Supplementary Information

Probing the Competition between Acetate and 2,2'-Bipyridine Ligands to Bind to d-Block 12 Group Metals: Molecular and Structural Diversity towards High-Efficiency Luminescent Materials

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Table S1. Crystal data and refinement parameters for the crystal structures of complexes reported in this work.

		1A	**1B**	**1C**	**1D**	**2A**	**2B**	**3A**	**3B**
Chemical formula		$C_{32}H_{34}N_4O_{12}Zn_3$	$C_{14}H_{20}N_2O_7Zn$	$C_{24}H_{23}N_4O_{4.5}Zn$	$C_{68}H_{86}N_{12}O_{21}Zn_2$	$C_{14}H_{20}N_2O_7Cd$	$C_{29}H_{32}N_5O_7Cd$	$C_{14}H_{16}N_2O_5Hg$	$C_{29}H_{42}N_5O_{12}Hg$
Fw ($g.mol^{-1}$)		862.80	393.71	504.85	1538.27	440.73	675.01	492.88	853.27
Cryst syst		Triclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group		*P -1*	*C 2/c*	*P -1*	*P 2₁/c*	*C 2/c*	*P -1*	*P 2₁/c*	*P 2₁/c*
Z		1	8	2	4	8	2	4	4
T (K)		296(2)	296(2)	293(2)	296(2)	296(2)	296(2)	296(2)	296(2)
Unit cell	*a* (Å)	8.0907(3)	20.1431(8)	9.316(13)	23.6688(15)	11.4204(12)	8.9084(10)	10.255(2)	12.380(2)
dimensions	*b* (Å)	9.8783(5)	8.0764(4)	13.037(18)	13.4856(9)	21.689(3)	12.5072(15)	12.619(2)	19.659(3)
	c (Å)	12.7432(6)	21.7544(9)	13.162(16)	24.0246(15)	15.3958(17)	14.9281(18)	13.064(2)	15.164(2)
	α (deg)	106.076(2)	90	61.74(3)	90	90	105.185(8)	90	90
	β (deg)	98.523(2)	97.401(2)	81.33(4)	105.012(3)	97.293(3)	99.615(8)	108.023(4)	108.148(9)
	γ (deg)	108.795(2)	90	85.11(4)	90	90	102.311(8)	90	90
V ($Å^3$)		894.34(7)	3509.6(3)	1392.0(3)	7406.7(8)	3782.6(8)	1523.8(3)	1607.7(5)	3507.0(9)
ρ_{calc} ($g.cm^{-3}$)		1.602	1.490	1.205	1.380	1.548	1.471	2.036	1.616
Absorption coefficient μ (mm^{-1})		2.062	1.436	0.916	0.728	1.189	0.769	9.598	4.454
absortpion correc.		multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
T_{min}/T_{max}		0.769	0.853	0.849	0.888	0.839	0.865	0.712	0.552
θ range for data collection (°)		1.723 - 25.366	2.039-25.398	1.774 - 26.172	1.747 - 25.096	2.03 – 25.53	1.455 - 25.072	2.301 - 25.367	1.731 - 25.41
index ranges	*h*	-9 to 9	-24 to 23	-11 to 11	-21 to 28	-13 to 13	-10 to 10	-11 to 12	-14 to 14
	k	-9 to 11	-4 to 9	-15 to 15	-16 to 15	-25 to 26	-12 to 14	-12 to 15	-23 to 23

l	-15 to 10	-26 to 26	-16 to 15	-28 to 25	-18 to 17	-17 to 17	-15 to 10	-18 to 18
Data collected	7034	8633	17146	35549	9433	14308	7450	27026
Unique reflections	3210	3188	5243	13019	3493	5339	2919	6429
Symmetry factor (R_{int})	0.0214	0.0324	0.0367	0.0727	0.0422	0.0432	0.0483	0.0713
Completeness to θ = 25° (%)	98.2	99.0	98.8	99.3	99.3	99.2	99.1	99.9
F(000)	440	1632	522	3224	1776	690	936	1708
Refined parameters	235	217	308	928	217	381	199	424
Goodness-of-fit on F^2 $(S)^a$	1.045	1.054	1.150	0.993	1.042	1.026	0.948	0.984
Final $R_1{}^b$ factor [$I > 2\sigma(I)$]	0.0245	0.0363	0.0970	0.0741	0.0619	0.0443	0.0411	0.0382
$wR_2{}^c$ factor (all data)	0.068	0.0963	0.2980	0.2383	0.1877	0.096	0.0917	0.0958
Largest diff. peak / hole (e Å^{-3})	0.325/-0.236	0.713/-0.375	1.977/-0.51	1.094/-0.528	2.493/-0.771	0.383/-0.446	0.973/-0.905	0.612/ -0.758
CCDC deposit no.	1538392	1522500	1522502	1538395	1522495	1538396	1538397	1522503

Table S2. Selected bond lengths and angles of the coordination complexes determined in this study.

Complex **1A**		Complex **1B**		Complex **1C**		Complex **1D**	
Zn1–O4	1.991(2)	Zn1 – N1	2.117(2)	Zn1 – N1	2.065(7)	Zn1–N1	2.139(5)
Zn1–O2	2.015(18)	Zn1 – N2	2.149(2)	Zn1 – N2	2.077(6)	Zn1–N2	2.157(5)
Zn1–O5	2.017(11)	Zn1 – O1	2.106(2)	Zn1 – N3	2.083(5)	Zn1–N3	2.158(5)
Zn1–N2	2.143(2)	Zn1 – O2	2.326(2)	Zn1 – N4	2.120(6)	Zn1–N4	2.142(4)
Zn1–N1	2.147(16)	Zn1 – O3W	2.079(2)	Zn1 – O1	2.164(7)	Zn1–N5	2.170(5)
Zn2–O1	2.068(15)	Zn1 – O4	2.046(2)	Zn1 – O2	2.188(6)	Zn1–N6	2.152(5)
Zn2–O3	2.093(18)						
Zn2–O5	2.185(17)	N1 – Zn1 – N2	76.585(9)	N1 – Zn1 – N2	76.867(5)	N1–Zn1–N2	76.906(2)
		N1 – Zn1 – O1	153.876(9)	N1 – Zn1 – N3	97.349(6)	N1–Zn1–N3	96.283(19)
O1–Zn2–O3	92.568(7)	N1—Zn1—O2	97.290(8)	N1 – Zn1 – N4	174.535(8)	N1–Zn1–N4	96.935(19)
O1–Zn2–O5	89.676(6)	N1 – Cd1 – O3W	92.664(9)	N1 – Zn1 – O1	93.111(6)	N1–Zn1–N5	166.032(2)
O3–Zn2–O5	88.041(6)	N1—Zn1—O4	105.277(9)	N1 – Zn1 – O2	94.522(7)	N1–Zn1–N6	94.417(2)
O4–Zn1–O2	97.528(7)	N2 – Zn1 – O1	92.728(9)	N2 – Zn1 – N3	103.743(5)	N2–Zn1–N3	94.713(19)
O4–Zn1–O5	98.296(7)	N2 – Zn1 – O2	90.344(9)	N2 – Zn1 – N4	103.150(6)	N2–Zn1–N5	93.835(19)
O4–Zn1–N2	161.002(7)	N2 – Zn1 – O3W	168.851(9)	N2 – Zn1 – O1	154.237(6)	N3–Zn1–N5	94.872(19)
O4–Zn1–N1	85.738(7)	N2 – Zn1 – O4	90.874(9)	N2 – Zn1 – O2	97.545(6)	N4–Zn1–N2	168.242(19)
O2–Zn1–O5	100.416(7)	O1 – Zn1 – O2	58.491(8)	N3 – Zn1 – N4	77.300(6)	N4–Zn1–N3	75.830(19)
O2–Zn1–N2	88.749(7)	O1 – Zn1 – O3W	95.845(9)	N3 – Zn1 – O1	101.025(6)	N4–Zn1–N5	93.923(19)
O2–Zn1–N1	117.760(6)	O1 – Zn1 – O4	98.563(9)	N3– Zn1 – O2	157.482(7)	N4–Zn1–N6	96.536(19)
O5–Zn1–N2	98.166(6)	O2 – Zn1 – O3W	88.082(9)	O1 – Zn1 – O2	59.152(5)	N6–Zn1–N2	93.943(19)
O5–Zn1–N1	140.830(6)	O2 – Zn1 – O4	157.054(7)			N6–Zn1–N3	167.524(19)
N2–Zn1–N1	75.502(6)	O3W – Zn1 – O4	94.873(9)			N6–Zn1–N5	75.585(19)

Complex **2A**		Complex **2B**		Complex **3A**		Complex **3B**	
Cd1—N1	2.337(7)	Cd1–O4	2.340(3)	Hg1–O1	2.1865(5)	Hg1 – N1	2.366(4)
Cd1—N2	2.352(7)	Cd1–O2	2.374(3)	Hg1–N2	2.3205(7)	Hg1 – N2	2.255(6)
Cd1 – O1	2.368(7)	Cd1–N4	2.395(4)	Hg1–N1	2.3292(7)	Hg1 – N3	2.380(4)
Cd1 – O2	2.463(7)	Cd1–N1	2.435(3)	Hg1–O3	2.3594(5)	Hg1 – N4	2.255(5)
Cd1 – O3	2.327(7)	Cd1–N2	2.437(4)			Hg1 – O3	2.534(4)
Cd1 – O4	2.478(5)	Cd1–N3	2.448(3)			Hg1 – O4	2.515(4)
Cd1 – O1W	2.259(6)						
						N1 – Hg1 – N2	71.974(16)
O1 – Cd1 – O2	53.035(2)	O4–Cd1–O2	87.501(11)	O1–Hg1–N2	127.772(2)	N1 – Hg1 – N3	124.489(15)
O1 – Cd1 – O3	85.222(2)	O4–Cd1–N4	128.099(10)	O1–Hg1–N1	129.231(2)	N1 – Hg1 – N4	102.662(16)
O1 – Cd1 – O4	138.456(18)	O4–Cd1–N1	97.312(12)	O1–Hg1–O3	116.895(2)	N1 – Hg1 – O3	98.181(14)
O2 – Cd1 – O3	127.041(2)	O4–Cd1–N2	78.687(11)	N2–Hg1–N1	70.929(2)	N1 – Hg1 – O4	138.089(14)
O2 – Cd1 – O4	157.656(18)	O4–Cd1–N3	164.301(10)	N2–Hg1–O3	104.563(2)	N2 – Hg1 – N3	104.258(16)
O3 – Cd1 – O4	53.767(2)	O2–Cd1–N4	112.936(12)	N1–Hg1–O3	96.749(2)	N2 – Hg1 – N4	170.002(18)
N1 – Cd1 – O1	114.970(2)	O2–Cd1–N1	148.020(12)			N2 – Hg1 – O3	101.453(15)
N1 – Cd1 – O2	81.383(2)	O2–Cd1–N2	82.815(12)			N2 – Hg1 – O4	86.171(14)

