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Electronic Supporting Information

Exploring Novel Cd(II) Complexes with 5-Methyl-4-Imidazolecarboxaldehyde: Synthesis, Structure, Computational Insights, and Affinity to DNA through switchSense Methodology

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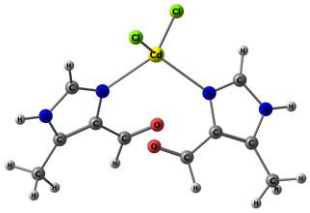
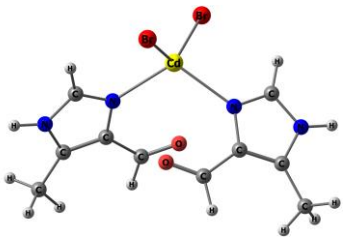
Keywords: Cd(II), imidazolecarboxaldehyde, crystal structure, computational analysis, switchSense technique

Table S1. Cartesian coordinates (in Å) of the gas-phase optimized structures of compounds **1**–**4**.

System	Cartesian Coordinates			
1 	C	-0.176260641497	2.972986080498	0.331911166905
	H	-0.739280333997	3.173820827066	1.241512591868
	C	0.710169499764	3.254429048004	-1.707313985996
	C	0.946556278958	1.956973054480	-1.230595591136
	C	1.579698764817	0.843217704382	-1.940326418836
	H	2.022711701644	1.094760209948	-2.930947080939
	C	1.055515530852	3.948521613766	-2.988062419698
	H	0.145600054009	4.245820520272	-3.534151871945
	H	1.638187281495	3.279629436996	-3.635002927152
	H	1.659376533398	4.850833446437	-2.799393294039
	C	0.176260641497	-2.972986080498	0.331911166905
	H	0.739280333997	-3.173820827066	1.241512591868
	C	-0.710169499764	-3.254429048004	-1.707313985996
	C	-0.946556278958	-1.956973054480	-1.230595591136
	C	-1.579698764817	-0.843217704382	-1.940326418836
	H	-2.022711701644	-1.094760209948	-2.930947080939
	C	-1.055515530852	-3.948521613766	-2.988062419698
	H	-0.145600054009	-4.245820520272	-3.534151871945
	H	-1.638187281495	-3.279629436996	-3.635002927152
	H	-1.659376533398	-4.850833446437	-2.799393294039
	Cd	0.000000000000	0.000000000000	1.366565515640
	Cl	-1.901973456323	1.018910943511	2.439998628302
	Cl	1.901973456323	-1.018910943511	2.439998628302
	N	0.396662063458	1.811214165803	0.031517840184
	N	0.000000000000	3.863669126703	-0.694939529824
	H	-0.352461136707	4.815695098126	-0.708121261012
	N	-0.396662063458	-1.811214165803	0.031517840184
	N	0.000000000000	-3.863669126703	-0.694939529824
	H	0.352461136707	-4.815695098126	-0.708121261012
	O	1.616361371151	-0.310529245270	-1.507646234014
	O	-1.616361371151	0.310529245270	-1.507646234014
2 	C	0.000000000000	3.024354639001	-0.026766630668
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	C	0.974602720781	3.277597025936	-2.029657761591
	C	1.080877197194	1.953057910145	-1.581909244021
	C	1.641350893593	0.799835224331	-2.290791308456
	H	2.141438480741	1.024101569062	-3.260267862767
	C	1.424837313067	3.970073135123	-3.278260333742
	H	0.565490746520	4.366586684986	-3.842879329538
	H	1.962972315785	3.265940637585	-3.926461420780
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	H	0.568860113316	-3.252742274356	0.872625936229
	C	-0.974602720781	-3.277597025936	-2.029657761591
	C	-1.080877197194	-1.953057910145	-1.581909244021
	C	-1.641350893593	-0.799835224331	-2.290791308456
	H	-2.141438480741	-1.024101569062	-3.260267862767
	C	-1.424837313067	-3.970073135123	-3.278260333742
	H	-0.565490746520	-4.366586684986	-3.842879329538
	H	-1.962972315785	-3.265940637585	-3.926461420780
	H	-2.104343436050	-4.805657775194	-3.044869306331
	Br	2.025065640801	-1.037650247629	2.045606126689
	Br	-2.025065640801	1.037650247629	2.045606126689
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	N	0.286780264586	3.921677483820	-1.022794697052
	H	0.021162938194	4.901608500905	-1.019720193111
	N	-0.478465145987	-1.825313776096	-0.342936162659
	N	-0.286780264586	-3.921677483820	-1.022794697052
	H	-0.021162938194	-4.901608500905	-1.019720193111
	O	1.561113313692	-0.357275385469	-1.873594818190
	O	-1.561113313692	0.357275385469	-1.873594818190
	C	3.065768219845	-0.290337020984	0.676084050133
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	C	4.026810292069	0.684207047908	-1.100844081403

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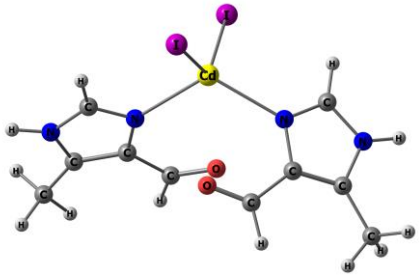

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O	0.624404044360	0.621069042334	-2.517752181404
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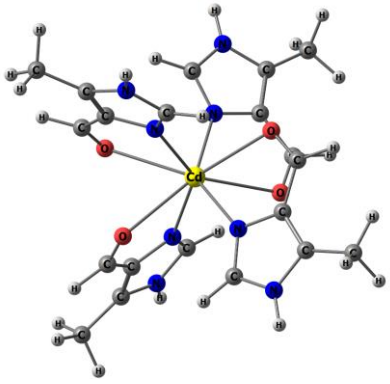
C	-3.174610227227	4.456998321928	-0.753640056076
H	-3.524932254866	4.720418337850	-1.764755128604
H	-2.351650168786	5.134559369264	-0.490510035107
H	-3.998505288950	4.629794331494	-0.042541003080
I	-1.212844086313	-2.640013192469	-1.153800081693
N	-1.560409111068	1.074094076214	-0.502475035925
N	-3.534321256291	1.963657139938	-0.957318066711
H	-4.517916323107	2.021281145036	-1.202701086685
O	0.878585064731	2.504874182082	-0.013652001008

4



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C	-1.902802153186	2.546211884199	0.929362214741
H	-2.358428246707	3.454218616588	1.380476463660
C	-4.302866790817	3.848768257386	-1.040426031013
H	-4.134464873331	4.574791087305	-1.852762104750
H	-4.114970740201	4.358956255978	-0.085227711305
H	-5.361990500866	3.543865063229	-1.062437253937
C	2.270021276061	0.071484976561	-2.513182174931
H	2.801884464732	0.966544404342	-2.195200317438
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C	0.858650095203	-1.562814745550	-2.685721618200
C	-0.319728489554	-2.343299556001	-2.319040419874
H	-0.550799447269	-3.242217341048	-2.930698584595
C	1.897016007435	-2.755468624272	-4.819557367070
H	1.845005890310	-2.283667968839	-5.814500232525
H	1.085959791209	-3.493921325052	-4.749763766942
H	2.855476086275	-3.294548631721	-4.741521164525
C	2.461906878626	0.126615894286	2.324266754305
H	2.356732577589	-0.891698325675	2.694543458033
C	3.238009942702	2.218347922046	2.165340946111
C	2.257257510232	1.965806054662	1.198101022944
C	1.722828208786	2.825261081378	0.145518114087
H	2.112881515167	3.864310103229	0.083756491130
C	4.060145828745	3.423109767816	2.494108753589
H	3.857600723098	3.768202915680	3.521356127935
H	3.826047661776	4.248217968382	1.806801679522
H	5.136805134008	3.202336506231	2.408857647887
C	-2.239384654482	-1.047784129534	2.315865943766
H	-2.832301012077	-0.135789126334	2.358757617210
C	-1.608673060736	-3.148121513889	2.756158412108
C	-0.722145050789	-2.527490577399	1.867307493958
C	0.500522472949	-3.028460250104	1.245752576949
H	0.797503494744	-4.076243808126	1.468218396090
C	-1.655725649597	-4.513815643936	3.362875114386
H	-1.625612849993	-4.458824650200	4.463451283931
H	-0.797720605586	-5.113591387536	3.028062774489
H	-2.576639628935	-5.043019050167	3.067554833365
Cd	0.000435123136	-0.000737307159	0.000750796935
N	-1.843990097538	1.001677974183	-0.977652649731

	N	-3.430206045308	1.831537080465	-2.281520022510
	H	-4.055970583208	1.927443387038	-3.080326642688
	N	1.183731161830	-0.439994396555	-1.941038643787
	N	2.644099541520	-0.682585744069	-3.588237586286
	H	3.444304840669	-0.491956221494	-4.190071067369
	N	1.789067383543	0.666262441015	1.311795157066
	N	3.335324072428	1.032314500510	2.854486900535
	H	3.964119065555	0.854194846108	3.636639709426
	N	-1.128561930613	-1.228269417909	1.606996722463
	N	-2.550881630000	-2.179864400922	3.012746649201
	H	-3.354852226363	-2.287714296214	3.629895123133
	O	-1.020723708970	1.918764139306	1.524214868932
	O	-1.042997927695	-2.019718267658	-1.371520387434
	O	0.875243384489	2.418917180388	-0.655784445729
	O	1.189721337161	-2.319036832052	0.505897296633

