# Paul A Dalby

List of Publications by Year
in descending order



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|---|---|---|---|
| 96 papers | 3,133 citations | 156536 32 h-index | 206121 51 g-index |
| 105 all docs | 105 docs citations | 105 times ranked | 2945 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Hot spots-making directed evolution easier. Biotechnology Advances, 2022, 56, 107926. | 6.0 | 35 |
| 2 | Protein Engineering and HDX Identify Structural Regions of G-CSF Critical to Its Stability and Aggregation. Molecular Pharmaceutics, 2022, 19, 616-629. | 2.3 | 4 |
| 3 | Fineâ€tuning the activity and stability of an evolved enzyme activeâ€site through noncanonical aminoâ€acids. FEBS Journal, 2021, 288, 1935-1955. | 2.2 | 7 |
| 4 | Comparison of the pH- and thermally-induced fluctuations of a therapeutic antibody Fab fragment by molecular dynamics simulation. Computational and Structural Biotechnology Journal, 2021, 19, 2726-2741. | 1.9 | 7 |
| 5 | Machine learning reveals hidden stability code in protein native fluorescence. Computational and Structural Biotechnology Journal, 2021, 19, 2750-2760. | 1.9 | 4 |
| 6 | Proof-of-concept analytical instrument for label-free optical deconvolution of protein species in a mixture. Journal of Chromatography A, 2021, 1641, 461968. | 1.8 | 2 |
| 7 | Solution structure of deglycosylated human IgG1 shows the role of CH2 glycans in its conformation. Biophysical Journal, 2021, 120, 1814-1834. | 0.2 | 3 |
| 8 | Reference Protocol to Assess Analytical Performance of Higher Order Structural Analysis Measurements: Results from an Interlaboratory Comparison. Analytical Chemistry, 2021, 93, 9041-9048. | 3.2 | 4 |
| 9 | Engineering improved ethylene production: Leveraging systems biology and adaptive laboratory evolution. Metabolic Engineering, 2021, 67, 308-320. | 3.6 | 8 |
| 10 | Biophysical characterization of the inactivation of E. coli transketolase by aqueous co-solvents. Scientific Reports, 2021, 11, 23584. | 1.6 | 1 |
| 11 | Engineering transketolase to accept both unnatural donor and acceptor substrates and produce Î±â€hydroxyketones. FEBS Journal, 2020, 287, 1758-1776. | 2.2 | 16 |
| 12 | Advancements in the co-formulation of biologic therapeutics. Journal of Controlled Release, 2020, 327, 397-405. | 4.8 | 21 |
| 13 | HDX and In Silico Docking Reveal that Excipients Stabilize G-CSF via a Combination of Preferential Exclusion and Specific Hotspot Interactions. Molecular Pharmaceutics, 2020, 17, 4637-4651. | 2.3 | 7 |
| 14 | Stability enhancement in a mAb and Fab coformulation. Scientific Reports, 2020, 10, 21129. | 1.6 | 7 |
| 15 | A beginner's guide to molecular dynamics simulations and the identification of cross-correlation networks for enzyme engineering. Methods in Enzymology, 2020, 643, 15-49. | 0.4 | 19 |
| 16 | The Two-Species Model of transketolase explains donor substrate-binding, inhibition and heat-activation. Scientific Reports, 2020, 10, 4148. | 1.6 | 7 |
| 17 | Functional and computational identification of a rescue mutation near the active site of an mRNA methyltransferase. Scientific Reports, 2020, 10, 21841. | 1.6 | 1 |
| 18 | Virus lasers for biological detection. Nature Communications, 2019, 10, 3594. | 5.8 | 27 |

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| 19 | Novel insights into transketolase activation by cofactor binding identifies two native species subpopulations. Scientific Reports, 2019, 9, 16116. | 1.6 | 9 |
| 20 | An Expanded Conformation of an Antibody Fab Region by X-Ray Scattering, Molecular Dynamics, and smFRET Identifies an Aggregation Mechanism. Journal of Molecular Biology, 2019, 431, 1409-1425. | 2.0 | 19 |
| 21 | Selective Stabilization and Destabilization of Protein Domains in Tissue-Type Plasminogen Activator Using Formulation Excipients. Molecular Pharmaceutics, 2019, 16, 744-755. | 2.3 | 6 |
| 22 | T<sub>m</sub>-Values and Unfolded Fraction Can Predict Aggregation Rates for Granulocyte Colony Stimulating Factor Variant Formulations but Not under Predominantly Native Conditions. Molecular Pharmaceutics, 2018, 15, 256-267. | 2.3 | 27 |
