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## **Supplementary Information**

# Light-induced self-assembly of bi-color CdTe Quantum Dots allows the discrimination of multiple proteins

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### **Results and Discussion**





Fig. S1. XPS analysis of S2p, Te3d and Cd3d in CdTe QDs before (left) and after (right) UV-light irradiation.

After UV-light irradiation, new peaks corresponding to S2p (BE = 168 eV) and Te3d (BE = 576.2eV) appear, whereas no significant change for Cd3d peak is found.

#### 2. The discrimination of different proteins without UV-light irradiation

The discrimination effect of the dual-channel fluorescent (FL) sensor without UVlight irradiation was also evaluated, the corresponding FL image was supplied in Fig. S2. The results show that UV-light is of vital importance to the identification of proteins, because almost no FL changes are found among the CdTe-protein complexes without the special irradiation of UV-light.



Fig. S2. FL images of G-QDs (A) and Y-QDs (B) in the presence and absence of ten proteins without special UV-light irradiation. The concentration of CdTe QDs is 0.25 mM and that of each protein is  $1.0 \text{ mg} \cdot \text{mL}^{-1}$ , all the protein samples are dissolved in PBS buffer (0.01 M, pH=7.4), the excitation wavelength is 302 nm.

# **3.** The effect of illumination time of UV-light and the concentration of CdTe QDs on the sensor

The effect of illumination time of UV-light on the sensor was discussed (0 min, 10 min, 20 min, 30 min, 40 min and 50 min). Here, G-QDs based sensor was chosen as an example, since the discriminating ability of the G-QDs based sensor is superior to that of Y-QDs based one. From Fig. S3, it is found that as the illumination time goes on, the distinguishing ability of the sensor grow better, too. It is also noticed that there is almost no difference between the FL response signals of the sensor when the illumination time is set at 40 min and 50 min. Hence, it is considered that 40 min is the best illumination time for the discrimination of native proteins.

The influence of the concentration of CdTe QDs (1.25 mM, 0.500 mM, 0.250 mM and 0.125 mM) was also researched, using G-QDs as an example. The results in Fig. S3 manifest that when CdTe QDs are at the concentration of 0.250 mM, the sensor display the best FL response patterns. It is hypothesized that the discriminating ability of the sensor has a great relation to the concentration ratio of CdTe QDs to proteins.



Fig. S3. FL images of G-QDs with the addition of ten proteins, illuminated by UV-light (302 nm) for a series of time. The proteins are dissolved in PBS buffer (0.01 M, pH=7.4) and concentrated at 0.25 mg·mL<sup>-1</sup>. From a to d, the concentration of CdTe QDs is 1.25 mM, 0.500 mM, 0.250 mM and 0.125 mM, respectively.

# 4. The determination and identification of 30 unknown protein samples at the concentration of 1.0 mg $\cdot$ mL<sup>-1</sup>.



Fig. S4. FL variation images of assembled G-QDs (a) and Y-QDs (b) in the presence and absence of 30 unknown proteins. The concentration of CdTe QDs is 0.25 mM and





Fig. S5. Canonical score plot for the corresponding  $\Delta$ RGB and  $\Delta$ I values obtained through the sensor against 30 unknown proteins.

Protein	R from G-QDs	G from G-QDs	B from G-QDs	I from G-QDs	R from Y-QDs	G from Y-QDs	B from Y-QDs	I from Y-QDs
Рар	249	157	67	32	254	61	76	37
Pap	246	163	69	35	253	64	71	35
Pap	248	169	64	33	252	66	66	33
Pap	245	167	57	36	255	59	62	36
Pap	247	168	60	34	254	56	75	31
Рер	244	91	122	25	253	0	132	21
Рер	242	84	126	22	254	1	135	18

Table S1. Training matrix of ten proteins at the concentration of 1.0 mg·mL<sup>-1</sup>

