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**Competitive formation of DNA linkage isomers by a trinuclear
platinum complex and the influence of pre-association**

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Supporting Information

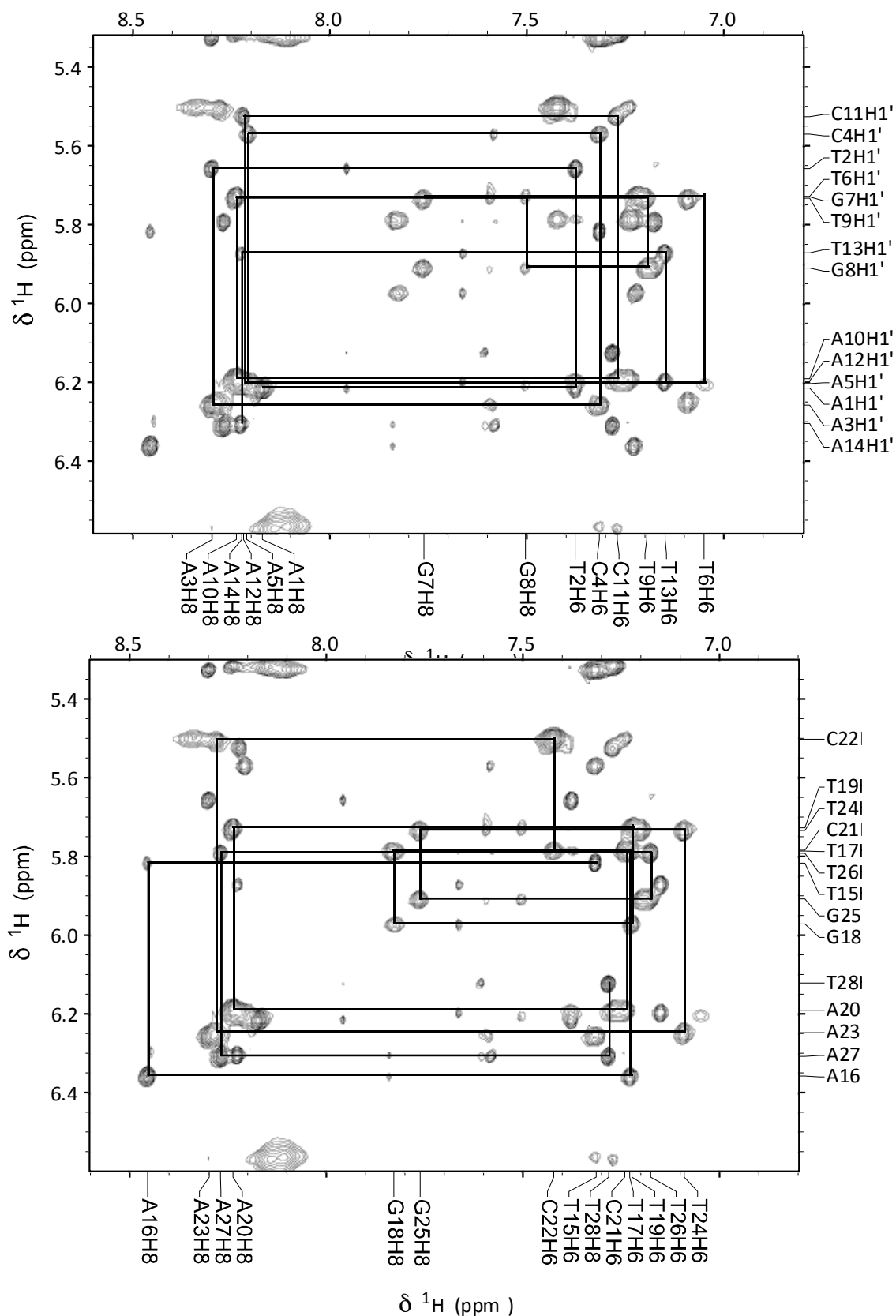


Figure S1a. Contour plot of the 2D ^1H NOESY NMR spectrum (mixing time = 150 ms) of duplex **I** (in 200 mM NaOAc, 5% D_2O in H_2O) at 298 K, showing the H6/H8 aromatic (8.5 – 6.9 ppm) to sugar ring $\text{H1}'$ (6.6 – 5.4 ppm) connectivities. The sequential NOESY assignment walks are shown for the –GG– strand (**Ia**) and for the complementary –CC– strand (**Ib**) and are in accordance with the published data (J. A. Parkinson, Y. Chen, Z. Guo, S. J. Berners-Price, T. Brown and P. J. Sadler, *Chem. Eur. J.*, 2000, 6, 3636-3644).

Table S1 – ¹H NMR chemical shifts of duplex **I** (298 K) showing the shifts that occur on addition of **0** (2:1 ratio).^a

	H6	H8	H2		Me	H1'	H2'	H2''	NH	H4(1)	H4(2)
A1		8.17 (0.00)	7.95 (-0.03)			6.20 (-0.02)	2.65 (-0.01)	2.80 (0.00)			
T2	7.37 (-0.01)				1.45 (-0.01)	5.58 (-0.06)	2.16 (-0.01)	2.40 (-0.03)			
A3		8.31 (0.00)	7.64 (0.03)			6.24 (-0.01)	2.75 (0.02)	2.90 (-0.01)			
C4	7.34 (0.01)			5.36 (0.03)		5.46 (-0.08)	2.06 (-0.01)	2.36 (-0.04)		6.58 (0.01)	8.07 (-0.04)
A5		8.25 (0.03)	7.53 (0.01)			6.20 (0.01)	2.68 (0.04)	2.88 (-0.01)			
T6	7.09 (0.04)				1.41 (0.05)	5.59 (-0.09)	1.87 (-0.03)	2.25 (-0.03)	13.50 (-0.01)		
G7		7.80 (0.03)				5.53 (-0.10)	2.68 (0.04)	2.68 (-0.01)	12.67 (0.08)		
G8		7.67 (0.05)				5.90 (-0.01)	2.51 (0.02)	2.70 (-0.01)	12.67 N/A		