| 23 | Coupled molecular dynamics mediate long- and short-range epistasis between mutations that affect stability and aggregation kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E11043-E11052. | 3.3 | 59 |
| 24 | Exploiting correlated molecular-dynamics networks to counteract enzyme activityâ€“stability trade-off. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E12192-E12200. | 3.3 | 65 |
| 25 | An Evaluation of the Potential of NMR Spectroscopy and Computational Modelling Methods to Inform Biopharmaceutical Formulations. Pharmaceutics, 2018, 10, 165. | 2.0 | 22 |
| 26 | Computational Design To Reduce Conformational Flexibility and Aggregation Rates of an Antibody Fab Fragment. Molecular Pharmaceutics, 2018, 15, 3079-3092. | 2.3 | 25 |
| 27 | Two strategies to engineer flexible loops for improved enzyme thermostability. Scientific Reports, 2017, 7, 41212. | 1.6 | 121 |
| 28 | An integrated biorefinery concept for conversion of sugar beet pulp into value-added chemicals and pharmaceutical intermediates. Faraday Discussions, 2017, 202, 415-431. | 1.6 | 41 |
| 29 | Identification of Proteinâ€“Excipient Interaction Hotspots Using Computational Approaches. International Journal of Molecular Sciences, 2016, 17, 853. | 1.8 | 18 |
| 30 | Impact of cofactor-binding loop mutations on thermotolerance and activity of E. coli transketolase. Enzyme and Microbial Technology, 2016, 89, 85-91. | 1.6 | 18 |
| 31 | Structural Analysis of an Evolved Transketolase Reveals Divergent Binding Modes. Scientific Reports, 2016, 6, 35716. | 1.6 | 16 |
| 32 | Transketolase catalysed upgrading of<scp>l</scp>-arabinose: the one-step stereoselective synthesis of<scp>l</scp>-gluco-heptulose. Green Chemistry, 2016, 18, 3158-3165. | 4.6 | 35 |
| 33 | Mapping the Aggregation Kinetics of a Therapeutic Antibody Fragment. Molecular Pharmaceutics, 2016, 13, 307-319. | 2.3 | 51 |
| 34 | Second generation engineering of transketolase for polar aromatic aldehyde substrates. Enzyme and Microbial Technology, 2015, 71, 45-52. | 1.6 | 28 |
| 35 | The Solution Structures of Two Human IgG1 Antibodies Show Conformational Stability and Accommodate Their C1q and FcÎ³R Ligands. Journal of Biological Chemistry, 2015, 290, 8420-8438. | 1.6 | 37 |
| 36 | Single activeâ€site mutants are sufficient to enhance serine:pyruvate Î±â€transaminase activity in an Ï‰â€transaminase. FEBS Journal, 2015, 282, 2512-2526. | 2.2 | 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. Chemical Engineering Science, 2015, 122, 360-372. | 1.9 | 37 |
| 38 | Evaluation of CV2025 Ï‰-transaminase for the bioconversion of lignin breakdown products into value-added chemicals: synthesis of vanillylamine from vanillin. Biocatalysis and Biotransformation, 2014, 32, 302-313. | 1.1 | 16 |
| 39 | The Fab Conformations in the Solution Structure of Human Immunoglobulin G4 (IgG4) Restrict Access to Its Fc Region. Journal of Biological Chemistry, 2014, 289, 20740-20756. | 1.6 | 34 |
| 40 | Identification and use of an alkane transporter plug-in for applications in biocatalysis and whole-cell biosensing of alkanes. Scientific Reports, 2014, 4, 5844. | 1.6 | 54 |
| 41 | The Solution Structure of Rabbit IgG Accounts for Its Interactions with the Fc Receptor and Complement C1q and Its Conformational Stability. Journal of Molecular Biology, 2013, 425, 506-523. | 2.0 | 28 |
| 42 | Optically Induced Thermal Gradients for Protein Characterization in Nanolitre-scale Samples in Microfluidic Devices. Scientific Reports, 2013, 3, 2130. | 1.6 | 10 |
| 43 | Rational substrate and enzyme engineering of transketolase for aromatics. Organic and Biomolecular Chemistry, 2012, 10, 9021. | 1.5 | 35 |
| 44 | An MILP formulation for the synthesis of protein purification processes. Chemical Engineering Research and Design, 2012, 90, 1262-1270. | 2.7 | 10 |
| 45 | Directed evolution to re-adapt a co-evolved network within an enzyme. Journal of Biotechnology, 2012, 157, 237-245. | 1.9 | 27 |
| 46 | A novel efficient optimisation system for purification process synthesis. Biochemical Engineering Journal, 2012, 67, 186-193. | 1.8 | 13 |
