

# Francesca Fanelli

## List of Publications by Year in descending order

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151  
papers

6,834  
citations

71061

41  
h-index

74108

75  
g-index

157  
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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.	1.9	17
2	Frontiers in Multiscale Modeling of Photoreceptor Proteins. Photochemistry and Photobiology, 2021, 97, 243-269.	1.3	26
3	Structural aspects of rod opsin and their implication in genetic diseases. Pflugers Archiv European Journal of Physiology, 2021, 473, 1339-1359.	1.3	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.	1.9	4
5	ETNK1 mutations induce a mutator phenotype that can be reverted with phosphoethanolamine. Nature Communications, 2020, 11, 5938.	5.8	22
6	Dynamics and structural communication in the ternary complex of fully phosphorylated V2 vasopressin receptor, vasopressin, and $\beta^2$ -arrestin 1. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183355.	1.4	6
7	webPSN v2.0: a webserver to infer fingerprints of structural communication in biomacromolecules. Nucleic Acids Research, 2020, 48, W94-W103.	6.5	56
8	Integrated structural modeling and super-resolution imaging resolve GPCR oligomers. Progress in Molecular Biology and Translational Science, 2020, 169, 151-179.	0.9	5
9	Membrane Estrogen Receptor (GPER) and Follicle-Stimulating Hormone Receptor (FSHR) Heteromeric Complexes Promote Human Ovarian Follicle Survival. IScience, 2020, 23, 101812.	1.9	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.	0.6	1
11	Interconnecting Flexibility, Structural Communication, and Function in RhoGEF Oncoproteins. Journal of Chemical Information and Modeling, 2019, 59, 4300-4313.	2.5	13
12	Frontal Variant of Alzheimer's Disease: A Report of a Novel PSEN1 Mutation. Journal of Alzheimer's Disease, 2019, 70, 11-15.	1.2	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.	13.5	65
14	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.	2.3	44
15	Computational modeling approaches to quantitative structure-binding kinetics relationships in drug discovery. Drug Discovery Today, 2018, 23, 1396-1406.	3.2	20
16	A Small Chaperone Improves Folding and Routing of Rhodopsin Mutants Linked to Inherited Blindness. IScience, 2018, 4, 1-19.	1.9	50
17	Structural Determinants of Constitutive Activation of G $\beta\gamma$ Proteins: Transducin as a Paradigm. Journal of Chemical Theory and Computation, 2017, 13, 886-899.	2.3	10
18	Epilepsy and intellectual disability linked protein Shrm4 interaction with GABABRs shapes inhibitory neurotransmission. Nature Communications, 2017, 8, 14536.	5.8	31

