Franca Fraternali

List of Publications by Year
in descending order

168 papers	5,680 citations	71061 41 h-index	106281 65 g-index
182 all docs	182 docs citations	182 times ranked	8793 citing authors

#	Article	IF	Citations
1	PDBe-KB: collaboratively defining the biological context of structural data. Nucleic Acids Research, 2022, 50, D534-D542.	6.5	46
2	Sulfated Progesterone Metabolites That Enhance Insulin Secretion via TRPM3 Are Reduced in Serum From Women With Gestational Diabetes Mellitus. Diabetes, 2022, 71, 837-852.	0.3	3
3	Editorial: Understanding and Engineering Antibody-Superantigen Interactions. Frontiers in Immunology, 2022, 13, 857339.	2.2	2
4	Allosteric Regulation of the Soluble Epoxide Hydrolase by Nitro Fatty Acids: a Combined Experimental and Computational Approach. Journal of Molecular Biology, 2022, 434, 167600.	2.0	3
5	Pandemic, Epidemic, Endemic: B Cell Repertoire Analysis Reveals Unique Anti-Viral Responses to SARS-CoV-2, Ebola and Respiratory Syncytial Virus. Frontiers in Immunology, 2022, 13, 807104.	2.2	6
6	Autosomal recessive hypotrichosis with loose anagen hairs associated with TKFC mutations*. British Journal of Dermatology, 2021, 184, 935-943.	1.4	7
7	Coarse-Grained Molecular Dynamics Simulations of Membrane Proteins: A Practical Guide. Methods in Molecular Biology, 2021, 2302, 253-273.	0.4	3
8	Nanocapsule designs for antimicrobial resistance. Nanoscale, 2021, 13, 10342-10355.	2.8	7
9	Short loop functional commonality identified in leukaemia proteome highlights crucial protein sub-networks. NAR Genomics and Bioinformatics, 2021, 3, lqab010.	1.5	0
10	Virus-inspired designs of antimicrobial nanocapsules. Faraday Discussions, 2021, , .	1.6	2
11	Single-Cell Transcriptomic Analyses Define Distinct Peripheral B Cell Subsets and Discrete Development Pathways. Frontiers in Immunology, 2021, 12, 602539.	2.2	83
12	Rapid inactivation of SARS-CoV-2 by titanium dioxide surface coating. Wellcome Open Research, 2021, 6, 56.	0.9	7
13	Pathogenic missense protein variants affect different functional pathways and proteomic features than healthy population variants. PLoS Biology, 2021, 19, e3001207.	2.6	13
14	Tumor-Infiltrating B Lymphocyte Profiling Identifies IgG-Biased, Clonally Expanded Prognostic Phenotypes in Triple-Negative Breast Cancer. Cancer Research, 2021, 81, 4290-4304.	0.4	40
15	Plating human iPSC lines on micropatterned substrates reveals role for ITGB1 nsSNV in endoderm formation. Stem Cell Reports, 2021, 16, 2628-2641.	2.3	4
16	Molecular Simulations Guidelines for Biological Nanomaterials: From Peptides to Membranes. Methods in Molecular Biology, 2021, 2208, 81-100.	0.4	0
17	PDBe-KB: a community-driven resource for structural and functional annotations. Nucleic Acids Research, 2020, 48, D344-D353.	6.5	87
18	Structure and Dynamics of Nanoconfined Water Between Surfactant Monolayers. Langmuir, 2020, 36, 447-455.	1.6	6

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19	Engineering Chirally Blind Protein Pseudocapsids into Antibacterial Persisters. ACS Nano, 2020, 14, 1609-1622.	7.3	42
20	SARS-CoV-2 spike protein predicted to form complexes with host receptor protein orthologues from a broad range of mammals. Scientific Reports, 2020, 10, 16471.	1.6	99
21	A New Crystal Form of the SARS-CoV-2 Receptor Binding Domain: CR3022 Complexâ€"An Ideal Target for In-Crystal Fragment Screening of the ACE2 Binding Site Surface. Frontiers in Pharmacology, 2020, 11, 615211.	1.6	7
22	Mining the PDB for Tractable Cases Where X-ray Crystallography Combined with Fragment Screens Can Be Used to Systematically Design Proteinâ€"Protein Inhibitors: Two Test Cases Illustrated by IL1Î²-IL1R and p38Î±â€"TAB1 Complexes. Journal of Medicinal Chemistry, 2020, 63, 7559-7568.	2.9	18
23	The Aurora B specificity switch is required to protect from non-disjunction at the metaphase/anaphase transition. Nature Communications, 2020, 11, 1396.	5.8	12
