

FIG. 1

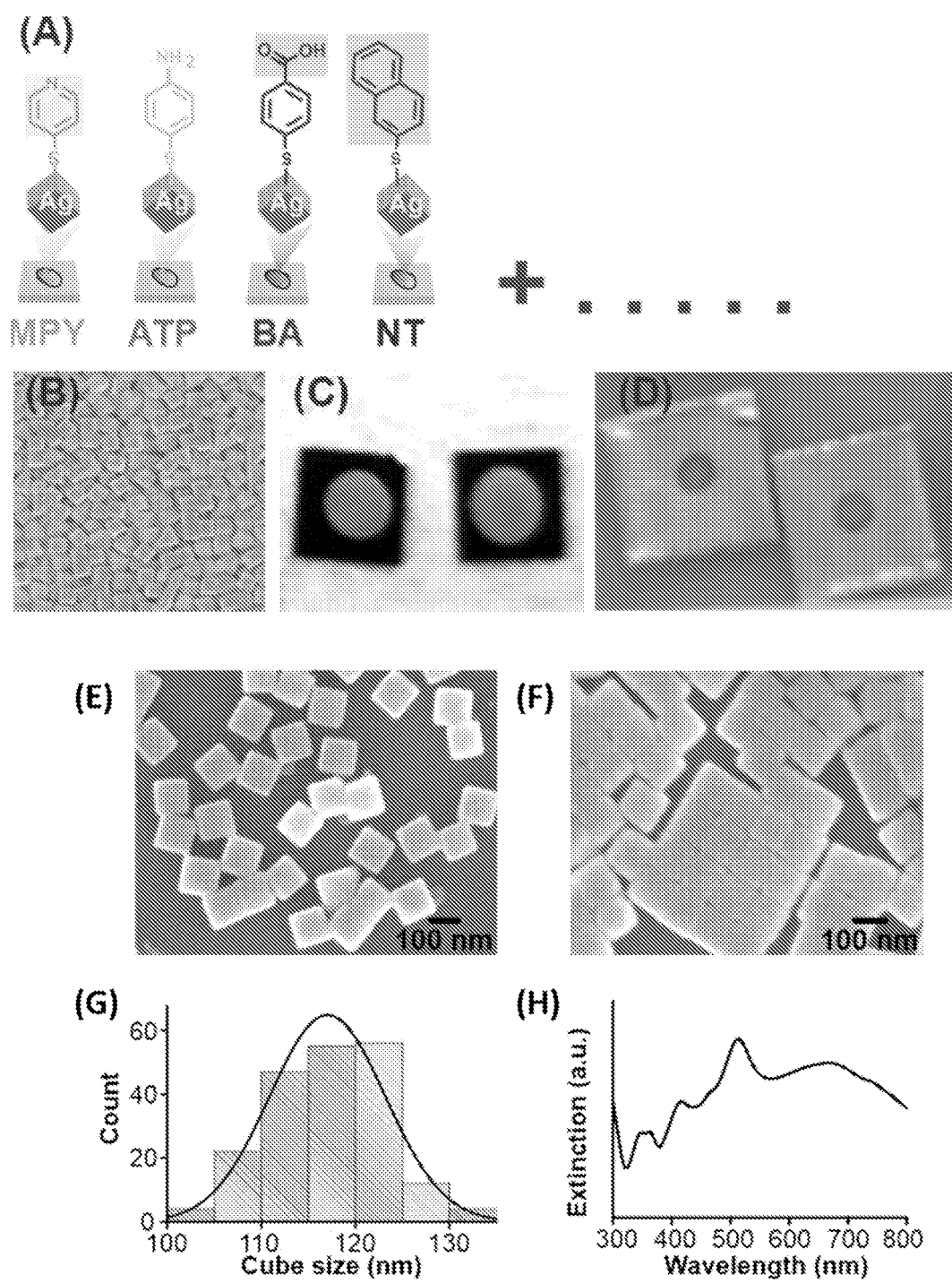


FIG. 2

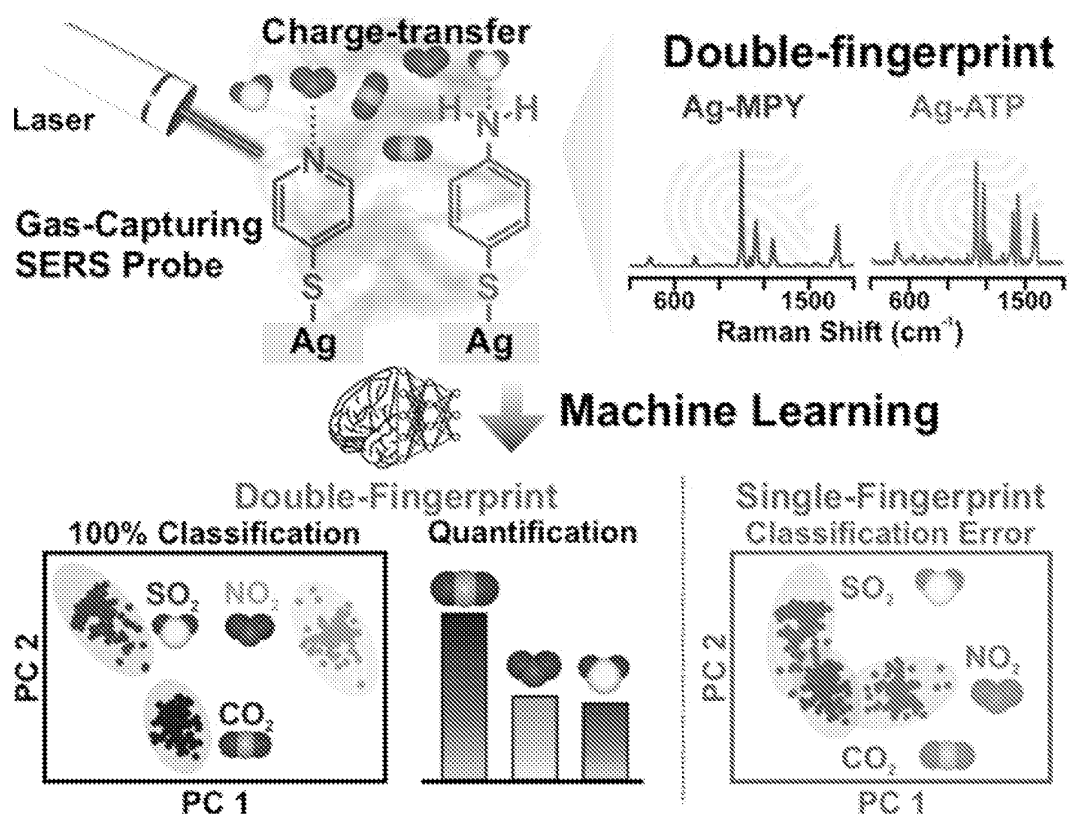


FIG. 3

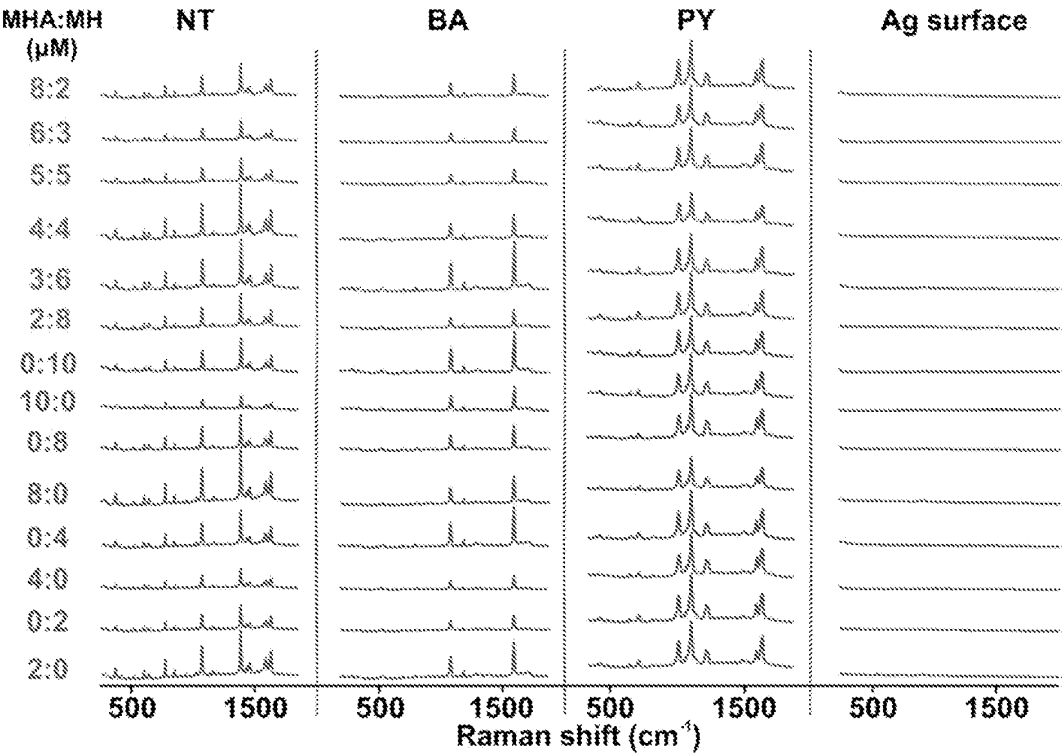


FIG. 4

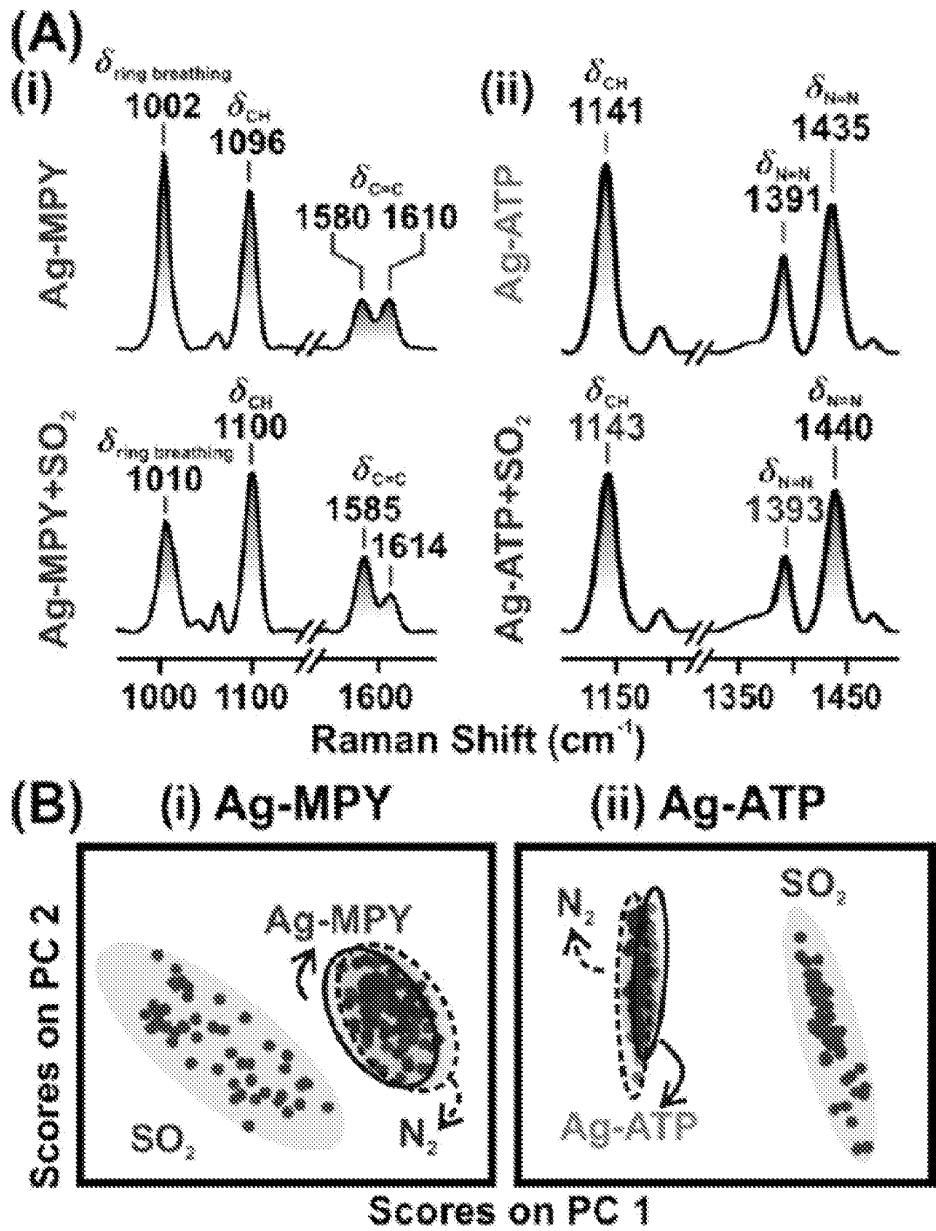


FIG. 5

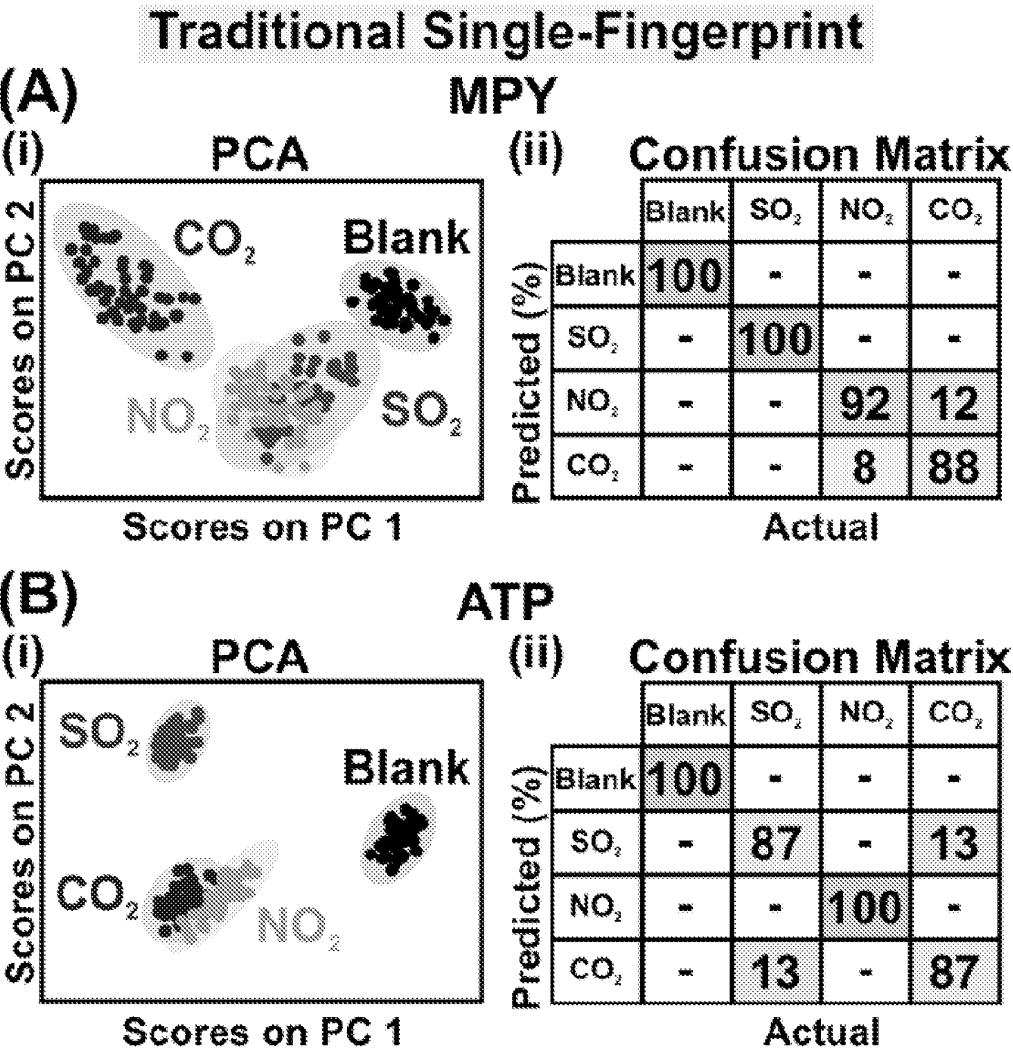


FIG. 5 (Continued)