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19	Dissecting intrinsic and ligand-induced structural communication in the $\hat{I}^{23}$ headpiece of integrins. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017, 1861, 2367-2381.	1.1	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. <i>Scientific Reports</i> , 2016, 6, 38425.	1.6	26
22	Small-Molecule Protein-Protein Interaction Inhibitor of Oncogenic Rho Signaling. <i>Cell Chemical Biology</i> , 2016, 23, 1135-1146.	2.5	28
23	Structure network analysis to gain insights into GPCR function. <i>Biochemical Society Transactions</i> , 2016, 44, 613-618.	1.6	21
24	WebPSN: a web server for high-throughput investigation of structural communication in biomacromolecules. <i>Bioinformatics</i> , 2015, 31, 779-781.	1.8	49
25	Single Molecule Analysis of Functionally Asymmetric G Protein-coupled Receptor (GPCR) Oligomers Reveals Diverse Spatial and Structural Assemblies. <i>Journal of Biological Chemistry</i> , 2015, 290, 3875-3892.	1.6	105
26	The intellectual disability protein RAB39B selectively regulates GluA2 trafficking to determine synaptic AMPAR composition. <i>Nature Communications</i> , 2015, 6, 6504.	5.8	93
27	Catching Functional Modes and Structural Communication in Dbl Family Rho Guanine Nucleotide Exchange Factors. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1878-1893.	2.5	24
28	Comparison of the isomerization mechanisms of human melanopsin and invertebrate and vertebrate rhodopsins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 1714-1719.	3.3	59
29	Multiscale quantum chemical approaches to QSAR modeling and drug design. <i>Drug Discovery Today</i> , 2014, 19, 1921-1927.	3.2	21
30	Quaternary Structure Predictions and Structural Communication Features of GPCR Dimers. <i>Progress in Molecular Biology and Translational Science</i> , 2013, 117, 105-142.	0.9	14
31	Network Analysis to Uncover the Structural Communication in GPCRs. <i>Methods in Cell Biology</i> , 2013, 117, 43-61.	0.5	19
32	The catalytic site structural gate of adenosine deaminase allosterically modulates ligand binding to adenosine receptors. <i>FASEB Journal</i> , 2013, 27, 1048-1061.	0.2	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. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2504-2518.	2.3	52
34	Network and Atomistic Simulations Unveil the Structural Determinants of Mutations Linked to Retinal Diseases. <i>PLoS Computational Biology</i> , 2013, 9, e1003207.	1.5	31
35	Light on the structural communication in Ras GTPases. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013, 31, 142-157.	2.0	19
36	Nucleotide Binding Affects Intrinsic Dynamics and Structural Communication in Ras GTPases. <i>Current Pharmaceutical Design</i> , 2013, 19, 4214-4225.	0.9	12

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37	The KDEL receptor couples to G $\alpha$ 11 to activate Src kinases and regulate transport through the Golgi. <i>EMBO Journal</i> , 2012, 31, 2869-2881.	3.5	105
38	Modeling the Structural Communication in Supramolecular Complexes Involving GPCRs. <i>Methods in Molecular Biology</i> , 2012, 914, 319-336.	0.4	4
39	Dimerization and ligand binding affect the structure network of A2A adenosine receptor. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2011, 1808, 1256-1266.	1.4	59
40	Update 1 of: Computational Modeling Approaches to Structure-Function Analysis of G Protein-Coupled Receptors. <i>Chemical Reviews</i> , 2011, 111, PR438-PR535.	23.0	71
41	Conserved amino acids participate in the structure networks deputed to intramolecular communication in the lutropin receptor. <i>Cellular and Molecular Life Sciences</i> , 2011, 68, 1227-1239.	2.4	54
42	Light on the structure of thromboxane A2 receptor heterodimers. <i>Cellular and Molecular Life Sciences</i> , 2011, 68, 3109-3120.	2.4	23
43	Wordom: A user-friendly program for the analysis of molecular structures, trajectories, and free energy surfaces. <i>Journal of Computational Chemistry</i> , 2011, 32, 1183-1194.	1.5	232
44	The Extreme C-Terminal Region of G $\alpha$ s Differentially Couples to the Luteinizing Hormone and $\beta$ 2-Adrenergic Receptors. <i>Molecular Endocrinology</i> , 2011, 25, 1416-1430.	3.7	9
45	Nucleotide Binding Switches the Information Flow in Ras GTPases. <i>PLoS Computational Biology</i> , 2011, 7, e1001098.	1.5	39
46	Superactive mutants of thromboxane prostanoid receptor: functional and computational analysis of an active form alternative to constitutively active mutants. <i>Cellular and Molecular Life Sciences</i> , 2010, 67, 2979-2989.	2.4	14
47	Deciphering the Deformation Modes Associated with Function Retention and Specialization in Members of the Ras Superfamily. <i>Structure</i> , 2010, 18, 402-414.	1.6	46
48	Computational quantum chemistry and adaptive ligand modeling in mechanistic QSAR. <i>Drug Discovery Today</i> , 2010, 15, 859-866.	3.2	25
49	Structure-activity relationships in 1,4-benzodioxan-related compounds. 10. Novel $\beta$ 1-adrenoreceptor antagonists related to openphendioxan: Synthesis, biological evaluation, and $\beta$ 1d computational study. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 7065-7077.	1.4	12
50	Structural insights into retinitis pigmentosa from unfolding simulations of rhodopsin mutants. <i>FASEB Journal</i> , 2010, 24, 3196-3209.	0.2	39
51	The luteinizing hormone receptor: Insights into structure-function relationships and hormone-receptor-mediated changes in gene expression in ovarian cancer cells. <i>Molecular and Cellular Endocrinology</i> , 2010, 329, 47-55.	1.6	32
52	Computational Screening of Rhodopsin Mutations Associated with Retinitis Pigmentosa. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2472-2485.	2.3	12
53	Network-level analysis of light adaptation in rod cells under normal and altered conditions. <i>Molecular BioSystems</i> , 2009, 5, 1232.	2.9	45
54	Adenosine A <sub>2A</sub> Receptor-Antagonist/Dopamine D <sub>2</sub> Receptor-Agonist Bivalent Ligands as Pharmacological Tools to Detect A <sub>2A</sub> -D <sub>2</sub> Receptor Heteromers. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 5590-5602.	2.9	129

