

# Alessandro Contini

## List of Publications by Year in descending order

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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	Virtual Screening Approach for the Identification of New Rac1 Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 4087-4090.	2.9	96
2	Biocatalytic Dynamic Kinetic Resolution for the Synthesis of Atropisomeric Biaryl N-oxide Lewis Base Catalysts. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 10755-10759.	7.2	87
3	Explicit Ligand Hydration Shells Improve the Correlation between MM-PB/GBSA Binding Energies and Experimental Activities. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2706-2717.	2.3	67
4	Improved Computation of Protein-Protein Relative Binding Energies with the Nwat-MMGBSA Method. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1692-1704.	2.5	59
5	An Efficient Implementation of the Nwat-MMGBSA Method to Rescore Docking Results in Medium-Throughput Virtual Screenings. <i>Frontiers in Chemistry</i> , 2018, 6, 43.	1.8	56
6	In Silico Drug Repurposing for SARS-CoV-2 Main Proteinase and Spike Proteins. <i>Journal of Proteome Research</i> , 2020, 19, 4637-4648.	1.8	50
7	Synthesis and "double-faced" antioxidant activity of polyhydroxylated 4-thiaflavans. <i>Organic and Biomolecular Chemistry</i> , 2005, 3, 3066.	1.5	49
8	SAR and QSAR study on 2-aminothiazole derivatives, modulators of transcriptional repression in Huntington's disease. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 5695-5703.	1.4	49
9	Binding of the repressor complex REST-SIN3b by small molecules restores neuronal gene transcription in Huntington's disease models. <i>Journal of Neurochemistry</i> , 2013, 127, 22-35.	2.1	44
10	$\beta$ -Hairpin mimics containing a piperidine-pyrrolidine scaffold modulate the $\beta$ -amyloid aggregation process preserving the monomer species. <i>Chemical Science</i> , 2017, 8, 1295-1302.	3.7	39
11	An Updated Test of AMBER Force Fields and Implicit Solvent Models in Predicting the Secondary Structure of Helical, $\beta$ -Hairpin, and Intrinsically Disordered Peptides. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 714-727.	2.3	38
12	A tendril perversion in a helical oligomer: trapping and characterizing a mobile screw-sense reversal. <i>Chemical Science</i> , 2017, 8, 3007-3018.	3.7	38
13	[2+4] and [4+2] Cycloadditions of o-Thioquinones with 1,3-Dienes: A Computational Study. <i>Journal of Organic Chemistry</i> , 2006, 71, 5507-5514.	1.7	32
14	Biocatalytic Dynamic Kinetic Resolution for the Synthesis of Atropisomeric Biaryl N-oxide Lewis Base Catalysts. <i>Angewandte Chemie</i> , 2016, 128, 10913-10917.	1.6	32
15	2-Amino-3-(phenylsulfanyl)norbormane-2-carboxylate: An Appealing Scaffold for the Design of Rac1-Tiam1 Protein-Protein Interaction Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 2953-2962.	2.9	31
16	1-Hydroxy-4-azepine-4-amino-4-carboxylic Acid: A New $\beta$ -Disubstituted Ornithine Analogue Capable of Inducing Helix Conformations in Short Ala-Aib Pentapeptides. <i>Chemistry - A European Journal</i> , 2012, 18, 8705-8715.	1.7	30
17	Role of Small GTPase Protein Rac1 in Cardiovascular Diseases. <i>Journal of Cardiovascular Pharmacology</i> , 2013, 62, 425-435.	0.8	30
18	Turning REST/NRSF Dysfunction in Huntingtons Disease into a Pharmaceutical Target. <i>Current Pharmaceutical Design</i> , 2009, 15, 3958-3967.	0.9	29

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19	Expedient chemical synthesis of 75mer DNA binding domain of MafA: an insight on its binding to insulin enhancer. <i>Amino Acids</i> , 2012, 43, 1995-2003.	1.2	27
