David G Lloyd

List of Publications by Year
in descending order

56 papers	1,654 citations	257429 24 h-index	302107 39 g-index
59 all docs	59 docs citations	59 times ranked	2370 citing authors

#	Article	IF	Citations
1	Comprehensive characterization of cytochrome P450 isozyme selectivity across chemical libraries. Nature Biotechnology, 2009, 27, 1050-1055.	17.5	154
2	Synthesis and Evaluation of Azetidinone Analogues of Combretastatin A-4 as Tubulin Targeting Agents. Journal of Medicinal Chemistry, 2010, 53, 8569-8584.	6.4	111
3	On the molecular pathology of neurodegeneration in IMPDH1-based retinitis pigmentosa. Human Molecular Genetics, 2004, 13, 641-650.	2.9	86
4	Scaffold Hopping in De Novo Design. Ligand Generation in the Absence of Receptor Information. Journal of Medicinal Chemistry, 2004, 47, 493-496.	6.4	69
5	Synthesis, evaluation and structural studies of antiproliferative tubulin-targeting azetidin-2-ones. Bioorganic and Medicinal Chemistry, 2011, 19, 2306-2325.	3.0	62
6	Lead identification of conformationally restricted Î²-lactam type combretastatin analogues: Synthesis, antiproliferative activity and tubulin targeting effects. European Journal of Medicinal Chemistry, 2010, 45, 5752-5766.	5.5	61
7	Considerations in Compound Database Preparationâ€œHiddenâ€•Impact on Virtual Screening Results. Journal of Chemical Information and Modeling, 2005, 45, 1908-1919.	5.4	59
8	Beyond the Ligand-Binding Pocket: Targeting Alternate Sites in Nuclear Receptors. Medicinal Research Reviews, 2013, 33, 1081-1118.	10.5	59
9	Screening for Inhibitors of Tau Protein Aggregation into Alzheimer Paired Helical Filaments: A Ligand Based Approach Results in Successful Scaffold Hopping. Current Alzheimer Research, 2007, 4, 315-323.	1.4	57
10	Flexible Estrogen Receptor Modulators:Â Design, Synthesis, and Antagonistic Effects in Human MCF-7 Breast Cancer Cells. Journal of Medicinal Chemistry, 2001, 44, 1072-1084.	6.4	52
11	Benzoxepin-Derived Estrogen Receptor Modulators:Â A Novel Molecular Scaffold for the Estrogen Receptor. Journal of Medicinal Chemistry, 2004, 47, 5612-5615.	6.4	48
12	Unbiasing Scoring Functions:â€‰ A New Normalization and Rescoring Strategy. Journal of Chemical Information and Modeling, 2007, 47, 1564-1571.	5.4	48
13	Synthesis, biological evaluation, structuralâ€“activity relationship, and docking study for a series of benzoxepin-derived estrogen receptor modulators. Bioorganic and Medicinal Chemistry, 2008, 16, 9554-9573.	3.0	47
14	â€œTrueâ€•Antiandrogensâ€”Selective Non-Ligand-Binding Pocket Disruptors of Androgen Receptorâ€“Coactivator Interactions: Novel Tools for Prostate Cancer. Journal of Medicinal Chemistry, 2012, 55, 1635-1644.	6.4	47
15	Macrophage Migration Inhibitory Factor (MIF) Enzymatic Activity and Lung Cancer. Molecular Medicine, 2014, 20, 729-735.	4.4	47
16	Oncology exploration: charting cancer medicinal chemistry space. Drug Discovery Today, 2006, 11, 149-159.	6.4	46
17	Synthesis, biochemical and molecular modelling studies of antiproliferative azetidinones causing microtubule disruption and mitotic catastrophe. European Journal of Medicinal Chemistry, 2011, 46, 4595-4607.	5.5	41
18	Integration of Ligand and Structure-Based Virtual Screening for the Identification of the First Dual Targeting Agent for Heat Shock Protein 90 (Hsp90) and Tubulin. Journal of Medicinal Chemistry, 2009, 52, 2177-2180.	6.4	38

