

# Egon L Willighagen

## List of Publications by Year in descending order

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Version: 2024-02-01

119  
papers

7,803  
citations

87723

38  
h-index

58464

82  
g-index

153  
all docs

153  
docs citations

153  
times ranked

11471  
citing authors

#	ARTICLE	IF	CITATIONS
1	The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics. <i>Journal of Chemical Information and Computer Sciences</i> , 2003, 43, 493-500.	2.8	904
2	WikiPathways: a multifaceted pathway database bridging metabolomics to other omics research. <i>Nucleic Acids Research</i> , 2018, 46, D661-D667.	6.5	708
3	WikiPathways: connecting communities. <i>Nucleic Acids Research</i> , 2021, 49, D613-D621.	6.5	519
4	Recent Developments of the Chemistry Development Kit (CDK) - An Open-Source Java Library for Chemo- and Bioinformatics. <i>Current Pharmaceutical Design</i> , 2006, 12, 2111-2120.	0.9	418
5	WikiPathways: capturing the full diversity of pathway knowledge. <i>Nucleic Acids Research</i> , 2016, 44, D488-D494.	6.5	380
6	The Blue Obelisk Interoperability in Chemical Informatics. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 991-998.	2.5	366
7	Adverse outcome pathways: opportunities, limitations and open questions. <i>Archives of Toxicology</i> , 2017, 91, 3477-3505.	1.9	282
8	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. <i>Journal of Cheminformatics</i> , 2017, 9, 33.	2.8	275
9	Open PHACTS: semantic interoperability for drug discovery. <i>Drug Discovery Today</i> , 2012, 17, 1188-1198.	3.2	274
10	Community assessment to advance computational prediction of cancer drug combinations in a pharmacogenomic screen. <i>Nature Communications</i> , 2019, 10, 2674.	5.8	240
11	FAIR Principles: Interpretations and Implementation Considerations. <i>Data Intelligence</i> , 2020, 2, 10-29.	0.8	149
12	Linked open drug data for pharmaceutical research and development. <i>Journal of Cheminformatics</i> , 2011, 3, 19.	2.8	148
13	OSCAR4: a flexible architecture for chemical text-mining. <i>Journal of Cheminformatics</i> , 2011, 3, 41.	2.8	145
14	The Chemical Translation Service a web-based tool to improve standardization of metabolomic reports. <i>Bioinformatics</i> , 2010, 26, 2647-2648.	1.8	117
15	Bioclipse: an open source workbench for chemo- and bioinformatics. <i>BMC Bioinformatics</i> , 2007, 8, 59.	1.2	111
16	A transcriptomics data-driven gene space accurately predicts liver cytopathology and drug-induced liver injury. <i>Nature Communications</i> , 2017, 8, 15932.	5.8	99
17	COVID-19 Disease Map, building a computational repository of SARS-CoV-2 virus-host interaction mechanisms. <i>Scientific Data</i> , 2020, 7, 136.	2.4	99
18	The ChEMBL database as linked open data. <i>Journal of Cheminformatics</i> , 2013, 5, 23.	2.8	96

