

Supporting Information

One-pot synthesis of dopamine dithiocarbamate functionalized gold nanoparticles for quantitative analysis of small molecules and phosphopeptides in SALDI- and MALDI-MS

Suresh Kumar Kailasa,^{a,b,c} and Hui-Fen Wu,^{a,b,d*}

^aDepartment of Chemistry, National Sun Yat-Sen University, Kaohsiung, 80424, Taiwan

^bCenter for Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung, 80424, Taiwan

^cDepartment of Applied Chemistry, S. V. National Institute of Technology, Surat – 395007, India

^dDoctoral Degree Program in Marine Biotechnology, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan

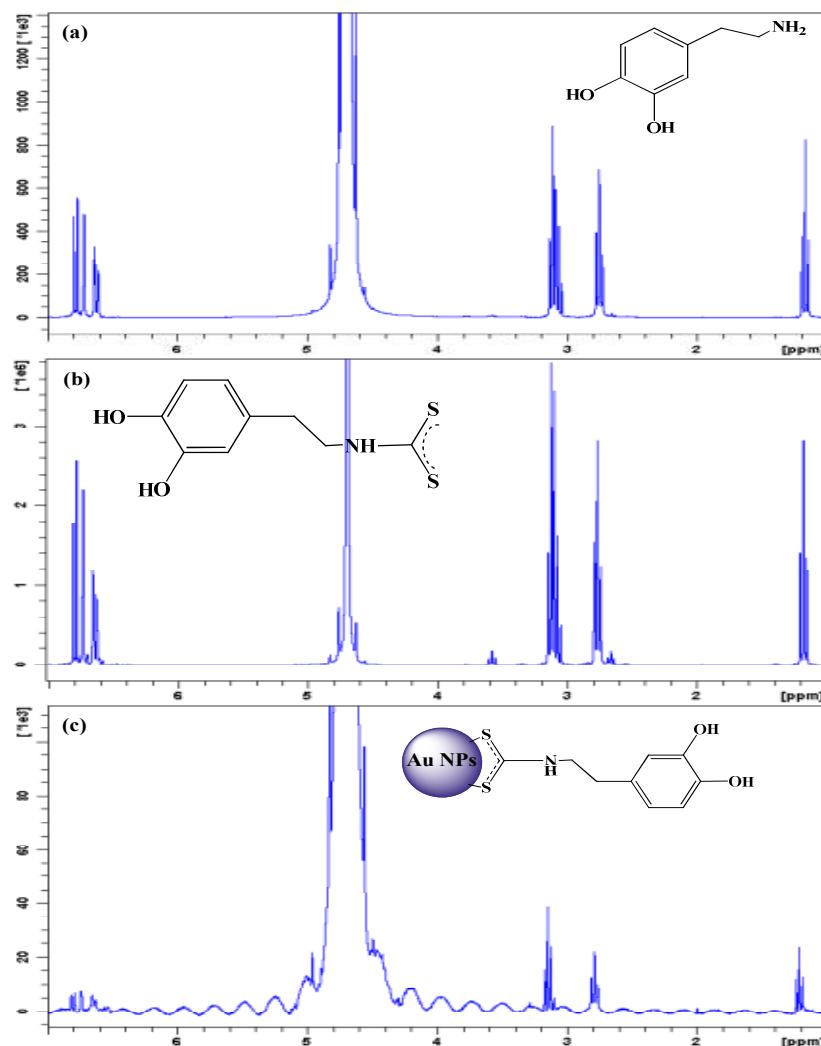


Figure S1. ¹H NMR spectra of (a) pure dopamine (b) dopamine dithiocarbamate and (c) DDTc-Au NPs.