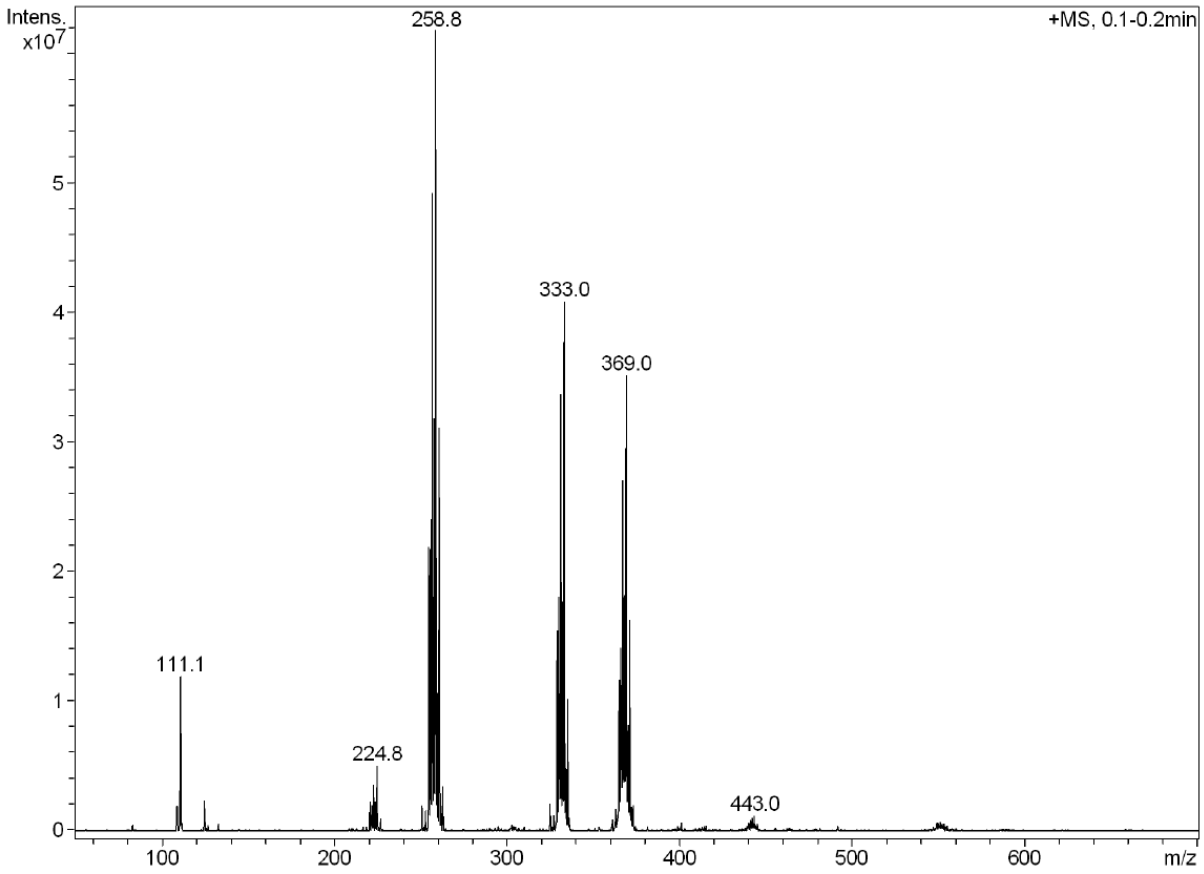


Figure S1. The ESI-MS spectrogram for CH_3OH/H_2O solution of complex **1**.

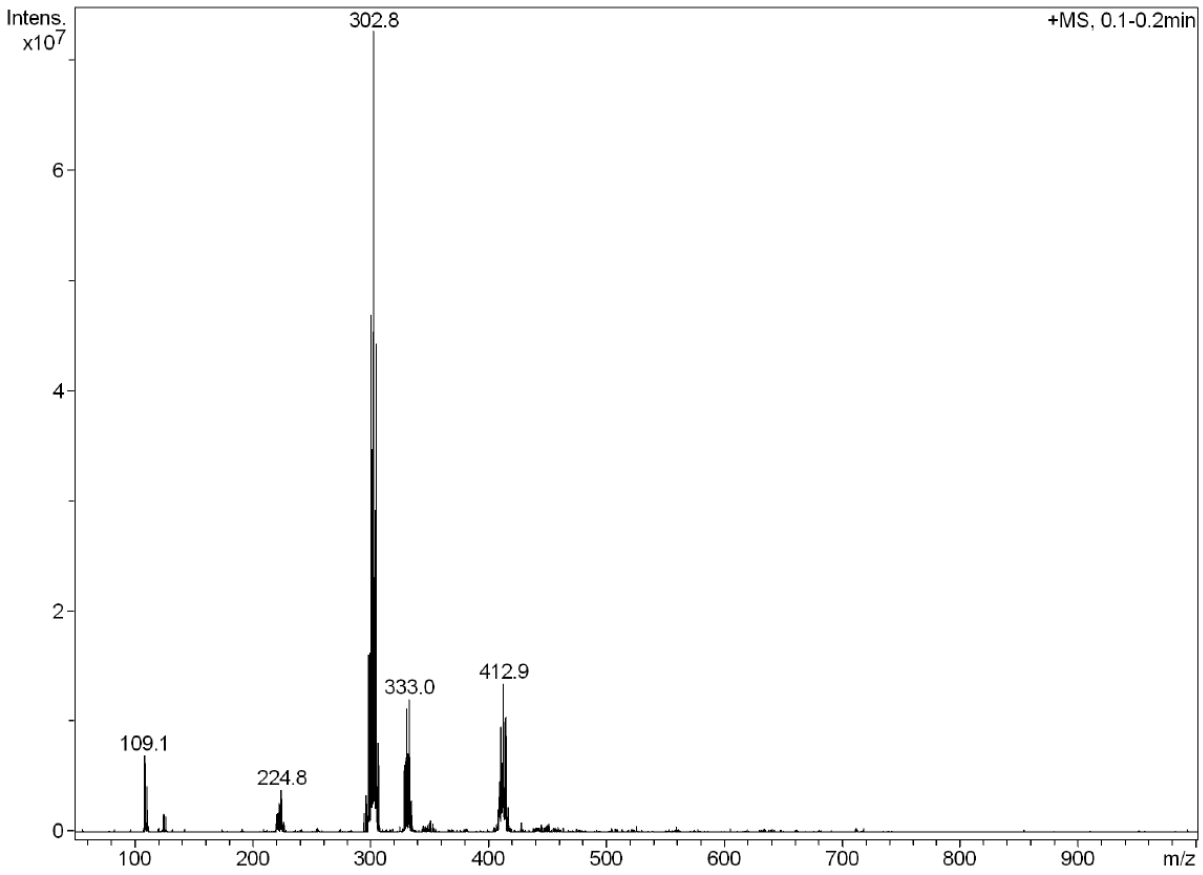


Figure S2. The ESI-MS spectrogram for CH_3OH/H_2O solution of complex **2**.

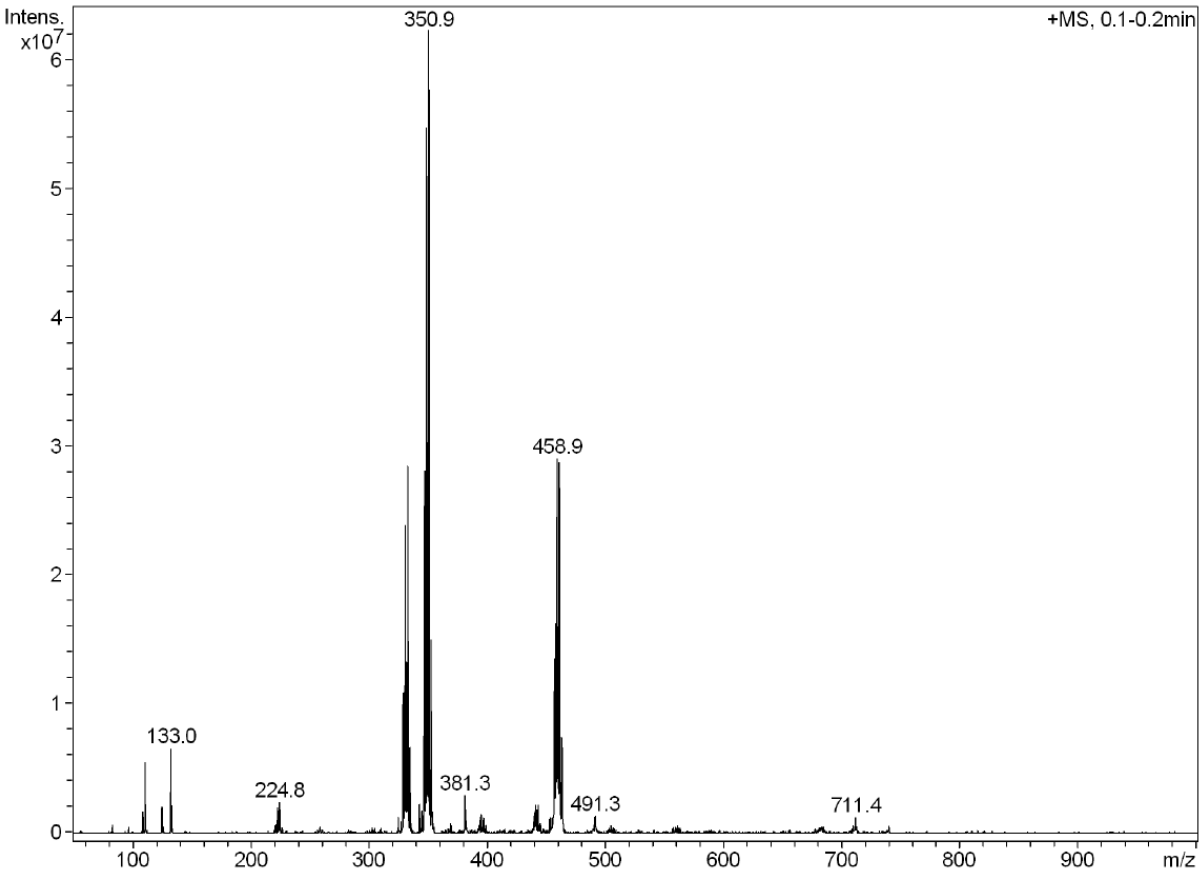


Figure S3. The ESI-MS spectrogram for CH_3OH/H_2O solution of complex **3**.

