Thomas R Caulfield

List of Publications by Year
in descending order

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79 papers	5,219 citations	159585 30 h-index	91884 69 g-index
82 all docs	82 docs citations	82 times ranked	9480 citing authors

#	Article	IF	Citations
1	Unconventional Translation of C9ORF72 GGGGCC Expansion Generates Insoluble Polypeptides Specific to c9FTD/ALS. Neuron, 2013, 77, 639-646.	8.1	962
2	Apolipoprotein E and Alzheimer disease: pathobiology and targeting strategies. Nature Reviews Neurology, 2019, 15, 501-518.	10.1	734
3	Antisense transcripts of the expanded C9ORF72 hexanucleotide repeat form nuclear RNA foci and undergo repeat-associated non-ATG translation in c9FTD/ALS. Acta Neuropathologica, 2013, 126, 829-844.	7.7	506
4	Aggregation-prone c9FTD/ALS poly(GA) RAN-translated proteins cause neurotoxicity by inducing ER stress. Acta Neuropathologica, 2014, 128, 505-524.	7.7	284
5	Stearoyl-CoA Desaturase 1 Is a Novel Molecular Therapeutic Target for Clear Cell Renal Cell Carcinoma. Clinical Cancer Research, 2013, 19, 2368-2380.	7.0	214
6	PINK1, Parkin, and Mitochondrial Quality Control: What can we Learn about Parkinsonâ€™s Disease Pathobiology?. Journal of Parkinson's Disease, 2017, 7, 13-29.	2.8	175
7	The dual functions of the extreme N-terminus of TDP-43 in regulating its biological activity and inclusion formation. Human Molecular Genetics, 2013, 22, 3112-3122.	2.9	156
8	Nanaomycin A Selectively Inhibits DNMT3B and Reactivates Silenced Tumor Suppressor Genes in Human Cancer Cells. Molecular Cancer Therapeutics, 2010, 9, 3015-3023.	4.1	154
9	(Pathoâ€)physiological relevance of <scp>PINK</scp> 1â€dependent ubiquitin phosphorylation. EMBO Reports, 2015, 16, 1114-1130.	4.5	147
10	Integrating Virtual Screening and Combinatorial Chemistry for Accelerated Drug Discovery. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 475-487.	1.1	122
11	Heterozygous PINK1 p.G411S increases risk of Parkinsonâ€™s disease via a dominant-negative mechanism. Brain, 2017, 140, 98-117.	7.6	116
12	Targeted manipulation of the sortilinâ€“progranulin axis rescues progranulin haploinsufficiency. Human Molecular Genetics, 2014, 23, 1467-1478.	2.9	96
13	Phosphorylation by PINK1 Releases the UBL Domain and Initializes the Conformational Opening of the E3 Ubiquitin Ligase Parkin. PLoS Computational Biology, 2014, 10, e1003935.	3.2	95
14	A Structural Model for the Large Subunit of the Mammalian Mitochondrial Ribosome. Journal of Molecular Biology, 2006, 358, 193-212.	4.2	85
15	Synthesis and Evaluation of Derivatives of the Proteasome Deubiquitinase Inhibitor bâ€<scp>AP</scp>15. Chemical Biology and Drug Design, 2015, 86, 1036-1048.	3.2	83
16	Advances in the computational development of DNA methyltransferase inhibitors. Drug Discovery Today, 2011, 16, 418-425.	6.4	80
17	Molecular dynamics simulations of human DNA methyltransferase 3B with selective inhibitor nanaomycin A. Journal of Structural Biology, 2011, 176, 185-191.	2.8	77
18	Molecular Dissection of FUS Points at Synergistic Effect of Low-Complexity Domains in Toxicity. Cell Reports, 2018, 24, 529-537.e4.	6.4	74

