Supporting Information

Neuronal proteins as targets of 3-hydroxykynurenine: Implications in neurodegenerative diseases

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Table S1. Residues of αSyn, $A\beta_{16}$, and $A\beta_{28}$, identified by LC-MS/MS in the conjugates 3OHKyn-Cu-$A\beta_{16}$, 3OHKyn-Fe-$A\beta_{16}$, 3OHKyn-Cu-$A\beta_{28}$, 3OHKyn-Fe-$A\beta_{28}$, 3OHKyn-Cu-αSyn, and 3OHKyn-Fe-αSyn, as adducts with 3OHKyn and its oxidation products pag S2
Figure S1. MS/MS spectrum of the $A\beta_{16}$ adduct with 3OHKyn at His13 pag S3
Figure S2. MS/MS spectrum of the $A\beta_{28}$ adducts with OHXan at His13 and 3OHKyn at His14 pag S4
Figure S3. MS/MS spectrum of the αSyn adducts with 3OHKyn at Lys6 and Xan at Lys10 pag S5
Figure S4. MS/MS spectrum of Aβ16 oxidized at His13 pag S6
Figure S5. Derivative absorption spectrum of 3OHKyn pag S7
Figure S6. Derivative absorption spectrum of oxidized 3OHKyn pag S7
Figure S7. Derivative absorption spectrum of 3OHKyn-αSyn pag S7
Figure S8. Absorption spectra of oxidized 3OHKyn, 3OHKyn-$A\beta_{16}$ and $A\beta_{16}$ pag S8
Figure S9. Absorption spectra of oxidized 3OHKyn, 3OHKyn-αSyn_6 and αSyn_6 pag S8
Figure S10. Absorption spectra of oxidized 3OHKyn, 3OHKyn-αSyn_{15} and αSyn_{15} pag S8
Figure S11. Proton NMR spectra of $A\beta_{16}$ and 3OHKyn-$A\beta_{16}$ pag S9
Figure S12. Proton NMR spectra of αSyn_6 and 3OHKyn-αSyn_6 pag S9
Figure S13. Proton NMR spectra of αSyn_{15} and 3OHKyn-αSyn_{15} pag S10

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Conjugates	**3OHKyn -aa (+207)**	**Xan-aa(A) (+406)**	**HXan-aa (+408)**	**OHXan-aa (+422)**	**Xan-aa(B) (+423)**	**DHQCA-aa (+235)**	**oxidation (+16)**
3OHKyn-Cu-$A\beta_{16}$		H13	H6 H13 H14	H13	H14		H13 Y10
3OHKyn-Fe-$A\beta_{16}$		H13	H6 H13 H14	H13	H14		H13 Y10
3OHKyn-Cu-$A\beta_{28}$		H13	H6 H13 H14	H13 H14	H14		H13 Y10
3OHKyn-Fe-$A\beta_{28}$		H13	H6 H13 H14	H13 H14	H14		H13 Y10
3OHKyn-Cu-αSyn	K21 K23	K21 K23 K45		K23		K23	M116 M127
3OHKyn-Fe-αSyn	K21 K23	K21 K23 K45		K23		K23	M116 M127

