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Supporting Information for

Development of a highly selective fluorescent probe for the rapid detection of HClO in living cells and zebrafish

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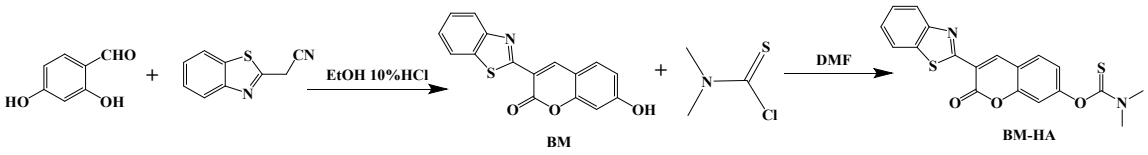

Scheme S1. The synthesis of fluorescent probe **BM-HA.**

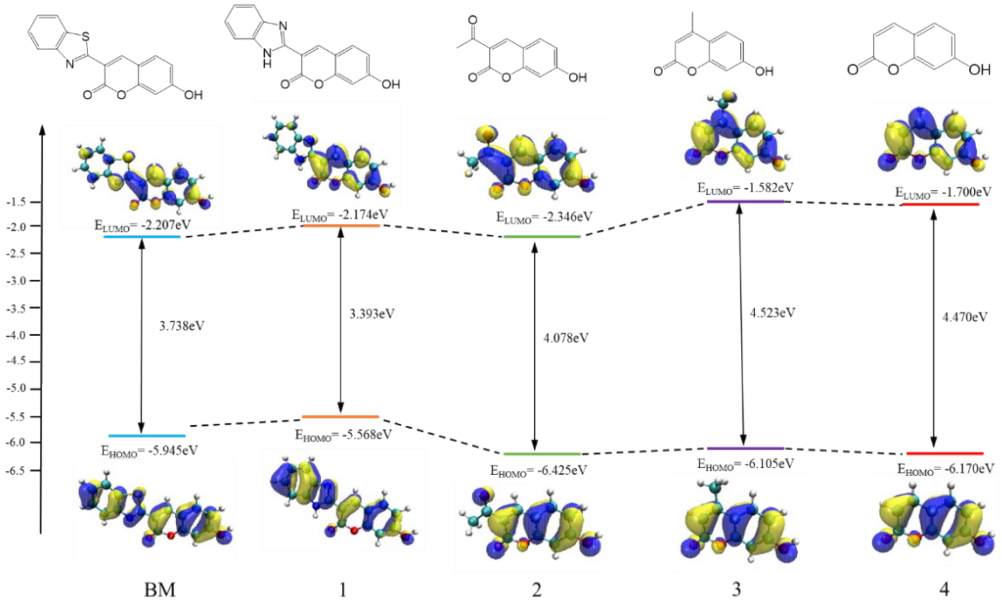

Fig. S1. DFT optimized structures and molecular orbital plots (LUMO and HOMO) of dyes **BM** and **1-4**.

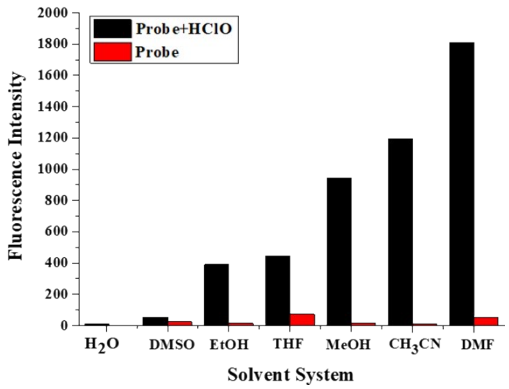

Fig. S2. The influence of different solvent system on the fluorescence intensity of probe **BM-HA** (10.0μM) with HClO (30.0μM).

