David M Ferguson

List of Publications by Year
in descending order

84 papers	18,849 citations	101543 36 h-index	69250 77 g-index
88 all docs	88 docs citations	88 times ranked	17392 citing authors

#	Article	IF	Citations
1	Toll-like receptor 7 and 8 imidazoquinoline-based agonist/antagonist pairs. Bioorganic and Medicinal Chemistry Letters, 2022, 59, 128548.	2.2	4
2	Parameterization and Application of the General Amber Force Field to Model Fluoro Substituted Furanose Moieties and Nucleosides. Molecules, 2022, 27, 2616.	3.8	0
3	In honor of Professor Robert Vince on the occasion of his 80th birthday. Medicinal Chemistry Research, 2021, 30, 303-304.	2.4	0
4	Structural modeling and analysis of the SARS-CoV-2 cell entry inhibitor camostat bound to the trypsin-like protease TMPRSS2. Medicinal Chemistry Research, 2021, 30, 399-409.	2.4	13
5	Novel TLR 7/8 agonists for improving NK cell mediated antibody-dependent cellular cytotoxicity (ADCC). Scientific Reports, 2021, 11, 3346.	3.3	17
6	4-Amino-2-butyl-7-methoxycarbonylthiazolo[4,5-c]quinoline. MolBank, 2021, 2021, M1305.	0.5	3
7	TLR7/8 Agonist-Loaded Nanoparticles Augment NK Cell-Mediated Antibody-Based Cancer Immunotherapy. Molecular Pharmaceutics, 2020, 17, 2109-2124.	4.6	28
8	A Cinchona Alkaloid Antibiotic That Appears To Target ATP Synthase in Streptococcus pneumoniae. Journal of Medicinal Chemistry, 2019, 62, 2305-2332.	6.4	24
9	Investigation of (S)-(â^')-Acidomycin: A Selective Antimycobacterial Natural Product That Inhibits Biotin Synthase. ACS Infectious Diseases, 2019, 5, 598-617.	3.8	22
10	Combination of Sunitinib and PD-L1 Blockade Enhances Anticancer Efficacy of TLR7/8 Agonist-Based Nanovaccine. Molecular Pharmaceutics, 2019, 16, 1200-1210.	4.6	30
11	Avoiding Antibiotic Inactivation in Mycobacterium tuberculosis by Rv3406 through Strategic Nucleoside Modification. ACS Infectious Diseases, 2018, 4, 1102-1113.	3.8	14
12	Polymeric nanoparticles encapsulating novel TLR7/8 agonists as immunostimulatory adjuvants for enhanced cancer immunotherapy. Biomaterials, 2018, 164, 38-53.	11.4	133
13	Acidic pH-responsive polymer nanoparticles as a TLR7/8 agonist delivery platform for cancer immunotherapy. Nanoscale, 2018, 10, 20851-20862.	5.6	59
14	Design and Synthesis of N1-Modified Imidazoquinoline Agonists for Selective Activation of Toll-like Receptors 7 and 8. ACS Medicinal Chemistry Letters, 2017, 8, 1148-1152.	2.8	32
15	Targeting Topoisomerase II Activity in NSCLC with 9-Aminoacridine Derivatives. Anticancer Research, 2015, 35, 5211-7.	1.1	4
16	Structureâ€"Activity Relationship Analysis of Imidazoquinolines with Toll-like Receptors 7 and 8 Selectivity and Enhanced Cytokine Induction. Journal of Medicinal Chemistry, 2014, 57, 339-347.	6.4	49
17	Synthesis and evaluation of N-alkyl-9-aminoacridines with antibacterial activity. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 3014-3017.	2.2	27
18	Structure and Stability of Human Telomeric G-Quadruplex with Preclinical 9-Amino Acridines. PLoS ONE, 2013, 8, e57701.	2.5	21

