Supporting Information

A Novel Photochemical Sensor Based on Quinoline Functionalized Phenazine Derivatives for Multiple Substrates Detection

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Calculation formula of LOD

Linear Equation: Y= aX + b

$$\delta = \sqrt{\frac{\sum_{i=1}^{N}(F_i - \bar{F})2}{N-1}} \quad (N = 20)$$

$$\text{LOD} = K \times \delta/S \ (K = 3,\ S = a \times 10^6)$$

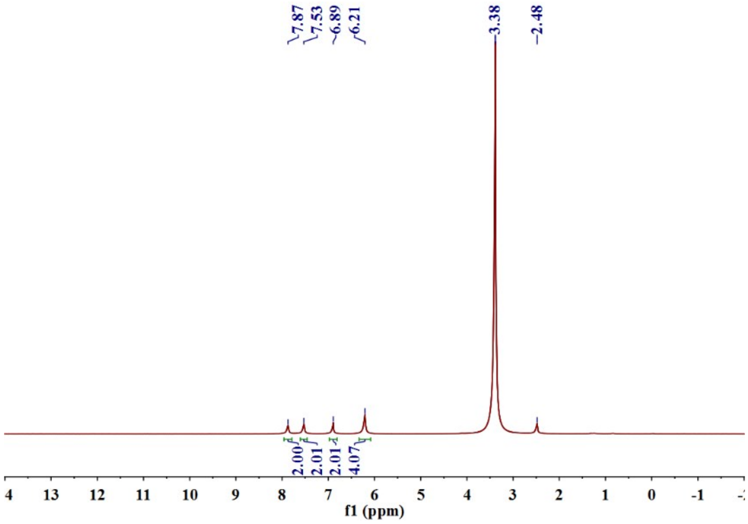

Fig. S1 ^{1}H NMR spectrum of **1** in DMSO-*d*6

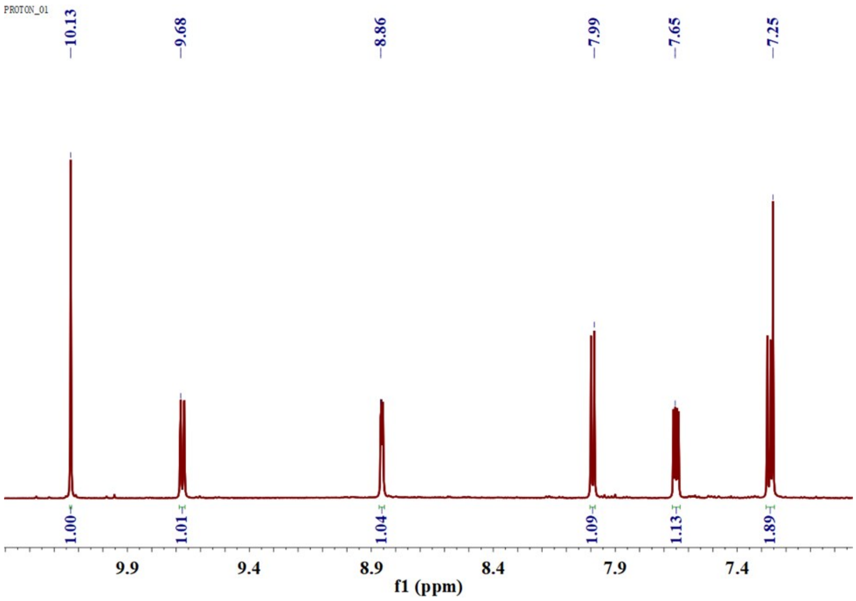

Fig. S2 ^{1}H NMR spectrum of **2** in $CDCl_3$

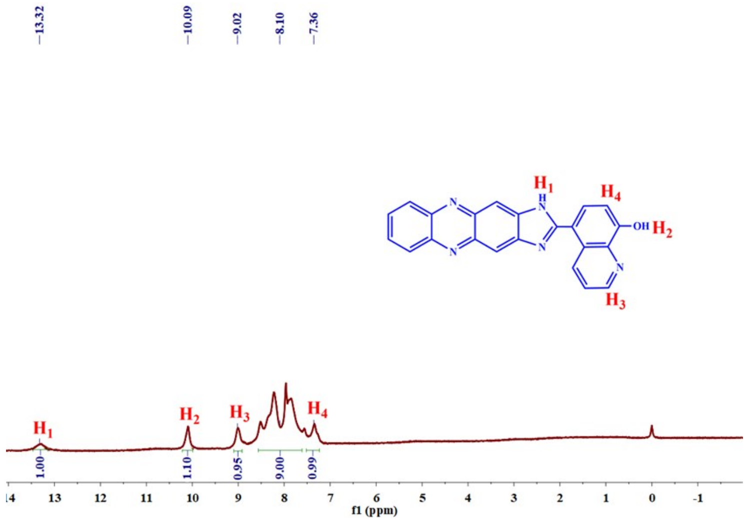

Fig. S3 ^{1}H NMR spectrum of **FQ-5** in DMSO-*d*6

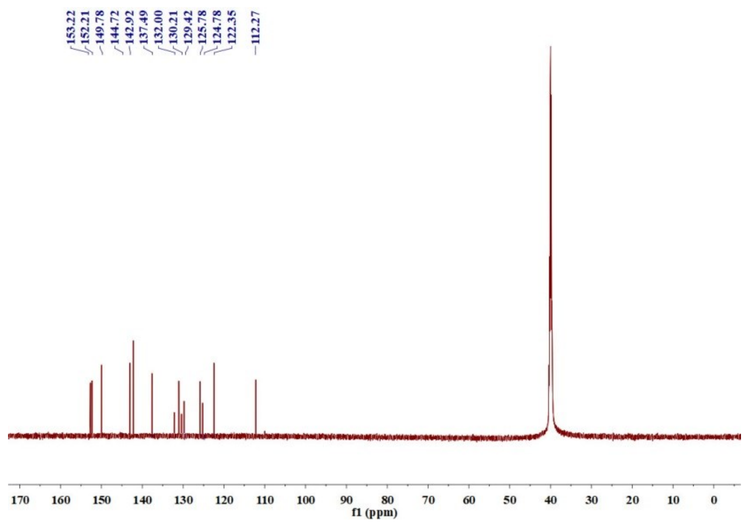

Fig. S4 ^{13}C NMR spectrum of **FQ-5** in DMSO-*d*6

