# R Rajasekaran

List of Publications by Year
in descending order

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| 97 | 1,118 | 471061 | 525886 |
|---|---|---|---|
| papers | citations | 17 h-index | 27 g-index |

| 97 | 97 | 97 | 1233 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Identification and in silico analysis of functional SNPs of the BRCA1 gene. Genomics, 2007, 90, 447-452. | 1.3 | 73 |
| 2 | Alpha-Synuclein Aggregation in Parkinson's Disease. Frontiers in Medicine, 2021, 8, 736978. | 1.2 | 58 |
| 3 | Studies on flexibility and binding affinity of Asp25 of HIV-1 protease mutants. International Journal of Biological Macromolecules, 2008, 42, 386-391. | 3.6 | 49 |
| 4 | A novel computational and structural analysis of nsSNPs in CFTR gene. Genomic Medicine, 2008, 2, 23-32. | 0.6 | 48 |
| 5 | Computational investigation of curcumin, a natural polyphenol that inhibits the destabilization and the aggregation of human SOD1 mutant (Ala4Val). RSC Advances, 2016, 6, 102744-102753. | 1.7 | 46 |
| 6 | Applications of computational algorithm tools to identify functional SNPs. Functional and Integrative Genomics, 2008, 8, 309-316. | 1.4 | 43 |
| 7 | Computational and Structural Investigation of Deleterious Functional SNPs in Breast Cancer BRCA2 Gene. Shengwu Gongcheng Xuebao/Chinese Journal of Biotechnology, 2008, 24, 851-856. | 0.2 | 39 |
| 8 | Comparative binding of kaempferol and kaempferide on inhibiting the aggregate formation of mutant (G85R) SOD1 protein in familial amyotrophic lateral sclerosis: A quantum chemical and molecular mechanics study. BioFactors, 2018, 44, 431-442. | 2.6 | 37 |
| 9 | Effect of deleterious nsSNP on the HER2 receptor based on stability and binding affinity with herceptin: A computational approach. Comptes Rendus - Biologies, 2008, 331, 409-417. | 0.1 | 33 |
| 10 | Probing the inhibitory activity of epigallocatechin-gallate on toxic aggregates of mutant (L84F) SOD1 protein through geometry based sampling and steered molecular dynamics. Journal of Molecular Graphics and Modelling, 2017, 74, 288-295. | 1.3 | 33 |
| 11 | Exploring the Cause of Oseltamivir Resistance Against Mutant H274Y Neuraminidase by Molecular Simulation Approach. Applied Biochemistry and Biotechnology, 2012, 167, 237-249. | 1.4 | 26 |
| 12 | Quantum chemical and molecular mechanics studies on the assessment of interactions between resveratrol and mutant SOD1 (G93A) protein. Journal of Computer-Aided Molecular Design, 2018, 32, 1347-1361. | 1.3 | 25 |
| 13 | Spectroscopic, Computational, Antimicrobial, DNA Interaction, In Vitro Anticancer and Molecular Docking Properties of Biochemically Active Cu(II) and Zn(II) Complexes of Pyrimidine-Ligand. Journal of Fluorescence, 2018, 28, 975-985. | 1.3 | 25 |
| 14 | Phenytoin-Bovine Serum Albumin interactions - modeling plasma protein â€“ drug binding: A multi-spectroscopy and in silico-based correlation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 193, 523-527. | 2.0 | 22 |
| 15 | Gramicidin Peptide to Combat Antibiotic Resistance: A Review. International Journal of Peptide Research and Therapeutics, 2020, 26, 191-199. | 0.9 | 20 |
| 16 | A Systematic and Comprehensive Review on Disease-Causing Genes in Amyotrophic Lateral Sclerosis. Journal of Molecular Neuroscience, 2020, 70, 1742-1770. | 1.1 | 20 |
| 17 | Cysteine to Serine Conversion at 111th Position Renders the Disaggregation and Retains the Stabilization of Detrimental SOD1 A4V Mutant Against Amyotrophic Lateral Sclerosis in Humanâ€”A Discrete Molecular Dynamics Study. Cell Biochemistry and Biophysics, 2018, 76, 231-241. | 0.9 | 19 |
| 18 | A systematic molecular dynamics approach to the structural characterization of amyloid aggregation propensity of Î²2-microglobulin mutant D76N. Molecular BioSystems, 2016, 12, 850-859. | 2.9 | 18 |

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|---|---|---|---|
| 19 | Exploring the cause of aggregation and reduced Zn binding affinity by G85R mutation in SOD1 rendering amyotrophic lateral sclerosis. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1276-1286. | 1.5 | 18 |