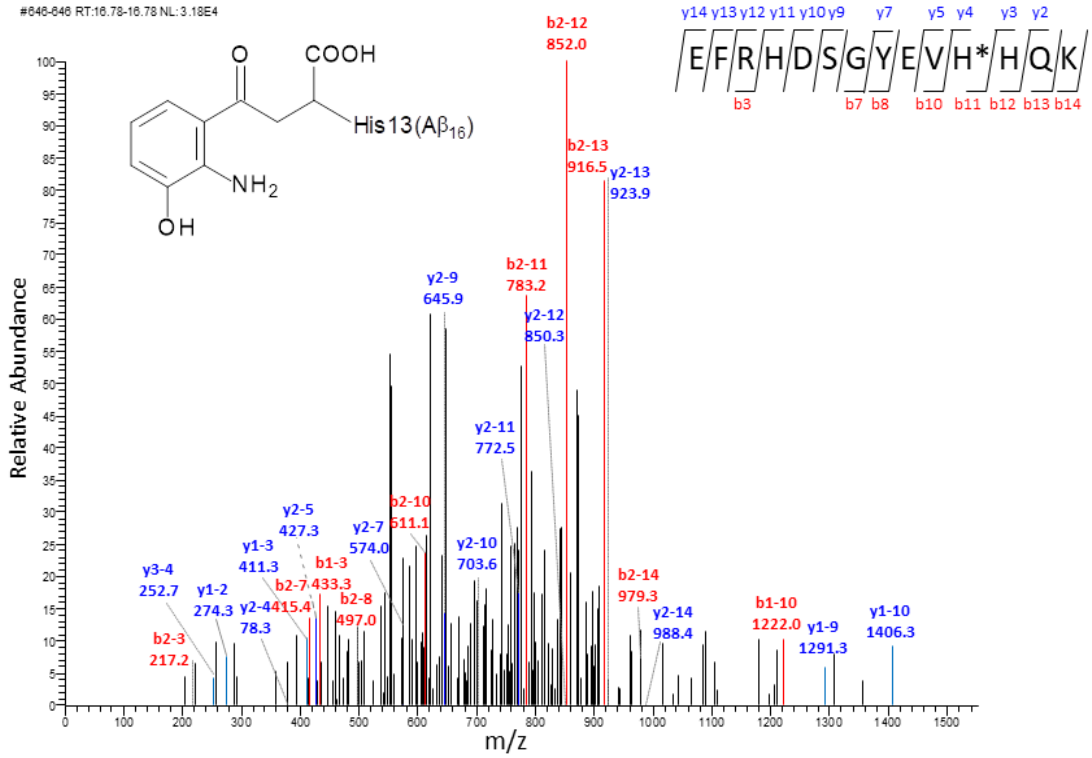

Figure S1. MS/MS spectrum of the m/z 659.7 peak assigned to the 3-16 peptide of $A\beta_{16}$ in a triple-charged state containing the adduct with 3OHKyn at His13 (peptide mass of 1975.8 amu, corresponding to a mass increase of 207 amu with respect to the unmodified peptide). The assignment of the y (in blue) and b (in red) ion series, in mono-, double-, or triple-charged states, is shown. Above the spectrum, the sequence of the peptide is shown with an asterisk on the modified residue and with the summary of the y and b ions found in the spectrum.

