## Jesus Mendieta

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Proton Transfer in Guanine-Cytosine Base Pairs in B-DNA. Journal of Chemical Theory and Computation, 2019, 15, 6984-6991.	2.3	21
2	Amino acid residues in HIV-2 reverse transcriptase that restrict the development of nucleoside analogue resistance through the excision pathway. Journal of Biological Chemistry, 2018, 293, 2247-2259.	1.6	9
3	Effect of water-DNA interactions on elastic properties of DNA self-assembled monolayers. Scientific Reports, 2017, 7, 536.	1.6	33
4	Two-step ATP-driven opening of cohesin head. Scientific Reports, 2017, 7, 3266.	1.6	19
5	Quantum Mechanics/Molecular Mechanics Free Energy Maps and Nonadiabatic Simulations for a Photochemical Reaction in DNA: Cyclobutane Thymine Dimer. Journal of Physical Chemistry Letters, 2016, 7, 4391-4397.	2.1	20
6	A Practical Quantum Mechanics Molecular Mechanics Method for the Dynamical Study of Reactions in Biomolecules. Advances in Protein Chemistry and Structural Biology, 2015, 100, 67-88.	1.0	5
7	MEPSA: minimum energy pathway analysis for energy landscapes. Bioinformatics, 2015, 31, 3853-3855.	1.8	84
8	Torsion and curvature of FtsZ filaments. Soft Matter, 2014, 10, 1977.	1.2	27
9	<scp>fireball</scp> / <scp>amber</scp> : An Efficient Local-Orbital DFT QM/MM Method for Biomolecular Systems. Journal of Chemical Theory and Computation, 2014, 10, 2185-2193.	2.3	42
10	Molecular basis of the association of H208Y and thymidine analogue resistance mutations M41L, L210W and T215Y in the HIV-1 reverse transcriptase of treated patients. Antiviral Research, 2014, 106, 42-52.	1.9	3
11	Simulation of Catalytic Water Activation in Mitochondrial F <sub>1</sub> -ATPase Using a Hybrid Quantum Mechanics/Molecular Mechanics Approach: An Alternative Role for β-Glu 188. Biochemistry, 2013, 52, 959-966.	1.2	6
12	Functional Specificity of a Protein-DNA Complex Mediated by Two Arginines Bound to the Minor Groove. Journal of Bacteriology, 2012, 194, 4727-4735.	1.0	4
13	Molecular dynamics analysis of conformational change of paramyxovirus F protein during the initial steps of membrane fusion. Biochemical and Biophysical Research Communications, 2012, 420, 42-47.	1.0	2
14	The Role of Gln61 in HRas GTP Hydrolysis: A Quantum Mechanics/Molecular Mechanics Study. Biophysical Journal, 2012, 102, 152-157.	0.2	48
15	Molecular dynamics simulation of GTPase activity in polymers of the cell division protein FtsZ. FEBS Letters, 2012, 586, 1236-1239.	1.3	9
16	Functional phosphoproteomics for current immunology research. Journal of Integrated OMICS, 2011, 1, .	0.5	3
17	Technical phosphoproteomic and bioinformatic tools useful in cancer research. Journal of Clinical Bioinformatics, 2011, 1, 26.	1.2	16
18	Nanomechanics of the Cadherin Ectodomain. Journal of Biological Chemistry. 2011. 286. 9405-9418.	1.6	45

