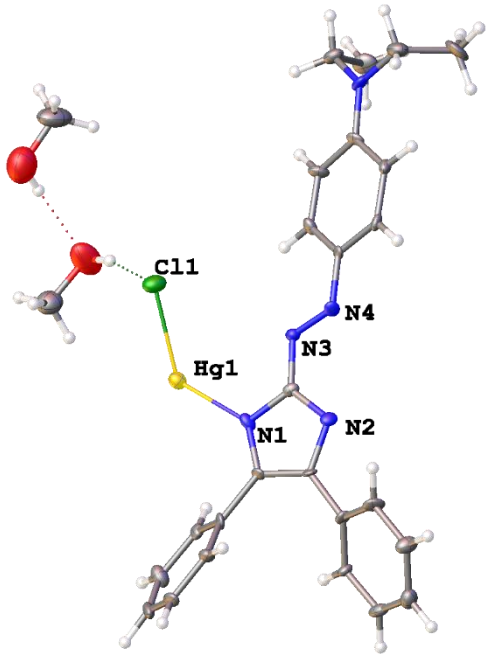


**Figure S1.** Asymmetric unit of **9Hg′** in representation of atoms with thermal ellipsoids (given at p = 50%).

**Table S1.** Crystallographic data and the refinement parameters for compounds.

| | **9Zn·CH$_3$OH** | **9Hg·CH$_3$OH** | **9Hg'·2CH$_3$OH** | **8·solvent** | **10** | **10Cd·1.75CH$_3$OH·0.75H$_2$O** |
|---|---|---|---|---|---|---|
| Empirical formula | $C_{26}H_{29}Cl_2N_5OZn$ | $C_{26}H_{29}Cl_2HgN_5O$ | $C_{27}H_{32}ClHgN_5O_2$ | $C_{24}H_{22}N_4O_3$ | C23 H19 N5 O4 | $C_{47.75}H_{46.5}Br_2CdN_{10}O_{10.5}$ |
| Fw | 563.81 | 699.03 | 694.61 | 414.45 | 429.43 | 1200.67 |
| Crystal system | Triclinic | Triclinic | Monoclinic | Monoclinic | Triclinic | Triclinic |
| Space group | $P\bar{1}$ | $P\bar{1}$ | $P2_1/c$ | $P2_1/c$ | $P\bar{1}$ | $P\bar{1}$ |
| Z | 2 | 2 | 4 | 4 | 2 | 4 |
| a, Å | 9.717(7) | 9.626(2) | 15.911(3) | 12.6640(15) | 9.4104(6) | 11.3012(11) |
| b, Å | 10.537(7) | 10.547(2) | 15.480(3) | 19.273(2) | 9.4575(7) | 17.9671(18) |
| c, Å | 14.692(13) | 14.916(3) | 11.104(2) | 9.5614(12) | 11.6949(8) | 29.382(3) |
| α, ° | 72.37(3) | 100.137(7) | 90 | 90 | 102.897(2) | 97.895(2) |
| β, ° | 71.17(3) | 108.617(9) | 108.76(3) | 91.540(3) | 90.055(2) | 99.032(2) |
| γ, ° | 79.99(2) | 98.811(8) | 90 | 90 | 91.925(2) | 102.104(2) |
| V, Å$^3$ | 1352.1(18) | 1376.8(5) | 2589.8(10) | 2332.9(5) | 1013.96(12) | 5670.9(10) |
| $D_{calc}$, g·cm$^{-3}$ | 1.385 | 1.686 | 1.781 | 1.180 | 1.407 | 1.406 |
| μ, cm$^{-1}$ | 1.134 | 5.811 | 6.081 | 0.080 | 0.099 | 1.855 |
| F(000) | 584 | 684 | 1368 | 872 | 448 | 2420 |
| No of measured reflections | 14193 | 20134 | 35134 | 27088 | 8652 | 77749 |
| No of independent reflections , $R_{int}$ | 7810, 0.023 | 9211, 0.030 | 8182, 0.175 | 7118, 0.100 | 4709, 0.041 | 34402, 0.159 |
| No of observed reflections with [I>2σ(I)] | 6731 | 8323 | 4027 | 3729 | 2496 | 13056 |
| No of parameters | 320 | 320 | 331 | 283 | 291 | 1309 |
| $R_1$ [I>2σ(I)] | 0.041 | 0.025 | 0.064 | 0.059 | 0.062 | 0.082 |
| $wR_2$ [all] | 0.110 | 0.066 | 0.127 | 0.127 | 0.149 | 0.185 |
| GOF | 1.04 | 1.13 | 0.93 | 1.01 | 1.03 | 1.07 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.98/-0.60 | 0.89/-1.36 | 2.07/-3.07 | 0.26/-0.28 | 0.27/-0.26 | 2.09/-2.04 |

