Julian Tirado-Rives

List of Publications by Year in Descending Order

93 papers	24,656 citations	46 h-index	95 g-index
95 ext. papers	27,688 ext. citations	6.7 avg, IF	7.02 L-index

#	Paper	IF	Citations
93	Potent Noncovalent Inhibitors of the Main Protease of SARS-CoV-2 from Molecular Sculpting of the Drug Perampanel Guided by Free Energy Perturbation Calculations. *ACS Central Science*, **2021**, 7, 467-475	16.8	70
92	Optimization of Triarylpyridinone Inhibitors of the Main Protease of SARS-CoV-2 to Low-Nanomolar Antiviral Potency. *ACS Medicinal Chemistry Letters*, **2021**, 12, 1325-1332	4.3	7
91	Metadynamics as a Postprocessing Method for Virtual Screening with Application to the Pseudokinase Domain of JAK2. *Journal of Chemical Information and Modeling*, **2020**, 60, 4403-4415	6.1	2
90	Identification of 14 Known Drugs as Inhibitors of the Main Protease of SARS-CoV-2 **2020**,		11
89	Explicit Representation of Cation-Interactions in Force Fields with 1/ Nonbonded Terms. *Journal of Chemical Theory and Computation*, **2020**, 16, 7184-7194	6.4	12
88	Identification of 14 Known Drugs as Inhibitors of the Main Protease of SARS-CoV-2. *ACS Medicinal Chemistry Letters*, **2020**, 11, 2526-2533	4.3	98
87	Absolute Free Energy of Binding Calculations for Macrophage Migration Inhibitory Factor in Complex with a Druglike Inhibitor. *Journal of Physical Chemistry B*, **2019**, 123, 8675-8685	3.4	10
86	QM/MM Calculations for the Cl + CHCl S2 Reaction in Water Using CM5 Charges and Density Functional Theory. *Journal of Physical Chemistry A*, **2019**, 123, 5713-5717	2.8	6
85	Robust Free Energy Perturbation Protocols for Creating Molecules in Solution. *Journal of Chemical Theory and Computation*, **2019**, 15, 3941-3948	6.4	9
84	Development and Testing of the OPLS-AA/M Force Field for RNA. *Journal of Chemical Theory and Computation*, **2019**, 15, 2734-2742	6.4	26
83	Unbinding Dynamics of Non-Nucleoside Inhibitors from HIV-1 Reverse Transcriptase. *Journal of Physical Chemistry B*, **2019**, 123, 1741-1748	3.4	13
82	Enhanced Monte Carlo Methods for Modeling Proteins Including Computation of Absolute Free Energies of Binding. *Journal of Chemical Theory and Computation*, **2018**, 14, 3279-3288	6.4	20
81	Molecular Dynamics Simulations of a Conformationally Mobile Peptide-Based Catalyst for Atroposelective Bromination. *ACS Catalysis*, **2018**, 8, 9968-9979	13.1	21
80	Improved Treatment of Nucleosides and Nucleotides in the OPLS-AA Force Field. *Chemical Physics Letters*, **2017**, 683, 276-280	2.5	13
79	1.14*CM1A-LBCC: Localized Bond-Charge Corrected CM1A Charges for Condensed-Phase Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 3864-3870	3.4	185
78	LigParGen web server: an automatic OPLS-AA parameter generator for organic ligands. *Nucleic Acids Research*, **2017**, 45, W331-W336	20.1	366
77	Improved Description of Sulfur Charge Anisotropy in OPLS Force Fields: Model Development and Parameterization. *Journal of Physical Chemistry B*, **2017**, 121, 6626-6636	3.4	18