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19	Structural and Functional Impact of Parkinson Disease-Associated Mutations in the E3 Ubiquitin Ligase Parkin. Human Mutation, 2015, 36, 774-786.	2.5	69
20	FAM111A protects replication forks from protein obstacles via its trypsin-like domain. Nature Communications, 2020, 11, 1318.	12.8	67
21	The PINK1 p.I368N mutation affects protein stability and ubiquitin kinase activity. Molecular Neurodegeneration, 2017, 12, 32.	10.8	62
22	Targeted inhibition of the deubiquitinating enzymes, <scp>USP</scp>14 and <scp>UCHL</scp>5, induces proteotoxic stress and apoptosis in <scp>W</scp>aldenstrÃ¶m macroglobulinaemia tumour cells. British Journal of Haematology, 2015, 169, 377-390.	2.5	55
23	Motion of transfer RNA from the A/T state into the Aâ€site using docking and simulations. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2489-2500.	2.6	52
24	Optimization of Peptide Hydroxamate Inhibitors of Insulin-Degrading Enzyme Reveals Marked Substrate-Selectivity. Journal of Medicinal Chemistry, 2013, 56, 2246-2255.	6.4	51
25	Multifaceted peptide assisted one-pot synthesis of gold nanoparticles for plectin-1 targeted gemcitabine delivery in pancreatic cancer. Nanoscale, 2017, 9, 15622-15634.	5.6	46
26	Activation of the E3 ubiquitin ligase Parkin. Biochemical Society Transactions, 2015, 43, 269-274.	3.4	45
27	Examinations of tRNA Range of Motion Using Simulations of Cryo-EM Microscopy and X-Ray Data. Journal of Biophysics, 2011, 2011, 1-11.	0.8	40
28	Development of multi-drug loaded PEGylated nanodiamonds to inhibit tumor growth and metastasis in genetically engineered mouse models of pancreatic cancer. Nanoscale, 2019, 11, 22006-22018.	5.6	40
29	Inter-ring rotation of apolipoprotein A-I protein monomers for the double-belt model using biased molecular dynamics. Journal of Molecular Graphics and Modelling, 2011, 29, 1006-1014.	2.4	38
30	APOE3 -Jacksonville (V236E) variant reduces self-aggregation and risk of dementia. Science Translational Medicine, 2021, 13, eabc9375.	12.4	37
31	Accelerated bottom-up drug design platform enables the discovery of novel stearoyl-CoA desaturase 1 inhibitors for cancer therapy. Oncotarget, 2018, 9, 3-20.	1.8	35
32	Long-range Electrostatic Complementarity Governs Substrate Recognition by Human Chymotrypsin C, a Key Regulator of Digestive Enzyme Activation. Journal of Biological Chemistry, 2013, 288, 9848-9859.	3.4	32
33	ACEI/ARB therapy in COVID-19: the double-edged sword of ACE2 and SARS-CoV-2 viral docking. Critical Care, 2020, 24, 475.	5.8	27
34	Inhibition of Prohormone Convertases PC1/3 and PC2 by 2,5-Dideoxystreptamine Derivatives. Molecular Pharmacology, 2012, 81, 440-454.	2.3	24
35	Comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA) of some benzimidazole derivatives with trichomonicidal activity. European Journal of Medicinal Chemistry, 2011, 46, 3499-3508.	5.5	23
36	Selective Targeting of Extracellular Insulin-Degrading Enzyme by Quasi-Irreversible Thiol-Modifying Inhibitors. ACS Chemical Biology, 2015, 10, 2716-2724.	3.4	22

