Electronic Supplementary Material (ESI) for CrystEngComm.
This journal is © The Royal Society of Chemistry 2019

# Water-assisted Ground State Intra-molecular Proton Transfer in *2,5*-dihydroxy-Substituted Azobenzenes: Experimental and Computational Studies

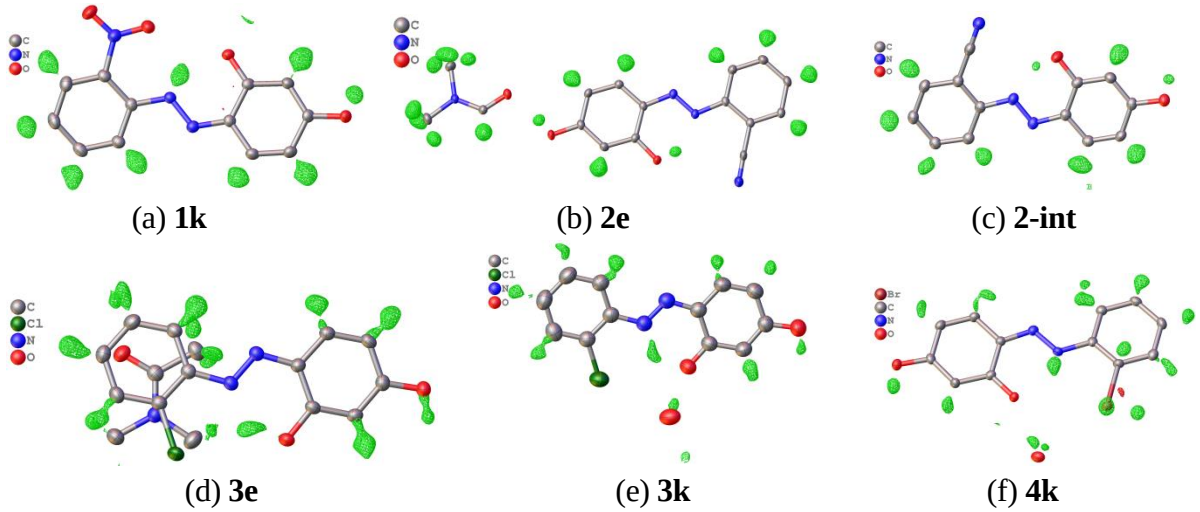
Dhiraj Das and Angshuman Roy Choudhury*

**Contents** **Page No.**

**Instrumentation**

All the recrystallized products were used for spectroscopic characterizations [$^{1}$H and $^{13}$C NMR (400 MHz, Bruker ultrashield plus Avance-III NMR spectrometer), FT-IR (PerkinElmer Spectrum 2), UV-Visible Spectrophotometer (LabIndia UV 3200)]. The melting points and melting enthalpies were determined based on DSC (PerkinElmer DSC 8000) traces recorded at a heating rate of 5 °C min$^{-1}$ under nitrogen atmosphere. The powder X-ray diffraction (PXRD) data were recorded on a Rigaku Ultima IV diffractometer with a parallel beam geometry, Cu $K_{\alpha}$ radiation, 2.5° primary and secondary solar slits, a 0.5° divergence slit with a 10 mm height limit slit, sample rotation stage (120 rpm) attachment and DTex Ultra detector at a tube voltage of 40 kV and current of 40 mA. The data sets were collected over 2θ values ranging from 5° to 50° with a scanning speed of 3° min$^{-1}$ and a 0.02° per step for all compounds. The simulated PXRD spectra were generated using Mercury 3.10.2 from solved single crystal X-ray data and compared with the observed PXRD patterns using WINPLOTR.

Single-crystal X-ray diffraction data of **1k**, **2e**, **3k**, and **4k** (except **2-int and 3e**) were recorded using a Rigaku XtaLAB mini diffractometer with Mercury375/M CCD detector, Mo-$K_{\alpha}$ radiation, a sample-to-detector distance of 4.95 cm, and $2\theta$ fixed at 29.85° using the CrysAlisPro software. The 100 K data were collected using Oxford Cryosystem. The data for **2-int** was collected on a Bruker D8 Venture and **3e** was on Bruker Kappa Apex II CCD diffractometer. All the crystal structures were solved using ShelXT and were refined using ShelXL available within Olex2. The crystal data and refinement parameters for all these compounds are listed in Table 1. All hydrogen atoms were geometrically fixed and refined using the riding model. The thermal ellipsoid plots and packing diagrams of all the molecules are drawn at 50% probability for non-H atoms using Olex 2 and Mercury 3.10.3. All the packing and interaction diagrams were generated using Mercury 3.10.3.



(a) **1k** (b) **2e** (c) **2-int**

(d) **3e** (e) **3k** (f) **4k**

**Figure S1**. Difference Fourier Map of the crystal structure excluding hydrogen atoms.

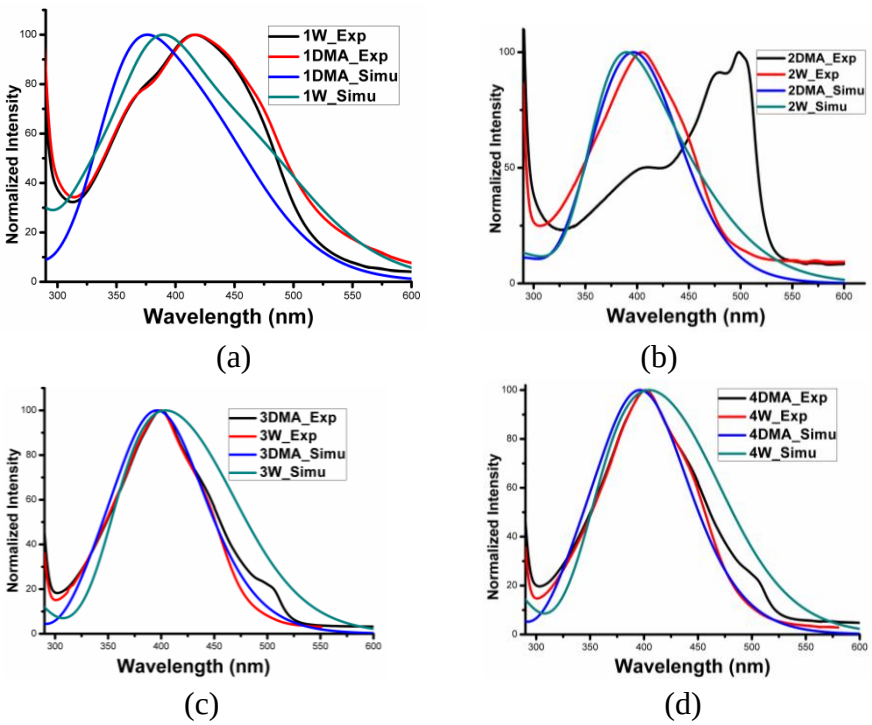



**Figure S2**. UV-Vis spectra and their theoretical fitting of (a) **1**, (b) **2**, (c) **3**, and (d) **4**.

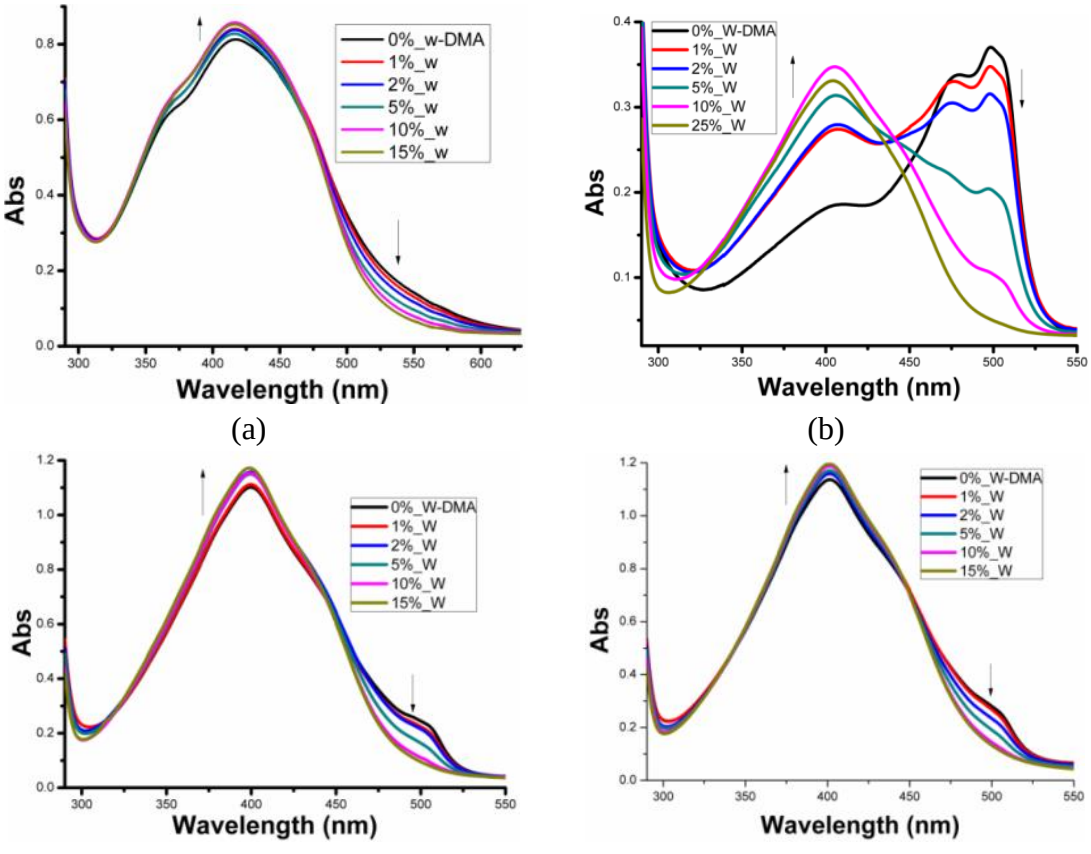
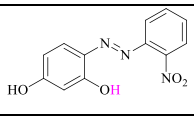
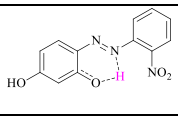
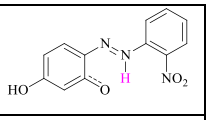
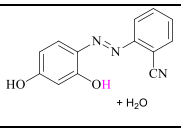
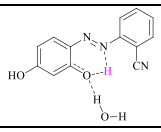
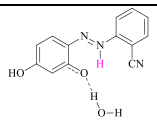
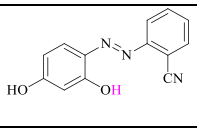
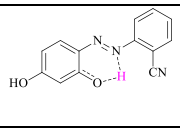
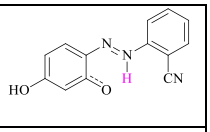



**Figure S3.** UV-Vis study of the compounds (a) **1**, (b) **2**, (c) **3**, and (d) **4** {0% w-DMA = 0 % water in 3 mL of Dimethyl acetamide, x%_w = x (= 1, 2, 5, 10, 15, 25) % water in 3 mL of Dimethyl acetamide}.

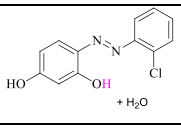
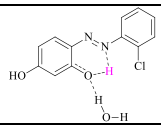
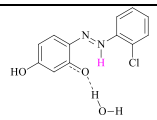
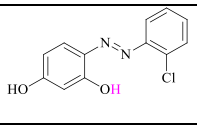
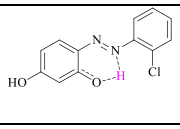
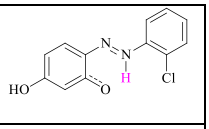
**Table S1a-d**. DFT calculated thermodynamics parameters at 298 K.

| **1** |  |  |  |
|---|---|---|---|
| | Reactant | TS | Product |
| $\Delta G_{298}$ (kcal/mol) | 0.0 | 1.20 | -1.31 |
| $\Delta H_{298}$ (kcal/mol) | 0.0 | 0.58 | -1.35 |
| $\Delta E_{298}$ (kcal/mol) | 0.0 | 0.58 | -1.35 |

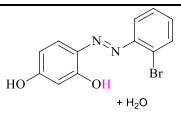
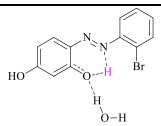
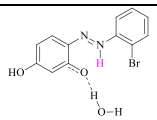
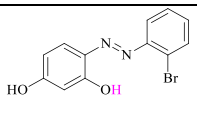
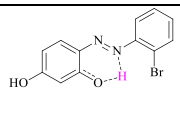
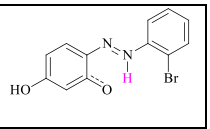
(a)

| **2** |  |  |  |  |  |  |
|---|---|---|---|---|---|---|
| | Reactants | TS | Product | Reactant | TS | Product |
| $\Delta G_{298}$ (kcal/mol) | 0.0 | 20.27 | 5.56 | 0.0 | 13.65 | 1.76 |
| $\Delta H_{298}$ (kcal/mol) | 0.0 | 11.09 | -2.06 | 0.0 | 13.25 | 1.84 |
| $\Delta E_{298}$ (kcal/mol) | 0.0 | 11.68 | -1.47 | 0.0 | 13.25 | 1.83 |

(b)

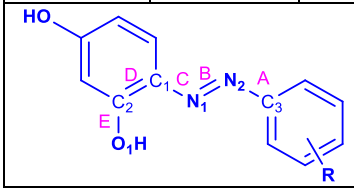
| **3** |  |  |  |  |  |  |
|---|---|---|---|---|---|---|
| | Reactants | TS | Product | Reactant | TS | Product |
| $\Delta G_{298}$ (kcal/mol) | 0.0 | 16.94 | 5.08 | 0.0 | 9.01 | 0.88 |
| $\Delta H_{298}$ (kcal/mol) | 0.0 | 7.83 | -2.85 | 0.0 | 8.23 | 0.68 |
| $\Delta E_{298}$ (kcal/mol) | 0.0 | 8.42 | -2.26 | 0.0 | 8.23 | 0.68 |

(c)

| **4** |  |  |  |  |  |  |
|---|---|---|---|---|---|---|
| | Reactants | TS | Product | Reactant | TS | Product |
| $\Delta G_{298}$ (kcal/mol) | 0.0 | 5.81 | 4.83 | 0.0 | 1.43 | 0.78 |
| $\Delta H_{298}$ (kcal/mol) | 0.0 | -2.03 | -2.91 | 0.0 | 0.92 | 0.88 |
| $\Delta E_{298}$ (kcal/mol) | 0.0 | -1.44 | -2.32 | 0.0 | 0.92 | 0.88 |

(d)

**Table S2**. Normal important bond distances in Azobenzenes reported in literature.

| Ref Code | CCDC no. | Bond distances (Å) |
|---|---|---|
| BIHLOU | 236353 | C7N1 (A) = 1.424(2)<br>N1N3 (B) = 1.274(2)<br>N3C13 (C) = 1.403(2)<br>C13C23 (D) = 1.421(2)<br>C23O12 (E) = 1.345(2) |
| BIHLUA | 236354 | C4N1 (A) = 1.420(3)<br>N1N2 (B) = 1.276(3)<br>N2C7 (C) = 1.397(3)<br>C7C12 (D) = 1.421(3)<br>C12O5 (E) = 1.343(3) |
| FONZEP | 993686 | C8N4 (A) = 1.279(11)<br>N4N1 (B) = 1.264(7)<br>N1C5 (C) = 1.292(10)<br>C5C4 (D) = 1.37(2)<br>C4O1 (E) = 1.38(2) |
| OQEREI | 814670 | C31N3 (A) = 1.400(4)<br>N3N4 (B) = 1.279(4)<br>N4C47 (C) = 1.359(4)<br>C47C48 (D) = 1.446(5)<br>C48O7 (E) = 1.306(4) |
| WALHAV | 1440778 | C3N4 (A) = 1.407(4)<br>N4N1 (B) = 1.289(4)<br>N1C7 (C) = 1.343(4)<br>C7C11 (D) = 1.442(4)<br>C11O1 (E) = 1.313(4) |
| YAZLEQ | 161659 | C4N1 (A) = 1.414(5)<br>N1N2 (B) = 1.281(4)<br>N2C7 (C) = 1.392(5)<br>C7C12 (D) = 1.413(5)<br>C12O5 (E) = 1.343(4) |
|  | | |

