Electronic Supplementary Material

Appendix

Table S1. Results of molecular docking of cationic *meso*-substituted thia- and oxacarbocyanine dyes (structures C1–C10) with proteases NSP3, NSP5, NSP12

Dye	Run	Aff.	E_{tot},	E_{VdW},	E_{el},
			kcal mol^{-1}		
			NSP3		
C1	1	–8.55	33.69 ± 0.39	–21.17 ± 1.41	–4.15 ± 1.73
C2	17	–8.68	33.07 ± 0.35	–21.25 ± 1.53	–4.42 ± 1.68
C3	4	–8.26	33.37 ± 1.10	–20.41 ± 1.11	–5.53 ± 1.51
C4	5	–8.85	26.54 ± 1.71	–22.04 ± 2.65	–4.67 ± 1.66
C5	8	–8.16	42.83 ± 0.55	–20.80 ± 1.51	–8.76 ± 1.58
C6	4	–8.67	117.81 ± 0.83	–24.25 ± 1.88	–3.83 ± 1.67
C7	16	–8.53	35.57 ± 0.73	–22.46 ± 1.17	–4.56 ± 1.08
C8	3	–8.063	23.48 ± 0.80	–19.33 ± 2.26	–6.00 ± 2.03
C9	14	–8.51	28.99 ± 0.57	–21.92 ± 0.85	–4.85 ± 1.61
C10	16	–8.00	134.73 ± 1.57	–21.85 ± 1.55	–5.56 ± 1.59
			NSP5		
C1	9	–8.39	26.71 ± 0.35	–26.17 ± 2.08	–6.46 ± 1.58
C2	8	–8.98	25.56 ± 0.69	–28.85 ± 3.49	–5.18 ± 2.67
C3	7	–7.99	25.78 ± 0.56	–26.90 ± 1.47	–7.19 ± 0.78
C4	17	–8.55	20.29 ± 0.56	–29.07 ± 2.06	–6.39 ± 1.36
C5	4	–8.41	36.27 ± 0.55	–24.56 ± 1.84	–12.50 ± 2.04
C6	12	–8.71	109.68 ± 1.37	–30.07 ± 1.36	–6.31 ± 2.96
C7	10	–8.10	27.35 ± 0.39	–29.24 ± 0.41	–7.04 ± 0.49
C8	24	–8.57	14.75 ± 1.50	–27.53 ± 1.42	–6.52 ± 0.42
C9	10	–8.28	21.46 ± 0.46	–28.83 ± 0.95	–5.34 ± 0.90
C10	8	–7.95	128.14 ± 0.77	–27.62 ± 1.87	–6.99 ± 1.27
			NSP12		
C1	4	–7.57	29.23 ± 1.36	–20.29 ± 1.33	–9.92 ± 3.00
C2	11	–7.53	28.69 ± 1.12	–22.39 ± 1.92	–7.62 ± 2.55
C3	18	–7.48	28.70 ± 1.90	–20.67 ± 2.10	–9.85±2.86
C4	14	–7.58	21.09 ± 1.31	–22.24 ± 2.66	–11.44 ± 3.26
C5	9	–7.29	35.91 ± 0.92	–18.80 ± 1.39	–18.89 ± 1.31
C6	18	–8.20	112.84 ± 0.62	–24.39 ± 2.71	–8.74 ± 2.62
C7	21	–7.58	30.21 ± 1.19	–21.67 ± 1.01	–11.92 ± 2.72
C8	19	–7.55	16.03 ± 1.75	–19.55 ± 2.15	–14.70 ± 1.08
C9	9	–7.61	23.88 ± 1.89	–21.91 ± 2.39	–10.92 ± 3.34
C10	12	–7.25	130.26 ± 0.84	–21.23 ± 1.62	–11.57 ± 1.95

Table S2. Results of molecular docking of uncharged squarylium dyes SQ1–SQ6 with proteases NSP3, NSP5, NSP12

