Electronic Supplementary Information for

Imaging of lysosomal pH changes with a novel quinoline/ benzothiazole probe

Li Fan *, Ming Nan, Jinyin Ge, Xiaodong, Wang, Bo Lin, Wenjia Zhang, Shaomin Shuang, Chuan Dong *

Institute of Environmental Science, College of Chemistry and Chemical Engineering, Shanxi University, Taiyuan 030006, China

E-mail: fanli128@sxu.edu.cn; dc@ sxu.edu.cn

We submit our manuscript to ***New Journal of chemistry***.

Table of Contents

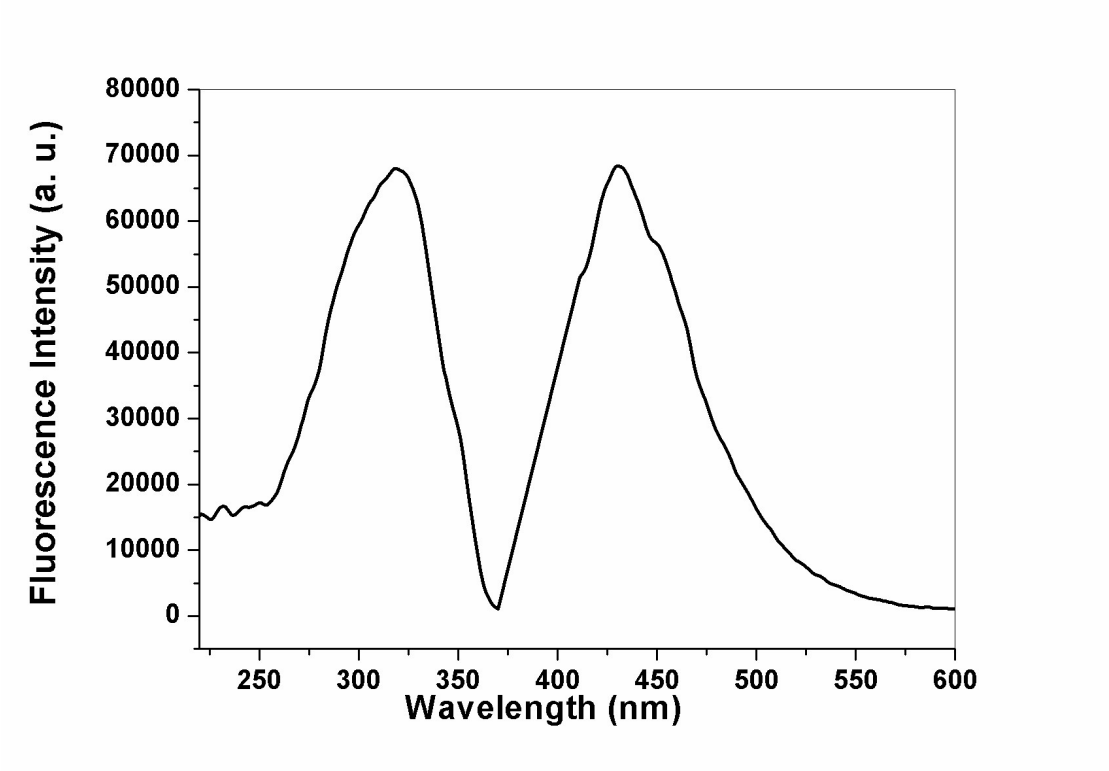


Fig. S1 The excitation and emission spectra of **BTVQ.**

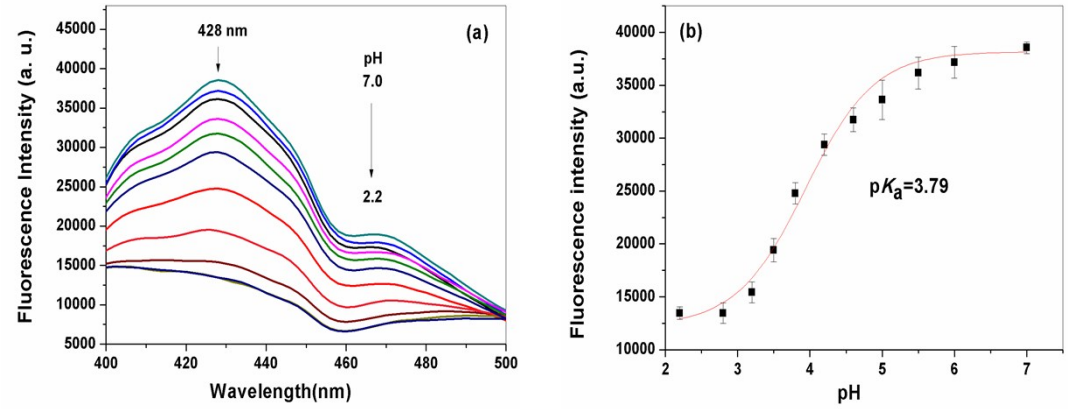


Fig. S2 (a) Changes of the fluorescent emissionspectra of **BTVQ** (5 μM) in ethanol/DMEM (1/4, v/v) medium with pH decreasing from 7.0 to 1.2. (b) Sigmoidal fittings of the pH-dependent fluorescent emission at 428 nm in the ethanol/DMEM (1/4, v/v) medium.

