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Electronic Supplementary Information for Biosensors and Bioelectronics

A bioinspired peptide matrix for the detection of 2,4,6-trinitrotoluene (TNT)

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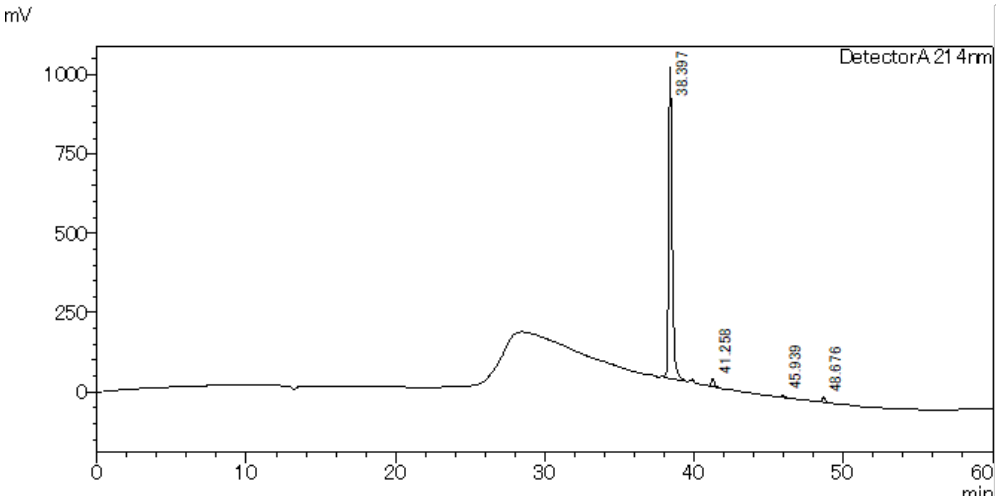
Table S1 The dissociation constants and limit of detection from reported TNT probes and sensing methodologies

Probe	Sensing mechanism	K_D	LOD	LDR	Reference
Peptide					
WHWQRPLMPVS	Isothermal titration	71.4 nM			Jaworski et al., 2008
WHWQRPLMPVS	FET		12.0 ppb		Kuang et al., 2010
WHWQRPLMPVS	Electrochemical impedance spectroscopy (EIS)		227 ppb		Zhang et al., 2015
ARGYSSFIYWFFDF	SPR	1.31 μM			Okochi et al., 2017
ARGYSSFIYWFFDF	SPR		3.4 ppm	4.0-250.8 ppm	Wang et al., 2018
ARGYSSFIYWFFDF	Potentiometric sensing		600 ppb	1.9-62.7 ppm	Wang et al., 2019
Peptide matrix					
ARGYSSFIYWFF	SPR	10.1 nM	0.62 ppb	0.68-18.3 ppb	This work
scFv					
2G5B5 scFv	SPR	0.48 nM			Liu et al., 2013
2G5B5 scFv	Fluorescence (Biosilica)		7.94 ppb		Zhen et al., 2016
2G5B5 scFv	Fluorescence (displacement immunoassay)		1 ppb	10-100 ppb	Charles et al., 2015
Antibody					
2G5B5 Ab	SPR	0.15 pM			Liu et al., 2013
Anti-TNT Ab	SPR		10 ppt	10 ppt-100 ppb	Kawaguchi et al., 2008

K_D: dissociation constant. LOD: limit of detection. LDR: linear dynamic range. ppm: parts-per-million. ppb: parts-per-billion. ppt: parts-per-trillion.

