Francesca Fanelli

List of Publications by Year in descending order

152 papers	6,834 citations	71102 41 h-index	74163 75 g-index
157 all docs	157 docs citations	157 times ranked	5874 citing authors

#	Article	IF	Citations
1	PSNtools for standalone and web-based structure network analyses of conformational ensembles. Computational and Structural Biotechnology Journal, 2022, 20, 640-649.	4.1	17
2	Frontiers in Multiscale Modeling of Photoreceptor Proteins. Photochemistry and Photobiology, 2021, 97, 243-269.	2.5	26
3	Structural aspects of rod opsin and their implication in genetic diseases. Pflugers Archiv European Journal of Physiology, 2021, 473, 1339-1359.	2.8	9
4	Structure network-based landscape of rhodopsin misfolding by mutations and algorithmic prediction of small chaperone action. Computational and Structural Biotechnology Journal, 2021, 19, 6020-6038.	4.1	4
5	ETNK1 mutations induce a mutator phenotype that can be reverted with phosphoethanolamine. Nature Communications, 2020, 11, 5938.	12.8	22
6	Dynamics and structural communication in the ternary complex of fully phosphorylated V2 vasopressin receptor, vasopressin, and Î²-arrestin 1. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183355.	2.6	6
7	webPSN v2.0: a webserver to infer fingerprints of structural communication in biomacromolecules. Nucleic Acids Research, 2020, 48, W94-W103.	14.5	56
8	Integrated structural modeling and super-resolution imaging resolve GPCR oligomers. Progress in Molecular Biology and Translational Science, 2020, 169, 151-179.	1.7	5
9	Membrane Estrogen Receptor (GPER) and Follicle-Stimulating Hormone Receptor (FSHR) Heteromeric Complexes Promote Human Ovarian Follicle Survival. IScience, 2020, 23, 101812.	4.1	29
10	ETNK1 Mutations in Atypical Chronic Myeloid Leukemia Induce a Mutator Phenotype That Can be Reverted with Phosphoethanolamine. Blood, 2020, 136, LBA-5-LBA-5.	1.4	1
11	Interconnecting Flexibility, Structural Communication, and Function in RhoGEF Oncoproteins. Journal of Chemical Information and Modeling, 2019, 59, 4300-4313.	5.4	13
12	Frontal Variant of Alzheimerâ€™s Disease: A Report of a Novel PSEN1 Mutation. Journal of Alzheimer's Disease, 2019, 70, 11-15.	2.6	8
13	Auto-regulation of Secretory Flux by Sensing and Responding to the Folded Cargo Protein Load in the Endoplasmic Reticulum. Cell, 2019, 176, 1461-1476.e23.	28.9	65
14	a-ARM: Automatic Rhodopsin Modeling with Chromophore Cavity Generation, Ionization State Selection, and External Counterion Placement. Journal of Chemical Theory and Computation, 2019, 15, 3134-3152.	5.3	44
15	Computational modeling approaches to quantitative structureâ€“binding kinetics relationships in drug discovery. Drug Discovery Today, 2018, 23, 1396-1406.	6.4	20
16	A Small Chaperone Improves Folding and Routing of Rhodopsin Mutants Linked to Inherited Blindness. IScience, 2018, 4, 1-19.	4.1	50
17	Structural Determinants of Constitutive Activation of GÎ± Proteins: Transducin as a Paradigm. Journal of Chemical Theory and Computation, 2017, 13, 886-899.	5.3	10
18	Epilepsy and intellectual disability linked protein Shrm4 interaction with GABABRs shapes inhibitory neurotransmission. Nature Communications, 2017, 8, 14536.	12.8	31

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19	Dissecting intrinsic and ligand-induced structural communication in the Î²3 headpiece of integrins. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 2367-2381.	2.4	13
20	Class A GPCR: Di/Oligomerization of Glycoprotein Hormone Receptors. , 2017, , 207-231.		2
21	Modulation of thermal noise and spectral sensitivity in Lake Baikal cottoid fish rhodopsins. Scientific Reports, 2016, 6, 38425.	3.3	26
22	Small-Molecule Protein-Protein Interaction Inhibitor of Oncogenic Rho Signaling. Cell Chemical Biology, 2016, 23, 1135-1146.	5.2	28