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19	The eNanoMapper database for nanomaterial safety information. Beilstein Journal of Nanotechnology, 2015, 6, 1609-1634.	1.5	92
20	The LOTUS initiative for open knowledge management in natural products research. ELife, 0, 11, .	2.8	90
21	The Chemical Information Ontology: Provenance and Disambiguation for Chemical Data on the Biological Semantic Web. PLoS ONE, 2011, 6, e25513.	1.1	86
22	PubChemRDF: towards the semantic annotation of PubChem compound and substance databases. Journal of Cheminformatics, 2015, 7, 34.	2.8	77
23	Wikidata as a knowledge graph for the life sciences. ELife, 2020, 9, .	2.8	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.	1.9	74
25	JChemPaint - Using the Collaborative Forces of the Internet to Develop a Free Editor for 2D Chemical Structures. Molecules, 2000, 5, 93-98.	1.7	70
26	The metaRbolomics Toolbox in Bioconductor and beyond. Metabolites, 2019, 9, 200.	1.3	64
27	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. Journal of Cheminformatics, 2011, 3, 37.	2.8	63
28	Elemental composition determination based on MS<i>n</i>. Bioinformatics, 2011, 27, 2376-2383.	1.8	63
29	eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. Journal of Biomedical Semantics, 2015, 6, 10.	0.9	63
30	SPLASH, a hashed identifier for mass spectra. Nature Biotechnology, 2016, 34, 1099-1101.	9.4	61
31	Integration among databases and data sets to support productive nanotechnology: Challenges and recommendations. Nanolmpact, 2018, 9, 85-101.	2.4	56
32	Scholia, Scientometrics and Wikidata. Lecture Notes in Computer Science, 2017, , 237-259.	1.0	55
33	CDK-Taverna: an open workflow environment for cheminformatics. BMC Bioinformatics, 2010, 11, 159.	1.2	54
34	COVID19 Disease Map, a computational knowledge repository of virus-host interaction mechanisms. Molecular Systems Biology, 2021, 17, e10387.	3.2	53
35	Bioclipse 2: A scriptable integration platform for the life sciences. BMC Bioinformatics, 2009, 10, 397.	1.2	52
36	A Data Fusion Pipeline for Generating and Enriching Adverse Outcome Pathway Descriptions. Toxicological Sciences, 2018, 162, 264-275.	1.4	51

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37	A Survey of Quantitative Descriptions of Molecular Structure. <i>Current Topics in Medicinal Chemistry</i> , 2012, 12, 1946-1956.	1.0	48
38	Emerging practices for mapping and linking life sciences data using RDF – A case series. <i>Web Semantics</i> , 2012, 14, 2-13.	2.2	48
39	RRegrs: an R package for computer-aided model selection with multiple regression models. <i>Journal of Cheminformatics</i> , 2015, 7, 46.	2.8	43
40	XMPP for cloud computing in bioinformatics supporting discovery and invocation of asynchronous web services. <i>BMC Bioinformatics</i> , 2009, 10, 279.	1.2	40
41	Towards interoperable and reproducible QSAR analyses: Exchange of datasets. <i>Journal of Cheminformatics</i> , 2010, 2, 5.	2.8	39
42	Cationic Gemini Surfactants Based on Tartaric Acid: Synthesis, Aggregation, Monolayer Behaviour, and Interaction with DNA. <i>European Journal of Organic Chemistry</i> , 2002, 2002, 1397-1406.	1.2	38
43	Chemical Markup, XML, and the World Wide Web. 5. Applications of Chemical Metadata in RSS Aggregators. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 462-469.	2.8	38
44	Method for the computational comparison of crystal structures. <i>Acta Crystallographica Section B: Structural Science</i> , 2005, 61, 29-36.	1.8	36
45	The ToxBank Data Warehouse: Supporting the Replacement of In Vivo Repeated Dose Systemic Toxicity Testing. <i>Molecular Informatics</i> , 2013, 32, 47-63.	1.4	35
46	Introducing WikiPathways as a Data-Source to Support Adverse Outcome Pathways for Regulatory Risk Assessment of Chemicals and Nanomaterials. <i>Frontiers in Genetics</i> , 2018, 9, 661.	1.1	34
47	Using the Semantic Web for Rapid Integration of WikiPathways with Other Biological Online Data Resources. <i>PLoS Computational Biology</i> , 2016, 12, e1004989.	1.5	33
48	Toward the Replacement of Animal Experiments through the Bioinformatics-driven Analysis of –Omics™ Data from Human Cell Cultures. <i>ATLA Alternatives To Laboratory Animals</i> , 2015, 43, 325-332.	0.7	29
49	Risk Governance of Emerging Technologies Demonstrated in Terms of its Applicability to Nanomaterials. <i>Small</i> , 2020, 16, e2003303.	5.2	28
50	Can an InChI for Nano Address the Need for a Simplified Representation of Complex Nanomaterials across Experimental and Nanoinformatics Studies?. <i>Nanomaterials</i> , 2020, 10, 2493.	1.9	28
51	Complex Portal 2022: new curation frontiers. <i>Nucleic Acids Research</i> , 2022, 50, D578-D586.	6.5	27
52	CyTargetLinker app update: A flexible solution for network extension in Cytoscape. <i>F1000Research</i> , 2018, 7, 743.	0.8	26
53	Chemical Markup, XML, and the World Wide Web. 7. CMLSpect, an XML Vocabulary for Spectral Data. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 2015-2034.	2.5	25
54	Linking the Resource Description Framework to cheminformatics and proteochemometrics. <i>Journal of Biomedical Semantics</i> , 2011, 2, S6.	0.9	24

