Elizabeth Yuriev

List of Publications by Year
in descending order

88 papers	2,943 citations	218677 26 h-index	175258 52 g-index
91 all docs	91 docs citations	91 times ranked	4178 citing authors

#	Article	IF	Citations
1	Challenges and advances in computational docking: 2009 in review. Journal of Molecular Recognition, 2011, 24, 149-164.	2.1	273
2	Status of GPCR Modeling and Docking as Reflected by Community-wide GPCR Dock 2010 Assessment. Structure, 2011, 19, 1108-1126.	3.3	269
3	Latest developments in molecular docking: 2010â€“2011 in review. Journal of Molecular Recognition, 2013, 26, 215-239.	2.1	263
4	The significance of acid/base properties in drug discovery. Chemical Society Reviews, 2013, 42, 485-496.	38.1	236
5	Improvements, trends, and new ideas in molecular docking: 2012â€“2013 in review. Journal of Molecular Recognition, 2015, 28, 581-604.	2.1	211
6	Free Energy Methods in Drug Design: Prospects of â€œAlchemical Perturbationâ€•in Medicinal Chemistry. Journal of Medicinal Chemistry, 2018, 61, 638-649.	6.4	125
7	Homology Modeling and Docking Evaluation of Aminergic G Protein-Coupled Receptors. Journal of Chemical Information and Modeling, 2010, 50, 626-637.	5.4	91
8	A glycopeptide in complex with MHC class I uses the GalNAc residue as an anchor. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 15029-15034.	7.1	82
9	Adopting an active learning approach to teaching in a research-intensive higher education context transformed staff teaching attitudes and behaviours. Higher Education Research and Development, 2016, 35, 619-633.	2.9	73
10	Threeâ€dimensional structures of carbohydrate determinants of Lewis system antigens: Implications for effective antibody targeting of cancer. Immunology and Cell Biology, 2005, 83, 709-717.	2.3	66
11	Molecular Docking of Carbohydrate Ligands to Antibodies: Structural Validation against Crystal Structures. Journal of Chemical Information and Modeling, 2009, 49, 2749-2760.	5.4	62
12	Flipped Classroom Implementation: A Case Report of Two Higher Education Institutions in the United States and Australia. Computers in the Schools, 2016, 33, 24-37.	1.0	56
13	Carbohydrate residues downstream of the terminal GalÎ±(1,3)Gal epitope modulate the specificity of xenoreactive antibodies. Immunology and Cell Biology, 2007, 85, 623-632.	2.3	45
14	Altered peptide ligands of myelin basic protein (MBP_{87â€“99}) conjugated to reduced mannan modulate immune responses in mice. Immunology, 2009, 128, 521-533.	4.4	42
15	Scaffolding the development of problem-solving skills in chemistry: guiding novice students out of dead ends and false starts. Chemistry Education Research and Practice, 2017, 18, 486-504.	2.5	42
16	Homobivalent Ligands of the Atypical Antipsychotic Clozapine: Design, Synthesis, and Pharmacological Evaluation. Journal of Medicinal Chemistry, 2012, 55, 1622-1634.	6.4	39
17	Student Engagement with a Flipped Classroom Teaching Design Affects Pharmacology Examination Performance in a Manner Dependent on Question Type. American Journal of Pharmaceutical Education, 2017, 81, 5931.	2.1	39
18	Structural basis for antibody targeting of the broadly expressed microbial polysaccharide poly-N-acetylglucosamine. Journal of Biological Chemistry, 2018, 293, 5079-5089.	3.4	39

