SUPPORTING INFORMATION

The reactive group effects on the photophysical and biological properties of the 2-phenyl-1*H*-phenanthro[9,10-*d*]imidazole derivatives as fluorescence markers

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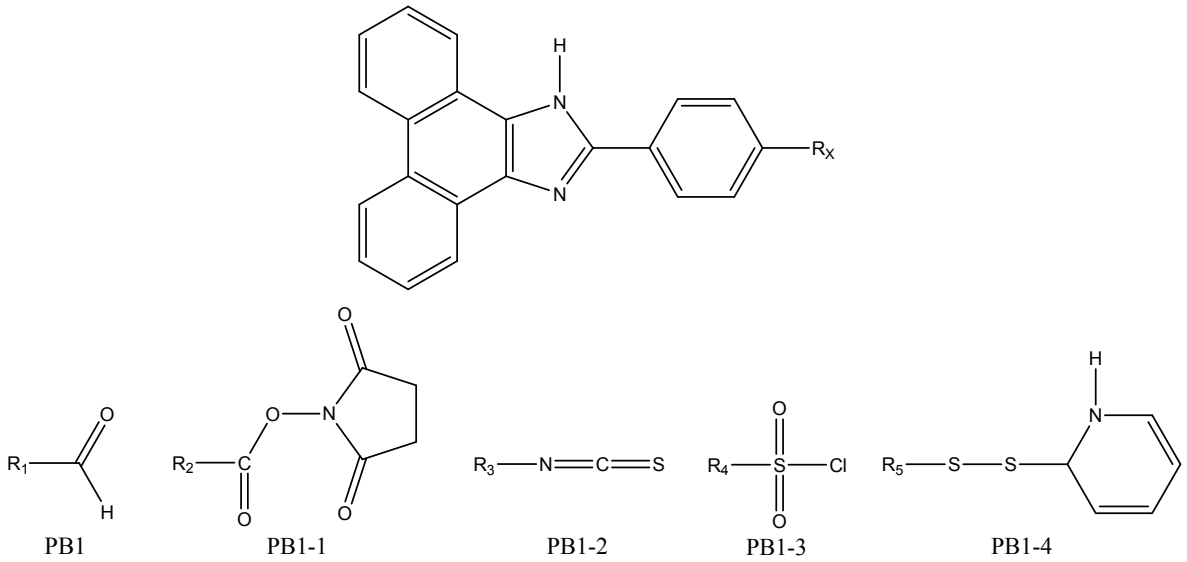