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55	On the Use of <sup>1</sup> H and <sup>13</sup> C 1D NMR Spectra as QSPR Descriptors. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 487-494.	2.5	23
56	New developments on the cheminformatics open workflow environment CDK-Taverna. <i>Journal of Cheminformatics</i> , 2011, 3, 54.	2.8	23
57	Cheminformatics. <i>Communications of the ACM</i> , 2012, 55, 65-75.	3.3	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. <i>Nanomaterials</i> , 2020, 10, 2068.	1.9	21
60	Fast and Scriptable Molecular Graphics in Web Browsers without Java3D. <i>Nature Precedings</i> , 2007, , .	0.1	19
61	The future of metabolomics in ELIXIR. <i>F1000Research</i> , 2017, 6, 1649.	0.8	19
62	CyTargetLinker app update: A flexible solution for network extension in Cytoscape. <i>F1000Research</i> , 2018, 7, 743.	0.8	18
63	Enabling Open Science: Wikidata for Research (Wiki4R). <i>Research Ideas and Outcomes</i> , 0, 1, e7573.	1.0	17
64	Computational toxicology using the OpenTox application programming interface and Bioclipse. <i>BMC Research Notes</i> , 2011, 4, 487.	0.6	16
65	Scientific Lenses to Support Multiple Views over Linked Chemistry Data. <i>Lecture Notes in Computer Science</i> , 2014, , 98-113.	1.0	16
66	<i>MECP2</i> variation in Rett syndrome-An overview of current coverage of genetic and phenotype data within existing databases. <i>Human Mutation</i> , 2018, 39, 914-924.	1.1	15
67	Userscripts for the Life Sciences. <i>BMC Bioinformatics</i> , 2007, 8, 487.	1.2	14
68	A protocol for adding knowledge to Wikidata: aligning resources on human coronaviruses. <i>BMC Biology</i> , 2021, 19, 12.	1.7	14
69	Automatically visualise and analyse data on pathways using PathVisioRPC from any programming environment. <i>BMC Bioinformatics</i> , 2015, 16, 267.	1.2	13
70	XMetDB: an open access database for xenobiotic metabolism. <i>Journal of Cheminformatics</i> , 2016, 8, 47.	2.8	13
71	Ten simple rules for creating reusable pathway models for computational analysis and visualization. <i>PLoS Computational Biology</i> , 2021, 17, e1009226.	1.5	13
72	CAS Common Chemistry in 2021: Expanding Access to Trusted Chemical Information for the Scientific Community. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2737-2743.	2.5	13

