Masateru Ohta

List of Publications by Year
in descending order

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40	728	623188	552369
papers	citations	14 h-index	26 g-index

44	44	44	772
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Effect of Water Molecules on the Activating S810L Mutation of the Mineralocorticoid Receptor. Journal of Chemical Information and Modeling, 2021, 61, 3583-3592.	2.5	0
2	Structure-based screening combined with computational and biochemical analyses identified the inhibitor targeting the binding of DNA Ligase 1 to UHRF1. Bioorganic and Medicinal Chemistry, 2021, 52, 116500.	1.4	8
3	Machine learning to estimate the local quality of protein crystal structures. Scientific Reports, 2021, 11, 23599.	1.6	2
4	Structure-based design and discovery of novel anti-tissue factor antibodies with cooperative double-point mutations, using interaction analysis. Scientific Reports, 2020, 10, 17590.	1.6	7
5	Comprehensive 3Dâ€RISM analysis of the hydration of small molecule binding sites in ligandâ€free protein structures. Journal of Computational Chemistry, 2020, 41, 2406-2419.	1.5	8
6	kGCN: a graph-based deep learning framework for chemical structures. Journal of Cheminformatics, 2020, 12, 32.	2.8	55
7	High-Precision Atomic Charge Prediction for Protein Systems Using Fragment Molecular Orbital Calculation and Machine Learning. Journal of Chemical Information and Modeling, 2020, 60, 3361-3368.	2.5	22
8	Lead Optimization and Avoidance of Reactive Metabolite Leading to PCO371, a Potent, Selective, and Orally Available Human Parathyroid Hormone Receptor 1 (hPTHR1) Agonist. Journal of Medicinal Chemistry, 2020, 63, 5089-5099.	2.9	17
9	Development of a Novel Human Parathyroid Hormone Receptor 1 (hPTHR1) Agonist (CH5447240), a Potent and Orally Available Small Molecule for Treatment of Hypoparathyroidism. Journal of Medicinal Chemistry, 2018, 61, 5949-5962.	2.9	9
10	Structure-Based Drug Design: A Key Technology for Drug Discovery in the Pharmaceutical Industry. Journal of Cardiac Failure, 2015, 21, S160.	0.7	0
11	CH5137291, an androgen receptor nuclear translocation-inhibiting compound, inhibits the growth of castration-resistant prostate cancer cells. International Journal of Oncology, 2015, 46, 1560-1572.	1.4	7
12	Monte Carlo Simulations on Atropisomerism of Thienotriazolodiazepines Applicable to Slow Transition Phenomena Using Potential Energy Surfaces by <i>ab initio</i> Molecular Orbital Calculations. Chemical and Pharmaceutical Bulletin, 2014, 62, 229-237.	0.6	0
13	Effects of fluorines on nonsecosteroidal vitamin D receptor agonists. Bioorganic and Medicinal Chemistry, 2013, 21, 712-721.	1.4	10
14	A series of nonsecosteroidal vitamin D receptor agonists for osteoporosis therapy. Bioorganic and Medicinal Chemistry, 2013, 21, 1823-1833.	1.4	10
15	Systematic SAR study of the side chain of nonsecosteroidal vitamin D3 analogs. Bioorganic and Medicinal Chemistry, 2012, 20, 4495-4506.	1.4	6
16	Pertuzumab in Combination with Trastuzumab Shows Significantly Enhanced Antitumor Activity in HER2-Positive Human Gastric Cancer Xenograft Models. Clinical Cancer Research, 2011, 17, 5060-5070.	3.2	158
17	Design and Synthesis of Peptidomimetic Factor VIIa Inhibitors. Chemical and Pharmaceutical Bulletin, 2010, 58, 38-44.	0.6	1
18	Design and synthesis of an androgen receptor pure antagonist (CH5137291) for the treatment of castration-resistant prostate cancer. Bioorganic and Medicinal Chemistry, 2010, 18, 8150-8157.	1.4	16

