Abby L Parrill

List of Publications by Year
in descending order

105 papers	3,947 citations	117453 34 h-index	133063 59 g-index
125 all docs	125 docs citations	125 times ranked	4080 citing authors

#	Article	IF	Citations
1	Ligand-based G Protein Coupled Receptor pharmacophore modeling: Assessing the role of ligand function in model development. Journal of Molecular Graphics and Modelling, 2022, 111, 108107.	1.3	11
2	Self-docking and cross-docking simulations of G protein-coupled receptor-ligand complexes: Impact of ligand type and receptor activation state. Journal of Molecular Graphics and Modelling, 2022, 112, 108119.	1.3	5
3	Discovery of agonistâ€“antagonist pairs for the modulation of Ca [2]+ and voltage-gated K+ channels of large conductance that contain beta1 subunits. Bioorganic and Medicinal Chemistry, 2022, 68, 116876.	1.4	1
4	Molecular modelling guided design, synthesis and QSAR analysis of new small molecule non-lipid autotaxin inhibitors. Bioorganic Chemistry, 2020, 103, 104188.	2.0	5
5	Benchmarking GPCR homology model templateÂselection in combination with de novo loop generation. Journal of Computer-Aided Molecular Design, 2020, 34, 1027-1044.	1.3	1
6	Optical Control of Lysophosphatidic Acid Signaling. Journal of the American Chemical Society, 2020, 142, 10612-10616.	6.6	37
7	A benchmark study of loop modeling methods applied to G protein-coupled receptors. Journal of Computer-Aided Molecular Design, 2019, 33, 573-595.	1.3	17
8	Optical control of sphingosine-1-phosphate formation and function. Nature Chemical Biology, 2019, 15, 623-631.	3.9	66
9	GPCR homology model template selection benchmarking: Global versus local similarity measures. Journal of Molecular Graphics and Modelling, 2019, 86, 235-246.	1.3	16
10	Highly Potent Non-Carboxylic Acid Autotaxin Inhibitors Reduce Melanoma Metastasis and Chemotherapeutic Resistance of Breast Cancer Stem Cells. Journal of Medicinal Chemistry, 2017, 60, 1309-1324.	2.9	45
11	G protein-coupled receptors: the evolution of structural insight. AIMS Biophysics, 2017, 4, 491-527.	0.3	56
12	Discovery and synthetic optimization of a novel scaffold for hydrophobic tunnel-targeted autotaxin inhibition. Bioorganic and Medicinal Chemistry, 2016, 24, 4660-4674.	1.4	6
13	Reprint of: â€œSynthetic lipids and their role in defining macromolecular assembliesâ€• Chemistry and Physics of Lipids, 2016, 194, 149-157.	1.5	0
14	Corrigendum to â€œMulti-generational pharmacophore modeling for ligands to the cholane steroid-recognition site in the Î²1 modulatory subunit of the BKCa channelâ€•[J. Mol. Graph. Model. 54 (2014) 174â€"183]. Journal of Molecular Graphics and Modelling, 2015, 55, 149.	1.3	0
15	Synthetic lipids and their role in defining macromolecular assemblies. Chemistry and Physics of Lipids, 2015, 191, 38-47.	1.5	1
16	Activation of Calcium- and Voltage-gated Potassium Channels of Large Conductance by Leukotriene B4. Journal of Biological Chemistry, 2014, 289, 35314-35325.	1.6	16
17	Design of anticancer lysophosphatidic acid agonists and antagonists. Future Medicinal Chemistry, 2014, 6, 871-883.	1.1	8
18	Targeting the hydrophobic pocket of autotaxin with virtual screening of inhibitors identifies a common aromatic sulfonamide structural motif. FEBS Journal, 2014, 281, 1017-1028.	2.2	22

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19	Multi-generational pharmacophore modeling for ligands to the cholane steroid-recognition site in the Î²1 modulatory subunit of the BKCa channel. Journal of Molecular Graphics and Modelling, 2014, 54, 174-183.	1.3	8
