PatchDock and SymmDock: servers for rigid and symmetric docking

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#	Paper	IF	Citations
2265	How Can Interleukin1 Receptor Antagonist Modulate Distinct Cell Death Pathways?.		
2264	Calmidazolium Chloride and Its Complex with Serum Albumin Prevent Huntingtin Exon1 Aggregation.		
2263	Does Fungicide Dodine Unfold Protein like Kosmo-Chaotropic Agent?.		
2262	Molecular Insights into Human Serum Albumin as a Receptor of Amyloid- in the Extracellular Region.		
2261	QM/MM Studies of Dph5 A Promiscuous Methyltransferase in the Eukaryotic Biosynthetic Pathway of Diphthamide.		
2260	Assessment of CAPRI predictions in rounds 3-5 shows progress in docking procedures. **2005**, 60, 150-69		281
2259	GRAMM-X public web server for protein-protein docking. *Nucleic Acids Research*, **2006**, 34, W310-4	20.1	556
2258	Formation of a soluble stable complex between pristine C60-fullerene and a native blood protein. **2006**, 7, 1783-9		45
2257	Structural modeling of protein interactions by analogy: application to PSD-95. **2006**, 2, e153		36
2256	Computational identification of inhibitors of protein-protein interactions. **2007**, 7, 63-82		77
2255	Ligand binding and circular permutation modify residue interaction network in DHFR. **2007**, 3, e117		39
2254	Free resources to assist structure-based virtual ligand screening experiments. **2007**, 8, 381-411		91
2253	An allosteric rheostat in HIV-1 gp120 reduces CCR5 stoichiometry required for membrane fusion and overcomes diverse entry limitations. **2007**, 374, 64-79		21
2252	Molecular determinants for the recruitment of the ubiquitin-ligase MuRF-1 onto M-line titin. **2007**, 21, 1383-92		81
2251	Protein structure analysis online. **2007**, Chapter 2, Unit 2.13		1
2250	Assessing the energy landscape of CAPRI targets by FunHunt. **2007**, 69, 809-15		14
2249	Automatic prediction of protein interactions with large scale motion. **2007**, 69, 764-73		46

2248	Analysis on multi-domain cooperation for predicting protein-protein interactions. **2007**, 8, 391		29
2247	Transient occurrence of an ebulin-related D-galactose-lectin in shoots of Sambucus ebulus L. **2008**, 69, 857-64		12
2246	On the inhibitory affect of some dementia drugs on DNA polymerase Beta activity. **2008**, 33, 2187-96		4
2245	Protein-protein docking by simulating the process of association subject to biochemical constraints. **2008**, 71, 1955-69		24
2244	An iterative knowledge-based scoring function for protein-protein recognition. **2008**, 72, 557-79		156
2243	Metabolic stereoselectivity of cytochrome P450 3A4 towards deoxypodophyllotoxin: In silico predictions and experimental validation. **2008**, 43, 1171-9		18
2242	Proposed arrangement of proteins forming a bacterial type II polyketide synthase. **2008**, 15, 1156-65		7
2241	Protein-protein docking: overview and performance analysis. **2008**, 413, 283-314		19
2240	Towards the development of universal, fast and highly accurate docking/scoring methods: a long way to go. **2008**, 153 Suppl 1, S7-26		349
2239	Protein-protein interaction and quaternary structure. **2008**, 41, 133-80		296
2238	The RosettaDock server for local protein-protein docking. *Nucleic Acids Research*, **2008**, 36, W233-8	20.1	389
2237	Studies on flexibility and binding affinity of Asp25 of HIV-1 protease mutants. **2008**, 42, 386-91		31
2236	Human platelet 12-lipoxygenase, new findings about its activity, membrane binding and low-resolution structure. **2008**, 376, 193-209		54
2235	Crystal structure of ST2348, a CBS domain protein, from hyperthermophilic archaeon Sulfolobus tokodaii. **2008**, 375, 124-8		11
2234	Molecular dynamics simulation of the cooperative adsorption of barley lipid transfer protein and cis-isocohumulone at the vacuum-water interface. **2008**, 9, 3024-32		25
2233	Platelet endothelial cell adhesion molecule 1 (PECAM-1) and its interactions with glycosaminoglycans: 1. Molecular modeling studies. **2008**, 47, 4851-62		35
2232	A survey of available tools and web servers for analysis of protein-protein interactions and interfaces. **2009**, 10, 217-32		118
2231	FireDock: a web server for fast interaction refinement in molecular docking. *Nucleic Acids Research*, **2008**, 36, W229-32	20.1	469

2230	3D-Garden: a system for modelling protein-protein complexes based on conformational refinement of ensembles generated with the marching cubes algorithm. **2008**, 24, 1137-44		53
2229	. **2008**,		6
2228	Solution structure of the silkworm betaGRP/GNBP3 N-terminal domain reveals the mechanism for beta-1,3-glucan-specific recognition. **2009**, 106, 11679-84		50
2227	FRODOCK: a new approach for fast rotational protein-protein docking. **2009**, 25, 2544-51		101
2226	Solution structures of cytosolic RNA sensor MDA5 and LGP2 C-terminal domains: identification of the RNA recognition loop in RIG-I-like receptors. **2009**, 284, 17465-74		147
2225	Crystal structure of the N-terminal domain of the secretin GspD from ETEC determined with the assistance of a nanobody. **2009**, 17, 255-65		148
2224	Protein-protein docking using region-based 3D Zernike descriptors. **2009**, 10, 407		116
2223	Anti-idiotypic antibodies: a new approach in prion research. **2009**, 10, 16		6
2222	Protein-protein docking dealing with the unknown. **2010**, 31, 317-42		85
2221	Computational modelling of protein interactions: energy minimization for the refinement and scoring of association decoys. **2009**, 57, 419-28		2
2220	In silico identification of catalytic residues in azobenzene reductase from Bacillus subtilis and its docking studies with azo dyes. **2009**, 1, 290-7		11
2219	Structural basis for the resilience of Darunavir (TMC114) resistance major flap mutations of HIV-1 protease. **2009**, 1, 320-8		44
2218	Structure based mechanism of the Ca(2+)-induced release of coelenterazine from the Renilla binding protein. **2009**, 74, 583-93		16
2217	Evolutionary conservation in multiple faces of protein interaction. **2009**, 77, 14-25		49
2216	Alanine substitutions of noncysteine residues in the cysteine-stabilized alphabeta motif. **2009**, 18, 1498-506		9
2215	RosettaAntibody: antibody variable region homology modeling server. *Nucleic Acids Research*, **2009**, 37, W474-9	20.1	123
2214	Mechanistic investigation of the endo-alpha-N-acetylgalactosaminidase from Streptococcus pneumoniae R6. **2009**, 48, 10334-41		16
2213	Docking and scoring: applications to drug discovery in the interactomics era. **2009**, 4, 673-86		11

2212	N- and C-terminal domains in human holocarboxylase synthetase participate in substrate recognition. **2009**, 96, 183-8	22
2211	Modelling of the membrane receptor CXCR3 and its complexes with CXCL9, CXCL10 and CXCL11 chemokines: putative target for new drug design. **2009**, 47, 332-9	22
2210	Molecular modeling studies of the interaction between Plasmodium falciparum HslU and HslV subunits. **2009**, 26, 473-9	25
2209	Prediction of localization and interactions of apoptotic proteins. **2009**, 16, 59	7
2208	Pseudomonas aeruginosa MurE amide ligase: enzyme kinetics and peptide inhibitor. **2009**, 421, 263-72	20
2207	Parallel Decomposition of 3D Surfaces in Images of Local Descriptors for Molecular Screening. **2009** ,	1
2206	Preliminary kinetic analysis of acyl carrier protein-ketoacylsynthase interactions in the actinorhodin minimal polyketide synthase. **2009**, 5, 511-8	7
2205	Evaluation of geometric complementarity between molecular surfaces using compactly supported radial basis functions. **2009**, 6, 689-94	2
2204	Theoretical characterization of substrate access/exit channels in the human cytochrome P450 3A4 enzyme: involvement of phenylalanine residues in the gating mechanism. **2009**, 113, 13018-25	87
2203	Characterization of 3-ketosteroid 9{alpha}-hydroxylase, a Rieske oxygenase in the cholesterol degradation pathway of Mycobacterium tuberculosis. **2009**, 284, 9937-46	114
2202	Proteomic analysis of streptomycin resistant and sensitive clinical isolates of Mycobacterium tuberculosis. **2010**, 8, 59	40
2201	CLE14/CLE20 peptides may interact with CLAVATA2/CORYNE receptor-like kinases to irreversibly inhibit cell division in the root meristem of Arabidopsis. **2010**, 232, 1061-74	59
2200	Exploring the cause of drug resistance by the detrimental missense mutations in KIT receptor: computational approach. **2010**, 39, 651-60	11
2199	In silico identification of significant detrimental missense mutations of EGFR and their effect with 4-anilinoquinazoline-based drugs. **2010**, 160, 1723-33	12
2198	Structural and functional analysis of A-type ketoreductases from the amphotericin modular polyketide synthase. **2010**, 18, 913-22	71
2197	Comparison of PGH2 binding site in prostaglandin synthases. **2010**, 11 Suppl 1, S51	3
2196	Potential immunoregulatory role of heme oxygenase-1 in human milk: a combined biochemical and molecular modeling approach. **2010**, 21, 865-71	18
2195	Computational approaches for protein function prediction: a combined strategy from multiple sequence alignment to molecular docking-based virtual screening. **2010**, 1804, 1695-712	68

2194	Structure of a membrane-attack complex/perforin (MACPF) family protein from the human gut symbiont Bacteroides thetaiotaomicron. **2010**, 66, 1297-305	26
2193	Recent advances in B-cell epitope prediction methods. **2010**, 6 Suppl 2, S2	100
2192	Structural modeling of histone methyltransferase complex Set1C from Saccharomyces cerevisiae using constraint-based docking. **2010**, 10, 4186-95	5
2191	Combining crystallography and molecular dynamics: the case of Schistosoma mansoni phospholipid glutathione peroxidase. **2010**, 78, 259-70	22
2190	FiberDock: Flexible induced-fit backbone refinement in molecular docking. **2010**, 78, 1503-19	144
2189	An integrated suite of fast docking algorithms. **2010**, 78, 3197-204	100
2188	MDockPP: A hierarchical approach for protein-protein docking and its application to CAPRI rounds 15-19. **2010**, 78, 3096-103	48
2187	ReplicOpter: a replicate optimizer for flexible docking. **2010**, 78, 3156-65	6
2186	Structure of the cholera toxin secretion channel in its closed state. **2010**, 17, 1226-32	112
2185	The HADDOCK web server for data-driven biomolecular docking. **2010**, 5, 883-97	936
2184	Measuring the cytochrome C nitrite reductase activity-practical considerations on the enzyme assays. **2010**,	9
2183	Molecular recognition between ketosynthase and acyl carrier protein domains of the 6-deoxyerythronolide B synthase. **2010**, 107, 22066-71	68
2182	Crystal structures of the lumazine protein from Photobacterium kishitanii in complexes with the authentic chromophore, 6,7-dimethyl- 8-(1'-D-ribityl) lumazine, and its analogues, riboflavin and flavin mononucleotide, at high resolution. **2010**, 192, 127-33	20
2181	Structural characterization of OxyD, a cytochrome P450 involved in beta-hydroxytyrosine formation in vancomycin biosynthesis. **2010**, 285, 24562-74	57
2180	A flavin-dependent monooxygenase from Mycobacterium tuberculosis involved in cholesterol catabolism. **2010**, 285, 22264-75	86
2179	SwarmDock and the use of normal modes in protein-protein docking. **2010**, 11, 3623-48	120
2178	Crystal structure of Legionella DotD: insights into the relationship between type IVB and type II/III secretion systems. **2010**, 6, e1001129	41
2177	In silico analysis of the apolipoprotein E and the amyloid beta peptide interaction: misfolding induced by frustration of the salt bridge network. **2010**, 6, e1000663	29

2176	Calmodulin binding to Arabidopsis cyclic nucleotide gated ion channels. **2010**, 5, 1147-9		8
2175	Building macromolecular assemblies by information-driven docking: introducing the HADDOCK multibody docking server. **2010**, 9, 1784-94		98
2174	Protein-protein docking tested in blind predictions: the CAPRI experiment. **2010**, 6, 2351-62		130
2173	Structural determination of Abeta25-35 micelles by molecular dynamics simulations. **2010**, 99, 666-74		21
2172	Interaction of mumps virus V protein variants with STAT1-STAT2 heterodimer: experimental and theoretical studies. **2010**, 7, 263		6
2171	Structural and biochemical characterization of the cytochrome P450 CypX (CYP134A1) from Bacillus subtilis: a cyclo-L-leucyl-L-leucyl dipeptide oxidase. **2010**, 49, 7282-96		66
2170	Protein-protein recognition between acyltransferases and acyl carrier proteins in multimodular polyketide synthases. **2010**, 49, 95-102		44
2169	Structure of the bacteriophage T4 long tail fiber receptor-binding tip. **2010**, 107, 20287-92		130
2168	FiberDock: a web server for flexible induced-fit backbone refinement in molecular docking. *Nucleic Acids Research*, **2010**, 38, W457-61	20.1	78
2167	Docking and Scoring in Drug Discovery. **2010**, 601-684		2
2166	Alzheimer Abeta(1-42) monomer adsorbed on the self-assembled monolayers. **2010**, 26, 12722-32		38
2165	Sialic acid-binding dwarf elder four-chain lectin displays nucleic acid N-glycosidase activity. **2010**, 92, 71-80		15
2164	Binding of YC-1/BAY 41-2272 to soluble guanylate cyclase: A new perspective to the mechanism of activation. **2010**, 397, 375-9		14
2163	The polypeptide Syn67 interacts physically with human holocarboxylase synthetase, but is not a target for biotinylation. **2010**, 495, 35-41		6
2162	Zinc ions promote Alzheimer Abeta aggregation via population shift of polymorphic states. **2010**, 107, 9490-5		234
2161	Spatio-temporal modeling of signaling protein recruitment to EGFR. **2010**, 4, 57		44
2160	Protein Interactions. **2010**, 247-302		0
2159	How does the reductase help to regulate the catalytic cycle of cytochrome P450 3A4 using the conserved water channel?. **2010**, 114, 5964-70		46

2158	FPGA acceleration of rigid-molecule docking codes. **2010**, 4, 184-195		12
2157	Allosteric regulation of glycogen synthase kinase 3□a theoretical study. **2010**, 49, 10890-901		24
2156	Current understanding of fatty acid biosynthesis and the acyl carrier protein. **2010**, 430, 1-19		215
2155	HexServer: an FFT-based protein docking server powered by graphics processors. *Nucleic Acids Research*, **2010**, 38, W445-9	20.1	436
2154	In silicon evaluation of nanoparticle cell interaction via human TLR3. **2010**,		0
2153	An accurate classification of native and non-native protein-protein interactions using supervised and semi-supervised learning approaches. **2010**,		
2152	A Parallel Algorithm for Molecular Surface Matching Through Image Representation. **2010**,		
2151	Image-based surface matching algorithm oriented to structural biology. **2011**, 8, 1004-16		17
2150	Novel NADPH-cysteine covalent adduct found in the active site of an aldehyde dehydrogenase. **2011**, 439, 443-52		17
2149	Crucial effect of the first CXXC motif of human QSOX 1b on the activity to different substrates. **2011**, 149, 293-300		7
2148	Protein docking with information on evolutionary conserved interfaces. **2011**,		3
2147	Structure and mechanism of the trans-acting acyltransferase from the disorazole synthase. **2011**, 50, 6539-48		64
2146	Isothermal titration calorimetric and computational studies on the binding of chitooligosaccharides to pumpkin (Cucurbita maxima) phloem exudate lectin. **2011**, 115, 4110-7		19
2145	AADS--an automated active site identification, docking, and scoring protocol for protein targets based on physicochemical descriptors. **2011**, 51, 2515-27		95
2144	Mass spectrometry of intact V-type ATPases reveals bound lipids and the effects of nucleotide binding. **2011**, 334, 380-385		224
2143	Accessory cholera enterotoxin, Ace, from Vibrio cholerae: structure, unfolding, and virstatin binding. **2011**, 50, 2962-72		20
2142	Characterisation of a mannose-binding C-type lectin from Oxyuranus scutellatus snake venom. **2011**, 93, 519-27		11
2141	A structural model of the HIV-1 Rev-integrase complex: the molecular basis of integrase regulation by Rev. **2011**, 416, 252-7		3

2140	Curcumin recognizes a unique binding site of tubulin. **2011**, 54, 6183-96	86
2139	Macromolecular docking restrained by a small angle X-ray scattering profile. **2011**, 173, 461-71	88
2138	Zinc binding to the Tyr402 and His402 allotypes of complement factor H: possible implications for age-related macular degeneration. **2011**, 408, 714-35	38
2137	Hotspot-centric de novo design of protein binders. **2011**, 413, 1047-62	32
2136	Computational interaction analysis of organophosphorus pesticides with different metabolic proteins in humans. **2011**, 25, 335-47	22
2135	Enhancement of the hydrolysis activity of □galactosidase from Geobacillus stearothermophilus by saturation mutagenesis. **2011**, 94, 1176-84	10
2134	Structural similarity and classification of protein interaction interfaces. **2011**, 6, e19554	9
2133	Concurrent proinflammatory and apoptotic activity of a Helicobacter pylori protein (HP986) points to its role in chronic persistence. **2011**, 6, e22530	29
2132	Hepatitis E virus ORF2 protein activates the pro-apoptotic gene CHOP and anti-apoptotic heat shock proteins. **2011**, 6, e25378	28
2131	Epitope-based immunoinformatics and molecular docking studies of nucleocapsid protein and ovarian tumor domain of crimean-congo hemorrhagic Fever virus. **2011**, 2, 72	11
2130	Molecular mechanism by which the nucleoid occlusion factor, SlmA, keeps cytokinesis in check. **2011**, 30, 154-64	119
2129	A multidomain flexible docking approach to deal with large conformational changes in the modeling of biomolecular complexes. **2011**, 19, 555-65	52
2128	Synthesis and bio-evaluation of human macrophage migration inhibitory factor inhibitor to develop anti-inflammatory agent. **2011**, 19, 7365-73	24
2127	Predicting protein-protein interactions on a proteome scale by matching evolutionary and structural similarities at interfaces using PRISM. **2011**, 6, 1341-54	206
2126	Molecular characterization of an h-type thioredoxin gene from grape. **2011**, 6, 1006-1022	1
2125	Computational design of proteins targeting the conserved stem region of influenza hemagglutinin. **2011**, 332, 816-21	441
2124	Prediction of protein binding sites and hot spots. **2011**, 1, 680-698	41
2123	Relationship between mutation of serine residue at 315th position in M. tuberculosis catalase-peroxidase enzyme and Isoniazid susceptibility: an in silico analysis. **2011**, 17, 869-77	63

2122	Comparative analysis of receptor binding by chicken and human interleukin-1. **2011**, 17, 1283-94		7
2121	Molecular dynamics simulation of the Staphylococcus aureus YsxC protein: molecular insights into ribosome assembly and allosteric inhibition of the protein. **2011**, 17, 3129-49		4
2120	Prediction of a new surface binding pocket and evaluation of inhibitors against huntingtin interacting protein 14: an insight using docking studies. **2011**, 17, 3047-56		13
2119	Drug discovery against H1N1 virus (influenza A virus) via computational virtual screening approach. **2011**, 20, 1445-1449		10
2118	Insights into structure and function of SHIP2-SH2: homology modeling, docking, and molecular dynamics study. **2011**, 4, 149-58		4
2117	Protein-protein complexation in bioluminescence. **2011**, 2, 957-72		12
2116	Protein-x of hepatitis B virus in interaction with CCAAT/enhancer-binding protein (C/EBP)-an in silico analysis approach. **2011**, 8, 41		4
2115	Prediction of conformational B-cell epitopes from 3D structures by random forests with a distance-based feature. **2011**, 12, 341		75
2114	Structure of the Mycobacterium tuberculosis OmpATb protein: a model of an oligomeric channel in the mycobacterial cell wall. **2011**, 79, 645-61		21
2113	SymmRef: a flexible refinement method for symmetric multimers. **2011**, 79, 2607-23		16
2112	Restricted sidechain plasticity in the structures of native proteins and complexes. **2011**, 20, 753-7		37
2111	Probing the interactions of an acyl carrier protein domain from the 6-deoxyerythronolide B synthase. **2011**, 20, 1244-55		42
2110	Feature-based classification of native and non-native protein-protein interactions: Comparing supervised and semi-supervised learning approaches. **2011**, 11, 4321-30		9
2109	The lipoproteins of cyanobacterial photosystem II. **2011**, 104, 191-203		46
2108	Oligomerization of G protein-coupled receptors: computational methods. **2011**, 18, 4588-605		28
2107	Rosetta FlexPepDock web server--high resolution modeling of peptide-protein interactions. *Nucleic Acids Research*, **2011**, 39, W249-53	20.1	273
2106	Cryptic parasite revealed improved prospects for treatment and control of human cryptosporidiosis through advanced technologies. **2011**, 77, 141-73		18
2105	A toll-like receptor-4-interacting surfactant protein-A-derived peptide suppresses tumor necrosis factor- release from mouse JAWS II dendritic cells. **2011**, 336, 672-81		20

2104	PRUNE and PROBE--two modular web services for protein-protein docking. *Nucleic Acids Research*, **2011**, 39, W229-34	20.1	12
2103	Identification and characterization of an immunogenic hybrid epitope formed by both HIV gp120 and human CD4 proteins. **2011**, 85, 13097-104		16
2102	Cross-linking measurements of in vivo protein complex topologies. **2011**, 10, M110.006841		69
2101	Comparative modeling: the state of the art and protein drug target structure prediction. **2011**, 14, 532-47		33
2100	Uncoupling charge movement from channel opening in voltage-gated potassium channels by ruthenium complexes. **2011**, 286, 16414-25		20
2099	Ebolavirus proteins suppress the effects of small interfering RNA by direct interaction with the mammalian RNA interference pathway. **2011**, 85, 2512-23		99
2098	Studies on adaptability of binding residues and flap region of TMC-114 resistance HIV-1 protease mutants. **2011**, 29, 137-52		58
2097	Partially glycosylated dendrimers block MD-2 and prevent TLR4-MD-2-LPS complex mediated cytokine responses. **2011**, 7, e1002095		28
2096	Separation of recombination and SOS response in Escherichia coli RecA suggests LexA interaction sites. **2011**, 7, e1002244		57
2095	GPU.proton.DOCK: Genuine Protein Ultrafast proton equilibria consistent DOCKing. *Nucleic Acids Research*, **2011**, 39, W223-8	20.1	7
2094	Identification and characterization of novel small-molecule inhibitors against hepatitis delta virus replication by using docking strategies. **2011**, 11, 803-9		6
2093	Characterization of flavonol inhibition of DnaB helicase: real-time monitoring, structural modeling, and proposed mechanism. **2012**, 2012, 735368		18
2092	Candida albicans scavenges host zinc via Pra1 during endothelial invasion. **2012**, 8, e1002777		157
2091	Identification and molecular characterization of an Alba-family protein from human malaria parasite Plasmodium falciparum. *Nucleic Acids Research*, **2012**, 40, 1174-90	20.1	61
2090	Dimerization of NKp46 receptor is essential for NKp46-mediated lysis: characterization of the dimerization site by epitope mapping. **2012**, 188, 6165-74		15
2089	A large-scale association study for nanoparticle C60 uncovers mechanisms of nanotoxicity disrupting the native conformations of DNA/RNA. *Nucleic Acids Research*, **2012**, 40, 7622-32	20.1	26
2088	Flexibility and binding affinity in protein-ligand, protein-protein and multi-component protein interactions: limitations of current computational approaches. **2012**, 9, 20-33		64
2087	Identification of the galactose binding domain of the adeno-associated virus serotype 9 capsid. **2012**, 86, 7326-33		79

2086	Reprogramming a module of the 6-deoxyerythronolide B synthase for iterative chain elongation. **2012**, 109, 4110-5	81
2085	Activation of p115-RhoGEF requires direct association of G13 and the Dbl homology domain. **2012**, 287, 25490-500	30
2084	Amino acid residues critical for the specificity for betaine aldehyde of the plant ALDH10 isoenzyme involved in the synthesis of glycine betaine. **2012**, 158, 1570-82	40
2083	Guiding protein docking with geometric and evolutionary information. **2012**, 10, 1242008	7
2082	Interaction of virstatin with human serum albumin: spectroscopic analysis and molecular modeling. **2012**, 7, e37468	95
2081	Protein-protein docking and hot-spot prediction for drug discovery. **2012**, 18, 4607-18	37
2080	Bovine lactoferrin-derived peptides as novel broad-spectrum inhibitors of influenza virus. **2012**, 106, 12-9	37
2079	Dietary polyphenol-derived protection against neurotoxic amyloid protein: from molecular to clinical. **2012**, 3, 1242-50	40
2078	Prediction of heparin binding sites in bone morphogenetic proteins (BMPs). **2012**, 1824, 1374-81	71
2077	Discovery of a multigene family of aquaporin silicon transporters in the primitive plant Equisetum arvense. **2012**, 72, 320-30	94
2076	In silico identification and characterization of 1-aminocyclopropane-1-carboxylate deaminase from Phytophthora sojae. **2012**, 18, 4101-11	20
2075	A calcium-dependent interaction between calmodulin and the calponin homology domain of human IQGAP1. **2012**, 371, 217-23	10
2074	Computational methods for prediction of protein-RNA interactions. **2012**, 179, 261-8	85
2073	In vivo application of photocleavable protein interaction reporter technology. **2012**, 11, 1027-41	25
2072	Cross-linking measurements of the Potato leafroll virus reveal protein interaction topologies required for virion stability, aphid transmission, and virus-plant interactions. **2012**, 11, 2968-81	53
2071	A basin hopping algorithm for protein-protein docking. **2012**,	3
2070	Amyloid-fibril disruption by C60-molecular guidance for rational drug design. **2012**, 14, 8599-607	47
2069	Evolving the [myoglobin, cytochrome b(5)] complex from dynamic toward simple docking: charging the electron transfer reactive patch. **2012**, 51, 8542-53	9

2068	Cholesterol promotes the interaction of Alzheimer amyloid monomer with lipid bilayer. **2012**, 421, 561-71	88
2067	Comparative structural modeling of a monothiol GRX from chickpea: insight in iron-sulfur cluster assembly. **2012**, 51, 266-73	14
2066	Novel protein-protein interactions between Entamoeba histolyticad-phosphoglycerate dehydrogenase and phosphoserine aminotransferase. **2012**, 94, 1676-86	5
2065	Inter-domain movements in polyketide synthases: a molecular dynamics study. **2012**, 8, 1157-71	7
2064	Probing the soybean Bowman-Birk inhibitor using recombinant antibody fragments. **2012**, 60, 6164-72	9
2063	Protein docking prediction using predicted protein-protein interface. **2012**, 13, 7	48
2062	Integrative structural modeling with small angle X-ray scattering profiles. **2012**, 12, 17	80
2061	Theoretical investigation on structural, functional and epitope of a 12 kDa excretory-secretory protein from Toxoplasma gondii. **2012**, 12, 30	3
2060	Computational design by evolving folds and assemblies over the alphabet in L- and D- amino acids. **2012**, 2, 3242	4
2059	Structural insights of rohu TLR3, its binding site analysis with fish reovirus dsRNA, poly I:C and zebrafish TRIF. **2012**, 51, 531-43	27
2058	Binding of single walled carbon nanotube to WT and mutant HIV-1 proteases: analysis of flap dynamics and binding mechanism. **2012**, 38, 430-45	12
2057	Detection and confirmation of alkaloids in leaves of Justicia adhatoda and bioinformatics approach to elicit its anti-tuberculosis activity. **2012**, 168, 980-90	30
2056	Synthesis, docking and anticancer activity studies of D-proline-incorporated wainunuamide. **2012**, 124, 1049-1055	1
2055	Computational analysis of deleterious missense mutations in aspartoacylase that cause Canavan's disease. **2012**, 55, 1109-19	5
2054	What in silico molecular docking can do for the 'bench-working biologists'. **2012**, 37, 1089-95	22
2053	Sanjeevini: a freely accessible web-server for target directed lead molecule discovery. **2012**, 13 Suppl 17, S7	100
2052	Mycobacterium tuberculosis DosR regulon gene Rv0079 encodes a putative, 'dormancy associated translation inhibitor (DATIN)'. **2012**, 7, e38709	21
2051	Modeling amyloid-beta as homogeneous dodecamers and in complex with cellular prion protein. **2012**, 7, e49375	11

2050	Basin Hopping as a General and Versatile Optimization Framework for the Characterization of Biological Macromolecules. **2012**, 2012, 1-19	24
2049	Pressure-selective modulation of NMDA receptor subtypes may reflect 3D structural differences. **2012**, 6, 37	10
2048	Computer Aided Drug Designing Using Phytochemicals- Bacoside A3 and Myricetin and Nitric Oxide Donors-S-Nitroso N-Acetylpenicillamine and Nitroglycerin as a Potential Treatment of Pancreatic Cancer. **2012**, 05,	1
2047	Human Serotonin 5-HT G Protein-Coupled Receptor Homology Model from the Adrenoceptor Structure: Ligand Docking and Mutagenesis Studies. **2012**, 112, 140	8
2046	Optimized grid-based protein-protein docking as a global search tool followed by incorporating experimentally derivable restraints. **2012**, 80, 691-702	2
2045	Fast and accurate modeling of protein-protein interactions by combining template-interface-based docking with flexible refinement. **2012**, 80, 1239-49	35
2044	Multi-LZerD: multiple protein docking for asymmetric complexes. **2012**, 80, 1818-33	53
2043	Molecular Determinants for Ligand Binding at Serotonin 5-HT and 5-HT GPCRs: Experimental Affinity Results Analyzed by Molecular Modeling and Ligand Docking Studies. **2012**, 112, 3807-3814	14
2042	Interpreting the structural mechanism of action for MT7 and human muscarinic acetylcholine receptor 1 complex by modeling protein-protein interaction. **2012**, 30, 30-44	6
2041	Identification of potential tumor differentiation factor (TDF) receptor from steroid-responsive and steroid-resistant breast cancer cells. **2012**, 287, 1719-33	43
2040	Networks of Protein?Protein Interactions: From Uncertainty to Molecular Details. **2012**, 31, 342-62	18
2039	Plasma membrane localization of Solanum tuberosum remorin from group 1, homolog 3 is mediated by conformational changes in a novel C-terminal anchor and required for the restriction of potato virus X movement]. **2012**, 160, 624-37	56
2038	Structure, orientation, and surface interaction of Alzheimer amyloid-peptides on the graphite. **2012**, 28, 6595-605	68
2037	Identification of a potential tumor differentiation factor receptor candidate in prostate cancer cells. **2012**, 279, 2579-94	33
2036	In silico characterization of atypical kinase PFD0975w from Plasmodium kinome: a suitable target for drug discovery. **2012**, 79, 600-9	9
2035	The N-terminal region of CXCL11 as structural template for CXCR3 molecular recognition: synthesis, conformational analysis, and binding studies. **2012**, 80, 254-65	11
2034	Nickel(II)-Schiff base complex recognizing domain II of bovine and human serum albumin: spectroscopic and docking studies. **2012**, 92, 164-74	85
2033	Spectral and electrochemical study of host-guest inclusion complex between 2,4-dinitrophenol and cyclodextrin. **2012**, 94, 89-100	52

2032	Constructing structural networks of signaling pathways on the proteome scale. **2012**, 22, 367-77	56
2031	Relationship between the structure and the enzymatic activity of crotoxin complex and its phospholipase A2 subunit: an in silico approach. **2012**, 35, 36-42	7
2030	[Interaction of sea amemone Heteractis crispa Kunitz type polypeptides with pain vanilloid receptor TRPV1: in silico investigation]. **2012**, 38, 185-98	8
2029	Ciprofloxacin-resistant Escherichia coli in hospital wastewater of Bangladesh and prediction of its mechanism of resistance. **2012**, 28, 827-34	16
2028	Isolation, identification and sequence analysis of a thioredoxin h gene, a member of subgroup III of h-type Trxs from grape (Vitis vinifera L. cv. Askari). **2012**, 39, 3683-93	3
2027	Macromolecular symmetric assembly prediction using swarm intelligence dynamic modeling. **2013**, 21, 1097-1106	27
2026	Characterization of tumor differentiation factor (TDF) and its receptor (TDF-R). **2013**, 70, 2835-48	19
2025	Human serum albumin interactions with C60 fullerene studied by spectroscopy, small-angle neutron scattering, and molecular dynamics simulations. **2013**, 15, 1	11
2024	A tandem Kunitz protease inhibitor (KPI106)-serine carboxypeptidase (SCP1) controls mycorrhiza establishment and arbuscule development in Medicago truncatula. **2013**, 75, 711-25	22
2023	Differential protease activity augments polyphagy in Helicoverpa armigera. **2013**, 22, 258-72	37
2022	Insights into molecular assembly of ACCase heteromeric complex in Chlorella variabilis--a homology modelling, docking and molecular dynamic simulation study. **2013**, 170, 1437-57	4
2021	A dodecameric ring-like structure of the N0 domain of the type II secretin from enterotoxigenic Escherichia coli. **2013**, 183, 354-362	14
2020	Pathogens use structural mimicry of native host ligands as a mechanism for host receptor engagement. **2013**, 14, 63-73	41
2019	A novel mechanism for antiglycative action of limonene through stabilization of protein conformation. **2013**, 9, 2463-72	32
2018	Modeling Complexes of Transmembrane Proteins: Systematic Analysis of Protein?Protein Docking Tools. **2013**, 32, 717-33	24
2017	Activation of nucleotide-binding oligomerization domain 1 (NOD1) receptor signaling in Labeo rohita by iE-DAP and identification of ligand-binding key motifs in NOD1 by molecular modeling and docking. **2013**, 170, 1282-309	20
2016	Identification of potential inhibitors of H5N1 influenza A virus neuraminidase by ligand-based virtual screening approach. **2013**, 66, 657-69	13
2015	Molecular dynamic simulations of Co(III) and Ru(II) polypyridyl complexes and docking studies with dsDNA. **2013**, 22, 5557-5565	9

2014	Evidence-based docking of the urease activation complex. **2013**, 31, 854-61	11
2013	Extrapolating the effect of deleterious nsSNPs in the binding adaptability of flavopiridol with CDK7 protein: a molecular dynamics approach. **2013**, 7, 10	40
2012	How good is automated protein docking?. **2013**, 81, 2159-66	385
2011	CyClus: a fast, comprehensive cylindrical interface approximation clustering/reranking method for rigid-body protein-protein docking decoys. **2013**, 81, 1005-16	9
2010	Structural templates for modeling homodimers. **2013**, 22, 1655-63	15
2009	A hydrolytic Eglutamyl transpeptidase from thermo-acidophilic archaeon Picrophilus torridus: binding pocket mutagenesis and transpeptidation. **2013**, 17, 29-41	18
2008	A structural modeling approach for the understanding of initiation and elongation of ALS-linked superoxide dismutase fibrils. **2013**, 19, 3695-704	4
2007	In silico discrimination of nsSNPs in hTERT gene by means of local DNA sequence context and regularity. **2013**, 19, 3517-27	6
2006	Bmcc1s interacts with the phosphate-activated glutaminase in the brain. **2013**, 95, 799-807	9
2005	Insight into structural and biochemical determinants of substrate specificity of PFI1625c: correlation analysis of protein-peptide molecular models. **2013**, 43, 21-30	5
2004	Functional characterization of an extracellular keratinolytic protease, Ker AP from Pseudomonas aeruginosa KS-1: A putative aminopeptidase with PA domain. **2013**, 91, 8-16	7
2003	OXA-162, a novel variant of OXA-48 displays extended hydrolytic activity towards imipenem, meropenem and doripenem. **2013**, 28, 990-6	23
2002	Spectroscopic and electrochemical studies on the interaction of an inclusion complex of Ecyclodextrin with 2,6-dinitrophenol in aqueous and solid phases. **2013**, 1036, 494-504	9
2001	Stable and potent analogues derived from the modification of the dicarbonyl moiety of curcumin. **2013**, 52, 7449-60	52
2000	A Minimalist Model of Protein Diffusion and Interactions: The Green Fluorescent Protein within the Cytoplasm. **2013**, 46, 8311-8322	16
1999	Understanding FtsZ assembly: cues from the behavior of its N- and C-terminal domains. **2013**, 52, 7071-81	6
1998	Structural analysis of guanylyl cyclase-activating protein-2 (GCAP-2) homodimer by stable isotope-labeling, chemical cross-linking, and mass spectrometry. **2013**, 24, 1969-79	25
1997	Dynamic switching of calmodulin interactions underlies Ca2+ regulation of CaV1.3 channels. **2013**, 4, 1717	83

1996	Antibody i-Patch prediction of the antibody binding site improves rigid local antibody-antigen docking. **2013**, 26, 621-9	55
1995	Computational design of a protein-based enzyme inhibitor. **2013**, 425, 3563-75	71
1994	Structural insights into functional overlapping and differentiation among myosin V motors. **2013**, 288, 34131-34145	25
1993	Intermolecular Contact Potentials for Protein-Protein Interactions Extracted from Binding Free Energy Changes upon Mutation. **2013**, 9, 3715-27	29
1992	Accurate SAXS profile computation and its assessment by contrast variation experiments. **2013**, 105, 962-74	359
1991	Spectral, electrochemical and docking studies of 5-indanol:□CD inclusion complex. **2013**, 51, 567-585	4
1990	Structural and functional studies on urease from pigeon pea (Cajanus cajan). **2013**, 58, 301-9	36
1989	A computational approach to explore the functional missense mutations in the spindle check point protein Mad1. **2013**, 8, 618-625	
1988	Structure-based protein-protein interaction networks and drug design. **2013**, 1, 183-191	7
1987	Molecular docking and simulation studies towards exploring antiviral compounds against envelope protein of Japanese encephalitis virus. **2013**, 2, 231-243	7
1986	Proteomic analysis of Mycobacterium tuberculosis isolates resistant to kanamycin and amikacin. **2013**, 94, 68-77	56
1985	In-silico screening of cancer associated mutation on PLK1 protein and its structural consequences. **2013**, 19, 5587-99	25
1984	Structure and assembly of an inner membrane platform for initiation of type IV pilus biogenesis. **2013**, 110, E4638-47	46
1983	Interaction between shrimp and white spot syndrome virus through PmRab7-VP28 complex: an insight using simulation and docking studies. **2013**, 19, 1285-94	16
1982	The role of lipids in defining membrane protein interactions: insights from mass spectrometry. **2013**, 23, 1-8	114
1981	pH- and heat-induced structural changes of bovine □actalbumin in response to oleic acid binding. **2013**, 236, 257-266	14
1980	The solution structure of rabbit IgG accounts for its interactions with the Fc receptor and complement C1q and its conformational stability. **2013**, 425, 506-23	22
1979	Comparative functional analysis of CYP71AV1 natural variants reveals an important residue for the successive oxidation of amorpha-4,11-diene. **2013**, 587, 278-84	19

