Supplementary Information to the manuscript

"A peptide-base trap for metal ions studied by electron paramagnetic resonance"

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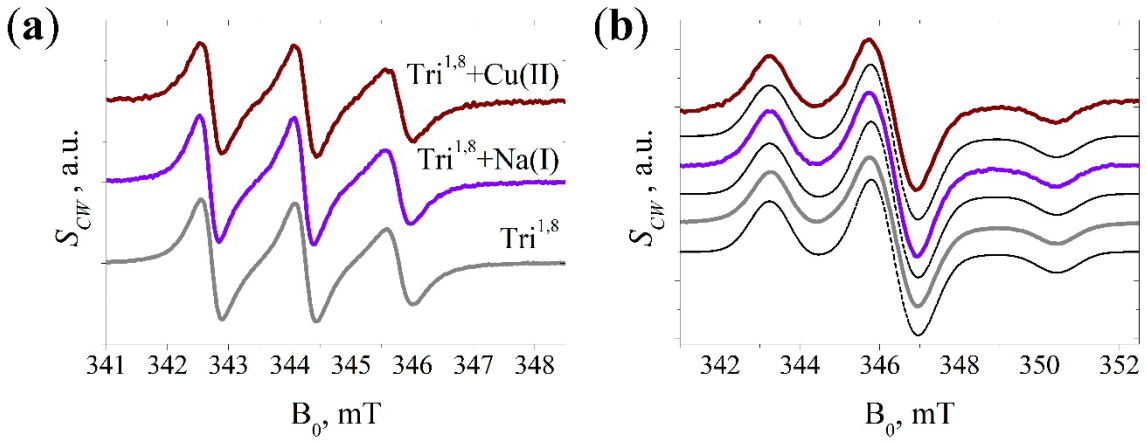

Figure S1. Continuous wave EPR spectra for $Tri^{1,8}$ with or without metal ions, acquired at room temperature (**a**), or at 100 K (**b**). The systems are identified by the same color in both panels. EPR spectra simulations are reported as dashed lines.

Table S1. *Best fit parameters for nitroxides and Cu(II) at 100K.*

Sample	*g*-tensor	A-tensor, MHz	linewidth, mT
$Tri^{1,8}$	[2.0093 2.0104 2.0045] ± 0.001	[15.6 15.02 100.2] ± 1	1.1 ($Tri^{1,8}$) 1.05-1.1 ($Tri^{1,8}$ + Na(I)) 1.05-1.1 ($Tri^{1,8}$ + Ca(II)) 1.1-1.12 ($Tri^{1,8}$ + Cu(II))
Cu(II)	[2.088 2.088 2.424]	A⊥ = 400	3-3.5
Tri-Cu(II)	[2.088 2.088 2.424]	A⊥ = 400	4-4.5

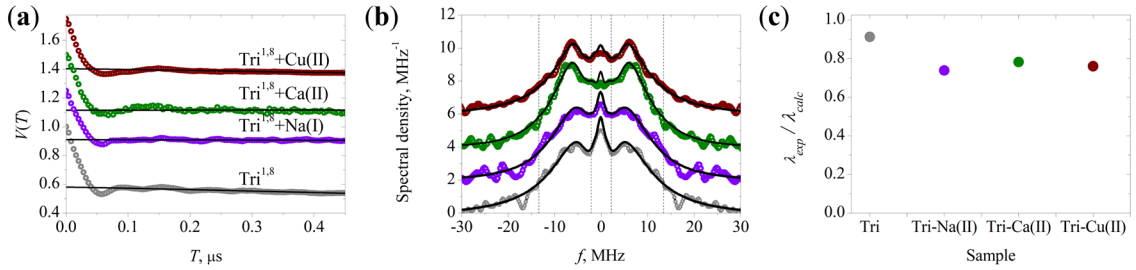

Figure S2. (**a**) Primary DEER traces for metal-ion free and metal-ion containing samples. Dashed lines show the background decay. Traces are shifted up for clarity. (**b**) Dipolar spectra in the frequency domain. Circles are experimental data; solid lines are best fit from the simulations. Spectra are shifted up for clarity. The vertical dashed lines show the area of the *open window* in the frequency domain. (**c**) The experimental modulation depth (λ_{exp}) *vs* the expected modulation depth (λ_{calc}). The systems are identified by the same color in all panels.

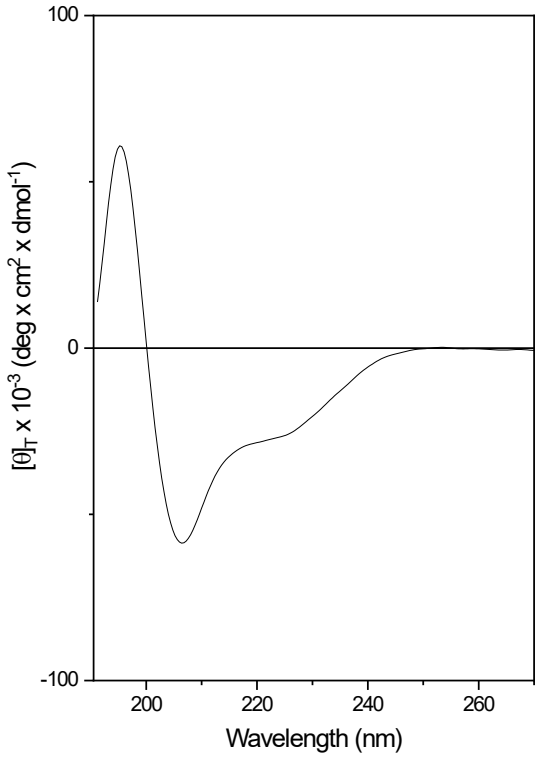

Figure S3. Circular dichroism spectrum acquired for Tri[1,8] under the same experimental condition as EPR. Peptide concentration: $2x10^{-4}$M in ethanol/methanol 95:5.