24	Symmetry-breaking transitions in the early steps of protein self-assembly. European Biophysics Journal, 2020, 49, 175-191.	1.2	28
25	Understanding the structural details of APOBEC3-DNA interactions using graph-based representations. Current Research in Structural Biology, 2020, 2, 130-143.	1.1	3
26	Prediction of Protein-Protein Interactions: Looking Through the Kaleidoscope. , 2019, , 834-848.		1
27	Lipid Head Group Parameterization for GROMOS 54A8: A Consistent Approach with Protein Force Field Description. Journal of Chemical Theory and Computation, 2019, 15, 5175-5193.	2.3	17
28	Lateral-Torsional Buckling of C-Beams with Varying Inertia. IOP Conference Series: Materials Science and Engineering, 2019, 473, 012011.	0.3	0
29	15-deoxy-Î"12,14-Prostaglandin J2 inhibits human soluble epoxide hydrolase by a dual orthosteric and allosteric mechanism. Communications Biology, 2019, 2, 188.	2.0	16
30	Green Design of Novel Metal Matrix Composites. IOP Conference Series: Materials Science and Engineering, 2019, 473, 012008.	0.3	0
31	Staging and Pretensioning of Cable-Stayed Bridges. IOP Conference Series: Materials Science and Engineering, 2019, 473, 012012.	0.3	0
32	Pan-cancer transcriptomic analysis dissects immune and proliferative functions of APOBEC3 cytidine deaminases. Nucleic Acids Research, 2019, 47, 1178-1194.	6.5	41
33	RhoBTB1 interacts with ROCKs and inhibits invasion. Biochemical Journal, 2019, 476, 2499-2514.	1.7	11
34	Functional cross-talk between allosteric effects of activating and inhibiting ligands underlies PKM2 regulation. ELife, 2019, 8, .	2.8	29
35	Tissue-specific shaping of the TCR repertoire and antigen specificity of iNKT cells. ELife, 2019, 8, .	2.8	16
36	BRepertoire: a user-friendly web server for analysing antibody repertoire data. Nucleic Acids Research, 2018, 46, W264-W270.	6.5	32

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37	In silico identification of rescue sites by double force scanning. Bioinformatics, 2018, 34, 207-214.	1.8	10
38	Genetic variants and proteinâ€“protein interactions: a multidimensional network-centric view. Current Opinion in Structural Biology, 2018, 50, 82-90.	2.6	19
39	Probing the early stages of prion protein (PrP) aggregation with atomistic molecular dynamics simulations. Chemical Communications, 2018, 54, 8007-8010.	2.2	12
40	Inhibitor-induced HER2-HER3 heterodimerisation promotes proliferation through a novel dimer interface. ELife, 2018, 7, .	2.8	55
41	ALIX Regulates Tumor-Mediated Immunosuppression by Controlling EGFR Activity and PD-L1 Presentation. Cell Reports, 2018, 24, 630-641.	2.9	103
42	Surface Accessibility and Dynamics of Macromolecular Assemblies Probed by Covalent Labeling Mass Spectrometry and Integrative Modeling. Analytical Chemistry, 2017, 89, 1459-1468.	3.2	46
43	Structural and Biophysical Analysis of Hypertrophic Cardiomyopathy-Linked Titin Missense Variants. Biophysical Journal, 2017, 112, 164a.	0.2	0
44	An engineered photoswitchable mammalian pyruvate kinase. FEBS Journal, 2017, 284, 2955-2980.	2.2	27
45	TITINdbâ€”a computational tool to assess titinâ€™s role as a disease gene. Bioinformatics, 2017, 33, 3482-3485.	1.8	34
46	Promiscuous antibodies characterised by their physico-chemical properties: From sequence to structure and back. Progress in Biophysics and Molecular Biology, 2017, 128, 47-56.	1.4	20
47	Investigating Ebola virus pathogenicity using molecular dynamics. BMC Genomics, 2017, 18, 566.	1.2	10
48	Significant Differences in Physicochemical Properties of Human Immunoglobulin Kappa and Lambda CDR3 Regions. Frontiers in Immunology, 2016, 7, 388.	2.2	56
49	Transitional B Cells in Early Human B Cell Development â€“ Time to Revisit the Paradigm?. Frontiers in Immunology, 2016, 7, 546.	2.2	53
50	Homology-Based Modeling of Universal Stress Protein from Listeria innocua Up-Regulated under Acid Stress Conditions. Frontiers in Microbiology, 2016, 7, 1998.	1.5	21
