Supporting information

INHIBITION OF AMYLOID-β AGGREGATION BY *p*-TERPHENYLS FROM THE MUSHROOM *POLYOZELLUS MULTIPLEX* AND THEIR NEUROPROTECTIVE EFFECTS

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S1. General Information

Infrared (IR) spectra were recorded with a Thermo FT-IR Nicolet iS5 spectrophotometer (ATR) and a Jasco IR Report-100 spectrophotometer (KBr). UV spectra were recorded with a Thermo GENESYS 10S UV-Vis spectrophotometer. ^{1}H NMR and ^{13}C NMR spectra were measured with a JEOL JNM-ECZ 500 MHz spectrometer using tetramethylsilane as the internal standard. Fast atom bombardment MS (FABMS) spectra were measured with a JEOL JMS-700 spectrometer. Electrospray ionization (ESIMS) spectra were measured with a JEOL JMS-T100LC spectrometer.

S2. Characterization Data of Compounds 1–7

polyozellin (1). Dark green amorphous; IR (ATR) 3438, 3292, 1745, 1629, 1613, 1221 cm^{-1}; positive HRFABMS *m/z* 438.0585 $[M]^+$ (calcd for $C_{22}H_{14}O_{10}$, 438.0579).

kynapcin-12 (2). Colorless amorphous; IR (ATR) 3356, 1719, 1612, 1525, 1460, 1424, 1369, 1217 cm^{-1}; positive HRESIMS *m/z* 433.0892 $[M + Na]^+$ (calcd for $C_{22}H_{18}NaO_8$, 433.0899).

NSC617425 (3). Pale brown amorphous; IR (ATR) 3446, 3343, 1761, 1749, 1524, 1427, 1372, 1231 cm^{-1}; positive HRESIMS *m/z* 449.0843 $[M + Na]^+$ (calcd for $C_{22}H_{18}NaO_9$, 449.0849).

cycloleucomelone (4). Brown amorphous; IR (KBr) 3270, 1680, 1635, 1602, 1566, 1518, 1480, 1340, 1298, 1028 cm^{-1}; positive HRESIMS *m/z* 361.0312 $[M + Na]^+$ (calcd for $C_{18}H_{10}NaO_7$, 461.0324).

Bl-V (5). Pale brown amorphous; IR (ATR) 3155, 1766, 1612, 1470, 1371, 1211, 1022 cm^{-1}; positive HRESIMS *m/z* 447.0694 $[M + Na]^+$ (calcd for $C_{22}H_{16}NaO_9$, 447.0692).

succinic acid (6). Colorless amorphous; IR (ATR) 2931, 2647, 2544, 1689, 1417, 1309, 1200 cm^{-1}; negative HRESIMS *m/z* 117.0189 $[M - H]^-$ (calcd for $C_4H_5O_4$, 117.0188).

protocatechuic acid (7). Colorless amorphous; IR (ATR) 3436, 2961, 2924, 1682, 1610, 1445, 1288, 1166 cm^{-1}; HREIMS *m/z* 150.0265 $[M]^+$. (calcd for $C_7H_6O_4$, 154.0266).

S3. Copies of ^1H and ^{13}C Spectra for Compounds 1–7

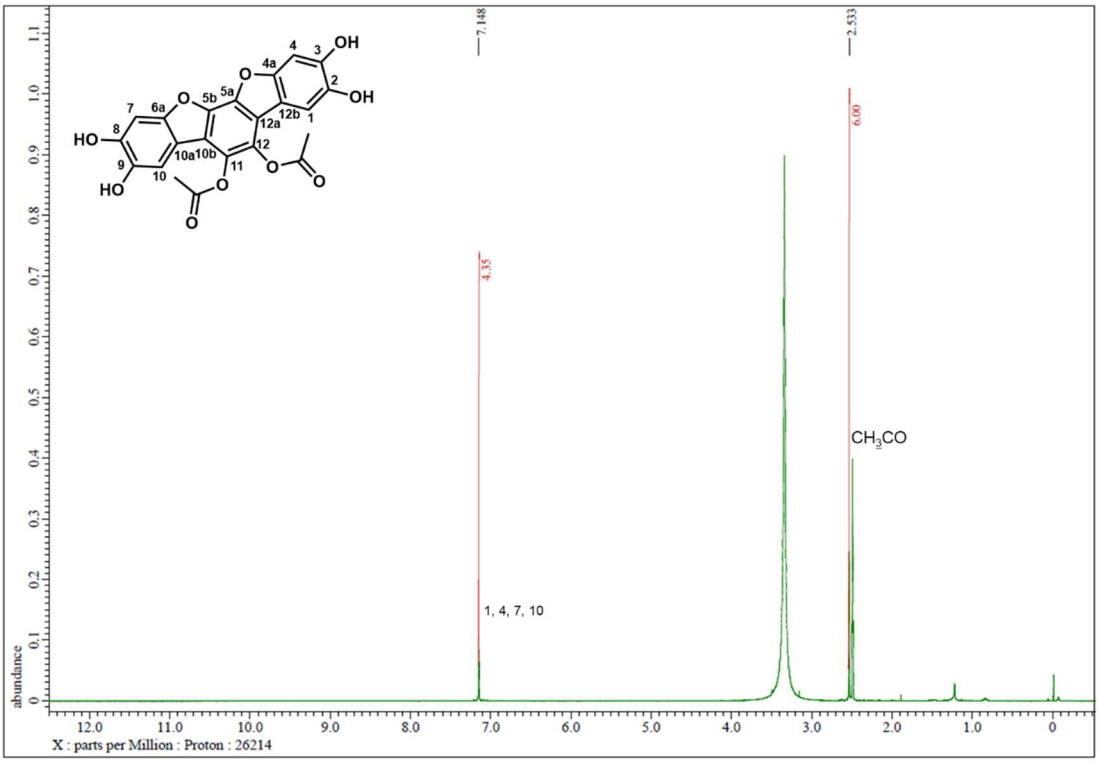

Fig. S1. ^1H NMR (500 MHz, DMSO-d_6) of polyozellin (1)

