

Elizabeth Yuriev

List of Publications by Year in descending order

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88
papers

2,943
citations

218381

26
h-index

174990

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. <i>Journal of Molecular Recognition</i> , 2011, 24, 149-164.	1.1	273
2	Status of GPCR Modeling and Docking as Reflected by Community-wide GPCR Dock 2010 Assessment. <i>Structure</i> , 2011, 19, 1108-1126.	1.6	269
3	Latest developments in molecular docking: 2010–2011 in review. <i>Journal of Molecular Recognition</i> , 2013, 26, 215-239.	1.1	263
4	The significance of acid/base properties in drug discovery. <i>Chemical Society Reviews</i> , 2013, 42, 485-496.	18.7	236
5	Improvements, trends, and new ideas in molecular docking: 2012–2013 in review. <i>Journal of Molecular Recognition</i> , 2015, 28, 581-604.	1.1	211
6	Free Energy Methods in Drug Design: Prospects of “Chemical Perturbation” in Medicinal Chemistry. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 638-649.	2.9	125
7	Homology Modeling and Docking Evaluation of Aminergic G Protein-Coupled Receptors. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 626-637.	2.5	91
8	A glycopeptide in complex with MHC class I uses the GalNAc residue as an anchor. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003, 100, 15029-15034.	3.3	82
9	Adopting an active learning approach to teaching in a research-intensive higher education context transformed staff teaching attitudes and behaviours. <i>Higher Education Research and Development</i> , 2016, 35, 619-633.	1.9	73
10	Three-dimensional structures of carbohydrate determinants of Lewis system antigens: Implications for effective antibody targeting of cancer. <i>Immunology and Cell Biology</i> , 2005, 83, 709-717.	1.0	66
11	Molecular Docking of Carbohydrate Ligands to Antibodies: Structural Validation against Crystal Structures. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 2749-2760.	2.5	62
12	Flipped Classroom Implementation: A Case Report of Two Higher Education Institutions in the United States and Australia. <i>Computers in the Schools</i> , 2016, 33, 24-37.	0.4	56
13	Carbohydrate residues downstream of the terminal Gal \pm (1,3)Gal epitope modulate the specificity of xenoreactive antibodies. <i>Immunology and Cell Biology</i> , 2007, 85, 623-632.	1.0	45
14	Altered peptide ligands of myelin basic protein (MBP _{87–99}) conjugated to reduced mannan modulate immune responses in mice. <i>Immunology</i> , 2009, 128, 521-533.	2.0	42
15	Scaffolding the development of problem-solving skills in chemistry: guiding novice students out of dead ends and false starts. <i>Chemistry Education Research and Practice</i> , 2017, 18, 486-504.	1.4	42
16	Homobivalent Ligands of the Atypical Antipsychotic Clozapine: Design, Synthesis, and Pharmacological Evaluation. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 1622-1634.	2.9	39
17	Student Engagement with a Flipped Classroom Teaching Design Affects Pharmacology Examination Performance in a Manner Dependent on Question Type. <i>American Journal of Pharmaceutical Education</i> , 2017, 81, 5931.	0.7	39
18	Structural basis for antibody targeting of the broadly expressed microbial polysaccharide poly-N-acetylglucosamine. <i>Journal of Biological Chemistry</i> , 2018, 293, 5079-5089.	1.6	39

