Andrew J Doig

List of Publications by Year
in descending order

102 papers	9,886 citations	66343 42 h-index	37204 96 g-index
110 all docs	110 docs citations	110 times ranked	12801 citing authors

#	Article	IF	Citations
1	Drug repurposing: progress, challenges and recommendations. Nature Reviews Drug Discovery, 2019, 18, 41-58.	46.4	2,689
2	Amyloid Î² Protein and Alzheimerâ€™s Disease: When Computer Simulations Complement Experimental Studies. Chemical Reviews, 2015, 115, 3518-3563.	47.7	530
3	Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimerâ€™s Disease, Parkinsonâ€™s Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. Chemical Reviews, 2021, 121, 2545-2647.	47.7	406
4	Distinguishing Enzyme Structures from Non-enzymes Without Alignments. Journal of Molecular Biology, 2003, 330, 771-783.	4.2	333
5	Nâ€and Câ€capping preferences for all 20 amino acids in Î±â€helical peptides. Protein Science, 1995, 4, 1325-1336.	6.6	328
6	Sideâ€chain conformational entropy in protein folding. Protein Science, 1995, 4, 2247-2251.	7.6	290
7	Properties and identification of human protein drug targets. Bioinformatics, 2009, 25, 451-457.	4.1	276
8	Inhibition of protein aggregation and amyloid formation by small molecules. Current Opinion in Structural Biology, 2015, 30, 50-56.	5.7	259
9	Is polyproline II helix the killer conformation? a raman optical activity study of the amyloidogenic prefibrillar intermediate of human lysozyme 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 2000, 301, 553-563.	4.2	214
10	Helix capping propensities in peptides parallel those in proteins. Proceedings of the National Academy of Sciences of the United States of America, 1993, 90, 11332-11336.	7.1	212
11	Toward the semiquantitative estimation of binding constants. Guides for peptide-peptide binding in aqueous solution. Journal of the American Chemical Society, 1991, 113, 7020-7030.	13.7	205
12	Inhibition of Toxicity in the Î²-Amyloid Peptide Fragment Î²-(25â€“35) Using N-Methylated Derivatives. Journal of Biological Chemistry, 2000, 275, 25109-25115.	3.4	203
13	Why Is Research on Amyloid-Î² Failing to Give New Drugs for Alzheimerâ€™s Disease?. ACS Chemical Neuroscience, 2017, 8, 1435-1437.	3.5	201
14	N-Methylated Peptide Inhibitors of Î²-Amyloid Aggregation and Toxicity. Optimization of the Inhibitor Structureâ€. Biochemistry, 2006, 45, 9906-9918.	2.5	181
15	Determination of Free Energies of N-Capping in .alpha.-Helixes by Modification of the Lifson-Roig Helix-Coil Theory To Include N- and C-Capping. Biochemistry, 1994, 33, 3396-3403.	2.5	180
16	Is the hydrophobic effect stabilizing or destabilizing in proteins?. Journal of Molecular Biology, 1991, 217, 389-398.	4.2	171
17	Predicting Enzyme Class From Protein Structure Without Alignments. Journal of Molecular Biology, 2005, 345, 187-199.	4.2	145
18	Effect of Phosphorylation on Î±-Helix Stability as a Function of Positionâ€. Biochemistry, 2002, 41, 1897-1905.	2.5	126

