Georgia Melagraki

List of Publications by Year
in descending order

96 papers	3,003 citations	126858 33 h-index	175177 52 g-index
97 all docs	97 docs citations	97 times ranked	3238 citing authors

#	Article	IF	Citations
1	Reducing health & environmental impacts of chemical warfare agents: Computational chemistry contributions. Chemosphere, 2022, 288, 132564.	4.2	0
2	Daphnia magna and mixture toxicity with nanomaterials â€“ Current status and perspectives in data-driven risk prediction. Nano Today, 2022, 43, 101430.	6.2	20
3	Using the Isalos platform to develop a (Q)SAR model that predicts metal oxide toxicity utilizing facet-based electronic, image analysis-based, and periodic table derived properties as descriptors. Structural Chemistry, 2022, 33, 527-538.	1.0	4
4	Prospects and challenges for FAIR toxicogenomics data. Nature Nanotechnology, 2022, 17, 17-18.	15.6	11
5	Editorial for the Special Issue From Nanoinformatics to Nanomaterials Risk Assessment and Governance. Nanomaterials, 2021, 11, 121.	1.9	4
6	NanoSolveIT integration of tools for assessment of human and environmental exposure to nanomaterials. , 2021, , 81-120.		1
7	Manually curated transcriptomics data collection for toxicogenomic assessment of engineered nanomaterials. Scientific Data, 2021, 8, 49.	2.4	19
8	Advances in De Novo Drug Design: From Conventional to Machine Learning Methods. International Journal of Molecular Sciences, 2021, 22, 1676.	1.8	131
9	Computational enrichment of physicochemical data for the development of a Î¶-potential read-across predictive model with Isalos Analytics Platform. NanoImpact, 2021, 22, 100308.	2.4	15
10	Nanotechnology and artificial intelligence to enable sustainable and precision agriculture. Nature Plants, 2021, 7, 864-876.	4.7	150
11	In Silico Identification and Evaluation of Natural Products as Potential Tumor Necrosis Factor Function Inhibitors Using Advanced Enalos Asclepios KNIME Nodes. International Journal of Molecular Sciences, 2021, 22, 10220.	1.8	10
12	Ecotoxicological read-across models for predicting acute toxicity of freshly dispersed versus medium-aged NMs to Daphnia magna. Chemosphere, 2021, 285, 131452.	4.2	16
13	Accelerating the Identification of Chemistryâ€“Driven Bioactive Compounds within a Multi-Objective Optimization Framework. Combinatorial Chemistry and High Throughput Screening, 2021, 25, .	0.6	0
14	Cheminformatics and virtual screening studies of COMT inhibitors as potential Parkinsonâ€™s disease therapeutics. Expert Opinion on Drug Discovery, 2020, 15, 53-62.	2.5	8
15	Risk Governance of Emerging Technologies Demonstrated in Terms of its Applicability to Nanomaterials. Small, 2020, 16, e2003303.	5.2	28
16	Predicting Cytotoxicity of Metal Oxide Nanoparticles Using Isalos Analytics Platform. Nanomaterials, 2020, 10, 2017.	1.9	34
17	Metadata Stewardship in Nanosafety Research: Community-Driven Organisation of Metadata Schemas to Support FAIR Nanoscience Data. Nanomaterials, 2020, 10, 2033.	1.9	41
18	Synthetic Analogues of Aminoadamantane as Influenza Viral Inhibitorsâ€”In Vitro, In Silico and QSAR Studies. Molecules, 2020, 25, 3989.	1.7	10

