

Andrei G Kutateladze

List of Publications by Year in descending order

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83
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#	ARTICLE	IF	CITATIONS
1	Maximizing Stepâ€Normalized Increases in Molecular Complexity: Formal [4+2+2+2] Photoinduced Cyclization Cascade to Access Polyheterocycles Possessing Privileged Substructures. <i>Angewandte Chemie</i> , 2022, 134, .	2.0	2
2	Maximizing Stepâ€Normalized Increases in Molecular Complexity: Formal [4+2+2+2] Photoinduced Cyclization Cascade to Access Polyheterocycles Possessing Privileged Substructures. <i>Angewandte Chemie - International Edition</i> , 2022, 61, e202112573.	13.8	6
3	DU8ML: Machine Learning-Augmented Density Functional Theory Nuclear Magnetic Resonance Computations for High-Throughput In Silico Solution Structure Validation and Revision of Complex Alkaloids. <i>Journal of Organic Chemistry</i> , 2022, 87, 4818-4828.	3.2	25
4	Peculiar Reaction Products and Mechanisms Revisited with Machine Learning-Augmented Computational NMR. <i>Journal of Organic Chemistry</i> , 2022, 87, 8589-8598.	3.2	8
5	Reassignment of Improbable Natural Products Identified through Chemical Principle Screening. <i>European Journal of Organic Chemistry</i> , 2022, 2022, .	2.4	10
6	Structure revision of ent-kaurane diterpenoids, isoserrins A, B, and D, enabled by DU8+ computation of their NMR spectral data. <i>Mendeleev Communications</i> , 2021, 31, 300-301.	1.6	1
7	Structure revision of ent-kaurane diterpenoids, isoserrins A, B, and D, enabled by DU8+ computation of their NMR spectral data. <i>Mendeleev Communications</i> , 2021, 31, 300-301.	1.6	0
8	DU8+ Computations Reveal a Common Challenge in the Structure Assignment of Natural Products Containing a Carboxylic Anhydride Moiety. <i>Journal of Organic Chemistry</i> , 2021, 86, 17511-17515.	3.2	5
9	EBCâ€232 and 323: A Structural Conundrum Necessitating Unification of Five In Silico Prediction and Elucidation Methods. <i>Chemistry - A European Journal</i> , 2020, 26, 11862-11867.	3.3	6
10	Stereochemical revision of xylogranatin F by GIAO and DU8+ NMR calculations. <i>Chirality</i> , 2020, 32, 515-523.	2.6	14
11	The Discreet Structural Diversity of Briarellins: DU8+ Guided Multiple Structure Revisions Yielded Two Unknown Structural Types. <i>Journal of Organic Chemistry</i> , 2020, 85, 6201-6205.	3.2	10
12	The value of universally available raw NMR data for transparency, reproducibility, and integrity in natural product research. <i>Natural Product Reports</i> , 2019, 36, 35-107.	10.3	92
13	Diastereoselective heterocyclization of geminal bromo-fluoro arylcyclopropanes by nitrosonium tetrafluoroborate: Access to 4-fluorinated isoxazolines and isoxazoles. <i>Tetrahedron</i> , 2019, 75, 130666.	1.9	3
14	Structure Validation of Complex Natural Products: Time to Change the Paradigm. What did Synthesis of Alstofoline A Prove?. <i>Journal of Organic Chemistry</i> , 2019, 84, 8297-8299.	3.2	26
15	Natural Products Containing the Oxetane and Related Moieties Present Additional Challenges for Structure Elucidation: A DU8+ Computational Case Study. <i>Journal of Organic Chemistry</i> , 2019, 84, 7575-7586.	3.2	30
16	Reassignments and Corroborations of Oxoâ€Bridged Natural Products Directed by OSE and DU8+ NMR Computation. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 7107-7112.	13.8	41
17	Reassignments and Corroborations of Oxoâ€Bridged Natural Products Directed by OSE and DU8+ NMR Computation. <i>Angewandte Chemie</i> , 2019, 131, 7181-7186.	2.0	5
18	Photoinitiated Cascade for Rapid Access to Pyrroloquinazolinone Core of Vasicinone, Luotonins, and Related Alkaloids. <i>Organic Letters</i> , 2019, 21, 2855-2858.	4.6	14