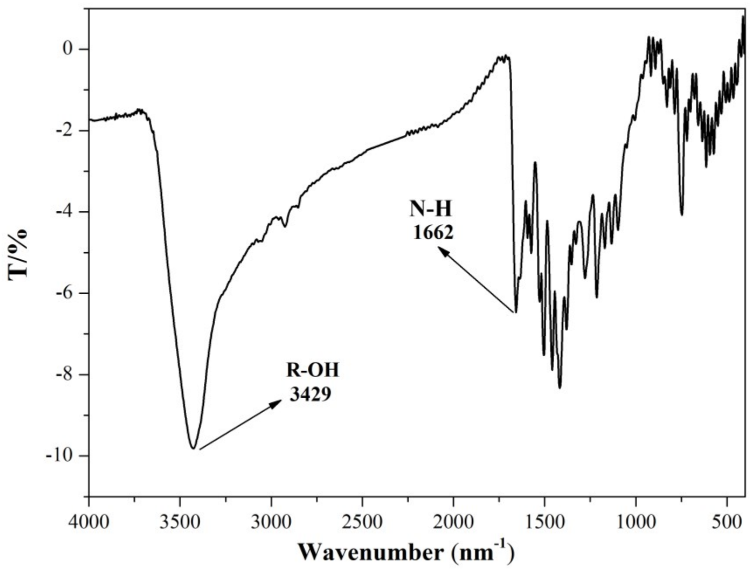

Fig. S5 IR spectrum of **FQ-5** in KBr disks

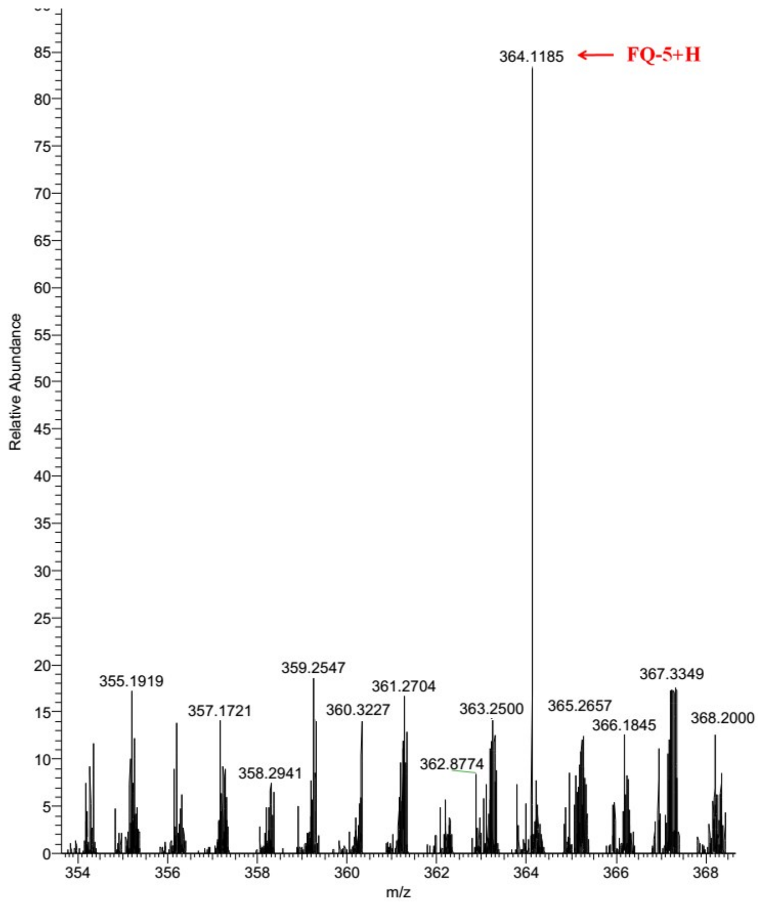

Fig. S6 ESI-MS spectrum of **FQ-5**

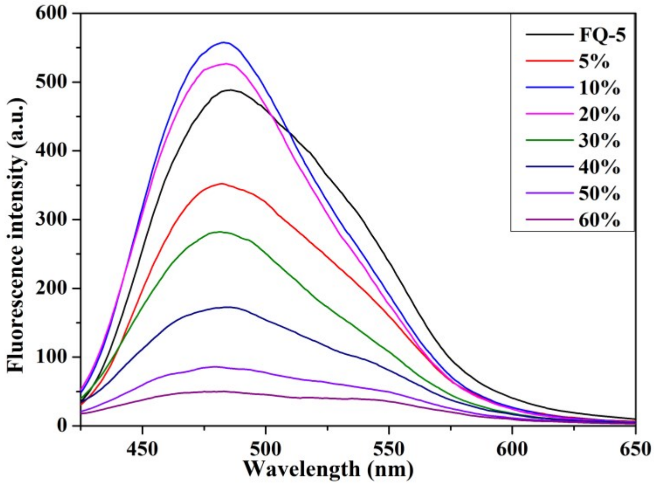

Fig.S7 Fluorescence emission spectra of **FQ-5** at different water ratios.(λ_{ex} = 400 nm, λ_{em}= 490 nm; ex=5nm, em=10nm)

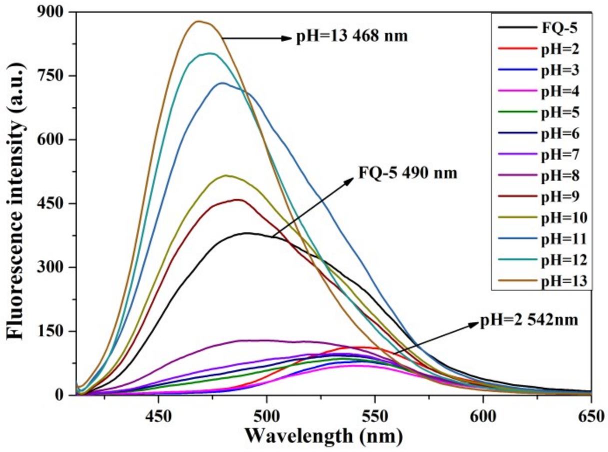

Fig. S8 Fluorescence spectra of **FQ-5** (1.0×10^{-4} M) in various pH values (pH ranged from 2.0 to13.0 DMF/H_2O (9:1, v/v) HEPES buffered solution (λ_{ex} = 400 nm, λ_{em}= 490 nm, ex= 5 nm, em= 10 nm)

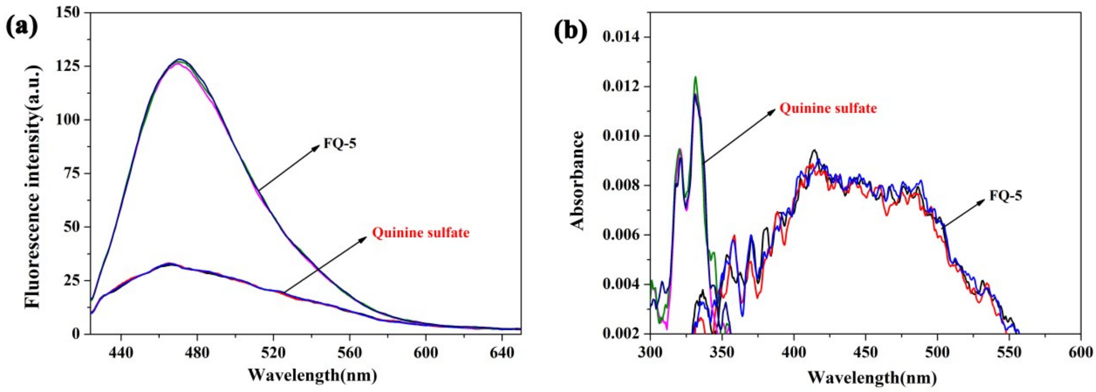

Fig. S9 Fluorescence quantum yield according to the corresponding formula, using quinine sulfate as standard (λ_{ex} = 400 nm; λ_{em}= 490 nm; ex=5 nm; em=10 nm.)

