Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Photophysics of push-pull based benzazoles: intramolecular proton transfer or charge transfer in the excited state?

Guilherme Wiethaus, Fabiano da Silveira Santos, Rodrigo da Costa Duarte, Josene Maria Toldo, Paulo Fernando Bruno Gonçalves and Fabiano Severo Rodembusch

Summary

Spectroscopic characterisation

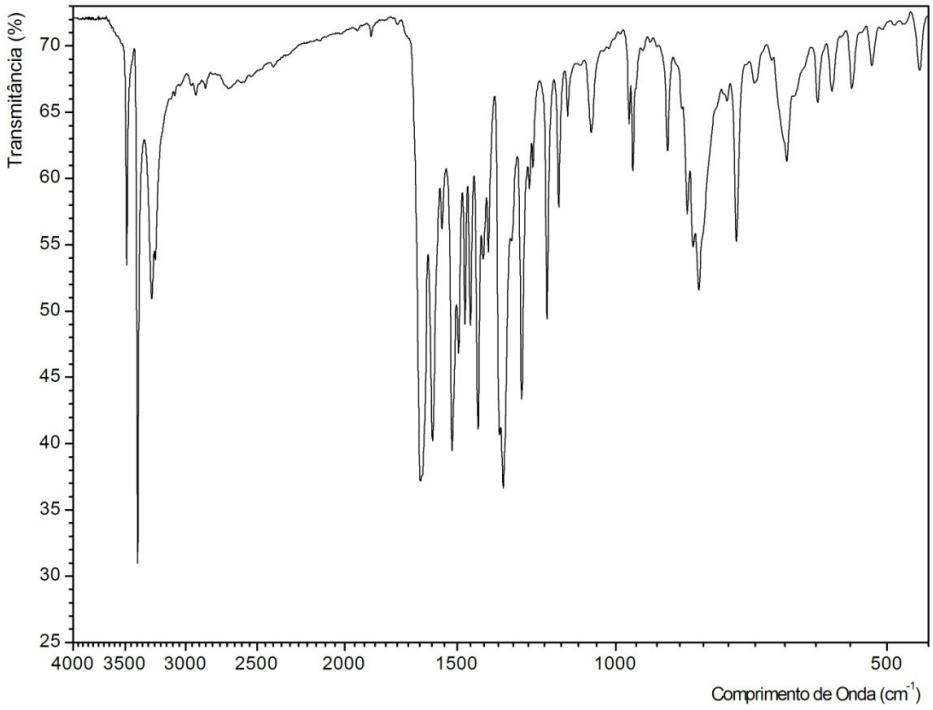


Figure S1. FTIR spectrum of **3a** in KBr pellets.

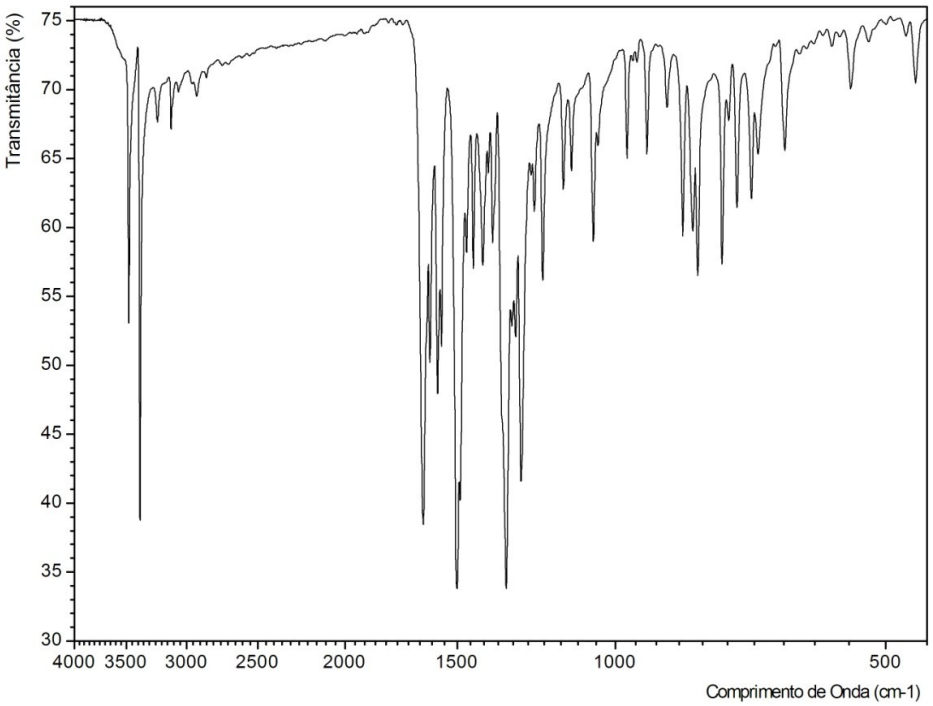


Figure S2. FTIR spectrum of **3a** in KBr pellets.

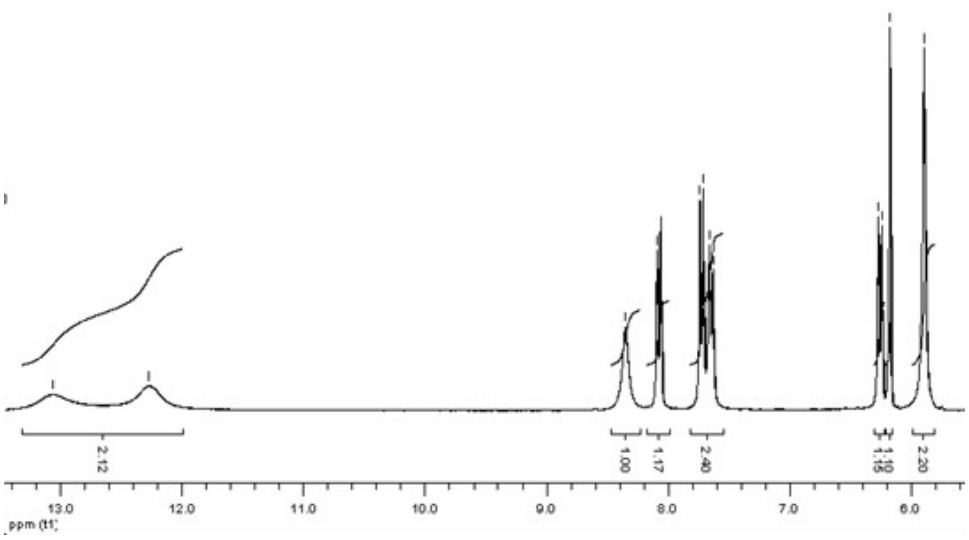


Figure S3. ^{1}H NMR spectrum (300 MHz) of **3a** in DMSO-d_6.

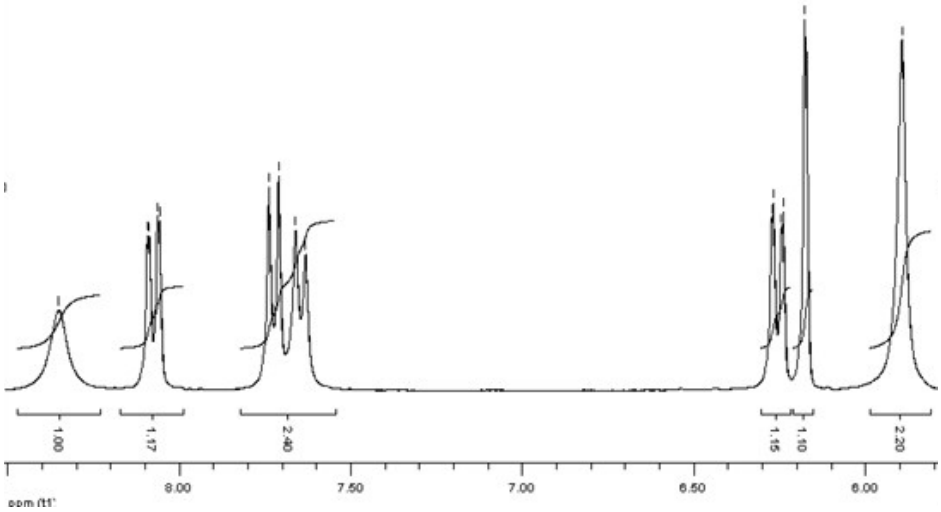


Figure S4. Amplification of the ^{1}H NMR spectrum (300 MHz) of **3a** in DMSO-d_6.

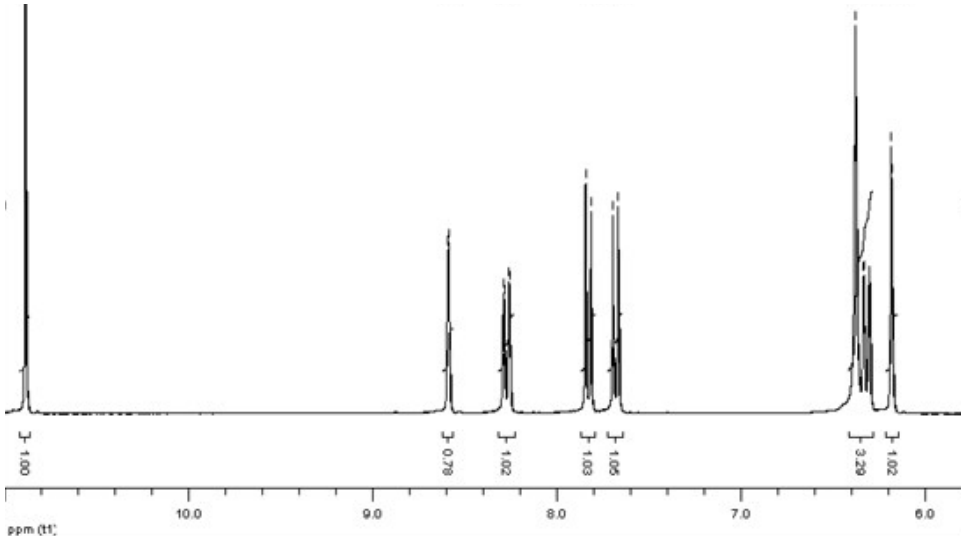


Figure S5. ^{1}H NMR spectrum (300 MHz) of **3a** in DMSO-d_6.

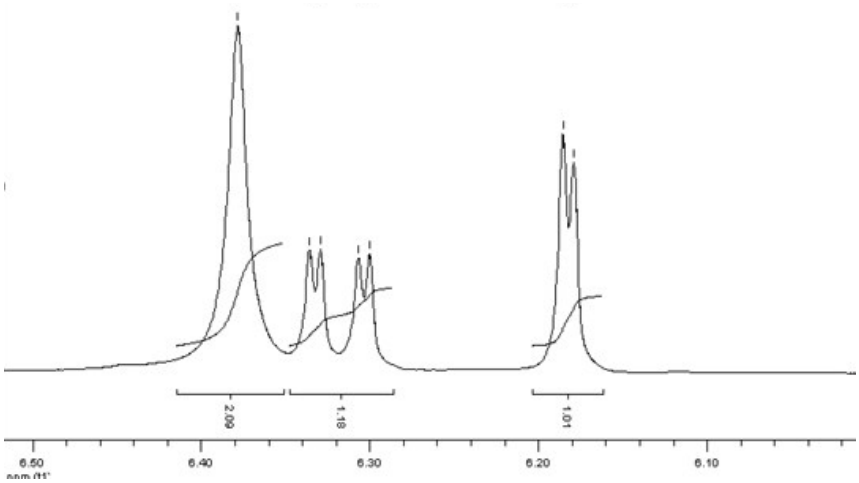


Figure S6. Amplification of the ^{1}H NMR spectrum (300 MHz) of **3b** in DMSO-d_6.

