Plant biomarker recognition by molecular imprinting based LSPR sensor array: Performance improvement by enhanced hotspot of Au nanostructure

Supplementary Information

Liang Shang,[†] Chuanjun Liu,[†,§] Bin Chen,[‡] Kenshi Hayashi[*,†]

[†]Department of Electronics, Graduate School of Information Science and Electrical Engineering, Kyushu University, Fukuoka 819-0395, Japan

[§]Research Laboratory, U.S.E. Co., Ltd., Tokyo 150-0013, Japan

[‡]College of Electronic and Information Engineering, Southwest University, Chongqing 400715, China

E-mail addresses:

shang.liang.100@s.kyushu-u.ac.jp (L. Shang); liu@o.ed.kyushu-u.ac.jp (C. Liu)

chenbin121@swu.edu.cn (B. Chen); hayashi@ed.kyushu-u.ac.jp (K. Hayashi)

* Corresponding author: Kenshi Hayashi, Ph.D., Professor, Tel.: +81-092-802-3629, Fax: +81-092-802-3629. E-mail: hayashi@ed.kyushu-u.ac.jp.

Supporting Figures and Tables.

Figures

Figure S1. Absorption spectra of MISG-coated samples with different size of Au nanoparticles.

Figure S2. SEM images of control (a) and MISGs with 10-nm (b), 20-nm (c), 30-nm (d), and 40-nm (e) AuNPs.

Figure S3. SEM images of bare (a), MISG$_{cis-jasmone}$- (b), MISG$_{\alpha-pinene}$- (c), MISG$_{limonene}$- (d), and MISG$_{\gamma-terpinene}$(e), NISG- (f), and AuNPs doped NISG-coated (g) sample.

Figure S4. Particle size distribution histogram of spherical gold nanoparticles determined from bare sample (Figure S3 a). SEM image was analyzed by ImageJ. The diameter of AuNPs was 34.13±9.41 nm.

Figure S5. Absorption spectra of MISG-coated samples different amount of 30-nm Au nanoparticles.

Figure S6. SEM images of control (a), and MISGs with 30 nm AuNPs 5-uL (b), 10-uL (c), 20-uL (d), 30-uL (e), 50-uL (f), 70-uL (g), and 90-uL (h).

Tables

Table S1. Standard performance measures of LDA, KNN, and NBC models for calibration set (%).

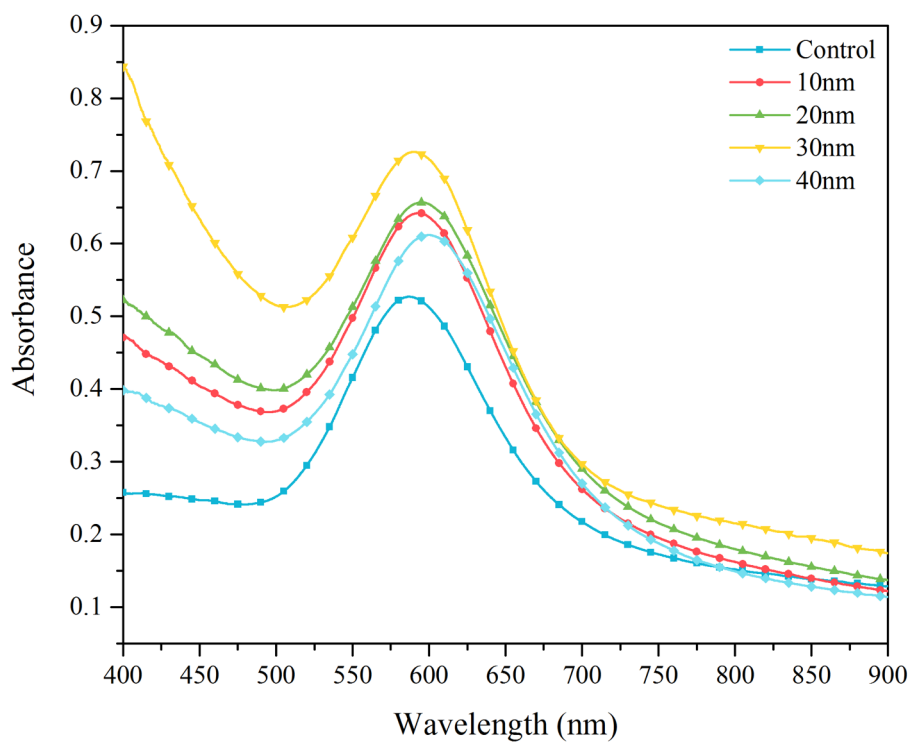Table S2. Standard performance measures of LDA, KNN, and NBC models for validation set (%).

