Rafael Dolezal

List of Publications by Year in descending order

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97 papers

1,612 citations

304368 22 h-index 36 g-index

102 all docs 102 docs citations

102 times ranked

1903 citing authors

#	Article	IF	CITATIONS
1	Accuracy and precision of binding free energy prediction for a tacrine related lead inhibitor of acetylcholinesterase with an arsenal of supercomputerized molecular modelling methods: a comparative study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11291-11319.	2.0	1
2	Low-contrast lesion segmentation in advanced MRI experiments by time-domain Ricker-type wavelets and fuzzy 2-means. Applied Intelligence, 2022, 52, 15237-15258.	3.3	6
3	Smallâ€molecule inhibitors of cyclophilin D as potential therapeutics in mitochondriaâ€related diseases. Medicinal Research Reviews, 2022, 42, 1822-1855.	5.0	11
4	Tacrine – Benzothiazoles: Novel class of potential multitarget anti-Alzheimeŕs drugs dealing with cholinergic, amyloid and mitochondrial systems. Bioorganic Chemistry, 2021, 107, 104596.	2.0	17
5	7-phenoxytacrine is a dually acting drug with neuroprotective efficacy in vivo. Biochemical Pharmacology, 2021, 186, 114460.	2.0	12
6	The Impact of Dextran Sodium Sulfate-Induced Gastrointestinal Injury on the Pharmacokinetic Parameters of Donepezil and Its Active Metabolite 6-O-desmethyldonepezil, and Gastric Myoelectric Activity in Experimental Pigs. Molecules, 2021, 26, 2160.	1.7	6
7	The Effect of Chemical Structure of OEG Ligand Shells with Quaternary Ammonium Moiety on the Colloidal Stabilization, Cellular Uptake and Photothermal Stability of Gold Nanorods. International Journal of Nanomedicine, 2021, Volume 16, 3407-3427.	3.3	O
8	Structure-activity relationships of dually-acting acetylcholinesterase inhibitors derived from tacrine on N-methyl-d-Aspartate receptors. European Journal of Medicinal Chemistry, 2021, 219, 113434.	2.6	9
9	Classification of Ataxic Gait. Sensors, 2021, 21, 5576.	2.1	2
10	Raman Spectroscopy as a Novel Method for the Characterization of Polydioxanone Medical Stents Biodegradation. Materials, 2021, 14, 5462.	1.3	7
11	Distribution-based imaging for multiple sclerosis lesion segmentation using specialized fuzzy 2-means powered by Nakagami transmutations. Applied Soft Computing Journal, 2021, 108, 107481.	4.1	7
12	Synthesis, <i>inÂvitro</i> screening and molecular docking of isoquinolinium-5-carbaldoximes as acetylcholinesterase and butyrylcholinesterase reactivators. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 478-488.	2.5	15
13	From orexin receptor agonist YNT-185 to novel antagonists with drug-like properties for the treatment of insomnia. Bioorganic Chemistry, 2020, 103, 104179.	2.0	5
14	The wide-spectrum antimicrobial effect of novel N-alkyl monoquaternary ammonium salts and their mixtures; the QSAR study against bacteria. European Journal of Medicinal Chemistry, 2020, 206, 112584.	2.6	22
15	Discovery of novel berberine derivatives with balanced cholinesterase and prolyl oligopeptidase inhibition profile. European Journal of Medicinal Chemistry, 2020, 203, 112593.	2.6	24
16	Wide-Antimicrobial Spectrum of Picolinium Salts. Molecules, 2020, 25, 2254.	1.7	8
17	Benzothiazolyl Ureas are Low Micromolar and Uncompetitive Inhibitors of 17β-HSD10 with Implications to Alzheimerမs Disease Treatment. International Journal of Molecular Sciences, 2020, 21, 2059.	1.8	14
18	The pharmacokinetic parameters and the effect of a single and repeated doses of memantine on gastric myoelectric activity in experimental pigs. PLoS ONE, 2020, 15, e0227781.	1.1	7

