Supplementary Material

Quinolin-2(1*H*-)-one-isoxazole dye as acceptor for mild addition of bisulfite in cationic or zwitterionic aqueous micellar solutions.

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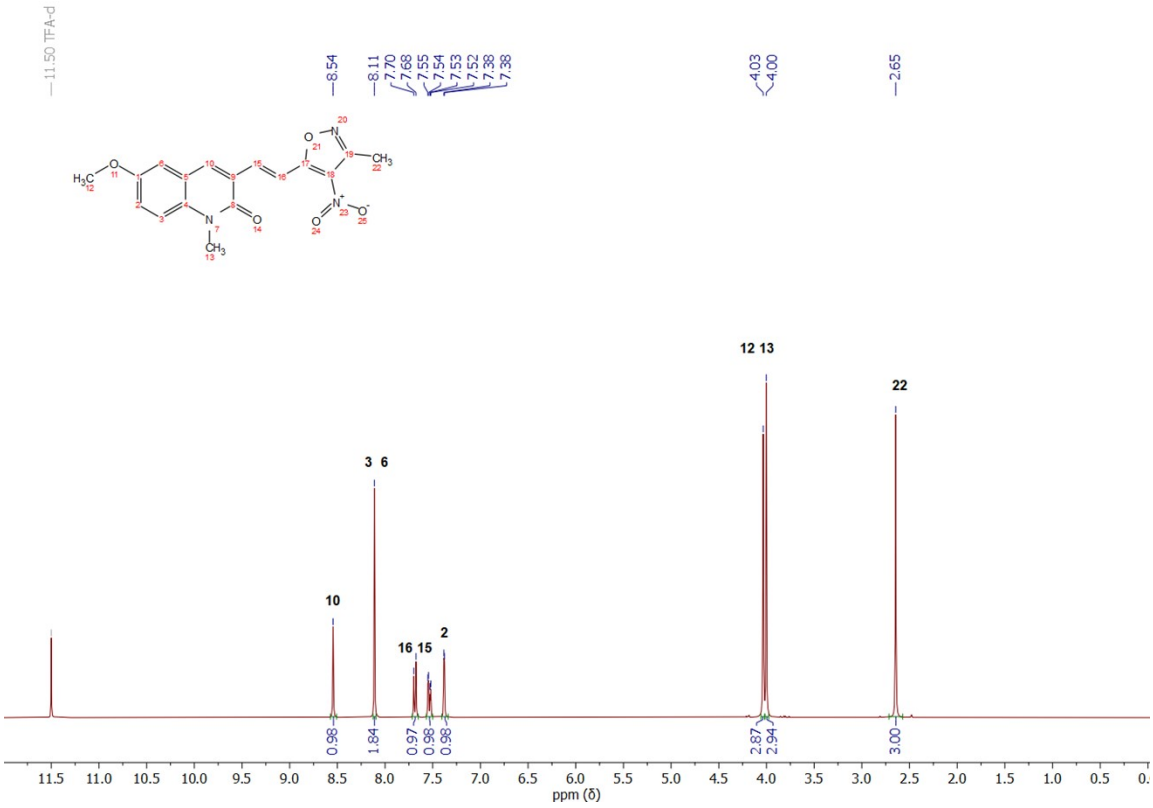

Figure S1. ^{1}H-NMR spectra of the (*E*)-6-methoxy-1-methyl-3-(2-(3-methyl-4-nitroisoxazol-5-yl)vinyl)quinolin-2(1*H*)-one dye (**MQI**) in TFA-*d*.

