

# Krishna Bisetty

## List of Publications by Year in Descending Order

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

104  
papers

2,365  
citations

26  
h-index

45  
g-index

111  
ext. papers

2,794  
ext. citations

3.8  
avg, IF

5.65  
L-index

#	Paper	IF	Citations
104	A combined experimental-computational approach for electrocatalytic detection of epinephrine using nanocomposite sensor based on polyaniline/nickel oxide. <i>Journal of Electroanalytical Chemistry</i> , <b>2022</b> , 911, 116204	4.1	
103	Electrocatalysis of Endosulfan Based on FeO: An Experimental and Computational Approach. <i>ACS Omega</i> , <b>2021</b> , 6, 30515-30525	3.9	0
102	Measurement of TiO <sub>2</sub> Nanoscale Ingredients in Sunscreens by Multidetector AF4, TEM, and spICP-MS Supported by Computational Modeling. <i>ACS Applied Nano Materials</i> , <b>2021</b> , 4, 4665-4675	5.6	5
101	Evaluation of the catalytic activity of graphene oxide and zinc oxide nanoparticles on the electrochemical sensing of T1R2-Rebaudioside A complex supported by in silico methods. <i>Pure and Applied Chemistry</i> , <b>2021</b> ,	2.1	1
100	Sensitivity Enhancement of Pre-Capillary Chelation Method for the Separation of Metal Ions: Experimental and DFT Study. <i>Current Analytical Chemistry</i> , <b>2021</b> , 17, 839-848	1.7	
99	Removal of Targeted Pharmaceuticals and Personal Care Products from Wastewater Treatment Plants using QSAR Model. <i>Current Analytical Chemistry</i> , <b>2021</b> , 17, 1003-1015	1.7	1
98	Separation of Sucralose in Food Samples using Amines as Background Electrolyte Supported with DFT Calculations. <i>Current Analytical Chemistry</i> , <b>2021</b> , 17, 989-1002	1.7	
97	Classification and functional analyses of putative virulence factors of Mycobacterium tuberculosis: A combined sequence and structure based study. <i>Computational Biology and Chemistry</i> , <b>2020</b> , 87, 107270	3.6	
96	Prospective computational design and in vitro bio-analytical tests of new chemical entities as potential selective CYP17A1 lyase inhibitors. <i>Bioorganic Chemistry</i> , <b>2020</b> , 94, 103462	5.1	3
95	Highly-efficient electrochemical label-free immunosensor for the detection of ochratoxin A in coffee samples. <i>Sensors and Actuators B: Chemical</i> , <b>2020</b> , 305, 127438	8.5	30
94	Photoelectrochemical Bisphenol S Sensor Based on ZnO-Nanoroads Modified by Molecularly Imprinted Polypyrrole. <i>Macromolecular Chemistry and Physics</i> , <b>2020</b> , 221, 1900232	2.6	35
93	Multivariate optimization of field-flow fractionation of nanoscale synthetic amorphous silica in processed foods supported by computational modelling. <i>New Journal of Chemistry</i> , <b>2020</b> , 44, 17542-17551	3.6	2
92	Nanostructured pencil graphite electrodes for application as high power biocathodes in miniaturized biofuel cells and bio-batteries. <i>Scientific Reports</i> , <b>2020</b> , 10, 16535	4.9	3
91	Electrochemical Enzymatic Biosensing of Neotame Supported by Computational Methods. <i>Electroanalysis</i> , <b>2020</b> , 32, 2669-2680	3	5
90	Experimental and Computational Studies of a Laccase Immobilized ZnONPs/GO-Based Electrochemical Enzymatic Biosensor for the Detection of Sucralose in Food Samples. <i>Food Analytical Methods</i> , <b>2020</b> , 13, 2014-2027	3.4	11
89	An in-silico layer-by-layer adsorption study of the interaction between Rebaudioside A and the T1R2 human sweet taste receptor: modelling and biosensing perspectives. <i>Scientific Reports</i> , <b>2020</b> , 10, 18391	4.9	2
88	High Performance Electrochemical Biosensor for Bisphenol A Using Screen Printed Electrodes Modified with Multiwalled Carbon Nanotubes Functionalized with Silver-Doped Zinc Oxide. <i>Waste and Biomass Valorization</i> , <b>2020</b> , 11, 1085-1096	3.2	18

