# Tudor I Oprea

## List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/5360997/publications.pdf

Version: 2024-02-01

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|---|---|---|---|
| 232 papers | 21,646 citations | 10979 71 h-index | 11601 135 g-index |
| 297 all docs | 297 docs citations | 297 times ranked | 22387 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Getting Started with the IDG KMC Datasets and Tools. Current Protocols, 2022, 2, e355. | 1.3 | 6 |
| 2 | GLUT3 inhibitor discovery through in silico ligand screening and in vivo validation in eukaryotic expression systems. Scientific Reports, 2022, 12, 1429. | 1.6 | 9 |
| 3 | A Workflow of Integrated Resources to Catalyze Network Pharmacology Driven COVID-19 Research. Journal of Chemical Information and Modeling, 2022, 62, 718-729. | 2.5 | 2 |
| 4 | Machine learning prediction and tau-based screening identifies potential Alzheimerâ€™s disease genes relevant to immunity. Communications Biology, 2022, 5, 125. | 2.0 | 18 |
| 5 | Diseases 2.0: a weekly updated database of diseaseâ€“gene associations from text mining and data integration. Database: the Journal of Biological Databases and Curation, 2022, 2022, . | 1.4 | 30 |
| 6 | A Comprehensive COVID-19 Daily News and Medical Literature Briefing to Inform Health Care and Policy in New Mexico: Implementation Study. JMIR Medical Education, 2022, 8, e23845. | 1.2 | 0 |
| 7 | State of the Art and Uses for the Biopharmaceutics Drug Disposition Classification System (BDDCS): New Additions, Revisions, and Citation References. AAPS Journal, 2022, 24, 37. | 2.2 | 22 |
| 8 | CACHE (Critical Assessment of Computational Hit-finding Experiments): A publicâ€“private partnership benchmarking initiative to enable the development of computational methods for hit-finding. Nature Reviews Chemistry, 2022, 6, 287-295. | 13.8 | 22 |
| 9 | AlphaFold illuminates half of the dark human proteins. Current Opinion in Structural Biology, 2022, 74, 102372. | 2.6 | 45 |
| 10 | TCRD and Pharos 2021: mining the human proteome for disease biology. Nucleic Acids Research, 2021, 49, D1334-D1346. | 6.5 | 109 |
| 11 | DrugCentral 2021 supports drug discovery and repositioning. Nucleic Acids Research, 2021, 49, D1160-D1169. | 6.5 | 129 |
| 12 | InContext: curation of medical context for drug indications. Journal of Biomedical Semantics, 2021, 12, 2. | 0.9 | 1 |
| 13 | A machine learning platform to estimate anti-SARS-CoV-2 activities. Nature Machine Intelligence, 2021, 3, 527-535. | 8.3 | 45 |
| 14 | TIGA: target illumination GWAS analytics. Bioinformatics, 2021, 37, 3865-3873. | 1.8 | 9 |
| 15 | Crowdsourced mapping of unexplored target space of kinase inhibitors. Nature Communications, 2021, 12, 3307. | 5.8 | 41 |
| 16 | Identification of new GLUT2-selective inhibitors through in silico ligand screening and validation in eukaryotic expression systems. Scientific Reports, 2021, 11, 13751. | 1.6 | 12 |
| 17 | COVIDomic: A multi-modal cloud-based platform for identification of risk factors associated with COVID-19 severity. PLoS Computational Biology, 2021, 17, e1009183. | 1.5 | 7 |
| 18 | A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151. | 18.7 | 128 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Supervised learning with word embeddings derived from PubMed captures latent knowledge about protein kinases and cancer. NAR Genomics and Bioinformatics, 2021, 3, lqab113. | 1.5 | 4 |