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19	Structural biology of antibody recognition of carbohydrate epitopes and potential uses for targeted cancer immunotherapies. Molecular Immunology, 2015, 67, 75-88.	2.2	38
20	A double mutation of MBP83â€“99 peptide induces IL-4 responses and antagonizes IFN-Î³ responses. Journal of Neuroimmunology, 2008, 200, 77-89.	2.3	34
21	Mannosylation of mutated MBP83â€“99 peptides diverts immune responses from Th1 to Th2. Molecular Immunology, 2008, 45, 3661-3670.	2.2	32
22	Antibody recognition of aberrant glycosylation on the surface of cancer cells. Current Opinion in Structural Biology, 2017, 44, 1-8.	5.7	32
23	Investigation of structureâ€“activity relationships in a series of glibenclamide analogues. European Journal of Medicinal Chemistry, 2004, 39, 835-847.	5.5	31
24	In silico analysis of antibodyâ€“carbohydrate interactions and its application to xenoreactive antibodies. Molecular Immunology, 2009, 47, 233-246.	2.2	31
25	Ligand Binding Pathways of Clozapine and Haloperidol in the Dopamine D₂ and D₃ Receptors. Journal of Chemical Information and Modeling, 2016, 56, 308-321.	5.4	31
26	The carbohydrate-binding promiscuity of Euonymus europaeus lectin is predicted to involve a single binding site. Glycobiology, 2015, 25, 101-114.	2.5	27
27	Novel adenosine A2A receptor ligands: A synthetic, functional and computational investigation of selected literature adenosine A2A receptor antagonists for extending into extracellular space. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 3427-3433.	2.2	26
28	Identification of preferred carbohydrate binding modes in xenoreactive antibodies by combining conformational filters and binding site maps. Glycobiology, 2010, 20, 724-735.	2.5	25
29	The cationic small molecule GW4869 is cytotoxic to high phosphatidylserine-expressing myeloma cells. British Journal of Haematology, 2017, 177, 423-440.	2.5	24
30	Molecular Characterization of Lipopolysaccharide Binding to HumanÎ±-1-Acid Glycoprotein. Journal of Lipids, 2012, 2012, 1-15.	4.8	23
31	Homology Modeling of Human Muscarinic Acetylcholine Receptors. Journal of Chemical Information and Modeling, 2014, 54, 243-253.	5.4	22
32	Characterization of the N-Methyltransferase Activities of the Multifunctional Polypeptide Cyclosporin Synthetase. Chemistry and Biology, 2011, 18, 464-475.	6.0	21
33	Ten Simple Rules for Developing a MOOC. PLoS Computational Biology, 2016, 12, e1005061.	3.2	21
34	Free Ig Light Chains Interact with Sphingomyelin and Are Found on the Surface of Myeloma Plasma Cells in an Aggregated Form. Journal of Immunology, 2010, 185, 4179-4188.	0.8	20
35	Gas-phase formation and reactions of radical cations of guanosine, deoxyguanosine and their homodimers and heterodimers. International Journal of Mass Spectrometry, 2011, 304, 74-82.	1.5	20
36	Carbohydrate-mimetic peptides: structural aspects of mimicry and therapeutic implications. Expert Opinion on Biological Therapy, 2011, 11, 211-224.	3.1	20

