Ye Hu

List of Publications by Year
in descending order

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	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
2	Structure-Promiscuity Relationship Puzzlesâ€”Extensively Assayed Analogs with Large Differences in Target Annotations. AAPS Journal, 2017, 19, 856-864.	4.4	14
3	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
4	Entering the â€˜big dataâ€™ era in medicinal chemistry: molecular promiscuity analysis revisited. Future Science OA, 2017, 3, FSO179.	1.9	53
5	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
6	Recent Advances in Scaffold Hopping. Journal of Medicinal Chemistry, 2017, 60, 1238-1246.	6.4	213
7	Determining the Degree of Promiscuity of Extensively Assayed Compounds. PLoS ONE, 2016, 11, e0153873.	2.5	43
8	Network Variants for Analyzing Target-Ligand Interactions. ACS Symposium Series, 2016, , 35-51.	0.5	1
9	Exploring Molecular Promiscuity from a Ligand and Target Perspective. ACS Symposium Series, 2016, , 19-34.	0.5	1
10	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
11	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
12	Computational Exploration of Molecular Scaffolds in Medicinal Chemistry. Journal of Medicinal Chemistry, 2016, 59, 4062-4076.	6.4	100
13	Activity-relevant similarity values for fingerprints and implications for similarity searching. F1000Research, 2016, 5, 591.	1.6	41
14	Analyzing compound activity records and promiscuity degrees in light of publication statistics. F1000Research, 2016, 5, 1227.	1.6	7
15	Analyzing compound activity records and promiscuity degrees in light of publication statistics. F1000Research, 2016, 5, 1227.	1.6	4
16	Identification of Interaction Hot Spots in Structures of Drug Targets on the Basis of Threeâ€Ðimensional Activity Cliff Information. Chemical Biology and Drug Design, 2015, 86, 1458-1465.	3.2	8
17	Structural and Activity Profile Relationships Between Drug Scaffolds. AAPS Journal, 2015, 17, 609-619.	4.4	6
18	Extension of three-dimensional activity cliff information through systematic mapping of active analogs. RSC Advances, 2015, 5, 43006-43015.	3.6	9

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19	Identification and analysis of the currently available high-confidence three-dimensional activity cliffs. RSC Advances, 2015, 5, 43660-43668.	3.6	11
20	Exploring the Scaffold Universe of Kinase Inhibitors. Journal of Medicinal Chemistry, 2015, 58, 315-332.	6.4	21
21	Current Compound Coverage of the Kinome. Journal of Medicinal Chemistry, 2015, 58, 30-40.	6.4	56
22	Promiscuity progression of bioactive compounds over time. F1000Research, 2015, 4, 118.	1.6	8
23	AnalogExplorer2 â€“ Stereochemistry sensitive graphical analysis of large analog series. F1000Research, 2015, 4, 1031.	1.6	3
24	Quantifying the Tendency of Therapeutic Target Proteins to Bind Promiscuous or Selective Compounds. PLoS ONE, 2015, 10, e0126838.	2.5	15
25	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
26	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
27	Learning from â€˜big dataâ€™: compounds and targets. Drug Discovery Today, 2014, 19, 357-360.	6.4	45
28	EXPLORING COMPOUND PROMISCUITY PATTERNS AND MULTI-TARGET ACTIVITY SPACES. Computational and Structural Biotechnology Journal, 2014, 9, e201401003.	4.1	54
29	Many Approved Drugs Have Bioactive Analogs With Different Target Annotations. AAPS Journal, 2014, 16, 847-859.	4.4	13
30	Matched molecular pair-based data sets for computer-aided medicinal chemistry. F1000Research, 2014, 3, 36.	1.6	5
31	Compound data sets and software tools for chemoinformatics and medicinal chemistry applications: update and data transfer. F1000Research, 2014, 3, 69.	1.6	4
32	Monitoring drug promiscuity over time. F1000Research, 2014, 3, 218.	1.6	17
33	Compound promiscuity: what can we learn from current data?. Drug Discovery Today, 2013, 18, 644-650.	6.4	135
34	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
35	Activity cliffs in PubChem confirmatory bioassays taking inactive compounds into account. Journal of Computer-Aided Molecular Design, 2013, 27, 115-124.	2.9	11
36	How Promiscuous Are Pharmaceutically Relevant Compounds? A Data-Driven Assessment. AAPS Journal, 2013, 15, 104-111.	4.4	32

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37	Activity profile relationships between structurally similar promiscuous compounds. European Journal of Medicinal Chemistry, 2013, 69, 393-398.	5.5	10
38	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
39	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
40	Visualization of Activity Landscapes and Chemogenomics Data. Molecular Informatics, 2013, 32, 954-963.	2.5	2
41	Advancing the activity cliff concept. F1000Research, 2013, 2, 199.	1.6	65
42	High-resolution view of compound promiscuity. F1000Research, 2013, 2, 144.	1.6	39
43	Many structurally related drugs bind different targets whereas distinct drugs display significant target overlap. RSC Advances, 2012, 2, 3481.	3.6	14
44	Systematic Identification and Classification of Three-Dimensional Activity Cliffs. Journal of Chemical Information and Modeling, 2012, 52, 1490-1498.	5.4	26
45	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
46	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
47	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
48	Rationalizing Structure and Target Relationships between Current Drugs. AAPS Journal, 2012, 14, 764-771.	4.4	3
49	Chemical Transformations That Yield Compounds with Distinct Activity Profiles. ACS Medicinal Chemistry Letters, 2011, 2, 523-527.	2.8	18
50	Target Family-Directed Exploration of Scaffolds with Different SAR Profiles. Journal of Chemical Information and Modeling, 2011, 51, 3138-3148.	5.4	9
51	Lessons Learned from Molecular Scaffold Analysis. Journal of Chemical Information and Modeling, 2011, 51, 1742-1753.	5.4	82
52	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
53	Exploring Target-Selectivity Patterns of Molecular Scaffolds. ACS Medicinal Chemistry Letters, 2010, 1, 54-58.	2.8	14
54	Scaffold Distributions in Bioactive Molecules, Clinical Trials Compounds, and Drugs. ChemMedChem, 2010, 5, 187-190.	3.2	22

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55	Molecular Scaffolds with High Propensity to Form Multi-Target Activity Cliffs. Journal of Chemical Information and Modeling, 2010, 50, 500-510.	5.4	45
56	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
57	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
58	Global assessment of scaffold hopping potential for current pharmaceutical targets. MedChemComm, 2010, 1, 339-344.	3.4	25
59	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
60	RelACCSâ€FP: A Structural Minimalist Approach to Fingerprint Design. Chemical Biology and Drug Design, 2008, 72, 341-349.	3.2	13