| 20 | Diabetes mellitus risk for 102 drugs and drug combinations used in patients with bipolar disorder. Psychoneuroendocrinology, 2020, 112, 104511. | 1.3 | 17 |
| 21 | How to Illuminate the Druggable Genome Using Pharos. Current Protocols in Bioinformatics, 2020, 69, e92. | 25.8 | 33 |
| 22 | Therapies for rare diseases: therapeutic modalities, progress and challenges ahead. Nature Reviews Drug Discovery, 2020, 19, 93-111. | 21.5 | 190 |
| 23 | Virtual and In Vitro Antiviral Screening Revive Therapeutic Drugs for COVID-19. ACS Pharmacology and Translational Science, 2020, 3, 1278-1292. | 2.5 | 43 |
| 24 | Off-Patent Drug Repositioning. Journal of Chemical Information and Modeling, 2020, 60, 5746-5753. | 2.5 | 14 |
| 25 | Artificial intelligence, drug repurposing and peer review. Nature Biotechnology, 2020, 38, 1127-1131. | 9.4 | 56 |
| 26 | Deciphering the Plasma Proteome of Type 2 Diabetes. Diabetes, 2020, 69, 2766-2778. | 0.3 | 34 |
| 27 | SmartGraph: a network pharmacology investigation platform. Journal of Cheminformatics, 2020, 12, 5. | 2.8 | 10 |
| 28 | Will Artificial Intelligence for Drug Discovery Impact Clinical Pharmacology?. Clinical Pharmacology and Therapeutics, 2020, 107, 780-785. | 2.3 | 77 |
| 29 | QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564. | 18.7 | 427 |
| 30 | How many rare diseases are there?. Nature Reviews Drug Discovery, 2020, 19, 77-78. | 21.5 | 204 |
| 31 | Novel drug targets in 2019. Nature Reviews Drug Discovery, 2020, 19, 300-300. | 21.5 | 12 |
| 32 | Exploring the dark genome: implications for precision medicine. Mammalian Genome, 2019, 30, 192-200. | 1.0 | 40 |
| 33 | A Selective Ligand for Estrogen Receptor Proteins Discriminates Rapid and Genomic Signaling. Cell Chemical Biology, 2019, 26, 1692-1702.e5. | 2.5 | 13 |
| 34 | Can BDDCS illuminate targets in drug design?. Drug Discovery Today, 2019, 24, 2299-2306. | 3.2 | 7 |
| 35 | Novel drug targets in 2018. Nature Reviews Drug Discovery, 2019, , . | 21.5 | 11 |
| 36 | The human endogenous metabolome as a pharmacology baseline for drug discovery. Drug Discovery Today, 2019, 24, 1806-1820. | 3.2 | 9 |

| # | Article | IF | Citations |
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| 37 | Comparison of 71 bipolar disorder pharmacotherapies for kidney disorder risk: The potential hazards of polypharmacy. Journal of Affective Disorders, 2019, 252, 201-211. | 2.0 | 8 |
| 38 | How to Prepare a Compound Collection Prior to Virtual Screening. Methods in Molecular Biology, 2019, 1939, 119-138. | 0.4 | 3 |
| 39 | DrugCentral 2018: an update. Nucleic Acids Research, 2019, 47, D963-D970. | 6.5 | 104 |
| 40 | Unexplored therapeutic opportunities in the human genome. Nature Reviews Drug Discovery, 2018, 17, 317-332. | 21.5 | 263 |
| 41 | In silico toxicology protocols. Regulatory Toxicology and Pharmacology, 2018, 96, 1-17. | 1.3 | 159 |
| 42 | Leaving us with fond memories, smiles, SMILES and, alas, tears: a tribute to David Weininger, 1952â€“2016. Journal of Computer-Aided Molecular Design, 2018, 32, 313-319. | 1.3 | 1 |
| 43 | Chronic obstructive pulmonary disease phenotypes using cluster analysis of electronic medical records. Health Informatics Journal, 2018, 24, 394-409. | 1.1 | 22 |
| 44 | High-Throughput Flow Cytometry Screening of Multidrug Efflux Systems. Methods in Molecular Biology, 2018, 1700, 293-318. | 0.4 | 12 |
| 45 | Proteomic analysis defines kinase taxonomies specific for subtypes of breast cancer. Oncotarget, 2018, 9, 15480-15497. | 0.8 | 24 |
