Supporting Information For:

Water-Soluble Pd Nanoparticles Synthesized from ω-Carboxyl-*S*-alkanethiosulfate Ligand Precursors as Unimolecular Micelle Catalysts

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I. Characterization of ω-Carboxyl-*S*-alkanethiosulfate Ligands

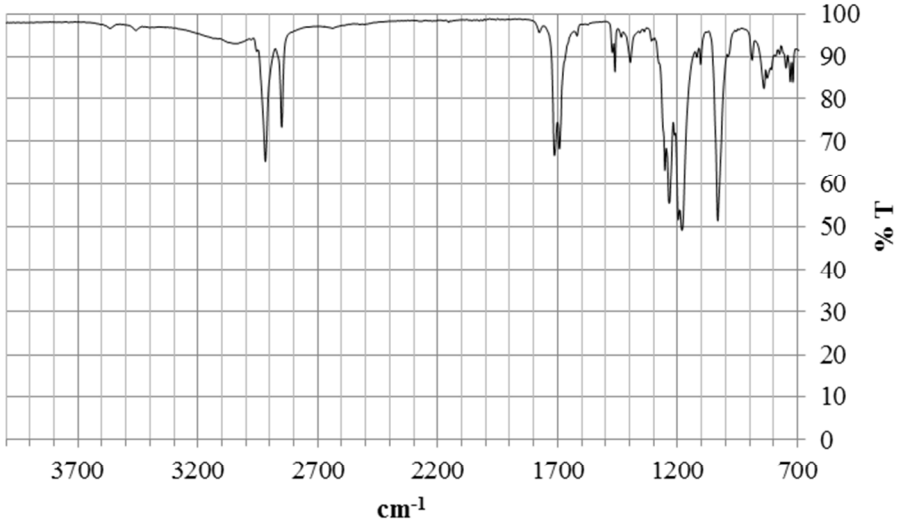

Figure S1. Infrared spectrum of sodium ω-carboxyl-*S*-undecanethiosulfate. The peaks at >3400 cm^{-1} is due to C=O overtone.

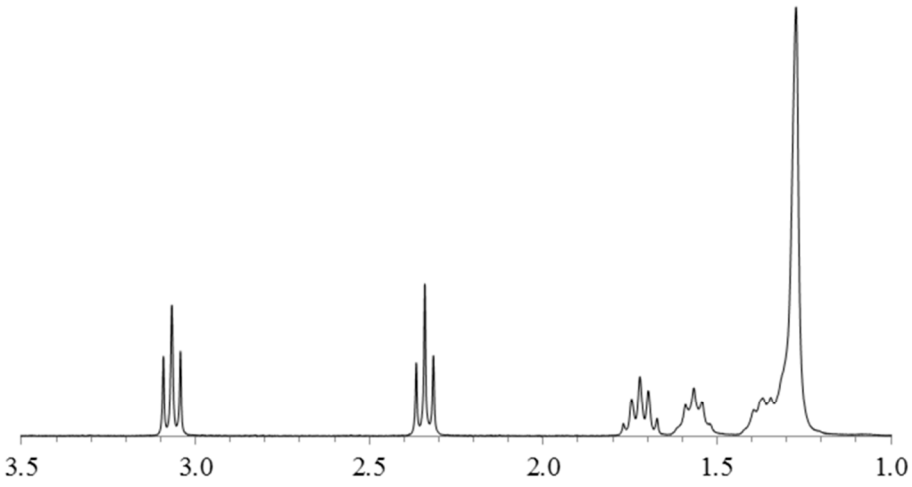

Figure S2. ^{1}H NMR spectrum of sodium ω-carboxyl-*S*-undecanethiosulfate in D_2O.

