Vladimir Baumruk

List of Publications by Citations

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	IR and Raman Spectra, Tautomeric Stabilities, and Scaled Quantum Mechanical Force Fields of Protonated Cytosine *The Journal of Physical Chemistry*, **1996**, 100, 5578-5589		128
77	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, 774-91	6.5	126
76	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		110
75	Demonstration of the ring conformation in polyproline by the Raman optical activity. *Journal of the American Chemical Society*, **2006**, 128, 2438-43	16.4	92
74	Conformational flexibility of L-alanine zwitterion determines shapes of Raman and Raman optical activity spectral bands. *Journal of Physical Chemistry A*, **2006**, 110, 4689-96	2.8	87
73	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		81
72	Vibrational circular dichroism of proteins in water solution. *Journal of the American Chemical Society* , **1993**, 115, 6939-6942	16.4	81
71	Proline zwitterion dynamics in solution, glass, and crystalline state. *Journal of the American Chemical Society*, **2006**, 128, 13451-62	16.4	77
70	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, 9719-9726		77
69	Structure of human alpha1-acid glycoprotein and its high-affinity binding site. *Biochemical and Biophysical Research Communications*, **2003**, 300, 41-6	3.4	74
68	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		66
67	Conformational study of sequential Lys and Leu based polymers and oligomers using vibrational and electronic CD spectra. *Biopolymers*, **1994**, 34, 1115-21	2.2	61
66	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	3.4	60
65	Anharmonic effects in IR, Raman, and Raman optical activity spectra of alanine and proline zwitterions. *Journal of Chemical Physics*, **2007**, 126, 224513	3.9	57
64	Interpretation of Raman and Raman optical activity spectra of a flexible sugar derivative, the gluconic acid anion. *Journal of Physical Chemistry A*, **2009**, 113, 3594-601	2.8	52
63	Measurement and Calculation of the Raman Optical Activity of Pinene and trans-Pinane. *Collection of Czechoslovak Chemical Communications*, **1997**, 62, 1384-1395		49
62	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	2.8	49

61	Comparison of quantitative conformer analyses by nuclear magnetic resonance and Raman optical activity spectra for model dipeptides. *Journal of Physical Chemistry A*, **2008**, 112, 8633-40	2.8	47
60	Structure of the ring in drop coating deposited proteins and its implication for Raman spectroscopy of biomolecules. *Vibrational Spectroscopy*, **2006**, 42, 184-187	2.1	46
59	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	2.3	44
58	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	2.8	42
57	Simulation of the Raman Optical Activity of l-Alanyl‖Alanine. *Journal of Physical Chemistry A*, **2001**, 105, 6362-6368	2.8	40
56	Side chain and flexibility contributions to the Raman optical activity spectra of a model cyclic hexapeptide. *Journal of Physical Chemistry A*, **2010**, 114, 7642-51	2.8	34
55	Unusual nucleotide conformations in GNRA and UNCG type tetraloop hairpins: evidence from Raman markers assignments. *Nucleic Acids Research*, **1999**, 27, 1398-404	20.1	33
54	Comparison between CUUG and UUCG tetraloops: thermodynamic stability and structural features analyzed by UV absorption and vibrational spectroscopy. *Nucleic Acids Research*, **2001**, 29, 4089-96	20.1	31
53	Protein structural segments and their interconnections derived from optical spectra. Thermal unfolding of ribonuclease T1 as an example. *Biochemistry*, **1996**, 35, 13094-106	3.2	31
52	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		31
51	Tracking of the polyproline folding by density functional computations and Raman optical activity spectra. *Journal of Physical Chemistry B*, **2011**, 115, 15079-89	3.4	30
50	Molecular characterization of binding of calcium and carbohydrates by an early activation antigen of lymphocytes CD69. *Biochemistry*, **2003**, 42, 9295-306	3.2	30
49	Structural features of the UCCG and UGCG tetraloops in very short hairpins as evidenced by optical spectroscopy. *Biochemistry*, **1998**, 37, 7878-84	3.2	29
48	Scaled Quantum Mechanical Force Fields and Vibrational Spectra of Nucleic Acid Constituents. 9. Tetrahydrofuran. *Journal of Physical Chemistry B*, **1998**, 102, 1314-1319	3.4	28
47	L-alanyl-L-alanine conformational changes induced by pH as monitored by the Raman optical activity spectra. *Journal of Physical Chemistry A*, **2009**, 113, 7760-8	2.8	27
46	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. *Journal of Organic Chemistry*, **2008**, 73, 1481-9	4.2	27
45	Structure of the dimeric N-glycosylated form of fungal beta-N-acetylhexosaminidase revealed by computer modeling, vibrational spectroscopy, and biochemical studies. *BMC Structural Biology*, **2007**, 7, 32	2.7	22
44	CH Stretching Region: Computational Modeling of Vibrational Optical Activity. *Journal of Chemical Theory and Computation*, **2013**, 9, 3096-108	6.4	21

