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SUPPLEMENTARY MATERIALS

Exploring the Iiteraction of curaxin CBL0137 with G-quadruplex DNA oligomers

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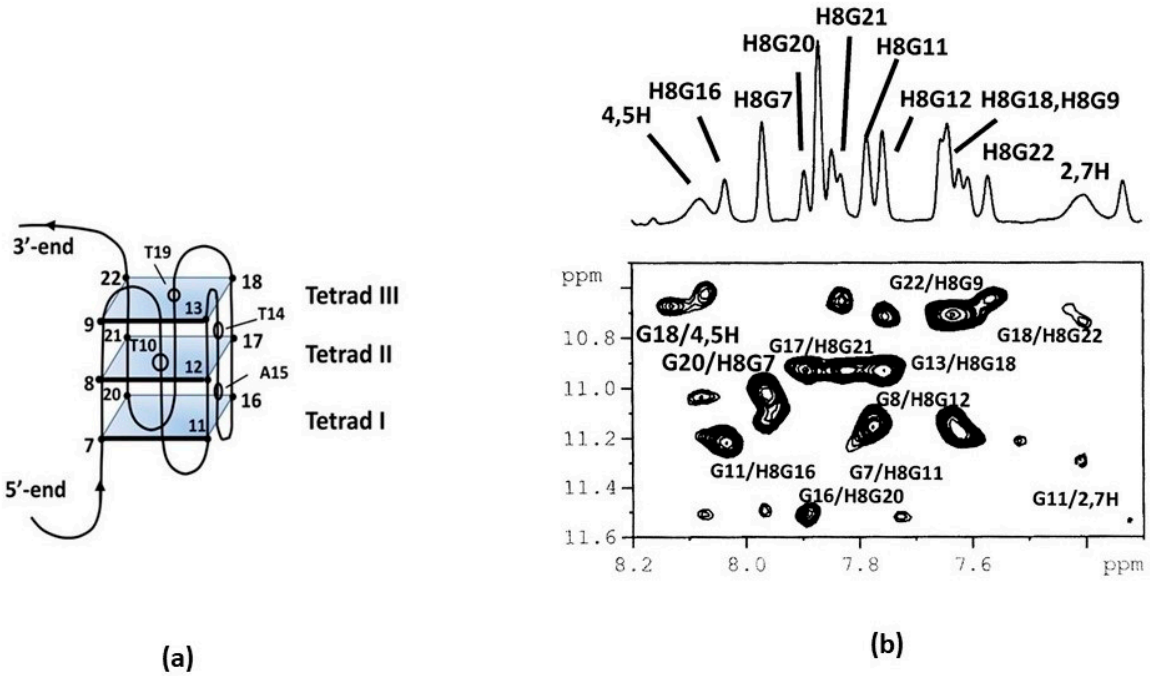