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19	Structural biology of antibody recognition of carbohydrate epitopes and potential uses for targeted cancer immunotherapies. <i>Molecular Immunology</i> , 2015, 67, 75-88.	1.0	38
20	A double mutation of MBP83â€™99 peptide induces IL-4 responses and antagonizes IFN-Î³ responses. <i>Journal of Neuroimmunology</i> , 2008, 200, 77-89.	1.1	34
21	Mannosylation of mutated MBP83â€™99 peptides diverts immune responses from Th1 to Th2. <i>Molecular Immunology</i> , 2008, 45, 3661-3670.	1.0	32
22	Antibody recognition of aberrant glycosylation on the surface of cancer cells. <i>Current Opinion in Structural Biology</i> , 2017, 44, 1-8.	2.6	32
23	Investigation of structureâ€™activity relationships in a series of glibenclamide analogues. <i>European Journal of Medicinal Chemistry</i> , 2004, 39, 835-847.	2.6	31
24	In silico analysis of antibodyâ€™carbohydrate interactions and its application to xenoreactive antibodies. <i>Molecular Immunology</i> , 2009, 47, 233-246.	1.0	31
25	Ligand Binding Pathways of Clozapine and Haloperidol in the Dopamine D ₂ and D ₃ Receptors. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 308-321.	2.5	31
26	The carbohydrate-binding promiscuity of <i>Euonymus europaeus</i> lectin is predicted to involve a single binding site. <i>Glycobiology</i> , 2015, 25, 101-114.	1.3	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. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 3427-3433.	1.0	26
28	Identification of preferred carbohydrate binding modes in xenoreactive antibodies by combining conformational filters and binding site maps. <i>Glycobiology</i> , 2010, 20, 724-735.	1.3	25
29	The cationic small molecule GW4869 is cytotoxic to high phosphatidylserine-expressing myeloma cells. <i>British Journal of Haematology</i> , 2017, 177, 423-440.	1.2	24
30	Molecular Characterization of Lipopolysaccharide Binding to Human Î±-1-Acid Glycoprotein. <i>Journal of Lipids</i> , 2012, 2012, 1-15.	1.9	23
31	Homology Modeling of Human Muscarinic Acetylcholine Receptors. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 243-253.	2.5	22
32	Characterization of the N-Methyltransferase Activities of the Multifunctional Polypeptide Cyclosporin Synthetase. <i>Chemistry and Biology</i> , 2011, 18, 464-475.	6.2	21
33	Ten Simple Rules for Developing a MOOC. <i>PLoS Computational Biology</i> , 2016, 12, e1005061.	1.5	21
34	Free Ig Light Chains Interact with Sphingomyelin and Are Found on the Surface of Myeloma Plasma Cells in an Aggregated Form. <i>Journal of Immunology</i> , 2010, 185, 4179-4188.	0.4	20
35	Gas-phase formation and reactions of radical cations of guanosine, deoxyguanosine and their homodimers and heterodimers. <i>International Journal of Mass Spectrometry</i> , 2011, 304, 74-82.	0.7	20
36	Carbohydrate-mimetic peptides: structural aspects of mimicry and therapeutic implications. <i>Expert Opinion on Biological Therapy</i> , 2011, 11, 211-224.	1.4	20

