

Paul A Dalby

List of Publications by Year in descending order

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Version: 2024-02-01

96
papers

3,133
citations

136950

32
h-index

182427

51
g-index

105
all docs

105
docs citations

105
times ranked

2629
citing authors

#	ARTICLE	IF	CITATIONS
1	Hot spots-making directed evolution easier. <i>Biotechnology Advances</i> , 2022, 56, 107926.	11.7	35
2	Protein Engineering and HDX Identify Structural Regions of G-CSF Critical to Its Stability and Aggregation. <i>Molecular Pharmaceutics</i> , 2022, 19, 616-629.	4.6	4
3	Fine-tuning the activity and stability of an evolved enzyme active site through noncanonical amino acids. <i>FEBS Journal</i> , 2021, 288, 1935-1955.	4.7	7
4	Comparison of the pH- and thermally-induced fluctuations of a therapeutic antibody Fab fragment by molecular dynamics simulation. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 2726-2741.	4.1	7
5	Machine learning reveals hidden stability code in protein native fluorescence. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 2750-2760.	4.1	4
6	Proof-of-concept analytical instrument for label-free optical deconvolution of protein species in a mixture. <i>Journal of Chromatography A</i> , 2021, 1641, 461968.	3.7	2
7	Solution structure of deglycosylated human IgG1 shows the role of CH2 glycans in its conformation. <i>Biophysical Journal</i> , 2021, 120, 1814-1834.	0.5	3
8	Reference Protocol to Assess Analytical Performance of Higher Order Structural Analysis Measurements: Results from an Interlaboratory Comparison. <i>Analytical Chemistry</i> , 2021, 93, 9041-9048.	6.5	4
9	Engineering improved ethylene production: Leveraging systems biology and adaptive laboratory evolution. <i>Metabolic Engineering</i> , 2021, 67, 308-320.	7.0	8
10	Biophysical characterization of the inactivation of <i>E. coli</i> transketolase by aqueous co-solvents. <i>Scientific Reports</i> , 2021, 11, 23584.	3.3	1
11	Engineering transketolase to accept both unnatural donor and acceptor substrates and produce \pm -hydroxyketones. <i>FEBS Journal</i> , 2020, 287, 1758-1776.	4.7	16
12	Advancements in the co-formulation of biologic therapeutics. <i>Journal of Controlled Release</i> , 2020, 327, 397-405.	9.9	21
13	HDX and In Silico Docking Reveal that Excipients Stabilize G-CSF via a Combination of Preferential Exclusion and Specific Hotspot Interactions. <i>Molecular Pharmaceutics</i> , 2020, 17, 4637-4651.	4.6	7
14	Stability enhancement in a mAb and Fab coformulation. <i>Scientific Reports</i> , 2020, 10, 21129.	3.3	7
15	A beginner's guide to molecular dynamics simulations and the identification of cross-correlation networks for enzyme engineering. <i>Methods in Enzymology</i> , 2020, 643, 15-49.	1.0	19
16	The Two-Species Model of transketolase explains donor substrate-binding, inhibition and heat-activation. <i>Scientific Reports</i> , 2020, 10, 4148.	3.3	7
17	Functional and computational identification of a rescue mutation near the active site of an mRNA methyltransferase. <i>Scientific Reports</i> , 2020, 10, 21841.	3.3	1
18	Virus lasers for biological detection. <i>Nature Communications</i> , 2019, 10, 3594.	12.8	27

