Iwan J P De Esch

List of Publications by Year
in descending order

65 papers	2,366 citations	201385 27 h-index	223531 46 g-index
68 all docs	68 docs citations	68 times ranked	3091 citing authors

#	Article	IF	Citations
1	Fragment-to-Lead Medicinal Chemistry Publications in 2020. Journal of Medicinal Chemistry, 2022, 65, 84-99.	2.9	52
2	Puckering the Planar Landscape of Fragments: Design and Synthesis of a 3D Cyclobutane Fragment Library. ChemMedChem, 2022, 17, .	1.6	6
3	Exploring the Activity Profile of TbrPDEB1 and hPDE4 Inhibitors Using Free Energy Perturbation. ACS Medicinal Chemistry Letters, 2022, 13, 904-910.	1.3	1
4	Escape from planarity in fragment-based drug discovery: A synthetic strategy analysis of synthetic 3D fragment libraries. Drug Discovery Today, 2022, 27, 2484-2496.	3.2	17
5	KLIFS: an overhaul after the first 5 years of supporting kinase research. Nucleic Acids Research, 2021, 49, D562-D569.	6.5	74
6	Vanishing white matter: Eukaryotic initiation factor 2B model and the impact of missense mutations. Molecular Genetics & Genomic Medicine, 2021, 9, e1593.	0.6	17
7	Structure Activity Relationship of N-Substituted Phenyldihydropyrazolones Against Trypanosoma cruzi Amastigotes. Frontiers in Chemistry, 2021, 9, 608438.	1.8	1
8	Exploring the Effect of Cyclization of Histamine H₁ Receptor Antagonists on Ligand Binding Kinetics. ACS Omega, 2021, 6, 12755-12768.	1.6	2
9	Discovery of fragments inducing conformational effects in dynamic proteins using a second-harmonic generation biosensor. RSC Advances, 2021, 11, 7527-7537.	1.7	4
10	Editorial to technologies in fragment-based drug discovery. Drug Discovery Today: Technologies, 2021, 40, 43.	4.0	0
11	Progress in Free Energy Perturbation: Options for Evolving Fragments. Drug Discovery Today: Technologies, 2021, 40, 36-42.	4.0	7
12	Fragment-to-Lead Medicinal Chemistry Publications in 2018. Journal of Medicinal Chemistry, 2020, 63, 4430-4444.	2.9	61
13	Identification of Phenylphthalazinones as a New Class of <i>Leishmania infantum</i> Inhibitors. ChemMedChem, 2020, 15, 219-227.	1.6	4
14	Fragment-to-Lead Medicinal Chemistry Publications in 2019. Journal of Medicinal Chemistry, 2020, 63, 15494-15507.	2.9	41
15	Bromo-Cyclobutenaminones as New Covalent UDP-N-Acetylglucosamine Enolpyruvyl Transferase (MurA) Inhibitors. Pharmaceuticals, 2020, 13, 362.	1.7	8
16	Structureâ€Activity Relationship of Phenylpyrazolones against Trypanosoma cruzi. ChemMedChem, 2020, 15, 1310-1321.	1.6	5
17	Escape from planarity in fragment-based drug discovery: A physicochemical and 3D property analysis of synthetic 3D fragment libraries. Drug Discovery Today: Technologies, 2020, 38, 77-90.	4.0	20
18	Discovery of Diaryl Ether Substituted Tetrahydrophthalazinones as TbrPDEB1 Inhibitors Following Structure-Based Virtual Screening. Frontiers in Chemistry, 2020, 8, 608030.	1.8	5

