

**Supplementary Data**

**TD-DFT study of the excited state intramolecular proton transfer (ESIPT) mechanism in the  
coumarin-benzothiazole derivatives: Substitution and solvent effects**

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Table S1. The selected topological parameters (au) of studied molecules in the gas phase.

	$S_0(E)$			$S_1(K)$		
	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$
<b>C1</b>						
O–H	0.3166	-2.1682	-0.6131	0.0423	0.1309	-0.0022
N $\cdots$ H	0.0642	0.1175	-0.0184	0.3157	-1.8237	-0.5000
d1	0.3585	-0.9709	-0.5395	0.3182	-0.8664	-0.4465
d2	0.2744	-0.7031	-0.2508	0.2746	-0.6875	-0.2602
d3	0.2949	-0.7873	-0.2886	0.2743	-0.6957	-0.2500
d4	0.3173	-0.3348	-0.4779	0.3747	-0.2788	-0.6082
d5	0.4263	-0.1025	-0.7345	0.4248	-0.1211	-0.7309
S–O	0.0197	0.0704	0.0012	0.0176	0.0622	0.0012
R–C	0.2817	-0.9826	-0.2806	0.2816	-0.9821	-0.2810
Ring A	0.0200	0.1271	0.0055	0.0166	0.1045	0.0047
<b>C2</b>						
O–H	0.3163	-2.1633	-0.6122	0.0452	0.1360	-0.0034
N $\cdots$ H	0.0647	0.1175	-0.0187	0.3132	-1.8026	-0.4953
d1	0.3580	-0.9711	-0.5382	0.3174	-0.8680	-0.4434
d2	0.2741	-0.7014	-0.2502	0.2755	-0.6924	-0.2620
d3	0.2965	-0.7955	-0.2917	0.2751	-0.6989	-0.2514
d4	0.3169	-0.3388	-0.4768	0.3732	-0.2883	-0.6064
d5	0.4239	-0.1464	-0.7290	0.4206	-0.1847	-0.7209
S–O	0.0209	0.0748	0.0013	0.0183	0.0650	0.0012
R–C	0.3171	-0.8295	-0.4552	0.3186	-0.8157	-0.4605
Ring A	0.0200	0.1276	0.0055	0.0170	0.1078	0.0049
<b>C3</b>						
O–H	0.3152	-2.1529	-0.6095	0.0431	0.1328	-0.0025
N $\cdots$ H	0.0651	0.1170	-0.0190	0.3152	-1.8200	-0.4992
d1	0.3583	-0.9696	-0.5391	0.3175	-0.8671	-0.4440
d2	0.2739	-0.7010	-0.2497	0.2753	-0.6918	-0.2612
d3	0.2961	-0.7937	-0.2909	0.2745	-0.6958	-0.2503
d4	0.3181	-0.3394	-0.4794	0.3747	-0.2833	-0.6083
d5	0.4265	-0.1192	-0.7352	0.4237	-0.1521	-0.7284
S–O	0.0204	0.0728	0.0013	0.0180	0.0638	0.0012
R–C	0.2989	-0.2690	-0.4382	0.3001	-0.2399	-0.4407
Ring A	0.0201	0.1279	0.0055	0.0167	0.1056	0.0048
<b>C4</b>						
O–H	0.3147	-2.1455	-0.6080	0.0458	0.1374	-0.0037
N $\cdots$ H	0.0660	0.1170	-0.0196	0.3133	-1.8050	-0.4961
d1	0.3578	-0.9698	-0.5379	0.3173	-0.8676	-0.4432
d2	0.2732	-0.6968	-0.2486	0.2752	-0.6911	-0.2610

Table S1. Continued

d3	0.2976	-0.8027	-0.2938	0.2756	-0.7021	-0.2522
d4	0.3181	-0.3349	-0.4795	0.3743	-0.2775	-0.6073
d5	0.4250	-0.1358	-0.7315	0.4216	-0.1753	-0.7231
S-O	0.0218	0.0783	0.0013	0.0193	0.0688	0.0012
R-C	0.2931	-0.2386	-0.4250	0.2960	-0.2026	-0.4309
Ring A	0.0201	0.1287	0.0055	0.0171	0.1088	0.0049
<b>C5</b>						
O-H	0.3169	-2.1706	-0.6138	0.0428	0.1314	-0.0024
N...H	0.0643	0.1178	-0.0184	0.3151	-1.8189	-0.4989
d1	0.3583	-0.9711	-0.5390	0.3179	-0.8674	-0.4452
d2	0.2740	-0.7011	-0.2502	0.2736	-0.6823	-0.2585
d3	0.2956	-0.7913	-0.2900	0.2757	-0.7031	-0.2526
d4	0.3169	-0.3359	-0.4768	0.3737	-0.2857	-0.6059
d5	0.4254	-0.1128	-0.7323	0.4241	-0.1290	-0.7291
S-O	0.0203	0.0727	0.0013	0.0179	0.0633	0.0012
R-C	0.2567	-0.6321	-0.2205	0.2556	-0.6269	-0.2185
Ring A	0.0200	0.1272	0.0055	0.0167	0.1051	0.0048

