

Nese Kurt-Yilmaz

List of Publications by Year in descending order

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59
papers

1,899
citations

279798

23
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302126

39
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all docs

67
docs citations

67
times ranked

2194
citing authors

#	ARTICLE	IF	CITATIONS
1	Deciphering the Molecular Mechanism of HCV Protease Inhibitor Fluorination as a General Approach to Avoid Drug Resistance. <i>Journal of Molecular Biology</i> , 2022, 434, 167503.	4.2	6
2	Defining the substrate envelope of SARS-CoV-2 main protease to predict and avoid drug resistance. <i>Nature Communications</i> , 2022, 13, .	12.8	63
3	Drug Design Strategies to Avoid Resistance in Direct-Acting Antivirals and Beyond. <i>Chemical Reviews</i> , 2021, 121, 3238-3270.	47.7	40
4	Crystal Structure of SARS-CoV-2 Main Protease in Complex with the Non-Covalent Inhibitor ML188. <i>Viruses</i> , 2021, 13, 174.	3.3	80
5	Inhibiting HTLV-1 Protease: A Viable Antiviral Target. <i>ACS Chemical Biology</i> , 2021, 16, 529-538.	3.4	12
6	Deciphering Complex Mechanisms of Resistance and Loss of Potency through Coupled Molecular Dynamics and Machine Learning. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2054-2064.	5.3	11
7	Introduction: Drug Resistance. <i>Chemical Reviews</i> , 2021, 121, 3235-3237.	47.7	53
8	Deciphering Antifungal Drug Resistance in <i>Pneumocystis jirovecii</i> DHFR with Molecular Dynamics and Machine Learning. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2537-2541.	5.4	6
9	Structural basis of substrate specificity in human cytidine deaminase family APOBEC3s. <i>Journal of Biological Chemistry</i> , 2021, 297, 100909.	3.4	14
10	Discovery of Quinoxaline-Based P1-P3 Macrocyclic NS3/4A Protease Inhibitors with Potent Activity against Drug-Resistant Hepatitis C Virus Variants. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 11972-11989.	6.4	15
11	Pan-3C Protease Inhibitor Rupintrivir Binds SARS-CoV-2 Main Protease in a Unique Binding Mode. <i>Biochemistry</i> , 2021, 60, 2925-2931.	2.5	21
12	Viral proteases: Structure, mechanism and inhibition. <i>The Enzymes</i> , 2021, 50, 301-333.	1.7	36
13	Molecular and Structural Mechanism of Pan-Genotypic HCV NS3/4A Protease Inhibition by Glecaprevir. <i>ACS Chemical Biology</i> , 2020, 15, 342-352.	3.4	11
14	Structural Analysis of Potent Hybrid HIV-1 Protease Inhibitors Containing Bis-tetrahydrofuran in a Pseudosymmetric Dipeptide Isostere. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 8296-8313.	6.4	6
15	Genome-scale in vivo CRISPR screen identifies RNLS as a target for beta cell protection in type 1 diabetes. <i>Nature Metabolism</i> , 2020, 2, 934-945.	11.9	53
16	Crystal Structure of a Soluble APOBEC3G Variant Suggests ssDNA to Bind in a Channel that Extends between the Two Domains. <i>Journal of Molecular Biology</i> , 2020, 432, 6042-6060.	4.2	12
17	A cross-reactive human IgA monoclonal antibody blocks SARS-CoV-2 spike-ACE2 interaction. <i>Nature Communications</i> , 2020, 11, 4198.	12.8	132
18	Optimizing the refinement of merohedrally twinned P61 HIV-1 protease-inhibitor cocrystal structures. <i>Acta Crystallographica Section D: Structural Biology</i> , 2020, 76, 302-310.	2.3	1

