Alessandro Contini

List of Publications by Year
in descending order

94 papers	1,858 citations	236833 25 h-index	345118 36 g-index
108 all docs	108 docs citations	108 times ranked	2298 citing authors

#	Article	IF	Citations
1	In Vitro Antimalarial Activity of Inhibitors of the Human GTPase Rac1. Antimicrobial Agents and Chemotherapy, 2022, 66, AAC0149821.	1.4	4
2	Modular synthesis of 2,4-diaminoanilines as CNS drug-like non-covalent inhibitors of asparagine endopeptidase. Bioorganic and Medicinal Chemistry, 2022, 63, 116746.	1.4	1
3	Identification of a novel off-target of paroxetine: Possible role in sexual dysfunction induced by this SSRI antidepressant drug. Journal of Molecular Structure, 2022, 1268, 133690.	1.8	4
4	Copper(II)â€Catalyzed Aminohalogenation of Alkynyl Carbamates. European Journal of Organic Chemistry, 2021, 2021, 1750-1757.	1.2	16
5	Morpholino-based peptide oligomers: Synthesis and DNA binding properties. Biochemical and Biophysical Research Communications, 2021, 549, 8-13.	1.0	3
6	Three-Dimensional Proteome-Wide Scale Screening for the 5-Alpha Reductase Inhibitor Finasteride: Identification of a Novel Off-Target. Journal of Medicinal Chemistry, 2021, 64, 4553-4566.	2.9	14
7	Central residues of FSHÎ² (89â€“97) peptide are not critical for FSHR binding: Implications for peptidomimetic design. Bioorganic and Medicinal Chemistry Letters, 2021, 44, 128132.	1.0	2
8	Targeting transdifferentiated hepatic stellate cells and monitoring the hepatic fibrogenic process by means of IGF2R-specific peptides designed in silico. Journal of Materials Chemistry B, 2021, 9, 2092-2106.	2.9	2
9	Discovery of a d-pro-lys peptidomimetic inhibitor of MMP9: Addressing the gelatinase selectivity beyond S1â€² subsite. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127467.	1.0	8
10	Non-natural 3-Arylmorpholino-Î²-amino Acid as a PPII Helix Inducer. Organic Letters, 2020, 22, 6197-6202.	2.4	13
11	In Silico Drug Repurposing for SARS-CoV-2 Main Proteinase and Spike Proteins. Journal of Proteome Research, 2020, 19, 4637-4648.	1.8	50
12	Enantioselective Synthesis of cis and trans 4â€Aminopipecolic Acids as Î³â€Amino Acids for the Construction of Cyclic RGDâ€Containing Peptidomimetics Antagonists of Î±_VÎ²₃ Integrin. European Journal of Organic Chemistry, 2020, 2020, 4371-4383.	1.2	1
13	Identification and in vivo validation of a 9-mer peptide derived from FSHÎ² with FSHR antagonist activity. Peptides, 2020, 132, 170367.	1.2	10
14	Advances in the Treatment of Explicit Water Molecules in Docking and Binding Free Energy Calculations. Current Medicinal Chemistry, 2020, 26, 7598-7622.	1.2	11
15	Editorial: Folded Synthetic Peptides for Biomedical Applications. Frontiers in Chemistry, 2019, 7, 448.	1.8	2
16	Identification of the first enantiopure Rac1â€“Tiam1 proteinâ€“protein interaction inhibitor and its optimized synthesis via phosphine free remote group directed hydroarylation. MedChemComm, 2019, 10, 310-314.	3.5	4
17	Rescoring Virtual Screening Results with the MM-PBSA Methods: Beware of Internal Dielectric Constants. Journal of Chemical Information and Modeling, 2019, 59, 2714-2728.	2.5	11
18	Discovery of small molecule binders of human FSHR(TMD) with novel structural scaffolds by integrating structural bioinformatics and machine learning algorithms. Journal of Molecular Graphics and Modelling, 2019, 89, 156-166.	1.3	5

