Egon L Willighagen

List of Publications by Citations

111 papers	5,264 citations	35 h-index	71 g-index
153 ext. papers	6,612 ext. citations	6.1 avg, IF	5.3 L-index

#	Paper	IF	Citations
111	The Chemistry Development Kit (CDK): an open-source Java library for Chemo- and Bioinformatics. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 493-500		731
110	WikiPathways: a multifaceted pathway database bridging metabolomics to other omics research. *Nucleic Acids Research*, **2018**, 46, D661-D667	20.1	421
109	Recent developments of the chemistry development kit (CDK) - an open-source java library for chemo- and bioinformatics. *Current Pharmaceutical Design*, **2006**, 12, 2111-20	3.3	373
108	The Blue Obelisk-interoperability in chemical informatics. *Journal of Chemical Information and Modeling*, **2006**, 46, 991-8	6.1	341
107	WikiPathways: capturing the full diversity of pathway knowledge. *Nucleic Acids Research*, **2016**, 44, D488-94	20.1	297
106	Open PHACTS: semantic interoperability for drug discovery. *Drug Discovery Today*, **2012**, 17, 1188-98	8.8	229
105	Adverse outcome pathways: opportunities, limitations and open questions. *Archives of Toxicology*, **2017**, 91, 3477-3505	5.8	174
104	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. *Journal of Cheminformatics*, **2017**, 9, 33	8.6	167
103	WikiPathways: connecting communities. *Nucleic Acids Research*, **2021**, 49, D613-D621	20.1	121
102	Community assessment to advance computational prediction of cancer drug combinations in a pharmacogenomic screen. *Nature Communications*, **2019**, 10, 2674	17.4	119
101	Linked open drug data for pharmaceutical research and development. *Journal of Cheminformatics*, **2011**, 3, 19	8.6	118
100	OSCAR4: a flexible architecture for chemical text-mining. *Journal of Cheminformatics*, **2011**, 3, 41	8.6	106
99	The Chemical Translation Service--a web-based tool to improve standardization of metabolomic reports. *Bioinformatics*, **2010**, 26, 2647-8	7.2	86
98	Bioclipse: an open source workbench for chemo- and bioinformatics. *BMC Bioinformatics*, **2007**, 8, 59	3.6	82
97	The ChEMBL database as linked open data. *Journal of Cheminformatics*, **2013**, 5, 23	8.6	78
96	COVID-19 Disease Map, building a computational repository of SARS-CoV-2 virus-host interaction mechanisms. *Scientific Data*, **2020**, 7, 136	8.2	71
95	FAIR Principles: Interpretations and Implementation Considerations. *Data Intelligence*, **2020**, 2, 10-29	3	66

