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	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
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	Towards scalable and accurate molecular dynamics using the SIBFA polarizable force field. AIP Conference Proceedings, 2017, , .	0.4	3
18	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

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19	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
20	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
21	Could the â€œJanusâ€ikeâ€•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
22	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
23	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
24	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
25	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
26	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
27	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
28	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
29	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
30	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
31	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
32	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
33	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
34	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
35	Rational Design, Synthesis, and DNA Binding Properties of Novel Sequenceâ€Selective Peptidyl Congeners of Ametantrone. ChemMedChem, 2010, 5, 1080-1091.	3.2	17
36	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

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37	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
38	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
39	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
40	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
41	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
42	Towards a force field based on density fitting. Journal of Chemical Physics, 2006, 124, 104101.	3.0	175
43	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
44	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
45	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
46	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
47	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
48	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
49	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
50	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
51	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
52	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
53	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
54	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

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55	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
56	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
57	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
58	A theoretical study of nonadditive effects in four water tetramers. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2745-2753.	1.7	64
59	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
60	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
61	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
62	Title is missing!. Journal of Computational Chemistry, 1996, 17, 1481.	3.3	69
63	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
64	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
65	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
66	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
67	Theoretical Design of Novel, 4 Base Pair Selective Derivatives of Mitoxantrone. Journal of Biomolecular Structure and Dynamics, 1990, 7, 1141-1160.	3.5	17
68	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
69	A theoretical investigation on the sequence selective binding of mitoxantrone to double-stranded tetranucleotides. Nucleic Acids Research, 1986, 14, 3799-3812.	14.5	55
70	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
71	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
72	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

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73	Cation binding to biomolecules. Theoretica Chimica Acta, 1977, 44, 151-163.	0.8	82
74	Spectrometric and computational studies of the binding of HIV-1 integrase inhibitors to viral DNA extremities. , 0, 1, e6.		2