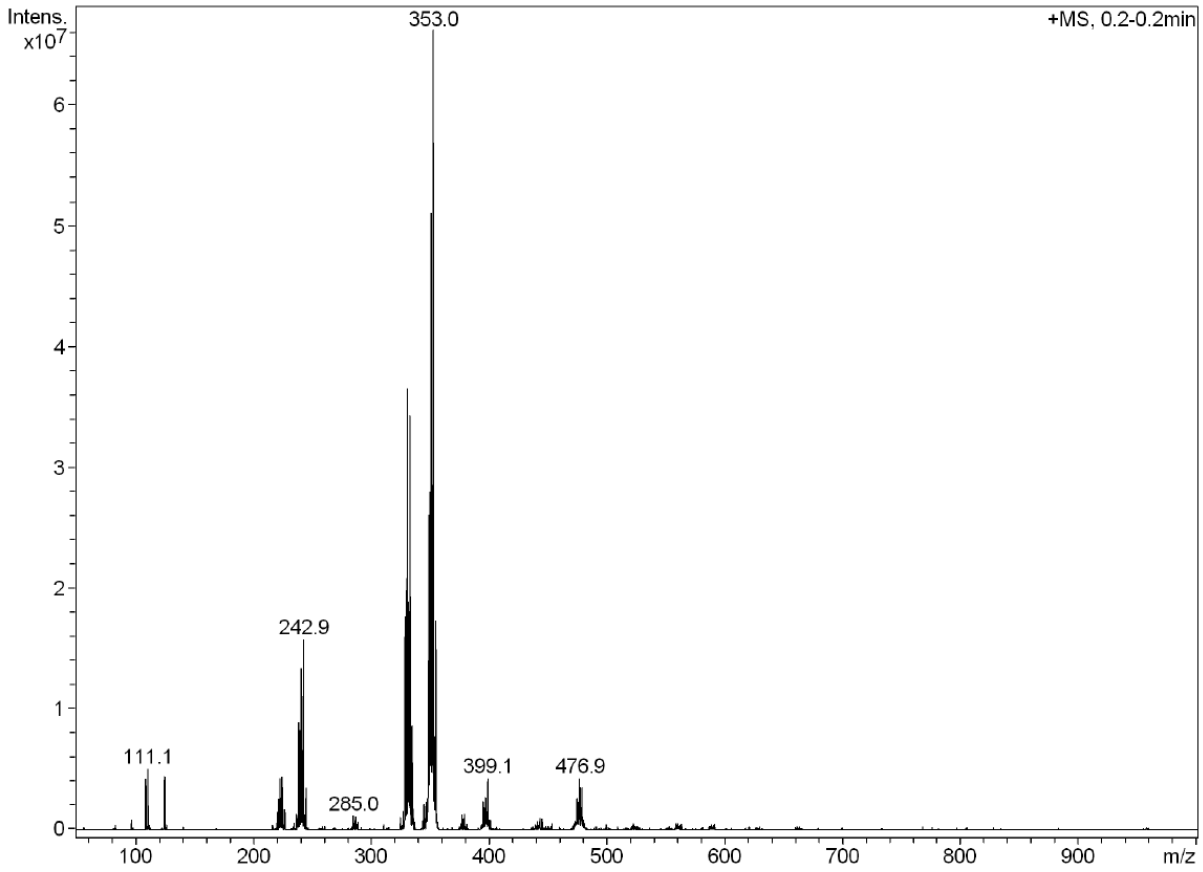


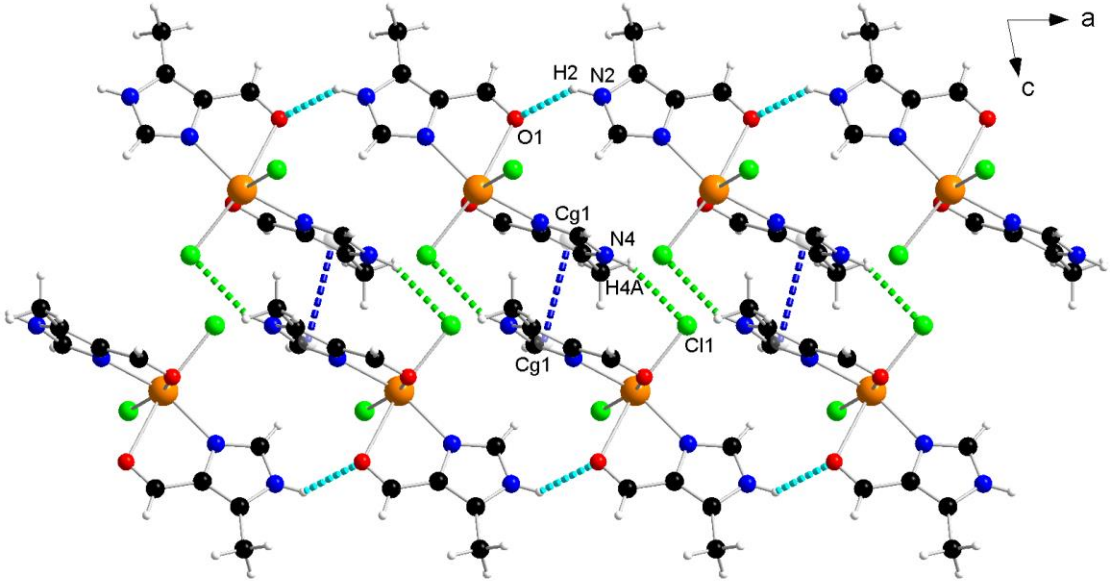
Figure S4. The ESI-MS spectrogram for CH_3OH/H_2O solution of complex **4**.

Table S2.
Bond lengths [Å] for complexes **1–4** obtained from X-ray analysis. Atoms numbering as in Fig. 1 (manuscript).

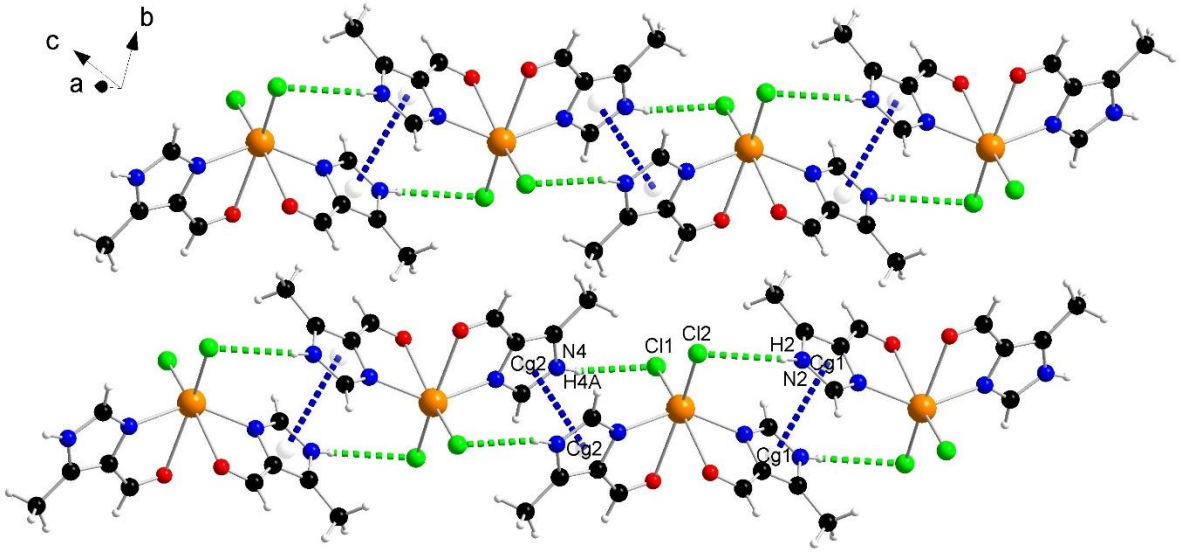
Bond lengths [Å]			
1			
Cd(1)-N(3)	2.248(5)	Cd(1)-Cl(2)	2.511(2)
Cd(1)-N(1)	2.260(5)	Cd(1)-O(2)	2.622(5)
Cd(1)-Cl(1)	2.504(2)	Cd(1)-O(1)	2.640(5)
2			
Cd(1)-N(3)	2.271(2)	Cd(1)-O(1)	2.609(2)
Cd(1)-N(1)	2.312(2)	Cd(1)-Br(2)	2.5970(4)
Cd(1)-O(2)	2.556(2)	Cd(1)-Br(1)	2.6587(4)
3			
Cd(1)-N(1)	2.270(3)	Cd(1)-O(1)a	2.718(3)
Cd(1)-N(1)a	2.270(3)	Cd(1)-I(1)	2.7874(4)
Cd(1)-O(1)	2.718(3)	Cd(1)-I(1)a	2.7874(4)
4			
Cd(1)-N(1)	2.260(3)	Cd(1)-O(2)	2.621(3)
Cd(1)-N(5)	2.263(3)	Cd(1)-O(3)	2.750(3)
Cd(1)-N(3)	2.299(3)	Cd(1)-O(4)	2.848(3)
Cd(1)-N(7)	2.307(3)	Cd(1)-O(1)	2.873(3)
a = 1-x, y, 0.5-z			

Table S3.
Valence angles [º] for complexes **1–4** obtained from X-ray analysis. Atoms numbering as in Fig. 1 (manuscript).

