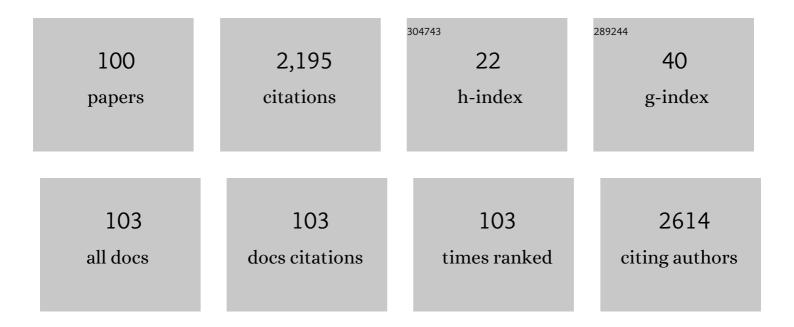
List of Publications by Year in descending order

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Υλή Ζηλής

#	Article	IF	CITATIONS
1	Modulating hemoglobin allostery for treatment of sickle cell disease: current progress and intellectual property. Expert Opinion on Therapeutic Patents, 2022, 32, 115-130.	5.0	9
2	Drug discovery efforts toward inhibitors of canonical Wnt/β-catenin signaling pathway in the treatment of cancer: A composition-of-matter review (2010–2020). Drug Discovery Today, 2022, 27, 1115-1127.	6.4	13
3	Novel bivalent ligands carrying potential antinociceptive effects by targeting putative mu opioid receptor and chemokine receptor CXCR4 heterodimers. Bioorganic Chemistry, 2022, 120, 105641.	4.1	5
4	Teaching an old dog new tricks: Drug discovery by repositioning natural products and their derivatives. Drug Discovery Today, 2022, 27, 1936-1944.	6.4	28
5	Rational Design, Chemical Syntheses, and Biological Evaluations of Peripherally Selective Mu Opioid Receptor Ligands as Potential Opioid Induced Constipation Treatment. Journal of Medicinal Chemistry, 2022, 65, 4991-5003.	6.4	3
6	Design, Synthesis, and Biological Evaluation of NAP Isosteres: A Switch from Peripheral to Central Nervous System Acting Mu-Opioid Receptor Antagonists. Journal of Medicinal Chemistry, 2022, 65, 5095-5112.	6.4	6
7	Exploration of naphthoquinone analogs in targeting the TCF-DNA interaction to inhibit the Wnt/β-catenin signaling pathway. Bioorganic Chemistry, 2022, 124, 105812.	4.1	4
8	Agonist-Promoted Phosphorylation and Internalization of the Kappa Opioid Receptor in Mouse Brains: Lack of Connection With Conditioned Place Aversion. Frontiers in Pharmacology, 2022, 13, .	3.5	1
9	Elucidating the binding mechanism of LPA species and analogs in an LPA4 receptor homology model. Journal of Molecular Graphics and Modelling, 2022, , 108274.	2.4	0
10	Design of bivalent ligands targeting putative GPCR dimers. Drug Discovery Today, 2021, 26, 189-199.	6.4	33
11	IOX1 Suppresses Wnt Target Gene Transcription and Colorectal Cancer Tumorigenesis through Inhibition of KDM3 Histone Demethylases. Molecular Cancer Therapeutics, 2021, 20, 191-202.	4.1	13
12	Development of structure-based pharmacophore to target the β-catenin-TCF protein–protein interaction. Medicinal Chemistry Research, 2021, 30, 429-439.	2.4	3
13	Exploring the putative mechanism of allosteric modulations by mixed-action kappa/mu opioid receptor bitopic modulators. Future Medicinal Chemistry, 2021, 13, 551-573.	2.3	4
14	Verifying the role of 3-hydroxy of 17-cyclopropylmethyl-4,5α-epoxy-3,14β-dihydroxy-6β-[(4′-pyridyl) carboxamido]morphinan derivatives via their binding affinity and selectivity profiles on opioid receptors. Bioorganic Chemistry, 2021, 109, 104702.	4.1	5
15	Structure-Based Design and Development of Chemical Probes Targeting Putative MOR-CCR5 Heterodimers to Inhibit Opioid Exacerbated HIV-1 Infectivity. Journal of Medicinal Chemistry, 2021, 64, 7702-7723.	6.4	8
16	Exploring naltrexamine derivatives featuring azaindole moiety via nitrogen-walk approach to investigate their in vitro pharmacological profiles at the mu opioid receptor. Bioorganic and Medicinal Chemistry Letters, 2021, 41, 127953.	2.2	2
17	Improving the Solubility and Oral Bioavailability of a Novel Aromatic Aldehyde Antisickling Agent (PP10) for the Treatment of Sickle Cell Disease. Pharmaceutics, 2021, 13, 1148.	4.5	4
