

Figure S1: Absorption spectrum of 3PBI in various solvents and at different H^+ concentrations.

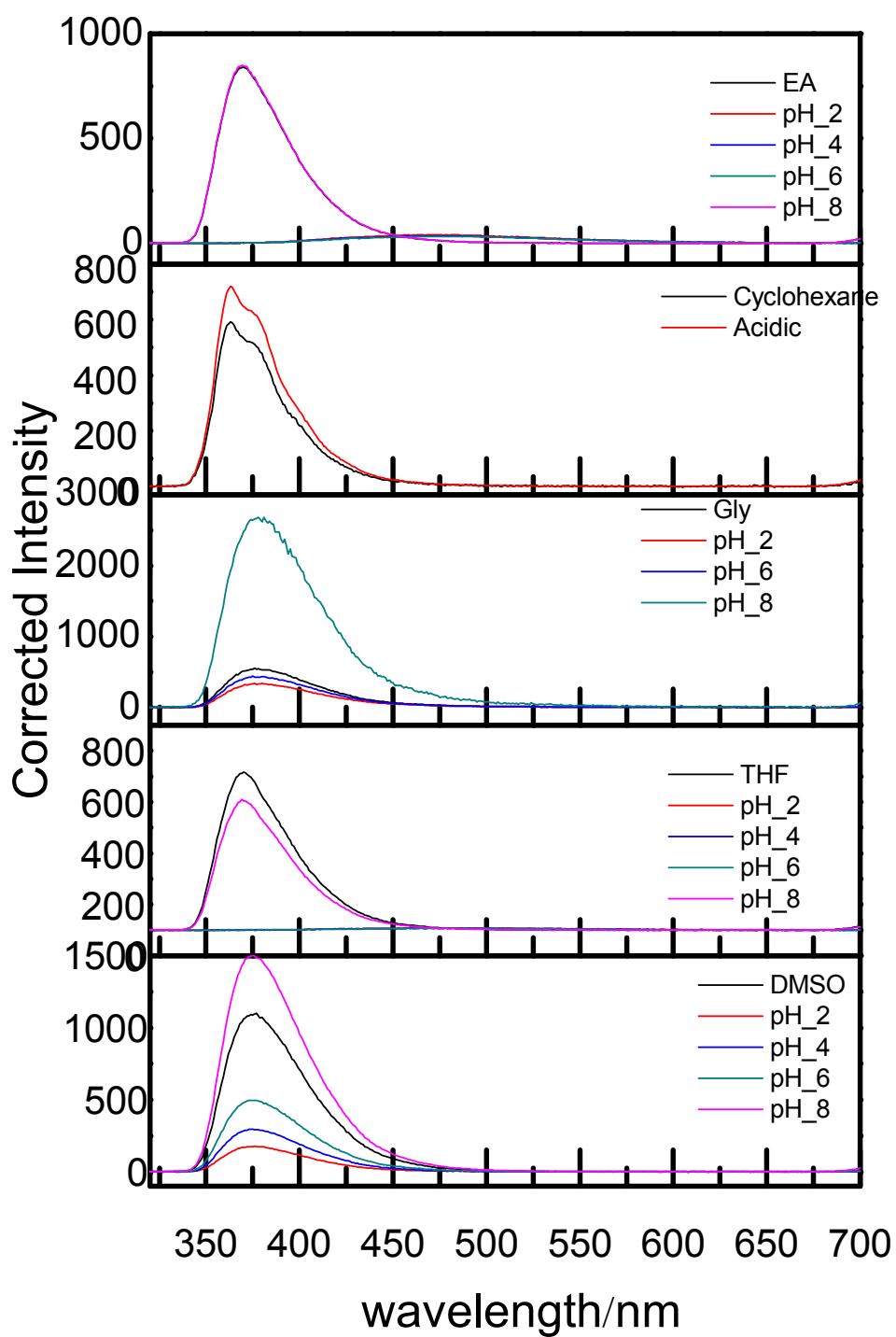


Figure: S2 Fluorescence spectrum of 3PBI in different solvents at different H^+ concentrations.

