Supporting Information

Synthesis of HBI-pBr

2-Hydroxy-5-bromobenzaldehyde (4.0 mmol), o-phenylenediamine (4.4 mol) and catalytic dose of silver nitrate ($AgNO_3$) were mixed in a 50 mL round-bottom flask with 20 mL dimethylsulfoxide (DMSO). Then, the mixture was stirred for 4 h in a water bath condition (35 ℃). The TLC template (PE:EA=3:1) was employed to monitor the progress of the reaction. The mixture was cooled to room temperature after finishing and then 60 mL dichloromethane (DCM) was added to the above room mixture, and then a large amount of saturated salt water was applied to extract the organic layer, which was span and dried to obtain the pure (Z)-2-(((2-hydroxyphenyl)imino)methyl)-4-bromophenol. Next, (Z)-2-(((2-hydroxyphenyl)imino)methyl)-4-bromophenol and 2,3-dichloro-5,6-difluoro-p-benzoquinone (DDQ) in a molar ratio of 1:1.1 were mixed in 60 mL dichloromethane. Similarly, the reaction was stirred at 40 ℃ for 4 h and monitored by TLC (PE:EA=5:1). Finally, by filtration the filtrate was retained and spin-dried and recrystallized with methanol to obtain the target product HBI-pBr, ^{1}H NMR (400 MHz, DMSO-*d6*) δ13.32 (s, 2H), 8.32 (d, J = 2.5 Hz, 1H), 7.71 (s, 2H), 7.55 (dd, J = 8.8, 2.5 Hz, 1H), 7.37-7.30 (m, 2H), 7.05 (d, J = 8.8 Hz, 1H).

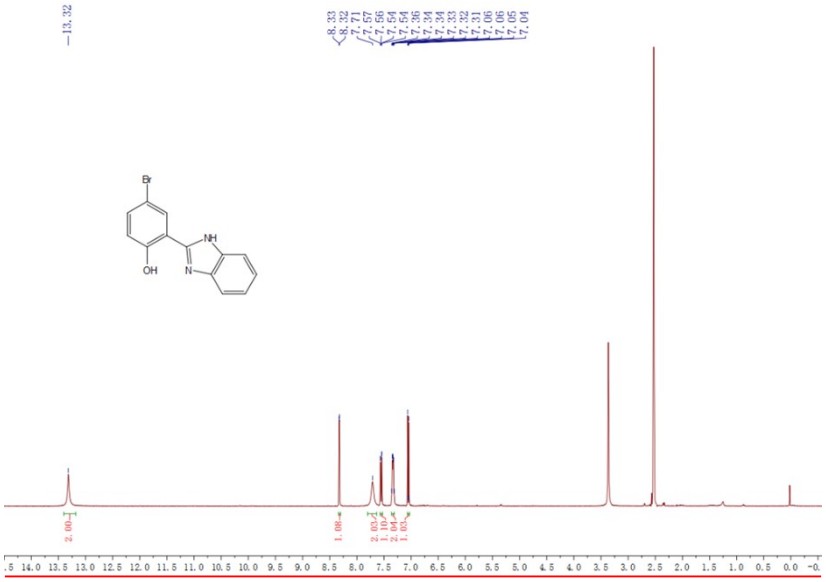


Figure S1. ^{1}H NMR spectrum of 2-(2'-hydroxy-5'-bromo)phenylbenzimidazole (HBI-pBr) (400 HZ, DMSO-*d6)*.

Preparation of sample solution

To investigate the effect of pH on molecular properties, we conducted titration experiments using standardized trifluoroacetic acid (2.0×10^{-4} M) and tetrabutylammonium hydroxide (2.0×10^{-4} M), recording the absorption and emission spectra. All solutions were freshly prepared in methanol, with the procedure involving the addition of 2.5×10^{-5} M HBI-pBr and varying volumes of TFA (0.000, 0.010, 0.020, 0.0035, 0.047, 0.080, 0.125 and 2.000 mL) and TBAOH (0.000, 0.085, 0.110, 0.145, 0.165, 0.185, 0.210, 0.225, 0.230, 0.350, 1.000, 3.000 and 6.000 mL) into several 10 ml volumetric flasks. The experiments were carried out at room temperature (25 ℃). The calibration procedure was repeated three times prior to each pK_a value determination.

