Structures of two coronavirus main proteases: implications for substrate binding and antiviral drug design

#	Paper	IF	Citations
352	.		
351	Crystal structures of the X-domains of a Group-1 and a Group-3 coronavirus reveal that ADP-ribose-binding may not be a conserved property. **2009**, 18, 6-16		33
350	A structural view of the inactivation of the SARS coronavirus main proteinase by benzotriazole esters. **2008**, 15, 597-606		68
349	Proteolytic processing of polyproteins 1a and 1ab between non-structural proteins 10 and 11/12 of Coronavirus infectious bronchitis virus is dispensable for viral replication in cultured cells. **2008**, 379, 175-80		41
348	Mechanism for controlling the dimer-monomer switch and coupling dimerization to catalysis of the severe acute respiratory syndrome coronavirus 3C-like protease. *Journal of Virology*, **2008**, 82, 4620-9	6.6	97
347	Structure of the main protease from a global infectious human coronavirus, HCoV-HKU1. *Journal of Virology*, **2008**, 82, 8647-55	6.6	60
346	Therapies for coronaviruses. Part 2: Inhibitors of intracellular life cycle. **2009**, 19, 415-31		20
345	Drug targets in severe acute respiratory syndrome (SARS) virus and other coronavirus infections. **2009**, 9, 223-45		34
344	Crystal structures of two coronavirus ADP-ribose-1″monophosphatases and their complexes with ADP-Ribose: a systematic structural analysis of the viral ADRP domain. *Journal of Virology*, **2009**, 83, 1083-92	6.6	44
343	Viral protease inhibitors. **2009**, 85-110		84
342	Liberation of SARS-CoV main protease from the viral polyprotein: N-terminal autocleavage does not depend on the mature dimerization mode. **2010**, 1, 59-74		40
341	Computational approaches for the discovery of cysteine protease inhibitors against malaria and SARS. **2010**, 6, 1-23		17
340	Profiling of substrate specificity of SARS-CoV 3CL. **2010**, 5, e13197		51
339	Essential covalent linkage between the chymotrypsin-like domain and the extra domain of the SARS-CoV main protease. **2010**, 148, 349-58		11
338	Functional and genetic studies of the substrate specificity of coronavirus infectious bronchitis virus 3C-like proteinase. *Journal of Virology*, **2010**, 84, 7325-36	6.6	20
337	The highly cited SARS research literature. **2010**, 36, 299-317		11
336	Mutation of Glu-166 blocks the substrate-induced dimerization of SARS coronavirus main protease. **2010**, 98, 1327-36		73

335	Insights into cleavage specificity from the crystal structure of foot-and-mouth disease virus 3C protease complexed with a peptide substrate. **2010**, 395, 375-89		47
334	Avian coronavirus infectious bronchitis virus susceptibility to botanical oleoresins and essential oils in vitro and in vivo. **2010**, 149, 86-94		32
333	Update 1 of: Proteases universally recognize beta strands in their active sites. **2010**, 110, PR1-31		129
332	Inhibitors of SARS-3CLpro: virtual screening, biological evaluation, and molecular dynamics simulation studies. **2011**, 51, 1376-92		28
331	Expression, crystallization and preliminary crystallographic study of the C-terminal half of nsp2 from SARS coronavirus. **2011**, 67, 790-3		2
330	Characterization of Bafinivirus main protease autoprocessing activities. *Journal of Virology*, **2011**, 85, 1348-59	6.6	17
329	Dynamically-driven inactivation of the catalytic machinery of the SARS 3C-like protease by the N214A mutation on the extra domain. **2011**, 7, e1001084		27
328	Temperature-sensitive mutants and revertants in the coronavirus nonstructural protein 5 protease (3CLpro) define residues involved in long-distance communication and regulation of protease activity. *Journal of Virology*, **2012**, 86, 4801-10	6.6	25
327	From head to toe of the norovirus 3C-like protease. **2012**, 3, 41-56		0
326	Structural basis of evasion of cellular adaptive immunity by HIV-1 Nef. **2012**, 19, 701-6		107
325	The newly emerged SARS-like coronavirus HCoV-EMC also has an "AchillesΡheel": current effective inhibitor targeting a 3C-like protease. **2013**, 4, 248-50		111
324	Discovery of N-(benzo[1,2,3]triazol-1-yl)-N-(benzyl)acetamido)phenyl) carboxamides as severe acute respiratory syndrome coronavirus (SARS-CoV) 3CLpro inhibitors: identification of ML300 and noncovalent nanomolar inhibitors with an induced-fit binding. **2013**, 23, 6172-7		76
323	From SARS to MERS: 10 years of research on highly pathogenic human coronaviruses. *Antiviral Research*, **2013**, 100, 286-95	10.8	226
322	Discovery, synthesis, and structure-based optimization of a series of N-(tert-butyl)-2-(N-arylamido)-2-(pyridin-3-yl) acetamides (ML188) as potent noncovalent small molecule inhibitors of the severe acute respiratory syndrome coronavirus (SARS-CoV) 3CL protease. **2013**, 56, 534-46		130
321	Chimeric exchange of coronavirus nsp5 proteases (3CLpro) identifies common and divergent regulatory determinants of protease activity. *Journal of Virology*, **2013**, 87, 12611-8	6.6	71
320	Mechanism for controlling the monomer-dimer conversion of SARS coronavirus main protease. **2013**, 69, 747-55		21
319	Assessing activity and inhibition of Middle East respiratory syndrome coronavirus papain-like and 3C-like proteases using luciferase-based biosensors. *Journal of Virology*, **2013**, 87, 11955-62	6.6	105
318	Dynamically-driven enhancement of the catalytic machinery of the SARS 3C-like protease by the S284-T285-I286/A mutations on the extra domain. **2014**, 9, e101941		45

