# 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 | 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 |
| 2 | 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 |
| 3 | 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 |
| 4 | Î±11Î²1 Integrin Recognizes the GFOGER Sequence in Interstitial Collagens. Journal of Biological Chemistry, 2003, 278, 7270-7277. | 3.4 | 143 |
| 5 | Structure of three tandem filamin domains reveals auto-inhibition of ligand binding. EMBO Journal, 2007, 26, 3993-4004. | 7.8 | 134 |
| 6 | A Peptide Inhibiting the Collagen Binding Function of Integrin Î±2I Domain. Journal of Biological Chemistry, 1999, 274, 3513-3521. | 3.4 | 81 |
| 7 | Rocker: Open source, easy-to-use tool for AUC and enrichment calculations and ROC visualization. Journal of Cheminformatics, 2016, 8, 45. | 6.1 | 80 |
| 8 | 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 |
| 9 | 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 |
| 10 | 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 |
| 11 | Modeling of interactions between xenobiotics and cytochrome P450 (CYP) enzymes. Frontiers in Pharmacology, 2015, 6, 123. | 3.5 | 65 |
| 12 | 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 |
| 13 | Vascular amine oxidases are needed for leukocyte extravasation into inflamed joints in vivo. Arthritis and Rheumatism, 2006, 54, 2852-2862. | 6.7 | 54 |
| 14 | 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 |
| 15 | 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 |
| 16 | New inhibitors of 17Î²-hydroxysteroid dehydrogenase type 1. Molecular and Cellular Endocrinology, 2006, 248, 192-198. | 3.2 | 51 |
| 17 | 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 |
| 18 | Characterization of Bile Salt/Cyclodextrin Interactions Using Isothermal Titration Calorimetry. Langmuir, 2001, 17, 7107-7111. | 3.5 | 48 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | 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 |
| 22 | Mammary-derived growth inhibitor (MDGI) interacts with integrin Î±-subunits and suppresses integrin activity and invasion. Oncogene, 2010, 29, 6452-6463. | 5.9 | 45 |
| 23 | 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 |
| 24 | 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 |
| 25 | 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 |
| 26 | 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 |
| 27 | 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 |
| 28 | Chicken avidin-related proteins show altered biotin-binding and physico-chemical properties as compared with avidin. Biochemical Journal, 2002, 363, 609. | 3.7 | 37 |
| 29 | 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 |
| 30 | Molecular and ecological signs of mitochondrial adaptation: consequences for introgression?. Heredity, 2014, 113, 277-286. | 2.6 | 37 |
| 31 | The Influence of Hydrogen Bonding on Sphingomyelin/Colipid Interactions in Bilayer Membranes. Biophysical Journal, 2016, 110, 431-440. | 0.5 | 37 |
| 32 | Binding Properties of HABA-Type Azo Derivatives to Avidin and Avidin-Related Protein 4. Chemistry and Biology, 2006, 13, 1029-1039. | 6.0 | 36 |
| 33 | Structure-Activity Relationship Analysis of 3-Phenylcoumarin-Based Monoamine Oxidase B Inhibitors. Frontiers in Chemistry, 2018, 6, 41. | 3.6 | 36 |
| 34 | 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 |
| 35 | Ultrafast protein structure-based virtual screening with Panther. Journal of Computer-Aided Molecular Design, 2015, 29, 989-1006. | 2.9 | 34 |
| 36 | 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 |

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|---|---|---|---|
| 37 | 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 |
| 38 | Cystic Fibrosis Transmembrane Conductance Regulator Interacts with Multiple Immunoglobulin Domains of Filamin A. Journal of Biological Chemistry, 2010, 285, 17156-17165. | 3.4 | 31 |
| 39 | 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 |
| 40 | Ligand-binding Domain Determines Endoplasmic Reticulum Exit of AMPA Receptors. Journal of Biological Chemistry, 2010, 285, 36032-36039. | 3.4 | 29 |
| 41 | Identification of estrogen receptor Î± ligands with virtual screening techniques. Journal of Molecular Graphics and Modelling, 2016, 64, 30-39. | 2.4 | 29 |
| 42 | 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 |
| 43 | 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 |
| 44 | 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 |
| 45 | 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 |
| 46 | 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 |
| 47 | 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 |
| 48 | 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 |
| 49 | The core domain of retrotransposon integrase in Hordeum: predicted structure and evolution. Molecular Biology and Evolution, 1998, 15, 1135-1144. | 8.9 | 25 |
| 50 | 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 |
| 51 | Blocking oestradiol synthesis pathways with potent and selective coumarin derivatives. Journal of Enzyme Inhibition and Medicinal Chemistry, 2018, 33, 743-754. | 5.2 | 25 |
| 52 | 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 |
| 53 | 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 |
| 54 | 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 |

