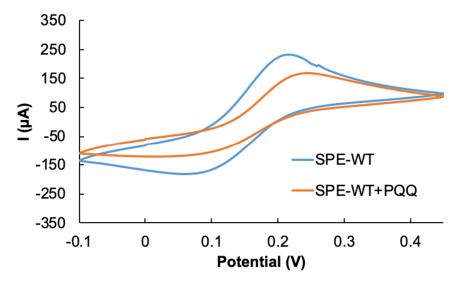
## Electronic Supplementary Information for

## Electrochemical flow injection analysis of interaction between pyrroloquinoline quinone (PQQ) and $\alpha$ -synuclein peptides related to Parkinson's disease

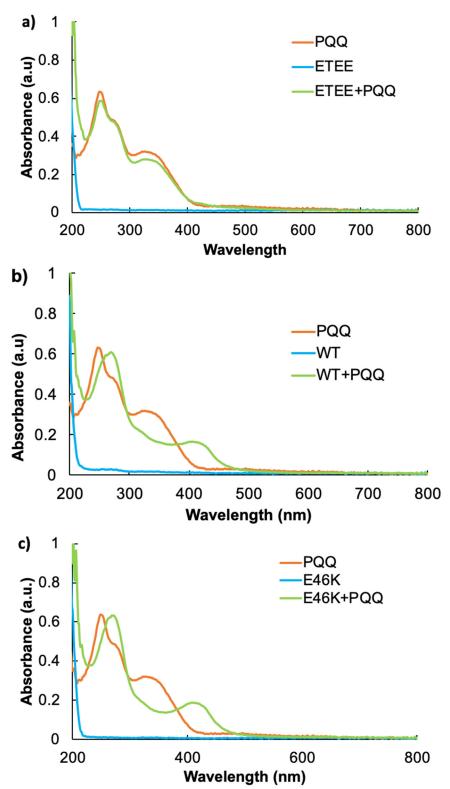
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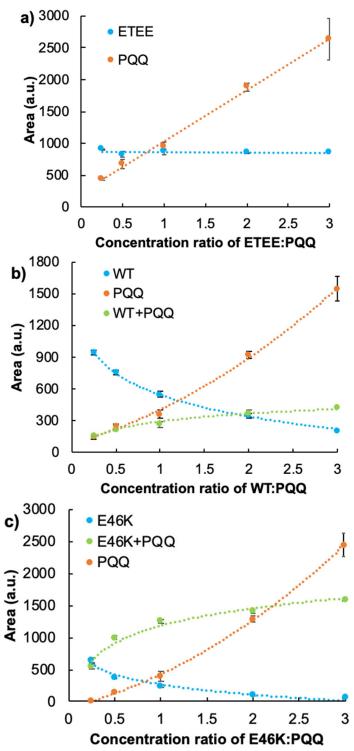
\*Corresponding author: <u>kagan.kerman@utoronto.ca</u>



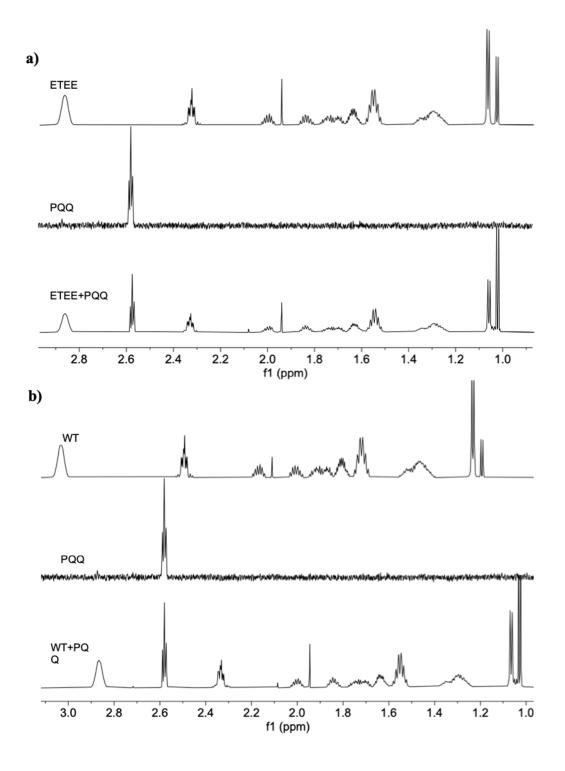
**Fig. S1** Cyclic voltammograms of the WT-modified SPE before (blue) and after (orange) interaction with PQQ at a scan rate of 100 mV/s with 10 mM  $[Fe(CN)_6]^{3-/4-}$  as the redox probe in 0.1 M NaClO<sub>4</sub> (pH 7.0).