N1 – Cd1 – O3	151.358(2)	O2–Cd1–N3	82.465(11)	N3 – Hg1 – N4	71.454(16)
N1 – Cd1 – O4	101.878(2)	N4–Cd1–N1	88.824(12)	N3 – Hg1 – O3	135.132(14)
N2 – Cd1 – O1	91.879(3)	N4–Cd1–N2	147.471(11)	N3– Hg1 – O4	94.968(14)
N2 – Cd1 – O2	118.125(2)	N4–Cd1–N3	67.295(10)	O3 – Zn1 – O4	50.831(13)
N2 – Cd1 – O3	90.678(2)	N1–Cd1–N2	67.372(12)		
N2 – Cd1 – O4	83.227(2)	N1–Cd1–N3	85.133(11)		
O1W – Cd1 – N1	95.956(3)	N2–Cd1–N3	88.069(11)		
O1W – Cd1 – N2	154.698(2)				
O1W – Cd1 – O1	113.285(3)				
O1W – Cd1 – O2	78.133(2)				
O1W – Cd1 – O3	93.897(3)				
O1W – Cd1 – O4	79.541(2)				
O1 – Cd1 – O2	53.035(2)				
O1 – Cd1 – O3	85.222(2)				
O1W – Cd1 – O4	79.541(2)				

Table S3. Geometry of selected hydrogen bonds found in crystal structures of coordination complexes determined here.

D—H···A	D—H (Å)	H···A (Å)	D···A (Å)	D—H···A (deg)
		Complex **1A**		
C_2—H_2···O_2	0.93	2.70	3.262(3)	120
C_4—H_4···O_6	0.93	2.49	3.390(4)	162
C_7—H_7···O_6	0.93	2.38	3.277(3)	162
		Complex **1B**		
O_{3w}—H_{13w}···O_{2w}	0.85	1.94	2.695(3)	148
O_{3W}—H_{23W}···O_3	0.85	1.98	2.646(3)	134
O_{2W}—H_{22W}···O_{1W}	0.85	2.12	2.769(4)	133
O_{2W}—H_{12W}···O_1	0.84	2.24	2.854(3)	130
O_{1W}—H_{11W}···O_2	0.85	1.92	2.773(3)	175
O_{1W}—H_{21W}···O_4	0.85	2.01	2.861(3)	175
		Complex **1C**		
O_{1W}—H_{11W}···O_2	0.99	2.08	2.86(2)	134
O_{1W}—H_{21W}···O_{1w}	0.99	2.57	3.17(3)	119
C_4—H_4···O_2	0.93	2.64	3.502(10)	154
C_7—H_7···O_2	0.93	2.70	3.540(10)	150
C_{14}—H_{14}···O_1	0.93	2.56	3.391(10)	148
C_{17}—H_{17}···O_1	0.93	2.46	3.375(7)	165
		Complex **1D**		
O_{2W}—H_{2A}···O_3	0.99	1.84	2.664(11)	138
O_{2W}—H_{2B}···O_8	0.99	1.79	2.657(9)	143
O_{3W}—H_{3A}···O_7	0.99	1.92	2.744(9)	139
O_{3W}—H_{3B}···O_{4W}	1.00	1.99	2.787(9)	135
O_{13W}—H_{13A}···O_{9W}	0.97	2.04	2.841(16)	138
O_{13W}—H_{13B}···O_5	0.96	1.80	2.577(18)	135
O_{1W}—H_{1A}···O_{1W}	0.99	2.14	2.748(12)	117
O_{1W}—H_{1B}···O_{2W}	1.00	2.02	2.883(9)	144
O_{4W}—H_{4A}···O_8	1.00	1.68	2.645(10)	160
O_{4W}—H_{4B}···O_{1W}	0.98	2.10	2.851(10)	132
O_{4W}—H_{4B}···O_{7W}	0.98	2.56	3.388(12)	142
O_{5W}—H_{5A}···O_5	0.99	1.88	2.676(12)	135
O_{5W}—H_{5B}···O_4	0.98	1.77	2.741(10)	167
O_{6W}—H_{6A}···O_{5W}	0.98	1.89	2.707(10)	139
O_{6W}—H_{6B}···O_{3W}	1.00	2.00	2.820(8)	137
O_{7W}—H_{7A}···O_3	0.99	1.76	2.619(15)	143
O_{7W}—H_{7B}···O_{6W}	1.00	1.86	2.822(12)	161
O_{8W}—H_{8A}···O_1	1.00	2.07	2.863(11)	135
O_{8W}—H_{8B}···O_{2W}	1.00	2.13	3.092(10)	162
O_{9W}—H_{9A}···O_4	0.99	1.71	2.663(14)	159
O_{9W}—H_{9B}···O_{11W}	0.99	1.81	2.656(17)	140
O_{10W}—H_{10A}···O_6	1.07	2.14	3.199(16)	169
O_{10W}—H_{10B}···O_{13W}	1.00	1.63	2.563(15)	153
O_{10W}—H_{10B}···O_5	1.00	2.54	3.249(17)	128
O_{11W}—H_{11B}···O_{12W}	1.00	2.19	3.030(2)	141
O_{12W}—H_{12A}···O_{10W}	0.96	2.41	3.090(2)	128
O_{12W}—H_{12B}···O_6	1.01	1.66	2.530(19)	141
		Complex **2A**		
O_{1w}—H_{11w}···O_2	0.85	1.96	2.644(9)	136
O_{1W}—H_{21W}···O_4	0.84	2.46	3.036(9)	126
O_{1W}—H_{21W}···O_4	0.84	2.09	2.706(8)	130
O_{2W}—H_{12W}···O_3	0.85	1.93	2.769(9)	170
O_{2W}—H_{22W}···O_1	0.85	1.93	2.764(11)	169
O_{3W}—H_{13W}···O_1	0.85	2.50	3.228(17)	144
O_{3W}—H_{23W}···O_{2W}	0.85	2.00	2.718(17)	141
		Complex **2B**		

O_{1W}—H_{11W}···O_1	0.87	1.97	2.830(5)	172
O_{1W}—H_{21W}···O_{2W}	0.99	1.83	2.805(5)	167
O_{2W}—H_{12W}···O_4	0.97	1.86	2.770(5)	154
O_{2W}—H_{22W}···O_{3W}	1.04	2.01	2.773(7)	128
O_{3W}—H_{13W}···O_{1W}	1.03	2.09	2.956(7)	141
O_{3W}—H_{23W}···O_3	0.96	2.24	2.960(7)	131
		Complex **3A**		
O_{1W}—H_{11W}···O_3	0.99	1.90	2.862(9)	162
O_{1W}—H_{21W}···O_4	0.99	2.11	2.840(1)	129
C_2—H_2···O_1	0.93	2.62	3.301(1)	131
		Complex **3B**		
O_{2w}—H_{12w}···O_4	1.02	2.05	2.817(6)	130
O_{3W}—H_{13W}···O_2	0.96	2.10	2.729(7)	121
O_{3W}—H_{23W}···O_{1W}	0.97	1.95	2.756(7)	139
O_{5W}—H_{15W}···O_{2w}	1.03	1.96	2.808(6)	138
O_{5W}—H_{15W}···O_{6W}	1.03	2.60	3.507(6)	147
O_{5W}—H_{25W}···O_{8W}	0.97	1.88	2.775(7)	152
O_{6W}—H_{26W}···O_{4W}	0.99	1.85	2.748(6)	149
O_{7W}—H_{17W}···O_{4W}	1.00	1.95	2.878(7)	154
O_{7W}—H_{27W}···O_{6W}	1.00	2.16	2.919(6)	132
O_{8W}—H_{18W}···O_3	1.01	2.03	2.837(6)	136
O_{8W}—H_{28W}···O_2	1.01	1.74	2.718(7)	162

Table S4. Time-dependent DFT wavelengths and oscillator strengths for the first ten vertical excitations of **2B** (partially optimized geometry)

Excited State	Main Transition (% contribution)	Wavelenght (nm)	f
S1	HOMO→LUMO (78.3%)	585.46	0.00090
S2	HOMO-1→LUMO (74.6%)	564.94	0.00010
S3	HOMO→LUMO+1 (76.1%)	551.01	0.00060
S4	HOMO-1→LUMO+1 (76.8%)	536.91	0.00010
S5	HOMO-2→LUMO (92.3%)	462.78	0.00050
S6	HOMO-2→LUMO+1 (65.7%) HOMO-3→LUMO (28.9%)	454.95	0.00130
S7	HOMO-3→LUMO (49.5%) HOMO-4→LUMO (29.0%)	440.15	0.00250
S8	HOMO-4→LUMO (51.5%) HOMO-2→LUMO+1 (22.3%)	436.48	0.00510
S9	HOMO-3→LUMO+1 (87.3%)	430.02	0.00230
S10	HOMO→LUMO+2 (87.2%)	428.43	0.00010

Table S5. Time-dependent DFT wavelengths and oscillator strengths for the first eleven vertical excitations of **1C** (fully optimized geometry)

