Assâ€Prof Denis Fourches

List of Publications by Year
in descending order

82 papers	8,176 citations	100601 38 h-index	66518 82 g-index
101 all docs	101 docs citations	101 times ranked	9768 citing authors

#	Article	IF	Citations
1	Cheminformatics Analysis of Fluoroquinolones and their Inhibition Potency Against Four Pathogens. Molecular Informatics, 2021, 40, 2000215.	1.4	0
2	SMILES Pair Encoding: A Data-Driven Substructure Tokenization Algorithm for Deep Learning. Journal of Chemical Information and Modeling, 2021, 61, 1560-1569.	2.5	41
3	The VKORC1 ER-luminal loop mutation (Leu76Pro) leads to a significant resistance to warfarin in black rats (Rattus rattus). Pesticide Biochemistry and Physiology, 2021, 173, 104774.	1.6	5
4	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	2.8	63
5	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	18.7	128
6	In vitro and in vivo Evaluation of in silico Predicted Pneumococcal UDPG:PP Inhibitors. Frontiers in Microbiology, 2020, 11, 1596.	1.5	5
7	Structural-based connectivity and omic phenotype evaluations (SCOPE): a cheminformatics toolbox for investigating lipidomic changes in complex systems. Analyst, The, 2020, 145, 7197-7209.	1.7	16
8	Unveiling molecular signatures of preeclampsia and gestational diabetes mellitus with multi-omics and innovative cheminformatics visualization tools. Molecular Omics, 2020, 16, 521-532.	1.4	16
9	Structure-based virtual screening of perfluoroalkyl and polyfluoroalkyl substances (PFASs) as endocrine disruptors of androgen receptor activity using molecular docking and machine learning. Environmental Research, 2020, 190, 109920.	3.7	21
10	SIME: synthetic insight-based macrolide enumerator to generate the V1B library of 1 billion macrolides. Journal of Cheminformatics, 2020, 12, 23.	2.8	6
11	Inductive transfer learning for molecular activity prediction: Next-Gen QSAR Models with MolPMoFiT. Journal of Cheminformatics, 2020, 12, 27.	2.8	74
12	Benchmarking 2D/3D/MD-QSAR Models for Imatinib Derivatives: How Far Can We Predict?. Journal of Chemical Information and Modeling, 2020, 60, 3342-3360.	2.5	12
13	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	2.8	120
14	Hierarchical Quantitative Structureâ€“Activity Relationship Modeling Approach for Integrating Binary, Multiclass, and Regression Models of Acute Oral Systemic Toxicity. Chemical Research in Toxicology, 2020, 33, 353-366.	1.7	20
15	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427
16	Novel peptide ligands for antibody purification provide superior clearance of host cell protein impurities. Journal of Chromatography A, 2020, 1625, 461237.	1.8	21
17	Integrative statistical methods for exposure mixtures and health. Annals of Applied Statistics, 2020, 14, 1945-1963.	0.5	5
18	Cheminformatics approach to exploring and modeling trait-associated metabolite profiles. Journal of Cheminformatics, 2019, 11, 43.	2.8	10

