

Vladimir Baumruk

List of Publications by Year in descending order

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172457

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80
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80
docs citations

80
times ranked

1894
citing authors

#	ARTICLE	IF	CITATIONS
1	IR and Raman Spectra, Tautomeric Stabilities, and Scaled Quantum Mechanical Force Fields of Protonated Cytosine. The Journal of Physical Chemistry, 1996, 100, 5578-5589.	2.9	137
2	Predictions of Secondary Structure using Statistical Analyses of Electronic and Vibrational Circular Dichroism and Fourier Transform Infrared Spectra of Proteins in H ₂ O. Journal of Molecular Biology, 1996, 259, 774-791.	4.2	131
3	The role of triton X-100 as an adsorbate and a molecular spacer on the surface of silver colloid: a surface-enhanced Raman scattering study. The Journal of Physical Chemistry, 1992, 96, 1361-1366.	2.9	126
4	Demonstration of the Ring Conformation in Polyproline by the Raman Optical Activity. Journal of the American Chemical Society, 2006, 128, 2438-2443.	13.7	94
5	Vibrational circular dichroism of proteins in water solution. Journal of the American Chemical Society, 1993, 115, 6939-6942.	13.7	93
6	Conformational Flexibility of α -Alanine Zwitterion Determines Shapes of Raman and Raman Optical Activity Spectral Bands. Journal of Physical Chemistry A, 2006, 110, 4689-4696.	2.5	90
7	Surface-enhanced resonance Raman spectra of free base 5,10,15,20-tetrakis(4-carboxyphenyl)porphyrin and its silver complex in systems with silver colloid: direct adsorption in comparison to adsorption via molecular spacer. The Journal of Physical Chemistry, 1993, 97, 9719-9729.	2.9	83
8	Neutron Inelastic Scattering, Optical Spectroscopies and Scaled Quantum Mechanical Force Fields for Analyzing the Vibrational Dynamics of Pyrimidine Nucleic Acid Bases. 1. Uracil. The Journal of Physical Chemistry, 1996, 100, 5224-5234.	2.9	83
9	Proline Zwitterion Dynamics in Solution, Glass, and Crystalline State. Journal of the American Chemical Society, 2006, 128, 13451-13462.	13.7	82
10	Structure of human β 1-acid glycoprotein and its high-affinity binding site. Biochemical and Biophysical Research Communications, 2003, 300, 41-46.	2.1	80
11	IR and Raman Spectra, Conformational Flexibility, and Scaled Quantum Mechanical Force Fields of Sodium Dimethyl Phosphate and Dimethyl Phosphate Anion. The Journal of Physical Chemistry, 1996, 100, 1559-1568.	2.9	72
12	Conformational study of sequential Lys and Leu based polymers and oligomers using vibrational and electronic CD spectra. Biopolymers, 1994, 34, 1115-1121.	2.4	64
13	Ground State Properties of the Nucleic Acid Constituents Studied by Density Functional Calculations. 2. Comparison between Calculated and Experimental Vibrational Spectra of Uridine and Cytidine. Journal of Physical Chemistry B, 1999, 103, 10934-10944.	2.6	62
14	Anharmonic effects in IR, Raman, and Raman optical activity spectra of alanine and proline zwitterions. Journal of Chemical Physics, 2007, 126, 224513.	3.0	61
15	Interpretation of Raman and Raman Optical Activity Spectra of a Flexible Sugar Derivative, the Gluconic Acid Anion. Journal of Physical Chemistry A, 2009, 113, 3594-3601.	2.5	56
16	Neutron Inelastic Scattering, Optical Spectroscopies and Scaled Quantum Mechanical Force Fields for Analyzing the Vibrational Dynamics of Pyrimidine Nucleic Acid Bases: 3. Cytosine. Journal of Physical Chemistry A, 1997, 101, 10063-10074.	2.5	54
17	Structure of the ring in drop coating deposited proteins and its implication for Raman spectroscopy of biomolecules. Vibrational Spectroscopy, 2006, 42, 184-187.	2.2	52
18	Measurement and Calculation of the Raman Optical Activity of β -Pinene and trans-Pinane. Collection of Czechoslovak Chemical Communications, 1997, 62, 1384-1395.	1.0	51

