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	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
2	Viral Involvement in Alzheimerâ€™s Disease. ACS Chemical Neuroscience, 2021, 12, 1049-1060.	3.5	38
3	Deconvolution of conformational exchange from Raman spectra of aqueous RNA nucleosides. Communications Chemistry, 2020, 3, .	4.5	7
4	Raman Spectroscopy to Monitor Post-Translational Modifications and Degradation in Monoclonal Antibody Therapeutics. Analytical Chemistry, 2020, 92, 10381-10389.	6.5	29
5	Quantification of protein glycation using vibrational spectroscopy. Analyst, The, 2020, 145, 3686-3696.	3.5	11
6	The Essentiality Status of Mouse Duplicate Gene Pairs Correlates with Developmental Co-Expression Patterns. Scientific Reports, 2019, 9, 3224.	3.3	8
7	Drug repurposing: progress, challenges and recommendations. Nature Reviews Drug Discovery, 2019, 18, 41-58.	46.4	2,689
8	Effect of IAPP on the proteome of cultured Rin-5F cells. BMC Biochemistry, 2018, 19, 9.	4.4	1
9	Identifying mouse developmental essential genes using machine learning. DMM Disease Models and Mechanisms, 2018, 11, .	2.4	18
10	Positive Feedback Loops in Alzheimerâ€™s Disease: The Alzheimerâ€™s Feedback Hypothesis. Journal of Alzheimer's Disease, 2018, 66, 25-36.	2.6	32
11	Amyloid-Î²/Drug Interactions from Computer Simulations and Cell-Based Assays. Journal of Alzheimer's Disease, 2018, 64, S659-S672.	2.6	5
12	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
13	Frozen, but no accident â€“ why the 20 standard amino acids were selected. FEBS Journal, 2017, 284, 1296-1305.	4.7	27
14	Properties of genes essential for mouse development. PLoS ONE, 2017, 12, e0178273.	2.5	17
15	Secondary Structure and Glycosylation of Mucus Glycoproteins by Raman Spectroscopies. Analytical Chemistry, 2016, 88, 11609-11615.	6.5	38
16	Determination of Protein Secondary Structure from Infrared Spectra Using Partial Least-Squares Regression. Biochemistry, 2016, 55, 3794-3802.	2.5	35
17	Properties of Protein Drug Target Classes. PLoS ONE, 2015, 10, e0117955.	2.5	97
18	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

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19	Inhibition of protein aggregation and amyloid formation by small molecules. Current Opinion in Structural Biology, 2015, 30, 50-56.	5.7	259
20	Amyloid Î² Protein and Alzheimerâ€™s Disease: When Computer Simulations Complement Experimental Studies. Chemical Reviews, 2015, 115, 3518-3563.	47.7	530
21	Molecular structure of the NQTrp inhibitor with the Alzheimer AÎ²1-28 monomer. European Journal of Medicinal Chemistry, 2015, 91, 43-50.	5.5	32
22	Inhibitor Design Against Cytotoxic Î²-Amyloid Species. Modecular Medicine and Medicinal, 2013, , 187-206.	0.4	0
23	Maximising the Size of Non-Redundant Protein Datasets Using Graph Theory. PLoS ONE, 2013, 8, e55484.	2.5	10
24	The N-Methylated Peptide SEN304 Powerfully Inhibits AÎ²(1â€“42) Toxicity by Perturbing Oligomer Formation. Biochemistry, 2012, 51, 8338-8352.	2.5	61
25	Determination of protein fold class from Raman or Raman optical activity spectra using random forests. Protein Science, 2011, 20, 1668-1674.	7.6	17
26	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
27	Properties and identification of antibiotic drug targets. BMC Bioinformatics, 2010, 11, 195.	2.6	39
28	Amyloidogenic sequences in native protein structures. Protein Science, 2010, 19, 327-348.	7.6	68
29	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
30	Using Machine Learning to Predict Protein Structure from Spectral Data. , 2010, , .		0
31	Accurate Determination of Protein Secondary Structure Content from Raman and Raman Optical Activity Spectra. Analytical Chemistry, 2010, 82, 6347-6349.	6.5	43
32	Properties and identification of human protein drug targets. Bioinformatics, 2009, 25, 451-457.	4.1	276
33	SitesIdentify: a protein functional site prediction tool. BMC Bioinformatics, 2009, 10, 379.	2.6	19
34	Sequence and Structural Features of Enzymes and their Active Sites by EC Class. Journal of Molecular Biology, 2009, 386, 1423-1436.	4.2	17
35	Inhibitors of protein aggregation and toxicity. Biochemical Society Transactions, 2009, 37, 692-696.	3.4	63
36	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