Рер	240	88	123	24	254	1	128	24
Рер	245	87	120	27	255	1	121	19
Рер	242	94	127	25	254	0	123	17
CAT	133	168	161	26	74	21	213	7
CAT	126	167	163	22	77	26	219	8
САТ	128	164	160	27	83	28	222	10
САТ	121	156	161	24	81	24	225	8
САТ	124	165	162	23	72	25	212	9
Ser	224	208	101	39	254	245	36	71
Ser	220	214	96	36	254	239	31	69
Ser	223	218	97	35	254	250	30	67
Ser	215	211	104	39	254	254	33	74
Ser	222	207	95	37	255	244	37	66
HSA	117	255	220	76	255	254	142	99
HSA	114	254	210	78	255	253	140	96
HSA	119	255	208	82	255	255	144	93
HSA	124	254	217	77	254	253	145	95
HSA	122	255	213	81	255	254	136	99
Col	125	53	126	13	177	54	102	7
Col	121	49	123	14	178	57	108	9
Col	126	50	127	12	183	53	109	8
Col	118	52	125	14	180	52	112	11
Col	128	54	122	15	173	48	105	10

Try	230	100	128	25	253	1	55	25
Try	227	96	125	23	254	2	45	24
Try	231	104	127	24	254	0	49	29
Try	232	95	122	20	254	4	42	22
Try	222	92	130	26	252	2	50	27
Lys	54	254	127	42	215	154	115	28
Lys	56	255	124	38	209	155	117	27
Lys	51	253	127	44	213	159	113	23
Lys	60	255	126	39	225	157	118	24
Lys	66	255	129	43	210	156	115	26
Muc	173	109	125	19	124	6	169	8
Muc	165	106	128	18	123	8	172	9
Muc	167	104	126	16	120	4	164	7
Muc	171	108	122	17	122	5	167	6
Muc	160	107	129	20	121	3	176	8
EA	226	254	169	73	254	254	94	78
EA	222	254	166	71	253	255	93	79
EA	224	255	163	70	252	253	91	81
EA	230	255	167	72	254	255	99	87
EA	222	255	168	75	253	254	97	83
Blank control	251	114	132	30	255	105	35	52
Blank control	248	110	136	29	252	112	39	50
Blank control	252	112	134	27	254	116	42	55

Blank control	253	115	126	31	253	109	34	51
Blank control	248	117	141	29	252	112	36	53

Table S2. The determination and identification of 30 unknown protein samples at the concentration of  $1.0 \text{ mg} \cdot \text{mL}^{-1}$ .

Sample	R from	G from	B from	I from	R from	G from	B from	I from	T1 /•0• /•	¥7 •0• /•
No.	G-QDs	G-QDs	G-QDs	G-QDs	Y-QDs	Y-QDs	Y-QDs	Y-QDs	Identification	verification
1	128	54	125	14	181	52	110	9	Col	Col
2	60	251	125	40	222	158	121	27	Lys	Lys
3	221	220	90	36	254	236	35	70	Ser	Ser
4	123	57	122	15	177	50	106	7	Col	Col
5	127	255	218	80	255	252	140	100	HSA	HSA
6	222	255	165	75	254	255	101	86	EA	EA
7	179	112	121	19	120	9	165	8	Muc	Muc
8	166	109	126	17	118	2	175	7	Muc	Muc
9	230	255	164	71	251	253	99	82	EA	EA
10	160	113	127	15	123	3	176	8	Muc	Muc
11	126	254	219	82	253	252	147	96	HSA	HSA
12	242	89	122	23	254	0	126	20	Рер	Рер
13	229	255	169	69	253	254	97	85	EA	EA
14	247	166	55	35	254	62	74	36	Рар	Рар
15	223	255	170	72	253	253	100	87	EA	EA
16	229	99	125	24	252	3	55	23	Try	Try
17	241	92	119	24	253	5	129	19	Pep	Рер
18	122	167	160	23	70	30	235	6	CAT	CAT

19	124	255	210	78	254	253	149	99	HSA	HSA
20	224	226	99	33	255	253	34	68	Ser	Ser
21	126	62	123	12	179	59	108	7	Col	Col
22	231	97	123	21	252	2	53	27	Try	Try
23	122	255	220	77	255	254	159	93	HSA	HSA
24	130	165	159	20	84	24	232	5	САТ	CAT
25	225	101	122	22	254	4	56	27	Try	Try
26	124	50	125	14	178	50	110	10	Col	Col
27	244	175	67	33	252	64	65	32	Pap	Pap
28	124	255	216	84	253	255	143	94	HSA	HSA
29	118	58	121	15	173	56	112	10	Col	Col
30	244	87	121	24	255	0	140	16	Рер	Рер
Blank control	250	118	131	27	252	111	40	51		

5. The discrimination of proteins at various concentration levels



Fig. S6. The FL images of G-QDs (A) and Y-QDs (B) in presence of ten proteins at various concentrations illuminated under UV-light (302 nm) for 40 min. The concentration of CdTe QDs is 0.25 mM, all the samples are dissolved in PBS buffer (0.01 M, pH=7.4).



