Olli T PentikÃ¤inen

List of Publications by Year
in descending order

101	3,373	126907	168389
papers	citations	33 h-index	53 g-index

102	102	102	3830
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Optimization of Cavity-Based Negative Images to Boost Docking Enrichment in Virtual Screening. Journal of Chemical Information and Modeling, 2022, , .	5.4	2
2	Rational design, optimization, and biological evaluation of novel Î±-Phosphonopropionic acids as covalent inhibitors of Rab geranylgeranyl transferase. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 940-951.	5.2	2
3	Computational Study on the Inhibitory Effect of Natural Compounds against the SARS-CoV-2 Proteins. Bioinorganic Chemistry and Applications, 2022, 2022, 1-19.	4.1	6
4	Sdfconf: A Novel, Flexible, and Robust Molecular Data Management Tool. Journal of Chemical Information and Modeling, 2022, 62, 9-15.	5.4	3
5	Ligand-Enhanced Negative Images Optimized for Docking Rescoring. International Journal of Molecular Sciences, 2022, 23, 7871.	4.1	1
6	Negative Image-Based Screening: Rigid Docking Using Cavity Information. Methods in Molecular Biology, 2021, 2266, 125-140.	0.9	1
7	Negative Image-Based Rescoring: Using Cavity Information to Improve Docking Screening. Methods in Molecular Biology, 2021, 2266, 141-154.	0.9	0
8	Molecular docking and oxidation kinetics of 3-phenyl coumarin derivatives by human CYP2A13. Xenobiotica, 2021, 51, 1207-1216.	1.1	6
9	Substrate Selectivity of Coumarin Derivatives by Human CYP1 Enzymes: In Vitro Enzyme Kinetics and In Silico Modeling. ACS Omega, 2021, 6, 11286-11296.	3.5	8
10	Detection of Binding Sites on SARS-CoV-2 Spike Protein Receptor-Binding Domain by Molecular Dynamics Simulations in Mixed Solvents. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2021, 18, 1281-1289.	3.0	3
11	A holistic view on c-Kit in cancer: Structure, signaling, pathophysiology and its inhibitors. Biochimica Et Biophysica Acta: Reviews on Cancer, 2021, 1876, 188631.	7.4	29
12	Coumarins as Tool Compounds to Aid the Discovery of Selective Function Modulators of Steroid Hormone Binding Proteins. Molecules, 2021, 26, .	3.8	0
13	Coumarins as Tool Compounds to Aid the Discovery of Selective Function Modulators of Steroid Hormone Binding Proteins. Molecules, 2021, 26, 5142.	3.8	6
14	In vitro glucuronidation of 7-hydroxycoumarin derivatives in intestine and liver microsomes of Beagle dogs. European Journal of Pharmaceutical Sciences, 2020, 141, 105118.	4.0	3
15	In vitro sulfonation of 7-hydroxycoumarin derivatives in liver cytosol of human and six animal species. Xenobiotica, 2020, 50, 885-893.	1.1	1
16	Coumarin-Based Profluorescent and Fluorescent Substrates for Determining Xenobiotic-Metabolizing Enzyme Activities In Vitro. International Journal of Molecular Sciences, 2020, 21, 4708.	4.1	26
17	Screening of Natural Products Targeting SARS-CoV-2â€“ACE2 Receptor Interface â€“ A MixMD Based HTVS Pipeline. Frontiers in Chemistry, 2020, 8, 589769.	3.6	14
18	Inhibition of Pneumolysin Cytotoxicity by Hydrolysable Tannins. Antibiotics, 2020, 9, 930.	3.7	7

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19	Inhibition of human CYP1 enzymes by a classical inhibitor Î±â€naphthoflavone and a novel inhibitor Nâ€(3, 5â€dichlorophenyl)cyclopropanecarboxamide: An in vitro and in silico study. Chemical Biology and Drug Design, 2020, 95, 520-533.	3.2	13
20	Cyanidinâ€3â€glucoside binds to talin and modulates colon cancer cell adhesions and 3D growth. FASEB Journal, 2020, 34, 2227-2237.	0.5	21
