**Data on multiple post-translational modifications in Alzheimer's disease**

Sayali Chandrashekhar Deolankar, Shashanka G. Koyangana, Arun H. Patil #, Yashwanth Subbannayya, Prashant Kumar Modi, and T. S. Keshava Prasad \*

Center for Systems Biology and Molecular Medicine, Yenepoya Research Centre, Yenepoya (Deemed to be University), Mangalore, India.

# Current address: Department of Pathology, Division of Cardiovascular Pathology, Johns Hopkins University School of Medicine, 720 Rutland Avenue, Ross Rm 626, Baltimore, MD.

\* Correspondence: keshav@yenepoya.edu.in; Tel: +91-9972250102

**Received:** 9 February 2022; **Accepted:** 23 May 2022; **Published:** 10 June 2022

**Edited by:** Indranath Chatterjee (Tongmyong University, South Korea)

**Reviewed by:** Jhinuk Chatterjee (PES University, India); Lilach Soreq University College London, UK)

<https://doi.org/10.31117/neuroscirn.v5i2.153>

**Supplementary Methods**

Details about the selection of proteomics data source, search parameters for identification of PTMs and downstream analysis steps used by Deolankar et al., 2019.

(Title: Dissecting Alzheimer's Disease Molecular Substrates by Proteomics and Discovery of Novel Post-translational Modifications. DOI: 10.1089/omi.2019.0085)

* 1. **Data source**

|  |  |  |
| --- | --- | --- |
| MS/MS data source | ProteomeXchange Consortium | via the PRoteomics IDEntifications (PRIDE) repository |
| Search term | Species - | *Homo sapiens* |
| Experiment type | shotgun proteomics |
| Disease | Alzheimer’s |
| Method | label-free quantification |
| Selected Dataset Identifiers | PXD004010 (prefrontal cortical region) | PMID: 27225868 |
| PXD002516 (region unknown) | PMID: 26892330 |
| PXD004863 (CSF) | PMID: 28044435 |

* 1. **Database search parameters**

|  |  |
| --- | --- |
| MS/MS raw files Searched against | NCBI Human RefSeq (release 89) protein database |
| Proteome Discoverer (Version 2.2) search Algorithm | SEQUEST HT |
| PD Search parameters | full tryptic specificity |
| up to 1 missed cleavage |
| Carbamidomethylation of cysteine was specified as static modification |
| oxidation of methionine, acetylation of protein N-termini along with phosphorylation of serine, threonine and tyrosine, O-GluNAcetylation of asparagines, serine and threonine, methylation of lysine and arginine, acetylation of lysine and citrullination of arginine were set as variable modification |
| Mass error: precursor ion- 10 ppmfragment ions- 0.05 Da |
| The probability of site modification was estimated by ptmRS node |
| q-value was calculated by Percolator |
| FDR- 1% at the peptide level |
| Downstream/bioinformatics analysis and Comparison of resulting PTMs with other resources | PTM-Pro tool was used to profile high confidence PTMs |
| Website: https://ptm-pro.inhouseprotocols.com/ |
| ptmRS site probabity > 75% for each PTM |
| PhosphoSitePlus database (Accessed on: 11.11.2018) |
| STRAP software and GOrilla tool were used for GO annotations |
| Pathway enrichment through KEGG pathways and DAVID v6.8 |
| Intensity Based Absolute Quantification (iBAQ): *in house* Perl script (PTM-Pro v2.0) |