Carlos A Montanari

List of Publications by Year
in descending order

122 papers	2,027 citations	218381 26 h-index	329751 37 g-index
130 all docs	130 docs citations	130 times ranked	2542 citing authors

#	Article	IF	Citations
1	CÃ¢ncer e agentes antineoplÃ¡sicos ciclo-celular especÃficos e ciclo-celular nÃ£o especÃficos que interagem com o DNA: uma introduÃ§Ã£o. Quimica Nova, 2005, 28, 118-129.	0.3	87
2	Inflation of correlation in the pursuit of drug-likeness. Journal of Computer-Aided Molecular Design, 2013, 27, 1-13.	1.3	72
3	Hologram QSAR model for the prediction of human oral bioavailability. Bioorganic and Medicinal Chemistry, 2007, 15, 7738-7745.	1.4	71
4	Discovery of novel Trypanosoma cruzi glyceraldehyde-3-phosphate dehydrogenase inhibitors. Bioorganic and Medicinal Chemistry, 2009, 17, 2476-2482.	1.4	67
5	Non-peptidic Cruzain Inhibitors with Trypanocidal Activity Discovered by Virtual Screening and In Vitro Assay. PLoS Neglected Tropical Diseases, 2013, 7, e2370.	1.3	63
6	Ligand efficiency metrics considered harmful. Journal of Computer-Aided Molecular Design, 2014, 28, 699-710.	1.3	54
7	Two- and three-dimensional quantitative structureâ€“activity relationships for a series of purine nucleoside phosphorylase inhibitors. Bioorganic and Medicinal Chemistry, 2006, 14, 516-527.	1.4	50
8	Molecular Design, Synthesis and Trypanocidal Activity of Dipeptidyl Nitriles as Cruzain Inhibitors. PLoS Neglected Tropical Diseases, 2015, 9, e0003916.	1.3	49
9	Hydrogen Bond Basicity Prediction for Medicinal Chemistry Design. Journal of Medicinal Chemistry, 2016, 59, 4278-4288.	2.9	48
10	Structural Basis for Selective Inhibition of Trypanosomatid Glyceraldehyde-3-Phosphate Dehydrogenase: Molecular Docking and 3D QSAR Studies. Journal of Chemical Information and Modeling, 2008, 48, 918-929.	2.5	47
11	Novel insights for dihydroorotate dehydrogenase class 1A inhibitors discovery. European Journal of Medicinal Chemistry, 2010, 45, 5899-5909.	2.6	47
12	Can Cysteine Protease Cross-Class Inhibitors Achieve Selectivity?. Journal of Medicinal Chemistry, 2019, 62, 10497-10525.	2.9	47
13	Effects of organic solvents on the enzyme activity of Trypanosoma cruzi glyceraldehyde-3-phosphate dehydrogenase in calorimetric assays. Analytical Biochemistry, 2007, 370, 107-114.	1.1	45
14	SeleÃ§Ã£o de variÃ¡veis em QSAR. Quimica Nova, 2002, 25, 439-448.	0.3	43
15	A QSERR study on enantioselective separation of enantiomeric sulphoxides. Analytica Chimica Acta, 2000, 419, 93-100.	2.6	41
16	Conformational differences between the wild type and V30M mutant transthyretin modulate its binding to genistein: Implications to tetramer stability and ligand-binding. Journal of Structural Biology, 2010, 170, 522-531.	1.3	39
17	Experimental study and computational modelling of cruzain cysteine protease inhibition by dipeptidyl nitriles. Physical Chemistry Chemical Physics, 2018, 20, 24317-24328.	1.3	38
18	3D QSAR studies on binding affinities of coumarin natural products for glycosomal GAPDH of Trypanosoma cruzi. Journal of Computer-Aided Molecular Design, 2003, 17, 277-290.	1.3	35

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19	Structure-Activity Relationships for the Design of Small-Molecule Inhibitors. Mini-Reviews in Medicinal Chemistry, 2005, 5, 585-593.	1.1	33
20	Pharmacophore Modeling for Anti-Chagas Drug Design Using the Fragment Molecular Orbital Method. PLoS ONE, 2015, 10, e0125829.	1.1	33
