Bruno O Villoutreix

List of Publications by Year
in descending order

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221 papers	9,172 citations	36303 51 h-index	58581 82 g-index
239 all docs	239 docs citations	239 times ranked	10334 citing authors

#	Article	IF	Citations
1	Regulation of Blood Coagulation by the Protein C Anticoagulant Pathway. Arteriosclerosis, Thrombosis, and Vascular Biology, 2005, 25, 1311-1320.	2.4	268
2	Druggable pockets and binding site centric chemical space: a paradigm shift in drug discovery. Drug Discovery Today, 2010, 15, 656-667.	6.4	249
3	The anticoagulant protein C pathway. FEBS Letters, 2005, 579, 3310-3316.	2.8	239
4	FAF-Drugs3: a web server for compound property calculation and chemical library design. Nucleic Acids Research, 2015, 43, W200-W207.	14.5	237
5	FAF-Drugs4: free ADME-tox filtering computations for chemical biology and early stages drug discovery. Bioinformatics, 2017, 33, 3658-3660.	4.1	230
6	FAF-Drugs2: Free ADME/tox filtering tool to assist drug discovery and chemical biology projects. BMC Bioinformatics, 2008, 9, 396.	2.6	221
7	Toward in silico structure-based ADMET prediction in drug discovery. Drug Discovery Today, 2012, 17, 44-55.	6.4	220
8	Rationalizing the chemical space of proteinâ€“protein interaction inhibitors. Drug Discovery Today, 2010, 15, 220-229.	6.4	185
9	Complement inhibitor C4b-binding proteinâ€”friend or foe in the innate immune system?. Molecular Immunology, 2004, 40, 1333-1346.	2.2	170
10	Mutations in components of complement influence the outcome of Factor I-associated atypical hemolytic uremic syndrome. Kidney International, 2010, 77, 339-349.	5.2	163
11	A Novel Interaction of Outer Membrane Protein A with C4b Binding Protein Mediates Serum Resistance of Escherichia coli K1. Journal of Immunology, 2002, 169, 6352-6360.	0.8	159
12	MTiOpenScreen: a web server for structure-based virtual screening. Nucleic Acids Research, 2015, 43, W448-W454.	14.5	159
13	3-Dimensional structure of membrane-bound coagulation factor VIII: modeling of the factor VIII heterodimer within a 3-dimensional density map derived by electron crystallography. Blood, 2002, 99, 1215-1223.	1.4	154
14	Computational analysis of calculated physicochemical and ADMET properties of protein-protein interaction inhibitors. Scientific Reports, 2017, 7, 46277.	3.3	128
15	FAF-Drugs: free ADME/tox filtering of compound collections. Nucleic Acids Research, 2006, 34, W738-W744.	14.5	115
16	Structure-Based Virtual Ligand Screening: Recent Success Stories. Combinatorial Chemistry and High Throughput Screening, 2009, 12, 1000-1016.	1.1	114
17	Designing Focused Chemical Libraries Enriched in Protein-Protein Interaction Inhibitors using Machine-Learning Methods. PLoS Computational Biology, 2010, 6, e1000695.	3.2	110
18	A Formylated Hexapeptide Ligand Mimics the Ability of Wnt-5a to Impair Migration of Human Breast Epithelial Cells. Journal of Biological Chemistry, 2006, 281, 2740-2749.	3.4	107

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19	Fast Structure-Based Virtual Ligand Screening Combining FRED, DOCK, and Surflex. Journal of Medicinal Chemistry, 2005, 48, 6012-6022.	6.4	106
20	Free Resources to Assist Structure-Based Virtual Ligand Screening Experiments. Current Protein and Peptide Science, 2007, 8, 381-411.	1.4	104
21	MS-DOCK: Accurate multiple conformation generator and rigid docking protocol for multi-step virtual ligand screening. BMC Bioinformatics, 2008, 9, 184.	2.6	102
