Alan Talevi

List of Publications by Year
in descending order

141 papers	1,947 citations	257450 24 h-index	302126 39 g-index
152 all docs	152 docs citations	152 times ranked	2556 citing authors

#	Article	IF	Citations
1	Potential medicinal effects and applications of stevia constituents. Phytochemistry Reviews, 2022, 21, 161-178.	6.5	6
2	Free Drug Theory. , 2022, , 1-6.		0
3	Antiseizure medication discovery: Recent and future paradigm shifts. Epilepsia Open, 2022, 7, .	2.4	3
4	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.	5.4	3
5	Central Nervous System Bioavailability. , 2022, , 233-242.		0
6	Drug Metabolism Functionalization (Phase I) Reactions. , 2022, , 387-394.		0
7	In Silico ADME: QSPR/QSAR. , 2022, , 525-531.		0
8	Site of Metabolism Predictions. , 2022, , 1073-1081.		0
9	Brain-to-Plasma Concentration Ratio and Unbound Partition Coefficient. , 2022, , 217-222.		0
10	Drug Metabolism. , 2022, , 362-368.		0
11	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.	5.4	7
12	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.	5.4	9
13	New anticonvulsant candidates prevent P-glycoprotein (P-gp) overexpression in a pharmacoresistant seizure model in mice. Epilepsy and Behavior, 2021, 121, 106451.	1.7	16
14	Can drug repurposing strategies be the solution to the COVID-19 crisis?. Expert Opinion on Drug Discovery, 2021, 16, 605-612.	5.0	19
15	Free Diffusion in Drug Absorption. , 2021, , 1-7.		0
16	Phase 0 and Phase III Transport. , 2021, , 1-8.		0
17	Drug Repurposing. , 2021, , .		4
18	Drug Distribution. , 2021, , 1-9.		0

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19	Transcytosis in Drug Absorption and Distribution. , 2021, , 1-7.		0
20	Drug Metabolism Functionalization (Phase I) Reactions. , 2021, , 1-7.		0
21	Drug Binding to Plasma Proteins. , 2021, , 1-12.		0
22	Zero-Order Drug Release. , 2021, , 1-6.		0
23	Active and Facilitated Transport in Drug Absorption. , 2021, , 1-7.		0
24	Central Nervous System Bioavailability. , 2021, , 1-10.		0
25	Free Drug Theory. , 2021, , 1-6.		1
26	Renal Drug Excretion. , 2021, , 1-7.		0
27	Peptide Transporters. , 2021, , 1-7.		0
28	Intestinal Perfusion Models. , 2021, , 1-9.		0
29	Drug Metabolism Synthetic (Phase II) Reactions. , 2021, , 1-8.		0
30	pKa Determination. , 2021, , 1-6.		0
31	Biorelevant Dissolution Media. , 2021, , 1-10.		0
32	Brain-to-Plasma Concentration Ratio and Unbound Partition Coefficient. , 2021, , 1-6.		0
33	Solute Carrier (SLC) Transporters: An Overview. , 2021, , 1-6.		1
34	Drug Release. , 2021, , 1-7.		5
35	Drug Absorption. , 2021, , 1-7.		0
36	Korsmeyer-Peppas, Peppas-Sahlin, and Brazel-Peppas: Models of Drug Release. , 2021, , 1-9.		1

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37	Cytochrome P450. , 2021, , 1-8.		0
38	Editorial: Lipid Nanoparticles as a Novel Strategy to Deliver Bioactive Molecules. Frontiers in Chemistry, 2021, 9, 655480.	3.6	1
39	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.	3.0	6
40	Ensemble learning application to discover new trypanothione synthetase inhibitors. Molecular Diversity, 2021, 25, 1361-1373.	3.9	2
41	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.	5.4	32
42	Drug Metabolism. , 2021, , 1-7.		0
43	Site of Metabolism Predictions. , 2021, , 1-9.		0
44	Unbound Brain-to-PlasmaÂPartition Coefficient Determination. , 2021, , 1-8.		0
45	Drug Excretion. , 2021, , 1-6.		0
46	Enzyme Induction and Drug Metabolism. , 2021, , 1-7.		0
47	Personalized Medicine and Drug Metabolism. , 2021, , 1-5.		0
48	Enterohepatic Recycling. , 2021, , 1-9.		1
49	Real and Apparent Volumes of Distribution. , 2021, , 1-9.		0
50	One-Compartment Pharmacokinetic Model. , 2021, , 1-8.		4
51	Organic Cation Transporters. , 2021, , 1-6.		0
52	Homology Modeling and Molecular Dynamics Simulations of Trypanosoma cruzi Phosphodiesterase b1. Chemistry and Biodiversity, 2021, , .	2.1	3
53	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.	5.2	13
54	Machine Learning in Drug Discovery and Development Part 1: A Primer. CPT: Pharmacometrics and Systems Pharmacology, 2020, 9, 129-142.	2.5	38

