## Ariel M Sarotti

## List of Publications by Year in descending order

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87 3,343 27 55
papers citations h-index g-index

87 87 87 2646
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#	Article	IF	CITATIONS
1	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. Natural Product Reports, 2022, 39, 58-76.	5.2	85
2	New and bioactive polyketides from Hawaiian marine-derived fungus <i>Trichoderma</i> sp. FM652. Natural Product Research, 2022, 36, 5984-5990.	1.0	6
3	Polyketides, diketopiperazines and an isochromanone from the marine-derived fungal strain Fusarium graminearum FM1010 from Hawaii. Phytochemistry, 2022, 198, 113138.	1.4	4
4	BOPHYâ€Fullerene C <sub>60</sub> Dyad as a Photosensitizer for Antimicrobial Photodynamic Therapy. Chemistry - A European Journal, 2022, 28, .	1.7	15
5	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
6	ML- <i>J</i> -DP4: An Integrated Quantum Mechanics-Machine Learning Approach for Ultrafast NMR Structural Elucidation. Organic Letters, 2022, 24, 7487-7491.	2.4	29
7	Thermal decomposition of hexamethylenetetramine: mechanistic study and identification of reaction intermediates <i>via</i> a computational and NMR approach. Organic and Biomolecular Chemistry, 2021, 19, 7374-7378.	1.5	6
8	BF3·OEt2-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
9	Sensitivity Analysis of DP4+ with the Probability Distribution Terms: Development of a Universal and Customizable Method. Journal of Organic Chemistry, 2021, 86, 8544-8548.	1.7	61
10	NF-κB inhibitory, antimicrobial and antiproliferative potentials of compounds from Hawaiian fungus Aspergillus polyporicola FS910. 3 Biotech, 2021, 11, 391.	1.1	0
11	New Alkaloids From a Hawaiian Fungal Strain Aspergillus felis FM324. Frontiers in Chemistry, 2021, 9, 724617.	1.8	1
12	Are Computational Methods Useful for Structure Elucidation of Large and Flexible Molecules? Belizentrin as a Case Study. Organic Letters, 2021, 23, 503-507.	2.4	14
13	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
14	Redefining the Impact of Boltzmann Analysis in the Stereochemical Assignment of Polar and Flexible Molecules by NMR Calculations. Organic Letters, 2020, 22, 52-56.	2.4	45
15	In Silico Reassignment of (+)-Diplopyrone by NMR Calculations: Use of a DP4/ <i>J</i> j-DP4/DP4+/DIP Tandem to Revise Both Relative and Absolute Configuration. Journal of Organic Chemistry, 2020, 85, 11566-11570.	1.7	19
16	NMR Calculations with Quantum Methods: Development of New Tools for Structural Elucidation and Beyond. Accounts of Chemical Research, 2020, 53, 1922-1932.	7.6	84
17	Waikikiamides A–C: Complex Diketopiperazine Dimer and Diketopiperazine–Polyketide Hybrids from a Hawaiian Marine Fungal Strain <i>Aspergillus</i> sp. FM242. Organic Letters, 2020, 22, 4408-4412.	2.4	25
18	Design, synthesis and evaluation of novel levoglucosenone derivatives as promising anticancer agents. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127247.	1.0	16

