

CITATION REPORT

List of articles citing

The 2.6 angstrom crystal structure of a human A2A adenosine receptor bound to an antagonist

DOI: 10.1126/science.1164772
Science, 2008, 322, 1211-7.

Source: <https://exaly.com/paper-pdf/43583328/citation-report.pdf>

Version: 2024-04-25

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
1628	Discovery of Novel Adenosine Receptor Antagonists through a Combined Structure- and Ligand-Based Approach Followed by Molecular Dynamics Investigation of Ligand Binding Mode.		
1627	.		
1626	Purification of the human G protein-coupled receptor adenosine A(2a)R in a stable and functional form expressed in <i>Pichia pastoris</i> . 2012 , Chapter 29, Unit 29.4		2
1625	Radioligand binding analysis as a tool for quality control of GPCR production for structural characterization: adenosine A(2a)R as a template for study. 2012 , Chapter 29, Unit 29.3		
1624	G Protein-Coupled Receptors. 2004 , 1-11		
1623	. 2009 ,		14
1622	Adenosine. 2009 , 158, S16-S17		78
1621	Computing highly correlated positions using mutual information and graph theory for G protein-coupled receptors. 2009 , 4, e4681		20
1620	Comparative sequence and structural analyses of G-protein-coupled receptor crystal structures and implications for molecular models. 2009 , 4, e7011		63
1619	Diseases associated with mutations of the human lutropin receptor. 2009 , 89, 97-114		27
1618	Molecular modeling and QSAR-based design of histamine receptor ligands. 2009 , 4, 1061-75		3
1617	Multifaceted approach to determine the antagonist molecular mechanism and interaction of ibodutant ([1-(2-phenyl-1R-[[1-(tetrahydropyran-4-ylmethyl)-piperidin-4-ylmethyl]-carbamoyl]-ethylcarbamoyl)-cyclopentyl]-amide) at the human tachykinin NK2 receptor. 2009 , 329, 486-95		12
1616	Helix 8 of leukotriene B4 type-2 receptor is required for the folding to pass the quality control in the endoplasmic reticulum. 2009 , 23, 1470-81		23
1615	Structural basis of the interaction between chemokine stromal cell-derived factor-1/CXCL12 and its G-protein-coupled receptor CXCR4. 2009 , 284, 35240-50		118
1614	Structural rearrangements of rhodopsin subunits in a dimer complex: a molecular dynamics simulation study. 2009 , 27, 127-47		40
1613	The effect of ligand efficacy on the formation and stability of a GPCR-G protein complex. 2009 , 106, 9501-6		186
1612	The magnitude of the light-induced conformational change in different rhodopsins correlates with their ability to activate G proteins. 2009 , 284, 20676-83		43

1611	Characterization of the A2B adenosine receptor from mouse, rabbit, and dog. 2009 , 329, 2-13	31
1610	Identification of two distinct inactive conformations of the beta2-adrenergic receptor reconciles structural and biochemical observations. 2009 , 106, 4689-94	247
1609	Probing the role of the cation-pi interaction in the binding sites of GPCRs using unnatural amino acids. 2009 , 106, 11919-24	61
1608	Conserved waters mediate structural and functional activation of family A (rhodopsin-like) G protein-coupled receptors. 2009 , 106, 8555-60	201
1607	The C-terminal tail of CRTH2 is a key molecular determinant that constrains G α and downstream signaling cascade activation. 2009 , 284, 1324-36	51
1606	Thyroid stimulating autoantibody M22 mimics TSH binding to the TSH receptor leucine rich domain: a comparative structural study of protein-protein interactions. 2009 , 42, 381-95	27
1605	Structural and kinetic modeling of an activating helix switch in the rhodopsin-transducin interface. 2009 , 106, 10660-5	43
1604	8-azapurine nucleus: a versatile scaffold for different targets. 2009 , 9, 1367-78	13
1603	Customizing G Protein-coupled receptor models for structure-based virtual screening. 2009 , 15, 4026-48	62
1602	Chapter 11 Bacterial Membrane Proteins. 2009 , 63, 269-297	0
1601	Elucidation of binding sites of dual antagonists in the human chemokine receptors CCR2 and CCR5. 2009 , 75, 1325-36	48
1600	Small-molecule agonists for the thyrotropin receptor stimulate thyroid function in human thyrocytes and mice. 2009 , 106, 12471-6	85
1599	Activation induces structural changes in the liganded angiotensin II type 1 receptor. 2009 , 284, 26603-12	12
1598	Position 5.46 of the serotonin 5-HT _{2A} receptor contributes to a species-dependent variation for the 5-HT _{2C} agonist (R)-9-ethyl-1,3,4,10b-tetrahydro-7-trifluoromethylpyrazino[2,1-a]isoindol-6(2H)-one: impact on selectivity and toxicological evaluation. 2009 , 76, 1211-9	9
1597	Rastering strategy for screening and centring of microcrystal samples of human membrane proteins with a sub-10 microm size X-ray synchrotron beam. 2009 , 6 Suppl 5, S587-97	138
1596	Selection and characterization of DARPins specific for the neurotensin receptor 1. 2009 , 22, 357-66	31
1595	Topology of class A G protein-coupled receptors: insights gained from crystal structures of rhodopsins, adrenergic and adenosine receptors. 2009 , 75, 1-12	97
1594	New directions in conventional methods of protein crystallization. 2009 , 101, 3-12	45

1593	Engineering of recombinant crystallization chaperones. 2009 , 19, 449-57	115
1592	Membrane protein crystallization from lipidic phases. 2009 , 19, 372-8	68
1591	Engineering G protein-coupled receptors to facilitate their structure determination. 2009 , 19, 386-95	157
1590	Structural snapshots of conformational changes in a seven-helix membrane protein: lessons from bacteriorhodopsin. 2009 , 19, 433-9	59
1589	Discovery of new GPCR biology: one receptor structure at a time. 2009 , 17, 8-14	165
1588	A role for a specific cholesterol interaction in stabilizing the Apo configuration of the human A(2A) adenosine receptor. 2009 , 17, 1660-1668	100
1587	Passing the baton in class B GPCRs: peptide hormone activation via helix induction?. 2009 , 34, 303-10	162
1586	A G protein-coupled receptor at work: the rhodopsin model. 2009 , 34, 540-52	289
1585	G-protein-coupled receptor-focused drug discovery using a target class platform approach. 2009 , 14, 231-40	138
1584	A chemogenomic approach to drug discovery: focus on cardiovascular diseases. 2009 , 14, 479-85	52
1583	Identification of transmembrane domain 6 & 7 residues that contribute to the binding pocket of the urotensin II receptor. 2009 , 77, 1374-82	10
1582	X-ray structure breakthroughs in the GPCR transmembrane region. 2009 , 78, 11-20	96
1581	Structures of micelle-bound selected insect neuropeptides and analogues: implications for receptor selection. 2009 , 10, 2644-53	5
1580	Adenosine A2A receptor antagonists: new 8-substituted 9-ethyladenines as tools for in vivo rat models of Parkinson's disease. 2009 , 4, 1010-9	27
1579	Ligand and structure-based models for the prediction of ligand-receptor affinities and virtual screenings: Development and application to the beta(2)-adrenergic receptor. 2010 , 31, 707-20	36
1578	Prokaryotic expression, in vitro folding, and molecular pharmacological characterization of the neuropeptide Y receptor type 2. 2009 , 25, 1732-9	20
1577	Homology modelling of the human adenosine A2B receptor based on X-ray structures of bovine rhodopsin, the beta2-adrenergic receptor and the human adenosine A2A receptor. 2009 , 23, 807-28	33
1576	Computation of 3D queries for ROCS based virtual screens. 2009 , 23, 853-68	23

1575	Structural determinants for selective recognition of peptide ligands for endothelin receptor subtypes ETA and ETB. 2009 , 15, 479-91	23
1574	G-protein-coupled receptor structures were not built in a day. 2009 , 18, 1335-42	26
1573	Progress toward heterologous expression of active G-protein-coupled receptors in <i>Saccharomyces cerevisiae</i> : Linking cellular stress response with translocation and trafficking. 2009 , 18, 2356-70	45
1572	Engineering a G protein-coupled receptor for structural studies: stabilization of the BLT1 receptor ground state. 2009 , 18, 727-34	13
1571	Biophysical dissection of membrane proteins. 2009 , 459, 344-6	223
1570	The structure and function of G-protein-coupled receptors. 2009 , 459, 356-63	1583
1569	GPCRs: insane in the membrane. 2009 , 6, 929-933	8
1568	Crystallizing membrane proteins using lipidic mesophases. 2009 , 4, 706-31	516
1567	Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. 2009 , 8, 455-63	236
1566	High-level production and characterization of a G-protein coupled receptor signaling complex. 2009 , 276, 4515-28	5
1565	Comparative analysis of GPCR crystal structures. 2009 , 85, 425-30	39
1564	G-protein-coupled receptor heteromers or how neurons can display differently flavoured patterns in response to the same neurotransmitter. 2009 , 158, 23-31	16
1563	7TM RECEPTORS. 2009 , 158, S5-S101	2
1562	A highly conserved tryptophan residue in the fourth transmembrane domain of the A adenosine receptor is essential for ligand binding but not receptor homodimerization. 2009 , 110, 1352-62	11
1561	Antagonists of the human A(2A) receptor. Part 5: Highly bio-available pyrimidine-4-carboxamides. 2009 , 19, 2664-7	25
1560	Recent Advances in the Application of Solution NMR Spectroscopy to Multi-Span Integral Membrane Proteins. 2009 , 55, 335-360	132
1559	Toward the three-dimensional structure and lysophosphatidic acid binding characteristics of the LPA(4)/p2y(9)/GPR23 receptor: a homology modeling study. 2009 , 28, 70-9	7
1558	Docking and chemoinformatic screens for new ligands and targets. 2009 , 20, 429-36	147

1557	8-Bromo-9-alkyl adenine derivatives as tools for developing new adenosine A2A and A2B receptors ligands. 2009 , 17, 2812-22	44
1556	Molecular recognition in the P2Y(14) receptor: Probing the structurally permissive terminal sugar moiety of uridine-5'-diphosphoglucose. 2009 , 17, 5298-311	29
1555	Introduction to adenosine receptors as therapeutic targets. 2009 , 1-24	78
1554	NMR characterization of membrane protein-detergent micelle solutions by use of microcoil equipment. 2009 , 131, 18450-6	23
1553	On transversal hydrophobicity of some proteins and their modules. 2009 , 49, 1821-30	6
1552	[Prediction of the spatial structure of proteins: emphasis on membrane targets]. 2009 , 35, 744-60	
1551	Functionalized congeners of A3 adenosine receptor-selective nucleosides containing a bicyclo[3.1.0]hexane ring system. 2009 , 52, 7580-92	40
1550	Allosteric functional switch of neurokinin A-mediated signaling at the neurokinin NK2 receptor: structural exploration. 2009 , 52, 5999-6011	12
1549	New insight into the binding mode of peptide ligands at Urotensin-II receptor: structure-activity relationships study on PSU and urantide. 2009 , 52, 3927-40	21
1548	Enhanced potency of nucleotide-dendrimer conjugates as agonists of the P2Y14 receptor: multivalent effect in G protein-coupled receptor recognition. 2009 , 20, 1650-9	21
1547	Pyrido[2,3-e]-1,2,4-triazolo[4,3-a]pyrazin-1-one as a new scaffold to develop potent and selective human A3 adenosine receptor antagonists. Synthesis, pharmacological evaluation, and ligand-receptor modeling studies. 2009 , 52, 2407-19	33
1546	PEGylated dendritic unimolecular micelles as versatile carriers for ligands of G protein-coupled receptors. 2009 , 20, 1888-98	30
1545	Functionalized congener approach to the design of ligands for G protein-coupled receptors (GPCRs). 2009 , 20, 1816-35	41
1544	Elucidation of the molecular basis of cholecystokinin Peptide docking to its receptor using site-specific intrinsic photoaffinity labeling and molecular modeling. 2009 , 48, 5303-12	22
1543	Amphipol-assisted in vitro folding of G protein-coupled receptors. 2009 , 48, 6516-21	90
1542	Anticonvulsant Met-enkephalin analogues containing backbone spacers reveal alternative non-opioid signaling in the brain. 2009 , 4, 659-71	11
1541	Chapter 13 Recent Advances in Adenosine Receptor (AR) Ligands in Pulmonary Diseases. 2009 , 265-277	5
1540	Nucleoside-5'-monophosphates as prodrugs of adenosine A2A receptor agonists activated by ecto-5'-nucleotidase. 2009 , 52, 7669-77	56

1539	Molecular basis of glucagon-like peptide 1 docking to its intact receptor studied with carboxyl-terminal photolabile probes. 2009 , 284, 34135-44	35
1538	From purified GPCRs to drug discovery: the promise of protein-based methodologies. 2009 , 9, 629-35	29
1537	Comparison of functional non-glycosylated GPCRs expression in <i>Pichia pastoris</i> . 2009 , 380, 271-6	34
1536	Fluorescence-based optimization of human bitter taste receptor expression in <i>Saccharomyces cerevisiae</i> . 2009 , 382, 704-10	13
1535	Ligand binding and micro-switches in 7TM receptor structures. 2009 , 30, 249-59	269
1534	Multiple switches in G protein-coupled receptor activation. 2009 , 30, 494-502	99
1533	The promiscuous mGlu5 receptor--a range of partners for therapeutic possibilities?. 2009 , 30, 617-23	40
1532	Distinct binding mode of 125I-AngII to AT1 receptor without the Cys18-Cys274 disulfide bridge. 2009 , 158, 14-8	2
1531	Expression, purification and in vitro functional reconstitution of the chemokine receptor CCR1. 2009 , 66, 73-81	26
1530	Role of helix 8 in G protein-coupled receptors based on structure-function studies on the type 1 angiotensin receptor. 2009 , 302, 118-27	47
1529	Thermostabilization of the neurotensin receptor NTS1. 2009 , 390, 262-77	133
1528	Uropathogenic <i>E. coli</i> adhesin-induced host cell receptor conformational changes: implications in transmembrane signaling transduction. 2009 , 392, 352-61	39
1527	Ligand entry and exit pathways in the beta2-adrenergic receptor. 2009 , 392, 1102-15	80
1526	In silico study of naphtha [1, 2-d] thiazol-2-amine with adenosine A2A receptor and its role in antagonism of haloperidol-induced motor impairments in mice. 2009 , 463, 215-8	14
1525	Evaluation of homology modeling of G-protein-coupled receptors in light of the A(2A) adenosine receptor crystallographic structure. 2009 , 52, 3284-92	85
1524	Identification of amino acids at two dimer interface regions of the alpha-factor receptor (Ste2). 2009 , 48, 7132-9	29
1523	Chapter 4 Monoacylglycerols. 2009 , 63, 83-108	27
1522	Structure of a double transmembrane fragment of a G-protein-coupled receptor in micelles. 2009 , 96, 3187-96	30

1521	Location, structure, and dynamics of the synthetic cannabinoid ligand CP-55,940 in lipid bilayers. 2009 , 96, 4916-24	32
1520	Overview of computational methods employed in early-stage drug discovery. 2009 , 1, 49-63	8
1519	2-Phenylpyrazolo[4,3-d]pyrimidin-7-one as a new scaffold to obtain potent and selective human A3 adenosine receptor antagonists: new insights into the receptor-antagonist recognition. 2009 , 52, 7640-52	51
1518	Tuning microbial hosts for membrane protein production. 2009 , 8, 69	60
1517	Crystallizing membrane proteins for structure determination: use of lipidic mesophases. 2009 , 38, 29-51	183
1516	Molecular modeling and docking studies of human 5-hydroxytryptamine 2A (5-HT _{2A}) receptor for the identification of hotspots for ligand binding. 2009 , 5, 1877-88	32
1515	Definition of the G protein-coupled receptor transmembrane bundle binding pocket and calculation of receptor similarities for drug design. 2009 , 52, 4429-42	86
1514	Strategies for the cloning and expression of membrane proteins. 2009 , 76, 43-86	10
1513	Predictions of binding for dopamine D2 receptor antagonists by the SIE method. 2009 , 49, 2369-75	22
1512	Modern homology modeling of G-protein coupled receptors: which structural template to use?. 2009 , 52, 5207-16	139
1511	Sequence-derived three-dimensional pharmacophore models for G-protein-coupled receptors and their application in virtual screening. 2009 , 52, 2923-32	60
1510	Dopamine D ₂ , D ₃ , and D ₄ selective phenylpiperazines as molecular probes to explore the origins of subtype specific receptor binding. 2009 , 52, 4923-35	75
1509	Computational Approaches in Peptide and Protein Design: An Overview. 2009 , 5-48	2
1508	Design of Cyclic Peptides. 2009 , 133-176	17
1507	Increasing selectivity of CC chemokine receptor 8 antagonists by engineering nondesolvation related interactions with the intended and off-target binding sites. 2009 , 52, 7706-23	26
1506	Computational molecular biology approaches to ligand-target interactions. 2009 , 3, 228-39	10
1505	High-throughput protein crystallization. 2009 , 77, 1-22	16
1504	GRIP: a server for predicting interfaces for GPCR oligomerization. 2009 , 29, 312-7	18

1503	Chapter 8. Activation mechanisms of chemokine receptors. 2009 , 461, 171-90	11
1502	Chapter 12. The use of receptor homology modeling to facilitate the design of selective chemokine receptor antagonists. 2009 , 461, 249-79	21
1501	Modeling small molecule-compound binding to G-protein-coupled receptors. 2009 , 460, 263-88	17
1500	Purification of recombinant G-protein-coupled receptors. 2009 , 463, 631-45	42
1499	Transferability of thermostabilizing mutations between beta-adrenergic receptors. 2009 , 26, 385-96	46
1498	Chemokine receptors and other G protein-coupled receptors. 2009 , 4, 88-95	32
1497	Current World Literature. 2009 , 4, 159-64	
1496	Unraveling the structure and function of G protein-coupled receptors through NMR spectroscopy. 2009 , 15, 4003-16	24
1495	The biology of CCR5 and CXCR4. 2009 , 4, 96-103	125
1494	Human A3 adenosine receptor as versatile G protein-coupled receptor example to validate the receptor homology modeling technology. 2009 , 15, 4069-84	9
1493	Progress in elucidating the structural and dynamic character of G Protein-Coupled Receptor oligomers for use in drug discovery. 2009 , 15, 4017-25	11
1492	Computer-aided identification of ligands for GPCR anti-obesity targets. 2009 , 9, 539-53	3
1491	G Protein-Coupled Receptors: target-based in silico screening. 2009 , 15, 4049-68	30
1490	Rhodopsin and the others: a historical perspective on structural studies of G protein-coupled receptors. 2009 , 15, 3994-4002	56
1489	G protein coupled receptors -in silico drug discovery and design. 2010 , 10, 638-56	23
1488	New tools for membrane protein research. 2010 , 11, 156-65	6
1487	GPR55, a lysophosphatidylinositol receptor with cannabinoid sensitivity?. 2010 , 10, 799-813	40
1486	GPCR Homology Model Development and Application. 2010 , 279-300	3

1485	Structural Genomics, Its Application in Chemistry, Biology, and Drug Discovery. 2010 , 569-600	
1484	Receptor Targets in Drug Discovery. 2010 , 499-548	
1483	Structure and Modeling of GPCRs: Implications for Drug Discovery. 2010 , 385-433	2
1482	X-Ray Structure Developments for GPCR Drug Targets. 2010 , 434-459	1
1481	The Evolving Pharmacology of GPCRs. 2010 , 27-60	2
1480	One-Micron Beams for Macromolecular Crystallography at GM/CA-CAT. 2010 ,	9
1479	Methods for combinatorial and parallel library design. 2011 , 672, 387-434	4
1478	Beyond rhodopsin: G protein-coupled receptor structure and modeling incorporating the beta2-adrenergic and adenosine A(2A) crystal structures. 2011 , 672, 359-86	13
1477	Structure-based discovery of novel chemotypes for adenosine A(2A) receptor antagonists. 2010 , 53, 1799-809	211
1476	Normal mode analysis of biomolecular structures: functional mechanisms of membrane proteins. 2010 , 110, 1463-97	383
1475	The significance of 2-furyl ring substitution with a 2-(para-substituted) aryl group in a new series of pyrazolo-triazolo-pyrimidines as potent and highly selective hA(3) adenosine receptors antagonists: new insights into structure-affinity relationship and receptor-antagonist recognition. 2010 , 53, 3361-75	36
1474	Crystallography of membrane proteins: from crystallization to structure. 2010 , 654, 79-103	3
1473	Structures of membrane proteins. 2010 , 43, 65-158	108
1472	Update 1 of: Over one hundred peptide-activated G protein-coupled receptors recognize ligands with turn structure. 2010 , 110, PR1-41	58
1471	Superactive mutants of thromboxane prostanoid receptor: functional and computational analysis of an active form alternative to constitutively active mutants. 2010 , 67, 2979-89	12
1470	Applications of fluorescence and bioluminescence resonance energy transfer to drug discovery at G protein coupled receptors. 2010 , 398, 167-80	32
1469	Insights into binding modes of adenosine A(2B) antagonists with ligand-based and receptor-based methods. 2010 , 45, 3459-71	27
1468	Novel 8-(furan-2-yl)-3-substituted thiazolo [5,4-e][1,2,4] triazolo[1,5-c] pyrimidine-2(3H)-thione derivatives as potential adenosine A(2A) receptor antagonists. 2010 , 18, 2491-500	25

1467	Design, synthesis, and binding of homologated truncated 4'-thioadenosine derivatives at the human A3 adenosine receptors. 2010 , 18, 7015-21	12
1466	New vistas in GPCR 3D structure prediction. 2010 , 16, 183-91	21
1465	Distinct interactions between the human adrenergic beta(2) receptor and Galpha(s)--an in silico study. 2010 , 16, 1307-18	6
1464	In silico binding characteristics between human histamine H1 receptor and antagonists. 2010 , 16, 1529-37	5
1463	Study of a structurally similar kappa opioid receptor agonist and antagonist pair by molecular dynamics simulations. 2010 , 16, 1567-76	24
1462	Pharmacophore modeling of human adenosine receptor A(A) antagonists. 2010 , 16, 1867-76	10
1461	A Plug-Based Microfluidic System for Dispensing Lipidic Cubic Phase (LCP) Material Validated by Crystallizing Membrane Proteins in Lipidic Mesophases. 2010 , 8, 789-798	30
1460	The N-terminal end truncated mu-opioid receptor: from expression to circular dichroism analysis. 2010 , 160, 2175-86	8
1459	Allosteric antagonist binding sites in class B GPCRs: corticotropin receptor 1. 2010 , 24, 659-74	10
1458	Ligand-guided optimization of CXCR4 homology models for virtual screening using a multiple chemotype approach. 2010 , 24, 1023-33	21
1457	Third joint Italian-German Purine Club meeting: "Purinergic receptors: new frontiers for novel therapies". 2010 , 6, 49-115	1
1456	Influence of MT7 toxin on the oligomerization state of the M1 muscarinic receptor. 2010 , 102, 409-20	10
1455	VPAC1 receptor binding site: contribution of photoaffinity labeling approach. 2010 , 44, 127-32	24
1454	The crystallographic structure of the human adenosine A2A receptor in a high-affinity antagonist-bound state: implications for GPCR drug screening and design. 2010 , 20, 401-14	39
1453	Unlocking the eukaryotic membrane protein structural proteome. 2010 , 20, 464-70	28
1452	Internally bridging water molecule in transmembrane alpha-helical kink. 2010 , 20, 456-63	14
1451	Oligomeric forms of G protein-coupled receptors (GPCRs). 2010 , 35, 595-600	79
1450	Lighting up multiprotein complexes: lessons from GPCR oligomerization. 2010 , 28, 407-15	72

1449	A novel chemogenomics analysis of G protein-coupled receptors (GPCRs) and their ligands: a potential strategy for receptor de-orphanization. 2010 , 11, 316	40
1448	Model of the complex of Parathyroid hormone-2 receptor and Tuberoinfundibular peptide of 39 residues. 2010 , 3, 270	3
1447	Modulation of bitter taste perception by a small molecule hTAS2R antagonist. 2010 , 20, 1104-9	118
1446	Dynamics and flexibility of G-protein-coupled receptor conformations and their relevance to drug design. 2010 , 15, 951-7	21
1445	Novel Alexa Fluor-488 labeled antagonist of the A(2A) adenosine receptor: Application to a fluorescence polarization-based receptor binding assay. 2010 , 80, 506-11	41
1444	Comparison of the pharmacological properties of human and rat histamine H(3)-receptors. 2010 , 80, 1437-49	27
1443	Role of the extracellular amino terminus and first membrane-spanning helix of dopamine D1 and D5 receptors in shaping ligand selectivity and efficacy. 2010 , 22, 106-16	12
1442	Site-directed mutagenesis and PBAN activation of the Helicoverpa zea PBAN-receptor. 2010 , 584, 1212-6	15
1441	Molecular modeling studies on the human neuropeptide S receptor and its antagonists. 2010 , 5, 371-83	15
1440	Agonist-selective signaling of G protein-coupled receptor: mechanisms and implications. 2010 , 62, 112-9	36
1439	Specific ligands as pharmacological chaperones: The transport of misfolded G-protein coupled receptors to the cell surface. 2010 , 62, 453-9	9
1438	The G-protein-coupled receptor, GPR84, is important for eye development in <i>Xenopus laevis</i> . 2010 , 239, 3024-37	10
1437	High Throughput Screening Approach to Lead Discovery. 2010 , 21-71	4
1436	Fragment-Based Lead Discovery. 2010 , 105-139	3
1435	Drug Design for G-Protein-Coupled Receptors by a Ligand-Based NMR Method. 2010 , 122, 1468-1471	8
1434	Drug design for G-protein-coupled receptors by a ligand-based NMR method. 2010 , 49, 1426-9	40
1433	An Improved Weighted-Residue Profile Based Method of Using Protein-Ligand Interaction Information in Increasing Hits Selection from Virtual Screening: A Study on Virtual Screening of Human GPCR A2A Receptor Antagonists. 2010 , 29, 781-91	2
1432	Molecular modelling of central nervous system receptors. 2010 , 20, 243-248	3