The fluorescence quantum yield of the sample was calculated using quinine sulfate as the standard

(Φ_{std} = 0.55). In this equation, Φ_{unk} and Φ_{std} are the fluorescence quantum yields of the sample and the standard, respectively; I_{unk} and I_{std} are the integral areas of the fluorescent spectra, respectively; A_{unk} and A_{std} are the absorbances of the sample and the standard at the excitation wavelength, respectively.

pH=12, $\Phi_{unk} = \Phi_{std} \times (I_{unk} / I_{std}) \times (A_{std} / A_{unk})$ $\Phi_{std} = 0.55$

I_{unk}:11.10 I_{std}: 10.89 A_{std} :0.013 A_{unk}: 0.009

$\Phi_{unk} =0.55 \times (11.10/10.89) \times (0.013/0.009)=0.809$

Fluorescence quantum yield: 80.9 %

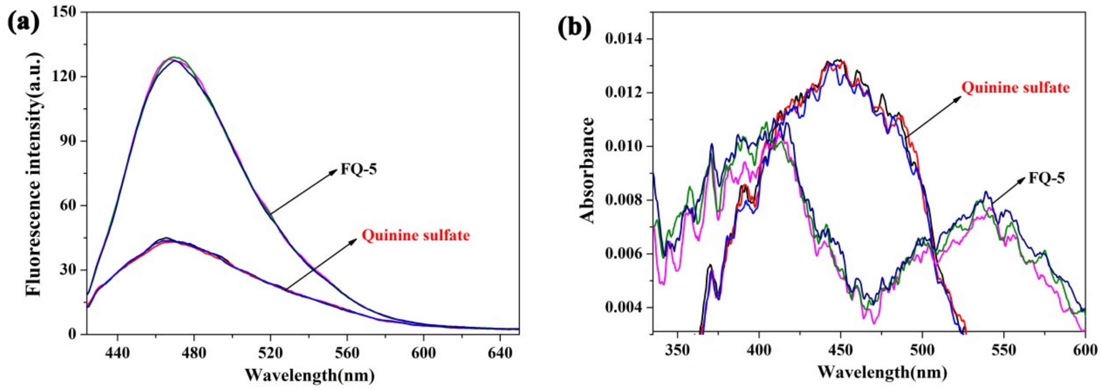

Fig. S10 Fluorescence quantum yield according to the corresponding formula, using quinine sulfate as standard (λ_{ex} = 400 nm; λ_{em}= 490 nm; ex=5 nm; em=10 nm.)

$\Phi_{unk} = \Phi_{std} \times (I_{unk} / I_{std}) \times (A_{std} / A_{unk})$ $\Phi_{std} = 0.55$

I_{unk}:11.11 I_{std}:10.87 A_{std}: 0.014 A_{unk}: 0.010

$\Phi_{unk} =0.55 \times (11.11/10.87) \times (0.014/0.010)=0.77$

Fluorescence quantum yield: 77.0 %

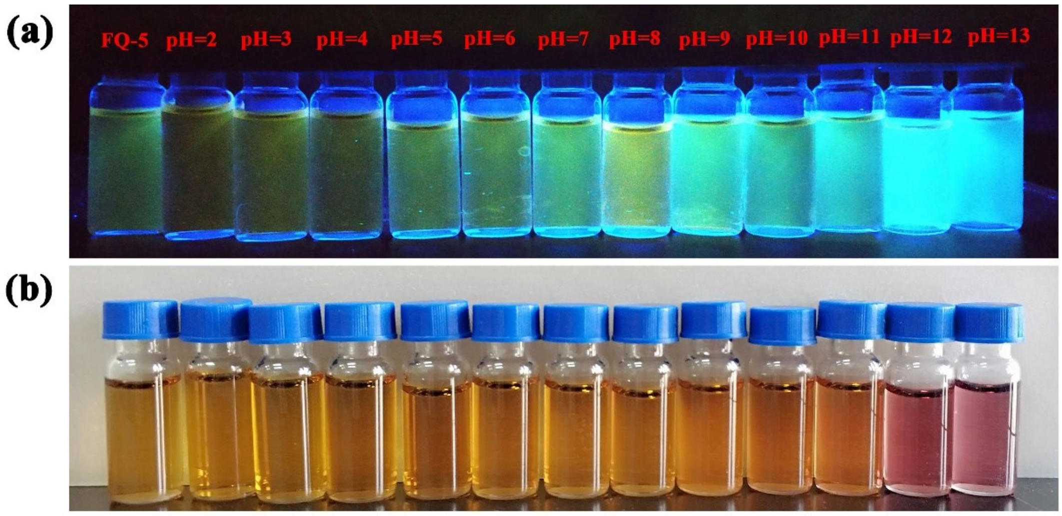

Fig.S11 (a) Photograph of **FQ-5** dispersed in different pH values (pH ranged from 2.0 to 13.0 DMF/H_2O (v/v, 9:1) HEPES buffered solution, $C_{FQ\text{-}5}$ = 1.0 × 10^{-4} M) taken under UV light illumination (λ_{ex} = 365 nm); (b) Photograph of **FQ-5** dispersed in different pH values (pH ranged from 2.0 to 13.0 DMF/H_2O (v/v, 9:1) HEPES buffered solution, $C_{FQ\text{-}5}$ = 1.0 × 10^{-4} M) taken under nature light.

