Andrew G Leach

List of Publications by Year
in descending order

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107 papers	5,626 citations	94269 37 h-index	79541 73 g-index
116 all docs	116 docs citations	116 times ranked	6391 citing authors

#	Article	IF	Citations
1	Multi-step organic synthesis using solid-supported reagents and scavengers: a new paradigm in chemical library generation. Journal of the Chemical Society, Perkin Transactions 1, 2000, , 3815-4195.	1.3	665
2	Binding Affinities of Hostâ€“Guest, Proteinâ€“Ligand, and Proteinâ€“Transition-State Complexes. Angewandte Chemie - International Edition, 2003, 42, 4872-4897.	7.2	511
3	A Standard Set of Pericyclic Reactions of Hydrocarbons for the Benchmarking of Computational Methods:Â The Performance of ab Initio, Density Functional, CASSCF, CASPT2, and CBS-QB3 Methods for the Prediction of Activation Barriers, Reaction Energetics, and Transition State Geometries. Journal of Physical Chemistry A, 2003, 107, 11445-11459.	1.1	342
4	Protodeboronation of Heteroaromatic, Vinyl, and Cyclopropyl Boronic Acids: pHâ€“Rate Profiles, Autocatalysis, and Disproportionation. Journal of the American Chemical Society, 2016, 138, 9145-9157.	6.6	262
5	Mechanism of Ene Reactions of Singlet Oxygen. A Two-Step No-Intermediate Mechanism. Journal of the American Chemical Society, 2003, 125, 1319-1328.	6.6	259
6	Matched Molecular Pairs as a Guide in the Optimization of Pharmaceutical Properties; a Study of Aqueous Solubility, Plasma Protein Binding and Oral Exposure. Journal of Medicinal Chemistry, 2006, 49, 6672-6682.	2.9	248
7	Matched Molecular Pairs as a Medicinal Chemistry Tool. Journal of Medicinal Chemistry, 2011, 54, 7739-7750.	2.9	238
8	Base-Catalyzed Aryl-B(OH)₂ Protodeboronation Revisited: From Concerted Proton Transfer to Liberation of a Transient Aryl Anion. Journal of the American Chemical Society, 2017, 139, 13156-13165.	6.6	214
9	Dielsâ€“Alder and ene reactions of singlet oxygen, nitroso compounds and triazolinediones: transition states and mechanisms from contemporary theory. Chemical Communications, 2002, , 1243-1255.	2.2	153
10	Beyond Picomolar Affinities: Quantitative Aspects of Noncovalent and Covalent Binding of Drugs to Proteins. Journal of Medicinal Chemistry, 2009, 52, 225-233.	2.9	150
11	Discovery of 4-Amino-N-[(1S)-1-(4-chlorophenyl)-3-hydroxypropyl]-1-(7H-pyrrolo[2,3-d]pyrimidin-4-yl)piperidine-4-carbox (AZD5363), an Orally Bioavailable, Potent Inhibitor of Akt Kinases. Journal of Medicinal Chemistry, 2013, 56, 2059-2073.	2.9	135
12	Matched Molecular Pair Analysis in drug discovery. Drug Discovery Today, 2013, 18, 724-731.	3.2	115
13	MIDA boronates are hydrolysed fast and slow by two different mechanisms. Nature Chemistry, 2016, 8, 1067-1075.	6.6	93
14	Transition States and Mechanisms of the Hetero-Dielsâ^'Alder Reactions of Hyponitrous Acid, Nitrosoalkanes, Nitrosoarenes, and Nitrosocarbonyl Compounds. Journal of Organic Chemistry, 2001, 66, 5192-5200.	1.7	90
15	Stereoselective glycosylation using oxathiane glycosyl donors. Chemical Communications, 2009, , 5841.	2.2	78
16	The Origins of Noncovalent Catalysis of Intermolecular Dielsâ^'Alder Reactions by Cyclodextrins, Self-Assembling Capsules, Antibodies, and RNAses. Journal of Organic Chemistry, 2002, 67, 4250-4260.	1.7	73
17	Use of Small-Molecule Crystal Structures To Address Solubility in a Novel Series of G Protein Coupled Receptor 119 Agonists: Optimization of a Lead and in Vivo Evaluation. Journal of Medicinal Chemistry, 2012, 55, 5361-5379.	2.9	65
18	The Ene Reactions of Nitroso Compounds Involve Polarized Diradical Intermediates. Journal of the American Chemical Society, 2002, 124, 14820-14821.	6.6	64

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19	Anion-Initiated Trifluoromethylation by TMSCF₃: Deconvolution of the Siliconateâ€“Carbanion Dichotomy by Stopped-Flow NMR/IR. Journal of the American Chemical Society, 2018, 140, 11112-11124.	6.6	63