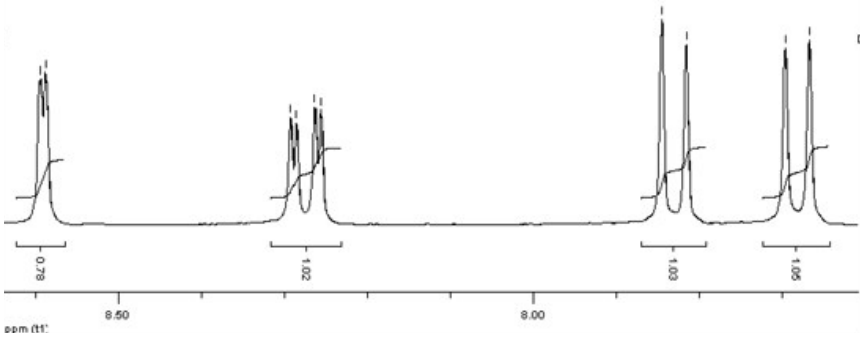
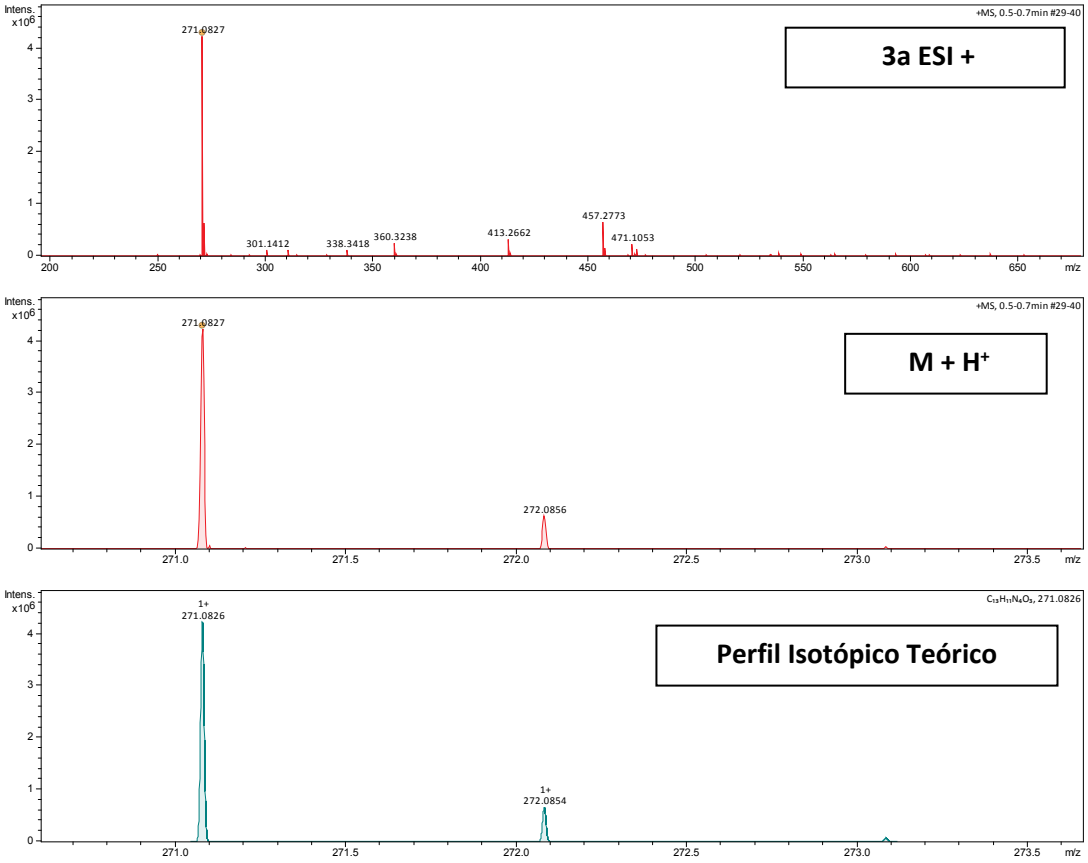
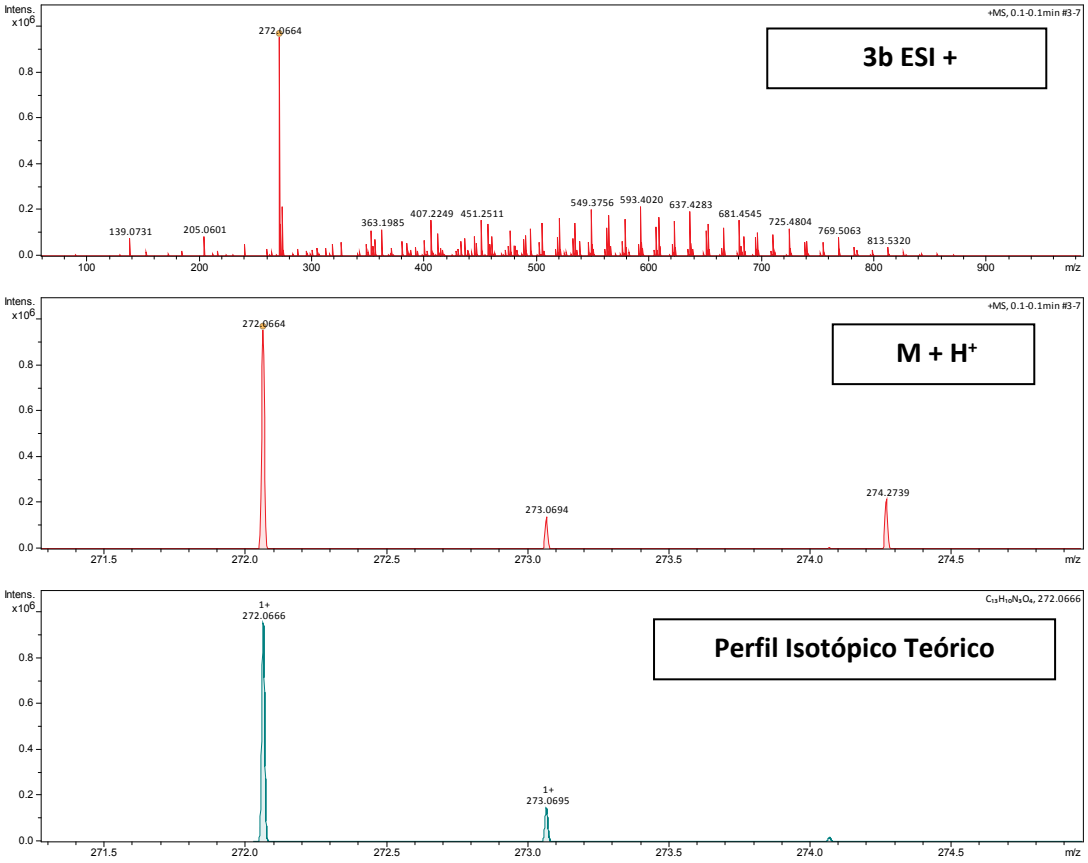


Figure S7. Amplification of the ^{1}H NMR spectrum (300 MHz) of **3b** in DMSO-d_6.



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
271.0827	C13H11N4O3	271.0826	-0.3	5.4	10.5	even	ok

Figure S8. HRMS data of **3a**.



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
272.0664	C13H10N3O4	272.0666	0.8	9	10.5	even	ok

Figure S9. HRMS data of **3b**.

Photophysical data

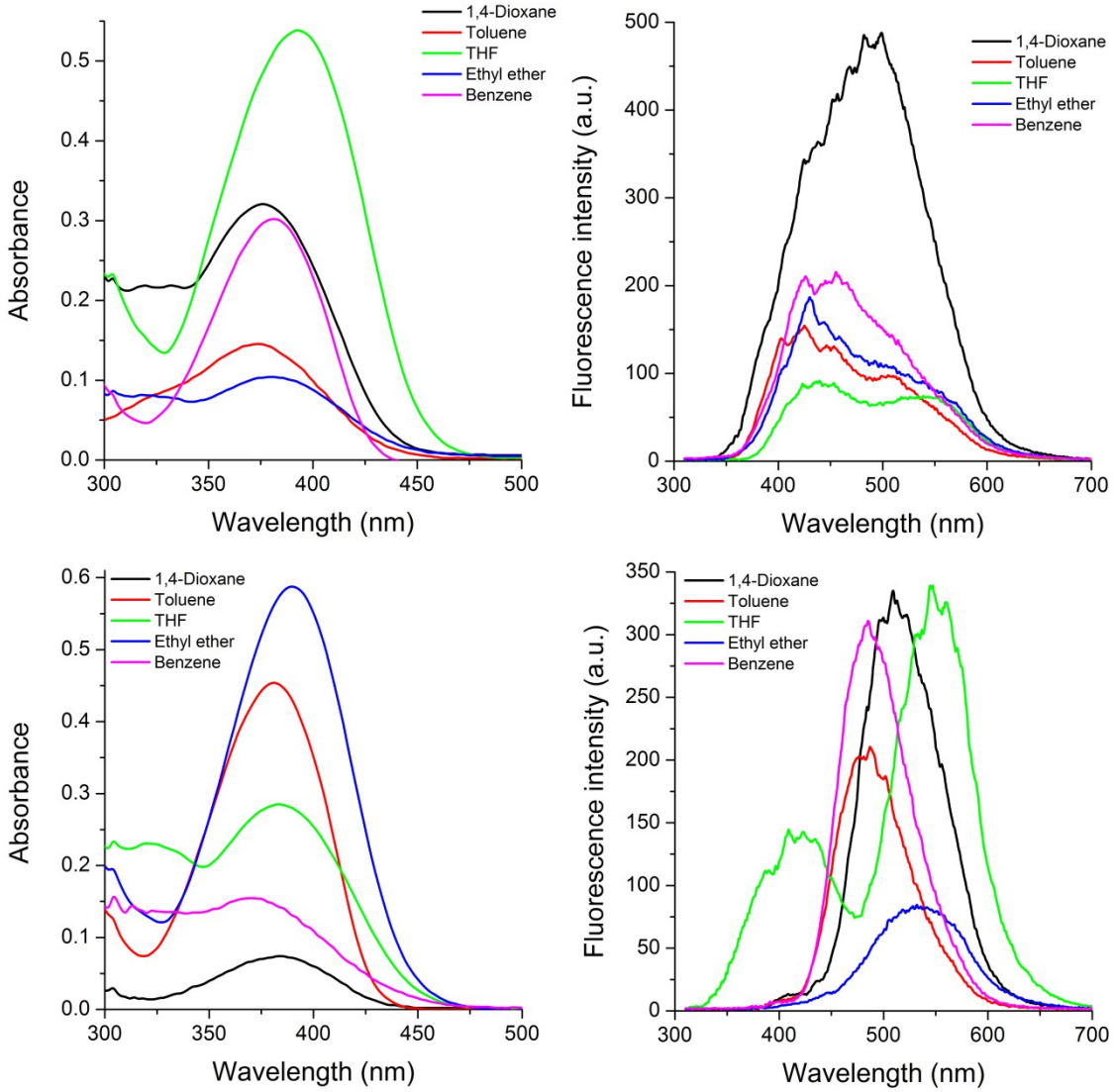


Figure S10. UV-Vis absorption and fluorescence emission spectra of **3a** (top) and **3b** (bottom) in different organic solvents at concentration of 10^{-5}M.

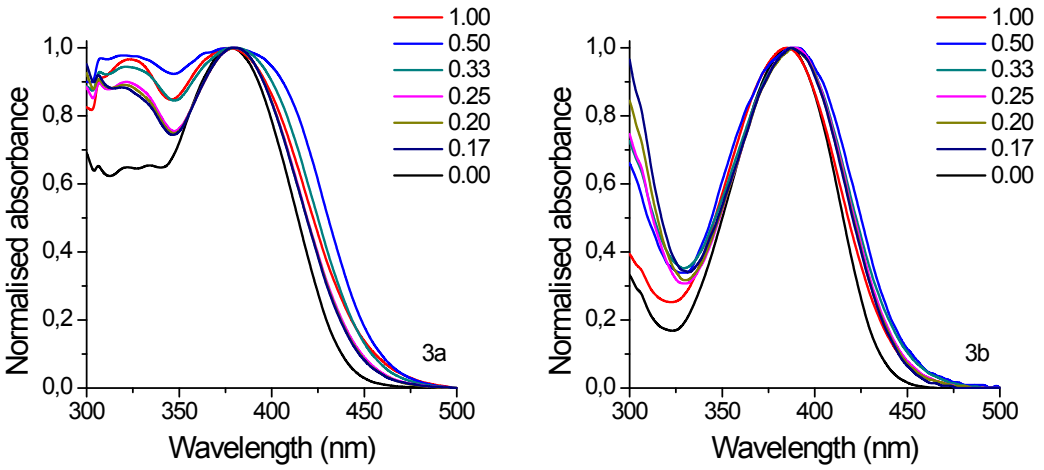


Figure S11. Solvent polarity plot function data. UV-Vis absorption spectra of **3a** and **3b** in acetonitrile:1,4-Dioxane mixtures. The acetonitrile volumetric fractions are indicated in both spectra.

