

## **Supplementary Material for ic-2013-01535s**

### **Gold(I)-Phosphine-N-heterocycles. Biological Activity and Specific (Ligand) Interactions on the C-terminal HIVNCp7 Zinc Finger.**

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**Table S2.** DNA melting temperatures expressed as a difference between treated and untreated DNA.

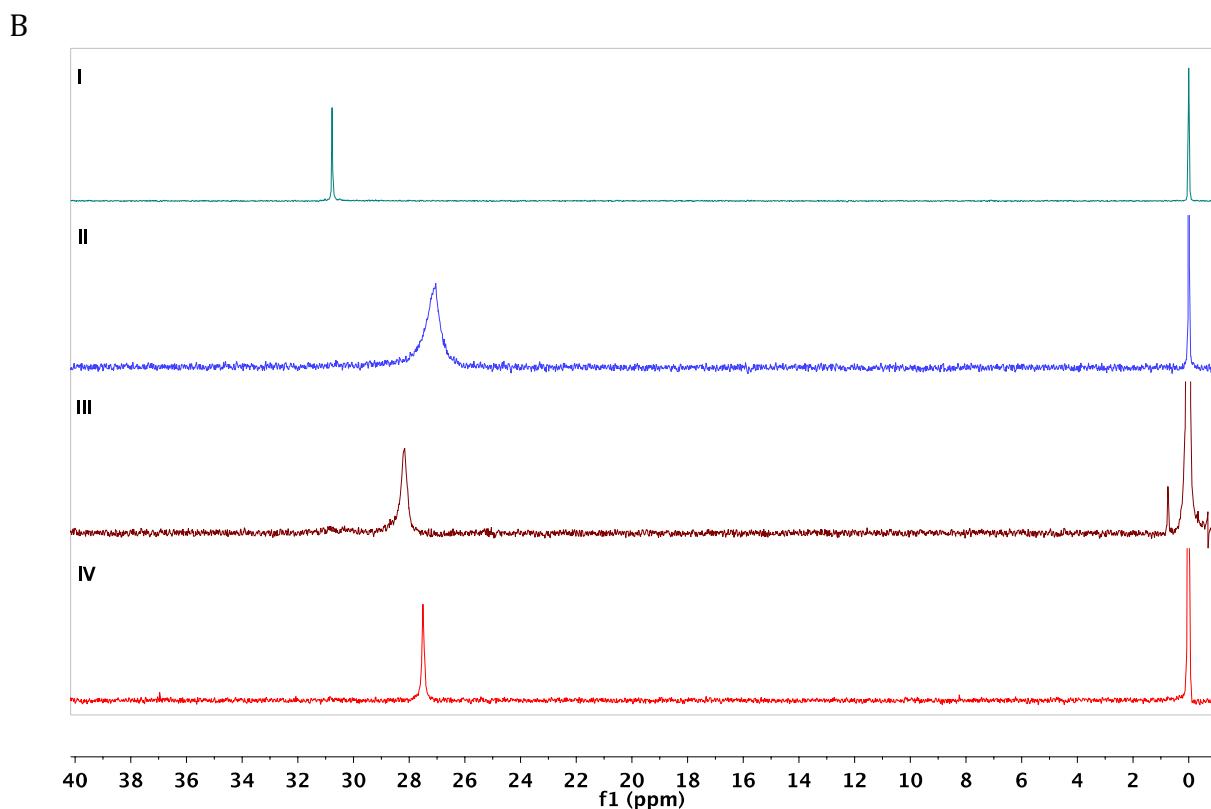
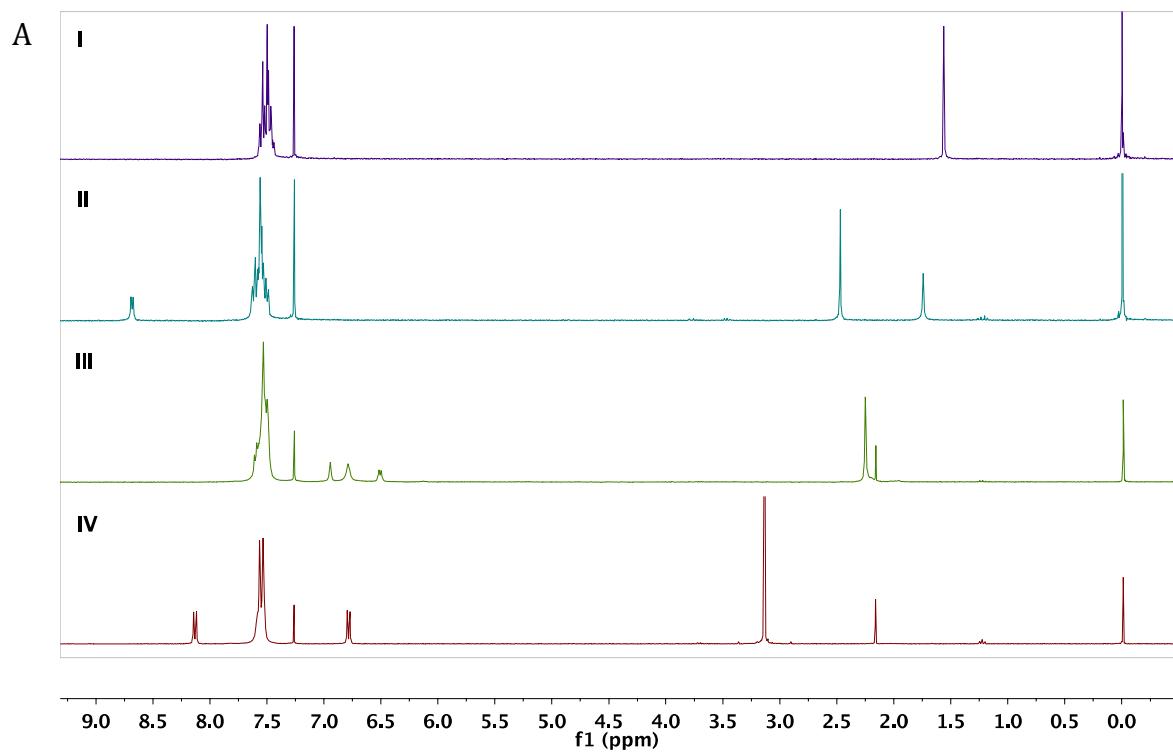


