ELECTRONIC SUPPLEMENTARY INFORMATION

Gas sensing and electrochemical properties of tetra and octa 2*H*-chromen-2-one substituted iron(II) phthalocyanines

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Table S1. Elemental analysis, spectral and MALDI-TOF data of coumarin substituted FePcs (**5-8**).

Pcs	Emprical Formula (MALDI-TOF (m/z))	Elemental Analysis (%) Found (Calc.)	UV-vis absorption in DMSO (λnm (logε))	IR Spectral Data (cm^{-1})	Yield (%)
5	$C_{100}H_{64}FeN_8O_{16}$ (1689.67)	C 71.09(69.91); H 3.82 (3.75); N 6.63(6.81)	315 (5.526), 605 (4.883), 669 (5.225)	742, 833, 956, 1083, 1175, 1244, 1366, 1421, 1480, 1511, 1582, 1603, 1723, 2837, 2927, 3000, 3069	7.62
6	$C_{100}H_{64}FeN_8O_{16}$ (1689.63)	C 71.09(70.89); H 3.82 (4.01); N 6.63(6.74)	328 (5.321), 631(5.115)	747, 832, 955, 1080, 1174, 1248, 1366, 1469, 1511, 1595, 1728, 2837, 2929, 3065	9.16
7	$C_{100}H_{64}FeN_8O_{16}$ (1827.26)	C 65.73(65.57); H 3.31 (3.43); N 6.13(5.95)	316 (5.557), 594 (4.739), 631(5.037), 656 (5.125)	744, 838, 897, 1045, 1085, 1178, 1250, 1369, 1410, 1456, 1513, 1604, 1731, 2854, 2926, 3007, 3071	19.66
8	$C_{168}H_{112}FeN_8O_{32}$ (2810.74)	C 71.79(71.61); H,4.02 (3.88); N, 3.99(4.11)	344 (5.243), 595 (4.602), 657 (5.090)	747, 836, 888, 1087, 1178, 1252, 1369, 1398, 1438, 1513, 1599, 1732, 2905, 2956, 2999, 3071	9.60

Tablo S2 The humidity dependence of the sensor parameters for the 60 nm **6** coated film kept at 298 K and exposed to various concentrations of CO_2 gas in air.

	200 ppm CO_2			400 ppm CO_2			600 ppm CO_2			800 ppm CO_2			1000 ppm CO_2		
RH	S $(ppm)^{-1}$	τ_{90} (s)	τ_{10} (s)	S $(ppm)^{-1}$	τ_{90} (s)	τ_{10} (s)	S $(ppm)^{-1}$	τ_{90} (s)	τ_{10} (s)	S $(ppm)^{-1}$	τ_{90} (s)	τ_{10} (s)	S $(ppm)^{-1}$	τ_{90} (s)	τ_{10} (s)
0%	$7.36x10^{-3}$	250	238	$8.30x10^{-3}$	240	215	$9.38x10^{-3}$	185	230	$1.10x10^{-2}$	135	200	$1.12x10^{-2}$	158	180
40%	$6.41x10^{-3}$	230	280	$6.93x10^{-3}$	240	200	$8.38x10^{-3}$	190	340	$8.54x10^{-3}$	140	205	$1.00x10^{-2}$	150	230
50%	$5.76x10^{-3}$	230	240	$6.00x10^{-3}$	220	185	$7.10x10^{-3}$	180	350	$7.85x10^{-3}$	130	180	$8.85x10^{-3}$	145	300
60%	$5.10x10^{-3}$	205	230	$5.23x10^{-3}$	210	210	$6.46x10^{-3}$	160	320	$7.04x10^{-3}$	120	160	$7.30x10^{-3}$	150	280
70%	$4.28x10^{-3}$	220	255	$4.67x10^{-3}$	225	200	$5.42x10^{-3}$	165	325	$6.45x10^{-3}$	125	175	$7.05x10^{-3}$	140	310
80%	$3.85x10^{-3}$	200	245	$4.11x10^{-3}$	215	190	$4.52x10^{-2}$	150	390	$6.14x10^{-3}$	110	140	$6.55x10^{-3}$	130	280

Tablo S3. The humidity dependence of the sensor parameters for the same sensor (60 nm **6** coated sensor) kept at 298 K and exposed to various concentrations of CO gas in N_2.