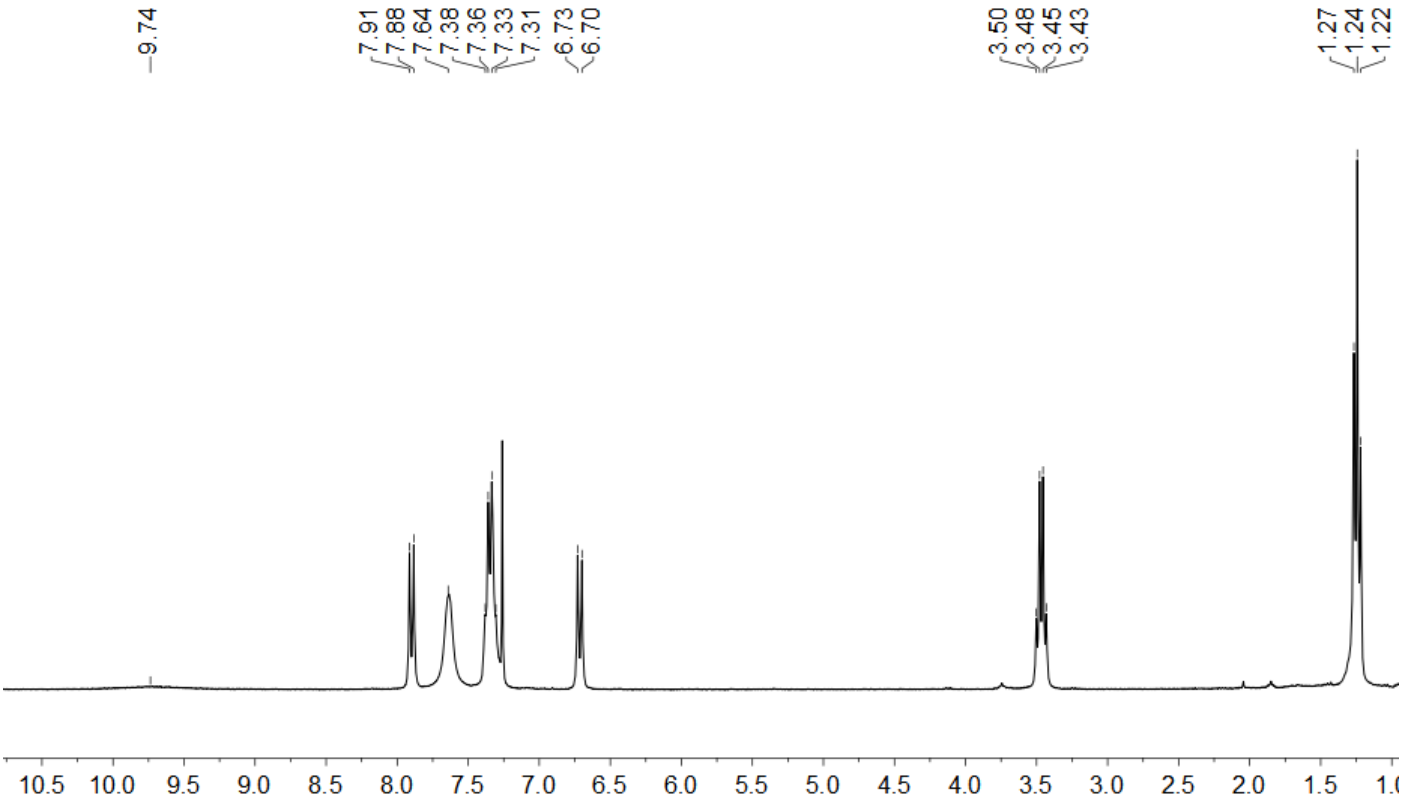


**Figure S2.** $^{1}$H NMR spectrum of **9** ($CDCl_3$).

