White Light Emitting Single Halochromic Hydrazine Bridged *Bis*(3-Pyrrolyl BODIPY) Fluorophore

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Supplementary information

MATERIALS AND METHODS

Materials:

The chemicals, such as $BF_3 \cdot Et_2O$ and 2,3- dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), hydrazine hydrate, TFA, DMF, and $POCl_3$, were used as obtained from Aldrich and TCI. All other chemicals used for the synthesis were reagent grade unless otherwise specified. Column chromatography was performed on silica gel (100-200) and basic alumina.

Methods:

- The ^1H and ^{13}C NMR spectra were recorded in $CDCl_3$ on Bruker 400 and 500 MHz instruments. The frequencies for the ^{13}C nucleus are 100.06 and 125.77 MHz for 400 and 500 MHz instruments, respectively.
- Absorption and steady state fluorescence spectra were obtained with PerkinElmer Lambda-35.
- Cyclic voltammetry (CV) studies were carried out with the BAS electrochemical system utilizing the three-electrode configuration consisting of glassy carbon (working electrode), platinum wire (auxiliary electrode), and saturated calomel (reference electrode) electrodes. The experiments were done in dry dichloromethane using tetrabutylammonium perchlorate as a supporting electrolyte.
- Mass spectra were recorded with a Q-TOF micro mass spectrometer.
- Fluorescence quantum yields were determined[S1] in each case by comparing the corrected spectrum with that of Rhodamine 6G (Φ =0.95) [S2] in EtOH by taking the area under total emission using the procedure reported earlier.
- The exponential decay curve of **10** and **10.2H**$^+$ were fitted appropriately with a mono/bi-exponential equation $Y = A+B_1 \exp(-t/\tau_1) +B_2 \exp(-t/\tau_2)$ to obtain best

goodness-of-fit χ^2 value. The average life time (τ_{av}) was calculated following the equations depicted in literature[S3].

- Rigaku Saturn 724 diffractometer was used for performing Single-crystal X-ray structure analysis which comprised of a low-temperature attachment. Data were collected at 100 K using graphite-monochromated MoK_α radiation (λ_α =0.71073 Å) by the ω-scan technique. Data were reduced by using Crystal Clear-SM Expert 2.1 b24 software. Structures were solved by direct methods and refined by least-squares against F2 utilizing the software packages SHELXL-97, SIR-92 and WINGX. All non-hydrogen atoms were refined anisotropically. X-ray data for the compound **10** was collected on a Bruker Kappa CCD diffractometer equipped with a graphite monochromated MoK_α radiation source at 200 K using the θ-2θ scan mode.
- Quantum chemical calculations (gas phase / vacuum) for ground state energy minimized structures for the probes **10** and **10.2H**$^+$ were done employing density functional theory (DFT) in a Gaussian 09W program package[S4]. The ground state structural elucidation involved in optimization using DFT based Beck-3 Lee Young Parr (B3LYP) functional where 6-311G basis sets were used. To obtain the oscillator strengths, identical basis and functional hybrid set were used whereas the vertical excitation energies were obtained by the help of TD-DFT techniques. Under the Polarisable Continuum Model (PCM) in the toluene media all the computations were done using the Self-Consistent Reaction Field (SCRF). The electronic absorption spectra as well as the oscillator strengths were thoroughly examined using TD-DFT with PCM model on the basis of the optimized structures in the S_0 state. [S5]

Compound Details

Cpd. 1: C42 H32 B2 F4 N8

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C42 H32 B2 F4 N8	747.2954	747.295361240274	-0.481003983622941	-0.646254938732369	99.47

Compound Spectra (Zoomed)

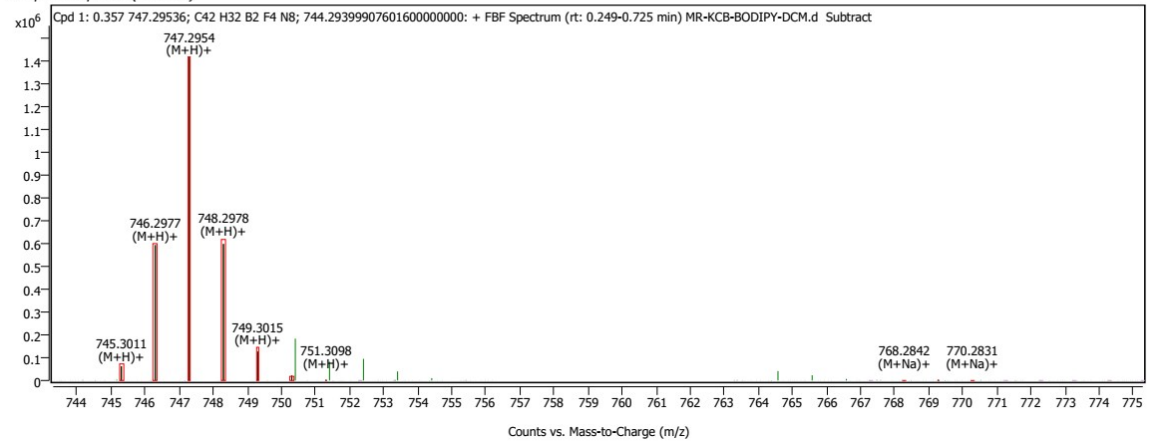

Fig. S1. High resolution mass spectrum of **10**.

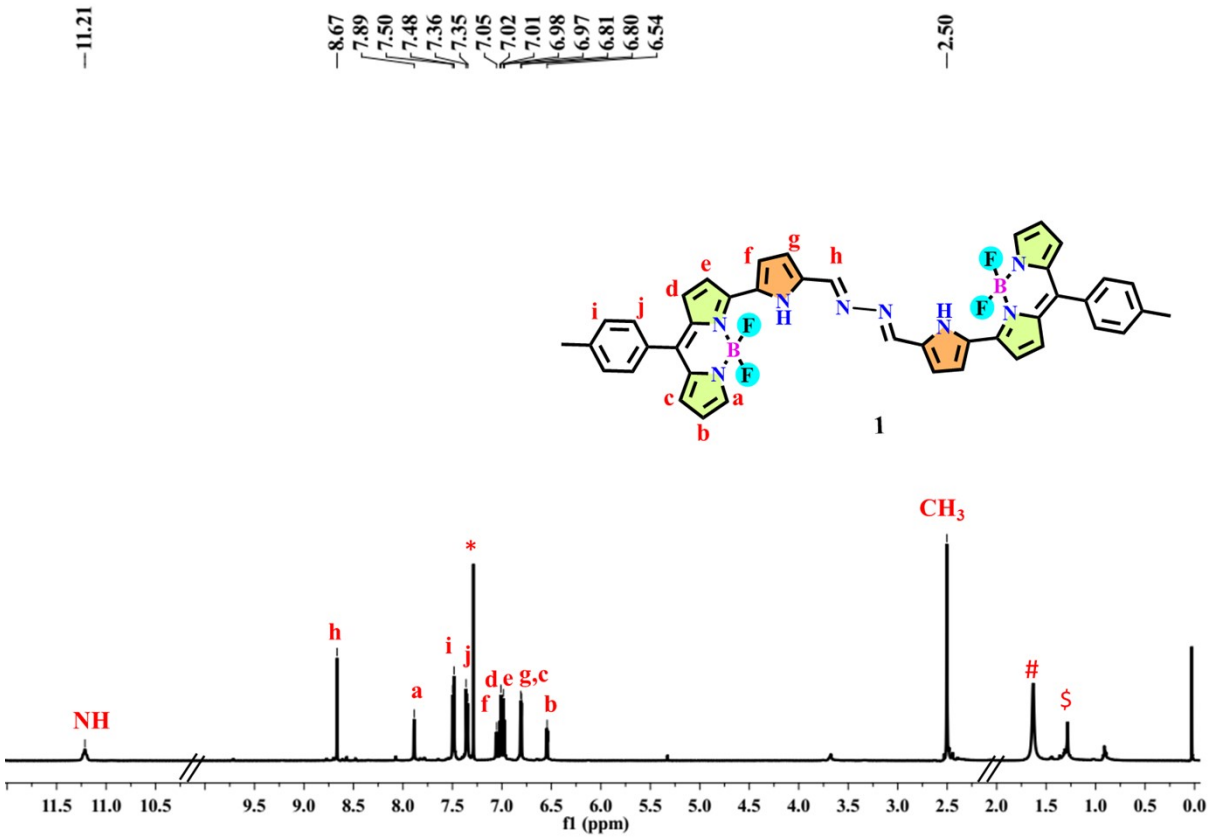

Fig. S2. ^{1}H NMR spectrum of **10** in $CDCl_3$ at room temperature. Note: Peaks marked with asterisk (*, #, $) are due to residual solvents.

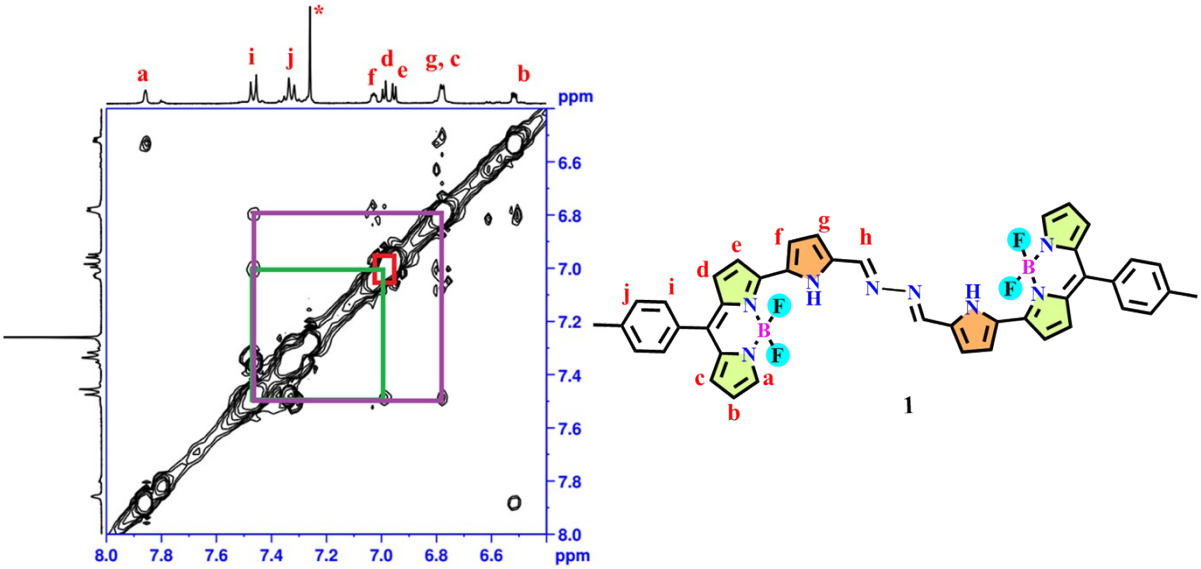

Fig. S3. ^{1}H-^{1}H COSY spectrum of compound **10** recorded in $CDCl_3$ at RT.