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19	Access to 5-fluoroisoxazoles via the nitrosation of geminal bromo-fluoro arylcyclopropanes. <i>Tetrahedron</i> , 2019, 75, 2861-2865.	1.9	8
20	Structural insights into the π - π stacking mechanism and DNA-binding activity of the YEATS domain. <i>Nature Communications</i> , 2018, 9, 4574.	12.8	45
21	Addressing the Challenges of Structure Elucidation in Natural Products Possessing the Oxirane Moiety. <i>Journal of Organic Chemistry</i> , 2018, 83, 8341-8352.	3.2	37
22	A novel withanolide with an unprecedented carbon skeleton from <i>Physalis angulata</i> . <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 1110-1114.	2.8	21
23	Polyheterocycle-carbohydrate chimeras: photoassisted synthesis of 2,5-epoxybenzoxacines and 2,5-epoxybenzazocine scaffolds and their postphotochemical hydroxylations. <i>Pure and Applied Chemistry</i> , 2017, 89, 259-268.	1.9	5
24	High-Throughput in Silico Structure Validation and Revision of Halogenated Natural Products Is Enabled by Parametric Corrections to DFT-Computed ^{13}C NMR Chemical Shifts and Spin-Spin Coupling Constants. <i>Journal of Organic Chemistry</i> , 2017, 82, 3368-3381.	3.2	121
25	Structure Determination and Mechanism of Formation of a <i>seco</i> -Moreliane Derivative Supported by Computational Analysis. <i>Journal of Natural Products</i> , 2017, 80, 1210-1214.	3.0	6
26	Step-Economical Photoassisted Diversity-Oriented Synthesis: Sustaining Cascade Photoreactions in Oxalyl Anilides to Access Complex Polyheterocyclic Molecular Architectures. <i>Journal of the American Chemical Society</i> , 2017, 139, 16584-16590.	13.7	34
27	Triquinanes and Related Sesquiterpenes Revisited Computationally: Structure Corrections of Hirsutanols B and D, Hirsutenol E, Cucumin B, Antrodins C-E, Chondroterpenes A and H, Chondrosterins C and E, Dichrocephone A, and Pethybrene. <i>Journal of Organic Chemistry</i> , 2017, 82, 10795-10802.	3.2	56
28	Photoassisted Synthesis of Complex Molecular Architectures: Dearomatization of Benzenoid Arenes with Azaxylidines via an Unprecedented [2+4] Reaction Topology. <i>Angewandte Chemie</i> , 2016, 128, 7102-7105.	2.0	7
29	Beyond the Dimer and Trimer: Tetraspiro[2.1.2.5.1.2.9.1.2.13.1.3] hexadecane-1,3,5,7-tetraone the Cyclic Tetramer of Carbonylcyclopropane. <i>Chemistry - A European Journal</i> , 2016, 22, 3996-3999.	3.3	6
30	Structure Revision of Decurrensides Enabled by the RFF Parametric Calculations of Proton Spin-Spin Coupling Constants. <i>Journal of Organic Chemistry</i> , 2016, 81, 8659-8661.	3.2	13
31	Structure Revision of an Acorane Sesquiterpene Cordycepol A. <i>Organic Letters</i> , 2016, 18, 4860-4863.	4.6	35
32	Computational structure revision of a longipinane derivative meridane. <i>Tetrahedron Letters</i> , 2016, 57, 4727-4729.	1.4	21
33	Photoassisted access to complex polyheterocycles containing a β -lactam moiety. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016, 329, 182-188.	3.9	8
34	Photoinduced Double Click-Cascade Offers Access to Complex Polyheterocycles from Readily Available Isatin-Based Photoprecursors. <i>Organic Letters</i> , 2016, 18, 3750-3753.	4.6	15
35	Photoassisted Synthesis of Complex Molecular Architectures: Dearomatization of Benzenoid Arenes with Azaxylidines via an Unprecedented [2+4] Reaction Topology. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 6988-6991.	13.8	40
36	Photoassisted Diversity-Oriented Synthesis: Intramolecular Cycloadditions of Photogenerated Azaxylidines with Oxazole Pendants, and Subsequent Postphotochemical Multicomponent Modifications. <i>Organic Letters</i> , 2016, 18, 460-463.	4.6	9