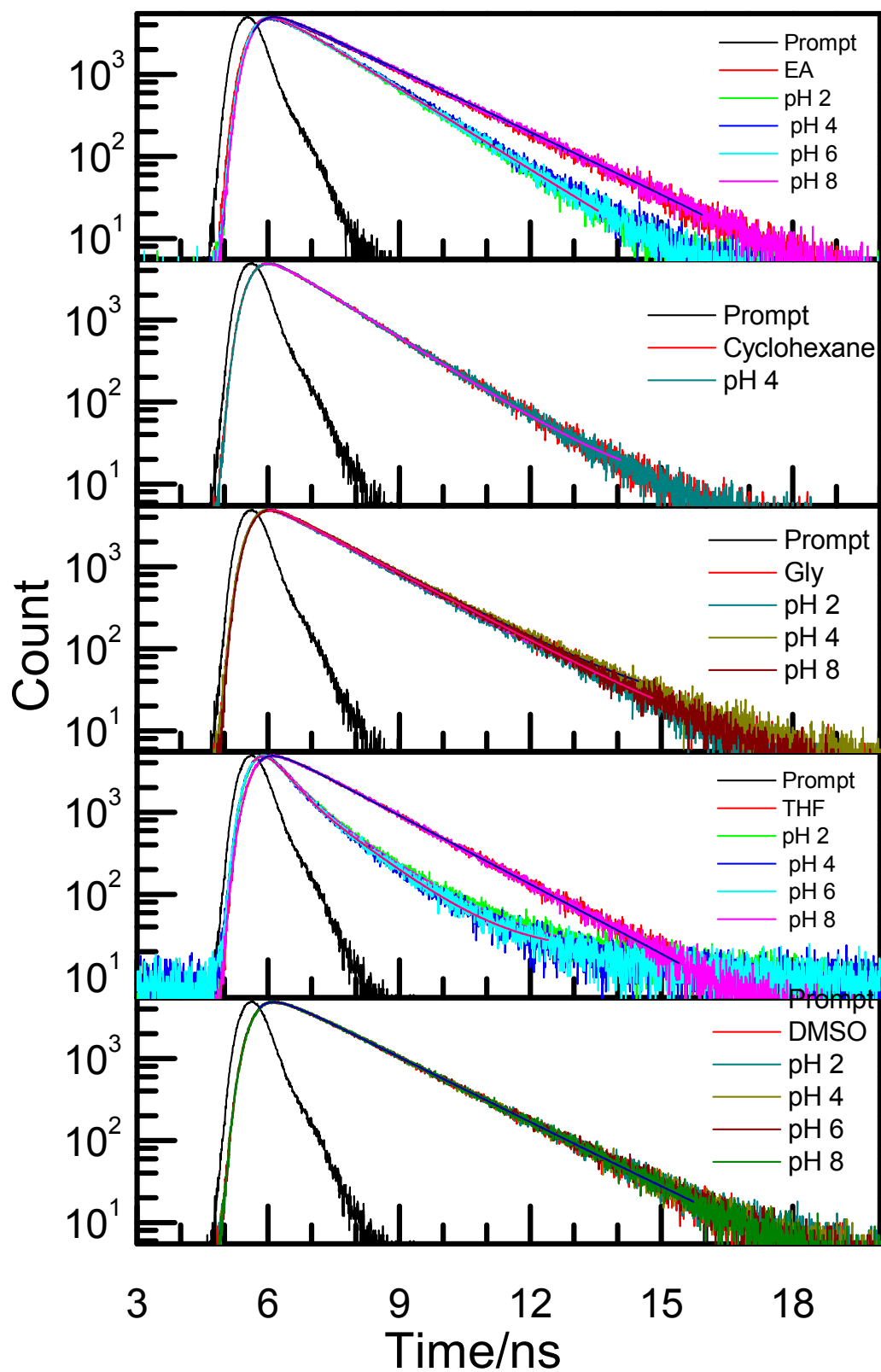


Figure S3. Temporal features of fluorescence of 3PBI

Figure S4. Optimized structure of 3PBI in ground state

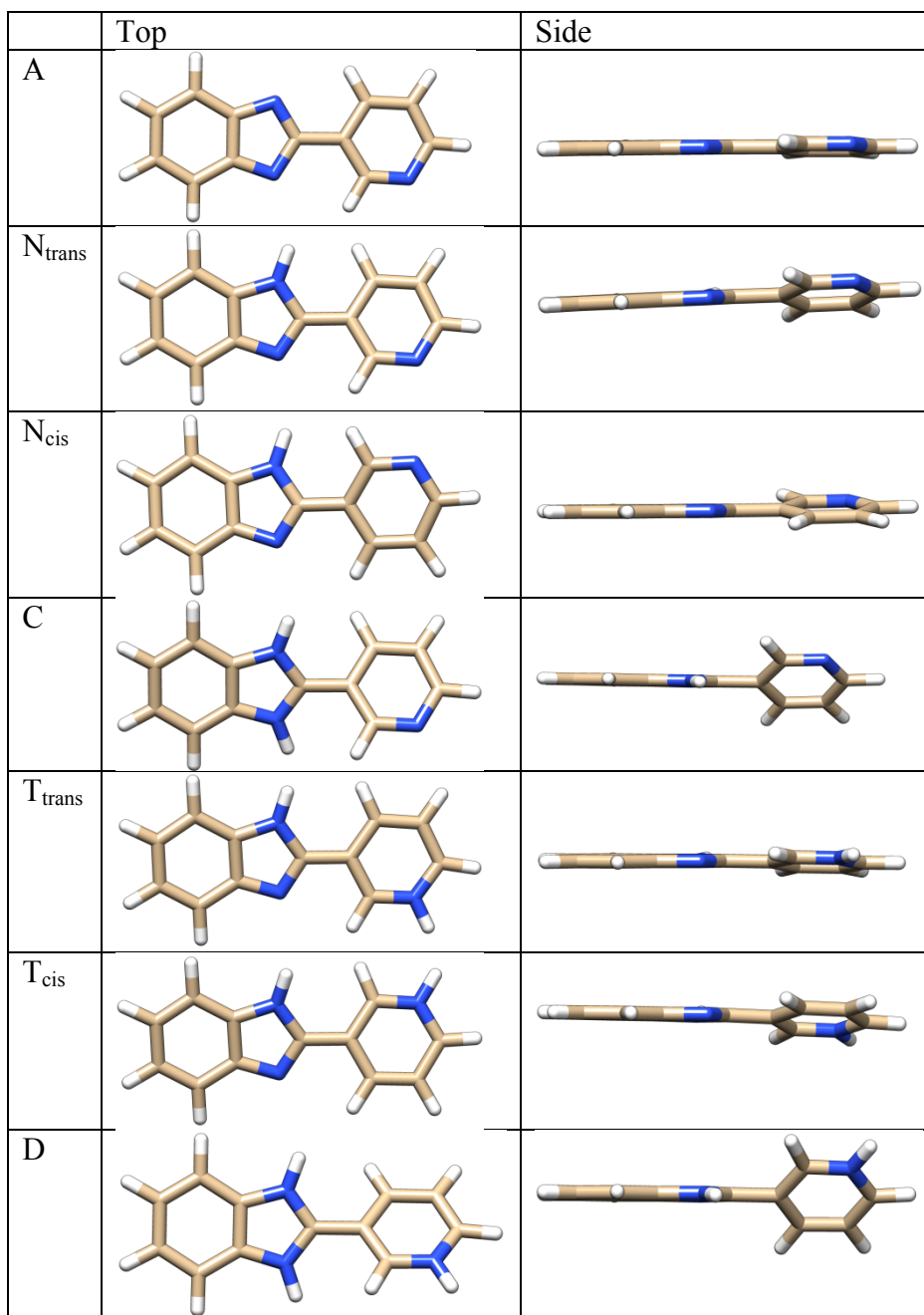


Figure S5. Optimized structure of 3PBI in excited state

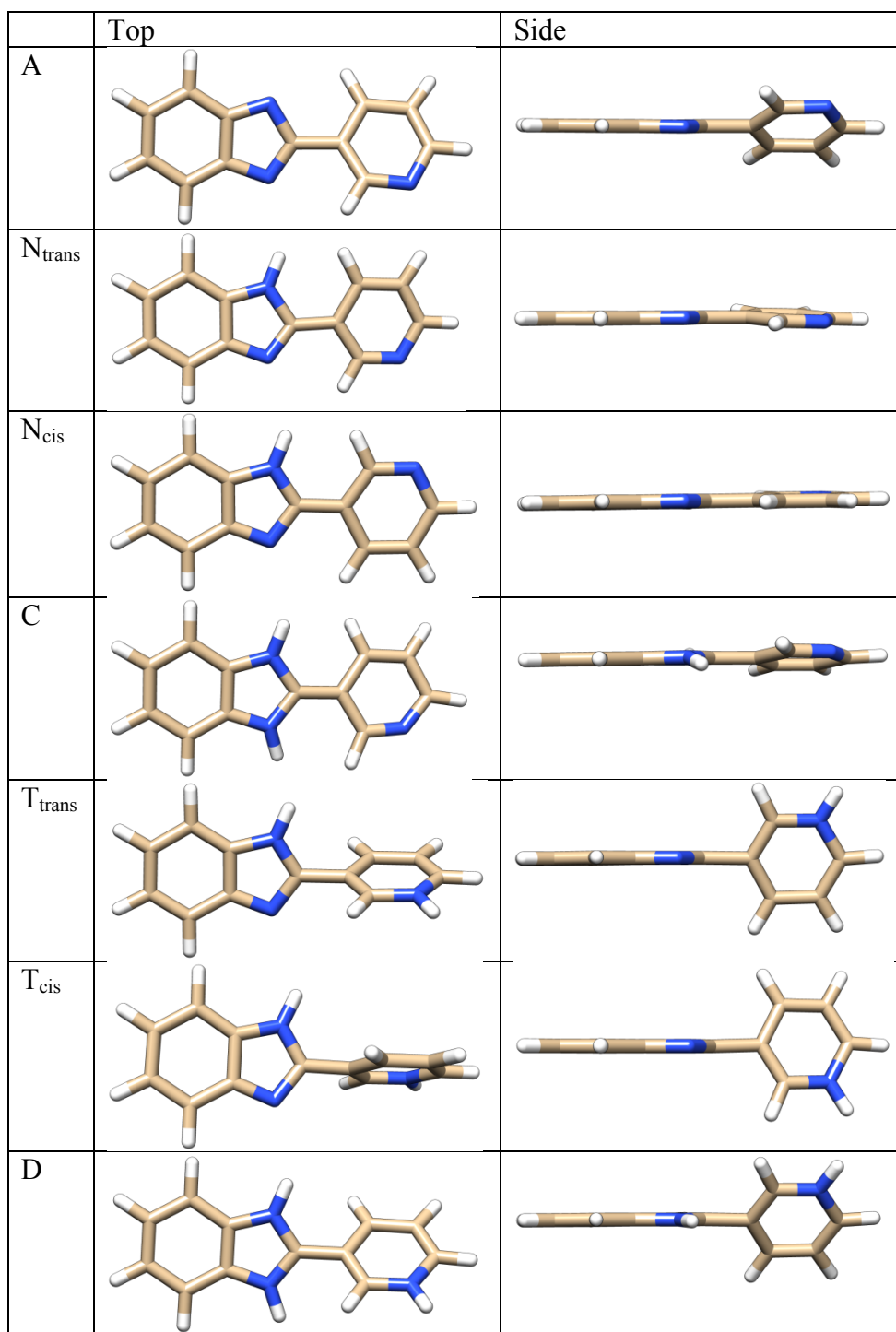


Table S1. Calculated photophysical properties of 3PBI using B3LYP/TZVP level.^a

Ground state	A	N _{trans}	C	T _{trans}	D
Optimized structure ^a	 -0.227 -0.231 -0.160	 -0.196 -0.173	 -0.157	 -0.178	 -0.197
HOMO					
LUMO					
ω^b	-4	-15	-36	-7	-42
PA ^c	-	-47.7	-29.8	-30.0	-23.5
Excited state	A*	N _{trans} *	C*	T _{trans} *	D*