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19	Computational Complexity of Kabsch and Quaternion Based Algorithms for Molecular Superimposition in Computational Chemistry. Proceedings of the International Neural Networks Society, 2020, , 473-486.	0.6	1
20	A Mini Review on Parallel Processing of Brain Magnetic Resonance Imaging. Lecture Notes in Computer Science, 2020, , 482-493.	1.0	1
21	OPCW BIOMEDICAL PROFICIENCY TEST IN THE LABORATORY OF ANALYTICAL CHEMISTRY AT THE DEPARTMENT OFÂTOXICOLOGY AND MILITARY PHARMACY. Military Medical Science Letters (Vojenske) Tj ETQq1	lo 0 :78431	l⊕rgBT /O√
22	Molecular modeling studies on the interactions of aflatoxin B1 and its metabolites with the peripheral anionic site of human acetylcholinesterase. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2041-2048.	2.0	16
23	Highly hydrophilic cationic gold nanorods stabilized by novel quaternary ammonium surfactant with negligible cytotoxicity. Journal of Biophotonics, 2019, 12, e201900024.	1.1	5
24	Synthesis, Antimicrobial Effect and Lipophilicityâ€Activity Dependence of Three Series of Dichained <i>N</i> â€Alkylammonium Salts. ChemistrySelect, 2019, 4, 12076-12084.	0.7	12
25	Surface screening, molecular modeling and in vitro studies on the interactions of aflatoxin M1 and human enzymes acetyl- and butyrylcholinesterase. Chemico-Biological Interactions, 2019, 308, 113-119.	1.7	4
26	In Vitro and In Silico Acetylcholinesterase Inhibitory Activity of Thalictricavine and Canadine and Their Predicted Penetration across the Blood-Brain Barrier. Molecules, 2019, 24, 1340.	1.7	23
27	Novel tacrine-tryptophan hybrids: Multi-target directed ligands as potential treatment for Alzheimer's disease. European Journal of Medicinal Chemistry, 2019, 168, 491-514.	2.6	75
28	Determination of Hypericin in <i>Hypericum perforatum</i> (St. John's Wort) Using Classical C18 and Pentafluorophenyl Stationary Phases: Contribution of Piâ€"Pi Interactions to High-Performance Liquid Chromatography (HPLC). Analytical Letters, 2019, 52, 1788-1812.	1.0	6
29	Non-peptide orexin 2 receptor modulators as promising way to treatment of narcolepsy/insomnia. Journal of the Neurological Sciences, 2019, 405, 98.	0.3	0
30	Orexin supplementation in narcolepsy treatment: A review. Medicinal Research Reviews, 2019, 39, 961-975.	5.0	31
31	Novel quinazolin-4-one derivatives as potentiating agents of doxorubicin cytotoxicity. Bioorganic Chemistry, 2019, 82, 204-210.	2.0	2
32	N-alkylated Tacrine Derivatives as Potential Agents in Alzheimer's Disease Therapy. Current Alzheimer Research, 2019, 16, 333-343.	0.7	5
33	Molecular Models in Chemistry Education at University and Upper Secondary School - Structure of Amides. Chemistry, Didactics, Ecology, Metrology, 2019, 24, 45-51.	0.1	O
34	Didactic Capacity of Selected Czech and Russian Organic Chemistry Textbooks. Chemistry, Didactics, Ecology, Metrology, 2019, 24, 61-76.	0.1	2
35	The concept of hybrid molecules of tacrine and benzyl quinolone carboxylic acid (BQCA) as multifunctional agents for Alzheimer's disease. European Journal of Medicinal Chemistry, 2018, 150, 292-306.	2.6	60
36	Characterization of the Penetration of the Blood–Brain Barrier by High-Performance Liquid Chromatography (HPLC) Using a Stationary Phase with an Immobilized Artificial Membrane. Analytical Letters, 2018, 51, 2401-2414.	1.0	6