18	Anibamine and Its Analogues: Potent Antiplasmodial Agents from Aniba citrifolia. Journal of Natural Products, 2020, 83, 569-577.	3.0	7

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19	Design and synthesis of a bivalent probe targeting the putative mu opioid receptor and chemokine receptor CXCR4 heterodimer. RSC Medicinal Chemistry, 2020, 11, 125-131.	3.9	6
20	Stereoselective syntheses of 3-dehydroxynaltrexamines and N-methyl-3-dehydroxynaltrexamines. Tetrahedron Letters, 2020, 61, 152379.	1.4	1
21	Structure activity relationship exploration of 5-hydroxy-2-(3-phenylpropyl)chromones as a unique 5-HT2B receptor antagonist scaffold. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127511.	2.2	5
22	Exploration of Structure–Activity Relationship of Aromatic Aldehydes Bearing Pyridinylmethoxy-Methyl Esters as Novel Antisickling Agents. Journal of Medicinal Chemistry, 2020, 63, 14724-14739.	6.4	7
23	Effective and Versatile Synthesis of Ginkgotoxin and Its 4′-O-Derivatives through Regioselective 4′-O-Alkylation and 4′-O-Chlorination of 3,5′-O-Dibenzylpyridoxine. SynOpen, 2020, 04, 51-54.	1.7	1
24	Bivalent Ligand Aiming Putative Mu Opioid Receptor and Chemokine Receptor CXCR4 Dimers in Opioid Enhanced HIV-1 Entry. ACS Medicinal Chemistry Letters, 2020, 11, 2318-2324.	2.8	7
25	Comparison of Pharmacological Properties between the Kappa Opioid Receptor Agonist Nalfurafine and 42B, Its 3-Dehydroxy Analogue: Disconnect between <i>in Vitro</i> Agonist Bias and <i>in Vivo</i> Pharmacological Effects. ACS Chemical Neuroscience, 2020, 11, 3036-3050.	3.5	17
26	VZHE-039, a novel antisickling agent that prevents erythrocyte sickling under both hypoxic and anoxic conditions. Scientific Reports, 2020, 10, 20277.	3.3	14
27	Computational insights into the molecular mechanisms of differentiated allosteric modulation at the mu opioid receptor by structurally similar bitopic modulators. Journal of Computer-Aided Molecular Design, 2020, 34, 879-895.	2.9	9
28	Structural elucidation and in vivo anti-arthritic activity of β-amyrin and polpunonic acid isolated from the root bark of Ziziphus abyssinica HochstEx. A Rich (Rhamnaceae). Bioorganic Chemistry, 2020, 98, 103744.	4.1	14
29	Recent advances in multitarget-directed ligands targeting G-protein-coupled receptors. Drug Discovery Today, 2020, 25, 1682-1692.	6.4	13
30	Insights into the Allosteric Mechanism of Setmelanotide (RM-493) as a Potent and First-in-Class Melanocortin-4 Receptor (MC4R) Agonist To Treat Rare Genetic Disorders of Obesity through an in Silico Approach. ACS Chemical Neuroscience, 2019, 10, 1055-1065.	3.5	20
31	Effectiveness comparisons of G-protein biased and unbiased mu opioid receptor ligands in warm water tail-withdrawal and drug discrimination in male and female rats. Neuropharmacology, 2019, 150, 200-209.	4.1	37
32	Characterization of 17-Cyclopropylmethyl-3,14β-dihydroxy-4,5α-epoxy-6α-(indole-7-carboxamido)morphinan (NAN) as a Novel Opioid Receptor Modulator for Opioid Use Disorder Treatment. ACS Chemical Neuroscience, 2019, 10, 2518-2532.	3.5	17
33	Application of Bivalent Bioisostere Concept on Design and Discovery of Potent Opioid Receptor Modulators. Journal of Medicinal Chemistry, 2019, 62, 11399-11415.	6.4	12
34	Pharmacological characterization of 17-cyclopropylmethyl-3,14-dihydroxy-4,5-epoxy-6-[(3′-fluoro-4′-pyridyl)acetamido]morphinan (NFP) as a dual selective MOR/KOR ligand with potential applications in treating opioid use disorder. European Journal of Pharmacology, 2019, 865, 172812.	3.5	2