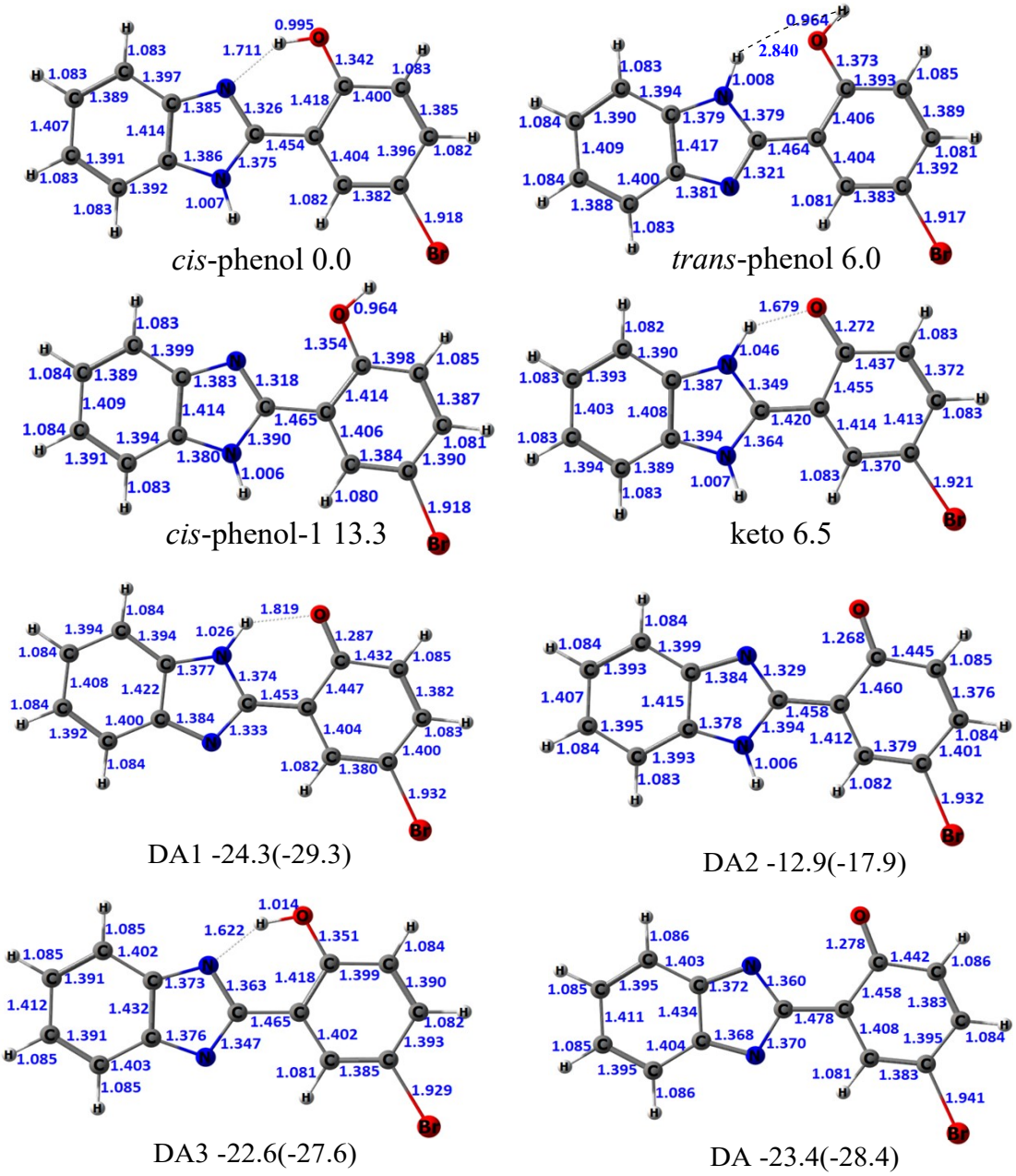


Figure S2. Optimized bond length/Å and relative zero-point correction energy/kcal·mol^{-1} for *cis*-phenol, keto, and anion of HBI-pBr in S_0 and S_1 at the B3LYP/6-311+G(d, p) level (solvent= methanol) model.

Notes: The data in parentheses represent the relative energy without zero-point correction.

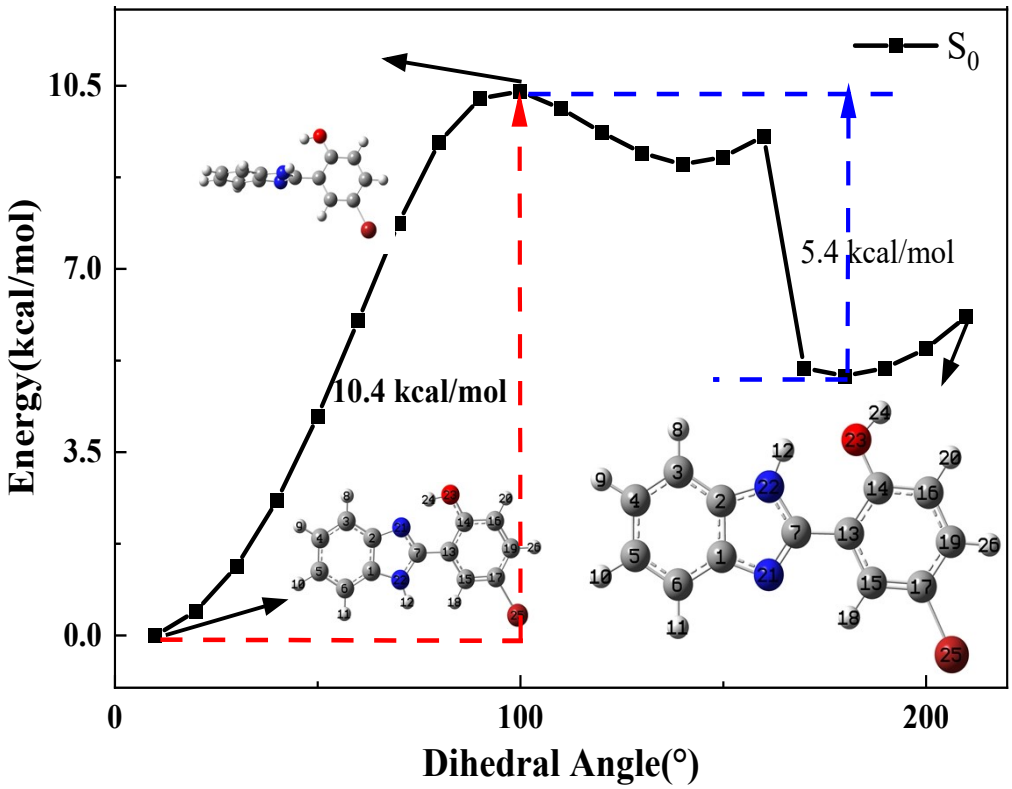


Figure S3. Isomerization potential energy surface curves of *cis*-phenol and *trans*-phenol calculated at B3LYP/6-311+G(d, p) level using PCM (solvent=methanol) model. (Note: dihedral angle: C_{15}-C_{13}-C_7-N_{21}

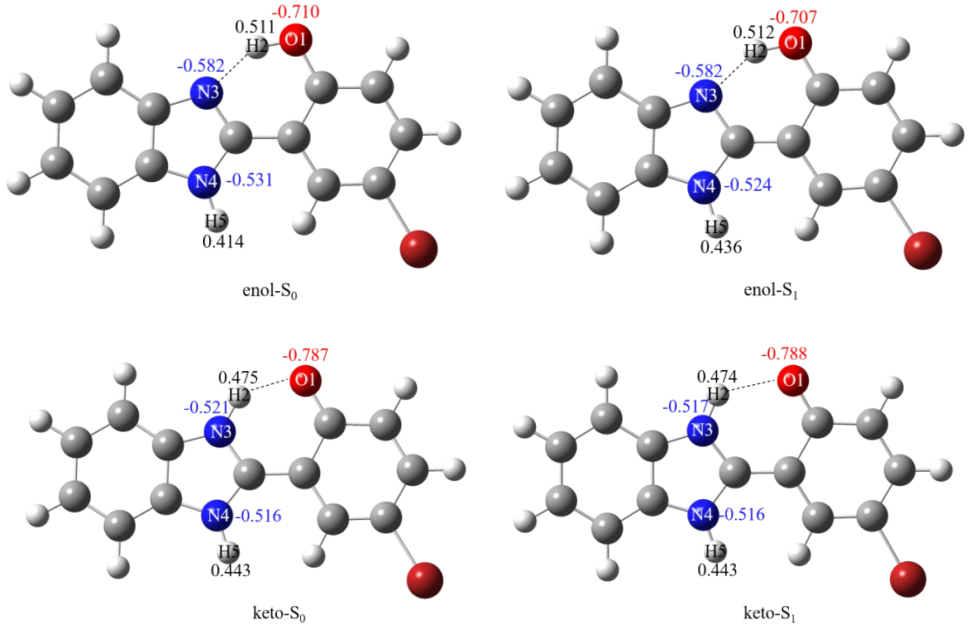


Figure S4. Charge distribution of ground HBI-pBr calculated at B3LYP/6-311+G(d, p) using PCM (solvent=methanol) model.