1978	Effects of surface curvature and surface characteristics of carbon-based nanomaterials on the adsorption and activity of acetylcholinesterase. **2013**, 62, 222-232	32
1977	X-ray structure of a superinfection exclusion lipoprotein from phage TP-J34 and identification of the tape measure protein as its target. **2013**, 89, 152-65	33
1976	Natural selection and population genetic structure of domain-I of Plasmodium falciparum apical membrane antigen-1 in India. **2013**, 18, 247-56	8
1975	The crystal structure of a novel phosphopantothenate synthetase from the hyperthermophilic archaea, Thermococcus onnurineus NA1. **2013**, 439, 533-8	4
1974	Diameter-selective dispersion of carbon nanotubes by Lactoglobulin whey protein. **2013**, 112, 16-22	12
1973	A computational protocol to predict suitable redox mediators for substitution of NAD(P)H in P450 monooxygenases. **2013**, 88, 47-51	14
1972	Purification, bio-chemical characterization, homology modeling and active site binding mode interactions of thermo-alkali-tolerant 1,4 endoxylanase from Coprinus cinereus LK-D-NCIM-1369. **2013**, 2, 267-277	10
1971	Effect of d-amino acids on collagen fibrillar assembly and stability: Experimental and modelling studies. **2013**, 75, 92-100	11
1970	Homology modeling and docking studies of FabH (Ketoacyl-ACP synthase III) enzyme involved in type II fatty acid biosynthesis of Chlorella variabilis: a potential algal feedstock for biofuel production. **2013**, 31, 241-57	10
1969	Insights into FlaI functions in archaeal motor assembly and motility from structures, conformations, and genetics. **2013**, 49, 1069-82	81
1968	Molecular modelling and simulations in cancer research. **2013**, 1836, 1-14	33
1967	Rational design of the survivin/CDK4 complex by combining protein-protein docking and molecular dynamics simulations. **2013**, 19, 1507-14	7
1966	A peptide derived from the C-terminus of PB1 inhibits influenza virus replication by interfering with viral polymerase assembly. **2013**, 280, 1139-49	27
1965	Computational design of novel protein binders and experimental affinity maturation. **2013**, 523, 1-19	30
1964	Creation of recombinant antigen-binding molecules derived from hybridomas secreting specific antibodies. **2013**, 8, 1125-48	27
1963	Studies on inclusion complexation between 4,4?-dihydroxybiphenyl and Cyclodextrin by experimental and theoretical approach. **2013**, 1048, 399-409	13
1962	Annexin A1 is regulated by domains cross-talk through post-translational phosphorylation and SUMOYlation. **2013**, 25, 1962-9	17
1961	Study of Q224K, V152G double mutation in bean PGIP2, an LRR protein for plant defense--an in silico approach. **2013**, 81, 852-62	4

1960	Common structural interactions between the receptors CXCR3, CXCR4 and CXCR7 complexed with their natural ligands, CXCL11 and CXCL12, by a modeling approach. **2013**, 64, 316-21	18
1959	Sampling and scoring: a marriage made in heaven. **2013**, 81, 1874-84	49
1958	Dissecting disease inheritance modes in a three-dimensional protein network challenges the "guilt-by-association" principle. **2013**, 93, 78-89	38
1957	Heme oxygenase-2/adiponectin protein-protein interaction in metabolic syndrome. **2013**, 432, 606-11	13
1956	Dormancy Associated Translation Inhibitor (DATIN/Rv0079) of Mycobacterium tuberculosis interacts with TLR2 and induces proinflammatory cytokine expression. **2013**, 64, 258-64	35
1955	Binding of aquo-ethylenediaminetetraacetatoruthenium(III) to apo-transferrin. Fluorescence, antiproliferative and in silico studies. **2013**, 404, 1-4	4
1954	Substrate preference of a Geobacillus maltogenic amylase: a kinetic and thermodynamic analysis. **2013**, 60, 1-9	10
1953	Galectin-3 regulates p21 stability in human prostate cancer cells. **2013**, 32, 5058-65	17
1952	HopDock: a probabilistic search algorithm for decoy sampling in protein-protein docking. **2013**, 11, S6	7
1951	Momordica charantia and its novel polypeptide regulate glucose homeostasis in mice via binding to insulin receptor. **2013**, 61, 2461-8	49
1950	The structure of Rv3717 reveals a novel amidase from Mycobacterium tuberculosis. **2013**, 69, 2543-54	22
1949	Molecular characterization of human melanocortin-5 receptor ligand-receptor interaction. **2013**, 52, 1737-45	11
1948	Cross-linking and mass spectrometry methodologies to facilitate structural biology: finding a path through the maze. **2013**, 14, 77-90	22
1947	Multidrug resistance protein P-gp interaction with nanoparticles (fullerenes and carbon nanotube) to assess their drug delivery potential: a theoretical molecular docking study. **2013**, 6, 343-57	27
1946	A suppressor screen of the chimeric AtCNGC11/12 reveals residues important for intersubunit interactions of cyclic nucleotide-gated ion channels. **2013**, 162, 1681-93	12
1945	Oligomeric properties of adeno-associated virus Rep68 reflect its multifunctionality. **2013**, 87, 1232-41	14
1944	Structure- and modeling-based identification of the adenovirus E4orf4 binding site in the protein phosphatase 2A B55 subunit. **2013**, 288, 13718-27	8
1943	Synthesis, Spectroscopic Characterization and Biological Activities of Transition Metal Complexes Derived from a Tridentate Schiff Base. **2013**, 2013, 1-10	8

1942	Cholesterol lowering drug may influence cellular immune response by altering MHC II function. **2013**, 54, 3106-15		20
1941	Details of ssDNA annealing revealed by an HSV-1 ICP8-ssDNA binary complex. *Nucleic Acids Research*, **2013**, 41, 5927-37	20.1	17
1940	Protein interactions, post-translational modifications and topologies in human cells. **2013**, 12, 1451-67		86
1939	Mutational analysis identifies residues crucial for homodimerization of myeloid differentiation factor 88 (MyD88) and for its function in immune cells. **2013**, 288, 30210-30222		37
1938	Informatics-driven Protein-protein Docking. **2013**,		1
1937	The Possible Role of TLR2 in Chronic Hepatitis B Patients with Precore Mutation. **2013**, 2013, 780319		9
1936	Structural insights into the extra cellular segment of integrin and molecular interaction studies. **2013**, 33, 319-24		4
1935	Allosteric lariat peptide inhibitors of Abl kinase. **2013**, 14, 2119-25		5
1934	Laminin 332 processing impacts cellular behavior. **2013**, 7, 122-34		90
1933	TanCAR: A Novel Bispecific Chimeric Antigen Receptor for Cancer Immunotherapy. **2013**, 2, e105		297
1932	Polymerase manager protein UmuD directly regulates Escherichia coli DNA polymerase III binding to ssDNA. *Nucleic Acids Research*, **2013**, 41, 8959-68	20.1	9
1931	Spectral Studies on the Supramolecular Assembly of 1H2NA: CD Complex and its Analytical Application as Chemosensor for the Selective Sensing of Cr3+. **2013**, 33, 221-235		6
1930	Protein-protein interaction network prediction by using rigid-body docking tools: application to bacterial chemotaxis. **2014**, 21, 790-8		11
1929	Tumor Differentiation Factor (TDF) and its Receptor (TDF-R): Is TDF-R an Inducible Complex with Multiple Docking Sites?. **2013**, 01,		1
1928	Characterization of the Leucine-Responsive Transcription Factor from Pathogenic Vibrio cholerae Using Molecular Modelling and Molecular Dynamics Simulations. **2013**, 02,		
1927	MEGADOCK: an all-to-all protein-protein interaction prediction system using tertiary structure data. **2014**, 21, 766-78		38
1926	Imperfect duplicate insertions type of mutations in plasmepsin V modulates binding properties of PEXEL motifs of export proteins in Indian Plasmodium vivax. **2013**, 8, e60077		5
1925	Tryptogalinin is a tick Kunitz serine protease inhibitor with a unique intrinsic disorder. **2013**, 8, e62562		28

1924	Comparative molecular docking analysis of cytoplasmic dynein light chain DYNLL1 with pilin to explore the molecular mechanism of pathogenesis caused by Pseudomonas aeruginosa PAO. **2013**, 8, e76730	11
1923	Identifying cytochrome p450 functional networks and their allosteric regulatory elements. **2013**, 8, e81980	23
1922	In silico, in vitro and in vivo analysis of binding affinity between N and C-domains of Clostridium perfringens alpha toxin. **2013**, 8, e82024	19
1921	Dynamics of Bcl-xL in water and membrane: molecular simulations. **2013**, 8, e76837	11
1920	Structural Analysis of Respirasomes in Electron Transfer Pathway of Acidithiobacillus ferrooxidans: A Computer-Aided Molecular Designing Study. **2013**, 2013, 1-14	4
1919	Computational design of binding proteins to EGFR domain II. **2014**, 9, e92513	7
1918	Biochemical and cellular evidence demonstrating AKT-1 as a binding partner for resveratrol targeting protein NQO2. **2014**, 9, e101070	25
1917	Surfactant protein D inhibits HIV-1 infection of target cells via interference with gp120-CD4 interaction and modulates pro-inflammatory cytokine production. **2014**, 9, e102395	24
1916	Differential binding of tenofovir and adefovir to reverse transcriptase of hepatitis B virus. **2014**, 9, e106324	17
1915	In silico and in vitro studies on the protein-protein interactions between Brugia malayi immunomodulatory protein calreticulin and human C1q. **2014**, 9, e106413	28
1914	Molecular handoffs in nitrergic neurotransmission. **2014**, 1, 8	11
1913	An In Silico Approach towards the Prediction of Druglikeness Properties of Inhibitors of Plasminogen Activator Inhibitor1. **2014**, 2014, 385418	2
1912	Structural Investigation of HSP70-HSP90 and HSP90-TDF Interactions. **2014**, 02,	
1911	In silico Interactive Study of Periplasmic and Outer Membrane Proteins of Type IV Secreting System (T4ss) in Helicobacter pylori. **2014**, 06,	0
1910	Identification of Novel Hepatitis C Virus NS3-4A Protease Inhibitors by Virtual Screening Approach. **2014**, 06,	1
1909	Computational drug designing of fungal pigments as potential aromatase inhibitors. **2014**, 9,	5
1908	A WXW motif is required for the anticancer activity of the TAT-RasGAP317-326 peptide. **2014**, 289, 23701-11	15
1907	Structural and functional characterization of the MERIT40 to understand its role in DNA repair. **2014**, 32, 2017-32	6

1906	Integrating in silico prediction methods, molecular docking, and molecular dynamics simulation to predict the impact of ALK missense mutations in structural perspective. **2014**, 2014, 895831		29
1905	Molecular Dynamics and Docking of Biphenyl: A Potential Attachment Inhibitor for HIV-1 gp120 Glycoprotein. **2014**, 13, 339		3
1904	CPB1 of Aedes aegypti interacts with DENV2 E protein and regulates intracellular viral accumulation and release from midgut cells. **2014**, 6, 5028-46		11
1903	Functional cross-talk between ras and rho pathways: a Ras-specific GTPase-activating protein (p120RasGAP) competitively inhibits the RhoGAP activity of deleted in liver cancer (DLC) tumor suppressor by masking the catalytic arginine finger. **2014**, 289, 6839-6849		22
1902	Knowledge-based search and multi-objective filters. **2014**,		
1901	Steric effect is a decisive factor on the orientation preference of guest into host: evidence from 5-indanol/ECD model. **2014**, 112, 1879-1891		7
1900	Chlorovirus Skp1-binding ankyrin repeat protein interplay and mimicry of cellular ubiquitin ligase machinery. **2014**, 88, 13798-810		7
1899	New strategies for integrative dynamic modeling of macromolecular assembly. **2014**, 96, 77-111		8
1898	Pleiotropic and epistatic behavior of a ring-hydroxylating oxygenase system in the polycyclic aromatic hydrocarbon metabolic network from Mycobacterium vanbaalenii PYR-1. **2014**, 196, 3503-15		26
1897	Accurate prediction of interfacial residues in two-domain proteins using evolutionary information: implications for three-dimensional modeling. **2014**, 82, 1219-34		6
1896	A real-time proximity querying algorithm for haptic-based molecular docking. **2014**, 169, 359-77		10
1895	A knowledge-based scoring function for protein-RNA interactions derived from a statistical mechanics-based iterative method. *Nucleic Acids Research*, **2014**, 42, e55	20.1	72
1894	Human protein Staufen-2 promotes HIV-1 proliferation by positively regulating RNA export activity of viral protein Rev. **2014**, 11, 18		13
1893	FK506-binding protein 12 modulates opioid receptor phosphorylation and protein kinase C()-dependent signaling by its direct interaction with the receptor. **2014**, 85, 37-49		9
1892	Cooperative gene regulation by microRNA pairs and their identification using a computational workflow. *Nucleic Acids Research*, **2014**, 42, 7539-52	20.1	61
1891	Metadynamics simulation study on the conformational transformation of HhaI methyltransferase: an induced-fit base-flipping hypothesis. **2014**, 2014, 304563		11
1890	The Bcl-2 homolog Nrz inhibits binding of IP3 to its receptor to control calcium signaling during zebrafish epiboly. **2014**, 7, ra14		30
1889	Structural insights into higher order assembly and function of the bacterial microcompartment protein PduA. **2014**, 289, 22377-84		54

1888	SAXS analysis of the tRNA-modifying enzyme complex MnmE/MnmG reveals a novel interaction mode and GTP-induced oligomerization. *Nucleic Acids Research*, **2014**, 42, 5978-92	20.1	21
1887	Structure-function correlation analysis of connexin50 missense mutations causing congenital cataract: electrostatic potential alteration could determine intracellular trafficking fate of mutants. **2014**, 2014, 673895		6
1886	Structure of a conserved Golgi complex-targeting signal in coronavirus envelope proteins. **2014**, 289, 12535-49		63
1885	Structural elucidation of a dual-activity PAP phosphatase-1 from Entamoeba histolytica capable of hydrolysing both 3'-phosphoadenosine 5'-phosphate and inositol 1,4-bisphosphate. **2014**, 70, 2019-31		6
1884	Drug resistance mechanism of PncA in Mycobacterium tuberculosis. **2014**, 32, 209-21		134
1883	Chicken MDA5 senses short double-stranded RNA with implications for antiviral response against avian influenza viruses in chicken. **2014**, 6, 58-71		45
1882	Clinically significant missense variants in human GALNT3, GALNT8, GALNT12, and GALNT13 genes: intriguing in silico findings. **2014**, 115, 313-27		13
1881	Reprogramming acyl carrier protein interactions of an Acyl-CoA promiscuous trans-acyltransferase. **2014**, 21, 636-46		33
1880	Alt a 1 from Alternaria interacts with PR5 thaumatin-like proteins. **2014**, 588, 1501-8		26
1879	Investigations towards understanding the thermal denaturation of lactoperoxidase. **2014**, 38, 47-54		8
1878	Modeling of Membrane Proteins. **2014**, 357-431		
1877	Identification of potential inhibitor targeting enoyl-acyl carrier protein reductase (InhA) in Mycobacterium tuberculosis: a computational approach. **2014**, 4, 253-261		1
1876	Insight into the oseltamivir resistance R292K mutation in H5N1 influenza virus: a molecular docking and molecular dynamics approach. **2014**, 68, 291-9		11
1875	Computational analysis of amprenavir resistance triple mutant (V32I, I47V and V82I) in HIV-1 protease. **2014**, 3, 1		
1874	Computational approaches and resources in single amino acid substitutions analysis toward clinical research. **2014**, 94, 365-423		19
1873	Molecular modeling of ABC transporter system - permease proteins from Microcoleus chthonoplastes PCC 7420 for effective binding against secreted aspartyl proteinases in Candida albicans - a therapeutic intervention. **2014**, 6, 63-70		5
1872	Differential antibiosis against Helicoverpa armigera exerted by distinct inhibitory repeat domains of Capsicum annuum proteinase inhibitors. **2014**, 101, 16-22		16
1871	On the use of knowledge-based potentials for the evaluation of models of protein-protein, protein-DNA, and protein-RNA interactions. **2014**, 94, 77-120		17

1870	Preparation and characterizations of solid/aqueous phases inclusion complex of 2,4-dinitroaniline with Ecyclodextrin. **2014**, 107, 72-84	26
1869	Integrative computational modeling of protein interactions. **2014**, 281, 1988-2003	77
1868	Spectral investigation and structural characterization of Dibenzalacetone: ECyclodextrin inclusion complex. **2014**, 1068, 155-163	22
1867	Study of inclusion complex between 2,6-dinitrobenzoic acid and Ecyclodextrin by 1H NMR, 2D 1H NMR (ROESY), FT-IR, XRD, SEM and photophysical methods. **2014**, 130, 105-15	26
1866	The role of pro-inflammatory S100A9 in Alzheimer's disease amyloid-neuroinflammatory cascade. **2014**, 127, 507-22	73
1865	Colorimetric engineered immunoprobe for the detection and quantification of microcystins. **2014**, 406, 124-30	7
1864	Antiviral activity of baicalin against influenza virus H1N1-pdm09 is due to modulation of NS1-mediated cellular innate immune responses. **2014**, 69, 1298-310	73
1863	Computational investigation of drug-resistant mutant of M2 proton channel (S31N) against rimantadine. **2014**, 70, 975-82	4
1862	Bordetella pertussis FbpA binds both unchelated iron and iron siderophore complexes. **2014**, 53, 3952-60	12
1861	Indicine N-oxide binds to tubulin at a distinct site and inhibits the assembly of microtubules: a mechanism for its cytotoxic activity. **2014**, 225, 66-77	19
1860	Computational modeling of protein-RNA complex structures. **2014**, 65, 310-9	24
1859	Molecular modeling of protein-protein interaction to decipher the structural mechanism of nonhost resistance in rice. **2014**, 32, 669-81	5
1858	In silico profiling and structural insights of missense mutations in RET protein kinase domain by molecular dynamics and docking approach. **2014**, 10, 421-36	21
1857	Inactivation of lipoxygenase and cyclooxygenase by natural betalains and semi-synthetic analogues. **2014**, 154, 246-54	71
1856	Computational design of a pH-sensitive IgG binding protein. **2014**, 111, 675-80	57
1855	Binding of the iminium and alkanolamine forms of sanguinarine to lysozyme: spectroscopic analysis, thermodynamics, and molecular modeling studies. **2014**, 118, 13077-91	50
1854	Berberine alters epigenetic modifications, disrupts microtubule network, and modulates HPV-18 E6-E7 oncoproteins by targeting p53 in cervical cancer cell HeLa: a mechanistic study including molecular docking. **2014**, 744, 132-46	33
1853	Predicting protein-ligand and protein-peptide interfaces. **2014**, 129, 1	4

1852	Pathway of human AS3MT arsenic methylation. **2014**, 27, 1979-89	85
1851	Comparative study of Plasmodium falciparum erythrocyte membrane protein 1-DBL□domain variants with respect to antigenic variations and docking interaction analysis with glycosaminoglycans. **2014**, 10, 2466-79	4
1850	Probabilistic models for capturing more physicochemical properties on protein-protein interface. **2014**, 54, 1798-809	13
1849	Immobilization of papain on nanoporous silica. **2014**, 4, 13304-13312	10
1848	A microscopic insight from conformational thermodynamics to functional ligand binding in proteins. **2014**, 10, 3280-9	16
1847	Peptides targeting chemokine receptor CXCR4: structural behavior and biological binding studies. **2014**, 20, 270-8	7
1846	The Fab conformations in the solution structure of human immunoglobulin G4 (IgG4) restrict access to its Fc region: implications for functional activity. **2014**, 289, 20740-56	30
1845	Aromatic interactions impact ligand binding and function at serotonin 5-HT G protein-coupled receptors: Receptor homology modeling, ligand docking, and molecular dynamics results validated by experimental studies. **2014**, 112, 398-407	11
1844	Attenuation of anti-tuberculosis therapy induced hepatotoxicity by Spirulina fusiformis, a candidate food supplement. **2014**, 24, 584-92	13
1843	Surface-induced conformational changes in doped bovine serum albumin self-assembled monolayers. **2014**, 136, 6151-4	14
1842	Selection of aptamers targeting the sialic acid receptor of hemagglutinin by epitope-specific SELEX. **2014**, 50, 8719-22	22
1841	2,6-Dinitroaniline and □cyclodextrin inclusion complex properties studied by different analytical methods. **2014**, 113, 577-87	23
1840	Binding mode analysis of a major T3SS translocator protein PopB with its chaperone PcrH from Pseudomonas aeruginosa. **2014**, 82, 3273-85	1
1839	Phosphorylation of an intrinsically disordered segment in Ets1 shifts conformational sampling toward binding-competent substates. **2014**, 22, 1196-1203	18
1838	Unexpected effects of the alteration of structure and stability of myoglobin and hemoglobin in ammonium-based ionic liquids. **2014**, 16, 5514-26	70
1837	Visual Analysis with Dynamic Geometric Complementarity and Physicochemical Matching in Protein Docking. **2014**,	1
1836	Identification of novel leads applying in silico studies for Mycobacterium multidrug resistant (MMR) protein. **2014**, 32, 1889-906	15
1835	Molecular docking of bacosides with tryptophan hydroxylase: a model to understand the bacosides mechanism. **2014**, 4, 251-5	7

1834	Architecture of the Saccharomyces cerevisiae RNA polymerase I Core Factor complex. **2014**, 21, 810-6	38
1833	A novel insulin receptor-binding protein from Momordica charantia enhances glucose uptake and glucose clearance in vitro and in vivo through triggering insulin receptor signaling pathway. **2014**, 62, 8952-61	35
1832	Exploring the structural and functional impact of the ALK F1174L mutation using bioinformatics approach. **2014**, 20, 2324	13
1831	Modelling the structure of full-length Epstein-Barr virus nuclear antigen 1. **2014**, 49, 358-72	11
1830	Modeling protein assemblies in the proteome. **2014**, 13, 887-96	13
1829	Communication of □phage lysin plyG enzymes binding toward SrtA for inhibition of Bacillus anthracis: protein-protein interaction and molecular dynamics study. **2014**, 21, 257-65	4
1828	Inhibition of the human respiratory syncytial virus small hydrophobic protein and structural variations in a bicelle environment. **2014**, 88, 11899-914	34
1827	Ribonomic approaches to study the RNA-binding proteome. **2014**, 588, 3649-64	29
1826	Conformational adaptation in the E. coli sigma 32 protein in response to heat shock. **2014**, 118, 4793-802	8
1825	Study of the cyclodextrin and its complexation with 2,4-dinitrobenzoic acid through photophysical properties and 2D NMR spectroscopy. **2014**, 1060, 239-250	6
1824	ZDOCK server: interactive docking prediction of protein-protein complexes and symmetric multimers. **2014**, 30, 1771-3	903
1823	Selective eradication of tumor vascular pericytes by peptide-conjugated nanoparticles for antiangiogenic therapy of melanoma lung metastasis. **2014**, 35, 3060-70	56
1822	Pesticides in mixture disrupt metabolic regulation: in silico and in vivo analysis of cumulative toxicity of mancozeb and imidacloprid on body weight of mice. **2014**, 205, 226-34	28
1821	Allantoinase and dihydroorotase binding and inhibition by flavonols and the substrates of cyclic amidohydrolases. **2014**, 101, 113-22	21
1820	Search strategies and evaluation in protein-protein docking: principles, advances and challenges. **2014**, 19, 1081-96	107
1819	Interaction between DNA and cationic diester-bonded Gemini surfactants. **2014**, 197, 322-327	25
1818	N-phenyl-1-naphthylamine/□cyclodextrin inclusion complex as a new fluorescent probe for rapid and visual detection of Pd(2+). **2014**, 133, 73-9	23
1817	In silico assessment of interaction of sea anemone toxin APETx2 and acid sensing ion channel 3. **2014**, 450, 384-9	5

1816	Mass spectrometry defines the C-terminal dimerization domain and enables modeling of the structure of full-length OmpA. **2014**, 22, 781-90	46
1815	Protein-protein interactions: switch from classical methods to proteomics and bioinformatics-based approaches. **2014**, 71, 205-28	84
1814	Neuroglobin as a regulator of mitochondrial-dependent apoptosis: a bioinformatics analysis. **2014**, 33, 111-6	26
1813	Large oligomeric complex structures can be computationally assembled by efficiently combining docked interfaces. **2015**, 83, 1887-99	2
1812	Different combinations of atomic interactions predict protein-small molecule and protein-DNA/RNA affinities with similar accuracy. **2015**, 83, 2100-14	11
1811	Discovery of small molecule inhibitors of MyD88-dependent signaling pathways using a computational screen. **2015**, 5, 14246	32
1810	Extension of resolution and oligomerization-state studies of 2,4'-dihydroxyacetophenone dioxygenase from Alcaligenes sp. 4HAP. **2015**, 71, 1258-63	5
1809	Assessing Structural Predictions of Protein-Protein Recognition: The CAPRI Experiment. **2015**, 137-173	3
1808	Applying Side-chain Flexibility in Motifs for Protein Docking. **2015**, 8, 1-10	3
1807	Structural analysis of Clostridium acetobutylicum ATCC 824 glycoside hydrolase from CAZy family GH105. **2015**, 71, 1100-8	1
1806	Force-sensitive autoinhibition of the von Willebrand factor is mediated by interdomain interactions. **2015**, 108, 2312-21	49
1805	Modeling of interaction between cytochrome c and the WD domains of Apaf-1: bifurcated salt bridges underlying apoptosome assembly. **2015**, 10, 29	11
1804	Novel p16 binding peptide development for p16-overexpressing cancer cell detection using phage display. **2015**, 21, 265-73	3
1803	Known structure, unknown function: An inquiry-based undergraduate biochemistry laboratory course. **2015**, 43, 245-62	29
1802	Mechanistic analysis elucidating the relationship between Lys96 mutation in Mycobacterium tuberculosis pyrazinamidase enzyme and pyrazinamide susceptibility. **2015**, 16 Suppl 2, S14	27
1801	Predicted binding site information improves model ranking in protein docking using experimental and computer-generated target structures. **2015**, 15, 23	6
1800	Mechanistic studies of the apical sodium-dependent bile acid transporter. **2015**, 83, 1107-17	6
1799	In Vivo Anti-Hyperglycemic Potential of Brahmi Gritham and Docking Studies of Its Active Components Against Protein Kinase C and CD38. **2015**, 39, 642-652	1

1798	AbDesign: An algorithm for combinatorial backbone design guided by natural conformations and sequences. **2015**, 83, 1385-406	55
1797	Structural determinants for the interactions between muscarinic toxin 7 and muscarinic acetylcholine receptors. **2015**, 28, 239-52	4
1796	Double Variational Binding--(SMILES) Conformational Analysis by Docking Mechanisms for Anti-HIV Pyrimidine Ligands. **2015**, 16, 19553-601	5
1795	Prediction of Protein-Ligand Binding Sites for Cisplatin and Transplatin based on Hydrogen Bonds. **2015**, 8,	
1794	Design of a Recombinant Hepatitis B Vaccine Based on Stably Binding HLA-I Peptides. **2015**, 04,	1
1793	Computational Prediction of RNA-Binding Proteins and Binding Sites. **2015**, 16, 26303-17	47
1792	Evolution of Macromolecular Docking Techniques: The Case Study of Nickel and Iron Metabolism in Pathogenic Bacteria. **2015**, 20, 14265-92	3
1791	Interaction pattern for the complex of B-DNA Fullerene compounds with a set of known replication proteins using docking study. **2015**, 11, 122-6	
1790	VORFFIP-driven dock: V-D2OCK, a fast and accurate protein docking strategy. **2015**, 10, e0118107	17
1789	Stability of the octameric structure affects plasminogen-binding capacity of streptococcal enolase. **2015**, 10, e0121764	8
1788	Structure, dynamics, and interaction of Mycobacterium tuberculosis (Mtb) DprE1 and DprE2 examined by molecular modeling, simulation, and electrostatic studies. **2015**, 10, e0119771	20
1787	Inhibition of a Putative Dihydropyrimidinase from Pseudomonas aeruginosa PAO1 by Flavonoids and Substrates of Cyclic Amidohydrolases. **2015**, 10, e0127634	15
1786	Suramin Inhibits Chikungunya Virus Entry and Transmission. **2015**, 10, e0133511	48
1785	Designing Second Generation Anti-Alzheimer Compounds as Inhibitors of Human Acetylcholinesterase: Computational Screening of Synthetic Molecules and Dietary Phytochemicals. **2015**, 10, e0136509	19
1784	Comparative Proteomic Analysis of Aminoglycosides Resistant and Susceptible Mycobacterium tuberculosis Clinical Isolates for Exploring Potential Drug Targets. **2015**, 10, e0139414	45
1783	The interaction of RNA helicase DDX3 with HIV-1 Rev-CRM1-RanGTP complex during the HIV replication cycle. **2015**, 10, e0112969	20
1782	Surfing the Protein-Protein Interaction Surface Using Docking Methods: Application to the Design of PPI Inhibitors. **2015**, 20, 11569-603	45
1781	Effect of Environmental Chemical Stress on Nuclear Noncoding RNA Involved in Epigenetic Control. **2015**, 2015, 761703	3

1780	Structure Analysis of Interacting Domains of RNA Dependent RNA Polymerase (Rdrp) Complex in Nipah Virus. **2015**, 04,		1
1779	The two paralogue phoN (phosphinothricin acetyl transferase) genes of Pseudomonas putida encode functionally different proteins. **2015**, 17, 3330-40		5
1778	New avenue in the treatment of temporal lobe epilepsy by classical anti-epileptics: A hypothetical establishment of executioner Caspase 3 inactivation by molecular modeling. **2015**, 6, 65-74		1
1777	Amiloride and GMQ Allosteric Modulation of the GABA-A ρ1 Receptor: Influences of the Intersubunit Site. **2015**, 353, 551-9		5
1776	A Computational Structural Biology of SoxR and DNA: A Modelling and Interactive Discern to Express the Sox Operon in Pseudaminobacter salicylatoxidans (KCT001) for Global Sulphur Oxidation. **2015**, 603-611		1
1775	Structural analysis of the interleukin-8/glycosaminoglycan interactions by amide hydrogen/deuterium exchange mass spectrometry. **2015**, 89, 45-53		16
1774	A differentially conserved residue (Ile42) of GH42 β-galactosidase from Geobacillus stearothermophilus BgaB is involved in both catalysis and thermostability. **2015**, 98, 2268-76		8
1773	Side-chain flexibility in protein docking. **2015**,		
1772	Crystal structures of the Gon7/Pcc1 and Bud32/Cgi121 complexes provide a model for the complete yeast KEOPS complex. *Nucleic Acids Research*, **2015**, 43, 3358-72	20.1	28
1771	Structure of the 34 kDa F-actin-bundling protein ABP34 from Dictyostelium discoideum. **2015**, 71, 1835-49		3
1770	UBE3A Regulates Synaptic Plasticity and Learning and Memory by Controlling SK2 Channel Endocytosis. **2015**, 12, 449-61		75
1769	Selection of effective and highly thermostable Bacillus subtilis lipase A template as an industrial biocatalyst-A modern computational approach. **2015**, 10, 508-519		9
1768	3D Reconstruction of a Full-Size GABAB Receptor. **2015**, 47, 364-375		3
1767	RACK1 (receptor for activated C-kinase 1) interactions with spectrin repeat elements. **2015**, 28, 49-58		3
1766	Adaptability in protein structures: structural dynamics and implications in ligand design. **2015**, 33, 298-321		6
1765	Selection and screening of microbial consortia for efficient and ecofriendly degradation of plastic garbage collected from urban and rural areas of Bangalore, India. **2015**, 187, 4174		31
1764	The conundrum of the high-affinity NGF binding site formation unveiled?. **2015**, 108, 687-97		15
1763	Characterization of ICAM-1 biophore to design cytoadherence blocking peptides. **2015**, 57, 27-35		8

1762	A web interface for easy flexible protein-protein docking with ATTRACT. **2015**, 108, 462-5	69
1761	Lipid regulation of the ABCB1 and ABCG2 multidrug transporters. **2015**, 125, 97-137	22
1760	Genetic and antigenic structural characterization for resistance of echovirus 11 to pleconaril in an immunocompromised patient. **2015**, 96, 571-579	11
1759	Molecular modeling and correlation of PFI1625c-peptide models of bioactive peptides with antimalarial properties. **2015**, 24, 1527-1533	6
1758	Cross talk between Leishmania donovani CpG DNA and Toll-like receptor 9: an immunoinformatics approach. **2015**, 459, 424-9	13
1757	Proteomic analysis of ofloxacin-mono resistant Mycobacterium tuberculosis isolates. **2015**, 127, 114-21	33
1756	RNA-LIM: a novel procedure for analyzing protein/single-stranded RNA propensity data with concomitant estimation of interface structure. **2015**, 472, 52-61	2
1755	Effect of graphene oxide on the conformational transitions of amyloid beta peptide: A molecular dynamics simulation study. **2015**, 61, 175-85	52
1754	Preparation, characterization and molecular modeling studies of the inclusion complex of Caffeine with Beta-cyclodextrin. **2015**, 1099, 616-624	39
1753	Molecular level biodegradation of phenol and its derivatives through dmp operon of Pseudomonas putida: A bio-molecular modeling and docking analysis. **2015**, 36, 144-51	10
1752	Preparation, physicochemical analysis and molecular modeling investigation of 2,2?-Bipyridine: □Cyclodextrin inclusion complex in solution and solid state. **2015**, 1100, 59-69	17
1751	□Synuclein dimer structures found from computational simulations. **2015**, 116, 133-40	9
1750	Engineering of a disulfide loop instead of a Zn binding loop restores the anti-proliferative, anti-angiogenic and anti-tumor activities of the N-terminal fragment of endostatin: Mechanistic and therapeutic insights. **2015**, 72, 73-82	9
1749	Biochemical and Structural Basis for Controlling Chemical Modularity in Fungal Polyketide Biosynthesis. **2015**, 137, 9885-93	44
1748	Synthesis, structure, protein binding of Cu(II) complexes with a tridentate NNO Schiff-base ligand. **2015**, 150, 290-300	10
1747	Evaluation of anti-diabetic and alpha glucosidase inhibitory action of anthraquinones from Rheum emodi. **2015**, 6, 2693-700	50
1746	DockStar: a novel ILP-based integrative method for structural modeling of multimolecular protein complexes. **2015**, 31, 2801-7	9
1745	Preparation and characterization of host-guest system between inosine and □cyclodextrin through inclusion mode. **2015**, 147, 151-7	18

1744	Study on the interaction of artificial and natural food colorants with human serum albumin: A computational point of view. **2015**, 56, 152-8		52
1743	Probing the protein interaction network of Pseudomonas aeruginosa cells by chemical cross-linking mass spectrometry. **2015**, 23, 762-73		59
1742	High-throughput screening-compatible assays of As(III) S-adenosylmethionine methyltransferase activity. **2015**, 480, 67-73		8
1741	Biochemical Characterization and Computational Identification of Mycobacterium tuberculosis Pyrazinamidase in Some Pyrazinamide-Resistant Isolates of Iran. **2015**, 34, 181-92		6
1740	In silico study of peptide inhibitors against BACE 1. **2015**, 9, 67-72		4
1739	The internal gene duplication and interrupted coding sequences in the MmpL genes of Mycobacterium tuberculosis: Towards understanding the multidrug transport in an evolutionary perspective. **2015**, 305, 413-23		30
1738	Assembling the pieces of macromolecular complexes: Hybrid structural biology approaches. **2015**, 15, 2792-803		15
1737	Cross-protection of influenza A virus infection by a DNA aptamer targeting the PA endonuclease domain. **2015**, 59, 4082-93		34
1736	Identifying a potential receptor for the antibacterial peptide of sponge Axinella donnani endosymbiont. **2015**, 566, 166-74		3
1735	The solution structures of two human IgG1 antibodies show conformational stability and accommodate their C1q and FcR ligands. **2015**, 290, 8420-38		25
1734	Exploring the potential of global protein-protein docking: an overview and critical assessment of current programs for automatic ab initio docking. **2015**, 20, 969-77		66
1733	Antibody specific epitope prediction-emergence of a new paradigm. **2015**, 11, 98-102		38
1732	Autophagy protein Ulk1 promotes mitochondrial apoptosis through reactive oxygen species. **2015**, 89, 311-21		30
1731	NPDock: a web server for protein-nucleic acid docking. *Nucleic Acids Research*, **2015**, 43, W425-30	20.1	133
1730	Inclusion Complexation of Acetanilide into the Cyclodextrin Nanocavity: A Computational Approach. **2015**, 10, 467-475		2
1729	Host-Microbe Protein Interactions during Bacterial Infection. **2015**, 22, 1521-1530		75
1728	The SPL7013 dendrimer destabilizes the HIV-1 gp120-CD4 complex. **2015**, 7, 18628-41		34
1727	Differential ubiquitin binding by the acidic loops of Ube2g1 and Ube2r1 enzymes distinguishes their Lys-48-ubiquitylation activities. **2015**, 290, 2251-63		16

1726	Computational elucidation of potential antigenic CTL epitopes in Ebola virus. **2015**, 36, 369-375	26
1725	Ca(2+) Interacts with Glu-22 of A(1-42) and Phospholipid Bilayers to Accelerate the A(1-42) Aggregation Below the Critical Micelle Concentration. **2015**, 54, 6323-32	12
1724	Algorithm to design inhibitors using stereochemically mixed l,d polypeptides: Validation against HIV protease. **2015**, 81, 410-7	1
1723	Prion Protein-Antibody Complexes Characterized by Chromatography-Coupled Small-Angle X-Ray Scattering. **2015**, 109, 793-805	28
1722	Photophysical and photoprototropic characteristics of phenothiazine in aqueous and cyclodextrin media. **2015**, 168, 245-255	5
1721	idDock+: Integrating Machine Learning in Probabilistic Search for Protein-Protein Docking. **2015**, 22, 806-22	5
1720	High-resolution protein-protein docking by global optimization: recent advances and future challenges. **2015**, 35, 24-31	30
1719	Comparative analysis of the mechanisms of sulfur anion oxidation and reduction by dsr operon to maintain environmental sulfur balance. **2015**, 59 Pt A, 177-84	2
1718	In silico prediction of ebolavirus RNA polymerase inhibition by specific combinations of approved nucleotide analogues. **2015**, 73, 89-94	3
1717	Fluorometric sensing of Pb2+ and CrO42 ions through hostguest inclusion for human lung cancer live cell imaging. **2015**, 5, 101802-101818	14
1716	Beware of docking!. **2015**, 36, 78-95	329
1715	Structural characterizations of metal ion binding transcriptional regulator CueR from opportunistic pathogen pseudomonas aeruginosa to identify its possible involvements in virulence. **2015**, 175, 649-56	6
1714	Overview of computational vaccinology: vaccine development through information technology. **2015**, 56, 381-91	9
1713	Enhancement of Internal Motions of Lysozyme through Interaction with Gold Nanoclusters and its Optical Imaging. **2015**, 119, 653-664	15
1712	Molecular interactions of agonist and inverse agonist ligands at serotonin 5-HT2C G protein-coupled receptors: computational ligand docking and molecular dynamics studies validated by experimental mutagenesis results. **2015**, 113, 348-358	3
1711	Global Optimization of Proteinpeptide Docking by a Filling Function Method. **2015**, 164, 1090-1108	3
1710	Fatty acid biosynthesis revisited: structure elucidation and metabolic engineering. **2015**, 11, 38-59	119
1709	Mapping of the interaction domains of the Crimean-Congo hemorrhagic fever virus nucleocapsid protein. **2015**, 96, 524-537	11