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37	Rational design of novel TLR4 ligands by in silico screening and their functional and structural characterization inÂvitro. European Journal of Medicinal Chemistry, 2018, 146, 38-46.	2.6	12
38	Profiling donepezil template into multipotent hybrids with antioxidant properties. Journal of Enzyme Inhibition and Medicinal Chemistry, 2018, 33, 583-606.	2.5	44
39	Investigation of New Orexin 2 Receptor Modulators Using In Silico and In Vitro Methods. Molecules, 2018, 23, 2926.	1.7	6
40	Molecular Modeling Studies on the Interactions of Aflatoxin B1 and Its Metabolites with Human Acetylcholinesterase. Part II: Interactions with the Catalytic Anionic Site (CAS). Toxins, 2018, 10, 389.	1.5	5
41	Rational Design of a New Class of Toll-Like Receptor 4 (TLR4) Tryptamine Related Agonists by Means of the Structure- and Ligand-Based Virtual Screening for Vaccine Adjuvant Discovery. Molecules, 2018, 23, 102.	1.7	8
42	A Review of the Synthesis of Quaternary Acetylcholinesterase Reactivators. Current Organic Chemistry, 2018, 22, 1619-1648.	0.9	6
43	Synthesis, Antimicrobial Effect and Surface Properties of Hydroxymethylsubstituted Pyridinium Salts. Letters in Drug Design and Discovery, 2018, 15, 828-842.	0.4	7
44	In vitro and in silico Evaluation of Non-Quaternary Reactivators of AChE as Antidotes of Organophosphorus Poisoning - a New Hope or a Blind Alley?. Medicinal Chemistry, 2018, 14, 281-292.	0.7	19
45	HPLC analysis and blood-brain penetration of 20-hydroxyecdysone diacetonide. Acta Chromatographica, 2017, 29, 375-383.	0.7	2
46	Progress in acetylcholinesterase reactivators and in the treatment of organophosphorus intoxication: a patent review (2006–2016). Expert Opinion on Therapeutic Patents, 2017, 27, 971-985.	2.4	28
47	Structure-Based Virtual Screening for Novel Modulators of Human Orexin 2 Receptor with Cloud Systems and Supercomputers. Studies in Computational Intelligence, 2017, , 161-171.	0.7	1
48	Tetroxime: reactivation potency – in vitro and in silico study. RSC Advances, 2017, 7, 7041-7045.	1.7	4
49	Synthesis and evaluation of frentizole-based indolyl thiourea analogues as MAO/ABAD inhibitors for Alzheimer's disease treatment. Bioorganic and Medicinal Chemistry, 2017, 25, 1143-1152.	1.4	45
50	Bis-isoquinolinium and bis-pyridinium acetylcholinesterase inhibitors: in vitro screening of probes for novel selective insecticides. RSC Advances, 2017, 7, 39279-39291.	1.7	6
51	Concentration of Donepezil in the Cerebrospinal Fluid of AD Patients: Evaluation of Dosage Sufficiency in Standard Treatment Strategy. Neurotoxicity Research, 2017, 31, 162-168.	1.3	23
52	Microwave synthesis of sulfanilic acid. Chemistry, Didactics, Ecology, Metrology, 2017, 22, 93-98.	0.1	3
53	Concentration of donepezil in the cerebrospinal fluid of AD patients: Evaluation of dosage sufficiency in standard treatment strategy. Journal of the Neurological Sciences, 2017, 381, 1027.	0.3	0
54	Multitarget Tacrine Hybrids with Neuroprotective Properties to Confront Alzheimer's Disease. Current Topics in Medicinal Chemistry, 2017, 17, 1006-1026.	1.0	75