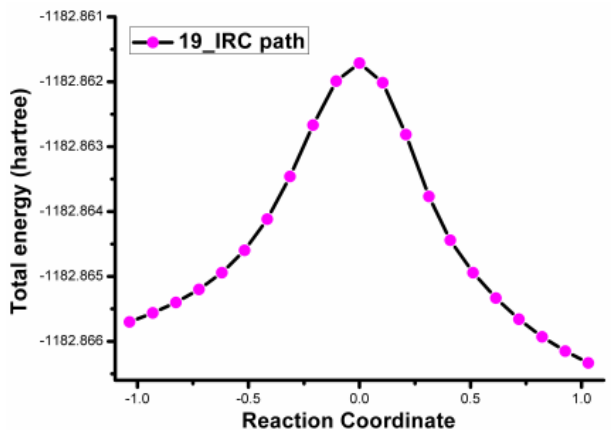



**Figure S4**. IRC calculation for **3.**

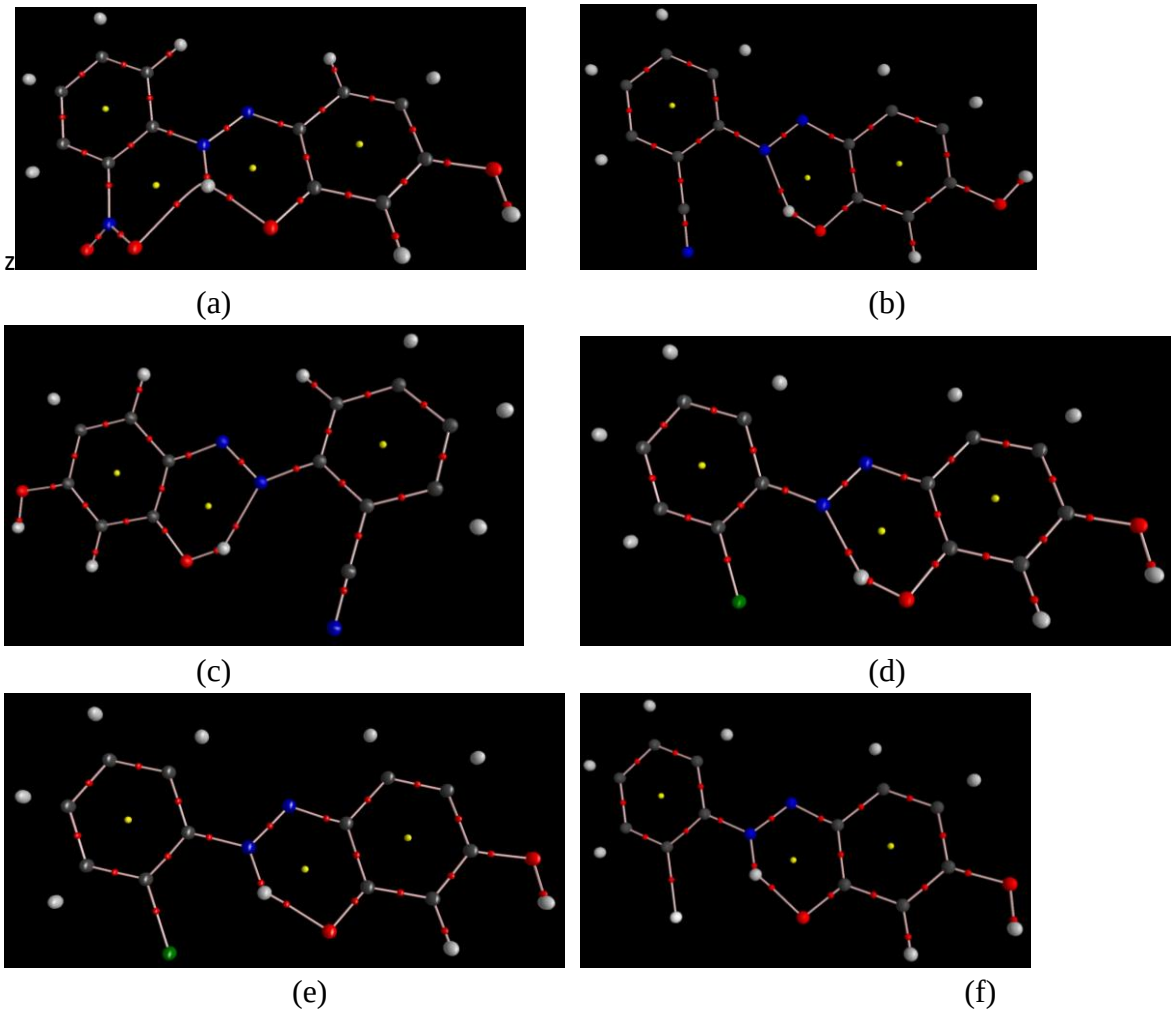
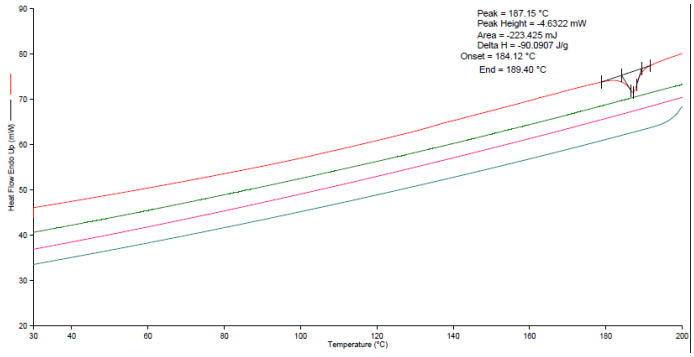
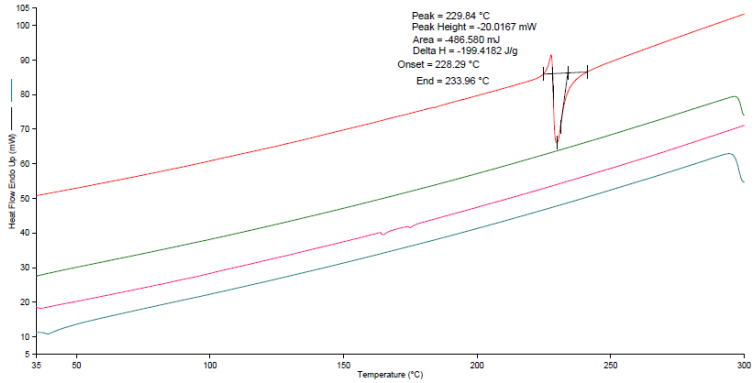


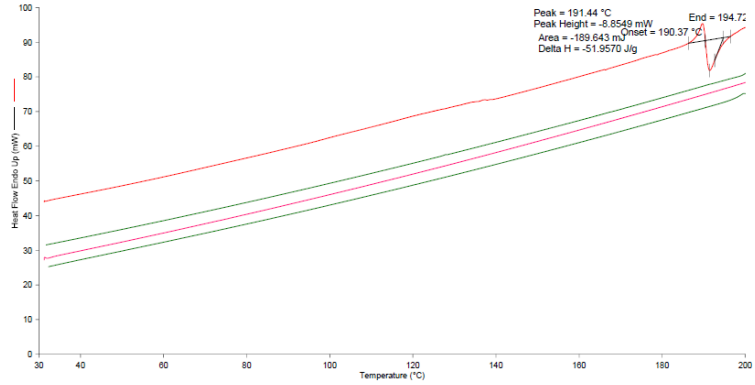

**Figure S5**. AIM analysis and bond path showing BCPs (red dots) and RCPs (yellow dots) (a) for **1k**, (b) for **2e**, (c) for **2-int**, (d) for **3e**, (e) for **3k** and (f) for **4k**.



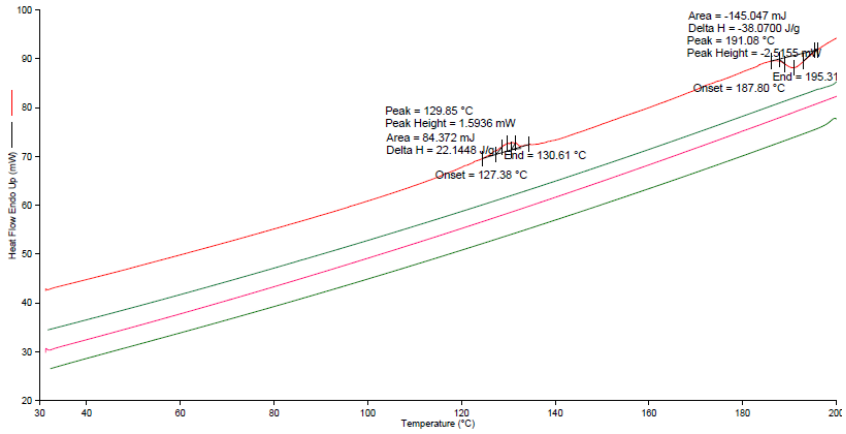

(a)




(b)




(c)

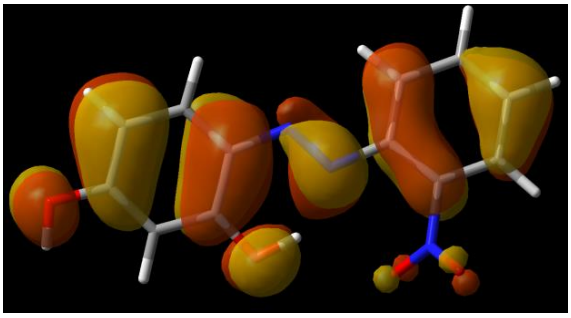



(d)

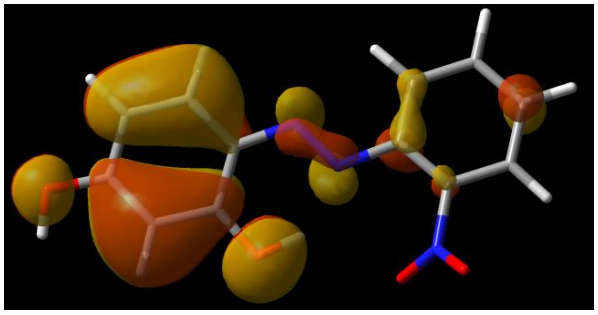
**Figure S6**. DSC curve of **1** (a), **2** (b), **3** (c), and **4** (d).

**Table S3**. Melting point of the compounds obtained from DSC measurement.

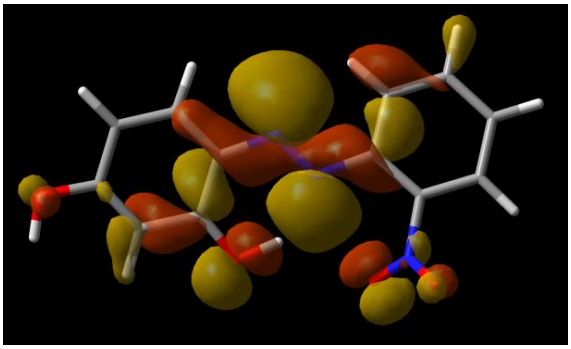
| Sample | Melting range (°*C*) | Enthalpy of melting ($J\ g^{-1}$) |
|---|---|---|
| **1** | 184-189 | -90.09 |
| **2** | 228-234 | -199.41 |
| **3** | 190-195 | -51.95 |
| **4** | 188-195 | -38.07 |



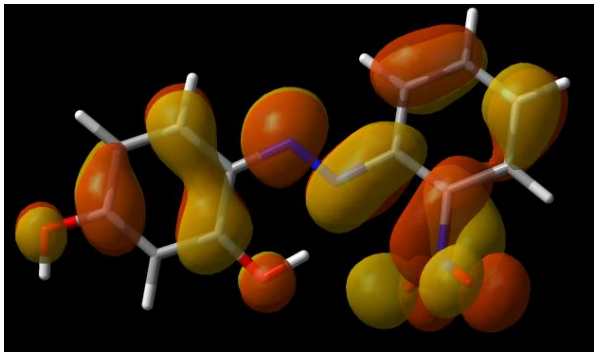
HOMO



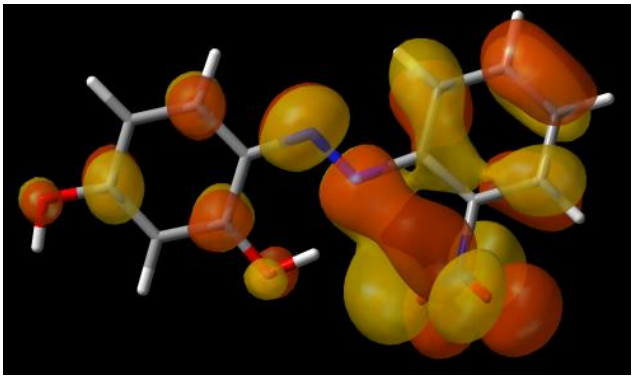
HOMO-1



HOMO-2

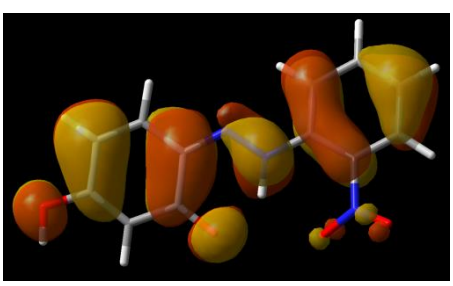


LUMO

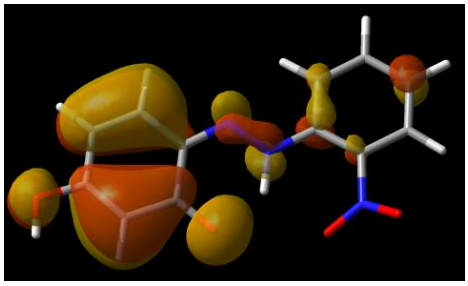


LUMO+1

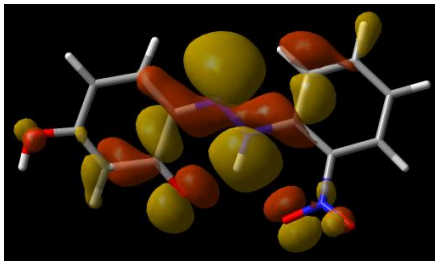
**Figure S7**. HOMO and LUMO for **1** in DMA.



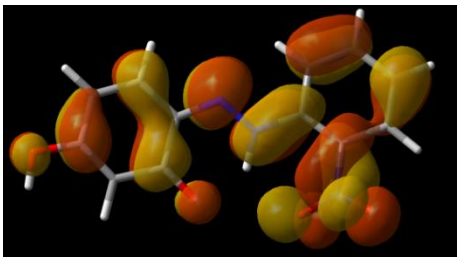
HOMO



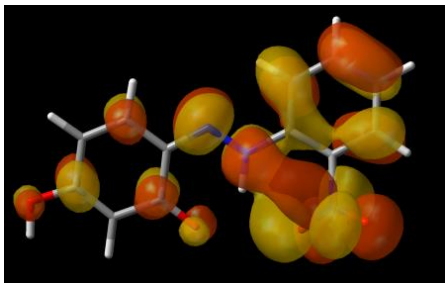
HOMO-1



HOMO-2

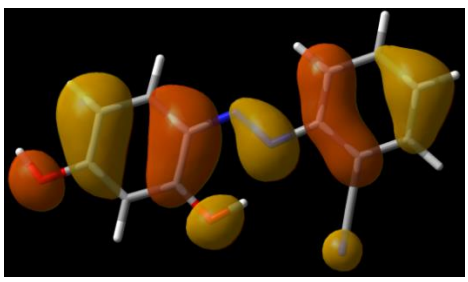


LUMO

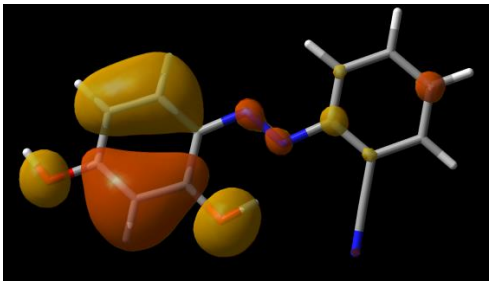


LUMO+1

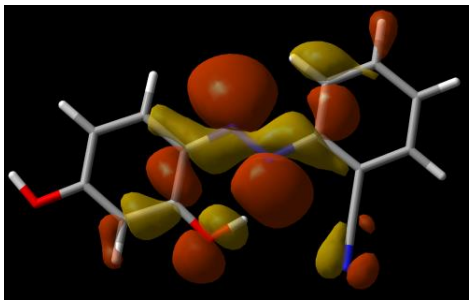
**Figure S8**. HOMO and LUMO for **1** in water.