23	Structure network analysis to gain insights into GPCR function. Biochemical Society Transactions, 2016, 44, 613-618.	3.4	21
24	WebPSN: a web server for high-throughput investigation of structural communication in biomacromolecules. Bioinformatics, 2015, 31, 779-781.	4.1	49
25	Single Molecule Analysis of Functionally Asymmetric G Protein-coupled Receptor (GPCR) Oligomers Reveals Diverse Spatial and Structural Assemblies. Journal of Biological Chemistry, 2015, 290, 3875-3892.	3.4	105
26	The intellectual disability protein RAB39B selectively regulates GluA2 trafficking to determine synaptic AMPAR composition. Nature Communications, 2015, 6, 6504.	12.8	93
27	Catching Functional Modes and Structural Communication in Dbl Family Rho Guanine Nucleotide Exchange Factors. Journal of Chemical Information and Modeling, 2015, 55, 1878-1893.	5.4	24
28	Comparison of the isomerization mechanisms of human melanopsin and invertebrate and vertebrate rhodopsins. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 1714-1719.	7.1	59
29	Multiscale quantum chemical approaches to QSAR modeling and drug design. Drug Discovery Today, 2014, 19, 1921-1927.	6.4	21
30	Quaternary Structure Predictions and Structural Communication Features of GPCR Dimers. Progress in Molecular Biology and Translational Science, 2013, 117, 105-142.	1.7	14
31	Network Analysis to Uncover the Structural Communication in GPCRs. Methods in Cell Biology, 2013, 117, 43-61.	1.1	19
32	The catalytic site structural gate of adenosine deaminase allosterically modulates ligand binding to adenosine receptors. FASEB Journal, 2013, 27, 1048-1061.	0.5	35
33	A Mixed Protein Structure Network and Elastic Network Model Approach to Predict the Structural Communication in Biomolecular Systems: The PDZ2 Domain from Tyrosine Phosphatase 1E As a Case Study. Journal of Chemical Theory and Computation, 2013, 9, 2504-2518.	5.3	52
34	Network and Atomistic Simulations Unveil the Structural Determinants of Mutations Linked to Retinal Diseases. PLoS Computational Biology, 2013, 9, e1003207.	3.2	31
35	Light on the structural communication in Ras GTPases. Journal of Biomolecular Structure and Dynamics, 2013, 31, 142-157.	3.5	19
36	Nucleotide Binding Affects Intrinsic Dynamics and Structural Communication in Ras GTPases. Current Pharmaceutical Design, 2013, 19, 4214-4225.	1.9	12

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37	The KDEL receptor couples to Gî±_{q/11}to activate Src kinases and regulate transport through the Golgi. EMBO Journal, 2012, 31, 2869-2881.	7.8	105
38	Modeling the Structural Communication in Supramolecular Complexes Involving GPCRs. Methods in Molecular Biology, 2012, 914, 319-336.	0.9	4
39	Dimerization and ligand binding affect the structure network of A2A adenosine receptor. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 1256-1266.	2.6	59
40	Update 1 of: Computational Modeling Approaches to Structureâ€"Function Analysis of G Protein-Coupled Receptors. Chemical Reviews, 2011, 111, PR438-PR535.	47.7	71
41	Conserved amino acids participate in the structure networks deputed to intramolecular communication in the lutropin receptor. Cellular and Molecular Life Sciences, 2011, 68, 1227-1239.	5.4	54
42	Light on the structure of thromboxane A2 receptor heterodimers. Cellular and Molecular Life Sciences, 2011, 68, 3109-3120.	5.4	23
43	Wordom: A userâ€friendly program for the analysis of molecular structures, trajectories, and free energy surfaces. Journal of Computational Chemistry, 2011, 32, 1183-1194.	3.3	232
44	The Extreme C-Terminal Region of Gî±s Differentially Couples to the Luteinizing Hormone and Î²2-Adrenergic Receptors. Molecular Endocrinology, 2011, 25, 1416-1430.	3.7	9
45	Nucleotide Binding Switches the Information Flow in Ras GTPases. PLoS Computational Biology, 2011, 7, e1001098.	3.2	39