1431	Enhancer and competitive allosteric modulation model for G-protein-coupled receptors. 2010 , 267, 663-75	6
1430	Structure and function of G protein-coupled receptors using NMR spectroscopy. 2010 , 57, 159-80	32
1429	Mammalian G protein-coupled receptor expression in Escherichia coli: II. Refolding and biophysical characterization of mouse cannabinoid receptor 1 and human parathyroid hormone receptor 1. 2010 , 401, 74-80	43
1428	2-Dialkynyl derivatives of (N)-methanocarba nucleosides: 'Clickable' A(3) adenosine receptor-selective agonists. 2010 , 18, 508-17	22
1427	Synthesis and pharmacological characterization of a new series of 5,7-disubstituted-[1,2,4]triazolo[1,5-a][1,3,5]triazine derivatives as adenosine receptor antagonists: A preliminary inspection of ligand-receptor recognition process. 2010 , 18, 2524-36	29
1426	Affinity of aporphines for the human 5-HT _{2A} receptor: insights from homology modeling and molecular docking studies. 2010 , 18, 5562-75	29
1425	Structure-activity relationships in 1,4-benzodioxan-related compounds. 10. Novel α -adrenoreceptor antagonists related to openphendioxan: synthesis, biological evaluation, and α d computational study. 2010 , 18, 7065-77	12
1424	Building a MCHR1 homology model provides insight into the receptor-antagonist contacts that are important for the development of new anti-obesity agents. 2010 , 18, 7365-79	8
1423	Synthesis of novel 7-imino-2-thioxo-3,7-dihydro-2H-thiazolo [4,5-d] pyrimidine derivatives as adenosine A _{2A} receptor antagonists. 2010 , 20, 1214-8	30
1422	Synthesis and evaluation of 1,2,4-triazolo[1,5-c]pyrimidine derivatives as A _{2A} receptor-selective antagonists. 2010 , 20, 5690-4	21
1421	Elucidation of the active conformation of the amino terminus of receptor-bound secretin using intramolecular disulfide bond constraints. 2010 , 20, 6040-4	5
1420	A reconstitution protocol for the in vitro folded human G protein-coupled Y ₂ receptor into lipid environment. 2010 , 150, 29-36	28
1419	Crystallization of small proteins assisted by green fluorescent protein. 2010 , 66, 1059-66	28
1418	Forced unbinding of GPR17 ligands from wild type and R255I mutant receptor models through a computational approach. 2010 , 10, 8	25
1417	Nucleoside conjugates of quantum dots for characterization of G protein-coupled receptors: strategies for immobilizing A _{2A} adenosine receptor agonists. 2010 , 8, 11	10
1416	The importance of valine 114 in ligand binding in beta(2)-adrenergic receptor. 2010 , 19, 85-93	8
1415	A synergistic approach to protein crystallization: combination of a fixed-arm carrier with surface entropy reduction. 2010 , 19, 901-13	112
1414	GPCR 3D homology models for ligand screening: lessons learned from blind predictions of adenosine A _{2a} receptor complex. 2010 , 78, 197-211	111

1413	Modeling the possible conformations of the extracellular loops in G-protein-coupled receptors. 2010 , 78, 271-85	25
1412	Modeling G protein-coupled receptors for structure-based drug discovery using low-frequency normal modes for refinement of homology models: application to H3 antagonists. 2010 , 78, 457-73	23
1411	FoldGPCR: structure prediction protocol for the transmembrane domain of G protein-coupled receptors from class A. 2010 , 78, 2189-201	31
1410	The impact of GPCR structures on pharmacology and structure-based drug design. 2010 , 159, 986-96	109
1409	Identification of a novel snake peptide toxin displaying high affinity and antagonist behaviour for the α -adrenoceptors. 2010 , 161, 1361-74	31
1408	Mapping the druggable allosteric space of G-protein coupled receptors: a fragment-based molecular dynamics approach. 2010 , 76, 201-17	91
1407	The birth and postnatal development of purinergic signalling. 2010 , 199, 93-147	89
1406	Structure determination of the seven-helix transmembrane receptor sensory rhodopsin II by solution NMR spectroscopy. 2010 , 17, 768-74	181
1405	The quest to understand heterotrimeric G protein signaling. 2010 , 17, 650-2	48
1404	Ligand-specific regulation of the extracellular surface of a G-protein-coupled receptor. 2010 , 463, 108-12	393
1403	Expression of G-protein coupled receptors in Escherichia coli for structural studies. 2010 , 75, 881-91	26
1402	Structural biology: The gatekeepers revealed. 2010 , 465, 823-6	11
1401	Structural basis of G protein-coupled receptor-G protein interactions. 2010 , 6, 541-8	68
1400	Functional studies of isolated GPCR-G protein complexes in the membrane bilayer of lipoprotein particles. 32-52	
1399	Interferon-gamma inhibits adenosine A2A receptor function in hepatic stellate cells by STAT1-mediated repression of adenylyl cyclase. 2010 , 2010, 113-126	7
1398	Insights into the binding of Phenyltiocarbamide (PTC) agonist to its target human TAS2R38 bitter receptor. 2010 , 5, e12394	87
1397	Mutational characterization of the bile acid receptor TGR5 in primary sclerosing cholangitis. 2010 , 5, e12403	90
1396	Static magnetic field exposure reproduces cellular effects of the Parkinson's disease drug candidate ZM241385. 2010 , 5, e13883	46

1395	Study of bioengineered zebra fish olfactory receptor 131-2: receptor purification and secondary structure analysis. 2010 , 5, e15027	13
1394	Hydrophobicity profiles in G protein-coupled receptor transmembrane helical domains. 2010 , 2010, 123-133	4
1393	Functional differences of invariant and highly conserved residues in the extracellular domain of the glycoprotein hormone receptors. 2010 , 285, 34813-27	15
1392	Analysis of transmembrane domains 1 and 4 of the human angiotensin II AT1 receptor by cysteine-scanning mutagenesis. 2010 , 285, 2284-93	12
1391	Impact of the DRY motif and the missing "ionic lock" on constitutive activity and G-protein coupling of the human histamine H4 receptor. 2010 , 333, 382-92	48
1390	Evolution-guided discovery and recoding of allosteric pathway specificity determinants in psychoactive bioamine receptors. 2010 , 107, 7787-92	72
1389	Proteins of the Hedgehog signaling pathway as therapeutic targets against cancer. 2010 , 7, 601-12	2
1388	Tasser-Based Protein Structure Prediction. 2010 , 219-242	2
1387	Reversible, allosteric small-molecule inhibitors of regulator of G protein signaling proteins. 2010 , 78, 524-33	65
1386	Ligand-supported purification of the urotensin-II receptor. 2010 , 78, 639-47	4
1385	International Union of Basic and Clinical Pharmacology. LXXX. The class Frizzled receptors. 2010 , 62, 632-67	161
1384	A conserved aromatic lock for the tryptophan rotameric switch in TM-VI of seven-transmembrane receptors. 2010 , 285, 3973-3985	107
1383	Ligand-induced rearrangements of the GABA(B) receptor revealed by fluorescence resonance energy transfer. 2010 , 285, 10291-9	29
1382	Third extracellular loop (EC3)-N terminus interaction is important for seven-transmembrane domain receptor function: implications for an activation microswitch region. 2010 , 285, 31472-83	19
1381	Nitro-oleic acid inhibits angiotensin II-induced hypertension. 2010 , 107, 540-8	96
1380	A lipid pathway for ligand binding is necessary for a cannabinoid G protein-coupled receptor. 2010 , 285, 17954-64	166
1379	Highly conserved tyrosine stabilizes the active state of rhodopsin. 2010 , 107, 19861-6	63
1378	Mapping the binding pocket of dual antagonist almorexant to human orexin 1 and orexin 2 receptors: comparison with the selective OX1 antagonist SB-674042 and the selective OX2 antagonist Methyl 2-[(4-methoxy-pyridin-3-yl)-(toluene-2-sulfonyl)-amino]N-pyridin-3-ylmethylacetamide (EMPA). 2010 , 78, 81-93	35

1377	Mobility of G proteins is heterogeneous and polarized during chemotaxis. 2010 , 123, 2922-30	15
1376	New Techniques to Express and Crystallize G Protein-Coupled Receptors. 2010 , 324-384	1
1375	Virtual Screening. 2010 , 1-46	1
1374	Evidence that interaction between conserved residues in transmembrane helices 2, 3, and 7 are crucial for human VPAC1 receptor activation. 2010 , 78, 394-401	28
1373	Adenosine A2A receptor is involved in cell surface expression of A2B receptor. 2010 , 285, 39271-88	59
1372	Characterization of the beta-D-glucopyranoside binding site of the human bitter taste receptor hTAS2R16. 2010 , 285, 28373-8	73
1371	Interactions between intracellular domains as key determinants of the quaternary structure and function of receptor heteromers. 2010 , 285, 27346-27359	86
1370	GPRC6A mediates the non-genomic effects of steroids. 2010 , 285, 39953-64	132
1369	In Cubo Crystallization of Membrane Proteins. 2010 , 237-272	5
1368	QSAR AND PHARMACOPHORE MODELING OF 4-ARYLTHIENO [3, 2-d] PYRIMIDINE DERIVATIVES AGAINST ADENOSINE RECEPTOR OF PARKINSON'S DISEASE. 2010 , 09, 975-991	10
1367	Conserved water-mediated hydrogen bond network between TM-I, -II, -VI, and -VII in 7TM receptor activation. 2010 , 285, 19625-36	39
1366	Ligand binding and subtype selectivity of the human A(2A) adenosine receptor: identification and characterization of essential amino acid residues. 2010 , 285, 13032-44	77
1365	The annexin I sequence gln(9)-ala(10)-trp(11)-phe(12) is a core structure for interaction with the formyl peptide receptor 1. 2010 , 285, 14338-45	28
1364	Ligand-specific conformation of extracellular loop-2 in the angiotensin II type 1 receptor. 2010 , 285, 16341-50	58
1363	Interaction of the human prostacyclin receptor with Rab11: characterization of a novel Rab11 binding domain within alpha-helix 8 that is regulated by palmitoylation. 2010 , 285, 18709-26	27
1362	Induced effects of sodium ions on dopaminergic G-protein coupled receptors. 2010 , 6, e1000884	77
1361	Structure and Function of G-Protein-Coupled Receptors. 2010 , 151-156	0
1360	Structural Bioinformatics of Membrane Proteins. 2010 ,	6

1359	GPCRRD: G protein-coupled receptor spatial restraint database for 3D structure modeling and function annotation. 2010 , 26, 3004-5	44
1358	Identification of determinants of glucose-dependent insulinotropic polypeptide receptor that interact with N-terminal biologically active region of the natural ligand. 2010 , 77, 547-58	48
1357	Ligand-based peptide design and combinatorial peptide libraries to target G protein-coupled receptors. 2010 , 16, 3071-88	78
1356	Receptor-driven identification of novel human A _{2A} adenosine receptor antagonists as potential therapeutic agents. 2010 , 485, 225-44	7
1355	Thyrotropin (TSH) receptor residue E251 in the extracellular leucine-rich repeat domain is critical for linking TSH binding to receptor activation. 2010 , 151, 1940-7	17
1354	Pharmacophoric models and 3D QSAR studies of the adenosine receptor ligands. 2010 , 10, 1019-35	7
1353	Endocannabinoid binding to the cannabinoid receptors: what is known and what remains unknown. 2010 , 17, 1468-86	111
1352	Adenosine receptor modeling: what does the A _{2A} crystal structure tell us?. 2010 , 10, 993-1018	39
1351	Understanding functional residues of the cannabinoid CB1. 2010 , 10, 779-98	24
1350	Modeling the interactions between alpha(1)-adrenergic receptors and their antagonists. 2010 , 6, 165-78	9
1349	The melanocortin-4 receptor: physiology, pharmacology, and pathophysiology. 2010 , 31, 506-43	357
1348	Hydration Site Thermodynamics Explain SARs for Triazolylpurines Analogues Binding to the A _{2A} Receptor. 2010 , 1, 160-4	91
1347	Subtlety of the structure-affinity and structure-efficacy relationships around a nonpeptide oxytocin receptor agonist. 2010 , 53, 1546-62	17
1346	Discovery of New Human A _{2A} Adenosine Receptor Agonists: Design, Synthesis, and Binding Mode of Truncated 2-Hexynyl-4'-thioadenosine. 2010 , 2010, 516-520	13
1345	Heterodimerization of the GABAB receptor-implications for GPCR signaling and drug discovery. 2010 , 58, 63-91	16
1344	Concerted interconversion between ionic lock substates of the beta(2) adrenergic receptor revealed by microsecond timescale molecular dynamics. 2010 , 98, 76-84	61
1343	LCP-Tm: an assay to measure and understand stability of membrane proteins in a membrane environment. 2010 , 98, 1539-48	55
1342	Platforms for the identification of GPCR targets, and of orthosteric and allosteric modulators. 2010 , 5, 391-403	5

1341	NMR analyses of the interaction between CCR5 and its ligand using functional reconstitution of CCR5 in lipid bilayers. 2010 , 132, 6768-77	65
1340	Scope and difficulty in generating theoretical insights regarding ligand recognition and activation of the beta 2 adrenergic receptor. 2010 , 53, 923-32	15
1339	Using the μ -Adrenoceptor for Structure-Based Drug Design. 2010 , 87, 625-627	6
1338	Hydrophobic residues in helix 8 of cannabinoid receptor 1 are critical for structural and functional properties. 2010 , 49, 502-11	33
1337	Structure of a GPCR ligand in its receptor-bound state: leukotriene B4 adopts a highly constrained conformation when associated to human BLT2. 2010 , 132, 9049-57	63
1336	Functionalized congeners of P2Y1 receptor antagonists: 2-alkynyl (N)-methanocarba 2'-deoxyadenosine 3',5'-bisphosphate analogues and conjugation to a polyamidoamine (PAMAM) dendrimer carrier. 2010 , 21, 1190-205	19
1335	Ligand-steered modeling and docking: A benchmarking study in class A G-protein-coupled receptors. 2010 , 50, 2119-28	57
1334	Molecular Dynamics Simulation at High Sodium Chloride Concentration: Toward the Inactive Conformation of the Human Adenosine A2A Receptor. 2010 , 1, 1008-1013	8
1333	Recombinant expression, in vitro refolding, and biophysical characterization of the human glucagon-like peptide-1 receptor. 2010 , 49, 7956-65	21
1332	Visualizing water molecules in transmembrane proteins using radiolytic labeling methods. 2010 , 49, 827-34	41
1331	Analysis of adenosine A β receptor stability: effects of ligands and disulfide bonds. 2010 , 49, 9181-9	20
1330	High-throughput virtual screening of proteins using GRID molecular interaction fields. 2010 , 50, 155-69	61
1329	Atom-centered interacting fragments and similarity search applications. 2010 , 50, 79-86	16
1328	Mass spectrometry-based GPCR proteomics: comprehensive characterization of the human cannabinoid 1 receptor. 2010 , 9, 1746-53	18
1327	Novel N2-substituted pyrazolo[3,4-d]pyrimidine adenosine A3 receptor antagonists: inhibition of A3-mediated human glioblastoma cell proliferation. 2010 , 53, 3954-63	46
1326	Structure of the human dopamine D3 receptor in complex with a D2/D3 selective antagonist. <i>Science</i> , 2010 , 330, 1091-5	33-3 938
1325	Seven transmembrane receptors as shapeshifting proteins: the impact of allosteric modulation and functional selectivity on new drug discovery. 2010 , 62, 265-304	491
1324	Frontal affinity chromatography-mass spectrometry useful for characterization of new ligands for GPR17 receptor. 2010 , 53, 3489-501	51

1323	Structures of the CXCR4 chemokine GPCR with small-molecule and cyclic peptide antagonists. <i>Science</i> , 2010 , 330, 1066-71	33-3	1432
1322	Predicted 3D structures for adenosine receptors bound to ligands: comparison to the crystal structure. 2010 , 170, 10-20		48
1321	The membrane complex between transducin and dark-state rhodopsin exhibits large-amplitude interface dynamics on the sub-microsecond timescale: insights from all-atom MD simulations. 2010 , 398, 161-73		19
1320	Increasingly accurate dynamic molecular models of G-protein coupled receptor oligomers: Panacea or Pandora's box for novel drug discovery?. 2010 , 86, 590-7		33
1319	Adenosine receptors interacting proteins (ARIPs): Behind the biology of adenosine signaling. 2010 , 1798, 9-20		51
1318	Purification of transmembrane proteins from <i>Saccharomyces cerevisiae</i> for X-ray crystallography. 2010 , 71, 207-23		30
1317	Expression, purification and characterization of leukotriene B(4) receptor, BLT1 in <i>Pichia pastoris</i> . 2010 , 72, 66-74		9
1316	A purified C-terminally truncated human adenosine A(2A) receptor construct is functionally stable and degradation resistant. 2010 , 74, 80-7		20
1315	Expression of neurotransmitter transporters for structural and biochemical studies. 2010 , 73, 152-60		6
1314	Heterologous high yield expression and purification of neurotensin and its functional fragment in <i>Escherichia coli</i> . 2010 , 74, 65-8		7
1313	Functional coupling of Cys-226 and Cys-296 in the glucagon-like peptide-1 (GLP-1) receptor indicates a disulfide bond that is close to the activation pocket. 2010 , 31, 2289-93		17
1312	The minor binding pocket: a major player in 7TM receptor activation. 2010 , 31, 567-74		93
1311	Multiple interests in structural models of DARC transmembrane protein. 2010 , 17, 184-96		8
1310	Mutagenesis of human neuropeptide Y/peptide YY receptor Y2 reveals additional differences to Y1 in interactions with highly conserved ligand positions. 2010 , 163, 120-9		14
1309	Recent progress in the structure determination of GPCRs, a membrane protein family with high potential as pharmaceutical targets. 2010 , 654, 141-68		49
1308	Practical considerations of membrane protein instability during purification and crystallisation. 2010 , 601, 187-203		88
1307	G Protein-Coupled Receptor Structures. 2010 , 129-138		
1306	Rational design of CCR2 antagonists: a survey of computational studies. 2010 , 5, 543-57		12

1305	Structure and activation of the visual pigment rhodopsin. 2010 , 39, 309-28	147
1304	Homology modeling and docking evaluation of aminergic G protein-coupled receptors. 2010 , 50, 626-37	88
1303	Hybrid ortho/allosteric ligands for the adenosine A(1) receptor. 2010 , 53, 3028-37	74
1302	Structure-based discovery of A2A adenosine receptor ligands. 2010 , 53, 3748-55	195
1301	In silico fragment-based drug design. 2010 , 5, 1047-65	19
1300	Nonlinear optical imaging of integral membrane protein crystals in lipidic mesophases. 2010 , 82, 491-7	66
1299	Probing the structural determinants for the function of intracellular loop 2 in structurally cognate G-protein-coupled receptors. 2010 , 49, 10691-701	16
1298	The year in G protein-coupled receptor research. 2010 , 24, 261-74	117
1297	Structural basis for ligand recognition of incretin receptors. 2010 , 84, 251-78	9
1296	Therapeutic and Diagnostic Agents for Parkinson's Disease. 2010 , 529-568	
1295	Neurotransmitter Receptors in the Basal Ganglia. 2010 , 75-96	3
1294	Membrane Protein Structure Determination. 2010 ,	4
1293	Heterologous Expression of Membrane Proteins. 2010 ,	2
1292	Modeling Protein-Ligand Binding by Mining Minima. 2010 , 6, 3540-3557	50
1291	Engineering a GPCR-ligand pair that simulates the activation of D(2L) by Dopamine. 2010 , 1, 25-35	19
1290	Dimerization of G protein-coupled purinergic receptors: increasing the diversity of purinergic receptor signal responses and receptor functions. 2010 , 30, 337-46	19
1289	Structural divergence and functional versatility of the rhodopsin superfamily. 2010 , 9, 1458-65	32
1288	Incorporation of the dopamine D2L receptor and bacteriorhodopsin within bicontinuous cubic lipid phases. 1. Relevance to in meso crystallization of integral membrane proteins in monoolein systems. 2010 , 6, 4828	39

1287	Incorporation of the dopamine D2L receptor and bacteriorhodopsin within bicontinuous cubic lipid phases. 2. Relevance to in meso crystallization of integral membrane proteins in novel lipid systems. 2010 , 6, 4838	33
1286	Functional analysis of the second extracellular loop of rhodopsin by characterizing split variants. 2010 , 9, 1490-7	9
1285	Preparation of an activated rhodopsin/transducin complex using a constitutively active mutant of rhodopsin. 2011 , 50, 10399-407	16
1284	Molecular modeling of the human serotonin(1A) receptor: role of membrane cholesterol in ligand binding of the receptor. 2011 , 7, 224-34	55
1283	International Union of Basic and Clinical Pharmacology. LXXXII: Nomenclature and Classification of Hydroxy-carboxylic Acid Receptors (GPR81, GPR109A, and GPR109B). 2011 , 63, 269-90	126
1282	Development of Polar Adenosine A2A Receptor Agonists for Inflammatory Bowel Disease: Synergism with A2B Antagonists. 2011 , 2, 890-5	30
1281	Adverse and protective influences of adenosine on the newborn and embryo: implications for preterm white matter injury and embryo protection. 2011 , 69, 271-8	59
1280	Identification of the GPR55 agonist binding site using a novel set of high-potency GPR55 selective ligands. 2011 , 50, 5633-47	55
1279	Discovery of phosphoric acid mono-{2-[(E/Z)-4-(3,3-dimethyl-butrylamino)-3,5-difluoro-benzoylimino]-thiazol-3-ylmethyl} ester (Lu AA47070): a phosphonooxymethylene prodrug of a potent and selective hA(2A) receptor antagonist. 2011 , 54, 751-64	26
1278	MIF-chemokine receptor interactions in atherogenesis are dependent on an N-loop-based 2-site binding mechanism. 2011 , 25, 894-906	40
1277	New 2-heterocycl-yl-imidazo[2,1-i]purin-5-one derivatives as potent and selective human A3 adenosine receptor antagonists. 2011 , 54, 5205-20	12
1276	Changes in conformation at the cytoplasmic ends of the fifth and sixth transmembrane helices of a yeast G protein-coupled receptor in response to ligand binding. 2011 , 50, 6841-54	20
1275	Structural elements of the signal propagation pathway in squid rhodopsin and bovine rhodopsin. 2011 , 115, 6172-9	9
1274	International Union of Basic and Clinical Pharmacology. LXXXI. Nomenclature and classification of adenosine receptors--an update. 2011 , 63, 1-34	948
1273	Homology Model Versus X-ray Structure in Receptor-based Drug Design: A Retrospective Analysis with the Dopamine D3 Receptor. 2011 , 2, 293-7	19
1272	The Implication of the First Agonist Bound Activated GPCR X-ray Structure on GPCR in Silico Modeling. 2011 , 2, 414-8	10
1271	Recombinant expression and functional characterization of mouse olfactory receptor mOR256-17 in mammalian cells. 2011 , 50, 7228-35	20
1270	Development of an Automated High Throughput LCP-FRAP Assay to Guide Membrane Protein Crystallization in Lipid Mesophases. 2011 , 11, 1193-1201	45

1269	Quantification of functional selectivity at the human β 1A)-adrenoceptor. 2011 , 79, 298-307	64
1268	The morphology and composition of cholesterol-rich micellar nanostructures determine transmembrane protein (GPCR) activity. 2011 , 100, L11-3	37
1267	Toward rational design of protein detergent complexes: determinants of mixed micelles that are critical for the in vitro stabilization of a G-protein coupled receptor. 2011 , 101, 1938-48	38
1266	Salt effects on the conformational stability of the visual G-protein-coupled receptor rhodopsin. 2011 , 101, 2798-806	11
1265	The use of GPCR structures in drug design. 2011 , 62, 1-36	34
1264	Molecular modeling of neurokinin B and tachykinin NK1 receptor complex. 2011 , 51, 2932-8	17
1263	Structural basis for the β -adrenergic receptor subtype selectivity of the representative agonists and antagonists. 2011 , 51, 1405-22	18
1262	Computational study of the binding modes of caffeine to the adenosine A2A receptor. 2011 , 115, 13880-90	15
1261	Fragment screening of stabilized G-protein-coupled receptors using biophysical methods. 2011 , 493, 115-36	91
1260	The use of G-protein coupled receptor models in lead optimization. 2011 , 3, 709-21	14
1259	G protein-coupled receptors: mutations and endocrine diseases. 2011 , 7, 362-72	110
1258	Synthesis, biological evaluation, and automated docking of constrained analogues of the opioid peptide H-Dmt-D-Ala-Phe-Gly-NH ₂ using the 4- or 5-methyl substituted 4-amino-1,2,4,5-tetrahydro-2-benzazepin-3-one scaffold. 2011 , 54, 6538-47	12
1257	Homology modeling of class a G protein-coupled receptors. 2012 , 857, 259-79	41
1256	Biological and pharmacological roles of HCA receptors. 2011 , 62, 219-50	38
1255	Genome-Wide Protein Structure Prediction. 2011 , 255-279	2
1254	Allosteric modulation of metabotropic glutamate receptors. 2011 , 62, 37-77	42
1253	A new drug design targeting the adenosinergic system for Huntington's disease. 2011 , 6, e20934	67
1252	The mouse eugenol odorant receptor: structural and functional plasticity of a broadly tuned odorant binding pocket. 2011 , 50, 843-53	72

1251	The identification of the 2-phenylphthalazin-1(2H)-one scaffold as a new decorable core skeleton for the design of potent and selective human A3 adenosine receptor antagonists. 2011 , 54, 2102-13	50
1250	Experimental challenges to targeting poorly characterized GPCRs: uncovering the therapeutic potential for free fatty acid receptors. 2011 , 62, 175-218	41
1249	The splice variant of the V2 vasopressin receptor adopts alternative topologies. 2011 , 50, 4981-6	6
1248	Virtual Screening on Homology Models. 2011 , 381-410	3
1247	Dissecting the functions of conserved prolines within transmembrane helices of the D2 dopamine receptor. 2011 , 6, 1063-8	21
1246	Cheminformatics and Computational Chemical Biology. 2011 ,	6
1245	Methods for the Discovery and Characterization of G Protein-Coupled Receptors. 2011 ,	
1244	Crystallizing Membrane Proteins in Lipidic Mesophases. A Host Lipid Screen. 2011 , 11, 530-537	43
1243	Structure-based prediction of subtype selectivity of histamine H3 receptor selective antagonists in clinical trials. 2011 , 51, 3262-74	36
1242	New QSAR prediction models derived from GPCR CB2-antagonistic triaryl bis-sulfone analogues by a combined molecular morphological and pharmacophoric approach. 2011 , 22, 525-44	9
1241	Ligand discovery from a dopamine D3 receptor homology model and crystal structure. 2011 , 7, 769-78	250
1240	From cradle to twilight: the carboxyl terminus directs the fate of the A(2A)-adenosine receptor. 2011 , 1808, 1350-7	30
1239	Structural features of adenosine receptors: from crystal to function. 2011 , 1808, 1233-44	47
1238	Allosteric modulation of adenosine receptors. 2011 , 1808, 1309-18	53
1237	Solution- and solid-state NMR studies of GPCRs and their ligands. 2011 , 1808, 1462-75	37
1236	Lipid-binding surfaces of membrane proteins: evidence from evolutionary and structural analysis. 2011 , 1808, 1092-102	63
1235	Recent developments in adenosine receptor ligands and their potential as novel drugs. 2011 , 1808, 1290-308	315
1234	Identification of a novel endoplasmic reticulum export motif within the eighth helical domain (H8) of the human prostacyclin receptor. 2011 , 1808, 1202-18	11