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19	Comparison of Quantitative Conformer Analyses by Nuclear Magnetic Resonance and Raman Optical Activity Spectra for Model Dipeptides. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8633-8640.	2.5	51
20	Metalation of 5,10,15,20-tetrakis(1-methyl-4-pyridyl)porphyrin in silver colloids studied via time dependence of surface-enhanced resonance Raman spectra. <i>Journal of Raman Spectroscopy</i> , 1998, 29, 575-584.	2.5	46
21	Conformation of the Dipeptide Cyclo(L-Pro-L-Pro) Monitored by the Nuclear Magnetic Resonance and Raman Optical Activity Spectra. Experimental and ab Initio Computational Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7321-7327.	2.5	44
22	Simulation of the Raman Optical Activity of L-Alanyl-L-Alanine. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6362-6368.	2.5	43
23	Side Chain and Flexibility Contributions to the Raman Optical Activity Spectra of a Model Cyclic Hexapeptide. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7642-7651.	2.5	37
24	Unusual nucleotide conformations in GNRA and UNCG type tetraloop hairpins: evidence from Raman markers assignments. <i>Nucleic Acids Research</i> , 1999, 27, 1398-1404.	14.5	36
25	Surface-Enhanced Raman Scattering (SERS) Spectroscopy with Borohydride-Reduced Silver Colloids: Controlling Adsorption of the Scattering Species by Surface Potential of Silver Colloid. <i>Collection of Czechoslovak Chemical Communications</i> , 1993, 58, 2682-2694.	1.0	34
26	Protein Structural Segments and Their Interconnections Derived from Optical Spectra. Thermal Unfolding of Ribonuclease T1 as an Example. <i>Biochemistry</i> , 1996, 35, 13094-13106.	2.5	33
27	Comparison between CUUG and UUCG tetraloops: thermodynamic stability and structural features analyzed by UV absorption and vibrational spectroscopy. <i>Nucleic Acids Research</i> , 2001, 29, 4089-4096.	14.5	33
28	Molecular Characterization of Binding of Calcium and Carbohydrates by an Early Activation Antigen of Lymphocytes CD69. <i>Biochemistry</i> , 2003, 42, 9295-9306.	2.5	33
29	Tracking of the Polyproline Folding by Density Functional Computations and Raman Optical Activity Spectra. <i>Journal of Physical Chemistry B</i> , 2011, 115, 15079-15089.	2.6	31
30	Structural Features of the UCCG and UGCG Tetraloops in Very Short Hairpins As Evidenced by Optical Spectroscopy. <i>Biochemistry</i> , 1998, 37, 7878-7884.	2.5	30
31	L-Alanyl-L-alanine Conformational Changes Induced by pH As Monitored by the Raman Optical Activity Spectra. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7760-7768.	2.5	29
32	CH Stretching Region: Computational Modeling of Vibrational Optical Activity. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3096-3108.	5.3	29
33	Scaled Quantum Mechanical Force Fields and Vibrational Spectra of Nucleic Acid Constituents. 9. Tetrahydrofuran. <i>Journal of Physical Chemistry B</i> , 1998, 102, 1314-1319.	2.6	28
34	Conformational Properties of the Pro-Gly Motif in the D-Ala-L-Pro-Gly-D-Ala Model Peptide Explored by a Statistical Analysis of the NMR, Raman, and Raman Optical Activity Spectra. <i>Journal of Organic Chemistry</i> , 2008, 73, 1481-1489.	3.2	28
35	Eight Amino Acids Form the ATP Recognition Site of Na ⁺ /K ⁺ -ATPase. <i>Biochemistry</i> , 2003, 42, 6446-6452.	2.5	27
36	Study of Chaperone-Like Activity of Human Haptoglobin: Conformational Changes under Heat Shock Conditions and Localization of Interaction Sites. <i>Biological Chemistry</i> , 2002, 383, 1667-76.	2.5	24

