Supporting Information

Synthesis and Characterization of *Cis* and *Trans* Cobalt (II) nalidixate Complexes Having 1-(4-chlorophenyl)-3-(pyridin-4-ylmethyl)urea Ligand

Rinki Brahma, Abhay Pratap Singh, Jubaraj Bikash Baruah*

Abbreviation used: *cis*-$[Co(L)_2(NALD)_2]\cdot 0.5DMF\cdot H_2O$ = ***CisCoNalurea***

trans-$[Co(L)_2(NALD)_2]\cdot 2DMF\cdot 2H_2O$ = ***TransCoNalurea***

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General:

Certain details on the crystal structure determination:

For CCDC no. 2265811 (***CisCoNalurea***), we used a solvent mask in Olex 2 (version 1.5) to reduce the effect of residual electron densities of the highly disordered solvent molecules of 0.5 DMF and one H_2O. 260 electrons were found in a volume of 1212 A^3 in one void per unit cell.

CCDC no. 2265812 (***TransCoNalurea***) has one DMF molecule with disordered O5, C26, and C27 atoms. Attempts were made to use SPLIT SAME for these disordered atoms, but this resulted in a wR_2 value of 19.10% and an increase of shift from 0.000 to 6.476. So, we have not corrected the disordered DMF molecule. This disordered DMF molecule affected the wR_2 value by 21.69%. We have also used a solvent mask in Olex 2 (version 1.5) to reduce the effect of residual electron densities of the highly disordered solvent molecules of one DMF and two H_2O. 444 electrons were found in a volume of 1586 A^3 in one void per unit cell.

Magnetic moment measurement of complexes *CisCoNalurea* and *TransCoNalurea* (in solid state):

The magnetic susceptibility (χ_M) of the bulk solid samples of both ***CisCoNalurea*** and ***TransCoNalurea*** were measured (at a temperature of 18°C ≈ 291.15K) in Sherwood Scientific magnetic susceptibility balance. Diamagnetic correction factors (χ_D) were calculated for both these complexes.[1] The respective magnetic moments (μ_{eff}) were finally calculated by using the formula,

$$\mu_{eff}=\sqrt{\frac{3k_B}{N_A\beta^2}(\chi_M-\chi_D)T}$$

Magnetic moment of *CisCoNalurea*, and *TransCoNalurea* in solution (Evans method):

The magnetic moments of both ***CisCoNalurea*** and ***TransCoNalurea*** [in CD_3OD-$(CD_3)_2CO$ (1:3 v/v) binary solvent] were determined by Evans method. A solution of ***CisCoNalurea*** (0.0010 g, 2.88 mM) [or, ***TransCoNalurea*** (0.0013 g, 2.88 mM)] in a 0.4 mL mixture of MeOH-d_4/Acetone-d_6 (1:3 v/v) and tert-butyl alcohol [2% in MeOH-d_4/Acetone-d_6 (1:3 v/v) mixture] was placed in an NMR tube. To the same NMR tube, a capillary containing 2% tert-butyl alcohol in MeOH-d_4/Acetone-d_6 (1:3 v/v) mixture was inserted. The NMR spectra were recorded in Bruker ASCEND 600 Nuclear Magnetic Resonance Spectrometer at 600 MHz at 25°C. A chemical shift difference of 12 Hz (for ***CisCoNalurea***) and 6 Hz (for ***TransCoNalurea***) for tert-butyl alcohol present in the inner and outer tubes were observed respectively. The magnetic moment of the respective samples was calculated by equation S2:

$$\chi_M = \frac{3 \times \Delta\nu}{1000 \times \nu \times c} \quad \text{……..(equation S1)}$$

where, $\Delta\nu$ = paramagnetic shift of tert-butyl alcohol in Hz

c = molar concentration of ***CisCoNalurea*** or ***TransCoNalurea***

ν = frequency of NMR instrument in Hz

$$\mu_{eff} = 798 \times \sqrt{(\chi_M \times T)} \quad \text{……..(equation S2)}$$

where, T = 25°C = 298.15 K

Table S1. Crystallographic and refinement parameters of the ligand **L**, ***CisCoNalurea***, and ***TransCoNalurea***.

Parameters	**L**	***CisCoNalurea***	***TransCoNalurea***
Formula	$C_{13}H_{12}ClN_3O$	$C_{50}H_{46}Cl_2CoN_{10}O_8$	$C_{56}H_{60}Cl_2CoN_{12}O_{10}$
CCDC	2265810	2265811	2265812
Mol. wt.	261.71	1044.80	1190.99
Crystal system, Space group	Monoclinic, *P*n	Monoclinic, *C*2/c	Monoclinic, *C*2/c
a (Å)	16.854(8)	13.3053(15)	19.691(4)
b (Å)	4.578(2)	20.015(2)	19.736(4)
c (Å)	18.262(9)	21.155(2)	18.462(4)
α (°)	90	90	90
β (°)	112.507(13)	90.540(3)	107.852(6)
γ (°)	90	90	90
V (Å³)	1301.8(11)	5633.4(11)	6829(3)
Density, g cm⁻³	1.335	1.232	1.158
Abs. coeff., mm⁻¹	0.285	0.456	0.387
F (000)	544	2164	2484
Total no. of reflections	4565	4963	6011
Reflections, I > 2σ(I)	3957	3622	4589
Max θ/ °	24.998	25.000	24.999
Ranges (h, k, l)	$-20 \le h \le 20$	$-15 \le h \le 15$	$-23 \le h \le 23$
	$-5 \le k \le 5$	$-23 \le k \le 23$	$-23 \le k \le 23$
	$-21 \le l \le 21$	$-25 \le l \le 25$	$-21 \le l \le 21$
Completed to 2θ (%)	99.1	99.9	99.7
Data/restraints/parameters	4565/2/334	4963/0/323	6011/0/371
GooF (F^2)	1.051	1.131	1.123
R indices [I > 2σ(I)]	0.0339	0.0561	0.0636
wR_2 [I > 2σ(I)]	0.0733	0.1499	0.1778
R indices (all data)	0.0433	0.0825	0.0841
wR_2 (all data)	0.0793	0.1897	0.2169

Table S2. Metal-ligand bond lengths of ***CisCoNalurea***, and ***TransCoNalurea*** compared with the bond lengths of the optimized structure.

Complex	Bond-length (Å)		
	Co1-N3	Co1-O2	Co1-O3
CisCoNalurea	2.141	2.041	2.119
	(1.944)	(2.2494)	(1.936)
TransCoNalurea	2.217	2.057	2.047
	(1.968)	(2.175)	(1.947)

[@] Bond lengths given inside the brackets are from the respective theoretically optimized structure given in Fig. S2 (calculation was done Gaussian 09W at B3LYP/6-31G level.

Table S3. Hydrogen bond parameters of **L**, ***CisCoNalurea***, and ***TransCoNalurea***.

Compound	D-H···A	d_{D-H} (Å)	$d_{H\cdots A}$ (Å)	$d_{D\cdots A}$ (Å)	∠D-H···A (º)
L	N(1) -H(1) ···O(1) [x, -1+y, z]	0.86	2.08	2.864(3)	152
	N(2) -H(2) ···O(1) [x, -1+y, z]	0.86	2.10	2.874(4)	149
	N(4) -H(4) ···O(2) [x, 1+y, z]	0.83(4)	2.13(4)	2.883(4)	152(3)
	N(5) -H(5A) ···O(2) [x, 1+y, z]	0.86 (4)	2.05(4)	2.848(4)	153(3)
CisCoNalurea	N(1) -H(1) ···O(3) [1/2+x, 1/2+y,z]	0.86	2.16	3.001(4)	164
	N(2) -H(2) ···O(4) [1/2+x, 1/2+y,z]	0.86	2.00	2.807(5)	156
TransCoNalurea	N(1) -H(1) ···O(4) [1-x, y,1/2-z]	0.86	2.12	2.882(5)	147
	N(2) -H(2) ···O(3) [1-x, y,1/2-z]	0.86	2.12	2.945(4)	160

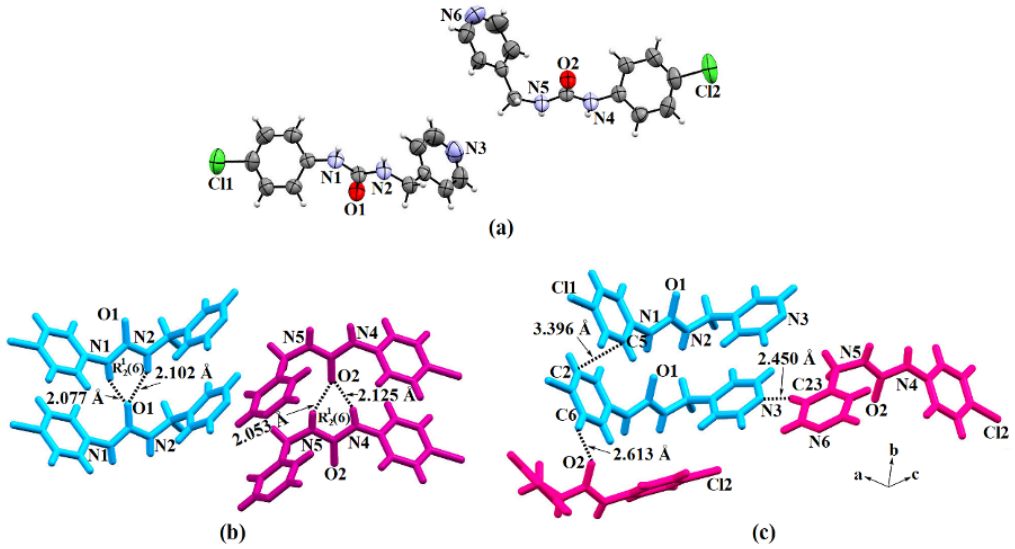


Figure S1. (a) Crystal structure of **L** determined by X-ray single crystal diffraction (Thermal ellipsoids are drawn at 50% probability); (b) Hydrogen bonds in symmetry non-equivalent molecules; and (c) π-interactions, C-H···O and C-H···N interactions in the crystal lattice.

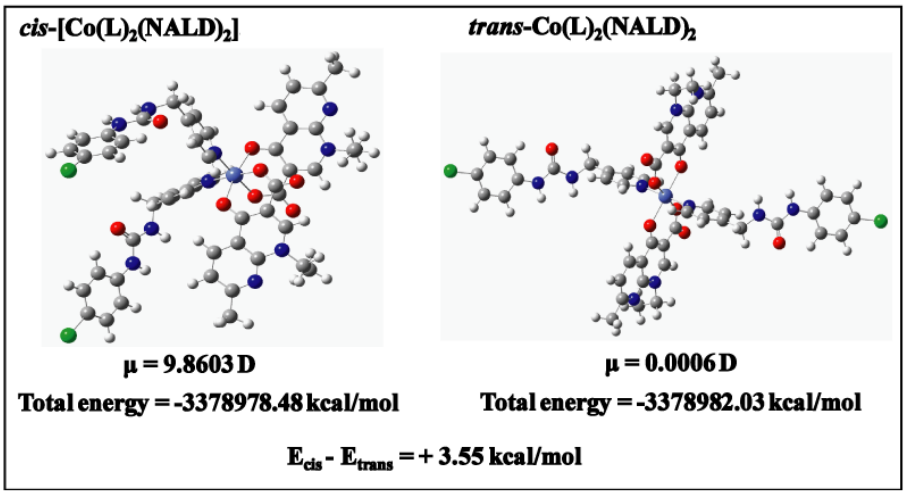


Figure S2. Optimized structures of ***CisCoNalurea***, and ***TransCoNalurea*** with their calculated dipole moments. (DFT calculation was done with B3LYP functional using 6-31G as the basis set).

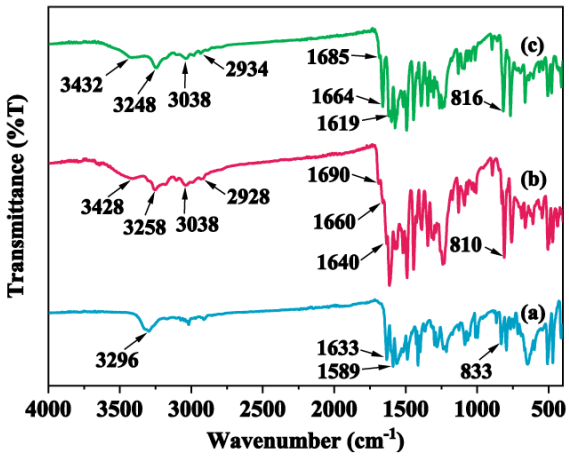


Figure S3. FTIR spectra of the solid samples of (a) **L**, (b) ***CisCoNalurea***, and (c) ***TransCoNalurea***.

