

# David M Ferguson

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/619597/publications.pdf>

Version: 2024-02-01

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	A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. <i>Journal of the American Chemical Society</i> , 1995, 117, 5179-5197.	13.7	12,116
2	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. <i>Computer Physics Communications</i> , 1995, 91, 1-41.	7.5	2,839
3	A new approach to probing conformational space with molecular mechanics: random incremental pulse search. <i>Journal of the American Chemical Society</i> , 1989, 111, 4371-4378.	13.7	198
4	Constant temperature simulations using the Langevin equation with velocity Verlet integration. <i>Chemical Physics</i> , 1998, 236, 243-252.	1.9	176
5	Isothermal-isobaric molecular dynamics simulations with Monte Carlo volume sampling. <i>Computer Physics Communications</i> , 1995, 91, 283-289.	7.5	141
6	Polymeric nanoparticles encapsulating novel TLR7/8 agonists as immunostimulatory adjuvants for enhanced cancer immunotherapy. <i>Biomaterials</i> , 2018, 164, 38-53.	11.4	133
7	Cation- $\pi$ Interactions: An Energy Decomposition Analysis and Its Implication in $\mu$ -Opioid Receptor-Ligand Binding. <i>Journal of the American Chemical Society</i> , 2002, 124, 4832-4837.	13.7	131
8	Synthesis and evaluation of acridine- and acridone-based anti-herpes agents with topoisomerase activity. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 5467-5480.	3.0	131
9	Identification of Compounds with Anti-West Nile Virus Activity. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 2127-2137.	6.4	128
10	Parameterization and evaluation of a flexible water model. <i>Journal of Computational Chemistry</i> , 1995, 16, 501-511.	3.3	122
11	Analysis of the Malondialdehyde-2'-Deoxyguanosine Adduct Pyrimidopurine in Human Leukocyte DNA by Gas Chromatography/Electron Capture/Negative Chemical Ionization/Mass Spectrometry. <i>Chemical Research in Toxicology</i> , 1997, 10, 181-188.	3.3	112
12	High-Throughput Assays Using a Luciferase-Expressing Replicon, Virus-Like Particles, and Full-Length Virus for West Nile Virus Drug Discovery. <i>Antimicrobial Agents and Chemotherapy</i> , 2005, 49, 4980-4988.	3.2	108
13	Triaryl Pyrazoline Compound Inhibits Flavivirus RNA Replication. <i>Antimicrobial Agents and Chemotherapy</i> , 2006, 50, 1320-1329.	3.2	107
14	Potent and Selective Indolomorphinan Antagonists of the Kappa-Opioid Receptor. <i>Journal of Medicinal Chemistry</i> , 2000, 43, 2759-2769.	6.4	106
15	Can the Lennard-Jones 6-12 function replace the 10-12 form in molecular mechanics calculations?. <i>Journal of Computational Chemistry</i> , 1991, 12, 620-626.	3.3	97
16	Acridine-Based Agents with Topoisomerase II Activity Inhibit Pancreatic Cancer Cell Proliferation and Induce Apoptosis. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 179-182.	6.4	94
17	Molecular Docking Reveals a Novel Binding Site Model for Fentanyl at the $\mu$ -Opioid Receptor. <i>Journal of Medicinal Chemistry</i> , 2000, 43, 381-391.	6.4	92
18	Synthesis and cancer cell cytotoxicity of substituted xanthenes. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 1456-1463.	3.0	89