Angles [º]			
1			
N(3)-Cd(1)-N(1)	141.31(18)	Cl(1)-Cd(1)-O(1)	161.09(11)
N(3)-Cd(1)-Cl(1)	103.43(14)	Cl(2)-Cd(1)-O(1)	91.63(12)
N(1)-Cd(1)-Cl(1)	98.77(14)	N(3)-Cd(1)-O(2)	68.86(16)
N(3)-Cd(1)-Cl(2)	95.86(14)	N(1)-Cd(1)-O(2)	80.19(16)
N(1)-Cd(1)-Cl(2)	107.79(14)	Cl(1)-Cd(1)-O(2)	89.48(12)
Cl(1)-Cd(1)-Cl(2)	106.21(7)	Cl(2)-Cd(1)-O(2)	160.58(11)
N(3)-Cd(1)-O(1)	80.39(16)	O(1)-Cd(1)-O(2)	74.48(12)
N(1)-Cd(1)-O(1)	69.11(16)		
2			
N(3)-Cd(1)-N(1)	139.08(8)	O(2)-Cd(1)-O(1)	80.84(7)
N(3)-Cd(1)-O(2)	69.82(7)	Br(2)-Cd(1)-O(1)	168.42(5)
N(1)-Cd(1)-O(2)	84.19(7)	N(3)-Cd(1)-Br(1)	101.17(6)
N(3)-Cd(1)-Br(2)	105.87(6)	N(1)-Cd(1)-Br(1)	97.01(6)
N(1)-Cd(1)-Br(2)	104.57(6)	O(2)-Cd(1)-Br(1)	165.86(5)
O(2)-Cd(1)-Br(2)	88.84(5)	Br(2)-Cd(1)-Br(1)	104.388(13)
N(3)-Cd(1)-O(1)	75.56(8)	O(1)-Cd(1)-Br(1)	86.39(5)
N(1)-Cd(1)-O(1)	69.34(7)		
3			
N(1)a-Cd(1)-N(1)	130.51(13)	N(1)-Cd(1)-O(1)	67.98(13)
N(1)a-Cd(1)-I(1)	106.48(7)	N(1)-Cd(1)-O(1)a	72.54(13)
N(1)-Cd(1)-I(1)	103.01(7)	O(1)-Cd(1)-I(1)	91.30(7)
N(1)a-Cd(1)-I(1)a	103.01(7)	O(1)-Cd(1)-I(1)a	163.16(7)
N(1)-Cd(1)-I(1)a	106.48(7)	O(1)a-Cd(1)-I(1)	163.16(7)
I(1)-Cd(1)-I(1)a	105.130(16)	O(1)a-Cd(1)-I(1)a	91.30(7)
N(1)a-Cd(1)-O(1)a	67.98(13)	O(1)-Cd(1)-O(1)a	72.60(13)
N(1)a-Cd(1)-O(1)	72.54(13)		
4			
N(1)-Cd(1)-O(3)	79.20(11)	O(1)-Cd(1)-N(7)	79.00(11)
N(1)-Cd(1)-O(1)	65.74(11)	O(1)-Cd(1)-O(4)	125.28(11)
N(1)-Cd(1)-N(5)	128.68(12)	O(1)-Cd(1)-O(2)	136.07(11)
N(1)-Cd(1)-N(7)	95.43(11)	O(1)-Cd(1)-N(3)	150.80(11)
N(1)-Cd(1)-O(4)	151.94(11)	N(5)-Cd(1)-N(7)	98.89(11)
N(1)-Cd(1)-O(2)	82.23(10)	N(5)-Cd(1)-O(4)	76.62(11)
N(1)-Cd(1)-N(3)	112.12(12)	N(5)-Cd(1)-O(2)	149.09(10)
O(3)-Cd(1)-O(1)	75.75(11)	N(5)-Cd(1)-N(3)	95.74(11)
O(3)-Cd(1)-N(5)	66.99(11)	N(7)-Cd(1)-O(4)	65.41(11)
O(3)-Cd(1)-N(7)	154.16(11)	N(7)-Cd(1)-O(2)	74.82(10)
O(3)-Cd(1)-O(4)	126.99(11)	N(7)-Cd(1)-N(3)	129.22(11)
O(3)-Cd(1)-O(2)	128.49(11)	O(4)-Cd(1)-O(2)	73.26(11)
O(3)-Cd(1)-N(3)	75.32(11)	O(4)-Cd(1)-N(3)	71.34(11)
O(1)-Cd(1)-N(5)	65.74(11)	O(2)-Cd(1)-N(3)	68.17(10)
a = 1-x, y, 0.5-z			

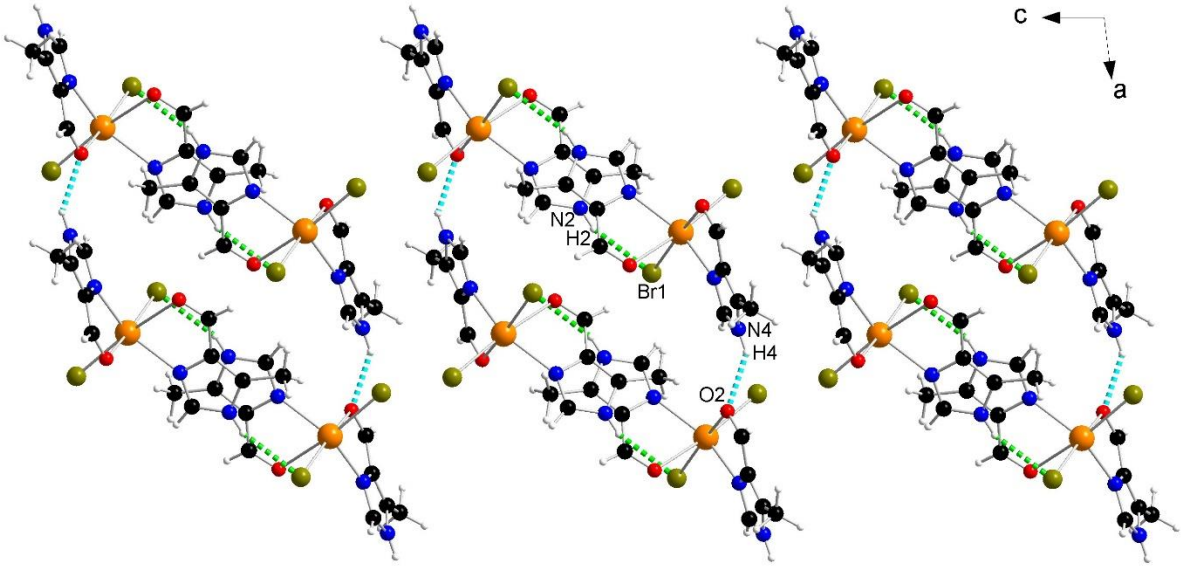


(a)

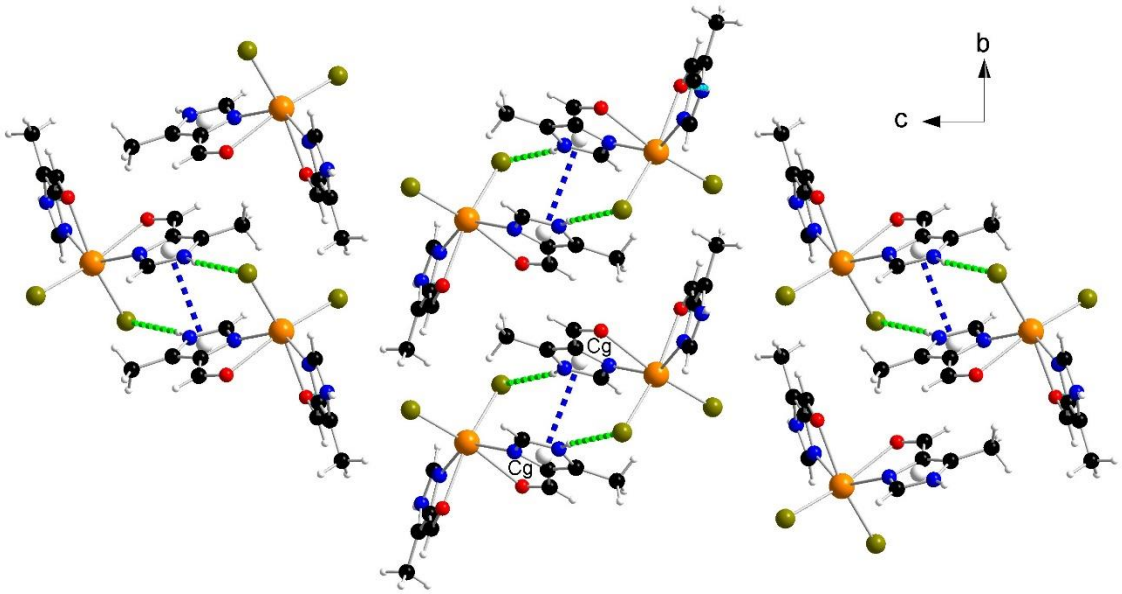


(b)

Figure S5. The geometry of non-covalent interactions in the crystal structure of complex **1**.



(a)



(b)

Figure S6. The geometry of hydrogen bonds (**a**) and π-π stacking interactions (**b**) in the crystal structure of complex **2**.

