

Calvin Yu-Chian Chen

List of Publications by Year in descending order

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129
papers

3,832
citations

136940

32
h-index

133244

59
g-index

131
all docs

131
docs citations

131
times ranked

3742
citing authors

#	ARTICLE	IF	CITATIONS
1	TCM Database@Taiwan: The World's Largest Traditional Chinese Medicine Database for Drug Screening In Silico. PLoS ONE, 2011, 6, e15939.	2.5	677
2	Beware of docking!. Trends in Pharmacological Sciences, 2015, 36, 78-95.	8.7	460
3	iScreen: world's first cloud-computing web server for virtual screening and de novo drug design based on TCM database@Taiwan. Journal of Computer-Aided Molecular Design, 2011, 25, 525-531.	2.9	127
4	Current developments of computer-aided drug design. Journal of the Taiwan Institute of Chemical Engineers, 2010, 41, 623-635.	5.3	123
5	Identification of Potent EGFR Inhibitors from TCM Database@Taiwan. PLoS Computational Biology, 2011, 7, e1002189.	3.2	85
6	Ligand-Based Dual Target Drug Design for H1N1: Swine Flu- A Preliminary First Study. Journal of Biomolecular Structure and Dynamics, 2009, 27, 171-178.	3.5	84
7	Structure-Based and Ligand-Based Drug Design for HER 2 Receptor. Journal of Biomolecular Structure and Dynamics, 2010, 28, 23-37.	3.5	84
8	Two Birds with One Stone? Possible Dual-Targeting H1N1 Inhibitors from Traditional Chinese Medicine. PLoS Computational Biology, 2011, 7, e1002315.	3.2	76
9	How to design a drug for the disordered proteins?. Drug Discovery Today, 2013, 18, 910-915.	6.4	71
10	Weighted Equation and Rules—A Novel Concept for Evaluating Protein-Ligand Interaction. Journal of Biomolecular Structure and Dynamics, 2009, 27, 271-282.	3.5	69
11	Insights into designing the dual-targeted HER2/HSP90 inhibitors. Journal of Molecular Graphics and Modelling, 2010, 29, 21-31.	2.4	63
12	A Novel Integrated Framework and Improved Methodology of Computer-Aided Drug Design. Current Topics in Medicinal Chemistry, 2013, 13, 965-988.	2.1	62
13	A Novel Strategy for Designing the Selective PPAR Agonist by the "Sum of Activity" Model. Journal of Biomolecular Structure and Dynamics, 2010, 28, 187-200.	3.5	59
14	iSMART: An Integrated Cloud Computing Web Server for Traditional Chinese Medicine for Online Virtual Screening, <i>de novo</i> Evolution and Drug Design. Journal of Biomolecular Structure and Dynamics, 2011, 29, 243-250.	3.5	59
15	Stroke prevention by traditional Chinese medicine? A genetic algorithm, support vector machine and molecular dynamics approach. Soft Matter, 2011, 7, 4001.	2.7	57
16	Drug Design for Neuropathic Pain Regulation from Traditional Chinese Medicine. Scientific Reports, 2013, 3, 844.	3.3	57
17	Potent Inhibitor Design Against H1N1 Swine Influenza: Structure-based and Molecular Dynamics Analysis for M2 Inhibitors from Traditional Chinese Medicine Database. Journal of Biomolecular Structure and Dynamics, 2011, 28, 471-482.	3.5	53
18	Computational screening and design of traditional Chinese medicine (TCM) to block phosphodiesterase-5. Journal of Molecular Graphics and Modelling, 2009, 28, 261-269.	2.4	52