Fig. SI1. Schematic representation of structures of studied PhI derivatives

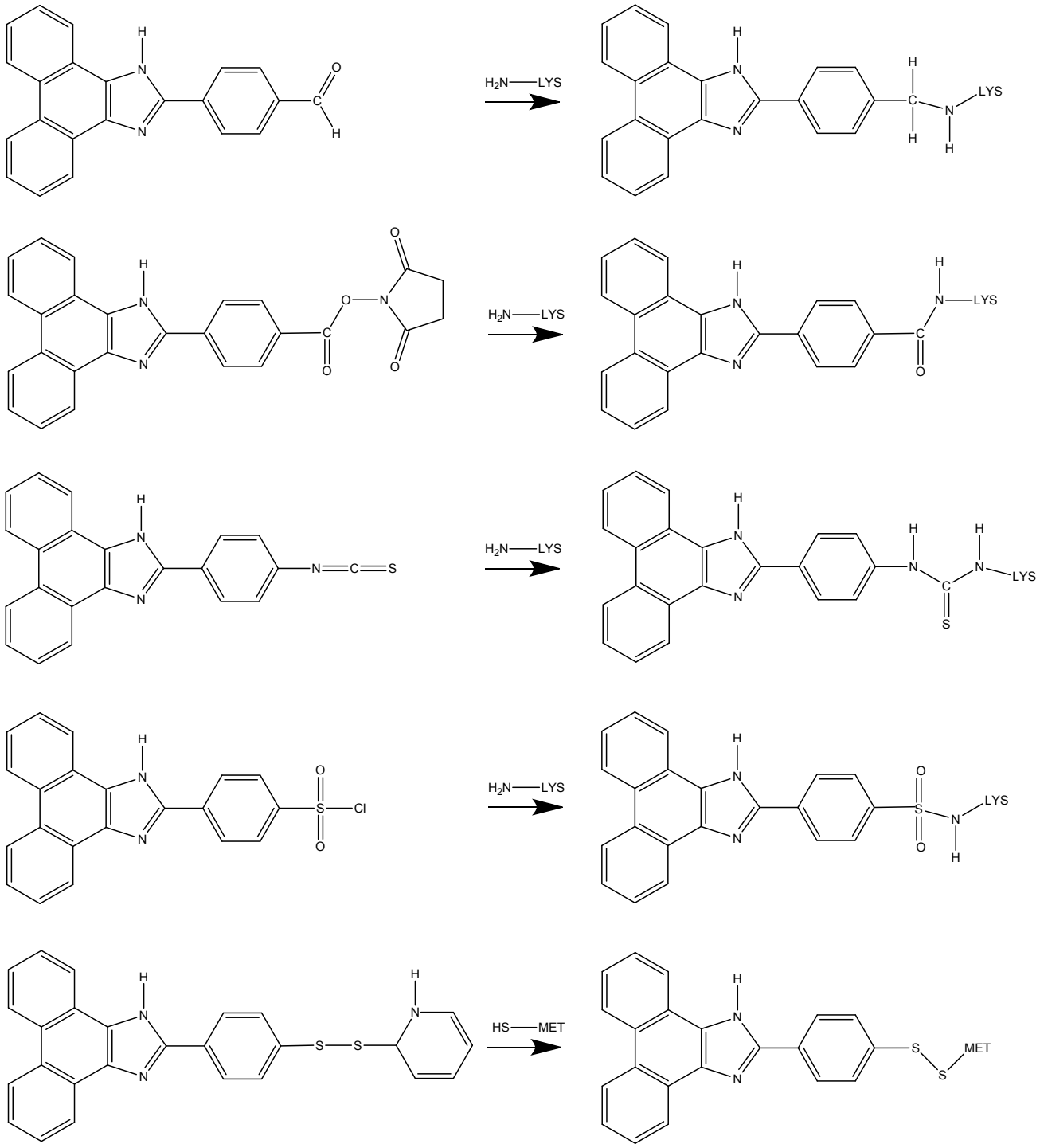


Fig. SI2. A route for bioconjugation of functional groups with protein

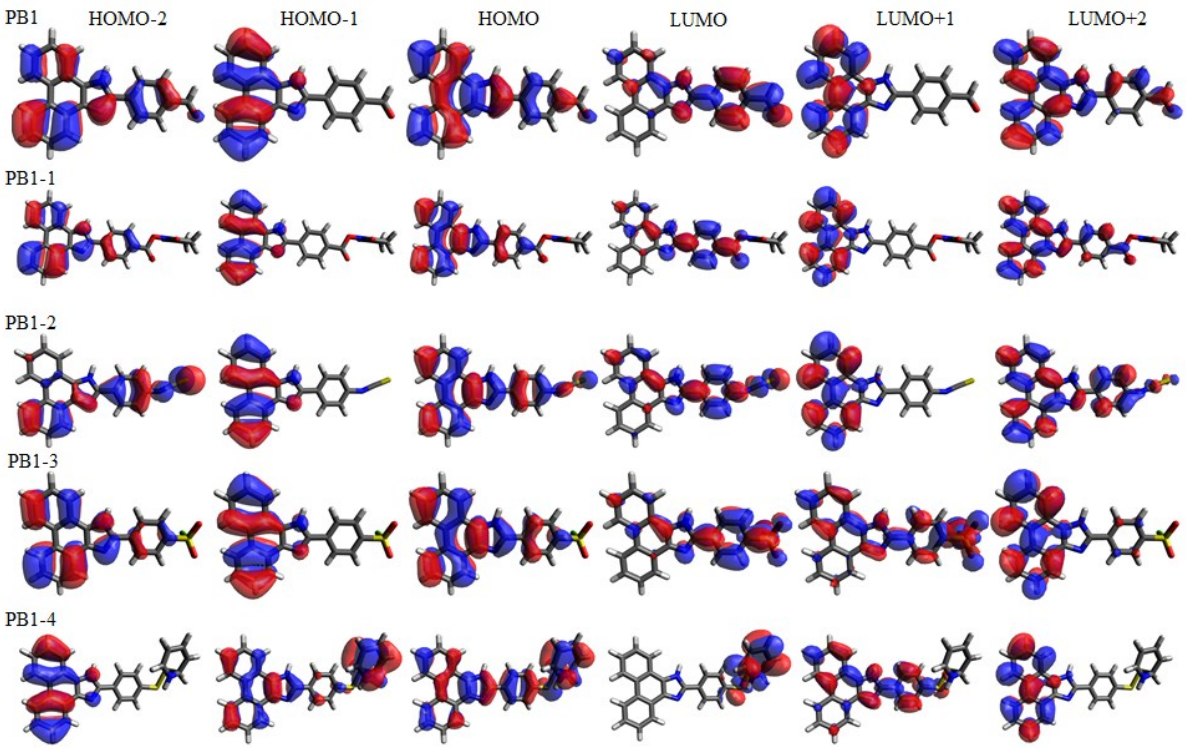


Fig. SI3. Molecular orbitals of PhI derivatives

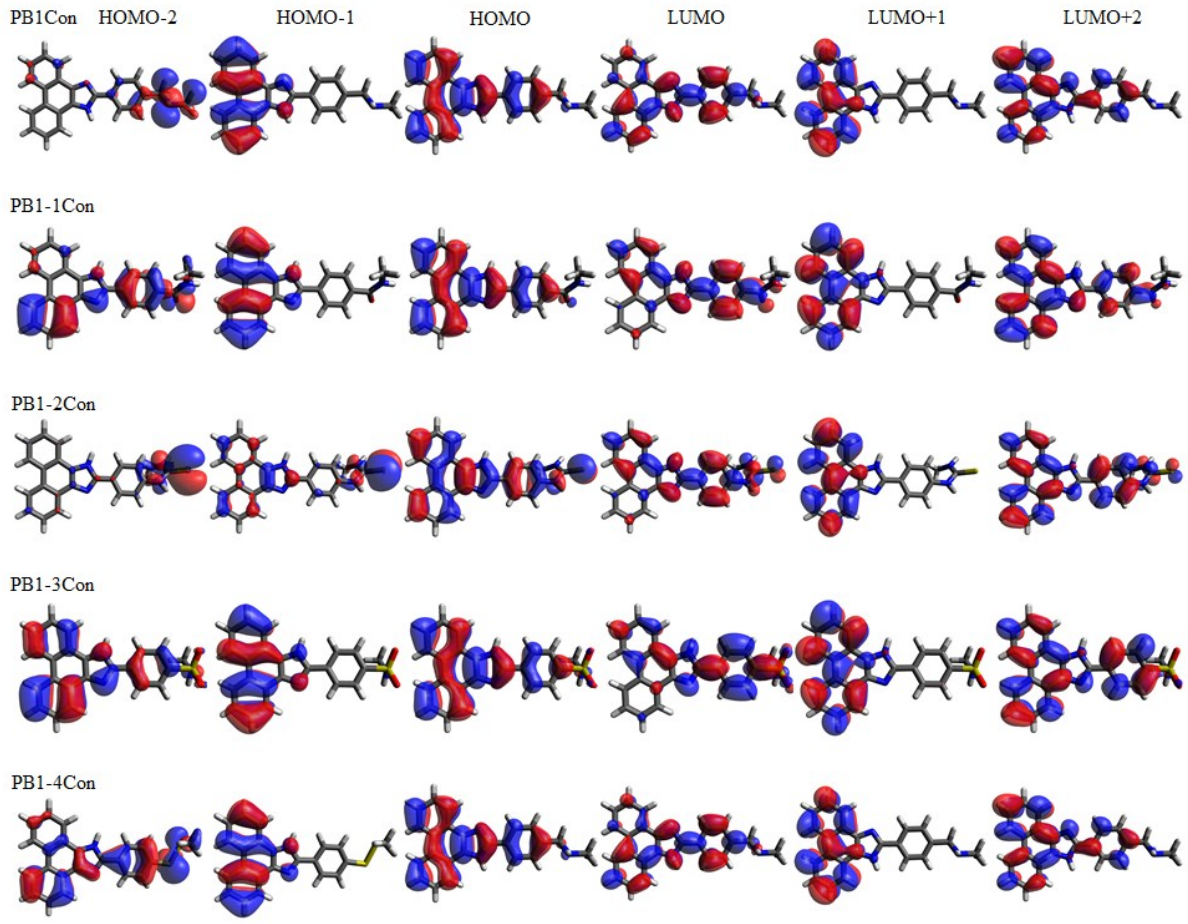


Fig. SI4. Molecular orbitals of biocomplexes

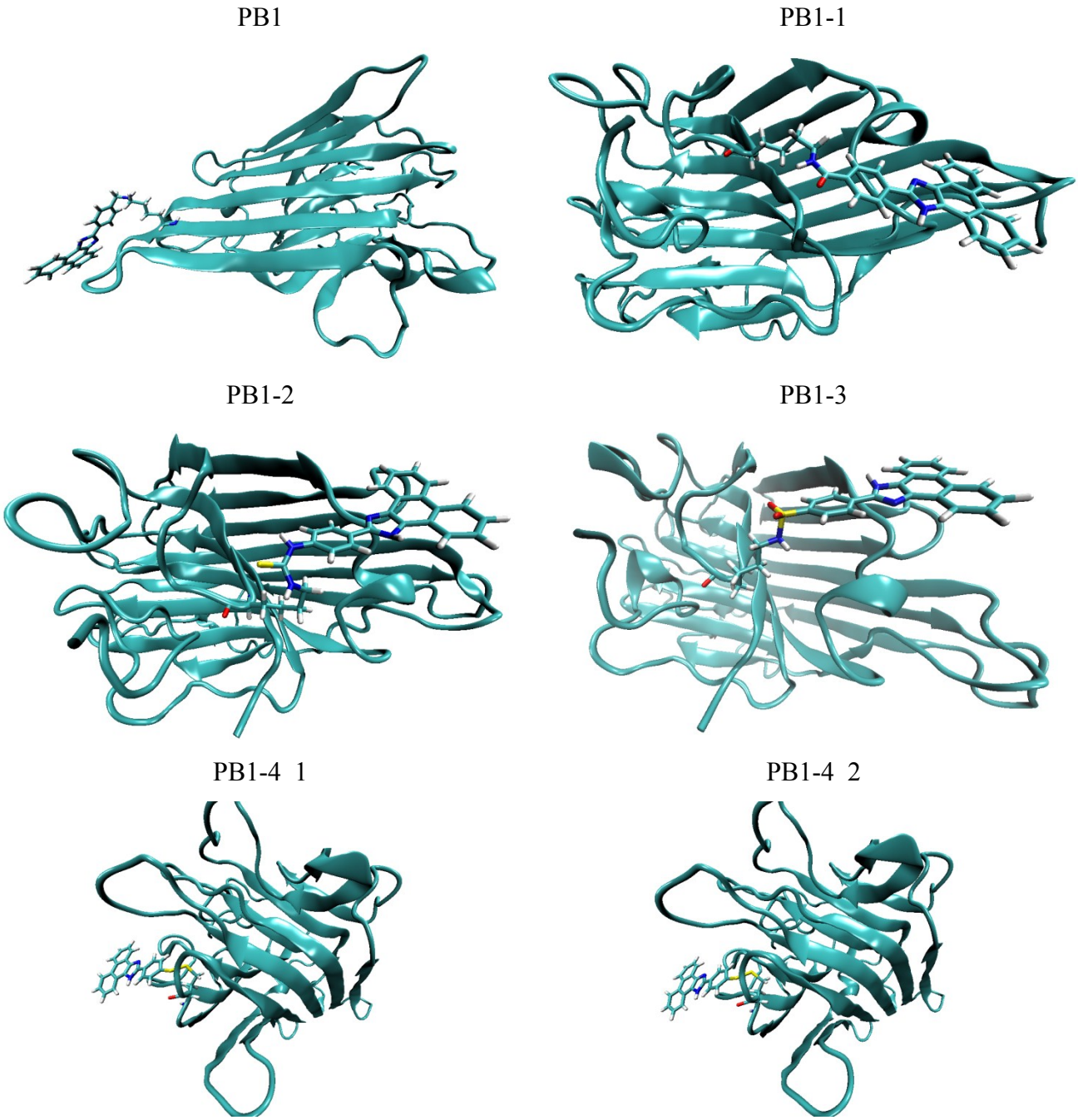


Fig. SI5. Graphic representations of concanavaline protein with probe molecules obtained during MD simulations. The PB1 molecule is bound with lysine LYS 116, the PB1-1-3 bound with lysine LYS 30 and PB1-4 with methionine 42

Tables:

Table SI1. The frontier orbital energies in selected solvents. All values are given in eV

	PB1						PB1Con					
	E_{HOMO}	E_{LUMO}	E_{GAP}	η [a]	μ [b]	χ [c]	E_{HOMO}	E_{LUMO}	E_{GAP}	η [a]	μ [b]	χ [c]
GP	-5.9016	-3.5133	2.3883	1.1942	-4.7074	4.7074	-5.6980	-1.3724	4.3256	2.1628	-3.5352	3.5352
Et_2O	-6.0377	-2.3881	3.6496	1.8256	-4.2129	4.2129	-5.8235	-1.4598	4.3637	2.1819	-3.6416	3.6416
THF	-6.0494	-2.3981	3.6512	1.8256	-4.2238	4.2238	-5.8591	-1.4870	4.3722	2.1861	-3.6731	3.6731
MeCN	-6.0684	-2.4126	3.6558	1.8279	-4.2405	4.2405	-5.9098	-1.5289	4.3809	2.1904	-3.7193	3.7193
DMF	-6.0687	-2.4130	3.6554	1.8277	-4.2407	4.2407	-5.9103	-1.5294	4.3809	2.1904	-3.7199	3.7199
DMSO	-6.0698	-2.4134	3.6564	1.8282	-4.2416	4.2416	-5.9136	-1.5321	4.3814	2.1907	-3.7229	3.7229
Water	-6.0717	-2.4150	3.6567	1.8283	-4.2433	4.2433	-5.9098	-1.5234	4.3863	2.1932	-3.7166	3.7166
	PB1-1						PB1-1Con					