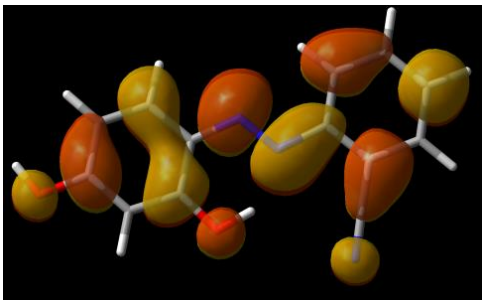
HOMO



HOMO-1

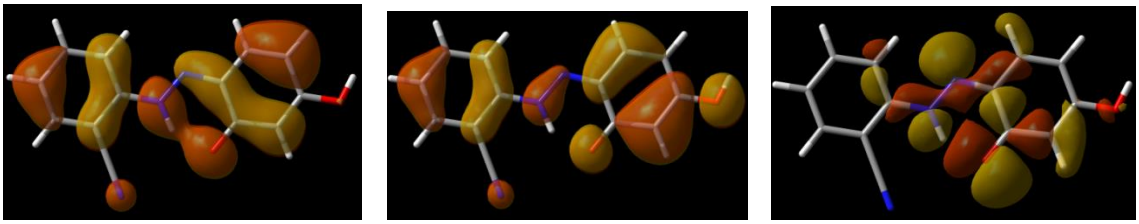


HOMO-2

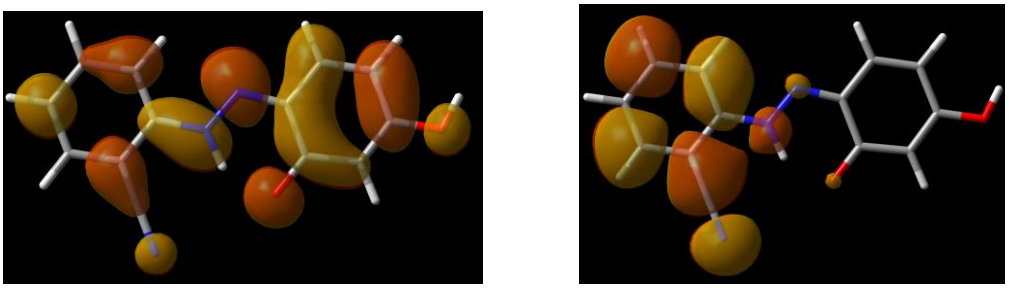


LUMO

**Figure S9**. HOMO and LUMO for **2** in DMA.

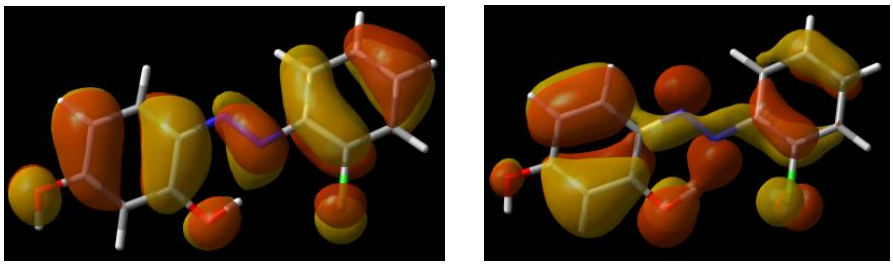


HOMO HOMO-1 HOMO-2

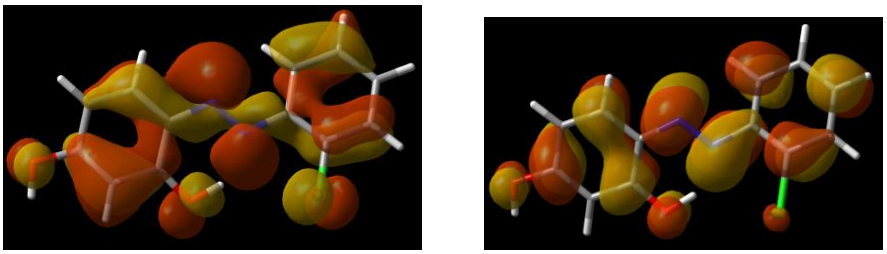


LUMO LUMO+1

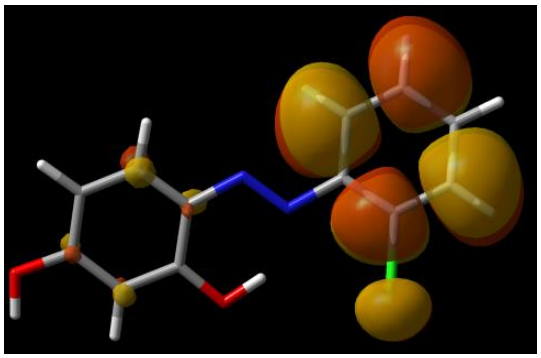
**Figure S10**. HOMO and LUMO for **2** in water.



HOMO HOMO-1



HOMO-2 LUMO



LUMO+1

**Figure S11**. HOMO and LUMO for **3** in DMA.

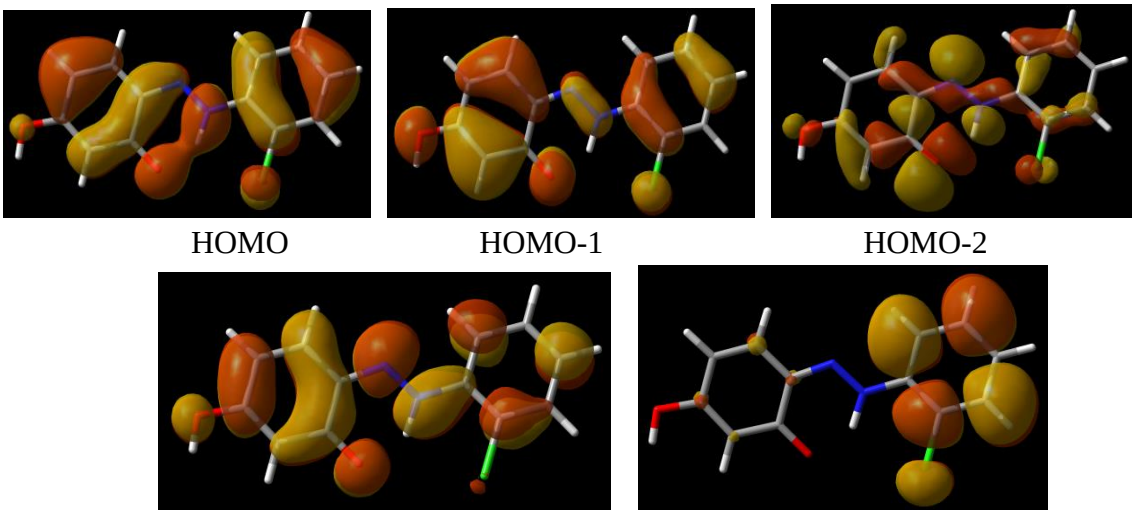



**Figure S12**. HOMO and LUMO for **3** in water.

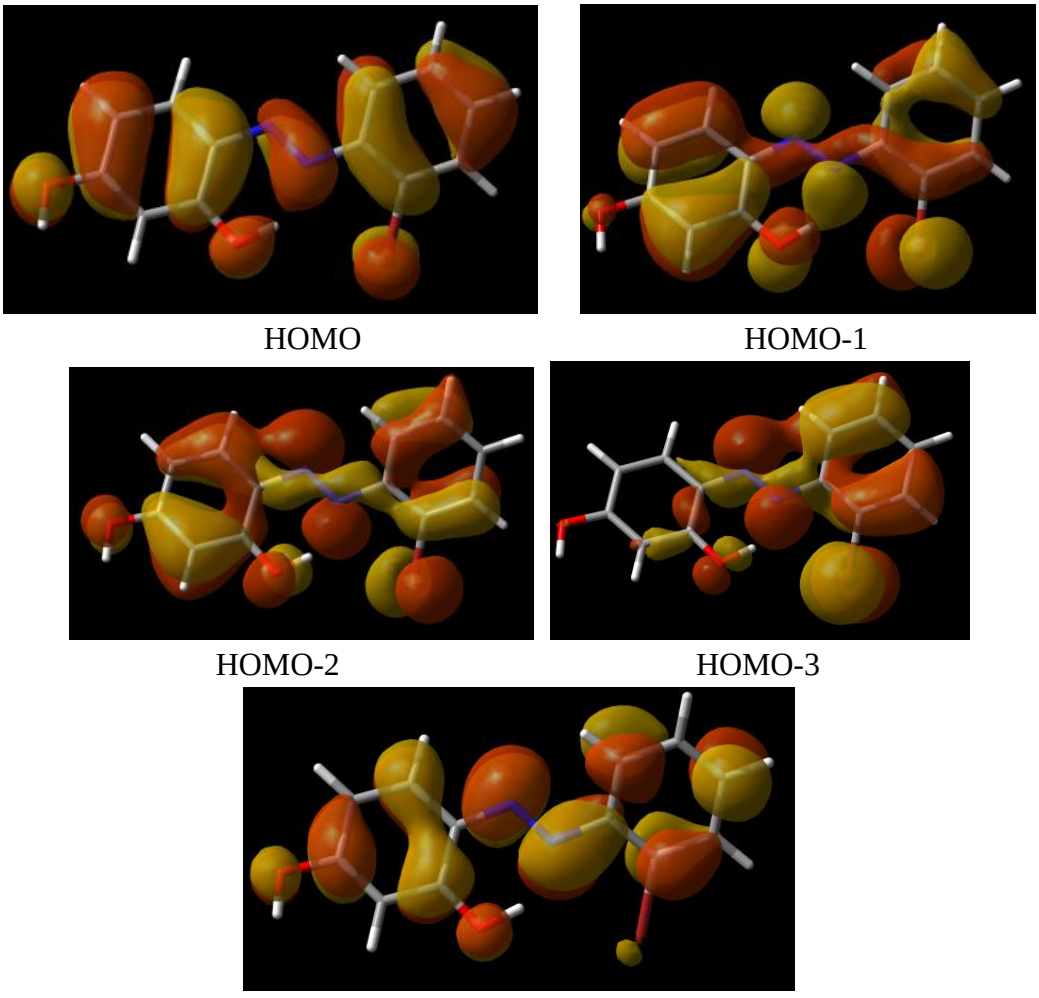
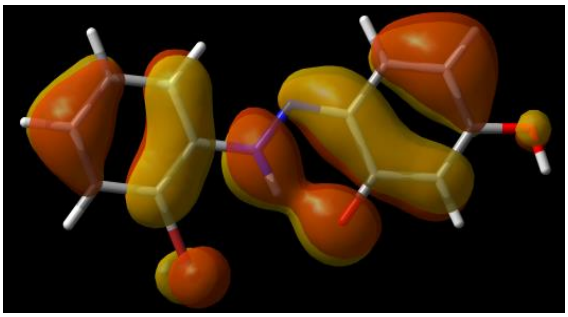
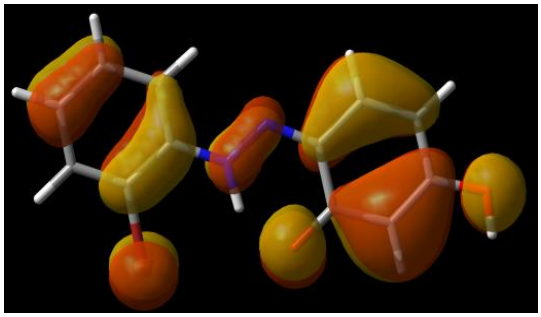


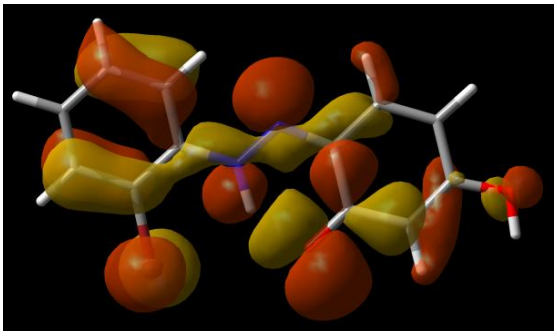

**Figure S13**. HOMO and LUMO for **4** in DMA.



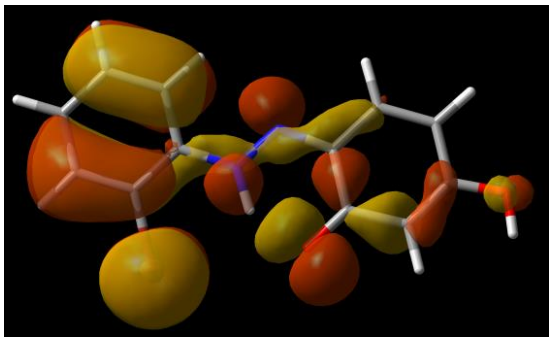
HOMO



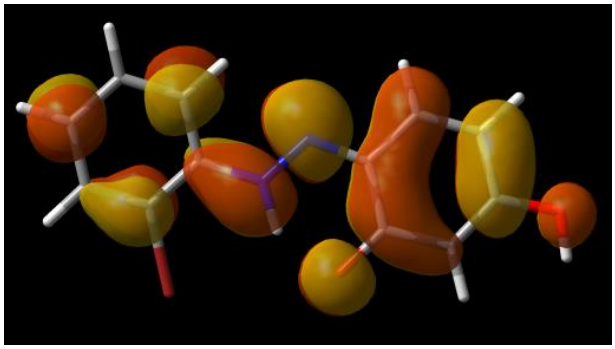
HOMO-1



HOMO-2

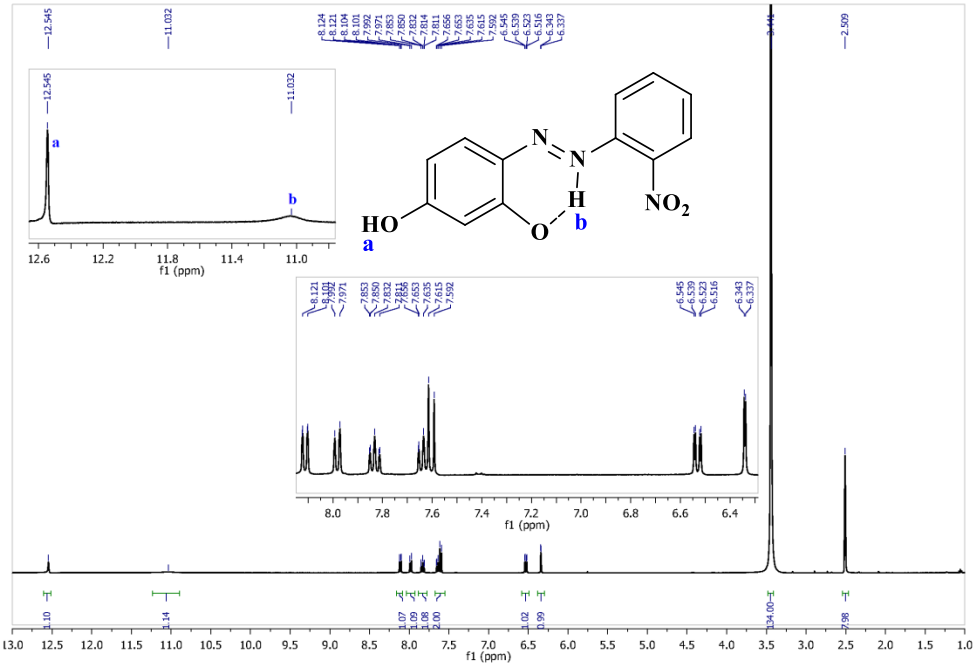


HOMO-3

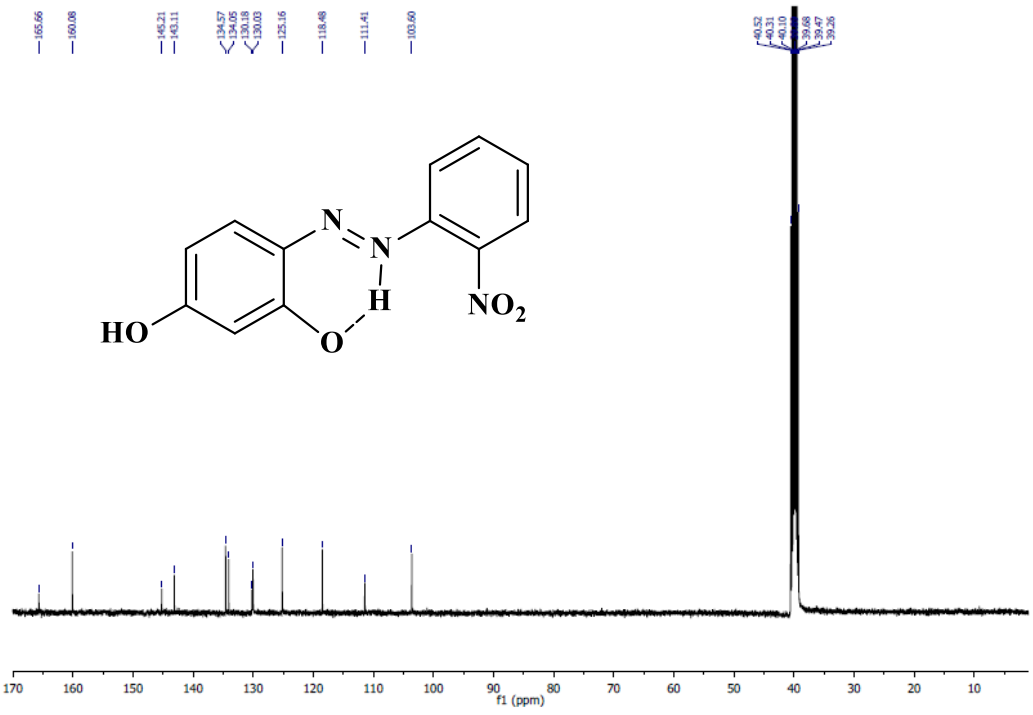


LUMO

**Figure S14**. HOMO and LUMO for **4** in water.

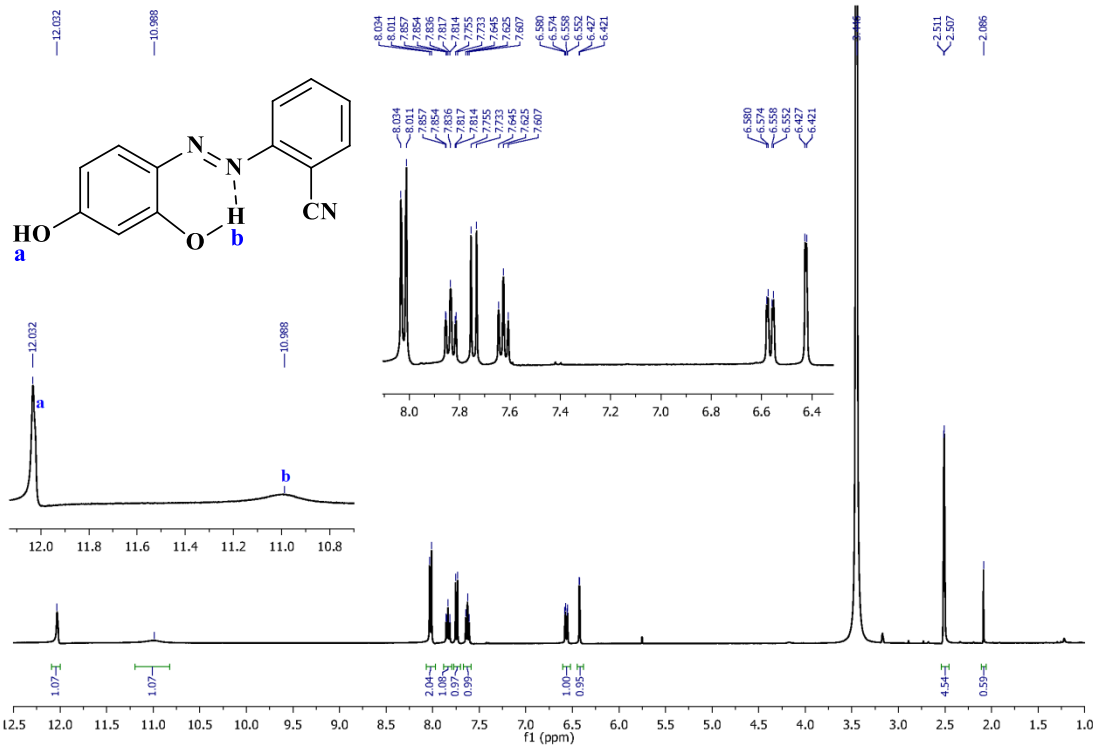



(a)