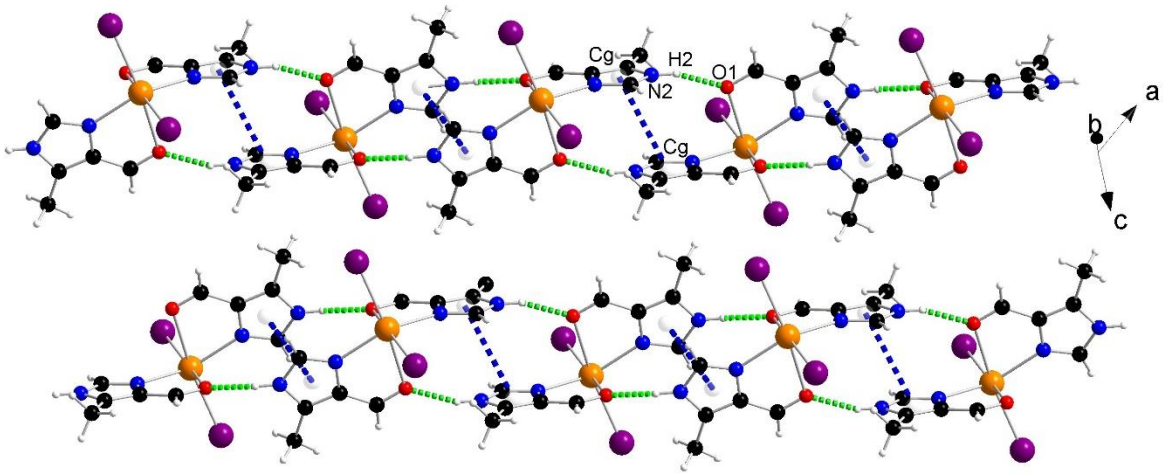
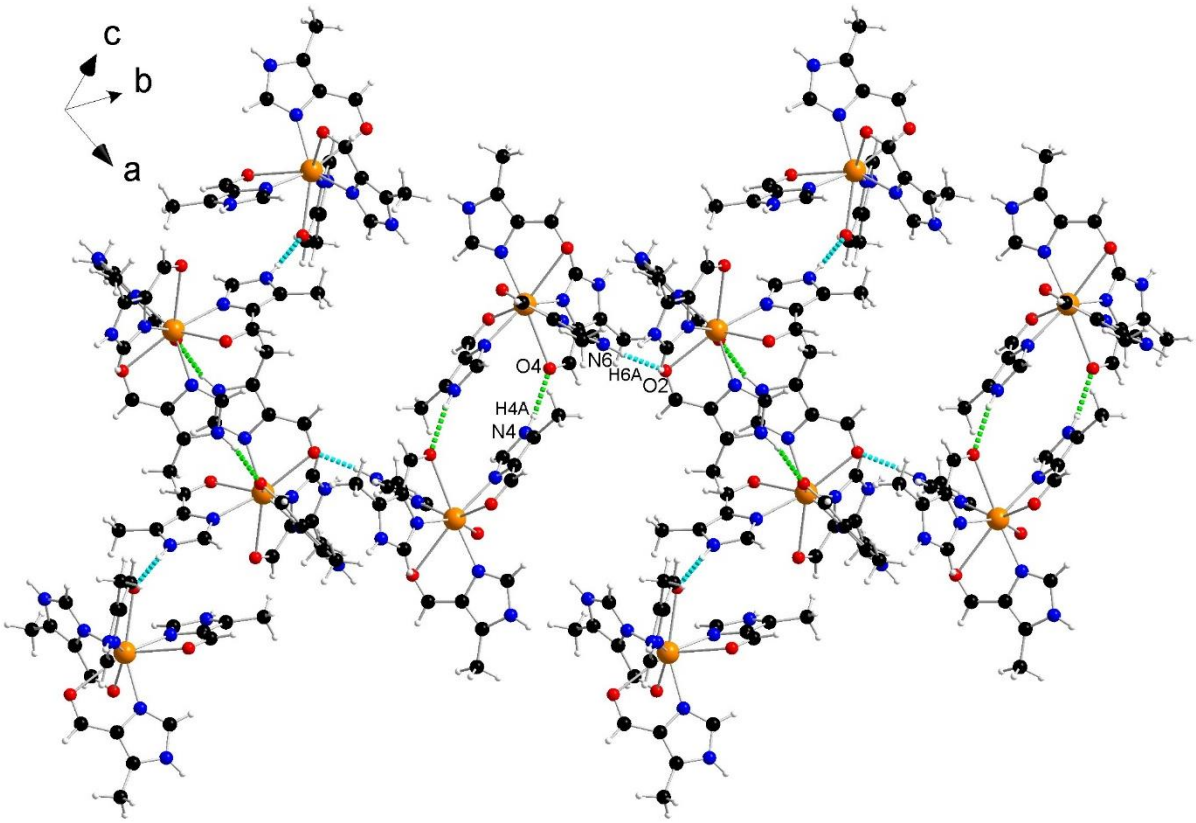
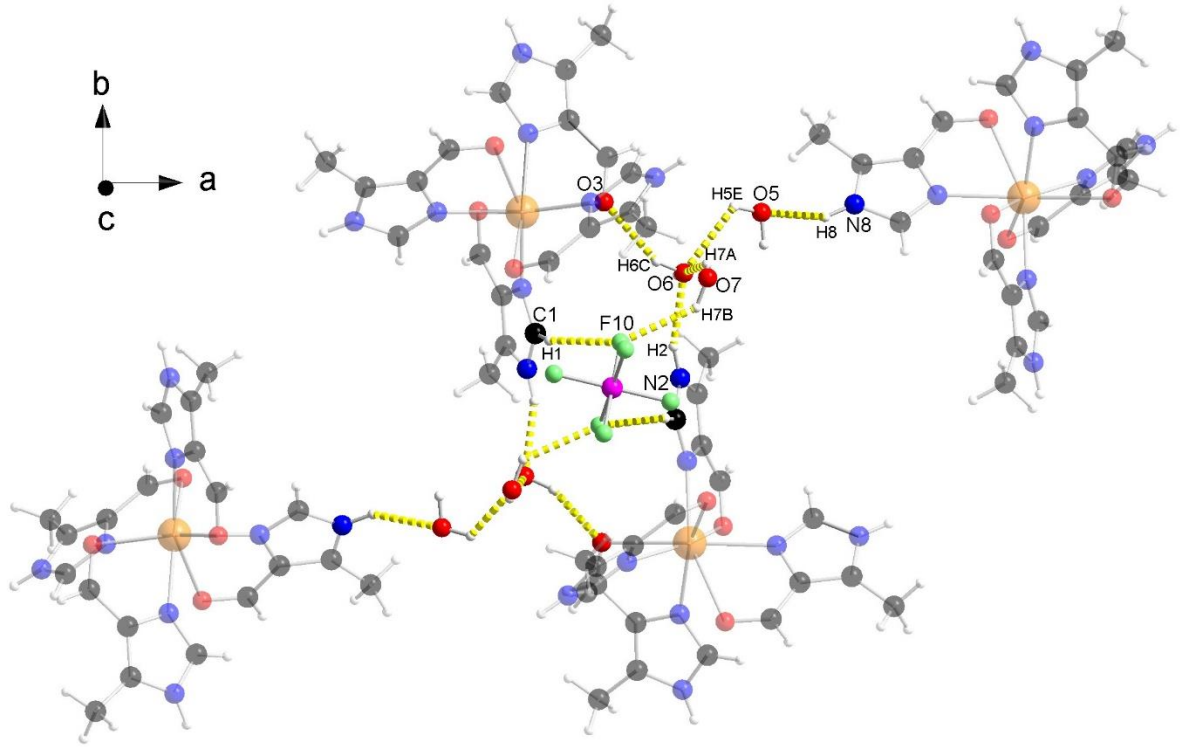


Figure S7. The geometry of non-covalent interactions in the crystal structure of complex **3**.



(a)



(b)

Figure S8. The geometry of N–H···O hydrogen bonds (**a**) and H-bonds formed by H_2O and PF_6^- anions (**b**) in the crystal structure of complex **4**.

Table S4.
The geometry of the most important hydrogen bonds in the crystal structures of complexes **1–4**. Atoms numbering as in Fig. 1 (manuscript).

D–H···A	D–H [Å]	H···A [Å]	D···A [Å]	D–H···A [º]	Symmetry code
1					
N2–H2···O1	0.880	2.432	3.061	128.83	-1+x, y, z
N4–H4A···Cl1	0.880	2.449	3.234	148.66	1-x, 1-y, 2-z
N2–H2···Cl2	0.880	2.626	3.340	139.04	-x, 2-y, 1-z
2					
N4–H4···O2	0.880	2.142	2.891	142.60	1+x, y, z
N2–H2···Br1	0.880	2.566	3.407	160.21	-x, -y, 1-z
3					
N2–H2···O1	0.880	1.990	2.811	154.66	0.5+x, 1.5-y, 0.5+z
4					
N6–H6A···O2	0.880	1.867	2.743	173.67	-0.25+x, 1.25-y, -0.25+z
N2–H2···O6	0.880	1.976	2.819	160.16	1-x, 1.5-y, z
N4–H4A···O4	0.880	2.030	2.858	156.49	1-x, 1-y, 1-z
N8–H8···O5	0.880	2.234	2.988	143.62	–
O6–H6C···O3	0.850	2.234	2.853	129.67	–
O7–H7A···O6	0.849	2.103	2.843	145.30	–
O5–H5E···O6	0.850	2.414	2.951	121.80	0.5+x, y, 0.5-z
O7–H7B···F10	0.850	2.205	2.864	134.26	–
C1–H1···F10	0.949	2.286	3.137	148.90	–

Table S5.
Selected FT-IR spectroscopic data for ligand (L) and complexes **1–4**.

Compound	Vibration band (cm^{-1})				$\Delta\nu$	
	$\nu(OH)_{H2O}$	ν(C=O)	ν(C=C, C=N)	$\nu(PF_6^-)$	(C=O)	(C=N)
L	-	1664	1512, 1439	-	-	-
1	-	1642, 1616	1516, 1436	-	48	3
2	-	1659, 1619	1512, 1445	-	45	6
3	-	1622 broad	1519, 1449	-	42	10
4	3653 broad	1650, 1623	1523, 1451	830	41	12

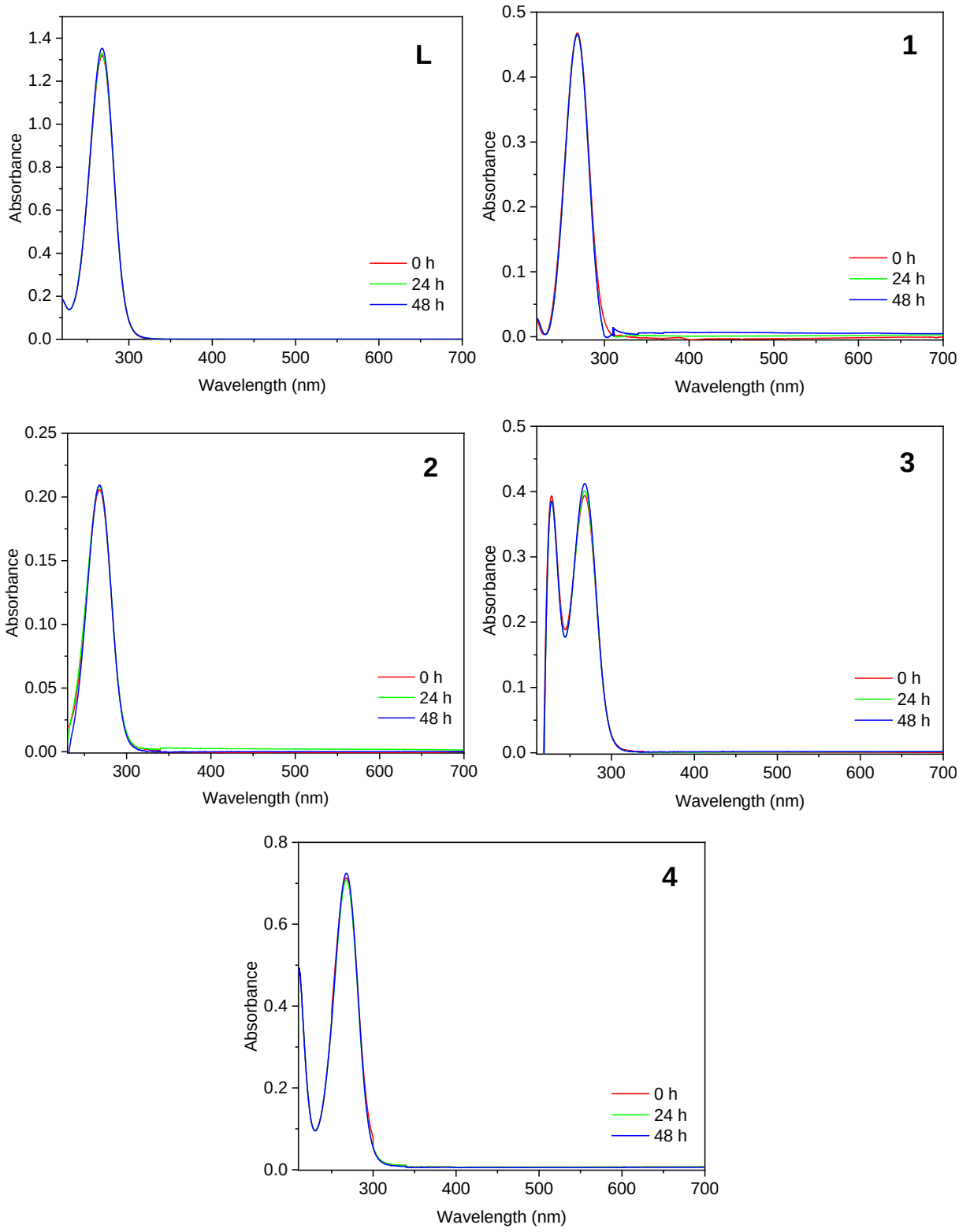


Figure S9. The stability studies of ligand (**L**) and complexes **1–4** in TE40 buffer monitored by UV-Vis at three different time points (0, 24, and 48h). [**L**] = $1 \cdot 10^{-4}$ M, [**1–4**] = $1 \cdot 10^{-5}$ M.

