Dimitrios Morikis

List of Publications by Citations

129 papers	3,561 citations	31 h-index	54 g-index
181 ext. papers	3,935 ext. citations	4.6 avg, IF	5 L-index

#	Paper	IF	Citations
129	Resonance raman investigations of site-directed mutants of myoglobin: effects of distal histidine replacement. *Biochemistry*, **1989**, 28, 4791-800	3.2	184
128	The molecular basis for protein kinase A anchoring revealed by solution NMR. *Nature Structural Biology*, **1999**, 6, 222-7		172
127	A novel mechanism of PKA anchoring revealed by solution structures of anchoring complexes. *EMBO Journal*, **2001**, 20, 1651-62	13	169
126	Spectroscopic studies of myoglobin at low pH: heme structure and ligation. *Biochemistry*, **1991**, 30, 1227-37	3.2	150
125	Adaptation of inorganic quantum dots for stable molecular beacons. *Sensors and Actuators B: Chemical*, **2004**, 102, 315-319	8.5	118
124	Alteration of sperm whale myoglobin heme axial ligation by site-directed mutagenesis. *Biochemistry*, **1990**, 29, 9783-91	3.2	108
123	Binding kinetics, structure-activity relationship, and biotransformation of the complement inhibitor compstatin. *Journal of Immunology*, **2000**, 165, 2491-9	5.3	92
122	Endosidin2 targets conserved exocyst complex subunit EXO70 to inhibit exocytosis. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E41-50	11.5	88
121	A gain-of-function mutation of Arabidopsis lipid transfer protein 5 disturbs pollen tube tip growth and fertilization. *Plant Cell*, **2009**, 21, 3902-14	11.6	84
120	Integrated computational and experimental approach for lead optimization and design of compstatin variants with improved activity. *Journal of the American Chemical Society*, **2003**, 125, 8422-3	16.4	76
119	Solution structure of Compstatin, a potent complement inhibitor. *Protein Science*, **1998**, 7, 619-27	6.3	75
118	Alteration of heme axial ligands by site-directed mutagenesis: a cytochrome becomes a catalytic demethylase. *Journal of the American Chemical Society*, **1987**, 109, 7896-7897	16.4	70
117	Compstatin, a peptide inhibitor of complement, exhibits species-specific binding to complement component C3. *Molecular Immunology*, **2003**, 39, 557-66	4.3	65
116	Electrostatic modeling predicts the activities of orthopoxvirus complement control proteins. *Journal of Immunology*, **2005**, 174, 2143-51	5.3	61
115	ADF/cofilin binds phosphoinositides in a multivalent manner to act as a PIP(2)-density sensor. *Biophysical Journal*, **2010**, 98, 2327-36	2.9	59
114	Design and NMR characterization of active analogues of compstatin containing non-natural amino acids. *Journal of Medicinal Chemistry*, **2005**, 48, 274-86	8.3	59
113	Related protein-protein interaction modules present drastically different surface topographies despite a conserved helical platform. *Journal of Molecular Biology*, **2003**, 330, 1117-29	6.5	56