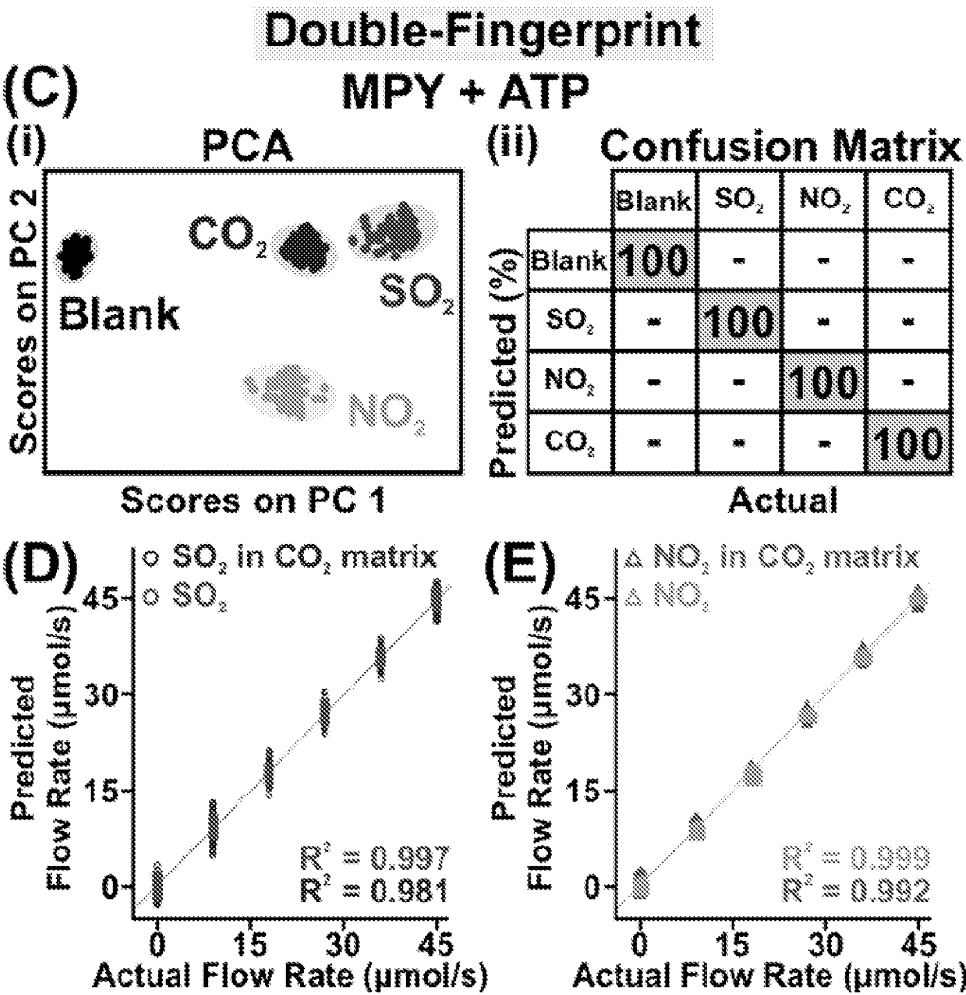


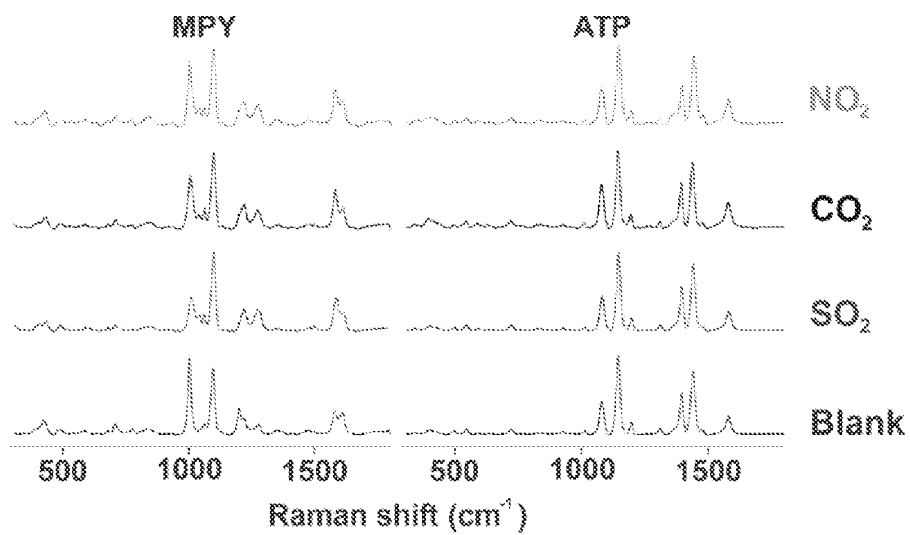
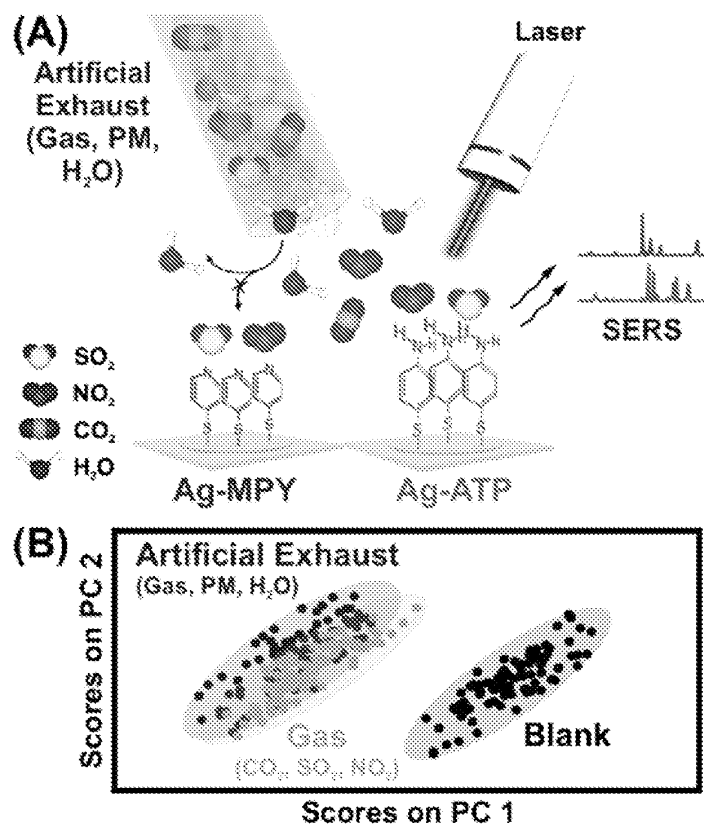
FIG. 6**FIG. 7**

FIG. 7 (Continued)

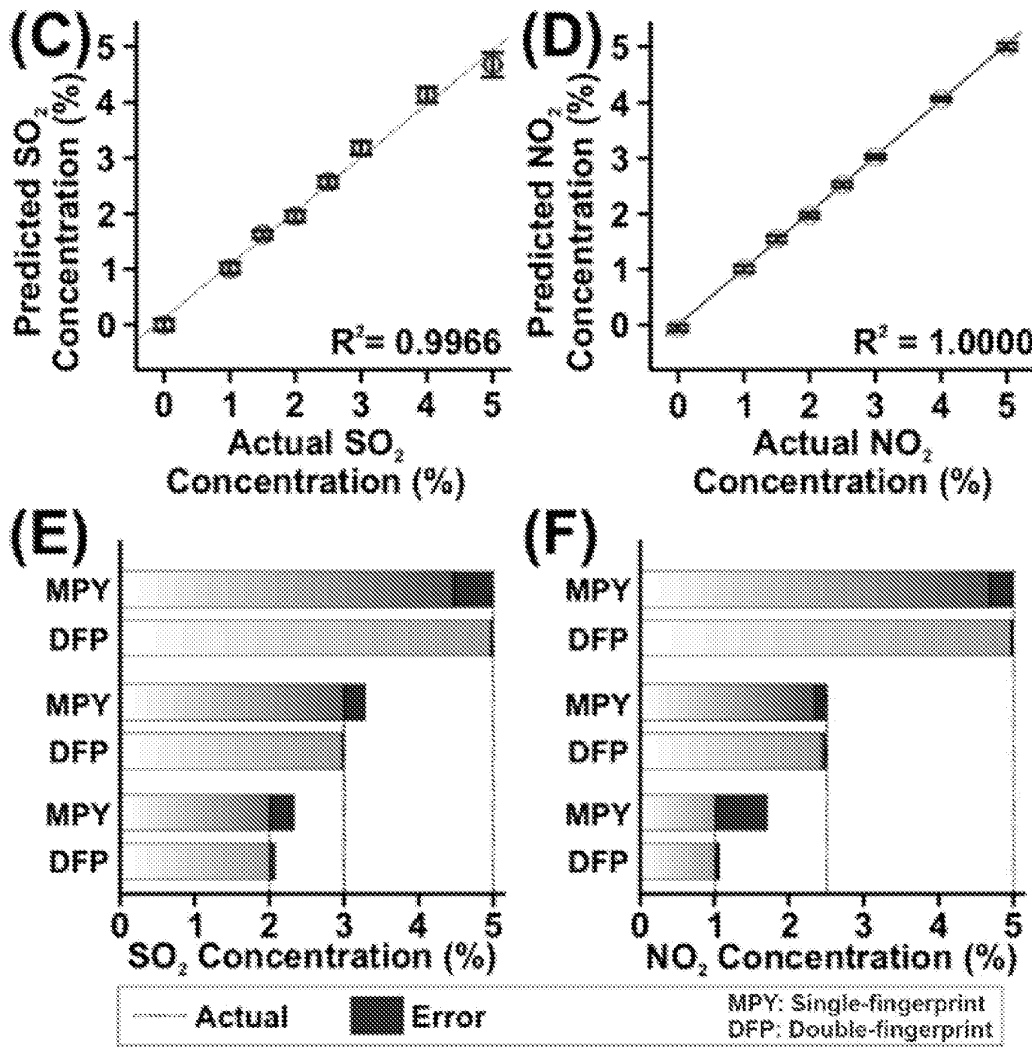


FIG. 8

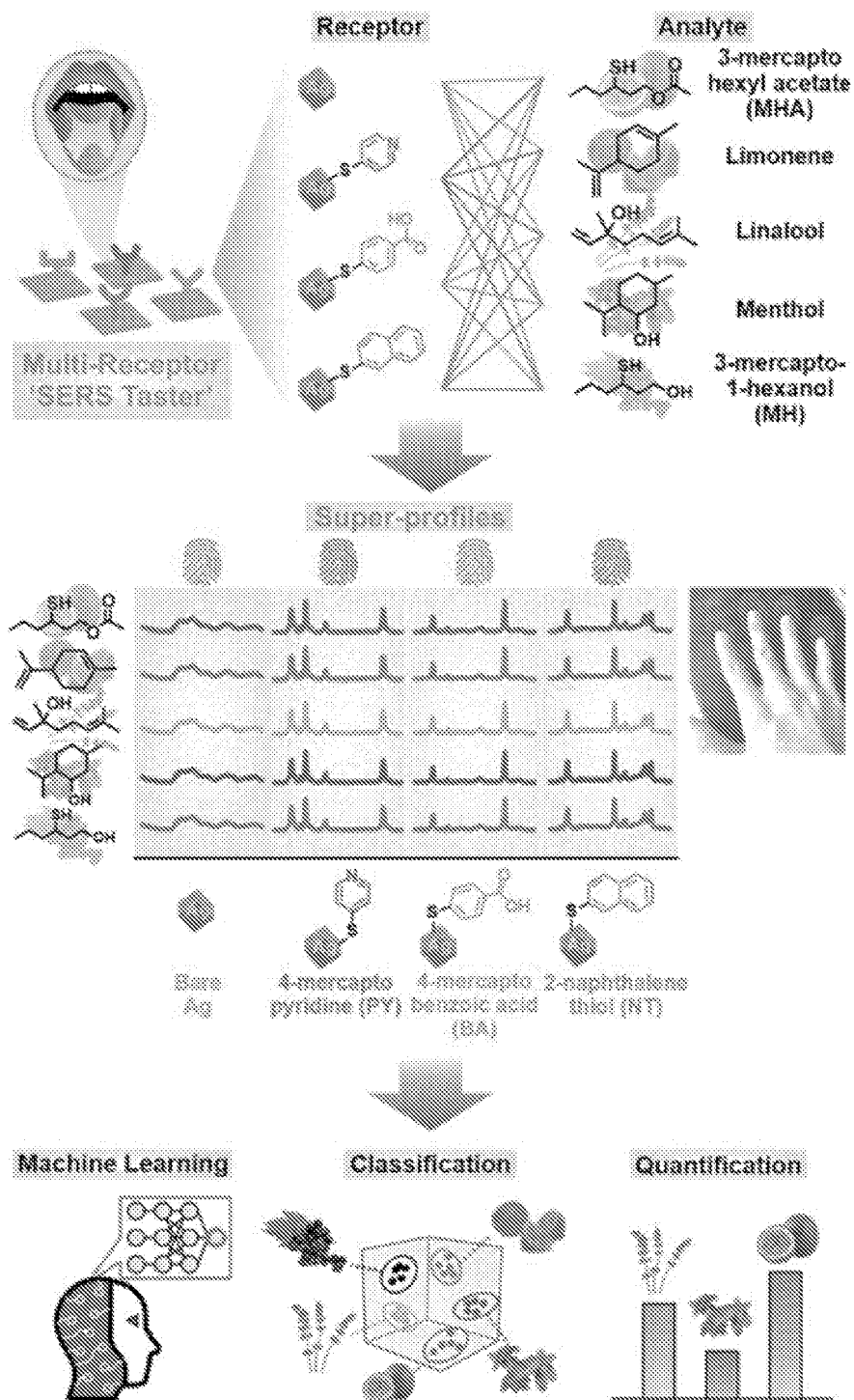


FIG. 9

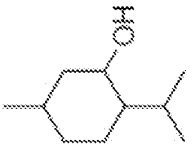
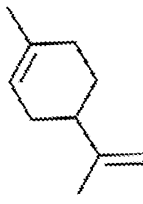
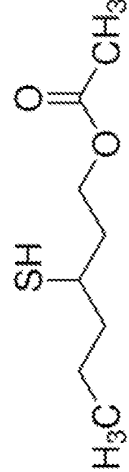
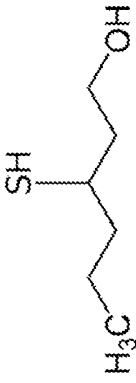
Wine flavor	Molecular structure	Types of wines present in	Possible intermolecular interactions
Menthol		Many red wine types such as Bordeaux, Cabernet Sauvignon, Shiraz	Hydrogen bonding; van der Waals' forces
Linalool		White wine types such as Muscat, Galicia	Hydrogen bonding; π - π interactions; van der Waals' forces
Limonene		White wine types such as Chardonnay, Viognier	π - π interactions; van der Waals' forces
3-mercaptohexyl acetate (MHA)		Red wine types, such as Cabernet Sauvignon, Merlot and white wine types such as Sauvignon Blanc and Semillon	Electrostatic interactions; van der Waals' forces; Ag-S bonding
3-mercapto-1-hexanol (MH)		Red wine types, such as Cabernet Sauvignon, white wine types such as Sauvignon Blanc and rosé wines	Hydrogen bonding; van der Waals' forces; Ag-S bonding

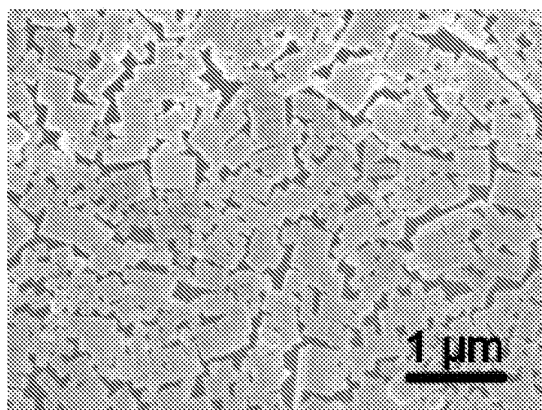
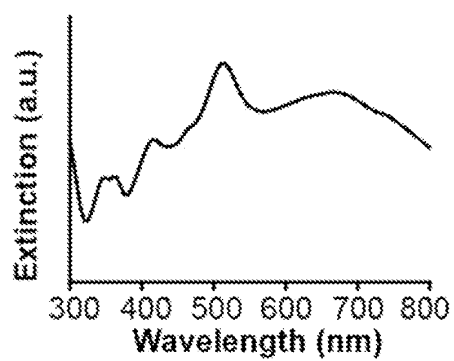
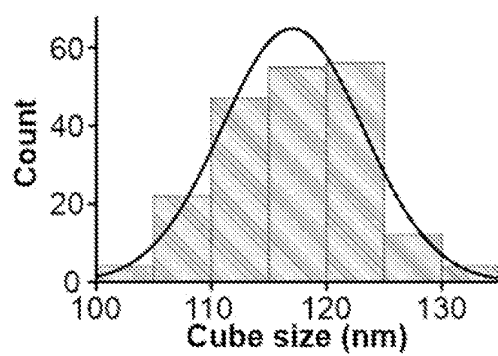
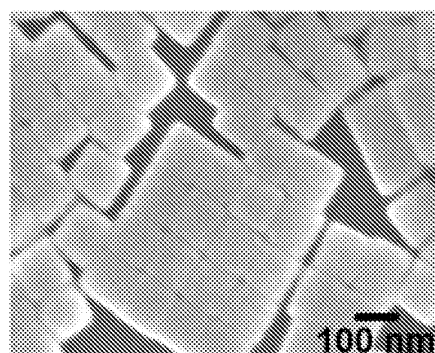
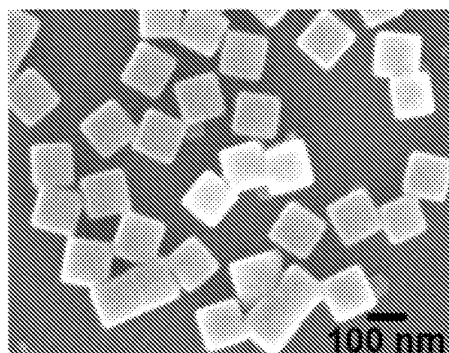
FIG. 10A**FIG. 10B**