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19	Target Specific Virtual Screening:â€‰ Optimization of an Estrogen Receptor Screening Platform. Journal of Medicinal Chemistry, 2007, 50, 5301-5310.	6.4	37
20	The effect of tightly bound water molecules on the structural interpretation of ligand-derived pharmacophore models. Journal of Computer-Aided Molecular Design, 2004, 18, 89-100.	2.9	34
21	Estrogen Receptors: Molecular Interactions, Virtual Screening and Future Prospects. Current Topics in Medicinal Chemistry, 2006, 6, 217-243.	2.1	29
22	Integrated Virtual Screening for the Identification of Novel and Selective Peroxisome Proliferator-Activated Receptor (PPAR) Scaffolds. Journal of Medicinal Chemistry, 2012, 55, 4978-4989.	6.4	28
23	The Vascular Targeting Agent Combretastatin-A4 and a Novelcis-Restricted Î²-Lactam Analogue, CA-432, Induce Apoptosis in Human Chronic Myeloid Leukemia Cells and Ex Vivo Patient Samples Including Those Displaying Multidrug Resistance. Journal of Pharmacology and Experimental Therapeutics, 2010, 335, 302-313.	2.5	26
24	Novel microtubule-targeting agents, pyrrolo-1,5-benzoxazepines, induce apoptosis in multi-drug-resistant cancer cells. Cancer Chemotherapy and Pharmacology, 2010, 66, 585-596.	2.3	24
25	Virtual Screening for the Identification of Novel Nonsteroidal Glucocorticoid Modulators. Journal of Medicinal Chemistry, 2010, 53, 3065-3074.	6.4	22
26	Guanidinium-based derivatives: Searching for new kinase inhibitors. European Journal of Medicinal Chemistry, 2014, 81, 427-441.	5.5	22
27	Synthesis and serotonin transporter activity of sulphur-substituted Î±-alkyl phenethylamines as a new class of anticancer agents. European Journal of Medicinal Chemistry, 2009, 44, 4862-4888.	5.5	20
28	Lead identification of Î²-lactam and related imine inhibitors of the molecular chaperone heat shock protein 90. Bioorganic and Medicinal Chemistry, 2011, 19, 6055-6068.	3.0	18
29	Identification of plasmepsin inhibitors as selective anti-malarial agents using ligand based drug design. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 3335-3341.	2.2	18
30	Î²-Lactam type molecular scaffolds for antiproliferative activity: Synthesis and cytotoxic effects in breast cancer cells. Journal of Enzyme Inhibition and Medicinal Chemistry, 2008, 23, 668-685.	5.2	17
31	Study of E/Z Isomerization in a Series of Novel Non-ligand Binding Pocket Androgen Receptor Antagonists. Journal of Chemical Information and Modeling, 2012, 52, 2387-2397.	5.4	16
32	Retinazone Inhibits Certain Blood-Borne Human Viruses Including Ebola Virus Zaire. Antiviral Chemistry and Chemotherapy, 2014, 23, 197-215.	0.6	16
33	T2* placental MRI in pregnancies complicated with fetal congenital heart disease. Placenta, 2021, 108, 23-31.	1.5	16
34	Design, Synthesis and Biochemical Evaluation of Novel Selective Estrogen Receptor Ligand Conjugates Incorporating an Endoxifen-Combretastatin Hybrid Scaffold. Biomedicines, 2016, 4, 15.	3.2	14
35	Synthesis, Structure-Activity Relationships and Antagonistic Effects in Human MCF-7 Breast Cancer Cells of Flexible Estrogen Receptor Modulators. Medicinal Chemistry, 2005, 1, 335-353.	1.5	14
36	Lead identification of conformationally restricted benzoxepin type combretastatin analogs: synthesis, antiproliferative activity, and tubulin effects. Journal of Enzyme Inhibition and Medicinal Chemistry, 2010, 25, 180-194.	5.2	13