1233	Recent progress in the study of G protein-coupled receptors with molecular dynamics computer simulations. 2011 , 1808, 1868-78	67
1232	Comparative NMR analysis of an 80-residue G protein-coupled receptor fragment in two membrane mimetic environments. 2011 , 1808, 2674-84	11
1231	Dimerization and ligand binding affect the structure network of A(2A) adenosine receptor. 2011 , 1808, 1256-66	53
1230	Molecular dynamics simulations reveal insights into key structural elements of adenosine receptors. 2011 , 50, 4194-208	60
1229	Novel 8-(furan-2-yl)-3-benzyl thiazolo [5,4-e][1,2,4] triazolo [1,5-c] pyrimidine-2(3H)-thione as selective adenosine A(2A) receptor antagonist. 2011 , 488, 1-5	8
1228	When simple agonism is not enough: emerging modalities of GPCR ligands. 2011 , 331, 241-7	49
1227	Evolution of three human GPCRs for higher expression and stability. 2011 , 408, 599-615	68
1226	Differential interactions of fluorescent agonists and antagonists with the yeast G protein coupled receptor Ste2p. 2011 , 409, 513-28	21
1225	Thermostabilisation of an agonist-bound conformation of the human adenosine A(2A) receptor. 2011 , 409, 298-310	98
1224	Engineering an ultra-thermostable $\alpha(1)$ -adrenoceptor. 2011 , 413, 628-38	45
1223	Chapter 18:Structure-based Virtual Screening for Ligands of G Protein-coupled Receptors. 2011 , 359-374	4
1222	Pyrimidine derivatives as potent and selective A3 adenosine receptor antagonists. 2011 , 54, 457-71	47
1221	Progress in structure based drug design for G protein-coupled receptors. 2011 , 54, 4283-311	191
1220	Ligand functional selectivity and quantitative pharmacology at G protein-coupled receptors. 2011 , 6, 811-25	61
1219	Crystallization chaperone strategies for membrane proteins. 2011 , 55, 293-302	28
1218	Characterization of lipid matrices for membrane protein crystallization by high-throughput small angle X-ray scattering. 2011 , 55, 342-9	28
1217	Production of the stable human histamine H ₁ receptor in Pichia pastoris for structural determination. 2011 , 55, 281-6	28
1216	New amphiphiles for membrane protein structural biology. 2011 , 55, 318-23	64

1215	Crystallizing membrane proteins using lipidic bicelles. 2011 , 55, 337-41	92
1214	GPCR stabilization using the bicelle-like architecture of mixed sterol-detergent micelles. 2011 , 55, 310-7	66
1213	Characterizing and predicting the functional and conformational diversity of seven-transmembrane proteins. 2011 , 55, 405-14	15
1212	Importance of the extracellular loops in G protein-coupled receptors for ligand recognition and receptor activation. 2011 , 32, 35-42	166
1211	Structural insights into adrenergic receptor function and pharmacology. 2011 , 32, 213-8	139
1210	Structural insights into RAMP modification of secretin family G protein-coupled receptors: implications for drug development. 2011 , 32, 591-600	63
1209	GPCR agonist binding revealed by modeling and crystallography. 2011 , 32, 637-43	52
1208	Optimization of Escherichia coli cultivation methods for high yield neuropeptide Y receptor type 2 production. 2011 , 76, 25-35	14
1207	Heterologous expression and purification of membrane-bound pyrophosphatases. 2011 , 79, 25-34	12
1206	Open conformation of adipokinetic hormone receptor from the malaria mosquito facilitates hormone binding. 2011 , 32, 553-9	10
1205	Analysis of the glucagon receptor first extracellular loop by the substituted cysteine accessibility method. 2011 , 32, 1593-9	17
1204	Role of membrane integrity on G protein-coupled receptors: Rhodopsin stability and function. 2011 , 50, 267-77	52
1203	Allosteric modulation of metabotropic glutamate receptors: structural insights and therapeutic potential. 2011 , 60, 66-81	99
1202	Structure based prediction of subtype-selectivity for adenosine receptor antagonists. 2011 , 60, 108-15	71
1201	Allosteric modulation of G protein-coupled receptors: a pharmacological perspective. 2011 , 60, 24-35	218
1200	Structure-based drug discovery and protein targets in the CNS. 2011 , 60, 7-23	21
1199	Transmembrane signaling by GPCRs: insight from rhodopsin and opsin structures. 2011 , 60, 52-7	42
1198	Exploration of structure-based drug design opportunities for mGluRs. 2011 , 60, 93-101	14

1197	Importance of receptor flexibility in binding of cyclam compounds to the chemokine receptor CXCR4. 2011 , 51, 139-47	14
1196	Leukotriene receptors. 2011 , 111, 6231-98	63
1195	Biophysical mapping of the adenosine A2A receptor. 2011 , 54, 4312-23	99
1194	Synthesis and biological evaluation of a new series of 1,2,4-triazolo[1,5-a]-1,3,5-triazines as human A(2A) adenosine receptor antagonists with improved water solubility. 2011 , 54, 877-89	30
1193	Exploring a model of a chemokine receptor/ligand complex in an explicit membrane environment by molecular dynamics simulation: the human CCR1 receptor. 2011 , 51, 2717-30	21
1192	Substituted pyrazolo[3,4-b]pyridines as human A1 adenosine antagonists: developments in understanding the receptor stereoselectivity. 2011 , 9, 4448-55	15
1191	Structure of an agonist-bound human A2A adenosine receptor. <i>Science</i> , 2011 , 332, 322-7	33.3 706
1190	Identification of essential cannabinoid-binding domains: structural insights into early dynamic events in receptor activation. 2011 , 286, 33422-35	30
1189	[Structure of the adenosine-bound conformation of the human adenosine A(2A) receptor]. 2011 , 27, 926-8	3
1188	Knowledge Based Membrane Protein Structure Prediction: From X-Ray Crystallography to Bioinformatics and Back to Molecular Biology. 2011 ,	
1187	Probing Structure and Dynamics of the Cell Membrane with Single Fluorescent Proteins. 2011 , 185-212	2
1186	Functional and Structural Overview of G-Protein-Coupled Receptors Comprehensively Obtained from Genome Sequences. 2011 , 4, 652-664	19
1185	High resolution structure of the ba3 cytochrome c oxidase from <i>Thermus thermophilus</i> in a lipidic environment. 2011 , 6, e22348	94
1184	Production of a bioengineered G-protein coupled receptor of human formyl peptide receptor 3. 2011 , 6, e23076	15
1183	Differential modulation of Beta-adrenergic receptor signaling by trace amine-associated receptor 1 agonists. 2011 , 6, e27073	42
1182	Modeling of human prokineticin receptors: interactions with novel small-molecule binders and potential off-target drugs. 2011 , 6, e27990	26
1181	The importance of alkynyl chain presence for the activity of adenine nucleosides/nucleotides on purinergic receptors. 2011 , 18, 1444-63	9
1180	P-glycoprotein inhibition: the past, the present and the future. 2011 , 12, 722-31	67

1179	Homology models in docking and high-throughput docking. 2011 , 11, 1528-34	36
1178	Collation and data-mining of literature bioactivity data for drug discovery. 2011 , 39, 1365-70	27
1177	Introduction. 2011 , 1-9	
1176	Heterologous Production of Active Mammalian G-Protein-Coupled Receptors Using Baculovirus-Infected Insect Cells. 2011 , 109-138	
1175	Expression of G-Protein-Coupled Receptors. 2011 , 219-248	3
1174	The cannabinoid type-1 receptor carboxyl-terminus, more than just a tail. 2011 , 117, 1-18	19
1173	Endocannabinoid tone versus constitutive activity of cannabinoid receptors. 2011 , 163, 1329-43	87
1172	Involvement of the first transmembrane segment of human β_2 -adrenoceptors in the subtype-selective binding of chlorpromazine, spiperone and spiroxatrine. 2011 , 164, 1558-72	10
1171	Guide to Receptors and Channels (GRAC), 5th edition. 2011 , 164 Suppl 1, S1-324	702
1170	Consultants. 2011 , 164, S3-S3	7
1169	G PROTEIN-COUPLED RECEPTORS. 2011 , 164, S5-S113	14
1168	LIGAND-GATED ION CHANNELS. 2011 , 164, S115-S135	5
1167	ION CHANNELS. 2011 , 164, S137-S174	9
1166	NUCLEAR RECEPTORS. 2011 , 164, S175-S188	78
1165	CATALYTIC RECEPTORS. 2011 , 164, S189-S212	1
1164	TRANSPORTERS. 2011 , 164, S213-S278	2
1163	ENZYMES. 2011 , 164, S279-S324	2
1162	Alterations in the photoactivation pathway of rhodopsin mutants associated with retinitis pigmentosa. 2011 , 278, 1493-505	8

1161	Structure of a nanobody-stabilized active state of the $\beta(2)$ adrenoceptor. 2011 , 469, 175-80	1299
1160	The structural basis of agonist-induced activation in constitutively active rhodopsin. 2011 , 471, 656-60	395
1159	Overcoming barriers to membrane protein structure determination. 2011 , 29, 335-40	293
1158	ePMV embeds molecular modeling into professional animation software environments. 2011 , 19, 293-303	60
1157	Status of GPCR modeling and docking as reflected by community-wide GPCR Dock 2010 assessment. 2011 , 19, 1108-26	243
1156	Structure of the adenosine A(2A) receptor in complex with ZM241385 and the xanthines XAC and caffeine. 2011 , 19, 1283-93	433
1155	Ligand-dependent perturbation of the conformational ensemble for the GPCR β adrenergic receptor revealed by HDX. 2011 , 19, 1424-32	111
1154	Structural basis for β opioid receptor binding and activation. 2011 , 19, 1683-90	23
1153	Assembling good amyloid: some structures at last. 2011 , 19, 1207-9	5
1152	Trapping small caffeine in a large GPCR pocket. 2011 , 19, 1204-7	5
1151	Allostery in GPCRs: 'MWC' revisited. 2011 , 36, 663-72	55
1150	New advances in production and functional folding of G-protein-coupled receptors. 2011 , 29, 314-22	68
1149	Identification of positions in the human neuropeptide Y/peptide YY receptor Y2 that contribute to pharmacological differences between receptor subtypes. 2011 , 45, 293-300	11
1148	Structural insights into agonist-induced activation of G-protein-coupled receptors. 2011 , 21, 541-51	180
1147	Nanobody stabilization of G protein-coupled receptor conformational states. 2011 , 21, 567-72	186
1146	High throughput platforms for structural genomics of integral membrane proteins. 2011 , 21, 517-22	23
1145	Uncovering the intimate relationship between lipids, cholesterol and GPCR activation. 2011 , 21, 802-7	183
1144	Past, present and future of A(2A) adenosine receptor antagonists in the therapy of Parkinson's disease. 2011 , 132, 280-99	143

1143	Comprehensive analysis of host gene expression in <i>Autographa californica</i> nucleopolyhedrovirus-infected <i>Spodoptera frugiperda</i> cells. 2011 , 412, 167-78	55
1142	Homology modeling in tandem with 3D-QSAR analyses: a computational approach to depict the agonist binding site of the human CB2 receptor. 2011 , 46, 4489-505	32
1141	Agonist-dependent effects of mutations in the sphingosine-1-phosphate type 1 receptor. 2011 , 667, 105-12	13
1140	The structure of active opsin as a basis for identification of GPCR agonists by dynamic homology modelling and virtual screening assays. 2011 , 585, 3587-92	12
1139	Strategies for the identification of allosteric modulators of G-protein-coupled receptors. 2011 , 81, 691-702	64
1138	The four cysteine residues in the second extracellular loop of the human adenosine A2B receptor: role in ligand binding and receptor function. 2011 , 82, 389-99	33
1137	CH/lydrogen bonds play a role in ligand recognition and equilibrium between active and inactive states of the α_2 adrenergic receptor: an ab initio fragment molecular orbital (FMO) study. 2011 , 19, 5231-7	40
1136	Does the combination of optimal substitutions at the C α , N β and N ϵ positions of the pyrazolo-triazolo-pyrimidine scaffold guarantee selective modulation of the human A α adenosine receptors?. 2011 , 19, 6120-34	10
1135	The hydrophobic amino acids in putative helix 8 in carboxy-terminus of histamine H(3) receptor are involved in receptor-G-protein coupling. 2011 , 23, 1843-9	7
1134	Enhanced Inter-helical Residue Contact Prediction in Transmembrane Proteins. 2011 , 66, 4356-4369	6
1133	Chemogenomic discovery of allosteric antagonists at the GPRC6A receptor. 2011 , 18, 1489-98	30
1132	Predicted structures and dynamics for agonists and antagonists bound to serotonin 5-HT2B and 5-HT2C receptors. 2011 , 51, 420-33	25
1131	Agonist-bound adenosine A2A receptor structures reveal common features of GPCR activation. 2011 , 474, 521-5	685
1130	Methods of protein structure comparison. 2012 , 857, 231-57	190
1129	The significance of G protein-coupled receptor crystallography for drug discovery. 2011 , 63, 901-37	163
1128	Prostanoid receptors. 2011 , 111, 6209-30	101
1127	Update 1 of: computational modeling approaches to structure-function analysis of G protein-coupled receptors. 2011 , 111, PR438-535	61
1126	Chapter 15:Activation of G Protein-Coupled Receptor (GPCR) Kinases by GPCRs. 2011 , 297-315	1

1125	Chapter 17: The Mechanics of Arrestin Receptor Interaction: How GPCRs and Arrestins Talk to Each Other. 2011 , 335-355	
1124	G protein- and agonist-bound serotonin 5-HT _{2A} receptor model activated by steered molecular dynamics simulations. 2011 , 51, 315-25	44
1123	Snooker: a structure-based pharmacophore generation tool applied to class A GPCRs. 2011 , 51, 2277-92	51
1122	Conformational dynamics of single G protein-coupled receptors in solution. 2011 , 115, 13328-38	81
1121	Structure of the human histamine H ₁ receptor complex with doxepin. 2011 , 475, 65-70	630
1120	Lipidic cubic phase technologies for membrane protein structural studies. 2011 , 21, 559-66	165
1119	Human cannabinoid 1 GPCR C-terminal domain interacts with bilayer phospholipids to modulate the structure of its membrane environment. 2011 , 13, 92-8	18
1118	Strategies to discover unexpected targets for drugs active at G protein-coupled receptors. 2011 , 51, 117-44	152
1117	Synthesis of heterologous G protein-coupled receptors in the methylotrophic yeast <i>P. pastoris</i> . 2011 , 441, 280-2	
1116	Comparison of three GPCR structural templates for modeling of the P2Y ₁₂ nucleotide receptor. 2011 , 25, 329-38	30
1115	In silico identification of new ligands for GPR17: a promising therapeutic target for neurodegenerative diseases. 2011 , 25, 743-52	45
1114	Pharmacology of the platelet purinergic receptors. 2011 , 7, 305-24	40
1113	Class A GPCRs: a multifaceted reality. 2011 , 7, 279-81	
1112	Homology model and docking studies on porcine β_2 adrenoceptor: description of two binding sites. 2011 , 17, 2525-38	8
1111	Modeling of ligand binding to G protein coupled receptors: cannabinoid CB ₁ , CB ₂ and adrenergic β_2 AR. 2011 , 17, 2353-66	27
1110	Conserved amino acids participate in the structure networks deputed to intramolecular communication in the lutropin receptor. 2011 , 68, 1227-39	46
1109	Homology modeling of human CCR ₂ receptor. 2011 , 20, 1704-1712	8
1108	Effects of lipid-analog detergent solubilization on the functionality and lipidic cubic phase mobility of the Torpedo californica nicotinic acetylcholine receptor. 2011 , 243, 47-58	8

1107	Structural determinants of the alpha2 adrenoceptor subtype selectivity. 2011 , 29, 1030-8	13
1106	Hydrogen/deuterium exchange mass spectrometry and optical spectroscopy as complementary tools for studying the structure and dynamics of a membrane protein. 2011 , 302, 3-11	20
1105	Cell-free synthesis of a functional G protein-coupled receptor complexed with nanometer scale bilayer discs. 2011 , 11, 57	48
1104	Evaluation of the <i>Pichia pastoris</i> expression system for the production of GPCRs for structural analysis. 2011 , 10, 24	28
1103	Automated sample-scanning methods for radiation damage mitigation and diffraction-based centering of macromolecular crystals. 2011 , 18, 717-22	57
1102	GPCR-SSFE: a comprehensive database of G-protein-coupled receptor template predictions and homology models. 2011 , 12, 185	46
1101	ss-TEA: Entropy based identification of receptor specific ligand binding residues from a multiple sequence alignment of class A GPCRs. 2011 , 12, 332	20
1100	Distinct second extracellular loop structures of the brain cannabinoid CB(1) receptor: implication in ligand binding and receptor function. 2011 , 79, 581-97	3
1099	Simplified modeling approach suggests structural mechanisms for constitutive activation of the C5a receptor. 2011 , 79, 787-802	6
1098	Modeling GPCR active state conformations: the $\beta(2)$ -adrenergic receptor. 2011 , 79, 1441-57	23
1097	Predicted structures of agonist and antagonist bound complexes of adenosine A3 receptor. 2011 , 79, 1878-97	27
1096	Progress in the structural prediction of G protein-coupled receptors: D3 receptor in complex with eticlopride. 2011 , 79, 1695-703	21
1095	Polymer-based cell-free expression of ligand-binding family B G-protein coupled receptors without detergents. 2011 , 20, 1030-41	41
1094	Challenges and advances in computational docking: 2009 in review. 2011 , 24, 149-64	210
1093	Differential Virtual Screening (DVS) with Active and Inactive Molecular Models for Finding and Profiling GPCR Modulators: Case of the CCK1 Receptor. 2011 , 30, 345-58	4
1092	Structure-based discovery of allosteric modulators of two related class B G-protein-coupled receptors. 2011 , 6, 2159-69	57
1091	Substructure-based virtual screening for adenosine A2A receptor ligands. 2011 , 6, 2302-11	21
1090	Applying in silico tools to the discovery of novel CXCR4 inhibitors. 2011 , 72, 95-111	3

1089	Solution conformation of non-mammalian tachykinin physalaemin in lipid micelles by nuclear magnetic resonance. 2011 , 96, 252-9	3
1088	Comparison analysis of primary ligand-binding sites in seven-helix membrane proteins. 2011 , 95, 31-8	1
1087	Expression and biophysical analysis of a triple-transmembrane domain-containing fragment from a yeast G protein-coupled receptor. 2011 , 96, 757-71	9
1086	A chimeric GPCR model mimicking the ligand binding site of the human Y1 receptor studied by NMR spectroscopy. 2011 , 12, 1690-3	4
1085	Site-specific in vitro and in vivo incorporation of molecular probes to study G-protein-coupled receptors. 2011 , 15, 392-8	37
1084	Structure-based druggability assessment--identifying suitable targets for small molecule therapeutics. 2011 , 15, 463-8	121
1083	Synthesis, structure-affinity relationships, and molecular modeling studies of novel pyrazolo[3,4-c]quinoline derivatives as adenosine receptor antagonists. 2011 , 19, 3757-68	20
1082	Molecular probes for the A2A adenosine receptor based on a pyrazolo[4,3-e][1,2,4]triazolo[1,5-c]pyrimidin-5-amine scaffold. 2011 , 21, 2740-5	22
1081	The structural and topological analysis of membrane-associated polypeptides by oriented solid-state NMR spectroscopy: established concepts and novel developments. 2011 , 153, 115-25	68
1080	Theoretical study of 3-D molecular similarity and ligand binding modes of orthologous human and rat D2 dopamine receptors. 2011 , 41, 537-45	13
1079	Biacore analysis with stabilized G-protein-coupled receptors. 2011 , 409, 267-72	56
1078	Lipoic acid stimulates cAMP production via G protein-coupled receptor-dependent and -independent mechanisms. 2011 , 22, 681-90	26
1077	Structure-function relationships of the human bitter taste receptor hTAS2R1: insights from molecular modeling studies. 2011 , 31, 229-40	17
1076	Regulation of G-Protein-Coupled Receptor Signalling by the Scaffolding Proteins Spinophilin/Neurabin 2 and Neurabin 1. 2011 , 5,	
1075	Organizational complexity of β -adrenergic receptor signaling systems. 2011 , 67, 19-49	3
1074	Molecular pharmacology, physiology, and structure of the P2Y receptors. 2011 , 61, 373-415	96
1073	Oligomerization of G protein-coupled receptors: computational methods. 2011 , 18, 4588-605	28
1072	Drug design of GPCR ligands using phylogenetics and chemogenomics--principles and case studies. 2011 , 11, 1882-901	12

1071	G protein-coupled receptor transmembrane binding pockets and their applications in GPCR research and drug discovery: a survey. 2011 , 11, 1902-24	17
1070	Chemogenomics approaches for receptor deorphanization and extensions of the chemogenomics concept to phenotypic space. 2011 , 11, 1964-77	18
1069	A ligand's view of target similarity: chemogenomic binding site-directed techniques for drug discovery. 2011 , 11, 1872-81	13
1068	Lipid cubic phase as a membrane mimetic for integral membrane protein enzymes. 2011 , 108, 8639-44	52
1067	Computational methods for the discovery of mood disorder therapies. 2011 , 6, 1227-45	7
1066	Molecular basis of secretin docking to its intact receptor using multiple photolabile probes distributed throughout the pharmacophore. 2011 , 286, 23888-99	28
1065	Solid-state ² H NMR relaxation illuminates functional dynamics of retinal cofactor in membrane activation of rhodopsin. 2011 , 108, 8263-8	47
1064	A structural insight into the reorientation of transmembrane domains 3 and 5 during family A G protein-coupled receptor activation. 2011 , 79, 262-9	53
1063	Role of the transmembrane domain 4/extracellular loop 2 junction of the human gonadotropin-releasing hormone receptor in ligand binding and receptor conformational selection. 2011 , 286, 34617-26	11
1062	Allosteric modulation of purine and pyrimidine receptors. 2011 , 61, 187-220	28
1061	GPCR Conformations: Implications for Rational Drug Design. 2011 , 4, 7-43	14
1060	In Silico Veritas: The Pitfalls and Challenges of Predicting GPCR-Ligand Interactions. 2011 , 4, 1196-1215	16
1059	Helix 8 of the M1 muscarinic acetylcholine receptor: scanning mutagenesis delineates a G protein recognition site. 2011 , 79, 701-9	23
1058	Structural model of ligand-G protein-coupled receptor (GPCR) complex based on experimental double mutant cycle data: MT7 snake toxin bound to dimeric hM1 muscarinic receptor. 2011 , 286, 31661-75	33
1057	Crystallizing membrane proteins for structure-function studies using lipidic mesophases. 2011 , 39, 725-32	41
1056	Cholesterol-induced conformational changes in the oxytocin receptor. 2011 , 437, 541-53	27
1055	Thematic Analysis—a chemogenomic approach to GPCR drug discovery. 2011 , 11, 1925-43	6
1054	Arrestin-rhodopsin binding stoichiometry in isolated rod outer segment membranes depends on the percentage of activated receptors. 2011 , 286, 7359-69	42

1053	From molecular details of the interplay between transmembrane helices of the thyrotropin receptor to general aspects of signal transduction in family A G-protein-coupled receptors (GPCRs). 2011 , 286, 25859-71	20
1052	Engineering a prokaryotic Cys-loop receptor with a third functional domain. 2011 , 286, 34635-42	27
1051	Recognition in the face of diversity: interactions of heterotrimeric G proteins and G protein-coupled receptor (GPCR) kinases with activated GPCRs. 2011 , 286, 7715-7721	49
1050	Allosteric and orthosteric sites in CC chemokine receptor (CCR5), a chimeric receptor approach. 2011 , 286, 37543-54	37
1049	Two distinct conformations of helix 6 observed in antagonist-bound structures of a beta1-adrenergic receptor. 2011 , 108, 8228-32	154
1048	Successful prediction of the intra- and extracellular loops of four G-protein-coupled receptors. 2011 , 108, 8275-80	58
1047	Unique interaction pattern for a functionally biased ghrelin receptor agonist. 2011 , 286, 20845-60	39
1046	GPCR structure and activation: an essential role for the first extracellular loop in activating the adenosine A2B receptor. 2011 , 25, 632-43	41
1045	Structural Biology of Membrane Proteins. 2011 , 249-273	2
1044	Structural Insights for Homology Modeling of Chemokine Receptors. 2011 , 33-50	
1043	Expression and Purification of G-Protein-Coupled Receptors for Nuclear Magnetic Resonance Structural Studies. 2011 , 297-316	3
1042	Efficient Synthesis of Unsaturated 1-Monoacyl Glycerols for in meso Crystallization of Membrane Proteins. 2010 , 2011, 809-812	7
1041	Molecular modelling study on human histamine H1 receptor and its applications in virtual lead identification for designing novel inverse agonists. 2011 , 37, 100-114	
1040	NMR structures of polytopic integral membrane proteins. 2011 , 28, 370-97	16
1039	GPCRs Revisited: New Insights Lead to Novel Drugs. 2011 , 4, 244-272	14
1038	Prediction of the Human EP1 Receptor Binding Site by Homology Modeling and Molecular Dynamics Simulation. 2011 , 79, 793-816	6
1037	The structure of the adenosine receptors: implications for drug discovery. 2011 , 61, 1-40	9
1036	Differential determinants for coupling of distinct G proteins with the class B secretin receptor. 2012 , 302, C1202-12	18

1035	Ligand-dependent conformations and dynamics of the serotonin 5-HT(2A) receptor determine its activation and membrane-driven oligomerization properties. 2012 , 8, e1002473	84
1034	Molecular modeling of the M3 acetylcholine muscarinic receptor and its binding site. 2012 , 2012, 789741	9
1033	Functions of transmembrane domain 3 of human melanocortin-4 receptor. 2012 , 49, 221-35	34
1032	Small molecule drug discovery at the glucagon-like peptide-1 receptor. 2012 , 2012, 709893	53
1031	The VPAC1 receptor: structure and function of a class B GPCR prototype. 2012 , 3, 139	13
1030	Pleiotropic functions of the transmembrane domain 6 of human melanocortin-4 receptor. 2012 , 49, 237-48	25
1029	Pocketome: an encyclopedia of small-molecule binding sites in 4D. 2012 , 40, D535-40	123
1028	GPCR heteromers and their allosteric receptor-receptor interactions. 2012 , 19, 356-63	71
1027	Structure-based design in the GPCR target space. 2012 , 19, 544-56	20
1026	Clinical implications of recent insights into the structural biology of beta2 adrenoceptors. 2012 , 13, 1336-46	6
1025	Compound activity prediction using models of binding pockets or ligand properties in 3D. 2012 , 12, 1869-82	33
1024	Functional selectivity in GPCR signaling: understanding the full spectrum of receptor conformations. 2012 , 12, 817-30	20
1023	The G-protein coupled receptor family: actors with many faces. 2012 , 18, 175-85	28
1022	Ice breaking in GPCR structural biology. 2012 , 33, 324-34	39
1021	The essential role for aromatic cluster in the β adrenergic receptor. 2012 , 33, 1062-8	3
1020	Recent Advances in the Rationale Design of GPER Ligands. 2012 , 19, 6199-6206	12
1019	Modeling and simulation studies of human β adrenergic receptor and its interactions with agonists. 2012 , 8, 283-95	4
1018	Automatic modeling of mammalian olfactory receptors and docking of odorants. 2012 , 25, 377-86	47

