Alan Talevi

List of Publications by Year
in descending order

141 papers	1,947 citations	257101 24 h-index	301761 39 g-index
152 all docs	152 docs citations	152 times ranked	2556 citing authors

#	Article	IF	Citations
1	Multi-target pharmacology: possibilities and limitations of the â€œskeleton key approachâ€•from a medicinal chemist perspective. Frontiers in Pharmacology, 2015, 6, 205.	1.6	250
2	Challenges and opportunities with drug repurposing: finding strategies to find alternative uses of therapeutics. Expert Opinion on Drug Discovery, 2020, 15, 397-401.	2.5	168
3	New QSPR study for the prediction of aqueous solubility of drug-like compounds. Bioorganic and Medicinal Chemistry, 2008, 16, 7944-7955.	1.4	86
4	Computer-guided drug repurposing: Identification of trypanocidal activity of clofazimine, benidipine and saquinavir. European Journal of Medicinal Chemistry, 2015, 93, 338-348.	2.6	63
5	Carbamazepine-loaded solid lipid nanoparticles and nanostructured lipid carriers: Physicochemical characterization and in vitro/in vivo evaluation. Colloids and Surfaces B: Biointerfaces, 2018, 167, 73-81.	2.5	63
6	Discovery of anticonvulsant activity of abietic acid through application of linear discriminant analysis. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 1684-1690.	1.0	48
7	Drug repositioning: current approaches and their implications in the precision medicine era. Expert Review of Precision Medicine and Drug Development, 2018, 3, 49-61.	0.4	48
8	Hybrid Ofloxacin/eugenol co-loaded solid lipid nanoparticles with enhanced and targetable antimicrobial properties. International Journal of Pharmaceutics, 2019, 569, 118575.	2.6	46
9	Prediction of drug intestinal absorption by new linear and non-linear QSPR. European Journal of Medicinal Chemistry, 2011, 46, 218-228.	2.6	45
10	An Integrated Drug Development Approach Applying Topological Descriptors. Current Computer-Aided Drug Design, 2012, 8, 172-181.	0.8	40
11	Application of descriptors based on Lipinskiâ€™s rules in the QSPR study of aqueous solubilities. Bioorganic and Medicinal Chemistry, 2007, 15, 3711-3719.	1.4	39
12	Discovery of novel polyamine analogs with anti-protozoal activity by computer guided drug repositioning. Journal of Computer-Aided Molecular Design, 2016, 30, 305-321.	1.3	39
13	Machine Learning in Drug Discovery and Development Part 1: A Primer. CPT: Pharmacometrics and Systems Pharmacology, 2020, 9, 129-142.	1.3	38
14	Neglected Tropical Protozoan Diseases: Drug Repositioning as a Rational Option. Current Topics in Medicinal Chemistry, 2016, 16, 2201-2222.	1.0	37
15	Application of Computer-Aided Drug Repurposing in the Search of New Cruzipain Inhibitors: Discovery of Amiodarone and Bromocriptine Inhibitory Effects. Journal of Chemical Information and Modeling, 2013, 53, 2402-2408.	2.5	36
16	Anticonvulsant activity of artificial sweeteners: A structural link between sweet-taste receptor T1R3 and brain glutamate receptors. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 4072-4074.	1.0	32
17	Strengths and Weaknesses of Docking Simulations in the SARS-CoV-2 Era: the Main Protease (Mpro) Case Study. Journal of Chemical Information and Modeling, 2021, 61, 3758-3770.	2.5	32
18	A successful virtual screening application: prediction of anticonvulsant activity in MES test of widely used pharmaceutical and food preservatives methylparaben and propylparaben. Journal of Computer-Aided Molecular Design, 2007, 21, 527-538.	1.3	31

