATAC-seq Data with Gene Perturbation"

Wei Shao, Yuti Liu, Shuang Zhang, Shuang Chen, Qiao Liu, and Wanwen Zeng

B1814 "Improving Genetic Perturbation Responses with A Comprehensive Biological Knowledge Graph"

Yang Li, Rui Chen, Yuting Tan, Xue Zhong, Bingshan Li, and Zhijun Yin

3. Next Generation Sequencing and High-throughput Methods

Regular Papers:

B275 "A Particle Swarm Optimization Algorithm Based on Multi-Population Mutual Learning for SNP-SNP Interaction Detection"

Lingian Zhao, Yahan Li, Junliang Shang, Qiangian Ren, Yuanyuan Zhang, and Jin-Xing Liu

B381 "scGDCC: Graph-based Dual Contrastive Calibration for Single Cell Multi-Omics Clustering"

Huayu Tao, Xinliang Sun, Yuxuan Chen, Min Li, and Ruiqing Zheng

B457 "A Single-Cell Clustering Algorithm Based on Structure Perturbation Non-Negative Matrix Factorization"

Hanjing Jiang, Meineng Wang, Luping Zhang, Yu-An Huang, Yangyuan Li, and Yabing Huang

B487 "SeqCCC: A Sequence-Informed Ligand-Receptor Interaction Prediction Method for Cell-Cell Communication Inference"

Bo-Ya Ji, Hong Xia, De-Bin Qiao, and Shao-Liang Peng

B702 "spGCLF: a versatile deep graph contrastive learning framework for spatial transcriptomics analysis"

Xiang Chen, Junnan Yu, and Min Li

B795 "MRF-XGBLC: Large-scale gene regulatory network inference based on multi-model fusion"

Liang Bai, Liwen Xu, Boya Ji, Shulin Wang, and Shaoliang Peng

B829 "GRNNLink: Predicting gene regulatory links from single-cell RNA-seq data using graph recurrent neural network"

Liang Bai and Shulin Wang

B913 "WFA-vect: a SIMD wavefront algorithm for gap-affine pairwise alignment"

Yifei Guo, Tao Tang, Qingzhe Wang, Canqun Yang, Zeyu Xia, Chenchen Peng, Yufei Guo, and Yingbo Cui

B983 "Spatial domains identification based on multi-view contrastive learning in spatial transcriptomics"

Yanru Gao, Feng Li, Fanhao Meng, Daohui Ge, Qianqian Ren, and Junliang Shang

B984 "Integrating Autoencoder and Multi-View Graph Convolutional Networks for Spatial Domains Identification"

Fanhao Meng, Feng Li, Yanru Gao, Daohui Ge, Rong Zhu, and Junliang Shang

B1074 "Multi-Slice Spatial Transcriptomics Data Integration Analysis with STG3Net"

Donghai Fang, Fangfang Zhu, and Wenwen Min

B1075 "Pretrained-Guided Conditional Diffusion Models for Microbiome Data Analysis"

Xinyuan Shi, Fangfang Zhu, and Wenwen Min

B1084 "Masked Graph Autoencoders with Contrastive Augmentation for Spatially Resolved Transcriptomics Data"

Donghai Fang, Fangfang Zhu, Dongting Xie, and Wenwen Min

B1214 "ViPER: Virus-Prokaryote intEraction prediction using foundation model with hieraRchical contrastive learning"

Feng Zhou, Yushuang He, Jiaxing Bai, Yichun Gao, and Ying Wang

B1386 "Integrating Local and Global Information to Decipher Spatial Domains of Spatial Transcriptomics by Attention-based Graph Convolutional Network"

Xuran Dou, Yue Gao, Junliang Shang, Chunhou Zheng, Yinglian Gao, and Jinxing Liu

B1476 "Sparse Attention-based Hierarchical Node Representation for Spatial Domain Identification"

Wei Peng, Zhihao Ping, Wei Dai, Xiaodong Fu, Li Liu, Lijun Liu, and Ning Yu

B1492 "scDCMAC:adaptive feedback clustering of scRNA-seq data with deep gene correlation mining"

