Vladimir Baumruk

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Chiroptical Properties and Conformation of Four Lasiocepsin-Related Antimicrobial Peptides: Structural Role of Disulfide Bridges. Symmetry, 2020, 12, 812.	2.2	1
2	Effects of sulfation and the environment on the structure of chondroitin sulfate studied <i>via</i> Raman optical activity. Physical Chemistry Chemical Physics, 2019, 21, 7367-7377.	2.8	21
3	Absolute Configuration Determination of a Taxol Precursor Based on Raman Optical Activity Spectra. Journal of Physical Chemistry B, 2017, 121, 1544-1551.	2.6	13
4	Influence of ligand binding on structure and thermostability of human α ₁ -acid glycoprotein. Journal of Molecular Recognition, 2016, 29, 70-79.	2.1	6
5	Relative intensity correction of Raman optical activity spectra facilitates extending the spectral region. Journal of Raman Spectroscopy, 2014, 45, 603-609.	2.5	13
6	Electronic Circular Dichroism of the Chiral Rigid Tricyclic Dilactam with Nonplanar Tertiary Amide Groups. Journal of Physical Chemistry B, 2014, 118, 11100-11108.	2.6	4
7	CH Stretching Region: Computational Modeling of Vibrational Optical Activity. Journal of Chemical Theory and Computation, 2013, 9, 3096-3108.	5.3	29
8	Protonation Effect of Tyrosine in a Segment of the SRF Transcription Factor: A Combined Optical Spectroscopy, Molecular Dynamics, and Density Functional Theory Calculation Study. Journal of Physical Chemistry B, 2013, 117, 16086-16095.	2.6	9
9	Nonplanar Tertiary Amides in Rigid Chiral Tricyclic Dilactams. Peptide Group Distortions and Vibrational Optical Activity. Journal of Physical Chemistry B, 2013, 117, 9626-9642.	2.6	7
10	Electronic and vibrational optical activity of several peptides related to neurohypophyseal hormones: Disulfide group conformation. Biopolymers, 2012, 97, 923-932.	2.4	9
11	Tracking of the Polyproline Folding by Density Functional Computations and Raman Optical Activity Spectra. Journal of Physical Chemistry B, 2011, 115, 15079-15089.	2.6	31
12	Disulfide chromophore and its optical activity. Chirality, 2010, 22, E47-55.	2.6	17
13	Raman optical activity study of poly-L-proline chains of various lengths. Spectroscopy, 2010, 24, 213-217.	0.8	9
14	Raman Optical Activity of Amide and Disulfide Groups in Peptides and Model Systems. , 2010, , .		0
15	Side Chain and Flexibility Contributions to the Raman Optical Activity Spectra of a Model Cyclic Hexapeptide. Journal of Physical Chemistry A, 2010, 114, 7642-7651.	2.5	37
16	A Fourier Transform Method for Generation of Anharmonic Vibrational Molecular Spectra. Journal of Chemical Theory and Computation, 2010, 6, 2095-2102.	5.3	5
17	<scp>l</scp> -Alanyl- <scp>l</scp> -alanine Conformational Changes Induced by pH As Monitored by the Raman Optical Activity Spectra. Journal of Physical Chemistry A, 2009, 113, 7760-7768.	2.5	29
18	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

