Supporting Information for

## In situ Real-time Identification of Packaged Chemicals using Dual-Offset Optical probe

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Figure S1. (a) The photographic image of an in-house SORS imaging system using the dual-offset optical probe. (b) The photographic image of probing head, laser input (SMA) and signal output terminal.



(a)

(b)



Figure S2. (a) The microscopic image of signal output terminal. There are 25 cores each in the sensing cores with 5 mm (right) and 10 mm (left) offsets. The sensing cores of the marked area were imaged by CCD in the probe imaging system. (b) The CCD image of the sensing core with 5 and 10 mm offsets.





Figure S3. Subtracted Raman spectra of various chemicals with DOOP system.









## Figure S4. Confusion matrix of (a) 5 mm, (b) 10 mm offset, and (c) subtracted spectra acquired the DOOP system.

## (a)

2-benzoylbenzoic acid	81	2	21	7	2	2	1	0	7	4	3	4	0	4	3	6	6	1	3	58
Acetaminophen	0	30	0	4	0	0	0	0	0	1	1	1	0	0	0	1	0	4	0	0
Benzophenone	0	0	11	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Biphenyl	0	0	0	50	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Cystamine	3	22	0	1	55	14	8	2	17	12	5	19	0	21	31	16	12	5	10	0
D-xylose	4	1	3	0	2	56	2	0	1	0	0	9	2	4	6	1	1	2	6	0
Glucose	0	2	1	1	5	25	98	1	19	12	10	5	2	37	9	8	23	10	12	0
PMMA	24	42	26	22	36	16	12	142	34	44	27	45	27	23	33	21	24	32	30	0
Polyvinyl alcohol	0	0	0	0	0	5	1	0	3	0	0	0	0	0	0	1	1	0	0	0
Pluronic	0	0	0	0	3	9	2	0	2	11	5	3	0	2	2	0	2	0	2	0
Poly(ethylene oxide)	1	1	0	1	1	0	0	2	4	29	78	4	0	3	3	1	6	1	3	0
Poly(sodium 4-styrenesulfonate)	0	0	0	1	0	1	0	0	2	1	0	4	0	1	1	0	2	1	0	0
Sodium acetate	4	2	1	5	4	7	1	0	4	1	2	3	107	3	9	0	1	2	7	0
Sucrose	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0
Sulfanilic acid	20	22	45	30	23	5	19	2	22	23	16	36	2	20	42	24	15	10	59	0
Titanium dioxide	8	21	21	3	17	10	4	1	33	6	0	15	10	26	10	70	12	8	8	0
Trisodium citrate	4	1	8	3	2	0	2	0	0	5	2	0	0	2	0	1	43	1	1	0
Trimesic acid	1	3	13	21	0	0	0	0	2	1	1	2	0	2	1	0	2	73	3	1
Urea	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0
Trans stilbene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	91
Trianesic e Trisoduum cittate Sustose Soduum acatate Soduum acatate Soduum acatate Soduum acatate Polyleathlene oxide Polyleathlene oxide Solucose Succose Succose Succose Solucose Succos Succos Su													Urea cid	Trans sur						

2-benzoylbenzoic acid	40	0	3	9	0	7	4	0	1	1	0	0	0	5	0	2	0	1	1	32
Acetaminophen	2	28	0	1	1	0	1	1	4	1	2	5	1	0	4	1	0	23	3	0
Benzophenone	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Biphenyl	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Cystamine	35	72	25	34	108	47	19	8	50	43	20	44	6	37	61	40	21	21	41	0
D-xylose	0	0	0	0	0	19	0	0	0	0	0	0	0	0	1	0	0	0	0	0
Glucose	0	0	0	0	0	0	35	0	0	0	0	0	0	3	0	0	0	0	1	0
PMMA	4	7	22	40	5	3	4	132	15	35	34	16	24	22	10	10	20	49	13	0
Polyvinyl alcohol	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Pluronic	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0
Poly(ethylene oxide)	0	0	0	0	1	1	2	0	0	6	65	0	0	1	1	0	2	0	0	0
Poly(sodium 4-styrenesulfonate)	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0
Sodium acetate	0	0	0	1	0	0	0	0	0	0	0	0	85	2	0	0	0	0	0	0
Sucrose	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sulfanilic acid	51	15	69	43	22	23	52	3	32	39	17	53	6	33	50	21	6	4	79	0
Titanium dioxide	18	26	23	16	12	49	28	5	46	22	8	27	28	43	23	75	53	42	10	0
Trisodium citrate	0	2	8	4	1	0	5	1	2	3	3	4	0	3	0	1	48	2	2	0
Trimesic acid	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	8	0	16
Urea	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Trans stilbene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	102
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(b)

