Bela Paizs

List of Publications by Year
in descending order

74 papers	5,098 citations	81900 39 h-index	85541 71 g-index
74 all docs	74 docs citations	74 times ranked	2742 citing authors

#	Article	IF	Citations
1	Fragmentation pathways of protonated peptides. Mass Spectrometry Reviews, 2005, 24, 508-548.	5.4	993
2	Infrared Spectroscopy and Theoretical Studies on Gas-Phase Protonated Leu-enkephalin and Its Fragments:Â Direct Experimental Evidence for the Mobile Proton. Journal of the American Chemical Society, 2007, 129, 5887-5897.	13.7	208
3	Scrambling of Sequence Information in Collision-Induced Dissociation of Peptides. Journal of the American Chemical Society, 2006, 128, 10364-10365.	13.7	180
4	Comparative study of BSSE correction methods at DFT and MP2 levels of theory. Journal of Computational Chemistry, 1998, 19, 575-584.	3.3	161
5	Towards understanding the tandem mass spectra of protonated oligopeptides. 1: Mechanism of amide bond cleavage. Journal of the American Society for Mass Spectrometry, 2004, 15, 103-113.	2.8	151
6	Spectroscopic and Theoretical Evidence for Oxazolone Ring Formation in Collision-Induced Dissociation of Peptides. Journal of the American Chemical Society, 2005, 127, 17154-17155.	13.7	150
7	Sequence-Scrambling Fragmentation Pathways of Protonated Peptides. Journal of the American Chemical Society, 2008, 130, 17774-17789.	13.7	145
8	Infrared Fingerprint Spectroscopy and Theoretical Studies of Potassium Ion Tagged Amino Acids and Peptides in the Gas Phase. Journal of the American Chemical Society, 2005, 127, 8571-8579.	13.7	141
9	Formation of b2+ ions from protonated peptides: anab initio study. Rapid Communications in Mass Spectrometry, 1999, 13, 525-533.	1.5	133
10	Revising the proton affinity scale of the naturally occurring Î±-amino acids. Journal of the American Society for Mass Spectrometry, 2006, 17, 1275-1281.	2.8	129
11	Stepwise Solvation of an Amino Acid:â€‰ The Appearance of Zwitterionic Structures. Journal of Physical Chemistry A, 2007, 111, 7309-7316.	2.5	123
12	Combined quantum chemical and RRKM modeling of the main fragmentation pathways of protonated GGG. II. Formation of b2, y1, and y2 ions. Rapid Communications in Mass Spectrometry, 2002, 16, 375-389.	1.5	120
13	Proton mobility in protonated peptides: a joint molecular orbital and RRKM study. , 2000, 14, 417-431.		99
14	On the effect of the BSSE on intermolecular potential energy surfaces. Comparison ofa priori anda posteriori BSSE correction schemes. Journal of Computational Chemistry, 2001, 22, 765-786.	3.3	93
15	Infrared Spectroscopy of Fragments of Protonated Peptides: Direct Evidence for Macrocyclic Structures of b₅ Ions. Journal of the American Chemical Society, 2009, 131, 11503-11508.	13.7	92
16	The Effect of the Initial Water of Hydration on the Energetics, Structures, and H/D Exchange Mechanism of a Family of Pentapeptides:Â An Experimental and Theoretical Study. Journal of the American Chemical Society, 2003, 125, 13768-13775.	13.7	88
17	Proton mobility in protonated glycylglycine andN-formylglycylglycinamide: a combined quantum chemical and RKKM study. Rapid Communications in Mass Spectrometry, 2001, 15, 637-650.	1.5	86
18	Proton-Driven Amide Bond-Cleavage Pathways of Gas-Phase Peptide Ions Lacking Mobile Protons. Journal of the American Chemical Society, 2009, 131, 14057-14065.	13.7	84