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19	Investigation into Potent Inflammation Inhibitors from Traditional Chinese Medicine. <i>Chemical Biology and Drug Design</i> , 2011, 78, 679-688.	3.2	52
20	Chemoinformatics and pharmacoinformatics approach for exploring the GABA-A agonist from Chinese herb suanzaoren. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2009, 40, 36-47.	5.3	47
21	In silico pharmacology suggests ginger extracts may reduce stroke risks. <i>Molecular BioSystems</i> , 2011, 7, 2702.	2.9	47
22	Screening from the World's Largest TCM Database Against H1N1 Virus. <i>Journal of Biomolecular Structure and Dynamics</i> , 2011, 28, 773-786.	3.5	44
23	Discovery of potent inhibitors for phosphodiesterase 5 by virtual screening and pharmacophore analysis. <i>Acta Pharmacologica Sinica</i> , 2009, 30, 1186-1194.	6.1	43
24	Three-in-one agonists for PPAR- α , PPAR- β , and PPAR- γ from traditional Chinese medicine. <i>Journal of Biomolecular Structure and Dynamics</i> , 2012, 30, 662-683.	3.5	43
25	Insights into the suanzaoren mechanism—From constructing the 3D structure of GABA-A receptor to its binding interaction analysis. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2008, 39, 663-671.	1.4	41
26	Traditional Chinese medicine, a solution for reducing dual stroke risk factors at once?. <i>Molecular BioSystems</i> , 2011, 7, 2711.	2.9	39
27	Application of bioactivity database of Chinese herbal medicine on the therapeutic prediction, drug development, and safety evaluation. <i>Journal of Ethnopharmacology</i> , 2010, 132, 429-437.	4.1	38
28	High performance screening, structural and molecular dynamics analysis to identify H1 inhibitors from TCM Database@Taiwan. <i>Molecular BioSystems</i> , 2011, 7, 3366.	2.9	38
29	May disordered protein cause serious drug side effect?. <i>Drug Discovery Today</i> , 2014, 19, 367-372.	6.4	37
30	Discovery of novel inhibitors for c-Met by virtual screening and pharmacophore analysis. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2008, 39, 617-624.	1.4	36
31	Identifying HER2 Inhibitors from Natural Products Database. <i>PLoS ONE</i> , 2011, 6, e28793.	2.5	36
32	Ligand-Based and Structure-Based Investigation for Alzheimer's Disease from Traditional Chinese Medicine. <i>Evidence-based Complementary and Alternative Medicine</i> , 2014, 2014, 1-16.	1.2	34
33	Pharmacoinformatics approach for mPGES-1 in anti-inflammation by 3D-QSAR pharmacophore mapping. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2009, 40, 155-161.	5.3	33
34	Novel selective inhibitors of hydroxyxanthone derivatives for human cyclooxygenase-2. <i>Acta Pharmacologica Sinica</i> , 2007, 28, 2027-2032.	6.1	30
35	Antiplatelet Effect and Selective Binding to Cyclooxygenase (COX) by Molecular Docking Analysis of Flavonoids and Lignans. <i>International Journal of Molecular Sciences</i> , 2007, 8, 830-841.	4.1	29
36	Bioinformatics, chemoinformatics, and pharmacoinformatics analysis of HER2/HSP90 dual-targeted inhibitors. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2010, 41, 143-149.	5.3	29

