# JÃ¼rgen Bajorath

List of Publications by Year
in descending order



| | | | |
|---|---|---|---|
| 573 papers | 20,094 citations | 26567 56 h-index | 19690 117 g-index |
| 662 all docs | 662 docs citations | 662 times ranked | 13876 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Docking and scoring in virtual screening for drug discovery: methods and applications. Nature Reviews Drug Discovery, 2004, 3, 935-949. | 21.5 | 2,697 |
| 2 | Polypharmacology: Challenges and Opportunities in Drug Discovery. Journal of Medicinal Chemistry, 2014, 57, 7874-7887. | 2.9 | 813 |
| 3 | Integration of virtual and high-throughput screening. Nature Reviews Drug Discovery, 2002, 1, 882-894. | 21.5 | 782 |
| 4 | Molecular Similarity in Medicinal Chemistry. Journal of Medicinal Chemistry, 2014, 57, 3186-3204. | 2.9 | 448 |
| 5 | QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564. | 18.7 | 427 |
| 6 | Molecular similarity analysis in virtual screening: foundations, limitations and novel approaches. Drug Discovery Today, 2007, 12, 225-233. | 3.2 | 409 |
| 7 | Current Trends in Ligand-Based Virtual Screening: Molecular Representations, Data Mining Methods, New Application Areas, and Performance Evaluation. Journal of Chemical Information and Modeling, 2010, 50, 205-216. | 2.5 | 306 |
| 8 | Exploring Activity Cliffs in Medicinal Chemistry. Journal of Medicinal Chemistry, 2012, 55, 2932-2942. | 2.9 | 282 |
| 9 | Application of Generative Autoencoder in De Novo Molecular Design. Molecular Informatics, 2018, 37, 1700123. | 1.4 | 276 |
| 10 | Interpretation of machine learning models using shapley values: application to compound potency and multi-target activity predictions. Journal of Computer-Aided Molecular Design, 2020, 34, 1013-1026. | 1.3 | 248 |
| 11 | Quo Vadis, Virtual Screening? A Comprehensive Survey of Prospective Applications. Journal of Medicinal Chemistry, 2010, 53, 8461-8467. | 2.9 | 223 |
| 12 | Selected Concepts and Investigations in Compound Classification, Molecular Descriptor Analysis, and Virtual Screening. Journal of Chemical Information and Computer Sciences, 2001, 41, 233-245. | 2.8 | 217 |
| 13 | Recent Advances in Scaffold Hopping. Journal of Medicinal Chemistry, 2017, 60, 1238-1246. | 2.9 | 213 |
| 14 | State-of-the-art in ligand-based virtual screening. Drug Discovery Today, 2011, 16, 372-376. | 3.2 | 196 |
| 15 | MMP-Cliffs: Systematic Identification of Activity Cliffs on the Basis of Matched Molecular Pairs. Journal of Chemical Information and Modeling, 2012, 52, 1138-1145. | 2.5 | 181 |
| 16 | Interpretation of Compound Activity Predictions from Complex Machine Learning Models Using Local Approximations and Shapley Values. Journal of Medicinal Chemistry, 2020, 63, 8761-8777. | 2.9 | 178 |
| 17 | Recent Progress in Understanding Activity Cliffs and Their Utility in Medicinal Chemistry. Journal of Medicinal Chemistry, 2014, 57, 18-28. | 2.9 | 174 |
| 18 | SAR Index:â€‰ Quantifying the Nature of Structureâ^'Activity Relationships. Journal of Medicinal Chemistry, 2007, 50, 5571-5578. | 2.9 | 172 |

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| 19 | Activity Landscape Representations for Structureâ˜Activity Relationship Analysis. Journal of Medicinal Chemistry, 2010, 53, 8209-8223. | 2.9 | 163 |
| 20 | Navigating structureâ€“activity landscapes. Drug Discovery Today, 2009, 14, 698-705. | 3.2 | 161 |
| 21 | Structureâ˜Activity Relationship Anatomy by Network-like Similarity Graphs and Local Structureâ˜Activity Relationship Indices. Journal of Medicinal Chemistry, 2008, 51, 6075-6084. | 2.9 | 143 |
| 22 | New Methodologies for Ligand-Based Virtual Screening. Current Pharmaceutical Design, 2005, 11, 1189-1202. | 0.9 | 139 |
| 23 | Combinatorial Preferences Affect Molecular Similarity/Diversity Calculations Using Binary Fingerprints and Tanimoto Coefficients. Journal of Chemical Information and Computer Sciences, 2000, 40, 163-166. | 2.8 | 138 |
