Luis A Montero

List of Publications by Year in Descending Order

72 papers	815 citations	17 h-index	24 g-index
74 ext. papers	890 ext. citations	3.5 avg, IF	3.64 L-index

#	Paper	IF	Citations
72	RCDPeaks: Memory-Efficient Density Peaks Clustering of Long Molecular Dynamics.. *Bioinformatics*, **2022**,	7.2	1
71	Prediction of molecular interactions and physicochemical properties relevant for vasopressin V2 receptor antagonism.. *Journal of Molecular Modeling*, **2022**, 28, 31	2	0
70	MCSS-Based Predictions of Binding Mode and Selectivity of Nucleotide Ligands. *Journal of Chemical Theory and Computation*, **2021**, 17, 2599-2618	6.4	1
69	BitQT: A Graph-Based Approach to the Quality Threshold Clustering of Molecular Dynamics. *Bioinformatics*, **2021**,	7.2	1
68	Theoretical Evaluation of the Molecular Inclusion Process between Chlordecone and Cyclodextrins: A New Method for Mitigating the Basis Set Superposition Error in the Case of an Implicit Solvation Model. *Journal of Chemical Information and Modeling*, **2020**, 60, 2115-2125	6.1	2
67	BitClust: Fast Geometrical Clustering of Long Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2020**, 60, 444-448	6.1	10
66	Role of Augmented Basis Sets and Quest for ab Initio Performance/Cost Alternative to Kohn-Sham Density Functional Theory. *Journal of Physical Chemistry A*, **2020**, 124, 126-134	2.8	5
65	In silico strategy for detailing the binding modes of a novel family of peptides proven as ghrelin receptor agonists. *Journal of Molecular Modeling*, **2020**, 26, 294	2	1
64	A computational strategy to understand structure-activity relationship of 1,3-disubstituted imidazole [1,5-▯pyrazine derivatives described as ATP competitive inhibitors of the IGF-1 receptor related to Ewing sarcoma. *Journal of Molecular Modeling*, **2020**, 26, 222	2	1
63	Quality Threshold Clustering of Molecular Dynamics: A Word of Caution. *Journal of Chemical Information and Modeling*, **2020**, 60, 467-472	6.1	12
62	Understanding the disrupting mechanism of the Tau aggregation motif " VQIVYK " by phenylthiazolyl-hydrazides inhibitors. *Journal of Molecular Recognition*, **2020**, 33, e2848	2.6	2
61	Kinetics of the condensation reaction of urea and furfural in a heterogeneous phase leading to difurfurylidenetriurea: A calorimetric study. *Thermochimica Acta*, **2019**, 672, 79-85	2.9	
60	Assessing How Correlated Molecular Orbital Calculations Can Perform versus Kohn-Sham DFT: Barrier Heights/Isomerizations. *Chemistry - A European Journal*, **2017**, 23, 9122-9129	4.8	11
59	Conceptual DFT analysis of the regioselectivity of 1,3-dipolar cycloadditions: nitrones as a case of study. *Journal of Molecular Modeling*, **2017**, 23, 236	2	10
58	Geometrical distortions and charge transfer in munchn▯e regio-selectivity: A conceptual density functional study. *International Journal of Quantum Chemistry*, **2017**, 117, e25444	2.1	3
57	Similarity measures between excited singlet and triplet electron densities in linear acenes: an application to singlet fission. *Molecular Physics*, **2016**, 114, 3650-3657	1.7	0
56	Integrating sampling techniques and inverse virtual screening: toward the discovery of artificial peptide-based receptors for ligands. *Molecular Diversity*, **2016**, 20, 421-38	3.1	3