46	Superactive mutants of thromboxane prostanoid receptor: functional and computational analysis of an active form alternative to constitutively active mutants. Cellular and Molecular Life Sciences, 2010, 67, 2979-2989.	5.4	14
47	Deciphering the Deformation Modes Associated with Function Retention and Specialization in Members of the Ras Superfamily. Structure, 2010, 18, 402-414.	3.3	46
48	Computational quantum chemistry and adaptive ligand modeling in mechanistic QSAR. Drug Discovery Today, 2010, 15, 859-866.	6.4	25
49	Structureâ€"activity relationships in 1,4-benzodioxan-related compounds. 10. Novel Î±1-adrenoreceptor antagonists related to openphendioxan: Synthesis, biological evaluation, and Î±1d computational study. Bioorganic and Medicinal Chemistry, 2010, 18, 7065-7077.	3.0	12
50	Structural insights into retinitis pigmentosa from unfolding simulations of rhodopsin mutants. FASEB Journal, 2010, 24, 3196-3209.	0.5	39
51	The luteinizing hormone receptor: Insights into structureâ€"function relationships and hormone-receptor-mediated changes in gene expression in ovarian cancer cells. Molecular and Cellular Endocrinology, 2010, 329, 47-55.	3.2	32
52	Computational Screening of Rhodopsin Mutations Associated with Retinitis Pigmentosa. Journal of Chemical Theory and Computation, 2009, 5, 2472-2485.	5.3	12
53	Network-level analysis of light adaptation in rod cells under normal and altered conditions. Molecular BioSystems, 2009, 5, 1232.	2.9	45
54	Adenosine A_{2A} Receptor-Antagonist/Dopamine D₂ Receptor-Agonist Bivalent Ligands as Pharmacological Tools to Detect A_{2A}-D₂ Receptor Heteromers. Journal of Medicinal Chemistry, 2009, 52, 5590-5602.	6.4	129

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55	Computational Modeling of Intramolecular and Intermolecular Communication in GPCRs. Current Protein and Peptide Science, 2009, 10, 173-185.	1.4	16
56	Ligand-Receptor Communication and Drug Design. Current Protein and Peptide Science, 2009, 10, 186-193.	1.4	7
57	Dark and photoactivated rhodopsin share common binding modes to transducin. FEBS Letters, 2008, 582, 991-996.	2.8	13
58	Homodimerization of Neurotensin 1 Receptor Involves Helices 1, 2, and 4: Insights from Quaternary Structure Predictions and Dimerization Free Energy Estimations. Journal of Chemical Information and Modeling, 2008, 48, 1669-1678.	5.4	31
59	Quaternary structure predictions and estimation of mutational effects on the free energy of dimerization of the OMPLA protein. Journal of Structural Biology, 2008, 163, 155-162.	2.8	8
60	Target Flexibility: An Emerging Consideration in Drug Discovery and Design. Journal of Medicinal Chemistry, 2008, 51, 6237-6255.	6.4	280
61	Mechanisms of Inter- and Intramolecular Communication in GPCRs and G Proteins. Journal of the American Chemical Society, 2008, 130, 4310-4325.	13.7	37
62	An Intracellular Loop (IL2) Residue Confers Different Basal Constitutive Activities to the Human Lutropin Receptor and Human Thyrotropin Receptor through Structural Communication between IL2 and Helix 6, via Helix 3. Endocrinology, 2008, 149, 1705-1717.	2.8	29
63	Contributions of Intracellular Loops 2 and 3 of the Lutropin Receptor in Gs Coupling. Molecular Endocrinology, 2008, 22, 126-138.	3.7	26
64	Intrinsic Differences in the Response of the Human Lutropin Receptor Versus the Human Follitropin Receptor to Activating Mutations. Journal of Biological Chemistry, 2007, 282, 25527-25539.	3.4	44
65	Dimerization of the lutropin receptor: Insights from computational modeling. Molecular and Cellular Endocrinology, 2007, 260-262, 59-64.	3.2	33
66	A functional transmembrane complex: The luteinizing hormone receptor with bound ligand and G protein. Molecular and Cellular Endocrinology, 2007, 260-262, 126-136.	3.2	63
67	Monomeric dark rhodopsin holds the molecular determinants for transducin recognition: Insights from computational analysis. FEBS Letters, 2007, 581, 944-948.	2.8	21