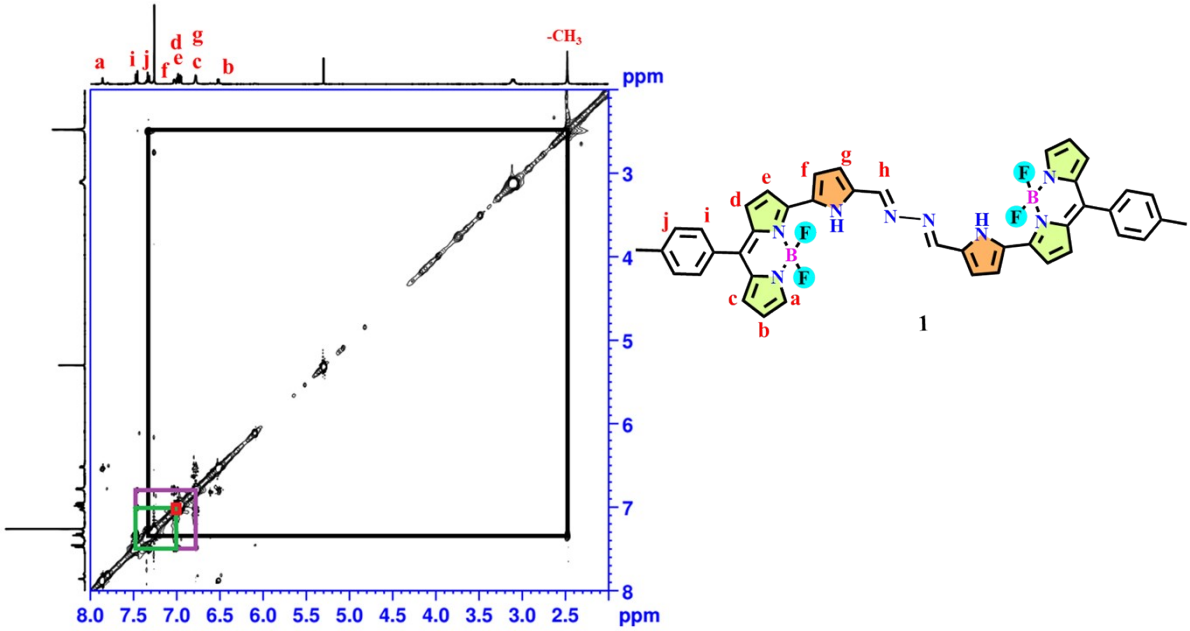

Fig. S4. ^{1}H-^{1}H NOESY spectrum of the compound **10** recorded in $CDCl_3$.

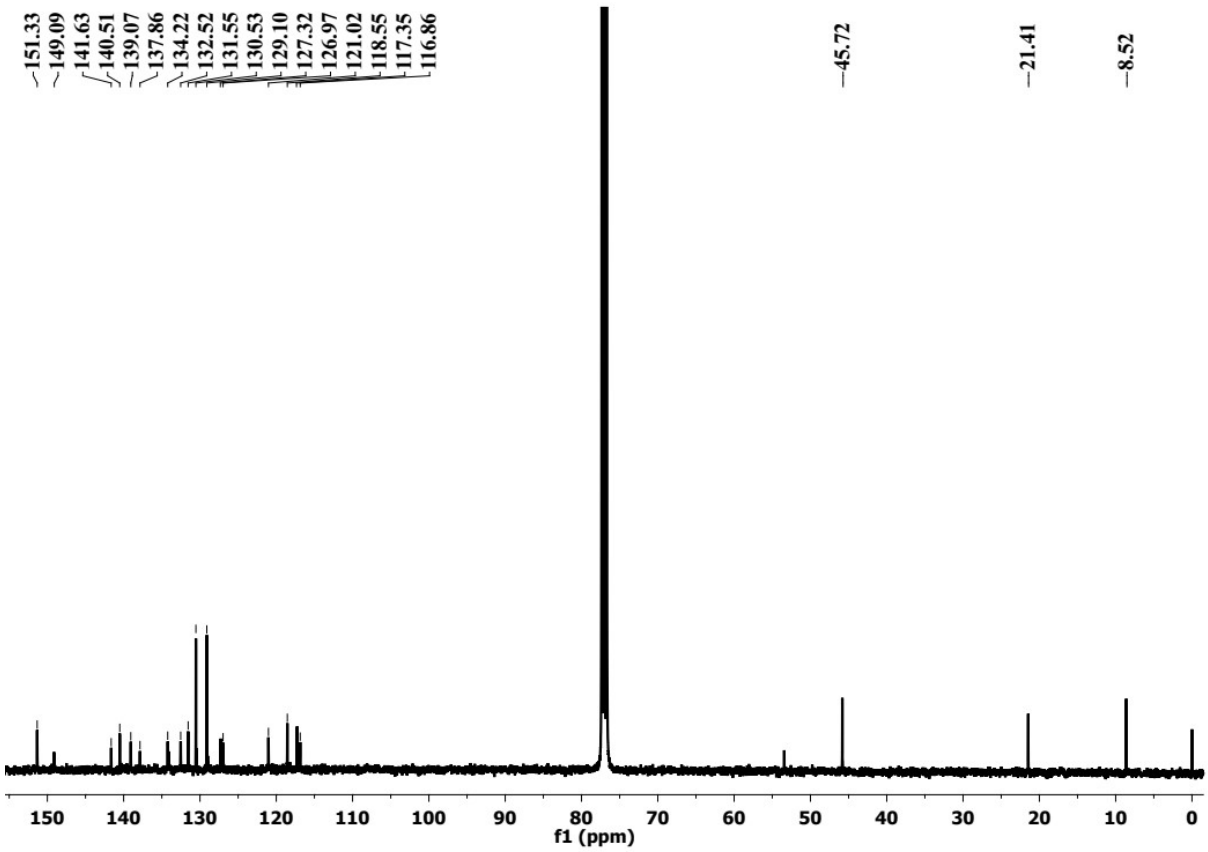

Fig. S5. ^{13}C NMR spectrum of the compound **10** recorded in $CDCl_3$.

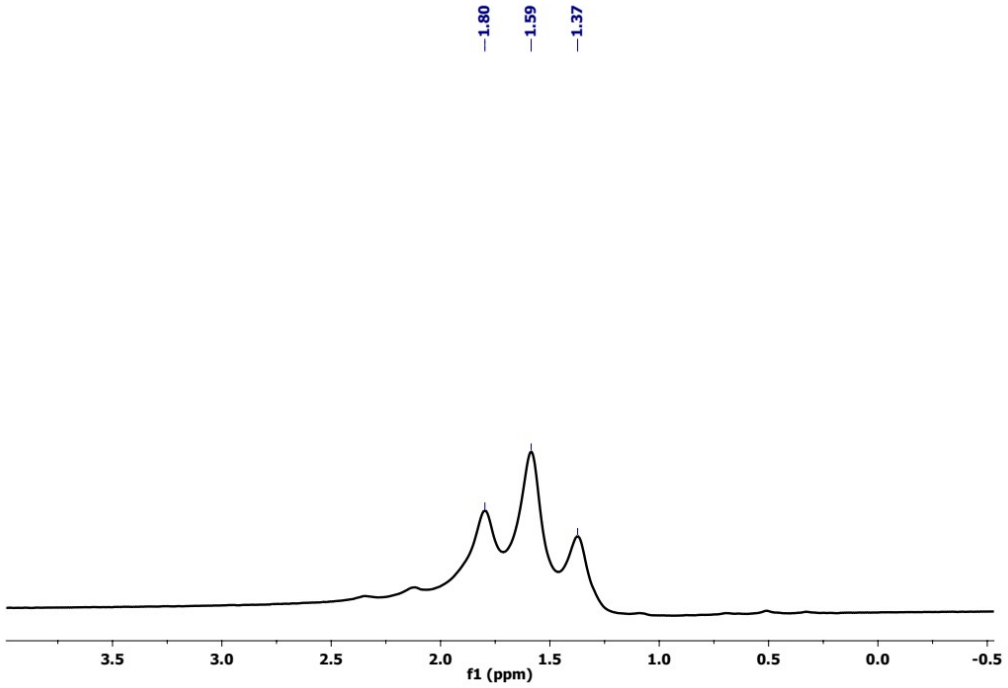

Fig. S6. ^{11}B NMR spectrum of **10** in $CDCl_3$ at room temperature.

