PtI_2(DACH), the Iodido Analogue of Oxaliplatin as a Candidate for Colorectal Cancer Treatment: Chemical and Biological Features

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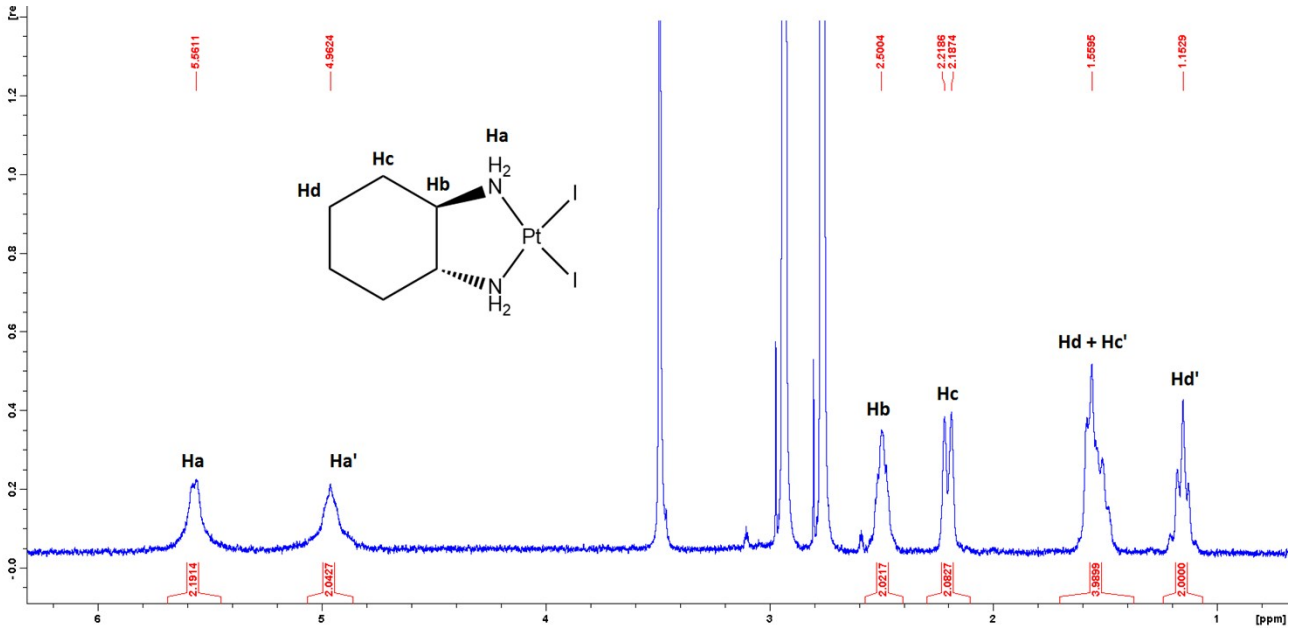
FIG. S1 ^{1}HNMR spectrum of PtI_2(DACH) in DMF-d_7 at 400.13 MHz: 5.56 (b, 1H); 4.96 (b, 1H); 2.50 (t, *J* = 8 Hz, 2H); 2.23 (d, *J* = 12 Hz, 2H); 1.56 (m, 4H); 1.15 (m, 2H).



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

FIG. S2 ^{13}CNMR spectrum of PtI_2(DACH) in DMF-d_7 at 100.01 MHz: 65.37; 33.23; 26.03.

