PtI₂(DACH), the Iodido Analogue of Oxaliplatin as a Candidate for Colorectal Cancer Treatment: Chemical and Biological Features

D. Cirri, S. Pillozzi, C. Gabbiani, J. Tricomi, G. Bartoli, M. Stefanini, E. Michelucci, A. Arcangeli, L. Messori* and T. Marzo* a

a Laboratory of Metals in Medicine (MetMed), Department of Chemistry, University of Florence, Via della Lastruccia 3, 50019, Sesto Fiorentino, Italy. E-mail: luigi.messori@unifi.it, tiziano.marzo@unifi.it.

b Department of Experimental and Clinical Medicine, University of Florence, Viale GB Morgagni 50, 50134 Firenze, Italy.

c Department of Chemistry and Industrial Chemistry, University of Pisa, via Moruzzi, 13, 56124 Pisa, Italy. E-mail: tiziano.marzo@dcci.unipi.it.

d DIVAL Toscana Srl, Via Madonna del Piano 6, 50119, Sesto Fiorentino, Firenze, Italy.

Mass Spectrometry Centre (CISM), University of Florence, Via U. Schiff 6, 50019 Sesto Fiorentino, Italy.

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FIG. S1 $^1$H NMR spectrum of PtI$_2$(DACH) in DMF-d$_7$ at 400.13 MHz: 5.56 (b, 1H); 4.96 (b, 1H); 2.50 (t, $J = 8$ Hz, 2H); 2.23 (d, $J = 12$ Hz, 2H); 1.56 (m, 4H); 1.15 (m, 2H).

Signals were attributed by comparison with the reported spectrum of oxaliplatin (Chem. Commun., 2012, 48, 847-849).

FIG. S2 $^{13}$C NMR spectrum of PtI$_2$(DACH) in DMF-d$_7$ at 100.01 MHz: 65.37; 33.23; 26.03.
FIG. S3 $^{155}$PtNMR spectrum of PtI$_2$(DACH) in DMF-d$_7$ at 86.01 MHz: -3413.26.

![FIG. S3 $^{155}$PtNMR spectrum of PtI$_2$(DACH) in DMF-d$_7$ at 86.01 MHz: -3413.26.](image)

FIG. S4 $^1$H NMR spectra comparison of PtCl$_2$(DACH) (blue) and PtI$_2$(DACH) (red) in DMF-d$_7$ + D$_2$O at 400.13 MHz.

![FIG. S4 $^1$H NMR spectra comparison of PtCl$_2$(DACH) (blue) and PtI$_2$(DACH) (red) in DMF-d$_7$ + D$_2$O at 400.13 MHz.](image)

D$_2$O completely suppress only the -NH$_2$ signals in the case of chlorido-analogue. This implies a lower mobility of amine protons upon replacement of chlorine with iodide.
Synthesis of PtCl$_2$(DACH): Diaminocyclohexane (1R,2R)-(−), DACH was solubilised in milli-q water and the obtained solution slowly added to K$_2$PtCl$_4$ water solution. After further four hours of stirring precipitate appeared, and complete precipitation of yellow crystals of PtI$_2$(DACH) allowed over night at room temperature. The solid was then collected through vacuum filtration and washed with hot water and ice-cooled ethanol and ether.
FIG. S5 Interaction with lysozyme and RNase (ESI-MS)
Comparison between the experimental (upper) and simulated (lower) spectra of 6- charge state of ODN2 + [Pt(DACH)]^{2+}.
We studied the antiproliferative effect of Oxaliplatin and PtI2(DACH) on HCT116 cells. The effects of both compounds used at the same concentration (50mM) were tested by the Trypan blue exclusion assay at different incubation times (24, 48, 72 hours). We found that PtI2(DACH) strongly inhibited proliferation, more than oxaliplatin.