Md Imtaiyaz Hassan

List of Publications by Citations

370 papers	7,114 citations	41 h-index	58 g-index
390 ext. papers	9,161 ext. citations	4.7 avg, IF	6.72 L-index

#	Paper	IF	Citations
370	Zinc alpha 2-glycoprotein: a multidisciplinary protein. *Molecular Cancer Research*, **2008**, 6, 892-906	6.6	167
369	Structure, function and applications of carbonic anhydrase isozymes. *Bioorganic and Medicinal Chemistry*, **2013**, 21, 1570-82	3.4	163
368	Luminol-based chemiluminescent signals: clinical and non-clinical application and future uses. *Applied Biochemistry and Biotechnology*, **2014**, 173, 333-55	3.2	158
367	A review of methods available to estimate solvent-accessible surface areas of soluble proteins in the folded and unfolded states. *Current Protein and Peptide Science*, **2014**, 15, 456-76	2.8	98
366	Glecaprevir and Maraviroc are high-affinity inhibitors of SARS-CoV-2 main protease: possible implication in COVID-19 therapy. *Bioscience Reports*, **2020**, 40,	4.1	90
365	The role of key residues in structure, function, and stability of cytochrome-c. *Cellular and Molecular Life Sciences*, **2014**, 71, 229-55	10.3	88
364	Protein aggregation and neurodegenerative diseases: From theory to therapy. *European Journal of Medicinal Chemistry*, **2016**, 124, 1105-1120	6.8	88
363	Current updates on computer aided protein modeling and designing. *International Journal of Biological Macromolecules*, **2016**, 85, 48-62	7.9	86
362	Spectroscopic and isothermal titration calorimetry studies of binding interaction of ferulic acid with bovine serum albumin. *Thermochimica Acta*, **2012**, 548, 56-64	2.9	79
361	Advancements in Docking and Molecular Dynamics Simulations Towards Ligand-receptor Interactions and Structure-function Relationships. *Current Topics in Medicinal Chemistry*, **2018**, 18, 1755-1768	3	79
360	Elucidation of Dietary Polyphenolics as Potential Inhibitor of Microtubule Affinity Regulating Kinase 4: In silico and In vitro Studies. *Scientific Reports*, **2017**, 7, 9470	4.9	78
359	Identification and evaluation of bioactive natural products as potential inhibitors of human microtubule affinity-regulating kinase 4 (MARK4). *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 1813-1829	3.6	77
358	Prolactin inducible protein in cancer, fertility and immunoregulation: structure, function and its clinical implications. *Cellular and Molecular Life Sciences*, **2009**, 66, 447-59	10.3	70
357	Large scale analysis of the mutational landscape in β-glucuronidase: A major player of mucopolysaccharidosis type VII. *Gene*, **2016**, 576, 36-44	3.8	67
356	Microtubule affinity-regulating kinase 4: structure, function, and regulation. *Cell Biochemistry and Biophysics*, **2013**, 67, 485-99	3.2	67
355	Investigation of molecular mechanism of recognition between citral and MARK4: A newer therapeutic approach to attenuate cancer cell progression. *International Journal of Biological Macromolecules*, **2018**, 107, 2580-2589	7.9	64
354	Size-dependent studies of macromolecular crowding on the thermodynamic stability, structure and functional activity of proteins: in vitro and in silico approaches. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 178-197	4	63