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19	Combined Virtual Screening Strategies. Current Computer-Aided Drug Design, 2009, 5, 23-37.	0.8	31
20	Synthesis of 2-Hydrazolyl-4-Thiazolidinones Based on Multicomponent Reactions and Biological Evaluation Against Trypanosoma Cruzi. Chemical Biology and Drug Design, 2011, 77, 166-172.	1.5	31
21	Applications of Nanosystems to Anticancer Drug Therapy (Part II. Dendrimers, Micelles, Lipid-based) Tj ETQq1 1 0.784314 rgBT /Overl	0.8	29
22	CNS Drug Development â€“ Lost in Translation?. Mini-Reviews in Medicinal Chemistry, 2012, 12, 959-970.	1.1	28
23	Novel cruzipain inhibitors for the chemotherapy of chronic Chagas disease. International Journal of Antimicrobial Agents, 2016, 48, 91-95.	1.1	26
24	Hybrid inhalable microparticles for dual controlled release of levofloxacin and DNase: physicochemical characterization and in vivo targeted delivery to the lungs. Journal of Materials Chemistry B, 2017, 5, 3132-3144.	2.9	26
25	Computer-Aided Drug Design: An Overview. Methods in Molecular Biology, 2018, 1762, 1-19.	0.4	25
26	In silico Guided Drug Repurposing: Discovery of New Competitive and Non-competitive Inhibitors of Falcipain-2. Frontiers in Chemistry, 2019, 7, 534.	1.8	23
27	Sulfamide derivatives with selective carbonic anhydrase VII inhibitory action. Bioorganic and Medicinal Chemistry, 2016, 24, 894-901.	1.4	22
28	Cascade Ligand- and Structure-Based Virtual Screening to Identify New Trypanocidal Compounds Inhibiting Putrescine Uptake. Frontiers in Cellular and Infection Microbiology, 2018, 8, 173.	1.8	22
29	The Thiol-polyamine Metabolism of Trypanosoma cruzi: Molecular Targets and Drug Repurposing Strategies. Current Medicinal Chemistry, 2019, 26, 6614-6635.	1.2	22
30	High-throughput Drug Repositioning for the Discovery of New Treatments for Chagas Disease. Mini-Reviews in Medicinal Chemistry, 2015, 15, 182-193.	1.1	22
31	Application of linear discriminant analysis in the virtual screening of antichagasic drugs through trypanothione reductase inhibition. Molecular Diversity, 2006, 10, 361-375.	2.1	20
32	A Combined Virtual Screening 2D and 3D QSAR Methodology for the Selection of New Anticonvulsant Candidates from a Natural Product Library. QSAR and Combinatorial Science, 2008, 27, 1120-1129.	1.5	20
33	Identification of Levothyroxine Antichagasic Activity through Computer-Aided Drug Repurposing. Scientific World Journal, The, 2014, 2014, 1-9.	0.8	19
34	Can drug repurposing strategies be the solution to the COVID-19 crisis?. Expert Opinion on Drug Discovery, 2021, 16, 605-612.	2.5	19
35	Applications of Nanosystems to Anticancer Drug Therapy (Part I. Nanogels, Nanospheres,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf	0.8	19
36	Cannabidiol (CBD) Inhibited Rhodamine-123 Efflux in Cultured Vascular Endothelial Cells and Astrocytes Under Hypoxic Conditions. Frontiers in Behavioral Neuroscience, 2020, 14, 32.	1.0	18