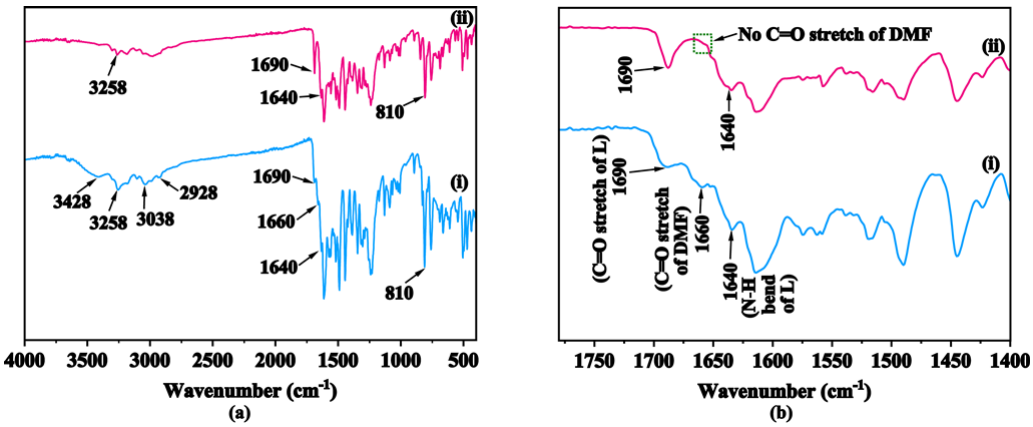


Figure S4. FTIR spectra of a solid sample of ***CisCoNalurea*** (a) (i) as synthesized, (ii) after heating at 180ºC for seven days, (b) expansion in the region 1780-1400 cm^{-1}.

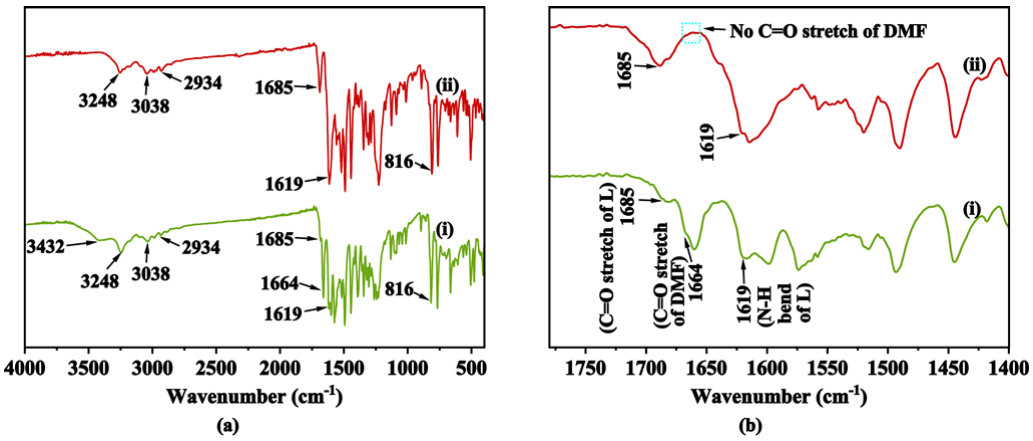


Figure S5. FTIR spectra of a solid sample of ***TransCoNalurea*** (a) (i) as synthesized, (ii) after heating in a laboratory oven at 110ºC for 14 days, (b) expansion in the region 1780-1400 cm^{-1}.

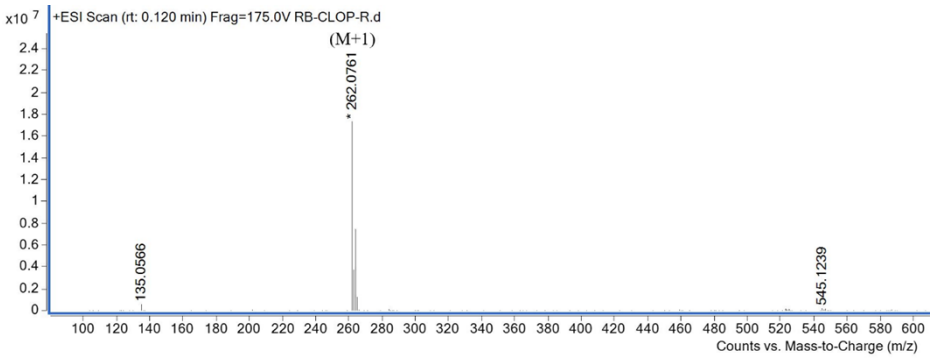


Figure S6. ESI-Mass spectrum of **L**.

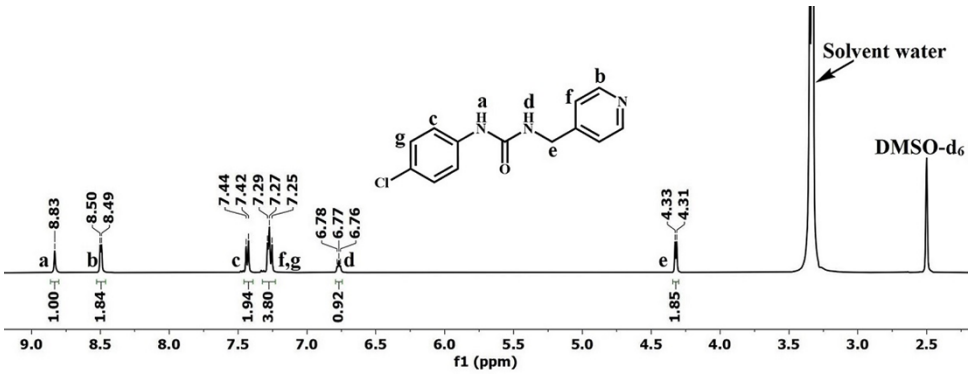


Figure S7. ^{1}H-NMR (DMSO-d_6, 500 MHz) spectrum of **L**.

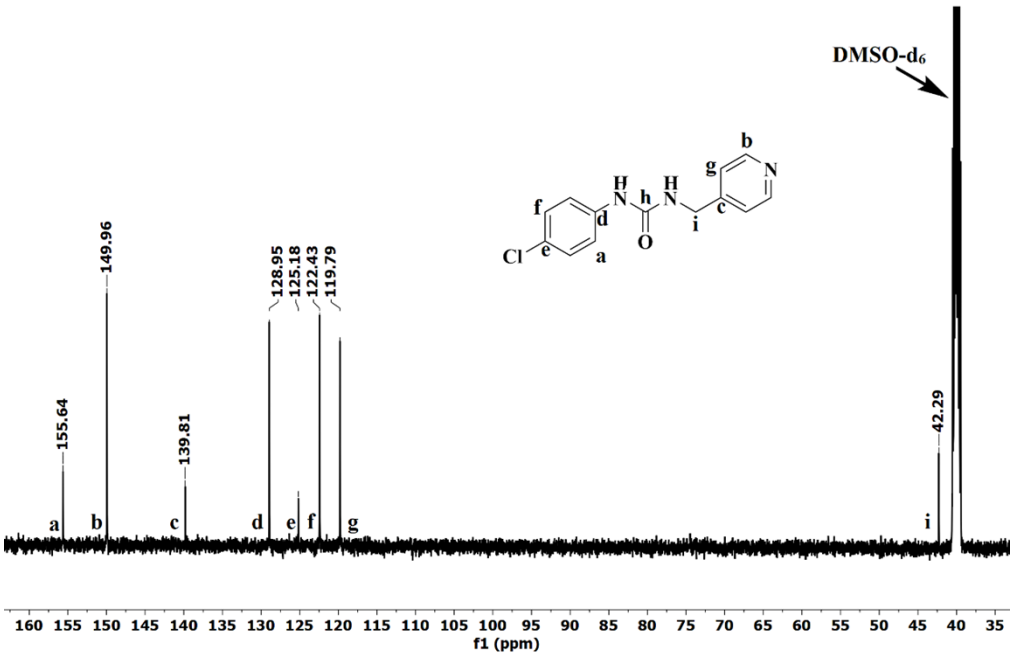


Figure S8. ^{13}C-NMR (DMSO-d$_6$, 125 MHz) spectrum of **L**.

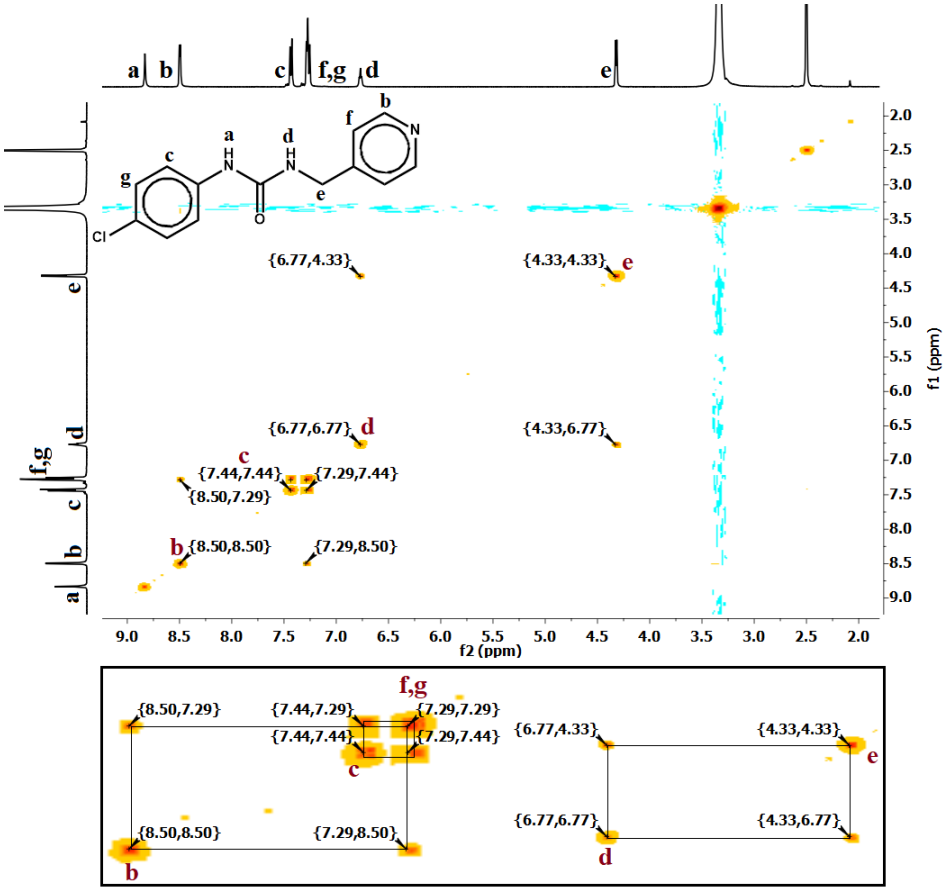


Figure S9. ^{1}H-HOMOCOSY (DMSO-d$_6$, 500 MHz) spectrum of **L** (the coupling correlations are explained at the bottom).

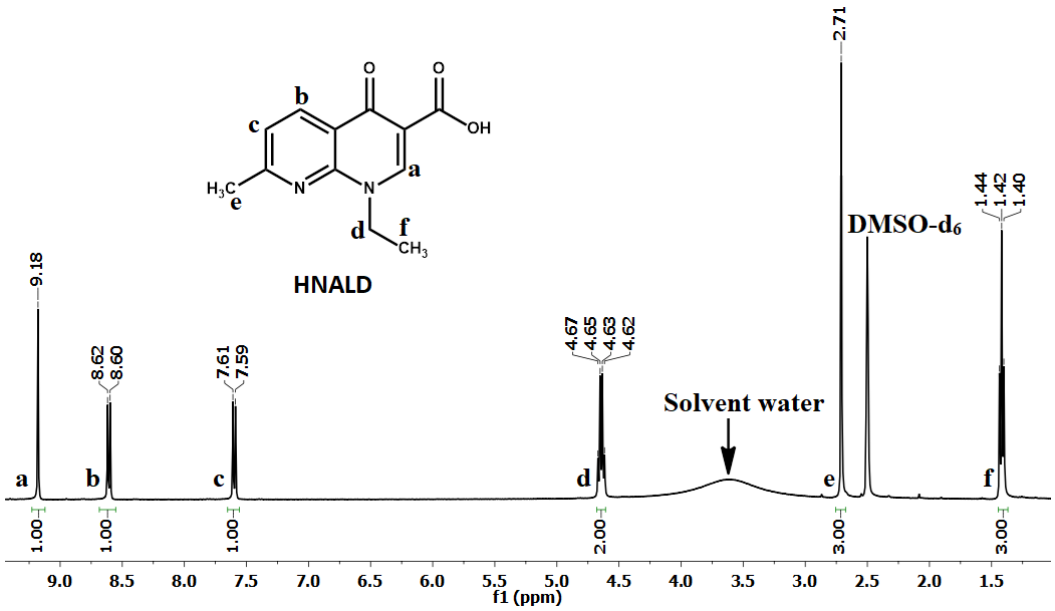


Figure S10. ^{1}H-NMR (DMSO-d_6, 400 MHz) spectrum of **HNALD**.