| 46 | Far away from the lamppost. PLoS Biology, 2018, 16, e3000067. | 2.6 | 10 |
| 47 | Activation of Rho Family GTPases by Small Molecules. ACS Chemical Biology, 2018, 13, 1514-1524. | 1.6 | 13 |
| 48 | Pharos: Collating protein information to shed light on the druggable genome. Nucleic Acids Research, 2017, 45, D995-D1002. | 6.5 | 271 |
| 49 | Protein biomarker druggability profiling. Journal of Biomedical Informatics, 2017, 66, 241-247. | 2.5 | 2 |
| 50 | TIN-X: target importance and novelty explorer. Bioinformatics, 2017, 33, 2601-2603. | 1.8 | 27 |
| 51 | DrugCentral: online drug compendium. Nucleic Acids Research, 2017, 45, D932-D939. | 6.5 | 215 |
| 52 | A comprehensive map of molecular drug targets. Nature Reviews Drug Discovery, 2017, 16, 19-34. | 21.5 | 1,608 |
| 53 | Formalizing drug indications on the road to therapeutic intent. Journal of the American Medical Informatics Association: JAMIA, 2017, 24, 1169-1172. | 2.2 | 8 |
| 54 | Learning reference-enriched approach towards large scale active ontology alignment and integration. , 2017, , . | | 1 |

| # | Article | IF | Citations |
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| 55 | The ontology reference model for visual selectivity analysis in drug-target interactions. , 2017, , . | | 1 |
| 56 | Drug target ontology to classify and integrate drug discovery data. Journal of Biomedical Semantics, 2017, 8, 50. | 0.9 | 63 |
| 57 | ChemProt-3.0: a global chemical biology diseases mapping. Database: the Journal of Biological Databases and Curation, 2016, 2016, bav123. | 1.4 | 75 |
| 58 | Glossary of terms used in computational drug design, part II (IUPAC Recommendations 2015). Pure and Applied Chemistry, 2016, 88, 239-264. | 0.9 | 12 |
| 59 | BDDCS, the Rule of 5 and drugability. Advanced Drug Delivery Reviews, 2016, 101, 89-98. | 6.6 | 475 |
| 60 | Badapple: promiscuity patterns from noisy evidence. Journal of Cheminformatics, 2016, 8, 29. | 2.8 | 85 |
| 61 | Discovery of a specific inhibitor of human GLUT5 by virtual screening and in vitro transport evaluation. Scientific Reports, 2016, 6, 24240. | 1.6 | 45 |
| 62 | Impact of similarity threshold on the topology of molecular similarity networks and clustering outcomes. Journal of Cheminformatics, 2016, 8, 16. | 2.8 | 15 |
| 63 | A pepducin designed to modulate P2Y 2 R function interacts with FPR2 in human neutrophils and transfers ATP to an NADPH-oxidase-activating ligand through a receptor cross-talk mechanism. Biochimica Et Biophysica Acta - Molecular Cell Research, 2016, 1863, 1228-1237. | 1.9 | 17 |
| 64 | Novel Activities of Select NSAID R-Enantiomers against Rac1 and Cdc42 GTPases. PLoS ONE, 2015, 10, e0142182. | 1.1 | 36 |
| 65 | Ligand-directed targeting of lymphatic vessels uncovers mechanistic insights in melanoma metastasis. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2521-2526. | 3.3 | 16 |
| 66 | Advancing Biological Understanding and Therapeutics Discovery with Small-Molecule Probes. Cell, 2015, 161, 1252-1265. | 13.5 | 135 |
| 67 | Ligandâ€Directed Profiling of Organelles with Internalizing Phage Libraries. Current Protocols in Protein Science, 2015, 79, 30.4.1-30.4.30. | 2.8 | 2 |
| 68 | Defining the microbial effluxome in the content of the host-microbiome interaction. Frontiers in Pharmacology, 2015, 6, 31. | 1.6 | 5 |
| 69 | P2Y2 receptor signaling in neutrophils is regulated from inside by a novel cytoskeleton-dependent mechanism. Experimental Cell Research, 2015, 336, 242-252. | 1.2 | 31 |
