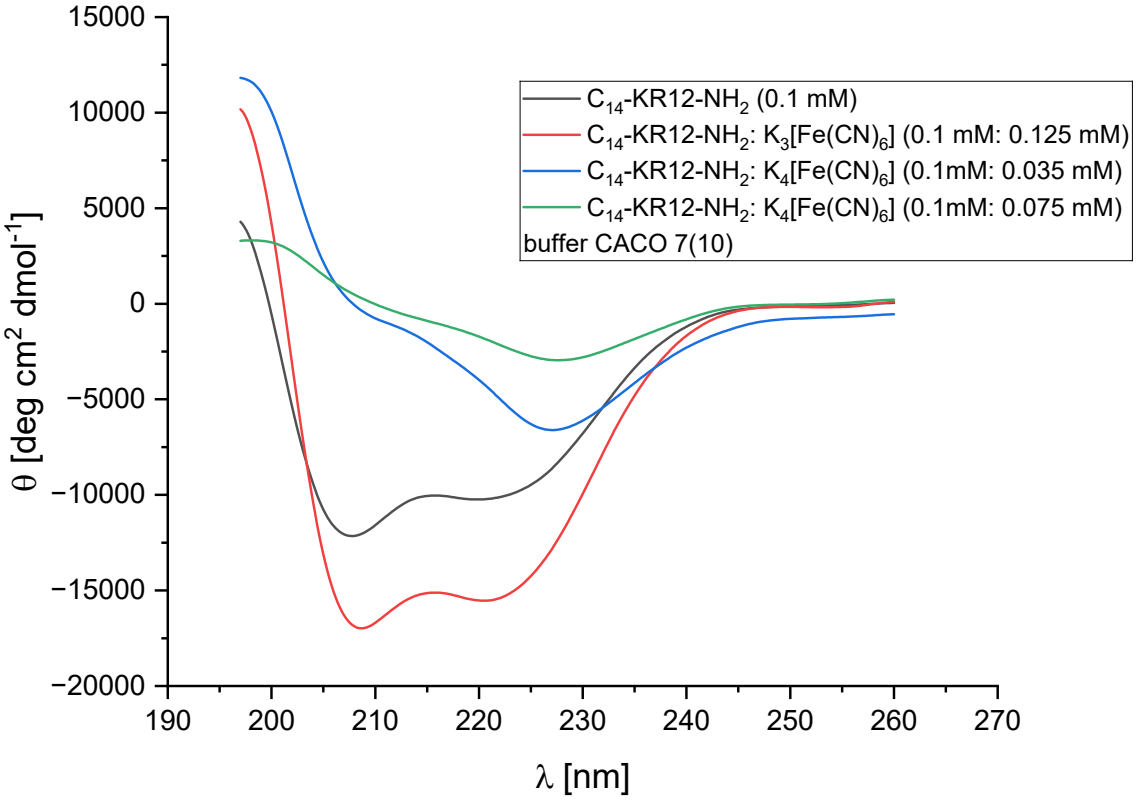


**Figure S1.** CD spectra of the C14-KR12 peptide in the presence of potassium ferricyanide ($K_3[Fe(CN)_6]$) and potassium ferrocyanide ($K_4[Fe(CN)_6]$) recorded in 10 mM sodium cacodylate buffer at pH 7 and 298.15 K.