| 20 | Identification and structural comparison of deleterious mutations in nsSNPs of ABL1 gene in chronic myeloid leukemia: A bio-informatics study. Journal of Biomedical Informatics, 2008, 41, 607-612. | 2.5 | 17 |
| 21 | Identification of Potential Inhibitors of H5N1 Influenza A Virus Neuraminidase by Ligand-Based Virtual Screening Approach. Cell Biochemistry and Biophysics, 2013, 66, 657-669. | 0.9 | 16 |
| 22 | Molecular binding response of naringin and naringenin to H46R mutant SOD1 protein in combating protein aggregation using density functional theory and discrete molecular dynamics. Progress in Biophysics and Molecular Biology, 2019, 145, 40-51. | 1.4 | 15 |
| 23 | In silico analysis of drug-resistant mutant of neuraminidase (N294S) against oseltamivir. Protoplasma, 2013, 250, 197-207. | 1.0 | 14 |
| 24 | Computational investigation of the human SOD1 mutant, Cys146Arg, that directs familial amyotrophic lateral sclerosis. Molecular BioSystems, 2017, 13, 1495-1503. | 2.9 | 14 |
| 25 | In Silico Analysis of Prion Protein Mutants: A Comparative Study by Molecular Dynamics Approach. Cell Biochemistry and Biophysics, 2013, 67, 1307-1318. | 0.9 | 13 |
| 26 | Detailed computational analysis revealed mutation V210I on PrP induced conformational conversion on Î²2â€“Î±2 loop and Î±2â€“Î±3. Molecular BioSystems, 2016, 12, 3223-3233. | 2.9 | 13 |
| 27 | Computational simulation analysis on human SOD1 mutant (H80R) exposes the structural destabilization and the deviation of Zn binding that directs familial amyotrophic lateral sclerosis. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2645-2653. | 2.0 | 13 |
| 28 | Investigation of structural stability and functionality of homodimeric gramicidin towards peptideâ€based drug: a molecular simulation approach. Journal of Cellular Biochemistry, 2019, 120, 4903-4911. | 1.2 | 13 |
| 29 | In silico analysis of structural and functional consequences in p16INK4A by deleterious nsSNPs associated CDKN2A gene in malignant melanoma. Biochimie, 2008, 90, 1523-1529. | 1.3 | 12 |
| 30 | In Silico Identification of Significant Detrimental Missense Mutations of EGFR and Their Effect with 4-Anilinoquinazoline-Based Drugs. Applied Biochemistry and Biotechnology, 2010, 160, 1723-1733. | 1.4 | 12 |
| 31 | Structural characterization of disease-causing mutations on SAP and the functional impact on the SLAM peptide: a molecular dynamics approach. Molecular BioSystems, 2014, 10, 1869. | 2.9 | 12 |
| 32 | Exploring the cause of drug resistance by the detrimental missense mutations in KIT receptor: computational approach. Amino Acids, 2010, 39, 651-660. | 1.2 | 11 |
| 33 | Prioritization of candidate SNPs in colon cancer using bioinformatics tools: An alternative approach for a cancer biologist. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 320-346. | 2.2 | 11 |
| 34 | Exploring the structural and functional effect of pRB by significant nsSNP in the coding region of RB1 gene causing retinoblastoma. Science China Life Sciences, 2010, 53, 234-240. | 2.3 | 11 |
| 35 | Computational Resources for Designing Peptide Based Drugs Preferred in the Field of Nanomedicine. Journal of Bionanoscience, 2016, 10, 1-14. | 0.4 | 11 |
| 36 | Rational design of linear tripeptides against the aggregation of human mutant SOD1 protein causing amyotrophic lateral sclerosis. Journal of the Neurological Sciences, 2019, 405, 116425. | 0.3 | 11 |

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|---|---|---|---|
| 37 | Selection of effective and highly thermostable Bacillus subtilis lipase A template as an industrial biocatalyst-A modern computational approach. Frontiers in Biology, 2015, 10, 508-519. | 0.7 | 10 |
| 38 | Analysis of the Structural Stability Among Cyclotide Members Through Cystine Knot Fold that Underpins Its Potential Use as a Drug Scaffold. International Journal of Peptide Research and Therapeutics, 2017, 23, 1-11. | 0.9 | 10 |