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19	Discovery of Imidazoquinolines with Toll-Like Receptor 7/8 Independent Cytokine Induction. ACS Medicinal Chemistry Letters, 2012, 3, 501-504.	2.8	33
20	Novel acridine-based agents with topoisomerase II inhibitor activity suppress mesothelioma cell proliferation and induce apoptosis. Investigational New Drugs, 2012, 30, 1443-1448.	2.6	15
21	9-Amino acridine pharmacokinetics, brain distribution, and in vitro/in vivo efficacy against malignant glioma. Cancer Chemotherapy and Pharmacology, 2012, 69, 1519-1527.	2.3	13
22	Synthesis and cancer cell cytotoxicity of substituted xanthenes. Bioorganic and Medicinal Chemistry, 2010, 18, 1456-1463.	3.0	89
23	Novel acridine-based compounds that exhibit an anti-pancreatic cancer activity are catalytic inhibitors of human topoisomerase II. European Journal of Pharmacology, 2009, 602, 223-229.	3.5	60
24	On the role of topoisomerase I in mediating the cytotoxicity of 9-aminoacridine-based anticancer agents. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 4459-4462.	2.2	13
25	Synthesis and evaluation of xanomeline analogsâ€"Probing the wash-resistant phenomenon at the M1 muscarinic acetylcholine receptor. Bioorganic and Medicinal Chemistry, 2008, 16, 1376-1392.	3.0	33
26	Acridine-Based Agents with Topoisomerase II Activity Inhibit Pancreatic Cancer Cell Proliferation and Induce Apoptosis. Journal of Medicinal Chemistry, 2008, 51, 179-182.	6.4	94
27	Toward a Structure-Based Model of Salvinorin A Recognition of the Î¹-Opioid Receptor. Journal of Medicinal Chemistry, 2008, 51, 1824-1830.	6.4	42
28	Quantitative Three Dimensional Structure Linear Interaction Energy Model of 5â€²-O-[N-(Salicyl)sulfamoyl]adenosine and the Aryl Acid Adenylating Enzyme MbtA. Journal of Medicinal Chemistry, 2008, 51, 7154-7160.	6.4	21
29	Molecular Recognition of Opioid Receptor Ligands. , 2008, , 585-608.		0
30	Simulated Annealing-Optimal Histogram Methods. Advances in Chemical Physics, 2007, , 311-336.	0.3	7
31	Triaryl Pyrazoline Compound Inhibits Flavivirus RNA Replication. Antimicrobial Agents and Chemotherapy, 2006, 50, 1320-1329.	3.2	107
32	Spectrophotometric Determination and Computational Evaluation of the Rates of Hydrolysis of 9-Amino-Substituted Acridines. Journal of Chemical Information and Modeling, 2006, 46, 876-883.	5.4	14
33	A unique binding epitope for salvinorinâ€ƒA, a non-nitrogenous kappa opioid receptor agonist. FEBS Journal, 2006, 273, 1966-1974.	4.7	35
34	Synthesis and evaluation of acridine- and acridone-based anti-herpes agents with topoisomerase activity. Bioorganic and Medicinal Chemistry, 2006, 14, 5467-5480.	3.0	131
35	Molecular recognition of opioid receptor ligands. AAPS Journal, 2006, 8, E126-E137.	4.4	71
36	Identification of Compounds with Anti-West Nile Virus Activity. Journal of Medicinal Chemistry, 2006, 49, 2127-2137.	6.4	128