21	Getting Docking into Shape Using Negative Image-Based Rescoring. Journal of Chemical Information and Modeling, 2019, 59, 3584-3599.	5.4	22
22	Fragmentâ€and negative imageâ€based screening of phosphodiesterase 10A inhibitors. Chemical Biology and Drug Design, 2019, 94, 1799-1812.	3.2	11
23	A Practical Perspective: The Effect of Ligand Conformers on the Negative Image-Based Screening. International Journal of Molecular Sciences, 2019, 20, 2779.	4.1	9
24	Suitability of <scp>MMGBSA</scp> for the selection of correct ligand binding modes from docking results. Chemical Biology and Drug Design, 2019, 93, 522-538.	3.2	38
25	Development of new Coumarin-based profluorescent substrates for human cytochrome P450 enzymes. Xenobiotica, 2019, 49, 1015-1024.	1.1	16
26	Blocking oestradiol synthesis pathways with potent and selective coumarin derivatives. Journal of Enzyme Inhibition and Medicinal Chemistry, 2018, 33, 743-754.	5.2	25
27	Molecular Docking-Based Design and Development of a Highly Selective Probe Substrate for UDP-glucuronosyltransferase 1A10. Molecular Pharmaceutics, 2018, 15, 923-933.	4.6	16
28	Effects of cold acclimation and dsRNA injections on Gs1l gene splicing in Drosophila montana. Scientific Reports, 2018, 8, 7577.	3.3	4
29	Improving Docking Performance Using Negative Image-Based Rescoring. Frontiers in Pharmacology, 2018, 9, 260.	3.5	20
30	Structure-Activity Relationship Analysis of 3-Phenylcoumarin-Based Monoamine Oxidase B Inhibitors. Frontiers in Chemistry, 2018, 6, 41.	3.6	36
31	Discovery of Retinoic Acid-Related Orphan Receptor Î³t Inverse Agonists via Docking and Negative Image-Based Screening. ACS Omega, 2018, 3, 6259-6266.	3.5	10
32	Identification of the Privileged Position in the Imidazo[1,2-a]pyridine Ring of Phosphonocarboxylates for Development of Rab Geranylgeranyl Transferase (RGGT) Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 8781-8800.	6.4	25
33	Skeletal Dysplasia Mutations Effect on Human Filaminsâ€™ Structure and Mechanosensing. Scientific Reports, 2017, 7, 4218.	3.3	13
34	Rocker: Open source, easy-to-use tool for AUC and enrichment calculations and ROC visualization. Journal of Cheminformatics, 2016, 8, 45.	6.1	80
35	Temperatureâ€dependent mutational robustness can explain faster molecular evolution at warm temperatures, affecting speciation rate and global patterns of species diversity. Ecography, 2016, 39, 1025-1033.	4.5	23
36	The Influence of Hydrogen Bonding on Sphingomyelin/Colipid Interactions in Bilayer Membranes. Biophysical Journal, 2016, 110, 431-440.	0.5	37

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37	Identification of estrogen receptor Î± ligands with virtual screening techniques. Journal of Molecular Graphics and Modelling, 2016, 64, 30-39.	2.4	29
38	Inhibitory effects and oxidation of 6-methylcoumarin, 7-methylcoumarin and 7-formylcoumarinviahuman CYP2A6 and its mouse and pig orthologous enzymes. Xenobiotica, 2016, 46, 14-24.	1.1	14
39	Modeling of interactions between xenobiotics and cytochrome P450 (CYP) enzymes. Frontiers in Pharmacology, 2015, 6, 123.	3.5	65
40	Ultrafast protein structure-based virtual screening with Panther. Journal of Computer-Aided Molecular Design, 2015, 29, 989-1006.	2.9	34
41	Case-specific performance of MM-PBSA, MM-GBSA, and SIE in virtual screening. Journal of Molecular Graphics and Modelling, 2015, 62, 303-318.	2.4	49
42	Reliability of Virtual Screening Methods in Prediction of PDE4Binhibitor Activity. Current Drug Discovery Technologies, 2015, 12, 117-126.	1.2	10