Figure S1 – A)  $^1\text{H}$  NMR of the compounds I – IV and B)  $^{31}\text{P}$  NMR of the compounds I - IV

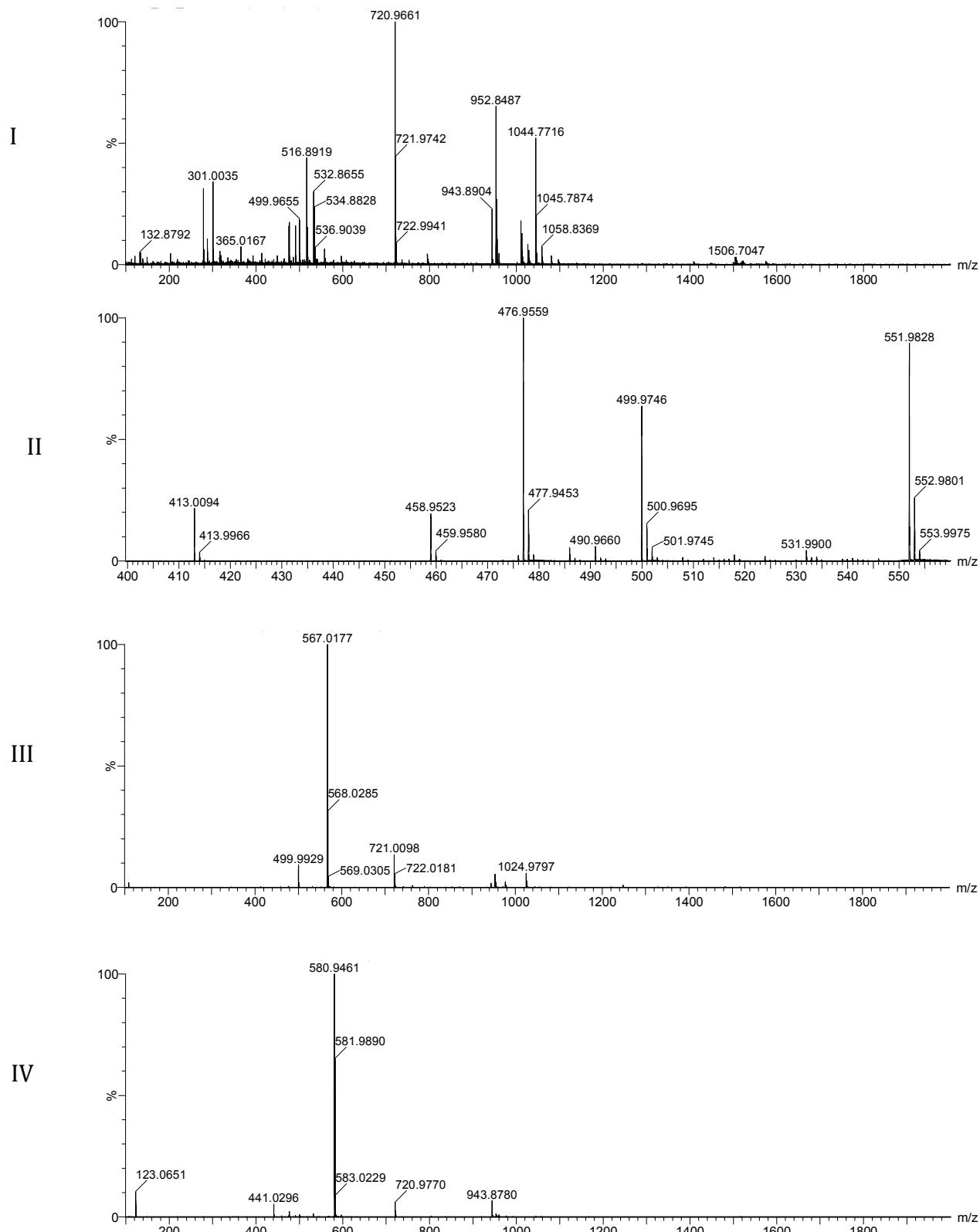


Figure S2. ESI-MS full scan (positive mode) of the gold(I) compounds **I-IV**

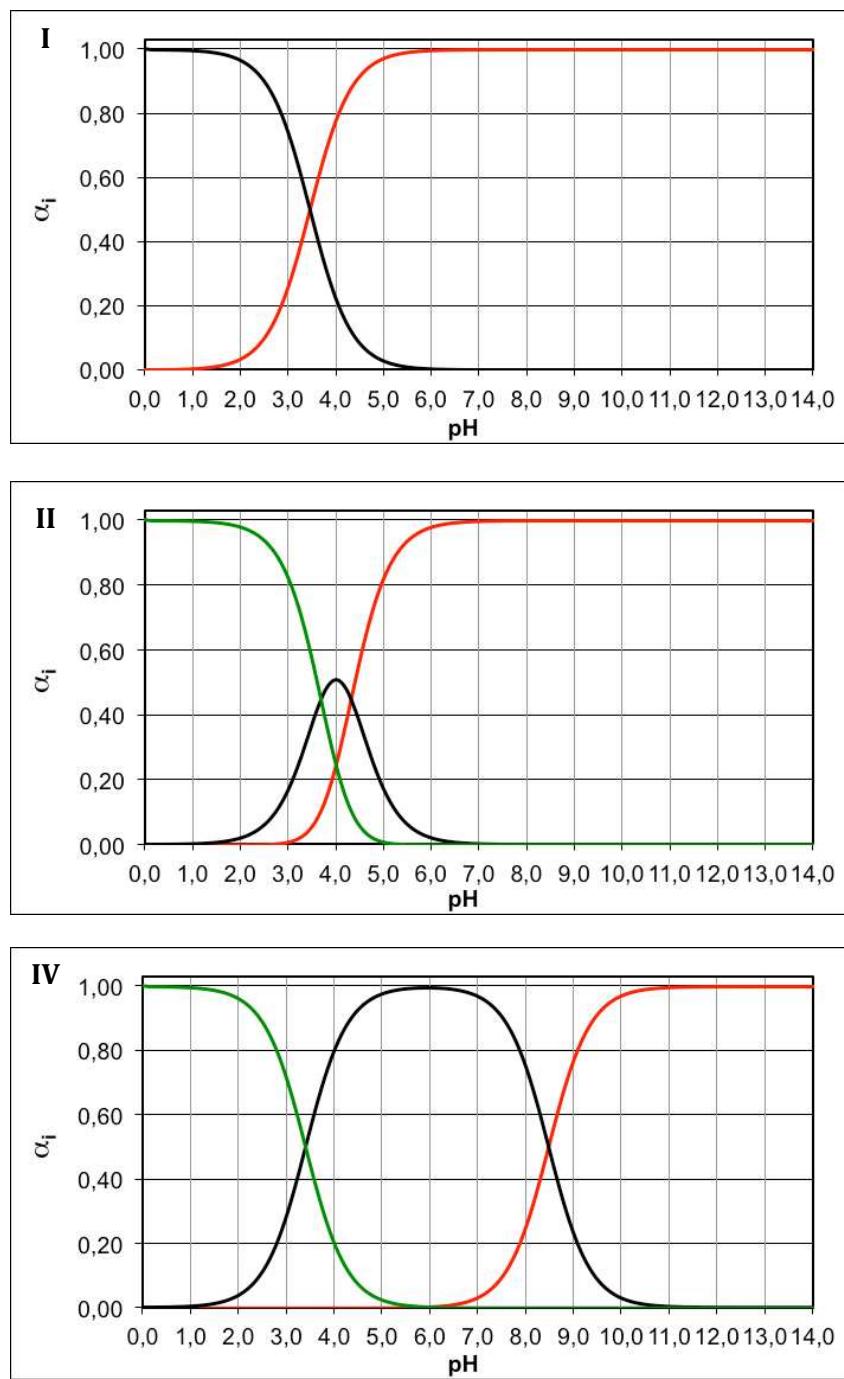