	E_{HOMO}	E_{LUMO}	E_{GAP}	η [a]	μ [b]	χ [c]	E_{HOMO}	E_{LUMO}	E_{GAP}	η [a]	μ [b]	χ [c]
GP	-60.276	-2.3042	3.7234	1.8617	-4.1659	4.1659	-5.8869	-17858	4.1011	2.0506	-3.8363	3.8363
Et_2O	-6.0466	-2.3573	3.6894	1.8447	-4.2020	4.2020	-5.9462	-1.8037	4.1425	2.0712	-3.8750	3.8750
THF	-6.0651	-2.3812	3.6839	1.8420	-4.2232	4.2232	-5.9680	-1.8233	4.1447	2.0723	-3.8957	3.8957
MeCN	-6.0937	-2.4158	3.6780	1.8390	-4.2547	4.2547	-6.0009	-1.8426	4.1583	2.0791	-3.9218	3.9218
DMF	-6.0940	-2.4160	3.6780	1.8390	-4.2550	4.2550	-6.0015	-1.8429	4.1585	2.0793	-3.9222	3.9222
DMSO	-6.0959	-2.4182	3.6777	1.8388	-4.2571	4.2571	-6.0034	-1.8440	4.1594	2.0797	-3.9237	3.9237
Water	-6.0986	-2.4215	3.6771	1.8386	-4.2601	4.2601	-6.0066	-1.8462	4.1605	2.0802	-3.9264	3.9364
	PB1-2						PB1-2Con					
	E_{HOMO}	E_{LUMO}	E_{GAP}	η [a]	μ [b]	χ [c]	E_{HOMO}	E_{LUMO}	E_{GAP}	η [a]	μ [b]	χ [c]
GP	-5.8893	-1.9980	3.8913	1.9457	-3.9437	3.9437	-5.7897	-1.6943	4.0954	2.0477	-3.7420	3.7420
Et_2O	-5.9136	-2.0021	3.9114	1.9557	-3.9578	3.9578	-5.8346	-1.6739	4.1607	2.0804	-3.7543	3.7543
THF	-5.9318	-2.0187	3.9131	1.9565	-3.9753	3.9753	-5.8523	-1.6780	4.1743	2.0872	-3.7652	3.7652
MeCN	-5.9252	-2.0244	3.9280	1.9640	-3.9885	3.9885	-5.8771	-1.6859	4.1912	2.0956	-3.7815	3.7815
DMF	-5.9528	-2.0247	3.9280	1.9640	-3.9887	3.9887	-5.8774	-1.6859	4.1915	2.0957	-3.7816	3.7816
DMSO	-5.9538	-2.0250	3.9289	1.9644	-3.9894	3.9894	-5.8787	-1.6864	4.1923	2.0961	-3.7826	3.7826
Water	-5.9560	-2.0258	3.9302	1.9651	-3.9909	3.9909	-5.8523	-1.6780	4.1743	2.0872	-3.7652	3.7652
	PB1-3						PB1-3Con					
