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	Complex Portal 2022: new curation frontiers. Nucleic Acids Research, 2022, 50, D578-D586.	14.5	27
2	Research Techniques Made Simple: Lipidomic Analysis in Skin Research. Journal of Investigative Dermatology, 2022, 142, 4-11.e1.	0.7	4
3	WikiPathways: Integrating Pathway Knowledge with Clinical Data. , 2022, , 1457-1466.		2
4	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
5	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
6	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
7	Understanding signaling and metabolic paths using semantified and harmonized information about biological interactions. PLoS ONE, 2022, 17, e0263057.	2.5	1
8	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
9	A protocol for adding knowledge to Wikidata: aligning resources on human coronaviruses. BMC Biology, 2021, 19, 12.	3.8	14
10	What is the role of cheminformatics in a pandemic?. Journal of Cheminformatics, 2021, 13, 16.	6.1	3
11	A resource to explore the discovery of rare diseases and their causative genes. Scientific Data, 2021, 8, 124.	5.3	11
12	Bacting: a next generation, command line version of Bioclipse. Journal of Open Source Software, 2021, 6, 2558.	4.6	6
13	Interpreting the lipidome: bioinformatic approaches to embrace the complexity. Metabolomics, 2021, 17, 55.	3.0	7
14	Reply to â€œFAIR chemical structure in the Journal of Cheminformaticsâ€• Journal of Cheminformatics, 2021, 13, 49.	6.1	3
15	Ten simple rules for creating reusable pathway models for computational analysis and visualization. PLoS Computational Biology, 2021, 17, e1009226.	3.2	13
16	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
17	A catalogue of 863 Rett-syndrome-causing MECP2 mutations and lessons learned from data integration. Scientific Data, 2021, 8, 10.	5.3	12
18	WikiPathways: connecting communities. Nucleic Acids Research, 2021, 49, D613-D621.	14.5	519

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19	COVID19 Disease Map, a computational knowledge repository of virusâ€“host interaction mechanisms. Molecular Systems Biology, 2021, 17, e10387.	7.2	53
20	Adoption of the Citation Typing Ontology by the Journal of Cheminformatics. Journal of Cheminformatics, 2020, 12, 47.	6.1	3
21	Risk Governance of Emerging Technologies Demonstrated in Terms of its Applicability to Nanomaterials. Small, 2020, 16, e2003303.	10.0	28
22	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
23	A Semi-Automated Workflow for FAIR Maturity Indicators in the Life Sciences. Nanomaterials, 2020, 10, 2068.	4.1	21
24	FAIR Principles: Interpretations and Implementation Considerations. Data Intelligence, 2020, 2, 10-29.	1.5	149
25	COVID-19 Disease Map, building a computational repository of SARS-CoV-2 virus-host interaction mechanisms. Scientific Data, 2020, 7, 136.	5.3	99
26	Learning cheminformatics. Journal of Cheminformatics, 2020, 12, 4.	6.1	7
27	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
28	Taking FAIR on the ChIN: The Chemistry Implementation Network. Data Intelligence, 2020, 2, 131-138.	1.5	12
29	Wikidata as a knowledge graph for the life sciences. ELife, 2020, 9, .	6.0	76
30	Journal of Cheminformatics, ORCID, and GitHub. Journal of Cheminformatics, 2019, 11, 44.	6.1	1
31	The metaRbolomics Toolbox in Bioconductor and beyond. Metabolites, 2019, 9, 200.	2.9	64
32	Community assessment to advance computational prediction of cancer drug combinations in a pharmacogenomic screen. Nature Communications, 2019, 10, 2674.	12.8	240
33	Beyond Pathway Analysis: Identification of Active Subnetworks in Rett Syndrome. Frontiers in Genetics, 2019, 10, 59.	2.3	10
34	WikiPathways: a multifaceted pathway database bridging metabolomics to other omics research. Nucleic Acids Research, 2018, 46, D661-D667.	14.5	708
35	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
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	Integration among databases and data sets to support productive nanotechnology: Challenges and recommendations. NanoImpact, 2018, 9, 85-101.	4.5	56
38	Nanopublications: A Growing Resource of Provenance-Centric Scientific Linked Data. , 2018, , .		21
39	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
40	Explicit interaction information from WikiPathways in RDF facilitates drug discovery in the Open PHACTS Discovery Platform. F1000Research, 2018, 7, 75.	1.6	7
41	Explicit interaction information from WikiPathways in RDF facilitates drug discovery in the Open PHACTS Discovery Platform. F1000Research, 2018, 7, 75.	1.6	6
42	CyTargetLinker app update: A flexible solution for network extension in Cytoscape. F1000Research, 2018, 7, 743.	1.6	26
43	CyTargetLinker app update: A flexible solution for network extension in Cytoscape. F1000Research, 2018, 7, 743.	1.6	18
44	Adverse outcome pathways: opportunities, limitations and open questions. Archives of Toxicology, 2017, 91, 3477-3505.	4.2	282
45	A transcriptomics data-driven gene space accurately predicts liver cytopathology and drug-induced liver injury. Nature Communications, 2017, 8, 15932.	12.8	99
46	Helping to improve the practice of cheminformatics. Journal of Cheminformatics, 2017, 9, 40.	6.1	3
47	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. Journal of Cheminformatics, 2017, 9, 33.	6.1	275
48	RDFIO: extending Semantic MediaWiki for interoperable biomedical data management. Journal of Biomedical Semantics, 2017, 8, 35.	1.6	5
49	Reliable Granular References to Changing Linked Data. Lecture Notes in Computer Science, 2017, , 436-451.	1.3	10
50	Scholia, Scientometrics and Wikidata. Lecture Notes in Computer Science, 2017, , 237-259.	1.3	55
51	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	1.6	19
52	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	1.6	11
53	Using the Semantic Web for Rapid Integration of WikiPathways with Other Biological Online Data Resources. PLoS Computational Biology, 2016, 12, e1004989.	3.2	33
54	WikiPathways: capturing the full diversity of pathway knowledge. Nucleic Acids Research, 2016, 44, D488-D494.	14.5	380