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19	Identification of Phenylpyrazolone Dimers as a New Class of Antiâ€•Trypanosoma cruzi Agents. ChemMedChem, 2019, 14, 1662-1668.	1.6	2
20	4-(3-Aminoazetidin-1-yl)pyrimidin-2-amines as High-Affinity Non-imidazole Histamine H3Receptor Agonists with in Vivo Central Nervous System Activity. Journal of Medicinal Chemistry, 2019, 62, 10848-10866.	2.9	6
21	The Landscape of Atypical and Eukaryotic Protein Kinases. Trends in Pharmacological Sciences, 2019, 40, 818-832.	4.0	87
22	Phenyldihydropyrazolones as Novel Lead Compounds Against <i>Trypanosoma cruzi</i>. ACS Omega, 2019, 4, 6585-6596.	1.6	6
23	A Photoswitchable Agonist for the Histamine H₃ Receptor, a Prototypic Family A Gâ€Proteinâ€Coupled Receptor. Angewandte Chemie - International Edition, 2019, 58, 4531-4535.	7.2	23
24	A toolbox of molecular photoswitches to modulate the CXCR3 chemokine receptor with light. Beilstein Journal of Organic Chemistry, 2019, 15, 2509-2523.	1.3	13
25	Covalent Inhibition of the Histamine H3 Receptor. Molecules, 2019, 24, 4541.	1.7	5
26	Fragment-to-Lead Medicinal Chemistry Publications in 2017. Journal of Medicinal Chemistry, 2019, 62, 3857-3872.	2.9	47
27	Structure-based exploration and pharmacological evaluation of N-substituted piperidin-4-yl-methanamine CXCR4 chemokine receptor antagonists. European Journal of Medicinal Chemistry, 2019, 162, 631-649.	2.6	12
28	Aminergic GPCRâ€“Ligand Interactions: A Chemical and Structural Map of Receptor Mutation Data. Journal of Medicinal Chemistry, 2019, 62, 3784-3839.	2.9	53
29	Synthesis and Characterization of a Bidirectional Photoswitchable Antagonist Toolbox for Real-Time GPCR Photopharmacology. Journal of the American Chemical Society, 2018, 140, 4232-4243.	6.6	50
30	Targeting a Subpocket in <i>Trypanosoma brucei</i> Phosphodiesterase B1 (TbrPDEB1) Enables the Structure-Based Discovery of Selective Inhibitors with Trypanocidal Activity. Journal of Medicinal Chemistry, 2018, 61, 3870-3888.	2.9	34
31	3Dâ€eâ€Chem: Structural Cheminformatics Workflows for Computerâ€Aided Drug Discovery. ChemMedChem, 2018, 13, 614-626.	1.6	17
32	When fragments link: a bibliometric perspective on the development of fragment-based drug discovery. Drug Discovery Today, 2018, 23, 1596-1609.	3.2	36
33	A Structural Framework for GPCR Chemogenomics: Whatâ€™s In a Residue Number?. Methods in Molecular Biology, 2018, 1705, 73-113.	0.4	6
34	Photoswitching the Efficacy of a Smallâ€Molecule Ligand for a Peptidergic GPCR: from Antagonism to Agonism. Angewandte Chemie - International Edition, 2018, 57, 11608-11612.	7.2	29
35	3D-e-Chem-VM: Structural Cheminformatics Research Infrastructure in a Freely Available Virtual Machine. Journal of Chemical Information and Modeling, 2017, 57, 115-121.	2.5	21
36	Structural Analysis of Chemokine Receptorâ€“Ligand Interactions. Journal of Medicinal Chemistry, 2017, 60, 4735-4779.	2.9	94