317	Structural insights into 5'flap DNA unwinding and incision by the human FAN1 dimer. **2014**, 5, 5726		23
316	Crystallization and preliminary crystallographic study of Porcine epidemic diarrhea virus main protease in complex with an inhibitor. **2014**, 70, 1608-11		
315	BacMam virus-based surface display of the infectious bronchitis virus (IBV) S1 glycoprotein confers strong protection against virulent IBV challenge in chickens. **2014**, 32, 664-70		25
314	Atlas of coronavirus replicase structure. **2014**, 194, 49-66		45
313	Identification of novel drug scaffolds for inhibition of SARS-CoV 3-Chymotrypsin-like protease using virtual and high-throughput screenings. **2014**, 22, 167-77		37
312	Coronaviruses resistant to a 3C-like protease inhibitor are attenuated for replication and pathogenesis, revealing a low genetic barrier but high fitness cost of resistance. *Journal of Virology*, **2014**, 88, 11886-98	6.6	61
311	Evidence for substrate binding-induced zwitterion formation in the catalytic Cys-His dyad of the SARS-CoV main protease. **2014**, 53, 5930-46		59
310	Potential Broad Spectrum Inhibitors of the Coronavirus 3CLpro: A Virtual Screening and Structure-Based Drug Design Study. **2015**, 7, 6642-60		43
309	Critical Assessment of the Important Residues Involved in the Dimerization and Catalysis of MERS Coronavirus Main Protease. **2015**, 10, e0144865		31
308	Structures of the Middle East respiratory syndrome coronavirus 3C-like protease reveal insights into substrate specificity. **2015**, 71, 1102-11		63
307	The SARS-coronavirus papain-like protease: structure, function and inhibition by designed antiviral compounds. *Antiviral Research*, **2015**, 115, 21-38	10.8	472
306	Human coronavirus OC43 3CL protease and the potential of ML188 as a broad-spectrum lead compound: homology modelling and molecular dynamic studies. **2015**, 15, 8		9
305	Conformational Flexibility of a Short Loop near the Active Site of the SARS-3CLpro is Essential to Maintain Catalytic Activity. **2016**, 6, 20918		13
304	A mechanistic study on the inhibition of □chymotrypsin by a macrocyclic peptidomimetic aldehyde. **2016**, 14, 6970-8		9
303	SARS-CoV 3CL protease cleaves its C-terminal autoprocessing site by novel subsite cooperativity. **2016**, 113, 12997-13002		143
302	Structure of Main Protease from Human Coronavirus NL63: Insights for Wide Spectrum Anti-Coronavirus Drug Design. **2016**, 6, 22677		108
301	Porcine Epidemic Diarrhea Virus 3C-Like Protease Regulates Its Interferon Antagonism by Cleaving NEMO. *Journal of Virology*, **2016**, 90, 2090-101	6.6	97
300	Crystal Structure of Feline Infectious Peritonitis Virus Main Protease in Complex with Synergetic Dual Inhibitors. *Journal of Virology*, **2016**, 90, 1910-7	6.6	23

299 Michael Acceptor-Based Peptidomimetic Inhibitor of Main Protease from Porcine Epidemic Diarrhea Virus. **2017**, 60, 3212-3216 — 18

298 Porcine deltacoronavirus nsp5 inhibits interferon-Ωproduction through the cleavage of NEMO. **2017**, 502, 33-38 — 63

297 Identification of two antiviral inhibitors targeting 3C-like serine/3C-like protease of porcine reproductive and respiratory syndrome virus and porcine epidemic diarrhea virus. **2018**, 213, 114-122 — 13

296 Phosphoserine acidic cluster motifs bind distinct basic regions on the Ωsubunits of clathrin adaptor protein complexes. **2018**, 293, 15678-15690 — 8

295 Structural basis for catalysis and substrate specificity of a 3C-like cysteine protease from a mosquito mesonivirus. **2019**, 533, 21-33 — 5

294 The crystal structure of main protease from mouse hepatitis virus A59 in complex with an inhibitor. **2019**, 511, 794-799 — 15

293 Prediction of potential inhibitors of the dimeric SARS-CoV2 main proteinase through the MM/GBSA approach. **2020**, 101, 107762 — 14

292 A multi-stage virtual screening of FDA-approved drugs reveals potential inhibitors of SARS-CoV-2 main protease. **2020**, 1-12 — 6

291 Crystallographic and electrophilic fragment screening of the SARS-CoV-2 main protease. **2020**, 11, 5047 — 188

290 A perspective on potential target proteins of COVID-19: Comparison with SARS-CoV for designing new small molecules. **2020**, 104, 104326 — 12

289 Molecular Docking and ADMET Study of Bioactive Compounds of Against Main Protease of SARS-CoV2. **2020**, 49, 2999-2999 — 21

288 Alkaloids from as Potential Inhibitors of SARS-CoV-2 Viral Proteins: An Study. *BioMed Research International*, **2020**, 2020, 5324560 — 3 — 30

287 Porcine epidemic diarrhea virus: Molecular mechanisms of attenuation and vaccines. **2020**, 149, 104553 — 10

286 Structure-Based Virtual Screening to Discover Potential Lead Molecules for the SARS-CoV-2 Main Protease. **2020**, 60, 5781-5793 — 49

285 drug repurposing and molecular dynamics puzzled out potential SARS-CoV-2 main protease inhibitors. **2021**, 39, 5756-5767 — 30

284 Evolving geographic diversity in SARS-CoV2 and in silico analysis of replicating enzyme 3CL targeting repurposed drug candidates. **2020**, 18, 278 — 22

283 Minireview of progress in the structural study of SARS-CoV-2 proteins. **2020**, 1, 53-61 — 23

282 Determination of potential inhibitors based on isatin derivatives against SARS-CoV-2 main protease (m): a molecular docking, molecular dynamics and structure-activity relationship studies. **2020**, 1-19 — 24

281   screening and molecular dynamics of phytochemicals from Indian cuisine against SARS-CoV-2 M. **2020**, 1-15   2

280   Exploring the Mechanism of Covalent Inhibition: Simulating the Binding Free Energy of α-Ketoamide Inhibitors of the Main Protease of SARS-CoV-2. **2020**, 59, 4601-4608   23

279   Antiviral agents against COVID-19: structure-based design of specific peptidomimetic inhibitors of SARS-CoV-2 main protease.. **2020**, 10, 40244-40263   11

278   Crystallographic structure of wild-type SARS-CoV-2 main protease acyl-enzyme intermediate with physiological C-terminal autoprocessing site. **2020**, 11, 5877   60

277   Docking Characterization and Inhibitory Activity of Flavan-3-ols and Dimeric Proanthocyanidins Against the Main Protease Activity of SARS-Cov-2. **2020**, 11, 601316   33

276   Targeting SARS-CoV-2 Proteases and Polymerase for COVID-19 Treatment: State of the Art and Future Opportunities. **2020**,   57

275   Interactive Molecular Dynamics in Virtual Reality Is an Effective Tool for Flexible Substrate and Inhibitor Docking to the SARS-CoV-2 Main Protease. **2020**, 60, 5803-5814   16

274   Probing the Dynamic Structure-Function and Structure-Free Energy Relationships of the Coronavirus Main Protease with Biodynamics Theory. **2020**, 3, 1111-1143   8

