(12) PATENT APPLICATION PUBLICATION
(19) INDIA
(22) Date of filing of Application :20/10/2022

(21) Application No.202231060095 A
(43) Publication Date : 04/11/2022

(54) Title of the invention : Computational approaches in altering the inhibition of Acetylcholinesterase Receptor in Alzheimer's disease treatment using Geranylgeraniol

(51) International classification :A61P0025280000, G16C0020500000, G16C0010000000, G16B0005000000, G16B0015300000
(86) International Application No :PCT//
Filing Date :01/01/1900
(87) International Publication No : NA
(61) Patent of Addition to Application Number :NA
Filing Date :NA
(62) Divisional to Application Number :NA
Filing Date :NA

(71)**Name of Applicant :**
1)Dr. Arabinda Ghosh
Address of Applicant :Assistant Professor Microbiology Division, Department of Botany, Gauhati University, Guwahati, Pin: 781014 Assam India ---------- ----------
2)Dr. Athanasios Alexiou
3)Mr. Nobendu Mukerjee
4)Mr. Somdatta Yashwant Chaudhari
5)Mr. Devesh Sharma
6)Vivek Digamber Rathod
7)Mr. Sandip Shrikishan Kshirsagar
8)Javed Ahmad Rais Ahmad Shaikh
9)Ms. Prapti Victoria Rozario
10)Mr. Bikram Dhara
Name of Applicant : NA
Address of Applicant : NA
(72)**Name of Inventor :**
1)Dr. Arabinda Ghosh
Address of Applicant :Assistant Professor Microbiology Division, Department of Botany, Gauhati University, Guwahati, Pin: 781014 Assam India ---------- ----------
2)Dr. Athanasios Alexiou
Address of Applicant :Assistant Professor Department of Science and Engineering, Novel Global Community Educational Foundation, Australia ---------- ----------
3)Mr. Nobendu Mukerjee
Address of Applicant :Student Department of Microbiology, West Bengal State University, Kolkata 700126 West Bengal India ---------- ----------
4)Mr. Somdatta Yashwant Chaudhari
Address of Applicant :Assistant Professor Department of Pharmaceutical Chemistry, P. E. S. Modern College of Pharmacy, Yamunanagar, Nigdi, Pin: 411044 Pune India ---------- ----------
5)Mr. Devesh Sharma
Address of Applicant :PhD Scholar Department of Biochemistry ICMR - National JALMA Institute for Leprosy & Other Mycobacterial Diseases, Agra (UP) Pin: 282001 Uttar Pradesh India ---------- ----------
6)Vivek Digamber Rathod
Address of Applicant :Assistant Professor Department of Chemical Technology, Dr Babasaheb Ambedkar Marathwada University Aurangabad Pin: 431004 Maharashtra India ---------- ----------
7)Mr. Sandip Shrikishan Kshirsagar
Address of Applicant :Assistant Professor Department of Pharmaceutical Chemistry, Dr. D. Y. Patil College of Pharmacy, Akurdi, Pune, Pin: 411044 Maharashtra India ---------- ----------
8)Javed Ahmad Rais Ahmad Shaikh
Address of Applicant :Assistant Professor Dept of Pharmacology Shastry Institute of Pharmacy, C/O- Dr. Firoz Shaikh, House no -2229, Sayyed Wada, At/Po-Erandol, Dist-Jalgaon, Pin: 425109 Maharashtra India ---------- ----------
9)Ms. Prapti Victoria Rozario
Address of Applicant :Intern Department of Microbiology, St. Xavier's College (Autonomous), Kolkata Pin: 700016 West Bengal India ---------- ----------
10)Mr. Bikram Dhara
Address of Applicant :Senior Research Fellow Department of Microbiology St. Xavier's College (Autonomous), Kolkata Pin: 700016 West Bengal India ---------- ----------

(57) Abstract :
Computational approaches in altering the inhibition of Acetylcholinesterase Receptor in Alzheimer's disease treatment using Geranylgeraniol Abstract Acetylcholinesterase (AChE) inhibitors have recently become the standard way to treat Alzheimer's disease (AD). By increasing synaptic concentrations of acetylcholine and decreasing acetylcholine turnover, these drugs counteract the effects of the loss of cholinergic neurons. On the other hand, AD has only been linked to AChE in the past few years. In particular, it looks like AChE may have a direct effect on amyloid-beta, causing more of this peptide to build up into hard plaques. This new function makes it more likely that AChE inhibitors, if made carefully, could be used to cure diseases instead of just making people feel better. Several studies have also shown that the cholinergic modulation and other functional effects of AChE inhibition may affect how amyloid precursor protein is processed and protect neurons from different stressors. So, it makes sense that new AChE inhibitors that take advantage of all of these benefits could be useful in the future to treat AD. Molecular docking and molecular dynamics modelling were used to examine the effectiveness of the drugs against AChE receptor. Geranylgeraniol's primary interactions were anticipated with the help of molecular docking investigations. With a binding affinity of -9.7 kcal/mol, it was the most promising of the candidates. By making substantial contact with the active site, Geranylgeraniol ensured the complex's structural integrity was maintained throughout its rapid expansion. In light of these findings, further research into Geranylgeraniol's potential as a lead drug for AChE receptors is warranted.

No. of Pages : 11 No. of Claims : 10