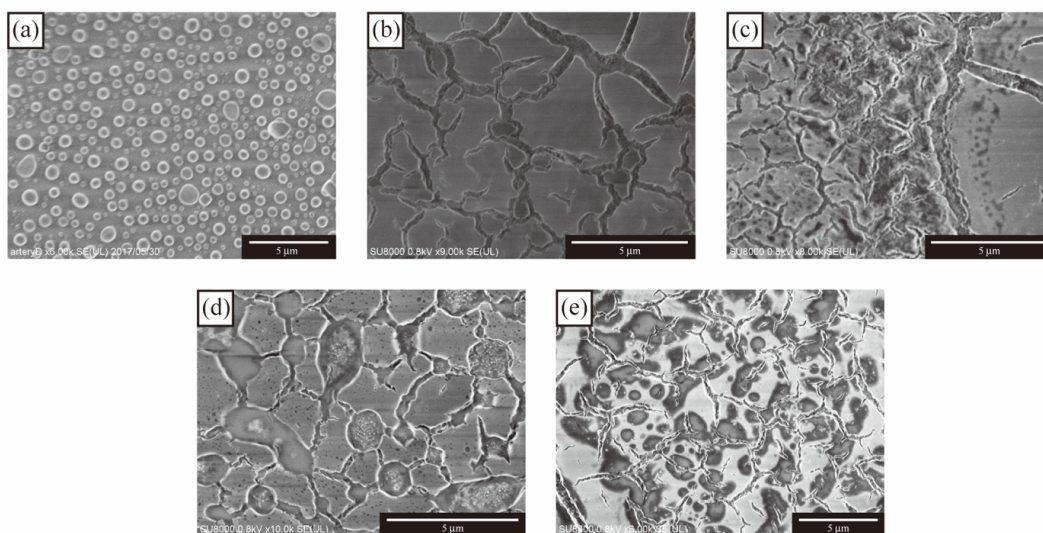Figure S1. Absorption spectra of MISG-coated samples with different size of Au nanoparticles.

Figure S2. SEM images of control (a) and MISGs with 10-nm (b), 20-nm (c), 30-nm (d) and 40-nm (e) AuNPs.
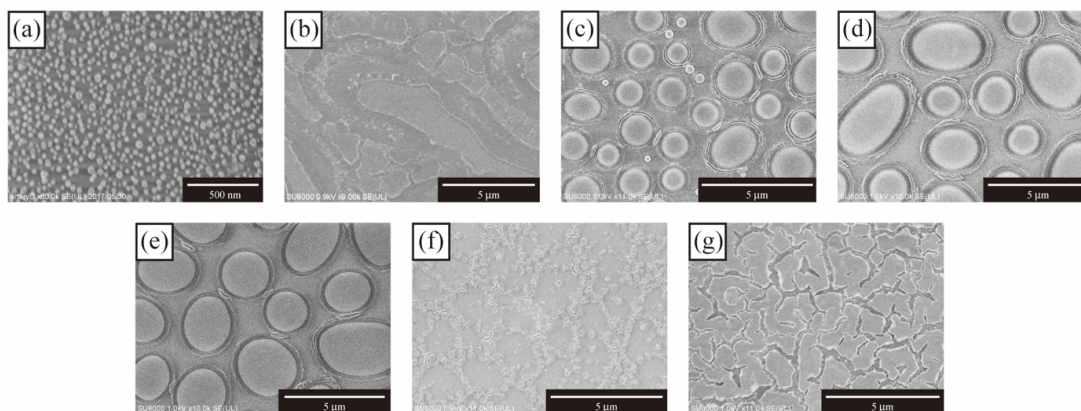
Figure S3. SEM images of bare (a), MISG$_{\text{cis-jasmone}}$- (b), MISG$_{\alpha\text{-pinene}}$- (c), MISG$_{\text{limonene}}$- (d), and MISG$_{\gamma\text{-terpiene}}$(e), NISG- (f), and AuNPs doped NISG-coated (g) sample.
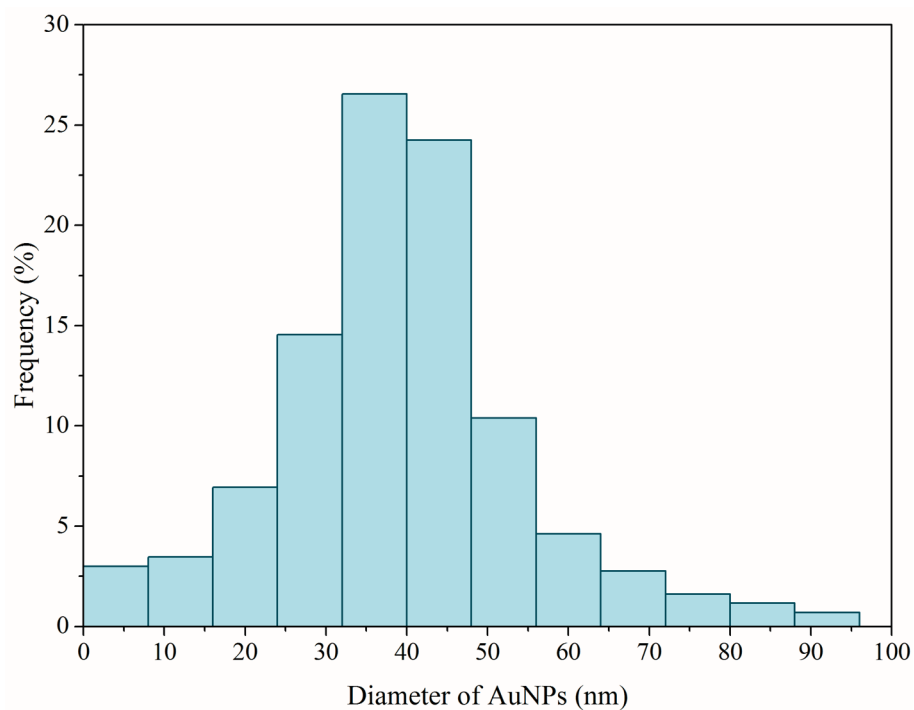