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55	XMetDB: an open access database for xenobiotic metabolism. Journal of Cheminformatics, 2016, 8, 47.	6.1	13
56	SPLASH, a hashed identifier for mass spectra. Nature Biotechnology, 2016, 34, 1099-1101.	17.5	61
57	PubChemRDF: towards the semantic annotation of PubChem compound and substance databases. Journal of Cheminformatics, 2015, 7, 34.	6.1	77
58	RRegrs: an R package for computer-aided model selection with multiple regression models. Journal of Cheminformatics, 2015, 7, 46.	6.1	43
59	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
60	The eNanoMapper database for nanomaterial safety information. Beilstein Journal of Nanotechnology, 2015, 6, 1609-1634.	2.8	92
61	Getting CAS registry numbers out of WikiData. The Winnower, 2015, , .	0.0	0
62	eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. Journal of Biomedical Semantics, 2015, 6, 10.	1.6	63
63	Automatically visualise and analyse data on pathways using PathVisioRPC from any programming environment. BMC Bioinformatics, 2015, 16, 267.	2.6	13
64	The first eNanoMapper prototype: A substance database to support safe-by-design. , 2014, , .		5
65	Scientific Lenses to Support Multiple Views over Linked Chemistry Data. Lecture Notes in Computer Science, 2014, , 98-113.	1.3	16
66	The ChEMBL database as linked open data. Journal of Cheminformatics, 2013, 5, 23.	6.1	96
67	Applications of the InChI in cheminformatics with the CDK and Bioclipse. Journal of Cheminformatics, 2013, 5, 14.	6.1	8
68	The ToxBank Data Warehouse: Supporting the Replacement of In Vivo Repeated Dose Systemic Toxicity Testing. Molecular Informatics, 2013, 32, 47-63.	2.5	35
69	Bioclipse-R: integrating management and visualization of life science data with statistical analysis. Bioinformatics, 2013, 29, 286-289.	4.1	8
70	A Survey of Quantitative Descriptions of Molecular Structure. Current Topics in Medicinal Chemistry, 2013, 12, 1946-1956.	2.1	6
71	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
72	Interactive predictive toxicology with Bioclipse and OpenTox. , 2012, , 35-61.		0