87	The structural basis of acid resistance in : insights from multiple pH regime molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2020</b> , 38, 4483-4492	3.6	2
86	Computational studies on the molecular insights of aptamer induced poly(N-isopropylacrylamide)-graft-graphene oxide for on/off- switchable whole-cell cancer diagnostics. <i>Scientific Reports</i> , <b>2019</b> , 9, 7873	4.9	8
85	Nanotechnology-based water quality management for wastewater treatment. <i>Environmental Chemistry Letters</i> , <b>2019</b> , 17, 65-121	13.3	70
84	Theoretical insights into the competitive metal bioaffinity of lactoferrin as a metal ion carrier: a DFT study. <i>New Journal of Chemistry</i> , <b>2019</b> , 43, 16374-16384	3.6	7
83	MWCNTs-Fe <sub>2</sub> O <sub>3</sub> nanoparticle nanohybrid-based highly sensitive electrochemicalsensor for the detection of kaempferol in broccoli samples. <i>Turkish Journal of Chemistry</i> , <b>2019</b> , 43, 1229-1243	1	4
82	Biogenic synthesis of nanoparticles: A review. <i>Arabian Journal of Chemistry</i> , <b>2019</b> , 12, 3576-3600	5.9	335
81	Removal of copper (II) from wastewater using green vegetable waste derived activated carbon: An approach to equilibrium and kinetic study. <i>Arabian Journal of Chemistry</i> , <b>2019</b> , 12, 4331-4339	5.9	40
80	Selectivity and sensitivity enhanced green energy waste based indirect- <del>E</del> solid phase extraction of carbaryl supported by DFT and molecular docking studies. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 257, 112-120	6	8
79	Membrane technology for water purification. <i>Environmental Chemistry Letters</i> , <b>2018</b> , 16, 343-365	13.3	38
78	One-pot biosynthesis of silver nanoparticles using Iboza Riparia and Ilex Mitis for cytotoxicity on human embryonic kidney cells. <i>Journal of Photochemistry and Photobiology B: Biology</i> , <b>2018</b> , 178, 560-567	6.7	17
77	Structural basis of pesticide detection by enzymatic biosensing: a molecular docking and MD simulation study. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2018</b> , 36, 1402-1416	3.6	13
76	Light induced DNA-functionalized TiO nanocrystalline interface: Theoretical and experimental insights towards DNA damage detection. <i>Journal of Photochemistry and Photobiology B: Biology</i> , <b>2018</b> , 188, 159-176	6.7	8
75	Special Properties of Nanomaterials for Chromatography <b>2018</b> , 37-54		
74	Role of Computational Tools in Designing Enzymatic Biosensors for the Detection of Pesticides in Environment <b>2018</b> , 287-311		
73	Smartphone based bioanalytical and diagnosis applications: A review. <i>Biosensors and Bioelectronics</i> , <b>2018</b> , 102, 136-149	11.8	174
72	Green synthesis, characterization and electrochemical sensing of silymarin by ZnO nanoparticles: Experimental and DFT studies. <i>Journal of Electroanalytical Chemistry</i> , <b>2018</b> , 808, 160-172	4.1	39
71	Structural insights into Rab21 GTPase activation mechanism by molecular dynamics simulations. <i>Molecular Simulation</i> , <b>2018</b> , 44, 179-189	2	12
70	Classification and Functional Analyses of Putative Conserved Proteins from Chlamydomonada pneumoniae CWL029. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , <b>2017</b> , 9, 96-106	3.5	1