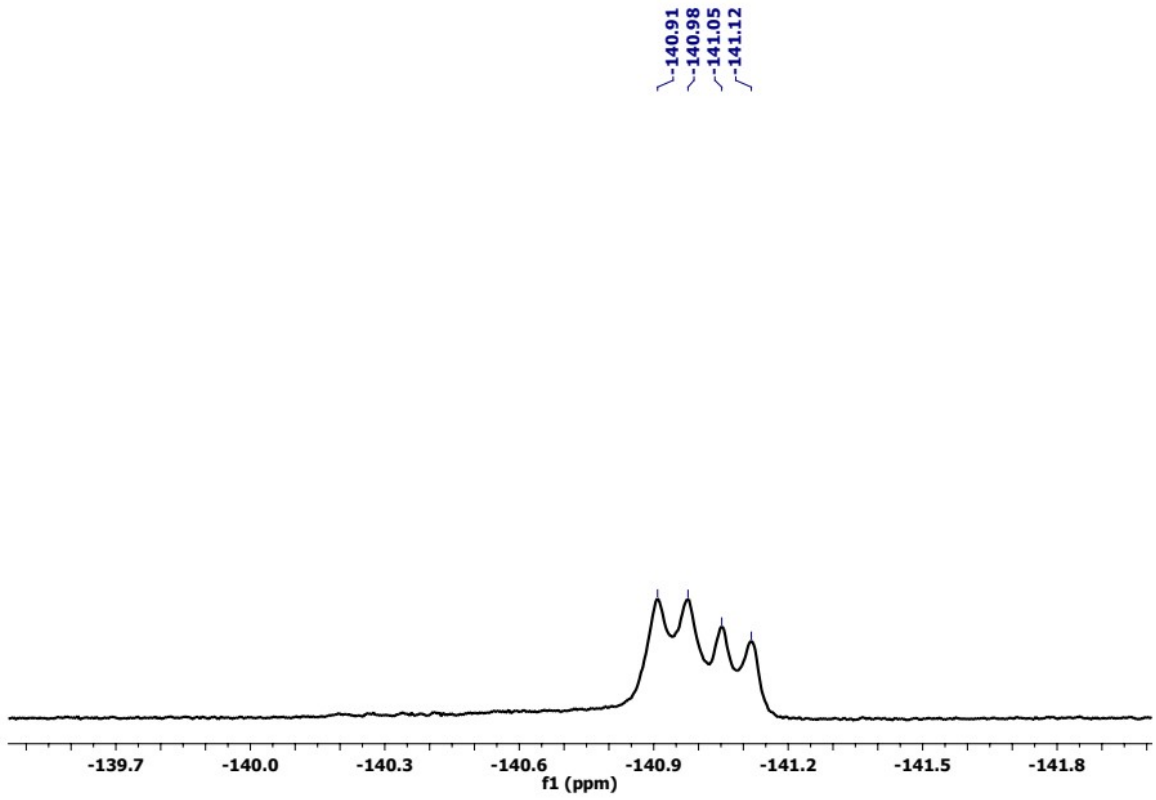

Fig. S7. ^{19}F NMR spectrum of **10** in $CDCl_3$ at room temperature.

Table S1 Crystallographic parameters and structure refinement of structure of compound **10**.

Empirical formula	$C_{42}H_{32}B_2F_4N_8$
Formula weight	746.37
Temperature/K	294.00
Crystal system	monoclinic
Space group	P21/c
a/Å	11.505(3)
b/Å	37.012(10)
c/Å	9.556(2)
α/°	90
β/°	111.920(5)
γ/°	90
Volume/Å3	3774.9(17)
Z	4
ρcalcg/cm3	1.313
μ/mm-1	0.093
F(000)	1544.0
Crystal size/mm3	0.4 × 0.3 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.816 to 49.998
Index ranges	-13 ≤ h ≤ 13, -44 ≤ k ≤ 44, -11 ≤ l ≤ 11
Reflections collected	70861
Independent reflections	6651 [Rint = 0.1905, Rsigma = 0.1049]
Data/restraints/parameters	6651/0/508
Goodness-of-fit on F2	1.052
Final R indexes [I>=2σ (I)]	R1 = 0.0974, wR2 = 0.1954
Final R indexes [all data]	R1 = z0.1607, wR2 = 0.2130
Largest diff. peak/hole / e Å-3	0.24/-0.24

Table S2. Bond Lengths for 10.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1	B1	1.379(6)	C12	C11	1.382(6)
F2	B1	1.397(6)	C13	C12	1.376(6)
F3	B2	1.383(7)	C14	C13	1.439(6)
F4	B2	1.403(7)	C15	C16	1.423(7)
N1	C1	1.360(6)	C16	C17	1.368(7)
N1	C4	1.389(5)	C17	C18	1.371(8)
N1	B1	1.525(6)	C19	C18	1.384(7)
N2	C6	1.393(5)	C20	C19	1.416(7)
N2	C9	1.351(5)	C20	C21	1.421(7)
N2	B1	1.550(6)	C22	C21	1.357(7)
N3	C10	1.363(5)	C23	C22	1.407(7)
N3	C13	1.362(5)	C23	C24	1.387(7)
N4	N5	1.402(5)	C24	C29	1.492(7)
N4	C14	1.280(6)	C25	C24	1.399(7)
N5	C15	1.281(6)	C25	C26	1.392(7)
N6	C16	1.361(6)	C27	C26	1.373(8)
N6	C19	1.384(6)	C28	C27	1.381(8)
N7	C20	1.361(6)	C29	C30	1.374(9)
N7	C23	1.402(6)	C29	C34	1.379(8)
N7	B2	1.548(7)	C30	C31	1.405(9)
N8	C25	1.386(6)	C32	C31	1.353(10)
N8	C28	1.348(6)	C32	C35	1.523(9)
N8	B2	1.516(7)	C33	C32	1.389(10)
C1	C2	1.366(7)	C34	C33	1.385(8)
C3	C2	1.376(7)	C36	C5	1.491(6)
C4	C3	1.400(6)	C36	C37	1.373(6)
C5	C4	1.405(6)	C36	C41	1.384(6)
C6	C5	1.390(6)	C37	C38	1.389(7)
C6	C7	1.416(6)	C39	C38	1.368(7)
C7	C8	1.356(6)	C39	C40	1.365(7)
C9	C8	1.415(6)	C39	C42	1.513(7)
C10	C9	1.440(6)	C41	C40	1.388(7)
C10	C11	1.392(6)			

Table S3. Bond Angles for 10

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C4	107.7(4)	C18	C19	C20	126.9(5)
C1	N1	B1	126.2(4)	N7	C20	C19	128.0(4)
C4	N1	B1	125.9(4)	N7	C20	C21	108.8(4)
C6	N2	B1	122.9(3)	C19	C20	C21	123.2(5)
C9	N2	C6	107.3(3)	C22	C21	C20	107.9(5)
C9	N2	B1	129.8(4)	C21	C22	C23	107.8(5)
C13	N3	C10	109.9(4)	N7	C23	C22	108.3(5)
C14	N4	N5	111.5(4)	C24	C23	N7	121.3(4)
C15	N5	N4	111.5(4)	C24	C23	C22	130.3(5)
C16	N6	C19	110.1(4)	C23	C24	C25	120.7(5)

C20	N7	C23	107.2(4)	C23	C24	C29	120.4(5)
C20	N7	B2	128.9(4)	C25	C24	C29	118.9(5)
C23	N7	B2	123.8(4)	N8	C25	C24	120.3(5)
C25	N8	B2	126.0(4)	N8	C25	C26	107.6(4)
C28	N8	C25	107.5(4)	C26	C25	C24	132.0(5)
C28	N8	B2	126.4(4)	C27	C26	C25	107.9(5)
N1	C1	C2	109.4(5)	C26	C27	C28	107.1(5)
C1	C2	C3	108.2(5)	N8	C28	C27	109.9(5)
C2	C3	C4	107.4(4)	C30	C29	C24	120.8(5)
N1	C4	C3	107.4(4)	C30	C29	C34	119.4(5)
N1	C4	C5	119.7(4)	C34	C29	C24	119.8(5)
C3	C4	C5	132.9(4)	C29	C30	C31	119.1(7)
C4	C5	C36	119.6(4)	C32	C31	C30	122.8(8)
C6	C5	C4	120.4(4)	C31	C32	C33	116.3(7)
C6	C5	C36	119.9(4)	C31	C32	C35	123.1(8)
N2	C6	C7	108.0(4)	C33	C32	C35	120.5(7)
C5	C6	N2	122.2(4)	C34	C33	C32	122.6(7)
C5	C6	C7	129.6(4)	C29	C34	C33	119.3(6)
C8	C7	C6	107.8(4)	C37	C36	C5	120.8(4)
C7	C8	C9	107.3(4)	C37	C36	C41	118.3(4)
N2	C9	C8	109.6(4)	C41	C36	C5	120.8(4)
N2	C9	C10	128.0(4)	C36	C37	C38	120.2(5)
C8	C9	C10	122.4(4)	C39	C38	C37	121.7(5)
N3	C10	C9	126.9(4)	C38	C39	C42	120.3(5)
N3	C10	C11	106.9(4)	C40	C39	C38	118.0(5)
C11	C10	C9	126.2(4)	C40	C39	C42	121.8(5)
C12	C11	C10	107.6(4)	C39	C40	C41	121.3(5)
C13	C12	C11	108.2(4)	C36	C41	C40	120.4(5)
N3	C13	C12	107.4(4)	F1	B1	F2	106.9(4)
N3	C13	C14	122.6(4)	F1	B1	N1	110.6(4)
C12	C13	C14	130.0(4)	F1	B1	N2	111.2(4)
N4	C14	C13	121.2(4)	F2	B1	N1	111.7(4)
N5	C15	C16	122.0(5)	F2	B1	N2	108.8(4)
N6	C16	C15	122.8(5)	N1	B1	N2	107.7(4)
N6	C16	C17	106.5(5)	F3	B2	F4	106.9(4)
C17	C16	C15	130.7(5)	F3	B2	N7	110.5(5)
C16	C17	C18	109.5(5)	F3	B2	N8	111.5(5)
C17	C18	C19	107.8(5)	F4	B2	N7	109.4(4)
N6	C19	C20	127.0(5)	F4	B2	N8	110.7(5)
C18	C19	N6	106.2(4)	N8	B2	N7	107.9(4)