112	Conformational interconversion in protein crystals. *Journal of Molecular Biology*, **1992**, 224, 207-15	6.5	55
111	The iron-histidine mode of myoglobin revisited: resonance Raman studies of isotopically labeled Escherichia coli-expressed myoglobin. *Journal of the American Chemical Society*, **1991**, 113, 9655-9660	16.4	55
110	Design of Peptide Analogues with Improved Activity Using a Novel de Novo Protein Design Approach. *Industrial & Engineering Chemistry Research*, **2004**, 43, 3817-3826	3.9	54
109	NMR evidence for multiple conformations in a highly helical model peptide. *Biochemistry*, **1993**, 32, 13089-97	3.2	54
108	A multifaceted study of stigma/style cysteine-rich adhesin (SCA)-like Arabidopsis lipid transfer proteins (LTPs) suggests diversified roles for these LTPs in plant growth and reproduction. *Journal of Experimental Botany*, **2010**, 61, 4277-90	7	49
107	Complement: structure, functions, evolution, and viral molecular mimicry. *Immunologic Research*, **2003**, 27, 367-86	4.3	48
106	The electrostatic nature of C3d-complement receptor 2 association. *Journal of Immunology*, **2004**, 172, 7537-47	5.3	47
105	Discovery of functionally selective C5aR2 ligands: novel modulators of C5a signalling. *Immunology and Cell Biology*, **2016**, 94, 787-95	5	47
104	Structural aspects and design of low-molecular-mass complement inhibitors. *Biochemical Society Transactions*, **2002**, 30, 1026-36	5.1	45
103	The structural basis of compstatin activity examined by structure-function-based design of peptide analogs and NMR. *Journal of Biological Chemistry*, **2002**, 277, 14942-53	5.4	43
102	Toward full-sequence de novo protein design with flexible templates for human beta-defensin-2. *Biophysical Journal*, **2008**, 94, 584-99	2.9	42
101	Immunophysical properties and prediction of activities for vaccinia virus complement control protein and smallpox inhibitor of complement enzymes using molecular dynamics and electrostatics. *Biophysical Journal*, **2006**, 90, 3106-19	2.9	39
100	Electrostatic clustering and free energy calculations provide a foundation for protein design and optimization. *Annals of Biomedical Engineering*, **2011**, 39, 1252-63	4.7	38
99	Species specificity of the complement inhibitor compstatin investigated by all-atom molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2655-67	4.2	32
98	Molecular dynamics in drug design: new generations of compstatin analogs. *Chemical Biology and Drug Design*, **2012**, 79, 703-18	2.9	31
97	Studies of structure-activity relations of complement inhibitor compstatin. *Journal of Immunology*, **2003**, 171, 1881-90	5.3	31
96	Resonance Raman scattering as a probe of electron-nuclear coupling: applications to heme proteins. *The Journal of Physical Chemistry*, **1991**, 95, 3391-3398		31
95	Two SCA (stigma/style cysteine-rich adhesin) isoforms show structural differences that correlate with their levels of in vitro pollen tube adhesion activity. *Journal of Biological Chemistry*, **2007**, 282, 33845-33858	5.4	30

94	Improvement of the anti-C3 activity of compstatin using rational and combinatorial approaches. *Biochemical Society Transactions*, **2004**, 32, 28-32	5.1	30
93	Quantitative Modeling of the Alternative Pathway of the Complement System. *PLoS ONE*, **2016**, 11, e0152337	3.7	30
92	De novo peptide design with C3a receptor agonist and antagonist activities: theoretical predictions and experimental validation. *Journal of Medicinal Chemistry*, **2012**, 55, 4159-68	8.3	29
91	Immunophysical exploration of C3d-CR2(CCP1-2) interaction using molecular dynamics and electrostatics. *Journal of Molecular Biology*, **2007**, 369, 567-83	6.5	29
90	New compstatin variants through two de novo protein design frameworks. *Biophysical Journal*, **2010**, 98, 2337-46	2.9	28
89	An evaluation of Poisson-Boltzmann electrostatic free energy calculations through comparison with experimental mutagenesis data. *Biopolymers*, **2011**, 95, 746-54	2.2	27
88	Synthetic small-molecule complement inhibitors. *Current Opinion in Investigational Drugs*, **2004**, 5, 1164-73		27
87	Influence of electrostatics on the complement regulatory functions of Kaposica, the complement inhibitor of Kaposi's sarcoma-associated herpesvirus. *Journal of Immunology*, **2010**, 184, 1956-67	5.3	26
86	Physical methods for structure, dynamics and binding in immunological research. *Trends in Immunology*, **2004**, 25, 700-7	14.4	26
85	Viral regulators of complement activation: structure, function and evolution. *Molecular Immunology* , **2014**, 61, 89-99	4.3	24
84	Automated computational framework for the analysis of electrostatic similarities of proteins. *Biotechnology Progress*, **2011**, 27, 316-25	2.8	24
83	Novel compstatin family peptides inhibit complement activation by drusen-like deposits in human retinal pigmented epithelial cell cultures. *Experimental Eye Research*, **2013**, 116, 96-108	3.7	23
82	Is the rigid-body assumption reasonable?: Insights into the effects of dynamics on the electrostatic analysis of barnase-barstar. *Journal of Non-Crystalline Solids*, **2011**, 357, 707-716	3.9	23
81	Design of a modified mouse protein with ligand binding properties of its human analog by molecular dynamics simulations: the case of C3 inhibition by compstatin. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 3166-79	4.2	23
80	The two sides of complement C3d: evolution of electrostatics in a link between innate and adaptive immunity. *PLoS Computational Biology*, **2012**, 8, e1002840	5	23
79	Resonance Raman studies of oriented chromophores: Metmyoglobin single crystals. *Journal of Chemical Physics*, **1989**, 90, 3015-3032	3.9	23
78	Contribution of specific amino acid changes in penicillin binding protein 1 to amoxicillin resistance in clinical Helicobacter pylori isolates. *Antimicrobial Agents and Chemotherapy*, **2011**, 55, 101-9	5.9	22
77	Thermodynamic studies on the interaction of the third complement component and its inhibitor, compstatin. *Journal of Biological Chemistry*, **2004**, 279, 54987-95	5.4	21

