Supplementary materials: Interaction and Redox Chemistry Between Iron, Dopamine and Alpha-Synuclein C-Terminal Peptides

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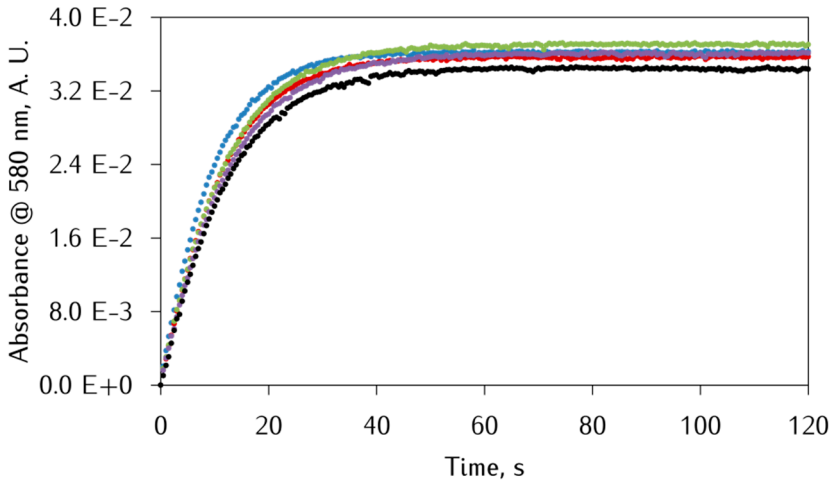


Figure S1. Kinetic traces of DA-Fe^{II} (20:1) interaction as a function of Ac-$_{\alpha Sp S119-132}$ concentration (λ_{max} = 580 nm) in 10 mM Mops buffer pH 7.0 and 37 °C, iron(II) 10 μM, DA 0.2 mM (blue) and increasing amount of Ac-$\alpha S^{P}S_{119-132}$ (0.5 equiv.: red, 1 equiv.: green, 1.5 equiv.: purple, 2 equiv.: black).

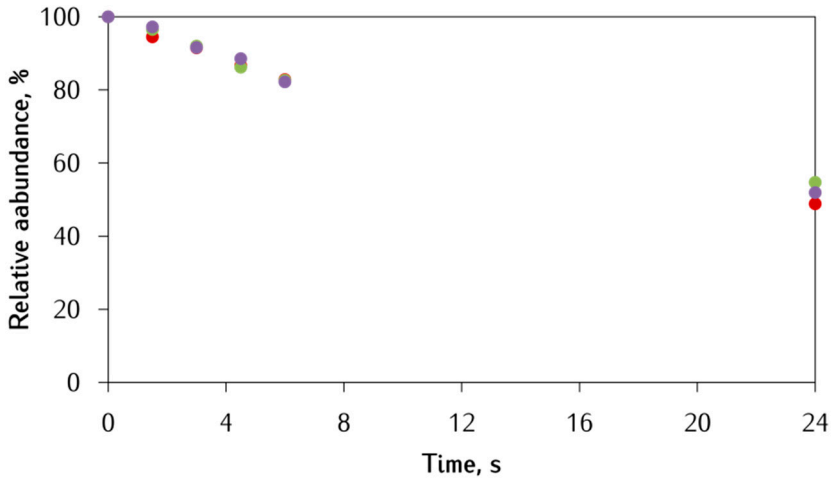


Figure S2. RP-HPLC kinetic traces of 200 μM DA in Mops buffer pH 7.0 and 37 °C (blue) in presence of 10 μM of iron(II) (red) and 2 equiv. of peptide (Ac-$\alpha S_{119-132}$: green, Ac-$\alpha S^{P}S_{119-132}$: purple, Ac-$\alpha S^{P}Y^{P}S_{119-132}$: cyan).

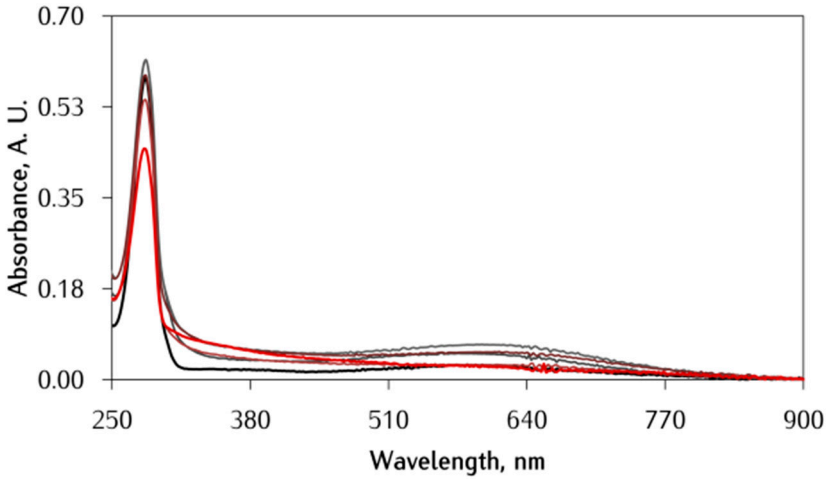


Figure S3. UV-Vis spectra of DA oxidation kinetics by Fe^{III}-Ac-αS119-132 complex (DA:Fe 20:1) in 10 mM Mops buffer pH 7.0 and SDS 20 mM, 37 °C; progression of time is rendered as color hue transition from black (0 h) towards red (24 h). Spectra were recorded at 0, 1.5, 3.0, 4.5, 6 and 24 h.