Figure S3A – pH dependent relative species distribution diagrams for compounds **I,II** and **IV**.

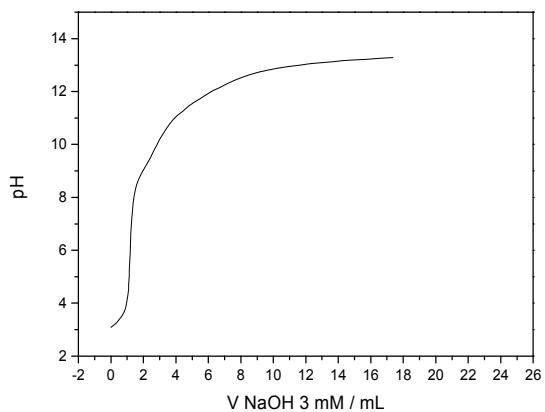
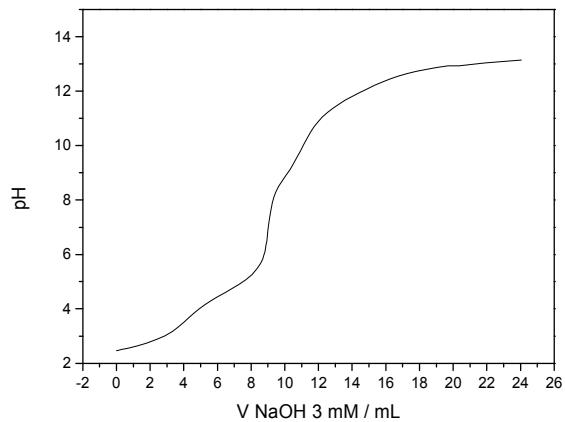
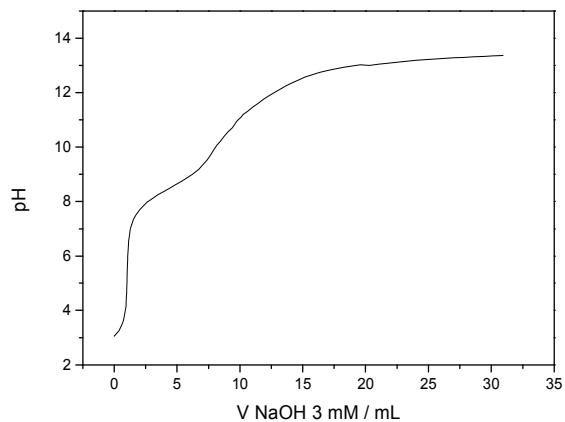
**I****II****IV**