35	Structure–Activity Relationship Studies of 6α- and 6β-Indolylacetamidonaltrexamine Derivatives as Bitopic Mu Opioid Receptor Modulators and Elaboration of the "Message-Address Concept―To Comprehend Their Functional Conversion. ACS Chemical Neuroscience, 2019, 10, 1075-1090.	3.5	28
36	Design, Synthesis, and Biological Evaluation of the Third Generation 17-Cyclopropylmethyl-3,14β-dihydroxy-4,5α-epoxy-6β-[(4′-pyridyl)carboxamido]morphinan (NAP) Derivatives as μ4∫κ Opioid Receptor Dual Selective Ligands. Journal of Medicinal Chemistry, 2019, 62, 561-574.	6.4	17

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37	Role of mu-opioid agonist efficacy on antinociceptive interactions between mu agonists and the nociceptin opioid peptide agonist Ro 64-6198 in rhesus monkeys. European Journal of Pharmacology, 2019, 844, 175-182.	3.5	7
38	Recent Advances in the Drug Discovery and Development of Dualsteric/ Bitopic Activators of G Protein-Coupled Receptors. Current Topics in Medicinal Chemistry, 2019, 19, 2378-2392.	2.1	14
39	Application of Receptor Theory to the Design and Use of Fixed-Proportion Mu-Opioid Agonist and Antagonist Mixtures in Rhesus Monkeys. Journal of Pharmacology and Experimental Therapeutics, 2018, 365, 37-47.	2.5	24
40	Rational design of pyridyl derivatives of vanillin for the treatment of sickle cell disease. Bioorganic and Medicinal Chemistry, 2018, 26, 2530-2538.	3.0	26
41	In vitro and in vivo functional profile characterization of 17-cyclopropylmethyl-3,14l²-dihydroxy-4,5l̂±-epoxy-6l̂±-(isoquinoline-3-carboxamido)morphinan (NAQ) as a low efficacy mu opioid receptor modulator. European Journal of Pharmacology, 2018, 827, 32-40.	3.5	15
42	Rational modification of vanillin derivatives to stereospecifically destabilize sickle hemoglobin polymer formation. Acta Crystallographica Section D: Structural Biology, 2018, 74, 956-964.	2.3	15
43	Understanding the role of glucose regulated protein 170 (GRP170) as a nucleotide exchange factor through molecular simulations. Journal of Molecular Graphics and Modelling, 2018, 85, 160-170.	2.4	7
44	Methylation Products of 6β- <i>N</i> -Heterocyclic Substituted Naltrexamine Derivatives as Potential Peripheral Opioid Receptor Modulators. ACS Chemical Neuroscience, 2018, 9, 3028-3037.	3.5	6
45	Exploring the binding mechanisms of diaminopimelic acid analogs to meso-diaminopimelate dehydrogenase by molecular modeling. Journal of Molecular Graphics and Modelling, 2018, 83, 100-111.	2.4	3
46	Structure of the µ-opioid receptor–Gi protein complex. Nature, 2018, 558, 547-552.	27.8	527
47	Nanoconjugated NAP as a Potent and Periphery Selective Mu Opioid Receptor Modulator To Treat Opioid-Induced Constipation. ACS Medicinal Chemistry Letters, 2017, 8, 78-83.	2.8	3
48	Binding mode analyses of NAP derivatives as mu opioid receptor selective ligands through docking studies and molecular dynamics simulation. Bioorganic and Medicinal Chemistry, 2017, 25, 2463-2471.	3.0	11
49	<scp>CRIP</scp> 1a inhibits endocytosis of Gâ€protein coupled receptors activated by endocannabinoids and glutamate by a common molecular mechanism. Journal of Neurochemistry, 2017, 141, 577-591.	3.9	19
50	Understanding molecular interactions between scavenger receptor A and its natural product inhibitors through molecular modeling studies. Journal of Molecular Graphics and Modelling, 2017, 77, 189-199.	2.4	4