353	Crystal structure of the novel complex formed between zinc alpha2-glycoprotein (ZAG) and prolactin-inducible protein (PIP) from human seminal plasma. *Journal of Molecular Biology*, **2008**, 384, 663-72	6.5	59
352	Functional annotation of conserved hypothetical proteins from Haemophilus influenzae Rd KW20. *PLoS ONE*, **2013**, 8, e84263	3.7	59
351	Curcumin specifically binds to the human calcium-calmodulin-dependent protein kinase IV: fluorescence and molecular dynamics simulation studies. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 572-84	3.6	58
350	Proteomic analysis of heparin-binding proteins from human seminal plasma: a step towards identification of molecular markers of male fertility. *Journal of Biosciences*, **2009**, 34, 899-908	2.3	54
349	Role of N-terminal residues on folding and stability of C-phycoerythrin: simulation and urea-induced denaturation studies. *Journal of Biomolecular Structure and Dynamics*, **2015**, 33, 121-33	3.6	53
348	Binding studies and biological evaluation of β-carotene as a potential inhibitor of human calcium/calmodulin-dependent protein kinase IV. *International Journal of Biological Macromolecules*, **2017**, 96, 161-170	7.9	52
347	A novel multicopper oxidase (laccase) from cyanobacteria: Purification, characterization with potential in the decolorization of anthraquinonic dye. *PLoS ONE*, **2017**, 12, e0175144	3.7	52
346	Rosmarinic Acid Exhibits Anticancer Effects via MARK4 Inhibition. *Scientific Reports*, **2020**, 10, 10300	4.9	51
345	Investigation of inhibitory potential of quercetin to the pyruvate dehydrogenase kinase 3: Towards implications in anticancer therapy. *International Journal of Biological Macromolecules*, **2019**, 136, 1076-1085	7.9	49
344	Evaluation of ellagic acid as an inhibitor of sphingosine kinase 1: A targeted approach towards anticancer therapy. *Biomedicine and Pharmacotherapy*, **2019**, 118, 109245	7.5	49
343	Synthesis, characterization and biological evaluation of tertiary sulfonamide derivatives of pyridyl-indole based heteroaryl chalcone as potential carbonic anhydrase IX inhibitors and anticancer agents. *European Journal of Medicinal Chemistry*, **2018**, 155, 13-23	6.8	49
342	High throughput screening, docking, and molecular dynamics studies to identify potential inhibitors of human calcium/calmodulin-dependent protein kinase IV. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 2179-2192	3.6	46
341	Biological evaluation of p-toluene sulphonylhydrazone as carbonic anhydrase IX inhibitors: An approach to fight hypoxia-induced tumors. *International Journal of Biological Macromolecules*, **2018**, 106, 840-850	7.9	45
340	Identification of γMangostin as a Potential Inhibitor of Microtubule Affinity Regulating Kinase 4. *Journal of Natural Products*, **2019**, 82, 2252-2261	4.9	44
339	Human β-glucuronidase: structure, function, and application in enzyme replacement therapy. *Rejuvenation Research*, **2013**, 16, 352-63	2.6	43
338	Structural characterization of MG and pre-MG states of proteins by MD simulations, NMR, and other techniques. *Journal of Biomolecular Structure and Dynamics*, **2015**, 33, 2267-84	3.6	43
337	Identification of high-affinity inhibitors of SARS-CoV-2 main protease: Towards the development of effective COVID-19 therapy. *Virus Research*, **2020**, 288, 198102	6.4	43
336	Therapeutic progress in amyotrophic lateral sclerosis-beginning to learning. *European Journal of Medicinal Chemistry*, **2016**, 121, 903-917	6.8	43

