Gabriel Cuevas

List of Publications by Year
in descending order

58	2,135	279798	223800
papers	citations	23 h-index	46 g-index

60	60	60	1890
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Effect of the nO â†' Ï€*Câ•O Interaction on the Conformational Preference of 1,3-Diketones: A Case Study of Riolozatrione Derivatives. Journal of Organic Chemistry, 2021, 86, 9540-9551.	3.2	1
2	Is the VCD spectrum a fingerprint of the conformational population? The conformation of perezone in the spotlight. Journal of Molecular Structure, 2020, 1202, 127273.	3.6	10
3	Experimental and theoretical study of the role of CH/Ïπ interactions in the aminolysis reaction of acetyl galactoside. Carbohydrate Research, 2019, 486, 107821.	2.3	5
4	Exploring the Role of Solvent on Carbohydrateâ€“Aryl Interactions by Diffusion NMR-Based Studies. ACS Omega, 2018, 3, 536-543.	3.5	2
5	Charge transfer and electron localization as the origin of the anomeric effect in the <scp>O</scp>â"€<scp>C</scp>â"€<scp>O</scp> segment of dimethoxymethane and spiroketals. Journal of Physical Organic Chemistry, 2018, 31, e3793.	1.9	5
6	Stereochemistry of a Second Riolozane and Other Diterpenoids from Jatropha dioica. Journal of Natural Products, 2017, 80, 2252-2262.	3.0	17
7	The influence of sulfur configuration in ¹H NMR chemical shifts of diasteromeric fiveâ€membered cyclic sulfites. Magnetic Resonance in Chemistry, 2017, 55, 233-238.	1.9	1
8	Biogenesis of Triterpene Dimers from Orthoquinones Related to Quinonemethides: Theoretical Study on the Reaction Mechanism. Molecules, 2016, 21, 1551.	3.8	4
9	The role of induced current density in Steroelectronic effects: Perlin effect. Journal of Computational Chemistry, 2015, 36, 1573-1578.	3.3	13
10	Vibrational Circular Dichroism (VCD), VCD Exciton Coupling, and Xâ€ray Determination of the Absolute Configuration of an Î±,Î²â€Unsaturated Germacranolide. Chirality, 2015, 27, 247-252.	2.6	13
11	The rotational barrier of ethane and some of its hexasubstituted derivatives in terms of the forces acting on the electron distribution. Physical Chemistry Chemical Physics, 2015, 17, 19021-19029.	2.8	17
12	ent-Kaurene Glycosides from Ageratina cylindrica. Journal of Natural Products, 2015, 78, 2580-2587.	3.0	21
13	A theoretical biogenesis overview of diterpenes isolated from Salvia microphylla. Journal of Molecular Modeling, 2015, 21, 306.	1.8	3
14	Assessment of hydrophobic interactions and their contributions through the analysis of the methane dimer. Journal of Computational Chemistry, 2015, 36, 361-375.	3.3	16
15	Properties of atoms in electronically excited molecules within the formalism of TDDFT. Journal of Computational Chemistry, 2014, 35, 820-828.	3.3	22
16	Dynamic Molecular Graphs: â€œHoppingâ€•Structures. Chemistry - A European Journal, 2014, 20, 5665-5672.	3.3	9
17	Structure, Absolute Configuration, and Antidiarrheal Activity of a Thymol Derivative from Ageratina cylindrica. Journal of Natural Products, 2014, 77, 358-363.	3.0	26
18	NMRâ€based conformational analysis of perezone and analogues. Magnetic Resonance in Chemistry, 2013, 51, 245-250.	1.9	12