68	In Silico Screening of Mutational Effects on Transmembrane Helix Dimerization:â€‰ Insights from Rigid-Body Docking and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 9114-9124.	2.6	20
69	In silico screening of mutational effects on enzyme-proteic inhibitor affinity: a docking-based approach. BMC Structural Biology, 2007, 7, 37.	2.3	17
70	Sequential Unfolding of Individual Helices of Bacterioopsin Observed in Molecular Dynamics Simulations of Extraction from the Purple Membrane. Biophysical Journal, 2006, 91, 3276-3284.	0.5	13
71	Prediction of MEF2Aâ€“DNA interface by rigid body docking: A tool for fast estimation of protein mutational effects on DNA binding. Journal of Structural Biology, 2006, 153, 278-283.	2.8	28
72	Inactive and active states and supramolecular organization of GPCRs: insights from computational modeling. Journal of Computer-Aided Molecular Design, 2006, 20, 449-461.	2.9	26

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73	Quaternary structure predictions of transmembrane proteins starting from the monomer: a docking-based approach. BMC Bioinformatics, 2006, 7, 340.	2.6	45
74	Structure-Function Relationships of the Luteinizing Hormone Receptor. Annals of the New York Academy of Sciences, 2005, 1061, 41-54.	3.8	26
75	Computational Modeling Approaches to Structureâ€"Function Analysis of G Protein-Coupled Receptors. ChemInform, 2005, 36, no.	0.0	0
76	Different Structural Requirements for the Constitutive and the Agonist-induced Activities of the Î²2-Adrenergic Receptor. Journal of Biological Chemistry, 2005, 280, 23464-23474.	3.4	13
77	The Formation of a Salt Bridge Between Helices 3 and 6 Is Responsible for the Constitutive Activity and Lack of Hormone Responsiveness of the Naturally Occurring L457R Mutation of the Human Lutropin Receptor. Journal of Biological Chemistry, 2005, 280, 26169-26176.	3.4	52
78	Rhodopsin Activation Follows Precoupling with Transducin:â€‰ Inferences from Computational Analysis,. Biochemistry, 2005, 44, 14695-14700.	2.5	40
79	The DRY Motif as a Molecular Switch of the Human Oxytocin Receptor. Biochemistry, 2005, 44, 9990-10008.	2.5	39
80	Probing Fragment Complementation by Rigid-Body Docking:â€‰ in Silico Reconstitution of Calbindin D9k. Journal of Chemical Information and Modeling, 2005, 45, 1429-1438.	5.4	15
81	Computational Modeling Approaches to Structureâ"Function Analysis of G Protein-Coupled Receptors. Chemical Reviews, 2005, 105, 3297-3351.	47.7	158
82	Insight into Mutation-Induced Activation of the Luteinizing Hormone Receptor: Molecular Simulations Predict the Functional Behavior of Engineered Mutants at M398. Molecular Endocrinology, 2004, 18, 1499-1508.	3.7	35
83	Structural determinants involved in the activation and regulation of G proteinâ€coupled receptors: lessons from the alpha1â€adrenegic receptor subtypes. Biology of the Cell, 2004, 96, 327-333.	2.0	13
84	Structural features of the inactive and active states of the melanin-concentrating hormone receptors: Insights from molecular simulations. Proteins: Structure, Function and Bioinformatics, 2004, 56, 430-448.	2.6	22
85	Synthesis, Screening, and Molecular Modeling of New Potent and Selective Antagonists at the Î±1dAdrenergic Receptor. Journal of Medicinal Chemistry, 2004, 47, 1900-1918.	6.4	52
86	Adenosine A2A-dopamine D2 receptorâ€"receptor heteromers. Targets for neuro-psychiatric disorders. Parkinsonism and Related Disorders, 2004, 10, 265-271.	2.2	132
87	Structural determinants involved in the activation and regulation of G protein-coupled receptors: lessons from the alpha1-adrenegic receptor subtypes. Biology of the Cell, 2004, 96, 327-333.	2.0	11
88	Molecular Dynamics Simulations of the Ligand-Induced Chemical Information Transfer in the 5-HT1A Receptor.. ChemInform, 2003, 34, no.	0.0	0