51	Design, Synthesis, and Biological Evaluation of Ester and Ether Derivatives of Antisickling Agent 5-HMF for the Treatment of Sickle Cell Disease. Molecular Pharmaceutics, 2017, 14, 3499-3511.	4.6	39
52	Diaminopimelic acid (DAP) analogs bearing isoxazoline moiety as selective inhibitors against meso-diaminopimelate dehydrogenase (m-Ddh) from Porphyromonas gingivalis. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 3840-3844.	2.2	6
53	Design, synthesis, and characterization of rhein analogs as novel inhibitors of scavenger receptor A. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 72-76.	2.2	3
54	San-Huang-Xie-Xin-Tang Constituents Exert Drug-Drug Interaction of Mutual Reinforcement at Both Pharmacodynamics and Pharmacokinetic Level: A Review. Frontiers in Pharmacology, 2016, 7, 448.	3.5	18

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55	Antinociceptive Interactions between the Imidazoline I2 Receptor Agonist 2-BFI and Opioids in Rats: Role of Efficacy at the Â-Opioid Receptor. Journal of Pharmacology and Experimental Therapeutics, 2016, 357, 509-519.	2.5	30
56	Exploration of bivalent ligands targeting putative mu opioid receptor and chemokine receptor CCR5 dimerization. Bioorganic and Medicinal Chemistry, 2016, 24, 5969-5987.	3.0	31
57	6β-N-Heterocyclic Substituted Naltrexamine Derivative BNAP: A Peripherally Selective Mixed MOR/KOR Ligand. ACS Chemical Neuroscience, 2016, 7, 1120-1129.	3.5	12
58	17-Cyclopropylmethyl-3,14β-dihydroxy-4,5α-epoxy-6β-(4′-pyridylcarboxamido)morphinan (NAP) Modulating the Mu Opioid Receptor in a Biased Fashion. ACS Chemical Neuroscience, 2016, 7, 297-304.	3.5	14
59	Effects of the novel, selective and low-efficacy mu opioid receptor ligand NAQ on intracranial self-stimulation in rats. Psychopharmacology, 2015, 232, 815-824.	3.1	18
60	Exploration on natural product anibamine side chain modification toward development of novel CCR5 antagonists and potential anti-prostate cancer agents. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 3721-3725.	2.2	8
61	Small molecule inhibits activity of scavenger receptor A: Lead identification and preliminary studies. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 3179-3183.	2.2	11
62	Design, syntheses, and pharmacological characterization of 17-cyclopropylmethyl-3,14β-dihydroxy-4,5α-epoxy-6α-(isoquinoline-3′-carboxamido)morphinan analogues as opioid receptor ligands. Bioorganic and Medicinal Chemistry, 2015, 23, 1701-1715.	3.0	19
63	Synthesis and Characterization of 5-Hydroxy-2-(2-phenylethyl)chromone (5-HPEC) and Its Analogues as Non-nitrogenous 5-HT2B Ligands. Journal of Natural Products, 2015, 78, 1859-1867.	3.0	12
64	Identification of Small-Molecule Inhibitors against Meso-2, 6-Diaminopimelate Dehydrogenase from Porphyromonas gingivalis. PLoS ONE, 2015, 10, e0141126.	2.5	13
65	Behavioral and cellular pharmacology characterization of 17-cyclopropylmethyl-3,14β-dihydroxy-4,5α-epoxy-6α-(isoquinoline-3′-carboxamido)morphinan (NAQ) as a mι opioid receptor selective ligand. European Journal of Pharmacology, 2014, 736, 124-130.	1 3.5	11
66	5-Hydroxy-2-(2-phenylethyl)chromone (5-HPEC): A novel non-nitrogenous ligand for 5-HT2B receptor. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 1489-1492.	2.2	17
67	Design, syntheses, and characterization of piperazine based chemokine receptor CCR5 antagonists as anti prostate cancer agents. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 2319-2323.	2.2	17