| 24 | Compound promiscuity: what can we learn from current data?. Drug Discovery Today, 2013, 18, 644-650. | 3.2 | 135 |
| 25 | Similarity searching. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 260-282. | 6.2 | 117 |
| 26 | Virtual Screening Methods that Complement HTS. Combinatorial Chemistry and High Throughput Screening, 2004, 7, 259-269. | 0.6 | 113 |
| 27 | Support vector machines for drug discovery. Expert Opinion on Drug Discovery, 2014, 9, 93-104. | 2.5 | 113 |
| 28 | Charting Biologically Relevant Spirocyclic Compound Space. Chemistry - A European Journal, 2017, 23, 703-710. | 1.7 | 107 |
| 29 | Computational Exploration of Molecular Scaffolds in Medicinal Chemistry. Journal of Medicinal Chemistry, 2016, 59, 4062-4076. | 2.9 | 100 |
| 30 | How Frequently Are Pan-Assay Interference Compounds Active? Large-Scale Analysis of Screening Data Reveals Diverse Activity Profiles, Low Global Hit Frequency, and Many Consistently Inactive Compounds. Journal of Medicinal Chemistry, 2017, 60, 3879-3886. | 2.9 | 97 |
| 31 | Development of Potent and Selective Inhibitors of ecto-5â€²-Nucleotidase Based on an Anthraquinone Scaffold. Journal of Medicinal Chemistry, 2010, 53, 2076-2086. | 2.9 | 88 |
| 32 | Scaffold Hopping Using Two-Dimensional Fingerprints: True Potential, Black Magic, or a Hopeless Endeavor? Guidelines for Virtual Screening. Journal of Medicinal Chemistry, 2010, 53, 5707-5715. | 2.9 | 84 |
| 33 | Lessons Learned from Molecular Scaffold Analysis. Journal of Chemical Information and Modeling, 2011, 51, 1742-1753. | 2.5 | 82 |
| 34 | Rationalizing Three-Dimensional Activity Landscapes and the Influence of Molecular Representations on Landscape Topology and the Formation of Activity Cliffs. Journal of Chemical Information and Modeling, 2010, 50, 1021-1033. | 2.5 | 80 |
| 35 | Computational analysis of ligand relationships within target families. Current Opinion in Chemical Biology, 2008, 12, 352-358. | 2.8 | 79 |
| 36 | Design and Evaluation of a Molecular Fingerprint Involving the Transformation of Property Descriptor Values into a Binary Classification Scheme. Journal of Chemical Information and Computer Sciences, 2003, 43, 1151-1157. | 2.8 | 78 |

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| 37 | SARANEA: A Freely Available Program To Mine Structureâ^'Activity and Structureâ^'Selectivity Relationship Information in Compound Data Sets. Journal of Chemical Information and Modeling, 2010, 50, 68-78. | 2.5 | 77 |
| 38 | Local Structural Changes, Global Data Views: Graphical Substructureâ^'Activity Relationship Trailing. Journal of Medicinal Chemistry, 2011, 54, 2944-2951. | 2.9 | 77 |
| 39 | Large-Scale Similarity Search Profiling of ChEMBL Compound Data Sets. Journal of Chemical Information and Modeling, 2011, 51, 1831-1839. | 2.5 | 76 |
| 40 | Evolving Concept of Activity Cliffs. ACS Omega, 2019, 4, 14360-14368. | 1.6 | 76 |
| 41 | Support Vector Machine Classification and Regression Prioritize Different Structural Features for Binary Compound Activity and Potency Value Prediction. ACS Omega, 2017, 2, 6371-6379. | 1.6 | 75 |
| 42 | The Future of Virtual Compound Screening. Chemical Biology and Drug Design, 2013, 81, 33-40. | 1.5 | 74 |
| 43 | Profile Scaling Increases the Similarity Search Performance of Molecular Fingerprints Containing Numerical Descriptors and Structural Keys. Journal of Chemical Information and Computer Sciences, 2003, 43, 1218-1225. | 2.8 | 69 |
| 44 | Identification of the First Low-Molecular-Weight Inhibitors of Matriptase-2. Journal of Medicinal Chemistry, 2010, 53, 5523-5535. | 2.9 | 67 |
| 45 | Database Searching for Compounds with Similar Biological Activity Using Short Binary Bit String Representations of Molecules. Journal of Chemical Information and Computer Sciences, 1999, 39, 881-886. | 2.8 | 65 |
| 46 | Advancing the activity cliff concept. F1000Research, 2013, 2, 199. | 0.8 | 65 |
