Nohad Gresh

List of Publications by Year
in descending order

74 papers	3,251 citations	159585 30 h-index	149698 56 g-index
74 all docs	74 docs citations	74 times ranked	1888 citing authors

#	Article	IF	Citations
1	Anisotropic, Polarizable Molecular Mechanics Studies of Inter- and Intramolecular Interactions and Ligandâ^'Macromolecule Complexes. A Bottom-Up Strategy. Journal of Chemical Theory and Computation, 2007, 3, 1960-1986.	5.3	312
2	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. Chemical Science, 2018, 9, 956-972.	7.4	190
3	Towards a force field based on density fitting. Journal of Chemical Physics, 2006, 124, 104101.	3.0	175
4	Theoretical studies of molecular conformation. Derivation of an additive procedure for the computation of intramolecular interaction energies. Comparison withab initio SCF computations. Theoretica Chimica Acta, 1984, 66, 1-20.	0.8	139
5	Improved Formulas for the Calculation of the Electrostatic Contribution to the Intermolecular Interaction Energy from Multipolar Expansion of the Electronic Distribution. Journal of Physical Chemistry A, 2003, 107, 10353-10359.	2.5	135
6	Energetics of Zn2+ binding to a series of biologically relevant ligands: A molecular mechanics investigation grounded onab initio self-consistent field supermolecular computations. Journal of Computational Chemistry, 1995, 16, 856-882.	3.3	129
7	A Comprehensive Energy Component Analysis of the Interaction of Hard and Soft Dications with Biological Ligands. Journal of the American Chemical Society, 1994, 116, 3556-3567.	13.7	105
8	Toward a Separate Reproduction of the Contributions to the Hartreeâ^'Fock and DFT Intermolecular Interaction Energies by Polarizable Molecular Mechanics with the SIBFA Potential. Journal of Chemical Theory and Computation, 2007, 3, 824-837.	5.3	104
9	Many-Body Effects in Systems of Peptide Hydrogen-Bonded Networks and Their Contributions to Ligand Binding:Â A Comparison of the Performances of DFT and Polarizable Molecular Mechanics. Journal of Physical Chemistry B, 2000, 104, 9746-9754.	2.6	93
10	General Model for Treating Short-Range Electrostatic Penetration in a Molecular Mechanics Force Field. Journal of Chemical Theory and Computation, 2015, 11, 2609-2618.	5.3	93
11	Interaction of neutral and zwitterionic glycine with Zn2+ in gas phase:ab initio and SIBFA molecular mechanics calculations. Journal of Computational Chemistry, 2000, 21, 963-973.	3.3	87
12	Cation binding to biomolecules. Theoretica Chimica Acta, 1977, 44, 151-163.	0.8	82
13	Theoretical Study of Binding of Hydrated Zn(II) and Mg(II) Cations to 5â€˜-Guanosine Monophosphate. Toward Polarizable Molecular Mechanics for DNA and RNA. Journal of Physical Chemistry B, 2003, 107, 8669-8681.	2.6	82
14	Representation of Zn(II) complexes in polarizable molecular mechanics. Further refinements of the electrostatic and short-range contributions. Comparisons with parallelab initiocomputations. Journal of Computational Chemistry, 2005, 26, 1113-1130.	3.3	79
15	Parallelab initio and molecular mechanics investigation of polycoordinated Zn(II) complexes with model hard and soft ligands: Variations of binding energy and of its components with number and charges of ligands. Journal of Computational Chemistry, 2000, 21, 1011-1039.	3.3	74
16	Title is missing!. Journal of Computational Chemistry, 1996, 17, 1481.	3.3	69
17	Model, Multiply Hydrogen-Bonded Water Oligomers (N= 3â^'20). How Closely Can a Separable, ab Initio-Grounded Molecular Mechanics Procedure Reproduce the Results of Supermolecule Quantum Chemical Computations?. Journal of Physical Chemistry A, 1997, 101, 8680-8694.	2.5	64
18	A theoretical study of nonadditive effects in four water tetramers. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2745-2753.	1.7	64