	200 ppm CO_2			400 ppm CO_2			600 ppm CO_2			800 ppm CO_2			1000 ppm CO_2		
RH	S $(ppm)^{-1}$	τ_{90} (s)	τ_{10} (s)	S $(ppm)^{-1}$	τ_{90} (s)	τ_{10} (s)	S $(ppm)^{-1}$	τ_{90} (s)	τ_{10} (s)	S $(ppm)^{-1}$	τ_{90} (s)	τ_{10} (s)	S $(ppm)^{-1}$	τ_{90} (s)	τ_{10} (s)
0%	1.99×10^{-3}	80	150	5.19×10^{-3}	300	310	5.17×10^{-3}	256	400	5.72×10^{-3}	250	500	6.49×10^{-3}	186	510
40%	2.75×10^{-3}	120	200	5.49×10^{-3}	311	450	5.85×10^{-3}	310	350	6.86×10^{-3}	320	550	8.42×10^{-3}	340	420
50%	3.45×10^{-3}	220	170	6.12×10^{-3}	270	550	7.22×10^{-3}	300	370	8.58×10^{-3}	415	500	9.24×10^{-3}	390	430
60%	3.90×10^{-3}	280	320	7.42×10^{-3}	300	500	9.04×10^{-3}	320	510	1.04×10^{-2}	350	530	1.47×10^{-2}	340	435
70%	3.05×10^{-3}	150	240	4.04×10^{-3}	300	440	6.84×10^{-3}	330	515	1.05×10^{-2}	265	550	9.54×10^{-3}	325	565
80%	4.11×10^{-3}	200	220	9.02×10^{-3}	300	480	1.27×10^{-2}	310	515	1.42×10^{-2}	320	555	1.73×10^{-2}	330	560

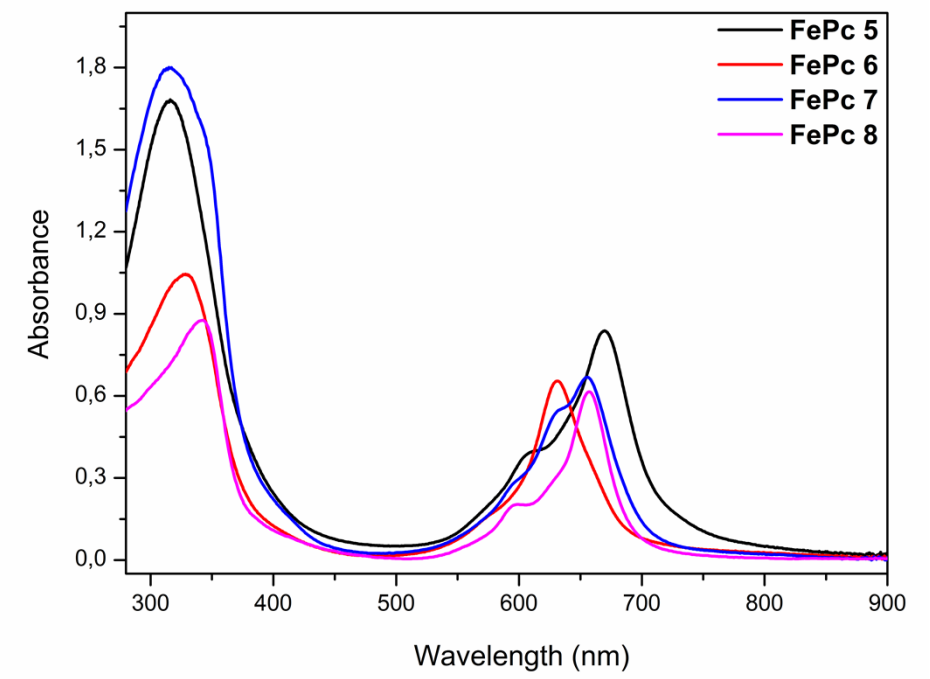

Fig. S1 Electronic absorption spectra of 5.0 x 10^{-6} M **5**, **6**, **7** and **8** in DMSO