FIG. 11A

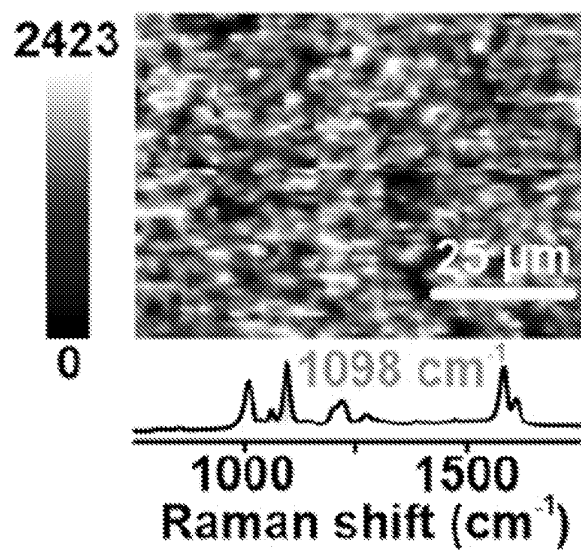


FIG. 11B

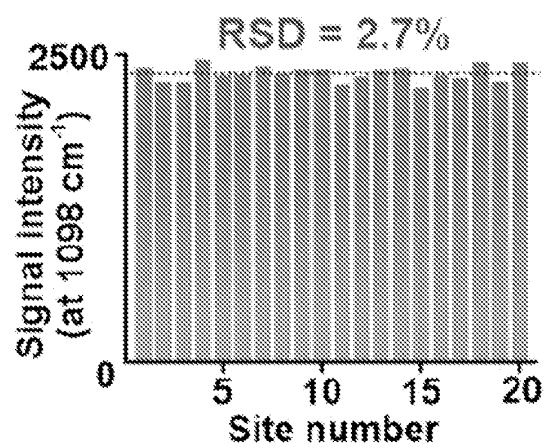


FIG. 11C

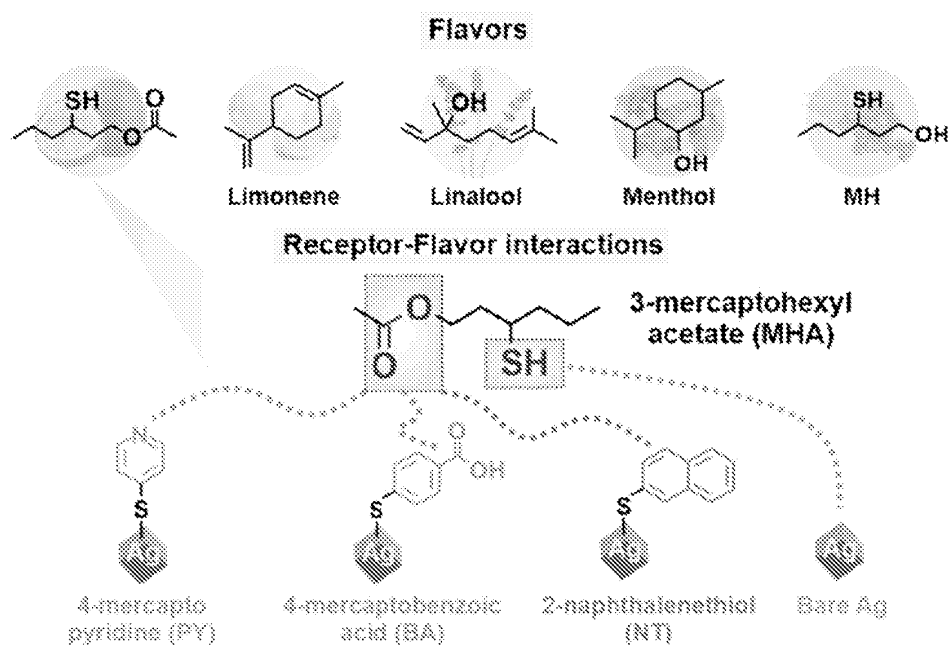


FIG. 11D

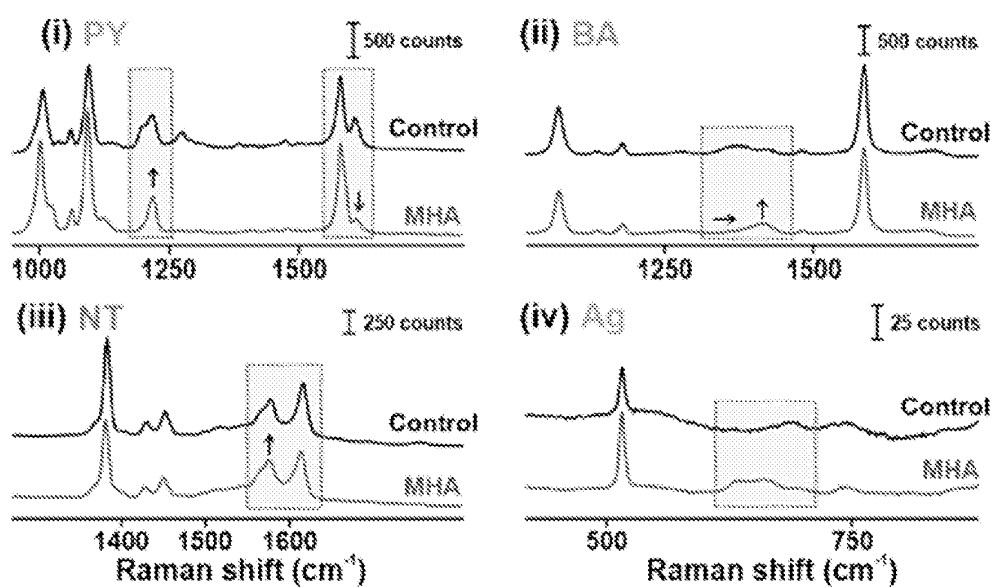


FIG. 11E

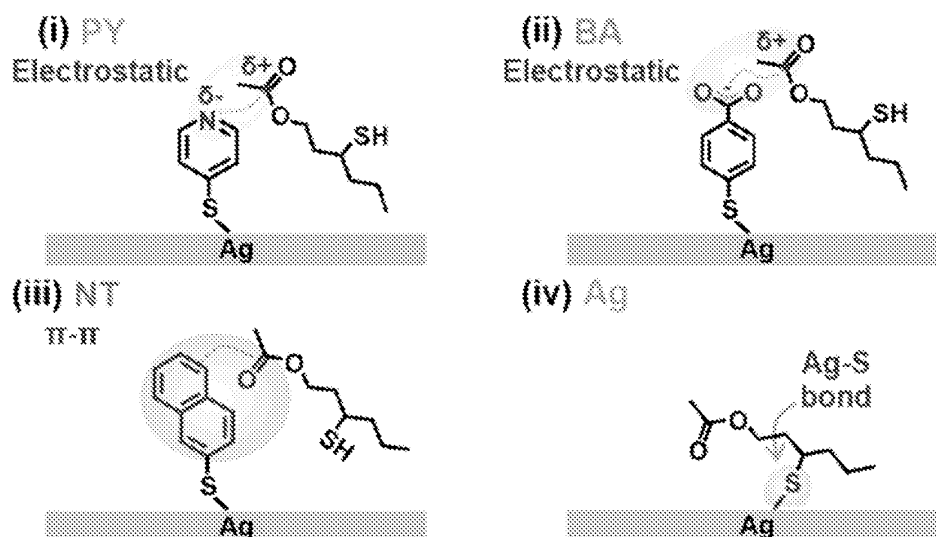


FIG. 12

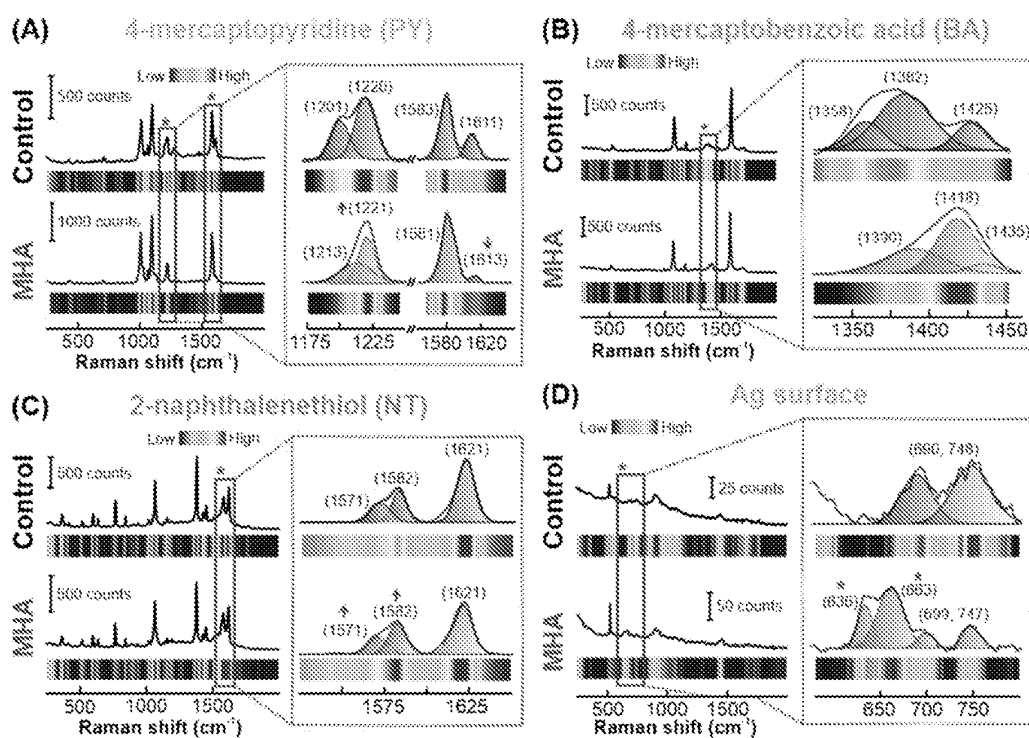


FIG. 13**Experimental spectrum**

	Peak 1: 1571 cm ⁻¹	Peak 2: 1582 cm ⁻¹	Peak 3: 1621 cm ⁻¹
MHA	142.35 ± 18.39	252.04 ± 20.73	403.04 ± 7.61
Control	153.54 ± 12.67	254.98 ± 24.35	494.03 ± 7.96
	Peak 1 : Peak 2	Peak 1 : Peak 3	Peak 2 : Peak 3
MHA	0.56	<u>0.35</u>	<u>0.63</u>
Control	0.60	0.31	0.52
Percentage change	6.7%	<u>12.9%</u>	<u>21.2%</u>

DFT simulated spectrum

	Peak 1: 1598 cm ⁻¹	Peak 2: 1632 cm ⁻¹	Peak 3: 1665 cm ⁻¹
MHA	684.21	197.25	618.82
Control	754.35	218.07	768.71
	Peak 1 : Peak 2	Peak 1 : Peak 3	Peak 2 : Peak 3
MHA	3.47	<u>1.11</u>	<u>0.32</u>
Control	3.46	0.98	0.28
Percentage change	0.3%	<u>13.3%</u>	<u>14.3%</u>