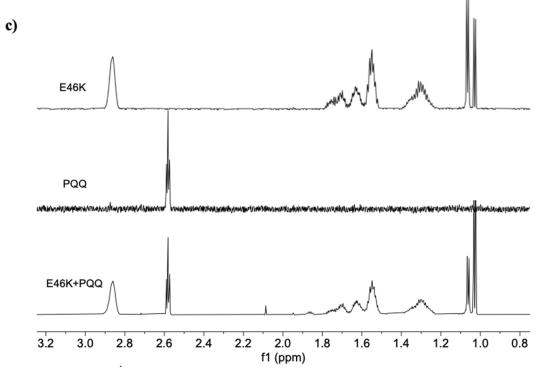


**Fig. S2** UV-vis spectra of 1 mM PQQ (orange), 1 mM peptide solution (blue), and peptide-PQQ complex (green) different species of  $\alpha$ -syn peptides a) ETEE, b) WT, and c) E46K.



**Fig. S3** Plots for the HPLC signals (area under the curve) analyzing the different peptide and PQQ ratios; with peptides alone in blue, peptides and PQQ in green, and PQQ alone in orange for different species of α-syn peptides a) ETEE, b) WT, and c) E46K. Error bars represent the standard deviation of triplicate measurements (n=3).





**Fig. S4** Up-field region H¹-NMR of peptides alone, PQQ alone, and peptide-PQQ complexes for a) ETEE, b) WT, and c) E46K.

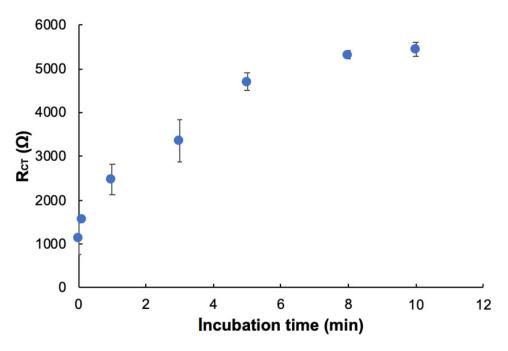
$$\mathbf{A}) \quad \overset{\mathsf{HO}}{\underset{\mathsf{NH}_2}{\mathsf{HO}}} \quad \overset{\mathsf{HO}}{\underset{\mathsf{N}}} \quad \overset{\mathsf{HO}}{\underset{\mathsf{N}}} \quad \overset{\mathsf{N}}{\underset{\mathsf{N}}} \quad \overset{\mathsf{N}}{\underset{\mathsf{N}$$

H<sub>2</sub>N-**GSKTKEG**-COOH

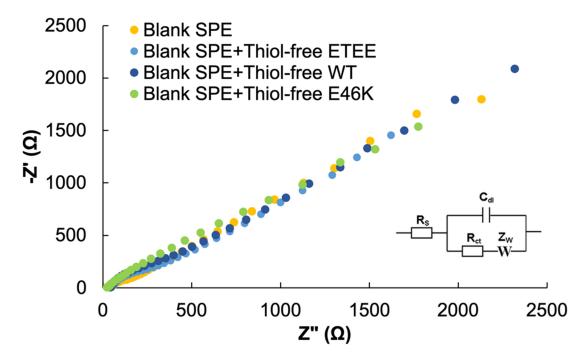
## Pyrroloquinoline quinone

## $H_2N$ -**GSKTKEG**-COOH x PQQ

**Fig. S5** Schematic illustration of A) WT peptide (GSKTKEG), B) Pyrroloquinoline quinone (PQQ) and C) the proposed structure of PQQ conjugated with WT peptide.



**Fig. S6** Plot for the dependence of  $R_{CT}$  on WT peptide-modified SPEs incubated with 0.01 μM PQQ for different durations of incubation. Error bars represent the standard deviation of triplicate measurements (n=3).



**Fig. S7** Nyquist plot of (yellow) blank gold screen-printed electrodes (SPEs) incubated with thiol-free (light blue) ETEE, (dark blue) WT and (green) E46K peptides. The redox probe was 10 mM  $[Fe(CN)_6]^{3-/4-}$  in 0.1 M NaClO<sub>4</sub> (pH 7.0).

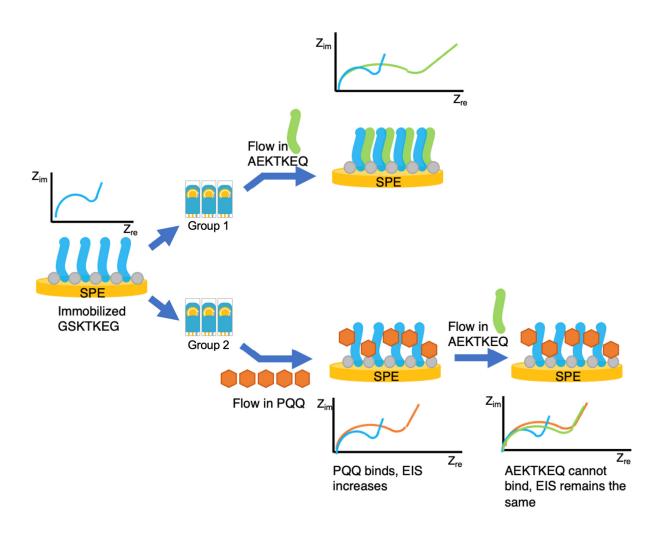


Fig. S8 Schematic illustration of the experimental design for studying the effects of PQQ on the intramolecular interactions of  $\alpha$ -syn misfolding as described in the results shown in Figure 8.