Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary Information

Analysis of fatty acids and triacylglycerides by Pd nanoparticle-assisted laser desorption/ionization mass spectrometry

Yuliya E. Silina,[1,2] Claudia Fink-Straube,[1] Heiko Hayen,[3] Dietrich A. Volmer[2]*

[1]*Leibniz Institute for New Materials (INM), Saarbrücken, Germany*

[2]*Institute of Bioanalytical Chemistry, Saarland University, Saarbrücken, Germany*

[3]*Institute of Inorganic and Analytical Chemistry, University of Münster, Germany*

*Corresponding author:

Prof. Dr. Dietrich A. Volmer
Saarland University
Institute of Bioanalytical Chemistry
D-66123 Saarbrücken, Germany
Tel +49 681 302 3433; Fax +49 681 302 2963
Email: Dietrich.Volmer@mx.uni-saarland.de

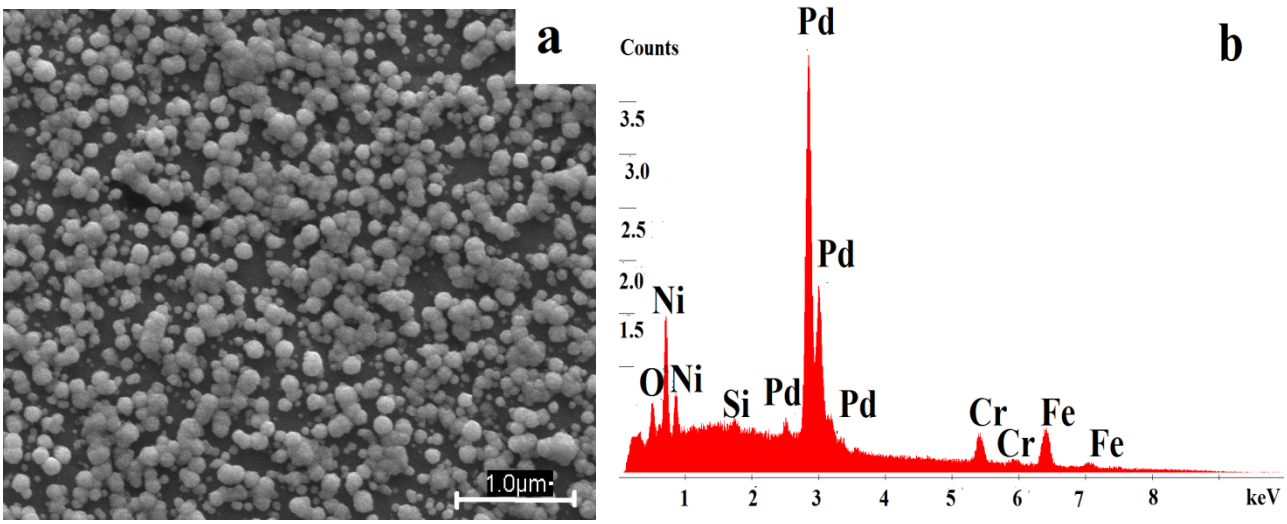

Figure S1. (a) SEM image of the Pd-NP surface; (b) EDX analysis of electroplated Pd target.

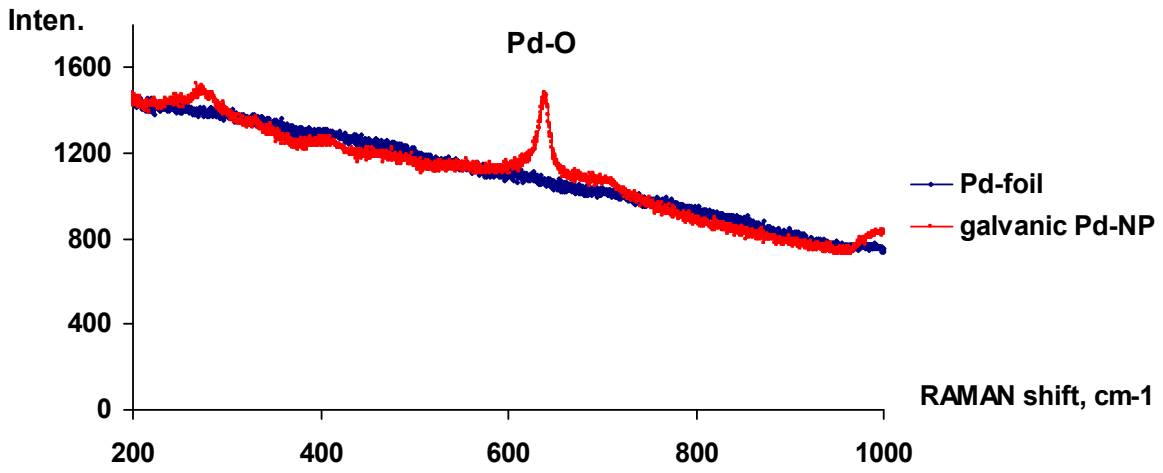

Figure S2. Raman spectra of Pd foil and electroplated Pd-NP (deposited on steel carrier material), indicating the presence of PdO at 639 nm^{-1} (excitation using a 633 nm HeNe laser).