21	A comparative study of warheads for design of cysteine protease inhibitors. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 5031-5035.	1.0	32
22	Structureâ€“activity relationships of novel inhibitors of glyceraldehyde-3-phosphate dehydrogenase. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 2199-2204.	1.0	30
23	ClogPalk: a method for predicting alkane/water partition coefficient. Journal of Computer-Aided Molecular Design, 2013, 27, 389-402.	1.3	30
24	Planejamento racional de fÃ¡rmacos baseado em produtos naturais. Quimica Nova, 2001, 24, .	0.3	30
25	2D QSAR and similarity studies on cruzain inhibitors aimed at improving selectivity over cathepsin L. Bioorganic and Medicinal Chemistry, 2008, 16, 838-853.	1.4	28
26	Assessment of the Cruzain Cysteine Protease Reversible and Irreversible Covalent Inhibition Mechanism. Journal of Chemical Information and Modeling, 2020, 60, 1666-1677.	2.5	26
27	Anti-trypanosomal activity of non-peptidic nitrile-based cysteine protease inhibitors. PLoS Neglected Tropical Diseases, 2017, 11, e0005343.	1.3	26
28	Determination of receptor-bound drug conformations by QSAR using flexible fitting to derive a molecular similarity index. Journal of Computer-Aided Molecular Design, 1996, 10, 67-73.	1.3	24
29	HEPT derivatives as non-nucleoside inhibitors of HIV-1 reverse transcriptase: QSAR studies agree with the crystal structures. Journal of Computer-Aided Molecular Design, 2002, 16, 287-295.	1.3	24
30	Multimilligram enantioresolution of sulfoxide proton pump inhibitors by liquid chromatography on polysaccharide-based chiral stationary phase. Journal of Pharmaceutical and Biomedical Analysis, 2008, 47, 81-87.	1.4	23
31	Integration of Ligandâ€•and Targetâ€Based Virtual Screening for the Discovery of Cruzain Inhibitors. Molecular Informatics, 2011, 30, 565-578.	1.4	23
32	New Class of Antitrypanosomal Agents Based on Imidazopyridines. ACS Medicinal Chemistry Letters, 2017, 8, 766-770.	1.3	21
33	QSAR and molecular modelling studies on B-DNA recognition of minor groove binders. European Journal of Medicinal Chemistry, 2003, 38, 141-155.	2.6	20
34	In Silico Prediction of Human Plasma Protein Binding Using Hologram QSAR. Letters in Drug Design and Discovery, 2007, 4, 502-509.	0.4	20
35	Leveraging the cruzain S3 subsite to increase affinity for reversible covalent inhibitors. Bioorganic Chemistry, 2018, 79, 285-292.	2.0	20
36	The influence of hydrogen bonding on partition coefficients. Journal of Computer-Aided Molecular Design, 2017, 31, 163-181.	1.3	19

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37	Evaluating QM/MM Free Energy Surfaces for Ranking Cysteine Protease Covalent Inhibitors. Journal of Chemical Information and Modeling, 2020, 60, 880-889.	2.5	19
38	Calorimetry and structureâ€“activity relationships for a series of antimicrobial hydrazides. Thermochimica Acta, 2004, 417, 283-294.	1.2	18
39	Synthesis and structure-activity relationship of nitrile-based cruzain inhibitors incorporating a trifluoroethylamine-based P2 amide replacement. Bioorganic and Medicinal Chemistry, 2019, 27, 115083.	1.4	18
40	Structural studies on some 1,3,4-thiadiazolium-2-aminides and their rearrangement isomers using 15N and 13C NMR spectroscopy. Journal of the Chemical Society Perkin Transactions II, 1994, , 2571.	0.9	17
41	Targeting the Shc-EGFR interaction with indomethacin inhibits MAP kinase pathway signalling. Cancer Letters, 2019, 457, 86-97.	3.2	17