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37	Docking of combinatorial peptide libraries into a broadly cross-reactive human IgM. Journal of Molecular Recognition, 2001, 14, 172-184.	2.1	19
38	Structural biology of carbohydrate xenoantigens. Expert Opinion on Biological Therapy, 2009, 9, 1017-1029.	3.1	18
39	Antibody Recognition of Cancer-Related Gangliosides and Their Mimics Investigated Using in silico Site Mapping. PLoS ONE, 2012, 7, e35457.	2.5	18
40	Conformational Analysis of Drug Molecules: A Practical Exercise in the Medicinal Chemistry Course. Journal of Chemical Education, 2009, 86, 477.	2.3	17
41	2-Methyl-4-(4-methylpiperazin-1-yl)-10H-thieno[2,3-b][1,5]benzodiazepine methanol solvate monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2003, 59, o1367-o1369.	0.2	16
42	Challenges and advances in structure-based virtual screening. Future Medicinal Chemistry, 2014, 6, 5-7.	2.3	16
43	The design, synthesis and biological evaluation of novel URB602 analogues as potential monoacylglycerol lipase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 6782-6787.	2.2	15
44	RNA-protein crosslinking to AMP residues at internal positions in RNA with a new photocrosslinking ATP analog. Nucleic Acids Research, 2000, 28, 1849-1858.	14.5	14
45	Antibodyâ€“ligand docking: insights into peptideâ€“carbohydrate mimicry. Molecular Simulation, 2008, 34, 461-469.	2.0	14
46	A Computational Approach for Exploring Carbohydrate Recognition by Lectins in Innate Immunity. Frontiers in Immunology, 2011, 2, 23.	4.8	14
47	AutoMap: A tool for analyzing proteinâ€“ligand recognition using multiple ligand binding modes. Journal of Molecular Graphics and Modelling, 2013, 40, 80-90.	2.4	14
48	Probing the environment of nascent RNA in Escherichia coli transcription elongation complexes utilizing a new fluorescent ribonucleotide analog. Nucleic Acids Research, 1999, 27, 1369-1376.	14.5	13
49	Toward activated homology models of the human M1 muscarinic acetylcholine receptor. Journal of Molecular Graphics and Modelling, 2014, 49, 91-98.	2.4	13
50	Recognition of IgG-Derived Peptides by a Human IgM with an Unusual Combining Site. Scandinavian Journal of Immunology, 2002, 55, 242-255.	2.7	12
51	Crossword puzzles for chemistry education: learning goals beyond vocabulary. Chemistry Education Research and Practice, 2016, 17, 532-554.	2.5	12
52	Steric Aspects of the Binding of Monofunctional Platinum(II) Complexes to Sites on Nucleobases:Â Metal Complex â€œFlatnessâ€•as a Structural Element of Speciation. Inorganic Chemistry, 1998, 37, 6269-6275.	4.0	11
53	Binding of synthetic peptides by a human monoclonal IgM with an unusual combining site structure. Journal of Molecular Recognition, 2001, 14, 229-238.	2.1	11
54	MHC and MHCâ€‘like molecules: Structural perspectives on the design of molecular vaccines. Hum Vaccin, 2008, 4, 400-409.	2.4	11

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55	Synthesis, molecular structure, NMR spectroscopic and computational analysis of a selective adenosine A2A antagonist, ZM 241385. Structural Chemistry, 2013, 24, 1241-1251.	2.0	11
56	The Acid/Base Profile of the Human Metabolome and Natural Products. Molecular Informatics, 2013, 32, 505-515.	2.5	11
57	Steric Parameters for Metal Binding Sites on Nucleobases. Inorganic Chemistry, 1996, 35, 7914-7915.	4.0	10
58	Peptide inhibitors of xenoreactive antibodies mimic the interaction profile of the native carbohydrate antigens. Biopolymers, 2011, 96, 193-206.	2.4	10
59	Detection and Prevention of Aggregation-based False Positives in STD-NMR-based Fragment Screening. Australian Journal of Chemistry, 2013, 66, 1518.	0.9	9
60	Virtual Screening Against Carbohydrate-Binding Proteins: Evaluation and Application to Bacterial Burkholderia ambifaria Lectin. Journal of Chemical Information and Modeling, 2018, 58, 1976-1989.	5.4	9
61	Sterically restrictive metal complexes. The synthesis and structural characterization of (1,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 to cytosine and guanine derivatives. Inorganica Chimica Acta, 1993, 214, 169-176.	2.4	8
62	Molecular Simulations of Carbohydrates with a Fucose-Binding Burkholderia ambifaria Lectin Suggest Modulation by Surface Residues Outside the Fucose-Binding Pocket. Frontiers in Pharmacology, 2017, 8, 393.	3.5	8
63	Immunoglobulin Cross-Reactivity Examined by Library Screening, Crystallography and Docking Studies. Combinatorial Chemistry and High Throughput Screening, 2001, 4, 397-408.	1.1	8
64	Using the Î²₂-Adrenoceptor for Structure-Based Drug Design. Journal of Chemical Education, 2010, 87, 625-627.	2.3	7
65	New hybrids of clozapine and haloperidol and their isosteric analogues: synthesis, X-ray crystallography, conformational analysis and preliminary pharmacological evaluation. Structural Chemistry, 2010, 21, 613-628.	2.0	6
66	Molecular Characterisation of the Haemagglutinin Glycan-Binding Specificity of Egg-Adapted Vaccine Strains of the Pandemic 2009 H1N1 Swine Influenza A Virus. Molecules, 2015, 20, 10415-10434.	3.8	6
67	Carbohydrates in Cyberspace. Frontiers in Immunology, 2015, 6, 300.	4.8	6
68	The influence and manipulation of acid/base properties in drug discovery. Drug Discovery Today: Technologies, 2018, 27, 41-47.	4.0	6
69	Problem solving in chemistry supported by metacognitive scaffolding: teaching associatesâ€™ perspectives and practices. Chemistry Education Research and Practice, 2022, 23, 436-451.	2.5	6
70	Markov State Model Analysis of Haloperidol Binding to the D3 Dopamine Receptor. Journal of Chemical Theory and Computation, 2020, 16, 3879-3888.	5.3	4
71	Structural Glycobiology of Antibody Recognition in Xenotransplantation and Cancer Immunotherapy. , 2012, , 203-228.		4
72	Effects of 5-[S-(2,4-dinitrophenyl)-thio]-2â€²-deoxyuridine analog incorporation on the structure and stability of DNA hybrids: implications for the design of nucleic acid probes. , 1999, 12, 337-345.		3