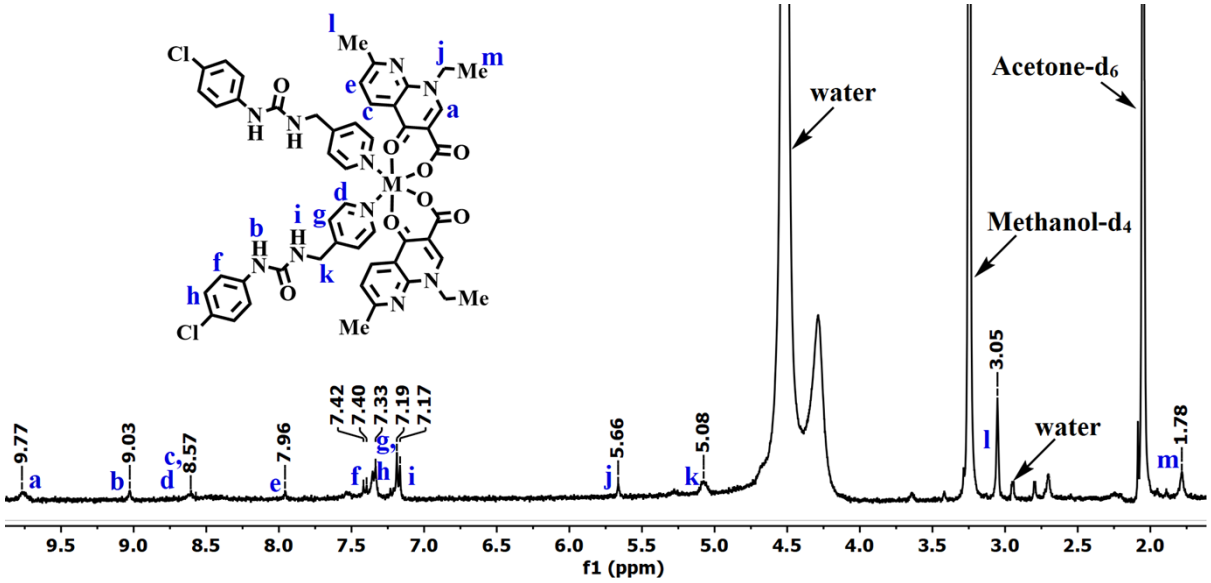


Figure S11. ^{1}H-NMR {Methanol-d_4/acetone-d_6 (1:3 v/v), 400MHz} spectrum of ***CisCoNalurea***.

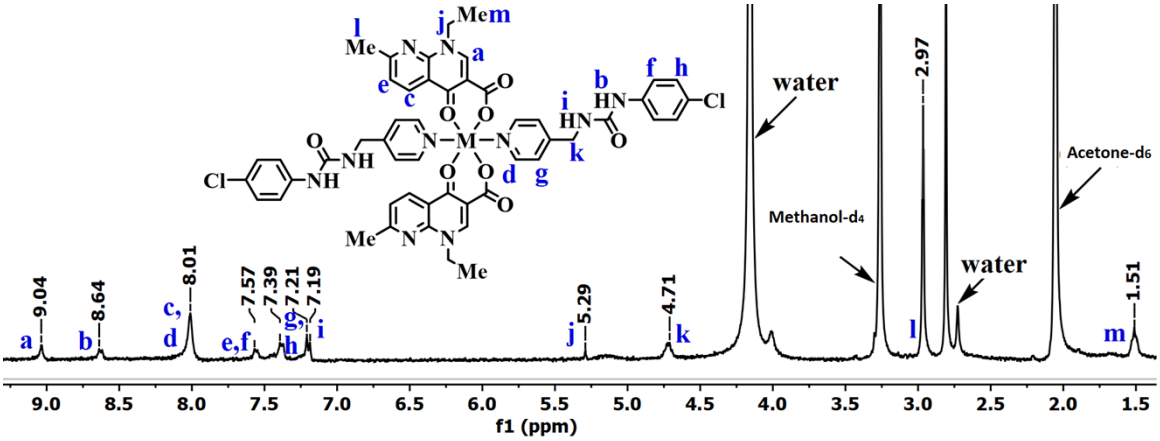


Figure S12. ^{1}H-NMR {Methanol-d_4/acetone-d_6 (1:3 v/v), 400MHz} spectrum of ***TransCoNalurea***.

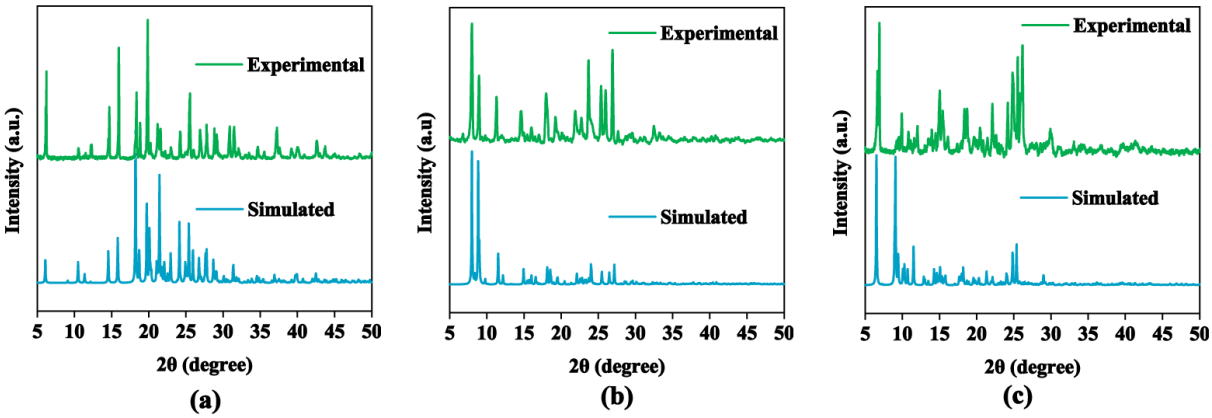


Figure S13. Powder X-ray diffraction pattern of (a) **L**, (b) ***CisCoNalurea***, and (c) ***TransCoNalurea***.

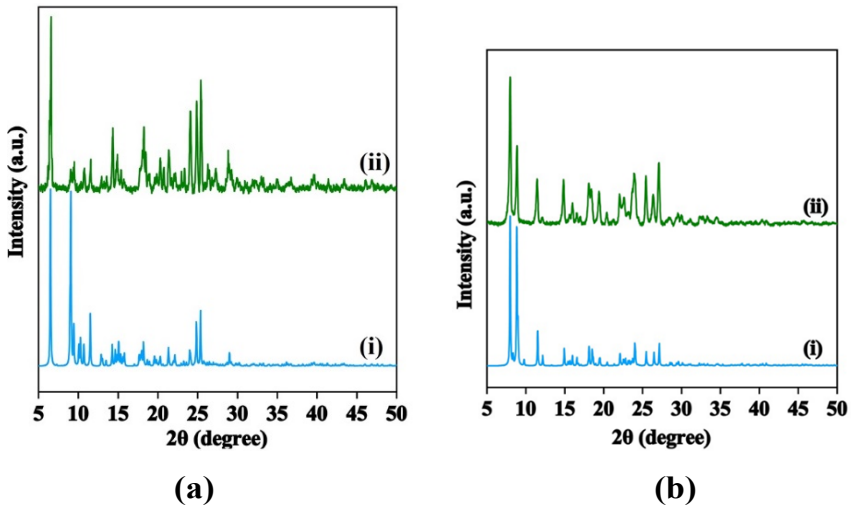


Figure S14. Powder X-ray diffraction patterns of the solid samples obtained from the heating reaction of **L**, **HNALD**, and $Co(NO_3)_2.6H_2O$ at 80ºC for (a) one hour giving

TransCoNalurea, and (b) two hours giving ***CisCoNalurea*** {(i) simulated and (ii) experimental patterns}.

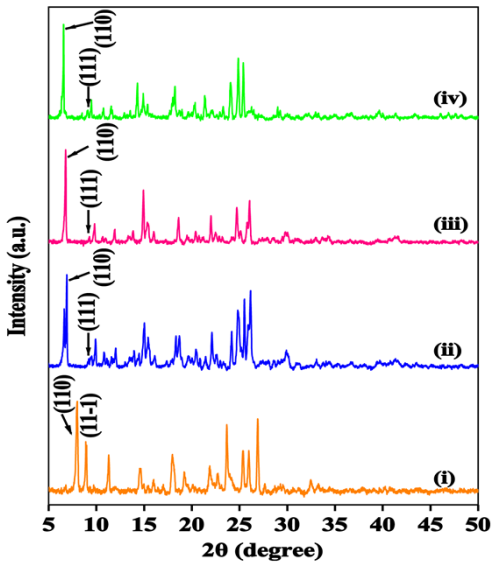


Figure S15. Comparison of the powder X-ray diffraction patterns of (i) ***CisCoNalurea***; (ii) ***TransCoNalurea***; (iii) and (iv) are the powder X-ray patterns of the products formed by using TBACl and TBABr salts for *cis*-to-*trans*-isomer conversion respectively.

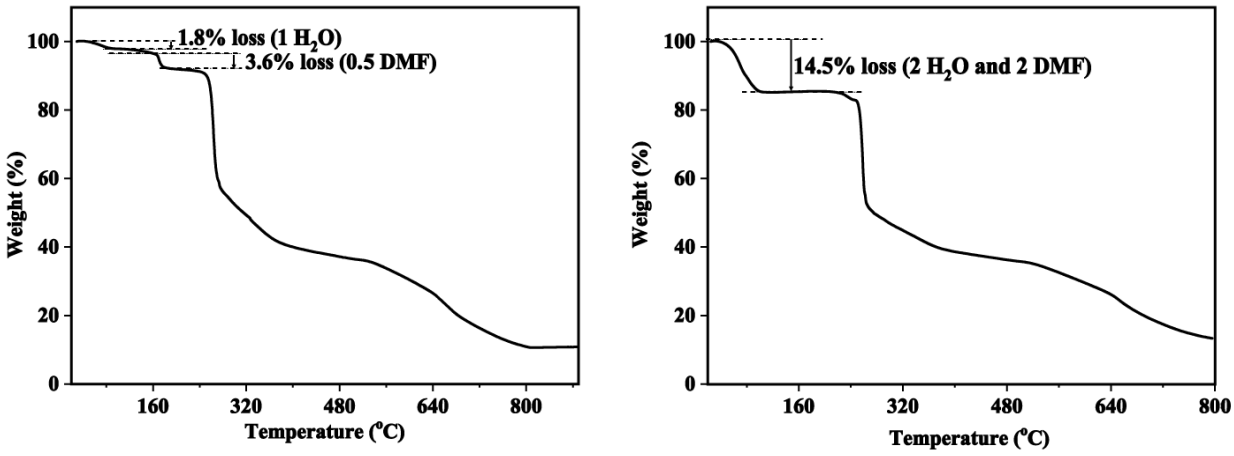


Figure S16. The plot of weight vs temperature observed from thermogravimetry of (a) ***CisCoNalurea***, and (b) ***TransCoNalurea***.