89	Molecular Dynamics Simulations of the Ligand-Induced Chemical Information Transfer in the 5-HT1AReceptor. Journal of Chemical Information and Computer Sciences, 2003, 43, 1520-1531.	2.8	29
90	Adenosine A2A-Dopamine D2 Receptor-Receptor Heteromerization. Journal of Biological Chemistry, 2003, 278, 46741-46749.	3.4	401

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91	Constitutively Active G Protein-Coupled Receptor Mutants: Implications on Receptor Function and Drug Action. Assay and Drug Development Technologies, 2003, 1, 311-316.	1.2	15
92	Mutagenesis and Modelling of the Î±1b-Adrenergic Receptor Highlight the Role of the Helix 3/Helix 6 Interface in Receptor Activation. Molecular Pharmacology, 2002, 61, 1025-1032.	2.3	114
93	A Model for Constitutive Lutropin Receptor Activation Based on Molecular Simulation and Engineered Mutations in Transmembrane Helices 6 and 7. Journal of Biological Chemistry, 2002, 277, 32202-32213.	3.4	67
94	The Lutropin/Choriogonadotropin Receptor, A 2002 Perspective. Endocrine Reviews, 2002, 23, 141-174.	20.1	671
95	THE Î±1b-ADRENERGIC RECEPTOR SUBTYPE: MOLECULAR PROPERTIES AND PHYSIOLOGICAL IMPLICATIONS. Journal of Receptor and Signal Transduction Research, 2002, 22, 1-16.	2.5	11
96	Structural Aspects of Luteinizing Hormone Receptor: Information from Molecular Modeling and Mutagenesis. Endocrine, 2002, 18, 285-294.	2.2	15
97	The Lutropin/Choriogonadotropin Receptor, A 2002 Perspective. , 2002, 23, 141-174.		167
98	Understanding the Mutation-Induced Activation of the Lutropin Receptor from Computer Simulation. , 2002, , 29-38.		0
99	Phenylpiperazinylalkylamino Substituted Pyridazinones as Potent Î±1Adrenoceptor Antagonists. Journal of Medicinal Chemistry, 2001, 44, 2403-2410.	6.4	28
100	Lutropin Receptor Function: Insights from Natural, Engineered, and Computer-Simulated Mutations. IUBMB Life, 2001, 51, 149-155.	3.4	21
101	Mutational and Computational Analysis of the Î±1b-Adrenergic Receptor. Journal of Biological Chemistry, 2001, 276, 46485-46494.	3.4	73
102	Pleiotropic Effects of Substitutions of a Highly Conserved Leucine in Transmembrane Helix III of the Human Lutropin/Choriogonadotropin Receptor with Respect to Constitutive Activation and Hormone Responsiveness. Molecular Endocrinology, 2001, 15, 972-984.	3.7	38
103	Pleiotropic Effects of Substitutions of a Highly Conserved Leucine in Transmembrane Helix III of the Human Lutropin/Choriogonadotropin Receptor with Respect to Constitutive Activation and Hormone Responsiveness. Molecular Endocrinology, 2001, 15, 972-984.	3.7	15
104	The Î±1a and Î±1b-adrenergic receptor subtypes: molecular mechanisms of receptor activation and of drug action. Pharmacochemistry Library, 2000, 31, 173-179.	0.1	0
105	Molecular basis of ligand binding and receptor activation in the oxytocin and vasopressin receptor family. Experimental Physiology, 2000, 85, 59s-66s.	2.0	30
106	The ad hoc supermolecule approach to receptor ligand design. Computational and Theoretical Chemistry, 2000, 503, 1-16.	1.5	7
107	The Î±1a and Î±1b-adrenergic receptor subtypes: molecular mechanisms of receptor activation and of drug action. Pharmaceutica Acta Helvetiae, 2000, 74, 173-179.	1.2	14
108	Theoretical investigation of substrate specificity for cytochromes P450 IA2, P450 IID6 and P450 IIIA4. Journal of Computer-Aided Molecular Design, 2000, 14, 93-116.	2.9	59

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109	Gonadotropin-Independent Precocious Puberty Due to Luteinizing Hormone Receptor Mutations in Brazilian Boys: A Novel Constitutively Activating Mutation in the First Transmembrane Helix1. Journal of Clinical Endocrinology and Metabolism, 2000, 85, 4799-4805.	3.6	49
110	Theoretical study on mutation-induced activation of the luteinizing hormone receptor 1 1Edited by F. E. Cohen. Journal of Molecular Biology, 2000, 296, 1333-1351.	4.2	45