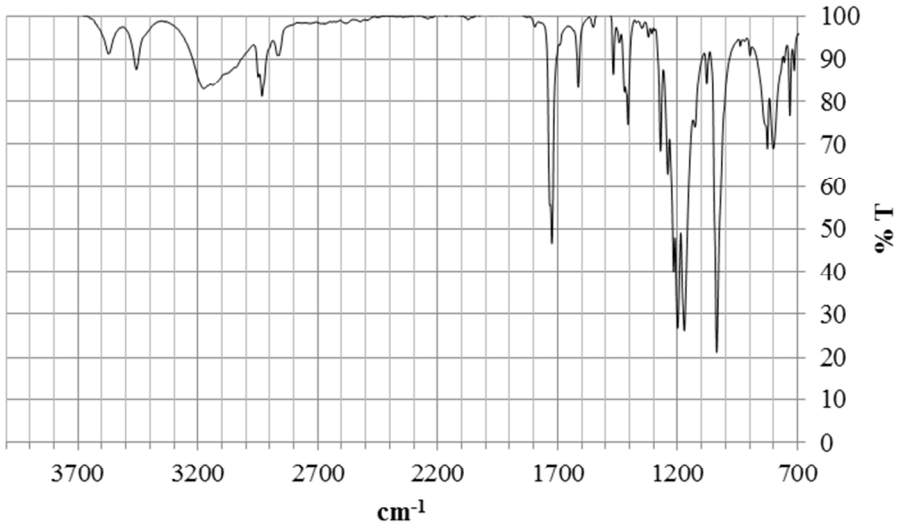

Figure S3. Infrared spectrum of sodium ω-carboxyl-*S*-hexanethiosulfate. The peaks at >3400 cm^{-1} is due to C=O overtone.

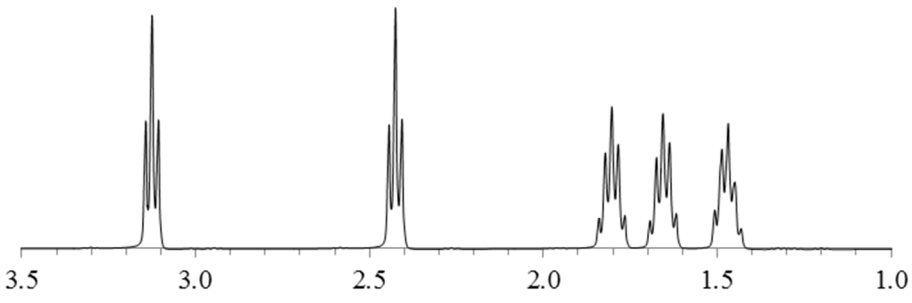

Figure S4. ^{1}H NMR spectrum of sodium ω-carboxyl-*S*-hexanethiosulfate in D_2O.

II. ^{1}H NMR Study of Thiosulfate Hydrolysis in Aqueous Solution

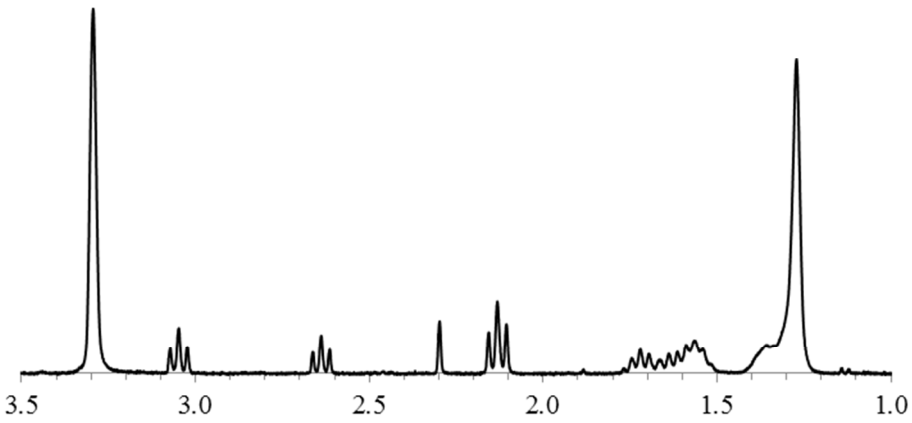

Figure S5. ^{1}H NMR spectra of sodium ω-carboxyl-*S*-undecanethiosulfate hydrolyzed by aqueous sodium borohydride solution in a one phase system of D_2O/MeOD. The resonances at 2.64 ppm indicate the formation of disulfide after the hydrolysis of thiosulfate.