1708	Structural characterization of Fis - A transcriptional regulator from pathogenic Pasteurella multocida essential for expression of virulence factors. **2015**, 554, 249-53	3
1707	Selective acquisition of host-derived ICAM-1 by HIV-1 is a matrix-dependent process. **2015**, 89, 323-36	10
1706	Investigation on inter molecular complexation between 4,4?-methylene-bis(N,N-dimethylaniline) and Ecyclodextrin: Preparation and characterization in aqueous medium and solid state. **2015**, 1080, 69-79	13
1705	Naturally Occurring Enzyme Inhibitors: A Smart Way to Fight against Micro- Inflammation in Human Gut. **2016**, 3,	
1704	Glycyrrhizic Acid Reduces Heart Rate and Blood Pressure by a Dual Mechanism. **2016**, 21,	7
1703	Structure-Based Pharmacophore Modeling, Virtual Screening and Molecular docking for the Treatment of ESR1 Mutations in Breast Cancer. **2016**, 05,	7
1702	In Silico Identification and Molecular Validation of Putative Antimicrobial Peptides for HIV Therapy. **2016**, 7,	10
1701	Geometric Simulation Approach for Grading and Assessing the Thermostability of CALBs. **2016**, 2016, 4101059	2
1700	Structural Stability, Transitions, and Interactions within SoxYZCD-Thiosulphate from : An Molecular Outlook for Maintaining Environmental Sulphur Cycle. **2016**, 2016, 8683713	0
1699	In Silico Approach for SAR Analysis of the Predicted Model of DEPDC1B: A Novel Target for Oral Cancer. **2016**, 2016, 3136024	9
1698	Probing Synechocystis-Arsenic Interactions through Extracellular Nanowires. **2016**, 7, 1134	12
1697	Cytosolic Proteome Profiling of Aminoglycosides Resistant Clinical Isolates Using MALDI-TOF/MS. **2016**, 7, 1816	29
1696	Role of Pea Enation Mosaic Virus Coat Protein in the Host Plant and Aphid Vector. **2016**, 8,	5
1695	Antibody Aggregation: Insights from Sequence and Structure. **2016**, 5,	47
1694	Identification of internalin-A-like virulent proteins in Leishmania donovani. **2016**, 9, 557	2
1693	Daboxin P, a Major Phospholipase A2 Enzyme from the Indian Daboia russelii russelii Venom Targets Factor X and Factor Xa for Its Anticoagulant Activity. **2016**, 11, e0153770	20
1692	Novel Nuclear Factor-KappaB Targeting Peptide Suppresses Amyloid Induced Inflammatory and Apoptotic Responses in Neuronal Cells. **2016**, 11, e0160314	12
1691	Coupling Genotyping and Computational Modeling in Prediction of Anti-epileptic Drugs that cause Stevens Johnson Syndrome and Toxic Epidermal Necrolysis for Carrier of HLA-B*15:02. **2016**, 19, 147-60	5

1690	Insights into HIV-1 proviral transcription from integrative structure and dynamics of the Tat:AFF4:P-TEFb:TAR complex. **2016**, 5,	28
1689	Structural and biochemical characterization of EDTA monooxygenase and its physical interaction with a partner flavin reductase. **2016**, 100, 989-1003	13
1688	The multiple stress responsive transcriptional regulator Rv3334 of Mycobacterium tuberculosis is an autorepressor and a positive regulator of kstR. **2016**, 283, 3056-71	7
1687	In planta chemical cross-linking and mass spectrometry analysis of protein structure and interaction in Arabidopsis. **2016**, 16, 1915-27	11
1686	Receptor Activity-modifying Proteins 2 and 3 Generate Adrenomedullin Receptor Subtypes with Distinct Molecular Properties. **2016**, 291, 11657-75	34
1685	Cloning, purification, and characterization of xylose isomerase from Thermotoga naphthophila RKU-10. **2016**, 56, 949-62	12
1684	3D Structure, Dimerization Modeling, and Lead Discovery by Ligand-protein Interaction Analysis of p60 Transcription Regulator Protein (p60TRP). **2016**, 35, 99-108	6
1683	Synthesis, spectroscopic and computational studies of 2-(thiophen-2-yl)-2,3-dihydro-1H-perimidine: An enzymes inhibition study. **2016**, 64, 185-201	25
1682	Mutational analysis and interactions of HBV preS1 with asialoglycoprotein receptor. **2016**, 11, 761-774	1
1681	Glycogen synthase kinase 3β suppresses polyglutamine aggregation by inhibiting Vaccinia-related kinase 2 activity. **2016**, 6, 29097	9
1680	A structural insight into the negative effects of opioids in analgesia by modulating the TLR4 signaling: An in silico approach. **2016**, 6, 39271	20
1679	Accelerating protein-protein complex validation by GPU based funnel generation. **2016**,	
1678	Acetylcholinesterase and Cytotoxic Activity of Chemical Constituents of Clutia lanceolata Leaves and its Molecular Docking Study. **2016**, 6, 267-278	10
1677	The drug ornidazole inhibits photosynthesis in a different mechanism described for protozoa and anaerobic bacteria. **2016**, 473, 4413-4426	7
1676	A putative nitroreductase from the DosR regulon of Mycobacterium tuberculosis induces pro-inflammatory cytokine expression via TLR2 signaling pathway. **2016**, 6, 24535	15
1675	Lipid-II Independent Antimicrobial Mechanism of Nisin Depends On Its Crowding And Degree Of Oligomerization. **2016**, 6, 37908	62
1674	A Novel PD-L1-targeting Antagonistic DNA Aptamer With Antitumor Effects. **2016**, 5, e397	72
1673	In silico selection of an aptamer to estrogen receptor alpha using computational docking employing estrogen response elements as aptamer-alike molecules. **2016**, 6, 21285	71

1672	Involvement of three putative glucosyltransferases from the UGT72 family in flavonol glucoside/rhamnoside biosynthesis in Lotus japonicus seeds. **2017**, 68, 597-612		23
1671	Binding interaction of a gamma-aminobutyric acid derivative with serum albumin: an insight by fluorescence and molecular modeling analysis. **2016**, 5, 1121		16
1670	Antimicrobial peptide Microcin C7 as an alternative drug candidate against Diphtheria toxin. **2016**,		
1669	Preparation and characterization of a imipramine-□cyclodextrin inclusion complex. **2016**, 44, 651-671		4
1668	Molecular determinants and interaction data of cyclic peptide inhibitor with the extracellular domain of TrkB receptor. **2016**, 6, 776-82		5
1667	Exploration of the binding modes of L-asparaginase complexed with its amino acid substrates by molecular docking, dynamics and simulation. **2016**, 6, 105		6
1666	Scratching the Surface: Resurfacing Proteins to Endow New Properties and Function. **2016**, 23, 543-553		16
1665	Amelioration of anti-tuberculosis drug induced oxidative stress in kidneys by Spirulina fusiformis in a rat model. **2016**, 38, 1115-21		13
1664	Effect of Silver Nanoparticles Against the Formation of Biofilm by Pseudomonas aeruginosa an In silico Approach. **2016**, 180, 426-437		18
1663	Bioinformatic analysis of human G□ Q209 missense mutations associated with uveal melanoma. **2016**,		2
1662	Predicting Protein-Protein Interactions from the Molecular to the Proteome Level. **2016**, 116, 4884-909		192
1661	Etodolac:□cyclodextrin inclusion complex as a novel fluorescent chemosensor probe for Ba2+. **2016**, 35, 118-130		13
1660	Fibromodulin: a master regulator of myostatin controlling progression of satellite cells through a myogenic program. **2016**, 30, 2708-19		40
1659	A study of host-guest complexation between amodiaquine and native cyclodextrin. Characterization in solid state and its in-vitro anticancer activity. **2016**, 53, 282-289		7
1658	Discovery of potential ALK inhibitors by virtual screening approach. **2016**, 6, 21		4
1657	New Bio-Based Cu(II) Complexes and Study of their Anti-Cancer Activities. **2016**, 26, 1183-97		3
1656	FoXS, FoXSDock and MultiFoXS: Single-state and multi-state structural modeling of proteins and their complexes based on SAXS profiles. *Nucleic Acids Research*, **2016**, 44, W424-9	20.1	260
1655	XLinkDB 2.0: integrated, large-scale structural analysis of protein crosslinking data. **2016**, 32, 2716-8		42

1654	Integrating error-prone PCR and DNA shuffling as an effective molecular evolution strategy for the production of □ketoglutaric acid by L-amino acid deaminase. **2016**, 6, 46149-46158		8
1653	Host-guest interaction of cytidine in □cyclodextrin microcavity: Characterization and docking study. **2016**, 219, 967-974		19
1652	Computational docking, molecular dynamics simulation and subsite structure analysis of a maltogenic amylase from Bacillus lehensis G1 provide insights into substrate and product specificity. **2016**, 67, 1-13		11
1651	Elucidation, functional clustering and structural characterization of □rCP1 substrates through a molecular dynamics study. **2016**, 12, 2233-46		10
1650	InterEvDock: a docking server to predict the structure of protein-protein interactions using evolutionary information. *Nucleic Acids Research*, **2016**, 44, W542-9	20.1	52
1649	Host-guest molecular recognition based fluorescence On-Off-On chemosensor for nanomolar level detection of Cu2+ and Cr2O72□ions: Application in XNOR logic gate and human lung cancer living cell imaging. **2016**, 234, 300-315		46
1648	Synthesis, characterization, molecular docking and biological studies of self assembled transition metal dithiocarbamates of substituted pyrrole-2-carboxaldehyde. **2016**, 160, 392-9		17
1647	Synergistic Neutralization of Pertussis Toxin by a Bispecific Antibody In Vitro and In Vivo. **2016**, 23, 851-862		11
1646	Single-walled carbon nanotube release affects the microbial enzyme-catalyzed oxidation processes of organic pollutants and lignin model compounds in nature. **2016**, 163, 217-226		46
1645	Spherical polar Fourier assembly of protein complexes with arbitrary point group symmetry. **2016**, 49, 158-167		28
1644	PRISM-EM: template interface-based modelling of multi-protein complexes guided by cryo-electron microscopy density maps. **2016**, 72, 1137-1148		12
1643	2H1NA/□cyclodextrin inclusion complex: Preparation, characterization and chemosensory application for detecting Ag+. **2016**, 53, 677-686		6
1642	Osteocalcin and Sex Hormone Binding Globulin Compete on a Specific Binding Site of GPRC6A. **2016**, 157, 4473-4486		36
1641	Ubiquitin Ligase COP1 Controls Hepatic Fat Metabolism by Targeting ATGL for Degradation. **2016**, 65, 3561-3572		24
1640	A far-red fluorescent protein evolved from a cyanobacterial phycobiliprotein. **2016**, 13, 763-9		119
1639	Normalization of NAD+ Redox Balance as a Therapy for Heart Failure. **2016**, 134, 883-94		164
1638	Studies on binding mechanism between carotenoids from sea buckthorn and thermally treated □actalbumin. **2016**, 1125, 721-729		17
1637	Characterization of molecular interactions between Escherichia coli RNA polymerase and topoisomerase I by molecular simulations. **2016**, 590, 2844-51		9

1636	Inhibition of sodium glucose cotransporters following status epilepticus induced by intrahippocampal pilocarpine affects neurodegeneration process in hippocampus. **2016**, 61, 258-268	12
1635	Dual targeting of MDM2 with a novel small-molecule inhibitor overcomes TRAIL resistance in cancer. **2016**, 37, 1027-1040	14
1634	Transporter engineering and enzyme evolution for pyruvate production from D/L-alanine with a whole-cell biocatalyst expressing L-amino acid deaminase from Proteus mirabilis. **2016**, 6, 82676-82684	15
1633	Computational prediction and analysis of potential antigenic CTL epitopes in Zika virus: A first step towards vaccine development. **2016**, 45, 187-197	36
1632	Elucidating modes of activation and herbicide resistance by sequence assembly and molecular modelling of the Acetolactate synthase complex in sugarcane. **2016**, 407, 184-197	6
1631	Structural and functional insights into the stationary-phase survival protein SurE, an important virulence factor of Brucella abortus. **2016**, 72, 386-96	
1630	High-throughput screening for the identification of small-molecule inhibitors of the flaviviral protease. **2016**, 134, 6-16	17
1629	A Novel Spirooxindole Derivative Inhibits the Growth of Leishmania donovani Parasites both In Vitro and In Vivo by Targeting Type IB Topoisomerase. **2016**, 60, 6281-93	36
1628	Interaction of Individual Structural Domains of hnRNP LL with the BCL2 Promoter i-Motif DNA. **2016**, 138, 10950-62	32
1627	Minicollagen cysteine-rich domains encode distinct modes of polymerization to form stable nematocyst capsules. **2016**, 6, 25709	11
1626	Protein-RNA interactions: structural biology and computational modeling techniques. **2016**, 8, 359-367	15
1625	InteractoMIX: a suite of computational tools to exploit interactomes in biological and clinical research. **2016**, 44, 917-24	3
1624	von Willebrand factor is dimerized by protein disulfide isomerase. **2016**, 127, 1183-91	33
1623	In-silico structural analysis of E509K mutation in LARGE and T192M mutation in Alpha Dystroglycan in the inhibition of glycosylation of Alpha Dystroglycan by LARGE. **2016**, 64, 313-321	2
1622	Atomic-Level Characterization of the Chain-Flipping Mechanism in Fatty-Acids Biosynthesis. **2016**, 7, 2899-904	15
1621	Anin silicoapproach predicted potential therapeutics that can confer protection from maximum pathogenic Hantaviruses. **2016**, 11, 411-428	3
1620	Identification of a novel splice site HSPG2 mutation and prenatal diagnosis in Schwartz Jampel Syndrome type 1 using whole exome sequencing. **2016**, 26, 809-814	7
1619	Encapsulation of dicinnamalacetone in □cyclodextrin: A physicochemical evaluation and molecular modeling approach on 1:2 inclusion complex. **2016**, 53, 546-556	6

1618	Gliptins in managing diabetes - Reviewing computational strategy. **2016**, 166, 108-120	22
1617	Rigid-Docking Approaches to Explore Protein-Protein Interaction Space. **2017**, 160, 33-55	4
1616	Inhibition of preS1-hepatocyte interaction by an array of recombinant human antibodies from naturally recovered individuals. **2016**, 6, 21240	16
1615	New cobalt(II) and nickel(II) complexes of benzyl carbazate Schiff bases: Syntheses, crystal structures, in vitro DNA and HSA binding studies. **2016**, 165, 220-231	39
1614	Translational Biomedical Informatics. **2016**,	1
1613	In vivo continuous evolution of genes and pathways in yeast. **2016**, 7, 13051	68
1612	Self-Assembly of Catenanes from Lasso Peptides. **2016**, 138, 14214-14217	28
1611	In Silico Aptamer Docking Studies: From a Retrospective Validation to a Prospective Case Study-TIM3 Aptamers Binding. **2016**, 5, e376	28
1610	Comparative Structural and Computational Analysis Supports Eighteen Cellulose Synthases in the Plant Cellulose Synthesis Complex. **2016**, 6, 28696	104
1609	Spectral characteristics of desipramine in □-cyclodextrin cavity through inclusion complex. **2016**, 53, 781-790	6
1608	GalaxyRefineComplex: Refinement of protein-protein complex model structures driven by interface repacking. **2016**, 6, 32153	55
1607	Exploring Human Diseases and Biological Mechanisms by Protein Structure Prediction and Modeling. **2016**, 939, 39-61	2
1606	Structural insights into functional amyloid inhibition in Gram -ve bacteria. **2016**, 44, 1643-1649	9
1605	Unraveling the Deleterious Effects of Cancer-Driven STK11 Mutants Through Conformational Sampling Approach. **2016**, 15, 35-44	3
1604	Computational study concerning the effect of some pesticides on the Proteus Mirabilis catalase activity. **2016**,	1
1603	Insights into the binding of ferulic acid to the thermally treated xanthine oxidase. **2016**, 31, 1259-1266	12
1602	A novel small-molecule compound disrupts influenza A virus PB2 cap-binding and inhibits viral replication. **2016**, 71, 2489-97	26
1601	In silico analysis for prediction of degradative capacity of Pseudomonas putida SF1. **2016**, 591, 382-92	20

1600	Neddylation requires glycyl-tRNA synthetase to protect activated E2. **2016**, 23, 730-7	29
1599	In Vivo Conformational Dynamics of Hsp90 and Its Interactors. **2016**, 23, 716-26	55
1598	Potent acetylcholinesterase inhibitors: Synthesis, biological assay and docking study of nitro acridone derivatives. **2016**, 161, 304-11	15
1597	Conformational Heterogeneity of Unbound Proteins Enhances Recognition in Protein-Protein Encounters. **2016**, 12, 3236-49	9
1596	Peptide-Mediated Interference of PB2-eIF4G1 Interaction Inhibits Influenza A Viruses' Replication in Vitro and in Vivo. **2016**, 2, 471-7	5
1595	HP- cyclodextrin as an inhibitor of amyloid- aggregation and toxicity. **2016**, 18, 20476-85	34
1594	Probing molecular basis of single-walled carbon nanotube degradation and nondegradation by enzymes based on manganese peroxidase and lignin peroxidase. **2016**, 6, 3592-3599	23
1593	Molecular principles behind pyrazinamide resistance due to mutations in panD gene in Mycobacterium tuberculosis. **2016**, 581, 31-42	29
1592	Leishmania donovani Encodes a Functional Selenocysteinyl-tRNA Synthase. **2016**, 291, 1203-20	10
1591	Interaction Mechanism of Doxorubicin and SWCNT: Protonation and Diameter Effects on the Drug Loading and Releasing. **2016**, 6, 314-322	51
1590	Visualization of Host-Polerovirus Interaction Topologies Using Protein Interaction Reporter Technology. **2016**, 90, 1973-87	33
1589	Silver(I) complexes with phthalazine and quinazoline as effective agents against pathogenic Pseudomonas aeruginosa strains. **2016**, 155, 115-28	53
1588	Ole e 13 is the unique food allergen in olive: Structure-functional, substrates docking, and molecular allergenicity comparative analysis. **2016**, 66, 26-40	15
1587	Architecture of the type IVa pilus machine. **2016**, 351, aad2001	233
1586	Docking and molecular dynamics simulation study of EGFR1 with EGF-like peptides to understand molecular interactions. **2016**, 12, 1987-95	8
1585	Synthesis, X-ray crystallography, spectroscopic (FT-IR, 1H &13C NMR and UV), computational (DFT/B3LYP) and enzymes inhibitory studies of 7-hydroximinocholest-5-en-3-ol acetate. **2016**, 1116, 317-332	13
1584	Cryo-EM Data Are Superior to Contact and Interface Information in Integrative Modeling. **2016**, 110, 785-97	12
1583	Gain-of-Function Mutation W493R in the Epithelial Sodium Channel Allosterically Reconfigures Intersubunit Coupling. **2016**, 291, 3682-92	6

1582	Enhanced intracellular delivery of small molecules and drugs via non-covalent ternary dispersions of single-wall carbon nanotubes. **2016**, 4, 1324-1330	10
1581	Anti-inflammatory effects of royal poinciana through inhibition of toll-like receptor 4 signaling pathway. **2016**, 34, 199-211	19
1580	Molecular association of glucose-6-phosphate isomerase and pyruvate kinase M2 with glyceraldehyde-3-phosphate dehydrogenase in cancer cells. **2016**, 16, 152	14
1579	The drug binding sites and transport mechanism of the RND pumps from Mycobacterium tuberculosis: Insights from molecular dynamics simulations. **2016**, 592, 38-49	22
1578	Molecular dynamic simulations of Escherichia coli L-asparaginase to illuminate its role in deamination of asparagine and glutamine residues. **2016**, 6, 2	6
1577	Biomimetic design: a programmed tetradecapeptide folds and auto-dimerizes as a stereochemically articulated receptor protein. **2016**, 6, 6077-6083	1
1576	EWGWS insert in Plasmodium falciparum ookinete surface enolase is involved in binding of PWWP containing peptides: Implications to mosquito midgut invasion by the parasite. **2016**, 68, 13-22	3
1575	Computational and anti-tumor studies of 7a-Aza-B-homostigmast-5-eno [7a, 7-d] tetrazole-3Ɛyl chloride. **2016**, 1108, 411-426	15
1574	Role of asparagine at position 562 in dimerization and immunogenicity of the hepatitis E virus capsid protein. **2016**, 37, 99-107	18
1573	Identification of a small-molecule inhibitor of influenza virus via disrupting the subunits interaction of the viral polymerase. **2016**, 125, 34-42	35
1572	A computational approach to determine susceptibility to cancer by evaluating the deleterious effect of nsSNP in XRCC1 gene on binding interaction of XRCC1 protein with ligase III. **2016**, 576, 141-9	16
1571	In silico identification of putative bifunctional Plk1 inhibitors by integrative virtual screening and structural dynamics approach. **2016**, 388, 72-84	8
1570	Computational Analysis of the Domain Architecture and Substrate-Gating Mechanism of Prolyl Oligopeptidases from Shewanella woodyi and Identification of Probable Lead Molecules. **2016**, 8, 284-93	1
1569	DARC: Mapping Surface Topography by Ray-Casting for Effective Virtual Screening at Protein Interaction Sites. **2016**, 59, 4152-70	16
1568	Titanium dioxide nanoparticles provide protection against polycyclic aromatic hydrocarbon BaP and chrysene-induced perturbation of DNA repair machinery: A computational biology approach. **2016**, 63, 497-513	13
1567	In silico characterization, homology modeling of Camellia sinensis chitinase and its evolutionary analyses with other plant chitinases. **2017**, 87, 685-695	4
1566	Nucleoplasmin-like domain of FKBP39 from Drosophila melanogaster forms a tetramer with partly disordered tentacle-like C-terminal segments. **2017**, 7, 40405	6
1565	Software for molecular docking: a review. **2017**, 9, 91-102	523

1564	Molecular dynamics exploration of the binding mechanism and properties of single-walled carbon nanotube to WT and mutant VP35 FBP region of Ebola virus. **2017**, 43, 149-165	6
1563	Synthesis, crystal structure and Hirschfeld surface analyses of an alkyl amine based salt, [C 5 H 16 N 2][ZnCl 4] and its enzyme inhibition activity. **2017**, 21, 481-486	2
1562	Computational analysis of nsSNPs of NPHS1 gene and their effect on protein structural stability. **2017**, 11, 98-103	
1561	Mutations at protein-protein interfaces: Small changes over big surfaces have large impacts on human health. **2017**, 128, 3-13	81
1560	Biodegradation of Carbon Nanotubes, Graphene, and Their Derivatives. **2017**, 35, 836-846	163
1559	Structural Insight into the Gene Expression Profiling of the hcn Operon in Pseudomonas aeruginosa. **2017**, 182, 1144-1157	7
1558	Geometry optimization of steroid sulfatase inhibitors - the influence on the free binding energy with STS. **2017**, 28, 1017-1032	10
1557	Surface Accessibility and Dynamics of Macromolecular Assemblies Probed by Covalent Labeling Mass Spectrometry and Integrative Modeling. **2017**, 89, 1459-1468	32
1556	Inhibition of Mammalian Glycoprotein YKL-40: IDENTIFICATION OF THE PHYSIOLOGICAL LIGAND. **2017**, 292, 2624-2636	15
1555	Recent Developments in 3D QSAR and Molecular Docking Studies of Organic and Nanostructures. **2017**, 2133-2161	3
1554	Understanding enzymatic degradation of single-walled carbon nanotubes triggered by functionalization using molecular dynamics simulation. **2017**, 4, 720-727	38
1553	The ClusPro web server for protein-protein docking. **2017**, 12, 255-278	1037
1552	Rescore protein-protein docked ensembles with an interface contact statistics. **2017**, 85, 235-241	5
1551	Bioisosteric modification of known fucosidase inhibitors to discover a novel inhibitor of β-L-fucosidase. **2017**, 7, 3563-3572	6
1550	Mitochondrial protein interactome elucidated by chemical cross-linking mass spectrometry. **2017**, 114, 1732-1737	114
1549	Characterization, purification, and temperature/pressure stability of polyphenol oxidase extracted from plums (Prunus domestica). **2017**, 56, 177-185	23
1548	Myosin B of Plasmodium falciparum (PfMyoB): in silico prediction of its three-dimensional structure and its possible interaction with MTIP. **2017**, 116, 1373-1382	2
1547	Insight into SNPs and epitopes of E protein of newly emerged genotype-I isolates of JEV from Midnapur, West Bengal, India. **2017**, 18, 13	8

1546	Prepore Stability Controls Productive Folding of the BAM-independent Multimeric Outer Membrane Secretin PulD. **2017**, 292, 328-338	11
1545	Elucidation of structural and functional integration of a novel antimicrobial peptide from Antheraea mylitta. **2017**, 27, 1686-1692	9
1544	Identification of New Lead Molecules Against UBE2NL Enzyme for Cancer Therapy. **2017**, 182, 1497-1517	8
1543	The dynamic mechanism of RASSF5 and MST kinase activation by Ras. **2017**, 19, 6470-6480	19
1542	Cyclin F/FBXO1 Interacts with HIV-1 Viral Infectivity Factor (Vif) and Restricts Progeny Virion Infectivity by Ubiquitination and Proteasomal Degradation of Vif Protein through SCF E3 Ligase Machinery. **2017**, 292, 5349-5363	15
1541	Structure of the mycobacterial ESX-5 type VII secretion system membrane complex by single-particle analysis. **2017**, 2, 17047	74
1540	Prediction of Biomolecular Complexes. **2017**, 265-292	5
1539	Comparative in silico analyses of Cannabis sativa, Prunella vulgaris and Withania somnifera compounds elucidating the medicinal properties against rheumatoid arthritis. **2017**, 74, 296-304	15
1538	Computational study on human sphingomyelin synthase 1 (hSMS1). **2017**, 1859, 1517-1525	9
1537	Screening the thermal stability of carotenoids–α-lactalbumin complex by spectroscopic and molecular modeling approach. **2017**, 54, 316-322	5
1536	Insights in luteovirid structural biology guided by chemical cross-linking and high resolution mass spectrometry. **2017**, 241, 42-52	12
1535	Fast and accurate grid representations for atom-based docking with partner flexibility. **2017**, 38, 1538-1546	1
1534	Targeted inhibition of Klotho binding to fibroblast growth factor 23 prevents hypophosphetemia. **2017**, 75, 9-19	8
1533	A bottom-up approach for encapsulation of sour cherries anthocyanins by using β-lactoglobulin as matrices. **2017**, 210, 83-90	31
1532	Computational Protein Design. **2017**,	5
1531	Looking "Under the Hood" of Cellular Mechanotransduction with Computational Tools: A Systems Biomechanics Approach across Multiple Scales. **2017**, 3, 2712-2726	8
1530	Selective Inhibition of Escherichia coli RNA and DNA Topoisomerase I by Hoechst 33258 Derived Mono- and Bisbenzimidazoles. **2017**, 60, 4904-4922	19
1529	Computational modeling of protein assemblies. **2017**, 44, 179-189	33

1528	HDOCK: a web server for protein-protein and protein-DNA/RNA docking based on a hybrid strategy. *Nucleic Acids Research*, **2017**, 45, W365-W373	20.1	278
1527	Genome-Wide Identification and Functional Characterization of UDP-Glucosyltransferase Genes Involved in Flavonoid Biosynthesis in Glycine max. **2017**, 58, 1558-1572		23
1526	The Binding mechanism of anthocyanins from sour cherries (Prunus cerasus L) skins to bovine β-lactoglobulin: A fluorescence and in silico-based approach. **2017**, 20, S3096-S3111		10
1525	Chicken interleukin-1β mutants are effective single-dose vaccine adjuvants that enhance mucosal immune response. **2017**, 87, 308-316		4
1524	Improvement of cytotoxic activity of local anesthetics against human breast cancer cell line through the cyclodextrin complexes. **2017**, 54, 402-410		3
1523	Interactions of carbon nanotubes and/or graphene with manganese peroxidase during biodegradation of endocrine disruptors and triclosan. **2017**, 184, 127-136		35
1522	Ferrocenylaniline based amide analogs of methoxybenzoic acids: Synthesis, structural characterization and butyrylcholinesterase (BChE) inhibition studies. **2017**, 1146, 130-137		7
1521	Nicotinic acetylcholine receptor alpha 1(nAChRα) subunit peptides as potential antiviral agents against rabies virus. **2017**, 104, 180-188		6
1520	Immuno-informatics based approaches to identify CD8+ T cell epitopes within the Leishmania donovani 3-ectonucleotidase in cured visceral leishmaniasis subjects. **2017**, 19, 358-369		25
1519	Potential entry inhibitors of the envelope protein (E2) of Chikungunya virus: in silico structural modeling, docking and molecular dynamic studies. **2017**, 28, 39-49		12
1518	A new fluorescent PET sensor probe for Co2+ ion detection: computational, logic device and living cell imaging applications. **2017**, 7, 16581-16593		41
1517	Secretory Proteome Analysis of Streptomycin-Resistant Mycobacterium tuberculosis Clinical Isolates. **2017**, 22, 1229-1238		22
1516	Structural insights into adiponectin receptors suggest ceramidase activity. **2017**, 544, 120-123		110
1515	Computational design of self-assembling cyclic protein homo-oligomers. **2017**, 9, 353-360		78
1514	Probing Oligomerized Conformations of Defensin in the Membrane. **2017**, 1529, 353-362		4
1513	Targeting the ubiquitin-conjugating enzyme E2D4 for cancer drug discovery-a structure-based approach. **2017**, 10, 51-67		5
1512	T8M mutation in connexin-26 impairs the connexon topology and shifts its interaction paradigm with lipid bilayer leading to non-syndromic hearing loss. **2017**, 227, 168-177		1
1511	Structural studies of RNA-protein complexes: A hybrid approach involving hydrodynamics, scattering, and computational methods. **2017**, 118-119, 146-162		23

1510	Docking and molecular dynamics studies for developing Microcin C7 as an alternative drug against diphtheria toxin. **2017**, 13, 292	
1509	Effect of calcium ions on structure and stability of the C1q-like domain of otolin-1 from human and zebrafish. **2017**, 284, 4278-4297	17
1508	In silico methods for design of biological therapeutics. **2017**, 131, 33-65	36
1507	Principles for computational design of binding antibodies. **2017**, 114, 10900-10905	73
1506	Functional efficiency of MerA protein among diverse mercury resistant bacteria for efficient use in bioremediation of inorganic mercury. **2017**, 142, 207-215	22
1505	Theoretical assessment of calix[n]arene as drug carriers for second generation tyrosine kinase inhibitors. **2017**, 247, 448-455	6
1504	KLK5 induces shedding of DPP4 from circulatory Th17 cells in type 2 diabetes. **2017**, 6, 1529-1539	28
1503	Exploring Heme and Hemoglobin Binding Regions of Plasmodium Heme Detoxification Protein for New Antimalarial Discovery. **2017**, 60, 8298-8308	14
1502	Testosterone/bicalutamide antagonism at the predicted extracellular androgen binding site of ZIP9. **2017**, 1864, 2402-2414	15
1501	Unraveling the Self-Assembly of the XcpQ Secretin Periplasmic Domain Provides New Molecular Insights into Type II Secretion System Secreton Architecture and Dynamics. **2017**, 8,	13
1500	Conformational analysis of the human chemokine receptor CXCR3. **2017**, 92, 76-86	1
1499	Panax ginseng genome examination for ginsenoside biosynthesis. **2017**, 6, 1-15	95
1498	Steered molecular dynamics simulation of the binding of the bovine auxilin J domain to the Hsc70 nucleotide-binding domain. **2017**, 23, 320	3
1497	modeling of the cryptic E2~ubiquitin-binding site of E6-associated protein (E6AP)/UBE3A reveals the mechanism of polyubiquitin chain assembly. **2017**, 292, 18006-18023	14
1496	Structure elucidation and in silico docking studies of a novel furopyrimidine antibiotics synthesized by endolithic bacterium Actinomadura sp. AL2. **2017**, 33, 178	7
1495	Biochemical Characterization of ArsI: A Novel C-As Lyase for Degradation of Environmental Organoarsenicals. **2017**, 51, 11115-11125	16
1494	Comparative analyses of enzymatic activity, structural study and docking of fungal cellulases. **2017**, 9, 54-60	8
1493	In Vitro Antimalarial Evaluation of Piperidine- and Piperazine-Based Chalcones: Inhibition of Falcipain-2 and Plasmepsin II Hemoglobinases Activities from Plasmodium falciparum. **2017**, 2, 7684-7690	7

1492	Modeling protein quaternary structure of homo- and hetero-oligomers beyond binary interactions by homology. **2017**, 7, 10480	357
1491	A computational protocol for the discovery of lead molecules targeting DNA unique to pathogens. **2017**, 131, 4-9	1
1490	Macrophage migration inhibitory factor (MIF) modulates trophic signaling through interaction with serine protease HTRA1. **2017**, 74, 4561-4572	11
1489	Interaction studies on catecholamines to cellular receptors using in silico approach. **2017**, 19, 29	0
1488	The design of target specific antibodies (scFv) by applying de novo workflow: Case study on BmR1 antigen from Brugia malayi. **2017**, 76, 543-550	3
1487	Characterization of NPHS2 gene polymorphisms associated to steroid resistance nephrotic syndrome in Indian children. **2017**, 628, 134-140	6
1486	Structure-function relationships in human d-aspartate oxidase: characterisation of variants corresponding to known single nucleotide polymorphisms. **2017**, 1865, 1129-1140	13
1485	DnrI of Streptomyces peucetius binds to the resistance genes, drrAB and drrC but is activated by daunorubicin. **2017**, 57, 862-872	5
1484	Identification of putative unique immunogenic ZIKV and DENV1-4 peptides for diagnostic cellular based tests. **2017**, 7, 6218	3
1483	Methylglyoxal and Advanced Glycation End products: Insight of the regulatory machinery affecting the myogenic program and of its modulation by natural compounds. **2017**, 7, 5916	29
1482	Enriching Traditional Protein-protein Interaction Networks with Alternative Conformations of Proteins. **2017**, 7, 7180	11
1481	The Vitality of Swivel Domain Motion in Performance of Enzyme I of Phosphotransferase System; A Comprehensive Molecular Dynamic Study. **2017**, 242, 1184-1198	7
1480	Identification of novel direct protein-protein interactions by irradiating living cells with femtosecond UV laser pulses. **2017**, 492, 67-73	6
1479	NLScore: a novel quantitative algorithm based on 3 dimensional structural determinants to predict the probability of nuclear localization in proteins containing classical nuclear localization signals. **2017**, 23, 258	2
1478	Syntheses, crystal structures, DFT calculations, protein interaction and anticancer activities of water soluble dipicolinic acid-imidazole based oxidovanadium(iv) complexes. **2017**, 46, 16682-16702	13
1477	Microencapsulation of Anthocyanins from Grape Skins by Whey Protein Isolates and Different Polymers. **2017**, 10, 1715-1726	30
1476	Binding of SoxR protein to two promoter-operator regions to regulate sox gene expression: A detailed molecular insight for structural changes and protein-DNA interactions. **2017**, 3-5, 34-40	
1475	Natural alkaloid Luotonin A and its affixed acceptor molecules: Serum albumin binding studies. **2017**, 173, 499-507	21

1474	Assessing the binding of cholinesterase inhibitors by docking and molecular dynamics studies. **2017**, 76, 36-42		16
1473	Inhibitors or toxins? Large library target-specific screening of fullerene-based nanoparticles for drug design purpose. **2017**, 9, 10263-10276		20
1472	Synthesis of novel 5-(aroylhydrazinocarbonyl)escitalopram as cholinesterase inhibitors. **2017**, 138, 396-406		12
1471	In silico analysis of candidate proteins sharing homology with Streptococcus agalactiae proteins and their role in male infertility. **2017**, 63, 15-28		5
1470	Identification of a novel small-molecule compound targeting the influenza A virus polymerase PB1-PB2 interface. **2017**, 137, 58-66		12
1469	Characteristics of C-terminal, β-amyloid peptide binding fragment of neuroprotective protease inhibitor, cystatin C. **2017**, 30, e2581		5
1468	Hydrophobic Interaction Between Domain I of Albumin and B Chain of Detemir May Support Myristate-Dependent Detemir-Albumin Binding. **2017**, 182, 82-96		10
1467	Putative model for heat shock protein 70 complexation with receptor of advanced glycation end products through fluorescence proximity assays and normal mode analyses. **2017**, 22, 99-111		9
1466	Pharmacoinformatics and molecular docking studies reveal potential novel Proline Dehydrogenase (PRODH) compounds for Schizophrenia inhibition. **2017**, 26, 314-326		12
1465	Thermal stability of the complex formed between carotenoids from sea buckthorn (Hippophae rhamnoides L.) and bovine β-lactoglobulin. **2017**, 173, 562-571		23
1464	Human and server docking prediction for CAPRI round 30-35 using LZerD with combined scoring functions. **2017**, 85, 513-527		15
1463	Template-based modeling and ab initio refinement of protein oligomer structures using GALAXY in CAPRI round 30. **2017**, 85, 399-407		9
1462	CD4-gp120 interaction interface - a gateway for HIV-1 infection in human: molecular network, modeling and docking studies. **2017**, 35, 2631-2644		5
1461	Design of novel lead molecules against RhoG protein as cancer target - a computational study. **2017**, 35, 3119-3139		17
1460	Photochemical and computational studies of inclusion complexes between β-cyclodextrin and 1,2-dihydroxyanthraquinones. **2017**, 16, 476-488		21
1459	PB2 substitutions V598T/I increase the virulence of H7N9 influenza A virus in mammals. **2017**, 501, 92-101		22
1458	Molecular docking analysis of imidazole derivatives and polybenzimidazole analogs as inhibitors of superoxide dismutase (SOD) and xanthine oxidase (XO). **2017**,		0
1457	GalaxyHomomer: a web server for protein homo-oligomer structure prediction from a monomer sequence or structure. *Nucleic Acids Research*, **2017**, 45, W320-W324	20.1	63

1456	Interfering with the high-affinity interaction between wheat amylase trypsin inhibitor CM3 and toll-like receptor 4: in silico and biosensor-based studies. **2017**, 7, 13169	23
1455	Targeting IL-17 AND IL-17D receptors of rheumatoid arthritis using phytocompounds: A Molecular Docking study. **2017**, 263, 022040	
1454	Antiquorum sensing activity of silver nanoparticles in . : an in silico study. **2017**, 5, 12	15
1453	The Immune Epitope Database and Analysis Resource in Epitope Discovery and Synthetic Vaccine Design. **2017**, 8, 278	202
1452	Identification of Potential MHC Class-II-Restricted Epitopes Derived from Antigens by Reverse Vaccinology and Evaluation of Their CD4+ T-Cell Responsiveness against Visceral Leishmaniasis. **2017**, 8, 1763	43
1451	Genome Wide Analysis of the Mismatch Repair Components of and Their Comparison with Human Host. **2017**, 8, 130	13
1450	Ribonucleotide Reductases from Bifidobacteria Contain Multiple Conserved Indels Distinguishing Them from All Other Organisms: Analysis of the Possible Role of a 43 aa Bifidobacteria-Specific Insert in the Class III RNR Homolog. **2017**, 8, 1409	6
1449	Controversial Effects of D-Amino Acid Oxidase Activator (DAOA)/G72 on D-Amino Acid Oxidase (DAO) Activity in Human Neuronal, Astrocyte and Kidney Cell Lines: The N-methyl D-aspartate (NMDA) Receptor Hypofunction Point of View. **2017**, 10, 342	4
1448	Pharmacoinformatics, Adaptive Evolution, and Elucidation of Six Novel Compounds for Schizophrenia Treatment by Targeting DAOA (G72) Isoforms. **2017**, 2017, 5925714	11
1447	Biomolecular changes that occur in the antennal gland of the giant freshwater prawn (Machrobrachium rosenbergii). **2017**, 12, e0177064	11
1446	Molecular docking studies of 3-bromopyruvate and its derivatives to metabolic regulatory enzymes: Implication in designing of novel anticancer therapeutic strategies. **2017**, 12, e0176403	30
1445	Identification and in silico characterization of a novel p.P208PfsX1 mutation in V-ATPase a3 subunit associated with autosomal recessive osteopetrosis in a Pakistani family. **2017**, 18, 148	7
1444	Repurposing of Modified Alpidem and Propoxyphene to Cure AURKA, BCAS1, GNAS and MLH1 Gene Mutations in Colorectal Cancer. **2017**, 06,	2
1443	Comparative Study on the Binding Affinity of Methimazole and Propylthiouracil to Thyroid Peroxidase as an Anti-Thyroid Drug: An Insilico Approach. **2017**, 07,	1
1442	PREDICTING THE BIODEGRADABILITY NATURE OF IMIDAZOLE AND ITS DERIVATIVES BY MODULATING TWO HISTIDINE DEGRADATION ENZYMES (UROCANASE AND FORMIMINOGLUTAMASE) ACTIVITIES. **2017**, 10, 383	9
1441	Abrus agglutinin stimulates BMP-2-dependent differentiation through autophagic degradation of □catenin in colon cancer stem cells. **2018**, 57, 664-677	23
1440	Interaction of Peptide Aptamers with Prion Protein Central Domain Promotes □Cleavage of PrP. **2018**, 55, 7758-7774	8
1439	Protein-Protein and Domain-Domain Interactions. **2018**,	7