Fig. S7. "Fingerprints" of ten proteins at various concentrations (from A to C: 0.50, 0.25 and 0.10 mg·mL<sup>-1</sup>), based on the corresponding  $\Delta$ RGB and  $\Delta$ I values extracted from their FL signals.



Fig. S8. Canonical score plots for the "fingerprints" of the ten proteins at various concentrations (from A to C: 0.50, 0.25 and 0.10 mg $\cdot$ mL<sup>-1</sup>).

In order to investigate the sensitivity of the sensor, experiments about recording the FL signals of the ten proteins at three various concentrations (0.50, 0.25 and 0.10 mg·mL<sup>-1</sup>) were performed (Fig. S6). The results reveal that the ten proteins possess apparent different "fingerprints" (Fig. S7) at each concentration level and no overlap exists in their corresponding canonical score plot (Fig.S8), indicating that the proteins are well distinguished. Considering the visual properties and accuracy of the sensor, it is concluded the detection limit of the sensor is around 0.10 mg·mL<sup>-1</sup>.

Protein	R from G-QDs	G from G-QDs	B from G-QDs	I from G-QDs	R from Y-QDs	G from Y-QDs	B from Y-QDs	I from Y-QDs
Pap	220	100	134	35	254	137	126	35
Pap	220	113	122	36	255	136	126	31
Pap	222	120	126	34	254	134	120	32
Pap	219	108	133	32	255	132	129	35
Pap	216	105	125	34	255	136	127	33
Pep	254	59	51	49	255	137	141	28
Pep	253	64	52	45	255	141	140	27
Pep	255	62	54	46	255	139	137	29
Pep	252	66	55	48	255	141	138	26

Table S3. Training matrix of ten proteins at the concentration of 0.50 mg·mL<sup>-1</sup>

Рер	249	67	53	44	255	134	141	27
CAT	155	117	159	14	237	105	162	23
CAT	156	118	156	16	238	108	161	20
CAT	160	124	157	14	236	106	168	24
CAT	154	115	158	15	239	110	163	26
CAT	155	117	152	14	237	102	165	22
Ser	255	216	46	35	255	207	148	45
Ser	253	228	48	31	255	201	146	44
Ser	255	218	47	34	255	203	145	46
Ser	255	217	42	36	255	208	148	47
Ser	254	213	45	33	255	202	149	49
HSA	0	255	255	73	255	255	231	100
HSA	1	255	250	79	255	255	234	93
HSA	0	255	254	76	255	255	239	95
HSA	1	255	254	74	254	255	229	98
HSA	0	255	252	72	255	255	226	100
Col	150	74	38	12	171	29	111	15
Col	148	72	36	13	178	32	114	16
Col	153	78	41	13	169	28	113	14
Col	154	76	42	14	175	30	111	17
Col	151	79	43	13	168	32	113	16
Try	212	127	37	20	204	51	129	15
Try	210	136	36	23	199	52	133	17

Try	213	118	42	22	201	56	131	16
Try	219	135	40	24	203	49	134	17
Try	206	135	44	21	208	51	131	16
Lys	0	255	146	20	171	178	176	20
Lys	0	255	137	18	174	181	183	22
Lys	0	255	147	19	173	177	176	23
Lys	0	255	148	21	171	179	183	20
Lys	0	255	135	22	169	180	176	22
Muc	127	111	75	14	166	22	149	15
Muc	131	110	76	13	174	21	141	13
Muc	129	111	82	12	178	21	153	15
Muc	128	107	74	13	175	22	151	12
Muc	124	108	73	13	175	20	150	13
EA	198	255	120	48	255	255	217	76
EA	204	254	113	50	255	255	216	78
EA	194	254	107	47	254	255	213	81
EA	200	254	116	51	255	255	216	82
EA	199	255	115	49	255	255	215	80
Blank control	255	182	31	60	254	101	150	26
Blank control	254	185	33	59	254	99	156	28
Blank control	252	184	31	57	252	102	154	29
Blank control	255	186	32	58	255	113	151	26
Blank control	255	187	37	53	254	93	153	27

