Supporting Information

## Platinum Binding Preferences Dominate the Binding of Novel Polyamide

## Amidine Anthraquinone Platinum(II) Complexes to DNA

## Anthony T.S. Lo<sup>1</sup>, Jon K. Chen<sup>2</sup>, Vincent Murray<sup>2</sup>, Matthew H. Todd<sup>3</sup>, and Trevor W. Hambley<sup>1</sup>

<sup>1</sup>School of Chemistry, The University of Sydney, Camperdown 2006, NSW, Australia.

<sup>2</sup>School of Biotechnology and Biomolecular Science, University of New South Wales, Sydney, NSW

2052, Australia.

<sup>3</sup>UCL School of Pharmacy, University College London, 29-39 Brunswick Square, London WC1N 1AX

## **Corresponding author**

Email: trevor.hambley@sydney.edu.au; Phone: +61 2 9036 9153

Seq2 Primer

1	5' - ATGTGCTGCA	AGGCGATTAA	GTTGGGTAAC	GCCAGGGTTT	TCCCAGTCAC	
	3' -TACACGACGT	TCCGCTAATT	CAACCCATTG	CGGTCCCAAA	AGGGTCAGTG	
51	GACGTTGTAA	AACGACGGCC	AGTGAATTGG	GGGGGGGGTA	ATTCGAGCTT	
	CTGCAACATT	TTGCTGCCGG	TCACTTAACC	CCCCCCCAT	TAAGCTCGAA	
101	TTCGGTTTCG	GTTTCGATTT	CGATTTTGAT	TTTGATTTAG	CTCGGTACCC	
	AAGCCAAAGC	CAAAGCTAAA	GCTAAAACTA	AAACTAAATC	GAGCCATGGG	
151	GGGGATCTTA	GGGTTAGGGT	TAGGGTTAGG	GTTAGGGTTA	GGGTTAGGGA	
	CCCCTAGAAT	CCCAATCCCA	ATCCCAATCC	CAATCCCAAT	CCCAATCCCT	
201	GCTTGGCGTA	ATCATGGTCA	TAGCTGTTTC	CTGTGTGAAA	TTGTTATCCG	
	CGAACCGCAT	TAGTACCAGT	ATCGACAAAG	GACACACTTT	AACAATAGGC	
251	CTCACAATTC	CACACAACAT	ACGAGCCGGA	AGCATAAAGT	GTAAAGCCTG	
	GAGTGTTAAG	GTGTGT <mark>TGTA</mark>	TGCTCGGCCT	TCGTATTTCA	CATTTCGGAC	
301	GGGTGCCTAA	TGAGTGAGCT	AACTCACATT	AATTGCGTTG	CGCTCACTGC	
	CCCACGGATT	ACTCACTCGA	TTGAG <mark>TGTA</mark> A	TTAACGCAAC	GCGAGTGACG	
351	CCGCTTTCCA	GTCGGGAAAC	CTGTCGTGCCAG			
	GGCGAAAGGT	CAGCCCTTTG	GACAGCACGGTC			

**Figure S1.** Sequence and fragment base pair lengths from 6-FAM Seq2 primer from the pUC19 with the  $T_7G_{10}CpG$  insert. The platinum adduct peaks observed at 3'-(T/A)GTA-5' regions are highlighted in red. The 5'-CGTA-3' sequence for which no platinum adduct peaks were observed is highlighted in orange. The observed peaks are representative of at least three independent experiments with the complex 1.

Mito15 primer

1	5' - ACTCAACATA	CTAGTCACAG	CCCTATACTC	CCTCTACATA	TTTACCACAA
	3' - TGAGTTGTAT	GATCAGTGTC	GGGATATGAG	GGAGATGTAT	AAATGGTGTT
51	CACAATGGGG	CTCACTCACC	CACCACATTA	АСААСАТААА	ACCCTCATTC
	GTGTTACCCC	GAGTGAGTGG	GTGGTGTAAT	TGTTGTATTT	TGGG <mark>AGTA</mark> AG
101	ACACGAGAAA	ACACCCTCAT	GTTCATACAC	CTATCCCCCA	TTCTCCGGGG
	TGTGCTCTTT	TGTGGGAGTA	CAAGTATGTG	GATAGGGGGT	AAGAGGCCCC
1 - 1					
121	ATCCTCTAGA	GTCGACCTGC	AGGCATGCAA	GCTTGGCGTA	ATCATGGTCA
	TAGGAGATCT	CAGCIGGACG	TCCGTACGTT	CGAACCGCAT	TAGTACCAGT
201	TAGC				
	ATCG				

Figure S2. Sequence and fragment base pair lengths from the 6-FAM Mito15 primer from pUC19 withthe HMHRV insert. The platinum adduct peaks corresponding to the sequence 3'-(T/A)GTA-5' arehighlighted in red, and a platinum adduct peak corresponding to the sequence 3'-CGTA-5' ishighlighted in orange. The observed peaks are representative of at least three independentexperimentswiththe[1C3-Pt(II)]+complex.



**Figure S3.** 2.0% agarose gel showing the electrophoretic mobility of (A) *Pvu*II cleaved pUC19  $T_7G_{10}CpG$  insert and (B) *Pvu*II cleaved pUC19 Mito15 insert; Lanes (A1-4, B1-B3) *Hinf*I digest of pUC19 (Lanes A1 and B1), pUC19  $T_7G_{10}CpG$  insert (Lane A3), *Pvu*II cleaved pUC19  $T_7G_{10}CpG$  insert (Lane A4), pUC19 HMHVR insert (Lane B2), *Pvu*II cleaved pUC19 Mito15 insert (Lane B3).



**Figure S4.** Electropherograms of cisplatin and polyamide-anthraquinone-platinum(II) complexes with *PvulI* digested  $T_7G_{10}CpG$  plasmid. A region of interest comparing the complexes with the same fragment length is indicated with purple dashed lines. Electropherograms of cisplatin and [1C3-Pt(II)]<sup>+</sup>) are boxed in red. The x-axis indicates the fragment size in nucleotides and the y-axis indicates relative fluorescence intensity.



**Figure S5.** Identification of the sequence specificity of  $[1C3-Pt(II)]^+$  complex (red) with the  $T_7G_{10}CpG/PvuII$  plasmid. Electropherograms from Figure S4 were overlaid with cisplatin (blue) to elucidate the sequence specificity of the platinum complex. The traces a) overlaid and b) zoomed, with the corresponding DNA sequence (from dideoxy sequencing) have been aligned with the zoomed overlay in b). Black underline indicate the sequence 3'-(A/T)GTA-5' and the orange underline indicates the sequence 3'-CGTA-5'. The x-axis indicates the fragment size in

nucleotides and the y-axis indicates relative fluorescence intensity.



**Figure S6.** Electropherograms of cisplatin and polyamide-anthraquinone-platinum(II) complexes with *Pvu*II digested Mito15 plasmid. A region of interest comparing the complexes with the same fragment length is indicated with purple dashed lines. Electropherograms of cisplatin and [1C3-Pt(II)]<sup>+</sup>) are boxed in red. The x-axis indicates the fragment size in nucleotides and the y-axis indicates relative fluorescence intensity.

