David Robert Westhead

List of Publications by Year in descending order

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111 papers 6,026 citations

66343 42 h-index 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. Bioinformatics, 2005, 21, 1487-1494.	4.1	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 Toxoplasma gondii. PLoS ONE, 2009, 4, e4801.	2.5	238
4	A Primer on Learning in Bayesian Networks for Computational Biology. PLoS Computational Biology, 2007, 3, e129.	3.2	220
5	Dynamic Gene Regulatory Networks Drive Hematopoietic Specification and Differentiation. Developmental Cell, 2016, 36, 572-587.	7.0	213
6	Ligand binding: functional site location, similarity and docking. Current Opinion in Structural Biology, 2003, 13, 389-395.	5.7	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. Lancet Oncology, The, 2019, 20, 649-662.	10.7	187
8	Molecular High-Grade B-Cell Lymphoma: Defining a Poor-Risk Group That Requires Different Approaches to Therapy. Journal of Clinical Oncology, 2019, 37, 202-212.	1.6	187
9	Depletion of RUNX1/ETO in t(8;21) AML cells leads to genome-wide changes in chromatin structure and transcription factor binding. Leukemia, 2012, 26, 1829-1841.	7.2	161
10	RUNX1 reshapes the epigenetic landscape at the onset of haematopoiesis. EMBO Journal, 2012, 31, 4318-4333.	7.8	158
11	Arabidopsis Co-expression Tool (ACT): web server tools for microarray-based gene expression analysis. Nucleic Acids Research, 2006, 34, W504-W509.	14.5	145
12	Chromatin Accessibility-Based Characterization of the Gene Regulatory Network Underlying Plasmodium falciparum Blood-Stage Development. Cell Host and Microbe, 2018, 23, 557-569.e9.	11.0	135
13	Identification of the REST regulon reveals extensive transposable element-mediated binding site duplication. Nucleic Acids Research, 2006, 34, 3862-3877.	14.5	121
14	Two distinct auto-regulatory loops operate at the PU.1 locus in B cells and myeloid cells. Blood, 2011, 117, 2827-2838.	1.4	120
15	Evolutionary algorithms in computer-aided molecular design. Journal of Computer-Aided Molecular Design, 1996, 10, 337-358.	2.9	119
16	PRO_LIGAND: An approach to de novo molecular design. 1. Application to the design of organic molecules. Journal of Computer-Aided Molecular Design, 1995, 9, 13-32.	2.9	118
17	In Vitro Generation of Long-lived Human Plasma Cells. Journal of Immunology, 2012, 189, 5773-5785.	0.8	111
18	A comparison of heuristic search algorithms for molecular docking. Journal of Computer-Aided Molecular Design, 1997, 11, 209-228.	2.9	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. Cell Reports, 2014, 8, 1974-1988.	6.4	106
20	Protein structural topology: Automated analysis and diagrammatic representation. Protein Science, 1999, 8, 897-904.	7.6	101
21	Insights into Protein–Protein Interfaces using a Bayesian Network Prediction Method. Journal of Molecular Biology, 2006, 362, 365-386.	4.2	99
22	Simple sequence-based kernels do not predict protein–protein interactions. Bioinformatics, 2010, 26, 2610-2614.	4.1	98
23	TOPS: an enhanced database of protein structural topology. Nucleic Acids Research, 2004, 32, 251D-254.	14.5	96
24	metaSHARK: software for automated metabolic network prediction from DNA sequence and its application to the genomes of Plasmodium falciparum and Eimeria tenella. Nucleic Acids Research, 2005, 33, 1399-1409.	14.5	91
25	Conservation, Convergence, and Divergence of Light-Responsive, Circadian-Regulated, and Tissue-Specific Expression Patterns during Evolution of the Arabidopsis GATA Gene Family. Plant Physiology, 2007, 143, 941-958.	4.8	87
26	Whole genome expression profiling based on paraffin embedded tissue can be used to classify diffuse large <scp>B</scp> â€cell lymphoma and predict clinical outcome. British Journal of Haematology, 2012, 159, 441-453.	2.5	81
27	Inference in Bayesian networks. Nature Biotechnology, 2006, 24, 51-53.	17.5	77