| 39 | Inâ€Silico Template Selection of Inâ€Vitro Evolved Kalata B1 of Oldenlandia Affinis for Scaffolding Peptideâ€Based Drug Design. Journal of Cellular Biochemistry, 2016, 117, 66-73. | 1.2 | 9 |
| 40 | In silico approach to explore the disruption in the molecular mechanism of human hyaluronidase 1 by mutant E268K that directs Natowicz syndrome. European Biophysics Journal, 2017, 46, 157-169. | 1.2 | 9 |
| 41 | Exploration of Structural and Functional Variations Owing to Point Mutations in Î±-NAGA. Interdisciplinary Sciences, Computational Life Sciences, 2018, 10, 81-92. | 2.2 | 9 |
| 42 | Structural distortions due to missense mutations in human formylglycine-generating enzyme leading to multiple sulfatase deficiency. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3575-3585. | 2.0 | 9 |
| 43 | Computational Investigation on Electrostatic Loop Mutants Instigating Destabilization and Aggregation on Human SOD1 Protein Causing Amyotrophic Lateral Sclerosis. Protein Journal, 2019, 38, 37-49. | 0.7 | 8 |
| 44 | Effect of Î²-cyclodextrin-EGCG complexion against aggregated a-synuclein through density functional theory and discrete molecular dynamics. Chemical Physics Letters, 2019, 717, 38-46. | 1.2 | 8 |
| 45 | Design, synthesis and exploration of in silico Î±-amylase and Î±-glucosidase binding studies of pyrrolidine-appended quinoline-constrained compounds. Research on Chemical Intermediates, 2020, 46, 1869-1880. | 1.3 | 8 |
| 46 | TTRMDB: A database for structural and functional analysis on the impact of SNPs over transthyretin (TTR) using bioinformatic tools. Computational Biology and Chemistry, 2020, 87, 107290. | 1.1 | 8 |
| 47 | Could Dermaseptin Analogue be a Competitive Inhibitor for ACE2 Towards Binding with Viral Spike Protein Causing COVID19?: Computational Investigation. International Journal of Peptide Research and Therapeutics, 2021, 27, 1043-1056. | 0.9 | 8 |
| 48 | Deciphering the loss of metal binding due to mutation D83G of human SOD1 protein causing FALS disease. International Journal of Biological Macromolecules, 2018, 107, 521-529. | 3.6 | 7 |
| 49 | Identification of protegrin-1 as a stable and nontoxic scaffold among protegrin family â€“ a computational approach. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2430-2439. | 2.0 | 7 |
| 50 | Analysis of binding residues between scorpion neurotoxins and D2 dopamine receptor: A computational docking study. Computers in Biology and Medicine, 2008, 38, 1056-1067. | 3.9 | 6 |
| 51 | In Silico Searching for Disease-Associated Functional DNA Variants. Methods in Molecular Biology, 2011, 760, 239-250. | 0.4 | 6 |
| 52 | Computational analysis of deleterious missense mutations in aspartoacylase that cause Canavanâ€™s disease. Science China Life Sciences, 2012, 55, 1109-1119. | 2.3 | 6 |
| 53 | In silico analysis of detrimental mutations in ADD domain of chromatin remodeling protein ATRX that cause ATR-X syndrome: X-linked disorder. Network Modeling Analysis in Health Informatics and Bioinformatics, 2013, 2, 123-135. | 1.2 | 5 |
| 54 | A theoretical study on Zn binding loop mutants instigating destabilization and metal binding loss in human SOD1 protein. Journal of Molecular Modeling, 2017, 23, 103. | 0.8 | 5 |

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|---|---|---|---|
| 55 | Molecular mechanics and quantum chemical calculations unveil the combating effect of baicalein on human islet amyloid polypeptide aggregates. Molecular Simulation, 2019, 45, 1538-1548. | 0.9 | 5 |
| 56 | Synthesis and exploration of in-silico and in-vitro Î±-glucosidase and Î±-amylase inhibitory activities of N-(3-acetyl-2-methyl-4-phenylquinolin-6-yl)arylamides. Journal of the Iranian Chemical Society, 2019, 16, 1071-1080. | 1.2 | 5 |
| 57 | A Review on Bioactive Porcine Peptide, Protegrin-1. International Journal of Peptide Research and Therapeutics, 2020, 26, 1493-1501. | 0.9 | 5 |