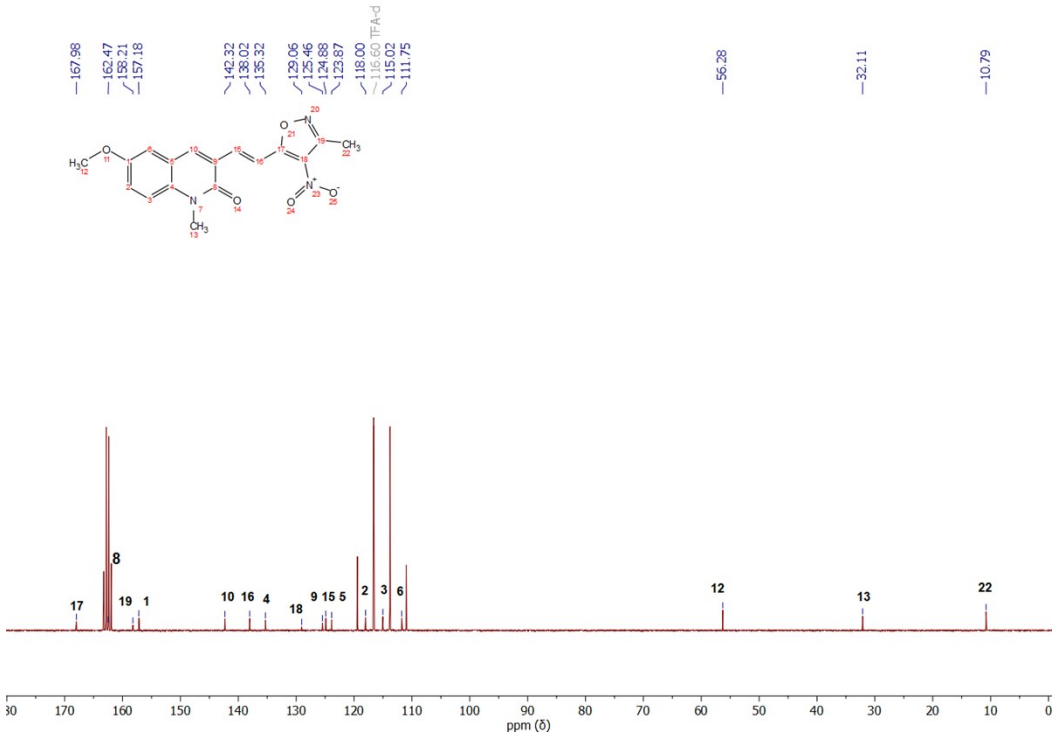

Figure S2. ^{13}C-NMR spectra of the (*E*)-6-methoxy-1-methyl-3-(2-(3-methyl-4-nitroisoxazol-5-yl)vinyl)quinolin-2(1*H*)-one dye (**MQI**) in TFA-*d*.