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19	Fluoro-Aryl Substituted Î±,Î²2,3-Peptides in the Development of Foldameric Antiparallel Î²-Sheets: A Conformational Study. Frontiers in Chemistry, 2019, 7, 192.	1.8	16
20	Identification of highly potent and selective MMP2 inhibitors addressing the S1â€² subsite with d-proline-based compounds. Bioorganic and Medicinal Chemistry, 2019, 27, 1891-1902.	1.4	13
21	From glucose to enantiopure morpholino Î²-amino acid: a new tool for stabilizing Î³-turns in peptides. Organic Chemistry Frontiers, 2019, 6, 972-982.	2.3	26
22	Tuning PFKFB3 Bisphosphatase Activity Through Allosteric Interference. Scientific Reports, 2019, 9, 20333.	1.6	17
23	Stereodivergent synthesis of 5-aminopipecolic acids and application in the preparation of a cyclic RGD peptidomimetic as a nanomolar Î±_VÎ²₃ integrin ligand. Organic and Biomolecular Chemistry, 2018, 16, 3402-3414.	1.5	4
24	Peptide modulators of Rac1/Tiam1 proteinâ€protein interaction: An alternative approach for cardiovascular diseases. Peptide Science, 2018, 110, e23089.	1.0	21
25	Tetrahydro-4H-(pyrrolo[3,4-d]isoxazol-3-yl)methanamine: A Bicyclic Diamino Scaffold Stabilizing Parallel Turn Conformations. Journal of Organic Chemistry, 2018, 83, 11493-11501.	1.7	17
26	An Efficient Implementation of the Nwat-MMGBSA Method to Rescore Docking Results in Medium-Throughput Virtual Screenings. Frontiers in Chemistry, 2018, 6, 43.	1.8	56
27	A tendril perversion in a helical oligomer: trapping and characterizing a mobile screw-sense reversal. Chemical Science, 2017, 8, 3007-3018.	3.7	38
28	Tandem Tetrahydroisoquinolineâ€4â€carboxylic Acid/Î²â€Alanine as a New Construct Able To Induce a Flexible Turn. Chemistry - A European Journal, 2017, 23, 10822-10831.	1.7	18
29	Synthesis and Biological Evaluation of New Natural Phenolic (2E,4E,6E)â€Octaâ€2,4,6â€trienoic Esters. Chemistry and Biodiversity, 2017, 14, e1700294.	1.0	6
30	Synthesis and conformational analysis of peptides embodying 2,3-methanopipecolic acids. Organic and Biomolecular Chemistry, 2017, 15, 6826-6836.	1.5	14
31	Pyrrolyl-silicon compounds with different alkyl spacer lengths: Synthesis, electrochemical behavior and binding properties. Synthetic Metals, 2017, 231, 127-136.	2.1	9
32	Î²-Hairpin mimics containing a piperidineâ€“pyrrolidine scaffold modulate the Î²-amyloid aggregation process preserving the monomer species. Chemical Science, 2017, 8, 1295-1302.	3.7	39
33	MOGLYNET â€“ Modulation of glycolytic flux as a new approach for treatment of atherosclerosis and plaque stabilization: a multidisciplinary study â€“ H2020. Impact, 2017, 2017, 26-28.	0.0	0
34	Evaluation of Chemical Diversity of Biotinylated Chiral 1,3â€Diamines as a Catalytic Moiety in Artificial Imine Reductase. ChemCatChem, 2016, 8, 1665-1670.	1.8	25
35	Biocatalytic Dynamic Kinetic Resolution for the Synthesis of Atropisomeric Biaryl Nâ€Oxide Lewis Base Catalysts. Angewandte Chemie - International Edition, 2016, 55, 10755-10759.	7.2	87
36	A new scaffold of topoisomerase I inhibitors: Design, synthesis and biological evaluation. European Journal of Medicinal Chemistry, 2016, 124, 326-339.	2.6	6

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37	Improved Computation of Proteinâ€“Protein Relative Binding Energies with the Nwat-MMGBSA Method. Journal of Chemical Information and Modeling, 2016, 56, 1692-1704.	2.5	59