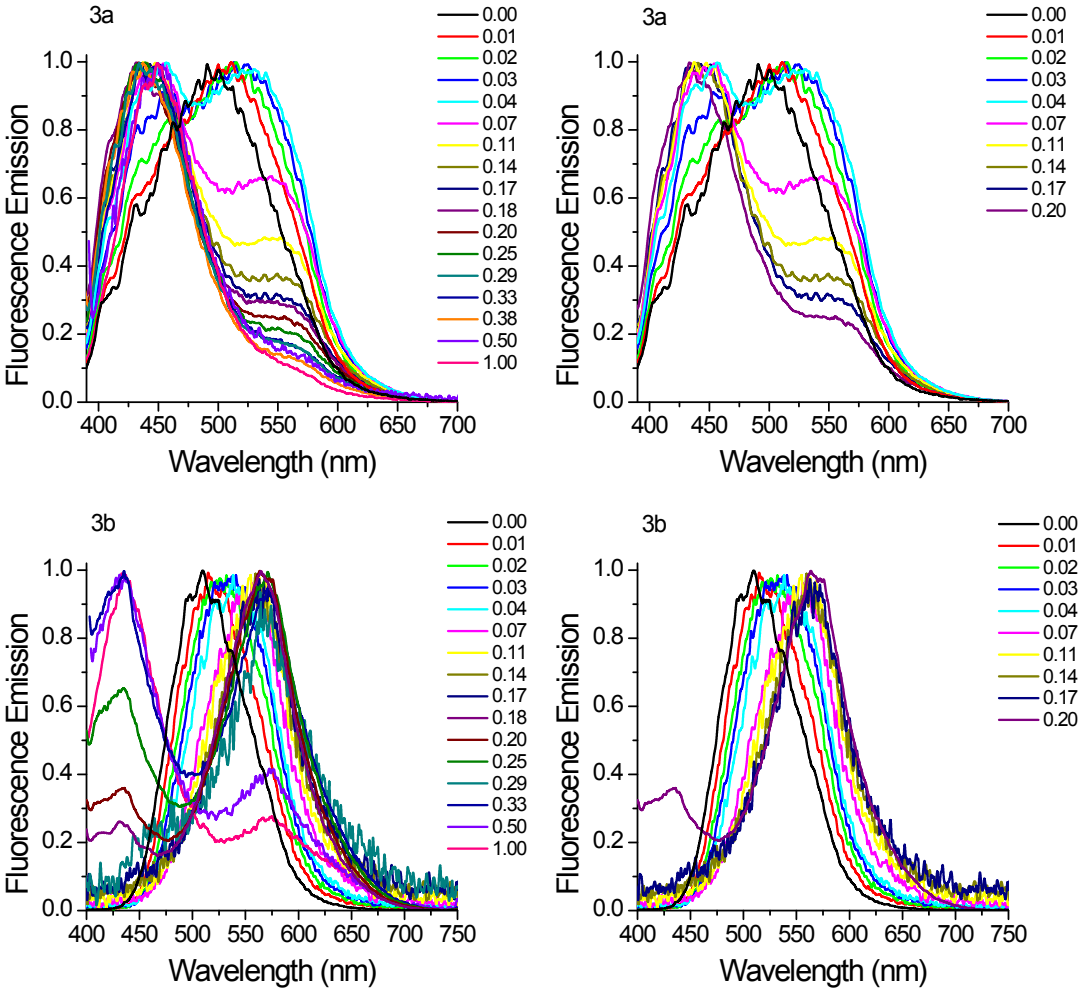


Figure S12. Solvent polarity plot function data. Normalised fluorescence emission spectra of **3a** and **3b** in acetonitrile:1,4-Dioxane mixtures. The acetonitrile volumetric fractions are indicated in the spectra.

Theoretical calculations

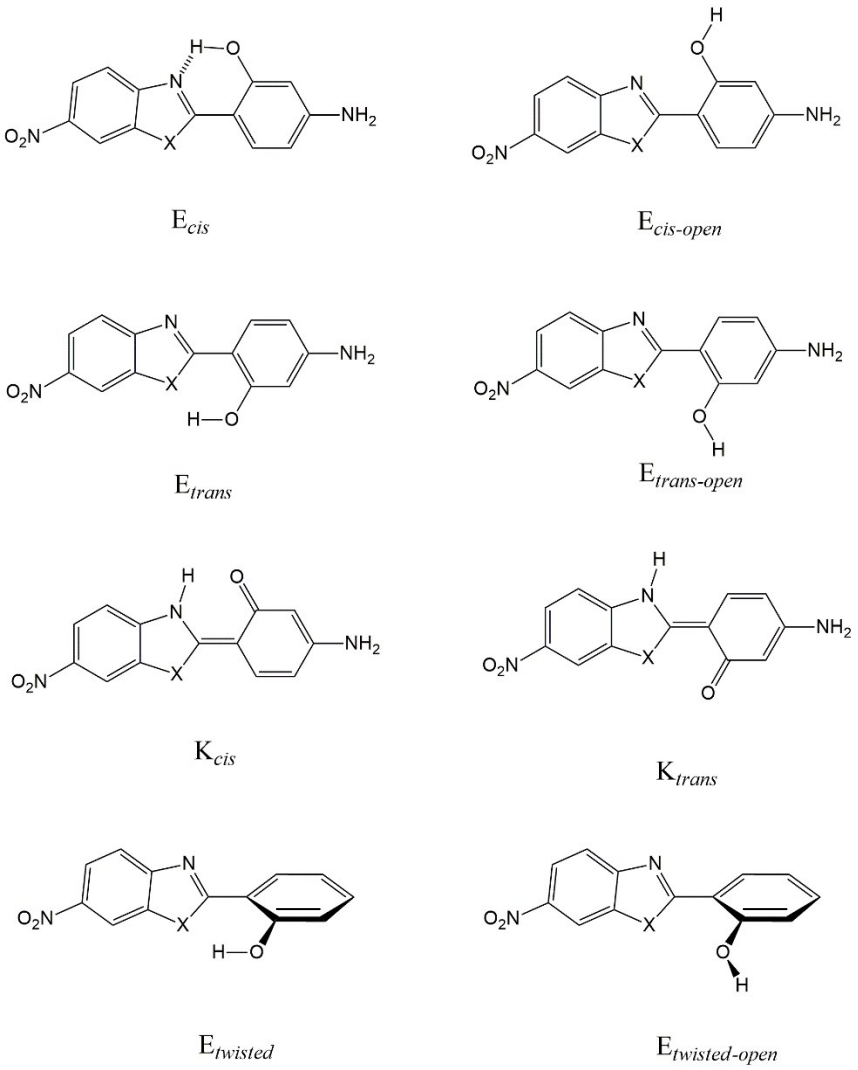


Figure S13 . Proposed conformations for the studied benzazole derivatives.

Table S1. Energies (in Hartree) obtained for all conformers found for **3b**, in 1,4-dioxane, in the ground state (E_{S0min}) and first singlet excited state (E_{S1min}). The energy differences are given in eV and were calculated with jun-cc-pVTZ in the cc-pVDZ geometries with the corresponding functionals.

	FUNC	E_{S0min} (Hartree)	E_{S1min} (Hartree)	$\Delta E_{min\text{-}min}$ (eV)	E_{abs} (eV)	E_{em} (eV)	$\Delta E_{rel\text{-}S0}$ (eV)	$\Delta E_{rel\text{-}S1}$ (eV)
E_{cis}	**PBE0**	-965.1732	-965.0669	2.89	3.08	2.70	0.00	0.00
	CAM	-965.8110	-965.6859	3.40	3.62	3.20	0.00	0.00
$E_{cis\text{-}open}$	**PBE0**	-965.1568	-965.0477	2.97	3.15	2.81	0.45	0.52
	CAM	-965.7951	-965.6693	3.42	3.68	3.18	0.43	0.45
K_{cis}	**PBE0**	-965.1530	-965.0685	2.30	2.73	1.83	0.55	-0.04
	CAM	-965.7908	-965.6747	3.16	3.34	2.89	0.55	0.30
E_{trans}	**PBE0**	-965.1634	-965.0564	2.91	3.09	2.74	0.27	0.29
	CAM	-965.8020	-965.6777	3.38	3.62	3.17	0.24	0.22
$E_{trans\text{-}open}$	**PBE0**	-965.1579	-965.0481	2.99	3.16	2.83	0.42	0.51
	CAM	-965.7961	-965.6702	3.43	3.68	3.19	0.40	0.43
K_{trans}	**PBE0**	-965.1290	-965.0645	1.76	2.60	066	1.20	0.07
	CAM	-965.7670	-965.6752	2.50	3.29	1.08	1.20	0.29

PBE0 = PBE1PBE; CAM = CAM-B3LYP; $\Delta E_{m\text{-}m} = ES_1 - ES_0$; E_{abs} = vertical absorption energy; E_{em} = vertical emission energy; $\Delta E_{rel\text{-}S0}$ = relative energy difference between conformers and E_{cis} at S_0; $\Delta E_{rel\text{-}S1}$ = relative energy difference between conformers E_{cis} at S_1.

Table S2. Absorption (λ_{abs}) and emission (λ_{em}) maxima wavelengths and respective oscillator forces found for all conformations obtained for **3a** with the functional PBE1PBE and CAM-B3LYP, varying the used solvent with PCM. The energies were calculated with jun-cc-pVTZ in the geometries calculated with cc-pVDZ.

		PBE1PBE				CAM-B3LYP			
	SOLV	**λ_{ABS} (nm)**	***f***	**λ_{EM} (nm)**	***f***	**λ_{ABS} (nm)**	***f***	**λ_{EM} (nm)**	***f***
ENOL CIS	DIOX	403.87	0.688	465.38	0.559	341.58	1.038	390.60	1.172
	DCM	422.14	0.633	507.12	0.715	349.53	0.994	427.17	1.341
	EtOH	425.86	0.602	520.28	0.757	350.59	0.960	438.59	1.383
	MeCN	426.39	0.595	522.75	0.765	350.67	0.951	440.67	1.390
ENOL CIS OPEN	DIOX	385.42	0.652	443.00	0.609	326.06	0.939	391.40	1.200
	DCM	410.66	0.588	496.09	0.723	337.96	0.898	431.80	1.358
	EtOH	417.01	0.567	512.23	0.754	340.38	0.869	444.36	1.397
	MeCN	418.01	0.562	515.24	0.760	340.73	0.862	446.72	1.404
ENOL TRANS	DIOX	398.39	0.233	494.95	0.162	325.82	0.646	388.13	0.438
	DCM	421.39	0.220	540.75	0.237	336.35	0.534	423.24	0.555
	EtOH	427.14	0.211	554.85	0.263	338.86	0.494	433.97	0.594
	MeCN	428.13	0.209	557.49	0.268	339.26	0.486	436.03	0.601
ENOL TRANS OPEN	DIOX	386.53	0.765	437.11	0.709	333.66	1.054	386.83	1.238
	DCM	411.91	0.683	490.43	0.821	346.23	1.003	427.22	1.397
	EtOH	417.70	0.646	506.70	0.854	348.51	0.969	439.96	1.439
	MeCN	418.61	0.638	509.74	0.861	348.80	0.960	442.36	1.446

Table S2. Continuation....

CETO CIS	DIOX	475.13	0.299	678.32	0.103	380.71	0.764	430.33	0.612
	DCM	478.26	0.315	646.95	0.217	379.50	0.776	440.97	0.898
	EtOH	477.55	0.309	641.41	0.262	377.78	0.758	446.47	0.966
	MeCN	477.29	0.306	640.60	0.271	377.34	0.752	447.58	0.978
CETO TRANS	DIOX	469.88	0.216	675.27	0.089	372.12	0.677	421.37	0.550
	DCM	474.86	0.243	644.33	0.189	372.73	0.686	432.60	0.807
	EtOH	475.00	0.244	638.91	0.231	371.93	0.670	438.68	0.871
	MeCN	474.95	0.243	638.11	0.240	371.69	0.665	439.93	0.882

DIOX=1,4-Dioxane; DCM=dichloromethane; EtOH=ethanol; MeCN=acetonitrile

Table S3. Absorption (λ_{abs}) and emission (λ_{em}) maxima wavelengths and respective oscillator forces found for all conformations obtained for **3a** with the functional PBE1PBE and CAM-B3LYP, varying the used solvent with PCM. The energies were calculated with jun-cc-pVTZ in the geometries calculated with cc-pVDZ.