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37	Structure of the dimeric N-glycosylated form of fungal β -N-acetylhexosaminidase revealed by computer modeling, vibrational spectroscopy, and biochemical studies. <i>BMC Structural Biology</i> , 2007, 7, 32.	2.3	24
38	Common Structural Features of <i>UUCG</i> and <i>UACG</i> Tetraloops in Very Short Hairpins Determined by UV Absorption, Raman, IR and NMR Spectroscopies. <i>Journal of Biomolecular Structure and Dynamics</i> , 1997, 14, 579-593.	3.5	23
39	Scaled quantum mechanical force fields and vibrational spectra of solid state nucleic acid constituents. 4. N7-Protonated guanine. <i>The Journal of Physical Chemistry</i> , 1992, 96, 9283-9287.	2.9	21
40	Raman optical activity spectrometer for peptide studies. <i>Journal of Molecular Structure</i> , 1999, 480-481, 431-435.	3.6	21
41	Effects of sulfation and the environment on the structure of chondroitin sulfate studied via Raman optical activity. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7367-7377.	2.8	21
42	Raman Optical Activity of the Central Part of Hinge Peptide. <i>Collection of Czechoslovak Chemical Communications</i> , 2005, 70, 403-409.	1.0	21
43	Metalation of positively charged water soluble mesoporphyrins studied via time-resolved SERRS spectroscopy. <i>Journal of Molecular Structure</i> , 1997, 410-411, 77-79.	3.6	20
44	Low temperature vibrational and vibronic spectra of adenine single crystals. <i>Journal of Molecular Structure</i> , 1990, 219, 299-304.	3.6	18
45	Surface-enhanced Raman spectra of 5,10,15,20-tetrakis(4-carboxyphenyl)porphyrin/silver colloid system: what information about the porphyrin do we obtain?. <i>Inorganic Chemistry</i> , 1991, 30, 4103-4105.	4.0	18
46	Enhanced raman spectra of 2,2'-bipyridine adsorbed on aggregated palladium colloidal particles. <i>Journal of Molecular Structure</i> , 1997, 410-411, 201-203.	3.6	17
47	Disulfide chromophore and its optical activity. <i>Chirality</i> , 2010, 22, E47-55.	2.6	17
48	Thermal stability, structural features, and B-to-Z transition in DNA tetraloop hairpins as determined by optical spectroscopy in d(CG)3T4(CG)3 and d(CG)3A4(CG)3 oligodeoxynucleotides. <i>Biopolymers</i> , 2005, 78, 21-34.	2.4	16
49	Raman optical activity of the hinge peptide. <i>Vibrational Spectroscopy</i> , 2006, 42, 88-92.	2.2	14
50	Relative intensity correction of Raman optical activity spectra facilitates extending the spectral region. <i>Journal of Raman Spectroscopy</i> , 2014, 45, 603-609.	2.5	13
51	Absolute Configuration Determination of a Taxol Precursor Based on Raman Optical Activity Spectra. <i>Journal of Physical Chemistry B</i> , 2017, 121, 1544-1551.	2.6	13
52	Aqueous phase structural features of GNRA tetraloops formed in short hairpins as evidenced by UV absorption and Raman spectroscopy. <i>Vibrational Spectroscopy</i> , 1999, 19, 335-340.	2.2	12
53	Interactions of Electronically Excited Copper(II) Porphyrin with DNA: Resonance Raman Evidence for the Exciplex Formation with Adenine and Cytosine Residues. <i>Journal of Physical Chemistry B</i> , 2003, 107, 7532-7535.	2.6	12
54	A universal computer-controlled UV-VIS spectrometer with high resolution monochromator. <i>Computer Physics Communications</i> , 1988, 50, 225-228.	7.5	11