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19	Re-Engineering Organocatalysts for Asymmetric Friedel–Crafts Alkylation of Indoles through Computational Studies. Journal of Organic Chemistry, 2020, 85, 9969-9978.	1.7	15
20	Quantum chemical computation and machine learning in NMR. Magnetic Resonance in Chemistry, 2020, 58, 477-477.	1.1	2
21	The Risks of Automation: A Study on DFT Energy Miscalculations and Its Consequences in NMR-based Structural Elucidation. Organic Letters, 2020, 22, 3561-3565.	2.4	19
22	Total Synthesis and Structural Validation of Phosdiecin A via Asymmetric Alcohol-Mediated Carbonyl Reductive Coupling. Journal of the American Chemical Society, 2019, 141, 13778-13782.	6.6	11
23	Exhaustive exploration of the conformational landscape of mono- and disubstituted five-membered rings by DFT and MP2 calculations. RSC Advances, 2019, 9, 24134-24145.	1.7	15
24	Palladium-Catalyzed Formation of Substituted Tetrahydropyrans: Mechanistic Insights and Structural Revision of Natural Products. Synthesis, 2019, 51, 1545-1560.	1.2	8
25	On the effect of intramolecular H-bonding in the configurational assessment of polyhydroxylated compounds with computational methods. The hyacinthacines case. Carbohydrate Research, 2019, 474, 72-79.	1.1	10
26	Combining the Power of <i>J</i> Coupling and DP4 Analysis on Stereochemical Assignments: The <i>J</i> -DP4 Methods. Organic Letters, 2019, 21, 4003-4007.	2.4	106
27	An Unusual Benzoisoquinoline-9-one Derivative and Other Related Compounds with Antiproliferative Activity from Hawaiian Endophytic Fungus Peyronellaea sp. FT431. Molecules, 2019, 24, 196.	1.7	11
28	Synthesis of Triazole Derivatives of Levoglucosenone As Promising Anticancer Agents: Effective Exploration of the Chemical Space through <i>retro</i> -aza-Michael//aza-Michael Isomerizations. Journal of Organic Chemistry, 2018, 83, 3516-3528.	1.7	25
29	Protonâ€Dependent Switching of a Novel Amino Chlorin Derivative as a Fluorescent Probe and Photosensitizer for Acidic Media. Chemistry - A European Journal, 2018, 24, 5950-5961.	1.7	13
30	NMR and experimental reinvestigation of the condensation reaction between $\hat{I}^3$ -methylene- $\hat{I}\pm,\hat{I}^2$ -unsaturated aldehydes and propargyl aldehydes. Organic and Biomolecular Chemistry, 2018, 16, 1442-1447.	1.5	7
31	Levoglucosenone and Its New Applications: Valorization of Cellulose Residues. European Journal of Organic Chemistry, 2018, 2018, 590-604.	1.2	89
32	Why lamivudine assembles into double-stranded helices in crystals: salt heterosynthon versus base-pairing homosynthon. CrystEngComm, 2018, 20, 3049-3057.	1.3	2
33	Structural revision of two unusual rhamnofolane diterpenes, curcusones I and J, by means of DFT calculations of NMR shifts and coupling constants. Organic and Biomolecular Chemistry, 2018, 16, 944-950.	1.5	37
34	A Domino Epoxide Ringâ€Opening Xanthate Migration Reaction: An Alternative Entry to Thiosugars. European Journal of Organic Chemistry, 2018, 2018, 6848-6856.	1.2	8
35	General Quantum-Based NMR Method for the Assignment of Absolute Configuration by Single or Double Derivatization: Scope and Limitations. Journal of Organic Chemistry, 2018, 83, 11839-11849.	1.7	21
36	Flabellipparicine, a Flabelliformide-Apparicine-Type Bisindole Alkaloid from <i>Tabernaemontana divaricata </i> . Journal of Natural Products, 2018, 81, 1976-1983.	1.5	32

