Bruno O Villoutreix

List of Publications by Year in Descending Order

Source: https://exaly.com/author-pdf/5485759/bruno-o-villoutreix-publications-by-year.pdf

Version: 2024-04-10

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

208 46 7,409 74 h-index g-index citations papers 6.1 6.11 8,223 239 avg, IF L-index ext. citations ext. papers

#	Paper	IF	Citations
208	Machine learning-driven identification of drugs inhibiting cytochrome P450 2C9 <i>PLoS</i> Computational Biology, 2022 , 18, e1009820	5	2
207	A new ChEMBL dataset for the similarity-based target fishing engine FastTargetPred: Annotation of an exhaustive list of linear tetrapeptides <i>Data in Brief</i> , 2022 , 42, 108159	1.2	
206	The first laminin G-like domain of protein S is essential for binding and activation of Tyro3 receptor and intracellular signalling <i>Biochemistry and Biophysics Reports</i> , 2022 , 30, 101263	2.2	
205	Antihistamine and cationic amphiphilic drugs, old molecules as new tools against the COVID-19?. <i>Medical Hypotheses</i> , 2021 , 148, 110508	3.8	9
204	Chemoinformatic Analysis of Psychotropic and Antihistaminic Drugs in the Light of Experimental Anti-SARS-CoV-2 Activities. <i>Advances and Applications in Bioinformatics and Chemistry</i> , 2021 , 14, 71-85	1.5	7
203	Role of Gly197 in the structure and function of protein C. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2021 , 1865, 129892	4	
202	Virtual screening web servers: designing chemical probes and drug candidates in the cyberspace. <i>Briefings in Bioinformatics</i> , 2021 , 22, 1790-1818	13.4	36
201	Resources and computational strategies to advance small molecule SARS-CoV-2 discovery: Lessons from the pandemic and preparing for future health crises. <i>Computational and Structural Biotechnology Journal</i> , 2021 , 19, 2537-2548	6.8	9
200	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 ACE2-Spike RBD Interface. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	54
199	PAK1-Dependent Antitumor Effect of AAC-11-Derived Peptides on Sary Syndrome Malignant CD4 T Lymphocytes. <i>Journal of Investigative Dermatology</i> , 2021 , 141, 2261-2271.e5	4.3	0
198	Anti-Factor B Antibodies and Acute Postinfectious GN in Children. <i>Journal of the American Society of Nephrology: JASN</i> , 2020 , 31, 829-840	12.7	20
197	FastTargetPred: a program enabling the fast prediction of putative protein targets for input chemical databases. <i>Bioinformatics</i> , 2020 , 36, 4225-4226	7.2	3
196	Gly197Arg mutation in protein C causes recurrent thrombosis in a heterozygous carrier. <i>Journal of Thrombosis and Haemostasis</i> , 2020 , 18, 1141-1153	15.4	2
195	Thr90Ser Mutation in Antithrombin is Associated with Recurrent Thrombosis in a Heterozygous Carrier. <i>Thrombosis and Haemostasis</i> , 2020 , 120, 1045-1055	7	2
194	Analysis of protein missense alterations by combining sequence- and structure-based methods. <i>Molecular Genetics & Denomic Medicine</i> , 2020 , 8, e1166	2.3	16
193	ELA/APELA precursor cleaved by furin displays tumor suppressor function in renal cell carcinoma through mTORC1 activation. <i>JCI Insight</i> , 2020 , 5,	9.9	15
192	Demystifying the Molecular Basis of Pyrazoloquinolinones Recognition at the Extracellular #+/B-Interface of the GABA Receptor by Molecular Modeling. <i>Frontiers in Pharmacology</i> , 2020 , 11, 561834	5.6	1