1438	Optimum Number of Anchored Clathrate Water and Its Instantaneous Fluctuations Dictate Ice Plane Recognition Specificities of Insect Antifreeze Protein. **2018**, 122, 3056-3067	21
1437	Exploring the deleterious SNPs in XRCC4 gene using computational approach and studying their association with breast cancer in the population of West India. **2018**, 655, 13-19	2
1436	Amodiaquine improves insulin resistance and lipid metabolism in diabetic model mice. **2018**, 20, 1688-1701	6
1435	Protein-Protein Docking: Methods and Tools. **2018**, 161-168	6
1434	Effect of reserpine on Pseudomonas aeruginosa quorum sensing mediated virulence factors and biofilm formation. **2018**, 34, 320-334	27
1433	A Terminally Capped Synthetic, Acyclic Tripeptide Forms Dimer in the Solid, Liquid and Gaseous States. **2018**, 3, 2523-2527	1
1432	A Highly Sensitive Detection System based on Proximity-dependent Hybridization with Computer-aided Affinity Maturation of a scFv Antibody. **2018**, 8, 3837	2
1431	Crystal structure, optical properties, DFT analysis of new morpholine based Schiff base ligands and their copper(II) complexes: DNA, protein docking analyses, antibacterial study and anticancer evaluation. **2018**, 90, 119-130	41
1430	Dinitrophenylhydrazine: Ecyclodextrin inclusion complex as a novel fluorescent chemosensor probe for Ce4+. **2018**, 44, 5301-5327	1
1429	Yeast aconitase mitochondrial import is modulated by interactions of its C and N terminal domains and Ssa1/2 (Hsp70). **2018**, 8, 5903	8
1428	Preparation, characterization and molecular modeling studies of the beta-cyclodextrin inclusion complex with benzoguanamine and its analytical application as chemosensor for the selective sensing of Ce. **2018**, 200, 212-225	18
1427	Mechanistic and structural insights into the in vitro inhibitory action of hypericin on glutathione reductase purified from baker's yeast. **2018**, 32, e22051	1
1426	Type IX secretion system PorM and gliding machinery GldM form arches spanning the periplasmic space. **2018**, 9, 429	38
1425	DFT/TD-DFT calculations, spectroscopic characterizations (FTIR, NMR, UV-vis), molecular docking and enzyme inhibition study of 7-benzoyloxycoumarin. **2018**, 73, 65-78	13
1424	Hedgehog Antagonist Pyrimidine-Indole Hybrid Molecule Inhibits Ciliogenesis through Microtubule Destabilisation. **2018**, 19, 723-735	7
1423	Hot-spot analysis for drug discovery targeting protein-protein interactions. **2018**, 13, 327-338	33
1422	Cellulose synthase 'class specific regions' are intrinsically disordered and functionally undifferentiated. **2018**, 60, 481-497	15
1421	Oxidation of SQSTM1/p62 mediates the link between redox state and protein homeostasis. **2018**, 9, 256	90

1420	KIX domain of AtMed15a, a Mediator subunit of Arabidopsis, is required for its interaction with different proteins. **2018**, 13, e1428514	12
1419	Novel coumarin rhenium(I) and -(V) complexes: Formation, DFT and DNA binding studies. **2018**, 144, 107-118	7
1418	Chemical Crosslinking Mass Spectrometry Analysis of Protein Conformations and Supercomplexes in Heart Tissue. **2018**, 6, 136-141.e5	73
1417	Investigation of nepetolide as a novel lead compound: Antioxidant, antimicrobial, cytotoxic, anticancer, anti-inflammatory, analgesic activities and molecular docking evaluation. **2018**, 26, 422-429	11
1416	Designing a polytope for use in a broad-spectrum dengue virus vaccine. **2018**, 13, 156-161	
1415	Designing of calixarene based drug carrier for dasatinib, lapatinib and nilotinib using multilevel molecular docking and dynamics simulations. **2018**, 90, 157-169	8
1414	A Structural Model of a P450-Ferredoxin Complex from Orientation-Selective Double Electron-Electron Resonance Spectroscopy. **2018**, 140, 2514-2527	17
1413	DmCatD, a cathepsin D-like peptidase of the hematophagous insect Dipetalogaster maxima (Hemiptera: Reduviidae): Purification, bioinformatic analyses and the significance of its interaction with lipophorin in the internalization by developing oocytes. **2018**, 105, 28-39	8
1412	Piperonylic acid stimulates keratinocyte growth and survival by activating epidermal growth factor receptor (EGFR). **2018**, 8, 162	8
1411	Computational analysis of sequential and structural variations in stromelysins as an insight towards matrix metalloproteinase research. **2018**, 11, 28-35	
1410	Structural characterization of β-catenin and RX-5902 binding to phospho-p68 RNA helicase by molecular dynamics simulation. **2018**, 140, 79-89	6
1409	Exploring Leptospiral proteomes to identify potential candidates for vaccine design against Leptospirosis using an immunoinformatics approach. **2018**, 8, 6935	21
1408	Protein-Induced Fluorescence Enhancement Based Detection of Plasmodium falciparum Glutamate Dehydrogenase Using Carbon Dot Coupled Specific Aptamer. **2018**, 20, 350-357	15
1407	Thrombin-like enzymes from snake venom: Structural characterization and mechanism of action. **2018**, 114, 788-811	24
1406	Protein-Protein Docking in Drug Design and Discovery. **2018**, 1762, 285-305	11
1405	Modeling Structure and Dynamics of Protein Complexes with SAXS Profiles. **2018**, 1764, 449-473	19
1404	Coordination susceptibilities of cinnamaldehyde and cuminaldehyde derived Schiff bases towards the fac-[Re(CO)3]+ core: Formation, computational and DNA interaction studies. **2018**, 477, 257-269	4
1403	On the mechanisms of protein interactions: predicting their affinity from unbound tertiary structures. **2018**, 34, 592-598	9

1402	Pharmacophore Modeling and Docking Studies of SNCA Receptor with Some Active Phytocompounds from Selected Ayurvedic Medicinal Plants Known for their CNS Activity. **2018**, 1-9	
1401	Small Molecule Interactome Mapping by Photoaffinity Labeling Reveals Binding Site Hotspots for the NSAIDs. **2018**, 140, 4259-4268	49
1400	Effects of pH and aggregation in the human prion conversion into scrapie form: a study using molecular dynamics with excited normal modes. **2018**, 47, 583-590	5
1399	Identification of an Arg-Leu-Arg tripeptide that contributes to the binding interface between the cytokine MIF and the chemokine receptor CXCR4. **2018**, 8, 5171	31
1398	Immunoinformatics approaches to design a novel multi-epitope subunit vaccine against HIV infection. **2018**, 36, 2262-2272	60
1397	The influence of pH and divalent/monovalent cations on the internal electron transfer (IET), enzymatic activity, and structure of fructose dehydrogenase. **2018**, 410, 3253-3264	27
1396	Alanine substitution mutations in the DNA binding region of a global staphylococcal virulence regulator affect its structure, function, and stability. **2018**, 113, 1221-1232	6
1395	Excavating chikungunya genome to design B and T cell multi-epitope subunit vaccine using comprehensive immunoinformatics approach to control chikungunya infection. **2018**, 61, 4-15	51
1394	Cross-linked peptide identification: A computational forest of algorithms. **2018**, 37, 738-749	17
1393	Spectral and proton transfer behavior of 1,4-dihydroxylanthraquinone in aqueous and confined media; molecular modelling strategy. **2018**, 259, 186-198	11
1392	Biophysical Studies on HCV 1a NS3/4A Protease and Its Catalytic Triad in Wild Type and Mutants by the In Silico Approach. **2018**, 10, 143-156	3
1391	Recognition dynamics of dopamine to human Monoamine oxidase B: role of Leu171/Gln206 and conserved water molecules in the active site cavity. **2018**, 36, 1439-1462	14
1390	Dynamics of fluoroquinolones induced resistance in DNA gyrase of Mycobacterium tuberculosis. **2018**, 36, 362-375	21
1389	In silico investigation on the inhibition of A□aggregation by A□peptide by potential of mean force study. **2018**, 36, 741-752	6
1388	Structural Evaluation and Binding Mode Analysis of CCL19 and CCR7 Proteins-Identification of Novel Leads for Rheumatic and Autoimmune Diseases: An Insilico study. **2018**, 10, 346-366	4
1387	Understanding the Interactions of High-Mobility Group of Protein Domain B1 with DNA Adducts Generated by Platinum Anticancer Molecules Using In Silico Approaches. **2018**, 10, 476-485	2
1386	Structural characterisation of medically relevant protein assemblies by integrating mass spectrometry with computational modelling. **2018**, 175, 34-41	16
1385	In Silico Structural Studies and Molecular Docking Analysis of Delta6-desaturase in HUFA Biosynthetic Pathway. **2018**, 29, 161-173	5

1384	Homology Modeling, Molecular Docking and Molecular Dynamics Based Functional Insights into Rice Urease Bound to Urea. **2018**, 88, 1539-1548	10
1383	Wild-type catalase peroxidase vs G279D mutant type: Molecular basis of Isoniazid drug resistance in Mycobacterium tuberculosis. **2018**, 641, 226-234	13
1382	Investigations on binding mechanism of bioactives from elderberry (Sambucus nigra L.) by whey proteins for efficient microencapsulation. **2018**, 223, 197-207	20
1381	Spider's venom phospholipases D: A structural review. **2018**, 107, 1054-1065	9
1380	Potential of ionic liquids for inhibiting the growth and □lactamase production by Bacillus cereus EMB20. **2018**, 107, 1915-1921	5
1379	Role of pncA gene mutations W68R and W68G in pyrazinamide resistance. **2018**, 119, 2567-2578	26
1378	Proteome and Structural Organization of the Knob Complex on the Surface of the Plasmodium Infected Red Blood Cell. **2018**, 12, e1600177	4
1377	Aromatic interactions at the ligand-protein interface: Implications for the development of docking scoring functions. **2018**, 91, 380-390	32
1376	Characterization of Ofloxacin Interaction with Mutated (A91V) Quinolone Resistance Determining Region of DNA Gyrase in Mycobacterium Leprae through Computational Simulation. **2018**, 76, 125-134	3
1375	Exploring the interaction between Mycobacterium tuberculosis enolase and human plasminogen using computational methods and experimental techniques. **2018**, 119, 2408-2417	8
1374	Rational evolution of the unusual Y-type oxyanion hole of Rhodococcus sp. CR53 lipase LipR. **2018**, 108, 26-33	4
1373	Automatic structure prediction of oligomeric assemblies using Robetta in CASP12. **2018**, 86 Suppl 1, 283-291	29
1372	Thermodynamic and first-principles biomolecular simulations applied to synthetic biology: promoter and aptamer designs. **2018**, 3, 19-37	8
1371	Role of catechins on ET-1-induced stimulation of PLD and NADPH oxidase activities in pulmonary smooth muscle cells: determination of the probable mechanism by molecular docking studies. **2018** , 96, 417-432	5
1370	Dihydroquercetin: known antioxidant□ew inhibitor of alpha-amylase activity. **2018**, 27, 966-971	2
1369	Structure analysis of capsid protein of Porcine circovirus type 2 from pigs with systemic disease. **2018**, 49, 351-357	7
1368	Arsenic methylation by a novel ArsM As(III) S-adenosylmethionine methyltransferase that requires only two conserved cysteine residues. **2018**, 107, 265-276	25
1367	□yclodextrin encapsulated polyphenols as effective antioxidants. **2018**, 109, e23084	15

1366	Identification of novel GPR17-agonists by structural bioinformatics and signaling activation. **2018**, 106, 901-907	11
1365	Role of curcumin in PLD activation by Arf6-cytohesin1 signaling axis in U46619-stimulated pulmonary artery smooth muscle cells. **2018**, 438, 97-109	4
1364	Structural basis for Cullins and RING component inhibition: Targeting E3 ubiquitin pathway conductors for cancer therapeutics. **2018**, 106, 532-543	10
1363	Extraction, purification and processing stability of peroxidase from plums (Prunus domestica). **2018** , 21, 2744-2757	6
1362	Synergistic AML Cell Death Induction by Marine Cytotoxin (+)-1(), 6(), 1'(), 6'(), 11(), 17()-Fistularin-3 and Bcl-2 Inhibitor Venetoclax. **2018**, 16,	12
1361	Inhibition potency of HMGR enzyme against hypercholesterolemia by bioactive peptides of CSN1S2 protein from caprine milk. **2018**,	1
1360	Molecular modeling, docking and protein-protein interaction analysis of MAPK signalling cascade involved in Camalexin biosynthesis in Brassica rapa. **2018**, 14, 145-152	6
1359	MOLECULAR DOCKING ANALYSIS OF THIRTEEN COMPOUNDS AS MODULATOR OF IONOTROPIC GLUTAMATE RECEPTOR. **2018**, 11, 114	
1358	STRUCTURE-BASED DRUG DESIGNING STUDIES TOWARDS EXPLORING THE POTENTIAL ANTICANCER ACTIVITY OF SELECTED PHYTOCOMPOUNDS AGAINST HISTONE DEACETYLASE 10 PROTEIN. **2018**, 11, 262	
1357	Identijication of potential inhibitors for identified novel drug targets of Aspergillus fumigatus. **2018**,	1
1356	Identification of promoter P, characterization of cadmium resistant gene and molecular cloning of promoter P from BC15. **2018**, 34, 819-833	3
1355	Novel mutation G324C in WNT1 mapped in a large Pakistani family with severe recessively inherited Osteogenesis Imperfecta. **2018**, 25, 82	6
1354	Molecular Docking, Computational, and Antithrombotic Studies of Novel 1,3,4-Oxadiazole Derivatives. **2018**, 19,	7
1353	Ubiquitin-conjugating enzyme E2 B regulates the ubiquitination of O-methylguanine-DNA methyltransferase and BCNU sensitivity in human nasopharyngeal carcinoma cells. **2018**, 158, 327-338	10
1352	Mutations in LZTR1 drive human disease by dysregulating RAS ubiquitination. **2018**, 362, 1177-1182	87
1351	Predicting CD4 T-cell epitopes based on antigen cleavage, MHCII presentation, and TCR recognition. **2018**, 13, e0206654	17
1350	Unintended specificity of an engineered ligand-binding protein facilitated by unpredicted plasticity of the protein fold. **2018**, 31, 375-387	5
1349	Role of K-Loop Cysteine Residues in the Marburg Virus Protein VP24–Human Keap1 Complex. **2018**, 3, 18639-18645	2

1348	Supramolecular assembly between adenocard and native beta-cyclodextrin: Preparation, characterization and in-vitro cytotoxic evaluation. **2018**, 51, 496-509	3
1347	Structural basis of development of multi-epitope vaccine against Middle East respiratory syndrome using in silico approach. **2018**, 11, 2377-2391	32
1346	COMPUTATIONAL APPROACHES FOR THE PREDICTION OF ANTIMICROBIAL POTENTIAL PEPTIDES FROM OCIMUM TENUIFLORUM.. **2018**, 11, 398	2
1345	COMPUTATIONAL DOCKING AND IN SILICO ANALYSIS OF POTENTIAL EFFLUX PUMP INHIBITOR PUNIGRATANE. **2018**, 10, 27	2
1344	Do environmentally induced DNA variations mediate adaptation in Aspergillus flavus exposed to chromium stress in tannery sludge?. **2018**, 19, 868	7
1343	Biomolecular docking, antimicrobial and cytotoxic studies on new bidentate schiff base ligand derived metal (II) complexes. **2018**, 33, e4753	12
1342	Synthesis, physicochemical characterization and structural studies of new Schiff base ligand and its metal (II) complexes: In silico molecular docking analysis, antimicrobial activity and cytotoxicity. **2018**, 32, e4538	13
1341	Insight into novel clinical mutants of RpsA-S324F, E325K, and G341R of associated with pyrazinamide resistance. **2018**, 16, 379-387	15
1340	Micafungin is a novel anti-viral agent of chikungunya virus through multiple mechanisms. **2018**, 159, 134-142	19
1339	ATRA reduces inflammation and improves alveolar epithelium regeneration in emphysematous rat lung. **2018**, 108, 1435-1450	9
1338	Maternal BDE-209 exposure during lactation perturbs steroidogenesis, germ cell kinetics and THRβ expression in testes of prepubertal mice offspring. **2018**, 122, 104-119	9
1337	A single epitope of Epstein-Barr Virus stimulate IgG production in mice. **2018**, 35, 55-58	1
1336	Bioinformatics Tools and Benchmarks for Computational Docking and 3D Structure Prediction of RNA-Protein Complexes. **2018**, 9,	21
1335	The potential HLA Class I-restricted epitopes derived from LeIF and TSA of Leishmania donovani evoke anti-leishmania CD8+ T lymphocyte response. **2018**, 8, 14175	17
1334	Immuno-informatics Analysis to Identify Novel Vaccine Candidates and Design of a Multi-Epitope Based Vaccine Candidate Against parasites. **2018**, 9, 2213	17
1333	Protein Dynamics in Solution by Quantitative Crosslinking/Mass Spectrometry. **2018**, 43, 908-920	34
1332	In silico-prediction of protein-protein interactions network about MAPKs and PP2Cs reveals a novel docking site variants in Brachypodium distachyon. **2018**, 8, 15083	6
1331	Phosphatidylinositol 4,5-bisphosphate (PIP) regulates KCNQ3 K channels by interacting with four cytoplasmic channel domains. **2018**, 293, 19411-19428	19

1330	Developing a Programmable, Self-Assembling (SLCCNV) Capsid Proteins into "Nanocargo"-like Architecture.. **2018**, 1, 1741-1757	2
1329	Methodologies and Application Issues of Contemporary Computing Framework. **2018**,	1
1328	Overview of the Maturation Machinery of the H-Cluster of [FeFe]-Hydrogenases with a Focus on HydF. **2018**, 19,	16
1327	Designing of CD8 and CD8-overlapped CD4 epitope vaccine by targeting late and early proteins of human papillomavirus. **2018**, 12, 107-125	17
1326	EpCAM homo-oligomerization is not the basis for its role in cell-cell adhesion. **2018**, 8, 13269	20
1325	Sedative-hypnotic like effect of 5-methoxyflavone in mice and investigation on possible mechanisms by in vivo and in silico methods. **2018**, 108, 85-94	6
1324	Designing of suitable linkers for the chimeric proteins to achieve the desired flexibility and extended conformation. **2018**, 11, 236	
1323	KnowVolution Campaign of an Aryl Sulfotransferase Increases Activity toward Cellobiose. **2018**, 24, 17117-17124	14
1322	Adenylate kinase potentiates the capsular polysaccharide by modulating Cps2D in Streptococcus pneumoniae D39. **2018**, 50, 1-14	4
1321	Identification and analyses of natural compounds as potential inhibitors of TRAF6-Basigin interactions in melanoma using structure-based virtual screening and molecular dynamics simulations. **2018**, 85, 281-293	2
1320	Discovering Selective Binders for Photoswitchable Proteins Using Phage Display. **2018**, 7, 2355-2364	20
1319	Molecular Modeling Applied to Nucleic Acid-Based Molecule Development. **2018**, 8,	13
1318	Decane-1,2-diol derivatives as potential antitumor agents for the treatment of glioblastoma. **2018**, 837, 105-116	3
1317	Epitope Mapping by HDX-MS Elucidates the Surface Coverage of Antigens Associated with High Blocking Efficiency of Antibodies to Birch Pollen Allergen. **2018**, 90, 11315-11323	15
1316	Supramolecular Interaction of Primaquine with Native Cyclodextrin. **2018**, 47, 906-929	6
1315	Copper(II)-sulfonamide Schiff base complexes: Structure, biological activity and theoretical interpretation. **2018**, 151, 344-354	18
1314	Characterization of a metagenomic serine metalloprotease and molecular docking studies. **2018**, 71, 69-75	5
1313	Chloramphenicol-borate/boronate complex for controlling infections by chloramphenicol-resistant bacteria.. **2018**, 8, 18016-18022	1

1312	The unequivocal preponderance of biocomputation in clinical virology.. **2018**, 8, 17334-17345		2
1311	Interactive structural analysis of TrCP1 and PER2 phosphoswitch binding through dynamics simulation assay. **2018**, 651, 34-42		5
1310	Cyclic trimer of human cystatin C, an amyloidogenic protein - molecular dynamics and experimental studies. **2018**, 123, 174701		2
1309	Shape complementarity at protein interfaces via global docking optimisation. **2018**, 84, 69-73		1
1308	A DFT study of inclusion complexes of substituted calix[n]arenes with dasatinib and lapatinib. **2018**, 84, 160-165		3
1307	A cylindrical assembly model and dynamics of the Ebola virus VP40 structural matrix. **2018**, 8, 9776		4
1306	SYNTHESIS, PHARMACOLOGICAL EVALUATION AND LIGAND-PROTEIN INTERACTION STUDY OF HYBRID UREA AND THIOUREA DERIVATIVES AS ANTIHYPERGLYCEMIC AGENTS. **2018**, 9, 36-44		
1305	Intrinsically disordered N-terminal domain of the Helicoverpa armigera Ultraspiracle stabilizes the dimeric form via a scorpion-like structure. **2018**, 183, 167-183		3
1304	Identification of ligand binding activity and DNA recognition by RhlR protein from opportunistic pathogen Pseudomonas aeruginosa-a molecular dynamic simulation approach. **2018**, 31, e2738		1
1303	Structural Prediction of Protein-Protein Interactions by Docking: Application to Biomedical Problems. **2018**, 110, 203-249		9
1302	QM/MM Studies of Dph5 - A Promiscuous Methyltransferase in the Eukaryotic Biosynthetic Pathway of Diphthamide. **2018**, 58, 1406-1414		5
1301	Development of in Planta Chemical Cross-Linking-Based Quantitative Interactomics in Arabidopsis. **2018**, 17, 3195-3213		8
1300	HSYMDOCK: a docking web server for predicting the structure of protein homo-oligomers with Cn or Dn symmetry. *Nucleic Acids Research*, **2018**, 46, W423-W431	20.1	20
1299	Algorithm 990. **2018**, 44, 1-30		6
1298	Computational and Pharmacological Evaluation of Ferrocene-Based Acyl Ureas and Homoleptic Cadmium Carboxylate Derivatives for Anti-diabetic Potential. **2017**, 8, 1001		8
1297	Ferrocene-based anilides: synthesis, structural characterization and inhibition of butyrylcholinesterase. **2018**, 47, 11769-11781		6
1296	Comparative Study of Carborane- and Phenyl-Modified Adenosine Derivatives as Ligands for the A2A and A3 Adenosine Receptors Based on a Rigid in Silico Docking and Radioligand Replacement Assay. **2018**, 23,		7
1295	Artificial intelligence in drug design. **2018**, 61, 1191-1204		72

1294	Calmodulin (CaM) Activates PI3K by Targeting the "Soft" CaM-Binding Motifs in Both the nSH2 and cSH2 Domains of p85. **2018**, 122, 11137-11146	11
1293	Evolutionary Analysis Provides Insight Into the Origin and Adaptation of HCV. **2018**, 9, 854	8
1292	Bi-allelic Mutations in Phe-tRNA Synthetase Associated with a Multi-system Pulmonary Disease Support Non-translational Function. **2018**, 103, 100-114	20
1291	An integrative approach to develop computational pipeline for drug-target interaction network analysis. **2018**, 8, 10238	6
1290	Calmidazolium Chloride and Its Complex with Serum Albumin Prevent Huntingtin Exon1 Aggregation. **2018**, 15, 3356-3368	3
1289	Binding mechanisms between lycopene extracted from tomato peels and bovine lactoglobulin. **2018**, 203, 582-589	6
1288	In silico and in vivo investigation of ferrocene-incorporated acyl ureas and homoleptic cadmium carboxylate derivatives for anticonvulsant, anxiolytic, and sedative potential. **2018**, 79, 184-197	6
1287	Antagonistic role of Klotho-derived peptides dynamics in the pancreatic cancer treatment through obstructing WNT-1 and Frizzled binding. **2018**, 240, 107-117	12
1286	Properties that rank protein:protein docking poses with high accuracy. **2018**, 20, 20927-20942	4
1285	Paradoxical Bactericidal Effects of Hydrophobic Lung Surfactant Proteins and Their Peptide Mimics Using Liposome Molecular Trojan. **2018**, 67, 1043-1057	4
1284	Protein-RNA Docking Using ICM. **2018**, 14, 4971-4984	7
1283	InterEvDock2: an expanded server for protein docking using evolutionary and biological information from homology models and multimeric inputs. *Nucleic Acids Research*, **2018**, 46, W408-W416 20.1	27
1282	Investigation of immunogenic properties of Hemolin from silkworm, Bombyx mori as carrier protein: an immunoinformatic approach. **2018**, 8, 6957	13
1281	Molecular Cloning and Docking of Gene Encoding Cysteine Protease With Antibiotic Interaction in NBMKU12 From the Clinical Isolates. **2018**, 9, 1658	
1280	Targeting the Tie2- integrin axis with bi-specific reagents for the inhibition of angiogenesis. **2018** , 16, 92	8
1279	A dual-specific macrophage colony-stimulating factor antagonist of c-FMS and 3 integrin for osteoporosis therapy. **2018**, 16, e2002979	15
1278	Inhibition of the Exoglucanase Cel7A by a Douglas-Fir-Condensed Tannin. **2018**, 122, 8665-8674	1
1277	Evolution of In Silico Strategies for Protein-Protein Interaction Drug Discovery. **2018**, 23,	50

1276	Structural Studies of Predicted Ligand Binding Sites and Molecular Docking Analysis of Slc2a4 as a Therapeutic Target for the Treatment of Cancer. **2018**, 19,	23
1275	Designing B- and T-cell multi-epitope based subunit vaccine using immunoinformatics approach to control Zika virus infection. **2018**, 119, 7631-7642	49
1274	Designing a new multifunctional peptide for metal chelation and A□inhibition. **2018**, 653, 1-9	7
1273	Nano-particle mediated inhibition of Parkinson's disease using computational biology approach. **2018**, 8, 9169	45
1272	Deleterious single nucleotide polymorphisms of protein kinase R identified by the computational approach. **2018**, 101, 65-73	1
1271	Evaluation of the inhibitory effect of abamectin on mammalian butyrylcholinesterase: Enzyme kinetic and molecular docking studies. **2018**, 53, 713-718	4
1270	In vitro and in silico analyses of Vicia faba L. on Peroxisome proliferator-activated receptor gamma. **2018**, 119, 7729-7737	2
1269	Direct Phosphorylation of SRC Homology 3 Domains by Tyrosine Kinase Receptors Disassembles Ligand-Induced Signaling Networks. **2018**, 70, 995-1007.e11	10
1268	Exploratory algorithm to devise multi-epitope subunit vaccine by investigating Leishmania donovani membrane proteins. **2019**, 37, 2381-2393	17
1267	Rational Structure-Based Drug Design. **2019**, 585-600	3
1266	Prediction of Protein-Protein Interactions: Looking Through the Kaleidoscope. **2019**, 834-848	
1265	Molecular Dynamics and Simulation. **2019**, 550-566	8
1264	Identification of lead molecules against potential drug target protein MAPK4 from L. donovani: An in-silico approach using docking, molecular dynamics and binding free energy calculation. **2019**, 14, e0221331	23
1263	Cloning and identification of Bartonella □enolase as a plasminogen-binding protein. **2019**, 135, 103651	1
1262	Assembly of B4GALT1/ST6GAL1 heteromers in the Golgi membranes involves lateral interactions via highly charged surface domains. **2019**, 294, 14383-14393	14
1261	Changes on the viral capsid surface during the evolution of porcine circovirus type 2 (PCV2) from 2009 till 2018 may lead to a better receptor binding. **2019**, 5, vez026	10
1260	Investigation of the effect of UV-B light on Arabidopsis MYB4 (AtMYB4) transcription factor stability and detection of a putative MYB4-binding motif in the promoter proximal region of AtMYB4. **2019**, 14, e0220123	5
1259	Ordered hydration layer mediated ice adsorption of a globular antifreeze protein: mechanistic insight. **2019**, 21, 19298-19310	13

1258	Integration of multiple computer modeling software programs for characterization of a brain natriuretic peptide sandwich DNA aptamer complex. **2019**, 32, e2809	3
1257	Archiving and disseminating integrative structure models. **2019**, 73, 385-398	9
1256	Enhanced solubility of guanosine by inclusion complexes with cyclodextrin derivatives: Preparation, characterization, and evaluation. **2019**, 224, 115166	31
1255	Salmonella Coiled-Coil- and TIR-Containing TcpS Evades the Innate Immune System and Subdues Inflammation. **2019**, 28, 804-818.e7	4
1254	Predicting Protein Complex Structure from Surface-Induced Dissociation Mass Spectrometry Data. **2019**, 5, 1330-1341	19
1253	GS-CA Compounds: First-In-Class HIV-1 Capsid Inhibitors Covering Multiple Grounds. **2019**, 10, 1227	27
1252	Discovery of human autophagy initiation kinase ULK1 inhibitors by multi-directional screening strategies. **2019**, 39, 122-133	17
1251	DNA interaction studies of rhenium compounds with Schiff base chelates encompassing biologically relevant moieties. **2019**, 38, 950-971	2
1250	A cross-reactive human monoclonal antibody targets the conserved H7 antigenic site A from fifth wave H7N9-infected humans. **2019**, 170, 104556	4
1249	Next-Generation Noncompetitive Nanosystems Based on Gambogic Acid: Identification of Transferrin Receptor Binding Sites, Regulatory Shelf Stability, and Their Preliminary Safety in Healthy Rodents. **2019**, 2, 3540-3550	5
1248	Exploring the mechanism of PPAR□phosphorylation mediated by CDK5. **2019**, 207, 317-326	10
1247	Proteomics and Non-proteomics Approaches to Study Stable and Transient Protein-Protein Interactions. **2019**, 1140, 121-142	1
1246	DR-SIP: protocols for higher order structure modeling with distance restraints- and cyclic symmetry-imposed packing. **2020**, 36, 449-461	
1245	CX3CL1 binding protein-2 (CBP2) of Plasmodium falciparum binds nucleic acids. **2019**, 138, 996-1005	1
1244	The Extent of Human Apolipoprotein A-I Lipidation Strongly Affects the □Amyloid Efflux Across the Blood-Brain Barrier. **2019**, 13, 419	31
1243	Calcium ion implicitly modulates the adsorption ability of ion-dependent type II antifreeze proteins on an ice/water interface: a structural insight. **2019**, 11, 1387-1400	6
1242	SYNTHESIS, CHARACTERIZATION, AND MOLECULAR DOCKING ANALYSIS OF PROLINE (PYRROLIDINE 2-CARBOXYLIC ACID) AND PROLINAMIDE (PYRROLIDINE 2-CARBOXYLIC ACID AMIDE) ISOMERS AS BACTERIAL COLLAGENASE INHIBITORS. **2019**, 12, 487	
1241	MicroRNA Assisted Gene Regulation in Colorectal Cancer. **2019**, 20,	13

1240	Guanylin, Uroguanylin and Guanylate Cyclase-C Are Expressed in the Gastrointestinal Tract of Horses. **2019**, 10, 1237	1
1239	Essentials of Bioinformatics, Volume II. **2019**,	1
1238	Identification of a Killer Toxin from with Glucanase Activity. **2019**, 11,	6
1237	Synthesis and characterization of manganese ferrite nanoparticles, and its interaction with bovine serum albumin: A spectroscopic and molecular docking approach. **2019**, 296, 111871	14
1236	B-cell epitopes: Discontinuity and conformational analysis. **2019**, 114, 643-650	9
1235	Effect of Kinase Inhibiting RNase Attenuator (KIRA) Compounds on the Formation of Face-to-Face Dimers of Inositol-Requiring Enzyme 1: Insights from Computational Modeling. **2019**, 20,	3
1234	Genomewide Analysis of Mode of Action of the -Adenosylmethionine Analogue Sinefungin in Leishmania infantum. **2019**, 4,	10
1233	Prediction of Deleterious Non-synonymous SNPs of Human STK11 Gene by Combining Algorithms, Molecular Docking, and Molecular Dynamics Simulation. **2019**, 9, 16426	27
1232	Proper evaluation of chemical cross-linking-based spatial restraints improves the precision of modeling homo-oligomeric protein complexes. **2019**, 20, 464	3
1231	Web Services for Molecular Docking Simulations. **2019**, 2053, 221-229	4
1230	Synthesis, crystal structure, DFT calculations, protein interaction, anticancer potential and bromoperoxidase mimicking activity of oxidoalkoxidovanadium(V) complexes. **2019**, 43, 17783-17800	3
1229	Computer-aided identification of lung cancer inhibitors through homology modeling and virtual screening. **2019**, 20,	16
1228	The effect of calcium and magnesium on the interaction between lactoglobulin and carotenoids from sea buckthorn berries. **2019**, 34, 739-748	2
1227	Biochemical insight into pseudouridine synthase 7 (PUS7) as a novel interactor of sirtuin, SIRT1. **2019**, 518, 598-604	0
1226	In silico evidence of de novo interactions between ribosomal and Epstein - Barr virus proteins. **2019** , 20, 34	1
1225	Palmatine inhibits Zika virus infection by disrupting virus binding, entry, and stability. **2019**, 518, 732-738	16
1224	Multi-input chemical control of protein dimerization for programming graded cellular responses. **2019**, 37, 1209-1216	21
1223	Structure-function relationship of an Urokinase Receptor-derived peptide which inhibits the Formyl Peptide Receptor type 1 activity. **2019**, 9, 12169	8

1222	Mechanistic Aspects of Fungicide-Induced DNA Damage: Spectroscopic and Molecular Dynamics Simulation Studies. **2019**, 123, 8653-8661		9
1221	Screening and Identification of PLK1-Polo Box Binding Peptides by High-Throughput Sequencing of Phage-Selected Libraries. **2019**, 26, 620-633		1
1220	Immunoinformatics approaches to explore Helicobacter Pylori proteome (Virulence Factors) to design B and T cell multi-epitope subunit vaccine. **2019**, 9, 13321		52
1219	Mycobacterium tuberculosis DosR regulon gene Rv2004c contributes to streptomycin resistance and intracellular survival. **2019**, 309, 151353		3
1218	Analysing non-synonymous mutations in XDR and MDR tuberculosis drugs. **2019**, 17, 100124		
1217	Elastin-like polypeptide fusions for high-level expression and purification of human IFN- in Escherichia coli. **2019**, 585, 113401		5
1216	From biomedicinal to models and back to therapeutics: a review on the advancement of peptidic modeling. **2019**, 11, 2313-2331		1
1215	Identification of a Novel Multifunctional Ligand for Simultaneous Inhibition of Amyloid-Beta (A) and Chelation of Zinc Metal Ion. **2019**, 10, 4619-4632		9
1214	New Functional Ingredients Based on Microencapsulation of Aqueous Anthocyanin-Rich Extracts Derived from Black Rice (L.). **2019**, 24,		15
1213	Spondias mombim L. (Anacardiaceae): Chemical fingerprints, inhibitory activities, and molecular docking on key enzymes relevant to erectile dysfunction and Alzheimer's diseases. **2019**, 43, e12772		13
1212	Self-assembled transition metal dithiocarbamates of pyridine-3-carboxamide: synthesis, spectral characterization, thermal and biological studies. **2019**, 43, 4413-4424		4
1211	Development of a dual-functional conjugate of antigenic peptide and Fc-III mimetics (DCAF) for targeted antibody blocking. **2019**, 10, 3271-3280		7
1210	3D Modeling of Tumor Necrosis Factor Receptor and Tumor Necrosis Factor-bound Receptor Systems. **2019**, 38, e1800011		8
1209	Modulation of aggregation of silk fibroin by synergistic effect of the complex of curcumin and cyclodextrin. **2019**, 1867, 416-425		5
1208	Biological action of molecular adduct pyrazole:trichloroacetic acid on Candida albicans and ctDNA - A combined experimental, Fukui functions calculation and molecular docking analysis. **2019**, 1184, 129-138		21
1207	Beacons Contribute Valuable Empirical Information to Theoretical 3-D Aptamer-Peptide Binding. **2019**, 29, 711-717		2
1206	HNADOCK: a nucleic acid docking server for modeling RNA/DNA-RNA/DNA 3D complex structures. *Nucleic Acids Research*, **2019**, 47, W35-W42	20.1	16
1205	Molecular Modeling-ased Delivery System Enhances Everolimus-Induced Apoptosis in Caco-2 Cells. **2019**, 4, 8767-8777		4

1204	Application of Novel Microbial Consortia for Environmental Site Remediation and Hazardous Waste Management Toward Low- and High-Density Polyethylene and Prioritizing the Cost-Effective, Eco-friendly, and Sustainable Biotechnological Intervention. **2019**, 431-478	
1203	Immunoinformatics approaches for designing a novel multi epitope peptide vaccine against human norovirus (Norwalk virus). **2019**, 74, 103936	31
1202	Structural studies of Staphylococcus aureus Sortase inhibiton via Conus venom peptides. **2019**, 671, 87-102	10
1201	RGD-independent binding of Russell's Viper venom Kunitz-type protease inhibitors to platelet GPIIb/IIIa receptor. **2019**, 9, 8316	9
1200	Association of BUD13-ZNF259-APOA5-APOA1-SIK3 cluster polymorphism in 11q23.3 and structure of APOA5 with increased plasma triglyceride levels in a Korean population. **2019**, 9, 8296	3
1199	GalaxyTongDock: Symmetric and asymmetric ab initio protein-protein docking web server with improved energy parameters. **2019**, 40, 2413-2417	20
1198	Specific keratinase derived designer peptides potently inhibit A aggregation resulting in reduced neuronal toxicity and apoptosis. **2019**, 476, 1817-1841	4
1197	Principles for Integrative Structural Biology Studies. **2019**, 177, 1384-1403	108
1196	Mutagenesis of DsbAss is Crucial for the Signal Recognition Particle Mechanism in : Insights from Molecular Dynamics Simulations. **2019**, 9,	7
1195	Immunoinformatics and structural vaccinology driven prediction of multi-epitope vaccine against Mayaro virus and validation through in-silico expression. **2019**, 73, 390-400	43
1194	Early impairment of epigenetic pattern in neurodegeneration: Additional mechanisms behind pyrethroid toxicity. **2019**, 124, 110629	18
1193	Interaction of acetaminophen and caffeine towards cyclooxygenase-2 (COX-2) in inhibition of prostaglandin (PGH2) synthesis. **2019**, 1146, 012004	
1192	A connection between reversible tyrosine phosphorylation and SNARE complex disassembly activity of N-ethylmaleimide-sensitive factor unveiled by the phosphomimetic mutant N-ethylmaleimide-sensitive factor-Y83E. **2019**, 25, 344-358	1
1191	Antihypertensive Effects of Corn Silk Extract and Its Novel Bioactive Constituent in Spontaneously Hypertensive Rats: The Involvement of Angiotensin-Converting Enzyme Inhibition. **2019**, 24,	13
1190	Characterization of phthalate reductase from Ralstonia eutropha CH34 and in silico study of phthalate dioxygenase and phthalate reductase interaction. **2019**, 90, 161-170	21
1189	Pyrene-based prospective biomaterial: In vitro bioimaging, protein binding studies and detection of bilirubin and Fe. **2019**, 221, 117150	15
1188	CHDOCK: a hierarchical docking approach for modeling Cn symmetric homo-oligomeric complexes. **2019**, 5, 65-72	6
1187	Anti-Inflammatory Effects of Different Astaxanthin Isomers and the Roles of Lipid Transporters in the Cellular Transport of Astaxanthin Isomers in Caco-2 Cell Monolayers. **2019**, 67, 6222-6231	39