76	Adding a Hydrogen Bond May Not Help: Naphthyridinone vs Quinoline Inhibitors of Macrophage Migration Inhibitory Factor. *ACS Medicinal Chemistry Letters*, **2017**, 8, 1287-1291	4.3	8
75	Performance of Protein-Ligand Force Fields for the Flavodoxin-Flavin Mononucleotide System. *Journal of Physical Chemistry Letters*, **2016**, 7, 3032-6	6.4	12
74	Hydration Properties and Solvent Effects for All-Atom Solutes in Polarizable Coarse-Grained Water. *Journal of Physical Chemistry B*, **2016**, 120, 8102-14	3.4	7
73	Biomolecular Force Field Parameterization via Atoms-in-Molecule Electron Density Partitioning. *Journal of Chemical Theory and Computation*, **2016**, 12, 2312-23	6.4	82
72	Determination of partial molar volumes from free energy perturbation theory. *Physical Chemistry Chemical Physics*, **2015**, 17, 8407-15	3.6	14
71	Molecular dynamics and Monte Carlo simulations for protein-ligand binding and inhibitor design. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 966-971	4	30
70	Application of a BOSS-Gaussian interface for QM/MM simulations of Henry and methyl transfer reactions. *Journal of Computational Chemistry*, **2015**, 36, 2064-74	3.5	11
69	Improved Peptide and Protein Torsional Energetics with the OPLSAA Force Field. *Journal of Chemical Theory and Computation*, **2015**, 11, 3499-509	6.4	391
68	Enhanced Monte Carlo Sampling through Replica Exchange with Solute Tempering. *Journal of Chemical Theory and Computation*, **2014**, 10, 565-571	6.4	32
67	Evaluation of CM5 Charges for Condensed-Phase Modeling. *Journal of Chemical Theory and Computation*, **2014**, 10, 2802-2812	6.4	44
66	Optimization of benzyloxazoles as non-nucleoside inhibitors of HIV-1 reverse transcriptase to enhance Y181C potency. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 1110-3	2.9	16
65	Bifunctional inhibition of human immunodeficiency virus type 1 reverse transcriptase: mechanism and proof-of-concept as a novel therapeutic design strategy. *Journal of Medicinal Chemistry*, **2013**, 56, 3959-68	8.3	21
64	Characterization of biaryl torsional energetics and its treatment in OPLS all-atom force fields. *Journal of Chemical Information and Modeling*, **2013**, 53, 1191-9	6.1	70
63	Virtual screening and optimization yield low-nanomolar inhibitors of the tautomerase activity of Plasmodium falciparum macrophage migration inhibitory factor. *Journal of Medicinal Chemistry*, **2012**, 55, 10148-59	8.3	30
62	Methyl effects on protein-ligand binding. *Journal of Medicinal Chemistry*, **2012**, 55, 4489-500	8.3	252
61	Improving MM-GB/SA Scoring through the Application of the Variable Dielectric Model. *Journal of Chemical Theory and Computation*, **2011**, 7, 3859-3865	6.4	29
60	Effects of Water Placement on Predictions of Binding Affinities for p38 MAP Kinase Inhibitors. *Journal of Chemical Theory and Computation*, **2010**, 6, 3850-3856	6.4	73
59	Synthesis and evaluation of selected key methyl ether derivatives of vancomycin aglycon. *Journal of Medicinal Chemistry*, **2010**, 53, 7229-35	8.3	17

58	Quantum mechanical/molecular mechanical modeling finds Diels-Alder reactions are accelerated less on the surface of water than in water. *Journal of the American Chemical Society*, **2010**, 132, 3097-104	16.4	50
57	Vancomycin analogs: Seeking improved binding of d-Ala-d-Ala and d-Ala-d-Lac peptides by side-chain and backbone modifications. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 5874-86	3.4	13
56	Vancomycin resistance: modeling backbone variants with D-Ala-D-Ala and D-Ala-D-Lac peptides. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 1236-9	2.9	13
55	Discovery of wild-type and Y181C mutant non-nucleoside HIV-1 reverse transcriptase inhibitors using virtual screening with multiple protein structures. *Journal of Chemical Information and Modeling*, **2009**, 49, 1272-9	6.1	37
54	Exploiting structural analysis, in silico screening, and serendipity to identify novel inhibitors of drug-resistant falciparum malaria. *ACS Chemical Biology*, **2009**, 4, 29-40	4.9	48
53	In Silico Improvement of beta3-peptide inhibitors of p53 x hDM2 and p53 x hDMX. *Journal of the American Chemical Society*, **2009**, 131, 6356-7	16.4	62
52	Energetics of displacing water molecules from protein binding sites: consequences for ligand optimization. *Journal of the American Chemical Society*, **2009**, 131, 15403-11	16.4	196
51	Prediction of the water content in protein binding sites. *Journal of Physical Chemistry B*, **2009**, 113, 13337-46	3.4	153
50	Optimization of azoles as anti-human immunodeficiency virus agents guided by free-energy calculations. *Journal of the American Chemical Society*, **2008**, 130, 9492-9	16.4	84
49	Pre-steady-state kinetic studies establish entecavir 5′-triphosphate as a substrate for HIV-1 reverse transcriptase. *Journal of Biological Chemistry*, **2008**, 283, 5452-9	5.4	34
48	Energetic effects for observed and unobserved HIV-1 reverse transcriptase mutations of residues L100, V106, and Y181 in the presence of nevirapine and efavirenz. *Bioorganic and Medicinal Chemistry Letters*, **2008**, 18, 969-72	2.9	6
47	Performance of B3LYP Density Functional Methods for a Large Set of Organic Molecules. *Journal of Chemical Theory and Computation*, **2008**, 4, 297-306	6.4	601
46	Search for non-nucleoside inhibitors of HIV-1 reverse transcriptase using chemical similarity, molecular docking, and MM-GB/SA scoring. *Journal of Chemical Information and Modeling*, **2007**, 47, 2416-28	6.1	61
45	The structures of antibiotics bound to the E site region of the 50 S ribosomal subunit of Haloarcula marismortui: 13-deoxytedanolide and girodazole. *Journal of Molecular Biology*, **2007**, 367, 1471-9	6.5	41
44	Computer-aided design of non-nucleoside inhibitors of HIV-1 reverse transcriptase. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 663-7	2.9	107
43	Comparison of SCC-DFTB and NDDO-based semiempirical molecular orbital methods for organic molecules. *Journal of Physical Chemistry A*, **2006**, 110, 13551-9	2.8	127
42	Contribution of conformer focusing to the uncertainty in predicting free energies for protein-ligand binding. *Journal of Medicinal Chemistry*, **2006**, 49, 5880-4	8.3	210
41	Relationship between side chain structure and 14-helix stability of beta3-peptides in water. *Journal of the American Chemical Society*, **2005**, 127, 167-78	16.4	88