94	The chemical information ontology: provenance and disambiguation for chemical data on the biological semantic web. *PLoS ONE*, **2011**, 6, e25513	3.7	65
93	The eNanoMapper database for nanomaterial safety information. *Beilstein Journal of Nanotechnology*, **2015**, 6, 1609-34	3	64
92	A transcriptomics data-driven gene space accurately predicts liver cytopathology and drug-induced liver injury. *Nature Communications*, **2017**, 8, 15932	17.4	60
91	Elemental composition determination based on MS(n). *Bioinformatics*, **2011**, 27, 2376-83	7.2	57
90	PubChemRDF: towards the semantic annotation of PubChem compound and substance databases. *Journal of Cheminformatics*, **2015**, 7, 34	8.6	55
89	JChemPaint - Using the Collaborative Forces of the Internet to Develop a Free Editor for 2D Chemical Structures. *Molecules*, **2000**, 5, 93-98	4.8	55
88	eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. *Journal of Biomedical Semantics*, **2015**, 6, 10	2.2	48
87	SPLASH, a hashed identifier for mass spectra. *Nature Biotechnology*, **2016**, 34, 1099-1101	44.5	48
86	CDK-Taverna: an open workflow environment for cheminformatics. *BMC Bioinformatics*, **2010**, 11, 159	3.6	47
85	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. *Journal of Cheminformatics*, **2011**, 3, 37	8.6	46
84	Bioclipse 2: a scriptable integration platform for the life sciences. *BMC Bioinformatics*, **2009**, 10, 397	3.6	46
83	A Data Fusion Pipeline for Generating and Enriching Adverse Outcome Pathway Descriptions. *Toxicological Sciences*, **2018**, 162, 264-275	4.4	43
82	NanoSolveIT Project: Driving nanoinformatics research to develop innovative and integrated tools for nanosafety assessment. *Computational and Structural Biotechnology Journal*, **2020**, 18, 583-602	6.8	41
81	Emerging practices for mapping and linking life sciences data using RDF A case series. *Web Semantics*, **2012**, 14, 2-13	2.9	41
80	Integration among databases and data sets to support productive nanotechnology: Challenges and recommendations. *NanoImpact*, **2018**, 9, 85-101	5.6	39
79	The metaRbolomics Toolbox in Bioconductor and beyond. *Metabolites*, **2019**, 9,	5.6	38
78	Scholia, Scientometrics and Wikidata. *Lecture Notes in Computer Science*, **2017**, 237-259	0.9	36
77	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, 462-9		35

76	The ToxBank Data Warehouse: Supporting the Replacement of In Vivo Repeated Dose Systemic Toxicity Testing. *Molecular Informatics*, **2013**, 32, 47-63	3.8	33
75	XMPP for cloud computing in bioinformatics supporting discovery and invocation of asynchronous web services. *BMC Bioinformatics*, **2009**, 10, 279	3.6	33
74	Towards interoperable and reproducible QSAR analyses: Exchange of datasets. *Journal of Cheminformatics*, **2010**, 2, 5	8.6	33
73	A survey of quantitative descriptions of molecular structure. *Current Topics in Medicinal Chemistry*, **2012**, 12, 1946-56	3	32
72	Cationic Gemini Surfactants Based on Tartaric Acid: Synthesis, Aggregation, Monolayer Behaviour, and Interaction with DNA. *European Journal of Organic Chemistry*, **2002**, 2002, 1397-1406	3.2	31
71	RRegrs: an R package for computer-aided model selection with multiple regression models. *Journal of Cheminformatics*, **2015**, 7, 46	8.6	30
70	Method for the computational comparison of crystal structures. *Acta Crystallographica Section B: Structural Science*, **2005**, 61, 29-36		30
69	Toward the Replacement of Animal Experiments through the Bioinformatics-driven Analysis of SOmicsSData from Human Cell Cultures. *ATLA Alternatives To Laboratory Animals*, **2015**, 43, 325-32	2.1	27
68	Using the Semantic Web for Rapid Integration of WikiPathways with Other Biological Online Data Resources. *PLoS Computational Biology*, **2016**, 12, e1004989	5	25
67	Wikidata as a knowledge graph for the life sciences. *ELife*, **2020**, 9,	8.9	24
66	Chemical Markup, XML, and the World Wide Web. 7. CMLSpect, an XML vocabulary for spectral data. *Journal of Chemical Information and Modeling*, **2007**, 47, 2015-34	6.1	22
65	Linking the Resource Description Framework to cheminformatics and proteochemometrics. *Journal of Biomedical Semantics*, **2011**, 2 Suppl 1, S6	2.2	21
64	New developments on the cheminformatics open workflow environment CDK-Taverna. *Journal of Cheminformatics*, **2011**, 3, 54	8.6	20
63	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	4.5	20
62	On the use of 1H and 13C 1D NMR spectra as QSPR descriptors. *Journal of Chemical Information and Modeling*, **2006**, 46, 487-94	6.1	18
61	The future of metabolomics in ELIXIR. *F1000Research*, **2017**, 6,	3.6	18
60	The LOTUS Initiative for Open Natural Products Research: Knowledge Management through Wikidata		15
59	Risk Governance of Emerging Technologies Demonstrated in Terms of its Applicability to Nanomaterials. *Small*, **2020**, 16, e2003303	11	14