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37	Traditional Chinese medicine application in HIV: an in silico study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014, 32, 1-12.	3.5	29
38	A novel perspective on designing the inhibitor of HER2 receptor. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2008, 39, 291-299.	1.4	28
39	Uroporphyrinogen Decarboxylase as a Potential Target for Specific Components of Traditional Chinese Medicine: A Virtual Screening and Molecular Dynamics Study. <i>PLoS ONE</i> , 2012, 7, e50087.	2.5	28
40	Treatment of Rheumatoid Arthritis with Traditional Chinese Medicine. <i>BioMed Research International</i> , 2014, 2014, 1-11.	1.9	27
41	Drug design for Influenza A virus subtype H1N1. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2010, 41, 8-15.	5.3	26
42	De novo design of novel selective COX-2 inhibitors: From virtual screening to pharmacophore analysis. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2009, 40, 55-69.	5.3	24
43	Network pharmacology-based approach of novel traditional Chinese medicine formula for treatment of acute skin inflammation in silico. <i>Computational Biology and Chemistry</i> , 2017, 71, 70-81.	2.3	23
44	In Silico Investigation of Potential Src Kinase Ligands from Traditional Chinese Medicine. <i>PLoS ONE</i> , 2012, 7, e33728.	2.5	22
45	In Silico Identification of Potent Pancreatic Triacylglycerol Lipase Inhibitors from Traditional Chinese Medicine. <i>PLoS ONE</i> , 2012, 7, e43932.	2.5	21
46	Pharmacological Chaperone Design for Reducing Risk Factor of Parkinson's Disease from Traditional Chinese Medicine. <i>Evidence-based Complementary and Alternative Medicine</i> , 2014, 2014, 1-12.	1.2	21
47	Discovery of novel insomnia leads from screening traditional Chinese medicine database. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014, 32, 776-791.	3.5	20
48	Investigation of silent information regulator 1 (Sirt1) agonists from Traditional Chinese Medicine. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013, 31, 1207-1218.	3.5	19
49	Inhibiting the vascular smooth muscle cells proliferation by EPC and DPPC liposomes encapsulated magnolol. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2008, 39, 407-411.	1.4	18
50	Han ethnicity-specific type 2 diabetic treatment from traditional Chinese medicine?. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013, 31, 1219-1235.	3.5	18
51	Lose Weight with Traditional Chinese Medicine? Potential Suppression of Fat Mass and Obesity-Associated Protein. <i>Journal of Biomolecular Structure and Dynamics</i> , 2011, 29, 471-483.	3.5	17
52	Treatment of Cardiovascular Disease by Traditional Chinese Medicine against Pregnane X Receptor. <i>BioMed Research International</i> , 2014, 2014, 1-17.	1.9	17
53	Chalcone Derivatives Inhibit Human Platelet Aggregation and Inhibit Growth in Human Bladder Cancer Cells. <i>Biological and Pharmaceutical Bulletin</i> , 2014, 37, 1191-1198.	1.4	17
54	Identification of tyrosinase inhibitors from traditional Chinese medicines for the management of hyperpigmentation. <i>SpringerPlus</i> , 2015, 4, 184.	1.2	17

