

## Supplementary Information

# Interaction of dpyatriz and Cu/Zn-dpyatriz complexes with human telomere DNA: The role of G-quadruplex formation and its effect on antitumor and antitelomerase activity

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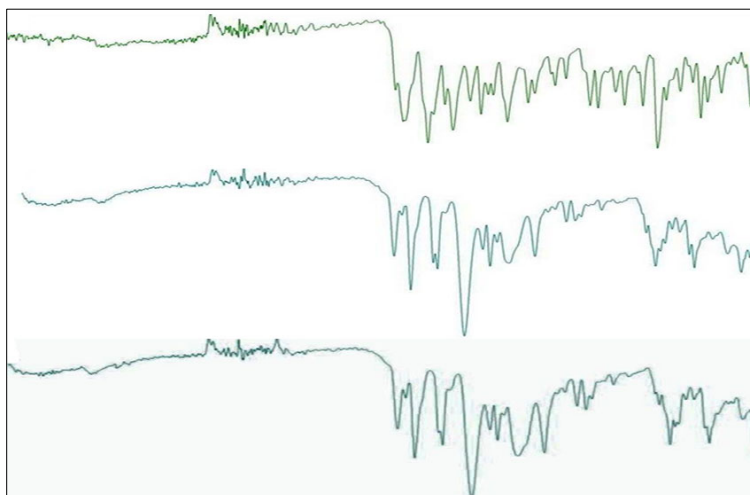
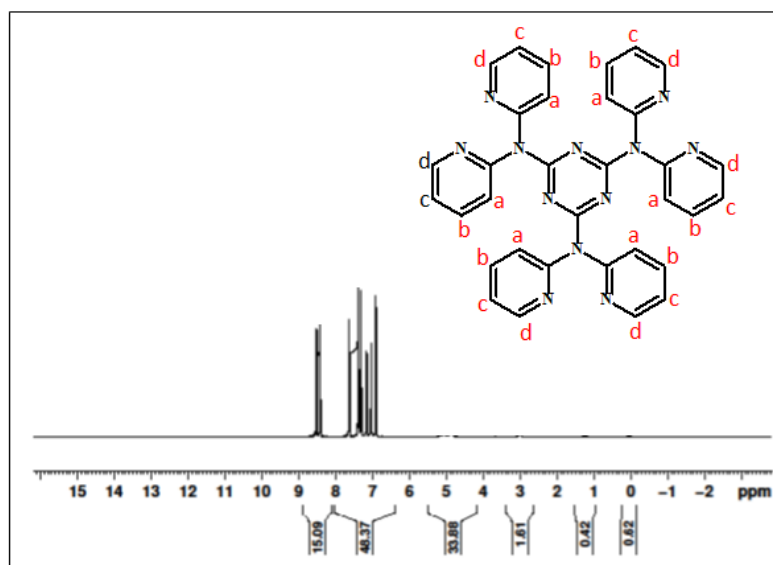
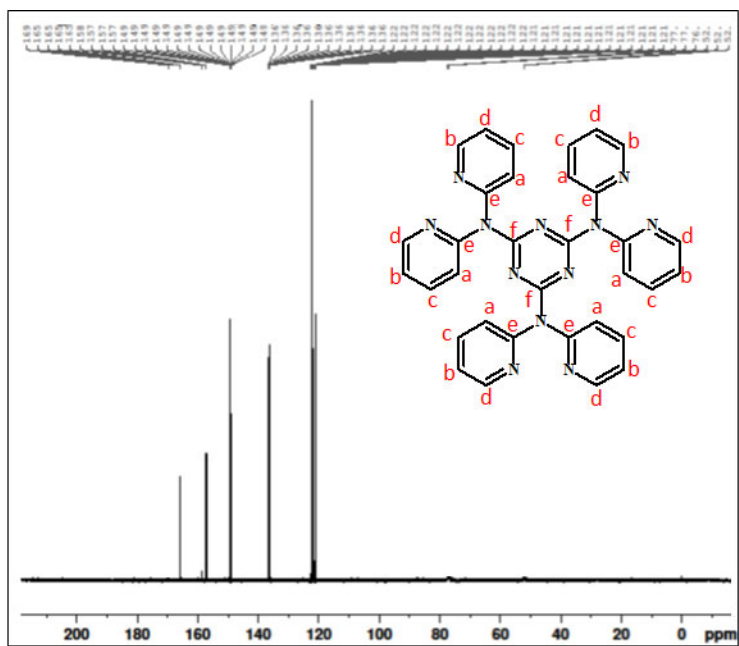