| 47 | Synthesis, biological evaluation and molecular docking of N-phenyl thiosemicarbazones as urease inhibitors. Bioorganic Chemistry, 2015, 61, 51-57. | 2.0 | 65 |
| 48 | Data structures and computational tools for the extraction of SAR information from large compound sets. Drug Discovery Today, 2010, 15, 630-639. | 3.2 | 64 |
| 49 | Ligand Prediction for Orphan Targets Using Support Vector Machines and Various Target-Ligand Kernels Is Dominated by Nearest Neighbor Effects. Journal of Chemical Information and Modeling, 2009, 49, 2155-2167. | 2.5 | 63 |
| 50 | Integrating Structureâ€•and Ligandâ€Based Virtual Screening: Comparison of Individual, Parallel, and Fused Molecular Docking and Similarity Search Calculations on Multiple Targets. ChemMedChem, 2008, 3, 1566-1571. | 1.6 | 62 |
| 51 | Support-Vector-Machine-Based Ranking Significantly Improves the Effectiveness of Similarity Searching Using 2D Fingerprints and Multiple Reference Compounds. Journal of Chemical Information and Modeling, 2008, 48, 742-746. | 2.5 | 61 |
| 52 | BindingDB and ChEMBL: online compound databases for drug discovery. Expert Opinion on Drug Discovery, 2011, 6, 683-687. | 2.5 | 60 |
| 53 | Fingerprint Scaling Increases the Probability of Identifying Molecules with Similar Activity in Virtual Screening Calculations. Journal of Chemical Information and Computer Sciences, 2001, 41, 746-753. | 2.8 | 59 |
| 54 | Molecular Similarity Analysis Uncovers Heterogeneous Structure-Activity Relationships and Variable Activity Landscapes. Chemistry and Biology, 2007, 14, 489-497. | 6.2 | 59 |

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| 55 | Chemical space networks: a powerful new paradigm for the description of chemical space. Journal of Computer-Aided Molecular Design, 2014, 28, 795-802. | 1.3 | 59 |
| 56 | Chemical Substitutions That Introduce Activity Cliffs Across Different Compound Classes and Biological Targets. Journal of Chemical Information and Modeling, 2010, 50, 1248-1256. | 2.5 | 57 |
| 57 | Searching for Target-Selective Compounds Using Different Combinations of Multiclass Support Vector Machine Ranking Methods, Kernel Functions, and Fingerprint Descriptors. Journal of Chemical Information and Modeling, 2009, 49, 582-592. | 2.5 | 56 |
| 58 | Polypharmacology Directed Compound Data Mining: Identification of Promiscuous Chemotypes with Different Activity Profiles and Comparison to Approved Drugs. Journal of Chemical Information and Modeling, 2010, 50, 2112-2118. | 2.5 | 56 |
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| 62 | Differential Shannon Entropy as a Sensitive Measure of Differences in Database Variability of Molecular Descriptors. Journal of Chemical Information and Computer Sciences, 2001, 41, 1060-1066. | 2.8 | 54 |
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| 64 | Active compounds from a diverse library of triazolothiadiazole and triazolothiadiazine scaffolds: Synthesis, crystal structure determination, cytotoxicity, cholinesterase inhibitory activity, and binding mode analysis. Bioorganic and Medicinal Chemistry, 2014, 22, 6163-6173. | 1.4 | 54 |
| 65 | EXPLORING COMPOUND PROMISCUITY PATTERNS AND MULTI-TARGET ACTIVITY SPACES. Computational and Structural Biotechnology Journal, 2014, 9, e201401003. | 1.9 | 54 |
| 66 | Entering the â€˜big dataâ€™ era in medicinal chemistry: molecular promiscuity analysis revisited. Future Science OA, 2017, 3, FSO179. | 0.9 | 53 |
| 67 | Memory-assisted reinforcement learning for diverse molecular de novo design. Journal of Cheminformatics, 2020, 12, 68. | 2.8 | 53 |
| 68 | Evaluation of Descriptors and Mini-Fingerprints for the Identification of Molecules with Similar Activity. Journal of Chemical Information and Computer Sciences, 2000, 40, 1227-1234. | 2.8 | 52 |
| 69 | From Structureâ€"Activity to Structureâ€"Selectivity Relationships: Quantitative Assessment, Selectivity Cliffs, and Key Compounds. ChemMedChem, 2009, 4, 1864-1873. | 1.6 | 51 |