1186	Selection of a Single Chain Variable Fragment Antibody (scFv) against Subtilisin BRC and its Interaction with Subtilisin BRC. **2019**, 8, 24-31		
1185	Structural and free energy landscape of novel mutations in ribosomal protein S1 (rpsA) associated with pyrazinamide resistance. **2019**, 9, 7482		20
1184	HawkDock: a web server to predict and analyze the protein-protein complex based on computational docking and MM/GBSA. *Nucleic Acids Research*, **2019**, 47, W322-W330	20.1	139
1183	Radicalic cleavage pathway and DNA docking studies of novel chemotherapic platinum agent of 5,6-di-2-ithienyl-2,3-dihydropyrazine. **2019**, 170, 25-33		1
1182	Binding of alpha-fodrin to gamma-tubulin accounts for its role in the inhibition of microtubule nucleation. **2019**, 593, 1154-1165		2
1181	Control of anterior GRadient 2 (AGR2) dimerization links endoplasmic reticulum proteostasis to inflammation. **2019**, 11,		29
1180	Fluorescent 1,4-Naphthoquinones To Visualize Diffuse and Dense-Core Amyloid Plaques in APP/PS1 Transgenic Mouse Brains. **2019**, 10, 3031-3044		9
1179	Immunoinformatics Approach for Multiepitopes Vaccine Prediction against Glycoprotein B of Avian Infectious Laryngotracheitis Virus. **2019**, 2019, 1270485		12
1178	Flexible Backbone Assembly and Refinement of Symmetrical Homomeric Complexes. **2019**, 27, 1041-1051.e8		8
1177	Molecular architecture, polar targeting and biogenesis of the Legionella Dot/Icm T4SS. **2019**, 4, 1173-1182		42
1176	Functional insights of a molecular complex pyrazolium 3,5-dinitrobenzoate:3,5-dinitrobenzoic acid on infectious agents and ctDNA - A comparative biological screening and complementary theoretical calculations. **2019**, 196, 111497		0
1175	Alternative interaction sites in the influenza A virus nucleoprotein mediate viral escape from the importin-α mediated nuclear import pathway. **2019**, 286, 3374-3388		2
1174	Flavonoid loaded nanoparticles as an effective measure to combat oxidative stress in Ribonuclease A. **2019**, 162, 185-197		8
1173	Modeling of Protein?Protein Interactions in Cytokinin Signal Transduction. **2019**, 20,		14
1172	Glyphaea brevis - In vitro antioxidant and in silico biological activity of major constituents and molecular docking analyses. **2019**, 59, 187-196		5
1171	An integrative approach using systems biology, mutational analysis with molecular dynamics simulation to challenge the functionality of a target protein. **2019**, 93, 1050-1060		10
1170	Molecular Docking: A Structure-Based Approach for Drug Repurposing. **2019**, 161-189		7
1169	Integrative Structure Modeling: Overview and Assessment. **2019**, 88, 113-135		29

1168	Vaccinomics strategy for developing a unique multi-epitope monovalent vaccine against Marburg marburgvirus. **2019**, 70, 140-157	22
1167	Further studies on sugar transporter (SWEET) genes in wheat (Triticum aestivum L.). **2019**, 46, 2327-2353	31
1166	DNA-protein interaction: identification, prediction and data analysis. **2019**, 46, 3571-3596	4
1165	Predicting Protein Dimer Structures Using MELD MD. **2019**, 15, 3381-3389	7
1164	In silico analyses of molecular interactions between groundnut bud necrosis virus and its vector,. **2019**, 30, 245-251	10
1163	A fully human anti-IL-7R antibody promotes antitumor activity against T-cell acute lymphoblastic leukemia. **2019**, 33, 2155-2168	30
1162	The mechanism of PI3K activation at the atomic level. **2019**, 10, 3671-3680	45
1161	A small molecule Nec-1 directly induces amyloid clearance in the brains of aged APP/PS1 mice. **2019**, 9, 4183	18
1160	Intrinsically disordered regions mediate macromolecular assembly of the Slit diaphragm proteins associated with Nephrotic syndrome. **2019**, 45, 603-613	4
1159	Anticancer evaluation of ruthenium(III) complexes with N-donor ligands tethered to coumarin or uracil moieties. **2019**, 492, 98-107	9
1158	Antibody antigen complex modelling in the era of immunoglobulin repertoire sequencing. **2019**, 4, 679-688	16
1157	Cloud-Based High Throughput Virtual Screening in Novel Drug Discovery. **2019**, 250-278	8
1156	X-ray radiolytic labeling reveals the molecular basis of orange carotenoid protein photoprotection and its interactions with fluorescence recovery protein. **2019**, 294, 8848-8860	13
1155	Combating tigecycline resistant Acinetobacter baumannii: A leap forward towards multi-epitope based vaccine discovery. **2019**, 132, 1-17	28
1154	Detection of ON1 and novel genotypes of human respiratory syncytial virus and emergence of palivizumab resistance in Lebanon. **2019**, 14, e0212687	15
1153	Structural study to analyze the DNA-binding properties of DsrC protein from the dsr operon of sulfur-oxidizing bacterium Allochromatium vinosum. **2019**, 25, 74	2
1152	Biofilm inhibition and anti-quorum sensing activity of phytosynthesized silver nanoparticles against the nosocomial pathogen Pseudomonas aeruginosa. **2019**, 35, 34-49	44
1151	Myxococcus xanthus truncated globin HbO: in silico analysis and functional characterization. **2019**, 46, 2101-2110	

1150	Shift in Bacillus sp. JR3 esterase LipJ activity profile after addition of essential residues from family I.5 thermophilic lipases. **2019**, 144, 166-176	2
1149	Benchmarking of different molecular docking methods for protein-peptide docking. **2019**, 19, 426	52
1148	Bioactivity of a radical scavenger bis(pyrazolium -toluenesulphonate) on ctDNA and certain microbes: a combined experimental and theoretical analysis. **2019**, 8, 421-431	0
1147	Reverse vaccinology approach to design a novel multi-epitope subunit vaccine against avian influenza A (H7N9) virus. **2019**, 130, 19-37	48
1146	Water soluble sulfaguanidine based Schiff base as a Turn-on Fluorescent probe for intracellular recognition of Zn2+ in living cells and exploration for biological activities. **2019**, 172, 28-38	14
1145	Interactions of flavonoids from yellow onion skins with whey proteins: Mechanisms of binding and microencapsulation with different combinations of polymers. **2019**, 215, 158-167	15
1144	Exploring the Pyrazinamide Drug Resistance Mechanism of Clinical Mutants T370P and W403G in Ribosomal Protein S1 of Mycobacterium tuberculosis. **2019**, 59, 1584-1597	19
1143	Microcin J25 inhibits ubiquinol oxidase activity of purified cytochrome bd-I from Escherichia coli. **2019**, 160, 141-147	9
1142	Biallelic mutations in valyl-tRNA synthetase gene VARS are associated with a progressive neurodevelopmental epileptic encephalopathy. **2019**, 10, 707	18
1141	Molecular encapsulation of lidocaine and procaine into cyclodexrin cavity: in vitro cytotoxic evaluation. **2019**, 56, 215-224	1
1140	Molecular docking studies of Vinca alkaloid derivatives on Tubulin. **2019**, 57, 702-706	1
1139	Structural Dynamics Behind Clinical Mutants of PncA-Asp12Ala, Pro54Leu, and His57Pro of Associated With Pyrazinamide Resistance. **2019**, 7, 404	10
1138	Secretagogin Regulates Insulin Signaling by Direct Insulin Binding. **2019**, 21, 736-753	7
1137	Molecular characterization, computational analysis and expression profiling of gene in Indian major carp, (Hamilton 1822). **2021**, 32, 413-426	5
1136	Molecular anatomy of the receptor binding module of a bacteriophage long tail fiber. **2019**, 15, e1008193	17
1135	In vivo structure of the Legionella type II secretion system by electron cryotomography. **2019**, 4, 2101-2108	15
1134	Federating Structural Models and Data: Outcomes from A Workshop on Archiving Integrative Structures. **2019**, 27, 1745-1759	22
1133	In silico characterization of Leptospira interrogans DNA ligase A and delineation of its antimicrobial stretches. **2019**, 69, 1329-1350	0

1132	Identifying protein-protein interface via a novel multi-scale local sequence and structural representation. **2019**, 20, 483	4
1131	GroScore: Accurate Scoring of Protein-Protein Binding Poses Using Explicit-Solvent Free-Energy Calculations. **2019**, 59, 5074-5085	6
1130	Protein-assisted RNA fragment docking (RnaX) for modeling RNA-protein interactions using ModelX. **2019**, 116, 24568-24573	5
1129	PMP-diketopiperazine adducts form at the active site of a PLP dependent enzyme involved in formycin biosynthesis. **2019**, 55, 14502-14505	4
1128	Isolation and Characterization of Cross-Neutralizing Human Anti-V3 Single-Chain Variable Fragments (scFvs) Against HIV-1 from an Antigen Preselected Phage Library. **2019**, 187, 1011-1027	6
1127	Interfering PLD1-PED/PEA15 interaction using self-inhibitory peptides: An study to discover novel therapeutic candidates against type 2 diabetes. **2019**, 26, 160-164	2
1126	Investigation of the probable homo-dimer model of the complementation group A (XPA) protein to represent the DNA-binding core. **2019**, 37, 3322-3336	1
1125	Engineering of serine protease for improved thermostability and catalytic activity using rational design. **2019**, 126, 229-237	19
1124	Ternary Copper (II) complex based chemical probes for DNA targeting: Cytotoxic activity under visible light. **2019**, 33, e4762	5
1123	How Can Interleukin-1 Receptor Antagonist Modulate Distinct Cell Death Pathways?. **2019**, 59, 351-359	12
1122	Molecular mechanics of caffeic acid in food profilin allergens. **2019**, 138, 1	
1121	Protein docking using constrained self-adaptive differential evolution algorithm. **2019**, 23, 11651-11669	1
1120	Insights into the Mechanisms of the Pyrazinamide Resistance of Three Pyrazinamidase Mutants N11K, P69T, and D126N. **2019**, 59, 498-508	12
1119	Direct SUMOylation of M1 muscarinic acetylcholine receptor increases its ligand-binding affinity and signal transduction. **2019**, 33, 3237-3251	6
1118	Proline functionalized gold nanoparticles modulates lysozyme fibrillation. **2019**, 174, 401-408	15
1117	Design of novel multi-epitope vaccines against severe acute respiratory syndrome validated through multistage molecular interaction and dynamics. **2019**, 37, 4345-4360	22
1116	How Ca1.2-bound verapamil blocks Ca influx into cardiomyocyte: Atomic level views. **2019**, 139, 153-157	7
1115	On identifying collective displacements in apo-proteins that reveal eventual binding pathways. **2019**, 15, e1006665	7

1114	Peptidyl-prolyl isomerase-B is involved in biofilm formation and a generic target for drug repurposing-based intervention. **2019**, 5, 3	17
1113	Structural basis for renal cancer by the dynamics of pVHL-dependent JADE1 stabilization and Ecatenin regulation. **2019**, 145, 65-77	2
1112	Biosynthesized Silver Nanoparticle (AgNP) From Leaf Extract Exhibits Anti-metastasis and Anti-biofilm Potentials. **2019**, 10, 8	40
1111	Molecular docking of anti-inflammatory drug diclofenac with metabolic targets: Potential applications in cancer therapeutics. **2019**, 465, 117-125	7
1110	Molecular Dynamics Simulation of Kynurenine Aminotransferase Type II with Nicotine as a Ligand: A Possible Biochemical Role of Nicotine in Schizophrenia. **2019**, 4, 710-717	1
1109	Assessment of the properties of chitin deacetylases showing different enzymatic action patterns. **2019**, 88, 41-48	6
1108	Structure-Based Docking Studies of GLUT4 Towards Exploring Selected Phytochemicals from Solanum xanthocarpum as a Therapeutic Target for the Treatment of Cancer. **2019**, 16, 406-416	16
1107	Evidence of human-like Ca channels and effects of Ca channel blockers in Acanthamoeba castellanii. **2019**, 93, 351-363	6
1106	Refinement of protein-protein complexes in contact map space with metadynamics simulations. **2019**, 87, 12-22	8
1105	Structural-dynamic insights into the cytotoxin-associated gene A (CagA) and its abrogation to interact with the tumor suppressor protein ASPP2 using decoy peptides. **2019**, 37, 4035-4050	13
1104	Synthesis, structural investigations and pharmacological properties of a new zinc complex with a N4-donor Schiff base incorporating 2-pyridyl ring. **2019**, 487, 97-106	6
1103	Styryl-cinnamate hybrid inhibits glioma by alleviating translation, bioenergetics and other key cellular responses leading to apoptosis. **2019**, 375, 11-21	
1102	PYRROLO isolated from marine sponge associated bacterium Halobacillus kuroshimensis SNSAB01 - Antifouling study based on molecular docking, diatom adhesion and mussel byssal thread inhibition. **2019**, 173, 9-17	4
1101	Quantitative Evaluation of Native Protein Folds and Assemblies by Hydrogen Deuterium Exchange Mass Spectrometry (HDX-MS). **2019**, 30, 58-66	8
1100	Mapping the minimum domain of the fibronectin binding site on transglutaminase 2 (TG2) and its importance in mediating signaling, adhesion, and migration in TG2-expressing cells. **2019**, 33, 2327-2342	7
1099	Novel missense mutations in gidB gene associated with streptomycin resistance in Mycobacterium tuberculosis: insights from molecular dynamics. **2019**, 37, 20-35	6
1098	Insight into a Transcriptional Adaptor Zinc Finger Encoded by a Putative Protein in the White Spot Syndrome Virus Genome. **2019**, 11, 145-151	3
1097	Coiled-coil oligomerization controls localization of the plasma membrane REMORINs. **2019**, 206, 12-19	14

1096	In-Silico Prediction of Peptide Based Vaccine Against Zika Virus. **2020**, 26, 85-91	9
1095	Computational approaches to therapeutic antibody design: established methods and emerging trends. **2020**, 21, 1549-1567	66
1094	Reserpine attenuates biofilm formation and virulence of Staphylococcus aureus. **2020**, 138, 103790	14
1093	Health Promoting Effects of Food-Derived Bioactive Peptides: A Review. **2020**, 26, 831-848	29
1092	Contriving a chimeric polyvalent vaccine to prevent infections caused by herpes simplex virus (type-1 and type-2): an exploratory immunoinformatic approach. **2020**, 38, 2898-2915	25
1091	Epitope-Based Vaccine Designing of Targeting the Virulence Factor Mce-Family Protein by Immunoinformatics Approach. **2020**, 26, 1165-1176	9
1090	Structural basis of the strong cell-cell junction formed by cadherin-23. **2019**, 287, 2328	1
1089	Biocomputational Analysis and In Silico Characterization of an Angiogenic Protein (RNase5) in Zebrafish (Danio rerio). **2020**, 26, 1687-1697	5
1088	Exploring the Molecular Mechanisms Underlying the in vitro Anticancer Effects of Multitarget-Directed Hydrazone Ruthenium(II)-Arene Complexes. **2020**, 15, 105-113	10
1087	Computational prediction of protein□protein binding affinities. **2020**, 10, e1448	44
1086	Potential druggable proteins and chimeric vaccine construct prioritization against Brucella melitensis from species core genome data. **2020**, 112, 1734-1745	7
1085	Docking Troponin T onto the Tropomyosin Overlapping Domain of Thin Filaments. **2020**, 118, 325-336	12
1084	Interaction of human dynein light chain 1 (DYNLL1) with enterochelin esterase () and protective antigen () might be the potential cause of human infection. **2020**, 27, 1396-1402	2
1083	Study of Anti-Apoptotic mechanism of Ruthenium (II)Polypyridyl Complexes via RT-PCR and DNA binding. **2020**, 34, e5332	7
1082	Characterization, molecular modeling and phylogenetic analysis of a long mammalian neurotoxin from the venom of the Iranian scorpion Androctonus crassicauda. **2020**, 75, 1029-1041	2
1081	Alterations in plasma membrane ion channel structures stimulate NLRP3 inflammasome activation in APOL1 risk milieu. **2020**, 287, 2000-2022	11
1080	Recombinant engineered phage-derived enzybiotic in Pichia pastoris X-33 as whole cell biocatalyst for effective biocontrol of Vibrio parahaemolyticus in aquaculture. **2020**, 154, 1576-1585	10
1079	Performance and enhancement of the LZerD protein assembly pipeline in CAPRI 38-46. **2020**, 88, 948-961	6

1078	Silica-supported heterogeneous catalysts-mediated synthesis of chalcones as potent urease inhibitors: in vitro and molecular docking studies. **2020**, 151, 123-133	4
1077	The Lazy Life of Lipid-Linked Oligosaccharides in All Life Domains. **2020**, 60, 631-643	2
1076	Application of an integrated cheminformatics-molecular docking approach for discovery for physicochemically similar analogs of fluoroquinolones as putative HCV inhibitors. **2020**, 84, 107167	2
1075	Removal of an atypical region from a staphylococcal cyclophilin affects its structure, function, stability, and shape. **2020**, 151, 1287-1298	2
1074	Micellization, anti-proliferative activity and binding study of cationic gemini surfactants with calf thymus DNA. **2020**, 34, 100221	9
1073	Structure prediction of biological assemblies using GALAXY in CAPRI rounds 38-45. **2020**, 88, 1009-1017	2
1072	Design, synthesis, antimycobacterial activity and molecular docking studies of novel 3-(N-substituted glycinamido) benzoic acid analogues as anti tubercular agents. **2020**, 30, 127603	2
1071	Identification and validation of novel and more effective choline kinase inhibitors against Streptococcus pneumoniae. **2020**, 10, 15418	2
1070	Evaluation of Human Cathelicidin LL-37 as a Novel Therapeutic Inhibitor of Panton-Valentine Leukocidin Toxin of Methicillin-Resistant. **2021**, 27, 602-615	1
1069	Synthesis, Molecular Docking, and In Vitro Boron Neutron Capture Therapy Assay of Carboranyl Sinomenine. **2020**, 25,	3
1068	PRosettaC: Rosetta Based Modeling of PROTAC Mediated Ternary Complexes. **2020**, 60, 4894-4903	33
1067	, Molecular Docking and Antimicrobial Activity of the Major Rapeseed Seed Storage Proteins. **2020**, 11, 1340	12
1066	Conformational ensembles of non-peptide □conotoxin mimetics and Ca ion binding to human voltage-gated N-type calcium channel Ca2.2. **2020**, 18, 2357-2372	1
1065	Enteroaggregative E. coli Adherence to Human Heparan Sulfate Proteoglycans Drives Segment and Host Specific Responses to Infection. **2020**, 16, e1008851	12
1064	GIP receptor suppresses PAC1receptor-mediated neuronal differentiation via formation of a receptor heterocomplex. **2021**, 157, 1850-1860	1
1063	Delineating blueprint of an epitope-based peptide vaccine against the multiple serovars of dengue virus: A hierarchical reverse vaccinology approach. **2020**, 20, 100430	3
1062	Antiviral Peptides as Promising Therapeutics against SARS-CoV-2. **2020**, 124, 9785-9792	33
1061	Immunoinformatics approach to understand molecular interaction between multi-epitopic regions of SARS-CoV-2 spike-protein with TLR4/MD-2 complex. **2020**, 85, 104587	36

1060	Computer-Aided Drug Design. **2020**,	4
1059	Mutational profiling of POT1 gene and its interaction with TPP1 in cancer- A computational approach. **2020**, 20, 100389	
1058	A peptide derived from phage-display limits psoriasis-like lesions in mice. **2020**, 6, e04162	2
1057	Comparative host-coronavirus protein interaction networks reveal pan-viral disease mechanisms. **2020**, 370,	261
1056	TAT-peptide conjugated repurposing drug against SARS-CoV-2 main protease (3CLpro): Potential therapeutic intervention to combat COVID-19.. **2020**, 13, 8069-8079	8
1055	Prediction of potential inhibitors for RNA-dependent RNA polymerase of SARS-CoV-2 using comprehensive drug repurposing and molecular docking approach. **2020**, 163, 1787-1797	34
1054	Guidelines To Predict Binding Poses of Antibody-Integrin Complexes. **2020**, 5, 16379-16385	1
1053	Methods for sequence and structural analysis of B and T cell receptor repertoires. **2020**, 18, 2000-2011	8
1052	Prediction of secondary, tertiary protein structure and interaction eIF4E from Capsicum annum with Rep Geminivirus. **2020**, 497, 012026	
1051	Structural study of letrozole and metronidazole and formation of self-assembly with graphene and fullerene with the enhancement of physical, chemical and biological activities. **2021**, 39, 5509-5515	23
1050	Porcine Parvovirus 7: Evolutionary Dynamics and Identification of Epitopes toward Vaccine Design. **2020**, 8,	4
1049	Performance of ZDOCK and IRAD in CAPRI rounds 39-45. **2020**, 88, 1050-1054	1
1048	Challenges and opportunities of automated protein-protein docking: HDOCK server vs human predictions in CAPRI Rounds 38-46. **2020**, 88, 1055-1069	8
1047	The potential antiviral effect of major royal jelly protein2 and its isoform X1 against severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2): Insight on their sialidase activity and molecular docking. **2020**, 75, 104282	8
1046	Atlasing of Assembly Landscapes using Distance Geometry and Graph Rigidity. **2020**, 60, 4924-4957	2
1045	Modelling the structural and reactivity landscapes of tucatinib with special reference to its wavefunction-dependent properties and screening for potential antiviral activity. **2020**, 26, 341	17
1044	Identification of biomarkers for the accurate and sensitive diagnosis of three bacterial pneumonia pathogens using in silico approaches. **2020**, 21, 82	4
1043	Probiotics-Derived Peptides and Their Immunomodulatory Molecules Can Play a Preventive Role Against Viral Diseases Including COVID-19. **2021**, 13, 611-623	12

1042	Core amino acid substitutions in HCV-3a isolates from Pakistan and opportunities for multi-epitopic vaccines. **2020**, 1-16	1
1041	Engineering a novel subunit vaccine against SARS-CoV-2 by exploring immunoinformatics approach. **2020**, 21, 100478	11
1040	Design of a multi-epitope-based vaccine targeting M-protein of SARS-CoV2: an immunoinformatics approach. **2020**, 1-15	17
1039	Docking-based identification of small-molecule binding sites at protein-protein interfaces. **2020**, 18, 3750-3761	4
1038	HDAC6 ZnF UBP as the Modifier of Tau Structure and Function. **2020**, 59, 4546-4562	7
1037	Bovine □lactoglobulin peptides as novel carriers for flavonoids extracted with supercritical fluids from yellow onion skins. **2020**, 85, 4290-4299	0
1036	Methods and Applications of In Silico Aptamer Design and Modeling. **2020**, 21,	25
1035	Designing novel epitope-based polyvalent vaccines against herpes simplex virus-1 and 2 exploiting the immunoinformatics approach. **2021**, 39, 6585-6605	6
1034	Characterization of the Proteins Involved in the DNA Repair Mechanism in. **2020**, 21,	
1033	Blueprint of epitope-based multivalent and multipathogenic vaccines: targeted against the dengue and zika viruses. **2021**, 39, 6882-6902	4
1032	The Interaction of Bovine □Lactoglobulin with Caffeic Acid: From Binding Mechanisms to Functional Complexes. **2020**, 10,	3
1031	Designing an efficient multi-epitope vaccine against Campylobacter jejuni using immunoinformatics and reverse vaccinology approach. **2020**, 147, 104398	15
1030	In silico analysis of PepYLCV-□1 protein interaction with pepper-SnRK1 for pathogenicity prediction. **2020**, 497, 012027	1
1029	Combination drug therapy for multimodal treatment of cancer by targeting mitochondrial transcriptional pathway: An in-silico approach. **2020**, 143, 110075	2
1028	Synthesis and characterization of host-guest inclusion complex of □cyclodextrin with 4,4?-methylenedianiline by diverse methodologies. **2020**, 316, 113843	4
1027	Molecular modeling and co-expression analysis of human stem cell factor as fusion partner to granulocyte colony stimulating factor for improving their bioactivity. **2021**, 39, 4990-5004	1
1026	Contriving Multi-Epitope Subunit of Vaccine for COVID-19: Immunoinformatics Approaches. **2020**, 11, 1784	54
1025	Structure of fish Toll-like receptors (TLR) and NOD-like receptors (NLR). **2020**, 161, 1602-1617	28

1024	Spectral analysis and DFT investigation of some benzopyran analogues and their self-assemblies with graphene. **2020**, 317, 113924	16
1023	Binuclear 3,3?,5,5?-tetramethyl-1H,H-4,4?-bipyrazole Ruthenium(II) complexes: Synthesis, characterization and biological studies. **2020**, 513, 119902	5
1022	Efficient elimination of primary B-ALL cells in vitro and in vivo using a novel 4-1BB-based CAR targeting a membrane-distal CD22 epitope. **2020**, 8,	6
1021	Prediction and evaluation of deleterious and disease causing non-synonymous SNPs (nsSNPs) in human NF2 gene responsible for neurofibromatosis type 2 (NF2). **2021**, 39, 7044-7055	2
1020	A dual and conflicting role for imiquimod in inflammation: A TLR7 agonist and a cAMP phosphodiesterase inhibitor. **2020**, 182, 114206	2
1019	Structural analysis of toll-like receptor 18 from soiny mullet (Liza haematocheila): Giving insights on the ligand binding mechanism of fish specific TLRs. **2020**, 107, 490-496	2
1018	Deciphering the Structural Enigma of HLA Class-II Binding Peptides for Enhanced Immunoinformatics-based Prediction of Vaccine Epitopes. **2020**, 19, 4655-4669	2
1017	New insights on human IRE1 tetramer structures based on molecular modeling. **2020**, 10, 17490	2
1016	Multi-epitope based vaccine design against Sarcoptes scabiei paramyosin using immunoinformatics approach. **2020**, 319, 114105	5
1015	Pleiotropic roles of cold shock proteins with special emphasis on unexplored cold shock protein member of Plasmodium falciparum. **2020**, 19, 382	2
1014	A novel strategy for molecular interfaces optimization: The case of Ferritin-Transferrin receptor interaction. **2020**, 18, 2678-2686	3
1013	Ultrasonic-assisted efficient synthesis of inclusion complexes of salsalate drug and □-cyclodextrin derivatives for potent biomedical applications. **2020**, 319, 114358	9
1012	Designing a multi-epitope peptide based vaccine against SARS-CoV-2. **2020**, 10, 16219	44
1011	Spectral analysis and detailed quantum mechanical investigation of some acetanilide analogues and their self-assemblies with graphene and fullerene. **2020**, 26, 254	11
1010	Active-site Molecular docking of Nigellidine with nucleocapsid- NSP2-MPro of COVID-19 and to human IL1R-IL6R and strong antioxidant role of Nigella-sativa in experimental rats. **2020**, 1-23	12
1009	Ebola Virus VP35 Protein: Modeling of the Tetrameric Structure and an Analysis of Its Interaction with Human PKR. **2020**, 19, 4533-4542	3
1008	Identification of zebrafish fumarate hydratase active site by molecular docking and simulation studies. **2020**, 1-13	
1007	The vital role of ditopic N□N bridging ligands with different lengths in the formation of new binuclear dioxomolybdenum(VI) complexes: synthesis, crystal structures, supramolecular framework and protein binding studies. **2020**, 44, 16645-16664	1

1006	A Poplar Rust Effector Protein Associates with Protein Disulfide Isomerase and Enhances Plant Susceptibility. **2020**, 9,	2
1005	Tetrapeptide Ac-HAEE-NH Protects 42 nAChR from Inhibition by A2020, 21,	3
1004	Structural and Molecular Docking Analytical Studies of the Predicted Ligand Binding Sites of Cadherin-1 in Cancer Prognostics. **2020**, 13, 1-9	1
1003	Structural Characterization of Covalently Stabilized Human Cystatin C Oligomers. **2020**, 21,	0
1002	Detecting the nature and solving the crystal structure of a contaminant protein from an opportunistic pathogen. **2020**, 76, 392-397	1
1001	Design of a multi-epitope peptide vaccine candidate against chandipura virus: an immuno-informatics study. **2020**, 1-12	4
1000	Harringtonine Inhibits Zika Virus Infection through Multiple Mechanisms. **2020**, 25,	4
999	Comprehensive genome based analysis of Vibrio parahaemolyticus for identifying novel drug and vaccine molecules: Subtractive proteomics and vaccinomics approach. **2020**, 15, e0237181	7
998	LncRNA-SLC16A1-AS1 induces metabolic reprogramming during Bladder Cancer progression as target and co-activator of E2F1. **2020**, 10, 9620-9643	26
997	DFT and MD simulations and molecular docking of co-crystals of octafluoro-1,4-diiodobutane with phenazine and acridine. **2020**, 31, 2525-2531	5
996	Binding of dipeptidyl peptidase III to the oxidative stress cell sensor Kelch-like ECH-associated protein 1 is a two-step process. **2021**, 39, 6870-6881	2
995	Structure-Based Virtual Screening and Biochemical Validation to Discover a Potential Inhibitor of the SARS-CoV-2 Main Protease. **2020**, 5, 33151-33161	14
994	PAR driven placenta EVT invasion act via LRP5/6 as coreceptors. **2020**, 34, 15701-15717	3
993	Prediction of putative regulatory elements in the subgenomic promoters of cucumber green mottle mosaic virus and their interactions with the RNA dependent RNA polymerase domain. **2020**, 31, 503-516	
992	Structure and dynamics of membrane protein in SARS-CoV-2. **2020**, 1-14	15
991	Structural insights and evaluation of the potential impact of missense variants on the interactions of SLIT2 with ROBO1/4 in cancer progression. **2020**, 10, 21909	1
990	Insight into the binding of PEG-400 with eye protein alpha-crystallin: Multi spectroscopic and computational approach: possible therapeutics targeting eye diseases. **2020**, 1-11	6
989	ITScore-NL: An Iterative Knowledge-Based Scoring Function for Nucleic Acid-Ligand Interactions. **2020**, 60, 6698-6708	6

988	Seeking the Source of Catalytic Efficiency of Lindane Dehydrochlorinase, LinA. **2020**, 124, 10353-10364	0
987	A substrate binding model for the KEOPS tRNA modifying complex. **2020**, 11, 6233	6
986	Genetic interaction mapping informs integrative structure determination of protein complexes. **2020**, 370,	11
985	A Web-Based Platform on Coronavirus Disease-19 to Maintain Predicted Diagnostic, Drug, and Vaccine Candidates. **2020**, 39, 204-216	17
984	Design of a multi-epitope subunit vaccine for immune-protection against Leishmania parasite. **2020** , 114, 471-481	11
983	In vitro anti-Helicobacter pylori and anti-gastric cancer activities of Acacia nilotica aqueous leaf extract and its validation using in silico molecular docking approach. **2020**, 51, 1675-1675	1
982	Recent Advances in Molecular Docking for the Research and Discovery of Potential Marine Drugs. **2020**, 18,	21
981	Computationally validated SARS-CoV-2 CTL and HTL Multi-Patch vaccines, designed by reverse epitomics approach, show potential to cover large ethnically distributed human population worldwide. **2020**, 1-20	6
980	Emerging of composition variations of SARS-CoV-2 spike protein and human ACE2 contribute to the level of infection: approaches. **2020**, 1-12	2
979	Structural prediction of protein interactions and docking using conservation and coevolution. **2020**, 10, e1470	4
978	Amantadine as a drug to mitigate the effects of COVID-19. **2020**, 140, 109755	38
977	The structure and reactivity of the HoxEFU complex from the cyanobacterium sp. PCC 6803. **2020**, 295, 9445-9454	3
976	CD95 Structure, Aggregation and Cell Signaling. **2020**, 8, 314	11
975	Novel ssDNA Ligand Against Ovarian Cancer Biomarker CA125 With Promising Diagnostic Potential. **2020**, 8, 400	4
974	Metagenomic Insight Towards Vanillin-Mediated Membrane Biofouling Prevention: In Silico Docking Validation. **2020**, 77, 2233-2247	3
973	Evaluation of anti-tuberculosis activity of some oxotitanium(IV) Schiff base complexes; molecular docking, dynamics simulation and ADMET studies. **2020**, 2, 1	4
972	Structure of nevanimibe-bound tetrameric human ACAT1. **2020**, 581, 339-343	24
971	Truncated human angiotensin converting enzyme 2; a potential inhibitor of SARS-CoV-2 spike glycoprotein and potent COVID-19 therapeutic agent. **2021**, 39, 3605-3614	40

970	Molecular Mechanisms Underlying the Absorption of Aglycone and Glycosidic Flavonoids in a Caco-2 BBe1 Cell Model. **2020**, 5, 10782-10793	13
969	In silico designing of peptide based vaccine for Hepatitis viruses using reverse vaccinology approach. **2020**, 84, 104388	5
968	Minimally altering a critical kinase for low-phytate maize. **2020**, 10, 6324	2
967	In Silico Characterization of a Unique Plant-Like "Loopful" GH19 Chitinase from Newly Isolated Chitinophaga sp. YS-16. **2020**, 77, 2248-2257	1
966	Comprehensive analysis of Translationally Controlled Tumor Protein (TCTP) provides insights for lineage-specific evolution and functional divergence. **2020**, 15, e0232029	2
965	Protein Network Studies on PCOS Biomarkers With S100A8, Druggability Assessment, and RNA Aptamer Designing to Control Its Cyst Migration Effect. **2020**, 8, 328	3
964	Rational targeting of Wzb phosphatase and Wzc kinase interaction inhibits extracellular polysaccharides synthesis and biofilm formation in Acinetobacter baumannii. **2020**, 492, 108025	8
963	Brain-Sparing Sympathofacilitators Mitigate Obesity without Adverse Cardiovascular Effects. **2020**, 31, 1120-1135.e7	8
962	Synthesis, characterization, molecular docking and antimicrobial activity of copper(II) complexes of metronidazole and 1,10 phenanthroline. **2020**, 510, 119744	13
961	Development and characterization of a fully human antibody targeting SCF/c-kit signaling. **2020**, 159, 66-78	3
960	Exploiting the reverse vaccinology approach to design novel subunit vaccines against Ebola virus. **2020**, 225, 151949	27
959	Plant Proteomics. **2020**,	2
958	Design of a Novel Multi Epitope-Based Vaccine for Pandemic Coronavirus Disease (COVID-19) by Vaccinomics and Probable Prevention Strategy against Avenging Zoonotics. **2020**, 151, 105387	21
957	A systematic and reverse vaccinology approach to design novel subunit vaccines against Dengue virus type-1 (DENV-1) and human Papillomavirus-16 (HPV-16). **2020**, 19, 100343	9
956	Synthesis, reactivity, in vitro boron neutron capture therapy assay, and molecular docking of fluorocyclocarboxyboranylamine. **2020**, 34, e5714	1
955	How repertoire data are changing antibody science. **2020**, 295, 9823-9837	19
954	Molecular Structure, Binding Affinity, and Biological Activity in the Epigenome. **2020**, 21,	3
953	Screening and druggability analysis of some plant metabolites against SARS-CoV-2: An integrative computational approach. **2020**, 20, 100367	28

952	A systematic strategy for the investigation of vaccines and drugs targeting bacteria. **2020**, 18, 1525-1538	7
951	Insight into the bovine milk peptide LPcin-YK3 selection in the proteolytic system of Lactobacillus species. **2020**, 26, e3268	1
950	Computer-Aided Ligand Discovery for Estrogen Receptor Alpha. **2020**, 21,	14
949	Structure-based drug designing and immunoinformatics approach for SARS-CoV-2. **2020**, 6, eabb8097	97
948	Characterization of Chenopodin Isoforms from Quinoa Seeds and Assessment of Their Potential Anti-Inflammatory Activity in Caco-2 Cells. **2020**, 10,	11
947	In silico structure prediction of full-length cotton cellulose synthase protein (GhCESA1) and its hierarchical complexes. **2020**, 27, 5597-5616	3
946	Molecular interactions of ceftazidime with bovine serum albumin: Spectroscopic, molecular docking, and DFT analyses. **2020**, 313, 113490	21
945	Analysis of binding affinity and docking of novel fatty acid-binding protein (FABP) ligands. **2020**, 143, 264-271	10
944	T cell epitope designing for dengue peptide vaccine using docking and molecular simulation studies. **2020**, 46, 787-795	13
943	Spectroscopic and Molecular Modeling Investigation on the Interaction between Folic Acid and Bovine Lactoferrin from Encapsulation Perspectives. **2020**, 9,	5
942	Mitochondrial protein interaction landscape of SS-31. **2020**, 117, 15363-15373	36
941	Green asymmetric synthesis of epoxypeptidomimetics and evaluation as human cathepsin K inhibitors. **2020**, 28, 115597	3
940	Anxiolytic-like activity of 5-methoxyflavone in mice with involvement of GABAergic and serotonergic systems - in vivo and in silico evidences. **2020**, 36, 100-110	4
939	Immunoinformatics characterization of SARS-CoV-2 spike glycoprotein for prioritization of epitope based multivalent peptide vaccine. **2020**, 314, 113612	24
938	Toward a chimeric vaccine against multiple isolates of Mycobacteroides - An integrative approach. **2020**, 250, 117541	5
937	Inhibition of □chymotrypsin by pristine single-wall carbon nanotubes: Clogging up the active site. **2020**, 571, 174-184	10
936	Enhancement of solubility, antibiofilm, and antioxidant activity of uridine by inclusion in □cyclodextrin derivatives. **2020**, 306, 112849	7
935	Identification and characterization of dihydropyrimidinase inhibited by plumbagin isolated from Nepenthes miranda extract. **2020**, 171-172, 124-135	9

934	Zn, Cd and Hg complexes with unsymmetric thiourea derivatives; syntheses, free radical scavenging and enzyme inhibition essay. **2020**, 1211, 128096		10
933	Molecular Docking in Modern Drug Discovery: Principles and Recent Applications. **2020**,		26
932	Structural motifs of oxacalix[4]arene for molecular recognition of nitroaromatic explosives: Experimental and computational investigations of host-guest complexes. **2020**, 306, 112809		6
931	Pleiotropic Functions and Biological Potentials of Silver Nanoparticles Synthesized by an Endophytic Fungus. **2020**, 8, 95		12
930	c-Phycocyanin primed silver nano conjugates: Studies on red blood cell stress resilience mechanism. **2020**, 194, 111211		15
929	Immunoinformatic Analysis of T- and B-Cell Epitopes for SARS-CoV-2 Vaccine Design. **2020**, 8,		29
928	Mass spectrometry reveals the chemistry of formaldehyde cross-linking in structured proteins. **2020**, 11, 3128		27
927	Computational structure modeling for diverse categories of macromolecular interactions. **2020**, 64, 1-8		9
926	3-Dimensional architecture of the human multi-tRNA synthetase complex. *Nucleic Acids Research*, **2020**, 48, 8740-8754	20.1	12
925	In Silico identification of angiotensin-converting enzyme inhibitory peptides from MRJP1. **2020**, 15, e0228265		8
924	Vaccinomics to design a novel single chimeric subunit vaccine for broad-spectrum immunological applications targeting nosocomial Enterobacteriaceae pathogens. **2020**, 146, 105258		17
923	In Silico Exploration of Conformational Dynamics and Novel Inhibitors for Targeting MEF2-Associated Transcriptional Activity. **2020**, 60, 1892-1909		2
922	Naringenin Inhibition of the Quorum Sensing Response Is Based on Its Time-Dependent Competition With -(3-Oxo-dodecanoyl)-L-homoserine Lactone for LasR Binding. **2020**, 7, 25		13
921	Mechanistic Model for the Hsp90-Driven Opening of Human Argonaute. **2020**, 60, 1469-1480		2
920	Fluorescence spectroscopy and molecular modeling of anthocyanins binding to bovine lactoferrin peptides. **2020**, 318, 126508		17
919	Receptor-ligand based molecular interaction to discover adjuvant for immune cell TLRs to develop next-generation vaccine. **2020**, 152, 535-545		10
918	User guide for the discovery of potential drugs via protein structure prediction and ligand docking simulation. **2020**, 58, 235-244		16
917	Development of epitope-based peptide vaccine against novel coronavirus 2019 (SARS-COV-2): Immunoinformatics approach. **2020**, 92, 618-631		237