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19	Novel insights into transketolase activation by cofactor binding identifies two native species subpopulations. <i>Scientific Reports</i> , 2019, 9, 16116.	3.3	9
20	An Expanded Conformation of an Antibody Fab Region by X-Ray Scattering, Molecular Dynamics, and smFRET Identifies an Aggregation Mechanism. <i>Journal of Molecular Biology</i> , 2019, 431, 1409-1425.	4.2	19
21	Selective Stabilization and Destabilization of Protein Domains in Tissue-Type Plasminogen Activator Using Formulation Excipients. <i>Molecular Pharmaceutics</i> , 2019, 16, 744-755.	4.6	6
22	ΔT_m -Values and Unfolded Fraction Can Predict Aggregation Rates for Granulocyte Colony Stimulating Factor Variant Formulations but Not under Predominantly Native Conditions. <i>Molecular Pharmaceutics</i> , 2018, 15, 256-267.	4.6	27
23	Coupled molecular dynamics mediate long- and short-range epistasis between mutations that affect stability and aggregation kinetics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E11043-E11052.	7.1	59
24	Exploiting correlated molecular-dynamics networks to counteract enzyme activity–stability trade-off. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E12192-E12200.	7.1	65
25	An Evaluation of the Potential of NMR Spectroscopy and Computational Modelling Methods to Inform Biopharmaceutical Formulations. <i>Pharmaceutics</i> , 2018, 10, 165.	4.5	22
26	Computational Design To Reduce Conformational Flexibility and Aggregation Rates of an Antibody Fab Fragment. <i>Molecular Pharmaceutics</i> , 2018, 15, 3079-3092.	4.6	25
27	Two strategies to engineer flexible loops for improved enzyme thermostability. <i>Scientific Reports</i> , 2017, 7, 41212.	3.3	121
28	An integrated biorefinery concept for conversion of sugar beet pulp into value-added chemicals and pharmaceutical intermediates. <i>Faraday Discussions</i> , 2017, 202, 415-431.	3.2	41
29	Identification of Protein–Excipient Interaction Hotspots Using Computational Approaches. <i>International Journal of Molecular Sciences</i> , 2016, 17, 853.	4.1	18
30	Impact of cofactor-binding loop mutations on thermotolerance and activity of <i>E. coli</i> transketolase. <i>Enzyme and Microbial Technology</i> , 2016, 89, 85-91.	3.2	18
31	Structural Analysis of an Evolved Transketolase Reveals Divergent Binding Modes. <i>Scientific Reports</i> , 2016, 6, 35716.	3.3	16
32	Transketolase catalysed upgrading of <i>D</i> -arabinose: the one-step stereoselective synthesis of <i>D</i> -gluco-heptulose. <i>Green Chemistry</i> , 2016, 18, 3158-3165.	9.0	35
33	Mapping the Aggregation Kinetics of a Therapeutic Antibody Fragment. <i>Molecular Pharmaceutics</i> , 2016, 13, 307-319.	4.6	51
34	Second generation engineering of transketolase for polar aromatic aldehyde substrates. <i>Enzyme and Microbial Technology</i> , 2015, 71, 45-52.	3.2	28
35	The Solution Structures of Two Human IgG1 Antibodies Show Conformational Stability and Accommodate Their C1q and FcγR Ligands. <i>Journal of Biological Chemistry</i> , 2015, 290, 8420-8438.	3.4	37
36	Single active-site mutants are sufficient to enhance serine:pyruvate transaminase activity in an <i>in vitro</i> transaminase. <i>FEBS Journal</i> , 2015, 282, 2512-2526.	4.7	23

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37	Modelling and optimisation of the one-pot, multi-enzymatic synthesis of chiral amino-alcohols based on microscale kinetic parameter determination. <i>Chemical Engineering Science</i> , 2015, 122, 360-372.	3.8	37
38	Evaluation of CV2025 α -transaminase for the bioconversion of lignin breakdown products into value-added chemicals: synthesis of vanillylamine from vanillin. <i>Biocatalysis and Biotransformation</i> , 2014, 32, 302-313.	2.0	16
39	The Fab Conformations in the Solution Structure of Human Immunoglobulin G4 (IgG4) Restrict Access to Its Fc Region. <i>Journal of Biological Chemistry</i> , 2014, 289, 20740-20756.	3.4	34
40	Identification and use of an alkane transporter plug-in for applications in biocatalysis and whole-cell biosensing of alkanes. <i>Scientific Reports</i> , 2014, 4, 5844.	3.3	54
41	The Solution Structure of Rabbit IgG Accounts for Its Interactions with the Fc Receptor and Complement C1q and Its Conformational Stability. <i>Journal of Molecular Biology</i> , 2013, 425, 506-523.	4.2	28
42	Optically Induced Thermal Gradients for Protein Characterization in Nanolitre-scale Samples in Microfluidic Devices. <i>Scientific Reports</i> , 2013, 3, 2130.	3.3	10
43	Rational substrate and enzyme engineering of transketolase for aromatics. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 9021.	2.8	35
44	An MILP formulation for the synthesis of protein purification processes. <i>Chemical Engineering Research and Design</i> , 2012, 90, 1262-1270.	5.6	10
45	Directed evolution to re-adapt a co-evolved network within an enzyme. <i>Journal of Biotechnology</i> , 2012, 157, 237-245.	3.8	27
46	A novel efficient optimisation system for purification process synthesis. <i>Biochemical Engineering Journal</i> , 2012, 67, 186-193.	3.6	13
47	Yeast-surface expressed BVDV E2 protein induces a Th1/Th2 response in naïve T cells. <i>Developmental and Comparative Immunology</i> , 2012, 37, 107-114.	2.3	20
48	A generic hierarchical screening method for the analysis of microscale refolds using an automated robotic platform. <i>Biotechnology Progress</i> , 2012, 28, 435-444.	2.6	13
49	Freeze drying formulation using microscale and design of experiment approaches: a case study using granulocyte colony-stimulating factor. <i>Biotechnology Letters</i> , 2012, 34, 641-648.	2.2	14
50	Directed evolution of a thermostable l-aminoacylase biocatalyst. <i>Journal of Biotechnology</i> , 2011, 155, 396-405.	3.8	10
51	Strategy and success for the directed evolution of enzymes. <i>Current Opinion in Structural Biology</i> , 2011, 21, 473-480.	5.7	161
52	Engineering and Design. <i>Current Opinion in Structural Biology</i> , 2011, 21, 450-451.	5.7	18
53	Optimal synthesis of chromatographic trains for downstream protein processing. <i>Biotechnology Progress</i> , 2011, 27, 1653-1660.	2.6	18
54	Thermodynamic parameters for salt-induced reversible protein precipitation from automated microscale experiments. <i>Biotechnology and Bioengineering</i> , 2011, 108, 322-332.	3.3	9