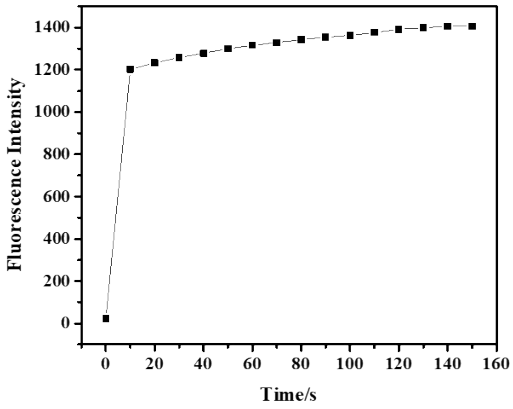

Fig. S3. Reaction-time profile of the probe **BM-HA** (10.0 μM) responses to HClO (30.0 μM). Fluorescence signals with λ_{ex} = 440 nm, λ_{em} = 490 nm.

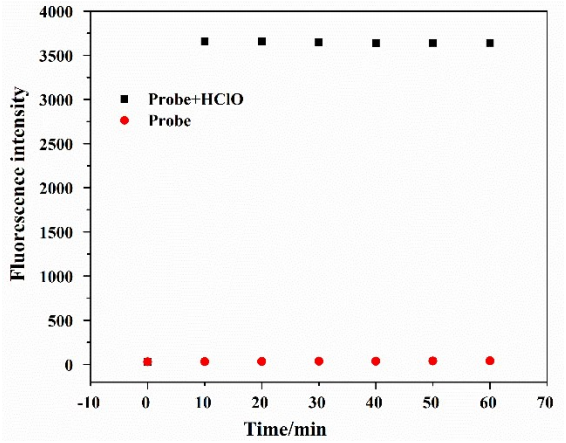

Fig. S4. The time-dependent fluorescence spectra of the probe **BM-HA** (10.0 μM) responses to HClO (40.0 μM). Fluorescence signals with λ_{ex} = 440 nm, λ_{em} = 490 nm.

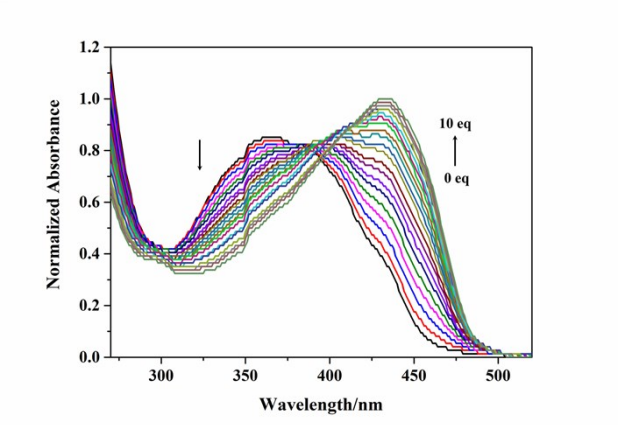

Fig. S5. UV-vis spectra of the probe **BM-HA** (10.0 μM) treated with different concentrations of HClO.

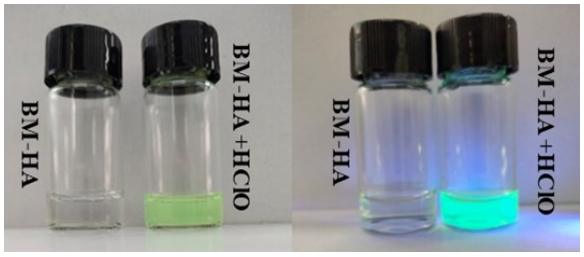

Fig. S6. The liquid fluorescence image of the probe **BM-HA** in the absence and presence of HClO in PBS buffer pH 7.4 that contained 1 % DMF, the left picture represented irradiation with natural light, the right picture showed irradiation with ultraviolet laser.

