

Selected List of Publications

Using Features Provided by PROFEAT

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Feature Group 1 & 2 [G1, G2]: Amino Acid Composition, Dipeptide Composition

- Reczko, M. and Bohr, H. (1994) The DEF data base of sequence based protein fold class predictions. *Nucleic Acids Res*, 22, 3616-3619.
- Grassmann, J., Reczko, M., Suhai, S. and Edler, L. (1999) Protein fold class prediction: new methods of statistical classification. *Proc Int Conf Intell Syst Mol Biol*, 106-112.
- Hua, S. and Sun, Z. (2001) Support vector machine approach for protein subcellular localization prediction. *Bioinformatics*, 17, 721-728.
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- Bhasin, M. and Raghava, G.P. (2004) Classification of nuclear receptors based on amino acid composition and dipeptide composition. *J Biol Chem*, 279, 23262-23266.

Feature Group 3 [G3]: Autocorrelation Descriptor

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Feature Group 4 [G4]: Composition, Transition, Distribution (CTD)

- Dubchak, I., Muchnik, I., Holbrook, S.R. and Kim, S.H. (1995) Prediction of protein folding class using global description of amino acid sequence. *Proc Natl Acad Sci USA*, 92, 8700-8704.
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- Han, L.Y., Cai, C.Z., Ji, Z.L., Cao, Z.W., Cui, J. and Chen, Y.Z. (2004) Predicting functional family of novel enzymes irrespective of sequence similarity: a statistical learning approach. *Nucleic Acids Res*, 32, 6437-6444.
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- Lin, H.H., Han, L.Y., Cai, C.Z., Ji, Z.L. and Chen, Y.Z. (2006) Prediction of transporter family from protein sequence by support vector machine approach. *Proteins*, 62, 218-231.
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- H.H. Lin, L.Y. Han, H.L. Zhang, C.J. Zheng, B. Xie, and Y.Z. Chen. (2006) Prediction of the Functional Class of Metal-Binding Proteins from Sequence Derived Physicochemical Properties by Support Vector Machine Approach. *BMC Bioinformatics* 7(Suppl 5): S13.
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Feature Group 5 [G5]: Quasi-Sequence-Order (QSO) Descriptors

- Chou, K.C. (2000) Prediction of protein subcellular locations by incorporating quasi-sequence-order effect. *Biochem Biophys Res Commun*, 278, 477-483.
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Feature Group 6 [G6]: Pseudo-Amino Acid Composition (PAAC)

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- Shen HB, Chou KC. (2005) Predicting protein subnuclear location with optimized evidence-theoretic K-nearest classifier and pseudo amino acid composition. *Biochem Biophys Res Commun.* 337(3):752-6.
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- Zhang T, Ding Y, Chou KC. (2006) Prediction of protein subcellular location using hydrophobic patterns of amino acid sequence. *Comput Biol Chem.* 30(5):367-71.
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Feature Group 7 [G7]: Amphiphilic Pseudo-Amino Acid Composition (APAAC)

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- Ding H, Luo L, Lin H. (2009). Prediction of cell wall lytic enzymes using Chou's amphiphilic pseudo amino acid composition. *Protein Pept Lett.* 16(4):351-5.

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Feature Group 8 [G8]: Topological Descriptors at Atomic Level

- Philip D.Mosier, Anne E. Counterman and Peter C. Jurs (2002) Prediction of peptide ion collision cross sections from topological molecular structure and amino acid parameters. *Anal Chem*,74:1360-1370
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Feature Group 9 [G9]: Total Amino Acid Properties (TAAP)

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Feature Group 10 & 11 [G10, G11]: Network Descriptors

- Barabási AL, Oltvai ZN. (2004) Network Biology: Understanding the Cell's Functional Organization. *Nat Rev Genet.* 5(2):101-13.
- Barabási AL, Gulbahce N, Loscalzo J. (2011) Network Medicine: a Network-Based Approach to Human Disease. *Nat Rev Genet.* 12(1):56-68
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- Yildirim MA, Goh KI, *et al.* (2007) Drug-target network. *Nat Biotechnol.* 25(10):1119-26.
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- Goh KI, Cusick ME, Valle D, Childs B, Vidal M, Barabási AL. (2007) The Human Disease Network. *Proc Natl Acad Sci USA.* 104(21):8685-90.
- Stelzl U, Worm U, *et al.* (2005) A Human Protein-Protein Interaction Network: a Resource for Annotating the Proteome. *Cell.* 122(6):957-68.
- Pujol A, Mosca R, Farrés J, Aloy P. (2010) Unveiling the Role of Network and Systems Biology in Drug Discovery. *Trends Pharmacol Sci.* 31(3):115-23.
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- Rubinov M, Sporns O. (2010) Complex Network Measures of Brain Connectivity: Uses and Interpretations. *Neuroimage.* 52(3):1059-69.
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List of Publications Citing PROFEAT (162 citations in Google Scholar, till Dec 2015)