22	Theileria parasites secrete a prolyl isomerase to maintain host leukocyte transformation. Nature, 2015, 520, 378-382.	27.8	100
23	A Cluster of Positively Charged Amino Acids in the C4BP Î±-Chain Is Crucial for C4b Binding and Factor I Cofactor Function. Journal of Biological Chemistry, 1999, 274, 19237-19245.	3.4	98
24	Drugâ€Like Proteinï£¿Protein Interaction Modulators: Challenges and Opportunities for Drug Discovery and Chemical Biology. Molecular Informatics, 2014, 33, 414-437.	2.5	93
25	iPPI-DB: a manually curated and interactive database of small non-peptide inhibitors of proteinâ€“protein interactions. Drug Discovery Today, 2013, 18, 958-968.	6.4	91
26	Frog: a FRee Online druG 3D conformation generator. Nucleic Acids Research, 2007, 35, W568-W572.	14.5	86
27	Development of Novel Thiazolopyrimidines as CDC25B Phosphatase Inhibitors. ChemMedChem, 2009, 4, 633-648.	3.2	84
28	Proposed lipocalin fold for apolipoprotein M based on bioinformatics and site-directed mutagenesis. FEBS Letters, 2001, 499, 127-132.	2.8	83
29	Structural investigation of the A domains of human blood coagulation factor V by molecular modeling. Protein Science, 1998, 7, 1317-1325.	7.6	82
30	Computational investigations of hERG channel blockers: New insights and current predictive models. Advanced Drug Delivery Reviews, 2015, 86, 72-82.	13.7	82
31	RPBS: a web resource for structural bioinformatics. Nucleic Acids Research, 2005, 33, W44-W49.	14.5	81
32	The FAF-Drugs2 server: a multistep engine to prepare electronic chemical compound collections. Bioinformatics, 2011, 27, 2018-2020.	4.1	81
33	Virtual screening web servers: designing chemical probes and drug candidates in the cyberspace. Briefings in Bioinformatics, 2021, 22, 1790-1818.	6.5	81
34	Molecular recognition in the protein C anticoagulant pathway. Journal of Thrombosis and Haemostasis, 2003, 1, 1525-1534.	3.8	76
35	One hundred thousand mouse clicks down the road: selected online resources supporting drug discovery collected over a decade. Drug Discovery Today, 2013, 18, 1081-1089.	6.4	76
36	Human C4b-Binding Protein Has Overlapping, But Not Identical, Binding Sites for C4b and Streptococcal M Proteins. Journal of Immunology, 2000, 164, 5328-5336.	0.8	74

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37	In Silico Investigation of the New UK (B.1.1.7) and South African (501Y.V2) SARS-CoV-2 Variants with a Focus at the ACE2â€“Spike RBD Interface. International Journal of Molecular Sciences, 2021, 22, 1695.	4.1	72
38	A structural model for the prostate disease marker, human prostateâ€specific antigen. Protein Science, 1994, 3, 2033-2044.	7.6	71
39	How to choose relevant multiple receptor conformations for virtual screening: a test case of Cdk2 and normal mode analysis. European Biophysics Journal, 2010, 39, 1365-1372.	2.2	68
40	Partial Glycosylation of Asn2181in Human Factor V as a Cause of Molecular and Functional Heterogeneity. Modulation of Glycosylation Efficiency by Mutagenesis of the Consensus Sequence for N-Linked Glycosylationâ€. Biochemistry, 1999, 38, 13584-13591.	2.5	64
41	A Leap into the Chemical Space of Protein-Protein Interaction Inhibitors. Current Pharmaceutical Design, 2012, 18, 4648-4667.	1.9	64
42	Antithrombin Phe229Leu: a new homozygous variant leading to spontaneous antithrombin polymerization in vivo associated with severe childhood thrombosis. Blood, 2003, 102, 919-925.	1.4	61
43	Determination and analysis of antigenic epitopes of prostate specific antigen (PSA) and human glandular kallikrein 2 (hK2) using synthetic peptides and computer modeling. Protein Science, 1998, 7, 259-269.	7.6	60