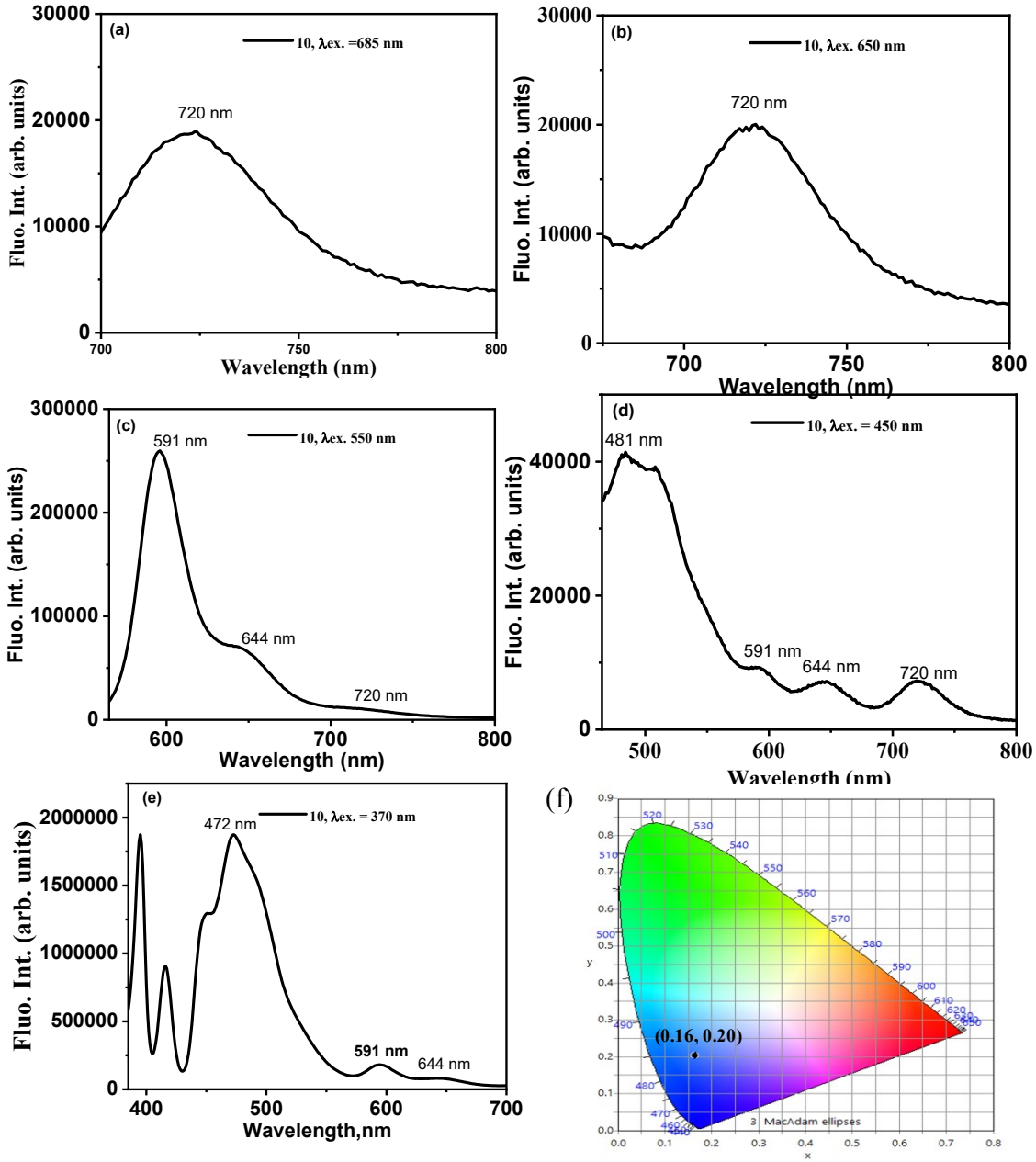

Fig. S8. (a-e) Emission profile of **10** at different excitation wavelengths and (f) CIE plot of **10** ($\lambda_{ex.}$ =370 nm) in dichloromethane *conditions*, [10] =1μM.

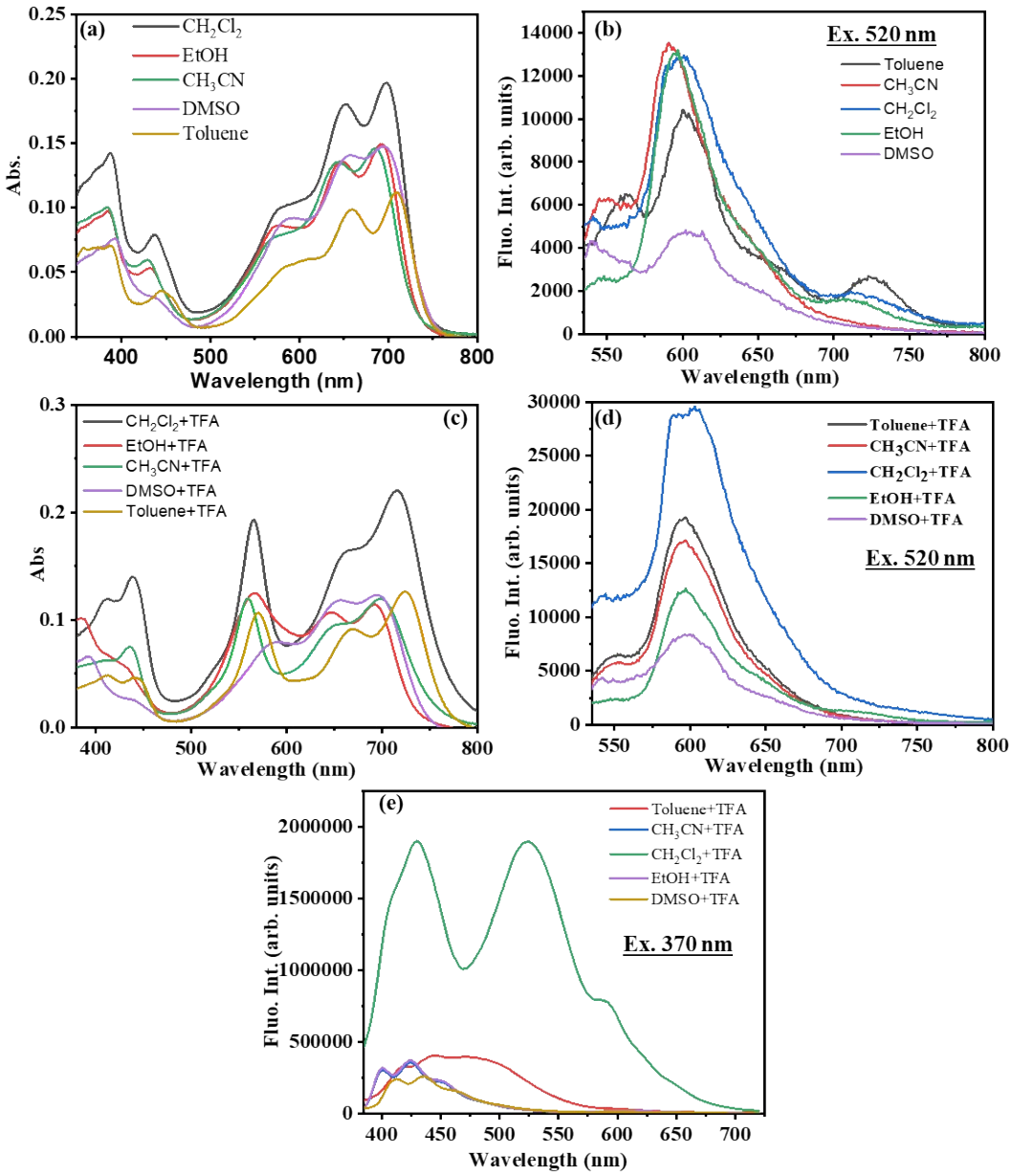

Fig. S9. (a) Absorption and (b) Emission profile of **10** at different solvents, (c) absorption, (d, e) emission profile of **10+TFA** at different solvents upon different excitation wavelengths *conditions*, [**10**] = [**10+TFA**] =10μM. for abs. and 1μM. for emission.

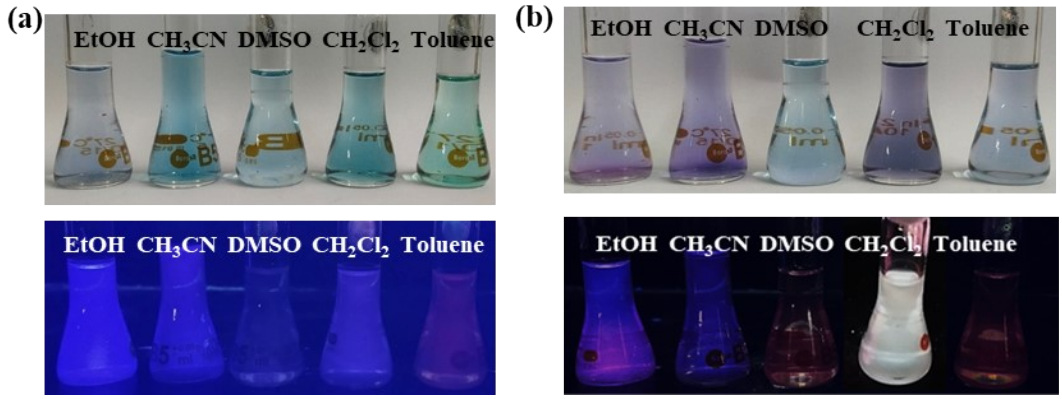

Fig. S10. Photographs depicting the change in colour of solution of (a) **10** and (b) **10+TFA** in visible (above) and UV light (below) in different solvents.

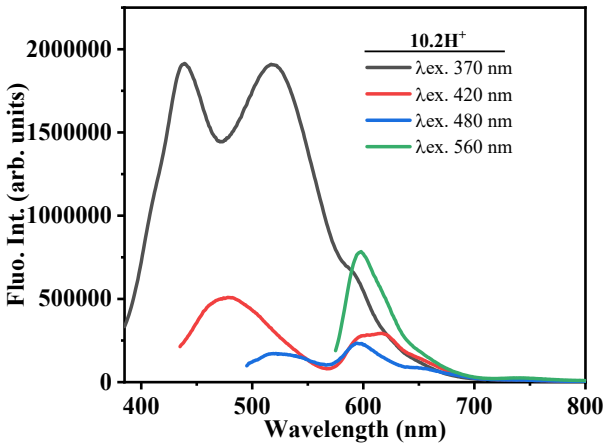

Fig. S11. Emission profile of **10.2H**$^+$ in CH_2Cl_2 at different excitation wavelengths *conditions*, [**10.2H**$^+$] =1μM.