69	Effect of pH on structure, function, and stability of mitochondrial carbonic anhydrase VA. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2017</b> , 35, 449-461	3.6	21
68	Urea-induced denaturation of human calcium/calmodulin-dependent protein kinase IV: a combined spectroscopic and MD simulation studies. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2017</b> , 35, 463-475	3.6	24
67	Structure prediction and functional analyses of a thermostable lipase obtained from <i>Shewanella putrefaciens</i> . <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2017</b> , 35, 2123-2135	3.6	30
66	Nanopolymer Chitosan in Cancer and Alzheimer Biomedical Application <b>2017</b> , 311-359		1
65	A Review of Gold and Silver Nanoparticle-Based Colorimetric Sensing Assays. <i>Advanced Engineering Materials</i> , <b>2017</b> , 19, 1700270	3.5	143
64	Molecular dynamics simulation of chitinase I from <i>Thermomyces lanuginosus</i> SSBP to ensure optimal activity. <i>Molecular Simulation</i> , <b>2017</b> , 43, 480-490	2	5
63	Robust adsorption of Direct Navy Blue-106 from textile industrial effluents by bio-hydrogen fermented waste derived activated carbon: Equilibrium and kinetic studies. <i>Arabian Journal of Chemistry</i> , <b>2017</b> , 10, S3084-S3096	5.9	9
62	Multivariate optimization of differential pulse polarographic catalytic hydrogen wave technique for the determination of nickel(II) in real samples. <i>Arabian Journal of Chemistry</i> , <b>2017</b> , 10, S2260-S2272	5.9	5
61	A Mini-Review on Enantiomeric Separation of Ofloxacin using Capillary Electrophoresis: Pharmaceutical Applications <b>2017</b> , 117-146		
60	Molecular Simulation of Chiral Selector-Enantiomer Interactions through Docking: Antimalarial Drugs as Case Study <b>2017</b> , 363-384		
59	Cloning, expression, and molecular dynamics simulations of a xylosidase obtained from <i>Thermomyces lanuginosus</i> . <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2016</b> , 34, 1681-92	3.6	38
58	Insight into the biosensing of graphene oxide: Present and future prospects. <i>Arabian Journal of Chemistry</i> , <b>2016</b> , 9, 238-261	5.9	76
57	Spectrophotometric determination of nickel (II) in waters and soils: Novel chelating agents and their biological applications supported by DFT method. <i>Karbala International Journal of Modern Science</i> , <b>2016</b> , 2, 239-250	4.6	13
56	Biosynthesis of ZnO nanoparticles using <i>Jacaranda mimosifolia</i> flowers extract: Synergistic antibacterial activity and molecular simulated facet specific adsorption studies. <i>Journal of Photochemistry and Photobiology B: Biology</i> , <b>2016</b> , 162, 199-207	6.7	96
55	Effect of pH on the structure, function, and stability of human calcium/calmodulin-dependent protein kinase IV: combined spectroscopic and MD simulation studies. <i>Biochemistry and Cell Biology</i> , <b>2016</b> , 94, 221-8	3.6	28
54	An ultrasensitive performance enhanced novel cytochrome c biosensor for the detection of rebaudioside A. <i>Biosensors and Bioelectronics</i> , <b>2016</b> , 77, 116-23	11.8	21
53	Large scale analysis of the mutational landscape in $\beta$ -glucuronidase: A major player of mucopolysaccharidosis type VII. <i>Gene</i> , <b>2016</b> , 576, 36-44	3.8	67
52	Monitoring of Cetylpyridinium Chloride Levels in Surface Waters: Patent Blue-V as Selective Ligand for Spectrophotometric Determination. <i>Asian Journal of Chemistry</i> , <b>2016</b> , 28, 1039-1042	0.4	4