	E_{HOMO}	E_{LUMO}	E_{GAP}	η [a]	μ [b]	χ [c]	E_{HOMO}	E_{LUMO}	E_{GAP}	η [a]	μ [b]	χ [c]
GP	-6.2420	-2.6365	3.6056	1.8028	-4.4393	4.4393	-6.0769	-2.0525	4.0244	2.0122	-4.0647	4.0647
Et_2O	-6.1590	-2.6746	3.4845	1.7422	-4.4168	4.4168	-6.0646	-2.0329	4.0317	2.0159	-4.0487	4.0487
THF	-6.1552	-2.6887	3.4665	1.7332	-4.4220	4.4220	-6.0717	-2.0351	4.0366	2.0183	-4.0534	4.0534
MeCN	-6.1558	-2.7056	3.4502	1.7251	-4.4307	4.4307	-6.0834	-2.0448	4.0385	2.0193	-4.0641	4.0641
DMF	-6.1558	-2.7056	3.4502	1.7251	-4.4307	4.4307	-6.0837	-2.0448	4.0388	2.0194	-4.0643	4.0643
DMSO	-6.1560	-2.7067	3.4494	1.7247	-4.4314	4.4314	-6.0845	-2.0454	4.0391	2.0195	-4.0649	4.0649
Water	-6.1563	-2.7075	3.4488	1.7244	-4.4319	4.4319	-6.0858	-2.0459	4.0399	2.0199	-4.0659	4.0659
	PB1-4						PB1-4Con					
	E_{HOMO}	E_{LUMO}	E_{GAP}	η [a]	μ [b]	χ [c]	E_{HOMO}	E_{LUMO}	E_{GAP}	η [a]	μ [b]	χ [c]
GP	-5.6210	-1.5071	4.1139	2.0570	-3.5641	3.5641	-5.7214	-1.5166	4.2048	2.1024	-3.6190	3.6190
Et_2O	5.6240	-1.5251	-4.1491	-3.5745	-2.0495	2.0495	-5.7957	-1.5525	4.2432	2.1216	-3.6741	3.6741
THF	-5.6292	-1.5403	4.0889	2.0444	-3.5847	3.5847	-5.8216	-1.5686	4.2530	2.1265	-3.6951	3.6951
MeCN	-5.6327	-1.5713	4.0614	2.0307	-3.6020	3.6020	-5.8583	-1.5817	4.2767	2.1383	-3.7200	3.7200
DMF	-5.6327	-1.5719	4.0608	2.0304	-3.6023	3.6023	-5.8589	-1.5819	4.2769	2.1385	-3.7204	3.7204
DMSO	-5.6346	-1.5762	4.0584	2.0292	-3.6054	3.6054	-5.8610	-1.5836	4.2775	2.1387	-3.7223	3.7223
Water	-5.6349	-1.5776	4.0573	2.0287	-3.6062	3.6062	-5.8616	-1.5877	4.2739	2.1370	-3.7246	3.7246