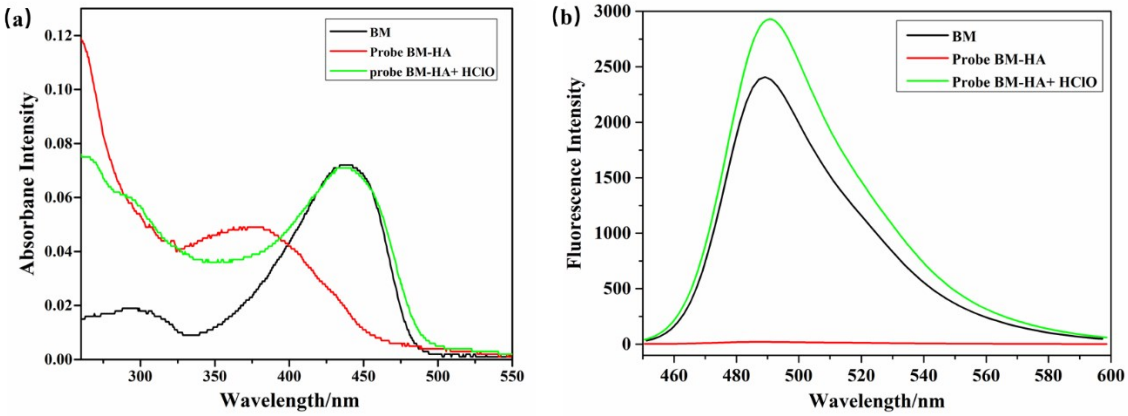

Fig. S7. Absorption spectra (a) and emission spectra (b) of the Compound **BM** (black line), the probe **BM-HA** (red line) and the probe **BM-HA** + HClO (green line).

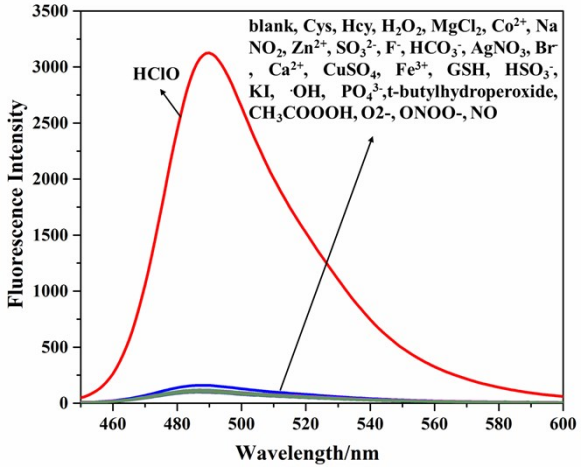

Fig. S8. Fluorescence spectra of the probe **BM-HA** (10.0 μM) to HClO (40.0 μM) over various relevant species (all 40.0 μM). Data shown in turn: blank, HClO, Cys, Hcy, H_2O_2, $MgCl_2$, Co^{2+}, $NaNO_2$, Zn^{2+}, SO_3^{2-}, F^-, HCO_3^-, $AgNO_3$, Br^-, Ca^{2+}, $CuSO_4$, Fe^{3+}, GSH, HSO_3^-, KI, $\cdot OH$, PO_4^{3-}, t-butylhydroperoxide, CH_3COOOH, O_2^-, $ONOO^-$, NO, respectively.

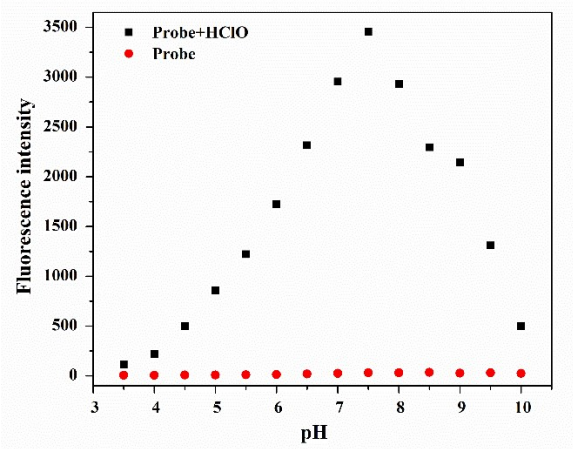

Fig. S9. The effects of pH on the fluorescence intensity of the probe **BM-HA** (10.0 μM) for HClO (40.0 μM).

Table S1. Compare the absorption and emission values of several functionals calculation and experiment of the compound **BM**.

	PBEPBE (nm)	CAM-B3LYP (nm)	B3PW91 (nm)	M062X (nm)	B3LYP (nm)	Experiment (nm)
absorption	435.15 nm	338.05nm	379.65 nm	337.80 nm	381.76 nm	440 nm
emission	527.65 nm	440.27 nm	476.64 nm	441.28 nm	482.34 nm	490 nm

Table S2. Comparison of experimental and calculated absorption and fluorescence emission for the compound **BM**.

		electronic transition	f^a	contrib	Calculation (nm)
BM	absorption	$S_0 \rightarrow S_1$	0.9707	HOMO→LUMO	381.76 nm
	emission	$S_1 \rightarrow S_0$	1.3103	LUMO→HOMO	482.34 nm

Table S3. The contribution percentage of each atom to HOMO, LUMO orbitals of compounds **BM-HA** and **BM**.