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55	Computational Modeling of Intramolecular and Intermolecular Communication in GPCRs. <i>Current Protein and Peptide Science</i> , 2009, 10, 173-185.	0.7	16
56	Ligand-Receptor Communication and Drug Design. <i>Current Protein and Peptide Science</i> , 2009, 10, 186-193.	0.7	7
57	Dark and photoactivated rhodopsin share common binding modes to transducin. <i>FEBS Letters</i> , 2008, 582, 991-996.	1.3	13
58	Homodimerization of Neurotensin 1 Receptor Involves Helices 1, 2, and 4: Insights from Quaternary Structure Predictions and Dimerization Free Energy Estimations. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1669-1678.	2.5	31
59	Quaternary structure predictions and estimation of mutational effects on the free energy of dimerization of the OMPLA protein. <i>Journal of Structural Biology</i> , 2008, 163, 155-162.	1.3	8
60	Target Flexibility: An Emerging Consideration in Drug Discovery and Design. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 6237-6255.	2.9	280
61	Mechanisms of Inter- and Intramolecular Communication in GPCRs and G Proteins. <i>Journal of the American Chemical Society</i> , 2008, 130, 4310-4325.	6.6	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. <i>Endocrinology</i> , 2008, 149, 1705-1717.	1.4	29
63	Contributions of Intracellular Loops 2 and 3 of the Lutropin Receptor in Gs Coupling. <i>Molecular Endocrinology</i> , 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. <i>Journal of Biological Chemistry</i> , 2007, 282, 25527-25539.	1.6	44
65	Dimerization of the lutropin receptor: Insights from computational modeling. <i>Molecular and Cellular Endocrinology</i> , 2007, 260-262, 59-64.	1.6	33
66	A functional transmembrane complex: The luteinizing hormone receptor with bound ligand and G protein. <i>Molecular and Cellular Endocrinology</i> , 2007, 260-262, 126-136.	1.6	63
67	Monomeric dark rhodopsin holds the molecular determinants for transducin recognition: Insights from computational analysis. <i>FEBS Letters</i> , 2007, 581, 944-948.	1.3	21
68	In Silico Screening of Mutational Effects on Transmembrane Helix Dimerization: Insights from Rigid-Body Docking and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9114-9124.	1.2	20
69	In silico screening of mutational effects on enzyme-proteic inhibitor affinity: a docking-based approach. <i>BMC Structural Biology</i> , 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. <i>Biophysical Journal</i> , 2006, 91, 3276-3284.	0.2	13
71	Prediction of MEF2A-DNA interface by rigid body docking: A tool for fast estimation of protein mutational effects on DNA binding. <i>Journal of Structural Biology</i> , 2006, 153, 278-283.	1.3	28
72	Inactive and active states and supramolecular organization of GPCRs: insights from computational modeling. <i>Journal of Computer-Aided Molecular Design</i> , 2006, 20, 449-461.	1.3	26