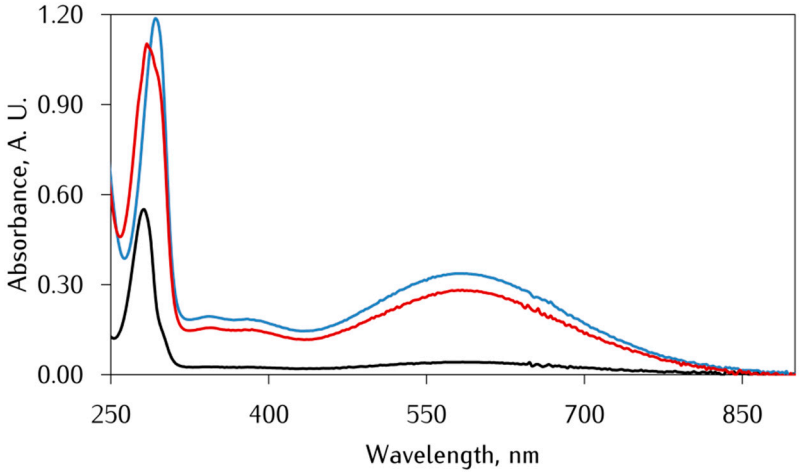


Figure S4. UV-Vis spectra of DA (200 μM) oxidation at 0 h in 10 mM Mops buffer pH 7.0 and 37 °C, in the presence of 10 μM of Fe^{II} (black), 100 μM of Fe^{II} (blue) or 100 μM Fe^{II} and 200 μM Ac-αS119-132 peptide (red).

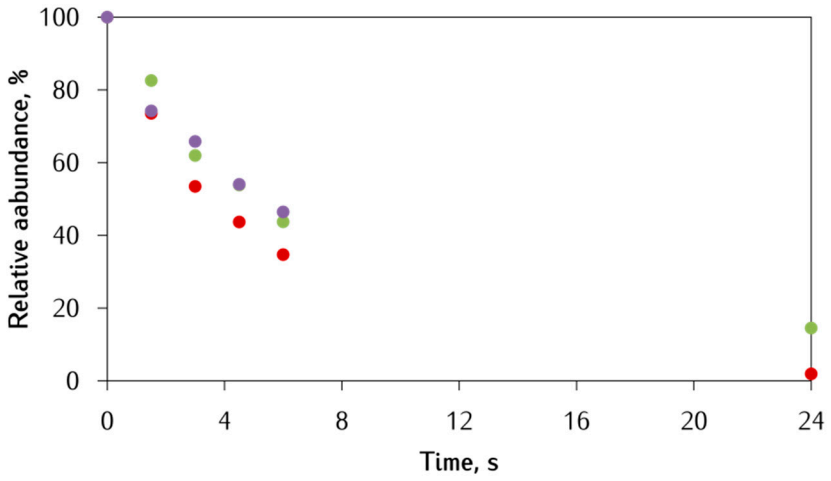
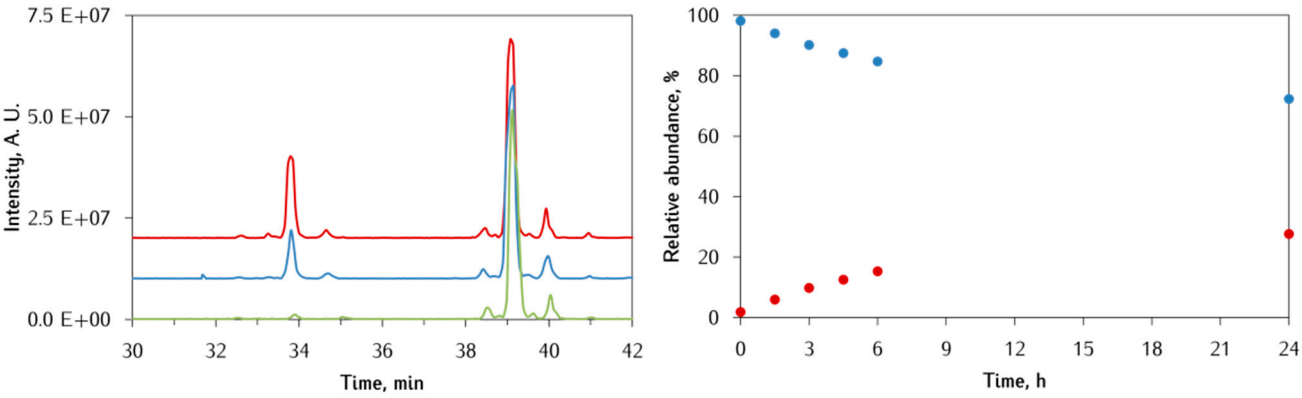
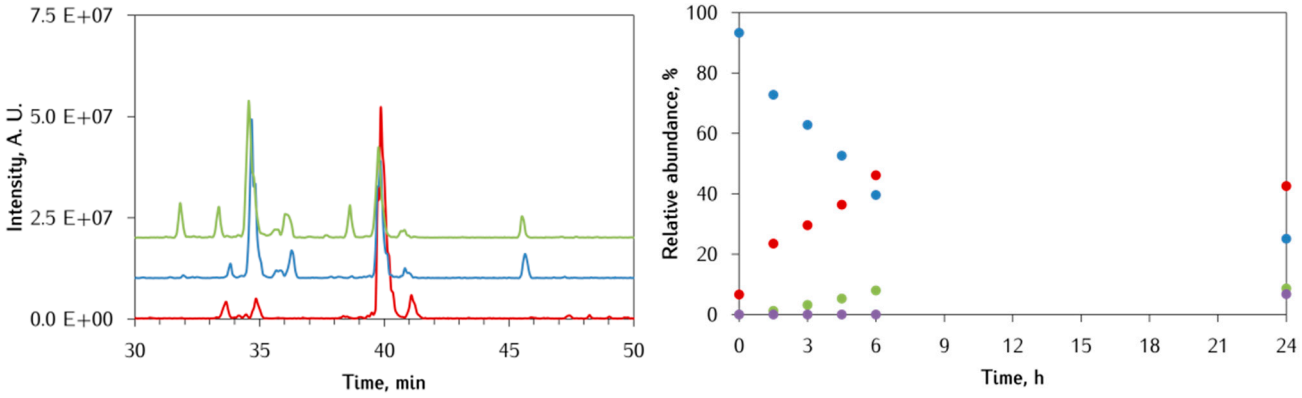