Figure S4. Particle size distribution histogram of spherical gold nanoparticles determined from bare sample (Figure S3 a). SEM image was analyzed by ImageJ. The diameter of AuNPs was 34.13±9.41 nm.
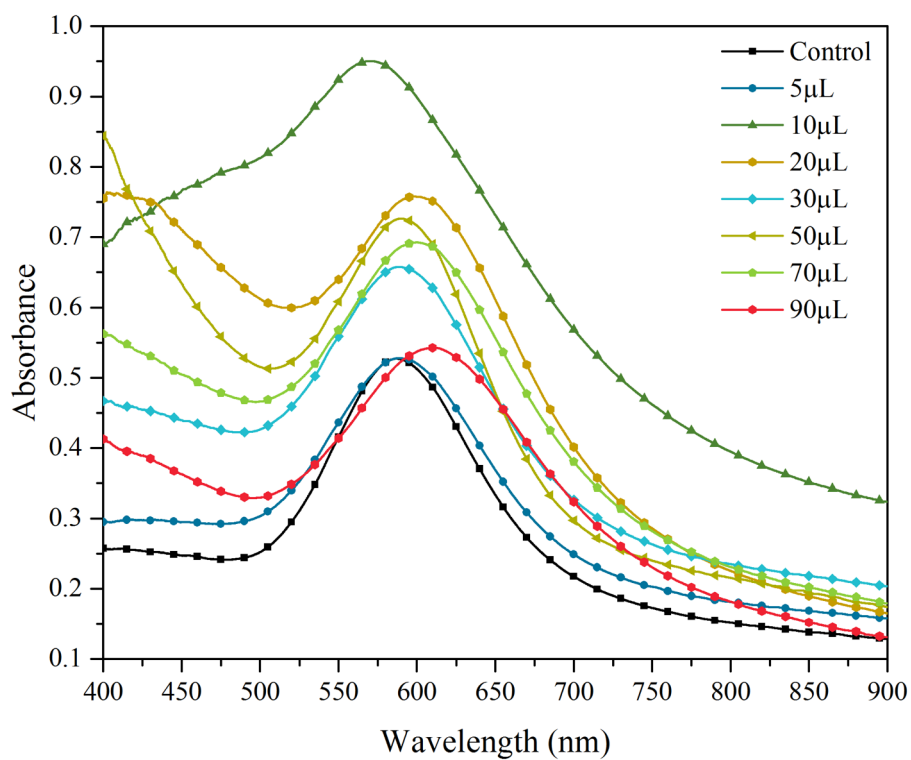
Figure S5. Absorption spectra of MISG-coated samples different amount of 30-nm Au nanoparticles.
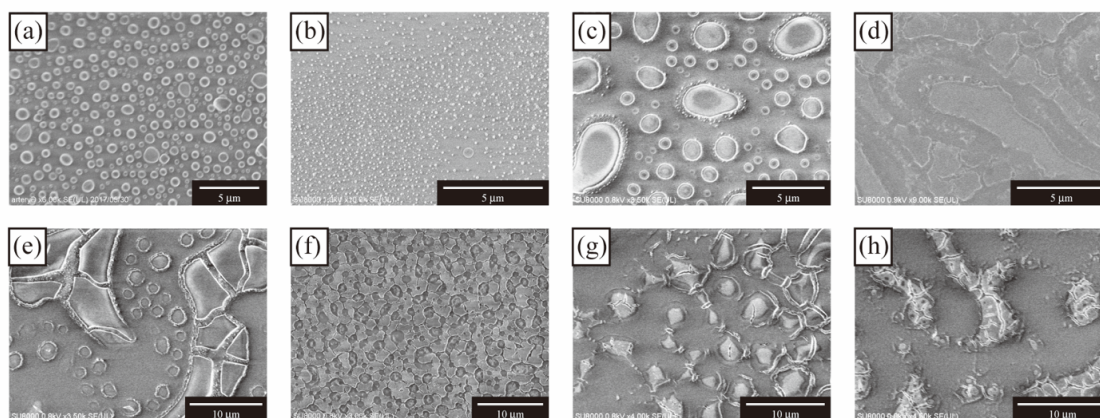