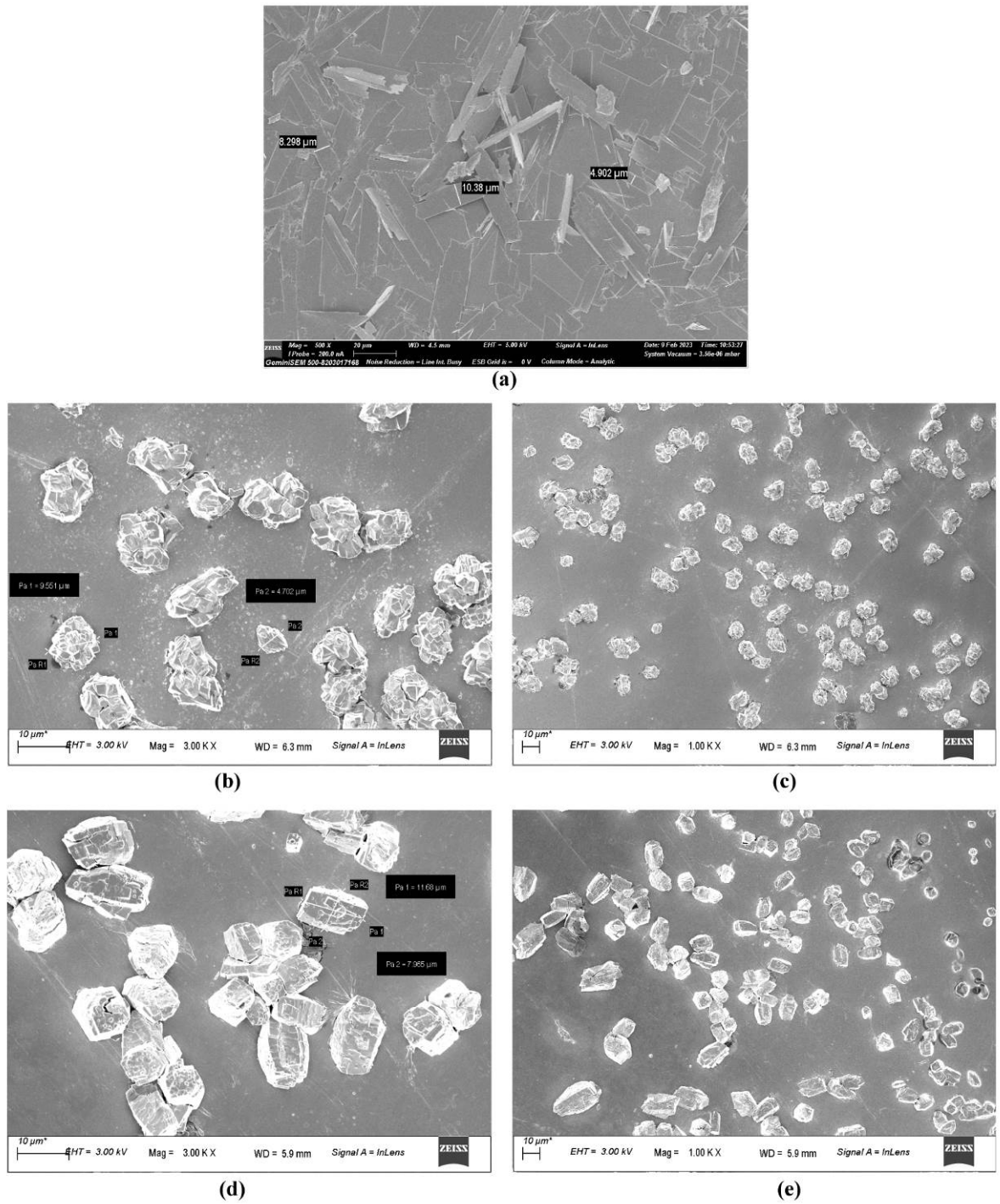


Figure S17. FESEM images of (a) **L**; (b) and (c) ***CisCoNalurea*** (at two magnifications); (d) and (e) ***TransCoNalurea*** (at two magnifications).

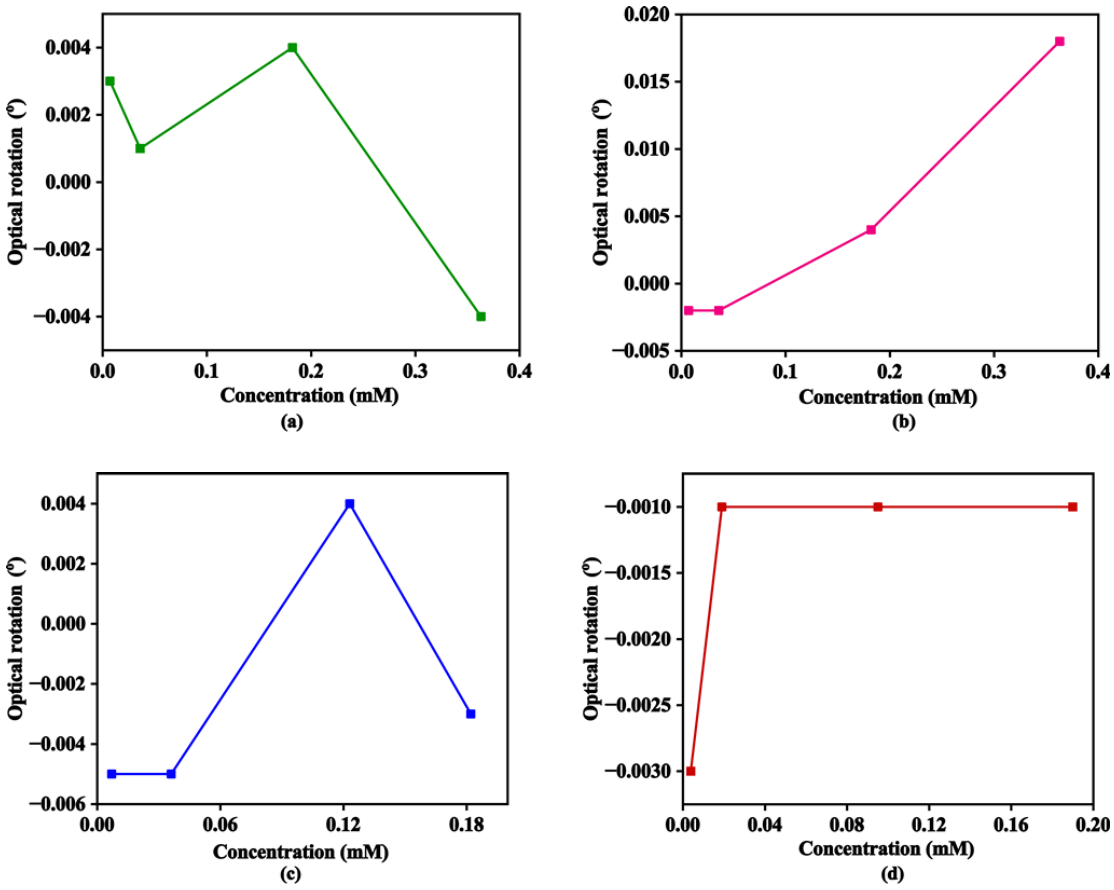
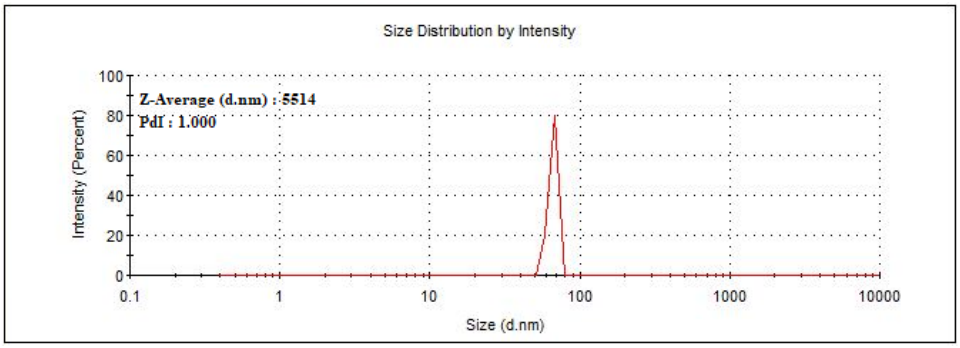
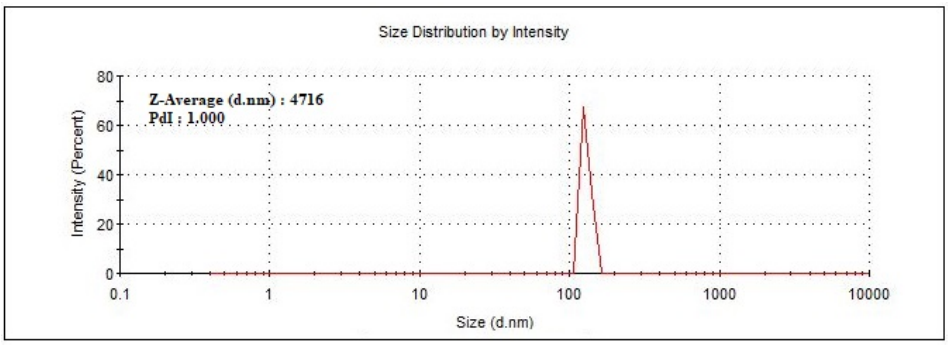


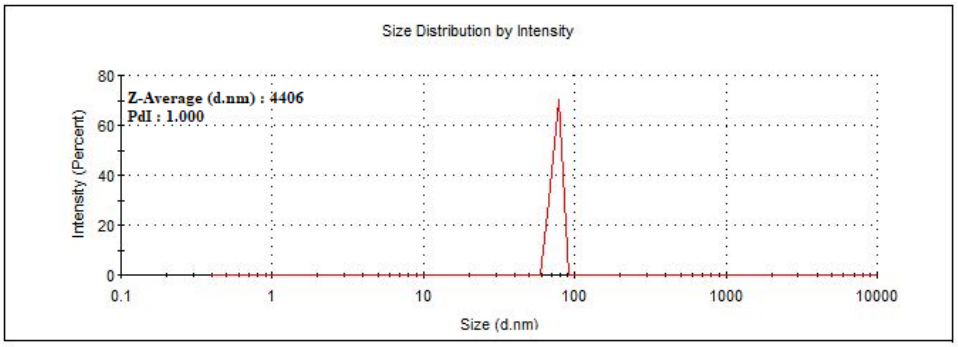
Figure S18. Optical rotation versus concentration plot of ***CisCoNalurea*** in binary solvents (a) THF-DMF (2:2 v/v), (b) DCM-acetone (1:3 v/v), (c) methanol-acetone (1:3 v/v), and (d) DMF.



(a)


Size Distribution by Intensity
Z-Average (d.nm) : 4716
PdI : 1.000
Intensity (Percent)
Size (d.nm)

(b)


Size Distribution by Intensity
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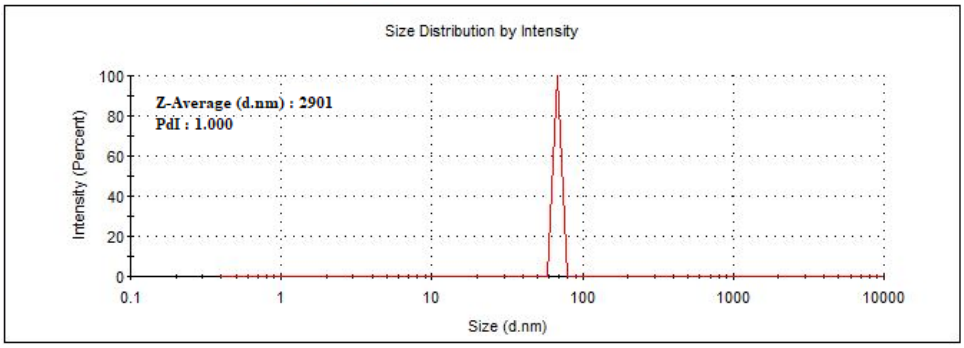
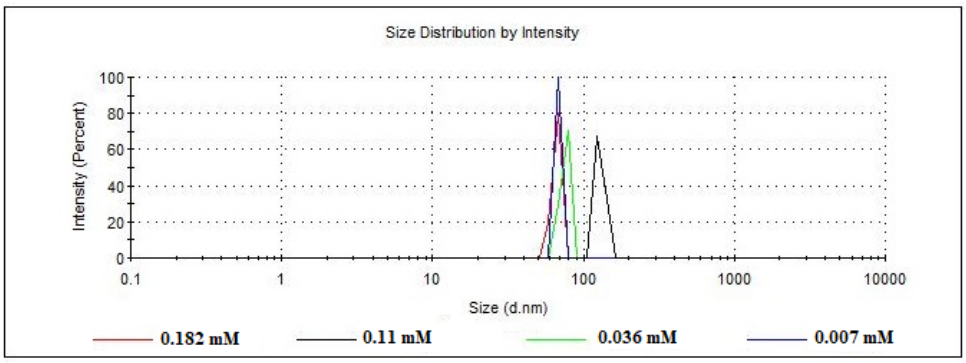
Intensity (Percent)
Size (d.nm)

(c)