68	Predicting the molecular interactions of CRIP1a–cannabinoid 1 receptor with integrated molecular modeling approaches. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 1158-1165.	2.2	13
69	Novel Structurally-Modified Allosteric Effectors of Hemoglobin Exhibit Superior Antisickling Properties. Blood, 2014, 124, 218-218.	1.4	2
70	Bivalent Ligands Targeting Chemokine Receptor Dimerization: Molecular Design and Functional Studies. Current Topics in Medicinal Chemistry, 2014, 14, 1606-1618.	2.1	16
71	Structure activity relationship studies of 17-cyclopropylmethyl-3,14β-dihydroxy-4,5α-epoxy-6α-(isoquinoline-3′-carboxamido)morphinan (NAQ) analogues as potent opioid receptor ligands: Preliminary results on the role of electronic characteristics for affinity and function. Bioorganic and Medicinal Chemistry Letters, 2013, 23,	2.2	13
72	5045-5040. Design, syntheses, and characterization of pharmacophore based chemokine receptor CCR5 antagonists as anti prostate cancer agents. European Journal of Medicinal Chemistry, 2013, 69, 647-658.	5.5	11

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73	Binding mode characterization of 6α- and 6β-N-heterocyclic substituted naltrexamine derivatives via docking in opioid receptor crystal structures and site-directed mutagenesis studies: Application of the â€message–address' concept in development of mu opioid receptor selective antagonists. Bioorganic and Medicinal Chemistry, 2013, 21, 6405-6413.	3.0	20
74	Design, Synthesis, and Biological Evaluation of 14-Heteroaromatic-Substituted Naltrexone Derivatives: Pharmacological Profile Switch from Mu Opioid Receptor Selectivity to Mu/Kappa Opioid Receptor Dual Selectivity. Journal of Medicinal Chemistry, 2013, 56, 9156-9169.	6.4	35
75	G Protein oupled Estrogen Receptor (GPER) Agonist Dual Binding Mode Analyses Toward Understanding of Its Activation Mechanism: A Comparative Homology Modeling Approach. Molecular Informatics, 2013, 32, 647-658.	2.5	28
76	A homology modeling study toward the understanding of three-dimensional structure and putative pharmacological profile of the G-protein coupled receptor GPR55. Journal of Molecular Graphics and Modelling, 2013, 39, 50-60.	2.4	24
77	A bivalent ligand targeting the putative mu opioid receptor and chemokine receptor CCR5 heterodimer: binding affinity versus functional activities. MedChemComm, 2013, 4, 847.	3.4	36
78	An efficient procedure for the preparation of natural products bearing the 2-(2-phenylethyl)chromone skeleton. Tetrahedron Letters, 2013, 54, 4292-4295.	1.4	10
79	Opioid receptor selectivity profile change via isosterism for 14-O-substituted naltrexone derivatives. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 3719-3722.	2.2	7
80	A novel bivalent HIV-1 entry inhibitor reveals fundamental differences in CCR5-μ-opioid receptor interactions between human astroglia and microglia. Aids, 2013, 27, 2181-2190.	2.2	31
81	Design, Synthesis, and Biological Evaluation of 17-Cyclopropylmethyl-3,14β-dihydroxy-4,5α-epoxy-6β-[(4′-pyridyl)carboxamido]morphinan Derivatives as Peripheral Selective μ Opioid Receptor Agents. Journal of Medicinal Chemistry, 2012, 55, 10118-10129.	6.4	22
82	6β-N-Heterocyclic substituted naltrexamine derivative NAP as a potential lead to develop peripheral mu opioid receptor selective antagonists. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 4731-4734.	2.2	21
83	The potential role of anibamine, a natural product CCR5 antagonist, and its analogues as leads toward development of anti-ovarian cancer agents. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 5093-5097.	2.2	17