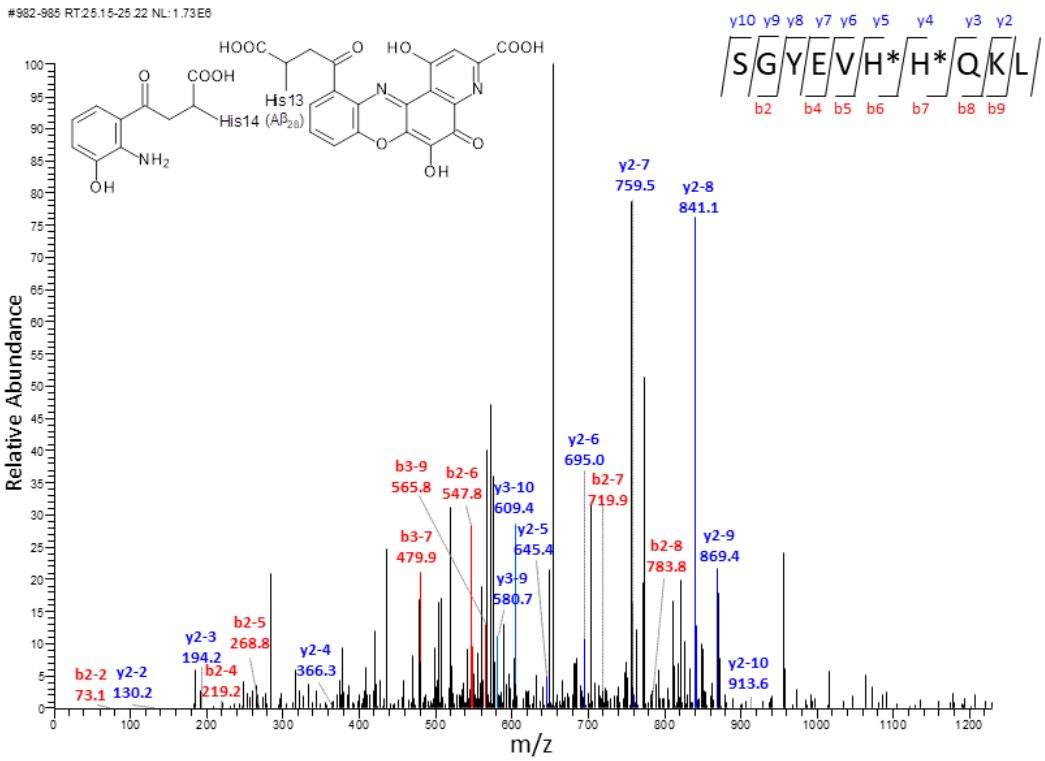

Figure S2. MS/MS spectrum of the m/z 610.0 peak assigned to the 8-17 peptide of $A\beta_{28}$ in a triple-charged state containing the adducts with OHXan at His13 and 3OHKyn at His14 (peptide mass of 1826.3 amu, corresponding to a mass increase of (422+207) amu with respect to the unmodified peptide). The assignment of the y (in blue) and b (in red) ion series, in double- or triple-charged states, is shown. Above the spectrum, the sequence of the peptide is shown with an asterisk on each modified residue and with the summary of the y and b ions found in the spectrum.

