Electronic Supplementary data

Exploring Charge Transfer Dynamics of Hydrogen Bonding Crystal of 2-Methyl-8-Quinolinol and Chloranilic Acid: Synthesis, Spectrophotometric, Single Crystal, DFT/PCM Analysis, Antimicrobial, and DNA Binding Studies

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Figures

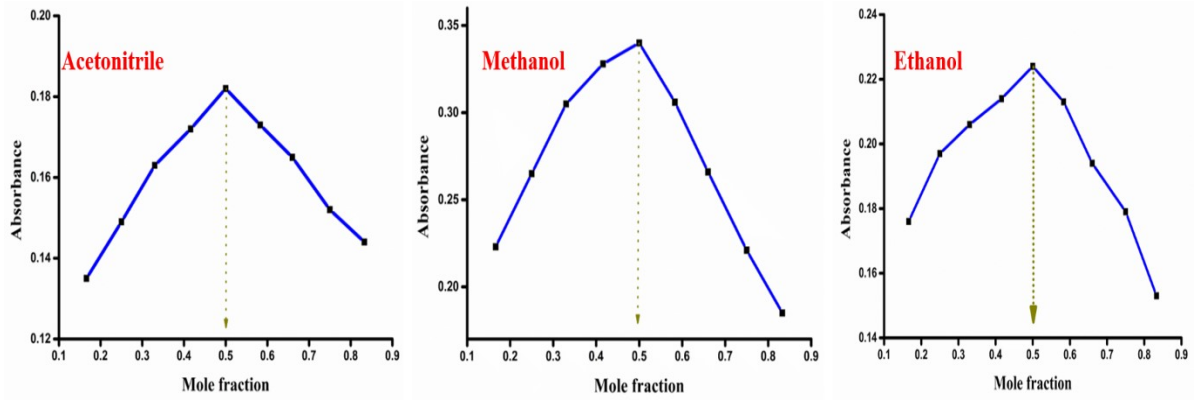

Fig. S1 Job's plot of the HBCT complex in different solvents.

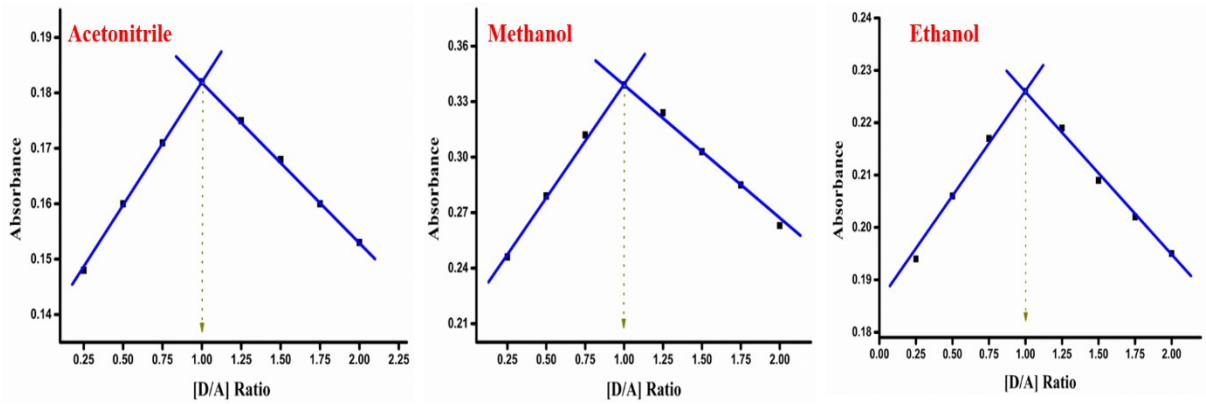

Fig. S2 Photometric titration plots of the HBCT complex in different solvents.

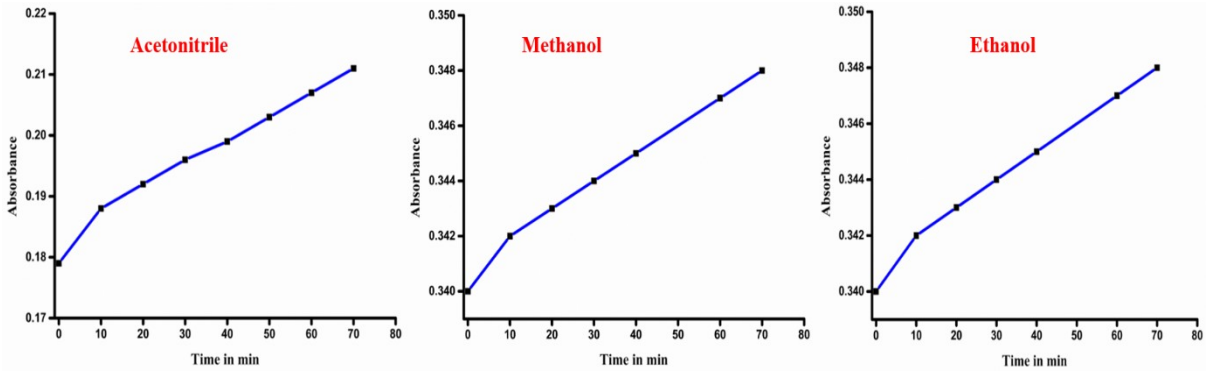

Fig. S3 Effect of time on the stability of HB CT complex in different solvents.