	407	0	10	0	0	0		0	0	0	0	0	0			0	0	0	0	0	
2-benzoylbenzoic acid	137	0	10	0	0	0	0	0	0	0	0	0	0	0	1	2	0	0	2	0	
Acetaminophen	0	139	1	0	0	0	0	0	1	2	0	0	0	1	1	5	0	0	2	0	
Benzophenone	0	0	90	0	2	0	0	1	1	1	0	1	0	0	1	0	2	0	2	0	
Biphenyl	0	0	1	139	1	0	0	1	1	1	0	0	0	0	1	1	0	0	0	0	
Cystamine	0	0	5	0	141	0	1	1	1	0	0	0	0	0	0	2	0	0	0	0	
D-xylose	0	1	4	0	0	120	0	3	3	1	0	0	0	3	0	1	0	0	2	0	
Glucose	0	1	1	0	1	1	137	3	1	1	0	1	0	6	2	4	4	0	1	0	
PMMA	0	0	3	0	0	1	4	128	0	0	0	0	0	1	3	5	0	0	0	0	
Polyvinyl alcohol	0	1	2	10	1	25	4	2	84	48	6	30	4	12	17	5	60	0	37	0	
Pluronic	7	4	11	0	0	1	0	0	1	43	6	0	3	2	1	5	3	0	0	0	
Poly(ethylene oxide)	2	0	1	0	1	0	1	0	3	30	137	1	0	0	2	6	1	0	2	0	
Poly(sodium 4-styrenesulfonate)	2	0	4	0	2	1	0	1	20	15	1	101	1	10	18	13	18	0	15	0	
Sodium acetate	0	0	2	0	0	0	0	0	3	1	0	1	137	0	1	0	0	0	6	0	
Sucrose	1	0	3	0	0	0	1	1	3	0	0	1	0	110	0	0	6	0	8	0	
Sulfanilic acid	1	3	3	0	1	0	2	1	23	7	0	13	4	3	100	8	7	3	38	0	
Titonium dioxido		0	1	0		1	-		20		0	10		0	0	06		0	0	0	
Triantum dioxide	0	0		0	0	1	0	0	3	0	0	1	0	0	0	00	0	0	0	0	
	0	0	1	0	0	0	0	2	1	0	0	0	0	1	1	2	46	0	5	0	
l rimesic acid	0	1	4	1	0	0	0	0	0	0	0	0	0	0	0	0	3	147	6	0	
Urea	0	0	3	0	0	0	0	6	1	0	0	0	0	1	1	4	0	0	24	0	
Trans stilbene	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	150	ļ
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Figure S5. The DOOP spectra of (a) 2-benzoylbenzoic acid, (b) PMMA, and (c) trisodium citrate used ANN prediction with signal to ratio: each spectra was obtained from single row of CCD sensor.



\* SN ratio : signal height (1587 cm  $^{-1}) /$  standard deviation (400 ~ 600 cm  $^{-1})$ 



\* SN ratio : signal height (1432 cm<sup>-1</sup>) / standard deviation (1600 ~ 1800 cm<sup>-1</sup>)

## (c) trisodium-citrate



Wavenumber (cm<sup>-1</sup>)

\* SN ratio : signal height (1435 cm<sup>-1</sup>) / standard deviation (1600 ~ 1800 cm<sup>-1</sup>)