Protein	R from G-QDs	G from G-QDs	B from G-QDs	I from G-QDs	R from Y-QDs	G from Y-QDs	B from Y-QDs	I from Y-QDs
Рар	254	141	124	52	255	101	159	30
Рар	252	138	129	53	255	100	163	28
Pap	251	133	125	51	254	107	157	29
Pap	255	143	123	54	254	106	159	27
Рар	254	134	131	52	254	105	160	30
Рер	253	89	62	60	246	54	152	23
Рер	252	91	58	62	245	58	151	20
Рер	251	92	59	58	241	57	154	22
Рер	248	92	57	59	246	56	149	21
Рер	250	88	66	61	237	58	153	20
CAT	156	88	153	17	232	52	121	19
CAT	157	92	166	16	225	49	123	22
CAT	154	93	153	19	224	50	126	21
CAT	150	89	154	18	222	48	119	20
CAT	151	93	160	16	230	46	120	22
Ser	255	181	79	41	255	140	113	29
Ser	253	180	83	39	254	141	116	31
Ser	255	179	78	37	255	144	114	33
Ser	254	175	81	40	255	142	117	31
Ser	255	173	82	36	255	140	115	34
HSA	207	255	255	87	254	255	212	100

Table S4. Training matrix of ten proteins at the concentration of 0.25  $mg{\cdot}mL^{\text{-1}}$ 

<ul> <li>93</li> <li>92</li> <li>95</li> <li>99</li> <li>14</li> <li>12</li> <li>13</li> <li>12</li> <li>14</li> <li>15</li> </ul>
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Muc	145	91	90	17	206	21	141	15
EA	201	187	111	39	254	158	171	40
EA	197	183	109	43	255	156	167	37
EA	198	190	114	41	255	154	174	38
EA	205	185	118	40	255	159	169	39
EA	199	186	109	38	255	164	172	36
Blank control	255	188	78	68	204	25	170	20
Blank control	255	169	61	62	202	23	166	22
Blank control	255	187	64	65	210	30	176	21
Blank control	255	190	62	69	206	32	157	18
Blank control	255	179	68	75	202	27	155	18

Table S5. Training matrix of ten proteins at the concentration of 0.10 mg  $\cdot$  mL<sup>-1</sup>

Ductoin	R from	G from	B from	I from	R from	G from	B from	I from
Frotein	G-QDs	G-QDs	G-QDs	G-QDs	Y-QDs	Y-QDs	Y-QDs	Y-QDs
Рар	255	255	52	62	254	116	151	32
Рар	255	254	49	60	255	115	150	33
Рар	255	255	50	58	254	113	152	30
Pap	255	255	49	63	254	118	151	32
Pap	255	254	51	61	254	114	159	34
Рер	254	221	45	77	255	100	133	24
Рер	254	220	47	79	255	102	139	23
Рер	252	227	49	76	255	104	136	22
Рер	253	224	48	74	255	100	132	21

Рер	254	226	46	77	255	107	136	25
CAT	212	110	133	23	211	41	149	18
CAT	214	112	129	20	210	39	146	17
CAT	206	114	135	21	207	39	141	17
CAT	209	113	134	24	209	37	140	19
CAT	211	115	125	22	217	38	138	17
Ser	228	146	96	49	222	61	144	19
Ser	230	147	99	42	224	58	145	18
Ser	235	137	99	46	220	59	143	17
Ser	236	139	102	43	220	64	145	19
Ser	234	141	97	48	215	57	139	18
HSA	255	227	55	100	255	255	187	68
HSA	255	222	58	99	254	255	184	64
HSA	255	220	57	100	254	255	183	65
HSA	255	219	56	99	255	255	180	67
HSA	255	225	59	100	255	255	179	69
Col	237	104	55	45	157	14	131	12
Col	229	112	56	46	154	13	139	13
Col	230	118	54	45	153	14	135	14
Col	234	113	59	44	152	12	131	15
Col	232	114	53	45	151	14	138	13
Try	199	104	100	35	181	28	152	15
Try	199	103	106	34	182	29	151	14