T9	7.20 (-0.01)				1.42 (0.05)	5.57 (-0.12)	2.03 (-0.03)	2.32 (-0.11)	13.45 (0.00)		
A10		8.29 (0.03)	7.62 (0.20)			6.14 (-0.04)	2.76 (0.07)	2.85 (-0.01)			
C11	7.33 (0.05)			5.41 (0.08)		5.43 (-0.06)	2.01 (0.01)	2.32 (-0.01)		6.62 (0.04)	8.11 (-0.04)
A12		8.25 (0.03)	7.71 (0.04)			6.19 (0.00)	2.63 (0.04)	2.82 (0.02)			
T13	7.16 (-0.00)				1.53 (0.03)	5.82 (-0.04)	1.89 (-0.02)	2.23 (-0.02)			
A14		8.22 (-0.01)	7.59 N/A			6.30 (0.00)	2.47 (0.01)	2.67 (0.01)			
T15	7.32 (0.01)				1.58 (0.02)	5.79 (-0.02)	1.79 (0.01)	2.20 (-0.00)			
A16		8.46 (0.00)	7.83 (-0.01)			6.33 (-0.01)	2.88 (0.00)	2.99 (-0.02)			
T17	7.25 (0.01)				1.45 (0.01)	5.71 (-0.05)	2.14 (-0.02)	2.43 (-0.04)	13.36 (0.03)		
G18		7.85 (0.03)				5.92 (-0.03)	2.61 (0.03)	2.69 (-0.03)	12.45 (0.05)		
T19	7.23 (0.01)				1.46 (0.05)	5.57 (-0.11)	2.04 (-0.03)	2.31 (-0.14)	13.48 (0.05)		
A20		8.29 (0.03)	7.60 (0.18)			6.14 (-0.04)	2.76 (0.09)	2.85 (-0.02)			
C21	7.31 (0.04)			5.32 (0.07)		5.79 (0.00)	1.97 (-0.03)	2.36 (-0.04)		6.45 (0.02)	7.91 (-0.04)
C22	7.45 (0.01)			5.57 (0.05)		5.30 (-0.15)	2.08 (-0.00)	2.35 (-0.04)		6.73 (0.04)	8.30 (-0.04)
A23		8.31 (0.02)	7.65 (0.10)			6.23 (0.00)	2.72 (0.05)	2.92 (-0.01)			
T24	7.14 (0.04)				1.48 (0.03)	5.64 (-0.04)	2.05 (-0.00)	2.37 (-0.01)	13.36 (-0.12)		
G25		7.80 (0.03)				5.89 (-0.00)	2.57 (0.02)	2.67 (-0.01)	12.41 (0.05)		
T26	7.19 (0.01)				1.45 (0.02)	5.73 (-0.03)	2.00 (0.01)	2.36 (-0.03)	13.48 (0.12)		
A27		8.30 (0.03)	7.65 (0.03)			6.31 (0.00)	2.77 (0.03)	2.85 (0.01)			
T28	7.29 (-0.01)				1.55 (0.00)	6.12 (0.00)	N/A N/A	N/A N/A			