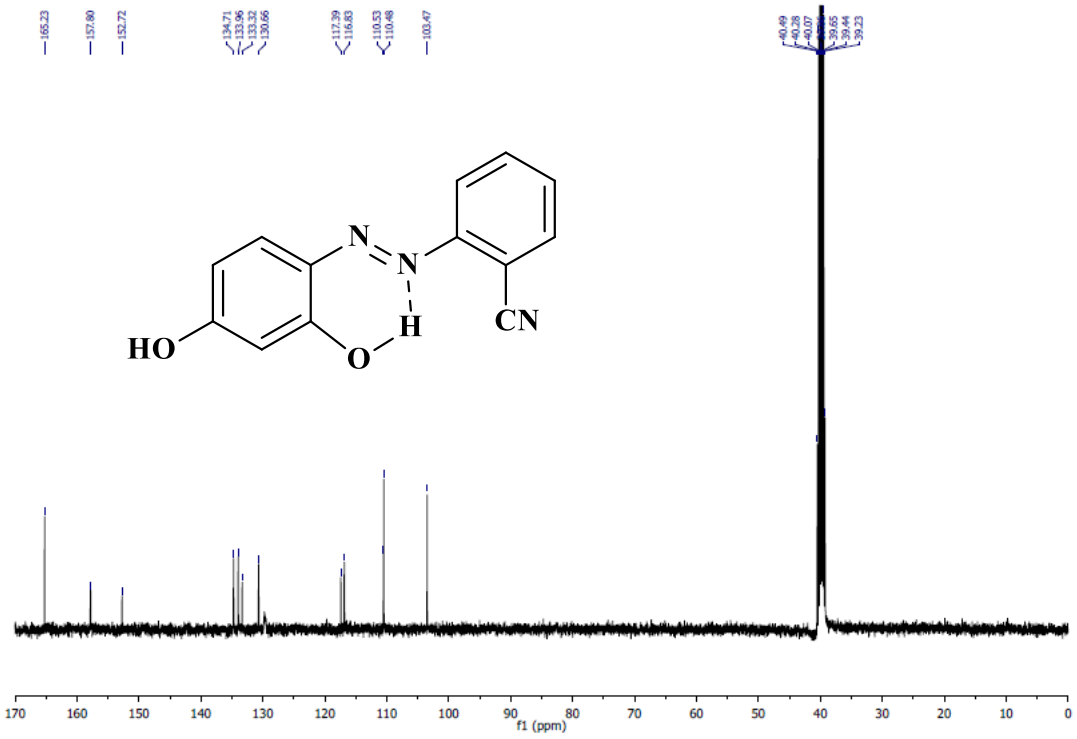



(b)

**Figure S15**. (a)$^{1}$H and (b) $^{13}$C NMR spectra of **1** in [d6-DMSO].

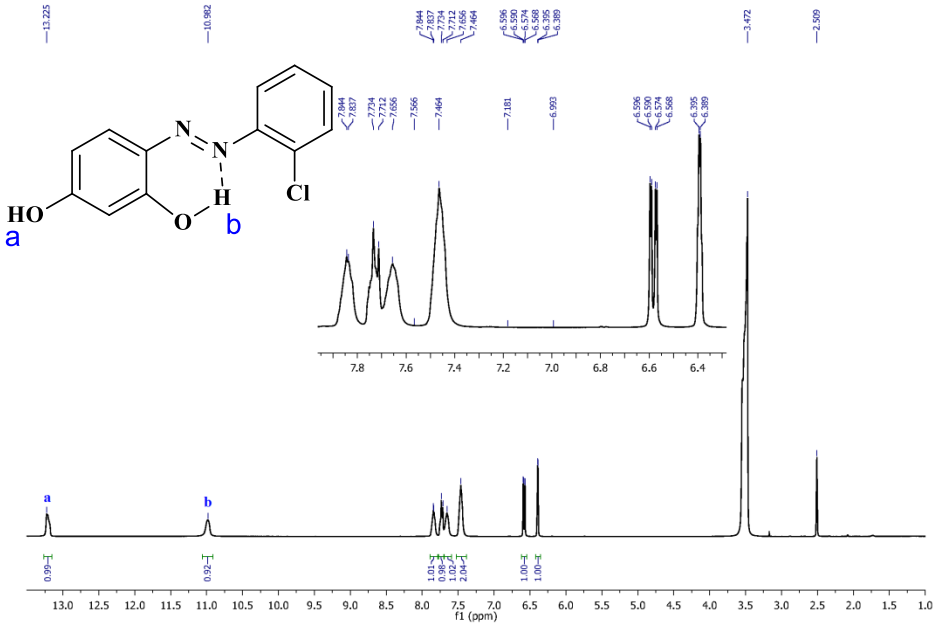



(a)

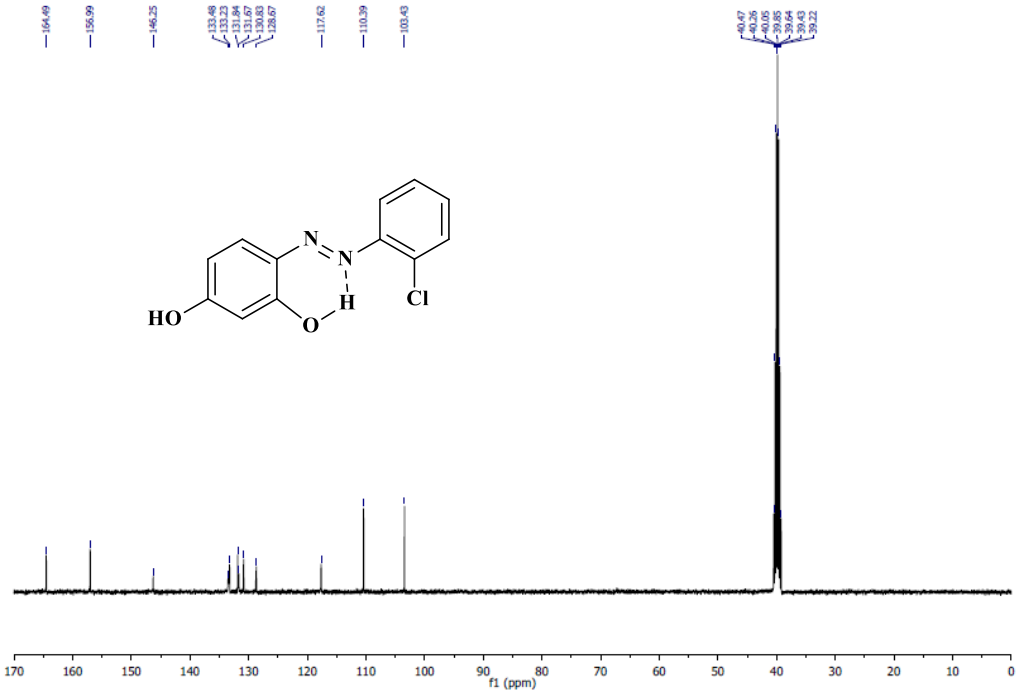



(b)

**Figure S16**. (a)$^{1}$H and (b) $^{13}$C NMR spectra of **2** in [d6-DMSO].

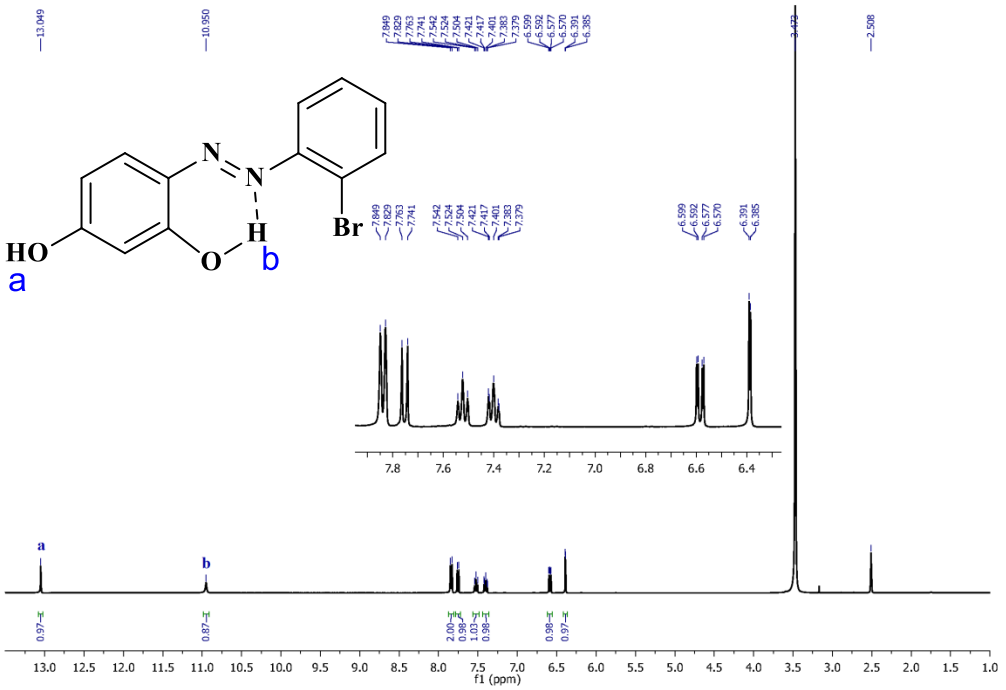



(a)

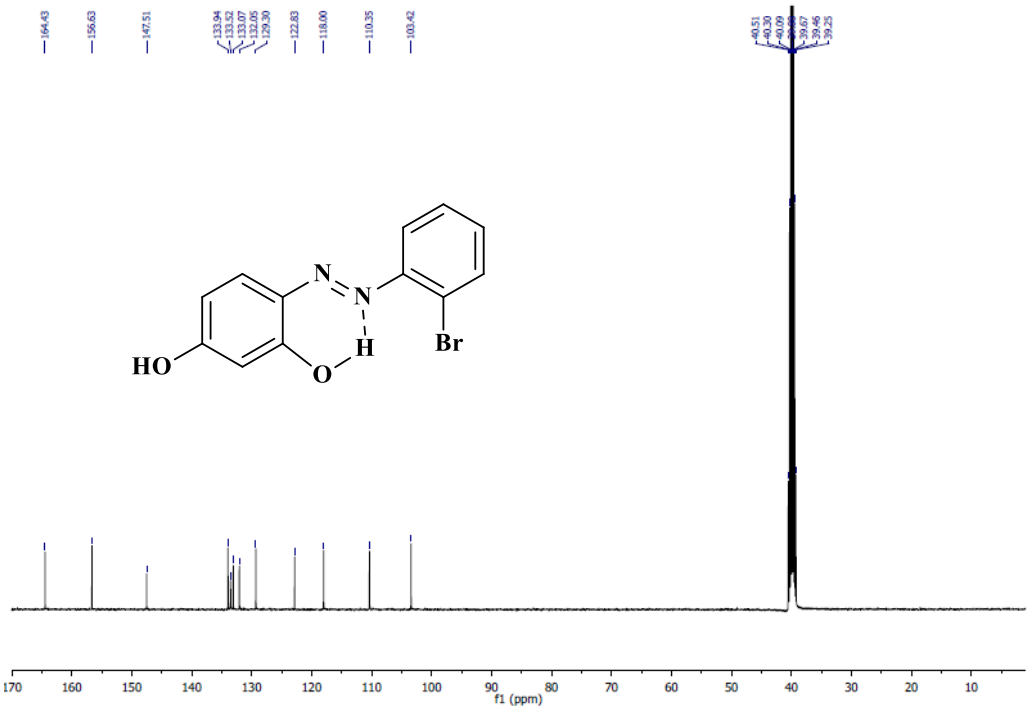



(b)

**Figure S17**. (a)[1]H and (b) [13]C NMR spectra of **3** in [d6-DMSO].




(a)




(b)