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37	Oxazolines as Dual-Function Traceless Chromophores and Chiral Auxiliaries: Enantioselective Photoassisted Synthesis of Polyheterocyclic Ketones. <i>Journal of the American Chemical Society</i> , 2016, 138, 2110-2113.	13.7	44
38	Amino Azaxyllylenes Photogenerated from <i>o</i> -Amido Imines: Photoassisted Access to Complex Spiro-Polyheterocycles. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 11516-11520.	13.8	52
39	An Acetyl-Methyl Switch Drives a Conformational Change in p53. <i>Structure</i> , 2015, 23, 322-331.	3.3	21
40	Intramolecular Cycloadditions of Photogenerated Azaxyllylenes with Oxadiazoles Provide Direct Access to Versatile Polyheterocyclic Ketopiperazines Containing a Spiro-oxirane Moiety. <i>Organic Letters</i> , 2015, 17, 438-441.	4.6	27
41	Computationally driven reassignment of the structures of aldingenins A and B. <i>Tetrahedron Letters</i> , 2015, 56, 4900-4903.	1.4	15
42	Minimalist Relativistic Force Field: Prediction of Proton-Proton Coupling Constants in ¹ H NMR Spectra Is Perfected with NBO Hybridization Parameters. <i>Journal of Organic Chemistry</i> , 2015, 80, 5218-5225.	3.2	89
43	Conformationally Constrained Penta(hetero)cyclic Molecular Architectures by Photoassisted Diversity-Oriented Synthesis. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 2205-2213.	2.4	22
44	Relativistic Force Field: Parametrization of ¹³ C- ¹ H Nuclear Spin-Spin Coupling Constants. <i>Journal of Organic Chemistry</i> , 2015, 80, 10838-10848.	3.2	59
45	Photoinduced Cycloadditions in the Diversity-Oriented Synthesis Toolbox: Increasing Complexity with Straightforward Post-Photochemical Modifications. <i>Australian Journal of Chemistry</i> , 2015, 68, 1672.	0.9	13
46	Intramolecular Photoassisted Cycloadditions of Azaxyllylenes and Postphotochemical Capstone Modifications via Suzuki Coupling Provide Access to Complex Polyheterocyclic Biaryls. <i>Journal of Organic Chemistry</i> , 2014, 79, 1235-1246.	3.2	31
47	Photoassisted Diversity-Oriented Synthesis: Accessing 2,6-Epoxyazocane (Oxamorphane) Cores. <i>Journal of Organic Chemistry</i> , 2014, 79, 10956-10971.	3.2	27
48	Relativistic Force Field: Parametric Computations of Proton-Proton Coupling Constants in ¹ H NMR Spectra. <i>Journal of Organic Chemistry</i> , 2014, 79, 8397-8406.	3.2	74
49	<i>o</i> -Tetramethylenecyclooctane: En Route to Polyspirocycles. <i>Journal of Organic Chemistry</i> , 2014, 79, 8163-8170.	3.2	13
50	Photoactive spatial proximity probes for binding pairs with epigenetic marks. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2014, 290, 101-108.	3.9	1
51	Intramolecular Cycloadditions of Photogenerated Azaxyllylenes: An Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10487-10496.	2.5	25
52	Photoinduced Intramolecular Cyclopentanation vs Photoprotolytic Oxametathesis in Polycyclic Alkenes Outfitted with Conformationally Constrained Aroylmethyl Chromophores. <i>Journal of Organic Chemistry</i> , 2013, 78, 2012-2025.	3.2	29
53	Cascade transformations involving thiocarbonyls: photoassisted access to bicyclic thiranes and oxapentalenes. <i>Journal of Sulfur Chemistry</i> , 2013, 34, 209-221.	2.0	2
54	Photoassisted Access to Enantiopure Conformationally Locked Ribofuranosylamines Spiro-Linked to Oxazolidino-Diketopiperazines. <i>ACS Combinatorial Science</i> , 2013, 15, 73-76.	3.8	31