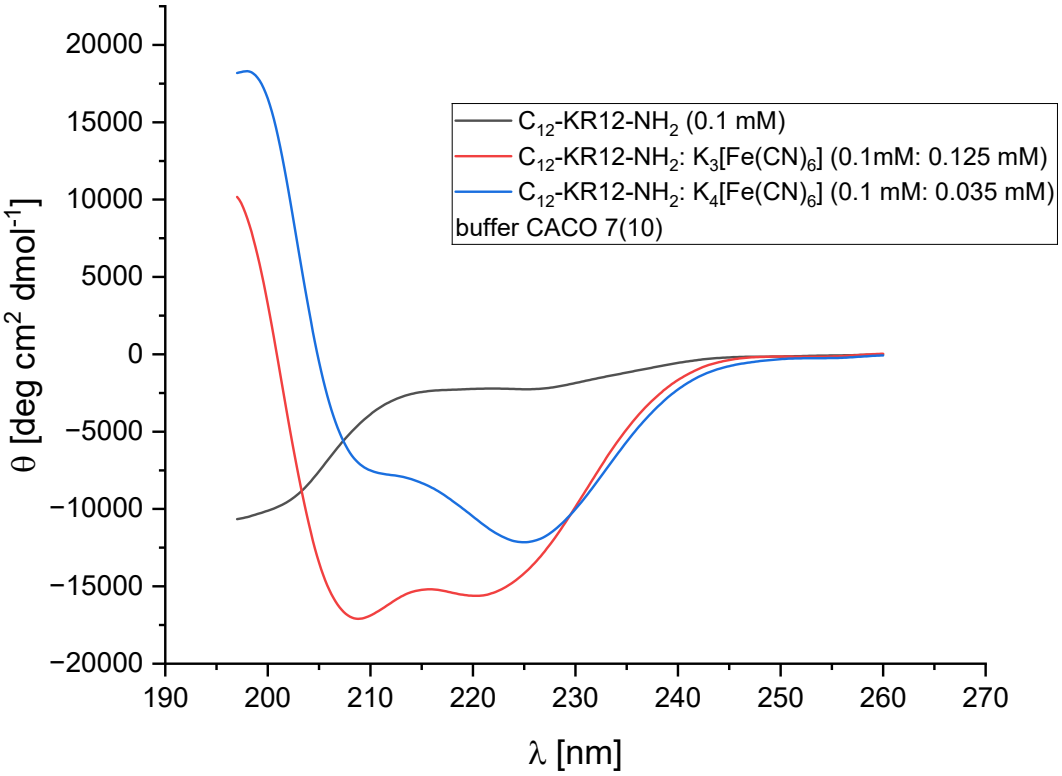


**Figure S2.** CD spectra of the C12-KR12 peptide in the presence of potassium ferricyanide ($K_3[Fe(CN)_6]$ and potassium ferrocyanide ($K_4[Fe(CN)_6]$) recorded in 10 mM sodium cacodylate buffer at pH 7 and 298.15 K.

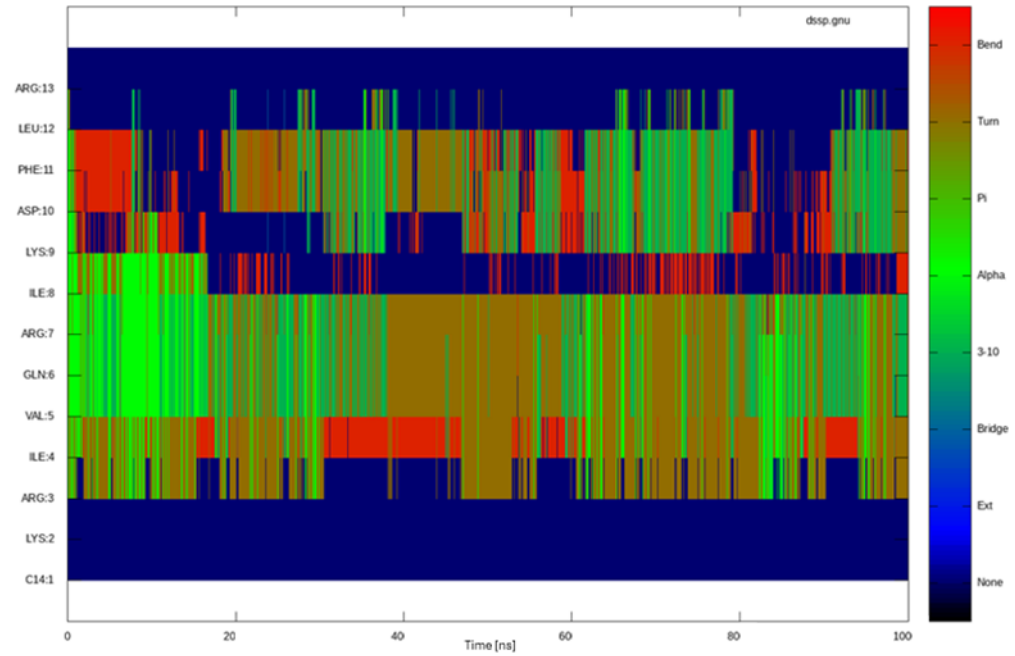


**Figure S3.** Time evolution of secondary structure elements of the C14-KR12 peptide in the presence of $[Fe(CN)_6]^{3-}$ obtained from the DSSP analysis for the MD simulation.

