Kemal Yelekci

List of Publications by Year
in descending order

57	1,575	394390 19	315719 38
papers	citations	h-index	g-index

57	57	57	2489
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Screening of novel and selective inhibitors for neuronal nitric oxide synthase (nNOS) via structure-based drug design techniques. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3607-3629.	3.5	4
2	Potential inhibitors of methionine aminopeptidase type II identified via structure-based pharmacophore modeling. Molecular Diversity, 2022, 26, 1005-1016.	3.9	3
3	Synthesis and molecular modeling of MetAP2 of thiosemicarbazides, 1,2,4-triazoles, thioethers derived from (S)-Naproxen as possible breast cancer agents. Journal of Molecular Structure, 2022, 1259, 132739.	3.6	6
4	Homology modeling and in silico design of novel and potential dual-acting inhibitors of human histone deacetylases HDAC5 and HDAC9 isozymes. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6396-6414.	3.5	87
5	Homology modeling of human GABA-AT and devise some novel and potent inhibitors via computer-aided drug design techniques. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4100-4110.	3.5	13
6	Drug repurposing for coronavirus (COVID-19): in silico screening of known drugs against coronavirus 3CL hydrolase and protease enzymes. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2980-2992.	3.5	284
7	New 2-Pyrazoline and Hydrazone Derivatives as Potent and Selective Monoamine Oxidase A Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 1989-2009.	6.4	20
8	Structure-based virtual screening for novel potential selective inhibitors of class IIa histone deacetylases for cancer treatment. Computational Biology and Chemistry, 2021, 92, 107491.	2.3	5
9	Discovery of novel isoform-selective histone deacetylases 5 and 9 inhibitors through combined ligand-based pharmacophore modeling, molecular mocking, and molecular dynamics simulations for cancer treatment. Journal of Molecular Graphics and Modelling, 2021, 106, 107937.	2.4	2
10	Examining the stability of binding modes of the co-crystallized inhibitors of human HDAC8 by molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1-10.	3.5	12
11	Crystallographic structure versus homology model: a case study of molecular dynamics simulation of human and zebrafish histone deacetylase 10. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4397-4406.	3.5	31
12	Synthesis, molecular modeling, inÂvivo study and anticancer activity against prostate cancer of (+) (S)-naproxen derivatives. European Journal of Medicinal Chemistry, 2020, 208, 112841.	5.5	21
13	Identification of potential inhibitors of human methionine aminopeptidase (type II) for cancer therapy: Structure-based virtual screening, ADMET prediction and molecular dynamics studies. Computational Biology and Chemistry, 2020, 86, 107244.	2.3	15
14	Synthesis, Anticancer Activity on Prostate Cancer Cell Lines and Molecular Modeling Studies of Flurbiprofen-Thioether Derivatives as Potential Target of MetAP (Type II). Medicinal Chemistry, 2020, 16, 735-749.	1.5	9
15	Synthesis, in silico studies and cytotoxicity evaluation of novel 1,3,4-oxadiazole derivatives designed as potential mPGES-1 inhibitors. Journal of Research in Pharmacy, 2020, 24, 436-451.	0.2	2
16	Synthesis, molecular modeling, in vivo study, and anticancer activity of 1,2,4â€triazole containing hydrazideâ€“hydrazones derived from (S)â€naproxen. Archiv Der Pharmazie, 2019, 352, e1800365.	4.1	44
17	Homology modeling of human histone deacetylase 10 and design of potential selective inhibitors. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3627-3636.	3.5	26
18	Absolute configuration and biological profile of pyrazoline enantiomers as MAO inhibitory activity. Chirality, 2019, 31, 21-33.	2.6	19