40	Potential energy functions for atomic-level simulations of water and organic and biomolecular systems. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6665-70	11.5	770
39	Molecular modeling of organic and biomolecular systems using BOSS and MCPRO. *Journal of Computational Chemistry*, **2005**, 26, 1689-700	3.5	324
38	Structural and energetic analyses of the effects of the K103N mutation of HIV-1 reverse transcriptase on efavirenz analogues. *Journal of Medicinal Chemistry*, **2004**, 47, 2389-92	8.3	36
37	Free Energies of Hydration from a Generalized Born Model and an All-Atom Force Field. *Journal of Physical Chemistry B*, **2004**, 108, 16264-16270	3.4	164
36	Activity predictions for efavirenz analogues with the K103N mutant of HIV reverse transcriptase. *Bioorganic and Medicinal Chemistry Letters*, **2003**, 13, 3337-40	2.9	29
35	Validation of a model for the complex of HIV-1 reverse transcriptase with nonnucleoside inhibitor TMC125. *Journal of the American Chemical Society*, **2003**, 125, 6016-7	16.4	66
34	Contributions of conformational compression and preferential transition state stabilization to the rate enhancement by chorismate mutase. *Journal of the American Chemical Society*, **2003**, 125, 6892-9	16.4	69
33	Investigation of solvent effects for the Claisen rearrangement of chorismate to prephenate: mechanistic interpretation via near attack conformations. *Journal of the American Chemical Society*, **2003**, 125, 6663-72	16.4	46
32	Molecular modeling calculations of HIV-1 reverse transcriptase nonnucleoside inhibitors: correlation of binding energy with biological activity for novel 2-aryl-substituted benzimidazole analogues. *Journal of Medicinal Chemistry*, **2003**, 46, 1940-7	8.3	39
31	Prediction of activity for nonnucleoside inhibitors with HIV-1 reverse transcriptase based on Monte Carlo simulations. *Journal of Medicinal Chemistry*, **2002**, 45, 2970-87	8.3	82
30	Antiviral drug design: computational analyses of the effects of the L100I mutation for HIV-RT on the binding of NNRTIs. *Bioorganic and Medicinal Chemistry Letters*, **2001**, 11, 2799-802	2.9	45
29	Estimation of binding affinities for HEPT and nevirapine analogues with HIV-1 reverse transcriptase via Monte Carlo simulations. *Journal of Medicinal Chemistry*, **2001**, 44, 145-54	8.3	94
28	Evaluation and Reparametrization of the OPLS-AA Force Field for Proteins via Comparison with Accurate Quantum Chemical Calculations on Peptides *Journal of Physical Chemistry B*, **2001**, 105, 6474-6487	3.4	2979
27	Monte Carlo calculations on HIV-1 reverse transcriptase complexed with the non-nucleoside inhibitor 8-Cl TIBO: contribution of the L100I and Y181C variants to protein stability and biological activity. *Protein Engineering, Design and Selection*, **2000**, 13, 413-21	1.9	24
26	Validation of a Model for the Complex of HIV-1 Reverse Transcriptase with Sustiva through Computation of Resistance Profiles. *Journal of the American Chemical Society*, **2000**, 122, 12898-12900	16.4	52
25	Estimation of the binding affinities of FKBP12 inhibitors using a linear response method. *Bioorganic and Medicinal Chemistry*, **1999**, 7, 851-60	3.4	73
24	Computational Studies of Molecular Recognition from Alkane Dimers to Protein-Ligand Complexes **1999**, 113-125		1
23	Prediction of binding affinities for TIBO inhibitors of HIV-1 reverse transcriptase using Monte Carlo simulations in a linear response method. *Journal of Medicinal Chemistry*, **1998**, 41, 5272-86	8.3	83