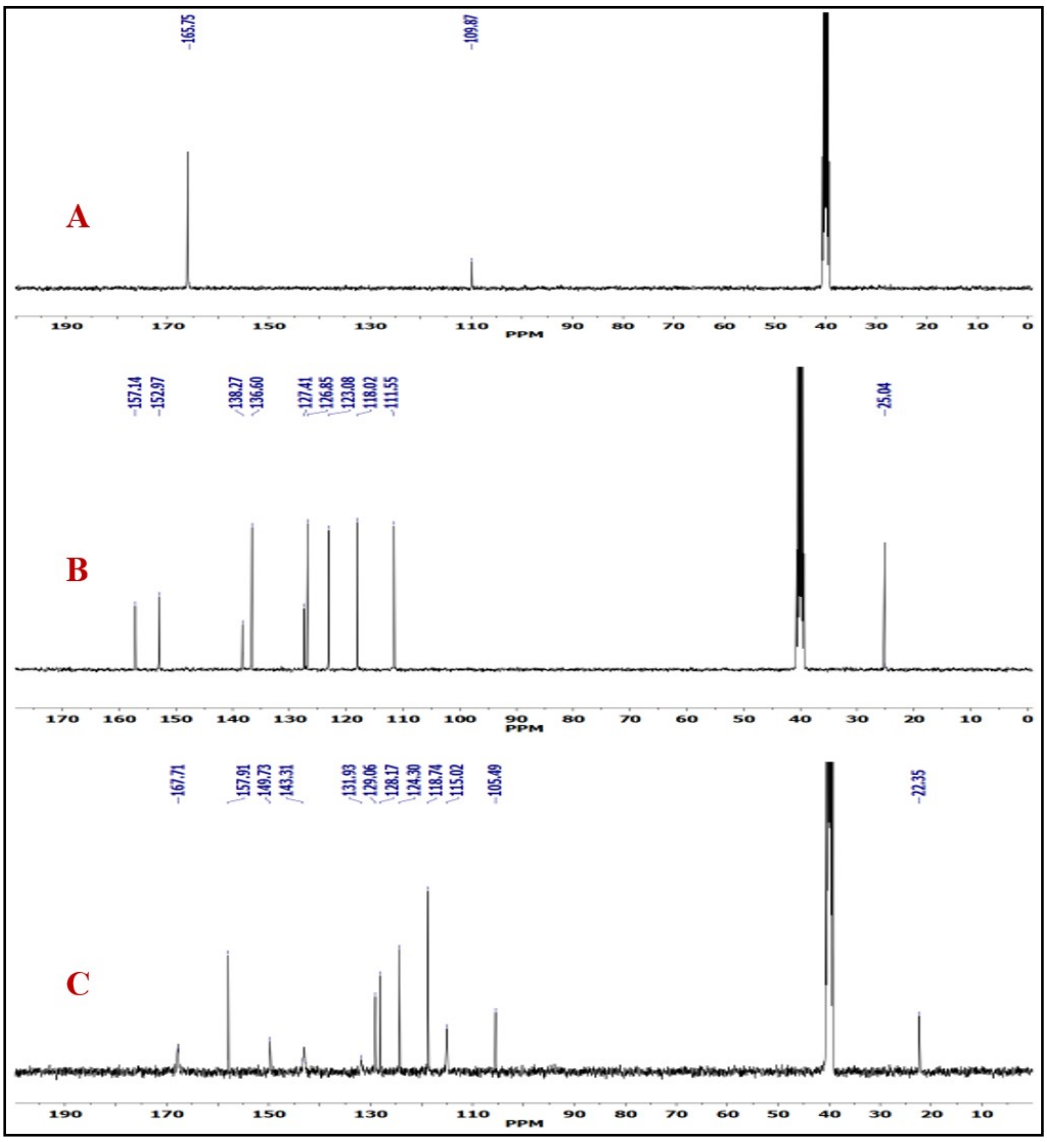

Fig. S4 ^{13}C NMR spectrum of (A) CHLA, (B) 2 MQ, and (C) HBCT complex in DMSO-d_6.