**Figure S18**. (a)$^{1}$H and (b) $^{13}$C NMR spectra of **4** in [d6-DMSO].

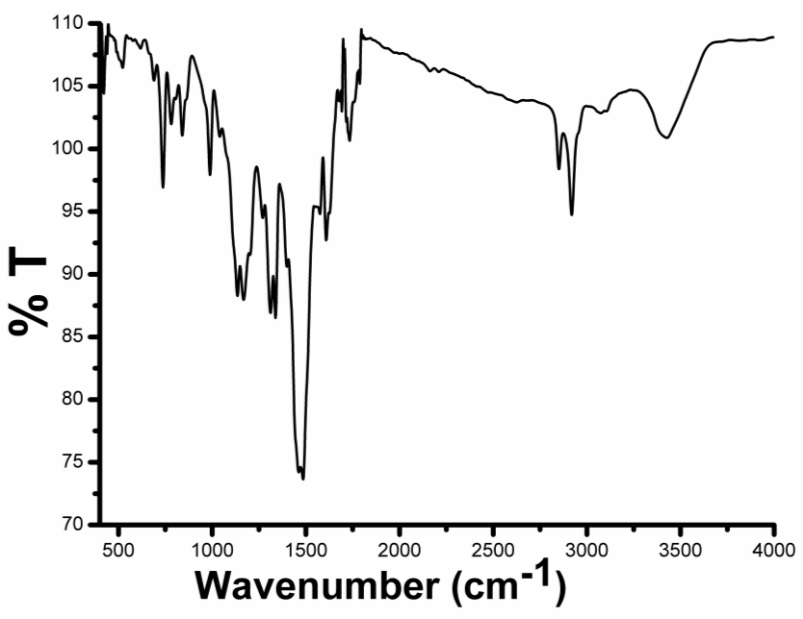



**Figure S19a**. FT-IR spectrum of **1.**

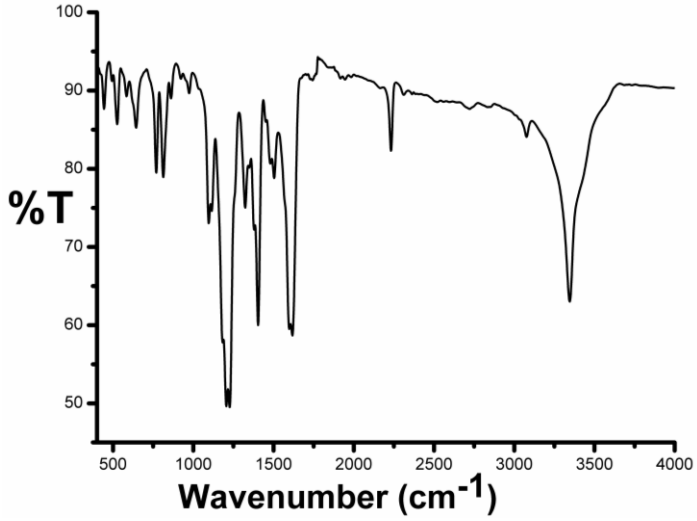



**Figure S19b**. FT-IR spectrum of **2.**

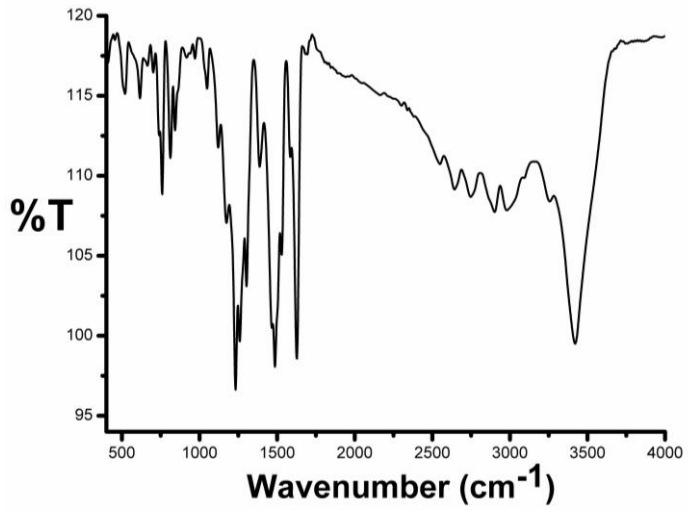



**Figure S19c**. FT-IR spectrum of **3.**

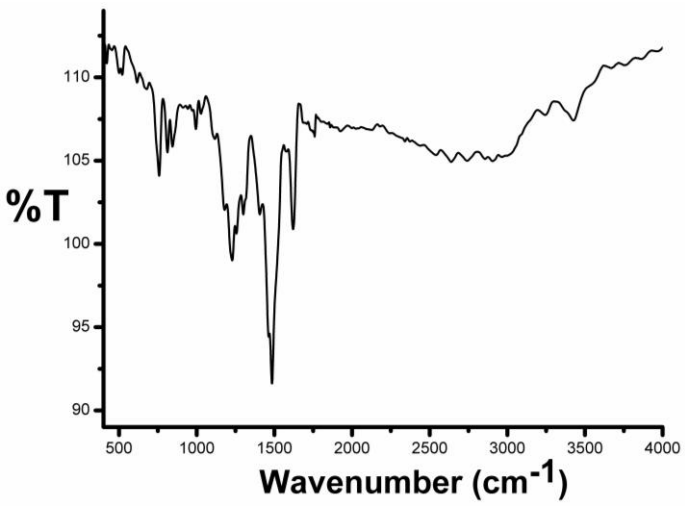



**Figure S19d**. FT-IR spectrum of **4.**

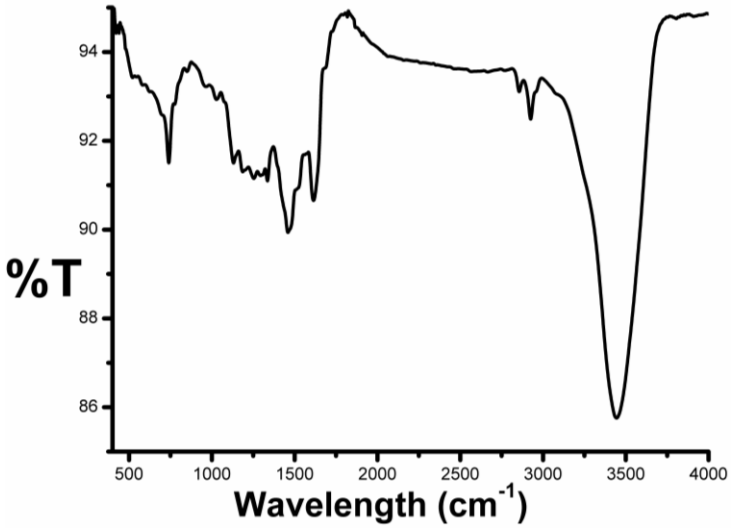



**Figure S19e**. FT-IR spectrum of **1** after DSC.

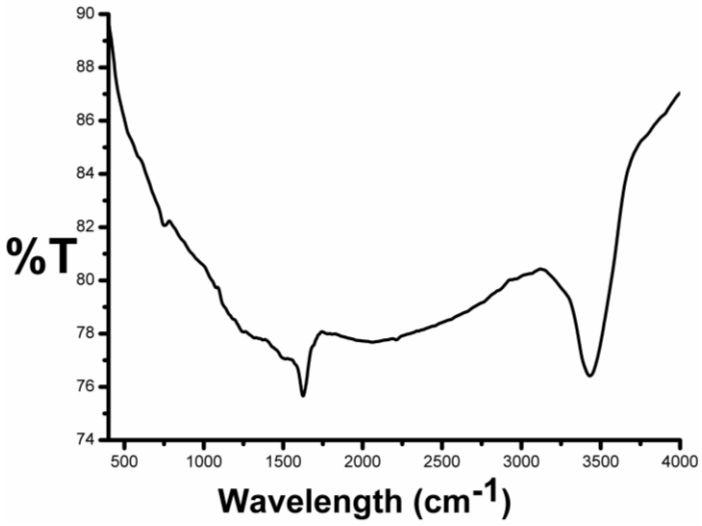



**Figure S19f**. FT-IR spectrum of **2** after DSC.

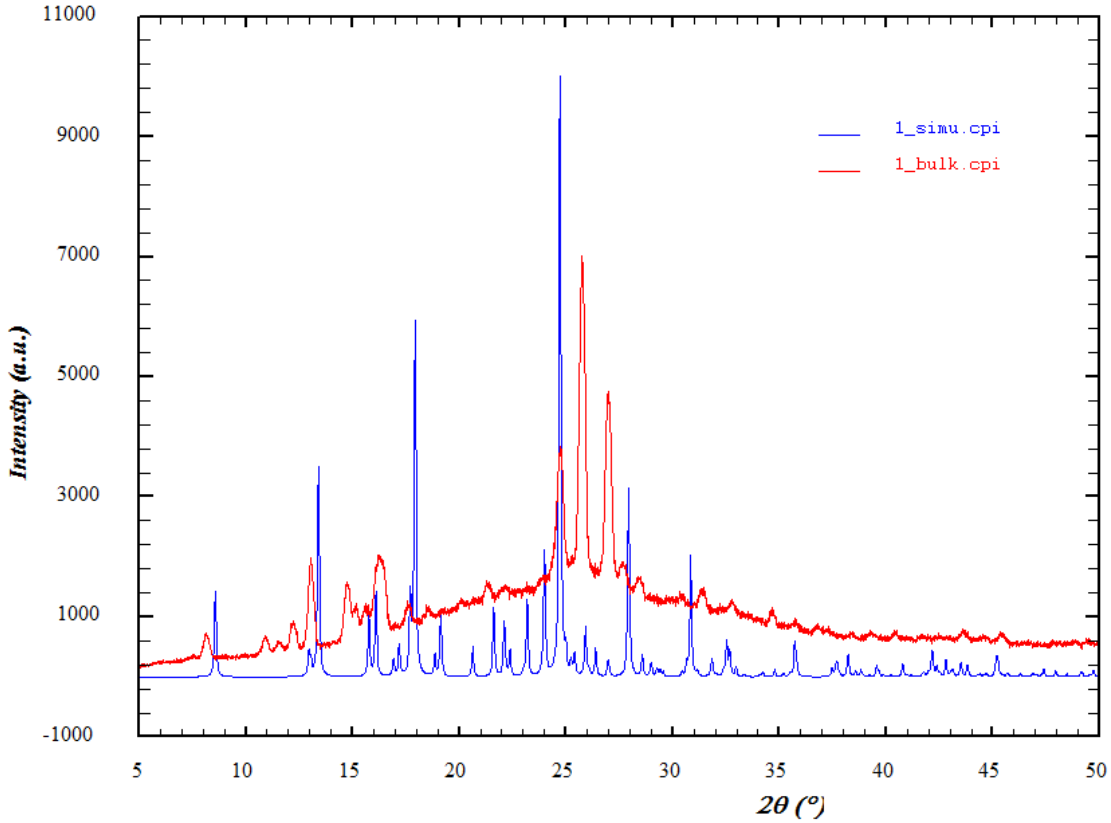



**Figure S20a**. PXRD of **1.**

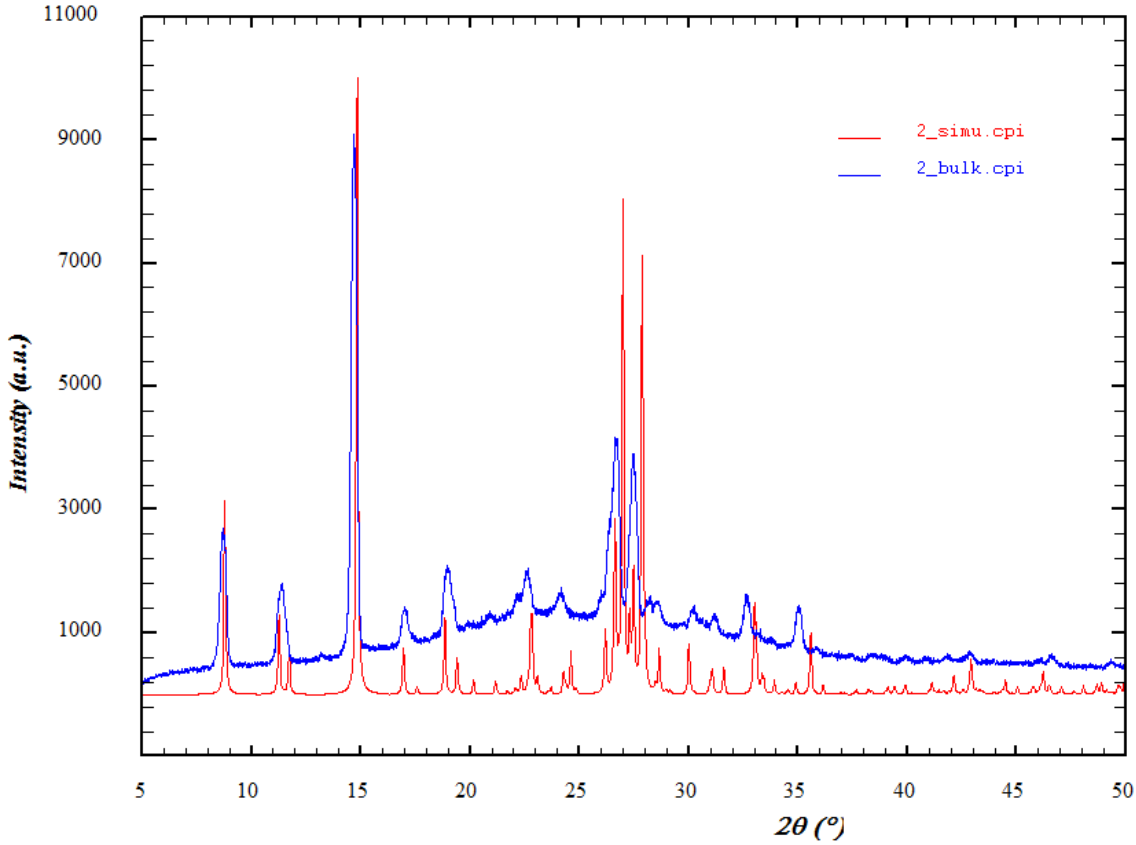



**Figure S20b**. PXRD of **2**

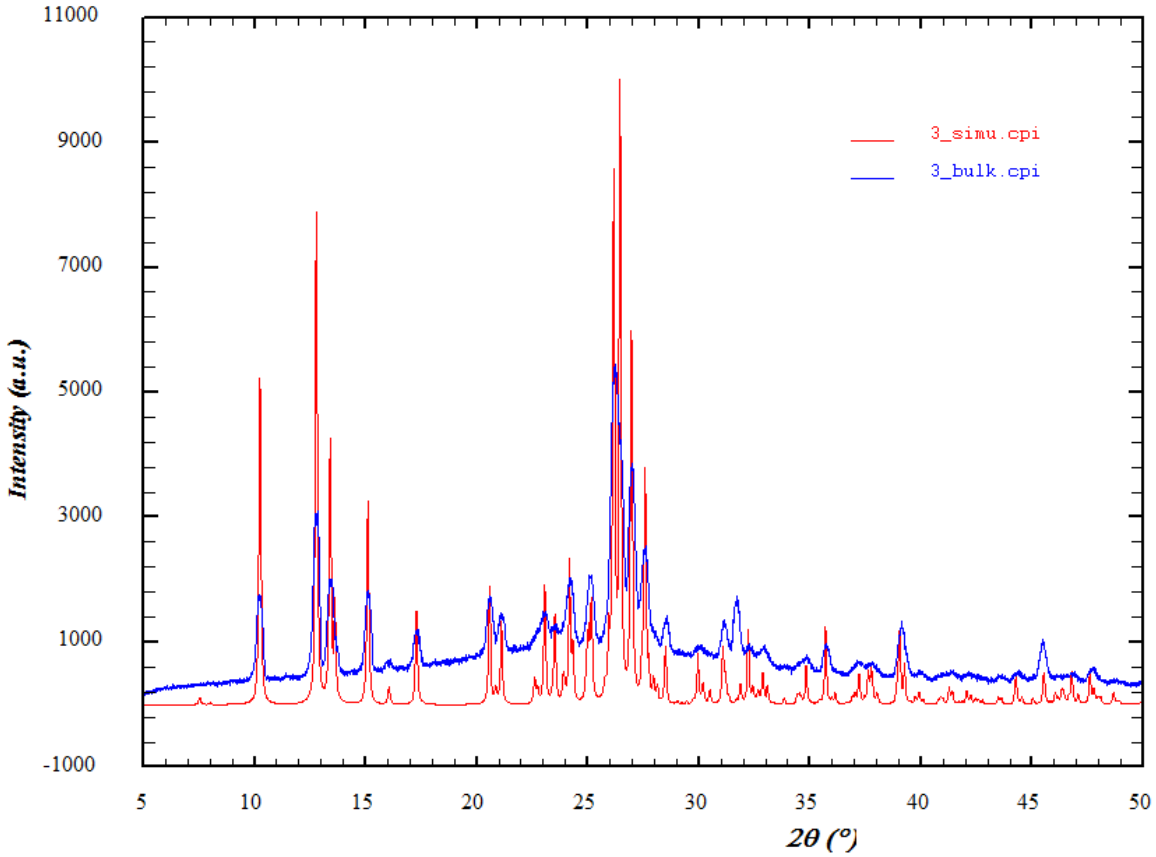



**Figure S20c**. PXRD of **3**

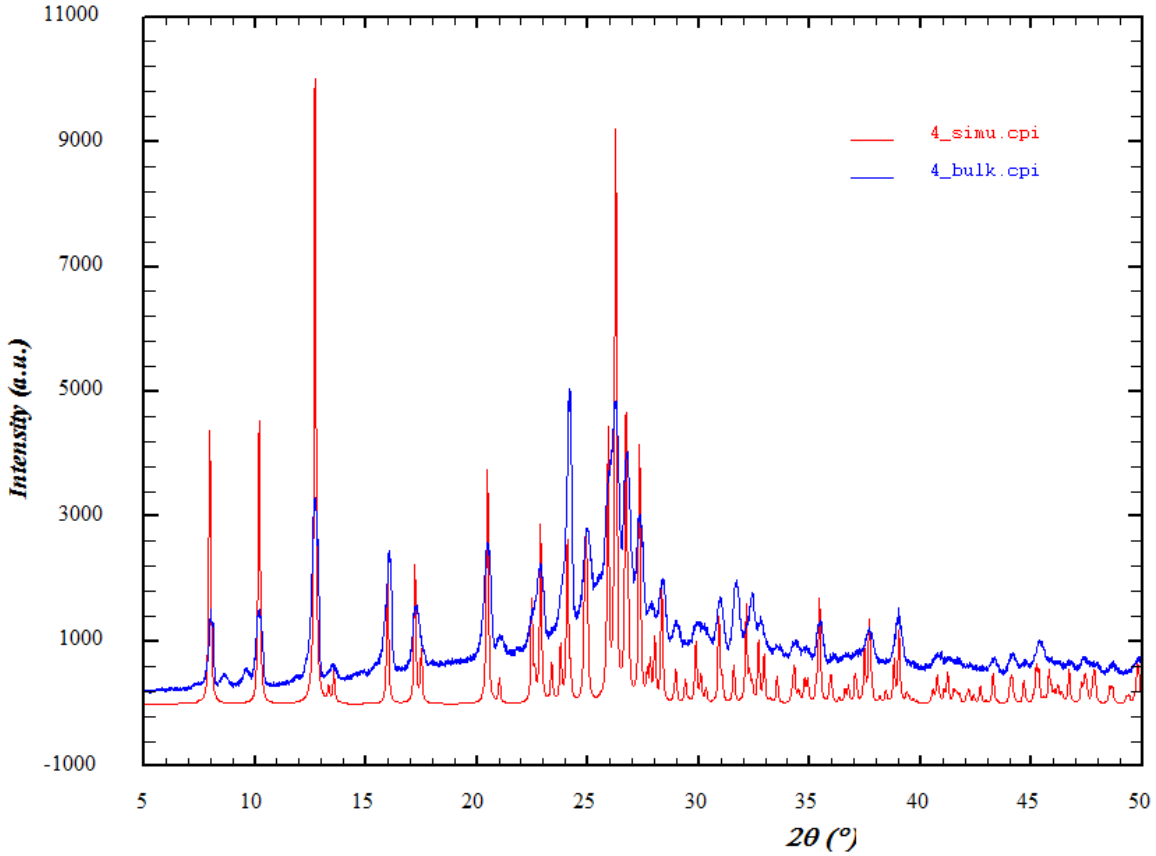
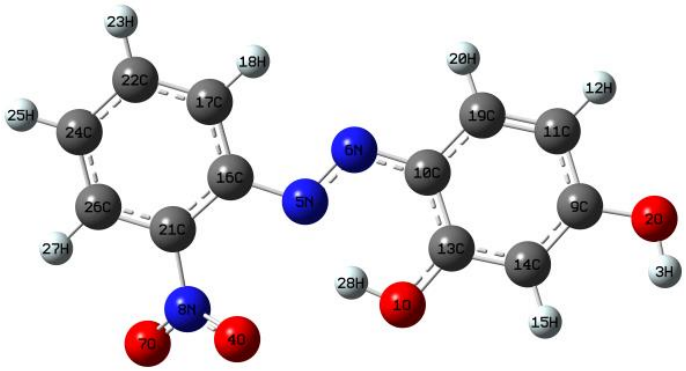