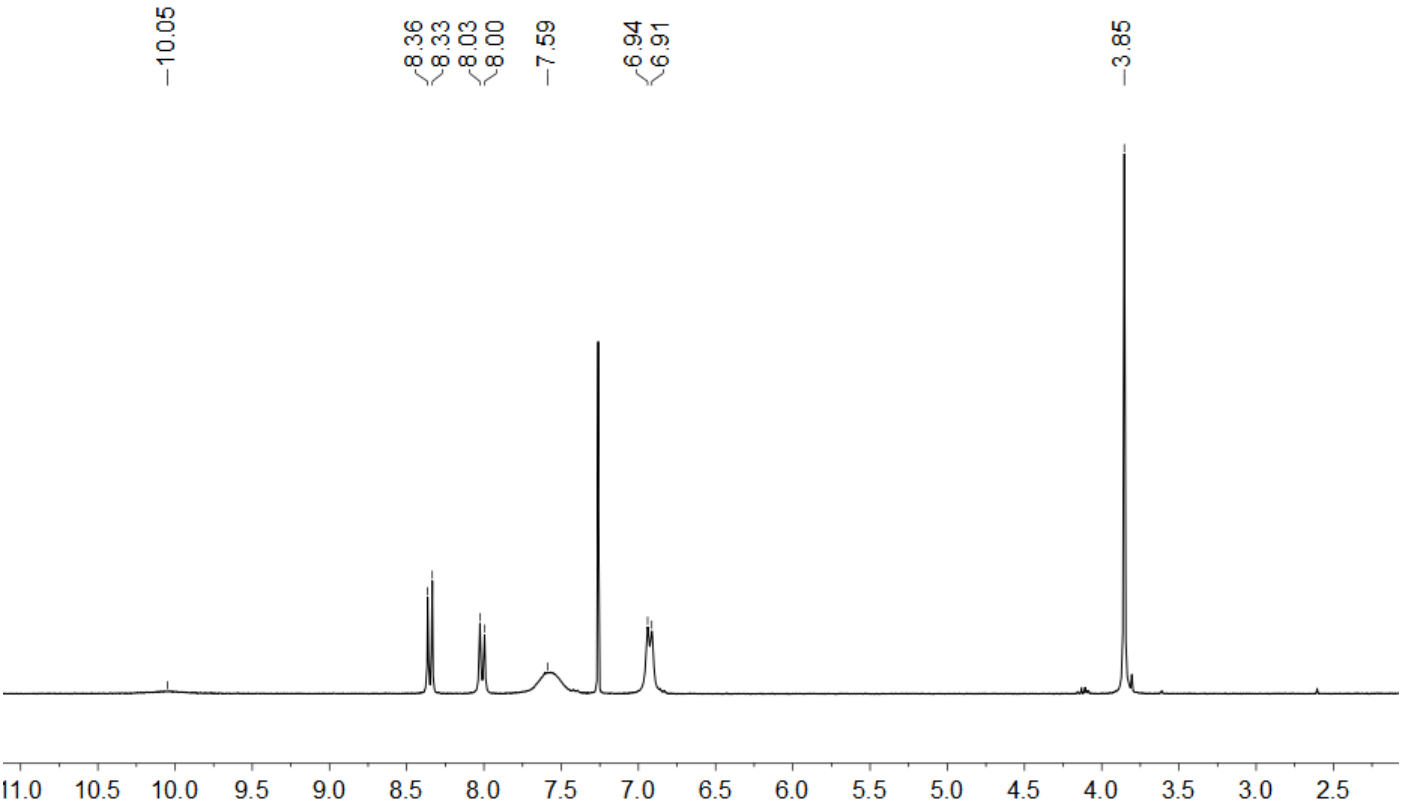


**Figure S3.** $^{1}$H NMR spectrum of **10** ($CDCl_3$).

