Amarda Shehu

List of Publications by Year
in descending order

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153 papers	2,136 citations	304602 22 h-index	302012 39 g-index
157 all docs	157 docs citations	157 times ranked	1922 citing authors

#	Article	IF	Citations
1	Small molecule generation via disentangled representation learning. Bioinformatics, 2022, 38, 3200-3208.	1.8	3
2	Data Size and Quality Matter: Generating Physically-Realistic Distance Maps of Protein Tertiary Structures. Biomolecules, 2022, 12, 908.	1.8	5
3	Generative deep learning for macromolecular structure and dynamics. Current Opinion in Structural Biology, 2021, 67, 170-177.	2.6	26
4	Unsupervised multi-instance learning for protein structure determination. Journal of Bioinformatics and Computational Biology, 2021, 19, 2140002.	0.3	5
5	Generative Adversarial Learning of Protein Tertiary Structures. Molecules, 2021, 26, 1209.	1.7	10
6	Editorial overview: Theory and simulation and their new friends. Current Opinion in Structural Biology, 2021, 67, iii-v.	2.6	0
7	Computing the Structural Dynamics of RVFV L Protein Domain in Aqueous Glycerol Solutions. Biomolecules, 2021, 11, 1427.	1.8	1
8	Improved Protein Decoy Selection via Non-Negative Matrix Factorization. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2021, PP, 1-1.	1.9	1
9	Generating tertiary protein structures via interpretable graph variational autoencoders. Bioinformatics Advances, 2021, 1, .	0.9	12
10	Antigen Binding Reshapes Antibody Energy Landscape and Conformation Dynamics. , 2021, , .		1
11	Generating Physically-Realistic Tertiary Protein Structures with Deep Latent Variable Models Learning Over Experimentally-available Structures. , 2021, , .		1
12	Decoy selection for protein structure prediction via extreme gradient boosting and ranking. BMC Bioinformatics, 2020, 21, 189.	1.2	5
13	Reducing Ensembles of Protein Tertiary Structures Generated De Novo via Clustering. Molecules, 2020, 25, 2228.	1.7	6
14	Anomaly Detection-Based Recognition of Near-Native Protein Structures. IEEE Transactions on Nanobioscience, 2020, 19, 562-570.	2.2	1
15	Evaluating Autoencoder-Based Featurization and Supervised Learning for Protein Decoy Selection. Molecules, 2020, 25, 1146.	1.7	9
16	A Multi-channel BiLSTM-CNN Model for Multilabel Emotion Classification of Informal Text. , 2020, , .		20
17	Deep Ranking in Template-free Protein Structure Prediction. , 2020, , .		5
18	Interpretable Molecule Generation via Disentanglement Learning. , 2020, , .		4

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19	Interpretable Deep Graph Generation with Node-edge Co-disentanglement. , 2020, , .		11
20	Reconstruction and Decomposition of High-Dimensional Landscapes via Unsupervised Learning. , 2020, , .		2
21	Variational Autoencoders for Protein Structure Prediction. , 2020, , .		6
22	From Interatomic Distances to Protein Tertiary Structures with a Deep Convolutional Neural Network. , 2020, , .		0
23	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.	1.9	0
24	Using subpopulation EAs to map molecular structure landscapes. , 2019, , .		4
25	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.	3.9	0
26	Attenuating dependence on structural data in computing protein energy landscapes. BMC Bioinformatics, 2019, 20, 280.	1.2	0
27	Modeling the Tertiary Structure of the Rift Valley Fever Virus L Protein. Molecules, 2019, 24, 1768.	1.7	5
28	Balancing multiple objectives in conformation sampling to control decoy diversity in template-free protein structure prediction. BMC Bioinformatics, 2019, 20, 211.	1.2	20
29	Unsupervised Learning for Decoy Selection in Protein Structure Prediction. Biophysical Journal, 2019, 116, 192a.	0.2	0
30	Graph-Based Community Detection for Decoy Selection in Template-Free Protein Structure Prediction. Molecules, 2019, 24, 854.	1.7	9
31	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.	0.4	2
32	Computational Structural Biology: Successes, Future Directions, and Challenges. Molecules, 2019, 24, 637.	1.7	16
33	A Multi-Objective Stochastic Optimization Approach for Decoy Generation in Template-Free Protein Structure Prediction. Biophysical Journal, 2019, 116, 59a.	0.2	0
34	Non-Negative Matrix Factorization for Selection of Near-Native Protein Tertiary Structures. , 2019, , .		6
35	Identifying Near-Native Protein Structures via Anomaly Detection. , 2019, , .		1
36	Building maps of protein structure spaces in template-free protein structure prediction. Journal of Bioinformatics and Computational Biology, 2019, 17, 1940013.	0.3	3