| 70 | Ligand Prediction from Protein Sequence and Small Molecule Information Using Support Vector Machines and Fingerprint Descriptors. Journal of Chemical Information and Modeling, 2009, 49, 767-779. | 2.5 | 50 |
| 71 | Prediction of Activity Cliffs Using Support Vector Machines. Journal of Chemical Information and Modeling, 2012, 52, 2354-2365. | 2.5 | 50 |
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| 74 | SAR Matrices: Automated Extraction of Information-Rich SAR Tables from Large Compound Data Sets. Journal of Chemical Information and Modeling, 2012, 52, 1769-1776. | 2.5 | 49 |
| 75 | Computer-aided drug discovery. F1000Research, 2015, 4, 630. | 0.8 | 49 |
| 76 | Multitask Machine Learning for Classifying Highly and Weakly Potent Kinase Inhibitors. ACS Omega, 2019, 4, 4367-4375. | 1.6 | 49 |
| 77 | Design of Multitarget Activity Landscapes That Capture Hierarchical Activity Cliff Distributions. Journal of Chemical Information and Modeling, 2011, 51, 258-266. | 2.5 | 48 |
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| 79 | Virtual Screening Identifies Novel Sulfonamide Inhibitors of ecto-5â€²-Nucleotidase. Journal of Medicinal Chemistry, 2012, 55, 6576-6581. | 2.9 | 47 |
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| 83 | Comparison of 2D Fingerprint Methods for Multiple-Template Similarity Searching on Compound Activity Classes of Increasing Structural Diversity. ChemMedChem, 2007, 2, 208-217. | 1.6 | 46 |
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| 86 | Methods for SAR visualization. RSC Advances, 2012, 2, 369-378. | 1.7 | 45 |
| 87 | Learning from â€˜big dataâ€™: compounds and targets. Drug Discovery Today, 2014, 19, 357-360. | 3.2 | 45 |
| 88 | A Coumarinâ€Labeled Vinyl Sulfone as Tripeptidomimetic Activityâ€Based Probe for Cysteine Cathepsins. ChemBioChem, 2014, 15, 955-959. | 1.3 | 45 |
| 89 | Emerging Chemical Patterns:â€‰ A New Methodology for Molecular Classification and Compound Selection. Journal of Chemical Information and Modeling, 2006, 46, 2502-2514. | 2.5 | 44 |
| 90 | Systematic computational analysis of structureâ€“activity relationships: concepts, challenges and recent advances. Future Medicinal Chemistry, 2009, 1, 451-466. | 1.1 | 44 |

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| 91 | Chemoinformatics: A view of the field and current trends in method development. Bioorganic and Medicinal Chemistry, 2012, 20, 5317-5323. | 1.4 | 44 |
| 92 | Virtual compound screening in drug discovery. Future Medicinal Chemistry, 2012, 4, 593-602. | 1.1 | 44 |
| 93 | Evolution of Support Vector Machine and Regression Modeling in Chemoinformatics and Drug Discovery. Journal of Computer-Aided Molecular Design, 2022, 36, 355-362. | 1.3 | 44 |
| 94 | Systematic Analysis of Public Domain Compound Potency Data Identifies Selective Molecular Scaffolds across Druggable Target Families. Journal of Medicinal Chemistry, 2010, 53, 752-758. | 2.9 | 43 |
| 95 | Large-scale exploration of bioisosteric replacements on the basis of matched molecular pairs. Future Medicinal Chemistry, 2011, 3, 425-436. | 1.1 | 43 |
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| 99 | Informatics for Chemistry, Biology, and Biomedical Sciences. Journal of Chemical Information and Modeling, 2021, 61, 26-35. | 2.5 | 42 |
| 100 | Molecular Similarity Analysis and Virtual Screening by Mapping of Consensus Positions in Binary-Transformed Chemical Descriptor Spaces with Variable Dimensionality. Journal of Chemical Information and Computer Sciences, 2004, 44, 21-29. | 2.8 | 41 |
| 101 | Matched Molecular Pair Analysis of Small Molecule Microarray Data Identifies Promiscuity Cliffs and Reveals Molecular Origins of Extreme Compound Promiscuity. Journal of Medicinal Chemistry, 2012, 55, 10220-10228. | 2.9 | 41 |
| 102 | Activity-relevant similarity values for fingerprints and implications for similarity searching. F1000Research, 2016, 5, 591. | 0.8 | 41 |