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19	Can an InChI for Nano Address the Need for a Simplified Representation of Complex Nanomaterials across Experimental and Nanoinformatics Studies?. Nanomaterials, 2020, 10, 2493.	1.9	28
20	Transcriptomics in Toxicogenomics, Part II: Preprocessing and Differential Expression Analysis for High Quality Data. Nanomaterials, 2020, 10, 903.	1.9	31
21	Development of Deep Learning Models for Predicting the Effects of Exposure to Engineered Nanomaterials on Daphnia magna. Small, 2020, 16, e2001080.	5.2	28
22	Zetaâ€Potential Readâ€Across Model Utilizing Nanodescriptors Extracted via the NanoXtract Image Analysis Tool Available on the Enalos Nanoinformatics Cloud Platform. Small, 2020, 16, e1906588.	5.2	35
23	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
24	Computer-Aided Drug Design of Î²-Secretase, Î³-Secretase and Anti-Tau Inhibitors for the Discovery of Novel Alzheimerâ€™s Therapeutics. International Journal of Molecular Sciences, 2020, 21, 703.	1.8	45
25	Transcriptomics in Toxicogenomics, Part III: Data Modelling for Risk Assessment. Nanomaterials, 2020, 10, 708.	1.9	38
26	Transcriptomics in Toxicogenomics, Part I: Experimental Design, Technologies, Publicly Available Data, and Regulatory Aspects. Nanomaterials, 2020, 10, 750.	1.9	42
27	Enalos Cloud Platform: Nanoinformatics and Cheminformatics Tools. Methods in Pharmacology and Toxicology, 2020, , 789-800.	0.1	4
28	Enalos Suite of Tools: Enhancing Cheminformatics and Nanoinfor - matics through KNIME. Current Medicinal Chemistry, 2020, 27, 6523-6535.	1.2	18
29	MS-275 Chemical Analogues Promote Hemoglobin Production and Erythroid Differentiation of K562 Cells. Hemoglobin, 2019, 43, 116-121.	0.4	2
30	Read-across predictions of nanoparticle hazard endpoints: a mathematical optimization approach. Nanoscale Advances, 2019, 1, 3485-3498.	2.2	9
31	A safe-by-design tool for functionalised nanomaterials through the Enalos Nanoinformatics Cloud platform. Nanoscale Advances, 2019, 1, 706-718.	2.2	33
32	A reaction limited in vivo dissolution model for the study of drug absorption: Towards a new paradigm for the biopharmaceutic classification of drugs. European Journal of Pharmaceutical Sciences, 2018, 117, 98-106.	1.9	13
33	Computational toxicology: From cheminformatics to nanoinformatics. Food and Chemical Toxicology, 2018, 112, 476-477.	1.8	3
34	Aqueous Solubility Enhancement for Bioassays of Insoluble Inhibitors and QSPR Analysis: A TNF-Î± Study. SLAS Discovery, 2018, 23, 84-93.	1.4	3
35	Consensus Predictive Model for Human K562 Cell Growth Inhibition through Enalos Cloud Platform. ChemMedChem, 2018, 13, 555-563.	1.6	2
36	A nanoinformatics decision support tool for the virtual screening of gold nanoparticle cellular association using protein corona fingerprints. Nanotoxicology, 2018, 12, 1148-1165.	1.6	40

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37	Enalos Suite: New Cheminformatics Platform for Drug Discovery and Computational Toxicology. Methods in Molecular Biology, 2018, 1800, 287-311.	0.4	3
38	Enalos+ KNIME Nodes: New Cheminformatics Tools for Drug Discovery. Methods in Molecular Biology, 2018, 1824, 113-138.	0.4	11
39	In Silico Discovery of Plant-Origin Natural Product Inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-Î¹B Ligand (RANKL). Frontiers in Pharmacology, 2018, 9, 800.	1.6	17
40	Current Status and Future Prospects of Smallâ€“molecule Proteinâ€“protein Interaction (PPI) Inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-Î¹B Ligand (RANKL). Current Topics in Medicinal Chemistry, 2018, 18, 661-673.	1.0	13
41	Open Source Chemoinformatics Software including KNIME Analytics. , 2017, , 2201-2230.		3
42	MouseTox: An online toxicity assessment tool for small molecules through Enalos Cloud platform. Food and Chemical Toxicology, 2017, 110, 83-93.	1.8	20
43	05.17â€…An integrated chemoinformatics-aided pipeline for the discovery of smallâ€“molecule dual inhibitors of tnf and rankl. , 2017, , .		0
44	Strategy for Identification of Nanomaterialsâ€™ Critical Properties Linked to Biological Impacts: Interlinking of Experimental and Computational Approaches. Challenges and Advances in Computational Chemistry and Physics, 2017, , 385-424.	0.6	5
45	Cheminformatics-aided discovery of small-molecule Protein-Protein Interaction (PPI) dual inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-Î¹B Ligand (RANKL). PLoS Computational Biology, 2017, 13, e1005372.	1.5	49
46	Searching for Novel Janus Kinase-2 Inhibitors Using a Combination of Pharmacophore Modeling, 3D-QSAR Studies and Virtual Screening. Mini-Reviews in Medicinal Chemistry, 2017, 17, 268-294.	1.1	9
47	Development of a Predictive Pharmacophore Model and a 3D-QSAR Study for an in silico Screening of New Potent Bcr-Abl Kinase Inhibitors. Mini-Reviews in Medicinal Chemistry, 2017, 17, 188-204.	1.1	10
48	Quantitative Nanostructure-Activity Relationship Models for the Risk Assessment of NanoMaterials. , 2017, , 1314-1338.		1
49	Quantitative Nanostructure-Activity Relationship Models for the Risk Assessment of NanoMaterials. , 2017, , 20-44.		0
50	Editorial: Towards Open Access for Cheminformatics. Combinatorial Chemistry and High Throughput Screening, 2016, 19, 260-261.	0.6	5
51	Searching for anthranilic acid-based thumb pocket 2 HCV NS5B polymerase inhibitors through a combination of molecular docking, 3D-QSAR and virtual screening. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 38-52.	2.5	30
52	Computer Aided Drug Design Approaches for Identification of Novel Autotaxin (ATX) Inhibitors. Current Medicinal Chemistry, 2016, 23, 1708-1724.	1.2	3
53	Open Source Chemoinformatics Software including KNIME Analytics Platform. , 2016, , 1-30.		0
54	Open-Source Chemoinformatics Software. , 2016, , 1-30.		0