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37	From molecular energy landscapes to equilibrium dynamics via landscape analysis and markov state models. Journal of Bioinformatics and Computational Biology, 2019, 17, 1940014.	0.3	6
38	Unsupervised and Supervised Learning over the
Energy Landscape for Protein Decoy Selection. Biomolecules, 2019, 9, 607.	1.8	6
39	Decoy Ensemble Reduction in Template-free Protein Structure Prediction. , 2019, , .		2
40	Learning Reduced Latent Representations of Protein Structure Data. , 2019, , .		8
41	Investigation of a dilated cardiomyopathyâ€“associated variant in BAG3 using genome-edited iPSC-derived cardiomyocytes. JCI Insight, 2019, 4, .	2.3	35
42	EML: A Scalable, Transparent Meta-Learning Paradigm for Big Data Applications. Intelligent Systems Reference Library, 2019, , 35-59.	1.0	1
43	Using Sequence-Predicted Contacts to Guide Template-free Protein Structure Prediction. , 2019, , .		2
44	Deep learning improves antimicrobial peptide recognition. Bioinformatics, 2018, 34, 2740-2747.	1.8	282
45	From Optimization to Mapping: An Evolutionary Algorithm for Protein Energy Landscapes. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2018, 15, 719-731.	1.9	11
46	Structure-Guided Protein Transition Modeling with a Probabilistic Roadmap Algorithm. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2018, 15, 1783-1796.	1.9	15
47	Sample-Based Models of Protein Energy Landscapes and Slow Structural Rearrangements. Journal of Computational Biology, 2018, 25, 33-50.	0.8	9
48	Reconstructing and Decomposing Protein Energy Landscapes to Organize Structure Spaces and Reveal Biologically-active States. , 2018, , .		1
49	Community Detection for Decoy Selection in Template-free Protein Structure Prediction. , 2018, , .		2
50	Guiding Exploration of Antimicrobial Peptide Space with a Deep Neural Network. , 2018, , .		0
51	An Energy Landscape Treatment of Decoy Selection in Template-Free Protein Structure Prediction. Computation, 2018, 6, 39.	1.0	13
52	Improved Decoy Selection via Machine Learning and Ranking. , 2018, , .		2
53	From mutations to mechanisms and dysfunction via computation and mining of protein energy landscapes. BMC Genomics, 2018, 19, 671.	1.2	6
54	From Extraction of Local Structures of Protein Energy Landscapes to Improved Decoy Selection in Template-Free Protein Structure Prediction. Molecules, 2018, 23, 216.	1.7	29

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55	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.	1.9	0
56	Statistical Analysis of Computed Energy Landscapes to Understand Dysfunction in Pathogenic Protein Variants. , 2017, , .		1
57	Evolving Conformation Paths to Model Protein Structural Transitions. , 2017, , .		0
58	Reconstructing and mining protein energy landscape to understand disease. , 2017, , .		1
59	Evolutionary search for paths on protein energy landscapes. , 2017, , .		0
60	Guest Editorial for Special Section on BIBM 2014. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2017, 14, 252-253.	1.9	0
61	Modeling protein structural transitions as a multiobjective optimization problem. , 2017, , .		0
62	Out of one, many: Exploiting intrinsic motions to explore protein structure spaces. , 2017, , .		0
63	Foreword on special issue on robotics methods for structural and dynamic modeling of molecular systems. Robotica, 2016, 34, 1677-1678.	1.3	0
64	A stochastic roadmap method to model protein structural transitions. Robotica, 2016, 34, 1705-1733.	1.3	11
65	A Survey of Computational Methods for Protein Function Prediction. , 2016, , 225-298.		42
66	A Novel EA-based Memetic Approach for Efficiently Mapping Complex Fitness Landscapes. , 2016, , .		6
67	Path-based Guidance of an Evolutionary Algorithm in Mapping a Fitness Landscape and its Connectivity. , 2016, , .		0
68	Sample-based Models of Protein Structural Transitions. , 2016, , .		5
69	Computing energy landscape maps and structural excursions of proteins. BMC Genomics, 2016, 17, 546.	1.2	20
70	A General, Adaptive, Roadmap-Based Algorithm for Protein Motion Computation. IEEE Transactions on Nanobioscience, 2016, 15, 158-165.	2.2	14
71	Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics. PLoS Computational Biology, 2016, 12, e1004619.	1.5	188
72	A Review of Evolutionary Algorithms for Computing Functional Conformations of Protein Molecules. Methods in Pharmacology and Toxicology, 2015, , 31-64.	0.1	16