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19	Toward accurate solvation dynamics of lanthanides and actinides in water using polarizable force fields: from gas-phase energetics to hydration free energies. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	62
20	Comparative binding energetics of Mg²⁺, Ca²⁺, Zn²⁺, and Cd²⁺ to biologically relevant ligands: Combined ab initio SCF supermolecule and molecular mechanics investigation. Journal of Computational Chemistry, 1996, 17, 1481-1495.	3.3	58
21	Binding of D- and L-captopril inhibitors to metallo-Î²-lactamase studied by polarizable molecular mechanics and quantum mechanics. Journal of Computational Chemistry, 2002, 23, 1281-1296.	3.3	57
22	Modeling of inhibitorâ€“metalloenzyme interactions and selectivity using molecular mechanics grounded in quantum chemistry. Proteins: Structure, Function and Bioinformatics, 1998, 31, 42-60.	2.6	56
23	A theoretical investigation on the sequence selective binding of mitoxantrone to double-stranded tetranucleotides. Nucleic Acids Research, 1986, 14, 3799-3812.	14.5	55
24	Polarizable Water Molecules in Ligandâ^'Macromolecule Recognition. Impact on the Relative Affinities of Competing Pyrrolopyrimidine Inhibitors for FAK Kinase. Journal of the American Chemical Society, 2010, 132, 3312-3320.	13.7	51
25	Mono- and poly-ligated complexes of Zn2+: Anab initio analysis of the metal-ligand interaction energy. Journal of Computational Chemistry, 1995, 16, 843-855.	3.3	47
26	Joint quantum chemical and polarizable molecular mechanics investigation of formate complexes with penta- and hexahydrated Zn2+: Comparison between energetics of model bidentate, monodentate, and through-water Zn2+ binding modes and evaluation of nonadditivity effects. Journal of Computational Chemistry, 1999, 20, 1379-1390.	3.3	47
27	Complexes of thiomandelate and captopril mercaptocarboxylate inhibitors to metallo-Î²-lactamase by polarizable molecular mechanics. Validation on model binding sites by quantum chemistry. Journal of Computational Chemistry, 2005, 26, 1131-1147.	3.3	47
28	Binding of 5-phospho-D-arabinonohydroxamate and 5-phospho-D-arabinonate inhibitors to zinc phosphomannose isomerase fromCandida albicans studied by polarizable molecular mechanics and quantum mechanics. Journal of Computational Chemistry, 2007, 28, 938-957.	3.3	44
29	Intramolecular interaction energies in model alanine and glycine tetrapeptides. Evaluation of anisotropy, polarization, and correlation effects. A parallelab initioHF/MP2, DFT, and polarizable molecular mechanics study. Journal of Computational Chemistry, 2004, 25, 823-834.	3.3	37
30	Polarizable Water Networks in Ligandâ€“Metalloprotein Recognition. Impact on the Relative Complexation Energies of Zn-Dependent Phosphomannose Isomerase with <scp>d</scp>-Mannose 6-Phosphate Surrogates. Journal of Physical Chemistry B, 2011, 115, 8304-8316.	2.6	31
31	Manyâ€body exchangeâ€repulsion in polarizable molecular mechanics. I. orbitalâ€based approximations and applications to hydrated metal cation complexes. Journal of Computational Chemistry, 2011, 32, 2949-2957.	3.3	30
32	4-Amino-1,2,4-triazole-3-thione-derived Schiff bases as metallo-Î²-lactamase inhibitors. European Journal of Medicinal Chemistry, 2020, 208, 112720.	5.5	29
33	Intramolecular chelation of Zn2+by Î±- and Î²-mercaptocarboxamides. A parallelab initioand polarizable molecular mechanics investigation. Assessment of the role of multipole transferability. Journal of Computational Chemistry, 2001, 22, 1038-1047.	3.3	28
34	Joint Molecular Modeling and Spectroscopic Studies of DNA Complexes of a Bis(arginyl) Conjugate of a Tricationic Porphyrin Designed to Target the Major Grooveâ€. Biochemistry, 1998, 37, 6165-6178.	2.5	26
35	Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general shortâ€range penetration correction up to quadrupoles. Journal of Computational Chemistry, 2016, 37, 494-506.	3.3	26
36	The reaction mechanism of type I phosphomannose isomerases: New information from inhibition and polarizable molecular mechanics studies. Proteins: Structure, Function and Bioinformatics, 2011, 79, 203-220.	2.6	24