43	Eight amino acids form the ATP recognition site of Na(+)/K(+)-ATPase. *Biochemistry*, **2003**, 42, 6446-52	3.2	20
42	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	4.5	20
41	Raman optical activity spectrometer for peptide studies. *Journal of Molecular Structure*, **1999**, 480-481, 431-435	3.4	20
40	Raman Optical Activity of the Central Part of Hinge Peptide. *Collection of Czechoslovak Chemical Communications*, **2005**, 70, 403-409		20
39	Metalation of positively charged water soluble mesoporphyrins studied via time-resolved SERRS spectroscopy. *Journal of Molecular Structure*, **1997**, 410-411, 77-79	3.4	19
38	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		19
37	Common structural features of UUCG and UACG tetraloops in very short hairpins determined by UV absorption, Raman, IR and NMR spectroscopies. *Journal of Biomolecular Structure and Dynamics*, **1997**, 14, 579-93	3.6	18
36	Enhanced raman spectra of 2,2?-bipyridine adsorbed on aggregated palladium colloidal particles. *Journal of Molecular Structure*, **1997**, 410-411, 201-203	3.4	17
35	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. *Biopolymers*, **2005**, 78, 21-34	2.2	16
34	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
33	Low temperature vibrational and vibronic spectra of adenine single crystals. *Journal of Molecular Structure*, **1990**, 219, 299-304	3.4	15
32	Effects of sulfation and the environment on the structure of chondroitin sulfate studied via Raman optical activity. *Physical Chemistry Chemical Physics*, **2019**, 21, 7367-7377	3.6	14
31	Disulfide chromophore and its optical activity. *Chirality*, **2010**, 22 Suppl 1, E47-55	2.1	14
30	Relative intensity correction of Raman optical activity spectra facilitates extending the spectral region. *Journal of Raman Spectroscopy*, **2014**, 45, 603-609	2.3	13
29	Raman optical activity of the hinge peptide. *Vibrational Spectroscopy*, **2006**, 42, 88-92	2.1	13
28	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	2.1	12
27	Interactions of Electronically Excited Copper(II) Porphyrin with DNA: Resonance Raman Evidence for the Exciplex Formation with Adenine and Cytosine Residues. *Journal of Physical Chemistry B*, **2003**, 107, 7532-7535	3.4	11
26	A universal computer-controlled UV-VIS spectrometer with high resolution monochromator. *Computer Physics Communications*, **1988**, 50, 225-228	4.2	11

25	Vibrational spectroscopy and computer modeling of proteins: solving structure of 1-acid glycoprotein. *Spectroscopy*, **2004**, 18, 323-330		10
24	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, 811-5	3.4	10
23	Absolute Configuration Determination of a Taxol Precursor Based on Raman Optical Activity Spectra. *Journal of Physical Chemistry B*, **2017**, 121, 1544-1551	3.4	9
22	Electronic and vibrational optical activity of several peptides related to neurohypophyseal hormones: disulfide group conformation. *Biopolymers*, **2012**, 97, 923-32	2.2	9
21	HOLE-BURNING SPECTROSCOPY OF ACTIVE AND INACTIVATEE) PHOTOSYSTEM II PARTICLES. *Photochemistry and Photobiology*, **1991**, 54, 127-132	3.6	9
20	Raman optical activity study of poly-L-proline chains of various lengths. *Spectroscopy*, **2010**, 24, 213-217		8
19	SERS spectroscopy with Ag colloids. *Journal of Molecular Structure*, **1997**, 408-409, 149-154	3.4	8
18	Vibrational spectra and quantum mechanical force fields of modified oligonucleotide linkages: 1. methyl methoxymethanphosphonate. *Journal of Molecular Structure*, **1997**, 415, 161-177	3.4	8
17	Thermodynamic and structural features of ultrastable DNA and RNA hairpins. *Journal of Molecular Structure*, **2003**, 651-653, 67-74	3.4	8
16	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, 16086-95	3.4	7
15	Nonplanar tertiary amides in rigid chiral tricyclic dilactams. Peptide group distortions and vibrational optical activity. *Journal of Physical Chemistry B*, **2013**, 117, 9626-42	3.4	6
14	Structure and Properties of Silicon Thin Films Deposited at Low Substrate Temperatures. *Japanese Journal of Applied Physics*, **2003**, 42, L987-L989	1.4	6
13	Structural features of two distinct molecular complexes of copper(II) cationic porphyrin and deoxyribonucleotides. *Biopolymers*, **2002**, 67, 278-81	2.2	6
12	A Fourier Transform Method for Generation of Anharmonic Vibrational Molecular Spectra. *Journal of Chemical Theory and Computation*, **2010**, 6, 2095-102	6.4	5
11	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	3.4	5
10	Changes in Na+,K(+)-ATPase structure induced by cation binding. Approach by Raman spectroscopy. *FEBS Letters*, **1992**, 312, 80-2	3.8	4
9	Electrical properties of some crystalline salts of adenine. *European Physical Journal D*, **1985**, 35, 670-676		4
8	Electronic circular dichroism of the chiral rigid tricyclic dilactam with nonplanar tertiary amide groups. *Journal of Physical Chemistry B*, **2014**, 118, 11100-8	3.4	3

7	Determination of Secondary Structures of Proteins Using Vibrational Circular Dichroism. *ACS Symposium Series*, **1994**, 61-70	0.4	3
6	Influence of ligand binding on structure and thermostability of human α1-acid glycoprotein. *Journal of Molecular Recognition*, **2016**, 29, 70-9	2.6	3
5	Raman Optical Activity of Biomolecules: From Simple Models to Complex Systems **2008**,		1
4	Resonance Raman spectra of bis (2,4-pentanedithionate) palladium (II) complex. *Journal of Molecular Structure*, **1992**, 265, 9-16	3.4	1
3	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
2	Chiroptical Properties and Conformation of Four Lasiocepsin-Related Antimicrobial Peptides: Structural Role of Disulfide Bridges. *Symmetry*, **2020**, 12, 812	2.7	
1	Polarized phosphorescence of adeninium hemisulphate hydrate single crystal. *Journal of Luminescence*, **1990**, 47, 93-98	3.8	