Excited State	Main Transition (% contribution)	Wavelenght (nm)	f
S1	HOMO→LUMO (99.6%)	348.38	0.0002
S2	HOMO→LUMO+1 (99.6%)	343.15	0.0012
S3	HOMO-1→LUMO (99.1%)	310.01	0.0014
S4	HOMO-1→LUMO+1 (99.0%)	305.68	0.0011
S5	HOMO-4→LUMO (95.8%)	290.48	0.0062
S6	HOMO-4→LUMO+1 (95.6%)	287.94	0.0043
S7	HOMO-2→LUMO (67.4%) HOMO-3→LUMO (13.8%)	282.73	0.0422
S8	HOMO-3→LUMO (66.8%) HOMO-2→LUMO (11.6%)	282.14	0.0285
S9	HOMO→LUMO+2 (93.0%)	279.97	0.0023
S10	HOMO-2→LUMO+1 (72.4%) HOMO-3→LUMO (13.7%)	278.22	0.1477

Table S6. Time-dependent DFT wavelengths and oscillator strengths for the first ten vertical excitations of **2B** (fully optimized geometry)

Excited State	Main Transition (% contribution)	Wavelenght (nm)	f
S1	HOMO→LUMO (92.2%)	394.62	0.0001
S2	HOMO-1→LUMO (62.5%) HOMO→LUMO+1 (36.8%)	389.08	0.0001
S3	HOMO-1→LUMO (62.2%) HOMO→LUMO+1 (36.8%)	377.19	0.0004
S4	HOMO-1→LUMO+1 (91.6%)	372.09	0.0020
S5	HOMO-2→LUMO (82.0%)	344.93	0.0013
S6	HOMO-3→LUMO (71.8%)	343.64	0.0007
S7	HOMO-4→LUMO (66.5%) HOMO-3→LUMO+1 (22.3%)	341.23	0.0007
S8	HOMO-2→LUMO+1 (82.3%)	337.25	0.0049
S9	HOMO-3→LUMO+1 (67.2%) HOMO-4→LUMO (29.0%)	330.84	0.0005
S10	HOMO-4→LUMO+1 (76.4%)	329.90	0.0001

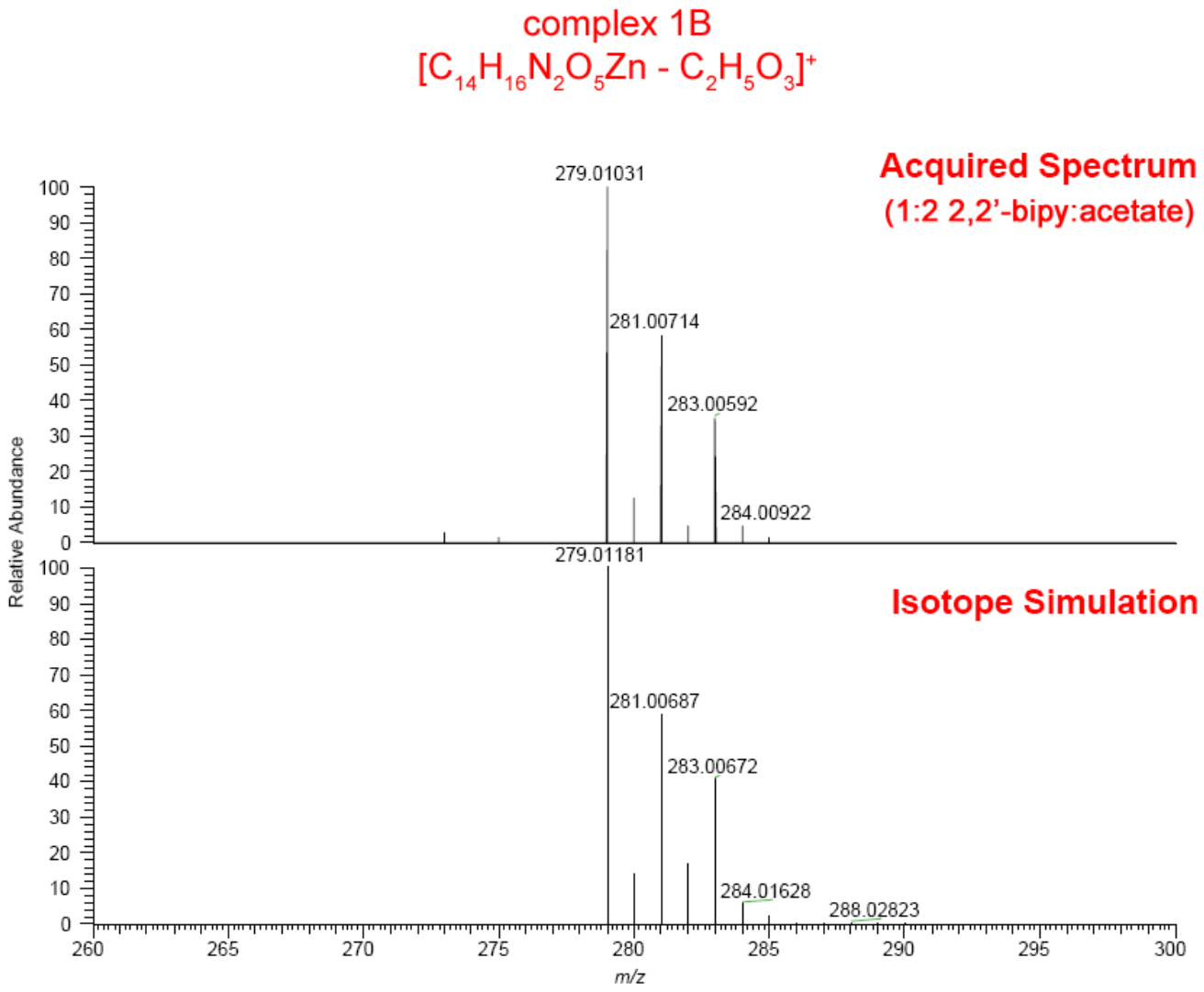


Figure S1. ESI(+)-orbitrap mass spectrum of complex **1B**. The $C_2H_5O_3$ formula refers to the eliminated ligands (one acetate and one water).

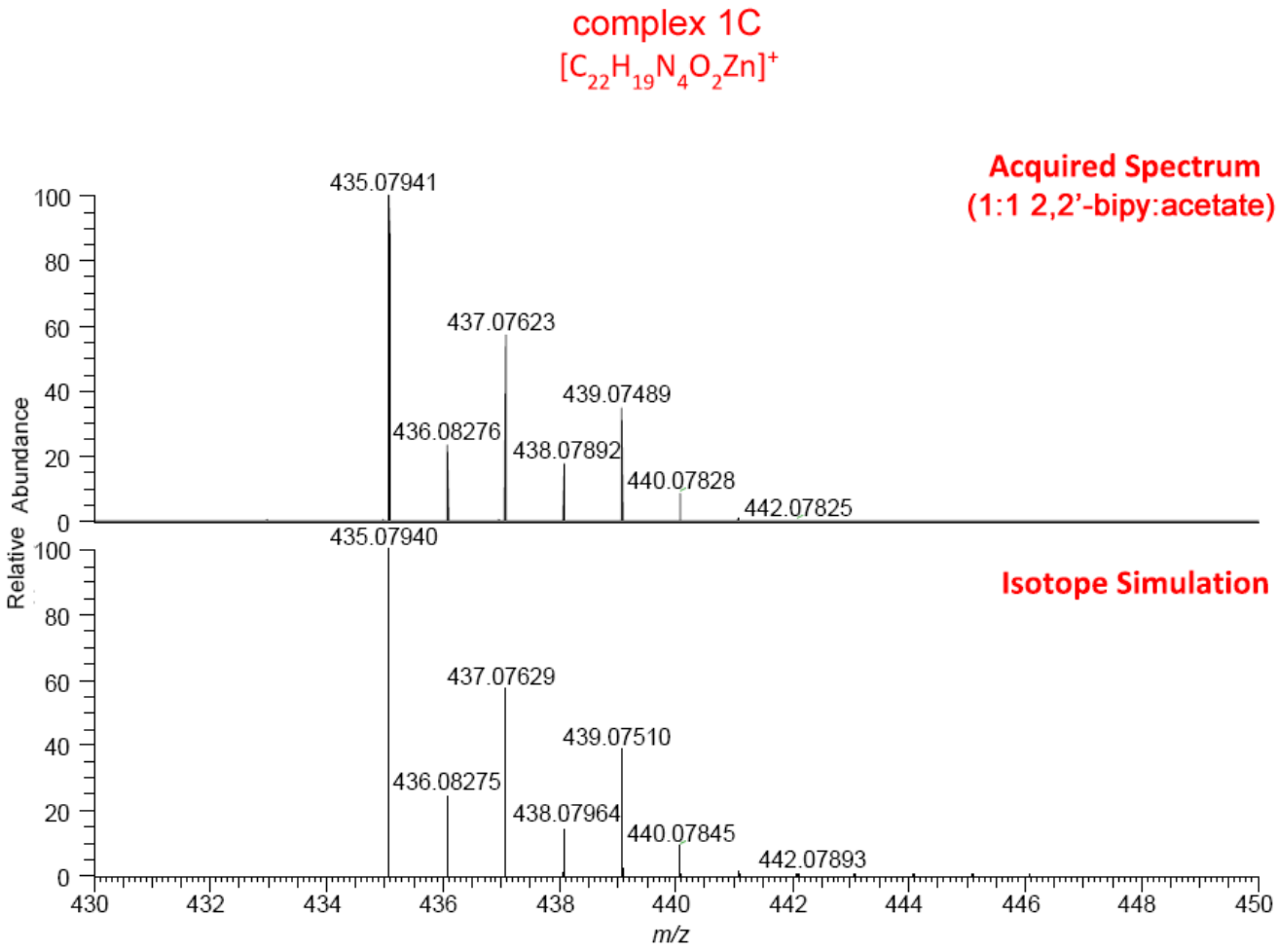


Figure S2. ESI(+)-orbitrap mass spectrum of complex **1C**.