20	Click-chemistry approach to azacycloalkene monosulfonyl diamines: synthesis and computational analysis of the reaction mechanism. <i>RSC Advances</i> , 2012, 2, 10652.	1.7	26
21	Synthesis, Molecular Characterization and Preliminary Antioxidant Activity Evaluation of Quercetin Fatty Esters. <i>JAOCs, Journal of the American Oil Chemists' Society</i> , 2013, 90, 1751-1759.	0.8	26
22	3-Aryl-N-aminoysulfonylphenyl-1H-pyrazole-5-carboxamides: a new class of selective Rac inhibitors. <i>MedChemComm</i> , 2013, 4, 537.	3.5	26
23	Asymmetric Modular Synthesis of a Semirigid Dipeptide Mimetic by Cascade Cycloaddition/Ring Rearrangement and Borohydride Reduction. <i>Journal of Organic Chemistry</i> , 2014, 79, 3094-3102.	1.7	26
24	From glucose to enantiopure morpholino $\beta^2$ -amino acid: a new tool for stabilizing $\beta^3$ -turns in peptides. <i>Organic Chemistry Frontiers</i> , 2019, 6, 972-982.	2.3	26
25	A Highly Diastereoselective Synthesis of $\beta^1$ -Hydroxy- $\beta^2$ -amino Acid Derivatives via a Lewis Acid Catalyzed Three-Component Condensation Reaction. <i>Journal of Organic Chemistry</i> , 2010, 75, 7099-7106.	1.7	25
26	Design, synthesis and pharmacophoric model building of novel substituted nicotinic acid hydrazones with potential antiproliferative activity. <i>Archives of Pharmacal Research</i> , 2012, 35, 1543-1552.	2.7	25
27	Mechanism of Stabilization of Helix Secondary Structure by Constrained $\beta^1$ -Tetrasubstituted $\beta^1$ -Amino Acids. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1350-1361.	1.2	25
28	Evaluation of Chemical Diversity of Biotinylated Chiral 1,3- $\beta^1$ -Diamines as a Catalytic Moiety in Artificial Imine Reductase. <i>ChemCatChem</i> , 2016, 8, 1665-1670.	1.8	25
29	Synthesis, structural, and biological evaluation of bis-heteroarylmaleimides and bis-heterofused imides. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 5291-5299.	1.4	24
30	1 <i>H</i> -Azepine-2-oxo-5-amino-5-carboxylic Acid: A $3 \times 10^3$ Helix Inducer and an Effective Tool for Functionalized Gold Nanoparticles. <i>Journal of Organic Chemistry</i> , 2015, 80, 5507-5516.	1.7	24
31	Antiproliferative effects on human tumor cells and rat aortic smooth muscular cells of 2,3-heteroarylmaleimides and heterofused imides. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 1691-1701.	1.4	23
32	Addition of sulfenic acids to monosubstituted acetylenes: a theoretical and experimental study. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 1048-1057.	0.9	23
33	New synthetic approach to [1]benzopyrano[4,3-b]pyridin-5-one derivatives. <i>Tetrahedron Letters</i> , 2004, 45, 3447-3449.	0.7	21
34	Synthesis of Enantiopure Highly Functionalized Pyrrolizines and Indolizines from Natural $\beta^1$ -Amino Acids: An Experimental and Theoretical Investigation. <i>European Journal of Organic Chemistry</i> , 2008, 2808-2816.	1.2	21
35	Ctr-1 Mets7 motif inspiring new peptide ligands for Cu( $\beta^1$ )-catalyzed asymmetric Henry reactions under green conditions. <i>RSC Advances</i> , 2016, 6, 71529-71533.	1.7	21
36	Peptide modulators of Rac1/Tiam1 protein-protein interaction: An alternative approach for cardiovascular diseases. <i>Peptide Science</i> , 2018, 110, e23089.	1.0	21

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37	Isothiazoles. Part 14: New 3-aminosubstituted isothiazole dioxides and their mono- and dihalogeno derivatives. <i>Tetrahedron</i> , 2003, 59, 9399-9408.	1.0	20