51	Promiscuity and Polyreactivity of Antibodies and their Binding Modes during B-Cell Differentiation. Biophysical Journal, 2016, 110, 207a.	0.2	0
52	Sarcomeric signalling proteins: Hubs for mechanosensation and hotspots for inherited myopathies. Neuromuscular Disorders, 2016, 26, S88.	0.3	3
53	Effect of RIC N-Terminal Tails on the Structure and Dynamics of Cardiac Myosin. Biophysical Journal, 2016, 110, 297a.	0.2	0
54	PinSnps: structural and functional analysis of SNPs in the context of protein interaction networks. Bioinformatics, 2016, 32, 2534-2536.	1.8	23

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55	On the reinforcement of cement mortars through 3D printed polymeric and metallic fibers. Composites Part B: Engineering, 2016, 90, 76-85.	5.9	123
56	Towards the identification of the allosteric Phe-binding site in phenylalanine hydroxylase. Journal of Biomolecular Structure and Dynamics, 2016, 34, 497-507.	2.0	7
57	Anatomy of protein disorder, flexibility and disease-related mutations. Frontiers in Molecular Biosciences, 2015, 2, 47.	1.6	16
58	Assembly of Influenza Hemagglutinin Fusion Peptides in a Phospholipid Bilayer by Coarse-grained Computer Simulations. Frontiers in Molecular Biosciences, 2015, 2, 66.	1.6	8
59	Pooled Sequencing of 531 Genes in Inflammatory Bowel Disease Identifies an Associated Rare Variant in BTNL2 and Implicates Other Immune Related Genes. PLoS Genetics, 2015, 11, e1004955.	1.5	59
60	Bridging topological and functional information in protein interaction networks by short loops profiling. Scientific Reports, 2015, 5, 8540.	1.6	19
61	Structural Properties of Green Tea Catechins. Journal of Physical Chemistry B, 2015, 119, 12860-12867.	1.2	93
62	BCRâ€ABL residues interacting with ponatinib are critical to preserve the tumorigenic potential of the oncoprotein. FASEB Journal, 2014, 28, 1221-1236.	0.2	29
63	Plasticity and conformational equilibria of influenza fusion peptides in model lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 1169-1179.	1.4	10
64	Mapping diseaseâ€related missense mutations in the immunoglobulinâ€like fold domain of lamin A/C reveals novel genotypeâ€“phenotype associations for laminopathies. Proteins: Structure, Function and Bioinformatics, 2014, 82, 904-915.	1.5	36
65	A discrete-to-continuum approach to the curvatures of membrane networks and parametric surfaces. Mechanics Research Communications, 2014, 56, 18-25.	1.0	15
66	Phosphorylation Modulates the Dynamics of the N-Terminal Tail in Cardiac RLC. Biophysical Journal, 2014, 106, 33a.	0.2	0
67	AP1S3 Mutations Are Associated with Pustular Psoriasis and Impaired Toll-like Receptor 3 Trafficking. American Journal of Human Genetics, 2014, 94, 790-797.	2.6	153
68	Gsatools: Analysis of Allosteric Communication and Functional Local Motions using a Structural Alphabet. Biophysical Journal, 2014, 106, 648a.	0.2	0
69	Design and application of implicit solvent models in biomolecular simulations. Current Opinion in Structural Biology, 2014, 25, 126-134.	2.6	124
70	Rate-independent dissipation and loading direction effects in compressed carbon nanotube arrays. Nanotechnology, 2013, 24, 255707.	1.3	22
71	Decrypting Prion Protein Conversion into a Î²-Rich Conformer by Molecular Dynamics. Journal of Chemical Theory and Computation, 2013, 9, 2455-2465.	2.3	32
72	Modeling microscale instabilities in compressed carbon nanotube bundles using multistable spring models. Composite Structures, 2013, 96, 745-750.	3.1	6

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73	Specialized Dynamical Properties of Promiscuous Residues Revealed by Simulated Conformational Ensembles. Journal of Chemical Theory and Computation, 2013, 9, 5127-5147.	2.3	39
74	GSATools: analysis of allosteric communication and functional local motions using a structural alphabet. Bioinformatics, 2013, 29, 2053-2055.	1.8	44