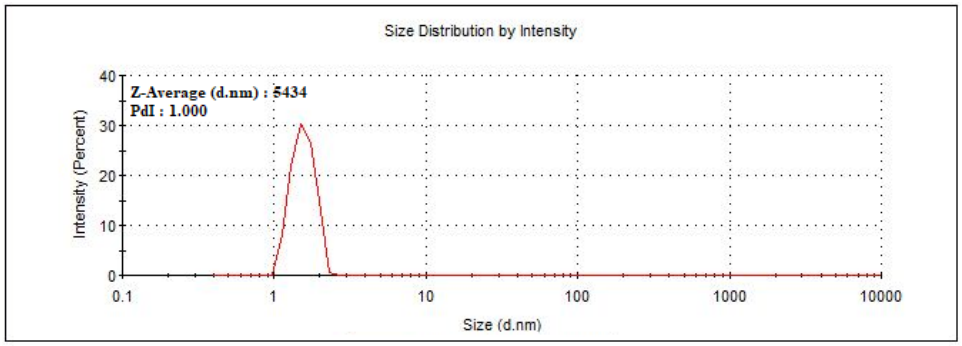

Size Distribution by Intensity
Z-Average (d.nm) : 2901
PdI : 1.000
Intensity (Percent)
Size (d.nm)

(d)

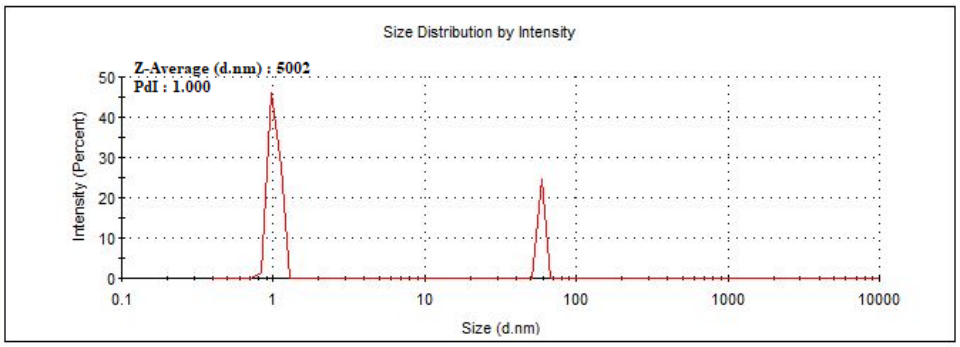

Size Distribution by Intensity
Intensity (Percent)
Size (d.nm)
0.182 mM
0.11 mM
0.036 mM
0.007 mM

(e)

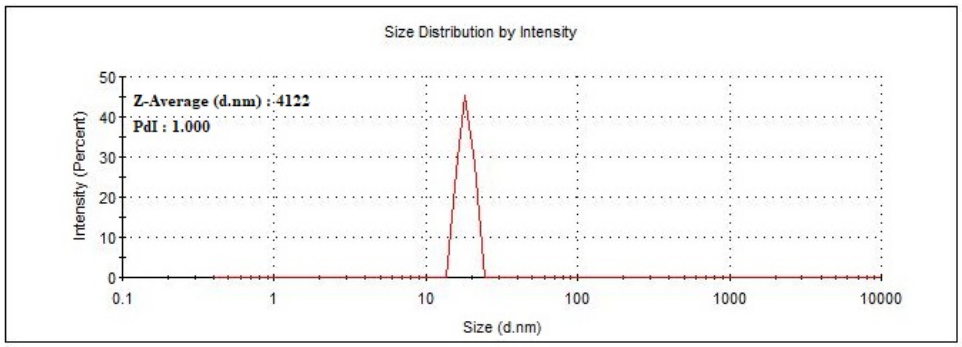
Figure S19. Size distribution plot of ***CisCoNalurea*** in THF-DMF (2:1 v/v) mixture at different concentrations (a) 0.182 mM, (b) 0.11 mM, (c) 0.036 mM, (d) 0.007 mM, and (e) comparative size distribution plot of these three concentrations (obtained from DLS data).



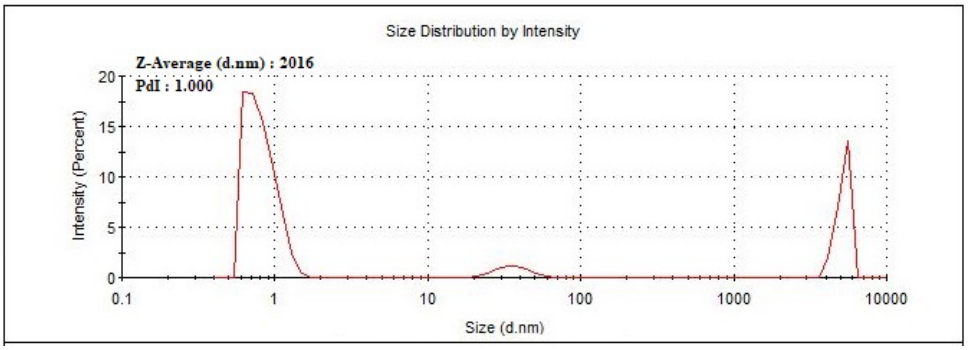
(a)



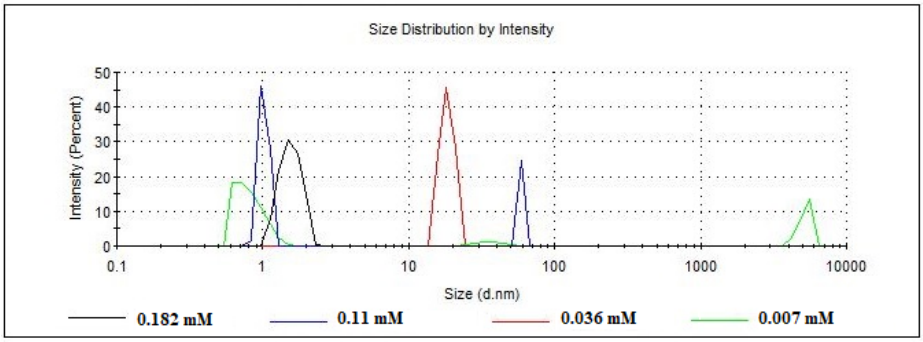
(b)



(c)

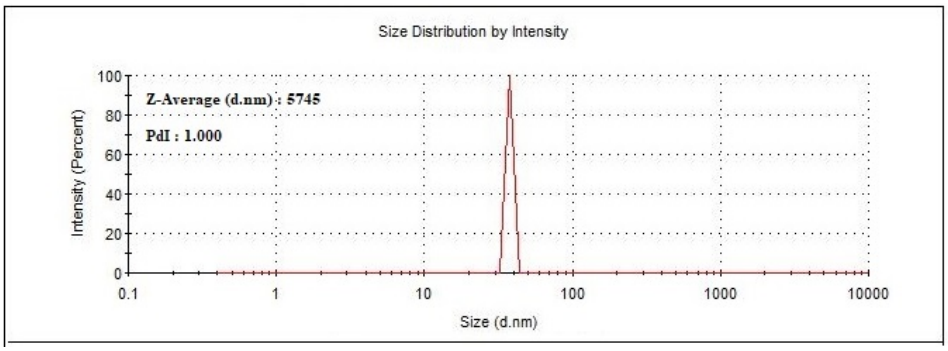


(d)

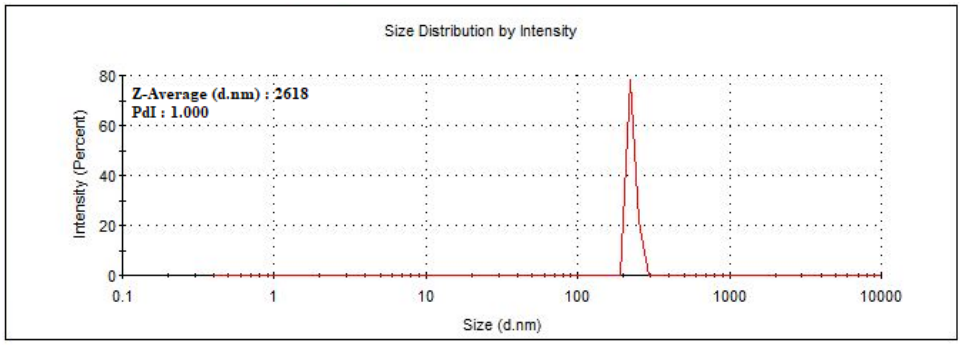


(e)

Figure S20. Size distribution plot of ***CisCoNalurea*** in methanol-acetone (1:3 v/v) mixture at different concentrations (a) 0.182 mM, (b) 0.11 mM, (c) 0.036 mM, (d) 0.007 mM, and (e) comparative size distribution plot of these three concentrations from dynamic light scattering.



(a)


Size Distribution by Intensity
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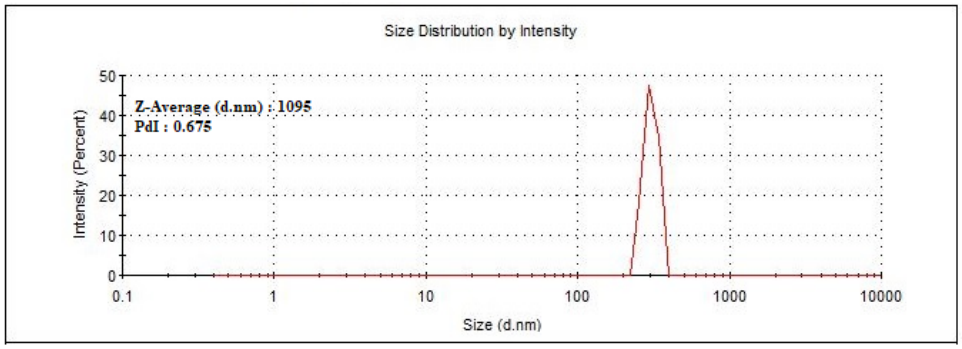
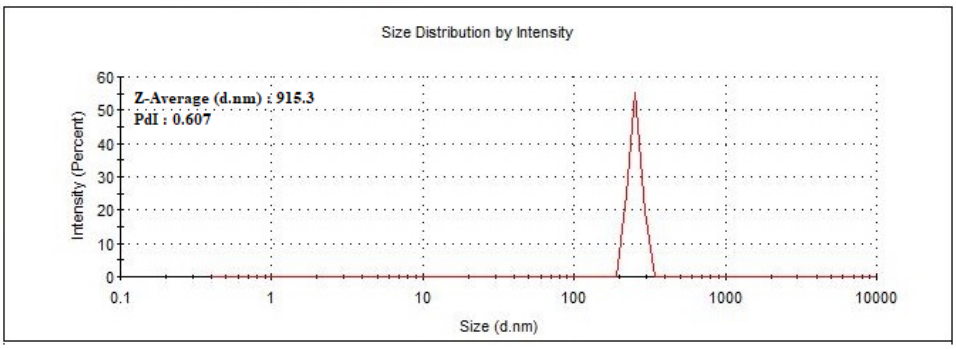
PdI : 1.000
Intensity (Percent)
Size (d.nm)

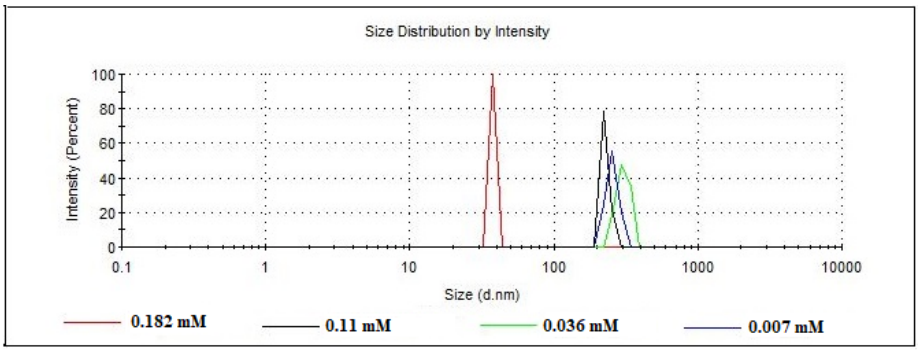
(b)


Size Distribution by Intensity
Z-Average (d.nm) : 1095
PdI : 0.675
Intensity (Percent)
Size (d.nm)

(c)