[a] Chemical hardness; [b] Chemical potential; [c] The Mulliken electronegativity

Table SI2. The values of vertical and cLR corrected excitation and de-excitation energies (in nm) for conjugates

	PB1Con				
	TDDFT			cLR-TDDFT	
	λ_{ABS}	f_{OS}	λ_{Em}	λ_{ABS}	λ_{Em}
GP	335.53	0.44	432.07		
Et_2O	338.68	0.66	444.61	335.46	467.59
THF	338.88	0.67	466.14	335.37	488.75
MeCN	338.02	0.62	495.1	335.1	500.46
DMF	338.76	0.67	497.05	335.16	500.49
DMSO	338.62	0.66	496.77	335.13	500.59
Water	337.87	0.59	494.87	335.29	500.77

	PB1-1Con					PB1-2Con				
	TDDFT			cLR-TDDFT		TDDFT			cLR-TDDFT	
	λ_{ABS}	f_{OS}	λ_{Em}	λ_{ABS}	λ_{Em}	λ_{ABS}	f_{OS}	λ_{Em}	λ_{ABS}	λ_{Em}
GP	349.82	0.76	441.07			357.84	0.73	414.99		
Et_2O	353.41	0.92	457.98	353.38	484.67	356.07	1.16	466.16	351.67	470.78
THF	354.01	0.94	460.45	354.17	489.18	355.52	1.19	467.6	367.33	472.08
MeCN	352.07	0.93	460.05	352.51	495.1	353.28	1.17	465.84	349.14	473.34
DMF	353.23	0.95	462.4	353.71	495.17	354.38	1.21	468.1	349.55	473.32
DMSO	352.99	0.95	462.12	353.49	494.52	354.14	1.2	467.76	349.41	473.04
Water	351.74	0.92	459.92	352.22	494.08	352.88	1.17	465.48	348.89	476.89

