

# Andrew G Leach

## List of Publications by Year in descending order

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107  
papers

5,626  
citations

94269

37  
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79541

73  
g-index

116  
all docs

116  
docs citations

116  
times ranked

6391  
citing authors

#	ARTICLE	IF	CITATIONS
1	Enantiomer stability of atropisomeric 1,5-disubstituted 1,2,3-triazoles. , 2022, 1, 100004.		5
2	Asymmetric Synthesis of Heterocyclic Chloroamines and Aziridines by Enantioselective Protonation of Catalytically Generated Enamines**. Chemistry - A European Journal, 2022, 28, .	1.7	4
3	A Lewis Base Nucleofugality Parameter, $N^{\dagger}F^{\dagger}B$ , and Its Application in an Analysis of MIDA-Boronate Hydrolysis Kinetics. Journal of Organic Chemistry, 2022, 87, 721-729.	1.7	3
4	<i>In Situ</i> Studies of Arylboronic Acids/Esters and $R_3SiCF_3$ Reagents: Kinetics, Speciation, and Dysfunction at the Carbanion $\pi$ -Ate Interface. Accounts of Chemical Research, 2022, 55, 1324-1336.	7.6	8
5	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
6	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
7	Boron and covalent inhibition. Annual Reports in Medicinal Chemistry, 2021, 56, 135-135.	0.5	1
8	Trialkylammonium salt degradation: implications for methylation and cross-coupling. Chemical Science, 2021, 12, 6949-6963.	3.7	12
9	Design, synthesis and evaluation of tryptophan analogues as tool compounds to study IDO1 activity. RSC Chemical Biology, 2021, 2, 1651-1660.	2.0	0
10	Physiological and Pathological Factors Affecting Drug Delivery to the Brain by Nanoparticles. Advanced Science, 2021, 8, e2002085.	5.6	25
11	Mapping Ligand-Shape Space for Protein $\pi$ -Ligand Systems: Distinguishing Key-in-Lock and Hand-in-Glove Proteins. Journal of Chemical Information and Modeling, 2021, 61, 1859-1874.	2.5	2
12	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
13	Microwave-assisted synthesis of 4-oxo-2-butenic acids by aldol-condensation of glyoxylic acid. RSC Advances, 2021, 11, 30229-30236.	1.7	1
14	Heavy-Atom Kinetic Isotope Effects: Primary Interest or Zero Point?. Journal of the American Chemical Society, 2021, 143, 21079-21099.	6.6	21
15	Racemisation in Chemistry and Biology. Chemistry - A European Journal, 2020, 26, 3661-3687.	1.7	9
16	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
17	Difluorocarbene Generation from $TMSCF_3$ : 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
18	Chemists: AI Is Here; Unite To Get the Benefits. Journal of Medicinal Chemistry, 2020, 63, 8695-8704.	2.9	28