335	Design, synthesis and biological evaluation of novel pyridine-thiazolidinone derivatives as anticancer agents: Targeting human carbonic anhydrase IX. *European Journal of Medicinal Chemistry* , **2018**, 144, 544-556	6.8	43
334	Virtual Screening Approach to Identify High-Affinity Inhibitors of Serum and Glucocorticoid-Regulated Kinase 1 among Bioactive Natural Products: Combined Molecular Docking and Simulation Studies. *Molecules*, **2020**, 25,	4.8	42
333	Calcium/calmodulin-dependent protein kinase IV: A multifunctional enzyme and potential therapeutic target. *Progress in Biophysics and Molecular Biology*, **2016**, 121, 54-65	4.7	42
332	Identification and Evaluation of Inhibitors of Lipase from using Virtual High-Throughput Screening and Molecular Dynamics Studies. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	42
331	Molecular mechanism of Ras-related protein Rab-5A and effect of mutations in the catalytically active phosphate-binding loop. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 105-118	3.6	41
330	Discovery of Hordenine as a Potential Inhibitor of Pyruvate Dehydrogenase Kinase 3: Implication in Lung Cancer Therapy. *Biomedicines*, **2020**, 8,	4.8	41
329	High resolution crystal structure of human -glucuronidase reveals structural basis of lysosome targeting. *PLoS ONE*, **2013**, 8, e79687	3.7	41
328	Design and development of Isatin-triazole hydrazones as potential inhibitors of microtubule affinity-regulating kinase 4 for the therapeutic management of cell proliferation and metastasis. *European Journal of Medicinal Chemistry*, **2019**, 163, 840-852	6.8	41
327	Structure-guided design of peptidic ligand for human prostate specific antigen. *Journal of Peptide Science*, **2007**, 13, 849-55	2.1	40
326	Implications of the second wave of COVID-19 in India. *Lancet Respiratory Medicine,the*, **2021**, 9, e93-e94	35.1	40
325	Designing New Kinase Inhibitor Derivatives as Therapeutics Against Common Complex Diseases: Structural Basis of Microtubule Affinity-Regulating Kinase 4 (MARK4) Inhibition. *OMICS A Journal of Integrative Biology*, **2015**, 19, 700-11	3.8	39
324	Binding mechanism of caffeic acid and simvastatin to the integrin linked kinase for therapeutic implications: a comparative docking and MD simulation studies. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 4327-4337	3.6	39
323	Search of potential inhibitor against New Delhi metallo-beta-lactamase 1 from a series of antibacterial natural compounds. *Journal of Natural Science, Biology and Medicine*, **2013**, 4, 51-6	0.8	38
322	Functional annotation of putative hypothetical proteins from Candida dubliniensis. *Gene*, **2014**, 543, 93-100	3.8	37
321	Structural and functional analysis of human prostatic acid phosphatase. *Expert Review of Anticancer Therapy*, **2010**, 10, 1055-68	3.5	37
320	Discovering a potent small molecule inhibitor for gankyrin using de novo drug design approach. *International Journal of Computational Biology and Drug Design*, **2011**, 4, 373-86	0.4	37
319	InstaDock: A single-click graphical user interface for molecular docking-based virtual high-throughput screening. *Briefings in Bioinformatics*, **2021**, 22,	13.4	37
318	Ellagic Acid Controls Cell Proliferation and Induces Apoptosis in Breast Cancer Cells via Inhibition of Cyclin-Dependent Kinase 6. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	36

