David R Langley

List of Publications by Year
in descending order

81	5,617	94433 37	79698 73
papers	citations	h-index	g-index

83	83	83	5323
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	PROTAC targeted protein degraders: the past is prologue. Nature Reviews Drug Discovery, 2022, 21, 181-200.	46.4	912
2	Chemical genetics strategy identifies an HCV NS5A inhibitor with a potent clinical effect. Nature, 2010, 465, 96-100.	27.8	882
3	Selective Interactions of Cationic Porphyrins with G-Quadruplex Structures. Journal of the American Chemical Society, 2001, 123, 8902-8913.	13.7	311
4	Inhibition of Hepatitis B Virus Polymerase by Entecavir. Journal of Virology, 2007, 81, 3992-4001.	3.4	167
5	Biochemical and Genetic Characterizations of a Novel Human Immunodeficiency Virus Type 1 Inhibitor That Blocks gp120-CD4 Interactions. Journal of Virology, 2003, 77, 10528-10536.	3.4	166
6	Pyrrolo[1,4]benzodiazepine antitumor antibiotics: relationship of DNA alkylation and sequence specificity to the biological activity of natural and synthetic compounds. Chemical Research in Toxicology, 1988, 1, 258-268.	3.3	144
7	Inhibition of influenza virus replication via small molecules that induce the formation of higher-order nucleoprotein oligomers. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 15366-15371.	7.1	116
8	Molecular Dynamic Simulations of Environment and Sequence Dependent DNA Conformations: The Development of the BMS Nucleic Acid Force Field and Comparison with Experimental Results. Journal of Biomolecular Structure and Dynamics, 1998, 16, 487-509.	3.5	111
9	Crystal structures of trimeric HIV envelope with entry inhibitors BMS-378806 and BMS-626529. Nature Chemical Biology, 2017, 13, 1115-1122.	8.0	110
10	Chemistry and structure elucidation of the kedarcidin chromophore. Journal of the American Chemical Society, 1993, 115, 8432-8443.	13.7	109
11	Targeting a binding pocket within the trimer-of-hairpins: Small-molecule inhibition of viral fusion. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 15046-15051.	7.1	102
12	Inhibitors of HIV-1 Attachment: The Discovery and Development of Temsavir and its Prodrug Fostemsavir. Journal of Medicinal Chemistry, 2018, 61, 62-80.	6.4	98
13	A General Amino Acid Synthesis Enabled by Innate Radical Crossâ€Coupling. Angewandte Chemie - International Edition, 2018, 57, 14560-14565.	13.8	97
14	The crystal structure of NS5A domain 1 from genotype 1a reveals new clues to the mechanism of action for dimeric HCV inhibitors. Protein Science, 2014, 23, 723-734.	7.6	96
15	Discovery of a 2,4-Disubstituted Pyrrolo[1,2-f][1,2,4]triazine Inhibitor (BMS-754807) of Insulin-like Growth Factor Receptor (IGF-1R) Kinase in Clinical Development. Journal of Medicinal Chemistry, 2009, 52, 7360-7363.	6.4	87
16	Isolation, Structure Determination, and Proposed Mechanism of Action for Artifacts of Maduropeptin Chromophore. Journal of the American Chemical Society, 1994, 116, 9351-9352.	13.7	82
17	A versatile and efficient synthesis of carbinolamine-containing pyrrolo[1,4]benzodiazepines via the cyclization of N-(2-aminobenzoyl)pyrrolidine-2-carboxaldehyde diethyl thioacetals: total synthesis of prothracarcin. Journal of Organic Chemistry, 1987, 52, 91-97.	3.2	78
18	Discovery of new acylaminopyridines as GSK-3 inhibitors by a structure guided in-depth exploration of chemical space around a pyrrolopyridinone core. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 1856-1863.	2.2	78