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37	Molecular interaction fingerprint approaches for GPCR drug discovery. Current Opinion in Pharmacology, 2016, 30, 59-68.	1.7	43
38	Identification of Ligand Binding Hot Spots of the Histamine H₁ Receptor following Structure-Based Fragment Optimization. Journal of Medicinal Chemistry, 2016, 59, 9047-9061.	2.9	26
39	Function-specific virtual screening for GPCR ligands using a combined scoring method. Scientific Reports, 2016, 6, 28288.	1.6	79
40	KLIFS: a structural kinase-ligand interaction database. Nucleic Acids Research, 2016, 44, D365-D371.	6.5	132
41	PDEStrIAn: A Phosphodiesterase Structure and Ligand Interaction Annotated Database As a Tool for Structure-Based Drug Design. Journal of Medicinal Chemistry, 2016, 59, 7029-7065.	2.9	54
42	Structure-based virtual screening for fragment-like ligands of the G protein-coupled histamine H₄receptor. MedChemComm, 2015, 6, 1003-1017.	3.5	33
43	Structure-Based Prediction of G-Protein-Coupled Receptor Ligand Function: A Î²-Adrenoceptor Case Study. Journal of Chemical Information and Modeling, 2015, 55, 1045-1061.	2.5	49
44	Fragment-Based Screening in Tandem with Phenotypic Screening Provides Novel Antiparasitic Hits. Journal of Biomolecular Screening, 2015, 20, 131-140.	2.6	23
45	Pharmacological Characterization of [³H]VUF11211, a Novel Radiolabeled Small-Molecule Inverse Agonist for the Chemokine Receptor CXCR3. Molecular Pharmacology, 2015, 87, 639-648.	1.0	14
46	Combinatorial Consensus Scoring for Ligand-Based Virtual Fragment Screening: A Comparative Case Study for Serotonin 5-HT₃A, Histamine H₁, and Histamine H₄Receptors. Journal of Chemical Information and Modeling, 2015, 55, 1030-1044.	2.5	17
47	EPHA4 is overexpressed but not functionally active in SÃ©zary syndrome. Oncotarget, 2015, 6, 31868-31876.	0.8	6
48	KLIFS: A Knowledge-Based Structural Database To Navigate Kinaseâ€“Ligand Interaction Space. Journal of Medicinal Chemistry, 2014, 57, 249-277.	2.9	243
49	Mapping histamine H4 receptorâ€“ligand binding modes. MedChemComm, 2013, 4, 193-204.	3.5	27
50	Small and colorful stones make beautiful mosaics: fragment-based chemogenomics. Drug Discovery Today, 2013, 18, 323-330.	3.2	30
51	From the protein's perspective: the benefits and challenges of protein structure-based pharmacophore modeling. MedChemComm, 2012, 3, 28-38.	3.5	81
52	Pharmacological characterization of a smallâ€molecule agonist for the chemokine receptor CXCR3. British Journal of Pharmacology, 2012, 166, 898-911.	2.7	44
53	Identification of novel Î±7 nicotinic receptor ligands by in silico screening against the crystal structure of a chimeric Î±7 receptor ligand binding domain. Bioorganic and Medicinal Chemistry, 2012, 20, 5992-6002.	1.4	11
54	A medicinal chemistry perspective on melting point: matched molecular pair analysis of the effects of simple descriptors on the melting point of drug-like compounds. MedChemComm, 2012, 3, 584.	3.5	26

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55	Fragment based lead discovery of small molecule inhibitors for the EPHA4 receptor tyrosine kinase. European Journal of Medicinal Chemistry, 2012, 47, 493-500.	2.6	23
56	Online parallel fragment screening and rapid hit exploration for nicotinic acetylcholine receptors. MedChemComm, 2011, 2, 590.	3.5	6
57	Crystal structure of the EphA4 protein tyrosine kinase domain in the apo- and dasatinib-bound state. FEBS Letters, 2011, 585, 3593-3599.	1.3	21
58	In Silico Veritas: The Pitfalls and Challenges of Predicting GPCR-Ligand Interactions. Pharmaceuticals, 2011, 4, 1196-1215.	1.7	16
59	Several down, a few to go: histamine H₃receptor ligands making the final push towards the market?. Expert Opinion on Investigational Drugs, 2011, 20, 1629-1648.	1.9	50
60	An efficient and information-rich biochemical method design for fragment library screening on ion channels. BioTechniques, 2010, 49, 822-829.	0.8	16
61	Histamine H3 receptor ligands with a 3-cyclobutoxy motif: a novel and versatile constraint of the classical 3-propoxy linker. MedChemComm, 2010, 1, 39.	3.5	8
62	Pharmacological characterization of the new histamine H₄ receptor agonist VUF 8430. British Journal of Pharmacology, 2009, 157, 34-43.	2.7	56
63	Molecular and biochemical pharmacology of the histamine H₄ receptor. British Journal of Pharmacology, 2009, 157, 14-23.	2.7	140
64	The histamine H receptor as a new therapeutic target for inflammation. Trends in Pharmacological Sciences, 2005, 26, 462-9.	4.0	189
65	A Qualitative Model for the Histamine H3 Receptor Explaining Agonistic and Antagonistic Activity Simultaneously. Archiv Der Pharmazie, 2000, 333, 254-260.	2.1	29