38	Model peptides containing the 3-sulfanyl-norbornene amino acid, a conformationally constrained cysteine analogue effective inducer of $3 \times 10^{-6}$ -helix secondary structures. <i>RSC Advances</i> , 2015, 5, 32643-32656.	1.7	20
39	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. <i>Tetrahedron</i> , 2005, 61, 4957-4964.	1.0	19
40	Origin of Helical Screw Sense Selectivity Induced by Chiral Constrained C $\pm$ -Tetrasubstituted $\alpha$ -Amino Acids in Aib-based Peptides. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14003-14013.	1.2	18
41	Tandem Tetrahydroisoquinoline-4-carboxylic Acid/ $\beta$ -Alanine as a New Construct Able To Induce a Flexible Turn. <i>Chemistry - A European Journal</i> , 2017, 23, 10822-10831.	1.7	18
42	Tetrahydro-4H-(pyrrolo[3,4-d]isoxazol-3-yl)methanamine: A Bicyclic Diamino Scaffold Stabilizing Parallel Turn Conformations. <i>Journal of Organic Chemistry</i> , 2018, 83, 11493-11501.	1.7	17
43	Tuning PFKFB3 Bisphosphatase Activity Through Allosteric Interference. <i>Scientific Reports</i> , 2019, 9, 20333.	1.6	17
44	3-Nitrocoumarin Amidines: A New Synthetic Strategy for Substituted [1]Benzopyrano[3,4-d]imidazol-4(3H)-ones. <i>European Journal of Organic Chemistry</i> , 2003, 2003, 3976-3984.	1.2	16
45	Intramolecular cycloadditions of nitrones derived from optically active 1-alkenyl-2-imidazolecarbaldehydes: regio- and diastereoselectivity. <i>Tetrahedron: Asymmetry</i> , 2004, 15, 3181-3187.	1.8	16
46	Tautomeric Equilibria of [1]Benzopyrano[3,4-d]imidazol-4(3H)-ones, a Theoretical and NMR Study. <i>Journal of Organic Chemistry</i> , 2006, 71, 159-166.	1.7	16
47	Fluoro-Aryl Substituted $\beta$ , $\gamma$ -Peptides in the Development of Foldameric Antiparallel $\beta$ -Sheets: A Conformational Study. <i>Frontiers in Chemistry</i> , 2019, 7, 192.	1.8	16
48	Copper(II)-Catalyzed Aminohalogenation of Alkynyl Carbamates. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 1750-1757.	1.2	16
49	Cycloaddition reactions of 1,3-diazabuta-1,3-dienes with alkynyl ketenes. <i>Tetrahedron</i> , 2009, 65, 4664-4670.	1.0	15
50	Synthesis and conformational analysis of peptides embodying 2,3-methanopipelic acids. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 6826-6836.	1.5	14
51	Three-Dimensional Proteome-Wide Scale Screening for the 5-Alpha Reductase Inhibitor Finasteride: Identification of a Novel Off-Target. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 4553-4566.	2.9	14
52	Isothiazoles. Part XV. A mild and efficient synthesis of new antiproliferative 5-sulfanylsubstituted 3-alkylaminoisothiazole 1,1-dioxides. <i>European Journal of Medicinal Chemistry</i> , 2006, 41, 675-682.	2.6	13
53	Chemoselective asymmetric synthesis of C-3a-(3-hydroxypropyl)tetrahydropyrrolo[2,3-b]indole and C-4a-(2-aminoethyl)-tetrahydropyrano[2,3-b]indole derivatives. <i>Tetrahedron</i> , 2009, 65, 1995-2004.	1.0	13
54	Molecular dynamics and tubulin polymerization kinetics study on 1,14-heterofused taxanes: evidence of stabilization of the tubulin head-to-tail dimer-dimer interaction. <i>Molecular BioSystems</i> , 2012, 8, 3254.	2.9	13

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55	Molecular insights into dimerization inhibition of c-Maf transcription factor. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2014, 1844, 2108-2115.	1.1	13
56	Identification of highly potent and selective MMP2 inhibitors addressing the S1â€² subsite with d-proline-based compounds. <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 1891-1902.	1.4	13