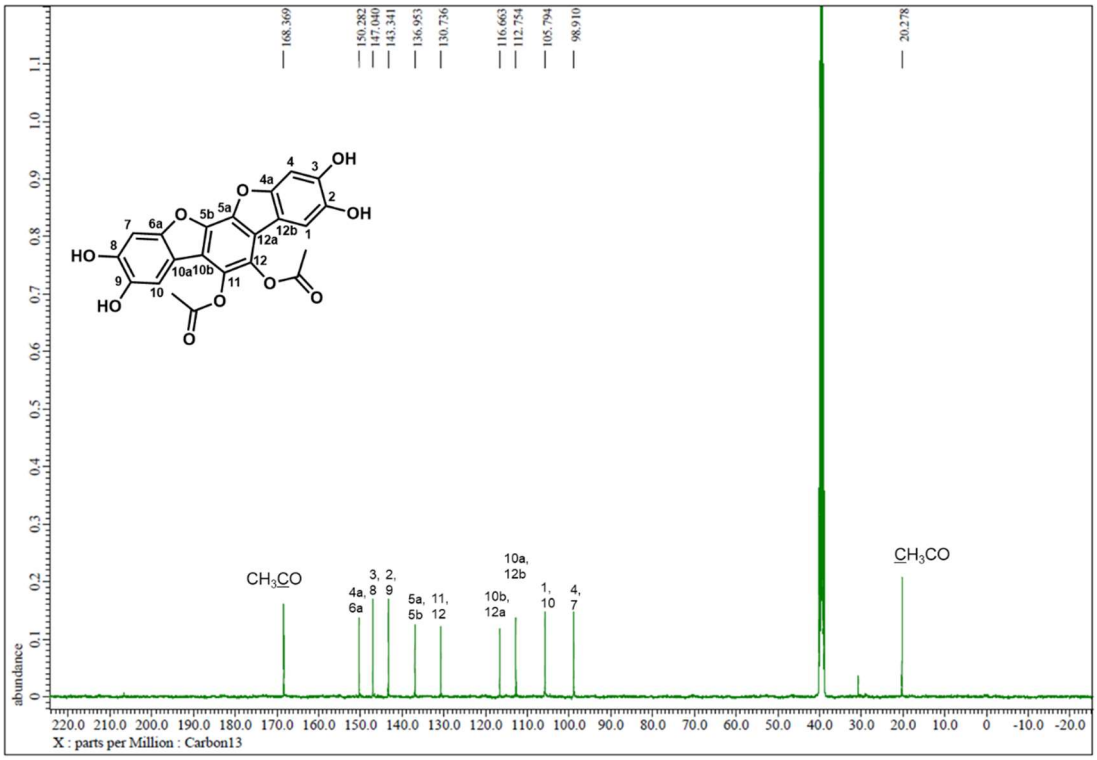

Fig. S2. ^{13}C NMR (500 MHz, DMSO-d_6) of polyozellin (1)

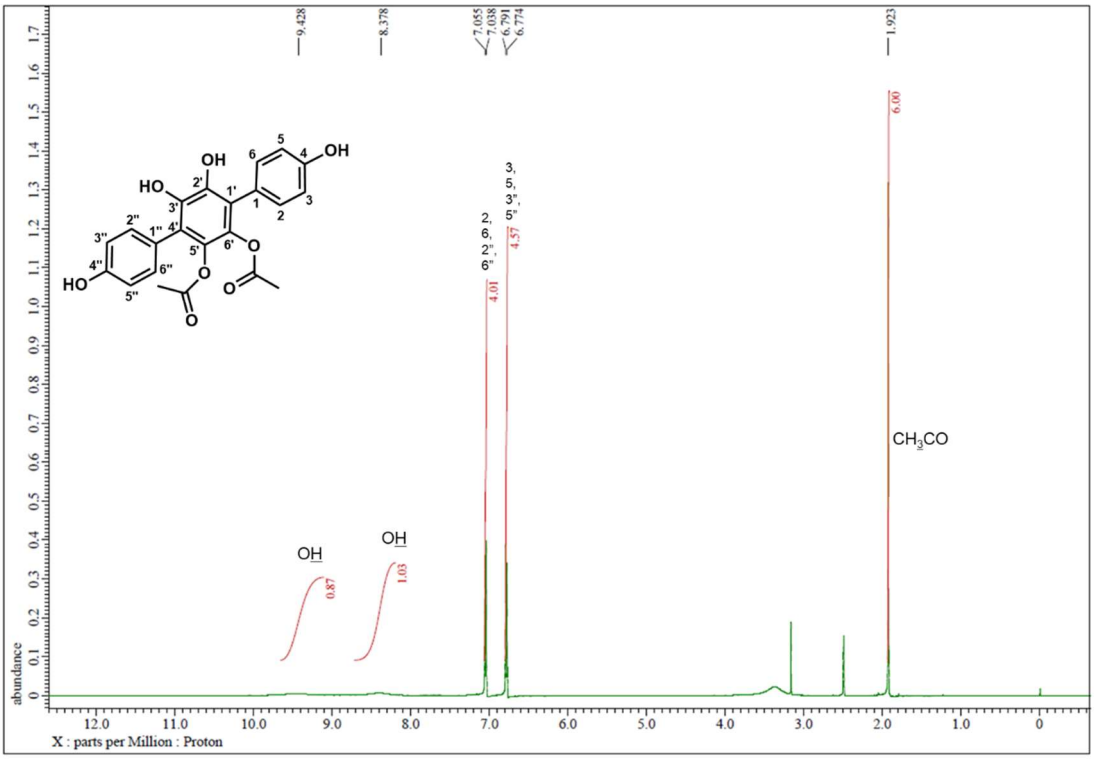

Fig. S3. ^{1}H NMR (500 MHz, DMSO-d_6) of kynapcin-12 (2)