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37	Fewer academics could be the answer to insufficient grants. Nature, 2008, 453, 978-978.	27.8	0
38	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
39	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
40	Stability and Design of Î±-Helical Peptides. Progress in Molecular Biology and Translational Science, 2008, 83, 1-52.	1.7	14
41	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
42	Peptide inhibitors of beta-amyloid aggregation. Current Opinion in Drug Discovery & Development, 2007, 10, 533-9.	1.9	12
43	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
44	N-Methylated Peptide Inhibitors of Î²-Amyloid Aggregation and Toxicity. Optimization of the Inhibitor Structureâ€. Biochemistry, 2006, 45, 9906-9918.	2.5	181
45	The CXXC motif at the N terminus of an Î±-helical peptide. Protein Science, 2006, 15, 1945-1950.	7.6	40
46	Structure and Stability of the Î±-Helix: Lessons for Design. , 2006, 340, 3-26.		17
47	Studies of the aggregation of an amyloidogenic Î±-synuclein peptide fragment. Biochemical Society Transactions, 2005, 33, 1113.	3.4	8
48	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
49	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
50	A Simple Approach to Normalization for Spectroscopic Data Mining. Applied Spectroscopy, 2005, 59, 542-544.	2.2	4
51	Predicting Enzyme Class From Protein Structure Without Alignments. Journal of Molecular Biology, 2005, 345, 187-199.	4.2	145
52	Anticooperativity in a Gluâ^'Lysâ^'Glu Salt Bridge Triplet in an Isolated Î±-Helical Peptideâ€. Biochemistry, 2005, 44, 10449-10456.	2.5	30
53	Prediction of Saccharomyces cerevisiae protein functional class from functional domain composition. Bioinformatics, 2004, 20, 1292-1300.	4.1	49
54	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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55	Improved prediction for N-termini of Î±-helices using empirical information. Proteins: Structure, Function and Bioinformatics, 2004, 57, 322-330.	2.6	14
56	Inhibitors of Amyloid Aggregation: Technologies for the Discovery of Novel Lead Compounds. Biotechnology and Genetic Engineering Reviews, 2004, 21, 197-214.	6.2	3
57	Effect of the N3 residue on the stability of the Â-helix. Protein Science, 2004, 13, 32-39.	7.6	28
58	The aggregation and membrane-binding properties of an Î±-synuclein peptide fragment. Biochemical Society Transactions, 2004, 32, 1127-1129.	3.4	13
59	Design strategies for anti-amyloid agents. Current Opinion in Structural Biology, 2003, 13, 526-532.	5.7	126
60	Distinguishing Enzyme Structures from Non-enzymes Without Alignments. Journal of Molecular Biology, 2003, 330, 771-783.	4.2	333
61	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
62	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
63	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
64	Effect of Phosphorylation on Î±-Helix Stability as a Function of Positionâ€. Biochemistry, 2002, 41, 1897-1905.	2.5	126
65	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
66	Information-Theoretic Analysis of Protein Sequences Shows that Amino Acids Self-cluster. Journal of Theoretical Biology, 2002, 218, 409-418.	1.7	10
67	Information-Theoretic Analysis of Protein Sequences Shows that Amino Acids Self-cluster. Journal of Theoretical Biology, 2002, 218, 409-418.	1.7	7
68	Recent advances in helixâ€“coil theory. Biophysical Chemistry, 2002, 101-102, 281-293.	2.8	97
69	Information-theoretic analysis of protein sequences shows that amino acids self-cluster. Journal of Theoretical Biology, 2002, 218, 409-18.	1.7	2
70	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
71	Stabilizing nonpolar/polar side-chain interactions in the ?-helix. Proteins: Structure, Function and Bioinformatics, 2001, 45, 449-455.	2.6	47
72	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

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73	Structure, stability and folding of the Î±-helix. Biochemical Society Symposia, 2001, 68, 95-110.	2.7	9
74	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
75	A Statistical Mechanical Model for Î²-Sheet Formation. Journal of Physical Chemistry B, 2000, 104, 1826-1836.	2.6	17
76	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
77	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
78	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
79	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
80	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
81	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
82	Molecular and chemical basis of prion-related diseases. Chemical Society Reviews, 1997, 26, 425.	38.1	25
83	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
84	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
85	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
86	Structures of Nâ€termini of helices in proteins. Protein Science, 1997, 6, 147-155.	7.6	104
87	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
88	Thermodynamics of amino acid side-chain internal rotations. Biophysical Chemistry, 1996, 61, 131-141.	2.8	13
89	Models for the 3₁₀â€helix/coil, Ïâ€helix/coil, and Î±â€helix/3₁₀â€helix/coil transitions in isolated peptides. Protein Science, 1996, 5, 1687-1696.	7.6	79
90	Nâ€and Câ€capping preferences for all 20 amino acids in Î±â€helical peptides. Protein Science, 1995, 4, 1325-1336.	7.6	328

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91	Sideâ€chain conformational entropy in protein folding. Protein Science, 1995, 4, 2247-2251.	7.6	290
92	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
93	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
94	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
95	Thermodynamics of Side Chain Internal Rotations â€“ Effects on Protein Structure and Stability. , 1993, , 557-566.		3
96	Why water-soluble, compact, globular proteins have similar specific enthalpies of unfolding at 110.degree.C. Biochemistry, 1992, 31, 9371-9375.	2.5	32
97	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
98	Hepatotoxic and nephrotoxic principles in Terminalia oblongata. Research in Veterinary Science, 1991, 50, 170-177.	1.9	54
99	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
100	Is the hydrophobic effect stabilizing or destabilizing in proteins?. Journal of Molecular Biology, 1991, 217, 389-398.	4.2	171
101	Surface areas of unfolded proteins. Nature, 1990, 348, 397-397.	27.8	0
102	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