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19	Conformational Properties of the Pro-Gly Motif in the <scp>d</scp> -Ala- <scp> </scp> -Pro-Gly- <scp>d</scp> -Ala Model Peptide Explored by a Statistical Analysis of the NMR, Raman, and Raman Optical Activity Spectra. Journal of Organic Chemistry, 2008, 73, 1481-1489.	3.2	28
20	Comparison of Quantitative Conformer Analyses by Nuclear Magnetic Resonance and Raman Optical Activity Spectra for Model Dipeptides. Journal of Physical Chemistry A, 2008, 112, 8633-8640.	2.5	51
21	Raman Optical Activity of Biomolecules: From Simple Models to Complex Systems. , 2008, , .		1
22	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
23	Structure of the dimeric N-glycosylated form of fungal β-N-acetylhexosaminidase revealed by computer modeling, vibrational spectroscopy, and biochemical studies. BMC Structural Biology, 2007, 7, 32.	2.3	24
24	Conformational Flexibility ofl-Alanine Zwitterion Determines Shapes of Raman and Raman Optical Activity Spectral Bands. Journal of Physical Chemistry A, 2006, 110, 4689-4696.	2.5	90
25	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
26	Proline Zwitterion Dynamics in Solution, Glass, and Crystalline State. Journal of the American Chemical Society, 2006, 128, 13451-13462.	13.7	82
27	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
28	Raman optical activity of the hinge peptide. Vibrational Spectroscopy, 2006, 42, 88-92.	2.2	14
29	Thermal stability, structural features, and B-to-Z transition in DNA tetraloop hairpins as determined by optical spectroscopy in d(CG)3T4(CG)3and d(CG)3A4(CG)3oligodeoxynucleotides. Biopolymers, 2005, 78, 21-34.	2.4	16
30	Raman Optical Activity of the Central Part of Hinge Peptide. Collection of Czechoslovak Chemical Communications, 2005, 70, 403-409.	1.0	21
31	Vibrational spectroscopy and computer modeling of proteins: solving structure of α ₁ -acid glycoprotein. Spectroscopy, 2004, 18, 323-330.	0.8	11
32	Thermodynamic and structural features of ultrastable DNA and RNA hairpins. Journal of Molecular Structure, 2003, 651-653, 67-74.	3.6	10
33	Eight Amino Acids Form the ATP Recognition Site of Na+/K+-ATPaseâ€. Biochemistry, 2003, 42, 6446-6452.	2.5	27
34	Interactions of Electronically Excited Copper(II)â^'Porphyrin with DNA: Resonance Raman Evidence for the Exciplex Formation with Adenine and Cytosine Residues. Journal of Physical Chemistry B, 2003, 107, 7532-7535.	2.6	12
35	Structure of human α1-acid glycoprotein and its high-affinity binding site. Biochemical and Biophysical Research Communications, 2003, 300, 41-46.	2.1	80
36	Molecular Characterization of Binding of Calcium and Carbohydrates by an Early Activation Antigen of Lymphocytes CD69â€. Biochemistry, 2003, 42, 9295-9306.	2.5	33

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37	Structure and Properties of Silicon Thin Films Deposited at Low Substrate Temperatures. Japanese Journal of Applied Physics, 2003, 42, L987-L989.	1.5	8
38	Study of Chaperone-Like Activity of Human Haptoglobin: Conformational Changes under Heat Shock Conditions and Localization of Interaction Sites. Biological Chemistry, 2002, 383, 1667-76.	2.5	24
39	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. Journal of Physical Chemistry A, 2002, 106, 7321-7327.	2.5	44
40	Structural features of two distinct molecular complexes of copper(II) cationic porphyrin and deoxyribonucleotides. Biopolymers, 2002, 67, 278-281.	2.4	7
41	Simulation of the Raman Optical Activity ofl-Alanylâ^'l-Alanine. Journal of Physical Chemistry A, 2001, 105, 6362-6368.	2.5	43
42	Comparison between CUUG and UUCG tetraloops: thermodynamic stability and structural features analyzed by UV absorption and vibrational spectroscopy. Nucleic Acids Research, 2001, 29, 4089-4096.	14.5	33
43	Unusual nucleotide conformations in GNRA and UNCG type tetraloop hairpins: evidence from Raman markers assignments. Nucleic Acids Research, 1999, 27, 1398-1404.	14.5	36
44	Raman optical activity spectrometer for peptide studies. Journal of Molecular Structure, 1999, 480-481, 431-435.	3.6	21
45	Aqueous phase structural features of GNRA tetraloops formed in short hairpins as evidenced by UV absorption and Raman spectroscopy. Vibrational Spectroscopy, 1999, 19, 335-340.	2.2	12
46	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
47	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. Journal of Raman Spectroscopy, 1998, 29, 575-584.	2.5	46
48	Scaled Quantum Mechanical Force Fields and Vibrational Spectra of Nucleic Acid Constituents. 9. Tetrahydrofuran. Journal of Physical Chemistry B, 1998, 102, 1314-1319.	2.6	28
49	Structural Features of the UCCC and UGCG Tetraloops in Very Short Hairpins As Evidenced by Optical Spectroscopyâ€. Biochemistry, 1998, 37, 7878-7884.	2.5	30
50	Catalytically Self-Sufficient P450 CYP102 (Cytochrome P450 BM-3): Resonance Raman Spectral Characterization of the Heme Domain and of the Holoenzyme. Biochemical and Biophysical Research Communications, 1998, 243, 811-815.	2.1	10
51	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
52	Measurement and Calculation of the Raman Optical Activity of α-Pinene and trans-Pinane. Collection of Czechoslovak Chemical Communications, 1997, 62, 1384-1395.	1.0	51
53	Common Structural Features of <u>UUCG</u> and <u>UACG</u> Tetraloops in Very Short Hairpins Determined by UV Absorption, Raman, IR and NMR Spectroscopies. Journal of Biomolecular Structure and Dynamics, 1997, 14, 579-593.	3.5	23
54	Neutron Inelastic Scattering, Optical Spectroscopies and Scaled Quantum Mechanical Force Fields for Analyzing the Vibrational Dynamics of Pyrimidine Nucleic Acid Bases:Â 3. Cytosine. Journal of Physical Chemistry A, 1997, 101, 10063-10074.	2.5	54