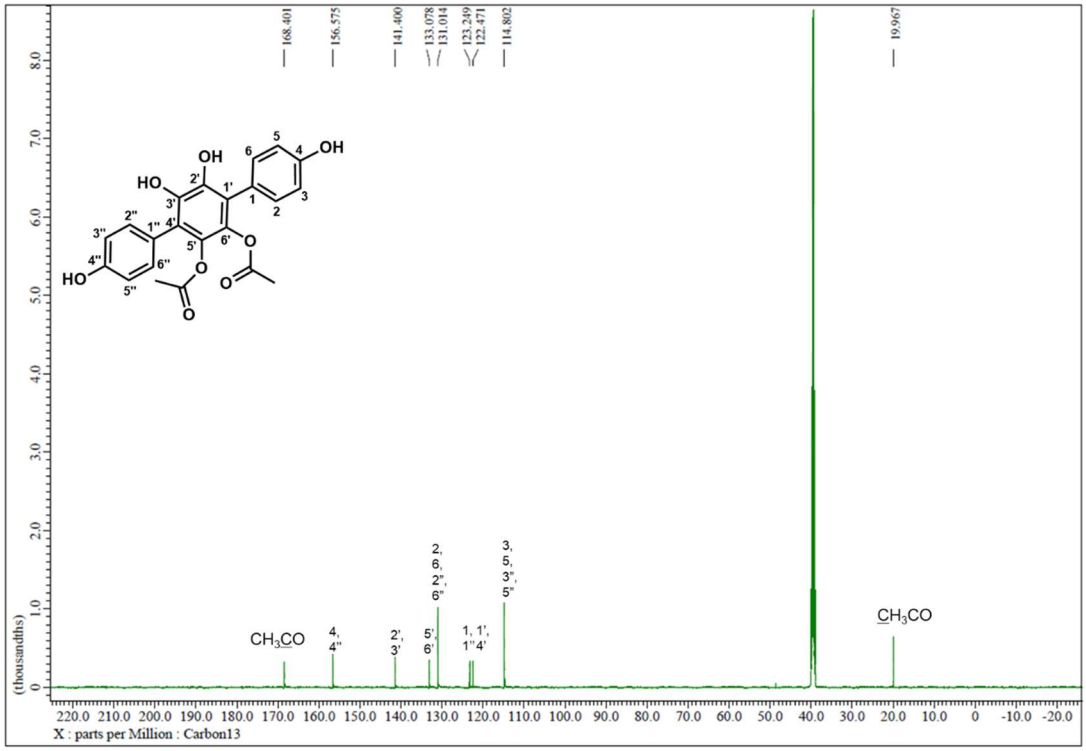

Fig. S4. ^{13}C NMR (500 MHz, DMSO-d_6) of kynapcin-12 (2)

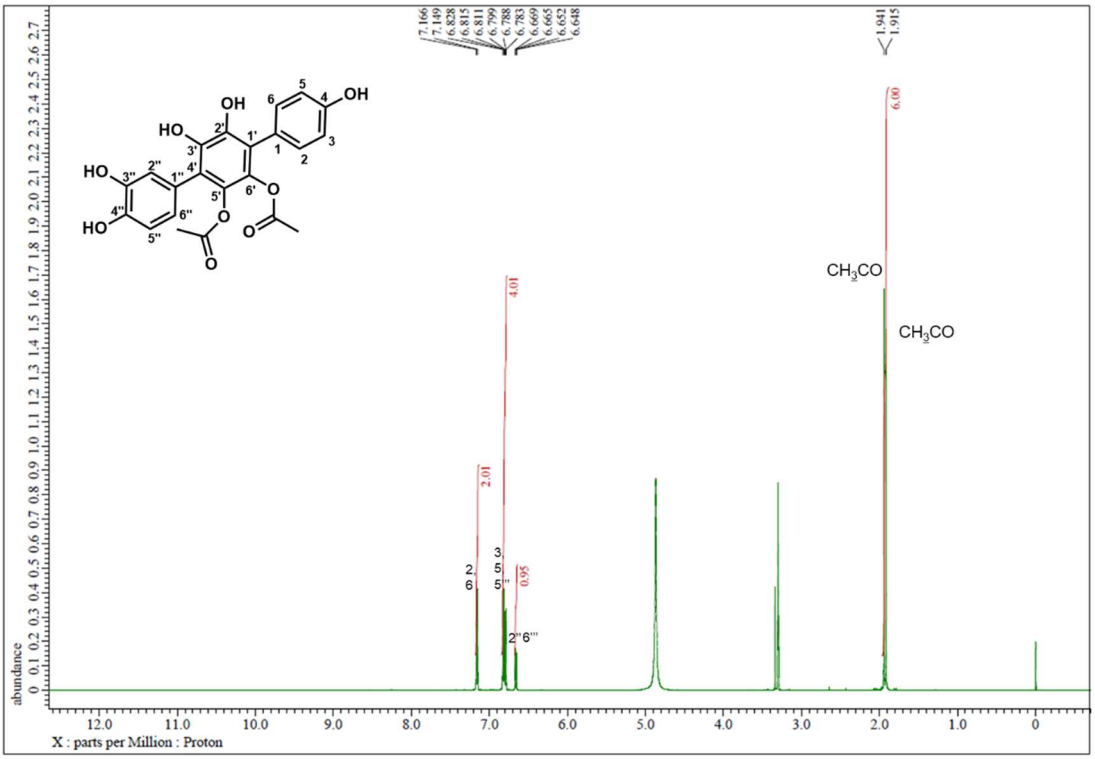

Fig. S5. ^{1}H NMR (500 MHz, CD_3OD) of NSC617425 (3)