44	Ligand Efficiency Driven Design of New Inhibitors of Mycobacterium tuberculosis Transcriptional Repressor EthR Using Fragment Growing, Merging, and Linking Approaches. Journal of Medicinal Chemistry, 2014, 57, 4876-4888.	6.4	59
45	In Silico-In Vitro Screening of Protein-Protein Interactions: Towards the Next Generation of Therapeutics. Current Pharmaceutical Biotechnology, 2008, 9, 103-122.	1.6	59
46	Mutations in complement factor I as found in atypical hemolytic uremic syndrome lead to either altered secretion or altered function of factor I. European Journal of Immunology, 2010, 40, 172-185.	2.9	58
47	Pharmacogenomics of the cytochrome P450 2C family: impacts of amino acid variations on drug metabolism. Drug Discovery Today, 2017, 22, 366-376.	6.4	58
48	Calcium binding to tandem repeats of EGFâ€like modules. Expression and characterization of the EGFâ€like modules of human Notchâ€1 implicated in receptorâ€ligand interactions. Protein Science, 1997, 6, 2059-2071.	7.6	57
49	Established and Emerging Trends in Computational Drug Discovery in the Structural Genomics Era. Chemistry and Biology, 2012, 19, 29-41.	6.0	57
50	In silico design of low molecular weight proteinâ€“protein interaction inhibitors: Overall concept and recent advances. Progress in Biophysics and Molecular Biology, 2015, 119, 20-32.	2.9	56
51	Genetic, molecular and functional analyses of complement factor I deficiency. European Journal of Immunology, 2009, 39, 310-323.	2.9	53
52	Structural and Energetic Characteristics of the Heparin-binding Site in Antithrombotic Protein C. Journal of Biological Chemistry, 2001, 276, 24122-24128.	3.4	52
53	PCE: web tools to compute protein continuum electrostatics. Nucleic Acids Research, 2005, 33, W372-W375.	14.5	51
54	A Cell-Penetrating Peptide Targeting AAC-11 Specifically Induces Cancer Cells Death. Cancer Research, 2016, 76, 5479-5490.	0.9	51

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55	Design of proteinâ€“membrane interaction inhibitors by virtual ligand screening, proof of concept with the C2 domain of factor V. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 12697-12702.	7.1	50
56	A Novel Non-Synonymous Polymorphism (p.Arg240His) in C4b-Binding Protein Is Associated with Atypical Hemolytic Uremic Syndrome and Leads to Impaired Alternative Pathway Cofactor Activity. Journal of Immunology, 2008, 180, 6385-6391.	0.8	50
57	Anti-Factor B Antibodies and Acute Postinfectious GN in Children. Journal of the American Society of Nephrology: JASN, 2020, 31, 829-840.	6.1	50
58	iPPI-DB: an online database of modulators of proteinâ€“protein interactions. Nucleic Acids Research, 2016, 44, D542-D547.	14.5	49
59	Proposed structural models of the prothrombinase (FXa-FVa) complex. Proteins: Structure, Function and Bioinformatics, 2006, 63, 440-450.	2.6	47
60	Receptor-Based Computational Screening of Compound Databases: The Main Docking-Scoring Engines. Current Protein and Peptide Science, 2006, 7, 369-393.	1.4	47
61	Secondary Substrate-binding Exosite in the Serine Protease Domain of Activated Protein C Important for Cleavage at Arg-506 but Not at Arg-306 in Factor Va. Journal of Biological Chemistry, 2001, 276, 23105-23108.	3.4	45
62	Structure-based virtual ligand screening with LigandFit: Pose prediction and enrichment of compound collections. Proteins: Structure, Function and Bioinformatics, 2007, 68, 712-725.	2.6	45