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19	Hepatitis C Virus NS5A Replication Complex Inhibitors: The Discovery of Daclatasvir. Journal of Medicinal Chemistry, 2014, 57, 2013-2032.	6.4	74
20	The dynemicin-DNA intercalation complex: a model based on DNA affinity cleavage and molecular dynamics simulation. Journal of the American Chemical Society, 1991, 113, 4395-4403.	13.7	72
21	Discovery and Development of Hepatitis C Virus NS5A Replication Complex Inhibitors. Journal of Medicinal Chemistry, 2014, 57, 1643-1672.	6.4	68
22	O-Debenzylation of a Pyrrolo[2,1-c][1,4]benzodiazepine in the Presence of a Carbinolamine Functionality: Synthesis of DC-81. Synthesis, 1990, 1990, 81-84.	2.3	65
23	Chemoselective synthesis of allyltrimethylsilanes by cross-coupling of vinyl triflates with tris((trimethylsilyl)methyl)aluminum catalyzed by palladium(0). Journal of the American Chemical Society, 1989, 111, 8320-8321.	13.7	59
24	Synthesis and evaluation of 2-anilino-3-phenylsulfonyl-6-methylpyridines as corticotropin-releasing factor1 receptor ligands. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 934-937.	2.2	56
25	Genotypic correlates of susceptibility to HIV-1 attachment inhibitor BMS-626529, the active agent of the prodrug BMS-663068. Journal of Antimicrobial Chemotherapy, 2014, 69, 573-581.	3.0	56
26	Diastereoselective addition of Grignard reagents to azetidine-2,3-dione: Synthesis of novel TaxolÂ® analogues. Tetrahedron Letters, 1996, 37, 6495-6498.	1.4	54
27	Lattice engineering enables definition of molecular features allowing for potent small-molecule inhibition of HIV-1 entry. Nature Communications, 2019, 10, 47.	12.8	50
28	Molecular Basis for Increased Susceptibility of Isolates with Atazanavir Resistance-Conferring Substitution I50L to Other Protease Inhibitors. Antimicrobial Agents and Chemotherapy, 2005, 49, 3825-3832.	3.2	49
29	Changes to the HIV Long Terminal Repeat and to HIV Integrase Differentially Impact HIV Integrase Assembly, Activity, and the Binding of Strand Transfer Inhibitors. Journal of Biological Chemistry, 2007, 282, 31186-31196.	3.4	49
30	In VivoPatterns of Resistance to the HIV Attachment Inhibitor BMS-488043. Antimicrobial Agents and Chemotherapy, 2011, 55, 729-737.	3.2	47
31	Inhibitors of Human Immunodeficiency Virus Type 1 (HIV-1) Attachment. 12. Structureâ€“Activity Relationships Associated with 4-Fluoro-6-azaindole Derivatives Leading to the Identification of 1-(4-Benzoylpiperazin-1-yl)-2-(4-fluoro-7-[1,2,3]triazol-1-yl-1H-pyrrolo[2,3-c]pyridin-3-yl)ethane-1,2-dione (BMS-585248). Journal of Medicinal Chemistry, 2013, 56, 1656-1669.	6.4	47
32	Homology models of the <scp>HIV</scp>â€1 attachment inhibitor <scp>BMS</scp>â€626529 bound to gp120 suggest a unique mechanism of action. Proteins: Structure, Function and Bioinformatics, 2015, 83, 331-350.	2.6	47
33	Discovery of Isonicotinamides as Highly Selective, Brain Penetrable, and Orally Active Glycogen Synthase Kinase-3 Inhibitors. Journal of Medicinal Chemistry, 2016, 59, 1041-1051.	6.4	47
34	Characterizations of HCV NS5A replication complex inhibitors. Virology, 2013, 444, 343-354.	2.4	44
35	Resensitizing daclatasvir-resistant hepatitis C variants by allosteric modulation of NS5A. Nature, 2015, 527, 245-248.	27.8	44
36	The Terminal (Catalytic) Adenosine of the HIV LTR Controls the Kinetics of Binding and Dissociation of HIV Integrase Strand Transfer Inhibitors. Biochemistry, 2008, 47, 13481-13488.	2.5	41