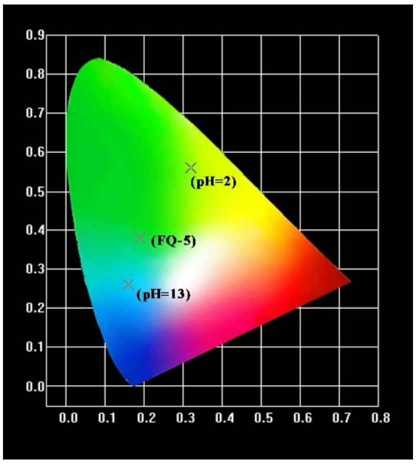

Fig.S12 The Commission Internationale de L'Eclairage (CIE) for **FQ-5**(1.0×10^{-4} M) in pH=2 and pH=13

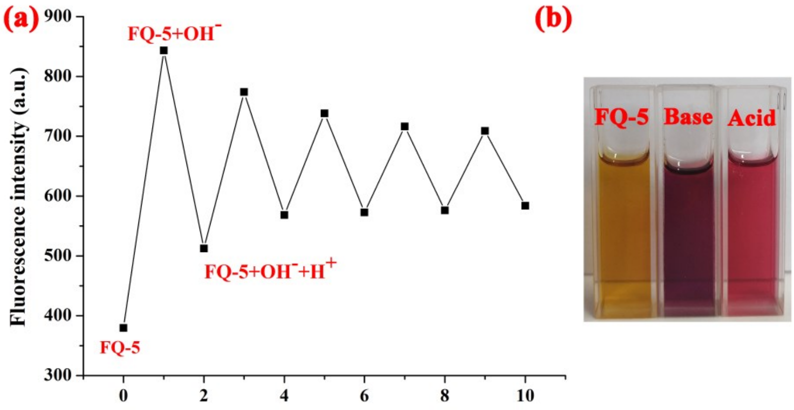

Fig.S13 (a) Fluorescence cycles of **FQ-5** in acid-base transformation; (b) Color changes observed for **FQ-5** upon the addition of acid-base.

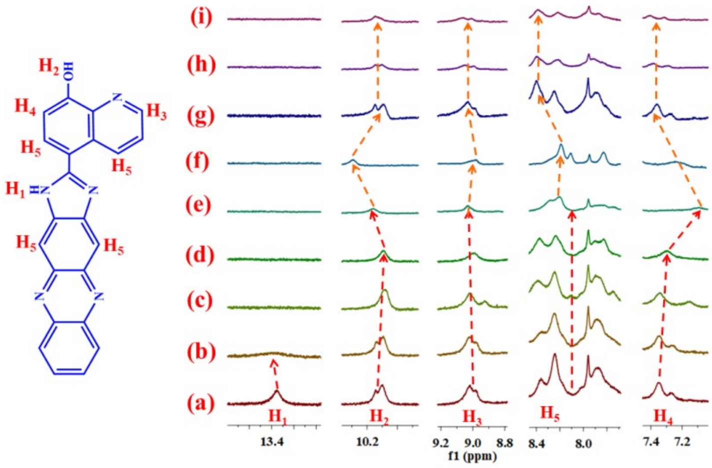

Fig.S14 Partial ^{1}H NMR spectra of **FQ-5** in DMSO-*d*6 with different equiv. of H^+/OH^- (a). FQ-5. (b). 0.5 equiv. OH^-. (c). 1.0 equiv. OH^- (d). 2.0 equiv. OH^- (e). 4.0 equiv. OH^- (f). 0.5 equiv. H^+ (g). 1.0 equiv. H^+ (h). 2.0 equiv. H^+ (i). 4.0 equiv. H^+

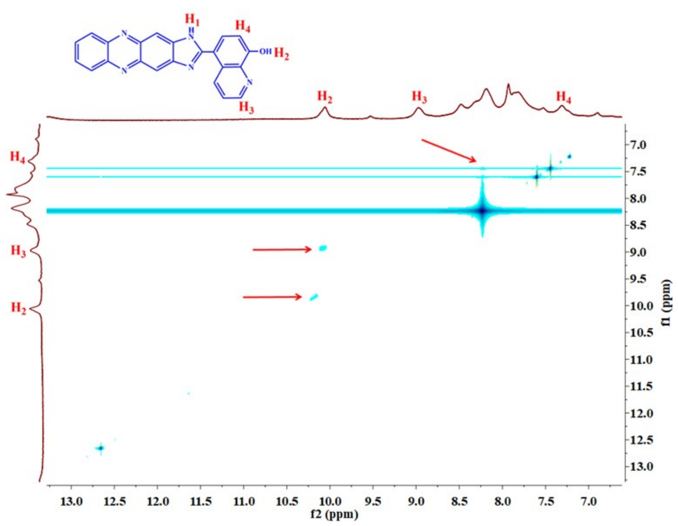

Fig. S15 2D NOESY spectrum of FQ-5 under acidic conditions (5mM) in DMSO-*d*6 solution

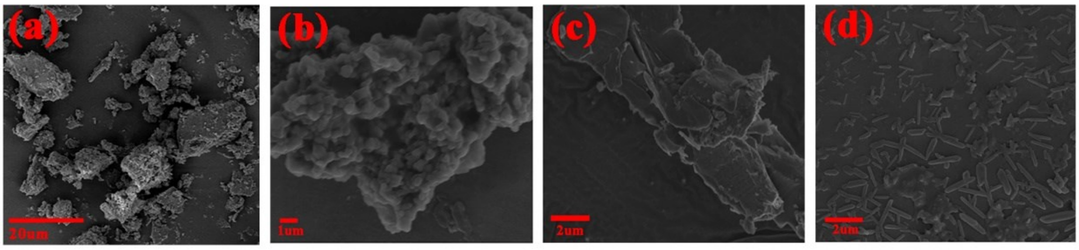

Fig.S16 SEM photos of (a-d) **FQ-5**; **FQ-5 (pH=2)**; **FQ-5 (pH=7)**; **FQ-5 (pH=12)**.