317	Evidence of vanillin binding to CAMKIV explains the anti-cancer mechanism in human hepatic carcinoma and neuroblastoma cells. *Molecular and Cellular Biochemistry*, **2018**, 438, 35-45	4.2	36
316	Structure and function of von Willebrand factor. *Blood Coagulation and Fibrinolysis*, **2012**, 23, 11-22	1	36
315	Structural model of human PSA: a target for prostate cancer therapy. *Chemical Biology and Drug Design*, **2007**, 70, 261-7	2.9	36
314	Spectroscopic, calorimetric and molecular docking insight into the interaction of Alzheimer's drug donepezil with human transferrin: implications of Alzheimer's drug. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 1094-1102	3.6	36
313	Implications of molecular diversity of chitin and its derivatives. *Applied Microbiology and Biotechnology*, **2017**, 101, 3513-3536	5.7	35
312	Structural and functional analysis of various globulin proteins from soy seed. *Critical Reviews in Food Science and Nutrition*, **2015**, 55, 1491-502	11.5	35
311	A single mutation induces molten globule formation and a drastic destabilization of wild-type cytochrome c at pH 6.0. *Journal of Biological Inorganic Chemistry*, **2009**, 14, 751-60	3.7	35
310	Structure-based identification of potential SARS-CoV-2 main protease inhibitors. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-14	3.6	35
309	Interaction of DNA minor groove binder Hoechst 33258 with bovine serum albumin. *Chemical and Pharmaceutical Bulletin*, **2009**, 57, 481-6	1.9	34
308	MARK4 Inhibited by AChE Inhibitors, Donepezil and Rivastigmine Tartrate: Insights into Alzheimer's Disease Therapy. *Biomolecules*, **2020**, 10,	5.9	34
307	Potential drug targets of SARS-CoV-2: From genomics to therapeutics. *International Journal of Biological Macromolecules*, **2021**, 177, 1-9	7.9	34
306	Unraveling the Role of RNA Mediated Toxicity of Repeats in C9-FTD/ALS. *Frontiers in Neuroscience*, **2017**, 11, 711	5.1	33
305	Evaluation of binding and inhibition mechanism of dietary phytochemicals with sphingosine kinase 1: Towards targeted anticancer therapy. *Scientific Reports*, **2019**, 9, 18727	4.9	33
304	Probing the Inhibition of Microtubule Affinity Regulating Kinase 4 by N-Substituted Acridones. *Scientific Reports*, **2019**, 9, 1676	4.9	32
303	Chitinase from Thermomyces lanuginosus SSBP and its biotechnological applications. *Extremophiles* , **2015**, 19, 1055-66	3	32
302	Relationship between protein stability and functional activity in the presence of macromolecular crowding agents alone and in mixture: An insight into stability-activity trade-off. *Archives of Biochemistry and Biophysics*, **2015**, 584, 42-50	4.1	32
301	Structure guided design of potential inhibitors of human calcium-calmodulin dependent protein kinase IV containing pyrimidine scaffold. *Bioorganic and Medicinal Chemistry Letters*, **2016**, 26, 782-788	2.9	32
300	Functional implications of pH-induced conformational changes in the Sphingosine kinase 1. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 225, 117453	4.4	32

299	Structural Analysis and Conformational Dynamics of Gene Mutations Involved in Coat Plus Syndrome. *Frontiers in Molecular Biosciences*, **2019**, 6, 41	5.6	31
298	Identification of functional candidates amongst hypothetical proteins of Treponema pallidum ssp. pallidum. *PLoS ONE*, **2015**, 10, e0124177	3.7	31
297	Proteomic approach for purification of seminal plasma proteins involved in tumor proliferation. *Journal of Separation Science*, **2007**, 30, 1979-88	3.4	31
296	Structure prediction and functional analyses of a thermostable lipase obtained from Shewanella putrefaciens. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 2123-2135	3.6	30
295	Probing the interaction of Rivastigmine Tartrate, an important Alzheimer's drug, with serum albumin: Attempting treatment of Alzheimer's disease. *International Journal of Biological Macromolecules*, **2020**, 148, 533-542	7.9	30
294	Structural diversity of class I MHC-like molecules and its implications in binding specificities. *Advances in Protein Chemistry and Structural Biology*, **2011**, 83, 223-70	5.3	30
293	Progastriscin: structure, function, and its role in tumor progression. *Journal of Molecular Cell Biology*, **2010**, 2, 118-27	6.3	30
292	Purification and characterization of zinc alpha2-glycoprotein-prolactin inducible protein complex from human seminal plasma. *Journal of Separation Science*, **2008**, 31, 2318-24	3.4	30
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289	Protein aggregation, misfolding and consequential human neurodegenerative diseases. *International Journal of Neuroscience*, **2017**, 127, 1047-1057	2	29
288	In vitro and in silico studies of urea-induced denaturation of yeast iso-1-cytochrome c and its deletants at pH 6.0 and 25 ℃. *Journal of Biomolecular Structure and Dynamics*, **2015**, 33, 1493-502	3.6	29
287	Exploring molecular insights into the interaction mechanism of cholesterol derivatives with the Mce4A: A combined spectroscopic and molecular dynamic simulation studies. *International Journal of Biological Macromolecules*, **2018**, 111, 548-560	7.9	29
286	Identification and evaluation of glutathione conjugate gamma-l-glutamyl-l-cysteine for improved drug delivery to the brain. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 3610-3620	3.6	29
285	Effect of pH on the structure, function, and stability of human calcium/calmodulin-dependent protein kinase IV: combined spectroscopic and MD simulation studies. *Biochemistry and Cell Biology*, **2016**, 94, 221-8	3.6	28
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282	Thermal Stabilization of Proteins by Mono- and Oligosaccharides: Measurement and Analysis in the Context of an Excluded Volume Model. *Biochemistry*, **2015**, 54, 3594-603	3.2	27

