

Analysis of Biomolecular Changes in HeLa Cervical Cancer Cell Line Induced by Interaction with [Pd(dach)Cl₂]

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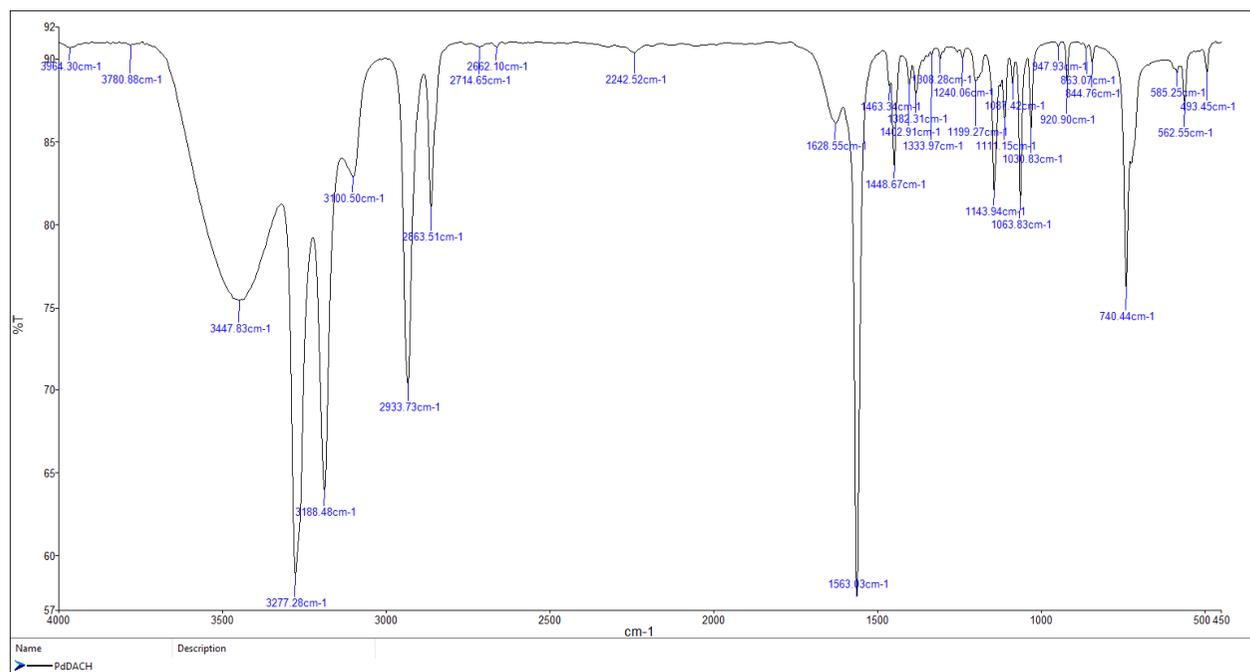