Dye	Run	Aff	E_{tot},	E_{VdW},	E_{el},
		kcal mol^{-1}			
			NSP3		
SQ1	15	–7.17	5.32 ± 0.66	–12.90 ± 2.46	–17.98 ± 2.39
SQ2	4	–7.61	17.32 ± 0.75	–15.45 ± 2.20	–14.14 ± 3.13
SQ3	5	–8.14	52.66 ± 0.30	–15.06 ± 3.42	–19.15 ± 2.38
SQ4	18	–7.14	7.15 ± 0.81	–8.08 ± 2.81	–24.25 ± 2.61
SQ5	24	–7.63	15.17 ± 0.64	–13.93 ± 1.20	–14.91 ± 1.35
SQ6	16	–7.38	49.02 ± 0.27	–15.31 ± 2.86	–18.55 ± 1.96
			NSP5		
SQ1	10	–7.91	–6.19 ± 1.36	–14.48 ± 3.27	–23.52 ± 3.68
SQ2	15	–7.39	12.10 ± 0.99	–20.18 ± 2.77	–14.55 ± 4.02
SQ3	8	–8.34	48.41± 1.93	–20.41 ± 3.23	–18.85 ± 5.18
SQ4	15	–8.064	–1.92 ± 1.48	–14.17 ± 6.39	–28.69 ± 7.48
SQ5	16	–7.92	9.88± 0.29	–23.89 ± 4.23	–10.80 ± 3.91
SQ6	19	–8.50	41.34± 0.31	–19.13 ± 7.03	–23.93 ± 7.16
			NSP12		
SQ1	8	–6.80	–3.51 ± 0.95	–7.56 ± 3.75	–27.86 ± 4.66
SQ2	8	–8.46	4.95 ± 1.57	–22.43 ± 2.32	–19.30 ± 2.63
SQ3	2	–8.26	36.71 ± 1.0	–13.60 ± 2.33	–36.24 ±1.69
SQ4	19	–7.40	–6.90 ± 1.33	–5.02 ± 3.55	–43.49 ± 5.70
SQ5	18	–7.76	5.74 ± 0.86	–15.03 ± 4.66	–23.29 ± 4.82
SQ6	20	–8.28	32.54 ± 1.02	–13.38 ± 6.57	–37.43 ± 7.51