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55	Photoassisted Synthesis of Enantiopure Alkaloid Mimics Possessing Unprecedented Polyheterocyclic Cores. <i>Journal of the American Chemical Society</i> , 2013, 135, 9608-9611.	13.7	62
56	Double-Tandem [4+2]-[2+2]-[4+2]-[2+2] Synthetic Sequence with Photoprotolytic Oxametathesis and Photoepoxidation in the Chromone Series. <i>Journal of Organic Chemistry</i> , 2011, 76, 1319-1332.	3.2	42
57	Rapid Photoassisted Access to N,O-Polyheterocycles with Benzoazocine and Hydroquinoline Cores: Intramolecular Cycloadditions of Photogenerated Azaxylenes. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 9423-9428.	13.8	77
58	First example of intramolecular [2+2] alkene-arene photocyclization in the chromone series and its synthetic utility. <i>Tetrahedron Letters</i> , 2010, 51, 3803-3806.	1.4	13
59	Strained to the Limit: When a Cyclobutyl Moiety Becomes a Thermodynamic Sink in a Protolytic Ring-Opening of Photogenerated Oxetanes. <i>Organic Letters</i> , 2010, 12, 3398-3401.	4.6	19
60	A peculiar quenching concentration dependence of photoinduced fragmentation in dithiane-carbonyl adducts: A mechanistic experimental and theoretical study. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2009, 206, 80-86.	3.9	3
61	Harvesting the Strain Installed by a Paternò-Büchi Step in a Synthetically Useful Way: High-Yielding Photoprotolytic Oxametathesis in Polycyclic Systems. <i>Organic Letters</i> , 2009, 11, 3886-3889.	4.6	49
62	2,6,7-Trithiabicyclo[2.2.2]octanes as Promising Photolabile Tags for Combinatorial Encoding. <i>Journal of Organic Chemistry</i> , 2008, 73, 335-338.	3.2	15
63	Photolabile amphiphiles with fluorogenic thioxanthone-dithiane functionality: synthesis and photoinduced fragmentation in micelles. <i>Journal of Sulfur Chemistry</i> , 2008, 29, 389-400.	2.0	7
64	Effect of β -Alkylthioethyl Substitution in 1,3-Dithianes: Quasi-anchimeric Assistance in Photoinduced Electron Transfer?. <i>Journal of Organic Chemistry</i> , 2008, 73, 6393-6396.	3.2	2
65	Photoactive Barbiturate Receptors: An Ultimate Lock-and-Key System in Which the Key Unlocks the Lock. <i>Organic Letters</i> , 2007, 9, 1077-1079.	4.6	14
66	Photoamplification and Multiple Tag Release in a Linear Peptide-Based Array of Dithiane Adducts. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 6137-6140.	13.8	14
67	Externally sensitized mesolytic fragmentations in dithiane-ketone adducts. <i>Tetrahedron</i> , 2006, 62, 6574-6580.	1.9	15
68	Direct screening of solution phase combinatorial libraries encoded with externally sensitized photolabile tags. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 13917-13921.	7.1	28
69	Dithiane, Trithiane, and Dithiazane-Based Photolabile Scaffolds for Molecular Recognition: Mechanism and Efficiency of the Photoinduced Fragmentation in Aqueous Reductive Environments. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2005, 180, 1379-1384.	1.6	2
70	Release and Report: A New Photolabile Caging System with a Two-Photon Fluorescence Reporting Function. <i>Journal of the American Chemical Society</i> , 2005, 127, 12458-12459.	13.7	50
71	Toward parameterization of spin-orbit coupling in triplet organic diradicals separated by a partially conjugated spacer. <i>Arkivoc</i> , 2005, 2005, 88-101.	0.5	9
72	Dithiane-Based Photolabile Amphiphiles: Toward Photolabile Liposomes. <i>Langmuir</i> , 2003, 19, 6381-6391.	3.5	24

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73	Anomalous C-C Bond Cleavage in Sulfur-Centered Cation Radicals Containing a Vicinal Hydroxy Group. <i>Journal of Organic Chemistry</i> , 2003, 68, 8236-8239.	3.2	30
74	Conformational Analysis of Singlet-Triplet State Mixing in Paternò-Büchi Diradicals. <i>Journal of the American Chemical Society</i> , 2001, 123, 9279-9282.	13.7	66
75	Dithiane- and Trithiane-Based Photolabile Scaffolds for Molecular Recognition. <i>Organic Letters</i> , 2001, 3, 1841-1844.	4.6	27
76	Synthesis and Liquid Membrane Transport Properties of Photolabile Molecular Clips Based on Dithiane-spiro-crown Ethers. <i>Organic Letters</i> , 2001, 3, 2633-2635.	4.6	13
77	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. <i>Journal of Chemical Education</i> , 2001, 78, 81.	2.3	3
78	Photoinduced C-C Bond Cleavage in Dithiane-Carbonyl Adducts: A Laser Flash Photolysis Study. <i>Journal of Organic Chemistry</i> , 2001, 66, 2887-2890.	3.2	38
79	Efficient Electrochemical Deprotection of Carboxylic and Amino Acids from Their 2-(Hydroxymethyl)-1,3-dithiane (Dim) Esters. <i>Organic Letters</i> , 2000, 2, 799-801.	4.6	17
80	Direct Transformation of 1,3-Dihalides into Dithianes and Dithiepins via a Novel One-Pot Reaction with Carbon Disulfide and Sodium Borohydride. <i>Organic Letters</i> , 2000, 2, 1133-1135.	4.6	19
81	Molecular Assembly and Disassembly: Novel Photolabile Molecular Hosts. <i>Organic Letters</i> , 2000, 2, 3817-3819.	4.6	28
82	Photooxidation of Methyl dithiepins into Dithiepin Carboxaldehydes in Carbon Tetrachloride. <i>Organic Letters</i> , 1999, 1, 937-939.	4.6	9
83	An Efficient Photo-SET-Induced Cleavage of Dithiane-Carbonyl Adducts and Its Relevance to the Development of Photoremovable Protecting Groups for Ketones and Aldehydes. <i>Journal of Organic Chemistry</i> , 1998, 63, 9924-9931.	3.2	64