20	Autotaxin inhibition: Development and application of computational tools to identify site-selective lead compounds. Bioorganic and Medicinal Chemistry, 2013, 21, 5548-5560.	1.4	16
21	Computational Design and Experimental Characterization of GPCR Segment Models. Methods in Enzymology, 2013, 522, 81-95.	0.4	0
22	Cerebrovascular Dilation via Selective Targeting of the Cholane Steroid-Recognition Site in the BK Channel <i>Î²</i>1-Subunit by a Novel Nonsteroidal Agent. Molecular Pharmacology, 2013, 83, 1030-1044.	1.0	38
23	Gold Nanorods Carrying Paclitaxel for Photothermal-Chemotherapy of Cancer. Bioconjugate Chemistry, 2013, 24, 376-386.	1.8	105
24	Integrating the puzzle pieces: The current atomistic picture of phospholipidâ€“G protein coupled receptor interactions. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2013, 1831, 2-12.	1.2	16
25	Structural Characterization of an LPA1 Second Extracellular Loop Mimetic with a Self-Assembling Coiled-Coil Folding Constraint. International Journal of Molecular Sciences, 2013, 14, 2788-2807.	1.8	3
26	Hits of a High-Throughput Screen Identify the Hydrophobic Pocket of Autotaxin/Lysophospholipase D As an Inhibitory Surface. Molecular Pharmacology, 2013, 84, 415-424.	1.0	32
27	Polymer Concepts Illustrated in the Context of Biopolymers. ACS Symposium Series, 2013, , 85-93.	0.5	0
28	Multiple Cholesterol Recognition/Interaction Amino Acid Consensus (CRAC) Motifs in Cytosolic C Tail of Slo1 Subunit Determine Cholesterol Sensitivity of Ca2+- and Voltage-gated K+ (BK) Channels. Journal of Biological Chemistry, 2012, 287, 20509-20521.	1.6	82
29	Virtual Screening for LPA₂-Specific Agonists Identifies a Nonlipid Compound with Antiapoptotic Actions. Molecular Pharmacology, 2012, 82, 1162-1173.	1.0	52
30	Comparative Modeling of Lipid Receptors. , 2012, 914, 207-218.		2
31	Introductory Molecular Orbital Theory: An Honors General Chemistry Computational Lab As Implemented Using Three-Dimensional Modeling Software. Journal of Chemical Education, 2012, 89, 1358-1363.	1.1	15
32	Sodium 3-Hydroxyolean-12-en-30-Oate is a Novel and Selective Activator of Î²1 Subunit-Containing BK Channels and thus Cerebral Artery Dilator. Biophysical Journal, 2012, 102, 133a-134a.	0.2	1
33	<i>JCE</i> Classroom Activity #113: An Interlocking Building Block Activity in Writing Formulas of Ionic Compounds. Journal of Chemical Education, 2012, 89, 1436-1438.	1.1	15
34	Structure of the First Sphingosine 1-Phosphate Receptor. Science Signaling, 2012, 5, pe23.	1.6	14
35	Mechanisms of Radiomitigative Cell Signaling Via Lysophosphatidic Acid Receptors. FASEB Journal, 2012, 26, 993.4.	0.2	0
36	Lysophosphatidic acid receptor agonists and antagonists (WO2010051053). Expert Opinion on Therapeutic Patents, 2011, 21, 281-286.	2.4	4

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37	Ligand-based autotaxin pharmacophore models reflect structure-based docking results. Journal of Molecular Graphics and Modelling, 2011, 31, 76-86.	1.3	12
38	Computational identification and experimental characterization of substrate binding determinants of nucleotide pyrophosphatase/phosphodiesterase 7. BMC Biochemistry, 2011, 12, 65.	4.4	7
39	Benzyl and Naphthalene Methylphosphonic Acid Inhibitors of Autotaxin with Antiâ€invasive and Antiâ€metastatic Activity. ChemMedChem, 2011, 6, 922-935.	1.6	56
40	GPCR Conformations: Implications for Rational Drug Design. Pharmaceuticals, 2011, 4, 7-43.	1.7	16