20	Learning Medicinal Chemistry Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) Rules from Cross-Company Matched Molecular Pairs Analysis (MMPA). Journal of Medicinal Chemistry, 2018, 61, 3277-3292.	2.9	59
21	The mechanism and regioselectivity of the ene reactions of nitroso compounds: a theoretical study of reactivity, regioselectivity, and kinetic isotope effects establishes a stepwise path involving polarized diradical intermediates. Organic and Biomolecular Chemistry, 2003, 1, 1389-1403.	1.5	58
22	Inhibitors of the tyrosine kinase EphB4. Part 1: Structure-based design and optimization of a series of 2,4-bis-anilinopyrimidines. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 2776-2780.	1.0	53
23	Neighbouring group participation vs. addition to oxacarbenium ions: studies on the synthesis of mycobacterial oligosaccharides. Organic and Biomolecular Chemistry, 2009, 7, 4842.	1.5	51
24	Theoretical Prediction of a Perepoxide Intermediate for the Reaction of Singlet Oxygen with trans-Cyclooctene Contrasts with the Two-Step No-Intermediate Ene Reaction for Acyclic Alkenes. Journal of Organic Chemistry, 2008, 73, 8511-8519.	1.7	49
25	Difluorocarbene Generation from TMSCF₃: Kinetics and Mechanism of NaI-Mediated and Si-Induced Anionic Chain Reactions. Journal of the American Chemical Society, 2020, 142, 14649-14663.	6.6	49
26	Inhibitors of the tyrosine kinase EphB4. Part 2: Structure-based discovery and optimisation of 3,5-bis substituted anilinopyrimidines. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 5717-5721.	1.0	48
27	A Cornucopia of Cycloadducts:â€‰ Theoretical Predictions of the Mechanisms and Products of the Reactions of Cyclopentadiene with Cycloheptatriene. Journal of the American Chemical Society, 2003, 125, 8330-8339.	6.6	46
28	Rationally Designing Safer Anilines: The Challenging Case of 4-Aminobiphenyls. Journal of Medicinal Chemistry, 2012, 55, 3923-3933.	2.9	46
29	Do Glycosyl Sulfonium Ions Engage in Neighbouringâ€Group Participation? A Study of Oxathiane Glycosyl Donors and the Basis for their Stereoselectivity. Chemistry - A European Journal, 2012, 18, 321-333.	1.7	45
30	Side Chain Flexibilities in the Human Ether-a-go-go Related Gene Potassium Channel (hERG) Together with Matched-Pair Binding Studies Suggest a New Binding Mode for Channel Blockers. Journal of Medicinal Chemistry, 2009, 52, 4266-4276.	2.9	44
31	Catalytic Enantioselective Synthesis of Î±â€Chiral Azaheteroaryl Ethylamines by Asymmetric Protonation. Angewandte Chemie - International Edition, 2018, 57, 11374-11377.	7.2	44
32	Inhibitors of epidermal growth factor receptor tyrosine kinase: Novel C-5 substituted anilinoquinazolines designed to target the ribose pocket. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 1633-1637.	1.0	42
33	Proteinâ€“Ligand Crystal Structures Can Guide the Design of Selective Inhibitors of the FGFR Tyrosine Kinase. Journal of Medicinal Chemistry, 2012, 55, 5003-5012.	2.9	42
34	Theoretical Elucidation of Kinetic and Thermodynamic Control of Radical Addition Regioselectivity. Journal of the American Chemical Society, 2003, 125, 4271-4278.	6.6	39
35	Shapes of Antibody Binding Sites:â€‰ Qualitative and Quantitative Analyses Based on a Geomorphic Classification Scheme. Journal of Organic Chemistry, 2006, 71, 5082-5092.	1.7	39
36	Kinetics and Mechanism of the Arase-Hoshi R₂BH-Catalyzed Alkyne Hydroboration: Alkenylboronate Generation via Bâ€“H/Câ€“B Metathesis. Journal of the American Chemical Society, 2019, 141, 18600-18611.	6.6	39

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37	Quantitatively Interpreted Enhanced Inhibition of Cytochrome P450s by Heteroaromatic Rings Containing Nitrogen. Journal of Chemical Information and Modeling, 2011, 51, 1048-1063.	2.5	37