38	Biocatalytic Dynamic Kinetic Resolution for the Synthesis of Atropisomeric Biaryl Nâ€Oxide Lewis Base Catalysts. Angewandte Chemie, 2016, 128, 10913-10917.	1.6	32
39	Ctr-1 Mets7 motif inspiring new peptide ligands for Cu(<scp>i</scp>)-catalyzed asymmetric Henry reactions under green conditions. RSC Advances, 2016, 6, 71529-71533.	1.7	21
40	An Updated Test of AMBER Force Fields and Implicit Solvent Models in Predicting the Secondary Structure of Helical, Î²-Hairpin, and Intrinsically Disordered Peptides. Journal of Chemical Theory and Computation, 2016, 12, 714-727.	2.3	38
41	Model peptides containing the 3-sulfanyl-norbornene amino acid, a conformationally constrained cysteine analogue effective inducer of 3₁₀-helix secondary structures. RSC Advances, 2015, 5, 32643-32656.	1.7	20
42	VCD spectroscopy as an excellent probe of chiral metal complexes containing a carbon monoxide vibrational chromophore. Chemical Communications, 2015, 51, 9385-9387.	2.2	10
43	1H-Azepine-2-oxo-5-amino-5-carboxylic Acid: A 3₁₀ Helix Inducer and an Effective Tool for Functionalized Gold Nanoparticles. Journal of Organic Chemistry, 2015, 80, 5507-5516.	1.7	24
44	Origin of Helical Screw Sense Selectivity Induced by Chiral Constrained CÎ±-Tetrasubstituted Î±-Amino Acids in Aib-based Peptides. Journal of Physical Chemistry B, 2015, 119, 14003-14013.	1.2	18
45	Mechanism of Stabilization of Helix Secondary Structure by Constrained CÎ±-Tetrasubstituted Î±-Amino Acids. Journal of Physical Chemistry B, 2015, 119, 1350-1361.	1.2	25
46	Molecular insights into dimerization inhibition of c-Maf transcription factor. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 2108-2115.	1.1	13
47	Asymmetric Modular Synthesis of a Semirigid Dipeptide Mimetic by Cascade Cycloaddition/Ring Rearrangement and Borohydride Reduction. Journal of Organic Chemistry, 2014, 79, 3094-3102.	1.7	26
48	2-Amino-3-(phenylsulfanyl)norbornane-2-carboxylate: An Appealing Scaffold for the Design of Rac1â€“Tiam1 Proteinâ€“Protein Interaction Inhibitors. Journal of Medicinal Chemistry, 2014, 57, 2953-2962.	2.9	31
49	Synthesis, Molecular Characterization and Preliminary Antioxidant Activity Evaluation of Quercetin Fatty Esters. JAOCS, Journal of the American Oil Chemists' Society, 2013, 90, 1751-1759.	0.8	26
50	Binding of the repressor complex RESTâ€<scp>mSIN</scp>3b by small molecules restores neuronal gene transcription in Huntington's disease models. Journal of Neurochemistry, 2013, 127, 22-35.	2.1	44
51	3-Aryl-N-aminoylsulfonylphenyl-1H-pyrazole-5-carboxamides: a new class of selective Rac inhibitors. MedChemComm, 2013, 4, 537.	3.5	26
52	Cross-talk between EGFR and T-cadherin: EGFR activation promotes T-cadherin localization to intercellular contacts. Cellular Signalling, 2013, 25, 1044-1053.	1.7	12
53	Explicit Ligand Hydration Shells Improve the Correlation between MM-PB/GBSA Binding Energies and Experimental Activities. Journal of Chemical Theory and Computation, 2013, 9, 2706-2717.	2.3	67
54	Molecular dynamic simulation of mGluR5 amino terminal domain: essential dynamics analysis captures the agonist or antagonist behaviour of ligands. Journal of Molecular Graphics and Modelling, 2013, 41, 72-78.	1.3	7

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55	Role of Small GTPase Protein Rac1 in Cardiovascular Diseases. Journal of Cardiovascular Pharmacology, 2013, 62, 425-435.	0.8	30