| 58 | Investigating the pernicious effects of heparan sulfate in serum amyloid A1 protein aggregation: a structural bioinformatics approach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1776-1790. | 2.0 | 5 |
| 59 | Probing the polyphenolic flavonoid, morin as a highly efficacious inhibitor against amyloid(A4V) mutant SOD1 in fatal amyotrophic lateral sclerosis. Archives of Biochemistry and Biophysics, 2022, 727, 109318. | 1.4 | 5 |
| 60 | In Silico Identification and Analysis of Drug Resistant Mutants of ABL Tyrosine Kinase Based on Detrimental Missense Mutations. Current Signal Transduction Therapy, 2011, 6, 396-404. | 0.3 | 4 |
| 61 | Computational Identification of Significant Missense Mutations in AKT1 Gene. Cell Biochemistry and Biophysics, 2014, 70, 957-965. | 0.9 | 4 |
| 62 | Influence of pleasant and unpleasant music on cardiovascular measures and task performance. International Journal of Biomedical Engineering and Technology, 2016, 21, 128. | 0.2 | 4 |
| 63 | Unraveling the Deleterious Effects of Cancer-Driven STK11 Mutants through Conformational Sampling Approach. Cancer Informatics, 2016, 15, CIN.S38044. | 0.9 | 4 |
| 64 | Unraveling the molecular effects of mutation L270P on Wiskkotâ€“Aldrich syndrome protein: insights from molecular dynamics approach. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2011-2022. | 2.0 | 4 |
| 65 | Structural Stability Among Hybrid Antimicrobial Peptide Cecropin A(1â€“8)â€“Magainin 2(1â€“12) and Its Analogues: A Computational Approach. Journal of Cluster Science, 2017, 28, 2549-2563. | 1.7 | 4 |
| 66 | Deciphering the Molecular Effects of Mutations on ATRX Cause ATRX Syndrome: A Molecular Dynamics Study. Journal of Cellular Biochemistry, 2017, 118, 3318-3327. | 1.2 | 4 |
| 67 | Hydrophobic Residues Confer the Helicity and Membrane Permeability of Ocellatin-1 Antimicrobial Peptide Scaffold Towards Therapeutics. International Journal of Peptide Research and Therapeutics, 2021, 27, 2459-2470. | 0.9 | 4 |
| 68 | Enhancement of Task Performance Aided by Music. Current Science, 2016, 111, 1794. | 0.4 | 4 |
| 69 | Decoding Conformational Imprint of Convoluted Molecular Interactions Between Prenylflavonoids and Aggregated Amyloid-Beta42 Peptide Causing Alzheimerâ€™s Disease. Frontiers in Chemistry, 2021, 9, 753146. | 1.8 | 4 |
| 70 | Probing the competitive inhibitor efficacy of frog-skin alpha helical AMPs identified against ACE2 binding to SARS-CoV-2 S1 spike protein as therapeutic scaffold to prevent COVID-19. Journal of Molecular Modeling, 2022, 28, 128. | 0.8 | 4 |
| 71 | Investigations on the interactions of scorpion neurotoxins with the predicted structure of D1 dopamine receptor by proteinâ€“protein docking method. A bioinformatics approach. Comptes Rendus - Biologies, 2008, 331, 489-499. | 0.1 | 3 |
| 72 | Computational identification and structural analysis of deleterious functional SNPs in MLL gene causing acute leukemia. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 247-255. | 2.2 | 3 |

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|---|---|---|---|
| 73 | Predicting Therapeutic Template by Evaluating the Structural Stability of Anti-Cancer Peptidesâ€"A Computational Approach. International Journal of Peptide Research and Therapeutics, 2011, 17, 31-38. | 0.9 | 3 |
| 74 | Geometric Simulation Approach for Grading and Assessing the Thermostability of CALBs. Biochemistry Research International, 2016, 2016, 1-7. | 1.5 | 3 |
| 75 | Identification of Effective Dimeric Gramicidin-D Peptide as Antimicrobial Therapeutics over Drug Resistance: In-Silico Approach. Interdisciplinary Sciences, Computational Life Sciences, 2019, 11, 575-583. | 2.2 | 3 |
| 76 | Hydrogen bonds in anoplin peptides aid in identification of a structurally stable therapeutic drug scaffold. Journal of Molecular Modeling, 2020, 26, 155. | 0.8 | 3 |
| 77 | Unravelling the molecular effect of ocellatin-1, F1, K1 and S1, the frog-skin antimicrobial peptides to enhance its therapeuticsâ€"quantum and molecular mechanical approaches. Journal of Molecular Modeling, 2021, 27, 10. | 0.8 | 3 |
