Andrei G Kutateladze

List of Publications by Year
in descending order

83	2,158	201674	265206
papers	citations	27 h-index	42 g-index

91	91	91	1863
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	High-Throughput in Silico Structure Validation and Revision of Halogenated Natural Products Is Enabled by Parametric Corrections to DFT-Computed ¹³C NMR Chemical Shifts and Spinâ€“Spin Coupling Constants. Journal of Organic Chemistry, 2017, 82, 3368-3381.	3.2	121
2	The value of universally available raw NMR data for transparency, reproducibility, and integrity in natural product research. Natural Product Reports, 2019, 36, 35-107.	10.3	92
3	Minimalist Relativistic Force Field: Prediction of Protonâ€“Proton Coupling Constants in ¹H NMR Spectra Is Perfected with NBO Hybridization Parameters. Journal of Organic Chemistry, 2015, 80, 5218-5225.	3.2	89
4	Rapid Photoassisted Access to N,O,Sâ€Polyheterocycles with Benzoazocine and Hydroquinoline Cores: Intramolecular Cycloadditions of Photogenerated Azaxylylenes. Angewandte Chemie - International Edition, 2011, 50, 9423-9428.	13.8	77
5	Relativistic Force Field: Parametric Computations of Protonâ€“Proton Coupling Constants in ¹H NMR Spectra. Journal of Organic Chemistry, 2014, 79, 8397-8406.	3.2	74
6	Conformational Analysis of Singletâ^'Triplet State Mixing in PaternÃ²â^'BÃ¼chi Diradicals. Journal of the American Chemical Society, 2001, 123, 9279-9282.	13.7	66
7	An Efficient Photo-SET-Induced Cleavage of Dithianeâ^'Carbonyl Adducts and Its Relevance to the Development of Photoremovable Protecting Groups for Ketones and Aldehydes. Journal of Organic Chemistry, 1998, 63, 9924-9931.	3.2	64
8	Photoassisted Synthesis of Enantiopure Alkaloid Mimics Possessing Unprecedented Polyheterocyclic Cores. Journal of the American Chemical Society, 2013, 135, 9608-9611.	13.7	62
9	Relativistic Force Field: Parametrization of ¹³Câ€“¹H Nuclear Spinâ€“Spin Coupling Constants. Journal of Organic Chemistry, 2015, 80, 10838-10848.	3.2	59
10	Triquinanes and Related Sesquiterpenes Revisited Computationally: Structure Corrections of Hirsutanols B and D, Hirsutenol E, Cucumin B, Antrodins Câ€“E, Chondroterpenes A and H, Chondrosterins C and E, Dichrocephone A, and Pethybrene. Journal of Organic Chemistry, 2017, 82, 10795-10802.	3.2	56
11	Amino Azaxylylenes Photogenerated from oâ€Amido Imines: Photoassisted Access to Complex Spiroâ€Polyâ€Heterocycles. Angewandte Chemie - International Edition, 2015, 54, 11516-11520.	13.8	52
12	Release and Report:â€‰ A New Photolabile Caging System with a Two-Photon Fluorescence Reporting Function. Journal of the American Chemical Society, 2005, 127, 12458-12459.	13.7	50
13	Harvesting the Strain Installed by a PaternÃ²â^'BÃ¼chi Step in a Synthetically Useful Way: High-Yielding Photoprotolytic Oxametathesis in Polycyclic Systems. Organic Letters, 2009, 11, 3886-3889.	4.6	49
14	Structural insights into the Ï€-Ï€-Ï€ stacking mechanism and DNA-binding activity of the YEATS domain. Nature Communications, 2018, 9, 4574.	12.8	45
15	Oxazolines as Dual-Function Traceless Chromophores and Chiral Auxiliaries: Enantioselective Photoassisted Synthesis of Polyheterocyclic Ketones. Journal of the American Chemical Society, 2016, 138, 2110-2113.	13.7	44
16	Double-Tandem [4Ï€+2Ï€]Â·[2Ï€+2Ï€]Â·[4Ï€+2Ï€]Â·[2Ï€+2Ï€] Synthetic Sequence with Photoprotolytic Oxametathesis and Photoepoxidation in the Chromone Series. Journal of Organic Chemistry, 2011, 76, 1319-1332.	3.2	42
17	Reassignments and Corroborations of Oxoâ€Bridged Natural Products Directed by OSE and DU8+ NMR Computation. Angewandte Chemie - International Edition, 2019, 58, 7107-7112.	13.8	41
18	Photoassisted Synthesis of Complex Molecular Architectures: Dearomatization of Benzenoid Arenes with Azaâ€oâ€xylylenes via an Unprecedented [2+4] Reaction Topology. Angewandte Chemie - International Edition, 2016, 55, 6988-6991.	13.8	40