Figure S3B – pH titration data diagrams for compounds **I,II** and **IV**. The original data was analyzed with CurTiPot 3.6.1, and the pKa obtained are listed in Table S1.

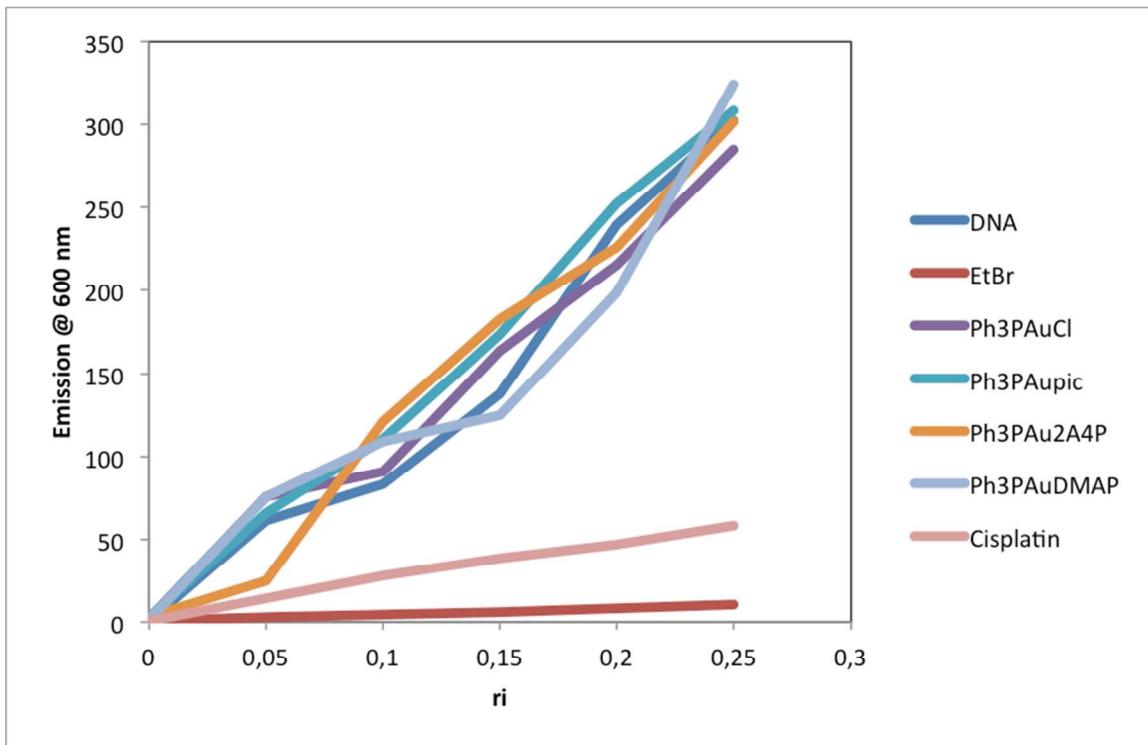


Figure S4. Ethidium bromide/DNA emission  $\lambda_{\text{em}} = 600$  nm after incubation with compounds I-IV and cisplatin for 24h. DNA was incubated with 1% DMSO for 24h . EtBr solution in buffer was measured as a control.