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55	Novel Tacrine-Scutellarin Hybrids as Multipotent Anti-Alzheimer's Agents: Design, Synthesis and Biological Evaluation. Molecules, 2017, 22, 1006.	1.7	32
56	Development of 2-Methoxyhuprine as Novel Lead for Alzheimer's Disease Therapy. Molecules, 2017, 22, 1265.	1.7	26
57	Novel Series of Quaternary Ammonium Surfactants Based on 2,3-Dihydro- [1,4]dioxino [2,3-b]pyridin-7-ol Ring: Synthesis, Analysis and Antimicrobial Evaluation. Letters in Organic Chemistry, 2017, 15, .	0.2	1
58	6-Benzothiazolyl Ureas, Thioureas and Guanidines are Potent Inhibitors of ABAD/ $17\hat{l}^2$ -HSD10 and Potential Drugs for Alzheimer"s Disease Treatment: Design, Synthesis and in vitro Evaluation. Medicinal Chemistry, 2017, 13, 345-358.	0.7	22
59	ANN and GMDH Algorithms in QSAR Analyses of Reactivation Potency for Acetylcholinesterase Inhibited by VX Warfare Agent. Lecture Notes in Computer Science, 2017, , 171-181.	1.0	O
60	6-benzothiazolyl ureas, thioureas and guanidines are potent inhibitors of ABAD/ $17\hat{l}^2$ -HSD10 and potential drugs for Alzheimer's disease treatment: Design, synthesis and in vitro evaluation. Medicinal Chemistry, 2017, , .	0.7	4
61	Towards understanding the mechanism of action of antibacterial N-alkyl-3-hydroxypyridinium salts: Biological activities, molecular modeling and QSAR studies. European Journal of Medicinal Chemistry, 2016, 121, 699-711.	2.6	37
62	A 7-methoxytacrine–4-pyridinealdoxime hybrid as a novel prophylactic agent with reactivation properties in organophosphate intoxication. Toxicology Research, 2016, 5, 1012-1016.	0.9	22
63	SAR study to find optimal cholinesterase reactivator against organophosphorous nerve agents and pesticides. Archives of Toxicology, 2016, 90, 2831-2859.	1.9	75
64	Simulations of Light Propagation and Thermal Response in Biological Tissues Accelerated by Graphics Processing Unit. Lecture Notes in Computer Science, 2016, , 242-251.	1.0	2
65	Rational Discovery of GSK3-Beta Modulators Aided by Protein Pocket Prediction and High-Throughput Molecular Docking. Lecture Notes in Computer Science, 2016, , 429-439.	1.0	1
66	Design, synthesis and in vitro evaluation of benzothiazole-based ureas as potential ABAD/17β-HSD10 modulators for Alzheimer's disease treatment. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 3675-3678.	1.0	29
67	Synthesis, antimicrobial evaluation and molecular modeling of 5-hydroxyisoquinolinium salt series; the effect of the hydroxyl moiety. Bioorganic and Medicinal Chemistry, 2016, 24, 841-848.	1.4	15
68	Novel caffeine derivatives with antiproliferative activity. RSC Advances, 2016, 6, 32534-32539.	1.7	12
69	Preparation of 7â€Methoxy Tacrine Dimer Analogs and Their <i>In vitro/In silico</i> Evaluation as Potential Cholinesterase Inhibitors. Bulletin of the Korean Chemical Society, 2015, 36, 1654-1660.	1.0	9
70	Comparative lipophilicity of morphine derivatives. Journal of Planar Chromatography - Modern TLC, 2015, 28, 126-132.	0.6	2
71	Synthesis and Disinfection Effect of the Pyridine-4-aldoxime Based Salts. Molecules, 2015, 20, 3681-3696.	1.7	22
72	7-Methoxytacrine-p-Anisidine Hybrids as Novel Dual Binding Site Acetylcholinesterase Inhibitors for Alzheimer's Disease Treatment. Molecules, 2015, 20, 22084-22101.	1.7	35