| 78 | Assortment of Tachystatin B of Tachypleus tridentatus as a Stable Scaffold in Antifungal Peptide Design. Trends in Bioinformatics, 2016, 9, 14-22. | 0.3 | 3 |
| 79 | Computational detection of deleterious SNPs and their effect on sequence and structural level of the VHL gene. Mammalian Genome, 2008, 19, 654-661. | 1.0 | 2 |
| 80 | The structural and functional reliability of Circulins of Chassalia parvifolia for peptide therapeutic scaffolding. Journal of Cellular Biochemistry, 2018, 119, 3999-4008. | 1.2 | 2 |
| 81 | In silico study on pH-based alanine scanning of Phylloseptin-2 helps determine potential mutant sites for futuristic therapeutic analogues. Molecular Simulation, 2020, 46, 1084-1093. | 0.9 | 2 |
| 82 | Molecular simulation unravels the amyloidogenic misfolding of nascent ApoA1 protein, driven by deleterious point mutations occurring in between 170â€"178 hotspot region. Journal of Biomolecular Structure and Dynamics, 2021, , 1-13. | 2.0 | 2 |
| 83 | A Review On Huntington Protein: Insight Into Protein Aggregation and Therapeutic Interventions. Current Drug Metabolism, 2022, 23, 260-282. | 0.7 | 2 |
| 84 | Exploring the Structural Stability of a Potential Antifungal Peptide Through Computational Analysis. Protein and Peptide Letters, 2009, 16, 1386-1392. | 0.4 | 1 |
| 85 | Application of Molecular Mechanics and Molecular Dynamics for Investigating the Detrimental Missense Mutations in Tumor Suppressor Protein SMAD4. Journal of Bionanoscience, 2009, 3, 80-87. | 0.4 | 1 |
| 86 | In Silico Template Selection of Short Antimicrobial Peptide Viscotoxin for Improving Its Antimicrobial Efficiency in Development of Potential Therapeutic Drugs. Applied Biochemistry and Biotechnology, 2017, 181, 898-913. | 1.4 | 1 |
| 87 | Identification of therapeutic peptide scaffold from tritrpticin family for urinary tract infections using in silico techniques. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4407-4417. | 2.0 | 1 |
| 88 | In Silico Therapeutic Peptide Design Against Pathogenic Domain Swapped Human Cystatin C Dimer. International Journal of Peptide Research and Therapeutics, 2021, 27, 1555-1575. | 0.9 | 1 |
| 89 | Molecular simulation probes the potency of resveratrol in regulating the toxic aggregation of mutant V30M TTR fibrils in Transthyretin mediated amyloidosis. Journal of Molecular Graphics and Modelling, 2022, 110, 108055. | 1.3 | 1 |
| 90 | Computational Evaluation of a Prospective Antimicrobial Peptide for Application in Nanomedicine. Journal of Computational and Theoretical Nanoscience, 2009, 6, 629-634. | 0.4 | 0 |

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|---|---|---|---|
| 91 | Comparative Binding Analysis of Monoclonal Antibodies Against Native and Mutant Type in ErbB2 Receptor: A Theoretical Modeling Approach. Current Pharmaceutical Biotechnology, 2009, 10, 701-708. | 0.9 | 0 |
| 92 | A computational approach to explore the functional missense mutations in the spindle check point protein Mad1. Frontiers in Biology, 2013, 8, 618-625. | 0.7 | 0 |
| 93 | In silico prediction of functional loss of cst3 gene in hereditary cerebral amyloid angiopathy. Bangladesh Journal of Pharmacology, 2013, 8, . | 0.1 | 0 |
| 94 | Computational Investigation to Explore the Detrimental Missense Mutations in Bruton's Tyrosine Kinase Aiding Nanotechnology Based Targeted Drug Delivery. Journal of Bionanoscience, 2015, 9, 281-291. | 0.4 | 0 |
| 95 | <I>In Silico</I> Analysis of Detrimental Missense Mutations in p110Î± That Cause Cancer. Journal of Bionanoscience, 2013, 7, 679-686. | 0.4 | 0 |
| 96 | Molecular Mechanics Approach of Leukodystrophy Causing E285A Mutation in Aspartoacylase Directs the Future Implementation of Nanomechanics. Journal of Bionanoscience, 2016, 10, 110-117. | 0.4 | 0 |
| 97 | Identifying the Deleterious Effects of Cancer Driven Mad1, BRAF and STK11 Mutants Through Conformational Sampling Approach. Journal of Bionanoscience, 2018, 12, 109-118. | 0.4 | 0 |