

Department of Chemistry

Dr. Deepti Goyal

Research Project-

- Name of the Project: Design, Synthesis and Evaluation of Modified Short Peptides as Inhibitors of Amyloid- β ($A\beta$) Peptide Aggregation
- Year of Award: 2015
- Funds provided: 24.4 Lakhs
- Duration of the project: 3 years
- Funding Agency: SERB-DST

Research Publications

Research Papers Published in International/National Journals:

Sr. No	Name of Author	Title of paper	Name of Journal	Year	ISBN/ISSN No.
1.	Anupamjeet Kaur, Suniba Shuaib, Deepti Goyal, Bhupesh Goyal	Interactions of a Multifunctional Di-Triazole Derivative with Alzheimer's $A\beta_{42}$ Monomer and $A\beta_{42}$ Protofibril: A Systematic Molecular Dynamics Study.	Physical Chemistry Chemical Physics, Vol. 22, Pg. No.1543	2020	463-9076 (print); 1463-9084 (web)
2.	Amandeep Kaur, A., Simranjeet Singh Narang, Anupamjeet Kaur, Sukhmani Mann, Nitesh Priyadarshi, Bhupesh Goyal, Nitin Kumar Singhal, Deepti Goyal	Multifunctional Mono-Triazole Derivatives Inhibit $A\beta_{42}$ Aggregation and Cu^{2+} -Mediated $A\beta_{42}$ Aggregation and Protect Against $A\beta_{42}$ -Induced Cytotoxicity.	Chemical Research in Toxicology, Vol.32, Pg. No.1824	2019	0893-228X (print) 1520-5010 (web)
3.	Sambasivarao Kotha, Arjun Shankar Chavan, A. Deepti Goyal	Diversity-Oriented Approaches to Polycycles and Heterocycles via Enyne Metathesis and Diels-Alder Reaction as Key Steps.	ACS Omega, Vol.4, Pg. No.22261	2019	2470-1343 (print) 2470-1343 (web)
4.	Simranjeet Singh Narang, Deepti Goyal, Bhupesh Goyal	Molecular Insights into the Inhibitory Mechanism of Bi-Functional Bis-	Amino acids, Vol.51, Pg. No.1593	2019	0939-4451 (Print) 1438-2199 (Online)

		Tryptoline Triazole Against β -Secretase (BACE1) Enzyme.			
5.	Anupamjeet Kaur, Sukhmani Mann, Amandeep Kaur, Nitesh Priyadarshi, Bhupesh Goyal, Nitin Kumar Singhal, Deepti Goyal	Multi-target-directed Triazole Derivatives as Promising Agents for the Treatment of Alzheimer's Disease.	Bioorganic Chemistry, Vol.87, Pg. No.572	2019	0045-2068
6.	Simranjeet SinghNarang, Suniba Shuaib, Deepti Goyal, Bhupesh Goyal	In Silico-Guided Identification of Potential Inhibitors Against β_2m Aggregation in Dialysis-Related Amyloidosis.	J. Biomolecular Structure & Dynamics, doi: 10.1080/07391102.2019.1668852	2019	1538-0254
7.	Simranjeet Singh Narang, Deepti Goyal, Bhupesh Goyal	Inhibition of Alzheimer's Amyloid- β_{42} Peptide Aggregation by a Bi-functional Bis-Tryptoline Triazole: Key Insights from Molecular Dynamics Simulations..	J. Biomolecular Structure & Dynamics, doi.org/10.1080/07391102.2019.1614093	2019	1538-0254
8.	Suniba Shuaib, Rajneet Kaur Saini, Deepti Goyal, Bhupesh Goyal	Impact of K16A and K28A Mutation on the Structure and Dynamics of Amyloid- β_{42} Peptide in Alzheimer's Disease: Key Insights from Molecular Dynamics Simulations.	J. Biomolecular Structure & Dynamics, doi.org/10.1080/07391102.2019.1586587	2019	1538-0254
9.	Suniba Shuaib, Simranjeet Singh Narang, Deepti Goyal, Bhupesh Goyal	Computational Design and Evaluation of β -Sheet Breaker Peptides for Destabilizing Alzheimer's Amyloid- β_{42} Protofibrils.	J. Cellular Biochemistry, doi:10.1002/jcb.29061	2019	1097-4644
10.	Rajneet Kaur Saini, Suniba Shuaib, Deepti Goyal, Bhupesh Goyal	Insights into the Inhibitory Mechanism of a Resveratrol and Clioquinol Hybrid against $A\beta_{42}$ Aggregation and Protofibril Destabilization: A Molecular Dynamics Simulation Study.	J. Biomolecular Structure & Dynamics, Vol.37, Pg. No.3183	2019	1538-0254
11.	Deepti Goyal,	Benzofuran and Indole:	Chem Med Chem,	2018	1860-7187

	Amandeep Kaur, Bhupesh Goyal	A Promising Scaffold for Drug Development in Alzheimer's Disease.	Vol.13, Pg. No.1275		
12.	Rajneet Kaur Saini, Suniba Shuaib, Deepti Goyal, Bhupesh Goyal	Molecular Insights into the Effect L17A/F19A Double Mutation on the Structure and Dynamics of A β 40: A Molecular Dynamics Simulation Study.	J. Cellular Biochemistry, Vol.119, Pg. No.8949	2018	1097-4644
13.	Simranjeet Singh Narang, Suniba Shuaib, Deepti Goyal, Bhupesh Goyal	Assessing the Effect of D59P Mutation in the DE Loop Region in Amyloid Aggregation Propensity of β 2-Microglobulin: A Molecular Dynamics Simulation Study.	J. Cellular Biochemistry, Vol.119, Pg. No.782	2018	1097-4644
14.	Suniba Shuaib, Rajneet Kaur Saini, Deepti Goyal, Bhupesh Goyal	Insights into the Inhibitory Mechanism of Dicyanovinyl-Substituted J147 Derivative against A β 42 Aggregation and Protofibril Destabilization: A Molecular Dynamics Simulation Study.	ChemistrySelect, Vol.2, Pg. No.1645	2017	2365-6549
15.	Deepti Goyal, Suniba Suniba, Sukhmani Mann, Bhupesh Goyal	Rationally Designed Peptides and Peptidomimetics as Inhibitors of Amyloid- β (A β) Aggregation: Potential Therapeutics of Alzheimer's Disease.	ACS Combinatorial Science, Vol.19, Pg. No.55	2017	2156-8952
16.	Anupamjeet Kaur, Sukhmani Mann, Bhupesh Goyal, Bhupinder Pal, Deepti Goyal	CuO Nanostructures of Variable Shapes as an Efficient Catalyst for [3+2] Cycloaddition of Azides with Terminal Alkyne.	RSC Advances, Vol.6, Pg. No.102733	2016	2046-2069
17.	Sambasivarao Kotha Arjun S. Chavan and Deepti Goyal	Diversity-Oriented Approaches to Polycyclics and Bioinspired Molecules via the Diels–Alder Strategy: Green Chemistry, Synthetic Economy, and Beyond	ACS Combinatorial Science, Vol.17, Pg. No.253	2015	1520-4766