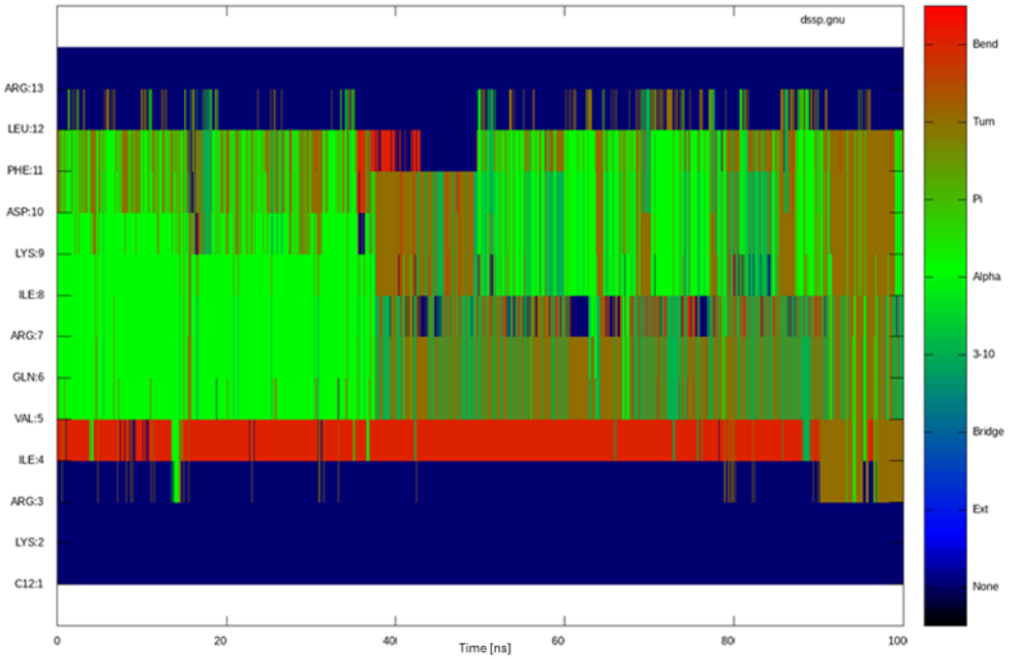


**Figure S4.** Time evolution of secondary structure elements of the C14-KR12 peptide in the presence of $[Fe(CN)_6]^{4-}$ obtained from the DSSP analysis for the MD simulation.