FIG. 14

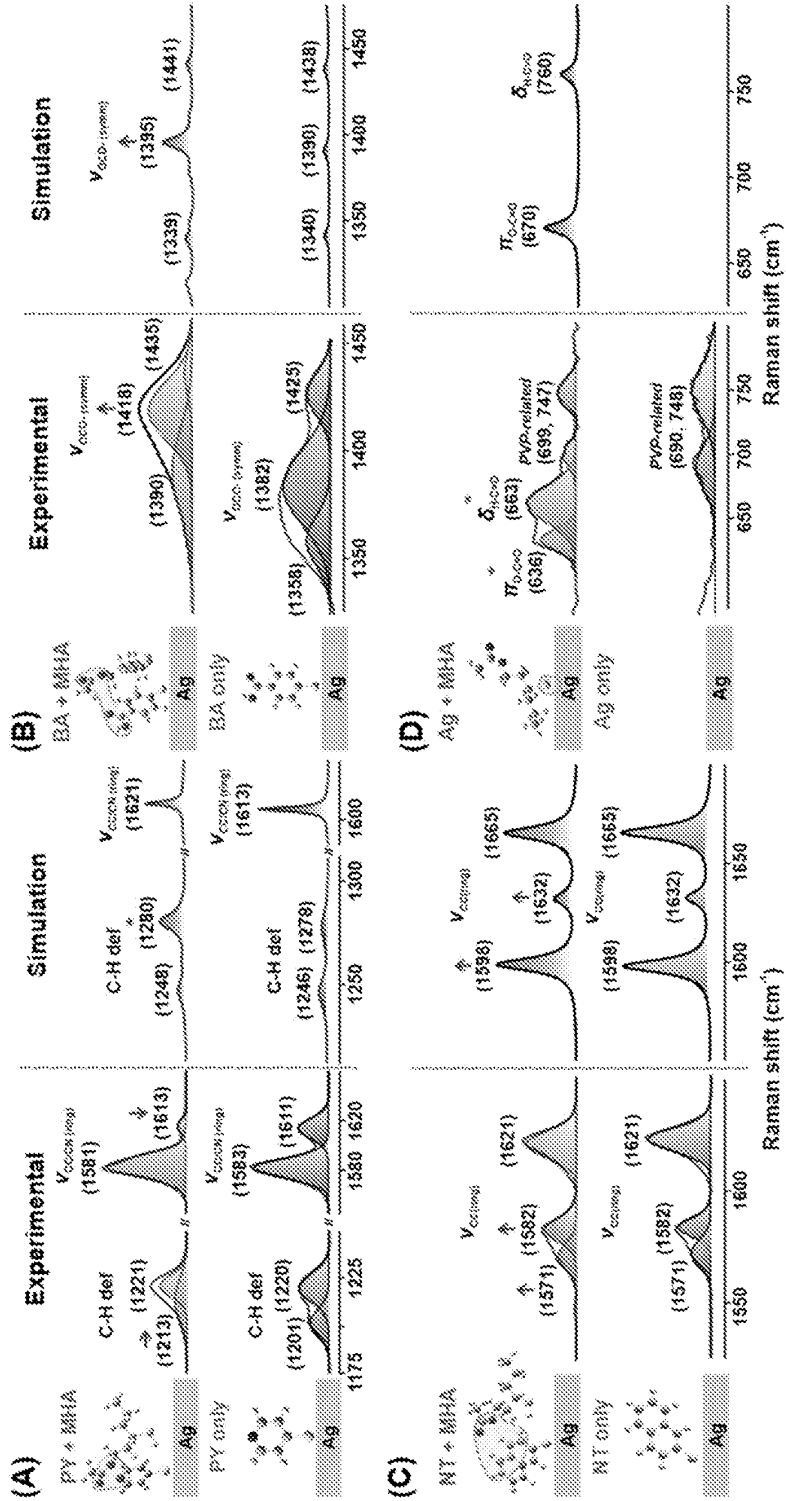


FIG. 15A

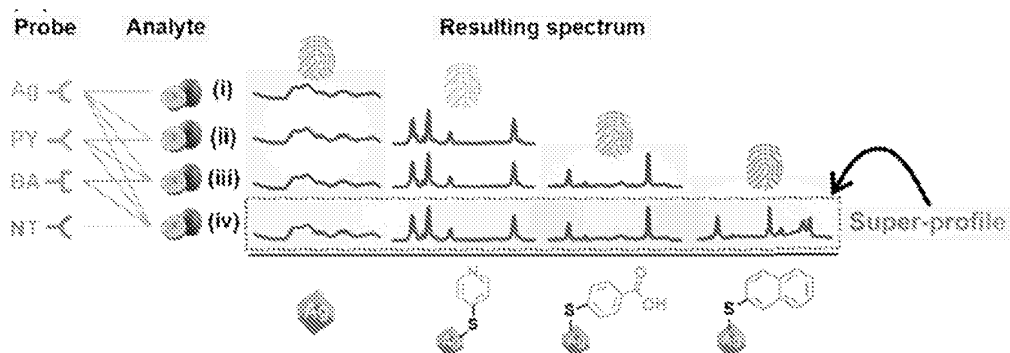


FIG. 15B

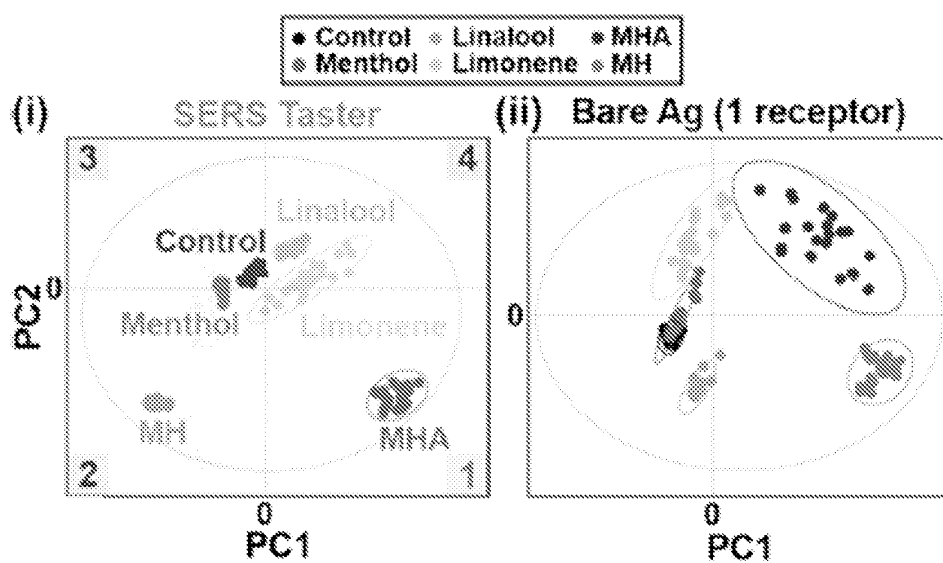


FIG. 15C

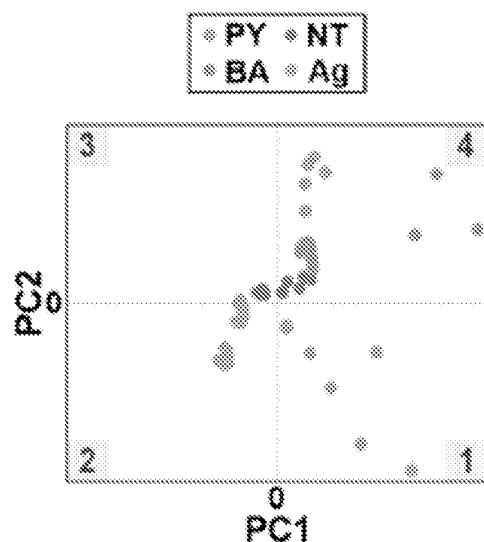


FIG. 15D

Quadrant	Flavor	Receptor-Flavor interactions		Receptor wavenumber	Assignment
(i)					
1	 MHA	 PY-MHA	 Ag-MHA	Electrostatic Ag-S bond	PY 1000-1008 Ag 630-670 (broad) $\pi_{\text{OCO}}, \delta_{\text{HCO}}$ (MHA)
(ii)					
2	 MH	 PY-MH	 Ag-MH	H-bond Ag-S bond	PY 416-424 Ag 630-670 (broad) Ring stretch + ν_{CS} ν_{CS} (MH)
(iii)					
3	 Menthol	 PY-Menthol	 NT-Menthol	H-bond van der Waals	PY 702-710 NT 630-638 out-of-plane C-H def δ_{CH}
(iv)					
4	 Linalool	 PY-Linalool	 BA-Linalool	H-bond H-bond	PY 1008-1016 BA 1350-1400 (broad) In-plane C-H def ν_{OCO}
	 Limonene	 BA-Limonene	 NT-Limonene	π - π π - π	BA 1584-1592 NT 764-770 ν_{CC} (ring) Ring breathing

FIG. 15E

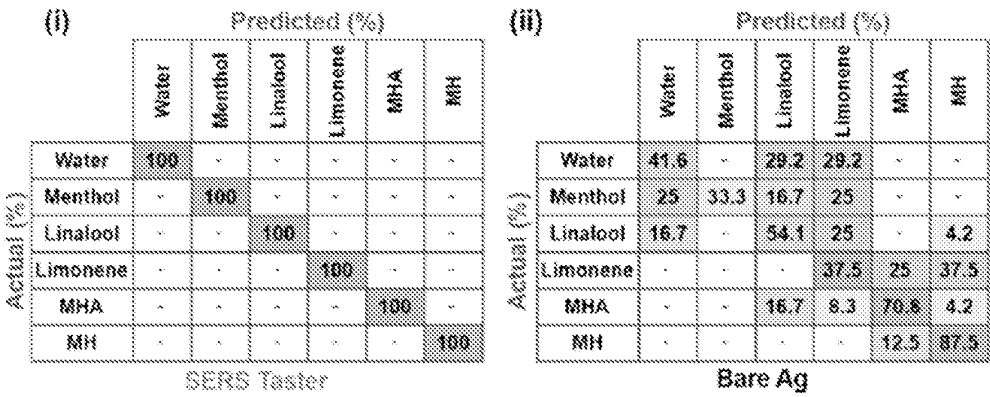


FIG. 16

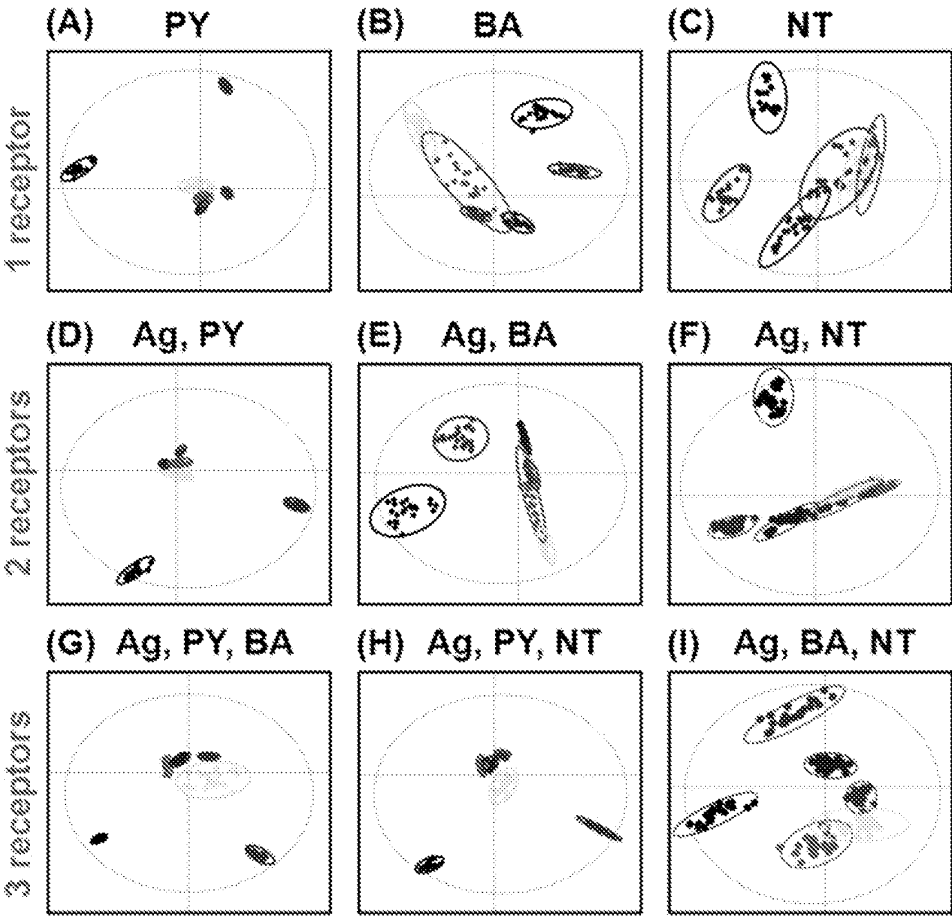


FIG. 17

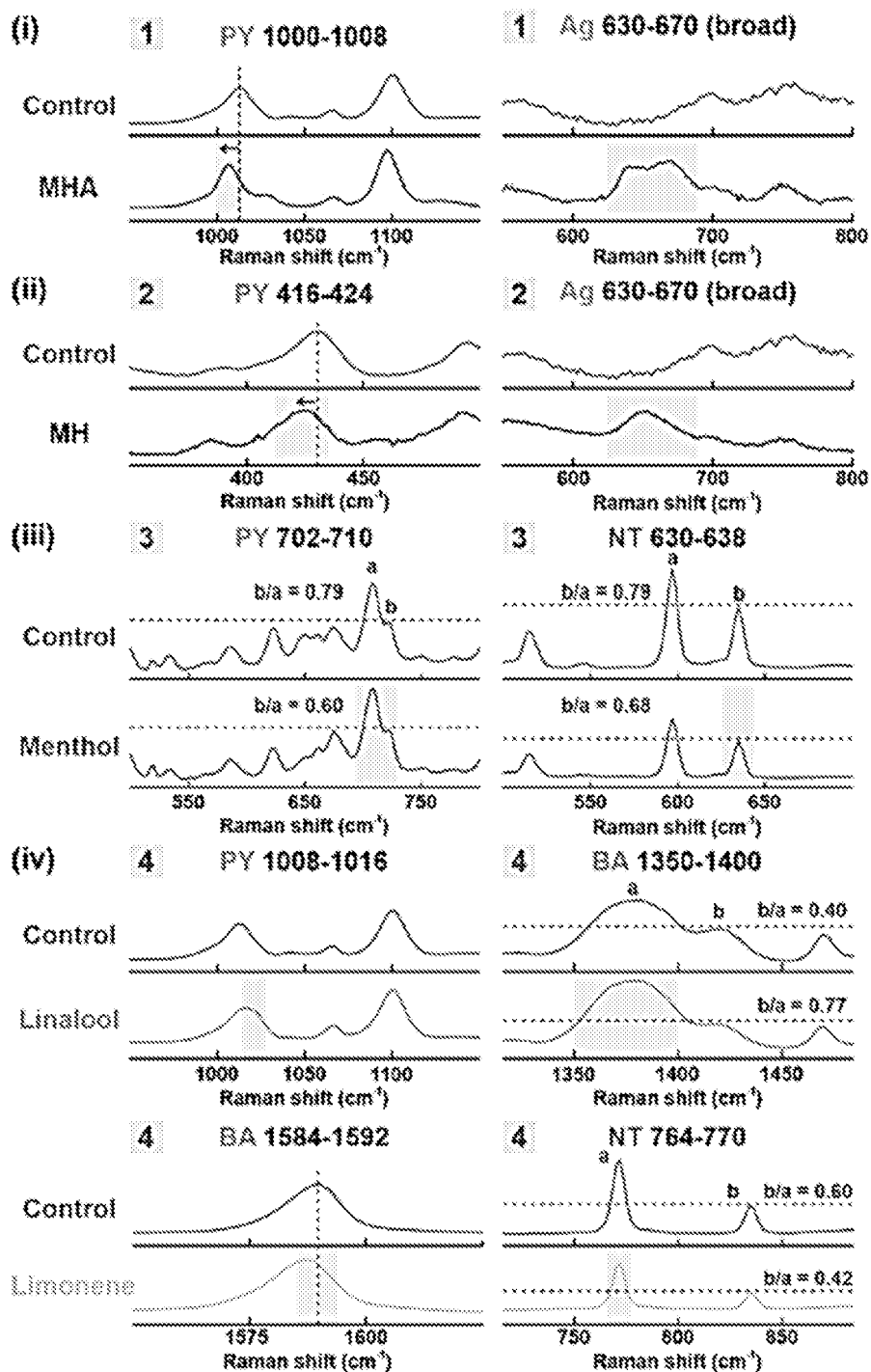


FIG. 18

	Ag surface only	SERS Taster
Average classification accuracy	54.2% (78/144)	100%
False negative	6.9% (10/144)	0%
False positive (for a single flavor molecule):		
Menthol	0%	0%
Linalool	10.4% (15/144)	0%
Limonene	14.6% (21/144)	0%
MHA	6.3% (9/144)	0%
MH	7.6% (11/144)	0%

FIG. 19

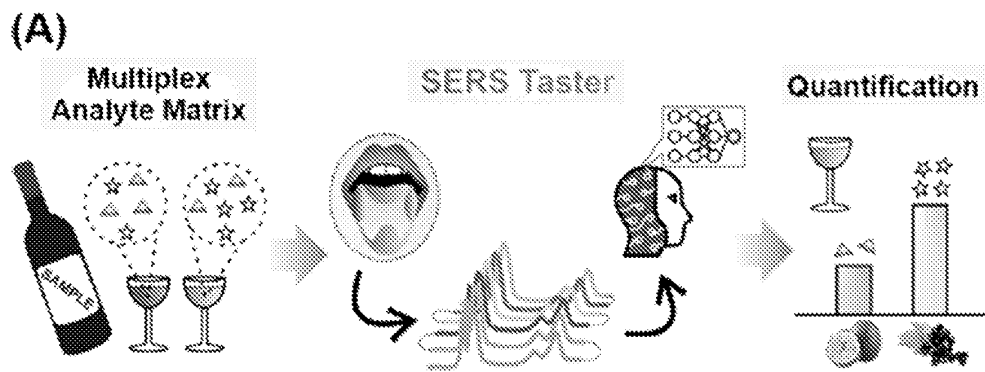


FIG. 19 (Continued)

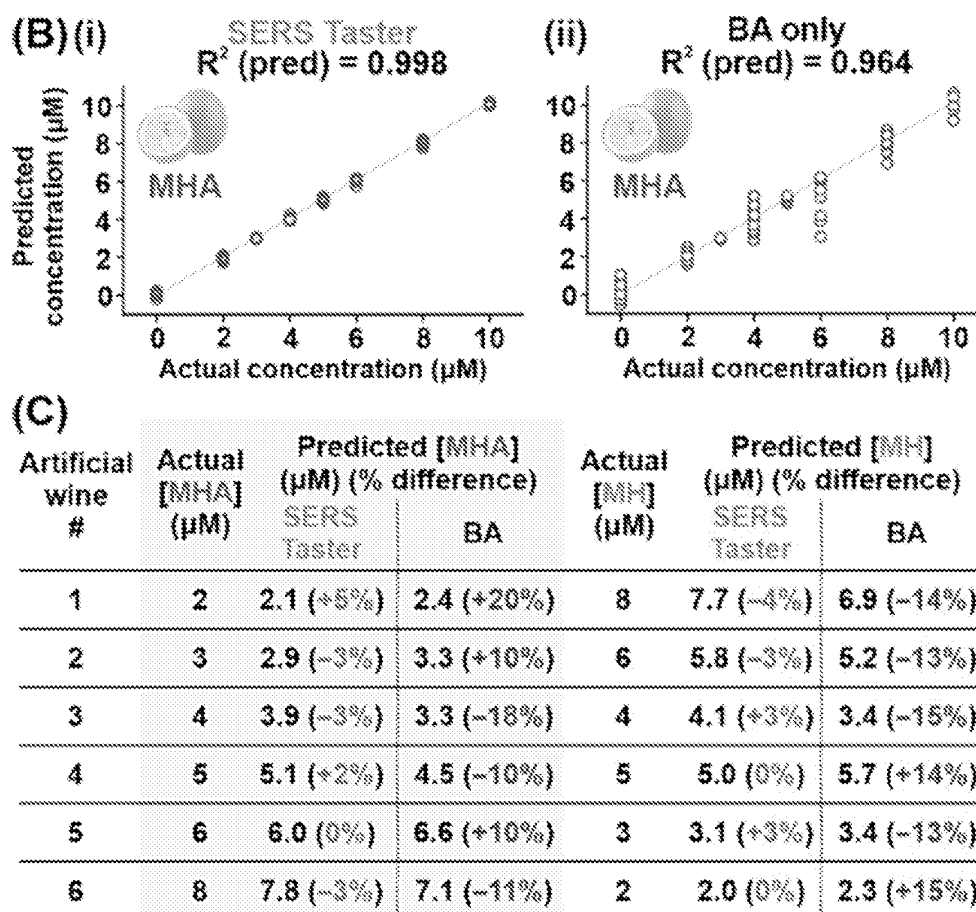


FIG. 20

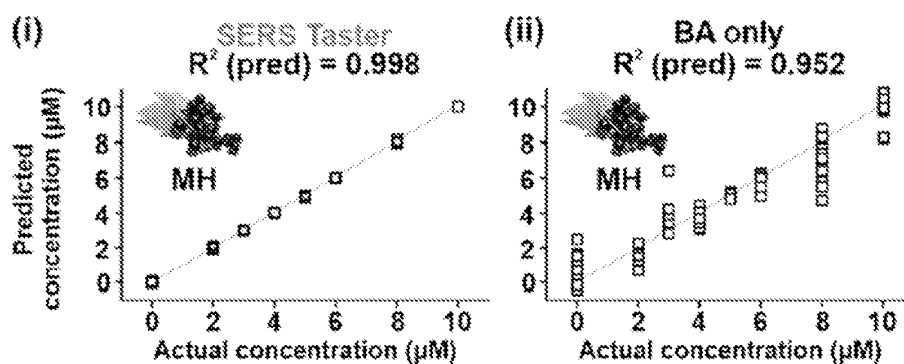


FIG. 21

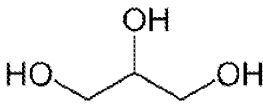
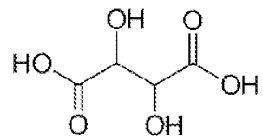
Potential interference	Molecular structure	Possible intermolecular interactions
Glycerol		Electrostatic interactions; Hydrogen bonding; van der Waals' forces
Tartaric acid		Electrostatic interactions; Hydrogen bonding; van der Waals' forces