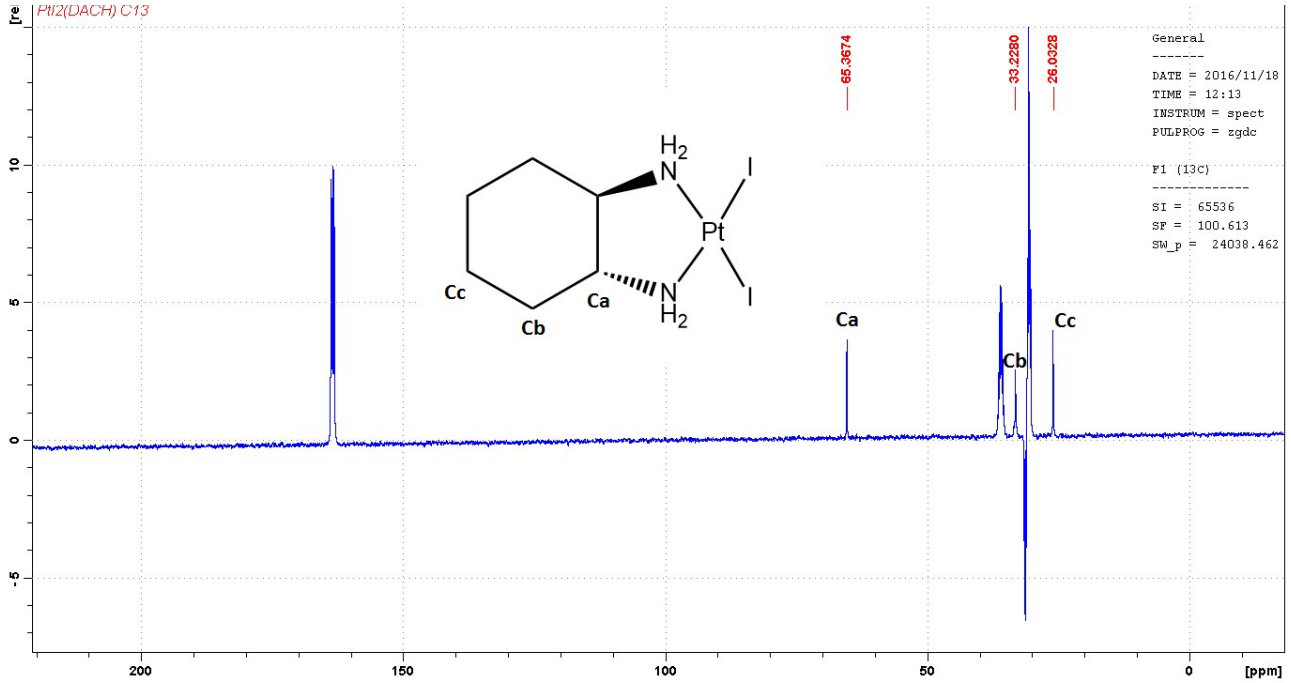


FIG. S3 ^{195}PtNMR spectrum of PtI_2(DACH) in DMF-d_7 at 86.01 MHz: -3413.26.