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55	Challenges and opportunities with drug repurposing: finding strategies to find alternative uses of therapeutics. Expert Opinion on Drug Discovery, 2020, 15, 397-401.	5.0	168
56	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.	2.9	11
57	Trypanosomatid-Caused Conditions: State of the Art of Therapeutics and Potential Applications of Lipid-Based Nanocarriers. Frontiers in Chemistry, 2020, 8, 601151.	3.6	9
58	Parabens inhibit hNaV 1.2 channels. Biomedicine and Pharmacotherapy, 2020, 128, 110250.	5.6	6
59	Cannabidiol (CBD) Inhibited Rhodamine-123 Efflux in Cultured Vascular Endothelial Cells and Astrocytes Under Hypoxic Conditions. Frontiers in Behavioral Neuroscience, 2020, 14, 32.	2.0	18
60	The Efficiency of Multi-target Drugs: A Network Approach. Human Perspectives in Health Sciences and Technology, 2020, , 63-75.	0.4	2
61	In Silico Drug Repositioning for Chagas Disease. Current Medicinal Chemistry, 2020, 27, 662-675.	2.4	12
62	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.	2.4	0
63	In silico Guided Drug Repurposing: Discovery of New Competitive and Non-competitive Inhibitors of Falcipain-2. Frontiers in Chemistry, 2019, 7, 534.	3.6	23
64	Hybrid Ofloxacin/eugenol co-loaded solid lipid nanoparticles with enhanced and targetable antimicrobial properties. International Journal of Pharmaceutics, 2019, 569, 118575.	5.2	46
65	Combined therapy with Benznidazole and repurposed drugs Clofazimine and Benidipine for chronic Chagas disease. European Journal of Medicinal Chemistry, 2019, 184, 111778.	5.5	4
66	Quantitative structureâ€“activity relationship models for compounds with anticonvulsant activity. Expert Opinion on Drug Discovery, 2019, 14, 653-665.	5.0	8
67	In Silico Modeling of FDA-Approved Drugs for Discovery of Therapies Against Neglected Diseases: A Drug Repurposing Approach. , 2019, , 625-648.		4
68	The Thiol-polyamine Metabolism of Trypanosoma cruzi: Molecular Targets and Drug Repurposing Strategies. Current Medicinal Chemistry, 2019, 26, 6614-6635.	2.4	22
69	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.	0.5	0
70	Computer-Aided Drug Design: An Overview. Methods in Molecular Biology, 2018, 1762, 1-19.	0.9	25
71	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.	5.5	15
72	Beneficial Effects of Stevia rebaudiana Bertoni and Steviol-Related Compounds on Health. Reference Series in Phytochemistry, 2018, , 263-284.	0.4	3