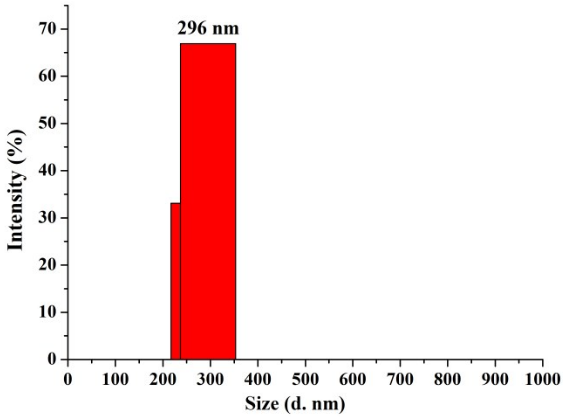

Fig.S17 DLS data of **FQ-5**-based aggregates in pH=2

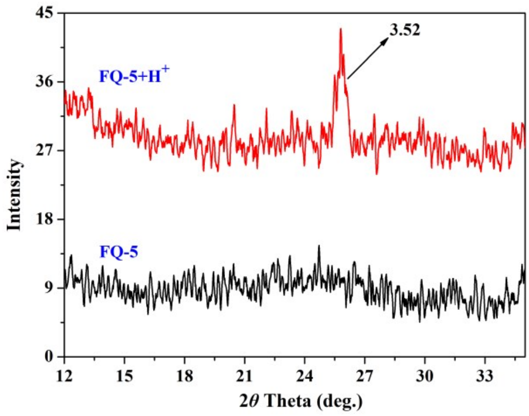

Fig.S18 The powder XRD patterns of the FQ-5 (black), FQ-5 (pH=2) (red)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-7.76825	-0.41479	0.24252
C	-6.63822	-1.15009	0.50378
C	-5.34592	-0.59403	0.24938
C	-5.24879	0.748	-0.28429
C	-6.44779	1.48108	-0.54333
C	-7.67184	0.91313	-0.28632
C	-2.93113	0.58741	-0.28084
C	-3.02778	-0.76685	0.25613
C	-1.85257	-1.52223	0.52021
H	-1.9435	-2.52546	0.9156
C	-0.6328	-0.94176	0.25567
C	-0.55128	0.40603	-0.267
C	-1.65877	1.17121	-0.53993
H	-8.74949	-0.83605	0.43538
H	-6.67985	-2.15695	0.90347
H	-6.34605	2.48365	-0.94314
H	-8.58233	1.46983	-0.4832
H	-1.62283	2.17936	-0.93444
N	-4.04773	1.31515	-0.53966
N	-4.24012	-1.32622	0.50947
N	0.81605	0.64778	-0.39152
N	0.66096	-1.46403	0.41651
C	1.49772	-0.50924	0.02539
H	1.23193	1.43427	-0.86159
C	4.82419	-2.20464	-0.44837
C	5.73124	-1.16772	-0.33389
C	5.27285	0.14984	-0.02924
C	3.87974	0.41748	0.14639
C	2.94976	-0.66273	-0.03823
C	3.45011	-1.9403	-0.30111

H	5.18021	-3.20394	-0.66403
C	3.55649	1.74488	0.55578
H	2.73618	-2.74865	-0.40633
C	4.55275	2.69332	0.69731
C	5.89993	2.33732	0.44478
H	2.53217	2.00338	0.79605
H	4.31517	3.70176	1.01626
H	6.69711	3.06685	0.53876
N	6.25019	1.10001	0.10611
O	7.0745	-1.36668	-0.49237
H	7.52209	-0.49551	-0.34899

Fig.S19 Cartesian coordinates of **FQ-5**

Symbolic Z-matrix:

Charge = 0 Multiplicity = 2

C	-7.76825	-0.41479	0.24252
C	-6.63822	-1.15009	0.50378
C	-5.34592	-0.59403	0.24938
C	-5.24879	0.748	-0.28429
C	-6.44779	1.48108	-0.54333
C	-7.67184	0.91313	-0.28632
C	-2.93113	0.58741	-0.28084
C	-3.02778	-0.76685	0.25613
C	-1.85257	-1.52223	0.52021
H	-1.9435	-2.52546	0.9156
C	-0.6328	-0.94176	0.25567
C	-0.55128	0.40603	-0.267
C	-1.65877	1.17121	-0.53993
H	-8.74949	-0.83605	0.43538
H	-6.67985	-2.15695	0.90347
H	-6.34605	2.48365	-0.94314

H	-8.58233	1.46983	-0.4832
H	-1.62283	2.17936	-0.93444
N	-4.04773	1.31515	-0.53966
N	-4.24012	-1.32622	0.50947
N	0.81605	0.64778	-0.39152
N	0.66096	-1.46403	0.41651
C	1.49772	-0.50924	0.02539
C	4.82419	-2.20464	-0.44837
C	5.73124	-1.16772	-0.33389
C	5.27285	0.14984	-0.02924
C	3.87974	0.41748	0.14639
C	2.94976	-0.66273	-0.03823
C	3.45011	-1.9403	-0.30111
H	5.18021	-3.20394	-0.66403
C	3.55649	1.74488	0.55578
H	2.73618	-2.74865	-0.40633
C	4.55275	2.69332	0.69731
C	5.89993	2.33732	0.44478
H	2.53217	2.00338	0.79605
H	4.31517	3.70176	1.01626
H	6.69711	3.06685	0.53876
N	6.25019	1.10001	0.10611
O	7.0745	-1.36668	-0.49237
H	7.52209	-0.49551	-0.34899

Fig.S20 Cartesian coordinates of **FQ-5** under alkaline conditions

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-6.48188	-4.99486	5.56349
C	-5.17085	-4.79099	5.90756

C	-4.29903	-4.08257	5.02604
C	-4.81904	-3.58772	3.77259
C	-6.18973	-3.81973	3.44974
C	-6.99678	-4.50399	4.32158
C	-2.73303	-2.70899	3.24675
C	-2.20627	-3.20854	4.51254
C	-0.84578	-2.99442	4.85765
H	-0.47178	-3.37449	5.79548
C	-0.04862	-2.30929	3.97215
C	-0.585	-1.81307	2.72387
C	-1.8911	-1.99715	2.34779
H	-7.14196	-5.53111	6.23205
H	-4.75257	-5.14859	6.83758
H	-6.54954	-3.43603	2.50578
H	-8.03582	-4.67864	4.07642
H	-2.31605	-1.63811	1.4222
N	-4.0305	-2.91193	2.90526
N	-3.00766	-3.88707	5.37519
N	0.49367	-1.18028	2.11181
N	1.30993	-1.97435	4.06617
C	1.6097	-1.31028	2.95066
H	0.51006	-0.81125	1.17849
C	5.34268	-1.28683	2.86652
C	5.61556	-0.18818	2.04893
C	4.58543	0.57018	1.49111
C	3.21494	0.28771	1.78167
C	2.95091	-0.8496	2.61393
C	4.01908	-1.60293	3.14148
H	6.15001	-1.87697	3.28116
C	2.2474	1.21937	1.29361

H	3.77602	-2.44467	3.77187
C	2.62575	2.23324	0.38051
C	3.94495	2.44439	0.07972
H	1.20983	1.1199	1.56229
H	1.8758	2.88074	-0.04741
H	4.29711	3.20232	-0.59926
N	4.90838	1.64377	0.66576
O	6.91114	0.24553	1.71953
H	7.59425	-0.36781	2.03301
H	5.93866	1.81745	0.39491
H	1.72401	-2.37329	4.97962

Fig.S21 Cartesian coordinates of **FQ-5** under acidic conditions

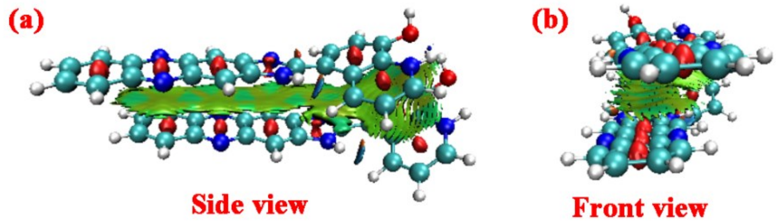

Fig. S22 The NCI graph dimers of **FQ-5** under acidic conditions

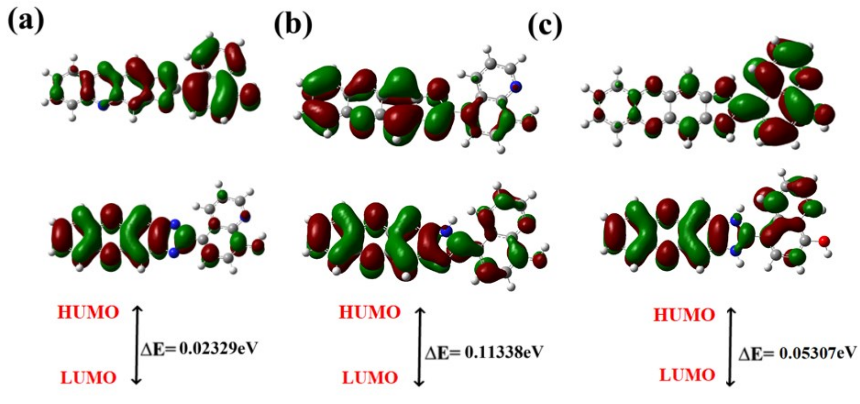

Fig.S23 The HOMO-LUMO energy gaps for (a) Alkaline; (b) **FQ-5** (Neutral) and (c) Acidic conditions.