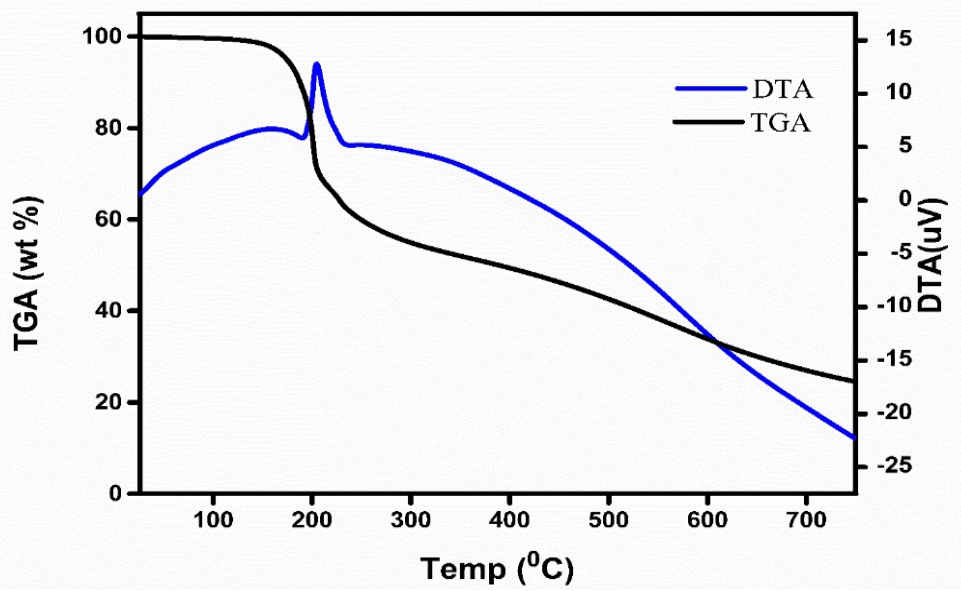

Fig. S5 The TGA-DTA curve of HB CT complex.

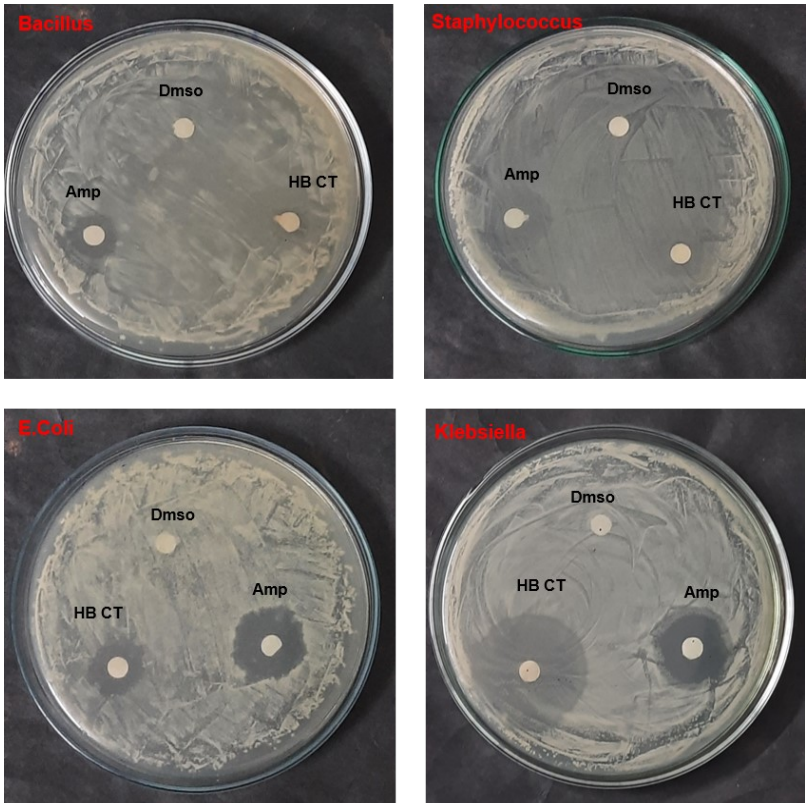

Fig. S6 Antibacterial activity of HB CT complex two-gram positive bacteria (top) and two gram negative bacteria (bottom)

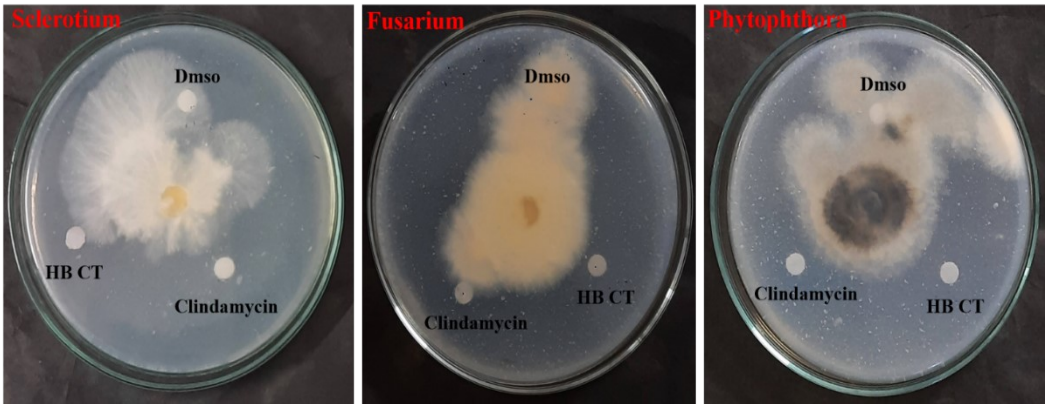

Fig. S7 Antifungal activity of HB CT complex in three different strains.