Shanchen Pang, Ruiqian Wang, Wenhao Wu, Hengxiao Li, Jiarui Wu, and Shudong Wang

B1494 "Deep Representation Learning for Electron Ionization Mass Spectra Retrieval"

Shibo Liu, Xuan Zhang, Anlei Jiao, Shiwei Sun, Longyang Dian, and Xuefeng Cui

B1688 "ULTR-asm: assembly of ultra long tandem repeat"

Xiaolin Li, Lianrong Pu, Kuanqiang Tang, Xianzhong Feng, and Daming Zhu

Short Papers:

B336 "Identification of cell-type-specific genes associated with autism by integrating gene expression and alternative polyadenylation profiles"

Xingyu Bi, Liping Kang, and Xiaohui Wu

B413 "Cluster Parallel Quality Score Data Lossless Compression via Sequence Multi-Partitioning and Redundant Encoding" Hui Sun, Yingfeng Zheng, Huidong Ma, Cheng Zhong, Meng Yan, Gang Wang, and Xiaoguang Liu

B437 "CLPLS: accurate deconvolution of spatial transcriptomic data via contrastive learning and partial least square regression"

Yuanyuan Mo, Juan Liu, and Lihua Zhang

B665 "A Flexible Subspace Parallel Evolutionary Framework for Epistatic Interaction Detection"

Fangting Li, Ying Yin, Yixiao Liu, Xin Wang, Changyong Yu, and Yuhai Zhao

B668 "GPU-Powered Evolutionary Auxiliary Multitasking for Fast SNP Interaction Detection"

Fangting Li, Ying Yin, Yixiao Liu, Xin Wang, Changyong Yu, and Yuhai Zhao

B728 "Multi-Population Ant Colony Optimization With Knowledge-Based Local Searches for Epistasis Detection"

Qianqian Ren, Shaoyi Liu, Lianlian Zhang, Junliang Shang, and Feng Li

B809 "KAS-former : a transformer-based model for predicting histone modifications using KAS-seq"

Lijuan Jia, Wen Wen, Zhaoxi Zhang, Jiaxin Zhong, Xiaoya Fan, Zengyou He, Ruitu Lyu, and Zhong Wang

B1020 "Thioproline Modulates Gut Microbiota to Resist Colorectal Cancer"

Jingjing Liu, Yixuan Wang, Jian Zhao, Quan Wang, Haiqing Si, and Xiaofeng Song

B1047 "scKADE: Single-Cell Multi-Omics Integration with Kolmogorov-Arnold Deep Embedding"

Shanchen Pang, Jiarui Wu, Wenhao Wu, Hengxiao Li, Ruiqian Wang, Yulin Zhang, and Shudong Wang

B1055 "Masked adversarial neural network for cell type deconvolution in spatial transcriptomics"

Lin Huang, Xiaofei Liu, shunfang wang, and Wenwen Min

B1197 "Comprehensive evaluation of haplotype phasing tools with different strategies across diverse sequence technologies"

Zhongbo Yang, Zhenhao Lu, Xin Li, Tao Jiang, Yadong Wang, and Yadong liu

B1289 "MATL: A deep neural network using multi-scale convolutions and transformer for transcription factor binding site prediction"

jinli fan, ruyi shen, xiaodi huang, and Yanju Zhang

B1530 "DeePSP-GIN: identification and classification of phage structural proteins using predicted protein structure, pretrained protein language model, and graph isomorphism network"

Muhit Islam Emon, Badhan Das, Ashrith Reddy Thukkaraju, and Liqing Zhang

B1711 "Deconvolution of spatial transcriptomics data based on multi-head dynamic GAT and optimal transport"

Yuqi Chen, Feng Yang, Peng Jiang, Yuan Wang, Qiang Zhang, and Juan Liu

B1732 "iTARGET: Interpretable Tailored Age Regression for Grouped Epigenetic Traits"

Zipeng Wu, Daniel Herring, Fabian Spill, and James Andrews

B1771 "m6A peak calling accounting for varying sequencing bias across regions and samples"

Lanyu Zhang, Zhenxing Guo, Zhaohui Qin, and Zhijin Wu

B1775 "Target-oriented Reference Construction for supervised cell type identification in scRNA-seq"

