Egon L Willighagen

List of Publications by Year
in descending order

119 papers	7,803 citations	87888 38 h-index	58581 82 g-index
153 all docs	153 docs citations	153 times ranked	11471 citing authors

#	Article	IF	Citations
1	The Chemistry Development Kit (CDK):â€‰An Open-Source Java Library for Chemo- and Bioinformatics. Journal of Chemical Information and Computer Sciences, 2003, 43, 493-500.	2.8	904
2	WikiPathways: a multifaceted pathway database bridging metabolomics to other omics research. Nucleic Acids Research, 2018, 46, D661-D667.	14.5	708
3	WikiPathways: connecting communities. Nucleic Acids Research, 2021, 49, D613-D621.	14.5	519
4	Recent Developments of the Chemistry Development Kit (CDK) - An Open-Source Java Library for Chemo- and Bioinformatics. Current Pharmaceutical Design, 2006, 12, 2111-2120.	1.9	418
5	WikiPathways: capturing the full diversity of pathway knowledge. Nucleic Acids Research, 2016, 44, D488-D494.	14.5	380
6	The Blue Obeliskâ€”Interoperability in Chemical Informatics. Journal of Chemical Information and Modeling, 2006, 46, 991-998.	5.4	366
7	Adverse outcome pathways: opportunities, limitations and open questions. Archives of Toxicology, 2017, 91, 3477-3505.	4.2	282
8	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. Journal of Cheminformatics, 2017, 9, 33.	6.1	275
9	Open PHACTS: semantic interoperability for drug discovery. Drug Discovery Today, 2012, 17, 1188-1198.	6.4	274
10	Community assessment to advance computational prediction of cancer drug combinations in a pharmacogenomic screen. Nature Communications, 2019, 10, 2674.	12.8	240
11	FAIR Principles: Interpretations and Implementation Considerations. Data Intelligence, 2020, 2, 10-29.	1.5	149
12	Linked open drug data for pharmaceutical research and development. Journal of Cheminformatics, 2011, 3, 19.	6.1	148
13	OSCAR4: a flexible architecture for chemical text-mining. Journal of Cheminformatics, 2011, 3, 41.	6.1	145
14	The Chemical Translation Serviceâ€”a web-based tool to improve standardization of metabolomic reports. Bioinformatics, 2010, 26, 2647-2648.	4.1	117
15	Bioclipse: an open source workbench for chemo- and bioinformatics. BMC Bioinformatics, 2007, 8, 59.	2.6	111
16	A transcriptomics data-driven gene space accurately predicts liver cytopathology and drug-induced liver injury. Nature Communications, 2017, 8, 15932.	12.8	99
17	COVID-19 Disease Map, building a computational repository of SARS-CoV-2 virus-host interaction mechanisms. Scientific Data, 2020, 7, 136.	5.3	99
18	The ChEMBL database as linked open data. Journal of Cheminformatics, 2013, 5, 23.	6.1	96

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19	The eNanoMapper database for nanomaterial safety information. Beilstein Journal of Nanotechnology, 2015, 6, 1609-1634.	2.8	92
20	The LOTUS initiative for open knowledge management in natural products research. ELife, 0, 11, .	6.0	90
21	The Chemical Information Ontology: Provenance and Disambiguation for Chemical Data on the Biological Semantic Web. PLoS ONE, 2011, 6, e25513.	2.5	86
22	PubChemRDF: towards the semantic annotation of PubChem compound and substance databases. Journal of Cheminformatics, 2015, 7, 34.	6.1	77
23	Wikidata as a knowledge graph for the life sciences. ELife, 2020, 9, .	6.0	76
24	NanoSolveIT Project: Driving nanoinformatics research to develop innovative and integrated tools for in silico nanosafety assessment. Computational and Structural Biotechnology Journal, 2020, 18, 583-602.	4.1	74
25	JChemPaint - Using the Collaborative Forces of the Internet to Develop a Free Editor for 2D Chemical Structures. Molecules, 2000, 5, 93-98.	3.8	70
26	The metaRbolomics Toolbox in Bioconductor and beyond. Metabolites, 2019, 9, 200.	2.9	64
27	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. Journal of Cheminformatics, 2011, 3, 37.	6.1	63
28	Elemental composition determination based on MSn. Bioinformatics, 2011, 27, 2376-2383.	4.1	63
29	eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. Journal of Biomedical Semantics, 2015, 6, 10.	1.6	63
30	SPLASH, a hashed identifier for mass spectra. Nature Biotechnology, 2016, 34, 1099-1101.	17.5	61
31	Integration among databases and data sets to support productive nanotechnology: Challenges and recommendations. NanoImpact, 2018, 9, 85-101.	4.5	56
32	Scholia, Scientometrics and Wikidata. Lecture Notes in Computer Science, 2017, , 237-259.	1.3	55
33	CDK-Taverna: an open workflow environment for cheminformatics. BMC Bioinformatics, 2010, 11, 159.	2.6	54
34	COVID19 Disease Map, a computational knowledge repository of virusâ€“host interaction mechanisms. Molecular Systems Biology, 2021, 17, e10387.	7.2	53
35	Bioclipse 2: A scriptable integration platform for the life sciences. BMC Bioinformatics, 2009, 10, 397.	2.6	52
36	A Data Fusion Pipeline for Generating and Enriching Adverse Outcome Pathway Descriptions. Toxicological Sciences, 2018, 162, 264-275.	3.1	51