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19	Theoretical study of the Diels-Alder reaction betweeno-benzoquinone and norbornadiene. IOP Conference Series: Materials Science and Engineering, 2013, 45, 012029.	0.6	1
20	The Rotational Barrier in Ethane: A Molecular Orbital Study. Molecules, 2012, 17, 4661-4671.	3.8	24
21	Role of Carbocationâ€™s Flexibility in Sesquiterpene Biosynthesis: Computational Study of the Formation Mechanism of Terrecyclene. Journal of Organic Chemistry, 2011, 76, 1572-1577.	3.2	16
22	AC-Glycosylflavone fromPiper ossanum, a Compound Conformationally Controlled by CH/Ï€ and Other Weak Intramolecular Interactions. Journal of Natural Products, 2010, 73, 1623-1627.	3.0	15
23	Conformational Properties of the Germacradienolide 6-Epidesacetyllaurenobiolide by Theory and NMR Analyses. Journal of Organic Chemistry, 2010, 75, 2139-2146.	3.2	7
24	Application of the additivity of group energies to understand conformational preference: the anomeric effect. Physical Chemistry Chemical Physics, 2010, 12, 13261.	2.8	11
25	Rotational Diffusion of Dihydroxy Coumarins: Effect of OH Groups and Their Relative Position on Soluteâ^'Solvent Interactions. Journal of Physical Chemistry B, 2009, 113, 8599-8606.	2.6	6
26	Enthalpic Nature of the CH/Ï€ Interaction Involved in the Recognition of Carbohydrates by Aromatic Compounds, Confirmed by a Novel Interplay of NMR, Calorimetry, and Theoretical Calculations. Journal of the American Chemical Society, 2009, 131, 18129-18138.	13.7	94
27	Biogenesis of Sesquiterpene Lactones Pseudoguaianolides from Germacranolides: Theoretical Study on the Reaction Mechanism of Terminal Biogenesis of 8-Epiconfertin. Journal of Organic Chemistry, 2009, 74, 874-883.	3.2	29
28	Aromaticâ€“Carbohydrate Interactions: An NMR and Computational Study of Model Systems. Chemistry - A European Journal, 2008, 14, 7570-7578.	3.3	75
29	Calorimetric Measurement of the CH/Ï€ Interaction Involved in the Molecular Recognition of Saccharides by Aromatic Compounds. Journal of Organic Chemistry, 2008, 73, 849-857.	3.2	37
30	Kinetic Studies of the Thermal cis-to-trans Isomerization of Dioxaphospholanes. Phosphorus, Sulfur and Silicon and the Related Elements, 2008, 183, 2421-2437.	1.6	14
31	On the role of aromatic-sugar interactions in the molecular recognition of carbohydrates: A 3D view by using NMR. Pure and Applied Chemistry, 2008, 80, 1827-1835.	1.9	26
32	Manifestations of Stereoelectronic Interactions in 1JCâ€“H One-Bond Coupling Constants. Accounts of Chemical Research, 2007, 40, 961-970.	15.6	49
33	Remote Position Substituents as Modulators of Conformational and Reactive Properties of Quinones. Relevance of the Ï€/Ï€ Intramolecular Interaction. Journal of Organic Chemistry, 2007, 72, 1883-1894.	3.2	20
34	Computational Study of 1,3-Dithiane 1,1-Dioxide (1,3-Dithiane Sulfone). Description of the Inversion Process and Manifestation of Stereoelectronic Effects on 1JC-H Coupling Constants. Journal of Physical Chemistry A, 2006, 110, 7703-7712.	2.5	22
35	Eremophilane esters ofRobinsonecio gerberifolius and their rearranged products. Study of the coupling constants2JH, H,3JH, H and4JH, H. Magnetic Resonance in Chemistry, 2006, 44, 30-34.	1.9	3
36	Toward the origin of the conformational preference of 2-methoxyoxane, a model useful to study the anomeric effect. Arkivoc, 2006, 2003, 132-148.	0.5	6