| 70 | A Novel Pharmacologic Activity of Ketorolac for Therapeutic Benefit in Ovarian Cancer Patients. Clinical Cancer Research, 2015, 21, 5064-5072. | 3.2 | 40 |
| 71 | Computational and Practical Aspects of Drug Repositioning. Drug Repurposing Rescue and Repositioning, 2015, 1, 28-35. | 0.0 | 6 |
| 72 | Computational and Practical Aspects of Drug Repositioning. Assay and Drug Development Technologies, 2015, 13, 299-306. | 0.6 | 89 |

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| 73 | FRET detection of lymphocyte functionâ€“associated antigen-1 conformational extension. Molecular Biology of the Cell, 2015, 26, 43-54. | 0.9 | 17 |
| 74 | CFP-10 from Mycobacterium tuberculosis Selectively Activates Human Neutrophils through a Pertussis Toxin-Sensitive Chemotactic Receptor. Infection and Immunity, 2015, 83, 205-213. | 1.0 | 36 |
| 75 | CHEMICAL AND BIOLOGICAL DESCRIPTOR INTEGRATION IMPROVES COMPUTATIONAL MODELING OF RAT TOXICITY. Revue Roumaine De Chimie, 2015, 60, 219-226. | 0.4 | 4 |
| 76 | An Automated High-Throughput Cell-Based Multiplexed Flow Cytometry Assay to Identify Novel Compounds to Target Candida albicans Virulence-Related Proteins. PLoS ONE, 2014, 9, e110354. | 1.1 | 15 |
| 77 | Antibacterial Activity of Pepducins, Allosterical Modulators of Formyl Peptide Receptor Signaling. Antimicrobial Agents and Chemotherapy, 2014, 58, 2985-2988. | 1.4 | 13 |
| 78 | Characterization of a Cdc42 protein inhibitor and its use as a molecular probe.. Journal of Biological Chemistry, 2014, 289, 6837. | 1.6 | 0 |
| 79 | An Overview of the Challenges in Designing, Integrating, and Delivering BARD: A Public Chemical-Biology Resource and Query Portal for Multiple Organizations, Locations, and Disciplines. Journal of Biomolecular Screening, 2014, 19, 614-627. | 2.6 | 22 |
| 80 | A novel receptor cross-talk between the ATP receptor P2Y2 and formyl peptide receptors reactivates desensitized neutrophils to produce superoxide. Experimental Cell Research, 2014, 323, 209-217. | 1.2 | 46 |
| 81 | Temporal disease trajectories condensed from population-wide registry data covering 6.2 million patients. Nature Communications, 2014, 5, 4022. | 5.8 | 289 |
| 82 | The University of New Mexico Center for Molecular Discovery. Combinatorial Chemistry and High Throughput Screening, 2014, 17, 256-265. | 0.6 | 8 |
| 83 | Emerging trends in the discovery of natural product antibacterials. Current Opinion in Pharmacology, 2013, 13, 678-687. | 1.7 | 42 |
| 84 | A Chemogenomic Analysis of Ionization Constantsâ€”Implications for Drug Discovery. ChemMedChem, 2013, 8, 242-255. | 1.6 | 40 |
| 85 | A systems chemical biology study of malate synthase and isocitrate lyase inhibition in Mycobacterium tuberculosis during active and NRP growth. Computational Biology and Chemistry, 2013, 47, 167-180. | 1.1 | 17 |
| 86 | The leukocyte chemotactic receptor FPR2, but not the closely related FPR1, is sensitive to cell-penetrating pepducins with amino acid sequences descending from the third intracellular receptor loop. Biochimica Et Biophysica Acta - Molecular Cell Research, 2013, 1833, 1914-1923. | 1.9 | 42 |
| 87 | Discovery of a Novel Selective PPARÎ³ Ligand with Partial Agonist Binding Properties by Integrated in Silico/in Vitro Work Flow. Journal of Chemical Information and Modeling, 2013, 53, 923-937. | 2.5 | 29 |
| 88 | Fluorescent substrates for flow cytometric evaluation of efflux inhibition in ABCB1, ABCC1, and ABCG2 transporters. Analytical Biochemistry, 2013, 437, 77-87. | 1.1 | 57 |