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37	A Survey of Quantitative Descriptions of Molecular Structure. Current Topics in Medicinal Chemistry, 2012, 12, 1946-1956.	2.1	48
38	Emerging practices for mapping and linking life sciences data using RDF â€" A case series. Web Semantics, 2012, 14, 2-13.	2.9	48
39	RRegrs: an R package for computer-aided model selection with multiple regression models. Journal of Cheminformatics, 2015, 7, 46.	6.1	43
40	XMPP for cloud computing in bioinformatics supporting discovery and invocation of asynchronous web services. BMC Bioinformatics, 2009, 10, 279.	2.6	40
41	Towards interoperable and reproducible QSAR analyses: Exchange of datasets. Journal of Cheminformatics, 2010, 2, 5.	6.1	39
42	Cationic Gemini Surfactants Based on Tartaric Acid: Synthesis, Aggregation, Monolayer Behaviour, and Interaction with DNA. European Journal of Organic Chemistry, 2002, 2002, 1397-1406.	2.4	38
43	Chemical Markup, XML, and the World Wide Web. 5. Applications of Chemical Metadata in RSS Aggregators. Journal of Chemical Information and Computer Sciences, 2004, 44, 462-469.	2.8	38
44	Method for the computational comparison of crystal structures. Acta Crystallographica Section B: Structural Science, 2005, 61, 29-36.	1.8	36
45	The ToxBank Data Warehouse: Supporting the Replacement of In Vivo Repeated Dose Systemic Toxicity Testing. Molecular Informatics, 2013, 32, 47-63.	2.5	35
46	Introducing WikiPathways as a Data-Source to Support Adverse Outcome Pathways for Regulatory Risk Assessment of Chemicals and Nanomaterials. Frontiers in Genetics, 2018, 9, 661.	2.3	34
47	Using the Semantic Web for Rapid Integration of WikiPathways with Other Biological Online Data Resources. PLoS Computational Biology, 2016, 12, e1004989.	3.2	33
48	Toward the Replacement of Animal Experiments through the Bioinformatics-driven Analysis of â€˜Omicsâ€™ Data from Human Cell Cultures. ATLA Alternatives To Laboratory Animals, 2015, 43, 325-332.	1.0	29
49	Risk Governance of Emerging Technologies Demonstrated in Terms of its Applicability to Nanomaterials. Small, 2020, 16, e2003303.	10.0	28
50	Can an InChI for Nano Address the Need for a Simplified Representation of Complex Nanomaterials across Experimental and Nanoinformatics Studies?. Nanomaterials, 2020, 10, 2493.	4.1	28
51	Complex Portal 2022: new curation frontiers. Nucleic Acids Research, 2022, 50, D578-D586.	14.5	27
52	CyTargetLinker app update: A flexible solution for network extension in Cytoscape. F1000Research, 2018, 7, 743.	1.6	26
53	Chemical Markup, XML, and the World Wide Web. 7. CMLSpect, an XML Vocabulary for Spectral Data. Journal of Chemical Information and Modeling, 2007, 47, 2015-2034.	5.4	25
54	Linking the Resource Description Framework to cheminformatics and proteochemometrics. Journal of Biomedical Semantics, 2011, 2, S6.	1.6	24