28	Annotating the Plasmodium genome and the enigma of the shikimate pathway. Trends in Parasitology, 2004, 20, 60-65.	3.3	70
29	The Arabidopsis co-expression tool (act): a WWW-based tool and database for microarray-based gene expression analysis. Plant Journal, 2006, 46, 336-348.	5.7	69
30	Distinct genetic changes reveal evolutionary history and heterogeneous molecular grade of DLBCL with MYC/BCL2 double-hit. Leukemia, 2020, 34, 1329-1341.	7.2	66
31	PRO_SELECT: combining structure-based drug design and combinatorial chemistry for rapid lead discovery. 1. Technology. Journal of Computer-Aided Molecular Design, 1997, 11, 193-207.	2.9	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. PLoS ONE, 2013, 8, e55895.	2.5	64
33	Chronic FLT3-ITD Signaling in Acute Myeloid Leukemia Is Connected to a Specific Chromatin Signature. Cell Reports, 2015, 12, 821-836.	6.4	63
34	TMB-Hunt: an amino acid composition based method to screen proteomes for beta-barrel transmembrane proteins. BMC Bioinformatics, 2005, 6, 56.	2.6	59
35	A PQM-1-Mediated Response Triggers Transcellular Chaperone Signaling and Regulates Organismal Proteostasis. Cell Reports, 2018, 23, 3905-3919.	6.4	58
36	PRO_LIGAND: An Approach to de Novo Molecular Design. 2. Design of Novel Molecules from Molecular Field Analysis (MFA) Models and Pharmacophores. Journal of Medicinal Chemistry, 1994, 37, 3994-4002.	6.4	56

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37	PRO_LIGAND: An approach to de novo molecular design. 3. A genetic algorithm for structure refinement. Journal of Computer-Aided Molecular Design, 1995, 9, 139-148.	2.9	56
38	The transferome of metabolic genes explored: analysis of the horizontal transfer of enzyme encoding genes in unicellular eukaryotes. Genome Biology, 2009, 10, R36.	9.6	56
39	Prediction of clinical outcome in glioblastoma using a biologically relevant nineâ€microRNA signature. Molecular Oncology, 2015, 9, 704-714.	4.6	56
40	An atlas of protein topology cartoons available on the world-wide web. Trends in Biochemical Sciences, 1998, 23, 35-36.	7.5	55
41	Deleterious SNP prediction: be mindful of your training data!. Bioinformatics, 2007, 23, 664-672.	4.1	54
42	An extended set of PRDM1/BLIMP1 target genes links binding motif type to dynamic repression. Nucleic Acids Research, 2010, 38, 5336-5350.	14.5	52
43	Network Analysis Identifies Proinflammatory Plasma Cell Polarization for Secretion of ISG15 in Human Autoimmunity. Journal of Immunology, 2016, 197, 1447-1459.	0.8	52
44	TMB-Hunt: a web server to screen sequence sets for transmembrane Â-barrel proteins. Nucleic Acids Research, 2005, 33, W188-W192.	14.5	51
45	A crucial role for the ubiquitously expressed transcription factor Sp1 at early stages of hematopoietic specification. Development (Cambridge), 2014, 141, 2391-2401.	2.5	51
46	Î ² Edge strands in protein structure prediction and aggregation. Protein Science, 2009, 12, 2348-2359.	7.6	48
47	SPIB and BATF provide alternate determinants of IRF4 occupancy in diffuse large B-cell lymphoma linked to disease heterogeneity. Nucleic Acids Research, 2014, 42, 7591-7610.	14.5	43
48	Protein structure prediction. Current Opinion in Biotechnology, 1998, 9, 383-389.	6.6	38
49	From gene expression to gene regulatory networks in Arabidopsis thaliana. BMC Systems Biology, 2009, 3, 85.	3.0	38
50	A computer system to perform structure comparison using TOPS representations of protein structure. Computers & Chemistry, 2001, 26, 23-30.	1.2	35
51	Metabolic reconstruction and analysis for parasite genomes. Trends in Parasitology, 2007, 23, 548-554.	3.3	33
52	metaTIGER: a metabolic evolution resource. Nucleic Acids Research, 2009, 37, D531-D538.	14.5	32
53	PRO_LIGAND: An approach to de novo molecular design. 4. Application to the design of peptides. Journal of Computer-Aided Molecular Design, 1995, 9, 213-225.	2.9	31
