



Library Indian Institute of Science Education and Research Mohali



DSpace@IISERMohali (/jspui/)

/ Publications of IISER Mohali (/jspui/handle/123456789/4)

/ Research Articles (/jspui/handle/123456789/9)


Please use this identifier to cite or link to this item: <http://hdl.handle.net/123456789/4483>

Title:	Pharmacophore-driven identification of N-methyl-D-receptor antagonists as potent neuroprotective agents validated using in vivo studies
Authors:	Jainarayanan, Ashwin K (/jspui/browse?type=author&value=Jainarayanan%2C+Ashwin+K)
Keywords:	Pharmacophore-driven N-methyl- D-receptor antagonists
Issue Date:	2021
Publisher:	Biology Methods and Protocols
Citation:	Biology Methods and Protocols, 5(1)
Abstract:	Alzheimer's disease (AD), apparently the most widespread reason behind dementia, is delineated by a continuous cognitive weakening in the aged. During its progression, N-methyl-D-aspartate receptor (NMDAR) antagonists are known to play a pivotal part in the mechanisms of learning and memory. Since there is an unmet medical need for the treatment of AD, we aim to identify possible chemical compounds targeted toward N-methyl-D-aspartate receptors. Three-dimensional models are developed to unveil some of the essential characteristics of the N-methyl-D-aspartate receptors by using a collection of already discovered N-methyl-D-aspartate receptor inhibitors. This is followed by virtual screening, which results in novel chemical compounds having the potential to inhibit N-methyl-D-aspartate receptors. Molecular docking studies and analysis promulgated two lead compounds with a high LibDock score. The compounds are shortlisted based on high estimated activity, fit values, LibDock score, no violation of Lipinski's, and availability for procuring. Finally, the shortlisted compounds are tested by employing in vivo studies, which we further propose as potential NMDA inhibitors for treating AD.
Description:	Only IISER Mohali authors are available in the record.
URI:	https://doi.org/10.1093/biomethods/bpaa013 (https://doi.org/10.1093/biomethods/bpaa013) http://hdl.handle.net/123456789/4483 (http://hdl.handle.net/123456789/4483)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need To Add...Full Text_PDF..pdf (/jspui/bitstream/123456789/4483/1/Need%20To%20Add%e2%80%a6Full%20Text_PDF..pdf)	Only IISER Mohali authors are available in the record.	15.36 kB	Adobe PDF	View/Open (/jspui/bitstream/123456789/4483/1/Need%20To%20Add%e2%80%a6Full%20Text_PDF..pdf)

Show full item record (</jspui/handle/123456789/4483?mode=full>)

 (</jspui/handle/123456789/4483/statistics>)

Items in DSpace are protected by copyright, with all rights reserved, unless otherwise indicated.