273   Pharmacophore modelling of vanillin derivatives, favipiravir, chloroquine, hydroxychloroquine, monolaurin and tetrodotoxin as M inhibitors of severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2). **2020**, 13, 527   8

272   Dynamical properties of enzyme-substrate complexes disclose substrate specificity of the SARS-CoV-2 main protease as characterized by the electron density descriptors. **2020**, 22, 19069-19079   13

271   In-Silico approach for identification of effective and stable inhibitors for COVID-19 main protease (M) from flavonoid based phytochemical constituents of. **2021**, 39, 6265-6280   38

270   Structural basis of CD4 downregulation by HIV-1 Nef. **2020**, 27, 822-828   18

269   Targeting severe acute respiratory syndrome-coronavirus (SARS-CoV-1) with structurally diverse inhibitors: a comprehensive review.. **2020**, 10, 28287-28299   10

268   Molecular Binding Mechanism and Pharmacology Comparative Analysis of Noscapine for Repurposing against SARS-CoV-2 Protease. **2020**, 19, 4678-4689   30

267   Understanding Severe Acute Respiratory Syndrome Coronavirus 2 Replication to Design Efficient Drug Combination Therapies. **2020**, 63, 2-9   11

266   Recent Advances in Pathophysiology, Drug Development and Future Perspectives of SARS-CoV-2. **2020**, 8, 580202   19

265   Interaction of small molecules with the SARS-CoV-2 main protease in silico and in vitro validation of potential lead compounds using an enzyme-linked immunosorbent assay. **2020**, 89, 107408   23

264   Rational approach toward COVID-19 main protease inhibitors via molecular docking, molecular dynamics simulation and free energy calculation. **2020**, 10, 17716   52

263 GRL-0920, an Indole Chloropyridinyl Ester, Completely Blocks SARS-CoV-2 Infection. *MBio*, **2020**, 11,   7.8   34

262 Discovery of potent inhibitors for SARS-CoV-2 main protease by ligand-based/structure-based virtual screening, MD simulations, and binding energy calculations. **2020**, 22, 23099-23106   18

261 Computational insight of dexamethasone against potential targets of SARS-CoV-2. **2020**, 1-11   11

260 screening of plant-derived antivirals against main protease, 3CL and endoribonuclease, NSP15 proteins of SARS-CoV-2. **2020**, 1-15   15

259 Impact of Early Pandemic Stage Mutations on Molecular Dynamics of SARS-CoV-2 M. **2020**, 60, 5080-5102   38

258 Repurposing Drugs, Ongoing Vaccine, and New Therapeutic Development Initiatives Against COVID-19. **2020**, 11, 1258   61

257 Antitussive noscapine and antiviral drug conjugates as arsenal against COVID-19: a comprehensive chemoinformatics analysis. **2020**, 1-16   14

256 Progress in Developing Inhibitors of SARS-CoV-2 3C-Like Protease. **2020**, 8,   61

255 Identification of Host Cellular Protein Substrates of SARS-COV-2 Main Protease. **2020**, 21,   13

254 Recent Progress in the Drug Development Targeting SARS-CoV-2 Main Protease as Treatment for COVID-19. **2020**, 7, 616341   38

253 Plausible mechanisms explaining the role of cucurbitacins as potential therapeutic drugs against coronavirus 2019. **2020**, 21, 100484   6

252 Remdesivir Strongly Binds to Both RNA-Dependent RNA Polymerase and Main Protease of SARS-CoV-2: Evidence from Molecular Simulations. **2020**, 124, 11337-11348   32

251 Anisotine and amarogentin as promising inhibitory candidates against SARS-CoV-2 proteins: a computational investigation. **2020**, 1-11   22

250 Computer aided identification of potential SARS CoV-2 main protease inhibitors from diterpenoids and biflavonoids of leaves. **2020**, 1-16   11

249 Structural basis for the inhibition of SARS-CoV-2 main protease by antineoplastic drug carmofur. **2020**, 27, 529-532   234

248 In silico fight against novel coronavirus by finding chromone derivatives as inhibitor of coronavirus main proteases enzyme. **2020**, 31, 1-10   21

247 Discovery of New Hydroxyethylamine Analogs against 3CL Protein Target of SARS-CoV-2: Molecular Docking, Molecular Dynamics Simulation, and Structure-Activity Relationship Studies. **2020**, 60, 5754-5770   56

246 Structure of M from SARS-CoV-2 and discovery of its inhibitors. **2020**, 582, 289-293   1836

245	Interaction of the prototypical βketoamide inhibitor with the SARS-CoV-2 main protease active site in silico: Molecular dynamic simulations highlight the stability of the ligand-protein complex. **2020**, 87, 107292	38
244	Molecular Targets in the Chemotherapy of Coronavirus Infection. **2020**, 85, 523-530	6
243	Repurposing cefuroxime for treatment of COVID-19: a scoping review of studies. **2021**, 39, 4547-4554	17
242	Boceprevir, GC-376, and calpain inhibitors II, XII inhibit SARS-CoV-2 viral replication by targeting the viral main protease. **2020**, 30, 678-692	384
241	Current Status of COVID-19 Therapies and Drug Repositioning Applications. **2020**, 23, 101303	54
240	Structure-based drug designing and immunoinformatics approach for SARS-CoV-2. **2020**, 6, eabb8097	97
239	An approach for identification of novel inhibitors as potential therapeutics targeting COVID-19 main protease. **2021**, 39, 4304-4315	23
238	screening of FDA approved drugs reveals ergotamine and dihydroergotamine as potential coronavirus main protease enzyme inhibitors. **2020**, 27, 2674-2682	13
237	NBCZone: Universal three-dimensional construction of eleven amino acids near the catalytic nucleophile and base in the superfamily of (chymo)trypsin-like serine fold proteases. **2020**, 153, 399-411	4
236	Identification of potential inhibitors of three key enzymes of SARS-CoV2 using computational approach. **2020**, 122, 103848	33
235	Repurposing drugs against the main protease of SARS-CoV-2: mechanism-based insights supported by available laboratory and clinical data. **2020**, 16, 474-491	22
234	Possibility of HIV-1 protease inhibitors-clinical trial drugs as repurposed drugs for SARS-CoV-2 main protease: a molecular docking, molecular dynamics and binding free energy simulation study. **2021**, 39, 5368-5375	14
233	Potential inhibitors against 2019-nCoV coronavirus M protease from clinically approved medicines. **2020**, 47, 119-121	252
232	Structural and Evolutionary Analysis Indicate That the SARS-CoV-2 Mpro Is a Challenging Target for Small-Molecule Inhibitor Design. **2020**, 21,	93
231	Natural Bioactive Compounds from Fungi as Potential Candidates for Protease Inhibitors and Immunomodulators to Apply for Coronaviruses. **2020**, 25,	35
230	Molecular Investigation of SARS-CoV-2 Proteins and Their Interactions with Antiviral Drugs. **2020**, 12,	72
229	Machine learning using intrinsic genomic signatures for rapid classification of novel pathogens: COVID-19 case study. **2020**, 15, e0232391	266
228	Déjvu: Stimulating open drug discovery for SARS-CoV-2. **2020**, 25, 928-941	63