56	Multicomponent Synthesis of Pentyl-Sulfonyl Amidines via Diazoalkane. Synlett, 2012, 23, 1523-1525.	1.0	8
57	Molecular dynamics and tubulin polymerization kinetics study on 1,14-heterofused taxanes: evidence of stabilization of the tubulin head-to-tail dimerâ€“dimer interaction. Molecular BioSystems, 2012, 8, 3254.	2.9	13
58	Click-chemistry approach to azacycloalkene monosulfonyl diamines: synthesis and computational analysis of the reaction mechanism. RSC Advances, 2012, 2, 10652.	1.7	26
59	Design, synthesis and pharmacophoric model building of novel substituted nicotinic acid hydrazones with potential antiproliferative activity. Archives of Pharmacal Research, 2012, 35, 1543-1552.	2.7	25
60	Expedient chemical synthesis of 75mer DNA binding domain of MafA: an insight on its binding to insulin enhancer. Amino Acids, 2012, 43, 1995-2003.	1.2	27
61	1Hâ€Azepineâ€4â€aminoâ€4â€carboxylic Acid: A New Î±,Î±â€Disubstituted Ornithine Analogue Capable of Inducing Helix Conformations in Short Alaâ€Aib Pentapeptides. Chemistry - A European Journal, 2012, 18, 8705-8715.	1.7	30
62	A New Series of Organocatalysts for Diels-Alder Cycloaddition Reactions and Theoretical Analysis. Current Organic Chemistry, 2011, 15, 3514-3522.	0.9	3
63	Synthesis, structural, and biological evaluation of bis-heteroarylmaleimides and bis-heterofused imides. Bioorganic and Medicinal Chemistry, 2011, 19, 5291-5299.	1.4	24
64	A Highly Diastereoselective Synthesis of Î±-Hydroxy-Î²-amino Acid Derivatives via a Lewis Acid Catalyzed Three-Component Condensation Reaction. Journal of Organic Chemistry, 2010, 75, 7099-7106.	1.7	25
65	Fused Isothiazole Sâ€Oxide Systems from Cycloaddition Reactions of Nâ€Benzylisothiazolâ€3â€amine 1â€Oxide. Helvetica Chimica Acta, 2009, 92, 779-789.	1.0	5
66	Addition of sulfenic acids to monosubstituted acetylenes: a theoretical and experimental study. Journal of Physical Organic Chemistry, 2009, 22, 1048-1057.	0.9	23
67	Chemoselective asymmetric synthesis of C-3a-(3-hydroxypropyl)tetrahydropyrrolo[2,3-b]indole and C-4a-(2-aminoethyl)-tetrahydropyrano[2,3-b]indole derivatives. Tetrahedron, 2009, 65, 1995-2004.	1.0	13
68	Cycloaddition reactions of 1,3-diazabuta-1,3-dienes with alkynyl ketenes. Tetrahedron, 2009, 65, 4664-4670.	1.0	15
69	Enantioselective synthesis, chiroptical properties and absolute configuration of 3-aminosubstituted isothiazole S-oxides. Tetrahedron: Asymmetry, 2009, 20, 2247-2256.	1.8	9
70	Virtual Screening Approach for the Identification of New Rac1 Inhibitors. Journal of Medicinal Chemistry, 2009, 52, 4087-4090.	2.9	96
71	Turning REST/NRSF Dysfunction in Huntingtons Disease into a Pharmaceutical Target. Current Pharmaceutical Design, 2009, 15, 3958-3967.	0.9	29
72	Efficient alkylation of N-Nâ€²disubstituted formamidines using Mitsunobuâ€™s reagents. Arkivoc, 2009, 2009, 126-131.	0.3	1

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73	Functionalization and molecular dynamics study of carboxyâ€terminated poly(1â€vinylpyrrolidinâ€2â€one): A potential soluble carrier of biomolecules. Journal of Polymer Science Part A, 2008, 46, 1683-1698.	2.5	7
74	Synthesis of Enantiopure Highly Functionalized Pyrrolizines and Indolizines from Natural Î±â€Amino Acids: An ExÂperimental and Theoretical Investigation. European Journal of Organic Chemistry, 2008, 2008, 2808-2816.	1.2	21