2015:

1. L Olsen, C Oostenbrink, FS Jorgensen. Prediction of cytochrome P450 mediated metabolism. *Advanced Drug Delivery Reviews*, 2015
2. N Xiao, DS Cao, MF Zhu, QS Xu. protr/ProtrWeb: R package and web server for generating various numerical representation schemes of protein sequences. *Bioinformatics*, 2015
3. YB Ruiz-Blanco, W Paz, J Green. ProtDCal: A program to compute general-purpose-numerical descriptors for sequences and 3D-structures of proteins. *BMC Bioinformatics*, 2015
4. Z Zinati, F Zamansani, AH KayvanJoo. New layers in understanding and predicting α -linolenic acid content in plants using amino acid characteristics of omega-3 fatty acid desaturase. *Computers in Biology and Medicine*, 2014
5. Y Liang, S Liu, S Zhang. Prediction of Protein Structural Class Based on Different Autocorrelation Descriptors of Position-Specific Scoring Matrix. *MATCH Commun. Math. Comput. Chem.* 2015
6. A Yousef, NM Charkari. SFM: A novel sequence-based fusion method for disease genes identification and prioritization. *Journal of Theoretical Biology*, 2015
7. W Zhang, L Ji, Y Chen, K Tang, H Wang. When drug discovery meets web search: Learning to Rank for ligand-based virtual screening. *Journal of Cheminformatics*, 2015
8. W Bao, D Wang, F Kong, R Han, Y Chen. Prediction of Protein Structure Classes. *Intelligent Computing Theories and Methodologies*, 2015
9. Y Wang, Y Guo, Q Kuang, X Pu, Y Ji, Z Zhang. A comparative study of family-specific protein-ligand complex affinity prediction based on random forest approach. *Journal of Computer-Aided Molecular Design*, 2015
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13. Y Marrero-Ponce, E Contreras-Torres. Novel 3D bio-macromolecular bilinear descriptors for protein science: Predicting protein structural classes. *Journal of theoretical biology*, 2015
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21. A Duardo-Sanchez, H Gonzalez-Diaz. MI-NODES Multiscale Models of Metabolic Reactions, Brain Connectome, Ecological, Epidemic, World Trade, and Legal-Social Networks. *Current Bioinformatics*, 2015
22. I Cortes-Ciriano, QU Ain, V Subramanian. Polypharmacology modelling using proteochemometrics (PCM): recent methodological developments, applications to target families, and future prospects. *MedChemComm*, 2015
23. D Ofer, N Rappoport, M Linial. The Little Known Universe of Short Proteins in Insects: A Machine Learning Approach. *Short Views on Insect Genomics and Proteomics*, 2015
24. L Li, J Li, W Xiao, Y Li, Y Qin, S Zhou, H Yang. Prediction the substrate specificities of membrane transport proteins based on support vector machine and hybrid features. *Computational Biology and Bioinformatics, IEEE/ACM Transactions*, 2015
25. AK Tiwari, R Srivastava. Feature based classification of nuclear receptors and their subfamilies using fuzzy K-nearest neighbor. *Computer Engineering and Applications (ICACEA) International Conference on Advances*, 2015
26. AK Tiwari, R Srivastava, S Srivastava. An Efficient Approach for the Prediction of G-Protein Coupled Receptors and Their Subfamilies. *Proceedings of 3rd International Conference on Advanced Computing, Networking and Informatics*, 2015
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28. D Wang, W Bao, S Han, Y Chen. Prediction of protein structure classes. *Informative and Cybernetics for Computational Social Systems (ICSS) International Conference*, 2015