38	Identification, optimisation and in vivo evaluation of oxadiazole DGAT-1 inhibitors for the treatment of obesity and diabetes. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 3873-3878.	1.0	36
39	Mechanism of the Forbidden [3s,5s]-Sigmatropic Shift: Orbital Symmetry Influences Stepwise Mechanisms Involving Diradical Intermediates. Chemistry - A European Journal, 2002, 8, 1290-1299.	1.7	34
40	Oxadiazole isomers: all bioisosteres are not created equal. MedChemComm, 2012, 3, 600.	3.5	33
41	The Origins of Periselectivity and Substituent Effects in Electrocyclizations ofo-Nitrososstyrenes: A Computational Study. Synthesis, 2005, 2005, 3463-3467.	1.2	32
42	Can we accelerate medicinal chemistry by augmenting the chemist with Big Data and artificial intelligence?. Drug Discovery Today, 2018, 23, 1373-1384.	3.2	32
43	Comparison of the ATP Binding Sites of Protein Kinases Using Conformationally Diverse Bisindolylmaleimides. Journal of the American Chemical Society, 2005, 127, 11699-11708.	6.6	31
44	Free-Wilson and Structural Approaches to Co-optimizing Human and Rodent Isoform Potency for 11Î²-Hydroxysteroid Dehydrogenase Type 1 (11Î²-HSD1) Inhibitors. Journal of Medicinal Chemistry, 2012, 55, 10652-10661.	2.9	31
45	Protodeboronation of (Hetero)Arylboronic Esters: Direct versus Prehydrolytic Pathways and Self-/Auto-Catalysis. Journal of the American Chemical Society, 2021, 143, 14814-14826.	6.6	29
46	Mechanistic Studies on a Sulfoxide Transfer Reaction Mediated by Diphenyl Sulfoxide/Triflic Anhydride. Chemistry - A European Journal, 2012, 18, 2987-2997.	1.7	28
47	Chemists: AI Is Here; Unite To Get the Benefits. Journal of Medicinal Chemistry, 2020, 63, 8695-8704.	2.9	28
48	A mechanistic proposal for the protodeboronation of neat boronic acids: boronic acid mediated reaction in the solid state. Organic and Biomolecular Chemistry, 2015, 13, 2555-2560.	1.5	25
49	Physiological and Pathological Factors Affecting Drug Delivery to the Brain by Nanoparticles. Advanced Science, 2021, 8, e2002085.	5.6	25
50	Enantiomeric pairs reveal that key medicinal chemistry parameters vary more than simple physical property based models can explain. MedChemComm, 2012, 3, 528.	3.5	24
51	Tuning the Binding Affinity and Selectivity of Perfluoroarylâ€Stapled Peptides by Cysteineâ€Editing. Chemistry - A European Journal, 2019, 25, 177-182.	1.7	23
52	Fragment-oriented synthesis: Î²-elaboration of cyclic amine fragments using enecarbamates as platform intermediates. Chemical Communications, 2020, 56, 8802-8805.	2.2	22
53	Heavy-Atom Kinetic Isotope Effects: Primary Interest or Zero Point?. Journal of the American Chemical Society, 2021, 143, 21079-21099.	6.6	21
54	Circumventing Seizure Activity in a Series of G Protein Coupled Receptor 119 (GPR119) Agonists. Journal of Medicinal Chemistry, 2014, 57, 8984-8998.	2.9	20

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55	Unexpected Syn Hydride Migration in the Non-aldol Aldol Reaction. Organic Letters, 2003, 5, 3375-3378.	2.4	19
56	Reaction energies computed with density functional theory correspond with a whole organism effect; modelling the Ames test for mutagenicity. Chemical Communications, 2009, , 1094.	2.2	19
57	Combined Application of Analytical Techniques for the Characterization of Polymer Supported Species. ACS Combinatorial Science, 2000, 2, 491-495.	3.3	18
58	Theoretical Investigation of the Origins of Catalysis of a Retro-Dielsâ^'Alder Reaction by Antibody 10F11. Journal of Organic Chemistry, 2004, 69, 3683-3692.	1.7	18
59	Catalytic Enantioselective Synthesis of Heterocyclic Vicinal Fluoroamines by Using Asymmetric Protonation: Method Development and Mechanistic Study. Chemistry - A European Journal, 2020, 26, 12249-12255.	1.7	18
60	NEW POLYETHYLENE GLYCOL POLYMERS AS KETAL PROTECTING GROUPS â€“ A POLYMER SUPPORTED APPROACH TO SYMMETRICALLY SUBSTITUTED SPIROKETALS. Synthetic Communications, 2001, 31, 2965-2977.	1.1	16