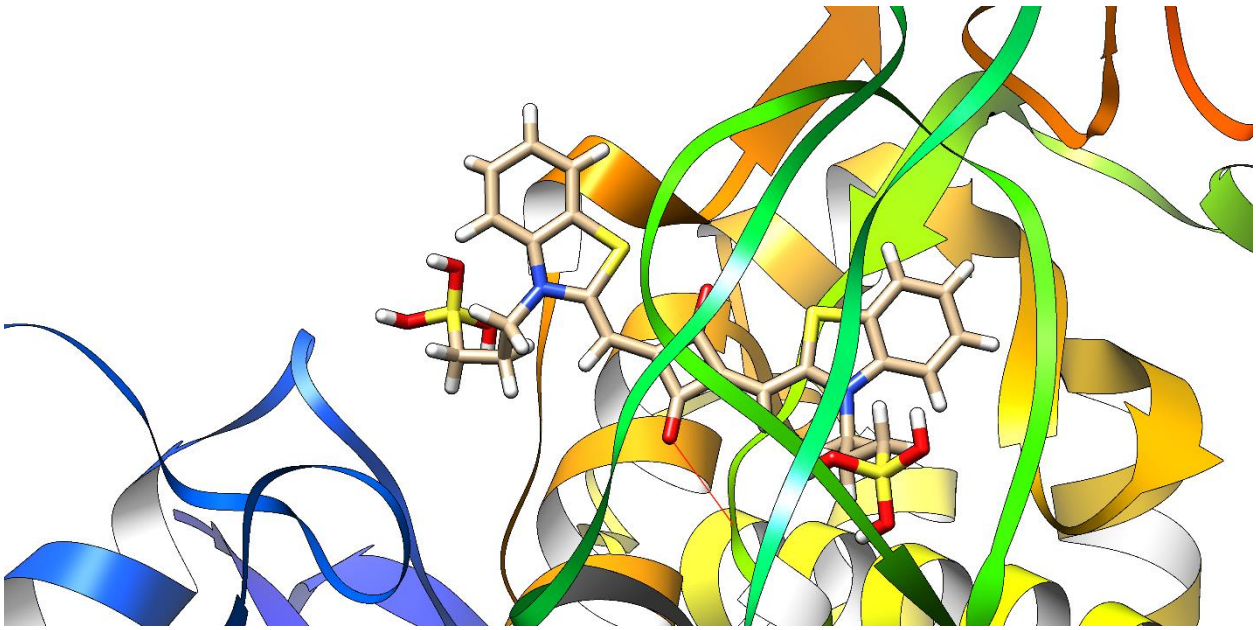

Fig. S1 Result of molecular docking of dye SQ1.3 with NSP12; the intermolecular hydrogen bond with LYS541 (2 Å) is shown by the red line; the initial configuration of dye SQ1.3 is given in **Fig. 2**.

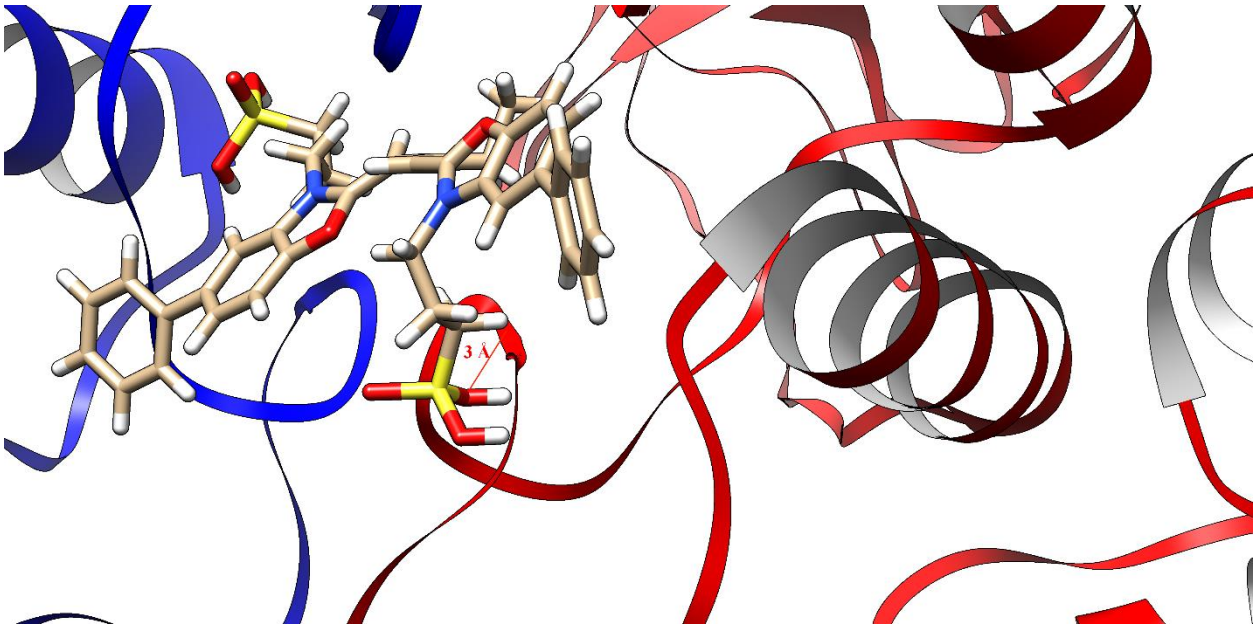

Fig. S2 Result of docking of dye 2.13 with NSP5; the intermolecular hydrogen bond with GLY282 (3 Å) is shown by the red line.