76	Insights into the mechanism of C5aR inhibition by PMX53 via implicit solvent molecular dynamics simulations and docking. *BMC Biophysics*, **2014**, 7, 5	0	20
75	Development of a quasi-dynamic pharmacophore model for anti-complement peptide analogues. *Journal of the American Chemical Society*, **2005**, 127, 10967-76	16.4	20
74	Conformational interconversion in compstatin probed with molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53, 130-41	4.2	20
73	Resonance Raman studies of myoglobin single crystals. *Journal of the American Chemical Society*, **1988**, 110, 6341-6342	16.4	19
72	Hybrid flagellin as a T cell independent vaccine scaffold. *BMC Biotechnology*, **2015**, 15, 71	3.5	18
71	Solvation effects in calculated electrostatic association free energies for the C3d-CR2 complex and comparison with experimental data. *Biopolymers*, **2010**, 93, 509-19	2.2	17
70	Insights into the structure, correlated motions, and electrostatic properties of two HIV-1 gp120 V3 loops. *PLoS ONE*, **2012**, 7, e49925	3.7	17
69	New compstatin peptides containing N-terminal extensions and non-natural amino acids exhibit potent complement inhibition and improved solubility characteristics. *Journal of Medicinal Chemistry*, **2015**, 58, 814-26	8.3	16
68	Exploring Protein-Protein and Protein-Ligand Interactions in the Immune System using Molecular Dynamics and Continuum Electrostatics. *Current Physical Chemistry*, **2012**, 2, 324-343	0.5	16
67	Molecular analysis of the interaction between staphylococcal virulence factor Sbi-IV and complement C3d. *Biophysical Journal*, **2014**, 106, 1164-73	2.9	15
66	Clustering of HIV-1 Subtypes Based on gp120 V3 Loop electrostatic properties. *BMC Biophysics*, **2012**, 5, 3	0	15
65	Molecular thermodynamics for charged biomacromolecules. *Fluid Phase Equilibria*, **2006**, 241, 317-333	2.5	15
64	A new generation of potent complement inhibitors of the Compstatin family. *Chemical Biology and Drug Design*, **2011**, 77, 431-40	2.9	14
63	Native-state conformational dynamics of GART: a regulatory pH-dependent coil-helix transition examined by electrostatic calculations. *Protein Science*, **2001**, 10, 2363-78	6.3	14
62	Hydration of the partially folded peptide RN-24 studied by multidimensional NMR. *Journal of Biomolecular NMR*, **1995**, 5, 353-6	3	14
61	Hydrogen exchange in the carbon monoxide complex of soybean leghemoglobin. *FEBS Journal*, **1996**, 237, 212-20		14
60	Electrostatic modeling of peptides derived from the V3-loop of HIV-1 gp120: implications of the interaction with chemokine receptor CCR5. *International Journal of Molecular Medicine*, **2007**, 19, 343-51	4.4	14
59	Complement Inhibition by Staphylococcus aureus: Electrostatics of C3d□fbC and C3d□hp Association. *Cellular and Molecular Bioengineering*, **2012**, 5, 32-43	3.9	13