42	QSAR based on biological microcalorimetry. Thermochimica Acta, 1999, 328, 91-97.	1.2	16
43	Organometallic Gold(III) Complex [Au(Hdamp)(L1⁴)]⁺ (L1 = SNS-Donating) Tj ETQq1 1 0.784314 rg BT Diseases, 2019, 5, 1698-1707.	1.8	16
44	Predicting the affinity of halogenated reversible covalent inhibitors through relative binding free energy. Physical Chemistry Chemical Physics, 2019, 21, 24723-24730.	1.3	16
45	The role of molecular interaction fields on enantioselective and nonselective separation of chiral sulfoxides. Journal of Chromatography A, 2006, 1121, 64-75.	1.8	15
46	Novel Application of 2D and 3D-Similarity Searches To Identify Substrates among Cytochrome P450 2C9, 2D6, and 3A4. Journal of Chemical Information and Modeling, 2010, 50, 97-109.	2.5	15
47	Molecular design, synthesis and biological evaluation of 1,4-dihydro-4-oxoquinoline ribonucleosides as TcGAPDH inhibitors with trypanocidal activity. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 4597-4601.	1.0	15
48	A neural networks study of quinone compounds with trypanocidal activity. Journal of Molecular Modeling, 2008, 14, 975-985.	0.8	14
49	Kinetic mechanism and catalysis of Trypanosoma cruzi dihydroorotate dehydrogenase enzyme evaluated by isothermal titration calorimetry. Analytical Biochemistry, 2010, 399, 13-22.	1.1	14
50	Estimation of the RP-HPLC Lipophilicity Parameters Log K', and Log K_W, A Comparison with the Hydrophobicity Index Ï•₀. Journal of Liquid Chromatography and Related Technologies, 1997, 20, 1703-1715.	0.5	13
51	Similarity search combined with docking and molecular dynamics for novel hAChE inhibitor scaffolds. Journal of Molecular Modeling, 2018, 24, 41.	0.8	13
52	Discovery of small molecule inhibitors of Leishmania braziliensis Hsp90 chaperone. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 639-649.	2.5	13
53	QSAR Based on Biological Microcalorimetry. Journal of Medicinal Chemistry, 2000, 43, 3448-3452.	2.9	12
54	Identification of chiral selectors for improved enantioseparation based on molecular interaction fields. Analytica Chimica Acta, 2005, 545, 33-45.	2.6	12

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55	Docking and molecular dynamics simulation of quinone compounds with trypanocidal activity. Journal of Molecular Modeling, 2009, 15, 1175-1184.	0.8	12
56	Expression, purification and kinetic characterization of His-tagged glyceraldehyde-3-phosphate dehydrogenase from Trypanosoma cruzi. Protein Expression and Purification, 2011, 76, 190-196.	0.6	12
57	The Open Form Inducer Approach for Structure-Based Drug Design. PLoS ONE, 2016, 11, e0167078.	1.1	12
58	Quantitative structure-retention relationships of antimicrobial hydrazides evaluated by reverse-phase liquid chromatography. Chromatographia, 2000, 51, 722-726.	0.7	11
59	ValidaÃ§Ã£o lateral em relaÃ§Ãµes quantitativas entre estrutura e atividade farmacolÃ³gica, QSAR. Quimica Nova, 2002, 25, 231-240.	0.3	11
60	Mapping the S1 and S1â€™ subsites of cysteine proteases with new dipeptidyl nitrile inhibitors as trypanocidal agents. PLoS Neglected Tropical Diseases, 2020, 14, e0007755.	1.3	11
61	Nitrile-based peptoids as cysteine protease inhibitors. Bioorganic and Medicinal Chemistry, 2021, 41, 116211.	1.4	11
62	DETERMINATION OF PARTITION COEFFICIENTS FOR SEVERAL PROPRANOLOL ANALOGUES BY REVERSED PHASE HIGH PERFORMANCE LIQUID CHROMATOGRAPHY. Journal of Liquid Chromatography and Related Technologies, 1999, 22, 2139-2149.	0.5	10