| 89 | The significance of acid/base properties in drug discovery. Chemical Society Reviews, 2013, 42, 485-496. | 18.7 | 236 |
| 90 | The CARLSBAD Database: A Confederated Database of Chemical Bioactivities. Database: the Journal of Biological Databases and Curation, 2013, 2013, bat044. | 1.4 | 30 |

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| 91 | Bradycardic effects mediated by activation of G proteinâ€coupled estrogen receptor in rat nucleus ambiguus. Experimental Physiology, 2013, 98, 679-691. | 0.9 | 23 |
| 92 | Characterization of a Cdc42 Protein Inhibitor and Its Use as a Molecular Probe. Journal of Biological Chemistry, 2013, 288, 8531-8543. | 1.6 | 134 |
| 93 | A Selective ATP-Binding Cassette Subfamily G Member 2 Efflux Inhibitor Revealed via High-Throughput Flow Cytometry. Journal of Biomolecular Screening, 2013, 18, 26-38. | 2.6 | 20 |
| 94 | A Novel Flow Cytometric HTS Assay Reveals Functional Modulators of ATP Binding Cassette Transporter ABCB6. PLoS ONE, 2012, 7, e40005. | 1.1 | 15 |
| 95 | ChemProt-2.0: visual navigation in a disease chemical biology database. Nucleic Acids Research, 2012, 41, D464-D469. | 6.5 | 50 |
| 96 | Targeting the Transposase Domain of the DNA Repair Component Metnase to Enhance Chemotherapy. Cancer Research, 2012, 72, 6200-6208. | 0.4 | 29 |
| 97 | Compound Collection Preparation for Virtual Screening. Methods in Molecular Biology, 2012, 910, 125-143. | 0.4 | 6 |
| 98 | Drug Repurposing: Far Beyond New Targets for Old Drugs. AAPS Journal, 2012, 14, 759-763. | 2.2 | 212 |
| 99 | Mechanisms of G Protein-Coupled Estrogen Receptor-Mediated Spinal Nociception. Journal of Pain, 2012, 13, 742-754. | 0.7 | 35 |
| 100 | Fitting the complexity of GPCRs modulation into simple hypotheses of ligand design. Journal of Molecular Graphics and Modelling, 2012, 38, 70-81. | 1.3 | 11 |
| 101 | A Competitive Nucleotide Binding Inhibitor: In Vitro Characterization of Rab7 GTPase Inhibition. ACS Chemical Biology, 2012, 7, 1095-1108. | 1.6 | 76 |
| 102 | BDDCS Class Prediction for New Molecular Entities. Molecular Pharmaceutics, 2012, 9, 570-580. | 2.3 | 78 |
| 103 | Improving the prediction of the brain disposition for orally administered drugs using BDDCS. Advanced Drug Delivery Reviews, 2012, 64, 95-109. | 6.6 | 65 |
| 104 | A non-peptide receptor inhibitor with selectivity for one of the neutrophil formyl peptide receptors, FPR 1. Biochemical Pharmacology, 2012, 83, 1655-1662. | 2.0 | 14 |
| 105 | Of possible cheminformatics futures. Journal of Computer-Aided Molecular Design, 2012, 26, 107-112. | 1.3 | 10 |
| 106 | Drug repurposing from an academic perspective. Drug Discovery Today: Therapeutic Strategies, 2011, 8, 61-69. | 0.5 | 240 |
| 107 | Identification of a GPER/GPR30 antagonist with improved estrogen receptor counterselectivity. Journal of Steroid Biochemistry and Molecular Biology, 2011, 127, 358-366. | 1.2 | 254 |
| 108 | Linking Pharmacology to Clinical Reports: Cyclobenzaprine and Its Possible Association With Serotonin Syndrome. Clinical Pharmacology and Therapeutics, 2011, 90, 662-665. | 2.3 | 46 |

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|---|---|---|---|
| 109 | Microbial Efflux Pump Inhibition: Tactics and Strategies. Current Pharmaceutical Design, 2011, 17, 1291-1302. | 0.9 | 140 |
| 110 | G protein-coupled estrogen receptor 1-mediated effects in the rat myometrium. American Journal of Physiology - Cell Physiology, 2011, 301, C1262-C1269. | 2.1 | 35 |