III. Characterization of 11-Mercaptoundecanoic acid-capped Palladium Nanoparticles (ws-MUA-PdNP)

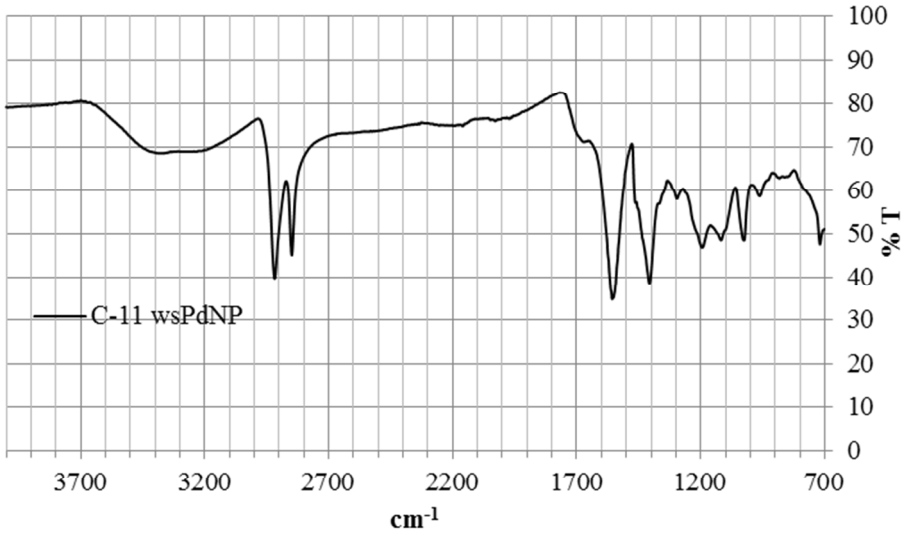

Figure S6. Infrared spectrum of ws-MUA-PdNP.

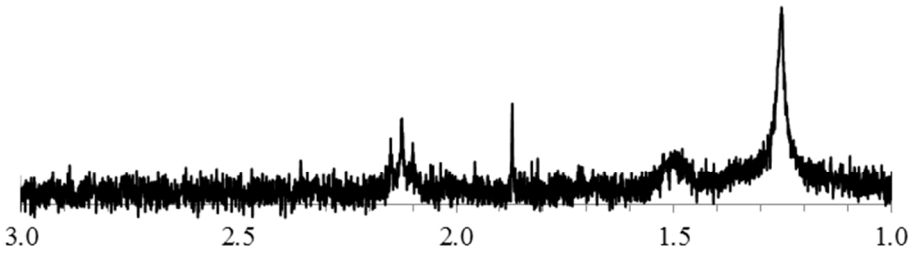

Figure S7. ^{1}H NMR spectrum of ws-MUA-PdNP.

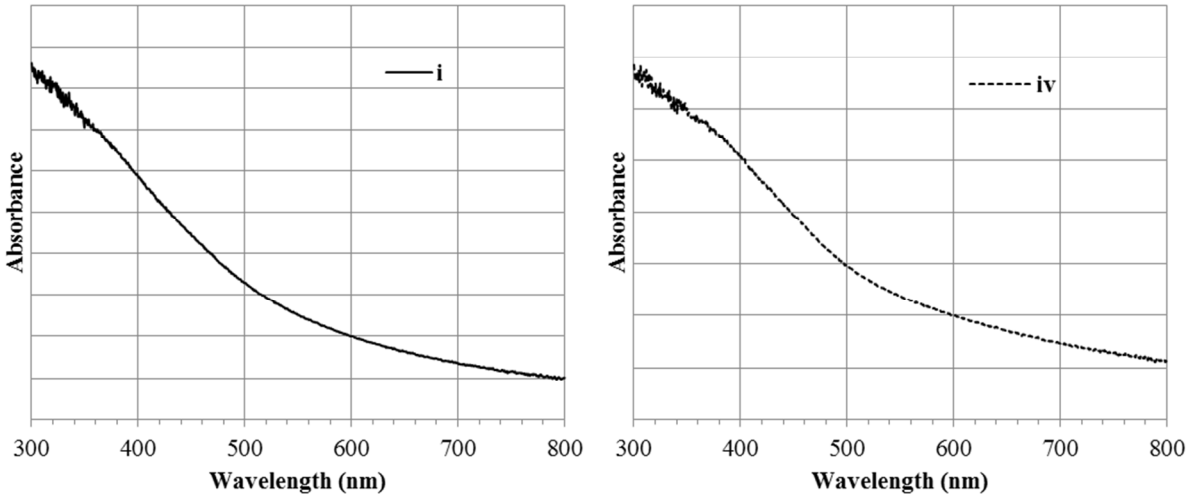

Figure S8. UV-Vis Spectra of ws-MUA-PdNPs (**i**) (left) and (**iv**) (right).