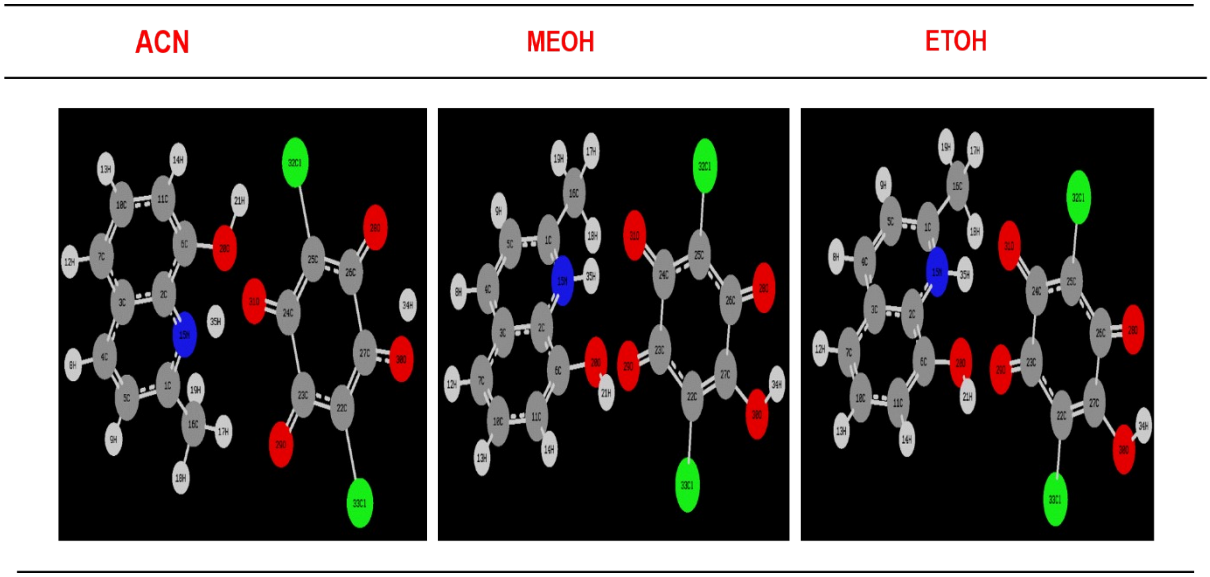

Fig. S8 The optimized structures of HB CT complex in IEF-PCM analysis.

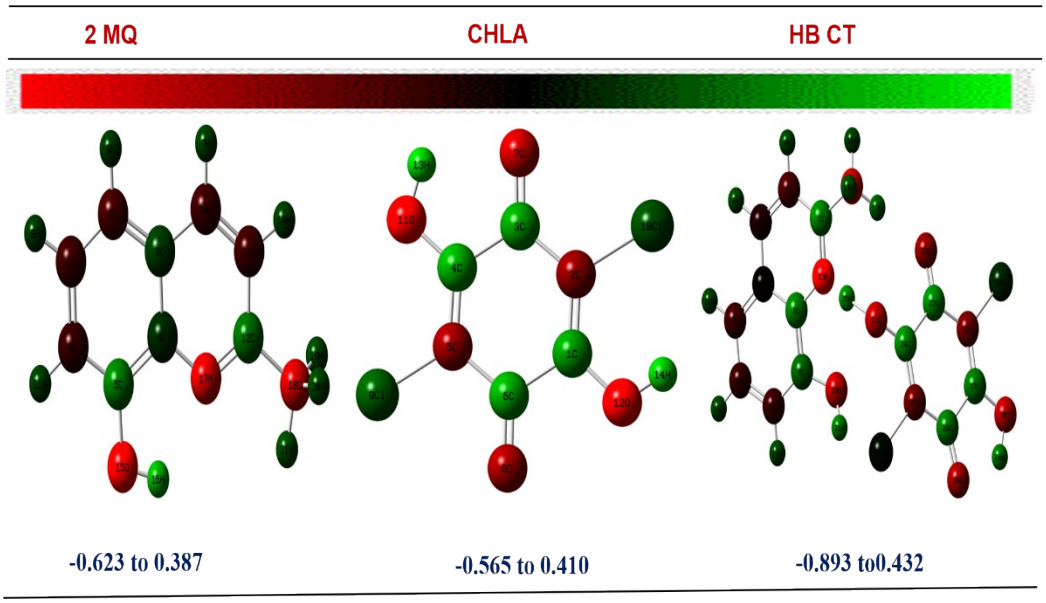

Fig. S9 Mulliken charge color range analysis of 2 MQ, CHLA, HB CT complex in the gas phase.