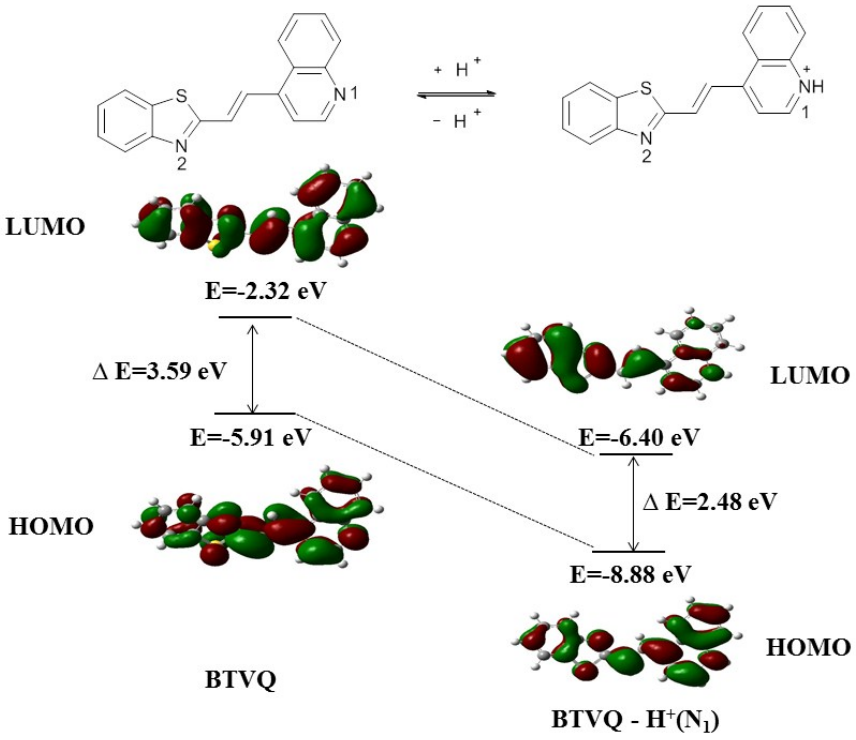


Fig. S3 Calculated HOMO and LUMO distributions of **BTVQ** and thire protonated products.

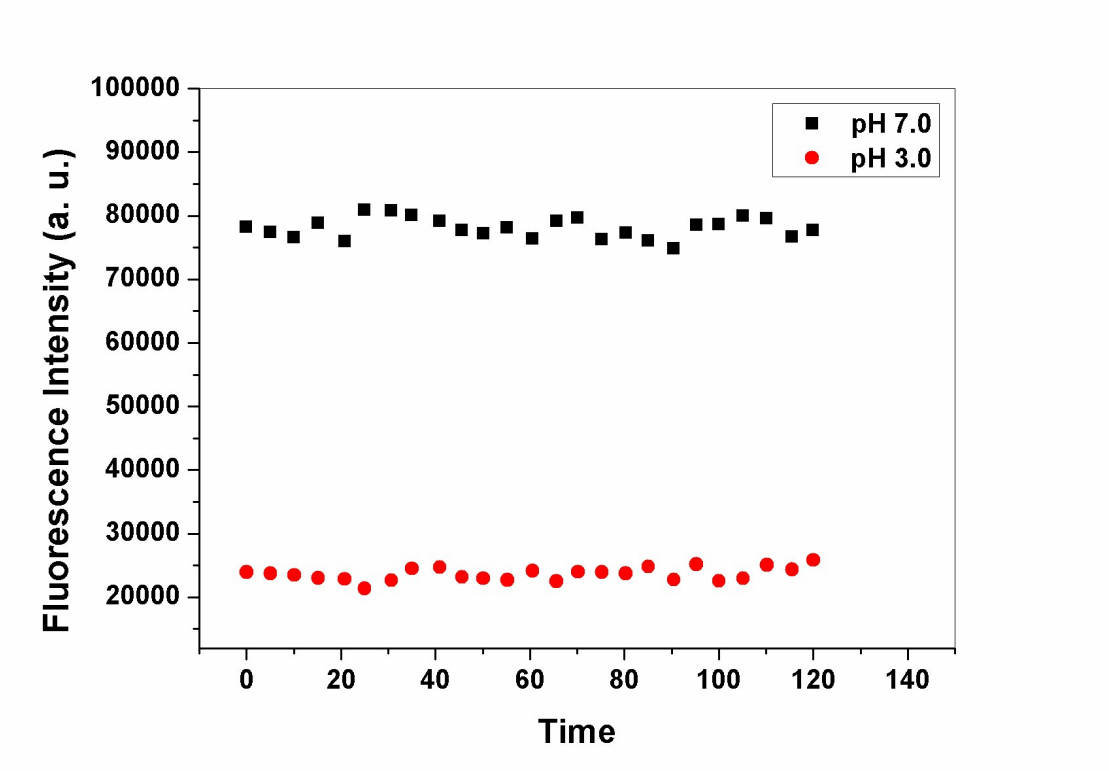


Fig. S4 Changes in fluorescence emission for **BTVQ** with times at pH 7.0 and 3.0, respectively. λ_{ex} = 318 nm. Excitation and emission bandwidths were both set at 2 nm.