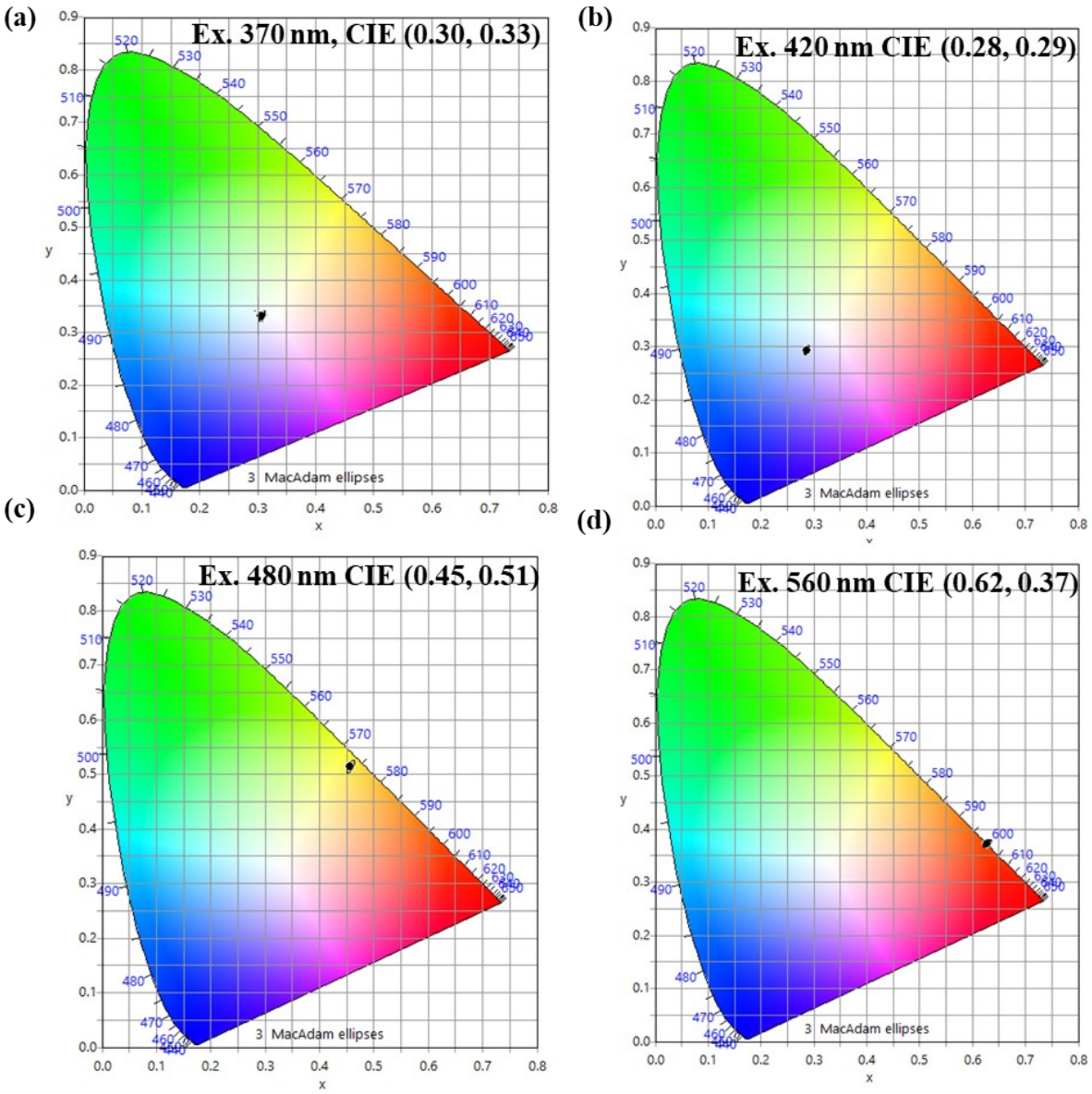

Fig. S12. (a-e) CIE plots of **10.2H**$^+$ in dichloromethane at different excitation wavelengths. *conditions*, [**10.2H**$^+$] =1μM.

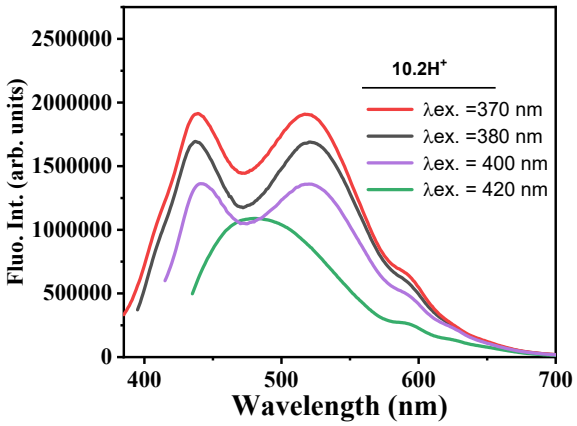

Fig. S13. Emission profile of **10** upon protonation (**10.2H**$^+$) at different excitation wavelengths in dichloromethane; *conditions*, [10] =1μM.

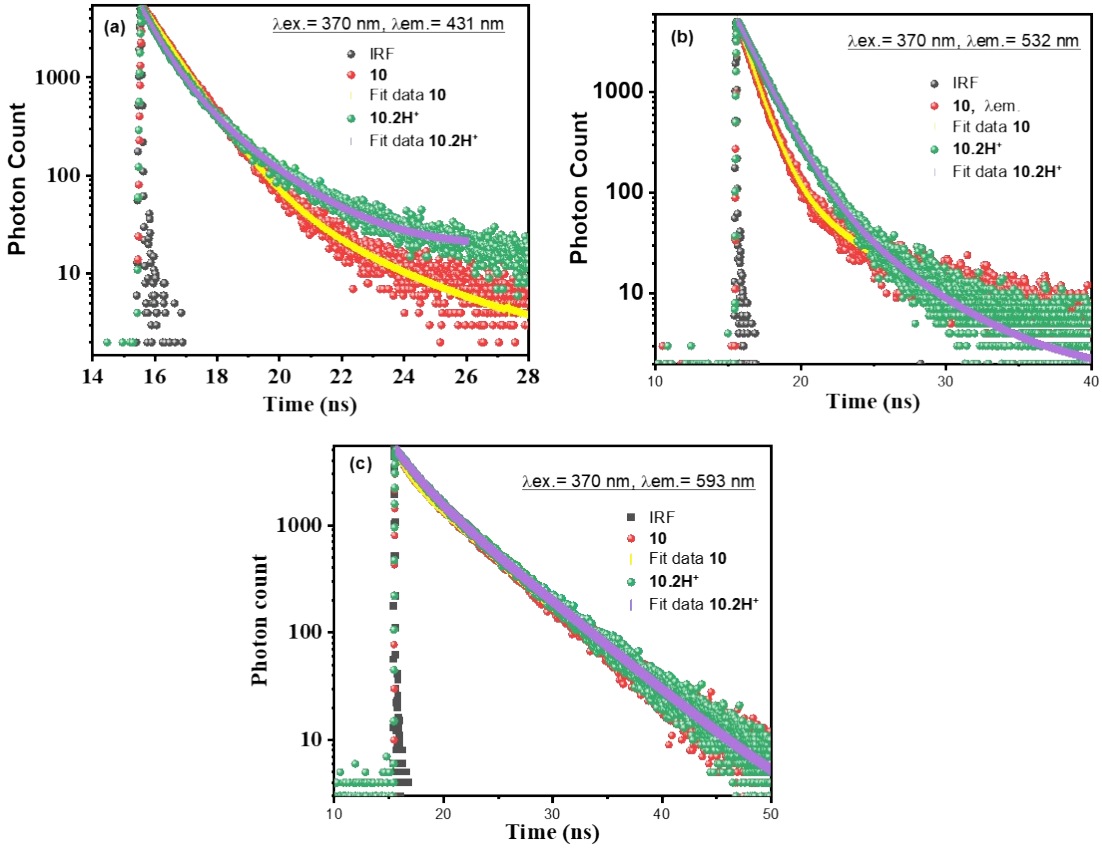

Fig. S14. (a-c) Emission decay profile (TCSPC data) of **10** alone and its protonation derivative **10.2H**$^+$ at different emission wavelengths (λex. = 370 nm) in dichloromethane; *conditions*, [**10**] =1μM.

Table S4: Fit-results to the exponential decay curve of **10** and **10.2H**$^+$ obtained with time-correlated single photon counting technique with exponential fit equation $A+B_1 \exp(-t/\tau_1) + B_2 \exp(-t/\tau_2)$.

Parameter	**10 ($\lambda_{ex.}$ =370 nm)**			**10.2H$^+$ ($\lambda_{ex.}$ =370 nm)**		
	λem. = 432	**523**	**594**	**λem. = 432**	**523**	**594**
τ_1, ns (%)	0.88 (91.62)	0.94 (87.46)	0.97 (9.62)	0.63 (55.94)	1.42 (88.64)	2.01 (21.94)
τ_2, ns (%)	2.91 (8.38)	3.96 (12.54)	4.76 (90.38)	1.71 (44.06)	4.17 (11.36)	5.25 (78.06)
τ_{av}, ns	**0.94**	**1.04**	**3.46**	**0.87**	**1.53**	**3.88**
χ^2	1.13	1.18	1.02	1.04	1.12	1.05