191	Fast Rescoring Protocols to Improve the Performance of Structure-Based Virtual Screening Performed on Protein-Protein Interfaces. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 3910	-3934	6
190	Structure-based drug repositioning over the human TMPRSS2 protease domain: search for chemical probes able to repress SARS-CoV-2 Spike protein cleavages. <i>European Journal of Pharmaceutical Sciences</i> , 2020 , 153, 105495	5.1	28
189	Ile73Asn mutation in protein C introduces a new N-linked glycosylation site on the first EGF-domain of protein C and causes thrombosis. <i>Haematologica</i> , 2020 , 105, 1712-1722	6.6	4
188	Fr-PPIChem: An Academic Compound Library Dedicated to Protein-Protein Interactions. <i>ACS Chemical Biology</i> , 2020 , 15, 1566-1574	4.9	13
187	A Free Web-Based Protocol to Assist Structure-Based Virtual Screening Experiments. <i>International Journal of Molecular Sciences</i> , 2019 , 20,	6.3	10
186	Rigorous sampling of docking poses unveils binding hypothesis for the halogenated ligands of L-type Amino acid Transporter 1 (LAT1). <i>Scientific Reports</i> , 2019 , 9, 15061	4.9	13
185	Analysis of solvent-exposed and buried co-crystallized ligands: a case study to support the design of novel protein-protein interaction inhibitors. <i>Drug Discovery Today</i> , 2019 , 24, 551-559	8.8	11
184	Breast Cancer Targeting through Inhibition of the Endoplasmic Reticulum-Based Apoptosis Regulator Nrh/BCL2L10. <i>Cancer Research</i> , 2018 , 78, 1404-1417	10.1	22
183	Expression and functional characterization of two natural heparin-binding site variants of antithrombin. <i>Journal of Thrombosis and Haemostasis</i> , 2018 , 16, 330-341	15.4	5
182	Insights into molecular mechanisms of drug metabolism dysfunction of human CYP2C9*30. <i>PLoS ONE</i> , 2018 , 13, e0197249	3.7	14
181	Online structure-based screening of purchasable approved drugs and natural compounds: retrospective examples of drug repositioning on cancer targets. <i>Oncotarget</i> , 2018 , 9, 32346-32361	3.3	15
180	Acute genetic ablation of pendrin lowers blood pressure in mice. <i>Nephrology Dialysis Transplantation</i> , 2017 , 32, 1137-1145	4.3	19
179	Computational Biology and Chemistry in MTi: Emphasis on the Prediction of Some ADMET Properties. <i>Molecular Informatics</i> , 2017 , 36, 1700008	3.8	2
178	Computational analysis of calculated physicochemical and ADMET properties of protein-protein interaction inhibitors. <i>Scientific Reports</i> , 2017 , 7, 46277	4.9	71
177	FAF-Drugs4: free ADME-tox filtering computations for chemical biology and early stages drug discovery. <i>Bioinformatics</i> , 2017 , 33, 3658-3660	7.2	141
176	In silico model of the human ClC-Kb chloride channel: pore mapping, biostructural pathology and drug screening. <i>Scientific Reports</i> , 2017 , 7, 7249	4.9	11
175	Identification of insulin-sensitizing molecules acting by disrupting the interaction between the Insulin Receptor and Grb14. <i>Scientific Reports</i> , 2017 , 7, 16901	4.9	3
174	AMMOS2: a web server for protein-ligand-water complexes refinement via molecular mechanics. <i>Nucleic Acids Research</i> , 2017 , 45, W350-W355	20.1	21

173	Pharmacogenomics of the cytochrome P450 2C family: impacts of amino acid variations on drug metabolism. <i>Drug Discovery Today</i> , 2017 , 22, 366-376	8.8	39
172	Gly74Ser mutation in protein C causes thrombosis due to a defect in protein S-dependent anticoagulant function. <i>Thrombosis and Haemostasis</i> , 2017 , 117, 1358-1369	7	5
171	Blockade of the malignant phenotype by Eubunit selective noncovalent inhibition of immuno- and constitutive proteasomes. <i>Oncotarget</i> , 2017 , 8, 10437-10449	3.3	8
170	Combining bioinformatics, chemoinformatics and experimental approaches to design chemical probes: Applications in the field of blood coagulation. <i>Annales Pharmaceutiques Francaises</i> , 2016 , 74, 253-66	1.3	1
169	iPPI-DB: an online database of modulators of protein-protein interactions. <i>Nucleic Acids Research</i> , 2016 , 44, D542-7	20.1	38
168	A Cell-Penetrating Peptide Targeting AAC-11 Specifically Induces Cancer Cells Death. <i>Cancer Research</i> , 2016 , 76, 5479-90	10.1	36
167	Discoidin Domains as Emerging Therapeutic Targets. <i>Trends in Pharmacological Sciences</i> , 2016 , 37, 641-6	5 59 .2	18
166	DNA damage-induced nuclear translocation of Apaf-1 is mediated by nucleoporin Nup107. <i>Cell Cycle</i> , 2015 , 14, 1242-51	4.7	19
165	Functional characterization of two novel non-synonymous alterations in CD46 and a Q950H change in factor H found in atypical hemolytic uremic syndrome patients. <i>Molecular Immunology</i> , 2015 , 65, 367-	76 ³	19
164	In silico design of low molecular weight protein-protein interaction inhibitors: Overall concept and recent advances. <i>Progress in Biophysics and Molecular Biology</i> , 2015 , 119, 20-32	4.7	46
163	Strategies in the Search for New Lead Compounds or Original Working Hypotheses 2015 , 73-99		6
162	Application Strategies for the Primary StructureActivity Relationship Exploration 2015, 301-318		2
161	MTiOpenScreen: a web server for structure-based virtual screening. <i>Nucleic Acids Research</i> , 2015 , 43, W448-54	20.1	101
160	Computational investigations of hERG channel blockers: New insights and current predictive models. <i>Advanced Drug Delivery Reviews</i> , 2015 , 86, 72-82	18.5	53
159	Therapeutic Targeting of Nuclear ETubulin in RB1-Negative Tumors. <i>Molecular Cancer Research</i> , 2015 , 13, 1073-82	6.6	11
158	Integrated structure- and ligand-based in silico approach to predict inhibition of cytochrome P450 2D6. <i>Bioinformatics</i> , 2015 , 31, 3930-7	7.2	12
157	An exploration of the 3D chemical space has highlighted a specific shape profile for the compounds intended to inhibit protein-protein interactions. <i>BMC Bioinformatics</i> , 2015 , 16, A5	3.6	2
156	In Silico Approaches Assisting the Rational Design of Low Molecular Weight Protein B rotein Interaction Modulators 2015 , 441-482		