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37	Development and Validation of a Computational Model Ensemble for the Early Detection of BCRP/ABCG2 Substrates during the Drug Design Stage. Journal of Chemical Information and Modeling, 2017, 57, 1868-1880.	2.5	17
38	Interaction of Solid Lipid Nanoparticles and Specific Proteins of the Corona Studied by Surface Plasmon Resonance. Journal of Nanomaterials, 2017, 2017, 1-11.	1.5	17
39	New anticonvulsant candidates prevent P-glycoprotein (P-gp) overexpression in a pharmacoresistant seizure model in mice. Epilepsy and Behavior, 2021, 121, 106451.	0.9	16
40	Propylparaben applied after pilocarpine-induced status epilepticus modifies hippocampal excitability and glutamate release in rats. NeuroToxicology, 2017, 59, 110-120.	1.4	15
41	Identification of cisapride as new inhibitor of putrescine uptake in Trypanosoma cruzi by combined ligand- and structure-based virtual screening. European Journal of Medicinal Chemistry, 2018, 149, 22-29.	2.6	15
42	Tailored Multi-Target Agents. Applications and Design Considerations. Current Pharmaceutical Design, 2016, 22, 3164-3170.	0.9	15
43	The Importance of Bioactivation in Computer-Guided Drug Repositioning. Why the Parent Drug is Not Always Enough. Current Topics in Medicinal Chemistry, 2016, 16, 2078-2087.	1.0	15
44	Several New Diverse Anticonvulsant Agents Discovered in a Virtual Screening Campaign Aimed at Novel Antiepileptic Drugs to Treat Refractory Epilepsy. Journal of Chemical Information and Modeling, 2012, 52, 3325-3330.	2.5	14
45	Development of Conformation Independent Computational Models for the Early Recognition of Breast Cancer Resistance Protein Substrates. BioMed Research International, 2013, 2013, 1-12.	0.9	13
46	Computational approaches for innovative antiepileptic drug discovery. Expert Opinion on Drug Discovery, 2016, 11, 1001-1016.	2.5	13
47	A structure-based approach towards the identification of novel antichagasic compounds: Trypanosoma cruzi carbonic anhydrase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 21-30.	2.5	13
48	Anticonvulsant effect of sodium cyclamate and propylparaben on pentylenetetrazolâ€induced seizures in zebrafish. Synapse, 2017, 71, e21961.	0.6	12
49	In Silico Drug Repositioning for Chagas Disease. Current Medicinal Chemistry, 2020, 27, 662-675.	1.2	12
50	Computer-Aided Recognition of ABC Transporters Substrates and Its Application to the Development of New Drugs for Refractory Epilepsy. Mini-Reviews in Medicinal Chemistry, 2017, 17, 205-215.	1.1	12
51	Hybrid Compounds as Anti-infective Agents. Current Topics in Medicinal Chemistry, 2017, 17, 1080-1095.	1.0	11
52	Application of target repositioning and in silico screening to exploit fatty acid binding proteins (FABPs) from Echinococcus multilocularis as possible drug targets. Journal of Computer-Aided Molecular Design, 2020, 34, 1275-1288.	1.3	11
53	Computer-Aided Identification of Anticonvulsant Effect of Natural Nonnutritive Sweeteners Stevioside and Rebaudioside A. Assay and Drug Development Technologies, 2015, 13, 313-318.	0.6	9
54	Trypanosomatid-Caused Conditions: State of the Art of Therapeutics and Potential Applications of Lipid-Based Nanocarriers. Frontiers in Chemistry, 2020, 8, 601151.	1.8	9

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55	iRaPCA and SOMoC: Development and Validation of Web Applications for New Approaches for the Clustering of Small Molecules. Journal of Chemical Information and Modeling, 2022, 62, 2987-2998.	2.5	9
56	Quantitative structureâ€“activity relationship models for compounds with anticonvulsant activity. Expert Opinion on Drug Discovery, 2019, 14, 653-665.	2.5	8
57	On the Development of New Antiepileptic Drugs for the Treatment of Pharmacoresistant Epilepsy: Different Approaches to Different Hypothesis. , 2013, , 207-224.		8
58	Development of a highly specific ensemble of topological models for early identification of Pâ€glycoprotein substrates. Journal of Chemometrics, 2011, 25, 313-322.	0.7	7
59	Modern Approaches for the Discovery of Anti-Infectious Drugs for the Treatment of Neglected Diseases. Current Topics in Medicinal Chemistry, 2018, 18, 369-381.	1.0	7
60	Structure-Based Virtual Screening Identifies Novobiocin, Montelukast, and Cinnarizine as TRPV1 Modulators with Anticonvulsant Activity In Vivo. Journal of Chemical Information and Modeling, 2022, 62, 3008-3022.	2.5	7
61	Parabens inhibit hNaV 1.2 channels. Biomedicine and Pharmacotherapy, 2020, 128, 110250.	2.5	6
62	Potential medicinal effects and applications of stevia constituents. Phytochemistry Reviews, 2022, 21, 161-178.	3.1	6
63	Preparation, physicochemical and biopharmaceutical characterization of oxcarbazepine-loaded nanostructured lipid carriers as potential antiepileptic devices. Journal of Drug Delivery Science and Technology, 2021, 63, 102470.	1.4	6
64	Drug Release. , 2021, , 1-7.		5
65	Combined therapy with Benznidazole and repurposed drugs Clofazimine and Benidipine for chronic Chagas disease. European Journal of Medicinal Chemistry, 2019, 184, 111778.	2.6	4
66	In Silico Modeling of FDA-Approved Drugs for Discovery of Therapies Against Neglected Diseases: A Drug Repurposing Approach. , 2019, , 625-648.		4
67	Drug Repurposing. , 2021, , .		4
68	One-Compartment Pharmacokinetic Model. , 2021, , 1-8.		4
69	Is There a Relationship Between Sweet Taste and Seizures? Anticonvulsant and Proconvulsant Effects of Non-Nutritive Sweeteners. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 335-345.	0.6	4
70	Integrated Application of Enhanced Replacement Method and Ensemble Learning for the Prediction of BCRP/ABCG2 Substrates. Current Bioinformatics, 2017, 12, 239-248.	0.7	4
71	The New Patient and Responsible Self-Medication Practices: A Critical Review. Current Drug Safety, 2010, 5, 342-353.	0.3	3
72	Beneficial Effects of Stevia rebaudiana Bertoni and Steviol-Related Compounds on Health. Reference Series in Phytochemistry, 2018, , 263-284.	0.2	3