Xin Wei, Wenjing Ma, Zhijin Wu, and Hao Wu

4. Cheminformatics and pharmacogenomics

Regular Papers:

B216 "Subgraph-based Self-Supervised Learning Framework for Enzymatic Reaction Feasibility Prediction"

Feng Yang, Juan Liu, Qiang Zhang, Zhihui Yang, Jianghang Liu, and Guangsheng Wu

B372 "MambaDTA: a novel Drug-Target Affinities prediction method with State-Space Model"

Dayan Liu, Tao Song, and Shudong Wang

B421 "Interpretable Multi-domain Awareness Scheme for Drug-target Interaction Prediction"

Xiaoqing Lian, Jie Zhu, Tianxu Lv, and Xiang Pan

B471 "DiffSim: Aligning Diffusion Model and Molecular Dynamics Simulation for Blind Docking"

Yanlin Fei, Yurui Li, Zhiling Zhou, and Haohan Wang

B524 "Application of Static Virus Spread Algorithm in Base-Balanced DNA Fragment Optimization"

Yao Yao, Yanfen Zheng, Xun Zhang, Xin Liu, Xiaokang Zhang, Bin Wang, and Qiang Zhang

B531 "Adaptive Drug Repositioning Prediction"

Zhenpeng Wu, Jiamin Chen, and Jianliang Gao

B586 "Diff4VS: HIV-inhibiting Molecules Generation with Classifier Guidance Diffusion for Virtual Screening"

Jiaqing Lyu, Changjie Chen, Bing Liang, and Yijia Zhang

B603 "MulMol: Transformer-based Multi-Task Molecular Representation Learning"

Dengdeng Huang and Shikui Tu

B626 "Molecular Property Prediction by Contrastive Learning from Joint-Aggregator Neural Network"

Zhihui Yang, Feng Yang, and Juan Liu

B992 "Novelty Encouraged Beam Clustering Search for Multi-Objective De Novo Diverse Drug Design"

Dengwei Zhao, Shikui Tu, and Lei Xu

B1062 "DPAGCN: Predicting Microbe-Drug Associations based on Dual Attention Graph Convolution"

Peng Wang, Xiangqiong Wu, Wen Li, Jiaxin Chu, and Nan Hu

B1070 "MFCM-DTI model of multimodal feature fusion: prediction of drug-target interaction"

WENJUN LI, Wanjun Ma, Mengyun Yang, and Xiwei Tang

B1245 "CSCL-DTI: predicting drug-target interaction through cross-view and self-supervised contrastive learning"

Xuan Lin, Xi Zhang, Zu-Guo Yu, Yahui Long, Xiangxiang Zeng, and Philip S Yu

B1299 "PretrainedBA: Enhancing Compound-Protein Binding Affinity Prediction Accuracy via Pre-training Large-Scale Interaction Information"

Sangmin Seo, Seungyeon Choi, Hwanhee Kim, and Sanghyun Park

B1302 "HGTRDA: Enhancing Prediction of ncRNA-Mediated Drug Resistance with Hypergraph Transformer"

Che Zhang, Ruohui He, Yanhao Fan, Xiaowen Hu, Yurong Qian, and Lei Deng

B1364 "Muli-Task Dual-view Model for Drug Combination Analysis: In Vivo and In Vitro Perspectives"

Yuhe YANG, Zhaoyue ZHANG, Xueqin XIE, Wei Su, Kejun Deng, and Hao Lin

B1388 "MLFF-DTA: A Multi-Level Feature Fusion Method for Predicting Drug-Target Binding Affinity"

Jiao Wang, Ge Kong, and Juan Wang

B1493 "Revolutionizing Enzyme Turnover Predictions with Non-Binary Reaction Fingerprints and AI"

Jibin Cheng, Cheng Chen, Guishan Cui, Haitao Jiang, and Xuefeng Cui

B1506 "How to Train Your Neural Network for Molecular Structure Generation from Mass Spectra?"