Jesus Mendieta

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19	Thymidine Analogue Excision and Discrimination Modulated by Mutational Complexes Including Single Amino Acid Deletions of Asp-67 or Thr-69 in HIV-1 Reverse Transcriptase. Journal of Biological Chemistry, 2011, 286, 20615-20624.	1.6	14
20	Structural and Functional Model for Ionic (K+/Na+) and pH Dependence of GTPase Activity and Polymerization of FtsZ, the Prokaryotic Ortholog of Tubulin. Journal of Molecular Biology, 2009, 390, 17-25.	2.0	38
21	A Mg <sup>2+</sup> â€induced conformational switch rendering a competent DNA polymerase catalytic complex. Proteins: Structure, Function and Bioinformatics, 2008, 71, 565-574.	1.5	28
22	Mechanistic Basis of Zidovudine Hypersusceptibility and Lamivudine Resistance Conferred by the Deletion of Codon 69 in the HIV-1 Reverse Transcriptase Coding Region. Journal of Molecular Biology, 2008, 382, 327-341.	2.0	18
23	Residues in human respiratory syncytial virus P protein that are essential for its activity on RNA viral synthesis. Virus Research, 2008, 132, 160-173.	1.1	20
24	Use of a Dominant rpsL Allele Conferring Streptomycin Dependence for Positive and Negative Selection in Thermus thermophilus. Applied and Environmental Microbiology, 2007, 73, 5138-5145.	1.4	14
25	DNA sequence-specific recognition by a transcriptional regulator requires indirect readout of A-tracts. Nucleic Acids Research, 2007, 35, 3252-3261.	6.5	10
26	Binding of 5â€~-GMP to the GluR2 AMPA Receptor: Insight from Targeted Molecular Dynamics Simulationsâ€. Biochemistry, 2005, 44, 14470-14476.	1.2	28
27	Phosphorylation modulates the alpha-helical structure and polymerization of a peptide from the third tau microtubule-binding repeat. Biochimica Et Biophysica Acta - General Subjects, 2005, 1721, 16-26.	1.1	22
28	In silico activation of Src tyrosine kinase reveals the molecular basis for intramolecular autophosphorylation. Journal of Molecular Graphics and Modelling, 2004, 23, 189-198.	1.3	21
29	Role of Histidine-85 in the Catalytic Mechanism of Thymidine Phosphorylase As Assessed by Targeted Molecular Dynamics Simulations and Quantum Mechanical Calculations. Biochemistry, 2004, 43, 405-414.	1.2	34
30	Towards New Thymidine Phosphorylase/PD-ECGF Inhibitors Based on the Transition State of the Enzyme Reaction. Nucleosides, Nucleotides and Nucleic Acids, 2003, 22, 951-953.	0.4	3
31	A 3·(ET743)-DNA Complex That Both Resembles an RNA-DNA Hybrid and Mimicks Zinc Finger-Induced DNA Structural Distortions. Journal of Medicinal Chemistry, 2002, 45, 871-880.	2.9	30
32	Combined Use of Differential Pulse Polarography and Multivariate Curve Resolution: As Applied to the Study of Metal Mixed Complexes of the Metallothionein Related Hexapeptide. Electroanalysis, 2002, 14, 50-56.	1.5	10
33	Molecular dynamics simulations of the conformational changes of the glutamate receptor ligand-binding core in the presence of glutamate and kainate. Proteins: Structure, Function and Bioinformatics, 2001, 44, 460-469.	1.5	37
34	Soft- and Hard-Modeling Approaches for the Determination of Stability Constants of Metal–Peptide Systems by Voltammetry. Analytical Biochemistry, 2000, 279, 189-201.	1.1	41
35	Zinc-binding properties of the C-terminal hexapeptide Lys–Cys–Thr–Cys–Cys–Ala from mouse metallothionein: analysis by differential pulse polarography and multivariate curve resolution. Analytica Chimica Acta, 1999, 385, 353-363.	2.6	17
36	Complexation of cadmium by the C-terminal hexapeptide Lys-Cys-Thr-Cys-Cys-Ala from mouse metallothionein: study by differential pulse polarography and circular dichroism spectroscopy with multivariate curve resolution analysis. Analytica Chimica Acta, 1999, 390, 15-25.	2.6	27

Jesus Mendieta

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37	Multivariate Curve Resolution of Cyclic Voltammetric Data:  Application to the Study of the Cadmium-Binding Properties of Glutathione. Analytical Chemistry, 1999, 71, 4629-4636.	3.2	53
38	Two-Phase Induction of the Nonnative α-Helical Form of β-Lactoglobulin in the Presence of Trifluoroethanol. Biophysical Journal, 1999, 76, 451-457.	0.2	38
39	Study of the zinc-binding properties of glutathione by differential pulse polarography and multivariate curve resolution. Journal of Inorganic Biochemistry, 1998, 70, 91-98.	1.5	58
40	Multivariate Curve Resolution: A Possible Tool in the Detection of Intermediate Structures in Protein Folding. Biophysical Journal, 1998, 74, 2876-2888.	0.2	53
41	Cadmium-binding properties of glutathione: A chemometrical analysis of voltammetric data. Journal of Inorganic Biochemistry, 1997, 66, 29-36.	1.5	77
42	Electrochemical study of the binding properties of a metallothionein I related peptide with cadmium or/and zinc. Electroanalysis, 1996, 8, 473-479.	1.5	25
43	Application of Multivariate Curve Resolution to Voltammetric Data. Analytical Biochemistry, 1996, 240, 134-141.	1.1	74
44	The electrochemical behaviour of Cd,Zn thioneins depending on the solution pH using differential pulse polarography. Analytica Chimica Acta, 1995, 305, 285-294.	2.6	32
45	Electrochemical behavior of metallothioneins and related molecules. Part I: Lys-Cys-Thr-Cys-Cys-Ala thionein fragment [56-61] MT I. Electroanalysis, 1995, 7, 663-669.	1.5	33
46	Transferrin-Binding Capacity by Rat Bone Marrow Populations Containing Different Proportions of Erythroid Cells. Biological Chemistry Hoppe-Seyler, 1994, 375, 135-140.	1.4	0
47	Transferrin binding capacity as a marker of differentiation and maturation of rat erythroid cells fractionated by counter current distribution in aqueous polymer two-phase systems. Bioscience Reports, 1994, 14, 119-130.	1.1	0
48	[33] Charge-directed affinity partitioning of cells. Methods in Enzymology, 1994, 228, 363-368.	0.4	0
49	Fractionation of erytroblasts with affinitymediated modifications of their electrical properties using counter-current distribution. Molecular and Cellular Biochemistry, 1993, 121, 93-98.	1.4	0
50	Rat bone marrow erythroid cell fractionation by counter current distribution in non-charge-sensitive two-phase systems. Bioscience Reports, 1992, 12, 77-85.	1.1	1
51	Ligand-receptor interactions in affinity cell partitioning. Journal of Chromatography A, 1992, 594, 97-103.	1.8	11
52	Affinity-mediated modification of electrical charge on a cell surface: A new approach to the affinity partitioning of biological particles. Analytical Biochemistry, 1992, 200, 280-285.	1.1	5
53	Analysis by partitioning in aqueous two-phase systems of the loss of transferrin-binding capacity during maturation of rat reticulocytes. Bioscience Reports, 1989, 9, 541-548.	1.1	10