	BM-FA			BM	
Atomic number	HOMO (%)	LUMO (%)	Atomic number	HOMO (%)	LUMO (%)
C1	1.93	1.80	C1	4.94	2.08
C2	3.33	7.46	C2	6.98	6.73
C3	0.72	2.60	C3	2.94	1.67
C4	1.37	5.11	C4	3.92	4.82
C5	0.92	4.57	C5	8.80	4.05
C6	0.42	6.39	C6	3.13	6.58
C7	0.35	3.38	C7	0.61	2.91
C8	0.56	4.10	C8	2.58	3.15
C9	2.02	11.97	C9	10.84	10.41
C10	0.81	20.02	**C10**	**4.60**	**20.95**
O11	0.25	2.93	O11	5.28	2.04
C12	0.80	6.13	C12	4.17	7.45
N13	0.91	6.04	N13	5.33	7.41
C14	0.99	1.13	C14	5.73	1.45
C15	0.90	1.53	C15	5.39	1.90
S16	0.43	3.68	S16	3.20	3.46
C17	0.45	1.79	C17	2.45	2.20
C18	0.49	0.54	C18	3.04	0.64
C19	0.11	2.07	C19	6.08	2.63
C20	0.23	0.80	C20	1.20	0.91
O21	1.73	1.30	O21	6.37	2.77
C22	4.65	0.57	H22	0.36	0.10
N23	1.09	0.08	H23	0.18	0.07
C24	1.39	0.02	H24	0.18	0.59
C25	0.73	0.04	H25	0.24	2.12
S26	**67.43**	**0.49**	H26	0.15	0.21
H27	0.15	0.08	H27	0.22	0.03
H28	0.05	0.16	H28	0.50	0.27
H29	0.01	0.58	H29	0.04	0.05
H30	0.04	1.97	H30	0.39	0.18
H31	0.03	0.17			
H32	0.03	0.03			
H33	0.09	0.21			
H34	0.01	0.06			
H35	0.41	0.01			
H36	0.83	0.01			
H37	0.29	0.01			
H38	0.05	0.01			
H39	0.04	0.02			
H40	0.08	0.01			

Table S4. The contribution percentage of molecular fragment to HOMO, LUMO orbitals of compounds **BM-HA** and **BM**.

	BM-FA			BM	
Molecular fragment	HOMO (%)	LUMO (%)	Molecular fragment	HOMO (%)	LUMO (%)
benzothiazole	6.41	24.18	benzothiazole	37.5	28.61
coumarin	12.93	73.12	coumarin	55.58	68.27
dimethylcarbamosulfonyl	78.72	2.57	Hydroxyl	6.76	2.95