63	Synthesis of Mesoionic 4â€(paraâ€substituted Phenylâ€5â€2,4â€dichlorophenyl)â€1,3â€4â€thiadiazoliumâ€2â€aminides by Direct Cyclization via Acylation of Thiosemicarbazides. Synthetic Communications, 2006, 36, 3359-3369.	1.1	10
64	Automated molecule editing in molecular design. Journal of Computer-Aided Molecular Design, 2013, 27, 655-664.	1.3	10
65	Integration of methods in cheminformatics and biocalorimetry for the design of trypanosomatid enzyme inhibitors. Future Medicinal Chemistry, 2014, 6, 17-33.	1.1	10
66	Quantitative structureâ€“retention relationships of flavonoids unraveled by immobilized artificial membrane chromatography. European Journal of Pharmaceutical Sciences, 2016, 88, 147-157.	1.9	10
67	Determination of Log Pappfor Drug Transfer to Microbial Cellular Systems via the Taylor-Aris Modified Diffusion Technique. QSAR and Combinatorial Science, 1998, 17, 102-108.	1.4	10
68	Predicting the Relative Binding Affinity for Reversible Covalent Inhibitors by Free Energy Perturbation Calculations. Journal of Chemical Information and Modeling, 2021, 61, 4733-4744.	2.5	9
69	Three-dimensional models of non-steroidal ligands: A comparative molecular field analysis. Steroids, 2006, 71, 417-428.	0.8	8
70	Synthesis, biochemical evaluation and molecular modeling studies of nonpeptidic nitrile-based fluorinated compounds. Future Medicinal Chemistry, 2021, 13, 25-43.	1.1	8
71	Structure Based Design, Synthesis, and Evaluation of Potential Inhibitors of Steroid Sulfatase. Current Topics in Medicinal Chemistry, 2014, 14, 1033-1044.	1.0	8
72	The Molecular Retention Mechanism in Reversed-Phase Liquid Chromatography of Meso-ionic Compounds by Quantitative Structure-Retention Relationships (QSRR). Chemistry and Biodiversity, 2005, 2, 1691-1700.	1.0	7

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73	In silico screening of HIV-1 non-nucleoside reverse transcriptase and protease inhibitors. European Journal of Medicinal Chemistry, 2008, 43, 1412-1422.	2.6	7
74	A new bianthron glycoside as inhibitor of Trypanosoma cruzi glyceraldehyde 3-phosphate dehydrogenase activity. Journal of the Brazilian Chemical Society, 2009, 20, 947-953.	0.6	7
75	On the intrinsic reactivity of highly potent trypanocidal cruzain inhibitors. RSC Medicinal Chemistry, 2020, 11, 1275-1284.	1.7	7
76	Optimization strategy of single-digit nanomolar cross-class inhibitors of mammalian and protozoa cysteine proteases. Bioorganic Chemistry, 2020, 101, 104039.	2.0	7
77	Structural, thermodynamic and functional studies of human 71ÂkDa heat shock cognate protein (HSPA8/hHsc70). Biochimica Et Biophysica Acta - Proteins and Proteomics, 2021, 1869, 140719.	1.1	7
78	Molecular Recognition of B-DNA Minor-Groove Binders: The Rigid Analogue Approach to Synthesise Antileishmaniasis Compounds: A Molecular Modeling Study. Journal of the Brazilian Chemical Society, 1998, 9, 175-180.	0.6	6
79	ON THE PARTITIONING OF SOME NEWLY SYNTHESIZED MESOIONIC 1,3,4-THIADIAZOLIUM-2-AMINIDE AND PRECURSORS EVALUATED BY RP-HPLC. Journal of Liquid Chromatography and Related Technologies, 1999, 22, 357-366.	0.5	6
80	Evaluation of the leishmanicidal and cytotoxic effects of inhibitors for microorganism metabolic pathway enzymes. Biomedicine and Pharmacotherapy, 2015, 74, 95-100.	2.5	6