916	Molecular aspects of the role of groove and stacked regions of DNA in binding with lipids: Spectroscopic and docking studies. **2020**, 303, 112672	2
915	Computer-Aided Drug Design for the Organic Chemistry Laboratory Using Accessible Molecular Modeling Tools. **2020**, 97, 760-763	14
914	Prospects of omics technologies and bioinformatics approaches in food science. **2020**, 317-340	0
913	Molecular Cloning of an Amino Acid Permease Gene and Structural Characterization of the Protein in Common Bean (Phaseolus vulgaris L.). **2020**, 62, 210-217	2
912	Structural Bioinformatics. **2020**,	2
911	Interaction of Isatin with Cytochrome P450 Isoenzymes: Investigation by Means of Spectral and Electrochemical Methods The role of Isatin in Cytochromes P450 Ligand-Protein Binding Events. **2020**, 10, 157-167	
910	Structure prediction of transferrin receptor protein 1 (TfR1) by homology modelling, docking, and molecular dynamics simulation studies. **2020**, 6, e03221	7
909	Cobalt ferrite nanoparticles for bimodal hyperthermia and their mechanistic interactions with lysozyme. **2020**, 310, 113194	10
908	Epitope based vaccine prediction for SARS-COV-2 by deploying immuno-informatics approach. **2020** , 19, 100338	47
907	Structural insights on binding mechanism of CAD complexes (CPSase, ATCase and DHOase). **2021**, 39, 3144-3157	
906	Identification and Design of a Next-Generation Multi Epitopes Bases Peptide Vaccine Candidate Against Prostate Cancer: An In Silico Approach. **2020**, 78, 495-509	8
905	Resveratrol as a nontoxic excipient stabilizes insulin in a bioactive hexameric form. **2020**, 34, 915-927	3
904	The HDOCK server for integrated protein-protein docking. **2020**, 15, 1829-1852	191
903	Tyrosine phosphorylation as a regulator of dystrophin and beta-dystroglycan interaction: A molecular insight. **2020**, 99, 107623	3
902	Glycated albumin based photonic crystal sensors for detection of lipopolysaccharides and discrimination of Gram-negative bacteria. **2020**, 1117, 1-8	15
901	Learning context-aware structural representations to predict antigen and antibody binding interfaces. **2020**, 36, 3996-4003	26
900	Designing of precise vaccine construct against visceral leishmaniasis through predicted epitope ensemble: A contemporary approach. **2020**, 86, 107259	8
899	In-silico elucidation of phytochemicals against diabetes mellitus. **2020**, 27, 2299-2307	9

898	Trimesic acid□theophylline and Isopthalic acid□caffeine Cocrystals: Synthesis, Characterization, Solubility, Molecular Docking, and Antimicrobial Activity. **2020**, 20, 3510-3522	10
897	Effects of the Hydrophobicity of Key Residues on the Characteristics and Stability of Glucose Oxidase on a Graphene Surface. **2020**, 6, 1899-1908	5
896	A computational model of ESAT-6 complex in membrane. **2020**, 19,	6
895	Computer aided novel antigenic epitopes selection from the outer membrane protein sequences of Aeromonas hydrophila and its analyses. **2020**, 82, 104320	9
894	Reverse vaccinology approach to design a novel multi-epitope vaccine candidate against COVID-19: an study. **2021**, 39, 2857-2872	134
893	In-Silico Proteomic Exploratory Quest: Crafting T-Cell Epitope Vaccine Against Whipple's Disease. **2020**, 27, 1-11	14
892	Structure-based drug design, synthesis and screening of MmaA1 inhibitors as novel anti-TB agents. **2021**, 25, 351-366	5
891	Screening and molecular characterization of lethal mutations of human homogentisate 1, 2 dioxigenase. **2021**, 39, 1661-1671	6
890	An in vitro model mimicking the complement system to favor directed phagocytosis of unwanted cells. **2021**, 49, 5-13	
889	A toxin complex protein from Photorhabdus akhurstii conferred oral insecticidal activity against Galleria mellonella by targeting the midgut epithelium. **2021**, 242, 126642	5
888	A computational study to disclose potential drugs and vaccine ensemble for COVID-19 conundrum. **2021**, 324, 114734	8
887	Host-guest inclusion complex of □cyclodextrin and 4,4?-(1,4-phenylenediisopropylidene)bisaniline: Spectral, structural and molecular modeling studies. **2021**, 1224, 129050	1
886	Alkaline phosphatase dual-binding sites for collagen dictate cell migration and microvessel assembly in vitro. **2021**, 122, 116-129	2
885	Spectroscopic, Structural, DFT and Molecular Docking Studies on Novel Cocrystal Salt Hydrate of Chromotropic Acid and Its Antibiofilm Activity. **2021**, 46, 353-364	8
884	Epigallocatechin gallate and theaflavin gallate interaction in SARS-CoV-2 spike-protein central channel with reference to the hydroxychloroquine interaction: Bioinformatics and molecular docking study. **2021**, 82, 86-96	28
883	DFT computational study towards investigating psychotropic drugs, promazine and trifluoperazine adsorption on graphene, fullerene and carbon cyclic ring nanoclusters. **2021**, 246, 119012	14
882	Uncovering DNA-PKcs ancient phylogeny, unique sequence motifs and insights for human disease. **2021**, 163, 87-108	18
881	Computational engineering the binding affinity of Adalimumab monoclonal antibody for designing potential biosimilar candidate. **2021**, 102, 107774	3

880	In silico molecular docking in DNA aptamer development. **2021**, 180, 54-67	10
879	Molecular characterization and modeling study of the Podr1 gene and genome-scale identification of whole ATP-binding cassette (ABC) transporters in Penicillium occitanis. **2021**, 113, 795-811	0
878	Drug designing against NSP15 of SARS-COV2 via high throughput computational screening and structural dynamics approach. **2021**, 892, 173779	5
877	Reinforcement of □mine-hydroxyl chelation pocket□by encapsulating into the □CD cavity for the sterically protective detection of Al3+. **2021**, 323, 114949	2
876	Conformational analysis and quantum descriptors of two bifonazole derivatives of immense anti-tuber potential by using vibrational spectroscopy and molecular docking studies. **2021**, 32, 859-867	5
875	In situ pepsin-assisted needle assembly of magnetic-graphitic-nanocapsules for enhanced gastric retention and mucus penetration. **2021**, 36, 101032	6
874	Heparin-mediated dimerization of follistatin. **2021**, 246, 467-482	2
873	Enantioseparation of ketoconazole and miconazole by capillary electrophoresis and a study on their inclusion interactions with □cyclodextrin and derivatives. **2021**, 33, 37-50	5
872	Towards a novel peptide vaccine for Middle East respiratory syndrome coronavirus and its possible use against pandemic COVID-19. **2021**, 324, 114706	5
871	Structural investigations, quantum mechanical studies on proton and metal affinity and biological activity predictions of selpercatinib. **2021**, 325, 114765	10
870	Determination of glycated albumin in serum and saliva by capillary electrophoresis utilizing affinity of 3-acrylamido phenylboronic acid selected by virtual screening and molecular docking. **2021**, 1636, 461793	0
869	Visualizing functional dynamicity in the DNA-dependent protein kinase holoenzyme DNA-PK complex by integrating SAXS with cryo-EM. **2021**, 163, 74-86	11
868	Leveraging the Entirety of the Protein Data Bank to Enable Improved Structure Prediction Based on Cross-Link Data. **2021**, 20, 1087-1095	3
867	Prediction of putative epitope-based vaccine against all corona virus strains for the Chinese population: Approach toward development of vaccine. **2021**, 65, 154-160	0
866	Essential interpretations of bioinformatics in COVID-19 pandemic. **2021**, 27, 100844	6
865	A MIF-Derived Cyclopeptide that Inhibits MIF Binding and Atherogenic Signaling via the Chemokine Receptor CXCR2. **2021**, 22, 1012-1019	7
864	Interaction mechanism of plant-based nanoarchitectured materials with digestive enzymes of termites as target for pest control: Evidence from molecular docking simulation and in vitro studies. **2021**, 403, 123840	5
863	Galaxy InteractoMIX: An Integrated Computational Platform for the Study of Protein-Protein Interaction Data. **2021**, 433, 166656	1

862	Discerning novel drug targets for treating Mycobacterium avium ss. paratuberculosis-associated autoimmune disorders: an in silico approach. **2021**, 22,	
861	Spectral Studies on the Supramolecular Assembly of Uridine with Cyclodextrin and Its In Vitro Cytotoxicity. **2021**, 41, 992-1011	3
860	Biochemical and molecular anticancer approaches for Boerhaavia diffusa root extracts in oral cancer. **2021**,	
859	RIG-I Has a Role in Immunity Against , a Gastrointestinal Parasite in : A Novel Report. **2020**, 11, 534705	3
858	Advances in structure-based drug design. **2021**, 55-103	0
857	Deciphering the architecture and interactome of hnRNP proteins and enigmRBPs. **2021**, 17, 503-516	0
856	Sugarcane cystatins: From discovery to biotechnological applications. **2021**, 167, 676-686	4
855	Prediction, Analysis, Visualization, and Storage of Protein Protein Interactions Using Computational Approaches. **2021**, 265-346	
854	Crosslinking mass spectrometry unveils novel interactions and structural distinctions in the model green alga. **2021**, 17, 917-928	
853	Designing a multi-epitope vaccine against the Lassa virus through reverse vaccinology, subtractive proteomics, and immunoinformatics approaches. **2021**, 25, 100683	0
852	Drebrin regulates cytoskeleton dynamics in migrating neurons through interaction with CXCR4. **2021**, 118,	5
851	2D Zernike polynomial expansion: Finding the protein-protein binding regions. **2021**, 19, 29-36	9
850	Identification of Novel Anticancer Agent by in silico Methods for Inhibition of KLK-12 Protein. **2021**, 6, 13-23	1
849	Computational Methods for the Elucidation of Protein Structure and Interactions. **2021**, 2305, 23-52	0
848	Resources for Docking-Based Virtual Screening. **2021**, 179-203	1
847	The Ras dimer structure. **2021**, 12, 8178-8189	5
846	[In silico specificity determination of neoantigen-reactive T-lymphocytes]. **2021**, 67, 251-258	2
845	design of multi-epitope-based peptide vaccine against SARS-CoV-2 using its spike protein. **2021**, 1-14	8

844	Antimicrobial β-defensins as multi-target inhibitors against amyloid formation and microbial infection. **2021**, 12, 9124-9139		9
843	Developing COVID-19 Vaccines by Innovative Bioinformatics Approaches. **2021**, 159-184		
842	In Silico Designing of a Multi-Epitope Based Vaccine Candidate Against Human Adenovirus Type B3 Respiratory Infections by Utilising Various Immunoinformatics Approaches. **2021**, 29,		
841	Update and Potential Opportunities in CBP [Cyclic Adenosine Monophosphate (cAMP) Response Element-Binding Protein (CREB)-Binding Protein] Research Using Computational Techniques. **2021**, 40, 19-27		
840	Borrelidin from Saltern-Derived Halophilic sp. Dissociates Amyloid- and Tau Fibrils. **2021**, 5, 7-13		2
839	SPServer: split-statistical potentials for the analysis of protein structures and protein-protein interactions. **2021**, 22, 4		3
838	Vibrio cholerae FruR facilitates binding of RNA polymerase to the fru promoter in the presence of fructose 1-phosphate. *Nucleic Acids Research*, **2021**, 49, 1397-1410	20.1	4
837	In-Silico analysis reveals lower transcription efficiency of C241T variant of SARS-CoV-2 with host replication factors MADP1 and hnRNP-1. **2021**, 25, 100670		5
836	Generalized linear models provide a measure of virulence for specific mutations in SARS-CoV-2 strains. **2021**, 16, e0238665		7
835	Classification and prediction of protein-protein interaction interface using machine learning algorithm. **2021**, 11, 1761		15
834	Immunoinformatics-guided design of a multi-epitope vaccine based on the structural proteins of severe acute respiratory syndrome coronavirus 2.. **2021**, 11, 18103-18121		14
833	Biomolecular Talks: Part 1: A Theoretical Revisit on Molecular Modeling and Docking Approaches. **2021**, 31-55		1
832	Computational identification and characterization of antigenic properties of Rv3899c of Mycobacterium tuberculosis and its interaction with Human leukocyte antigen (HLA).		
831	Identification of potential antivirals against SARS-CoV-2 using virtual screening method. **2021**, 23, 100531		8
830	Polypyridyl iron(III) complexes containing long alkyl chains: synthesis, characterization, DFT calculations and biological activity. **2021**, 45, 12902-12914		0
829	Time-dependent conformational analysis of ALK5-lumican complex in presence of graphene and graphene oxide employing molecular dynamics and MMPBSA calculation. **2021**, 1-24		
828	Computational drug repurposing strategy predicted peptide-based drugs that can potentially inhibit the interaction of SARS-CoV-2 spike protein with its target (humanACE2). **2021**, 16, e0245258		9
827	Reverse vaccinology approach towards the in-silico multiepitope vaccine development against SARS-CoV-2. **2021**, 10, 44		3

826	Utilization of O/S-doped graphene nanoclusters for ultrasensitive detection of flurane derivatives-DFT investigations. **2021**, 1-8	1
825	Modified Snake Neurotoxin Averts Amyloid Binding to 7 Nicotinic Acetylcholine Receptor and Reverses Cognitive Deficits in Alzheimer's Disease Mice. **2021**, 58, 2322-2341	2
824	Improving Blind Docking in DOCK6 through an Automated Preliminary Fragment Probing Strategy. **2021**, 26,	7
823	Pan-Cancer Analysis and Drug Formulation for GPR139 and GPR142. **2020**, 11, 521245	1
822	Ovine CD14- an immune response gene has a role against gastrointesinal nematode Haemonchus contortus -a novel report.	1
821	Mycobacterium tuberculosis Peptidyl Prolyl Isomerase A Interacts With Host Integrin Receptor to Exacerbate Disease Progression. **2021**, 224, 1383-1393	1
820	Baseline Comparisons of Complementary Sampling Methods for Assembly Driven by Short-Ranged Pair Potentials toward Fast and Flexible Hybridization. **2021**, 17, 1967-1987	0
819	Cryo-EM structures of engineered active bc-cbb type CIIICIV super-complexes and electronic communication between the complexes. **2021**, 12, 929	7
818	Comparative Genomics and Integrated Network Approach Unveiled Undirected Phylogeny Patterns, Co-mutational Hot Spots, Functional Cross Talk, and Regulatory Interactions in SARS-CoV-2. **2021**, 6,	8
817	Structural Characterization of the Hidden Peptide SHPRH-146aa Encoded by Non-Coding circ-SHPRH to Act as Tumor Suppressor. **2021**, 193, 2076-2086	2
816	Intrinsic atomic interaction at molecular proximal vicinity infer cellular biocompatibility of antibacterial nanopepper. **2021**, 16, 307-322	5
815	Designing of multiepitope-based vaccine against Leptospirosis using Immuno-Informatics approaches.	1
814	Interaction of TLR4 and TLR8 in the Innate Immune Response against Mycobacterium Tuberculosis. **2021**, 22,	4
813	Estimation of drug-likeness properties of GC-MS separated bioactive compounds in rare medicinal using molecular docking technique and SwissADME in silico tools. **2021**, 10, 14	2
812	Excited-state electronic properties, structural studies, noncovalent interactions, and inhibition of the novel severe acute respiratory syndrome coronavirus 2 proteins in Ripretinib by first-principle simulations. **2021**, 324, 115134	13
811	Evolution and Diversity of Semaphorins and Plexins in Choanoflagellates. **2021**, 13,	1
810	Elucidation of the hetero-dimeric binding activity of LasR and RhlR proteins with the promoter DNA and the role of a specific Phe residue during the biosynthesis of HCN synthase from opportunistic pathogen Pseudomonas aeruginosa. **2021**, 27, 76	0
809	Evaluating the Multifunctionality of a New Modulator of Zinc-Induced A Aggregation Using a Novel Computational Approach. **2021**, 61, 1383-1401	2

808	Structural Characterization of Receptor-Receptor Interactions in the Allosteric Modulation of G Protein-Coupled Receptor (GPCR) Dimers. **2021**, 22,	1
807	Implementation of computational approaches to explore the deleterious effects of non-synonymous SNPs on pRB protein. **2021**, 1-18	3
806	Protein sequence optimization with a pairwise decomposable penalty for buried unsatisfied hydrogen bonds. **2021**, 17, e1008061	8
805	Structural characterization and functional annotation of microbial proteases mined from solid tannery waste metagenome. **2021**, 76, 1829-1842	3
804	Dravet syndrome-associated mutations in , and define the genetic landscape of defects of GABA receptors. **2021**, 3, fcab033	3
803	Immunoinformatics approach for a novel multi-epitope subunit vaccine design against various subtypes of Influenza A virus. **2021**, 226, 152053	4
802	Immunoinformatic approach to design a multiepitope vaccine targeting non-mutational hotspot regions of structural and non-structural proteins of the SARS CoV2. **2021**, 9, e11126	2
801	Development of new vaccine target against SARS-CoV2 using envelope (E) protein: An evolutionary, molecular modeling and docking based study. **2021**, 172, 74-81	4
800	In Silico and In Vitro Tailoring of a Chitosan Nanoformulation of a Human Metabolic Enzyme. **2021**, 13,	3
799	Structure-Function Analyses of New SARS-CoV-2 Variants B.1.1.7, B.1.351 and B.1.1.28.1: Clinical, Diagnostic, Therapeutic and Public Health Implications. **2021**, 13,	68
798	Massively parallel, computationally-guided design of a pro-enzyme.	
797	A novel peptide isolated from garlic shows anticancer effect against leukemic cell lines via interaction with Bcl-2 family proteins. **2021**, 97, 1017-1028	3
796	Adsorption of adipic acid in Al/B-N/P nanocages: DFT investigations. **2021**, 27, 113	14
795	In-silico structural analysis of Pseudomonas syringae effector HopZ3 reveals ligand binding activity and virulence function. **2021**, 134, 599-611	
794	Spectroscopic and DFT investigations of 8-hydroxy quinoline-5-sulfonic acid-5-chloro-8-hydroxyquinoline cocrystal. **2021**, 75, 3387-3399	1
793	Structural based screening of potential inhibitors of SMAD4: a step towards personalized medicine for gall bladder and other associated cancers. **2021**, 25, 1945-1961	
792	ZEAL: Protein structure alignment based on shape similarity. **2021**,	1
791	RNA and DNA G-quadruplexes bind to human dicer and inhibit its activity. **2021**, 78, 3709-3724	5

790	Oxidation shuts down an auto-inhibitory mechanism of von Willebrand factor. **2021**, 89, 731-741	0
789	Jacalin domain-containing protein OsSalT interacts with OsDREB2A and OsNAC1 to impart drought stress tolerance in planta. **2021**, 183, 104362	1
788	Synergistically improved methane production from anaerobic wastewater treatment by iron/polyaniline composite. **2021**, 4, 265-273	23
787	Optimized structure of monoubiquitinated FANCD2 (human) at Lys 561: a theoretical approach.	
786	Immunoinformatic Approach for the identification of T Cell and B Cell Epitopes in the Surface Glycoprotein and Designing a Potent Multiepitope Vaccine Construct Against SARS-CoV-2 including the new UK variant.	0
785	Structural and Drug Screening Analysis of the Non-structural Proteins of Severe Acute Respiratory Syndrome Coronavirus 2 Virus Extracted From Indian Coronavirus Disease 2019 Patients. **2021**, 12, 626642	4
784	Protein Interaction Interface Region Prediction by Geometric Deep Learning. **2021**,	14
783	Prediction of B- and T-cell epitopes using in-silico approaches: a solution to the development of recombinant vaccines against COVID-19. **2021**, 33,	1
782	Immunoinformatics analysis to design novel epitope based vaccine candidate targeting the glycoprotein and nucleoprotein of Lassa mammarenavirus (LASMV) using strains from Nigeria. **2021** , 1-20	0
781	Integrative proteomics identifies thousands of distinct, multi-epitope, and high-affinity nanobodies. **2021**, 12, 220-234.e9	12
780	Molecular docking and density functional theory studies of potent 1,3-disubstituted-9H-pyrido[3,4-b]indoles antifilarial compounds. **2021**, 32, 1925-1947	1
779	Xanthone glucoside 2-□D-glucopyranosyl-1,3,6,7-tetrahydroxy-9H-xanthen-9-one binds to the ATP-binding pocket of glycogen synthase kinase 3□and inhibits its activity: implications in prostate cancer and associated cardiovascular disease risk. **2021**, 1-17	1
778	Molecules against Covid-19: An in silico approach for drug development. **2021**, 19, 100095	6
777	ROS Dependent Antifungal and Anticancer Modulations of Osmotin. **2021**, 26,	0
776	Inhibition of SARS-CoV-2 3CL M by Natural and Synthetic Inhibitors: Potential Implication for Vaccine Production Against COVID-19. **2021**, 8, 640819	2
775	Epitope-based universal vaccine for Human T-lymphotropic virus-1 (HTLV-1). **2021**, 16, e0248001	7
774	Butea monosperma seed extract mediated biosynthesis of ZnO NPs and their antibacterial, antibiofilm and anti-quorum sensing potentialities. **2021**, 14, 103044	11
773	PR-1-Like Protein as a Potential Target for the Identification of Fusarium oxysporum: An In Silico Approach. **2021**, 10, 8	1

772	Effect of Chelate Ring Size of Binuclear Copper(II) Complexes on Catecholase Activity and DNA Cleavage. **2021**, 2021, 1710-1721	2
771	Structural Model for Recruitment of RIT1 to the LZTR1 E3 Ligase: Evidences from an Integrated Computational Approach. **2021**, 61, 1875-1888	
770	Micafungin Inhibits Dengue Virus Infection through the Disruption of Virus Binding, Entry, and Stability. **2021**, 14,	4
769	An interplay of microglia and matrix metalloproteinase MMP9 under hypoxic stress regulates the opticin expression in retina. **2021**, 11, 7444	3
768	Conserved in 186 countries the RBD fraction of SARS CoV-2 S-protein with in-silicoT500S mutation strongly blocks ACE2 rejecting the viral spike; A Molecular-docking analysis.	0
767	Molecular docking simulation of interaction between insulin and silica nanoparticle. **2021**, 1869, 012062	
766	Formation of Kiss1R/GPER Heterocomplexes Negatively Regulates Kiss1R-mediated Signalling through Limiting Receptor Cell Surface Expression. **2021**, 433, 166843	2
765	A resource of high-quality and versatile nanobodies for drug delivery. **2021**, 24, 103014	4
764	Computational screening of 645 antiviral peptides against the receptor-binding domain of the spike protein in SARS-CoV-2. **2021**, 136, 104759	8
763	Computational Identification of Dithymoquinone as a Potential Inhibitor of Myostatin and Regulator of Muscle Mass. **2021**, 26,	1
762	Robust de novo design of protein binding proteins from target structural information alone.	1
761	Pan-vaccinomics approach towards a universal vaccine candidate against WHO priority pathogens to address growing global antibiotic resistance. **2021**, 136, 104705	14
760	A Comprehensive Computer Aided Vaccine Design Approach to Propose a Multi-Epitopes Subunit Vaccine against Genus Using Pan-Genomics, Reverse Vaccinology, and Biophysical Techniques. **2021**, 9,	3
759	Antiviral peptides against the main protease of SARS-CoV-2: A molecular docking and dynamics study.. **2021**, 14, 103315	12
758	Designing multi-epitope vaccine candidates against functional amyloids in Pseudomonas aeruginosa through immunoinformatic and structural bioinformatics approach. **2021**, 93, 104982	1
757	Cyclophilin A: a possible host modulator in Chandipura virus infection. **2021**, 166, 3143-3150	1
756	Computational Insights into the Interaction between Cytoadherence Receptor gC1qR and the DBL𝛽12 Domain of a PfEMP1 Ligand. **2021**, 11,	1
755	Subtractive Proteomics and Immuno-informatics Approaches for Multi-peptide Vaccine Prediction Against and Validation Through In Silico Expression. **2021**, 1-17	1

754	Inhibitory potential of plant-derived metabolites against Zika virus: a computational-aided approach **2021**, 100129	3
753	Ebola virus protein VP40 binding to Sec24c for transport to the plasma membrane. **2021**,	0
752	Targeting the actin nucleation promoting factor WASp provides a therapeutic approach for hematopoietic malignancies. **2021**, 12, 5581	1
751	Structural basis for UFM1 transfer from UBA5 to UFC1. **2021**, 12, 5708	1
750	Repurposing proteases: An analysis of the binding potential of extracellular fungal proteases with selected viral proteins. **2021**, 15, 100756	1
749	Exploring the structural basis to develop efficient multi-epitope vaccines displaying interaction with HLA and TAP and TLR3 molecules to prevent NIPAH infection, a global threat to human health.	0
748	Immunogenic profiling and designing of a novel vaccine from capsid proteins of FMDV serotype Asia-1 through reverse vaccinology. **2021**, 93, 104925	
747	Identification of potential antileishmanial agents via structure-based molecular simulations. **2022**, 110, 108039	0
746	Proteomic Tools for the Analysis of Cytoskeleton Proteins. **2022**, 2364, 363-425	0
745	Theaflavin-3'-O-gallate a Black-tea Constituent Blocked SARS CoV-2 RNA dependant RNA Polymerase Active-site with Better Docking Results than Remdesivir. **2021**, 71, 462-472	1
744	Computational analysis of human host binding partners of chikungunya and dengue viruses during coinfection. **2021**, 79,	0
743	Teaching Aspects of Antibiotics and Antimicrobials to the Food Science Student through a Combination Wet Lab and Activity. **2021**, 22,	
742	Cloning and expression analysis of fused holin-endolysin from RL bacteriophage; Exhibits broad activity against multi drug resistant pathogens. **2021**, 149, 109846	5
741	NLDock: a Fast Nucleic Acid-Ligand Docking Algorithm for Modeling RNA/DNA-Ligand Complexes. **2021**, 61, 4771-4782	3
740	Synthesis, anti-diabetic and QSAR analysis of flavone hydrazide Schiff base derivatives. **2021**, 1-16	2
739	Chlamydia trachomatis core genome data mining for promising novel drug targets and chimeric vaccine candidates identification. **2021**, 136, 104701	2
738	In silico vaccine design and epitope mapping of New Delhi metallo-beta-lactamase (NDM): an immunoinformatics approach. **2021**, 22, 458	2
737	Identification of vaccine targets in pathogens and design of a vaccine using computational approaches. **2021**, 11, 17626	7

736	Structural and ATPase activity analysis of nucleotide binding domain of Rv3870 enzyme of M. tuberculosis ESX-1 system. **2021**, 189, 879-889	
735	In Silico Analysis of Peptide Macrocycle -Protein Interactions. **2022**, 2371, 317-334	
734	Immunoinformatics analysis of antigenic epitopes and designing of a multi-epitope peptide vaccine from putative nitro-reductases of Mycobacterium tuberculosis DosR. **2021**, 94, 105017	2
733	Synthesis, spectroscopic and crystal structure of nickel(II) complex of thiosemicarbazone basedSchiff base: Antimicrobial, anticancer and molecular docking studies. **2021**, 132, 108850	0
732	In silico methods and tools for drug discovery. **2021**, 137, 104851	23
731	Evaluation of selected carotenoids of Lycopersicon esculentum variants as therapeutic targets for 'Alzheimer's disease: an in silico approach. **2021**, 22, 49	1
730	Systematic transition modeling analysis in the MEF2B-DNA binding interface due to Y69H and K4E variants. **2021**, 108, 108009	1
729	Discovery of Taroxaz-104: The first potent antidote of SARS-CoV-2 VOC-202012/01 strain. **2021**, 1246, 131106	7
728	Sodium fusidate prevents protein aggregation of silk fibroin and offers new perspectives for human lens material disaggregation. **2021**, 279, 106680	3
727	Evidence of cluster formation of croconic acid with Ag, Au and Cu cages, enhancement of electronic properties and Raman activity. **2022**, 264, 120233	6
726	A Spatial and Functional Interaction of a Heterotetramer Survivin-DNA-PKcs Complex in DNA Damage Response. **2021**, 81, 2304-2317	5
725	Immunoinformatics aided design of peptide-based vaccines against ebolaviruses. **2021**, 117, 157-187	
724	Spectroscopic and computational study of chromone derivatives with antitumor activity: detailed DFT, QTAIM and docking investigations. **2021**, 3, 1	2
723	A comprehensive screening of the whole proteome of hantavirus and designing a multi-epitope subunit vaccine for cross-protection against hantavirus: Structural vaccinology and immunoinformatics study. **2021**, 150, 104705	7
722	Immunoinformatics designed T cell multi epitope dengue peptide vaccine derived from non structural proteome. **2021**, 150, 104728	18
721	Biomolecular TalksPart 2: Applications and Challenges of Molecular Docking Approaches. **2021**, 245-269	1
720	Methods for Molecular Modelling of Protein Complexes. **2021**, 2305, 53-80	1
719	MDock: A Suite for Molecular Inverse Docking and Target Prediction. **2021**, 2266, 313-322	2

718	Guardians of the Cell: State-of-the-Art of Membrane Proteins from a Computational Point-of-View. **2021**, 2315, 3-28	
717	From integrative structural biology to cell biology. **2021**, 296, 100743	13
716	A computational perspective on the dynamic behaviour of recurrent drug resistance mutations in the pncA gene from .. **2021**, 11, 2476-2486	3
715	Vaccine Design and Immunoinformatics. **2021**, 137-149	
714	Probing the interactions of novel europium coordination complexes with serum albumin. **2021**, 36, 795-801	1
713	Coupling 6-chloro-3-methyluracil with copper: structural features, theoretical analysis, and biofunctional properties. **2021**, 50, 13533-13542	1
712	Mining the Proteome of Leishmania donovani for the Development of Novel MHC Class I Restricted Epitope for the Control of Visceral Leishmaniasis. **2018**, 119, 378-391	16
711	Sampling and energy evaluation challenges in ligand binding protein design. **2017**, 26, 2426-2437	23
710	Structure Prediction of Protein Complexes. **2007**, 109-134	3
709	Modeling of Multimolecular Complexes. **2020**, 2112, 163-174	8
708	In Silico Analysis of Class III Peroxidases: Hypothetical Structure, Ligand Binding Sites, Posttranslational Modifications, and Interaction with Substrates. **2020**, 2139, 325-339	2
707	Cathepsins B1 and B2 of Trichobilharzia SPP., bird schistosomes causing cercarial dermatitis. **2011**, 712, 136-54	8
706	Pairwise and multimeric protein-protein docking using the LZerD program suite. **2014**, 1137, 209-34	29
705	Computer-aided drug designing. **2014**, 1168, 313-21	7
704	Sketching of CD95 Oligomers by In Silico Investigations. **2017**, 1557, 153-171	1
703	Analysis and prediction of protein quaternary structure. **2010**, 609, 349-64	20
702	Synchrotron Small-Angle X-Ray Scattering on Biological Macromolecules in Solution. **2020**, 1645-1672	1
701	Modeling of Membrane Proteins. **2019**, 371-451	2

700	Prediction of Protein-Protein Binding Interfaces. **2013**, 105-133	4
699	Investigation on the interaction of heated soy proteins with anthocyanins from cornelian cherry fruits. **2020**, 231, 118114	10
698	iScore: An MPI supported software for ranking protein-protein docking models based on a random walk graph kernel and support vector machines.. **2020**, 11, 100462-100462	3
697	Hybrid methods for combined experimental and computational determination of protein structure. **2020**, 153, 240901	13
696	Chlorovirus PBCV-1 protein A064R has three of the transferase activities necessary to synthesize its capsid protein N-linked glycans. **2020**, 117, 28735-28742	6
695	Computational approach to explore the inhibitory potential of biologically derived compounds against vitellogenin receptor (VgR) using structure based virtual screening and molecular dynamics. **2020**, 1-7	1
694	Virtual repurposing of ursodeoxycholate and chenodeoxycholate as lead candidates against SARS-Cov2-Envelope protein: A molecular dynamics investigation. **2020**, 1-12	11
693	Lysine as a potential low molecular weight angiogen: its clinical, experimental and in-silico validation- A brief study.	2
692	Designing Novel Subunit Vaccines against Herpes Simplex Virus-1 using Reverse Vaccinology Approach.	5
691	The Essential Facts of Wuhan Novel Coronavirus Outbreak in China and Epitope-based Vaccine Designing against COVID-19.	13
690	Structural basis to design multi-epitope vaccines against Novel Coronavirus 19 (COVID19) infection, the ongoing pandemic emergency: an in silico approach.	5
689	Immuno-informatics Characterization SARS-CoV-2 Spike Glycoprotein for Prioritization of Epitope based Multivalent Peptide Vaccine.	2
688	ACE2 polymorphisms and individual susceptibility to SARS-CoV-2 infection: insights from an in silico study.	22
687	RNA and DNA G-quadruplexes bind to human Dicer and inhibit its activity.	0
686	Comparative Genomics and Integrated Network Approach Unveiled Undirected Phylogeny Patterns, Co-mutational Hotspots, Functional Crosstalk and Regulatory Interactions in SARS-CoV-2.	2
685	IG-VAE: Generative Modeling of Immunoglobulin Proteins by Direct 3D Coordinate Generation.	13
684	A robust and versatile nanobody platform for drug delivery.	4
683	Integrative proteomics reveals exceptional diversity and versatility of mammalian humoral immunity.	3

682	Identification of potential inhibitory analogs of metastasis tumor antigens (MTAs) using bioactive compounds: revealing therapeutic option to prevent malignancy.	2
681	Plant derived bioactive compounds as potential inhibitors of ZIKA virus: an in silico investigation.	3
680	Evaluation of protein-ligand docking methods on peptide-ligand complexes for docking small ligands to peptides.	5
679	Molecular architecture of theLegionellaDot/Icm type IV secretion system.	6
678	A Rev-CBP80-eIF4AI complex drives Gag synthesis from the HIV-1 unspliced mRNA.	2
677	Reverse vaccinology approach to design a novel multi-epitope subunit vaccine against avian influenza A (H7N9) virus.	2
676	In vivo structure of the Legionella type II secretion system by electron cryotomography.	3
675	Learning Context-aware Structural Representations to Predict Antigen and Antibody Binding Interfaces.	2
674	Mitochondrial protein interaction landscape of SS-31.	5
673	Structural analysis of the PATZ1 BTB domain homodimer. **2020**, 76, 581-593	2
672	An Immunoinformatics Study to Predict Epitopes in the Envelope Protein of SARS-CoV-2. **2020**, 2020, 7079356	5
671	Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics. **2016**, 12, e1004619	124
670	Structural and functional similarities between osmotin from Nicotiana tabacum seeds and human adiponectin. **2011**, 6, e16690	32
669	Protein X of hepatitis B virus: origin and structure similarity with the central domain of DNA glycosylase. **2011**, 6, e23392	21
668	Structural insight of dopamine β-hydroxylase, a drug target for complex traits, and functional significance of exonic single nucleotide polymorphisms. **2011**, 6, e26509	25
667	Structure of an MmyB-like regulator from C. aurantiacus, member of a new transcription factor family linked to antibiotic metabolism in actinomycetes. **2012**, 7, e41359	12
666	ATTRACT-EM: a new method for the computational assembly of large molecular machines using cryo-EM maps. **2012**, 7, e49733	40
665	Prediction of structure of human WNT-CRD (FZD) complex for computational drug repurposing. **2013**, 8, e54630	7

664	Use of a small peptide fragment as an inhibitor of insulin fibrillation process: a study by high and low resolution spectroscopy. **2013**, 8, e72318	52
663	GOMoDo: A GPCRs online modeling and docking webserver. **2013**, 8, e74092	65
662	Titanium dioxide nanoparticles as guardian against environmental carcinogen benzo[alpha]pyrene. **2014**, 9, e107068	25
661	The Interaction of FABP with Kap**2015**, 10, e0132138	6
660	Cloning and Expression of Defensin from Soiny Mullet (Liza haematocheila), with Insights of its Antibacterial Mechanism. **2016**, 11, e0157544	14
659	In silico and in vitro studies on the anti-cancer activity of andrographolide targeting survivin in human breast cancer stem cells. **2020**, 15, e0240020	6
658	Pentafluoropropionic Anhydride Functionalized PAMAM Dendrimer as miRNA Delivery Reagent. 1295-1302	4
657	In vitro transfection potential of fluorinated G5 PAMAM dendrimers for miRNA delivery to MRC-5 cells.	2
656	Gelsolin-Cu/ZnSOD interaction alters intracellular reactive oxygen species levels to promote cancer cell invasion. **2016**, 7, 52832-52848	15
655	Carnitine palmitoyl transferase-1A (CPT1A): a new tumor specific target in human breast cancer. **2016**, 7, 19982-96	47
654	Discovery and characterization of Isofistularin-3, a marine brominated alkaloid, as a new DNA demethylating agent inducing cell cycle arrest and sensitization to TRAIL in cancer cells. **2016**, 7, 24027-49	41
653	Inhibitory Mechanism of An Anticancer Drug, Bexarotene Against Amyloid Peptide Aggregation: Repurposing Via Neuroinformatics Approach. **2019**, 25, 2989-2995	6
652	Consensus Analyses in Molecular Docking Studies Applied to Medicinal Chemistry. **2020**, 20, 1322-1340	4
651	Targeting Kinase Interaction Networks: A New Paradigm in PPI Based Design of Kinase Inhibitors. **2019**, 19, 467-485	8
650	Decoding Protein-protein Interactions: An Overview. **2020**, 20, 855-882	5
649	Synthesis, Docking Study, Cytotoxicity, Antioxidant, and Anti-microbial Activities of Novel 2,4-Disubstituted Thiazoles Based on Phenothiazine. **2020**, 17, 151-159	1
648	Integrated Cheminformatics-Molecular Docking Approach to Drug Discovery Against Viruses. **2020**, 20, 150-159	1
647	Structural Basis for Designing Multiepitope Vaccines Against COVID-19 Infection: In Silico Vaccine Design and Validation. **2020**, 1, e19371	11