58	Nanopublications: A Growing Resource of Provenance-Centric Scientific Linked Data **2018**,		14
57	Computational toxicology using the OpenTox application programming interface and Bioclipse. *BMC Research Notes*, **2011**, 4, 487	2.3	13
56	Cheminformatics. *Communications of the ACM*, **2012**, 55, 65-75	2.5	13
55	Fast and Scriptable Molecular Graphics in Web Browsers without Java3D. *Nature Precedings*, **2007**,		13
54	CyTargetLinker app update: A flexible solution for network extension in Cytoscape. *F1000Research*, **2018**, 7,	3.6	13
53	MECP2 variation in Rett syndrome-An overview of current coverage of genetic and phenotype data within existing databases. *Human Mutation*, **2018**, 39, 914-924	4.7	12
52	Enabling Open Science: Wikidata for Research (Wiki4R). *Research Ideas and Outcomes*, **2015**, 1, e7573	2.5	12
51	CyTargetLinker app update: A flexible solution for network extension in Cytoscape. *F1000Research*, **2018**, 7, 743	3.6	12
50	Scientific Lenses to Support Multiple Views over Linked Chemistry Data. *Lecture Notes in Computer Science*, **2014**, 98-113	0.9	12
49	Automatically visualise and analyse data on pathways using PathVisioRPC from any programming environment. *BMC Bioinformatics*, **2015**, 16, 267	3.6	11
48	Userscripts for the life sciences. *BMC Bioinformatics*, **2007**, 8, 487	3.6	11
47	Can an InChI for Nano Address the Need for a Simplified Representation of Complex Nanomaterials across Experimental and Nanoinformatics Studies?. *Nanomaterials*, **2020**, 10,	5.4	10
46	The future of metabolomics in ELIXIR. *F1000Research*, **2017**, 6, 1649	3.6	10
45	A Semi-Automated Workflow for FAIR Maturity Indicators in the Life Sciences. *Nanomaterials*, **2020**, 10,	5.4	9
44	Resource description framework technologies in chemistry. *Journal of Cheminformatics*, **2011**, 3, 15	8.6	9
43	Open source drug discovery with bioclipse. *Current Topics in Medicinal Chemistry*, **2012**, 12, 1980-6	3	9
42	Supervised Self-Organizing Maps in Crystal Property and Structure Prediction. *Crystal Growth and Design*, **2007**, 7, 1738-1745	3.5	9
41	COVID19 Disease Map, a computational knowledge repository of virus-host interaction mechanisms. *Molecular Systems Biology*, **2021**, 17, e10387	12.2	9