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Table S1. Continued

	S <sub>0</sub> (E)			S <sub>1</sub> (E)			S <sub>1</sub> (K)		
	$\rho$ (r)	$\nabla^2 \rho(r)$	H (r)	$\rho$ (r)	$\nabla^2 \rho(r)$	H (r)	$\rho$ (r)	$\nabla^2 \rho(r)$	H (r)
<b>C6</b>									
O–H	0.3153	-2.1547	-0.6098	0.3350	-2.3911	-0.6662	0.0408	0.1290	-0.0015
N...H	0.0651	0.1169	-0.0190	0.0515	0.1158	-0.0100	0.3180	-1.8464	-0.5054
d1	0.3587	-0.9699	-0.5400	0.3368	-0.9747	-0.4649	0.3178	-0.8648	-0.4453
d2	0.2736	-0.6988	-0.2491	0.2998	-0.8427	-0.3000	0.2749	-0.6895	-0.2603
d3	0.2958	-0.7929	-0.2902	0.2794	-0.7020	-0.2583	0.2748	-0.6993	-0.2510
d4	0.3193	-0.3310	-0.4821	0.3116	-0.3587	-0.4652	0.3763	-0.2698	-0.6121
d5	0.4274	-0.0927	-0.7374	0.4221	-0.1319	-0.7243	0.4258	-0.1130	-0.7335
S–O	0.0200	0.0722	0.0013	0.0272	0.0990	0.0013	0.0185	0.0659	0.0013
R–C	0.2664	-0.6982	-0.2327	0.2865	-0.8189	-0.2704	0.2656	-0.6950	-0.2320
Ring A	0.0201	0.1280	0.0055	0.0183	0.1134	0.0050	0.0165	0.1031	0.0047
<b>C7</b>									
O–H	0.3145	-2.1472	-0.6080	0.3350	-2.3914	-0.6662	0.0414	0.1311	-0.0017
N...H	0.0655	0.1166	-0.0193	0.0514	0.1158	-0.0100	0.3178	-1.8432	-0.5047
d1	0.3588	-0.9693	-0.5404	0.3369	-0.9747	-0.4654	0.3199	-0.8652	-0.4512
d2	0.2738	-0.7002	-0.2494	0.2996	-0.8418	-0.2996	0.2792	-0.7126	-0.2686
d3	0.2948	-0.7876	-0.2882	0.2802	-0.7067	-0.2600	0.2732	-0.6898	-0.2479
d4	0.3198	-0.3308	-0.4834	0.3123	-0.3539	-0.4667	0.3775	-0.259	-0.6150
d5	0.4276	-0.0920	-0.7379	0.4234	-0.1202	-0.7276	0.4249	-0.1237	-0.7313
S–O	0.0195	0.0702	0.0013	0.0266	0.0965	0.0014	0.0188	0.0669	0.0012
R–C	0.2800	-0.7801	-0.2751	0.3003	-0.8990	-0.3149	0.2837	-0.8027	-0.2834
Ring A	0.0201	0.1282	0.0055	0.0183	0.1136	0.0051	0.0166	0.1048	0.0048
<b>C8</b>									
O–H	0.3135	-2.1343	-0.6052	0.3313	-2.3500	-0.6564	0.0581	0.1520	-0.0101
N...H	0.0667	0.1165	-0.0201	0.0544	0.1171	-0.0118	0.2986	-1.6556	-0.4610
d1	0.3586	-0.9688	-0.5398	0.3374	-0.9748	-0.4673	0.3355	-0.8624	-0.4947
d2	0.2728	-0.6946	-0.2477	0.2985	-0.8348	-0.2947	0.2866	-0.7518	-0.2826
d3	0.2965	-0.7977	-0.2915	0.2812	-0.7113	-0.2116	0.2716	-0.6768	-0.2446
d4	0.3205	-0.3269	-0.4849	0.3167	-0.3233	-0.4765	0.3753	-0.2489	-0.6095
d5	0.4278	-0.0921	-0.7385	0.4263	-0.1001	-0.7349	0.4271	-0.0971	-0.7366
S–O	0.0206	0.0744	0.0013	0.0261	0.0958	0.0014	0.0220	0.0797	0.0014
R–C	0.2507	-0.6474	-0.2688	0.2987	-0.7699	-0.4232	0.2890	-0.7580	-0.3978
Ring A	0.0202	0.1294	0.0056	0.0187	0.1172	0.0052	0.0189	0.1242	0.0055