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37	Theoretical Study of Inversion and Topomerization Processes of Substituted Cyclohexanes: The Relevance of the Energy 3D Hypersurface. ChemPhysChem, 2005, 6, 671-680.	2.1	27
38	The Origin of One-Bond C-H Coupling Constants in OCH Fragments: Not Primarily nOâ†'${{m sigma}{{ast hfill atop {m CH}hfill}}}$ Delocalization. Angewandte Chemie - International Edition, 2005, 44, 2360-2364.	13.8	48
39	Molecular Recognition of Saccharides by Proteins. Insights on the Origin of the Carbohydrateâ^'Aromatic Interactions. Journal of the American Chemical Society, 2005, 127, 7379-7386.	13.7	214
40	Manifestation of Stereoelectronic Effects on the Calculated Carbonâ^'Hydrogen Bond Lengths and One-Bond 1JC-H NMR Coupling Constants. Relative Acceptor Ability of the Carbonyl (CO), Thiocarbonyl (CS), and Methylidene (CCH2) Groups toward Câ^'H Donor Bonds. Journal of Organic Chemistry, 2004, 69, 7266-7276.	3.2	29
41	G2 and DFT Rigorous Description of the Inversion Process of Oxane and Thiane used as Simple Ring Systems to Model Sugar Components. ChemPhysChem, 2003, 4, 754-757.	2.1	11
42	The Nonexistence of Repulsive 1,3-Diaxial Interactions in Monosubstituted Cyclohexanes. Journal of Physical Chemistry A, 2003, 107, 9253-9256.	2.5	66
43	Manifestation of Stereoelectronic Effects on the Calculated Carbonâ^'Hydrogen Bond Lengths and One Bond1JC-HNMR Coupling Constants in Cyclohexane, Six-Membered Heterocycles, and Cyclohexanone Derivatives. Journal of the American Chemical Society, 2002, 124, 13088-13096.	13.7	92
44	Electronic Delocalization Contribution to the Anomeric Effect Evaluated by Computational Methods. Journal of Organic Chemistry, 2001, 66, 2918-2924.	3.2	45
45	Rigorous Interpretation of Electronic Density Functions of Axial and Equatorial Conformers of Dimethylphosphinoylcyclohexane, 2-(Dimethylphosphinoyl)-1,3,5-trithiane, and 2-(Dimethylphosphinoyl)-1,3-dithiane-1,1,3,3-tetraoxide. Journal of Organic Chemistry, 2001, 66, 2925-2931.	3.2	13
46	Hydrogen Bond Type Contributions to the Anomeric Effect in Sâ^'Câ^'P(O) and Sâ^'Câ^'P(S) Segmentsâ€. Journal of the American Chemical Society, 2000, 122, 692-698.	13.7	25
47	Density Functional Calculation of 1JC-H Coupling Constants in Cyclohexane and Diheterocyclohexanes. Repercussion of Stereoelectronic Effects on Coupling Constants. Journal of Physical Chemistry A, 1999, 103, 932-937.	2.5	68
48	A Density Functional Study of 2-Lithio-1,3-dithiane and 2-Lithio-2-phenyl-1,3-dithiane:Â Conformational Preference of the Câ^'Li Bond and Structural Analysis. Journal of the American Chemical Society, 1997, 119, 7545-7549.	13.7	42
49	Rationalization of the anomalous 1H NMR chemical shifts in 1,3-diheterocyclohexanes. Computational and Theoretical Chemistry, 1997, 418, 231-241.	1.5	37
50	Calorimetric study of the anomeric effect in 2-carboethoxy-1,3-dithianes. Journal of Physical Organic Chemistry, 1994, 7, 561-566.	1.9	2
51	Stereoelectronic Interpretation for the Anomalous 1H NMR Chemical Shifts and One-Bond C-H Coupling Constants (Perlin Effects) in 1,3-Dioxanes, 1,3-Oxathianes, and 1,3-Dithianes. Spectroscopic and Theoretical Observations. Journal of the American Chemical Society, 1994, 116, 5796-5804.	13.7	87
52	Conformational analysis of 1,3-dithian-2-yltrimethylphosphonium chloride. Origin of the S-C-P anomeric effect. Journal of the American Chemical Society, 1993, 115, 1313-1316.	13.7	21
53	Stereoelectronic interpretation of the unusual perlin effects and 1H NMR chemical shifts in 1,3-oxathiane. Tetrahedron Letters, 1992, 33, 6927-6930.	1.4	43
54	Reverse Perlin effects for all Cî—¸H bonds in 1,3-Dithiane.. Tetrahedron Letters, 1992, 33, 1847-1850.	1.4	42

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55	Enthalpic and entropic contributions to the s-c-p-(o) anomeric effect. Tetrahedron Letters, 1992, 33, 2271-2274.	1.4	13
56	Recent studies of the anomeric effect. Tetrahedron, 1992, 48, 5019-5087.	1.9	535
57	Diterpenes from Salvia brevifloraâ˜†. Phytochemistry, 1987, 26, 2019-2021.	2.9	18
58	Applications of the Quantum Theory of Atoms in Molecules in Organic Chemistryâ€“ Charge Distribution, Conformational Analysis and Molecular Interactions. , 0, , 375-397.		3