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73	Molecular Topology and Other Promiscuity Determinants as Predictors of Therapeutic Class - A Theoretical Framework to Guide Drug Repositioning?. Current Topics in Medicinal Chemistry, 2018, 18, 1110-1122.	1.0	3
74	Dissolution Studies of Generic Medications: New Evidence of Deviations from the Transitivity Principle. Dissolution Technologies, 2012, 19, 13-24.	0.2	3
75	Virtual Screening. , 0, , 229-245.		3
76	Homology Modeling and Molecular Dynamics Simulations of Trypanosoma cruzi Phosphodiesterase b1. Chemistry and Biodiversity, 2021, , .	1.0	3
77	Antiseizure medication discovery: Recent and future paradigm shifts. Epilepsia Open, 2022, 7, .	1.3	3
78	Tetracycline Derivatives Inhibit Plasmodial Cysteine Protease Falcipain-2 through Binding to a Distal Allosteric Site. Journal of Chemical Information and Modeling, 2022, 62, 159-175.	2.5	3
79	New similarity-based algorithm and its application to classification of anticonvulsant compounds. Journal of Enzyme Inhibition and Medicinal Chemistry, 2007, 22, 253-265.	2.5	2
80	The application of molecular topology for ulcerative colitis drug discovery. Expert Opinion on Drug Discovery, 2018, 13, 89-101.	2.5	2
81	Introduction. Biopharmaceutics and Pharmacokinetics. , 2018, , 3-10.		2
82	Drug Distribution. , 2018, , 33-53.		2
83	Drug Excretion. , 2018, , 81-96.		2
84	Ensemble learning application to discover new trypanothione synthetase inhibitors. Molecular Diversity, 2021, 25, 1361-1373.	2.1	2
85	The Efficiency of Multi-target Drugs: A Network Approach. Human Perspectives in Health Sciences and Technology, 2020, , 63-75.	0.2	2
86	Editorial [Towards Responsible, Safe Self-Medication (Guest Editor: Alan Talevi)]. Current Drug Safety, 2010, 5, 314-314.	0.3	1
87	Virtual Screening Applications in the Search of Novel Antiepileptic Drug Candidates. Methods in Pharmacology and Toxicology, 2016, , 237-258.	0.1	1
88	Network Pharmacology and Epilepsy. Methods in Pharmacology and Toxicology, 2016, , 351-364.	0.1	1
89	The Importance of Drug Repurposing in the Field of Antiepileptic Drug Development. Methods in Pharmacology and Toxicology, 2016, , 365-377.	0.1	1
90	Beneficial Effects of Stevia rebaudiana Bertoni and Steviol-Related Compounds on Health. Reference Series in Phytochemistry, 2016, , 1-22.	0.2	1

