Grace Brannigan

List of Publications by Year
in descending order

70	1,739	304743 22	315739 38
papers	citations	h-index	g-index

78	78	78	1953
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	2.1	157
2	Embedded cholesterol in the nicotinic acetylcholine receptor. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 14418-14423.	7.1	148
3	A Consistent Model for Thermal Fluctuations and Protein-Induced Deformations in Lipid Bilayers. Biophysical Journal, 2006, 90, 1501-1520.	0.5	134
4	Implicit solvent simulation models for biomembranes. European Biophysics Journal, 2006, 35, 104-124.	2.2	132
5	Solvent-free simulations of fluid membrane bilayers. Journal of Chemical Physics, 2004, 120, 1059-1071.	3.0	114
6	Flexible lipid bilayers in implicit solvent. Physical Review E, 2005, 72, 011915.	2.1	109
7	Multiple binding sites for the general anesthetic isoflurane identified in the nicotinic acetylcholine receptor transmembrane domain. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 14122-14127.	7.1	103
8	A Predicted Binding Site for Cholesterol on the GABAA Receptor. Biophysical Journal, 2014, 106, 1938-1949.	0.5	73
9	Contributions of Gaussian Curvature and Nonconstant Lipid Volume to Protein Deformation of Lipid Bilayers. Biophysical Journal, 2007, 92, 864-876.	0.5	72
10	A Unitary Anesthetic Binding Site at High Resolution. Journal of Biological Chemistry, 2009, 284, 24176-24184.	3.4	67
11	General Anesthetics Predicted to Block the GLIC Pore with Micromolar Affinity. PLoS Computational Biology, 2012, 8, e1002532.	3.2	59
12	Identification of a fluorescent general anesthetic, 1-aminoanthracene. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 6501-6506.	7.1	44
13	Computational Investigation of Cholesterol Binding Sites on Mitochondrial VDAC. Journal of Physical Chemistry B, 2014, 118, 9852-9860.	2.6	43
14	A lipid site shapes the agonist response of a pentameric ligand-gated ion channel. Nature Chemical Biology, 2019, 15, 1156-1164.	8.0	43
15	A Streamlined, General Approach for Computing Ligand Binding Free Energies and Its Application to GPCR-Bound Cholesterol. Journal of Chemical Theory and Computation, 2018, 14, 6560-6573.	5.3	42
16	The role of molecular shape in bilayer elasticity and phase behavior. Journal of Chemical Physics, 2004, 121, 3259-3271.	3.0	36
17	Direct binding of phosphatidylglycerol at specific sites modulates desensitization of a ligand-gated ion channel. ELife, 2019, 8, .	6.0	34
18	Evolution of the <scp>SARSâ€CoV</scp>â€2 proteome in three dimensions (3D) during the first 6 months of the <scp>COVID</scp>â€19 pandemic. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1054-1080.	2.6	31