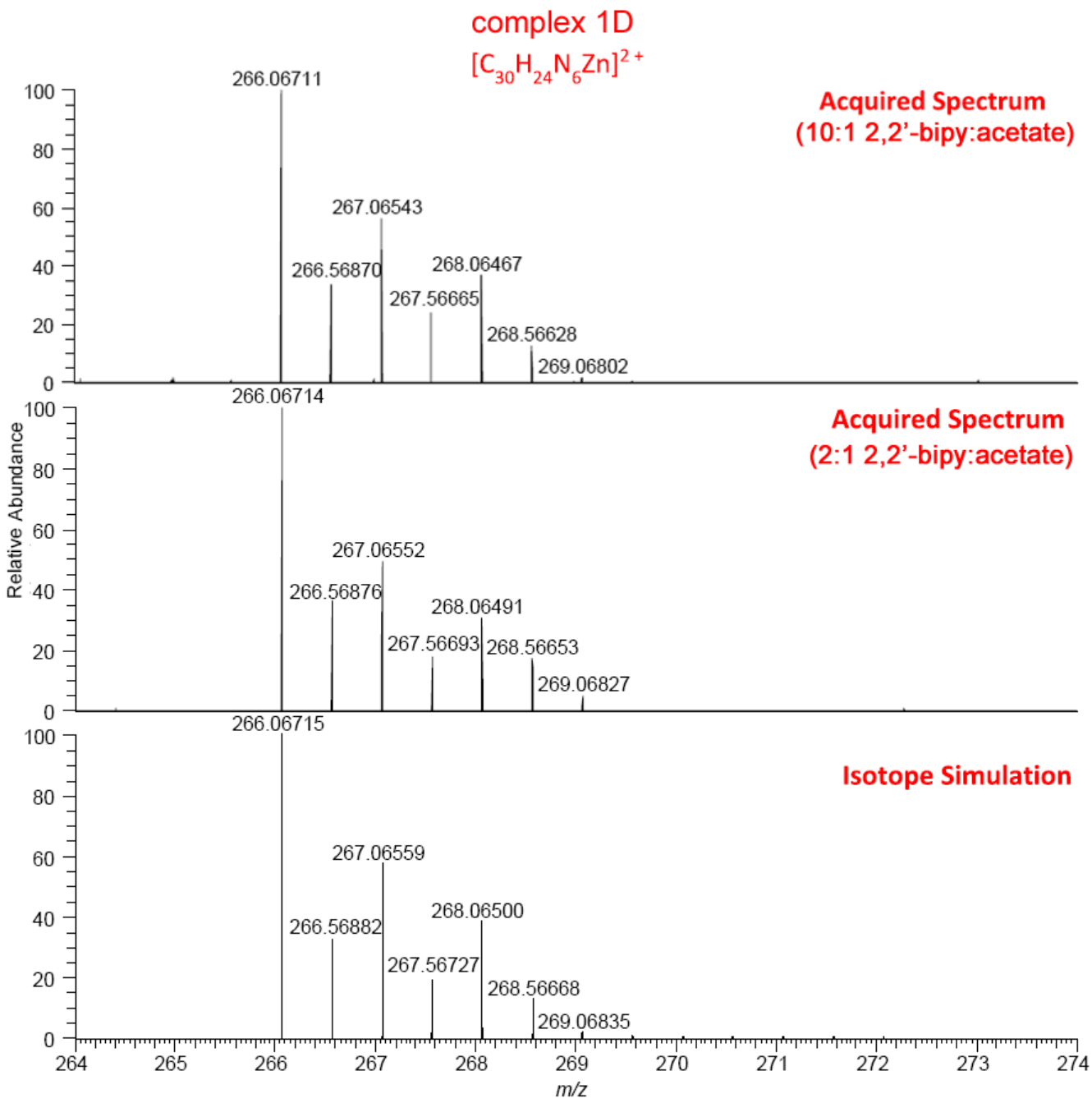


Figure S3. ESI(+)-orbitrap mass spectrum of complex **1D**.

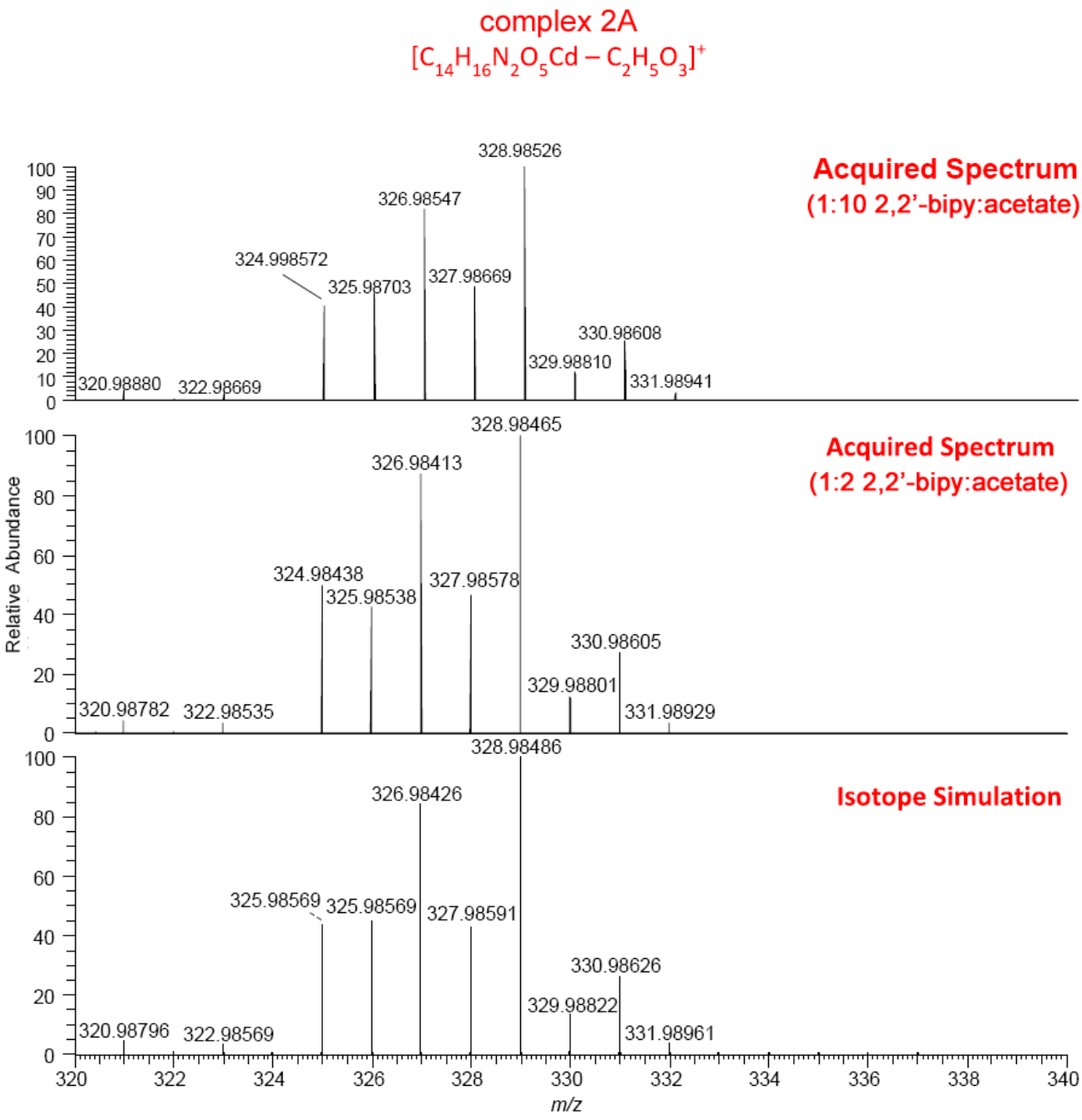


Figure S4. ESI(+)-orbitrap mass spectrum of complex **2A**. The $C_2H_5O_3$ formula refers to the eliminated ligands (one acetate and one water).

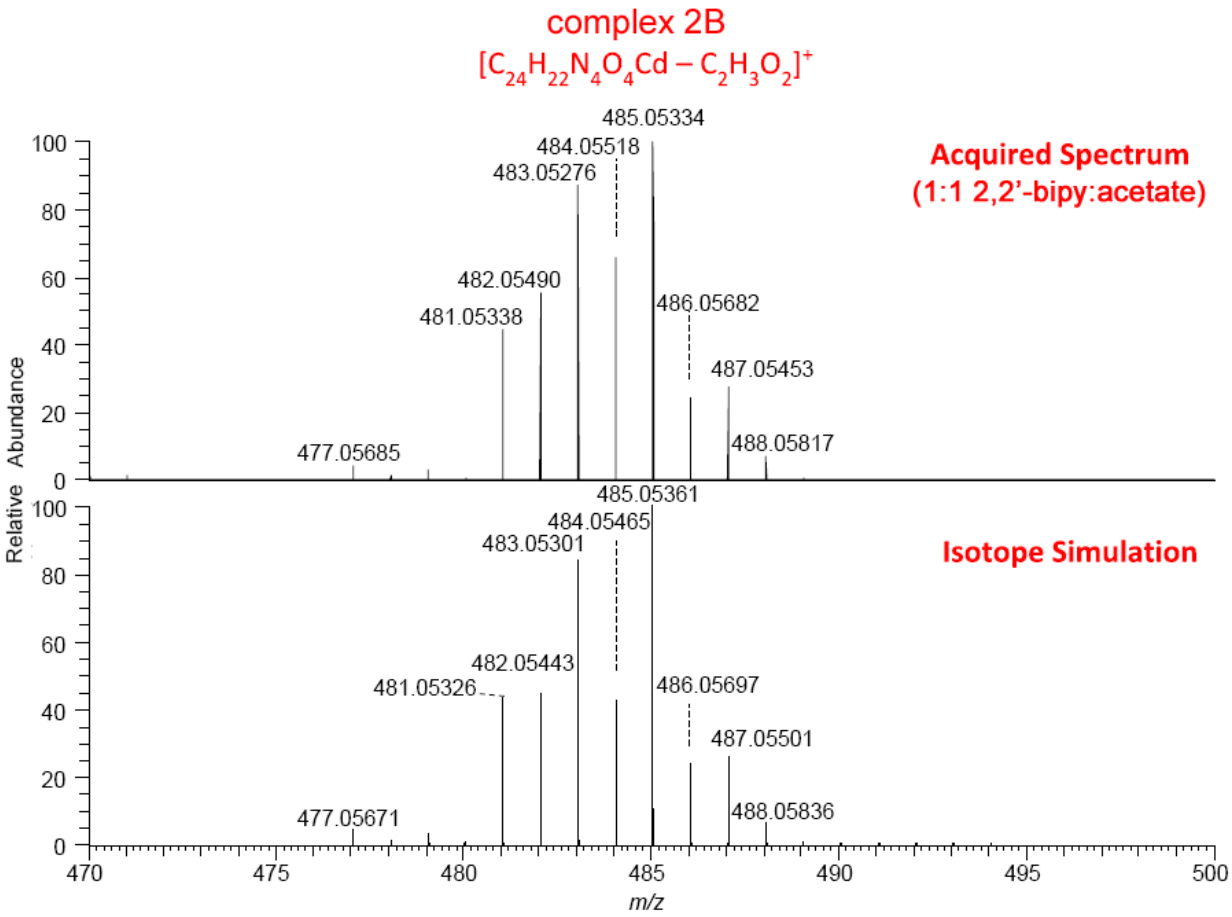


Figure S5. ESI(+)-orbitrap mass spectrum of complex **2B**. The $C_2H_3O_2$ formula refers to the eliminated ligand (one acetate).