| 47 | Yeast-surface expressed BVDV E2 protein induces a Th1/Th2 response in naÃ¯ve T cells. Developmental and Comparative Immunology, 2012, 37, 107-114. | 1.0 | 20 |
| 48 | A generic hierarchical screening method for the analysis of microscale refolds using an automated robotic platform. Biotechnology Progress, 2012, 28, 435-444. | 1.3 | 13 |
| 49 | Freeze drying formulation using microscale and design of experiment approaches: a case study using granulocyte colony-stimulating factor. Biotechnology Letters, 2012, 34, 641-648. | 1.1 | 14 |
| 50 | Directed evolution of a thermostable l-aminoacylase biocatalyst. Journal of Biotechnology, 2011, 155, 396-405. | 1.9 | 10 |
| 51 | Strategy and success for the directed evolution of enzymes. Current Opinion in Structural Biology, 2011, 21, 473-480. | 2.6 | 161 |
| 52 | Engineering and Design. Current Opinion in Structural Biology, 2011, 21, 450-451. | 2.6 | 18 |
| 53 | Optimal synthesis of chromatographic trains for downstream protein processing. Biotechnology Progress, 2011, 27, 1653-1660. | 1.3 | 18 |
| 54 | Thermodynamic parameters for saltâ€induced reversible protein precipitation from automated microscale experiments. Biotechnology and Bioengineering, 2011, 108, 322-332. | 1.7 | 9 |

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| 55 | A high-throughput fluorescence chemical denaturation assay as a general screen for proteinâ€“ligand binding. Analytical Biochemistry, 2011, 411, 155-157. | 1.1 | 29 |
| 56 | Structural stability of E. coli transketolase to temperature and pH denaturation. Journal of Biotechnology, 2011, 155, 209-216. | 1.9 | 17 |
| 57 | A toolbox approach for the rapid evaluation of multi-step enzymatic syntheses comprising a â€˜mix and matchâ€™E. coliexpression system with microscale experimentation. Biocatalysis and Biotransformation, 2011, 29, 192-203. | 1.1 | 18 |
| 58 | Protein denaturation and protein:drugs interactions from intrinsic protein fluorescence measurements at the nanolitre scale. Protein Science, 2010, 19, 1544-1554. | 3.1 | 22 |
| 59 | Masking of the Fc region in human IgG4 by constrained X-ray scattering modelling: implications for antibody function and therapy. Biochemical Journal, 2010, 432, 101-114. | 1.7 | 40 |
| 60 | A Multidisciplinary Approach Toward the Rapid and Preparative-Scale Biocatalytic Synthesis of Chiral Amino Alcohols: A Concise Transketolase-/Ĩ‰-Transaminase-Mediated Synthesis of (2S,3S)-2-Aminopentane-1,3-diol. Organic Process Research and Development, 2010, 14, 99-107. | 1.3 | 80 |
| 61 | Î±,Î±â€²-Dihydroxyketone formation using aromatic and heteroaromatic aldehydes with evolved transketolase enzymes. Chemical Communications, 2010, 46, 7608. | 2.2 | 45 |
| 62 | Non-Î±-hydroxylated aldehydes with evolved transketolase enzymes. Organic and Biomolecular Chemistry, 2010, 8, 1301. | 1.5 | 68 |
| 63 | An MINLP Formulation for the Synthesis of Chromatographic Protein Purification Processes with Product Loss. Computer Aided Chemical Engineering, 2009, 26, 1057-1062. | 0.3 | 2 |
| 64 | Distributions of enzyme residues yielding mutants with improved substrate specificities from two different directed evolution strategies. Protein Engineering, Design and Selection, 2009, 22, 401-411. | 1.0 | 38 |
| 65 | Ultra scaleâ€down of protein refold screening in microwells: Challenges, solutions and application. Biotechnology and Bioengineering, 2009, 103, 329-340. | 1.7 | 16 |
| 66 | Rapid optimization of protein freezeâ€drying formulations using ultra scaleâ€down and factorial design of experiment in microplates. Biotechnology and Bioengineering, 2009, 104, 957-964. | 1.7 | 30 |
| 67 | Evolutionary Analysis of the TPP-Dependent Enzyme Family. Journal of Molecular Evolution, 2008, 66, 36-49. | 0.8 | 66 |
| 68 | A microplateâ€based evaluation of complex denaturation pathways: Structural stability of Escherichia coli transketolase. Biotechnology and Bioengineering, 2008, 99, 1303-1310. | 1.7 | 16 |
| 69 | Enhancing and Reversing the Stereoselectivity of Escherichia coli Transketolase via Singleâ€Point Mutations. Advanced Synthesis and Catalysis, 2008, 350, 2631-2638. | 2.1 | 65 |