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19	Avoiding Drug Resistance by Substrate Envelope-Guided Design: Toward Potent and Robust HCV NS3/4A Protease Inhibitors. <i>MBio</i> , 2020, 11, .	4.1	15
20	HIV-1 Protease Inhibitors Incorporating Stereochemically Defined P2 ^{â€²} Ligands To Optimize Hydrogen Bonding in the Substrate Envelope. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 8062-8079.	6.4	21
21	Molecular Determinants of Epistasis in HIV-1 Protease: Elucidating the Interdependence of L89V and L90M Mutations in Resistance. <i>Biochemistry</i> , 2019, 58, 3711-3726.	2.5	15
22	Picomolar to Micromolar: Elucidating the Role of Distal Mutations in HIV-1 Protease in Conferring Drug Resistance. <i>ACS Chemical Biology</i> , 2019, 14, 2441-2452.	3.4	36
23	Target-Specific Prediction of Ligand Affinity with Structure-Based Interaction Fingerprints. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3679-3691.	5.4	16
24	Mechanism for APOBEC3G catalytic exclusion of RNA and non-substrate DNA. <i>Nucleic Acids Research</i> , 2019, 47, 7676-7689.	14.5	7
25	NMR and MD studies combined to elucidate inhibitor and water interactions of HIV-1 protease and their modulations with resistance mutations. <i>Journal of Biomolecular NMR</i> , 2019, 73, 365-374.	2.8	9
26	Structural Adaptation of Darunavir Analogues against Primary Mutations in HIV-1 Protease. <i>ACS Infectious Diseases</i> , 2019, 5, 316-325.	3.8	27
27	Structural Analysis of the Active Site and DNA Binding of Human Cytidine Deaminase APOBEC3B. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 637-647.	5.3	16
28	Mutations in Influenza A Virus Neuraminidase and Hemagglutinin Confer Resistance against a Broadly Neutralizing Hemagglutinin Stem Antibody. <i>Journal of Virology</i> , 2019, 93, .	3.4	37
29	Probing Structural Changes among Analogous Inhibitor-Bound Forms of HIV-1 Protease and a Drug-Resistant Mutant in Solution by Nuclear Magnetic Resonance. <i>Biochemistry</i> , 2018, 57, 1652-1662.	2.5	12
30	Hydration Structure and Dynamics of Inhibitor-Bound HIV-1 Protease. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2784-2796.	5.3	28
31	Mavyret: A Pan-Genotypic Combination Therapy for the Treatment of Hepatitis C Infection. <i>Biochemistry</i> , 2018, 57, 481-482.	2.5	9
32	HIV-1 Protease Uses Bi-Specific S2/S2 ^{â€²} Subsites to Optimize Cleavage of Two Classes of Target Sites. <i>Journal of Molecular Biology</i> , 2018, 430, 5182-5195.	4.2	13
33	Quinoxaline-Based Linear HCV NS3/4A Protease Inhibitors Exhibit Potent Activity against Drug Resistant Variants. <i>ACS Medicinal Chemistry Letters</i> , 2018, 9, 691-696.	2.8	16
34	Substrate sequence selectivity of APOBEC3A implicates intra-DNA interactions. <i>Scientific Reports</i> , 2018, 8, 7511.	3.3	47
35	T cell epitope engineering: an avian H7N9 influenza vaccine strategy for pandemic preparedness and response. <i>Human Vaccines and Immunotherapeutics</i> , 2018, 14, 2203-2207.	3.3	10
36	Structural analysis of the active site and DNA binding of human cytidine deaminase APOBEC3B. <i>FASEB Journal</i> , 2018, 32, 792.31.	0.5	0