Try	197	101	104	32	180	28	150	14
Try	195	105	99	33	182	27	149	15
Try	200	99	103	37	179	29	148	16
Lys	79	109	118	10	45	16	174	10
Lys	84	115	119	12	41	18	169	11
Lys	76	108	106	11	38	19	173	12
Lys	80	106	115	12	46	17	169	10
Lys	77	107	114	10	47	16	172	9
Muc	191	108	95	27	193	21	127	16
Muc	188	114	94	28	194	23	130	15
Muc	189	113	91	26	189	20	137	14
Muc	190	117	92	29	191	22	134	15
Muc	181	109	96	24	190	22	139	17
EA	218	120	108	28	226	46	169	18
EA	216	114	112	29	223	42	165	20
EA	214	122	115	27	227	43	166	21
EA	215	117	110	30	226	48	163	19
EA	213	118	113	27	219	51	169	17
Blank control	255	220	53	71	192	19	146	16
Blank control	255	211	51	74	193	23	165	15
Blank control	252	218	54	73	187	17	148	16
Blank control	254	210	51	70	186	25	161	18
Blank control	255	207	52	72	180	16	155	17

### 6. The discrimination of HSA and Muc at various concentrations

Protein	R from	G from	B from	I from	R from	G from	B from	I from
Frotein	G-QDs	G-QDs	G-QDs	G-QDs	Y-QDs	Y-QDs	Y-QDs	Y-QDs
HSA (1.0 mg·mL <sup>-1</sup> )	116	254	221	77	255	253	141	98
HSA (1.0 mg·mL <sup>-1</sup> )	113	255	211	76	254	254	142	95
HSA (1.0 mg·mL <sup>-1</sup> )	117	254	207	81	255	253	145	94
HSA (1.0 mg·mL <sup>-1</sup> )	123	254	219	79	254	254	144	96
HSA (1.0 mg·mL <sup>-1</sup> )	121	255	212	80	255	255	137	98
HSA (0.50 mg·mL <sup>-1</sup> )	1	255	250	72	255	255	233	99
HSA (0.50 mg·mL <sup>-1</sup> )	0	255	255	78	255	255	232	94
HSA (0.50 mg·mL <sup>-1</sup> )	1	255	253	75	254	255	238	96
HSA (0.50 mg·mL <sup>-1</sup> )	0	255	254	76	254	255	228	99
HSA 0.50 mg·mL <sup>-1</sup> )	0	255	254	71	253	255	227	100
HSA (0.25 mg·mL <sup>-1</sup> )	206	254	254	88	254	255	211	101
HSA (0.25 mg·mL <sup>-1</sup> )	205	255	255	92	255	255	210	92
HSA (0.25 mg·mL <sup>-1</sup> )	200	255	251	94	254	255	209	93
HSA (0.25 mg·mL <sup>-1</sup> )	202	254	253	93	254	255	207	96
HSA (0.25 mg·mL <sup>-1</sup> )	196	255	249	92	255	255	211	97
Muc (1.0 mg·mL <sup>-1</sup> )	172	108	126	18	122	7	170	9
Muc (1.0 mg·mL <sup>-1</sup> )	164	107	127	19	124	6	173	8
Muc (1.0 mg·mL <sup>-1</sup> )	166	105	128	17	121	8	165	6
Muc (1.0 mg·mL <sup>-1</sup> )	170	109	121	20	120	5	168	7
Muc (1.0 mg·mL <sup>-1</sup> )	159	105	129	16	122	4	175	8