| 103 | Improving the Search Performance of Extended Connectivity Fingerprints through Activityâ€Oriented Feature Filtering and Application of a Bitâ€Densityâ€Dependent Similarity Function. ChemMedChem, 2009, 4, 540-548. | 1.6 | 40 |
| 104 | Composition and Topology of Activity Cliff Clusters Formed by Bioactive Compounds. Journal of Chemical Information and Modeling, 2014, 54, 451-461. | 2.5 | 40 |
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| 107 | Comparison of Confirmed Inactive and Randomly Selected Compounds as Negative Training Examples in Support Vector Machine-Based Virtual Screening. Journal of Chemical Information and Modeling, 2013, 53, 1595-1601. | 2.5 | 39 |
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| 109 | Design and Evaluation of a Novel Class-Directed 2D Fingerprint to Search for Structurally Diverse Active Compounds. Journal of Chemical Information and Modeling, 2006, 46, 2515-2526. | 2.5 | 38 |
| 110 | Design of chemical space networks using a Tanimoto similarity variant based upon maximum common substructures. Journal of Computer-Aided Molecular Design, 2015, 29, 937-950. | 1.3 | 38 |
| 111 | Highly Promiscuous Small Molecules from Biological Screening Assays Include Many Pan-Assay Interference Compounds but Also Candidates for Polypharmacology. Journal of Medicinal Chemistry, 2016, 59, 10285-10290. | 2.9 | 38 |
| 112 | Three-Dimensional Similarity in Molecular Docking: Prioritizing Ligand Poses on the Basis of Experimental Binding Modes. Journal of Chemical Information and Modeling, 2016, 56, 580-587. | 2.5 | 38 |
| 113 | Methods for Computerâ€aided Chemical Biology. Part 2: Evaluation of Compound Selectivity Using 2D Molecular Fingerprints. Chemical Biology and Drug Design, 2007, 70, 195-205. | 1.5 | 37 |
| 114 | Similarity Searching Using Fingerprints of Molecular Fragments Involved in Proteinâ^'Ligand Interactions. Journal of Chemical Information and Modeling, 2008, 48, 2308-2312. | 2.5 | 37 |
| 115 | Molecular Fingerprint Recombination: Generating Hybrid Fingerprints for Similarity Searching from Different Fingerprint Types. ChemMedChem, 2009, 4, 1859-1863. | 1.6 | 37 |
| 116 | Growth of Ligandâ€“Target Interaction Data in ChEMBL Is Associated with Increasing and Activity Measurement-Dependent Compound Promiscuity. Journal of Chemical Information and Modeling, 2012, 52, 2550-2558. | 2.5 | 37 |
| 117 | Visualization and Interpretation of Support Vector Machine Activity Predictions. Journal of Chemical Information and Modeling, 2015, 55, 1136-1147. | 2.5 | 37 |
| 118 | Activity-relevant similarity values for fingerprints and implications for similarity searching. F1000Research, 2016, 5, 591. | 0.8 | 37 |
| 119 | Accurate Partitioning of Compounds Belonging to Diverse Activity Classes. Journal of Chemical Information and Computer Sciences, 2002, 42, 757-764. | 2.8 | 36 |
| 120 | Recursive Median Partitioning for Virtual Screening of Large Databases. Journal of Chemical Information and Computer Sciences, 2003, 43, 182-188. | 2.8 | 36 |
| 121 | Structural Interpretation of Activity Cliffs Revealed by Systematic Analysis of Structureâ^'Activity Relationships in Analog Series. Journal of Chemical Information and Modeling, 2009, 49, 2179-2189. | 2.5 | 36 |
| 122 | What is the Likelihood of an Active Compound to Be Promiscuous? Systematic Assessment of Compound Promiscuity on the Basis of PubChem Confirmatory Bioassay Data. AAPS Journal, 2013, 15, 808-815. | 2.2 | 36 |
| 123 | Assessment of Molecular Similarity from the Analysis of Randomly Generated Structural Fragment Populations. Journal of Chemical Information and Modeling, 2006, 46, 1937-1944. | 2.5 | 34 |
| 124 | Methods for Computerâ€Aided Chemical Biology. Part 3: Analysis of Structureâ€“Selectivity Relationships through Singleâ€•or Dualâ€Step Selectivity Searching and Bayesian Classification. Chemical Biology and Drug Design, 2008, 71, 518-528. | 1.5 | 34 |