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73	A Survey of Quantitative Descriptions of Molecular Structure. Current Topics in Medicinal Chemistry, 2012, 12, 1946-1956.	2.1	48
74	Cheminformatics. Communications of the ACM, 2012, 55, 65-75.	4.5	21
75	Open Source Drug Discovery with Bioclipse. Current Topics in Medicinal Chemistry, 2012, 12, 1980-1986.	2.1	11
76	Emerging practices for mapping and linking life sciences data using RDF â€" A case series. Web Semantics, 2012, 14, 2-13.	2.9	48
77	Changing computational research. The challenges ahead. Source Code for Biology and Medicine, 2012, 7, 2.	1.7	8
78	Open PHACTS: semantic interoperability for drug discovery. Drug Discovery Today, 2012, 17, 1188-1198.	6.4	274
79	Emerging Practices for Mapping and Linking Life Sciences Data Using RDF - A Case Series. SSRN Electronic Journal, 2012, , .	0.4	0
80	Accessing, Using, and Creating Chemical Property Databases for Computational Toxicology Modeling. Methods in Molecular Biology, 2012, 929, 221-241.	0.9	7
81	Linking the Resource Description Framework to cheminformatics and proteochemometrics. Journal of Biomedical Semantics, 2011, 2, S6.	1.6	24
82	New developments on the cheminformatics open workflow environment CDK-Taverna. Journal of Cheminformatics, 2011, 3, 54.	6.1	23
83	Computational toxicology using the OpenTox application programming interface and Bioclipse. BMC Research Notes, 2011, 4, 487.	1.4	16
84	Resource description framework technologies in chemistry. Journal of Cheminformatics, 2011, 3, 15.	6.1	11
85	Linked open drug data for pharmaceutical research and development. Journal of Cheminformatics, 2011, 3, 19.	6.1	148
86	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. Journal of Cheminformatics, 2011, 3, 37.	6.1	63
87	OSCAR4: a flexible architecture for chemical text-mining. Journal of Cheminformatics, 2011, 3, 41.	6.1	145
88	Elemental composition determination based on MSn. Bioinformatics, 2011, 27, 2376-2383.	4.1	63
89	The Chemical Information Ontology: Provenance and Disambiguation for Chemical Data on the Biological Semantic Web. PLoS ONE, 2011, 6, e25513.	2.5	86
90	CDK-Taverna: an open workflow environment for cheminformatics. BMC Bioinformatics, 2010, 11, 159.	2.6	54

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91	Towards interoperable and reproducible QSAR analyses: Exchange of datasets. Journal of Cheminformatics, 2010, 2, 5.	6.1	39
92	Beautifying Data in the Real World. Nature Precedings, 2010, , .	0.1	1
93	The Chemical Translation Serviceâ€"a web-based tool to improve standardization of metabolomic reports. Bioinformatics, 2010, 26, 2647-2648.	4.1	117
94	Three-Dimensional (3D) Molecular Representations. Chapman & Hall/CRC Mathematical and Computational Biology Series, 2010, , 65-87.	0.1	0
95	XMPP for cloud computing in bioinformatics supporting discovery and invocation of asynchronous web services. BMC Bioinformatics, 2009, 10, 279.	2.6	40
96	Bioclipse 2: A scriptable integration platform for the life sciences. BMC Bioinformatics, 2009, 10, 397.	2.6	52
97	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
98	Supervised Self-Organizing Maps in Crystal Property and Structure Prediction. Crystal Growth and Design, 2007, 7, 1738-1745.	3.0	9
99	Fast and Scriptable Molecular Graphics in Web Browsers without Java3D. Nature Precedings, 2007, , .	0.1	19
100	Userscripts for the Life Sciences. BMC Bioinformatics, 2007, 8, 487.	2.6	14
101	Bioclipse: an open source workbench for chemo- and bioinformatics. BMC Bioinformatics, 2007, 8, 59.	2.6	111
102	Molecular Chemometrics. Critical Reviews in Analytical Chemistry, 2006, 36, 189-198.	3.5	8
103	The Blue Obeliskâ€"Interoperability in Chemical Informatics. Journal of Chemical Information and Modeling, 2006, 46, 991-998.	5.4	366
104	On the Use of1H and13C 1D NMR Spectra as QSPR Descriptors. Journal of Chemical Information and Modeling, 2006, 46, 487-494.	5.4	23
105	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
106	Method for the computational comparison of crystal structures. Acta Crystallographica Section B: Structural Science, 2005, 61, 29-36.	1.8	36
107	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
108	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

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109	The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics.. ChemInform, 2003, 34, no.	0.0	9
110	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
111	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
112	Enabling Open Science: Wikidata for Research (Wiki4R). Research Ideas and Outcomes, 0, 1, e7573.	1.0	17
113	Using the RRegrs R package for automating predictive modelling. , 0, , .		2
114	Robustifying Scholia: paving the way for knowledge discovery and research assessment through Wikidata. Research Ideas and Outcomes, 0, 5, .	1.0	7
115	Providing gene-to-variant and variant-to-gene database identifier mappings to use with BridgeDb mapping services.. F1000Research, 0, 7, 1390.	1.6	1
116	ELIXIR and Toxicology: a community in development. F1000Research, 0, 10, 1129.	1.6	3
117	BridgeDb and Wikidata: a powerful combination generating interoperable open research (BridgeDb). Research Ideas and Outcomes, 0, 8, .	1.0	1
118	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
119	The LOTUS initiative for open knowledge management in natural products research. ELife, 0, 11, .	6.0	90