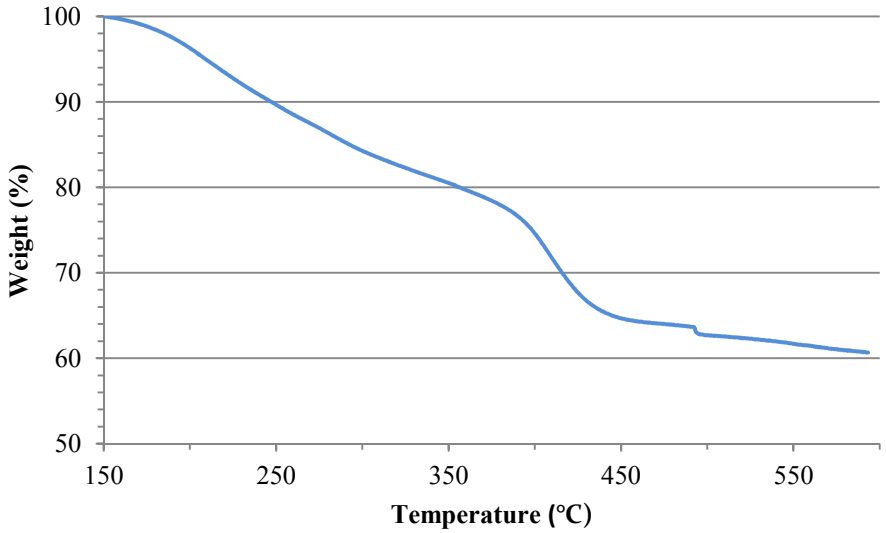

Figure S9. Thermogravimetric profile of ws-MUA-PdNP (**i**).

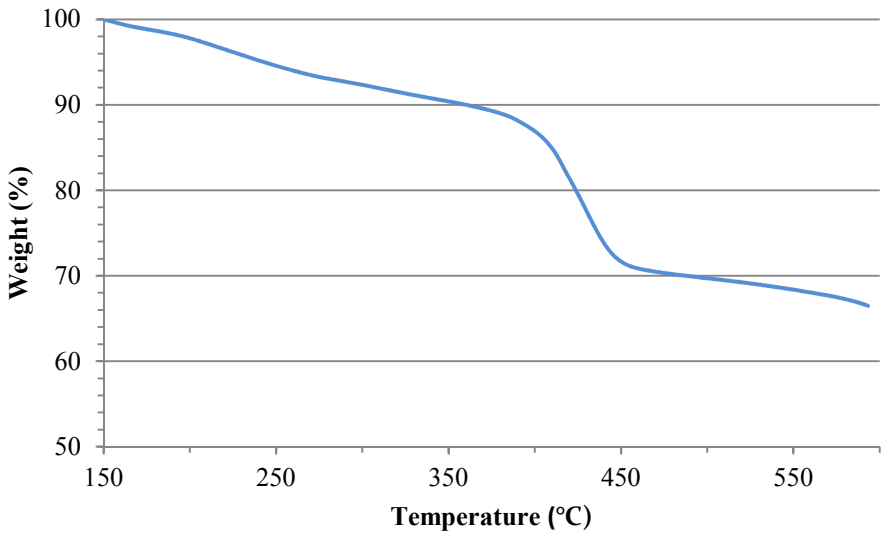

Figure S10. Thermogravimetric profile of ws-MUA-PdNP (**iv**).