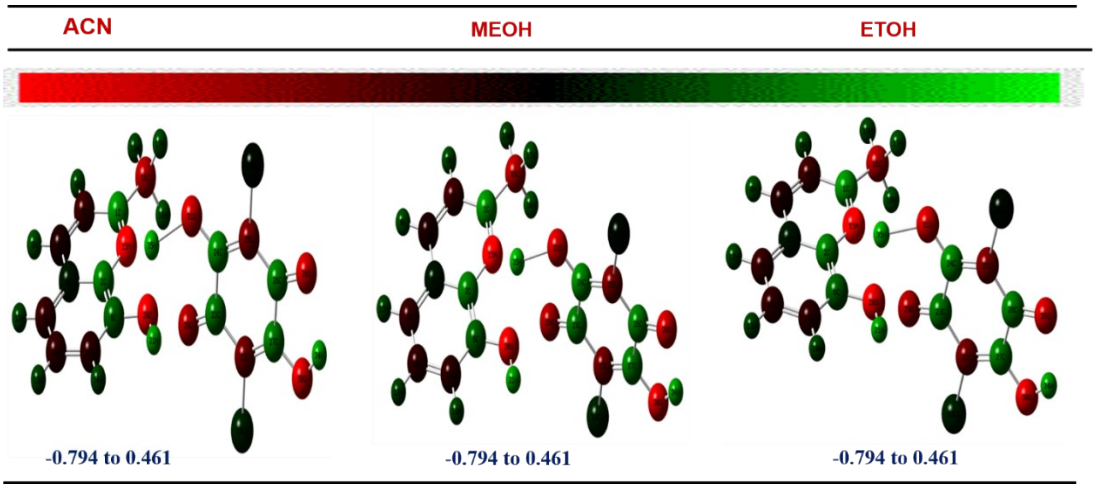

Fig. S10 Mulliken charge color range analysis of HB CT complex in the PCM analysis.

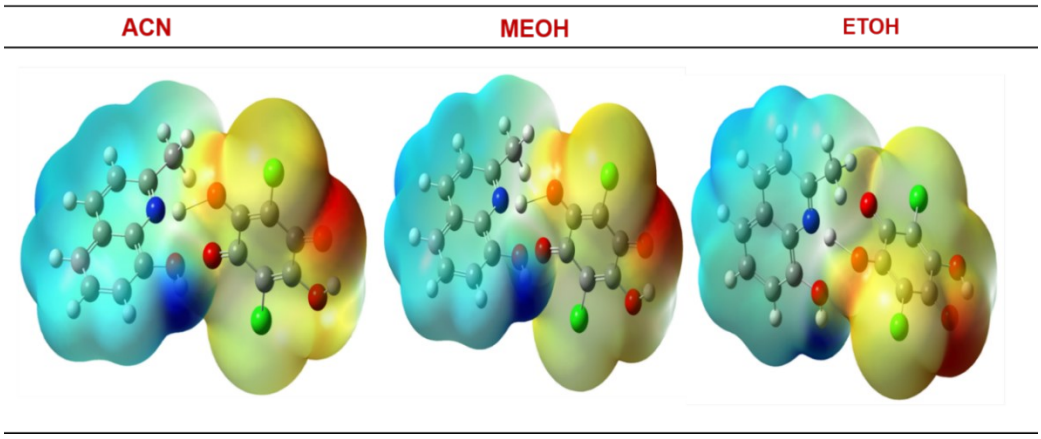

Fig. S11 Electrostatic potential surface maps HB CT complex in the PCM analysis.

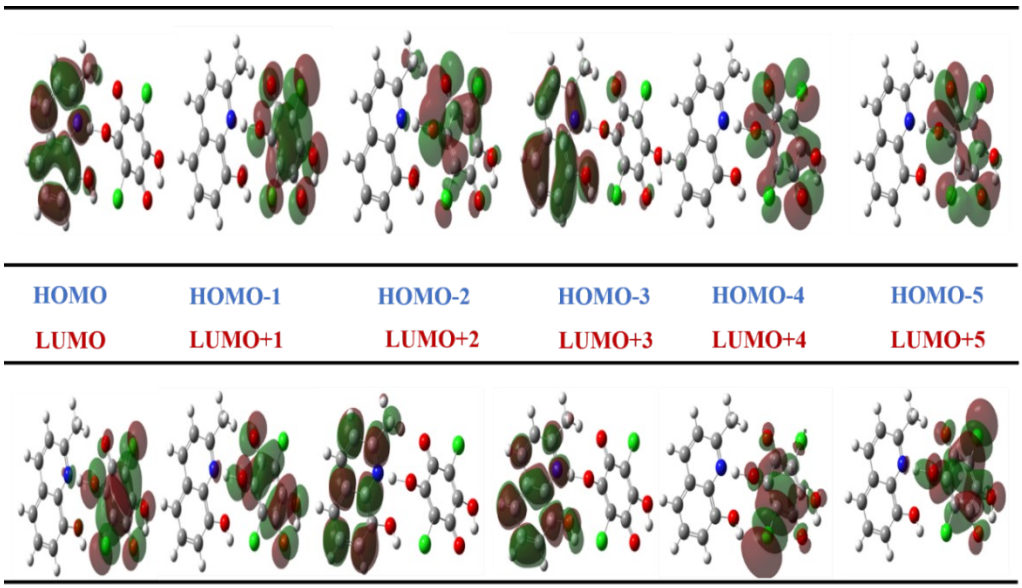

Fig. S12 FMO surfaces HB CT complex in the gas phase.