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19	Role of the Fourth Transmembrane Î± Helix in the Allosteric Modulation of Pentameric Ligand-Gated Ion Channels. Structure, 2015, 23, 1655-1664.	3.3	29
20	Composition dependence of bilayer elasticity. Journal of Chemical Physics, 2005, 122, 074905.	3.0	28
21	The Structural Basis for Low Conductance in the Membrane Protein VDAC upon Î²-NADH Binding and Voltage Gating. Structure, 2020, 28, 206-214.e4.	3.3	28
22	A Novel Bifunctional Alkylphenol Anesthetic Allows Characterization of Î³-Aminobutyric Acid, Type A (GABAA), Receptor Subunit Binding Selectivity in Synaptosomes. Journal of Biological Chemistry, 2016, 291, 20473-20486.	3.4	26
23	An Atomistic Model for Simulations of the General Anesthetic Isoflurane. Journal of Physical Chemistry B, 2010, 114, 604-612.	2.6	24
24	Shedding Light on Anesthetic Mechanisms: Application of Photoaffinity Ligands. Anesthesia and Analgesia, 2016, 123, 1253-1262.	2.2	24
25	Boundary lipids of the nicotinic acetylcholine receptor: Spontaneous partitioning via coarse-grained molecular dynamics simulation. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 887-896.	2.6	18
26	Boundary effects on forced drainage through aqueous foam. Philosophical Magazine Letters, 2001, 81, 197-201.	1.2	17
27	Spontaneous lipid binding to the nicotinic acetylcholine receptor in a native membrane. Journal of Chemical Physics, 2021, 154, 185102.	3.0	15
28	Sequence specificity despite intrinsic disorder: How a disease-associated Val/Met polymorphism rearranges tertiary interactions in a long disordered protein. PLoS Computational Biology, 2019, 15, e1007390.	3.2	13
29	Ketamine Metabolite (2R,6R)-Hydroxynorketamine Interacts with Î¼ and Îº Opioid Receptors. ACS Chemical Neuroscience, 2021, 12, 1487-1497.	3.5	13
30	Pentameric ligand-gated ion channels: insights from computation. Molecular Simulation, 2014, 40, 821-829.	2.0	12
31	Polyunsaturated fatty acids inhibit a pentameric ligand-gated ion channel through one of two binding sites. ELife, 2022, 11, .	6.0	11
32	Direct Interactions of Cholesterol With Pentameric Ligand-Gated Ion Channels: Testable Hypotheses From Computational Predictions. Current Topics in Membranes, 2017, 80, 163-186.	0.9	10
33	Interactions of L-3,5,3'-Triiodothyronine, Allopregnanolone, and Ivermectin with the GABAA Receptor: Evidence for Overlapping Intersubunit Binding Modes. PLoS ONE, 2015, 10, e0139072.	2.5	8
34	Azi-medetomidine: Synthesis and Characterization of a Novel Î±2 Adrenergic Photoaffinity Ligand. ACS Chemical Neuroscience, 2019, 10, 4716-4728.	3.5	5
35	Untangling Direct and Domain-Mediated Interactions Between Nicotinic Acetylcholine Receptors in DHA-Rich Membranes. Journal of Membrane Biology, 2019, 252, 385-396.	2.1	4
36	L-3,3â€™,5-triiodothyronine and pregnenolone sulfate inhibit Torpedo nicotinic acetylcholine receptors. PLoS ONE, 2019, 14, e0223272.	2.5	3

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37	Analysis of the Interactions between GABA(A) Receptors and T3 using Electrophysiology and Molecular Dynamics Simulations. Biophysical Journal, 2013, 104, 638a.	0.5	1
38	Physical Accuracy Leads to Biological Relevance: Best Practices For Simulating Ligand-Gated Ion Channels Interacting With General Anesthetics. Methods in Enzymology, 2018, 602, 3-24.	1.0	1
39	A Model for Lipid Bilayers in Implicit Solvent. , 2008, , 41-58.		1
40	Contiguously hydrophobic sequences are functionally significant throughout the human exome. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2116267119.	7.1	1
41	Effects of Isoflurane Binding in the Pore of a Ligand-Gated Ion Channel. Biophysical Journal, 2010, 98, 133a.	0.5	0
42	Multiple Modes of Interaction between the Nicotinic Acetylcholine Receptor and Isoflurane Observed Through Long Time Simulations. Biophysical Journal, 2010, 98, 134a.	0.5	0
43	Transmembrane Domain Packing in Cys-Loop Receptors: What Can we Learn from Prokaryotes?. Biophysical Journal, 2011, 100, 277a.	0.5	0
44	Dominant Site Involved in Inhibition of Targets by Anesthetics Suggested Through Novel Free Energy Perturbation Calculations. Biophysical Journal, 2011, 100, 195a.	0.5	0
45	Interactions of GABAA Receptors with Steroid-Like Positive and Negative Modulators. Biophysical Journal, 2012, 102, 111a.	0.5	0
46	A Mechanism for Potentiation of the GABA(A) Receptor by Bound Cholesterol. Biophysical Journal, 2013, 104, 638a.	0.5	0
47	Calculation of Cholesterol Binding Affinity for Pentameric Ligand-Gated Ion Channels. Biophysical Journal, 2014, 106, 340a.	0.5	0
48	Effects of Disease-Associated Mutations on the Conformations of GABA(A) Receptors. Biophysical Journal, 2014, 106, 550a.	0.5	0
49	Prediction of the Effects of the Val66Met Polymorphism on the Conformational Ensemble of an Intrinsically Disordered Protein, Brain-Derived Neurotrophic Factor. Biophysical Journal, 2014, 106, 425a.	0.5	0
50	Calculation of Cholesterol Binding Affinity for Pentameric Ligand-Gated Ion Channels. Biophysical Journal, 2015, 108, 317a.	0.5	0
51	Prediction of the Effects of the Val66Met Polymorphism and Adjacent Structured Domains on the Conformational Ensemble of an Intrinsically Disordered Protein, Brain-Derived Neurotrophic Factor. Biophysical Journal, 2015, 108, 386a-387a.	0.5	0
52	Role of the Transmembrane Î±-Helix M4 in the Potentiation of Pentameric Ligand-Gated Ion Channels. Biophysical Journal, 2015, 108, 432a.	0.5	0
53	Affinity Calculations for Lipophilic Modulators Binding to Isolated Sites on GABA(A) Receptors. Biophysical Journal, 2015, 108, 19a.	0.5	0
54	Effects of a Structured Domain on the Conformational Ensemble of Disordered Regions in Brain-Derived Neurotrophic Factor. Biophysical Journal, 2016, 110, 559a.	0.5	0