61	Antibody-Catalyzed Oxy-Cope Rearrangement:Â Mechanism and Origins of Catalysis and Stereoselectivity from DFT Quantum Mechanics and Flexible Docking. Journal of the American Chemical Society, 2004, 126, 9695-9708.	6.6	16
62	Enhancing the kinetics of hydrazone exchange processes: an experimental and computational study. Organic and Biomolecular Chemistry, 2019, 17, 3218-3224.	1.5	16
63	Discovery, optimisation and in vivo evaluation of novel GPR119 agonists. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 7310-7316.	1.0	15
64	Rigid and concave, 2,4-cis-substituted azetidine derivatives: A platform for asymmetric catalysis. Scientific Reports, 2018, 8, 6541.	1.6	15
65	Derivatisation of parthenolide to address chemoresistant chronic lymphocytic leukaemia. MedChemComm, 2019, 10, 1379-1390.	3.5	15
66	A System for Encoding and Searching Markush Structures. Journal of Chemical Information and Modeling, 2012, 52, 1936-1947.	2.5	14
67	Achieving improved permeability by hydrogen bond donor modulation in a series of MGAT2 inhibitors. MedChemComm, 2013, 4, 1305.	3.5	12
68	Catalytic Enantioselective Synthesis of Î±â€Chiral Azaheteroaryl Ethylamines by Asymmetric Protonation. Angewandte Chemie, 2018, 130, 11544-11547.	1.6	12
69	Trialkylammonium salt degradation: implications for methylation and cross-coupling. Chemical Science, 2021, 12, 6949-6963.	3.7	12
70	Optimisation of aqueous solubility in a series of G protein coupled receptor 119 (GPR119) agonists. MedChemComm, 2013, 4, 95-100.	3.5	11
71	Turbocharging Matched Molecular Pair Analysis: Optimizing the Identification and Analysis of Pairs. Journal of Chemical Information and Modeling, 2017, 57, 2424-2436.	2.5	11
72	Quantitative Prediction of Rate Constants for Aqueous Racemization To Avoid Pointless Stereoselective Syntheses. Angewandte Chemie - International Edition, 2018, 57, 982-985.	7.2	11

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73	Predicting proteinâ€“ligand binding affinity and correcting crystal structures with quantum mechanical calculations: lactate dehydrogenase A. Chemical Science, 2019, 10, 2218-2227.	3.7	11
74	The problem of racemization in drug discovery and tools to predict it. Expert Opinion on Drug Discovery, 2019, 14, 527-539.	2.5	10
75	The discovery of benzanilides as c-Met receptor tyrosine kinase inhibitors by a directed screening approach. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 5224-5229.	1.0	9
76	Racemisation in Chemistry and Biology. Chemistry - A European Journal, 2020, 26, 3661-3687.	1.7	9
77	Optimisation of biphenyl acetic acid inhibitors of diacylglycerol acetyl transferase 1 â€“ the discovery of AZD2353. MedChemComm, 2013, 4, 159-164.	3.5	8
78	Design and synthesis of a novel series of cyclohexyloxy-pyridyl derivatives as inhibitors of diacylglycerol acyl transferase 1. MedChemComm, 2013, 4, 151-158.	3.5	8
79	Experimental Testing of Quantum Mechanical Predictions of Mutagenicity: Aminopyrazoles. Chemical Research in Toxicology, 2013, 26, 703-709.	1.7	8
80	Development of Brain Targeting Peptide Based MMP-9 Inhibiting Nanoparticles for the Treatment of Brain Diseases with Elevated MMP-9 Activity. Journal of Pharmaceutical Sciences, 2020, 109, 3134-3144.	1.6	8
81	In Situ Studies of Arylboronic Acids/Esters and R₃SiCF₃ Reagents: Kinetics, Speciation, and Dysfunction at the Carbanionâ€“Ate Interface. Accounts of Chemical Research, 2022, 55, 1324-1336.	7.6	8
82	Data-Driven Derivation of Molecular Substructures That Enhance Drug Activity in Gram-Negative Bacteria. Journal of Medicinal Chemistry, 2022, 65, 6088-6099.	2.9	8
83	Investigation of the Origins of Regiochemical Control in [4+2] Cycloadditions of 2-Pyrones and Alkynylboronates. Synthesis, 2012, 44, 1964-1973.	1.2	7