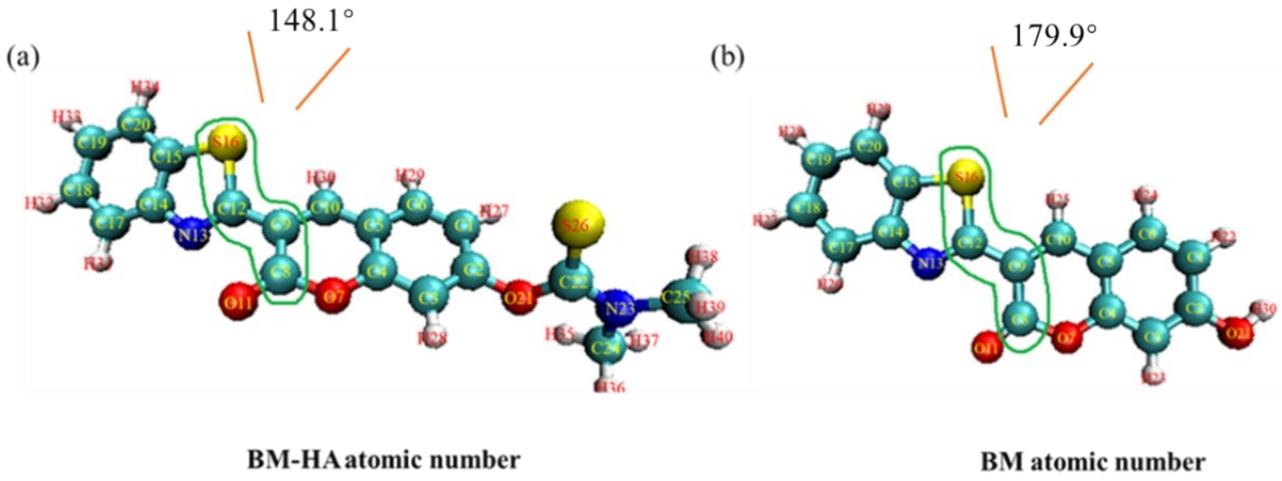

Fig. S10. The atomic numbers of the probe (a) **BM-HA** and the compound (b) **BM**.

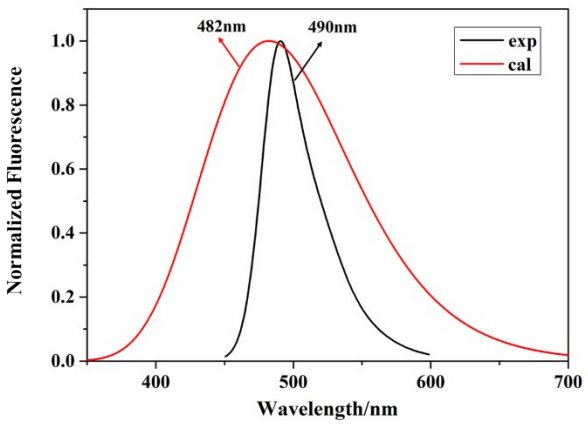

Fig. S11. Experimental and theory calculated fluorescence spectra of the compound **BM**.

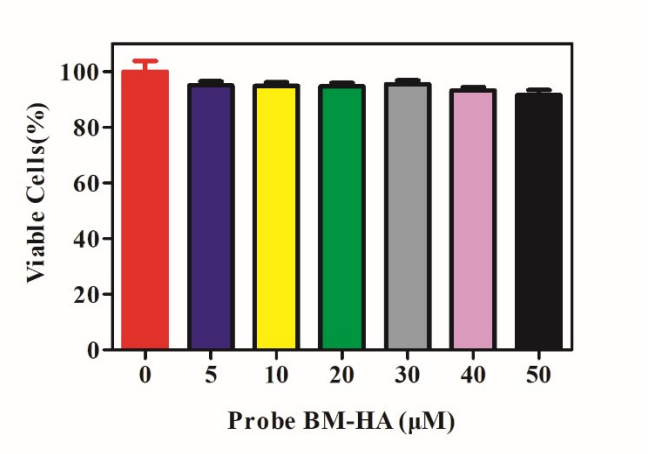

Fig. S12. Cytotoxicity assays of probe at different concentrations for HeLa cells.