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55	Editorial (Thematic Issue: Advances in Cheminformatics: Drug Discovery, Computational Toxicology) Tj ETQq1 1 0.784314 rgBT /Over	0.6	0
56	Editorial (Thematic Issue: Advances in Cheminformatics: Drug Discovery, Computational Toxicology) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.6	2
57	Exploiting ChEMBL database to identify indole analogs as HCV replication inhibitors. Methods, 2015, 71, 4-13.	1.9	20
58	Stability and binding effects of silver(I) complexes at lipoxygenase-1. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 30, 539-549.	2.5	3
59	Rational Drug Design Paradigms: The Odyssey for Designing Better Drugs. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 238-256.	0.6	8
60	A Risk Assessment Tool for the Virtual Screening of Metal Oxide Nanoparticles through Enalos InSilicoNano Platform. Current Topics in Medicinal Chemistry, 2015, 15, 1827-1836.	1.0	39
61	Quantitative Nanostructure-Activity Relationship Models for the Risk Assessment of NanoMaterials. Advances in Chemical and Materials Engineering Book Series, 2015, , 535-559.	0.2	0
62	Antiproliferative novel isoxazoles: Modeling, virtual screening, synthesis, and bioactivity evaluation. European Journal of Medicinal Chemistry, 2014, 81, 139-149.	2.6	32
63	Enalos InSilicoNano platform: an online decision support tool for the design and virtual screening of nanoparticles. RSC Advances, 2014, 4, 50713-50725.	1.7	68
64	Enalos KNIME nodes: Exploring corrosion inhibition of steel in acidic medium. Chemometrics and Intelligent Laboratory Systems, 2013, 123, 9-14.	1.8	70
65	Identification of putative estrogen receptor-mediated endocrine disrupting chemicals using QSAR- and structure-based virtual screening approaches. Toxicology and Applied Pharmacology, 2013, 272, 67-76.	1.3	78
66	Rational design, efficient syntheses and biological evaluation of N , N â€²-symmetrically bis-substituted butylimidazole analogs as a new class of potent Angiotensin II receptor blockers. European Journal of Medicinal Chemistry, 2013, 62, 352-370.	2.6	28
67	Molecular Modeling on Pyrimidine-Urea Inhibitors of TNF-Î± Production: An Integrated Approach Using a Combination of Molecular Docking, Classification Techniques, and 3D-QSAR CoMSIA. Journal of Chemical Information and Modeling, 2012, 52, 711-723.	2.5	57
68	Comparative Binding Effects of Aspirin and Anti-Inflammatory Cu Complex in the Active Site of LOX-1. Journal of Chemical Information and Modeling, 2012, 52, 3293-3301.	2.5	10
69	Comparative study of the AT1 receptor prodrug antagonist candesartan cilexetil with other sartans on the interactions with membrane bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 3107-3120.	1.4	19
70	Functionalized 4-Hydroxy Coumarins: Novel Synthesis, Crystal Structure and DFT Calculations. Molecules, 2011, 16, 384-402.	1.7	22
71	Ligand - based virtual screening procedure for the prediction and the identification of novel Î²-amyloid aggregation inhibitors using Kohonen maps and Counterpropagation Artificial Neural Networks. European Journal of Medicinal Chemistry, 2011, 46, 497-508.	2.6	93
72	Ligand and Structure Based Virtual Screening Strategies for Hit-Finding and Optimization of Hepatitis C Virus (HCV) Inhibitors. Current Medicinal Chemistry, 2011, 18, 2612-2619.	1.2	29