| 111 | Computational Systems Chemical Biology. Methods in Molecular Biology, 2011, 672, 459-488. | 0.4 | 19 |
| 112 | A Novel Approach for Predicting P-Glycoprotein (ABCB1) Inhibition Using Molecular Interaction Fields. Journal of Medicinal Chemistry, 2011, 54, 1740-1751. | 2.9 | 141 |
| 113 | BDDCS Applied to Over 900 Drugs. AAPS Journal, 2011, 13, 519-547. | 2.2 | 532 |
| 114 | Understanding drugâ€likeness. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 760-781. | 6.2 | 152 |
| 115 | Associating Drugs, Targets and Clinical Outcomes into an Integrated Network Affords a New Platform for Computerâ€Aided Drug Repurposing. Molecular Informatics, 2011, 30, 100-111. | 1.4 | 100 |
| 116 | Nextâ€generation QSAR. Molecular Informatics, 2011, 30, 89-89. | 1.4 | 1 |
| 117 | Cross-Pharmacology Analysis of G Protein-Coupled Receptors. Current Topics in Medicinal Chemistry, 2011, 11, 1956-1963. | 1.0 | 33 |
| 118 | High-Throughput Screen for the Chemical Inhibitors of Antiapoptotic Bcl-2 Family Proteins by Multiplex Flow Cytometry. Assay and Drug Development Technologies, 2011, 9, 465-474. | 0.6 | 24 |
| 119 | ChemProt: a disease chemical biology database. Nucleic Acids Research, 2011, 39, D367-D372. | 6.5 | 71 |
| 120 | Intracellular Cannabinoid Type 1 (CB1) Receptors Are Activated by Anandamide. Journal of Biological Chemistry, 2011, 286, 29166-29174. | 1.6 | 83 |
| 121 | Novel derivatives of 1,3,4-oxadiazoles are potent mitostatic agents featuring strong microtubule depolymerizing activity in the sea urchin embryo and cell culture assays. European Journal of Medicinal Chemistry, 2010, 45, 1683-1697. | 2.6 | 70 |
| 122 | Modulation of Bitter Taste Perception by a Small Molecule hTAS2R Antagonist. Current Biology, 2010, 20, 1104-1109. | 1.8 | 142 |
| 123 | A Scaffoldâ€Treeâ€Merging Strategy for Prospective Bioactivity Annotation of Î³â€Pyrones. Angewandte Chemie - International Edition, 2010, 49, 3666-3670. | 7.2 | 41 |
| 124 | Transporterâ€Mediated Efflux Influences CNS Side Effects: ABCB1, from Antitarget to Target. Molecular Informatics, 2010, 29, 16-26. | 1.4 | 35 |
| 125 | Small molecule inhibitors of hantavirus infection. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 7085-7091. | 1.0 | 23 |
| 126 | iPHACE: integrative navigation in pharmacological space. Bioinformatics, 2010, 26, 985-986. | 1.8 | 24 |

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| 127 | Model-Free Drug-Likeness from Fragments. Journal of Chemical Information and Modeling, 2010, 50, 1387-1394. | 2.5 | 28 |
| 128 | The G Proteinâ€“Coupled Receptor GPR30 Inhibits Proliferation of Estrogen Receptorâ€“Positive Breast Cancer Cells. Cancer Research, 2010, 70, 1184-1194. | 0.4 | 204 |
| 129 | High-Throughput Multiplex Flow Cytometry Screening for Botulinum Neurotoxin Type A Light Chain Protease Inhibitors. Assay and Drug Development Technologies, 2010, 8, 37-46. | 0.6 | 20 |
| 130 | Highly efficient synthesis and characterization of the GPR30-selective agonist G-1 and related tetrahydroquinoline analogs. Organic and Biomolecular Chemistry, 2010, 8, 2252. | 1.5 | 40 |
| 131 | Conformational mAb as a Tool for Integrin Ligand Discovery. Assay and Drug Development Technologies, 2009, 7, 507-515. | 0.6 | 18 |
| 132 | Detection of Intracellular Granularity Induction in Prostate Cancer Cell Lines by Small Molecules Using the HyperCytÂ® High-Throughput Flow Cytometry System. Journal of Biomolecular Screening, 2009, 14, 596-609. | 2.6 | 28 |