58	A theoretical view of the C3d:CR2 binding controversy. *Molecular Immunology*, **2015**, 64, 112-22	4.3	13
57	Proton transfer dynamics of GART: the pH-dependent catalytic mechanism examined by electrostatic calculations. *Protein Science*, **2001**, 10, 2379-92	6.3	13
56	A computational model for the evaluation of complement system regulation under homeostasis, disease, and drug intervention. *PLoS ONE*, **2018**, 13, e0198644	3.7	13
55	Derivation of ligands for the complement C3a receptor from the C-terminus of C5a. *European Journal of Pharmacology*, **2014**, 745, 176-81	5.3	12
54	The effect of electrostatics on factor H function and related pathologies. *Journal of Molecular Graphics and Modelling*, **2011**, 29, 1047-55	2.8	12
53	M13 bacteriophage spheroids as scaffolds for directed synthesis of spiky gold nanostructures. *Nanoscale*, **2018**, 10, 13055-13063	7.7	12
52	Molecular Mechanism of Biased Ligand Conformational Changes in CC Chemokine Receptor 7. *Journal of Chemical Information and Modeling*, **2016**, 56, 1808-22	6.1	11
51	Virtual Screening of Chemical Compounds for Discovery of Complement C3 Ligands. *ACS Omega*, **2018**, 3, 6427-6438	3.9	11
50	Conformational analysis of compstatin analogues with molecular dynamics simulations in explicit water. *Journal of Molecular Graphics and Modelling*, **2007**, 26, 571-80	2.8	11
49	Applications of Molecular Dynamics Simulations in Immunology: A Useful Computational Method in Aiding Vaccine Design. *Current Proteomics*, **2006**, 3, 259-270	0.7	11
48	Electrostatic properties of the structure of the docking and dimerization domain of protein kinase A IIalpha. *FEBS Journal*, **2002**, 269, 2040-51		11
47	Energetic evaluation of binding modes in the C3d and Factor H (CCP 19-20) complex. *Protein Science*, **2015**, 24, 789-802	6.3	10
46	Complement Inhibitors Targeting C3, C4, and C575-112		10
45	AESOP: A Python Library for Investigating Electrostatics in Protein Interactions. *Biophysical Journal*, **2017**, 112, 1761-1766	2.9	9
44	Electrostatic exploration of the C3d-FH4 interaction using a computational alanine scan. *Molecular Immunology*, **2011**, 48, 1844-50	4.3	9
43	Discovery of Small Molecules for Fluorescent Detection of Complement Activation Product C3d. *Journal of Medicinal Chemistry*, **2015**, 58, 9535-45	8.3	8
42	Engineering pre-SUMO4 as efficient substrate of SENP2. *Protein Engineering, Design and Selection*, **2014**, 27, 117-26	1.9	8
41	Structural study of Ac-Phe-[Orn-Pro-dCha-Trp-Arg], a potent C5a receptor antagonist, by NMR. *Biopolymers*, **2008**, 90, 803-15	2.2	8

40	Characterization of the interaction between peptides derived from the gp120/V3 domain of HIV-1 and the amino terminal of the chemokine receptor CCR5 by NMR spectroscopy and light scattering. *Journal of Non-Crystalline Solids*, **2006**, 352, 4451-4458	3.9	8
39	From atoms to systems: a cross-disciplinary approach to complement-mediated functions. *Molecular Immunology*, **2004**, 41, 153-64	4.3	8
38	Structure-Based Integrative Computational and Experimental Approach for the Optimization of Drug Design. *Lecture Notes in Computer Science*, **2005**, 680-688	0.9	8
37	Determination of local ligand conformations in slowly tumbling proteins by homonuclear 2D and 3D NMR: application to heme propionates in leghemoglobin. *Journal of the American Chemical Society*, **1993**, 115, 6238-6246	16.4	8
36	1H resonance assignments and secondary structure of the carbon monoxide complex of soybean leghemoglobin determined by homonuclear two-dimensional and three-dimensional NMR spectroscopy. *FEBS Journal*, **1994**, 219, 611-26		8
35	Low pH myoglobin photoproducts. *Biophysical Journal*, **1992**, 61, 1041-4	2.9	8
34	Detection of Side Chain Rearrangements Mediating the Motions of Transmembrane Helices in Molecular Dynamics Simulations of G Protein-Coupled Receptors. *Computational and Structural Biotechnology Journal*, **2017**, 15, 131-137	6.8	7
33	Electrostatic Steering Accelerates C3d:CR2 Association. *Journal of Physical Chemistry B*, **2016**, 120, 8416-23	3.4	7
32	An immunophysical study of the complement system: Examples for the pH dependence of protein binding and stability. *Journal of Non-Crystalline Solids*, **2006**, 352, 4445-4450	3.9	7
31	Characterization, Dynamics, and Mechanism of CXCR4 Antagonists on a Constitutively Active Mutant. *Cell Chemical Biology*, **2019**, 26, 662-673.e7	8.2	7
30	Dissecting Distinct Roles of NEDDylation E1 Ligase Heterodimer APPBP1 and UBA3 Reveals Potential Evolution Process for Activation of Ubiquitin-related Pathways. *Scientific Reports*, **2018**, 8, 10108	4.9	6
29	The pH dependence of stability of the activation helix and the catalytic site of GART. *Biophysical Chemistry*, **2003**, 105, 279-91	3.5	6
28	Hybrid Inorganic-Organic Molecular Beacons. *Sensor Letters*, **2004**, 2, 85-90	0.9	6
27	pH dependence of stability of the 10th human fibronectin type III domain: a computational study. *Biotechnology Progress*, **2008**, 24, 48-55	2.8	5
26	Peptide redesign for inhibition of the complement system: Targeting age-related macular degeneration. *Molecular Vision*, **2016**, 22, 1280-1290	2.3	5
25	Conformational heterogeneity in CCR7 undergoes transitions to specific states upon ligand binding. *Journal of Molecular Graphics and Modelling*, **2017**, 74, 352-358	2.8	4
24	Crosslinked flagella as a stabilized vaccine adjuvant scaffold. *BMC Biotechnology*, **2019**, 19, 48	3.5	4
23	De novo protein design of agonists and antagonists of C5a receptors. *Immunobiology*, **2012**, 217, 1162-1163	3.4	4