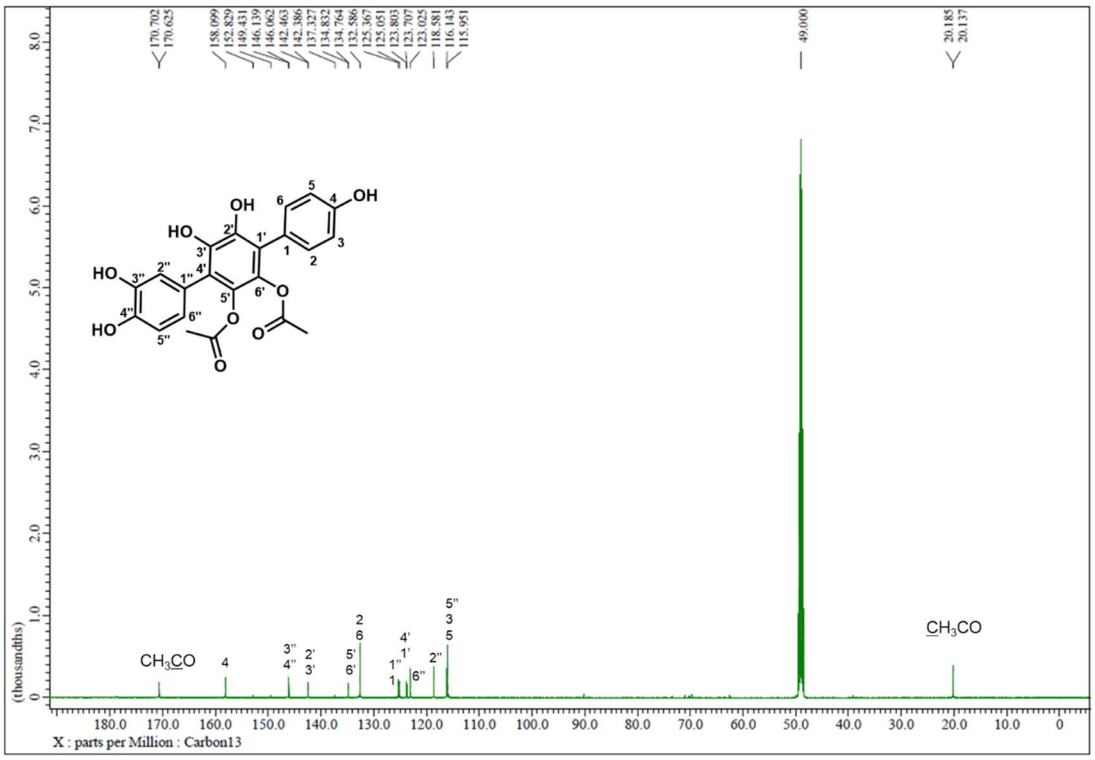

Fig. S6. ^{13}C NMR (500 MHz, CD_3OD) of NSC617425 (3)

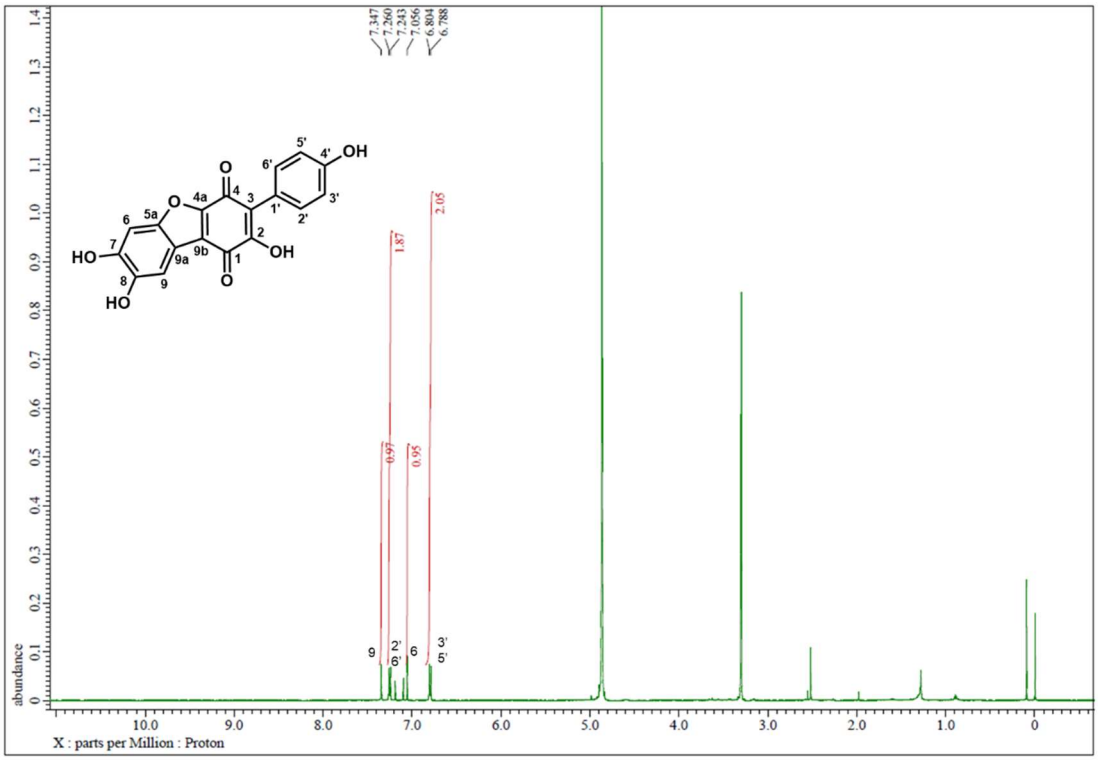

Fig. S7. ^{1}H NMR (500 MHz, CD_3OD) of cycloleucomelone (4)