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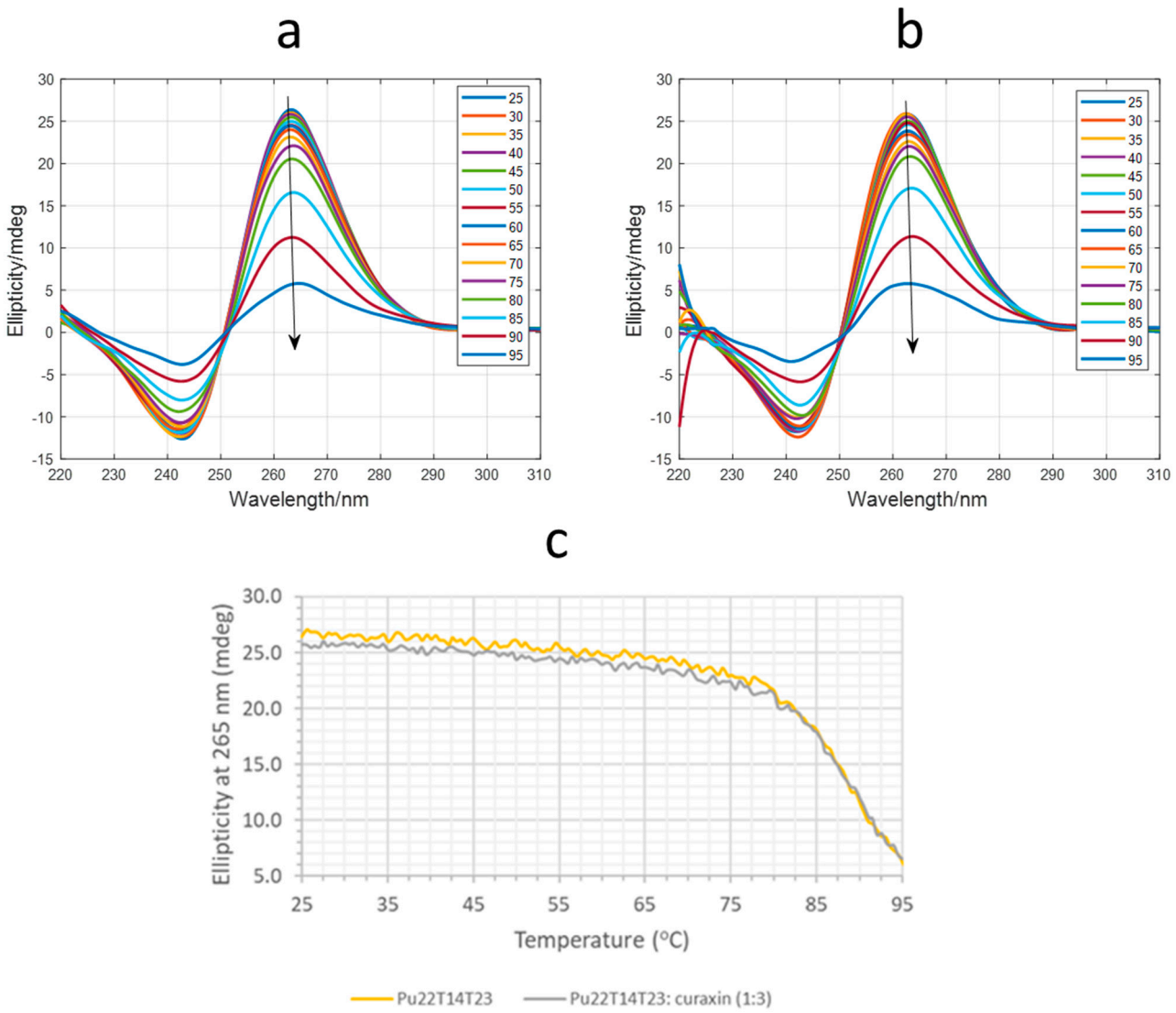

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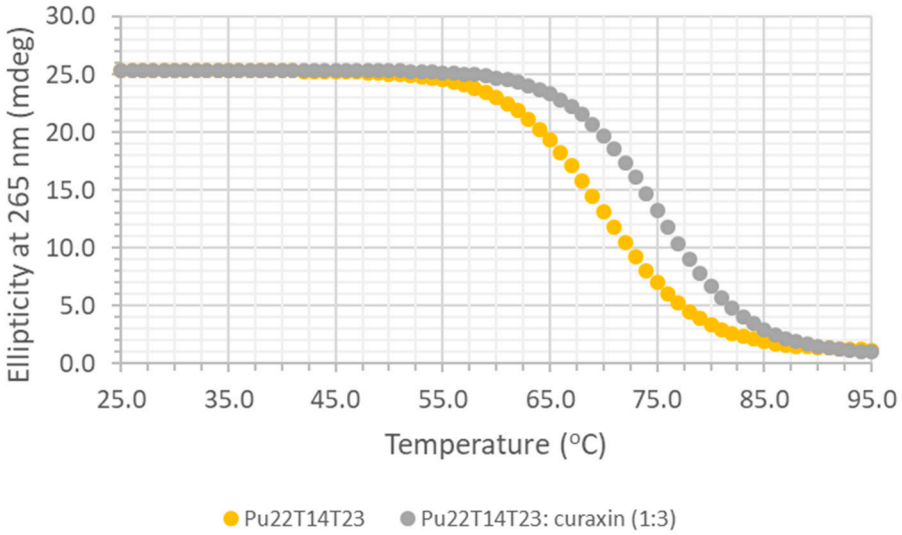