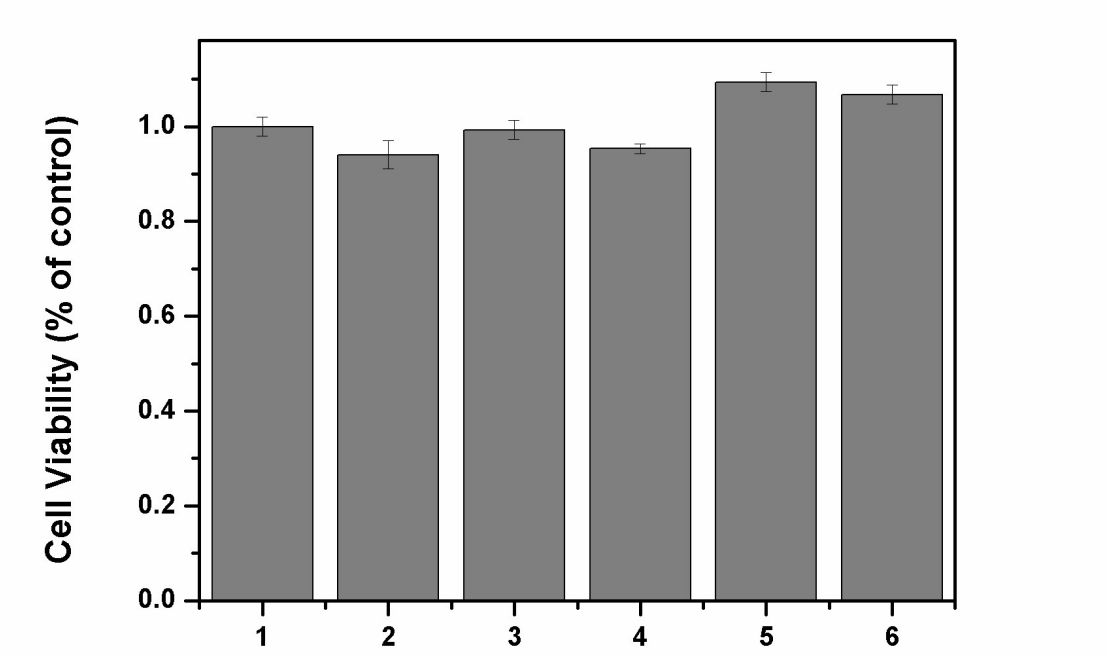


Fig. S5 Cell cytotoxic effect of **BTVQ** on SiHa cells. 1, control; 2, 0.5 μM; 3, 1 μM; 4, 10 μM; 5, 20 μM; 6, 50 μM. Data are expressed as mean values ± standard error of the mean of three independent experiments, each performed in three triplicate.

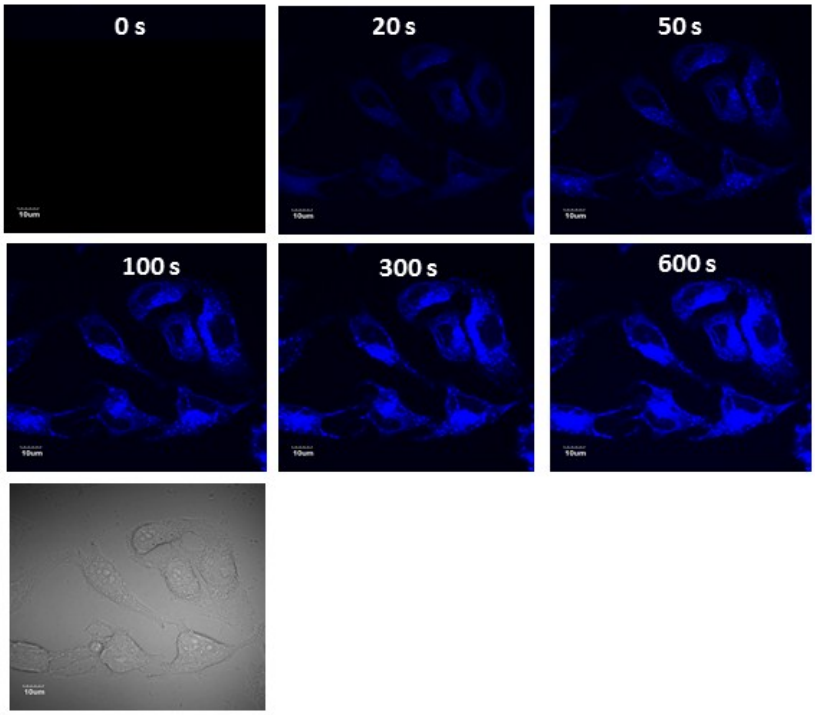


Fig. S6 The dynamic fluorescence imaging of **BTVQ** in HeLa cells (0-600s). The fluorescence images are acquired on an Olympus FV1000 confocal laser scanning microscope with blue channel (Ex = 405 nm, Em = 420-480 nm)

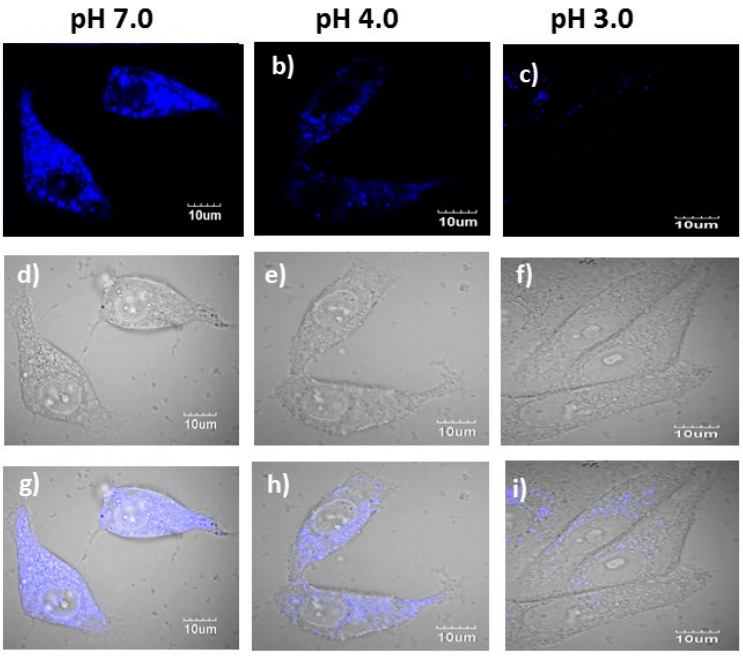
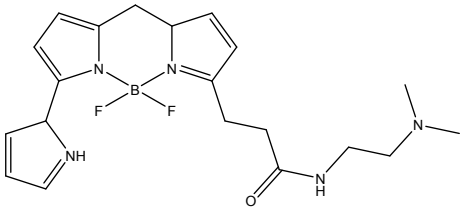