FIG. 22

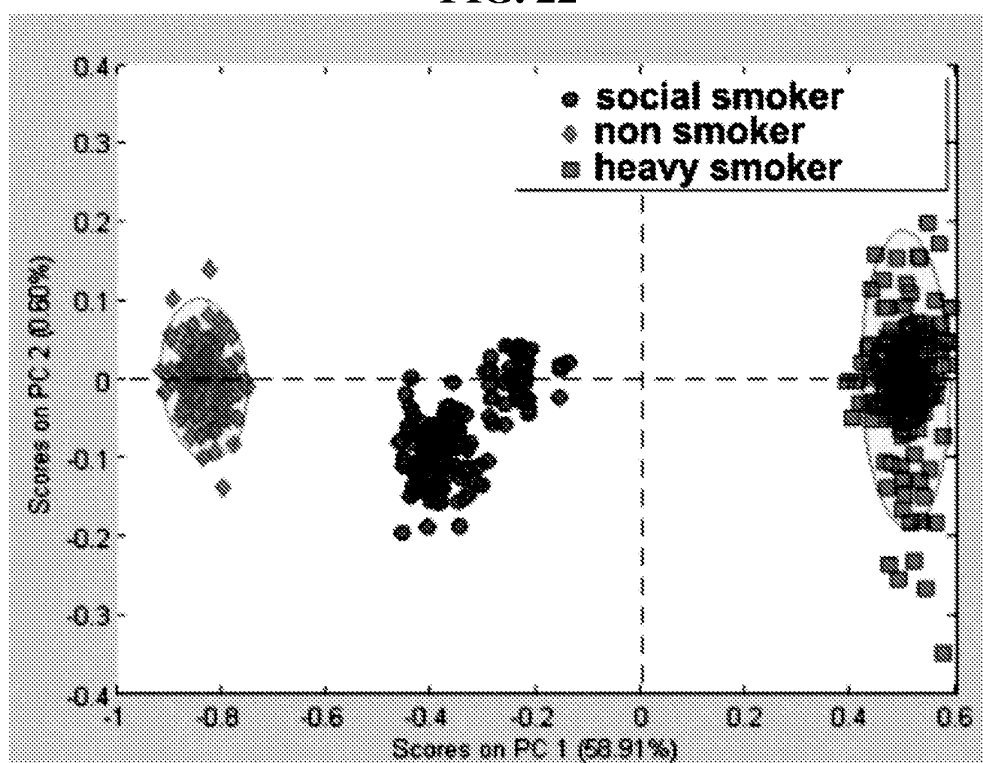


FIG. 23

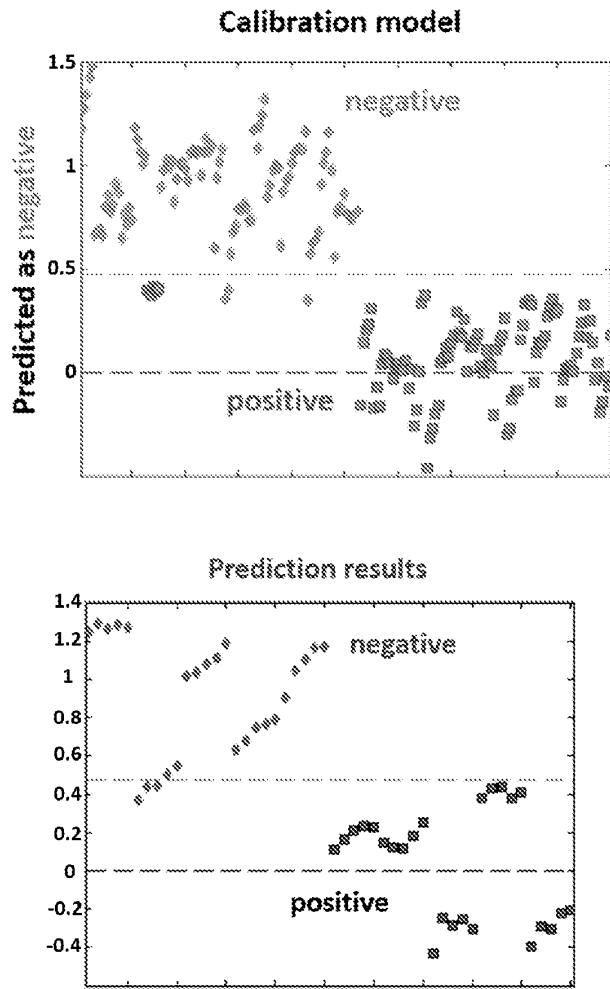


FIG. 24

	Actual	
	Positive	Negative
Predicted	5	1
Negative	0	4

FIG. 25

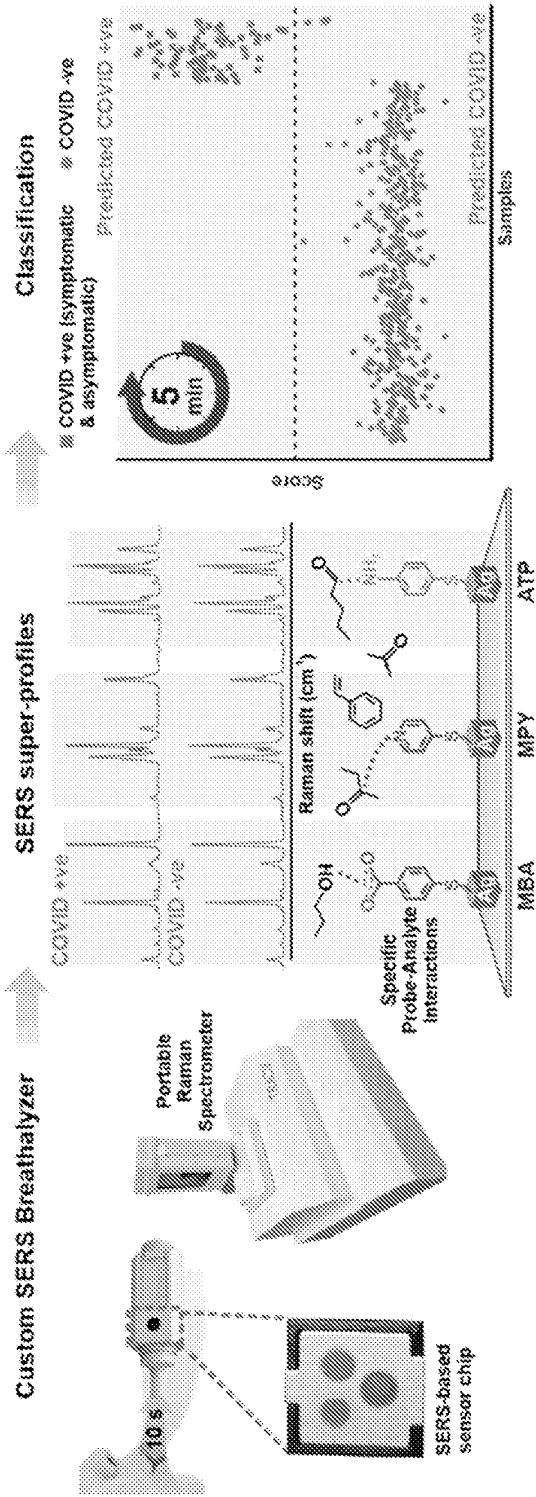


FIG. 26

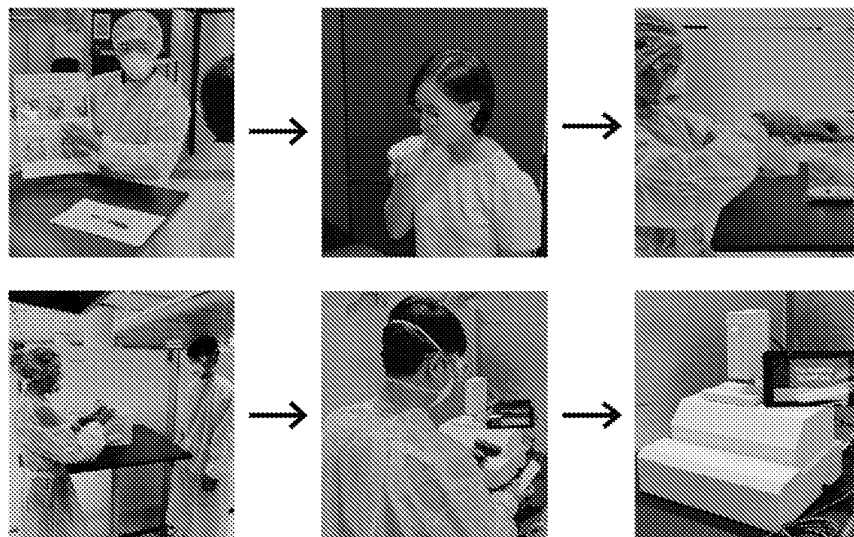


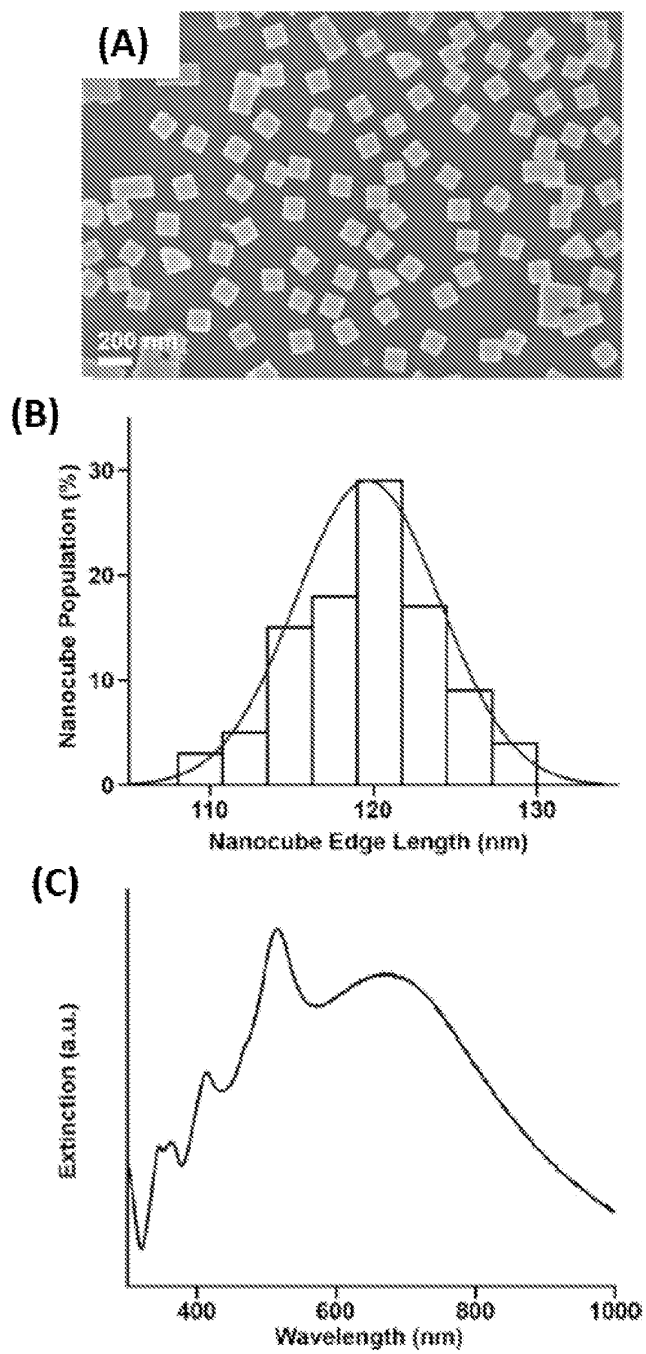
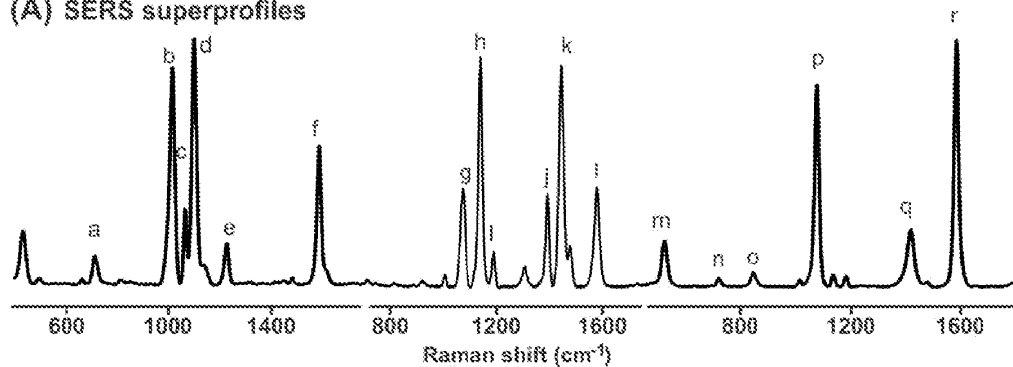
FIG. 27

FIG. 28**(A) SERS superprofiles****(B)**

	Peak position	Experimental (cm ⁻¹)	Assignment
MPY	a	714	$\nu(\text{C-S})$
	b	1014	Ring breathing
	c	1064	$\delta(\text{CH})$
	d	1100	Ring breathing + $\nu(\text{C-S})$
	e	1224	$\beta(\text{CH}) + \delta(\text{NH})$
	f	1586	$\nu(\text{C=C})$ *de-protonated pyridine
ATP	g	1075	$\nu(\text{C=C}) + \nu(\text{C-S})$
	h	1143	$\beta(\text{C-H}) + \nu(\text{C-N})$
	i	1186	$\beta(\text{C-H})$
	j	1393	$\nu(\text{N=N}) + \nu(\text{C-N})$
	k	1441	$\nu(\text{N=N}) + \beta(\text{C-H})$
	l	1560	$\nu(\text{C=C})$
MBA	m	521	$\nu(\text{C-S})$
	n	717	$\gamma(\text{CCC})$
	o	842	$\delta(\text{COO-})$
	p	1077	Ring breathing + $\nu(\text{C-S})$
	q	1418	$\nu(\text{COO-})$
	r	1586	$\nu(\text{C=C})$

ν , stretching; δ , bending; ρ , rocking; β , X-H bending (where X is C, N, O); γ , out of plane bending