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19	Design strategies for anti-amyloid agents. Current Opinion in Structural Biology, 2003, 13, 526-532.	5.7	126
20	The Â-helix folds on the millisecond time scale. Proceedings of the National Academy of Sciences of the United States of America, 1999, 96, 7232-7237.	7.1	115
21	Structures of Nâ€termini of helices in proteins. Protein Science, 1997, 6, 147-155.	7.6	104
22	Recent advances in helixâ€“coil theory. Biophysical Chemistry, 2002, 101-102, 281-293.	2.8	97
23	Properties of Protein Drug Target Classes. PLoS ONE, 2015, 10, e0117955.	2.5	97
24	Binding energy of an amide-amide hydrogen bond in aqueous and nonpolar solvents. Journal of the American Chemical Society, 1992, 114, 338-343.	13.7	96
25	Addition of side chain interactions to modified Lifsonâ€Roig helixâ€coil theory: Application to energetics of Phenylalanineâ€Methionine interactions. Protein Science, 1995, 4, 2383-2391.	7.6	96
26	Side-chain structures in the first turn of the Î±-helix 1 1Edited by J. M. Thornton. Journal of Molecular Biology, 1999, 287, 127-143.	4.2	93
27	Design of an N-Methylated Peptide Inhibitor of Î±-Synuclein Aggregation Guided by Solid-State NMR. Journal of the American Chemical Society, 2008, 130, 7873-7881.	13.7	86
28	Stabilizing Interactions between Aromatic and Basic Side Chains in Î±-Helical Peptides and Proteins. Tyrosine Effects on Helix Circular Dichroism. Journal of the American Chemical Society, 2002, 124, 12706-12714.	13.7	82
29	Models for the 3₁₀â€helix/coil, Ï€â€helix/coil, and Î±â€helix/3₁₀â€helix/coil transitions in isolated peptides. Protein Science, 1996, 5, 1687-1696.	7.6	79
30	Effect of the N1 residue on the stability of the alpha-helix for all 20 amino acids. Protein Science, 2001, 10, 463-470.	7.6	76
31	Amyloidogenic sequences in native protein structures. Protein Science, 2010, 19, 327-348.	7.6	68
32	Inhibitors of protein aggregation and toxicity. Biochemical Society Transactions, 2009, 37, 692-696.	3.4	63
33	A Phosphoserineâ^'Lysine Salt Bridge within an Î±-Helical Peptide, the Strongest Î±-Helix Side-Chain Interaction Measured to Dateâ€. Biochemistry, 2005, 44, 7553-7558.	2.5	61
34	The N-Methylated Peptide SEN304 Powerfully Inhibits Aβ(1â€“42) Toxicity by Perturbing Oligomer Formation. Biochemistry, 2012, 51, 8338-8352.	2.5	61
35	Hydrogen bonding interactions between glutamine and asparagine in Î±-helical peptides 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 1997, 272, 465-473.	4.2	60
36	Prediction of Protein Function in the Absence of Significant Sequence Similarity. Current Medicinal Chemistry, 2004, 11, 2135-2142.	2.4	57

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37	Hepatotoxic and nephrotoxic principles in Terminalia oblongata. Research in Veterinary Science, 1991, 50, 170-177.	1.9	54
38	Effect of the N2 residue on the stability of the Î±-helix for all 20 amino acids. Protein Science, 2008, 10, 1305-1311.	7.6	53
39	Prediction of Saccharomyces cerevisiae protein functional class from functional domain composition. Bioinformatics, 2004, 20, 1292-1300.	4.1	49
40	Periodicity in Î±-helix lengths and C-capping preferences 1 1Edited by J. M. Thornton. Journal of Molecular Biology, 1999, 293, 1211-1219.	4.2	48
41	Stabilizing nonpolar/polar side-chain interactions in the ?-helix. Proteins: Structure, Function and Bioinformatics, 2001, 45, 449-455.	2.6	47
42	A Study of the Regional Effects of Î±-Synuclein on the Organization and Stability of Phospholipid Bilayers. Biochemistry, 2006, 45, 5783-5792.	2.5	47
43	Accurate Determination of Protein Secondary Structure Content from Raman and Raman Optical Activity Spectra. Analytical Chemistry, 2010, 82, 6347-6349.	6.5	43
44	Isolation and structure elucidation of punicalagin, a toxic hydrolysable tannin, from Terminalia oblongata. Journal of the Chemical Society Perkin Transactions 1, 1990, , 2317.	0.9	42
45	The CXXC motif at the N terminus of an Î±-helical peptide. Protein Science, 2006, 15, 1945-1950.	7.6	40
46	Properties and identification of antibiotic drug targets. BMC Bioinformatics, 2010, 11, 195.	2.6	39
47	Local control of a disorderâ€“order transition in 4E-BP1 underpins regulation of translation via eIF4E. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 17627-17632.	7.1	38
48	Secondary Structure and Glycosylation of Mucus Glycoproteins by Raman Spectroscopies. Analytical Chemistry, 2016, 88, 11609-11615.	6.5	38
49	Viral Involvement in Alzheimerâ€™s Disease. ACS Chemical Neuroscience, 2021, 12, 1049-1060.	3.5	38
50	Determination of Protein Secondary Structure from Infrared Spectra Using Partial Least-Squares Regression. Biochemistry, 2016, 55, 3794-3802.	2.5	35
51	Length preferences and periodicity in Â-strands. Antiparallel edge Â-sheets are more likely to finish in non-hydrogen bonded rings. Protein Engineering, Design and Selection, 2003, 16, 957-961.	2.1	34
52	Why water-soluble, compact, globular proteins have similar specific enthalpies of unfolding at 110.degree.C. Biochemistry, 1992, 31, 9371-9375.	2.5	32
53	Free energies of amino acid side-chain rotamers in Î±-helices, Î²-sheets and Î±-helix N-caps 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 1997, 272, 456-464.	4.2	32
54	Molecular structure of the NQTrp inhibitor with the Alzheimer AÎ²1-28 monomer. European Journal of Medicinal Chemistry, 2015, 91, 43-50.	5.5	32

