

Vladimir Baumruk

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

78
papers

2,342
citations

29
h-index

46
g-index

80
ext. papers

2,422
ext. citations

4.2
avg, IF

4.32
L-index

#	Paper	IF	Citations
78	Chiroptical Properties and Conformation of Four Lasiocepsin-Related Antimicrobial Peptides: Structural Role of Disulfide Bridges. <i>Symmetry</i> , 2020 , 12, 812	2.7	
77	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	3.6	14
76	Absolute Configuration Determination of a Taxol Precursor Based on Raman Optical Activity Spectra. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 1544-1551	3.4	9
75	Influence of ligand binding on structure and thermostability of human α -acid glycoprotein. <i>Journal of Molecular Recognition</i> , 2016 , 29, 70-9	2.6	3
74	Electronic circular dichroism of the chiral rigid tricyclic dilactam with nonplanar tertiary amide groups. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 11100-8	3.4	3
73	Relative intensity correction of Raman optical activity spectra facilitates extending the spectral region. <i>Journal of Raman Spectroscopy</i> , 2014 , 45, 603-609	2.3	13
72	CH Stretching Region: Computational Modeling of Vibrational Optical Activity. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3096-108	6.4	21
71	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, 16086-95	3.4	7
70	Nonplanar tertiary amides in rigid chiral tricyclic dilactams. Peptide group distortions and vibrational optical activity. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 9626-42	3.4	6
69	Electronic and vibrational optical activity of several peptides related to neurohypophyseal hormones: disulfide group conformation. <i>Biopolymers</i> , 2012 , 97, 923-32	2.2	9
68	Tracking of the polyproline folding by density functional computations and Raman optical activity spectra. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 15079-89	3.4	30
67	Raman optical activity study of poly-L-proline chains of various lengths. <i>Spectroscopy</i> , 2010 , 24, 213-217		8
66	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, 7642-51	2.8	34
65	A Fourier Transform Method for Generation of Anharmonic Vibrational Molecular Spectra. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2095-102	6.4	5
64	Disulfide chromophore and its optical activity. <i>Chirality</i> , 2010 , 22 Suppl 1, E47-55	2.1	14
63	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, 7760-8	2.8	27
62	Interpretation of Raman and Raman optical activity spectra of a flexible sugar derivative, the gluconic acid anion. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 3594-601	2.8	52

61	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, 1481-9	4.2	27
60	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, 8633-40	2.8	47
59	Raman Optical Activity of Biomolecules: From Simple Models to Complex Systems 2008 ,		1
58	Anharmonic effects in IR, Raman, and Raman optical activity spectra of alanine and proline zwitterions. <i>Journal of Chemical Physics</i> , 2007 , 126, 224513	3.9	57
57	Structure of the dimeric N-glycosylated form of fungal beta-N-acetylhexosaminidase revealed by computer modeling, vibrational spectroscopy, and biochemical studies. <i>BMC Structural Biology</i> , 2007 , 7, 32	2.7	22
56	Conformational flexibility of L-alanine zwitterion determines shapes of Raman and Raman optical activity spectral bands. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 4689-96	2.8	87
55	Demonstration of the ring conformation in polyproline by the Raman optical activity. <i>Journal of the American Chemical Society</i> , 2006 , 128, 2438-43	16.4	92
54	Proline zwitterion dynamics in solution, glass, and crystalline state. <i>Journal of the American Chemical Society</i> , 2006 , 128, 13451-62	16.4	77
53	Structure of the ring in drop coating deposited proteins and its implication for Raman spectroscopy of biomolecules. <i>Vibrational Spectroscopy</i> , 2006 , 42, 184-187	2.1	46
52	Raman optical activity of the hinge peptide. <i>Vibrational Spectroscopy</i> , 2006 , 42, 88-92	2.1	13
51	Thermal stability, structural features, and B-to-Z transition in DNA tetraloop hairpins as determined by optical spectroscopy in d(CG)(3)T(4)(CG)(3) and d(CG)(3)A(4)(CG)(3) oligodeoxynucleotides. <i>Biopolymers</i> , 2005 , 78, 21-34	2.2	16
50	Raman Optical Activity of the Central Part of Hinge Peptide. <i>Collection of Czechoslovak Chemical Communications</i> , 2005 , 70, 403-409		20
49	Vibrational spectroscopy and computer modeling of proteins: solving structure of β -acid glycoprotein. <i>Spectroscopy</i> , 2004 , 18, 323-330		10
48	Structure and Properties of Silicon Thin Films Deposited at Low Substrate Temperatures. <i>Japanese Journal of Applied Physics</i> , 2003 , 42, L987-L989	1.4	6
47	Thermodynamic and structural features of ultrastable DNA and RNA hairpins. <i>Journal of Molecular Structure</i> , 2003 , 651-653, 67-74	3.4	8
46	Eight amino acids form the ATP recognition site of Na(+)/K(+)-ATPase. <i>Biochemistry</i> , 2003 , 42, 6446-52	3.2	20
45	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	3.4	11
44	Structure of human alpha1-acid glycoprotein and its high-affinity binding site. <i>Biochemical and Biophysical Research Communications</i> , 2003 , 300, 41-6	3.4	74