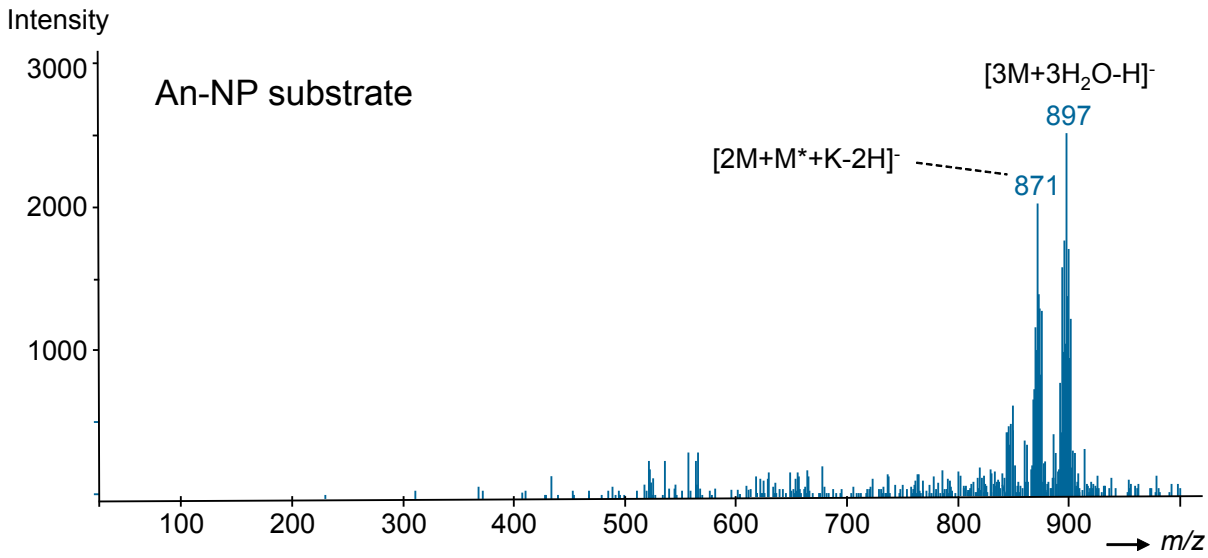

Figure S3. Ag-NP-assisted LDI mass spectrum of a fatty acid mixture (C16:0, C18:0-C18:3, at 200 ng/µL each) in negative ion mode. Note: M* is used as designator for the analyte in hetero trimeric clusters, when two different fatty acid species (M and M*) are present the same cluster ion (laser fluence, 45 %).

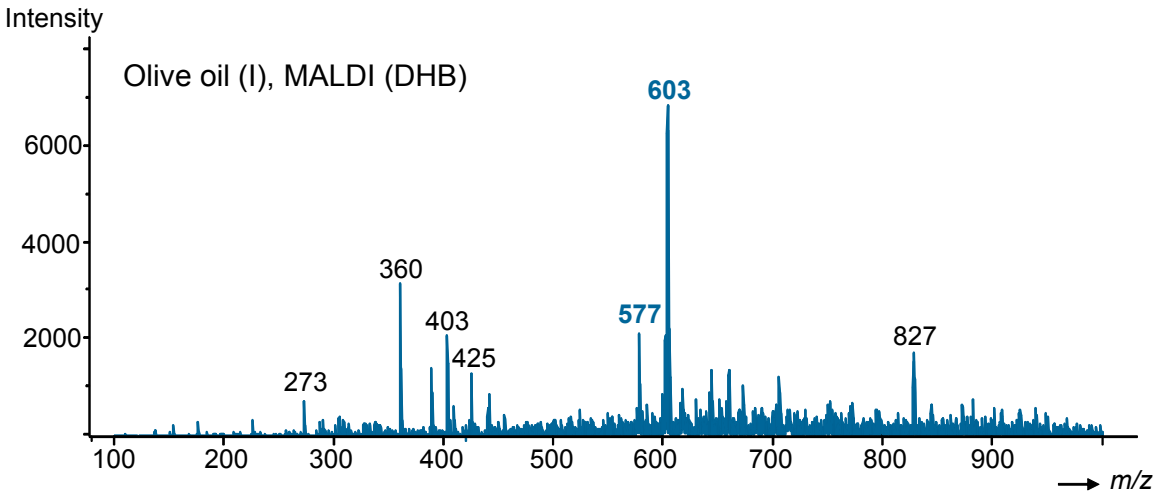

Figure S4. MALDI mass spectrum of cold-extracted olive oil (I) using DHB as matrix compound. The intact TAGs are almost completely degraded and DAG-like fragments (e.g. *m/z* 577, 601 and 603) dominate the spectrum in addition to MALDI matrix ions (laser fluence, 45 %).

Table S1. Analytical figures of merit (n=5) for fatty acid standards from Pd-NP substrates (d_p=60-80 nm, laser fluence 45 %), in the concentration range from 5-10000 ng/µL (ion currents extracted from full scan mass spectra).

Analyte	***Positive ion mode***			***Negative ion mode***		
	$[M+K]^+$ ***m/z***	***y* = a*x* + b**	R^2	**$[3M+3H_2O-H]^-$** ***m/z***	***y* = a*x* + b**	R^2
C16:0	295	y=337*x*–5234	0.996	821	y=32.2*x*+3956	0.924
C18:0	323	y=852*x*+242123	0.988	905	y=613.8*x*+11128	0.896
C18:1	321	y=889*x*+57482	0.942	899	y=1554.9*x*+81590	0.960
C18:2	319	y=1402*x*+47094	0.983	893	y=538.5*x*+34615	0.942
C18:3	317	y=1055*x*+31104	0.987	887	y=164.8*x*+19780	0.930