Amarda Shehu

List of Publications by Year
in descending order

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153 papers	2,136 citations	304743 22 h-index	302126 39 g-index
157 all docs	157 docs citations	157 times ranked	1922 citing authors

#	Article	IF	Citations
1	Deep learning improves antimicrobial peptide recognition. Bioinformatics, 2018, 34, 2740-2747.	4.1	282
2	Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics. PLoS Computational Biology, 2016, 12, e1004619.	3.2	188
3	Are nicotinic acetylcholine receptors coupled to G proteins?. BioEssays, 2013, 35, 1025-1034.	2.5	72
4	Modeling protein conformational ensembles: From missing loops to equilibrium fluctuations. Proteins: Structure, Function and Bioinformatics, 2006, 65, 164-179.	2.6	71
5	Menthol Binding and Inhibition of Î±7-Nicotinic Acetylcholine Receptors. PLoS ONE, 2013, 8, e67674.	2.5	64
6	Multiscale characterization of protein conformational ensembles. Proteins: Structure, Function and Bioinformatics, 2009, 76, 837-851.	2.6	63
7	Basin Hopping as a General and Versatile Optimization Framework for the Characterization of Biological Macromolecules. Advances in Artificial Intelligence, 2012, 2012, 1-19.	0.9	58
8	Guiding the Search for Native-like Protein Conformations with an Ab-initio Tree-based Exploration. International Journal of Robotics Research, 2010, 29, 1106-1127.	8.5	50
9	Effective Automated Feature Construction and Selection for Classification of Biological Sequences. PLoS ONE, 2014, 9, e99982.	2.5	48
10	Mapping the Conformation Space of Wildtype and Mutant H-Ras with a Memetic, Cellular, and Multiscale Evolutionary Algorithm. PLoS Computational Biology, 2015, 11, e1004470.	3.2	47
11	A Survey of Computational Methods for Protein Function Prediction. , 2016, , 225-298.		42
12	Modeling Structures and Motions of Loops in Protein Molecules. Entropy, 2012, 14, 252-290.	2.2	41
13	Menthol Inhibits 5-HT₃Receptorâ€“Mediated Currents. Journal of Pharmacology and Experimental Therapeutics, 2013, 347, 398-409.	2.5	40
14	On the Characterization of Protein Native State Ensembles. Biophysical Journal, 2007, 92, 1503-1511.	0.5	36
15	Probabilistic Search and Energy Guidance for Biased Decoy Sampling in Ab Initio Protein Structure Prediction. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2013, 10, 1162-1175.	3.0	36
16	Investigation of a dilated cardiomyopathyâ€“associated variant in BAG3 using genome-edited iPSC-derived cardiomyocytes. JCI Insight, 2019, 4, .	5.0	35
17	Restriction versus guidance in protein structure prediction. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15302-15307.	7.1	34
18	Evolutionary-inspired probabilistic search for enhancing sampling of local minima in the protein energy surface. Proteome Science, 2012, 10, S5.	1.7	34

