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	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
2	Design, synthesis and stepwise optimization of nitrile-based inhibitors of cathepsins B and L. Bioorganic and Medicinal Chemistry, 2021, 29, 115827.	1.4	6
3	Synthesis, biochemical evaluation and molecular modeling studies of nonpeptidic nitrile-based fluorinated compounds. Future Medicinal Chemistry, 2021, 13, 25-43.	1.1	8
4	Nitrile-based peptoids as cysteine protease inhibitors. Bioorganic and Medicinal Chemistry, 2021, 41, 116211.	1.4	11
5	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
6	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
7	The Effect of Dipeptidyl Nitrile Derivatives on Pancreatic Ductal Adenocarcinoma Cells In Vitro. Current Chemical Biology, 2021, 15, 278-286.	0.2	1
8	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
9	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
10	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
11	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
12	On the intrinsic reactivity of highly potent trypanocidal cruzain inhibitors. RSC Medicinal Chemistry, 2020, 11, 1275-1284.	1.7	7
13	Dipeptidyl nitrile derivatives suppress the Trypanosoma cruzi in vitro infection. Experimental Parasitology, 2020, 219, 108032.	0.5	3
14	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
15	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
16	Optimization strategy of single-digit nanomolar cross-class inhibitors of mammalian and protozoa cysteine proteases. Bioorganic Chemistry, 2020, 101, 104039.	2.0	7
17	Discovery of small molecule inhibitors of Leishmania braziliensis Hsp90 chaperone. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 639-649.	2.5	13
18	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

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19	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
20	Organometallic Gold(III) Complex [Au(Hdamp)(L1⁴)]⁺ (L1 = SNS-Donating) Tj ETQq0 0 0 rgBT /Overloc Diseases, 2019, 5, 1698-1707.	1.8	16
21	Can Cysteine Protease Cross-Class Inhibitors Achieve Selectivity?. Journal of Medicinal Chemistry, 2019, 62, 10497-10525.	2.9	47
22	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
23	Targeting the Shc-EGFR interaction with indomethacin inhibits MAP kinase pathway signalling. Cancer Letters, 2019, 457, 86-97.	3.2	17
24	Dipeptidyl nitrile derivatives have cytostatic effects against Leishmania spp. promastigotes. Experimental Parasitology, 2019, 200, 84-91.	0.5	3
25	Ligand-induced conformational selection predicts the selectivity of cysteine protease inhibitors. PLoS ONE, 2019, 14, e0222055.	1.1	6
26	Predicting the affinity of halogenated reversible covalent inhibitors through relative binding free energy. Physical Chemistry Chemical Physics, 2019, 21, 24723-24730.	1.3	16
27	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
28	Similarity search combined with docking and molecular dynamics for novel hAChE inhibitor scaffolds. Journal of Molecular Modeling, 2018, 24, 41.	0.8	13
29	Leveraging the cruzain S3 subsite to increase affinity for reversible covalent inhibitors. Bioorganic Chemistry, 2018, 79, 285-292.	2.0	20
30	Experimental study and computational modelling of cruzain cysteine protease inhibition by dipeptidyl nitriles. Physical Chemistry Chemical Physics, 2018, 20, 24317-24328.	1.3	38
31	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
32	The influence of hydrogen bonding on partition coefficients. Journal of Computer-Aided Molecular Design, 2017, 31, 163-181.	1.3	19
33	A comparative study of warheads for design of cysteine protease inhibitors. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 5031-5035.	1.0	32
34	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
35	New Class of Antitrypanosomal Agents Based on Imidazopyridines. ACS Medicinal Chemistry Letters, 2017, 8, 766-770.	1.3	21
36	Highly predictive hologram QSAR models of nitrile-containing cruzain inhibitors. Journal of Biomolecular Structure and Dynamics, 2017, 35, 3232-3249.	2.0	4