IV. Characterization of 6-Mercaptohexanoic acid-capped Palladium Nanoparticles (ws-MHA-PdNP)

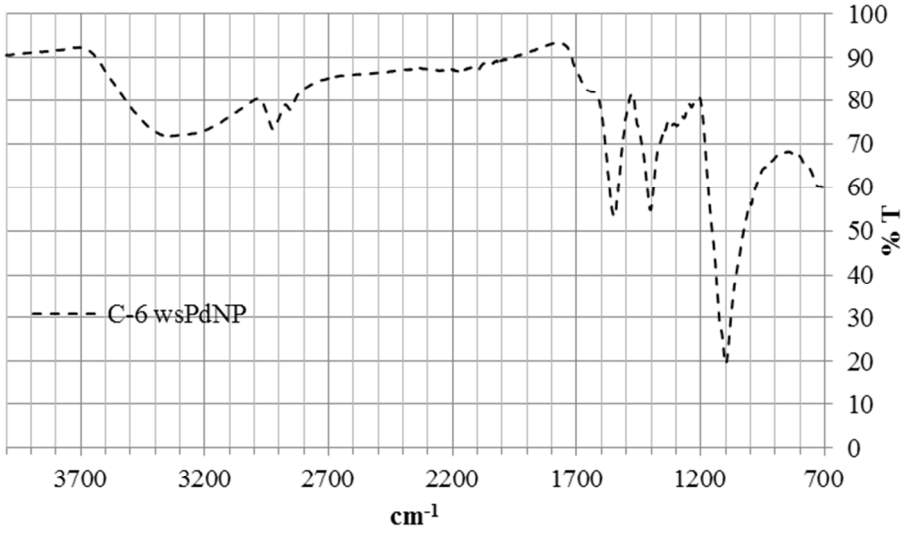

Figure S11. Infrared spectrum of ws-MHA-PdNP.

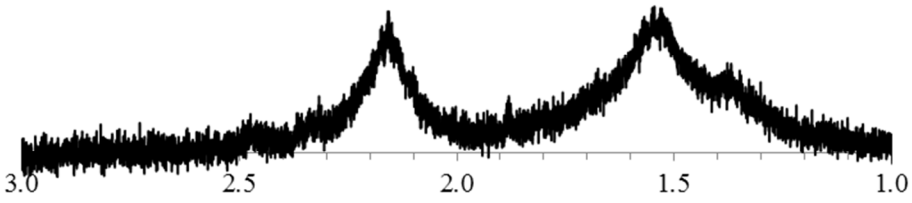

Figure S12. ^{1}H NMR spectrum of ws-MHA-PdNP in D_2O.

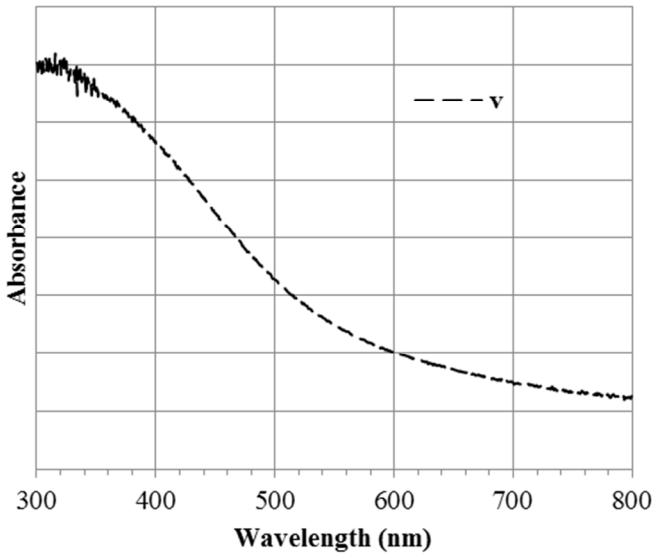

Figure S13. UV-Vis Spectra of ws-MHA-PdNP (**v**).