227	Novel 2019 coronavirus structure, mechanism of action, antiviral drug promises and rule out against its treatment. **2021**, 39, 3409-3418		275
226	Computational studies of drug repurposing and synergism of lopinavir, oseltamivir and ritonavir binding with SARS-CoV-2 protease against COVID-19. **2021**, 39, 2673-2678		247
225	Structural Basis of SARS-CoV-2- and SARS-CoV-Receptor Binding and Small-Molecule Blockers as Potential Therapeutics. **2021**, 61, 465-493		19
224	Screening Malaria-box compounds to identify potential inhibitors against SARS-CoV-2 M, using molecular docking and dynamics simulation studies. **2021**, 890, 173664		11
223	Synthesis, characterization and computational study on potential inhibitory action of novel azo imidazole derivatives against COVID-19 main protease (M: 6LU7). *Journal of Molecular Structure*, **2021**, 1225, 129230	3.4	15
222	Computational Intelligence Methods in COVID-19: Surveillance, Prevention, Prediction and Diagnosis. **2021**,		
221	Repurposing potential of FDA-approved and investigational drugs for COVID-19 targeting SARS-CoV-2 spike and main protease and validation by machine learning algorithm. **2021**, 97, 836-853		15
220	The main protease and RNA-dependent RNA polymerase are two prime targets for SARS-CoV-2. **2021**, 538, 63-71		11
219	Potential molecular targets of nonstructural proteins for the development of antiviral drugs against SARS-CoV-2 infection. **2021**, 133, 111035		9
218	The potential effects of clinical antidiabetic agents on SARS-CoV-2. **2021**, 13, 243-252		8
217	Potential SARS-CoV-2 main protease inhibitors. **2021**, 26, 804-816		52
216	Diamond Light Source: contributions to SARS-CoV-2 biology and therapeutics. **2021**, 538, 40-46		4
215	Union is strength: antiviral and anti-inflammatory drugs for COVID-19. **2021**, 26, 229-239		15
214	The recent outbreaks of human coronaviruses: A medicinal chemistry perspective. **2021**, 41, 72-135		15
213	COVID-19 drug repurposing: A review of computational screening methods, clinical trials, and protein interaction assays. **2021**, 41, 5-28		43
212	Ligand-Based Approaches for the Development of Drugs Against SARS-CoV-2. **2021**, 117		1
211	Inhibition mechanism and hot-spot prediction of nine potential drugs for SARS-CoV-2 M by large-scale molecular dynamic simulations combined with accurate binding free energy calculations. **2021**, 13, 8313-8332		4
210	Evaluation of drug repositioning by molecular docking of pharmaceutical resources available in the Brazilian healthcare system against SARS-CoV-2. **2021**, 23, 100539		6

191   Ginkgolic acid and anacardic acid are specific covalent inhibitors of SARS-CoV-2 cysteine proteases. **2021**, 11, 45   16

190   Protein structural heterogeneity: A hypothesis for the basis of proteolytic recognition by the main protease of SARS-CoV and SARS-CoV-2. **2021**, 182, 177-184   10

189   Structural insights of key enzymes into therapeutic intervention against SARS-CoV-2. **2021**, 213, 107690   2

188   A Blueprint for High Affinity SARS-CoV-2 Mpro Inhibitors from Activity-Based Compound Library Screening Guided by Analysis of Protein Dynamics. **2021**, 4, 1079-1095   15

187   Inhibition of S-protein RBD and hACE2 Interaction for Control of SARSCoV- 2 Infection (COVID-19). **2021**, 21, 689-703   3

186   Virtual Screening and Molecular Design of Potential SARS-COV-2 Inhibitors. **2021**, 76, 95-113   0

185   Diverse SARS-CoV-2 variants preceded the initial COVID-19 outbreak in Croatia. **2021**, 166, 1735-1739

184   Structure-based virtual screening, molecular dynamics and binding affinity calculations of some potential phytocompounds against SARS-CoV-2. **2021**, 1-18   7

183   Targeting novel structural and functional features of coronavirus protease nsp5 (3CL, M) in the age of COVID-19. **2021**, 102,   18

182   Is PF-00835231 a Pan-SARS-CoV-2 Mpro Inhibitor? A Comparative Study. **2021**, 26,   8

181   High Throughput Virtual Screening and Validation of a SARS-CoV-2 Main Protease Non-Covalent Inhibitor.   9

180   Computational guided approach for drug repurposing against SARS-CoV-2. **2021**, 16, 211-243   3

179   A novel conformational state for SARS-CoV-2 main protease.   3

178   Knowing and combating the enemy: a brief review on SARS-CoV-2 and computational approaches applied to the discovery of drug candidates. **2021**, 41,   6

177   Structural Basis of Potential Inhibitors Targeting SARS-CoV-2 Main Protease. **2021**, 9, 622898   75

176   Prevention of SARS-CoV-2 Proliferation with a Novel and Potent Main Protease Inhibitor by Docking, ADMET, MM-PBSA, and Molecular Dynamics Simulation. **2021**, 20, 305-322   3

175   Insights into SARS-CoV-2: Medicinal Chemistry Approaches to Combat Its Structural and Functional Biology. **2021**, 379, 23   2

174   An Updated Review on SARS-CoV-2 Main Proteinase (M): Protein Structure and Small-Molecule Inhibitors. **2021**, 21, 442-460   12

173 Molecular dynamics and in silico mutagenesis on the reversible inhibitor-bound SARS-CoV-2 main protease complexes reveal the role of lateral pocket in enhancing the ligand affinity. **2021**, 11, 7429   7

172 Recognition of Divergent Viral Substrates by the SARS-CoV-2 Main Protease.

171 Rutin: A Potential Antiviral for Repurposing as a SARS-CoV-2 Main Protease (Mpro) Inhibitor. **2021**, 16, 1934578X2199172   5

170 Multi-conformation representation of Mpro identifies promising candidates for drug repurposing against COVID-19. **2021**, 27, 128   4