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55	On the Use of1H and13C 1D NMR Spectra as QSPR Descriptors. Journal of Chemical Information and Modeling, 2006, 46, 487-494.	5.4	23
56	New developments on the cheminformatics open workflow environment CDK-Taverna. Journal of Cheminformatics, 2011, 3, 54.	6.1	23
57	Cheminformatics. Communications of the ACM, 2012, 55, 65-75.	4.5	21
58	Nanopublications: A Growing Resource of Provenance-Centric Scientific Linked Data. , 2018, , .		21
59	A Semi-Automated Workflow for FAIR Maturity Indicators in the Life Sciences. Nanomaterials, 2020, 10, 2068.	4.1	21
60	Fast and Scriptable Molecular Graphics in Web Browsers without Java3D. Nature Precedings, 2007, , .	0.1	19
61	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	1.6	19
62	CyTargetLinker app update: A flexible solution for network extension in Cytoscape. F1000Research, 2018, 7, 743.	1.6	18
63	Enabling Open Science: Wikidata for Research (Wiki4R). Research Ideas and Outcomes, 0, 1, e7573.	1.0	17
64	Computational toxicology using the OpenTox application programming interface and Bioclipse. BMC Research Notes, 2011, 4, 487.	1.4	16
65	Scientific Lenses to Support Multiple Views over Linked Chemistry Data. Lecture Notes in Computer Science, 2014, , 98-113.	1.3	16
66	MECP2 variation in Rett syndrome-An overview of current coverage of genetic and phenotype data within existing databases. Human Mutation, 2018, 39, 914-924.	2.5	15
67	Userscripts for the Life Sciences. BMC Bioinformatics, 2007, 8, 487.	2.6	14
68	A protocol for adding knowledge to Wikidata: aligning resources on human coronaviruses. BMC Biology, 2021, 19, 12.	3.8	14
69	Automatically visualise and analyse data on pathways using PathVisioRPC from any programming environment. BMC Bioinformatics, 2015, 16, 267.	2.6	13
70	XMetDB: an open access database for xenobiotic metabolism. Journal of Cheminformatics, 2016, 8, 47.	6.1	13
71	Ten simple rules for creating reusable pathway models for computational analysis and visualization. PLoS Computational Biology, 2021, 17, e1009226.	3.2	13
72	CAS Common Chemistry in 2021: Expanding Access to Trusted Chemical Information for the Scientific Community. Journal of Chemical Information and Modeling, 2022, 62, 2737-2743.	5.4	13

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73	A catalogue of 863 Rett-syndrome-causing MECP2 mutations and lessons learned from data integration. Scientific Data, 2021, 8, 10.	5.3	12
74	Taking FAIR on the ChIN: The Chemistry Implementation Network. Data Intelligence, 2020, 2, 131-138.	1.5	12
75	Resource description framework technologies in chemistry. Journal of Cheminformatics, 2011, 3, 15.	6.1	11
76	Open Source Drug Discovery with Bioclipse. Current Topics in Medicinal Chemistry, 2012, 12, 1980-1986.	2.1	11
77	A resource to explore the discovery of rare diseases and their causative genes. Scientific Data, 2021, 8, 124.	5.3	11
78	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	1.6	11
79	Beyond Pathway Analysis: Identification of Active Subnetworks in Rett Syndrome. Frontiers in Genetics, 2019, 10, 59.	2.3	10
80	Reliable Granular References to Changing Linked Data. Lecture Notes in Computer Science, 2017, , 436-451.	1.3	10
81	Providing Adverse Outcome Pathways from the AOP-Wiki in a Semantic Web Format to Increase Usability and Accessibility of the Content. Applied in Vitro Toxicology, 2022, 8, 2-13.	1.1	10
82	The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics.. ChemInform, 2003, 34, no.	0.0	9
83	Supervised Self-Organizing Maps in Crystal Property and Structure Prediction. Crystal Growth and Design, 2007, 7, 1738-1745.	3.0	9
84	Molecular Chemometrics. Critical Reviews in Analytical Chemistry, 2006, 36, 189-198.	3.5	8
85	Changing computational research. The challenges ahead. Source Code for Biology and Medicine, 2012, 7, 2.	1.7	8
86	Applications of the InChI in cheminformatics with the CDK and Bioclipse. Journal of Cheminformatics, 2013, 5, 14.	6.1	8
87	Bioclipse-R: integrating management and visualization of life science data with statistical analysis. Bioinformatics, 2013, 29, 286-289.	4.1	8
88	Learning cheminformatics. Journal of Cheminformatics, 2020, 12, 4.	6.1	7
89	Interpreting the lipidome: bioinformatic approaches to embrace the complexity. Metabolomics, 2021, 17, 55.	3.0	7
90	Accessing, Using, and Creating Chemical Property Databases for Computational Toxicology Modeling. Methods in Molecular Biology, 2012, 929, 221-241.	0.9	7