Figure S1. FTIR spectrum of the [Pd(dach)Cl₂] complex

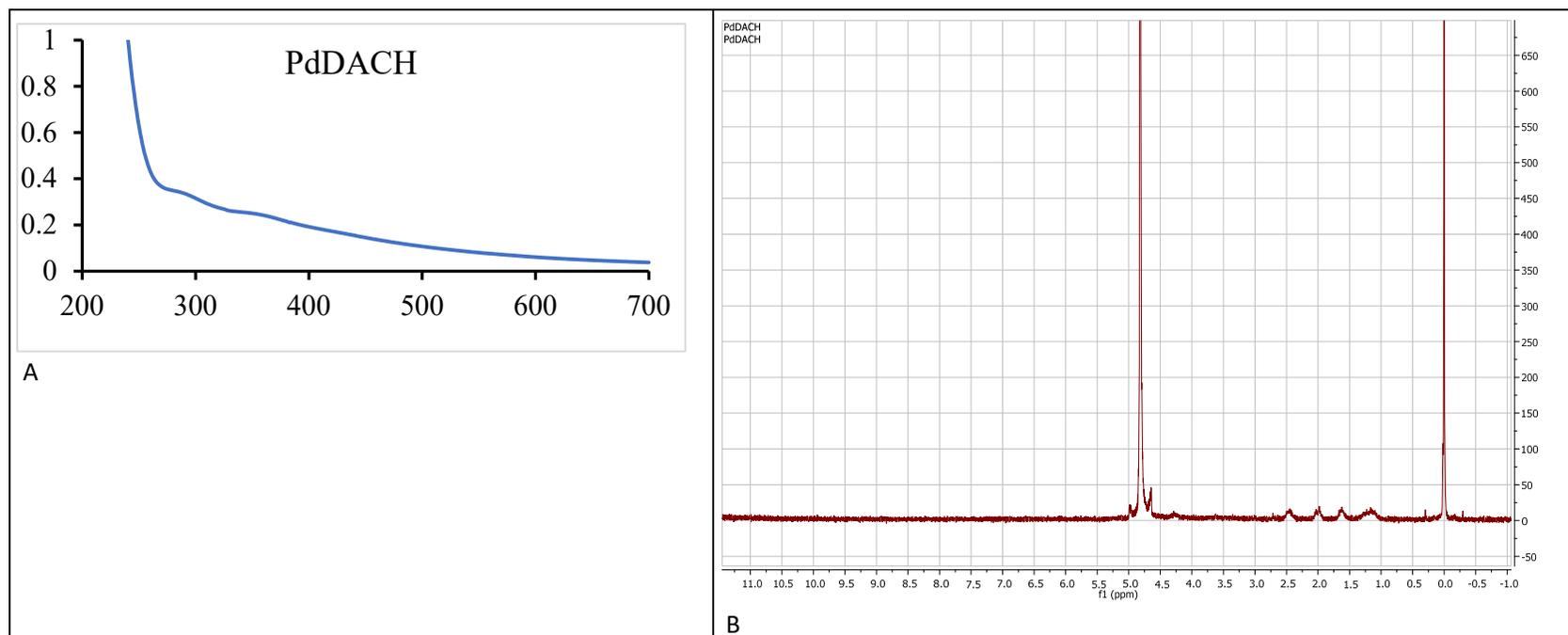


Figure S2. UV/Vis spectrum of the $[Pd(dach)Cl_2]$ complex (A) and the proton NMR spectrum of Pd(II).

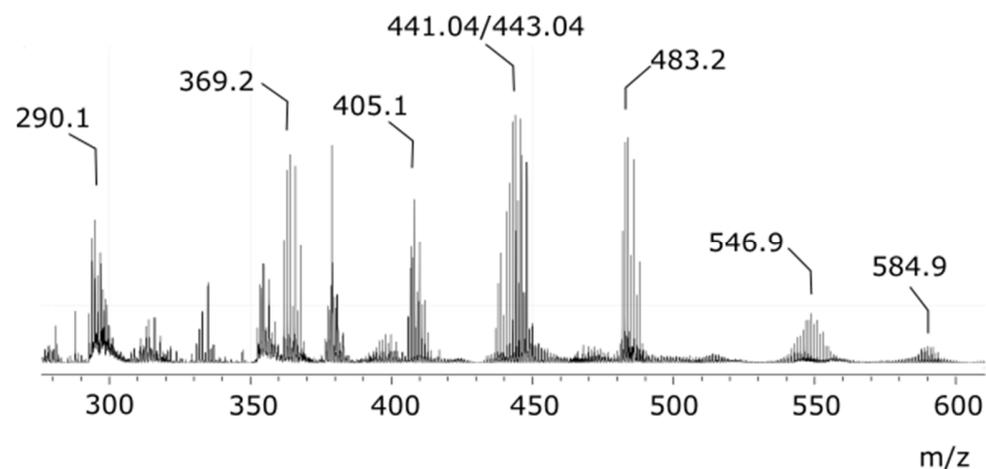


Figure S3. Positive ion MALDI TOF mass spectrum of Pd(dach) complex acquired with α -hydroxy-cinnamic acid (CHCA) as the matrix. Spectrum represents the average of 200 individual laser shots. The peak position is identified by the m/z ratio indicated in the Figure. The identity of signals is given in the table below.

Table S1. The position and identification of signals observed in MALDI TOF mass spectra given in Fig. S3.

Peak position (m/z)*	Isotopic distribution (m/z)	Signal identity
290.1	288.1-296.9	$\text{Pd(dach)Cl}_2+\text{H}^+$
369.2	367.2-375.2	$\text{Pd(dach)}_2\text{Cl}$
405.1	403.1-411.1	$\text{Pd(dach)}_2\text{Cl}_2+\text{H}^+$
441.1/443.1 [#]	437.1-445.1/438.1-447.1	$\text{Pd(dach)}_2\text{Cl}_3+\text{H}^+$ / $(\text{Pd(dach)Cl}_2)_2+\text{H}^+$
483.2	481.2-489.2	$\text{Pd(dach)Cl}_2+\text{H}^+$
546.9	541.9-553.9	$(\text{Pd(dach)})_2\text{Cl}_3$
584.9	577.9-590.9	$(\text{Pd(dach)Cl}_2)_2+\text{H}^+$

*The position of the maximum is indicated

[#]This signal represents most likely the overlapping ion species. Due to a higher number of signals arising from a high number of isotopes, both signals are probable.