a



b

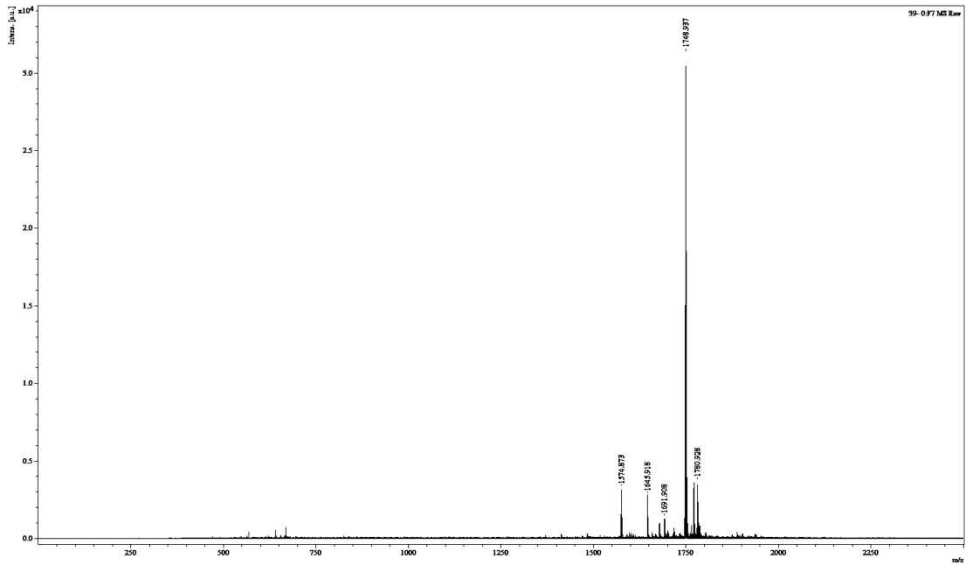


Fig. S1 a Confirmation of purity of Cys-TNT-BP (CARGYSSFIYWFFC) by using analytical HPLC system. The product was eluted at 38.4 min and its purity was calculated to 95.6%. **b** MS spectrum of Cys-TNT-BP. The main peak (1748.937) was correspond with the predicted molecular weight of the peptide (1748.755).