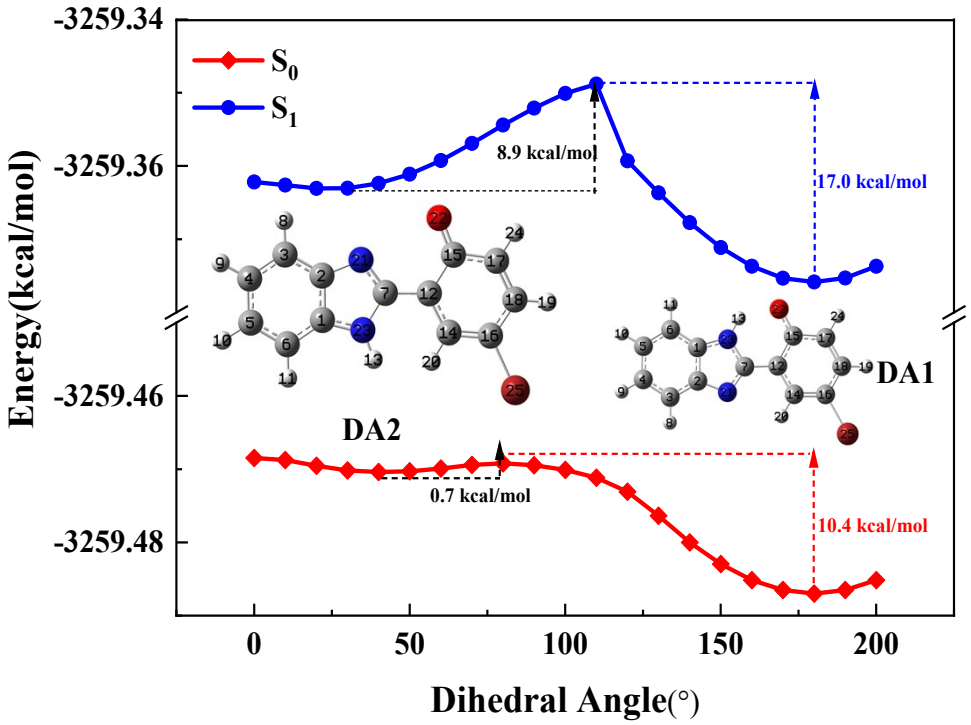


Figure S5. Isomerization potential energy surface curves of DA1 and DA2 calculated at TD-B3LYP/6-311+G(d, p) level using PCM (solvent=methanol) model.
(Note: Dihedral angle: C_{14}-C_{12}-C_7-N_{23}).

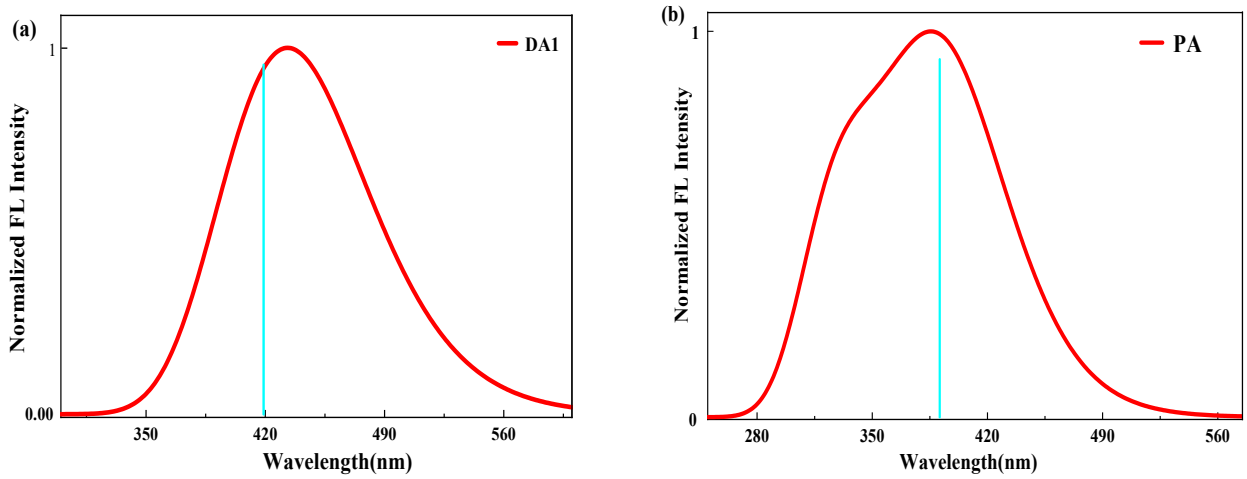


Figure S6. Emission spectra of DA1 (a) and PA (b) calculated at the B3LYP-TD/6-311+G(d, p) level using PCM (solvent=methanol) model. Notes: The vertical line represents the maximum emission bands observed experimentally.