43	A Novel Structural Unit in the N-terminal Region of Filamins. Journal of Biological Chemistry, 2014, 289, 8588-8598.	3.4	18
44	l-Arabinose/d-galactose 1-dehydrogenase of Rhizobium leguminosarum bv. trifolii characterised and applied for bioconversion of l-arabinose to l-arabonate with Saccharomyces cerevisiae. Applied Microbiology and Biotechnology, 2014, 98, 9653-9665.	3.6	15
45	Molecular and ecological signs of mitochondrial adaptation: consequences for introgression?. Heredity, 2014, 113, 277-286.	2.6	37
46	Molecular mechanism of T-cell protein tyrosine phosphatase (TCPTP) activation by mitoxantrone. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 1988-1997.	2.3	14
47	MMGBSA As a Tool To Understand the Binding Affinities of Filaminâ€“Peptide Interactions. Journal of Chemical Information and Modeling, 2013, 53, 2626-2633.	5.4	205
48	2NH and 3OH are crucial structural requirements in sphingomyelin for sticholysin II binding and pore formation in bilayer membranes. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 1390-1395.	2.6	44
49	Novel Î±2Î²1 Integrin Inhibitors Reveal That Integrin Binding to Collagen under Shear Stress Conditions Does Not Require Receptor Preactivation. Journal of Biological Chemistry, 2012, 287, 44694-44702.	3.4	37
50	Structureâ€“activity relationship of sphingomyelin analogs with sphingomyelinase from Bacillus cereus. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 474-480.	2.6	7
51	Structural Mechanism of N-Methyl-D-Aspartate Receptor Type 1 Partial Agonism. PLoS ONE, 2012, 7, e47604.	2.5	16
52	Novel Hydrazine Molecules as Tools To Understand the Flexibility of Vascular Adhesion Protein-1 Ligand-Binding Site: Toward More Selective Inhibitors. Journal of Medicinal Chemistry, 2011, 54, 2143-2154.	6.4	24
53	Comparison of Virtual High-Throughput Screening Methods for the Identification of Phosphodiesterase-5 Inhibitors. Journal of Chemical Information and Modeling, 2011, 51, 1353-1363.	5.4	28
54	Fluorescent Small Molecule Probe to Modulate and Explore Î±2Î²1 Integrin Function. Journal of the American Chemical Society, 2011, 133, 14558-14561.	13.7	15

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55	Blockage of collagen binding to integrin Î±2Î²1: structureâ€“activity relationship of proteinâ€“protein interaction inhibitors. MedChemComm, 2011, 2, 764.	3.4	6
56	Full and Partial Agonism of Ionotropic Glutamate Receptors Indicated by Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2011, 51, 1037-1047.	5.4	26
57	A small-molecule inhibitor of integrin Î±2Î²1 introduces a new strategy for antithrombotic therapy. Thrombosis and Haemostasis, 2010, 103, 387-397.	3.4	40
58	Mammary-derived growth inhibitor (MDGI) interacts with integrin Î±-subunits and suppresses integrin activity and invasion. Oncogene, 2010, 29, 6452-6463.	5.9	45
59	Cystic Fibrosis Transmembrane Conductance Regulator Interacts with Multiple Immunoglobulin Domains of Filamin A. Journal of Biological Chemistry, 2010, 285, 17156-17165.	3.4	31
60	Pro-prion Binds Filamin A, Facilitating Its Interaction with Integrin Î²1, and Contributes to Melanomagenesis. Journal of Biological Chemistry, 2010, 285, 30328-30339.	3.4	46
61	Ligand-binding Domain Determines Endoplasmic Reticulum Exit of AMPA Receptors. Journal of Biological Chemistry, 2010, 285, 36032-36039.	3.4	29
62	Synthesis, in Vitro Activity, and Three-Dimensional Quantitative Structureâ^'Activity Relationship of Novel Hydrazine Inhibitors of Human Vascular Adhesion Protein-1. Journal of Medicinal Chemistry, 2010, 53, 6301-6315.	6.4	26