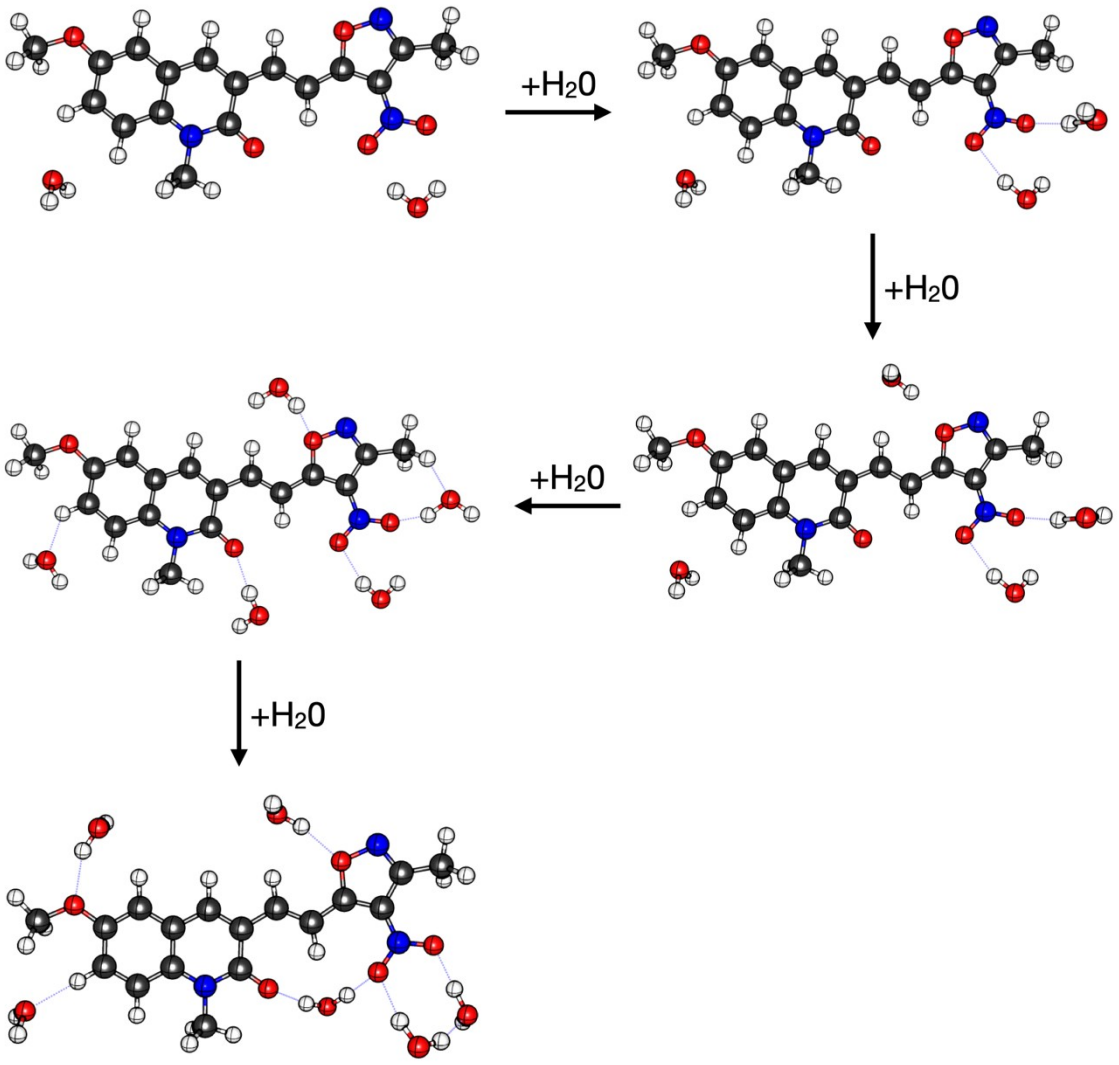

Figure S3. Addition of two to six water molecules to MQI while maintaining PCM as an implicit solvent model.

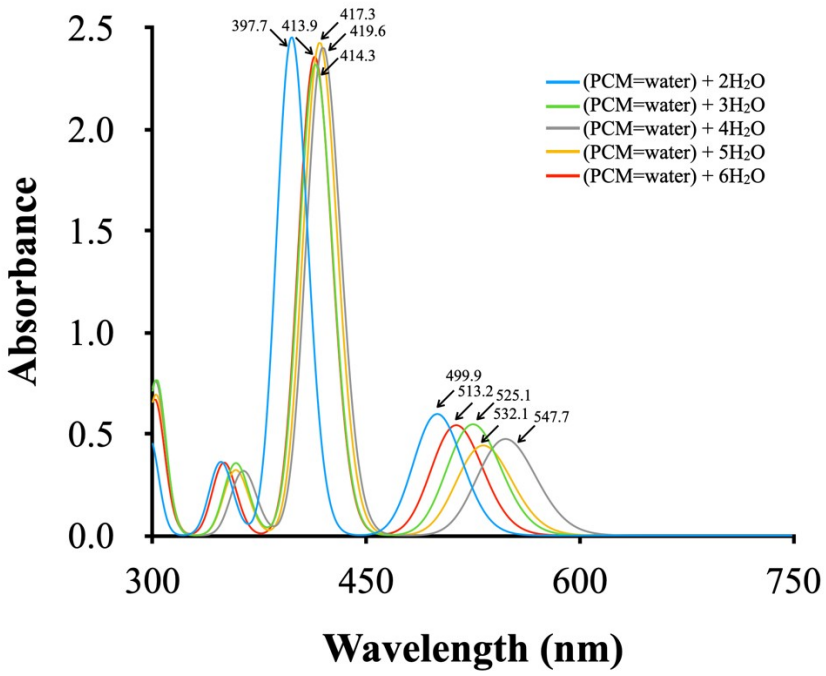

Figure S4. Calculated UV-vis spectra of **MQI** using two to six water molecules undermining PCM with water as the implicit solvent.

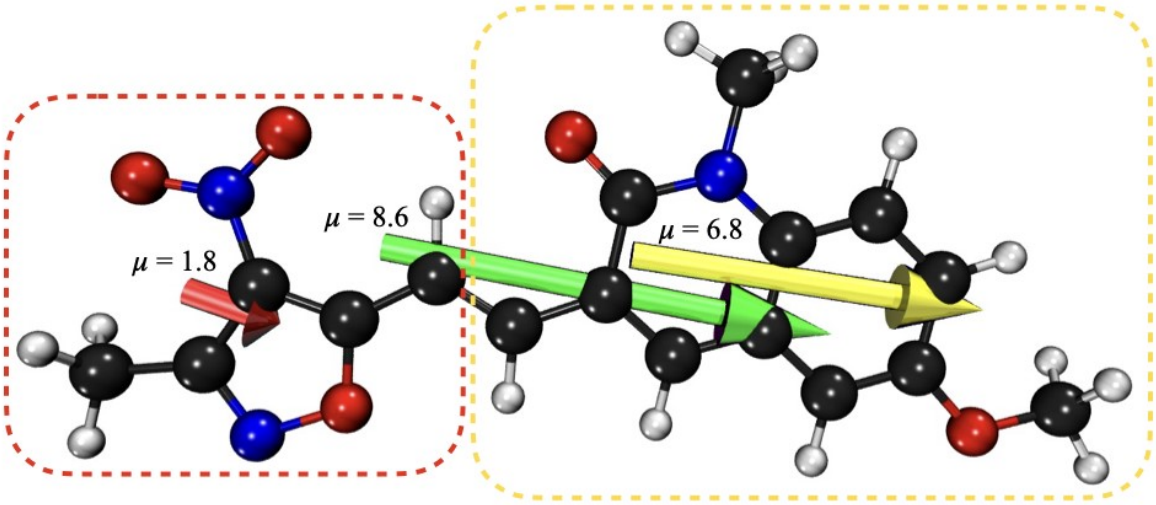

Figure S5. Magnitudes and vectors of dipole moments μ (in D) of **MQI** (green arrow) and local polarity in each fragment (red and yellow arrow) were calculated at the PBE0,6-311G** level. Oxygen is red, nitrogen is dark blue, carbon is dark gray, and hydrogen is white.