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55	Antiplatelet Effect and Selective Binding to Cyclooxygenase by Molecular Docking Analysis of 3-Alkylaminopropoxy-9,10-anthraquinone Derivatives. <i>Biological and Pharmaceutical Bulletin</i> , 2008, 31, 1547-1551.	1.4	16
56	<i>In Silico</i> Identification of Potent PPAR- α Agonists from Traditional Chinese Medicine: A Bioactivity Prediction, Virtual Screening, and Molecular Dynamics Study. <i>Evidence-based Complementary and Alternative Medicine</i> , 2014, 2014, 1-19.	1.2	16
57	Computational screening and QSAR analysis for design of AMP-activated protein kinase agonist. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2010, 41, 352-359.	5.3	15
58	Developing Hypothetical Inhibition Mechanism of Novel Urea Transporter B Inhibitor. <i>Scientific Reports</i> , 2014, 4, 5775.	3.3	15
59	Finding Inhibitors of Mutant Superoxide Dismutase-1 for Amyotrophic Lateral Sclerosis Therapy from Traditional Chinese Medicine. <i>Evidence-based Complementary and Alternative Medicine</i> , 2014, 2014, 1-12.	1.2	14
60	Evaluation of Correlation of Cell Cycle Proteins and Ki-67 Interaction in Paranasal Sinus Inverted Papilloma Prognosis and Squamous Cell Carcinoma Transformation. <i>BioMed Research International</i> , 2014, 2014, 1-16.	1.9	14
61	Insight into molecular dynamics simulation of BRAF(V600E) and potent novel inhibitors for malignant melanoma. <i>International Journal of Nanomedicine</i> , 2015, 10, 3131.	6.7	14
62	Traditional Chinese medicine as dual guardians against hypertension and cancer?. <i>Journal of Biomolecular Structure and Dynamics</i> , 2012, 30, 299-317.	3.5	13
63	Mechanism of BAG1 repair on Parkinson's disease-linked DJ1 mutation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2012, 30, 1-12.	3.5	12
64	<i>In Silico</i> Investigation of Traditional Chinese Medicine Compounds to Inhibit Human Histone Deacetylase 2 for Patients with Alzheimer's Disease. <i>BioMed Research International</i> , 2014, 2014, 1-15.	1.9	12
65	Drug design for hemagglutinin: Screening and molecular dynamics from traditional Chinese medicine database. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2011, 42, 563-571.	5.3	11
66	Computational Design of Apolipoprotein E4 Inhibitors for Alzheimer's Disease Therapy from Traditional Chinese Medicine. <i>BioMed Research International</i> , 2014, 2014, 1-13.	1.9	11
67	Investigation of the Novel Lead of Melanocortin 1 Receptor for Pigmentary Disorders. <i>Evidence-based Complementary and Alternative Medicine</i> , 2014, 2014, 1-13.	1.2	11
68	Drug Design of Cyclin-Dependent Kinase 2 Inhibitor for Melanoma from Traditional Chinese Medicine. <i>BioMed Research International</i> , 2014, 2014, 1-17.	1.9	11
69	Molecular dynamics analysis of potent inhibitors of M2 proton channel against H1N1 swine influenza virus. <i>Molecular Simulation</i> , 2011, 37, 250-256.	2.0	10
70	Osteoponin Promoter Controlled by DNA Methylation: Aberrant Methylation in Cloned Porcine Genome. <i>BioMed Research International</i> , 2014, 2014, 1-16.	1.9	10
71	Drug design for mPGES-1 from traditional Chinese medicine database: A screening, docking, QSAR, molecular dynamics, and pharmacophore mapping study. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2011, 42, 580-591.	5.3	9
72	<i>In Silico</i> Design of BACE1 Inhibitor for Alzheimer's Disease by Traditional Chinese Medicine. <i>BioMed Research International</i> , 2014, 2014, 1-14.	1.9	9

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73	Lead Discovery for Alzheimer's Disease Related Target Protein RbAp48 from Traditional Chinese Medicine. <i>BioMed Research International</i> , 2014, 2014, 1-14.	1.9	9
74	Molecular level activation insights from a NR2A/NR2B agonist. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014, 32, 683-693.	3.5	9
75	Novel hemagglutinin inhibitors for H1N1 influenza virus screening from TCM database. <i>Molecular Simulation</i> , 2011, 37, 361-368.	2.0	8
76	<i>In Silico</i> Insight into Potent of Anthocyanin Regulation of FKBP52 to Prevent Alzheimer's Disease. <i>Evidence-based Complementary and Alternative Medicine</i> , 2014, 2014, 1-20.	1.2	8
77	Screening from TCM Database@Taiwan and QSAR model for identifying HER2 inhibitors. <i>Molecular Simulation</i> , 2011, 37, 884-892.	2.0	7
78	A possible strategy against head and neck cancer: <i>in silico</i> investigation of three-in-one inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013, 31, 1358-1369.	3.5	7
79	Potential Mitochondrial Isocitrate Dehydrogenase R140Q Mutant Inhibitor from Traditional Chinese Medicine against Cancers. <i>BioMed Research International</i> , 2014, 2014, 1-10.	1.9	7
80	Magnolol encapsulated by different acyl chain length of liposomes on inhibiting proliferation of smooth muscle cells. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2009, 40, 380-386.	5.3	6
81	Structure-based and ligand-based drug design for microsomal prostaglandin E synthase-1 inhibitors. <i>Molecular Simulation</i> , 2011, 37, 226-236.	2.0	6
82	Key features for designing M2 proton channel anti swine flu inhibitors. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2011, 42, 701-708.	5.3	6
83	Memory enhancement by traditional Chinese medicine?. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013, 31, 1411-1439.	3.5	6
84	<i>In Silico</i> Design for Adenosine Monophosphate-Activated Protein Kinase Agonist from Traditional Chinese Medicine for Treatment of Metabolic Syndromes. <i>Evidence-based Complementary and Alternative Medicine</i> , 2014, 2014, 1-16.	1.2	6
85	Potential Retinoid X Receptor Agonists for Treating Alzheimer's Disease from Traditional Chinese Medicine. <i>Evidence-based Complementary and Alternative Medicine</i> , 2014, 2014, 1-13.	1.2	6
86	<i>In Silico</i> Investigation of Potential mTOR Inhibitors from Traditional Chinese Medicine for Treatment of Leigh Syndrome. <i>BioMed Research International</i> , 2014, 2014, 1-9.	1.9	6
87	<i>In Silico</i> Investigation of Potential PARP-1 Inhibitors from Traditional Chinese Medicine. <i>Evidence-based Complementary and Alternative Medicine</i> , 2014, 2014, 1-13.	1.2	6
88	Potential Protein Phosphatase 2A Agents from Traditional Chinese Medicine against Cancer. <i>Evidence-based Complementary and Alternative Medicine</i> , 2014, 2014, 1-10.	1.2	6
89	Treatment of Acute Lymphoblastic Leukemia from Traditional Chinese Medicine. <i>Evidence-based Complementary and Alternative Medicine</i> , 2014, 2014, 1-21.	1.2	5
90	Potential Smoothed Inhibitor from Traditional Chinese Medicine against the Disease of Diabetes, Obesity, and Cancer. <i>BioMed Research International</i> , 2014, 2014, 1-12.	1.9	5