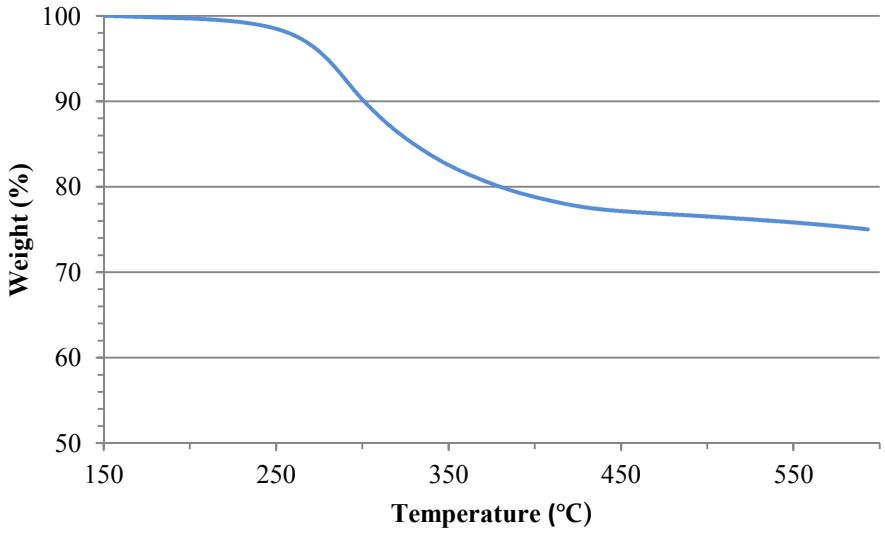

Figure S14. Thermogravimetric profile of ws-MHA-PdNP (**v**).

V. Post-Catalysis Characterization of 6-Mercaptohexanoic acid-capped Palladium Nanoparticles (ws-MHA-PdNP)

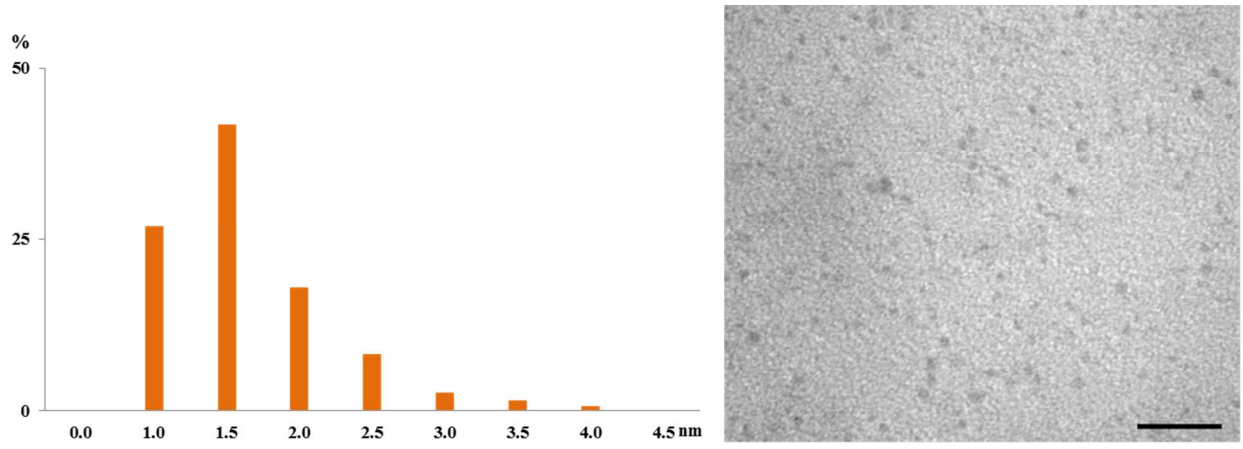

Figure S15. TEM image and size histogram of ws-MHA-PdNP (**v**) after 4 hour reaction. Histogram documents at least 400 counts (1.60 ± 0.56 nm). Scale bar in TEM image is 20 nm.

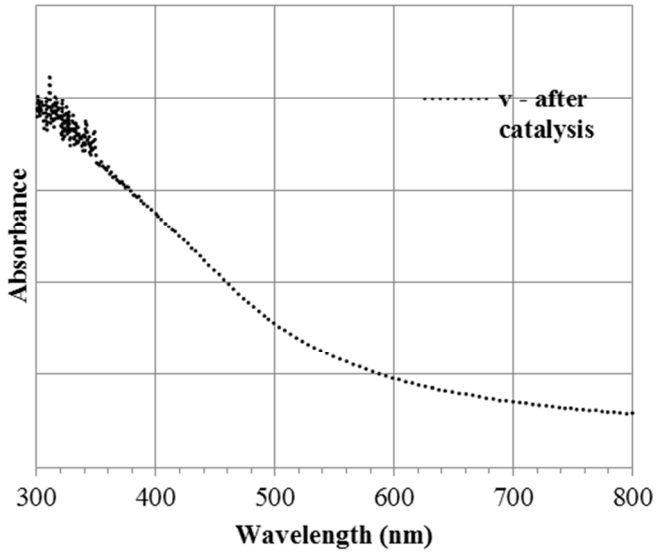

Figure S16. UV-vis spectrum of ws-MHA-PdNP (**v**) after 4 hour reaction.