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55	A high-throughput fluorescence chemical denaturation assay as a general screen for protein-ligand binding. <i>Analytical Biochemistry</i> , 2011, 411, 155-157.	2.4	29
56	Structural stability of <i>E. coli</i> transketolase to temperature and pH denaturation. <i>Journal of Biotechnology</i> , 2011, 155, 209-216.	3.8	17
57	A toolbox approach for the rapid evaluation of multi-step enzymatic syntheses comprising a mix and match <i>E. coli</i> expression system with microscale experimentation. <i>Biocatalysis and Biotransformation</i> , 2011, 29, 192-203.	2.0	18
58	Protein denaturation and protein:drugs interactions from intrinsic protein fluorescence measurements at the nanolitre scale. <i>Protein Science</i> , 2010, 19, 1544-1554.	7.6	22
59	Masking of the Fc region in human IgG4 by constrained X-ray scattering modelling: implications for antibody function and therapy. <i>Biochemical Journal</i> , 2010, 432, 101-114.	3.7	40
60	A Multidisciplinary Approach Toward the Rapid and Preparative-Scale Biocatalytic Synthesis of Chiral Amino Alcohols: A Concise Transketolase-Transaminase-Mediated Synthesis of (2 <i>S</i> ,3 <i>S</i>)-2-Aminopentane-1,3-diol. <i>Organic Process Research and Development</i> , 2010, 14, 99-107.	2.7	80
61	β -Dihydroxyketone formation using aromatic and heteroaromatic aldehydes with evolved transketolase enzymes. <i>Chemical Communications</i> , 2010, 46, 7608.	4.1	45
62	Non-hydroxylated aldehydes with evolved transketolase enzymes. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 1301.	2.8	68
63	An MINLP Formulation for the Synthesis of Chromatographic Protein Purification Processes with Product Loss. <i>Computer Aided Chemical Engineering</i> , 2009, 26, 1057-1062.	0.5	2
64	Distributions of enzyme residues yielding mutants with improved substrate specificities from two different directed evolution strategies. <i>Protein Engineering, Design and Selection</i> , 2009, 22, 401-411.	2.1	38
65	Ultra scale-down of protein refold screening in microwells: Challenges, solutions and application. <i>Biotechnology and Bioengineering</i> , 2009, 103, 329-340.	3.3	16
66	Rapid optimization of protein freeze-drying formulations using ultra scale-down and factorial design of experiment in microplates. <i>Biotechnology and Bioengineering</i> , 2009, 104, 957-964.	3.3	30
67	Evolutionary Analysis of the TPP-Dependent Enzyme Family. <i>Journal of Molecular Evolution</i> , 2008, 66, 36-49.	1.8	66
68	A microplate-based evaluation of complex denaturation pathways: Structural stability of <i>Escherichia coli</i> transketolase. <i>Biotechnology and Bioengineering</i> , 2008, 99, 1303-1310.	3.3	16
69	Enhancing and Reversing the Stereoselectivity of <i>Escherichia coli</i> Transketolase via Single-Point Mutations. <i>Advanced Synthesis and Catalysis</i> , 2008, 350, 2631-2638.	4.3	65
70	A new approach to bioconversion reaction kinetic parameter identification. <i>AIChE Journal</i> , 2008, 54, 2155-2163.	3.6	31
71	Directed evolution of transketolase substrate specificity towards an aliphatic aldehyde. <i>Journal of Biotechnology</i> , 2008, 134, 240-245.	3.8	69
72	Engineering Enzymes for Biocatalysis. <i>Recent Patents on Biotechnology</i> , 2007, 1, 1-9.	0.8	50