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91	Lead Screening for HIV-1 Integrase (IN) Inhibited by Traditional Chinese Medicine. BioMed Research International, 2014, 2014, 1-12.	1.9	5
92	The Inhibition of Folylpolyglutamate Synthetase (folC) in the Prevention of Drug Resistance in <i>Mycobacterium tuberculosis</i> by Traditional Chinese Medicine. BioMed Research International, 2014, 2014, 1-14.	1.9	5
93	Investigation of Estrogen Receptor (ESR1) for Breast Cancer from Traditional Chinese Medicine. BioMed Research International, 2014, 2014, 1-12.	1.9	5
94	Lead Screening for Chronic Obstructive Pulmonary Disease of IKK2 Inhibited by Traditional Chinese Medicine. Evidence-based Complementary and Alternative Medicine, 2014, 2014, 1-16.	1.2	5
95	Insight into two antioxidants binding to the catalase NADPH binding site from traditional Chinese medicines. RSC Advances, 2015, 5, 6625-6635.	3.6	5
96	Susceptible gene of stasis-stagnation constitution from genome-wide association study related to cardiovascular disturbance and possible regulated traditional Chinese medicine. BMC Complementary and Alternative Medicine, 2015, 15, 229.	3.7	5
97	Drug discovery for DNA break repair system by screening from TCM database and molecular dynamics approach. Molecular Simulation, 2011, 37, 804-811.	2.0	4
98	A possible solution for hair loss by inhibiting corticotropin-releasing factor (CRF) receptor from traditional Chinese medicine. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1613-1623.	3.5	4
99	Investigation of Anti-Infection Mechanism of Lactoferricin and Splunc-1. Evidence-based Complementary and Alternative Medicine, 2014, 2014, 1-10.	1.2	4
100	In SilicoInvestigation of Potential TRAF6 Inhibitor from Traditional Chinese Medicine against Cancers. BioMed Research International, 2014, 2014, 1-14.	1.9	4
101	When Modern Technology Meets Ancient Traditional Chinese Medicine. Evidence-based Complementary and Alternative Medicine, 2015, 2015, 1-2.	1.2	4
102	Molecular insight and resolution for tumors harboring the H-ras(G12V) mutation. RSC Advances, 2015, 5, 20623-20633.	3.6	4
103	A Novel Algorithm for Identification of Activated Cryptic 5â€² Splice Sites. Journal of Biomolecular Structure and Dynamics, 2012, 29, 1089-1099.	3.5	3
104	Investigation of Potent Lead for Acquired Immunodeficiency Syndrome from Traditional Chinese Medicine. BioMed Research International, 2014, 2014, 1-11.	1.9	3
105	Exploring 3D-QSAR pharmacophore mapping of azaphenanthrene derivatives for mPGES-1 inhibition Using HypoGen technique. , 2008, , .		2
106	Screening from the world's largest TCM database for inhibiting DNA repair protein XRCC4. Molecular Simulation, 2011, 37, 503-509.	2.0	2
107	Treat Alzheimer's disease by traditional Chinese medicine?. Molecular Simulation, 2011, 37, 923-931.	2.0	2
108	Lead Screening for CXCR4 of the Human HIV Infection Receptor Inhibited by Traditional Chinese Medicine. BioMed Research International, 2014, 2014, 1-13.	1.9	2