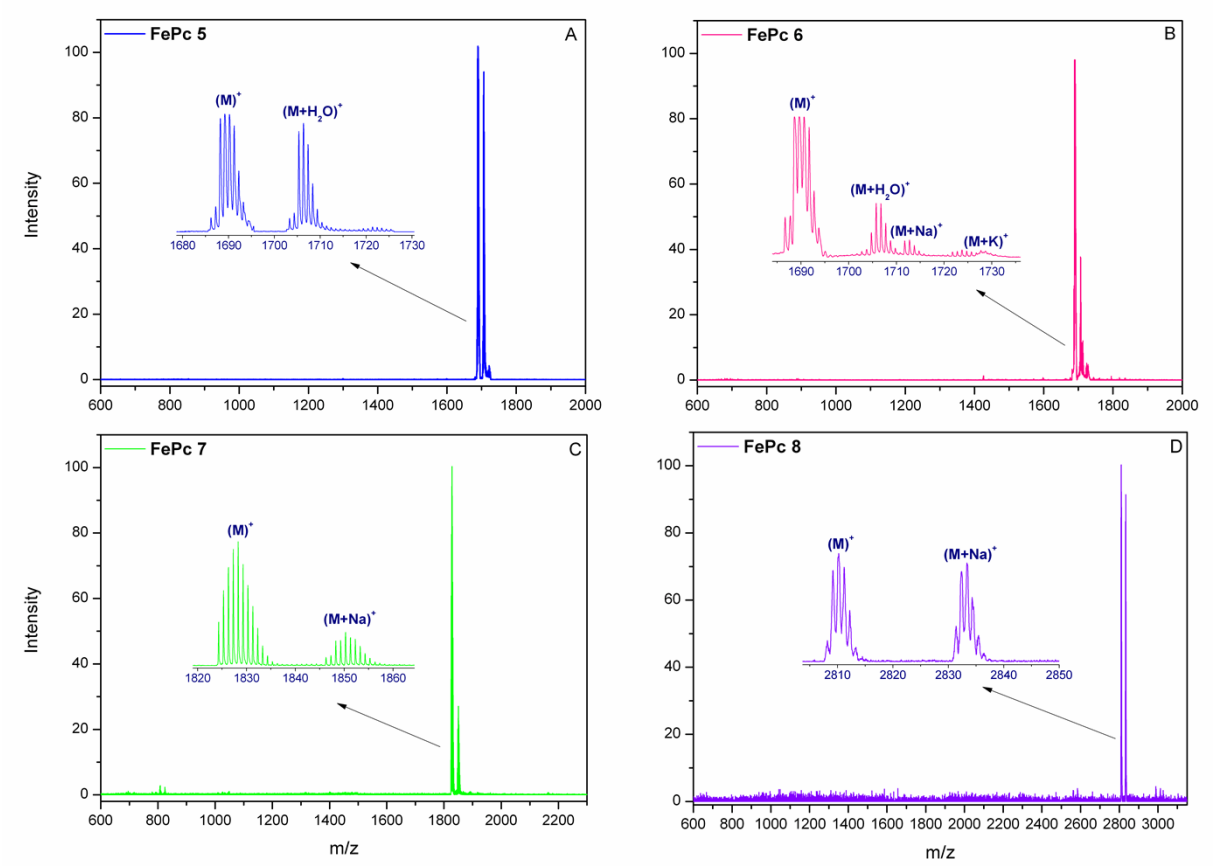

Fig. S2 Positive ion and reflectron mode MALDI-TOF-MS spectrum of (A) **6**, (B) **7**, (C) **8** and (D) **9** in α-cyano-4-hydroxycinnamic acid MALDI matrix using nitrogen laser (at 337 nm wavelength) accumulating 50 laser shots.