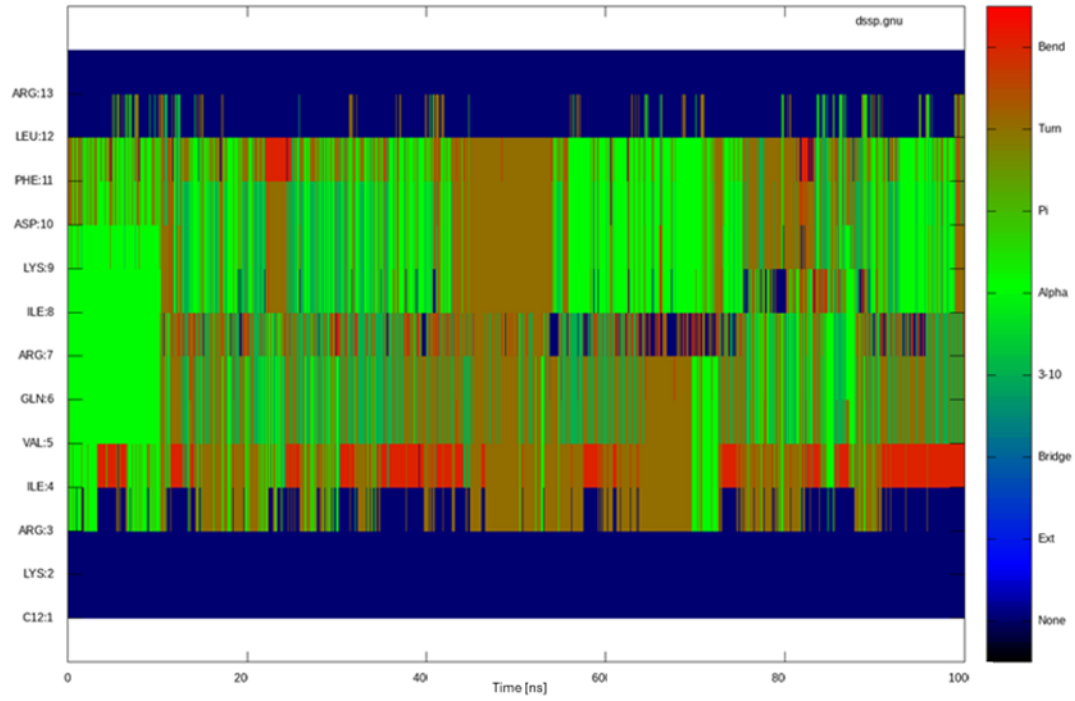


**Figure S5.** Time evolution of secondary structure elements of the C12-KR12 peptide in the presence of $[Fe(CN)_6]^{3-}$ obtained from the DSSP analysis for the MD simulation.

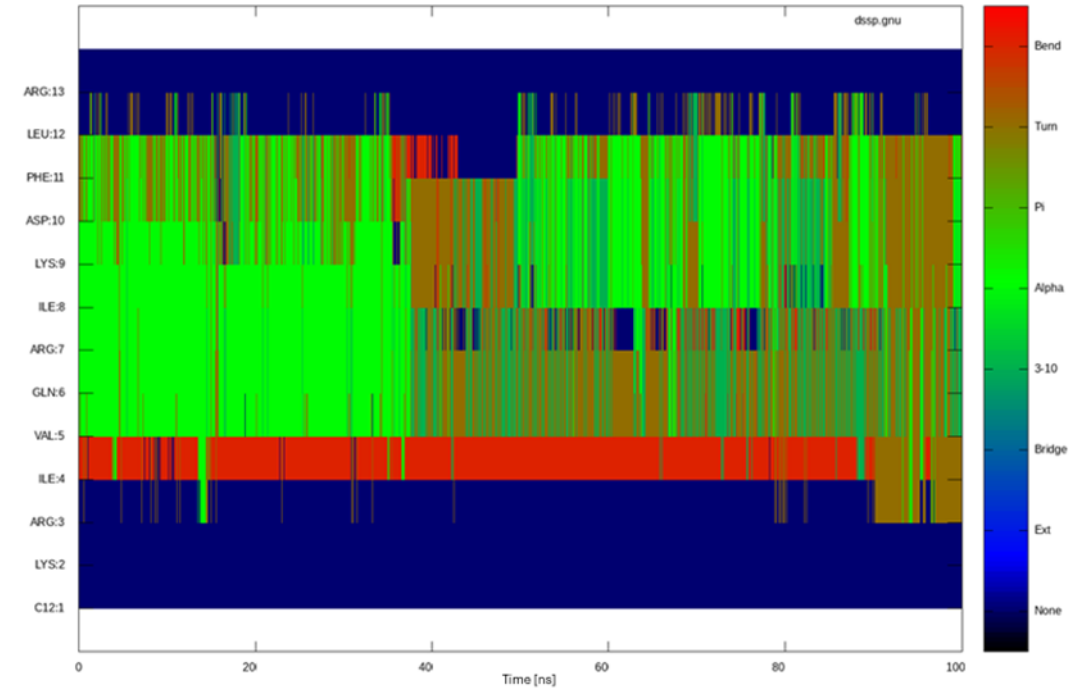


**Figure S6.** Time evolution of secondary structure elements of the C12-KR12 peptide in the presence of $[Fe(CN)_6]^{4-}$ obtained from the DSSP analysis for the MD simulation.