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73	Quaternary structure predictions of transmembrane proteins starting from the monomer: a docking-based approach. <i>BMC Bioinformatics</i> , 2006, 7, 340.	1.2	45
74	Structure-Function Relationships of the Luteinizing Hormone Receptor. <i>Annals of the New York Academy of Sciences</i> , 2005, 1061, 41-54.	1.8	26
75	Computational Modeling Approaches to Structure-Function Analysis of G Protein-Coupled Receptors. <i>ChemInform</i> , 2005, 36, no.	0.1	0
76	Different Structural Requirements for the Constitutive and the Agonist-induced Activities of the $\beta$ 2-Adrenergic Receptor. <i>Journal of Biological Chemistry</i> , 2005, 280, 23464-23474.	1.6	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. <i>Journal of Biological Chemistry</i> , 2005, 280, 26169-26176.	1.6	52
78	Rhodopsin Activation Follows Precoupling with Transducin: Inferences from Computational Analysis. <i>Biochemistry</i> , 2005, 44, 14695-14700.	1.2	40
79	The DRY Motif as a Molecular Switch of the Human Oxytocin Receptor. <i>Biochemistry</i> , 2005, 44, 9990-10008.	1.2	39
80	Probing Fragment Complementation by Rigid-Body Docking: In Silico Reconstitution of Calbindin D9k. <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 1429-1438.	2.5	15
81	Computational Modeling Approaches to Structure-Function Analysis of G Protein-Coupled Receptors. <i>Chemical Reviews</i> , 2005, 105, 3297-3351.	23.0	158
82	Insight into Mutation-Induced Activation of the Luteinizing Hormone Receptor: Molecular Simulations Predict the Functional Behavior of Engineered Mutants at M398. <i>Molecular Endocrinology</i> , 2004, 18, 1499-1508.	3.7	35
83	Structural determinants involved in the activation and regulation of G protein-coupled receptors: lessons from the $\alpha$ 1-adrenergic receptor subtypes. <i>Biology of the Cell</i> , 2004, 96, 327-333.	0.7	13
84	Structural features of the inactive and active states of the melanin-concentrating hormone receptors: Insights from molecular simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 56, 430-448.	1.5	22
85	Synthesis, Screening, and Molecular Modeling of New Potent and Selective Antagonists at the $\beta$ 1-Adrenergic Receptor. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 1900-1918.	2.9	52
86	Adenosine A2A-dopamine D2 receptor-receptor heteromers. Targets for neuro-psychiatric disorders. <i>Parkinsonism and Related Disorders</i> , 2004, 10, 265-271.	1.1	132
87	Structural determinants involved in the activation and regulation of G protein-coupled receptors: lessons from the $\alpha$ 1-adrenergic receptor subtypes. <i>Biology of the Cell</i> , 2004, 96, 327-333.	0.7	11
88	Molecular Dynamics Simulations of the Ligand-Induced Chemical Information Transfer in the 5-HT1A Receptor. <i>ChemInform</i> , 2003, 34, no.	0.1	0
89	Molecular Dynamics Simulations of the Ligand-Induced Chemical Information Transfer in the 5-HT1A Receptor. <i>Journal of Chemical Information and Computer Sciences</i> , 2003, 43, 1520-1531.	2.8	29
90	Adenosine A2A-Dopamine D2 Receptor-Receptor Heteromerization. <i>Journal of Biological Chemistry</i> , 2003, 278, 46741-46749.	1.6	401