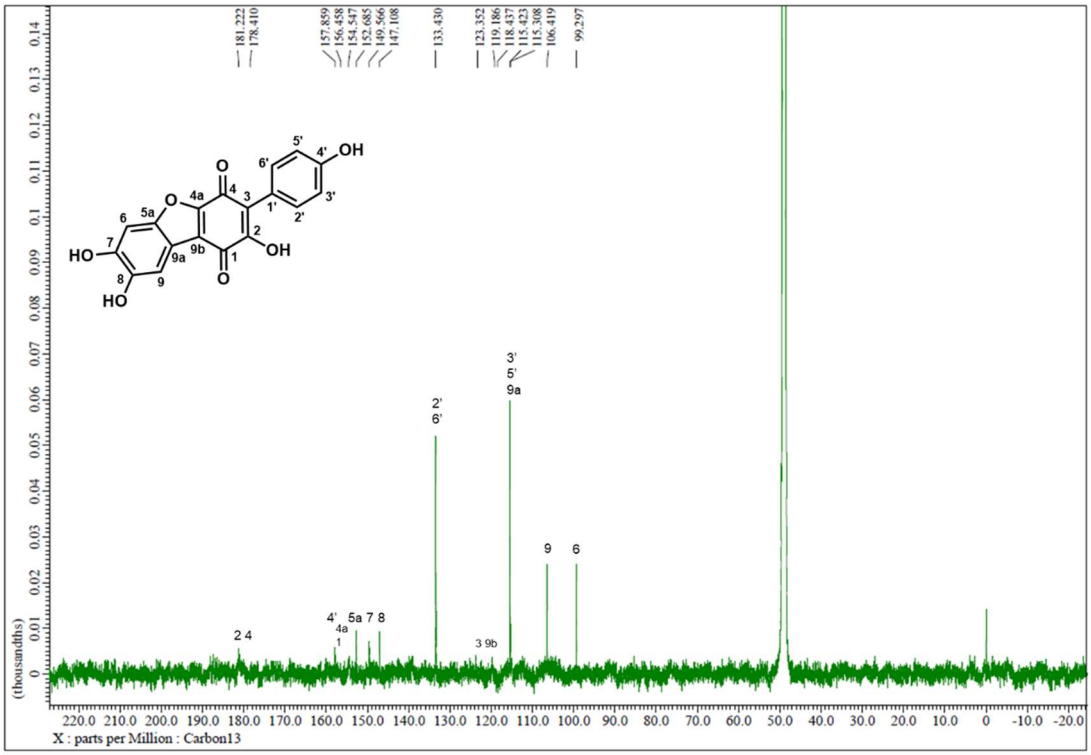

Fig. S8. ^{13}C NMR (500 MHz, CD_3OD) of cycloleucomelone (4)

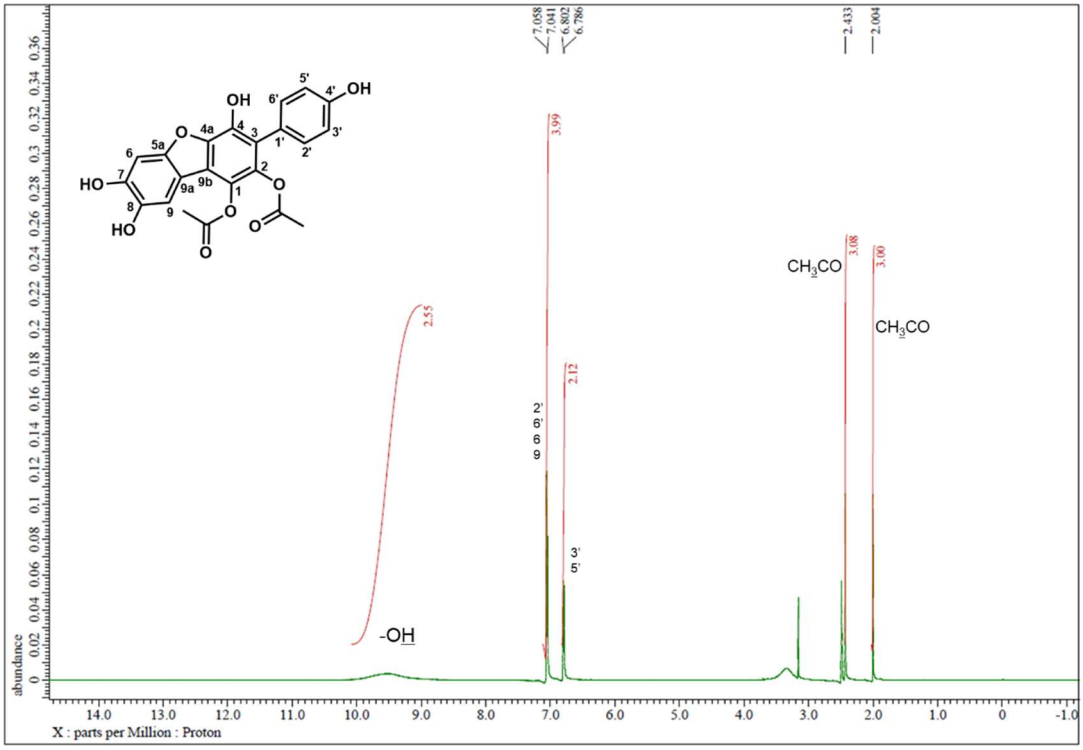

Fig. S9. ^{1}H NMR (500 MHz, DMSO-d_6) of Bl-V (5)

