Bruno O Villoutreix

List of Publications by Citations

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

#	Paper	IF	Citations
208	Druggable pockets and binding site centric chemical space: a paradigm shift in drug discovery. *Drug Discovery Today*, **2010**, 15, 656-67	8.8	214
207	Regulation of blood coagulation by the protein C anticoagulant pathway: novel insights into structure-function relationships and molecular recognition. *Arteriosclerosis, Thrombosis, and Vascular Biology*, **2005**, 25, 1311-20	9.4	205
206	FAF-Drugs3: a web server for compound property calculation and chemical library design. *Nucleic Acids Research*, **2015**, 43, W200-7	20.1	192
205	FAF-Drugs2: free ADME/tox filtering tool to assist drug discovery and chemical biology projects. *BMC Bioinformatics*, **2008**, 9, 396	3.6	192
204	The anticoagulant protein C pathway. *FEBS Letters*, **2005**, 579, 3310-6	3.8	189
203	Toward in silico structure-based ADMET prediction in drug discovery. *Drug Discovery Today*, **2012**, 17, 44-55	8.8	171
202	Rationalizing the chemical space of protein-protein interaction inhibitors. *Drug Discovery Today*, **2010**, 15, 220-9	8.8	158
201	Complement inhibitor C4b-binding protein-friend or foe in the innate immune system?. *Molecular Immunology*, **2004**, 40, 1333-46	4.3	147
200	FAF-Drugs4: free ADME-tox filtering computations for chemical biology and early stages drug discovery. *Bioinformatics*, **2017**, 33, 3658-3660	7.2	141
199	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, 1215-23	2.2	137
198	A novel interaction of outer membrane protein A with C4b binding protein mediates serum resistance of Escherichia coli K1. *Journal of Immunology*, **2002**, 169, 6352-60	5.3	136
197	Mutations in components of complement influence the outcome of Factor I-associated atypical hemolytic uremic syndrome. *Kidney International*, **2010**, 77, 339-49	9.9	131
196	MTiOpenScreen: a web server for structure-based virtual screening. *Nucleic Acids Research*, **2015**, 43, W448-54	20.1	101
195	Structure-based virtual ligand screening: recent success stories. *Combinatorial Chemistry and High Throughput Screening*, **2009**, 12, 1000-16	1.3	101
194	FAF-Drugs: free ADME/tox filtering of compound collections. *Nucleic Acids Research*, **2006**, 34, W738-44	20.1	96
193	Fast structure-based virtual ligand screening combining FRED, DOCK, and Surflex. *Journal of Medicinal Chemistry*, **2005**, 48, 6012-22	8.3	96
192	Designing focused chemical libraries enriched in protein-protein interaction inhibitors using machine-learning methods. *PLoS Computational Biology*, **2010**, 6, e1000695	5	94