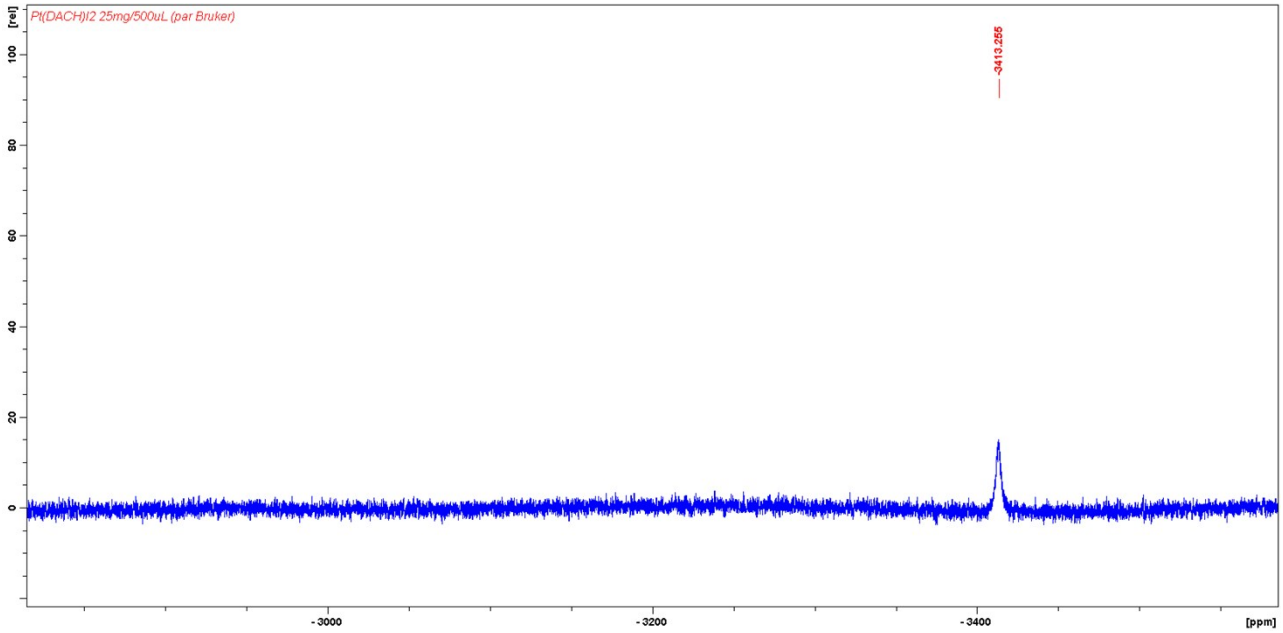
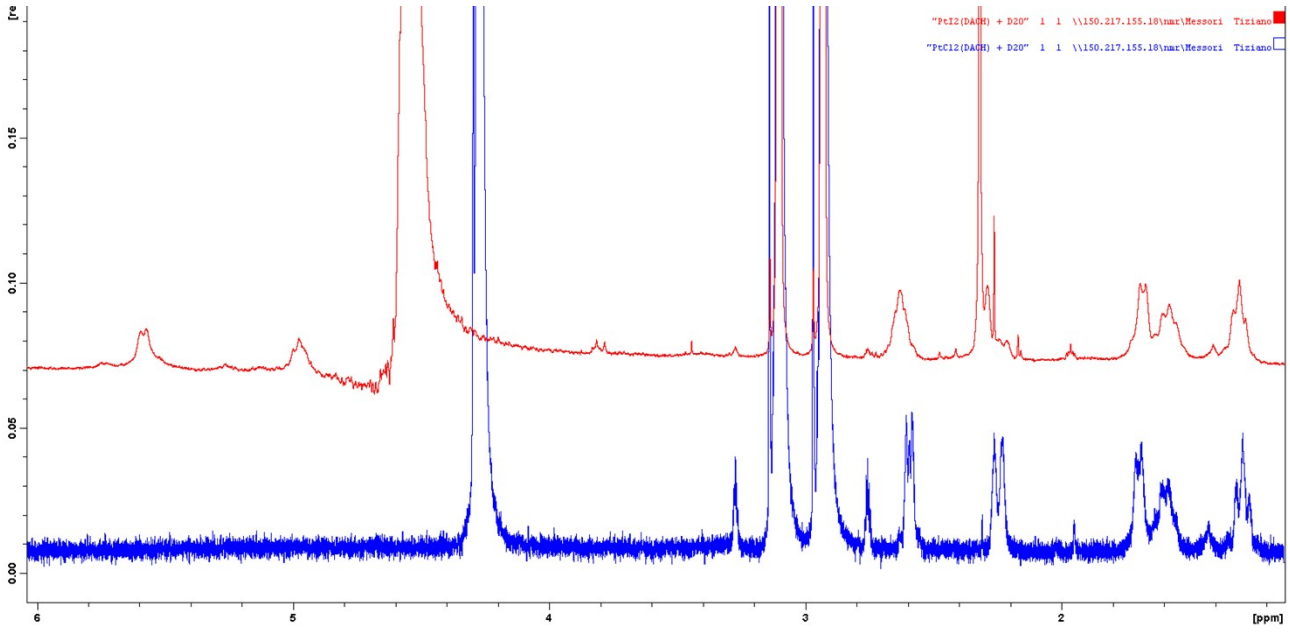


FIG. S4 ^{1}HNMR spectra comparison of $PtCl_2$(DACH) (blue) and PtI_2(DACH) (red) in DMF-d_7 + D_2O at 400.13 MHz.