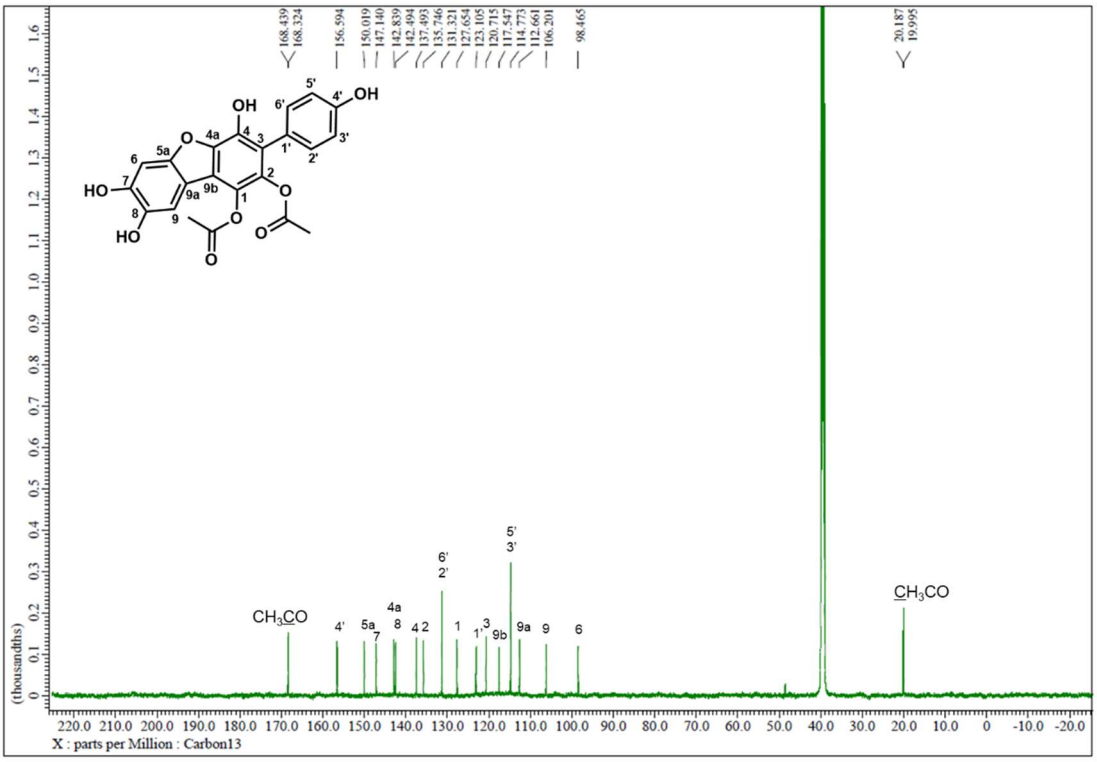

Fig. S10. ^{13}C NMR (500 MHz, DMSO-d_6) of Bl-V (5)

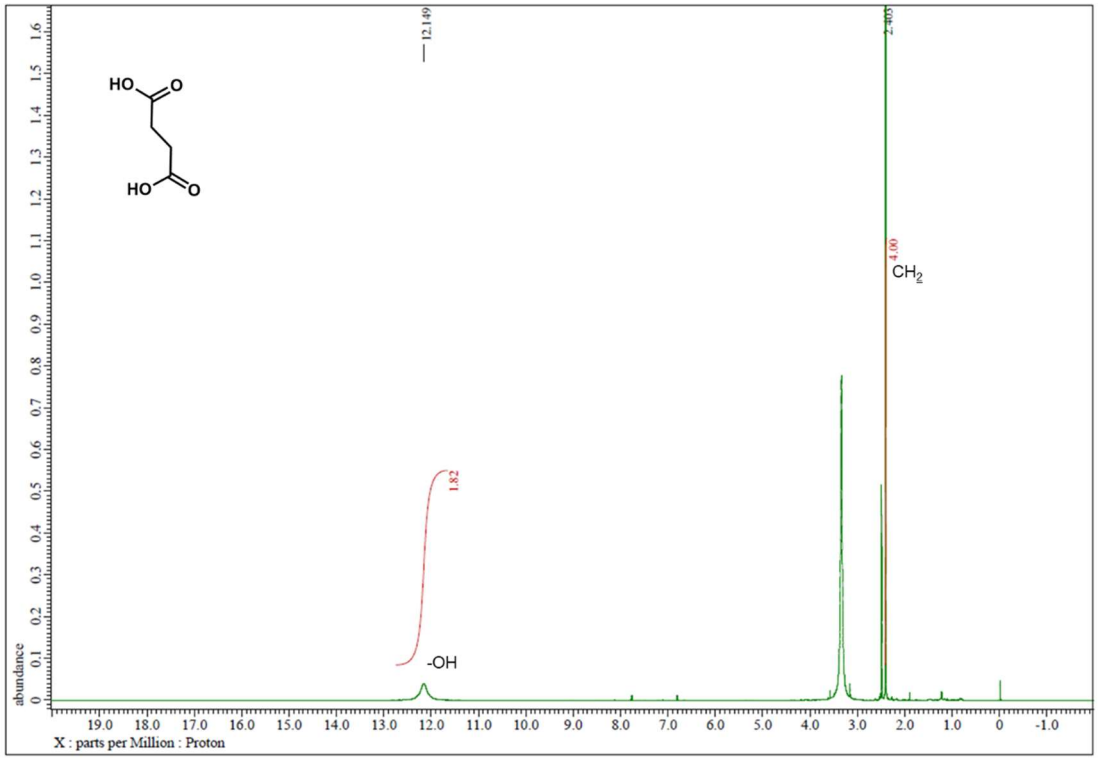

Fig. S11. ^{1}H NMR (500 MHz, DMSO-d_6) of succinic acid (6)