191	A formylated hexapeptide ligand mimics the ability of Wnt-5a to impair migration of human breast epithelial cells. *Journal of Biological Chemistry*, **2006**, 281, 2740-9	5.4	92
190	Free resources to assist structure-based virtual ligand screening experiments. *Current Protein and Peptide Science*, **2007**, 8, 381-411	2.8	91
189	Drug-Like Protein-Protein Interaction Modulators: Challenges and Opportunities for Drug Discovery and Chemical Biology. *Molecular Informatics*, **2014**, 33, 414-437	3.8	84
188	MS-DOCK: accurate multiple conformation generator and rigid docking protocol for multi-step virtual ligand screening. *BMC Bioinformatics*, **2008**, 9, 184	3.6	84
187	A cluster of positively charged amino acids in the C4BP alpha-chain is crucial for C4b binding and factor I cofactor function. *Journal of Biological Chemistry*, **1999**, 274, 19237-45	5.4	82
186	iPPI-DB: a manually curated and interactive database of small non-peptide inhibitors of protein-protein interactions. *Drug Discovery Today*, **2013**, 18, 958-68	8.8	79
185	Proposed lipocalin fold for apolipoprotein M based on bioinformatics and site-directed mutagenesis. *FEBS Letters*, **2001**, 499, 127-32	3.8	76
184	Structural investigation of the A domains of human blood coagulation factor V by molecular modeling. *Protein Science*, **1998**, 7, 1317-25	6.3	75
183	Computational analysis of calculated physicochemical and ADMET properties of protein-protein interaction inhibitors. *Scientific Reports*, **2017**, 7, 46277	4.9	71
182	Theileria parasites secrete a prolyl isomerase to maintain host leukocyte transformation. *Nature*, **2015**, 520, 378-82	50.4	71
181	Development of novel thiazolopyrimidines as CDC25B phosphatase inhibitors. *ChemMedChem*, **2009**, 4, 633-48	3.7	71
180	The FAF-Drugs2 server: a multistep engine to prepare electronic chemical compound collections. *Bioinformatics*, **2011**, 27, 2018-20	7.2	70
179	One hundred thousand mouse clicks down the road: selected online resources supporting drug discovery collected over a decade. *Drug Discovery Today*, **2013**, 18, 1081-9	8.8	68
178	RPBS: a web resource for structural bioinformatics. *Nucleic Acids Research*, **2005**, 33, W44-9	20.1	68
177	Molecular recognition in the protein C anticoagulant pathway. *Journal of Thrombosis and Haemostasis*, **2003**, 1, 1525-34	15.4	68
176	Human C4b-binding protein has overlapping, but not identical, binding sites for C4b and streptococcal M proteins. *Journal of Immunology*, **2000**, 164, 5328-36	5.3	68
175	Frog: a FRee Online druG 3D conformation generator. *Nucleic Acids Research*, **2007**, 35, W568-72	20.1	67
174	How to choose relevant multiple receptor conformations for virtual screening: a test case of Cdk2 and normal mode analysis. *European Biophysics Journal*, **2010**, 39, 1365-72	1.9	65

173	A structural model for the prostate disease marker, human prostate-specific antigen. *Protein Science*, **1994**, 3, 2033-44	6.3	65
172	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. *Biochemistry*, **1999**, 38, 13584-91	3.2	58
171	Established and emerging trends in computational drug discovery in the structural genomics era. *Chemistry and Biology*, **2012**, 19, 29-41		54
170	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. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	54
169	Computational investigations of hERG channel blockers: New insights and current predictive models. *Advanced Drug Delivery Reviews*, **2015**, 86, 72-82	18.5	53
168	A leap into the chemical space of protein-protein interaction inhibitors. *Current Pharmaceutical Design*, **2012**, 18, 4648-67	3.3	53
167	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, 259-69	6.3	51
166	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, 4876-88	8.3	50
165	PCE: web tools to compute protein continuum electrostatics. *Nucleic Acids Research*, **2005**, 33, W372-5	20.1	49
164	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, 172-85	6.1	48
163	In silico-in vitro screening of protein-protein interactions: towards the next generation of therapeutics. *Current Pharmaceutical Biotechnology*, **2008**, 9, 103-22	2.6	47
162	In silico design of low molecular weight protein-protein interaction inhibitors: Overall concept and recent advances. *Progress in Biophysics and Molecular Biology*, **2015**, 119, 20-32	4.7	46
161	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. *Protein Science*, **1997**, 6, 2059-71	6.3	46
160	Antithrombin Phe229Leu: a new homozygous variant leading to spontaneous antithrombin polymerization in vivo associated with severe childhood thrombosis. *Blood*, **2003**, 102, 919-25	2.2	46
159	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
158	Structural and energetic characteristics of the heparin-binding site in antithrombotic protein C. *Journal of Biological Chemistry*, **2001**, 276, 24122-8	5.4	44
157	Structure-based virtual ligand screening with LigandFit: pose prediction and enrichment of compound collections. *Proteins: Structure, Function and Bioinformatics*, **2007**, 68, 712-25	4.2	41
156	Design of protein 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, 12697-702	11.5	41