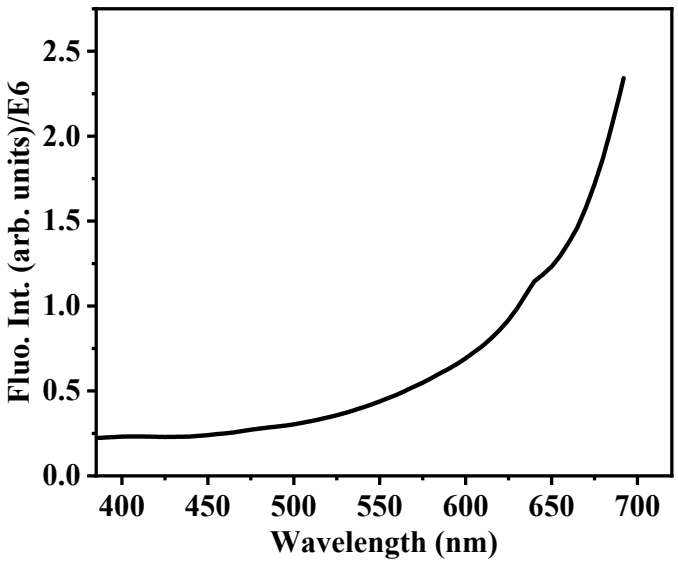

Fig. S15. Solid state fluorescence spectrum of compound **10.**

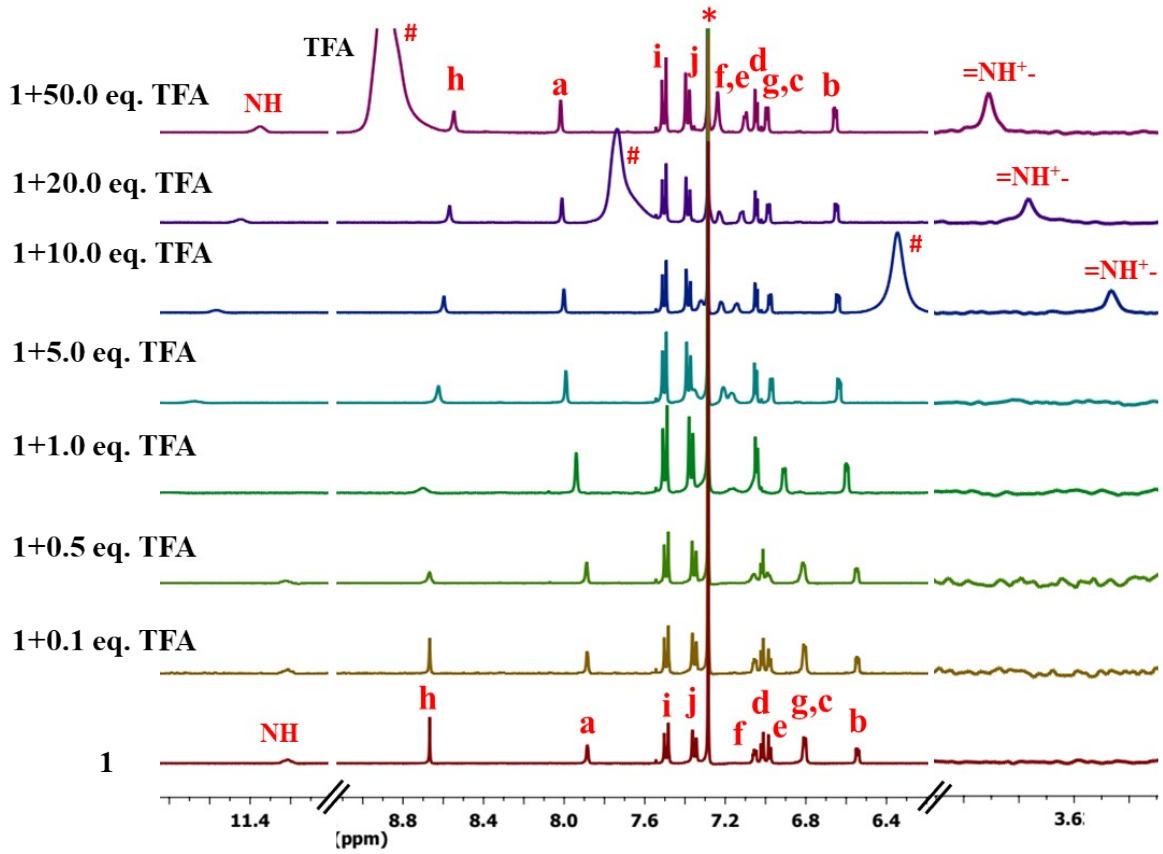

Fig. S16. Partial ^{1}H-NMR titration of **10** (400 MHz) in the presence of TFA.

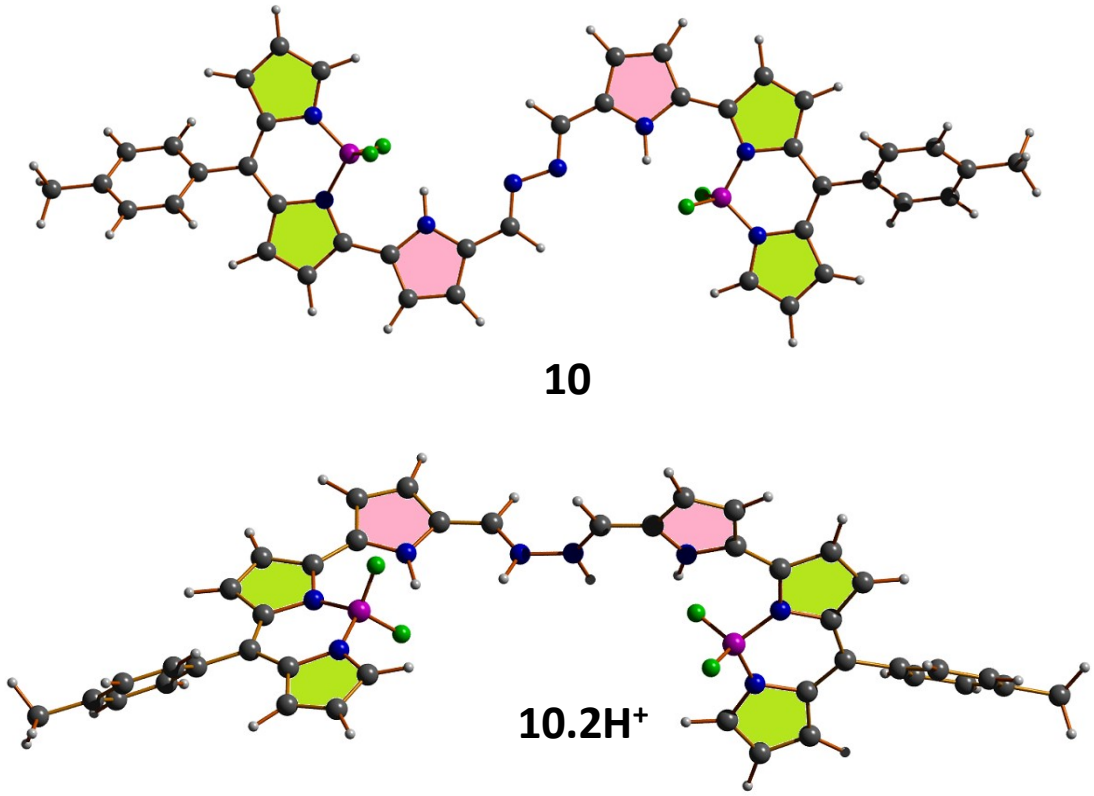

Fig. S17. DFT Optimized structure of **10** and **10.2H**$^{+}$

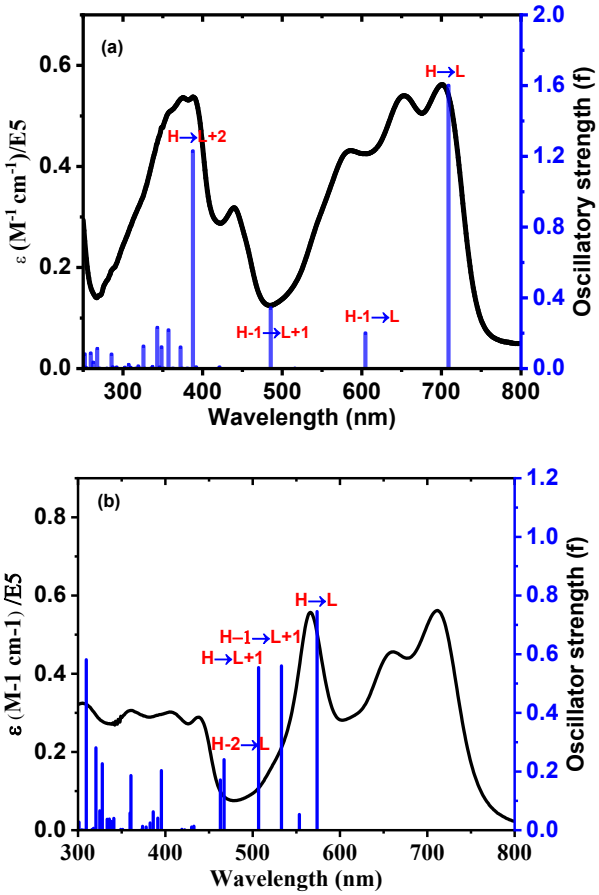

Fig. S18. Calculated excitation (blue vertical lines) and experimental UV/vis absorption spectra (black lines) for (a) **10** and (b) **10.2H$^+$.**

Table S5. S_0 optimized geometry of the compound **10** at B3LYP/6-31g (d,p)/LANL2DZ level of theory.

Total Energy (hartree) = - 2506.660609

Atom	X	Y	Z	Atom	X	Y	Z
C	-9.870970000	0.102575000	-0.077032000	C	-8.413196000	0.281875000	0.068111000
C	-7.558623000	-0.827700000	0.055197000	C	-2.014511000	-2.124643000	0.297680000
C	-7.875942000	1.577904000	0.222778000	C	-0.733962000	-1.487189000	0.213992000
H	0.156314000	-2.106934000	0.348667000	C	-4.248495000	-2.300237000	0.250973000
C	-5.635137000	-1.952599000	0.143569000	C	-7.864108000	-2.205652000	-0.121775000
H	-8.853209000	-2.600652000	-0.298083000	C	-12.668779000	-0.233178000	-0.362469000
C	-3.722590000	-3.588306000	0.469804000	H	-4.312230000	-4.482831000	0.610221000