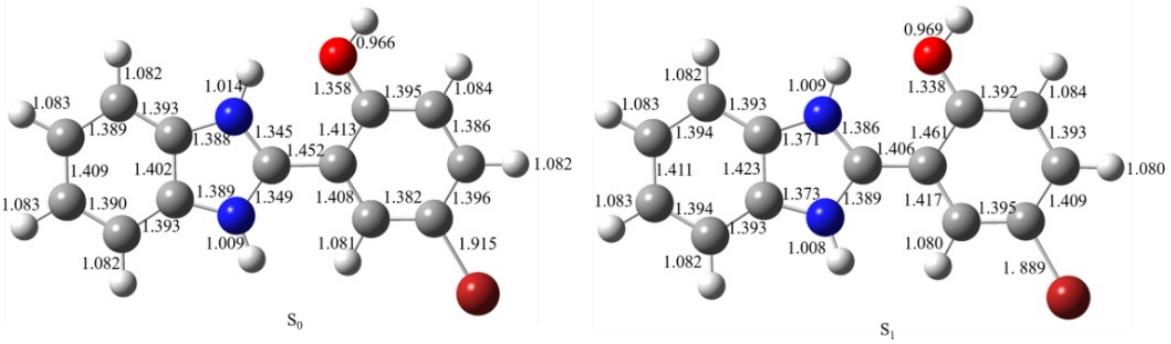


Figure S7. Optimized bond length in Å of PA in S_0 and S_1 at B3LYP and TD-B3LYP with the 6-311+G(d, p) basis using PCM (solvent=methanol) model.

Table S1. Frontier molecular orbitals (FMO) and their charge distribution composition of 2-(2'-hydroxy)phenylbenzimidazole (HBI) and 2-(2'-hydroxy-5'-bromo)phenylbenzimidazole (HBI-pBr) structures in the optimized S_1 state calculated at the B3LYP/6-311+G(d, p) level.

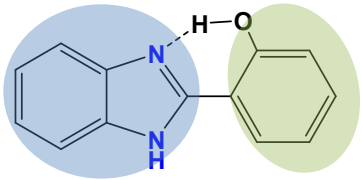
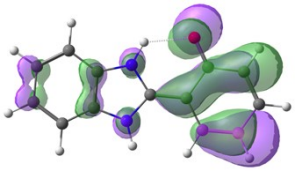
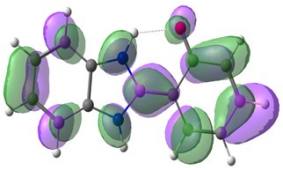
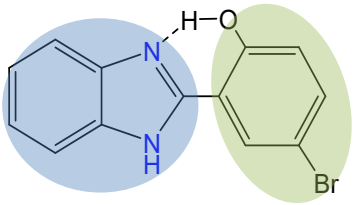
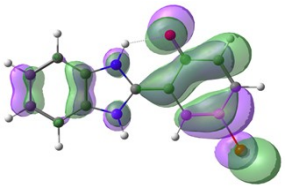
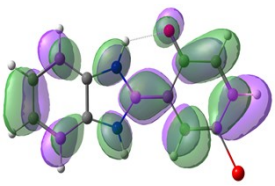
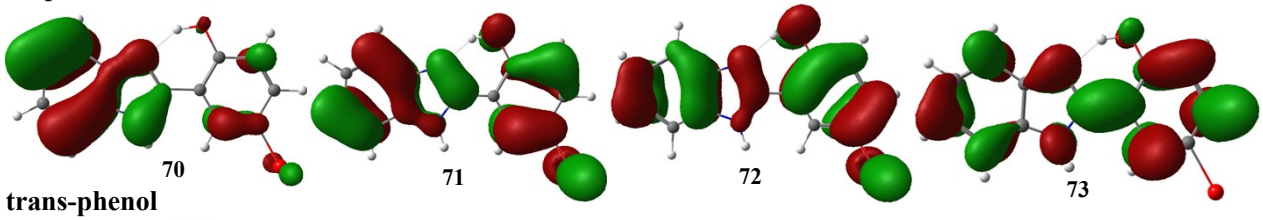
		HOMO	LUMO
HBI			
	Fragment1 (blue)	53.74%	47.25%
	Fragment2 (green)	46.26%	52.75%
HBI-pBr			
	Fragment1 (blue)	42.88%	44.37%
	Fragment2 (green)	57.12%	55.38%

Table S2. Experimental and calculated singlet electronic transition energies (λ_{abs}^{max}/nm), the corresponding orbital character and oscillator strengths of the *cis*-phenol, *trans*-phenol and keto at the B3LYP-TD/6-311+G(d, p) level using PCM (solvent=cyclohexane) model.

Species	States	Orbitals (coefff.)	Electronic Transition	Transition Energies(nm)/ Oscillator strength(f)	
				Cal	Exp
cis-phenol	**S_1**	**π→π***	**72→73(0.69325)**	**333(0.5647)**	**344(0.4528)/ 330 (0.5580)**
	S_2	**π→π***	**70→73(0.51455)** **71→73 (0.5580)**	**287(0.2415)**	**298 (0.0318)**
	S_3	π→π*	72→73(0.69453)	283(0.1252)	288 (0.0630)
trans-phenol	S_1	π→π*	72→73(0.69453)	322 (0.7558)	
	S_2	π→π*	71→73(0.69172)	297(0.0297)	
	S_3	π→π*	70→73(0.61932) 72→73 (0.29059)	286 (0.0994)	
Keto	S_1	π→π*	72→73(0.70423)	406.0(0.4371)	
	S_4	π→π*	72→74(0.69740)	293.7(0.0019)	
	S_5	π→π*	70→73(0.69748)	286.6(0.4370)	

cis-phenol



trans-phenol

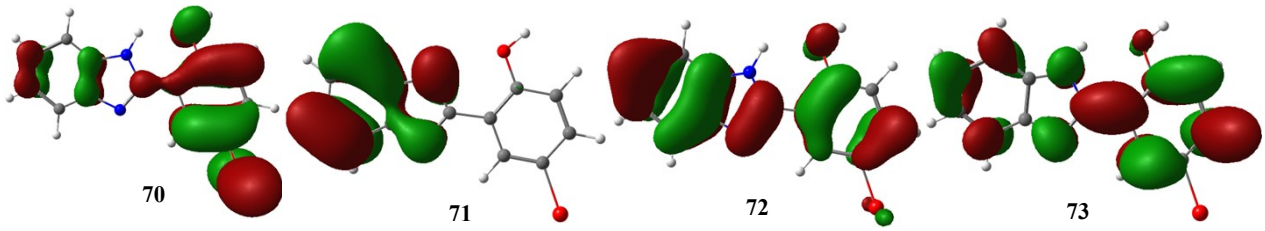


Table S3. Experimental and calculated singlet electronic transition energies (λ_{abs}^{max}/nm), the corresponding orbital character and oscillator strengths of the DA1, DA2, DA3 and DA at the B3LYP-TD/6-311+G(d, p) level using PCM (solvent=methanol) model.

