Supporting Information.

Title:
Structure of *trans*-resveratrol in complex with the cardiac regulatory protein troponin C.

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Figure 1: Oxidation rate determined by following the chemical shift change of H2/H6 over time. The initial starting chemical shift was normalized to one, and the chemical shift was measured at each time point. Since the H2/H6 is a doublet, the chemical shift from the further downfield peak of the doublet was measured.

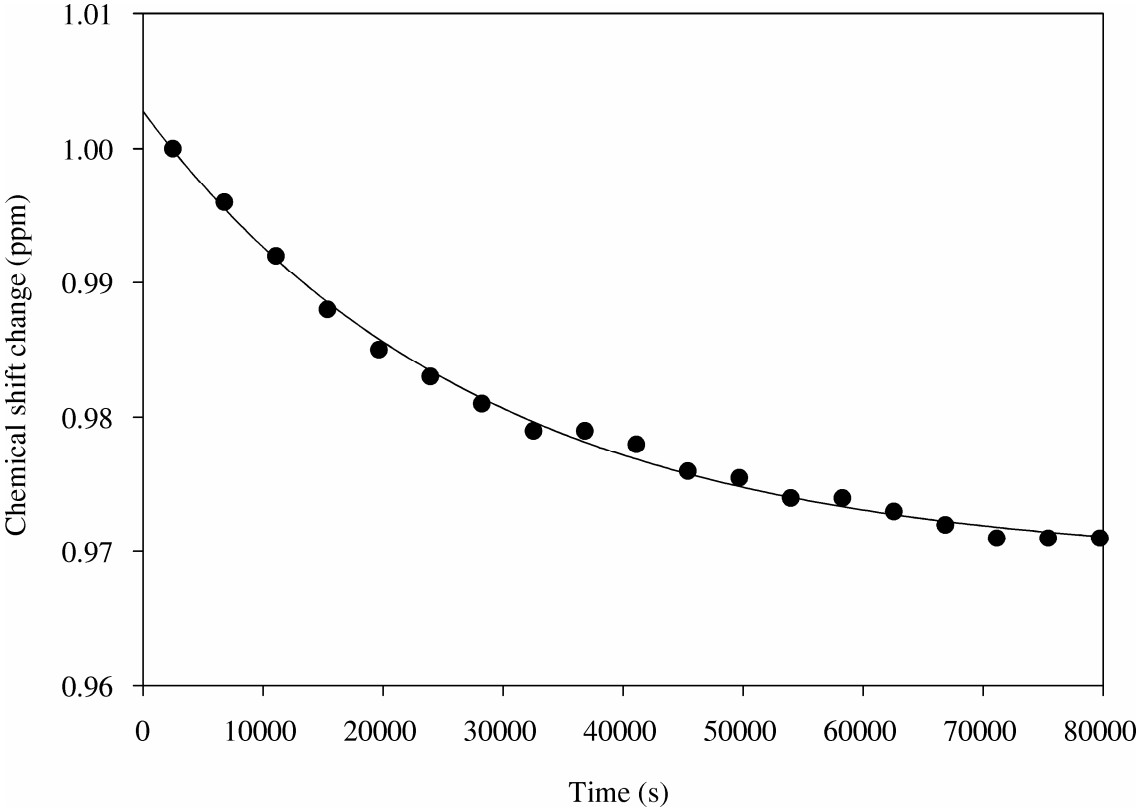

Figure 2: ROEs measured at each mixing time.