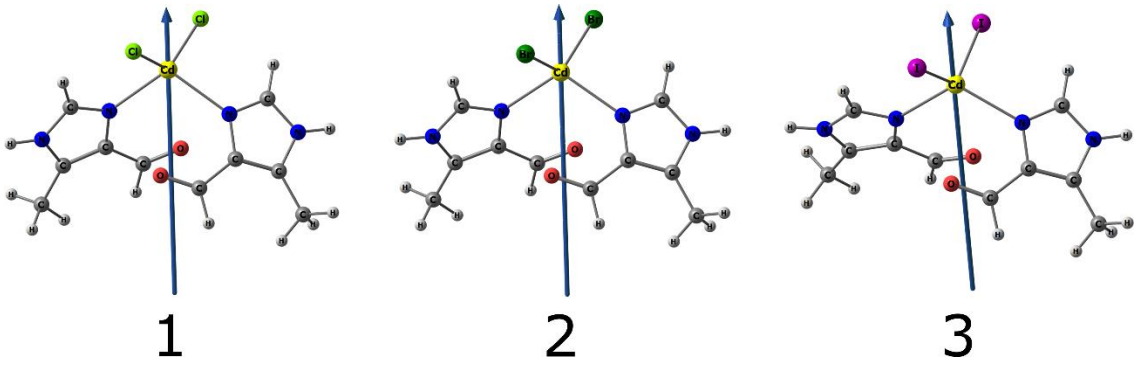


Figure S10. The equilibrium geometries of gas-phase optimized **1**–**3** compounds with corresponding dipole moment vectors.

Table S6.
Results of the FBO analysis of the bonds formed by Cd(II) ion within the studied coordination compounds. The bond lengths are given in Å, whereas FBO is a dimensionless quantity.

System	Bond	Crystal structure		Gas phase structure	
		Bond Length	FBO	Bond Length	FBO
1	Cd-Cl	2.504	1.160	2.410	1.280
	Cd-Cl	2.513	1.151	2.410	1.280
	Cd-N	2.261	0.813	2.285	0.819
	Cd-N	2.247	0.822	2.285	0.819
	Cd-O	2.630	0.489	3.312	0.162
	Cd-O	2.629	0.491	3.312	0.162
2	Cd-Br	2.658	1.146	2.532	1.317
	Cd-Br	2.597	1.230	2.532	1.317
	Cd-N	2.312	0.774	2.279	0.823
	Cd-N	2.272	0.799	2.279	0.823
	Cd-O	2.610	0.503	3.232	0.188
	Cd-O	2.557	0.543	3.232	0.188
3	Cd-I	2.787	1.194	2.700	1.319
	Cd-I	2.786	1.195	2.734	1.252
	Cd-N	2.271	0.811	2.267	0.833
	Cd-N	2.271	0.811	2.281	0.813
	Cd-O	2.7079	0.440	3.214	0.187
	Cd-O	2.7079	0.440	3.001	0.286
4	Cd-N	2.255	0.851	2.316	0.692
	Cd-N	2.298	0.808	2.316	0.692
	Cd-N	2.266	0.840	2.316	0.692
	Cd-N	2.304	0.804	2.315	0.692
	Cd-O	2.753	0.431	2.655	0.371
	Cd-O	2.874	0.351	2.655	0.372
	Cd-O	2.620	0.514	2.655	0.372
	Cd-O	2.847	0.373	2.654	0.372

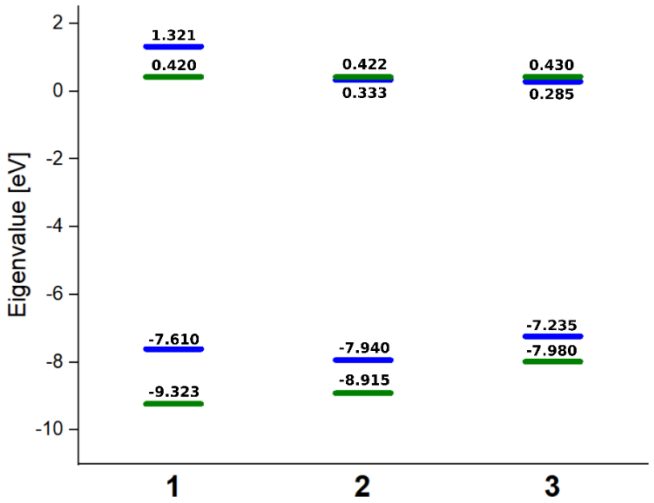


Figure S11. The eigenvalues of **1**–**3** compounds' frontier orbitals. The values marked by green and blue correspond to gas-phase and crystal structures respectively.

Table S7.
The molecular volumes of **1**–**4** systems calculated numerically with the use of the marching terathedra method (in $Å^3$).

System	Volume	
	Crystal structure	Gas-phase structure
1	349.10	361.04
2	365.86	377.62
3	392.39	404.96
4	849.80*	537.67

*value affected by a presence of hexafluorophosphate anions and water molecules in a crystal structure **Table S8.**

Table S8.
The values of Molecular Polarity Index (MPI) of **1**–**4** systems (in $kcal \cdot mol^{-1}$).

System	MPI	
	Crystal structure	Gas-phase structure
1	34.62	27.94
2	34.40	27.74
3	33.19	26.97

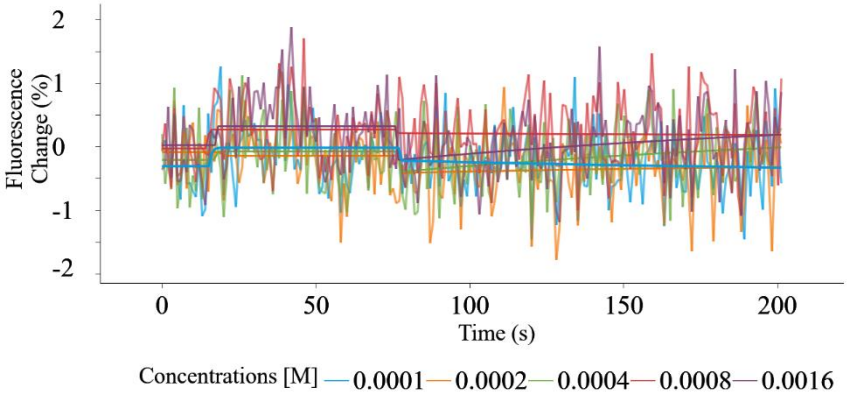


Figure S12. Results showing changes in fluorescence over time occurring during the analysis of the interactions of the ligand with the DNA helix performed in the static mode (weak binders) at a temperature of 25 °C.

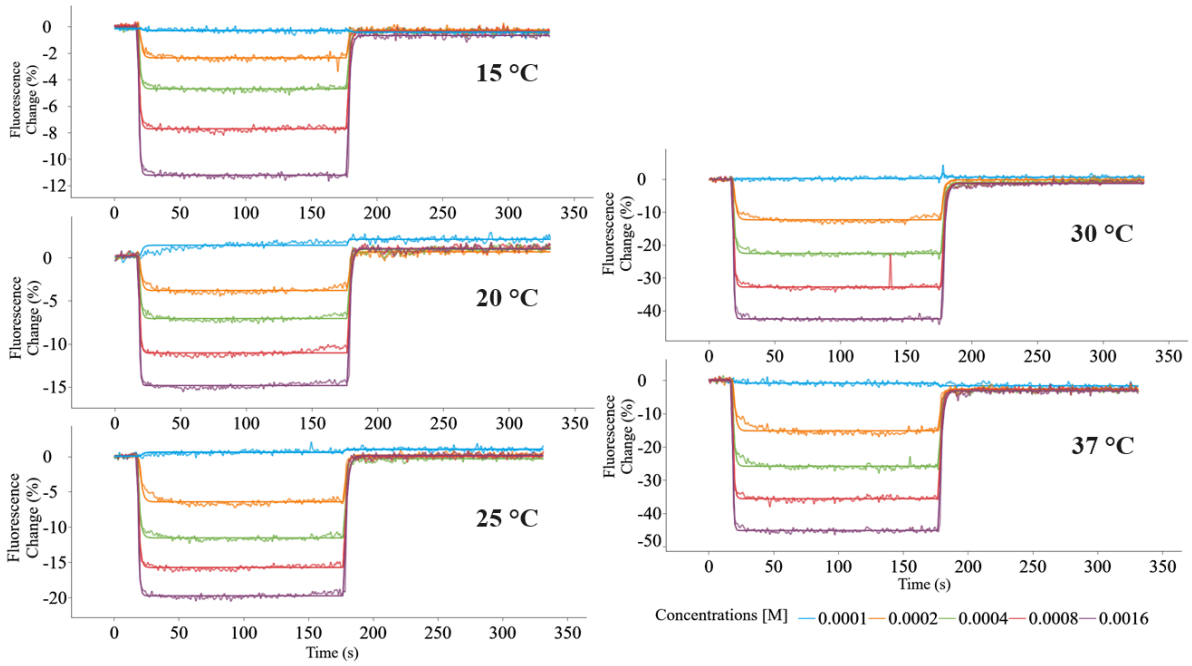


Figure S13. Representative results showing changes in fluorescence over time occurring during the analysis of the interactions of the complex **2** with the DNA helix performed in the static mode (weak binders) at temperatures: 15, 20, 25, 30, and 37 °C. The thinner lines in each color represent the measurement points and the bold line represents the fitted data from which the kinetic parameters are calculated.

