Ye Hu

List of Publications by Year
in descending order

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60 papers	1,805 citations	257450 24 h-index	276875 41 g-index
61 all docs	61 docs citations	61 times ranked	1892 citing authors

#	Article	IF	Citations
1	Recent Advances in Scaffold Hopping. Journal of Medicinal Chemistry, 2017, 60, 1238-1246.	6.4	213
2	Compound promiscuity: what can we learn from current data?. Drug Discovery Today, 2013, 18, 644-650.	6.4	135
3	Computational Exploration of Molecular Scaffolds in Medicinal Chemistry. Journal of Medicinal Chemistry, 2016, 59, 4062-4076.	6.4	100
4	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.	6.4	97
5	Lessons Learned from Molecular Scaffold Analysis. Journal of Chemical Information and Modeling, 2011, 51, 1742-1753.	5.4	82
6	Advancing the activity cliff concept. F1000Research, 2013, 2, 199.	1.6	65
7	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.	5.4	56
8	Current Compound Coverage of the Kinome. Journal of Medicinal Chemistry, 2015, 58, 30-40.	6.4	56
9	Extending the Activity Cliff Concept: Structural Categorization of Activity Cliffs and Systematic Identification of Different Types of Cliffs in the ChEMBL Database. Journal of Chemical Information and Modeling, 2012, 52, 1806-1811.	5.4	54
10	EXPLORING COMPOUND PROMISCUITY PATTERNS AND MULTI-TARGET ACTIVITY SPACES. Computational and Structural Biotechnology Journal, 2014, 9, e201401003.	4.1	54
11	Entering the â€˜big dataâ€™ era in medicinal chemistry: molecular promiscuity analysis revisited. Future Science OA, 2017, 3, FSO179.	1.9	53
12	Molecular Scaffolds with High Propensity to Form Multi-Target Activity Cliffs. Journal of Chemical Information and Modeling, 2010, 50, 500-510.	5.4	45
13	Learning from â€˜big dataâ€™: compounds and targets. Drug Discovery Today, 2014, 19, 357-360.	6.4	45
14	Systematic Analysis of Public Domain Compound Potency Data Identifies Selective Molecular Scaffolds across Druggable Target Families. Journal of Medicinal Chemistry, 2010, 53, 752-758.	6.4	43
15	Determining the Degree of Promiscuity of Extensively Assayed Compounds. PLoS ONE, 2016, 11, e0153873.	2.5	43
16	Activity-relevant similarity values for fingerprints and implications for similarity searching. F1000Research, 2016, 5, 591.	1.6	41
17	High-resolution view of compound promiscuity. F1000Research, 2013, 2, 144.	1.6	39
18	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.	5.4	37

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19	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.	4.4	36
20	How Promiscuous Are Pharmaceutically Relevant Compounds? A Data-Driven Assessment. AAPS Journal, 2013, 15, 104-111.	4.4	32
21	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.	5.4	32
22	Analog series-based scaffolds: computational design and exploration of a new type of molecular scaffolds for medicinal chemistry. Future Science OA, 2016, 2, FSO149.	1.9	28
23	Systematic Identification and Classification of Three-Dimensional Activity Cliffs. Journal of Chemical Information and Modeling, 2012, 52, 1490-1498.	5.4	26
24	Global assessment of scaffold hopping potential for current pharmaceutical targets. MedChemComm, 2010, 1, 339-344.	3.4	25
25	Exploration of 3D Activity Cliffs on the Basis of Compound Binding Modes and Comparison of 2D and 3D Cliffs. Journal of Chemical Information and Modeling, 2012, 52, 670-677.	5.4	23
26	Systematic Identification of Scaffolds Representing Compounds Active against Individual Targets and Single or Multiple Target Families. Journal of Chemical Information and Modeling, 2013, 53, 312-326.	5.4	23
27	Scaffold Distributions in Bioactive Molecules, Clinical Trials Compounds, and Drugs. ChemMedChem, 2010, 5, 187-190.	3.2	22
28	Exploring the Scaffold Universe of Kinase Inhibitors. Journal of Medicinal Chemistry, 2015, 58, 315-332.	6.4	21
29	Chemical Transformations That Yield Compounds with Distinct Activity Profiles. ACS Medicinal Chemistry Letters, 2011, 2, 523-527.	2.8	18
30	Monitoring drug promiscuity over time. F1000Research, 2014, 3, 218.	1.6	17
31	Assessing the Growth of Bioactive Compounds and Scaffolds over Time: Implications for Lead Discovery and Scaffold Hopping. Journal of Chemical Information and Modeling, 2016, 56, 300-307.	5.4	16
32	Mapping of inhibitors and activity data to the human kinome and exploring promiscuity from a ligand and target perspective. Chemical Biology and Drug Design, 2017, 89, 834-845.	3.2	16
33	Quantifying the Tendency of Therapeutic Target Proteins to Bind Promiscuous or Selective Compounds. PLoS ONE, 2015, 10, e0126838.	2.5	15
34	Exploring Target-Selectivity Patterns of Molecular Scaffolds. ACS Medicinal Chemistry Letters, 2010, 1, 54-58.	2.8	14
35	Many structurally related drugs bind different targets whereas distinct drugs display significant target overlap. RSC Advances, 2012, 2, 3481.	3.6	14
36	Structure-Promiscuity Relationship Puzzlesâ€"Extensively Assayed Analogs with Large Differences in Target Annotations. AAPS Journal, 2017, 19, 856-864.	4.4	14

