

Ariel M Sarotti

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Beyond DP4: an Improved Probability for the Stereochemical Assignment of Isomeric Compounds using Quantum Chemical Calculations of NMR Shifts. <i>Journal of Organic Chemistry</i> , 2015, 80, 12526-12534.	1.7	890
2	A Multi-standard Approach for GIAO ¹³ C NMR Calculations. <i>Journal of Organic Chemistry</i> , 2009, 74, 7254-7260.	1.7	208
3	Computational Chemistry to the Rescue: Modern Toolboxes for the Assignment of Complex Molecules by GIAO NMR Calculations. <i>Chemistry - A European Journal</i> , 2016, 22, 12246-12261.	1.7	177
4	Combining the Power of <i>J</i> Coupling and DP4 Analysis on Stereochemical Assignments: The <i>J</i> -DP4 Methods. <i>Organic Letters</i> , 2019, 21, 4003-4007.	2.4	106
5	An efficient microwave-assisted green transformation of cellulose into levoglucosenone. Advantages of the use of an experimental design approach. <i>Green Chemistry</i> , 2007, 9, 1137.	4.6	94
6	Levoglucosenone and Its New Applications: Valorization of Cellulose Residues. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 590-604.	1.2	89
7	Successful combination of computationally inexpensive GIAO ¹³ C NMR calculations and artificial neural network pattern recognition: a new strategy for simple and rapid detection of structural misassignments. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 4847.	1.5	86
8	A critical review on the use of DP4+ in the structural elucidation of natural products: the good, the bad and the ugly. A practical guide. <i>Natural Product Reports</i> , 2022, 39, 58-76.	5.2	85
9	NMR Calculations with Quantum Methods: Development of New Tools for Structural Elucidation and Beyond. <i>Accounts of Chemical Research</i> , 2020, 53, 1922-1932.	7.6	84
10	Application of the Multi-standard Methodology for Calculating ¹ H NMR Chemical Shifts. <i>Journal of Organic Chemistry</i> , 2012, 77, 6059-6065.	1.7	83
11	Recent Applications of Levoglucosenone as Chiral Synthone. <i>Current Organic Synthesis</i> , 2012, 9, 439-459.	0.7	81
12	GIAO ¹ H COSY Simulations Merged with Artificial Neural Networks Pattern Recognition Analysis. Pushing the Structural Validation a Step Forward. <i>Journal of Organic Chemistry</i> , 2015, 80, 9371-9378.	1.7	69
13	Sensitivity Analysis of DP4+ with the Probability Distribution Terms: Development of a Universal and Customizable Method. <i>Journal of Organic Chemistry</i> , 2021, 86, 8544-8548.	1.7	61
14	Determination of the Relative Configuration of Terminal and Spiroepoxides by Computational Methods. Advantages of the Inclusion of Unscaled Data. <i>Journal of Organic Chemistry</i> , 2017, 82, 1873-1879.	1.7	51
15	Redefining the Impact of Boltzmann Analysis in the Stereochemical Assignment of Polar and Flexible Molecules by NMR Calculations. <i>Organic Letters</i> , 2020, 22, 52-56.	2.4	45
16	1,3-Dipolar Cycloaddition Reactions of Azomethine Ylides with a Cellulose-Derived Chiral Enone. A Novel Route for Organocatalysts Development. <i>Organic Letters</i> , 2012, 14, 2556-2559.	2.4	43
17	Computational Chemistry Driven Solution to Rubriflordilactone B. <i>Organic Letters</i> , 2016, 18, 6420-6423.	2.4	42
18	Structural revision of two unusual rhamnofolane diterpenes, curcusones I and J, by means of DFT calculations of NMR shifts and coupling constants. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 944-950.	1.5	37

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19	Highly Diastereoselective Diels-Alder Reaction Using a Chiral Auxiliary Derived from Levoglucosenone. <i>Organic Letters</i> , 2006, 8, 1487-1490.	2.4	36
20	π-Stacking Effect on Levoglucosenone Derived Internal Chiral Auxiliaries. A Case of Complete Enantioselectivity Inversion on the Diels-Alder Reaction. <i>Organic Letters</i> , 2008, 10, 3389-3392.	2.4	35
21	Flabelliparicine, a Flabelliformide-Apparicine-Type Bisindole Alkaloid from <i>Tabernaemontana divaricata</i> . <i>Journal of Natural Products</i> , 2018, 81, 1976-1983.	1.5	32