63	Exploring kainate receptor pharmacology using molecular dynamics simulations. Neuropharmacology, 2010, 58, 515-527.	4.1	22
64	Pharmacological activity of C10-substituted analogs of the high-affinity kainate receptor agonist dysiherbaine. Neuropharmacology, 2010, 58, 640-649.	4.1	15
65	Efficient Virtual Screening Using Multiple Protein Conformations Described as Negative Images of the Ligand-Binding Site. Journal of Chemical Information and Modeling, 2010, 50, 1005-1011.	5.4	20
66	Molecular Basis of Filamin A-FilGAP Interaction and Its Impairment in Congenital Disorders Associated with Filamin A Mutations. PLoS ONE, 2009, 4, e4928.	2.5	65
67	Full Domain Closure of the Ligand-binding Core of the Ionotropic Glutamate Receptor iGluR5 Induced by the High Affinity Agonist Dysiherbaine and the Functional Antagonist 8,9-Dideoxyneodysiherbaine. Journal of Biological Chemistry, 2009, 284, 14219-14229.	3.4	53
68	Cooperative symmetric to asymmetric conformational transition of the apoâ€form of scavenger decapping enzyme revealed by simulations. Proteins: Structure, Function and Bioinformatics, 2008, 70, 498-508.	2.6	26
69	Novel Analogs and Stereoisomers of the Marine Toxin Neodysiherbaine with Specificity for Kainate Receptors. Journal of Pharmacology and Experimental Therapeutics, 2008, 324, 484-496.	2.5	33
70	Synthesis and Pharmacological Characterization of N3-Substituted Willardiine Derivatives:Â Role of the Substituent at the 5-Position of the Uracil Ring in the Development of Highly Potent and Selective GLUK5Kainate Receptor Antagonists. Journal of Medicinal Chemistry, 2007, 50, 1558-1570.	6.4	70
71	Small Molecule Designed to Target Metal Binding Site in the Î±2I Domain Inhibits Integrin Function. Journal of Medicinal Chemistry, 2007, 50, 2742-2746.	6.4	24
72	Structure of three tandem filamin domains reveals auto-inhibition of ligand binding. EMBO Journal, 2007, 26, 3993-4004.	7.8	134

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73	Subtype selectivity and flexibility of ionotropic glutamate receptors upon antagonist ligand binding. Organic and Biomolecular Chemistry, 2006, 4, 1058.	2.8	20
74	New inhibitors of 17Î²-hydroxysteroid dehydrogenase type 1. Molecular and Cellular Endocrinology, 2006, 248, 192-198.	3.2	51
75	Binding Properties of HABA-Type Azo Derivatives to Avidin and Avidin-Related Protein 4. Chemistry and Biology, 2006, 13, 1029-1039.	6.0	36
76	Vascular amine oxidases are needed for leukocyte extravasation into inflamed joints in vivo. Arthritis and Rheumatism, 2006, 54, 2852-2862.	6.7	54
77	Determination of Binding Site Residues Responsible for the Subunit Selectivity of Novel Marine-Derived Compounds on Kainate Receptors. Molecular Pharmacology, 2006, 69, 1849-1860.	2.3	30
78	Divergent Pharmacological Activity of Novel Marine-Derived Excitatory Amino Acids on Glutamate Receptors. Journal of Pharmacology and Experimental Therapeutics, 2005, 314, 1068-1078.	2.5	52
79	Functional Display of an Î±2 Integrin-Specific Motif (RKK) on the Surface of Baculovirus Particles. Technology in Cancer Research and Treatment, 2005, 4, 437-445.	1.9	9
80	Construction of Hevein (Hev b 6.02) with Reduced Allergenicity for Immunotherapy of Latex Allergy by Comutation of Six Amino Acid Residues on the Conformational IgE Epitopes. Journal of Immunology, 2004, 172, 2621-2628.	0.8	47
81	Jararhagin-derived RKKH Peptides Induce Structural Changes in Î±1I Domain of Human Integrin Î±1Î²1. Journal of Biological Chemistry, 2004, 279, 7962-7970.	3.4	35