51	Current Advances in the Identification and Characterization of Putative Drug and Vaccine Targets in the Bacterial Genomes. <i>Current Topics in Medicinal Chemistry</i> , <b>2016</b> , 16, 1040-69	3	18
50	Hybrid of ZnONPs/MWCNTs for electrochemical detection of aspartame in food and beverage samples. <i>Journal of Electroanalytical Chemistry</i> , <b>2016</b> , 774, 51-57	4.1	19
49	A pH based molecular dynamics simulations of chitinase II isolated from <i>Thermomyces lanuginosus</i> SSBP. <i>Cogent Biology</i> , <b>2016</b> , 2, 1168336	1.6	2
48	Electrochemical sensing platform amplified with a nanobiocomposite of L-phenylalanine ammonia-lyase enzyme for the detection of capsaicin. <i>Biosensors and Bioelectronics</i> , <b>2016</b> , 83, 45-53	11.8	29
47	Towards New Drug Targets? Function Prediction of Putative Proteins of <i>Neisseria meningitidis</i> MC58 and Their Virulence Characterization. <i>OMICS A Journal of Integrative Biology</i> , <b>2015</b> , 19, 416-34	3.8	17
46	Thermostable chitinase II from <i>Thermomyces lanuginosus</i> SSBP: Cloning, structure prediction and molecular dynamics simulations. <i>Journal of Theoretical Biology</i> , <b>2015</b> , 374, 107-14	2.3	47
45	In silico approaches for the identification of virulence candidates amongst hypothetical proteins of <i>Mycoplasma pneumoniae</i> 309. <i>Computational Biology and Chemistry</i> , <b>2015</b> , 59 Pt A, 67-80	3.6	22
44	PKR-inhibitor binds efficiently with human microtubule affinity-regulating kinase 4. <i>Journal of Molecular Graphics and Modelling</i> , <b>2015</b> , 62, 245-252	2.8	25
43	Studies on Bacterial Proteins Corona Interaction with Saponin Imprinted ZnO Nanohoneycombs and Their Toxic Responses. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2015</b> , 7, 23848-56	9.5	11
42	Chitinase from <i>Thermomyces lanuginosus</i> SSBP and its biotechnological applications. <i>Extremophiles</i> , <b>2015</b> , 19, 1055-66	3	32
41	Fabrication of copper nanoparticles decorated multiwalled carbon nanotubes as a high performance electrochemical sensor for the detection of neotame. <i>Biosensors and Bioelectronics</i> , <b>2015</b> , 67, 200-7	11.8	28
40	Analytical evaluation of steviol glycosides by capillary electrophoresis supported with molecular docking studies. <i>Journal of the Iranian Chemical Society</i> , <b>2015</b> , 12, 127-136	2	10
39	Seasonal Variation and Distribution of Anionic Surfactants in and around Tirupati: A Famous Pilgrim Centre in South India. <i>Asian Journal of Chemistry</i> , <b>2015</b> , 27, 3655-3657	0.4	2
38	Designing New Kinase Inhibitor Derivatives as Therapeutics Against Common Complex Diseases: Structural Basis of Microtubule Affinity-Regulating Kinase 4 (MARK4) Inhibition. <i>OMICS A Journal of Integrative Biology</i> , <b>2015</b> , 19, 700-11	3.8	39
37	Role of N-terminal residues on folding and stability of C-phycoerythrin: simulation and urea-induced denaturation studies. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2015</b> , 33, 121-33	3.6	53
36	Functional Insight into Putative Conserved Proteins of <i>Rickettsia rickettsii</i> and their Virulence Characterization. <i>Current Proteomics</i> , <b>2015</b> , 12, 101-116	0.7	5
35	Development of Green Energy Waste Activated Carbon for Removal of Trivalent Chromium: Equilibrium and Kinetic Modeling. <i>Separation Science and Technology</i> , <b>2014</b> , 49, 513-522	2.5	11
34	Triflic acid promoted Fries rearrangement of C-3 vinyl/isopropenyl-azetid-2-ones: single-pot synthesis of C-3 functionalized-2-aryl-2,3-dihydro-quinoline-4(1H)-ones. <i>RSC Advances</i> , <b>2014</b> , 4, 41793-41801	3.7	7

33	Creation of thermostable and alkaline stable xylanase variants by DNA shuffling. <i>Journal of Biotechnology</i> , <b>2014</b> , 187, 139-46	3.7	53
32	Electrochemical Determination of Capsaicin and Silymarin Using a Glassy Carbon Electrode Modified by Gold Nanoparticle Decorated Multiwalled Carbon Nanotubes. <i>Analytical Letters</i> , <b>2014</b> , 47, 2813-2828	2.2	34
31	Determination of Neotame by High-Performance Capillary Electrophoresis Using Cyclodextrin as a Chiral Selector. <i>Analytical Letters</i> , <b>2014</b> , 47, 2795-2812	2.2	8
30	Dithiocarbamates as hazardous remediation agent: A critical review on progress in environmental chemistry for inorganic species studies of 20th century. <i>Arabian Journal of Chemistry</i> , <b>2014</b> , 7, 11-25	5.9	108
29	Lactam-Syntho-Interceded Synthesis of Isatin-Imidazolidine-2-thione Conjugates with Structural Validation using Molecular Dynamic Simulations and Cytotoxic Evaluation. <i>Synlett</i> , <b>2013</b> , 24, 1865-1869	2.2	7
28	Synthesis, docking and in vitro antimalarial evaluation of bifunctional hybrids derived from Lactams and 7-chloroquinoline using click chemistry. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2012</b> , 22, 57-61	2.9	54
27	Connecting simulated, bioanalytical, and molecular docking data on the stereoselective binding of (E)-catechin to human serum albumin. <i>Analytical and Bioanalytical Chemistry</i> , <b>2012</b> , 402, 1899-909	4.4	9
26	Synthetic Studies on the Role of Substituents at C-3 Position on C3-C4 Bond Cleavage of Lactam Ring: Convenient Route for Diastereoselective Synthesis of Pyridin-2-ones. <i>Heterocycles</i> , <b>2012</b> , 86, 1301	0.8	4
25	Experimental-like affinity constants and enantioselectivity estimates from flexible docking. <i>Journal of Chemical Information and Modeling</i> , <b>2012</b> , 52, 2754-9	6.1	10
24	Theoretical study on the formation of a pentacyclo-undecane cage lactam. <i>Computational and Theoretical Chemistry</i> , <b>2012</b> , 986, 63-70	2	8
23	Regio- and Diastereoselective Nitroso Diels-Alder Cycloaddition Reactions of 3-dienyl-2-azetidinones with Nitrosoarenes. <i>Letters in Organic Chemistry</i> , <b>2012</b> , 9, 411-421	0.6	3
22	Preparation, spectrochemical, and computational analysis of L-carnosine (2-[(3-aminopropanoyl)amino]-3-(1H-imidazol-5-yl)propanoic acid) and its ruthenium (II) coordination complexes in aqueous solution. <i>Molecules</i> , <b>2011</b> , 16, 10269-91	4.8	18
21	A computational study of Neuromedin B. <i>Computational and Theoretical Chemistry</i> , <b>2011</b> , 971, 1-7	2	
20	Comparative structural studies of T-20 analogues using molecular dynamics. <i>Computational and Theoretical Chemistry</i> , <b>2011</b> , 974, 122-132	2	2
19	Conformational space search of Neuromedin C using replica exchange molecular dynamics and molecular dynamics. <i>Journal of Peptide Science</i> , <b>2011</b> , 17, 174-83	2.1	1
18	Computational study of the free energy landscape of the miniprotein CLN025 in explicit and implicit solvent. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 1440-9	3.4	11
17	Synthesis and docking studies of thiophene scaffolds in COX-2. <i>Arkivoc</i> , <b>2011</b> , 2011, 55-70	0.9	10
16	Molecular dynamics simulations of Ac-3Aib-Cage-3Aib-NHMe. <i>Molecular Simulation</i> , <b>2010</b> , 36, 1035-1044		9