1017	Allostery. 2012 ,	4
1016	Tools for GPCR drug discovery. 2012 , 33, 372-84	214
1015	Identification of three residues essential for 5-hydroxytryptamine 2A-metabotropic glutamate 2 (5-HT _{2A} /mGlu ₂) receptor heteromerization and its psychoactive behavioral function. 2012 , 287, 44301-19	94
1014	Reengineering the collision coupling and diffusion mode of the A _{2A} -adenosine receptor: palmitoylation in helix 8 relieves confinement. 2012 , 287, 42104-18	8
1013	Turning receptors on and off with intracellular pepducins: new insights into G-protein-coupled receptor drug development. 2012 , 287, 12787-96	113
1012	A novel nonribose agonist, LUF5834, engages residues that are distinct from those of adenosine-like ligands to activate the adenosine A _{2a} receptor. 2012 , 81, 475-87	31
1011	Modulation of constitutive activity and signaling bias of the ghrelin receptor by conformational constraint in the second extracellular loop. 2012 , 287, 33488-502	30
1010	Naturally evolved G protein-coupled receptors adopt metastable conformations. 2012 , 109, 13284-9	40
1009	Pharmacological characterization and modeling of the binding sites of novel 1,3-bis(pyridinylethynyl)benzenes as metabotropic glutamate receptor 5-selective negative allosteric modulators. 2012 , 82, 929-37	32
1008	The thyrotropin receptor hinge region as a surrogate ligand: identification of loci contributing to the coupling of thyrotropin binding and receptor activation. 2012 , 153, 5058-67	9
1007	Spatial proximity between the VPAC1 receptor and the amino terminus of agonist and antagonist peptides reveals distinct sites of interaction. 2012 , 26, 2060-71	21
1006	Limits of ligand selectivity from docking to models: in silico screening for A ₁ adenosine receptor antagonists. 2012 , 7, e49910	46
1005	Intracellular Loop 2 Peptides of the Human 5HT _{1a} Receptor are Differential Activators of Gi. 2012 , 2012, 490734	2
1004	The arginine of the DRY motif in transmembrane segment III functions as a balancing micro-switch in the activation of the α_2 -adrenergic receptor. 2012 , 287, 31973-82	24
1003	Ligand-mimicking receptor variant discloses binding and activation mode of prolactin-releasing peptide. 2012 , 287, 32181-94	7
1002	PheVI:09 (Phe _{6.44}) as a sliding microswitch in seven-transmembrane (7TM) G protein-coupled receptor activation. 2012 , 287, 43516-26	27
1001	The importance of the adenosine A _{2A} receptor-dopamine D ₂ receptor interaction in drug addiction. 2012 , 19, 317-55	63
1000	Evolution of class A G-protein-coupled receptors: implications for molecular modeling. 2012 , 19, 1110-8	10

999	Homology Modeling and Antagonist Binding Site Study of the Human Histamine H2 Receptor. 2012 , 8, 1084-1092	2
998	A closer look into G protein coupled receptor activation: X-ray crystallography and long-scale molecular dynamics simulations. 2012 , 19, 1135-45	16
997	The family B1 GPCR: structural aspects and interaction with accessory proteins. 2012 , 13, 103-15	36
996	Structure-Based Design, Synthesis and Molecular Modeling Studies of Thiazolyl Urea Derivatives as Novel Anti-Parkinsonian Agents. 2012 , 8, 1057-1068	0
995	Action of molecular switches in GPCRs--theoretical and experimental studies. 2012 , 19, 1090-109	298
994	Harvesting and cryo-cooling crystals of membrane proteins grown in lipidic mesophases for structure determination by macromolecular crystallography. 2012 , e4001	35
993	9.8 G Protein Coupled Receptors. 2012 , 123-148	
992	Adenosiland: walking through adenosine receptors landscape. 2012 , 58, 248-57	27
991	Allosteric modulation of seven transmembrane spanning receptors: theory, practice, and opportunities for central nervous system drug discovery. 2012 , 55, 1445-64	184
990	Membrane protein structure determination using crystallography and lipidic mesophases: recent advances and successes. 2012 , 51, 6266-88	96
989	Structural basis for allosteric regulation of GPCRs by sodium ions. <i>Science</i> , 2012 , 337, 232-6	33.3 714
988	Exploring the directionality of 5-substitutions in a new series of 5-alkylaminopyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine as a strategy to design novel human $\alpha(3)$ adenosine receptor antagonists. 2012 , 55, 9654-68	16
987	Molecular dynamics simulations reveal specific interactions of post-translational palmitoyl modifications with rhodopsin in membranes. 2012 , 134, 4324-31	29
986	Homology modeling of cannabinoid receptors: discovery of cannabinoid analogues for therapeutic use. 2012 , 819, 595-613	8
985	Critical features for biosynthesis, stability, and functionality of a G protein-coupled receptor uncovered by all-versus-all mutations. 2012 , 109, 9810-5	62
984	Identification of residues involved in homodimer formation located within a β -strand region of the N-terminus of a Yeast G protein-coupled receptor. 2012 , 32, 65-75	20
983	Target based virtual screening by docking into automatically generated GPCR models. 2012 , 914, 255-70	1
982	Chapter 7:A Nuclear G Protein-coupled Estrogen Receptor, GPER. Homology Modeling Studies Toward Its Ligand-binding Mode Characterization. 2012 , 117-137	5

981	C(X)CR in silico: Computer-aided prediction of chemokine receptor-ligand interactions. 2012 , 9, e227-314	16
980	Predicted structure of agonist-bound glucagon-like peptide 1 receptor, a class B G protein-coupled receptor. 2012 , 109, 19988-93	41
979	Crystal structure of a lipid G protein-coupled receptor. <i>Science</i> , 2012 , 335, 851-5	33-3 538
978	Comparison of the binding and functional properties of two structurally different D2 dopamine receptor subtype selective compounds. 2012 , 3, 1050-62	25
977	Structure of the human M2 muscarinic acetylcholine receptor bound to an antagonist. 2012 , 482, 547-51	625
976	Current assessment of docking into GPCR crystal structures and homology models: successes, challenges, and guidelines. 2012 , 52, 3263-77	74
975	Ligand-, structure- and pharmacophore-based molecular fingerprints: a case study on adenosine A(1), A (2A), A (2B), and A (3) receptor antagonists. 2012 , 26, 1247-66	41
974	Structure-based design, synthesis, and molecular modeling studies of 1-(benzo[d]thiazol-2-yl)-3-(substituted aryl)urea derivatives as novel anti-Parkinsonian agents. 2012 , 21, 2630-2643	13
973	Homology modeling of the human 5-HT1A, 5-HT 2A, D1, and D2 receptors: model refinement with molecular dynamics simulations and docking evaluation. 2012 , 18, 3639-55	24
972	Fractal dimension as a measure of surface roughness of G protein-coupled receptors: implications for structure and function. 2012 , 18, 4465-75	14
971	Restructuring G-protein- coupled receptor activation. 2012 , 151, 14-23	208
970	Fragment screening at adenosine-A(3) receptors in living cells using a fluorescence-based binding assay. 2012 , 19, 1105-15	67
969	Ligand and decoy sets for docking to G protein-coupled receptors. 2012 , 52, 1-6	88
968	Fabrication of X-ray compatible microfluidic platforms for protein crystallization. 2012 , 174, 1-9	53
967	The role of protein structural analysis in the next generation sequencing era. 2014 , 336, 67-98	12
966	Pharmacophore mapping and in silico screening to identify new potent leads for A(2A) adenosine receptor as antagonists. 2012 , 32, 102-13	10
965	Insertion of T4-lysozyme (T4L) can be a useful tool for studying olfactory-related GPCRs. 2012 , 8, 1750-9	11
964	Post-translational modifications of the serotonin type 4 receptor heterologously expressed in mouse rod cells. 2012 , 51, 214-24	12

963	An aromatic region to induce a switch between agonism and inverse agonism at the ghrelin receptor. 2012 , 55, 7437-49	39
962	Second extracellular loop of human glucagon-like peptide-1 receptor (GLP-1R) has a critical role in GLP-1 peptide binding and receptor activation. 2012 , 287, 3642-58	74
961	New insights for drug design from the X-ray crystallographic structures of G-protein-coupled receptors. 2012 , 82, 361-71	75
960	A structure-based approach to understanding somatostatin receptor-4 agonism (sst4). 2012 , 52, 171-86	16
959	Synthesis and pharmacological evaluation of dual acting antioxidant A(2A) adenosine receptor agonists. 2012 , 55, 3521-34	17
958	Predictions for cholesterol interaction sites on the A2A adenosine receptor. 2012 , 134, 16512-5	81
957	Structural transitions of transmembrane helix 6 in the formation of metarhodopsin I. 2012 , 116, 10477-89	16
956	Microscopic binding of M5 muscarinic acetylcholine receptor with antagonists by homology modeling, molecular docking, and molecular dynamics simulation. 2012 , 116, 532-41	10
955	Homology model-assisted elucidation of binding sites in GPCRs. 2012 , 914, 179-205	31
954	Mistic and TarCF as fusion protein partners for functional expression of the cannabinoid receptor 2 in Escherichia coli. 2012 , 83, 128-34	13
953	An expression and purification system for the biosynthesis of adenosine receptor peptides for biophysical and structural characterization. 2012 , 84, 224-35	3
952	Ligand-specific interactions modulate kinetic, energetic, and mechanical properties of the human α_2 adrenergic receptor. 2012 , 20, 1391-402	79
951	Diversity and modularity of G protein-coupled receptor structures. 2012 , 33, 17-27	348
950	Domain coupling in GPCRs: the engine for induced conformational changes. 2012 , 33, 79-88	59
949	New insights from structural biology into the druggability of G protein-coupled receptors. 2012 , 33, 249-60	150
948	Biomolecular membrane protein crystallization. 2012 , 92, 2648-2661	9
947	Ligand binding and activation of the secretin receptor, a prototypic family B G protein-coupled receptor. 2012 , 166, 18-26	13
946	Conformational switches in the VPAC(1) receptor. 2012 , 166, 79-84	5

945	Reversed binding of a small molecule ligand in homologous chemokine receptors - differential role of extracellular loop 2. 2012 , 166, 258-75	13
944	Functional efficacy of adenosine A _{2A} receptor agonists is positively correlated to their receptor residence time. 2012 , 166, 1846-59	124
943	Vibrationally assisted electron transfer mechanism of olfaction: myth or reality?. 2012 , 14, 13861-71	47
942	Comparative modeling of lipid receptors. 2012 , 914, 207-18	2
941	Structure prediction of G protein-coupled receptors and their ensemble of functionally important conformations. 2012 , 914, 237-54	22
940	Dopamine D1 receptor and serotonin 5-HT _{1A} receptor agonist effects of the natural product (R)-stapholidine: molecular modelling and dynamics simulations. 2012 , 38, 970-979	1
939	Modeling of mammalian olfactory receptors and docking of odorants. 2012 , 4, 255-269	15
938	Maximizing detergent stability and functional expression of a GPCR by exhaustive recombination and evolution. 2012 , 422, 414-28	46
937	Artificial membrane-like environments for in vitro studies of purified G-protein coupled receptors. 2012 , 1818, 225-33	65
936	Molecular simulations and solid-state NMR investigate dynamical structure in rhodopsin activation. 2012 , 1818, 241-51	26
935	Optimization of purification and refolding of the human chemokine receptor CXCR1 improves the stability of proteoliposomes for structure determination. 2012 , 1818, 584-91	30
934	The role of cholesterol on the activity and stability of neurotensin receptor 1. 2012 , 1818, 2228-33	58
933	Structure and activation of rhodopsin. 2012 , 33, 291-9	42
932	Structure-activity relationships and molecular modeling of 1,2,4-triazoles as adenosine receptor antagonists. 2012 , 3, 715-720	15
931	Structure-based drug screening for G-protein-coupled receptors. 2012 , 33, 268-72	229
930	Large multiple transmembrane domain fragments of a G protein-coupled receptor: biosynthesis, purification, and biophysical studies. 2012 , 98, 485-500	6
929	MT1-selective melatonin receptor ligands: synthesis, pharmacological evaluation, and molecular dynamics investigation of N-[(3-O-substituted)anilino]alkyl]amides. 2012 , 7, 1954-64	21
928	Platform for the rapid construction and evaluation of GPCRs for crystallography in <i>Saccharomyces cerevisiae</i> . 2012 , 11, 78	37

927	Identifying novel adenosine receptor ligands by simultaneous proteochemometric modeling of rat and human bioactivity data. 2012 , 55, 7010-20	42
926	Structure-function studies of muscarinic acetylcholine receptors. 2012 , 29-48	14
925	G Protein-Coupled Receptors. 2012 , 31-70	
924	Ligand-receptor interaction platforms and their applications for drug discovery. 2012 , 7, 969-88	81
923	The best of both worlds? Bitopic orthosteric/allosteric ligands of g protein-coupled receptors. 2012 , 52, 153-78	133
922	Non-HLA-antibodies targeting Angiotensin type 1 receptor and antibody mediated rejection. 2012 , 73, 1282-6	37
921	Topogenesis of heterologously expressed fragments of the human Y4 GPCR. 2012 , 1818, 3055-63	5
920	Agonist dynamics and conformational selection during microsecond simulations of the A(2A) adenosine receptor. 2012 , 102, 2114-20	32
919	Comparison of fragments comprising the first two helices of the human Y4 and the yeast Ste2p G-protein-coupled receptors. 2012 , 103, 817-26	4
918	New chromene scaffolds for adenosine A(2A) receptors: synthesis, pharmacology and structure-activity relationships. 2012 , 54, 303-10	28
917	Antihypertensive profile of 2-thienyl-3,4-methylenedioxybenzoylhydrazine is mediated by activation of the A2A adenosine receptor. 2012 , 55, 49-57	26
916	Agonist-bound structures of G protein-coupled receptors. 2012 , 22, 482-90	85
915	Ligand-specific homology modeling of human cannabinoid (CB1) receptor. 2012 , 38, 155-64	13
914	Identification of structural determinants of ligand selectivity in 5-HT ₂ receptor subtypes on the basis of protein-ligand interactions. 2012 , 38, 342-53	1
913	Receptors for Purines and Pyrimidines. 2012 , 119-244	12
912	Modeling the structural communication in supramolecular complexes involving GPCRs. 2012 , 914, 319-36	4
911	[Handling G-protein-coupled receptors: expression, purification and in vitro stabilization]. 2012 , 28, 837-44	2
910	Early History of Purinergic Signalling. 2012 , 7-66	2

909	Highly potent and selective fluorescent antagonists of the human adenosine A ₁ receptor based on the 1,2,4-triazolo[4,3-a]quinoxalin-1-one scaffold. 2012 , 55, 1771-82	36
908	Comparative pharmacophore modeling of human adenosine receptor A ₁ and A ₃ antagonists. 2012 , 55, 2407-2418	1
907	Contributions of fluorescence techniques to understanding G protein-coupled receptor dimerisation. 2012 , 4, 291-298	12
906	Molecular Docking and Prediction of Pharmacokinetic Properties of Dual Mechanism Drugs that Block MAO-B and Adenosine A _{2A} Receptors for the Treatment of Parkinson's Disease. 2012 , 4, 184-92	32
905	Water-soluble pyrazolo[4,3-e][1,2,4]triazolo[1,5-c]pyrimidines as human A _{1A} adenosine receptor antagonists. 2012 , 55, 5380-90	10
904	Screening for high-yielding <i>Pichia pastoris</i> clones: the production of G protein-coupled receptors as a case study. 2012 , 866, 65-73	6
903	1.4 X-Ray Crystallography: Crystallization. 2012 , 34-63	
902	Neuroendocrine GPCR Signaling. 2012 , 21-53	4
901	Cannabinoid receptor type 2 (CB ₂)-selective N-aryl-oxadiazolyl-propionamides: synthesis, radiolabelling, molecular modelling and biological evaluation. 2012 , 2, 32	30
900	Identification of a crucial amino acid in the helix position 6.51 of human tachykinin neurokinin 1 and 3 receptors contributing to the insurmountable mode of antagonism by dual NK ₁ /NK ₃ antagonists. 2012 , 55, 5061-76	5
899	3-aryl-[1,2,4]triazino[4,3-a]benzimidazol-4(10H)-one: a novel template for the design of highly selective A _{2B} adenosine receptor antagonists. 2012 , 55, 1490-9	23
898	Molecular evolution of a peptide GPCR ligand driven by artificial neural networks. 2012 , 7, e36948	10
897	N-terminal T4 lysozyme fusion facilitates crystallization of a G protein coupled receptor. 2012 , 7, e46039	99
896	Stabilization of functional recombinant cannabinoid receptor CB ₂ in detergent micelles and lipid bilayers. 2012 , 7, e46290	38
895	Structural Diversity in Conserved Regions Like the DRY-Motif among Viral 7TM Receptors-A Consequence of Evolutionary Pressure?. 2012 , 2012, 231813	12
894	Beyond modeling: all-atom olfactory receptor model simulations. 2012 , 3, 61	20
893	[G protein-coupled receptors in the spotlight]. 2012 , 28, 876-82	3
892	Purinergic signalling: what is missing and needed next? The use of transgenic mice, crystallographic analysis and MicroRNA. 2012 , 11, 751-67	6

891	Farnesyl pyrophosphate is an endogenous antagonist to ADP-stimulated P2Y ₁ receptor-mediated platelet aggregation. 2012 , 108, 119-32	8
890	Novel computational methodologies for structural modeling of spacious ligand binding sites of G-protein-coupled receptors: development and application to human leukotriene B4 receptor. 2012 , 2012, 691579	1
889	Human Serotonin 5-HT G Protein-Coupled Receptor Homology Model from the Adrenoceptor Structure: Ligand Docking and Mutagenesis Studies. 2012 , 112, 140	8
888	Bihelix: Towards de novo structure prediction of an ensemble of G-protein coupled receptor conformations. 2012 , 80, 505-18	37
887	Do crystal structures obviate the need for theoretical models of GPCRs for structure-based virtual screening?. 2012 , 80, 1503-21	26
886	Homology modeling and molecular dynamics simulations of the active state of the nociceptin receptor reveal new insights into agonist binding and activation. 2012 , 80, 1948-61	26
885	Molecular Determinants for Ligand Binding at Serotonin 5-HT and 5-HT GPCRs: Experimental Affinity Results Analyzed by Molecular Modeling and Ligand Docking Studies. 2012 , 112, 3807-3814	14
884	Structure of the first sphingosine 1-phosphate receptor. 2012 , 5, pe23	13
883	Chemistry and biology of multicomponent reactions. 2012 , 112, 3083-135	1678
882	Characterization of adenosine receptor in its native environment: insights from molecular dynamics simulations of palmitoylated/glycosylated, membrane-integrated human A(2B) adenosine receptor. 2012 , 18, 4309-24	15
881	Structure of the human μ opioid receptor in complex with JDTic. 2012 , 485, 327-32	695
880	Optimization of adenosine 5'-carboxamide derivatives as adenosine receptor agonists using structure-based ligand design and fragment screening. 2012 , 55, 4297-308	55
879	A prospective cross-screening study on G-protein-coupled receptors: lessons learned in virtual compound library design. 2012 , 55, 5311-25	28
878	Chapter 2: Thermodynamics of Ligand Binding. 2012 , 23-79	4
877	A new era of GPCR structural and chemical biology. 2012 , 8, 670-3	160
876	Interpreting the structural mechanism of action for MT7 and human muscarinic acetylcholine receptor 1 complex by modeling protein-protein interaction. 2012 , 30, 30-44	6
875	G-protein-coupled receptor dynamics: dimerization and activation models compared with experiment. 2012 , 40, 394-9	13
874	Structural insights into human GPCR protein OA1: a computational perspective. 2012 , 18, 2117-33	9

873	Evaluation of molecular modeling of agonist binding in light of the crystallographic structure of an agonist-bound A _{2A} adenosine receptor. 2012 , 55, 538-52	36
872	G-protein-coupled receptor inactivation by an allosteric inverse-agonist antibody. 2012 , 482, 237-40	240
871	Computational studies of the binding modes of CCR1 antagonists. 2012 , 38, 953-960	1
870	Molecular Dynamics Simulations of G Protein-Coupled Receptors. 2012 , 31, 222-30	15
869	Structure-activity relationships of truncated C2- or C8-substituted adenosine derivatives as dual acting A _{2A} and A _{2B} adenosine receptor ligands. 2012 , 55, 342-56	31
868	Molecular insights into the D1R agonist and D2R/D3R antagonist effects of the natural product (-)-stepholidine: molecular modeling and dynamics simulations. 2012 , 116, 8121-30	12
867	Vorhersage der Ligandenerkennung in einem Geruchsrezeptor durch Kombination von ortsgerechter Mutagenese und dynamischer Homologie-Modellierung. 2012 , 124, 1300-1304	9
866	Biosynthesis and spectroscopic characterization of 2-TM fragments encompassing the sequence of a human GPCR, the Y4 receptor. 2012 , 13, 818-28	6
865	Impact of helix irregularities on sequence alignment and homology modeling of G protein-coupled receptors. 2012 , 13, 1393-9	35
864	Investigation of D ₁ receptor-agonist interactions using a combination of pharmacophore and receptor homology modeling. 2012 , 7, 471-82, 338	11
863	Structure-activity relationships for negative allosteric mGluR5 modulators. 2012 , 7, 440-51	16
862	Allostery and the Monod-Wyman-Changeux model after 50 years. 2012 , 41, 103-33	265
861	Allosteric mechanisms of G protein-Coupled Receptor signaling: a structural perspective. 2012 , 796, 133-74	11
860	Fragment-based approaches in drug discovery and chemical biology. 2012 , 51, 4990-5003	315
859	Ligand-based virtual screening approach using a new scoring function. 2012 , 52, 963-74	58
858	Molecular mechanism of β -arrestin-biased agonism at seven-transmembrane receptors. 2012 , 52, 179-97	461
857	G protein-coupled adenosine (P1) and P2Y receptors: ligand design and receptor interactions. 2012 , 8, 419-36	71
856	h β 2R-G β complex: prediction versus crystal structure--how valuable are predictions based on molecular modeling studies?. 2012 , 18, 3439-44	1

855	Structural modelling and dynamics of proteins for insights into drug interactions. 2012 , 64, 323-43	24
854	Characterization of the Drosophila adenosine receptor: the effect of adenosine analogs on cAMP signaling in Drosophila cells and their utility for in vivo experiments. 2012 , 121, 383-95	5
853	Pharmacological modulation of chemokine receptor function. 2012 , 165, 1617-1643	175
852	Lifting the lid on GPCRs: the role of extracellular loops. 2012 , 165, 1688-1703	190
851	Identification and analysis of functionally important amino acids in human purinergic 12 receptor using a Saccharomyces cerevisiae expression system. 2012 , 279, 180-91	16
850	Binding sites in membrane proteins--diversity, druggability and prospects. 2012 , 91, 326-39	6
849	Specification of the cholesterol interaction with the oxytocin receptor using a chimeric receptor approach. 2012 , 676, 12-9	13
848	Novel fluorescent antagonist as a molecular probe in A(3) adenosine receptor binding assays using flow cytometry. 2012 , 83, 1552-61	28
847	Discovery of novel A3 adenosine receptor ligands based on chromone scaffold. 2012 , 84, 21-9	41
846	The role of the second and third extracellular loops of the adenosine A1 receptor in activation and allosteric modulation. 2012 , 84, 76-87	45
845	Determination of different putative allosteric binding pockets at the lutropin receptor by using diverse drug-like low molecular weight ligands. 2012 , 351, 326-36	28
844	Computational design of membrane proteins. 2012 , 20, 5-14	31
843	Fusion partner toolchest for the stabilization and crystallization of G protein-coupled receptors. 2012 , 20, 967-76	272
842	G protein-coupled receptors in the hypothalamic paraventricular and supraoptic nuclei--serpentine gateways to neuroendocrine homeostasis. 2012 , 33, 45-66	57
841	Crystallographic study and molecular modeling on the oxidation product of N-[(8R)-2-methoxy-5,6,7,8,9,10-hexahydro-6,9-methanocyclohepta[b]indol-8-yl]acetamide. 2012 , 48, 552-555	1
840	Palmitoylation and membrane cholesterol stabilize Ebpioid receptor homodimerization and G protein coupling. 2012 , 13, 6	77
839	Prediction of a ligand-binding niche within a human olfactory receptor by combining site-directed mutagenesis with dynamic homology modeling. 2012 , 51, 1274-8	74
838	Three "hotspots" important for adenosine A(2B) receptor activation: a mutational analysis of transmembrane domains 4 and 5 and the second extracellular loop. 2012 , 8, 23-38	17

837	The A3 adenosine receptor as multifaceted therapeutic target: pharmacology, medicinal chemistry, and in silico approaches. 2013 , 33, 235-335	35
836	endoCANNABINOIDS. 2013 ,	6
835	Development of new chromatographic tools based on A2A adenosine receptor subtype for ligand characterization and screening by FAC-MS. 2013 , 405, 837-45	15
834	Design, synthesis, binding and docking-based 3D-QSAR studies of 2-pyridylbenzimidazoles--a new family of high affinity CB1 cannabinoid ligands. 2013 , 18, 3972-4001	17
833	Synthesis, biological activity and molecular modelling studies of tricyclic alkylimidazo-, pyrimido- and diazepinopurinediones. 2013 , 9, 395-414	12
832	Quaternary structure predictions and structural communication features of GPCR dimers. 2013 , 117, 105-42	12
831	Probing GPCR structure: adenosine and P2Y nucleotide receptors. 2013 , 520, 199-217	4
830	In vitro modification of substituted cysteines as tool to study receptor functionality and structure-activity relationships. 2013 , 439, 173-83	3
829	Production of GPCR and GPCR complexes for structure determination. 2013 , 23, 381-92	30
828	A microfluidic approach for protein structure determination at room temperature via on-chip anomalous diffraction. 2013 , 13, 3183-7	35
827	Structure of the human glucagon class B G-protein-coupled receptor. 2013 , 499, 444-9	312
826	Conversion of a non-selective adenosine receptor antagonist into A3-selective high affinity fluorescent probes using peptide-based linkers. 2013 , 11, 5673-82	40
825	Development of 7TM receptor-ligand complex models using ligand-biased, semi-empirical helix-bundle repacking in torsion space: application to the agonist interaction of the human dopamine D2 receptor. 2013 , 27, 277-91	3
824	Synthesis of substituted diphenyl sulfones and their structure-activity relationship with the antagonism of 5-HT _{2A} receptors. 2013 , 21, 4614-27	17
823	Molecular modeling of adenosine receptors. 2013 , 522, 37-59	3
822	Functionally biased signalling properties of 7TM receptors - opportunities for drug development for the ghrelin receptor. 2013 , 170, 1349-62	50
821	Olfactory Receptors. 2013 ,	1
820	Conformational ensemble view of G protein-coupled receptors and the effect of mutations and ligand binding. 2013 , 520, 31-48	14