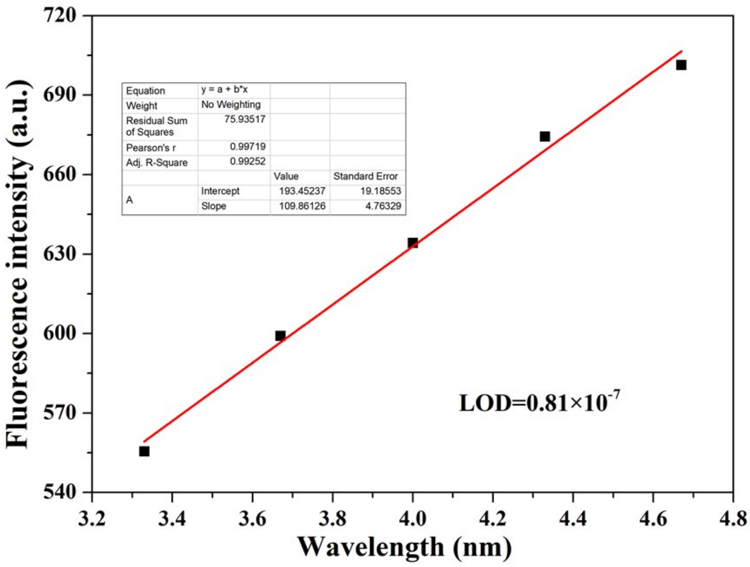

Fig. S24 Photograph of the linear range for L-Arg

The result of the analysis as follows:

Linear Equation: Y = 109.86X + 193.45, R^2 = 0.9925,

S = 109.86×10^6

LOD = K × δ/S =0.81×10^{-7} M (K = 3)

LOD=0.81×10^{-7} M

Table S1

Comparison of detection limit of sensor for L-Arg with previously reported L-Arg sensors

No	Journal, Year, Volume, Page	LOD (M)	Solvent	Ref.
1	*Sens. Actuators B: Chem.*, 2014, 192, 496-502	2.3 × 10^{-6}	CH_3OH/Tris buffer (pH=7)	57(a)
2	*Chem. Commun.*, 2011, 47, 3921-3923	2.0 × 10^{-6}	HEPES (pH=7.4)	57(b)
3	*Biosens. Bioelectron.*,2017, 87, 772-778	3.4 × 10^{-8}	Phosphate buffer (pH=7.4)	57(c)
4	*Macromol. Res.*, 2012, 20, 344-346	1.0 × 10^{-5}	Water	57(d)

5	*Talanta,* 2012, 97, 16-22	2.3 × 10^{-6}	CH_3COOH-CH_3COONa buffer(pH=6.0)	58(a)
6	*New J. Chem*., 2020, 44, 4842-4849	1.5 × 10^{-7}	Tris/HCl buffer (pH=4.0)	58(b)
7	*New J. Chem*., 2017, 41, 15216-15228	2.85 ×10^{-8}	pH 7.4 adjusted solution	58(c)
8	*Langmuir*, 2014, 30, 15364-1537	1.7 × 10^{-7}	HEPES buffe (pH=7.4)	58(d)
	This work	8.1 × 10^{-8}	DMF/Tris HEPES (pH=7.4)	

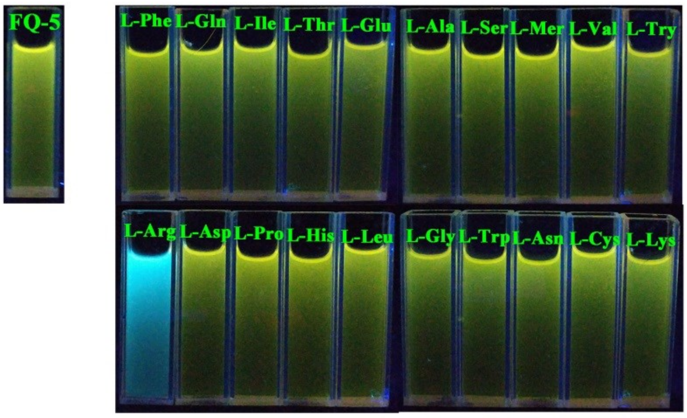

Fig. S25 Photograph of **FQ-5** dispersed in different amino acids (pH =7 DMF/H_2O (v/v, 9:1) HEPES buffered solution, $C_{FQ\text{-}5}$ = 1.0 × 10^{-4} M) taken under UV light illumination (λ_{ex} = 365 nm)

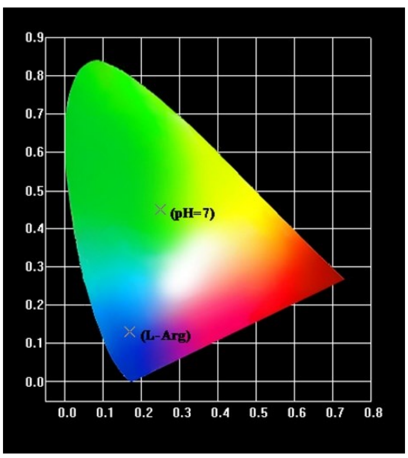

Fig. S26 The Commission Internationale de L'Eclairage (CIE) for **FQ-5** (1.0×10^{-4} M) in DMF/H_2O (9:1, v/v) binary solution