#	Article	IF	Citations
19	4D- quantitative structureâ€“activity relationship modeling: making a comeback. Expert Opinion on Drug Discovery, 2019, 14, 1227-1235.	2.5	23
20	Student-Guided Three-Dimensional Printing Activity in Large Lecture Courses: A Practical Guideline. Journal of Chemical Education, 2019, 96, 291-295.	1.1	25
21	Binding of peanut allergen Ara h 2 with Vaccinium fruit polyphenols. Food Chemistry, 2019, 284, 287-295.	4.2	23
22	Cheminformatics Analysis of Dynamic WNKâ€Inhibitor Interactions. Molecular Informatics, 2018, 37, e1700138.	1.4	7
23	Toward the Rational Design of Sustainable Hair Dyes Using Cheminformatics Approaches: Step 1. Database Development and Analysis. ACS Sustainable Chemistry and Engineering, 2018, 6, 2344-2352.	3.2	15
24	In silico Predicted Glucoseâ€1â€phosphate Uridylyltransferase (GalU) Inhibitors Block a Key Pathway Required for Listeria Virulence. Molecular Informatics, 2018, 37, e1800004.	1.4	15
25	Cheminformatics-based enumeration and analysis of large libraries of macrolide scaffolds. Journal of Cheminformatics, 2018, 10, 53.	2.8	8
26	Toward the Rational Design of Sustainable Hair Dyes Using Cheminformatics Approaches: Step 2. Identification of Hair Dye Substance Database Analogs in the Max Weaver Dye Library. ACS Sustainable Chemistry and Engineering, 2018, 6, 14248-14256.	3.2	7
27	Chemistry-Wide Association Studies (CWAS): A Novel Framework for Identifying and Interpreting Structureâ€“Activity Relationships. Journal of Chemical Information and Modeling, 2018, 58, 2203-2213.	2.5	7
28	Exploring drug space with ChemMaps.com. Bioinformatics, 2018, 34, 3773-3775.	1.8	15
29	Adverse drug reactions triggered by the common HLA-B*57:01 variant: virtual screening of DrugBank using 3D molecular docking. Journal of Cheminformatics, 2018, 10, 3.	2.8	4
30	Predicting Adverse Drug Effects from Literature- and Database-Mined Assertions. Drug Safety, 2018, 41, 1059-1072.	1.4	3
31	Confirmation of high-throughput screening data and novel mechanistic insights into VDR-xenobiotic interactions by orthogonal assays. Scientific Reports, 2018, 8, 8883.	1.6	8
32	Adverse drug reactions triggered by the common HLA-B*57:01 variant: a molecular docking study. Journal of Cheminformatics, 2017, 9, 13.	2.8	44
33	Cheminformatics Modeling of Amine Solutions for Assessing their CO₂Absorption Properties. Molecular Informatics, 2017, 36, 1600143.	1.4	12
34	Characterizing the Chemical Space of ERK2 Kinase Inhibitors Using Descriptors Computed from Molecular Dynamics Trajectories. Journal of Chemical Information and Modeling, 2017, 57, 1286-1299.	2.5	75
35	Weaver's historic accessible collection of synthetic dyes: a cheminformatics analysis. Chemical Science, 2017, 8, 4334-4339.	3.7	32
36	Quantitative Nanostructureâ€“Activity Relationships: Methods, Case Studies, and Perspectives. Nanomedicine and Nanotoxicology, 2017, , 361-376.	0.1	2

#	Article	IF	Citations
37	Reaction: Molecular Modeling for Novel Antibacterials. CheM, 2017, 3, 13-14.	5.8	3
38	RealityConvert: a tool for preparing 3D models of biochemical structures for augmented and virtual reality. Bioinformatics, 2017, 33, 3816-3818.	1.8	27
39	Computer-Assisted Decision Support for Student Admissions Based on Their Predicted Academic Performance. American Journal of Pharmaceutical Education, 2017, 81, 46.	0.7	16
40	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	2.8	264
41	QSAR models of human data can enrich or replace LLNA testing for human skin sensitization. Green Chemistry, 2016, 18, 6501-6515.	4.6	42
42	Activity prediction and identification of misâ€annotated chemical compounds using extreme descriptors. Journal of Chemometrics, 2016, 30, 99-108.	0.7	2
43	Trust, but Verify II: A Practical Guide to Chemogenomics Data Curation. Journal of Chemical Information and Modeling, 2016, 56, 1243-1252.	2.5	228
44	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	2.8	1
45	Alarms about structural alerts. Green Chemistry, 2016, 18, 4348-4360.	4.6	103
46	QSAR Modeling and Prediction of Drugâ€“Drug Interactions. Molecular Pharmaceutics, 2016, 13, 545-556.	2.3	65
47	Computer-aided design of carbon nanotubes with the desired bioactivity and safety profiles. Nanotoxicology, 2016, 10, 374-383.	1.6	29
48	Cheminformatics-aided pharmacovigilance: application to Stevens-Johnson Syndrome. Journal of the American Medical Informatics Association: JAMIA, 2016, 23, 968-978.	2.2	13
49	Comprehensive characterization of the Published Kinase Inhibitor Set. Nature Biotechnology, 2016, 34, 95-103.	9.4	289
50	Predâ€hERG: A Novel webâ€Accessible Computational Tool for Predicting Cardiac Toxicity. Molecular Informatics, 2015, 34, 698-701.	1.4	159
51	Drug Side Effect Profiles as Molecular Descriptors for Predictive Modeling of Target Bioactivity. Molecular Informatics, 2015, 34, 160-170.	1.4	6
52	Predicting chemically-induced skin reactions. Part II: QSAR models of skin permeability and the relationships between skin permeability and skin sensitization. Toxicology and Applied Pharmacology, 2015, 284, 273-280.	1.3	53
53	Predicting chemically-induced skin reactions. Part I: QSAR models of skin sensitization and their application to identify potentially hazardous compounds. Toxicology and Applied Pharmacology, 2015, 284, 262-272.	1.3	72
54	Curation of chemogenomics data. Nature Chemical Biology, 2015, 11, 535-535.	3.9	158

