

# David Robert Westhead

## List of Publications by Year in descending order

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111  
papers

6,026  
citations

66234

42  
h-index

85405

71  
g-index

116  
all docs

116  
docs citations

116  
times ranked

9484  
citing authors

#	ARTICLE	IF	CITATIONS
1	Improved prediction of protein-protein binding sites using a support vector machines approach. <i>Bioinformatics</i> , 2005, 21, 1487-1494.	1.8	347
2	Flexible docking using tabu search and an empirical estimate of binding affinity. , 1998, 33, 367-382.		328
3	A Unique Dual Activity Amino Acid Hydroxylase in <i>Toxoplasma gondii</i> . <i>PLoS ONE</i> , 2009, 4, e4801.	1.1	238
4	A Primer on Learning in Bayesian Networks for Computational Biology. <i>PLoS Computational Biology</i> , 2007, 3, e129.	1.5	220
5	Dynamic Gene Regulatory Networks Drive Hematopoietic Specification and Differentiation. <i>Developmental Cell</i> , 2016, 36, 572-587.	3.1	213
6	Ligand binding: functional site location, similarity and docking. <i>Current Opinion in Structural Biology</i> , 2003, 13, 389-395.	2.6	191
7	Gene-expression profiling of bortezomib added to standard chemoimmunotherapy for diffuse large B-cell lymphoma (REMoDL-B): an open-label, randomised, phase 3 trial. <i>Lancet Oncology</i> , The, 2019, 20, 649-662.	5.1	187
8	Molecular High-Grade B-Cell Lymphoma: Defining a Poor-Risk Group That Requires Different Approaches to Therapy. <i>Journal of Clinical Oncology</i> , 2019, 37, 202-212.	0.8	187
9	Depletion of RUNX1/ETO in t(8;21) AML cells leads to genome-wide changes in chromatin structure and transcription factor binding. <i>Leukemia</i> , 2012, 26, 1829-1841.	3.3	161
10	RUNX1 reshapes the epigenetic landscape at the onset of haematopoiesis. <i>EMBO Journal</i> , 2012, 31, 4318-4333.	3.5	158
11	Arabidopsis Co-expression Tool (ACT): web server tools for microarray-based gene expression analysis. <i>Nucleic Acids Research</i> , 2006, 34, W504-W509.	6.5	145
12	Chromatin Accessibility-Based Characterization of the Gene Regulatory Network Underlying <i>Plasmodium falciparum</i> Blood-Stage Development. <i>Cell Host and Microbe</i> , 2018, 23, 557-569.e9.	5.1	135
13	Identification of the REST regulon reveals extensive transposable element-mediated binding site duplication. <i>Nucleic Acids Research</i> , 2006, 34, 3862-3877.	6.5	121
14	Two distinct auto-regulatory loops operate at the PU.1 locus in B cells and myeloid cells. <i>Blood</i> , 2011, 117, 2827-2838.	0.6	120
15	Evolutionary algorithms in computer-aided molecular design. <i>Journal of Computer-Aided Molecular Design</i> , 1996, 10, 337-358.	1.3	119
16	PRO_LIGAND: An approach to de novo molecular design. 1. Application to the design of organic molecules. <i>Journal of Computer-Aided Molecular Design</i> , 1995, 9, 13-32.	1.3	118
17	In Vitro Generation of Long-lived Human Plasma Cells. <i>Journal of Immunology</i> , 2012, 189, 5773-5785.	0.4	111
18	A comparison of heuristic search algorithms for molecular docking. <i>Journal of Computer-Aided Molecular Design</i> , 1997, 11, 209-228.	1.3	106