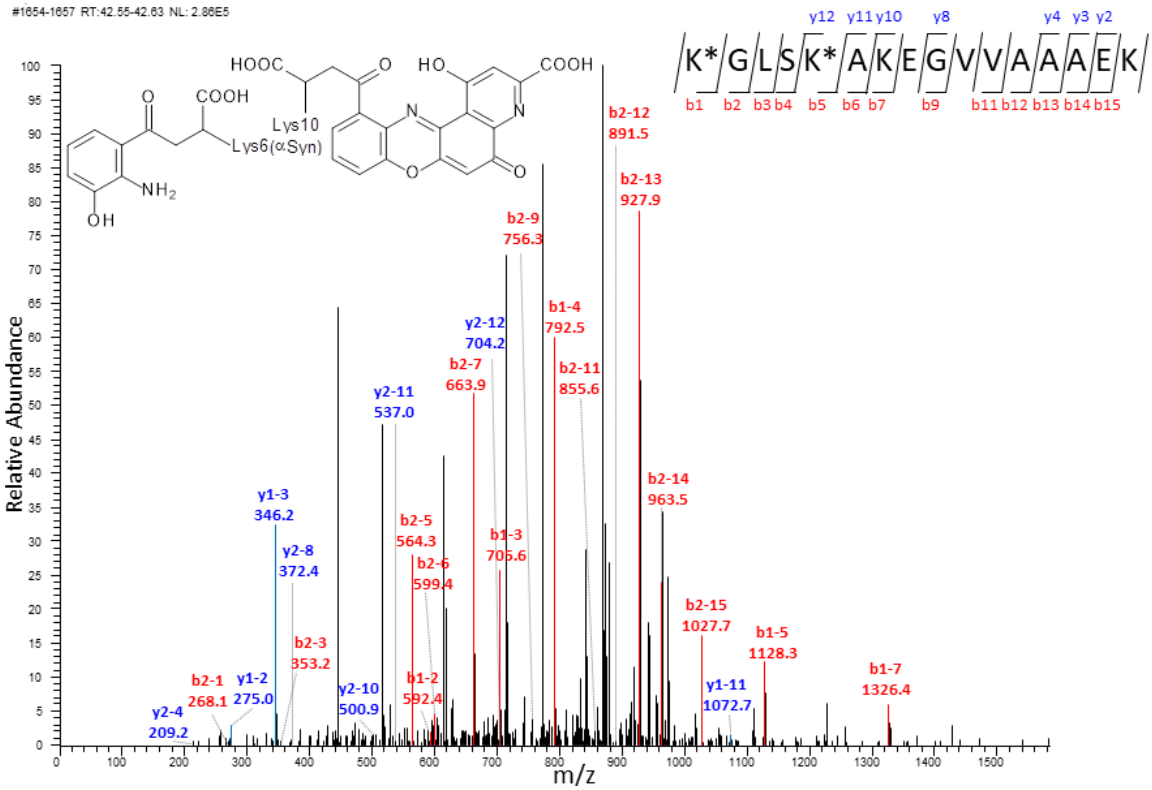

Figure S3. MS/MS spectrum of the m/z 734.0 peak assigned to the 6-21 peptide of αSyn in a triple-charged state containing the adducts with 3OHKyn at Lys6 and Xan at Lys10 (peptide mass of 2198.8 amu, corresponding to a mass increase of (207+406) amu with respect to the unmodified peptide). The assignment of the y (in blue) and b (in red) ion series, in mono- or double-charged states, is shown. Above the spectrum, the sequence of the peptide is shown with an asterisk on each modified residue and with the summary of the y and b ions found in the spectrum.