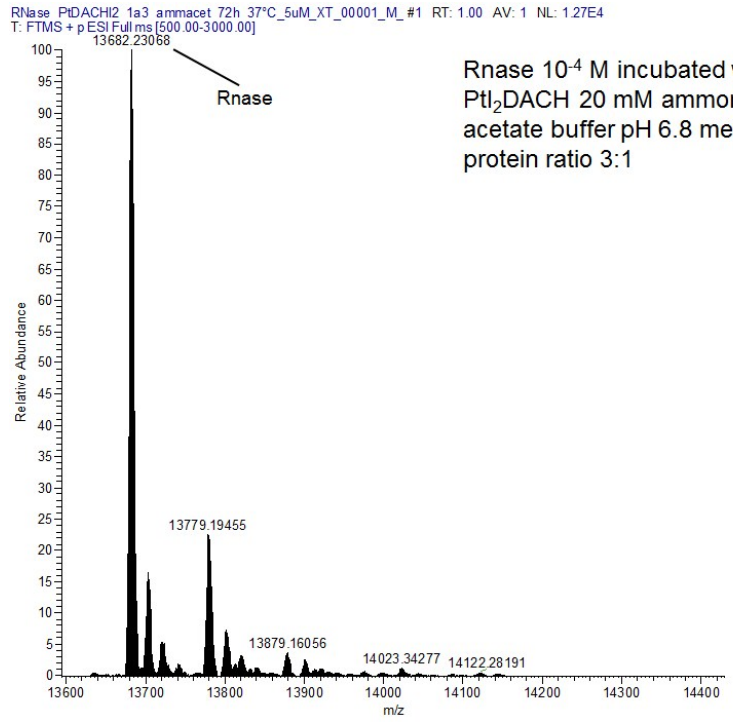


D_2O completely suppress only the -NH_2 signals in the case of chlorido-analogue. This implies a lower mobility of amine protons upon replacement of chlorine with iodide.

S4

Synthesis of $PtCl_2$(DACH): Diaminocyclohexane (1R,2R)-(-), DACH was solubilised in milli-q water and the obtained solution slowly added to K_2PtCl_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)