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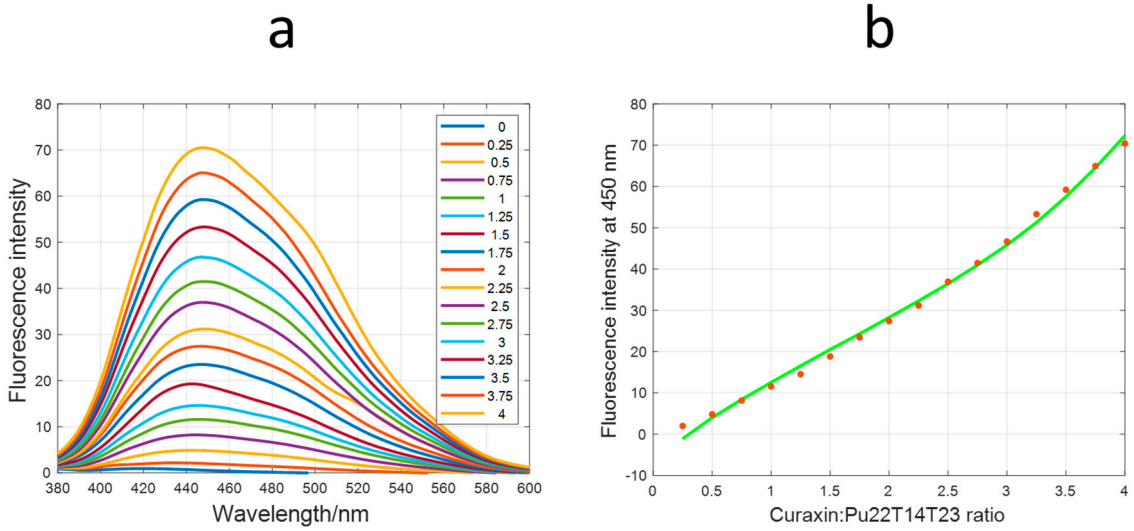

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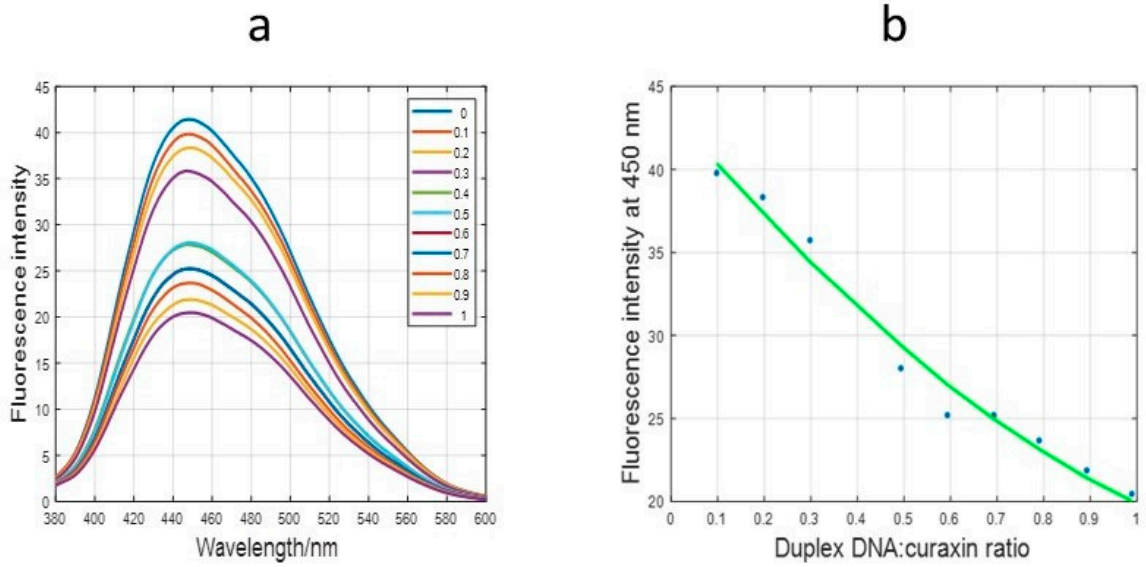