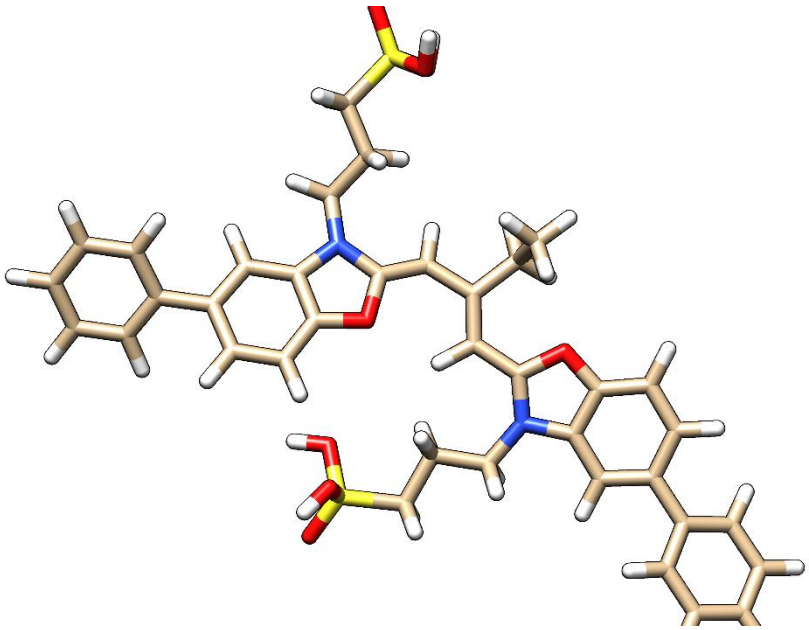

Fig. S3 Initial configuration of dye 2.13.

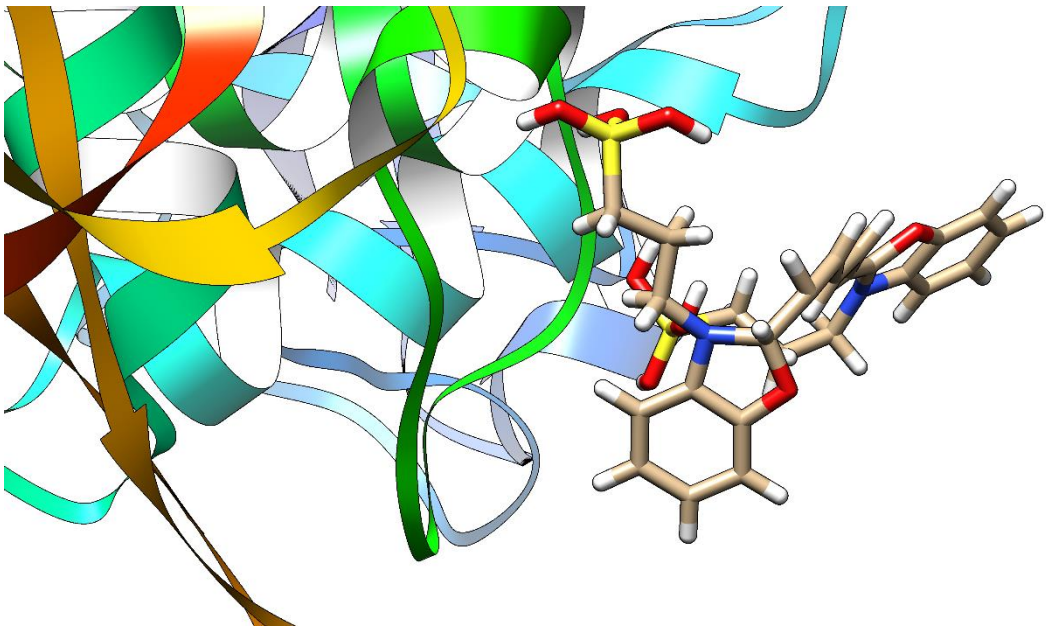

Fig. S4 Result of docking of dye 3.4 with NSP3.