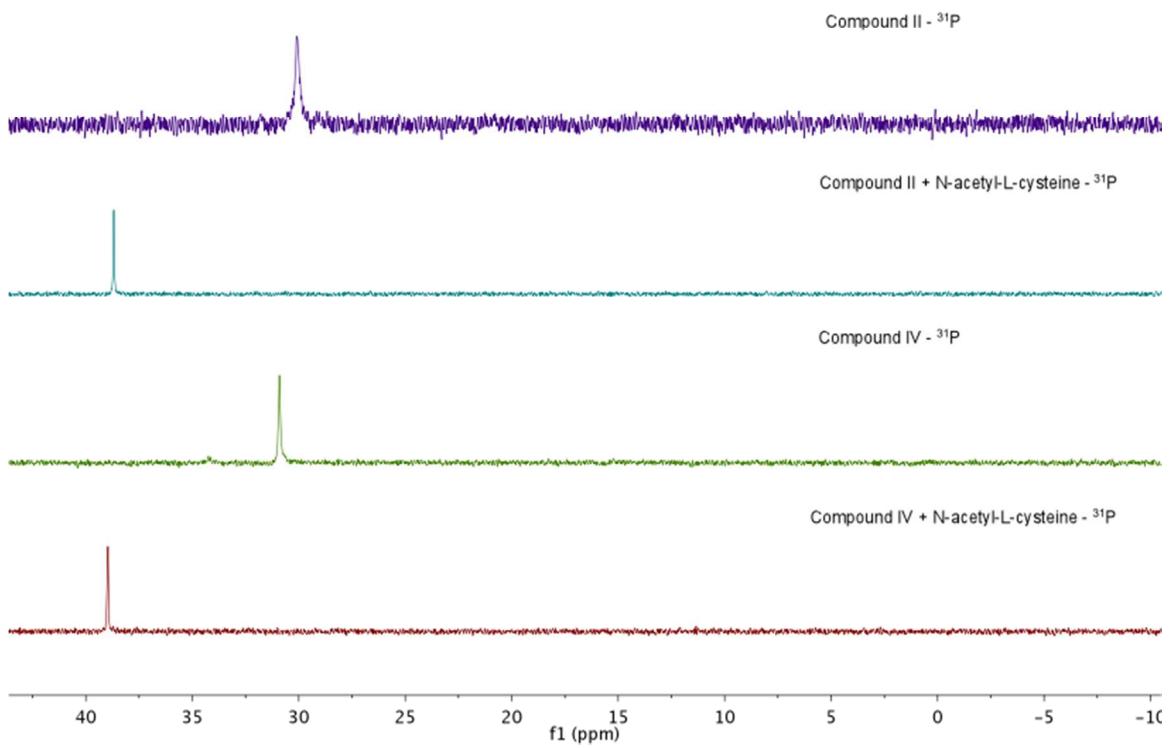


Figure S5.  $^{31}\text{P}$  NMR spectra of N-acetylcysteine interaction with gold(I) compounds. A) compound **II** B) compound **IV**

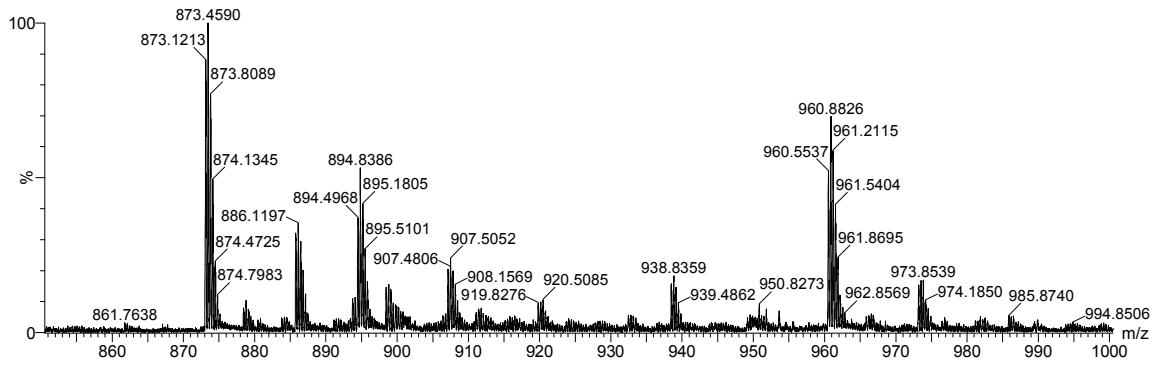


Figure S6. ESI-MS of reaction between  $[(\text{PPh}_3)\text{PAuDMAP}]^+$ , IV, and ZF NCp7 after 78h.