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37	A combined ligand-based and target-based drug design approach for G-protein coupled receptors: application to salvinorin A, a selective kappa opioid receptor agonist. Journal of Computer-Aided Molecular Design, 2006, 20, 471-493.	2.9	43
38	Editorial [Hot Topic:Opioid Receptors (Guest Editor: David M. Ferguson)]. Current Topics in Medicinal Chemistry, 2005, 5, 301-302.	2.1	0
39	High-Throughput Assays Using a Luciferase-Expressing Replicon, Virus-Like Particles, and Full-Length Virus for West Nile Virus Drug Discovery. Antimicrobial Agents and Chemotherapy, 2005, 49, 4980-4988.	3.2	108
40	3'-Exonuclease resistance of DNA oligodeoxynucleotides containing O6-[4-oxo-4-(3-pyridyl)butyl]guanine. Nucleic Acids Research, 2003, 31, 1984-1994.	14.5	17
41	4 Molecular Modeling of Opioid Receptor-Ligand Complexes. Progress in Medicinal Chemistry, 2002, 40, 107-135.	10.4	8
42	Cationâˆ'Ï€ Interactions:â€‰ An Energy Decomposition Analysis and Its Implication in Î´-Opioid Receptorâˆ'Ligand Binding. Journal of the American Chemical Society, 2002, 124, 4832-4837.	13.7	131
43	Stereochemical requirements for receptor recognition of the Î¼-opioid peptide endomorphin-1: Biological activity, NMR and conformational analysis of D-amino acid substituted analogs. , 2002, , 624-625.		0
44	Covalently Induced Activation of the Î´ Opioid Receptor by a Fluorogenic Affinity Label, 7â€²-(Phthalaldehydecarboxamido)naltrindole (PNTI). Journal of Medicinal Chemistry, 2001, 44, 1017-1020.	6.4	16
45	Investigation of the Selectivity of Oxymorphone- and Naltrexone-Derived Ligands via Site-Directed Mutagenesis of Opioid Receptors:Â Exploring the â€˜Address' Recognition Locus. Journal of Medicinal Chemistry, 2001, 44, 857-862.	6.4	79
46	Transformation of a Îº-Opioid Receptor Antagonist to a Îº-Agonist by Transfer of a Guanidinium Group from the 5â€²- to 6â€²-Position of Naltrindole. Journal of Medicinal Chemistry, 2001, 44, 2073-2079.	6.4	62
47	Exploring the unique pharmacology of a novel opioid receptor, ZFOR1, using molecular modeling and the `messageâ€"address' concept. Protein Engineering, Design and Selection, 2001, 14, 953-960.	2.1	6
48	Molecular Docking Reveals a Novel Binding Site Model for Fentanyl at the Î¼-Opioid Receptor. Journal of Medicinal Chemistry, 2000, 43, 381-391.	6.4	92
49	Stereochemical Requirements for Receptor Recognition of the Î¼-Opioid Peptide Endomorphin-1. Biophysical Journal, 2000, 78, 590-599.	0.5	75
50	Potent and Selective Indolomorphinan Antagonists of the Kappa-Opioid Receptor. Journal of Medicinal Chemistry, 2000, 43, 2759-2769.	6.4	106
51	Isosteric Replacement of Acidic with Neutral Residues in Extracellular Loop-2 of the Îº-Opioid Receptor Does Not Affect Dynorphin A(1âˆ'13) Affinity and Function. Journal of Medicinal Chemistry, 2000, 43, 1251-1252.	6.4	24
52	Structural properties of DNA:RNA duplexes containing 2'-O-methyl and 2'-S-methyl substitutions: a molecular dynamics investigation. Nucleic Acids Research, 1999, 27, 2189-2195.	14.5	42
53	Effects of C2â€²-Substitution on Arabinonucleic Acid Structure and Conformation. Journal of the American Chemical Society, 1999, 121, 5609-5610.	13.7	25
54	Constant temperature simulations using the Langevin equation with velocity Verlet integration. Chemical Physics, 1998, 236, 243-252.	1.9	176