Kai Zhao, Yanmin Liu, Longyang Dian, Shiwei Sun, and Xuefeng Cui

B1521 "Causal Invariant Hierarchical Molecular Representation for Out-of-distribution Molecular Property Prediction"

Xinlong Wen, Yifei Guo, Shuoying Wei, Wenhan Long, Lida Zhu, and Rongbo Zhu

B1528 "Semi-Template Retrosynthesis Prediction with 3D Spatial Structures and Reaction Center Disconnection Rules"

Xin Li, Zishuai Wei, Shuang Wang, Peifu Han, Xue Li, and Tao Song

B1543 "Mamba-DTA: Drug-Target Binding Affinity Prediction with State Space Model"

Yulong Wu, Jin Xie, Jing Nie, Xiaohong Zhang, and Yuansong Zeng

B1664 "Advancing Flexible Docking of P450-Heme Complexes via JAX MD"

Rongxu Guo, Cheng Chen, Jiaheng Sang, Guishan Cui, Fa Zhang, Xuefeng Cui, and Shengying Li

B1870 "AffinityLM: Binding-Site Informed Multitask Language Model for Drug-Target Affinity Prediction"

Tyler Rose, Charlotte Zhou, and Nicolo Monti

Short Papers:

B277 "MolCLW: Molecular Contrastive Learning With Learnable Weighted Substructures"

Jiahe Li, Wenjie Du, and Yang Wang

B350 "APK-MRL: An Adaptive Pre-training Framework with Knowledge-enhanced for Molecular Representation Learning"

Xu Gong, Qun Liu, Rui Han, Li Liu, Yike Guo, and Guoyin Wang

B990 "Unveiling HDAC8 antagonists for breast cancer therapy via molecular modeling"

Vaishali Pankaj, Inderjeet Bhogal, and Sudeep Roy

B1129 "Cycle-Configuration: A Novel Graph-theoretic Descriptor Set for Molecular Inference"

Bowen Song, Jianshen Zhu, Naveed Azam, Kazuya Haraguchi, Liang Zhao, and Tatsuya Akutsu

B1145 "A Multi Target Drug Design Method Based on Target Protein Sequence and Feature Similarity"

Haoran Liu, Xiaoli Lin, Jing Hu, and Xiaolong Zhang

B1178 "Dual Interaction and Kernel-Diverse Network for Accurate Drug-Target Binding Affinity Prediction"

Yulong Wu, Jin Xie, Jing Nie, Jian Hu, and Yuansong Zeng

B1290 "MBC-DTA: A Multi-Scale Bilinear Attention with Contrastive Learning Framework for Drug-Target Binding Affinity Prediction"

Huiting Li, Weiyu Zhang, Yong Shang, and Wenpeng Lu

B1417 "Exploring Latent Space for Generating Peptide Analogs Using Protein Language Models"

Po-Yu Liang, Xueting Huang, Tibo Duran, Andrew Wiemer, and Jun Bai

B1623 "LEMTL: Enhancing the pharmacokinetic predictions of multitask learning with existing pharmacokinetics"

Ying Li, Xiao Deng, Jingsong Lv, Hongyang Chen, and Yao Yang

B1833 "PARank: Pocket-based Drug-target Affinity Ranking with Heterogeneous GNN"

Bin Feng, Zijing Liu, Jiying Zhang, Yu Li, and Lei Zhang

5. Cross-Cutting Computational Methods and Bioinformatics of Disease

Regular Papers:

B238 "MVLncStack: A novel method for lncRNA subcellular localization prediction based on multi-view features"

Ziqi Liu, Tao Bai, Dongdong Jiang, Bin Liu, and Liang Yu

B239 "MTTSCL: protein subcellular localization prediction using multi-task learning"

Liang Yu, Xiang Wu, Yan Li, Zhaoyang Huang, and Zigi Liu

B260 "DeepTAPE Enhancing Systemic Lupus Erythematosus Diagnosis with Deep Learning Based on TCRβ CDR3 Sequences"

Tongfei Shen, Miaozhe Huo, Wan Nie, Kaiqi Li, Ziwei Ma, Xikang Feng, and Shuai Cheng Li

B267 "Identification of disease-related genetic variants and imaging factors leveraging summary statistics"

Duo Xi, Dingnan Cui, Minjianan Zhang, Jin Zhang, Muheng Shang, Lei Guo, Lei Du, and Junwei Han

B276 "Bimodality Approach to Mental Disorder Diagnosis via Dual-pathway Fusion Perceptual Network"

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