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29. H Wang, M Wang, H Tan, Y Li, Z Zhang, J Song. PredPPCrys: Accurate Prediction of Sequence Cloning, Protein Production, Purification and Crystallization Propensity from Protein Sequences Using Multi-Step Heterogeneous Feature Fusion and Selection. *PLOS one*, 2014
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32. L Li, S Yu, W Xiao, Y Li, M Li, L Huang, X Zheng. Prediction of bacterial protein subcellular localization by incorporating various features into Chou's PseAAC and a backward feature selection approach. *Biochimie*, 2014
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36. QU Ain, O Mendez-Lucio, IC Ciriano, T Malliavin. Modelling ligand selectivity of serine proteases using integrative proteochemometric approaches improves model performance and allows the multi-target dependent interpretation of features. *Integrative Biology*, 2014
37. BA van den Berg, MJT Reinders, JA Roubos. SPiCE: a web-based tool for sequence-based protein classification and exploration. *BMC Bioinformatics*, 2014
38. CO Sakar, O Kursun, H Seker. Combining multiple clusterings for protein structure prediction. *International Journal of Data Mining and Bioinformatics*, 2014
39. X Du, J Cheng, T Zheng, Z Duan, F Qian. A Novel Feature Extraction Scheme with Ensemble Coding for Protein-Protein Interaction Prediction. *International Journal of Molecular Sciences*, 2014
40. S Datta, S Mukhopadhyay. An ensemble method approach to investigate kinase-specific phosphorylation sites. *International journal of Nanomedicine*, 2014
41. N Habibi, SZM Hashim, A Norouzi. A review of machine learning methods to predict the solubility of overexpressed recombinant proteins in Escherichia coli. *BMC Bioinformatics*, 2014
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43. AN Mbah, ISRN Computational Biology, 2014. Application of Hybrid Functional Group to ATP binding Protein Prediction. *ISRN Computational Biology*, 2014
44. W Huang, G Yang, X Zhao, Z Li. Prediction of HLA-DRB1 0401 binding peptides using support vector machine. *International Journal of Data Mining and Bioinformatics*, 2014
45. B Ma, AO Charkowski, JD Glasner, NT Perna. Identification of host-microbe interaction factors in the genomes of soft rot-associated pathogens *Dickeya dadantii* 3937 and *Pectobacterium carotovorum* WPP14 with supervised machine learning. *BMC Genomics*, 2014
46. CO Sakar, O Kursun, H Seker, F Gurgun. Combining multiple views: Case studies on protein and arrhythmia features. *Engineering Applications of Artificial Intelligence*, 2014
47. N Xiao, Q Xu, D Cao. protr: Protein Sequence Descriptor Calculation and Similarity Computation with R. *R Package*, 2014
48. Y Liu, Y Li, Z Huang, Z Xu, Z Yang, Z Chen. Multi-algorithm and multi-model based drug target prediction and web server. *Acta Pharmacologica Sinica*, 2014
49. SE Richards, E Holmes. Transcriptomics, proteomics, metabolomics, and metagenomics datasets. *Metabolomics as a Tool in Nutrition Research*, 2014
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51. P Klus, B Bolognesi, F Agostini, D Marchese. The cleverSuite approach for protein characterization: predictions of structural properties, solubility, chaperone requirements and RNA-binding abilities. *Bioinformatics*, 2014
52. L Li, S Yu, W Xiao, Y Li, W Hu, L Huang, X Zheng. Protein submitochondria localization from integrated sequence representation and SVM-based backward feature extraction. *Molecular BioSystems*, 2014

53. JB Brown, Y Okuno, G Marcou, A Varnek. Computational chemogenomics: Is it more than inductive transfer? *Journal of Computer-Aided Molecular Design*, 2014
54. RD Roy, D Dash. Selection of relevant features from amino acids enables development of robust classifiers. *Amino Acids*, 2014
55. W Zhang, M Ke. Protein Encoding: A Matlab toolbox of representing or encoding protein sequences as numerical vectors for bioinformatics. *Journal of Chemical & Pharmaceutical Research*, 2014

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57. GS Han, ZG Yu, V Anh, AP Krishnajith, YC Tian. An ensemble method for predicting subnuclear localizations from primary protein structures. *PLOS One*, 2013
58. M Lapins, A Worachartcheewan, O Spjuth, V Georgiev. A unified proteochemometric model for prediction of inhibition of cytochrome P450 isoforms. *PLOS One*, 2013
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60. DS Cao, QS Xu, YZ Liang. propy: a tool to generate various modes of Chou's PseAAC. *Bioinformatics*, 2013
61. TH Chang, LC Wu, TY Lee, SP Chen. EuLoc: a web-server for accurately predict protein subcellular localization in eukaryotes by incorporating various features of sequence segments into the general form of Chou's PseAAC. *Journal of Computer-Aided Molecular Design*, 2013
62. GT Valente, ML Acencio, C Martins, N Lemke. The development of a universal in silico predictor of protein-protein interactions. *PLOS One*, 2013
63. GJP van Westen, RF Swier, I Cortes-Ciriano. Benchmarking of protein descriptor sets in proteochemometric modeling (part 2): modeling performance of 13 amino acid descriptor sets. *Journal of Cheminformatics*, 2013
64. F Hosseinzadeh, AH KayvanJoo, M Ebrahimi. Prediction of lung tumor types based on protein attributes by machine learning algorithms. *Springerplus*, 2013
65. DS Cao, YZ Liang, J Yan, GS Tan. PyDPI: freely available Python package for chemoinformatics, bioinformatics, and chemogenomics studies. *Journal of Chemical Information and Modeling*, 2013
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