55	Pyrrolyl-Silicon Compounds as Precursors for Donor-Acceptor Systems Stabilized by Noncovalent Interactions. *Journal of Physical Chemistry A*, **2015**, 119, 7038-51	2.8	5
54	Integration of ligand and structure-based virtual screening for identification of leading anabolic steroids. *Journal of Steroid Biochemistry and Molecular Biology*, **2013**, 138, 348-58	5.1	3
53	Electron density deformations provide new insights into the spectral shift of rhodopsins. *Journal of Computational Chemistry*, **2013**, 34, 2460-71	3.5	5
52	Anabolic and androgenic activities of 19-nor-testosterone steroids: QSAR study using quantum and physicochemical molecular descriptors. *Journal of Steroid Biochemistry and Molecular Biology*, **2011**, 126, 35-45	5.1	6
51	Coulomb and Exchange contributions to electronic excitations of benzene aggregates. *Chemical Physics Letters*, **2011**, 502, 271-276	2.5	3
50	Influence of diosgenin structure on the polymerization kinetics of acrylamide: An experimental and theoretical approach. *Journal of Molecular Structure*, **2011**, 985, 34-47	3.4	2
49	A DFT periodic study on the interaction between O2 and cation exchanged chabazite MCHA (M = H+, Na+ or Cu+): effects in the triplet-singlet energy gap. *Physical Chemistry Chemical Physics*, **2010**, 12, 442-52	3.6	16
48	Quantum relativistic investigation about the coordination and bonding effects of different ligands on uranyl complexes. *Polyhedron*, **2010**, 29, 975-984	2.7	17
47	Interaction of brassinolide with essential amino acid residues: a theoretical approach. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 604-11	2.8	2
46	Molecular orbital model of the influence of interaction between O2 and aluminosilicate sites on the triplet-singlet energy gap and reactivity. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 746-54	2.8	2
45	Zur Lichtabsorption und Aeichromic vinyloger Furfurole. *Zeitschrift F Chemie*, **2010**, 17, 266-267		1
44	Multiple minima hypersurfaces studies of aluminosilicate hydration. *International Journal of Quantum Chemistry*, **2010**, 110, 586-594	2.1	2
43	Theoretical study of imidazole...NO complexes. *Journal of Physical Chemistry A*, **2009**, 113, 14595-605	2.8	2
42	A theoretical approach to the solvation of brassinosteroids. *Journal of Molecular Graphics and Modelling*, **2009**, 27, 600-10	2.8	6
41	MMH-2 as a new approach for the prediction of intermolecular interactions: the crystal packing of acetamide. *CrystEngComm*, **2009**, 11, 2358	3.3	7
40	An approach to hydration of model silica materials by exploring their multiple minima hypersurfaces. The role of entropy of association. *Journal of Physical Chemistry A*, **2008**, 112, 2880-7	2.8	12
39	Ab initio and matrix isolation study of the acetylenefuran dimer. *Chemical Physics*, **2008**, 343, 168-185	2.3	27
38	DFT modelling of cobalt and nickel complexes with dithiophosphinic acid. *Computational and Theoretical Chemistry*, **2008**, 859, 93-97		9

37	Quantum mechanical model for Maya Blue. *International Journal of Quantum Chemistry*, **2008**, 108, 1664-1673	1.6	26
36	In silico study of the human rhodopsin and meta rhodopsin II/S-arrestin complexes: impact of single point mutations related to retina degenerative diseases. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 1133-41	4.2	6
35	Applying pattern recognition methods plus quantum and physico-chemical molecular descriptors to analyze the anabolic activity of structurally diverse steroids. *Journal of Computational Chemistry*, **2008**, 29, 317-33	3.5	17
34	Chemometric and chemoinformatic analyses of anabolic and androgenic activities of testosterone and dihydrotestosterone analogues. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 6448-59	3.4	11
33	Interactions between simple radicals and water. *Chemical Physics*, **2008**, 353, 193-201	2.3	25
32	DFT analysis of rotational barriers, 1H and 13C NMR chemical shifts in neutral and protonated furfurylidenanilines. *Computational and Theoretical Chemistry*, **2008**, 852, 78-82		3
31	Theoretical study of m-dansylaminophenylboronic acid and their species: A sugar chemosensor. *Computational and Theoretical Chemistry*, **2008**, 852, 71-77		2
30	Validation of performances of some semiempirical Hamiltonians for predicting molecular structure calculation of natural brassinosteroids: Towards understanding their biological activity by electron exchange effects. *Computational and Theoretical Chemistry*, **2007**, 819, 109-120		7
29	Theoretical affinity order among flavonoids and amino acid residues: An approach to understand flavonoid–protein interactions. *Computational and Theoretical Chemistry*, **2007**, 819, 121-129		11
28	Exploring the potential energy surfaces of association of NO with aminoacids and related organic functional groups: the role of entropy of association. *Theoretical Chemistry Accounts*, **2007**, 118, 649-663	1.9	11
27	Computational biology in Cuba: an opportunity to promote science in a developing country. *PLoS Computational Biology*, **2007**, 3, e227	5	6
26	CNDOL: A fast and reliable method for the calculation of electronic properties of very large systems. Applications to retinal binding pocket in rhodopsin and gas phase porphine. *Journal of Chemical Physics*, **2007**, 127, 145102	3.9	17
25	Furan-formic acid dimers: an ab initio and matrix isolation study. *Journal of Physical Chemistry A*, **2006**, 110, 13775-85	2.8	18
24	Computational study of noncovalent complexes between formamide and formic acid. *Journal of Physical Chemistry A*, **2006**, 110, 12613-22	2.8	21
23	Excited state acidity of bifunctional compounds: 9. Excited state intramolecular proton transfer in 3,5-dihydroxy-7,4?-dimethoxyflavone and 3,5-dihydroxy-7,4?-dimethoxyflavanone: spectral and fluorescence decay results. *Journal of Photochemistry and Photobiology A: Chemistry*, **2006**, 181, 370-377	4.7	5
22	Structure–activity analysis on ecdysteroids: A structural and quantum chemical approach based on two biological systems. *Computational and Theoretical Chemistry*, **2006**, 758, 263-274		8
21	Bonding and solvation preferences of nickel complexes [Ni(S2PR2)2] (R=H, Me, OMe) according a natural bond orbital analysis. *Computational and Theoretical Chemistry*, **2006**, 767, 37-41		12
20	Ab initio modelling of crosslinking in polymers. A case of chains with furan rings. *Computational and Theoretical Chemistry*, **2006**, 770, 99-106		17