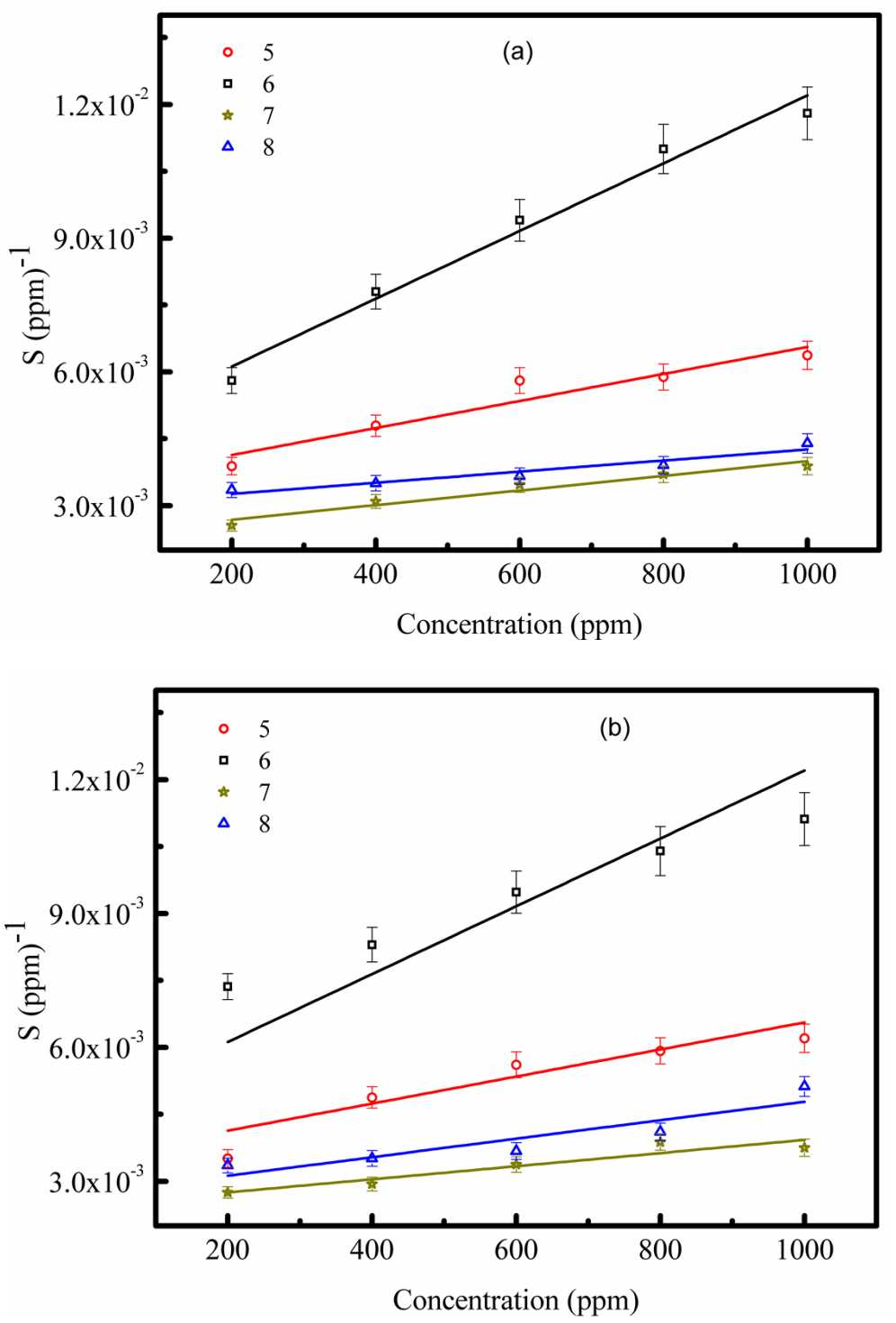

Fig. S3 Concentration dependence of the sensitivity of of the 60 nm **5-8** coated sensors at 298 K in (a) N_2 and (b) air atmosphere.