41	FTY720 (Gilenya) Phosphate Selectivity of Sphingosine 1-Phosphate Receptor Subtype 1 (S1P1) G Protein-coupled Receptor Requires Motifs in Intracellular Loop 1 and Transmembrane Domain 2. Journal of Biological Chemistry, 2011, 286, 30513-30525.	1.6	15
42	The steroid interaction site in transmembrane domain 2 of the large conductance, voltage- and calcium-gated potassium (BK) channel accessory Î²1 subunit. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 20207-20212.	3.3	45
43	(S)-FTY720-Vinylphosphonate, an analogue of the immunosuppressive agent FTY720, is a pan-antagonist of sphingosine 1-phosphate GPCR signaling and inhibits autotaxin activity. Cellular Signalling, 2010, 22, 1543-1553.	1.7	50
44	2D binary QSAR modeling of LPA3 receptor antagonism. Journal of Molecular Graphics and Modelling, 2010, 28, 828-833.	1.3	6
45	Characterization of non-lipid autotaxin inhibitors. Bioorganic and Medicinal Chemistry, 2010, 18, 769-776.	1.4	23
46	Synthesis and pharmacological evaluation of the stereoisomers of 3-carba cyclic-phosphatidic acid. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 7525-7528.	1.0	24
47	GPRC6A Mediates the Non-genomic Effects of Steroids. Journal of Biological Chemistry, 2010, 285, 39953-39964.	1.6	163
48	Pharmacophore Development and Application Toward the Identification of Novel, Small-Molecule Autotaxin Inhibitors. Journal of Medicinal Chemistry, 2010, 53, 3095-3105.	2.9	32
49	Optimization of a Pipemidic Acid Autotaxin Inhibitor. Journal of Medicinal Chemistry, 2010, 53, 1056-1066.	2.9	38
50	Phospholipase D2-Dependent Inhibition of the Nuclear Hormone Receptor PPARÎ³ by Cyclic Phosphatidic Acid. Molecular Cell, 2010, 39, 421-432.	4.5	117
51	Autotaxin inhibitors: a perspective on initial medicinal chemistry efforts. Expert Opinion on Therapeutic Patents, 2010, 20, 1619-1625.	2.4	17
52	Unique Ligand Selectivity of the GPR92/LPA5 Lysophosphatidate Receptor Indicates Role in Human Platelet Activation. Journal of Biological Chemistry, 2009, 284, 17304-17319.	1.6	131
53	Dual Activity Lysophosphatidic Acid Receptor Pan-Antagonist/Autotaxin Inhibitor Reduces Breast Cancer Cell Migration <i>In vitro</i> and Causes Tumor Regression <i>In vivo</i>. Cancer Research, 2009, 69, 5441-5449.	0.4	148
54	Structure-based drug design identifies novel LPA3 antagonists. Bioorganic and Medicinal Chemistry, 2009, 17, 7457-7464.	1.4	25

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55	Autotaxin structureâ€"activity relationships revealed through lysophosphatidylcholine analogs. Bioorganic and Medicinal Chemistry, 2009, 17, 3433-3442.	1.4	27
56	Crystal Structures of a Second Gâ€…Proteinâ€Coupled Receptor: Triumphs and Implications. ChemMedChem, 2008, 3, 1021-1023.	1.6	6
57	Molecular recognition in the sphingosine 1-phosphate receptor family. Journal of Molecular Graphics and Modelling, 2008, 26, 1189-1201.	1.3	31
58	Virtual screening approaches for the identification of non-lipid autotaxin inhibitors. Bioorganic and Medicinal Chemistry, 2008, 16, 1784-1795.	1.4	48
59	Identification of non-lipid LPA3 antagonists by virtual screening. Bioorganic and Medicinal Chemistry, 2008, 16, 6207-6217.	1.4	29
60	Lysophospholipid interactions with protein targets. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2008, 1781, 540-546.	1.2	34
61	Subtype-specific Residues Involved in Ligand Activation of the Endothelial Differentiation Gene Family Lysophosphatidic Acid Receptors. Journal of Biological Chemistry, 2008, 283, 12175-12187.	1.6	34