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37	Sphaerialactonam, a γ-lactam–isochromanone from the Hawaiian endophytic fungus Paraphaeosphaeria sp. FT462. Tetrahedron Letters, 2017, 58, 1330-1333.	0.7	22
38	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
39	Verbenanone, an octahydro-5 H -chromen-5-one from a Hawaiian-plant associated fungus FT431. Tetrahedron Letters, 2017, 58, 2290-2293.	0.7	16
40	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
41	Mechanistic insight into the acid-catalyzed isomerization of biomass-derived polysubstituted pyrrolidines: an experimental and DFT study. Organic and Biomolecular Chemistry, 2017, 15, 426-434.	1.5	12
42	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
43	NF-κB inhibitors, unique γ-pyranol-γ-lactams with sulfide and sulfoxide moieties from Hawaiian plant Lycopodiella cernua derived fungus Paraphaeosphaeria neglecta FT462. Scientific Reports, 2017, 7, 10424.	1.6	24
44	Winged-Cone Conformation in Hexa- <i>p-tert</i> butylcalix[6]arene Driven by the Unusually Strong Guest Encapsulation. ACS Omega, 2017, 2, 5315-5323.	1.6	4
45	Catalytic Asymmetric Synthesis and Stereochemical Revision of (+)-Cryptoconcatone H. Journal of Organic Chemistry, 2017, 82, 9191-9197.	1.7	21
46	Determination of the Relative Configuration of Terminal and Spiroepoxides by Computational Methods. Advantages of the Inclusion of Unscaled Data. Journal of Organic Chemistry, 2017, 82, 1873-1879.	1.7	51
47	A New N-methoxypyridone from the Co-Cultivation of Hawaiian Endophytic Fungi Camporesia sambuci FT1061 and Epicoccum sorghinum FT1062. Molecules, 2017, 22, 1166.	1.7	27
48	Experimental and theoretical insights in the alkene–arene intramolecular π-stacking interaction. Beilstein Journal of Organic Chemistry, 2016, 12, 1616-1623.	1.3	20
49	Computational Chemistry Driven Solution to Rubriflordilactone B. Organic Letters, 2016, 18, 6420-6423.	2.4	42
50	Synthesis of a 3-Thiomannoside. Organic Letters, 2016, 18, 1748-1751.	2.4	11
51	Thermodynamically driven, syn-selective vinylogous aldol reaction of tetronamides. Organic and Biomolecular Chemistry, 2016, 14, 4897-4907.	1.5	13
52	Substituent-Modulated Conformation and Supramolecular Assembly of Tetronamides. Crystal Growth and Design, 2016, 16, 5798-5810.	1.4	6
53	Computational Chemistry to the Rescue: Modern Toolboxes for the Assignment of Complex Molecules by GIAO NMR Calculations. Chemistry - A European Journal, 2016, 22, 12246-12261.	1.7	177
54	A theoretical study of the Duff reaction: insights into its selectivity. Organic and Biomolecular Chemistry, 2016, 14, 10496-10501.	1.5	26

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55	Total synthesis and stereochemical assignment of cryptolatifolione. RSC Advances, 2015, 5, 53471-53476.	1.7	8
56	Beyond DP4: an Improved Probability for the Stereochemical Assignment of Isomeric Compounds using Quantum Chemical Calculations of NMR Shifts. Journal of Organic Chemistry, 2015, 80, 12526-12534.	1.7	890
57	Cascade cyclization triggered by imine formation. Formal synthesis of the alkaloid $(\hat{A}\pm)$ -stemoamide and its 9a-epimer. Tetrahedron Letters, 2015, 56, 6664-6668.	0.7	16
58	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
59	Joint Experimental, in Silico, and NMR Studies toward the Rational Design of Iminium-Based Organocatalyst Derived from Renewable Sources. Journal of Organic Chemistry, 2015, 80, 7626-7634.	1.7	28
60	Total Synthesis and Tentative Structural Elucidation of Cryptomoscatone E3: Interplay of Experimental and Computational Studies. Journal of Organic Chemistry, 2015, 80, 12027-12037.	1.7	27
61	GIAO C–H COSY Simulations Merged with Artificial Neural Networks Pattern Recognition Analysis. Pushing the Structural Validation a Step Forward. Journal of Organic Chemistry, 2015, 80, 9371-9378.	1.7	69
62	Montmorillonite K-10 promoted synthesis of chiral dioxa-caged compounds derived from levoglucosenone. Carbohydrate Research, 2015, 402, 67-70.	1.1	6
63	Unraveling polar Diels–Alder reactions with conceptual DFT analysis and the distortion/interaction model. Organic and Biomolecular Chemistry, 2014, 12, 187-199.	1.5	31
64	Asymmetric construction of substituted pyrrolidines via 1,3-dipolar cycloaddition of azomethine ylides and chiral acrylates derived from biomass. Tetrahedron Letters, 2014, 55, 2394-2397.	0.7	11
65	Theoretical insight into the pyrolytic deformylation of levoglucosenone and isolevoglucosenone. Carbohydrate Research, 2014, 390, 76-80.	1.1	16
66	Successful combination of computationally inexpensive GIAO 13C NMR calculations and artificial neural network pattern recognition: a new strategy for simple and rapid detection of structural misassignments. Organic and Biomolecular Chemistry, 2013, 11, 4847.	1.5	86
67	Cellulose recycling as a source of raw chirality. Pure and Applied Chemistry, 2013, 85, 1683-1692.	0.9	29
68	Recent Applications of Levoglucosenone as Chiral Synthon. Current Organic Synthesis, 2012, 9, 439-459.	0.7	81
69	Application of the Multi-standard Methodology for Calculating <sup>1</sup> H NMR Chemical Shifts. Journal of Organic Chemistry, 2012, 77, 6059-6065.	1.7	83
70	1,3-Dipolar Cycloaddition Reactions of Azomethine Ylides with a Cellulose-Derived Chiral Enone. A Novel Route for Organocatalysts Development. Organic Letters, 2012, 14, 2556-2559.	2.4	43
71	Experimental and theoretical study of a Diels–Alder reaction between a sugar-derived nitroalkene and cyclopentadiene. Carbohydrate Research, 2011, 346, 460-464.	1.1	8
72	DFT calculations induced a regiochemical outcome revision of the Diels–Alder reaction between levoglucosenone and isoprene. Tetrahedron Letters, 2011, 52, 3116-3119.	0.7	21