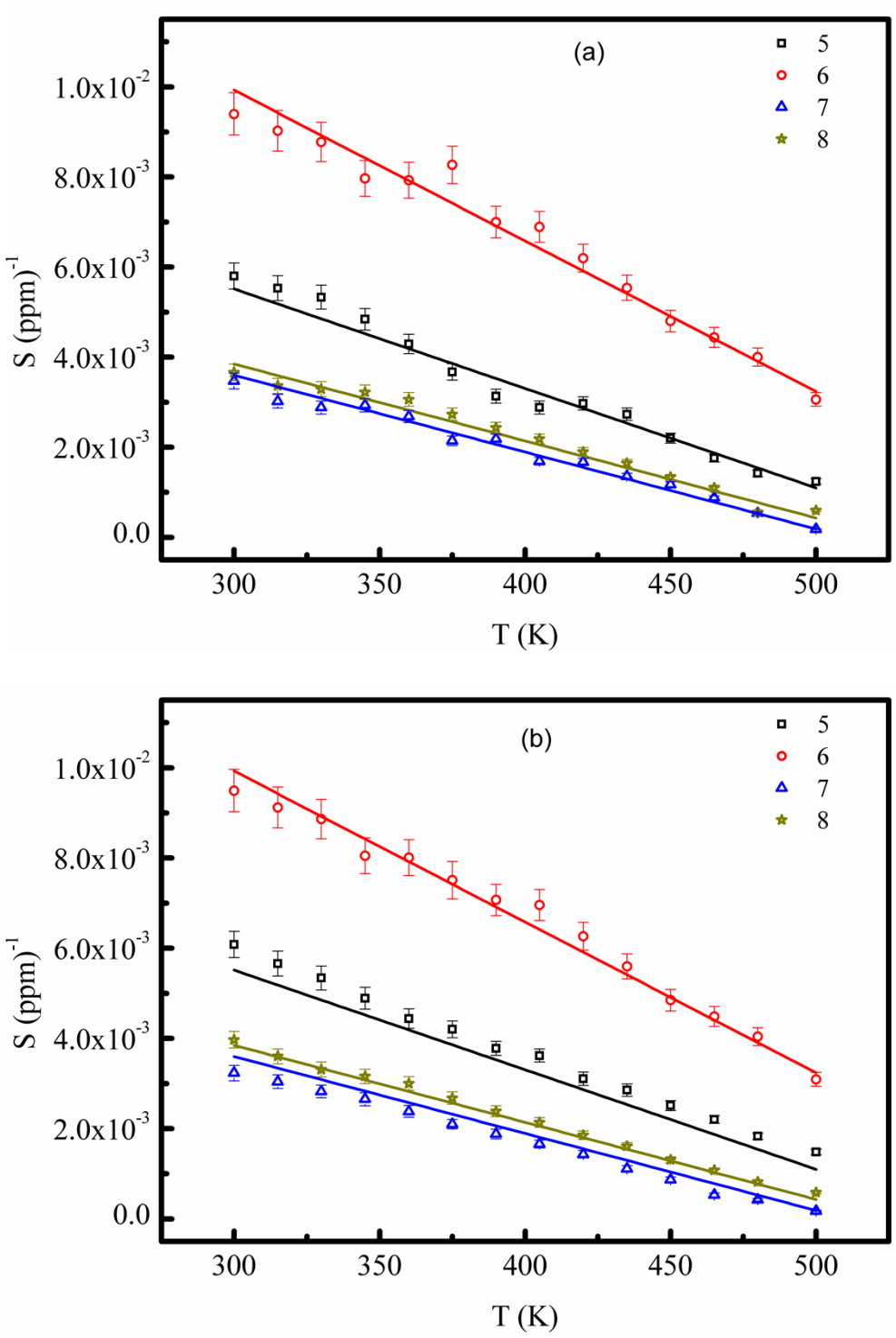

Fig. S4 The effect of the operating temperature on the sensitivity of the sensors for 600 ppm CO_2 (a) in N_2 (b) in air.