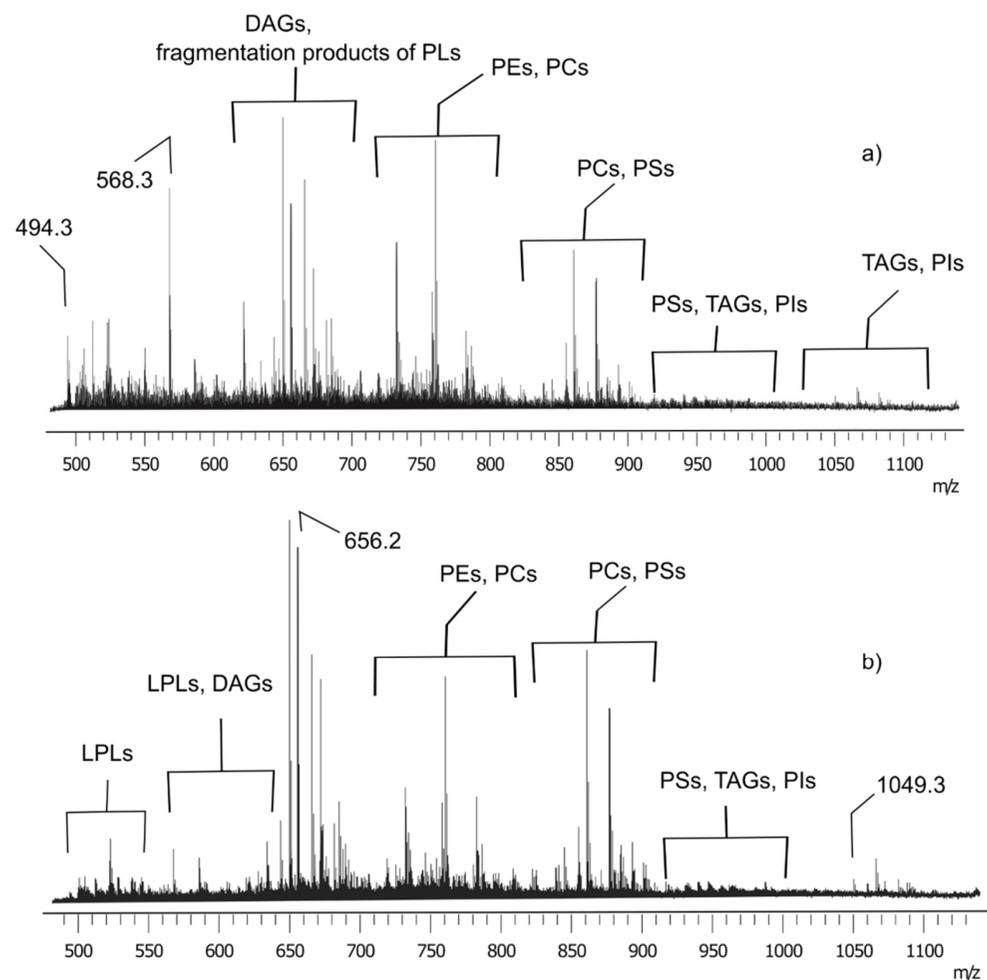


Figure S4. Positive ion MALDI TOF mass spectra of organic extract of untreated HeLa cells (a) and treated with Pd(dach) (b). Spectra are acquired with the CHCA matrix and in the reflector mode. Representative spectra are presented and the region in which the major phospholipid classes are detectable is indicated. The numbers represent the position of signals that differ in abundance between the two preparations. Their identity is given in the text. Abbreviations: LPLs-lysophospholipids; DAGs-diacylglycerols; PLs-phospholipids; PEs-phosphatidylethanolamines; PCs-phosphatidylcholines; PSs-phosphatidylserine; TAGs-triacylglycerols; PIs-phosphatidylinositols;

The signal at m/z 1049.3 might arise from phosphatidylinositol phosphate, but its identity could not be confirmed with certainty. The signal at m/z 494.3 [1] most likely corresponds to the proton adduct of LPC 16:1, whereas that at m/z 568.3 is the sodium adduct of DAG 36:0 [2]. Significant changes in other m/z regions are not detectable. Signal at m/z 1049 is detectable only in Pd(dach)-treated cells, and corresponds to the phosphatidylinositol phosphate.

References

1. Silva CL, Perestrelo R, Sousa-Ferreira I, et al (2020) Lipid biosignature of breast cancer tissues by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry. *Breast Cancer Res Treat* 182:9–19. <https://doi.org/10.1007/s10549-020-05672-9>
2. Benard S, Arnhold J, Lehnert M, et al (1999) Experiments towards quantification of saturated and polyunsaturated diacylglycerols by matrix-assisted laser desorption and ionization time-of-flight mass spectrometry. *Chem Phys Lipids* 100:115–125. [https://doi.org/https://doi.org/10.1016/S0009-3084\(99\)00045-6](https://doi.org/https://doi.org/10.1016/S0009-3084(99)00045-6)