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19	Identification of a Dynamic Core Transcriptional Network in t(8;21) AML that Regulates Differentiation Block and Self-Renewal. <i>Cell Reports</i> , 2014, 8, 1974-1988.	2.9	106
20	Protein structural topology: Automated analysis and diagrammatic representation. <i>Protein Science</i> , 1999, 8, 897-904.	3.1	101
21	Insights into Protein-Protein Interfaces using a Bayesian Network Prediction Method. <i>Journal of Molecular Biology</i> , 2006, 362, 365-386.	2.0	99
22	Simple sequence-based kernels do not predict protein-protein interactions. <i>Bioinformatics</i> , 2010, 26, 2610-2614.	1.8	98
23	TOPS: an enhanced database of protein structural topology. <i>Nucleic Acids Research</i> , 2004, 32, 251D-254.	6.5	96
24	metaSHARK: software for automated metabolic network prediction from DNA sequence and its application to the genomes of <i>Plasmodium falciparum</i> and <i>Eimeria tenella</i> . <i>Nucleic Acids Research</i> , 2005, 33, 1399-1409.	6.5	91
25	Conservation, Convergence, and Divergence of Light-Responsive, Circadian-Regulated, and Tissue-Specific Expression Patterns during Evolution of the Arabidopsis GATA Gene Family. <i>Plant Physiology</i> , 2007, 143, 941-958.	2.3	87
26	Whole genome expression profiling based on paraffin embedded tissue can be used to classify diffuse large B-cell lymphoma and predict clinical outcome. <i>British Journal of Haematology</i> , 2012, 159, 441-453.	1.2	81
27	Inference in Bayesian networks. <i>Nature Biotechnology</i> , 2006, 24, 51-53.	9.4	77
28	Annotating the Plasmodium genome and the enigma of the shikimate pathway. <i>Trends in Parasitology</i> , 2004, 20, 60-65.	1.5	70
29	The Arabidopsis co-expression tool (act): a WWW-based tool and database for microarray-based gene expression analysis. <i>Plant Journal</i> , 2006, 46, 336-348.	2.8	69
30	Distinct genetic changes reveal evolutionary history and heterogeneous molecular grade of DLBCL with MYC/BCL2 double-hit. <i>Leukemia</i> , 2020, 34, 1329-1341.	3.3	66
31	PRO_SELECT: combining structure-based drug design and combinatorial chemistry for rapid lead discovery. 1. Technology. <i>Journal of Computer-Aided Molecular Design</i> , 1997, 11, 193-207.	1.3	65
32	A Microarray Platform-Independent Classification Tool for Cell of Origin Class Allows Comparative Analysis of Gene Expression in Diffuse Large B-cell Lymphoma. <i>PLoS ONE</i> , 2013, 8, e55895.	1.1	64
33	Chronic FLT3-ITD Signaling in Acute Myeloid Leukemia Is Connected to a Specific Chromatin Signature. <i>Cell Reports</i> , 2015, 12, 821-836.	2.9	63
34	TMB-Hunt: an amino acid composition based method to screen proteomes for beta-barrel transmembrane proteins. <i>BMC Bioinformatics</i> , 2005, 6, 56.	1.2	59
35	A PQM-1-Mediated Response Triggers Transcellular Chaperone Signaling and Regulates Organismal Proteostasis. <i>Cell Reports</i> , 2018, 23, 3905-3919.	2.9	58
36	PRO_LIGAND: An Approach to de Novo Molecular Design. 2. Design of Novel Molecules from Molecular Field Analysis (MFA) Models and Pharmacophores. <i>Journal of Medicinal Chemistry</i> , 1994, 37, 3994-4002.	2.9	56