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73	A combined LS-SVM & MLR QSAR workflow for predicting the inhibition of CXCR3 receptor by quinazolinone analogs. Molecular Diversity, 2010, 14, 225-235.	2.1	48
74	Collaborative development of predictive toxicology applications. Journal of Cheminformatics, 2010, 2, 7.	2.8	91
75	In Silico Exploration for Identifying Structureâ€“Activity Relationship of MEK Inhibition and Oral Bioavailability for Isothiazole Derivatives. Chemical Biology and Drug Design, 2010, 76, 397-406.	1.5	56
76	A novel QSAR model for predicting the inhibition of CXCR3ÂreceptorÂbyÂ4-N-aryl-[1,4] diazepane ureas. European Journal of Medicinal Chemistry, 2009, 44, 877-884.	2.6	51
77	Synthesis and evaluation of the antioxidant and anti-inflammatory activity of novel coumarin-3-aminoamides and their alpha-lipoic acid adducts. European Journal of Medicinal Chemistry, 2009, 44, 3020-3026.	2.6	244
78	Predictive QSAR workflow for the in silico identification and screening of novel HDAC inhibitors. Molecular Diversity, 2009, 13, 301-311.	2.1	59
79	Development and Evaluation of a QSPR Model for the Prediction of Diamagnetic Susceptibility. QSAR and Combinatorial Science, 2008, 27, 432-436.	1.5	44
80	Design and Synthesis of Novel Quinolinone-3-aminoamides and Their Î±-Lipoic Acid Adducts as Antioxidant and Anti-inflammatory Agents. Journal of Medicinal Chemistry, 2007, 50, 2450-2458.	2.9	94
81	Identification of a series of novel derivatives as potent HCV inhibitors by a ligand-based virtual screening optimized procedure. Bioorganic and Medicinal Chemistry, 2007, 15, 7237-7247.	1.4	37
82	Optimization of biaryl piperidine and 4-amino-2-biarylurea MCH1 receptor antagonists using QSAR modeling, classification techniques and virtual screening. Journal of Computer-Aided Molecular Design, 2007, 21, 251-267.	1.3	31
83	A Novel QSAR Model for Evaluating and Predicting the Inhibition Activity of Dipeptidyl Aspartyl Fluoromethylketones. QSAR and Combinatorial Science, 2006, 25, 928-935.	1.5	27
84	A novel QSAR model for predicting induction of apoptosis by 4-aryl-4H-chromenes. Bioorganic and Medicinal Chemistry, 2006, 14, 6686-6694.	1.4	88
85	QSAR study on para-substituted aromatic sulfonamides as carbonic anhydrase II inhibitors using topological information indices. Bioorganic and Medicinal Chemistry, 2006, 14, 1108-1114.	1.4	63
86	Prediction of intrinsic viscosity in polymerâ€“solvent combinations using a QSPR model. Polymer, 2006, 47, 3240-3248.	1.8	68
87	Investigation of substituent effect of 1-(3,3-diphenylpropyl)-piperidinyl phenylacetamides on CCR5 binding affinity using QSAR and virtual screening techniques. Journal of Computer-Aided Molecular Design, 2006, 20, 83-95.	1.3	36
88	A Novel RBF Neural Network Training Methodology to Predict Toxicity to Vibrio Fischeri. Molecular Diversity, 2006, 10, 213-221.	2.1	32
89	A novel simple QSAR model for the prediction of anti-HIV activity using multiple linear regression analysis. Molecular Diversity, 2006, 10, 405-414.	2.1	55
90	Prediction of toxicity using a novel RBF neural network training methodology. Journal of Molecular Modeling, 2006, 12, 297-305.	0.8	39

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91	A novel QSPR model for predicting Î¸ (lower critical solution temperature) in polymer solutions using molecular descriptors. Journal of Molecular Modeling, 2006, 13, 55-64.	0.8	28
92	A simple synthesis of functionalized 2-amino-3-cyano-4-chromones by application of the N-hydroxybenzotriazole methodology. Arkivoc, 2006, 2006, 28-34.	0.3	20
93	Prediction of high weight polymers glass transition temperature using RBF neural networks. Computational and Theoretical Chemistry, 2005, 716, 193-198.	1.5	80
94	Novel Short-Step Synthesis of Functionalized Î³-Phenyl-Î²-hydroxybutenoates and Their Cyclization to 4-Hydroxycoumarins via the N-Hydroxybenzotriazole Methodology.. ChemInform, 2005, 36, no.	0.1	0
95	Novel Short-Step Synthesis of Functionalized Î³-Phenyl-Î²-hydroxybutenoates and their Cyclization to 4-Hydroxycoumarins via the N-Hydroxybenzotriazole Methodology. Synthesis, 2004, 2004, 1775-1782.	1.2	3
96	Towards an in silico integrated approach for testing and assessment of nanomaterials: from predicted indoor air concentrations to lung dose and biodistribution. Environmental Science: Nano, 0, , .	2.2	2