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91	Constitutively Active G Protein-Coupled Receptor Mutants: Implications on Receptor Function and Drug Action. <i>Assay and Drug Development Technologies</i> , 2003, 1, 311-316.	0.6	15
92	Mutagenesis and Modelling of the $\hat{1}\pm 1b$ -Adrenergic Receptor Highlight the Role of the Helix 3/Helix 6 Interface in Receptor Activation. <i>Molecular Pharmacology</i> , 2002, 61, 1025-1032.	1.0	114
93	A Model for Constitutive Lutropin Receptor Activation Based on Molecular Simulation and Engineered Mutations in Transmembrane Helices 6 and 7. <i>Journal of Biological Chemistry</i> , 2002, 277, 32202-32213.	1.6	67
94	The Lutropin/Choriogonadotropin Receptor, A 2002 Perspective. <i>Endocrine Reviews</i> , 2002, 23, 141-174.	8.9	671
95	THE $\hat{1}\pm 1b$ -ADRENERGIC RECEPTOR SUBTYPE: MOLECULAR PROPERTIES AND PHYSIOLOGICAL IMPLICATIONS. <i>Journal of Receptor and Signal Transduction Research</i> , 2002, 22, 1-16.	1.3	11
96	Structural Aspects of Luteinizing Hormone Receptor: Information from Molecular Modeling and Mutagenesis. <i>Endocrine</i> , 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	Phenylpiperazinyllalkylamino Substituted Pyridazinones as Potent $\hat{1}\pm 1$ Adrenoceptor Antagonists. <i>Journal of Medicinal Chemistry</i> , 2001, 44, 2403-2410.	2.9	28
100	Lutropin Receptor Function: Insights from Natural, Engineered, and Computer-Simulated Mutations. <i>IUBMB Life</i> , 2001, 51, 149-155.	1.5	21
101	Mutational and Computational Analysis of the $\hat{1}\pm 1b$ -Adrenergic Receptor. <i>Journal of Biological Chemistry</i> , 2001, 276, 46485-46494.	1.6	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. <i>Molecular Endocrinology</i> , 2001, 15, 972-984.	3.7	38
103	The $\hat{1}\pm 1a$ and $\hat{1}\pm 1b$ -adrenergic receptor subtypes: molecular mechanisms of receptor activation and of drug action. <i>Pharmacochemistry Library</i> , 2000, 31, 173-179.	0.1	0
104	Molecular basis of ligand binding and receptor activation in the oxytocin and vasopressin receptor family. <i>Experimental Physiology</i> , 2000, 85, 59s-66s.	0.9	30
105	The ad hoc supermolecule approach to receptor ligand design. <i>Computational and Theoretical Chemistry</i> , 2000, 503, 1-16.	1.5	7
106	The $\hat{1}\pm 1a$ and $\hat{1}\pm 1b$ -adrenergic receptor subtypes: molecular mechanisms of receptor activation and of drug action. <i>Pharmaceutica Acta Helvetiae</i> , 2000, 74, 173-179.	1.2	14
107	Theoretical investigation of substrate specificity for cytochromes P450 IA2, P450 IID6 and P450 IIIA4. <i>Journal of Computer-Aided Molecular Design</i> , 2000, 14, 93-116.	1.3	59
108	Gonadotropin-Independent Precocious Puberty Due to Luteinizing Hormone Receptor Mutations in Brazilian Boys: A Novel Constitutively Activating Mutation in the First Transmembrane Helix1. <i>Journal of Clinical Endocrinology and Metabolism</i> , 2000, 85, 4799-4805.	1.8	49