75	Antiproliferative effects on human tumor cells and rat aortic smooth muscular cells of 2,3-heteroarylmaleimides and heterofused imides. Bioorganic and Medicinal Chemistry, 2008, 16, 1691-1701.	1.4	23
76	SAR and QSAR study on 2-aminothiazole derivatives, modulators of transcriptional repression in Huntingtonâ€™s disease. Bioorganic and Medicinal Chemistry, 2008, 16, 5695-5703.	1.4	49
77	Synthesis of 4-nitromethylene-1,4-dihydropyrimidine derivatives as pyrimidine nucleoside analogues. Tetrahedron, 2008, 64, 11067-11073.	1.0	5
78	A Mild and Efficient Synthesis of 3-Aminosubstituted Isothiazole S-Oxides and their 5-Sulfanylsubstituted Derivatives. Letters in Organic Chemistry, 2008, 5, 623-627.	0.2	4
79	Synthesis of phenylacetaldehyde amidines and their intramolecular cyclization. Arkivoc, 2008, 2008, 136-147.	0.3	8
80	Synthesis of 4-dialkylaminopyridine derivatives through ring-rearrangement of 3-nitro-2H-pyran-2-one acetamidines. Tetrahedron, 2007, 63, 9652-9662.	1.0	7
81	[2Â+Â4] and [4Â+Â2] Cycloadditions ofo-Thioquinones with 1,3-Dienes:Â A Computational Study. Journal of Organic Chemistry, 2006, 71, 5507-5514.	1.7	32
82	Tautomeric Equilibria of [1]Benzopyrano[3,4-d]imidazol-4(3H)-ones, a Theoretical and NMR Study. Journal of Organic Chemistry, 2006, 71, 159-166.	1.7	16
83	Isothiazoles. Part XV. A mild andÂefficient synthesis ofÂnew antiproliferative 5-sulfanylsubstituted 3-alkylaminoisothiazole 1,1-dioxides. European Journal of Medicinal Chemistry, 2006, 41, 675-682.	2.6	13
84	Computational investigation of the nucleophilic reaction between methylthiolate and 4-bromo-3-methylamino-isothiazole 1,1-dioxide. Computational and Theoretical Chemistry, 2005, 726, 107-113.	1.5	2
85	Substituted coumarin amidines: useful building blocks for the preparation of [1]benzopyrano[4,3-b]pyridin-5-one and [1]benzopyrano[4,3-d]pyrimidin-5-one derivatives. Tetrahedron, 2005, 61, 4957-4964.	1.0	19
86	Substituted Coumarin Amidines: Useful Building Blocks for the Preparation of [1]Benzopyrano[4,3-b]pyridin-5-one and [1]Benzopyrano[4,3-d]pyrimidin-5-one Derivatives.. ChemInform, 2005, 36, no.	0.1	1
87	Synthesis and â€œdouble-facedâ€•antioxidant activity of polyhydroxylated 4-thiaflavans. Organic and Biomolecular Chemistry, 2005, 3, 3066.	1.5	49
88	Isothiazoles. Part 14. New 3-Aminosubstituted Isothiazole Dioxides and Their Mono- and Dihalogeno Derivatives.. ChemInform, 2004, 35, no.	0.1	0
89	New Synthetic Approach to [1]Benzopyrano[4,3-b]pyridin-5-one Derivatives.. ChemInform, 2004, 35, no.	0.1	0
90	Intramolecular cycloadditions of nitrones derived from optically active 1-alkenyl-2-imidazolecarbaldehydes: regio- and diastereoselectivity. Tetrahedron: Asymmetry, 2004, 15, 3181-3187.	1.8	16

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91	New synthetic approach to [1]benzopyrano[4,3-b]pyridin-5-one derivatives. Tetrahedron Letters, 2004, 45, 3447-3449.	0.7	21
92	3-Nitrocoumarin Amidines: A New Synthetic Strategy for Substituted [1]Benzopyrano[3,4-d]imidazol-4(3H)-ones. European Journal of Organic Chemistry, 2003, 2003, 3976-3984.	1.2	16
93	Isothiazoles. Part 14: New 3-aminosubstituted isothiazole dioxides and their mono- and dihalogeno derivatives. Tetrahedron, 2003, 59, 9399-9408.	1.0	20
94	An effective contribution to functionalized pyridines synthesis by way of an unusual rearrangement of amidines. Tetrahedron, 2002, 58, 1213-1221.	1.0	10