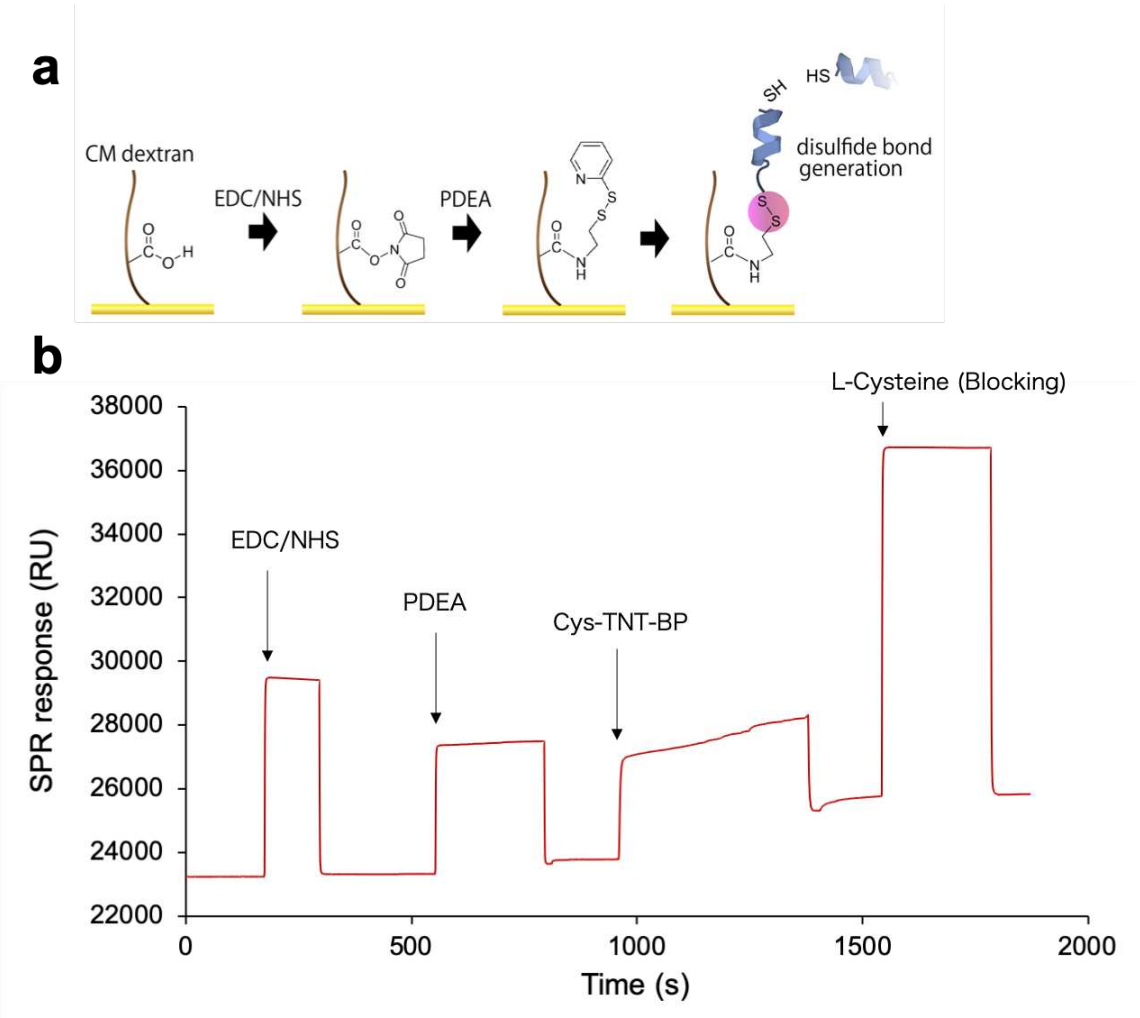


Fig. S2 a Schematic illustration of the activation of sensor chip surface and the immobilization of Cys-TNT-BP fragments. **b** SPR sensorgram during the activation of carboxyl groups of CM-dextran and the fabrication of the matrix. After starting Cys-TNT-BP injection, sensor response gradually and constantly increased, which indicated that the peptide matrix was successfully constructed. L-Cysteine solution is applied after matrix formation for blocking remaining thiol groups at the ends of polypeptide chains.