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19	Multi-Objective Stochastic Search for Sampling Local Minima in the Protein Energy Surface. , 2013, , .		34
20	A Data-Driven Evolutionary Algorithm for Mapping Multibasin Protein Energy Landscapes. Journal of Computational Biology, 2015, 22, 844-860.	1.6	31
21	An Evolutionary Algorithm Approach for Feature Generation from Sequence Data and Its Application to DNA Splice Site Prediction. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2012, 9, 1387-1398.	3.0	29
22	From Extraction of Local Structures of Protein Energy Landscapes to Improved Decoy Selection in Template-Free Protein Structure Prediction. Molecules, 2018, 23, 216.	3.8	29
23	Off-lattice protein structure prediction with homologous crossover. , 2013, , .		28
24	Generative deep learning for macromolecular structure and dynamics. Current Opinion in Structural Biology, 2021, 67, 170-177.	5.7	26
25	Elucidating the ensemble of functionally-relevant transitions in protein systems with a robotics-inspired method. BMC Structural Biology, 2013, 13, S8.	2.3	25
26	IN SEARCH OF THE PROTEIN NATIVE STATE WITH A PROBABILISTIC SAMPLING APPROACH. Journal of Bioinformatics and Computational Biology, 2011, 09, 383-398.	0.8	23
27	Characterizing Energy Landscapes of Peptides Using a Combination of Stochastic Algorithms. IEEE Transactions on Nanobioscience, 2015, 14, 545-552.	3.3	23
28	Unfolding the fold of cyclic cysteineâ€rich peptides. Protein Science, 2008, 17, 482-493.	7.6	22
29	Computing energy landscape maps and structural excursions of proteins. BMC Genomics, 2016, 17, 546.	2.8	20
30	Balancing multiple objectives in conformation sampling to control decoy diversity in template-free protein structure prediction. BMC Bioinformatics, 2019, 20, 211.	2.6	20
31	A Multi-channel BiLSTM-CNN Model for Multilabel Emotion Classification of Informal Text. , 2020, , .		20
32	A Survey of Computational Treatments of Biomolecules by Robotics-Inspired Methods Modeling Equilibrium Structure and Dynamic. Journal of Artificial Intelligence Research, 0, 57, 509-572.	7.0	20
33	AN EVOLUTIONARY CONSERVATION-BASED METHOD FOR REFINING AND RERANKING PROTEIN COMPLEX STRUCTURES. Journal of Bioinformatics and Computational Biology, 2012, 10, 1242002.	0.8	19
34	A population-based evolutionary search approach to the multiple minima problem in de novo protein structure prediction. BMC Structural Biology, 2013, 13, S4.	2.3	18
35	Sampling Conformation Space to Model Equilibrium Fluctuations in Proteins. Algorithmica, 2007, 48, 303-327.	1.3	17
36	A Review of Evolutionary Algorithms for Computing Functional Conformations of Protein Molecules. Methods in Pharmacology and Toxicology, 2015, , 31-64.	0.2	16

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37	Computational Structural Biology: Successes, Future Directions, and Challenges. Molecules, 2019, 24, 637.	3.8	16
38	Structure-Guided Protein Transition Modeling with a Probabilistic Roadmap Algorithm. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2018, 15, 1783-1796.	3.0	15
39	A multiscale hybrid evolutionary algorithm to obtain sample-based representations of multi-basin protein energy landscapes. , 2014, , .		14
40	A General, Adaptive, Roadmap-Based Algorithm for Protein Motion Computation. IEEE Transactions on Nanobioscience, 2016, 15, 158-165.	3.3	14
41	GUIDING PROBABILISTIC SEARCH OF THE PROTEIN CONFORMATIONAL SPACE WITH STRUCTURAL PROFILES. Journal of Bioinformatics and Computational Biology, 2012, 10, 1242005.	0.8	13
42	Computational Methods for Exploration and Analysis of Macromolecular Structure and Dynamics. PLoS Computational Biology, 2015, 11, e1004585.	3.2	13
43	An Energy Landscape Treatment of Decoy Selection in Template-Free Protein Structure Prediction. Computation, 2018, 6, 39.	2.0	13
44	Efficient basin hopping in the protein energy surface. , 2012, , .		12
45	Generating tertiary protein structures via interpretable graph variational autoencoders. Bioinformatics Advances, 2021, 1, .	2.4	12
46	GUIDING PROTEIN DOCKING WITH GEOMETRIC AND EVOLUTIONARY INFORMATION. Journal of Bioinformatics and Computational Biology, 2012, 10, 1242008.	0.8	11
47	Binary Response Models for Recognition of Antimicrobial Peptides. , 2013, , .		11
48	A stochastic roadmap method to model protein structural transitions. Robotica, 2016, 34, 1705-1733.	1.9	11
49	From Optimization to Mapping: An Evolutionary Algorithm for Protein Energy Landscapes. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2018, 15, 719-731.	3.0	11
50	Interpretable Deep Graph Generation with Node-edge Co-disentanglement. , 2020, , .		11
51	Using evolutionary computation to improve SVM classification. , 2010, , .		10
52	HopDock: a probabilistic search algorithm for decoy sampling in protein-protein docking. Proteome Science, 2013, 11, S6.	1.7	10
53	Computing transition paths in multiple-basin proteins with a probabilistic roadmap algorithm guided by structure data. , 2015, , .		10
54	Generative Adversarial Learning of Protein Tertiary Structures. Molecules, 2021, 26, 1209.	3.8	10