| 125 | Targeting Multifunctional Proteins by Virtual Screening: Structurally Diverse Cytohesin Inhibitors with Differentiated Biological Functions. ACS Chemical Biology, 2010, 5, 839-849. | 1.6 | 34 |
| 126 | Novel structural hybrids of pyrazolobenzothiazines with benzimidazoles as cholinesterase inhibitors. European Journal of Medicinal Chemistry, 2014, 78, 106-117. | 2.6 | 34 |

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| 127 | Machine Learning Models for Accurate Prediction of Kinase Inhibitors with Different Binding Modes. Journal of Medicinal Chemistry, 2020, 63, 8738-8748. | 2.9 | 34 |
| 128 | Current Trends, Overlooked Issues, and Unmet Challenges in Virtual Screening. Journal of Chemical Information and Modeling, 2020, 60, 4112-4115. | 2.5 | 34 |
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| 131 | Median Partitioning:â€‰ A Novel Method for the Selection of Representative Subsets from Large Compound Pools. Journal of Chemical Information and Computer Sciences, 2002, 42, 885-893. | 2.8 | 33 |
| 132 | Anatomy of Fingerprint Search Calculations on Structurally Diverse Sets of Active Compounds. Journal of Chemical Information and Modeling, 2005, 45, 1812-1819. | 2.5 | 33 |
| 133 | Ligand-Target Interaction-Based Weighting of Substructures for Virtual Screening. Journal of Chemical Information and Modeling, 2008, 48, 1955-1964. | 2.5 | 33 |
| 134 | Identification of sulfonic acids as efficient ecto-5â€²-nucleotidase inhibitors. European Journal of Medicinal Chemistry, 2013, 70, 685-691. | 2.6 | 33 |
| 135 | Structure- and Similarity-Based Survey of Allosteric Kinase Inhibitors, Activators, and Closely Related Compounds. Journal of Medicinal Chemistry, 2022, 65, 922-934. | 2.9 | 33 |
| 136 | Identification of Structurally Diverse Growth Hormone Secretagogue Agonists by Virtual Screening and Structureâ^'Activity Relationship Analysis of 2-Formylaminoacetamide Derivatives. Journal of Medicinal Chemistry, 2004, 47, 4286-4290. | 2.9 | 32 |
| 137 | How Promiscuous Are Pharmaceutically Relevant Compounds? A Data-Driven Assessment. AAPS Journal, 2013, 15, 104-111. | 2.2 | 32 |
| 138 | Influence of Search Parameters and Criteria on Compound Selection, Promiscuity, and Pan Assay Interference Characteristics. Journal of Chemical Information and Modeling, 2014, 54, 3056-3066. | 2.5 | 32 |
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| 141 | Formal Concept Analysis for the Identification of Molecular Fragment Combinations Specific for Active and Highly Potent Compounds. Journal of Medicinal Chemistry, 2008, 51, 5342-5348. | 2.9 | 31 |
| 142 | Inhibition of Human Leukocyte Elastase by Brunsvicamidesâ€…Aâ€“C: Cyanobacterial Cyclic Peptides. ChemMedChem, 2009, 4, 1425-1429. | 1.6 | 31 |
| 143 | Computational Polypharmacology Analysis of the Heat Shock Protein 90 Interactome. Journal of Chemical Information and Modeling, 2015, 55, 676-686. | 2.5 | 31 |
| 144 | Similarity Search Profiling Reveals Effects of Fingerprint Scaling in Virtual Screening. Journal of Chemical Information and Computer Sciences, 2004, 44, 2032-2039. | 2.8 | 30 |

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| 146 | Chemical Database Mining through Entropy-Based Molecular Similarity Assessment of Randomly Generated Structural Fragment Populations. Journal of Chemical Information and Modeling, 2007, 47, 59-68. | 2.5 | 30 |
| 147 | How Do 2D Fingerprints Detect Structurally Diverse Active Compounds? Revealing Compound Subset-Specific Fingerprint Features through Systematic Selection. Journal of Chemical Information and Modeling, 2011, 51, 2254-2265. | 2.5 | 30 |
| 148 | Comprehensive Analysis of Singleâ€•and Multiâ€Target Activity Cliffs Formed by Currently Available Bioactive Compounds. Chemical Biology and Drug Design, 2011, 78, 224-228. | 1.5 | 30 |
| 149 | Design and characterization of chemical space networks for different compound data sets. Journal of Computer-Aided Molecular Design, 2015, 29, 113-125. | 1.3 | 30 |
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