Optimized structure ^a	 -0.309 -0.259 -0.199	 -0.185 -0.174	 -0.160	 -0.197	
ω^b	-28	4	-9	-77	-49
PA ^c	-	-39.4	-41.2	-49.9	-12.6

^a Löwdin charges (in a.u) on nitrogens are shown

^b ω denotes dihedral angles (in degrees) between the two heterocyclic rings

^c PA denotes proton affinity (kcal mol⁻¹)

Table S2: Anisotropy of 3PBI in various solvents and nafion at different hydration levels

System	Anisotropy
Cyclohexane	0.0224
DMSO	0.04174
EA	0.01674
THF	0.02899
Gly	0.29812
Nafion ($\lambda = 6$)	0.00601
Nafion ($\lambda = 1$)	0.32509

Table S3: Temporal features of fluorescence of 3PBI in various solvents at different acid concentrations.

Solvents		τ_1/ps	τ_2/ps	a_1	a_2	χ^2
Cyclohexane	Neat solvent	1340±2				1.08
	pH4	1300±2				1.09
Glycerol	Neat solvent	1560±2				1.07
	pH2	1500±3				1.19
	pH6	1580±2				1.06
	pH8	1560±2				1.16
DMSO	Neat solvent	1628±2				1.05
	pH2	1638±2				1.06
	pH4	1635±2				1.02
	pH6	1628±2				1.03
Ethyl acetete	pH8	1644±2				1.00
	Neat solvent	1711±2				1.01
	pH2	1299±2				1.03
	pH4	1359±2				1.11
THF	pH6	1321±2				1.10
	pH8	1733±2				1.03
	Neat solvent	1526±2	--	--	--	1.12
	pH2	1315±18	500±4	0.27	0.73	1.11
	pH4	1180±18	300±4	0.19	0.81	1.63
	pH6	1328±52	500±6	0.25	0.75	1.66
	pH8	1555±2	--	--	--	1.07