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55	SERS spectroscopy with Ag colloids. Journal of Molecular Structure, 1997, 408-409, 149-154.	3.6	8
56	UNCG tetraloops in short oligoribonucleotides reveal high thermodynamic stability and unusual structural properties in aqueous phase as confirmed by optical and NMR spectroscopies. Journal of Molecular Structure, 1997, 408-409, 241-245.	3.6	5
57	Metalation of positively charged water soluble mesoporphyrins studied via time-resolved SERRS spectroscopy. Journal of Molecular Structure, 1997, 410-411, 77-79.	3.6	20
58	Enhanced raman spectra of 2,2′-bipyridine adsorbed on aggregated palladium colloidal particles. Journal of Molecular Structure, 1997, 410-411, 201-203.	3.6	17
59	Vibrational spectra and quantum mechanical force fields of modified oligonucleotide linkages: 1. methyl methoxymethanphosphonate. Journal of Molecular Structure, 1997, 415, 161-177.	3.6	9
60	Protein Structural Segments and Their Interconnections Derived from Optical Spectra. Thermal Unfolding of Ribonuclease T1as an Exampleâ€. Biochemistry, 1996, 35, 13094-13106.	2.5	33
61	Predictions of Secondary Structure using Statistical Analyses of Electronic and Vibrational Circular Dichroism and Fourier Transform Infrared Spectra of Proteins in H2O. Journal of Molecular Biology, 1996, 259, 774-791.	4.2	131
62	IR and Raman Spectra, Tautomeric Stabilities, and Scaled Quantum Mechanical Force Fields of Protonated Cytosineâ€. The Journal of Physical Chemistry, 1996, 100, 5578-5589.	2.9	137
63	IR and Raman Spectra, Conformational Flexibility, and Scaled Quantum Mechanical Force Fields of Sodium Dimethyl Phosphate and Dimethyl Phosphate Anionâ€. The Journal of Physical Chemistry, 1996, 100, 1559-1568.	2.9	72
64	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
65	Determination of Secondary Structures of Proteins Using Vibrational Circular Dichroism. ACS Symposium Series, 1994, , 61-70.	0.5	3
66	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
67	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
68	Vibrational circular dichroism of proteins in water solution. Journal of the American Chemical Society, 1993, 115, 6939-6942.	13.7	93
69	Surface-Enhanced Raman Scattering (SERS) Spectroscopy with Borohydride-Reduced Silver Colloids: Controlling Adsorption of the Scattering Species by Surface Potential of Silver Colloid. Collection of Czechoslovak Chemical Communications, 1993, 58, 2682-2694.	1.0	34
70	Scaled quantum mechanical force fields and vibrational spectra of solid state nucleic acid constituents. 4. N7-Protonated guanine. The Journal of Physical Chemistry, 1992, 96, 9283-9287.	2.9	21
71	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
72	Changes in Na+,K+-ATPase structure induced by cation binding Approach by Raman spectroscopy. FEBS Letters, 1992, 312, 80-82.	2.8	4

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73	Resonance Raman spectra of bis (2,4-pentanedithionate) palladium (II) complex. Journal of Molecular Structure, 1992, 265, 9-16.	3.6	1
74	Surface-enhanced Raman spectra of 5,10,15,20-tetrakis(4-carboxyphenyl)porphyrin/silver colloid system: what information about the porphyrin do we obtain?. Inorganic Chemistry, 1991, 30, 4103-4105.	4.0	18
75	and Photobiology, 1991, 54, 127-132.	2.5	10
76	Polarized phosphorescence of adeninium hemisulphate hydrate single crystal. Journal of Luminescence, 1990, 47, 93-98.	3.1	0
77	Low temperature vibrational and vibronic spectra of adenine single crystals. Journal of Molecular Structure, 1990, 219, 299-304.	3.6	18
78	A universal computer-controlled UV-VIS spectrometer with high resolution monochromator. Computer Physics Communications, 1988, 50, 225-228.	7.5	11
79	Electrical properties of some crystalline salts of adenine. European Physical Journal D, 1985, 35, 670-676.	0.4	4