75	Multiscale Mass-Spring Models of Carbon Nanotube Arrays Accounting for Mullins-like Behavior and Permanent Deformation. Multiscale Modeling and Simulation, 2013, 11, 545-565.	0.6	4
76	Proteinâ€“protein interaction networks studies and importance of 3D structure knowledge. Expert Review of Proteomics, 2013, 10, 511-520.	1.3	17
77	Large-Scale Modelling of the Divergent Spectrin Repeats in Nesprins: Giant Modular Proteins. PLoS ONE, 2013, 8, e63633.	1.1	35
78	Structural Features of the Regulatory ACT Domain of Phenylalanine Hydroxylase. PLoS ONE, 2013, 8, e79482.	1.1	17
79	A Computational Exploration of the Interactions of the Green Tea Polyphenol (â€“)-Epigallocatechin 3-Gallate with Cardiac Muscle Troponin C. PLoS ONE, 2013, 8, e70556.	1.1	9
80	Structure and Stability Insights into Tumour Suppressor p53 Evolutionary Related Proteins. PLoS ONE, 2013, 8, e76014.	1.1	20
81	Emerging Role of the Ubiquitin-proteasome System as Drug Targets. Current Pharmaceutical Design, 2013, 19, 3175-3189.	0.9	16
82	Detection of Allosteric Signal Transmission by Information-Theoretic Analysis of Protein Dynamics. Biophysical Journal, 2012, 102, 225a.	0.2	0
83	Intrinsic Dynamics of the Regulatory Light Chain: Implications on Muscle Contraction. Biophysical Journal, 2012, 102, 451a.	0.2	0
84	Detection of allosteric signal transmission by informationâ€theoretic analysis of protein dynamics. FASEB Journal, 2012, 26, 868-881.	0.2	97
85	Ureaâ€“Water Solvation Forces on Prion Structures. Journal of Chemical Theory and Computation, 2012, 8, 3977-3984.	2.3	2
86	Proteinâ€“Water Interactions in MD Simulations: POPS/POPSCOMP Solvent Accessibility Analysis, Solvation Forces and Hydration Sites. Methods in Molecular Biology, 2012, 819, 375-392.	0.4	22
87	A Multiscale View of Protein-Protein Interactions. Biophysical Journal, 2012, 102, 184a-185a.	0.2	1
88	Continuum limits of bistable spring models of carbon nanotube arrays accounting for material damage. Mechanics Research Communications, 2012, 45, 58-63.	1.0	31
89	B-RAF Mutant Alleles Associated with Langerhans Cell Histiocytosis, a Granulomatous Pediatric Disease. PLoS ONE, 2012, 7, e33891.	1.1	132
90	Implicit Solvation Parameters Derived from Explicit Water Forces in Large-Scale Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 2391-2403.	2.3	18

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91	Abstract P2-10-29: Time dependent breast cancer metastasis prediction using novel biological imaging, clinico-pathological and genomic data combined with Bayesian modeling to reduce over-fitting and improve on inter-cohort reproducibility.. , 2012, , .		0
92	A Refined, Efficient Mean Solvation Force Model that Includes the Interior Volume Contribution. Journal of Physical Chemistry B, 2011, 115, 4547-4557.	1.2	14
93	When a module is not a domain: the case of the REJ module and the redefinition of the architecture of polycystin-1. Biochemical Journal, 2011, 435, 651-660.	1.7	14
94	A CASEâ€BYâ€CASE EVOLUTIONARY ANALYSIS OF FOUR IMPRINTED RETROGENES. Evolution; International Journal of Organic Evolution, 2011, 65, 1413-1427.	1.1	26
95	How FÃ¶rster Resonance Energy Transfer Imaging Improves the Understanding of Protein Interaction Networks in Cancer Biology. ChemPhysChem, 2011, 12, 442-461.	1.0	46
96	Modeling and in situ identification of material parameters for layered structures based on carbon nanotube arrays. Composite Structures, 2011, 93, 3013-3018.	3.1	50
97	Multiscale mass-spring models of carbon nanotube foams. Journal of the Mechanics and Physics of Solids, 2011, 59, 89-102.	2.3	68
98	A Targeted siRNA Screen Identifies Regulators of Cdc42 Activity at the Natural Killer Cell Immunological Synapse. Science Signaling, 2011, 4, ra81.	1.6	46
99	Mutants of the tumour suppressor p53 L1 loop as second-site suppressors for restoring DNA binding to oncogenic p53 mutations: structural and biochemical insights. Biochemical Journal, 2010, 427, 225-236.	1.7	29