54	Calculation of helix packing angles in protein structures. Bioinformatics, 2003, 19, 1298-1299.	4.1	30

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55	Active-site-directed 3D database searching: Pharmacophore extraction and validation of hits. Journal of Computer-Aided Molecular Design, 1996, 10, 397-416.	2.9	24
56	Gene expression meta-analysis reveals immune response convergence on the IFNÎ ³ -STAT1-IRF1 axis and adaptive immune resistance mechanisms in lymphoma. Genome Medicine, 2015, 7, 96.	8.2	24
57	metaSHARK: a WWW platform for interactive exploration of metabolic networks. Nucleic Acids Research, 2006, 34, W725-W728.	14.5	23
58	Heat Stress Enhances the Accumulation of Polyadenylated Mitochondrial Transcripts in Arabidopsis thaliana. PLoS ONE, 2008, 3, e2889.	2.5	23
59	Parsimonious Gene Correlation Network Analysis (PGCNA): a tool to define modular gene co-expression for refined molecular stratification in cancer. Npj Systems Biology and Applications, 2019, 5, 13.	3.0	22
60	The Role of SurA PPlase Domains in Preventing Aggregation of the Outer-Membrane Proteins tOmpA and OmpT. Journal of Molecular Biology, 2019, 431, 1267-1283.	4.2	22
61	Predicting the effect of missense mutations on protein function: analysis with Bayesian networks. BMC Bioinformatics, 2006, 7, 405.	2.6	21
62	Asymmetric mutation rates at enzyme-inhibitor interfaces: Implications for the protein-protein docking problem. Protein Science, 2003, 12, 2099-2103.	7.6	20
63	Transferring genomics to the clinic: distinguishing Burkitt and diffuse large B cell lymphomas. Genome Medicine, 2015, 7, 64.	8.2	20
64	Cut-and-Run: A Distinct Mechanism by which $V(D)J$ Recombination Causes Genome Instability. Molecular Cell, 2019, 74, 584-597.e9.	9.7	20
65	New Tools and Resources for Analysing Protein Structures and Their Interactions. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 1132-1138.	2.5	19
66	Differential expression and extent of fungal/plant and fungal/bacterial chitinases of Aspergillus fumigatus. Archives of Microbiology, 2005, 184, 78-81.	2.2	19
67	Prediction of horizontal gene transfers in eukaryotes: approaches and challenges. Biochemical Society Transactions, 2009, 37, 792-795.	3.4	19
68	A validated microRNA profile with predictive potential in glioblastoma patients treated with bevacizumab. Molecular Oncology, 2016, 10, 1296-1304.	4.6	19
69	Cellâ€ofâ€origin in diffuse large Bâ€cell lymphoma: findings from the <scp>UK</scp> 's populationâ€based Haematological Malignancy Research Network. British Journal of Haematology, 2019, 185, 781-784.	2.5	19
70	TmaDB: a repository for tissue microarray data. BMC Bioinformatics, 2005, 6, 218.	2.6	18
71	Combining the interactome and deleterious SNP predictions to improve disease gene identification. Human Mutation, 2009, 30, 485-492.	2.5	18
72	The transcriptional regulation of protein complexes; a cross-species perspective. Genomics, 2009, 94, 369-376.	2.9	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. PLoS Computational Biology, 2019, 15, e1007337.	3.2	18
74	Al-based algorithms for protein surface comparisons. Computers & Chemistry, 2001, 26, 79-84.	1.2	17
75	GO-At :in silicoprediction of gene function inArabidopsis thalianaby combining heterogeneous data. Plant Journal, 2010, 61, 713-721.	5 . 7	17
76	MetNetMaker: a free and open-source tool for the creation of novel metabolic networks in SBML format. Bioinformatics, 2010, 26, 2352-2353.	4.1	17
77	Gene function prediction using semantic similarity clustering and enrichment analysis in the malaria parasite <i>Plasmodium falciparum</i> . Bioinformatics, 2010, 26, 2431-2437.	4.1	17
78	Prognostic microRNAs in high-grade glioma reveal a link to oligodendrocyte precursor differentiation. Oncoscience, 2014, 2, 252-262.	2.2	12
79	Growth Factor–like Gene Regulation Is Separable from Survival and Maturation in Antibody-Secreting Cells. Journal of Immunology, 2019, 202, 1287-1300.	0.8	11