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109	Theoretical study on mutation-induced activation of the luteinizing hormone receptor 1 Edited by F. E. Cohen. <i>Journal of Molecular Biology</i> , 2000, 296, 1333-1351.	2.0	45
110	Gonadotropin-Independent Precocious Puberty Due to Luteinizing Hormone Receptor Mutations in Brazilian Boys: A Novel Constitutively Activating Mutation in the First Transmembrane Helix. <i>Journal of Clinical Endocrinology and Metabolism</i> , 2000, 85, 4799-4805.	1.8	50
111	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. <i>Molecular Pharmacology</i> , 2000, 57, 219-31.	1.0	93
112	Inverse Agonism and Neutral Antagonism at $\hat{1}\alpha$ - and $\hat{1}\beta$ -Adrenergic Receptor Subtypes. <i>Molecular Pharmacology</i> , 1999, 56, 858-866.	1.0	86
113	Activation Mechanism of Human Oxytocin Receptor: A Combined Study of Experimental and Computer-Simulated Mutagenesis. <i>Molecular Pharmacology</i> , 1999, 56, 214-225.	1.0	88
114	Theoretical study on receptor-G protein recognition: New insights into the mechanism of the $\beta$ -adrenergic receptor activation. <i>International Journal of Quantum Chemistry</i> , 1999, 73, 71-83.	1.0	19
115	Theoretical study of the electrostatically driven step of receptor-G protein recognition. , 1999, 37, 145-156.		31
116	Structure-Function Relationships of the $\alpha$ - $\beta$ -Adrenergic Receptor. <i>European Urology</i> , 1999, 36, 11-16.	0.9	7
117	Theoretical study on receptor-G protein recognition: New insights into the mechanism of the $\hat{1}\beta$ -adrenergic receptor activation. , 1999, 73, 71.		1
118	Theoretical study of the electrostatically driven step of receptor-G protein recognition. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 37, 145-56.	1.5	9
119	Molecular mechanisms involved in the activation and regulation of the $\hat{1}\beta$ -adrenergic receptor subtypes. <i>Il Farmaco</i> , 1998, 53, 273-277.	0.9	9
120	Isoxazolo-[3,4-d]-pyridazin-7-(6H)-ones and their Corresponding 4,5-Disubstituted-3-(2H)-Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 307 T Modeling, and Binding Studies. <i>Bioorganic and Medicinal Chemistry</i> , 1998, 6, 925-935.	1.4	33
121	Hydrophobicity of Residue 351 of the G Protein $\hat{1}\beta$ Determines the Extent of Activation by the $\hat{1}\beta$ -Adrenoceptor. <i>Biochemistry</i> , 1998, 37, 11555-11562.	1.2	87
122	Computer Modeling of Size and Shape Descriptors of $\hat{1}\beta$ -Adrenergic Receptor Antagonists and Quantitative Structure-Affinity/Selectivity Relationships. <i>Methods</i> , 1998, 14, 239-254.	1.9	14
123	Ab Initio Modeling and Molecular Dynamics Simulation of the $\hat{1}\beta$ -Adrenergic Receptor Activation. <i>Methods</i> , 1998, 14, 302-317.	1.9	38
124	Identification of a Constitutively Active Mutant of the Human Oxytocin Receptor. <i>Advances in Experimental Medicine and Biology</i> , 1998, 449, 367-369.	0.8	3
125	The activation process of the $\hat{1}\beta$ -adrenergic receptor: Potential role of protonation and hydrophobicity of a highly conserved aspartate. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1997, 94, 808-813.	3.3	207
126	Constitutively active $\hat{1}\beta$ -adrenergic receptor mutants: Potential mechanisms underlying receptor activation. <i>Pharmacology Library</i> , 1997, 28, 421-431.	0.1	0