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91	Editorial (Thematic Issue: Targeted Therapies). Mini-Reviews in Medicinal Chemistry, 2017, 17, 186-187.	1.1	1
92	Free Drug Theory. , 2021, , 1-6.		1
93	Solute Carrier (SLC) Transporters: An Overview. , 2021, , 1-6.		1
94	Korsmeyer-Peppas, Peppas-Sahlin, and Brazel-Peppas: Models of Drug Release. , 2021, , 1-9.		1
95	Editorial: Lipid Nanoparticles as a Novel Strategy to Deliver Bioactive Molecules. Frontiers in Chemistry, 2021, 9, 655480.	1.8	1
96	Enterohepatic Recycling. , 2021, , 1-9.		1
97	Systematic Comparison of the Performance of Different 2D and 3D Ligand-Based Virtual Screening Methodologies to Discover Anticonvulsant Drugs. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 387-398.	0.6	1
98	Computer-aided search of novel inhibitors of n-myristoyl transferase with trypanocidal effects. International Journal of Infectious Diseases, 2018, 73, 311.	1.5	0
99	Drug Transporters. , 2018, , 331-348.		0
100	Drug Absorption. , 2018, , 11-31.		0
101	Drug Metabolism. , 2018, , 55-80.		0
102	Free Diffusion in Drug Absorption. , 2021, , 1-7.		0
103	Phase 0 and Phase III Transport. , 2021, , 1-8.		0
104	Drug Distribution. , 2021, , 1-9.		0
105	Transcytosis in Drug Absorption and Distribution. , 2021, , 1-7.		0
106	Drug Metabolism Functionalization (Phase I) Reactions. , 2021, , 1-7.		0
107	Drug Binding to Plasma Proteins. , 2021, , 1-12.		0
108	Zero-Order Drug Release. , 2021, , 1-6.		0

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109	Active and Facilitated Transport in Drug Absorption. , 2021, , 1-7.		0
110	Central Nervous System Bioavailability. , 2021, , 1-10.		0
111	Renal Drug Excretion. , 2021, , 1-7.		0
112	Peptide Transporters. , 2021, , 1-7.		0
113	Intestinal Perfusion Models. , 2021, , 1-9.		0
114	Drug Metabolism Synthetic (Phase II) Reactions. , 2021, , 1-8.		0
115	pKa Determination. , 2021, , 1-6.		0
116	Biorelevant Dissolution Media. , 2021, , 1-10.		0
117	Brain-to-Plasma Concentration Ratio and Unbound Partition Coefficient. , 2021, , 1-6.		0
118	Drug Absorption. , 2021, , 1-7.		0
119	Cytochrome P450. , 2021, , 1-8.		0
120	Drug Metabolism. , 2021, , 1-7.		0
121	Site of Metabolism Predictions. , 2021, , 1-9.		0
122	Unbound Brain-to-PlasmaÂPartition Coefficient Determination. , 2021, , 1-8.		0
123	Drug Excretion. , 2021, , 1-6.		0
124	Enzyme Induction and Drug Metabolism. , 2021, , 1-7.		0
125	Personalized Medicine and Drug Metabolism. , 2021, , 1-5.		0
126	Real and Apparent Volumes of Distribution. , 2021, , 1-9.		0

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127	Organic Cation Transporters. , 2021, , 1-6.		0
128	Recent Studies on Similarity Measures and its Applications to Chemoinformatics and Drug Design. , 2012, , 272-297.		0
129	Computer-Based Strategies Towards the Discovery of New Antiepileptic Agents. , 2012, , 99-118.		0
130	Recent Patents on Polymeric Nanosystems Applications for Anticancer Drug Delivery. , 2015, , 524-601.		0
131	Recent Patents on Nanosystems Applications to Anticancer Drug Therapy: Lipid-based Systems. , 2015, , 602-659.		0
132	An Introduction toÂPharmacokinetics. , 2017, , 13-46.		0
133	Application of Machine Learning Approaches to Identify New Anticonvulsant Compounds Active in the 6ÂHz Seizure Model. Communications in Computer and Information Science, 2019, , 3-19.	0.4	0
134	Positive Predictive Value Surfaces as a Complementary Tool to Assess the Performance of Virtual Screening Methods. Mini-Reviews in Medicinal Chemistry, 2020, 20, 1447-1460.	1.1	0
135	Free Drug Theory. , 2022, , 1-6.		0
136	Central Nervous System Bioavailability. , 2022, , 233-242.		0
137	Drug Metabolism Functionalization (Phase I) Reactions. , 2022, , 387-394.		0
138	In Silico ADME: QSPR/QSAR. , 2022, , 525-531.		0
139	Site of Metabolism Predictions. , 2022, , 1073-1081.		0
140	Brain-to-Plasma Concentration Ratio and Unbound Partition Coefficient. , 2022, , 217-222.		0
141	Drug Metabolism. , 2022, , 362-368.		0