Tables

Table S1. Characteristic FT-IR frequencies (cm^{-1}) and tentative band assignments.

2MQ	CHLA	HB CT	Assignments
3344 br	-	3411 br	υ(OH)
	3229 s	2970 br	υ(OH)
3052 w	-		$υ_{as}$(CH)
	1663 s	1635 s	υ(C = O)
2955 w	-		$υ_{s}$(CH)
	1628 s	1599 ms	υ(C = C)
2921 w	-	2865 br	$υ_{as}(CH_3)$
1569 s	-	1558 s	υ(CC)
1426 ms	-	1384 ms	δ (CH_3)
1325 s	-		υ(CN)
	1365 s	1358 s	υ(C-O)
	1259 s	1285 s	υ(C-C)
1246	-	1237 s	υ(C-O)
1156 vs	-		δ (CH)
1094 ms	-	1089 s	δ (CH)
1048 w	-	1044 w	$γ(CH_3)$
	979 s	982 s	δ(OH)
	845 s	836 s	υ(C-Cl)
	752 s	745 s	υ(C-Cl)
	690 s	693 s	γ(C-O)

Abbreviations: 2 MQ (2-Methyl-8-quinolinol); CHLA (chloranilic acid), HB CT; s, strong; m, medium; w, weak; υ, stretching; δ, bending

Table. S2 Elemental analysis by EDX spectrum of HB CT complex

Element	Weight (Experimental) %	Atomic (Theoritical) %
C	53.16	52.20
N	3.52	3.80
O	22.75	21.73
Cl	17.52	19.26

Table S3. The bond lengths (A^0) of 2 MQ, CHLA, and HB CT complex in gas phase/PCM analysis

	CHLA				2MQ				HBCT			
Bond length(A^0)	GAS	ACN	MeOH	EtOH	GAS	ACN	MeOH	EtOH	GAS	ACN	MeOH	EtOH
C(1)-O(12)	1.349	1.3463	1.3463	1.3463					1.3397	1.3463	1.3463	1.3463
C(4)-O(11)	1.3526	1.349	1.349	1.3491					1.2723	1.2741	1.2741	1.2742
C(2)-Cl(10)	1.8081	1.8054	1.8054	1.8055					1.812	1.8125	1.8125	1.8124
C(5)-Cl(9)	1.7874	1.7962	1.7961	1.796					1.8377	1.8226	1.8226	1.8223
C(1)-C(6)	1.5158	1,5145	1.5145	1.5146					1.525	1.5159	1.5159	1.5159
C(1)-C(2)	1.3577	1.3581	1.3581	1.3581					1,3435	1.3531	1.3531	1.3531
C(3)-O(7)	1.2527	1.2527	1.2527	1.2527					1.2432	1.2498	1.2498	1.2498
C(6)-O(8)	1.24	1.2436	1.2436	1.2435					1.2639	1.2762	1.2762	1.2762
O(12)-H(14)	0.9825	0.9824	0.9824	0.9824					1.032	1.0	1.0	1.0001
O(11)-H(13)	0.9899	0.98996	0.9896	0.9896					1.4673	1.7236	1.7233	1.721
C(1)-C(2)					1.3851	1.3852	1.3852	1.3852	1.3789	1.3816	1.3816	1.3816
C(2-C(3)					1.4212	1.4224	1.4224	1.4224	1.4178	1.4205	1.4205	1.4205
C(3)-C(4)					1.4249	1.4242	1.4242	1.4243	1.4191	1.4258	1.4258	1.4258
C(4)-C(5)					1.4259	1.4252	1.4252	1.4252	1.4234	1.4194	1.4194	1.4194
C(5)-C(6)					1.3821	1.3816	1.3816	1.3816	1.3816	1.3845	1.3845	1.3845
C(5)-O(15)					1.3748	1.3813	1.3813	1.3812	1.3659	1.379	1.379	1.3789
C(4)-N(17)					1.3723	1.3737	1.3737	1.3737	1.3729	1.3797	1.3797	1.3796
C(12)-N(17)					1.3337	1.3354	1.3354	1.3354	1.3375	1.3466	1.3466	1.3465
C(12)-C(18)					1.506	1.505	1.505	1.505	1.5025	1.4978	1.4978	1.4978
O(15)-H(16)					0.9889	0.9898	0.9898	0.9898	0.998	0.9767	0.9767	0.9766

Table S4. The bond angle of 2 MQ, CHLA, and HB CT complex in gas phase/PCM analysis