Species	State	Electronic Transition	Orbitals (coefff.)	Transition Energies(nm)/ Oscillator strength(f)	
				Cal	Exp
DA1	**S_1**	**π→π***	**72→73(0.70040)**	**374(0.4398)**	**360(0.4234)**
	S_4	π→π*	71→73(0.46298)	286(0.1426)	298 (0.0008)
			72→75(0.48994)		
	S_5	π→π*	71→73(0.49678)	282(0.1314)	289 (0.1014)
	S_{11}	π→π*	72→79(0.63511)	248(0.3057)	253 (0.1112)
	S_{15}	π→π*	67→73(0.63485)	231(0.0003)	225 (0.0011)
			72→82(0.27972)		
DA2	S_1	π→π*	72→73(0.70218)	393(0.4670)	
	S_4	π→π*	72→75(0.68941)	298(0.0036)	
	S_6	π→π*	70→73(0.63431)	283(0.2591)	
	S_{12}	π→π*	72→79(0.58786)	256(0.2961)	
	S_{14}	π→π*	72→81(0.60400)	252(0.0344)	
DA3	**S_1**	**π→π***	**72→73(0.69280)**	**331(0.6356)**	
	S_2	π→π*	71→73(0.94810)	308(0.0658)	
	S_4	π→π*	70→73(0.52836)	285(0.0749)	
	S_6	π→π*	71→75(0.67129)	258(0.0284)	
DA	**S_1**	**π→π***	**72→73(0.69902)**	**379(0.4995)**	
	S_6	π→π*	72→76(0.63649)	297(0.0533)	
	S_8	π→π*	70→73(0.63117)	291(0.1519)	
	S_{12}	π→π*	72→79(0.60933)	267(0.1012)	

Table S4. Calculated singlet electronic transition orbitals of the DA1 at the B3LYP-TD/6-311+G(d, p) level using PCM (solvent=methanol) model.

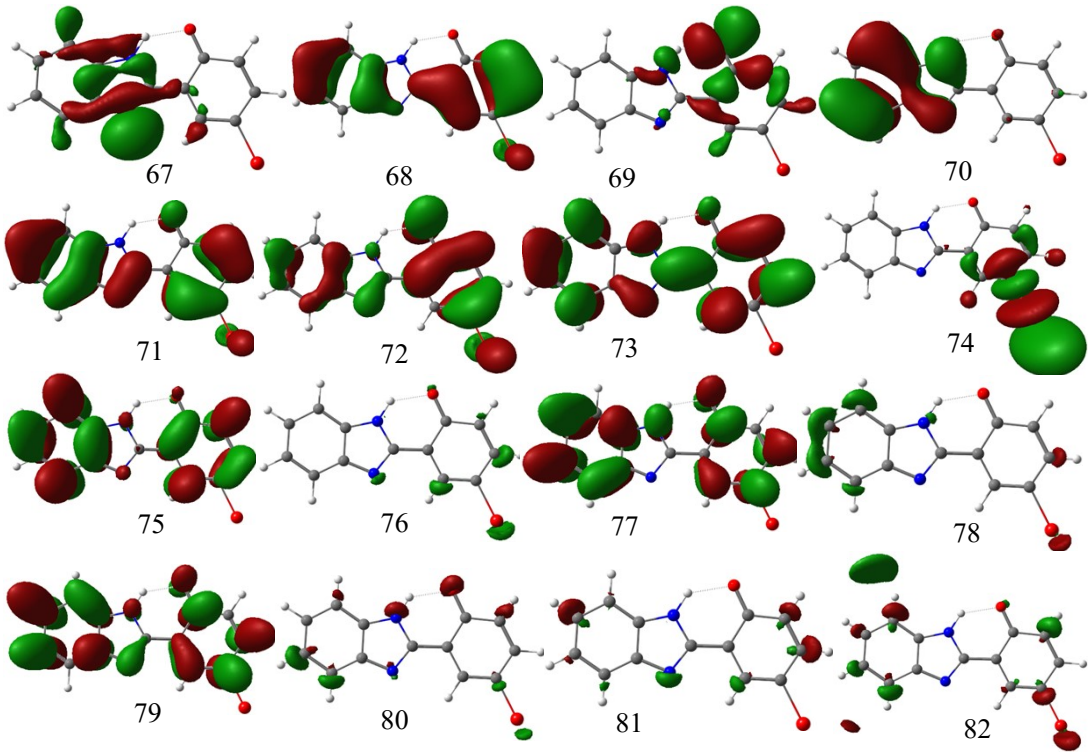


Table S5. Experimental and calculated singlet electronic transition energies (λ_{abs}^{max}/nm), the corresponding orbital character and oscillator strengths of PA at the B3LYP-TD/6-311+G(d, p) level using PCM (solvent=methanol) model.

States	Orbitals(coefff.)	ElectronicTransition	Transition Energies(nm)/Oscillator strength(f)	
			Cal.	Exp.
S_1	π→π*	72→73(0.68823)	339(0.3969)	346/338
S_2	π→π*	71→73(0.66324)	300 (0.4017)	300
S_3	π→π*	70→73(0.67595)	295 (0.1230)	289
		72→75(0.41797)		
S_7	π→π*	72→74(0.25093)	236(0.0194)	240
		70→77(0.25036)		
S_{10}	π→π*	71→74(0.56672)	218(0.2541)	217
		72→77(0.21126)		

Table S6. Calculated singlet electronic transition orbitals of the PA at the B3LYP-TD/6-311+G(d, p) level using PCM (solvent=methanol) model.