84	Structure activity relationship studies of natural product chemokine receptor CCR5 antagonist anibamine toward the development of novel anti prostate cancer agents. European Journal of Medicinal Chemistry, 2012, 55, 395-408.	5.5	18
85	Design and synthesis of a bivalent ligand to explore the putative heterodimerization of the mu opioid receptor and the chemokine receptor CCR5. Organic and Biomolecular Chemistry, 2012, 10, 2633.	2.8	35
86	Facile synthesis of 2,3,5,6-tetrabromo-4-methyl-nitrocyclohexa-2,5-dien-1-one, a mild nitration reagent. Tetrahedron Letters, 2012, 53, 1592-1594.	1.4	5
87	Regio- and Stereoselective Syntheses of the Natural Product CCR5 Antagonist Anibamine and its Three Olefin Isomers. Journal of Organic Chemistry, 2011, 76, 7945-7952.	3.2	16
88	Characterization of 6α- and 6β- <i>N</i> -Heterocyclic Substituted Naltrexamine Derivatives as Novel Leads to Development of Mu Opioid Receptor Selective Antagonists. ACS Chemical Neuroscience, 2011, 2, 346-351.	3.5	33
89	Preclinical Disposition (In Vitro) of Novel μ-Opioid Receptor Selective Antagonists. Drug Metabolism and Disposition, 2011, 39, 1589-1596.	3.3	21
90	Structure selectivity relationship studies of 17-cyclopropylmethyl-3,14β-dihydroxy-4,5α-epoxy-6β-[(4′-pyridyl)carboxamido]morphinan derivatives toward the development of the mu opioid receptor antagonists. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 5625-5629.	2.2	15

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91	The natural product CCR5 antagonist anibamine and its analogs as anti-prostate cancer agents. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 5159-5163.	2.2	15
92	Huperzine A as Potential Treatment of <i>Alzheimer</i> 's Disease: An Assessment on Chemistry, Pharmacology, and Clinical Studies. Chemistry and Biodiversity, 2011, 8, 1189-1204.	2.1	108
93	Anibamine, a natural product CCR5 antagonist, as a novel lead for the development of anti-prostate cancer agents. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 4627-4630.	2.2	39
94	Toward the three-dimensional structure and lysophosphatidic acid binding characteristics of the LPA4/p2y9/GPR23 receptor: A homology modeling study. Journal of Molecular Graphics and Modelling, 2009, 28, 70-79.	2.4	12
95	14-O-Heterocyclic-substituted naltrexone derivatives as non-peptide mu opioid receptor selective antagonists: Design, synthesis, and biological studies. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 1825-1829.	2.2	19
96	Comparative Docking Study of Anibamine as the First Natural Product CCR5 Antagonist in CCR5 Homology Models. Journal of Chemical Information and Modeling, 2009, 49, 120-132.	5.4	34
97	Design, Synthesis, and Biological Evaluation of 6α- and 6β- <i>N</i> -Heterocyclic Substituted Naltrexamine Derivatives as 1¼ Opioid Receptor Selective Antagonists. Journal of Medicinal Chemistry, 2009, 52, 1416-1427.	6.4	70
98	Stereoselective synthesis of the two major metabolites of spironolactone, 3α- and 3β-hydroxy-7α-methylthio-17α-pregn-4-ene-21,17-carbolactone. Steroids, 2007, 72, 569-572.	1.8	6
99	Total Synthesis of Anibamine, a Novel Natural Product as a Chemokine Receptor CCR5 Antagonist. Organic Letters, 2007, 9, 2043-2046.	4.6	62
100	Homology Modeling and Molecular Dynamics Simulations of the Mu Opioid Receptor in a Membrane-Aqueous System. ChemBioChem, 2005, 6, 853-859.	2.6	46