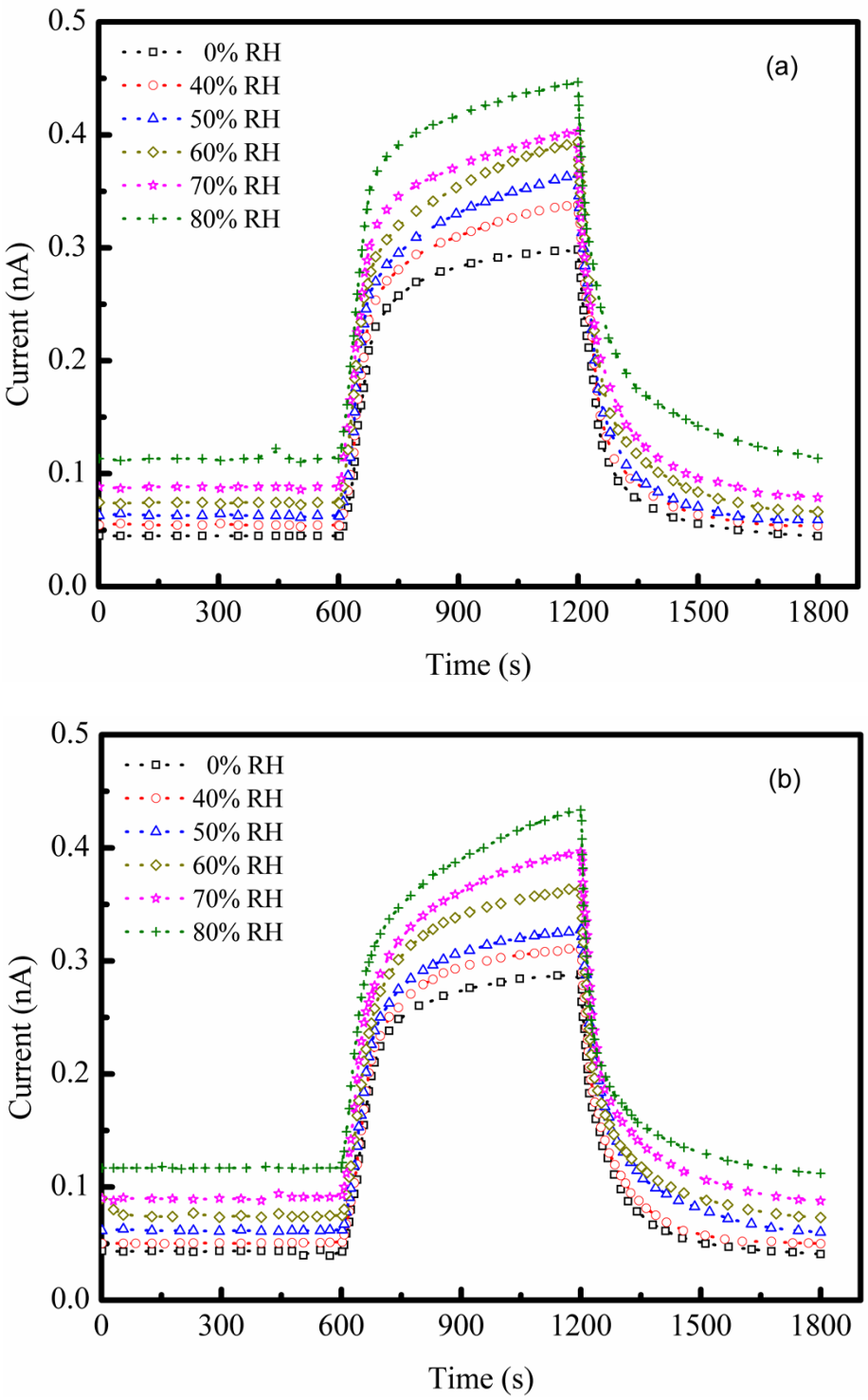

Fig. S5 Variation of the sensor current vs. the time exposition 600 ppm CO_2 gas and varying RH condition for **6** coated sensor at 298 K in (a) N_2 (b) air.