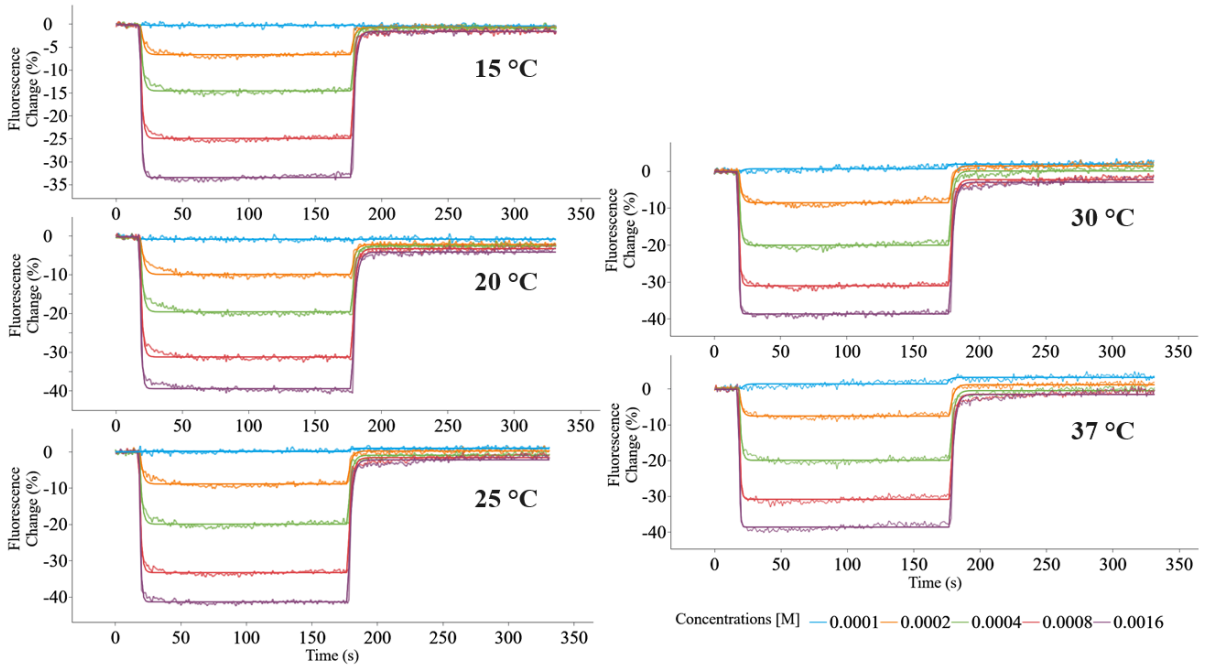


Figure S14. Representative results showing changes in fluorescence over time occurring during the analysis of the interactions of the complex **3** with the DNA helix performed in the static mode (weak binders) at temperatures: 15, 20, 25, 30, and 37 °C. The thinner lines in each color represent the measurement points and the bold line represents the fitted data from which the kinetic parameters are calculated.

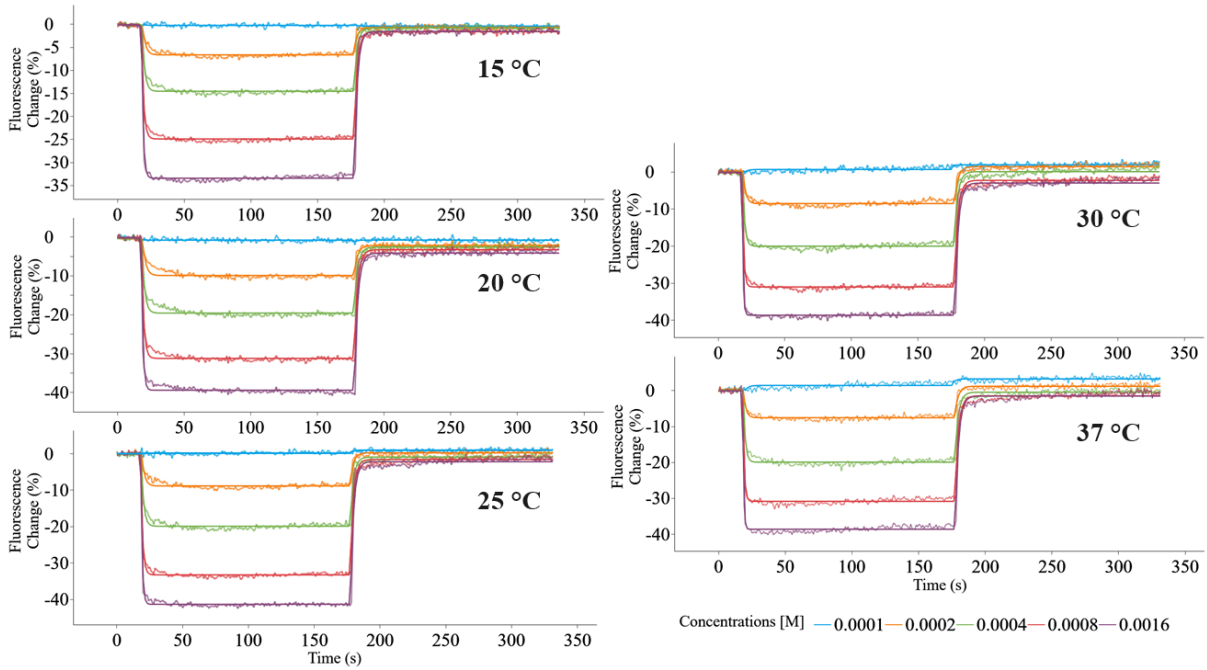


Figure S15. Representative results showing changes in fluorescence over time occurring during the analysis of the interactions of the complex **4** with the DNA helix performed in the static mode (weak binders) at temperatures: 15, 20, 25, 30, and 37 °C. The thinner lines in each color represent the measurement points and the bold line represents the fitted data from which the kinetic parameters are calculated.

Table S9. The determined values of thermodynamic parameters ΔG (Gibbs free energy), ΔH (enthalpy), and ΔS (entropy) for **1–4** are based on their association constant K_A. All thermodynamic parameters were computed as given in eqs. 1–3, respectively.

Compound	Temp. [°C]	ΔG [kJ·mol^{-1}]	ΔS [kJ·mol^{-1}·K^{-1}]	ΔH [kJ·mol^{-1}]
1	15	–15.08	–	–
	20	–16.08	0.20	42.07
	25	–17.30	0.24	55.45
	30	–17.42	0.02	–10.06
	37	–18.13	0.10	13.50
2	15	–14.90	–	–
	20	–16.57	0.33	81.20
	25	–16.33	–0.05	–30.34
	30	–17.75	0.28	68.00
	37	–18.53	0.11	16.22
3	15	–13.35	–	–
	20	–14.55	0.24	55.62
	25	–15.07	0.10	15.69
	30	–16.44	0.27	66.77
	37	–17.52	0.15	30.19
4	15	–15.29	–	–
	20	–16.32	0.21	44.19
	25	–16.75	0.09	8.82
	30	–18.89	0.43	110.80
	37	–19.34	0.06	0.61

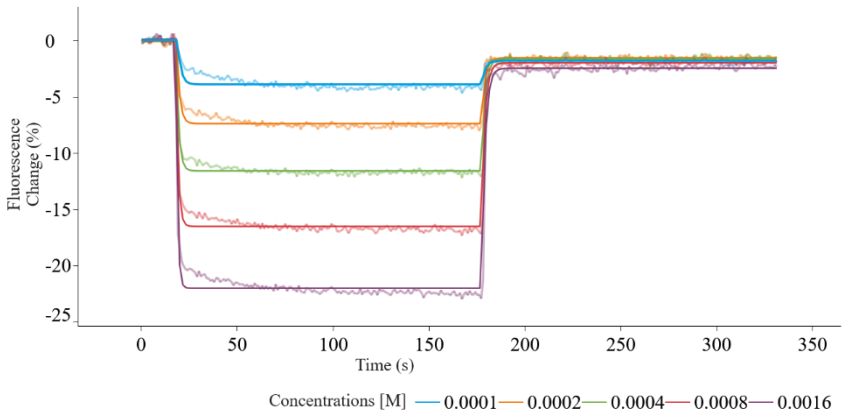


Figure S16. Result showing changes in fluorescence over time occurring during the analysis of the interactions of the salt $CdCl_2$ with the DNA helix performed in the static mode (weak binders) at temperature 25 °C.

Table S10. Values (along with their standard deviations in the parentheses) of determined association rates k_a (in $[M^{-1} \cdot s^{-1}]$), dissociation rates k_d (in $[s^{-1}]$), associations constants K_A (in $[M^{-1}]$), and dissociation constants K_D (in [M]) for salt $CdCl_2$ interactions with DNA measured by switchSense technique at temperature 25 °C.