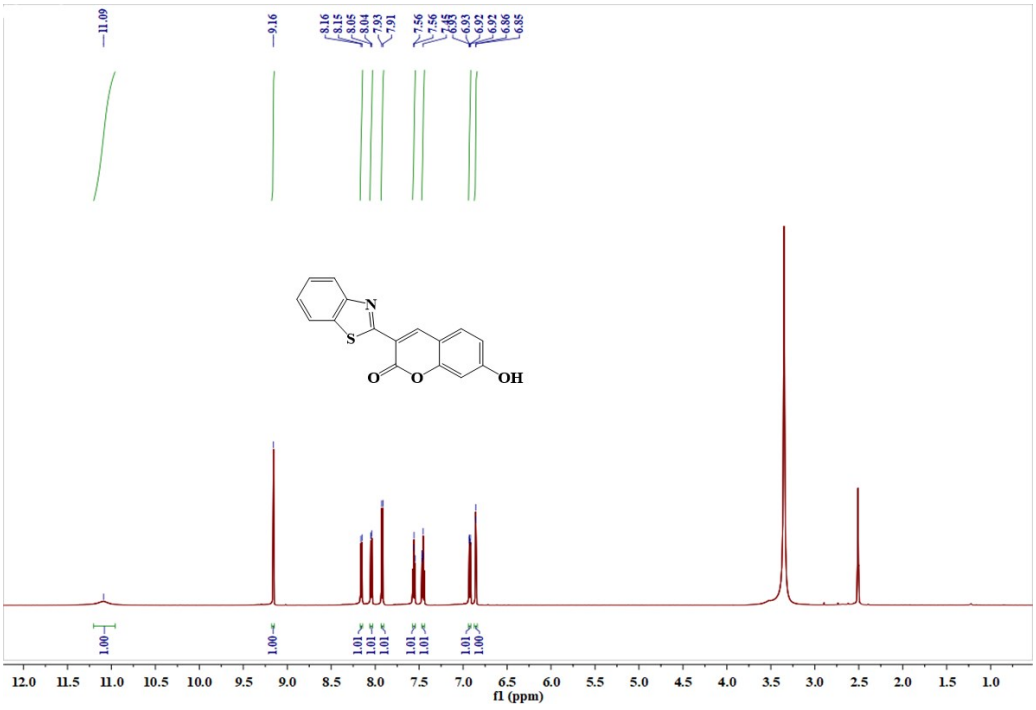

Fig. S13. ^{1}H NMR spectra of the compound **BM** in DMSO-*d*6**.**

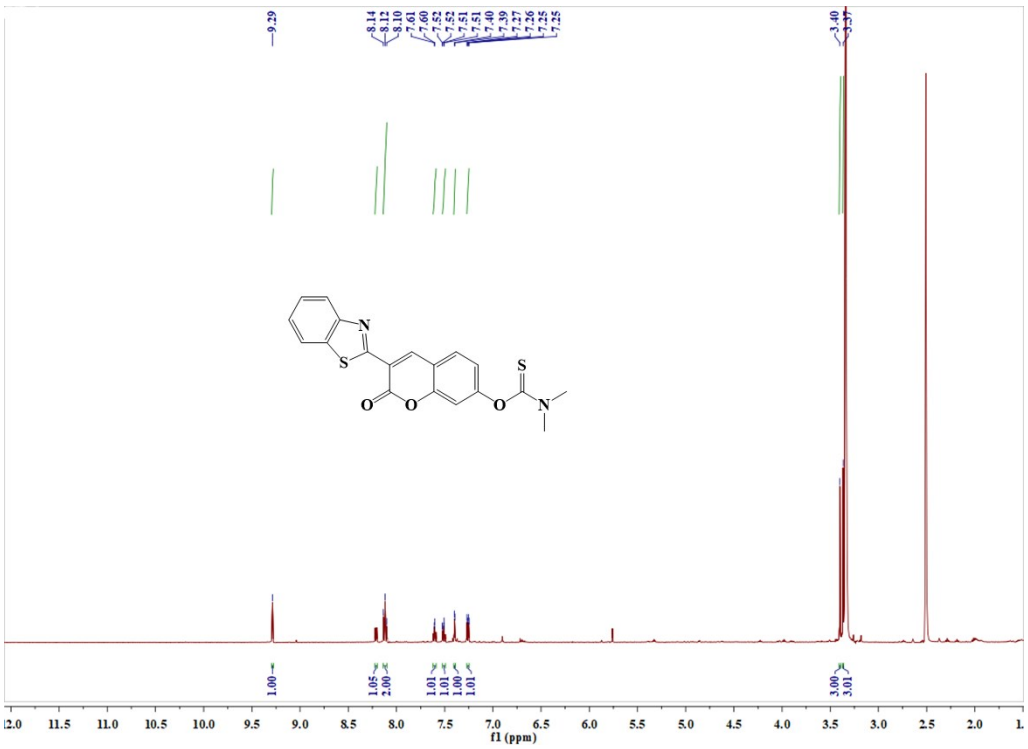

Fig. S14. ^{1}H NMR spectra of the compound **BM-HA** DMSO-*d*6**.**