		PBE1PBE				CAM-B3LYP			
	SOLV	**λ_{ABS} (nm)**	***f***	**λ_{EM} (nm)**	***f***	**λ_{ABS} (nm)**	***f***	**λ_{EM} (nm)**	***f***
ENOLCIS	DIOX	402.75	0.754	459.33	0.591	342.48	1.117	386.85	1.263
	DCM	419.90	0.711	496.04	0.777	349.95	1.095	421.95	1.448
	EtOH	423.38	0.682	507.63	0.827	350.82	1.067	432.82	1.494
	MeCN	423.86	0.676	509.84	0.837	350.85	1.060	434.86	1.502
ENOLCIS OPEN	DIOX	393.59	0.776	441.36	0.691	336.77	1.097	389.62	1.266
	DCM	416.46	0.716	490.02	0.826	347.79	1.065	428.44	1.433
	EtOH	421.50	0.685	504.69	0.863	349.64	1.038	440.52	1.475
	MeCN	422.28	0.678	507.41	0.871	349.85	1.031	442.67	1.481
ENOL TRANS	DIOX	401.73	0.788	451.86	0.660	342.53	1.133	390.83	1.301
	DCM	419.19	0.742	491.28	0.841	350.47	1.107	427.00	1.486
	EtOH	422.54	0.713	503.28	0.894	351.40	1.079	438.20	1.533
	MeCN	423.00	0.706	505.54	0.903	351.45	1.072	440.30	1.541

Table S3. Continuation...

		PBE1PBE				CAM-B3LYP			
	SOLV	**λ_{ABS} (nm)**	***f***	**λ_{EM} (nm)**	***f***	**λ_{ABS} (nm)**	***f***	**λ_{EM} (nm)**	***f***
ENOL TRANSOPEN	DIOX	392.07	0.806	438.59	0.721	336.77	1.130	388.46	1.312
	DCM	415.38	0.746	487.11	0.868	348.37	1.100	427.37	1.486
	EtOH	420.52	0.715	501.75	0.912	350.38	1.073	439.57	1.532
	MeCN	421.31	0.708	504.45	0.919	350.62	1.066	441.84	1.540
-CETOCIS	DIOX	453.99	0.288	677.26	0.059	371.02	0.781	428.81	0.497
	DCM	455.44	0.329	635.99	0.144	370.94	0.840	429.64	0.857
	EtOH	454.54	0.329	626.24	0.196	369.68	0.835	432.16	0.959
	MeCN	454.27	0.328	624.66	0.207	369.33	0.832	432.77	0.977
CETO TRANS	DIOX	476.35	0.1878	1871.7	0.000	376.76	0.604	1147.51	0.0000
	DCM	474.89	0.2155	1180.6	0.000	376.86	0.679	918.44	0.0000
	EtOH	473.00	0.2184	1087.3	0.000	375.69	0.686	869.63	0.0001
	MeCN	472.54	0.2182	1072.6	0.000	375.36	0.686	862.17	0.0002

DIOX=1,4-Dioxane; DCM=dichloromethane; EtOH=ethanol; MeCN=acetonitrile

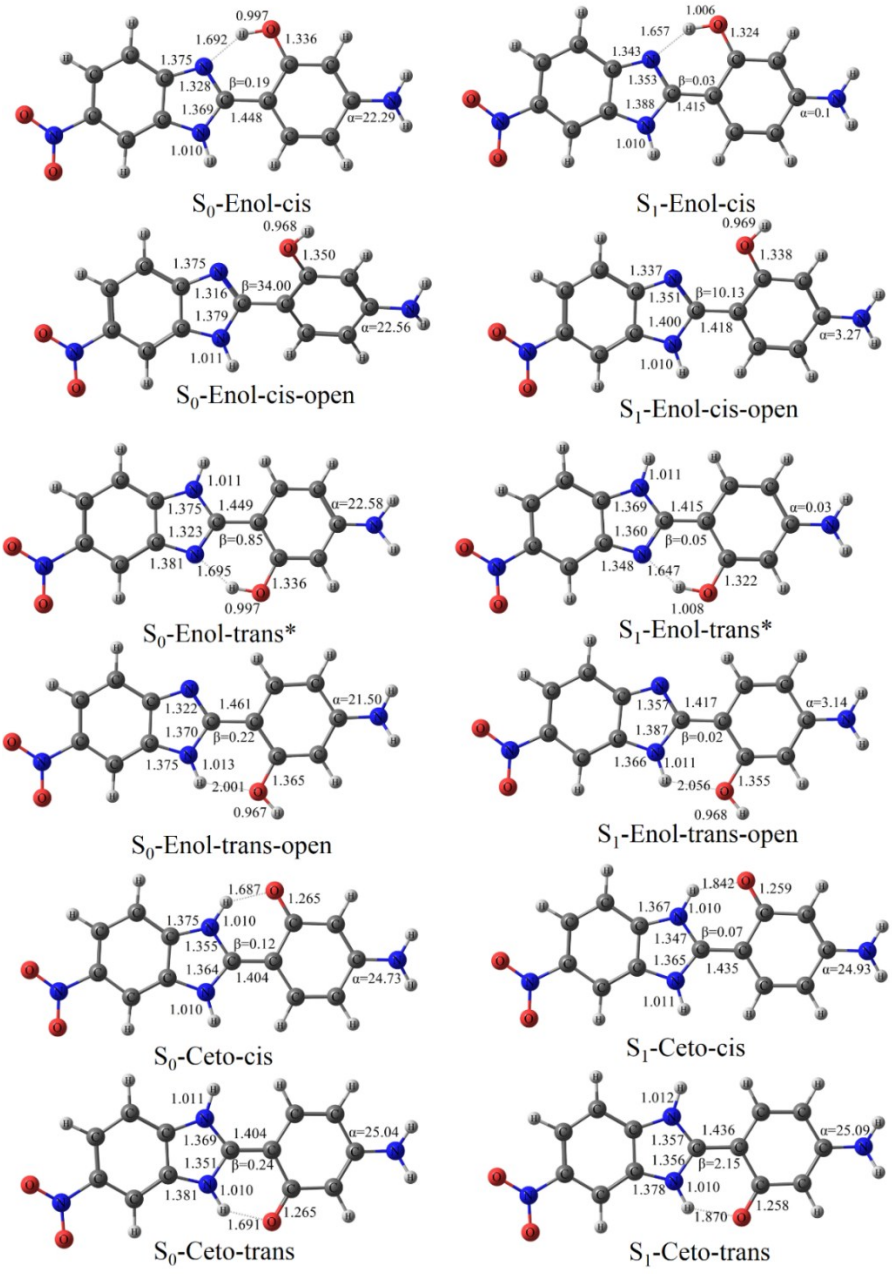


Figure S14. **3a** conformers optimized in the ground (S_0) and the excited states (S_1) using CAM-B3LYP/cc-pVDZ and PCM/1,4-dioxane. The bond lengths are given in angstroms and the dihedral angles in degrees (α = $C_{5'}$—C_4'—N—H; β= N_3—C_2—$C_{1'}$—$C_{2'}$).

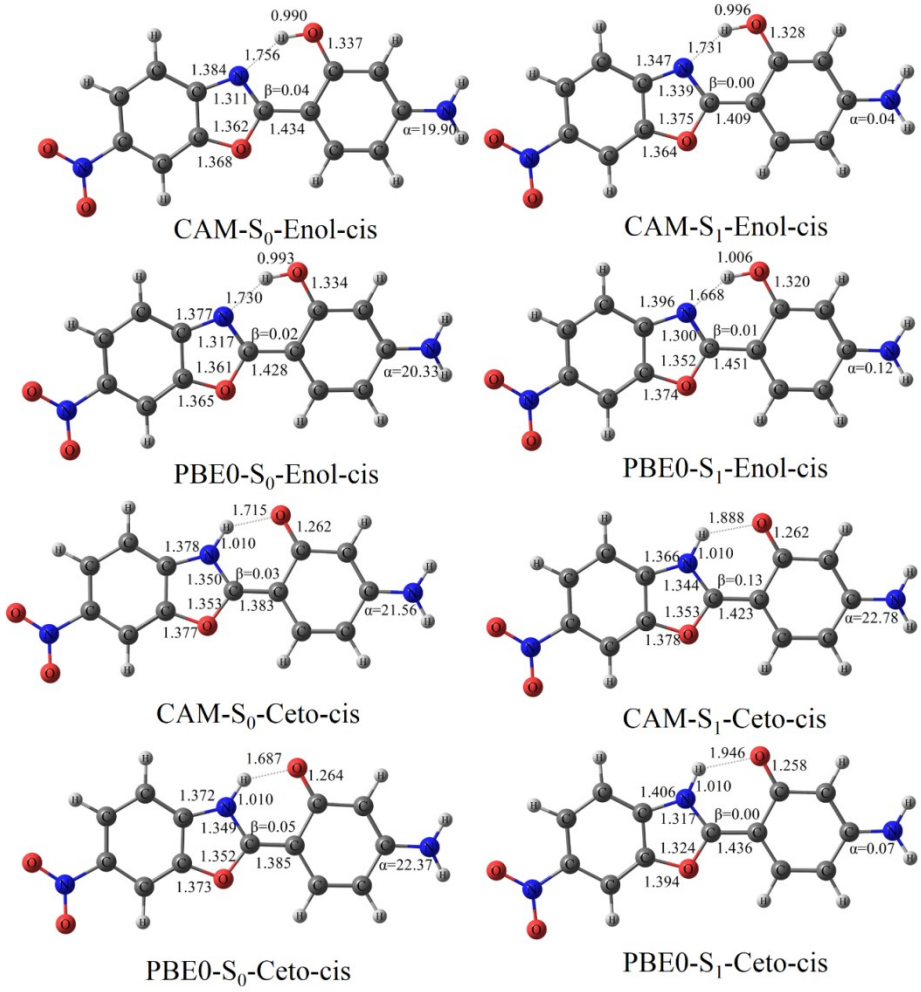


Figure S15. Minimized energies for the ground (left) and excited (right) states for **3b** using PCM and 1,4-dioxane as solvent. The major bond lengths (in Angstroms) and angles (in degrees) are presented and were calculated using CAM-B3LYP and PBE1PBE with the base set cc-pVDZ.

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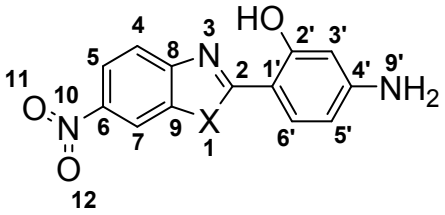
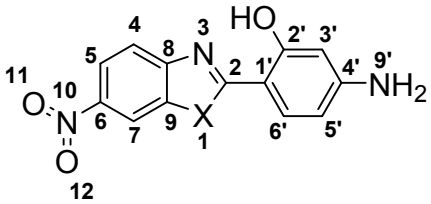
Table S4. Partial charges (in ua) and dipole moments (in debye) calculated for HBO, **3a** and **3b** using CAM-B3LYP and PBE1PBE (values in red), juncec-pVTZ and 1,4-dioxane as solvent. Population analysis was done using ChelpG.



Estrutura	μ	N_3	$O_{7'}$	$H_{8'}$	X_1	$N_{9'}$	N_{10}	O_{11}	O_{12}
HBO-S_0	2,6	-0,508	-0,567	0,345	-0,290				
	2,5	-0,479	-0,536	0,337	-0,264				
HBO-S_1-E	1,6	-0,545	-0,528	0,373	-0,303				
	1,4	-0,526	-0,499	0,373	-0,276				
HBO-S_1-K	3,7	-0,466	-0,655	0,420	-0,275				
	2,7	-0,459	-0,630	0,427	-0,253				

Table S4. Continuation...