80	Arabidopsis Coexpression Tool: a tool for gene coexpression analysis in Arabidopsis thaliana. IScience, 2021, 24, 102848.	4.1	11
81	The fibril_one on-line database: Mutations, experimental conditions, and trends associated with amyloid fibril formation. Protein Science, 2009, 11 , $1862-1866$.	7.6	10
82	Ibrutinib induces chromatin reorganisation of chronic lymphocytic leukaemia cells. Oncogenesis, 2019, 8, 32.	4.9	10
83	Benchmarking pipelines for subclonal deconvolution of bulk tumour sequencing data. Nature Communications, 2021, 12, 6396.	12.8	10
84	Bayesian refinement of protein functional site matching. BMC Bioinformatics, 2007, 8, 257.	2.6	9
85	Small RNA analysis in Petunia hybrida identifies unusual tissue-specific expression patterns of conserved miRNAs and of a 24mer RNA. Rna, 2009, 15, 1012-1020.	3 . 5	9
86	Dysregulation of the miRâ€30c/DLL4 axis by circHIPK3 is essential for KSHV lytic replication. EMBO Reports, 2022, 23, e54117.	4.5	9
87	Modelling the pH-dependent Properties of Kv1 Potassium Channels. Journal of Molecular Biology, 2007, 368, 328-335.	4.2	8
88	A consensus algorithm to screen genomes for novel families of transmembrane \hat{l}^2 barrel proteins. Proteins: Structure, Function and Bioinformatics, 2007, 69, 8-18.	2.6	7
89	Comparative analysis of gene expression platforms for cellâ€ofâ€origin classification of diffuse large Bâ€cell lymphoma shows high concordance. British Journal of Haematology, 2021, 192, 599-604.	2.5	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. Blood, 2013, 122, 74-74.	1.4	7

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91	Bridging the gap with the UK Genomics Pathology Imaging Collection. Nature Medicine, 2022, 28, 1107-1108.	30.7	7
92	Flexible model-based clustering of mixed binary and continuous data: application to genetic regulation and cancer. Nucleic Acids Research, 2016, 45, gkw1270.	14.5	4
93	PlasmoPredict: a gene function prediction website for Plasmodium falciparum. Trends in Parasitology, 2010, 26, 107-110.	3.3	3
94	KvDB; mining and mapping sequence variants in voltage-gated potassium channels. Human Mutation, 2010, 31, 908-917.	2.5	3
95	Cancer somatic mutations cluster in a subset of regulatory sites predicted from the ENCODE data. Molecular Cancer, 2016, 15, 76.	19.2	3
96	Simulation of heterogeneous tumour genomes with HeteroGenesis and in silico whole exome sequencing. Bioinformatics, 2019, 35, 2850-2852.	4.1	3
97	Alio intuitu: the automated reconstruction of the metabolic networks of parasites. Trends in Parasitology, 2009, 25, 396-397.	3.3	2
98	Similarity Search Methods As an Alternative to Sub-Type Characterisation in Aggressive Lymphomas. Blood, 2016, 128, 3052-3052.	1.4	2
99	Bayesian Data Integration and Enrichment Analysis for Predicting Gene Function in Malaria. Lecture Notes in Computer Science, 2009, , 457-466.	1.3	1
100	Ligand: A new automated system for de novo drug design. AIP Conference Proceedings, 1995, , .	0.4	0
101	Automated derivation and refinement of sequence length patterns for protein sequences using evolutionary computation. BioSystems, 2005, 81, 247-254.	2.0	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. Experimental Hematology, 2013, 41, S16.	0.4	0
105	Using common variants to indicate cancer genes. International Journal of Cancer, 2015, 136, 241-245.	5.1	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,. Blood, 2011, 118, 3682-3682.	1.4	0
108	Identification of a Dynamic Core Transcriptional Network in t(8;21) AML Regulating Differentiation Block and Self-Renewal. Blood, 2014, 124, 1061-1061.	1.4	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.	1.4	o
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.	1.4	0
111	Bioinformatic approaches to biological systems. SEB Experimental Biology Series, 2008, 61, 1-16.	0.1	o