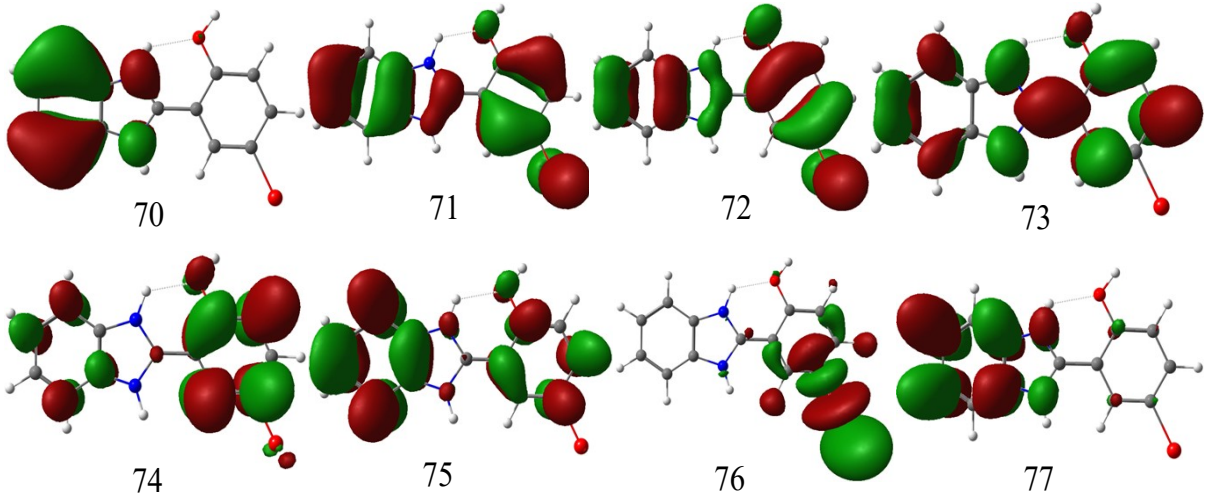
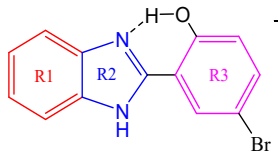


Table S7. NICS(1)_ZZ values (in ppm) of every ring in HBI-pBr structures in the optimized S_0 and S_1 states calculated at the B3LYP/6-311+G(d, p) level.



System	S_0[a]			S_1[a]		
	R1	R2	R3	R1	R2	R3
Phenol	-28.53	-22.87	-20.40	15.64	0.51	21.88
Keto	-28.55	-18.42	-14.26	-19.74	7.07	10.82
Anion	-28.26	-24.88	-16.30	-12.20	-8.89	24.87
Cation	-29.05	-20.39	-20.22	-8.36	-3.45	22.54

[a] Corresponding the benzyl, imizole and phenol rings indicated in left structure.

Table S8. Cartesian coordinates of phenol, keto, DA1, DA2, DA3, DA and PA of HBI-pBr in the optimized S_0 and S_1 states calculated at the B3LYP/6-311+G(d, p) level using PCM (solvent=methanol) model.

HBI-pBr							
Phenol							
	S_0				S_1		
C	-2.923718	-1.013599	-0.000069	C	-2.92307	-1.027107	0.000076
C	-3.251582	0.361916	0.000203	C	-3.24011	0.383007	-0.0001
C	-4.589999	0.765757	0.000247	C	-4.59292	0.791679	-0.0001
C	-5.563972	-0.22582	0.000079	C	-5.56579	-0.196382	0.000139
C	-5.222383	-1.592302	-0.000165	C	-5.23484	-1.572625	0.000358
C	-3.89568	-2.011707	-0.000291	C	-3.90585	-2.009159	0.00032
C	-1.079915	0.236646	0.000132	C	-1.05336	0.216914	-0.000023
H	-4.851317	1.816829	0.000413	H	-4.84758	1.843761	-0.000236
H	-6.61028	0.055182	0.00013	H	-6.61181	0.086528	0.000171
H	-6.011386	-2.334613	-0.000292	H	-6.03249	-2.305509	0.000546
H	-3.633233	-3.062294	-0.000535	H	-3.65603	-3.062424	0.00047
H	-0.980121	-1.893559	0.001343	H	-1.00782	-1.936824	0.001343
C	0.31956	0.636148	0.000038	C	0.29153	0.58594	0.000016
C	0.645972	2.016170	-0.000093	C	0.64705	2.009634	0.000257
C	1.358109	-0.309322	0.000109	C	1.36864	-0.359608	-0.000178
C	1.990002	2.404806	-0.000241	C	1.98173	2.409787	0.000329
C	2.677048	0.10604	-0.000032	C	2.67142	0.097025	-0.000062
H	1.138181	-1.368019	0.000267	H	1.16847	-1.421013	-0.000464
C	3.006143	1.461737	-0.000216	C	3.01257	1.463945	0.000198
H	2.222110	3.462470	-0.000377	H	2.20006	3.470158	0.00051
N	-2.08416	1.107065	0.000367	N	-2.10407	1.108097	-0.000183
N	-1.540064	-1.055441	-0.000466	N	-1.55464	-1.090397	-0.000176
O	-0.292327	2.981608	-0.000106	O	-0.30212	2.939439	0.000445
H	-1.187743	2.540186	0.000184	H	-1.20625	2.47869	0.00034
Br	4.078962	-1.206483	0.000073	Br	4.09231	-1.180687	-0.000325
H	4.040808	1.777689	-0.000339	H	4.04821	1.77297	0.000281

Keto							
	S_0				S_1		
C	-2.93823	-1.00878	0.000472	C	-2.92378	-0.9817	0.000463
C	-3.26748	0.360244	0.000449	C	-3.2961	0.386638	0.000408
C	-4.59191	0.783109	0.000609	C	-4.63767	0.770115	0.000588
C	-5.57396	-0.20500	0.000804	C	-5.59092	-0.25319	0.000842
C	-5.24300	-1.56815	0.000828	C	-5.22113	-1.60496	0.000908
C	-3.91606	-1.99516	0.000655	C	-3.87626	-1.99593	0.000717
C	-1.03036	0.191492	0.000137	C	-1.03565	0.276446	0.000063
H	-4.84479	1.835331	0.000579	H	-4.9226	1.814048	0.000541
H	-6.61683	0.086578	0.000933	H	-6.64246	0.007316	0.000991
H	-6.03501	-2.30658	0.000979	H	-5.99172	-2.36605	0.001108