	PB1-3Con					PB1-4Con				
	TDDFT			cLR-TDDFT		TDDFT			cLR-TDDFT	
	λ_{ABS}	f_{OS}	λ_{Em}	λ_{ABS}	λ_{Em}	λ_{ABS}	f_{OS}	λ_{Em}	λ_{ABS}	λ_{Em}
GP	356.87	0.76	487.32			343.47	0.85	537.81		
Et_2O	363.47	0.92	504.38	365.37	508.43	347.62	1.03	582.71	342.55	592.08
THF	363.82	0.94	506.89	366.48	510.12	347.71	1.05	591.38	342.13	592.99
MeCN	362.7	0.94	506.58	365.63	511.28	345.43	0.99	596.47	340.6	600.99
DMF	363.98	0.96	508.93	367.33	511.36	346.46	1.03	600.23	340.8	614
DMSO	363.75	0.96	508.66	367.09	510.74	346.27	1.02	600.12	340.73	613.1
Water	362.42	0.93	506.47	365.38	508.33	345.54	0.98	597.16	340.78	612.18

Table SI3. Calculated values of dipole moments (in D) for the ground and CT excited state

	PB1		PB1-1		PB1-2		PB1-3		PB1-4	
	μ_g	μ_{CT}	μ_g	μ_{CT}	μ_g	μ_{CT}	μ_g	μ_{CT}	μ_g	μ_{CT}
GP	5.62	16.86	3.47	13.92	3.62	13.19	7.08	22.38	3.15	9.38
Et_2O	7.23	21.09	4.92	17.01	5.57	16.39	8.47	28.57	4.22	13.65
THF	7.61	21.92	5.32	17.65	5.89	17.14	8.76	29.77	4.55	14.71
MeCN	8.11	22.86	5.87	18.45	6.29	17.69	9.12	31.22	5.60	16.42
DMF	8.13	22.90	5.88	18.46	6.29	17.65	9.12	31.18	5.61	16.42
DMSO	8.16	22.96	5.91	18.51	6.31	17.68	9.14	31.27	5.85	16.47
Water	8.21	23.04	5.96	18.57	6.34	17.77	9.17	31.44	5.91	16.66
	PB1Con		PB1-1Con		PB1-2Con		PB1-3Con		PB1-4Con	
	μ_g	μ_{CT}	μ_g	μ_{CT}	μ_g	μ_{CT}	μ_g	μ_{CT}	μ_g	μ_{CT}
GP	2.89	4.47	5.65	11.17	4.77	4.83	6.33	15.04	3.44	5.77
Et_2O	3.71	6.97	7.60	13.41	6.35	9.76	7.85	18.39	4.92	7.65
THF	3.89	7.50	8.31	13.99	6.75	10.55	8.22	19.01	5.29	7.89
MeCN	4.02	7.95	9.01	14.50	7.27	11.11	8.98	19.81	5.69	7.59
DMF	4.03	8.01	9.02	14.55	7.28	11.21	8.99	19.83	5.70	7.87
DMSO	4.03	8.03	9.06	14.58	7.31	11.22	9.02	19.87	5.73	7.84
Water	4.27	8.40	9.13	14.58	7.24	11.15	9.07	19.92	6.14	7.85

Table SI4. CT parameters for the bright low-lying excited state

	D_{CT}	q_{CT}	D_{CT}	q_{CT}	D_{CT}	q_{CT}	D_{CT}	q_{CT}	D_{CT}	q_{CT}
	PB1		PB1-1		PB1-2		PB1-3		PB1-4	
GP	3.997	0.680	3.960	0.702	3.762	0.585	4.4250	0.744	1.393	0.532
Et_2O	4.739	0.721	4.585	0.738	4.258	0.604	5.340	0.816	1.553	0.574
THF	4.870	0.729	4.702	0.745	4.369	0.607	5.506	0.831	1.824	0.585
MeCN	5.032	0.736	4.865	0.750	4.484	0.608	5.706	0.848	2.431	0.608
DMF	5.024	0.738	4.889	0.752	4.469	0.608	5.736	0.848	2.474	0.611
DMSO	5.022	0.738	4.868	0.752	4.460	0.608	5.705	0.849	2.468	0.613
Water	5.015	0.737	4.864	0.751	4.460	0.607	5.692	0.848	2.465	0.613
	PB1Con		PB1-1 Con		PB1-2 Con		PB1-3 Con		PB1-4 Con	
GP	0.293	0.427	3.311	0.593	0.482	0.594	3.361	0.623	1.829	0.473
Et_2O	1.172	0.441	3.699	0.604	2.186	0.538	3.878	0.657	1.504	0.471
THF	1.089	0.443	3.760	0.604	2.338	0.533	3.971	0.661	1.361	0.469
MeCN	1.202	0.444	3.825	0.601	2.409	0.524	4.078	0.661	1.828	0.459
DMF	1.060	0.446	3.824	0.604	2.409	0.527	4.071	0.663	1.904	0.463
DMSO	1.044	0.446	3.836	0.604	2.455	0.526	4.077	0.663	1.902	0.463
Water	1.089	0.446	3.829	0.600	2.466	0.523	4.094	0.661	1.852	0.459

Table SI5. Two-photon absorption cross section (δ_{TSM}^{OF}) expressed in a.u.