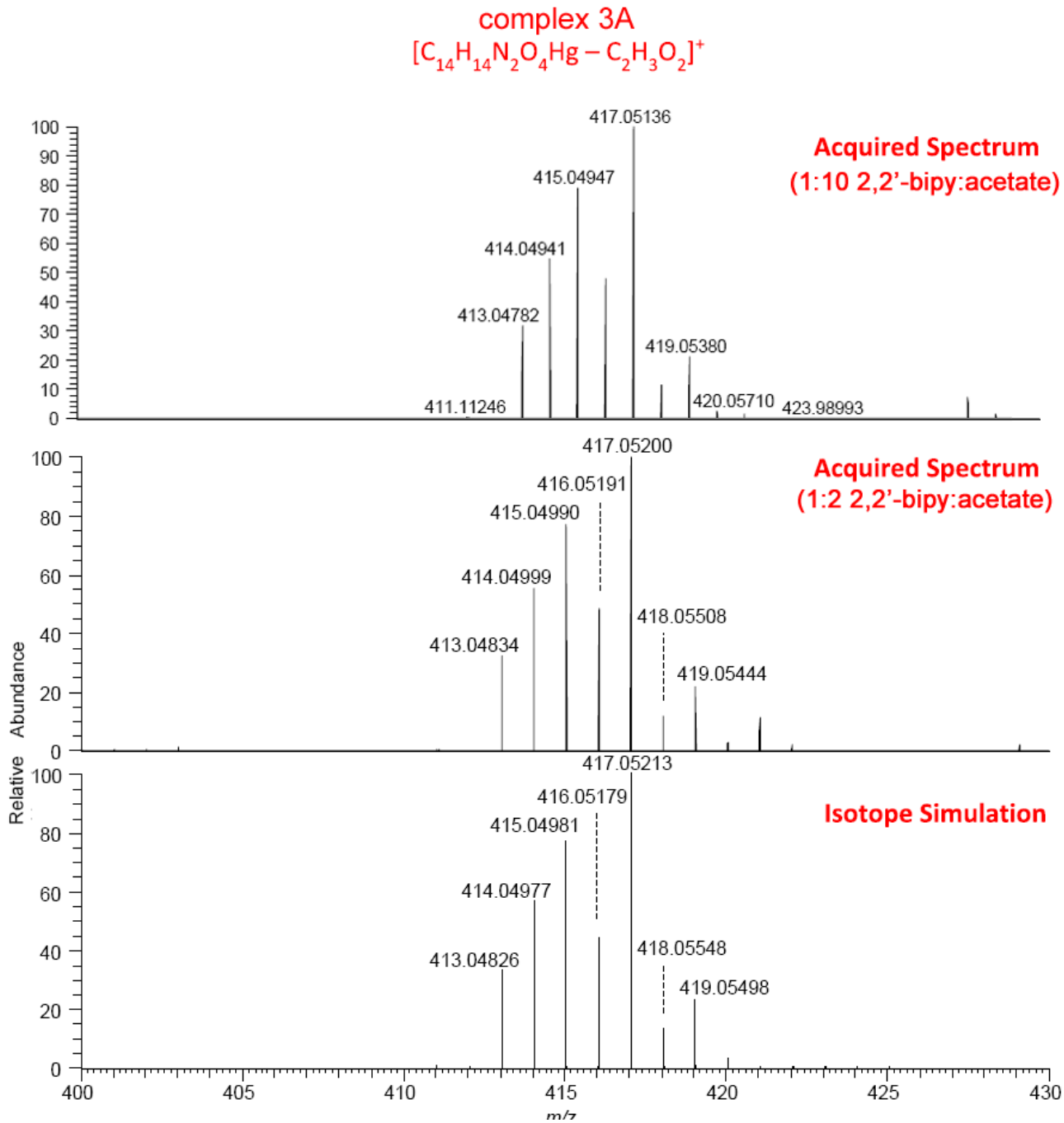


Figure S6. ESI(+)-orbitrap mass spectrum of complex **3A**. The $C_2H_3O_2$ formula refers to the eliminated ligand (one acetate).

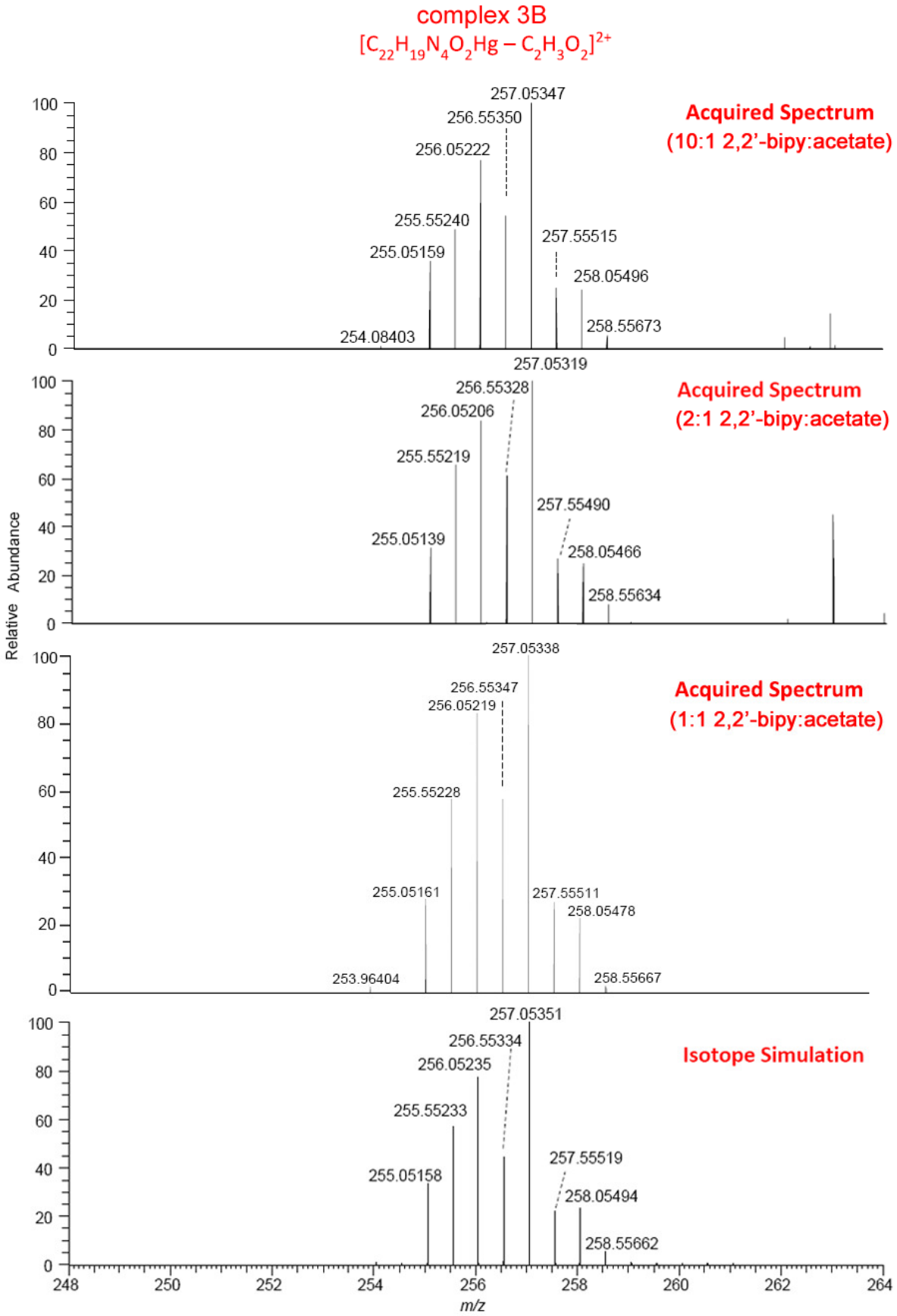


Figure S7. ESI(+)-orbitrap mass spectrum of complex **3B**. The $C_2H_3O_2$ formula refers to the eliminated ligand (one acetate).