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37	Crystal structure of APOBEC3A bound to single-stranded DNA reveals structural basis for cytidine deamination and specificity. <i>Nature Communications</i> , 2017, 8, 15024.	12.8	130
38	Hepatitis C Virus NS3/4A Protease Inhibitors Incorporating Flexible P2 Quinoxalines Target Drug Resistant Viral Variants. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 5699-5716.	6.4	36
39	Interdependence of Inhibitor Recognition in HIV-1 Protease. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2300-2309.	5.3	27
40	Dengue Virus NS2B/NS3 Protease Inhibitors Exploiting the Prime Side. <i>Journal of Virology</i> , 2017, 91, .	3.4	42
41	Elucidating the Interdependence of Drug Resistance from Combinations of Mutations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5671-5682.	5.3	27
42	Structural Determination of the Broadly Reactive Anti-IGHV1-69 Anti-idiotypic Antibody G6 and Its Idiotope. <i>Cell Reports</i> , 2017, 21, 3243-3255.	6.4	13
43	Structural and molecular analysis of a protective epitope of <scp>Lyme</scp> disease antigen <scp>OspA</scp> and antibody interactions. <i>Journal of Molecular Recognition</i> , 2017, 30, e2595.	2.1	8
44	Drug Resistance to HIV-1 Protease Inhibitors: Molecular Mechanisms and Substrate Coevolution. , 2017, , 535-544.		5
45	Improving Viral Protease Inhibitors to Counter Drug Resistance. <i>Trends in Microbiology</i> , 2016, 24, 547-557.	7.7	81
46	Dengue Protease Substrate Recognition: Binding of the Prime Side. <i>ACS Infectious Diseases</i> , 2016, 2, 734-743.	3.8	19
47	Molecular and Dynamic Mechanism Underlying Drug Resistance in Genotype 3 Hepatitis C NS3/4A Protease. <i>Journal of the American Chemical Society</i> , 2016, 138, 11850-11859.	13.7	55
48	Molecular Basis for Differential Patterns of Drug Resistance in Influenza N1 and N2 Neuraminidase. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 6098-6108.	5.3	20
49	Structural and Thermodynamic Effects of Macrocyclization in HCV NS3/4A Inhibitor MK-5172. <i>ACS Chemical Biology</i> , 2016, 11, 900-909.	3.4	39
50	The ssDNA Mutator APOBEC3A Is Regulated by Cooperative Dimerization. <i>Structure</i> , 2015, 23, 903-911.	3.3	79
51	Structural basis and distal effects of Gag substrate coevolution in drug resistance to HIV-1 protease. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 15993-15998.	7.1	40
52	HIV-1 Protease-Substrate Coevolution in Nelfinavir Resistance. <i>Journal of Virology</i> , 2014, 88, 7145-7154.	3.4	22
53	Drug Resistance Conferred by Mutations Outside the Active Site through Alterations in the Dynamic and Structural Ensemble of HIV-1 Protease. <i>Journal of the American Chemical Society</i> , 2014, 136, 11956-11963.	13.7	83
54	Drug Resistance Mutations Alter Dynamics of Inhibitor-Bound HIV-1 Protease. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3438-3448.	5.3	34

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55	Substrate Envelope-Designed Potent HIV-1 Protease Inhibitors to Avoid Drug Resistance. <i>Chemistry and Biology</i> , 2013, 20, 1116-1124.	6.0	52
56	Cooperative Effects of Drug-Resistance Mutations in the Flap Region of HIV-1 Protease. <i>ACS Chemical Biology</i> , 2013, 8, 513-518.	3.4	18
57	Structural and Thermodynamic Basis of Amprenavir/Darunavir and Atazanavir Resistance in HIV-1 Protease with Mutations at Residue 50. <i>Journal of Virology</i> , 2013, 87, 4176-4184.	3.4	26
58	Differential Flap Dynamics in Wild-Type and a Drug Resistant Variant of HIV-1 Protease Revealed by Molecular Dynamics and NMR Relaxation. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3452-3462.	5.3	55
59	Extreme Entropy-Enthalpy Compensation in a Drug-Resistant Variant of HIV-1 Protease. <i>ACS Chemical Biology</i> , 2012, 7, 1536-1546.	3.4	72