Noriyuki Yamaotsu

List of Publications by Year
in descending order

51	1,053	471371	434063
papers	citations	17 h-index	31 g-index

54	54	54	1745
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Synthesis and Evaluation of Habiterpenol Analogs. Chemical and Pharmaceutical Bulletin, 2022, 70, 261-268.	0.6	3
2	Identification of novel EED-EZH2 PPI inhibitors using an in silico fragment mapping method. Journal of Computer-Aided Molecular Design, 2021, 35, 601-611.	1.3	5
3	Structure-based virtual screening for novel chymase inhibitors by in silico fragment mapping. Journal of Molecular Graphics and Modelling, 2019, 89, 102-108.	1.3	3
4	Linear Discriminant Analysis for the <i>in Silico</i> Discovery of Mechanism-Based Reversible Covalent Inhibitors of a Serine Protease: Application of Hydration Thermodynamics Analysis and Semi-empirical Molecular Orbital Calculation. Chemical and Pharmaceutical Bulletin, 2018, 66, 399-409.	0.6	1
5	Validation of molecular force field parameters for peptides including isomerized amino acids. Chirality, 2018, 30, 332-341.	1.3	6
6	Design of a New Î±-1-C-Alkyl-DAB Derivative Acting as a Pharmacological Chaperone for Î²-Glucocerebrosidase Using Ligand Docking and Molecular Dynamics Simulation. Molecules, 2018, 23, 2683.	1.7	10
7	In silico fragment-mapping method: a new tool for fragment-based/structure-based drug discovery. Journal of Computer-Aided Molecular Design, 2018, 32, 1229-1245.	1.3	11
8	Multi-step virtual screening to develop selective DYRK1A inhibitors. Journal of Molecular Graphics and Modelling, 2017, 72, 229-239.	1.3	10
9	Precise prediction of activators for the human constitutive androstane receptor using structure-based three-dimensional quantitative structureâ€“activity relationship methods. Drug Metabolism and Pharmacokinetics, 2017, 32, 179-188.	1.1	8
10	Investigation of substrate recognition for cytochrome P450 1A2 mediated by water molecules using docking and molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2017, 74, 326-336.	1.3	16
11	In silico analyses of the effects of a point mutation and a pharmacological chaperone on the thermal fluctuation of phenylalanine hydroxylase. Biophysical Chemistry, 2017, 228, 47-54.	1.5	0
12	Gibbs Free Energy of Hydrolytic Water Molecule in Acyl-Enzyme Intermediates of a Serine Protease: A Potential Application for Computer-Aided Discovery of Mechanism-Based Reversible Covalent Inhibitors. Chemical and Pharmaceutical Bulletin, 2017, 65, 889-892.	0.6	3
13	Long chain fatty acids alter the interactive binding of ligands to the two principal drug binding sites of human serum albumin. PLoS ONE, 2017, 12, e0180404.	1.1	42
14	Prediction of three-dimensional structures and structural flexibilities of wild-type and mutant cytochrome P450 1A2 using molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2016, 68, 48-56.	1.3	15
15	Molecular Dynamics Simulations to Investigate the Influences of Amino Acid Mutations on Protein Three-Dimensional Structures of Cytochrome P450 2D6.1, 2, 10, 14A, 51, and 62. PLoS ONE, 2016, 11, e0152946.	1.1	27
16	Identification of Novel <scp>d</scp>-Aspartate Oxidase Inhibitors by in Silico Screening and Their Functional and Structural Characterization in Vitro. Journal of Medicinal Chemistry, 2015, 58, 7328-7340.	2.9	20
17	Effects of initial settings on computational proteinâ€“ligand docking accuracies for several docking programs. Molecular Simulation, 2015, 41, 1027-1034.	0.9	5
18	Three-Dimensional Quantitative Structureâ€“Activity Relationship Analysis for Human Pregnane X Receptor for the Prediction of CYP3A4 Induction in Human Hepatocytes: Structure-Based Comparative Molecular Field Analysis. Journal of Pharmaceutical Sciences, 2015, 104, 223-232.	1.6	8