C	-6.679141000	-2.902179000	-0.050900000	H	-6.529255000	-3.966320000	-0.161313000
C	-2.329615000	-3.476193000	0.506193000	H	-1.609086000	-4.266379000	0.665628000
C	-10.566568000	-0.834888000	0.705679000	H	-10.022977000	-1.419608000	1.440073000
C	-6.272755000	3.080045000	0.520925000	H	-5.264037000	3.443505000	0.660051000
C	-10.596904000	0.870859000	-1.003782000	H	-10.069741000	1.583515000	-1.628952000
C	0.747997000	1.497044000	-0.316262000	H	-0.141627000	2.114964000	-0.463135000
C	-11.942608000	-0.995265000	0.562959000	H	-12.464268000	-1.719608000	1.182932000
C	-8.496630000	2.845639000	0.307096000	H	-9.560587000	3.021654000	0.251804000
C	2.028947000	2.133402000	-0.401767000	C	9.859320000	-0.115394000	0.171625000
C	6.266002000	-3.073827000	-0.538414000	H	5.260402000	-3.431570000	-0.710701000
C	4.262688000	2.309881000	-0.348967000	N	6.514080000	-1.750716000	-0.455904000
N	3.202519000	1.451031000	-0.236671000	H	3.266581000	0.461300000	-0.012591000
N	6.174164000	0.706871000	-0.196217000	B	-5.439141000	0.648761000	0.459711000
B	5.452715000	-0.633316000	-0.553182000	C	7.455277000	-3.796106000	-0.357897000
H	7.549624000	-4.872963000	-0.370543000	C	3.738031000	3.592900000	-0.598594000
H	4.327838000	4.484902000	-0.753293000	C	2.345304000	3.480354000	-0.637325000
H	1.625547000	4.267214000	-0.815587000	C	10.783292000	-0.766884000	-0.663981000
H	10.417105000	-1.382843000	-1.478222000	C	12.645704000	0.198332000	0.569520000
C	12.152200000	-0.606478000	-0.466746000	H	12.851719000	-1.110659000	-1.128259000
C	10.351340000	0.689816000	1.213874000	H	9.649789000	1.173167000	1.885411000
C	11.722041000	0.837600000	1.408380000	H	12.083725000	1.450072000	2.230115000
C	14.129195000	0.389370000	0.763204000	H	14.690516000	-0.481101000	0.408521000
H	14.372480000	0.556504000	1.817568000	H	14.485726000	1.262790000	0.201183000
F	4.429519000	-0.904186000	0.380055000	F	-4.463156000	0.865634000	-0.535448000
F	-4.831958000	0.640122000	1.706160000	F	4.909029000	-0.554920000	-1.825973000
N	-6.174673000	-0.704794000	0.202300000	N	-3.188997000	-1.438783000	0.154312000
H	-3.254035000	-0.449169000	-0.067702000	N	-0.646610000	-0.214266000	-0.020308000
N	-6.506508000	1.760931000	0.365373000	N	0.659784000	0.226683000	-0.068770000
C	-11.971169000	0.697483000	-1.145180000	H	-12.512424000	1.287689000	-1.879930000
C	5.646496000	1.961771000	-0.217089000	C	7.871465000	-1.578811000	-0.218125000
C	7.558659000	0.826859000	-0.048001000	C	-7.483258000	3.788530000	0.484215000
H	-7.593149000	4.859247000	0.585009000	C	8.408946000	-0.286495000	-0.034736000
C	-14.163068000	-0.390719000	-0.493745000	H	-14.478038000	-1.409079000	-0.243884000
H	-14.497566000	-0.161528000	-1.510744000	H	-14.687829000	0.292524000	0.187128000
C	7.879430000	2.211048000	0.013415000	H	8.877925000	2.609067000	0.113827000
C	8.467828000	-2.859038000	-0.148122000	H	9.512196000	-3.047751000	0.051589000
C	6.698905000	2.912132000	-0.085732000	H	6.561270000	3.983273000	-0.056671000

Table S6. S_0 optimized geometry of the protonated derivative **10.2H**$^+$ at B3LYP/6-31g (d,p)/LANL2DZ level of theory.

Total Energy (hartree) = -2507.444162

Atom	X	Y	Z	Atotm	X	Y	Z
C	9.523521000	-1.096574000	-0.185214000	C	8.070489000	-0.899879000	-0.212720000
C	7.478132000	0.196673000	0.490944000	C	2.428848000	2.626607000	1.297711000
C	7.250422000	-1.769798000	-0.928850000	C	1.136783000	2.588483000	0.841252000
H	0.393658000	3.236651000	1.291599000	C	4.607620000	2.136715000	1.492164000
C	5.882057000	1.537511000	1.249063000	C	8.107976000	1.210533000	1.247692000
H	9.172360000	1.315308000	1.386807000	C	12.320958000	-1.513450000	-0.143667000
C	4.294669000	3.124754000	2.479946000	H	4.997473000	3.525007000	3.195164000
C	7.108179000	2.033249000	1.740558000	H	7.226278000	2.917265000	2.350373000
C	2.959992000	3.422287000	2.362397000	H	2.382103000	4.111305000	2.963023000
C	10.239469000	-1.049540000	1.028535000	H	9.706051000	-0.885047000	1.958344000
C	5.337188000	-2.582613000	-1.692709000	H	4.267678000	-2.648244000	-1.839362000
C	10.229790000	-1.352967000	-1.375784000	H	9.697336000	-1.356977000	-2.320653000
C	-1.159444000	2.471366000	-1.485829000	H	-0.450730000	3.110820000	-1.999645000
C	11.611494000	-1.264274000	1.043245000	H	12.145942000	-1.246124000	1.988700000
C	7.549332000	-2.957630000	-1.659027000	H	8.536170000	-3.378831000	-1.777499000
C	-2.471852000	2.463494000	-1.884177000	C	-9.423973000	-1.219289000	0.202641000
C	-5.495223000	-1.221905000	2.767816000	H	-4.487875000	-1.003317000	3.095097000
C	-4.657530000	1.967337000	-1.921976000	N	-5.989852000	-0.657815000	1.656422000
N	-3.478807000	1.681140000	-1.331049000	H	-3.384128000	0.917388000	-0.658976000
N	-6.128515000	0.492878000	-0.549391000	B	5.072390000	-0.518174000	-0.199268000
B	-5.235210000	0.298160000	0.718195000	C	-6.450703000	-2.085739000	3.346485000
H	-6.308243000	-2.673082000	4.242088000	C	-4.425574000	2.981235000	-2.904922000
H	-5.189589000	3.426310000	-3.524247000	C	-3.086674000	3.283018000	-2.883124000
H	-2.567715000	4.019883000	-3.480579000	C	-10.315994000	-1.176670000	1.293150000
H	-9.982158000	-0.761073000	2.237684000	C	-12.088965000	-2.126124000	-0.074731000
C	-11.626196000	-1.616698000	1.148555000	H	-12.306801000	-1.559652000	1.993035000

C	-9.886879000	-1.724784000	-1.028662000	H	-9.203588000	-1.798699000	-1.867580000
C	-11.193905000	-2.179610000	-1.155066000	H	-11.528465000	-2.591252000	-2.102795000
C	-13.516801000	-2.577175000	-0.232062000	H	-13.915074000	-2.968571000	0.709062000
H	-13.606296000	-3.348751000	-1.002638000	H	-14.152193000	-1.733946000	-0.533213000
F	-3.992966000	-0.308482000	0.361910000	F	4.279556000	0.223164000	-1.125443000
F	4.229283000	-1.078041000	0.741844000	F	-4.969053000	1.520067000	1.305859000
N	6.114979000	0.420323000	0.483279000	N	3.479353000	1.860231000	0.806116000
H	3.489034000	1.265712000	-0.024299000	N	0.692807000	1.802348000	-0.165961000
N	5.866968000	-1.584077000	-0.972042000	N	-0.651103000	1.743581000	-0.468192000
C	11.607091000	-1.547434000	-1.349879000	H	12.141268000	-1.720388000	-2.279305000
C	-5.900190000	1.333793000	-1.613129000	C	-7.289084000	-1.135079000	1.472002000
C	-7.445604000	0.082109000	-0.631809000	C	6.352860000	-3.452804000	-2.146953000
H	6.201384000	-4.340758000	-2.743569000	C	-8.040774000	-0.762514000	0.358488000
C	13.807934000	-1.749081000	-0.110071000	H	14.314152000	-0.976610000	0.479470000
H	14.233860000	-1.755747000	-1.117216000	H	14.033367000	-2.714248000	0.360702000
C	-8.047737000	0.681020000	-1.760811000	H	-9.076695000	0.555429000	-2.059301000
C	-7.570167000	-2.043676000	2.533689000	H	-8.487453000	-2.602394000	2.642587000
C	-7.079906000	1.459375000	-2.375576000	H	-7.184736000	2.045595000	-3.277185000
H	1.280503000	1.096019000	-0.595974000	H	-1.224714000	1.134941000	0.106371000

Table S7. Major transitions were calculated using TD-DFT studies of **10**.

Energy (cm-1)	**Wavelength (nm)**	**Osc. Strength**	**Major contribs**
14105.8304088	708.926714004	1.5999	HOMO->LUMO (99%)
16540.8182299	604.565013713	0.0001	H-1->LUMO (12%), HOMO->L+1 (87%)
19383.9225922	515.891453469	0.0005	H-1->LUMO (88%), HOMO->L+1 (13%)
20596.1738989	485.527071633	0.3423	H-1->L+1 (92%)
23735.2837366	421.313691084	0.008	H-4->LUMO (34%), H-2->LUMO (40%), HOMO->L+2 (21%)
23785.2901112	420.42791798	0.003	H-4->LUMO (57%), H-2->LUMO (23%), HOMO->L+2 (12%)
25520.188688	391.846632572	0.0085	H-3->LUMO (58%), H-2->L+1 (29%)
25783.9319863	387.838441605	1.2301	H-5->LUMO (20%), H-3->L+1 (12%), H-2->LUMO (18%), HOMO->L+2 (37%)
26296.0940487	380.28461495	0.0002	H-3->LUMO (28%), H-2->L+1 (57%)