	δ_{TSM}^{OF}				
	PB1	PB1-1	PB1-2	PB1-3	PB1-4
GP	150608	30432	25529	41591	1819
Et_2O	178243	43689	35362	96255	4883
THF	98437	44596	38807	102506	5997
MeCN	48218	44395	37735	74098	7412
DMF	49930	45131	38428	80139	7797
DMSO	49449	45197	38163	89393	7387
Water	48387	44357	37722	96392	7271

Table SI6. The values of free energies (DGsolv) of solvation in kcal/mol obtained using SMD solvation model

	PB1	PB1-1	PB1-2	PB1-3	PB1-4	PB1Con	PB1-1 Con	PB1-2 Con	PB1-3 Con	PB1-4 Con
Et_2O		-28.81	-22.01	-24.34	-26.10	-21.19	-25.48	-29.63	-27.02	-21.30
THF		-30.36	-21.74	-25.34	-27.27	-22.02	-25.76	-31.00	-28.81	-21.82
MeCN	-22.70	-33.66	-24.46	-27.73	-30.20	-25.59	-30.64	-33.39	-31.72	-24.98
DMF	-21.30	-32.90	-22.28	-26.95	-27.73	-23.30	-28.67	-31.33	-31.27	-22.86
DMSO	-19.11	-30.30	-19.61	-24.65	-25.08	-20.66	-26.20	-28.64	-28.80	-22.36
Water	-13.48	-22.93	-11.24	-18.91	-17.86	-15.78	-21.48	-22.02	-24.31	-14.60

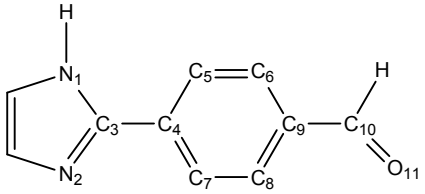
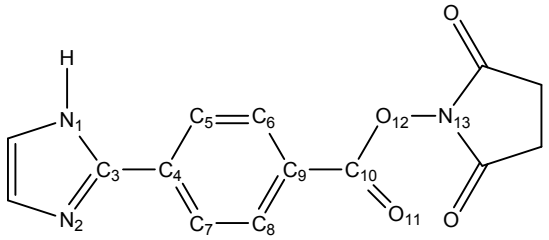
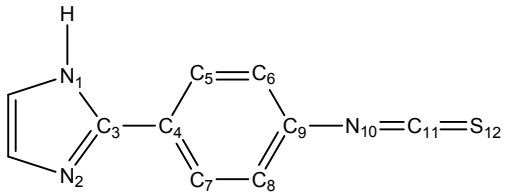
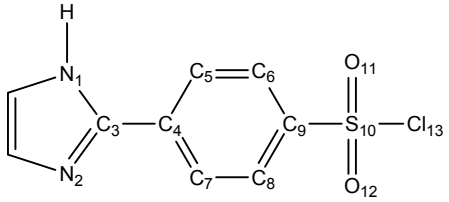
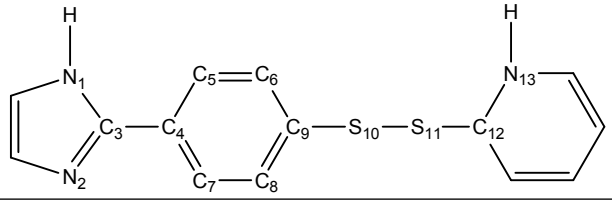
Table SI7. Calculated probability of the biological activity

	PB1	PB1-1	PB1-2	PB1-3	PB1-4	PB1 Con	PB1-1 Con	PB1-2 Con	PB1-3 Con	PB1-4 Con
Alpha-Radioprotector activity	0.95	0.96	0.93	0.98	0.74	0.85	0.87	0.93	0.97	0.93
Gamma-radioprotector activity mechanism I	0.63	0.77	0.72	0.76	0.78	0.26	0.28	0.88	0.91	0.54
Analgetic activity	0.69	0.36	0.00	0.00	0.00	0.95	0.93	0.00	0.10	0.98
Anti-infectious_laryngotracheitis_activity	0.85	0.77	0.76	0.85	0.00	0.99	1.00	0.57	0.96	0.65
Anti-Adenovirus activity	0.00	0.00	0.00	0.00	0.00	0.92	0.11	0.00	0.00	0.00
Anti-Arrhytmic activity	0.00	0.09	0.00	0.00	0.84	0.62	0.12	0.06	0.00	0.80
Anti-Bacterial activity	0.00	0.00	0.00	0.00	0.00	0.61	0.98	0.00	0.06	0.00
Anti-Oxidant activity	0.00	0.00	0.00	0.00	0.00	0.02	0.14	0.00	0.00	0.01
Anti-Psychotic activity diazepine site	0.47	0.80	0.50	0.90	0.98	0.00	0.16	0.59	0.88	0.39
Anti-Tumor Alkylic activity	0.40	0.76	0.24	0.17	0.53	0.90	0.51	0.05	0.22	0.61
Anti-Tumor Antimitotic activity	0.44	0.05	0.10	0.14	0.39	0.24	0.01	0.15	0.00	0.25
Anti-Tumor Cycline-dependent kinase 4 inhibitory activity	0.99	0.91	1.00	0.99	0.98	0.53	0.61	1.00	0.98	0.99
Anti-Tumor Dihydrofolate reductase inhibitory activity	0.01	0.02	0.00	0.01	0.00	0.40	0.22	0.01	0.06	0.00
Anti-Tumor DNA anti-metabolitic activity	0.99	0.00	0.98	1.00	0.69	0.89	0.16	0.99	1.00	0.96
Anti-Tumor Topoisomerase I inhibitory activity	0.63	0.06	0.06	0.01	0.03	1.00	0.98	0.97	0.21	0.98
Anti-Tumor Topoisomerase II inhibitory activity	0.72	0.14	0.89	0.36	0.26	0.93	0.00	0.00	0.00	0.00
HIV1-proteaze inhibitory activity	0.60	0.59	0.60	0.66	0.06	0.13	0.02	0.36	0.62	0.46
HT51 A inhibitory activity	0.89	0.95	0.95	0.98	0.61	0.03	0.00	0.95	0.99	0.85
Tuberculostatic Dihydrofolate reductase inhibitory activity	0.98	0.98	0.91	0.87	0.96	0.98	0.81	0.93	0.89	0.97
Human factor XA Inhibitory activity	0.99	0.00	0.65	0.00	0.00	1.00	0.82	0.93	0.00	0.65
Metabolism at CYP450 2D6	0.77	0.96	0.92	0.90	0.43	0.87	0.71	0.87	0.92	0.66
Metabolism at CYP450 3A4	0.99	0.99	0.99	0.96	0.24	0.82	0.73	0.96	0.95	0.99
Progestagenic activity	0.99	1.00	1.00	1.00	1.00	0.00	0.00	0.91	0.95	1.00
Vasorelaxant_activity	0.12	0.64	0.39	0.35	0.00	0.28	0.00	0.00	0.18	0.00
COX1 inhibitory activity	0.75	0.59	0.92	0.75	0.93	0.05	1.00	0.64	0.86	0.00
COX2 inhibitory activity	0.98	0.95	0.99	0.98	0.00	0.96	0.00	1.00	1.00	0.97