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37	An Acrobatic Substrate Metamorphosis Reveals a Requirement for Substrate Conformational Dynamics in Trypsin Proteolysis. Journal of Biological Chemistry, 2016, 291, 26304-26319.	3.4	22
38	Disulfide engineering of human Kunitz-type serine protease inhibitors enhances proteolytic stability and target affinity toward mesotrypsin. Journal of Biological Chemistry, 2019, 294, 5105-5120.	3.4	20
39	An integrated approach to the discovery of potent agelastatin A analogues for brain tumors: chemical synthesis and biological, physicochemical and CNS pharmacokinetic analyses. MedChemComm, 2013, 4, 1093.	3.4	19
40	Protein molecular modeling techniques investigating novel <scp>TAB</scp>2 variant R347X causing cardiomyopathy and congenital heart defects in multigenerational family. Molecular Genetics & Genomic Medicine, 2018, 6, 666-672.	1.2	19
41	Molecular Inhibitor of QSOX1 Suppresses Tumor Growth In Vivo. Molecular Cancer Therapeutics, 2020, 19, 112-122.	4.1	17
42	Small molecule inhibitors of mesotrypsin from a structure-based docking screen. PLoS ONE, 2017, 12, e0176694.	2.5	16
43	Pharmacokinetics of Agelastatin A in the central nervous system. MedChemComm, 2012, 3, 233-237.	3.4	15
44	A novel splice site variant in <scp>CYP</scp>11A1 in trans with the p.E314K variant in a male patient with congenital adrenal insufficiency. Molecular Genetics & Genomic Medicine, 2017, 5, 781-787.	1.2	14
45	Attacking COVID-19 Progression Using Multi-Drug Therapy for Synergetic Target Engagement. Biomolecules, 2021, 11, 787.	4.0	14
46	Design and Evaluation of PEGylated Liposomal Formulation of a Novel Multikinase Inhibitor for Enhanced Chemosensitivity and Inhibition of Metastatic Pancreatic Ductal Adenocarcinoma. Bioconjugate Chemistry, 2019, 30, 2703-2713.	3.6	12
47	Molecular Dynamics Simulations Suggest a Non-Doublet Decoding Model of â€“1 Frameshifting by tRNASer3. Biomolecules, 2019, 9, 745.	4.0	11
48	Functional Analysis of the SIM1 Variant p.G715V in 2 Patients With Obesity. Journal of Clinical Endocrinology and Metabolism, 2020, 105, 355-361.	3.6	11
49	Endotheliitis, endothelin, and endothelin receptor blockers in COVID-19. Medical Hypotheses, 2021, 150, 110564.	1.5	11
50	Integrative data fusion for comprehensive assessment of a novel CHEK2 variant using combined genomics, imaging, and functionalâ€“structural assessments via protein informatics. Molecular Omics, 2019, 15, 59-66.	2.8	9
51	Pharmacokinetics of bendamustine in the central nervous system: chemoinformatic screening followed by validation in a murine model. MedChemComm, 2012, 3, 1526.	3.4	8
52	Protein informatics combined with multiple data sources enriches the clinical characterization of novel <scp>TRPV</scp>4 variant causing an intermediate skeletal dysplasia. Molecular Genetics & Genomic Medicine, 2019, 7, e566.	1.2	8
53	Protein modeling and clinical description of a novel inâ€frame <scp>GLB</scp>1 deletion causing <scp>GM</scp>1 gangliosidosis type <scp>II</scp>. Molecular Genetics & Genomic Medicine, 2018, 6, 1229-1235.	1.2	6
54	Protein molecular modeling shows residue T599 is critical to wild-type function of POLG and description of a novel variant associated with the SANDO phenotype. Human Genome Variation, 2018, 5, 18016.	0.7	6