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280	Design and synthesis of a novel class of carbonic anhydrase-IX inhibitor 1-(3-(phenyl/4-fluorophenyl)-7-imino-3H-[1,2,3]triazolo[4,5d]pyrimidin 6(7H)yl)urea. *Journal of Molecular Graphics and Modelling*, **2016**, 64, 101-109	2.8	26
279	Molecular interaction studies on ellagic acid for its anticancer potential targeting pyruvate dehydrogenase kinase 3.. *RSC Advances*, **2019**, 9, 23302-23315	3.7	26
278	Conformational and thermodynamic characterization of the premolten globule state occurring during unfolding of the molten globule state of cytochrome c. *Journal of Biological Inorganic Chemistry*, **2010**, 15, 1319-29	3.7	26
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276	Identification of High-Affinity Inhibitors of Cyclin-Dependent Kinase 2 Towards Anticancer Therapy. *Molecules*, **2019**, 24,	4.8	26
275	First evidence of formation of pre-molten globule state in myoglobin: A macromolecular crowding approach towards protein folding in vivo. *International Journal of Biological Macromolecules*, **2019**, 126, 1288-1294	7.9	26
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273	PKR-inhibitor binds efficiently with human microtubule affinity-regulating kinase 4. *Journal of Molecular Graphics and Modelling*, **2015**, 62, 245-252	2.8	25
272	Characterisation of mutations and molecular studies of type 2 von Willebrand disease. *Thrombosis and Haemostasis*, **2013**, 109, 39-46	7	25
271	Effect of sequential deletion of extra N-terminal residues on the structure and stability of yeast iso-1-cytochrome-c. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 2005-16	3.6	25
270	Investigation of deleterious effects of nsSNPs in the POT1 gene: a structural genomics-based approach to understand the mechanism of cancer development. *Journal of Cellular Biochemistry*, **2019**, 120, 10281-10294	4.7	25
269	Urea-induced denaturation of human calcium/calmodulin-dependent protein kinase IV: a combined spectroscopic and MD simulation studies. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 463-475	3.6	24
268	Unraveling Binding Mechanism of Alzheimer's Drug Rivastigmine Tartrate with Human Transferrin: Molecular Docking and Multi-Spectroscopic Approach towards Neurodegenerative Diseases. *Biomolecules*, **2019**, 9,	5.9	24
267	Insight of the Interaction between 2,4-thiazolidinedione and Human Serum Albumin: A Spectroscopic, Thermodynamic and Molecular Docking Study. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	24
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265	Computing disease-linked SOD1 mutations: deciphering protein stability and patient-phenotype relations. *Scientific Reports*, **2017**, 7, 4678	4.9	24
264	Fragile histidine triad protein: structure, function, and its association with tumorogenesis. *Journal of Cancer Research and Clinical Oncology*, **2010**, 136, 333-50	4.9	24