Fig. S1 — IR spectra of dpyatriz, Cu- dpyatriz, Zn- dpyatriz



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz) 6.90 (d, 6H, a-py-H), 7.33 (m, 6H, c-py-H), 7.66 (m, 6H, b-py-H), 8.51 (d, 6H, d-py-H) ppm;

Fig. S2 —  $^1\text{H}$  NMR spectrum of dpyatriz



$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 500 MHz) 121.1(a), 122.9(b), 137.4(c), 145.2(d), 157.9(e), 164.4(f)ppm.

Fig. S3 —  $^{13}\text{C}$  NMR spectrum of dpyatriz

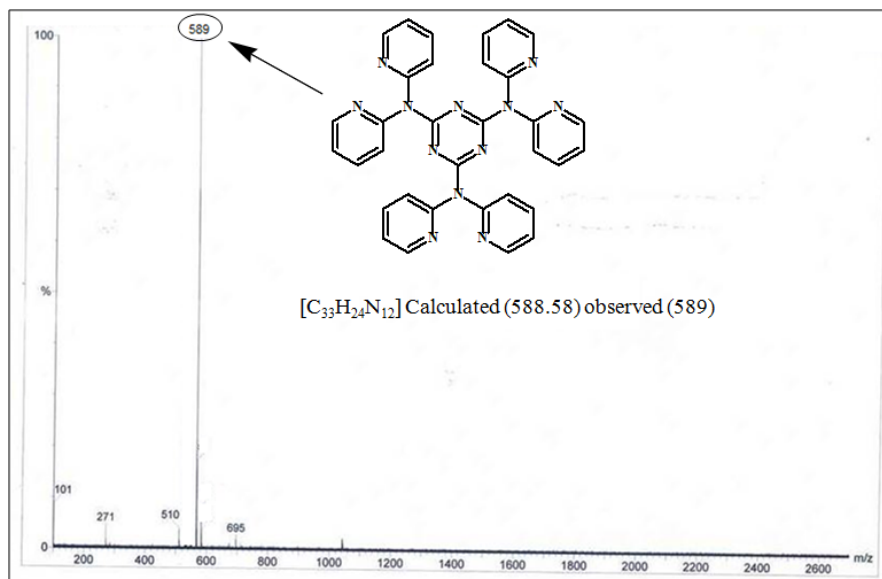


Fig. S4 — Mass spectrum of dpyatriz

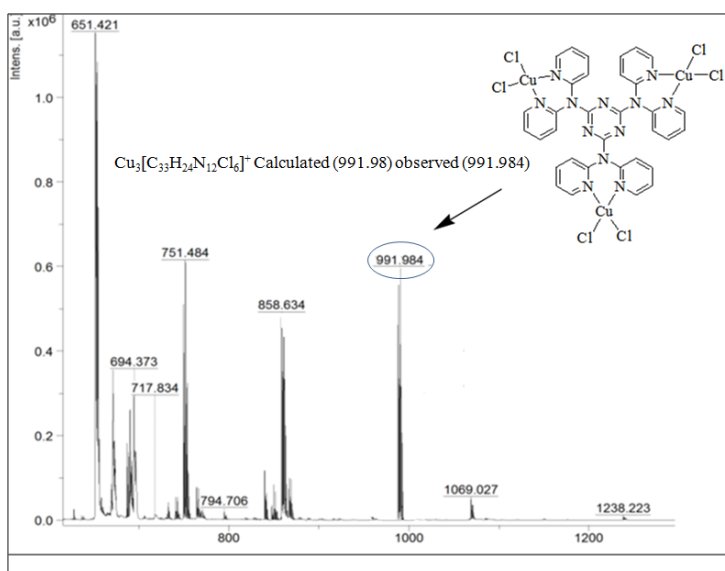