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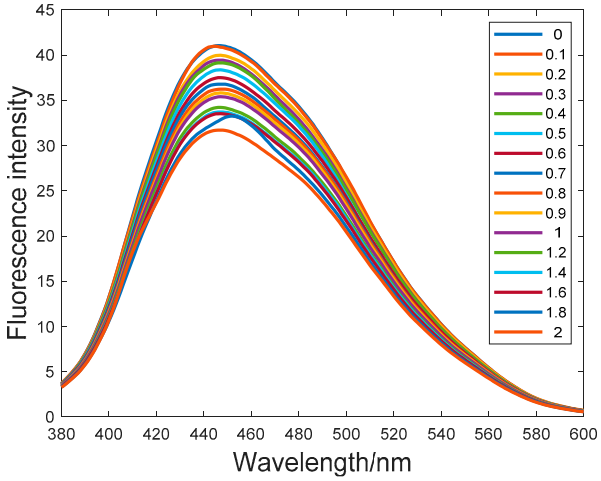

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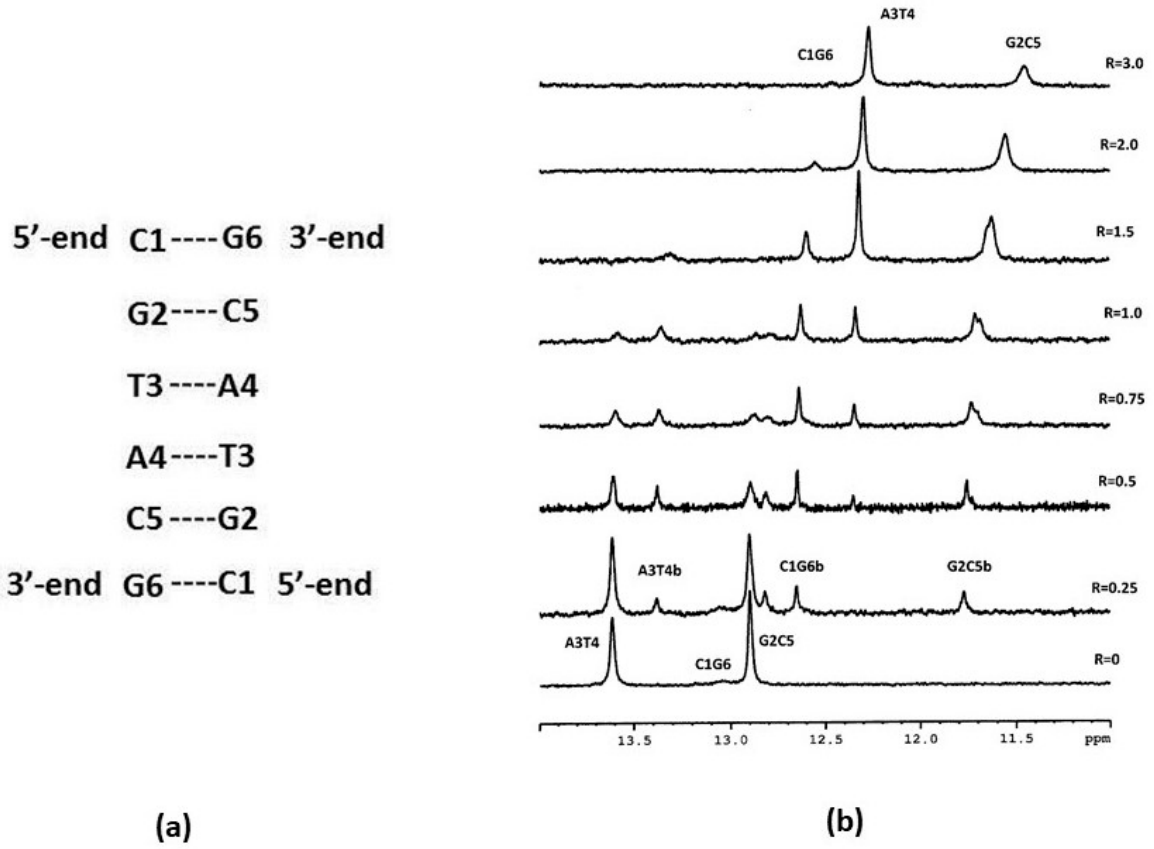