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73	Drug repositioning: current approaches and their implications in the precision medicine era. Expert Review of Precision Medicine and Drug Development, 2018, 3, 49-61.	0.7	48
74	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.	5.0	63
75	The application of molecular topology for ulcerative colitis drug discovery. Expert Opinion on Drug Discovery, 2018, 13, 89-101.	5.0	2
76	Computer-aided search of novel inhibitors of n-myristoyl transferase with trypanocidal effects. International Journal of Infectious Diseases, 2018, 73, 311.	3.3	0
77	Introduction. Biopharmaceutics and Pharmacokinetics. , 2018, , 3-10.		2
78	Drug Transporters. , 2018, , 331-348.		0
79	Drug Absorption. , 2018, , 11-31.		0
80	Drug Distribution. , 2018, , 33-53.		2
81	Drug Metabolism. , 2018, , 55-80.		0
82	Drug Excretion. , 2018, , 81-96.		2
83	Cascade Ligand- and Structure-Based Virtual Screening to Identify New Trypanocidal Compounds Inhibiting Putrescine Uptake. Frontiers in Cellular and Infection Microbiology, 2018, 8, 173.	3.9	22
84	Modern Approaches for the Discovery of Anti-Infectious Drugs for the Treatment of Neglected Diseases. Current Topics in Medicinal Chemistry, 2018, 18, 369-381.	2.1	7
85	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.	2.1	3
86	Propylparaben applied after pilocarpine-induced status epilepticus modifies hippocampal excitability and glutamate release in rats. NeuroToxicology, 2017, 59, 110-120.	3.0	15
87	Anticonvulsant effect of sodium cyclamate and propylparaben on pentylenetetrazolâ€induced seizures in zebrafish. Synapse, 2017, 71, e21961.	1.2	12
88	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.	5.8	26
89	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.	5.4	17
90	Editorial (Thematic Issue: Targeted Therapies). Mini-Reviews in Medicinal Chemistry, 2017, 17, 186-187.	2.4	1

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91	Hybrid Compounds as Anti-infective Agents. Current Topics in Medicinal Chemistry, 2017, 17, 1080-1095.	2.1	11
92	Interaction of Solid Lipid Nanoparticles and Specific Proteins of the Corona Studied by Surface Plasmon Resonance. Journal of Nanomaterials, 2017, 2017, 1-11.	2.7	17
93	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.	2.4	12
94	Integrated Application of Enhanced Replacement Method and Ensemble Learning for the Prediction of BCRP/ABCG2 Substrates. Current Bioinformatics, 2017, 12, 239-248.	1.5	4
95	An Introduction toÂPharmacokinetics. , 2017, , 13-46.		0
96	Novel cruzipain inhibitors for the chemotherapy of chronic Chagas disease. International Journal of Antimicrobial Agents, 2016, 48, 91-95.	2.5	26
97	Virtual Screening Applications in the Search of Novel Antiepileptic Drug Candidates. Methods in Pharmacology and Toxicology, 2016, , 237-258.	0.2	1
98	Network Pharmacology and Epilepsy. Methods in Pharmacology and Toxicology, 2016, , 351-364.	0.2	1
99	The Importance of Drug Repurposing in the Field of Antiepileptic Drug Development. Methods in Pharmacology and Toxicology, 2016, , 365-377.	0.2	1
100	Computational approaches for innovative antiepileptic drug discovery. Expert Opinion on Drug Discovery, 2016, 11, 1001-1016.	5.0	13
101	Beneficial Effects of Stevia rebaudiana Bertoni and Steviol-Related Compounds on Health. Reference Series in Phytochemistry, 2016, , 1-22.	0.4	1
102	Discovery of novel polyamine analogs with anti-protozoal activity by computer guided drug repositioning. Journal of Computer-Aided Molecular Design, 2016, 30, 305-321.	2.9	39
103	Sulfamide derivatives with selective carbonic anhydrase VII inhibitory action. Bioorganic and Medicinal Chemistry, 2016, 24, 894-901.	3.0	22
104	Tailored Multi-Target Agents. Applications and Design Considerations. Current Pharmaceutical Design, 2016, 22, 3164-3170.	1.9	15
105	Neglected Tropical Protozoan Diseases: Drug Repositioning as a Rational Option. Current Topics in Medicinal Chemistry, 2016, 16, 2201-2222.	2.1	37
106	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.	2.1	15
107	Multi-target pharmacology: possibilities and limitations of the â€œskeleton key approachâ€•from a medicinal chemist perspective. Frontiers in Pharmacology, 2015, 6, 205.	3.5	250
108	Computer-guided drug repurposing: Identification of trypanocidal activity of clofazimine, benidipine and saquinavir. European Journal of Medicinal Chemistry, 2015, 93, 338-348.	5.5	63