819	Novel approaches to drug design for the treatment of schizophrenia. 2013 , 8, 1285-96	19
818	Synthesis, molecular structure, NMR spectroscopic and computational analysis of a selective adenosine A2A antagonist, ZM 241385. 2013 , 24, 1241-1251	9
817	Structure-based virtual screening of MT2 melatonin receptor: influence of template choice and structural refinement. 2013 , 53, 821-35	28
816	The role of a sodium ion binding site in the allosteric modulation of the A(2A) adenosine G protein-coupled receptor. 2013 , 21, 2175-85	98
815	Ligand-dependent cholesterol interactions with the human A(2A) adenosine receptor. 2013 , 169, 39-45	22
814	Molecular modeling of vasopressin receptor and in silico screening of V1b receptor antagonists. 2013 , 8, 951-64	1
813	Design and evaluation of xanthine based adenosine receptor antagonists: potential hypoxia targeted immunotherapies. 2013 , 21, 7453-64	8
812	Kink characterization and modeling in transmembrane protein structures. 2013 , 53, 2926-36	6
811	G protein-coupled receptors as regulators of energy homeostasis. 2013 , 114, 1-43	13
810	Development of a cysteine-deprived and C-terminally truncated GLP-1 receptor. 2013 , 49, 100-8	6
809	Unlocking the secrets of the gatekeeper: methods for stabilizing and crystallizing GPCRs. 2013 , 1828, 2583-91	27
808	Conformational restriction of G-proteins Coupled Receptors (GPCRs) upon complexation to G-proteins: a putative activation mode of GPCRs?. 2013 , 587, 2656-61	10
807	4th International Conference on Biomedical Engineering in Vietnam. 2013 ,	3
806	The protein local optimization program and G-protein-coupled receptors: loop restoration and applications to homology modeling. 2013 , 522, 1-20	1
805	Computational design and experimental characterization of GPCR segment models. 2013 , 522, 81-95	
804	Magic angle spinning nuclear magnetic resonance spectroscopy of G protein-coupled receptors. 2013 , 522, 365-89	8
803	Amino acid residues of G-protein-coupled receptors critical for endoplasmic reticulum export and trafficking. 2013 , 521, 203-16	3
802	An overview of biological macromolecule crystallization. 2013 , 14, 11643-91	83

801	8-(2-Furyl)adenine derivatives as A _{2A} adenosine receptor ligands. 2013 , 70, 525-35	11
800	GPCR activation: protonation and membrane potential. 2013 , 4, 747-60	17
799	Study of the selectivity of α -adrenergic antagonists by molecular modeling of α _{1a} -, α _{1b} -, and α ₂ -adrenergic receptor subtypes and docking simulations. 2013 , 144, 903-912	1
798	Implementing the "Best Template Searching" tool into Adenosiland platform. 2013 , 1, 25	10
797	Crystal structures of the A adenosine receptor and their use in medicinal chemistry. 2013 , 1, 22	8
796	Simulation and comparative analysis of binding modes of nucleoside and non-nucleoside agonists at the A _{2B} adenosine receptor. 2013 , 1, 24	19
795	Advances in the study of structure and function of G protein-coupled receptors (about awarding the Nobel Prize for Chemistry in 2012 to Robert Lefkowitz and Brian Kobilka). 2013 , 49, 469-480	0
794	Solid-state NMR spectroscopy structure determination of a lipid-embedded heptahelical membrane protein. 2013 , 10, 1007-12	172
793	Modulation of A _{2B} receptor antagonist on D ₁ receptor internalization and ERK phosphorylation. 2013 , 34, 1292-300	15
792	α -adrenergic receptor activation by agonists studied with ^{19}F NMR spectroscopy. 2013 , 52, 10762-5	60
791	Complementarity between in silico and biophysical screening approaches in fragment-based lead discovery against the A _{2A} adenosine receptor. 2013 , 53, 2701-14	55
790	To fuse or not to fuse: what is your purpose?. 2013 , 22, 1466-77	76
789	G Protein-Coupled Estrogen Receptor (GPER) Agonist Dual Binding Mode Analyses toward Understanding of its Activation Mechanism: A Comparative Homology Modeling Approach. 2013 , 32, 647-658	22
788	The Concise Guide to PHARMACOLOGY 2013/14: G protein-coupled receptors. 2013 , 170, 1459-581	509
787	A Strategy Combining Differential Low-Throughput Screening and Virtual Screening (DLS-VS) Accelerating the Discovery of new Modulators for the Orphan GPR34 Receptor. 2013 , 32, 213-29	10
786	The role of hydrophobic amino acids in the structure and function of the rhodopsin family of G protein-coupled receptors. 2013 , 520, 99-115	10
785	Conopeptide α 1A defines a new allosteric site on the extracellular surface of the α _{2B} -adrenoceptor. 2013 , 288, 1814-27	20
784	The GPCR Network: a large-scale collaboration to determine human GPCR structure and function. 2013 , 12, 25-34	207

783	Molecular alliance-from orthosteric and allosteric ligands to dualsteric/bitopic agonists at G protein coupled receptors. 2013 , 52, 508-16	64
782	Molecular basis for dramatic changes in cannabinoid CB1 G protein-coupled receptor activation upon single and double point mutations. 2013 , 22, 101-13	33
781	Ligand-specific binding and activation of the human adenosine A(2B) receptor. 2013 , 52, 726-40	35
780	Mapping the functional binding sites of cholesterol in β_2 -adrenergic receptor by long-time molecular dynamics simulations. 2013 , 117, 1085-94	65
779	Identification of novel amino acid derived CCK-2R antagonists as potential antiulcer agent: homology modeling, design, synthesis, and pharmacology. 2013 , 53, 176-87	12
778	Biophysical and structural investigation of bacterially expressed and engineered CCR5, a G protein-coupled receptor. 2013 , 55, 79-95	16
777	Molecular signatures of G-protein-coupled receptors. 2013 , 494, 185-94	1071
776	Characterization of the dynamic events of GPCRs by automated computational simulations. 2013 , 41, 205-12	35
775	Computationally-predicted CB1 cannabinoid receptor mutants show distinct patterns of salt-bridges that correlate with their level of constitutive activity reflected in G protein coupling levels, thermal stability, and ligand binding. 2013 , 81, 1304-17	30
774	Structure-function of the G protein-coupled receptor superfamily. 2013 , 53, 531-56	758
773	Loop prediction for a GPCR homology model: algorithms and results. 2013 , 81, 214-28	18
772	Molekulare Allianz von orthosterischen und allosterischen Liganden zu dualsterischen/bitopischen Agonisten G-Protein-gekoppelter Rezeptoren. 2013 , 125, 530-538	5
771	A structural chemogenomics analysis of aminergic GPCRs: lessons for histamine receptor ligand design. 2013 , 170, 101-26	60
770	Modulation of A2B adenosine receptor by 1-Benzyl-3-ketoindole derivatives. 2013 , 69, 331-7	24
769	Identification of transmembrane domain 3, 4 & 5 residues that contribute to the formation of the ligand-binding pocket of the urotensin-II receptor. 2013 , 86, 1584-93	7
768	The second extracellular loop of GPCRs determines subtype-selectivity and controls efficacy as evidenced by loop exchange study at A2 adenosine receptors. 2013 , 85, 1317-29	30
767	Structure of β -adrenergic receptors. 2013 , 520, 117-51	7
766	Directed evolution of G-protein-coupled receptors for high functional expression and detergent stability. 2013 , 520, 67-97	15

765	Enrichment factor analyses on G-protein coupled receptors with known crystal structure. 2013 , 53, 739-43	19
764	Loss of constitutive activity is correlated with increased thermostability of the human adenosine A2A receptor. 2013 , 169, 988-98	24
763	Endogenous lipid activated G protein-coupled receptors: emerging structural features from crystallography and molecular dynamics simulations. 2013 , 169, 46-56	30
762	Structural features of the apelin receptor N-terminal tail and first transmembrane segment implicated in ligand binding and receptor trafficking. 2013 , 1828, 1471-83	29
761	Optimising the combination of thermostabilising mutations in the neurotensin receptor for structure determination. 2013 , 1828, 1293-301	28
760	Antagonist binding and induced conformational dynamics of GPCR A2A adenosine receptor. 2013 , 81, 1399-410	17
759	Paracrine Regulation of Renal Function by Dopamine. 2013 , 539-591	1
758	2-Arylpyrazolo[4,3-d]pyrimidin-7-amino derivatives as new potent and selective human A3 adenosine receptor antagonists. Molecular modeling studies and pharmacological evaluation. 2013 , 56, 2256-69	24
757	From heptahelical bundle to hits from the Haystack: structure-based virtual screening for GPCR ligands. 2013 , 522, 279-336	44
756	Crystal structure of oligomeric α 1-adrenergic G protein-coupled receptors in ligand-free basal state. 2013 , 20, 419-25	207
755	Design, synthesis and biological evaluation of bivalent ligands against A(1)-D(1) receptor heteromers. 2013 , 34, 441-52	14
754	A homology modeling study toward the understanding of three-dimensional structure and putative pharmacological profile of the G-protein coupled receptor GPR55. 2013 , 39, 50-60	21
753	Bridging the gap: bitopic ligands of G-protein-coupled receptors. 2013 , 34, 59-66	132
752	Critical analysis of the successes and failures of homology models of G protein-coupled receptors. 2013 , 81, 729-39	20
751	GPCR activation: a mutagenic spotlight on crystal structures. 2013 , 34, 67-84	57
750	Adenosine receptors as drug targets--what are the challenges?. 2013 , 12, 265-86	573
749	Molecular dynamics simulations of the adenosine A2a receptor: structural stability, sampling, and convergence. 2013 , 53, 1168-78	36
748	X-ray structural information of GPCRs in drug design: what are the limitations and where do we go?. 2013 , 8, 607-20	15

747	Interactions of the β subunits of heterotrimeric G-proteins with GPCRs, effectors and RGS proteins: a critical review and analysis of interacting surfaces, conformational shifts, structural diversity and electrostatic potentials. 2013 , 182, 209-18	50
746	Conformational flexibility and structural dynamics in GPCR-mediated G protein activation: a perspective. 2013 , 425, 2288-98	72
745	Synthesis and structure-activity relationships of 2-hydrazinyladenosine derivatives as A(2A) adenosine receptor ligands. 2013 , 21, 436-47	4
744	Structure-based approaches to ligands for G-protein-coupled adenosine and P2Y receptors, from small molecules to nanoconjugates. 2013 , 56, 3749-67	27
743	Biophysical fragment screening of the α_1 -adrenergic receptor: identification of high affinity arylpiperazine leads using structure-based drug design. 2013 , 56, 3446-55	129
742	Novel adenosine A(2A) receptor ligands: a synthetic, functional and computational investigation of selected literature adenosine A(2A) receptor antagonists for extending into extracellular space. 2013 , 23, 3427-33	22
741	Breaking the barriers in membrane protein crystallography. 2013 , 45, 636-44	73
740	A3 adenosine receptor: homology modeling and 3D-QSAR studies. 2013 , 42, 60-72	24
739	Synthesis and biological evaluation of metabolites of 2-n-butyl-9-methyl-8-[1,2,3]triazol-2-yl-9H-purin-6-ylamine (ST1535), a potent antagonist of the A2A adenosine receptor for the treatment of Parkinson's disease. 2013 , 56, 5456-63	13
738	Water network perturbation in ligand binding: adenosine A(2A) antagonists as a case study. 2013 , 53, 1700-13	103
737	Generation of functional antibodies for mammalian membrane protein crystallography. 2013 , 23, 563-8	29
736	Ligand-dependent activation and deactivation of the human adenosine A(2A) receptor. 2013 , 135, 8749-59	83
735	Development of M1 mAChR allosteric and bitopic ligands: prospective therapeutics for the treatment of cognitive deficits. 2013 , 4, 1026-48	54
734	Retinal conformation governs pKa of protonated Schiff base in rhodopsin activation. 2013 , 135, 9391-8	30
733	Stabilizing membrane proteins through protein engineering. 2013 , 17, 427-35	65
732	Revisiting a receptor-based pharmacophore hypothesis for human A(2A) adenosine receptor antagonists. 2013 , 53, 1620-37	12
731	Expression of GPCRs in <i>Pichia pastoris</i> for structural studies. 2013 , 520, 1-29	10
730	Binding site exploration of CCR5 using in silico methodologies: a 3D-QSAR approach. 2013 , 36, 6-31	9

729	Structure-based studies of chemokine receptors. 2013 , 23, 539-46	19
728	Rational design of sulfonated A3 adenosine receptor-selective nucleosides as pharmacological tools to study chronic neuropathic pain. 2013 , 56, 5949-63	37
727	G-protein-coupled receptor structure, ligand binding and activation as studied by solid-state NMR spectroscopy. 2013 , 450, 443-57	31
726	Optimized method of G-protein-coupled receptor homology modeling: its application to the discovery of novel CXCR7 ligands. 2013 , 56, 4236-51	32
725	Molecular modelling of odorant/olfactory receptor complexes. 2013 , 1003, 53-65	15
724	Chemical genomics approach for GPCR-ligand interaction prediction and extraction of ligand binding determinants. 2013 , 53, 1253-62	8
723	Pyrazolo[1,5-c]quinazoline derivatives and their simplified analogues as adenosine receptor antagonists: synthesis, structure-affinity relationships and molecular modeling studies. 2013 , 21, 283-94	37
722	Methods for recombinant expression and functional characterization of human cannabinoid receptor CB2. 2013 , 6, e201303011	6
721	Distinct CCK-2 receptor conformations associated with β -arrestin-2 recruitment or phospholipase-C activation revealed by a biased antagonist. 2013 , 135, 2560-73	25
720	Mutagenesis and computational modeling of human G-protein-coupled receptor Y2 for neuropeptide Y and peptide YY. 2013 , 52, 7987-98	20
719	Self-organized criticality in proteins: Hydrophobic roughening profiles of G-protein-coupled receptors. 2013 , 87,	5
718	Selective and potent adenosine A3 receptor antagonists by methoxyaryl substitution on the N-(2,6-diarylpyrimidin-4-yl)acetamide scaffold. 2013 , 59, 235-42	11
717	Structural determinants of arrestin functions. 2013 , 118, 57-92	52
716	Synthesis of novel pyrido[3,2-e][1,2,4]triazolo[1,5-c]pyrimidine derivatives: potent and selective adenosine A3 receptor antagonists. 2013 , 346, 699-707	8
715	Emerging opportunities for allosteric modulation of G-protein coupled receptors. 2013 , 85, 153-62	43
714	Stabilised G protein-coupled receptors in structure-based drug design: a case study with adenosine A2A receptor. 2013 , 4, 52-67	23
713	Advances in methods to characterize ligand-induced ionic lock and rotamer toggle molecular switch in G protein-coupled receptors. 2013 , 520, 153-74	7
712	Strategies for studying the ligand binding site of GPCRs: photoaffinity labeling of the VPAC1 receptor, a prototype of class B GPCRs. 2013 , 520, 219-37	4

711	Preparation of purified GPCRs for structural studies. 2013 , 41, 185-90	11
710	Functional fusions of T4 lysozyme in the third intracellular loop of a G protein-coupled receptor identified by a random screening approach in yeast. 2013 , 26, 59-71	12
709	Insights into the molecular evolution of oxytocin receptor ligand binding. 2013 , 41, 197-204	45
708	Structural Characterization of an LPA1 Second Extracellular Loop Mimetic with a Self-Assembling Coiled-Coil Folding Constraint. 2013 , 14, 2788-807	3
707	An efficient nanolitre-volume multi-channel device for highly viscous materials used in membrane protein crystallization. 2013 , 46, 829-831	
706	Extracellular disulfide bridges serve different purposes in two homologous chemokine receptors, CCR1 and CCR5. 2013 , 84, 335-45	17
705	Biased and constitutive signaling in the CC-chemokine receptor CCR5 by manipulating the interface between transmembrane helices 6 and 7. 2013 , 288, 12511-21	51
704	Modelling of GPCRs. 2013 ,	2
703	Visualization of membrane protein crystals in lipid cubic phase using X-ray imaging. 2013 , 69, 1252-9	19
702	Crystallogenesis of adenosine A(2A) receptor-T4 lysozyme fusion protein: a practical route for the structure. 2013 , 520, 175-98	3
701	Efficient isotopic tryptophan labeling of membrane proteins by an indole controlled process conduct. 2013 , 110, 1681-90	5
700	Detailed analysis of biased histamine H ₁ receptor signalling by JNJ 7777120 analogues. 2013 , 170, 78-88	26
699	Structure of the human angiotensin II type 1 (AT1) receptor bound to angiotensin II from multiple chemoselective photoprobe contacts reveals a unique peptide binding mode. 2013 , 288, 8187-8197	37
698	[Strategies for the structural determination of G protein-coupled receptors: from an example of histamine H ₁ receptor]. 2013 , 133, 539-47	
697	β ₂ -Adrenergic Receptor Activation by Agonists Studied with 19F NMR Spectroscopy. 2013 , 125, 10962-10965	11
696	Computational approaches for ligand discovery and design in class-A G protein- coupled receptors. 2013 , 19, 2216-36	15
695	A computationally designed water-soluble variant of a G-protein-coupled receptor: the human mu opioid receptor. 2013 , 8, e66009	28
694	Assessment and challenges of ligand docking into comparative models of G-protein coupled receptors. 2013 , 8, e67302	29

693	The therapeutic potential of allosteric ligands for free fatty acid sensitive GPCRs. 2013 , 13, 14-25	24
692	The 2.1 Å resolution structure of cyanopindolol-bound β_1 -adrenoceptor identifies an intramembrane Na ⁺ ion that stabilises the ligand-free receptor. 2014 , 9, e92727	129
691	Pharmacology of Adenosine Receptors and Their Signaling Role in Immunity and Inflammation. 2014 ,	3
690	. 2014 ,	20
689	GPCR A2AAR Agonist Binding and Induced Conformation Changes of Functional Switches. 2014 , 27, 29-38	1
688	Molecular dynamics simulations reveal initial structural and dynamic features for the A2AR as a result of ligand binding. 2014 , 40, 996-1014	4
687	Structural basis for constitutive activity and agonist-induced activation of the enteroendocrine fat sensor GPR119. 2014 , 171, 5774-89	17
686	Identification of functionally important residues of the silkworm pheromone biosynthesis-activating neuropeptide receptor, an insect ortholog of the vertebrate neuromedin U receptor. 2014 , 289, 19150-63	18
685	The identification of high-affinity G protein-coupled receptor ligands from large combinatorial libraries using multicolor quantum dot-labeled cell-based screening. 2014 , 6, 809-23	4
684	Reflections on the Many Facets of Protein Microcrystallography. 2014 , 67, 1793	6
683	A combination of in vitro techniques for efficient discovery of functional monoclonal antibodies against human CXC chemokine receptor-2 (CXCR2). 2014 , 6, 1415-24	19
682	Functions of the DRY motif and intracellular loop 2 of human melanocortin 3 receptor. 2014 , 53, 319-30	16
681	Discovery of GPCR ligands for probing signal transduction pathways. 2014 , 5, 255	25
680	Structural basis of G protein-coupled receptor-Gi protein interaction: formation of the cannabinoid CB2 receptor-Gi protein complex. 2014 , 289, 20259-72	27
679	Somatostatin Receptor-4 Agonists as Candidates for Treatment of Alzheimer's Disease. 2014 , 566-597	2
678	Computational prediction of alanine scanning and ligand binding energetics in G-protein coupled receptors. 2014 , 10, e1003585	52
677	Alpha-bulges in G protein-coupled receptors. 2014 , 15, 7841-64	27
676	Membrane Protein Production for Structural Analysis. 2014 , 1-44	1

675	Applications for mass spectrometry in the study of ion channel structure and function. 2014 , 806, 237-61	1
674	Insight into the interactions between novel coumarin derivatives and human A3 adenosine receptors. 2014 , 9, 2245-53	11
673	Allosteric interactions at adenosine A(1) and A(3) receptors: new insights into the role of small molecules and receptor dimerization. 2014 , 171, 1102-13	47
672	Insights into the role of Asp79(2.50) in β_2 adrenergic receptor activation from molecular dynamics simulations. 2014 , 53, 7283-96	40
671	The molecular basis of ligand interaction at free fatty acid receptor 4 (FFA4/GPR120). 2014 , 289, 20345-58	52
670	Pancreatic polypeptide is recognized by two hydrophobic domains of the human Y4 receptor binding pocket. 2014 , 289, 5846-59	24
669	Mapping the intramolecular signal transduction of G-protein coupled receptors. 2014 , 82, 727-43	35
668	Global fold of human cannabinoid type 2 receptor probed by solid-state ^{13}C -, ^{15}N -MAS NMR and molecular dynamics simulations. 2014 , 82, 452-65	16
667	Structure-based drug design for G protein-coupled receptors. 2014 , 53, 1-63	57
666	CHAPTER 8:Macrocyclic Inhibitors of GPCR's, Integrins and ProteinProtein Interactions. 2014 , 283-338	2
665	Abstracts from Purines 2014, an International Conference on Nucleotides, Nucleosides and Nucleobases, held in Bonn, Germany, from July 23-27, 2014. 2014 , 10, 657-854	4
664	Do plants contain g protein-coupled receptors?. 2014 , 164, 287-307	45
663	W246(6.48) opens a gate for a continuous intrinsic water pathway during activation of the adenosine A2A receptor. 2015 , 54, 556-9	46
662	From three-dimensional GPCR structure to rational ligand discovery. 2014 , 796, 129-57	26
661	Structural biology of the S1P1 receptor. 2014 , 378, 23-53	4
660	Proteochemometric modeling in a Bayesian framework. 2014 , 6, 35	32
659	Chlorogenic acid inhibits human platelet activation and thrombus formation. 2014 , 9, e90699	59
658	GPCRDB: an information system for G protein-coupled receptors. 2014 , 42, D422-5	82

657	Structural basis for the binding of the membrane-proximal C-terminal region of chemokine receptor CCR2 with the cytosolic regulator FROUNT. 2014 , 281, 5552-66	8
656	Isothermal titration calorimetry in membrane protein research. 2014 , 87, 313-25	25
655	Fluorescent approaches for understanding interactions of ligands with G protein coupled receptors. 2014 , 1838, 15-33	78
654	T4-lysozyme fusion for the production of human formyl peptide receptors for structural determination. 2014 , 172, 2571-81	1
653	Protein Conformational Dynamics. 2014 ,	9
652	Structure-based and fragment-based GPCR drug discovery. 2014 , 9, 256-75	53
651	mGluR5: exploration of orthosteric and allosteric ligand binding pockets and their applications to drug discovery. 2014 , 39, 1862-75	24
650	Protease-activated-receptor-2 affects protease-activated-receptor-1-driven breast cancer. 2014 , 71, 2517-33	29
649	Surface plasmon resonance spectroscopy for characterisation of membrane protein-ligand interactions and its potential for drug discovery. 2014 , 1838, 43-55	268
648	Membrane Transport Mechanism. 2014 ,	2
647	Structural features of the G-protein/GPCR interactions. 2014 , 1840, 16-33	73
646	Allosteric sodium in class A GPCR signaling. 2014 , 39, 233-44	314
645	The Mechanism of Olfaction. 2014 , 32-187	1
644	8-Substituted 2-alkynyl-N(9)-propargyladenines as A2A adenosine receptor antagonists. 2014 , 22, 3072-82	8
643	Impact of template choice on homology model efficiency in virtual screening. 2014 , 54, 1661-8	34
642	SuperBiHelix method for predicting the pleiotropic ensemble of G-protein-coupled receptor conformations. 2014 , 111, E72-8	25
641	Adenosine A2A receptor as a drug discovery target. 2014 , 57, 3623-50	185
640	G Protein-Coupled Receptors - Modeling and Simulation. 2014 ,	7

639	Amino acid conservation and interactions in rhodopsin: probing receptor activation by NMR spectroscopy. 2014 , 1837, 683-93	14
638	Multiscale modelling to understand the self-assembly mechanism of human β_2 -adrenergic receptor in lipid bilayer. 2014 , 48, 29-39	26
637	Bridging molecular docking to membrane molecular dynamics to investigate GPCR-ligand recognition: the human A_{2A} adenosine receptor as a key study. 2014 , 54, 169-83	54
636	Adenosine A_{2A} Receptor Antagonists. 2014 , 1-42	
635	Elastic network normal mode dynamics reveal the GPCR activation mechanism. 2014 , 82, 579-86	15
634	Identification of transmembrane domain 1 & 2 residues that contribute to the formation of the ligand-binding pocket of the urotensin-II receptor. 2014 , 92, 280-8	4
633	Crucial positively charged residues for ligand activation of the GPR35 receptor. 2014 , 289, 3625-38	13
632	Computational Studies of Smell and Taste Receptors. 2014 , 54, 1205-1218	31
631	Predicted ligands for the human urotensin-II G protein-coupled receptor with some experimental validation. 2014 , 9, 1732-43	5
630	Ligand induced change of β_2 adrenergic receptor from active to inactive conformation and its implication for the closed/open state of the water channel: insight from molecular dynamics simulation, free energy calculation and Markov state model analysis. 2014 , 16, 15874-85	33
629	Design, synthesis and evaluation of N6-substituted 2-aminoadenosine-5'-N-methylcarboxamides as A_3 adenosine receptor agonists. 2014 , 5, 192-196	6
628	Mapping the binding pocket of a novel, high-affinity, slow dissociating tachykinin NK3 receptor antagonist: biochemical and electrophysiological characterization. 2014 , 86, 259-72	3
627	Predicted 3D structures of olfactory receptors with details of odorant binding to OR1G1. 2014 , 28, 1175-90	12
626	Advancements of Mass Spectrometry in Biomedical Research. 2014 ,	4
625	Structural basis for Smoothed receptor modulation and chemoresistance to anticancer drugs. 2014 , 5, 4355	175
624	Development of [^{18}F]-labeled pyrazolo[4,3-e]-1,2,4- triazolo[1,5-c]pyrimidine (SCH442416) analogs for the imaging of cerebral adenosine A_{2A} receptors with positron emission tomography. 2014 , 57, 6765-80	24
623	Exploration of the antagonist CP-376395 escape pathway for the corticotropin-releasing factor receptor 1 by random acceleration molecular dynamics simulations. 2014 , 10, 1958-67	20
622	Aromatic interactions impact ligand binding and function at serotonin 5-HT G protein-coupled receptors: Receptor homology modeling, ligand docking, and molecular dynamics results validated by experimental studies. 2014 , 112, 398-407	11

621	Moonlighting proteins and protein-protein interactions as neurotherapeutic targets in the G protein-coupled receptor field. 2014 , 39, 131-55	78
620	Selecting an optimal number of binding site waters to improve virtual screening enrichments against the adenosine A2A receptor. 2014 , 54, 1737-46	43
619	Intelligent Computing in Bioinformatics. 2014 ,	3
618	Overexpression of membrane proteins from higher eukaryotes in yeasts. 2014 , 98, 7671-98	23
617	Constitutive activities in the thyrotropin receptor: regulation and significance. 2014 , 70, 81-119	20
616	Improving the apo-state detergent stability of NTS1 with CHES for pharmacological and structural studies. 2014 , 1838, 2817-24	28
615	Recent advances in magic angle spinning solid state NMR of membrane proteins. 2014 , 82, 1-26	70
614	Strategies for improved modeling of GPCR-drug complexes: blind predictions of serotonin receptors bound to ergotamine. 2014 , 54, 2004-21	19
613	1,3,5-Triazine-based analogues of purine: from isosteres to privileged scaffolds in medicinal chemistry. 2014 , 85, 371-90	59
612	Biased agonism at G protein-coupled receptors: the promise and the challenges--a medicinal chemistry perspective. 2014 , 34, 1286-330	81
611	Adenosine receptor neurobiology: overview. 2014 , 119, 1-49	81
610	The recombinant expression systems for structure determination of eukaryotic membrane proteins. 2014 , 5, 658-72	66
609	Adenosine-insensitive right ventricular tachycardia: novel variant of idiopathic outflow tract tachycardia. 2014 , 11, 1770-8	9
608	Examining the critical roles of human CB2 receptor residues Valine 3.32 (113) and Leucine 5.41 (192) in ligand recognition and downstream signaling activities. 2014 , 452, 334-9	6
607	Domains for activation and inactivation in G protein-coupled receptors--a mutational analysis of constitutive activity of the adenosine A2B receptor. 2014 , 92, 348-57	9
606	Invited review: GPCR structural characterization: Using fragments as building blocks to determine a complete structure. 2014 , 102, 223-43	8
605	Elucidation of conformational states, dynamics, and mechanism of binding in human μ opioid receptor complexes. 2014 , 54, 2294-308	25
604	Extended N(6) substitution of rigid C2-arylethynyl nucleosides for exploring the role of extracellular loops in ligand recognition at the A3 adenosine receptor. 2014 , 24, 3302-6	7