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19	Photoinduced Câ^'C Bond Cleavage in Dithianeâ^'Carbonyl Adducts:Â A Laser Flash Photolysis Study. Journal of Organic Chemistry, 2001, 66, 2887-2890.	3.2	38
20	Addressing the Challenges of Structure Elucidation in Natural Products Possessing the Oxirane Moiety. Journal of Organic Chemistry, 2018, 83, 8341-8352.	3.2	37
21	Structure Revision of an Acorane Sesquiterpene Cordycepol A. Organic Letters, 2016, 18, 4860-4863.	4.6	35
22	Step-Economical Photoassisted Diversity-Oriented Synthesis: Sustaining Cascade Photoreactions in Oxalyl Anilides to Access Complex Polyheterocyclic Molecular Architectures. Journal of the American Chemical Society, 2017, 139, 16584-16590.	13.7	34
23	Photoassisted Access to Enantiopure Conformationally Locked Ribofuranosylamines Spiro-Linked to Oxazolidino-Diketopiperazines.. ACS Combinatorial Science, 2013, 15, 73-76.	3.8	31
24	Intramolecular Photoassisted Cycloadditions of Azaxylylenes and Postphotochemical Capstone Modifications via Suzuki Coupling Provide Access to Complex Polyheterocyclic Biaryls. Journal of Organic Chemistry, 2014, 79, 1235-1246.	3.2	31
25	Anomalous Câ^'C Bond Cleavage in Sulfur-Centered Cation Radicals Containing a Vicinal Hydroxy Group. Journal of Organic Chemistry, 2003, 68, 8236-8239.	3.2	30
26	Natural Products Containing the Oxetane and Related Moieties Present Additional Challenges for Structure Elucidation: A DU8+ Computational Case Study. Journal of Organic Chemistry, 2019, 84, 7575-7586.	3.2	30
27	Photoinduced Intramolecular Cyclopentanation vs Photoprotolytic Oxametathesis in Polycyclic Alkenes Outfitted with Conformationally Constrained Aroylmethyl Chromophores. Journal of Organic Chemistry, 2013, 78, 2012-2025.	3.2	29
28	Molecular Assembly and Disassembly:â€‰ Novel Photolabile Molecular Hosts. Organic Letters, 2000, 2, 3817-3819.	4.6	28
29	Direct screening of solution phase combinatorial libraries encoded with externally sensitized photolabile tags. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 13917-13921.	7.1	28
30	Dithiane- and Trithiane-Based Photolabile Scaffolds for Molecular Recognition. Organic Letters, 2001, 3, 1841-1844.	4.6	27
31	Photoassisted Diversity-Oriented Synthesis: Accessing 2,6-Epoxyazocane (Oxamorphan) Cores. Journal of Organic Chemistry, 2014, 79, 10956-10971.	3.2	27
32	Intramolecular Cycloadditions of Photogenerated Azaxylylenes with Oxadiazoles Provide Direct Access to Versatile Polyheterocyclic Ketopiperazines Containing a Spiro-oxirane Moiety. Organic Letters, 2015, 17, 438-441.	4.6	27
33	Structure Validation of Complex Natural Products: Time to Change the Paradigm. What did Synthesis of Alstofolinine A Prove?. Journal of Organic Chemistry, 2019, 84, 8297-8299.	3.2	26
34	Intramolecular Cycloadditions of Photogenerated Azaxylylenes: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2014, 118, 10487-10496.	2.5	25
35	DU8ML: Machine Learning-Augmented Density Functional Theory Nuclear Magnetic Resonance Computations for High-Throughput In Silico Solution Structure Validation and Revision of Complex Alkaloids. Journal of Organic Chemistry, 2022, 87, 4818-4828.	3.2	25
36	Dithiane-Based Photolabile Amphiphiles:Â Toward Photolabile Liposomes1,2. Langmuir, 2003, 19, 6381-6391.	3.5	24