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37	New C-5 substituted pyrrolotriazine dual inhibitors of EGFR and HER2 protein tyrosine kinases. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 2036-2042.	2.2	38
38	Respiratory syncytial virus fusion inhibitors. Part 6: An examination of the effect of structural variation of the benzimidazol-2-one heterocycle moiety. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 4784-4790.	2.2	38
39	Discovery and initial SAR of 3-(1H-benzo[d]imidazol-2-yl)pyridin-2(1H)-ones as inhibitors of insulin-like growth factor 1-receptor (IGF-1R). Bioorganic and Medicinal Chemistry Letters, 2007, 17, 2317-2321.	2.2	37
40	Expanding GPCR homology model binding sites via a balloon potential: A molecular dynamics refinement approach. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1919-1929.	2.6	37
41	Synthesis of etoposide phosphate, BMY-40481: A water-soluble clinically active prodrug of etoposide. Bioorganic and Medicinal Chemistry Letters, 1994, 4, 2567-2572.	2.2	35
42	The DNA-esperamicin A1 complex. A model based on solvated molecular dynamics simulations. Journal of the American Chemical Society, 1994, 116, 15-29.	13.7	34
43	Discovery of the Human Immunodeficiency Virus Type 1 (HIV-1) Attachment Inhibitor Temsavir and Its Phosphonooxymethyl Prodrug Fostemsavir. Journal of Medicinal Chemistry, 2018, 61, 6308-6327.	6.4	34
44	Discovery of a Fluoroindolo[2,3-a]carbazole Clinical Candidate with Broad Spectrum Antitumor Activity in Preclinical Tumor Models Superior to the Marketed Oncology Drug, CPT-11â€. Journal of Medicinal Chemistry, 2005, 48, 2258-2261.	6.4	33
45	Mechanistic Characterization and Molecular Modeling of Hepatitis B Virus Polymerase Resistance to Entecavir. PLoS ONE, 2010, 5, e9195.	2.5	33
46	Respiratory syncytial virus fusion inhibitors. Part 5: Optimization of benzimidazole substitution patterns towards derivatives with improved activity. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 4592-4598.	2.2	32
47	E-Novo: An Automated Workflow for Efficient Structure-Based Lead Optimization. Journal of Chemical Information and Modeling, 2009, 49, 1797-1809.	5.4	32
48	E-ring desoxy analogs of etoposide. Journal of Medicinal Chemistry, 1989, 32, 1418-1420.	6.4	31
49	X-Ray Crystal Structures of Human Immunodeficiency Virus Type 1 Protease Mutants Complexed with Atazanavir. Journal of Virology, 2007, 81, 9525-9535.	3.4	29
50	Synthesis and stereochemistry of carbinolamine-containing pyrrolo[1,4]benzodiazepines by reductive cyclization of N-(2-nitrobenzoyl)pyrrolidine-2-carboxaldehydes. Journal of Organic Chemistry, 1986, 51, 705-712.	3.2	28
51	Facile Synthesis of a Simplified Bicyclo[7.3.1] Esperamicin-Calicheamicin Enediyne Core. Tetrahedron, 1994, 50, 1519-1538.	1.9	28
52	Novel C-5 aminomethyl pyrrolotriazine dual inhibitors of EGFR and HER2 protein tyrosine kinases. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 2828-2833.	2.2	27
53	5-((4-Aminopiperidin-1-yl)methyl)pyrrolotriazine dual inhibitors of EGFR and HER2 protein tyrosine kinases. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 4947-4954.	2.2	27
54	A General Amino Acid Synthesis Enabled by Innate Radical Crossâ€Coupling. Angewandte Chemie, 2018, 130, 14768-14773.	2.0	25