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55	Relative Affinities of Positive and Negative Modulators of Heteromeric GABA(A) Receptors for Pseudo-Symmetric Intersubunit Binding Sites. Biophysical Journal, 2016, 110, 454a.	0.5	0
56	Effects of Quasi-Native Lipid Composition on Membrane Domain Formation Induced by Nicotinic Acetylcholine Receptors. Biophysical Journal, 2016, 110, 604a.	0.5	0
57	Absolute Affinity Calculations for Cholesterol Binding to G-Protein Coupled Receptors (GPCR). Biophysical Journal, 2016, 110, 423a.	0.5	0
58	Effects of Excluded Volume and Induced N-Terminal Conformational Change on Ion Translocation across VDAC. Biophysical Journal, 2016, 110, 609a.	0.5	0
59	Mechanism Underlying Conformational Effects of a Disease-Associated Hydrophobic-to-Hydrophobic Substitution on an Intrinsically Disordered Region. Biophysical Journal, 2017, 112, 207a.	0.5	0
60	Interactions of Nicotinic Acetylcholine Receptors with Liquid-Disordered Domains Rich in n-3 Polyunsaturated Fatty Acids. Biophysical Journal, 2017, 112, 225a.	0.5	0
61	Modulation of Gaba(A) Receptors by General Anesthetics: A Combinatoric Model Predicts Twenty Years of Concentration-Response Data (With a Few Interesting Exceptions). Biophysical Journal, 2017, 112, 413a.	0.5	0
62	Relative Affinities of General Anesthetics for Pseudo-Symmetric Intersubunit Binding Sites of Heteromeric GABA(A) Receptors. Biophysical Journal, 2017, 112, 555a.	0.5	0
63	The pH Dependence of Ketamine Binding to G-Protein Coupled Receptors. Biophysical Journal, 2018, 114, 226a.	0.5	0
64	Oligomerization of Nicotinic Acetylcholine Receptors in Domain-Forming Membranes. Biophysical Journal, 2018, 114, 340a.	0.5	0
65	Conformational Effects of Various Hydrophobic-to-Hydrophobic Substitution Located at the Midpoint of the Intrinsically Disordered Region of ProBDNF. Biophysical Journal, 2018, 114, 591a.	0.5	0
66	Nicotinic Acetylcholine Receptor Clustering in DHA-Enriched Domains. Biophysical Journal, 2019, 116, 434a.	0.5	0
67	Conformational Effects of a Disease-Associated Hydrophobic-to-Hydrophobic Substitution and Histidine Protonation State Located at the Midpoint of the Intrinsically Disordered Region of proBDNF. Biophysical Journal, 2019, 116, 179a.	0.5	0
68	Boundary Lipids of the Nicotinic Acetylcholine Receptor in Quasi-Native Membranes. Biophysical Journal, 2019, 116, 220a.	0.5	0
69	New Tools for Conformational and Binding Free Energy Simulations. Biophysical Journal, 2019, 116, 142a.	0.5	0
70	Disease Associated Mutations in Intrinsically Disordered Proteins Show Evidence of Enrichment in Hydrophobic Blobs. Biophysical Journal, 2020, 118, 215a.	0.5	0