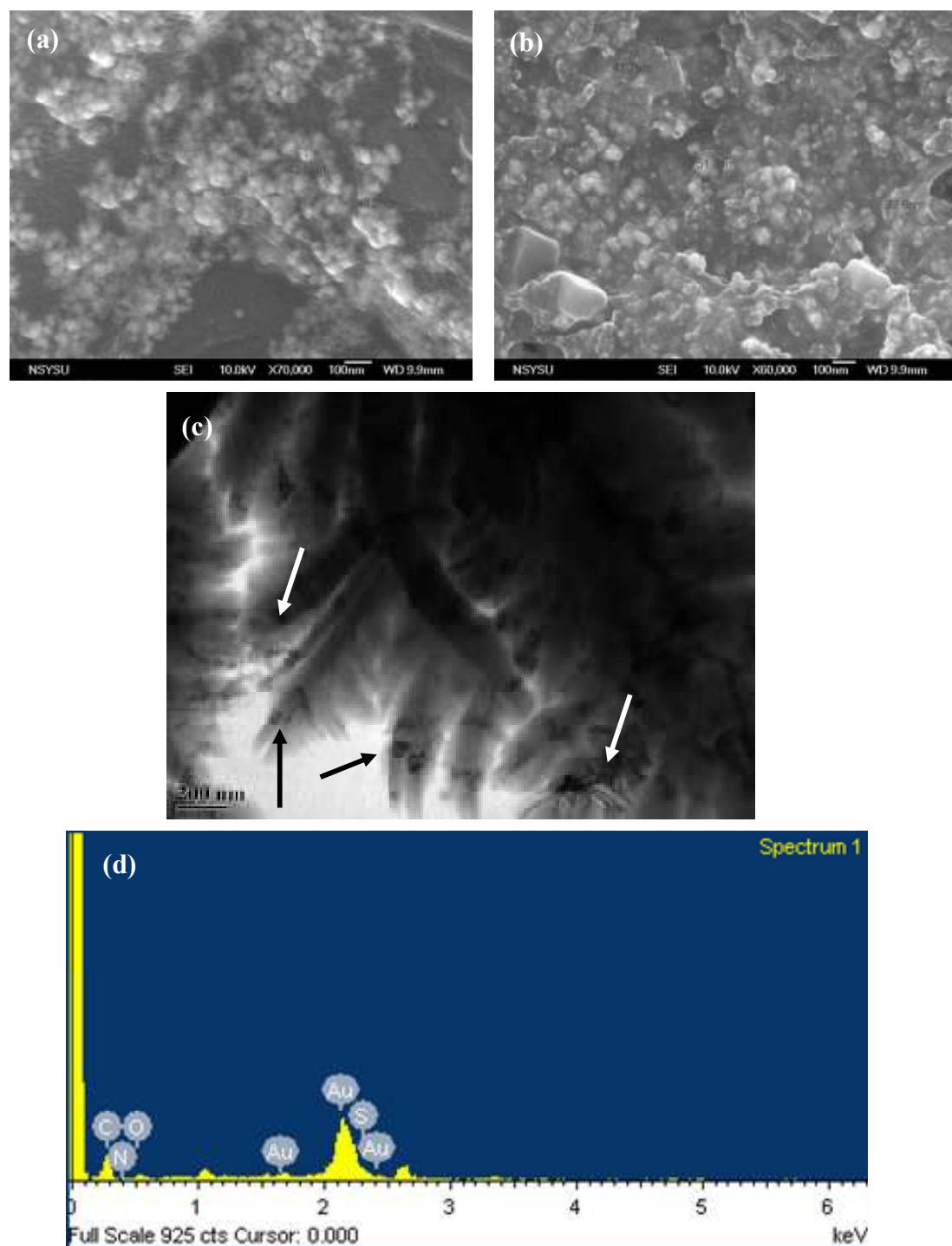


Figure S2. SEM images of (a) bare Au NPs and (b) DDTC-Au NPs. (c) TEM image of DDTC-Au NPs. (d) The energy dispersive X-ray spectra (EDXS) of DDTC-Au NPs and the spectrum has shown the elemental signals of dopamine dithiocarbamate functionalized-Au NPs.