15	Conformational profile of bombesin assessed using different computational protocols. <i>Journal of Molecular Graphics and Modelling</i> , <b>2010</b> , 29, 581-90	2.8	1
14	Molecular dynamics (MD) simulations of VIP and PACAP27. <i>Biopolymers</i> , <b>2009</b> , 91, 391-400	2.2	6
13	Cycloaddition reactions of cross-conjugated enaminones. <i>Tetrahedron</i> , <b>2009</b> , 65, 8478-8485	2.4	22
12	Conformational study of the PCU cage mono-peptide: a key role of some force-field parameters. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 5234-8	3.4	
11	Determination of lead and cadmium in seawater by differential pulse anodic stripping voltammetry: fit-for-purpose partial validation and internal quality aspects. <i>Analytical and Bioanalytical Chemistry</i> , <b>2008</b> , 392, 277-86	4.4	2
10	Trishomocubane amino acid as a beta-turn scaffold. <i>Chemical Biology and Drug Design</i> , <b>2008</b> , 71, 125-30	2.9	20
9	A molecular dynamics study of the pentacyclo-undecane (PCU) cage polypeptides of the type Ac-3Ala-Cage-3Ala-NHMe. <i>Molecular Simulation</i> , <b>2007</b> , 33, 1105-1108	2	6
8	Analysis of the conformational profile of trishomocubane amino acid dipeptide. <i>Biopolymers</i> , <b>2006</b> , 81, 339-49	2.2	15
7	A theoretical study of pentacyclo-undecane cage peptides of the type [Ac-X-Y-NHMe]. <i>Journal of Peptide Science</i> , <b>2006</b> , 12, 92-105	2.1	21
6	Simulated annealing study of the pentacyclo-undecane cage amino acid tripeptides of the type [Ac-X-Y-Z-NHMe]. <i>Computational and Theoretical Chemistry</i> , <b>2006</b> , 759, 145-157		12
5	A molecular dynamics study of the pentacyclo-undecane cage amino acid tripeptide. <i>Computational and Theoretical Chemistry</i> , <b>2006</b> , 770, 221-228		8
4	Conformational analysis of small peptides of the type Ac-X-NHMe, where X=Gly, Ala, Aib and Cage. <i>Computational and Theoretical Chemistry</i> , <b>2005</b> , 731, 127-137		26
3	Computational study of the conformational preferences of the (R)-8-amino-pentacyclo[5.4.0.0(2,6).0(3,10).0(5,9)]undecane-8-carboxylic acid mono-peptide. <i>Journal of Peptide Science</i> , <b>2004</b> , 10, 274-84	2.1	18
2	Functionalized Electrochemical Aptasensor for Sensing of Ochratoxin A in Cereals Supported by in Silico Adsorption Studies. <i>ACS Food Science &amp; Technology</i> ,		1
1	CHAPTER 1: Perspective on Analytical Sciences and Nanotechnology. <i>RSC Detection Science</i> , 1-34	0.4	5