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37	RelACCSâ€FP: A Structural Minimalist Approach to Fingerprint Design. Chemical Biology and Drug Design, 2008, 72, 341-349.	3.2	13
38	Many Approved Drugs Have Bioactive Analogs With Different Target Annotations. AAPS Journal, 2014, 16, 847-859.	4.4	13
39	Many drugs contain unique scaffolds with varying structural relationships to scaffolds of currently available bioactive compounds. European Journal of Medicinal Chemistry, 2014, 76, 427-434.	5.5	12
40	Activity cliffs in PubChem confirmatory bioassays taking inactive compounds into account. Journal of Computer-Aided Molecular Design, 2013, 27, 115-124.	2.9	11
41	Identification and analysis of the currently available high-confidence three-dimensional activity cliffs. RSC Advances, 2015, 5, 43660-43668.	3.6	11
42	Activity profile relationships between structurally similar promiscuous compounds. European Journal of Medicinal Chemistry, 2013, 69, 393-398.	5.5	10
43	Target Family-Directed Exploration of Scaffolds with Different SAR Profiles. Journal of Chemical Information and Modeling, 2011, 51, 3138-3148.	5.4	9
44	Extension of three-dimensional activity cliff information through systematic mapping of active analogs. RSC Advances, 2015, 5, 43006-43015.	3.6	9
45	Introduction of Target Cliffs as a Concept To Identify and Describe Complex Molecular Selectivity Patterns. Journal of Chemical Information and Modeling, 2013, 53, 545-552.	5.4	8
46	Identification of Interaction Hot Spots in Structures of Drug Targets on the Basis of Threeâ€Đimensional Activity Cliff Information. Chemical Biology and Drug Design, 2015, 86, 1458-1465.	3.2	8
47	Promiscuity progression of bioactive compounds over time. F1000Research, 2015, 4, 118.	1.6	8
48	Analyzing compound activity records and promiscuity degrees in light of publication statistics. F1000Research, 2016, 5, 1227.	1.6	7
49	Structural and Activity Profile Relationships Between Drug Scaffolds. AAPS Journal, 2015, 17, 609-619.	4.4	6
50	Matched molecular pair-based data sets for computer-aided medicinal chemistry. F1000Research, 2014, 3, 36.	1.6	5
51	Activity Profile Sequences: a Concept to Account for the Progression of Compound Activity in Target Space and to Extract SAR Information from Analogue Series with Multiple Target Annotations. ChemMedChem, 2011, 6, 2150-2154.	3.2	4
52	Compound data sets and software tools for chemoinformatics and medicinal chemistry applications: update and data transfer. F1000Research, 2014, 3, 69.	1.6	4
53	Analyzing compound activity records and promiscuity degrees in light of publication statistics. F1000Research, 2016, 5, 1227.	1.6	4
54	Rationalizing Structure and Target Relationships between Current Drugs. AAPS Journal, 2012, 14, 764-771.	4.4	3

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55	AnalogExplorer2 â€“ Stereochemistry sensitive graphical analysis of large analog series. F1000Research, 2015, 4, 1031.	1.6	3
56	Visualization of Activity Landscapes and Chemogenomics Data. Molecular Informatics, 2013, 32, 954-963.	2.5	2
57	SAR Matrix Method for Large-Scale Analysis of Compound Structureâ€“Activity Relationships and Exploration of Multitarget Activity Spaces. Methods in Molecular Biology, 2018, 1825, 339-352.	0.9	2
58	Network Variants for Analyzing Target-Ligand Interactions. ACS Symposium Series, 2016, , 35-51.	0.5	1
59	Exploring Molecular Promiscuity from a Ligand and Target Perspective. ACS Symposium Series, 2016, , 19-34.	0.5	1
60	Inside Cover: From Structure-Activity to Structure-Selectivity Relationships: Quantitative Assessment, Selectivity Cliffs, and Key Compounds (ChemMedChem 11/2009). ChemMedChem, 2009, 4, 1766-1766.	3.2	0