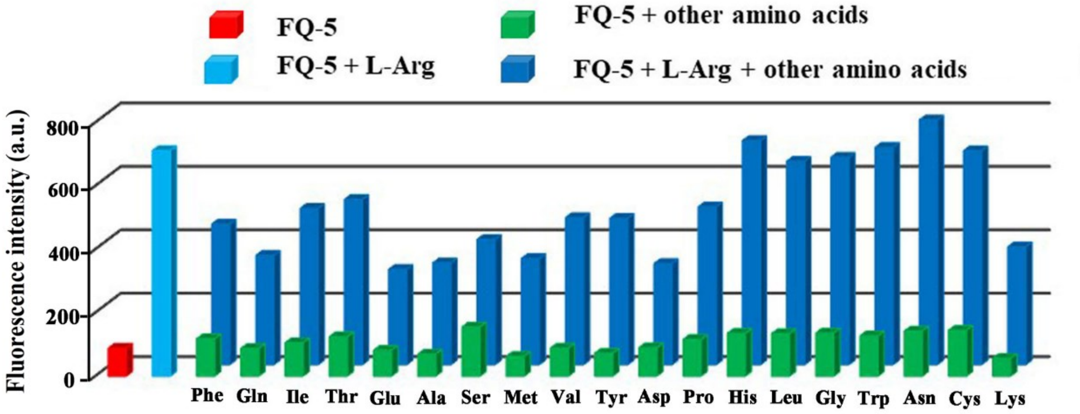

Fig. S27 Fluorescence intensity of **FQ-5** (1×10^{-4} M) and L-Arg (6 equiv.) in the presence of an excess (6 equiv.) of various other amino acids.

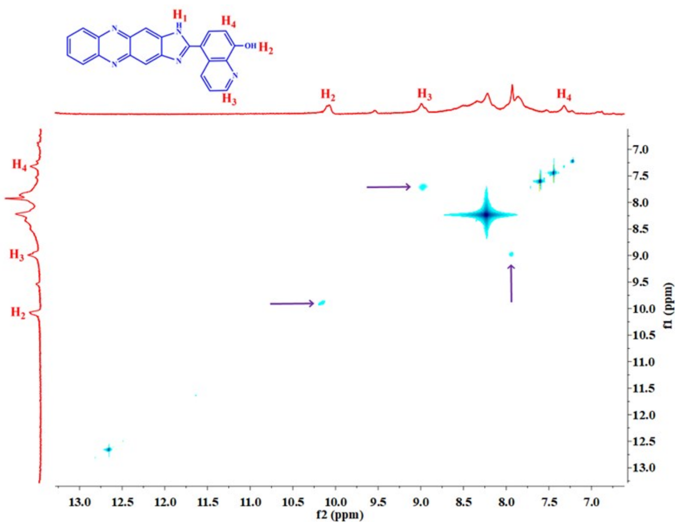

Fig.S28 2D NOESY spectrum of **L-Arg+FQ-5**

Symbolic Z-matrix:

Charge = 0 Multiplicity = 2

C	-7.18342	0.16431	-5.10334
C	-5.89692	0.555	-5.36682
C	-4.80093	-0.12491	-4.75364

C	-5.06959	-1.2255	-3.85634
C	-6.42364	-1.60212	-3.60674
C	-7.4493	-0.92538	-4.21359
C	-2.78901	-1.51201	-3.51624
C	-2.51684	-0.40078	-4.4201
C	-1.17988	-0.00136	-4.68464
H	-0.99578	0.82447	-5.35352
C	-0.16279	-0.68886	-4.06925
C	-0.44528	-1.79473	-3.18271
C	-1.71902	-2.21356	-2.89528
H	-8.01332	0.67908	-5.56777
H	-5.66346	1.37318	-6.0325
H	-6.59365	-2.42811	-2.93144
H	-8.4749	-1.2113	-4.0238
H	-1.95838	-3.03399	-2.2353
N	-4.06358	-1.89923	-3.25428
N	-3.53608	0.26849	-5.01984
N	0.81087	-2.23784	-2.77104
N	1.22633	-0.49531	-4.15364
C	1.77734	-1.41986	-3.37822
H	0.98461	-2.89811	-2.03545
C	5.33551	-0.3407	-2.80641

C	5.98455	-1.52281	-2.51904
C	5.27121	-2.75594	-2.56233
C	3.88101	-2.78411	-2.88543
C	3.21179	-1.53576	-3.12098
C	3.96114	-0.3605	-3.10177
H	5.88769	0.58633	-2.78756
C	3.3043	-4.08155	-3.00557
H	3.44827	0.56572	-3.31433
C	4.06179	-5.20678	-2.75406
C	5.4199	-5.06902	-2.38543
H	2.28045	-4.18899	-3.33127
H	3.63237	-6.19327	-2.85269
H	6.03247	-5.93348	-2.17171
N	6.0109	-3.8816	-2.30571
O	7.31598	-1.55199	-2.20198
H	7.57038	-2.4908	-2.05473
N	-2.31987	-1.14258	0.50968
H	-2.96721	-1.34671	-0.22468
C	-1.32805	-0.10119	0.33248
H	-1.46594	0.66603	1.09435
C	0.08476	-0.66192	0.45566
C	-1.45326	0.54709	-1.03885

H	0.2161	-1.10356	1.44348
H	0.24106	-1.42513	-0.30669
C	1.09656	0.46278	0.26344
O	-2.31511	0.17107	-1.83022
O	-0.69404	1.45449	-1.3715
H	0.96614	0.90463	-0.72441
H	0.94118	1.22621	1.02576
C	2.50938	-0.09795	0.38662
H	2.64071	-0.53959	1.37444
H	2.66567	-0.86116	-0.37573
N	3.52053	0.96746	0.20528
H	3.20176	1.90924	0.0277
C	4.82979	0.74137	0.2655
N	5.3258	-0.47109	0.49535
N	5.65037	1.77283	0.08768
H	4.69988	-1.25224	0.62995
H	6.32612	-0.60509	0.53424
H	5.27043	2.69226	-0.08667
H	6.6497	1.63196	0.12782
H	-2.35701	-1.65715	1.36632
H	-1.55229	-1.62247	0.08479
C	-6.51253	0.51321	3.10079

C	-5.30286	0.14077	3.62531
C	-4.14126	0.93589	3.38466
C	-4.26213	2.13288	2.58389
C	-5.53958	2.48701	2.05446
C	-6.63177	1.69853	2.3067
C	-1.99166	2.54776	2.85159
C	-1.86823	1.3395	3.65829
C	-0.60934	0.96019	4.19523
H	-0.53453	0.06194	4.78753
C	0.47586	1.76012	3.93391
C	0.33865	2.96042	3.14071
C	-0.85485	3.36434	2.59958
H	-7.39215	-0.08882	3.28314
H	-5.18	-0.74761	4.22759
H	-5.59922	3.3868	1.45946
H	-7.59922	1.96749	1.90506
H	-0.98495	4.25399	2.00161
N	-3.18991	2.91702	2.33107
N	-2.95302	0.55959	3.90615
N	1.62337	3.5008	3.10568
N	1.81427	1.61021	4.33444
C	2.47013	2.6481	3.83213