| 133 | Discovery of Selective Probes and Antagonists for G Protein-Coupled Receptors FPR/FPRL1 and GPR30. Current Topics in Medicinal Chemistry, 2009, 9, 1227-1236. | 1.0 | 25 |
| 134 | Duplex highâ€throughput flow cytometry screen identifies two novel formylpeptide receptor family probes. Cytometry Part A: the Journal of the International Society for Analytical Cytology, 2009, 75A, 253-263. | 1.1 | 32 |
| 135 | Expression of estrogen receptor GPR30 in the rat spinal cord and in autonomic and sensory ganglia. Journal of Neuroscience Research, 2009, 87, 1610-1619. | 1.3 | 83 |
| 136 | In vivo effects of a GPR30 antagonist. Nature Chemical Biology, 2009, 5, 421-427. | 3.9 | 461 |
| 137 | Interactive exploration of chemical space with Scaffold Hunter. Nature Chemical Biology, 2009, 5, 581-583. | 3.9 | 207 |
| 138 | Bioactivity-guided mapping and navigation of chemical space. Nature Chemical Biology, 2009, 5, 585-592. | 3.9 | 129 |
| 139 | A crowdsourcing evaluation of the NIH chemical probes. Nature Chemical Biology, 2009, 5, 441-447. | 3.9 | 111 |
| 140 | Novel Chemical Space Exploration via Natural Products. Journal of Medicinal Chemistry, 2009, 52, 1953-1962. | 2.9 | 248 |
| 141 | Estrogen Rapidly Modulates 5-Hydroxytrytophan-Induced Visceral Hypersensitivity via GPR30 in Rats. Gastroenterology, 2009, 137, 1040-1050. | 0.6 | 48 |
| 142 | QSAR Modeling of the Bloodâ€“Brain Barrier Permeability for Diverse Organic Compounds. Pharmaceutical Research, 2008, 25, 1902-1914. | 1.7 | 163 |
| 143 | Optimization of CAMD techniques 3. Virtual screening enrichment studies: a help or hindrance in tool selection?. Journal of Computer-Aided Molecular Design, 2008, 22, 169-178. | 1.3 | 163 |
| 144 | Black Swans and white tablets. Chemistry Central Journal, 2008, 2, . | 2.6 | 0 |

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|---|---|---|---|
| 145 | 2D QSAR and similarity studies on cruzain inhibitors aimed at improving selectivity over cathepsin L. Bioorganic and Medicinal Chemistry, 2008, 16, 838-853. | 1.4 | 28 |
| 146 | hERG Classification Model Based on a Combination of Support Vector Machine Method and GRIND Descriptors. Molecular Pharmaceutics, 2008, 5, 117-127. | 2.3 | 91 |
| 147 | Scaffold Topologies. 1. Exhaustive Enumeration up to Eight Rings. Journal of Chemical Information and Modeling, 2008, 48, 1304-1310. | 2.5 | 43 |
| 148 | Corrigendum to â€œActivation of dioxin response element (DRE)-associated genes by benzo(a)pyrene 3,6-quinone and benzo(a)pyrene 1,6-quinone in MCF-10A human mammary epithelial cellsâ€•[Toxicol. Appl. Pharmacol. 221 (2007) 203â€“214]. Toxicology and Applied Pharmacology, 2008, 226, 345-346. | 1.3 | 0 |
| 149 | Scaffold Topologies. 2. Analysis of Chemical Databases. Journal of Chemical Information and Modeling, 2008, 48, 1311-1324. | 2.5 | 44 |
| 150 | High-Throughput Flow Cytometry to Detect Selective Inhibitors of ABCB1, ABCC1, and ABCG2 Transporters. Assay and Drug Development Technologies, 2008, 6, 263-276. | 0.6 | 67 |
| 151 | Estrogen Signaling through the Transmembrane G Proteinâ€“Coupled Receptor GPR30. Annual Review of Physiology, 2008, 70, 165-190. | 5.6 | 539 |
| 152 | Understanding virulence mechanisms in M. tuberculosis infection via A circuit-based simulation framework. , 2008, 2008, 4953-5. | | 2 |
| 153 | GPR30: a novel therapeutic target in estrogen-related disease. Trends in Pharmacological Sciences, 2008, 29, 116-123. | 4.0 | 122 |