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55	Conformational analysis of the endogenous Î¼-opioid agonist endomorphin-1 using NMR spectroscopy and molecular modeling. FEBS Letters, 1998, 439, 13-20.	2.8	72
56	Conformational Analysis and Automated Receptor Docking of Selective Arylacetamide-Based Î¼-Opioid Agonists. Journal of Medicinal Chemistry, 1998, 41, 4777-4789.	6.4	56
57	Structural characteristics of 2'-O-(2-methoxyethyl)-modified nucleic acids from molecular dynamics simulations. Nucleic Acids Research, 1998, 26, 3694-3699.	14.5	31
58	Parameterization and Simulation of the Physical Properties of Phosphorothioate Nucleic Acids. ACS Symposium Series, 1997, , 41-54.	0.5	1
59	Molecular Simulation of Dynorphin A-(1â^'10) Binding to Extracellular Loop 2 of the Î¼-Opioid Receptor. A Model for Receptor Activation. Journal of Medicinal Chemistry, 1997, 40, 3254-3262.	6.4	78
60	Analysis of the Malondialdehydeâ^'2â€˜- Deoxyguanosine Adduct Pyrimidopurinone in Human Leukocyte DNA by Gas Chromatography/Electron Capture/Negative Chemical Ionization/Mass Spectrometry. Chemical Research in Toxicology, 1997, 10, 181-188.	3.3	112
61	A computational analysis of interaction energies in methane and neopentane dimer systems. Journal of Computational Chemistry, 1997, 18, 70-79.	3.3	24
62	Knowledge-based modeling of a bacterial dichloromethane dehalogenase. , 1997, 28, 217-226.		27
63	An Analysis of the Conserved Residues between Halobacterial Retinal Proteins and G-Protein Coupled Receptors:â€‰ Implications for GPCR Modeling. Journal of Chemical Information and Computer Sciences, 1996, 36, 857-861.	2.8	15
64	Identification of Helical Packing Motifs Common to Bacteriorhodopsin and G Protein-Coupled Receptors. Journal of Molecular Modeling, 1996, 3, 70.	1.8	0
65	Application of the message-address concept to the docking of naltrexone and selective naltrexone-derived opioid antagonists into opioid receptor models. Neurochemical Research, 1996, 21, 1287-1294.	3.3	87
66	AMBER, a package of computer programs for applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules. Computer Physics Communications, 1995, 91, 1-41.	7.5	2,839
67	Parameterization and evaluation of a flexible water model. Journal of Computational Chemistry, 1995, 16, 501-511.	3.3	122
68	Isothermal-isobaric molecular dynamics simulations with Monte Carlo volume sampling. Computer Physics Communications, 1995, 91, 283-289.	7.5	141
69	A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. Journal of the American Chemical Society, 1995, 117, 5179-5197.	13.7	12,116
70	On the role of extracellular loops of opioid receptors in conferring ligand selectivity. FEBS Letters, 1995, 375, 1-4.	2.8	66
71	Conformational searches for the global minimum of protein models. Journal of Global Optimization, 1994, 4, 209-227.	1.8	7
72	On the use of acceptance ratio methods in free energy calculations. Journal of Chemical Physics, 1993, 99, 10086-10087.	3.0	13

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73	New results on protein folding from simulated annealing. Journal of the American Chemical Society, 1992, 114, 6555-6556.	13.7	20
74	Free energy perturbation calculations involving potential function changes. Journal of Computational Chemistry, 1992, 13, 362-370.	3.3	29
75	Comparison ofab initio, semiempirical, and molecular mechanics calculations for the conformational analysis of ring systems. Journal of Computational Chemistry, 1992, 13, 525-532.	3.3	51
76	Alternative expressions for energies and forces due to angle bending and torsional energy. Journal of Computational Chemistry, 1992, 13, 585-594.	3.3	19
77	How transferable are hydrogen parameters in molecular mechanics calculations?. Journal of Computational Chemistry, 1992, 13, 971-978.	3.3	33
78	Determination of the relative binding free energies of peptide inhibitors to the HIV-1 protease. Journal of Medicinal Chemistry, 1991, 34, 2654-2659.	6.4	87
79	Application of Free-Energy Decomposition to Determine the Relative Stability of R and S Oligodeoxyribonucleotide Methylphosphonates. Antisense Research and Development, 1991, 1, 243-254.	3.1	10
80	Can the Lennard-Jones 6-12 function replace the 10-12 form in molecular mechanics calculations?. Journal of Computational Chemistry, 1991, 12, 620-626.	3.3	97
81	Molecular mechanics calculations of several lanthanide complexes: An application of the random incremental pulse search. Journal of Computational Chemistry, 1990, 11, 1061-1071.	3.3	34
82	Molecular mechanics conformational analysis of cyclononane using the RIPS method and comparison with quantum-mechanical calculations. Journal of Computational Chemistry, 1989, 10, 903-910.	3.3	39
83	A new approach to probing conformational space with molecular mechanics: random incremental pulse search. Journal of the American Chemical Society, 1989, 111, 4371-4378.	13.7	198
84	Structures of lanthanide shift reagent complexes by molecular mechanics computations. Computational and Theoretical Chemistry, 1985, 124, 343-351.	1.5	26