Figure S6. SEM images of control (a), and MISGs with 30 nm AuNPs 5-uL (b), 10-uL (c), 20-uL (d), 30-uL (e), 50-uL (f), 70-uL (g) and 90-uL (h).

Table S1. Standard performance measures of LDA, KNN, and NBC models for calibration set (%).

Models	PVOCs	Sensitivity	Specificity	Precision	Recall	F1 score	Accuracy
KNN	*cis*-Jasmone	96.55±12.23	97.09±4.56	77.5±35.8	96.55±12.23	91.11±15.66	97.54±6.63
	α-Pinene	82.89±22.24	99.07±2.95	93±22.5	82.89±22.24	88.72±13.54	91.1±11.69
	Limonene	95.58±12.1	98.81±2.85	91±21.77	95.58±12.1	92.86±13.37	97.31±6.29
	γ-Terpinene	96±12.34	99.2±2.18	94±16.33	96±12.34	93.47±12.68	97.6±6.13
	cis-Jasmone+ α-Pinene	89.61±21.69	95.74±4.12	68±31.4	89.61±21.69	77.72±17.84	92.98±11.17
	cis-Jasmone+Limonene	98.23±7.52	98.92±3.24	91.5±25.68	98.23±7.52	97.16±8.55	98.94±3.79
	α-Pinene+Limonene	80.17±21.15	99.65±1.52	97.5±10.95	80.17±21.15	86.2±15.21	89.91±10.69
	Limonene+ γ-Terpniene	98.96±5.83	99.1±2.86	93±22.5	98.96±5.83	97.29±8.68	99.27±2.99
LDA	*cis*-Jasmone	99.88±1.25	99.98±0.2	99.86±1.43	99.88±1.25	99.86±1.01	99.93±0.63
	α-Pinene	80.19±8.24	99.77±0.66	98.43±4.49	80.19±8.24	88.15±5.54	89.98±4.2
	Limonene	99.57±2.45	98±1.35	85.57±9.84	99.57±2.45	91.73±5.85	98.78±1.4
	γ-Terpinene	100±0	99.74±0.68	98.14±4.83	100±0	99±2.6	99.87±0.34
	cis-Jasmone+ α-Pinene	78.01±8.15	98.25±0.77	88±5.26	78.01±8.15	82.56±6.15	88.13±4.32
	cis-Jasmone+Limonene	99.13±3.21	99.98±0.2	99.86±1.43	99.13±3.21	99.46±1.86	99.55±1.6
	α-Pinene+Limonene	98.7±4.5	96.55±1.31	74.86±9.76	98.7±4.5	84.7±6.07	97.62±2.2
	Limonene+ γ-Terpinene	98.75±3.77	100±0	100±0	98.75±3.77	99.33±2.01	99.38±1.88
NBC	*cis*-Jasmone	95.55±6.86	98.4±1.17	88.57±8.37	95.55±6.86	91.63±5.75	96.98±3.53
	α-Pinene	79.36±8.74	97.73±1.34	84.14±9.5	79.36±8.74	81.28±6.89	88.55±4.55
	Limonene	99.75±1.76	99.9±0.44	99.29±3.13	99.75±1.76	99.48±1.9	99.83±0.9
	γ-Terpinene	99.88±1.25	100±0	100±0	99.88±1.25	99.93±0.67	99.94±0.63
	cis-Jasmone+ α-Pinene	94.54±8.22	98.42±0.84	88.86±5.95	94.54±8.22	91.42±5.87	96.48±4.29
	cis-Jasmone+Limonene	100±0	100±0	100±0	100±0	100±0	100±0
	α-Pinene+Limonene	89.61±5.95	99.19±1.24	94.29±8.85	89.61±5.95	91.61±5.65	94.4±3.11
	Limonene+ γ-Terpinene	100±0	100±0	100±0	100±0	100±0	100±0