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55	Sample-Based Models of Protein Energy Landscapes and Slow Structural Rearrangements. Journal of Computational Biology, 2018, 25, 33-50.	1.6	9
56	Graph-Based Community Detection for Decoy Selection in Template-Free Protein Structure Prediction. Molecules, 2019, 24, 854.	3.8	9
57	Evaluating Autoencoder-Based Featurization and Supervised Learning for Protein Decoy Selection. Molecules, 2020, 25, 1146.	3.8	9
58	Exploring representations of protein structure for automated remote homology detection and mapping of protein structure space. BMC Bioinformatics, 2014, 15, S4.	2.6	8
59	Learning Reduced Latent Representations of Protein Structure Data. , 2019, , .		8
60	Populating Local Minima in the Protein Conformational Space. , 2011, , .		7
61	Rapid sampling of local minima in protein energy surface and effective reduction through a multi-objective filter. Proteome Science, 2013, 11, S12.	1.7	6
62	A Novel EA-based Memetic Approach for Efficiently Mapping Complex Fitness Landscapes. , 2016, , .		6
63	From mutations to mechanisms and dysfunction via computation and mining of protein energy landscapes. BMC Genomics, 2018, 19, 671.	2.8	6
64	Non-Negative Matrix Factorization for Selection of Near-Native Protein Tertiary Structures. , 2019, , .		6
65	From molecular energy landscapes to equilibrium dynamics via landscape analysis and markov state models. Journal of Bioinformatics and Computational Biology, 2019, 17, 1940014.	0.8	6
66	Unsupervised and Supervised Learning over the
Energy Landscape for Protein Decoy Selection. Biomolecules, 2019, 9, 607.	4.0	6
67	Reducing Ensembles of Protein Tertiary Structures Generated De Novo via Clustering. Molecules, 2020, 25, 2228.	3.8	6
68	Variational Autoencoders for Protein Structure Prediction. , 2020, , .		6
69	Selecting predictive features for recognition of hypersensitive sites of regulatory genomic sequences with an evolutionary algorithm. , 2010, , .		5
70	Refinement of docked protein complex structures using evolutionary traces. , 2011, , .		5
71	Protein docking with information on evolutionary conserved interfaces. , 2011, , .		5
72	A TWO-STAGE EVOLUTIONARY APPROACH FOR EFFECTIVE CLASSIFICATION OF HYPERSENSITIVE DNA SEQUENCES. Journal of Bioinformatics and Computational Biology, 2011, 09, 399-413.	0.8	5

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73	A robotics-inspired method to sample conformational paths connecting known functionally-relevant structures in protein systems. , 2012, , .		5
74	A basin hopping algorithm for protein-protein docking. , 2012, , .		5
75	Evolution Strategies for Exploring Protein Energy Landscapes. , 2015, , .		5
76	idDock+: Integrating Machine Learning in Probabilistic Search for Proteinâ€“Protein Docking. Journal of Computational Biology, 2015, 22, 806-822.	1.6	5
77	Sample-based Models of Protein Structural Transitions. , 2016, , .		5
78	Modeling the Tertiary Structure of the Rift Valley Fever Virus L Protein. Molecules, 2019, 24, 1768.	3.8	5
79	Decoy selection for protein structure prediction via extreme gradient boosting and ranking. BMC Bioinformatics, 2020, 21, 189.	2.6	5
80	Unsupervised multi-instance learning for protein structure determination. Journal of Bioinformatics and Computational Biology, 2021, 19, 2140002.	0.8	5
81	Deep Ranking in Template-free Protein Structure Prediction. , 2020, , .		5
82	Data Size and Quality Matter: Generating Physically-Realistic Distance Maps of Protein Tertiary Structures. Biomolecules, 2022, 12, 908.	4.0	5
83	A population-based evolutionary algorithm for sampling minima in the protein energy surface. , 2012, , .		4
84	Systematic analysis of global features and model building for recognition of antimicrobial peptides. , 2013, , .		4
85	Using subpopulation EAs to map molecular structure landscapes. , 2019, , .		4
86	Interpretable Molecule Generation via Disentanglement Learning. , 2020, , .		4
87	Enhancing Sampling of the Conformational Space Near the Protein Native State. Lecture Notes of the Institute for Computer Sciences, Social-Informatics and Telecommunications Engineering, 2012, , 249-263.	0.3	4
88	Biased decoy sampling to aid the selection of near-native protein conformations. , 2012, , .		3
89	Exploring the Structure Space of Wildtype Ras Guided by Experimental Data. , 2013, , .		3
90	Informatics-driven Protein-protein Docking. , 2013, , .		3