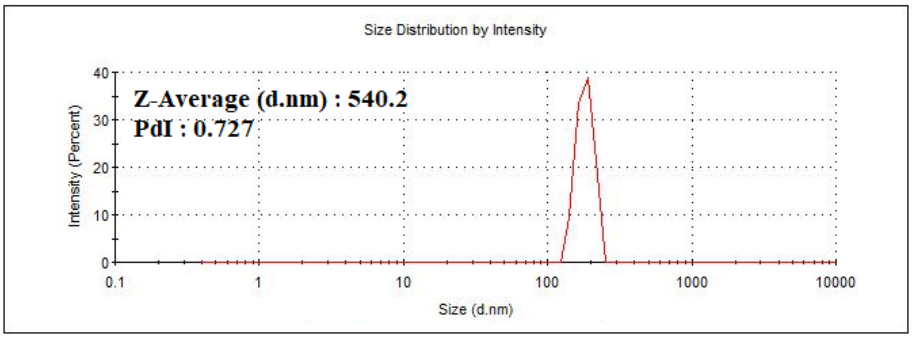

Size Distribution by Intensity
Z-Average (d.nm) : 915.3
PdI : 0.607
Intensity (Percent)
Size (d.nm)

(d)

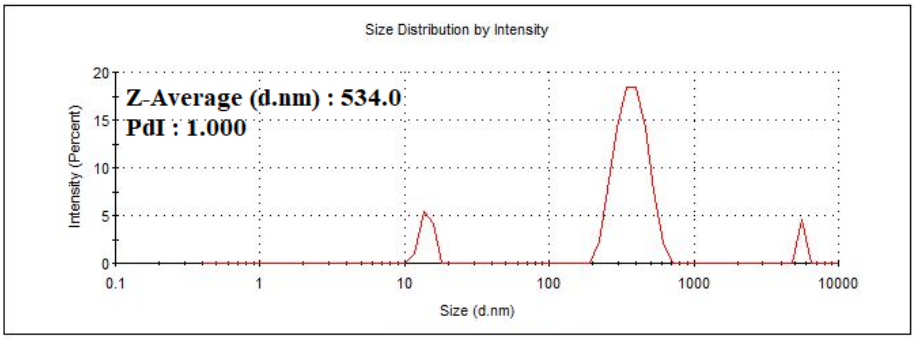

Size Distribution by Intensity
Intensity (Percent)
Size (d.nm)
0.182 mM
0.11 mM
0.036 mM
0.007 mM

(e)

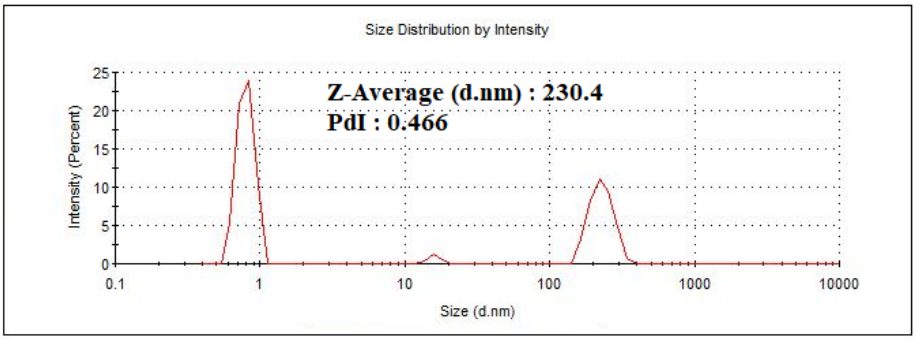
Figure S21. Size distribution plot of ***CisCoNalurea*** in DCM-acetone (1:3 v/v) mixture at different concentrations (a) 0.182 mM, (b) 0.11 mM, (c) 0.036 mM, (d) 0.007 mM and (e) comparative size distribution plot of these three concentrations from dynamic light scattering.



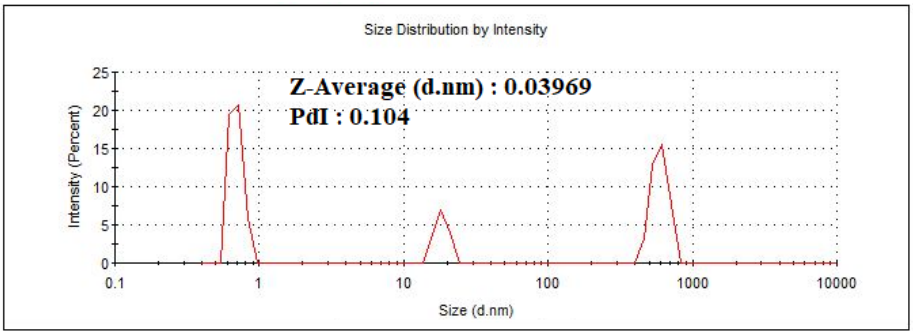
(a)



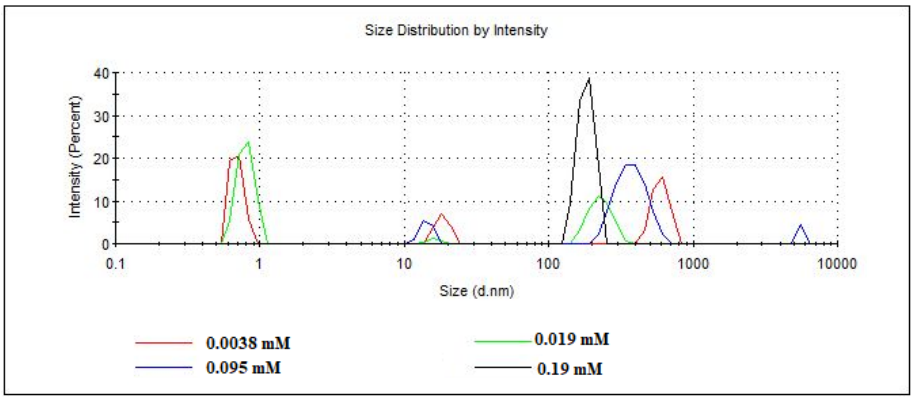
(b)



(c)



(d)



(e)

Figure S22. Size distribution plot of ***CisCoNalurea*** in DMF at different concentrations (a) 0.182 mM, (b) 0.11 mM, (c) 0.036 mM, (d) 0.007 mM, and (e) comparative size distribution plot of these three concentrations from dynamic light scattering.

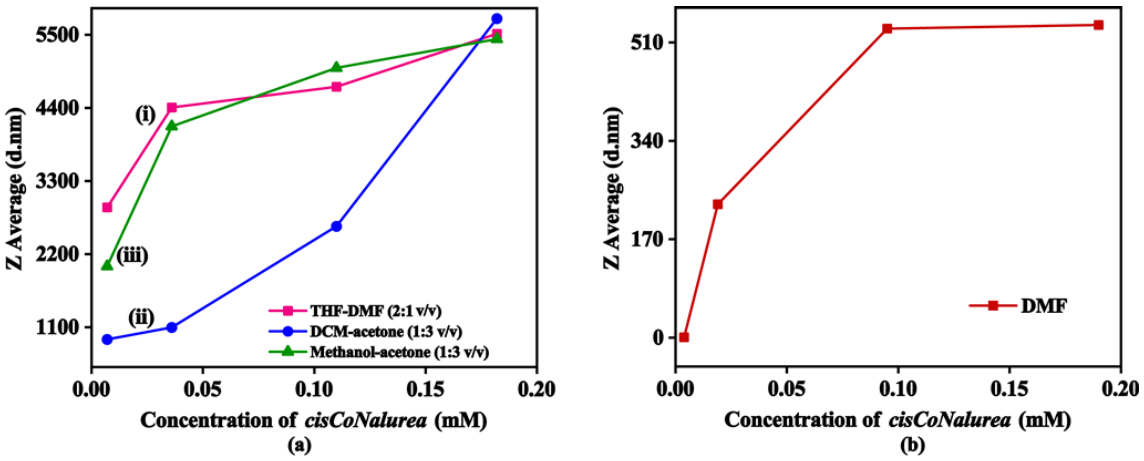


Figure S23. Plots of average paticle size (Z_{av}) versus concentration of ***CisCoNalurea*** at different concentrations (a) (i) THF-DMF (2:1 v/v), (ii) DCM-acetone (1:3 v/v), (iii) methanol-acetone (1:3 v/v), and (b) DMF.

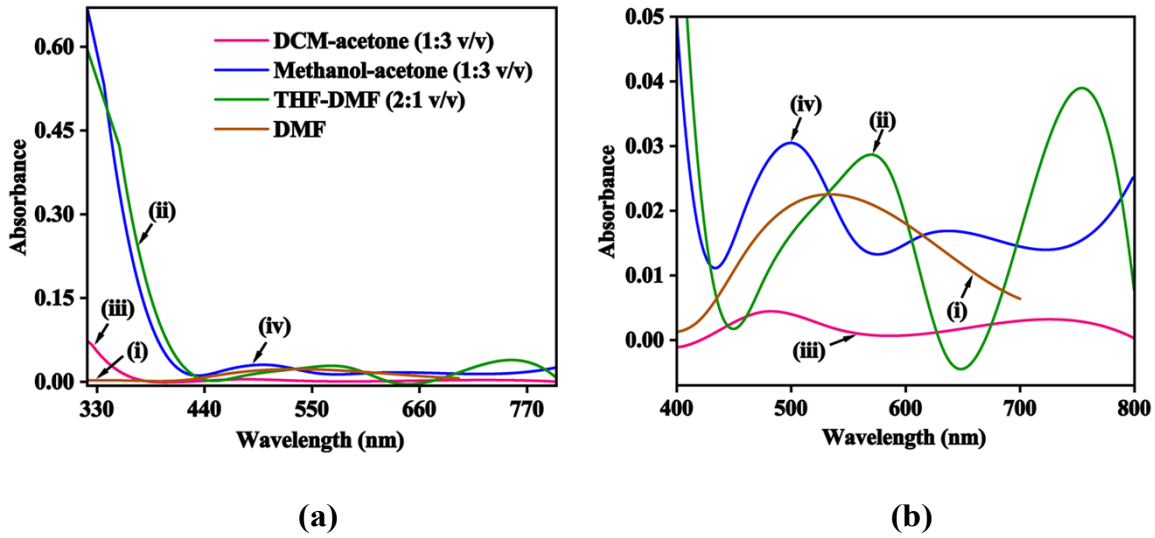


Figure S24. UV-visible spectra, and (b) visible spectra of ***CisCoNalurea*** in (a) DMF (1.14×10^{-3} M), and in binary solvents (b) THF-DMF (2:2 v/v), (c) DCM-acetone (1:3 v/v), and (d) methanol-acetone (1:3 v/v); concentration of ***CisCoNalurea*** in binary solvents = 1.5×10^{-2} M (cuvette used: 1mm path-length).