19	Effect of the Si/Al distribution on the UV–vis spectrum of propene–zeolite system. A theoretical approach. *Computational and Theoretical Chemistry*, **2006**, 769, 77-82		1
18	A combined experimental and quantum chemical study on the putative protonophoric activity of thiocyanate. *Biophysical Journal*, **2005**, 89, 1504-15	2.9	9
17	MO-calculations on the solvation effects on the structure of natural flavonoids in aqueous and acetone phases. *Computational and Theoretical Chemistry*, **2005**, 715, 227-239		10
16	Noncovalent complexes between dimethyl ether and formic acid--an ab initio and matrix isolation study. *ChemPhysChem*, **2005**, 6, 618-24	3.2	20
15	A novel in-silico approach for QSAR Studies of Anabolic and Androgenic Activities in the 17β-hydroxy-5α-androstane Steroid Family. *QSAR and Combinatorial Science*, **2005**, 24, 218-226		21
14	Essential amino acids interacting with flavonoids: A theoretical approach. *International Journal of Quantum Chemistry*, **2005**, 103, 82-104	2.1	20
13	Patterns of retinal light absorption related to retinitis pigmentosa mutants from in silico model structures of rhodopsin. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 392-9	4.2	14
12	Theoretical model of internal rotation in monosubstituted derivatives of furfural. *Journal of Computational Chemistry*, **2004**, 25, 429-38	3.5	8
11	1:2 Formic Acid/Acetylene Complexes: Ab Initio and Matrix Isolation Studies of Weakly Interacting Systems. *Journal of Physical Chemistry A*, **2004**, 108, 11846-11854	2.8	26
10	Theoretical study of flavonoids and proline interactions. Aqueous and gas phases. *Computational and Theoretical Chemistry*, **2003**, 623, 63-73		24
9	UV–vis spectrum of simple hydrocarbons in a zeolite cavity. A supramolecular charge transfer. *Chemical Physics Letters*, **2002**, 364, 176-179	2.5	8
8	OH hydrogen abstraction reactions from alanine and glycine: A quantum mechanical approach. *Journal of Computational Chemistry*, **2001**, 22, 1138-1153	3.5	55
7	Multiple minima hypersurfaces of water clusters for calculations of association energy. *International Journal of Quantum Chemistry*, **2000**, 79, 8-16	2.1	48
6	Clinoptilolite–heulandite polymorphism: structural features from computer simulation. *Physical Chemistry Chemical Physics*, **2000**, 2, 1803-1813	3.6	22
5	Silicon–aluminium distribution in dehydrated calcium heulandite. *Physical Chemistry Chemical Physics*, **1999**, 1, 1679-1685	3.6	18
4	A Theoretical Approach to Analytical Properties of 2,4-Diamino-5-phenylthiazole in Water Solution. Tautomerism and Dependence on pH. *Journal of the American Chemical Society*, **1998**, 120, 12023-12033	16.4	63
3	Theoretical approach to cationic polymerization of alkenylfurans. II. Ab initio and semiempirical study of relevant steps in the reaction mechanism. *Journal of Polymer Science Part A*, **1992**, 30, 2497-2502	2.5	
2	The site of radical attack at the furan ring from MNDO calculations. *Die Makromolekulare Chemie Theory and Simulations*, **1992**, 1, 99-103		5

1 From PPP-MO theory to all-valence electron calculations of ionic and excited states in organic molecules. *International Journal of Quantum Chemistry*, **1990**, 37, 465-483 2.1 22