63	AMMOS: Automated Molecular Mechanics Optimization tool for in silico Screening. BMC Bioinformatics, 2008, 9, 438.	2.6	44
64	Receptor-Based Virtual Ligand Screening for the Identification of Novel CDC25 Phosphatase Inhibitors. Journal of Chemical Information and Modeling, 2008, 48, 157-165.	5.4	43
65	Structural basis for type I and type II deficiencies of antithrombotic plasma protein C: Patterns revealed by three-dimensional molecular modelling of mutations of the protease domain. Proteins: Structure, Function and Bioinformatics, 1994, 18, 367-380.	2.6	42
66	The Kaposi's sarcoma-associated herpesvirus complement control protein (KCP) binds to heparin and cell surfaces via positively charged amino acids in CCP1â€“2. Molecular Immunology, 2006, 43, 1665-1675.	2.2	42
67	Novel Organic Proteasome Inhibitors Identified by Virtual and in Vitro Screening. Journal of Medicinal Chemistry, 2010, 53, 509-513.	6.4	42
68	Mutations within the cyclooxygenase-1 gene in aspirin non-responders with recurrence of stroke. Thrombosis Research, 2003, 112, 275-283.	1.7	41
69	Structure-based drug repositioning over the human TMPRSS2 protease domain: search for chemical probes able to repress SARS-CoV-2 Spike protein cleavages. European Journal of Pharmaceutical Sciences, 2020, 153, 105495.	4.0	40
70	Structural investigation of C4b-binding protein by molecular modeling: Localization of putative binding sites. , 1998, 31, 391-405.		39
71	DG-AMMOS: A New tool to generate 3D conformation of small molecules using Distance Geometry and Automated Molecular Mechanics Optimization for in silico Screening. BMC Chemical Biology, 2009, 9, 6.	1.6	38
72	Targeting the Proangiogenic VEGF-VEGFR Protein-Protein Interface with Drug-like Compounds by In Silico and InÂVitro Screening. Chemistry and Biology, 2011, 18, 1631-1639.	6.0	38

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73	Which Three-Dimensional Characteristics Make Efficient Inhibitors of Proteinâ€“Protein Interactions?. Journal of Chemical Information and Modeling, 2014, 54, 3067-3079.	5.4	38
74	Defining the Factor Xa-binding Site on Factor Va by Site-directed Glycosylation. Journal of Biological Chemistry, 2002, 277, 50022-50029.	3.4	36
75	Two Clusters of Charged Residues Located in the Electropositive Face of the Von Willebrand Factor A1 Domain Are Essential for Heparin Bindingâ€. Biochemistry, 2002, 41, 6668-6678.	2.5	36
76	A theoretical model for the Gla-TSR-EGF-1 region of the anticoagulant cofactor protein S: from biostructural pathology to species-specific cofactor activity. Journal of Computer-Aided Molecular Design, 1997, 11, 293-304.	2.9	35
77	Amino Acid Residues in Thrombin-sensitive Region and First Epidermal Growth Factor Domain of Vitamin K-dependent Protein S Determining Specificity of the Activated Protein C Cofactor Function. Journal of Biological Chemistry, 1998, 273, 27449-27458.	3.4	35
78	The Kaposi's Sarcoma-associated Herpesvirus Complement Control Protein Mimics Human Molecular Mechanisms for Inhibition of the Complement System. Journal of Biological Chemistry, 2004, 279, 45093-45101.	3.4	35
79	Discovery of novel inhibitors of vascular endothelial growth factor-Aâ€“Neuropilin-1 interaction by structure-based virtual screening. Bioorganic and Medicinal Chemistry, 2014, 22, 4042-4048.	3.0	35
80	Probing the activation of protein C by the thrombin-thrombomodulin complex using structural analysis, site-directed mutagenesis, and computer modeling. Proteins: Structure, Function and Bioinformatics, 1999, 35, 218-234.	2.6	34