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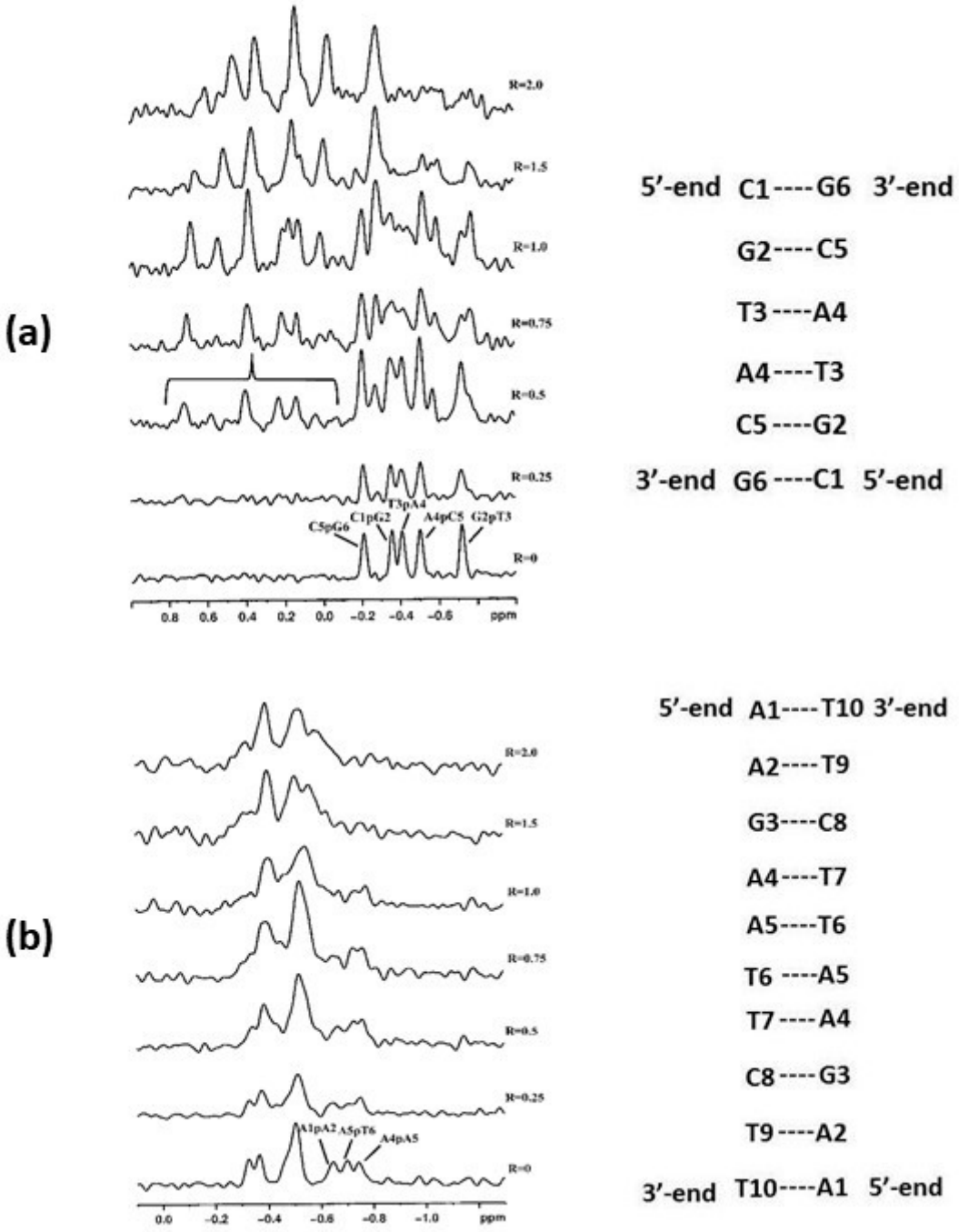