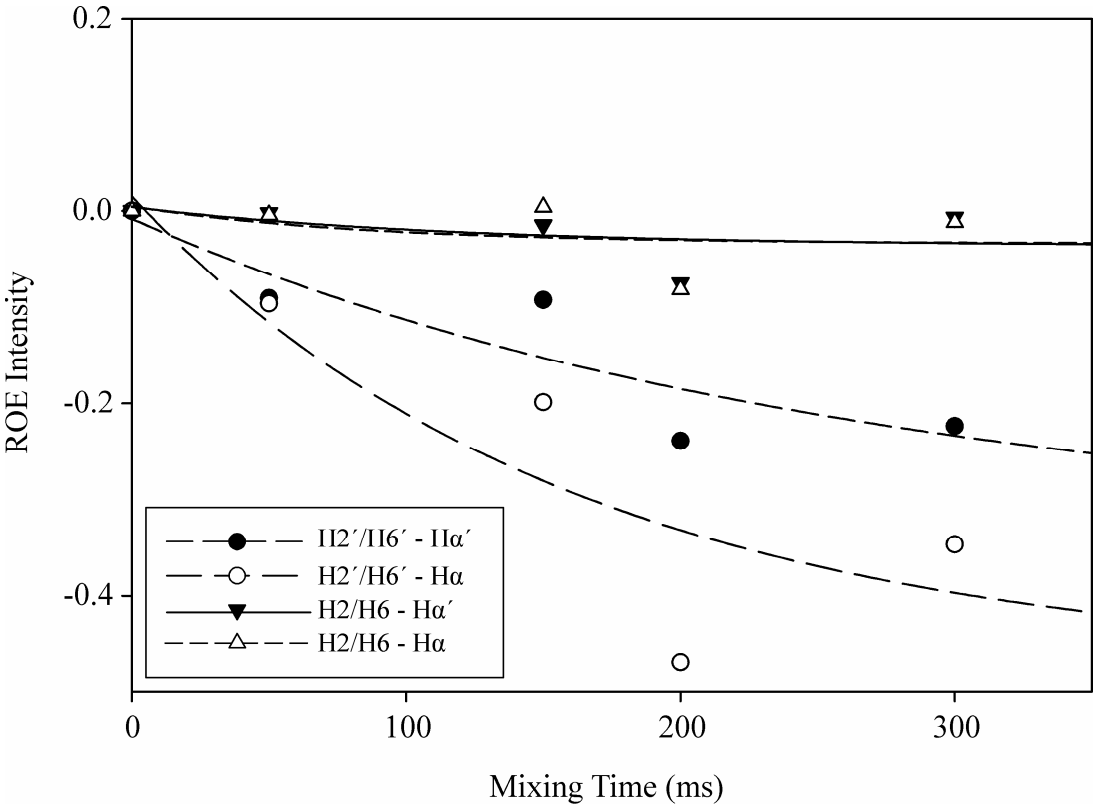

Figure 3: Binding of resveratrol to cTnC. a. $^{1}H,^{15}N$-HSQC spectra of cCTnC acquired throughout the titration with resveratrol. The first point in the titration is represented with 20 contours; whereas, each titration point with resveratrol is represented by a single contour (O). Direction of CSPs are indicated by arrows for several peaks. **b.** fitting of $^{1}H,^{15}N$-HSQC with xcrvfit to determine the dissociation constant. **c.** Bar graph of the total chemical shift change ($\Delta\delta = \sqrt{(\Delta\delta_H)^2 + \frac{1}{25}(\Delta\delta_N)^2}$) versus residue number for the titration of resveratrol into cTnC (light grey) and cCTnC (dark grey).