(3a) X=NH
(3b) X=O

Estrutura	μ	N_3	$O_{7'}$	$H_{8'}$	X_1	$N_{9'}$	N_{10}	O_{11}	O_{12}
3a-S_0	8,6	-0,562	-0,592	0,365	-0,598	-0,794	0,739	-0,457	-0,472
	9,2	*-0,533*	*-0,558*	*0,355*	*-0,574*	*-0,752*	*0,703*	*-0,444*	*-0,457*
3a-S_1-E	20,8	-0,528	-0,551	0,368	-0,583	-0,898	0,661	-0,565	-0,570
	28,0	*-0,484*	*-0,509*	*0,357*	*-0,544*	*-0,805*	*0,597*	*-0,580*	*-0,596*
3a-S_1-K	16,3	-0,467	-0,638	0,434	-0,504	-0,769	0,672	-0,557	-0,557
	24,4	*-0,473*	*-0,581*	*0,44*	*-0,522*	*-0,761*	*0,585*	*-0,584*	*-0,598*
NAHBO-S_0	7,8	-0,533	-0,569	0,352	-0,287	-0,798	0,740	-0,454	-0,463
	8,5	*-0,503*	*-0,537*	*0,342*	*-0,254*	*-0,760*	*0,705*	*-0,440*	*-0,449*
NAHBO-S_1-E	19,6	-0,489	-0,539	0,358	-0,300	-0,899	0,690	-0,556	-0,558
	27,8	*-0,442*	*-0,487*	*0,340*	*-0,265*	*-0,789*	*0,617*	*-0,579*	*-0,589*
NAHBO-S_1-K	12,7	-0,491	-0,637	0,447	-0,262	-0,779	0,699	-0,519	-0,519
	25,5	*-0,510*	*-0,577*	*0,454*	*-0,239*	*-0,903*	*0,594*	*-0,581*	*-0,591*

Spectra, orbitals, and electronic transitions

3a ABSORPTION: 1,4-dioxane

Main transitions:

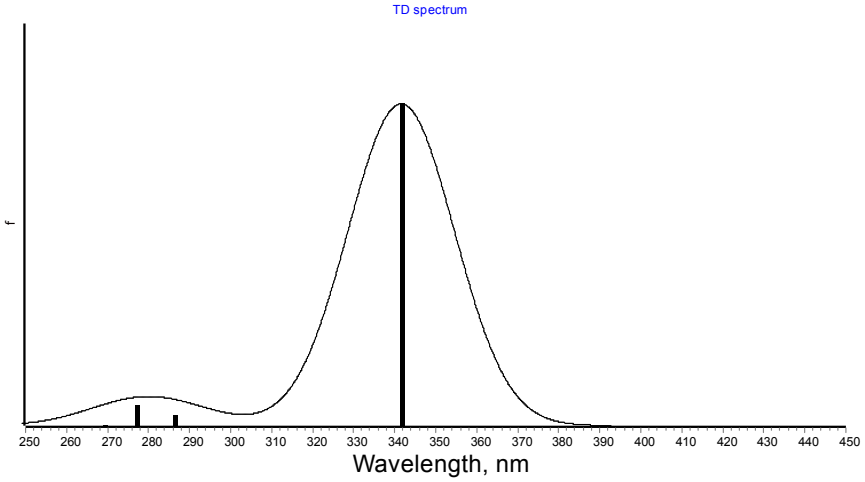
Excited State 1: Singlet-A 3.6298 eV 341.58 nm f=1.0384 <S**2>=0.000 70 -> 71 0.63062

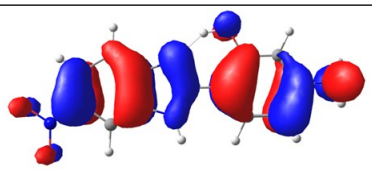
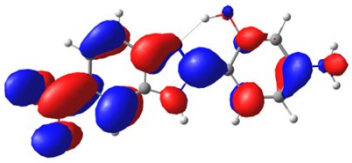
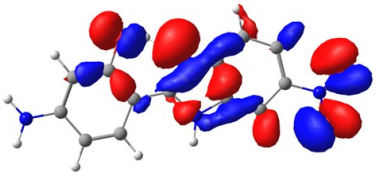
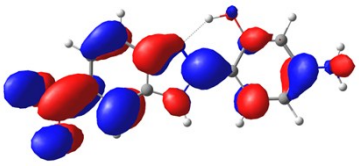
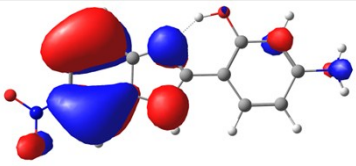
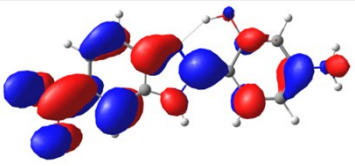
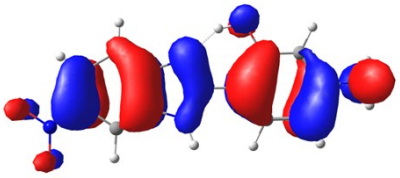
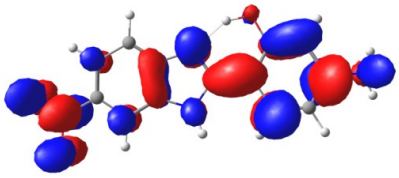
Excited State 2: Singlet-A 4.0579 eV 305.54 nm f=0.0000 <S**2>=0.000 66 -> 71 0.58349

Excited State 3: Singlet-A 4.3286 eV 286.43 nm f=0.0344 <S**2>=0.000 68 -> 71 0.64612

Excited State 4: Singlet-A 4.4755 eV 277.03 nm f=0.0650 <S**2>=0.000 70 -> 72 0.42519

Excited State 5: Singlet-A 4.6030 eV 269.36 nm f=0.0005 <S**2>=0.000 62 -> 71 0.64750



MO 70		**MO 71**	
MO 66		**MO 71**	
MO68		**MO 71**	
MO 70		**MO 72**	

3a EMISSION:1,4-Dioxane

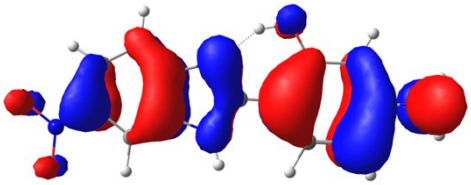
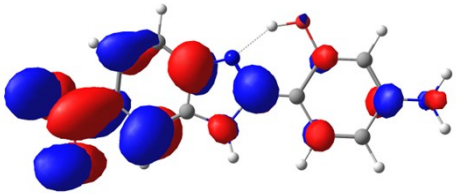
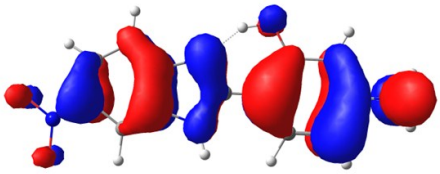
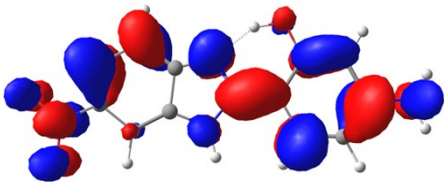
Main transitions:

Excited State 1: Singlet-A 3.1742 eV 390.60 nm f=1.1718 <S**2>=0.000 70 -> 71 0.65780

Excited State 2: Singlet-A 3.7491 eV 330.70 nm f=0.0000 <S**2>=0.000 66 -> 71 0.59244

Excited State 3: Singlet-A 4.1170 eV 301.15 nm f=0.0068 <S**2>=0.000 68 -> 71 0.60394

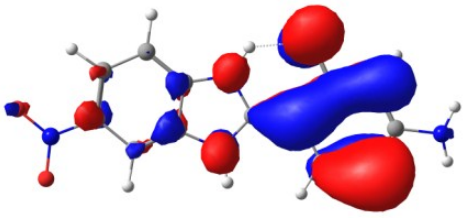
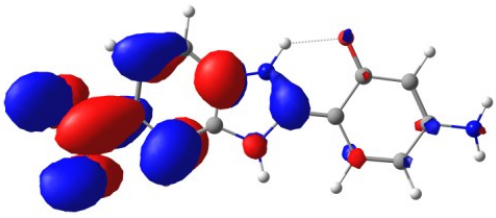
Excited State 4: Singlet-A 4.2566 eV 291.27 nm f=0.2084 <S**2>=0.000 70 -> 72 0.50696

MO 70	MO 71
	
MO 70	**MO 72**
	

3a: KETO Emission: 1,4-dioxane

Main transition:

Excited State 1: Singlet-A 2.8811 eV 430.33 nm f=0.6123 <S**2>=0.000 70 -> 71 0.62942

MO 70	MO 71
	

3a ENOL ABSORPTION: Acetonitrile

Main transitions:

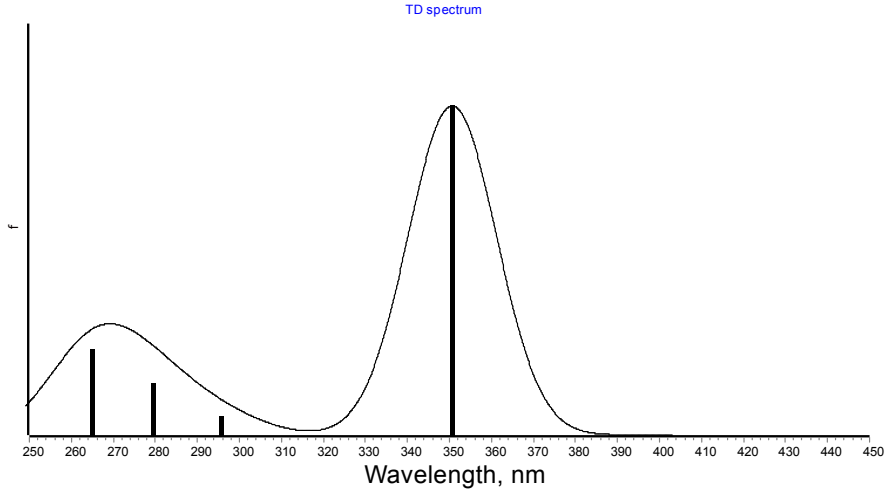
Excited State 1: Singlet-A 3.5356 eV 350.67 nm f=0.9509 <S**2>=0.000 70 -> 71 0.63551

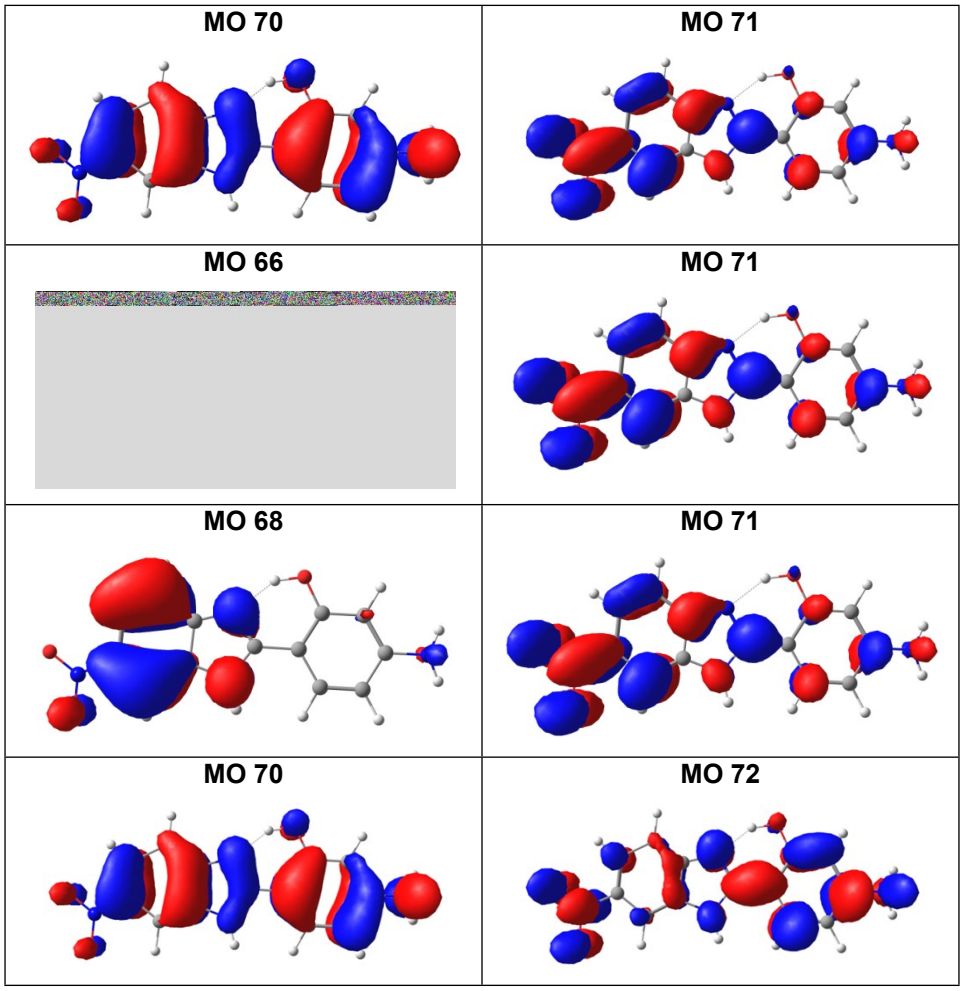
Excited State 2: Singlet-A 4.0769 eV 304.11 nm f=0.0000 <S**2>=0.000 66 -> 71 0.64261