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Table S1. ^{1}H chemical shift assignments of curaxin in absence and in presence of d(T_2AG_3T)$_4$ [a] and Pu22T14T23[b]

protons	δ curaxin free (ppm)	δ d(T_2AG_3T)$_4$ /curaxin (ppm)	Δδ[b]	δ Pu22T14T23 /curaxin (ppm)	Δδ[b]
1,8-H	7.50	7.00	-0.50	7.00	-0.50
2,7-H	8.05	7.44	-0.61	7.41	-0.64
4,5-H	8.41	8.17	-0.24	8.08	-0.33
CH_2(9)	4.55	4.19	-0.36	4.32	-0.23
CH_2	3.42	3.24	-0.18	3.32	-0.10
CH (isopropyl)	3.42	3.24	-0.18	3.32	-0.10
CH_3CO	2.68	2.26	-0.42	2.27	-0.41
CH_3 (isopropyl)	1.30	1.16	-0.14	1.19	-0.11

[a] Acquired at 25°C in H_2O-D_2O (90:10 v/v), 25 mM K-phosphate buffer, 150 mM KCl, 1mMEDTA, pH 6.7. [b] Acquired at 25°C in H_2O-D_2O (90:10 v/v), 25 mM KH_2PO_4, 70 mM KCl, pH 6.9. [c] $\Delta\delta=\delta_{bound}-\delta_{free}$

Table S2. ^{1}H chemical shift values of d(T_2AG_3T)$_4$ in the presence of curaxin[a]

d(T_2AG_3T)$_4$ /curaxin	H1 free	bound	Δδ	H8/H6 free	bound	Δδ	H2/Me free	bound	Δδ
T1	-	-	-	7.39	7.49	0.10	1.66	1.68	0.02
T2	-	-	-	7.30	7.31	0.01	1.76	1.77	0.01
A3	-	-		8.43	8.38	-0.05	8.09	n.d.	
G4	11.61	11.33	**-0.28**	7.95	7.78	**-0.17**	-	-	
G5	11.23	11.00	**-0.23**	7.79	7.61	**-0.18**	-	-	
G6	11.15	10.60	**-0.55**	7.70	7.69	-0.01	-	-	
T7	-	-	-	7.36	7.49	**0.13**	1.60	1.68	0.02

d(T_2AG_3T)$_4$ /curaxin	H1′ free	bound	Δδ	H2′/H2″ free	bound	Δδ
T1	6.00	6.11	0.11	2.10;2.34	2.27;2.27	0.17; -0.07
T2	6.23	5.93	-0.30	2.03;2.32	2.06;2.33	0.03;0.01
A3	6.28	6.26	-0.02	2.86;2.92	2.87;2.87	0.01;-0.05
G4	6.01	5.96	-0.05	2.67;2.91	2.60;2.82	-0.07;-0.03
G5	6.03	5.99	-0.04	2.66;2.74	2.60;2.82	-0.06;-0.09
G6	6.27	6.29	0.02	2.57;2.70	2.60;2.69	0.03;-0.01
T7	6.07	6.11	0.04	2.17;2.19	2.27;2.27	0.10;0.08

d(T_2AG_3T)$_4$ /curaxin	H3′ free	bound	Δδ	H4′ free	bound	Δδ
T1	4.64	n.d.	-	4.00	n.d.	-
T2	4.72	n.d.	-	4.06	n.d.	-
A3	5.10	5.08	-0.02	4.44	4.45	0.01
G4	5.05	4.98	-0.07	4.49	4.45	-0.04
G5	5.04	4.98	-0.06	4.51	4.45	-0.06

G6	4.91	4.98	0.07	4.52	4.46	-0.06
T7	4.49	5.02	0.03	4.23	4.21	-0.02

$d(T_2AG_3T)_4$ /curaxin	H5′/H5″ free	bound	Δδ
T1	3.65;3.65	n.d.	-
T2	3.90;3.90	n.d.	-
A3	4.15;4.10	4.12;4.12	-0.03, 0.02
G4	4.27;4.27	4.24;4.24	-0.03; -0.03
G5	4.30;4.30	4.27;4.27	-0.03; -0.03
G6	4.27;4.27	4.24;4.24	-0.03; -0.03
T7	4.07;4.07	4.12;4.12	0.05; 0.05