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19	Catalytic Enantioselective Synthesis of Heterocyclic Vicinal Fluoroamines by Using Asymmetric Protonation: Method Development and Mechanistic Study. <i>Chemistry - A European Journal</i> , 2020, 26, 12249-12255.	1.7	18
20	Fragment-oriented synthesis: $\hat{I}^2$ -elaboration of cyclic amine fragments using enecarbamates as platform intermediates. <i>Chemical Communications</i> , 2020, 56, 8802-8805.	2.2	22
21	Frontispiece: Racemisation in Chemistry and Biology. <i>Chemistry - A European Journal</i> , 2020, 26, .	1.7	0
22	Derivatisation of parthenolide to address chemoresistant chronic lymphocytic leukaemia. <i>MedChemComm</i> , 2019, 10, 1379-1390.	3.5	15
23	Kinetics and Mechanism of the Arase-Hoshi $R_{2<sub>2</sub>}$ -BH-Catalyzed Alkyne Hydroboration: Alkenylboronate Generation via $B\hat{H}/C\hat{B}$ Metathesis. <i>Journal of the American Chemical Society</i> , 2019, 141, 18600-18611.	6.6	39
24	Predicting protein-ligand binding affinity and correcting crystal structures with quantum mechanical calculations: lactate dehydrogenase A. <i>Chemical Science</i> , 2019, 10, 2218-2227.	3.7	11
25	The problem of racemization in drug discovery and tools to predict it. <i>Expert Opinion on Drug Discovery</i> , 2019, 14, 527-539.	2.5	10
26	Enhancing the kinetics of hydrazone exchange processes: an experimental and computational study. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 3218-3224.	1.5	16
27	Tuning the Binding Affinity and Selectivity of Perfluoroaryl-stapled Peptides by Cysteine-editing. <i>Chemistry - A European Journal</i> , 2019, 25, 177-182.	1.7	23
28	An investigation into drug partitioning behaviour in simulated pulmonary surfactant monolayers with associated molecular modelling. <i>Surface and Interface Analysis</i> , 2018, 50, 369-377.	0.8	1
29	Rigid and concave, 2,4-cis-substituted azetidines: A platform for asymmetric catalysis. <i>Scientific Reports</i> , 2018, 8, 6541.	1.6	15
30	Can we accelerate medicinal chemistry by augmenting the chemist with Big Data and artificial intelligence?. <i>Drug Discovery Today</i> , 2018, 23, 1373-1384.	3.2	32
31	Quantitative Prediction of Rate Constants for Aqueous Racemization To Avoid Pointless Stereoselective Syntheses. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 982-985.	7.2	11
32	Learning Medicinal Chemistry Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) Rules from Cross-Company Matched Molecular Pairs Analysis (MMPA). <i>Journal of Medicinal Chemistry</i> , 2018, 61, 3277-3292.	2.9	59
33	Quantitative Prediction of Rate Constants for Aqueous Racemization To Avoid Pointless Stereoselective Syntheses. <i>Angewandte Chemie</i> , 2018, 130, 994-997.	1.6	4
34	Catalytic Enantioselective Synthesis of $\hat{I}^{\pm}$ -Chiral Azaheteroaryl Ethylamines by Asymmetric Protonation. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 11374-11377.	7.2	44
35	Catalytic Enantioselective Synthesis of $\hat{I}^{\pm}$ -Chiral Azaheteroaryl Ethylamines by Asymmetric Protonation. <i>Angewandte Chemie</i> , 2018, 130, 11544-11547.	1.6	12
36	Anion-Initiated Trifluoromethylation by $TMSCF_3$ : Deconvolution of the Silicate-Carbanion Dichotomy by Stopped-Flow NMR/IR. <i>Journal of the American Chemical Society</i> , 2018, 140, 11112-11124.	6.6	63