	CHLA				2MQ				HBCT			
Bond angle(A^0)	GAS	ACN	MeOH	EtOH	GAS	ACN	MeOH	EtOH	GAS	ACN	MeOH	EtOH
C(1)-C(6)-O(8)	119.5771	119.5721	119.572	119.5725					113.5988	114.2449	114.2413	114.2373
C(1)-O(12)-H(14)	112.4048	113.4774	113.474	113.4616					102.3998	106.4555	106.4515	106.433
C(1)-C(2)-Cl(10)	120.1477	120.5638	120.5624	120.5576					120.0823	120.785	120.7885	120.8022
C(2)-C(3)-O(7)	125.5509	125.479	125.4792	125.48					124.5935	123.8141	123.8111	123.8028
C(4)-C(3)-O(7)	117.1462	117.0879	117.0881	117.0888					118.5088	118.2127	118.2108	118.2094
C(3)-C(4)-O(11)	114.6101	115.1768	115.1738	115.1629					116.5654	116.6796	116.6788	116.6716
C(4)-O(11)-H(13)	108.8329	109.6834	109.6796	109.6661					128.7916	124.2958	124.2973	124.2847
C(5)-C(4)-O(11)	123.653	123.4934	123.4943	123.4977					126.4604	125.6116	125.613	125.618
C(4)-C(5)-Cl(9)	121.1836	120.9378	120.9392	120.9443					117.7828	118.4659	118.4713	118.4868
C(6)-C(5)-Cl(9	117.366	117.3456	117.3456	117.3457					116.4053	117.7346	117.7308	117.7259
C(1)-C(2)-C(3)					119.6425	119.7252	119.7268	119.7252	119.4558	119.7316	119.7312	119.7317
C(1)-C(6)-C(5)					119.5738	119.4965	119.497	119.4987	120.8554	120.5331	120.5325	120.5315
C(6)-C(5)-O(15)					121.695	121.7621	121.7619	121.7612	126.9228	124.7847	124,7878	124.7965
C(4)-C(5)-O(15)					118,1826	117.8904	117.8917	117.8965	114.707	115.6965	115.694	115.6862
C(5)-C(4)-N(17)					116.5447	116.6326	116.6322	116.6308	119.0722	120.6688	120.6665	120.6583
C(3)-C(4)-N(17)					123.4517	123.4947	123.4945	123.4938	119.9102	119.3413	119.3424	119.3488
C(4)-N(17)-C(12)					119.3108	119.1932	119.1937	119.1957	123.4069	123.3866	123.3876	123.3866
C(18)-C(12)-N(17)					118.0729	118.2592	118.2584	118.2554	118.1352	118.4191	118.4227	118.4288
C(13)-C(12)-N(17)					120.9534	120.9606	120.9606	120.9605	118.506	118.6976	118.6965	118.6951
C(13)-C(12)-C(18)					120.9736	120.7802	120.781	120.784	118.1352	122.8774	122.8749	122.8697

Table S5. Mullican charge distribution of 2 MQ, CHLA, and HB CT complex in the gas phase and PCM analysis

	CHLA				2MQ				HBCT			
CHLA	GAS	ACN	MeOH	EtOH	GAS	ACN	MeOH	EtOH	GAS	ACN	MeOH	EtOH
C(1)	0.3128	0.3354	0.3352	0.3348					0.3737	0.3290	0.3289	0.3286
C(2)	-0.2938	-0.2766	-0.2767	-0.2771					-0.3690	-0.2928	-0.2928	-0.2930
C(3)	0.3172	0.3432	0.3430	0.3425					0.4216	0.3102	0.3101	0.3098
C(4)	0.3410	0.3645	0.3643	0.3639					0.4231	0.3672	0.3672	0.3673
C(5)	-0.3213	-0.3062	-0.3063	-0.3066					-0.3406	-0.3243	-0.3243	-0.3244
C(6)	0.3388	0.3599	0.3598	0.3594					0.3813	0.3330	0.3330	0.3328
O(7)	-0.4127	-0.4361	-0.4360	-0.4356					-0.4600	-0.4545	-0.4545	-0.4544
O(8)	-0.3393	-0.4009	-0.4006	-0.3994					-0.5125	-0.5377	-0.5375	-0.5369
Cl(9)	-0.1935	0.1463	0.1465	0.1474					0.0374	0.0269	0.0271	0.0279
Cl(10)	-0.1572	0.1545	0.1545	0.1547					-0.1284	0.0906	0.0907	0.0911
O(11)	-0.1548	-0.1506	-0.1506	-0.1507					-0.5896	-0.5563	-0.5563	-0.5564
O(12)	-0.1386	-0.1332	-0.1332	-0.1332					-0.1997	-0.1724	-0.1724	-0.1724
2 MQ												
C(1)					-0.0069	-0.0027	-0.0027	-0.0028	0.0385	0.0366	0.0366	0.0365
C(2)					-0.0274	-0.0145	-0.0145	-0.0148	0.0038	0.0280	0.0279	0.0275
C(3)					0.1344	0.1205	0.1206	0.1209	-0.0238	0.0631	0.0632	0.0634
C(4)					0.0966	0.0964	0.0964	0.0964	0.3963	0.3410	0.3410	0.3410
C(5)					0.2763	0.2672	0.2672	0.2674	0.3171	0.0299	0.2581	0.2582
C(6)					0.0220	0.0114	0.0114	0.0116	-0.0381	0.0582	0.0581	0.0577
C(10)					0.0064	0.0270	0.0269	0.0265	0.1229	0.1133	0.1131	0.1124
C(12)					0.2391	0.2365	0.2365	0.2365	0.4126	0.3938	0.3938	0.3939
C(13)					-0.0045	0.0154	0.0153	0.0149	-0.0152	0.0299	0.0297	0.0293
O(15)					-0.2364	-0.2595	-0.2594	-0.2591	-0.2166	-0.2146	-0.2145	-0.2142
N(17)					-0.5096	-0.5259	-0.5258	-0.5255	-0.4607	-0.3329	-0.3327	-0.3320
C(18)					0.0099	0.0280	0.0279	0.0276	0.1012	0.1061	0.1061	0.1061