^a Numbers in brackets are the changes in chemical shift of the protons of the duplex upon addition of 2 mol. equiv. of the complex, i.e. $\Delta\delta = \delta(\mathbf{I:0}) - \delta(\mathbf{I})$.

Table S2 – Energies of minimised structures from the production dynamics simulation of **0** (non-relativistic DFT Hirshfeld charges) docked at the G18 site of duplex **I**.

Time (ps)	Energy (cal mol⁻¹)
491 – 520	-1.7770 × 10 ⁵
1631 – 1660	-1.7818 × 10 ⁵
4601 – 4630	-1.7781 × 10 ⁵
4961 – 4990	-1.7789 × 10 ⁵
6371 – 6400	-1.7769 × 10 ⁵
6731 – 6760	-1.7767 × 10 ⁵
7871 – 7900	-1.7780 × 10 ⁵
9161 – 9190	-1.7790 × 10 ⁵

Table S3 – Energies of minimised structures selected from the production dynamics simulation of **0** (non-relativistic DFT Hirshfeld charges) with the GG duplex with the complex docked at the G25 site.

Time (ps)	Energy (cal mol⁻¹)
491 – 520	-2.0295 × 10 ⁵
1181 – 1210	-2.0283 × 10 ⁵
1631 – 1660	-2.0252 × 10 ⁵
3161 – 3190	-2.0238 × 10 ⁵
4481 – 4510	-2.0261 × 10 ⁵
6191 – 6220	-2.0291 × 10 ⁵
6761 – 6790	-2.0243 × 10 ⁵
7811 – 7840	-2.0293 × 10 ⁵
8831 – 8860	-2.0248 × 10 ⁵
9551 – 9580	-2.0302 × 10 ⁵

Scientist equation file used in the fitting of combined monofunctional and combined product species of $^{15}\text{N-1}$ with duplex **I**.

```
// MicroMath Scientist Model File
// Simplified - combined total for product and monofunctional
IndVars: T
DepVars: A, B, C, D, L
Params: KAB, KBC, KCD,
A'=-KAB*A
B'=KAB*A-KBC*B*L
C'=KBC*B*L-KCD*C
D'=KCD*C
L'=-KBC*B*L
// A=1, B=aqua/Cl (2), C=monofunctional (3,4), D=product (5), L= duplex I
// Initial Conditions
T=0.0
A=0.0016
B=0.000
C=0.000
D=0.0
L=0.002
***
```