FIG. 29

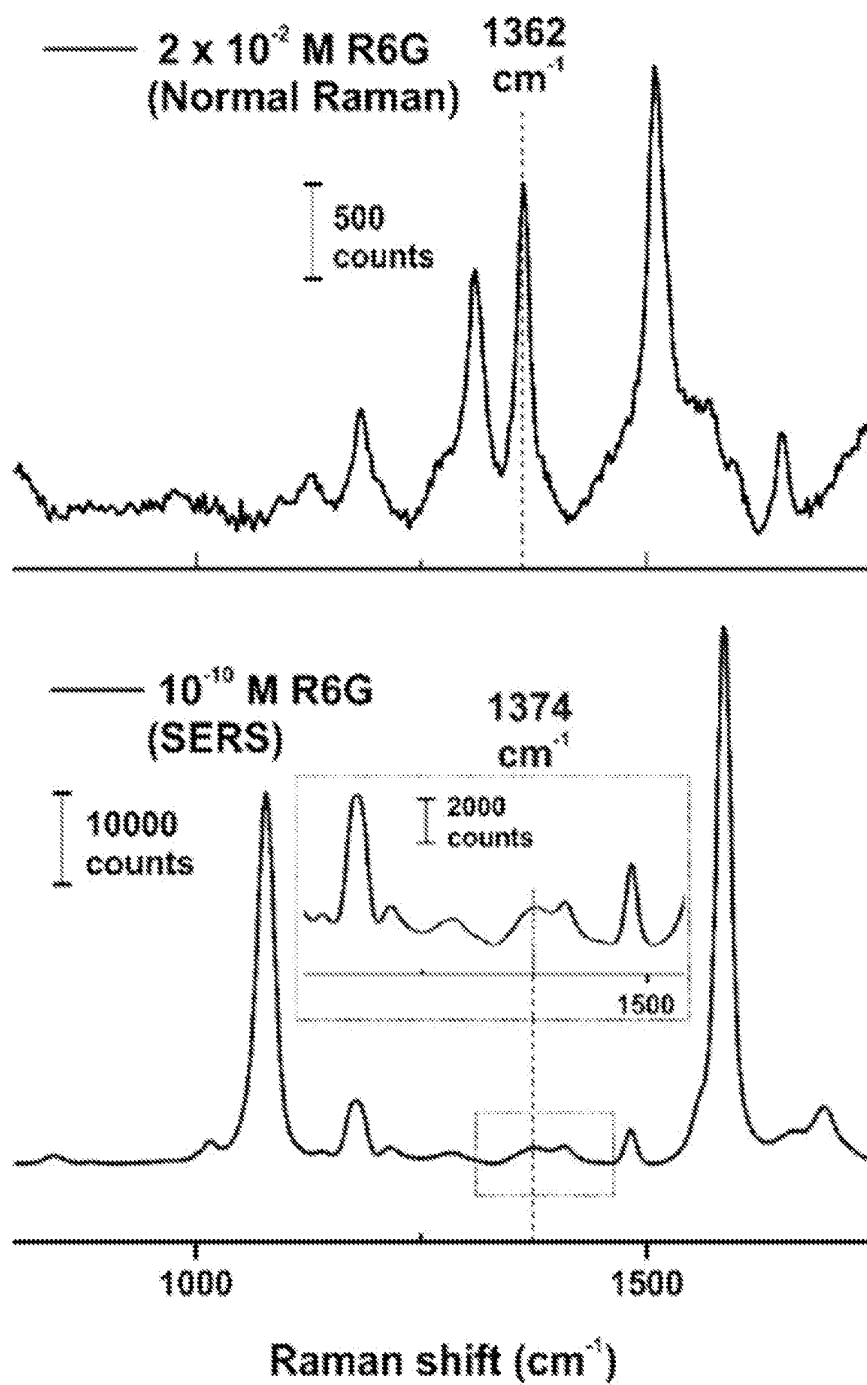


FIG. 30

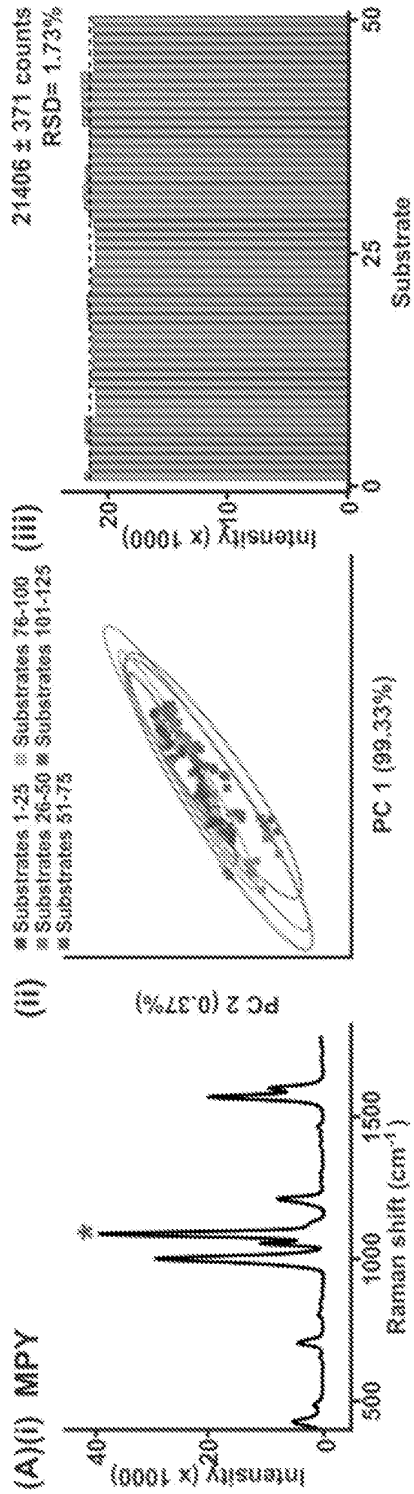


FIG. 30 (Continued)

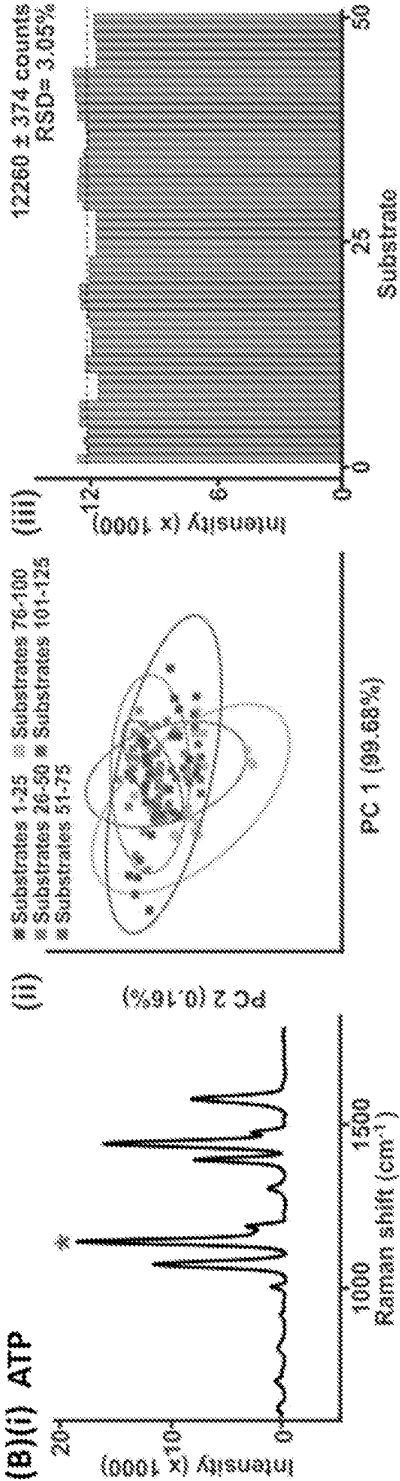


FIG. 30 (Continued)

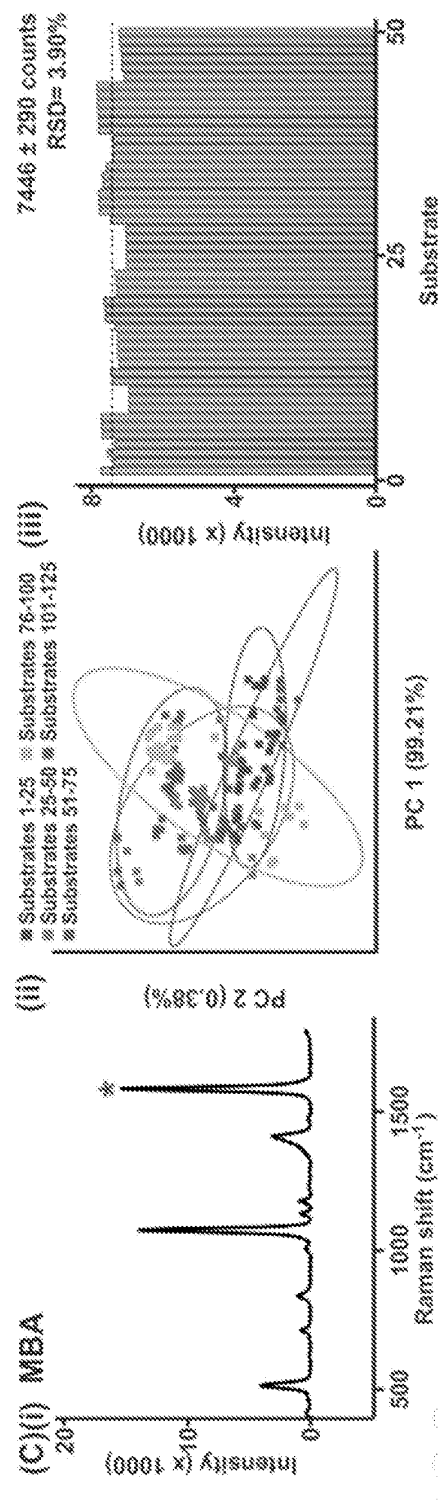


FIG. 31

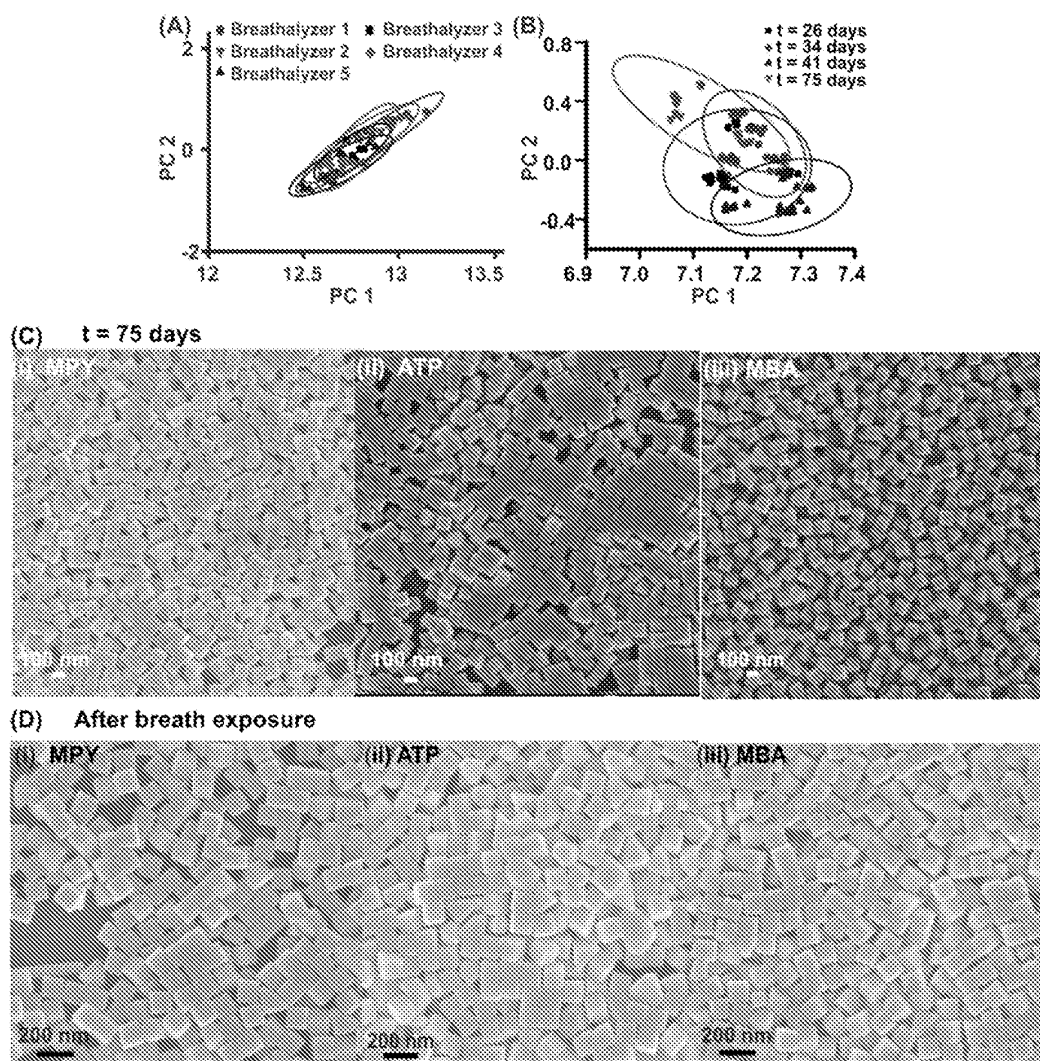


FIG. 32

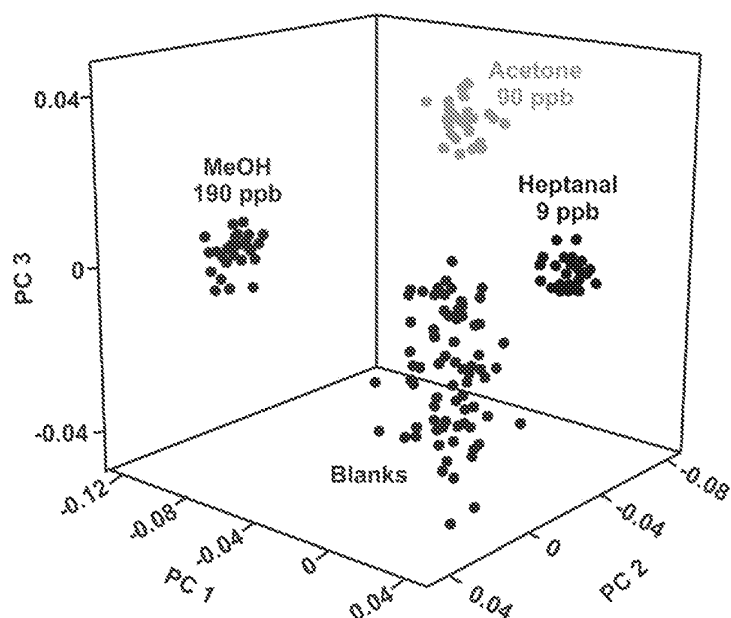


FIG. 33

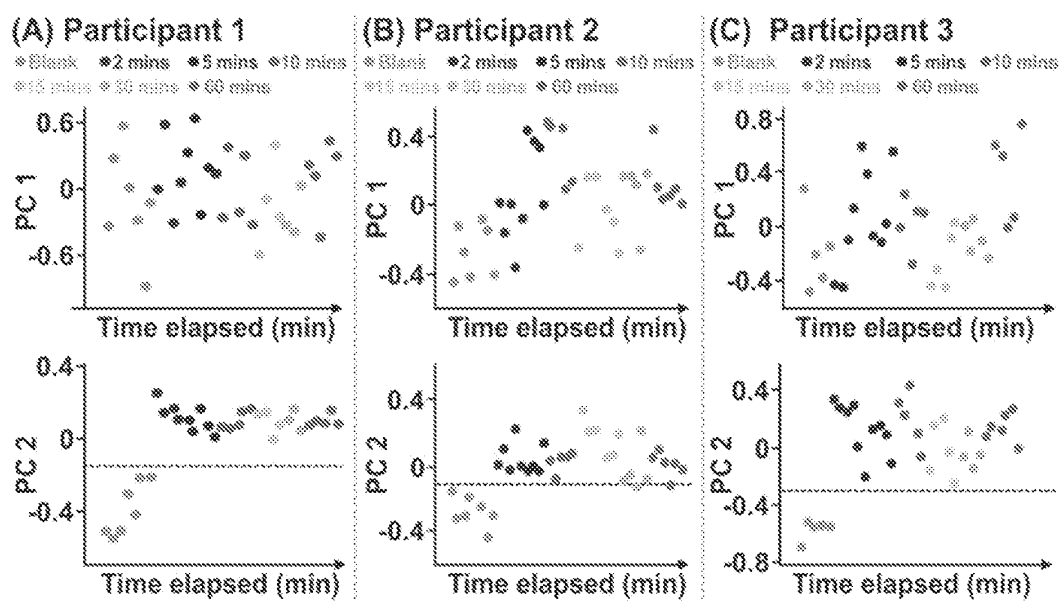


FIG. 34

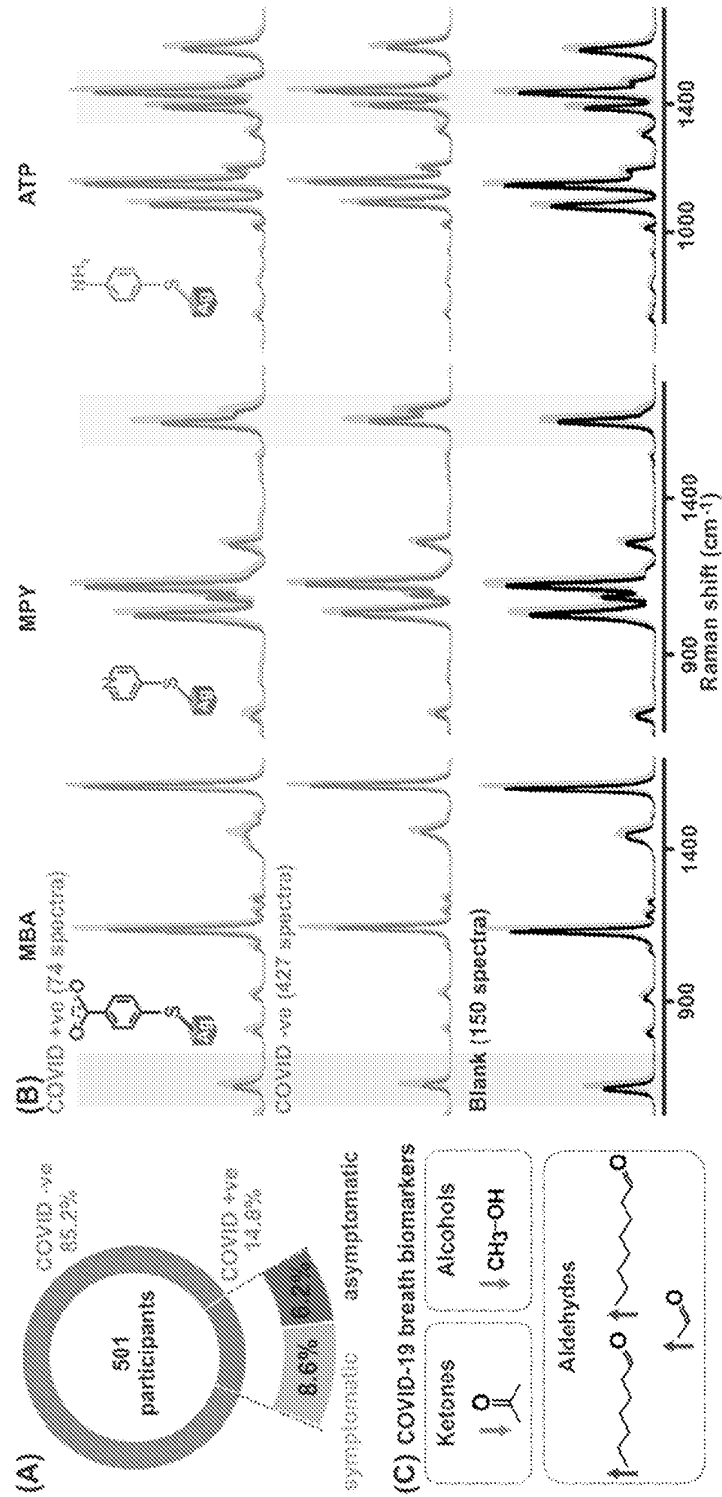


FIG. 35A

Compound	MW (g mol ⁻¹)	Saturated vapor pressure (Pa)	Saturated vapor concentration (ppm)
ethanal	44.05	143,280	2465
heptanal	100.21	569	22
octanal	128.212	80	4
acetone	58.08	37,519	851
methanol	32.04	21,697	271
water	18.02	5,626	40