#	Article	IF	Citations
19	The design of potent HIV-1 integrase inhibitors by a combined approach of structure-based virtual screening and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4644-4650.	3.5	8
20	Human dopamine transporter: the first implementation of a combined in silico/in vitro approach revealing the substrate and inhibitor specificities. Journal of Biomolecular Structure and Dynamics, 2019, 37, 291-306.	3.5	8
21	Synthesis, Molecular Modelling and Antibacterial Activity Against Helicobacter pylori of Novel Diflunisal Derivatives as Urease Enzyme Inhibitors. Letters in Drug Design and Discovery, 2019, 16, 392-400.	0.7	6
22	Synthesis, anticancer activity, and molecular modeling of etodolacâ€thioether derivatives as potent methionine aminopeptidase (type II) inhibitors. Archiv Der Pharmazie, 2018, 351, e1700195.	4.1	16
23	Identification of potential isoform-selective histone deacetylase inhibitors for cancer therapy: a combined approach of structure-based virtual screening, ADMET prediction and molecular dynamics simulation assay. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3231-3245.	3.5	29
24	Pharmacophore-based virtual screening for identification of potential selective inhibitors of human histone deacetylase 6. Computational Biology and Chemistry, 2018, 77, 318-330.	2.3	16
25	Carboxylic acid derivatives display potential selectivity for human histone deacetylase 6: Structure-based virtual screening, molecular docking and dynamics simulation studies. Computational Biology and Chemistry, 2018, 75, 131-142.	2.3	20
26	Synthesis, Molecular Docking and Anticancer Activity of Diflunisal Derivatives as Cyclooxygenase Enzyme Inhibitors. Molecules, 2018, 23, 1969.	3.8	20
27	Investigation of Synthesis, Molecular Modeling and Monoaminoxidase Inhibitor Activity of a New 2-Pyrazoline Compound. Turk Hijiyen Ve Deneysel Biyoloji Dergisi Turkish Bulletin of Hygiene and Experimental Biology, 2018, 75, 253-264.	0.2	1
28	Corrected Panel-Reactive Antibody Positivity Rates for Hypersensitized Patients in Turkish Population With Calculated Panel-Reactive Antibody Software. Transplantation Proceedings, 2017, 49, 445-447.	0.6	2
29	Exploration of the binding pocket of histone deacetylases: the design of potent and isoform-selective inhibitors. Turkish Journal of Biology, 2017, 41, 901-918.	0.8	17
30	New Human Monoamine Oxidase A Inhibitors with Potential Anti- Depressant Activity: Design, Synthesis, Biological Screening and Evaluation of Pharmacological Activity. Combinatorial Chemistry and High Throughput Screening, 2017, 20, 461-473.	1.1	11
31	Design, Synthesis and hMAO Inhibitory Screening of Novel 2-Pyrazoline Analogues. Combinatorial Chemistry and High Throughput Screening, 2017, 20, 510-521.	1.1	7
32	Drug Design for CNS Diseases: Polypharmacological Profiling of Compounds Using Cheminformatic, 3D-QSAR and Virtual Screening Methodologies. Frontiers in Neuroscience, 2016, 10, 265.	2.8	62
33	Synthesis and Screening of Human Monoamine Oxidaseâ€A Inhibitor Effect of New 2â€Pyrazoline and Hydrazone Derivatives. Archiv Der Pharmazie, 2015, 348, 743-756.	4.1	20
34	Flavonoids from Sideritis Species: Human Monoamine Oxidase (hMAO) Inhibitory Activities, Molecular Docking Studies and Crystal Structure of Xanthomicrol. Molecules, 2015, 20, 7454-7473.	3.8	25
35	cisâ€cyclopropylamines as mechanismâ€based inhibitors of monoamine oxidases. FEBS Journal, 2015, 282, 3190-3198.	4.7	31
36	De Novo Design of Potent and Selective Neuronal Nitric Oxide Synthase (nNOS) Inhibitors by a Fragment-Based Approach. Journal of Pharmaceutical Chemistry, 2015, 1, 68.	0.2	0