155	The Kaposi's sarcoma-associated herpesvirus complement control protein (KCP) binds to heparin and cell surfaces via positively charged amino acids in CCP1-2. *Molecular Immunology*, **2006**, 43, 1665-75	4.3	41
154	Novel organic proteasome inhibitors identified by virtual and in vitro screening. *Journal of Medicinal Chemistry*, **2010**, 53, 509-13	8.3	40
153	Receptor-based computational screening of compound databases: the main docking-scoring engines. *Current Protein and Peptide Science*, **2006**, 7, 369-93	2.8	40
152	Pharmacogenomics of the cytochrome P450 2C family: impacts of amino acid variations on drug metabolism. *Drug Discovery Today*, **2017**, 22, 366-376	8.8	39
151	Genetic, molecular and functional analyses of complement factor I deficiency. *European Journal of Immunology*, **2009**, 39, 310-23	6.1	39
150	AMMOS: Automated Molecular Mechanics Optimization tool for in silico Screening. *BMC Bioinformatics*, **2008**, 9, 438	3.6	39
149	Proposed structural models of the prothrombinase (FXa-FVa) complex. *Proteins: Structure, Function and Bioinformatics*, **2006**, 63, 440-50	4.2	39
148	iPPI-DB: an online database of modulators of protein-protein interactions. *Nucleic Acids Research*, **2016**, 44, D542-7	20.1	38
147	Mutations within the cyclooxygenase-1 gene in aspirin non-responders with recurrence of stroke. *Thrombosis Research*, **2003**, 112, 275-83	8.2	38
146	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, 23105-8	5.4	38
145	Structural investigation of C4b-binding protein by molecular modeling: localization of putative binding sites. *Proteins: Structure, Function and Bioinformatics*, **1998**, 31, 391-405	4.2	36
144	Receptor-based virtual ligand screening for the identification of novel CDC25 phosphatase inhibitors. *Journal of Chemical Information and Modeling*, **2008**, 48, 157-65	6.1	36
143	A Cell-Penetrating Peptide Targeting AAC-11 Specifically Induces Cancer Cells Death. *Cancer Research*, **2016**, 76, 5479-90	10.1	36
142	Virtual screening web servers: designing chemical probes and drug candidates in the cyberspace. *Briefings in Bioinformatics*, **2021**, 22, 1790-1818	13.4	36
141	Targeting the proangiogenic VEGF-VEGFR protein-protein interface with drug-like compounds by in silico and in vitro screening. *Chemistry and Biology*, **2011**, 18, 1631-9		35
140	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, 45093-101	5.4	34
139	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, 367-80	4.2	34
138	Which three-dimensional characteristics make efficient inhibitors of protein-protein interactions?. *Journal of Chemical Information and Modeling*, **2014**, 54, 3067-79	6.1	33

137	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	4.2	32
136	The gamma-carboxyglutamic acid domain of anticoagulant protein S is involved in activated protein C cofactor activity, independently of phospholipid binding. *Blood*, **2005**, 105, 122-30	2.2	32
135	Defining the factor Xa-binding site on factor Va by site-directed glycosylation. *Journal of Biological Chemistry*, **2002**, 277, 50022-9	5.4	32
134	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		31
133	MED-SuMoLig: a new ligand-based screening tool for efficient scaffold hopping. *Journal of Chemical Information and Modeling*, **2007**, 47, 1097-110	6.1	31
132	Discovery of novel inhibitors of vascular endothelial growth factor-A-Neuropilin-1 interaction by structure-based virtual screening. *Bioorganic and Medicinal Chemistry*, **2014**, 22, 4042-8	3.4	30
131	Positively charged amino acids at the interface between alpha-chain CCP1 and CCP2 of C4BP are required for regulation of the classical C3-convertase. *Molecular Immunology*, **2000**, 37, 445-53	4.3	30
130	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, 27449-58	5.4	30
129	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, 218-34	4.2	29
128	Structural stability and heat-induced conformational change of two complement inhibitors: C4b-binding protein and factor H. *Protein Science*, **2004**, 13, 1356-64	6.3	28
127	Structural investigation of the alpha-1-antichymotrypsin: prostate-specific antigen complex by comparative model building. *Protein Science*, **1996**, 5, 836-51	6.3	28
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125	1,2,4-Triazole derivatives as transient inactivators of kallikreins involved in skin diseases. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 4547-51	2.9	27
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123	Mutations in alpha-chain of C4BP that selectively affect its factor I cofactor function. *Journal of Biological Chemistry*, **2003**, 278, 43437-42	5.4	27
122	Factor V New Brunswick: Ala221Val associated with FV deficiency reproduced in vitro and functionally characterized. *Blood*, **2003**, 102, 1316-22	2.2	27
121	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	7	27
120	Molecular models of the procoagulant factor VIIIa-factor IXa complex. *Journal of Thrombosis and Haemostasis*, **2005**, 3, 2044-56	15.4	25