43	Molecular characterization of binding of calcium and carbohydrates by an early activation antigen of lymphocytes CD69. <i>Biochemistry</i> , 2003 , 42, 9295-306	3.2	30
42	Structural features of two distinct molecular complexes of copper(II) cationic porphyrin and deoxyribonucleotides. <i>Biopolymers</i> , 2002 , 67, 278-81	2.2	6
41	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	4.5	20
40	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	2.8	42
39	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, 4089-96	20.1	31
38	Simulation of the Raman Optical Activity of L-Alanyl-L-Alanine. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 6362-6368	2.8	40
37	Unusual nucleotide conformations in GNRA and UCG type tetraloop hairpins: evidence from Raman markers assignments. <i>Nucleic Acids Research</i> , 1999 , 27, 1398-404	20.1	33
36	Raman optical activity spectrometer for peptide studies. <i>Journal of Molecular Structure</i> , 1999 , 480-481, 431-435	3.4	20
35	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	2.1	12
34	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. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 10934-10944	3.4	60
33	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	2.3	44
32	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	3.4	28
31	Structural features of the UCCG and UGCG tetraloops in very short hairpins as evidenced by optical spectroscopy. <i>Biochemistry</i> , 1998 , 37, 7878-84	3.2	29
30	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, 811-5	3.4	10
29	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
28	Measurement and Calculation of the Raman Optical Activity of β -Pinene and trans-Pinane. <i>Collection of Czechoslovak Chemical Communications</i> , 1997 , 62, 1384-1395		49
27	Common structural features of UUCG and UACG tetraloops in very short hairpins determined by UV absorption, Raman, IR and NMR spectroscopies. <i>Journal of Biomolecular Structure and Dynamics</i> , 1997 , 14, 579-93	3.6	18
26	Neutron Inelastic Scattering, Optical Spectroscopies and Scaled Quantum Mechanical Force Fields for Analyzing the Vibrational Dynamics of Pyrimidine Nucleic Acid Bases: 3. Cytosine. <i>Journal of Physical Chemistry A</i> , 1997 , 101, 10063-10074	2.8	49

25	SERS spectroscopy with Ag colloids. <i>Journal of Molecular Structure</i> , 1997 , 408-409, 149-154	3.4	8
24	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	3.4	5
23	Metalation of positively charged water soluble mesoporphyrins studied via time-resolved SERRS spectroscopy. <i>Journal of Molecular Structure</i> , 1997 , 410-411, 77-79	3.4	19
22	Enhanced raman spectra of 2,2'-bipyridine adsorbed on aggregated palladium colloidal particles. <i>Journal of Molecular Structure</i> , 1997 , 410-411, 201-203	3.4	17
21	Vibrational spectra and quantum mechanical force fields of modified oligonucleotide linkages: 1. methyl methoxymethanphosphonate. <i>Journal of Molecular Structure</i> , 1997 , 415, 161-177	3.4	8
20	Neutron Inelastic Scattering, Optical Spectroscopies and Scaled Quantum Mechanical Force Fields for Analyzing the Vibrational Dynamics of Pyrimidine Nucleic Acid Bases. 1. Uracil. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 5224-5234		81
19	Protein structural segments and their interconnections derived from optical spectra. Thermal unfolding of ribonuclease T1 as an example. <i>Biochemistry</i> , 1996 , 35, 13094-106	3.2	31
18	Predictions of secondary structure using statistical analyses of electronic and vibrational circular dichroism and Fourier transform infrared spectra of proteins in H ₂ O. <i>Journal of Molecular Biology</i> , 1996 , 259, 774-91	6.5	126
17	IR and Raman Spectra, Tautomeric Stabilities, and Scaled Quantum Mechanical Force Fields of Protonated Cytosine. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 5578-5589		128
16	IR and Raman Spectra, Conformational Flexibility, and Scaled Quantum Mechanical Force Fields of Sodium Dimethyl Phosphate and Dimethyl Phosphate Anion. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 1559-1568		66
15	Determination of Secondary Structures of Proteins Using Vibrational Circular Dichroism. <i>ACS Symposium Series</i> , 1994 , 61-70	0.4	3
14	Conformational study of sequential Lys and Leu based polymers and oligomers using vibrational and electronic CD spectra. <i>Biopolymers</i> , 1994 , 34, 1115-21	2.2	61
13	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. <i>The Journal of Physical Chemistry</i> , 1993 , 97, 9719-9729		77
12	Vibrational circular dichroism of proteins in water solution. <i>Journal of the American Chemical Society</i> , 1993 , 115, 6939-6942	16.4	81
11	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		31
10	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		19
9	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. <i>The Journal of Physical Chemistry</i> , 1992 , 96, 1361-1366		110
8	Changes in Na ⁺ ,K ⁽⁺⁾ -ATPase structure induced by cation binding. Approach by Raman spectroscopy. <i>FEBS Letters</i> , 1992 , 312, 80-2	3.8	4

- 7 Resonance Raman spectra of bis (2,4-pentanedithionate) palladium (II) complex. *Journal of Molecular Structure*, **1992**, 265, 9-16 3.4 1
- 6 HOLE-BURNING SPECTROSCOPY OF ACTIVE AND INACTIVATED PHOTOSYSTEM II PARTICLES. *Photochemistry and Photobiology*, **1991**, 54, 127-132 3.6 9
- 5 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 5.1 16
- 4 Polarized phosphorescence of adeninium hemisulphate hydrate single crystal. *Journal of Luminescence*, **1990**, 47, 93-98 3.8
- 3 Low temperature vibrational and vibronic spectra of adenine single crystals. *Journal of Molecular Structure*, **1990**, 219, 299-304 3.4 15
- 2 A universal computer-controlled UV-VIS spectrometer with high resolution monochromator. *Computer Physics Communications*, **1988**, 50, 225-228 4.2 11
- 1 Electrical properties of some crystalline salts of adenine. *European Physical Journal D*, **1985**, 35, 670-676 4