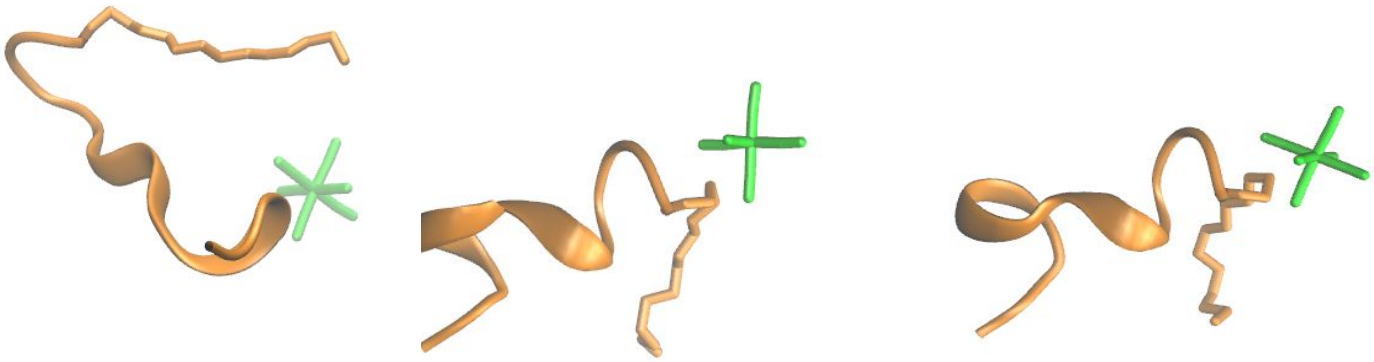

**Figure S7.** Representative MD snapshot of C14-KR12 in the presence of $[Fe(CN)_6]^{3-}$, showing a predominantly disordered structure with only transient helical elements.

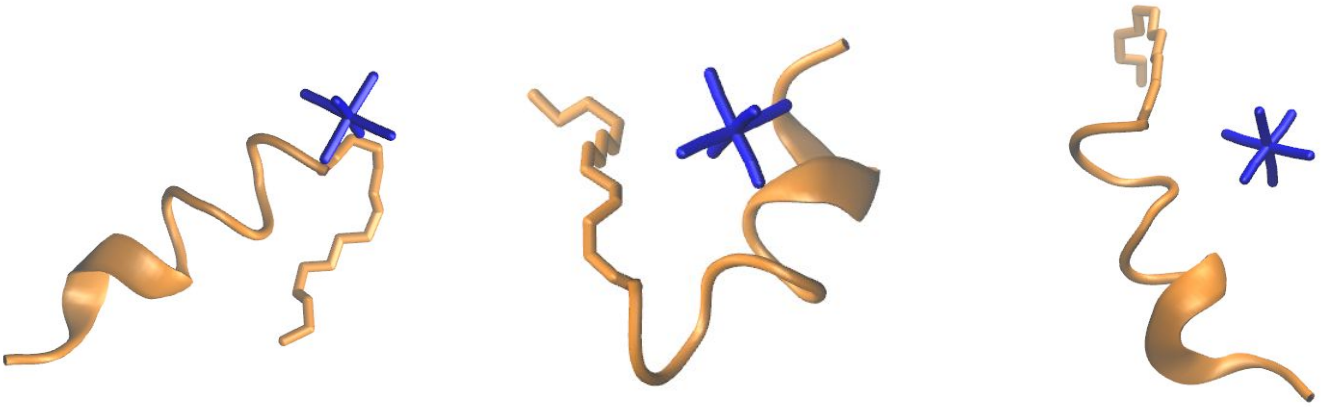

**Figure S8.** Representative MD snapshot of C14-KR12 in the presence of $[Fe(CN)_6]^{4-}$, illustrating partial stabilization and increased helical content.