Table SI8. Binding free energies (ΔG_b, kcal/mol) and values of the inhibitor constants (K_i in mM) obtained during AutoDock simulations

	PB1		PB1-1		PB1-2		PB1-3		PB1-4		
LYS	ΔG_b	K_i	ΔG_b	K_i	ΔG_b	K_i	ΔG_b	K_i	MET	ΔG_b	K_i
30	-5.33	0.35	-5.44	0.77	-5.25	0.39	-5.63	0.20	42	-5.22	0.15
35	-4.31	1.21	-4.97	1.71	-4.24	2.12	-4.89	0.71	129	-4.67	0.38
36	-4.27	2.68	-4.89	1.95	-3.85	4.12	-4.49	1.41			
39	-3.70	9.99	-3.69	14.68	-3.02	16.79	-3.29	10.65			
46	-4.62	0.98	-5.19	1.17	-4.42	1.57	-4.52	1.33			
59	-4.14	5.67	-3.59	17.45	-3.04	16.29	-3.64	5.93			
101	-5.63	0.49	-4.64	3.00	-4.38	1.70	-5.23	0.54			
114	-4.80	1.35	-5.10	1.37	-4.43	1.54	-4.55	1.27			
116	-5.84	0.79	-5.03	1.54	-4.70	0.99	-5.17	0.44			
135	-3.79	10.70	-3.29	28.82	-3.27	10.99	-3.27	10.89			
138	-3.97	3.41	-3.47	21.27	-3.86	4.07	-3.74	4.99			
200	-3.24	16.58	-3.17	35.27	-3.08	15.18	-3.21	12.18			
TER	-4.51	1.02	-4.34	4.95	-3.88	3.92	-3.99	3.25			

Table SI9. Change of structural parameters after docking simulation

PB1			PB1-1		
					
	output	AutoDock		output	AutoDock
N1-C3-C4-C7	-179.99953	-173.84678	N1-C3-C4-C7	-176.42603	80.24600
N2-C3-C4-C5	-179.99926	-173.74735	N2-C3-C4-C5	-176.66506	79.93283
C6-C9-C10-O11	179.99050	-62.26327	C6-C9-C10-O12	0.93464	53.97451
N1-O11	7.51221	7.23555	C6-C9-C10-O11	-179.00352	-125.99654
			C8-C9-C10-O12	-179.27950	-125.81530
			C8-C9-C10-O11	0.78234	54.21365
			C9-C10-O12-N13	-179.30279	118.56210
			O11-C10-O12-N13	0.63942	-61.46497
			N1-N13	8.42422	7.75775
			C9-N13	3.58451	3.32495
			C10-N13	2.29407	2.29419
PB1-2			PB1-3		
					
N1-C3-C4-C7	-179.93550	-160.91580	N1-C3-C4-C7	-179.16998	-110.93957
N2-C3-C4-C5	-179.93329	-160.83276	N2-C3-C4-C5	-179.64054	-110.74302
C9-N10-C11-S12	179.89729	177.12026	C6-C9-S10-Cl13	-90.46260	38.34579
N1-S12	9.26157	9.25485	C8-C9-S10-Cl13	90.04492	-142.22705
N1-N10	5.16158	6.50367	C6-C9-S10-O12	157.83271	149.98615
			C8-C9-S10-O11	-158.22939	106.07361
			N1-Cl13	7.58784	7.62153
PB1-4					
					
	N1-C3-C4-C7	176.86030	171.98689		
	N2-C3-C4-C5	176.90453	172.03220		
	C9-S10-S11-C12	91.25539	81.81705		
	C6-C9-S10-S11	14.20259	-166.47000		
	C8-C9-S10-S11	-168.13967	15.90356		
	S10-S11-C12-N13	-54.85169	-134.93924		
	C9-N13	3.59341	4.52755		
	C9-C12	3.95677	3.81541		
	N1-N13	71.8635	8.55496		