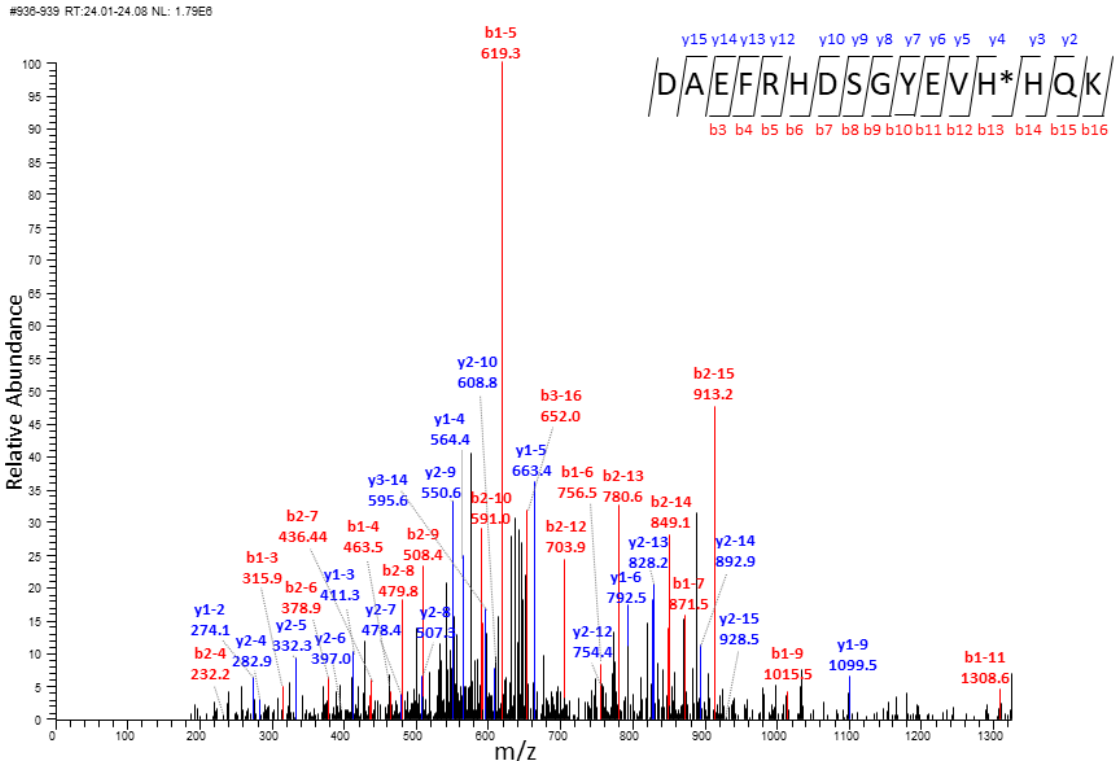

Figure S4. MS/MS spectrum of the m/z 657.3 peak assigned to the $A\beta_{16}$ peptide in a triple-charged state containing oxidized His13 (peptide mass of 1970.0 amu, corresponding to a mass increase of 16 amu with respect to the unmodified peptide). The assignment of the y (in blue) and b (in red) ion series, in mono-, double-, or triple-charged states, is shown. Above the spectrum, the sequence of the peptide is shown with an asterisk on the modified residue and with the summary of the y and b ions found in the spectrum.

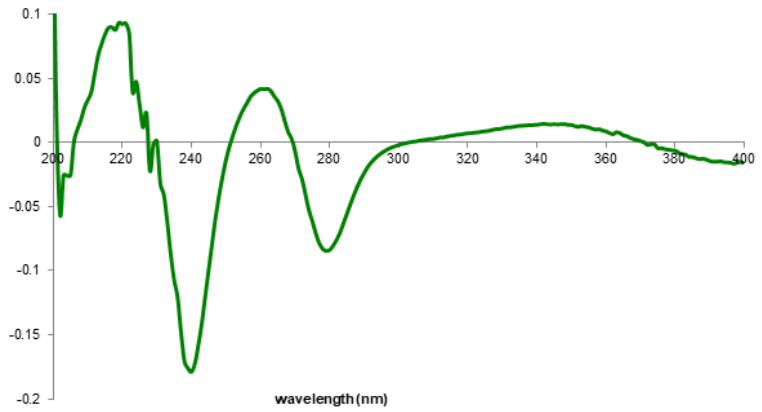

Figure S5. Derivative absorption spectrum of 3OHKyn.

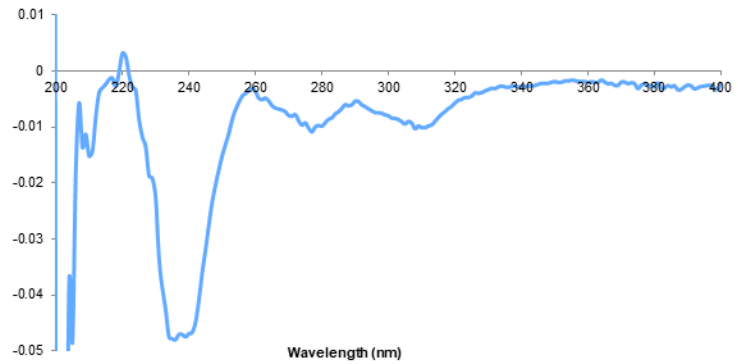

Figure S6. Derivative absorption spectrum of oxidized 3OHKyn.

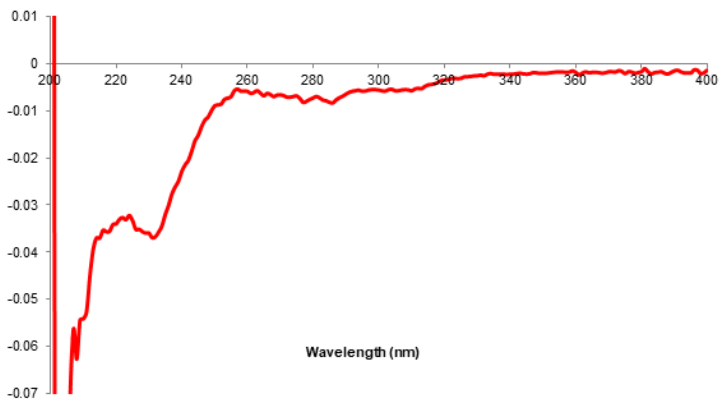

Figure S7. Derivative absorption spectrum of 3OHKyn-αSyn.