#	Article	IF	Citations
55	Target-Specific Native/Decoy Pose Classifier Improves the Accuracy of Ligand Ranking in the CSAR 2013 Benchmark. Journal of Chemical Information and Modeling, 2015, 55, 63-71.	2.5	14
56	Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. Chemistry of Materials, 2015, 27, 735-743.	3.2	209
57	Clozapine-induced agranulocytosis is associated with rare HLA-DQB1 and HLA-B alleles. Nature Communications, 2014, 5, 4757.	5.8	153
58	Modelability Criteria: Statistical Characteristics Estimating Feasibility to Build Predictive QSAR Models for a Dataset. , 2014, , 187-230.		11
59	Short Communication: Cheminformatics Analysis to Identify Predictors of Antiviral Drug Penetration into the Female Genital Tract. AIDS Research and Human Retroviruses, 2014, 30, 1058-1064.	0.5	14
60	HTS navigator: freely accessible cheminformatics software for analyzing high-throughput screening data. Bioinformatics, 2014, 30, 588-589.	1.8	16
61	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	2.9	1,401
62	Data Set Modelability by QSAR. Journal of Chemical Information and Modeling, 2014, 54, 1-4.	2.5	105
63	Expanding the scope of drug repurposing in pediatrics: The Children's Pharmacy Collaborativeâ„¢. Drug Discovery Today, 2014, 19, 1696-1698.	3.2	22
64	Chemical Basis of Interactions Between Engineered Nanoparticles and Biological Systems. Chemical Reviews, 2014, 114, 7740-7781.	23.0	478
65	Cheminformatics: At the Crossroad of Eras. Challenges and Advances in Computational Chemistry and Physics, 2014, , 539-546.	0.6	4
66	Tuning hERG Out: Antitarget QSAR Models for Drug Development. Current Topics in Medicinal Chemistry, 2014, 14, 1399-1415.	1.0	82
67	Predicting Binding Affinity of CSAR Ligands Using Both Structure-Based and Ligand-Based Approaches. Journal of Chemical Information and Modeling, 2013, 53, 1915-1922.	2.5	20
68	Human Intestinal Transporter Database: QSAR Modeling and Virtual Profiling of Drug Uptake, Efflux and Interactions. Pharmaceutical Research, 2013, 30, 996-1007.	1.7	76
69	Integrative Chemicalâ€"Biological Read-Across Approach for Chemical Hazard Classification. Chemical Research in Toxicology, 2013, 26, 1199-1208.	1.7	107
70	Discovery of Novel Antimalarial Compounds Enabled by QSAR-Based Virtual Screening. Journal of Chemical Information and Modeling, 2013, 53, 475-492.	2.5	77
71	Using Graph Indices for the Analysis and Comparison of Chemical Datasets. Molecular Informatics, 2013, 32, 827-842.	1.4	21
72	Predicting Drug-Induced Hepatotoxicity Using QSAR and Toxicogenomics Approaches. Chemical Research in Toxicology, 2011, 24, 1251-1262.	1.7	190

#	Article	IF	Citations
73	Exploring Quantitative Nanostructure-Activity Relationships (QNAR) Modeling as a Tool for Predicting Biological Effects of Manufactured Nanoparticles. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 217-225.	0.6	79
74	Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set. Journal of Chemical Information and Modeling, 2010, 50, 2094-2111.	2.5	202
75	Trust, But Verify: On the Importance of Chemical Structure Curation in Cheminformatics and QSAR Modeling Research. Journal of Chemical Information and Modeling, 2010, 50, 1189-1204.	2.5	611
76	Quantitative Nanostructureâ^'Activity Relationship Modeling. ACS Nano, 2010, 4, 5703-5712.	7.3	342
77	Modeling Liver-Related Adverse Effects of Drugs Using kNearest Neighbor Quantitative Structureâ^'Activity Relationship Method. Chemical Research in Toxicology, 2010, 23, 724-732.	1.7	104
78	Cheminformatics Analysis of Assertions Mined from Literature That Describe Drug-Induced Liver Injury in Different Species. Chemical Research in Toxicology, 2010, 23, 171-183.	1.7	117
79	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	2.5	258
80	Critical Assessment of QSAR Models of Environmental Toxicity against Tetrahymena pyriformis: Focusing on Applicability Domain and Overfitting by Variable Selection. Journal of Chemical Information and Modeling, 2008, 48, 1733-1746.	2.5	350
81	ISIDA - Platform for Virtual Screening Based on Fragment and Pharmacophoric Descriptors. Current Computer-Aided Drug Design, 2008, 4, 191-198.	0.8	173
82	Benchmarking of Linear and Nonlinear Approaches for Quantitative Structureâ^'Property Relationship Studies of Metal Complexation with Ionophores. Journal of Chemical Information and Modeling, 2006, 46, 808-819.	2.5	68