H	1.92246	4.25732	2.51792
C	6.12713	1.78867	4.0317
C	6.74339	3.02196	4.05323
C	5.95754	4.21093	4.06347
C	4.53185	4.1439	4.0354
C	3.91301	2.85097	3.95131
C	4.724	1.71757	3.97986
H	6.73005	0.89366	4.04108
C	3.8555	5.39179	4.16076
H	4.23997	0.75273	3.9498
C	4.57211	6.56818	4.23682
C	5.98513	6.53132	4.20037
H	2.77856	5.41691	4.23464
H	4.0649	7.51638	4.34138
H	6.57024	7.43891	4.24663
N	6.65809	5.38772	4.1303
O	8.10677	3.14277	4.07934
H	8.32397	4.10175	4.11008

Fig.S29 Cartesian coordinates of **FQ-5**+L-Arg

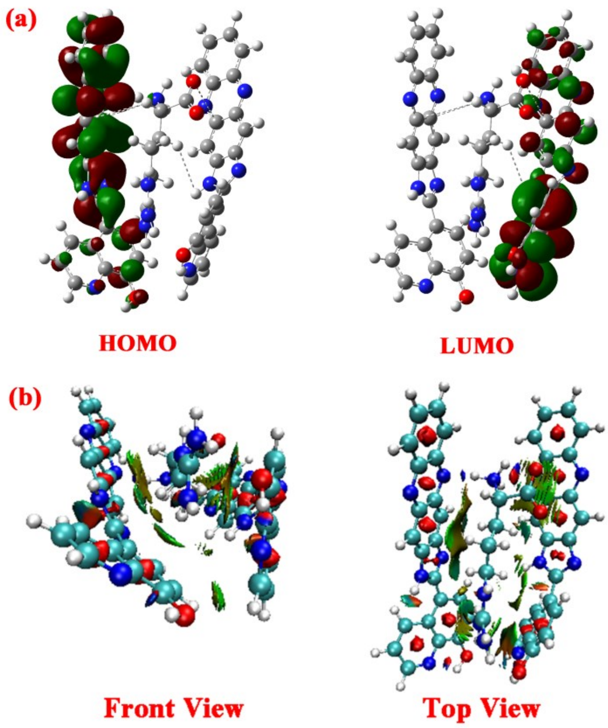

Fig.S30 (a) The HOMO-LUMO energy gaps for **FQ-5+L-Arg**, (b) The NCI graph of **FQ-5+L-Arg**.

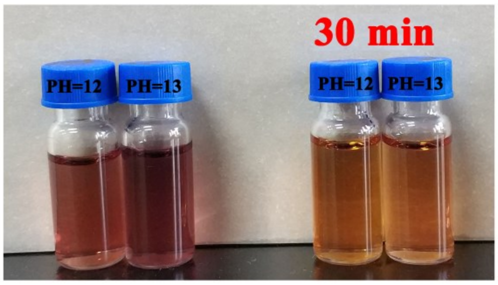

Fig. S31 UV-Vis Photos of = 12/13 solution before and after being placed in the air for 30 min

Fig. S32 Carbon dioxide reactor, please refer to the multimedia file for details

Equipment: Three-necked flask, constant pressure funnel, catheter, HCl (dilute), $CaCO_3$, beaker, magneton, stirrer, FQ-5(1.0 × 10^{-4} M, DMF/H_2O (9:1, v/v)) and HEPES buffered solution (pH=12/13)

Describe: First, we designed a carbon dioxide reactor through chemical reactions: $CaCO_3$+2HCl (dilute) =$CaCl_2$+CO_2+H_2O. A small amount of $CaCO_3$ is placed in a three-necked flask with one end sealed and the other end inserted into a catheter. In addition, pour a little into HCl (dilute) the constant pressure funnel. Then, the funnel pistons and stirrer were opened to allow the reaction to take place, and the catheter was passed into **FQ-5** with pH 12/13, and it was obvious that the solution changed from purple to orange.

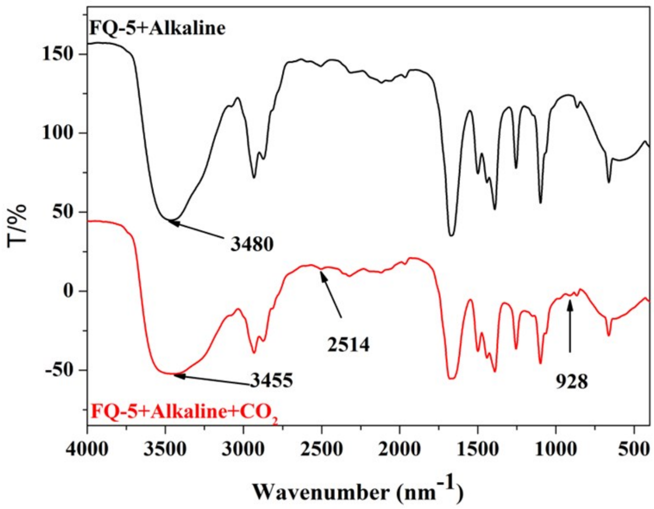

Fig. S33 FT-IR spectroscopy of powder **FQ-5-OH** and **FQ-5-OH** +CO_2

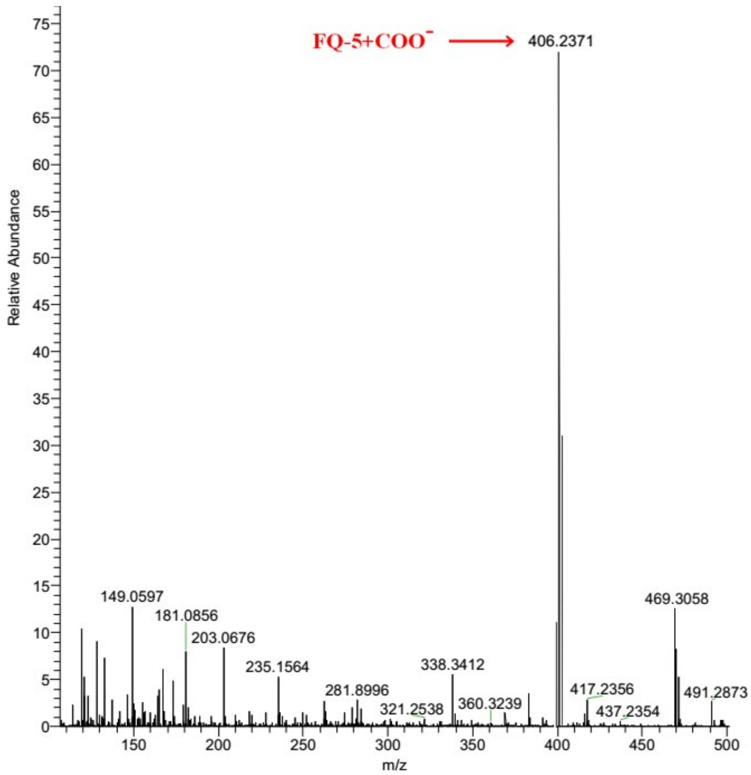

Fig. S34 ESI-MS spectrum of **FQ-5**+COO^-