Fig. S7 Fluorescence images of 10 μM **BTVQ** in HepG2 cells clamped at pH 7.0 (a, d and g), 4.0 (b, e and h) and 3.0 (c, f and i), respectively. The blue channel images were collected at 420-480 nm (first row, λ_{ex} = 405 nm). The second row shows the corresponding bright-field transmission images. The third row shows the merged images of the first low and second low.

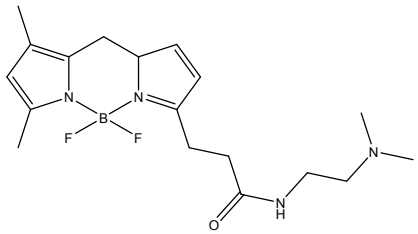
Table S1 Comparison of some reported pH sensors with BTVQ

Probes	Em (nm)	Stokes'hift (nm)	pH range	pK_a	Biological imaging applications
LysoTracker Red (LTR)	590	13	4.0-8.0	-	Lysosome
LysoTracker Green (LTG)	511	7	4.0-8.0	-	Lysosome
Naphthalimide-based					
1	529 /580	139/190	3.0-7.0	4.82	Lysosome
2	525	118	2.0-11.0	6.18 ± 0.049	Mitochondria (0.87)
Quinolone-based					
3	494 /570	89/165	3.0-6.0	4.20±0.015	lysosomes (0.81)
Benzoxadiazole-based					
4	530	85	2.0-9.0	4.10	Lysosome
Rhodamine-based					
5	573	50	4.5-7.4	5.23	Lysosome
6	650	70	4.0-7.0	5.04	Lysosome (0.92)
7	578	53	4.5-7.4	5.47	Lysosome
BODIPY-based					
8	786	36	4.97-7.32	5.08	late endosomes
9	707	32	4.5-7.4	4.0	lysosomes (0.79)
Hemicyanine-based					
10	448/490	88/130	3.5-7.2	5.82	Lysosome (0.91)
11	655	109	4.0-7.4	5.0	Lysosome
12	670/708	35/73	4.0-7.4	5.00±0.01	Lysosome
13	680	150	5.0-8.0	6.3	Mitochondria (0.91)
14	525/607	128/140	5.0-7.0	5.88	Mitochondria (0.93)
15	600	110/40	6.15-8.38	7.33±0.33	Mitochondria (0.93)
16	522	110	1.5-6.7	3.18	*E. coli cells*
17	523/650	100/123	0.50-7.00	2.44	*E. coli cells*
BTVQ	***428***	***110***	***2.2-7.0***	***3.52***	***Lysosome*** (0.94) / ***E. coli cells***

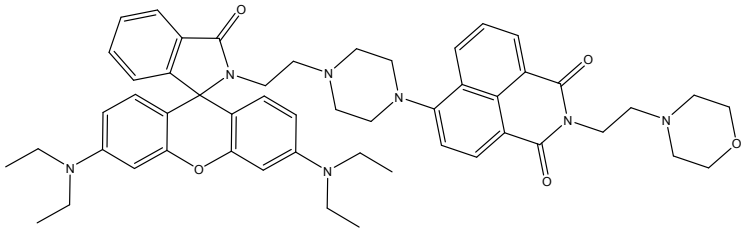
The performance of our sensor **BTVQ** has been compared with some reported pH sensors based on other materials (**Fig. S6**). As listed in Table S1, compared with some reported representative pH sensors, the significant advantage of **BTVQ** is that it may avoid the influence of reduce the excitation interference due to the large Stokes'hift of 110 nm. Furthermore, the probe has the ability of selective imaging of lysosome with the average Pearson's co-localization coefficient of 0.94 with Lyso Tracker Red. Even more importantly, **BTVQ** win out on the unique behavior for sensing extreme acidity (pH < 4) in E. coli cells. As far as we known, there is very limited probes which could simultaneously selectively stain weak acidic lysosome and image extreme acidity changes in *E. coli* cells.