#	Article	IF	Citations
19	Structureâ€“activity relationships of bioisosteric replacement of the carboxylic acid in novel androgen receptor pure antagonists. Bioorganic and Medicinal Chemistry, 2010, 18, 3159-3168.	1.4	14
20	Structure-Based Drug Design of Peptide Mimetics Containing Large P3 Moieties as Inhibitors of Factor VIIa. Letters in Drug Design and Discovery, 2009, 6, 86-92.	0.4	2
21	Abstract A220: Design and synthesis of an androgen receptor pure antagonist (CH5137291) for treatment of castrationâ€resistant prostate cancer. , 2009, , .		0
22	Abstract A219: Universal efficacy of novel androgen receptor pure antagonist, CH5137291, against broad spectrum prostate cancer including castrationâ€resistant prostate cancers. , 2009, , .		0
23	Factor VIIa inhibitors: Target hopping in the serine protease family using X-ray structure determination. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 4533-4537.	1.0	14
24	Discovery of an Orally-Active Nonsteroidal Androgen Receptor Pure Antagonist and the Structure-Activity Relationships of Its Derivatives. Chemical and Pharmaceutical Bulletin, 2008, 56, 1555-1561.	0.6	19
25	Discovery and structureâ€“activity relationships of new steroidal compounds bearing a carboxy-terminal side chain as androgen receptor pure antagonists. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 5573-5576.	1.0	13
26	Discovery of 7Î±-substituted dihydrotestosterones as androgen receptor pure antagonists and their structureâ€“activity relationships. Bioorganic and Medicinal Chemistry, 2007, 15, 174-185.	1.4	17
27	Structure of human factor VIIa/tissue factor in complex with a peptide-mimetic inhibitor: high selectivity against thrombin by introducing two charged groups in P2 and P4. Acta Crystallographica Section F: Structural Biology Communications, 2005, 61, 169-173.	0.7	7
28	Novel interactions of large P3 moiety and small P4 moiety in the binding of the peptide mimetic factor VIIa inhibitor. Biochemical and Biophysical Research Communications, 2005, 326, 859-865.	1.0	7
29	Structure-based design of P3 moieties in the peptide mimetic factor VIIa inhibitor. Biochemical and Biophysical Research Communications, 2005, 327, 589-596.	1.0	11
30	Crystal structure of human factor VIIa/tissue factor in complex with peptide mimetic inhibitor. Biochemical and Biophysical Research Communications, 2004, 324, 1227-1233.	1.0	12
31	Physicochemical parameters responsible for the affinity of methotrexate analogs for rat canalicular multispecific organic anion transporter (cMOAT/MRP2). Pharmaceutical Research, 2001, 18, 579-586.	1.7	19
32	Conformationâ^'Function Relationship of Vitamin D:Â Conformational Analysis Predicts Potential Side-Chain Structure. Journal of Medicinal Chemistry, 1998, 41, 1467-1475.	2.9	65
33	Conformationally Restricted Analogs of 1Î±,25-Dihydroxyvitamin D3and Its 20-Epimer:Â Compounds for Study of the Three-Dimensional Structure of Vitamin D Responsible for Binding to the Receptor. Journal of Medicinal Chemistry, 1996, 39, 2727-2737.	2.9	69
34	Three-dimensional structure-activity relationships and receptor mapping of quinolone antibacterials. Pharmacochemistry Library, 1995, 23, 97-124.	0.1	0
35	Background and features of emil, a system for database-aided bioanalogous structural transformation of bioactive compounds. Pharmacochemistry Library, 1995, 23, 235-273.	0.1	6
36	On the side chain conformation of 1Î±,25-dihydroxyvitamin D3 responsible for binding to the receptor. Bioorganic and Medicinal Chemistry Letters, 1995, 5, 979-984.	1.0	20

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37	Comparative molecular field analysis of benzopyran-4-carbothioamide potassium channel openers. Bioorganic and Medicinal Chemistry Letters, 1994, 4, 2903-2906.	1.0	8
38	Structure-activity relationships of 6-substituted benzopyran-4-carbothioamide potassium channel openers. Bioorganic and Medicinal Chemistry Letters, 1993, 3, 1659-1662.	1.0	14
39	Design of potent K+ channel openers by pharmacophore model. Bioorganic and Medicinal Chemistry Letters, 1993, 3, 625-631.	1.0	30
40	Three-dimensional structure-activity relationships and receptor mapping of N1-substituents of quinolone antibacterials. Journal of Medicinal Chemistry, 1991, 34, 131-139.	2.9	44