111	Gonadotropin-Independent Precocious Puberty Due to Luteinizing Hormone Receptor Mutations in Brazilian Boys: A Novel Constitutively Activating Mutation in the First Transmembrane Helix. Journal of Clinical Endocrinology and Metabolism, 2000, 85, 4799-4805.	3.6	50
112	Mutational analysis of the highly conserved arginine within the Glu/Asp-Arg-Tyr motif of the alpha(1b)-adrenergic receptor: effects on receptor isomerization and activation. Molecular Pharmacology, 2000, 57, 219-31.	2.3	93
113	Inverse Agonism and Neutral Antagonism at Î±_{1a}- and Î±_{1b}-Adrenergic Receptor Subtypes. Molecular Pharmacology, 1999, 56, 858-866.	2.3	86
114	Activation Mechanism of Human Oxytocin Receptor: A Combined Study of Experimental and Computer-Simulated Mutagenesis. Molecular Pharmacology, 1999, 56, 214-225.	2.3	88
115	Theoretical study on receptor-G protein recognition: New insights into the mechanism of the ?1b-adrenergic receptor activation. International Journal of Quantum Chemistry, 1999, 73, 71-83.	2.0	19
116	Theoretical study of the electrostatically driven step of receptor-G protein recognition. , 1999, 37, 145-156.		31
117	Structure-Function Relationships of the α_{1b}-Adrenergic Receptor. European Urology, 1999, 36, 11-16.	1.9	7
118	Theoretical study on receptorâ€“G protein recognition: New insights into the mechanism of the Î±1bâ€adrenergic receptor activation. International Journal of Quantum Chemistry, 1999, 73, 71-83.	2.0	1
119	Theoretical study of the electrostatically driven step of receptor-G protein recognition. Proteins: Structure, Function and Bioinformatics, 1999, 37, 145-56.	2.6	9
120	Molecular mechanisms involved in the activation and regulation of the Î±1-adrenergic receptor subtypes. Il Farmaco, 1998, 53, 273-277.	0.9	9
121	Isoxazolo-[3,4- d]-pyridazin-7-(6 H)-ones and their Corresponding 4,5-Disubstituted-3-(2 H) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T f 5 Modeling, and Binding Studies. Bioorganic and Medicinal Chemistry, 1998, 6, 925-935.	3.0	33
122	Hydrophobicity of Residue351of the G Protein Gi1Î± Determines the Extent of Activation by the Î±2A-Adrenoceptorâ€. Biochemistry, 1998, 37, 11555-11562.	2.5	87
123	Computer Modeling of Size and Shape Descriptors of Î±1-Adrenergic Receptor Antagonists and Quantitative Structureâ€“Affinity/Selectivity Relationships. Methods, 1998, 14, 239-254.	3.8	14
124	Ab InitioModeling and Molecular Dynamics Simulation of the Î±1b-Adrenergic Receptor Activation. Methods, 1998, 14, 302-317.	3.8	38
125	Identification of a Constitutively Active Mutant of the Human Oxytocin Receptor. Advances in Experimental Medicine and Biology, 1998, 449, 367-369.	1.6	3
126	The activation process of the Â1B-adrenergic receptor: Potential role of protonation and hydrophobicity of a highly conserved aspartate. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 808-813.	7.1	207

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127	Constitutively active Î±1B-adrenergic receptor mutants: Potential mechanisms underlying receptor activation. Pharmacochemistry Library, 1997, 28, 421-431.	0.1	0
128	Conformational analysis and theoretical quantitative size and shape-affinity relationships of N4-protonated N1-arylpiperazine 5-HT1A serotoninergic ligands. Computational and Theoretical Chemistry, 1997, 397, 129-145.	1.5	11
129	Î±1-Adrenoceptor subtype selectivity: Molecular modelling and theoretical quantitative structureâ€"affinity relationships. Bioorganic and Medicinal Chemistry, 1997, 5, 809-816.	3.0	27
130	Theoretical investigation of IL-6 multiprotein receptor assembly. , 1997, 29, 528-548.		9
131	Amino acids of theÎ±1B-adrenergic receptor involved in agonist binding: differences in docking catecholamines to receptor subtypes. FEBS Letters, 1996, 399, 9-13.	2.8	70
132	Molecular mechanisms underlying the activation and regulation of the Î±1B-adrenergic receptor. Biochemical Society Transactions, 1996, 24, 959-963.	3.4	2