Table S6. Training matrix of HSA and Muc at different concentrations

Muc (0.50 mg·mL <sup>-1</sup> )	126	110	76	13	167	21	148	13
Muc (0.50 mg·mL <sup>-1</sup> )	130	111	75	14	173	22	142	15
Muc (0.50 mg·mL <sup>-1</sup> )	128	112	81	13	179	21	152	14
Muc (0.50 mg·mL <sup>-1</sup> )	127	106	75	13	176	22	150	13
Muc (0.50 mg·mL <sup>-1</sup> )	123	109	74	13	175	20	151	12
Muc (0.25 mg·mL <sup>-1</sup> )	141	81	95	15	196	18	127	14
Muc (0.25 mg·mL <sup>-1</sup> )	142	82	88	17	202	16	132	15
Muc (0.25 mg·mL <sup>-1</sup>	145	85	86	16	194	15	133	14
Muc (0.25 mg·mL <sup>-1</sup> )	148	82	91	18	192	18	136	16
Muc (0.25 mg·mL <sup>-1</sup> )	144	90	92	18	204	20	140	15
Blank control	255	187	77	67	203	24	171	22
Blank control	255	168	62	63	204	25	167	20
Blank control	255	189	63	64	208	31	175	18
Blank control	255	191	61	68	205	33	158	19
Blank control	255	178	69	76	201	28	154	21

## 7. The detection of the mixtures of proteins



Fig. S9. FL color (A) and intensity (B) variation images of assembled G-QDs (a) and Y-QDs (b) in the presence of the mixtures of Pap and Pep at different concentration levels. The concentration of CdTe QDs is 0.25 mM and all the protein samples are dissolved in PBS buffer (0.01 M, pH=7.4), the UV-light (302 nm) irradiation time is 40 min.

Protein	R from	G from	B from	I from	R from	G from	B from	I from
	G-QDs	G-QDs	G-QDs	G-QDs	Y-QDs	Y-QDs	Y-QDs	Y-QDs
Pap (1.0 mg·mL <sup>-1</sup> )	252	161	64	41	253	72	80	55
Pap (1.0 mg⋅mL <sup>-1</sup> )	251	158	60	40	253	70	79	52
Pap (1.0 mg⋅mL <sup>-1</sup> )	250	158	65	43	252	71	80	54
Pap (1.0 mg·mL <sup>-1</sup> )	251	157	62	42	253	72	74	54
Pap (1.0 mg·mL <sup>-1</sup> )	250	160	63	42	252	68	75	50
Pap (0.5mg·mL <sup>-1</sup> )+Pep (0.5mg·mL <sup>-1</sup> )	255	130	37	38	255	33	32	40
Pap (0.5mg·mL <sup>-1</sup> )+Pep (0.5mg·mL <sup>-1</sup> )	255	131	39	39	255	29	31	44
Pap (0.5mg⋅mL <sup>-1</sup> )+pep (0.5mg⋅mL <sup>-1</sup> )	255	128	36	39	254	31	33	43
Pap $(0.5 \text{mg} \cdot \text{mL}^{-1})$ +pep $(0.5 \text{mg} \cdot \text{mL}^{-1})$	255	130	40	39	254	32	31	44
Pap $(0.5 \text{mg} \cdot \text{mL}^{-1})$ +Pep $(0.5 \text{mg} \cdot \text{mL}^{-1})$	255	128	39	40	255	27	30	38
Pap (0.25mg·mL <sup>-1</sup> )+Pep (0.75mg·mL <sup>-1</sup> )	254	85	20	31	254	27	18	45
Pap (0.25mg·mL <sup>-1</sup> )+Pep (0.75mg·mL <sup>-1</sup> )	255	88	24	31	254	26	19	42

Table S7. Training matrix of the mixtures of Pap and Pep at different concentration levels

Pap (0.25mg·mL <sup>-1</sup> )+Pep (0.75mg·mL <sup>-1</sup> )	254	85	22	30	255	31	23	43
Pap (0.25mg·mL <sup>-1</sup> )+Pep (0.75mg·mL <sup>-1</sup> )	255	88	26	32	254	33	20	46
Pap (0.25mg·mL <sup>-1</sup> )+Pep (0.75mg·mL <sup>-1</sup> )	254	86	24	32	254	25	18	44
Pep (1.0 mg·mL <sup>-1</sup> )	250	87	128	31	253	9	128	43
Pep (1.0 mg·mL <sup>-1</sup> )	250	86	127	30	253	8	127	44
Pep (1.0 mg·mL <sup>-1</sup> )	251	87	125	31	253	7	123	45
Pep (1.0 mg·mL <sup>-1</sup> )	251	88	127	30	253	7	124	40
Pep (1.0 mg·mL <sup>-1</sup> )	250	86	126	32	253	5	127	38
Blank control	255	108	122	38	253	126	31	77
Blank control	255	101	129	33	253	109	37	73
Blank control	254	105	121	35	253	128	28	66
Blank control	255	104	148	40	252	112	40	71
Blank control	243	114	153	38	255	115	44	78