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73	Mapping the Conformation Space of Wildtype and Mutant H-Ras with a Memetic, Cellular, and Multiscale Evolutionary Algorithm. PLoS Computational Biology, 2015, 11, e1004470.	1.5	47
74	Computational Methods for Exploration and Analysis of Macromolecular Structure and Dynamics. PLoS Computational Biology, 2015, 11, e1004585.	1.5	13
75	Computing transition paths in multiple-basin proteins with a probabilistic roadmap algorithm guided by structure data. , 2015, , .		10
76	A Data-Driven Evolutionary Algorithm for Mapping Multibasin Protein Energy Landscapes. Journal of Computational Biology, 2015, 22, 844-860.	0.8	31
77	Characterizing Energy Landscapes of Peptides Using a Combination of Stochastic Algorithms. IEEE Transactions on Nanobioscience, 2015, 14, 545-552.	2.2	23
78	The 7th Computational Structural Bioinformatics Workshop. Journal of Computational Biology, 2015, 22, 785-786.	0.8	0
79	Evolution Strategies for Exploring Protein Energy Landscapes. , 2015, , .		5
80	Mapping Multiple Minima in Protein Energy Landscapes with Evolutionary Algorithms. , 2015, , .		1
81	idDock+: Integrating Machine Learning in Probabilistic Search for Proteinâ€“Protein Docking. Journal of Computational Biology, 2015, 22, 806-822.	0.8	5
82	Evolutionary Algorithms for Protein Structure Modeling. , 2015, , .		1
83	Effective Automated Feature Construction and Selection for Classification of Biological Sequences. PLoS ONE, 2014, 9, e99982.	1.1	48
84	A novel method to improve recognition of antimicrobial peptides through distal sequence-based features. , 2014, , .		3
85	A multiscale hybrid evolutionary algorithm to obtain sample-based representations of multi-basin protein energy landscapes. , 2014, , .		14
86	Knowledge-based search and multi-objective filters. , 2014, , .		0
87	Sampling-based methods for a full characterization of energy landscapes of small peptides. , 2014, , .		2
88	Evolutionary search algorithms for protein modeling. , 2014, , .		1
89	Exploring representations of protein structure for automated remote homology detection and mapping of protein structure space. BMC Bioinformatics, 2014, 15, S4.	1.2	8
90	Computer scientist in profile. ACM SIGBioinformatics Record, 2014, 4, 5-7.	0.3	0

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91	Binary Response Models for Recognition of Antimicrobial Peptides. , 2013, , .		11
92	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.	1.9	36
93	The 6th Computational Structural Bioinformatics Workshop. BMC Structural Biology, 2013, 13, I1.	2.3	1
94	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
95	Elucidating the ensemble of functionally-relevant transitions in protein systems with a robotics-inspired method. BMC Structural Biology, 2013, 13, S8.	2.3	25
96	HopDock: a probabilistic search algorithm for decoy sampling in protein-protein docking. Proteome Science, 2013, 11, S6.	0.7	10
97	Rapid sampling of local minima in protein energy surface and effective reduction through a multi-objective filter. Proteome Science, 2013, 11, S12.	0.7	6
98	Multi-Objective Stochastic Search for Sampling Local Minima in the Protein Energy Surface. , 2013, , .		34
99	A PCA-guided Search Algorithm to Probe the Conformational Space of the Ras Protein. , 2013, , .		0
100	Exploring the Structure Space of Wildtype Ras Guided by Experimental Data. , 2013, , .		3
101	Menthol Inhibits 5-HT₃Receptorâ€“Mediated Currents. Journal of Pharmacology and Experimental Therapeutics, 2013, 347, 398-409.	1.3	40
102	Informatics-driven Protein-protein Docking. , 2013, , .		3
103	Higher-order representations of protein structure space. , 2013, , .		0
104	Are nicotinic acetylcholine receptors coupled to G proteins?. BioEssays, 2013, 35, 1025-1034.	1.2	72
105	Protein-protein Docking Using Information from Native Interaction Interfaces. , 2013, , .		0
106	Systematic analysis of global features and model building for recognition of antimicrobial peptides. , 2013, , .		4
107	Off-lattice protein structure prediction with homologous crossover. , 2013, , .		28
108	Computer scientist in profile. ACM SIGBioinformatics Record, 2013, 3, 26-27.	0.3	0