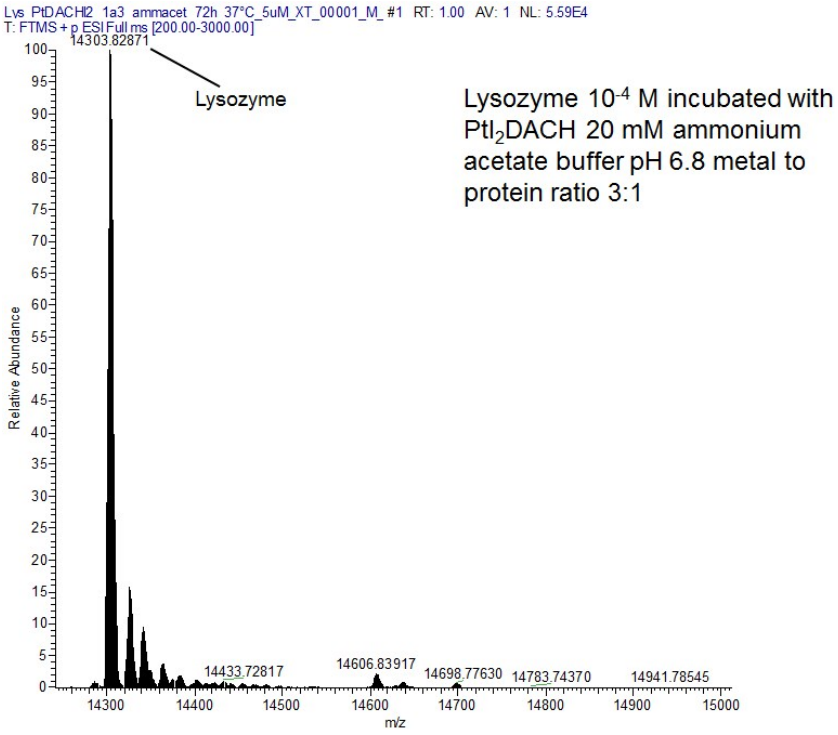
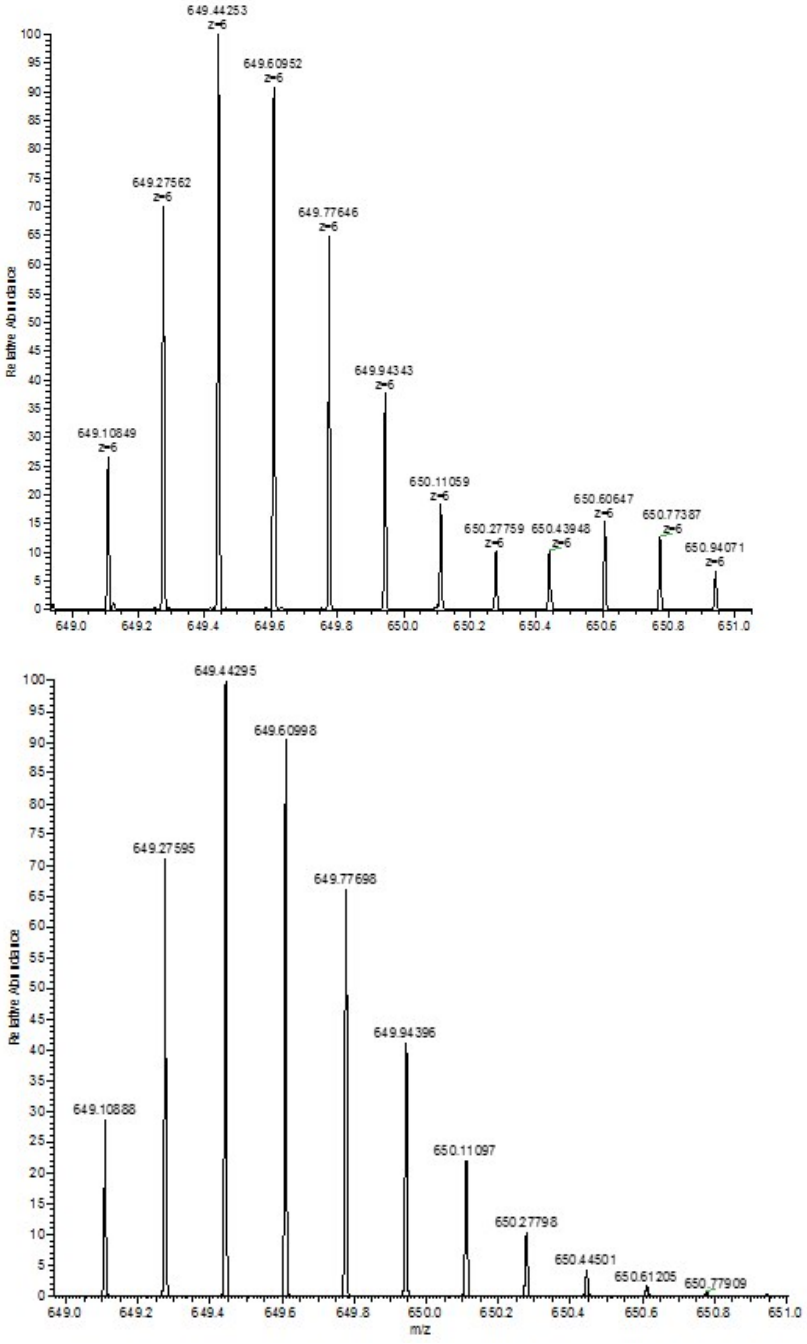
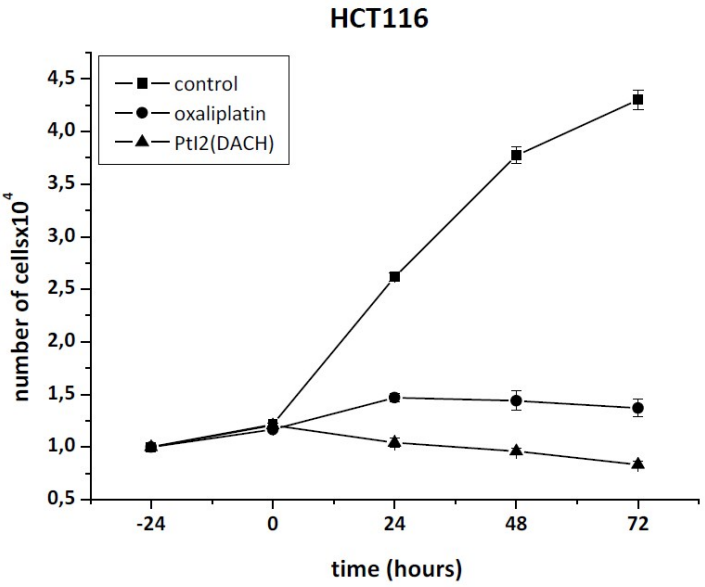


FIG. S6 ESI-MS theoretical calculations



Comparison between the experimental (upper) and simulated (lower) spectra of 6^- charge state of ODN2 + $[Pt(DACH)]^{2+}$.

S7 Effects of Oxaliplatin and PtI2(DACH) on HCT116 cell proliferation after a single treatment at time 0 (50mM for both compounds), given as the number of Trypan Blue negative cells. Values are means ± sem of three independent experiments.



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 .