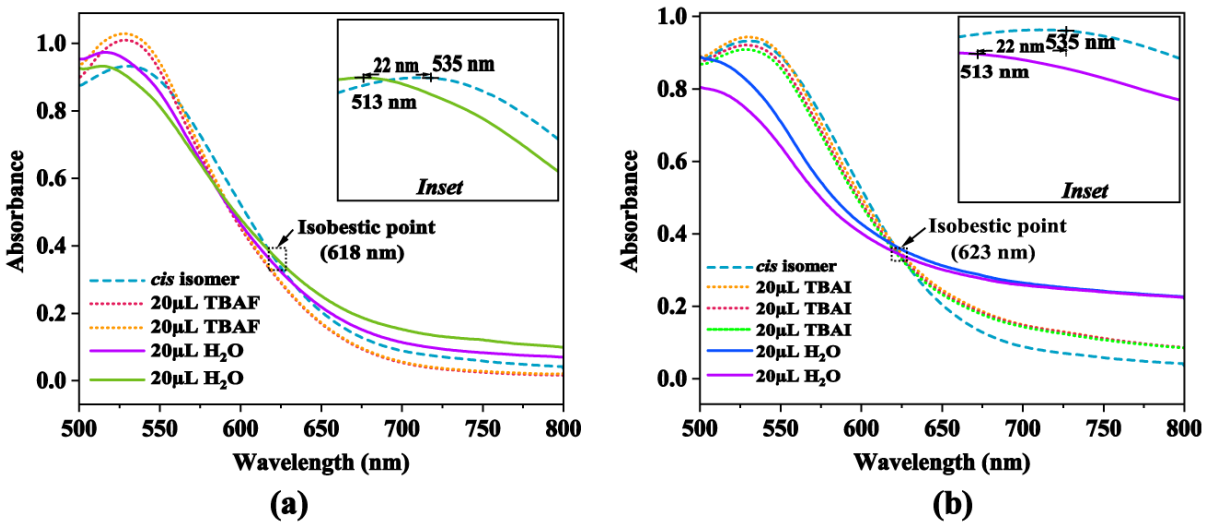
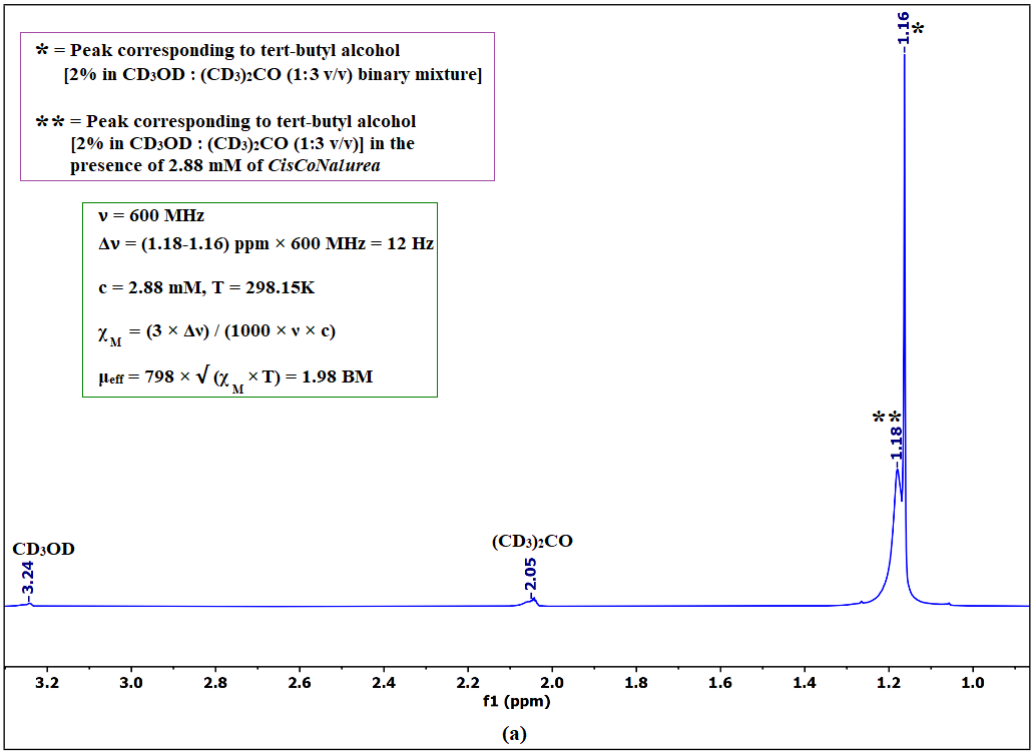


Figure S25. Visible absorption titration of ***CisCoNalurea*** in DMF (23×10^{-4} M) with (a) 20μL aliquot of TBAF in DMF (46×10^{-4} M) followed by 20μL aliquot of water, (b) 20μL aliquot of TBAI in DMF (46×10^{-4} M) followed by 20μL aliquot of water.



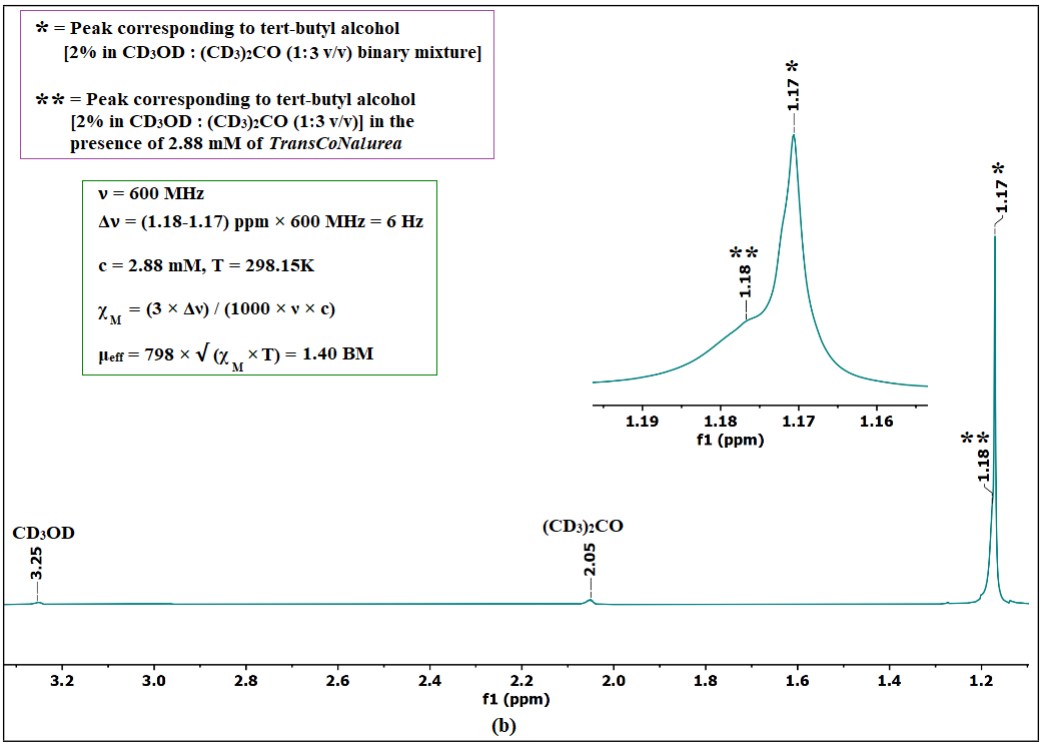


Figure S26. Determination of magnetic moment of (a) ***CisCoNalurea*** and (b) ***TransCoNalurea***.

Table S4. List of torsion angles of two symmetry independent **L**.

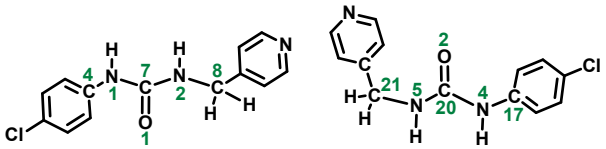
Torsion	Torsion angle (º)
	
N1-C7-N2-C8	-180.0(3)
N4-C20-N5-C21	175.8(3)
C4-N1-C7-O1	-0.8(5)
C17-N4-C20-O2	-0.8(5)
C4-N1-C7-N2	178.8(3)
C17-N4-C20-N5	179.8(3)

Table S5. Optical rotation and specific rotation of ***CisCoNalurea*** in THF-DMF (2:1 v/v) at different concentrations at 25 ºC.

Concentration (mM)	**Optical rotation (º)**	**Specific rotation (º)**
0.363	-0.004	-10.0
0.182	0.004	20.0
0.036	0.001	25.0
0.007	0.003	375.0

Table S6. Optical rotation and specific rotation of ***CisCoNalurea*** in methanol-acetone (1:3 v/v) at different concentrations at 25 ºC.

Concentration (mM)	**Optical rotation (º)**	**Specific rotation (º)**
0.182	-0.003	-15.0
0.123	0.004	+ 29.6
0.036	-0.005	-125.0
0.007	-0.005	-625.0

Table S7. Optical rotation and specific rotation of ***CisCoNalurea*** in DCM-acetone (1:3 v/v) at different concentrations at 25 ºC.

Concentration (mM)	**Optical rotation (º)**	**Specific rotation (º)**
0.363	0.018	+ 45.0
0.182	0.004	20.0
0.036	-0.002	-50.0
0.007	-0.002	-250.0

Table S8. Optical rotation and specific rotations of ***CisCoNalurea*** in DMF at different concentrations at 20 ºC.

Concentration (mM)	**Optical rotation (º)**	**Specific rotation (º)**
0.190	-0.001	-4.7
0.095	-0.001	-9.6
0.019	-0.001	-47.6
0.0038	-0.003	-714.3

Table S9. Z-average values of ***CisCoNalurea*** in different solvent mixtures at different concentrations.

Solvent mixture	**Z-average value (nm) at different concentration (mM)**			
	0.182 mM	**0.11 mM**	**0.036 mM**	**0.007 mM**
THF-DMF (2:1 v/v)	5514	4716	4406	2901
Methanol-acetone (1:3 v/v)	5434	5002	4122	2016
DCM-acetone (1:3 v/v)	5745	2618	1095	915.3

Table S10. Z-average values of ***CisCoNalurea*** from dynamic light scattering in DMF at different concentrations.

Concentration of *CisCoNalurea* in DMF (mM)	**Z-average value (nm)**
0.19	540.2
0.095	534
0.019	230.4
0.0038	0.4

Table S11. Coordinates of the optimized structure of **L**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-11.507042	-0.568516	-2.696048
2	8	0	-5.377584	-2.046222	0.289338

3	7	0	-4.943042	-1.067981	2.331151
4	1	0	-5.190592	-0.358300	3.005113
5	7	0	-6.998085	-0.707680	1.306067
6	1	0	-7.228528	-0.214085	2.157014
7	6	0	-8.021881	-0.716148	0.328620
8	6	0	-1.505724	-0.290423	2.775170
9	1	0	-1.520099	-0.521939	3.835956
10	6	0	-2.490657	-0.800194	1.917847
11	6	0	-7.922291	-1.402719	-0.895358
12	1	0	-7.029846	-1.967743	-1.118875
13	6	0	-5.754858	-1.319831	1.241315
14	6	0	-8.981984	-1.351721	-1.806723
15	1	0	-8.907523	-1.879734	-2.749515
16	7	0	-0.412381	0.840696	0.941975
17	6	0	-0.492782	0.519580	2.252479
18	1	0	0.282118	0.926611	2.892841
19	6	0	-10.249182	0.057748	-0.290191
20	1	0	-11.146916	0.618342	-0.060883
21	6	0	-3.614521	-1.681462	2.437785
22	1	0	-3.655971	-2.609438	1.860852
23	1	0	-3.435069	-1.939180	3.486528
24	6	0	-9.192094	0.010279	0.619443
25	1	0	-9.279351	0.545033	1.561672
26	6	0	-2.408751	-0.470145	0.553316

27	1	0	-3.146679	-0.853062	-0.143207
28	6	0	-10.128443	-0.626172	-1.497167
29	6	0	-1.364882	0.344398	0.114442
30	1	0	-1.272918	0.614778	-0.931687
31	17	0	11.161420	-3.337905	-0.478831
32	8	0	5.533954	0.410693	1.224892
33	7	0	6.000518	-0.254834	-0.963704
34	7	0	4.096633	0.987406	-0.487091
35	6	0	5.232515	0.381194	0.008331
36	6	0	3.154954	1.688720	0.388431
37	1	0	3.578639	1.610176	1.395820
38	1	0	2.184224	1.179453	0.394210
39	6	0	2.955683	3.145109	0.009238
40	6	0	7.208797	-0.965079	-0.786164
41	7	0	2.550317	5.864963	-0.640202
42	6	0	1.668372	3.704786	0.005512
43	1	0	0.808203	3.087997	0.249771
44	6	0	7.839171	-1.128395	0.461840
45	1	0	7.390995	-0.695311	1.343570
46	6	0	1.515257	5.055970	-0.320545
47	1	0	0.531856	5.515211	-0.334205
48	6	0	9.596007	-2.398483	-0.602246
49	6	0	4.034746	3.980288	-0.322078
50	1	0	5.047954	3.592707	-0.333469

51	6	0	7.796905	-1.531776	-1.933599
52	1	0	7.319572	-1.412336	-2.902805
53	6	0	8.990531	-2.249345	-1.847135
54	1	0	9.437193	-2.682207	-2.733742
55	6	0	9.035296	-1.848094	0.546338
56	1	0	9.521328	-1.974173	1.506169
57	6	0	3.788908	5.318932	-0.635587
58	1	0	4.603910	5.988045	-0.892314
59	1	0	3.871875	0.937597	-1.470133
60	1	0	5.667958	-0.215132	-1.916854

Table S12. Coordinates of the optimized structure of ***CisCoNalurea***.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	1.876461	0.178647	0.512064
2	17	0	-7.353460	-8.550917	-3.016125
3	8	0	2.464271	1.997987	0.182872
4	8	0	3.608393	0.151211	1.971041
5	7	0	1.339076	-1.650314	0.895356
6	8	0	3.976179	3.452038	-0.697166
7	8	0	-1.117739	-6.737798	-0.469881
8	7	0	8.270427	-0.732085	1.147921