169 Novel 1,2,3-Triazole Derivatives as Potential Inhibitors against Covid-19 Main Protease: Synthesis, Characterization, Molecular Docking and DFT Studies. **2021**, 6, 3468-3486   12

168 SARS-CoV-2 M: A Potential Target for Peptidomimetics and Small-Molecule Inhibitors. **2021**, 11,   30

167 Modeling the binding of protoporphyrin IX, verteporfin, and chlorin e6 to SARS-CoV-2 proteins. **2021**, 57, 1-9   5

166 Discovery of potent Covid-19 main protease inhibitors using integrated drug-repurposing strategy. **2021**, 68, 712-725   2

165 Epigallocatechin-3-gallate, an active ingredient of Traditional Chinese Medicines, inhibits the 3CLpro activity of SARS-CoV-2. **2021**, 176, 1-12   39

164 A higher flexibility at the SARS-CoV-2 main protease active site compared to SARS-CoV and its potentialities for new inhibitor virtual screening targeting multi-conformers. **2021**, 1-21   1

163 Virtual High Throughput Screening to find Suitable Inhibitors for SARSCoV- 2 Main Protease. **2021**, 19, 209-214

162 SARS-CoV-2 main protease inhibition by compounds isolated from Luffa cylindrica using molecular docking. **2021**, 40, 127972   4

161 Binding mode characterization of 13b in the monomeric and dimeric states of SARS-CoV-2 main protease using molecular dynamics simulations. **2021**, 1-19   3

160 The missing link: covalent linkages in structural models. **2021**, 77, 727-745   6

159 The Contribution of Biophysics and Structural Biology to Current Advances in COVID-19. **2021**, 50, 493-523   3

158 In silico analysis of selected components of grapefruit seed extract against SARS-CoV-2 main protease. **2021**, 5, 5-12   2

157 Discovery of SARS-CoV-2 Mpro Peptide Inhibitors from Modelling Substrate and Ligand Binding.   1

156 SARS-CoV-2: Origin, Evolution, and Targeting Inhibition. **2021**, 11, 676451   6

(2021-2021)

155 "Identification of Nafamostat and VR23 as COVID-19 drug candidates by targeting 3CL and PL.". *Journal of Molecular Structure*, **2021**, 1233, 130094 — 3.4 — 7

154 Novel Coronavirus Disease 2019 (COVID-19) Current Update: Perspective on Epidemiology, Diagnosis, Drug Targets and Vaccines. **2021**, 2, — 1

153 Virtual screening, ADMET profiling, PASS prediction, and bioactivity studies of potential inhibitory roles of alkaloids, phytosterols, and flavonoids against COVID-19 main protease (M). **2021**, 1-7 — 9

152 Target-based drug discovery, ADMET profiling and bioactivity studies of antibiotics as potential inhibitors of SARS-CoV-2 main protease (M). **2021**, 1-15 — 7

151 The interaction of the bioflavonoids with five SARS-CoV-2 proteins targets: An in silico study. **2021**, 134, 104464 — 1

150 Docking-based virtual screening and identification of potential COVID-19 main protease inhibitors from brown algae. **2021**, — 3

149 Structurally modified compounds of hydroxychloroquine, remdesivir and tetrahydrocannabinol against main protease of SARS-CoV-2, a possible hope for COVID-19: Docking and molecular dynamics simulation studies. **2021**, 335, 116185 — 14

148 Recognition of Divergent Viral Substrates by the SARS-CoV-2 Main Protease. **2021**, 7, 2591-2595 — 15

147 Discovery of Novel Small-Molecule Inhibitors of SARS-CoV-2 Main Protease as Potential Leads for COVID-19 Treatment. **2021**, 61, 4745-4757 — 3

146 Exploring the Binding Mechanism of PF-07321332 SARS-CoV-2 Protease Inhibitor through Molecular Dynamics and Binding Free Energy Simulations. **2021**, 22, — 20

145 Molecular Docking Analysis of the Phytochemicals from Tinospora Cordifolia as Potential Inhibitor Against Multi Targeted SARS-CoV-2 & Cytokine Storm. **2021**, 20, 559-580 — 0

144 Rutaretin1R(6?-sinapoylglucoside): promising inhibitor of COVID 19 m catalytic dyad from the leaves of miq (Pittosporaceae). **2021**, 1-17 — 2

143 Discovery of novel inhibitors of SARS-CoV-2 main protease. **2021**, 1-9 — 1

142 Mechanistic Insights into the Inhibition of SARS-CoV-2 Main Protease by Clovamide and Its Derivatives: In Silico Studies. **2021**, 1, 377-404 — 4

141 Chitosan derivatives: A suggestive evaluation for novel inhibitor discovery against wild type and variants of SARS-CoV-2 virus. **2021**, 187, 492-512 — 8

140 Crystal structures of human coronavirus NL63 main protease at different pH values. **2021**, 77, 348-355 — 2

139 Structural biology of SARS-CoV-2 and implications for therapeutic development. **2021**, 19, 685-700 — 38

138 New 1,2,3-Triazole Scaffold Schiff Bases as Potential Anti-COVID-19: Design, Synthesis, DFT-Molecular Docking, and Cytotoxicity Aspects. **2021**, 9, — 5

137	A cyclic peptide inhibitor of the SARS-CoV-2 main protease. **2021**, 221, 113530	5
136	Natural medicinal plant products as an immune-boosters: A possible role to lessen the impact of Covid-19. **2021**, 4, 100105	7
135	Discovery of SARS-CoV-2 M peptide inhibitors from modelling substrate and ligand binding. **2021**, 12, 13686-13703	14
134	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease.. **2021**, 12, 1513-1527	29
133	Molecular mechanism of inhibition of COVID-19 main protease by adrenoceptor agonists and adenosine deaminase inhibitors using methods. **2021**, 1-16	1
132	Expression and Functions of SARS Coronavirus Replicative Proteins. **2010**, 75-98	10
131	Computational Intelligence in Drug Repurposing for COVID-19. **2021**, 273-294	3
130	Druggable targets of SARS-CoV-2 and treatment opportunities for COVID-19. **2020**, 104, 104269	37
129	1,2,4 triazolo[1,5-a] pyrimidin-7-ones as novel SARS-CoV-2 Main protease inhibitors: In silico screening and molecular dynamics simulation of potential COVID-19 drug candidates. **2020**, 267, 106478	11
128	Unravelling lead antiviral phytochemicals for the inhibition of SARS-CoV-2 M enzyme through in silico approach. **2020**, 255, 117831	72
127	Glecaprevir and Maraviroc are high-affinity inhibitors of SARS-CoV-2 main protease: possible implication in COVID-19 therapy. **2020**, 40,	90
126	A pocket guide on how to structure SARS-CoV-2 drugs and therapies. **2020**, 48, 2625-2641	5
125	Dual inhibition of SARS-CoV-2 spike and main protease through a repurposed drug, rutin. **2020**, 1-13	8
124	Potential inhibitors for 2019-nCoV coronavirus M protease from clinically approved medicines.	35
123	Machine learning using intrinsic genomic signatures for rapid classification of novel pathogens: COVID-19 case study.	26
122	Structure of Mpro from COVID-19 virus and discovery of its inhibitors.	65
121	Structural and Evolutionary Analysis Indicate that the SARS-CoV-2 Mpro is an Inconvenient Target for Small-Molecule Inhibitors Design.	11
120	Structural basis for the inhibition of SARS-CoV-2 main protease by antineoplastic drug Carmofur.	7