82	Chicken Avidin-related Protein 4/5 Shows Superior Thermal Stability when Compared with Avidin while Retaining High Affinity to Biotin. Journal of Biological Chemistry, 2004, 279, 9337-9343.	3.4	44
83	BODIL: a molecular modeling environment for structure-function analysis and drug design. Journal of Computer-Aided Molecular Design, 2004, 18, 401-419.	2.9	200
84	Model structures of the N-methyl-d-aspartate receptor subunit NR1 explain the molecular recognition of agonist and antagonist ligands. Journal of Structural Biology, 2004, 145, 205-215.	2.8	10
85	Selective agonist binding of (S)-2-amino-3-(3-hydroxy-5-methyl-4-isoxazolyl)propionic acid (AMPA) and 2S-(2Î±,3Î²,4Î²)-2-carboxy-4-(1-methylethenyl)-3-pyrrolidineacetic acid (kainate) receptors: a molecular modeling study. Biochemical Pharmacology, 2003, 66, 2413-2425.	4.4	26
86	Î±11Î²1 Integrin Recognizes the GFOGER Sequence in Interstitial Collagens. Journal of Biological Chemistry, 2003, 278, 7270-7277.	3.4	143
87	The Major Conformational IgE-binding Epitopes of Hevein (Hev b6.02) Are Identified by a Novel Chimera-based Allergen Epitope Mapping Strategy. Journal of Biological Chemistry, 2002, 277, 22656-22661.	3.4	37
88	Discrimination between Agonists and Antagonists by the Î±-Amino-3-hydroxy-5-methyl-4-isoxazole Propionic Acid-selective Glutamate Receptor. Journal of Biological Chemistry, 2002, 277, 41940-41947.	3.4	10
89	Chicken avidin-related proteins show altered biotin-binding and physico-chemical properties as compared with avidin. Biochemical Journal, 2002, 363, 609.	3.7	37
90	Chicken avidin-related proteins show altered biotin-binding and physico-chemical properties as compared with avidin. Biochemical Journal, 2002, 363, 609-617.	3.7	47

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91	Antiferritin VL homodimer binds human spleen ferritin with high specificity. Journal of Structural Biology, 2002, 138, 171-186.	2.8	9
92	Determinants of antagonist binding at the Î±-amino-3-hydroxy-5-methyl-4-isoxazolepropionic acid receptor subunit, GluR-D. FEBS Journal, 2002, 269, 6261-6270.	0.2	8
93	Characterization of Bile Salt/Cyclodextrin Interactions Using Isothermal Titration Calorimetry. Langmuir, 2001, 17, 7107-7111.	3.5	48
94	Selective Binding of Collagen Subtypes by Integrin Î±1I, Î±2I, and Î±10I Domains. Journal of Biological Chemistry, 2001, 276, 48206-48212.	3.4	221
95	Integrin Î±2I Domain Recognizes Type I and Type IV Collagens by Different Mechanisms. Journal of Biological Chemistry, 2000, 275, 3348-3354.	3.4	65
96	A Peptide Inhibiting the Collagen Binding Function of Integrin Î±2I Domain. Journal of Biological Chemistry, 1999, 274, 3513-3521.	3.4	81
97	â€œRKKHâ€•Peptides from the Snake Venom Metalloproteinase ofBothrops jararaca Bind Near the Metal Ion-dependent Adhesion Site of the Human Integrin Î±2 I-domain. Journal of Biological Chemistry, 1999, 274, 31493-31505.	3.4	33
98	A dimeric ternary complex of FGFR1, heparin and FGF-1 leads to an â€˜electrostatic sandwichâ€™ model for heparin binding. Structure, 1999, 7, 699-709.	3.3	24
99	A dimeric ternary complex of FGFR1, heparin and FGF-1 leads to an â€˜electrostatic sandwichâ€™ model for heparin binding. Structure, 1999, 7, R198.	3.3	0
100	AMPA receptors and bacterial periplasmic amino acid-binding proteins share the ionic mechanism of ligand recognition. EMBO Journal, 1998, 17, 4704-4711.	7.8	61
101	The core domain of retrotransposon integrase in Hordeum: predicted structure and evolution. Molecular Biology and Evolution, 1998, 15, 1135-1144.	8.9	25