Excited State 3: Singlet-A 4.1968 eV 295.43 nm f=0.0552 <S**2>=0.000 68 -> 71 0.66867

Excited State 4: Singlet-A 4.4382 eV 279.36 nm f=0.1497 <S**2>=0.000 70 -> 72 0.49651

Excited State 5: Singlet-A 4.6843 eV 264.68 nm f=0.2472 <S**2>=0.000 69 -> 71 0.38580





3a EMISSION: Acetonitrile

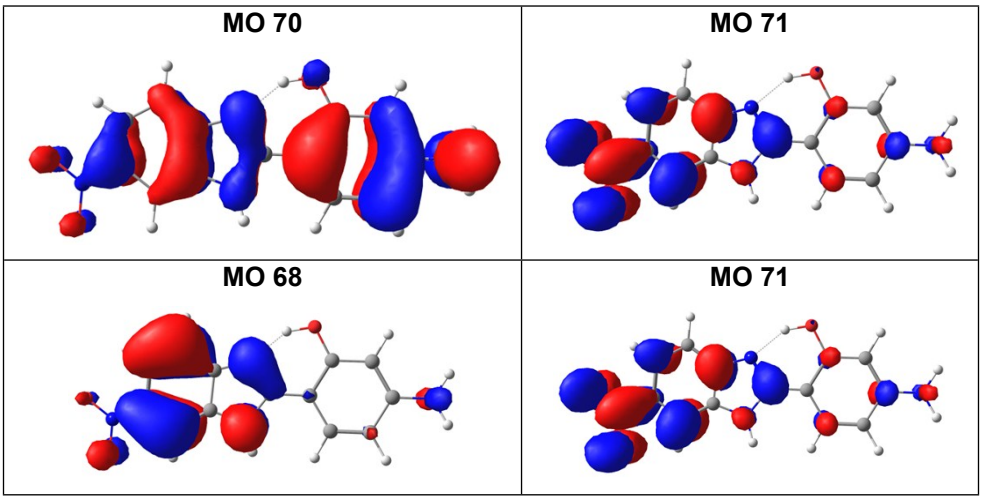
Main transitions:

Excited State 1: Singlet-A 2.8135 eV 440.67 nm f=1.3904 <S**2>=0.000 70 -> 71 0.65735

Excited State 2: Singlet-A 3.7081 eV 334.36 nm f=0.0000 <S**2>=0.000 66 -> 71 0.49888

Excited State 3: Singlet-A 3.8853 eV 319.11 nm f=0.0162 <S**2>=0.000 68 -> 71 0.63885

Excited State 4: Singlet-A 4.0528 eV 305.93 nm f=0.4397 <S**2>=0.000 70 -> 72 0.57688



3b ENOL ABSORPTION: 1,4-dioxane

Main transitions:

Excited State 1: Singlet-A 3.6202 eV 342.48 nm f=1.1165 <S**2>=0.000 70 -> 71 0.62906

Excited State 2: Singlet-A 4.0564 eV 305.65 nm f=0.0000 <S**2>=0.000 66 -> 71 0.62454

Excited State 3: Singlet-A 4.4777 eV 276.89 nm f=0.0010 <S**2>=0.000 70 -> 72 0.35145

Excited State 4: Singlet-A 4.5681 eV 271.41 nm f=0.0010 <S**2>=0.000 68 -> 71 0.44533

Excited State 5: Singlet-A 4.7073 eV 263.39 nm f=0.2876 <S**2>=0.000 70 -> 72 0.45019

ABSORPTION ENOL IN ACETONITRILE

Main transitions:

Excited State 1: Singlet-A 3.5338 eV 350.85 nm f=1.0601 <S**2>=0.000 70 -> 71 0.63310

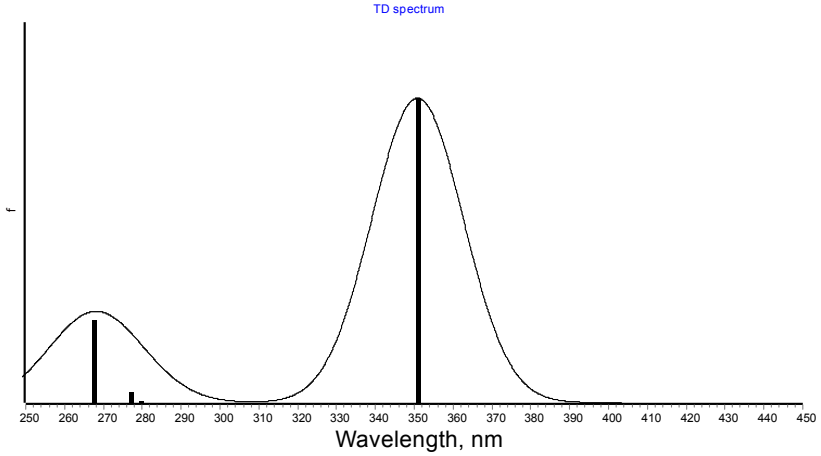
Excited State 2: Singlet-A 4.0758 eV 304.19 nm f=0.0000 <S**2>=0.000 66 -> 71 0.53525

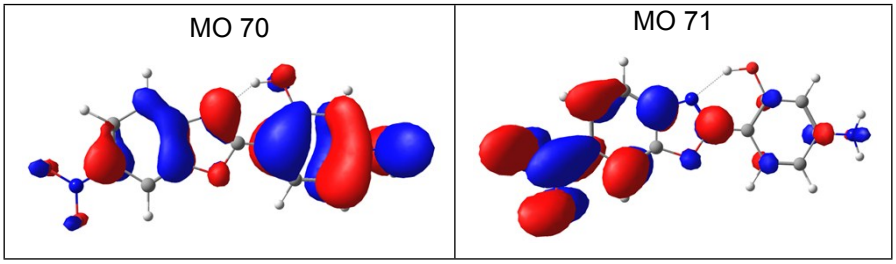
Excited State 3: Singlet-A 4.4359 eV 279.50 nm f=0.0045 <S**2>=0.000 68 -> 71 0.40086

Excited State 4: Singlet-A 4.4789 eV 276.82 nm f=0.0365 <S**2>=0.000 67 -> 71 0.42659

Excited State 5: Singlet-A 4.6404 eV 267.18 nm f=0.2885 <S**2>=0.000 70 -> 72 0.34450

Absorption spectra in acetonitrile





EMISSION IN 1,4-DIOXANE:

Main transitions:

Excited State 1: Singlet-A 3.2050 eV 386.85 nm f=1.2634 <S**2>=0.000 70 -> 71 0.65632

Excited State 2: Singlet-A 3.7663 eV 329.19 nm f=0.0000 <S**2>=0.000 66 -> 71 0.63230

Excited State 3: Singlet-A 4.2715 eV 290.26 nm f=0.0349 <S**2>=0.000 70 -> 72 0.51105

Excited State 4: Singlet-A 4.4015 eV 281.69 nm f=0.0005 <S**2>=0.000 63 -> 71 0.62691

Excited State 5: Singlet-A 4.4103 eV 281.12 nm f=0.0038 <S**2>=0.000 67 -> 71 0.48631

EMISSION – ACETONITRILE:

Main transitions:

Excited State 1: Singlet-A 2.8511 eV 434.86 nm f=1.5020 <S**2>=0.000 70 -> 71 0.65465

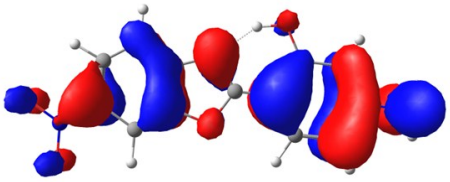
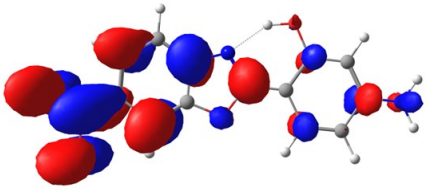
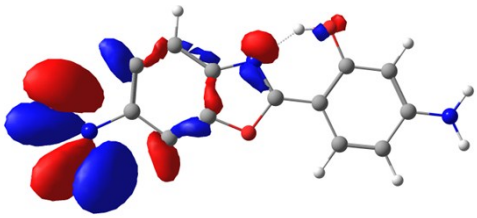
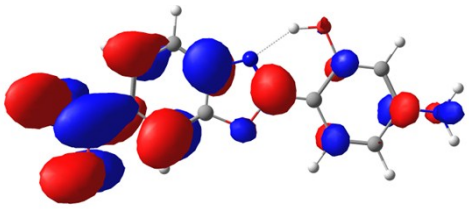
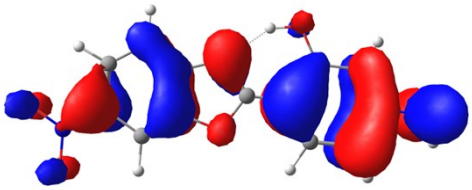
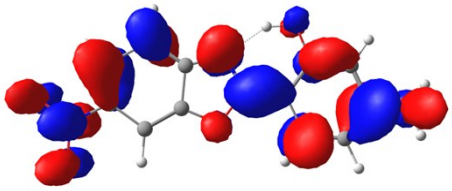
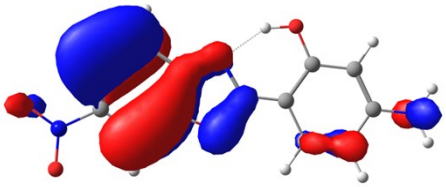
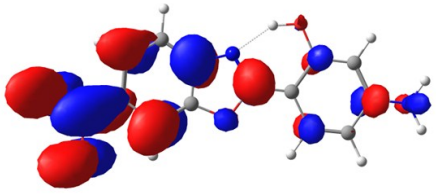
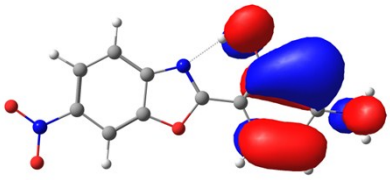
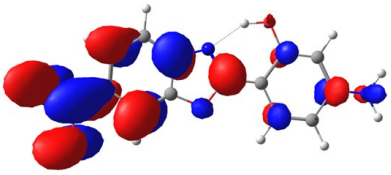
Excited State 2: Singlet-A 3.7348 eV 331.97 nm f=0.0000 <S**2>=0.000 66 -> 71 0.63933

Excited State 3: Singlet-A 4.0621 eV 305.22 nm f=0.1407 <S**2>=0.000 70 -> 72 0.56615

Excited State 4: Singlet-A 4.2468 eV 291.95 nm f=0.1557 <S**2>=0.000 67 -> 71 0.60139

Excited State 5: Singlet-A 4.3491 eV 285.08 nm f=0.1421 <S**2>=0.000 69 -> 71 0.54068

MO in acetonitrile:

MO 70	**MO 71**
	
66	**71**
	
70	**72**
	
67	**71**
	
69	**71**
	

Characterisation of the non-ESIPT benzazoles

Figure S16. FTIR spectrum of **3c** in KBr pellets.