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91	A novel method to improve recognition of antimicrobial peptides through distal sequence-based features. , 2014, , .		3
92	Building maps of protein structure spaces in template-free protein structure prediction. Journal of Bioinformatics and Computational Biology, 2019, 17, 1940013.	0.8	3
93	Automated Design of Assemblable, Modular, Synthetic Chromosomes. Lecture Notes in Computer Science, 2010, , 280-289.	1.3	3
94	Small molecule generation via disentangled representation learning. Bioinformatics, 2022, 38, 3200-3208.	4.1	3
95	An evolutionary-based approach for feature generation: Eukaryotic promoter recognition. , 2011, , .		2
96	Feature and Kernel Evolution for Recognition of Hypersensitive Sites in DNA Sequences. Lecture Notes of the Institute for Computer Sciences, Social-Informatics and Telecommunications Engineering, 2012, , 213-228.	0.3	2
97	Computational biologist in profile. ACM SIGBioinformatics Record, 2013, 3, 12-14.	0.3	2
98	Sampling-based methods for a full characterization of energy landscapes of small peptides. , 2014, , .		2
99	Community Detection for Decoy Selection in Template-free Protein Structure Prediction. , 2018, , .		2
100	Improved Decoy Selection via Machine Learning and Ranking. , 2018, , .		2
101	Learning Organizations of Protein Energy Landscapes: An Application on Decoy Selection in Template-Free Protein Structure Prediction. Methods in Molecular Biology, 2019, 1958, 147-171.	0.9	2
102	Decoy Ensemble Reduction in Template-free Protein Structure Prediction. , 2019, , .		2
103	Using Sequence-Predicted Contacts to Guide Template-free Protein Structure Prediction. , 2019, , .		2
104	Reconstruction and Decomposition of High-Dimensional Landscapes via Unsupervised Learning. , 2020, , .		2
105	The 6th Computational Structural Bioinformatics Workshop. BMC Structural Biology, 2013, 13, I1.	2.3	1
106	Evolutionary search algorithms for protein modeling. , 2014, , .		1
107	Mapping Multiple Minima in Protein Energy Landscapes with Evolutionary Algorithms. , 2015, , .		1
108	Evolutionary Algorithms for Protein Structure Modeling. , 2015, , .		1

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109	Statistical Analysis of Computed Energy Landscapes to Understand Dysfunction in Pathogenic Protein Variants. , 2017, , .		1
110	Reconstructing and mining protein energy landscape to understand disease. , 2017, , .		1
111	Reconstructing and Decomposing Protein Energy Landscapes to Organize Structure Spaces and Reveal Biologically-active States. , 2018, , .		1
112	Identifying Near-Native Protein Structures via Anomaly Detection. , 2019, , .		1
113	Anomaly Detection-Based Recognition of Near-Native Protein Structures. IEEE Transactions on Nanobioscience, 2020, 19, 562-570.	3.3	1
114	Computing the Structural Dynamics of RVFV L Protein Domain in Aqueous Glycerol Solutions. Biomolecules, 2021, 11, 1427.	4.0	1
115	Improved Protein Decoy Selection via Non-Negative Matrix Factorization. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2021, PP, 1-1.	3.0	1
116	Connecting Molecular Energy Landscape Analysis with Markov Model-based Analysis of Equilibrium Structural Dynamics. , 0, , .		1
117	EML: A Scalable, Transparent Meta-Learning Paradigm for Big Data Applications. Intelligent Systems Reference Library, 2019, , 35-59.	1.2	1
118	Antigen Binding Reshapes Antibody Energy Landscape and Conformation Dynamics. , 2021, , .		1
119	Generating Physically-Realistic Tertiary Protein Structures with Deep Latent Variable Models Learning Over Experimentally-available Structures. , 2021, , .		1
120	Protein conformational search with geometric projections. , 2011, , .		0
121	Mapping the Protein Conformational Landscape with Adaptive Probabilistic Search. Biophysical Journal, 2011, 100, 377a.	0.5	0
122	Assembly of low-energy protein conformations with heterogeneous fragments. , 2011, , .		0
123	THE 5TH INTERNATIONAL CONFERENCE ON BIO-INSPIRED MODELS OF NETWORK, INFORMATION AND COMPUTING SYSTEMS (BIONETICS 2010) SPECIAL TRACK ON BIOINFORMATICS. Journal of Bioinformatics and Computational Biology, 2011, 09, v-vii.	0.8	0
124	An evolutionary search framework to efficiently sample local minima in the protein conformational space. , 2012, , .		0
125	Jumping low, jumping high: Controlling hopping in the protein energy surface. , 2012, , .		0
126	Sampling low-energy protein-protein configurations with basin hopping. , 2012, , .		0

