Elena Cichero

List of Publications by Year
in descending order

81	1,386	304743 22	454955 30
papers	citations	h-index	g-index

82	82	82	1694
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Magnolol and Luteolin Inhibition of Î±-Glucosidase Activity: Kinetics and Type of Interaction Detected by In Vitro and In Silico Studies. Pharmaceuticals, 2022, 15, 205.	3.8	15
2	Journey on VX-809-Based Hybrid Derivatives towards Drug-like F508del-CFTR Correctors: From Molecular Modeling to Chemical Synthesis and Biological Assays. Pharmaceuticals, 2022, 15, 274.	3.8	3
3	Discovery of Novel Trace Amine-Associated Receptor 5 (TAAR5) Antagonists Using a Deep Convolutional Neural Network. International Journal of Molecular Sciences, 2022, 23, 3127.	4.1	5
4	In silico drug repositioning on F508del-CFTR: A proof-of-concept study on the AIFA library. European Journal of Medicinal Chemistry, 2021, 213, 113186.	5.5	4
5	NBD2 Is Required for the Rescue of Mutant F508del CFTR by a Thiazole-Based Molecule: A Class II Corrector for the Multi-Drug Therapy of Cystic Fibrosis. Biomolecules, 2021, 11, 1417.	4.0	9
6	Synthesis and Structure-activity Relationship of Aminoarylthiazole Derivatives as Potential Potentiators of the Chloride Transport Defect in Cystic Fibrosis. Medicinal Chemistry, 2021, 17, 646-657.	1.5	3
7	Exploring the Selectivity Profile of Sigma Receptor Ligands by Molecular Docking and Pharmacophore Analyses. Medicinal Chemistry, 2021, 17, 1151-1165.	1.5	3
8	Probing In Silico the Benzimidazole Privileged Scaffold for the Development of Drug-like Anti-RSV Agents. Pharmaceuticals, 2021, 14, 1307.	3.8	17
9	Probing Allosteric Hsp70 Inhibitors by Molecular Modelling Studies to Expedite the Development of Novel Combined F508del CFTR Modulators. Pharmaceuticals, 2021, 14, 1296.	3.8	4
10	Trace amine associated receptor 1 (TAAR1) modulators: a patent review (2010-present). Expert Opinion on Therapeutic Patents, 2020, 30, 137-145.	5.0	18
11	Discovery of novel VX-809 hybrid derivatives as F508del-CFTR correctors by molecular modeling, chemical synthesis and biological assays. European Journal of Medicinal Chemistry, 2020, 208, 112833.	5.5	8
12	Novel 1-Amidino-4-Phenylpiperazines as Potent Agonists at Human TAAR1 Receptor: Rational Design, Synthesis, Biological Evaluation and Molecular Docking Studies. Pharmaceuticals, 2020, 13, 391.	3.8	20
13	Identification of a Potent and Selective 5-HT_{1A} Receptor Agonist with In Vitro and In Vivo Antinociceptive Activity. ACS Chemical Neuroscience, 2020, 11, 4111-4127.	3.5	8
14	Molecular Docking and QSAR Studies as Computational Tools Exploring the Rescue Ability of F508del CFTR Correctors. International Journal of Molecular Sciences, 2020, 21, 8084.	4.1	10
15	New Insights into the Binding Features of F508del CFTR Potentiators: A Molecular Docking, Pharmacophore Mapping and QSAR Analysis Approach. Pharmaceuticals, 2020, 13, 445.	3.8	8
16	Recent Strategic Advances in CFTR Drug Discovery: An Overview. International Journal of Molecular Sciences, 2020, 21, 2407.	4.1	6
17	Charcot-Marie-Tooth Type 2B: A New Phenotype Associated with a Novel RAB7A Mutation and Inhibited EGFR Degradation. Cells, 2020, 9, 1028.	4.1	20
18	Synthesis and Biological Evaluation of Novel (thio)semicarbazone-Based Benzimidazoles as Antiviral Agents against Human Respiratory Viruses. Molecules, 2020, 25, 1487.	3.8	44