(2013-2015)

155	Amino acid residues in the laminin G domains of protein S involved in tissue factor pathway inhibitor interaction. <i>Thrombosis and Haemostasis</i> , 2015 , 113, 976-87	7	8
154	Genetic polymorphisms associated with increased risk of developing chronic myelogenous leukemia. <i>Oncotarget</i> , 2015 , 6, 36269-77	3.3	23
153	FAF-Drugs3: a web server for compound property calculation and chemical library design. <i>Nucleic Acids Research</i> , 2015 , 43, W200-7	20.1	192
152	Theileria parasites secrete a prolyl isomerase to maintain host leukocyte transformation. <i>Nature</i> , 2015 , 520, 378-82	50.4	71
151	Which three-dimensional characteristics make efficient inhibitors of protein-protein interactions?. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 3067-79	6.1	33
150	Identification of Small Inhibitory Molecules Targeting the Bfl-1 Anti-Apoptotic Protein That Alleviates Resistance to ABT-737. <i>Journal of Biomolecular Screening</i> , 2014 , 19, 1035-46		10
149	Ligand efficiency driven design of new inhibitors of Mycobacterium tuberculosis transcriptional repressor EthR using fragment growing, merging, and linking approaches. <i>Journal of Medicinal Chemistry</i> , 2014 , 57, 4876-88	8.3	50
148	Discovery of novel inhibitors of vascular endothelial growth factor-A-Neuropilin-1 interaction by structure-based virtual screening. <i>Bioorganic and Medicinal Chemistry</i> , 2014 , 22, 4042-8	3.4	30
147	Identification of novel small molecule inhibitors of activated protein C. <i>Thrombosis Research</i> , 2014 , 133, 1105-14	8.2	12
146	Rational design of small molecules targeting the C2 domain of coagulation factor VIII. <i>Blood</i> , 2014 , 123, 113-20	2.2	17
145	Drug-Like Protein-Protein Interaction Modulators: Challenges and Opportunities for Drug Discovery and Chemical Biology. <i>Molecular Informatics</i> , 2014 , 33, 414-437	3.8	84
144	EFFICIENCY OF A HIERARCHICAL DOCKING PROTOCOL FOR COMPUTATIONAL LIGAND SCREENING AGAINST HOMOLOGY MODELS. <i>Biomedical Engineering - Applications, Basis and Communications</i> , 2014 , 26, 1450024	0.6	1
143	1,2,4-Triazole derivatives as transient inactivators of kallikreins involved in skin diseases. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013 , 23, 4547-51	2.9	27
142	Identification by in silico and in vitro screenings of small organic molecules acting as reversible inhibitors of kallikreins. <i>European Journal of Medicinal Chemistry</i> , 2013 , 70, 661-8	6.8	17
141	Aggrecanase-2 inhibitors based on the acylthiosemicarbazide zinc-binding group. <i>European Journal of Medicinal Chemistry</i> , 2013 , 69, 244-61	6.8	10
140	A Leap into the Chemical Space of Protein P rotein Interaction Inhibitors 2013 , 63-83		1
139	iPPI-DB: a manually curated and interactive database of small non-peptide inhibitors of protein-protein interactions. <i>Drug Discovery Today</i> , 2013 , 18, 958-68	8.8	79
138	Molecular basis of coagulation factor V deficiency caused by the R1698W inter-domain mutation. <i>Thrombosis and Haemostasis</i> , 2013 , 110, 31-8	7	2