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19	Cyclization and Rearrangement Reactions ofanFragment Ions of Protonated Peptides. Journal of the American Chemical Society, 2010, 132, 14766-14779.	13.7	84
20	On the Dynamics of Fragment Isomerization in Collision-Induced Dissociation of Peptides. Journal of Physical Chemistry A, 2008, 112, 1286-1293.	2.5	82
21	Combined quantum chemical and RRKM modeling of the main fragmentation pathways of protonated GGG. I.Cis-trans isomerization around protonated amide bonds. Rapid Communications in Mass Spectrometry, 2001, 15, 2307-2323.	1.5	81
22	Theoretical study of the main fragmentation pathways for protonated glycylglycine. Rapid Communications in Mass Spectrometry, 2001, 15, 651-663.	1.5	80
23	Infrared Spectroscopy of Fragments from Doubly Protonated Tryptic Peptides. ChemPhysChem, 2009, 10, 883-885.	2.1	74
24	Vibrational Spectroscopy and Conformational Structure of Protonated Polyalanine Peptides Isolated in the Gas Phase. Journal of Physical Chemistry A, 2008, 112, 4608-4616.	2.5	66
25	What is the structure of b₂ ions generated from doubly protonated tryptic peptides?. Journal of the American Society for Mass Spectrometry, 2009, 20, 618-624.	2.8	65
26	Gas-Phase Structure and Fragmentation Pathways of Singly Protonated Peptides with N-Terminal Arginine. Journal of Physical Chemistry B, 2010, 114, 15092-15105.	2.6	65
27	Hidden Histidine Radical Rearrangements upon Electron Transfer to Gas-Phase Peptide Ions. Experimental Evidence and Theoretical Analysis. Journal of the American Chemical Society, 2008, 130, 14584-14596.	13.7	64
28	The Histidine Effect. Electron Transfer and Capture Cause Different Dissociations and Rearrangements of Histidine Peptide Cation-Radicals. Journal of the American Chemical Society, 2010, 132, 10728-10740.	13.7	55
29	Towards Understanding the Tandem Mass Spectra of Protonated Oligopeptides. 2: The Proline Effect in Collision-Induced Dissociation of Protonated Ala-Ala-Xxx-Pro-Ala (Xxx = Ala, Ser, Leu, Val, Phe, and) Tj ETQq1 1 0.784314 rgBT /Overlock	4.3	
30	Role of Isomerization Barriers in the pKaControl of the Retinal Schiff Base:Â A Density Functional Study. Journal of Physical Chemistry B, 1999, 103, 4518-4527.	2.6	52
31	Conformational Effects on the Proton Affinity of the Schiff Base in Bacteriorhodopsin:Â A Density Functional Study. Journal of Physical Chemistry B, 1997, 101, 8021-8028.	2.6	51
32	Ab initio and MS/MS studies on protonated peptides containing basic and acidic amino acid residues. International Journal of Mass Spectrometry, 2002, 219, 203-232.	1.5	50
33	Geometry optimization of large biomolecules in redundant internal coordinates. Journal of Chemical Physics, 2000, 113, 6566-6572.	3.0	49
34	Proton mobility and main fragmentation pathways of protonated lysylglycine. Rapid Communications in Mass Spectrometry, 2001, 15, 1457-1472.	1.5	49
35	Intermolecular bond lengths: extrapolation to the basis set limit on uncorrected and BSSE-corrected potential energy hypersurfaces. Journal of Computational Chemistry, 2001, 22, 196-207.	3.3	49
36	An efficient direct method for geometry optimization of large molecules in internal coordinates. Journal of Chemical Physics, 1998, 109, 6571-6576.	3.0	47

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37	Assigning Structures to Gas-Phase Peptide Cations and Cation-Radicals. An Infrared Multiphoton Dissociation, Ion Mobility, Electron Transfer, and Computational Study of a Histidine Peptide Ion. Journal of Physical Chemistry B, 2012, 116, 3445-3456.	2.6	47
38	Towards understanding some ion intensity relationships for the tandem mass spectra of protonated peptides. Rapid Communications in Mass Spectrometry, 2002, 16, 1699-1702.	1.5	40
39	Backbone cleavages and sequential loss of carbon monoxide and ammonia from protonated AGG: A combined tandem mass spectrometry, isotope labeling, and theoretical study. Journal of the American Society for Mass Spectrometry, 2007, 18, 1291-1303.	2.8	40
40	Effect of the his residue on the cyclization of b ions. Journal of the American Society for Mass Spectrometry, 2010, 21, 1352-1363.	2.8	40
41	Why are a₃ ions rarely observed?. Journal of the American Society for Mass Spectrometry, 2008, 19, 1764-1770.	2.8	39
42	Modeling of the gas-phase ion chemistry of protonated arginine. Journal of Mass Spectrometry, 2004, 39, 1025-1035.	1.6	38
43	Cleavage of the amide bond of protonated dipeptides. Physical Chemistry Chemical Physics, 2004, 6, 2691-2699.	2.8	36
44	Isotope labeling and theoretical study of the formation of a3* ions from protonated tetraglycine. Journal of the American Society for Mass Spectrometry, 2006, 17, 1654-1664.	2.8	36
45	Experimental and theoretical investigation of the main fragmentation pathways of protonated H-Gly-Gly-Sar-OH and H-Gly-Sar-Sar-OH. Journal of the American Society for Mass Spectrometry, 2003, 14, 1454-1469.	2.8	35
46	Conformation-Specific Spectroscopy of Peptide Fragment Ions in a Low-Temperature Ion Trap. Journal of the American Society for Mass Spectrometry, 2012, 23, 1029-1045.	2.8	32
47	Structure and Reactivity of an and an Peptide Fragments Investigated Using Isotope Labeling, Tandem Mass Spectrometry, and Density Functional Theory Calculationsâ Ž. Journal of the American Society for Mass Spectrometry, 2008, 19, 1788-1798.	2.8	31
48	Intramolecular condensation reactions in protonated dipeptides: Carbon monoxide, water, and ammonia losses in competition. Journal of the American Society for Mass Spectrometry, 2004, 15, 1025-1038.	2.8	30
49	Structure of [M + H â˜ H₂O]⁺ from Protonated Tetraglycine Revealed by Tandem Mass Spectrometry and IRMPD Spectroscopy. Journal of Physical Chemistry A, 2010, 114, 5076-5082.	2.5	30
50	Rearrangement Pathways of the a 4 Ion of Protonated YGGFL Characterized by IR Spectroscopy and Modeling. Journal of the American Society for Mass Spectrometry, 2012, 23, 664-675.	2.8	29
51	Carboxyl-Catalyzed Prototropic Rearrangements in Histidine Peptide Radicals upon Electron Transfer: Effects of Peptide Sequence and Conformation. Journal of the American Chemical Society, 2009, 131, 16472-16487.	13.7	26
52	Fragmentation of doubly-protonated Pro-His-Xaa tripeptides: Formation of b₂²⁺ ions. Journal of the American Society for Mass Spectrometry, 2009, 20, 2135-2143.	2.8	25
53	Extraribosomal cyclic tetradepsipeptides beauverolides: profiling and modeling the fragmentation pathways. Journal of Mass Spectrometry, 2004, 39, 949-960.	1.6	23
54	Extension of SCF and DFT versions of chemical Hamiltonian approach toN interacting subsystems and an algorithm for their efficient implementation. Journal of Computational Chemistry, 1997, 18, 694-701.	3.3	21