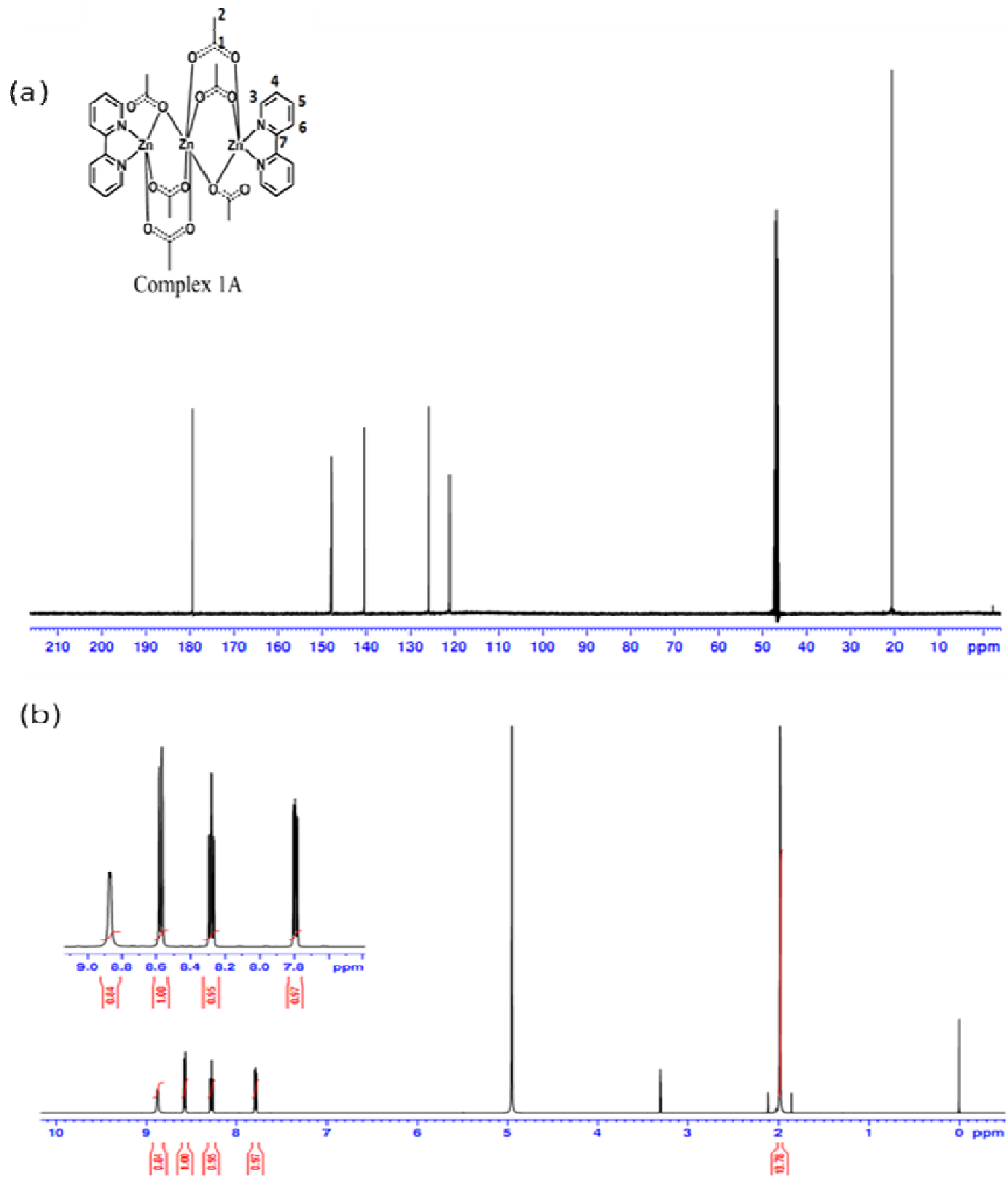


Figure S8. (a) ^{13}C NMR and (b) ^{1}H NMR spectra of **1A**. ^{1}H NMR (500 MHz, Methanol-d4) δ (ppm): 8.87 (dt, 1H, *J* 7.82; 0.98, H-3), 8.58 (dt, 1H, *J* 7.64; 0.98, H-6), 8.30 (td, 1H, *J* 7.82; 1.71, H-4), 7.78 (ddd, 1H, *J* 7.64; 5.16; 0.98, H-5), 1.99 (s, 3H, H-2). ^{13}C NMR (125 MHz, Methanol-d4) δ (ppm): 179.7 (C-1), 148.2 (C-7), 148.0 (C-5), 140.7 (C-3), 126.1 (C-4), 121.3 (C-6), 20.6 (C-2).

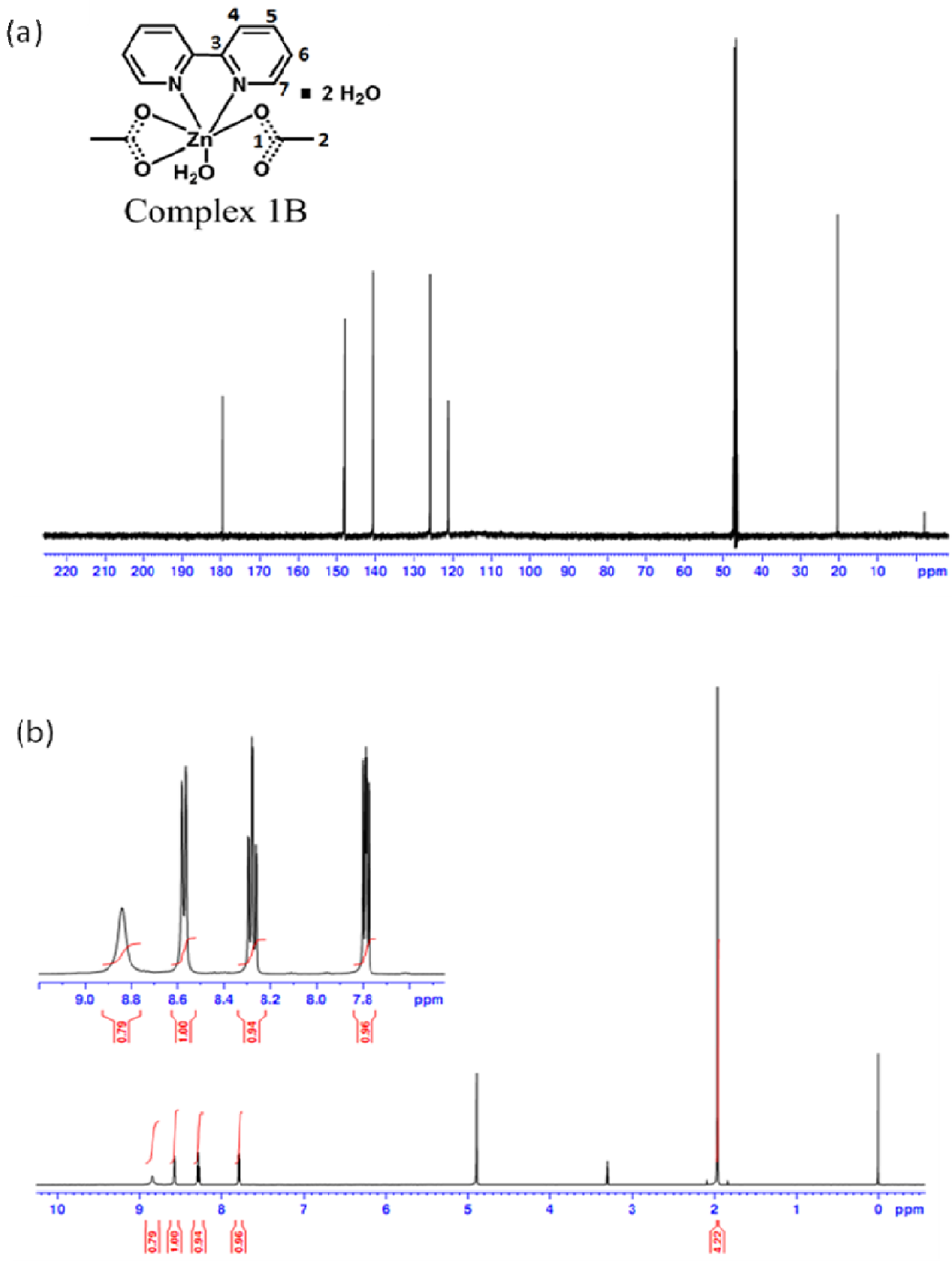


Figure S9. (a) ^{13}C NMR and (b) ^{1}H NMR spectra of **1B**. ^{1}H NMR (500 MHz, Methanol-d4) δ (ppm): 8.84 (sl, 1H, H-7), 8.58 (dl, 1H, *J* 7.68, H-4), 8.28 (td, 1H, *J* 7.80; 1.61, H-6), 7.78 (ddd, 1H, *J* 7.68; 5.16; 0.98, H-5), 1.97 (s, 3H, H-2). ^{13}C NMR (125 MHz, Methanol-d4) δ (ppm): 179.4 (C-1), 148.3 (C-3), 148.0 (C-5), 140.4 (C-7), 125.9 (C-6), 121.1 (C-4), 20.6 (C-2).