603	Mapping substance P binding sites on the neurokinin-1 receptor using genetic incorporation of a photoreactive amino acid. 2014 , 289, 18045-54	43
602	Ligand- and mutation-induced conformational selection in the CCR5 chemokine G protein-coupled receptor. 2014 , 111, 13040-5	28
601	Dualsteric muscarinic antagonists--orthosteric binding pose controls allosteric subtype selectivity. 2014 , 57, 6739-50	25
600	Perturbation of fluid dynamics properties of water molecules during G protein-coupled receptor-ligand recognition: the human A2A adenosine receptor as a key study. 2014 , 54, 2846-55	23
599	Alternative quality assessment strategy to compare performances of GPCR-ligand docking protocols: the human adenosine A(2A) receptor as a case study. 2014 , 54, 2243-54	22
598	Optimization of 6-heterocyclic-2-(1H-pyrazol-1-yl)-N-(pyridin-2-yl)pyrimidin-4-amine as potent adenosine A2A receptor antagonists for the treatment of Parkinson's disease. 2014 , 5, 674-82	15
597	Supervised molecular dynamics (SuMD) as a helpful tool to depict GPCR-ligand recognition pathway in a nanosecond time scale. 2014 , 54, 372-6	97
596	Dynamic behavior of the active and inactive states of the adenosine A(2A) receptor. 2014 , 118, 3355-65	21
595	Expression, stabilization and purification of membrane proteins via diverse protein synthesis systems and detergents involving cell-free associated with self-assembly peptide surfactants. 2014 , 32, 564-74	14
594	N-acylhydrazone derivative ameliorates monocrotaline-induced pulmonary hypertension through the modulation of adenosine AA2R activity. 2014 , 173, 154-62	28
593	Conserved residues in RF-NH ₂ receptor models identify predicted contact sites in ligand-receptor binding. 2014 , 53, 278-85	13
592	Different efficacy of adenosine and NECA derivatives at the human A3 adenosine receptor: insight into the receptor activation switch. 2014 , 87, 321-31	16
591	Unifying family A GPCR theories of activation. 2014 , 143, 51-60	141
590	Computational insights into the binding mechanism of antagonists with neuropeptide B/W receptor 1. 2014 , 10, 2236-46	1
589	Computational study of possible complexes of caffeine and adenosine with adenosine receptor fragments. 2014 , 1043, 17-23	
588	Agonist-bound structure of the human P2Y12 receptor. 2014 , 509, 119-22	222
587	Molecular dynamics simulations of the adenosine A2a receptor in POPC and POPE lipid bilayers: effects of membrane on protein behavior. 2014 , 54, 573-81	31
586	Comparative genomic analysis of eutherian Mas-related G protein-coupled receptor genes. 2014 , 540, 16-9	7

585	Discovery of simplified N-substituted pyrazolo[3,4-d]pyrimidine derivatives as novel adenosine receptor antagonists: efficient synthetic approaches, biological evaluations and molecular docking studies. 2014 , 22, 1751-65	12
584	Insight into the binding mode and the structural features of the pyrimidine derivatives as human A2A adenosine receptor antagonists. 2014 , 115, 13-22	11
583	Structural and biophysical characterisation of G protein-coupled receptor ligand binding using resonance energy transfer and fluorescent labelling techniques. 2014 , 1838, 3-14	25
582	Nonlamellar Lipid Aggregates. 2014 , 48-65	1
581	Functional importance of two conserved residues in intracellular loop 1 and transmembrane region 2 of Family A GPCRs: insights from ligand binding and signal transduction responses of D1 and D5 dopaminergic receptor mutants. 2015 , 27, 2014-25	5
580	Molecular interaction studies of green tea catechins as multitarget drug candidates for the treatment of Parkinson's disease: computational and structural insights. 2015 , 26, 97-115	20
579	Investigation of Inhibition Mechanism of Chemokine Receptor CCR5 by Micro-second Molecular Dynamics Simulations. 2015 , 5, 13180	33
578	Helix 8 of the angiotensin- II type 1A receptor interacts with phosphatidylinositol phosphates and modulates membrane insertion. 2015 , 5, 9972	10
577	Structure-Based Design Strategies for Targeting G-Protein-Coupled Receptors (GPCRs). 2015 , 199-216	
576	Micelle-Enhanced Bioorthogonal Labeling of Genetically Encoded Azido Groups on the Lipid-Embedded Surface of a GPCR. 2015 , 16, 1314-22	16
575	In-Membrane Chemical Modification (IMCM) for Site-Specific Chromophore Labeling of GPCRs. 2015 , 127, 15461-15464	2
574	In-Membrane Chemical Modification (IMCM) for Site-Specific Chromophore Labeling of GPCRs. 2015 , 54, 15246-9	9
573	Potent, Metabolically Stable 2-Alkyl-8-(2H-1,2,3-triazol-2-yl)-9H-adenines as Adenosine A2A Receptor Ligands. 2015 , 10, 1149-52	2
572	Integrating Pharmacophore into Membrane Molecular Dynamics Simulations to Improve Homology Modeling of G Protein-coupled Receptors with Ligand Selectivity: A2A Adenosine Receptor as an Example. 2015 , 86, 1438-50	5
571	Investigation of the conformational dynamics of the apo A2A adenosine receptor. 2015 , 24, 1004-12	10
570	Structural characterization of triple transmembrane domain containing fragments of a yeast G protein-coupled receptor in an organic : aqueous environment by solution-state NMR spectroscopy. 2015 , 21, 212-22	3
569	Structural Studies of G Protein-Coupled Receptors. 2015 , 38, 836-42	64
568	Charting a Path to Success in Virtual Screening. 2015 , 20, 18732-58	52

567	Cardiac contractility structure-activity relationship and ligand-receptor interactions; the discovery of unique and novel molecular switches in myosuppressin signaling. 2015 , 10, e0120492	10
566	Discovery and cardioprotective effects of the first non-Peptide agonists of the G protein-coupled prokineticin receptor-1. 2015 , 10, e0121027	39
565	Sequence, structure and ligand binding evolution of rhodopsin-like G protein-coupled receptors: a crystal structure-based phylogenetic analysis. 2015 , 10, e0123533	33
564	Binding of the Antagonist Caffeine to the Human Adenosine Receptor hA2AR in Nearly Physiological Conditions. 2015 , 10, e0126833	11
563	Transmembrane signal transduction by peptide hormones via family B G protein-coupled receptors. 2015 , 6, 264	45
562	Free energy calculations of A(2A) adenosine receptor mutation effects on agonist binding. 2015 , 51, 3522-5	27
561	Molecular recognition of ketamine by a subset of olfactory G protein-coupled receptors. 2015 , 8, ra33	14
560	Use of molecular modeling aided design to dial out hERG liability in adenosine A(2A) receptor antagonists. 2015 , 25, 2958-62	9
559	Opioid receptors: Structural and mechanistic insights into pharmacology and signaling. 2015 , 763, 206-13	47
558	References. 2015 , 633-722	
557	Development of novel adenosine receptor ligands based on the 3-amidocoumarin scaffold. 2015 , 61, 1-6	8
556	Studying the binding interactions of allosteric agonists and antagonists of the CXCR4 receptor. 2015 , 60, 1-14	15
555	Quantifying conformational changes in GPCRs: glimpse of a common functional mechanism. 2015 , 16, 124	35
554	New substituted 9-propyladenine derivatives as A2A adenosine receptor antagonists. 2015 , 6, 963-970	8
553	The molecular basis of oligomeric organization of the human M3 muscarinic acetylcholine receptor. 2015 , 87, 936-53	17
552	Selectivity in the Use of Gi/o Proteins Is Determined by the DRF Motif in CXCR6 and Is Cell-Type Specific. 2015 , 88, 894-910	8
551	GPCR crystal structures: Medicinal chemistry in the pocket. 2015 , 23, 3880-906	88
550	Characteristic molecular vibrations of adenosine receptor ligands. 2015 , 589, 548-52	6

549	Modeling and protein engineering studies of active and inactive states of human dopamine D2 receptor (D2R) and investigation of drug/receptor interactions. 2015 , 19, 321-32	25
548	Human adenosine A2A receptor binds calmodulin with high affinity in a calcium-dependent manner. 2015 , 108, 903-917	11
547	Molecular docking screening using agonist-bound GPCR structures: probing the A2A adenosine receptor. 2015 , 55, 550-63	55
546	Identification of destabilizing and stabilizing mutations of Ste2p, a G protein-coupled receptor in <i>Saccharomyces cerevisiae</i> . 2015 , 54, 1787-806	6
545	Crystallization Optimization of Pharmaceutical Solid Forms with X-ray Compatible Microfluidic Platforms. 2015 , 15, 1201-1209	23
544	Structure and function of serotonin G protein-coupled receptors. 2015 , 150, 129-42	200
543	The importance of ligands for G protein-coupled receptor stability. 2015 , 40, 79-87	53
542	A facile and novel synthesis of N(2)-, C(6)-substituted pyrazolo[3,4-d]pyrimidine-4 carboxylate derivatives as adenosine receptor antagonists. 2015 , 92, 784-98	5
541	Methodological advances: the unsung heroes of the GPCR structural revolution. 2015 , 16, 69-81	146
540	G Protein-Coupled Receptor Screening Assays. 2015 ,	
539	Extracellular surface residues of the β B-adrenoceptor critical for G protein-coupled receptor function. 2015 , 87, 121-9	9
538	The role of experimental and computational structural approaches in 7TM drug discovery. 2015 , 10, 1071-84	12
537	From G Protein-coupled Receptor Structure Resolution to Rational Drug Design. 2015 , 290, 19489-95	74
536	Selectivity is species-dependent: Characterization of standard agonists and antagonists at human, rat, and mouse adenosine receptors. 2015 , 11, 389-407	81
535	Characterization of G protein coupling mediated by the conserved D134(3.49) of DRY motif, M241(6.34), and F251(6.44) residues on human CXCR1. 2015 , 5, 182-90	12
534	X-ray structure of a mammalian stearyl-CoA desaturase. 2015 , 524, 252-6	136
533	Communication over the network of binary switches regulates the activation of A2A adenosine receptor. 2015 , 11, e1004044	24
532	Role of Lipids in Folding, Misfolding and Function of Integral Membrane Proteins. 2015 , 855, 1-31	7

531	Selective Protonation of Acidic Residues Triggers Opsin Activation. 2015 , 119, 9510-9	8
530	GPCR-I-TASSER: A Hybrid Approach to G Protein-Coupled Receptor Structure Modeling and the Application to the Human Genome. 2015 , 23, 1538-1549	121
529	Expanding the horizons of G protein-coupled receptor structure-based ligand discovery and optimization using homology models. 2015 , 51, 13576-94	36
528	Insights into the human A1 adenosine receptor from molecular dynamics simulation: structural study in the presence of lipid membrane. 2015 , 24, 3645-3659	13
527	A Molecular Pharmacologist's Guide to G Protein-Coupled Receptor Crystallography. 2015 , 88, 536-51	45
526	G-protein coupled receptor solubilization and purification for biophysical analysis and functional studies, in the total absence of detergent. 2015 , 35,	121
525	Inhibition and Reversal of Microbial Attachment by an Antibody with Parasteric Activity against the FimH Adhesin of Uropathogenic E. coli. 2015 , 11, e1004857	35
524	Capture-stabilize approach for membrane protein SPR assays. 2014 , 4, 7360	20
523	Large-scale production and protein engineering of G protein-coupled receptors for structural studies. 2015 , 6, 66	46
522	Cross-linking strategies to study peptide ligand-receptor interactions. 2015 , 556, 527-47	4
521	Molecular Determinants of CGS21680 Binding to the Human Adenosine A2A Receptor. 2015 , 87, 907-15	95
520	Structure-Based Prediction of G-Protein-Coupled Receptor Ligand Function: A β -Adrenoceptor Case Study. 2015 , 55, 1045-61	35
519	Exploring the 7-oxo-thiazolo[5,4-d]pyrimidine core for the design of new human adenosine A3 receptor antagonists. Synthesis, molecular modeling studies and pharmacological evaluation. 2015 , 96, 105-21	19
518	Design, synthesis, and biological evaluation of novel 2-((2-(4-(substituted)phenyl)piperazin-1-yl)ethyl)amino)-5'-N-ethylcarboxamidoadenosines as potent and selective agonists of the A2A adenosine receptor. 2015 , 58, 3253-67	13
517	Fingerprint-based consensus virtual screening towards structurally new 5-HT(6)R ligands. 2015 , 25, 1827-30	13
516	Engineering G Protein-Coupled Receptors for Drug Design. 2015 , 1-18	2
515	An insight into antagonist binding and induced conformational dynamics of class B GPCR corticotropin-releasing factor receptor 1. 2015 , 11, 2042-50	8
514	A Novel Screening Approach for Optimal and Functional Fusion of T4 Lysozyme in GPCRs. 2015 , 557, 27-43	1

513	History and perspectives of A2A adenosine receptor antagonists as potential therapeutic agents. 2015 , 35, 790-848	74
512	Studying G protein-coupled receptors: immunoblotting, immunoprecipitation, phosphorylation, surface labeling, and cross-linking protocols. 2015 , 127, 303-22	8
511	Molecular modeling of the human P2Y14 receptor: A template for structure-based design of selective agonist ligands. 2015 , 23, 4056-64	18
510	Mutational mapping of the transmembrane binding site of the G-protein coupled receptor TGR5 and binding mode prediction of TGR5 agonists. 2015 , 104, 57-72	22
509	GPCRtm: An amino acid substitution matrix for the transmembrane region of class A G Protein-Coupled Receptors. 2015 , 16, 206	15
508	Biased Gs versus Gq proteins and β -arrestin signaling in the NK1 receptor determined by interactions in the water hydrogen bond network. 2015 , 290, 24495-508	25
507	Defining thermostability of membrane proteins by western blotting. 2015 , 28, 539-42	20
506	Purification and Crystallization of a Thermostabilized Agonist-Bound Conformation of the Human Adenosine A(2A) Receptor. 2015 , 1335, 17-27	2
505	Helix 3 acts as a conformational hinge in Class A GPCR activation: An analysis of interhelical interaction energies in crystal structures. 2015 , 192, 545-553	15
504	Design and synthesis of fused tetrahydroisoquinoline-iminoimidazolines. 2015 , 106, 15-25	1
503	Paeoniflorin ameliorates ischemic neuronal damage in vitro via adenosine A1 receptor-mediated transactivation of epidermal growth factor receptor. 2015 , 36, 298-310	21
502	Emerging Approaches to GPCR Ligand Screening for Drug Discovery. 2015 , 21, 687-701	62
501	Adenosine A2A Receptor Antagonists in Drug Development. 2015 , 39-56	1
500	Structures of G protein-coupled receptors reveal new opportunities for drug discovery. 2015 , 20, 1355-64	111
499	Expression, purification and functional characterization of human equilibrative nucleoside transporter subtype-1 (hENT1) protein from Sf9 insect cells. 2015 , 114, 99-107	21
498	Navigating in chromone chemical space: discovery of novel and distinct A3 adenosine receptor ligands. 2015 , 5, 78572-78585	10
497	A Pipeline To Enhance Ligand Virtual Screening: Integrating Molecular Dynamics and Fingerprints for Ligand and Proteins. 2015 , 55, 2256-74	52
496	Post-expression strategies for structural investigations of membrane proteins. 2015 , 32, 131-8	14

495	Pyrazin-2(1H)-ones as a novel class of selective A3 adenosine receptor antagonists. 2015 , 7, 1373-80	7
494	Discovery of Novel Potent and Selective Agonists at the Melanocortin-3 Receptor. 2015 , 58, 9773-8	15
493	John Daly Lecture: Structure-guided Drug Design for Adenosine and P2Y Receptors. 2015 , 13, 286-98	14
492	Structure and function of G protein-coupled receptor oligomers: implications for drug discovery. 2015 , 7, 408-27	18
491	Mammalian olfactory receptors: molecular mechanisms of odorant detection, 3D-modeling, and structure-activity relationships. 2015 , 130, 1-36	11
490	A Conformational Analysis Study on the Melanocortin 4 Receptor Using Multiple Molecular Dynamics Simulations. 2015 , 86, 309-21	8
489	Molecular interactions of agonist and inverse agonist ligands at serotonin 5-HT _{2C} G protein-coupled receptors: computational ligand docking and molecular dynamics studies validated by experimental mutagenesis results. 2015 , 113, 348-358	3
488	Synthesis and pharmacological evaluation of dual acting ligands targeting the adenosine A _{2A} and dopamine D ₂ receptors for the potential treatment of Parkinson's disease. 2015 , 58, 718-38	37
487	Uptake of the butyrate receptors, GPR41 and GPR43, in lipidic bicontinuous cubic phases suitable for in meso crystallization. 2015 , 441, 78-84	8
486	Conserved disulfide bond is not essential for the adenosine A _{2A} receptor: Extracellular cysteines influence receptor distribution within the cell and ligand-binding recognition. 2015 , 1848, 603-14	15
485	Biochemical Roles of Eukaryotic Cell Surface Macromolecules. 2015 ,	4
484	W2466.48 Opens a Gate for a Continuous Intrinsic Water Pathway during Activation of the Adenosine A _{2A} Receptor. 2015 , 127, 566-569	13
483	Pyrazoloquinazolines: Synthetic strategies and bioactivities. 2015 , 97, 444-61	33
482	Hologram quantitative structure activity relationship, docking, and molecular dynamics studies of inhibitors for CXCR4. 2015 , 85, 119-36	16
481	Moonlighting adenosine deaminase: a target protein for drug development. 2015 , 35, 85-125	40
480	A new crystal structure fragment-based pharmacophore method for G protein-coupled receptors. 2015 , 71, 104-12	15
479	Novel approaches for targeting the adenosine A _{2A} receptor. 2015 , 10, 63-80	9
478	QSAR and docking analysis of A _{2B} adenosine receptor antagonists based on non-xanthine scaffold. 2015 , 24, 394-407	15

477	In Silico ADMET Profiling. 2016 , 225-268	1
476	In silico modeling techniques for predicting the tertiary structure of human H4 receptor. 2016 , 21, 597-619	11
475	Cholesterol and nicotinic acetylcholine receptor: An intimate nanometer-scale spatial relationship spanning the billion year time-scale. 2016 , 5, S67-S86	1
474	Homology Modeling and Ligand-Based Molecule Design. 2016 , 109-160	0
473	G Protein-Coupled Receptors (GPCRs) in Alzheimer's Disease: A Focus on BACE1 Related GPCRs. 2016 , 8, 58	39
472	Structure-Based Sequence Alignment of the Transmembrane Domains of All Human GPCRs: Phylogenetic, Structural and Functional Implications. 2016 , 12, e1004805	56
471	Macrophage Migration Inhibitory Factor-CXCR4 Receptor Interactions: EVIDENCE FOR PARTIAL ALLOSTERIC AGONISM IN COMPARISON WITH CXCL12 CHEMOKINE. 2016 , 291, 15881-95	46
470	Novel Scaffold Identification of mGlu1 Receptor Negative Allosteric Modulators Using a Hierarchical Virtual Screening Approach. 2016 , 87, 239-56	14
469	The Length and Flexibility of the 2-Substituent of 9-Ethyladenine Derivatives Modulate Affinity and Selectivity for the Human A2A Adenosine Receptor. 2016 , 11, 1829-39	8
468	Extracellular Loop 2 of the Adenosine A1 Receptor Has a Key Role in Orthosteric Ligand Affinity and Agonist Efficacy. 2016 , 90, 703-714	39
467	Role of the Second Extracellular Loop of the Adenosine A1 Receptor on Allosteric Modulator Binding, Signaling, and Cooperativity. 2016 , 90, 715-725	35
466	Novel Irreversible Agonists Acting at the A Adenosine Receptor. 2016 , 59, 11182-11194	15
465	Effect of Lipidic Cubic Phase Structure on Functionality of the Dopamine 2L Receptor: Implications for in Meso Crystallization. 2016 , 16, 5014-5022	10
464	Nanodisc-Tm: Rapid functional assessment of nanodisc reconstituted membrane proteins by CPM assay. 2016 , 3, 212-8	6
463	Non-equivalence of Key Positively Charged Residues of the Free Fatty Acid 2 Receptor in the Recognition and Function of Agonist Versus Antagonist Ligands. 2016 , 291, 303-17	35
462	Activation of the A2A adenosine G-protein-coupled receptor by conformational selection. 2016 , 533, 265-8	202
461	Exploring the 2- and 5-positions of the pyrazolo[4,3-d]pyrimidin-7-amino scaffold to target human A1 and A2A adenosine receptors. 2016 , 24, 2794-808	13
460	Ultraslow Water-Mediated Transmembrane Interactions Regulate the Activation of A2A Adenosine Receptor. 2016 , 111, 1180-1191	22

459	How does adenosine control neuronal dysfunction and neurodegeneration?. 2016 , 139, 1019-1055	222
458	Synthesis, binding assays, cytotoxic activity and docking studies of benzimidazole and benzothiophene derivatives with selective affinity for the CB2 cannabinoid receptor. 2016 , 124, 17-35	17
457	Adenosine A2a receptors form distinct oligomers in protein detergent complexes. 2016 , 590, 3295-306	9
456	How to Choose the Suitable Template for Homology Modelling of GPCRs: 5-HT7 Receptor as a Test Case. 2016 , 35, 414-23	11
455	Similarities and differences in affinity and binding modes of tricyclic pyrimido- and pyrazinoxanthines at human and rat adenosine receptors. 2016 , 24, 4347-4362	13
454	[Structural Life Science towards the Regulation of Selective GPCR Signaling]. 2016 , 136, 179-84	
453	[In Silico Drug Design Using an Evolutionary Algorithm and Compound Database]. 2016 , 136, 107-12	
452	In search of novel ligands using a structure-based approach: a case study on the adenosine A receptor. 2016 , 30, 863-874	13
451	More than Meets the Eye: Hidden Structures in the Proteome. 2016 , 3, 373-386	8
450	Structure of the adenosine A(2A) receptor bound to an engineered G protein. 2016 , 536, 104-7	283
449	New Trends in Inspecting GPCR-ligand Recognition Process: the Contribution of the Molecular Modeling Section (MMS) at the University of Padova. 2016 , 35, 440-8	3
448	An Fc-Small Molecule Conjugate for Targeted Inhibition of the Adenosine 2A Receptor. 2016 , 17, 1951-1960	1
447	Multivalent approaches and beyond: novel tools for the investigation of dopamine D2 receptor pharmacology. 2016 , 8, 1349-72	5
446	Structural Analysis of the Histamine H Receptor. 2017 , 241, 21-30	6
445	⌊Adrenergic Receptor Conformational Response to Fusion Protein in the Third Intracellular Loop. 2016 , 24, 2190-2197	37
444	Structural assemblies of the di- and oligomeric G-protein coupled receptor TGR5 in live cells: an MFIS-FRET and integrative modelling study. 2016 , 6, 36792	17
443	Predicting Subtype Selectivity for Adenosine Receptor Ligands with Three-Dimensional Biologically Relevant Spectrum (BRS-3D). 2016 , 6, 36595	10
442	Structural studies of G protein-coupled receptors. 2016 , 68, 894-903	27

441	Pharmacophore-Map-Pick: A Method to Generate Pharmacophore Models for All Human GPCRs. 2016 , 35, 81-91	4
440	Structure-Activity Analysis of Biased Agonism at the Human Adenosine A3 Receptor. 2016 , 90, 12-22	31
439	Conformational and Thermodynamic Landscape of GPCR Activation from Theory and Computation. 2016 , 110, 2618-2629	7
438	Novel Therapeutic Approaches to the Treatment of Parkinson's Disease. 2016 ,	
437	Binding mode similarity measures for ranking of docking poses: a case study on the adenosine A2A receptor. 2016 , 30, 447-56	10
436	Controlling the Dissociation of Ligands from the Adenosine A2A Receptor through Modulation of Salt Bridge Strength. 2016 , 59, 6470-9	115
435	Role of Conserved Disulfide Bridges and Aromatic Residues in Extracellular Loop 2 of Chemokine Receptor CCR8 for Chemokine and Small Molecule Binding. 2016 , 291, 16208-20	10
434	Carbamate substituted 2-amino-4,6-diphenylpyrimidines as adenosine receptor antagonists. 2016 , 26, 734-738	11
433	Computational Prediction and Biochemical Analyses of New Inverse Agonists for the CB1 Receptor. 2016 , 56, 201-12	4
432	Prediction of Loops in G Protein-Coupled Receptor Homology Models: Effect of Imprecise Surroundings and Constraints. 2016 , 56, 671-86	6
431	Role of extracellular cysteine residues in the adenosine A2A receptor. 2016 , 12, 313-29	20
430	Homology modeling and molecular docking studies of Drosophila and Aedes sex peptide receptors. 2016 , 66, 115-22	5
429	Towards a structural understanding of allosteric drugs at the human calcium-sensing receptor. 2016 , 26, 574-92	56
428	Progress in the development of small molecules as new human A3 adenosine receptor ligands based on the 3-thiophenylcoumarin core. 2016 , 7, 845-852	2
427	Discovery of Potent and Highly Selective A2B Adenosine Receptor Antagonist Chemotypes. 2016 , 59, 1967-83	44
426	Molecular Basis of Ligand Dissociation from the Adenosine A2A Receptor. 2016 , 89, 485-91	63
425	Synthesis and structure activity relationship investigation of triazolo[1,5-a]pyrimidines as CB2 cannabinoid receptor inverse agonists. 2016 , 113, 11-27	27
424	Understanding the molecular basis of agonist/antagonist mechanism of GPER1/GPR30 through structural and energetic analyses. 2016 , 158, 104-116	18