81	MED-SuMoLig:â€‰A New Ligand-Based Screening Tool for Efficient Scaffold Hopping. Journal of Chemical Information and Modeling, 2007, 47, 1097-1110.	5.4	34
82	Breast Cancer Targeting through Inhibition of the Endoplasmic Reticulum-Based Apoptosis Regulator Nrh/BCL2L10. Cancer Research, 2018, 78, 1404-1417.	0.9	34
83	The Î³-carboxyglutamic acid domain of anticoagulant protein S is involved in activated protein C cofactor activity, independently of phospholipid binding. Blood, 2005, 105, 122-130.	1.4	33
84	In Silico Prediction of Aqueous Solubility: A Multimodel Protocol Based on Chemical Similarity. Molecular Pharmaceutics, 2012, 9, 3127-3135.	4.6	33
85	Structural investigation of the alphaâ€1â€antichymotrypsin: Prostateâ€specific antigen complex by comparative model building. Protein Science, 1996, 5, 836-851.	7.6	32
86	SHBG region of the anticoagulant cofactor protein S: Secondary structure prediction, circular dichroism spectroscopy, and analysis of naturally occurring mutations. , 1997, 29, 478-491.		32
87	Positively charged amino acids at the interface between Î±-chain CCP1 and CCP2 of C4BP are required for regulation of the classical C3-convertase. Molecular Immunology, 2000, 37, 445-453.	2.2	31
88	Mutations in Î±-Chain of C4BP That Selectively Affect Its Factor I Cofactor Function. Journal of Biological Chemistry, 2003, 278, 43437-43442.	3.4	31
89	Factor V New Brunswick: Ala221Val associated with FV deficiency reproduced in vitro and functionally characterized. Blood, 2003, 102, 1316-1322.	1.4	31
90	Structural stability and heat-induced conformational change of two complement inhibitors: C4b-binding protein and factor H. Protein Science, 2004, 13, 1356-1364.	7.6	31

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91	Molecular models of the procoagulant Factor VIIIa-Factor IXa complex. Journal of Thrombosis and Haemostasis, 2005, 3, 2044-2056.	3.8	31
92	Acute genetic ablation of pendrin lowers blood pressure in mice. Nephrology Dialysis Transplantation, 2017, 32, gfw393.	0.7	31
93	Molecular Models for the two Discoidin Domains of Human Blood Coagulation Factor V. Journal of Molecular Modeling, 1998, 4, 268-275.	1.8	30
94	Involvement of Lys 62[217] and Lys 63[218] of Human Anticoagulant Protein C in Heparin Stimulation of Inhibition by the Protein C Inhibitor. Thrombosis and Haemostasis, 1999, 82, 72-79.	3.4	29
95	1,2,4-Triazole derivatives as transient inactivators of kallikreins involved in skin diseases. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 4547-4551.	2.2	29
96	Fr-PPIChem: An Academic Compound Library Dedicated to Proteinâ€“Protein Interactions. ACS Chemical Biology, 2020, 15, 1566-1574.	3.4	29
97	Analysis of Binding Sites on Complement Factor I That Are Required for Its Activity. Journal of Biological Chemistry, 2010, 285, 6235-6245.	3.4	28
98	A novel druglike spleen tyrosine kinase binder prevents anaphylactic shock when administered orally. Journal of Allergy and Clinical Immunology, 2008, 122, 188-194.e3.	2.9	27
99	Genetic polymorphisms associated with increased risk of developing chronic myelogenous leukemia. Oncotarget, 2015, 6, 36269-36277.	1.8	27
100	Integrated structure- and ligand-based in silico approach to predict inhibition of cytochrome P450 2D6. Bioinformatics, 2015, 31, 3930-3937.	4.1	27
101	Combining Ligand- and Structure-Based Methods in Drug Design Projects. Current Computer-Aided Drug Design, 2008, 4, 250-258.	1.2	27