119	Functions of human complement inhibitor C4b-binding protein in relation to its structure. *Archivum Immunologiae Et Therapiae Experimentalis*, **2004**, 52, 83-95	4	25
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117	Genetic polymorphisms associated with increased risk of developing chronic myelogenous leukemia. *Oncotarget*, **2015**, 6, 36269-77	3.3	23
116	1,2,4-Oxadiazoles identified by virtual screening and their non-covalent inhibition of the human 20S proteasome. *Current Medicinal Chemistry*, **2013**, 20, 2351-62	4.3	23
115	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, 1405-9	6.8	23
114	Molecular Models for the two Discoidin Domains of Human Blood Coagulation Factor V. *Journal of Molecular Modeling*, **1998**, 4, 268-275	2	23
113	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	4.2	23
112	Breast Cancer Targeting through Inhibition of the Endoplasmic Reticulum-Based Apoptosis Regulator Nrh/BCL2L10. *Cancer Research*, **2018**, 78, 1404-1417	10.1	22
111	In silico prediction of aqueous solubility: a multimodel protocol based on chemical similarity. *Molecular Pharmaceutics*, **2012**, 9, 3127-35	5.6	22
110	Two clusters of charged residues located in the electropositive face of the von Willebrand factor A1 domain are essential for heparin binding. *Biochemistry*, **2002**, 41, 6668-78	3.2	22
109	Quaternary structure of the HSC70 cochaperone HIP. *Biochemistry*, **2000**, 39, 307-15	3.2	22
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106	Structural prediction and analysis of endothelial cell protein C/activated protein C receptor. *Protein Engineering, Design and Selection*, **1999**, 12, 833-40	1.9	21
105	Combining Ligand- and Structure-Based Methods in Drug Design Projects. *Current Computer-Aided Drug Design*, **2008**, 4, 250-258	1.4	21
104	Anti-Factor B Antibodies and Acute Postinfectious GN in Children. *Journal of the American Society of Nephrology: JASN*, **2020**, 31, 829-840	12.7	20
103	Analysis of binding sites on complement factor I that are required for its activity. *Journal of Biological Chemistry*, **2010**, 285, 6235-45	5.4	20
102	Structural analysis of an anti-estradiol antibody. *Molecular Immunology*, **1997**, 34, 1215-26	4.3	20