646	Bioinformatics Techniques used in Hepatitis C Virus Research. **2017**, 11, 921-932	1
645	Molecular docking study of L-Asparaginase I from Vibrio campbellii in the treatment of acute lymphoblastic leukemia (ALL). **2020**, 4, 8-16	4
644	Molecular Mechanism of Cancer Susceptibility Associated with Fok1 Single Nucleotide Polymorphism of VDR in Relation to Breast Cancer. **2019**, 20, 199-206	5
643	Lithium: a potential estrogen signaling modulator. **2009**, 7, 175-188	3
642	Supramolecular Encapsulation of a Neurotransmitter Serotonin by Cucurbit[7]uril. **2020**, 8, 582757	4
641	Protein-Protein Docking. **2016**, 173-195	2
640	Molecular Docking Technique to Understand Enzyme-Ligand Interactions. **2017**, 727-746	1
639	Implications of Molecular Docking Assay for Bioremediation. **2017**, 24-45	2
638	Implications of Molecular Docking Assay for Bioremediation. **2020**, 1556-1577	1
637	Evaluation of the Anti-Inflammatory Activities of 5,8,11-<i>cis</i>-Eicosatrienoic Acid. **2013**, 04, 113-119	2
636	Structural Modeling and Analysis of Pregnancy-Associated Glycoprotein-1 of Buffalo (Bubalus bubalis). **2012**, 2012, 481539	2
635	Inhibition on JAK-STAT3 Signaling Transduction Cascade Is Taken by Bioactive Peptide Alpha-S2 Casein Protein from Goat Ethawah Breed Milk. **2015**, 23, 233-8	6
634	Elucidation of the Molecular Interaction between miRNAs and the HOXA9 Gene, Involved in Acute Myeloid Leukemia, by the Assistance of Argonaute Protein through a Computational Approach. **2015**, 13, 45-52	6
633	Study of miRNA Based Gene Regulation, Involved in Solid Cancer, by the Assistance of Argonaute Protein. **2016**, 14, 112-124	6
632	Identification and Characterization of Novel Small-Molecule Inhibitors against Hepatitis Delta Virus Replication by Using Docking Strategies. **2011**, 11, 803-809	7
631	Modeling of the potential coiled-coil structure of snapin protein and its interaction with SNARE complex. **2006**, 1, 269-75	4
630	Predictive inference on cytoplasmic and mitochondrial thioredoxin peroxidases in the highly radioresistant Lepidopteran insect Spodoptera frugiperda. **2010**, 4, 399-404	5
629	Structure modeling of novel DNA glycosylase enzyme from oral pathogen Streptococcus sanguinis. **2010**, 5, 136-40	3

628	Structure modeling and comparative genomics for epimerase enzyme (Gal10p). **2010**, 5, 266-70	1
627	Structure based prediction of functional sites with potential inhibitors to Nudix enzymes from disease causing microbes. **2011**, 5, 341-9	0
626	Molecular modelling of urease accessory interaction proteins of Helicobacter Pylori J 99 and predicting an interruption in interaction by Vigna radiata Defensins. **2011**, 5, 410-5	2
625	Structure modeling and inhibitor prediction ofNADP oxidoreductase enzyme from Methanobrevibacter smithii. **2011**, 6, 15-9	16
624	Insights of interaction between small and large subunits of ADP-glucose pyrophosphorylase from bread wheat (Triticum aestivum L.). **2011**, 6, 144-8	8
623	Identification of EPAC (Exchange Protein Activated by cAMP) bioinformatically as a potential signalling biomarker in Cardiovascular Disease (CVD) and its molecular docking by a lead molecule. **2011**, 6, 176-8	5
622	Identification of novel sweet protein for nutritional applications. **2011**, 7, 112-4	2
621	Mobility in the structure of E.coli recQ helicase upon substrate binding as seen from molecular dynamics simulations. **2011**, 7, 371-4	1
620	Homology modeling, docking studies and functional analysis of various azoreductase accessory interacting proteins of Nostoc sp.PCC7120. **2012**, 8, 296-300	6
619	Linear epitope prediction in HPV type 16 E7 antigen and their docked interaction with human TMEM 50A structural model. **2017**, 13, 122-130	1
618	Design of peptide epitope from the neuraminidase protein of influenza A and influenza B towards short peptide vaccine development. **2018**, 14, 183-189	4
617	Structure to function analysis with antigenic characterization of a hypothetical protein,HPAG1_0576 from Helicobacter pylori HPAG1. **2019**, 15, 456-466	4
616	Molecular docking analysis of alkaloid compounds with beta-catenin towards the treatment of colon cancer. **2020**, 16, 283-287	1
615	Molecular docking analysis of piperine with CDK2,CDK4,Cyclin D and Cyclin T proteins. **2020**, 16, 359-362	2
614	Molecular docking analysis of Bcl-2 with phyto-compounds. **2020**, 16, 468-473	1
613	Molecular docking analysis of amyloid precursor protein with compounds from the Australian cowplant. **2020**, 16, 561-566	3
612	Identification and Pharmacological Analysis of High Efficacy Small Molecule Inhibitors of EGF-EGFR Interactions in Clinical Treatment of Non-Small Cell Lung Carcinoma: a Computational Approach. **2015**, 16, 8191-6	15
611	Identification of High Affinity Non-Peptidic Small Molecule Inhibitors of MDM2-p53 Interactions through Structure-Based Virtual Screening Strategies. **2015**, 16, 3759-65	14

610	Wss1 metalloprotease partners with Cdc48/Doa1 in processing genotoxic SUMO conjugates. **2015**, 4,	52
609	Structure and organisation of the archaellum machinery. **2017**, 6,	51
608	Computational design of environmental sensors for the potent opioid fentanyl. **2017**, 6,	44
607	Localized surface plasmon resonance aptasensor for selective detection of SARS-CoV-2 S1 protein. **2021**, 146, 7207-7217	3
606	TRICLOSAN IS A KCNQ3 POTASSIUM CHANNEL ACTIVATOR.	
605	Docking and ADMET studies for investigating the anticancer potency of Moscatilin on APC10/DOC1 and PKM2 against five clinical drugs. **2021**, 19, 161	1
604	Synthesis, In Silico Study, and Anti-Cancer Activity of Thiosemicarbazone Derivatives. **2021**, 9,	2
603	A conserved NAG motif is critical to the catalytic activity of galactinol synthase, a key regulatory enzyme of RFO biosynthesis. **2021**, 478, 3939-3955	1
602	In Silico Modeling as a Perspective in Developing Potential Vaccine Candidates and Therapeutics for COVID-19. **2021**, 11, 1273	4
601	Rational Design of a Modality-Specific Inhibitor of TRPM8 Channel against Oxaliplatin-Induced Cold Allodynia. **2021**, 8, e2101717	2
600	Theoretical model study of adsorbed antimalarial-graphene dimers: doping effects, photophysical parameters, intermolecular interactions, edge adsorption, and SERS. **2021**, 1-12	4
599	Towards A Novel Multi-Epitopes Chimeric Vaccine for Simulating Strong Immune Responses and Protection against. **2021**, 18,	10
598	Identification of binding interaction between Curcumin derivative and PERK13 Proline rich receptor like protein kinase protein using In silico docking techniques to help plants tackle salt water.	
597	Immunoinformatics and Immunogenetics-Based Design of Immunogenic Peptides Vaccine against the Emerging Tick-Borne Encephalitis Virus (TBEV) and Its Validation through In Silico Cloning and Immune Simulation. **2021**, 9,	1
596	Structure and Topology Prediction of Phage Adhesion Devices Using AlphaFold2: The Case of Two Phages. **2021**, 9,	3
595	Development of synthetic antigen vaccines for COVID-19. **2021**, 1-16	0
594	Building HMM and molecular docking analysis for the sensitive detection of anti-viral pneumonia antimicrobial peptides (AMPs). **2021**, 11, 20621	1
593	Synergistic in-vitro antiviral effects of combination treatment using anidulafungin and T-1105 against Zika virus infection. **2021**, 195, 105188	2

592 Neutralization of Daboxin P activities by rationally designed aptamers. **2021**, 203, 93-103

591 Identification of immunodominant epitopes in allelic variants VK210 and VK247 of Plasmodium Vivax Circumsporozoite immunogen. **2021**, 96, 105120 4

590 Comparative modeling and genomics for galactokinase (Gal1p) enzyme. **2011**, 5, 422-9

589 Drug Designing Approaches Using In-Silico Techniques [Book Review]. **2012**, 4, 1-9

588 Variation in Active Site Amino Residues of H1N1 Swine Flu Neuraminidase. **2013**, 575-583

587 Role of Protein Aggregation and Interactions between Synuclein and Calbindin in Parkinson Disease. **2013**, 677-684

586 Sequence and structural characterization of Trx-Grx type of monothiol glutaredoxins from Ashbya gossypii. **2013**, 9, 243-9

585 LCMV Interaction Changes with T192M Mutation in Alpha-Dystroglycan. **2015**, 11-23

584 Structural Insights into IbpA IbpB Interactions to Predict Their Roles in Heat Shock Response. **2015**, 41-51

583 Synchrotron Small-Angle X-Ray Scattering on Biological Macromolecules in Solution. **2015**, 1-25

582 Recent Developments in 3D QSAR and Molecular Docking Studies of Organic and Nanostructures. **2016**, 1-29 1

581 Synchrotron Small-Angle X-Ray Scattering on Biological Macromolecules in Solution. **2016**, 1393-1420

580 Molecular-Docking-Based Anti-Allergic Drug Design. **2016**, 232-248 1

579 Molecular Docking Technique to Understand Enzyme-Ligand Interactions. **2016**, 246-266

578 Role of Molecular Docking in Computer-Aided Drug Design and Development. **2016**, 1-28 1

577 Applying Computational Scoring Functions to Assess Biomolecular Interactions in Food Science: Applications to the Estrogen Receptors. **2016**, 3,

576 Online Molecular Docking Resources. **2016**, 360-379

575 (3E)-5-Chloro-3-(2-phenylhydrazinylidene)-1H-indol-2(3H)-one. **2016**, 1, 1

574 The Wnt segment polarity pathway and TMED2 protein may interact via a lectin- and decoy-type mechanism.

573 Structure, interaction and post-translational modification study of arsenic reduction system in Bifidobacterium longum.

572 In-silico studies of facilitated VEGF(s) VEGFR(s) bindings for assessment of Lysine as an indirect Low-Mol-Wt angiogen: Experimental validation of a potential synthetic Low-Mol-Wt angiogen

571 Computational Pharmacogenetics of P-Glycoprotein Mediated Antiepileptic Drug Resistance.

570 Online Molecular Docking Resources. **2017**, 941-959

569 Structure Modeling and Molecular Docking Studies of Schizophrenia Candidate Genes, Synapsins 2 (SYN2) and Trace Amino Acid Receptor (TAAR6). **2017**, 291-301 1

568 Molecular-Docking-Based Anti-Allergic Drug Design. **2017**, 711-726

567 Role of Molecular Docking in Computer-Aided Drug Design and Development. **2017**, 683-710

566 Protein-Protein Docking. **2017**, 1092-1114

565 Molecular mechanism of cell-cell adhesion mediated by cadherin-23.

564 Glutathione redox cycle enzymes as potential targets for heme-mediated oxidation under hemolysis: in silico analysis. **2018**,

563 Application of Novel Microbial Consortia for Environmental Site Remediation and Hazardous Waste Management Toward Low- and High-Density Polyethylene and Prioritizing the Cost-Effective, Eco-friendly, and Sustainable Biotechnological Intervention. **2018**, 1-48

562 Evolutionary Analysis Provides Insight into the Origin and Adaptation of HCV.

561 Structural Interactions Between H-NS and IHF with DNA. **2018**, 1-11

560 Molecular Mechanism of the Strong Cell-Adhesion by Cadherin-23. 0

559 Mutation in DsbA signal sequence hampers the SRP mechanism: A new strategy to combat virulence factor.

558 Protein Docking using Constrained Self-adaptive Differential Evolution Algorithm.

557 On identifying collective displacements in apo-proteins that reveal eventual binding pathways.

556 Computational evidence of a new allosteric communication pathway between active sites and putative regulatory sites in the alanine racemase ofMycobacterium tuberculosis. 1

555 Phosphatidylinositol 4,5-Bisphosphate (PIP2) Regulates KCNQ3 K+ Channels through Multiple Sites of Action.

554 Computational Pharmacogenetics of P-Glycoprotein Mediated Antiepileptic Drug Resistance. **2018**, 11, 197-207 0

553 Predicting CD4 T-cell epitopes based on antigen cleavage, MHCII presentation, and TCR recognition.

552 Flexible backbone assembly and refinement of symmetrical homomeric complexes.

551 In silico Structural Characterization of Plasmodium falciparum helicase, PfBrr2. **2018**, 15, 517-527

550 Alternative interaction sites in the influenza A virus nucleoprotein mediate viral escape from the importin-α mediated nuclear import pathway.

549 CBP/EP300-dependent acetylation and stabilization of HSF2 are compromised in the rare disorder, Rubinstein-Taybi syndrome.

548 Protein Docking and Drug Design. **2019**, 889-922

547 Design and Development of Small Molecules from Somatic, Stem Cell Reprogramming, and Therapy. **2019**, 167-183

546 Combinatorial Designing of Novel Lead Molecules Towards the Putative Drug Targets of Extreme Drug-Resistant Mycobacterium tuberculosis: A Future Insight for Molecular Medicine. **2019**, 233-281

545 A Complex Interplay of Anionic Phospholipid Binding Regulates 3-Phosphoinositide-Dependent-Kinase-1 Homodimer Activation.

544 Identification of target candidate in Polycystic ovarian syndrome and invitro evaluation of therapeutic activity of the designed RNA Aptamer.

543 Resveratrol prevents amyloid fibrillation of insulin by arresting it in a bioactive oligomeric form.

542 Structural characterization of covalently stabilized human cystatin C oligomers.

541 CX3CL1 binding protein-2 (CBP2) of Plasmodium falciparum binds nucleic acids.

540 Contriving a chimeric polyvalent vaccine to prevent infections caused by Herpes Simplex Virus (Type-1 and Type-2): an exploratory immunoinformatic approach.

539 Molecular modelling and docking of Mus musculus HMGB1 inflammatory protein with CGA. **2019**, 15, 467-473 1

538	Structural distortions induced by Kinase Inhibiting RNase Attenuator (KIRA) compounds prevent the formation of face-to-face dimers of Inositol Requiring Enzyme 1.	
537	iScore: an MPI supported software for ranking protein-protein docking models based on a random walk graph kernel and support vector machines.	
536	Oxidation shuts down an auto-inhibitory mechanism of von Willebrand factor.	
535	Molecular docking analysis of flavonoid compounds with HIV-1 Reverse transcriptase for the identification of potential effective inhibitors. **2019**, 15, 646-656	
534	Towards a Chimeric Vaccine against Multiple Isolates ofMycobacteroides- An Integrative Approach.	
533	A study of the effect of Paclitaxel, Docetaxel and Tamoxifen citrate coumpounds found in Taxus wallichiana on the Beta-tubulin and Estrogen Receptor (ESR) proteins in humans using a bioinformatics approach. 103-114	
532	Cavity/Binding Site Prediction Approaches and Their Applications. **2020**, 49-69	
531	Ecotoxicological QSAR Modeling of Nanomaterials: Methods in 3D-QSARs and Combined Docking Studies for Carbon Nanostructures. **2020**, 215-233	
530	Stress-induced tyrosine phosphorylation of RtcB modulates IRE1 activity and signaling outputs.	1
529	Structural Basis for Designing Multiepitope Vaccines Against COVID-19 Infection: In Silico Vaccine Design and Validation (Preprint).	
528	PRosettaC: Rosetta based modeling of PROTAC mediated ternary complexes.	3
527	An Immunoinformatics Study to Predict Epitopes in the Envelope Protein of SARS-COV-2.	0
526	Molecular docking data of piperine with Bax, Caspase 3, Cox 2 and Caspase 9. **2020**, 16, 458-461	0
525	Immunoglobulin interface redesigning to enhance lebrikizumab mediated immunomodulation of IL-13 hyper-response. **2021**, 39, 4051-4065	0
524	Molecular docking analysis of docetaxel analogues as duel lipocalin 2 inhibitors. **2020**, 16, 438-443	0
523	SARS-CoV-2 ORF8 can fold into human factor 1 catalytic domain binding site on complement C3b: Predict functional mimicry.	1
522	Cryo-EM Structures of Respiratorybc1-cbb3type CIII2CIV Supercomplex and Electronic Communication Between the Complexes.	
521	Generalized linear models provide a measure of virulence for specific mutations in SARS-CoV-2 strains.	1

520	Computational screening of potential MHC class I restricted cytotoxic T lymphocytes-based common multi-epitopes of major arboviral diseases. **2020**, 15, 497-505	
519	A non-synonymous single nucleotide polymorphism in FASN gene alters FASN enzyme activity in subcutaneous and intramuscular adipose tissue in Holstein Friesian steers. **2020**,	1
518	Molecular docking analysis of aspirin analogues with Ecatenin. **2020**, 16, 725-730	
517	Whey Protein Isolate-Xylose Maillard-Based Conjugates with Tailored Microencapsulation Capacity of Flavonoids from Yellow Onions Skins. **2021**, 10,	0
516	Structural and Functional Analysis of Female Sex Hormones against SARS-CoV-2 Cell Entry. **2021**, 22,	5
515	Identification and characterization of DNA aptamers specific to VP2 protein of canine parvovirus. **2021**, 105, 8895-8906	0
514	Bioactive's Characterization, Biological Activities, and In Silico Studies of Red Onion (L.) Skin Extracts. **2021**, 10,	3
513	Immunoinformatic identification of the epitope-based vaccine candidates from Maltoporin, FepA and OmpW of Shigella Spp, with molecular docking confirmation. **2021**, 96, 105129	0
512	Binding interactions of cationic gemini surfactants with gold nanoparticles-conjugated bovine serum albumin: A FRET/NSET, spectroscopic, and docking study. **2021**, 225, 112351	4
511	Structural analysis of Sub16 sedolisin of Trichophyton rubrum reveals a flexible nature of its pro domain.	
510	In-Silico Study on Apoptosis Inducing Mechanism of Phytochemicals to Regulate RAS Related G-Proteins Using FDBB Approach.	
509	A recombinant fragment of Human surfactant protein D binds Spike protein and inhibits infectivity and replication of SARS-CoV-2 in clinical samples.	1
508	Bioinformatics in Plant Pathology. **2021**, 725-844	
507	Ferrocene-functionalized anilines as potent anticancer and antidiabetic agents: Synthesis, spectroscopic elucidation, and DFT calculations. **2022**, 1249, 131632	1
506	Structural Analysis of the PATZ1 BTB domain homodimer.	
505	Exploiting the Reverse Vaccinology Approach to Design Novel Subunit Vaccine against Ebola Virus.	3
504	Proteome Exploration of Legionella pneumophila for Identifying Novel Therapeutics: A Hierarchical Subtractive Genomics and Reverse Vaccinology Approach.	
503	Docking analysis of importin-11 homology model with the phyto compounds towards colorectal cancer treatment. **2020**, 16, 153-159	1

502	Designing a multi-epitope peptide-based vaccine against SARS-CoV-2.	2
501	Comprehensive Genome Based Analysis of Vibrio parahaemolyticus for Identifying Novel Drug and Vaccine Molecules: Subtractive Proteomics and Vaccinomics Approach.	0
500	In silico design of Multi-epitope-based peptide vaccine against SARS-CoV-2 using its spike protein.	5
499	Jacalin domain-containing protein OsSalT interacts with OsDREB2A and OsNAC1 to impart drought stress tolerance in planta.	
498	Identification of potential inhibitory analogs of metastasis tumor antigens (MTAs) using bioactive compounds: revealing therapeutic option to prevent malignancy. **2021**, 1	
497	Computational and structural based approach to identify malignant nonsynonymous single nucleotide polymorphisms associated with CDK4 gene. **2021**, 16, e0259691	1
496	An integrated computational framework to design a multi-epitopes vaccine against Mycobacterium tuberculosis. **2021**, 11, 21929	5
495	Structural and functional analysis of female sex hormones against SARS-Cov2 cell entry. **2020**,	1
494	Synthesis, crystal structure and docking studies of tetracyclic 10-iodo-1,2-dihydroisoquinolino[2,1-b][1,2,4]benzothiadiazine 12,12-dioxide and its precursors. **2020**, 76, 810-820	0
493	Supercomputers in Modeling of Biological Systems. 201-222	
492	Wide variabilities identified among spike proteins of SARS Cov2 globally-dominant variant identified.	1
491	Molecular characterization of RIGI, TLR7 and TLR3 as immune response gene of indigenous ducks in response to Avian influenza.	3
490	RIG-I has a role in immunity against Haemonchus contortus, a gastrointestinal parasite in Ovis aries- a novel report.	0
489	COVID19: Exploring uncommon epitopes for a stable immune response through MHC1 binding.	
488	Computationally validated SARS-CoV-2 CTL and HTL Multi-Patch Vaccines designed by reverse epitomics approach, shows potential to cover large ethnically distributed human population worldwide.	0
487	A vaccine built from potential immunogenic pieces derived from the SARS-CoV-2 spike glycoprotein.	
486	Molecular Elucidation of Pancreatic Elastase Inhibition by Baicalein.	2
485	Molecular docking and simulation investigation: effect of beta-sesquiphellandrene with ionic integration on SARS-CoV2 and SFTS viruses. **2020**, 18, 78	10

484	In silico Techniques for Prospecting and Characterizing Monoclonal Antibodies.	
483	Evidence for NAD-dependent histone dynamics and tunneling associated conformational transitions in circadian deacetylase SIRT1. **2020**, 99, 107646	0
482	An Epithelial Sodium Channel (ENaC)-Specific Aptamer Determined through Structure-Based Virtual Screening for the Development of Hypertension Early Detection System. **2020**, 27, 67-75	0
481	Systematic protein-protein docking and molecular dynamics studies of HIV-1 gp120 and CD4: insights for new drug development. **2011**, 19, 469-75	6
480	Molecular determinants of ligand binding at the human histamine H receptor: Site-directed mutagenesis results analyzed with ligand docking and molecular dynamics studies at H homology and crystal structure models. **2012**, 4, 2937-2951	10
479	Molecular docking analysis of compounds from Lycopersicon esculentum with the insulin receptor to combat type 2 diabetes. **2020**, 16, 748-752	
478	Molecular docking and molecular dynamics simulation. **2022**, 291-304	3
477	Systems biology and big data analytics. **2022**, 425-442	
476	Binder design for targeting SARS-CoV-2 spike protein: An in silico perspective. **2022**, 26, 101452	1
475	Designing a Multi-epitope Peptide Vaccine Against COVID-19 Variants Utilizing In-silico Tools. **2021**, 15, 592-605	0
474	New system for archiving integrative structures. **2021**, 77, 1486-1496	2
473	Annotation of Potential Vaccine Targets and Design of a Multi-Epitope Subunit Vaccine against through Reverse Vaccinology and Validation through an Agent-Based Modeling Approach. **2021**, 9,	0
472	Selected Derivatives of Erythromycin B- and Anti-Malarial Studies. **2021**, 14,	1
471	Pan-Genome Reverse Vaccinology Approach for the Design of Multi-Epitope Vaccine Construct against. **2021**, 22,	1
470	A Novel Type of PD-L1 Inhibitor rU1 snRNPA From Human-Derived Protein Scaffolds Library.. **2021**, 11, 781046	0
469	Protein-Protein Docking: Past, Present, and Future. **2021**, 1	1
468	A Combined Spectroscopic and In Silico Approach to Evaluate the Interaction of Human Frataxin with Mitochondrial Superoxide Dismutase.. **2021**, 9,	0
467	rRNA Platform Technology for Drug Discovery Methods for Identifying Ligands That Target Plasmodium RNA Structural Motifs.	

466	Antibacterial prophylaxis and molecular docking studies of ketone and ester compounds isolated from Cyperus rotundus L. against Aeromonas veronii.	1
465	Whey Proteins Isolate-Based Biopolymeric Combinations to Microencapsulate Supercritical Fluid Extracted Oleoresins from Sea Buckthorn Pomace.. **2021**, 14,	
464	Computational Evaluation of Molecular Structures and Spectroscopic Properties of Tryptamine Derivatives on Its Binding With Novel Corona Virus Proteins. 1-10	
463	Molecular interaction of nitrate transporter proteins with recombinant glycinebetaine results in efficient nitrate uptake in the cyanobacterium Anabaena PCC 7120. **2021**, 16, e0257870	
462	In-Silico Vaccine Design Based on a Novel Vaccine Candidate Against Infections Caused by. **2022**, 28, 16	2
461	Synergistic collagen-condiment: Streptococcal collagen-like (Scl) protein in cell-adhesion and diabetic wound-closure matrix.	
460	C-terminal modified Enkephalin-like tetrapeptides with enhanced affinities at the kappa opioid receptor and monoamine transporters. **2021**, 51, 116509	0
459	Thermal Stability and Inhibitory Action of Red Grape Skin Phytochemicals against Enzymes Associated with Metabolic Syndrome.. **2022**, 11,	0
458	The novel EhHSTF7 transcription factor displays an oligomer state and recognizes a heat shock element in the Entamoeba histolytica parasite. **2021**, 162, 105349	1
457	Epicatechin is a promising novel inhibitor of SARS-CoV-2 entry by disrupting interactions between angiotensin-converting enzyme type 2 and the viral receptor binding domain: A computational/simulation study.. **2021**, 141, 105155	2
456	Structural insights into the activation of blood coagulation factor XI zymogen by thrombin: A computational molecular dynamics study.. **2021**, 281, 106737	
455	Anticancer chiral and racemic ternary copper(II) complexes: Multiple mechanisms and epigenetic histone methyltransferase enzymes as novel targets. **2022**, 213, 115617	0
454	Antioxidant, molecular docking and computational investigation of new flavonoids. **2022**, 1254, 132189	2
453	Spectroscopic and molecular modeling methods to investigate the interaction between psycho-stimulant modafinil and calf thymus DNA using ethidium bromide as a fluorescence probe.. **2021**, 270, 120787	4
452	CORRELATION BETWEEN PHARMACOKINETIC PROPERTIES AND 15N-NMR AND 13C-NMR CHEMICAL SHIFTS OF ANGIOTENSIN CONVERTING ENZYME INHIBITORS. **2019**, 56, 26-32	
451	Shape tracing: An extension of sphere tracing for 3D non-convex collision in protein docking. **2020**,	
450	Molecular docking analysis of compounds from Lycopersicon esculentum with the insulin receptor to combat type 2 diabetes. **2020**, 16, 748-752	
449	Immunoinformatics approaches to design: A novel multi-epitope vaccine candidate against SARS-CoV-2 and its in silico expression (Preprint).	

448	Extensive modelling and quantum chemical study of sterol C-22 desaturase mechanism: A commercially important cytochrome P450 family. **2021**,	
447	RIGI, TLR7, and TLR3 Genes Were Predicted to Have Immune Response Against Avian Influenza in Indigenous Ducks.. **2021**, 8, 633283	1
446	Thyroid-Stimulating Hormone Favors Runx2-Mediated Matrix Mineralization in HOS and SaOS2 Cells: An In Vitro and In Silico Approach.. **2022**, 27,	
445	Repurposing Based Identification of Novel Inhibitors against MmpS5-MmpL5 Efflux Pump of : A Combined In Silico and In Vitro Study.. **2022**, 10,	
444	Role of RIGI, MDA5 and interferon alpha of duck in Duck Plague infection a novel report.	0
443	Plant-Based Vaccines: Antigen Design, Diversity, and Strategies for High Level Production.. **2022**, 10,	2
442	Oxidative stress, DNA, and membranes targets as modes of antibacterial and antibiofilm activity of facile synthesized biocompatible keratin-copper nanoparticles against multidrug resistant uro-pathogens.. **2022**, 38, 20	3
441	MITOL-mediated DRP1 ubiquitylation and degradation promotes mitochondrial hyperfusion in CMT2A-linked MFN2 mutant. **2021**,	1
440	Synthesis of Nucleoside-like Molecules from a Pyrolysis Product of Cellulose and Their Computational Prediction as Potential SARS-CoV-2 RNA-Dependent RNA Polymerase Inhibitors.. **2022**, 23,	1
439	Structural and Dynamic Insights into the W68L, L85P, and T87A Mutations of Inducing Resistance to Pyrazinamide.. **2022**, 19,	
438	Bioactivity assessment of essential oils of Cymbopogon species using a network pharmacology approach.. **2022**, 73, 107	
437	Computational designing of a novel subunit vaccine for human cytomegalovirus by employing the immunoinformatics framework. 1-23	0
436	Electrostatically charged rutile TiO2 surfaces with enhanced photocatalytic activity for bacteria inactivation. **2022**,	1
435	A novel DNA aptamer targeting lung cancer stem cells exerts a therapeutic effect by binding and neutralizing Annexin A2.. **2022**, 27, 956-968	0
434	Targeting mucormycosis polyprotein (RVT_1 region) through antifungal phytochemicals: An in-silico perspective. **2022**, 29, 100851	1
433	Tracking the circulating SARS-CoV-2 variant of concern in South Africa using wastewater-based epidemiology.. **2022**, 12, 1182	3
432	Food and human health: An outlook of the journey of food from hunger satisfaction to health-promoting agent. **2022**, 1-30	
431	Inclusion of Desolvation Energy into Protein-Protein Docking through Atomic Contact Potentials.. **2022**,	0

430	Methyltransferase as Antibiotics Against Foodborne Pathogens: An Approach for Exploring Enzyme as Enzymobiotics.. **2021**, 12, 800587	
429	In Silico Analysis of Honeybee Venom Protein Interaction with Wild Type and Mutant (A82V + P375S) Ebola Virus Spike Protein. **2022**, 2, 45-55	0
428	Molecular Determinants for OMF Selectivity in Tripartite RND Multidrug Efflux Systems.. **2022**, 11,	1
427	Screening and potent applicability analysis of commonly used pesticides against Schistocerca gregaria and Locusta migratoria: an integrative computational approach. **2022**, 42, 1971	
426	A stepwise docking molecular dynamics approach for simulating antibody recognition with substantial conformational changes.. **2022**, 20, 710-720	
425	Synthesis, Spectroscopic and Biological Investigation of a New Ca(II) Complex of Meloxicam as Potential COX-2 Inhibitor.. **2022**, 1-18	0
424	Mechanical strain stimulates COPII-dependent trafficking via Rac1.	
423	Design of a multi-epitope vaccine against SARS-CoV-2: immunoinformatic and computational methods.. **2022**, 12, 4288-4310	2
422	An in silico study to unveil potential drugs and vaccine chimera for HBV capsid assembly protein: combined molecular docking and dynamics simulation approach.. **2022**, 28, 51	0
421	Synthesis, characterization, docking and biological studies of M(II) (M= Mg, Ca, Sr) Piroxicam complexes. **2022**, 1254, 132256	0
420	Global conserved RBD fraction of SARS-CoV-2 S-protein with T500S mutation in silico significantly blocks ACE2 and rejects viral spike.. **2022**, 7, 2	1
419	Phosphorylation of guanosine monophosphate reductase triggers a GTP-dependent switch from pro- to anti-oncogenic function of EPHA4.. **2022**,	0
418	Plasma Bead Entrapped Liposomes as a Potential Drug Delivery System to Combat Fungal Infections.. **2022**, 27,	
417	Integration of software tools for integrative modeling of biomolecular systems.. **2022**, 107841	0
416	A Synthetically Accessible Small-Molecule Inhibitor of USP5-Cav3.2 Calcium Channel Interactions with Analgesic Properties.. **2022**,	1
415	TN strain proteome mediated therapeutic target mapping and multi-epitopic peptide-based vaccine development for Mycobacterium leprae.. **2022**, 99, 105245	2
414	Cotranslational interaction of human EBP50 and ezrin overcomes masked binding site during complex assembly.. **2022**, 119,	2
413	Protein Binding of Benzofuran Derivatives: A CD Spectroscopic and In Silico Comparative Study of the Effects of 4-Nitrophenyl Functionalized Benzofurans and Benzodifurans on BSA Protein Structure.. **2022**, 12,	0

412	How fullerene derivatives (FDs) act on therapeutically important targets associated with diabetic diseases.. **2022**, 20, 913-924	3
411	An integrated in silico based subtractive genomics and reverse vaccinology approach for the identification of novel vaccine candidate and chimeric vaccine against XDR Salmonella typhi H58.. **2022**, 114, 110301	1
410	In-Silico Design of a Novel Tridecapeptide Targeting Spike Protein of SARS-CoV-2 Variants of Concern.. **2022**, 28, 28	3
409	Computational Intelligence-Based Cheminformatics Model as Cancer Therapeutics. **2022**, 251-269	
408	Tools for Characterizing Proteins: Circular Variance, Mutual Proximity, Chameleon Sequences, and Subsequence Propensities.. **2022**, 2405, 39-61	
407	Three-Dimensional Structure Characterization and Inhibition Study of Exfoliative Toxin D From .. **2022**, 13, 800970	0
406	Neprosin belongs to a new family of glutamic peptidase based on in silico evidence.	
405	Computational Design of a Multi-Epitope Vaccine Against .. **2022**, 13, 806825	0
404	Design of a Multi-Epitopes Vaccine against Hantaviruses: An Immunoinformatics and Molecular Modelling Approach.. **2022**, 10,	2
403	Human Growth Factor/Immunoglobulin Complexes for Treatment of Myocardial Ischemia-Reperfusion Injury.. **2022**, 10, 749787	0
402	Quantum Mechanical Investigation into the Adsorption Pattern of Clomipramine and Methotrimeprazine HCl with Graphene and Fullerene. 1-14	1
401	Stress-induced tyrosine phosphorylation of RtcB modulates IRE1 activity and signaling outputs.. **2022**, 5,	0
400	Fullerenes against COVID-19: Repurposing C and C to Clog the Active Site of SARS-CoV-2 Protease.. **2022**, 27,	3
399	A novel strategy for developing a tetravalent vaccine (dvac) against dengue utilizing conserved regions from all DENV proteins.. **2022**, 164, 105447	0
398	Nanofibers from hydroxypropyl □cyclodextrin/pantothenic acid supramolecular complexes: Physicochemical characterization and potential biomedical applications. 152808372210820	
397	Designing of a Recombinant Multi-Epitopes Based Vaccine against Using Bioinformatics and Immunoinformatics Approaches.. **2022**, 19,	6
396	New type of RNA virus replication inhibitor based on decahydro-closo-decaborate anion containing amino acid ester pendant group.. **2022**, 1	1
395	Immunogenic Epitope-Based Vaccine Prediction from Surface Glycoprotein of MERS-CoV by Deploying Immunoinformatics Approach.. **2022**, 28, 77	1

394	Evaluation of Cyc protein stability in Acidithiobacillus ferrooxidans bacterium alter E121D mutation by molecular dynamics simulation to improve electron transfer.. **2022**, 1	0
393	Progress and challenges for the machine learning-based design of fit-for-purpose monoclonal antibodies.. **2022**, 14, 2008790	4
392	Binding and Photocleavage Studies of Ru (II) Polypyridyl Complexes with DNA: An In Silico and Antibacterial activity. **2022**, 12, 266-282	0
391	Targeting the HIV-1 Tat and Human Tat protein complex through natural products: An in silico docking and Molecular Dynamics Simulation Approach. **2022**, 19,	2
390	Impact of Chromate and Dichromate on Lysozyme Stability: A Spectroscopic and Molecular Docking Investigation.. **2022**,	0
389	Codon usage studies and epitope-based peptide vaccine prediction against Tropheryma whipplei.. **2022**, 20, 41	3
388	Ligand-Dependent Modulation of the Dynamics of Intracellular Loops Dictates Functional Selectivity of 5-HTR.. **2022**,	0
387	In-vivo Studies and Molecular Docking of Modeled Mus musculas 8S Lipoxygenase Protein Using Some Natural Bioactive Compounds. 1	
386	PLO3S : Protein LOcal Surficial Similarity Screening.	
385	Modeling the Dynamics of Protein-Protein Interfaces, How and Why?. **2022**, 27,	1
384	Drug Discovery of Plausible Lead Natural Compounds That Target the Insulin Signaling Pathway: Bioinformatics Approaches.. **2022**, 2022, 2832889	1
383	Crucial role and mechanism of transcription-coupled DNA repair in bacteria.. **2022**,	2
382	In Silico Analysis of the Multi-Targeted Mode of Action of Ivermectin and Related Compounds. **2022**, 10, 51	0
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359	Evaluation of anticancer activity of N H/N-Me Aziridine derivatives as a potential poly (ADP-ribose) polymerase 1 inhibitor. **2022**, 1258, 132689	0

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357	DFT of 5-Fluoro-2-Oxo-1H-Pyrazine-3-Carboxamide (OPC) Adsorption, Spectroscopic, Solvent Effect, and SERS Analysis. **2022**, 357, 119076	3
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354	A Geometric Complementarity-Based Tool for Protein–Protein Docking. **2022**, 21, 35-46	
353	T-cell epitope-based vaccine designing against Orthohantavirus: a causative agent of deadly cardio-pulmonary disease.. **2022**, 11, 2	4
352	Oligomeric States and Hydrodynamic Properties of Lysyl Oxidase-Like 2.. **2021**, 11,	1
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350	The Effects of Tetrapeptides Designed to Fit the Androgen Binding Site of ZIP9 on Myogenic and Osteogenic Cells.. **2021**, 11,	2
349	Investigating the role of carbohydrate-binding module 34 in cyclomaltodextrinase from : structural and functional analyses.. **2022**, 12, 25	0
348	Molecular Basis of Selective Cytokine Signaling Inhibition by Antibodies Targeting a Shared Receptor.. **2021**, 12, 779100	1
347	Therapeutic potential of methylxanthine drug on alpha synuclein protein in Parkinson's disease.	
346	Structural Characterization of Enolase and Its Interaction with Human Plasminogen by In Silico and In Vitro Assays.. **2021**, 10,	0
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344	Reverse vaccinology approach to design a vaccine targeting membrane lipoproteins of .. **2021**, 1-16	0
343	Elucidating the role of silicon dioxide and titanium dioxide nanoparticles in mitigating the disease of the eggplant caused by Phomopsis vexans, Ralstonia solanacearum, and root-knot nematode Meloidogyne incognita. **2022**, 11, 1606-1619	0
342	T-Cell Epitopes Based Vaccine Candidate's Prediction for Treatment Against Burkholderia pseudomallei: Causative Agent of Melioidosis. **2022**, 28, 1	0
341	MIF1 and MIF2 Myostatin Peptide Inhibitors as Potent Muscle Mass Regulators.. **2022**, 23,	0

340	Anticancer, Antibacterial, Antioxidant, and DNA-Binding Study of Metal-Phenalenyl Complexes.. **2022**, 2022, 8453159	1
339	COMPLEX EFFECT OF LOW-INTENSITY LASER RADIATION AND POTASSIUM CHANNEL PEPTIDE INHIBITOR ON MELANOMA CELL SURVIVAL. **2022**, 94-104	
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336	A dual action small molecule enhances azoles and overcomes resistance through co-targeting Pdr5 and Vma1: Osimertinib targets Pdr5 and Vma1.. **2022**,	
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333	Image_1.pdf. **2020**,	
332	Table_1.xlsx. **2020**,	
331	Data_Sheet_1.docx. **2020**,	
330	Data_Sheet_1.XLSX. **2018**,	
329	Data_Sheet_2.XLSX. **2018**,	
328	Data_Sheet_3.XLSX. **2018**,	
327	Data_Sheet_4.XLSX. **2018**,	
326	Data_Sheet_5.XLSX. **2018**,	
325	Data_Sheet_6.XLSX. **2018**,	
324	Data_Sheet_7.XLSX. **2018**,	
323	Data_Sheet_8.XLSX. **2018**,	