**Figure S20d**. PXRD of **4.**

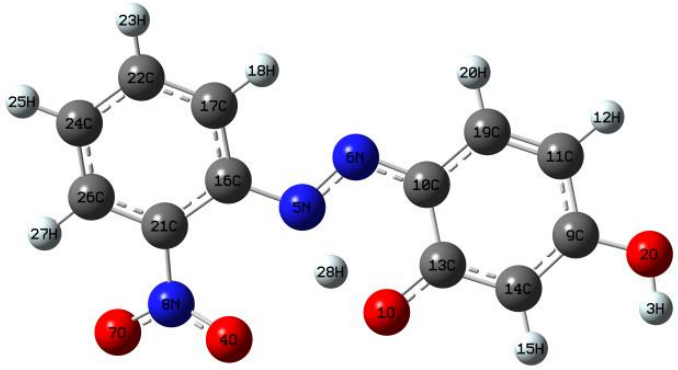
**Figure S21a**. Optimized geometry and coordinates of **1e (**enol form of **1)**




**C12H9N3O4**

| | | | |
|---|---|---|---|
| O | -0.031311000 | -0.017887000 | 0.005849000 |
| O | 0.097776000 | 0.012972000 | 4.769032000 |
| H | 1.048723000 | 0.123360000 | 4.618320000 |
| O | -0.504572000 | -0.011917000 | -2.986372000 |
| N | -2.374114000 | -0.293756000 | -0.990843000 |
| N | -2.927377000 | -0.395102000 | 0.158404000 |
| O | -1.328583000 | 1.257152000 | -4.547402000 |
| N | -1.454892000 | 0.419811000 | -3.646544000 |
| C | -0.575481000 | -0.072823000 | 3.595557000 |
| C | -2.093763000 | -0.273808000 | 1.247796000 |
| C | -1.975191000 | -0.251757000 | 3.684567000 |
| H | -2.442912000 | -0.310476000 | 4.660559000 |
| C | -0.672357000 | -0.089945000 | 1.179836000 |
| C | 0.069753000 | 0.007922000 | 2.359711000 |
| H | 1.144918000 | 0.143890000 | 2.293990000 |
| C | -3.236230000 | -0.458146000 | -2.091253000 |
| C | -4.549299000 | -0.950711000 | -1.966766000 |
| H | -4.897898000 | -1.232034000 | -0.981001000 |
| C | -2.708222000 | -0.351117000 | 2.522714000 |
| H | -3.783789000 | -0.491645000 | 2.554859000 |
| C | -2.801441000 | -0.096166000 | -3.388913000 |
| C | -5.379076000 | -1.077076000 | -3.074965000 |
| H | -6.381724000 | -1.472948000 | -2.948297000 |
| C | -4.931117000 | -0.699305000 | -4.347978000 |
| H | -5.576758000 | -0.800914000 | -5.213342000 |
| C | -3.644101000 | -0.195709000 | -4.500470000 |
| H | -3.272416000 | 0.105416000 | -5.471980000 |
| H | -0.723531000 | -0.096680000 | -0.716719000 |

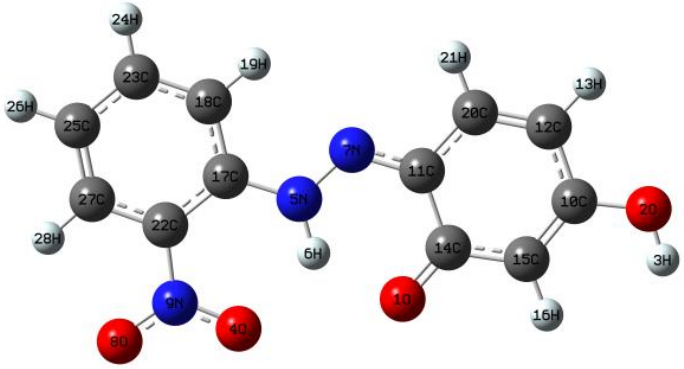
**Figure S21b**. Optimized geometry and coordinates of **1ts (**transition state of **1)**




**C12H9N3O4**

| | | | |
|---|---|---|---|
| O | -0.182226000 | -0.072150000 | -0.061994000 |
| O | 0.131041000 | -0.047756000 | 4.707784000 |
| H | 1.084447000 | 0.023060000 | 4.546520000 |
| O | -0.532106000 | 0.258817000 | -2.877588000 |
| N | -2.382838000 | -0.272127000 | -0.979156000 |
| N | -2.967582000 | -0.333738000 | 0.181016000 |
| O | -1.281869000 | 1.126751000 | -4.724177000 |
| N | -1.444404000 | 0.476804000 | -3.683246000 |
| C | -0.556207000 | -0.104270000 | 3.543916000 |
| C | -2.151733000 | -0.246663000 | 1.254022000 |
| C | -1.973115000 | -0.223333000 | 3.676278000 |
| H | -2.403834000 | -0.258691000 | 4.670230000 |
| C | -0.708232000 | -0.118222000 | 1.128922000 |
| C | 0.068023000 | -0.051514000 | 2.304429000 |
| H | 1.146403000 | 0.040637000 | 2.218281000 |
| C | -3.198199000 | -0.427875000 | -2.108678000 |
| C | -4.505214000 | -0.941105000 | -1.982738000 |
| H | -4.847203000 | -1.227490000 | -0.996738000 |
| C | -2.746644000 | -0.293200000 | 2.549217000 |
| H | -3.825972000 | -0.387037000 | 2.612283000 |
| C | -2.769818000 | -0.066500000 | -3.412703000 |
| C | -5.336034000 | -1.086933000 | -3.085586000 |
| H | -6.331743000 | -1.496842000 | -2.949611000 |
| C | -4.895970000 | -0.719422000 | -4.364705000 |
| H | -5.540111000 | -0.840507000 | -5.228472000 |
| C | -3.617171000 | -0.203806000 | -4.520505000 |
| H | -3.247579000 | 0.088892000 | -5.494729000 |
| H | -1.149607000 | -0.148817000 | -0.810858000 |

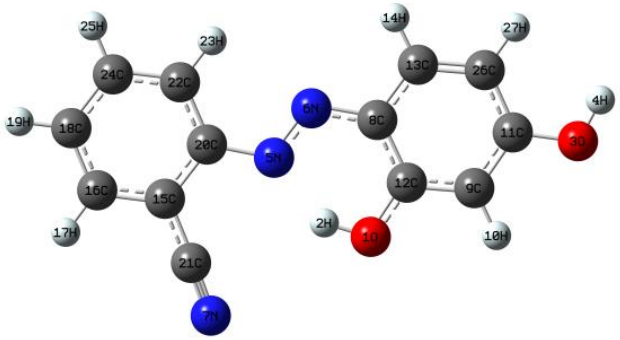
**Figure S21c**. Optimized geometry and coordinates of **1k (**keto form of **1)**




**C12H9N3O4**

| | | | |
|---|---|---|---|
| O | -0.039660000 | 0.260645000 | 0.027190000 |
| O | 0.010753000 | -0.068484000 | 4.781179000 |
| H | 0.947203000 | 0.170292000 | 4.697417000 |
| O | -0.584015000 | 0.403888000 | -2.950602000 |
| N | -2.353659000 | -0.229993000 | -1.091363000 |
| H | -1.360158000 | 0.030298000 | -1.192941000 |
| N | -2.836387000 | -0.439316000 | 0.115034000 |
| O | -1.126596000 | 0.468043000 | -5.052658000 |
| N | -1.413775000 | 0.268942000 | -3.866161000 |
| C | -0.584686000 | -0.129078000 | 3.568453000 |
| C | -2.051780000 | -0.320277000 | 1.174095000 |
| C | -1.984139000 | -0.477691000 | 3.608359000 |
| H | -2.444396000 | -0.660272000 | 4.572698000 |
| C | -0.607422000 | 0.040150000 | 1.130950000 |
| C | 0.077107000 | 0.118536000 | 2.388328000 |
| H | 1.130847000 | 0.379828000 | 2.375328000 |
| C | -3.194393000 | -0.367333000 | -2.195518000 |
| C | -4.537424000 | -0.752779000 | -2.005376000 |
| H | -4.878732000 | -0.932716000 | -0.995074000 |
| C | -2.683681000 | -0.567942000 | 2.447959000 |
| H | -3.737053000 | -0.828414000 | 2.443219000 |
| C | -2.766334000 | -0.136126000 | -3.532452000 |
| C | -5.403361000 | -0.901340000 | -3.078069000 |
| H | -6.429482000 | -1.200723000 | -2.890093000 |
| C | -4.967388000 | -0.671972000 | -4.392266000 |
| H | -5.645074000 | -0.790186000 | -5.230154000 |
| C | -3.654423000 | -0.291130000 | -4.610087000 |
| H | -3.284619000 | -0.105685000 | -5.609690000 |

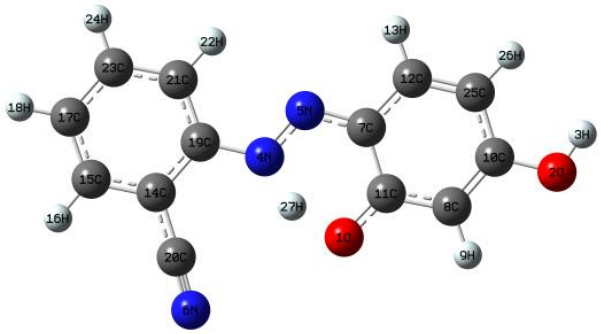
**Figure S21d**. Optimized geometry and coordinates of **2e (**enol form of **2)**




**C13N3H9O2**

| | | | |
|---|---|---|---|
| O | -0.007562000 | -0.078833000 | -0.005949000 |
| H | 0.051314000 | -0.068026000 | 0.991669000 |
| O | 2.903823000 | -0.021503000 | -3.699150000 |
| H | 3.839215000 | 0.004275000 | -3.950642000 |
| N | 1.122617000 | -0.022249000 | 2.314202000 |
| N | 2.292889000 | 0.008432000 | 1.803542000 |
| N | -2.355020000 | -0.114540000 | 2.821684000 |
| C | 2.373109000 | -0.001050000 | 0.426152000 |
| C | 1.466060000 | -0.049507000 | -1.846388000 |
| H | 0.618884000 | -0.081956000 | -2.522471000 |
| C | 2.768542000 | -0.013541000 | -2.349252000 |
| C | 1.252939000 | -0.043716000 | -0.468352000 |
| C | 3.676399000 | 0.034423000 | -0.123592000 |
| H | 4.513564000 | 0.066474000 | 0.566233000 |
| C | -0.223627000 | -0.044228000 | 4.304279000 |
| C | -0.375054000 | -0.038018000 | 5.701952000 |
| H | -1.370773000 | -0.062826000 | 6.130732000 |
| C | 0.750525000 | -0.000381000 | 6.520196000 |
| H | 0.634045000 | 0.004322000 | 7.598672000 |
| C | 1.067209000 | -0.012416000 | 3.722543000 |
| C | -1.388254000 | -0.082828000 | 3.471171000 |
| C | 2.190822000 | 0.025367000 | 4.563629000 |
| H | 3.178284000 | 0.049450000 | 4.119349000 |
| C | 2.029670000 | 0.031251000 | 5.946114000 |
| H | 2.906876000 | 0.060501000 | 6.584970000 |
| C | 3.887340000 | 0.028863000 | -1.487434000 |
| H | 4.892395000 | 0.056358000 | -1.896226000 |

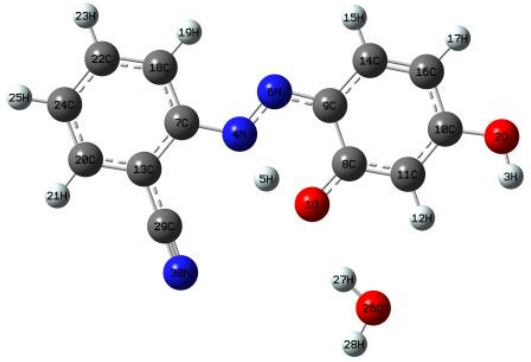
**Figure S21e**. Optimized geometry and coordinates of **2ts (**transition state of **2)**




**C13N3H9O2**

| | | | |
|---|---|---|---|
| O | 0.165318000 | 0.081973000 | -0.129568000 |
| O | -0.085377000 | 0.025253000 | 4.583562000 |
| H | 0.482421000 | 0.012911000 | 5.365865000 |
| N | 2.344823000 | 0.084219000 | -1.131673000 |
| N | 2.970844000 | 0.067197000 | 0.007582000 |
| N | -0.166455000 | 0.125965000 | -3.711055000 |
| C | 2.189403000 | 0.057333000 | 1.107088000 |
| C | -0.003781000 | 0.053800000 | 2.241146000 |
| H | -1.086870000 | 0.059297000 | 2.206381000 |
| C | 0.664706000 | 0.035713000 | 3.450154000 |
| C | 0.730237000 | 0.065147000 | 1.029575000 |
| C | 2.832431000 | 0.038599000 | 2.377854000 |
| H | 3.917644000 | 0.033163000 | 2.400018000 |
| C | 2.424683000 | 0.112812000 | -3.550856000 |
| C | 3.159936000 | 0.123882000 | -4.749642000 |
| H | 2.622289000 | 0.137490000 | -5.691623000 |
| C | 4.550540000 | 0.117515000 | -4.724188000 |
| H | 5.109869000 | 0.126205000 | -5.653882000 |
| C | 3.104201000 | 0.095021000 | -2.308491000 |
| C | 0.993787000 | 0.119805000 | -3.616787000 |
| C | 4.509061000 | 0.088797000 | -2.297452000 |
| H | 5.020991000 | 0.075122000 | -1.343363000 |
| C | 5.219266000 | 0.099947000 | -3.492720000 |
| H | 6.304861000 | 0.094922000 | -3.466028000 |
| C | 2.093933000 | 0.027908000 | 3.530817000 |
| H | 2.578329000 | 0.013506000 | 4.503482000 |
| H | 1.157258000 | 0.087235000 | -0.940977000 |

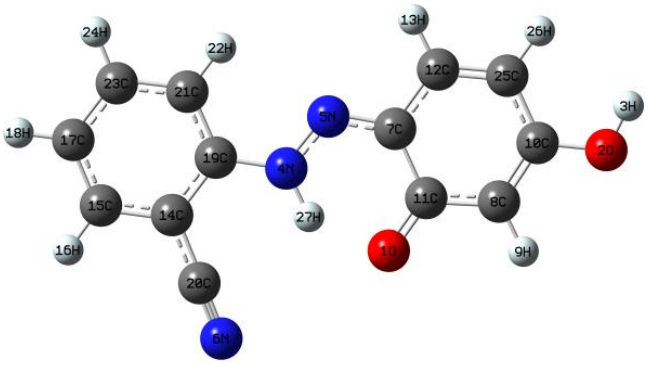
**Figure S21f**. Optimized geometry and coordinates of **2ts_w (**transition state of **2** with water**)**



**C13N3H11O3**

| | | | |
|---|---|---|---|
| O | 0.000821000 | -0.007532000 | 0.003628000 |
| O | -0.006071000 | -0.003977000 | 4.780566000 |
| H | 0.955644000 | -0.007574000 | 4.667963000 |
| N | -2.138738000 | -0.000127000 | -1.062693000 |
| H | -0.929542000 | -0.004582000 | -0.813797000 |
| N | -2.804922000 | 0.003206000 | 0.051009000 |
| C | -2.852927000 | 0.001987000 | -2.267044000 |
| C | -0.607239000 | -0.004401000 | 1.157218000 |
| C | -2.060631000 | 0.001124000 | 1.180457000 |
| C | -0.620216000 | -0.002574000 | 3.572378000 |
| C | 0.091264000 | -0.006130000 | 2.381919000 |
| H | 1.177848000 | -0.010226000 | 2.359765000 |
| C | -2.117210000 | -0.002039000 | -3.477506000 |
| C | -2.743965000 | 0.004600000 | 2.431203000 |
| H | -3.829163000 | 0.008679000 | 2.415936000 |
| C | -2.046701000 | 0.002825000 | 3.609522000 |
| H | -2.542187000 | 0.005413000 | 4.573342000 |
| C | -4.256435000 | 0.007957000 | -2.318728000 |
| H | -4.811358000 | 0.011042000 | -1.388775000 |
| C | -2.794918000 | -0.000028000 | -4.709210000 |
| H | -2.215507000 | -0.003178000 | -5.626173000 |
| C | -4.910297000 | 0.009856000 | -3.546010000 |
| H | -5.995899000 | 0.014477000 | -3.570021000 |
| C | -4.185537000 | 0.005897000 | -4.745740000 |
| H | -4.702343000 | 0.007430000 | -5.699721000 |
| O | 2.794326000 | -0.017879000 | 0.554655000 |
| H | 1.923371000 | -0.014750000 | 0.116173000 |
| H | 3.450634000 | -0.021976000 | -0.151606000 |
| C | -0.684808000 | -0.008203000 | -3.465777000 |
| N | 0.479344000 | -0.013238000 | -3.477891000 |