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55	Sequential 1H, 13C, and 15N-NMR Assignments and Solution Conformation of Apokedarcidin. Biochemistry, 1994, 33, 11438-11452.	2.5	24
56	Balancing oral exposure with Cyp3A4 inhibition in benzimidazole-based IGF-IR inhibitors. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 4075-4080.	2.2	24
57	Convergent approach to intermediates used for the synthesis of the enediyne structure of the esperamicins and calicheamicins. Tetrahedron Letters, 1989, 30, 3499-3500.	1.4	21
58	Treatment of Counterions in Computer Simulations of DNA. Reviews in Computational Chemistry, 2007, , 317-372.	1.5	21
59	Uncialamycin as a novel payload for antibody drug conjugate (ADC) based targeted cancer therapy. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 466-470.	2.2	21
60	Discovery and Optimization of Novel Pyrazolopyrimidines as Potent and Orally Bioavailable Allosteric HIV-1 Integrase Inhibitors. Journal of Medicinal Chemistry, 2020, 63, 2620-2637.	6.4	21
61	Electrostatic interaction of Ï€-Acidic amides with hydrogen-Bond acceptors. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 3261-3266.	2.2	20
62	2-(1H-Imidazol-4-yl)ethanamine and 2-(1H-pyrazol-1-yl)ethanamine side chain variants of the IGF-1R inhibitor BMS-536924. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 1702-1707.	2.2	20
63	The synthesis and biological activity of enediyne minor groove binding hybrids. Bioorganic and Medicinal Chemistry Letters, 1995, 5, 1049-1052.	2.2	17
64	Novel 3â€˜,6â€˜-Anhydro and N12,N13-Bridged Glycosylated Fluoroindolo[2,3-a]carbazoles as Topoisomerase I Inhibitors. Fluorine as a Leaving Group from sp3Carbon. Organic Letters, 2005, 7, 1271-1274.	4.6	16
65	Synthesis and antitumor properties of novel 14-Î²-hydroxytaxol and related analogues. Bioorganic and Medicinal Chemistry Letters, 1994, 4, 1565-1570.	2.2	15
66	Structure activity relationship studies of 3-arylsulfonyl-pyrido[1,2-a]pyrimidin-4-imines as potent 5-HT6 antagonists. Bioorganic and Medicinal Chemistry, 2014, 22, 1782-1790.	3.0	13
67	A Functional Na_V1.7-Na_VAb Chimera with a Reconstituted High-Affinity ProTx-II Binding Site. Molecular Pharmacology, 2017, 92, 310-317.	2.3	11
68	Reassignment of the structure for the antitumor agent RR-150.. Journal of Antibiotics, 1988, 41, 199-201.	2.0	10
69	Chemistry and structure elucidation of the kedarcidin chromophore. [Erratum to document cited in CA119(21):226387u]. Journal of the American Chemical Society, 1994, 116, 2233-2233.	13.7	9
70	MORPH: A New Tool for Ligand Design. Journal of Chemical Information and Modeling, 2010, 50, 1159-1164.	5.4	9
71	Probing the Underlying Basis for the Binding Specificity of Calicheamicin Î³1I. A Molecular Dynamics Study. Tetrahedron, 1994, 50, 1379-1396.	1.9	8
72	Nucleophilic Capture of the Imino-Quinone Methide Type Intermediates Generated from 2-Aminothiazol-5-yl Carbinols. Organic Letters, 2009, 11, 5154-5157.	4.6	8

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73	Heterocycle amide isosteres: An approach to overcoming resistance for HIV-1 integrase strand transfer inhibitors. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 126784.	2.2	7
74	Design, Synthesis, and Structureâ€“Activity Relationships of Novel Tetrahydroisoquinolino Benzodiazepine Dimer Antitumor Agents and Their Application in Antibodyâ€“Drug Conjugates. Journal of Medicinal Chemistry, 2020, 63, 13913-13950.	6.4	7
75	Communication: Quantum polarized fluctuating charge model: A practical method to include ligand polarizability in biomolecular simulations. Journal of Chemical Physics, 2011, 135, 231101.	3.0	6
76	Structure-based amelioration of PXR transactivation in a novel series of macrocyclic allosteric inhibitors of HIV-1 integrase. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127531.	2.2	6
77	Cloning, purification, crystallization and preliminary X-ray analysis of the catalytic domain of human receptor-like protein tyrosine phosphatase Î³ in three different crystal forms. Acta Crystallographica Section F: Structural Biology Communications, 2011, 67, 768-774.	0.7	3
78	Inhibitors of Protein-Protein Interactions in Paramyxovirus Fusion: A Focus on Respiratory Syncytial Virus. Topics in Medicinal Chemistry, 2012, , 167-196.	0.8	3
79	Efficient synthesis of (Z)- and (E)-methyl 2-(methoxyimino)-2-phenylacetate. Tetrahedron Letters, 2010, 51, 2144-2147.	1.4	2
80	DNA-Model-Based Design and Execution of Some Fused Benzodiazepine Hybrid Payloads for Antibodyâ€“Drug Conjugate Modality. ACS Medicinal Chemistry Letters, 2021, 12, 404-412.	2.8	2
81	Protein-Protein Interaction Targets to Inhibit HIV-1 Infection. Topics in Medicinal Chemistry, 2012, , 105-165.	0.8	0