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73	A catalogue of 863 Rett-syndrome-causing MECP2 mutations and lessons learned from data integration. <i>Scientific Data</i> , 2021, 8, 10.	2.4	12
74	Taking FAIR on the ChIN: The Chemistry Implementation Network. <i>Data Intelligence</i> , 2020, 2, 131-138.	0.8	12
75	Resource description framework technologies in chemistry. <i>Journal of Cheminformatics</i> , 2011, 3, 15.	2.8	11
76	Open Source Drug Discovery with Bioclipse. <i>Current Topics in Medicinal Chemistry</i> , 2012, 12, 1980-1986.	1.0	11
77	A resource to explore the discovery of rare diseases and their causative genes. <i>Scientific Data</i> , 2021, 8, 124.	2.4	11
78	The future of metabolomics in ELIXIR. <i>F1000Research</i> , 2017, 6, 1649.	0.8	11
79	Beyond Pathway Analysis: Identification of Active Subnetworks in Rett Syndrome. <i>Frontiers in Genetics</i> , 2019, 10, 59.	1.1	10
80	Reliable Granular References to Changing Linked Data. <i>Lecture Notes in Computer Science</i> , 2017, , 436-451.	1.0	10
81	Providing Adverse Outcome Pathways from the AOP-Wiki in a Semantic Web Format to Increase Usability and Accessibility of the Content. <i>Applied in Vitro Toxicology</i> , 2022, 8, 2-13.	0.6	10
82	The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics.. <i>ChemInform</i> , 2003, 34, no.	0.1	9
83	Supervised Self-Organizing Maps in Crystal Property and Structure Prediction. <i>Crystal Growth and Design</i> , 2007, 7, 1738-1745.	1.4	9
84	Molecular Chemometrics. <i>Critical Reviews in Analytical Chemistry</i> , 2006, 36, 189-198.	1.8	8
85	Changing computational research. The challenges ahead. <i>Source Code for Biology and Medicine</i> , 2012, 7, 2.	1.7	8
86	Applications of the InChI in cheminformatics with the CDK and Bioclipse. <i>Journal of Cheminformatics</i> , 2013, 5, 14.	2.8	8
87	Bioclipse-R: integrating management and visualization of life science data with statistical analysis. <i>Bioinformatics</i> , 2013, 29, 286-289.	1.8	8
88	Learning cheminformatics. <i>Journal of Cheminformatics</i> , 2020, 12, 4.	2.8	7
89	Interpreting the lipidome: bioinformatic approaches to embrace the complexity. <i>Metabolomics</i> , 2021, 17, 55.	1.4	7
90	Accessing, Using, and Creating Chemical Property Databases for Computational Toxicology Modeling. <i>Methods in Molecular Biology</i> , 2012, 929, 221-241.	0.4	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.	0.8	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.	1.0	6
94	Bacting: a next generation, command line version of Bioclipse. Journal of Open Source Software, 2021, 6, 2558.	2.0	6
95	Explicit interaction information from WikiPathways in RDF facilitates drug discovery in the Open PHACTS Discovery Platform. F1000Research, 2018, 7, 75.	0.8	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.	0.9	5
98	Incorporating Commercial and Private Data into an Open Linked Data Platform for Drug Discovery. Lecture Notes in Computer Science, 2013, , 65-80.	1.0	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.	1.6	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.	2.8	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.	0.3	4
103	Helping to improve the practice of cheminformatics. Journal of Cheminformatics, 2017, 9, 40.	2.8	3
104	Adoption of the Citation Typing Ontology by the Journal of Cheminformatics. Journal of Cheminformatics, 2020, 12, 47.	2.8	3
105	What is the role of cheminformatics in a pandemic?. Journal of Cheminformatics, 2021, 13, 16.	2.8	3
106	Reply to â€œFAIR chemical structure in the Journal of Cheminformaticsâ€• Journal of Cheminformatics, 2021, 13, 49.	2.8	3
107	ELIXIR and Toxicology: a community in development. F1000Research, 0, 10, 1129.	0.8	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.	2.8	1
112	Investigating the Molecular Processes behind the Cell-Specific Toxicity Response to Titanium Dioxide Nanobelts. International Journal of Molecular Sciences, 2021, 22, 9432.	1.8	1
113	Providing gene-to-variant and variant-to-gene database identifier mappings to use with BridgeDb mapping services.. F1000Research, 0, 7, 1390.	0.8	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.	1.1	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