Rodrigo Galindo-Murillo

List of Publications by Year
in descending order

49 papers	1,741 citations	586496 16 h-index	325983 40 g-index
50 all docs	50 docs citations	50 times ranked	2662 citing authors

#	Article	IF	Citations
1	Backbone Hydrocarbon-Constrained Nucleic Acids Modulate Hybridization Kinetics for RNA. Journal of the American Chemical Society, 2022, 144, 1941-1950.	6.6	5
2	Riboflavin Stabilizes Abasic, Oxidized G-Quadruplex Structures. Biochemistry, 2022, 61, 265-275.	1.2	3
3	Transient Hoogsteen Base Pairs Observed in Unbiased Molecular Dynamics Simulations of DNA. Journal of Physical Chemistry Letters, 2022, 13, 6283-6287.	2.1	2
4	Molecular dynamics simulations of acyclic analogs of nucleic acids for antisense inhibition. Molecular Therapy - Nucleic Acids, 2021, 23, 527-535.	2.3	2
5	Ethidium bromide interactions with DNA: an exploration of a classic DNAâ€“ligand complex with unbiased molecular dynamics simulations. Nucleic Acids Research, 2021, 49, 3735-3747.	6.5	55
6	Elucidating Molecular Interactions of Ten Natural Compounds Targeting E6 HPV High Risk Oncoproteins Using Microsecond Molecular Dynamics Simulations. Medicinal Chemistry, 2021, 17, 587-600.	0.7	2
7	Sequence-dependent structural properties of B-DNA: what have we learned in 40Âyears?. Biophysical Reviews, 2021, 13, 995-1005.	1.5	13
8	Hydrophobic unnatural base pairs show a Watson-Crick pairing in micro-second molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4098-4106.	2.0	5
9	Effect of 4-HNE Modification on ZU5-ANK Domain and the Formation of Their Complex with Î²-Spectrin: A Molecular Dynamics Simulation Study. Journal of Chemical Information and Modeling, 2020, 60, 805-820.	2.5	13
10	Novel Blocker of Onco SK3 Channels Derived from Scorpion Toxin Tamapin and Active against Migration of Cancer Cells. ACS Medicinal Chemistry Letters, 2020, 11, 1627-1633.	1.3	11
11	AMBER parameters and topology data of 2-pentylpyrrole adduct of arginine with 4-hydroxy-2-nonenal. Data in Brief, 2020, 29, 105294.	0.5	1
12	Heteroleptic NiII complexes: Synthesis, structural characterization, computational studies and amoebicidal activity evaluation. Journal of Inorganic Biochemistry, 2020, 206, 111043.	1.5	3
13	Ancillary Ligand in Ternary CuII Complexes Guides Binding Selectivity toward Minor-Groove DNA. Journal of Physical Chemistry B, 2020, 124, 11648-11658.	1.2	6
14	Exploring potentially alternative non-canonical DNA duplex structures through simulation. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2201-2210.	2.0	5
15	Antigiardiasic activity of Cu(II) coordination compounds: Redox imbalance and membrane damage after a short exposure time. Journal of Inorganic Biochemistry, 2019, 195, 83-90.	1.5	14
16	4-HNE carbonylation induces local conformational changes on bovine serum albumin and thioredoxin. A molecular dynamics study. Journal of Molecular Graphics and Modelling, 2019, 86, 298-307.	1.3	17
17	Lessons learned in atomistic simulation of double-stranded DNA: Solvation and salt concerns [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	2.2	12
18	Defining a conformational ensemble that directs activation of PPARÎ³. Nature Communications, 2018, 9, 1794.	5.8	53

