Antreas Afantitis

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2863288/publications.pdf

Version: 2024-02-01

		126858	175177
106	3,130	33	52
papers	citations	h-index	g-index

107	107	107	3330
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	Nanotechnology and artificial intelligence to enable sustainable and precision agriculture. Nature Plants, 2021, 7, 864-876.	4.7	150
3	Advances in De Novo Drug Design: From Conventional to Machine Learning Methods. International Journal of Molecular Sciences, 2021, 22, 1676.	1.8	131
4	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
5	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
6	Collaborative development of predictive toxicology applications. Journal of Cheminformatics, 2010, 2, 7.	2.8	91
7	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
8	Prediction of high weight polymers glass transition temperature using RBF neural networks. Computational and Theoretical Chemistry, 2005, 716, 193-198.	1.5	80
9	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
10	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
11	Enalos KNIME nodes: Exploring corrosion inhibition of steel in acidic medium. Chemometrics and Intelligent Laboratory Systems, 2013, 123, 9-14.	1.8	70
12	Prediction of intrinsic viscosity in polymerâ€“solvent combinations using a QSPR model. Polymer, 2006, 47, 3240-3248.	1.8	68
13	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
14	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
15	Predictive QSAR workflow for the in silico identification and screening of novel HDAC inhibitors. Molecular Diversity, 2009, 13, 301-311.	2.1	59
16	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
17	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
18	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

#	Article	IF	Citations
19	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
20	Cheminformatics-aided discovery of small-molecule Protein-Protein Interaction (PPI) dual inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-Î²B Ligand (RANKL). PLoS Computational Biology, 2017, 13, e1005372.	1.5	49
21	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
22	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
23	Development and Evaluation of a QSPR Model for the Prediction of Diamagnetic Susceptibility. QSAR and Combinatorial Science, 2008, 27, 432-436.	1.5	44
24	Transcriptomics in Toxicogenomics, Part I: Experimental Design, Technologies, Publicly Available Data, and Regulatory Aspects. Nanomaterials, 2020, 10, 750.	1.9	42
25	Metadata Stewardship in Nanosafety Research: Community-Driven Organisation of Metadata Schemas to Support FAIR Nanoscience Data. Nanomaterials, 2020, 10, 2033.	1.9	41
26	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
27	Prediction of toxicity using a novel RBF neural network training methodology. Journal of Molecular Modeling, 2006, 12, 297-305.	0.8	39
28	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
29	Transcriptomics in Toxicogenomics, Part III: Data Modelling for Risk Assessment. Nanomaterials, 2020, 10, 708.	1.9	38
30	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
31	Development and therapeutic potential of autotaxin small molecule inhibitors: From bench to advanced clinical trials. Medicinal Research Reviews, 2019, 39, 976-1013.	5.0	37
32	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
33	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
34	Predicting Cytotoxicity of Metal Oxide Nanoparticles Using Isalos Analytics Platform. Nanomaterials, 2020, 10, 2017.	1.9	34
35	Surface Functionalization of Grapheneâ€Based Materials: Biological Behavior, Toxicology, and Safeâ€Byâ€Design Aspects. Advanced Biology, 2021, 5, e2100637.	1.4	34
36	A safe-by-design tool for functionalised nanomaterials through the Enalos Nanoinformatics Cloud platform. Nanoscale Advances, 2019, 1, 706-718.	2.2	33

#	Article	IF	Citations
37	A Novel RBF Neural Network Training Methodology to Predict Toxicity to Vibrio Fischeri. Molecular Diversity, 2006, 10, 213-221.	2.1	32
38	Antiproliferative novel isoxazoles: Modeling, virtual screening, synthesis, and bioactivity evaluation. European Journal of Medicinal Chemistry, 2014, 81, 139-149.	2.6	32
39	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
40	Transcriptomics in Toxicogenomics, Part II: Preprocessing and Differential Expression Analysis for High Quality Data. Nanomaterials, 2020, 10, 903.	1.9	31
41	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
42	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
43	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
44	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
45	Risk Governance of Emerging Technologies Demonstrated in Terms of its Applicability to Nanomaterials. Small, 2020, 16, e2003303.	5.2	28
46	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
47	Development of Deep Learning Models for Predicting the Effects of Exposure to Engineered Nanomaterials on Daphnia magna. Small, 2020, 16, e2001080.	5.2	28
48	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
49	Hydroxamic Acids Constitute a Novel Class of Autotaxin Inhibitors that Exhibit in Vivo Efficacy in a Pulmonary Fibrosis Model. Journal of Medicinal Chemistry, 2018, 61, 3697-3711.	2.9	27
50	Functionalized 4-Hydroxy Coumarins: Novel Synthesis, Crystal Structure and DFT Calculations. Molecules, 2011, 16, 384-402.	1.7	22
51	Exploiting ChEMBL database to identify indole analogs as HCV replication inhibitors. Methods, 2015, 71, 4-13.	1.9	20
52	MouseTox: An online toxicity assessment tool for small molecules through Enalos Cloud platform. Food and Chemical Toxicology, 2017, 110, 83-93.	1.8	20
53	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
54	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