| 70 | A new approach to bioconversion reaction kinetic parameter identification. AICHE Journal, 2008, 54, 2155-2163. | 1.8 | 31 |
| 71 | Directed evolution of transketolase substrate specificity towards an aliphatic aldehyde. Journal of Biotechnology, 2008, 134, 240-245. | 1.9 | 69 |
| 72 | Engineering Enzymes for Biocatalysis. Recent Patents on Biotechnology, 2007, 1, 1-9. | 0.4 | 50 |

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| 73 | Structural stability of an enzyme biocatalyst. Biochemical Society Transactions, 2007, 35, 1606-1609. | 1.6 | 8 |
| 74 | Accelerating biocatalytic process design: Integrating new tools from biology, chemistry and engineering. Journal of Biotechnology, 2007, 131, S78. | 1.9 | 0 |
| 75 | Directed evolution of transketolase activity on non-phosphorylated substrates. Journal of Biotechnology, 2007, 131, 425-432. | 1.9 | 74 |
| 76 | One-pot synthesis of amino-alcohols using a de-novo transketolase and Î²-alanine: Pyruvate transaminase pathway inEscherichia coli. Biotechnology and Bioengineering, 2007, 96, 559-569. | 1.7 | 132 |
| 77 | Factors affecting protein refolding yields in a fed-batch and batch-refolding system. Biotechnology and Bioengineering, 2007, 97, 1523-1534. | 1.7 | 20 |
| 78 | Integration of biocatalytic conversions into chemical syntheses. Journal of Chemical Technology and Biotechnology, 2007, 82, 1063-1066. | 1.6 | 40 |
| 79 | Structural stability of E. coli transketolase to urea denaturation. Enzyme and Microbial Technology, 2007, 41, 653-662. | 1.6 | 23 |
| 80 | Optimisation and evaluation of a generic microplate-based HPLC screen for transketolase activity. Biotechnology Letters, 2007, 29, 1759-1770. | 1.1 | 20 |
| 81 | Reaction modelling and simulation to assess the integrated use of transketolase and Ï‰-transaminase for the synthesis of an aminotriol. Biocatalysis and Biotransformation, 2006, 24, 449-457. | 1.1 | 28 |
| 82 | A critical assessment of the impact of mixing on dilution refolding. Biotechnology and Bioengineering, 2006, 93, 955-963. | 1.7 | 26 |
| 83 | The First Mimetic of the Transketolase Reaction. European Journal of Organic Chemistry, 2006, 2006, 1121-1123. | 1.2 | 30 |
| 84 | Directed evolution of biocatalytic processes. New Biotechnology, 2005, 22, 11-19. | 2.7 | 107 |
| 85 | High-throughput measurement of protein stability in microtiter plates. Biotechnology and Bioengineering, 2005, 89, 599-607. | 1.7 | 52 |
| 86 | Directed evolution strategies for improved enzymatic performance. Microbial Cell Factories, 2005, 4, 29. | 1.9 | 79 |
| 87 | One-Pot Synthesis and the Integration of Chemical and Biocatalytic Conversions. , 2005, , 419-428. | | 6 |
| 88 | Exposing relationships using directed evolution. Trends in Biotechnology, 2004, 22, 203-205. | 4.9 | 2 |
| 89 | Optimising enzyme function by directed evolution. Current Opinion in Structural Biology, 2003, 13, 500-505. | 2.6 | 105 |
| 90 | Accelerated design of bioconversion processes using automated microscale processing techniques. Trends in Biotechnology, 2003, 21, 29-37. | 4.9 | 129 |

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| 91 | Better Biocatalytic Processes Faster:Â New Tools for the Implementation of Biocatalysis in Organic Synthesis. Organic Process Research and Development, 2002, 6, 434-440. | 1.3 | 41 |
| 92 | Evolution of binding affinity in a WW domain probed by phage display. Protein Science, 2000, 9, 2366-2376. | 3.1 | 34 |
| 93 | Evolution of binding affinity in a WW domain probed by phage display. , 2000, 9, 2366. | | 5 |
| 94 | Movement of the Intermediate and Rate Determining Transition State of Barnase on the Energy Landscape with Changing Temperature. Biochemistry, 1998, 37, 4674-4679. | 1.2 | 44 |
| 95 | Folding intermediates of wild-type and mutants of barnase. I. use of Ï†-value analysis and m-values to probe the cooperative nature of the folding pre-equilibrium. Journal of Molecular Biology, 1998, 276, 625-646. | 2.0 | 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. Journal of Molecular Biology, 1998, 276, 647-656. | 2.0 | 33 |