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37	PRO_LIGAND: An approach to de novo molecular design. 3. A genetic algorithm for structure refinement. <i>Journal of Computer-Aided Molecular Design</i> , 1995, 9, 139-148.	1.3	56
38	The transferome of metabolic genes explored: analysis of the horizontal transfer of enzyme encoding genes in unicellular eukaryotes. <i>Genome Biology</i> , 2009, 10, R36.	13.9	56
39	Prediction of clinical outcome in glioblastoma using a biologically relevant nine- $\mu$ RNA signature. <i>Molecular Oncology</i> , 2015, 9, 704-714.	2.1	56
40	An atlas of protein topology cartoons available on the world-wide web. <i>Trends in Biochemical Sciences</i> , 1998, 23, 35-36.	3.7	55
41	Deleterious SNP prediction: be mindful of your training data!. <i>Bioinformatics</i> , 2007, 23, 664-672.	1.8	54
42	An extended set of PRDM1/BLIMP1 target genes links binding motif type to dynamic repression. <i>Nucleic Acids Research</i> , 2010, 38, 5336-5350.	6.5	52
43	Network Analysis Identifies Proinflammatory Plasma Cell Polarization for Secretion of ISG15 in Human Autoimmunity. <i>Journal of Immunology</i> , 2016, 197, 1447-1459.	0.4	52
44	TMB-Hunt: a web server to screen sequence sets for transmembrane $\alpha$ -barrel proteins. <i>Nucleic Acids Research</i> , 2005, 33, W188-W192.	6.5	51
45	A crucial role for the ubiquitously expressed transcription factor Sp1 at early stages of hematopoietic specification. <i>Development (Cambridge)</i> , 2014, 141, 2391-2401.	1.2	51
46	$\hat{\rho}^2$ Edge strands in protein structure prediction and aggregation. <i>Protein Science</i> , 2009, 12, 2348-2359.	3.1	48
47	SPIB and BATF provide alternate determinants of IRF4 occupancy in diffuse large B-cell lymphoma linked to disease heterogeneity. <i>Nucleic Acids Research</i> , 2014, 42, 7591-7610.	6.5	43
48	Protein structure prediction. <i>Current Opinion in Biotechnology</i> , 1998, 9, 383-389.	3.3	38
49	From gene expression to gene regulatory networks in <i>Arabidopsis thaliana</i> . <i>BMC Systems Biology</i> , 2009, 3, 85.	3.0	38
50	A computer system to perform structure comparison using TOPS representations of protein structure. <i>Computers &amp; Chemistry</i> , 2001, 26, 23-30.	1.2	35
51	Metabolic reconstruction and analysis for parasite genomes. <i>Trends in Parasitology</i> , 2007, 23, 548-554.	1.5	33
52	metaTIGER: a metabolic evolution resource. <i>Nucleic Acids Research</i> , 2009, 37, D531-D538.	6.5	32
53	PRO_LIGAND: An approach to de novo molecular design. 4. Application to the design of peptides. <i>Journal of Computer-Aided Molecular Design</i> , 1995, 9, 213-225.	1.3	31
54	Calculation of helix packing angles in protein structures. <i>Bioinformatics</i> , 2003, 19, 1298-1299.	1.8	30

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55	Active-site-directed 3D database searching: Pharmacophore extraction and validation of hits. <i>Journal of Computer-Aided Molecular Design</i> , 1996, 10, 397-416.	1.3	24
56	Gene expression meta-analysis reveals immune response convergence on the IFN $\beta$ -STAT1-IRF1 axis and adaptive immune resistance mechanisms in lymphoma. <i>Genome Medicine</i> , 2015, 7, 96.	3.6	24
57	metaSHARK: a WWW platform for interactive exploration of metabolic networks. <i>Nucleic Acids Research</i> , 2006, 34, W725-W728.	6.5	23
58	Heat Stress Enhances the Accumulation of Polyadenylated Mitochondrial Transcripts in <i>Arabidopsis thaliana</i> . <i>PLoS ONE</i> , 2008, 3, e2889.	1.1	23
59	Parsimonious Gene Correlation Network Analysis (PGCNA): a tool to define modular gene co-expression for refined molecular stratification in cancer. <i>Npj Systems Biology and Applications</i> , 2019, 5, 13.	1.4	22
60	The Role of SurA PPlase Domains in Preventing Aggregation of the Outer-Membrane Proteins tOmpA and OmpT. <i>Journal of Molecular Biology</i> , 2019, 431, 1267-1283.	2.0	22
61	Predicting the effect of missense mutations on protein function: analysis with Bayesian networks. <i>BMC Bioinformatics</i> , 2006, 7, 405.	1.2	21
62	Asymmetric mutation rates at enzyme-inhibitor interfaces: Implications for the protein-protein docking problem. <i>Protein Science</i> , 2003, 12, 2099-2103.	3.1	20
63	Transferring genomics to the clinic: distinguishing Burkitt and diffuse large B cell lymphomas. <i>Genome Medicine</i> , 2015, 7, 64.	3.6	20
64	Cut-and-Run: A Distinct Mechanism by which V(D)J Recombination Causes Genome Instability. <i>Molecular Cell</i> , 2019, 74, 584-597.e9.	4.5	20
65	New Tools and Resources for Analysing Protein Structures and Their Interactions. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1998, 54, 1132-1138.	2.5	19
66	Differential expression and extent of fungal/plant and fungal/bacterial chitinases of <i>Aspergillus fumigatus</i> . <i>Archives of Microbiology</i> , 2005, 184, 78-81.	1.0	19
67	Prediction of horizontal gene transfers in eukaryotes: approaches and challenges. <i>Biochemical Society Transactions</i> , 2009, 37, 792-795.	1.6	19
68	A validated microRNA profile with predictive potential in glioblastoma patients treated with bevacizumab. <i>Molecular Oncology</i> , 2016, 10, 1296-1304.	2.1	19
69	Cell-of-origin in diffuse large B-cell lymphoma: findings from the UK's population-based Haematological Malignancy Research Network. <i>British Journal of Haematology</i> , 2019, 185, 781-784.	1.2	19
70	TmaDB: a repository for tissue microarray data. <i>BMC Bioinformatics</i> , 2005, 6, 218.	1.2	18
71	Combining the interactome and deleterious SNP predictions to improve disease gene identification. <i>Human Mutation</i> , 2009, 30, 485-492.	1.1	18
72	The transcriptional regulation of protein complexes; a cross-species perspective. <i>Genomics</i> , 2009, 94, 369-376.	1.3	18

