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Supplementary Material

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Machine Learning Neuroprotective Strategy Reveals a Unique Set of Parkinson Therapeutic Nicotine Analogs

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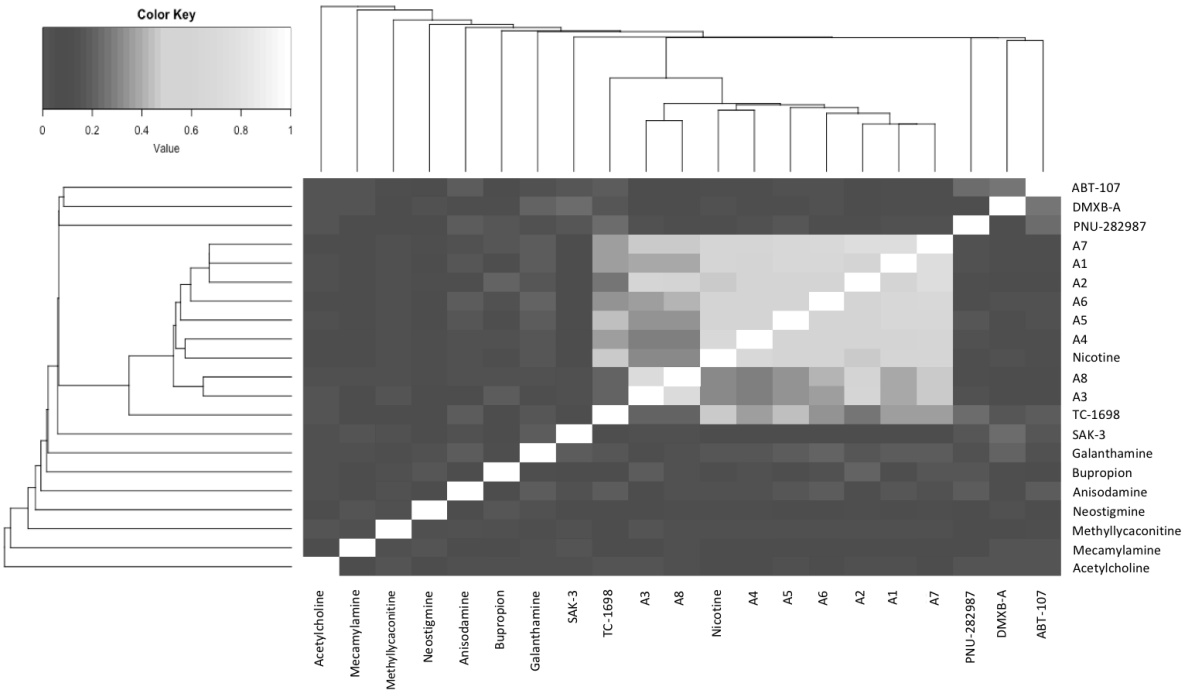
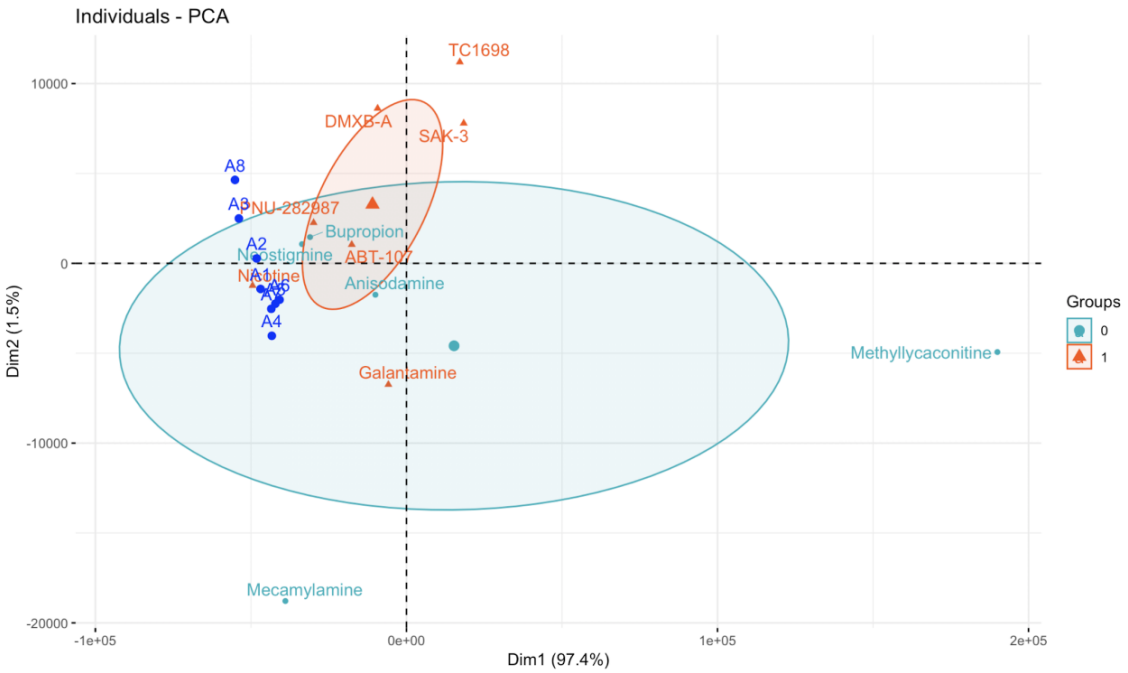
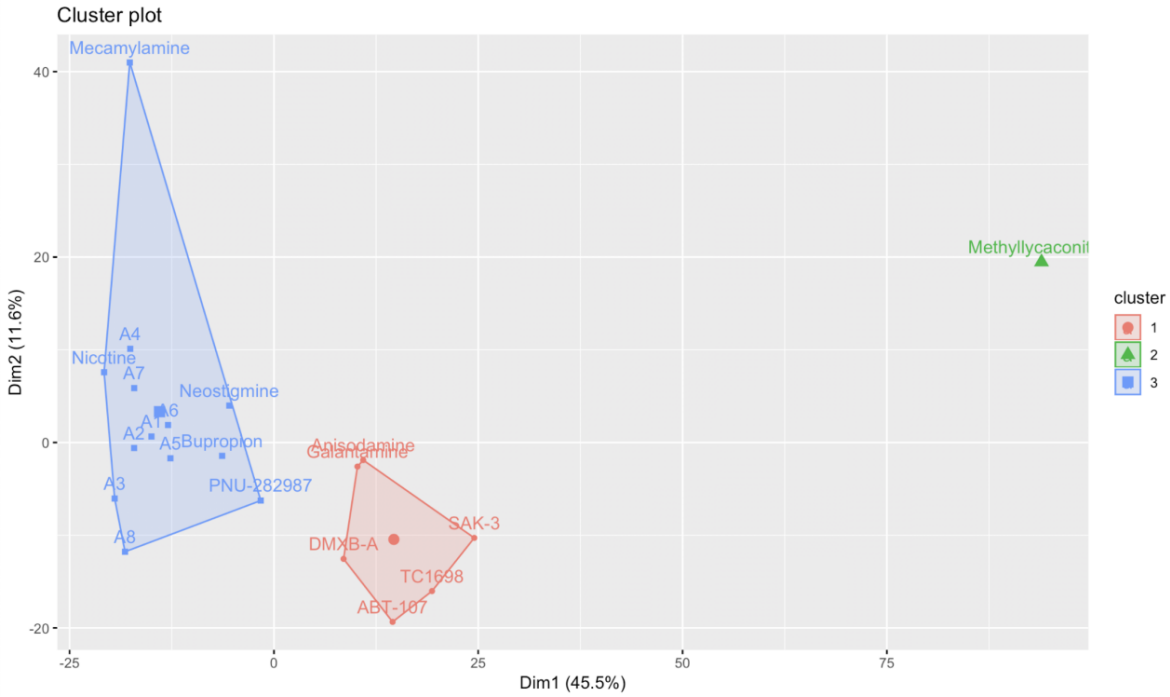
SUPPLEMENTARY FIGURES



Supplementary Fig. (1). Similarity of molecules related to their potential neuroprotective response. The central cluster of the heatmap contains the analogs of nicotine, nicotine and TC-1698, both related to a neuroprotective *in vitro* positive activity over α7 nAChR.



Supplementary Fig. (2). Principal component analysis of the manually curated dataset. 0 represents the antagonist function over the receptor (no neuroprotection) and 1 indicates the molecules related with a positive response of α7 nAChR and putative induction of PI3K/AKT Bcl-2.



Supplementary Fig. (3). K-mean analysis of the manually curated dataset. The number of clusters were set to be self-organized and the clusters tend to organize the molecules by the activity over the receptor.