Fig. S5 — Mass spectrum of Cu-dpyatriz

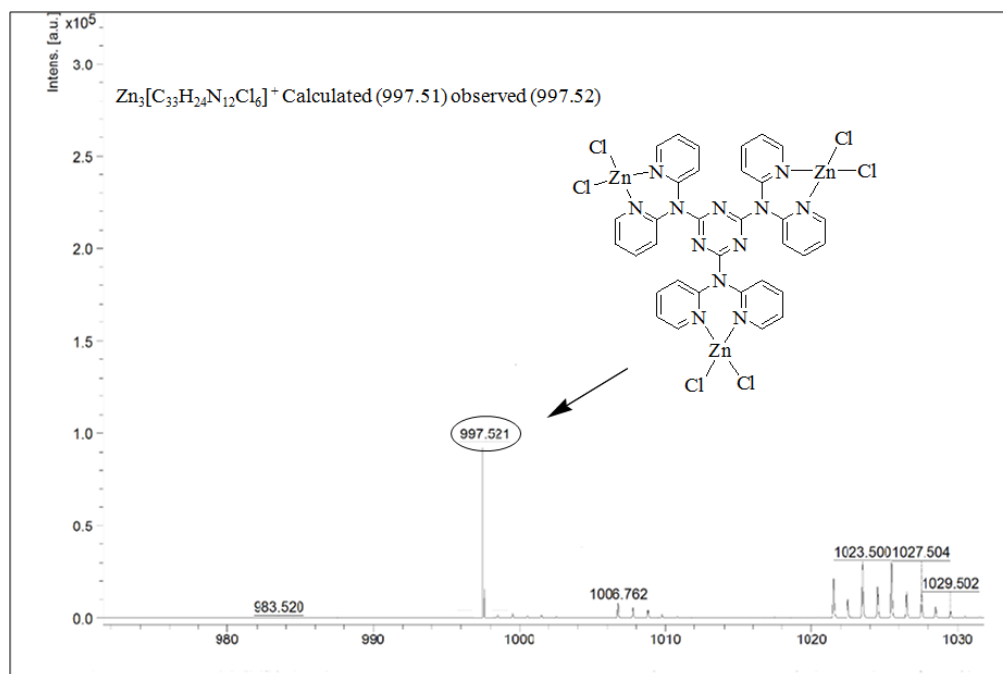


Fig. S6 — Mass spectrum of Zn-dpyatriz

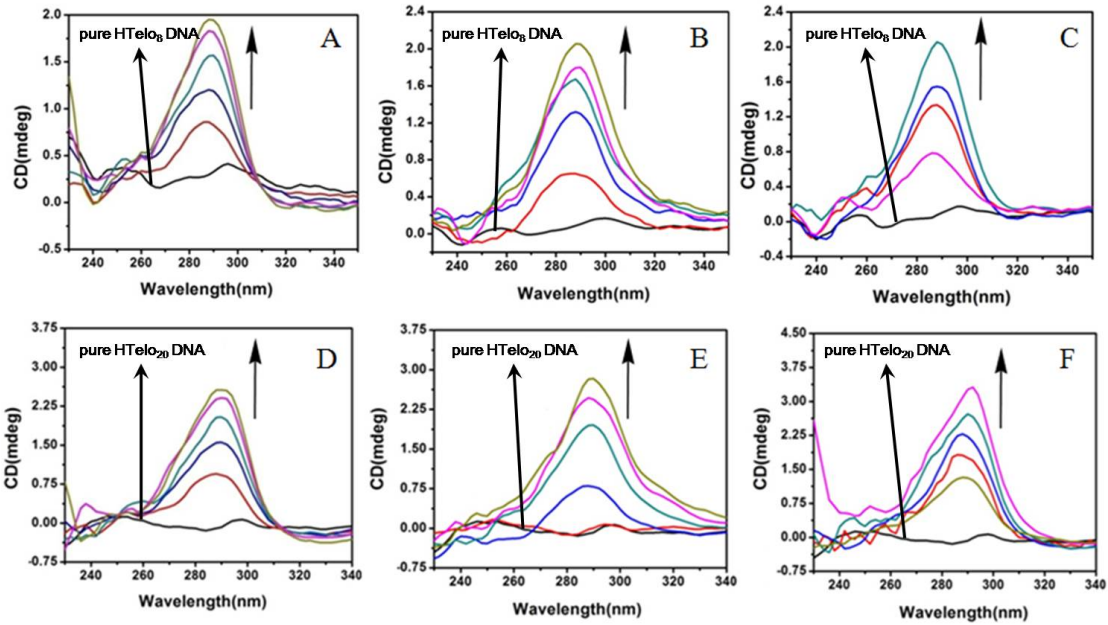


Fig. S7 — CD spectra of HTelo<sub>8</sub> under no salt conditions ( $4 \times 10^{-5}$ M) treated upto 5 equivalents of dpyatriz (A), Cu-dpyatriz (B) and Zn-dpyatriz (C); CD spectra of HTelo<sub>20</sub> under no salt conditions ( $7 \times 10^{-5}$ M) treated upto 5 equivalents of dpyatriz (D), Cu-dpyatriz (E) and Zn-dpyatriz (F)

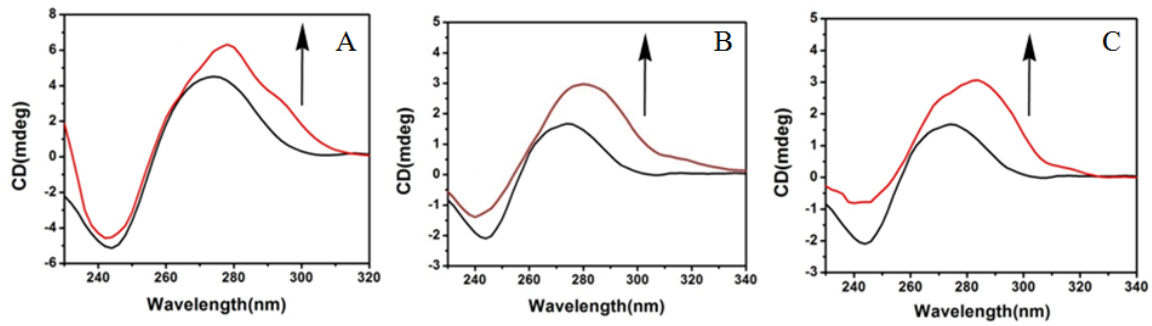


Fig. S8 — CD spectra of CT DNA ( $5 \times 10^{-5}$  M) in the presence of dpyatriz (A), Cu-dpyatriz (B) and Zn-dpyatriz (C)

Table S1 — C,H,N analysis report for dpyatriz, Cu- dpyatriz, Zn- dpyatriz

## Elemental Analysis For dpyatriz Ligand

S.No	Element	Calculated (%)	Observed (%)
1	C	67.33	67.16
2	H	4.10	4.48
3	N	28.55	28.74

## Elemental Analysis For Cu-dpyatriz complex

S.No	Element	Calculated (%)	Observed (%)
1	C	39.96	39.13
2	H	2.44	2.48
3	N	16.94	16.12

## Elemental Analysis For Zn-dpyatriz complex

S.No	Element	Calculated (%)	Observed (%)
1	C	39.73	39.12
2	H	2.42	2.46
3	N	16.85	16.11