Table S6. HOMO-LUMO (Ha) energies for 2 MQ, CHLA, and HB CT complex in gas phase/PCM analysis

	2MQ				CHLA				HBCT			
FMO	GAS	ACN	MeOH	EtOH	GAS	ACN	MeOH	EtOH	GAS	ACN	MeOH	EtOH
HOMO	-0.21071	-0.21737	-0.21733	-0.21720	-0.27103	-0.26625	-0.26627	-0.26636	-0.20977	-0.22423	-0.22413	-0.22375
HOMO-1	-0.25277	-0.25543	-0.25541	-0.25535	-0.30033	-0.29215	-0.29219	-0.29231	-0.23773	-0.24273	-0.24280	-0.24303
HOMO-2	-0.26654	-0.26998	-0.26996	-0.26987	-0.30505	-0.30472	-0.30471	-0.30470	-0.24029	-0.26504	-0.26496	-0.26466
HOMO-3	-0.29220	-0.29522	-0.29520	-0.29513	-0.32266	-0.31910	-0.31912	-0.31920	-0.26058	-0.26588	-0.26579	-0.26545
HOMO-4	-0.32971	-0.33311	-0.33309	-0.33302	-0.33455	-0.33783	-0.33780	-0.33770	-0.26366	-0.28176	-0.28181	-0.28183
HOMO-5	-0.33749	-0.34513	-0.34509	-0.34496	-0.35766	-0.35119	-0.35125	-0.35143	-0.28164	-0.28253	-0.28245	-0.28231
LUMO	-0.05129	-0.05355	-0.05353	-0.05348	-0.15776	-0.15148	-0.15151	-0.15162	-0.10913	-0.11851	-0.11843	-0.11812
LUMO+1	-0.01813	-0.02070	-0.02069	-0.02062	-0.03533	-0.02424	-0.02428	-0.02444	-0.09261	-0.09449	-0.09455	-0.09475
LUMO+2	0.03003	0.02541	0.02543	0.02553	-0.03346	-0.02350	-0.02355	-0.02372	-0.06264	-0.04303	-0.04311	-0.04339
LUMO+3	0.08272	0.08093	0.08094	0.08099	-0.02358	-0.01724	-0.01727	-0.01738	-0.01991	-0.00175	-0.00182	-0.00206
LUMO+4	0.09626	0.09610	0.09612	0.09620	-0.00937	-0.01048	-0.01048	-0.01044	-0.02301	-0.00069	-0.00059	-0.00021
LUMO+5	0.09965	0.10553	0.10550	0.10539	0.03778	0.06108	0.06098	0.06060	-0.03008	0.00837	0.00845	0.00877

Table S7. Reactivity parameters (eV) energies for 2 MQ, CHLA, and HB CT complex in gas phase/PCM analysis

	2 MQ				CHLA				HB CT			
B3LYP	GAS	ACN	MEOH	ETOH	GAS	ACN	MEOH	ETOH	GAS	ACN	MEOH	ETOH
E_{HOMO}	-5.73	-5.91	-5.91	-5.90	-7.37	-7.24	-7.24	-7.24	-5.70	-6.09	-6.09	-6.09
E_{LUMO}	-1.39	-1,45	-1.45	-1.45	-4.29	-4.12	-4.12	-4.12	-2.96	-3.22	-3.22	-3.22
IP	5.73	5.91	5.91	5.90	7.37	7.24	7.24	7.24	5.70	6.09	6.09	6.09
A	1.39	1.45	1.45	1.45	4.29	4.12	4.12	4.12	2.96	3.22	3.22	3.22
η	2.17	2.23	2.23	2.22	1.54	1.56	1.56	1.56	1.37	1.43	1.43	1.43
μ	3.56	3.68	3.68	3.67	5.83	5.68	5.68	5.68	4.33	4.65	4.65	4.65
ω	13.75	15.09	15.09	14.95	26.17	25.16	25.16	25.16	12.84	15.46	15.46	15.46
σ	0.46	0.44	0.44	0.45	0.64	0.64	0.64	0.64	0.72	0.69	0.69	0.69