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73	Identification of gene specific cis-regulatory elements during differentiation of mouse embryonic stem cells: An integrative approach using high-throughput datasets. <i>PLoS Computational Biology</i> , 2019, 15, e1007337.	1.5	18
74	AI-based algorithms for protein surface comparisons. <i>Computers &amp; Chemistry</i> , 2001, 26, 79-84.	1.2	17
75	GO-At&#x2013;in silicoprediction of gene function in <i>Arabidopsis thaliana</i> by combining heterogeneous data. <i>Plant Journal</i> , 2010, 61, 713-721.	2.8	17
76	MetNetMaker: a free and open-source tool for the creation of novel metabolic networks in SBML format. <i>Bioinformatics</i> , 2010, 26, 2352-2353.	1.8	17
77	Gene function prediction using semantic similarity clustering and enrichment analysis in the malaria parasite <i>Plasmodium falciparum</i> . <i>Bioinformatics</i> , 2010, 26, 2431-2437.	1.8	17
78	Prognostic microRNAs in high-grade glioma reveal a link to oligodendrocyte precursor differentiation. <i>Oncoscience</i> , 2014, 2, 252-262.	0.9	12
79	Growth Factor&#x201c;like Gene Regulation Is Separable from Survival and Maturation in Antibody-Secreting Cells. <i>Journal of Immunology</i> , 2019, 202, 1287-1300.	0.4	11
80	<i>Arabidopsis</i> Coexpression Tool: a tool for gene coexpression analysis in <i>Arabidopsis thaliana</i> . <i>IScience</i> , 2021, 24, 102848.	1.9	11
81	The fibril_one on-line database: Mutations, experimental conditions, and trends associated with amyloid fibril formation. <i>Protein Science</i> , 2009, 11, 1862-1866.	3.1	10
82	Ibrutinib induces chromatin reorganisation of chronic lymphocytic leukaemia cells. <i>Oncogenesis</i> , 2019, 8, 32.	2.1	10
83	Benchmarking pipelines for subclonal deconvolution of bulk tumour sequencing data. <i>Nature Communications</i> , 2021, 12, 6396.	5.8	10
84	Bayesian refinement of protein functional site matching. <i>BMC Bioinformatics</i> , 2007, 8, 257.	1.2	9
85	Small RNA analysis in <i>Petunia hybrida</i> identifies unusual tissue-specific expression patterns of conserved miRNAs and of a 24mer RNA. <i>Rna</i> , 2009, 15, 1012-1020.	1.6	9
86	Dysregulation of the miR&#x2013;0c/DLL4 axis by circHIPK3 is essential for KSHV lytic replication. <i>EMBO Reports</i> , 2022, 23, e54117.	2.0	9
87	Modelling the pH-dependent Properties of Kv1 Potassium Channels. <i>Journal of Molecular Biology</i> , 2007, 368, 328-335.	2.0	8
88	A consensus algorithm to screen genomes for novel families of transmembrane $\beta$ barrel proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 69, 8-18.	1.5	7
89	Comparative analysis of gene expression platforms for cell&#x2013;of&#x2013;origin classification of diffuse large B&#x2013;cell lymphoma shows high concordance. <i>British Journal of Haematology</i> , 2021, 192, 599-604.	1.2	7
90	Development Of A Cross Platform, 2-Way Gene Expression Classifier To Distinguish Burkitt Lymphoma From DLBCL, and Assessment Of The Potential Impact Of Its Use In Treatment Decision Making. <i>Blood</i> , 2013, 122, 74-74.	0.6	7