119 | Boceprevir, GC-376, and calpain inhibitors II, XII inhibit SARS-CoV-2 viral replication by targeting the viral main protease. **2020**, | 15

118 | Structural Basis of CD4 Downregulation by HIV-1 Nef. | 0

117 | Crystallographic and electrophilic fragment screening of the SARS-CoV-2 main protease. | 9

116 | SARS-CoV-2 structural coverage map reveals state changes that disrupt host immunity. | 5

115 | Structure-Based Design of a Cyclic Peptide Inhibitor of the SARS-CoV-2 Main Protease. | 1

114 | SARS-CoV-2 3CLpro whole human proteome cleavage prediction and enrichment/depletion analysis. | 2

113 | Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. **2020**, | 2

112 | A blueprint for high affinity SARS-CoV-2 Mpro inhibitors from activity-based compound library screening guided by analysis of protein dynamics. | 0

111 | A comprehensive review on promising anti-viral therapeutic candidates identified against main protease from SARS-CoV-2 through various computational methods. **2020**, 18, 69 | 20

110 | Profiling of substrate specificities of 3C-like proteases from group 1, 2a, 2b, and 3 coronaviruses. **2011**, 6, e27228 | 48

109 | Therapeutic Targets and Computational Approaches on Drug Development for COVID-19. **2020**, 20, 2210-2220 | 11

108 | Computational studies of drugs for possible action against Covid-19 infections. **2020**, 10, 99-105 | 1

107 | A Computational Approach to Explore the Interaction of Semisynthetic Nitrogenous Heterocyclic Compounds with the SARS-CoV-2 Main Protease. **2020**, 11, | 4

106 | Comprehensive analysis of drugs to treat SARS-CoV-2 infection: Mechanistic insights into current COVID-19 therapies (Review). **2020**, 46, 467-488 | 86

105 | Structural basis of HIV-1 Vpu-mediated BST2 antagonism via hijacking of the clathrin adaptor protein complex 1. **2014**, 3, e02362 | 67

104 | Identification of therapeutic drugs against COVID-19 through computational investigation on drug repurposing and structural modification. **2020**, 34, 458-469 | 3

103 | **2020**, 3-15 | 4

102 | An outlook on suicide enzyme inhibition and drug design. 1 | 1

101	Pharmacological Significance of Hesperidin and Hesperetin, Two Citrus Flavonoids, as Promising Antiviral Compounds for Prophylaxis Against and Combating COVID-19. **2021**, 16, 1934578X2110425	7
100	Michaelis-like complex of SARS-CoV-2 main protease visualized by room-temperature X-ray crystallography. **2021**, 8, 973-979	5
99	Seven compounds from tumeric essential oil inhibits three key proteins involved in SARS-CoV-2 cell entry and replication in silico.	1
98	A Comprehensive Review about the Molecular Structure of Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2): Insights into Natural Products against COVID-19. **2021**, 13,	6
97	Crystal-structures-guided design of fragment-based drugs for inhibiting the main protease of SARS-CoV-2. **2021**,	3
96	Zingiber officinale: Ayurvedic Uses of the Plant and In Silico Binding Studies of Selected Phytochemicals With Mpro of SARS-CoV-2. **2021**, 16, 1934578X2110317	1
95	Viral Cysteine Peptidases and Cysteine Peptidase Inhibitors. 1	
94	Phosphoserine acidic cluster motifs in the cytoplasmic domains of transmembrane proteins bind distinct basic regions on the subunits of clathrin adaptor protein complexes.	
93	Identification of a critical horseshoe-shaped region in the nsp5 (Mpro, 3CLpro) protease interdomain loop (IDL) of coronavirus mouse hepatitis virus (MHV).	1
92	Coronavirus infection: principles of ethyotropic chemotherapy. **2020**, 18-39	
91	Flexibility and mobility of SARS-CoV-2-related protein structures.	1
90	Using serpins cysteine protease cross-specificity to possibly trap SARS-CoV-2 Mpro with reactive center loop chimera. **2020**, 134, 2235-2241	0
89	SARS-CoV-2: Potential Drug Targets and Its Virtual Screening. **2022**, 203-244	0
88	Screening of Kabasura Kudineer Chooranam against COVID-19 through Targeting of Main Protease and RNA-Dependent RNA Polymerase of SARS-CoV-2 by Molecular Docking Studies. **2021**, 5, 319-331	
87	Strategies for search of pharmacological drugs against SARS-CoV-2 on the base of studying the structural-genetic features of coronaviruses SARS-CoV, MERS-CoV and SARS-CoV-2. **2020**, 18, 269-296	0
86	Unveiling the Effect of Low pH on the SARS-CoV-2 Main Protease by Molecular Dynamics Simulations. **2021**, 13,	3
85	Identification and Development of Therapeutics for COVID-19. **2021**, e0023321	5
84	Determination the binding ability of N-acetyl cysteine and its derivatives with SARS-COV-2 main protease using molecular docking and molecular dynamics studies. **2021**, 93, 43-51	