#	ARTICLE	IF	CITATIONS
19	Determination of the relative binding free energies of peptide inhibitors to the HIV-1 protease. <i>Journal of Medicinal Chemistry</i> , 1991, 34, 2654-2659.	6.4	87
20	Application of the message-address concept to the docking of naltrexone and selective naltrexone-derived opioid antagonists into opioid receptor models. <i>Neurochemical Research</i> , 1996, 21, 1287-1294.	3.3	87
21	Investigation of the Selectivity of Oxymorphone- and Naltrexone-Derived Ligands via Site-Directed Mutagenesis of Opioid Receptors: Exploring the "Address" Recognition Locus. <i>Journal of Medicinal Chemistry</i> , 2001, 44, 857-862.	6.4	79
22	Molecular Simulation of Dynorphin A-(1-10) Binding to Extracellular Loop 2 of the $\mu$ -Opioid Receptor. A Model for Receptor Activation. <i>Journal of Medicinal Chemistry</i> , 1997, 40, 3254-3262.	6.4	78
23	Stereochemical Requirements for Receptor Recognition of the $\mu$ -Opioid Peptide Endomorphin-1. <i>Biophysical Journal</i> , 2000, 78, 590-599.	0.5	75
24	Conformational analysis of the endogenous $\mu$ -opioid agonist endomorphin-1 using NMR spectroscopy and molecular modeling. <i>FEBS Letters</i> , 1998, 439, 13-20.	2.8	72
25	Molecular recognition of opioid receptor ligands. <i>AAPS Journal</i> , 2006, 8, E126-E137.	4.4	71
26	On the role of extracellular loops of opioid receptors in conferring ligand selectivity. <i>FEBS Letters</i> , 1995, 375, 1-4.	2.8	66
27	Transformation of a $\mu$ -Opioid Receptor Antagonist to a $\mu$ -Agonist by Transfer of a Guanidinium Group from the 5 $\alpha$ - to 6 $\alpha$ -Position of Naltrindole. <i>Journal of Medicinal Chemistry</i> , 2001, 44, 2073-2079.	6.4	62
28	Novel acridine-based compounds that exhibit an anti-pancreatic cancer activity are catalytic inhibitors of human topoisomerase II. <i>European Journal of Pharmacology</i> , 2009, 602, 223-229.	3.5	60
29	Acidic pH-responsive polymer nanoparticles as a TLR7/8 agonist delivery platform for cancer immunotherapy. <i>Nanoscale</i> , 2018, 10, 20851-20862.	5.6	59
30	Conformational Analysis and Automated Receptor Docking of Selective Arylacetamide-Based $\mu$ -Opioid Agonists. <i>Journal of Medicinal Chemistry</i> , 1998, 41, 4777-4789.	6.4	56
31	Comparison of ab initio, semiempirical, and molecular mechanics calculations for the conformational analysis of ring systems. <i>Journal of Computational Chemistry</i> , 1992, 13, 525-532.	3.3	51
32	Structure-Activity Relationship Analysis of Imidazoquinolines with Toll-like Receptors 7 and 8 Selectivity and Enhanced Cytokine Induction. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 339-347.	6.4	49
33	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. <i>Journal of Computer-Aided Molecular Design</i> , 2006, 20, 471-493.	2.9	43
34	Structural properties of DNA:RNA duplexes containing 2'-O-methyl and 2'-S-methyl substitutions: a molecular dynamics investigation. <i>Nucleic Acids Research</i> , 1999, 27, 2189-2195.	14.5	42
35	Toward a Structure-Based Model of Salvinorin A Recognition of the $\mu$ -Opioid Receptor. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 1824-1830.	6.4	42
36	Molecular mechanics conformational analysis of cyclononane using the RIPS method and comparison with quantum-mechanical calculations. <i>Journal of Computational Chemistry</i> , 1989, 10, 903-910.	3.3	39

#	ARTICLE	IF	CITATIONS
37	A unique binding epitope for salvinorinâ€fA, a non-nitrogenous kappa opioid receptor agonist. FEBS Journal, 2006, 273, 1966-1974.	4.7	35
38	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
39	How transferable are hydrogen parameters in molecular mechanics calculations?. Journal of Computational Chemistry, 1992, 13, 971-978.	3.3	33
40	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
41	Discovery of Imidazoquinolines with Toll-Like Receptor 7/8 Independent Cytokine Induction. ACS Medicinal Chemistry Letters, 2012, 3, 501-504.	2.8	33
42	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
43	Structural characteristics of 2'-O-(2-methoxyethyl)-modified nucleic acids from molecular dynamics simulations. Nucleic Acids Research, 1998, 26, 3694-3699.	14.5	31
44	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
45	Free energy perturbation calculations involving potential function changes. Journal of Computational Chemistry, 1992, 13, 362-370.	3.3	29
46	TLR7/8 Agonist-Loaded Nanoparticles Augment NK Cell-Mediated Antibody-Based Cancer Immunotherapy. Molecular Pharmaceutics, 2020, 17, 2109-2124.	4.6	28
47	Knowledge-based modeling of a bacterial dichloromethane dehalogenase. , 1997, 28, 217-226.		27
48	Synthesis and evaluation of N-alkyl-9-aminoacridines with antibacterial activity. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 3014-3017.	2.2	27
49	Structures of lanthanide shift reagent complexes by molecular mechanics computations. Computational and Theoretical Chemistry, 1985, 124, 343-351.	1.5	26
50	Effects of C2â€-Substitution on Arabinonucleic Acid Structure and Conformation. Journal of the American Chemical Society, 1999, 121, 5609-5610.	13.7	25
51	A computational analysis of interaction energies in methane and neopentane dimer systems. Journal of Computational Chemistry, 1997, 18, 70-79.	3.3	24
52	Isosteric Replacement of Acidic with Neutral Residues in Extracellular Loop-2 of the Î²-Opioid Receptor Does Not Affect Dynorphin A(1âˆˆ13) Affinity and Function. Journal of Medicinal Chemistry, 2000, 43, 1251-1252.	6.4	24
53	A Cinchona Alkaloid Antibiotic That Appears To Target ATP Synthase in <i>Streptococcus pneumoniae</i> . Journal of Medicinal Chemistry, 2019, 62, 2305-2332.	6.4	24
54	Investigation of ( <i>S</i> )-â€-Acidomycin: A Selective Antimycobacterial Natural Product That Inhibits Biotin Synthase. ACS Infectious Diseases, 2019, 5, 598-617.	3.8	22