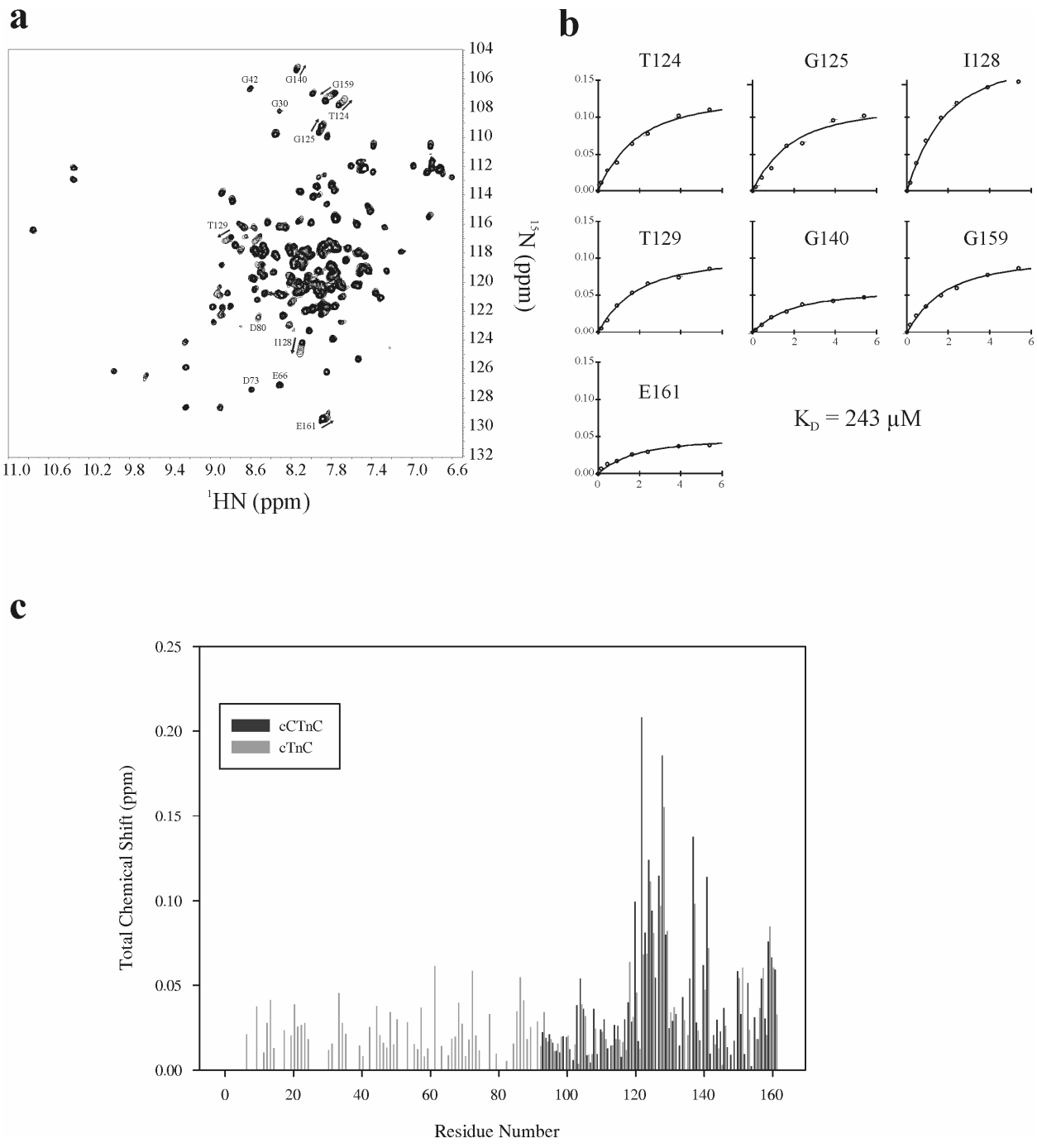

Figure 4: Ligand dependant chemical shift perturbations of cCTnC. Bar graph of the total chemical shift change ($\Delta\delta = \sqrt{(\Delta\delta_H)^2 + \frac{1}{25}(\Delta\delta_N)^2}$) versus residue number for the titration of $cTnI_{34\text{-}71}$ (red), EGCg (orange), EMD 57033 (yellow), and resveratrol (green) into cCTnC. Chart on the right is an expansion of the bar chart; $cTnI_{34\text{-}71}$ CSPs have been removed for clarity.