[a] Acquired at 25°C in 25 mM KH_2PO4, 150 mM KCl and 1 mM EDTA, pH 6.7, 10% D_2O, R=2.0

Table S3 . Selected ^{1}H chemical shift values for the complex of curaxin with Pu22T14T23.[a]

	H1/H2/Me	Δδ[b]	H6/H8	Δδ
T4	1.79	+0.14	7.33	+0.12
G5	n.d.	-	8.24	+0.24
A6	7.97	+0.17	n.d.	-
G7	11.20	**- 0.56**	7.97	-0.07
G8	10.94	- 0.28	7.60	-0.12
G9	10.30	-0.30	7.71	-0.11
T10	n.d.	-	n.d.	
G11	11.23	**-0.48**	7.78	-0.21
G12	11.17	-0.33	7.76	-0.24
G13	10.70	**-0.36**	7.78	-0.08
T14	1.94	+0.02	7.64	-0.01
A15	8.36	-0.02	8.55	+0.02
G16	11.50	**- 0.40**	8.04	-0.07
G17	10.93	- 0.32	7.63	- 0.17
G18	10.64	**- 0.38**	7.66	- 0.13

T19	2.00	+0.01	7.86	0.00
G20	11.03	-0.24	7.90	0.00
G21	11.13	-0.24	7.83	-0.08
G22	10.72	**-0.32**	7.57	-0.04
T23	1.30	-0.18	7.09	-0.05
A24	7.23	+0.13	n.d.	-
A25	7.60	+0.21	n.d.	-

[a] Measured at 25°C in ppm (δ) from external DSS. Solvent H_2O-D_2O (90:10 v/v), 25 mM K-phosphate buffer, 70 mM KCl, pH 6.9, *R* = 2.0.

[b] $\Delta\delta = \delta_{bound} - \delta_{free}$

Table S4. Inter-residue NOE interactions of Pu22T14T23 in the complex with curaxin[a]

G-tetrad I	*G-tetrad II*	*Tetrad III*
G7H1-G11H8	G8H1-G12H8	G9H1-G13H8
G11H1-G16H8	G12H1-G17H8	G13H1-G18H8
G16H1-G20H8	G17H1-G21H8	G18H1-G22H8
G20H1-G7H8	G21H1-G8H8	G22H1-G9H8

[a] Acquired at 25°C in H_2O-D_2O (90:10 v/v), 25 mM K-phosphate buffer, 70 mM KCl, pH 6.9; R=2.0

Table S5. Selected ^{1}H chemical shift values for the complex of curaxin with and d(CGTACG)2[a]

"CG"	H2/H5/CH_3	$\Delta\delta^b$	H6/H8	$\Delta\delta^b$
C1	5.44		7.35	-0.12
G2	-	-	7.53	-0.12
T3	1.61		7.15	-0.07

A4	6.97		8.06	-0.06
C5	5.52		7.32	-0.11
G6	-		7.79	-0.09
	NH			
C1G6	12.45	-0.60		
G2C5	11.45	**-1.45**		
T3A4	12.27	**-1.34**		

[a] Measured at 15°C in ppm (δ) from external DSS. Solvent H_2O-D_2O (90:10 v/v), of 0.1 M NaCl and 10 mM sodium phosphate buffer solution, pH = 7.0; R = 3.0. [b] $\Delta\delta = \delta_{bound} - \delta_{free}$; [c] Very broad signal.

Table S6. Intermolecular NOE in the curaxin-d(CGTACG)$_2$[a] complex

NOE	
Curaxin	d(CGTACG)$_2$
1,8-H	G2H8
2,7-H	G2H8
4,5-H	G2H8
CH_3 iso	A4H8
CH_3CO	A4H8
1,8-H	A4H8
2,7-H	A4H8
1,8-H	A4H8
2,7-H	T3H6
4,5-H	T3H6

[a] Measured at 15°C in ppm (δ) from external DSS. Solvent H_2O-D_2O (90:10 v/v), of 0.1 M NaCl and 10 mM sodium phosphate buffer solution, pH = 7.0; R = 3.0.