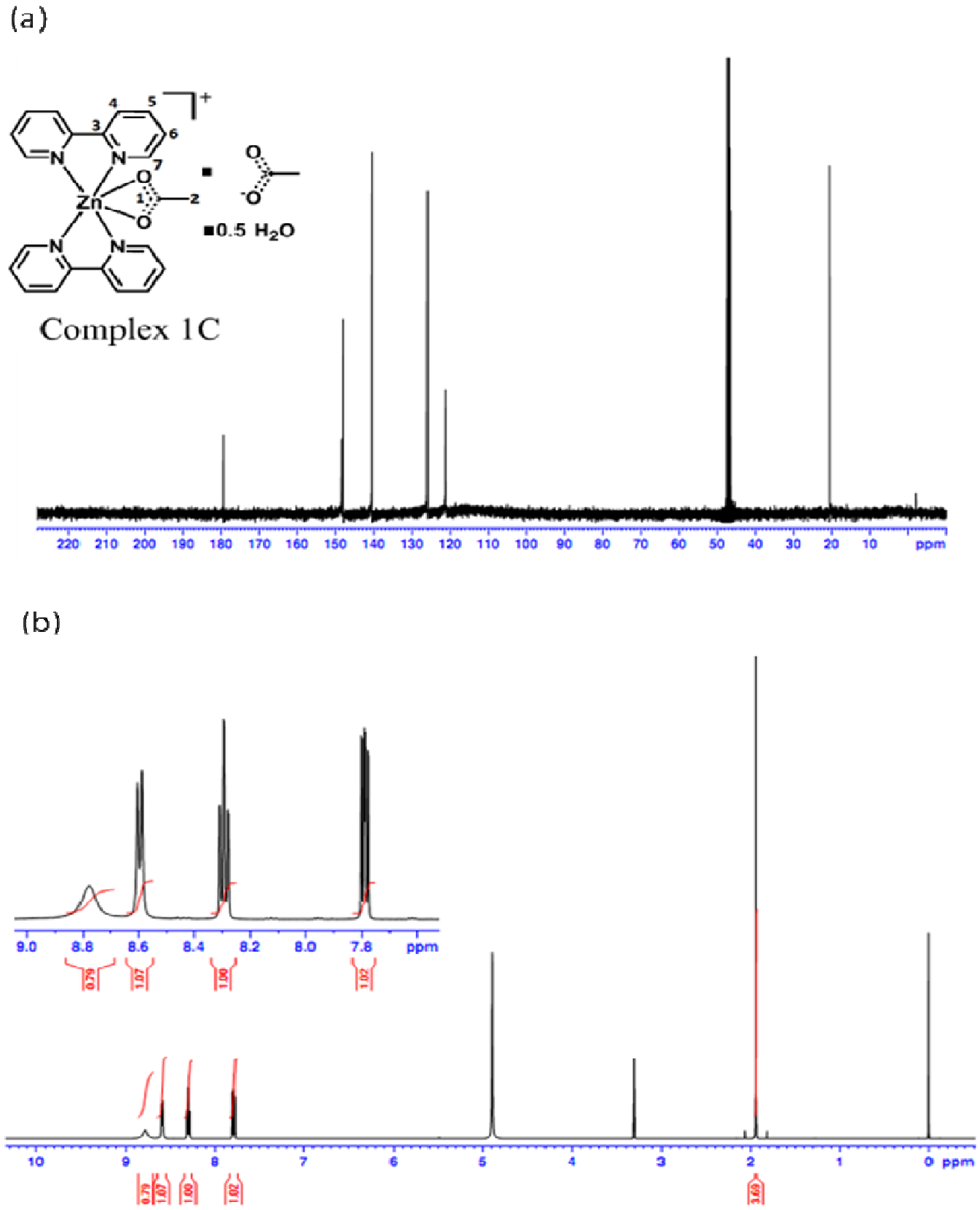


Figure S10. (a) ^{13}C NMR and (b) ^{1}H NMR spectra of **1C**. ^{1}H NMR (500 MHz, Methanol-d4) δ (ppm): 8.78 (sl, 1H, H-7), 8.59 (dl, 1H, *J* 7.61, H-4), 8.28 (td, 1H, *J* 7.89; 1.64, H-6), 7.78 (ddd, 1H, *J* 7.61; 5.15; 0.96, H-5), 1.94 (s, 3H, H-2). ^{13}C NMR (125 MHz, Methanol-d4) δ (ppm): 178.9 (C-1), 149.9 (C-3), 148.4 (C-5), 140.5 (C-7), 125.9 (C-6), 121.2 (C-4), 20.6 (C-2).

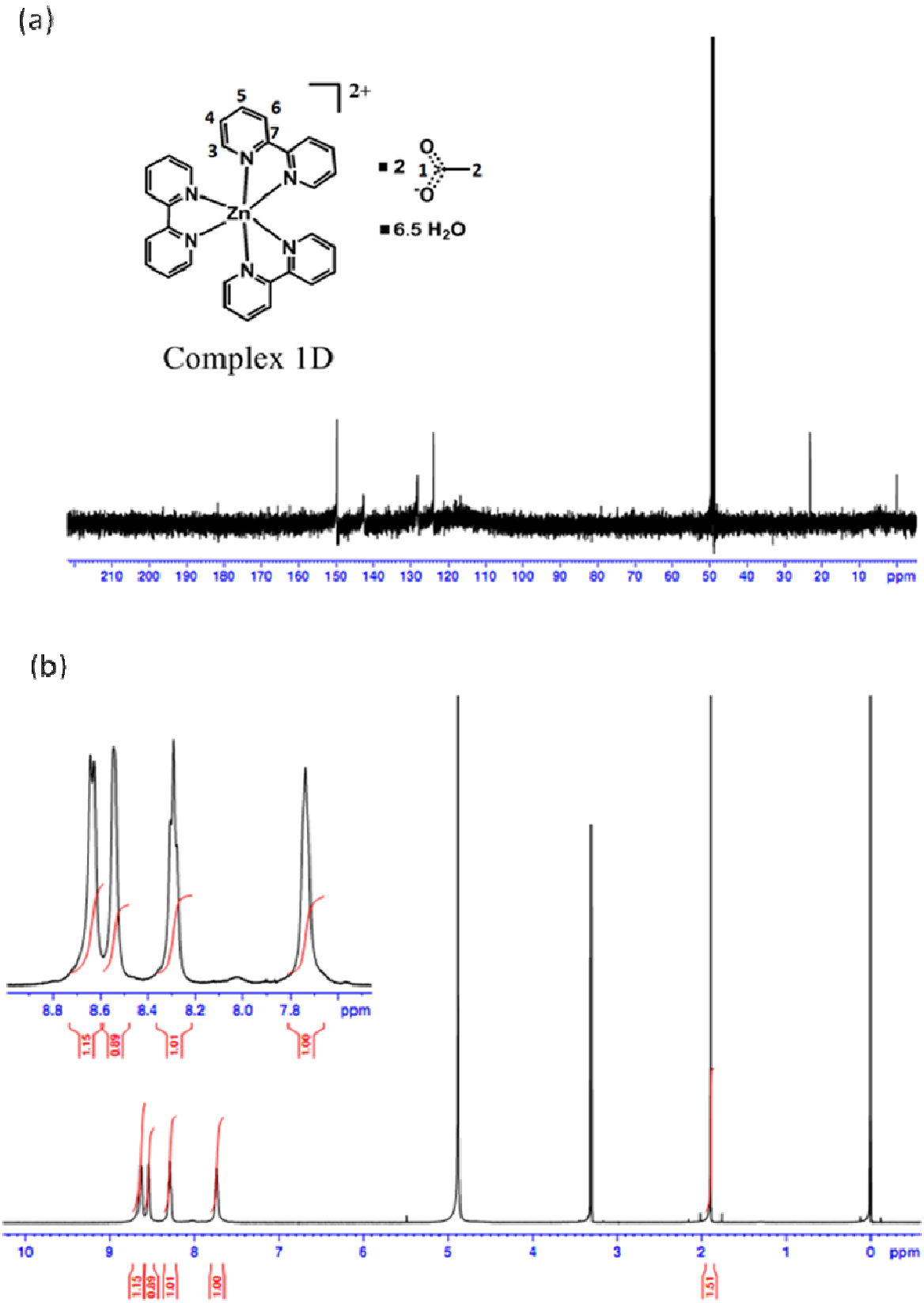


Figure S11. (a) ^{13}C NMR and (b) ^{1}H NMR spectra of **1D**. ^{1}H NMR (500 MHz, Methanol-d4) δ (ppm): 8.64 (dl, 1H, *J* 7.48, H-3), 8.54 (sl, 1H, H-6), 8.29 (tl, 1H, *J* 7.48, H-4), 7.73 (sl, 1H, H-5), 1.89 (s, 3H, H-2). ^{13}C NMR (125 MHz, Methanol-d4) δ (ppm): 181.8 (C-1), 149.8 (C-7), 149.3 (C-5), 143.0 (C-3), 128.2 (C-4), 123.9 (C-6), 23.6 (C-2).

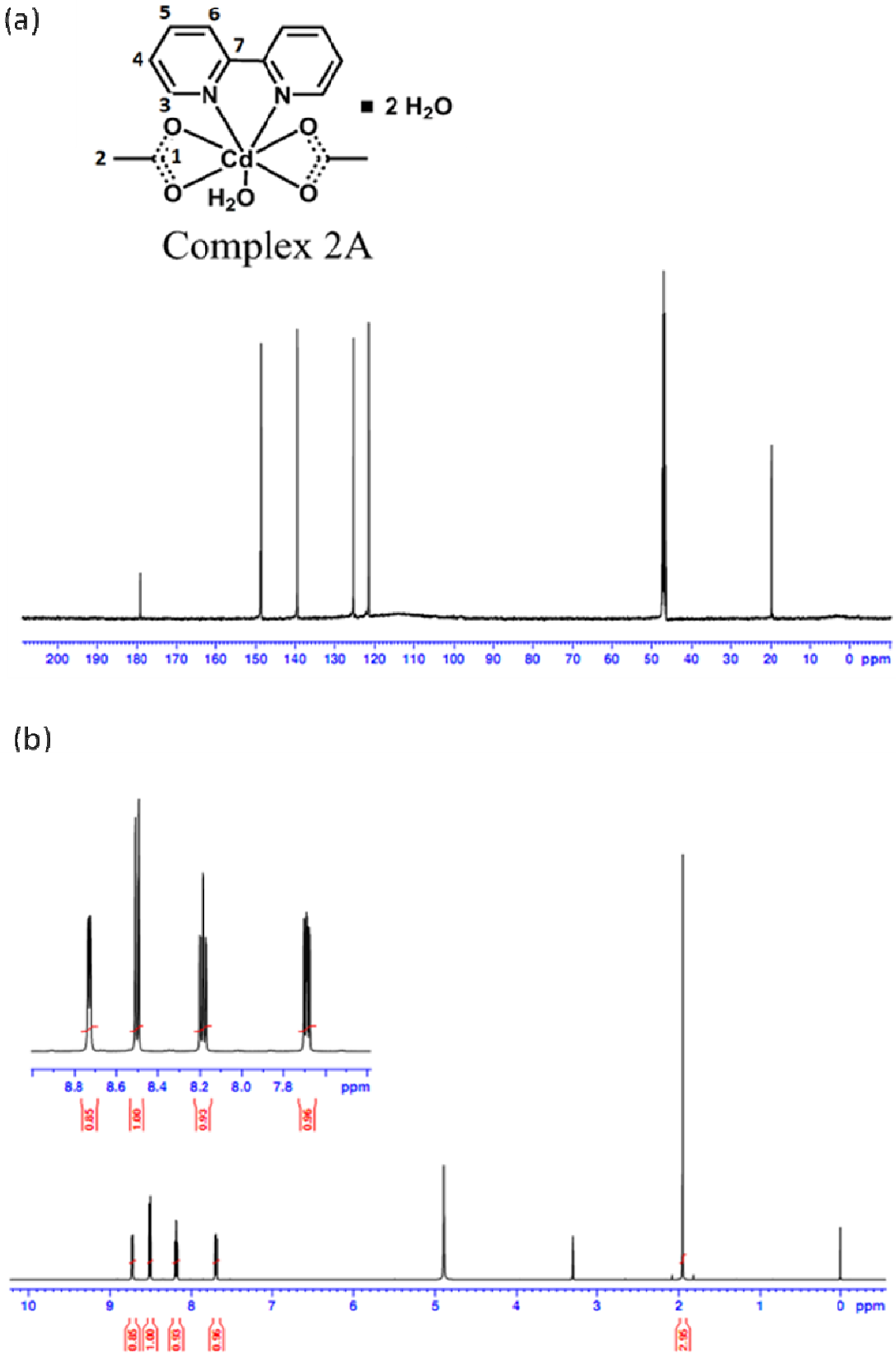


Figure S12. (a) ^{13}C NMR and (b) ^{1}H NMR spectra of **2A**. ^{1}H NMR (500 MHz, Methanol-d4) δ (ppm): 8.72 (dq, 1H, *J* 5.07; 0.95, H-3), 8.50 (dt, 1H, *J* 8.61; 0.95, H-6), 8.18 (td, 1H, *J* 7.88; 1.71, H-4), 7.68 (ddd, 1H, *J* 8.61; 5.07; 0.95, H-5), 1.94 (s, 3H, H-2). ^{13}C NMR (125 MHz, Methanol-d4) δ (ppm): 179.2 (C-1), 148.9 (C-7), 148.7 (C-5), 139.5 (C-3), 125.3 (C-4), 121.4 (C-6), 19.9 (C-2).