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109	Computer-Aided Identification of Anticonvulsant Effect of Natural Nonnutritive Sweeteners Stevioside and Rebaudioside A. Assay and Drug Development Technologies, 2015, 13, 313-318.	1.2	9
110	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.	1.1	1
111	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.	1.1	4
112	High-throughput Drug Repositioning for the Discovery of New Treatments for Chagas Disease. Mini-Reviews in Medicinal Chemistry, 2015, 15, 182-193.	2.4	22
113	Recent Patents on Polymeric Nanosystems Applications for Anticancer Drug Delivery. , 2015, , 524-601.		0
114	Recent Patents on Nanosystems Applications to Anticancer Drug Therapy: Lipid-based Systems. , 2015, , 602-659.		0
115	Identification of Levothyroxine Antichagasic Activity through Computer-Aided Drug Repurposing. Scientific World Journal, The, 2014, 2014, 1-9.	2.1	19
116	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.	5.4	36
117	Development of Conformation Independent Computational Models for the Early Recognition of Breast Cancer Resistance Protein Substrates. BioMed Research International, 2013, 2013, 1-12.	1.9	13
118	Applications of Nanosystems to Anticancer Drug Therapy (Part II. Dendrimers, Micelles, Lipid-based) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.6	29
119	On the Development of New Antiepileptic Drugs for the Treatment of Pharmacoresistant Epilepsy: Different Approaches to Different Hypothesis. , 2013, , 207-224.		8
120	Applications of Nanosystems to Anticancer Drug Therapy (Part I. Nanogels, Nanospheres,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 302 Td	1.6	19
121	CNS Drug Development â€“ Lost in Translation?. Mini-Reviews in Medicinal Chemistry, 2012, 12, 959-970.	2.4	28
122	An Integrated Drug Development Approach Applying Topological Descriptors. Current Computer-Aided Drug Design, 2012, 8, 172-181.	1.2	40
123	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.	5.4	14
124	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.	2.2	32
125	Dissolution Studies of Generic Medications: New Evidence of Deviations from the Transitivity Principle. Dissolution Technologies, 2012, 19, 13-24.	0.6	3
126	Recent Studies on Similarity Measures and its Applications to Chemoinformatics and Drug Design. , 2012, , 272-297.		0

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127	Computer-Based Strategies Towards the Discovery of New Antiepileptic Agents. , 2012, , 99-118.		0
128	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.	3.2	31
129	Development of a highly specific ensemble of topological models for early identification of Pâ€glycoprotein substrates. Journal of Chemometrics, 2011, 25, 313-322.	1.3	7
130	Prediction of drug intestinal absorption by new linear and non-linear QSPR. European Journal of Medicinal Chemistry, 2011, 46, 218-228.	5.5	45
131	Editorial [Towards Responsible, Safe Self-Medication (Guest Editor: Alan Talevi)]. Current Drug Safety, 2010, 5, 314-314.	0.6	1
132	The New Patient and Responsible Self-Medication Practices: A Critical Review. Current Drug Safety, 2010, 5, 342-353.	0.6	3
133	Combined Virtual Screening Strategies. Current Computer-Aided Drug Design, 2009, 5, 23-37.	1.2	31
134	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.	1.4	20
135	New QSPR study for the prediction of aqueous solubility of drug-like compounds. Bioorganic and Medicinal Chemistry, 2008, 16, 7944-7955.	3.0	86
136	New similarity-based algorithm and its application to classification of anticonvulsant compounds. Journal of Enzyme Inhibition and Medicinal Chemistry, 2007, 22, 253-265.	5.2	2
137	Application of descriptors based on Lipinskiâ€™s rules in the QSPR study of aqueous solubilities. Bioorganic and Medicinal Chemistry, 2007, 15, 3711-3719.	3.0	39
138	Discovery of anticonvulsant activity of abietic acid through application of linear discriminant analysis. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 1684-1690.	2.2	48
139	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.	2.9	31
140	Application of linear discriminant analysis in the virtual screening of antichagasic drugs through trypanothione reductase inhibition. Molecular Diversity, 2006, 10, 361-375.	3.9	20
141	Virtual Screening. , 0, , 229-245.		3