

SUPPORTING INFORMATION

Pyridoxamine as a potential scavenger of neurotoxic dopamine quinone: Inhibition of dopamine-induced α -synuclein oligomerization

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Table of contents

Table S1. ^1H NMR, ^1H - ^{13}C HMQC, and ^1H - ^1H COSY assignments for the PL–DA adduct. Please refer to Fig. S2A for numbering.

Table S2. V8 α -Syn peptides identified by LC/ESI-MS/MS analysis followed by database search ([XLSX](#)).

Table S3. Tryptic α -Syn peptides identified by LC/ESI-MS/MS analysis followed by database search ([XLSX](#)).

Figure S1. LC/ESI-MS/MS and UV analyses of PL produced by the reaction between PM and DA. **(A)** MS/MS spectrum of $[\text{M} + \text{H}]^+$ at m/z 168.1. **(B)** UV spectrum showing λ_{max} at 288.0 nm.

Figure S2. **(A)** ^1H NMR, **(B)** ^1H - ^{13}C HMQC, and **(C)** ^1H - ^1H COSY spectra of the PL–DA adduct (1-[3-hydroxy-5-(hydroxymethyl)-2-methylpyridin-4-yl]-1,2,3,4-tetrahydroisoquinoline-6,7-diol).

Figure S3. MS/MS spectra of V8 α -Syn peptides containing oxidized Met.

Table S1. ^1H NMR, ^1H - ^{13}C HMQC, and ^1H - ^1H COSY assignments for the PL-DA adduct. Please refer to Fig. S2A for numbering.

Atom number	δ H (ppm)	HMQC	COSY
1	7.91 (s, 1H)	C(1)	H(8)
2	6.44 (s, 1H)	C(2)	
3	6.01 (s, 1H)	C(3)	H(4)
4	5.20 (s, 1H)	C(4)	H(6') or H(7)
5	4.62 (dd, $J = 7.2, 13.2$ Hz, 1H)	C(5)	
5'	4.54 (dd, $J = 8.4, 13.2$ Hz, 1H)	C(5)	
6	3.19-3.21 (m, 1H)	C(6)	H(7'), H(6') or H(7)
6'	2.81-2.85 (m, 2H)*	C(6)	
7	2.81-2.85 (m, 2H)*	C(7)	
7'	2.50-2.52 (m, 1H)	C(7)	H(6') or H(7)
8	2.18 (s, 3H)	C(8)	

* Peaks for H-6' and H-7 in ^1H -NMR spectrum were overlapped due to their close chemical shifts.