**Table S1.** Average per-residue distances between the C14-KR12/ C12-KR12 peptides residues and the center of mass of $K_4[Fe(CN)_6]$/ $K_3[Fe(CN)_6]$.

| **C14-KR12 + $[Fe(CN)_6]^{4-}$** | |
|---|---|
| *Residue* | *Distance [Å]* |
| Lys1 | 7.1± 1.2 |
| Arg2 | 7.8± 1.4 |
| Ile3 | 13.3± 1.1 |
| Val4 | 13.3± 1.6 |
| Gln5 | 11.2± 2.4 |
| Arg6 | 14.2± 2.7 |
| Ile7 | 17.4± 1.6 |

| | |
|---|---|
| Lys8 | 19.0± 2.2 |
| Asp9 | 21.9± 1.5 |
| Phe10 | 18.2± 2.3 |
| Leu11 | 19.5± 2.7 |
| Arg12 | 21.0± 4.2 |
| **C14-KR12 + $[Fe(CN)_6]^{3-}$** | |
| *Residue* | *Distance [Å]* |
| Lys1 | 22.5±10.2 |
| Arg2 | 23.2±9.7 |
| Ile3 | 22.7±9.2 |
| Val4 | 22.8±9.6 |
| Gln5 | 23.9±9.5 |
| Arg6 | 23.9±9.5 |
| Ile7 | 23.3±9.5 |
| Lys8 | 23.9±9.2 |
| Asp9 | 24.9±8.6 |
| Phe10 | 25.2±8.5 |
| Leu11 | 25.9±8.1 |
| Arg12 | 27.6±6.9 |
| **C12-KR12 + $[Fe(CN)_6]^{4-}$** | |
| *Residue* | *Distance [Å]* |
| Lys1 | 8.7± 5.2 |
| Arg2 | 9.7± 5.8 |
| Ile3 | 14.5± 4.9 |
| Val4 | 14.8± 4.7 |
| Gln5 | 14.3± 5.7 |
| Arg6 | 16.2± 5.4 |
| Ile7 | 19.0± 4.3 |
| Lys8 | 22.3± 4.2 |
| Asp9 | 21.2± 4.8 |
| Phe10 | 20.0± 4.5 |
| Leu11 | 22.0± 4.3 |
| Arg12 | 25.9± 3.4 |
| **C12-KR12 + $[Fe(CN)_6]^{3-}$** | |
| *Residue* | *Distance [Å]* |

| | |
|---|---|
| Lys1 | 9.6± 6.3 |
| Arg2 | 10.3± 6.1 |
| Ile3 | 13.0± 5.4 |
| Val4 | 13.4± 4.8 |
| Gln5 | 13.6± 4.5 |
| Arg6 | 15.6± 4.5 |
| Ile7 | 16.7± 4.2 |
| Lys8 | 18.7± 4.5 |
| Asp9 | 19.4± 3.3 |
| Phe10 | 18.3± 4.3 |
| Leu11 | 19.2± 4.4 |
| Arg12 | 22.1± 4.2 |

**Table S2.** Radius of gyration (Rg) of single peptide systems (C12-KR12 and C14-KR12) in the presence of $[Fe(CN)_6]^{3-}$ and $[Fe(CN)_6]^{4-}$.

| *System* | *Rg [Å]* |
|---|---|
| C12-KR12 + $[Fe(CN)_6]^{3-}$ | 7.9± 0.4 |
| C12-KR12 + $[Fe(CN)_6]^{4-}$ | 7.8 ±0.3 |
| C14-KR12 + $[Fe(CN)_6]^{3-}$ | 7.9± 0.6 |
| C14-KR12 + $[Fe(CN)_6]^{4-}$ | 7.8 ±0.4 |

**Table S3.** Radius of gyration (Rg) of two peptide systems (C12-KR12 and C14-KR12) in complex with $[Fe(CN)_6]^{3-}$ and $[Fe(CN)_6]^{4-}$, including values for the entire complex and individual peptides.