22	NMR evidence of charge-dependent interaction between various PND V3 and CCR5 N-terminal peptides. *Biopolymers*, **2009**, 92, 94-109	2.2	4
21	Computational studies of CXCR1, the receptor of IL-8/CXCL8, using molecular dynamics and electrostatics. *Biopolymers*, **2008**, 89, 52-61	2.2	4
20	Structure, Dynamics, Activity, and Function of Compstatin and Design of More Potent Analogues **2005**, 317-340		4
19	Molecular Mechanisms of Macular Degeneration Associated with the Complement Factor H Y402H Mutation. *Biophysical Journal*, **2019**, 116, 215-226	2.9	4
18	A predictive model for HIV type 1 coreceptor selectivity. *AIDS Research and Human Retroviruses*, **2013**, 29, 1386-94	1.6	3
17	Electrostatic Similarity Determination Using Multiresolution Analysis. *Molecular Informatics*, **2011**, 30, 733-46	3.8	3
16	Solution structure of a bent alpha-helix. *Biochemistry*, **2007**, 46, 12959-67	3.2	3
15	Immunophysical Evaluation of the Initiating Step in the Formation of the Membrane Attack Complex. *Frontiers in Physics*, **2018**, 6,	3.9	3
14	Ionic tethering contributes to the conformational stability and function of complement C3b. *Molecular Immunology*, **2017**, 85, 137-147	4.3	2
13	Factor H-Inspired Design of Peptide Biomarkers of the Complement C3d Protein. *ACS Medicinal Chemistry Letters*, **2020**, 11, 1054-1059	4.3	2
12	Electrostatic modeling of peptides derived from the V3-loop of HIV-1 gp120: Implications of the interaction with chemokine receptor CCR5. *International Journal of Molecular Medicine*,	4.4	2
11	SPARC coordinates extracellular matrix remodeling and efficient recruitment to and migration of antigen-specific T cells in the brain following infection. *Scientific Reports*, **2021**, 11, 4549	4.9	2
10	Electrostatic Interactions between Complement Regulator CD46(SCR1-2) and Adenovirus Ad11/Ad21 Fiber Protein Knob. *Molecular Biology International*, **2015**, 2015, 967465		1
9	Structure, Dynamics, Activity, and Function of Compstatin and Design of More Potent Analogues **2005**, 317-340		1
8	Structure of the Anaphylatoxins C3a and C5a **2005**, 161-178		1
7	The Building Blocks of the Complement System **2005**, 1-18		1
6	Overcoming the Key Challenges in De Novo Protein Design: Enhancing Computational Efficiency and Incorporating True Backbone Flexibility **2008**, 133-183		1
5	A Computational Model for the Evaluation of Complement System Regulation under Homeostasis, Disease, and Drug Intervention		1

4	Role of Electrostatic Hotspots in the Selectivity of Complement Control Proteins Toward Human and Bovine Complement Inhibition. *Frontiers in Molecular Biosciences*, **2021**, 8, 618068	5.6	1
3	Systems Biology Modeling of the Complement System Under Immune Susceptible Pathogens.. *Frontiers in Physics*, **2021**, 9,	3.9	1
2	Structure Calculations of Symmetric Dimers using Molecular Dynamics/Simulated Annealing and NMR Restraints: The Case of the RIIβ Subunit of Protein Kinase A. *Nonconvex Optimization and Its Applications*, **2000**, 141-156		1
1	Structure of the Anaphylatoxins C3a and C5a **2005**, 161-177		