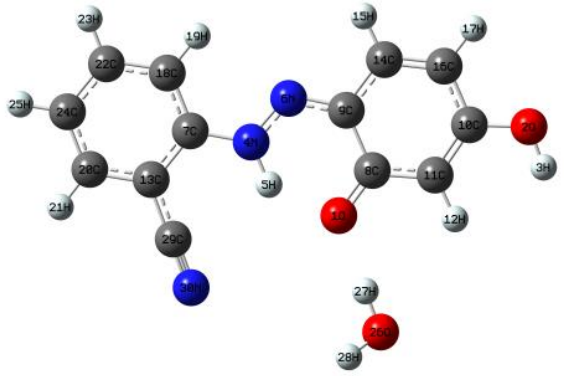
**Figure S21g**. Optimized geometry and coordinates of **2k (**keto form of **2)**




**C13N3H9O2**

| | | | |
|---|---|---|---|
| O | 0.025956000 | 0.086955000 | -0.040438000 |
| O | -0.003642000 | 0.024576000 | 4.669658000 |
| H | 0.591840000 | 0.010913000 | 5.433907000 |
| N | 2.331865000 | 0.085292000 | -1.170290000 |
| N | 2.898504000 | 0.065367000 | 0.009270000 |
| N | -0.132998000 | 0.121454000 | -3.752206000 |
| C | 2.127982000 | 0.056154000 | 1.093961000 |
| C | -0.022009000 | 0.055945000 | 2.329884000 |
| H | -1.106418000 | 0.064077000 | 2.345638000 |
| C | 0.692511000 | 0.034689000 | 3.508022000 |
| C | 0.645718000 | 0.067563000 | 1.067870000 |
| C | 2.818159000 | 0.033732000 | 2.355054000 |
| H | 3.903182000 | 0.025602000 | 2.336673000 |
| C | 2.457154000 | 0.112211000 | -3.591431000 |
| C | 3.217538000 | 0.123178000 | -4.775613000 |
| H | 2.703975000 | 0.135730000 | -5.730586000 |
| C | 4.606673000 | 0.117796000 | -4.715994000 |
| H | 5.188396000 | 0.126410000 | -5.631115000 |
| C | 3.108197000 | 0.095704000 | -2.332820000 |
| C | 1.029832000 | 0.117372000 | -3.677756000 |
| C | 4.509654000 | 0.090268000 | -2.286403000 |
| H | 5.005067000 | 0.077576000 | -1.324028000 |
| C | 5.244823000 | 0.101273000 | -3.468010000 |
| H | 6.328874000 | 0.097058000 | -3.415127000 |
| C | 2.132334000 | 0.022967000 | 3.531105000 |
| H | 2.653555000 | 0.005540000 | 4.483085000 |
| H | 1.289260000 | 0.092463000 | -1.173672000 |

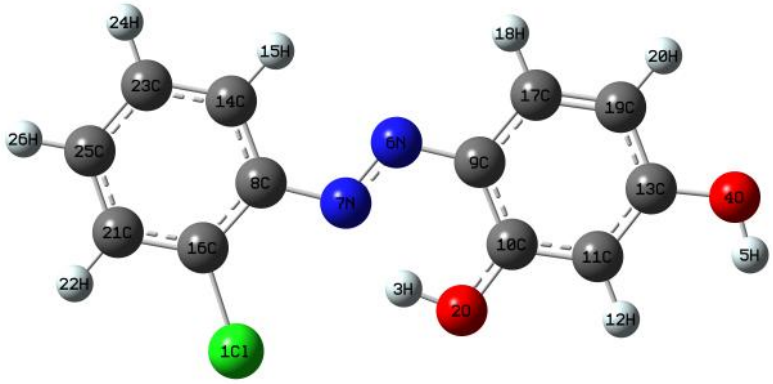
**Figure S21h**. Optimized geometry and coordinates of **2k_w (**keto form of **2** with water**)**



**C13N3H11O3**

| | | | |
|---|---|---|---|
| O | 0.001623000 | -0.014665000 | 0.009286000 |
| O | -0.010351000 | -0.002584000 | 4.779945000 |
| H | 0.955324000 | -0.009711000 | 4.688380000 |
| N | -2.331142000 | -0.000259000 | -1.086973000 |
| H | -1.293153000 | -0.008794000 | -1.126910000 |
| N | -2.866531000 | 0.007379000 | 0.104563000 |
| C | -3.136342000 | 0.004745000 | -2.231388000 |
| C | -0.601327000 | -0.007931000 | 1.133862000 |
| C | -2.078235000 | 0.003706000 | 1.177459000 |
| C | -0.614045000 | -0.001139000 | 3.571401000 |
| C | 0.086481000 | -0.008987000 | 2.381145000 |
| H | 1.172093000 | -0.017564000 | 2.369513000 |
| C | -2.514890000 | -0.007407000 | -3.504525000 |
| C | -2.751030000 | 0.012100000 | 2.448974000 |
| H | -3.836036000 | 0.020390000 | 2.443070000 |
| C | -2.050323000 | 0.009786000 | 3.615545000 |
| H | -2.541476000 | 0.016033000 | 4.581693000 |
| C | -4.535493000 | 0.021606000 | -2.149984000 |
| H | -5.007293000 | 0.031172000 | -1.175771000 |
| C | -3.303166000 | -0.002514000 | -4.670029000 |
| H | -2.812796000 | -0.012040000 | -5.637083000 |
| C | -5.298796000 | 0.026133000 | -3.313862000 |
| H | -6.381141000 | 0.039257000 | -3.235228000 |
| C | -4.690480000 | 0.014145000 | -4.576564000 |
| H | -5.293945000 | 0.017864000 | -5.477504000 |
| O | 2.773637000 | -0.037441000 | -0.249818000 |
| H | 1.793903000 | -0.045458000 | -0.167298000 |
| H | 2.967200000 | -0.490233000 | -1.080739000 |
| C | -1.089908000 | -0.025350000 | -3.623577000 |
| N | 0.071014000 | -0.040453000 | -3.721665000 |

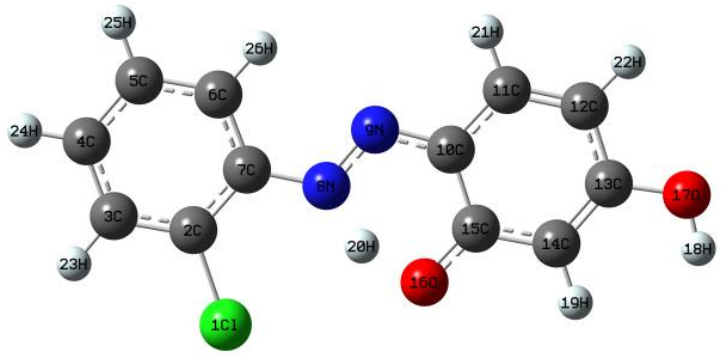
**Figure S21i**. Optimized geometry and coordinates of **3e (**enol form of **3)**




**C12H9N2O2Cl**

| | | | |
|---|---|---|---|
| Cl | -0.091291000 | -0.207219000 | -0.024796000 |
| O | -0.017232000 | -0.025311000 | 3.674018000 |
| H | 0.475707000 | -0.133331000 | 2.806444000 |
| O | 1.093624000 | 0.084853000 | 8.312518000 |
| H | 0.138283000 | 0.213359000 | 8.408154000 |
| N | 2.816399000 | -0.411763000 | 3.070035000 |
| N | 1.982360000 | -0.360144000 | 2.105739000 |
| C | 2.518822000 | -0.499357000 | 0.810009000 |
| C | 2.293170000 | -0.276920000 | 4.343840000 |
| C | 0.907097000 | -0.087830000 | 4.646575000 |
| C | 0.496424000 | 0.034210000 | 5.976713000 |
| H | -0.558782000 | 0.176492000 | 6.189711000 |
| C | 1.440485000 | -0.028055000 | 7.003974000 |
| C | 3.889424000 | -0.691643000 | 0.546601000 |
| H | 4.572445000 | -0.735013000 | 1.386814000 |
| C | 1.633618000 | -0.444170000 | -0.284672000 |
| C | 3.217040000 | -0.334462000 | 5.413949000 |
| H | 4.264455000 | -0.477938000 | 5.168140000 |
| C | 2.812310000 | -0.213527000 | 6.727511000 |
| H | 3.520171000 | -0.257332000 | 7.547390000 |
| C | 2.092991000 | -0.574578000 | -1.595183000 |
| H | 1.388108000 | -0.527789000 | -2.417798000 |
| C | 4.352267000 | -0.822390000 | -0.757516000 |
| H | 5.411997000 | -0.970117000 | -0.940303000 |
| C | 3.455104000 | -0.764162000 | -1.832238000 |
| H | 3.811390000 | -0.865688000 | -2.852390000 |

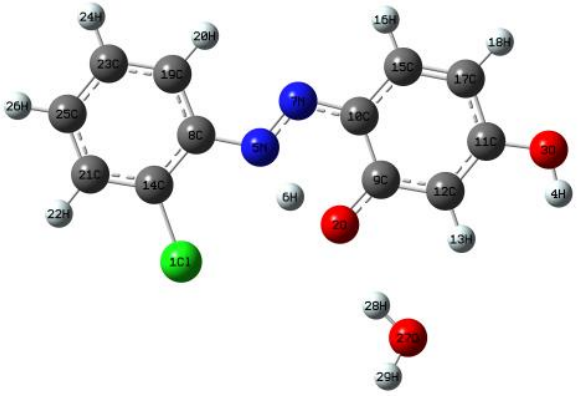
**Figure S21j**. Optimized geometry and coordinates of **3ts (**transition state of **3)**




**C12H9N2O2Cl**

| | | | |
|---|---|---|---|
| Cl | -0.028604000 | 0.001331000 | -0.023459000 |
| C | -0.006593000 | 0.000681000 | 1.729028000 |
| C | 1.224241000 | 0.000657000 | 2.385594000 |
| C | 1.269452000 | 0.000139000 | 3.779397000 |
| C | 0.078251000 | -0.000349000 | 4.515185000 |
| C | -1.148575000 | -0.000323000 | 3.862440000 |
| C | -1.212651000 | 0.000193000 | 2.456504000 |
| N | -2.431514000 | 0.000212000 | 1.762290000 |
| N | -3.532729000 | -0.000101000 | 2.443474000 |
| C | -4.673041000 | -0.000170000 | 1.710322000 |
| C | -5.913533000 | -0.000513000 | 2.407400000 |
| C | -7.103221000 | -0.000617000 | 1.726634000 |
| C | -7.085035000 | -0.000379000 | 0.301429000 |
| C | -5.903037000 | -0.000039000 | -0.421194000 |
| C | -4.659760000 | 0.000084000 | 0.256283000 |
| O | -3.524977000 | 0.000403000 | -0.368956000 |
| O | -8.305776000 | -0.000539000 | -0.297621000 |
| H | -8.206399000 | -0.000190000 | -1.259925000 |
| H | -5.896917000 | 0.000137000 | -1.507553000 |
| H | -2.688549000 | 0.000383000 | 0.567770000 |
| H | -5.884684000 | -0.000693000 | 3.492527000 |
| H | -8.059844000 | -0.000883000 | 2.235783000 |
| H | 2.135964000 | 0.001043000 | 1.798432000 |
| H | 2.229682000 | 0.000119000 | 4.285433000 |
| H | 0.107510000 | -0.000755000 | 5.600398000 |
| H | -2.079014000 | -0.000701000 | 4.417296000 |

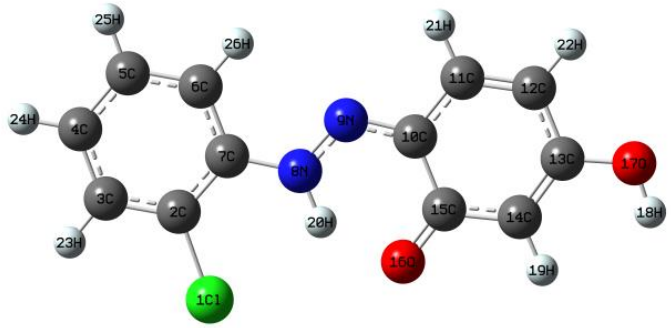
**Figure S21k**. Optimized geometry and coordinates of **3ts_w** (transition state of **3** with water)



**C12H11N2O3Cl**

| | | | |
|---|---|---|---|
| Cl | 0.269452000 | 0.757085000 | -0.184023000 |
| O | 0.283151000 | 0.623617000 | 3.330334000 |
| O | 0.825431000 | 0.288601000 | 8.070331000 |
| H | -0.109989000 | 0.537757000 | 8.074914000 |
| N | 2.220104000 | 0.153462000 | 2.008084000 |
| H | 1.076487000 | 0.444712000 | 2.413788000 |
| N | 2.982862000 | -0.091532000 | 3.022272000 |
| C | 2.770362000 | 0.056618000 | 0.720636000 |
| C | 1.000781000 | 0.388967000 | 4.401333000 |
| C | 2.392269000 | 0.019905000 | 4.241126000 |
| C | 1.284344000 | 0.216273000 | 6.795008000 |
| C | 0.469009000 | 0.480294000 | 5.702466000 |
| H | -0.574764000 | 0.758976000 | 5.820869000 |
| C | 1.953892000 | 0.317620000 | -0.396767000 |
| C | 3.187142000 | -0.239928000 | 5.391230000 |
| H | 4.226022000 | -0.514092000 | 5.237499000 |
| C | 2.652924000 | -0.146632000 | 6.651190000 |
| H | 3.238934000 | -0.340708000 | 7.541925000 |
| C | 4.115860000 | -0.293430000 | 0.501215000 |
| H | 4.739952000 | -0.493374000 | 1.363889000 |
| C | 2.464424000 | 0.231935000 | -1.691977000 |
| H | 1.811280000 | 0.438451000 | -2.532545000 |
| C | 4.623731000 | -0.378658000 | -0.789332000 |
| H | 5.664093000 | -0.650265000 | -0.938878000 |
| C | 3.800061000 | -0.116258000 | -1.890774000 |
| H | 4.192921000 | -0.181790000 | -2.900470000 |
| O | -2.336068000 | 1.268630000 | 4.237021000 |
| H | -1.529934000 | 1.090932000 | 3.716104000 |
| H | -2.939500000 | 1.744446000 | 3.655029000 |

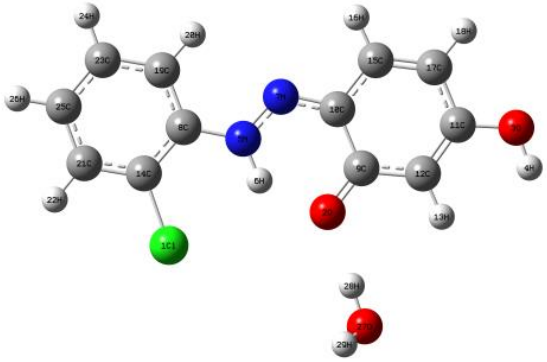
**Figure S21l**. Optimized geometry and coordinates of **3k** (keto form of **3**)




**C12H9N2O2Cl**

| | | | |
|---|---|---|---|
| Cl | 0.060055000 | 0.048861000 | -0.027292000 |
| C | 0.027945000 | -0.001319000 | 1.731960000 |
| C | 1.235563000 | 0.006613000 | 2.427828000 |
| C | 1.231516000 | -0.033602000 | 3.822904000 |
| C | 0.014983000 | -0.081634000 | 4.513785000 |
| C | -1.190674000 | -0.089260000 | 3.819609000 |
| C | -1.201576000 | -0.048923000 | 2.414871000 |
| N | -2.399615000 | -0.055108000 | 1.687883000 |
| N | -3.552122000 | -0.103398000 | 2.298456000 |
| C | -4.670895000 | -0.106304000 | 1.572504000 |
| C | -5.901041000 | -0.160272000 | 2.313798000 |
| C | -7.106458000 | -0.166812000 | 1.679935000 |
| C | -7.144352000 | -0.119016000 | 0.244369000 |
| C | -5.998388000 | -0.067252000 | -0.520490000 |
| C | -4.706647000 | -0.057681000 | 0.094182000 |
| O | -3.628287000 | -0.010010000 | -0.575296000 |
| O | -8.389097000 | -0.129212000 | -0.290949000 |
| H | -8.347824000 | -0.095443000 | -1.259037000 |
| H | -6.046212000 | -0.033046000 | -1.605161000 |
| H | -2.427523000 | -0.021264000 | 0.649120000 |
| H | -5.834932000 | -0.195279000 | 3.396573000 |
| H | -8.042429000 | -0.207216000 | 2.225210000 |
| H | 2.167996000 | 0.044055000 | 1.875582000 |
| H | 2.172776000 | -0.027256000 | 4.362385000 |
| H | 0.004725000 | -0.113024000 | 5.598462000 |
| H | -2.136546000 | -0.126235000 | 4.345818000 |