100	Mutation of the RAD51C gene in a Fanconi anemiaâ€“like disorder. Nature Genetics, 2010, 42, 406-409.	9.4	360
101	Rationalisation of the Differences between APOBEC3G Structures from Crystallography and NMR Studies by Molecular Dynamics Simulations. PLoS ONE, 2010, 5, e11515.	1.1	17
102	The oligomerization properties of prion protein are restricted to the H2H3 domain. FASEB Journal, 2010, 24, 3222-3231.	0.2	74
103	Interface Dynamics In Hub Proteins. Biophysical Journal, 2010, 98, 239a.	0.2	0
104	In Silico Phosphorylation of the Autoinhibited Form of p47phox: Insights into the Mechanism of Activation. Biophysical Journal, 2010, 99, 3716-3725.	0.2	15
105	Protein Networks Reveal Detection Bias and Species Consistency When Analysed by Information-Theoretic Methods. PLoS ONE, 2010, 5, e12083.	1.1	20
106	Tailored graph ensembles as proxies or null models for real networks I: tools for quantifying structure. Journal of Physics A: Mathematical and Theoretical, 2009, 42, 485001.	0.7	38
107	RNA-Dependent Oligomerization of APOBEC3G Is Required for Restriction of HIV-1. PLoS Pathogens, 2009, 5, e1000330.	2.1	155
108	Josephin domain of ataxinâ€3 contains two distinct ubiquitinâ€binding sites. Biopolymers, 2009, 91, 1203-1214.	1.2	77

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109	Molecular determinants of peculiar properties of a Pleurotus ostreatus laccase: Analysis by site-directed mutagenesis. Enzyme and Microbial Technology, 2009, 45, 507-513.	1.6	42
110	Development of new laccases by directed evolution: Functional and computational analyses. Proteins: Structure, Function and Bioinformatics, 2008, 72, 25-34.	1.5	85
111	The p73 DNA Binding Domain Displays Enhanced Stability Relative to Its Homologue, the Tumor Suppressor p53, and Exhibits Cooperative DNA Binding. Biochemistry, 2008, 47, 3235-3244.	1.2	24
112	Stability and Cations Coordination of DNA and RNA 14-Mer G-Quadruplexes: A Multiscale Computational Approach. Journal of Physical Chemistry B, 2008, 112, 12115-12123.	1.2	34
113	Conformation and Dynamics of a Rhodamine Probe Attached at Two Sites on a Protein: Implications for Molecular Structure Determination in situ. Journal of the American Chemical Society, 2008, 130, 17120-17128.	6.6	13
114	Multi-Scale Simulations Provide Supporting Evidence for the Hypothesis of Intramolecular Protein Translocation in GroEL/GroES Complexes. PLoS Computational Biology, 2008, 4, e1000006.	1.5	8
115	Molecular interactions of ASPP1 and ASPP2 with the p53 protein family and the apoptotic promoters PUMA and Bax. Nucleic Acids Research, 2008, 36, 5139-5151.	6.5	49
116	A solvable model of the genesis of amino-acid sequences via coupled dynamics of folding and slow-genetic variation. Journal of Physics A: Mathematical and Theoretical, 2008, 41, 285004.	0.7	8
117	MinSet: a general approach to derive maximally representative database subsets by using fragment dictionaries and its application to the SCOP database. Bioinformatics, 2007, 23, 515-516.	1.8	16
118	Structural insight into theh TERTintron 6 sequence d(GGGGTGAAAGGGG) from¹H-NMR study. Nucleosides, Nucleotides and Nucleic Acids, 2007, 26, 1133-1137.	0.4	5
119	Toward the Understanding of MNEI Sweetness from Hydration Map Surfaces. Biophysical Journal, 2006, 90, 3052-3061.	0.2	42
120	Water molecules as structural determinants among prions of low sequence identity. FEBS Letters, 2006, 580, 2488-2494.	1.3	23
121	Dynamic domain threading. Proteins: Structure, Function and Bioinformatics, 2006, 64, 601-614.	1.5	9
122	Interactions of the C2 domain of human factor V with a model membrane. Proteins: Structure, Function and Bioinformatics, 2006, 64, 363-375.	1.5	12
123	Interaction of malaria parasite-inhibitory antibodies with the merozoite surface protein MSP119 by computational docking. Proteins: Structure, Function and Bioinformatics, 2006, 66, 513-527.	1.5	9