8. The discrimination of thermally denatured proteins



Fig. S10. The FL images of G-QDs (A) and Y-QDs (B) in presence of ten thermally

denatured proteins at the concentration of 1.0 mg·mL<sup>-1</sup>, illuminated under UV-light (302 nm) for 40 min. The concentration of CdTe QDs is 0.25 mM, all the samples are dissolved in PBS buffer (0.01 M, pH=7.4).

Ductoin	R from	G from	B from	I from	R from	G from	B from	I from
riotein	G-QDs	G-QDs	G-QDs	G-QDs	Y-QDs	Y-QDs	Y-QDs	Y-QDs
Pap	217	214	133	25	255	169	171	82
Pap	218	209	139	29	255	171	168	78
Pap	206	200	144	28	255	180	176	80
Pap	214	211	134	26	255	180	164	79
Рар	218	213	132	30	255	182	171	84
Рер	252	255	57	70	255	51	161	33
Pep	253	249	49	67	254	54	164	34
Pep	254	252	47	72	249	49	157	31
Pep	254	255	52	73	255	59	163	38
Pep	250	252	46	69	255	51	169	35
САТ	21	143	180	6	226	125	218	35
CAT	35	145	187	7	231	132	221	37
САТ	29	147	183	6	235	137	214	38
CAT	32	145	183	6	230	130	223	33
CAT	32	142	185	8	228	133	218	32
Ser	197	255	127	60	255	188	175	71
Ser	185	255	124	56	255	183	178	68
Ser	183	253	133	53	255	192	180	64

Table S8. Training matrix of ten thermally denatured proteins at the concentration of  $1.0 \text{ mg} \cdot \text{mL}^{-1}$ 

Ser	193	255	132	55	255	190	185	66
Ser	187	255	134	57	255	186	183	70
HSA	67	255	203	19	255	255	221	99
HSA	70	255	207	20	255	255	226	100
HSA	64	255	203	22	255	255	231	96
HSA	66	255	205	21	255	255	225	98
HSA	67	255	206	20	255	255	226	97
Col	212	151	164	42	173	37	76	17
Col	214	156	160	40	178	42	80	16
Col	215	159	167	43	166	38	82	18
Col	213	152	166	42	169	44	85	16
Col	213	153	168	39	172	40	78	17
Try	231	176	95	94	255	80	118	35
Try	229	171	99	99	254	78	121	37
Try	234	169	108	93	250	82	116	36
Try	228	171	102	92	255	85	119	35
Try	233	175	103	95	252	83	117	39
Lys	140	110	180	10	166	114	175	27
Lys	130	101	189	12	159	111	182	29
Lys	133	102	196	13	156	121	190	25
Lys	136	113	186	12	160	122	188	26
Lys	131	109	188	11	154	125	185	30
Muc	131	125	182	5	132	32	159	16

Muc	128	122	183	4	135	30	152	18
Muc	129	126	174	5	133	37	156	15
Muc	127	120	179	6	133	35	159	17
Muc	123	123	175	5	136	31	155	15
EA	217	255	206	30	255	255	250	77
EA	225	255	212	34	255	255	254	73
EA	212	255	203	33	255	255	252	70
EA	210	255	200	36	255	255	255	76
EA	211	255	201	35	255	255	247	74
Blank control	255	166	175	64	255	164	168	99
Blank control	255	165	168	69	255	171	166	97
Blank control	255	164	172	66	255	166	169	98
Blank control	255	169	179	65	255	171	166	99
Blank control	255	167	167	70	255	169	163	100



Fig. S11. Hierarchical cluster analysis of the sensor of native and thermally denatured proteins at 1.0 mg·mL<sup>-1</sup>. Asterisk (\*) stands for thermally denatured protein.