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37	Anti-trypanosomal activity of non-peptidic nitrile-based cysteine protease inhibitors. PLoS Neglected Tropical Diseases, 2017, 11, e0005343.	1.3	26
38	The Open Form Inducer Approach for Structure-Based Drug Design. PLoS ONE, 2016, 11, e0167078.	1.1	12
39	Hydrogen Bond Basicity Prediction for Medicinal Chemistry Design. Journal of Medicinal Chemistry, 2016, 59, 4278-4288.	2.9	48
40	Quantitative structureâ€“retention relationships of flavonoids unraveled by immobilized artificial membrane chromatography. European Journal of Pharmaceutical Sciences, 2016, 88, 147-157.	1.9	10
41	Pharmacophore Modeling for Anti-Chagas Drug Design Using the Fragment Molecular Orbital Method. PLoS ONE, 2015, 10, e0125829.	1.1	33
42	Evaluation of the leishmanicidal and cytotoxic effects of inhibitors for microorganism metabolic pathway enzymes. Biomedicine and Pharmacotherapy, 2015, 74, 95-100.	2.5	6
43	Molecular Design, Synthesis and Trypanocidal Activity of Dipeptidyl Nitriles as Cruzain Inhibitors. PLoS Neglected Tropical Diseases, 2015, 9, e0003916.	1.3	49
44	Molecular Design, Synthesis and Evaluation of 2,3-Diarylquinoxalines as Estrogen Receptor Ligands. Medicinal Chemistry, 2015, 11, 736-746.	0.7	1
45	Integration of methods in cheminformatics and biocalorimetry for the design of trypanosomatid enzyme inhibitors. Future Medicinal Chemistry, 2014, 6, 17-33.	1.1	10
46	Ligand efficiency metrics considered harmful. Journal of Computer-Aided Molecular Design, 2014, 28, 699-710.	1.3	54
47	Structure Based Design, Synthesis, and Evaluation of Potential Inhibitors of Steroid Sulfatase. Current Topics in Medicinal Chemistry, 2014, 14, 1033-1044.	1.0	8
48	ClogPalk: a method for predicting alkane/water partition coefficient. Journal of Computer-Aided Molecular Design, 2013, 27, 389-402.	1.3	30
49	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
50	Inflation of correlation in the pursuit of drug-likeness. Journal of Computer-Aided Molecular Design, 2013, 27, 1-13.	1.3	72
51	Automated molecule editing in molecular design. Journal of Computer-Aided Molecular Design, 2013, 27, 655-664.	1.3	10
52	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
53	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
54	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

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55	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
56	Antifungal activity of triâ€•and tetraâ€‘thioureido amino derivatives against different Candida species. Mycoses, 2011, 54, e389-93.	1.8	1
57	Integration of Ligandâ€•and Targetâ€Based Virtual Screening for the Discovery of Cruzain Inhibitors. Molecular Informatics, 2011, 30, 565-578.	1.4	23
58	Comparative Molecular Field Analysis of a Series of Inhibitors of HIV-1 Protease. Medicinal Chemistry, 2011, 7, 71-79.	0.7	4
59	Structure-based design of anti-trypanosomal drugs. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C294-C294.	0.3	0
60	Kinetic mechanism and catalysis of Trypanosoma cruzi dihydroorotate dehydrogenase enzyme evaluated by isothermal titration calorimetry. Analytical Biochemistry, 2010, 399, 13-22.	1.1	14
61	Novel insights for dihydroorotate dehydrogenase class 1A inhibitors discovery. European Journal of Medicinal Chemistry, 2010, 45, 5899-5909.	2.6	47
62	Estudos de relaÃ§Ãµes estrutura-atividade quantitativas (QSAR) de bis-benzamidinas com atividade antifÃºngica. Quimica Nova, 2010, 33, 1482-1489.	0.3	2
63	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
64	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
65	The GRID/CPCA approach in drug discovery. Expert Opinion on Drug Discovery, 2010, 5, 333-346.	2.5	5
66	Structure Based Design of Potential Inhibitors of Steroid Sulfatase. Advances in Intelligent and Soft Computing, 2010, , 151-156.	0.2	0
67	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
68	Docking and molecular dynamics simulation of quinone compounds with trypanocidal activity. Journal of Molecular Modeling, 2009, 15, 1175-1184.	0.8	12
69	Discovery of novel Trypanosoma cruzi glyceraldehyde-3-phosphate dehydrogenase inhibitors. Bioorganic and Medicinal Chemistry, 2009, 17, 2476-2482.	1.4	67
70	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
71	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
72	A neural networks study of quinone compounds with trypanocidal activity. Journal of Molecular Modeling, 2008, 14, 975-985.	0.8	14