322 Image_1.TIF. **2018**,

321 Image_2.TIF. **2018**,

320 Image_3.TIF. **2018**,

319 Data_Sheet_1.PDF. **2020**,

318 Image_1.TIF. **2020**,

317 Data_Sheet_1.docx. **2019**,

316 Table_1.doc. **2020**,

315 Image_1.PDF. **2018**,

314 Table_1.PDF. **2018**,

313 Table_2.PDF. **2018**,

312 Table_3.PDF. **2018**,

311 Table_4.PDF. **2018**,

310 Table_5.PDF. **2018**,

309 Table_6.PDF. **2018**,

308 Data_Sheet_1.pdf. **2020**,

307 DataSheet_1.docx. **2020**,

306 DataSheet_2.docx. **2020**,

305 DataSheet1.DOCX. **2018**,

304 Image1.TIF. **2018**,

303 Image10.TIF. **2018**,

302 Image11.TIF. **2018**,

301 Image12.TIF. **2018**,

300 Image13.TIF. **2018**,

299 Image14.TIF. **2018**,

298 Image15.TIF. **2018**,

297 Image2.TIF. **2018**,

296 Image3.TIF. **2018**,

295 Image4.TIF. **2018**,

294 Image5.TIF. **2018**,

293 Image6.TIF. **2018**,

292 Image7.TIF. **2018**,

291 Image8.TIF. **2018**,

290 Image9.TIF. **2018**,

289 Table_1.docx. **2019**,

288 Image_1.pdf. **2019**,

287 Image_2.png. **2019**,

286	Triclosan is a KCNQ3 potassium channel activator.. **2022**, 1	
285	[Efficient screening for 8-oxoguanine DNA glycosylase binding aptamers via capillary electrophoresis]. **2021**, 39, 721-729	0
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276	CoLab: A Workshop-Based Undergraduate Research Experience for Entering College Students.	0
275	Cell membrane enolase of Aedes albopictus C6/36 cells is involved in the entrance mechanism of dengue virus (DENV). **2022**, 25, 101924	
274	Neprosin belongs to a new family of glutamic peptidase based on in silico evidence.. **2022**, 183, 23-35	2
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268	Immunoinformatic paradigm predicts macrophage and T-cells epitope responses against globally conserved spike fragments of SARS CoV-2 for universal vaccination. **2022**, 108847	
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265	Human serum albumin adsorption on cellulose nanocrystal: A spectroscopy and molecular dynamics simulation research. **2022**, 597, 153749	0
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263	Immunoinformatic Design of a Multivalent Peptide Vaccine Against Mucormycosis: Targeting FTR1 Protein of Major Causative Fungi. **2022**, 13,	1
262	Evaluating the conformational space of the active site of D 2 dopamine receptor. Scope and limitations of the standard docking methods.	0
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260	Insight into the mechanism of allergenicity decreasing in recombinant sarcoplasmic calcium-binding protein from shrimp (Litopenaeus vannamei) with thermal processing via spectroscopy and molecular dynamics simulation techniques. **2022**, 111427	1
259	Computational Structure Prediction for Antibody-Antigen Complexes From Hydrogen-Deuterium Exchange Mass Spectrometry: Challenges and Outlook. **2022**, 13,	1
258	Targeting Akt/NF-□/p53 Pathway and Apoptosis Inducing Potential of 1,2-Benzenedicarboxylic Acid, Bis (2-Methyl Propyl) Ester Isolated from Onosma bracteata Wall. against Human Osteosarcoma (MG-63) Cells. **2022**, 27, 3478	0
257	SARS CoV2 Kerala Isolate Spike Protein Induces Cancer Proliferating Markers for Lung and Breast Cancer An In Silico Approach. **2022**, 03,	
256	Identification of vaccine targets & design of vaccine against SARS-CoV-2 coronavirus using computational and deep learning-based approaches. 10, e13380	2
255	A Molecular Docking Study of Human STEAP2 for the Discovery of New Potential Anti-Prostate Cancer Chemotherapeutic Candidates. **2022**, 2,	
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251	Design of a Multi-Epitopes Based Chimeric Vaccine against Enterobacter cloacae Using Pan-Genome and Reverse Vaccinology Approaches. **2022**, 10, 886	1

250	Mincle-binding DNA aptamer demonstrates therapeutic potential in a model of inflammatory bowel disease. **2022**,	1
249	Combined in Silico Prediction Methods, Molecular Dynamic Simulation, and Molecular Docking of FOXG1 Missense Mutations: Effect on FoxG1 Structure and Its Interactions with DNA and Bmi-1 Protein.	0
248	E2UbcH5B-derived peptide ligands target HECT E3-E2 binding site and block the Ub-dependent SARS-CoV-2 egression: A computational study. **2022**, 146, 105660	1
247	Execution and Design of an Anti HPIV-1 Vaccine with Multiple Epitopes Triggering Innate and Adaptive Immune Responses: An Immunoinformatic Approach. **2022**, 10, 869	2
246	Genome-Wide Characterization of Superoxide Dismutase (SOD) Genes in Daucus carota: Novel Insights Into Structure, Expression, and Binding Interaction With Hydrogen Peroxide (H2O2) Under Abiotic Stress Condition. 13,	1
245	Heme Detoxification protein (Pf HDP) is essential for the hemoglobin uptake and metabolism in Plasmodium falciparum.	
244	Biochemical Properties and Physiological Functions of pLG72: Twenty Years of Investigations. **2022**, 12, 858	
243	Chrysin-Loaded Chitosan Nanoparticle-Mediated Neuroprotection in A□□2-Induced Neurodegenerative Conditions in Zebrafish.	0
242	Mechanistic interaction studies of synthesized ZIF-8 nanoparticles with bovine serum albumin using spectroscopic and molecular docking approaches. **2022**, 12,	4
241	Development of Multi-epitope Based Subunit Vaccine Against Crimean-Congo Hemorrhagic Fever Virus Using Reverse Vaccinology Approach. **2022**, 28,	0
240	Cryo-EM structure of a type IV secretion system.	1
239	Development of S-aryl dithiocarbamate derived novel antiproliferative compound exhibiting tubulin bundling. **2022**, 68, 116874	0
238	Identification and structural analysis of novel malathion-specific DNA aptameric sensors designed for food testing. **2022**, 287, 121617	4
237	Structural and electronic investigation of 3,4-dihydropyrimidin-2(1H)-ones (DHPMs): Correlations between spectroscopic and molecular docking features upon salmon sperm DNA. **2022**, 1266, 133546	
236	Laminins and Matrix Metalloproteinases Connection: A Subtle Relationship That Can Go Wrong in a Tumor Context, Particularly If CD44 Gets Involved. **2022**, 219-246	0
235	Immunoinformatics- and Bioinformatics-Assisted Computational Designing of a Novel Multiepitopes Vaccine Against Cancer-Causing Merkel Cell Polyomavirus. 13,	0
234	HrpA anchors meningococci to the dynein motor and affects the balance between apoptosis and pyroptosis. **2022**, 29,	
233	Binding of the M. tuberculosis EccC ATPase double hexameric ring to the EsxAB virulence factor is enhanced by ATP.	

232	Reverse Vaccinology and Immunoinformatic Assisted Designing of a Multi-Epitopes Based Vaccine Against Nosocomial Burkholderia cepacia. 13,	0
231	Identifying the potential role of curcumin analogues as anti-breast cancer agents; an in silico approach. **2022**, 23,	
230	In silico Analysis of Peptide-Based Biomarkers for the Diagnosis and Prevention of Latent Tuberculosis Infection. 13,	1
229	Novel In Silico Insights into Rv1417 and Rv2617c as Potential Protein Targets: The Importance of the Medium on the Structural Interactions with Exported Repetitive Protein (Erp) of Mycobacterium tuberculosis. **2022**, 14, 2577	1
228	In Silico Characterization, Identification, and Molecular-level Analysis of Holotricin-3: A Dynamic Study. **2022**, 38, 671-675	
227	Application of Mathematical Modeling and Computational Tools in the Modern Drug Design and Development Process. **2022**, 27, 4169	1
226	Ig-VAE: Generative modeling of protein structure by direct 3D coordinate generation. **2022**, 18, e1010271	1
225	Analytical Studies of Antimicrobial Peptides as Diagnostic Biomarkers for the Detection of Bacterial and Viral Pneumonia. **2022**, 9, 305	0
224	Pan-Genome Analysis of Oral Bacterial Pathogens to Predict a Potential Novel Multi-Epitopes Vaccine Candidate. **2022**, 19, 8408	2
223	Proteome Exploration of Legionella pneumophila To Identify Novel Therapeutics: a Hierarchical Subtractive Genomics and Reverse Vaccinology Approach.	0
222	In Silico Study: Combination of □Mangostin and Chitosan Conjugated with Trastuzumab against Human Epidermal Growth Factor Receptor 2. **2022**, 14, 2747	
221	Machine-designed biotherapeutics: opportunities, feasibility and advantages of deep learning in computational antibody discovery. **2022**, 23,	1
220	Human malaria parasite cold shock protein plays an essential role in asexual and sexual stage development and presents an excellent druggable target.	
219	Molecular Interaction analysis of SPARC-Collagen with human serum albumin.	
218	An In-Silico Investigation to Design a Multi-Epitopes Vaccine against Multi-Drug Resistant Hafnia alvei. **2022**, 10, 1127	0
217	Interaction Interface of A□2 with Human Na,K-ATPase Studied by MD and ITC and Inhibitor Screening by MD. **2022**, 10, 1663	0
216	Insights into the phylogeny of transporters coded within biosynthetic gene clusters for glycopeptides and related antibiotics. **2022**, 33-46	
215	Structure Prediction and Analysis of Hepatitis E Virus Non-Structural Proteins from the Replication and Transcription Machinery by AlphaFold2. **2022**, 14, 1537	1

214	Antibody CDR amino acids underlying the functionality of antibody repertoires in recognizing diverse protein antigens. **2022**, 12,	0
213	Open-Source Browser-Based Tools for Structure-Based Computer-Aided Drug Discovery. **2022**, 27, 4623	
212	An Insulin Receptor-Binding Multifunctional Protein from Tamarindus indica L. Presents a Hypoglycemic Effect in a Diet-Induced Type 2 Diabetes Preclinical Study. **2022**, 11, 2207	0
211	Recombinant production and characterization of L-glutaminase (glsA) as a promiscuity therapeutic enzyme. **2022**, 106, 5511-5524	
210	Evidence for Plant-Conserved Region Mediated Trimeric CESAs in Plant Cellulose Synthase Complexes.	0
209	CD, UV, and In Silico Insights on the Effect of 1,3-Bis(1?-uracilyl)-2-propanone on Serum Albumin Structure. **2022**, 12, 1071	1
208	Multi-epitope chimeric vaccine designing and novel drug targets prioritization against multi-drug resistant Staphylococcus pseudintermedius. 13,	0
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206	Efficient DNA-ligand interaction framework using fuzzy C-means clustering based glowworm swarm optimization (FCMGSO) method. 1-13	
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204	An Immunoinformatic Study on Exploration of Membrane Proteins to Develop Epitope Based Vaccine Against Streptococcus pneumoniae. **2022**, 28,	
203	Establishing the Taxa with Phylogenetic Profile and in-silico Ayurvedic Remedy of Human Oropharynx Microbiome.	
202	Augmenting apoptosis-mediated anticancer activity of lactoperoxidase and lactoferrin by nanocombination with copper and iron hybrid nanometals. **2022**, 12,	1
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198	Mechanical strain stimulates COPII -dependent secretory trafficking via Rac1.	3
197	Multi-epitope chimeric vaccine design against emerging Monkeypox virus via reverse vaccinology techniques- a bioinformatics and immunoinformatics approach. 13,	4

196	A Computational Study on the Interaction of NSP10 and NSP14: Unraveling the RNA Synthesis Proofreading Mechanism in SARS-CoV-2, SARS-CoV, and MERS-CoV.	1
195	Identification of therapeutic miRNAs from the Arsenic induced gene expression profile of hepatocellular carcinoma.	1
194	Host Virus Interactions in Japanese Encephalitis Virus. **2022**, 2, 117-125	1
193	Molecular docking study on vitamin D supplements to understand their interaction with VDR-RXR heterodimer and VDRE of TAGAP gene. 1-10	
192	Cupressus sempervirens L. flavonoids as potent inhibitors to xanthine oxidase: in vitro, molecular docking, ADMET and PASS studies. 1-14	
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190	Smart electrochemical immunosensor for detection of aspartame in dietary products supported by in silico methods. **2022**, 11, 100203	0
189	Enhancing the biological properties of zinc complexes with bis(indolyl)methane groups: Synthesis, characterization, DNA interaction, and biocide activity. **2022**, 236, 111973	1
188	Biosynthesis and characterization of Serratia marcescens derived silver nanoparticles: Investigating its antibacterial, anti-biofilm potency and molecular docking analysis with biofilm-associated proteins. **2022**, 365, 120094	0
187	Higher affinity binding alleles and copy number variation of inhibitory KIR2DL1 gene influence the immune surveillance in head and neck squamous cell carcinoma in the population of Assam, North-East India. **2022**, 34, 201086	
186	Exploiting reverse vaccinology approach for the design of a multiepitope subunit vaccine against the major SARS-CoV-2 variants. **2022**, 101, 107754	0
185	Functionalized carbon nanotubes as an alternative to traditional anti-HIV-1 protease inhibitors: An understanding towards Nano-medicine development through MD simulations. **2022**, 117, 108280	0
184	Pan-Genome-Assisted Computational Design of a Multi-Epitopes-Based Vaccine Candidate against Helicobacter cinaedi. **2022**, 19, 11579	0
183	Designing a vaccine-based therapy against Epstein-Barr virus-associated tumors using immunoinformatics approach. **2022**, 150, 106128	0
182	TPGS loaded triphenyltin (IV) micelles induced apoptosis by upregulating p53 in breast cancer cells and inhibit tumor progression in T-cell lymphoma bearing mice. **2022**, 308, 120937	0
181	SARS-CoV-2 main protease (3CLpro) interaction with acyclovir antiviral drug/methyl- cyclodextrin complex: Physiochemical characterization and molecular docking. **2022**, 366, 120292	0
180	Modeling and simulation of peptides. **2023**, 35-56	0
179	Search for putative heme binding sites in the integrated membrane protein of human erythrocytes SLC4A1 and protein kinases SYK and LYN. **2021**, 4-15	0

178	Identification of promising nutraceuticals against filarial immune-modulatory proteins: insights from in silico and ex vivo studies. **2022**, 12, 22542-22554	0
177	Computational design and characterization of a multiepitope vaccine against carbapenemase-producing Klebsiella pneumoniae strains, derived from antigens identified through reverse vaccinology. **2022**, 20, 4446-4463	1
176	Potent and selective anticancer activity of half-sandwich ruthenium and osmium complexes with modified curcuminoid ligands. **2022**, 51, 13311-13321	3
175	Rational incorporation of any unnatural amino acid into proteins by machine learning on existing experimental proofs. **2022**, 20, 4930-4941	0
174	Novel Chimeric Vaccine Candidate Development against Leptotrichia buccalis. **2022**, 19, 10742	0
173	Immunoinformatics Studies and Design of a Potential Multi-Epitope Peptide Vaccine to Combat the Fatal Visceral Leishmaniasis. **2022**, 10, 1598	2
172	Elucidation of the Anticancer Potential of Selected Citrus Flavonoids Against NEDD4-1 in Breast Cancer. **2022**, 32, 796-804	0
171	Accelerated rational PROTAC design via deep learning and molecular simulations. **2022**, 4, 739-748	2
170	Molecular Docking of Monomethine Cyanine Dyes to Lysozyme Amyloid Fibrils. **2022**, 142-148	0
169	Deciphering the molecular insight behind the inhibitory role of copper and silver nanocomposite on important bacterial and fungal pathogens in rice (oryza sativa).	0
168	Oleanolic Acid as a Possible Inhibitor of Pfn2: In silico Approach.	0
167	Structure and Biological Properties of Ribosome-Inactivating Proteins and Lectins from Elder (Sambucus nigra L.) Leaves. **2022**, 14, 611	2
166	Study of the Effects of Nicotine and Caffeine for the Treatment of Parkinson Disease.	0
165	Multiple Docking of Fluorescent Dyes to Fibrillar Insulin. **2022**, 115-120	0
164	Immunoinformatics Approach to Design Novel Subunit Vaccine against the Epstein-Barr Virus.	0
163	Kinetics and computational study of butyrylcholinesterase inhibition by methylrosmarinate: relevance to Alzheimer disease treatment. **2022**, 8, e10613	1
162	Fusarium verticillioides NAT1 (FDB2) N -malonyltransferase is structurally, functionally and phylogenetically distinct from its N -acetyltransferase (NAT) homologues.	0
161	Na,K-ATPase Acts as a Beta-Amyloid Receptor Triggering Src Kinase Activation. **2022**, 11, 2753	0

160	Multi-Epitope-Based Vaccine Candidate for Monkeypox: An In Silico Approach. **2022**, 10, 1564	3
159	Structure of the two-component S-layer of the archaeon Sulfolobus acidocaldarius.	0
158	Potential antiviral peptides against the nucleoprotein of SARS-CoV-2.	0
157	pyDockDNA: A new web server for energy-based protein-DNA docking and scoring. 9,	0
156	A candidate multi-epitope vaccine against Lumpy Skin Disease.	0
155	Analyses of biosynthesized silver nanoparticles produced from strawberry fruit pomace extracts in terms of biocompatibility, cytotoxicity, antioxidant ability, photodegradation, and in-silico studies. **2022**, 34, 102327	0
154	Big dynorphin is a neuroprotector scaffold against amyloid peptide aggregation and cell toxicity. **2022**, 20, 5672-5679	1
153	Docking-Based Virtual Screening for the Discovery of 1,3,4-Oxadiazoles as Aminoacyl-tRNA Synthetase Inhibitors. **2022**, 14, 83-92	0
152	Docking and Molecular Dynamics-Based Identification of Interaction between Various Beta-Amyloid Isoforms and RAGE Receptor. **2022**, 23, 11816	0
151	Fast and versatile sequence-independent protein docking for nanomaterials design using RPXDock.	1
150	Exploring Facile Synthesis and Cholinesterase Inhibiting Potential of Heteroaryl Substituted Imidazole Derivatives for the Treatment of Alzheimer Disease. **2022**, 104384	0
149	From Genome Mining to Protein Engineering: A Structural Bioinformatics Route. **2023**, 79-94	0
148	The structural basis for the self-inhibition of DNA binding by apo-0.	0
147	Vaccinomics-Aided Development of a Next-Generation Chimeric Vaccine against an Emerging Threat: Mycoplasma genitalium. **2022**, 10, 1720	0
146	Computational Studies on Selected Macrolides Active against Escherichia coli Combined with the NMR Study of Tylosin A in Deuterated Chloroform. **2022**, 27, 7280	0
145	Blockage of ATPase-mediated energy supply inducing metabolic disturbances in algal cells under silver nanoparticles stress. **2022**,	0
144	Structural Prediction and Characterization of Canavalia grandiflora (ConGF) Lectin Complexed with MMP1: Unveiling the Antiglioma Potential of Legume Lectins. **2022**, 27, 7089	0
143	Omicron SARS-CoV-2 Spike-1 Protein Decreased Binding Affinity to nAChr: Implications for Autonomic Dysregulation of the Parasympathetic Nervous System and the Cholinergic Anti-Inflammatory Pathway An In Silico Analysis. **2022**, 2, 553-564	0

142	The antimicrobial peptide Magainin-2 interacts with BamA impairing folding of E. coli membrane proteins. 10,	0
141	In Silico Methods for Identification of Potential Active Sites of Therapeutic Targets. **2022**, 27, 7103	0
140	In-Silico Exploration of Plant Metabolites as Potential Remedies of Norovirus. **2022**, 2022, 1-13	0
139	In silico bioprospecting of receptors for Doderlin: an antimicrobial peptide isolated from Lactobacillus acidophilus.	0
138	Rab7 Investigation Insights into the Existence of White Spot Syndrome Virus in Crustaceans: An In Silico Approach. **2022**, 2022, 1-16	0
137	Computationally Designed Anti-LuxP DNA Aptamer Suppressed Flagellar Assembly- and Quorum Sensing-Related Gene Expression in Vibrio parahaemolyticus. **2022**, 11, 1600	0
136	Immuno-informatics profiling of monkeypox virus cell surface binding protein for designing a next generation multi-valent peptide-based vaccine. 13,	2
135	In silico designing of a novel polyvalent multi-subunit peptide vaccine leveraging cross- immunity against human visceral & cutaneous leishmaniasis: An Immunoinformatics-based approach.	0
134	Immunogenic analysis of epitope-based vaccine candidate induced by photodynamic therapy in MDA-MB-231 triple-negative breast cancer cells. **2022**, 40, 103174	0
133	Insights into the reactivity properties, docking, DFT and MD simulations of orphenadrinium dihydrogen citrate in different solvents. **2022**, 367, 120583	3
132	Bi(III) complexes of piroxicam and meloxicam: Synthesis, characterization, antioxidant, anti-inflammatory and DNA cleavage studies. **2023**, 1272, 134234	0
131	3D Modeling of Non-coding RNA Interactions. **2022**, 281-317	0
130	Bio functional molecular complexes, ferrocenyl hydrazone based binuclear Cu (II) derivatives: Synthesis, spectral, DNA/BSA binding & in-silico analyses. **2022**, 4, 100624	0
129	Targeting apoptosis in MCF-7 and Ehrlich ascites carcinoma cells by saponifiable fractions from green and black Vitis vinifera seed oil. **2023**, 157, 114017	0
128	Development of Nucleic Acid Targeting Molecules: Molecular Docking Approaches and Recent Advances.	0
127	An in vitro and computational validation of a novel loss-of-functional mutation in PAX9 associated with non-syndromic tooth agenesis.	0
126	Molecular docking study on europium nanoparticles and mussel adhesive protein for effective detection of latent fingerprints. 1-33	0
125	Mutational analysis of phospholipase C epsilon 1 gene in Egyptian children with steroid-resistant nephrotic syndrome. **2022**, 23,	0

124	Multi-Epitope Vaccine for Monkeypox Using Pan-Genome and Reverse Vaccinology Approaches. **2022**, 14, 2504	1
123	Antigenic mapping reveals sites of vulnerability on HCoV spike protein. **2022**, 5,	0
122	Molecular exposition of broad-spectrum antibacterial efficacy by p-coumaric acid from an edible mushroom Termitomyces heimii: in vitro and in silico approach.	0
121	Fabrication of Functional bioMOF-100 Prototype as Drug Delivery System for Breast Cancer Therapy. **2022**, 14, 2458	1
120	Integrativesubtractive proteomics, immunoinformatics, docking, and simulation approaches reveal candidate vaccine against Sin Nombre orthohantavirus. 13,	0
119	Design of a multi-epitope protein as a subunit vaccine against lumpy skin disease using an immunoinformatics approach. **2022**, 12,	2
118	Hydrophobicity Effects of Glutamyl Transpeptidase-Responsive Polymers on the Catalytic Activity and Transcytosis Efficacy. **2022**, 33, 2132-2142	0
117	Computational Design of a Chimeric Vaccine against Plesiomonas shigelloides Using Pan-Genome and Reverse Vaccinology. **2022**, 10, 1886	0
116	Anti-Sporotrichotic Activity, Lambert-W Inhibition Kinetics and 3D Structural Characterization of Sporothrix schenckii Catalase as Target of Glucosinolates from Moringa oleifera. **2022**, 90, 70	0
115	Differential interactions of synuclein conformers affect refolding and activity of proteins.	0
114	Theoretical Study at the Molecular Mechanics Level of the Interaction of Tetracycline and Chloramphenicol with the Antibiotic Receptors Present in Enterococcus faecalis (Q839F7) and Streptococcus mutans (Q8DS20). **2022**, 11, 1640	0
113	Multimodal approach to characterize the tetrameric form of human PML-RBCC domain and ATO-mediated conformational changes. **2022**, 223, 468-478	0
112	Structural, functional and evolutionary analysis of wheat WRKY45 protein: A combined bioinformatics and MD simulation approach.	0
111	Multi-state modeling of antibody-antigen complexes with SAXS profiles and deep-learning models. **2022**,	0
110	Structure Prediction and In-silico Designing of Drugs against Plant Homeodomain Finger Protein 14 for Suppression of Malignant Transformation and Tumorigenicity of Non Small Cell Lung Cancer. **2022**, 4621-4626	0
109	Deciphering the anti-filarial potential of bioactive compounds from Ocimum sanctum: a combined experimental and computational study. **2022**, 60, 2237-2252	0
108	N-Linked Glycosylation in Chinese Hamster Ovary Cells Is Critical for Insulin-like Growth Factor 1 Signaling. **2022**, 23, 14952	0
107	Molecular Cloning, Expression, Sequence Characterization and Structural Insight of Bubalus bubalis Growth Hormone-Receptor.	0

106	Successes and Failures of Static Aptamer-Target 3D Docking Models. **2022**, 23, 14410	0
105	Tsukushi proteoglycan maintains RNA splicing and developmental signaling network in GFAP-expressing subventricular zone neural stem/progenitor cells. 10,	0
104	Molecular docking simulation, drug pharmacokinetics and synthesis of carbon nanodots from phytochemicals against isoenzymes of cancer. **2022**,	0
103	Label-Free Analysis of Binding and Inhibition of SARS-Cov-19 Spike Proteins to ACE2 Receptor with ACE2-Derived Peptides by Surface Plasmon Resonance.	0
102	GDockScore: a graph-based protein-protein docking scoring function.	0
101	Multi Epitopic Peptide Based Vaccine Development Targeting Immobilization Antigen of Ichthyophthirius multifiliis: A Computational Approach. **2023**, 29,	0
100	Mechano-cytoskeleton remodeling mechanism and molecular docking studies on nanosurface technology - Titania nanotube arrays.	0
99	One enzyme, many faces: urease is also canatoxin. 1-12	0
98	In Silico and In Vitro Antiviral Activity Evaluation of Prodigiosin from Serratia marcescens Against Enterovirus 71. **2022**, 51, 113-128	0
97	Homozygous GRHPR C.494G>A mutation is deleterious that causes early onset of nephrolithiasis in West Bengal, India. 9,	0
96	Synthesis, molecular docking, bio-evaluation and quantitative structure activity relationship of new chalcone derivatives as antioxidants. **2022**, 134814	0
95	Protein□protein interaction prediction methods: from docking-based to AI-based approaches.	0
94	Large scale peptide screening against main protease of SARS CoV -2.	0
93	In Silico functional and phylogenetic analyses of fungal immunomodulatory proteins of some edible mushrooms. **2022**, 12,	0
92	TMPRSS6 rs855791 polymorphism is associated with iron deficiency in a cohort of Sri Lankan pregnant women. **2022**, 23,	0
91	In Silico Comparative Exploration of Allergens of Periplaneta Americana, Blattella Germanica and Phoenix Dactylifera for the Diagnosis of Patients Suffering from IgE-Mediated Allergic Respiratory Diseases. **2022**, 27, 8740	0
90	ADMET profiling and molecular docking of potential antimicrobial peptides previously isolated from African catfish, Clarias gariepinus. 9,	0
89	Improved docking of peptides and small molecules in iMOLSDOCK. **2023**, 29,	1

88	Emergence of a unique SARS-CoV-2 Delta sub-cluster harboring a constellation of co-appearing non-Spike mutations.	0
87	Ursolic acid and rosmarinic acid ameliorate alterations in hippocampal neurogenesis and social memory induced by amyloid beta in mouse model of Alzheimer disease. 13,	0
86	Molecular characterization of glutor-GLUT interaction and prediction of glutor drug-likeness: implications for its utility as an antineoplastic agent. 1-12	0
85	In vitro anti-Leishmania activity of new isomeric cobalt(II)complexes and in silico insights: Mitochondria impairment and apoptosis-like cell death of the parasite. **2022**, 112088	0
84	SHP-1 tyrosine phosphatase binding to c-Src kinase phosphor-dependent conformations: A comparative structural framework. **2023**, 18, e0278448	0
83	Protein protein interfaces in molecular glue-induced ternary complexes: classification, characterization, and prediction.	0
82	Virtual screening of truncated single stranded DNA aptamers for Staphylococcal enterotoxin type A. 1-10	0
81	Design of a dual-function agent by fusing a designed anti-VEGF-A binder and CPG-2 enzyme. 1-8	0
80	In silico design of a promiscuous chimeric multi-epitope vaccine against Mycobacterium tuberculosis. **2023**,	0
79	Synthesis, spectroscopic, in vitro, in vivo biological evaluation, and in silico docking analysis of new meloxicam metal complexes.	0
78	Effect of proton ion concentration on the supramolecular interaction between phenoxazine and cyclodextrin. **2023**, 100229	0
77	An in silico reverse vaccinology approach to design a novel multiepitope peptide vaccine for non-small cell lung cancers. **2023**, 37, 101169	0
76	The formation of HuR/YB1 complex is required for the stabilization of target mRNA to promote myogenesis.	1
75	In silico peptide-based therapeutics against human colorectal cancer by the activation of TLR5 signaling pathways. **2023**, 29,	0
74	Conformational and mechanical stability of the isolated large subunit of membrane-bound [NiFe]-hydrogenase from Cupriavidus necator. 13,	0
73	Identification of Potential Druggable Targets and Structure-Based Virtual Screening for Drug-like Molecules against the Shrimp Pathogen Enterocytozoon hepatopenaei. **2023**, 24, 1412	0
72	Interactions of Nanomaterials with Plant Pigments. **2023**, 93-131	0
71	Major royal jelly proteins elicited suppression of SARS-CoV-2 entry and replication with halting lung injury. **2023**, 228, 715-731	0

70	Purification, molecular docking and in vivo analyses of novel angiotensin-converting enzyme inhibitory peptides from protein hydrolysate of moth bean (Vigna aconitifolia (Jacq.) M□rechal) seeds. **2023**, 230, 123138	0
69	Carrying Temoporfin with Human Serum Albumin: A New Perspective for Photodynamic Application in Head and Neck Cancer. **2023**, 13, 68	2
68	Ultra-Short Cyclized □Boomerang Peptides: Structures, Interactions with Lipopolysaccharide, Antibiotic Potentiator and Wound Healing. **2023**, 24, 263	0
67	In silico Design of Multi-epitope Vaccines Targeting Iron-regulated lipoproteins of Staphylococcus aureus Using Immunoinformactics. **2022**, 52, 170-183	0
66	Dimerisation of the Yeast K+ Translocation Protein Trk1 Depends on the K+ Concentration. **2023**, 24, 398	0
65	Biofilm Inhibitory Activity of Actinomycete-Synthesized AgNPs with Low Cytotoxic Effect: Experimental and In Silico Study. **2023**, 11, 102	0
64	Design and Prediction of Aptamers Assisted by In Silico Methods. **2023**, 11, 356	0
63	Self-assembly of thiolato-bridged ester-functionalized Re(i)-based tetranuclear spiro-metallacyclophanes.	0
62	Immunoinformatics Approach to Design a Multi-Epitope Nanovaccine against Leishmania Parasite: Elicitation of Cellular Immune Responses. **2023**, 11, 304	0
61	Glycosylated and Succinylated Macrocyclic Lactones with Amyloid-□Aggregation-Regulating Activity from a Marine Bacillus sp.. **2023**, 21, 67	0
60	Artificial Intelligence and Machine Learning Technology Driven Modern Drug Discovery and Development. **2023**, 24, 2026	2
59	Recent advances in the area of plant-based anti-cancer drug discovery using computational approaches.	0
58	Proteome-wide Screening of Potential Vaccine Targets against Brucella melitensis. **2023**, 11, 263	0
57	Study of the Rv1417 and Rv2617c Membrane Proteins and Their Interactions with Nicotine Derivatives as Potential Inhibitors of Erp Virulence-Associated Factor in Mycobacterium tuberculosis: An In Silico Approach. **2023**, 13, 248	0
56	Applications of alignment-free sequence descriptors in the characterization of sequences in the age of big data: a case study with Zika virus, SARS, MERS, and COVID-19. **2023**, 359-390	0
55	Synthesis, Characterization, and Evaluation of Antimicrobial Efficacy of Reduced Graphene□nO□Copper Nanocomplex. **2023**, 12, 246	0
54	S-Adenosyl-l-Homocysteine Exhibits Potential Antiviral Activity Against Dengue Virus Serotype-3 (DENV-3) in Bangladesh: A Viroinformatics-Based Approach. **2023**, 17, 117793222311582	0
53	Exploring the structural basis to develop efficient multi-epitope vaccines displaying interaction with HLA and TAP and TLR3 molecules to prevent NIPAH infection, a global threat to human health. **2023**, 18, e0282580	0

52	The structure of the neurotoxin palytoxin determined by MicroED.	0
51	USP7 imparts partial EMT state in colorectal cancer by stabilizing the RNA helicase DDX3X and augmenting Wnt/β-catenin signaling. **2023**, 1870, 119446	0
50	AR13 peptide-conjugated liposomes improve the antitumor efficacy of doxorubicin in mice bearing C26 colon carcinoma; in silico, in vitro, and in vivo study. **2023**, 466, 116470	0
49	Tenofovir antiviral drug solubility enhancement with β-cyclodextrin inclusion complex and in silico study of potential inhibitor against SARS-CoV-2 main protease (Mpro). **2023**, 377, 121544	0
48	Immunogenic multi-epitope-based vaccine development to combat cyclosporiasis of immunocompromised patients applying computational biology method. **2023**, 248, 108497	0
47	Phylogenetic distribution, structural analysis and interaction of nucleotide excision repair proteins in cyanobacteria. **2023**, 126, 103487	0
46	In silico toxicity studies of traditional Chinese herbal medicine: A mini review. **2023**, 80, 102588	0
45	Synthesis of novel Schiff base metal complexes and their spectroscopic characterization, biological activity and molecular docking investigation. **2023**, 1282, 135161	0
44	Computational insight into stability-enhanced systems of anthocyanin with protein/peptide. **2023**, 6, 100168	0
43	Gold(III) assisted C-N bond dissociation; Synthesis, structure, photoluminescence, and pharmacokinetic studies of 1,10/- phenanthroline-gold(III)-N-heterocyclic carbene. **2023**, 1285, 135442	0
42	Deciphering the mechanism of resistance by novel double mutations in pncA in Mycobacterium tuberculosis using protein structural graphs (PSG) and structural bioinformatic approaches. **2023**, 154, 106599	0
41	In-silico selection employing rigid–docking and molecular–dynamic simulation in selecting DNA aptamers against androgen receptor. **2023**, 18,	0
40	A novel heterozygote allele in caprine melanocortin 1 receptor (MC1R) gene: an association with heat stress traits. **2023**, 55,	0
39	An engineered miRNA PS-OMe miR130 inhibits acute lung injury by targeting eCIRP in sepsis. **2023**, 29,	0
38	Classification of GTP-dependent K-Ras4B active and inactive conformational states. **2023**, 158, 091104	0
37	Vitexin isolated from Acanthus ilicifolius L. leaf enhances GLUT-4 translocation in experimental diabetic rats.	0
36	Production of a Fungal Punicalagin-Degrading Enzyme by Solid-State Fermentation: Studies of Purification and Characterization. **2023**, 12, 903	0
35	A guide to current methodology and usage of reverse vaccinology towardsin silicovaccine discovery. **2023**, 47,	0

34	Synthesis and Antiaggregant and Anticoagulant Activity of Amino-Acid Salts and Computer Simulation of the Interaction of Their Structures with the Surface of Cyclooxygenase. **2023**, 56, 1451-1456	0
33	Molecular Dynamic Simulations Unravel the Underlying Impact of Missense Mutation in Autoimmunity Gene PTPN22 on Predisposition to Rheumatoid Arthritis. **2023**, 43, 121-132	0
32	Designing multi-epitope vaccine against important colorectal cancer (CRC) associated pathogens based on immunoinformatics approach. **2023**, 24,	0
31	Molecular Docking and ADMET Study of Spice-Derived Potential Phytochemicals against Human DNA Topoisomerase III Alpha. **2023**, 407,	0
30	Tumor Necrosis Factor Family Members and Myocardial Ischemia-Reperfusion Injury: State of the Art and Therapeutic Implications. **2023**, 24, 4606	0
29	Docking strategies. **2023**, 243-258	0
28	Comparison of the DNA-binding interactions of 5-hydroxymethylfurfural and its synthesized derivative, 5, 5[oxy-bis(methylene)]bis-2-furfural: experimental, DFT and docking studies. **2023**, 17,	0
27	Immunoselective progression of a multi-epitope-based subunit vaccine candidate to convey protection against the parasite Onchocerca lupi. **2023**, 38, 101209	0
26	In Silico Methodologies to Improve Antioxidants Characterization from Marine Organisms. **2023**, 12, 710	0
25	A Comparative Study of the Inhibitory Action of Berberine Derivatives on the Recombinant Protein FtsZ of E. coli. **2023**, 24, 5674	0
24	Mitochondrial Haemoglobin Is Upregulated with Hypoxia in Skeletal Muscle and Has a Conserved Interaction with ATP Synthase and Inhibitory Factor 1. **2023**, 12, 912	0
23	Targeting Ras-binding domain of ELMO1 by computational nanobody design. **2023**, 6,	0
22	Discrete Molecular Aggregates Based on ZnII and SbIII/V Ions Displaying Efficient Antibacterial and Antioxidant Properties. **2023**, 62, 5237-5247	0
21	CM2D3: Furnishing the Human Interactome with Structural Models of Protein Complexes Derived by Comparative Modeling and Docking. **2023**, 168055	0
20	Molecular encapsulation of nortriptyline in the cyclodextrin cavity: In-vitro cytotoxic potential against MCF-7 cell line.	0
19	In silico designing of a novel polyvalent multi-subunit peptide vaccine leveraging cross-immunity against human visceral and cutaneous leishmaniasis: an immunoinformatics-based approach. **2023**, 29,	0
18	Effect of cyclodextrin on benzophenones and its impact on UVR filtration of cotton fabric through guest absorber host enhancer mechanism. **2023**, 103, 131-145	0
17	An In-depth Genomic Investigation to Design a Multi-Epitope Based Vaccine against Brucellosis.	0

16	Bovine serum albumin prevents human hemoglobin aggregation and retains its chaperone-like activity. 1-16	0
15	Cancer Therapeutics: Structure-Based Drug Design of Inhibitors for a Novel Angiogenic Growth Factor. **2023**, 18, 72-88	0
14	Early cellular events and potential regulators of cellulase induction in Penicillium janthinellum NCIM 1366. **2023**, 13,	0
13	DNA Binding and Cleavage, Stopped-Flow Kinetic, Mechanistic, and Molecular Docking Studies of Cationic Ruthenium(II) Nitrosyl Complexes Containing N_2S_4 Core. **2023**, 28, 3028	0
12	Identification and Biological Evaluation of a Water-Soluble Fullerene Nanomaterial as BTK Kinase Inhibitor. Volume 18, 1709-1724	0
11	Investigation of Peptidoglycan-Associated Lipoprotein of Acinetobacter baumannii and Its Interaction with Fibronectin To Find Its Therapeutic Potential.	0
10	Biophysical and computational approaches to study ternary complexes: A 'cooperative relationship' to rationalize targeted protein degradation.	0
9	Repurposing immune boosting and anti-viral efficacy of Parkia bioactive entities as multi-target directed therapeutic approach for SARS-CoV-2: exploration of lead drugs by drug likeness, molecular docking and molecular dynamics simulation methods. 1-39	0
8	Mechanism of sphingolipid homeostasis revealed by structural analysis of Arabidopsis SPT-ORM1 complex. **2023**, 9,	0
7	Insights on adsorption properties of a DNA base, guanine on nano metal cages (Ag24/Au24/Cu24): DFT, SERS, NCI and solvent effects. **2023**, 1285, 135541	0
6	Immunoinformatics approach to design next-generation epitope-based peptide vaccine against Peste des Petits Ruminants Virus (PPRV). **2023**,	0
5	Elucidation of conserved multi-epitope vaccine against Leishmania donovani using reverse vaccinology. 1-14	0
4	Integrated Omics approach for Prediction of Operons like gene clusters in plants: Tools, Techniques, and Future aspects. **2023**, 947-954	0
3	A subunit vaccine against pneumonia: targeting Streptococcus pneumoniae and Klebsiella pneumoniae. **2023**, 12,	0
2	An in silico approach for prediction of B cell and T cell epitope candidates against Chikungunya virus. 1-12	0
1	The Diagnostic Potential of RNA Aptamers against the NS1 Protein of Dengue Virus Serotype 2. **2023**, 12, 722	0