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37	Conformationally Constrained Penta(hetero)cyclic Molecular Architectures by Photoassisted Diversityâ€Oriented Synthesis. European Journal of Organic Chemistry, 2015, 2015, 2205-2213.	2.4	22
38	An Acetyl-Methyl Switch Drives a Conformational Change in p53. Structure, 2015, 23, 322-331.	3.3	21
39	Computational structure revision of a longipinane derivative meridane. Tetrahedron Letters, 2016, 57, 4727-4729.	1.4	21
40	A novel withanolide with an unprecedented carbon skeleton from Physalis angulata. Organic and Biomolecular Chemistry, 2017, 15, 1110-1114.	2.8	21
41	Direct Transformation of 1,3-Dihalides into Dithianes and Dithiepines via a Novel One-Pot Reaction with Carbon Disulfide and Sodium Borohydride. Organic Letters, 2000, 2, 1133-1135.	4.6	19
42	Strained to the Limit: When a Cyclobutyl Moiety Becomes a Thermodynamic Sink in a Protolytic Ring-Opening of Photogenerated Oxetanes. Organic Letters, 2010, 12, 3398-3401.	4.6	19
43	Efficient Electrochemical Deprotection of Carboxylic and Amino Acids from Their 2-(Hydroxymethyl)-1,3-dithiane (Dim) Esters. Organic Letters, 2000, 2, 799-801.	4.6	17
44	Externally sensitized mesolytic fragmentations in dithianeâ€“ketone adducts. Tetrahedron, 2006, 62, 6574-6580.	1.9	15
45	2,6,7-Trithiabicyclo[2.2.2]octanes as Promising Photolabile Tags for Combinatorial Encoding. Journal of Organic Chemistry, 2008, 73, 335-338.	3.2	15
46	Computationally driven reassignment of the structures of aldingenins A and B. Tetrahedron Letters, 2015, 56, 4900-4903.	1.4	15
47	Photoinduced â€œDouble Clickâ€•Cascade Offers Access to Complex Polyheterocycles from Readily Available Isatin-Based Photoprecursors. Organic Letters, 2016, 18, 3750-3753.	4.6	15
48	Photoactive Barbiturate Receptors:Â An Ultimate Lock-and-Key System in Which the Key Unlocks the Lock. Organic Letters, 2007, 9, 1077-1079.	4.6	14
49	Photoamplification and Multiple Tag Release in a Linear Peptideâ€Based Array of Dithiane Adducts. Angewandte Chemie - International Edition, 2007, 46, 6137-6140.	13.8	14
50	Photoinitiated Cascade for Rapid Access to Pyrroloquinazolinone Core of Vasicinone, Luotonins, and Related Alkaloids. Organic Letters, 2019, 21, 2855-2858.	4.6	14
51	Stereochemical revision of xylogranatin F by GIAO and DU8+ NMR calculations. Chirality, 2020, 32, 515-523.	2.6	14
52	Synthesis and Liquid Membrane Transport Properties of Photolabile Molecular Clips Based on Dithiane-spiro-crown Ethers. Organic Letters, 2001, 3, 2633-2635.	4.6	13
53	First example of intramolecular [2Ï€+2Ï€] alkeneâ€“arene photocyclization in the chromone series and its synthetic utility. Tetrahedron Letters, 2010, 51, 3803-3806.	1.4	13
54	symm-Tetramethylenecyclooctane: En Route to Polyspirocycles. Journal of Organic Chemistry, 2014, 79, 8163-8170.	3.2	13