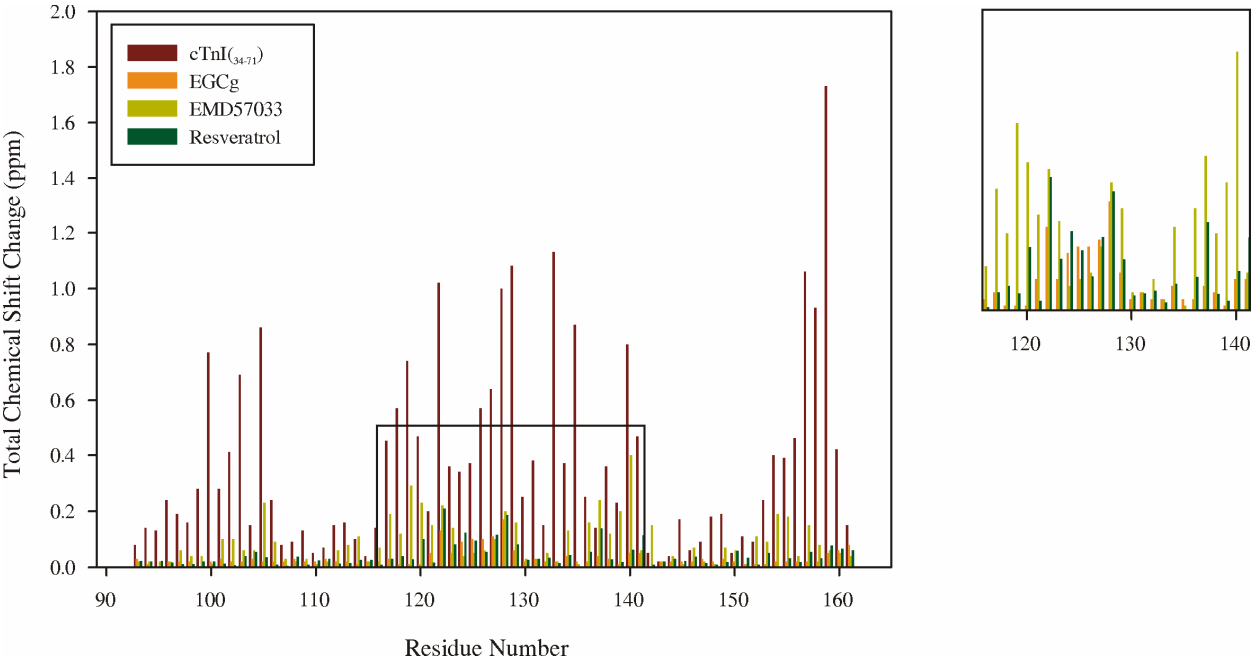

Figure 5: Intramolecular NOEs of resveratrol in complex with cCTnC.

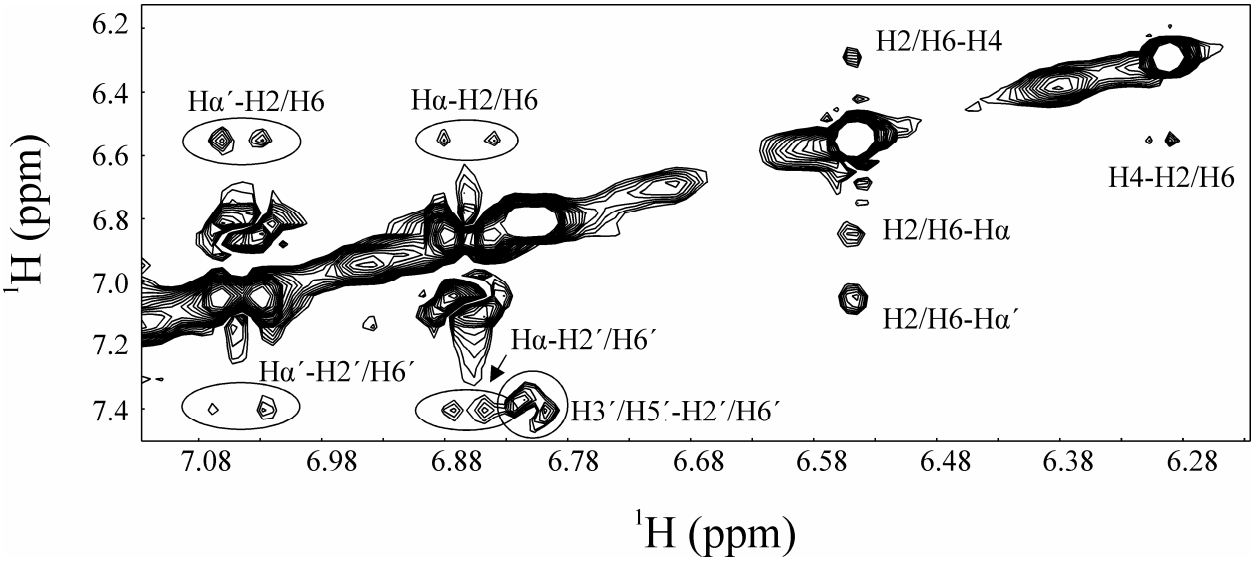

Table 1: Structural statistics for 20 NMR structures of cCTnC•resveratrol.

	Backbone atoms	**Heavy Atoms**
R.m.s.d. from the average structure		
All residues (Å)	0.93 ± 0.14	1.42 ± 0.13
Ordered residues [a] (Å)	0.72 ± 0.11	1.21 ± 0.13
Total Distance Restraints	925	
Short range (|*i-j*|=1) NOEs	519	
Medium range (1<|*i-j*|<5) NOEs	201	
Long range (|*i-j*|≥5) NOEs	179	
Intermolecular NOEs	23	
Intramolecular NOEs	4	
Ca^{2+} distance restraints	12	
Dihedral restraints (ϕ/ψ)	106	
NOE violations per structure		
> 0.5 Å	0	
> 0.3 Å	0	
> 0.1 Å	2.15	
Dihedral Violations > 5º	0	
Ramachadran plot statistics [b]		
ϕ/ψ in most favored regions (%)	83.2 %	
ϕ/ψ in additionally allowed regions (%)	15.3 %	
ϕ/ψ generously allowed regions (%)	1.4 %	
ϕ/ψ in disallowed regions (%)	0.1 %	

[a] Residues 92-105,111-124,and 131-158

[b] For all residues as determined by PROCHECK