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73	Assessing the halogen effect in Diels–Alder reactions involving chiral α-halo enones. A combined experimental and DFT computational approach. Tetrahedron Letters, 2011, 52, 4145-4148.	0.7	13
74	A facile microwave-assisted Diels–Alder reaction of vinylboronates. Organic and Biomolecular Chemistry, 2010, 8, 5069.	1.5	30
75	Second generation levoglucosenone-derived chiral auxiliaries. Scope and application in asymmetric Diels–Alder reactions. Tetrahedron, 2009, 65, 3502-3508.	1.0	27
76	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. Tetrahedron Letters, 2009, 50, 6121-6125.	0.7	10
77	Asymmetric Allylboration Reactions with Soderquist's Chiral 10-Substituted-9-borabicyclo[3.3.2]decanes: A Theoretical Study. Journal of Organic Chemistry, 2009, 74, 3562-3565.	1.7	9
78	A Multi-standard Approach for GIAO <sup>13</sup> C NMR Calculations. Journal of Organic Chemistry, 2009, 74, 7254-7260.	1.7	208
79	Ï€-Stacking Effect on Levoglucosenone Derived Internal Chiral Auxiliaries. A Case of Complete Enantioselectivity Inversion on the Dielsâ° Alder Reaction. Organic Letters, 2008, 10, 3389-3392.	2.4	35
80	An efficient microwave-assisted green transformation of cellulose into levoglucosenone. Advantages of the use of an experimental design approach. Green Chemistry, 2007, 9, 1137.	4.6	94
81	Exploring structural effects of levoglucosenone derived chiral auxiliaries in asymmetric Diels–Alder cycloadditions. Tetrahedron, 2007, 63, 241-251.	1.0	23
82	Highly Diastereoselective Dielsâ^'Alder Reaction Using a Chiral Auxiliary Derived from Levoglucosenone. Organic Letters, 2006, 8, 1487-1490.	2.4	36
83	Microwave-Assisted Regioselective Cycloaddition Reactions between 9-Substituted Anthracenes and Levoglucosenone. Organic Letters, 2006, 8, 5561-5564.	2.4	27
84	A chiral auxiliary derived from levoglucosenone in asymmetric Diels–Alder transformations. Tetrahedron Letters, 2005, 46, 6987-6990.	0.7	15
85	A novel design of a levoglucosenone derived chiral auxiliary. Tetrahedron Letters, 2004, 45, 8203-8206.	0.7	17
86	Computer-Guided Total Synthesis of Natural Products. Recent Examples and Future Perspectives. Journal of the Brazilian Chemical Society, 0, , .	0.6	4
87	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