102	Functions of human complement inhibitor C4b-binding protein in relation to its structure. Archivum Immunologiae Et Therapiae Experimentalis, 2004, 52, 83-95.	2.3	27
103	Three-dimensional model of the SHBG-like region of anticoagulant protein S: New structure-function insights. Proteins: Structure, Function and Bioinformatics, 2001, 43, 203-216.	2.6	26
104	MED-3DMC: A new tool to generate 3D conformation ensembles of small molecules with a Monte Carlo sampling of the conformational space. European Journal of Medicinal Chemistry, 2009, 44, 1405-1409.	5.5	26
105	Editorial [Hot topic: Structure-Based Virtual Screening (Guest Editor: Walter Filgueira De Azevedo) Tj ETQq1 1 0.784314 rgBT /Overlo	2.1	26
106	DNA damage-induced nuclear translocation of Apaf-1 is mediated by nucleoporin Nup107. Cell Cycle, 2015, 14, 1242-1251.	2.6	26
107	Pan-assay interference compounds (PAINS) that may not be too painful for chemical biology projects. Drug Discovery Today, 2017, 22, 1131-1133.	6.4	26
108	Prevention of COVID-19 by drug repurposing: rationale from drugs prescribed for mental disorders. Drug Discovery Today, 2020, 25, 1287-1290.	6.4	26

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109	Defining the structure of membraneâ€bound human blood coagulation factor Va. Journal of Thrombosis and Haemostasis, 2008, 6, 76-82.	3.8	25
110	1,2,4-Oxadiazoles Identified by Virtual Screening and their Non-Covalent Inhibition of the Human 20S Proteasome. Current Medicinal Chemistry, 2013, 20, 2351-2362.	2.4	25
111	Online structure-based screening of purchasable approved drugs and natural compounds: retrospective examples of drug repositioning on cancer targets. Oncotarget, 2018, 9, 32346-32361.	1.8	25
112	Analysis of protein missense alterations by combining sequenceâ€•and structureâ€based methods. Molecular Genetics & Genomic Medicine, 2020, 8, e1166.	1.2	25
113	ELA/APELA precursor cleaved by furin displays tumor suppressor function in renal cell carcinoma through mTORC1 activation. JCI Insight, 2020, 5, .	5.0	25
114	Structural Requirements of Anticoagulant Protein S for Its Binding to the Complement Regulator C4b-binding Protein. Journal of Biological Chemistry, 2002, 277, 15099-15106.	3.4	24
115	Functional characterization of two novel non-synonymous alterations in CD46 and a Q950H change in factor H found in atypical hemolytic uremic syndrome patients. Molecular Immunology, 2015, 65, 367-376.	2.2	24
116	AMMOS2: a web server for proteinâ€“ligandâ€“water complexes refinement via molecular mechanics. Nucleic Acids Research, 2017, 45, W350-W355.	14.5	24
117	Insights into molecular mechanisms of drug metabolism dysfunction of human CYP2C9*30. PLoS ONE, 2018, 13, e0197249.	2.5	24
118	Quaternary Structure of the HSC70 Cochaperone HIP. Biochemistry, 2000, 39, 307-315.	2.5	23
119	Characterization of the Complement Inhibitory Function of Rhesus Rhadinovirus Complement Control Protein (RCP). Journal of Biological Chemistry, 2009, 284, 505-514.	3.4	23
120	Tyrosine Kinase Syk Non-Enzymatic Inhibitors and Potential Anti-Allergic Drug-Like Compounds Discovered by Virtual and In Vitro Screening. PLoS ONE, 2011, 6, e21117.	2.5	23
121	Rigorous sampling of docking poses unveils binding hypothesis for the halogenated ligands of L-type Amino acid Transporter 1 (LAT1). Scientific Reports, 2019, 9, 15061.	3.3	23
122	In Silico Mechanistic Profiling to Probe Small Molecule Binding to Sulfotransferases. PLoS ONE, 2013, 8, e73587.	2.5	23
123	Structural prediction and analysis of endothelial cell protein C/activated protein C receptor. Protein Engineering, Design and Selection, 1999, 12, 833-840.	2.1	22
