Electronic Supplementary Material (ESI) for Dalton Transactions.

Interaction of a Gold(I) Dicarbene Anticancer Drug with Human Telomeric DNA G-Quadruplex: Solution and Computationally Aided X-ray Diffraction Analysis

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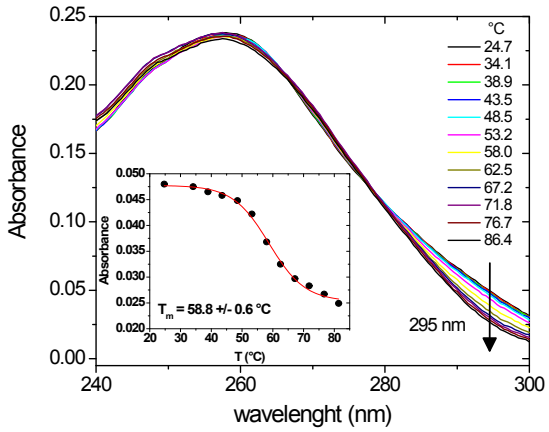

Figure S0. Example of variation of absorbance profile for the $[Au(NHC)_2]^+$/Tel 23 system at different temperatures; [Tel23] = 1.0 µM, r = $[Au(NHC)_2]^+$/Tel 23 = 5.0, 50 mM potassium phosphate buffer, pH = 7.0, cell path 1.0 cm. Inset is the simoidal fit of the absorbance at 292 nm vs. temperature plot which provides the melting temperature, T_m.

Table S1. Data collection and data refinement about the crystal structure of the adduct formed by the complex $[Au(NHC)_2]^+$ and the human telomeric sequence Tel24.

Data collection	
Wavelength	0.872900 Å
Cell parameters	a = 36.600 b = 71.370 Å c = 27.050 Å β = 92.42°
Crystal system	monoclininc
Space Group	C 2
Resolution limits	35.62-1.6(1.70-1.60) Å
Number of reflections	48359 (5872)
Rsym	11.0 (265.5)
Multiplicity	5.4 (4.5)
Completeness (%)	97.6 (90.4)
< I / σ(I) >	6.04(0.45)
CC (1/2)	99.2 (22.5)
Refinement	

Resolution range	35.62-2.00Å
Unique reflections (working/free)	4178/517
Rfactor	22.8%
Rfree factor	25.3%
Non-hydrogen atoms	567
Drug atoms	21
Water molecules	39
RMSD bonds	0.004
RMSD angles	1.114

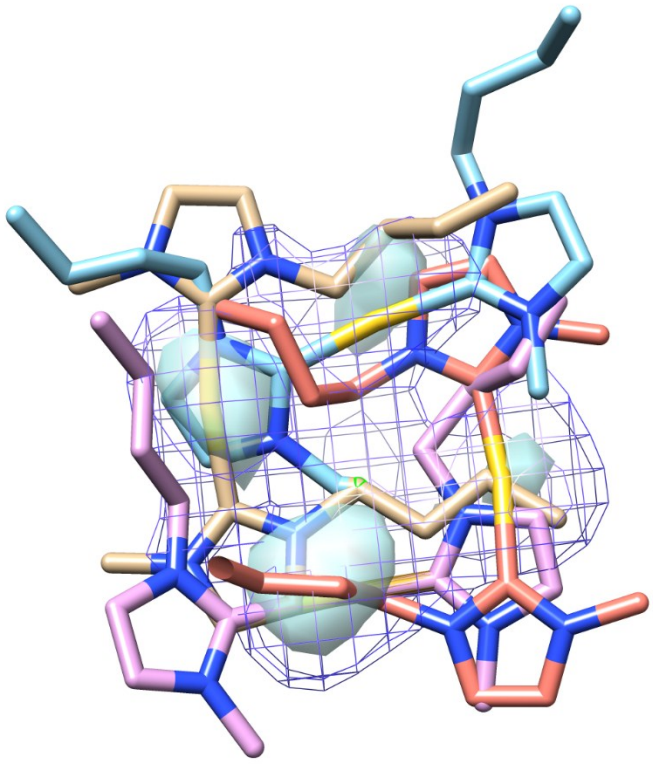

Figure S1 Skeleton of the disordered [Au(NHC)2]+ complex, spread over four crystallographic positions. The following color code has been used to identify each single position: salmon (Au1), tan (Au2), light brown (Au3), light pink (Au4). OMIT electron density map (meshed) and anomalous Fourier difference map for the gold ions (continuous) contoured at 1.5σ and 3σ levels, respectively.