81	Novel anti-prostate cancer scaffold identified by the combination of in silico and cell-based assays targeting the PI3K-AKT-mTOR pathway. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 4001-4006.	1.0	6
82	Ligand-induced conformational selection predicts the selectivity of cysteine protease inhibitors. PLoS ONE, 2019, 14, e0222055.	1.1	6
83	Crystal structure of Leishmania mexicana cysteine protease B in complex with a high-affinity azadipeptide nitrile inhibitor. Bioorganic and Medicinal Chemistry, 2020, 28, 115743.	1.4	6
84	Design, synthesis and stepwise optimization of nitrile-based inhibitors of cathepsins B and L. Bioorganic and Medicinal Chemistry, 2021, 29, 115827.	1.4	6
85	Biological Activity and Physicochemical Properties of Dipeptidyl Nitrile Derivatives Against Pancreatic Ductal Adenocarcinoma Cells. Anti-Cancer Agents in Medicinal Chemistry, 2019, 19, 112-120.	0.9	6
86	The GRID/CPCA approach in drug discovery. Expert Opinion on Drug Discovery, 2010, 5, 333-346.	2.5	5
87	3D-WHIM pattern recognition study for bisamidines. A structure-property relationship study. Journal of the Brazilian Chemical Society, 2000, 11, 393-397.	0.6	5
88	Bioactivity of a series of substituted N(3-phenyl-2-propenylidene)benzeneamines: a microcalorimetric study. International Journal of Pharmaceutics, 1992, 85, 199-202.	2.6	4
89	On Flexible Fitting Using The Molecular Similarity Index. A neural network analysis for antileishmaniasis compounds. QSAR and Combinatorial Science, 1997, 16, 480-481.	1.4	4
90	Sistemas transportadores de drogas. Quimica Nova, 1998, 21, 470-476.	0.3	4

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91	Sobre o uso de mÃ©todos quimiomÃ©tricos em quÃmica combinatÃ³ria. Quimica Nova, 2000, 23, 178-184.	0.3	4
92	Hologram Quantitative Structure-Activity Relationships for a Class of Inhibitors of HIV-1 Protease. Letters in Drug Design and Discovery, 2007, 4, 356-364.	0.4	4
93	Comparative Molecular Field Analysis of a Series of Inhibitors of HIV-1 Protease. Medicinal Chemistry, 2011, 7, 71-79.	0.7	4
94	In silico selection and cell-based characterization of selective and bioactive compounds for androgen-dependent prostate cancer cell. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 546-550.	1.0	4
95	Highly predictive hologram QSAR models of nitrile-containing cruzain inhibitors. Journal of Biomolecular Structure and Dynamics, 2017, 35, 3232-3249.	2.0	4
96	N-Sulfonyl dipeptide nitriles as inhibitors of human cathepsin S: In silico design, synthesis and biochemical characterization. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127420.	1.0	4
97	QuÃmica Medicinal: 25 anos de planejamento racional de fÃ¡rmacos. Quimica Nova, 0, 25, 39-44.	0.3	4
98	A patent review on cathepsin K inhibitors to treat osteoporosis (2011 â€“ 2021). Expert Opinion on Therapeutic Patents, 2022, 32, 561-573.	2.4	4
99	A Combined Study Using Ligandâ€Based Design, Synthesis, and Pharmacological Evaluation of Analogues of the Acetaminophen Orthoâ€Regioisomer with Potent Analgesic Activity. Chemical Biology and Drug Design, 2012, 80, 99-105.	1.5	3
100	Dipeptidyl nitrile derivatives have cytostatic effects against Leishmania spp. promastigotes. Experimental Parasitology, 2019, 200, 84-91.	0.5	3
101	Dipeptidyl nitrile derivatives suppress the Trypanosoma cruzi in vitro infection. Experimental Parasitology, 2020, 219, 108032.	0.5	3
102	A quÃmica medicinal na prÃ³xima dÃ©cada. Quimica Nova, 2000, 23, 134-137.	0.3	2