124	Rational design of small molecules targeting the C2 domain of coagulation factor VIII. Blood, 2014, 123, 113-120.	1.4	22
125	Prothrombin deficiency caused by compound heterozygosity for two novel mutations in the prothrombin gene associated with a bleeding tendency. Thrombosis and Haemostasis, 2006, 95, 195-198.	3.4	21
126	New non-hydroxamic ADAMTS-5 inhibitors based on the 1,2,4-triazole-3-thiol scaffold. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 6213-6216.	2.2	21

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127	Discoidin Domains as Emerging Therapeutic Targets. Trends in Pharmacological Sciences, 2016, 37, 641-659.	8.7	21
128	Analysis of Protein S C4b-Binding Protein Interactions by Homology Modeling and Inhibitory Antibodies. Biochemistry, 1994, 33, 11073-11078.	2.5	20
129	Structural analysis of an anti-estradiol antibody. Molecular Immunology, 1997, 34, 1215-1226.	2.2	20
130	Activated Protein Câ^'Protein C Inhibitor Complex Formation:Â Characterization of a Neoepitope Provides Evidence for Extensive Insertion of the Reactive Center Loop. Biochemistry, 2000, 39, 15713-15720.	2.5	20
131	Analysis of solvent-exposed and buried co-crystallized ligands: a case study to support the design of novel proteinâ€“protein interaction inhibitors. Drug Discovery Today, 2019, 24, 551-559.	6.4	20
132	Interspecies Loop Grafting in the Protease Domain of Human Protein C Yielding Enhanced Catalytic and Anticoagulant Activity. Thrombosis and Haemostasis, 1999, 82, 1078-1087.	3.4	20
133	Topological Studies of the Amino Terminal Modules of Vitamin K-dependent Protein S Using Monoclonal Antibody Epitope Mapping and Molecular Modeling. Thrombosis and Haemostasis, 1998, 80, 798-804.	3.4	20
134	Zebrafish ProVEGF-C Expression, Proteolytic Processing and Inhibitory Effect of Unprocessed ProVEGF-C during Fin Regeneration. PLoS ONE, 2010, 5, e11438.	2.5	20
135	The complement regulator C4b-binding protein analyzed by molecular modeling, bioinformatics and computer-aided experimental design. Immunopharmacology, 1999, 42, 121-134.	2.0	19
136	Localization of a Hydrophobic Binding Site for Anticoagulant Protein S on the Î²-Chain of Complement Regulator C4b-binding Protein. Journal of Biological Chemistry, 2001, 276, 4330-4337.	3.4	19
137	Molecular Characterization of the Interaction between Porins of Neisseria gonorrhoeae and C4b-Binding Protein. Journal of Immunology, 2007, 179, 540-547.	0.8	19
138	Mapping of the Factor Xa Binding Site on Factor Va by Site-directed Mutagenesis. Journal of Biological Chemistry, 2008, 283, 20805-20812.	3.4	19
139	Design and synthesis of novel bis-thiazolone derivatives as micromolar CDC25 phosphatase inhibitors: Effect of dimerisation on phosphatase inhibition. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 7345-7350.	2.2	19
140	Identification by in silico and inÂvitro screenings of small organic molecules acting as reversible inhibitors of kallikreins. European Journal of Medicinal Chemistry, 2013, 70, 661-668.	5.5	19
141	The C4b-binding proteinâ€“protein S interaction is hydrophobic in nature. BBA - Proteins and Proteomics, 1998, 1388, 181-189.	2.1	18
142	Structural Bioinformatics: Methods, Concepts and Applications to Blood Coagulation Proteins. Current Protein and Peptide Science, 2002, 3, 341-364.	1.4	18
143	Theoretical and Experimental Study of the D2194G Mutation in the C2 Domain of Coagulation Factor V. Biophysical Journal, 2004, 86, 488-498.	0.5	18