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19	Differential Effects of Methoxy Group on the Interaction of Curcuminoids with Two Major Ligand Binding Sites of Human Serum Albumin. PLoS ONE, 2014, 9, e87919.	1.1	20
20	Evaluation of Influence of Single Nucleotide Polymorphisms in Cytochrome P450 2B6 on Substrate Recognition Using Computational Docking and Molecular Dynamics Simulation. PLoS ONE, 2014, 9, e96789.	1.1	25
21	In Silieo Study on the Inhibitory Interaction of Drugs with Wild-type CYP2D6.1 and the Natural Variant CYP2D6.17. Drug Metabolism and Pharmacokinetics, 2014, 29, 52-60.	1.1	14
22	Synthesis of a novel universal opioid receptor agonist with the 1,3,5-trioxazatriquinane skeleton and its pharmacologies. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 4895-4898.	1.0	9
23	3P026 Computational studies for the influences of protein flexibilities on enzymatic activities of the wild type and mutants of CYP2B6(01B. Protein: Structure & Function,Poster,The 52nd Annual Meeting) Tj ETQq1 1 0.784314 rgBT /Ov		
24	Three-dimensional Quantitative Structureâ€“Activity Relationship Analysis of Inhibitors of Human and Rat Cytochrome P4503A Enzymes. Drug Metabolism and Pharmacokinetics, 2013, 28, 345-355.	1.1	14
25	Evaluations of the conformational search accuracy of CAMDAS using experimental three-dimensional structures of protein-ligand complexes. Journal of Physics: Conference Series, 2013, 454, 012028.	0.3	4
26	AMF-26, a Novel Inhibitor of the Golgi System, Targeting ADP-ribosylation Factor 1 (Arf1) with Potential for Cancer Therapy. Journal of Biological Chemistry, 2012, 287, 3885-3897.	1.6	68
27	Quantitative Structure-Activity Relationship (QSAR) Analysis to Predict Drug-Drug Interactions of ABC Transporter ABCG2. Mini-Reviews in Medicinal Chemistry, 2012, 12, 505-514.	1.1	13
28	Essential Structure of Opioid Îº Receptor Agonist Nalfurafine for Binding to Îº Receptor 1: Synthesis of Decahydroisoquinoline Derivatives and Their Pharmacologies. Chemical and Pharmaceutical Bulletin, 2012, 60, 945-948.	0.6	15
29	513 Development of a Novel Inhibitor of ADP-Ribosylation Factor 1 (Arf1) That Has Potential for Cancer Therapy. European Journal of Cancer, 2012, 48, 158.	1.3	0
30	Abstract LB-357: Identification of a new inhibitor of the Golgi system, targeting ADP-ribosylation Factor 1 (Arf1) with potential for cancer therapy. , 2012, , .		0
31	Brazilian propolis-derived components inhibit TNF-Î±-mediated downregulation of adiponectin expression via different mechanisms in 3T3-L1 adipocytes. Biochimica Et Biophysica Acta - General Subjects, 2011, 1810, 695-703.	1.1	33
32	Identification of the three-dimensional pharmacophore of Îº-opioid receptor agonists. Bioorganic and Medicinal Chemistry, 2010, 18, 4446-4452.	1.4	30
33	NMR spectroscopy and computational analysis of interaction between Serratia marcescens chitinase B and a dipeptide derived from natural-product cyclopentapeptide chitinase inhibitor argifin. Bioorganic and Medicinal Chemistry, 2010, 18, 5835-5844.	1.4	9
34	Drug design and synthesis of a novel Îº opioid receptor agonist with an oxabicyclo[2.2.2]octane skeleton and its pharmacology. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 121-124.	1.0	33
35	3D-Pharmacophore Identification for Îº-Opioid Agonists Using Ligand-Based Drug-Design Techniques. Topics in Current Chemistry, 2010, 299, 277-307.	4.0	23
36	Evaluation of the searching abilities of HBOP and HBSITE for binding pocket detection. Journal of Computational Chemistry, 2009, 30, 2728-2737.	1.5	16

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37	Structure-Based CoMFA As a Predictive Model - CYP2C9 Inhibitors As a Test Case. Journal of Chemical Information and Modeling, 2009, 49, 853-864.	2.5	25
38	In silico multi-filter screening approaches for developing novel Î²-secretase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 2771-2775.	1.0	11
39	Determination of Ligand-Binding Sites on Proteins Using Long-Range Hydrophobic Potential. Biological and Pharmaceutical Bulletin, 2008, 31, 1552-1558.	0.6	16
40	Brownian Dynamics Simulations of a Wild Type and Mutants of Bovine Pancreatic Trypsin Inhibitors. Biological and Pharmaceutical Bulletin, 2008, 31, 2182-2186.	0.6	1
41	Comparison of Consensus Scoring Strategies for Evaluating Computational Models of Proteinâ~'Ligand Complexes. Journal of Chemical Information and Modeling, 2006, 46, 380-391.	2.5	141
42	New AMBER force field parameters of heme iron for cytochrome P450s determined by quantum chemical calculations of simplified models. Journal of Computational Chemistry, 2005, 26, 818-826.	1.5	107
43	Use of Photoaffinity Labeling and Site-directed Mutagenesis for Identification of the Key Residue Responsible for Extraordinarily High Affinity Binding of UCN-01 in Human Î±1-Acid Glycoprotein. Journal of Biological Chemistry, 2005, 280, 1384-1391.	1.6	22
44	Hydrolysis of Angiotensin II Receptor Blocker Prodrug Olmesartan Medoxomil by Human Serum Albumin and Identification of Its Catalytic Active Sites. Drug Metabolism and Disposition, 2005, 33, 1911-9.	1.7	26
45	Esterase-Like Activity of Serum Albumin: Characterization of Its Structural Chemistry Using p-Nitrophenyl Esters as Substrates. Pharmaceutical Research, 2004, 21, 285-292.	1.7	121
46	Studies of Binding Modes of (S)-Mephenytoin to Wild Types and Mutants of Cytochrome P450 2C19 and 2C9 Using Homology Modeling and Computational Docking. Pharmaceutical Research, 2004, 21, 2270-2278.	1.7	21
47	Molecular dynamics simulation of the calmodulin-trifluoperazine complex in aqueous solution. Biopolymers, 2001, 58, 410-421.	1.2	12
48	Analysis of Affinities of Penicillins for a Class C Î²-Lactamase by Molecular Dynamics Simulations. , 2000, , 399-400.		1
49	Solvation Free Energies of Amino Acids Calculated by Molecular Dynamics/Free Energy Perturbation Method.. Chemical and Pharmaceutical Bulletin, 1995, 43, 717-721.	0.6	0
50	Estimation of stabilities of staphylococcal nuclease mutants (Met32 â†' Ala and Met32 â†' Leu) using molecular dynamics/free energy perturbation. BBA - Proteins and Proteomics, 1993, 1203, 243-250.	2.1	12
51	Molecular dynamics study of the stability of staphylococcal nuclease mutants: component analysis of the free energy difference of denaturation. BBA - Proteins and Proteomics, 1993, 1163, 81-88.	2.1	15