22	Unraveling polar Diels-Alder reactions with conceptual DFT analysis and the distortion/interaction model. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 187-199.	1.5	31
23	A facile microwave-assisted Diels-Alder reaction of vinylboronates. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 5069.	1.5	30
24	Cellulose recycling as a source of raw chirality. <i>Pure and Applied Chemistry</i> , 2013, 85, 1683-1692.	0.9	29
25	ML-DP4: An Integrated Quantum Mechanics-Machine Learning Approach for Ultrafast NMR Structural Elucidation. <i>Organic Letters</i> , 2022, 24, 7487-7491.	2.4	29
26	Joint Experimental, in Silico, and NMR Studies toward the Rational Design of Iminium-Based Organocatalyst Derived from Renewable Sources. <i>Journal of Organic Chemistry</i> , 2015, 80, 7626-7634.	1.7	28
27	Microwave-Assisted Regioselective Cycloaddition Reactions between 9-Substituted Anthracenes and Levoglucosenone. <i>Organic Letters</i> , 2006, 8, 5561-5564.	2.4	27
28	Second generation levoglucosenone-derived chiral auxiliaries. Scope and application in asymmetric Diels-Alder reactions. <i>Tetrahedron</i> , 2009, 65, 3502-3508.	1.0	27
29	Total Synthesis and Tentative Structural Elucidation of Cryptomoscatone E3: Interplay of Experimental and Computational Studies. <i>Journal of Organic Chemistry</i> , 2015, 80, 12027-12037.	1.7	27
30	A New N-methoxypyridone from the Co-Cultivation of Hawaiian Endophytic Fungi <i>Camporesia sambuci</i> FT1061 and <i>Epicoccum sorghinum</i> FT1062. <i>Molecules</i> , 2017, 22, 1166.	1.7	27
31	A theoretical study of the Duff reaction: insights into its selectivity. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 10496-10501.	1.5	26
32	Synthesis of Triazole Derivatives of Levoglucosenone As Promising Anticancer Agents: Effective Exploration of the Chemical Space through retro-aza-Michael/aza-Michael Isomerizations. <i>Journal of Organic Chemistry</i> , 2018, 83, 3516-3528.	1.7	25
33	Waikikiamides C: Complex Diketopiperazine Dimer and Diketopiperazine-Polyketide Hybrids from a Hawaiian Marine Fungal Strain <i>Aspergillus</i> sp. FM242. <i>Organic Letters</i> , 2020, 22, 4408-4412.	2.4	25
34	NF-β inhibitors, unique β-pyranol-β-lactams with sulfide and sulfoxide moieties from Hawaiian plant <i>Lycopodiella cernua</i> derived fungus <i>Paraphaeosphaeria neglecta</i> FT462. <i>Scientific Reports</i> , 2017, 7, 10424.	1.6	24
35	Exploring structural effects of levoglucosenone derived chiral auxiliaries in asymmetric Diels-Alder cycloadditions. <i>Tetrahedron</i> , 2007, 63, 241-251.	1.0	23
36	Sphaerialactonam, a β-lactam-isochromanone from the Hawaiian endophytic fungus <i>Paraphaeosphaeria</i> sp. FT462. <i>Tetrahedron Letters</i> , 2017, 58, 1330-1333.	0.7	22

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37	DFT calculations induced a regiochemical outcome revision of the Diels–Alder reaction between levoglucosenone and isoprene. <i>Tetrahedron Letters</i> , 2011, 52, 3116-3119.	0.7	21
38	Catalytic Asymmetric Synthesis and Stereochemical Revision of (+)-Cryptoconcatone H. <i>Journal of Organic Chemistry</i> , 2017, 82, 9191-9197.	1.7	21
39	General Quantum-Based NMR Method for the Assignment of Absolute Configuration by Single or Double Derivatization: Scope and Limitations. <i>Journal of Organic Chemistry</i> , 2018, 83, 11839-11849.	1.7	21
40	Experimental and theoretical insights in the alkene–arene intramolecular π -stacking interaction. <i>Beilstein Journal of Organic Chemistry</i> , 2016, 12, 1616-1623.	1.3	20
41	In Silico Reassignment of (+)-Diplopyrone by NMR Calculations: Use of a DP4+/DIP Tandem to Revise Both Relative and Absolute Configuration. <i>Journal of Organic Chemistry</i> , 2020, 85, 11566-11570.	1.7	19
42	The Risks of Automation: A Study on DFT Energy Miscalculations and Its Consequences in NMR-based Structural Elucidation. <i>Organic Letters</i> , 2020, 22, 3561-3565.	2.4	19
43	A novel design of a levoglucosenone derived chiral auxiliary. <i>Tetrahedron Letters</i> , 2004, 45, 8203-8206.	0.7	17