FIG. 35B

Comparison	U	Z	Probability > U
MPY 1617 cm ⁻¹ / 1586 cm ⁻¹			
Blank vs. COVID-negative	0	-18.15465	1.17973×10^{-73}
Blank vs. COVID-positive	0	-11.83178	2.67425×10^{-32}
COVID-positive vs. COVID negative	4078	-9.30333	1.36118×10^{-20}
DMAB 1143 cm ⁻¹ / 1075 cm ⁻¹			
Blank vs. COVID-negative	29326	-14.83242	9.04155×10^{-50}
Blank vs. COVID-positive	8771	-2.67483	0.00748
COVID-positive vs. COVID negative	21821	4.79878	1.59638×10^{-6}
DMAB 1186 cm ⁻¹ / 1075 cm ⁻¹			
Blank vs. COVID-negative	4021	-16.44439	9.20048×10^{-61}
Blank vs. COVID-positive	1660	-8.41441	3.94867×10^{-17}
COVID-positive vs. COVID negative	22441	8.2616	2.22045×10^{-16}
DMAB 1393 cm ⁻¹ / 1075 cm ⁻¹			
Blank vs. COVID-negative	48708	-16.49396	4.05455×10^{-61}
Blank vs. COVID-positive	12136	-7.54075	4.67281×10^{-14}
COVID-positive vs. COVID negative	67632	4.20121	2.65494×10^{-5}
DMAB 1441 cm ⁻¹ / 1075 cm ⁻¹			
Blank vs. COVID-negative	32088	-13.89048	7.23536×10^{-44}
Blank vs. COVID-positive	7859	-3.65652	2.55667×10^{-4}
COVID-positive vs. COVID negative	20555	3.67522	2.37645×10^{-4}
MBA 521 cm ⁻¹ / 1077 cm ⁻¹			
Blank vs. COVID-negative	19015	5.71197	1.1678×10^{-8}
Blank vs. COVID-positive	4331	9.54477	1.125×10^{-30}
COVID-positive vs. COVID negative	16276	2.36422	1.807×10^{-2}

FIG. 35C**Experimental**

	Peak intensity (a.u.)	
	$\nu(\text{CS})$ at 521 cm^{-1} / ring breathing at 1077 cm^{-1}	% Change with analyte incubation
MBA only	0.2451 ± 0.0318	-
MBA-acetone	0.2111 ± 0.0202	-13.91 %
MBA-ethanal	0.1601 ± 0.006	-34.71 %
MBA-heptanal	0.2445 ± 0.0170	-0.28 %
MBA-octanal	0.2160 ± 0.0109	-11.91 %
MBA-MeOH	0.2659 ± 0.0323	+8.45 %
MBA-water	0.3063 ± 0.0061	+24.95 %

DFT simulated

	Peak intensity (a.u.)			
	$\nu(\text{CS})$ at 296 cm^{-1}	Ring breathing at 1099 cm^{-1}	$\nu(\text{CS})$ / ring breathing	% Change with analyte
MBA only	648.8	4053.4	0.1600	-
MBA-acetone	35125.1	222790.5	0.1577	-1.48 %
MBA-ethanal	34160.4	216723.4	0.1576	-1.50 %
MBA-heptanal	38964.9	244067.1	0.1596	-0.23 %
MBA-octanal	25947.8	228943	0.1133	-29.17 %
MBA-MeOH	46121.9	218295.6	0.2113	+32.03 %
MBA-water	29796.6	167335.1	0.1781	+11.27 %