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37	Palladium and Platinum 2,4-cis-amino Azetidine and Related Complexes. <i>Frontiers in Chemistry</i> , 2018, 6, 211.	1.8	5
38	Crystallisation of aspirin via simulated pulmonary surfactant monolayers and lung-specific additives. <i>Surface and Interface Analysis</i> , 2017, 49, 864-872.	0.8	0
39	Turbocharging Matched Molecular Pair Analysis: Optimizing the Identification and Analysis of Pairs. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2424-2436.	2.5	11
40	Base-Catalyzed Aryl-B(OH) <sub>2</sub> Protodeboronation Revisited: From Concerted Proton Transfer to Liberation of a Transient Aryl Anion. <i>Journal of the American Chemical Society</i> , 2017, 139, 13156-13165.	6.6	214
41	The pH dependent interaction between nicotine and simulated pulmonary surfactant monolayers with associated molecular modelling. <i>Surface and Interface Analysis</i> , 2017, 49, 919-927.	0.8	4
42	Protodeboronation of Heteroaromatic, Vinyl, and Cyclopropyl Boronic Acids: pH-Dependent Rate Profiles, Autocatalysis, and Disproportionation. <i>Journal of the American Chemical Society</i> , 2016, 138, 9145-9157.	6.6	262
43	MIDA boronates are hydrolysed fast and slow by two different mechanisms. <i>Nature Chemistry</i> , 2016, 8, 1067-1075.	6.6	93
44	Designing Hydroxamates and Reversed Hydroxamates to Inhibit Zinc-containing Proteases but not Cytochrome P450s: Insights from Quantum Mechanics and Protein-Ligand Crystal Structures. <i>Molecular Informatics</i> , 2015, 34, 608-614.	1.4	1
45	A mechanistic proposal for the protodeboronation of neat boronic acids: boronic acid mediated reaction in the solid state. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 2555-2560.	1.5	25
46	Novel N-thiazolyl piperazine-1-carboxamide CCR2 antagonists – investigation of an unexpected reaction with glutathione. <i>MedChemComm</i> , 2015, 6, 2140-2145.	3.5	2
47	Circumventing Seizure Activity in a Series of G Protein Coupled Receptor 119 (GPR119) Agonists. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 8984-8998.	2.9	20
48	Predicting the activity and toxicity of new psychoactive substances: a pharmaceutical industry perspective. <i>Drug Testing and Analysis</i> , 2014, 6, 739-745.	1.6	5
49	A monomeric form of iNOS can rationalise observed SAR for inhibitors of dimerisation: quantum mechanics and docking compared. <i>MedChemComm</i> , 2013, 4, 180-186.	3.5	2
50	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. <i>MedChemComm</i> , 2013, 4, 165-174.	3.5	6
51	Optimisation of biphenyl acetic acid inhibitors of diacylglycerol acetyl transferase 1 – the discovery of AZD2353. <i>MedChemComm</i> , 2013, 4, 159-164.	3.5	8
52	Design and synthesis of a novel series of cyclohexyloxy-pyridyl derivatives as inhibitors of diacylglycerol acyl transferase 1. <i>MedChemComm</i> , 2013, 4, 151-158.	3.5	8
53	Discovery of 4-Amino-N-[(1S)-1-(4-chlorophenyl)-3-hydroxypropyl]-1-(7H-pyrrolo[2,3-d]pyrimidin-4-yl)piperidine-4-carboxamide (AZD5363), an Orally Bioavailable, Potent Inhibitor of Akt Kinases. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 2059-2073.	2.9	135
54	Matched Molecular Pair Analysis in drug discovery. <i>Drug Discovery Today</i> , 2013, 18, 724-731.	3.2	115

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55	Experimental Testing of Quantum Mechanical Predictions of Mutagenicity: Aminopyrazoles. <i>Chemical Research in Toxicology</i> , 2013, 26, 703-709.	1.7	8
56	Optimisation of aqueous solubility in a series of G protein coupled receptor 119 (GPR119) agonists. <i>MedChemComm</i> , 2013, 4, 95-100.	3.5	11
57	Tactics to Avoid Inhibition of Cytochrome P450s. <i>Topics in Medicinal Chemistry</i> , 2013, , 107-158.	0.4	3
58	Achieving improved permeability by hydrogen bond donor modulation in a series of MGAT2 inhibitors. <i>MedChemComm</i> , 2013, 4, 1305.	3.5	12
59	Investigation of the Origins of Regiochemical Control in [4+2] Cycloadditions of 2-Pyrones and Alkynylboronates. <i>Synthesis</i> , 2012, 44, 1964-1973.	1.2	7
60	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. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 5361-5379.	2.9	65
61	Furanyl cyclic amines: a diastereoselective synthesis of 2,6-syn-disubstituted piperidines under thermodynamic control. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 2392.	1.5	3
62	Enantiomeric pairs reveal that key medicinal chemistry parameters vary more than simple physical property based models can explain. <i>MedChemComm</i> , 2012, 3, 528.	3.5	24
63	A System for Encoding and Searching Markush Structures. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1936-1947.	2.5	14
64	Free-Wilson and Structural Approaches to Co-optimizing Human and Rodent Isoform Potency for 11 $\beta$ -Hydroxysteroid Dehydrogenase Type 1 (11 $\beta$ -HSD1) Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 10652-10661.	2.9	31
65	Rationally Designing Safer Anilines: The Challenging Case of 4-Aminobiphenyls. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 3923-3933.	2.9	46
66	Oxadiazole isomers: all bioisosteres are not created equal. <i>MedChemComm</i> , 2012, 3, 600.	3.5	33
67	Protein-Ligand Crystal Structures Can Guide the Design of Selective Inhibitors of the FGFR Tyrosine Kinase. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 5003-5012.	2.9	42
68	Identification, optimisation and in vivo evaluation of oxadiazole DGAT-1 inhibitors for the treatment of obesity and diabetes. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 3873-3878.	1.0	36
69	Do Glycosyl Sulfonium Ions Engage in Neighbouring-Group Participation? A Study of Oxathiane Glycosyl Donors and the Basis for their Stereoselectivity. <i>Chemistry - A European Journal</i> , 2012, 18, 321-333.	1.7	45
70	Mechanistic Studies on a Sulfoxide Transfer Reaction Mediated by Diphenyl Sulfoxide/Triflic Anhydride. <i>Chemistry - A European Journal</i> , 2012, 18, 2987-2997.	1.7	28
71	Matched Molecular Pairs as a Medicinal Chemistry Tool. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 7739-7750.	2.9	238
72	The discovery of benzanilides as c-Met receptor tyrosine kinase inhibitors by a directed screening approach. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2011, 21, 5224-5229.	1.0	9