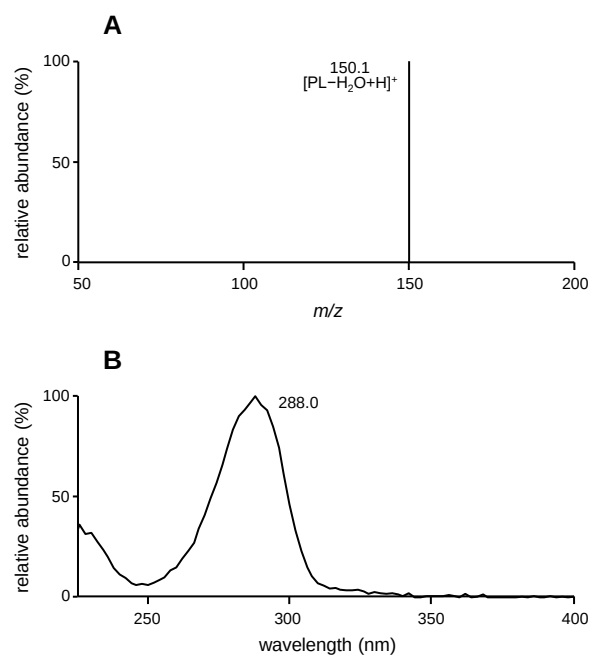


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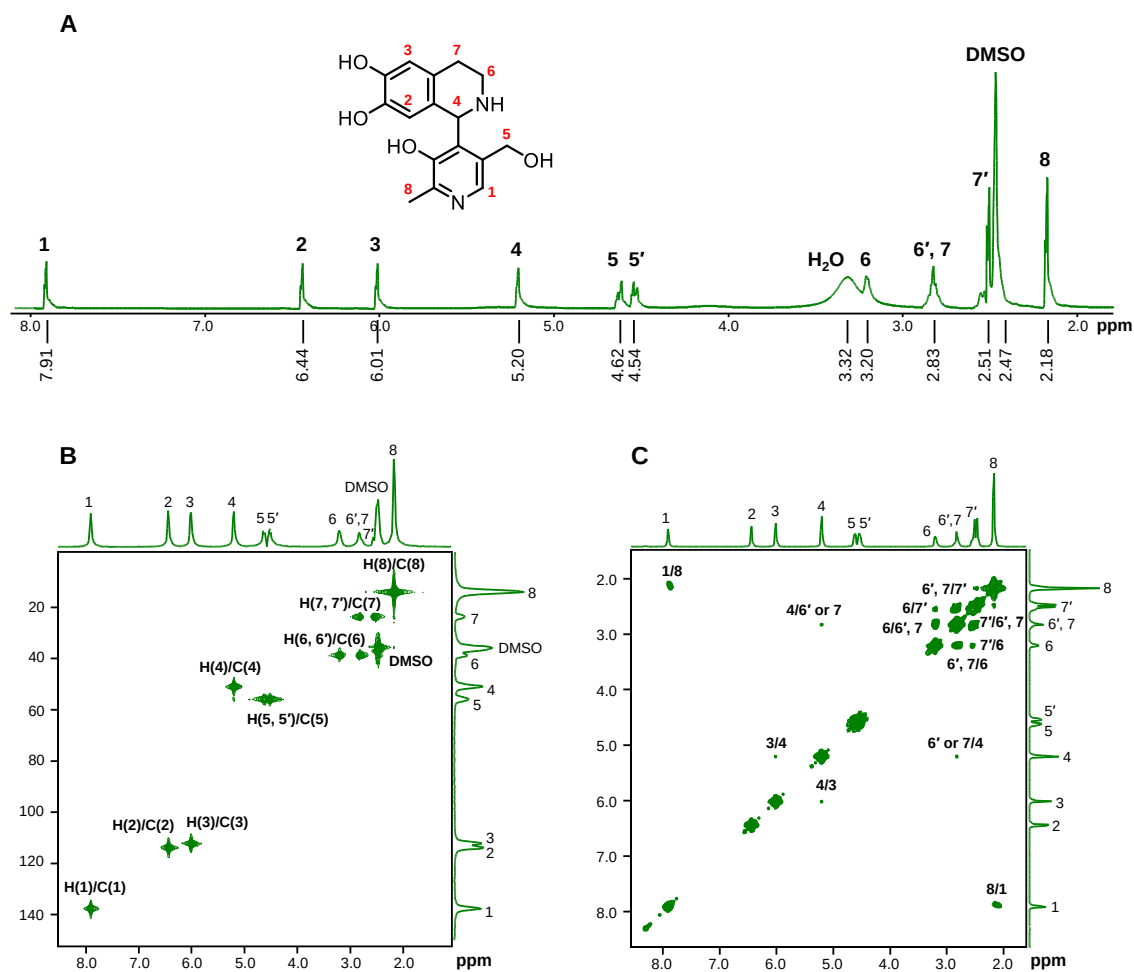


Figure S2. (A) ^1H NMR, (B) ^1H - ^{13}C HMQC, and (C) ^1H - ^1H COSY spectra of the PL-DA adduct (1-[3-hydroxy-5-(hydroxymethyl)-2-methylpyridin-4-yl]-1,2,3,4-tetrahydroisoquinoline-6,7-diol).

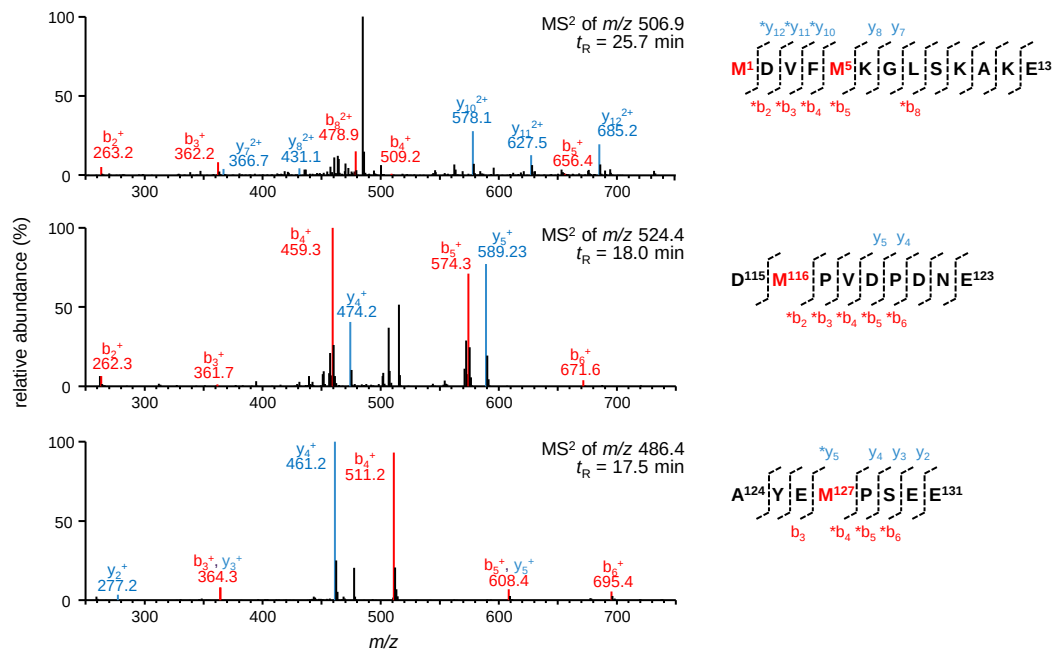


Figure S3. MS/MS spectra of V8 α -Syn peptides containing oxidized Met.