84	Discovery and optimization of efficacious neutral 4-amino-6-biphenyl-7,8-dihydropyrimido[5,4-f][1,4]oxazepin-5-one diacylglycerol acyl transferase-1 (DGAT1) inhibitors. MedChemComm, 2013, 4, 165-174.	3.5	6
85	Predicting the activity and toxicity of new psychoactive substances: a pharmaceutical industry perspective. Drug Testing and Analysis, 2014, 6, 739-745.	1.6	5
86	Palladium and Platinum 2,4-cis-amino Azetidine and Related Complexes. Frontiers in Chemistry, 2018, 6, 211.	1.8	5
87	Enantiomer stability of atropisomeric 1,5-disubstituted 1,2,3-triazoles. , 2022, 1, 100004.		5
88	The pH dependent interaction between nicotine and simulated pulmonary surfactant monolayers with associated molecular modelling. Surface and Interface Analysis, 2017, 49, 919-927.	0.8	4
89	Quantitative Prediction of Rate Constants for Aqueous Racemization To Avoid Pointless Stereoselective Syntheses. Angewandte Chemie, 2018, 130, 994-997.	1.6	4
90	Asymmetric Synthesis of Heterocyclic Chloroamines and Aziridines by Enantioselective Protonation of Catalytically Generated Enamines**. Chemistry - A European Journal, 2022, 28, .	1.7	4

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91	Furanyl cyclic amines: a diastereoselective synthesis of 2,6-syn-disubstituted piperidines under thermodynamic control. Organic and Biomolecular Chemistry, 2012, 10, 2392.	1.5	3
92	Tactics to Avoid Inhibition of Cytochrome P450s. Topics in Medicinal Chemistry, 2013, , 107-158.	0.4	3
93	A Lewis Base Nucleofugality Parameter, N^F_B, and Its Application in an Analysis of MIDA-Boronate Hydrolysis Kinetics. Journal of Organic Chemistry, 2022, 87, 721-729.	1.7	3
94	Energy Contour Plots: Slices through the Potential Energy Surface That Simplify Quantum Mechanical Studies of Reacting Systems. Journal of Chemical Education, 2006, 83, 451.	1.1	2
95	A monomeric form of iNOS can rationalise observed SAR for inhibitors of dimerisation: quantum mechanics and docking compared. MedChemComm, 2013, 4, 180-186.	3.5	2
96	Novel N-thiazolyl piperazine-1-carboxamide CCR2 antagonists â€“ investigation of an unexpected reaction with glutathione. MedChemComm, 2015, 6, 2140-2145.	3.5	2
97	The Inclusion of a Matrix Metalloproteinase-9 Responsive Sequence in Self-assembled Peptide-based Brain-Targeting Nanoparticles Improves the Efficiency of Nanoparticles Crossing the Blood-Brain Barrier at Elevated MMP-9 Levels. Journal of Pharmaceutical Sciences, 2021, 110, 1349-1364.	1.6	2
98	Mapping Ligand-Shape Space for Proteinâ€“Ligand Systems: Distinguishing Key-in-Lock and Hand-in-Glove Proteins. Journal of Chemical Information and Modeling, 2021, 61, 1859-1874.	2.5	2
99	Theoretical Studies of Antibody Catalysis. , 2005, , 72-117.		1
100	Designing Hydroxamates and Reversed Hydroxamates to Inhibit Zincâ€containing Proteases but not Cytochrome P450s: Insights from Quantum Mechanics and Proteinâ€ligand Crystal Structures. Molecular Informatics, 2015, 34, 608-614.	1.4	1
101	An investigation into drug partitioning behaviour in simulated pulmonary surfactant monolayers with associated molecular modelling. Surface and Interface Analysis, 2018, 50, 369-377.	0.8	1
102	Boron and covalent inhibition. Annual Reports in Medicinal Chemistry, 2021, 56, 135-135.	0.5	1
103	Microwave-assisted synthesis of 4-oxo-2-butenoic acids by aldol-condensation of glyoxylic acid. RSC Advances, 2021, 11, 30229-30236.	1.7	1
104	Binding Affinities of Hostâ”Guest, Proteinâ”Ligand, and Proteinâ”Transition-State Complexes. ChemInform, 2004, 35, no.	0.1	0
105	Crystallisation of aspirin via simulated pulmonary surfactant monolayers and lungâ€specific additives. Surface and Interface Analysis, 2017, 49, 864-872.	0.8	0
106	Frontispiece: Racemisation in Chemistry and Biology. Chemistry - A European Journal, 2020, 26, .	1.7	0
107	Design, synthesis and evaluation of tryptophan analogues as tool compounds to study IDO1 activity. RSC Chemical Biology, 2021, 2, 1651-1660.	2.0	0