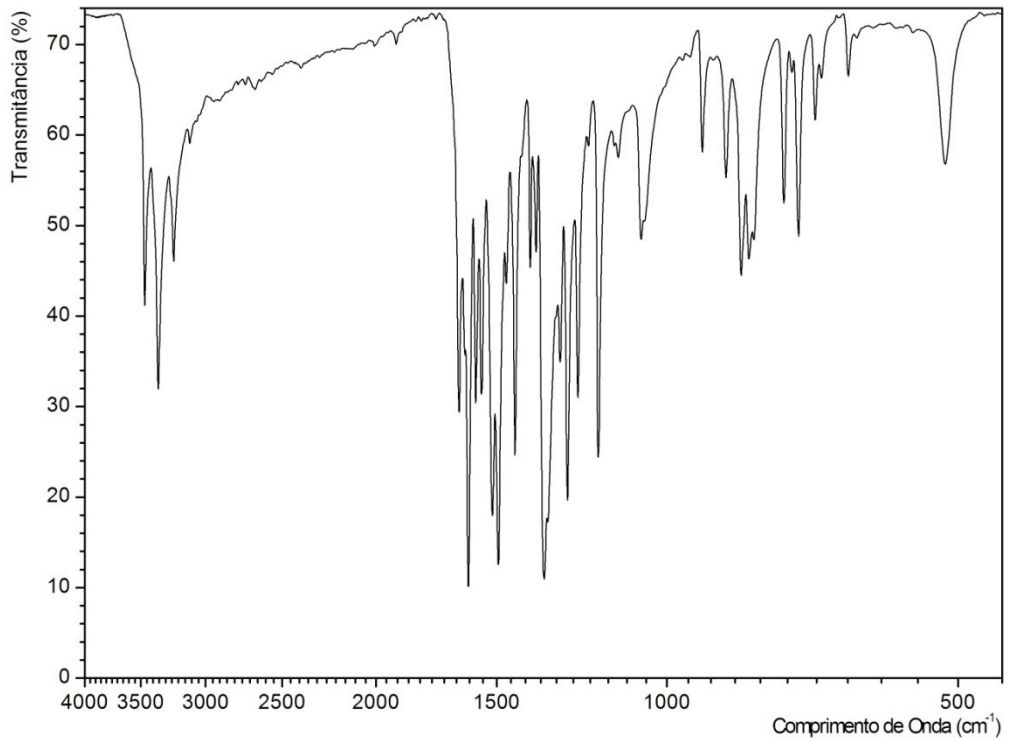


Figure S17. FTIR spectrum of **3d** in KBr pellets.

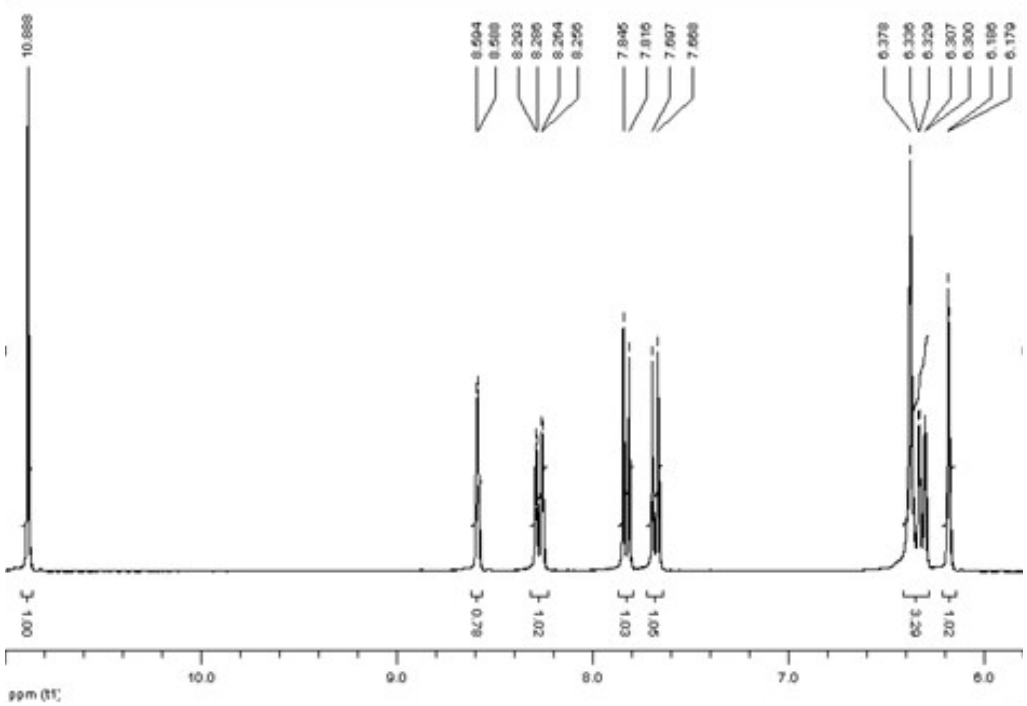


Figure S18. ^{1}H NMR spectrum (300 MHz) of **3c** in DMSO-d_6.

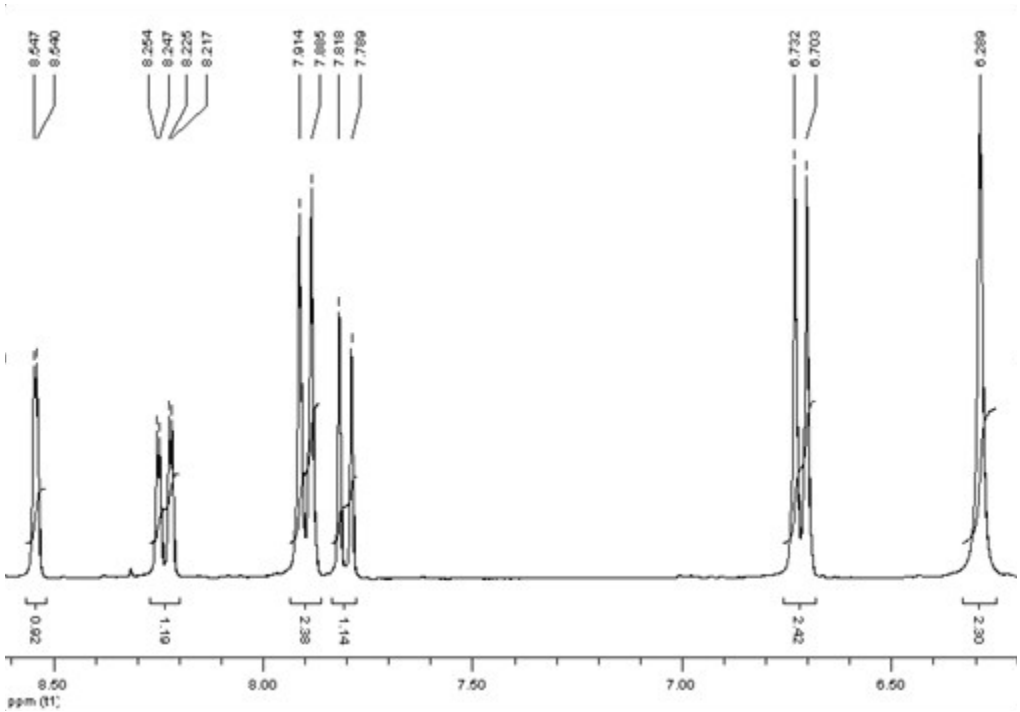
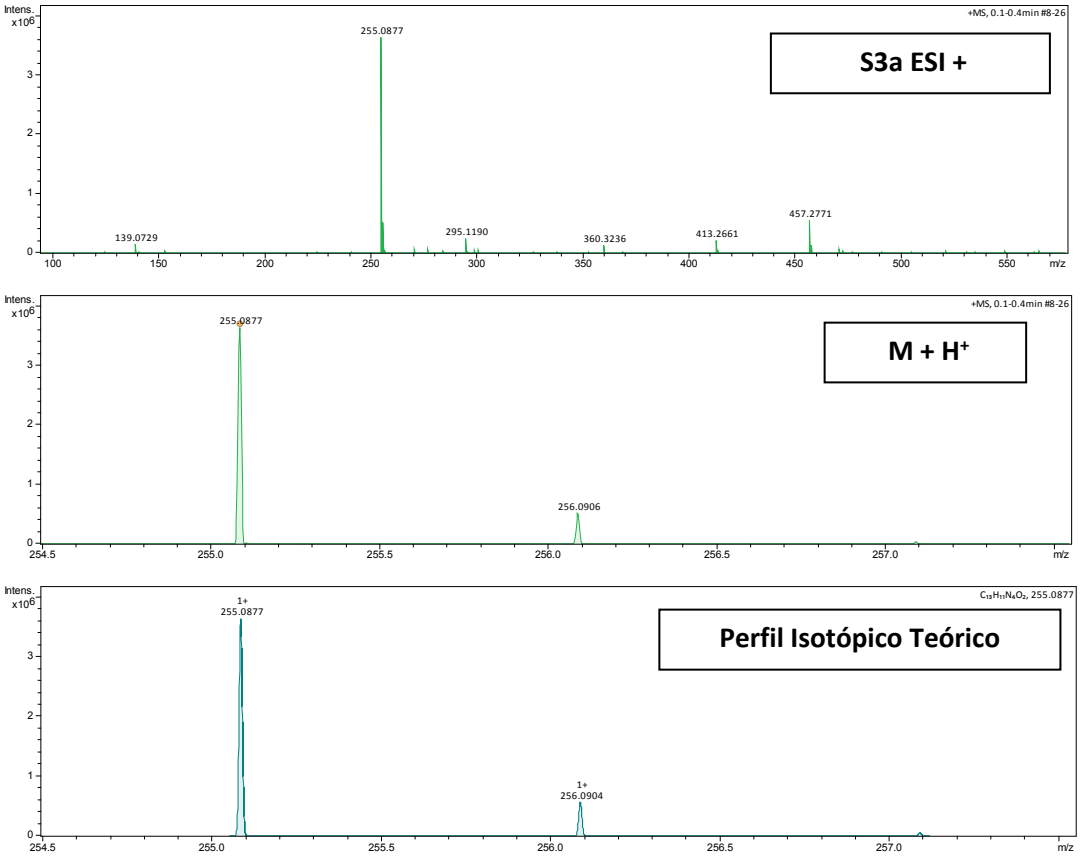
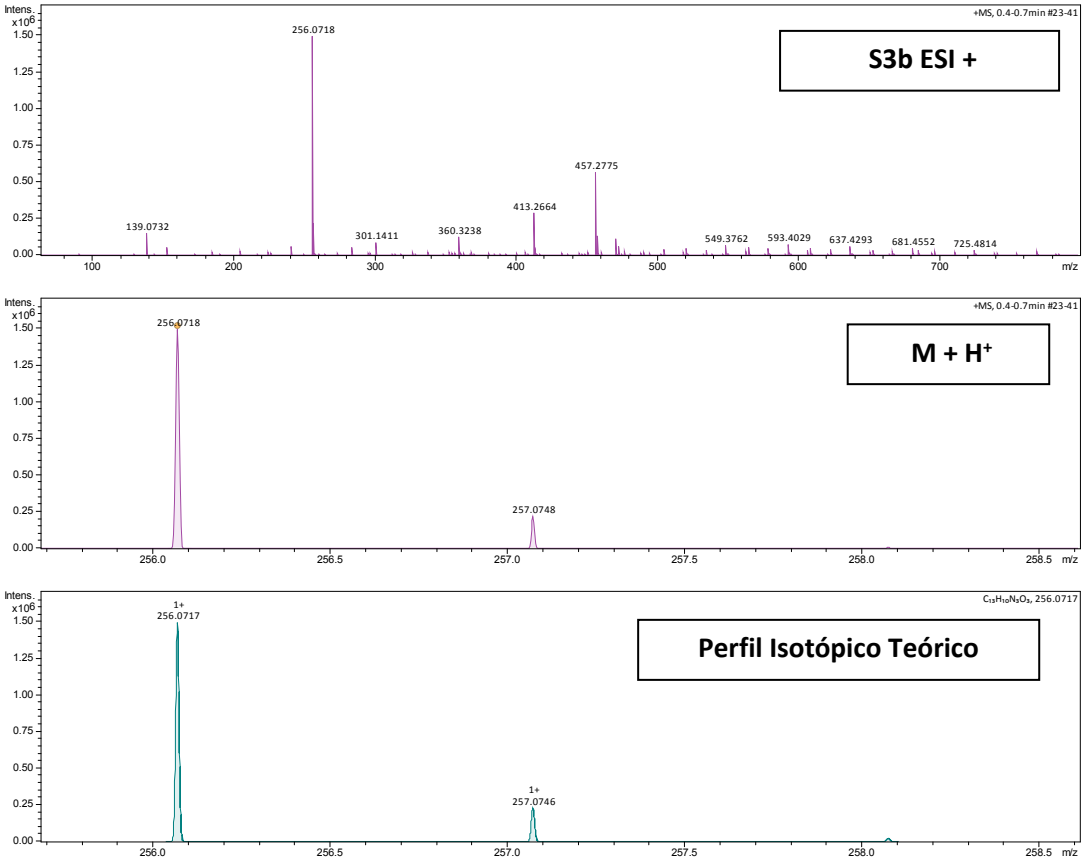


Figure S19. ^{1}H NMR spectrum (300 MHz) of **3d** in DMSO-d_6.