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19	Identification of a high affinity binding site for abscisic acid on human lanthionine synthetase component C-like protein 2. International Journal of Biochemistry and Cell Biology, 2018, 97, 52-61.	2.8	13
20	Rational design, chemical synthesis and biological evaluation of novel biguanides exploring species-specificity responsiveness of TAAR1 agonists. European Journal of Medicinal Chemistry, 2018, 146, 171-184.	5.5	28
21	Synthesis and biological evaluation of novel thiazole- VX-809 hybrid derivatives as F508del correctors by QSAR-based filtering tools. European Journal of Medicinal Chemistry, 2018, 144, 179-200.	5.5	29
22	Novel sulfenamides and sulfonamides based on pyridazinone and pyridazine scaffolds as CB 1 receptor ligand antagonists. Bioorganic and Medicinal Chemistry, 2018, 26, 295-307.	3.0	8
23	Fluorometric detection of protein-ligand engagement: The case of phosphodiesterase5. Journal of Pharmaceutical and Biomedical Analysis, 2018, 149, 335-342.	2.8	6
24	Novel pyrrolocycloalkylpyrazole analogues as CB₁ ligands. Chemical Biology and Drug Design, 2018, 91, 181-193.	3.2	4
25	Exploring the effectiveness of novel benzimidazoles as CB2 ligands: synthesis, biological evaluation, molecular docking studies and ADMET prediction. MedChemComm, 2018, 9, 2045-2054.	3.4	12
26	Opportunities and challenges in the design of selective TAAR1 agonists: an editorial. Expert Opinion on Therapeutic Patents, 2018, 28, 437-440.	5.0	3
27	Synthesis and biological evaluation of 1,3-dioxolane-based 5-HT_{1A} receptor agonists for CNS disorders and neuropathic pain. Future Medicinal Chemistry, 2018, 10, 2137-2154.	2.3	8
28	Speeding Up the Identification of Cystic Fibrosis Transmembrane Conductance Regulator-Targeted Drugs: An Approach Based on Bioinformatics Strategies and Surface Plasmon Resonance. Molecules, 2018, 23, 120.	3.8	14
29	Synthesis, biological evaluation and molecular modeling of novel azaspiro dihydrotriazines as influenza virus inhibitors targeting the host factor dihydrofolate reductase (DHFR). European Journal of Medicinal Chemistry, 2018, 155, 229-243.	5.5	19
30	New pyridazinone-4-carboxamides as new cannabinoid receptor type-2 inverse agonists: Synthesis, pharmacological data and molecular docking. European Journal of Medicinal Chemistry, 2017, 127, 398-412.	5.5	15
31	New arylsparteine derivatives as positive inotropic drugs. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 588-599.	5.2	4
32	Host dihydrofolate reductase (DHFR)-directed cycloguanil analogues endowed with activity against influenza virus and respiratory syncytial virus. European Journal of Medicinal Chemistry, 2017, 135, 467-478.	5.5	28
33	Exhaustive CoMFA and CoMSIA analyses around different chemical entities: a ligand-based study exploring the affinity and selectivity profiles of 5-HT_{1A} ligands. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 214-230.	5.2	10
34	Benzimidazole-based derivatives as privileged scaffold developed for the treatment of the RSV infection: a computational study exploring the potency and cytotoxicity profiles. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 375-402.	5.2	10
35	Structureâ€“Activity Relationships within a Series of Ïƒ₁ and Ïƒ₂ Receptor Ligands: Identification of a Ïƒ₂ Receptor Agonist (BS148) with Selective Toxicity against Metastatic Melanoma. ChemMedChem, 2017, 12, 1893-1905.	3.2	6
36	Targeting species-specific trace amine-associated receptor 1 ligands: to date perspective of the rational drug design process. Future Medicinal Chemistry, 2017, 9, 1507-1527.	2.3	12