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55	Formation of iminium ions by fragmentation of a2 ions. Rapid Communications in Mass Spectrometry, 2004, 18, 1635-1640.	1.5	21
56	Rearrangement chemistry of a ions probed by IR spectroscopy. International Journal of Mass Spectrometry, 2015, 377, 172-178.	1.5	21
57	A divide-and-conquer approach to compute collision cross sections in the projection approximation method. International Journal of Mass Spectrometry, 2015, 378, 360-363.	1.5	19
58	Electronic Effects on the Ground-State Rotational Barrier of Polyene Schiff Bases:Â A Molecular Orbital Study. Journal of Physical Chemistry B, 1999, 103, 5388-5395.	2.6	18
59	Unimolecular chemistry of metal ion-coordinated Î±-dipeptide radicals. International Journal of Mass Spectrometry, 2007, 265, 251-260.	1.5	16
60	Competing gas-phase fragmentation pathways of asparagine-, glutamine-, and lysine-containing protonated dipeptides. Theoretical Chemistry Accounts, 2010, 125, 387-396.	1.4	16
61	IR Spectroscopy of b₄ Fragment Ions of Protonated Pentapeptides in the Xâ€“H (X = C, N, O) Region. Journal of Physical Chemistry A, 2013, 117, 2508-2516.	2.5	16
62	Newtonian molecular dynamics in general curvilinear internal coordinates. Chemical Physics Letters, 2002, 353, 400-406.	2.6	12
63	Using Gas-Phase Guestâ€“Host Chemistry to Probe the Structures of b Ions of Peptides. Journal of the American Society for Mass Spectrometry, 2012, 23, 2055-2058.	2.8	12
64	Coupled perturbed Hartreeâ€”Fock equations. An alternative derivation and generalization to non-orthogonal orbitals. Chemical Physics Letters, 1994, 220, 97-101.	2.6	11
65	Focus issue on peptide fragmentation. Journal of the American Society for Mass Spectrometry, 2008, 19, 1717-1718.	2.8	8
66	Mre11 exonuclease activity removes the chain-terminating nucleoside analog gemcitabine from the nascent strand during DNA replication. Science Advances, 2020, 6, eaaz4126.	10.3	8
67	Various energy minima and corresponding fragmentation processes: Alkylsilanes. Organic Mass Spectrometry, 1993, 28, 1491-1497.	1.3	6
68	Evaluating the formation of salt-bridges: a molecular orbital study. Chemical Physics Letters, 2000, 326, 129-142.	2.6	5
69	Zundel-Type H-Bonding in Biomolecular Ions. Journal of the American Society for Mass Spectrometry, 2014, 25, 1511-1514.	2.8	5
70	The environmental release and ecosystem risks of illicit drugs during Glastonbury Festival.. Environmental Research, 2022, 204, 112061.	7.5	5
71	Localization maps by orbital partitioning of the electron density. Theoretica Chimica Acta, 1993, 86, 379-389.	0.8	4
72	An exploratory study of 1,2-cis- and 1,2-trans-thiocarbamates of glucofuranosyl- and glucopyranosylamine. Computational and Theoretical Chemistry, 1998, 455, 267-274.	1.5	3

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73	23rd Sanibel Conference on Mass Spectrometry: From Fragmentation Mechanisms to Sequencing: Tandem Mass Spectrometry Based Peptide and Protein Identification. Journal of the American Society for Mass Spectrometry, 2012, 23, 575-576.	2.8	2
74	Alexander George Harrison (1931â€“2018). Journal of the American Society for Mass Spectrometry, 2019, 30, 2183-2184.	2.8	0