40	Applications of the InChI in cheminformatics with the CDK and Bioclipse. *Journal of Cheminformatics*, **2013**, 5, 14	8.6	8
39	Bioclipse-R: integrating management and visualization of life science data with statistical analysis. *Bioinformatics*, **2013**, 29, 286-9	7.2	8
38	Molecular Chemometrics. *Critical Reviews in Analytical Chemistry*, **2006**, 36, 189-198	5.2	7
37	Taking FAIR on the ChIN: The Chemistry Implementation Network. *Data Intelligence*, **2020**, 2, 131-138	3	7
36	Accessing, using, and creating chemical property databases for computational toxicology modeling. *Methods in Molecular Biology*, **2012**, 929, 221-41	1.4	7
35	Reliable Granular References to Changing Linked Data. *Lecture Notes in Computer Science*, **2017**, 436-451	0.9	7
34	A protocol for adding knowledge to Wikidata: aligning resources on human coronaviruses. *BMC Biology*, **2021**, 19, 12	7.3	7
33	Beyond Pathway Analysis: Identification of Active Subnetworks in Rett Syndrome. *Frontiers in Genetics*, **2019**, 10, 59	4.5	6
32	The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics.. *ChemInform*, **2003**, 34, no		6
31	Explicit interaction information from WikiPathways in RDF facilitates drug discovery in the Open PHACTS Discovery Platform. *F1000Research*, **2018**, 7, 75	3.6	6
30	XMetDB: an open access database for xenobiotic metabolism. *Journal of Cheminformatics*, **2016**, 8, 47	8.6	5
29	Changing computational research. The challenges ahead. *Source Code for Biology and Medicine*, **2012**, 7, 2	1.9	5
28	Incorporating Commercial and Private Data into an Open Linked Data Platform for Drug Discovery. *Lecture Notes in Computer Science*, **2013**, 65-80	0.9	5
27	A Survey of Quantitative Descriptions of Molecular Structure. *Current Topics in Medicinal Chemistry*, **2013**, 12, 1946-1956	3	4
26	The first eNanoMapper prototype: A substance database to support safe-by-design **2014**,		4
25	Explicit interaction information from WikiPathways in RDF facilitates drug discovery in the Open PHACTS Discovery Platform. *F1000Research*, **2018**, 7, 75	3.6	4
24	Complex Portal 2022: new curation frontiers. *Nucleic Acids Research*, **2021**,	20.1	4
23	A catalogue of 863 Rett-syndrome-causing MECP2 mutations and lessons learned from data integration. *Scientific Data*, **2021**, 8, 10	8.2	4

22	A protocol for adding knowledge to Wikidata, a case report		3
21	Robustifying Scholia: paving the way for knowledge discovery and research assessment through Wikidata. *Research Ideas and Outcomes*,5,	2.5	3
20	Accessing biological data in R with semantic web technologies		3
19	Automatic OpenAPI to Bio.tools Conversion		3
18	RDFIO: extending Semantic MediaWiki for interoperable biomedical data management. *Journal of Biomedical Semantics*, **2017**, 8, 35	2.2	2
17	Using the RRegrs R package for automating predictive modelling		2
16	Two real use cases of FAIR maturity indicators in the life sciences		2
15	Reply to "FAIR chemical structure in the Journal of Cheminformatics". *Journal of Cheminformatics*, **2021**, 13, 49	8.6	2
14	Collaborative Cheminformatics Applications399-422		2
13	Research Techniques Made Simple: Lipidomic Analysis in Skin Research.. *Journal of Investigative Dermatology*, **2022**, 142, 4-11.e1	4.3	1
12	Wikidata as a FAIR knowledge graph for the life sciences		1
11	Bacting: a next generation, command line version of Bioclipse. *Journal of Open Source Software*, **2021**, 6, 2558	5.2	1
10	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	1.3	1
9	ELIXIR and Toxicology: a community in development. *F1000Research*, **2021**, 10, 1129	3.6	0
8	Providing gene-to-variant and variant-to-gene database identifier mappings to use with BridgeDb mapping services.. *F1000Research*,7, 1390	3.6	0
7	A resource to explore the discovery of rare diseases and their causative genes. *Scientific Data*, **2021**, 8, 124	8.2	0
6	Interpreting the lipidome: bioinformatic approaches to embrace the complexity. *Metabolomics*, **2021**, 17, 55	4.7	0
5	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	0

4	PSnpBind: a database of mutated binding site protein-ligand complexes constructed using a multithreaded virtual screening workflow.. *Journal of Cheminformatics*, **2022**, 14, 8	8.6	0
3	Interactive predictive toxicology with Bioclipse and OpenTox **2012**, 35-61		
2	WikiPathways: Integrating Pathway Knowledge with Clinical Data **2022**, 1457-1466		
1	Understanding signaling and metabolic paths using semantified and harmonized information about biological interactions.. *PLoS ONE*, **2022**, 17, e0263057	3.7	