#	Article	IF	Citations
37	Aryl butenoic acid derivatives as a new class of histone deacetylase inhibitors: synthesis, in vitro evaluation, and molecular docking studies. Turkish Journal of Chemistry, 2014, 38, 338-344.	1.2	2
38	Synthesis of some novel hydrazone and 2-pyrazoline derivatives: Monoamine oxidase inhibitory activities and docking studies. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 3278-3284.	2.2	44
39	In silico identification of novel and selective monoamine oxidase B inhibitors. Journal of Neural Transmission, 2013, 120, 853-858.	2.8	10
40	Synthesis, molecular modeling, and in vitro screening of monoamine oxidase inhibitory activities of some novel hydrazone derivatives. Journal of Neural Transmission, 2013, 120, 883-891.	2.8	13
41	Insights into the binding mode of new N-substituted pyrazoline derivatives to MAO-A: docking and quantum chemical calculations. Journal of Neural Transmission, 2013, 120, 859-862.	2.8	6
42	Evaluation of selective human MAO inhibitory activities of some novel pyrazoline derivatives. Journal of Neural Transmission, 2013, 120, 863-873.	2.8	13
43	Synthesis and molecular modeling of some novel hexahydroindazole derivatives as potent monoamine oxidase inhibitors. Bioorganic and Medicinal Chemistry, 2009, 17, 6761-6772.	3.0	34
44	Histone Deacetylase Inhibition Activity and Molecular Docking of (Eâ€Š)â€Resveratrol: Its Therapeutic Potential in Spinal Muscular Atrophy. Chemical Biology and Drug Design, 2009, 73, 355-364.	3.2	42
45	New pyrazoline bearing 4(3H)-quinazolinone inhibitors of monoamine oxidase: Synthesis, biological evaluation, and structural determinants of MAO-A and MAO-B selectivity. Bioorganic and Medicinal Chemistry, 2009, 17, 675-689.	3.0	133
46	Molecular modifications on carboxylic acid derivatives as potent histone deacetylase inhibitors: Activity and docking studies. Bioorganic and Medicinal Chemistry, 2009, 17, 5219-5228.	3.0	160
47	Thermal rearrangement of 2-acetoxy-2,6,6-trimethylbicyclo[3.1.0]hexane: Theoretical elucidation of the mechanism. Computational and Theoretical Chemistry, 2007, 814, 61-73.	1.5	2
48	Docking of novel reversible monoamine oxidase-B inhibitors: efficient prediction of ligand binding sites and estimation of inhibitors thermodynamic properties. Journal of Neural Transmission, 2007, 114, 725-732.	2.8	23
49	A computational study on the amine-oxidation mechanism of monoamine oxidase: Insight into the polar nucleophilic mechanism. Organic and Biomolecular Chemistry, 2006, 4, 646.	2.8	54
50	Docking studies on monoamine oxidase-B inhibitors: Estimation of inhibition constants (Ki) of a series of experimentally tested compounds. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 4438-4446.	2.2	49
51	Computer modeling of oxygen containing heptylamines as monoamine oxidase inactivators. Computational and Theoretical Chemistry, 2001, 572, 97-106.	1.5	11
52	Effect of The Locus of The Oxygen Atom in Amino Ethers on the Inactivation of Monoamine Oxidase B. Journal of Enzyme Inhibition and Medicinal Chemistry, 1998, 13, 31-39.	0.5	4
53	Observation of a Flavin Semiquinone in the Resting State of Monoamine Oxidase B by Electron Paramagnetic Resonance and Electron Nuclear Double Resonance Spectroscopyâ€,â€¡. Biochemistry, 1996, 35, 11085-11091.	2.5	30
54	Electron spin resonance studies of monoamine oxidase B. First direct evidence for a substrate radical intermediate. Journal of the American Chemical Society, 1989, 111, 1138-1140.	13.7	29

#	Article	IF	Citations
55	Thermal aromatization of alkylidenecyclopentenes and related hydrocarbons. Journal of Organic Chemistry, 1988, 53, 4357-4363.	3.2	9
56	In silico design of novel and highly selective lysine-specific histone demethylase inhibitors. Turkish Journal of Chemistry, 0, , .	1.2	5
57	Are Coumarin Derivatives The New Keys in Depression Treatment? In silico Key-lock Fitting Analysis of Coumarin Derivatives with Monoamine Oxidase-A. Journal of Pharmaceutical Chemistry, 0, 7, .	0.2	0