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109	Lead Screening for HIV of C-C Chemokine Receptor Type 5 Receptor Inhibited by Traditional Chinese Medicine. Evidence-based Complementary and Alternative Medicine, 2014, 2014, 1-10.	1.2	2
110	In Silico Investigation of Cytochrome P450 2C9 in relation to Aging Using Traditional Chinese Medicine. Evidence-based Complementary and Alternative Medicine, 2014, 2014, 1-14.	1.2	2
111	Recent Novel High-Tech Researches in Molecular Biology. BioMed Research International, 2015, 2015, 1-3.	1.9	2
112	Reducing without Side Effects? A Novel Strategy for Designing the PPAR Agonists. , 2009, , .		1
113	Chemical engineering research in Taiwan in 2007â€“2009. Journal of the Taiwan Institute of Chemical Engineers, 2010, 41, 244-245.	5.3	1
114	Design of Glucagon-Like Peptide-1 Receptor Agonist for Diabetes Mellitus from Traditional Chinese Medicine. Evidence-based Complementary and Alternative Medicine, 2014, 2014, 1-17.	1.2	1
115	In Silico Investigation of Potential Pyruvate Kinase M2 Regulators from Traditional Chinese Medicine against Cancers. BioMed Research International, 2014, 2014, 1-14.	1.9	1
116	An Investigation of Small GTPases in relation to Liver Tumorigenesis Using Traditional Chinese Medicine. BioMed Research International, 2014, 2014, 1-11.	1.9	1
117	Possible Inhibitor from Traditional Chinese Medicine for the β Form of Calcium-Dependent Protein Kinase Type II in the Treatment of Major Depressive Disorder. BioMed Research International, 2014, 2014, 1-14.	1.9	1
118	Residue-based design of small molecule inhibitor for H1N1, H5N1 and H7N1 mutants. Journal of Molecular Modeling, 2016, 22, 4.	1.8	1
119	Is that Possible to Design the Versatile Inhibitors for H1N1, H5N1, H5N2, and H5N7?. , 2009, , .		0
120	Could Traditional Chinese Medicine Used for Curing Erectile Dysfunction?. , 2009, , .		0
121	What is the Key Point for Designing HER2 Inhibitors?. , 2009, , .		0
122	Drug Design for AMP-Activated Protein Kinase Agonists in Silico. , 2009, , .		0
123	Drug Design for XRCC4 in Silico. , 2009, , .		0
124	Drug Design for KU86 in DNA Break Repair System. , 2009, , .		0
125	Drug Design for the Influenza A Virus Subtype H1N1. , 2009, , .		0
126	A Novel Strategy for Designing Dual-Target Inhibitors of KU86 and XRCC4. , 2009, , .		0

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127	Dual-Targeted Drug Design of HER2 and HSP90 by CoMFA Model and Pharmacophore Analysis. , 2009, , .		0
128	Chapter 5. When Modern Computational Systems Biology Meets Traditional Chinese Medicine. RSC Drug Discovery Series, 2013, , 61-80.	0.3	0
129	Insight into HIV of IFN-Induced Myxovirus Resistance 2 (MX2) Expressed by Traditional Chinese Medicine. BioMed Research International, 2014, 2014, 1-14.	1.9	0