83	Design of New Bis-triazolyl Structure for Identification of Inhibitory Activity on COVID-19 Main Protease by Molecular Docking Approach. *Journal of Molecular Structure*, **2021**, 1250, 131858	3.4	0
82	Phenylethanoid glycosides as a possible COVID-19 protease inhibitor: a virtual screening approach. **2021**, 27, 341		1
81	Probing the dynamic structure-function and structure-free energy relationships of the corona virus main protease with Biodynamics theory.		
80	Molecular dynamics and in silico mutagenesis on the reversible inhibitor-bound SARS-CoV-2 Main Protease complexes reveal the role of a lateral pocket in enhancing the ligand affinity.		
79	Discovery of five HIV nucleoside analog reverse-transcriptase inhibitors (NRTIs) as potent inhibitors against the RNA-dependent RNA polymerase (RdRp) of SARS-CoV and 2019-nCoV.		1
78	High-throughput Virtual Screening Web Service Development for SARS-CoV-2 Drug Design. **2020**,		0
77	In Silico Study of Pacific oyster Antiviral Polypeptides as Potential Inhibitory Compounds for SARS-CoV-2 Main Protease. **2020**, 11,		2
76	Approaches for the Treatment of SARS-CoV-2 Infection: A Pharmacologic View and Literature Review. **2020**, 19, 258-281		1
75	identification of promising inhibitor against RNA-dependent RNA polymerase target of SARS-CoV-2. **2021**, 10, 131-140		1
74	Viral proteases: Structure, mechanism and inhibition. **2021**, 50, 301-333		3
73	Structure-Function Characteristics of SARS-CoV-2 Proteases and Their Potential Inhibitors from Microbial Sources.. **2021**, 9,		4
72	High-Throughput Virtual Screening and Validation of a SARS-CoV-2 Main Protease Noncovalent Inhibitor. **2021**,		12
71	COVID-19 Syndrome: Nexus with Herbivory and Exposure Dynamics for Monitoring Livestock Welfare and Agro-Environment. **2021**, 13, 12381		
70	A Focus on Severe Acute Respiratory Syndrome (SARS) Coronavirus (SARS-CoVs) 1 and 2. **2022**, 449-485		
69	Analysis of flavonoid compounds of Orange (Citrus sp.) peel as anti-main protease of SARS-CoV-2: A molecular docking study. **2022**, 951, 012078		0
68	Structure-based identification of naphthoquinones and derivatives as novel inhibitors of main protease Mpro and papain-like protease PLpro of SARS-CoV-2.. **2022**,		1
67	SARS-CoV-2 main protease and papain-like protease inhibition by abietane-type diterpenes isolated from the branches of using molecular docking studies.. **2022**, 1-8		1
66	A Genetically encoded BRET-based SARS-CoV-2 Mpro protease activity sensor.		0

| 65 | De Novo In-silico Pharmacological Analysis of Herbal Phytoconstituents for COVID-19 Treatment. **2022**, 257-262 | | 1 |

| 64 | In silico studies on structural inhibition of SARS-CoV-2 main protease M by major secondary metabolites of Andrographis paniculata and Cinchona officinalis.. **2022**, 77, 1-17 | | 1 |

| 63 | Targeting Angiotensin-Converting Enzyme 2 (ACE2) for the Discovery of Anticoronaviral Drugs. **2022**, 03, | | |

| 62 | The Structure of the Porcine Deltacoronavirus Main Protease Reveals a Conserved Target for the Design of Antivirals.. **2022**, 14, | | 1 |

| 61 | A new inactive conformation of SARS-CoV-2 main protease.. **2022**, 78, 363-378 | | 5 |

| 60 | Genetic surveillance of SARS-CoV-2 Mpro reveals high sequence and structural conservation prior to the introduction of protease inhibitor Paxlovid. | | 0 |

| 59 | Implication of in silico studies in the search for novel inhibitors against SARS-CoV-2.. **2022**, e2100360 | | 1 |

| 58 | Computational Screening of Phenylamino-Phenoxy-Quinoline Derivatives against the Main Protease of SARS-CoV-2 Using Molecular Docking and the ONIOM Method.. **2022**, 27, | | 1 |

| 57 | Computational studies on the design of NCI natural products as inhibitors to SARS-CoV-2 main protease.. **2022**, 1-11 | | 0 |

| 56 | Harnessing the Natural Toxic Metabolites in COVID-19.. **2022**, 2022, 3954944 | | |

| 55 | SARS-CoV-2 3CLpro whole human proteome cleavage prediction and enrichment/depletion analysis.. **2022**, 98, 107671 | | 0 |

| 54 | Potential Resistance of SARS-CoV-2 Main Protease (Mpro) against Protease Inhibitors: Lessons Learned from HIV-1 Protease.. **2022**, 23, | | 7 |

| 53 | Repurposing dyphylline as a pan-coronavirus antiviral therapy.. **2022**, | | 0 |

| 52 | Label-free duplex SAMDI-MS screen reveals novel SARS-CoV-2 3CLpro inhibitors.. *Antiviral Research*, **2022**, 105279 | 10.8 | 0 |

| 51 | Synthesis, crystal structure, DFT and molecular docking studies of N-acetyl-2,4-[diaryl-3-azabicyclo[3.3.1]nonan-9-yl]-9-spiro-4Racetyl-2R(acetylamino)-4R9-dihydro-[1R3R4R]thiadiazoles: A potential SARS-nCoV-2 Mpro (COVID-19) inhibitor.. *Journal of Molecular Structure*, **2022**, 132747 | 3.4 | |

| 50 | Virtual Screening of Phytochemicals Targeting the Main Protease and Spike Protein of SARS-CoV-2: An In silico Approach. *Journal of Biomedical Research & Environmental Sciences*, **2021**, 2, 1121-1131 | 0.3 | 0 |

| 49 | The Inhibition of SARS-CoV-2 3CL M by Graphene and Its Derivatives from Molecular Dynamics Simulations.. *ACS Applied Materials & Interfaces*, **2021**, | 9.5 | 1 |

| 48 | Exploration of Luteolin as Potential Anti-COVID19 agent: Molecular Docking, Molecular Dynamic Simulation, ADMET and DFT analysis. *Letters in Drug Design and Discovery*, **2021**, 19, | 0.8 | 2 |

47   Investigation on the Impact of Potential Phytocompounds from Curcuma longa Against COVID-19. *Journal of Plant Sciences*, **2022**, 17, 33-52   0.2

46   Phillygenin activates PKR/eIF2 pathway and induces stress granule to exert anti-avian infectious bronchitis virus.. *International Immunopharmacology*, **2022**, 108, 108764   5.8

45   Data_Sheet_1.PDF. **2020**,

44   Inhibitory effect of thymoquinone from Nigella sativa against SARS-CoV-2 main protease. An in-silico study.. *Brazilian Journal of Biology*, **2022**, 84, e250667   1.5   2

43   A Proteomics-MM/PBSA Dual Approach for the Analysis of SARS-CoV-2 Main Protease Substrate Peptide Specificity. *Peptides*, **2022**, 170814   3.8

42   Natural compounds may contribute in preventing SARS-CoV-2 infection: a narrative review. *Food Science and Human Wellness*, **2022**, 11, 1134-1142   8.3   0