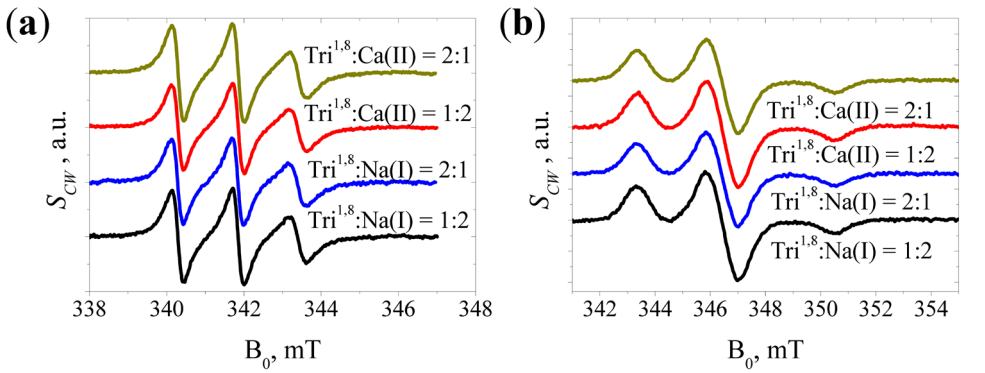

Figure S4. Continuous wave EPR spectra acquired at room temperature (**a**) and at 100 K (**b**) for the double-labeled peptide $Tri^{1,8}$ with sodium or calcium ions.

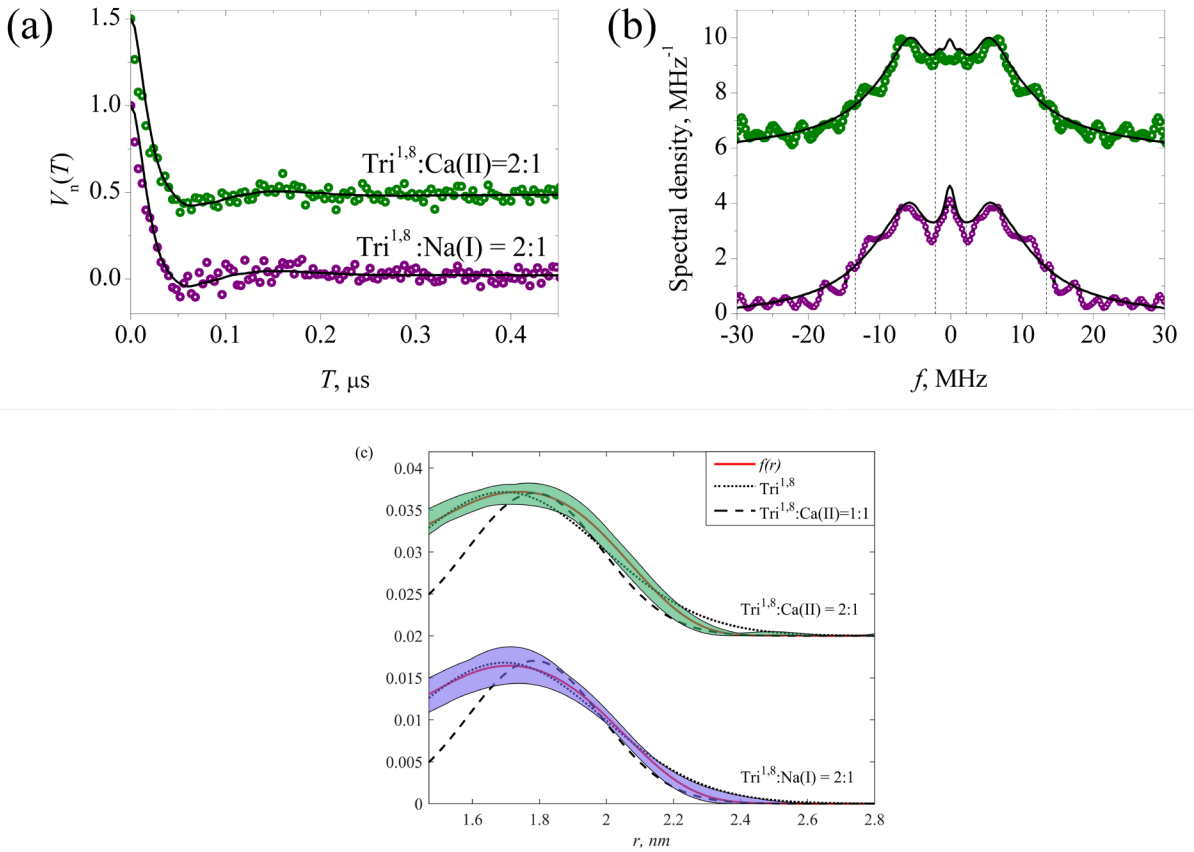

Figure S5. Normalized dipolar traces for Tri^{1,8} with sodium or calcium ions (experimental data are shown as magenta or green circles, respectively) in the time- (**a**) and frequency-domain (**b**), and their fits. The distance distribution functions (red curves) with confidence interval (shaded areas), evaluated by the validation tool of the DeerAnalysis software (version 2018) are reported in panel (**c**). The distance distribution function obtained for Tri^{1,8} without ions (black dotted line) is reported as a reference, while the black, dashed line is the distance distribution function obtained for the system Tri^{1,8}/Ca(II) 1:1. Spectra are shifted for clarity.