9	7	0	7.132432	0.918655	-0.067486
10	6	0	5.936617	-0.262977	1.674291
11	6	0	7.123383	-0.043824	0.936378
12	6	0	4.702506	0.461351	1.367736
13	7	0	-3.060532	-6.766067	0.824937
14	1	0	-3.413496	-6.648851	1.764304
15	6	0	4.822604	1.501361	0.381841
16	7	0	-1.039873	-6.064944	1.734585
17	1	0	-1.552678	-5.752081	2.546046
18	6	0	0.793721	-2.435525	-0.070318
19	1	0	0.615521	-1.947470	-1.017034
20	6	0	0.743828	-4.345363	1.412375
21	6	0	8.301442	-1.666845	2.113176
22	6	0	6.013394	1.664282	-0.286106
23	1	0	6.073306	2.422985	-1.055458
24	6	0	7.163482	-1.947643	2.906615
25	1	0	7.220176	-2.708578	3.677170
26	6	0	3.692413	2.395191	-0.067910
27	6	0	0.483206	-3.773022	0.155822
28	1	0	0.049389	-4.373895	-0.635616
29	6	0	1.607356	-2.194785	2.107447
30	1	0	2.079417	-1.538617	2.825340
31	6	0	5.989064	-1.249531	2.678158
32	1	0	5.088218	-1.439333	3.249287

33	6	0	-1.706589	-6.536640	0.619644
34	6	0	1.321309	-3.527984	2.394304
35	1	0	1.556896	-3.925539	3.376581
36	6	0	-4.021985	-7.189756	-0.122609
37	6	0	8.272107	1.009651	-1.018415
38	1	0	8.272004	2.032675	-1.405305
39	1	0	9.188476	0.845238	-0.451562
40	6	0	0.403406	-5.798594	1.692795
41	1	0	0.810943	-6.436962	0.904462
42	1	0	0.841498	-6.110555	2.646539
43	6	0	9.597307	-2.408539	2.309658
44	1	0	10.361531	-1.997157	1.648027
45	1	0	9.478017	-3.475921	2.083999
46	1	0	9.946134	-2.332529	3.346750
47	6	0	-3.717317	-7.465605	-1.468326
48	1	0	-2.700481	-7.362266	-1.816374
49	6	0	-4.732201	-7.875900	-2.338815
50	1	0	-4.499467	-8.088840	-3.375002
51	6	0	-6.035236	-8.011441	-1.869402
52	6	0	-5.347762	-7.334236	0.328396
53	1	0	-5.594614	-7.122247	1.365485
54	6	0	-6.358424	-7.745879	-0.541290
55	1	0	-7.376384	-7.855330	-0.188418
56	6	0	8.128632	-0.013319	-2.153105

57	1	0	8.263123	-1.028641	-1.768417
58	1	0	8.891484	0.167544	-2.919299
59	1	0	7.136306	0.046513	-2.613282
60	17	0	-10.043817	5.292092	-0.109203
61	8	0	3.050788	-0.517831	-0.861152
62	8	0	0.399071	0.370370	-1.173234
63	7	0	0.658774	0.904665	1.839929
64	8	0	4.355533	-0.152843	-2.688476
65	8	0	-4.664063	2.623611	3.441384
66	7	0	-0.147165	3.818389	-4.488079
67	7	0	1.941987	2.811312	-4.140720
68	6	0	0.046169	2.004949	-2.870041
69	6	0	0.586629	2.885588	-3.836095
70	6	0	0.892256	1.056796	-2.143325
71	7	0	-4.716782	4.830572	2.679828
72	1	0	-4.213737	5.706776	2.689791
73	6	0	2.255332	0.970292	-2.594576
74	7	0	-2.847544	4.003397	3.783705
75	1	0	-2.357408	4.843785	3.512743
76	6	0	1.128964	1.687193	2.841185
77	1	0	2.204358	1.758459	2.908369
78	6	0	-1.116020	2.221874	3.571418
79	6	0	-1.462521	3.912517	-4.226465
80	6	0	2.707216	1.853312	-3.546760

81	1	0	3.747767	1.805588	-3.840522
82	6	0	-2.090144	3.067757	-3.280226
83	1	0	-3.152807	3.169733	-3.089829
84	6	0	3.292797	0.028855	-2.032047
85	6	0	0.271339	2.349761	3.717947
86	1	0	0.690021	2.968995	4.504885
87	6	0	-0.685531	0.765135	1.692227
88	1	0	-1.006098	0.151871	0.861925
89	6	0	-1.331888	2.125301	-2.604580
90	1	0	-1.764689	1.466743	-1.861062
91	6	0	-4.117409	3.745970	3.305645
92	6	0	-1.591784	1.400597	2.533958
93	1	0	-2.658580	1.271621	2.388470
94	6	0	-5.978472	4.876823	2.042218
95	6	0	2.593409	3.866277	-4.960859
96	1	0	3.475518	3.406259	-5.415252
97	1	0	1.895588	4.149197	-5.748859
98	6	0	-2.079763	2.964024	4.480237
99	1	0	-2.813636	2.271686	4.901533
100	1	0	-1.534052	3.430060	5.306982
101	6	0	-2.241602	4.950586	-4.990429
102	1	0	-1.557298	5.573484	-5.569160
103	1	0	-2.822675	5.589622	-4.315009
104	1	0	-2.951431	4.478963	-5.682326

105	6	0	-6.859894	3.781603	1.982316
106	1	0	-6.580843	2.847476	2.446307
107	6	0	-8.088573	3.915308	1.327624
108	1	0	-8.768572	3.073506	1.280814
109	6	0	-8.433787	5.129704	0.742248
110	6	0	-6.350571	6.095128	1.442472
111	1	0	-5.676984	6.947215	1.481738
112	6	0	-7.578009	6.227032	0.791853
113	1	0	-7.858457	7.166969	0.332908
114	6	0	2.979933	5.076082	-4.099754
115	1	0	2.082882	5.601847	-3.759221
116	1	0	3.586266	5.775768	-4.686614
117	1	0	3.547712	4.764418	-3.216095

Table S13. Coordinates of the optimized structure of ***TransCoNalurea***.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.000025	0.000016	-0.000030
2	17	0	14.205870	-0.579411	-1.525255
3	8	0	-0.793527	-1.919383	0.645412
4	8	0	0.472619	-0.834888	-1.694648
5	8	0	8.014270	-2.360584	1.147026

6	7	0	-0.589364	-5.557075	-1.331672
7	8	0	0.781540	-2.339960	-3.360668
8	7	0	1.756682	-0.489823	0.738447
9	7	0	8.772249	-0.154516	1.056559
10	1	0	8.530925	0.800490	1.281071
11	7	0	-1.584821	-6.656601	0.486518
12	6	0	4.267793	-1.161322	1.800963
13	7	0	6.694968	-0.654313	1.968609
14	1	0	6.582780	0.332285	2.151541
15	6	0	4.119301	-0.823876	0.445544
16	1	0	4.977004	-0.818656	-0.217389
17	6	0	-0.163571	-3.161421	-1.336640
18	6	0	0.401000	-2.043871	-2.195091
19	6	0	-1.202631	-4.253125	0.613424
20	6	0	-0.708800	-3.015771	-0.007519
21	6	0	3.117859	-1.149198	2.603950
22	1	0	3.178687	-1.394565	3.659220
23	6	0	-1.138963	-5.497582	-0.051908
24	6	0	-0.136852	-4.410705	-1.916623
25	1	0	0.276533	-4.490084	-2.915494
26	6	0	10.037657	-0.318939	0.447676
27	6	0	5.614553	-1.549107	2.380284
28	1	0	5.546748	-1.588258	3.475268
29	1	0	5.911843	-2.546694	2.037482

30	6	0	-1.761633	-4.253105	1.906896
31	1	0	-1.817155	-3.308134	2.434981
32	6	0	1.884497	-0.812011	2.049307
33	1	0	0.974893	-0.760038	2.631612
34	6	0	2.861064	-0.497277	-0.052268
35	1	0	2.688698	-0.252379	-1.091313
36	6	0	7.844451	-1.140050	1.373687
37	6	0	-0.532043	-6.847192	-2.067984
38	1	0	0.304499	-6.770027	-2.767653
39	1	0	-0.310467	-7.626973	-1.338817
40	6	0	10.551435	-1.566274	0.046857
41	1	0	9.964359	-2.458689	0.204243
42	6	0	-2.114763	-6.638523	1.723458
43	6	0	-2.217518	-5.437480	2.464300
44	1	0	-2.649810	-5.454412	3.458545
45	6	0	11.814427	-1.636807	-0.549795
46	1	0	12.211063	-2.596129	-0.859077
47	6	0	10.806603	0.842210	0.240243
48	1	0	10.419857	1.810902	0.546045
49	6	0	12.555177	-0.474854	-0.743977
50	6	0	12.066291	0.769671	-0.355625
51	1	0	12.652652	1.666510	-0.512672
52	6	0	-2.592656	-7.951170	2.285215
53	1	0	-3.659895	-7.909842	2.535761

54	1	0	-2.053747	-8.206239	3.206143
55	1	0	-2.433290	-8.746183	1.554787
56	6	0	-1.838235	-7.159763	-2.804955
57	1	0	-2.661605	-7.267432	-2.093310
58	1	0	-1.736637	-8.100621	-3.357671
59	1	0	-2.088356	-6.368769	-3.520290
60	17	0	-14.205735	0.579268	1.525545
61	8	0	0.793477	1.919416	-0.645475
62	8	0	-0.472667	0.834919	1.694587
63	8	0	-8.014217	2.360566	-1.146885
64	7	0	0.589364	5.557098	1.331635
65	8	0	-0.781571	2.339987	3.360615
66	7	0	-1.756731	0.489857	-0.738510
67	7	0	-8.772260	0.154511	-1.056600
68	1	0	-8.530985	-0.800476	-1.281246
69	7	0	1.584827	6.656624	-0.486551
70	6	0	-4.267838	1.161357	-1.801035
71	7	0	-6.695015	0.654337	-1.968715
72	1	0	-6.582852	-0.332250	-2.151717
73	6	0	-4.119351	0.823914	-0.445615
74	1	0	-4.977056	0.818698	0.217316
75	6	0	0.163545	3.161448	1.336589
76	6	0	-0.401036	2.043899	2.195035
77	6	0	1.202610	4.253153	-0.613472

78	6	0	0.708767	3.015801	0.007465
79	6	0	-3.117901	1.149231	-2.604018
80	1	0	-3.178726	1.394597	-3.659289
81	6	0	1.138958	5.497606	0.051868
82	6	0	0.136842	4.410729	1.916580
83	1	0	-0.276539	4.490106	2.915453
84	6	0	-10.037631	0.318903	-0.447631
85	6	0	-5.614597	1.549140	-2.380363
86	1	0	-5.546782	1.588301	-3.475346
87	1	0	-5.911894	2.546721	-2.037549
88	6	0	1.761606	4.253135	-1.906946
89	1	0	1.817115	3.308167	-2.435038
90	6	0	-1.884541	0.812044	-2.049371
91	1	0	-0.974935	0.760069	-2.631673
92	6	0	-2.861116	0.497315	0.052201
93	1	0	-2.688753	0.252418	1.091247
94	6	0	-7.844448	1.140048	-1.373675
95	6	0	0.532059	6.847211	2.067955
96	1	0	-0.304481	6.770049	2.767627
97	1	0	0.310486	7.626998	1.338794
98	6	0	-10.551350	1.566206	-0.046637
99	1	0	-9.964256	2.458622	-0.203948
100	6	0	2.114764	6.638548	-1.723494
101	6	0	2.217502	5.437508	-2.464344

102	1	0	2.649790	5.454442	-3.458592
103	6	0	-11.814310	1.636707	0.550089
104	1	0	-12.210900	2.596005	0.859505
105	6	0	-10.806602	-0.842247	-0.240295
106	1	0	-10.419901	-1.810915	-0.546232
107	6	0	-12.555085	0.474754	0.744170
108	6	0	-12.066257	-0.769740	0.355646
109	1	0	-12.652638	-1.666579	0.512616
110	6	0	2.592672	7.951193	-2.285244
111	1	0	3.659919	7.909865	-2.535756
112	1	0	2.053791	8.206256	-3.206189
113	1	0	2.433284	8.746209	-1.554823
114	6	0	1.838257	7.159765	2.804922
115	1	0	2.661624	7.267432	2.093273
116	1	0	1.736669	8.100621	3.357644
117	1	0	2.088374	6.368766	3.520251

Reference:

1. G. A. Bain and J. F. Berry, *J. Chem. Educ.*, 2008, **85**, 532–536.

2. D. F. Evans, *J. Chem. Soc.*, 1959, 2003–2005.

3. K. De Buysser, G. G. Herman, E. Bruneel, S. Hoste and I. Van Driessche, *Chem. Phys.*, 2005, **315**, 286–292.