124	Calcium regulates scallop muscle by changing myosin flexibility. European Biophysics Journal, 2006, 35, 302-312.	1.2	7
125	Molecular simulations in structure prediction. , 2005, , .		0
126	Prion and water: Tight and dynamical hydration sites have a key role in structural stability. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 7535-7540.	3.3	145

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127	POPSCOMP: an automated interaction analysis of biomolecular complexes. Nucleic Acids Research, 2005, 33, W342-W346.	6.5	50
128	Plasticity of Influenza Haemagglutinin Fusion Peptides and Their Interaction with Lipid Bilayers. Biophysical Journal, 2005, 88, 25-36.	0.2	78
129	Reorganization in apo- and holo-Î²-lactoglobulin upon protonation of Glu89: Molecular dynamics and pKa calculations. Proteins: Structure, Function and Bioinformatics, 2004, 54, 744-758.	1.5	50
130	Mode of binding of camptothecins to double helix oligonucleotidesElectronic supplementary information (ESI) available: Chemical shift values, inter-proton distances obtained from MD simulations of CAP model for the complex d(CGTATACG)2/Cpt 6 and molecular dynamics figures. See http://www.rsc.org/suppdata/ob/b3/b312780j/Dedicated to Professors Luciano Caglioti and Domenico Misiti on occasion of their 70th birthdays.. Organic and Biomolecular Chemistry, 2004, 2, 505.	1.5	18
131	Quantum Mechanics Calculations on Rhodamine Dyes Require Inclusion of Solvent Water for Accurate Representation of the Structure. Journal of Physical Chemistry A, 2004, 108, 7744-7751.	1.1	27
132	Thermal unfolding simulations of apo-calmodulin using leap-dynamics. Proteins: Structure, Function and Bioinformatics, 2003, 50, 648-656.	1.5	18
133	Effects of pathological mutations on the stability of a conserved amino acid triad in retinoschisin. FEBS Letters, 2003, 544, 21-26.	1.3	31
134	Hydrogen-Bonding Propensities of Sphingomyelin in Solution and in a Bilayer Assembly: A Molecular Dynamics Study. Biophysical Journal, 2003, 84, 1507-1517.	0.2	121
135	POPS: a fast algorithm for solvent accessible surface areas at atomic and residue level. Nucleic Acids Research, 2003, 31, 3364-3366.	6.5	212
136	Parameter optimized surfaces (POPS): analysis of key interactions and conformational changes in the ribosome. Nucleic Acids Research, 2002, 30, 2950-2960.	6.5	94
137	Modularity and homology: modelling of the titin type I modules and their interfaces. Journal of Molecular Biology, 2001, 311, 283-296.	2.0	29
138	Leap-dynamics: efficient sampling of conformational space of proteins and peptides in solution. FEBS Letters, 2000, 470, 257-262.	1.3	18
139	An immunoglobulin-like fold in a major plant allergen: the solution structure of Phl p 2 from timothy grass pollen. Structure, 1999, 7, 943-952.	1.6	46
140	Novel RNA-binding motif: The KH module. , 1999, 51, 153-164.		60
141	Exploring protein interiors: The role of a buried histidine in the KH module fold. , 1999, 34, 484-496.		13
142	Neurologically active plant compounds and peptide hormones: a chirality connection. FEBS Letters, 1999, 448, 217-220.	1.3	3
143	Modularity and homology: modelling of the type II module family from titin. Journal of Molecular Biology, 1999, 290, 581-593.	2.0	30
144	Exploring protein interiors: The role of a buried histidine in the KH module fold. , 1999, 34, 484.		1

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145	A conformational study in solution of pro-somatostatin fragments by NMR and computational methods. , 1998, 4, 305-318.		2
146	A Molecular Dynamics Study of the First Five Generations of Poly(Propylene Imine) Dendrimers Modified with N-tBoc-L-Phenylalanine. Chemistry - A European Journal, 1998, 4, 927-934.	1.7	63
147	Mapping the active site of factor Xa by selective inhibitors: An NMR and MD study. , 1998, 30, 264-274.		11