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
255.0877	C13H11N4O2	255.0877	0	8.3	10.5	even	ok

Figure S20. HRMS data of **3c**.



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
256.0718	C13H10N3O3	256.0717	-0.5	7.5	10.5	even	ok

Figure S21. HRMS data of **3d**.

Calculations with explicit solvation

NAHBN in acetonitrile: Emission with explicit solvation

Excited State 1: Singlet-A 2.6270 eV 471.96 nm f=1.3370 <S**2>=0.000
114 -> 115 0.66187
Excited State 2: Singlet-A 3.7003 eV 335.06 nm f=0.0000 <S**2>=0.000
109 -> 115 0.65842
Excited State 3: Singlet-A 3.7194 eV 333.34 nm f=0.0636 <S**2>=0.000
112 -> 115 0.66697
Excited State 4: Singlet-A 3.9737 eV 312.01 nm f=0.5089 <S**2>=0.000
114 -> 116 0.61030

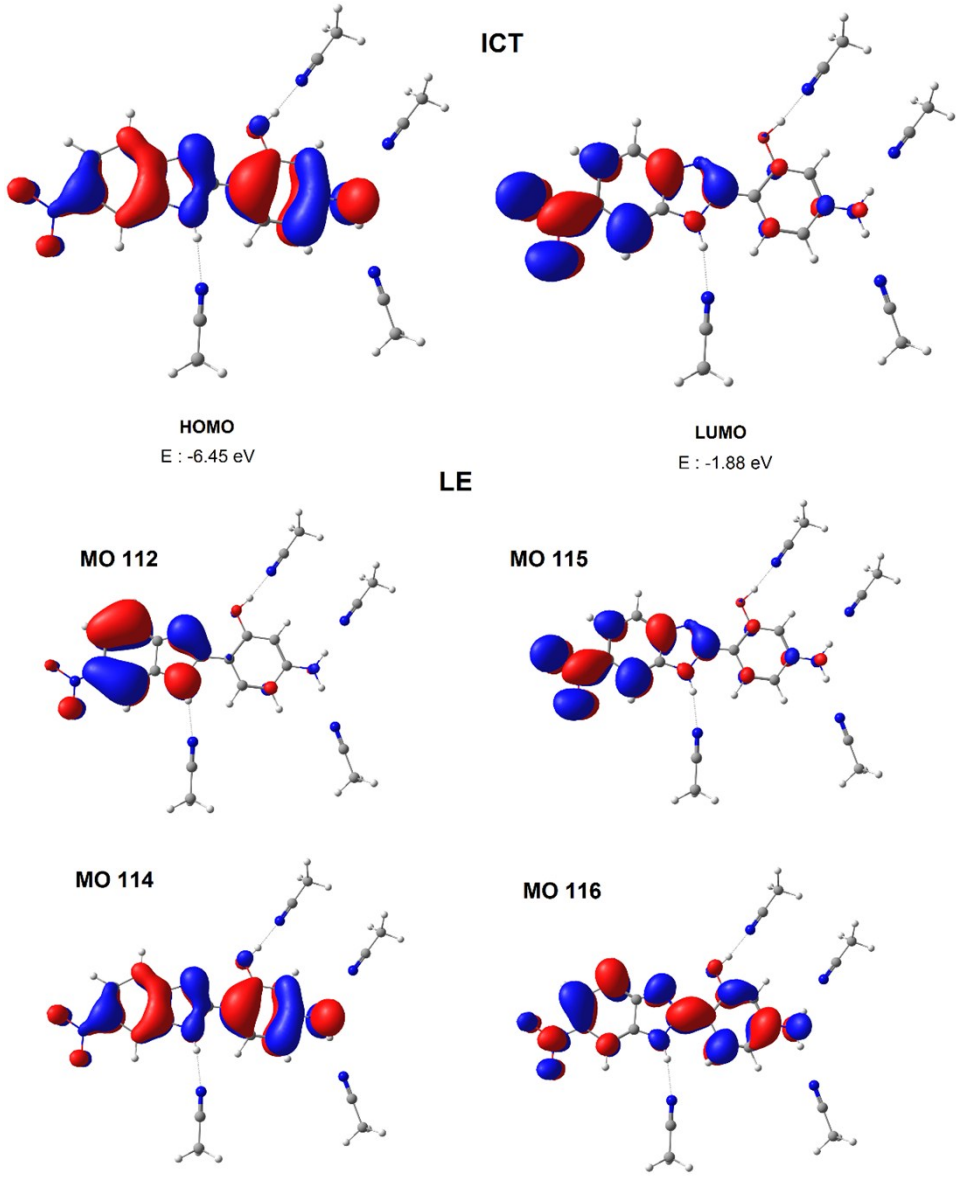


Figure S22. Emission with explicit solvation of **3a** in acetonitrile.

NAHBO in acetonitrile: Emission with explicit solvation

Excited State 1: Singlet-A 2.6797 eV 462.68 nm f=1.4674 <S**2>=0.000
103 -> 104 0.65765
Excited State 2: Singlet-A 3.7137 eV 333.85 nm f=0.0000 <S**2>=0.000
98 -> 104 0.62198
Excited State 3: Singlet-A 4.0049 eV 309.58 nm f=0.2119 <S**2>=0.000
103 -> 105 0.55872
Excited State 4: Singlet-A 4.1450 eV 299.12 nm f=0.2241 <S**2>=0.000
100 -> 104 0.61504

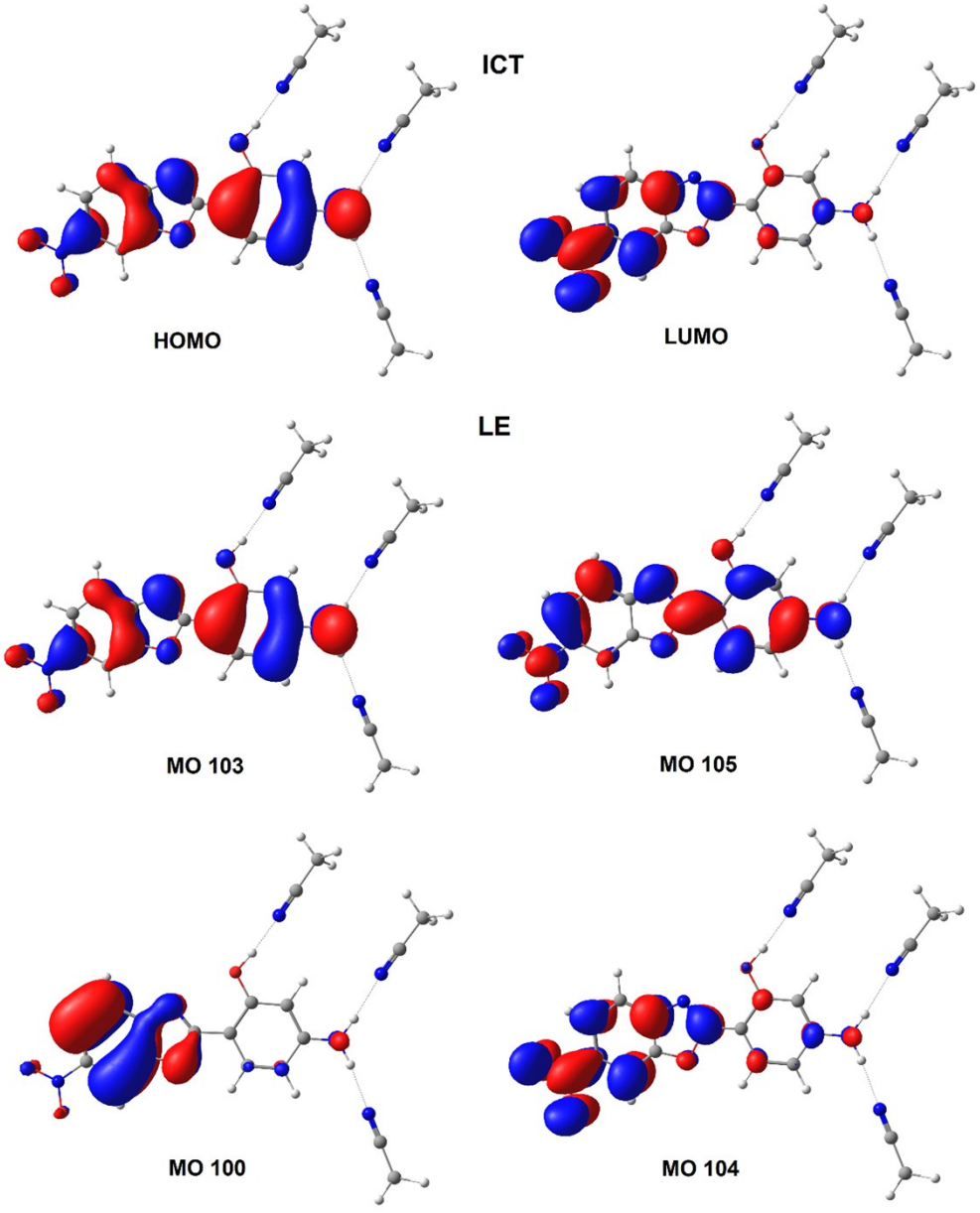


Figure S23. Emission with explicit solvation of **3b** in acetonitrile.

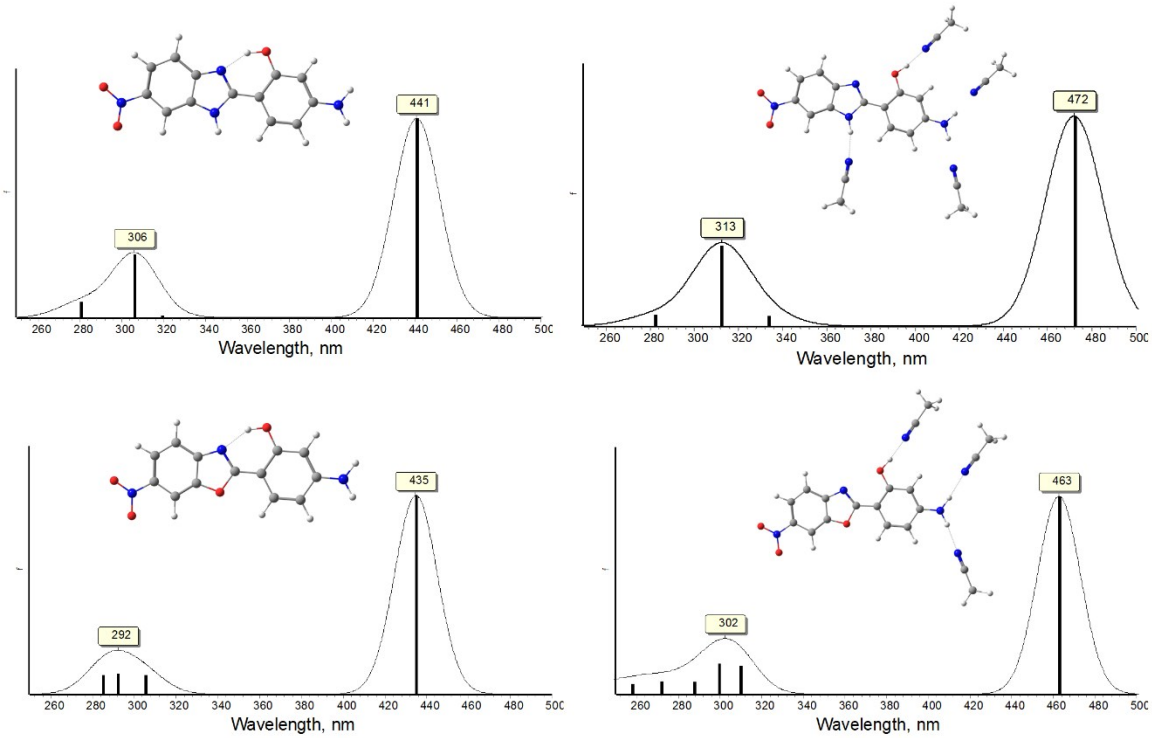


Figure S24. Comparison between emission spectra using implicit solvent and using explicit solvent. The spectra were computed using CAM-B3LYP functional.