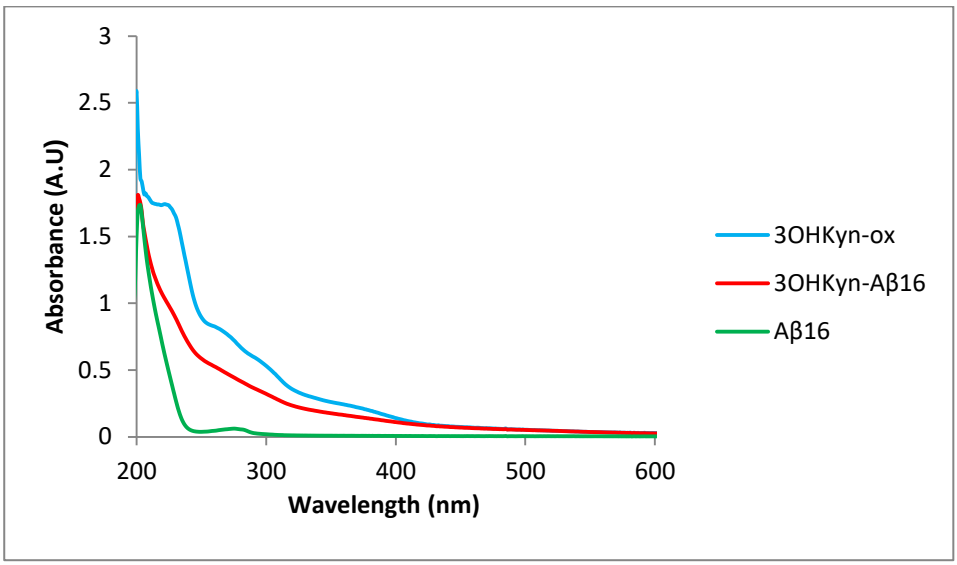

Figure S8. Absorption spectra of oxidized 3OHKyn, 3OHKyn-Aβ_{16} and Aβ_{16}.

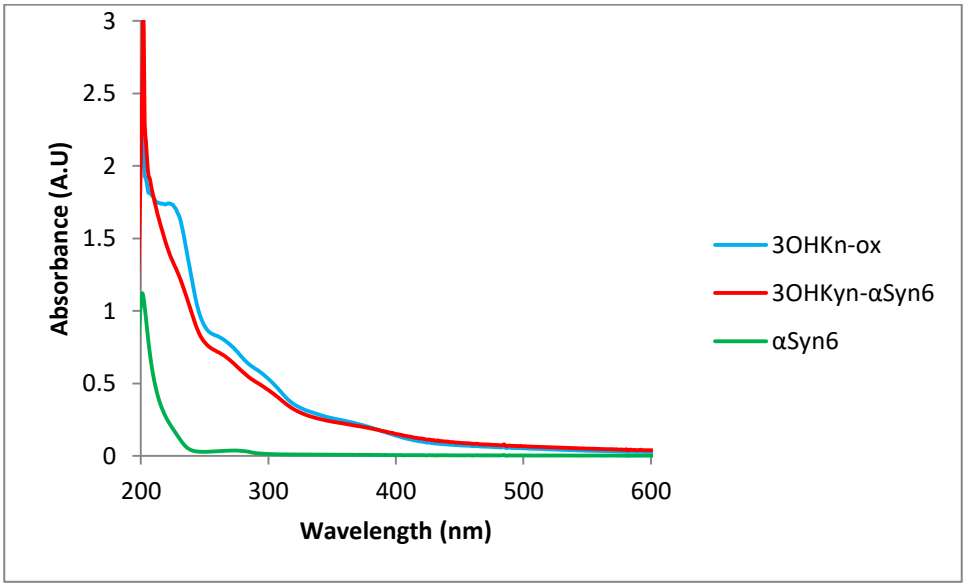

Figure S9. Absorption spectra of oxidized 3OHKyn, 3OHKyn-αSyn_6 and αSyn_6.