137	One hundred thousand mouse clicks down the road: selected online resources supporting drug discovery collected over a decade. <i>Drug Discovery Today</i> , 2013 , 18, 1081-9	8.8	68
136	Insights into an original pocket-ligand pair classification: a promising tool for ligand profile prediction. <i>PLoS ONE</i> , 2013 , 8, e63730	3.7	15
135	1,2,4-Oxadiazoles identified by virtual screening and their non-covalent inhibition of the human 20S proteasome. <i>Current Medicinal Chemistry</i> , 2013 , 20, 2351-62	4.3	23
134	In silico mechanistic profiling to probe small molecule binding to sulfotransferases. <i>PLoS ONE</i> , 2013 , 8, e73587	3.7	14
133	Toward in silico structure-based ADMET prediction in drug discovery. <i>Drug Discovery Today</i> , 2012 , 17, 44-55	8.8	171
132	Design and synthesis of novel bis-thiazolone derivatives as micromolar CDC25 phosphatase inhibitors: effect of dimerisation on phosphatase inhibition. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012 , 22, 7345-50	2.9	16
131	In silico prediction of aqueous solubility: a multimodel protocol based on chemical similarity. <i>Molecular Pharmaceutics</i> , 2012 , 9, 3127-35	5.6	22
130	Established and emerging trends in computational drug discovery in the structural genomics era. <i>Chemistry and Biology</i> , 2012 , 19, 29-41		54
129	Analysis of binding sites on complement factor I using artificial N-linked glycosylation. <i>Journal of Biological Chemistry</i> , 2012 , 287, 13572-83	5.4	8
128	A leap into the chemical space of protein-protein interaction inhibitors. <i>Current Pharmaceutical Design</i> , 2012 , 18, 4648-67	3.3	53
127	AMMOS software: method and application. <i>Methods in Molecular Biology</i> , 2012 , 819, 127-41	1.4	2
126	Tyrosine kinase syk non-enzymatic inhibitors and potential anti-allergic drug-like compounds discovered by virtual and in vitro screening. <i>PLoS ONE</i> , 2011 , 6, e21117	3.7	17
125	Targeting the proangiogenic VEGF-VEGFR protein-protein interface with drug-like compounds by in silico and in vitro screening. <i>Chemistry and Biology</i> , 2011 , 18, 1631-9		35
124	Three-dimensional structure generators of drug-like compounds: DG-AMMOS, an open-source package. <i>Expert Opinion on Drug Discovery</i> , 2011 , 6, 339-51	6.2	9
123	Target-Based Virtual Screening to Address Protein B rotein Interfaces. <i>Methods and Principles in Medicinal Chemistry</i> , 2011 , 435-465	0.4	
122	The FAF-Drugs2 server: a multistep engine to prepare electronic chemical compound collections. <i>Bioinformatics</i> , 2011 , 27, 2018-20	7.2	70
121	Analysis of binding sites on complement factor I that are required for its activity. <i>Journal of Biological Chemistry</i> , 2010 , 285, 6235-45	5.4	20
120	Mutations in components of complement influence the outcome of Factor I-associated atypical hemolytic uremic syndrome. <i>Kidney International</i> , 2010 , 77, 339-49	9.9	131

In Silico ADME/Tox Predictions 2010, 29-124 119 4 Tensin2 reduces intracellular phosphatidylinositol 3,4,5-trisphosphate levels at the plasma 118 12 3.4 membrane. Biochemical and Biophysical Research Communications, 2010, 399, 396-401 Designing focused chemical libraries enriched in protein-protein interaction inhibitors using 117 5 94 machine-learning methods. PLoS Computational Biology, 2010, 6, e1000695 Mutations in complement factor I as found in atypical hemolytic uremic syndrome lead to either 116 6.1 48 altered secretion or altered function of factor I. European Journal of Immunology, 2010, 40, 172-85 Novel organic proteasome inhibitors identified by virtual and in vitro screening. Journal of 8.3 115 40 Medicinal Chemistry, 2010, 53, 509-13 How to choose relevant multiple receptor conformations for virtual screening: a test case of Cdk2 1.9 65 and normal mode analysis. European Biophysics Journal, 2010, 39, 1365-72 In silico studies of blood coagulation proteins: from mosaic proteases to nonenzymatic cofactor 8.1 113 14 inhibitors. Current Opinion in Structural Biology, 2010, 20, 168-79 Rationalizing the chemical space of protein-protein interaction inhibitors. Drug Discovery Today, 8.8 112 158 **2010**, 15, 220-9 Druggable pockets and binding site centric chemical space: a paradigm shift in drug discovery. Drug 8.8 111 214 Discovery Today, 2010, 15, 656-67 New non-hydroxamic ADAMTS-5 inhibitors based on the 1,2,4-triazole-3-thiol scaffold. Bioorganic 110 2.9 19 and Medicinal Chemistry Letters, 2010, 20, 6213-6 Zebrafish ProVEGF-C expression, proteolytic processing and inhibitory effect of unprocessed 109 17 3.7 ProVEGF-C during fin regeneration. PLoS ONE, 2010, 5, e11438 Characterization of the complement inhibitory function of rhesus rhadinovirus complement control 108 5.4 21 protein (RCP). Journal of Biological Chemistry, 2009, 284, 505-514 Development of novel thiazolopyrimidines as CDC25B phosphatase inhibitors. ChemMedChem, 107 3.7 71 2009, 4, 633-48 Genetic, molecular and functional analyses of complement factor I deficiency. European Journal of 106 6.1 39 Immunology, 2009, 39, 310-23 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, 105 31 **2009**, 9, 6 MED-3DMC: a new tool to generate 3D conformation ensembles of small molecules with a Monte 104 6.8 Carlo sampling of the conformational space. European Journal of Medicinal Chemistry, 2009, 44, 1405-9 Structure-based virtual ligand screening: recent success stories. Combinatorial Chemistry and High 103 1.3 101 Throughput Screening, 2009, 12, 1000-16 MS-DOCK: accurate multiple conformation generator and rigid docking protocol for multi-step 3.6 84 102 virtual ligand screening. BMC Bioinformatics, 2008, 9, 184