144	Kaposi's sarcoma-associated herpes virus complement control protein: KCP â€“ complement inhibition and more. Molecular Immunology, 2007, 44, 11-22.	2.2	18

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145	Insights into an Original Pocket-Ligand Pair Classification: A Promising Tool for Ligand Profile Prediction. PLoS ONE, 2013, 8, e63730.	2.5	18
146	Resources and computational strategies to advance small molecule SARS-CoV-2 discovery: Lessons from the pandemic and preparing for future health crises. Computational and Structural Biotechnology Journal, 2021, 19, 2537-2548.	4.1	18
147	In Vitro Characterisation of Two Naturally Occurring Mutations in the Thrombin-sensitive Region of Anticoagulant Protein S. Thrombosis and Haemostasis, 1999, 82, 1627-1633.	3.4	17
148	Tracking Structural Features Leading to Resistance of Activated Protein C to Î±1-antitrypsinâ€. Biochemistry, 2000, 39, 2853-2860.	2.5	17
149	Screening Outside the Catalytic Site: Inhibition of Macromolecular Interactions Through Structure-Based Virtual Ligand Screening Experiments. The Open Biochemistry Journal, 2008, 2, 29-37.	0.5	17
150	Characterization and Structural Impact of Five Novel PROS1 Mutations in Eleven Protein S-deficient Families. Thrombosis and Haemostasis, 2001, 86, 1392-1399.	3.4	16
151	A Free Web-Based Protocol to Assist Structure-Based Virtual Screening Experiments. International Journal of Molecular Sciences, 2019, 20, 4648.	4.1	16
152	Structural modeling and electrostatic properties of aspartate transcarbamylase fromSaccharomyces cerevisiae. Proteins: Structure, Function and Bioinformatics, 1994, 19, 230-243.	2.6	15
153	Comparative modeling of the three CP modules of the ÃŸ-chain of C4BP and evaluation of potential sites of interaction with protein S. Protein Engineering, Design and Selection, 1995, 8, 1253-1258.	2.1	15
154	Noonan syndrome type I with PTPN11 3 bp deletion: Structureâ€“function implications. Proteins: Structure, Function and Bioinformatics, 2005, 58, 7-13.	2.6	15
155	Tensin2 reduces intracellular phosphatidylinositol 3,4,5-trisphosphate levels at the plasma membrane. Biochemical and Biophysical Research Communications, 2010, 399, 396-401.	2.1	15
156	Strategies in the Search for New Lead Compounds or Original Working Hypotheses. , 2015, , 73-99.		15
157	In silico model of the human ClC-Kb chloride channel: pore mapping, biostructural pathology and drug screening. Scientific Reports, 2017, 7, 7249.	3.3	15
158	The N-terminal Epidermal Growth Factor-like Domain of Coagulation Factor IX. Journal of Biological Chemistry, 2002, 277, 35616-35624.	3.4	14
159	Altered inactivation pathway of factor Va by activated protein C in the presence of heparin. FEBS Journal, 2004, 271, 2724-2736.	0.2	14
160	In silico studies of blood coagulation proteins: from mosaic proteases to nonenzymatic cofactor inhibitors. Current Opinion in Structural Biology, 2010, 20, 168-179.	5.7	14
161	Identification of novel small molecule inhibitors of activated protein C. Thrombosis Research, 2014, 133, 1105-1114.	1.7	14
162	Fast Rescoring Protocols to Improve the Performance of Structure-Based Virtual Screening Performed on Proteinâ€“Protein Interfaces. Journal of Chemical Information and Modeling, 2020, 60, 3910-3934.	5.4	14

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163	Molecular Model for the C-type Lectin Domain of Human Thrombomodulin. Journal of Molecular Modeling, 1998, 4, 310-322.	1.8	13
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