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37	New insights into the structure of the trace amineâ€associated receptor 2: Homology modelling studies exploring the binding mode of 3â€iodothyronamine. Chemical Biology and Drug Design, 2017, 89, 790-796.	3.2	18
38	Novel biguanide-based derivatives scouted as TAAR1 agonists: Synthesis, biological evaluation, ADME prediction and molecular docking studies. European Journal of Medicinal Chemistry, 2017, 127, 781-792.	5.5	38
39	Synthesis, biological evaluation and molecular modeling of 1-oxa-4-thiaspiro- and 1,4-dithiaspiro[4.5]decane derivatives asÂpotent and selective 5-HT1A receptor agonists. European Journal of Medicinal Chemistry, 2017, 125, 435-452.	5.5	31
40	Further Insights in the Binding Mode of Selective Inhibitors to Human PDE4D Enzyme Combining Docking and Molecular Dynamics. Molecular Informatics, 2016, 35, 369-381.	2.5	17
41	Titelbild: Impaired Chaperone Activity of Human Heat Shock Protein Hsp27 Siteâ€Specifically Modified with Argpyrimidine (Angew. Chem. 38/2016). Angewandte Chemie, 2016, 128, 11473-11473.	2.0	0
42	Hit-to-Lead Optimization of Mouse Trace Amine Associated Receptor 1 (mTAAR1) Agonists with a Diphenylmethane-Scaffold: Design, Synthesis, and Biological Study. Journal of Medicinal Chemistry, 2016, 59, 9825-9836.	6.4	19
43	Molecular Chaperones in the Pathogenesis of Amyotrophic Lateral Sclerosis: The Role of HSPB1. Human Mutation, 2016, 37, 1202-1208.	2.5	45
44	Impaired Chaperone Activity of Human Heat Shock Protein Hsp27 Siteâ€Specifically Modified with Argpyrimidine. Angewandte Chemie - International Edition, 2016, 55, 11397-11402.	13.8	19
45	Impaired Chaperone Activity of Human Heat Shock Protein Hsp27 Siteâ€Specifically Modified with Argpyrimidine. Angewandte Chemie, 2016, 128, 11569-11574.	2.0	5
46	New insights into selective PDE4D inhibitors: 3-(Cyclopentyloxy)-4-methoxybenzaldehyde O-(2-(2,6-dimethylmorpholino)-2-oxoethyl) oxime (GEBR-7b) structural development and promising activities to restore memory impairment. European Journal of Medicinal Chemistry, 2016, 124, 82-102.	5.5	31
47	Synthesis, molecular modeling and SAR study of novel pyrazolo[5,1-f][1,6]naphthyridines as CB 2 receptor antagonists/inverse agonists. Bioorganic and Medicinal Chemistry, 2016, 24, 5291-5301.	3.0	15
48	Exhaustive 3D-QSAR analyses as a computational tool to explore the potency and selectivity profiles of thieno[3,2-d]pyrimidin-4(3H)-one derivatives as PDE7 inhibitors. RSC Advances, 2016, 6, 61088-61108.	3.6	9
49	Tricyclic pyrazoles. Part 8. Synthesis, biological evaluation and modelling of tricyclic pyrazole carboxamides as potential CB2 receptor ligands with antagonist/inverse agonist properties. European Journal of Medicinal Chemistry, 2016, 112, 66-80.	5.5	18
50	Scouting new sigma receptor ligands: Synthesis, pharmacological evaluation and molecular modeling of 1,3-dioxolane-based structures and derivatives. European Journal of Medicinal Chemistry, 2016, 112, 1-19.	5.5	25
51	A homology modelling-driven study leading to the discovery of the first mouse trace amine-associated receptor 5 (TAAR5) antagonists. MedChemComm, 2016, 7, 353-364.	3.4	30
52	New insights into PDE4B inhibitor selectivity: CoMFA analyses and molecular docking studies. Molecular Diversity, 2016, 20, 77-92.	3.9	19
53	Fight Against H1N1 Influenza A Virus: Recent Insights Towards the Development of Druggable Compounds. Current Medicinal Chemistry, 2016, 23, 1802-1817.	2.4	21
54	Design, Synthesis, and Evaluation of Thyronamine Analogues as Novel Potent Mouse Trace Amine Associated Receptor 1 (mTAAR1) Agonists. Journal of Medicinal Chemistry, 2015, 58, 5096-5107.	6.4	42