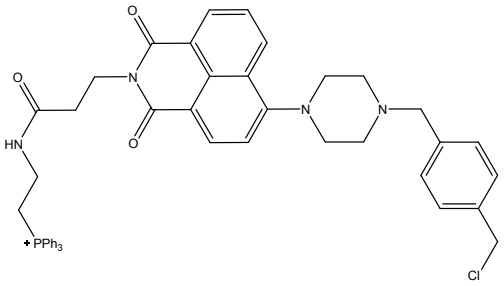
LTR *Anal. Biochem.,* 2001, **294**, 118



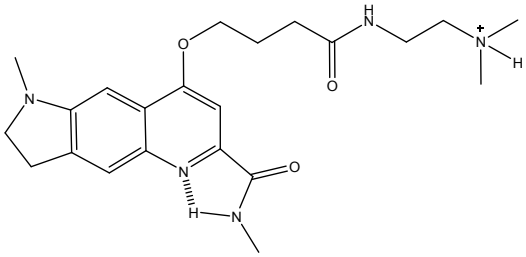
LTG *Angew. Chem., Int. Ed.,* 2005, **44**, 6504



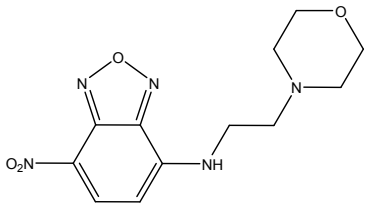
1 *J. Mater. Chem. B*, 2015, **3**, 3260



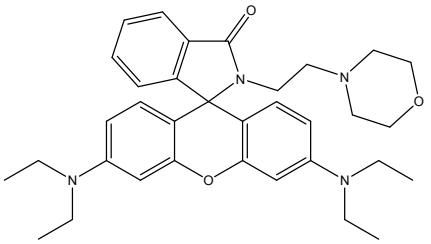
2 *J. Am. Chem.Soc.,* 2014, **136**, 14136



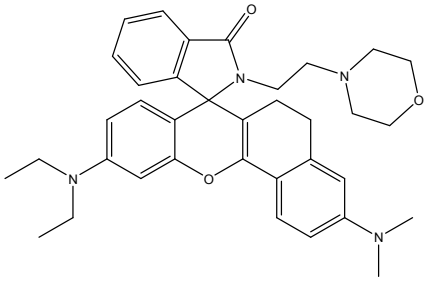
3 *Org. Lett.*, 2013, **15**, 5020



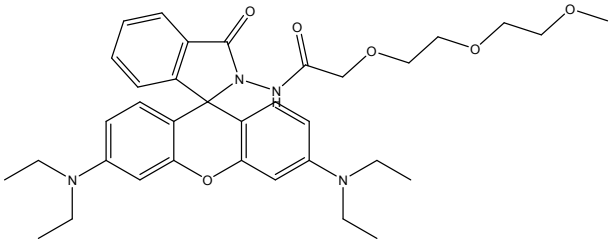
4 *Anal. Chim. Acta*, 2016,**920**, 86



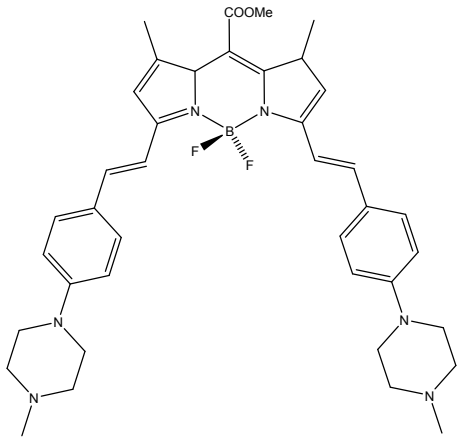
5 *J. Mater. Chem. B*, 2015, **3**, 919



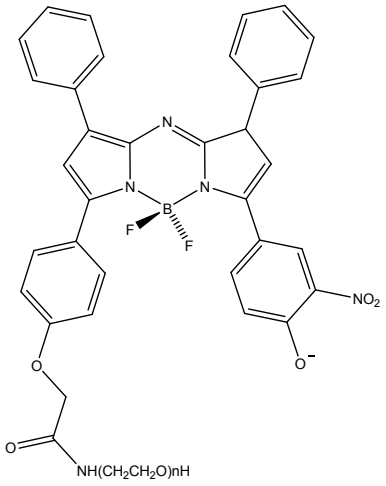
6 *Anal. Chem.*, 2017, **89**, 1922



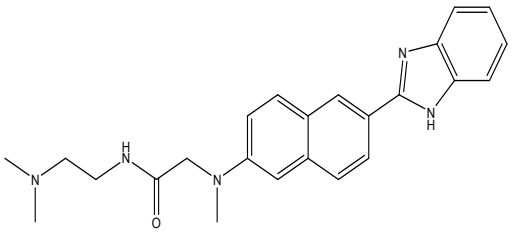
7 *Chem. Commun*., 2012, **48**, 11766



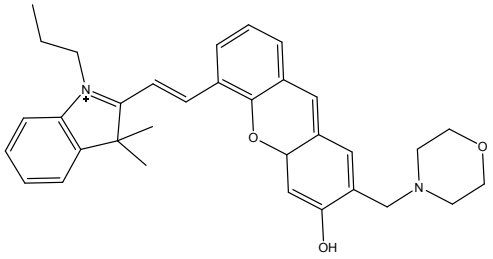
8 *ChemPlusChem*, 2016, **81**, 1209



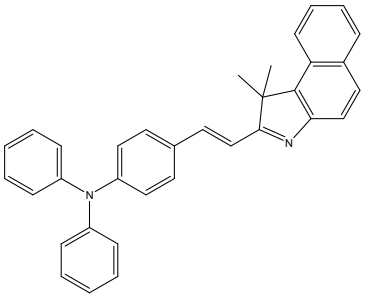
9 *Nat. Commun*., 2016, **7**, 10855



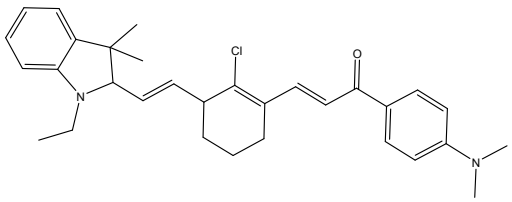
10 *J. Am. Chem. Soc.,* 2013,**135**, 17969