Table S1. Sulfite concentration effects on the observed rate constant (k_{obsd}) for its reaction with **MQI** (25 μM) in an aqueous micellar cationic CTACl and CTABr media (0.01 M).

10^4 [HSO_3^-]/M	*Cationic aqueous micellar solutions*	
	CTACl $10^3 k_{obsd}/s^{-1}$	**CTABr** $10^3 k_{obsd}/s^{-1}$
0.2	0.55	8.07
0.4	2.24	-
0.6	2.76	9.43
0.8	3.01	11.60
1.0	-	19.70
1.2	-	23.30
1.4	10.50	25.70
1.6	9.87	30.30
1.8	11.40	35.80
2.0	14.90	–
2.2	14.30	–
2.4	16.30	–
2.6	17.40	–

Table S2. Sulfite concentration effects on the observed rate constant (k_{obsd}) for its reaction with **MQI** (25 μM) in an aqueous micellar zwitterionic SB3-10 (0.1 M), SB3-14, and SB3-16 media (0.01 M).

10^4 [HSO_3^-]/M	*Zwitterionic aqueous micellar solutions*		
	SB3-10 $10^4 k_{obsd}/s^{-1}$	**SB3-14** $10^4 k_{obsd}/s^{-1}$	**SB3-16** $10^4 k_{obsd}/s^{-1}$
0	0.67	1.14	1.72
1.0	0.67	1.21	1.65
2.0	1.69	2.12	3.33
3.0	2.17	3.22	5.10
4.0	3.21	4.03	6.13
6.0	4.41	6.32	9.88
7.0	–	–	11.10
8.0	5.94	6.97	12.90
10.0	8.45	9.10	14.70
12.0	8.78	10.70	15.80
13.0	–	11.30	–
14.0	10.40	11.80	–
15.0	–	13.30	–

Table S3. Effect of Concentration of cationic aqueous micellar solution (D_n)[a] on the observed rate constant (k_{obsd}) for the addition reaction of **MQI** (25 μM) by bisulfite ion (300 μM) at 25 °C.

CTACl		CTABr		CPBr	
$10^3[D_n]$	$10^2k_{obsd}/s^{-1}$	$10^3[D_n]$	$10^2k_{obsd}/s^{-1}$	$10^3[D_n]$	$10^2k_{obsd}/s^{-1}$
0.5	4.12	1.1	4.08	2.8	0.997
0.9	4.39	1.5	4.78	2.9	1.132
1.7	4.80	1.9	5.30	13.0	1.341
2.5	4.93	2.7	5.36	33.0	1.341
3.3	5.00	3.1	5.45	53.0	1.401
4.1	4.91	4.3	5.68	73.0	1.381
4.5	5.14	5.1	5.74	–	–
6.5	4.98	5.5	5.74	–	–
7.7	4.83	–	–	–	–
8.1	4.81	–	–	–	–

[a]The concentration of micellized surfactant.

Table S4. Effect of Concentration of zwitterionic surfactants (D_T)[a] on the observed rate constant (k_{obsd}) for the addition reaction of **MQI** (25 μM) by bisulfite ion (300 μM) at 25 °C.

SB3-10		SB3-14		SB3-16	
$10^2[D_T]$	$10^4 k_{obsd}/s^{-1}$	$10^3[D_T]$	$10^4 k_{obsd}/s^{-1}$	$10^3[D_T]$	$10^4 k_{obsd}/s^{-1}$
5.1	4.18	3.2	2.03	0.4	1.55
6.1	4.74	3.6	2.71	1.2	2.13
6.4	4.90	4.4	3.49	2.0	3.80
7.2	6.20	4.8	3.89	2.8	4.50
8.0	7.21	6.0	4.75	4.0	5.18
8.5	8.89	6.8	4.93	4.8	6.50
9.3	8.39	8.0	5.97	6.8	9.68
9.8	9.01	8.8	6.49	8.0	10.10
10.0	9.94	9.2	7.64	9.6	10.30

[a]The stoichiometric surfactant concentration.