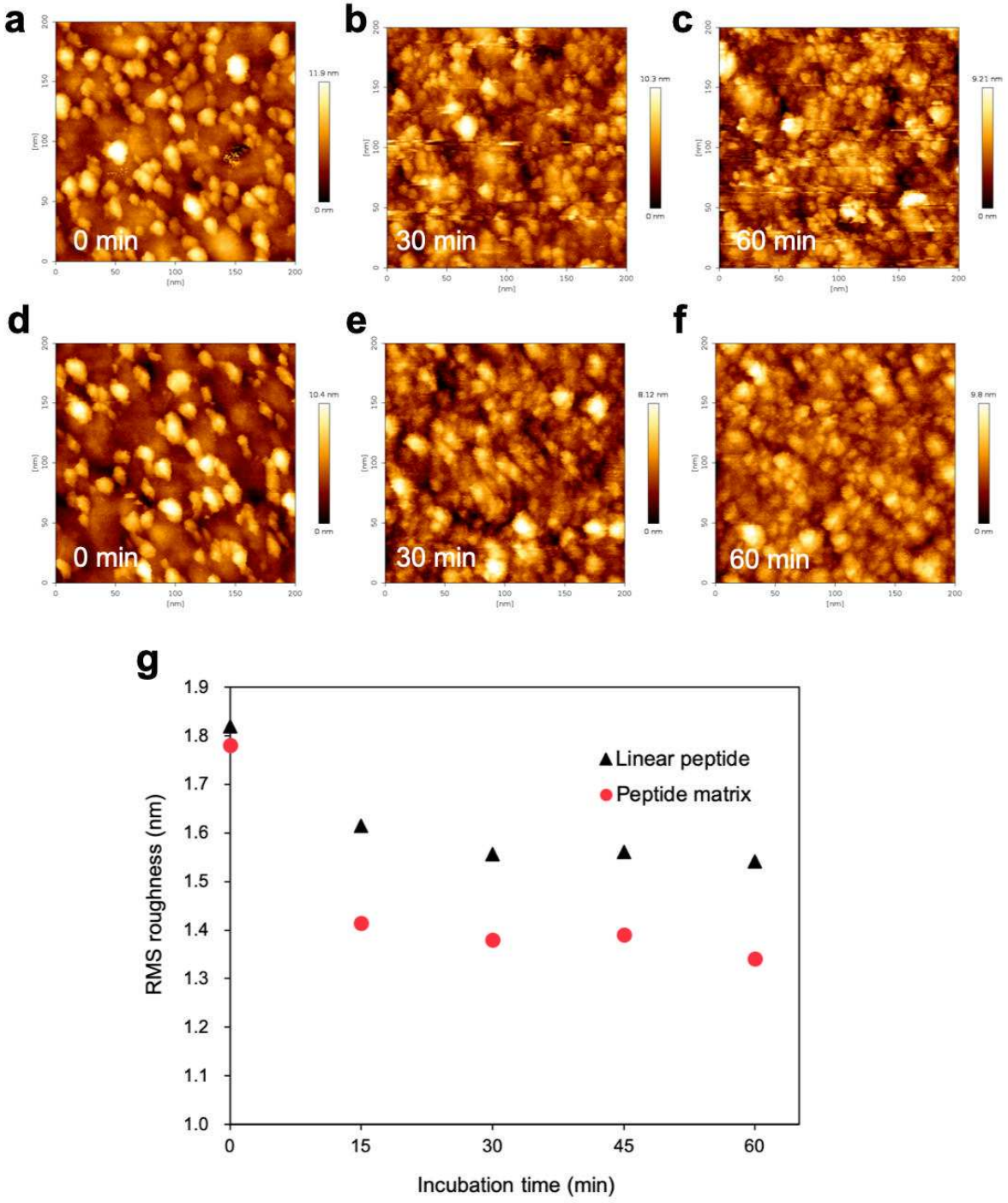


Fig. S3 AFM analysis of linear TNT-BP layer and TNT-BP matrix formation on gold surfaces. **a-f** Representative AFM images of bare gold substrate (a, d), linear TNT-BP peptide layer (b, c) and TNT-BP matrix (e, f) in 5 μM of peptide solution. Incubation times are indicated on the lower position of each images. For each experiment (a-c and d-f), same position of substrate was observed. **g** Relationship between the root-mean-square (RMS) roughness and incubation time evaluated from AFM images.

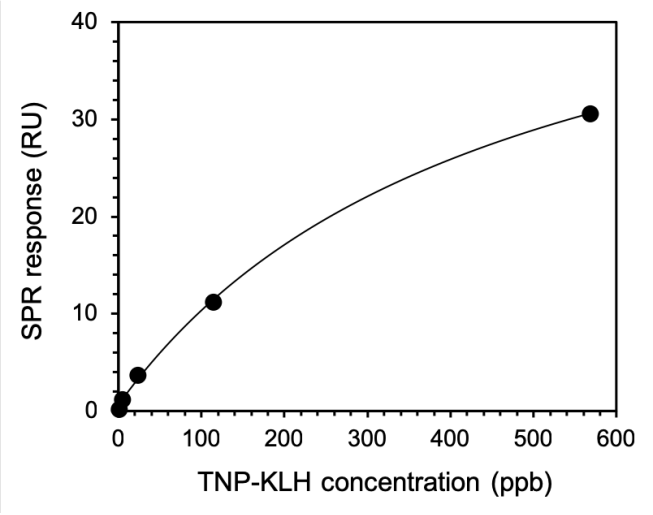


Fig. S4 SPR sensorgram of the affinity measurement of TNT-BP linear peptide layer to TNP-KLH as a control measurement. SPR response as a function of equivalent concentration to TNP.

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