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37	Synthesis and evaluation of non-hydrolyzable d-mannose 6-phosphate surrogates reveal 6-deoxy-6-dicarboxymethyl-d-mannose as a new strong inhibitor of phosphomannose isomerases. Bioorganic and Medicinal Chemistry, 2009, 17, 7100-7107.	3.0	23
38	S/G-1: An ab Initio Force-Field Blending Frozen Hermite Gaussian Densities and Distributed Multipoles. Proof of Concept and First Applications to Metal Cations. Journal of Physical Chemistry A, 2014, 118, 7598-7612.	2.5	22
39	A supervised fitting approach to force field parametrization with application to the SIBFA polarizable force field. Journal of Computational Chemistry, 2014, 35, 1577-1591.	3.3	21
40	Channeling through Two Stacked Guanine Quartets of One and Two Alkali Cations in the Li⁺, Na⁺, K⁺, and Rb⁺ Series. Assessment of the Accuracy of the SIBFA Anisotropic Polarizable Molecular Mechanics Potential. Journal of Physical Chemistry B, 2017, 121, 3997-4014.	2.6	20
41	Assessment of SAPT and Supermolecular EDA Approaches for the Development of Separable and Polarizable Force Fields. Journal of Chemical Theory and Computation, 2021, 17, 2759-2774.	5.3	20
42	Bis- and Tris-DNA Intercalating Porphyrins Designed to Target the Major Groove: Synthesis of Acridylbis-arginyl-porphyrins, Molecular Modelling of Their DNA Complexes, and Experimental Tests. European Journal of Organic Chemistry, 2004, 2004, 1781-1797.	2.4	19
43	Conformation-dependent intermolecular interaction energies of the triphosphate anion with divalent metal cations. Application to the ATP-binding site of a binuclear bacterial enzyme. A parallel quantum chemical and polarizable molecular mechanics investigation. Journal of Computational Chemistry, 2004, 25, 160-168.	3.3	19
44	Stacked and H-Bonded Cytosine Dimers. Analysis of the Intermolecular Interaction Energies by Parallel Quantum Chemistry and Polarizable Molecular Mechanics.. Journal of Physical Chemistry B, 2015, 119, 9477-9495.	2.6	19
45	Analysis of the Interactions Taking Place in the Recognition Site of a Bimetallic Mg(II)â^'Zn(II) Enzyme, Isopentenyl Diphosphate Isomerase. A Parallel Quantum-Chemical and Polarizable Molecular Mechanics Study. Journal of Physical Chemistry B, 2010, 114, 4884-4895.	2.6	18
46	Theoretical Design of Novel, 4 Base Pair Selective Derivatives of Mitoxantrone. Journal of Biomolecular Structure and Dynamics, 1990, 7, 1141-1160.	3.5	17
47	Rational Design, Synthesis, and DNA Binding Properties of Novel Sequenceâ€Selective Peptidyl Congeners of Ametantrone. ChemMedChem, 2010, 5, 1080-1091.	3.2	17
48	4-(N-Alkyl- and -Acyl-amino)-1,2,4-triazole-3-thione Analogs as Metallo-Î²-Lactamase Inhibitors: Impact of 4-Linker on Potency and Spectrum of Inhibition. Biomolecules, 2020, 10, 1094.	4.0	15
49	Substituent-Modulated Affinities of Halobenzene Derivatives to the HIV-1 Integrase Recognition Site. Analyses of the Interaction Energies by Parallel Quantum Chemical and Polarizable Molecular Mechanics. Journal of Physical Chemistry A, 2014, 118, 9772-9782.	2.5	14
50	Could the â€œJanusâ€likeâ€•properties of the halobenzene CX bond (Xï£¾Cl, Br) be leveraged to enhance molecular recognition?. Journal of Computational Chemistry, 2015, 36, 210-221.	3.3	14
51	Interfacial Water Many-Body Effects Drive Structural Dynamics and Allosteric Interactions in SARS-CoV-2 Main Protease Dimerization Interface. Journal of Physical Chemistry Letters, 2021, 12, 6218-6226.	4.6	13
52	Theoretical study of the binding of aliphatic diamines to the minor groove of a B-DNA (dA-dT)11 oligomer. Biopolymers, 1985, 24, 1527-1542.	2.4	12
53	Theoretical Design of a Bistetrapeptide Derivative of Mitoxantrone Targeted Towards the Double-Stranded Hexanucleotide Sequence d(GGCGCC)₂. Journal of Biomolecular Structure and Dynamics, 1991, 8, 827-846.	3.5	12
54	Quantumâ€chemistry based calibration of the alkali metal cation series (Li⁺ï£¿Cs⁺) for largeâ€scale polarizable molecular mechanics/dynamics simulations. Journal of Computational Chemistry, 2015, 36, 285-302.	3.3	12