148	The solution structure of the first KH domain of FMR1, the protein responsible for the fragile X syndrome. Nature Structural Biology, 1997, 4, 712-716.	9.7	80
149	Design and Solution Structure of a Partially Rigid Opioid Antagonist Lacking the Basic Center - Models of Antagonism. FEBS Journal, 1997, 247, 66-73.	0.2	24
150	Title is missing!. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 1997, 28, 63-78.	1.6	6
151	Calix[4]Arene Podands and Barrelands Incorporating 2,2â€³â€²Bipyridine Moieties and Their Lanthanide Complexes: Luminescence Properties. Chemistry - A European Journal, 1997, 3, 1815-1822.	1.7	52
152	MOLECULAR DYNAMICS STUDY OF THE COMPLEXATION OF LUMINESCENT CATIONS BY ENCAPSULATING LIGANDS WITH BIPYRIDINE UNITS. Journal of Physical Organic Chemistry, 1997, 10, 292-304.	0.9	13
153	An Efficient Mean Solvation Force Model for Use in Molecular Dynamics Simulations of Proteins in Aqueous Solution. Journal of Molecular Biology, 1996, 256, 939-948.	2.0	118
154	Conformational analysis of dolastatin 10: An nmr and theoretical approach. Biopolymers, 1995, 36, 525-538.	1.2	10
155	Conformational transitions of a dipeptide in water: Effects of imposed pathways using umbrella sampling techniques. Biopolymers, 1994, 34, 347-355.	1.2	18
156	First observation of a helical peptide containing chiral Î±-monosubstituted residues without a preferred screw sense. Journal of the Chemical Society Perkin Transactions II, 1992, , 971-977.	0.9	6
157	Preferred conformation of peptides from C?,?-symmetrically disubstituted glycines: Aromatic residues. Biopolymers, 1991, 31, 637-641.	1.2	50
158	Restrained and unrestrained molecular dynamics simulations in the NVT ensemble of alamethicin. Biopolymers, 1990, 30, 1083-1099.	1.2	52
159	A microscopic approach to the structure and thermodynamic properties of peptides and proteins. Thermochimica Acta, 1990, 162, 141-154.	1.2	4
160	Structural versatility of peptides from CÎ±,Î±-disubstituted glycines. Preferred conformation of the CÎ±,Î±-dibenzylglycine residue. Journal of the Chemical Society Perkin Transactions II, 1990, , 1481-1487.	0.9	16
161	Sensitivity of peptide conformation to methods and geometrical parameters. A comparative ab initio and molecular mechanics study of oligomers of .alpha.-aminoisobutyric acid. Macromolecules, 1990, 23, 2038-2044.	2.2	26
162	Structural versatility of peptides containing CÎ±,Î±-dialkylated glycines: conformational energy computations, i.r. absorption and 1H n.m.r. analysis of 1-aminocyclopropane-1-carboxylic acid homopeptides. International Journal of Biological Macromolecules, 1989, 11, 345-352.	3.6	32

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163	Structural versatility of peptides containing CÎ±,Î±-dialkylated glycines. An X-ray diffraction study of six 1-aminocyclopropane-1-carboxylic acid rich peptides. International Journal of Biological Macromolecules, 1989, 11, 353-360.	3.6	53
164	Conformational behavior of ?,?-dialkylated peptides: Ab initio and empirical results for cyclopropylglycine. Biopolymers, 1988, 27, 1673-1685.	1.2	42
165	Structural versatility of peptides from CÎ±,Î±-dialkylated glycines: a conformational energy calculation and X-ray diffraction study of homopeptides from 1-aminocyclopentane-1-carboxylic acid. International Journal of Biological Macromolecules, 1988, 10, 292-299.	3.6	45
166	Conformational preferences and selfâ€association modes of two diastereomeric statine derivatives. International Journal of Peptide and Protein Research, 1987, 30, 583-595.	0.1	5
167	Mechanical and Experimental Study on the use of Sustainable Materials for Additive Manufacturing. IOP Conference Series: Materials Science and Engineering, 0, 473, 012010.	0.3	2
168	Mathematical Modeling of Surface Roughness in the Forming of Innovative Materials. IOP Conference Series: Materials Science and Engineering, 0, 473, 012009.	0.3	0