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127	A tree-based search to bias sampling of protein decoy conformations. , 2012, , .		0
128	Mapping conformational pathways between known functional protein states. , 2012, , .		0
129	Physico-chemical features for recognition of antimicrobial peptides. , 2012, , .		0
130	An evolutionary framework to sample near-native protein conformations. , 2012, , .		0
131	A PCA-guided Search Algorithm to Probe the Conformational Space of the Ras Protein. , 2013, , .		0
132	Higher-order representations of protein structure space. , 2013, , .		0
133	Protein-protein Docking Using Information from Native Interaction Interfaces. , 2013, , .		0
134	Computer scientist in profile. ACM SIGBioinformatics Record, 2013, 3, 26-27.	0.3	0
135	Knowledge-based search and multi-objective filters. , 2014, , .		0
136	Computer scientist in profile. ACM SIGBioinformatics Record, 2014, 4, 5-7.	0.3	0
137	The 7th Computational Structural Bioinformatics Workshop. Journal of Computational Biology, 2015, 22, 785-786.	1.6	0
138	Foreword on special issue on robotics methods for structural and dynamic modeling of molecular systems. Robotica, 2016, 34, 1677-1678.	1.9	0
139	Path-based Guidance of an Evolutionary Algorithm in Mapping a Fitness Landscape and its Connectivity. , 2016, , .		0
140	Evolving Conformation Paths to Model Protein Structural Transitions. , 2017, , .		0
141	Evolutionary search for paths on protein energy landscapes. , 2017, , .		0
142	Guest Editorial for Special Section on BIBM 2014. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2017, 14, 252-253.	3.0	0
143	Modeling protein structural transitions as a multiobjective optimization problem. , 2017, , .		0
144	Out of one, many: Exploiting intrinsic motions to explore protein structure spaces. , 2017, , .		0

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145	Guiding Exploration of Antimicrobial Peptide Space with a Deep Neural Network. , 2018, , .		0
146	Advances in the Application and Development of Non-Linear Global Optimization Techniques in Computational Structural Biology. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2018, 15, 688-689.	3.0	0
147	Guest Editorial for the ACM International Conference on Bioinformatics, Computational Biology, and Health Informatics. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2019, 16, 1409-1409.	3.0	0
148	Guest Editorial on the Special Issue on Informatics on Biomedical Data Learning, Reasoning, and Representation. IEEE Journal of Biomedical and Health Informatics, 2019, 23, 81-82.	6.3	0
149	Attenuating dependence on structural data in computing protein energy landscapes. BMC Bioinformatics, 2019, 20, 280.	2.6	0
150	Unsupervised Learning for Decoy Selection in Protein Structure Prediction. Biophysical Journal, 2019, 116, 192a.	0.5	0
151	A Multi-Objective Stochastic Optimization Approach for Decoy Generation in Template-Free Protein Structure Prediction. Biophysical Journal, 2019, 116, 59a.	0.5	0
152	Editorial overview: Theory and simulation and their new friends. Current Opinion in Structural Biology, 2021, 67, iii-v.	5.7	0
153	From Interatomic Distances to Protein Tertiary Structures with a Deep Convolutional Neural Network. , 2020, , .		0