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73	Ligand-based 3D QSAR analysis of reactivation potency of mono- and bis-pyridinium aldoximes toward VX-inhibited rat acetylcholinesterase. Journal of Molecular Graphics and Modelling, 2015, 56, 113-129.	1.3	17
74	Design, synthesis and in vitro testing of 7-methoxytacrine-amantadine analogues: a novel cholinesterase inhibitors for the treatment of Alzheimer's disease. Medicinal Chemistry Research, 2015, 24, 2645-2655.	1.1	28
75	HPC Cloud Technologies for Virtual Screening in Drug Discovery. Lecture Notes in Computer Science, 2015, , 440-449.	1.0	10
76	Tacrine–Trolox Hybrids: A Novel Class of Centrally Active, Nonhepatotoxic Multi-Target-Directed Ligands Exerting Anticholinesterase and Antioxidant Activities with Low In Vivo Toxicity. Journal of Medicinal Chemistry, 2015, 58, 8985-9003.	2.9	121
77	Variable Elimination Approaches for Data-Noise Reduction in 3D QSAR Calculations. Lecture Notes in Computer Science, 2015, , 313-325.	1.0	3
78	Endpoint Firewall for Local Security Hardening in Academic Research Environment. Lecture Notes in Computer Science, 2015, , 246-255.	1.0	2
79	Parallel Flexible Molecular Docking in Computational Chemistry on High Performance Computing Clusters. Lecture Notes in Computer Science, 2015, , 418-427.	1.0	10
80	Structural Properties of Potential Synthetic Vaccine Adjuvants - TLR Agonists. Current Medicinal Chemistry, 2015, 22, 3306-3325.	1.2	10
81	A Review of the Total Synthesis of (+)-Lactacystin and its Analogs. Current Organic Chemistry, 2015, 19, 1980-2001.	0.9	5
82	ACID DISSOCIATION CONSTANTS AND MOLECULAR DESCRIPTORS OF SOME XYLENE LINKED BISPYRIDINIUM OXIMES. Military Medical Science Letters (Vojenske Zdravotnicke Listy), 2015, 84, 94-103.	0.2	1
83	6-Hydroxyquinolinium salts differing in the length of alkyl side-chain: Synthesis and antimicrobial activity. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 5238-5241.	1.0	35
84	7-MEOTA–donepezil like compounds as cholinesterase inhibitors: Synthesis, pharmacological evaluation, molecular modeling and QSAR studies. European Journal of Medicinal Chemistry, 2014, 82, 426-438.	2.6	80
85	From Pyridinium-based to Centrally Active Acetylcholinesterase Reactivators. Mini-Reviews in Medicinal Chemistry, 2014, 14, 215-221.	1.1	44
86	Preparation, In Vitro Screening and Molecular Modelling of Monoquaternary Compounds Related to the Selective Acetylcholinesterase Inhibitor BW284c51. Medicinal Chemistry, 2014, 11, 21-29.	0.7	4
87	Oximes: Inhibitors of Human Recombinant Acetylcholinesterase. A Structure-Activity Relationship (SAR) Study. International Journal of Molecular Sciences, 2013, 14, 16882-16900.	1.8	38
88	Comparison of Novel Tacrine and 7-MEOTA Derivatives with Aromatic and Alicyclic Residues: Synthesis, Biological Evaluation and Docking Studies. Letters in Organic Chemistry, 2013, 10, 291-297.	0.2	3
89	Antimycobacterial 3-phenyl-4-thioxo-2H-1,3-benzoxazine-2(3H)-ones and 3-phenyl-2H-1,3-benzoxazine-2,4(3H)-dithiones substituted on phenyl and benzoxazine moiety in position 6. Chemical Papers, 2011, 65, .	1.0	4
90	Quantitative Structure–Electrochemistry Relationship of 1â€Phenylâ€5â€benzylâ€sulfanyltetrazoles and Their Electrooxidation as a Metabolic Model. Electroanalysis, 2010, 22, 2117-2122.	1.5	13

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91	<i>Nâ€</i> Benzylsalicylthioamides: Highly Active Potential Antituberculotics. Archiv Der Pharmazie, 2009, 342, 113-119.	2.1	17
92	New antituberculotics originated from salicylanilides with promising in vitro activity against atypical mycobacterial strains. Bioorganic and Medicinal Chemistry, 2009, 17, 3572-3579.	1.4	46
93	QSAR analysis of salicylamide isosteres with the use of quantum chemical molecular descriptors. European Journal of Medicinal Chemistry, 2009, 44, 869-876.	2.6	17
94	Highly Active Potential Antituberculotics: 3-(4-Alkylphenyl)-4-thioxo-2H-1,3-benzoxazine-2(3H)-ones and 3-(4-Alkylphenyl)-2H-1,3-benzoxazine-2,4(3H)-dihiones Substituted in Ring-B by Halogen. Archiv Der Pharmazie, 2008, 341, 800-803.	2.1	8
95	The antimycobacterial derivatives against potential pathogenic strains: 2-Hydroxy-3-(4-phenylpiperazin-1-yl)-propylphenylcarbamates. Scientia Pharmaceutica, 2007, 75, 55-61.	0.7	4
96	QSAR study of antimycobacterial activity of quaternary ammonium salts of piperidinylethyl esters of alkoxysubstituted phenylcarbamic acids. Folia Microbiologica, 2006, 51, 21-4.	1.1	15
97	1-Aryl-5-benzylsulfanyltetrazoles, a new group of antimycobacterial compounds against potentially pathogenic strains. Folia Microbiologica, 2005, 50, 195-197.	1.1	12