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55	Positive Feedback Loops in Alzheimerâ€™s Disease: The Alzheimerâ€™s Feedback Hypothesis. Journal of Alzheimer's Disease, 2018, 66, 25-36.	2.6	32
56	Anticooperativity in a Gluâ^'Lysâ^'Glu Salt Bridge Triplet in an Isolated Î±-Helical Peptideâ€. Biochemistry, 2005, 44, 10449-10456.	2.5	30
57	Raman Spectroscopy to Monitor Post-Translational Modifications and Degradation in Monoclonal Antibody Therapeutics. Analytical Chemistry, 2020, 92, 10381-10389.	6.5	29
58	Inhibition of toxicity and protofibril formation in the amyloid-Î² peptide Î²(25â€“35) using N-Methylated derivatives. Biochemical Society Transactions, 2002, 30, 537-542.	3.4	28
59	Effect of the N3 residue on the stability of the Â-helix. Protein Science, 2004, 13, 32-39.	7.6	28
60	Frozen, but no accident â€“ why the 20 standard amino acids were selected. FEBS Journal, 2017, 284, 1296-1305.	4.7	27
61	Molecular and chemical basis of prion-related diseases. Chemical Society Reviews, 1997, 26, 425.	38.1	25
62	Rotamer strain energy in protein helices - quantification of a major force opposing protein folding. Journal of Molecular Biology, 2001, 305, 961-968.	4.2	25
63	A three stranded Î²-sheet peptide in aqueous solution containing N-methyl amino acids to prevent aggregation. Chemical Communications, 1997, , 2153-2154.	4.1	24
64	The effects of Î±-synuclein on phospholipid vesicle integrity: a study using31P NMR and electron microscopy. Molecular Membrane Biology, 2008, 25, 518-527.	2.0	24
65	Combined Experimental and Simulation Studies Suggest a Revised Mode of Action of the Antiâ€Alzheimer Disease Drug NQâ€Trp. Chemistry - A European Journal, 2015, 21, 12657-12666.	3.3	20
66	Addition of sideâ€chain interactions to 3₁₀â€helix/coil and Î±â€helix/3₁₀â€helix/coil theory. Protein Science, 1998, 7, 2374-2383.	7.6	19
67	SitesIdentify: a protein functional site prediction tool. BMC Bioinformatics, 2009, 10, 379.	2.6	19
68	Identifying mouse developmental essential genes using machine learning. DMM Disease Models and Mechanisms, 2018, 11, .	2.4	18
69	A Statistical Mechanical Model for Î²-Sheet Formation. Journal of Physical Chemistry B, 2000, 104, 1826-1836.	2.6	17
70	Structure and Stability of the Î±-Helix: Lessons for Design. , 2006, 340, 3-26.		17
71	Sequence and Structural Features of Enzymes and their Active Sites by EC Class. Journal of Molecular Biology, 2009, 386, 1423-1436.	4.2	17
72	Determination of protein fold class from Raman or Raman optical activity spectra using random forests. Protein Science, 2011, 20, 1668-1674.	7.6	17