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19	Computational DNA binding studies of (â€“)-epigallocatechin-3-gallate. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3311-3323.	2.0	15
20	Development and benchmark to obtain AMBER parameters dataset for non-standard amino acids modified with 4-hydroxy-2-nonenal. Data in Brief, 2018, 21, 2581-2589.	0.5	7
21	Water-Soluble Ruthenium (II) Chiral Heteroleptic Complexes with Amoebicidal in Vitro and in Vivo Activity. Journal of Medicinal Chemistry, 2017, 60, 899-912.	2.9	15
22	The Role of the DNA Backbone in Minorâ€Groove Ligand Binding. ChemPhysChem, 2017, 18, 1909-1915.	1.0	14
23	Structural and dynamical instability of DNA caused by high occurrence of d5SICS and dNaM unnatural nucleotides. Physical Chemistry Chemical Physics, 2017, 19, 10571-10580.	1.3	11
24	Computational Assessment of Potassium and Magnesium Ion Binding to a Buried Pocket in GTPase-Associating Center RNA. Journal of Physical Chemistry B, 2017, 121, 451-462.	1.2	15
25	A User-Friendly DNA Modeling Software for the Interpretation of Cryo-Electron Microscopy Data. Methods in Molecular Biology, 2017, 1624, 193-210.	0.4	2
26	Effect of tunable redox behavior of bis chelate substituted 1,10-phenantroline Cu(II) complexes on its reaction with superoxide anion in DMSO. Toward a simple criterion to identify a SOD-like mechanism. Journal of Inorganic Biochemistry, 2017, 175, 118-128.	1.5	7
27	Dissociative reactions of benzonorbornadienes with tetrazines: scope of leaving groups and mechanistic insights. Organic and Biomolecular Chemistry, 2017, 15, 9855-9865.	1.5	28
28	Isomeric Effect on the Pharmacokinetic Behavior of Anticancer Cu^{II} Mixed Chelate Complexes: Experimental and Theoretical Approach. European Journal of Inorganic Chemistry, 2017, 2017, 1728-1736.	1.0	20
29	Polycyclic ferrocenyl(dihydro)thiazepine derivatives: Diastereo-selective synthesis, characterization, electrochemical behavior, theoretical and biological investigation. Journal of Inorganic Biochemistry, 2017, 166, 141-149.	1.5	7
30	Metal-Based Drug-DNA Interactions. Journal of the Mexican Chemical Society, 2017, 57, .	0.2	3
31	Transitions of Double-Stranded DNA Between the A- and B-Forms. Journal of Physical Chemistry B, 2016, 120, 8449-8456.	1.2	38
32	Assessing the Current State of Amber Force Field Modifications for DNA. Journal of Chemical Theory and Computation, 2016, 12, 4114-4127.	2.3	351
33	Using Wavelet Analysis To Assist in Identification of Significant Events in Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2016, 56, 1282-1291.	2.5	17
34	A mixed <scp>DFTâ€MD</scp> methodology for the in silico development of drug releasing macrocycles. Calix and thiaâ€calix[N]arenes as carriers for Bosutinib and Sorafenib. Journal of Computational Chemistry, 2016, 37, 940-946.	1.5	9
35	Probing the influence of hypermodified residues within the tRNA3Lys anticodon stem loop interacting with the A-loop primer sequence from HIV-1. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 607-617.	1.1	5
36	A Range of Nitrato Coordination Modes in Ni^{II} Complexes with the Versatile Ligand 1,8â€Bis(2â€pyridyl)â€3,6â€dithiaoctane: Structural, Spectroscopic, Electrochemical, and Theoretical Studies. European Journal of Inorganic Chemistry, 2015, 2015, 3307-3316.	1.0	3

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37	Convergence and reproducibility in molecular dynamics simulations of the DNA duplex d(GCACGAACGAACGAACGC). Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 1041-1058.	1.1	136
38	Potential Amoebicidal Activity of Hydrazone Derivatives: Synthesis, Characterization, Electrochemical Behavior, Theoretical Study and Evaluation of the Biological Activity. Molecules, 2015, 20, 9929-9948.	1.7	12
39	Intercalation processes of copper complexes in DNA. Nucleic Acids Research, 2015, 43, 5364-5376.	6.5	137
40	Refinement of the Sugarâ€“Phosphate Backbone Torsion Beta for AMBER Force Fields Improves the Description of Z- and B-DNA. Journal of Chemical Theory and Computation, 2015, 11, 5723-5736.	2.3	392
41	On the absence of intrahelical DNA dynamics on the Î¼s to ms timescale. Nature Communications, 2014, 5, 5152.	5.8	70
42	The Ï€â€Backâ€Bonding Modulation and Its Impact in the Electronic Properties of Cu^{II} Antineoplastic Compounds: An Experimental and Theoretical Study. Chemistry - A European Journal, 2014, 20, 13730-13741.	1.7	35
43	DNA Binding Dynamics and Energetics of Cobalt, Nickel, and Copper Metallopeptides. ChemMedChem, 2014, 9, 1252-1259.	1.6	17
44	Calix[n]arene-based drug carriers: A DFT study of their electronic interactions with a chemotherapeutic agent used against leukemia. Computational and Theoretical Chemistry, 2014, 1035, 84-91.	1.1	24
45	In Silico Design of Monomolecular Drug Carriers for the Tyrosine Kinase Inhibitor Drug Imatinib Based on Calix- and Thiacalix[n]arene Host Molecules: A DFT and Molecular Dynamics Study. Journal of Chemical Theory and Computation, 2014, 10, 825-834.	2.3	26
46	Molecular Modeling of Nucleic Acid Structure. Current Protocols in Nucleic Acid Chemistry, 2013, 54, 7.5.1-7.5.13.	0.5	10
47	Molecular Modeling of Nucleic Acid Structure: Energy and Sampling. Current Protocols in Nucleic Acid Chemistry, 2013, 54, 7.8.1-7.8.21.	0.5	2
48	Molecular recognition between DNA and a copper-based anticancer complex. Physical Chemistry Chemical Physics, 2012, 14, 15539.	1.3	55
49	Ï€-Stacking between CasiopeinasÂ® and DNA bases. Physical Chemistry Chemical Physics, 2011, 13, 14510.	1.3	36