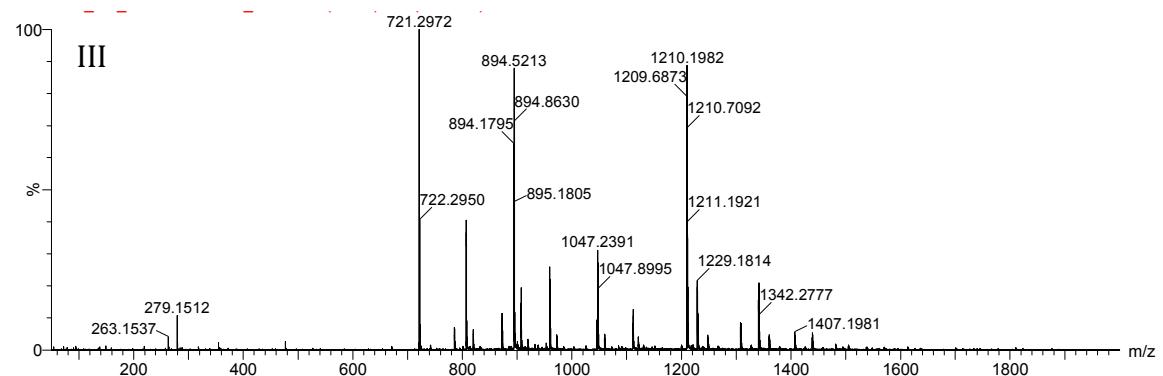
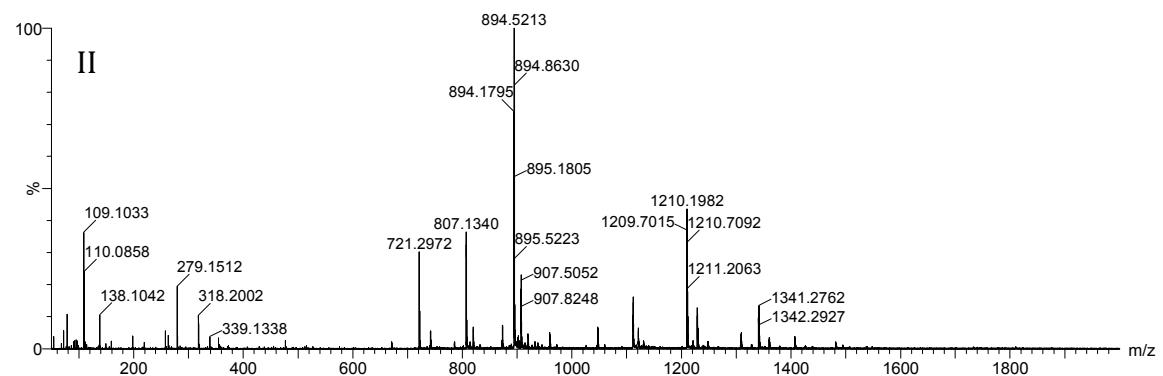
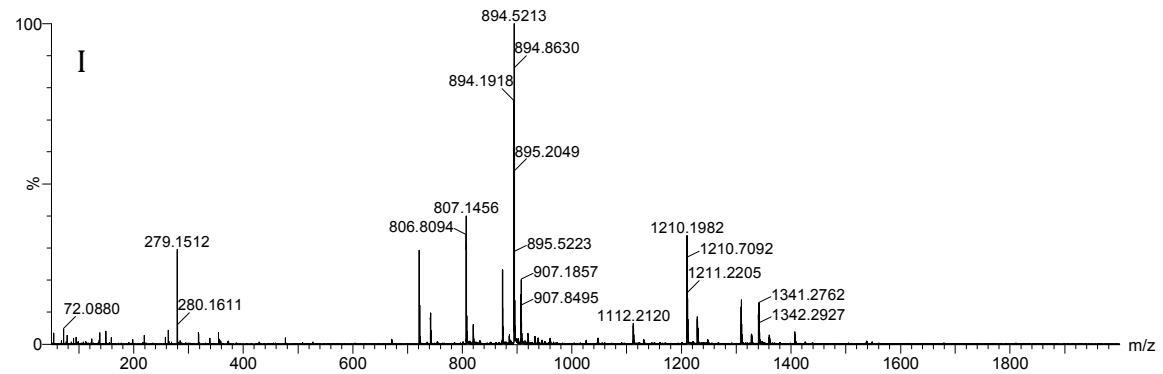


Figure S7. The ESI-MS full scan (positive mode) of reaction between compounds I-III with ZF NCp7 immediately upon incubation.

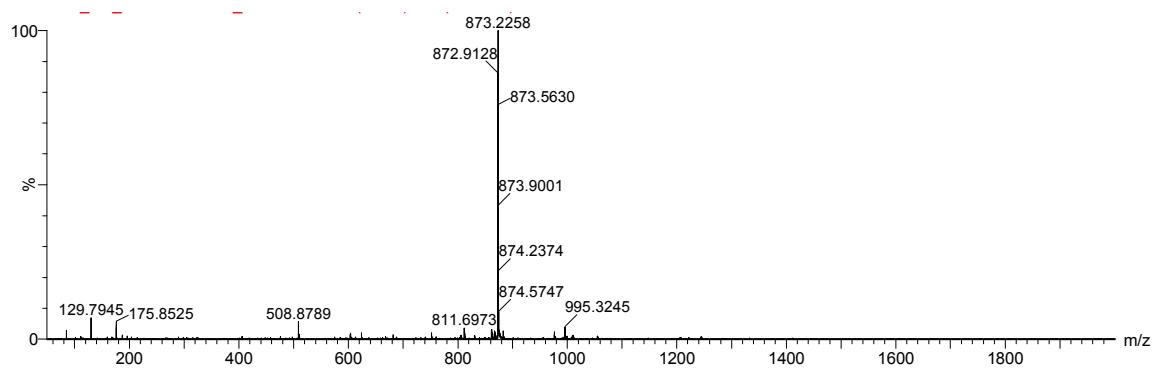


Figure S8. MSMS of peak m/z 873 (corresponding to Au<sub>2</sub>F) of reaction between [(PPh<sub>3</sub>)Au(DMAP)]<sup>+</sup> and ZFNCp7.