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55	Photoinduced Cycloadditions in the Diversity-Oriented Synthesis Toolbox: Increasing Complexity with Straightforward Post-Photochemical Modifications. Australian Journal of Chemistry, 2015, 68, 1672.	0.9	13
56	Structure Revision of Decurrensides Aâ€“E Enabled by the RFF Parametric Calculations of Proton Spinâ€“Spin Coupling Constants. Journal of Organic Chemistry, 2016, 81, 8659-8661.	3.2	13
57	The Discreet Structural Diversity of Briarellins: DU8+ Guided Multiple Structure Revisions Yielded Two Unknown Structural Types. Journal of Organic Chemistry, 2020, 85, 6201-6205.	3.2	10
58	Reassignment of Improbable Natural Products Identified through Chemical Principle Screening. European Journal of Organic Chemistry, 2022, 2022, .	2.4	10
59	Photooxidation of Methyldithiepins into Dithiepin Carboxaldehydes in Carbon Tetrachloride. Organic Letters, 1999, 1, 937-939.	4.6	9
60	Photoassisted Diversity-Oriented Synthesis: Intramolecular Cycloadditions of Photogenerated Azaxylylenes with Oxazole Pendants, and Subsequent Postphotochemical Multicomponent Modifications. Organic Letters, 2016, 18, 460-463.	4.6	9
61	Toward parameterization of spin-orbit coupling in triplet organic diradicals separated by a partially conjugated spacer. Arkivoc, 2005, 2005, 88-101.	0.5	9
62	Photoassisted access to complex polyheterocycles containing a Î²-lactam moiety. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 329, 182-188.	3.9	8
63	Access to 5-fluoroisoxazoles via the nitrosation of geminal bromo-fluoro arylcyclopropanes. Tetrahedron, 2019, 75, 2861-2865.	1.9	8
64	Peculiar Reaction Products and Mechanisms Revisited with Machine Learning-Augmented Computational NMR. Journal of Organic Chemistry, 2022, 87, 8589-8598.	3.2	8
65	Photolabile amphiphiles with fluorogenic thioxanthone-dithiane functionality: synthesis and photoinduced fragmentation in micelles. Journal of Sulfur Chemistry, 2008, 29, 389-400.	2.0	7
66	Photoassisted Synthesis of Complex Molecular Architectures: Dearomatization of Benzenoid Arenes with Azaâ€oâ€xylylenes via an Unprecedented [2+4] Reaction Topology. Angewandte Chemie, 2016, 128, 7102-7105.	2.0	7
67	Beyond the Dimer and Trimer: Tetraspiro[2.1.2 5 .1.2 9 .1.2 13 .1 3] hexadecaneâ€1,3,5,7â€tetraoneâ€”the Cyclic Tetramer of Carbonylcyclopropane. Chemistry - A European Journal, 2016, 22, 3996-3999.	3.3	6
68	Structure Determination and Mechanism of Formation of a seco-Moreliane Derivative Supported by Computational Analysis. Journal of Natural Products, 2017, 80, 1210-1214.	3.0	6
69	EBCâ€232 and 323: A Structural Conundrum Necessitating Unification of Five In Silico Prediction and Elucidation Methods. Chemistry - A European Journal, 2020, 26, 11862-11867.	3.3	6
70	Maximizing Stepâ€Normalized Increases in Molecular Complexity: Formal [4+2+2+2] Photoinduced Cyclization Cascade to Access Polyheterocycles Possessing Privileged Substructures. Angewandte Chemie - International Edition, 2022, 61, e202112573.	13.8	6
71	Polyheterocycle-carbohydrate chimeras: photoassisted synthesis of 2,5-epoxybenzoxacines and 2,5-epoxybenzazocine scaffolds and their postphotochemical hydroxylations. Pure and Applied Chemistry, 2017, 89, 259-268.	1.9	5
72	Reassignments and Corroborations of Oxoâ€Bridged Natural Products Directed by OSE and DU8+ NMR Computation. Angewandte Chemie, 2019, 131, 7181-7186.	2.0	5

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73	DU8+ Computations Reveal a Common Challenge in the Structure Assignment of Natural Products Containing a Carboxylic Anhydride Moiety. Journal of Organic Chemistry, 2021, 86, 17511-17515.	3.2	5
74	Determination of the Position of the Conformational Equilibrium of a Trans 1,2-Disubstituted Cyclohexane by NMR Spectroscopy. An Experiment in Physical Organic Chemistry for Undergraduate Students. Journal of Chemical Education, 2001, 78, 81.	2.3	3
75	A peculiar quenching concentration dependence of photoinduced fragmentation in dithianeâ€“carbonyl adducts: A mechanistic experimental and theoretical study. Journal of Photochemistry and Photobiology A: Chemistry, 2009, 206, 80-86.	3.9	3
76	Diastereoselective heterocyclization of geminal bromo-fluoro arylcyclopropanes by nitrosonium tetrafluoroborate: Access to 4-fluorinated isoxazolines and isoxazoles. Tetrahedron, 2019, 75, 130666.	1.9	3
77	Dithiane, Trithiane, and Dithiazane-Based Photolabile Scaffolds for Molecular Recognition: Mechanism and Efficiency of the Photoinduced Fragmentation in Aqueous Reductive Environments. Phosphorus, Sulfur and Silicon and the Related Elements, 2005, 180, 1379-1384.	1.6	2
78	Effect of Î²-Alkylthioethyl Substitution in 1,3-Dithianes: Quasianchimeric Assistance in Photoinduced Electron Transfer?. Journal of Organic Chemistry, 2008, 73, 6393-6396.	3.2	2
79	Cascade transformations involving thiocarbonyls: photoassisted access to bicyclic thiiranes and oxapentalenes. Journal of Sulfur Chemistry, 2013, 34, 209-221.	2.0	2
80	Maximizing Stepâ€Normalized Increases in Molecular Complexity: Formal [4+2+2+2] Photoinduced Cyclization Cascade to Access Polyheterocycles Possessing Privileged Substructures. Angewandte Chemie, 2022, 134, .	2.0	2
81	Photoactive spatial proximity probes for binding pairs with epigenetic marks. Journal of Photochemistry and Photobiology A: Chemistry, 2014, 290, 101-108.	3.9	1
82	Structure revision of ent-kaurane diterpenoids, isoserrins A, B, and D, enabled by DU8+ computation of their NMR spectral data. Mendeleev Communications, 2021, 31, 300-301.	1.6	1
83	Structure revision of ent-kaurane diterpenoids, isoserrins A, B, and D, enabled by DU8+ computation of their NMR spectral data. Mendeleev Communications, 2021, 31, 300-301.	1.6	0