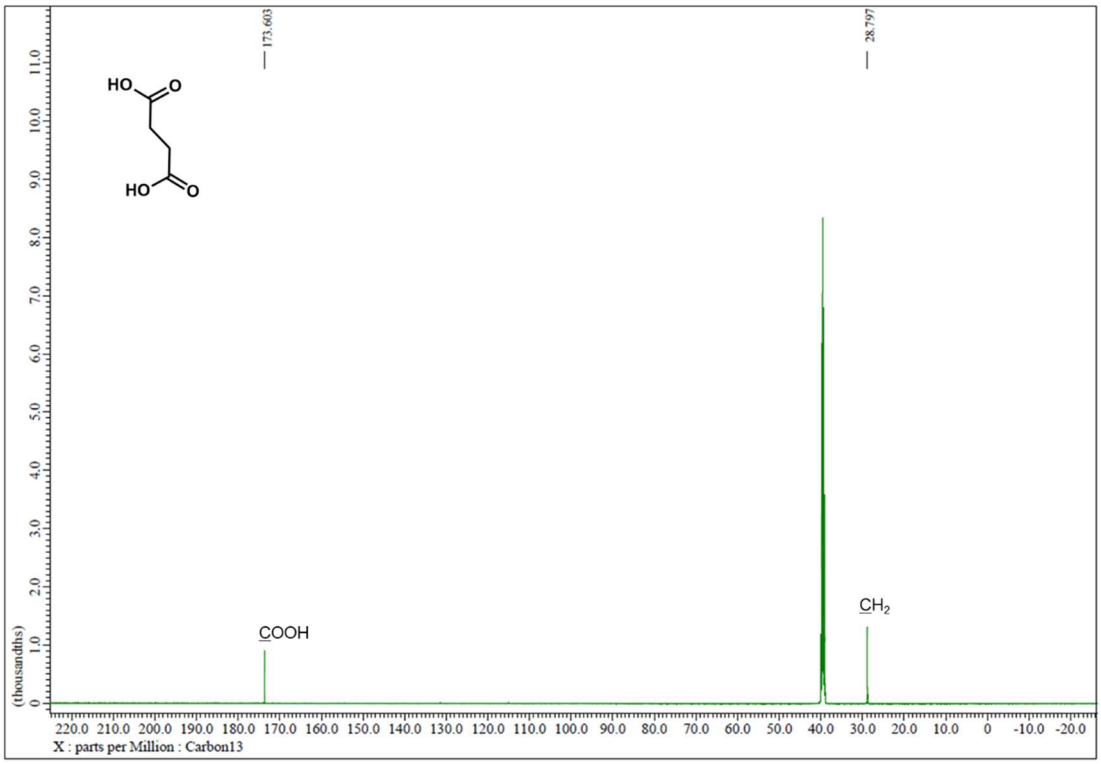

Fig. S12. ^{13}C NMR (500 MHz, DMSO-d_6) of succinic acid (6)

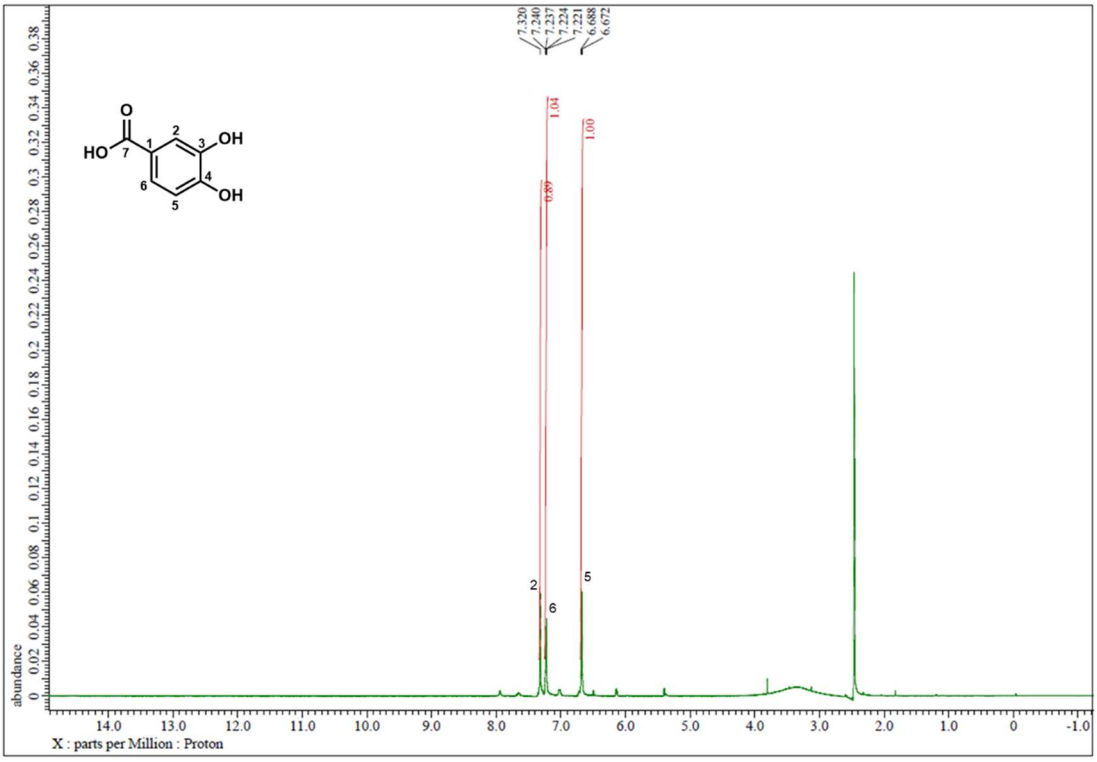

Fig. S13. ^{1}H NMR (500 MHz, DMSO-d_6) of protocatechuic acid (7)

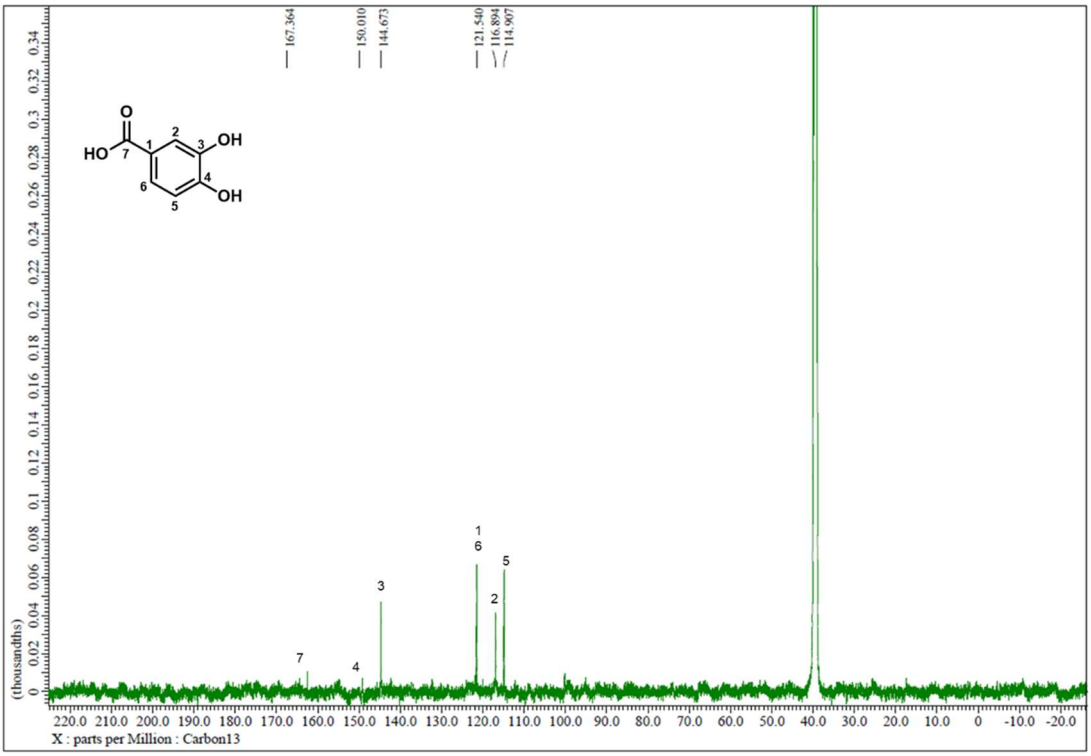

Fig. S14. ^{13}C NMR (500 MHz, DMSO-d_6) of protocatechuic acid (7)