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73	Properties of genes essential for mouse development. PLoS ONE, 2017, 12, e0178273.	2.5	17
74	A critical assessment of the secondary structure Î±-helices and their termini in proteins. Protein Engineering, Design and Selection, 2002, 15, 545-554.	2.1	15
75	Determination of Î±â€helix N1 energies after addition of N1, N2, and N3 preferences to helix/coil theory. Protein Science, 2000, 9, 750-754.	7.6	15
76	Improving the Efficiency of the Genetic Code by Varying the Codon Lengthâ€"The Perfect Genetic Code. Journal of Theoretical Biology, 1997, 188, 355-360.	1.7	14
77	Improved prediction for N-termini of Î±-helices using empirical information. Proteins: Structure, Function and Bioinformatics, 2004, 57, 322-330.	2.6	14
78	Stability and Design of Î±-Helical Peptides. Progress in Molecular Biology and Translational Science, 2008, 83, 1-52.	1.7	14
79	Randomâ€Coil:Î±â€Helix Equilibria as a Reporter for the Lewis^Xâ€"Lewis^X Interaction. Angewandte Chemie - International Edition, 2011, 50, 11167-11171.	13.8	14
80	Thermodynamics of amino acid side-chain internal rotations. Biophysical Chemistry, 1996, 61, 131-141.	2.8	13
81	The aggregation and membrane-binding properties of an Î±-synuclein peptide fragment. Biochemical Society Transactions, 2004, 32, 1127-1129.	3.4	13
82	Pairwise Coupling in an Arg-Phe-Met Triplet Stabilizes Î±-Helical Peptide via Shared Rotamer Preferences. Journal of the American Chemical Society, 2005, 127, 5002-5003.	13.7	12
83	Peptide inhibitors of beta-amyloid aggregation. Current Opinion in Drug Discovery & Development, 2007, 10, 533-9.	1.9	12
84	Quantification of protein glycation using vibrational spectroscopy. Analyst, The, 2020, 145, 3686-3696.	3.5	11
85	Information-Theoretic Analysis of Protein Sequences Shows that Amino Acids Self-cluster. Journal of Theoretical Biology, 2002, 218, 409-418.	1.7	10
86	Maximising the Size of Non-Redundant Protein Datasets Using Graph Theory. PLoS ONE, 2013, 8, e55484.	2.5	10
87	Structure, stability and folding of the Î±-helix. Biochemical Society Symposia, 2001, 68, 95-110.	2.7	9
88	Studies of the aggregation of an amyloidogenic Î±-synuclein peptide fragment. Biochemical Society Transactions, 2005, 33, 1113.	3.4	8
89	The Essentiality Status of Mouse Duplicate Gene Pairs Correlates with Developmental Co-Expression Patterns. Scientific Reports, 2019, 9, 3224.	3.3	8
90	Information-Theoretic Analysis of Protein Sequences Shows that Amino Acids Self-cluster. Journal of Theoretical Biology, 2002, 218, 409-418.	1.7	7

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91	Deconvolution of conformational exchange from Raman spectra of aqueous RNA nucleosides. Communications Chemistry, 2020, 3, .	4.5	7
92	Amyloid-Î²/Drug Interactions from Computer Simulations and Cell-Based Assays. Journal of Alzheimer's Disease, 2018, 64, S659-S672.	2.6	5
93	A Simple Approach to Normalization for Spectroscopic Data Mining. Applied Spectroscopy, 2005, 59, 542-544.	2.2	4
94	Inhibitors of Amyloid Aggregation: Technologies for the Discovery of Novel Lead Compounds. Biotechnology and Genetic Engineering Reviews, 2004, 21, 197-214.	6.2	3
95	Thermodynamics of Side Chain Internal Rotations â€“ Effects on Protein Structure and Stability. , 1993, , 557-566.		3
96	Statistical Thermodynamics of the Collagen Triple-Helix/Coil Transition. Free Energies for Amino Acid Substitutions within the Triple-Helix. Journal of Physical Chemistry B, 2008, 112, 15029-15033.	2.6	2
97	Information-theoretic analysis of protein sequences shows that amino acids self-cluster. Journal of Theoretical Biology, 2002, 218, 409-18.	1.7	2
98	Effect of IAPP on the proteome of cultured Rin-5F cells. BMC Biochemistry, 2018, 19, 9.	4.4	1
99	Surface areas of unfolded proteins. Nature, 1990, 348, 397-397.	27.8	0
100	Fewer academics could be the answer to insufficient grants. Nature, 2008, 453, 978-978.	27.8	0
101	Using Machine Learning to Predict Protein Structure from Spectral Data. , 2010, , .		0
102	Inhibitor Design Against Cytotoxic Î²-Amyloid Species. Modecular Medicine and Medicinal, 2013, , 187-206.	0.4	0