**Appendix A.**

**Supplementary table 1:** GC-MS/MS detected phytoconstituents in the methanolic bark extract of *N. cadamba* and their binding energy with two AD receptor targets.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Compound. No** | **R.Time** | **Name of the compound** | **%**  **Peak** | **Binding Energy (K/cal)** | |
| **2LMN**  **(Aβ receptor)** | **3LII**  **(ACHE receptor)** |
|  | 3.267 | 2,2’-Bioxirane | 2.63 | -56.3 | -43.1 |
|  | 3.442 | Ethanol, 2-nitro-, propionate (ester) | 0.97 | -82.2 | -69.3 |
|  | 3.688 | L-Alanine, N-methoxycarbonyl-, methyl ester | 0.89 | -89.2 | -62.6 |
|  | 3.911 | 1,3,5-Pentanetriol | 0.62 | -66.4 | -60.6 |
|  | 4.357 | 7-Oxabicyclo[2.2.1]heptanes | 0.67 | -54.9 | -49.2 |
|  | 4.437 | Furfural | 1.44 | -61.7 | -63.8 |
|  | 4.883 | 2-Furanmethanol | 2.65 | -63.8 | -62.8 |
|  | 5.373 | 4-Cyclopenetene-1,3-doine | 0.84 | -64 | -51.7 |
|  | 6.251 | 2(3H)-Furanone, 5-methyl | 1.25 | -61.6 | -50.5 |
|  | 6.981 | Benzaldehyde | 3.96 | -69.3 | -50.4 |
|  | 7.226 | 2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one | 0.31 | -66.2 | -63.4 |
|  | 7.763 | Aniline | 1.70 | -66.6 | -47.9 |
|  | 7.983 | Formic acid, 2-propenyl ester | 2.03 | -54.1 | -50.9 |
|  | 9.351 | 2,5-Anhydro-1,6-dideoxyhexo-3,4-diulose | 2.56 | -52.9 | -52.2 |
|  | 9.613 | Phenol, 2-methoxy | 5.71 | -76.5 | -60.1 |
|  | 9.902 | 3-Buten-2-ol | 1.75 | -48.9 | -47.4 |
|  | 10.252 | 4H-Pyran-4-one, 3-hydroxy-2-methyl | 0.68 | -70.9 | -57.6 |
|  | 11.058 | 1,5-Anhydro-6-deoxyhexo-2,3-diulose | 5.56 | -68.8 | -61 |
|  | 11.561 | 2-Propenal, 3-(2-furanyl) | 0.84 | -78.8 | -55.9 |
|  | 12.011 | Benzoic acid | 4.19 | -70.8 | -48.9 |
|  | 12.277 | (S)-(+)-2',3'-dideoxyribonolactone | 0.59 | -67.1 | -58.2 |
|  | 12.745 | Benzene-1,2-diol | 5.08 | -71 | -60.2 |
|  | 12.957 | 5-Hydroxymethylfurfural | 15.38 | -74.6 | -64.5 |
|  | 13.674 | 3,4-Dihydroxyacetophenone | 0.13 | -75.5 | -71.8 |
|  | 13.838 | 2H-Pyran-5-carboxylic acid, 2-oxo-, methyl ester | 0.33 | -66.7 | -64.2 |
|  | 14.396 | 1,4-Benzenediol | 9.32 | -73.3 | -62.8 |
|  | 14.970 | Phenol, 2,6-dimethoxy | 1.20 | -82.5 | -65.6 |
|  | 15.114 | Neric acid | 0.33 | -62 | -60.8 |
|  | 15.375 | Benzoic acid, 4-formyl-, methyl ester | 2.29 | -93.6 | -66.2 |
|  | 15.978 | 2-Oxabicyclo[2.2.1]heptan-3-one, 1,7,7-trimethyl | 0.24 | -62.1 | -60.9 |
|  | 16.692 | 1-Methyl-4-(2-methyl-2-oxiranyl)-7-oxabicyclo[4.1.0]heptanes | 0.15 | -71 | -66.8 |
|  | 17.023 | 2-Hexynal, 4-ethyl | 0.26 | -58.6 | -56.9 |
|  | 18.081 | Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester | 0.31 | -93.8 | -68.9 |
|  | 18.265 | Beta-d-glucopyranose, 1,6-anhydro- | 1.73 | -71.8 | -70.2 |
|  | 19.071 | 1-Tetradecene | 0.22 | -91.1 | -66.2 |
|  | 19.159 | Diethyl phthalate | 0.12 | -80.9 | -74.6 |
|  | 19.738 | Phenol, 3,4,5-trimethoxy | 1.31 | -80.2 | -72.1 |
|  | 22.239 | 1-Hexadecanol, 2-methyl- | 0.35 | -96.3 | -82.1 |
|  | 22.380 | 2H-Benzocyclohepten-2-one, 3,4,4a,5,6,7,8,9-octahydro | 1.46 | -73.8 | -67.2 |
|  | 24.171 | Hexadecanoic acid, methyl ester | 4.60 | -120.2 | -81.2 |
|  | 25.098 | Pentadec-7-ene, 7-bromomethyl | 0.50 | -97.1 | -74.9 |
|  | 25.282 | 2(1H)-Naphthalenone, octahydro-1-methyl-, (1.alpha.,4a.beta.,8a.alpha.) | 0.48 | -74.4 | -66.2 |
|  | 25.548 | Hexadecanoic acid | 0.12 | -112.4 | -77.3 |
|  | 26.045 | Bicyclo[2.2.2]octane-1-carboxylic acid, 4-methyl- | 0.58 | -67.9 | -61.1 |
|  | 26.386 | 1-Hexadecanol | 0.12 | -109.3 | -72.4 |
|  | 26.464 | 9,12-Octadecadienoic acid, methyl ester, (E,E)- | 1.90 | -131.4 | -87 |
|  | 26.546 | (9E,12E)-9,12-octadecadienoyl chloride | 1.63 | -102.4 | -83.4 |
|  | 26.709 | Phytol | 0.12 | -75.1 | -78.3 |
|  | 26.864 | Heptadecanoic acid, 16-methyl-, methyl ester | 0.69 | -123.5 | -86.1 |
|  | 27.705 | Trichloroacetic acid, pentadecyl ester | 0.13 | -118.6 | -85.6 |
|  | 29.335 | Eicosanoic acid, methyl ester | 0.41 | -141.4 | -90.3 |
|  | 31.583 | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl | 2.26 | -95.8 | -85.1 |
|  | 31.676 | Hexadecanal | 0.21 | -111.1 | -74.6 |
|  | 32.562 | Hexadecanoic acid, (3-bromoprop-2-ynyl) ester | 0.14 | -109.3 | -80.9 |
|  | 33.043  35.115 | Hexadecanoic acid, 2-hydroxy-, methyl ester | 0.23  0.38 | -103 | -80.6 |
|  | 33.500 | 9,12-Octadecadienoic acid (Z,Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 1.79 | -91 | -82.7 |
|  | 34.075 | Octadecanoic acid, 2-hydroxy-, methyl ester | 0.12 | -110.4 | -88.9 |
|  | 34.369 | 9-Octadecenamide | 0.34 | -137.1 | -91.3 |
|  | 34.555 | Squalene | 0.42 | -97.7 | -77.1 |
|  | 38.343 | Beta-sitosterol acetate | 0.28 | -94.5 | -93.9 |
|  | 38.637 | Vitamin E | 0.48 | -61.6 | -78.9 |
| - | - | Curcumin | - | -110.2 | - |
| - | - | Galantamine | - | - | -74.5 |