57	Non-natural 3-Arylmorpholino-Î²-amino Acid as a PPII Helix Inducer. <i>Organic Letters</i> , 2020, 22, 6197-6202.	2.4	13
58	Cross-talk between EGFR and T-cadherin: EGFR activation promotes T-cadherin localization to intercellular contacts. <i>Cellular Signalling</i> , 2013, 25, 1044-1053.	1.7	12
59	Rescoring Virtual Screening Results with the MM-PBSA Methods: Beware of Internal Dielectric Constants. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2714-2728.	2.5	11
60	Advances in the Treatment of Explicit Water Molecules in Docking and Binding Free Energy Calculations. <i>Current Medicinal Chemistry</i> , 2020, 26, 7598-7622.	1.2	11
61	An effective contribution to functionalized pyridines synthesis by way of an unusual rearrangement of amidines. <i>Tetrahedron</i> , 2002, 58, 1213-1221.	1.0	10
62	VCD spectroscopy as an excellent probe of chiral metal complexes containing a carbon monoxide vibrational chromophore. <i>Chemical Communications</i> , 2015, 51, 9385-9387.	2.2	10
63	Identification and in vivo validation of a 9-mer peptide derived from FSHÎ² with FSHR antagonist activity. <i>Peptides</i> , 2020, 132, 170367.	1.2	10
64	Enantioselective synthesis, chiroptical properties and absolute configuration of 3-aminosubstituted isothiazole S-oxides. <i>Tetrahedron: Asymmetry</i> , 2009, 20, 2247-2256.	1.8	9
65	Pyrrolyl-silicon compounds with different alkyl spacer lengths: Synthesis, electrochemical behavior and binding properties. <i>Synthetic Metals</i> , 2017, 231, 127-136.	2.1	9
66	Multicomponent Synthesis of Pentyl-Sulfonyl Amidines via Diazoalkane. <i>Synlett</i> , 2012, 23, 1523-1525.	1.0	8
67	Discovery of a d-pro-lys peptidomimetic inhibitor of MMP9: Addressing the gelatinase selectivity beyond S1â€² subsite. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2020, 30, 127467.	1.0	8
68	Synthesis of phenylacetaldehyde amidines and their intramolecular cyclization. <i>Arkivoc</i> , 2008, 2008, 136-147.	0.3	8
69	Synthesis of 4-dialkylaminopyridine derivatives through ring-rearrangement of 3-nitro-2H-pyran-2-one acetamidines. <i>Tetrahedron</i> , 2007, 63, 9652-9662.	1.0	7
70	Functionalization and molecular dynamics study of carboxyâ€²-terminated poly(1â€²-vinylpyrrolidinâ€²-2-one): A potential soluble carrier of biomolecules. <i>Journal of Polymer Science Part A</i> , 2008, 46, 1683-1698.	2.5	7
71	Molecular dynamic simulation of mGluR5 amino terminal domain: essential dynamics analysis captures the agonist or antagonist behaviour of ligands. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 41, 72-78.	1.3	7
72	A new scaffold of topoisomerase I inhibitors: Design, synthesis and biological evaluation. <i>European Journal of Medicinal Chemistry</i> , 2016, 124, 326-339.	2.6	6

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73	Synthesis and Biological Evaluation of New Natural Phenolic (2 <i>E</i> ,4 <i>E</i> ,6 <i>E</i> )-Octa-2,4,6-trienoic Esters. <i>Chemistry and Biodiversity</i> , 2017, 14, e1700294.	1.0	6
74	Synthesis of 4-nitromethylene-1,4-dihydropyrimidine derivatives as pyrimidine nucleoside analogues. <i>Tetrahedron</i> , 2008, 64, 11067-11073.	1.0	5
75	Fused Isothiazole <i>S</i> -Oxide Systems from Cycloaddition Reactions of <i>N</i> -Benzylisothiazol-3-amine 1-oxide. <i>Helvetica Chimica Acta</i> , 2009, 92, 779-789.	1.0	5
76	Discovery of small molecule binders of human FSHR(TMD) with novel structural scaffolds by integrating structural bioinformatics and machine learning algorithms. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 89, 156-166.	1.3	5