101	FAF-Drugs2: free ADME/tox filtering tool to assist drug discovery and chemical biology projects. <i>BMC Bioinformatics</i> , 2008 , 9, 396	3.6	192
100	AMMOS: Automated Molecular Mechanics Optimization tool for in silico Screening. <i>BMC Bioinformatics</i> , 2008 , 9, 438	3.6	39
99	A novel druglike spleen tyrosine kinase binder prevents anaphylactic shock when administered orally. <i>Journal of Allergy and Clinical Immunology</i> , 2008 , 122, 188-94, 194.e1-3	11.5	24
98	Receptor-based virtual ligand screening for the identification of novel CDC25 phosphatase inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2008 , 48, 157-65	6.1	36
97	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, 6385-91	5.3	45
96	Mapping of the factor Xa binding site on factor Va by site-directed mutagenesis. <i>Journal of Biological Chemistry</i> , 2008 , 283, 20805-12	5.4	14
95	Defining the structure of membrane-bound human blood coagulation factor Va. <i>Journal of Thrombosis and Haemostasis</i> , 2008 , 6, 76-82	15.4	20
94	In silico-in vitro screening of protein-protein interactions: towards the next generation of therapeutics. <i>Current Pharmaceutical Biotechnology</i> , 2008 , 9, 103-22	2.6	47
93	Combining Ligand- and Structure-Based Methods in Drug Design Projects. <i>Current Computer-Aided Drug Design</i> , 2008 , 4, 250-258	1.4	21
92	Screening Outside the Catalytic Site: Inhibition of Macromolecular Inter-actions Through Structure-Based Virtual Ligand Screening Experiments. <i>The Open Biochemistry Journal</i> , 2008 , 2, 29-37	0.9	14
91	MED-SuMoLig: a new ligand-based screening tool for efficient scaffold hopping. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 1097-110	6.1	31
90	Protein structure analysis online. <i>Current Protocols in Protein Science</i> , 2007 , Chapter 2, Unit 2.13	3.1	1
89	Structure-based virtual ligand screening with LigandFit: pose prediction and enrichment of compound collections. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 68, 712-25	4.2	41
88	Molecular characterization of the interaction between porins of Neisseria gonorrhoeae and C4b-binding protein. <i>Journal of Immunology</i> , 2007 , 179, 540-7	5.3	16
87	Free resources to assist structure-based virtual ligand screening experiments. <i>Current Protein and Peptide Science</i> , 2007 , 8, 381-411	2.8	91
86	Frog: a FRee Online druG 3D conformation generator. <i>Nucleic Acids Research</i> , 2007 , 35, W568-72	20.1	67
85	Kaposiß sarcoma-associated herpes virus complement control protein: KCPcomplement inhibition and more. <i>Molecular Immunology</i> , 2007 , 44, 11-22	4.3	16
84	Design of protein membrane interaction inhibitors by virtual ligand screening, proof of concept with the C2 domain of factor V. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 12697-702	11.5	41

(2004-2006)