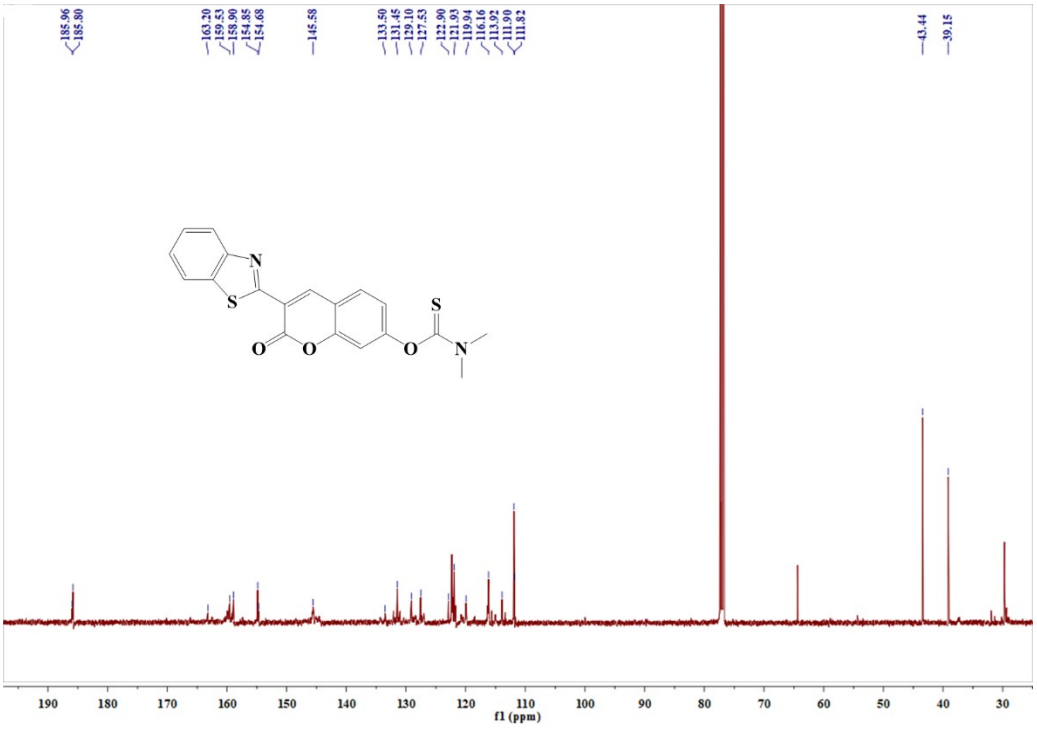

Fig. S15. ^{13}C NMR spectra of the compound **BM-HA** in $CDCl_3$**.**

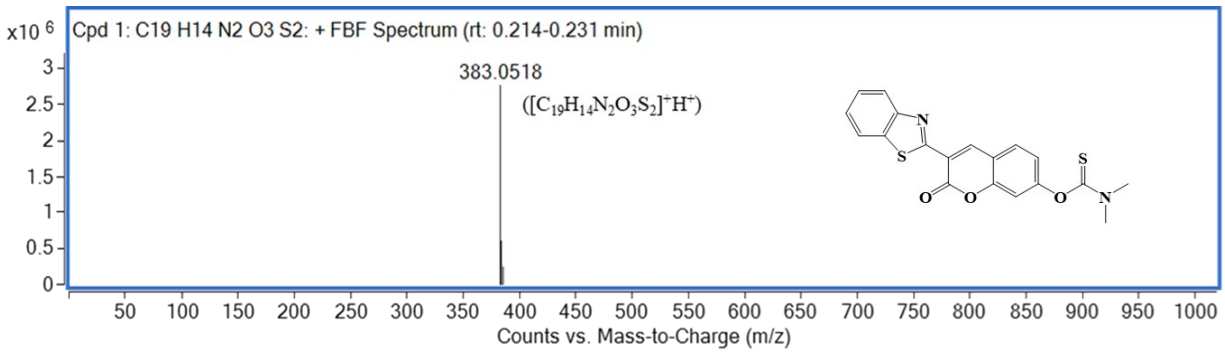

Fig. S16. HRMS spectra of the compound **BM-HA.**