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109	Computational biologist in profile. ACM SIGBioinformatics Record, 2013, 3, 12-14.	0.3	2
110	Menthol Binding and Inhibition of Î±7-Nicotinic Acetylcholine Receptors. PLoS ONE, 2013, 8, e67674.	1.1	64
111	Modeling Structures and Motions of Loops in Protein Molecules. Entropy, 2012, 14, 252-290.	1.1	41
112	AN EVOLUTIONARY CONSERVATION-BASED METHOD FOR REFINING AND RERANKING PROTEIN COMPLEX STRUCTURES. Journal of Bioinformatics and Computational Biology, 2012, 10, 1242002.	0.3	19
113	GUIDING PROBABILISTIC SEARCH OF THE PROTEIN CONFORMATIONAL SPACE WITH STRUCTURAL PROFILES. Journal of Bioinformatics and Computational Biology, 2012, 10, 1242005.	0.3	13
114	Biased decoy sampling to aid the selection of near-native protein conformations. , 2012, , .		3
115	An evolutionary search framework to efficiently sample local minima in the protein conformational space. , 2012, , .		0
116	Jumping low, jumping high: Controlling hopping in the protein energy surface. , 2012, , .		0
117	A population-based evolutionary algorithm for sampling minima in the protein energy surface. , 2012, , .		4
118	A robotics-inspired method to sample conformational paths connecting known functionally-relevant structures in protein systems. , 2012, , .		5
119	Sampling low-energy protein-protein configurations with basin hopping. , 2012, , .		0
120	A tree-based search to bias sampling of protein decoy conformations. , 2012, , .		0
121	Mapping conformational pathways between known functional protein states. , 2012, , .		0
122	GUIDING PROTEIN DOCKING WITH GEOMETRIC AND EVOLUTIONARY INFORMATION. Journal of Bioinformatics and Computational Biology, 2012, 10, 1242008.	0.3	11
123	A basin hopping algorithm for protein-protein docking. , 2012, , .		5
124	Efficient basin hopping in the protein energy surface. , 2012, , .		12
125	Physico-chemical features for recognition of antimicrobial peptides. , 2012, , .		0
126	An evolutionary framework to sample near-native protein conformations. , 2012, , .		0

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127	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.	0.2	2
128	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
129	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.	1.9	29
130	Evolutionary-inspired probabilistic search for enhancing sampling of local minima in the protein energy surface. Proteome Science, 2012, 10, S5.	0.7	34
131	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.	0.2	4
132	Refinement of docked protein complex structures using evolutionary traces. , 2011, , .		5
133	Populating Local Minima in the Protein Conformational Space. , 2011, , .		7
134	Protein conformational search with geometric projections. , 2011, , .		0
135	Protein docking with information on evolutionary conserved interfaces. , 2011, , .		5
136	An evolutionary-based approach for feature generation: Eukaryotic promoter recognition. , 2011, , .		2
137	Mapping the Protein Conformational Landscape with Adaptive Probabilistic Search. Biophysical Journal, 2011, 100, 377a.	0.2	0
138	A TWO-STAGE EVOLUTIONARY APPROACH FOR EFFECTIVE CLASSIFICATION OF HYPERSENSITIVE DNA SEQUENCES. Journal of Bioinformatics and Computational Biology, 2011, 09, 399-413.	0.3	5
139	IN SEARCH OF THE PROTEIN NATIVE STATE WITH A PROBABILISTIC SAMPLING APPROACH. Journal of Bioinformatics and Computational Biology, 2011, 09, 383-398.	0.3	23
140	Assembly of low-energy protein conformations with heterogeneous fragments. , 2011, , .		0
141	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.	0.3	0
142	Selecting predictive features for recognition of hypersensitive sites of regulatory genomic sequences with an evolutionary algorithm. , 2010, , .		5
143	Guiding the Search for Native-like Protein Conformations with an Ab-initio Tree-based Exploration. International Journal of Robotics Research, 2010, 29, 1106-1127.	5.8	50
144	Using evolutionary computation to improve SVM classification. , 2010, , .		10

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145	Automated Design of Assemblable, Modular, Synthetic Chromosomes. Lecture Notes in Computer Science, 2010, , 280-289.	1.0	3
146	Restriction versus guidance in protein structure prediction. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15302-15307.	3.3	34
147	Multiscale characterization of protein conformational ensembles. Proteins: Structure, Function and Bioinformatics, 2009, 76, 837-851.	1.5	63
148	Unfolding the fold of cyclic cysteineâ€rich peptides. Protein Science, 2008, 17, 482-493.	3.1	22
149	On the Characterization of Protein Native State Ensembles. Biophysical Journal, 2007, 92, 1503-1511.	0.2	36
150	Sampling Conformation Space to Model Equilibrium Fluctuations in Proteins. Algorithmica, 2007, 48, 303-327.	1.0	17
151	Modeling protein conformational ensembles: From missing loops to equilibrium fluctuations. Proteins: Structure, Function and Bioinformatics, 2006, 65, 164-179.	1.5	71
152	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
153	Connecting Molecular Energy Landscape Analysis with Markov Model-based Analysis of Equilibrium Structural Dynamics. , 0, , .		1