FIG. 36

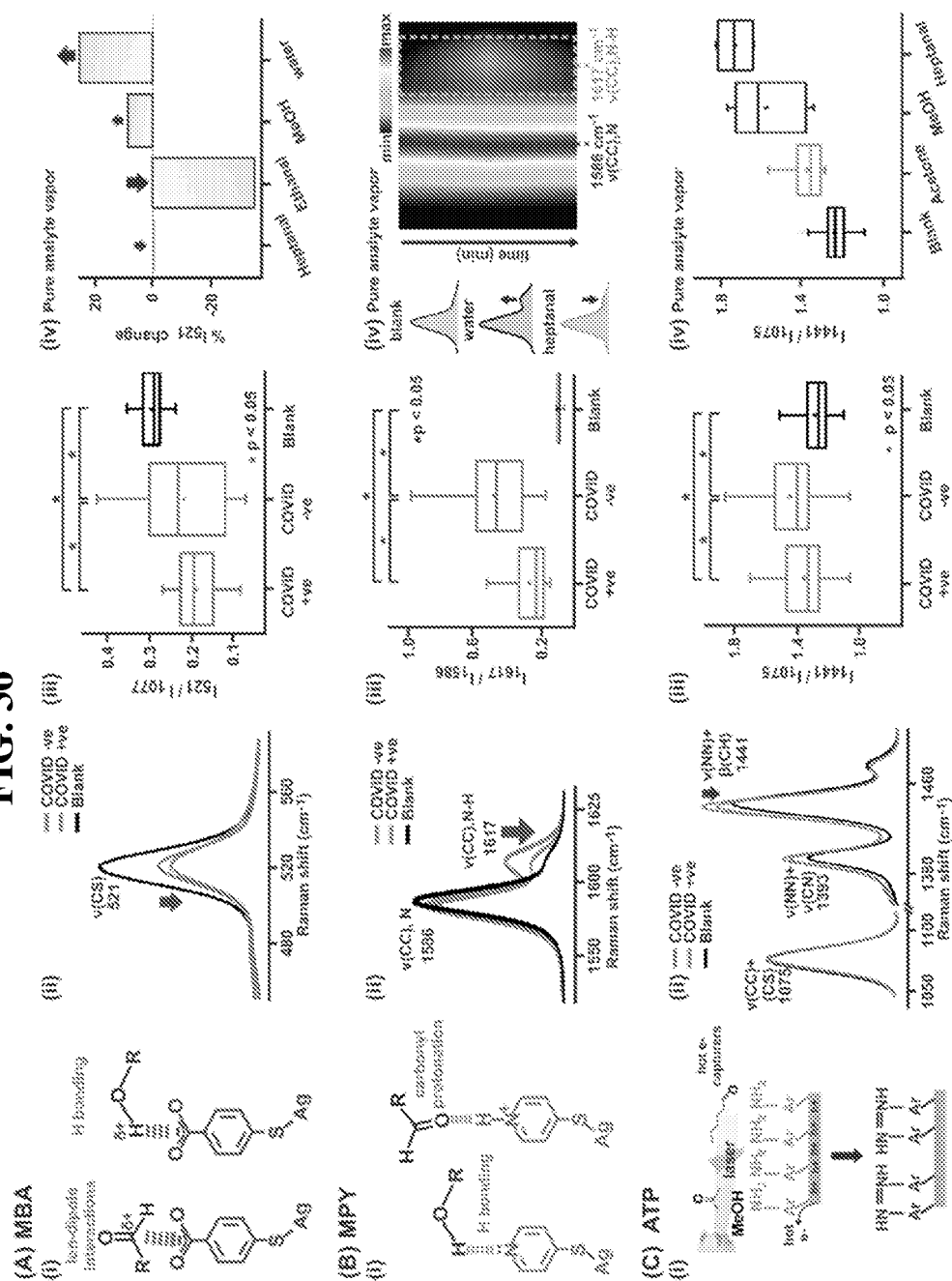


FIG. 37

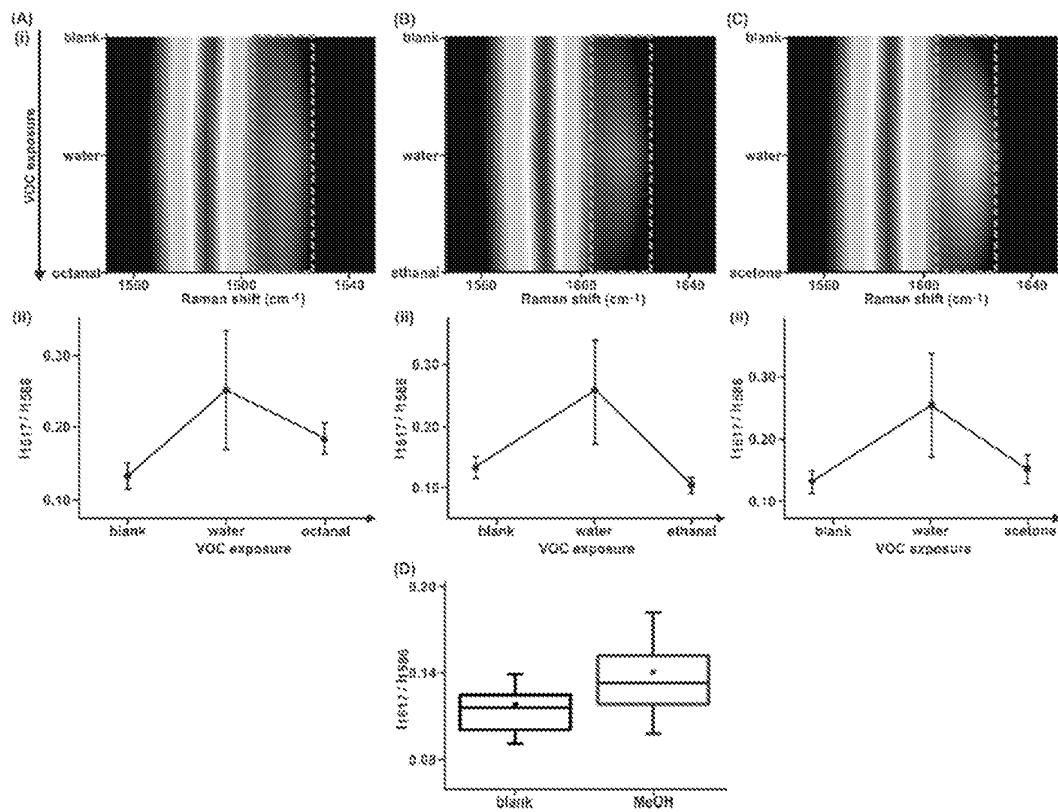


FIG. 38

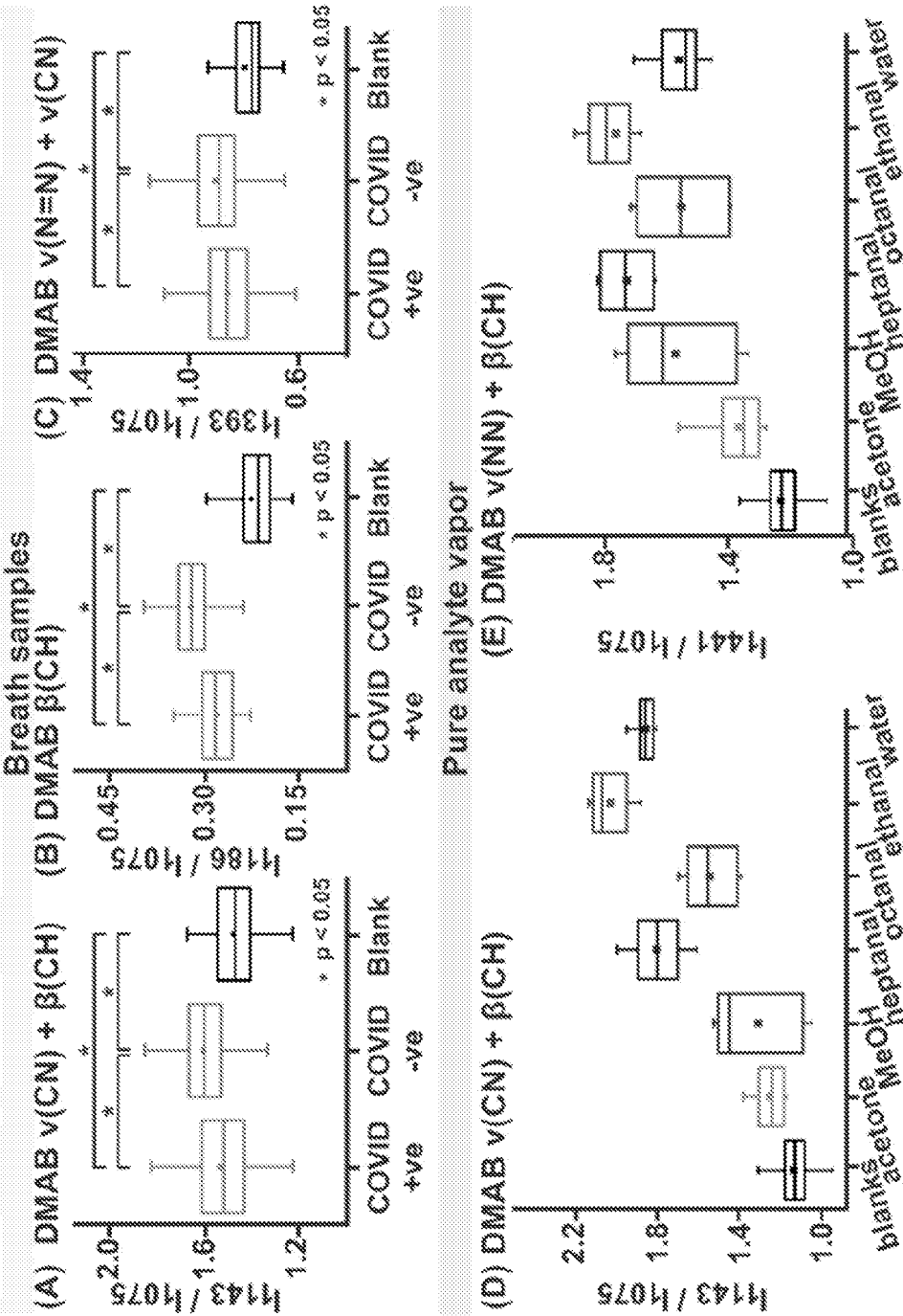


FIG. 39

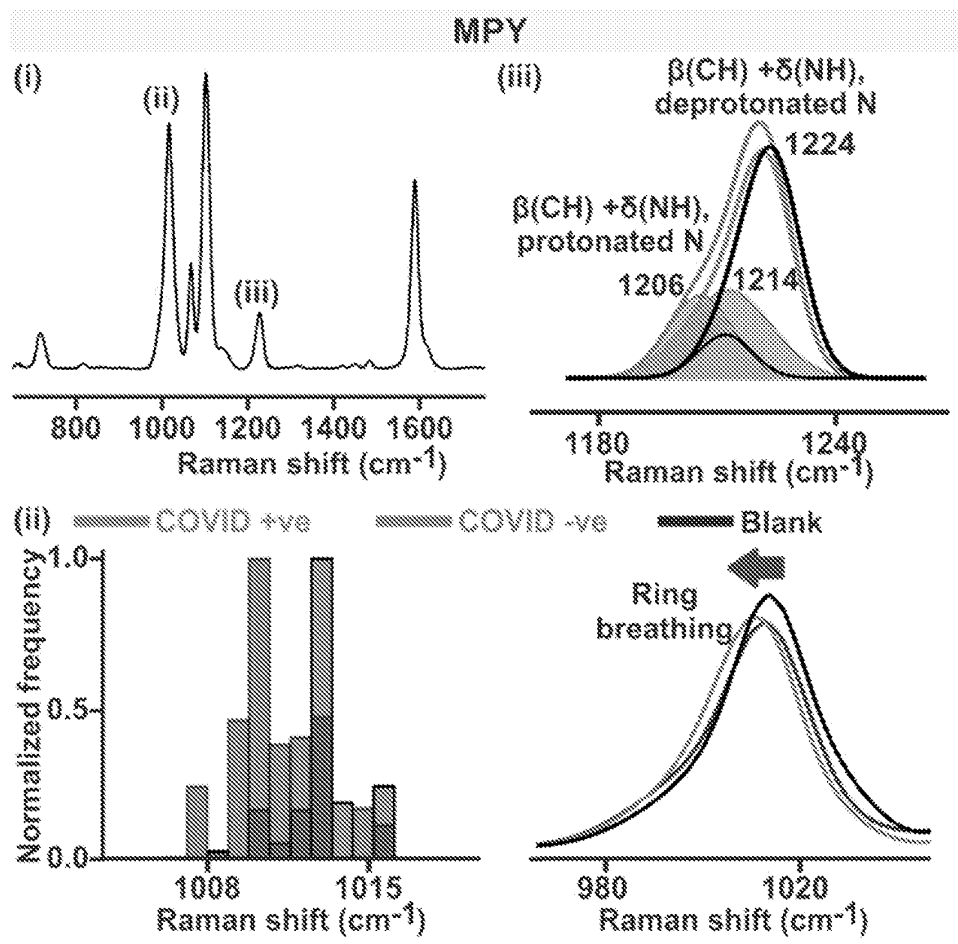


FIG. 40

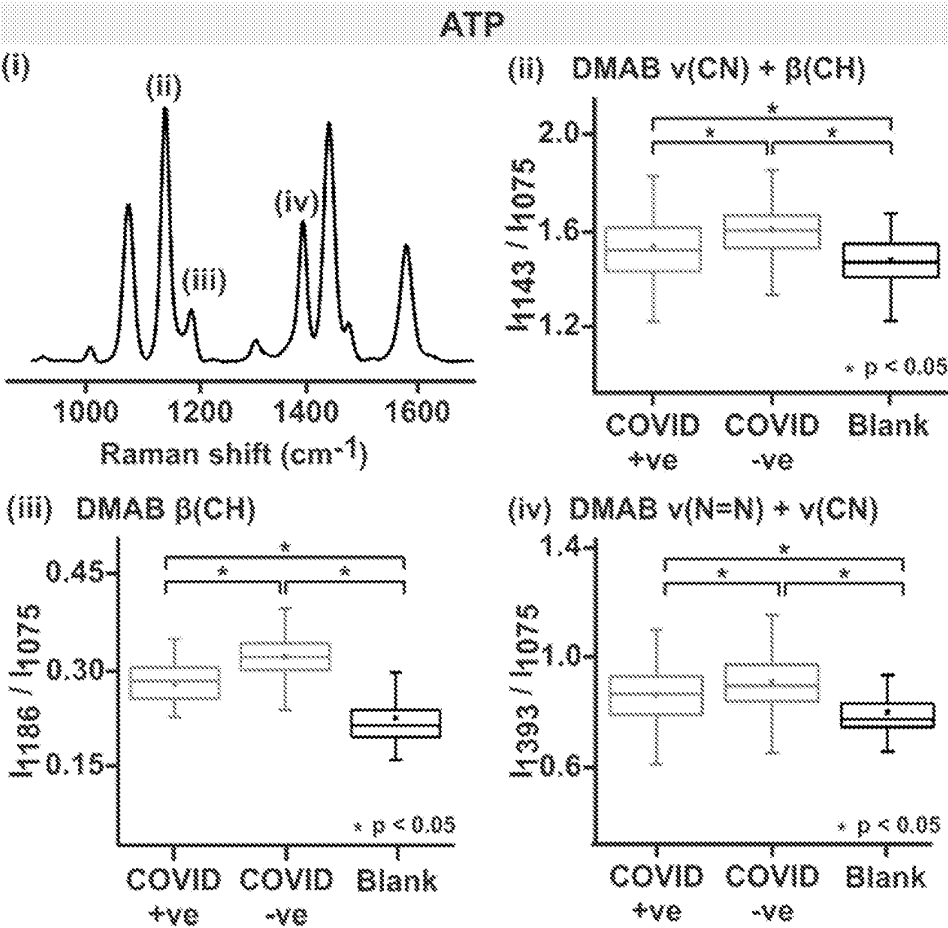


FIG. 41

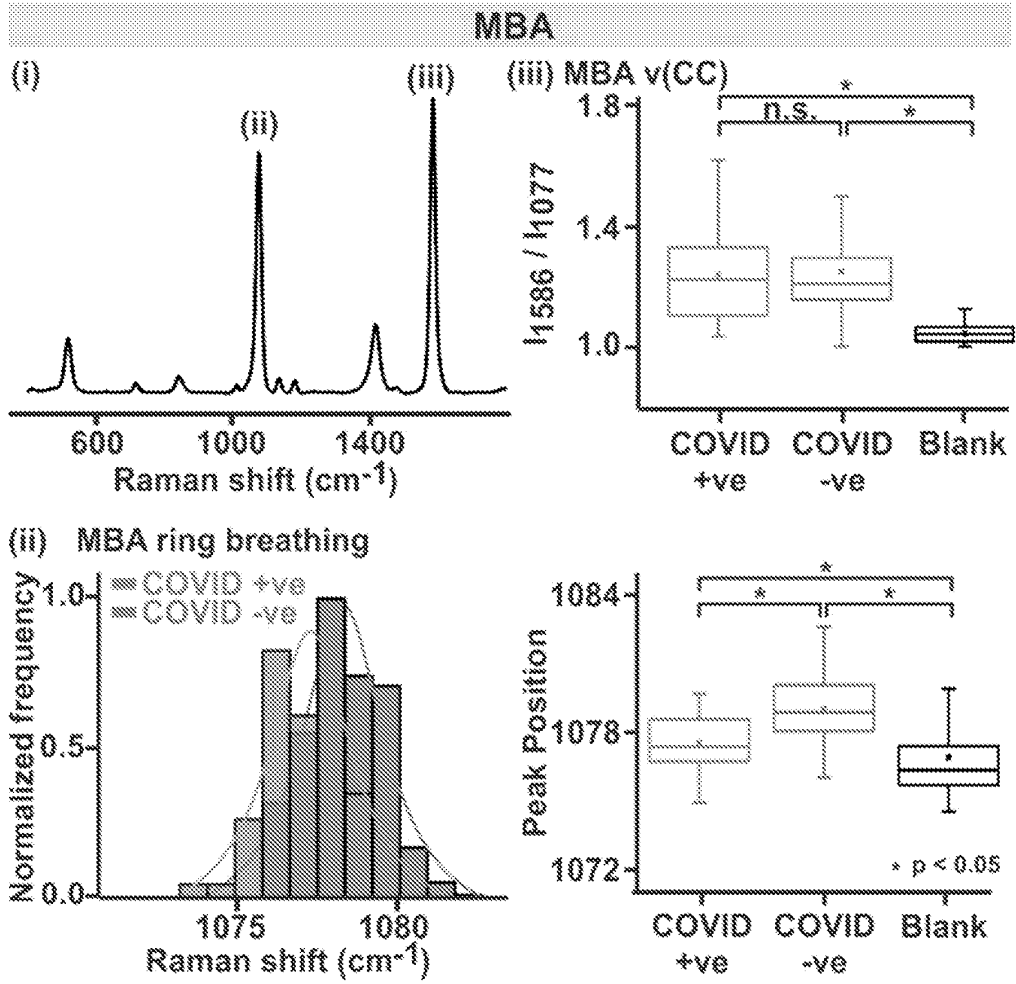


FIG. 42

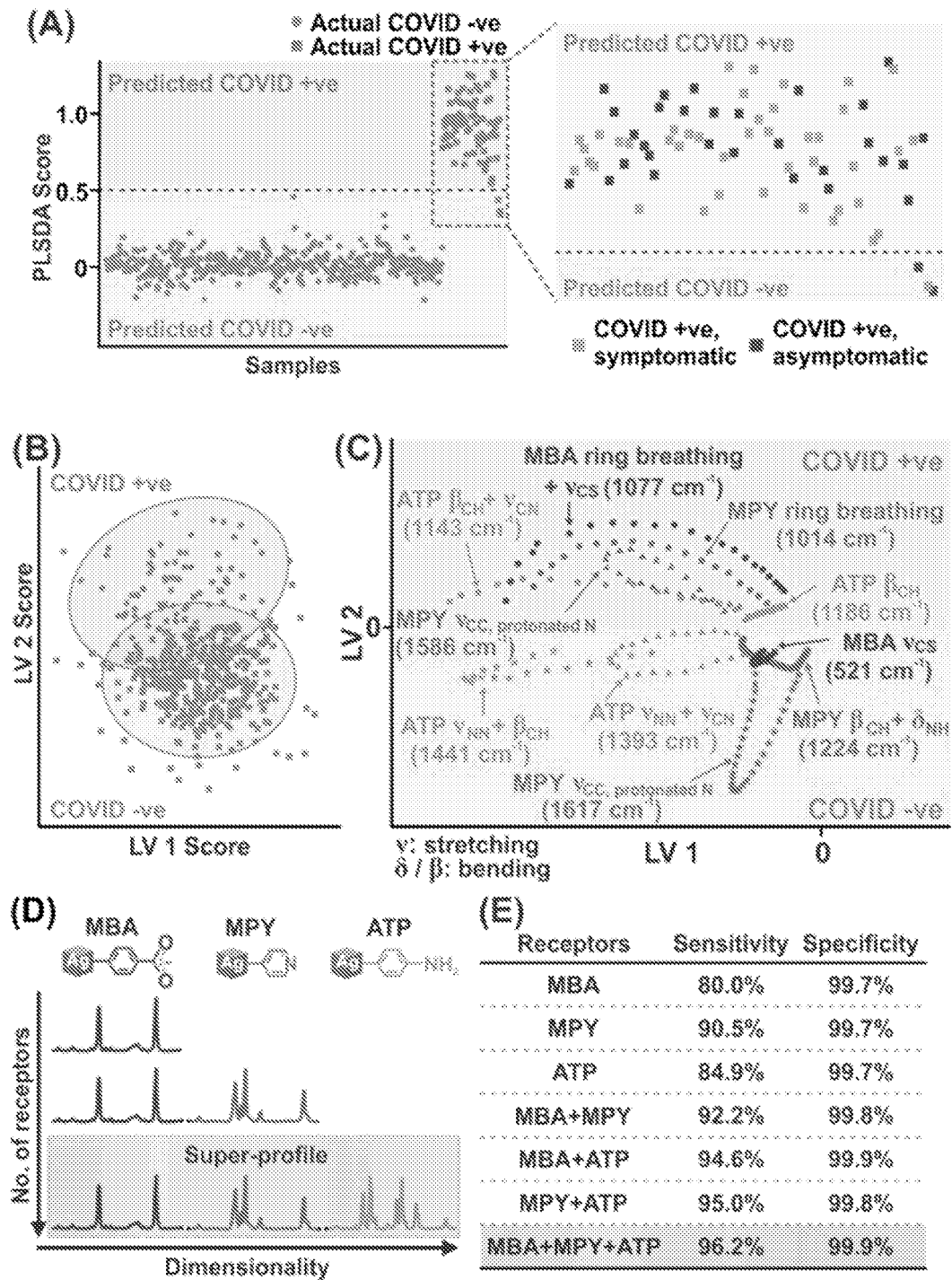


FIG. 43

Model no.	Sensitivity (%)	Specificity (%)
1	89.19	100
2	100	100
3	100	100
4	97.3	99.07
5	94.59	100
6	100	100
7	94.59	99.53
8	91.89	100
9	100	100
10	91.89	100
11	91.89	100
12	93.33	100
13	100	100
14	91.89	100
15	100	100
16	94.59	100
17	97.3	99.53
18	100	100
19	94.59	100
20	100	100
21	94.59	100
22	97.3	99.07
23	100	100
24	100	100
25	97.3	100
26	97.3	100
27	97.3	100
28	91.89	100
29	100	100
30	97.3	100
31	94.59	100
32	91.89	100
33	97.3	100
34	94.59	100
35	100	100
36	94.59	100
37	97.3	100
38	93.33	100
39	91.89	100
40	100	99.53
41	94.59	100
42	100	100
43	97.3	100
44	100	100
45	100	100
46	86.49	100
47	94.59	100
48	94.59	100
49	100	100
50	89.19	100

FIG. 44

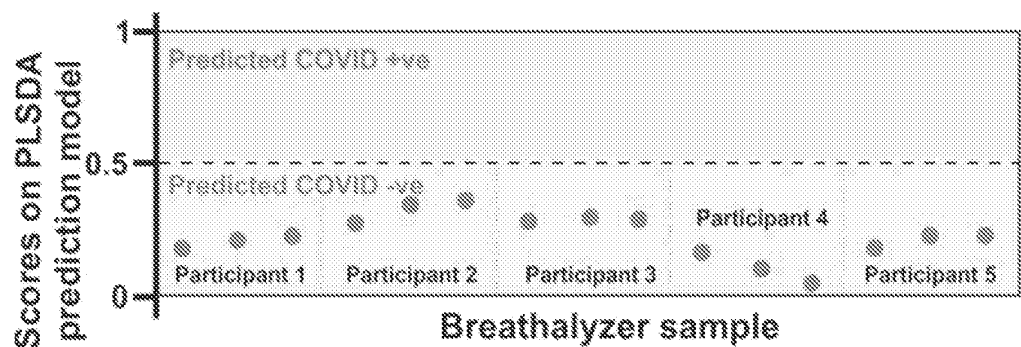


FIG. 45

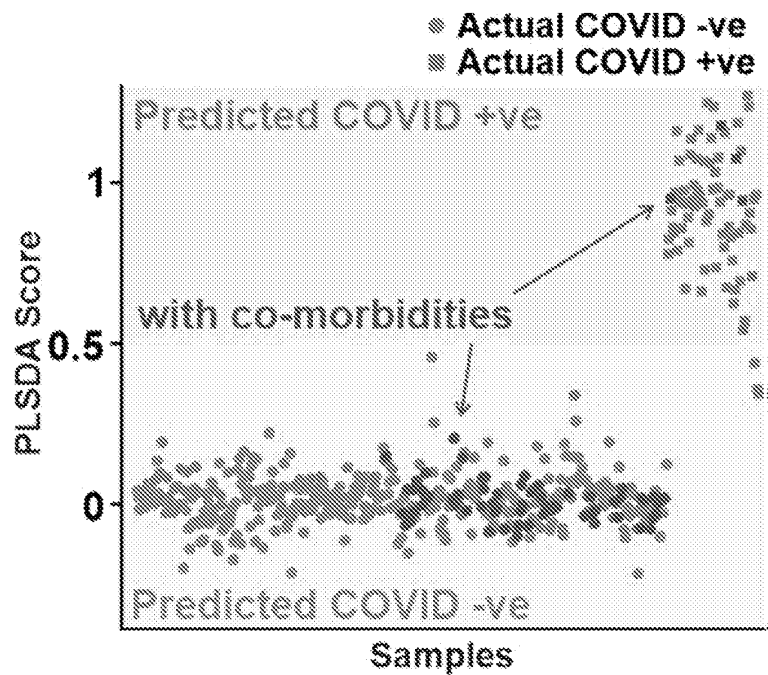
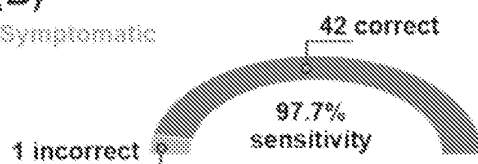


FIG. 46**(A)**

	Actual positive	Actual negative	
Predicted positive	71 (71.16)	0 (0.28)	PPV = 99.6% (98.2-100%)
Predicted negative	3 (2.84)	427 (426.72)	NPV = 99.3% (98.6-100%)
	Sensitivity = 96.2% (91.8-100%)	Specificity = 99.9% (99.7-100%)	

(B)

Symptomatic



Asymptomatic

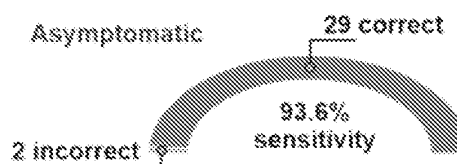
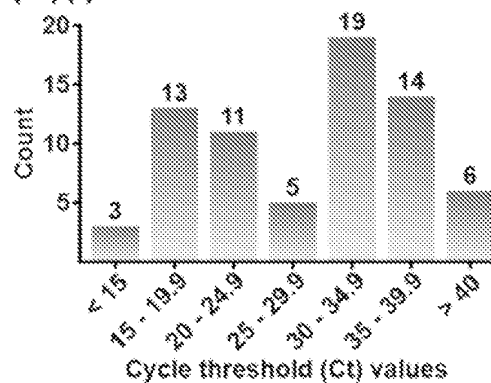
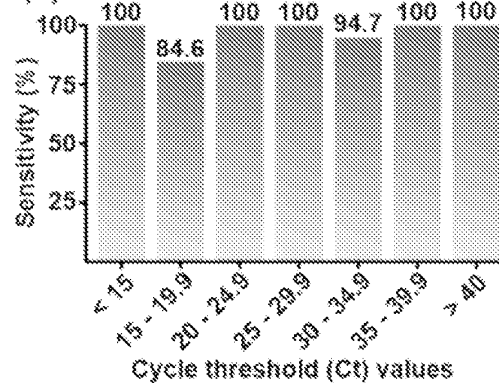
**(C)(i)****(ii)**

FIG. 46 (Continued)

