

# Kirk E Hevener

## List of Publications by Year in descending order

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39  
papers

1,687  
citations

430442

18  
h-index

315357

38  
g-index

39  
all docs

39  
docs citations

39  
times ranked

2872  
citing authors

#	ARTICLE	IF	CITATIONS
1	Validation of Molecular Docking Programs for Virtual Screening against Dihydropteroate Synthase. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 444-460.	2.5	367
2	Hit Identification and Optimization in Virtual Screening: Practical Recommendations Based on a Critical Literature Analysis. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 6560-6572.	2.9	215
3	Recent developments in topoisomerase-targeted cancer chemotherapy. <i>Acta Pharmaceutica Sinica B</i> , 2018, 8, 844-861.	5.7	166
4	Comparison of radii sets, entropy, QM methods, and sampling on MM-PBSA, MM-GBSA, and QM/MM-GBSA ligand binding energies of <i>F. tularensis</i> enoyl-ACP reductase (FabI). <i>Journal of Computational Chemistry</i> , 2015, 36, 1859-1873.	1.5	91
5	Synthesis and Evaluation of Nitrofuranylamides as Novel Antituberculosis Agents. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 5276-5283.	2.9	81
6	A statistical framework to evaluate virtual screening. <i>BMC Bioinformatics</i> , 2009, 10, 225.	1.2	81
7	Structural Studies of Pterin-Based Inhibitors of Dihydropteroate Synthase. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 166-177.	2.9	81
8	Structure-activity relationships and enzyme inhibition of pantothenamide-type pantothenate kinase inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 1007-1020.	1.4	61
9	Discovery of a Novel and Potent Class of <i>F. tularensis</i> Enoyl-Reductase (FabI) Inhibitors by Molecular Shape and Electrostatic Matching. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 268-279.	2.9	57
10	The Structure of the Pantothenate Kinase-ADP-Pantothenate Ternary Complex Reveals the Relationship between the Binding Sites for Substrate, Allosteric Regulator, and Antimetabolites. <i>Journal of Biological Chemistry</i> , 2004, 279, 35622-35629.	1.6	47
11	Quantitative structure-activity relationship studies on nitrofuranyl anti-tubercular agents. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 8042-8053.	1.4	46
12	Constitutive expression of the cryptic vanGcd operon promotes vancomycin resistance in <i>Clostridioides difficile</i> clinical isolates. <i>Journal of Antimicrobial Chemotherapy</i> , 2020, 75, 859-867.	1.3	39
13	The Fatty Acid Synthesis Protein Enoyl-ACP Reductase II (FabK) is a Target for Narrow-Spectrum Antibacterials for <i>Clostridium difficile</i> Infection. <i>ACS Infectious Diseases</i> , 2019, 5, 208-217.	1.8	30
14	Hit-to-Lead: Hit Validation and Assessment. <i>Methods in Enzymology</i> , 2018, 610, 265-309.	0.4	23
15	High-Throughput Screening (HTS) and Hit Validation to Identify Small Molecule Inhibitors with Activity against NS3/4A proteases from Multiple Hepatitis C Virus Genotypes. <i>PLoS ONE</i> , 2013, 8, e75144.	1.1	21
16	Structural and Enzymatic Analyses Reveal the Binding Mode of a Novel Series of <i>Francisella tularensis</i> Enoyl Reductase (FabI) Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 5933-5941.	2.9	20
17	Pharmacophore Modeling, Synthesis, and Antibacterial Evaluation of Chalcones and Derivatives. <i>ACS Omega</i> , 2018, 3, 18343-18360.	1.6	20
18	Second-Generation Antidiabetic Sulfonylureas Inhibit <i>Candida albicans</i> and Candidalysin-Mediated Activation of the NLRP3 Inflammasome. <i>Antimicrobial Agents and Chemotherapy</i> , 2020, 64, .	1.4	20