#	Article	IF	Citations
55	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
56	Manually curated transcriptomics data collection for toxicogenomic assessment of engineered nanomaterials. Scientific Data, 2021, 8, 49.	2.4	19
57	Enalos Suite of Tools: Enhancing Cheminformatics and Nanoinfor - matics through KNIME. Current Medicinal Chemistry, 2020, 27, 6523-6535.	1.2	18
58	In Silico Discovery of Plant-Origin Natural Product Inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-ÎºB Ligand (RANKL). Frontiers in Pharmacology, 2018, 9, 800.	1.6	17
59	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
60	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
61	Current Status and Future Prospects of Smallâ€“molecule Proteinâ€“protein Interaction (PPI) Inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-ÎºB Ligand (RANKL). Current Topics in Medicinal Chemistry, 2018, 18, 661-673.	1.0	13
62	Synthesis of novel 2-pyrrolidinone and pyrrolidine derivatives and study of their inhibitory activity against autotaxin enzyme. Bioorganic and Medicinal Chemistry, 2020, 28, 115216.	1.4	12
63	Enalos+ KNIME Nodes: New Cheminformatics Tools for Drug Discovery. Methods in Molecular Biology, 2018, 1824, 113-138.	0.4	11
64	Prospects and challenges for FAIR toxicogenomics data. Nature Nanotechnology, 2022, 17, 17-18.	15.6	11
65	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
66	Nanoinformatics: Artificial Intelligence and Nanotechnology in the New Decade. Combinatorial Chemistry and High Throughput Screening, 2020, 23, 4-5.	0.6	10
67	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
68	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
69	Cyclisation of Novel Amino Oxo Esters to Tetramic Acidsâ^' Density Functional Theory Study of the Reaction Mechanism. European Journal of Organic Chemistry, 2003, 2003, 4593-4600.	1.2	9
70	Read-across predictions of nanoparticle hazard endpoints: a mathematical optimization approach. Nanoscale Advances, 2019, 1, 3485-3498.	2.2	9
71	Importance of Surface Topography in Both Biological Activity and Catalysis of Nanomaterials: Can Catalysis by Design Guide Safe by Design?. International Journal of Molecular Sciences, 2021, 22, 8347.	1.8	9
72	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

#	Article	IF	Citations
73	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
74	Structure-Based Discovery of Novel Chemical Classes of Autotaxin Inhibitors. International Journal of Molecular Sciences, 2020, 21, 7002.	1.8	8
75	Rational Drug Design Paradigms: The Odyssey for Designing Better Drugs. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 238-256.	0.6	8
76	Editorial: Towards Open Access for Cheminformatics. Combinatorial Chemistry and High Throughput Screening, 2016, 19, 260-261.	0.6	5
77	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
78	Editorial for the Special Issue From Nanoinformatics to Nanomaterials Risk Assessment and Governance. Nanomaterials, 2021, 11, 121.	1.9	4
79	Enalos Cloud Platform: Nanoinformatics and Cheminformatics Tools. Methods in Pharmacology and Toxicology, 2020, , 789-800.	0.1	4
80	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
81	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
82	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
83	Open Source Chemoinformatics Software including KNIME Analytics. , 2017, , 2201-2230.		3
84	Computational toxicology: From cheminformatics to nanoinformatics. Food and Chemical Toxicology, 2018, 112, 476-477.	1.8	3
85	Aqueous Solubility Enhancement for Bioassays of Insoluble Inhibitors and QSPR Analysis: A TNF-Î± Study. SLAS Discovery, 2018, 23, 84-93.	1.4	3
86	Enalos Suite: New Cheminformatics Platform for Drug Discovery and Computational Toxicology. Methods in Molecular Biology, 2018, 1800, 287-311.	0.4	3
87	Computer Aided Drug Design Approaches for Identification of Novel Autotaxin (ATX) Inhibitors. Current Medicinal Chemistry, 2016, 23, 1708-1724.	1.2	3
88	Editorial (Thematic Issue: Advances in Cheminformatics: Drug Discovery, Computational Toxicology) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.6	2
89	Consensus Predictive Model for Human K562 Cell Growth Inhibition through Enalos Cloud Platform. ChemMedChem, 2018, 13, 555-563.	1.6	2
90	Cheminformatics Toolboxes and Workflows within KNIME Analytics. Current Medicinal Chemistry, 2020, 27, 6442-6443.	1.2	2

#	Article	IF	Citations
91	Methods, models, mechanisms and metadata: Introducing the Nanotoxicology collection at F1000Research. F1000Research, 2021, 10, 1196.	0.8	2
92	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
93	Development of nonlinear quantitative structure-activity relationships using rbf networks and evolutionary computing. Computer Aided Chemical Engineering, 2004, , 265-270.	0.3	1
94	Editorial. Combinatorial Chemistry and High Throughput Screening, 2013, 16, 763-763.	0.6	1
95	NanoSolveIT integration of tools for assessment of human and environmental exposure to nanomaterials. , 2021, , 81-120.		1
96	Quantitative Nanostructure-Activity Relationship Models for the Risk Assessment of NanoMaterials. , 2017, , 1314-1338.		1
97	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
98	Editorial. Combinatorial Chemistry and High Throughput Screening, 2014, 17, 395-395.	0.6	0
99	Editorial (Thematic Issue: Advances in Cheminformatics: Drug Discovery, Computational Toxicology) Tj ETQq1 1 0.784314 rgBT /Over	0.6	0
100	05.17â€...An integrated chemoinformatics-aided pipeline for the discovery of smallâ€“molecule dual inhibitors of tnf and rankl. , 2017, , .		0
101	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
102	Meet our Editorial Board Members. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 235-235.	0.6	0
103	Open Source Chemoinformatics Software including KNIME Analytics Platform. , 2016, , 1-30.		0
104	Open-Source Chemoinformatics Software. , 2016, , 1-30.		0
105	Quantitative Nanostructure-Activity Relationship Models for the Risk Assessment of NanoMaterials. , 2017, , 20-44.		0
106	Computational chemistry in the search for improved therapeutics for inflammatory and autoimmune diseases. Biochemist, 2017, 39, 20-23.	0.2	0