Table S2. Standard performance measures of LDA, KNN, and NBC models for validation set (%).

Models	PVOCs	Sensitivity	Specificity	Precision	Recall	F1 score	Accuracy
KNN	*cis*-Jasmone	95.55±6.86	98.4±1.17	88.57±8.37	95.55±6.86	91.63±5.75	96.98±3.53
	α-Pinene	79.36±8.74	97.73±1.34	84.14±9.5	79.36±8.74	81.28±6.89	88.55±4.55
	Limonene	99.75±1.76	99.9±0.44	99.29±3.13	99.75±1.76	99.48±1.9	99.83±0.9
	γ-Terpinene	99.88±1.25	100±0	100±0	99.88±1.25	99.93±0.67	99.94±0.63
	cis-Jasmone+ α-Pinene	94.54±8.22	98.42±0.84	88.86±5.95	94.54±8.22	91.42±5.87	96.48±4.29
	cis-Jasmone+Limonene	100±0	100±0	100±0	100±0	100±0	100±0
	α-Pinene+Limonene	89.61±5.95	99.19±1.24	94.29±8.85	89.61±5.95	91.61±5.65	94.4±3.11
	Limonene+ γ-Terpinene	100±0	100±0	100±0	100±0	100±0	100±0
LDA	*cis*-Jasmone	98.64±8.18	98.87±2.8	91.5±21.39	98.64±8.18	94.9±12.51	98.87±4.48
	α-Pinene	74.74±24.83	98.72±3.37	90.5±25.32	74.74±24.83	83.05±15.4	86.85±13.13
	Limonene	89.82±23.48	96.79±4.26	76±32.16	89.82±23.48	85.04±18.39	93.55±12.81
	γ-Terpinene	100±0	98.16±3.34	86±25.7	100±0	92.44±14.03	99.24±1.4
	cis-Jasmone+ α-Pinene	75.29±22.66	98.33±3.12	88±22.61	75.29±22.66	78.63±17.65	86.86±11.59
	cis-Jasmone+Limonene	95.62±11.32	99.74±1.55	98±12.14	95.62±11.32	96.7±8.05	97.74±5.65
	α-Pinene+Limonene	98.24±8.14	95.12±4.46	62.5±35.09	98.24±8.14	81.45±16.67	97.35±4.28
	Limonene+ γ-Terpinene	94.67±12.28	100±0	100±0	94.67±12.28	96.8±7.37	97.33±6.14
NBC	*cis*-Jasmone	86.29±21.78	97.09±3.74	78.5±27.76	86.29±21.78	80.66±17.79	91.79±11.3
	α-Pinene	69.39±29.74	95.74±4.48	69±33.17	69.39±29.74	71.32±18.07	82.74±15.86
	Limonene	89.65±18.38	98.83±3.37	91±26	89.65±18.38	92.3±12.05	94.54±9.6
	γ-Terpinene	97.94±9.08	98.16±3.34	86±25.7	97.94±9.08	91.13±14.52	98.21±4.58
	cis-Jasmone+ α-Pinene	89.52±16.37	98.36±3.25	87.5±25	89.52±16.37	87.08±13.94	94.11±7.87
	cis-Jasmone+Limonene	100±0	100±0	100±0	100±0	100±0	100±0
	α-Pinene+Limonene	89.29±20.2	97.91±3.51	84.5±26.3	89.29±20.2	86.53±17.51	93.71±10.77
	Limonene+ γ-Terpinene	99.75±1.76	98±14.07	100±0	100±0	100±0	100±0