44	Theoretical insight into the pyrolytic deformylation of levoglucosenone and isolevoglucosenone. <i>Carbohydrate Research</i> , 2014, 390, 76-80.	1.1	16
45	Cascade cyclization triggered by imine formation. Formal synthesis of the alkaloid (Δ^{\pm})-stemoamide and its 9a-epimer. <i>Tetrahedron Letters</i> , 2015, 56, 6664-6668.	0.7	16
46	Verbenanone, an octahydro-5 H -chromen-5-one from a Hawaiian-plant associated fungus FT431. <i>Tetrahedron Letters</i> , 2017, 58, 2290-2293.	0.7	16
47	Design, synthesis and evaluation of novel levoglucosenone derivatives as promising anticancer agents. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2020, 30, 127247.	1.0	16
48	A chiral auxiliary derived from levoglucosenone in asymmetric Diels–Alder transformations. <i>Tetrahedron Letters</i> , 2005, 46, 6987-6990.	0.7	15
49	Exhaustive exploration of the conformational landscape of mono- and disubstituted five-membered rings by DFT and MP2 calculations. <i>RSC Advances</i> , 2019, 9, 24134-24145.	1.7	15
50	Re-Engineering Organocatalysts for Asymmetric Friedel–Crafts Alkylation of Indoles through Computational Studies. <i>Journal of Organic Chemistry</i> , 2020, 85, 9969-9978.	1.7	15
51	BOPHY–Fullerene C ₆₀ Dyad as a Photosensitizer for Antimicrobial Photodynamic Therapy. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	15
52	Are Computational Methods Useful for Structure Elucidation of Large and Flexible Molecules? Belizentrin as a Case Study. <i>Organic Letters</i> , 2021, 23, 503-507.	2.4	14
53	Assessing the halogen effect in Diels–Alder reactions involving chiral $\hat{\pi}$ -halo enones. A combined experimental and DFT computational approach. <i>Tetrahedron Letters</i> , 2011, 52, 4145-4148.	0.7	13
54	Thermodynamically driven, syn-selective vinylogous aldol reaction of tetronamides. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 4897-4907.	1.5	13

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55	Proton-Dependent Switching of a Novel Amino Chlorin Derivative as a Fluorescent Probe and Photosensitizer for Acidic Media. <i>Chemistry - A European Journal</i> , 2018, 24, 5950-5961.	1.7	13
56	Mechanistic insight into the acid-catalyzed isomerization of biomass-derived polysubstituted pyrrolidines: an experimental and DFT study. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 426-434.	1.5	12
57	Asymmetric construction of substituted pyrrolidines via 1,3-dipolar cycloaddition of azomethine ylides and chiral acrylates derived from biomass. <i>Tetrahedron Letters</i> , 2014, 55, 2394-2397.	0.7	11
58	Synthesis of a 3-Thiomannoside. <i>Organic Letters</i> , 2016, 18, 1748-1751.	2.4	11
59	Total Synthesis and Structural Validation of Phosdiecin A via Asymmetric Alcohol-Mediated Carbonyl Reductive Coupling. <i>Journal of the American Chemical Society</i> , 2019, 141, 13778-13782.	6.6	11
60	An Unusual Benzoisoquinoline-9-one Derivative and Other Related Compounds with Antiproliferative Activity from Hawaiian Endophytic Fungus <i>Peyronellaea</i> sp. FT431. <i>Molecules</i> , 2019, 24, 196.	1.7	11
61	An experimental/theoretical approach to determine the optical purity and the absolute configuration of endo- and exo-norborn-5-en-2-ol using mandelate derivatives. <i>Tetrahedron Letters</i> , 2009, 50, 6121-6125.	0.7	10
62	On the effect of intramolecular H-bonding in the configurational assessment of polyhydroxylated compounds with computational methods. The hyacinthacines case. <i>Carbohydrate Research</i> , 2019, 474, 72-79.	1.1	10
63	Asymmetric Allylboration Reactions with Soderquist's Chiral 10-Substituted-9-borabicyclo[3.3.2]decanes: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2009, 74, 3562-3565.	1.7	9
64	Experimental and theoretical study of a Diels-Alder reaction between a sugar-derived nitroalkene and cyclopentadiene. <i>Carbohydrate Research</i> , 2011, 346, 460-464.	1.1	8
65	Total synthesis and stereochemical assignment of cryptolatifolione. <i>RSC Advances</i> , 2015, 5, 53471-53476.	1.7	8
66	A Domino Epoxide Ring-Opening Xanthate Migration Reaction: An Alternative Entry to Thiosugars. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 6848-6856.	1.2	8