423	Medicinal chemistry of adenosine, P2Y and P2X receptors. 2016 , 104, 31-49	158
422	Discovery of aminoquinazoline derivatives as human A(2A) adenosine receptor antagonists. 2016 , 26, 1348-54	10
421	Structural refinement of pyrazolo[4,3-d]pyrimidine derivatives to obtain highly potent and selective antagonists for the human A3 adenosine receptor. 2016 , 108, 117-133	16
420	Biased signaling: potential agonist and antagonist of PAR2. 2016 , 34, 1363-76	4
419	Structurally Enabled Discovery of Adenosine A Receptor Antagonists. 2017 , 117, 21-37	54
418	Labeling and Single-Molecule Methods To Monitor G Protein-Coupled Receptor Dynamics. 2017 , 117, 186-245	75
417	Kinetic Aspects of the Interaction between Ligand and G Protein-Coupled Receptor: The Case of the Adenosine Receptors. 2017 , 117, 38-66	41
416	The signaling pathway of dopamine D2 receptor (D2R) activation using normal mode analysis (NMA) and the construction of pharmacophore models for D2R ligands. 2017 , 35, 2040-2048	9
415	From Homology Models to a Set of Predictive Binding Pockets-a 5-HT Receptor Case Study. 2017 , 57, 311-321	22
414	An update on the physiological and therapeutic relevance of GPCR oligomers. 2017 , 117, 303-327	71
413	Prediction of consensus binding mode geometries for related chemical series of positive allosteric modulators of adenosine and muscarinic acetylcholine receptors. 2017 , 38, 1209-1228	5
412	Membrane cholesterol access into a G-protein-coupled receptor. 2017 , 8, 14505	89
411	7 σ RMSD matrix: A new method for quantitative comparison of the transmembrane domain structures in the G-protein coupled receptors. 2017 , 199, 87-101	3
410	Structure of the Adenosine A Receptor Reveals the Basis for Subtype Selectivity. 2017 , 168, 867-877.e13	167
409	Crystal structure of the adenosine A receptor bound to an antagonist reveals a potential allosteric pocket. 2017 , 114, 2066-2071	87
408	Method for rapid optimization of recombinant GPCR protein expression and stability using virus-like particles. 2017 , 133, 41-49	6
407	Fast iodide-SAD phasing for high-throughput membrane protein structure determination. 2017 , 3, e1602952	27
406	Chemically Stable Lipids for Membrane Protein Crystallization. 2017 , 17, 3502-3511	19

405	Active state structures of G protein-coupled receptors highlight the similarities and differences in the G protein and arrestin coupling interfaces. 2017 , 45, 124-132	42
404	Homology-based Modeling of Rhodopsin-like Family Members in the Inactive State: Structural Analysis and Deduction of Tips for Modeling and Optimization. 2017 , 36, 1700014	7
403	Discovery of Novel and Selective Adenosine A Receptor Antagonists for Treating Parkinson's Disease through Comparative Structure-Based Virtual Screening. 2017 , 57, 1474-1487	35
402	The Roles of Water in the Protein Matrix: A Largely Untapped Resource for Drug Discovery. 2017 , 60, 6781-6827	77
401	Understanding the common themes and diverse roles of the second extracellular loop (ECL2) of the GPCR super-family. 2017 , 449, 3-11	35
400	Identification of potent cholecystokinin-B receptor antagonists: synthesis, molecular modeling and anti-cancer activity against pancreatic cancer cells. 2017 , 8, 1561-1574	5
399	Structural Basis for Apelin Control of the Human Apelin Receptor. 2017 , 25, 858-866.e4	74
398	Binding Kinetics and Pathways of Ligands to GPCRs. 2017 , 38, 717-732	42
397	Classification Models. 2017 , 175-192	0
396	Regression Models. 2017 , 193-208	1
395	Structure-Based Discovery of GPCR Ligands from Crystal Structures and Homology Models. 2017 , 65-99	1
394	The 1,2,4-Triazolo[4,3-a]pyrazin-3-one as a Versatile Scaffold for the Design of Potent Adenosine Human Receptor Antagonists. Structural Investigations to Target the A Receptor Subtype. 2017 , 60, 5772-5790	27
393	Photoaffinity Labeling of the Human A Adenosine Receptor and Cross-link Position Analysis by Mass Spectrometry. 2017 , 8, 660-665	13
392	New approaches towards the understanding of integral membrane proteins: A structural perspective on G protein-coupled receptors. 2017 , 26, 1493-1504	34
391	An Ensemble-Based Protocol for the Computational Prediction of Helix-Helix Interactions in G Protein-Coupled Receptors using Coarse-Grained Molecular Dynamics. 2017 , 13, 2254-2270	21
390	Enantiospecific Recognition at the A Adenosine Receptor by Alkyl 2-Cyanoimino-4-substituted-6-methyl-1,2,3,4-tetrahydropyrimidine-5-carboxylates. 2017 , 60, 3372-3382	19
389	Metal ions-binding T4 lysozyme as an intramolecular protein purification tag compatible with X-ray crystallography. 2017 , 26, 1116-1123	5
388	Pharmacological Characterization of Human Histamine Receptors and Histamine Receptor Mutants in the Sf9 Cell Expression System. 2017 , 241, 63-118	3

387	Integration on Ligand and Structure Based Approaches in GPCRs. 2017 , 101-161	0
386	A covalent antagonist for the human adenosine A receptor. 2017 , 13, 191-201	17
385	Structure and activation of the TSH receptor transmembrane domain. 2017 , 8, 2	14
384	Functional characterization of human equilibrative nucleoside transporter 1. 2017 , 8, 284-295	22
383	Photoaffinity Labeling in Drug Discovery Research. 2017 , 241-265	1
382	Targeting immunosuppressive adenosine in cancer. 2017 , 17, 709-724	304
381	A kinetic view of GPCR allostery and biased agonism. 2017 , 13, 929-937	89
380	A New Class of Fluorinated A Adenosine Receptor Agonist with Application to Last-Step Enzymatic [F]Fluorination for PET Imaging. 2017 , 18, 2156-2164	12
379	Overexpression and purification of Dicer and accessory proteins for biochemical and structural studies. 2017 , 126, 54-65	5
378	Structures of Human A and A Adenosine Receptors with Xanthenes Reveal Determinants of Selectivity. 2017 , 25, 1275-1285.e4	126
377	Identification of Helix 4 (H4) of Rab11a as a novel Rab11-binding domain (RBD): Interaction of Rab11a with the Prostacyclin Receptor. 2017 , 1864, 1819-1832	3
376	Effects of 4(1H)-quinolinone derivative, a novel non-nucleotide allosteric purinergic P2Y agonist, on cardiomyocytes in neonatal rats. 2017 , 7, 6050	8
375	Effect of Nitrogen Atom Substitution in A Adenosine Receptor Binding: N-(4,6-Diarylpyridin-2-yl)acetamides as Potent and Selective Antagonists. 2017 , 60, 7502-7511	10
374	Allosteric Communication Networks in Proteins Revealed through Pocket Crosstalk Analysis. 2017 , 3, 949-960	37
373	Machine learning unifies the modeling of materials and molecules. 2017 , 3, e1701816	346
372	Hot-Spot Residues to be Mutated Common in G Protein-Coupled Receptors of Class A: Identification of Thermostabilizing Mutations Followed by Determination of Three-Dimensional Structures for Two Example Receptors. 2017 , 121, 6341-6350	19
371	Bitopic fluorescent antagonists of the A adenosine receptor based on pyrazolo[4,3-][1,2,4]triazolo[1,5-]pyrimidin-5-amine functionalized congeners. 2017 , 8, 1659-1667	10
370	Design, synthesis and evaluation of 2-aryl benzoxazoles as promising hit for the A receptor. 2017 , 32, 850-864	8

369	Structural basis for the cooperative allosteric activation of the free fatty acid receptor GPR40. 2017 , 24, 570-577	99
368	Prodrug approach: An overview of recent cases. 2017 , 127, 810-827	73
367	Imidazo[1,2-a]pyrazin-8-amine core for the design of new adenosine receptor antagonists: Structural exploration to target the A and A subtypes. 2017 , 125, 611-628	15
366	Impact of protein-ligand solvation and desolvation on transition state thermodynamic properties of adenosine A ligand binding kinetics. 2017 , 5, 16	15
365	Structures of Non-rhodopsin GPCRs Elucidated Through X-Ray Crystallography. 2017 , 1-26	
364	Human Adenosine A Receptor: Molecular Mechanism of Ligand Binding and Activation. 2017 , 8, 898	42
363	Expression, Purification, and Monitoring of Conformational Changes of hCB2 TMH67H8 in Different Membrane-Mimetic Lipid Mixtures Using Circular Dichroism and NMR Techniques. 2017 , 7,	2
362	Exploring Adenosine Receptor Ligands: Potential Role in the Treatment of Cardiovascular Diseases. 2017 , 22,	16
361	Structure-Based Design of Potent and Selective Ligands at the Four Adenosine Receptors. 2017 , 22,	18
360	Gonadotropin-Releasing Hormone (GnRH) Receptor Structure and GnRH Binding. 2017 , 8, 274	31
359	Adenosine ?. 2017 ,	
358	Fluorinated Adenosine A Receptor Antagonists Inspired by Preladenant as Potential Cancer Immunotherapeutics. 2017 , 2017, 4852537	5
357	Ligand modulation of sidechain dynamics in a wild-type human GPCR. 2017 , 6,	49
356	Structural Probing and Molecular Modeling of the A ₁ Adenosine Receptor: A Focus on Agonist Binding. 2017 , 22,	20
355	Modeling and Design for Membrane Protein Targets. 2017 , 145-188	2
354	GPCR Modulation of Thieno[2,3-b]pyridine Anti-Proliferative Agents. 2017 , 22,	8
353	Structural features embedded in G protein-coupled receptor co-crystal structures are key to their success in virtual screening. 2017 , 12, e0174719	9
352	Improving virtual screening of G protein-coupled receptors via ligand-directed modeling. 2017 , 13, e1005819	7

351	Computer-aided design of multi-target ligands at AR, AR and PDE10A, key proteins in neurodegenerative diseases. 2017 , 9, 67	10
350	Emerging Roles for MAS-Related G Protein-Coupled Receptor-X2 in Host Defense Peptide, Opioid, and Neuropeptide-Mediated Inflammatory Reactions. 2017 , 136, 123-162	45
349	Molecular Affinity of Mabolo Extracts to an Octopamine Receptor of a Fruit Fly. 2017 , 22,	4
348	Discovery of Novel Adenosine Receptor Antagonists through a Combined Structure- and Ligand-Based Approach Followed by Molecular Dynamics Investigation of Ligand Binding Mode. 2018 , 58, 794-815	14
347	Structural Basis for G Protein-Coupled Receptor Signaling. 2018 , 47, 1-18	72
346	Fluorescent-Labeled Selective Adenosine A Receptor Antagonist Enables Competition Binding Assay by Flow Cytometry. 2018 , 61, 4301-4316	18
345	Microbial expression systems for membrane proteins. 2018 , 147, 3-39	39
344	Structural Connection between Activation Microswitch and Allosteric Sodium Site in GPCR Signaling. 2018 , 26, 259-269.e5	77
343	An efficient screening method for purifying and crystallizing membrane proteins using modified clear-native PAGE. 2018 , 548, 7-14	10
342	Yeast surface display platform for rapid discovery of conformationally selective nanobodies. 2018 , 25, 289-296	193
341	Allosteric Coupling of Drug Binding and Intracellular Signaling in the A Adenosine Receptor. 2018 , 172, 68-80.e12	119
340	Purinergic Receptors: Novel Targets for Cancer Immunotherapy. 2018 , 115-141	2
339	Increasing the Stability of Recombinant Human Green Cone Pigment. 2018 , 57, 1022-1030	2
338	Biased signalling: from simple switches to allosteric microprocessors. 2018 , 17, 243-260	319
337	Structural Properties of the Human Protease-Activated Receptor 1 Changing by a Strong Antagonist. 2018 , 26, 829-838.e4	6
336	Design and synthesis of 2,6-disubstituted-8-amino imidazo[1,2a]pyridines, a promising privileged structure. 2018 , 26, 3296-3307	4
335	The yin and yang of solubilization and stabilization for wild-type and full-length membrane protein. 2018 , 147, 118-125	25
334	New potent and selective A adenosine receptor antagonists as potential tools for the treatment of gastrointestinal diseases. 2018 , 151, 199-213	11

333	Chemical Diversity in the G Protein-Coupled Receptor Superfamily. 2018 , 39, 494-512	54
332	Discovery of benzothiazolylquinoline conjugates as novel human A receptor antagonists: biological evaluations and molecular docking studies. 2018 , 5, 171622	4
331	Adenosine A receptor agonists with potent antiplatelet activity. 2018 , 29, 292-300	14
330	Adenosine and adenosine receptors in the immunopathogenesis and treatment of cancer. 2018 , 233, 2032-2057	80
329	Recent Advances in Structure-Based Drug Design Targeting Class A G Protein-Coupled Receptors Utilizing Crystal Structures and Computational Simulations. 2018 , 61, 1-46	55
328	Mapping the allosteric sites of the A adenosine receptor. 2018 , 91, 5-16	18
327	Coumarins and adenosine receptors: New perceptions in structure-affinity relationships. 2018 , 91, 245-256	5
326	Biased signaling of G protein-coupled receptors - From a chemokine receptor CCR7 perspective. 2018 , 258, 4-14	18
325	Characterisation of endogenous A and A receptor-mediated cyclic AMP responses in HEK 293 cells using the GloSensor biosensor: Evidence for an allosteric mechanism of action for the A-selective antagonist PSB 603. 2018 , 147, 55-66	14
324	Natural product modulators of human sensations and mood: molecular mechanisms and therapeutic potential. 2018 , 47, 1592-1637	18
323	Importance of the second extracellular loop for melatonin MT receptor function and absence of melatonin binding in GPR50. 2018 , 175, 3281-3297	18
322	Assessment of the transmembrane domain structures in GPCR Dock 2013 models. 2018 , 201, 210-220	1
321	Solid-State Nuclear Magnetic Resonance Spectroscopy of Membrane Proteins. 2018 , 251-283	
320	AquaMMapS: An Alternative Tool to Monitor the Role of Water Molecules During Protein-Ligand Association. 2018 , 13, 522-531	17
319	Current and Future Challenges in GPCR Drug Discovery. 2018 , 1705, 1-21	11
318	Modeling and Deorphanization of Orphan GPCRs. 2018 , 1705, 413-429	3
317	Breakthrough in GPCR Crystallography and Its Impact on Computer-Aided Drug Design. 2018 , 1705, 45-72	12
316	A Structural Framework for GPCR Chemogenomics: What's In a Residue Number?. 2018 , 1705, 73-113	6

315	GPCRs: What Can We Learn from Molecular Dynamics Simulations?. 2018 , 1705, 133-158	9
314	AMP and adenosine are both ligands for adenosine 2B receptor signaling. 2018 , 28, 202-206	7
313	Structural Mapping of Adenosine Receptor Mutations: Ligand Binding and Signaling Mechanisms. 2018 , 39, 75-89	40
312	A monoclonal antibody raised against a thermo-stabilised β -adrenoceptor interacts with extracellular loop 2 and acts as a negative allosteric modulator of a sub-set of β -adrenoceptors expressed in stable cell lines. 2018 , 147, 38-54	11
311	Membrane Biophysics. 2018 ,	
310	Muscarinic receptor oligomerization. 2018 , 136, 401-410	10
309	. 2018 ,	0
308	Structure activity relationship of 2-arylalkynyl-adenine derivatives as human A adenosine receptor antagonists. 2018 , 9, 1920-1932	3
307	Structural Basis for Binding of Allosteric Drug Leads in the Adenosine A Receptor. 2018 , 8, 16836	38
306	A adenosine receptor functional states characterized by F-NMR. 2018 , 115, 12733-12738	56
305	Targeting the Oncoprotein Smoothened by Small Molecules: Focus on Novel Acylguanidine Derivatives as Potent Smoothened Inhibitors. 2018 , 7,	27
304	New Expression Systems for GPCRs. 2018 , 29-69	
303	Probing structure-activity relationship in β -arrestin2 recruitment of diversely substituted adenosine derivatives. 2018 , 158, 103-113	8
302	Computational Studies for Structure-Based Drug Designing Against Transmembrane Receptors: pLGICs and Class A GPCRs. 2018 , 6,	4
301	Role of Extracellular Loops and Membrane Lipids for Ligand Recognition in the Neuronal Adenosine Receptor Type 2A: An Enhanced Sampling Simulation Study. 2018 , 23,	9
300	Could the presence of sodium ion influence the accuracy and precision of the ligand-posing in the human A adenosine receptor orthosteric binding site using a molecular docking approach? Insights from Dockbench. 2018 , 32, 1337-1346	6
299	Targeting adenosine A receptor antagonism for treatment of cancer. 2018 , 13, 997-1003	30
298	Molecular Determinants for Ligand Selectivity of the Cell-Free Synthesized Human Endothelin B Receptor. 2018 , 430, 5105-5119	3

297	The A2aR C-terminus provides improved total and active expression yields for adenosine receptor chimeras. 2018 , 64, 4297-4307	4
296	Cannabidiol skews biased agonism at cannabinoid CB and CB receptors with smaller effect in CB-CB heteroreceptor complexes. 2018 , 157, 148-158	51
295	Born This Way: Using Intrinsic Disorder to Map the Connections between SLITRKs, TSHR, and Male Sexual Orientation. 2018 , 18, e1800307	0
294	Functional roles of tyrosine 185 during the bacteriorhodopsin photocycle as revealed by in situ spectroscopic studies. 2018 , 1859, 1006-1014	6
293	Tritium-labeled agonists as tools for studying adenosine A receptors. 2018 , 14, 223-233	13
292	Enabling STD-NMR fragment screening using stabilized native GPCR: A case study of adenosine receptor. 2018 , 8, 8142	35
291	Cryo-EM structure of the adenosine A receptor coupled to an engineered heterotrimeric G protein. 2018 , 7,	137
290	Identifying G protein-coupled receptor dimers from crystal packings. 2018 , 74, 655-670	13
289	Medicinal Chemistry of A2B Adenosine Receptors. 2018 , 137-168	9
288	Adenosine Receptors: Structure, Distribution, and Signal Transduction. 2018 , 33-57	9
287	An Affinity-Based Probe for the Human Adenosine A Receptor. 2018 , 61, 7892-7901	27
286	The Role of Adenosine Receptors in Psychostimulant Addiction. 2017 , 8, 985	46
285	Molecular Evidence of Adenosine Deaminase Linking Adenosine A Receptor and CD26 Proteins. 2018 , 9, 106	34
284	Exploring G Protein-Coupled Receptors (GPCRs) Ligand Space via Cheminformatics Approaches: Impact on Rational Drug Design. 2018 , 9, 128	43
283	Pharmacology of Adenosine Receptors: The State of the Art. 2018 , 98, 1591-1625	259
282	Supervised Molecular Dynamics (SuMD) Approaches in Drug Design. 2018 , 1824, 287-298	9
281	Investigation into Improving the Aqueous Solubility of the Thieno[2,3-b]pyridine Anti-Proliferative Agents. 2018 , 23,	11
280	A Transmembrane Single-Polypeptide-Chain (sc) Linker to Connect the Two G-Protein-Coupled Receptors in Tandem and the Design for an In Vivo Analysis of Their Allosteric Receptor- Receptor Interactions. 2018 ,	

279	Extrinsic Tryptophans as NMR Probes of Allosteric Coupling in Membrane Proteins: Application to the A Adenosine Receptor. 2018 , 140, 8228-8235	24
278	Prediction of Conformation Specific Thermostabilizing Mutations for Class A G Protein-Coupled Receptors. 2019 , 59, 3744-3754	1
277	G-protein-coupled receptor-based sensors for imaging neurochemicals with high sensitivity and specificity. 2019 , 151, 279-288	21
276	High-throughput identification of peptide agonists against GPCRs by co-culture of mammalian reporter cells and peptide-secreting yeast cells using droplet microfluidics. 2019 , 9, 10920	9
275	Use of syngeneic cells expressing membrane-bound GM-CSF as an adjuvant to induce antibodies against native multi-pass transmembrane protein. 2019 , 9, 9931	4
274	Free-Energy Calculations for Bioisosteric Modifications of A Adenosine Receptor Antagonists. 2019 , 20,	1
273	Structure and Function of GPCRs. 2019 ,	
272	Structural Insights from Recent CB1 X-Ray Crystal Structures. 2019 ,	1
271	Identification of functional divergence sites in dopamine receptors of vertebrates. 2019 , 83, 107140	7
270	Adenosine A2A Receptor as a Potential Drug Target - Current Status and Future Perspectives. 2019 , 25, 2716-2740	12
269	Antioxidant-Conjugated 1,2,4-Triazolo[4,3-]pyrazin-3-one Derivatives: Highly Potent and Selective Human A Adenosine Receptor Antagonists Possessing Protective Efficacy in Neuropathic Pain. 2019 , 62, 8511-8531	9
268	Structural Characterization of Agonist Binding to an A Adenosine Receptor through Biomolecular Simulations and Mutagenesis Experiments. 2019 , 62, 8831-8846	6
267	Reconstruction of apo A2A receptor activation pathways reveal ligand-competent intermediates and state-dependent cholesterol hotspots. 2019 , 9, 14199	15
266	Progress in the Development of Agonists, Antagonists and Allosteric Modulators of Adenosine Receptors. 2019 , 25, 2695-2696	5
265	Studying the collective motions of the adenosine A2A receptor as a result of ligand binding using principal component analysis. 2019 , 37, 4685-4700	7
264	Dynamic Role of the G Protein in Stabilizing the Active State of the Adenosine A Receptor. 2019 , 27, 703-712.e3	18
263	Recent Updates in the Computer Aided Drug Design Strategies for the Discovery of Agonists and Antagonists of Adenosine Receptors. 2019 , 25, 747-749	17
262	Understanding Ligand Binding Selectivity in a Prototypical GPCR Family. 2019 , 59, 2830-2836	16

261	Design, synthesis and biological evaluation of 2-hydrazinyladenosine derivatives as A adenosine receptor ligands. 2019 , 179, 310-324	3
260	Computational prediction of GPCR oligomerization. 2019 , 55, 178-184	7
259	Structure and Activation Mechanism of GPCRs. 2019 , 53-64	3
258	An exploration strategy improves the diversity of de novo ligands using deep reinforcement learning: a case for the adenosine A receptor. 2019 , 11, 35	29
257	Reduced level of docosahexaenoic acid shifts GPCR neuroreceptors to less ordered membrane regions. 2019 , 15, e1007033	11
256	A benchmark study of loop modeling methods applied to G protein-coupled receptors. 2019 , 33, 573-595	9
255	The role of NMR spectroscopy in mapping the conformational landscape of GPCRs. 2019 , 57, 145-156	18
254	Revealing the Mechanism of Agonist-Mediated Cannabinoid Receptor 1 (CB1) Activation and Phospholipid-Mediated Allosteric Modulation. 2019 , 62, 5638-5654	10
253	Molecular modeling approaches for the discovery of adenosine A receptor antagonists: current status and future perspectives. 2019 , 24, 1854-1864	21
252	The lipid phase preference of the adenosine A receptor depends on its ligand binding state. 2019 , 55, 5724-5727	6
251	Structural and energetic basis for novel epicatechin derivatives acting as GPER agonists through the MMGBSA method. 2019 , 189, 176-186	7
250	Mutations in the NPxxY motif stabilize pharmacologically distinct conformational states of the β_1 and β_2 -adrenoceptors. 2019 , 12,	11
249	The Transmembrane Conformation of the Influenza B Virus M2 Protein in Lipid Bilayers. 2019 , 9, 3725	10
248	Molecular Dynamics Simulations of the Allosteric Modulation of the Adenosine A2A Receptor by a Mini-G Protein. 2019 , 9, 5495	8
247	A Chemical Strategy for Amphiphile Replacement in Membrane Protein Research. 2019 , 35, 4319-4327	2
246	Emerging Diversity in Lipid-Protein Interactions. 2019 , 119, 5775-5848	163
245	Hydrogenated Diglucose Detergents for Membrane-Protein Extraction and Stabilization. 2019 , 35, 4287-4295	10
244	Insights to the Binding of a Selective Adenosine A Receptor Antagonist Using Molecular Dynamic Simulations, MM-PBSA and MM-GBSA Free Energy Calculations, and Mutagenesis. 2019 , 59, 5183-5197	8

243	A adenosine receptor activation mechanisms: molecular dynamics analysis of inactive, active, and fully active states. 2019 , 33, 983-996	7
242	Site-selective modification of tryptophan and protein tryptophan residues through PdNP bionanohybrid-catalysed C-H activation in aqueous media. 2019 , 55, 12928-12931	12
241	State-dependent Lipid Interactions with the A2a Receptor Revealed by MD Simulations Using InVivo-Mimetic Membranes. 2019 , 27, 392-403.e3	42
240	Isotopic Labeling of Eukaryotic Membrane Proteins for NMR Studies of Interactions and Dynamics. 2019 , 614, 37-65	6
239	GPCR drug discovery: integrating solution NMR data with crystal and cryo-EM structures. 2019 , 18, 59-82	109
238	Seeing and sensing single G protein-coupled receptors by atomic force microscopy. 2019 , 57, 25-32	12
237	Membrane cholesterol depletion reduces downstream signaling activity of the adenosine A receptor. 2019 , 1861, 760-767	21
236	Probe dependence of allosteric enhancers on the binding affinity of adenosine A _{2A} -receptor agonists at rat and human A _{2A} -receptors measured using NanoBRET. 2019 , 176, 864-878	13
235	Conducting Nanomaterial Sensor Using Natural Receptors. 2019 , 119, 36-93	100
234	Computer-aided drug design in new druggable targets for the next generation of immune-oncology therapies. 2019 , 9, e1397	2
233	Emerging structural biology of lipid G protein-coupled receptors. 2019 , 28, 292-304	33
232	In-silico studies on conformational stability of flagellin-receptor complexes. 2020 , 38, 2240-2252	1
231	Progress in GPCR structure determination. 2020 , 3-22	2
230	Subtype-Selective Fluorescent Ligands as Pharmacological Research Tools for the Human Adenosine A Receptor. 2020 , 63, 2656-2672	14
229	Role of cholesterol-mediated effects in GPCR heterodimers. 2020 , 227, 104852	15
228	Structure-Based Optimization of Coumarin hA Adenosine Receptor Antagonists. 2020 , 63, 2577-2587	9
227	Cholesterol impacts chemokine CCR5 receptor ligand-binding activity. 2020 , 287, 2367-2385	5
226	Adenosine Receptor Ligands: Coumarin-Chalcone Hybrids as Modulating Agents on the Activity of ARs. 2020 , 25,	3