103	The role of ion pairing in the chromatographic study of propranolol analogues. Chromatographia, 2001, 53, 11-16.	0.7	2
104	Estudos de relaÃ§Ãµes estrutura-atividade quantitativas (QSAR) de bis-benzamidinas com atividade antifÃºngica. Quimica Nova, 2010, 33, 1482-1489.	0.3	2
105	Synthesis and matched molecular pair analysis of covalent reversible inhibitors of the cysteine protease CPB. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127439.	1.0	2
106	Estudos de QSAR baseados em dados de atividade biolÃ³gica obtidos por microcalorimetria: III interaÃ§Ã£o de m-alcoxifenÃ³is e p-hidroxibenzoatos de alquila com Escherichia coli. Quimica Nova, 1997, 20, 125-131.	0.3	2
107	A QSAR Study on Pneumocystis carinii Topoisomerases of bis-Benzimidazoles. QSAR and Combinatorial Science, 2000, 19, 173-175.	1.4	1
108	InteraÃ§Ã£o de compostos organossulfurados derivados do alho com o citocromo-c: um estudo eletroquÃmico. Quimica Nova, 2002, 25, 5-9.	0.3	1

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109	Um novo modelo para os sÃ±tios de interaÃ§Ã£o dos antagonistas H2, baseado na caracterizaÃ§Ã£o quÃmica dos sÃ±tios primÃ¡rio e secundÃ¡rio por QSAR- 3D. Quimica Nova, 2003, 26, 499-506.	0.3	1
110	Preparation and Chemical and Biological Studies of the Novel ComplexÂÎ¼-1,4,5-triphenyl-1,3,4-triazole-2-thiolate-bis[dichlorotriethylphosphineplatinum(II)]a. Transition Metal Chemistry, 2005, 30, 733-737.	0.7	1
111	Chemometric Characterization of Chromatographic Retention Parameters of Mesoionic 1,3,4â€¯Thiadiazoliumâ€³â€Aminides by Molecular Interaction Fields. Journal of Liquid Chromatography and Related Technologies, 2006, 29, 307-327.	0.5	1
112	Antifungal activity of triâ€•and tetraâ€‡thioureido amino derivatives against different Candida species. Mycoses, 2011, 54, e389-93.	1.8	1
113	InvestigaÃ§Ã£o eletroquÃmica e calorimÃ©trica da interaÃ§Ã£o de novos agentes antitumorais biscatiÃ´nicos com DNA. Quimica Nova, 2012, 35, 1318-1324.	0.3	1
114	Molecular design aided by random forests and synthesis of potent trypanocidal agents as cruzain inhibitors for Chagas disease treatment. Chemical Biology and Drug Design, 2020, 96, 948-960.	1.5	1
115	Estrogen Receptor: Structural Differences and Potential Implications on Selectivity Examined by the GRID/CPCA Approach. Letters in Drug Design and Discovery, 2008, 5, 182-192.	0.4	1
116	Molecular Design, Synthesis and Evaluation of 2,3-Diarylquinoxalines as Estrogen Receptor Ligands. Medicinal Chemistry, 2015, 11, 736-746.	0.7	1
117	The Effect of Dipeptidyl Nitrile Derivatives on Pancreatic Ductal Adenocarcinoma Cells In Vitro. Current Chemical Biology, 2021, 15, 278-286.	0.2	1
118	A CoMFA study on antileishmaniasis bisamidines. , 2000, , 314-315.		0
119	The history, evolution and importance of lipophilicity in medicinal chemistry: from Hippocrates and Galeno to Paracelsus and the contributions of Overton and Hansch. Revista Virtual De Quimica, 2009, 1, .	0.1	0
120	Structure Based Design of Potential Inhibitors of Steroid Sulfatase. Advances in Intelligent and Soft Computing, 2010, , 151-156.	0.2	0
121	Structure-based design of anti-trypanosomal drugs. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C294-C294.	0.3	0
122	Discovery of 2-aminopyridine Derivatives with Antichagasic and Antileishmanial Activity Using Phenotypic Assays. Letters in Drug Design and Discovery, 2020, 17, 867-872.	0.4	0