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

Palnati Manojkumar¹, Harilal², Varukolu Mahipal¹, Gangadhari Suresh¹, Nampally Venkatesh¹, Macha Ramesh³, Tigulla Parthasarathy¹*

¹Department of Chemistry, Osmania University, Hyderabad-500007.
²School of Chemistry, University of Hyderabad, Gachibowli, Hyderabad-500046.
³University College of Science, Saifabad, Osmania University, Hyderabad-500004.
*Corresponding author

E-mail: sarathym@gmail.com

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.

| ACN | MEOH | ETOH |
|-----|------|------|

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| \(\nu(\text{OH})\) |
| 3229 s   | 2970 br|        | \(\nu(\text{OH})\) |
| 3052 w   | -     | 1635 s | \(\nu(C = O)\) |
| 1663 s   | 1628 s| 1599 ms| \(\nu(C = C)\) |
| 2955 w   | -     | 2865 br| \(\nu_{as}(\text{CH}_3)\) |
| 1569 s   | -     | 1558 s | \(\nu(\text{CC})\) |
| 1426 ms  | -     | 1384 ms| \(\delta(\text{CH}_3)\) |
| 1325 s   | -     | 1358 s | \(\nu(C-O)\) |
| 1365 s   | 1259 s| 1285 s | \(\nu(C-C)\) |
| 1246     | -     | 1237 s | \(\nu(C-O)\) |
| 1156 vs  | -     |        | \(\delta(\text{CH})\) |
| 1094 ms  | -     | 1089 s | \(\delta(\text{CH})\) |
| 1048 w   | -     | 1044 w | \(\gamma(\text{CH}_3)\) |
| 979 s    | 982 s |        | \(\delta(\text{OH})\) |
| 845 s    | 836 s |        | \(\nu(C-\text{Cl})\) |
| 752 s    | 745 s |        | \(\nu(C-\text{Cl})\) |
| 690 s    | 693 s |        | \(\gamma(C-O)\) |

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

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

| Element | Weight (Experimental) % | Atomic (Theoretical) % |
|---------|-------------------------|------------------------|
| 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 (Å) of 2 MQ, CHLA, and HB CT complex in gas phase/PCM analysis

| Bond length(A°) | CHLA  | 2MQ   | HBCT  |
|-----------------|-------|-------|-------|
|                 | 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(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| 0.9896| 0.9896| 0.9896| 1.4673| 1.7236| 1.7233| 1.721 |
| C(1)-C(2)       | 1.385 | 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| 1.3816| 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|
| Bond angle (°) | CHLA   | 2MQ    | HBCT   |
|--------------|--------|--------|--------|
|              | 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)-C(3) | 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(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(4)-C(5)-O(15) | 117.366 | 117.3456 | 117.3456 | 117.3457 | 116.4053 | 117.7346 | 117.7308 | 117.7259 |

Table S4. The bond angle of 2 MQ, CHLA, and HB CT complex in gas phase/PCM analysis
Table S5. Mullican charge distribution of 2 MQ, CHLA, and HB CT complex in the gas phase and PCM analysis

|        | CHLA       | 2MQ        | HBCT       |        |        |        |        |        |        |
|--------|------------|------------|------------|--------|--------|--------|--------|--------|--------|
| 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

|        | CHLA       | 2MQ        |        |        |        |        |        |        |        |
|--------|------------|------------|--------|--------|--------|--------|--------|--------|--------|
| 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

| FMO          | GAS      | ACN      | MeOH     | EtOH     | GAS      | ACN      | MeOH     | EtOH     | GAS      | ACN      | MeOH     | EtOH     |
|--------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| HOMO         | -0.21071 | -0.21733 | -0.21733 | -0.21720 | -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 | -0.26987 | -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 | -0.02355 | -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 | -0.01717 | -0.01812 | -0.0206 |
| LUMO+4       | 0.09626  | 0.09610  | 0.09612  | 0.09620  | -0.00937 | -0.01048 | -0.01044 | -0.02304 | -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    |           |           |           |
| E_{HOMO} | -5.73     | -5.91     | -6.09     |
| E_{LUMO} | -1.39     | -1.45     | -1.45     |
| IP       | 5.73      | 5.90      | 6.09      |
| A        | 1.39      | 1.45      | 1.45      |
| η        | 2.17      | 2.23      | 2.23      |
| μ        | 3.56      | 3.68      | 3.68      |
| ω        | 13.75     | 15.09     | 15.09     |
| σ        | 0.46      | 0.44      | 0.44      |