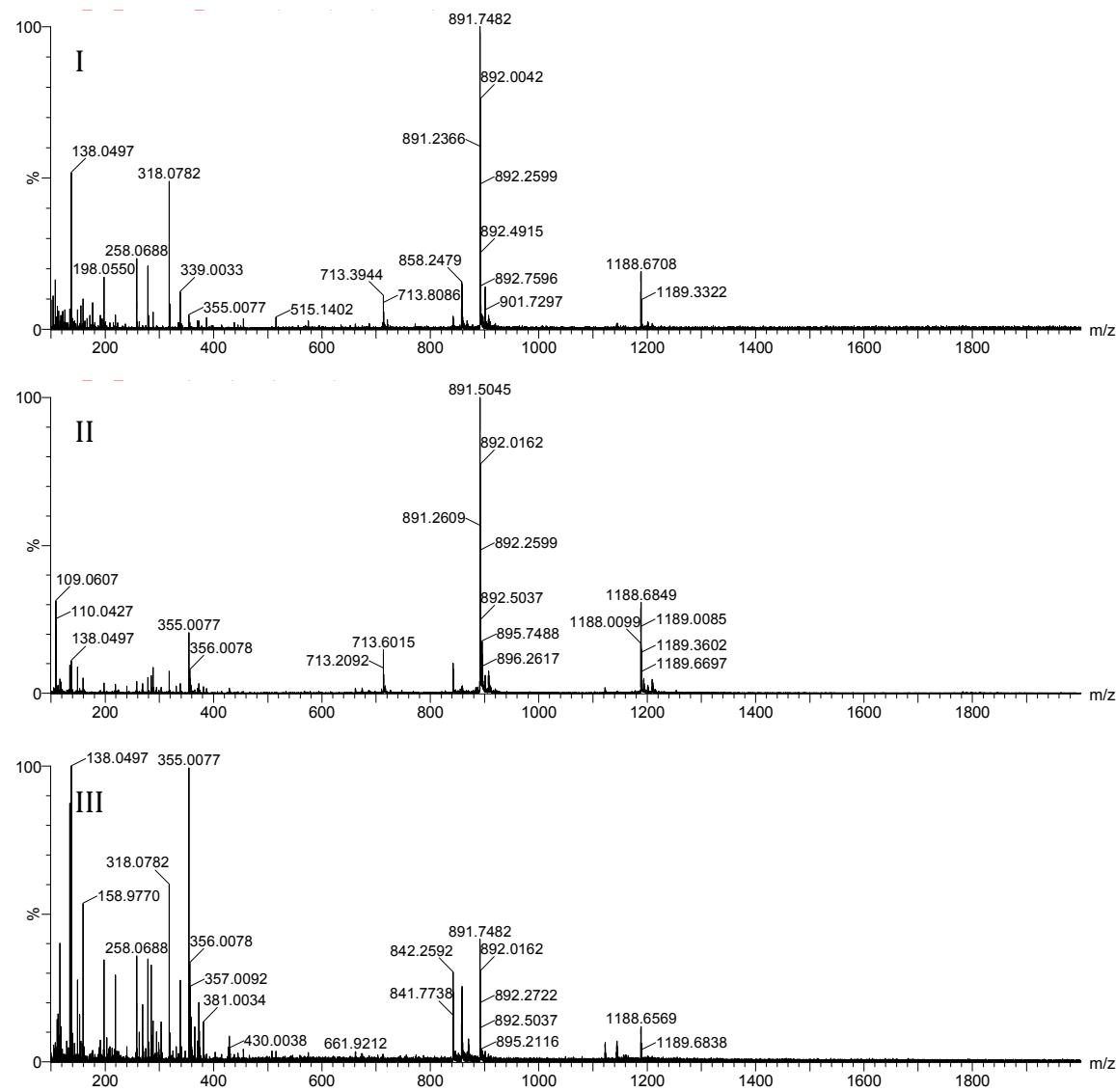


Figure S9. ESI-MS full scan (positive mode) of reaction between compounds **I-III** with ZF Sp1 immediately upon incubation.

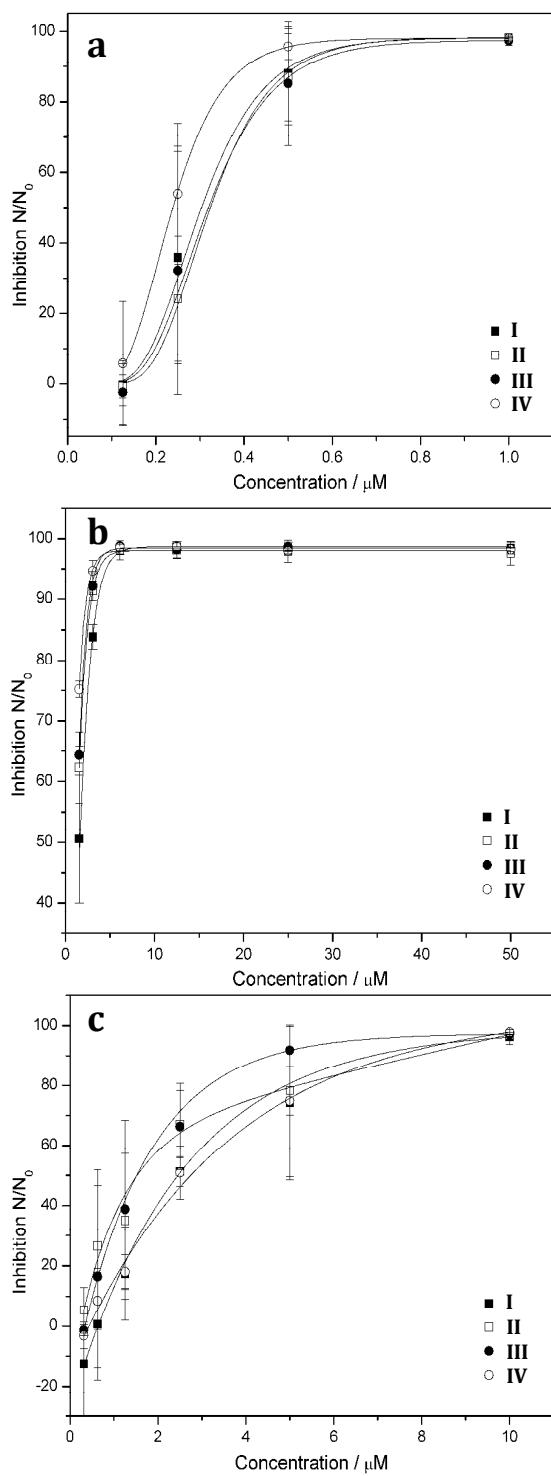


Figure S10. Cytotoxicity curves of the complexes **I**, **II**, **III** and **IV** in three cell lines: a) A2780; b) HCT116 and c) MCF7