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55	Development of the Quantum-Inspired SIBFA Many-Body Polarizable Force Field: Enabling Condensed-Phase Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2022, 18, 3607-3621.	5.3	12
56	Complexes of a Znâ€metalloenzyme binding site with hydroxamateâ€containing ligands. A case for detailed benchmarkings of polarizable molecular mechanics/dynamics potentials when the experimental binding structure is unknown. Journal of Computational Chemistry, 2016, 37, 2770-2782.	3.3	11
57	Calibration of 1,2,4-Triazole-3-Thione, an Original Zn-Binding Group of Metallo-Î²-Lactamase Inhibitors. Validation of a Polarizable MM/MD Potential by Quantum Chemistry. Journal of Physical Chemistry B, 2017, 121, 6295-6312.	2.6	11
58	Importance of explicit smeared lone-pairs in anisotropic polarizable molecular mechanics. Torture track angular tests for exchange-repulsion and charge transfer contributions. Journal of Computational Chemistry, 2017, 38, 1897-1920.	3.3	11
59	Further refinements of next-generation force fields â€" Nonempirical localization of off-centered points in molecules. Canadian Journal of Chemistry, 2013, 91, 804-810.	1.1	10
60	Polarizable molecular mechanics studies of <scp>Cu(I)/Zn(II)</scp> superoxide dismutase: Bimetallic binding site and structured waters. Journal of Computational Chemistry, 2014, 35, 2096-2106.	3.3	9
61	A Simple Isomerization of the Purine Scaffold of a Kinase Inhibitor, Roscovitine, Affords a Four- to Seven-Fold Enhancement of Its Affinity for Four CDKs. Could This Be Traced Back to Conjugation-Induced Stiffenings/Loosenings of Rotational Barriers?. ACS Omega, 2017, 2, 3467-3474.	3.5	8
62	Conformational analysis of a polyconjugated protein-binding ligand by joint quantum chemistry and polarizable molecular mechanics. Addressing the issues of anisotropy, conjugation, polarization, and multipole transferability. Journal of Molecular Modeling, 2014, 20, 2472.	1.8	7
63	Design and synthesis of a peptide derivative of ametantrone targeting the major groove of the d(GGCGCC)2palindromic sequence. New Journal of Chemistry, 2020, 44, 3624-3631.	2.8	6
64	The inhibition process of HIV-1 integrase by diketoacids molecules: Understanding the factors governing the better efficiency of dolutegravir. Biochemical and Biophysical Research Communications, 2017, 488, 433-438.	2.1	4
65	Calibration of the dianionic phosphate group: Validation on the recognition site of the homodimeric enzyme phosphoglucose isomerase. Journal of Computational Chemistry, 2020, 41, 839-854.	3.3	4
66	Intermolecular interactions of the extended recognition site of <scp>VIM</scp>â€2 <scp>metalloâ€Î²â€lactamase</scp> with 1,2,4â€triazoleâ€3â€thione inhibitors. Validations of a polarizable molecular mechanics potential by ab initio <scp>QC</scp>. Journal of Computational Chemistry, 2021, 42, 86-106.	3.3	4
67	A theoretical study of the selective entrapment of alkali and ammonium cations between guanine tetramers. International Journal of Quantum Chemistry, 1985, 28, 49-56.	2.0	3
68	Towards scalable and accurate molecular dynamics using the SIBFA polarizable force field. AIP Conference Proceedings, 2017, , .	0.4	3
69	Parallel ab initio and molecular mechanics investigation of polycoordinated Zn(II) complexes with model hard and soft ligands: Variations of binding energy and of its components with number and charges of ligands. Journal of Computational Chemistry, 2000, 21, 1011.	3.3	3
70	Approaching the double-faceted nature of the CX bond in halobenzenes with a bifunctional probe. Chemical Physics Letters, 2015, 637, 51-57.	2.6	2
71	Quantum-Chemistry Based Design of Halobenzene Derivatives With Augmented Affinities for the HIV-1 Viral G4/C16 Base-Pair. Frontiers in Chemistry, 2020, 8, 440.	3.6	2
72	Spectrometric and computational studies of the binding of HIV-1 integrase inhibitors to viral DNA extremities. , 0, 1, e6.		2

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73	A Joint 2D NMR and Theoretical Investigation of Ca²⁺Binding Loops III and IV of Calmodulin. Journal of Biomolecular Structure and Dynamics, 1990, 7, 1003-1018.	3.5	1
74	Multimolecular complexes of the phosphodiester anion with Zn(II) or Mg(II) and water moleculesâ€"Preliminary validations of a polarizable potential by ab initio quantum chemistry. Journal of Computational Chemistry, 2021, 42, 1430-1446.	3.3	0