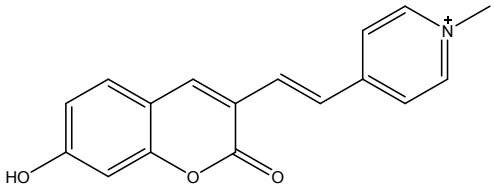
11 *Angew. Chem. Int. Ed*., 2014, **53**, 10916



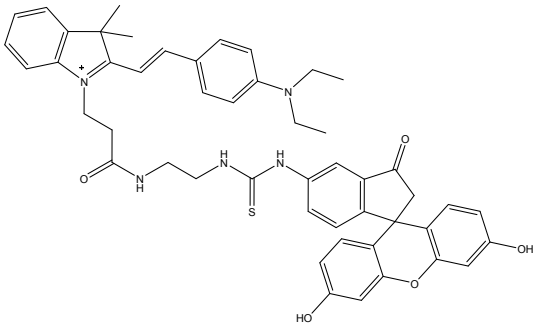
12 *Chem. Commun.*, 2012, **48**, 11202



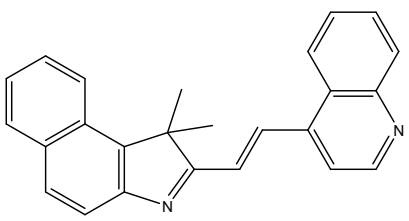
13 *Chem. Commun.,* 2014, **50**, 7184

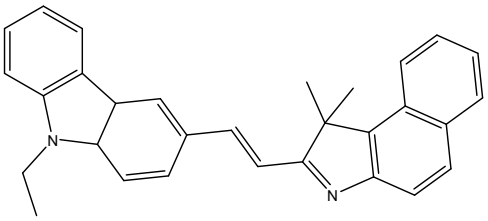