For further studying the discriminating capability of our senor for native and thermally denatured proteins, hierarchical cluster analysis (HCA) was performed using the euclidean distance to process the raw data. From the results in Fig. S11, it is found that HCA can successfully classify all the protein samples into different categories without any mistake (in five replicates), and the native proteins are quite distant from their corresponding thermally denatured ones. This illustrates that our sensor is rather sensitive for the surface characteristics and 3D spatial conformations of proteins. In order to distinguish the native and denatured proteins more clearly, the raw data were also processed using PCA to generate eight canonical factors (42.777%, 28.220%, 12.051%, 6.195%, 4.765%, 3.550%, 1.670% and 0.772% of the variation), and the first three most significant factors were used to generate a 3D plot (Fig. S12). From Fig. S12, it can be seen that the 20 different protein groups show excellent separation without any overlap, which clearly demonstrates the discriminating capability of our senor for native and thermally denatured proteins.



Fig. S12. Canonical score plot of the corresponding  $\Delta$ RGB and  $\Delta$ I values obtained through the sensor against native and their corresponding thermally denatured proteins at 1.0 mg·mL<sup>-1</sup>. Asterisk (\*) stands for thermally denatured protein.

#### 9. The discrimination of proteins artificially added in human urine



Fig. S13. the FL images of G-QDs (A) and Y-QDs (B) in presence of eight proteins  $(1.0 \text{ mg} \cdot \text{mL}^{-1})$  dissolved in human urine, illuminated under UV-light (302 nm) for 10 min. The concentration of CdTe QDs is 0.25 mM.

Table S9. Training matrix of eight native proteins added in human urine at the concentration of  $1.0 \text{ mg} \cdot \text{mL}^{-1}$ 

Protein	R from	G from	B from	I from	R from	G from	B from	I from
riotein	G-QDs	G-QDs	G-QDs	G-QDs	Y-QDs	Y-QDs	Y-QDs	Y-QDs
Pap	111	178	100	20	99	46	226	27
Pap	113	172	106	25	100	55	219	28
Pap	119	181	94	19	97	53	223	32
Рар	106	175	100	18	94	45	220	30
Pap	123	172	99	20	101	54	221	29
Pep	160	252	83	41	93	81	224	32
Pep	162	254	86	43	98	80	219	34
Pep	159	255	87	40	94	86	224	35
Pep	165	254	85	41	91	87	216	36
Pep	169	254	90	40	99	81	221	34
CAT	64	161	150	7	3	51	216	25

САТ	63	160	149	8	5	55	219	26
CAT	65	159	149	8	6	56	211	24
CAT	67	165	153	7	5	49	213	27
CAT	63	165	147	7	4	52	215	28
Ser	56	229	110	23	97	120	180	37
Ser	60	224	117	20	94	123	183	41
Ser	63	221	113	19	90	120	179	39
Ser	68	222	106	19	91	118	182	41
Ser	59	226	112	20	92	119	183	38
Col	108	250	60	31	205	146	141	66
Col	113	253	65	30	202	144	140	69
Col	100	248	61	33	205	147	145	67
Col	101	249	63	30	206	144	141	64
Col	105	247	66	28	202	143	140	65
Try	210	255	5	64	184	140	152	54
Try	216	255	9	63	179	139	147	56
Try	202	255	5	68	183	141	148	55
Try	215	255	7	69	179	142	147	53
Try	205	255	8	65	180	138	151	57
Lys	143	231	71	33	43	56	228	29
Lys	142	233	66	35	46	51	229	28
Lys	141	229	67	34	41	55	221	27
Lys	145	230	69	37	44	49	226	30

Lys	144	234	70	35	45	52	225	25
Muc	193	243	56	44	148	89	217	33
Muc	192	237	54	46	149	86	218	34
Muc	195	244	61	45	144	85	219	31
Muc	194	232	59	44	149	88	224	37
Muc	188	244	58	49	147	87	227	34
Blank control	168	255	82	58	152	51	238	40
Blank control	167	254	81	55	154	56	236	39
Blank control	180	255	87	59	156	58	239	42
Blank control	182	254	85	55	153	56	233	41
Blank control	174	255	81	53	160	65	242	39