H	-3.66132	-3.04742	0.000667	H	-3.58782	-3.03914	0.000768
H	-0.99641	-1.91515	0.00034	H	-0.98564	-1.84761	0.000295
C	0.326719	0.609087	-0.000067	C	0.334833	0.653213	-0.00016
C	0.587908	2.039968	-0.000066	C	0.697913	2.088461	-0.00022
C	1.383889	-0.33036	-0.000264	C	1.359569	-0.29795	-0.00036
C	1.975988	2.411692	-0.000169	C	2.082086	2.423608	-0.00012
C	2.683858	0.10226	-0.000428	C	2.711874	0.114488	-0.00044
H	1.176443	-1.39377	-0.000291	H	1.146989	-1.35793	-0.00045
C	2.98495	1.482515	-0.00037	C	3.090144	1.453384	-0.00027
H	2.201193	3.471297	-0.000091	H	2.333654	3.477463	0.000069
N	-2.06694	1.054073	0.000211	N	-2.12998	1.109412	0.00015
N	-1.54586	-1.07147	0.000256	N	-1.54322	-1.00861	0.000225
O	-0.34006	2.910397	0.000308	O	-0.21055	2.975964	0.000272
H	-1.78917	2.062527	0.000098	H	-1.98662	2.115324	0.000055
Br	4.121779	-1.17126	-0.000686	Br	4.049412	-1.23563	-0.00064
H	4.019791	1.802271	-0.000475	H	4.134127	1.734605	-0.00024

DA1

S_0				S_1			
C	3.3036	0.36279	0.000044	C	3.284429	0.360931	0.000048
C	2.844587	-0.974686	0.000316	C	2.871323	-0.99963	0.000148
C	3.759211	-2.032	0.00036	C	3.83619	-2.014265	0.000196
C	5.112593	-1.715449	0.000192	C	5.179224	-1.646718	0.000144
C	5.555177	-0.37826	-0.000052	C	5.570425	-0.294392	0.000041
C	4.658778	0.685934	-0.000178	C	4.627707	0.732285	-0.000019
C	1.076972	0.293134	0.000245	C	1.067814	0.187932	0.000016
H	3.417579	-3.059777	0.000526	H	3.539593	-3.056968	0.000271
H	5.846167	-2.512688	0.000243	H	5.942543	-2.416478	0.000187
H	6.618921	-0.17332	-0.000179	H	6.625579	-0.046813	0.000008
H	4.999196	1.713906	-0.000422	H	4.928006	1.773416	-0.000104
H	2.132471	2.146146	0.001456	H	1.896445	2.084694	0.000183
C	-0.319078	0.704446	0.000151	C	-0.30861	0.653398	0.000034
C	-1.33324	-0.286756	0.00002	C	-1.34324	-0.2959	-0.000036
C	-0.690561	2.058882	0.000222	C	-0.60045	2.071147	0.000182
C	-2.676635	0.104069	-0.000128	C	-2.6632	0.107589	-0.000064
C	-2.02706	2.413703	0.000081	C	-1.99105	2.413947	0.000069
C	-3.030473	1.444487	-0.000103	C	-2.99784	1.467413	-0.000033
N	1.459633	-0.979544	0.00048	N	1.489802	-1.07673	0.000184
N	2.157065	1.138489	-0.000353	N	2.111583	1.08169	-0.000038
H	-4.073623	1.731185	-0.000226	H	-4.03649	1.775719	-0.000073
H	-1.073268	-1.324694	0.000034	H	-1.08102	-1.345743	-0.000085
O	0.304306	3.086081	0.000431	O	0.312565	2.978698	0.000172
H	-2.296219	3.449297	0.000113	H	-2.24301	3.469057	0.000091
Br	-4.020737	-1.252945	-0.000368	Br	-4.0708	-1.216103	-0.000207

DA2

	S_0				S_1		
C	-2.934359	-0.988933	-0.000068	C	-2.862038	-0.948364	0.000419
C	-3.258986	0.38735	0.000204	C	-3.273455	0.405447	0.000065
C	-4.596448	0.794339	0.000248	C	-4.638059	0.714275	-0.000105
C	-5.572752	-0.194943	0.00008	C	-5.550535	-0.338169	0.000113
C	-5.23438	-1.562225	-0.000164	C	-5.122344	-1.678285	0.000479
C	-3.908667	-1.984751	-0.00029	C	-3.7669	-2.007174	0.000623
C	-1.087619	0.25697	0.000133	C	-1.100723	0.449647	0.000189
H	-4.855292	1.846023	0.000414	H	-4.969237	1.746408	-0.000399
H	-6.618395	0.08852	0.000131	H	-6.613028	-0.123733	-0.000012
H	-6.025127	-2.302678	-0.000291	H	-5.860492	-2.471802	0.000635
H	-3.648693	-3.035953	-0.000534	H	-3.437102	-3.039251	0.000883
H	-0.992838	-1.873464	0.001344	H	-0.876972	-1.691578	0.001598
C	0.312792	0.653177	0.000039	C	0.305338	0.835933	0.000143
C	0.64245	2.032427	-0.000092	C	0.728103	2.233184	0.000487
C	1.349113	-0.294734	0.00011	C	1.280178	-0.184986	-0.000256
C	1.987391	2.417899	-0.00024	C	2.158171	2.43956	0.000558
C	2.669026	0.117523	-0.000031	C	2.630237	0.096064	-0.000204
H	1.126694	-1.352911	0.000268	H	0.987202	-1.226489	-0.000717
C	3.00131	1.472442	-0.000215	C	3.084052	1.421492	0.00023
H	2.221988	3.475014	-0.000376	H	2.493795	3.471344	0.000873
N	-2.089813	1.129749	0.000368	N	-2.169433	1.239966	-0.000073
N	-1.550808	-1.034031	-0.000465	N	-1.485536	-0.890687	0.000335
O	-0.293574	3.000071	-0.000105	O	-0.056493	3.229365	0.000756
Br	4.067847	-1.198295	0.000074	Br	3.912435	-1.349066	-0.000785
H	4.036716	1.785958	-0.000338	H	4.145178	1.640798	0.000281

DA3

	S_0				S_1		
C	2.92908	-1.031089	0.00006	C	-2.86942	-1.014668	-0.000015
C	3.258938	0.343949	-0.000212	C	-3.25338	0.364661	0.00009
C	4.59794	0.745848	-0.000256	C	-4.605142	0.735477	0.000179
C	5.570474	-0.24714	-0.000088	C	-5.559939	-0.27671	0.000162
C	5.226903	-1.613125	0.000156	C	-5.185491	-1.638106	0.000055
C	3.899594	-2.030606	0.000282	C	-3.84786	-2.020564	-0.000035
C	1.087092	0.221828	-0.000141	C	-1.104261	0.191266	-0.000015
H	4.860781	1.79654	-0.000422	H	-4.897556	1.780258	0.00026
H	6.617187	0.032344	-0.000139	H	-6.613283	-0.018451	0.000231
H	6.014829	-2.35658	0.000283	H	-5.959304	-2.398102	0.000044
H	3.635623	-3.080811	0.000526	H	-3.566478	-3.068468	-0.000113
C	-0.311802	0.623359	-0.000047	C	0.294653	0.626372	-0.000019
C	-0.636213	2.003853	0.000084	C	0.620462	2.006071	0.000048
C	-1.351721	-0.320604	-0.000118	C	1.335887	-0.312542	-0.00007
C	-1.979678	2.394438	0.000232	C	1.962438	2.401377	0.000071