83	Functional analysis of the factor IX epidermal growth factor-like domain mutation Ile66Thr associated with mild hemophilia B. <i>Pathophysiology of Haemostasis and Thrombosis: International Journal on Haemostasis and Thrombosis Research</i> , 2006 , 35, 370-5		2
82	FAF-Drugs: free ADME/tox filtering of compound collections. <i>Nucleic Acids Research</i> , 2006 , 34, W738-44	20.1	96
81	Receptor-based computational screening of compound databases: the main docking-scoring engines. <i>Current Protein and Peptide Science</i> , 2006 , 7, 369-93	2.8	40
80	A formylated hexapeptide ligand mimics the ability of Wnt-5a to impair migration of human breast epithelial cells. <i>Journal of Biological Chemistry</i> , 2006 , 281, 2740-9	5.4	92
79	The Kaposiß sarcoma-associated herpesvirus complement control protein (KCP) binds to heparin and cell surfaces via positively charged amino acids in CCP1-2. <i>Molecular Immunology</i> , 2006 , 43, 1665-75	4.3	41
78	Prothrombin deficiency caused by compound heterozygosity for two novel mutations in the prothrombin gene associated with a bleeding tendency. <i>Thrombosis and Haemostasis</i> , 2006 , 95, 195-198	7	19
77	Proposed structural models of the prothrombinase (FXa-FVa) complex. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006 , 63, 440-50	4.2	39
76	PCE: web tools to compute protein continuum electrostatics. <i>Nucleic Acids Research</i> , 2005 , 33, W372-5	20.1	49
75	RPBS: a web resource for structural bioinformatics. <i>Nucleic Acids Research</i> , 2005 , 33, W44-9	20.1	68
74	The anticoagulant protein C pathway. FEBS Letters, 2005, 579, 3310-6	3.8	189
73	Noonan syndrome type I with PTPN11 3 bp deletion: structure-function implications. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005 , 58, 7-13	4.2	13
72	The gamma-carboxyglutamic acid domain of anticoagulant protein S is involved in activated protein C cofactor activity, independently of phospholipid binding. <i>Blood</i> , 2005 , 105, 122-30	2.2	32
71	Fast structure-based virtual ligand screening combining FRED, DOCK, and Surflex. <i>Journal of Medicinal Chemistry</i> , 2005 , 48, 6012-22	8.3	96
70	A critical role for Gly25 in the B chain of human thrombin. <i>Journal of Thrombosis and Haemostasis</i> , 2005 , 3, 139-45	15.4	9
69	Molecular models of the procoagulant factor VIIIa-factor IXa complex. <i>Journal of Thrombosis and Haemostasis</i> , 2005 , 3, 2044-56	15.4	25
68	Regulation of blood coagulation by the protein C anticoagulant pathway: novel insights into structure-function relationships and molecular recognition. <i>Arteriosclerosis, Thrombosis, and Vascular Biology</i> , 2005 , 25, 1311-20	9.4	205
67	The Kaposiß sarcoma-associated herpesvirus complement control protein mimics human molecular	5-4.	34
	mechanisms for inhibition of the complement system. Journal of Biological Chemistry, 2004, 279, 45093-	101	<i>3</i> 1

65	Structural stability and heat-induced conformational change of two complement inhibitors: C4b-binding protein and factor H. <i>Protein Science</i> , 2004 , 13, 1356-64	6.3	28
64	Functional properties of recombinant factor V mutated in a potential calcium-binding site. <i>Biochemistry</i> , 2004 , 43, 5803-10	3.2	10
63	Complement inhibitor C4b-binding protein-friend or foe in the innate immune system?. <i>Molecular Immunology</i> , 2004 , 40, 1333-46	4.3	147
62	Theoretical and experimental study of the D2194G mutation in the C2 domain of coagulation factor V. <i>Biophysical Journal</i> , 2004 , 86, 488-98	2.9	16
61	Functions of human complement inhibitor C4b-binding protein in relation to its structure. <i>Archivum Immunologiae Et Therapiae Experimentalis</i> , 2004 , 52, 83-95	4	25
60	Mutations in alpha-chain of C4BP that selectively affect its factor I cofactor function. <i>Journal of Biological Chemistry</i> , 2003 , 278, 43437-42	5.4	27
59	Factor V New Brunswick: Ala221Val associated with FV deficiency reproduced in vitro and functionally characterized. <i>Blood</i> , 2003 , 102, 1316-22	2.2	27
58	Antithrombin Phe229Leu: a new homozygous variant leading to spontaneous antithrombin polymerization in vivo associated with severe childhood thrombosis. <i>Blood</i> , 2003 , 102, 919-25	2.2	46
57	Role of CCP2 of the C4b-binding protein beta-chain in protein S binding evaluated by mutagenesis and monoclonal antibodies. <i>FEBS Journal</i> , 2003 , 270, 93-100		5
56	Probing plasma clearance of the thrombin-antithrombin complex with a monoclonal antibody against the putative serpin-enzyme complex receptor-binding site. <i>FEBS Journal</i> , 2003 , 270, 4059-69		8
55	Functional analysis of the EGF-like domain mutations Pro55Ser and Pro55Leu, which cause mild hemophilia B. <i>Journal of Thrombosis and Haemostasis</i> , 2003 , 1, 782-90	15.4	8
54	Molecular recognition in the protein C anticoagulant pathway. <i>Journal of Thrombosis and Haemostasis</i> , 2003 , 1, 1525-34	15.4	68
53	Mutations within the cyclooxygenase-1 gene in aspirin non-responders with recurrence of stroke. <i>Thrombosis Research</i> , 2003 , 112, 275-83	8.2	38
52	Protein C Deficiency caused by Homozygosity for a Novel PROC D180G Mutation In vitro Expression and Structural Analysis of the Mutation. <i>Thrombosis and Haemostasis</i> , 2002 , 88, 632-638	7	7
51	Structural requirements of anticoagulant protein S for its binding to the complement regulator C4b-binding protein. <i>Journal of Biological Chemistry</i> , 2002 , 277, 15099-106	5.4	19
50	Defining the factor Xa-binding site on factor Va by site-directed glycosylation. <i>Journal of Biological Chemistry</i> , 2002 , 277, 50022-9	5.4	32
49	A novel interaction of outer membrane protein A with C4b binding protein mediates serum resistance of Escherichia coli K1. <i>Journal of Immunology</i> , 2002 , 169, 6352-60	5.3	136
48	The N-terminal epidermal growth factor-like domain of coagulation factor IX. Probing its functions in the activation of factor IX and factor X with a monoclonal antibody. <i>Journal of Biological Chemistry</i> , 2002 , 277, 35616-24	5.4	13