14 *Biomaterials ,* 2015,**53**, 669



15 *Chem. Sci.*, 2015, **6**, 3187

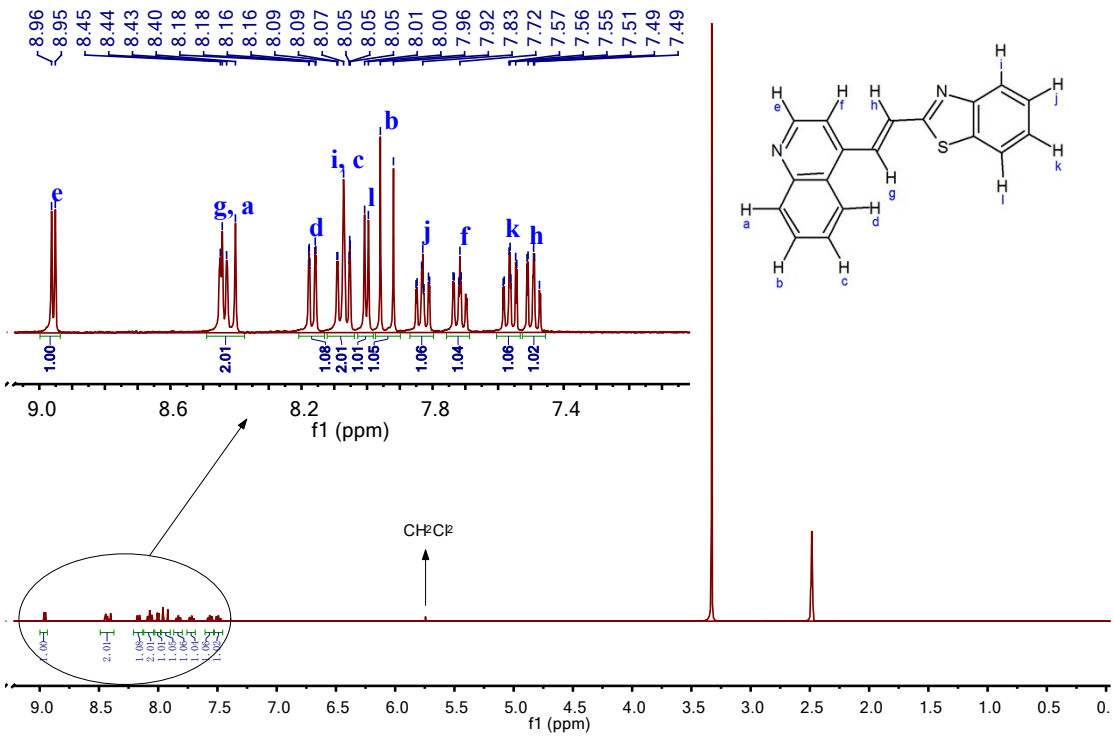


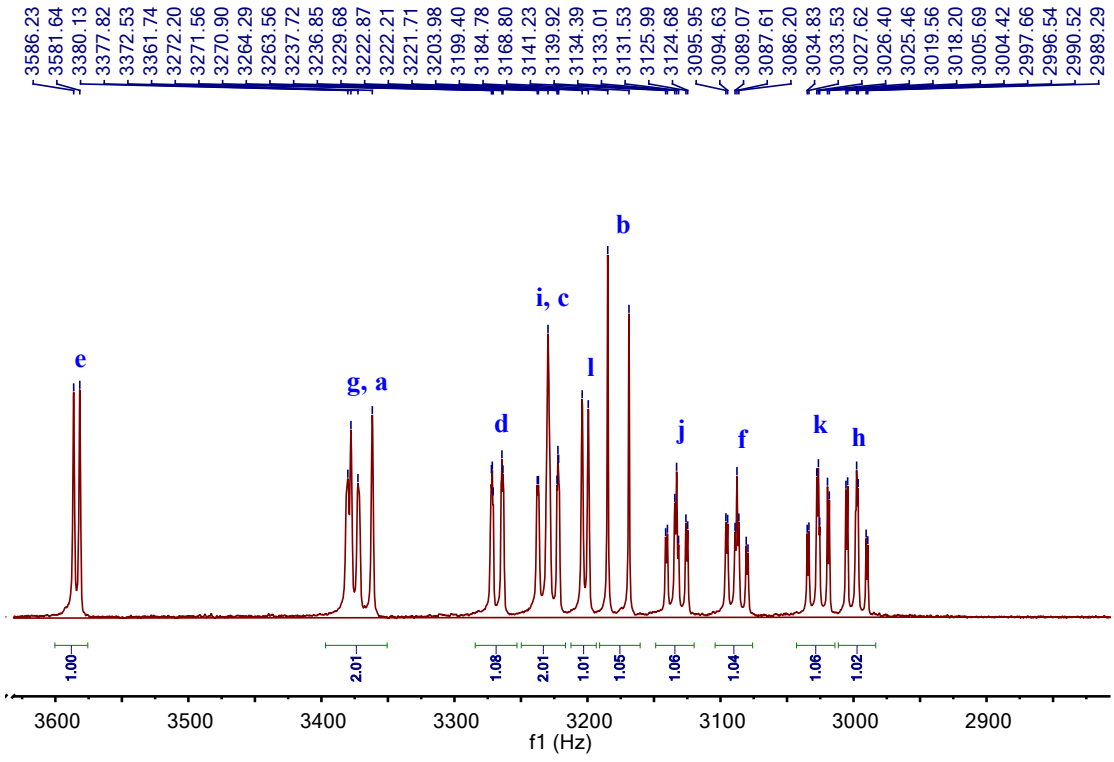


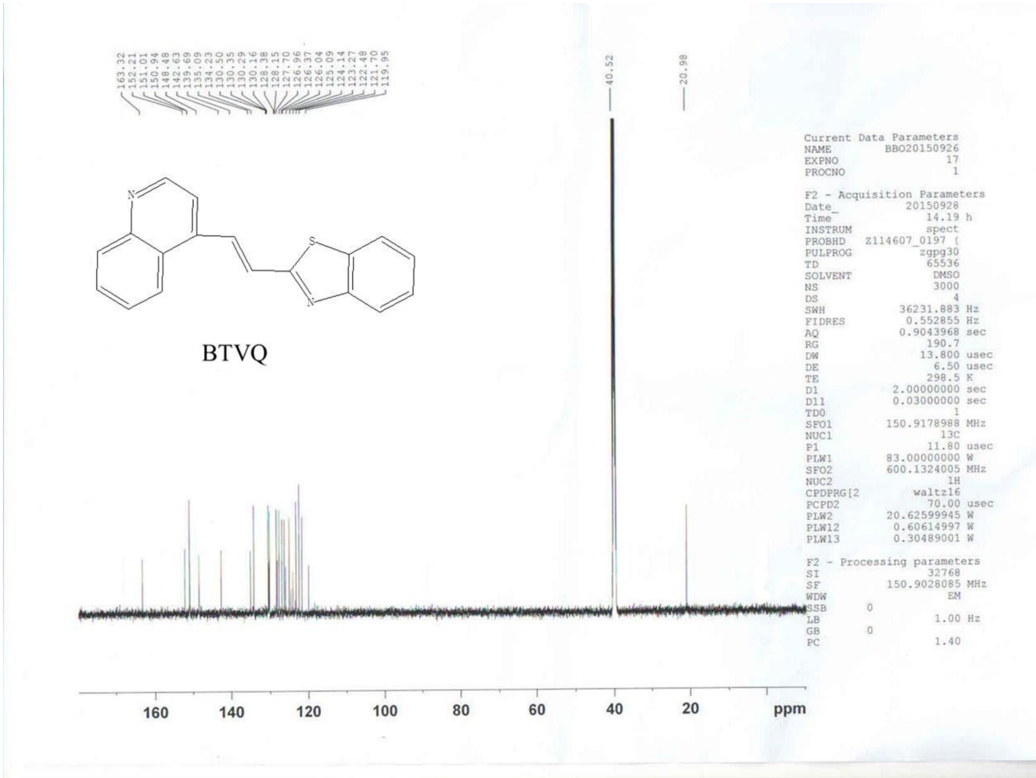
16 *Anal. Chem*., 2015, **87**, 2788 **17** Sens. Actuators, B,2015, **221**,1069