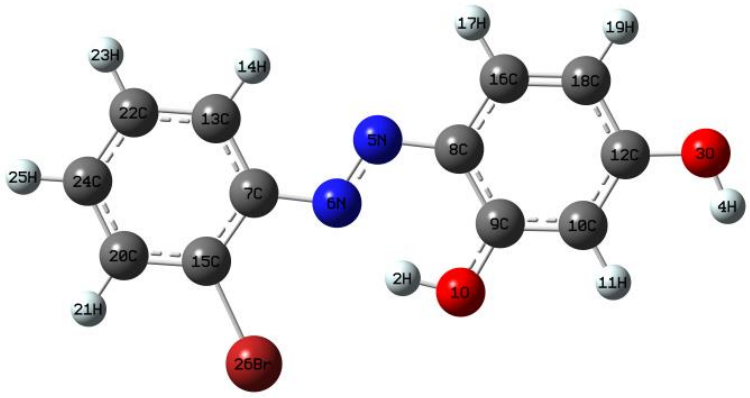
**Figure S21m**. Optimized geometry and coordinates of **3k_w** (keto form of **3** with water)



**C12H11N2O3Cl**

| | | | |
|---|---|---|---|
| Cl | 0.252150000 | 0.727990000 | -0.226514000 |
| O | 0.141068000 | 0.617491000 | 3.512989000 |
| O | 0.979213000 | 0.232071000 | 8.195757000 |
| H | 0.041556000 | 0.464295000 | 8.281186000 |
| N | 2.180380000 | 0.157750000 | 2.000677000 |
| H | 1.183822000 | 0.405889000 | 2.149117000 |
| N | 2.894950000 | -0.063951000 | 3.066042000 |
| C | 2.746462000 | 0.060448000 | 0.721094000 |
| C | 0.914012000 | 0.386032000 | 4.503959000 |
| C | 2.327060000 | 0.035872000 | 4.270742000 |
| C | 1.349318000 | 0.186534000 | 6.895384000 |
| C | 0.474727000 | 0.446284000 | 5.857887000 |
| H | -0.562390000 | 0.703129000 | 6.051473000 |
| C | 1.949797000 | 0.304376000 | -0.412677000 |
| C | 3.188549000 | -0.224103000 | 5.390303000 |
| H | 4.222288000 | -0.478651000 | 5.180034000 |
| C | 2.724492000 | -0.153875000 | 6.669502000 |
| H | 3.362116000 | -0.347355000 | 7.524361000 |
| C | 4.098025000 | -0.276728000 | 0.537776000 |
| H | 4.710434000 | -0.464774000 | 1.411012000 |
| C | 2.484943000 | 0.215518000 | -1.696507000 |
| H | 1.848666000 | 0.408591000 | -2.552912000 |
| C | 4.631382000 | -0.365351000 | -0.743945000 |
| H | 5.677083000 | -0.627001000 | -0.868479000 |
| C | 3.829135000 | -0.120037000 | -1.864630000 |
| H | 4.243326000 | -0.188722000 | -2.864995000 |
| O | -2.549526000 | 1.255100000 | 3.746388000 |
| H | -1.589547000 | 1.052572000 | 3.669047000 |
| H | -2.692928000 | 2.042234000 | 3.205369000 |

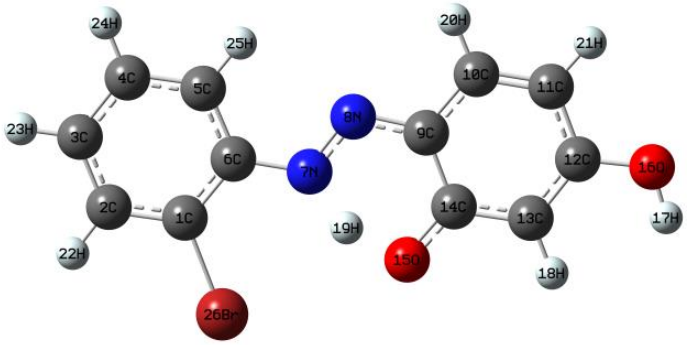
**Figure S21n**. Optimized geometry and coordinates of **4e** (enol form of **4**)




**C12H9N2O2Br**

| | | | |
|---|---|---|---|
| O | -0.003054000 | -0.003288000 | -0.006540000 |
| H | -0.009619000 | -0.001801000 | 0.996604000 |
| O | 3.276386000 | -0.002959000 | -3.471918000 |
| H | 2.492378000 | -0.005901000 | -4.041356000 |
| N | 2.164408000 | 0.003566000 | 1.954902000 |
| N | 0.959124000 | 0.002302000 | 2.372195000 |
| C | 0.785070000 | 0.004723000 | 3.771082000 |
| C | 2.342170000 | 0.001710000 | 0.583228000 |
| C | 1.286127000 | -0.001631000 | -0.382541000 |
| C | 1.591533000 | -0.003232000 | -1.746194000 |
| H | 0.779169000 | -0.005723000 | -2.466562000 |
| C | 2.925626000 | -0.001589000 | -2.159591000 |
| C | 1.855516000 | 0.008331000 | 4.687308000 |
| H | 2.865784000 | 0.009280000 | 4.295512000 |
| C | -0.525519000 | 0.003659000 | 4.280376000 |
| C | 3.679863000 | 0.003306000 | 0.122796000 |
| H | 4.468954000 | 0.005820000 | 0.867891000 |
| C | 3.982145000 | 0.001711000 | -1.223355000 |
| H | 5.007160000 | 0.002897000 | -1.576138000 |
| C | -0.768010000 | 0.005783000 | 5.653522000 |
| H | -1.787824000 | 0.004762000 | 6.021341000 |
| C | 1.620797000 | 0.010603000 | 6.056434000 |
| H | 2.458421000 | 0.013336000 | 6.746806000 |
| C | 0.306951000 | 0.009260000 | 6.543137000 |
| H | 0.117337000 | 0.010971000 | 7.611884000 |
| Br | -2.017591000 | -0.001265000 | 3.096099000 |

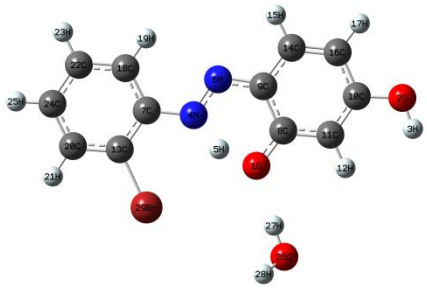
**Figure S21o**. Optimized geometry and coordinates of **4ts** (transition state of **4**)




**C12H9N2O2Br**

| | | | |
|---|---|---|---|
| C | -0.001937000 | 0.000118000 | 0.006347000 |
| C | 0.000986000 | 0.000054000 | 1.400523000 |
| C | 1.212900000 | -0.000083000 | 2.091302000 |
| C | 2.420716000 | -0.000156000 | 1.382525000 |
| C | 2.415397000 | -0.000093000 | -0.006563000 |
| C | 1.201612000 | 0.000045000 | -0.720748000 |
| N | 1.163130000 | 0.000111000 | -2.124114000 |
| N | 2.280998000 | 0.000033000 | -2.773988000 |
| C | 2.174291000 | 0.000101000 | -4.127793000 |
| C | 3.376054000 | 0.000019000 | -4.888812000 |
| C | 3.339194000 | 0.000077000 | -6.259973000 |
| C | 2.076821000 | 0.000221000 | -6.919877000 |
| C | 0.878217000 | 0.000309000 | -6.217080000 |
| C | 0.892177000 | 0.000250000 | -4.806619000 |
| O | -0.201705000 | 0.000325000 | -4.093185000 |
| O | 2.124219000 | 0.000268000 | -8.275234000 |
| H | 1.231247000 | 0.000351000 | -8.652361000 |
| H | -0.077147000 | 0.000421000 | -6.732898000 |
| H | 0.227362000 | 0.000235000 | -2.928175000 |
| H | 4.320156000 | -0.000093000 | -4.353280000 |
| H | 4.244138000 | 0.000014000 | -6.856683000 |
| H | -0.940004000 | 0.000113000 | 1.938569000 |
| H | 1.211672000 | -0.000131000 | 3.176548000 |
| H | 3.366553000 | -0.000264000 | 1.914887000 |
| H | 3.342863000 | -0.000150000 | -0.566221000 |
| Br | -1.675598000 | 0.000306000 | -0.898464000 |

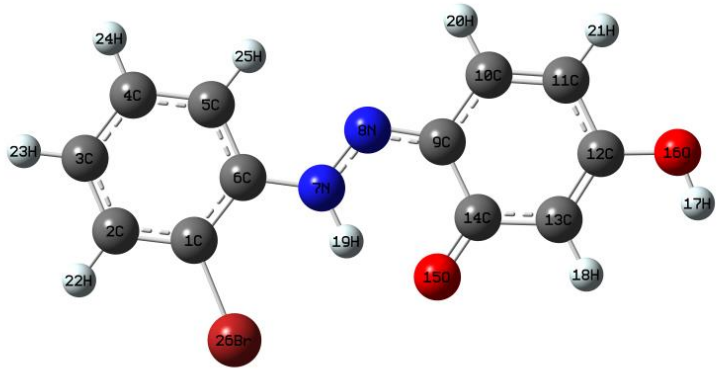
**Figure S21p**. Optimized geometry and coordinates of **4ts_w** (transition state of **4** with water)



**C12H11N2O3Br**

| | | | |
|---|---|---|---|
| O | -0.000685000 | 0.007277000 | -0.016800000 |
| O | 0.015951000 | 0.009847000 | 4.773798000 |
| H | 0.979424000 | 0.019561000 | 4.667313000 |
| N | -2.154010000 | -0.019302000 | -1.062111000 |
| H | -0.919657000 | -0.004987000 | -0.808683000 |
| N | -2.810438000 | -0.024799000 | 0.047424000 |
| C | -2.872537000 | -0.027294000 | -2.268609000 |
| C | -0.608171000 | 0.000758000 | 1.152209000 |
| C | -2.052688000 | -0.015283000 | 1.180231000 |
| C | -0.607183000 | 0.002620000 | 3.570471000 |
| C | 0.095746000 | 0.009969000 | 2.368108000 |
| H | 1.181199000 | 0.021574000 | 2.351616000 |
| C | -2.170535000 | -0.021671000 | -3.487559000 |
| C | -2.729275000 | -0.021600000 | 2.429001000 |
| H | -3.814485000 | -0.033541000 | 2.421787000 |
| C | -2.027883000 | -0.012867000 | 3.609700000 |
| H | -2.528129000 | -0.017773000 | 4.571256000 |
| C | -4.279880000 | -0.040508000 | -2.304874000 |
| H | -4.820945000 | -0.044481000 | -1.366413000 |
| C | -2.847155000 | -0.029730000 | -4.706088000 |
| H | -2.284528000 | -0.025123000 | -5.632632000 |
| C | -4.956362000 | -0.048063000 | -3.518296000 |
| H | -6.041640000 | -0.058155000 | -3.526960000 |
| C | -4.242204000 | -0.042931000 | -4.722928000 |
| H | -4.766663000 | -0.048730000 | -5.672985000 |
| O | 2.799859000 | 0.037595000 | -0.419289000 |
| H | 1.829030000 | 0.002130000 | -0.299910000 |
| H | 2.990633000 | -0.556880000 | -1.156390000 |
| Br | -0.266598000 | -0.006573000 | -3.503347000 |

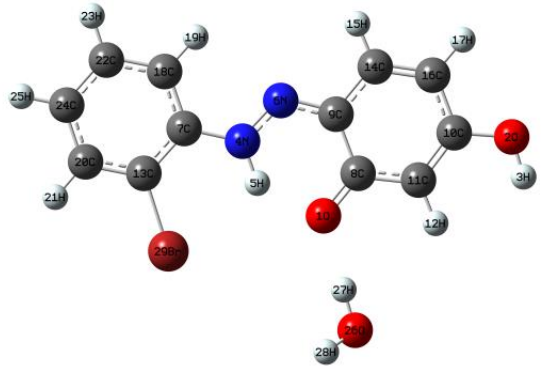
**Figure S21q**. Optimized geometry and coordinates of **4k** (keto form of **4**)




**C12H9N2O2Br**

| | | | |
|---|---|---|---|
| C | -0.007018000 | -0.002470000 | 0.007394000 |
| C | 0.006378000 | -0.001338000 | 1.401151000 |
| C | 1.223376000 | 0.001789000 | 2.083333000 |
| C | 2.424262000 | 0.003742000 | 1.363986000 |
| C | 2.410582000 | 0.002319000 | -0.025954000 |
| C | 1.190997000 | -0.000986000 | -0.725743000 |
| N | 1.157378000 | -0.002293000 | -2.126871000 |
| N | 2.263646000 | -0.000573000 | -2.818995000 |
| C | 2.200027000 | -0.001902000 | -4.150326000 |
| C | 3.462084000 | 0.000029000 | -4.838132000 |
| C | 3.522737000 | -0.001124000 | -6.198315000 |
| C | 2.301265000 | -0.004271000 | -6.955558000 |
| C | 1.061490000 | -0.006179000 | -6.352317000 |
| C | 0.940553000 | -0.005146000 | -4.926512000 |
| O | -0.180942000 | -0.006583000 | -4.331522000 |
| O | 2.469122000 | -0.005178000 | -8.300174000 |
| H | 1.612864000 | -0.007455000 | -8.754892000 |
| H | 0.148209000 | -0.008504000 | -6.940675000 |
| H | 0.269972000 | -0.004725000 | -2.667511000 |
| H | 4.364050000 | 0.002407000 | -4.234509000 |
| H | 4.466367000 | 0.000292000 | -6.731868000 |
| H | -0.931282000 | -0.002886000 | 1.944996000 |
| H | 1.230863000 | 0.002771000 | 3.168377000 |
| H | 3.374888000 | 0.006230000 | 1.887580000 |
| H | 3.333699000 | 0.003730000 | -0.592279000 |
| Br | -1.681940000 | -0.007510000 | -0.897559000 |

**Figure S21r**. Optimized geometry and coordinates of **4k_w** (keto form of **4** with water)



**C12H11N2O3Br**

| | | | |
|---|---|---|---|
| O | -0.001153000 | -0.022512000 | 0.017289000 |
| O | -0.015457000 | -0.001168000 | 4.790867000 |
| H | 0.949717000 | -0.011246000 | 4.696447000 |
| N | -2.336119000 | -0.003904000 | -1.077207000 |
| H | -1.299513000 | -0.015985000 | -1.125441000 |
| N | -2.871100000 | 0.007929000 | 0.109029000 |
| C | -3.133928000 | 0.001567000 | -2.230115000 |
| C | -0.606946000 | -0.011654000 | 1.142043000 |
| C | -2.080414000 | 0.004177000 | 1.185376000 |
| C | -0.621545000 | -0.000257000 | 3.581261000 |
| C | 0.079340000 | -0.012583000 | 2.390686000 |
| H | 1.165076000 | -0.024136000 | 2.380029000 |
| C | -2.527219000 | -0.011163000 | -3.497981000 |
| C | -2.753929000 | 0.016917000 | 2.453828000 |
| H | -3.839001000 | 0.028160000 | 2.446139000 |
| C | -2.055590000 | 0.014857000 | 3.623724000 |
| H | -2.549689000 | 0.024341000 | 4.588425000 |
| C | -4.536611000 | 0.019922000 | -2.150435000 |
| H | -5.001629000 | 0.030089000 | -1.172329000 |
| C | -3.298018000 | -0.006429000 | -4.658489000 |
| H | -2.808677000 | -0.016518000 | -5.625636000 |
| C | -5.305196000 | 0.024870000 | -3.308982000 |
| H | -6.387535000 | 0.039008000 | -3.230602000 |
| C | -4.690187000 | 0.011631000 | -4.566184000 |
| H | -5.288031000 | 0.015542000 | -5.471649000 |
| O | 2.751611000 | -0.042556000 | -0.305688000 |
| H | 1.773571000 | -0.052010000 | -0.196068000 |
| H | 2.922310000 | -0.477166000 | -1.151162000 |
| Br | -0.628839000 | -0.037881000 | -3.654332000 |

Water molecule

H2O

| | | | |
|---|---|---|---|
| O | 0.000000000 | 0.000000000 | 0.000000000 |
| H | 0.000000000 | 0.000000000 | 0.966850000 |
| H | 0.934181000 | 0.000000000 | -0.249227000 |

17: Safety and hazards

The chemicals used in this research have their own safety requirements (as prescribed in their MSDS) and handling procedure as prescribed in MSDS should be followed. Local rules of handling X-ray diffractometer and UV-VIS instruments should be followed.