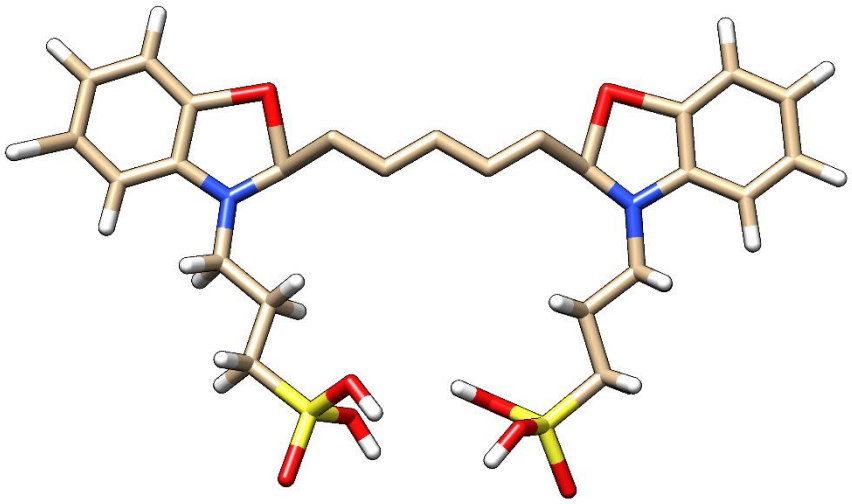

Fig. S5 Initial configuration of dye 3.4.

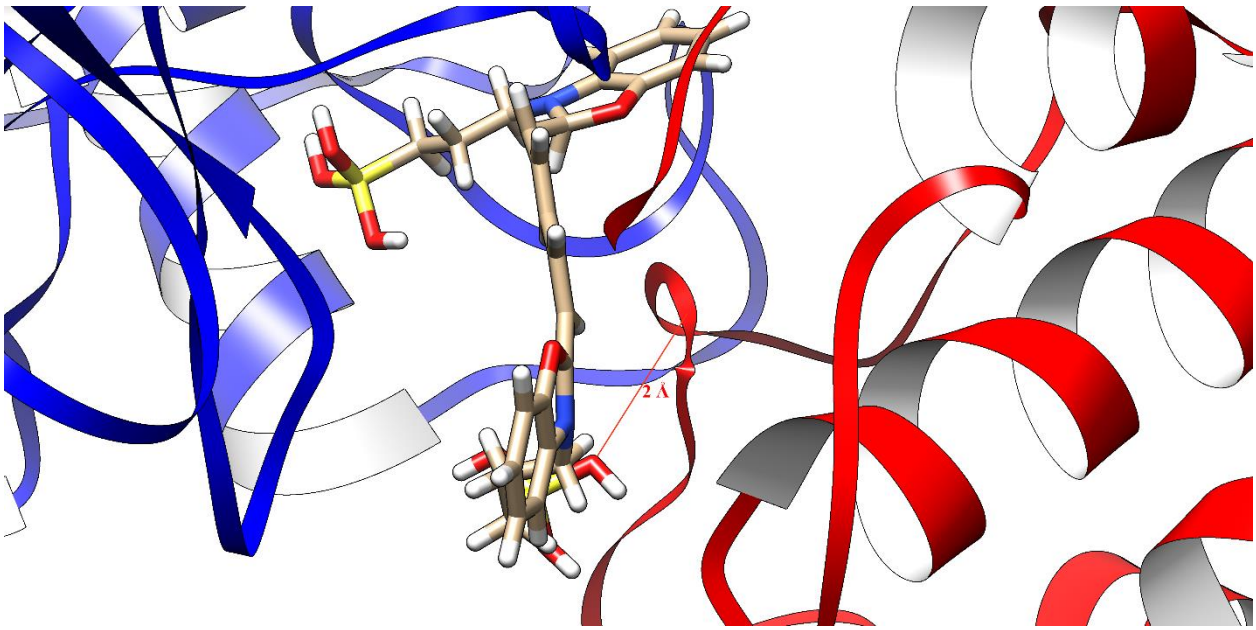

Fig. S6 Result of docking of dye 3.4 with NSP5; the intermolecular hydrogen bond with LEU282 (2 Å) is shown by the red line; the initial configuration of dye 3.4 is given in **Fig. S5**.