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73	Mcg light chain dimer as a model system for ligand design: a docking study. Journal of Molecular Recognition, 2002, 15, 331-340.	2.1	3
74	Binding Mode Prediction of PDE4 Inhibitors: A Comparison of Modelling Methods. Australian Journal of Chemistry, 2010, 63, 396.	0.9	3
75	Effect of Changing From Closed-Book to Formulary-Allowed Examinations. American Journal of Pharmaceutical Education, 2021, 85, 7990.	2.1	3
76	'HELPA': a rapid means of student evaluation of lecturing performance in higher education. Assessment and Evaluation in Higher Education, 1995, 20, 191-202.	5.6	2
77	Gas phase supramolecular cluster ions of deoxyguanosine induced by binding to (2,2â€²:6â€²2â€³-terpyridine)-platinum(II) and (diethylenetriamine)-platinum(II). Dalton Transactions, 2009, , 1542.	3.3	2
78	The Synthesis and Preliminary Pharmacological Evaluation of a Series of Substituted 4'-Phenoxypropyl Analogues of the Atypical Antipsychotic Clozapine. Australian Journal of Chemistry, 2010, 63, 116.	0.9	2
79	Antibody-Carbohydrate Recognition from Docked Ensembles Using the AutoMap Procedure. Methods in Molecular Biology, 2015, 1331, 41-55.	0.9	2
80	Teaching Chemistry Down Under in an â€œUpside Downâ€•World: Lessons Learned and Stakeholder Perspectives. ACS Symposium Series, 0, , 105-122.	0.5	2
81	5,5â€²-(Piperazine-1,4-diyl)bis(8-chloropyrido[2,3-b][1,5]benzoxazepine). Acta Crystallographica Section E: Structure Reports Online, 2006, 62, o5434-o5436.	0.2	1
82	Reply to â€˜Response to Milland et al.: Carbohydrate residues downstream of the terminal galÎ±(1,3)gal epitope modulate the specificity of xenoreactive antibodiesâ€™. Immunology and Cell Biology, 2008, 86, 633-634.	2.3	1
83	Homology Modeling and Docking Evaluation of Human Muscarinic Acetylcholine Receptors. Neuromethods, 2016, , 15-35.	0.3	1
84	Geometric forms of 8-chloro-11-[4-(8-chloro-5H-dibenzo[b,e][1,4]diazepin-11-yl)piperazin-1-yl]-5H-dibenzo[b,e][1,4]diazepineâ€“acetoneâ€“pentane (2/1/1). Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o4034-o4034.	0.2	0
85	8-Chloro-5-(4-phenethylpiperazin-1-yl)pyrido[2,3-b][1,5]benzoxazepine. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o1865-o1866.	0.2	0
86	Molecular Modelling: Advances in Biomolecular and Materials Modelling. Australian Journal of Chemistry, 2011, 64, 885.	0.9	0
87	Editorial: Structural and Computational Glycobiology â€“ Immunity and Infection. Frontiers in Immunology, 2015, 6, 359.	4.8	0
88	Antibody Recognition of a Polysaccharide Common to many Microbes and Biofilms. FASEB Journal, 2019, 33, 351.1.	0.5	0