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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	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
75	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
76	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
77	In Silico Prediction of Human Plasma Protein Binding Using Hologram QSAR. Letters in Drug Design and Discovery, 2007, 4, 502-509.	0.4	20
78	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
79	Hologram QSAR model for the prediction of human oral bioavailability. Bioorganic and Medicinal Chemistry, 2007, 15, 7738-7745.	1.4	71
80	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
81	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
82	Three-dimensional models of non-steroidal ligands: A comparative molecular field analysis. Steroids, 2006, 71, 417-428.	0.8	8
83	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
84	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
85	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
86	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
87	Identification of chiral selectors for improved enantioseparation based on molecular interaction fields. Analytica Chimica Acta, 2005, 545, 33-45.	2.6	12
88	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
89	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
90	Structure-Activity Relationships for the Design of Small-Molecule Inhibitors. Mini-Reviews in Medicinal Chemistry, 2005, 5, 585-593.	1.1	33

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91	Calorimetry and structureâ€“activity relationships for a series of antimicrobial hydrazides. Thermochimica Acta, 2004, 417, 283-294.	1.2	18
92	Structureâ€“activity relationships of novel inhibitors of glyceraldehyde-3-phosphate dehydrogenase. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 2199-2204.	1.0	30
93	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
94	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
95	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
96	SeleÃ§Ã£o de variÃ¡veis em QSAR. Quimica Nova, 2002, 25, 439-448.	0.3	43
97	ValidaÃ§Ã£o lateral em relaÃ§Ãµes quantitativas entre estrutura e atividade farmacolÃ³gica, QSAR. Quimica Nova, 2002, 25, 231-240.	0.3	11
98	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
99	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
100	The role of ion pairing in the chromatographic study of propranolol analogues. Chromatographia, 2001, 53, 11-16.	0.7	2
101	Planejamento racional de fÃ¡rmacos baseado em produtos naturais. Quimica Nova, 2001, 24, .	0.3	30
102	A QSERR study on enantioselective separation of enantiomeric sulphoxides. Analytica Chimica Acta, 2000, 419, 93-100.	2.6	41
103	Quantitative structure-retention relationships of antimicrobial hydrazides evaluated by reverse-phase liquid chromatography. Chromatographia, 2000, 51, 722-726.	0.7	11
104	A quÃmica medicinal na prÃ³xima dÃ©cada. Quimica Nova, 2000, 23, 134-137.	0.3	2
105	Sobre o uso de mÃ©todos quimiomÃ©tricos em quÃmica combinatÃ³ria. Quimica Nova, 2000, 23, 178-184.	0.3	4
106	A QSAR Study on Pneumocystis carinii Topoisomerases of bis-Benzimidazoles. QSAR and Combinatorial Science, 2000, 19, 173-175.	1.4	1
107	QSAR Based on Biological Microcalorimetry. Journal of Medicinal Chemistry, 2000, 43, 3448-3452.	2.9	12
108	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

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109	A CoMFA study on antileishmaniasis bisamidines. , 2000, , 314-315.		0
110	QSAR based on biological microcalorimetry. Thermochimica Acta, 1999, 328, 91-97.	1.2	16
111	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
112	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
113	Sistemas transportadores de drogas. Quimica Nova, 1998, 21, 470-476.	0.3	4
114	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
115	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
116	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
117	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
118	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
119	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
120	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
121	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
122	QuÃmica Medicinal: 25 anos de planejamento racional de fÃ¡rmacos. Quimica Nova, 0, 25, 39-44.	0.3	4