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	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
2	Molecular Chaperones in the Pathogenesis of Amyotrophic Lateral Sclerosis: The Role of HSPB1. Human Mutation, 2016, 37, 1202-1208.	2.5	45
3	Synthesis and Biological Evaluation of Novel (thio)semicarbazone-Based Benzimidazoles as Antiviral Agents against Human Respiratory Viruses. Molecules, 2020, 25, 1487.	3.8	44
4	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
5	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
6	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
7	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
8	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
9	Homology Modeling, Docking Studies and Molecular Dynamic Simulations Using Graphical Processing Unit Architecture to Probe the Typeâ€11 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
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	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

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19	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
20	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
21	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
22	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
23	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
24	Fight Against H1N1 Influenza A Virus: Recent Insights Towards the Development of Druggable Compounds. Current Medicinal Chemistry, 2016, 23, 1802-1817.	2.4	21
25	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
26	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
27	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
28	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
29	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
30	New insights into PDE4B inhibitor selectivity: CoMFA analyses and molecular docking studies. Molecular Diversity, 2016, 20, 77-92.	3.9	19
31	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
32	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
33	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
34	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
35	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
36	Trace amine associated receptor 1 (TAAR1) modulators: a patent review (2010-present). Expert Opinion on Therapeutic Patents, 2020, 30, 137-145.	5.0	18

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37	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
38	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
39	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
40	Probing In Silico the Benzimidazole Privileged Scaffold for the Development of Drug-like Anti-RSV Agents. Pharmaceuticals, 2021, 14, 1307.	3.8	17
41	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
42	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
43	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
44	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
45	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
46	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
47	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
48	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
49	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
50	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
51	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
52	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
53	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
54	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

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55	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
56	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
57	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
58	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
59	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
60	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
61	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
62	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
63	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
64	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
65	Fluorometric detection of protein-ligand engagement: The case of phosphodiesterase5. Journal of Pharmaceutical and Biomedical Analysis, 2018, 149, 335-342.	2.8	6
66	Recent Strategic Advances in CFTR Drug Discovery: An Overview. International Journal of Molecular Sciences, 2020, 21, 2407.	4.1	6
67	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
68	Impaired Chaperone Activity of Human Heat Shock Protein Hsp27 Siteâ€Specifically Modified with Argpyrimidine. Angewandte Chemie, 2016, 128, 11569-11574.	2.0	5
69	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
70	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
71	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
72	New arylsparteine derivatives as positive inotropic drugs. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 588-599.	5.2	4

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73	Novel pyrrolocycloalkylpyrazole analogues as CB₁ ligands. Chemical Biology and Drug Design, 2018, 91, 181-193.	3.2	4
74	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
75	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
76	Opportunities and challenges in the design of selective TAAR1 agonists: an editorial. Expert Opinion on Therapeutic Patents, 2018, 28, 437-440.	5.0	3
77	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
78	Exploring the Selectivity Profile of Sigma Receptor Ligands by Molecular Docking and Pharmacophore Analyses. Medicinal Chemistry, 2021, 17, 1151-1165.	1.5	3
79	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
80	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
81	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