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| 55 | 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 |
| 56 | Exploring kainate receptor pharmacology using molecular dynamics simulations. Neuropharmacology, 2010, 58, 515-527. | 4.1 | 22 |
| 57 | Getting Docking into Shape Using Negative Image-Based Rescoring. Journal of Chemical Information and Modeling, 2019, 59, 3584-3599. | 5.4 | 22 |
| 58 | Cyanidinâ€3â€glucoside binds to talin and modulates colon cancer cell adhesions and 3D growth. FASEB Journal, 2020, 34, 2227-2237. | 0.5 | 21 |
| 59 | Subtype selectivity and flexibility of ionotropic glutamate receptors upon antagonist ligand binding. Organic and Biomolecular Chemistry, 2006, 4, 1058. | 2.8 | 20 |
| 60 | 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 |
| 61 | Improving Docking Performance Using Negative Image-Based Rescoring. Frontiers in Pharmacology, 2018, 9, 260. | 3.5 | 20 |
| 62 | A Novel Structural Unit in the N-terminal Region of Filamins. Journal of Biological Chemistry, 2014, 289, 8588-8598. | 3.4 | 18 |
| 63 | 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 |
| 64 | Development of new Coumarin-based profluorescent substrates for human cytochrome P450 enzymes. Xenobiotica, 2019, 49, 1015-1024. | 1.1 | 16 |
| 65 | Structural Mechanism of N-Methyl-D-Aspartate Receptor Type 1 Partial Agonism. PLoS ONE, 2012, 7, e47604. | 2.5 | 16 |
| 66 | Pharmacological activity of C10-substituted analogs of the high-affinity kainate receptor agonist dysiherbaine. Neuropharmacology, 2010, 58, 640-649. | 4.1 | 15 |
| 67 | 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 |
| 68 | 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 |
| 69 | 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 |
| 70 | 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 |
| 71 | 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 |
| 72 | Skeletal Dysplasia Mutations Effect on Human Filaminsâ€™ Structure and Mechanosensing. Scientific Reports, 2017, 7, 4218. | 3.3 | 13 |

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| 73 | 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 |
| 74 | Fragmentâ€and negative imageâ€based screening of phosphodiesterase 10A inhibitors. Chemical Biology and Drug Design, 2019, 94, 1799-1812. | 3.2 | 11 |
| 75 | 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 |
| 76 | 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 |
| 77 | 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 |
| 78 | Reliability of Virtual Screening Methods in Prediction of PDE4Binhibitor Activity. Current Drug Discovery Technologies, 2015, 12, 117-126. | 1.2 | 10 |
| 79 | Antiferritin VL homodimer binds human spleen ferritin with high specificity. Journal of Structural Biology, 2002, 138, 171-186. | 2.8 | 9 |
| 80 | 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 |
| 81 | 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 |
| 82 | 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 |
| 83 | 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 |
| 84 | Structureâ€“activity relationship of sphingomyelin analogs with sphingomyelinase from Bacillus cereus. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 474-480. | 2.6 | 7 |
| 85 | Inhibition of Pneumolysin Cytotoxicity by Hydrolysable Tannins. Antibiotics, 2020, 9, 930. | 3.7 | 7 |
| 86 | Blockage of collagen binding to integrin Î±2Î²1: structureâ€“activity relationship of proteinâ€“protein interaction inhibitors. MedChemComm, 2011, 2, 764. | 3.4 | 6 |
| 87 | Molecular docking and oxidation kinetics of 3-phenyl coumarin derivatives by human CYP2A13. Xenobiotica, 2021, 51, 1207-1216. | 1.1 | 6 |
| 88 | Coumarins as Tool Compounds to Aid the Discovery of Selective Function Modulators of Steroid Hormone Binding Proteins. Molecules, 2021, 26, 5142. | 3.8 | 6 |
| 89 | 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 |
| 90 | Effects of cold acclimation and dsRNA injections on Gs1l gene splicing in Drosophila montana. Scientific Reports, 2018, 8, 7577. | 3.3 | 4 |

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| 91 | 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 |
| 92 | 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 |
| 93 | Sdfconf: A Novel, Flexible, and Robust Molecular Data Management Tool. Journal of Chemical Information and Modeling, 2022, 62, 9-15. | 5.4 | 3 |
| 94 | Optimization of Cavity-Based Negative Images to Boost Docking Enrichment in Virtual Screening. Journal of Chemical Information and Modeling, 2022, , . | 5.4 | 2 |
| 95 | 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 |
| 96 | In vitro sulfonation of 7-hydroxycoumarin derivatives in liver cytosol of human and six animal species. Xenobiotica, 2020, 50, 885-893. | 1.1 | 1 |
| 97 | Negative Image-Based Screening: Rigid Docking Using Cavity Information. Methods in Molecular Biology, 2021, 2266, 125-140. | 0.9 | 1 |
| 98 | Ligand-Enhanced Negative Images Optimized for Docking Rescoring. International Journal of Molecular Sciences, 2022, 23, 7871. | 4.1 | 1 |
| 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 | Negative Image-Based Rescoring: Using Cavity Information to Improve Docking Screening. Methods in Molecular Biology, 2021, 2266, 141-154. | 0.9 | 0 |
| 101 | Coumarins as Tool Compounds to Aid the Discovery of Selective Function Modulators of Steroid Hormone Binding Proteins. Molecules, 2021, 26, . | 3.8 | 0 |