C	-2.670057	0.09667	0.000023	C	2.655065	0.10811	-0.000046
H	-1.133329	-1.379619	-0.000276	H	1.081549	-1.363278	-0.000119
C	-2.997185	1.452843	0.000207	C	2.986545	1.461235	0.000027
H	-2.210252	3.452437	0.000368	H	2.192652	3.460146	0.000123
N	2.092598	1.09079	-0.000376	N	-2.10484	1.117383	0.000088
N	1.545367	-1.070925	0.000457	N	-1.495793	-1.097964	-0.000076
O	0.303485	2.967929	0.000097	O	-0.334035	2.961752	0.000081
H	1.19826	2.525209	-0.000193	H	-1.227345	2.481034	0.000021
Br	-4.073872	-1.213818	-0.000082	Br	4.064818	-1.207857	-0.000109
H	-4.031391	1.770295	0.00033	H	4.020488	1.780041	0.000046

DA

S_0				S_1			
C	3.317207	0.39009	0.000054	C	3.280453	0.410821	-0.00005
C	2.863109	-0.949063	0.000326	C	2.800694	-0.940048	0.000164
C	3.78161	-2.00301	0.00037	C	3.705528	-2.013784	0.000292
C	5.133821	-1.681491	0.000202	C	5.071075	-1.730543	0.000211
C	5.571491	-0.342685	-0.000042	C	5.542757	-0.400508	0.00001
C	4.671189	0.718209	-0.000168	C	4.657587	0.677502	-0.000121
C	1.09085	0.312256	0.000255	C	1.128102	0.422836	0.000019
H	3.443756	-3.032036	0.000536	H	3.35145	-3.040576	0.000431
H	5.870318	-2.47603	0.000253	H	5.787216	-2.545981	0.000299
H	6.634475	-0.13384	-0.000169	H	6.612318	-0.217443	-0.00004
H	5.007829	1.747425	-0.000412	H	5.02507	1.69968	-0.000261
C	-0.306701	0.718438	0.000161	C	-0.284699	0.85703	-0.000005
C	-1.317216	-0.276482	0.00003	C	-1.24884	-0.168438	-0.000056
C	-0.683157	2.071501	0.000232	C	-0.726286	2.246211	0.000033
C	-2.662037	0.109407	-0.000118	C	-2.606386	0.095802	-0.00005
C	-2.020949	2.421411	0.000091	C	-2.155955	2.436652	0.000078
C	-3.020796	1.448516	-0.000093	C	-3.08004	1.408335	0.000024
N	1.478183	-0.959008	0.00049	N	1.433404	-0.912267	0.000155
N	2.167831	1.161572	-0.000343	N	2.200819	1.258068	-0.000102
H	-4.064992	1.73138	-0.000216	H	-4.143192	1.619456	0.000043
H	-1.053434	-1.313458	0.000044	H	-0.888482	-1.187848	-0.000091
O	0.307932	3.102347	0.000441	O	0.044078	3.265988	0.000102
H	-2.29391	3.456008	0.000124	H	-2.503723	3.465321	0.00015
Br	-4.001146	-1.252536	-0.000358	Br	-3.87248	-1.375781	-0.000143

PA							
		S_0				S_1	
C	-2.9184	-1.038657	-0.000071	C	-2.89979	-1.000997	0.000338
C	-3.24701	0.336682	0.000201	C	-3.2954	0.345357	0.000067
C	-4.58564	0.739804	0.000245	C	-4.63814	0.714126	-0.000079
C	-5.55908	-0.252296	0.000077	C	-5.56455	-0.320999	0.00007
C	-5.21676	-1.618595	-0.000167	C	-5.1666	-1.671739	0.000342
C	-3.88983	-2.037287	-0.000293	C	-3.82679	-2.039435	0.000467
C	-1.07527	0.212578	0.00013	C	-1.05203	0.276497	0.00017
H	-4.84752	1.790735	0.000411	H	-4.94023	1.752903	-0.000301
H	-6.60554	0.028144	0.000128	H	-6.62075	-0.083545	-0.000033
H	-6.00536	-2.361329	-0.000294	H	-5.92514	-2.444123	0.000444
H	-3.62682	-3.087733	-0.000537	H	-3.51652	-3.075753	0.000668
H	-0.97433	-1.917573	0.001341	H	-0.92895	-1.817731	0.001171
C	0.323988	0.612832	0.000036	C	0.340095	0.680398	0.000122
C	0.649659	1.993029	-0.000095	C	0.712577	2.041672	0.000347
C	1.363044	-0.332081	0.000107	C	1.353111	-0.296395	-0.000174
C	1.99348	2.382386	-0.000243	C	2.060569	2.397214	0.00035
C	2.68176	0.08399	-0.000034	C	2.682432	0.077974	-0.000173
H	1.143685	-1.390896	0.000265	H	1.107527	-1.348694	-0.000487
C	3.010127	1.439863	-0.000218	C	3.047692	1.424614	0.0001
H	2.22502	3.440175	-0.000379	H	2.335189	3.445197	0.000547
N	-2.07999	1.082458	0.000365	N	-2.12332	1.090359	-0.000015
N	-1.53473	-1.079756	-0.000468	N	-1.5098	-0.992439	0.0003
O	-0.28916	2.957963	-0.000108	O	-0.27215	2.975578	0.000562
Br	4.084379	-1.22778	0.000071	Br	4.040936	-1.267801	-0.000593
H	4.044622	1.756371	-0.000341	H	4.089888	1.71335	0.0001
H	-2.00757	2.079832	0.000612	H	-2.03261	2.100042	-0.000254
H	0.136411	3.81848	-0.00012	H	0.088757	3.871598	0.000733