| *System* | *Rg (complex) [Å]* | *Rg (peptide 1) [Å]* | *Rg (peptide 2) [Å]* |
|---|---|---|---|
| 1. C12-KR12 + $[Fe(CN)_6]^{3-}$ (initial orientation of hydrophobic tails parallel to each other) | 10.7 ± 1.3 | 8.7 ± 0.6 | 7.9 ± 0.3 |
| 2. C12-KR12 + $[Fe(CN)_6]^{3-}$ | Peptides dissociation | - | - |
| 3. C12-KR12 + $[Fe(CN)_6]^{3-}$ | Peptides dissociation | - | - |
| 1. C12-KR12 + $[Fe(CN)_6]^{3-}$ (initial orientation of hydrophobic tails antiparallel to each other) | 11.5 ± 2.7 | 10.7 ± 1.1 | 8.2 ± 0.3 |
| 2. C12-KR12 + $[Fe(CN)_6]^{3-}$ | Peptides dissociation | - | - |

| | | | |
|---|---|---|---|
| 3. C12-KR12 + $[Fe(CN)_6]^{3-}$ | Peptides dissociation | - | - |
| 1. C12-KR12 + $[Fe(CN)_6]^{4-}$ (initial orientation of hydrophobic tails parallel to each other) | 9.8 ± .4 | 8.0 ± 0.3 | 8.1 ± 0.3 |
| 2. C12-KR12 + $[Fe(CN)_6]^{4-}$ | 9.9 ± 04 | 8.1 ± 0.3 | 8.1 ± 0.2 |
| 3. C12-KR12 + $[Fe(CN)_6]^{4-}$ | Peptides dissociation | - | - |
| 1. C12-KR12 + $[Fe(CN)_6]^{4-}$ (initial orientation of hydrophobic tails antiparallel to each other) | 8.7 ± 0.2 | 8.2 ± 0.3 | 8.2 ± 0.3 |
| 2. C12-KR12 + $[Fe(CN)_6]^{4-}$ | 9.8 ± 1.3 | 8.1 ± 03 | 8.0 ± 0.3 |
| 3. C12-KR12 + $[Fe(CN)_6]^{4-}$ | 9.7 ± 0.4 | 8.0 ± 0.2 | 8.2 ± 0.3 |
| 1. C14-KR12 + $[Fe(CN)_6]^{3-}$ (initial orientation of hydrophobic tails parallel to each other) | Peptides dissociation | - | - |
| 2. C14-KR12 + $[Fe(CN)_6]^{3-}$ | Peptides dissociation | - | - |
| 3. C14-KR12 + $[Fe(CN)_6]^{3-}$ | 9.9 ± 0.8 | 8.3 ± 0.3 | 8.3 ± 0.3 |
| 1. C14-KR12 + $[Fe(CN)_6]^{3-}$ (initial orientation of hydrophobic tails antiparallel to each other) | Peptides dissociation | - | - |
| 2. C14-KR12 + $[Fe(CN)_6]^{3-}$ | 23.5 ± 10.9 | 7.9 ± 0.3 | 8.6 ± 0.5 |
| 3. C14-KR12 + $[Fe(CN)_6]^{3-}$ | 10.8 ± 1.7 | 8.4 ± 0.5 | 8.0 ± 0.3 |
| 1. C14-KR12 + $[Fe(CN)_6]^{4-}$ (initial orientation of hydrophobic tails parallel to each other) | Peptides dissociation | - | - |
| 2. C14-KR12 + $[Fe(CN)_6]^{4-}$ | 12.6 ± 2.9 | 8.1 ± 0.3 | 8.8 ± 0.7 |
| 3. C14-KR12 + $[Fe(CN)_6]^{4-}$ | Peptides dissociation | - | - |
| 1. C14-KR12 + $[Fe(CN)_6]^{4-}$ (initial orientation of hydrophobic tails antiparallel to each | Peptides dissociation | - | - |

| | | | |
|---|---|---|---|
| other) | | | |
| 2. C14-KR12 + $[Fe(CN)_6]^{4-}$ | Peptides dissociation | - | - |
| 3. C14-KR12 + $[Fe(CN)_6]^{4-}$ | Peptides dissociation | - | - |