41   COVID-19 and the Importance of Being Prepared: A Multidisciplinary Strategy for the Discovery of Antivirals to Combat Pandemics. *Biomedicines*, **2022**, 10, 1342   4.8   1

40   Maturation of the SARS-CoV-2 virus is regulated by dimerization of its main protease. *Computational and Structural Biotechnology Journal*, **2022**,   6.8   0

39   Review on development of potential inhibitors of SARS-CoV-2 main protease (MPro). *Future Journal of Pharmaceutical Sciences*, **2022**, 8,   2.1   0

38   The Life of SARS-CoV-2 Inside Cells: Replication Transcription Complex Assembly and Function. *Annual Review of Biochemistry*, **2022**, 91, 381-401   29.1   0

37   Primer for Designing Main Protease (Mpro) Inhibitors of SARS-CoV-2. *Journal of Physical Chemistry Letters*, 5776-5786   6.4   0

36   Binding and unbinding pathways of peptide substrate on SARS-CoV-2 3CL protease.   0

35   Will the Use of Pharmacogenetics Improve Treatment Efficiency in COVID-19?. *Pharmaceuticals*, **2022**, 15, 739   5.2   2

34   Genomic, proteomic and metabolomic profiling of severe acute respiratory syndrome-Coronavirus-2. **2022**, 49-76

33   Paxlovid: Mechanism of Action, Synthesis, and In Silico Study. *BioMed Research International*, **2022**, 2022, 1-16   3   7

32   Large library docking for novel SARS-CoV-2 main protease non-covalent and covalent inhibitors.   0

31   The SARS-CoV-2 main protease (M pro): Structure, function, and emerging therapies for COVID-19. *MedComm*, **2022**, 3,   2.2   4

30   Genetic Surveillance of SARS-CoV-2 M pro Reveals High Sequence and Structural Conservation Prior to the Introduction of Protease Inhibitor Paxlovid. *MBio*,   7.8   3

29	Structure-Based Identification of Naphthoquinones and Derivatives as Novel Inhibitors of Main Protease Mpro and Papain-like Protease PLpro of SARS-CoV-2.	2
28	Multiple pathways for SARS-CoV-2 resistance to nirmatrelvir.	1
27	A yeast-based system to study SARS-CoV-2 Mpro structure and to identify nirmatrelvir resistant mutations.	
26	Proteolytic Processing of the Coronavirus Replicase Nonstructural Protein 14 Exonuclease Is Not Required for Virus Replication but Alters RNA Synthesis and Viral Fitness. **2022**, 96,	2
25	An integrated metabolomic and proteomic approach for the identification of covalent inhibitors of the main protease (Mpro) of SARS-COV-2 from crude natural extracts. **2023**, 252, 123824	
24	In Silico Evaluation of Sesquiterpenes and Benzoxazinoids Phytotoxins against Mpro, RNA Replicase and Spike Protein of SARS-CoV-2 by Molecular Dynamics. Inspired by Nature. **2022**, 14, 599	0
23	Structural and functional characterization of NEMO cleavage by SARS-CoV-2 3CLpro. **2022**, 13,	3
22	A computational insight on the inhibitory potential of 8-Hydroxydihydrosanguinarine (8-HDS), a pyridone containing analogue of sanguinarine, against SARS CoV2..	1
21	Individual and Synergistic Potential of Bioactive Compounds from Chrysopogon Zizanioides Against Main-Protease of SARSCov-2 using Computational Approach. **2022**, 19, 657-670	0
20	Antiviral activity of Cenostigma pluviosum var. peltophoroides extract and fractions against SARS-CoV-2. 1-12	1
19	A genetically encoded BRET-based SARS-CoV-2 Mpro protease activity sensor. **2022**, 5,	0
18	Decamethoxin virucidal activity: in vitro and in silico studies. **2022**, 94, 81-91	0
17	The Discovery of Small Allosteric and Active Site Inhibitors of the SARS-CoV-2 Main Protease via Structure-Based Virtual Screening and Biological Evaluation. **2022**, 27, 6710	1
16	Repositioning of anti-dengue compounds against SARS-CoV-2 as viral polyprotein processing inhibitor. **2022**, 17, e0277328	0
15	Multiple pathways for SARS-CoV-2 resistance to nirmatrelvir.	8
14	Identification of multi-targeting natural antiviral peptides to impede SARS-CoV-2 infection.	0
13	Functional dynamics of SARS-CoV-2 3C-like protease as a member of clan PA.	0
12	Binding and Unbinding Pathways of Peptide Substrates on the SARS-CoV-2 3CL Protease.	0

| 11 | Potential Inhibitors of SARS-CoV-2 Main Protease (Mpro) Identified from the Library of FDA-Approved Drugs Using Molecular Docking Studies. **2023**, 11, 85 | 0 |

| 10 | Artificial intelligence based virtual screening study for competitive and allosteric inhibitors of the SARS-CoV-2 main protease. 1-19 | 0 |

| 9 | Broad-spectrum coronavirus 3C-like protease peptidomimetic inhibitors effectively block SARS-CoV-2 replication in cells: Design, synthesis, biological evaluation, and X-ray structure determination. **2023**, 253, 115311 | 0 |

| 8 | Crystal Structures of Inhibitor-Bound Main Protease from Delta- and Gamma-Coronaviruses. | 0 |

| 7 | Repurposing of US-FDA approved drugs against SARS-CoV-2 main protease (Mpro) by using STD-NMR spectroscopy, in silico studies and antiviral assays. **2023**, 234, 123540 | 0 |

| 6 | Lessons Learnt from COVID-19: Computational Strategies for Facing Present and Future Pandemics. **2023**, 24, 4401 | 0 |

| 5 | Antitarget, Anti-SARS-CoV-2 Leads, Drugs, and the Drug Discovery–Genetics Alliance Perspective. **2023**, 66, 3664-3702 | 0 |

| 4 | In silico application of data science, genomics, and bioinformatics in screening drug candidates against COVID-19. **2023**, 107-128 | 0 |

| 3 | Crystal Structures of Inhibitor-Bound Main Protease from Delta- and Gamma-Coronaviruses. **2023**, 15, 781 | 0 |

| 2 | Impact of Drug Repurposing on SARS-Cov-2 Main Protease. **2022**, 96, 3311-3330 | 0 |

| 1 | An Investigation of the Antiviral Potential of Phytocompounds against Avian Infectious Bronchitis Virus through Template-Based Molecular Docking and Molecular Dynamics Simulation Analysis. **2023**, 15, 847 | 0 |