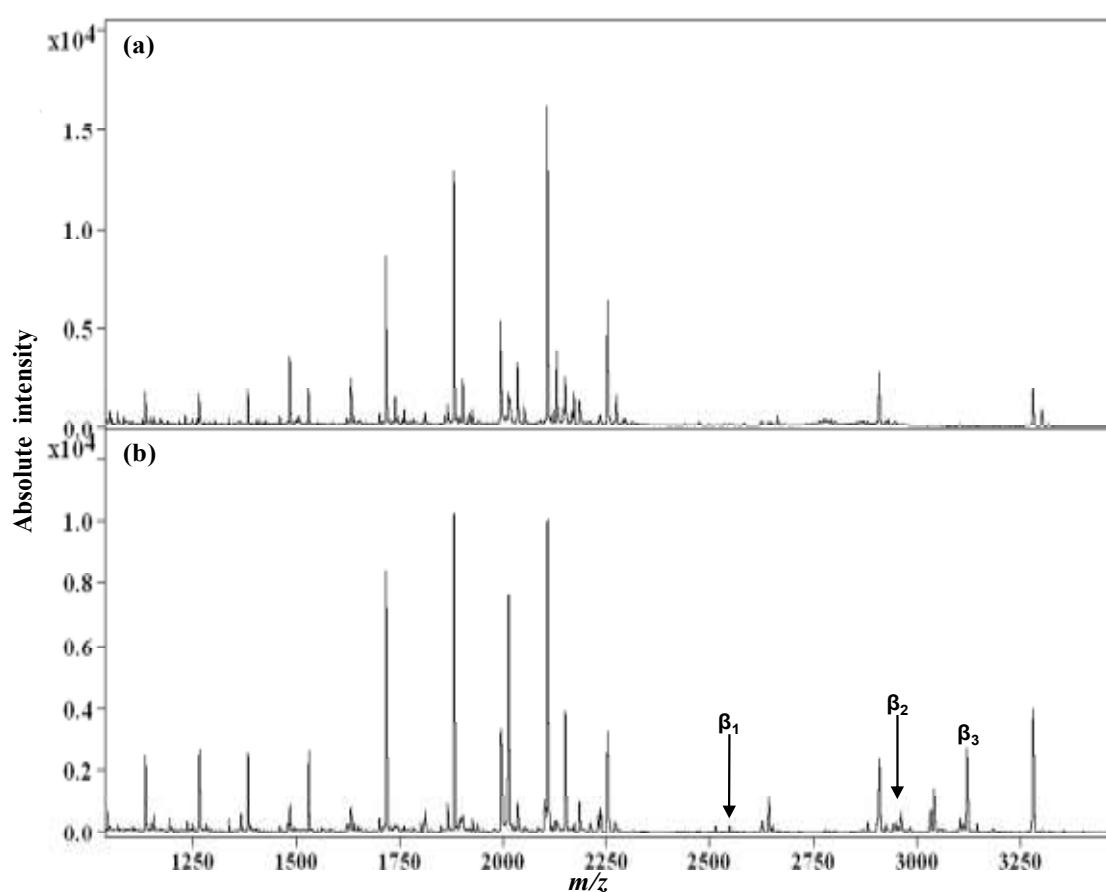


Figure S3. MALDI mass spectra of microwave tryptic digest of β -casein at 50 s microwave irradiating time using (a) 2,5-DHB and (b) using DDTc-Au NPs as affinity probes along with 2,5-DHB as the matrix. Microwave conditions are same those shown in Figure 6.

Table S1. List of phosphopeptides ion peaks detected from microwave tryptic digests of α -casein and β -casein using DDTC-Au NPs as affinity probes.

Protein	Peak number	Observed <i>m/z</i>	Phosphopeptide sequences
α -casein	α_1	924.4	DIGpSESTEDQAMEDIK (α -S1/58-73)
	α_2	952.7	EKVNELpSKDIGpSESTEDQAMEDIK (α -S1/52-73)
	α_3	976.2	YKVPQLEIVPNpSAEER (α -S1/119-134)
	α_4	1003.3	NANEEYSIGpSpSpSEEpSAEVATEEVK (α -S2/61-85)
	α_5	1103.7	GNAEGpSpSDEEGKLVIDEPAK (α -S1/180-188)
	α_6	1251.6	TKVIPYVRYL (α -S2-(213-222))
	α_7	1267.1	YLGYLEQLLR (α -S1/106-115)
	α_8	1337.5	VNELpSKDIGpSEpSTEDQAMEDIK (α -S1/52-73)
	α_9	1367.1	QM#EAEPsiPSpSpSEEIVPNpSVEQK (α -S1/74-94)
	α_{10}	1384.5	FFVAPFPEVFGK (α -S1/38-49)
	α_{11}	1410.3	EQLpSTpSEENSK (α -S2/141-151)
	α_{12}	1660.1	VPQLEIVPNpSAEER (α -S1/121-134)
	α_{13}	1759.8	HQGLPQEVLNENLLR (α -S1/23-37)
	α_{14}	1847.4	DIGpSETEDQAMEDIK (α -S1/58-73)
	α_{15}	1951.6	YKVPQLEIVPNpSAEER (α -S1/119-134)
	α_{16}	2080.1	KYKVPQLEIVPNpSAEER (α -S1/118-134)
	α_{17}	2105.0	TDAPSFSIDIPNPIGSENSEK (α -S1/189-208)
	α_{18}	2618.7	NTMEHVpSpSpSEESIIpSQETYK (α -S1/17-36)
	α_{19}	2678.0	VNELpSKDIGpSEpSTEDQAMEDIK (α -S1/52-73)
	α_{20}	3008.1	NANEEYSIGpSpSpSEEpSAEVATEEVK (α -S1/46-70)
β -casein	β_1	2556.9	FQpSEEQQQTEDELQDKIHPF (β /33-52)
	β_2	2965.6	ELEELNVPGEIVEpSLpSpSpSEESITR (β /2-25)
	β_3	3122.5	RELEELNVPGEIVEpSLpSpSpSEESITR (β /1-25)

pS refers to phosphorylated serine unit; M# oxidation on methionine.