77	A Mild and Efficient Synthesis of 3-Aminosubstituted Isothiazole <i>S</i> -Oxides and their 5-Sulfanylsubstituted Derivatives. <i>Letters in Organic Chemistry</i> , 2008, 5, 623-627.	0.2	4
78	Stereodivergent synthesis of 5-aminopipericolic acids and application in the preparation of a cyclic RGD peptidomimetic as a nanomolar $\alpha V\beta 3$ integrin ligand. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 3402-3414.	1.5	4
79	Identification of the first enantiopure Rac1 "Tiam1 protein" protein interaction inhibitor and its optimized synthesis <i>via</i> phosphine free remote group directed hydroarylation. <i>MedChemComm</i> , 2019, 10, 310-314.	3.5	4
80	<i>In Vitro</i> Antimalarial Activity of Inhibitors of the Human GTPase Rac1. <i>Antimicrobial Agents and Chemotherapy</i> , 2022, 66, AAC0149821.	1.4	4
81	Identification of a novel off-target of paroxetine: Possible role in sexual dysfunction induced by this SSRI antidepressant drug. <i>Journal of Molecular Structure</i> , 2022, 1268, 133690.	1.8	4
82	A New Series of Organocatalysts for Diels-Alder Cycloaddition Reactions and Theoretical Analysis. <i>Current Organic Chemistry</i> , 2011, 15, 3514-3522.	0.9	3
83	Morpholino-based peptide oligomers: Synthesis and DNA binding properties. <i>Biochemical and Biophysical Research Communications</i> , 2021, 549, 8-13.	1.0	3
84	Computational investigation of the nucleophilic reaction between methylthiolate and 4-bromo-3-methylamino-isothiazole 1,1-dioxide. <i>Computational and Theoretical Chemistry</i> , 2005, 726, 107-113.	1.5	2
85	Editorial: Folded Synthetic Peptides for Biomedical Applications. <i>Frontiers in Chemistry</i> , 2019, 7, 448.	1.8	2
86	Central residues of FSH $\beta$ (89-97) peptide are not critical for FSHR binding: Implications for peptidomimetic design. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2021, 44, 128132.	1.0	2
87	Targeting transdifferentiated hepatic stellate cells and monitoring the hepatic fibrogenic process by means of IGF2R-specific peptides designed <i>in silico</i> . <i>Journal of Materials Chemistry B</i> , 2021, 9, 2092-2106.	2.9	2
88	Substituted Coumarin Amidines: Useful Building Blocks for the Preparation of [1]Benzopyrano[4,3- <i>b</i> ]pyridin-5-one and [1]Benzopyrano[4,3- <i>d</i> ]pyrimidin-5-one Derivatives.. <i>ChemInform</i> , 2005, 36, no.	0.1	1
89	Enantioselective Synthesis of <i>cis</i> and <i>trans</i> 4-Aminopipericolic Acids as $\beta$ -Amino Acids for the Construction of Cyclic RGD-Containing Peptidomimetics Antagonists of $\alpha V\beta 3$ Integrin. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 4371-4383.	1.2	1
90	Efficient alkylation of <i>N</i> -disubstituted formamidines using Mitsunobu's reagents. <i>Arkivoc</i> , 2009, 2009, 126-131.	0.3	1

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91	Modular synthesis of 2,4-diaminoanilines as CNS drug-like non-covalent inhibitors of asparagine endopeptidase. <i>Bioorganic and Medicinal Chemistry</i> , 2022, 63, 116746.	1.4	1
92	Isothiazoles. Part 14. New 3-Aminosubstituted Isothiazole Dioxides and Their Mono- and Dihalogeno Derivatives.. <i>ChemInform</i> , 2004, 35, no.	0.1	0
93	New Synthetic Approach to [1]Benzopyrano[4,3-b]pyridin-5-one Derivatives.. <i>ChemInform</i> , 2004, 35, no.	0.1	0
94	MOGLYNET â€“ Modulation of glycolytic flux as a new approach for treatment of atherosclerosis and plaque stabilization: a multidisciplinary study â€“ H2020. <i>Impact</i> , 2017, 2017, 26-28.	0.0	0