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55	TRIO gene segregation in a family with cerebellar ataxia. Neurologia I Neurochirurgia Polska, 2018, 52, 743-749.	1.2	5
56	Whole Exome Sequencing and Molecular Modeling of a Missense Variant in TNFAIP3 That Segregates with Disease in a Family with Chronic Urticaria and Angioedema. Case Reports in Genetics, 2018, 2018, 1-6.	0.2	5
57	Personalized molecular modeling for pinpointing associations of protein dysfunction and variants associated with hereditary cancer syndromes. Molecular Genetics & Genomic Medicine, 2018, 6, 805-810.	1.2	4
58	Genomic Observations of a Rare/Pathogenic SMAD3 Variant in Loeysâ€“Dietz Syndrome 3 Confirmed by Protein Informatics and Structural Investigations. Medicina (Lithuania), 2019, 55, 137.	2.0	4
59	Structural And Computational Perspectives of Selectively Targeting Mutant Proteins. Current Drug Discovery Technologies, 2021, 18, 365-378.	1.2	4
60	Platforms for Personalized Polytherapeutics Discovery in COVID-19. Journal of Molecular Biology, 2021, 433, 166945.	4.2	4
61	Role of PLEXIND1/TGFÎ² Signaling Axis in Pancreatic Ductal Adenocarcinoma Progression Correlates with the Mutational Status of KRAS. Cancers, 2021, 13, 4048.	3.7	4
62	Three-tier stratification for CNS COVID-19 to help decide which patients should undergo lumbar puncture with CSF analysis: A case report and literature review. Romanian Journal of Internal Medicine = Revue Roumaine De Medecine Interne, 2020, 59, 88-92.	0.6	4
63	An Induced-Fit Docking Method for Refining Drug-Receptor Interactions Derived from Maxwellian-Assessor Nanoprobes (Quantum Mechanics-Based Criterion Assessment) Placed Over Adaptive Intervals of Molecular Dynamics Sampling. Biophysical Journal, 2012, 102, 171a-172a.	0.5	3
64	An activating germline IDH1 variant associated with a tumor entity characterized by unilateral and bilateral chondrosarcoma of the mastoid. Human Genetics and Genomics Advances, 2020, 1, 100006.	1.7	3
65	Structural Models for the Dynamic Effects of Loss-of-Function Variants in the Human SIM1 Protein Transcriptional Activation Domain. Biomolecules, 2020, 10, 1314.	4.0	3
66	Reply: Heterozygous PINK1 p.G411S in rapid eye movement sleep behaviour disorder. Brain, 2017, 140, e33-e33.	7.6	2
67	Examination of Molecular Effects of MYLK Deletion in a Patient with Extensive Aortic, Carotid, and Abdominal Dissections That Underlie the Genetic Dysfunction. Case Reports in Medicine, 2020, 2020, 1-7.	0.7	2
68	Characterization of a Pathogenic Variant in the ABCD1 Gene Through Protein Molecular Modeling. Case Reports in Genetics, 2020, 2020, 1-7.	0.2	2
69	Clinical description & molecular modeling of novel MAX pathogenic variant causing pheochromocytoma in family, supports paternal parent-of-origin effect. Cancer Genetics, 2021, 252-253, 107-110.	0.4	2
70	A novel, germline, deactivating CBL variant p.L493F alters domain orientation and is associated with multiple childhood cancers. Cancer Genetics, 2021, 254-255, 18-24.	0.4	2
71	A Virtual Screening Platform Identifies Chloroethylagelastatin A as a Potential Ribosomal Inhibitor. Biomolecules, 2020, 10, 1407.	4.0	1
72	Genomics combined with a protein informatics platform to assess a novel pathogenic variant c.1024 A>G (p.K342E) in OPA1 in a patient with autosomal dominant optic atrophy. Ophthalmic Genetics, 2020, 41, 563-569.	1.2	1

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73	The PINK1 p.I368N Mutation Affects Protein Stability and Kinase Activity with Its Structural Change. Juntendo Medical Journal, 2018, 64, 17-30.	0.1	0
74	Inhibition of PC1/3 and PC2 by 2,5â€dideoxystreptamine derivatives. FASEB Journal, 2012, 26, 557.2.	0.5	0
75	Parkin. , 2016, , 1-9.		0
76	Parkin. , 2017, , 1-9.		0
77	Parkin. , 2018, , 3786-3794.		0
78	Structural Basis for Improved Proteolytic Stability and Target Affinity of Disulfide engineered Human Kunitzâ€type Serine Protease Inhibitors. FASEB Journal, 2019, 33, 472.1.	0.5	0
79	Molecular Modeling and Phenotypic Description of a Patient with a Novel Exonic Deletion of <i>GALNS</i> with Resultant Morquio Syndrome with Two Successful Pregnancies. Molecular Syndromology, 0, , 1-8.	0.8	0