(1999-2002)

47	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. <i>Blood</i> , 2002 , 99, 1215-23	2.2	137
46	Structural bioinformatics: methods, concepts and applications to blood coagulation proteins. <i>Current Protein and Peptide Science</i> , 2002 , 3, 341-64	2.8	16
45	Two clusters of charged residues located in the electropositive face of the von Willebrand factor A1 domain are essential for heparin binding. <i>Biochemistry</i> , 2002 , 41, 6668-78	3.2	22
44	Three-dimensional model of the SHBG-like region of anticoagulant protein S: New structure f unction insights. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001 , 43, 203-216	4.2	23
43	Screening the molecular surface of human anticoagulant protein C: a search for interaction sites. Journal of Computer-Aided Molecular Design, 2001 , 15, 13-27	4.2	11
42	Localization of a hydrophobic binding site for anticoagulant protein S on the beta -chain of complement regulator C4b-binding protein. <i>Journal of Biological Chemistry</i> , 2001 , 276, 4330-7	5.4	18
41	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. <i>Journal of Biological Chemistry</i> , 2001 , 276, 23105-8	5.4	38
40	Structural and energetic characteristics of the heparin-binding site in antithrombotic protein C. <i>Journal of Biological Chemistry</i> , 2001 , 276, 24122-8	5.4	44
39	Proposed lipocalin fold for apolipoprotein M based on bioinformatics and site-directed mutagenesis. <i>FEBS Letters</i> , 2001 , 499, 127-32	3.8	76
38	Characterization and Structural Impact of Five Novel PROS1 Mutations in Eleven Protein S-deficient Families. <i>Thrombosis and Haemostasis</i> , 2001 , 86, 1392-1399	7	13
37	Defect of Heparin Binding in Plasma and Recombinant von Willebrand Factor with Type 2 von Willebrand Disease Mutations. <i>Thrombosis and Haemostasis</i> , 2001 , 86, 1459-1465	7	2
36	Factor VIII inhibitors in two families with mild haemophilia A: structural analysis of the mutations. <i>Pathophysiology of Haemostasis and Thrombosis: International Journal on Haemostasis and Thrombosis Research</i> , 2000 , 30, 268-79		9
35	Human C4b-binding protein has overlapping, but not identical, binding sites for C4b and streptococcal M proteins. <i>Journal of Immunology</i> , 2000 , 164, 5328-36	5.3	68
34	Positively charged amino acids at the interface between alpha-chain CCP1 and CCP2 of C4BP are required for regulation of the classical C3-convertase. <i>Molecular Immunology</i> , 2000 , 37, 445-53	4.3	30
33	Quaternary structure of the HSC70 cochaperone HIP. <i>Biochemistry</i> , 2000 , 39, 307-15	3.2	22
32	Tracking structural features leading to resistance of activated protein C to alpha 1-antitrypsin. <i>Biochemistry</i> , 2000 , 39, 2853-60	3.2	17
31	Activated protein C-protein C inhibitor complex formation: characterization of a neoepitope provides evidence for extensive insertion of the reactive center loop. <i>Biochemistry</i> , 2000 , 39, 15713-20	3.2	19
30	In Vitro Characterisation of Two Naturally Occurring Mutations in the Thrombin-sensitive Region of Anticoagulant Protein S. <i>Thrombosis and Haemostasis</i> , 1999 , 82, 1627-1633	7	16