**Table S4.** Solvent-accessible surface area (SASA) of single-peptide systems (C12-KR12 and C14-KR12) in the presence of $[Fe(CN)_6]^{3-}$ and $[Fe(CN)_6]^{4-}$.

| *System* | *SASA[Å²]* |
|---|---|
| C12-KR12 + $[Fe(CN)_6]^{3-}$ | 1836.1 ± 102.1 |
| C12-KR12 + $[Fe(CN)_6]^{4-}$ | 1768.9 ± 92.2 |
| C14-KR12 + $[Fe(CN)_6]^{3-}$ | 1818.3 ± 118.3 |
| C14-KR12 + $[Fe(CN)_6]^{4-}$ | 1739.4 ± 99.8 |

**Table S5**. Solvent-accessible surface area (SASA) of two peptide systems (C12-KR12 and C14-KR12) in the presence of $[Fe(CN)_6]^{3-}$ and $[Fe(CN)_6]^{4-}$.

| *System* | *SASA[Å²]* |
|---|---|
| 1. C12-KR12 + $[Fe(CN)_6]^{3-}$ (initial orientation of hydrophobic tails parallel to each other) | 3183.0 ±189.6 |
| 2. C12-KR12 + $[Fe(CN)_6]^{3-}$ | Peptides dissociation |
| 3. C12-KR12 + $[Fe(CN)_6]^{3-}$ | Peptides dissociation |
| 1. C12-KR12 + $[Fe(CN)_6]^{3-}$ (initial orientation of hydrophobic tails antiparallel to each other) | 3365.2 ± 304.3 |
| 2. C12-KR12 + $[Fe(CN)_6]^{3-}$ | Peptides dissociation |
| 3. C12-KR12 + $[Fe(CN)_6]^{3-}$ | Peptides dissociation |
| 1. C12-KR12 + $[Fe(CN)_6]^{4-}$ (initial orientation of hydrophobic tails parallel to each other) | 3572.5 ±137.9 |
| 2. C12-KR12 + $[Fe(CN)_6]^{4-}$ | 3589.0 ± 182.3 |
| 3. C12-KR12 + $[Fe(CN)_6]^{4-}$ | Peptides dissociation |
| 1. C12-KR12 + $[Fe(CN)_6]^{4-}$ (initial orientation of hydrophobic tails antiparallel to each other) | 2929.5 ± 178.6 |
| 2. C12-KR12 + $[Fe(CN)_6]^{4-}$ | 2955.5 ± 168.8 |
| 3. C12-KR12 + $[Fe(CN)_6]^{4-}$ | 3065.8 ± 229.4 |
| 1. C14-KR12 + $[Fe(CN)_6]^{3-}$ (initial orientation of hydrophobic tails parallel to each other) | Peptides dissociation |
| 2. C14-KR12 + $[Fe(CN)_6]^{3-}$ | Peptides dissociation |
| 3. C14-KR12 + $[Fe(CN)_6]^{3-}$ | 3108 ± 132.9 |
| 1. C14-KR12 + $[Fe(CN)_6]^{3-}$ (initial orientation of hydrophobic tails antiparallel to each other) | Peptides dissociation |
| 2. C14-KR12 + $[Fe(CN)_6]^{3-}$ | 3268.0 ± 184.8 |
| 3. C14-KR12 + $[Fe(CN)_6]^{3-}$ | 3315.4 ± 306.4 |
| 1. C14-KR12 + $[Fe(CN)_6]^{4-}$ (initial orientation of hydrophobic tails parallel to each other) | Peptides dissociation |
| 2. C14-KR12 + $[Fe(CN)_6]^{4-}$ | 3455.6 ± 142.3 |
| 3. C14-KR12 + $[Fe(CN)_6]^{4-}$ | Peptides dissociation |
| 1. C14-KR12 + $[Fe(CN)_6]^{4-}$ | Peptides dissociation |

| | |
|---|---|
| (initial orientation of hydrophobic tails antiparallel to each other) | |
| 2. C14-KR12 + $[Fe(CN)_6]^{4-}$ | Peptides dissociation |
| 3. C14-KR12 + $[Fe(CN)_6]^{4-}$ | Peptides dissociation |