62	Ethanol Modulates BK_{Ca}Channels by Acting as an Adjuvant of Calcium. Molecular Pharmacology, 2008, 74, 628-640.	1.0	51
63	Structural determinants of monohydroxylated bile acids to activate Î²1 subunit-containing BK channels. Journal of Lipid Research, 2008, 49, 2441-2451.	2.0	28
64	Autotaxin Inhibition: Challenges and Progress Toward Novel Anti-Cancer Agents. Anti-Cancer Agents in Medicinal Chemistry, 2008, 8, 917-923.	0.9	35
65	Identification of the Hydrophobic Ligand Binding Pocket of the S1P1 Receptor. Journal of Biological Chemistry, 2007, 282, 2374-2385.	1.6	49
66	The Lysophosphatidic Acid Type 2 Receptor Is Required for Protection Against Radiation-Induced Intestinal Injury. Gastroenterology, 2007, 132, 1834-1851.	0.6	113
67	Peptide design and structural characterization of a GPCR loop mimetic. Biopolymers, 2007, 86, 298-310.	1.2	18
68	Sphingosine 1-phosphate pKa and binding constants: Intramolecular and intermolecular influences. Journal of Molecular Graphics and Modelling, 2007, 26, 519-528.	1.3	19
69	Synthesis and pharmacological evaluation of second-generation phosphatidic acid derivatives as lysophosphatidic acid receptor ligands. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 633-640.	1.0	47
70	Different Residues Mediate Recognition of 1-O-Oleyllysophosphatidic Acid and Rosiglitazone in the Ligand Binding Domain of Peroxisome Proliferator-activated Receptor Î³. Journal of Biological Chemistry, 2006, 281, 3398-3407.	1.6	81
71	Structural characteristics of lysophosphatidic acid biological targets. Biochemical Society Transactions, 2005, 33, 1366.	1.6	17
72	Sphingosine 1-phosphate analogue recognition and selectivity at S1P4 within the endothelial differentiation gene family of receptors. Biochemical Journal, 2005, 389, 187-195.	1.7	47

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73	Cluster analysis and three-dimensional QSAR studies of HIV-1 integrase inhibitors. Journal of Molecular Graphics and Modelling, 2005, 23, 317-328.	1.3	18
74	S1P1-Selective In Vivo-Active Agonists from High- Throughput Screening: Off-the-Shelf Chemical Probes of Receptor Interactions, Signaling, and Fate. Chemistry and Biology, 2005, 12, 703-715.	6.2	227
75	Identification of Residues Responsible for Ligand Recognition and Regioisomeric Selectivity of Lysophosphatidic Acid Receptors Expressed in Mammalian Cells*. Journal of Biological Chemistry, 2005, 280, 35038-35050.	1.6	79
76	Functional Dissection and Molecular Characterization of Calcium-sensitive Actin-capping and Actin-depolymerizing Sites in Villin. Journal of Biological Chemistry, 2004, 279, 45036-45046.	1.6	33
77	A single amino acid determines preference between phospholipids and reveals length restriction for activation of the S1P4 receptor. BMC Biochemistry, 2004, 5, 12.	4.4	20
78	Sphingosine 1-phosphate and lysophosphatidic acid receptors: agonist and antagonist binding and progress toward development of receptor-specific ligands. Seminars in Cell and Developmental Biology, 2004, 15, 467-476.	2.3	39
79	Molecular mechanisms of lysophosphatidic acid action. Progress in Lipid Research, 2003, 42, 498-526.	5.3	171
80	Fatty Alcohol Phosphates are Subtype-Selective Agonists and Antagonists of Lysophosphatidic Acid Receptors. Molecular Pharmacology, 2003, 63, 1032-1042.	1.0	85
81	HIV-1 Integrase Inhibition: Binding Sites, Structure Activity Relationships and Future Perspectives. Current Medicinal Chemistry, 2003, 10, 1811-1824.	1.2	23