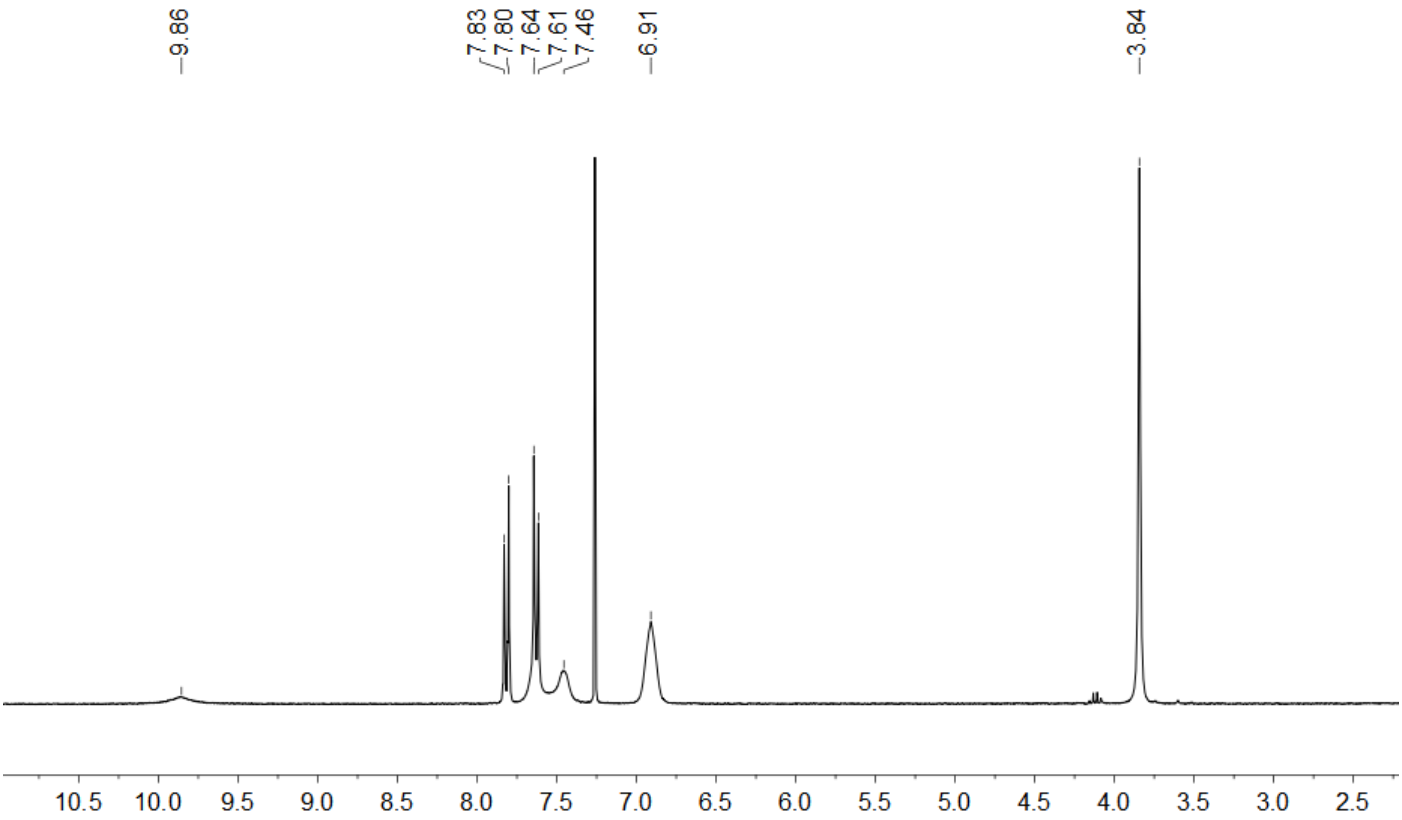


**Figure S4.** $^{1}$H NMR spectrum of **11** ($CDCl_3$).