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73	Discovery, optimisation and in vivo evaluation of novel GPR119 agonists. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2011, 21, 7310-7316.	1.0	15
74	Quantitatively Interpreted Enhanced Inhibition of Cytochrome P450s by Heteroaromatic Rings Containing Nitrogen. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 1048-1063.	2.5	37
75	Reaction energies computed with density functional theory correspond with a whole organism effect; modelling the Ames test for mutagenicity. <i>Chemical Communications</i> , 2009, , 1094.	2.2	19
76	Stereoselective glycosylation using oxathiane glycosyl donors. <i>Chemical Communications</i> , 2009, , 5841.	2.2	78
77	Beyond Picomolar Affinities: Quantitative Aspects of Noncovalent and Covalent Binding of Drugs to Proteins. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 225-233.	2.9	150
78	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. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 4266-4276.	2.9	44
79	Neighbouring group participation vs. addition to oxacarbenium ions: studies on the synthesis of mycobacterial oligosaccharides. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 4842.	1.5	51
80	Inhibitors of the tyrosine kinase EphB4. Part 1: Structure-based design and optimization of a series of 2,4-bis-anilinopyrimidines. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2008, 18, 2776-2780.	1.0	53
81	Inhibitors of the tyrosine kinase EphB4. Part 2: Structure-based discovery and optimisation of 3,5-bis substituted anilinopyrimidines. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2008, 18, 5717-5721.	1.0	48
82	Theoretical Prediction of a Peroxide Intermediate for the Reaction of Singlet Oxygen with <i>trans</i> -Cyclooctene Contrasts with the Two-Step No-Intermediate Ene Reaction for Acyclic Alkenes. <i>Journal of Organic Chemistry</i> , 2008, 73, 8511-8519.	1.7	49
83	Energy Contour Plots: Slices through the Potential Energy Surface That Simplify Quantum Mechanical Studies of Reacting Systems. <i>Journal of Chemical Education</i> , 2006, 83, 451.	1.1	2
84	Matched Molecular Pairs as a Guide in the Optimization of Pharmaceutical Properties; a Study of Aqueous Solubility, Plasma Protein Binding and Oral Exposure. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 6672-6682.	2.9	248
85	Shapes of Antibody Binding Sites: Qualitative and Quantitative Analyses Based on a Geomorphic Classification Scheme. <i>Journal of Organic Chemistry</i> , 2006, 71, 5082-5092.	1.7	39
86	Inhibitors of epidermal growth factor receptor tyrosine kinase: Novel C-5 substituted anilinoquinazolines designed to target the ribose pocket. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006, 16, 1633-1637.	1.0	42
87	Theoretical Studies of Antibody Catalysis. , 2005, , 72-117.		1
88	The Origins of Periselectivity and Substituent Effects in Electrocyclizations of <i>o</i> -Nitrostyrenes: A Computational Study. <i>Synthesis</i> , 2005, 2005, 3463-3467.	1.2	32
89	Comparison of the ATP Binding Sites of Protein Kinases Using Conformationally Diverse Bisindolylmaleimides. <i>Journal of the American Chemical Society</i> , 2005, 127, 11699-11708.	6.6	31
90	Binding Affinities of Host-Guest, Protein-Ligand, and Protein-Transition-State Complexes. <i>ChemInform</i> , 2004, 35, no.	0.1	0