82	Three-Dimensional Quantitative Structure-Activity Relationship and Comparative Molecular Field Analysis of Dipeptide Hydroxamic Acid Helicobacter pylori Urease Inhibitors. Antimicrobial Agents and Chemotherapy, 2002, 46, 2613-2618.	1.4	26
83	Regulation of Actin Dynamics by Tyrosine Phosphorylation:Â Identification of Tyrosine Phosphorylation Sites within the Actin-Severing Domain of Villinâ€. Biochemistry, 2002, 41, 11750-11760.	1.2	26
84	Molecular basis for lysophosphatidic acid receptor antagonist selectivity. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2002, 1582, 309-317.	1.2	78
85	QSAR studies of HIV-1 integrase inhibition. Bioorganic and Medicinal Chemistry, 2002, 10, 4169-4183.	1.4	59
86	Molecular Models ofN-Benzyladriamycin-14-valerate (AD 198) in Complex with the Phorbol Ester-Binding C1b Domain of Protein Kinase C-Î´. Journal of Medicinal Chemistry, 2001, 44, 1028-1034.	2.9	15
87	A Single Amino Acid Determines Lysophospholipid Specificity of the S1P1 (EDG1) and LPA1 (EDG2) Phospholipid Growth Factor Receptors. Journal of Biological Chemistry, 2001, 276, 49213-49220.	1.6	99
88	Dynamic modeling of EDG1 receptor structural changes induced by site-directed mutations. Computational and Theoretical Chemistry, 2000, 529, 219-224.	1.5	14
89	QSAR development to describe HIV-1 integrase inhibition. Computational and Theoretical Chemistry, 2000, 529, 273-282.	1.5	13
90	Identification of Edg1 Receptor Residues That Recognize Sphingosine 1-Phosphate. Journal of Biological Chemistry, 2000, 275, 39379-39384.	1.6	147

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91	Everyday Chemical Reactions: A Writing Assignment to Promote Synthesis of Concepts and Relevance in Chemistry. Journal of Chemical Education, 2000, 77, 1303.	1.1	8
92	Pharmacological Characterization of Phospholipid Growthâ€Factor Receptors. Annals of the New York Academy of Sciences, 2000, 905, 34-53.	1.8	18
93	Structural Features of EDG1 Receptorâ€Ligand Complexes Revealed by Computational Modeling and Mutagenesis. Annals of the New York Academy of Sciences, 2000, 905, 330-339.	1.8	23
94	Overview of Rational Drug Design. ACS Symposium Series, 1999, , 1-11.	0.5	9
95	Solid Phase Synthesis and Secondary Structural Studies of (1â†'5) Amide-Linked Sialooligomers1. Journal of Organic Chemistry, 1998, 63, 1074-1078.	1.7	118
96	Recent advances in computer-aided drug design methods. Expert Opinion on Therapeutic Patents, 1997, 7, 937-945.	2.4	4
97	Fostering Curiosity-Driven Learning through Interactive Multimedia Representations of Biological Molecules. Journal of Chemical Education, 1997, 74, 1141.	1.1	3
98	Periodic 2.0 for Macintosh. Journal of Chemical Information and Computer Sciences, 1997, 37, 820-820.	2.8	1
99	Discovery-Based Stereochemistry Tutorials Available on the World Wide Web. Journal of Chemical Education, 1997, 74, 329.	1.1	6
100	Computational studies of sialyllactones: methods and uses. Glycoconjugate Journal, 1997, 14, 523-529.	1.4	9
101	gNMR version 3 for Macintosh. Journal of Chemical Information and Computer Sciences, 1996, 36, 153-153.	2.8	1
102	The Stereochem Game: Making Chemistry More Fun. The Chemical Educator, 1996, 1, 1-7.	0.0	5
103	The â€œFacilitated Transitionâ€• hypothesis as an explanation for the gemdialkyl effect. Computational and Theoretical Chemistry, 1996, 370, 187-202.	1.5	26
104	Evolutionary and genetic methods in drug design. Drug Discovery Today, 1996, 1, 514-521.	3.2	33
105	Evidence against the reactive rotamer explanation of the gem-dialkyl effect. Tetrahedron Letters, 1994, 35, 7319-7322.	0.7	27