225	Adenosine A Receptor Antagonists for Cancer Immunotherapy. 2020 , 63, 12196-12212	21
224	An investigation into the allosteric mechanism of GPCR A adenosine receptor with trajectory-based information theory and complex network model. 2021 , 39, 6431-6439	1
223	Targeting G Protein-Coupled Receptors with Magnetic Carbon Nanotubes: The Case of the A Adenosine Receptor. 2020 , 15, 1909-1920	2
222	Experimental and computational analysis of biased agonism on full-length and a C-terminally truncated adenosine A receptor. 2020 , 18, 2723-2732	9
221	Thermostability of a recombinant G protein-coupled receptor expressed at high level in mammalian cell culture. 2020 , 10, 16805	3
220	Purinergic Signaling: Impact of GPCR Structures on Rational Drug Design. 2020 , 15, 1958-1973	7
219	Tumor Immunotherapy Using A Adenosine Receptor Antagonists. 2020 , 13,	10
218	Pharmacological characterisation of novel adenosine A receptor antagonists. 2020 , 10, 20781	5
217	A guide to membrane protein X-ray crystallography. 2021 , 288, 5788-5804	10
216	The Specificity of Downstream Signaling for A and AR Does Not Depend on the C-Terminus, Despite the Importance of This Domain in Downstream Signaling Strength. 2020 , 8,	1
215	D-limonene Inhibits Pentylentetrazole-Induced Seizure via Adenosine A2A Receptor Modulation on GABAergic Neuronal Activity. 2020 , 21,	3
214	In silico characterization of adipokinetic hormone receptor and screening for pesticide candidates against stick insect, <i>Carausius morosus</i> . 2020 , 101, 107720	2
213	Adenosine A receptor antagonists: from caffeine to selective non-xanthines. 2020 ,	19
212	In Silico Drug Design for Purinergic GPCRs: Overview on Molecular Dynamics Applied to Adenosine and P2Y Receptors. 2020 , 10,	9
211	X-Ray Crystallography and Free Energy Calculations Reveal the Binding Mechanism of A Adenosine Receptor Antagonists. 2020 , 59, 16536-16543	13
210	Nitrogen-Walk Approach to Explore Bioisosteric Replacements in a Series of Potent A Adenosine Receptor Antagonists. 2020 , 63, 7721-7739	10
209	Lipid-Protein Interactions Are a Unique Property and Defining Feature of G Protein-Coupled Receptors. 2020 , 118, 1887-1900	27
208	Exploring the Activation Mechanism of the mGlu5 Transmembrane Domain. 2020 , 7, 38	2

207	P2Y1-like nucleotide receptors Structures, molecular modeling, mutagenesis, and oligomerization. 2020 , 10, e1464	7
206	Activation of adenosine A receptor by lipids from docosahexaenoic acid revealed by NMR. 2020 , 6, eaay8544	15
205	X-Ray Crystallography and Free Energy Calculations Reveal the Binding Mechanism of A2A Adenosine Receptor Antagonists. 2020 , 132, 16679	1
204	A Taxicab geometry quantification system to evaluate the performance of in silico methods: a case study on adenosine receptors ligands. 2020 , 34, 697-707	
203	Computer simulations of protein-membrane systems. 2020 , 170, 273-403	15
202	Ligand-induced conformational changes in a SMALP-encapsulated GPCR. 2020 , 1862, 183235	16
201	High-Throughput Macromolecular Crystallography in Drug Discovery. 2020 , 211-251	
200	Impact of Recently Determined Crystallographic Structures of GPCRs on Drug Discovery. 2020 , 449-477	1
199	Insights into adenosine A2A receptor activation through cooperative modulation of agonist and allosteric lipid interactions. 2020 , 16, e1007818	11
198	Exploring the molecular structures that confer ligand selectivity for galanin type II and III receptors. 2020 , 15, e0230872	3
197	Discovery of novel 1,3,5-triazine as adenosine A receptor antagonist for benefit in Parkinson's disease. 2021 , 35, e22659	0
196	A Adenosine Receptor Partial Agonism Related to Structural Rearrangements in an Activation Microswitch. 2021 , 29, 170-176.e3	7
195	Therapeutic Path to Double Knockout: Investigating the Selective Dual-Inhibitory Mechanisms of Adenosine Receptors A1 and A2 by a Novel Methoxy-Substituted Benzofuran Derivative in the Treatment of Parkinson's Disease. 2021 , 79, 25-36	0
194	G protein-coupled receptor-G protein interactions: a single-molecule perspective. 2021 , 101, 857-906	10
193	Molecular probes for the human adenosine receptors. 2021 , 17, 85-108	3
192	Medicinal chemistry of P2 and adenosine receptors: Common scaffolds adapted for multiple targets. 2021 , 187, 114311	15
191	Role of Cardiac A Receptors Under Normal and Pathophysiological Conditions. 2020 , 11, 627838	4
190	Synthesis and Biological Evaluation of a Novel F-Labeled Radiotracer for PET Imaging of the Adenosine A Receptor. 2021 , 22,	3

189	Adenosine receptors as promising targets for the management of ocular diseases. 2021 , 30, 1-18	7
188	Development of F-Labeled Radiotracers for PET Imaging of the Adenosine A Receptor: Synthesis, Radiolabeling and Preliminary Biological Evaluation. 2021 , 22,	3
187	Structure and function of adenosine receptor heteromers. 2021 , 78, 3957-3968	5
186	Ligand modulation of the conformational dynamics of the A adenosine receptor revealed by single-molecule fluorescence. 2021 , 11, 5910	5
185	Crystal Structure and Subsequent Ligand Design of a Nonriboside Partial Agonist Bound to the Adenosine A Receptor. 2021 , 64, 3827-3842	5
184	Discovery of novel dual adenosine A1/A2A receptor antagonists using deep learning, pharmacophore modeling and molecular docking. 2021 , 17, e1008821	6
183	Computational evaluation of interactions between olfactory receptor OR2W1 and its ligands. 2021 , 19, e9	0
182	Structure-Based Drug Design for G Protein-Coupled Receptors. 1-59	
181	Pathways and Mechanism of Caffeine Binding to Human Adenosine A Receptor. 2021 , 8, 673170	2
180	Structure-Based Drug Design. 1-54	0
179	Heterologous Expression and Biochemical Characterization of the Human Zinc Transporter 1 (ZnT1) and Its Soluble C-Terminal Domain. 2021 , 9, 667803	2
178	Fragment-Based Lead Discovery. 1-35	
177	Affinity Mass Spectrometry-Based Fragment Screening Identified a New Negative Allosteric Modulator of the Adenosine A Receptor Targeting the Sodium Ion Pocket. 2021 , 16, 991-1002	4
176	Characterization of binding kinetics of AR to G β protein by surface plasmon resonance. 2021 , 120, 1641-1649	3
175	Biased agonism at adenosine receptors. 2021 , 82, 109954	8
174	Lighting Up the Plasma Membrane: Development and Applications of Fluorescent Ligands for Transmembrane Proteins. 2021 , 27, 8605-8641	1
173	In Vitro and In Silico Characterization of G-Protein Coupled Receptor (GPCR) Targets of Phlorofuofuroeckol-A and Dieckol. 2021 , 19,	2
172	Critical APJ receptor residues in extracellular domains that influence effector selectivity. 2021 , 288, 6543-6562	0

171	Structure-Based Molecular Generator Combined with Artificial Intelligence and Docking Simulations. 2021 , 61, 3304-3313	4
170	Homo-oligomerization of the human adenosine A receptor is driven by the intrinsically disordered C-terminus. 2021 , 10,	5
169	A novel high-throughput screen for identifying lipids that stabilise membrane proteins in detergent based solution. 2021 , 16, e0254118	4
168	Modulation of adenosine A2a receptor oligomerization by receptor activation and PIP interactions. 2021 , 29, 1312-1325.e3	2
167	Filling of a water-free void explains the allosteric regulation of the β_1 -adrenergic receptor by cholesterol.	0
166	Subtle Chemical Changes Cross the Boundary between Agonist and Antagonist: New A Adenosine Receptor Homology Models and Structural Network Analysis Can Predict This Boundary. 2021 , 64, 12525-12536	3
165	Structure determination of GPCRs: cryo-EM compared with X-ray crystallography. 2021 , 49, 2345-2355	10
164	Computational design of highly signaling active membrane receptors through de novo solvent-mediated allosteric networks.	
163	PFOA regulate adenosine receptors and downstream concentration-response cAMP-PKA pathway revealed by integrated omics and molecular dynamics analyses. 2022 , 803, 149910	1
162	Structural Insights into Cholesterol Interactions with G-Protein-Coupled Receptors. 231-253	2
161	Mechanism of GPCR-directed autoantibodies in diseases. 2012 , 749, 187-99	18
160	Overview of Non-CB1/CB2 Cannabinoid Receptors: Chemistry and Modeling. 2013 , 29-51	1
159	Computer-aided design of GPCR ligands. 2015 , 1272, 271-91	8
158	Structural Basis of Dopamine Receptor Activation. 2010 , 47-73	3
157	The family of G protein-coupled receptors: an example of membrane proteins. 2010 , 654, 441-54	5
156	Novel Assay Technologies for the Discovery of G Protein-Coupled Receptor Drugs. 2011 , 231-253	1
155	Chemosensory G-proteins-coupled receptors: a perspective from computational methods. 2014 , 805, 441-57	4
154	Role of lipid-mediated effects in β_1 -adrenergic receptor dimerization. 2015 , 842, 247-61	19

153	Molecular Aspects of Histamine Receptors. 2016 , 1-49	3
152	Computer Assisted Peptide Design and Optimization with Topology Preserving Neural Networks. 2010 , 132-139	1
151	Development of Refined Homology Models: Adding the Missing Information to the Medically Relevant Neurotransmitter Transporters. 2014 , 99-120	2
150	GPCRs: Past, present, and future. 2010 , 251-278	1
149	A3 Adenosine Receptor Agonists: History and Future Perspectives. 2010 , 93-120	1
148	Functional and structural studies of TRP channels heterologously expressed in budding yeast. 2011 , 704, 25-40	14
147	The GPCR crystallography boom: providing an invaluable source of structural information and expanding the scope of homology modeling. 2014 , 796, 3-13	20
146	Modeling of G protein-coupled receptors using crystal structures: from monomers to signaling complexes. 2014 , 796, 15-33	11
145	How the dynamic properties and functional mechanisms of GPCRs are modulated by their coupling to the membrane environment. 2014 , 796, 55-74	21
144	Chemometric modeling of PET imaging agents for diagnosis of Parkinson's disease: a QSAR approach. 2020 , 31, 1969-1981	2
143	Structures, Limitations, and Pitfalls. 2016 , 3-14	2
142	3,4-Dihydropyrimidin-2(1)-ones as Antagonists of the Human A Adenosine Receptor: Optimization, Structure-Activity Relationship Studies, and Enantiospecific Recognition. 2021 , 64, 458-480	12
141	CHAPTER 5: Fragment Screening of G Protein-Coupled Receptors. 2015 , 101-125	1
140	Membrane protein crystallography in the era of modern structural biology. 2020 , 48, 2505-2524	3
139	Design: An assay based on single-polypeptide-chain heterodimeric A2AR/D2R and non-oligomerized fusions for in vivo analysis of their allosteric receptor-receptor interactions.	0
138	Cryo-EM structure of the adenosine A2A receptor coupled to an engineered heterotrimeric G protein.	2
137	State-Dependent Lipid Interactions with the A2a Receptor Revealed by MD Simulations Using In Vivo-Mimetic Membranes.	10
136	Pharmacological Characterisation of Novel Adenosine Receptor A3R Antagonists.	5

135	3D-printed holders for fixed-target serial X-ray crystallography. 2020 , 53, 854-859	3
134	Using sequence similarity networks for visualization of relationships across diverse protein superfamilies. 2009 , 4, e4345	287
133	Stability of the neurotensin receptor NTS1 free in detergent solution and immobilized to affinity resin. 2010 , 5, e12579	10
132	Monoolein lipid phases as incorporation and enrichment materials for membrane protein crystallization. 2011 , 6, e24488	13
131	The E92K melanocortin 1 receptor mutant induces cAMP production and arrestin recruitment but not ERK activity indicating biased constitutive signaling. 2011 , 6, e24644	23
130	Novel information on the epitope of an inverse agonist monoclonal antibody provides insight into the structure of the TSH receptor. 2012 , 7, e31973	5
129	Membrane-sensitive conformational states of helix 8 in the metabotropic Glu2 receptor, a class C GPCR. 2012 , 7, e42023	25
128	Recombinant production of human Aquaporin-1 to an exceptional high membrane density in <i>Saccharomyces cerevisiae</i> . 2013 , 8, e56431	25
127	GOMoDo: A GPCRs online modeling and docking webserver. 2013 , 8, e74092	65
126	<i>Saccharomyces cerevisiae</i> -based platform for rapid production and evaluation of eukaryotic nutrient transporters and transceptors for biochemical studies and crystallography. 2013 , 8, e76851	13
125	Arginine 199 and leucine 208 have key roles in the control of adenosine A2A receptor signalling function. 2014 , 9, e89613	5
124	Structural and energetic effects of A2A adenosine receptor mutations on agonist and antagonist binding. 2014 , 9, e108492	44
123	Structure-Activity Relationship Studies of N- and C-Terminally Modified Secretin Analogs for the Human Secretin Receptor. 2016 , 11, e0149359	5
122	Structural and Functional Effect of an Oscillating Electric Field on the Dopamine-D3 Receptor: A Molecular Dynamics Simulation Study. 2016 , 11, e0166412	2
121	An Anti-Parkinson's Disease Drug via Targeting Adenosine A2A Receptor Enhances Amyloid- β Generation and β -Secretase Activity. 2016 , 11, e0166415	14
120	Symmetry based assembly of a 2 dimensional protein lattice. 2017 , 12, e0174485	4
119	Epigenetically silenced GNG4 inhibits SDF1/CXCR4 signaling in mesenchymal glioblastoma. 2016 , 7, 136-47	21
118	Molecular Dynamics Simulations of Adenosine Receptors: Advances, Applications and Trends. 2019 , 25, 783-816	17

117	Recent Advances of In-Silico Modeling of Potent Antagonists for the Adenosine Receptors. 2019 , 25, 750-773	11
116	Recent Advances in the In-silico Structure-based and Ligand-based Approaches for the Design and Discovery of Agonists and Antagonists of A2A Adenosine Receptor. 2019 , 25, 774-782	12
115	Understanding Membrane Protein Drug Targets in Computational Perspective. 2019 , 20, 551-564	16
114	Bivalent ligands targeting chemokine receptor dimerization: molecular design and functional studies. 2014 , 14, 1606-18	14
113	Recent Advances of Small Molecular Regulators Targeting G Protein- Coupled Receptors Family for Oncology Immunotherapy. 2019 , 19, 1464-1483	1
112	In Silico Studies Targeting G-protein Coupled Receptors for Drug Research Against Parkinson's Disease. 2018 , 16, 786-848	10
111	The Protein Structure Initiative: achievements and visions for the future. 2012 , 4, 7	37
110	G protein-coupled receptors: the evolution of structural insight. 2017 , 4, 491-527	26
109	Insights into the structural biology of G-protein coupled receptors impacts drug design for central nervous system neurodegenerative processes. 2013 , 8, 2290-302	6
108	Molecular-Docking-Based Drug Design and Discovery. 2016 , 158-185	2
107	Human μ Opioid Receptor Models with Evaluation of the Accuracy Using the Crystal Structure of the Murine μ Opioid Receptor. 2012 , 3, 218	5
106	Prediction of Binding Mode between Chemokine Receptor CCR2 and Its Known Antagonists using Ligand Supported Homology Modeling. 2012 , 33, 717-720	2
105	Impact of the Protein Data Bank Across Scientific Disciplines. 2020 , 19, 25	9
104	Molecular docking studies of 1-(substituted phenyl)-3-(naphtha [1, 2-d] thiazol-2-yl) urea/thiourea derivatives with human adenosine A(2A) receptor. 2011 , 6, 330-4	7
103	Common activation mechanism of class A GPCRs. 2019 , 8,	117
102	Predicting the Activities of Drug Excipients on Biological Targets using One-Shot Learning.	
101	Synthesis, QSAR modeling, and molecular docking of novel fused 7-deazaxanthine derivatives as adenosine A receptor antagonists. 2021 ,	2
100	Molecular Modeling and Reengineering of A3 Adenosine Receptors. 2010 , 149-161	

- 99 Membrane-Protein Crystallography and Potentiality for Drug Design-An Example from Neurotransmitter Transporter Homolog LeuT. **2010**, 52, 76-80
- 98 Recent Advances in Biology of Crysteinyl Leukotriene. **2010**, 52, 69-75 1
- 97 Prediction of three-dimensional transmembrane helical protein structures. **2010**, 231-249
- 96 Hormone Signaling Via G Protein-Coupled Receptors. **2010**, 83-105 0
- 95 Modeling workshops and methods. **2010**,
- 94 Homology Modeling of 5-HT_{2C} Receptors. **2011**, 97-127
- 93 Crystal Structure Analysis of Adenosine A_{2A} Receptor in Complex with Functional Antibody Fragment. **2013**, 55, 103-109
- 92 Inducing Conformational Changes in G Protein-Coupled Receptors by Domain Coupling. **2014**, 219-237
- 91 Predicting Potential Ligands for Orphan GPCRs Based on the Improved Laplacian Regularized Least Squares Method. **2014**, 280-287
- 90 Olfactory Receptor Proteins. **2014**, 47-68
- 89 Effects of Adenosine Receptors. **2015**, 1-29
- 88 Adenosine Receptors. **2015**, 1-29
- 87 Adenosine Receptor. **2016**, 473-496
- 86 Ultraslow water-mediated transmembrane interactions regulate the activation of A_{2A} adenosine receptor.
- 85 Molecular-Docking-Based Drug Design and Discovery. **2017**, 656-682
- 84 Overview of Arrestin Mediated Signaling with Receptors and Non-receptor Binding Partners. **2017**, 19-29
- 83 Identifying G protein-coupled receptor dimers from crystal packings.
- 82 Protein-Ligand Docking with Protein-based and Ligand-based Structure Activity Relationships.

81	Adenosine Receptors and Drug Discovery in the Cardiovascular System. 2019 , 65-82	
80	Nonantimicrobial Actions of Macrolides: Overview and Perspectives for Future Development. 2021 , 73, 233-262	5
79	Pharmacology of Adenosine Receptors. 2020 , 325-359	
78	Oligomerization of the Human Adenosine A _{2A} Receptor is Driven by the Intrinsically Disordered C-terminus.	1
77	Adenosine receptor antagonists: Recent advances and therapeutic perspective. 2022 , 227, 113907	3
76	Membrane Protein Production and Purification from Escherichia coli and Sf9 Insect Cells. 2020 , 2168, 3-49	
75	G-Protein-Coupled Receptor Expression and Purification. 2021 , 2178, 439-467	1
74	Ligand Modulation of the Conformational Dynamics of the A _{2A} Adenosine Receptor Revealed by Single-Molecule Fluorescence.	
73	Sub-millisecond conformational dynamics of the A _{2A} adenosine receptor revealed by single-molecule FRET.	
72	Modeling G Protein-Coupled Receptors: a Concrete Possibility. 2010 , 28, 26-31	17
71	Molecular determinants of ligand binding at the human histamine H receptor: Site-directed mutagenesis results analyzed with ligand docking and molecular dynamics studies at H homology and crystal structure models. 2012 , 4, 2937-2951	10
70	G protein-coupled receptors--recent advances. 2012 , 59, 515-29	36
69	Structure-Based Design of Dual-Acting Compounds Targeting Adenosine A Receptor and Histone Deacetylase as Novel Tumor Immunotherapeutic Agents. 2021 , 64, 16573-16597	4
68	State-Targeting Stabilization of Adenosine A Receptor by Fusing a Custom-Made De Novo Designed α -Helical Protein. 2021 , 22,	2
67	Purinergic GPCR transmembrane residues involved in ligand recognition and dimerization. 2021 , 166, 133-159	
66	Structure-Based Virtual Screening for Ligands of G Protein-Coupled Receptors: What Can Molecular Docking Do for You?. 2021 , 73, 527-565	4
65	Novel Molecular Targets of Antidepressants.. 2022 , 27,	3
64	Recent developments in the management of Huntington's disease.. 2022 , 120, 105642	2

63	Predicting the Activities of Drug Excipients on Biological Targets using One-Shot Learning.. 2022,	0
62	Discovery of Pyridone-Substituted Triazolopyrimidine Dual A/A AR Antagonists for the Treatment of Ischemic Stroke.. 2022, 13, 436-442	
61	A2A Adenosine Receptor Antagonists and their Potential in Neurological Disorders.. 2022,	1
60	International Union of Basic and Clinical Pharmacology. CXII: Adenosine Receptors: A Further Update.. 2022, 74, 340-372	7
59	Discovery of HTL26119. 2022, 179-200	
58	Single Stabilizing Point Mutation Enables High-Resolution Co-Crystal Structures of the Adenosine A2A Receptor with Preladenant Conjugates.. 2022,	2
57	Eine einzige stabilisierende Punktmutation ermöglicht hochaufgelöste Co-Kristallstrukturen des Adenosin-A 2A -Rezeptors mit Preladenant-Konjugaten.	
56	SINAPs: A Software Tool for Analysis and Visualization of Interaction Networks of Molecular Dynamics Simulations.. 2022,	0
55	Cathepsin D interacts with adenosine A2A receptors in mouse macrophages to modulate cell surface localization and inflammatory signaling.. 2022, 101888	
54	A Adenosine Receptor Antagonists: Are Triazolotriazine and Purine Scaffolds Interchangeable?. 2022, 27,	2
53	The Pharmacological Potential of Adenosine A Receptor Antagonists for Treating Parkinson's Disease.. 2022, 27,	2
52	Wearable Bioelectronics for Chronic Wound Management. 2111022	19
51	Attenuation of Tumor Development in Mammary Carcinoma Rats by Theacrine, an Antagonist of Adenosine 2A Receptor.. 2021, 26,	3
50	The Structural Basis of Peptide Binding at Class A G Protein-Coupled Receptors.. 2021, 27,	1
49	CHAPTER 6. A Unifying Approach to the Duality of Energetic Versus Conformational Formulations of Allosteric Coupling: Mechanistic Implications for GPCR Allostery. 131-155	
48	Table_1.pdf. 2020,	
47	Video_1.MP4. 2020,	
46	Table_1.XLSX. 2018,	

45	Table_2.XLSX. 2018,		
44	Table_3.XLSX. 2018,		
43	Determination of key residues in MRGPRX2 to enhance pseudo-allergic reactions induced by fluoroquinolones.. 2022, 12, 6650		0
42	Molecular Simulations and Drug Discovery of Adenosine Receptors.. 2022, 27,		1
41	Purinergic receptors modulators: An emerging pharmacological tool for disease management.. 2022,		0
40	A adenosine receptor antagonists rescue lymphocyte activity in adenosine-producing patient-derived cancer models.. 2022, 10,		2
39	Superconserved receptors expressed in the brain: Expression, function, motifs and evolution of an orphan receptor family. 2022, 108217		
38	Design, synthesis, and biological evaluation of triazole-pyrimidine-methylbenzotrile derivatives as dual A2A/A2B adenosine receptor antagonists. 2022, 37, 1514-1526		0
37	Structural mass spectrometry of membrane proteins. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2022, 140813	4	4
36	CryoEM Structures of the Human HIV-1 Restriction Factor SERINC3 and Function as a Lipid Transporter.		2
35	A robust approach for MicroED sample preparation of lipidic cubic phase embedded membrane protein crystals.		0
34	Cancer-Associated Mutations of the Adenosine A2A Receptor Have Diverse Influences on Ligand Binding and Receptor Functions. 2022, 27, 4676		0
33	Filling of a water-free void explains the allosteric regulation of the β_1 -adrenergic receptor by cholesterol.		2
32	GPCR Agonist-to-Antagonist Conversion: Enabling the Design of Nucleoside Functional Switches for the A2A Adenosine Receptor.		1
31	Ten Years of GPCR Structures. 2022, 299-345		0
30	Comparative Study of State-Dependent Cholesterol Binding Sites in Adenosine A2A and A1 Receptors Using Coarse-Grained Molecular Dynamics Simulations in Biologically Relevant Membranes.		0
29	Bell-Evans model and steered molecular dynamics in uncovering the dissociation kinetics of ligands targeting G-protein-coupled receptors. 2022, 12,		0
28	Dual A1/A3 Adenosine Receptor Antagonists: Binding Kinetics and Structure-Activity Relationship Studies Using Mutagenesis and Alchemical Binding Free Energy Calculations.		0

- 27 Synthesis, Molecular Docking, and Neuroprotective Effect of 2-Methylcinnamic Acid Amide in 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP) An Induced Parkinson Disease Model. **2022**, 12, 1518 ○
- 26 Nucleoside transporters and immunosuppressive adenosine signaling in the tumor microenvironment: Potential therapeutic opportunities. **2022**, 240, 108300 ○
- 25 Activation and signaling mechanism revealed by GPR119-Gs complex structures. **2022**, 13, ○
- 24 Bifunctional Tools to Study Adenosine Receptors. **2022**, ○
- 23 Global insights into the fine tuning of human A2AAR conformational dynamics in a ternary complex with an engineered G protein viewed by NMR. **2022**, 41, 111844 ○
- 22 Transactivation of receptor tyrosine kinases by purinergic P2Y and adenosine receptors. ○
- 21 Cryo-EM structure of the human adenosine A_{2B} receptor's signaling complex. **2022**, 8, ○
- 20 Comparative Study of Receptor-, Receptor State-, and Membrane-Dependent Cholesterol Binding Sites in A_{2A} and A₁ Adenosine Receptors Using Coarse-Grained Molecular Dynamics Simulations. ○
- 19 Cryo-EM structures of orphan GPR21 signaling complexes. **2023**, 14, ○
- 18 Anionic Phospholipids Control Mechanisms of GPCR-G Protein Recognition. ○
- 17 Systematic analyses of the sequence conservation and ligand interaction patterns of purinergic P₁ and P_{2Y} receptors provide a structural basis for receptor selectivity. **2023**, 21, 889-898 1
- 16 Non-ionic cholesterol-based additives for the stabilization of membrane proteins. **2022**, ○
- 15 G Protein-Coupled Receptors: Conformational Gatekeepers of Transmembrane Signal Transduction and Diversification. **2011**, 188-229 ○
- 14 NMR of Membrane Proteins. **2012**, 271-317 ○
- 13 Modeling of Olfactory Receptors. **2023**, 183-193 ○
- 12 Role of adenosine A_{2a} receptor in cancers and autoimmune diseases. **2023**, 11, ○
- 11 Sub-millisecond conformational dynamics of the A_{2A} adenosine receptor revealed by single-molecule FRET. **2023**, 6, ○
- 10 Biophysical Dissection of Isolated GPCRs: The Adenosine A_{2A} Receptor under the Bistouries. **2023**, 2, 47-92 ○

- 9 Anionic phospholipids control mechanisms of GPCR-G protein recognition. **2023**, 14,
- 8 A robust approach for MicroED sample preparation of lipidic cubic phase embedded membrane protein crystals. **2023**, 14,
- 7 G Protein-Coupled Receptors. **2023**, 1-28
- 6 Once Upon a Time Adenosine and Its Receptors: Historical Survey and Perspectives as Potential Targets for Therapy in Human Diseases. **2023**,
- 5 Bioengineered Exosomes Bearing Adenosine A2a Receptor for the Treatment of Neuroinflammation. **2022**, 18, 2642-2650
- 4 Structural insights into the human niacin receptor HCA2-Gi signalling complex. **2023**, 14,
- 3 Machine Learning-aided Discovery of Novel Chemotype Antagonists for G Protein-coupled Receptors: The Case of the Adenosine A2A Receptor.
- 2 Structural insight into an anti-BRIL Fab as a G-protein-coupled receptor crystallization chaperone. **2023**, 79, 435-441
- 1 Conformational dynamics of the μ opioid receptor determine ligand intrinsic efficacy.