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19	Synergistic Inhibitor Binding to the Papain-Like Protease of Human SARS Coronavirus: Mechanistic and Inhibitor Design Implications. <i>ChemMedChem</i> , 2013, 8, 1361-1372.	1.6	19
20	Recent advances in the rational design and optimization of antibacterial agents. <i>MedChemComm</i> , 2016, 7, 1694-1715.	3.5	19
21	Fragment-Based Drug Discovery Using a Multidomain, Parallel MD-MM/PBSA Screening Protocol. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 560-572.	2.5	18
22	Structural and biological evaluation of a novel series of benzimidazole inhibitors of <i>Francisella tularensis</i> enoyl-ACP reductase (FabI). <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015, 25, 1292-1296.	1.0	18
23	Computational Toxicology Methods in Chemical Library Design and High-Throughput Screening Hit Validation. <i>Methods in Molecular Biology</i> , 2018, 1800, 275-285.	0.4	18
24	High-level expression, purification, and characterization of <i>Staphylococcus aureus</i> dihydroorotase (PyrC) as a cleavable His-SUMO fusion. <i>Protein Expression and Purification</i> , 2013, 88, 98-106.	0.6	16
25	Rifamycin Resistance in <i>Clostridium difficile</i> Is Generally Associated with a Low Fitness Burden. <i>Antimicrobial Agents and Chemotherapy</i> , 2016, 60, 5604-5607.	1.4	16
26	The Vacuolar Ca <sup>2+</sup> ATPase Pump Pmc1p Is Required for <i>Candida albicans</i> Pathogenesis. <i>MSphere</i> , 2019, 4, .	1.3	14
27	Structural characterization of <i>Porphyromonas gingivalis</i> enoyl-ACP reductase II (FabK). <i>Acta Crystallographica Section F, Structural Biology Communications</i> , 2018, 74, 105-112.	0.4	11
28	Identification of Small Molecules Exhibiting Oxacillin Synergy through a Novel Assay for Inhibition of <i>vraTSR</i> Expression in Methicillin-Resistant <i>Staphylococcus aureus</i> . <i>Antimicrobial Agents and Chemotherapy</i> , 2019, 63, .	1.4	10
29	DPAGT1 Inhibitors of Capuramycin Analogues and Their Antimigratory Activities of Solid Tumors. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 10855-10878.	2.9	10
30	Antibacterial kaneoeic acids A-F from a Hawaiian fungus <i>Fusarium</i> sp. FM701. <i>Phytochemistry</i> , 2021, 181, 112545.	1.4	9
31	Small-Molecule Inhibition of the <i>C. difficile</i> FAS-II Enzyme, FabK, Results in Selective Activity. <i>ACS Chemical Biology</i> , 2019, 14, 1528-1535.	1.6	8
32	Concise Synthesis of Tunicamycin and Discovery of a Cytostatic DPAGT1 Inhibitor. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	7
33	Special Challenges to the Rational Design of Antibacterial Agents. <i>Annual Reports in Medicinal Chemistry</i> , 2013, 48, 283-298.	0.5	6
34	The Discovery and Development of Thienopyrimidines as Inhibitors of <i>Helicobacter pylori</i> That Act through Inhibition of the Respiratory Complex I. <i>ACS Infectious Diseases</i> , 2021, 7, 1044-1058.	1.8	6
35	Expression, purification and characterization of enoyl-ACP reductase II, FabK, from <i>Porphyromonas gingivalis</i> . <i>Protein Expression and Purification</i> , 2012, 85, 100-108.	0.6	5
36	Crystal structure of the 65-kilodalton amino-terminal fragment of DNA topoisomerase I from the gram-positive model organism <i>Streptococcus mutans</i> . <i>Biochemical and Biophysical Research Communications</i> , 2019, 516, 333-338.	1.0	5

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37	A simplified protocol for high-yield expression and purification of bacterial topoisomerase I. <i>Protein Expression and Purification</i> , 2016, 124, 32-40.	0.6	2
38	Identification of Dual-Target Compounds with Antifungal and Anti-NLRP3 Inflammasome Activity. <i>ACS Infectious Diseases</i> , 2021, 7, 2522-2535.	1.8	2
39	Concise Synthesis of Tunicamycin V and Discovery of a Cytostatic DPAGT1 Inhibitor. <i>Angewandte Chemie</i> , 0, , .	1.6	2