29	Involvement of Lys 62[217] and Lys 63[218] of Human Anticoagulant Protein C in Heparin Stimulation of Inhibition by the Protein C Inhibitor. <i>Thrombosis and Haemostasis</i> , 1999 , 82, 72-79	7	27
28	Structural prediction and analysis of endothelial cell protein C/activated protein C receptor. <i>Protein Engineering, Design and Selection</i> , 1999 , 12, 833-40	1.9	21
27	A cluster of positively charged amino acids in the C4BP alpha-chain is crucial for C4b binding and factor I cofactor function. <i>Journal of Biological Chemistry</i> , 1999 , 274, 19237-45	5.4	82
26	The complement regulator C4b-binding protein analyzed by molecular modeling, bioinformatics and computer-aided experimental design. <i>Immunopharmacology</i> , 1999 , 42, 121-34		16
25	Probing the activation of protein C by the thrombin-thrombomodulin complex using structural analysis, site-directed mutagenesis, and computer modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999 , 35, 218-34	4.2	29
24	Partial glycosylation of Asn2181 in human factor V as a cause of molecular and functional heterogeneity. Modulation of glycosylation efficiency by mutagenesis of the consensus sequence for N-linked glycosylation. <i>Biochemistry</i> , 1999 , 38, 13584-91	3.2	58
23	Interspecies Loop Grafting in the Protease Domain of Human Protein C Yielding Enhanced Catalytic and Anticoagulant Activity. <i>Thrombosis and Haemostasis</i> , 1999 , 82, 1078-1087	7	15
22	The C4b-binding protein-protein S interaction is hydrophobic in nature. <i>BBA - Proteins and Proteomics</i> , 1998 , 1388, 181-9		16
21	Structural investigation of C4b-binding protein by molecular modeling: localization of putative binding sites. <i>Proteins: Structure, Function and Bioinformatics</i> , 1998 , 31, 391-405	4.2	36
20	Molecular Models for the two Discoidin Domains of Human Blood Coagulation Factor V. <i>Journal of Molecular Modeling</i> , 1998 , 4, 268-275	2	23
19	Molecular Model for the C-type Lectin Domain of Human Thrombomodulin. <i>Journal of Molecular Modeling</i> , 1998 , 4, 310-322	2	12
18	Determination and analysis of antigenic epitopes of prostate specific antigen (PSA) and human glandular kallikrein 2 (hK2) using synthetic peptides and computer modeling. <i>Protein Science</i> , 1998 , 7, 259-69	6.3	51
17	Structural investigation of the A domains of human blood coagulation factor V by molecular modeling. <i>Protein Science</i> , 1998 , 7, 1317-25	6.3	75
16	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. <i>Journal of Biological Chemistry</i> , 1998 , 273, 27449-58	5.4	30
15	Topological Studies of the Amino Terminal Modules of Vitamin K-dependent Protein S Using Monoclonal Antibody Epitope Mapping and Molecular Modeling. <i>Thrombosis and Haemostasis</i> , 1998 , 80, 798-804	7	16
14	Structural analysis of an anti-estradiol antibody. <i>Molecular Immunology</i> , 1997 , 34, 1215-26	4.3	20
13	A theoretical model for the Gla-TSR-EGF-1 region of the anticoagulant cofactor protein S: from biostructural pathology to species-specific cofactor activity. <i>Journal of Computer-Aided Molecular Design</i> , 1997 , 11, 293-304	4.2	32
12	Local electrostatic potentials in pyridoxal phosphate labelled horse heart cytochrome c. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 1997 , 37, 74-83	6.7	9

LIST OF PUBLICATIONS

11	SHBG region of the anticoagulant cofactor protein S: Secondary structure prediction, circular dichroism spectroscopy, and analysis of naturally occurring mutations 1997 , 29, 478-491		27	
10	Calcium binding to tandem repeats of EGF-like modules. Expression and characterization of the EGF-like modules of human Notch-1 implicated in receptor-ligand interactions. <i>Protein Science</i> , 1997 , 6, 2059-71	6.3	46	
9	Structural investigation of the alpha-1-antichymotrypsin: prostate-specific antigen complex by comparative model building. <i>Protein Science</i> , 1996 , 5, 836-51	6.3	28	
8	A Two-Allele Polymorphism in Protein C Inhibitor with Varying Frequencies in Different Ethnic Populations. <i>Thrombosis and Haemostasis</i> , 1996 , 75, 062-069	7	5	
7	Comparative modeling of the three CP modules of the beta-chain of C4BP and evaluation of potential sites of interaction with protein S. <i>Protein Engineering, Design and Selection</i> , 1995 , 8, 1253-8	1.9	13	
6	Characterization of a cDNA for Rhesus Monkey Protein C Inhibitor Evidence for N-Terminal Involvement in Heparin Stimulation. <i>Thrombosis and Haemostasis</i> , 1995 , 74, 1079-1087	7	8	
5	A structural model for the prostate disease marker, human prostate-specific antigen. <i>Protein Science</i> , 1994 , 3, 2033-44	6.3	65	
4	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. <i>Proteins: Structure, Function and Bioinformatics</i> , 1994 , 18, 367-80	4.2	34	
3	Structural modeling and electrostatic properties of aspartate transcarbamylase from Saccharomyces cerevisiae. <i>Proteins: Structure, Function and Bioinformatics</i> , 1994 , 19, 230-43	4.2	12	
2	Analysis of protein S C4b-binding protein interactions by homology modeling and inhibitory antibodies. <i>Biochemistry</i> , 1994 , 33, 11073-8	3.2	19	
1	Targeting furin activity through in silico and in vitro drug repurposing strategy for SARS-CoV-2 spike glycoprotein cleavage repression		2	