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73	Structural stability of an enzyme biocatalyst. <i>Biochemical Society Transactions</i> , 2007, 35, 1606-1609.	3.4	8
74	Accelerating biocatalytic process design: Integrating new tools from biology, chemistry and engineering. <i>Journal of Biotechnology</i> , 2007, 131, S78.	3.8	0
75	Directed evolution of transketolase activity on non-phosphorylated substrates. <i>Journal of Biotechnology</i> , 2007, 131, 425-432.	3.8	74
76	One-pot synthesis of amino-alcohols using a de-novo transketolase and α -alanine: Pyruvate transaminase pathway in <i>Escherichia coli</i> . <i>Biotechnology and Bioengineering</i> , 2007, 96, 559-569.	3.3	132
77	Factors affecting protein refolding yields in a fed-batch and batch-refolding system. <i>Biotechnology and Bioengineering</i> , 2007, 97, 1523-1534.	3.3	20
78	Integration of biocatalytic conversions into chemical syntheses. <i>Journal of Chemical Technology and Biotechnology</i> , 2007, 82, 1063-1066.	3.2	40
79	Structural stability of <i>E. coli</i> transketolase to urea denaturation. <i>Enzyme and Microbial Technology</i> , 2007, 41, 653-662.	3.2	23
80	Optimisation and evaluation of a generic microplate-based HPLC screen for transketolase activity. <i>Biotechnology Letters</i> , 2007, 29, 1759-1770.	2.2	20
81	Reaction modelling and simulation to assess the integrated use of transketolase and α -transaminase for the synthesis of an aminotriol. <i>Biocatalysis and Biotransformation</i> , 2006, 24, 449-457.	2.0	28
82	A critical assessment of the impact of mixing on dilution refolding. <i>Biotechnology and Bioengineering</i> , 2006, 93, 955-963.	3.3	26
83	The First Mimetic of the Transketolase Reaction. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 1121-1123.	2.4	30
84	Directed evolution of biocatalytic processes. <i>New Biotechnology</i> , 2005, 22, 11-19.	2.7	107
85	High-throughput measurement of protein stability in microtiter plates. <i>Biotechnology and Bioengineering</i> , 2005, 89, 599-607.	3.3	52
86	Directed evolution strategies for improved enzymatic performance. <i>Microbial Cell Factories</i> , 2005, 4, 29.	4.0	79
87	One-Pot Synthesis and the Integration of Chemical and Biocatalytic Conversions. , 2005, , 419-428.		6
88	Exposing relationships using directed evolution. <i>Trends in Biotechnology</i> , 2004, 22, 203-205.	9.3	2
89	Optimising enzyme function by directed evolution. <i>Current Opinion in Structural Biology</i> , 2003, 13, 500-505.	5.7	105
90	Accelerated design of bioconversion processes using automated microscale processing techniques. <i>Trends in Biotechnology</i> , 2003, 21, 29-37.	9.3	129

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91	Better Biocatalytic Processes Faster: New Tools for the Implementation of Biocatalysis in Organic Synthesis. <i>Organic Process Research and Development</i> , 2002, 6, 434-440.	2.7	41
92	Evolution of binding affinity in a WW domain probed by phage display. <i>Protein Science</i> , 2000, 9, 2366-2376.	7.6	34
93	Evolution of binding affinity in a WW domain probed by phage display. <i>Protein Science</i> , 2000, 9, 2366-2376.	7.6	5
94	Movement of the Intermediate and Rate Determining Transition State of Barnase on the Energy Landscape with Changing Temperature. <i>Biochemistry</i> , 1998, 37, 4674-4679.	2.5	44
95	Folding intermediates of wild-type and mutants of barnase. I. use of $\Delta\ddagger$ -value analysis and m-values to probe the cooperative nature of the folding pre-equilibrium. <i>Journal of Molecular Biology</i> , 1998, 276, 625-646.	4.2	56
96	Folding intermediates of wild-type and mutants of barnase. II. correlation of changes in equilibrium amide exchange kinetics with the population of the folding intermediate. <i>Journal of Molecular Biology</i> , 1998, 276, 647-656.	4.2	33