26767.1218352	373.592650774	0.0002	H-4->L+1 (98%)
26860.682149	372.291364178	0.1207	H-7->LUMO (14%), H-6->L+1 (11%), H-5->LUMO (44%), H-3->L+1 (12%), HOMO->L+2 (12%)
27614.0039857	362.135096569	0.0002	H-7->L+1 (17%), H-6->LUMO (66%)
27995.5042306	357.200210349	0.2177	H-7->LUMO (31%), H-6->L+1 (11%), H-3->L+1 (36%), H-2->LUMO (11%)
28489.9220956	351.001310795	0.0003	H-8->LUMO (20%), H-5->L+1 (19%), H-1->L+2 (43%)
28709.3049003	348.319126316	0.1214	H-9->LUMO (24%), H-8->L+1 (13%), H-7->LUMO (16%), H-5->LUMO (15%), H-3->L+1 (24%)
28902.8779632	345.986306718	0.0074	H-12->LUMO (14%), H-9->L+1 (24%), H-8->LUMO (38%)
29160.9753805	342.924057564	0.2309	H-9->LUMO (43%), H-5->LUMO (13%), H-3->L+1 (11%)
29662.6522353	337.124270637	0.0095	H-11->LUMO (43%), H-10->LUMO (29%), H-10->L+1 (11%)
29690.8816403	336.803740661	0.0033	H-12->LUMO (14%), H-11->LUMO (30%), H-11->L+1 (13%), H-10->LUMO (31%)
29870.743278	334.775733798	0.0003	H-5->L+1 (41%), H-1->L+2 (24%)
30555.5079882	327.273236755	0.0006	H-12->LUMO (31%), H-8->LUMO (11%), H-5->L+1 (17%)
30709.5598842	325.631498391	0.1256	H-14->LUMO (21%), H-14->L+1 (15%), H-13->LUMO (42%)
31074.9290405	321.802826548	0.0003	H-14->LUMO (30%), H-13->LUMO (12%), HOMO->L+3 (11%)
31328.9936856	319.193144227	0.0134	H-7->LUMO (21%), H-6->L+1 (69%)
31658.0678927	315.875246522	0.0	H-7->L+1 (68%), H-6->LUMO (13%)
32279.114803	309.797838665	0.005	H-11->L+1 (10%), H-10->L+1 (65%)
32302.5048814	309.573515636	0.0025	H-11->L+1 (59%), H-10->L+1 (10%), H-9->L+1 (10%)
32413.0028382	308.518160132	0.0007	H-4->L+2 (89%)
32535.5991114	307.355643452	0.0212	H-12->L+1 (13%), H-8->L+1 (67%)
32944.5222069	303.540598865	0.0005	H-12->LUMO (12%), H-11->L+1 (10%), H-9->L+1 (59%), H-8->LUMO (14%)
33074.37747	302.348850226	0.0057	H-12->L+1 (60%), H-9->LUMO (17%)
34210.8126605	292.305245691	0.0029	H-13->LUMO (16%), H-13->L+1 (43%), HOMO->L+3 (24%)
34247.9141642	291.988585117	0.0073	H-14->L+1 (36%), H-13->LUMO (10%), H-13->L+1 (13%), HOMO->L+3 (17%)
34297.1139844	291.569722297	0.0021	H-14->LUMO (13%), H-14->L+1 (32%), H-13->L+1 (14%), HOMO->L+3 (25%)
34756.8500089	287.713069436	0.0017	H-2->L+2 (10%), HOMO->L+4 (78%)
34797.1777303	287.379628241	0.0033	H-2->L+2 (14%), HOMO->L+5 (67%)
34837.5054518	287.046959026	0.0087	H-2->L+2 (42%), HOMO->L+5 (24%), HOMO->L+6 (16%)
35022.206416	285.53312379	0.0802	H-2->L+2 (19%), HOMO->L+6 (68%)
35752.1381743	279.703550911	0.0007	HOMO->L+7 (76%)
37072.4677746	269.741956775	0.0001	H-3->L+2 (90%)
37383.7977841	267.495562054	0.1116	H-15->LUMO (26%), H-1->L+3 (65%)
38066.9493855	262.695071747	0.0347	H-15->LUMO (40%), H-1->L+3 (21%), HOMO->L+8 (29%)
38529.9116278	259.538617597	0.0864	H-5->L+2 (80%), HOMO->L+8 (12%)
39356.6299175	254.086796074	0.0024	H-1->L+5 (88%)

39373.5675605	253.977493521	0.0017	H-1->L+4 (89%)
39484.0655173	253.266725931	0.0003	H-15->L+1 (14%), H-1->L+6 (66%)
39634.8911955	252.302950718	0.007	H-15->L+1 (43%), H-1->L+6 (20%)
39671.9926992	252.066995369	0.0814	H-15->LUMO (11%), H-11->L+2 (14%), H-7->L+2 (12%), HOMO->L+8 (23%)
39842.9822382	250.985228471	0.0007	H-6->L+2 (88%)
40016.3914404	249.897595461	0.0745	H-7->L+2 (24%), H-1->L+7 (65%)

Table S8. Major and minor transitions were calculated using TD-DFT studies of **10.2H**$^{+}$.

Energy (cm-1)	Wavelength (nm)	Osc. Strength	Major contribs
17428.0281018	573.788379361	0.7455	HOMO->LUMO (98%)
18068.4323185	553.451446354	0.0537	H-1->LUMO (58%), HOMO->L+1 (41%)
18762.0691274	532.990254545	0.5601	H-1->L+1 (97%)
19730.7409966	506.823337335	0.5545	H-1->LUMO (41%), HOMO->L+1 (57%)
21400.3086647	467.282979732	0.2405	H-3->LUMO (25%), H-3->L+1 (13%), H-2->LUMO (48%), H-2->L+1 (10%)
21598.7210542	462.990376833	0.1712	H-3->LUMO (42%), H-3->L+1 (16%), H-2->LUMO (20%), H-2->L+1 (19%)
23108.5909453	432.739496046	0.0137	H-3->LUMO (22%), H-3->L+1 (33%), H-2->LUMO (15%), H-2->L+1 (29%)
23252.9641881	430.05269862	0.0107	H-3->LUMO (10%), H-3->L+1 (35%), H-2->LUMO (14%), H-2->L+1 (40%)
23692.5363519	422.073848552	0.0015	H-4->LUMO (66%), H-4->L+1 (31%)
23869.1717718	418.95043932	0.003	H-5->LUMO (50%), H-5->L+1 (48%)
25283.8682403	395.509101098	0.2031	H-7->LUMO (18%), H-7->L+1 (16%), H-6->LUMO (17%), HOMO->L+2 (33%)
25554.063974	391.327188121	0.0411	H-7->LUMO (32%), H-6->LUMO (14%), H-6->L+1 (27%)
25898.4627152	386.123304305	0.0629	H-6->LUMO (18%), HOMO->L+2 (51%)
26134.7831629	382.63183351	0.0246	H-1->L+2 (66%)
26453.3721623	378.023638674	0.0108	HOMO->L+3 (72%)
26741.3120935	373.953228811	0.0132	H-1->L+3 (69%)
26807.4495567	373.030637579	0.0004	H-5->LUMO (49%), H-5->L+1 (50%)
26893.7508806	371.833592287	0.0001	H-4->LUMO (32%), H-4->L+1 (66%)
27732.5674867	360.586880561	0.1861	H-10->LUMO (13%), H-9->LUMO (28%), H-9->L+1 (19%), H-8->LUMO (13%)
27813.2229296	359.541216252	0.0582	H-10->L+1 (12%), H-9->LUMO (16%), H-8->LUMO (20%), H-8->L+1 (23%)
28481.8565513	351.100707989	0.0026	H-6->LUMO (43%), H-6->L+1 (51%)
28661.7181889	348.897436437	0.0026	H-7->LUMO (28%), H-7->L+1 (66%)
29325.512484	341.000008285	0.0405	H-3->L+2 (25%), H-3->L+3 (12%), H-2->L+2 (51%)
29539.2494077	338.532637102	0.0298	H-3->L+2 (43%), H-3->L+3 (15%), H-2->L+2 (20%), H-2->L+3 (18%)
29774.763301	335.85489493	0.038	H-10->LUMO (12%), H-8->LUMO (42%), H-8->L+1 (29%)
29998.9854322	333.34460669	0.0374	H-9->LUMO (28%), H-9->L+1 (35%), H-8->L+1 (16%)
30503.8885048	327.827057145	0.2268	H-10->LUMO (53%), H-9->L+1 (17%)
30777.3104562	324.91468071	0.0661	H-11->LUMO (38%), H-10->L+1 (36%)
31203.9777492	320.471962914	0.281	H-12->LUMO (10%), H-11->L+1 (66%)
31436.2654247	318.103943484	0.0007	H-13->LUMO (29%), H-12->LUMO (15%), H-12-

			>L+1 (13%), H-10->L+1 (19%)
31468.5276019	317.777816824	0.0065	H-3->L+2 (20%), H-3->L+3 (29%), H-2->L+2 (12%), H-2->L+3 (32%)
31650.0023484	315.955742749	0.0023	H-3->L+3 (38%), H-2->L+2 (13%), H-2->L+3 (38%)
32313.7966435	309.46533799	0.5813	H-13->LUMO (26%), H-12->LUMO (33%), H-11->L+1 (14%)
32606.5759012	306.686603043	0.0003	H-4->L+2 (74%), H-4->L+3 (22%)
32854.1881109	304.375197654	0.0015	H-5->L+2 (60%), H-5->L+3 (36%)
33209.0720596	301.122536096	0.0275	H-13->LUMO (19%), H-12->LUMO (17%), H-11->LUMO (13%), H-10->L+1 (13%)
33651.0638867	297.167424889	0.0267	H-12->LUMO (21%), H-12->L+1 (70%)
33858.348375	295.34813362	0.003	H-13->LUMO (15%), H-13->L+1 (70%)
34038.2100127	293.787481665	0.0659	H-7->L+2 (29%), H-7->L+3 (17%), H-6->L+2 (21%)
34239.0420655	292.064245865	0.0148	H-7->L+2 (14%), H-6->L+2 (25%), H-6->L+3 (25%)
35176.258312	284.28265199	0.0001	H-5->L+2 (38%), H-5->L+3 (62%)
35294.821813	283.327680558	0.0001	H-4->L+2 (23%), H-4->L+3 (77%)
35881.9934374	278.691316787	0.0178	H-9->L+2 (33%), H-9->L+3 (19%), H-8->L+2 (22%), H-7->L+2 (10%)
35966.6816524	278.035101949	0.0173	H-9->L+2 (21%), H-8->L+2 (25%), H-8->L+3 (24%), H-6->L+2 (11%)
36834.534218	271.48436141	0.0007	H-6->L+2 (33%), H-6->L+3 (60%)
37040.2055974	269.976903171	0.0006	H-7->L+2 (20%), H-7->L+3 (72%)
37100.6971796	269.536713868	0.1109	H-15->L+1 (10%), H-14->LUMO (23%), H-11->L+3 (11%), H-10->L+2 (39%)
37343.4700627	267.784434152	0.0076	H-15->LUMO (34%), H-14->L+1 (18%), H-11->L+2 (20%), H-10->L+3 (13%)
37970.9694085	263.359091321	0.0032	H-14->LUMO (30%), H-10->L+2 (13%), H-8->L+2 (25%), H-8->L+3 (12%)
38190.3522131	261.846236562	0.0025	H-11->L+2 (16%), H-9->L+2 (21%), H-8->L+3 (28%)

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