67	Palladium-Catalyzed Formation of Substituted Tetrahydropyrans: Mechanistic Insights and Structural Revision of Natural Products. <i>Synthesis</i> , 2019, 51, 1545-1560.	1.2	8
68	NMR and experimental reinvestigation of the condensation reaction between β^3 -methylene- β^2 -unsaturated aldehydes and propargyl aldehydes. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 1442-1447.	1.5	7
69	Montmorillonite K-10 promoted synthesis of chiral dioxo-caged compounds derived from levoglucosenone. <i>Carbohydrate Research</i> , 2015, 402, 67-70.	1.1	6
70	Substituent-Modulated Conformation and Supramolecular Assembly of Tetronamides. <i>Crystal Growth and Design</i> , 2016, 16, 5798-5810.	1.4	6
71	Thermal decomposition of hexamethylenetetramine: mechanistic study and identification of reaction intermediates via a computational and NMR approach. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 7374-7378.	1.5	6
72	New and bioactive polyketides from Hawaiian marine-derived fungus <i>Trichoderma</i> sp. FM652. <i>Natural Product Research</i> , 2022, 36, 5984-5990.	1.0	6

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73	Discovery of unusual dimeric piperazyl cyclopeptides encoded by a <i>Lentzea flaviverrucosa</i> DSM 44664 biosynthetic supercluster. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2117941119.	3.3	6
74	Solvatomorphs of 25,26,27,28-tetrahydroxycalix[4]arene and 5,11,17,23-tetramino-25,26,27,28-tetrabutoxycalix[4]arene: quenching photoluminescence through switching the guest. CrystEngComm, 2017, 19, 1792-1800.	1.3	5
75	Experimental and theoretical second harmonic generation and photoluminescence from the pseudo-centrosymmetric dihydrochloride salt dihydrate of trans-1,2-bis(4-pyridyl)ethene. CrystEngComm, 2017, 19, 346-354.	1.3	5
76	Heliotropiumides A and B, new phenolamides with N-carbamoyl putrescine moiety from Heliotropium foertherianum collected in Hawaii and their biological activities. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 4630-4634.	1.0	4
77	Winged-Cone Conformation in Hexa- <i>p</i> -tert-butylcalix[6]arene Driven by the Unusually Strong Guest Encapsulation. ACS Omega, 2017, 2, 5315-5323.	1.6	4
78	Computer-Guided Total Synthesis of Natural Products. Recent Examples and Future Perspectives. Journal of the Brazilian Chemical Society, 0, , .	0.6	4
79	Looking at the big picture in activation strain model/energy decomposition analysis: the case of the <i>ortho</i> / <i>para</i> regioselectivity rule in Diels-Alder reactions. Organic and Biomolecular Chemistry, 2020, 18, 1104-1111.	1.5	4
80	Polyketides, diketopiperazines and an isochromanone from the marine-derived fungal strain <i>Fusarium graminearum</i> FM1010 from Hawaii. Phytochemistry, 2022, 198, 113138.	1.4	4
81	Understanding reactivity and regioselectivity in Diels-Alder reactions of a sugar-derived dienophile bearing two competing EWGs. An experimental and computational study. Carbohydrate Research, 2015, 415, 54-59.	1.1	2
82	Why lamivudine assembles into double-stranded helices in crystals: salt heterosynthon versus base-pairing homosynthon. CrystEngComm, 2018, 20, 3049-3057.	1.3	2
83	Quantum chemical computation and machine learning in NMR. Magnetic Resonance in Chemistry, 2020, 58, 477-477.	1.1	2
84	BF ₃ ·OEt ₂ -Catalyzed Unexpected Stereoselective Formation of 2,4-trans-Diallyl-2-methyl-6-aryltetrahydro-2H-pyrans with Quaternary Stereocenters. Journal of Organic Chemistry, 2021, 86, 6518-6527.	1.7	2
85	New Alkaloids From a Hawaiian Fungal Strain <i>Aspergillus felis</i> FM324. Frontiers in Chemistry, 2021, 9, 724617.	1.8	1
86	Towards the Synthesis of Highly Hindered Pyrrolidines by Intramolecular AAC Click Reactions: What Can Be Learned from DFT Calculations?. European Journal of Organic Chemistry, 0, , .	1.2	1
87	NF- κ B inhibitory, antimicrobial and antiproliferative potentials of compounds from Hawaiian fungus <i>Aspergillus polyporicola</i> FS910. 3 Biotech, 2021, 11, 391.	1.1	0