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127	Conformational analysis and theoretical quantitative size and shape-affinity relationships of N4-protonated N1-arylpiperazine 5-HT1A serotonergic ligands. Computational and Theoretical Chemistry, 1997, 397, 129-145.	1.5	11
128	$\hat{1}$ -Adrenoceptor subtype selectivity: Molecular modelling and theoretical quantitative structure-affinity relationships. Bioorganic and Medicinal Chemistry, 1997, 5, 809-816.	1.4	27
129	Theoretical investigation of IL-6 multiprotein receptor assembly. , 1997, 29, 528-548.		9
130	Amino acids of the $\hat{1}$ B-adrenergic receptor involved in agonist binding: differences in docking catecholamines to receptor subtypes. FEBS Letters, 1996, 399, 9-13.	1.3	70
131	Molecular mechanisms underlying the activation and regulation of the $\hat{1}$ B-adrenergic receptor. Biochemical Society Transactions, 1996, 24, 959-963.	1.6	2
132	MOLECULAR MECHANISMS UNDERLYING THE ACTIVATION AND REGULATION OF THE $\hat{1}$ -ADRENERGIC RECEPTOR. Biochemical Society Transactions, 1996, 24, 517S-517S.	1.6	0
133	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.	3.5	338
134	Computational simulations of stem-cell factor/c-Kit receptor interaction. , 1996, 26, 42-54.		2
135	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.	3.5	95
136	Molecular dynamics simulations of m3-muscarinic receptor activation and QSAR analysis. Bioorganic and Medicinal Chemistry, 1995, 3, 1465-1477.	1.4	20
137	Theoretical quantitative structure-activity relationship analysis of congeneric and non-congeneric $\hat{1}$ -adrenoceptor antagonists: a chemometric study. Computational and Theoretical Chemistry, 1995, 331, 79-93.	1.5	26
138	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
139	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
140	Prototropic molecular forms and theoretical descriptors in QSAR analysis. Computational and Theoretical Chemistry, 1995, 333, 1-17.	1.5	11
141	Computer simulations of signal transduction mechanism in $\hat{1}$ B-adrenergic and m3-muscarinic receptors. Protein Engineering, Design and Selection, 1995, 8, 557-564.	1.0	20
142	Theoretical quantitative structure-activity relationship analysis on three dimensional models of ligand-m1 muscarinic receptor complexes. Bioorganic and Medicinal Chemistry, 1994, 2, 195-211.	1.4	23
143	The heuristic-direct approach to theoretical quantitative structure-activity relationship analysis of $\hat{1}$ -adrenoceptor ligands. Computational and Theoretical Chemistry, 1994, 314, 265-276.	1.5	13
144	Theoretical quantitative size and shape activity and selectivity analyses of 5-HT1A serotonin and $\hat{1}$ -adrenergic receptor ligands. Computational and Theoretical Chemistry, 1994, 305, 101-110.	1.5	16

#	ARTICLE	IF	CITATIONS
145	Enantiomeric resolution of sulfoxides on a DACH-DNB chiral stationary phase: A quantitative structure-enantioselective retention relationship (QSERR) study. <i>Chirality</i> , 1993, 5, 527-537.	1.3	44
146	Theoretical quantitative structure-activity analysis and pharmacophore modelling of selective non-congeneric $\hat{1}\pm 1\alpha$ -adrenergic antagonists. <i>Computational and Theoretical Chemistry</i> , 1993, 280, 283-290.	1.5	14
147	The heuristic-direct approach to quantitative structure-activity relationship analysis. <i>Computational and Theoretical Chemistry</i> , 1993, 285, 147-153.	1.5	18
148	Theoretical quantitative structure-activity analysis of quinuclidine-based muscarinic cholinergic receptor ligands. <i>Computational and Theoretical Chemistry</i> , 1993, 283, 63-71.	1.5	11
149	Molecular modelling and quantitative structure- activity relationship analysis using theoretical descriptors of 1,4-benzodioxan (WB-4101) related compounds $\hat{1}\pm 1$ -adrenergic antagonists. <i>Computational and Theoretical Chemistry</i> , 1992, 276, 327-340.	1.5	20
150	Conformational analysis, molecular modeling and quantitative structure-activity relationship studies of 2,4-diamino-6,7-dimethoxy-2-substituted quinazoline $\hat{1}\pm 1$ -adrenergic antagonists. <i>Computational and Theoretical Chemistry</i> , 1991, 251, 307-318.	1.5	20
151	Chapter 8. Uncovering GPCR and G Protein Function by Protein Structure Network Analysis. <i>Chemical Biology</i> , 0, , 198-220.	0.1	1