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37	Docking of combinatorial peptide libraries into a broadly cross-reactive human IgM. <i>Journal of Molecular Recognition</i> , 2001, 14, 172-184.	1.1	19
38	Structural biology of carbohydrate xenoantigens. <i>Expert Opinion on Biological Therapy</i> , 2009, 9, 1017-1029.	1.4	18
39	Antibody Recognition of Cancer-Related Gangliosides and Their Mimics Investigated Using in silico Site Mapping. <i>PLoS ONE</i> , 2012, 7, e35457.	1.1	18
40	Conformational Analysis of Drug Molecules: A Practical Exercise in the Medicinal Chemistry Course. <i>Journal of Chemical Education</i> , 2009, 86, 477.	1.1	17
41	2-Methyl-4-(4-methylpiperazin-1-yl)-10H-thieno[2,3-b][1,5]benzodiazepine methanol solvate monohydrate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2003, 59, o1367-o1369.	0.2	16
42	Challenges and advances in structure-based virtual screening. <i>Future Medicinal Chemistry</i> , 2014, 6, 5-7.	1.1	16
43	The design, synthesis and biological evaluation of novel URB602 analogues as potential monoacylglycerol lipase inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2011, 21, 6782-6787.	1.0	15
44	RNA-protein crosslinking to AMP residues at internal positions in RNA with a new photocrosslinking ATP analog. <i>Nucleic Acids Research</i> , 2000, 28, 1849-1858.	6.5	14
45	Antibody-ligand docking: insights into peptide-carbohydrate mimicry. <i>Molecular Simulation</i> , 2008, 34, 461-469.	0.9	14
46	A Computational Approach for Exploring Carbohydrate Recognition by Lectins in Innate Immunity. <i>Frontiers in Immunology</i> , 2011, 2, 23.	2.2	14
47	AutoMap: A tool for analyzing protein-ligand recognition using multiple ligand binding modes. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 40, 80-90.	1.3	14
48	Probing the environment of nascent RNA in Escherichia coli transcription elongation complexes utilizing a new fluorescent ribonucleotide analog. <i>Nucleic Acids Research</i> , 1999, 27, 1369-1376.	6.5	13
49	Toward activated homology models of the human M1 muscarinic acetylcholine receptor. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 49, 91-98.	1.3	13
50	Recognition of IgG-Derived Peptides by a Human IgM with an Unusual Combining Site. <i>Scandinavian Journal of Immunology</i> , 2002, 55, 242-255.	1.3	12
51	Crossword puzzles for chemistry education: learning goals beyond vocabulary. <i>Chemistry Education Research and Practice</i> , 2016, 17, 532-554.	1.4	12
52	Steric Aspects of the Binding of Monofunctional Platinum(II) Complexes to Sites on Nucleobases: A Metal Complex's Flatness as a Structural Element of Speciation. <i>Inorganic Chemistry</i> , 1998, 37, 6269-6275.	1.9	11
53	Binding of synthetic peptides by a human monoclonal IgM with an unusual combining site structure. <i>Journal of Molecular Recognition</i> , 2001, 14, 229-238.	1.1	11
54	MHC and MHC-like molecules: Structural perspectives on the design of molecular vaccines. <i>Hum Vaccin</i> , 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. <i>Structural Chemistry</i> , 2013, 24, 1241-1251.	1.0	11
56	The Acid/Base Profile of the Human Metabolome and Natural Products. <i>Molecular Informatics</i> , 2013, 32, 505-515.	1.4	11
57	Steric Parameters for Metal Binding Sites on Nucleobases. <i>Inorganic Chemistry</i> , 1996, 35, 7914-7915.	1.9	10
58	Peptide inhibitors of xenoreactive antibodies mimic the interaction profile of the native carbohydrate antigens. <i>Biopolymers</i> , 2011, 96, 193-206.	1.2	10
59	Detection and Prevention of Aggregation-based False Positives in STD-NMR-based Fragment Screening. <i>Australian Journal of Chemistry</i> , 2013, 66, 1518.	0.5	9
60	Virtual Screening Against Carbohydrate-Binding Proteins: Evaluation and Application to Bacterial <i>Burkholderia ambifaria</i> Lectin. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1976-1989.	2.5	9
61	Sterically restrictive metal complexes. The synthesis and structural characterization of (1,1'-Tj) ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 to cytosine and guanine derivatives. <i>Inorganica Chimica Acta</i> , 1993, 214, 169-176.	1.2	8
62	Molecular Simulations of Carbohydrates with a Fucose-Binding <i>Burkholderia ambifaria</i> Lectin Suggest Modulation by Surface Residues Outside the Fucose-Binding Pocket. <i>Frontiers in Pharmacology</i> , 2017, 8, 393.	1.6	8
63	Immunoglobulin Cross-Reactivity Examined by Library Screening, Crystallography and Docking Studies. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2001, 4, 397-408.	0.6	8
64	Using the β -Adrenoceptor for Structure-Based Drug Design. <i>Journal of Chemical Education</i> , 2010, 87, 625-627.	1.1	7
65	New hybrids of clozapine and haloperidol and their isosteric analogues: synthesis, X-ray crystallography, conformational analysis and preliminary pharmacological evaluation. <i>Structural Chemistry</i> , 2010, 21, 613-628.	1.0	6
66	Molecular Characterisation of the Haemagglutinin Glycan-Binding Specificity of Egg-Adapted Vaccine Strains of the Pandemic 2009 H1N1 Swine Influenza A Virus. <i>Molecules</i> , 2015, 20, 10415-10434.	1.7	6
67	Carbohydrates in Cyberspace. <i>Frontiers in Immunology</i> , 2015, 6, 300.	2.2	6
68	The influence and manipulation of acid/base properties in drug discovery. <i>Drug Discovery Today: Technologies</i> , 2018, 27, 41-47.	4.0	6
69	Problem solving in chemistry supported by metacognitive scaffolding: teaching associates'™ perspectives and practices. <i>Chemistry Education Research and Practice</i> , 2022, 23, 436-451.	1.4	6
70	Markov State Model Analysis of Haloperidol Binding to the D3 Dopamine Receptor. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3879-3888.	2.3	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]-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.	1.1	3
74	Binding Mode Prediction of PDE4 Inhibitors: A Comparison of Modelling Methods. Australian Journal of Chemistry, 2010, 63, 396.	0.5	3
75	Effect of Changing From Closed-Book to Formulary-Allowed Examinations. American Journal of Pharmaceutical Education, 2021, 85, 7990.	0.7	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.	3.9	2
77	Gas phase supramolecular cluster ions of deoxyguanosine induced by binding to (2,2,6,6-tetramethyl-3-terpyridine)-platinum(II) and (diethylenetriamine)-platinum(II). Dalton Transactions, 2009, , 1542.	1.6	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.	0.5	2
79	Antibody-Carbohydrate Recognition from Docked Ensembles Using the AutoMap Procedure. Methods in Molecular Biology, 2015, 1331, 41-55.	0.4	2
80	Teaching Chemistry Down Under in an "Upside Down" World: Lessons Learned and Stakeholder Perspectives. ACS Symposium Series, 0, , 105-122.	0.5	2
81	5,5-(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 "Response to Milland et al.": Carbohydrate residues downstream of the terminal gal(1,3)gal epitope modulate the specificity of xenoreactive antibodies. Immunology and Cell Biology, 2008, 86, 633-634.	1.0	1
83	Homology Modeling and Docking Evaluation of Human Muscarinic Acetylcholine Receptors. Neuromethods, 2016, , 15-35.	0.2	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]diazepine acetone 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.	0.5	0
87	Editorial: Structural and Computational Glycobiology "Immunity and Infection. Frontiers in Immunology, 2015, 6, 359.	2.2	0
88	Antibody Recognition of a Polysaccharide Common to many Microbes and Biofilms. FASEB Journal, 2019, 33, 351.1.	0.2	0