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91	Explicit interaction information from WikiPathways in RDF facilitates drug discovery in the Open PHACTS Discovery Platform. F1000Research, 2018, 7, 75.	1.6	7
92	Robustifying Scholia: paving the way for knowledge discovery and research assessment through Wikidata. Research Ideas and Outcomes, 0, 5, .	1.0	7
93	A Survey of Quantitative Descriptions of Molecular Structure. Current Topics in Medicinal Chemistry, 2013, 12, 1946-1956.	2.1	6
94	Bacting: a next generation, command line version of Bioclipse. Journal of Open Source Software, 2021, 6, 2558.	4.6	6
95	Explicit interaction information from WikiPathways in RDF facilitates drug discovery in the Open PHACTS Discovery Platform. F1000Research, 2018, 7, 75.	1.6	6
96	The first eNanoMapper prototype: A substance database to support safe-by-design. , 2014, , .		5
97	RDFIO: extending Semantic MediaWiki for interoperable biomedical data management. Journal of Biomedical Semantics, 2017, 8, 35.	1.6	5
98	Incorporating Commercial and Private Data into an Open Linked Data Platform for Drug Discovery. Lecture Notes in Computer Science, 2013, , 65-80.	1.3	5
99	The AOP-DB RDF: Applying FAIR Principles to the Semantic Integration of AOP Data Using the Research Description Framework. Frontiers in Toxicology, 2022, 4, 803983.	3.1	5
100	PSnpBind: a database of mutated binding site proteinâ€“ligand complexes constructed using a multithreaded virtual screening workflow. Journal of Cheminformatics, 2022, 14, 8.	6.1	5
101	SKG4EOSC - Scholarly Knowledge Graphs for EOSC: Establishing a backbone of knowledge graphs for FAIR Scholarly Information in EOSC. Research Ideas and Outcomes, 0, 8, .	1.0	5
102	Research Techniques Made Simple: Lipidomic Analysis in Skin Research. Journal of Investigative Dermatology, 2022, 142, 4-11.e1.	0.7	4
103	Helping to improve the practice of cheminformatics. Journal of Cheminformatics, 2017, 9, 40.	6.1	3
104	Adoption of the Citation Typing Ontology by the Journal of Cheminformatics. Journal of Cheminformatics, 2020, 12, 47.	6.1	3
105	What is the role of cheminformatics in a pandemic?. Journal of Cheminformatics, 2021, 13, 16.	6.1	3
106	Reply to â€œFAIR chemical structure in the Journal of Cheminformaticsâ€• Journal of Cheminformatics, 2021, 13, 49.	6.1	3
107	ELIXIR and Toxicology: a community in development. F1000Research, 0, 10, 1129.	1.6	3
108	Using the RRegrs R package for automating predictive modelling. , 0, , .		2

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109	WikiPathways: Integrating Pathway Knowledge with Clinical Data. , 2022, , 1457-1466.		2
110	Beautifying Data in the Real World. Nature Precedings, 2010, , .	0.1	1
111	Journal of Cheminformatics, ORCID, and GitHub. Journal of Cheminformatics, 2019, 11, 44.	6.1	1
112	Investigating the Molecular Processes behind the Cell-Specific Toxicity Response to Titanium Dioxide Nanobelts. International Journal of Molecular Sciences, 2021, 22, 9432.	4.1	1
113	Providing gene-to-variant and variant-to-gene database identifier mappings to use with BridgeDb mapping services.. F1000Research, 0, 7, 1390.	1.6	1
114	BridgeDb and Wikidata: a powerful combination generating interoperable open research (BridgeDb). Research Ideas and Outcomes, 0, 8, .	1.0	1
115	Understanding signaling and metabolic paths using semantified and harmonized information about biological interactions. PLoS ONE, 2022, 17, e0263057.	2.5	1
116	Interactive predictive toxicology with Bioclipse and OpenTox. , 2012, , 35-61.		0
117	Emerging Practices for Mapping and Linking Life Sciences Data Using RDF - A Case Series. SSRN Electronic Journal, 2012, , .	0.4	0
118	Getting CAS registry numbers out of WikiData. The Winnower, 2015, , .	0.0	0
119	Three-Dimensional (3D) Molecular Representations. Chapman & Hall/CRC Mathematical and Computational Biology Series, 2010, , 65-87.	0.1	0