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91	Bridging the gap with the UK Genomics Pathology Imaging Collection. <i>Nature Medicine</i> , 2022, 28, 1107-1108.	15.2	7
92	Flexible model-based clustering of mixed binary and continuous data: application to genetic regulation and cancer. <i>Nucleic Acids Research</i> , 2016, 45, gkw1270.	6.5	4
93	PlasmoPredict: a gene function prediction website for <i>Plasmodium falciparum</i> . <i>Trends in Parasitology</i> , 2010, 26, 107-110.	1.5	3
94	KvDB; mining and mapping sequence variants in voltage-gated potassium channels. <i>Human Mutation</i> , 2010, 31, 908-917.	1.1	3
95	Cancer somatic mutations cluster in a subset of regulatory sites predicted from the ENCODE data. <i>Molecular Cancer</i> , 2016, 15, 76.	7.9	3
96	Simulation of heterogeneous tumour genomes with HeteroGenesis and in silico whole exome sequencing. <i>Bioinformatics</i> , 2019, 35, 2850-2852.	1.8	3
97	Alio intuitu: the automated reconstruction of the metabolic networks of parasites. <i>Trends in Parasitology</i> , 2009, 25, 396-397.	1.5	2
98	Similarity Search Methods As an Alternative to Sub-Type Characterisation in Aggressive Lymphomas. <i>Blood</i> , 2016, 128, 3052-3052.	0.6	2
99	Bayesian Data Integration and Enrichment Analysis for Predicting Gene Function in Malaria. <i>Lecture Notes in Computer Science</i> , 2009, , 457-466.	1.0	1
100	Ligand: A new automated system for de novo drug design. <i>AIP Conference Proceedings</i> , 1995, , .	0.3	0
101	Automated derivation and refinement of sequence length patterns for protein sequences using evolutionary computation. <i>BioSystems</i> , 2005, 81, 247-254.	0.9	0
102	Fundamentals of protein structure and function. , 2005, , .		0
103	Functional Gene Networks: A Preliminary Study on a Modified Genetic Algorithm for Candidate Discovery in Large Microarray Datasets. , 2007, , .		0
104	Identification of a dynamic core transcriptional regulatory network for t(8;21) AML. <i>Experimental Hematology</i> , 2013, 41, S16.	0.2	0
105	Using common variants to indicate cancer genes. <i>International Journal of Cancer</i> , 2015, 136, 241-245.	2.3	0
106	Transferomics: Seeing the Evolutionary Forest Using Phylogenetic Trees. , 2010, , 101-114.		0
107	Meta-Analysis of Diffuse Large B-Cell Lymphoma Gene Expression Identifies Novel and Recurrent Biological Connections,. <i>Blood</i> , 2011, 118, 3682-3682.	0.6	0
108	Identification of a Dynamic Core Transcriptional Network in t(8;21) AML Regulating Differentiation Block and Self-Renewal. <i>Blood</i> , 2014, 124, 1061-1061.	0.6	0

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109	Defining Immune Response Signatures in DLBCL As Potential Predictive Biomarkers for Outcome to Immunotherapy. Blood, 2015, 126, 2663-2663.	0.6	0
110	Longitudinal Analyses of Diagnostic-Relapse Biopsies of Diffuse Large B Cell Lymphoma Reveal a Poor Risk Subset of ABC Patients Based on the Expression of a 30 Gene Panel. Blood, 2019, 134, 2769-2769.	0.6	0
111	Bioinformatic approaches to biological systems. SEB Experimental Biology Series, 2008, 61, 1-16.	0.1	0