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55	Synthesis and structureâ€“activity relationship of aminoarylthiazole derivatives as correctors of the chloride transport defect in cystic fibrosis. European Journal of Medicinal Chemistry, 2015, 99, 14-35.	5.5	31
56	In silico evaluation of human small heat shock protein HSP27: Homology modeling, mutation analyses and docking studies. Bioorganic and Medicinal Chemistry, 2015, 23, 3215-3220.	3.0	23
57	Enantiomeric resolution of [(2,2-diphenyl-1,3-dioxolan-4-yl)methyl](2-phenoxyethyl)amine, a potent Î±₁and 5-HT_{1A}receptor ligand: an in vitro and computational study. MedChemComm, 2015, 6, 677-690.	3.4	5
58	Ligand-based homology modelling of the human CB₂ receptor SR144528 antagonist binding site: a computational approach to explore the 1,5-diaryl pyrazole scaffold. MedChemComm, 2015, 6, 1978-1986.	3.4	10
59	Further Insights Into the Pharmacology of the Human Trace Amineâ€Associated Receptors: Discovery of Novel Ligands for <scp>TAAR</scp>1 by a Virtual Screening Approach. Chemical Biology and Drug Design, 2014, 84, 712-720.	3.2	41
60	Structureâ€“affinity/activity relationships of 1,4-dioxa-spiro[4.5]decane based ligands at Î±<alpha>1 and 5-HT1A receptors. European Journal of Medicinal Chemistry, 2014, 87, 248-266.	5.5	13
61	Synthesis, inÂvitro antiplatelet activity and molecular modelling studies of 10-substituted 2-(1-piperazinyl)pyrimido[1,2- a]benzimidazol-4(10 H)-ones. European Journal of Medicinal Chemistry, 2013, 62, 564-578.	5.5	20
62	Insights into the Structure and Pharmacology of the Human Trace Amineâ€Associated Receptor 1 (hTAAR1): Homology Modelling and Docking Studies. Chemical Biology and Drug Design, 2013, 81, 509-516.	3.2	52
63	Homology Modeling, Docking Studies and Molecular Dynamic Simulations Using Graphical Processing Unit Architecture to Probe the Typeâ€1 Phosphodiesterase Catalytic Site: A Computational Approach for the Rational Design of Selective Inhibitors. Chemical Biology and Drug Design, 2013, 82, 718-731.	3.2	33
64	T137A variant is a pathogenetic SOD1 mutation associated with a slowly progressive ALS phenotype. Amyotrophic Lateral Sclerosis and Other Motor Neuron Disorders, 2012, 13, 398-399.	2.1	4
65	Synthesis, Biological Evaluation, and Docking Studies of Tetrahydrofuran- Cyclopentanone- and Cyclopentanol-Based Ligands Acting at Adrenergic Î±₁- and Serotonine 5-HT_{1A} Receptors. Journal of Medicinal Chemistry, 2012, 55, 23-36.	6.4	38
66	Scouting new molecular targets for CFTR therapy: the HSC70/BAG-1 complex. A computational study. Medicinal Chemistry Research, 2012, 21, 4430-4436.	2.4	2
67	Fast course ALS presenting with vocal cord paralysis: Clinical features, bioinformatic and modelling analysis of the novel SOD1 Gly147Ser mutation. Amyotrophic Lateral Sclerosis and Other Motor Neuron Disorders, 2012, 13, 144-148.	2.1	14
68	Docking-based CoMFA and CoMSIA analyses of tetrahydro-Î²-carboline derivatives as type-5 phosphodiesterase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2012, 27, 730-743.	5.2	11
69	Docking-based 3D-QSAR analyses of pyrazole derivatives as HIV-1 non-nucleoside reverse transcriptase inhibitors. Journal of Molecular Modeling, 2012, 18, 1573-1582.	1.8	27
70	Synthesis of new 5,6-dihydrobenzo[h]quinazoline 2,4-diamino substituted and antiplatelet/antiphlogistic activities evaluation. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 1125-1129.	2.2	17
71	Homology modeling in tandem with 3D-QSAR analyses: A computational approach to depict the agonist binding site of the human CB2 receptor. European Journal of Medicinal Chemistry, 2011, 46, 4489-4505.	5.5	36
72	3,4,5-Trisubstituted-1,2,4-4H-triazoles as WT and Y188L mutant HIV-1 non-nucleoside reverse transcriptase inhibitors: docking-based CoMFA and CoMSIA analyses. Journal of Molecular Modeling, 2011, 17, 1537-1550.	1.8	18

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73	1,3-Dioxolane-based ligands incorporating a lactam or imide moiety: Structureâ€“affinity/activity relationship at Î±1-adrenoceptor subtypes and at 5-HT1A receptors. European Journal of Medicinal Chemistry, 2010, 45, 3740-3751.	5.5	21
74	CoMFA and CoMSIA analyses on 4-oxo-1,4-dihydroquinoline and 4-oxo-1,4-dihydro-1,5-, -1,6- and -1,8-naphthyridine derivatives as selective CB2 receptor agonists. Journal of Molecular Modeling, 2010, 16, 677-691.	1.8	17
75	CoMFA and CoMSIA analyses on 1,2,3,4-tetrahydropyrrolo[3,4-b]indole and benzimidazole derivatives as selective CB2 receptor agonists. Journal of Molecular Modeling, 2010, 16, 1481-1498.	1.8	26
76	Computational studies of the binding mode and 3D-QSAR analyses of symmetric formimidoester disulfides: a new class of non-nucleoside HIV-1 reverse transcriptase inhibitor. Journal of Molecular Modeling, 2009, 15, 357-367.	1.8	7
77	Acylthiocarbamates as non-nucleoside HIV-1 reverse transcriptase inhibitors: docking studies and ligand-based CoMFA and CoMSIA analyses. Journal of Molecular Modeling, 2009, 15, 871-884.	1.8	18
78	Exploring the QSAR of Pyrazolo[3,4â€b]Pyridine, Pyrazolo[3,4â€b]Pyridone and Pyrazolo[3,4â€b]Pyrimidine Derivatives as Antagonists for A₁ Adenosine Receptor. QSAR and Combinatorial Science, 2009, 28, 426-435.	1.4	4
79	Thiocarbamates as non-nucleoside HIV-1 reverse transcriptase inhibitors: Docking-based CoMFA and CoMSIA analyses. European Journal of Medicinal Chemistry, 2009, 44, 2059-2070.	5.5	24
80	Exploring the binding features of rimonabant analogues and acyclic CB1 antagonists: docking studies and QSAR analysis. Journal of Molecular Modeling, 2008, 14, 1131-1145.	1.8	12
81	Rational design, synthesis and biological evaluation of new 1,5-diarylpyrazole derivatives as CB1 receptor antagonists, structurally related to rimonabant. European Journal of Medicinal Chemistry, 2008, 43, 2627-2638.	5.5	26