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55	Vibrational spectroscopy and computer modeling of proteins: solving structure of $\hat{I}_{\pm 1}$ -acid glycoprotein. <i>Spectroscopy</i> , 2004, 18, 323-330.	0.8	11
56	and <i>Photobiology</i> , 1991, 54, 127-132.	2.5	10
57	Catalytically Self-Sufficient P450 CYP102 (Cytochrome P450 BM-3): Resonance Raman Spectral Characterization of the Heme Domain and of the Holoenzyme. <i>Biochemical and Biophysical Research Communications</i> , 1998, 243, 811-815.	2.1	10
58	Thermodynamic and structural features of ultrastable DNA and RNA hairpins. <i>Journal of Molecular Structure</i> , 2003, 651-653, 67-74.	3.6	10
59	Vibrational spectra and quantum mechanical force fields of modified oligonucleotide linkages: 1. methyl methoxymethanphosphonate. <i>Journal of Molecular Structure</i> , 1997, 415, 161-177.	3.6	9
60	Raman optical activity study of poly-L-proline chains of various lengths. <i>Spectroscopy</i> , 2010, 24, 213-217.	0.8	9
61	Electronic and vibrational optical activity of several peptides related to neurohypophyseal hormones: Disulfide group conformation. <i>Biopolymers</i> , 2012, 97, 923-932.	2.4	9
62	Protonation Effect of Tyrosine in a Segment of the SRF Transcription Factor: A Combined Optical Spectroscopy, Molecular Dynamics, and Density Functional Theory Calculation Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 16086-16095.	2.6	9
63	SERS spectroscopy with Ag colloids. <i>Journal of Molecular Structure</i> , 1997, 408-409, 149-154.	3.6	8
64	Structure and Properties of Silicon Thin Films Deposited at Low Substrate Temperatures. <i>Japanese Journal of Applied Physics</i> , 2003, 42, L987-L989.	1.5	8
65	Structural features of two distinct molecular complexes of copper(II) cationic porphyrin and deoxyribonucleotides. <i>Biopolymers</i> , 2002, 67, 278-281.	2.4	7
66	Nonplanar Tertiary Amides in Rigid Chiral Tricyclic Dilactams. Peptide Group Distortions and Vibrational Optical Activity. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9626-9642.	2.6	7
67	Influence of ligand binding on structure and thermostability of human $\hat{I}_{\pm 1}$ -acid glycoprotein. <i>Journal of Molecular Recognition</i> , 2016, 29, 70-79.	2.1	6
68	UNCG tetraloops in short oligoribonucleotides reveal high thermodynamic stability and unusual structural properties in aqueous phase as confirmed by optical and NMR spectroscopies. <i>Journal of Molecular Structure</i> , 1997, 408-409, 241-245.	3.6	5
69	A Fourier Transform Method for Generation of Anharmonic Vibrational Molecular Spectra. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2095-2102.	5.3	5
70	Electrical properties of some crystalline salts of adenine. <i>European Physical Journal D</i> , 1985, 35, 670-676.	0.4	4
71	Changes in Na ⁺ ,K ⁺ -ATPase structure induced by cation binding Approach by Raman spectroscopy. <i>FEBS Letters</i> , 1992, 312, 80-82.	2.8	4
72	Electronic Circular Dichroism of the Chiral Rigid Tricyclic Dilactam with Nonplanar Tertiary Amide Groups. <i>Journal of Physical Chemistry B</i> , 2014, 118, 11100-11108.	2.6	4

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73	Determination of Secondary Structures of Proteins Using Vibrational Circular Dichroism. ACS Symposium Series, 1994, , 61-70.	0.5	3
74	Resonance Raman spectra of bis (2,4-pentanedithionate) palladium (II) complex. Journal of Molecular Structure, 1992, 265, 9-16.	3.6	1
75	Raman Optical Activity of Biomolecules: From Simple Models to Complex Systems. , 2008, , .		1
76	Chiroptical Properties and Conformation of Four Lasiocepsin-Related Antimicrobial Peptides: Structural Role of Disulfide Bridges. Symmetry, 2020, 12, 812.	2.2	1
77	Metalation of 5,10,15,20-tetrakis(1-methyl-4-pyridyl)porphyrin in silver colloids studied via time dependence of surface-enhanced resonance Raman spectra. , 1998, 29, 575.		1
78	Polarized phosphorescence of adeninium hemisulphate hydrate single crystal. Journal of Luminescence, 1990, 47, 93-98.	3.1	0
79	Raman Optical Activity of Amide and Disulfide Groups in Peptides and Model Systems. , 2010, , .		0