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37	Permuting input for more effective sampling of 3D conformer space. Journal of Computer-Aided Molecular Design, 2006, 20, 179-190.	2.9	11
38	Molecular Topology Applied to the Discovery of 1-Benzyl-2-(3-fluorophenyl)-4-hydroxy-3-(3-phenylpropanoyl)-2H-pyrrole-5-one as a Non-Ligand-Binding-Pocket Antiandrogen. Journal of Chemical Information and Modeling, 2014, 54, 2953-2966.	5.4	11
39	Structureâ€“activity studies with high-affinity inhibitors of pyroglutamyl-peptidase II. Biochemical Journal, 2005, 389, 569-576.	3.7	10
40	On the Effects of Permuted Input on Conformational Sampling of Drugâ€like Molecules: an Evaluation of Stochastic Proximity Embedding. Chemical Biology and Drug Design, 2007, 70, 123-133.	3.2	10
41	Theoretical studies of parent 1-, 2-, 3-pyrazolines and their methylated derivatives. Structural Chemistry, 2013, 24, 421-432.	2.0	10
42	Benzothiepin-derived molecular scaffolds for estrogen receptor modulators: synthesis and antagonistic effects in breast cancer cells. Journal of Enzyme Inhibition and Medicinal Chemistry, 2007, 22, 655-666.	5.2	9
43	Rational ligand-based virtual screening and structureâ€“activity relationship studies in the ligand-binding domain of the glucocorticoid receptor-Î±. Future Medicinal Chemistry, 2009, 1, 483-499.	2.3	8
44	Structureâ€“Activity Relationships in Non-Ligand Binding Pocket (Non-LBP) Diarylhydrazide Antiandrogens. Journal of Chemical Information and Modeling, 2013, 53, 2116-2130.	5.4	8
45	A topological study of prodrugs of 5-fluorouracil. International Journal of Pharmaceutics, 2002, 231, 241-251.	5.2	7
46	â€˜tieredScreenâ€™ â€“ Layered Virtual Screening Tool for the Identification of Novel Estrogen Receptor Alpha Modulators. Molecular Informatics, 2010, 29, 421-430.	2.5	7
47	Optimisation of estrogen receptor subtype-selectivity of a 4-Aryl-4H-chromene scaffold previously identified by virtual screening. Bioorganic and Medicinal Chemistry, 2020, 28, 115261.	3.0	7
48	Consensus Computational Ligandâ€Based Design for the Identification of Novel Modulators of Human Estrogen Receptor Alpha. Molecular Informatics, 2012, 31, 246-258.	2.5	6
49	Neutral Alkaline-Metal and Alkaline-Earth-Metal Derivatives of Imidazole and Benzimidazole. Journal of Physical Chemistry A, 2014, 118, 4195-4204.	2.5	6
50	Antiestrogenically Active 2-benzyl-1,1-diarylbut-2-enes: Synthesis, Structure- Activity Relationships and Molecular Modeling Study for Flexible Estrogen Receptor Antagonists. Medicinal Chemistry, 2006, 2, 147-168.	1.5	5
51	Flexible Estrogen Receptor Modulators: Synthesis, Biochemistry and Molecular Modeling Studies for 3-Benzyl-4,6-diarylhex-3-ene and 3,4,6-Triarylhex-3-ene Derivatives. Medicinal Chemistry, 2007, 3, 135-155.	1.5	5
52	Rational structure-based drug design and optimization in the ligand-binding domain of the glucocorticoid receptor-Î±. Future Medicinal Chemistry, 2009, 1, 345-359.	2.3	5
53	Development of the Î²-lactam type molecular scaffold for selective estrogen receptor Î± modulator action: synthesis and cytotoxic effects in MCF-7 breast cancer cells. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 117-130.	5.2	4
54	Virtual screening of the estrogen receptor. Expert Opinion on Drug Discovery, 2008, 3, 853-866.	5.0	3

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55	Fetal magnetic resonance imaging (MRI) enhances the diagnosis of congenital body anomalies. Journal of Pediatric Surgery, 2022, 57, 239-244.	1.6	3
56	Approaches to Scaffold Hopping. Drug Discovery Today: Technologies, 2013, 10, e451-e452.	4.0	2