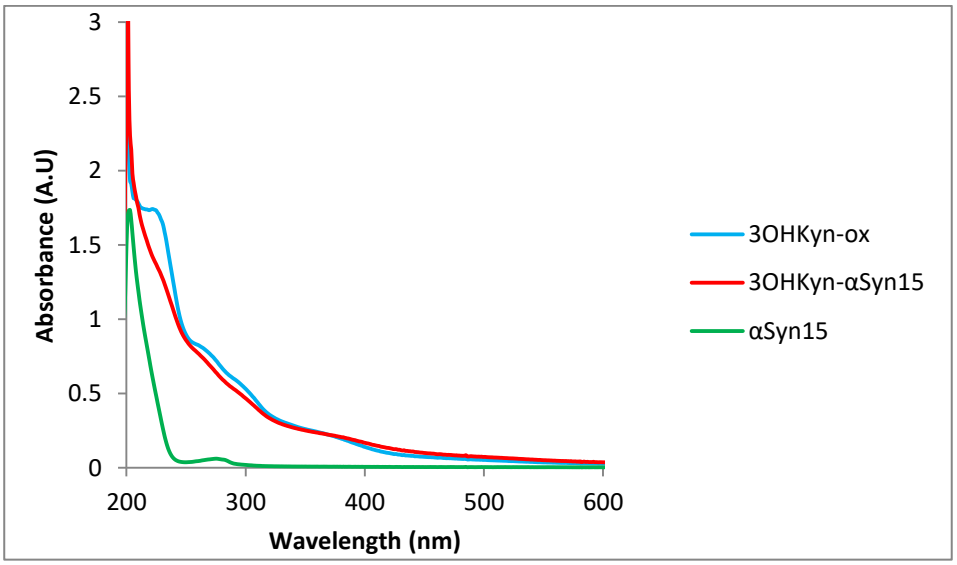

Figure S10. Absorption spectra of oxidized 3OHKyn, 3OHKyn-αSyn_{15} and αSyn_{15}.

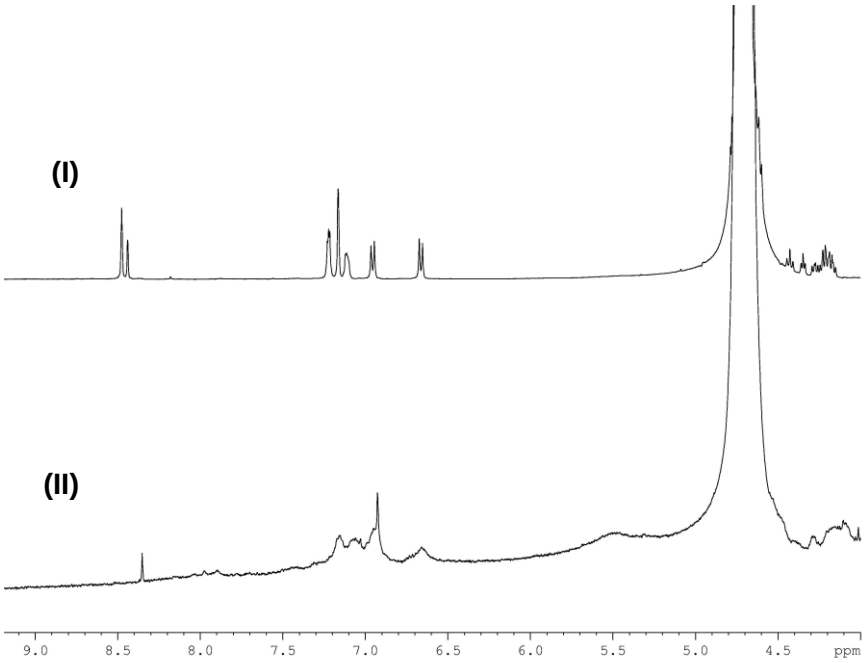

Figure S11. Proton NMR spectra of (I) $A\beta_{16}$ and (II) 3OHKyn-$A\beta_{16}$.