| 154 | The ins and outs of GPR30: A transmembrane estrogen receptor. Journal of Steroid Biochemistry and Molecular Biology, 2008, 109, 350-353. | 1.2 | 136 |
| 155 | Quantifying the Relationships among Drug Classes. Journal of Chemical Information and Modeling, 2008, 48, 755-765. | 2.5 | 160 |
| 156 | Efficient Calculation of Molecular Properties from Simulation Using Kernel Molecular Dynamics. Journal of Chemical Information and Modeling, 2008, 48, 1626-1637. | 2.5 | 5 |
| 157 | High-Throughput Screening for Daunorubicin-Mediated Drug Resistance Identifies Mometasone Furoate as a Novel ABCB1-Reversal Agent. Journal of Biomolecular Screening, 2008, 13, 185-193. | 2.6 | 29 |
| 158 | On a Riemannian Invariant of Chen Type. Rocky Mountain Journal of Mathematics, 2008, 38, . | 0.2 | 6 |
| 159 | Early ADME/T Predictions: Toy or Tool?. , 2008, , 240-267. | | 4 |
| 160 | High-throughput flow cytometry for drug discovery. Expert Opinion on Drug Discovery, 2007, 2, 685-696. | 2.5 | 30 |
| 161 | Distribution and characterization of estrogen receptor G protein-coupled receptor 30 in the rat central nervous system. Journal of Endocrinology, 2007, 193, 311-321. | 1.2 | 433 |
| 162 | G Proteinâ€“Coupled Receptor 30 (GPR30) Mediates Gene Expression Changes and Growth Response to 17Î²-Estradiol and Selective GPR30 Ligand G-1 in Ovarian Cancer Cells. Cancer Research, 2007, 67, 1859-1866. | 0.4 | 383 |

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|---|---|---|---|
| 163 | Exemestane's 17-hydroxylated metabolite exerts biological effects as an androgen. Molecular Cancer Therapeutics, 2007, 6, 2817-2827. | 1.9 | 58 |
| 164 | Theoretical and Practical Aspects of Three-Dimensional Quantitative Structure-Activity Relationships. Reviews in Computational Chemistry, 2007, , 127-182. | 1.5 | 37 |
| 165 | Ligand-Based Virtual Screening by Novelty Detection with Self-Organizing Maps. Journal of Chemical Information and Modeling, 2007, 47, 2044-2062. | 2.5 | 29 |
| 166 | Systems chemical biology. Nature Chemical Biology, 2007, 3, 447-450. | 3.9 | 129 |
| 167 | In vitro differentiation of human mesenchymal stem cells to epithelial lineage. Journal of Cellular and Molecular Medicine, 2007, 11, 502-508. | 1.6 | 147 |
| 168 | Activation of dioxin response element (DRE)-associated genes by benzo(a)pyrene 3,6-quinone and benzo(a)pyrene 1,6-quinone in MCF-10A human mammary epithelial cells. Toxicology and Applied Pharmacology, 2007, 221, 203-214. | 1.3 | 52 |
| 169 | Lead-like, drug-like or â€œPub-likeâ€: how different are they?. Journal of Computer-Aided Molecular Design, 2007, 21, 113-119. | 1.3 | 98 |
| 170 | Virtual screening applications: a study of ligand-based methods and different structure representations in four different scenarios. Journal of Computer-Aided Molecular Design, 2007, 21, 617-640. | 1.3 | 38 |
| 171 | Integration of virtual and physical screening. Drug Discovery Today: Technologies, 2006, 3, 377-385. | 4.0 | 22 |
| 172 | Target, chemical and bioactivity databases â€“ integration is key. Drug Discovery Today: Technologies, 2006, 3, 357-365. | 4.0 | 53 |
| 173 | Virtual and biomolecular screening converge on a selective agonist for GPR30. Nature Chemical Biology, 2006, 2, 207-212. | 3.9 | 730 |
| 174 | Biomolecular screening of formylpeptide receptor ligands with a sensitive, quantitative, high-throughput flow cytometry platform. Nature Protocols, 2006, 1, 59-66. | 5.5 | 33 |
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