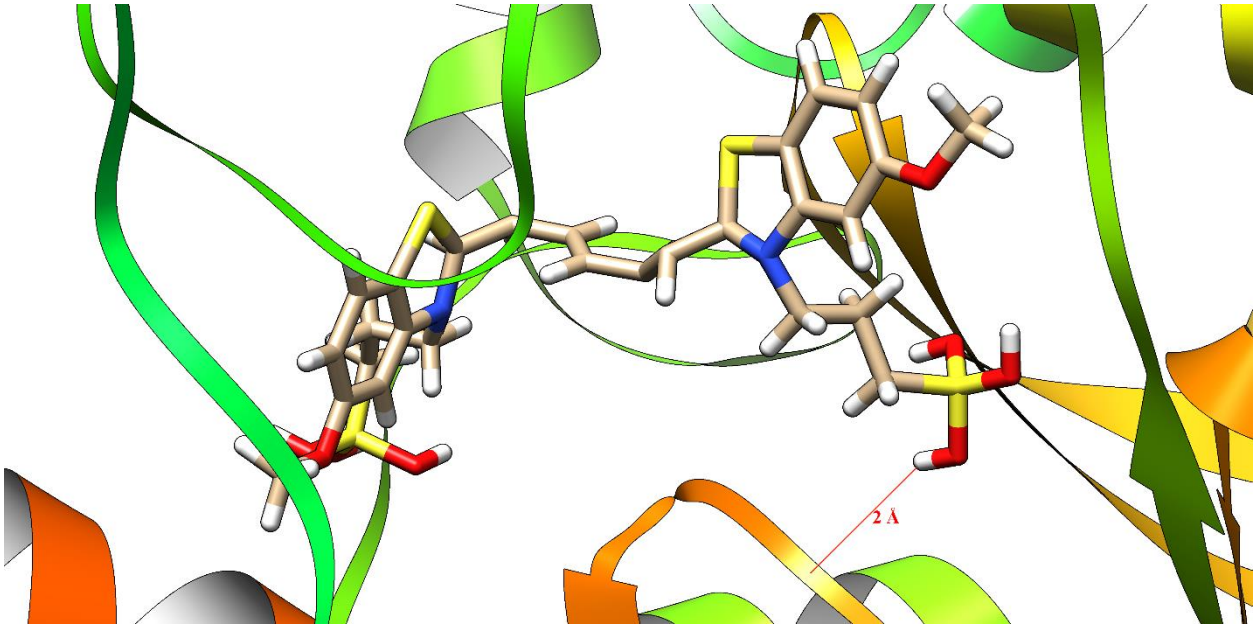

Fig. S7 Result of docking of dye 3.3 with NSP12; the intermolecular hydrogen bond with GLU731 is shown by the red line.

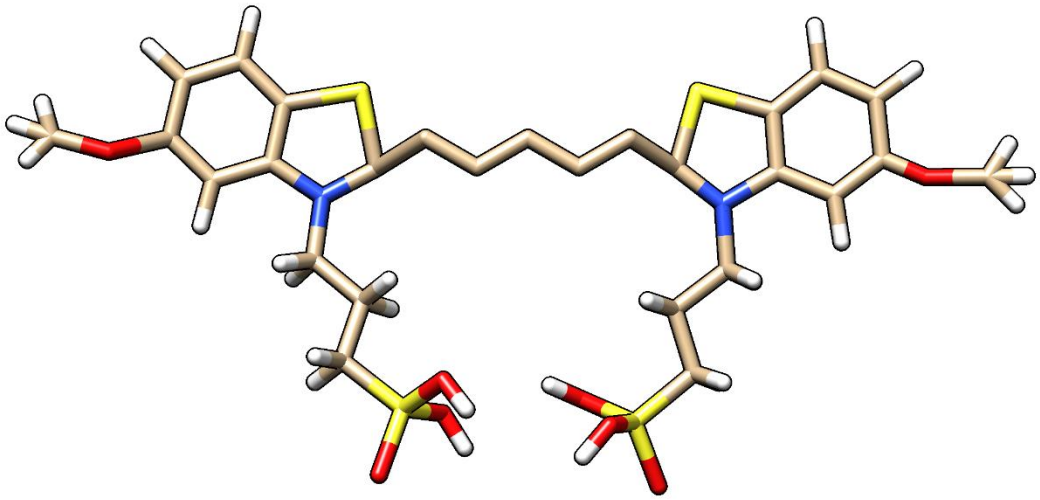

Fig. S8 The initial configuration of dye 3.3.