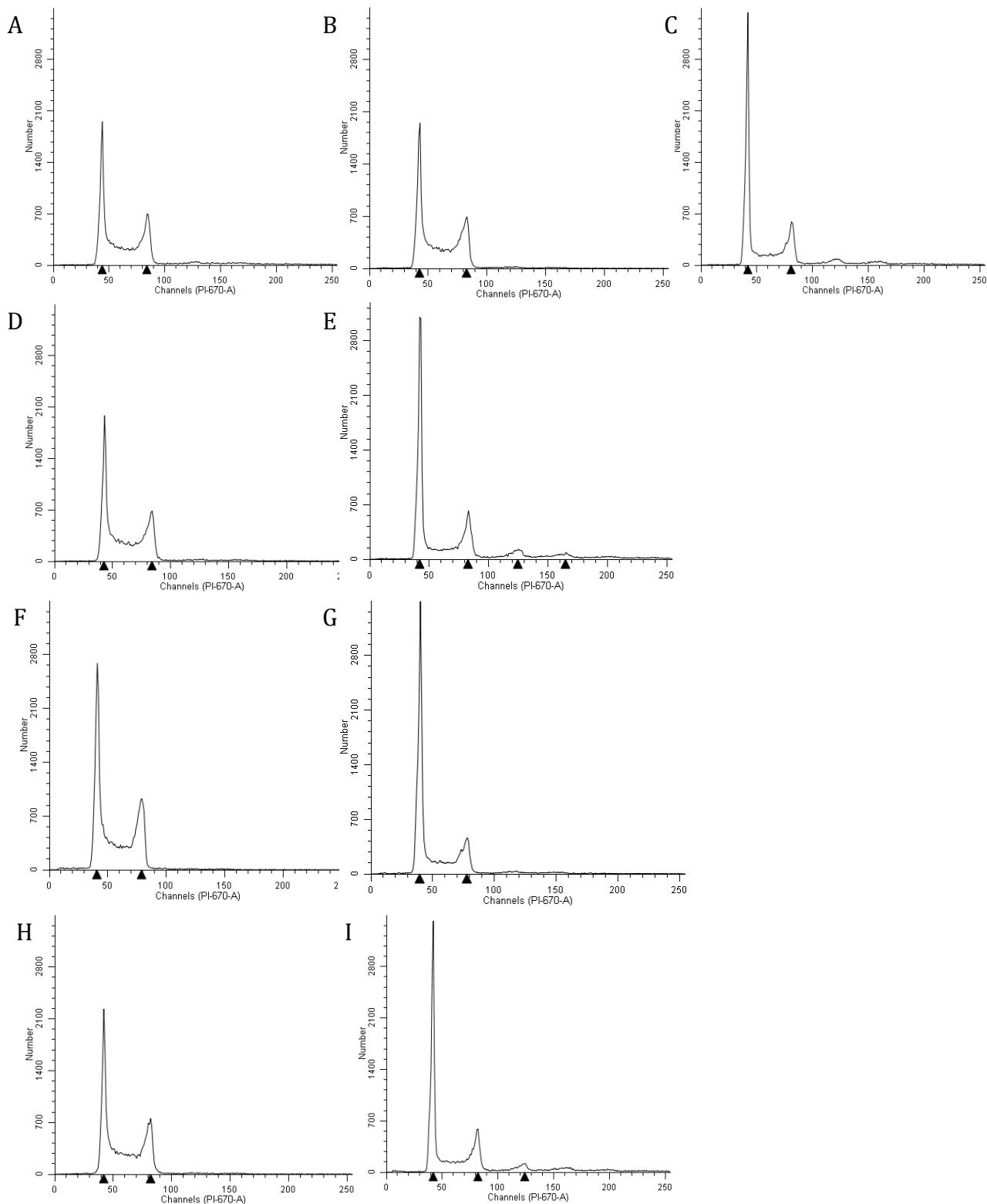


Figure S11. Cell cycle effects of gold(I) compounds in HCT 116 cells in 24h and 48h treatment. A) Control (Untreated); B) Compound I - 24h; C) I - 48h; D) II - 24h; E) II - 48h; F) III - 24h; G) III - 48h; H) IV - 24h and I) IV - 48h.

Table S1. pKa values of Compounds **I**, **II** and **IV**.

Compound	pKa	
	P(Ph) <sub>3</sub>	Py
<b>I</b>	3.45	-
<b>II</b>	3.68	4.31
<b>IV</b>	3.39	8.42

Table S2. DNA melting temperatures after incubation of the compounds I-IV in different DNA:compound molar ratios. Results are a difference between treated and untreated DNA\*.

$r_i$	I $\Delta T$ (°C)	II $\Delta T$ (°C)	III $\Delta T$ (°C)	IV $\Delta T$ (°C)
0,01	-0,25	-0,84	-1,30	-1,09
0,03	0,84	0,63	0,59	0,05
0,05	0,38	1,90	1,38	1,64
0,075	1,22	2,60	1,72	0,17
0,1	1,68	3,07	2,22	1,51

\* untreated DNA was measured after incubation with 1% (v/v) DMSO