133	MOLECULAR MECHANISMS UNDERLYING THE ACTIVATION AND REGULATION OF THE Î±1-ADRENERGIC RECEPTOR. Biochemical Society Transactions, 1996, 24, 517S-517S.	3.4	0
134	Constitutively active mutants of the alpha 1B-adrenergic receptor: role of highly conserved polar amino acids in receptor activation.. EMBO Journal, 1996, 15, 3566-3578.	7.8	338
135	Computational simulations of stem-cell factor/c-Kit receptor interaction. , 1996, 26, 42-54.		2
136	Constitutively active mutants of the alpha 1B-adrenergic receptor: role of highly conserved polar amino acids in receptor activation. EMBO Journal, 1996, 15, 3566-78.	7.8	95
137	Molecular dynamics simulations of m3-muscarinic receptor activation and QSAR analysis. Bioorganic and Medicinal Chemistry, 1995, 3, 1465-1477.	3.0	20
138	Theoretical quantitative structure-activity relationship analysis of congeneric and non-congeneric Î±1-adrenoceptor antagonists: a chemometric study. Computational and Theoretical Chemistry, 1995, 331, 79-93.	1.5	26
139	Quantitative structure-affinity/selectivity relationship analysis on three-dimensional models of the complexes between the ETA and ETB receptors and C-terminal endothelin hexapeptide antagonists. Computational and Theoretical Chemistry, 1995, 333, 243-248.	1.5	5
140	Comparative molecular dynamics study of the seven-helix bundle arrangement of G-protein coupled receptors. Computational and Theoretical Chemistry, 1995, 333, 49-69.	1.5	18
141	Prototropic molecular forms and theoretical descriptors in QSAR analysis. Computational and Theoretical Chemistry, 1995, 333, 1-17.	1.5	11
142	Computer simulations of signal transduction mechanism in Î±1B-adrenergic and m3-muscarinic receptors. Protein Engineering, Design and Selection, 1995, 8, 557-564.	2.1	20
143	Theoretical quantitative structureâ€"activity relationship analysis on three dimensional models of ligandâ€"m1 muscarinic receptor complexes. Bioorganic and Medicinal Chemistry, 1994, 2, 195-211.	3.0	23
144	The heuristic-direct approach to theoretical quantitative structure-activity relationship analysis of Î±1-adrenoceptor ligands. Computational and Theoretical Chemistry, 1994, 314, 265-276.	1.5	13

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145	Theoretical quantitative size and shape activity and selectivity analyses of 5-HT1A serotonin and Î±1-adrenergic receptor ligands. Computational and Theoretical Chemistry, 1994, 305, 101-110.	1.5	16
146	Enantiomeric resolution of sulfoxides on a DACH-DNB chiral stationary phase: A quantitative structure-enantioselective retention relationship (QSERR) study. Chirality, 1993, 5, 527-537.	2.6	44
147	Theoretical quantitative structure-activity analysis and pharmacophore modelling of selective non-congeneric Î±1a-adrenergic antagonists. Computational and Theoretical Chemistry, 1993, 280, 283-290.	1.5	14
148	The heuristic-direct approach to quantitative structure-activity relationship analysis. Computational and Theoretical Chemistry, 1993, 285, 147-153.	1.5	18
149	Theoretical quantitative structure-activity analysis of quinuclidine-based muscarinic cholinergic receptor ligands. Computational and Theoretical Chemistry, 1993, 283, 63-71.	1.5	11
150	Molecular modelling and quantitative structure- activity relationship analysis using theoretical descriptors of 1,4-benzodioxan (WB-4101) related compounds Î±1-adrenergic antagonists. Computational and Theoretical Chemistry, 1992, 276, 327-340.	1.5	20
151	Conformational analysis, molecular modeling and quantitative structure-activity relationship studies of 2,4-diamino-6,7-dimethoxy-2-substituted quinazoline Î±1-adrenergic antagonists. Computational and Theoretical Chemistry, 1991, 251, 307-318.	1.5	20
152	Chapter 8. Uncovering GPCR and G Protein Function by Protein Structure Network Analysis. Chemical Biology, 0, , 198-220.	0.2	1