22	Molecular dynamics simulations of the unfolding of barnase in water and 8 M aqueous urea. *Biochemistry*, **1997**, 36, 7313-29	3.2	162
21	Monte Carlo Simulations for Proteins: Binding Affinities for Trypsin−Benzamidine Complexes via Free-Energy Perturbations. *Journal of Physical Chemistry B*, **1997**, 101, 9663-9669	3.4	83
20	OPLS all-atom force field for carbohydrates. *Journal of Computational Chemistry*, **1997**, 18, 1955-1970	3.5	535
19	Approaches to Protein-Ligand Binding from Computer Simulations **1997**, 21-34		0
18	Viability of molecular modeling with pentium-based PCs. *Journal of Computational Chemistry*, **1996**, 17, 1385-6	3.5	18
17	Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids. *Journal of the American Chemical Society*, **1996**, 118, 11225-11236	16.4	9849
16	Monte Carlo vs Molecular Dynamics for Conformational Sampling. *The Journal of Physical Chemistry*, **1996**, 100, 14508-14513		119
15	A comprehensive study of the rotational energy profiles of organic systems by ab initio MO theory, forming a basis for peptide torsional parameters. *Journal of Computational Chemistry*, **1995**, 16, 984-1010	3.5	69
14	Free energies of hydration for organic molecules from Monte Carlo simulations. *Journal of Computer - Aided Molecular Design*, **1995**, 3, 123-138		35
13	Molecular dynamics simulations of the unfolding of apomyoglobin in water. *Biochemistry*, **1993**, 32, 4175-84	3.2	118
12	Mechanism for the rotamase activity of FK506 binding protein from molecular dynamics simulations. *Biochemistry*, **1993**, 32, 12864-74	3.2	42
11	Molecular dynamics and Monte Carlo simulations favor the .alpha.-helical form for alanine-based peptides in water. *Journal of the American Chemical Society*, **1993**, 115, 11590-11593	16.4	96
10	Monte Carlo simulations of pure liquid substituted benzenes with OPLS potential functions. *Journal of Computational Chemistry*, **1993**, 14, 206-215	3.5	145
9	Molecular dynamics simulations of the unfolding of an alpha-helical analogue of ribonuclease A S-peptide in water. *Biochemistry*, **1991**, 30, 3864-71	3.2	207
8	Molecular dynamics of proteins with the OPLS potential functions. Simulation of the third domain of silver pheasant ovomucoid in water. *Journal of the American Chemical Society*, **1990**, 112, 2773-2781	16.4	88
7	The OPLS [optimized potentials for liquid simulations] potential functions for proteins, energy minimizations for crystals of cyclic peptides and crambin. *Journal of the American Chemical Society*, **1988**, 110, 1657-66	16.4	3825
6	A CONVENIENT SYNTHESIS OF 10, 10?-DIMETHYL-9, 9?-BIACRIDYLIDENE. *Organic Preparations and Procedures International*, **1988**, 20, 295-298	1.1	4
5	Efficient computation of absolute free energies of binding by computer simulations. Application to the methane dimer in water. *Journal of Chemical Physics*, **1988**, 89, 3742-3746	3.9	269

4	Crystal structures of isomeric (2,6-dioxacyclohexyl)phenols: models for preassociation complexes in acid-catalyzed solvolysis of acetals. *Journal of Organic Chemistry*, **1986**, 51, 1987-1991	4.2	6
3	ONE-STEP PREPARATIONS OF ISOMERIC (2,6-DIOXACYCLOHEXYL)PHENOLS. *Organic Preparations and Procedures International*, **1985**, 17, 62-64	1.1	1
2	Synthesis and structures of stilbene cycles. 2. Low-valent titanium-induced ring closures of aromatic bis(carbonyls). *Journal of Organic Chemistry*, **1984**, 49, 1627-1634	4.2	30
1	Synthesis and structure of stilbene crowns.. *Tetrahedron Letters*, **1982**, 23, 1639-1642	2	18