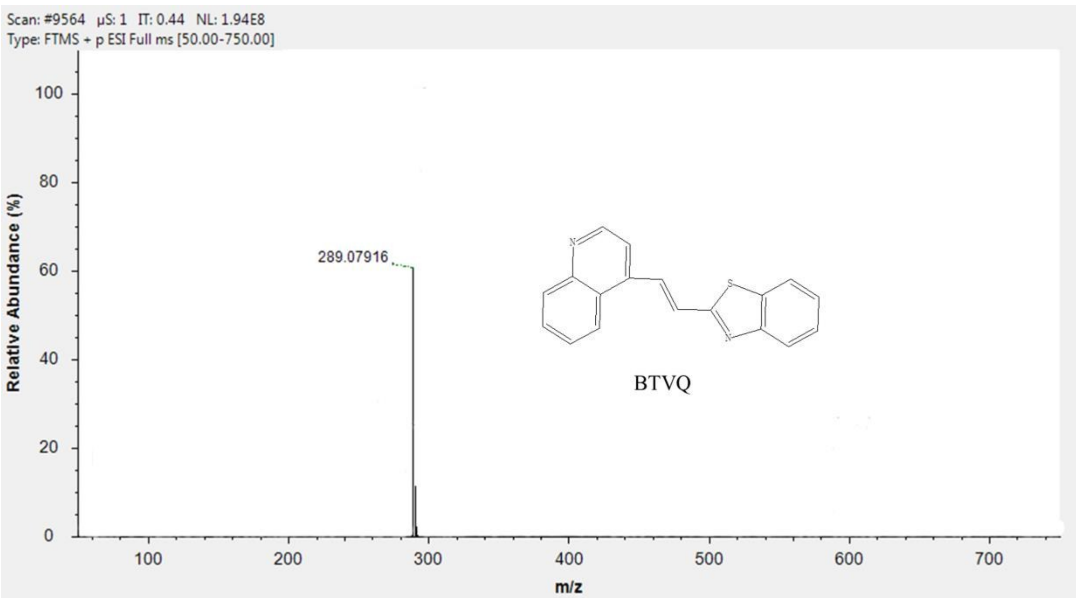
Fig. S8 Chemical structures of the sensors based on other materials listed in **Table S1**.

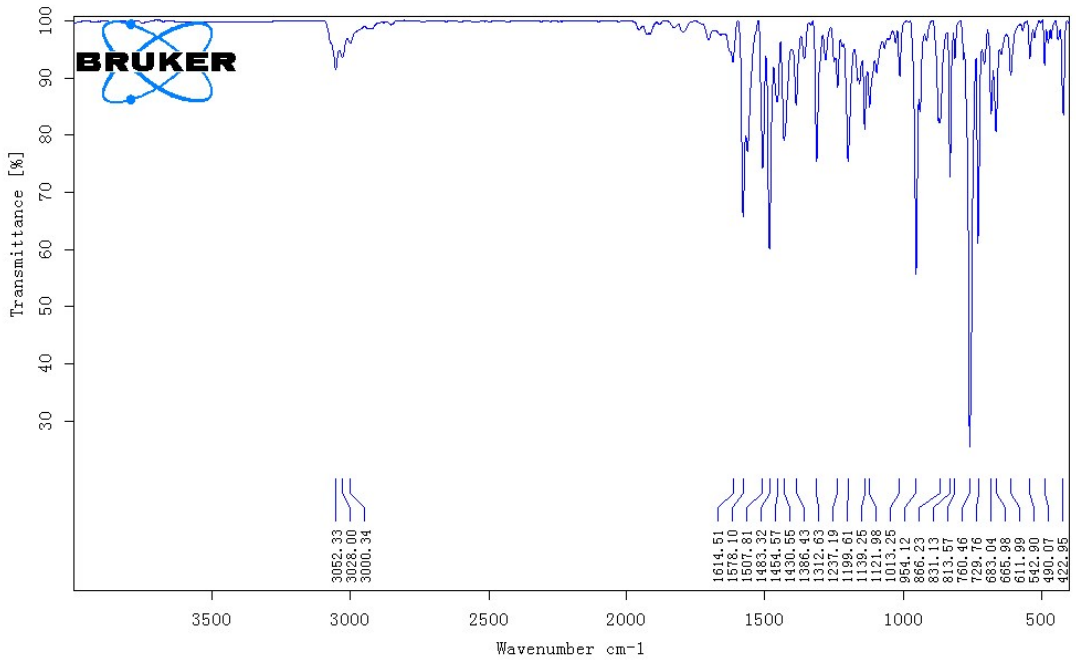
^{1}H NMR, ^{13}C NMR, MS and IR spectra analysis reports of BTVQ.






163.32
152.21
151.01
150.94
148.48
142.63
139.69
135.09
134.23
130.50
130.35
130.29
130.16
128.38
128.15
127.70
126.96
126.37
126.04
125.09
124.14
123.27
122.48
121.70
119.95
40.52
20.98
BTVQ
Current Data Parameters
NAME BBO20150926
EXPNO 17
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150928
Time 14.19 h
INSTRUM spect
PROBHD Z114607_0197 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3000
DS 4
SWH 36231.883 Hz
FIDRES 0.552855 Hz
AQ 0.9043968 sec
RG 190.7
DW 13.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178988 MHz
NUC1 13C
P1 11.80 usec
PLW1 83.00000000 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 20.62599945 W
PLW12 0.60614997 W
PLW13 0.30489001 W
F2 - Processing parameters
SI 32768
SF 150.9028085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160
140
120
100
80
60
40
20
ppm


Scan: #9564 µS: 1 IT: 0.44 NL: 1.94E8
Type: FTMS + p ESI Full ms [50.00-750.00]
Relative Abundance (%)
289.07916
BTVQ
m/z


BRUKER
Transmittance [%]
100
90
80
70
60
50
40
30
3052.33
3028.00
3000.34
1614.51
1578.10
1507.81
1483.32
1454.57
1430.55
1386.43
1312.63
1237.19
1199.61
1139.25
1121.98
1013.25
954.12
866.23
831.13
813.57
760.46
729.76
683.04
665.98
611.99
542.90
490.07
422.95
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1