101	Defining the structure of membrane-bound human blood coagulation factor Va. *Journal of Thrombosis and Haemostasis*, **2008**, 6, 76-82	15.4	20
100	Acute genetic ablation of pendrin lowers blood pressure in mice. *Nephrology Dialysis Transplantation*, **2017**, 32, 1137-1145	4.3	19
99	DNA damage-induced nuclear translocation of Apaf-1 is mediated by nucleoporin Nup107. *Cell Cycle*, **2015**, 14, 1242-51	4.7	19
98	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, 367-76	4.3	19
97	New non-hydroxamic ADAMTS-5 inhibitors based on the 1,2,4-triazole-3-thiol scaffold. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 6213-6	2.9	19
96	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	7	19
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94	Activated protein C-protein C inhibitor complex formation: characterization of a neoepitope provides evidence for extensive insertion of the reactive center loop. *Biochemistry*, **2000**, 39, 15713-20	3.2	19
93	Analysis of protein S C4b-binding protein interactions by homology modeling and inhibitory antibodies. *Biochemistry*, **1994**, 33, 11073-8	3.2	19
92	Localization of a hydrophobic binding site for anticoagulant protein S on the beta -chain of complement regulator C4b-binding protein. *Journal of Biological Chemistry*, **2001**, 276, 4330-7	5.4	18
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90	Rational design of small molecules targeting the C2 domain of coagulation factor VIII. *Blood*, **2014**, 123, 113-20	2.2	17
89	Identification by in silico and in vitro screenings of small organic molecules acting as reversible inhibitors of kallikreins. *European Journal of Medicinal Chemistry*, **2013**, 70, 661-8	6.8	17
88	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	3.7	17
87	Tracking structural features leading to resistance of activated protein C to alpha 1-antitrypsin. *Biochemistry*, **2000**, 39, 2853-60	3.2	17
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85	Analysis of protein missense alterations by combining sequence- and structure-based methods. *Molecular Genetics & Genomic Medicine*, **2020**, 8, e1166	2.3	16
84	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, 7345-50	2.9	16

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82	Molecular characterization of the interaction between porins of Neisseria gonorrhoeae and C4b-binding protein. *Journal of Immunology*, **2007**, 179, 540-7	5.3	16
81	Kaposi's sarcoma-associated herpes virus complement control protein: KCP--complement inhibition and more. *Molecular Immunology*, **2007**, 44, 11-22	4.3	16
80	Theoretical and experimental study of the D2194G mutation in the C2 domain of coagulation factor V. *Biophysical Journal*, **2004**, 86, 488-98	2.9	16
79	Structural bioinformatics: methods, concepts and applications to blood coagulation proteins. *Current Protein and Peptide Science*, **2002**, 3, 341-64	2.8	16
78	In Vitro Characterisation of Two Naturally Occurring Mutations in the Thrombin-sensitive Region of Anticoagulant Protein S. *Thrombosis and Haemostasis*, **1999**, 82, 1627-1633	7	16
77	The complement regulator C4b-binding protein analyzed by molecular modeling, bioinformatics and computer-aided experimental design. *Immunopharmacology*, **1999**, 42, 121-34		16
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71	In silico studies of blood coagulation proteins: from mosaic proteases to nonenzymatic cofactor inhibitors. *Current Opinion in Structural Biology*, **2010**, 20, 168-79	8.1	14
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64	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. *Journal of Biological Chemistry*, **2002**, 277, 35616-24	5.4	13
63	Characterization and Structural Impact of Five Novel PROS1 Mutations in Eleven Protein S-deficient Families. *Thrombosis and Haemostasis*, **2001**, 86, 1392-1399	7	13
62	Comparative modeling of the three CP modules of the beta-chain of C4BP and evaluation of potential sites of interaction with protein S. *Protein Engineering, Design and Selection*, **1995**, 8, 1253-8	1.9	13
61	Fr-PPIChem: An Academic Compound Library Dedicated to Protein-Protein Interactions. *ACS Chemical Biology*, **2020**, 15, 1566-1574	4.9	13
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57	Molecular Model for the C-type Lectin Domain of Human Thrombomodulin. *Journal of Molecular Modeling*, **1998**, 4, 310-322	2	12
56	Structural modeling and electrostatic properties of aspartate transcarbamylase from Saccharomyces cerevisiae. *Proteins: Structure, Function and Bioinformatics*, **1994**, 19, 230-43	4.2	12
55	Therapeutic Targeting of Nuclear Tubulin in RB1-Negative Tumors. *Molecular Cancer Research*, **2015**, 13, 1073-82	6.6	11
54	In silico model of the human ClC-Kb chloride channel: pore mapping, biostructural pathology and drug screening. *Scientific Reports*, **2017**, 7, 7249	4.9	11
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