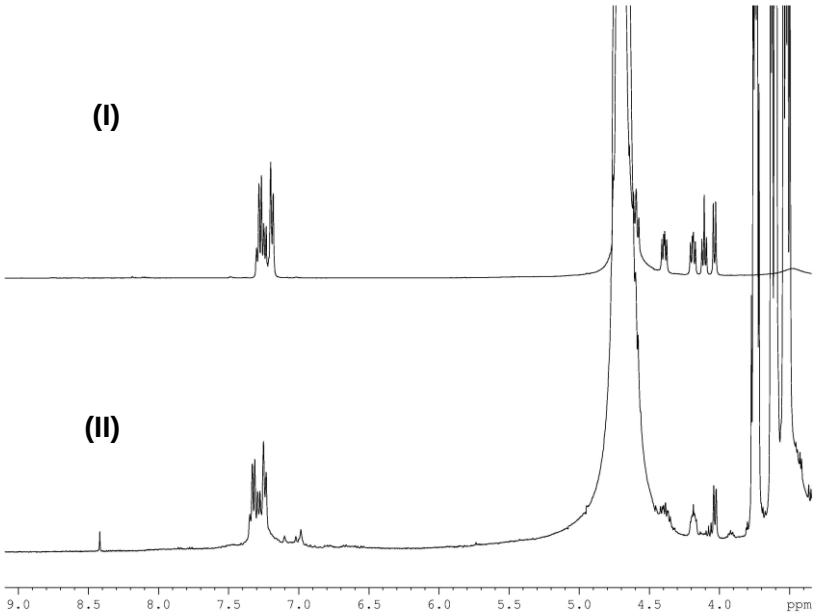

Figure S12. Proton NMR spectra of (I) αSyn_6 and (II) 3OHKyn-αSyn_6.

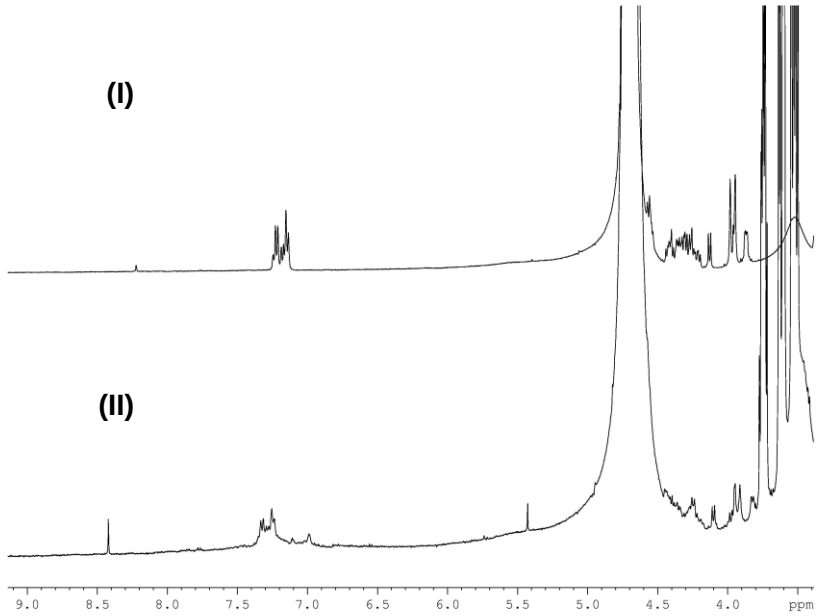

Figure S13. Proton NMR spectra of (I) αSyn_{15} and (II) 3OHKyn-αSyn_{15}.