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262	Design, synthesis, and biological evaluation of pyrimidine derivatives as potential inhibitors of human calcium/calmodulin-dependent protein kinase IV. *Chemical Biology and Drug Design*, **2017**, 89, 741-754	2.9	23
261	Molecular Basis of Pathogenesis of Coronaviruses: A Comparative Genomics Approach to Planetary Health to Prevent Zoonotic Outbreaks in the 21st Century. *OMICS A Journal of Integrative Biology*, **2020**, 24, 634-644	3.8	23
260	Molecular basis of the structural stability of hemochromatosis factor E: A combined molecular dynamic simulation and GdmCl-induced denaturation study. *Biopolymers*, **2016**, 105, 133-42	2.2	23
259	SARS-CoV-2 mediated lung inflammatory responses in host: targeting the cytokine storm for therapeutic interventions. *Molecular and Cellular Biochemistry*, **2021**, 476, 675-687	4.2	23
258	Characterization of intermediate state of myoglobin in the presence of PEG 10 under physiological conditions. *International Journal of Biological Macromolecules*, **2017**, 99, 241-248	7.9	22
257	In silico approaches for the identification of virulence candidates amongst hypothetical proteins of Mycoplasma pneumoniae 309. *Computational Biology and Chemistry*, **2015**, 59 Pt A, 67-80	3.6	22
256	Synthesis and SAR studies of novel 1,2,4-oxadiazole-sulfonamide based compounds as potential anticancer agents for colorectal cancer therapy. *Bioorganic Chemistry*, **2020**, 98, 103754	5.1	22
255	Comparison of the thermal stabilization of proteins by oligosaccharides and monosaccharide mixtures: Measurement and analysis in the context of excluded volume theory. *Biophysical Chemistry*, **2018**, 237, 31-37	3.5	22
254	Inhibiting CDK6 Activity by Quercetin Is an Attractive Strategy for Cancer Therapy. *ACS Omega*, **2020**, 5, 27480-27491	3.9	22
253	Impact of Gln94Glu mutation on the structure and function of protection of telomere 1, a cause of cutaneous familial melanoma. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 1514-1524	3.6	22
252	Effect of pH on structure, function, and stability of mitochondrial carbonic anhydrase VA. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 449-461	3.6	21
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250	2/3D-QSAR, molecular docking and MD simulation studies of FtsZ protein targeting benzimidazoles derivatives. *Computational Biology and Chemistry*, **2019**, 78, 398-413	3.6	21
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247	Hesperidin-CAMKIV interaction and its impact on cell proliferation and apoptosis in the human hepatic carcinoma and neuroblastoma cells. *Journal of Cellular Biochemistry*, **2019**, 120, 15119-15130	4.7	20
246	Design, synthesis & biological evaluation of ferulic acid-based small molecule inhibitors against tumor-associated carbonic anhydrase IX. *Bioorganic and Medicinal Chemistry*, **2020**, 28, 115424	3.4	20

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241	Structure-based functional annotation of hypothetical proteins from Candida dubliniensis: a quest for potential drug targets. *3 Biotech*, **2015**, 5, 561-576	2.8	19
240	Characterization of pre-molten globule state of yeast iso-1-cytochrome c and its deletants at pH 6.0 and 25 ℃. *International Journal of Biological Macromolecules*, **2015**, 72, 1406-18	7.9	19
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231	Atypical PKC phosphorylates microtubule affinity-regulating kinase 4 in vitro. *Molecular and Cellular Biochemistry*, **2015**, 410, 223-8	4.2	18
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229	Characterisation of molten globule-like state of sheep serum albumin at physiological pH. *International Journal of Biological Macromolecules*, **2016**, 89, 605-13	7.9	18
228	Testing the ability of non-methylamine osmolytes present in kidney cells to counteract the deleterious effects of urea on structure, stability and function of proteins. *PLoS ONE*, **2013**, 8, e72533	3.7	18

227	Cooperative Unfolding of Residual Structure in Heat Denatured Proteins by Urea and Guanidinium Chloride. *PLoS ONE*, **2015**, 10, e0128740	3.7	18
226	Current Advances in the Identification and Characterization of Putative Drug and Vaccine Targets in the Bacterial Genomes. *Current Topics in Medicinal Chemistry*, **2016**, 16, 1040-69	3	18
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