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91	Antibody-Catalyzed Oxy-Cope Rearrangement: A Mechanism and Origins of Catalysis and Stereoselectivity from DFT Quantum Mechanics and Flexible Docking. <i>Journal of the American Chemical Society</i> , 2004, 126, 9695-9708.	6.6	16
92	Theoretical Investigation of the Origins of Catalysis of a Retro-Diels-Alder Reaction by Antibody 10F11. <i>Journal of Organic Chemistry</i> , 2004, 69, 3683-3692.	1.7	18
93	A Standard Set of Pericyclic Reactions of Hydrocarbons for the Benchmarking of Computational Methods: 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. <i>Journal of Physical Chemistry A</i> , 2003, 107, 11445-11459.	1.1	342
94	Binding Affinities of Host-Guest, Protein-Ligand, and Protein-Transition-State Complexes. <i>Angewandte Chemie - International Edition</i> , 2003, 42, 4872-4897.	7.2	511
95	Mechanism of Ene Reactions of Singlet Oxygen. A Two-Step No-Intermediate Mechanism. <i>Journal of the American Chemical Society</i> , 2003, 125, 1319-1328.	6.6	259
96	A Cornucopia of Cycloadducts: Theoretical Predictions of the Mechanisms and Products of the Reactions of Cyclopentadiene with Cycloheptatriene. <i>Journal of the American Chemical Society</i> , 2003, 125, 8330-8339.	6.6	46
97	Theoretical Elucidation of Kinetic and Thermodynamic Control of Radical Addition Regioselectivity. <i>Journal of the American Chemical Society</i> , 2003, 125, 4271-4278.	6.6	39
98	Unexpected Syn Hydride Migration in the Non-aldol Aldol Reaction. <i>Organic Letters</i> , 2003, 5, 3375-3378.	2.4	19
99	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. <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 1389-1403.	1.5	58
100	The Ene Reactions of Nitroso Compounds Involve Polarized Diradical Intermediates. <i>Journal of the American Chemical Society</i> , 2002, 124, 14820-14821.	6.6	64
101	Mechanism of the Forbidden [3s,5s]-Sigmatropic Shift: Orbital Symmetry Influences Stepwise Mechanisms Involving Diradical Intermediates. <i>Chemistry - A European Journal</i> , 2002, 8, 1290-1299.	1.7	34
102	The Origins of Noncovalent Catalysis of Intermolecular Diels-Alder Reactions by Cyclodextrins, Self-Assembling Capsules, Antibodies, and RNAses. <i>Journal of Organic Chemistry</i> , 2002, 67, 4250-4260.	1.7	73
103	Diels-Alder and ene reactions of singlet oxygen, nitroso compounds and triazolinediones: transition states and mechanisms from contemporary theory. <i>Chemical Communications</i> , 2002, , 1243-1255.	2.2	153
104	Transition States and Mechanisms of the Hetero-Diels-Alder Reactions of Hyponitrous Acid, Nitrosoalkanes, Nitrosoarenes, and Nitrosocarbonyl Compounds. <i>Journal of Organic Chemistry</i> , 2001, 66, 5192-5200.	1.7	90
105	NEW POLYETHYLENE GLYCOL POLYMERS AS KETAL PROTECTING GROUPS - A POLYMER SUPPORTED APPROACH TO SYMMETRICALLY SUBSTITUTED SPIROKETALS. <i>Synthetic Communications</i> , 2001, 31, 2965-2977.	1.1	16
106	Combined Application of Analytical Techniques for the Characterization of Polymer Supported Species. <i>ACS Combinatorial Science</i> , 2000, 2, 491-495.	3.3	18
107	Multi-step organic synthesis using solid-supported reagents and scavengers: a new paradigm in chemical library generation. <i>Journal of the Chemical Society, Perkin Transactions 1</i> , 2000, , 3815-4195.	1.3	665