Compound	Temp. [°C]	k_a $[M^{-1} \cdot s^{-1}]$	k_d $[s^{-1}]$	K_A $[M^{-1}]$	K_D [M]
$CdCl_2$	25	373 ± 35	$(5.78 \pm 0.14) \cdot 10^{-1}$	644 ± 62	$(1.55 \pm 0.15) \cdot 10^{-3}$

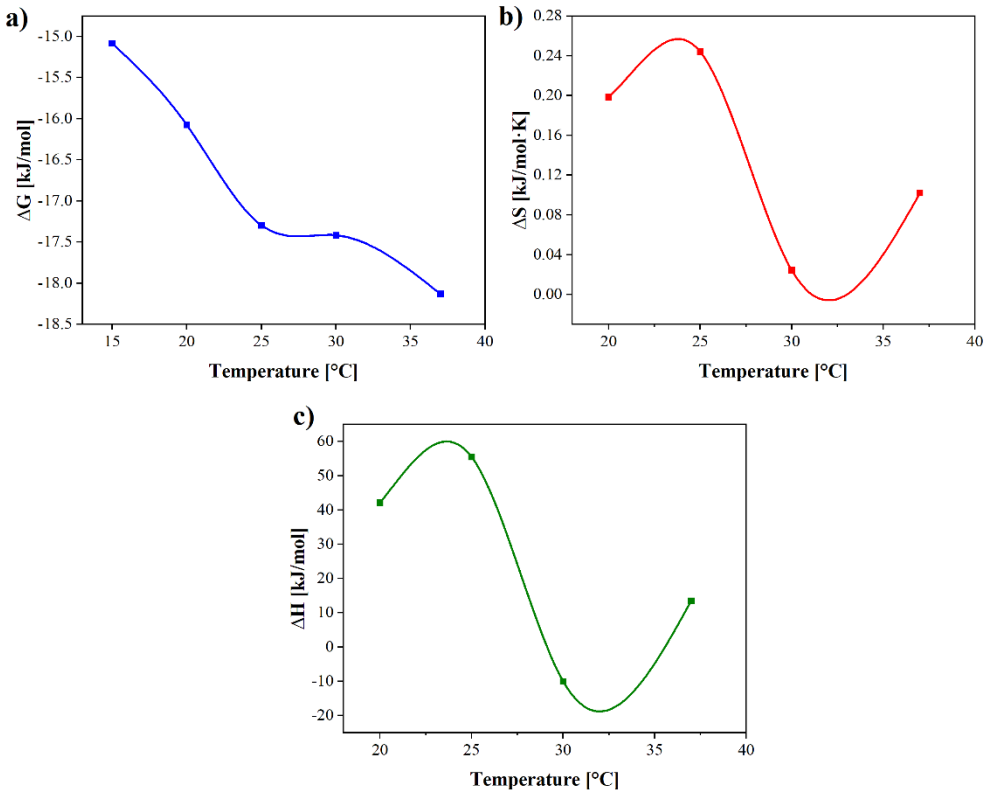


Figure S17. Dependence of the change of **a)** Gibbs free energy (ΔG), **b)** enthalpy (ΔH), and **c)** entropy (ΔS) as a function of temperature for the complex **1**.

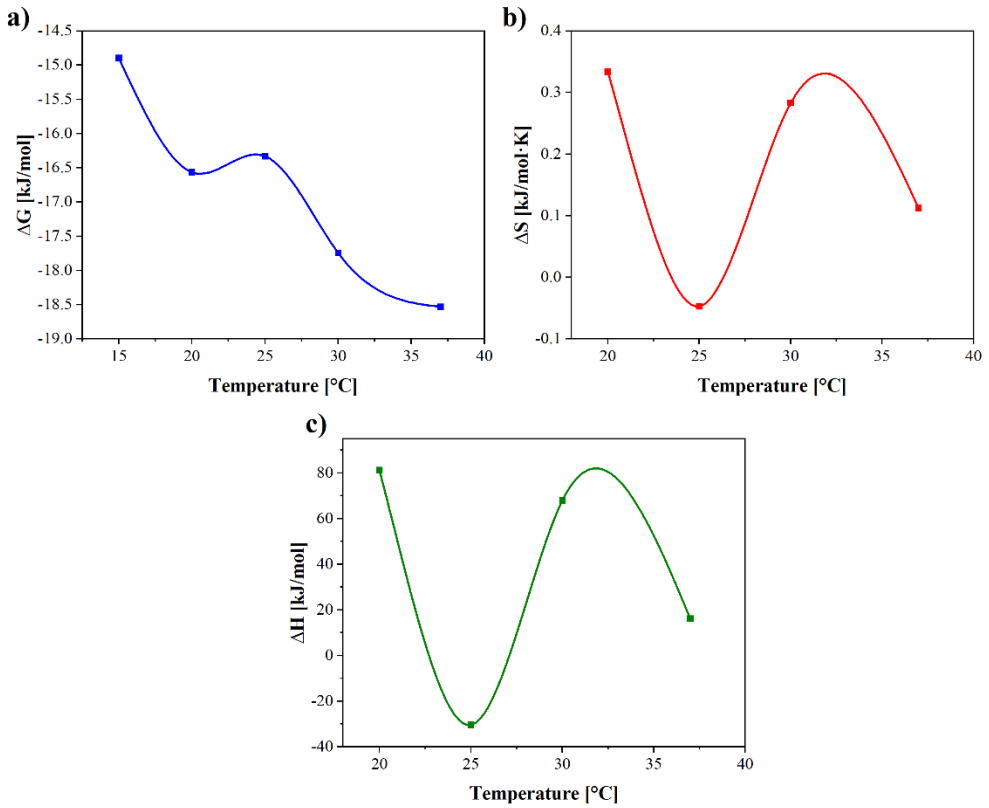


Figure S18. Dependence of the change of **a)** Gibbs free energy (ΔG), **b)** enthalpy (ΔH), and **c)** entropy (ΔS) as a function of temperature for the complex **2**.

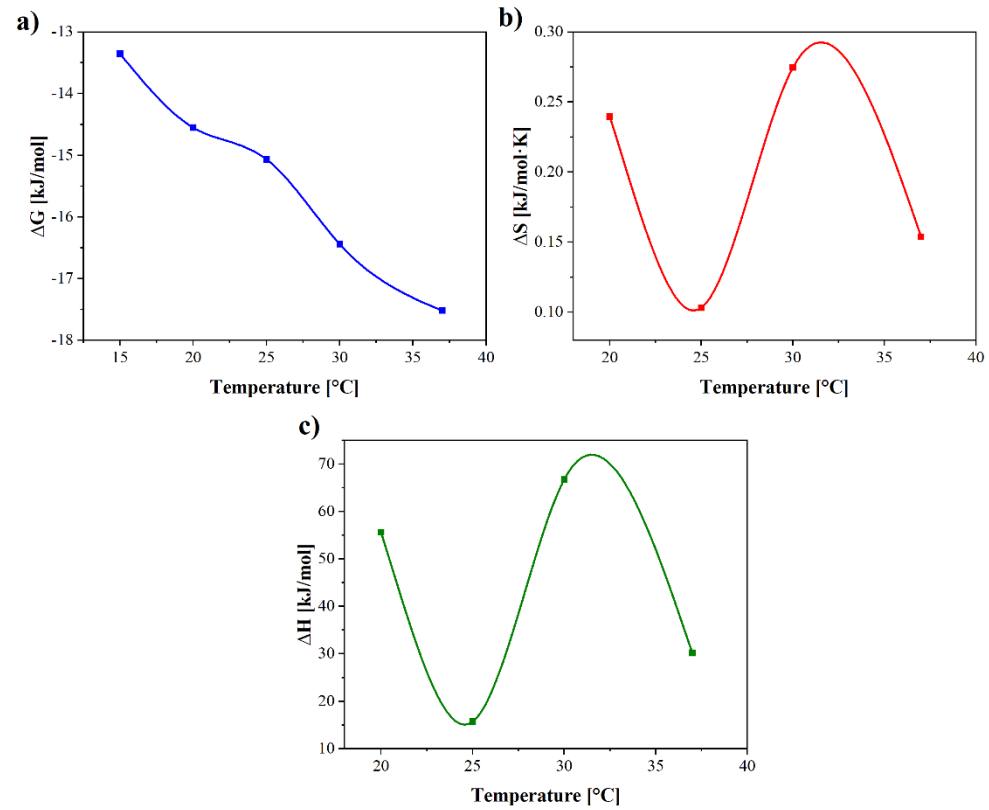


Figure S19. Dependence of the change of **a)** Gibbs free energy (ΔG), **b)** enthalpy (ΔH), and **c)** entropy (ΔS) as a function of temperature for the complex **3**.

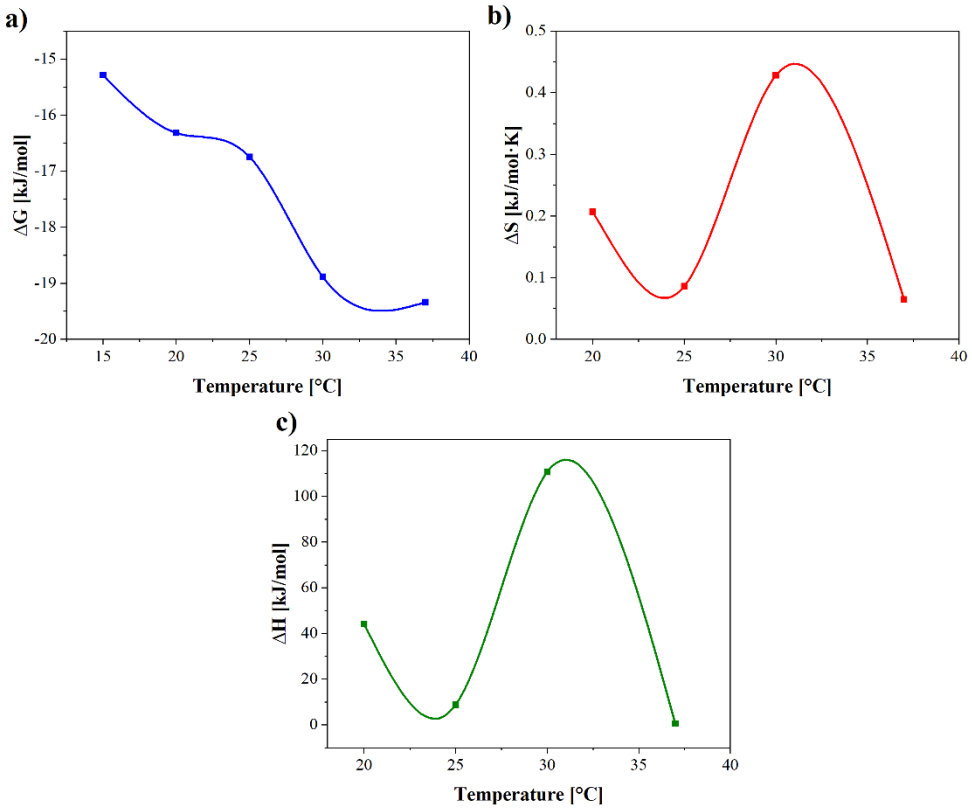


Figure S20. Dependence of the change of **a)** Gibbs free energy (ΔG), **b)** enthalpy (ΔH), and **c)** entropy (ΔS) as a function of temperature for the complex **4**.