Kemal Yelekci

List of Publications by Citations

53 papers	1,227 citations	18 h-index	34 g-index
57 ext. papers	1,394 ext. citations	3.5 avg, IF	5.82 L-index

#	Paper	IF	Citations
53	Drug repurposing for coronavirus (COVID-19): screening of known drugs against coronavirus 3CL hydrolase and protease enzymes. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 2980-2992	3.6	216
52	Molecular modifications on carboxylic acid derivatives as potent histone deacetylase inhibitors: Activity and docking studies. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 5219-28	3.4	128
51	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, 675-89	3.4	117
50	Homology modeling and 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	3.6	80
49	Drug Design for CNS Diseases: Polypharmacological Profiling of Compounds Using Cheminformatic, 3D-QSAR and Virtual Screening Methodologies. *Frontiers in Neuroscience*, **2016**, 10, 265	5.1	49
48	A computational study on the amine-oxidation mechanism of monoamine oxidase: insight into the polar nucleophilic mechanism. *Organic and Biomolecular Chemistry*, **2006**, 4, 646-58	3.9	48
47	Docking studies on monoamine oxidase-B inhibitors: estimation of inhibition constants (K(i)) of a series of experimentally tested compounds. *Bioorganic and Medicinal Chemistry Letters*, **2005**, 15, 4438-46	2.9	45
46	Histone deacetylase inhibition activity and molecular docking of (e)-resveratrol: its therapeutic potential in spinal muscular atrophy. *Chemical Biology and Drug Design*, **2009**, 73, 355-64	2.9	38
45	Synthesis of some novel hydrazone and 2-pyrazoline derivatives: monoamine oxidase inhibitory activities and docking studies. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 3278-84	2.9	37
44	Synthesis and molecular modeling of some novel hexahydroindazole derivatives as potent monoamine oxidase inhibitors. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 6761-72	3.4	30
43	Observation of a flavin semiquinone in the resting state of monoamine oxidase B by electron paramagnetic resonance and electron nuclear double resonance spectroscopy. *Biochemistry*, **1996**, 35, 11085-91	3.2	28
42	cis-Cyclopropylamines as mechanism-based inhibitors of monoamine oxidases. *FEBS Journal*, **2015**, 282, 3190-8	5.7	26
41	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	16.4	26
40	Synthesis, molecular modeling, in vivo study, and anticancer activity of 1,2,4-triazole containing hydrazide-hydrazones derived from (S)-naproxen. *Archiv Der Pharmazie*, **2019**, 352, e1800365	4.3	25
39	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	3.6	20
38	Flavonoids from Sideritis Species: Human Monoamine Oxidase (hMAO) Inhibitory Activities, Molecular Docking Studies and Crystal Structure of Xanthomicrol. *Molecules*, **2015**, 20, 7454-73	4.8	20
37	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, 725-32	4.3	20

36	Homology modeling of human histone deacetylase 10 and design of potential selective inhibitors. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 3627-3636	3.6	20
35	Synthesis and Screening of Human Monoamine Oxidase-A Inhibitor Effect of New 2-Pyrazoline and Hydrazone Derivatives. *Archiv Der Pharmazie*, **2015**, 348, 743-56	4.3	18
34	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	3.6	17
33	Synthesis, anticancer activity, and molecular modeling of etodolac-thioether derivatives as potent methionine aminopeptidase (type II) inhibitors. *Archiv Der Pharmazie*, **2018**, 351, e1700195	4.3	15
32	Absolute configuration and biological profile of pyrazoline enantiomers as MAO inhibitory activity. *Chirality*, **2019**, 31, 21-33	2.1	15
31	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	3.6	15
30	Synthesis, Molecular Docking and Anticancer Activity of Diflunisal Derivatives as Cyclooxygenase Enzyme Inhibitors. *Molecules*, **2018**, 23,	4.8	12
29	Evaluation of selective human MAO inhibitory activities of some novel pyrazoline derivatives. *Journal of Neural Transmission*, **2013**, 120, 863-73	4.3	11
28	Computer modeling of oxygen containing heptylamines as monoamine oxidase inactivators. *Computational and Theoretical Chemistry*, **2001**, 572, 97-106		11
27	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	1.3	11
26	Synthesis, molecular modeling, in vivo study and anticancer activity against prostate cancer of (+) (S)-naproxen derivatives. *European Journal of Medicinal Chemistry*, **2020**, 208, 112841	6.8	11
25	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	3.6	10
24	Synthesis, molecular modeling, and in vitro screening of monoamine oxidase inhibitory activities of some novel hydrazone derivatives. *Journal of Neural Transmission*, **2013**, 120, 883-91	4.3	10
23	Exploration of the binding pocket of histone deacetylases: the design of potent and isoform-selective inhibitors. *Turkish Journal of Biology*, **2017**, 41, 901-918	3.1	9
22	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, 1751-1760	3.6	8
21	In silico identification of novel and selective monoamine oxidase B inhibitors. *Journal of Neural Transmission*, **2013**, 120, 853-8	4.3	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	3.6	7
19	New 2-Pyrazoline and Hydrazone Derivatives as Potent and Selective Monoamine Oxidase A Inhibitors. *Journal of Medicinal Chemistry*, **2021**, 64, 1989-2009	8.3	7

18	Pharmacophore-based virtual screening for identification of potential selective inhibitors of human histone deacetylase 6. *Computational Biology and Chemistry*, **2018**, 77, 318-330	3.6	7
17	Thermal aromatization of alkylidenecyclopentenes and related hydrocarbons. *Journal of Organic Chemistry*, **1988**, 53, 4357-4363	4.2	6
16	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	1.8	6
15	Design, Synthesis and hMAO Inhibitory Screening of Novel 2-Pyrazoline Analogues. *Combinatorial Chemistry and High Throughput Screening*, **2017**, 20, 510-521	1.3	6
14	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	3.6	5
13	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, 859-62	4.3	5
12	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	3.6	5
11	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, 31-9		4
10	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	0.8	4
9	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
8	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		2
7	Corrected Panel-Reactive Antibody Positivity Rates for Hypersensitized Patients in Turkish Population With Calculated Panel-Reactive Antibody Software. *Transplantation Proceedings*, **2017**, 49, 445-447	1.1	1
6	Structure-based virtual screening for novel potential selective inhibitors of class IIa histone deacetylases for cancer treatment. *Computational Biology and Chemistry*, **2021**, 92, 107491	3.6	1
5	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	2.8	1
4	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	3.4	1
3	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	Potential inhibitors of methionine aminopeptidase type II identified via structure-based pharmacophore modeling. *Molecular Diversity*, **2021**, 1	3.1	
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*, **2022**, 1-23	3.6	