#	ARTICLE	IF	CITATIONS
55	Quantitative Three Dimensional Structure Linear Interaction Energy Model of 5â€²-(Salicyl)sulfamoyl]adenosine and the Aryl Acid Adenylating Enzyme MbtA. Journal of Medicinal Chemistry, 2008, 51, 7154-7160.	6.4	21
56	Structure and Stability of Human Telomeric G-Quadruplex with Preclinical 9-Amino Acridines. PLoS ONE, 2013, 8, e57701.	2.5	21
57	New results on protein folding from simulated annealing. Journal of the American Chemical Society, 1992, 114, 6555-6556.	13.7	20
58	Alternative expressions for energies and forces due to angle bending and torsional energy. Journal of Computational Chemistry, 1992, 13, 585-594.	3.3	19
59	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
60	Novel TLR 7/8 agonists for improving NK cell mediated antibody-dependent cellular cytotoxicity (ADCC). Scientific Reports, 2021, 11, 3346.	3.3	17
61	Covalently Induced Activation of the Î Opioid Receptor by a Fluorogenic Affinity Label, 7â€³-(Phthalaldehydecaboxamido)naltrexone (PNTI). Journal of Medicinal Chemistry, 2001, 44, 1017-1020.	6.4	16
62	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
63	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
64	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
65	Avoiding Antibiotic Inactivation in <i>Mycobacterium tuberculosis</i> by Rv3406 through Strategic Nucleoside Modification. ACS Infectious Diseases, 2018, 4, 1102-1113.	3.8	14
66	On the use of acceptance ratio methods in free energy calculations. Journal of Chemical Physics, 1993, 99, 10086-10087.	3.0	13
67	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
68	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
69	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
70	Application of Free-Energy Decomposition to Determine the Relative Stability of <i>R</i> and <i>S</i> Oligodeoxyribonucleotide Methylphosphonates. Antisense Research and Development, 1991, 1, 243-254.	3.1	10
71	4 Molecular Modeling of Opioid Receptor-Ligand Complexes. Progress in Medicinal Chemistry, 2002, 40, 107-135.	10.4	8
72	Conformational searches for the global minimum of protein models. Journal of Global Optimization, 1994, 4, 209-227.	1.8	7

#	ARTICLE	IF	CITATIONS
73	Simulated Annealing-Optimal Histogram Methods. <i>Advances in Chemical Physics</i> , 2007, , 311-336.	0.3	7
74	Exploring the unique pharmacology of a novel opioid receptor, ZFOR1, using molecular modeling and the 'message-address' concept. <i>Protein Engineering, Design and Selection</i> , 2001, 14, 953-960.	2.1	6
75	Toll-like receptor 7 and 8 imidazoquinoline-based agonist/antagonist pairs. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2022, 59, 128548.	2.2	4
76	Targeting Topoisomerase II Activity in NSCLC with 9-Aminoacridine Derivatives. <i>Anticancer Research</i> , 2015, 35, 5211-7.	1.1	4
77	4-Amino-2-butyl-7-methoxycarbonylthiazolo[4,5-c]quinoline. <i>MolBank</i> , 2021, 2021, M1305.	0.5	3
78	Parameterization and Simulation of the Physical Properties of Phosphorothioate Nucleic Acids. <i>ACS Symposium Series</i> , 1997, , 41-54.	0.5	1
79	Identification of Helical Packing Motifs Common to Bacteriorhodopsin and G Protein-Coupled Receptors. <i>Journal of Molecular Modeling</i> , 1996, 3, 70.	1.8	0
80	Editorial [Hot Topic:Opioid Receptors (Guest Editor: David M. Ferguson)]. <i>Current Topics in Medicinal Chemistry</i> , 2005, 5, 301-302.	2.1	0
81	In honor of Professor Robert Vince on the occasion of his 80th birthday. <i>Medicinal Chemistry Research</i> , 2021, 30, 303-304.	2.4	0
82	Molecular Recognition of Opioid Receptor Ligands. , 2008, , 585-608.		0
83	Stereochemical requirements for receptor recognition of the $\mu$ -opioid peptide endomorphin-1: Biological activity, NMR and conformational analysis of D-amino acid substituted analogs. , 2002, , 624-625.		0
84	Parameterization and Application of the General Amber Force Field to Model Fluoro Substituted Furanose Moieties and Nucleosides. <i>Molecules</i> , 2022, 27, 2616.	3.8	0