Table S2 — Interaction report for parallel DNA docking with dpyatriz

Ligand	Receptor	base	Interaction	Distance	E (kcal/mol)
C 43	6-ring	DG 16 (A)	H-pi	4.39	-0.5
6-ring	C2'	DG 16 (A)	pi-H	4.74	-0.9
6-ring	5-ring	DG 16 (A)	pi-pi	3.70	-0.0

Table S3 — Interaction report for parallel DNA docking with Cu- dpyatriz

Ligand	Receptor	base	Interaction	Distance	E (kcal/mol)
N 56	OP1	DG 14 (A)	H-donor	3.20	-1.9
6-ring	6-ring	DG 14 (A)	pi-pi	3.85	-0.0

Table S4 — Interaction report for parallel DNA docking with Zn- dpyatriz					
Ligand	Receptor	base	Interaction	Distance	E (kcal/mol)
6-ring	6-ring	DG 8 (A)	pi-pi	3.99	-0.0

Table S5 — Interaction report for antiparallel DNA docking with dpyatriz					
Ligand	Receptor	base	Interaction	Distance	E (kcal/mol)
N 51	C1'	DT 12 (A)	H-acceptor	3.50	-0.7
C 49	5-ring	DA 13 (A)	H-pi	4.66	-0.7
6-ring	C4'	DT 12 (A)	pi-H	4.00	-1.1
6-ring	6-ring	DG 22 (A)	pi-pi	3.92	-0.0
6-ring	6-ring	DG 10 (A)	pi-pi	3.62	-0.0
6-ring	5-ring	DG 14 (A)	pi-pi	3.52	-0.0

Table S6 — Interaction report for antiparallel DNA docking with Cu- dpyatriz					
Ligand	Receptor	base	Interaction	Distance	E (kcal/mol)
N 34	OP2	DT 11 (A)	H-donor	3.07	-3.1
N 36	O4'	DG 22 (A)	H-donor	3.50	-1.2
Cu 76	OP2)	DG 10 (A)	Metal	2.54	-1.2
C 72	5-ring	DG 14 (A)	H-pi	3.56	-0.5

Table S7 — Interaction report for antiparallel DNA docking with Zn- dpyatriz					
Ligand	Receptor	base	Interaction	Distance	E (kcal/mol)
N 16	O4'	DT 12 (A)	H-donor	2.95	-3.0
N 36	OP2	DT 12 (A)	H-donor	3.29	-7.5
Zn 79	OP2	DT 11 (A)	Metal	2.00	-3.0
N 16	6-ring	DT 12 (A)	H-pi	4.57	-0.6

Table S8 — Interaction report for Hybrid DNA docking with dpyatriz					
Ligand	Receptor	base	Interaction	Distance	E (kcal/mol)
C 35	6-ring	DT 2 (A)	H-pi	3.36	-0.5
C 41	6-ring	DG 12 (A)	H-pi	4.29	-0.6
6-ring	6-ring	DG 12 (A)	pi-pi	3.72	-0.0
6-ring	6-ring	DT 13 (A)	pi-pi	3.92	-0.0

Table S9 — Interaction report for Hybrid DNA docking with Cu- dpyatriz					
Ligand	Receptor	base	Interaction	Distance	E (kcal/mol)
Cl 81	O6	DG 16 (A)	H-donor	3.03	-3.8
Cl 84	N7	DG 4 (A)	H-donor	3.59	-0.7
N 3	N2	DG 12 (A)	H-acceptor	2.81	-5.1
Cu 80	OP1	DG 6 (A)	Metal	2.65	-1.0
N 36	6-ring	DT 13 (A)	H-pi	4.01	-5.5

Table S10 — Interaction report for Hybrid DNA docking with Zn- dpyatriz					
Ligand	Receptor	base	Interaction	Distance	E (kcal/mol)
N 74	OP2	DT 14 (A)	H-donor	2.81	-11.6
Zn 76	OP1	DG 12 (A)	Metal	2.07	-2.0