S4. Thin layer chromatography (TLC) of Methanol Extract from the Fruiting Body of *P. multiplex*

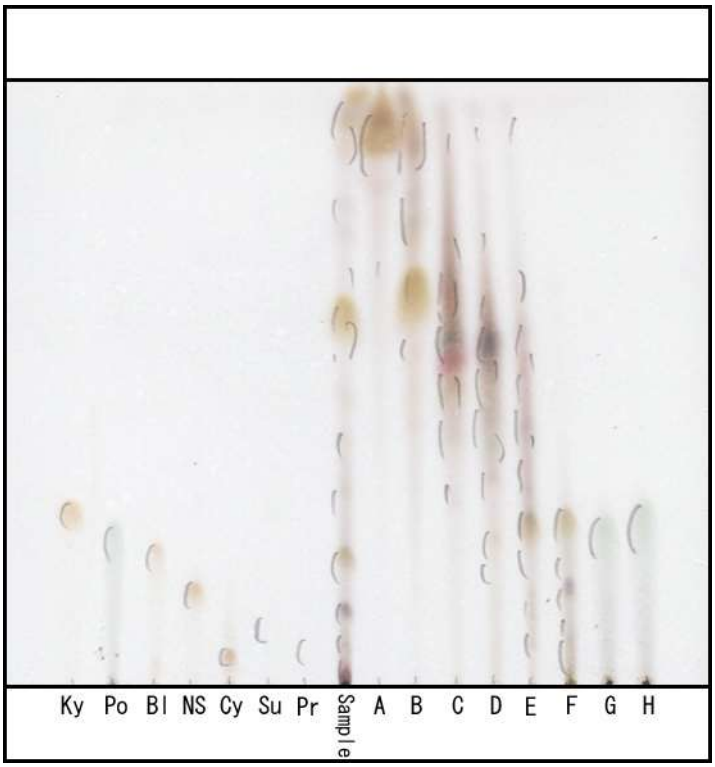

Fig. S15.

Separation with $CHCl_3$-MeOH (5:1). 50% solution of sulfuric acid in MeOH were used separately as visualization reagents. Ky: kynapcin-12, Po: polyozellin, Bl: Bl-V, NS: NSC617425, Cy: cycloleucomelone, Su: succinic acid, Pr: protocatechuic acid, Sample: methanol extract from the fruiting body of *P. multiplex*, A–H: each fraction A–H.

S5. Inhibitory Activity of Aβ aggregation

Values are expressed as mean ± SD, n=3. The half-maximal inhibitory concentration (IC_{50}) values of compounds **1**–**11** were 0.615 ± 0.347, 6.76 ± 5.14, 6.45 ± 2.34, 2.17 ± 0.770, 3.61 ± 1.10, >100, >100, 12.62 ± 0.813, 1.29 ± 0.207, 1.96 ± 0.793, and 21.61 ± 3.91 μM, respectively.

S6. Inhibitory Activity Against BACE1

Values are expressed as mean ± SD, n=3. The IC_{50} values of compounds **3**–**7, 10** and **11** were >100, 66.62 ± 28.66, >100, >100, >100, 34.49 ± 13.26 and >100 μM, respectively.

S7. Cytotoxicity of Compounds 1–7 on SH-SY5Y Cells

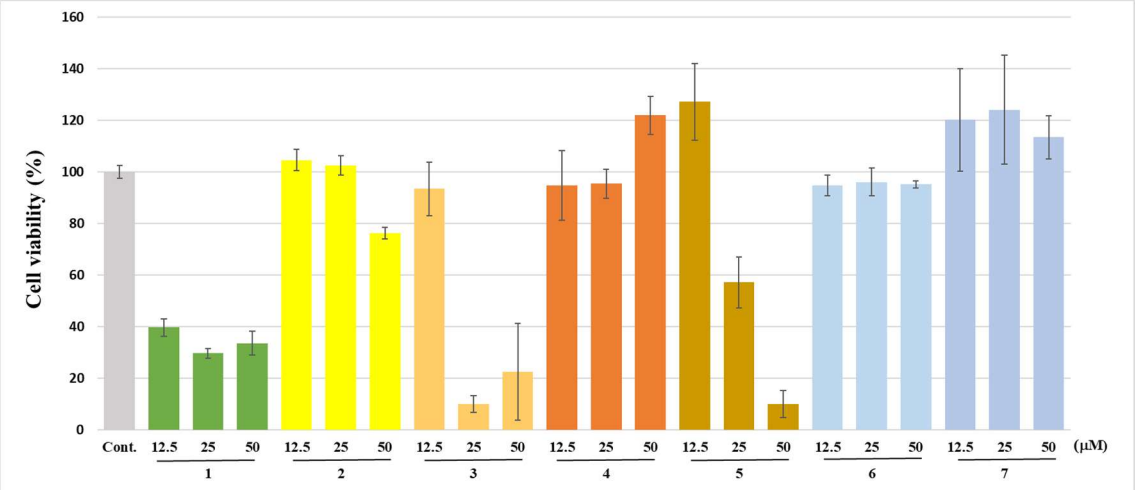

Fig. S16. Cytotoxicity of compounds 1–7 on SH-SY5Y cells

Cont. indicates the control group (cells in the absence of compounds **1**–**7**). **1**–**7** indicate the groups treated with each compound (**1**–**7**). Values are expressed as mean ± SD, n=3.