Figure S5. RP-HPLC kinetic traces of DA (200 μM) oxidation in Mops buffer pH 7.0 and 37 °C (blue) in the presence of 100 μM of Fe^{II} (red) and 2 equiv. of peptide (Ac-$\alpha S_{119-132}$: green, Ac-$\alpha S^{P}S_{119-132}$: purple).



(a) (b)

Figure S6. (a) HPLC-MS elution profiles of Ac-αS$_{119-132}$ (20 μM) in Mops buffer pH 7.0 at 37 °C, in the presence of Fe^{II} (10 μM) and DA (200 μM) at the beginning (blue), and after 6 h (red) and 24 h of incubation (green). (b) Percent modification detected by the HPLC-MS analysis: Ac-αS$_{119-132}$ (t_r 39 min, blue), Ac-αS$_{119-132}$ +16 (t_r 33.8 min, red).



(a) (b)

Figure S7. (a) HPLC-MS elution profiles of Ac-αSpS$_{119-132}$ (20 μM) in Mops buffer pH 7.0 at 37 °C, in the presence of Fe^{II} (10 μM) and DA (200 μM) at the beginning (blue), and after 6 h (red) and 24 h of incubation (green). (b) percent modification detected by HPLC-MS analysis: Ac-αS^{p}S$_{119-132}$ (t_r 40 min, blue), Ac-αS^{p}S$_{119-132}$ +16 (t_r 34.6 min, red), Ac-αS^{p}S$_{119-132}$ +32 (t_r 36.4 min, green), Ac-^{119}DPDNEAYEM*^{127} fragment (t_r 32 min, purple).

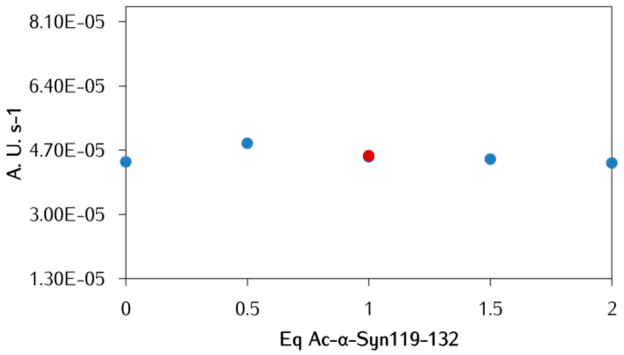


Figure S8. Slope of the kinetic traces of 3 mM DA oxidation by 25 μM Cu^{II} and 0-2 eq of Ac-$\alpha S_{119-132}$ in Hepes buffer pH 7.4, 37 °C. Red circle refers to DA autoxidation, while blue ones to Cu^{II}-Ac-$\alpha S_{119-132}$.