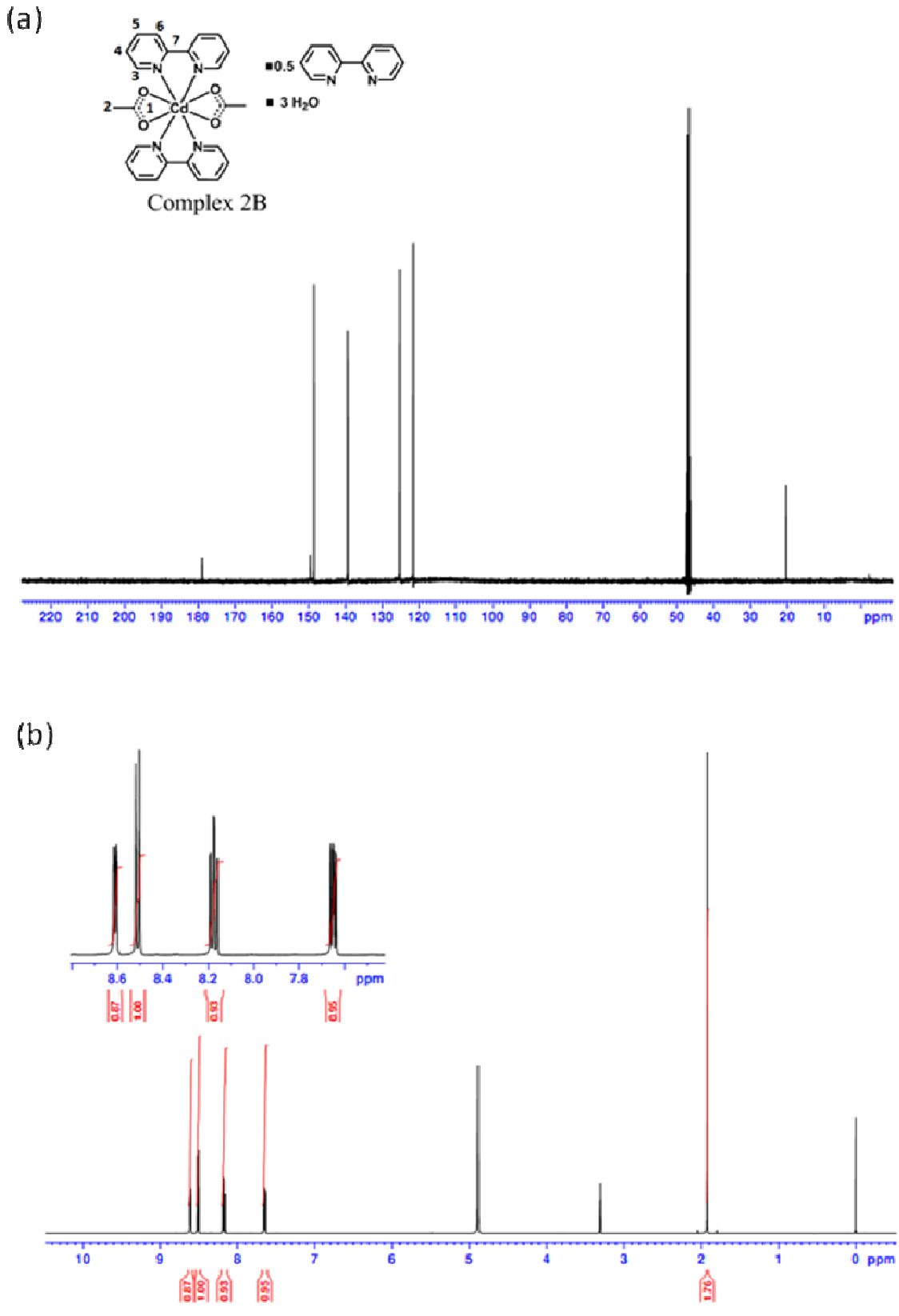


Figure S13. (a) ^{13}C NMR and (b) ^{1}H NMR spectra of **2B**. ^{1}H NMR (500 MHz, Methanol-d4) *δ* (ppm): 8.61 (dq, 1H, *J* 5.04; 0.82, H-3), 8.51 (dt, 1H, *J* 7.62; 0.82, H-6), 8.18 (td, 1H, *J* 7.80; 1.77, H-4), 7.64 (ddd, 1H, *J* 7.62; 5.04; 1.77, H-5), 1.94 (s, 3H, H-2). ^{13}C NMR (125 MHz, Methanol-d4) *δ* (ppm): 178.9 (C-1), 149.5 (C-7), 148.5 (C-5), 139.4 (C-3), 125.2 (C-4), 121.6 (C-6), 20.3 (C-2).

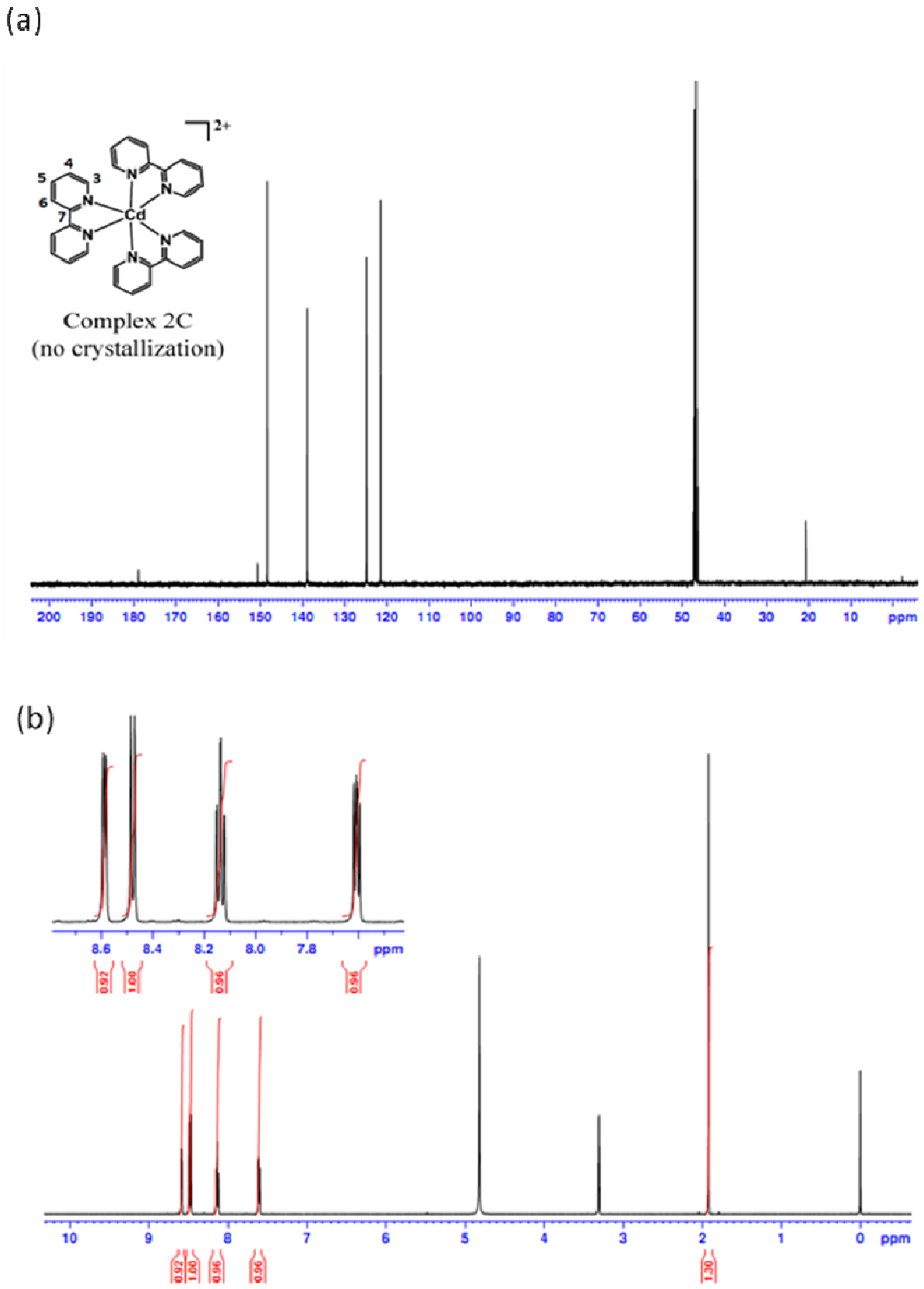


Figure S14. (a) ^{13}C NMR and (b) ^{1}H NMR spectra of **2C**. ^{1}H NMR (500 MHz, Methanol-d4) δ (ppm): 8.58 (dl, 1H, *J* 5.05, H-3), 8.47 (dl, 1H, *J* 7.58, H-6), 8.13 (td, 1H, *J* 7.83; 1.62, H-4), 7.60 (ddd, 1H, *J* 7.58; 5.05; 1.03, H-5). ^{13}C NMR (125 MHz, Methanol-d4) δ (ppm): 150.6 (C-7), 148.3 (C-5), 138.9 (C-3), 124.9 (C-4), 121.4 (C-6).

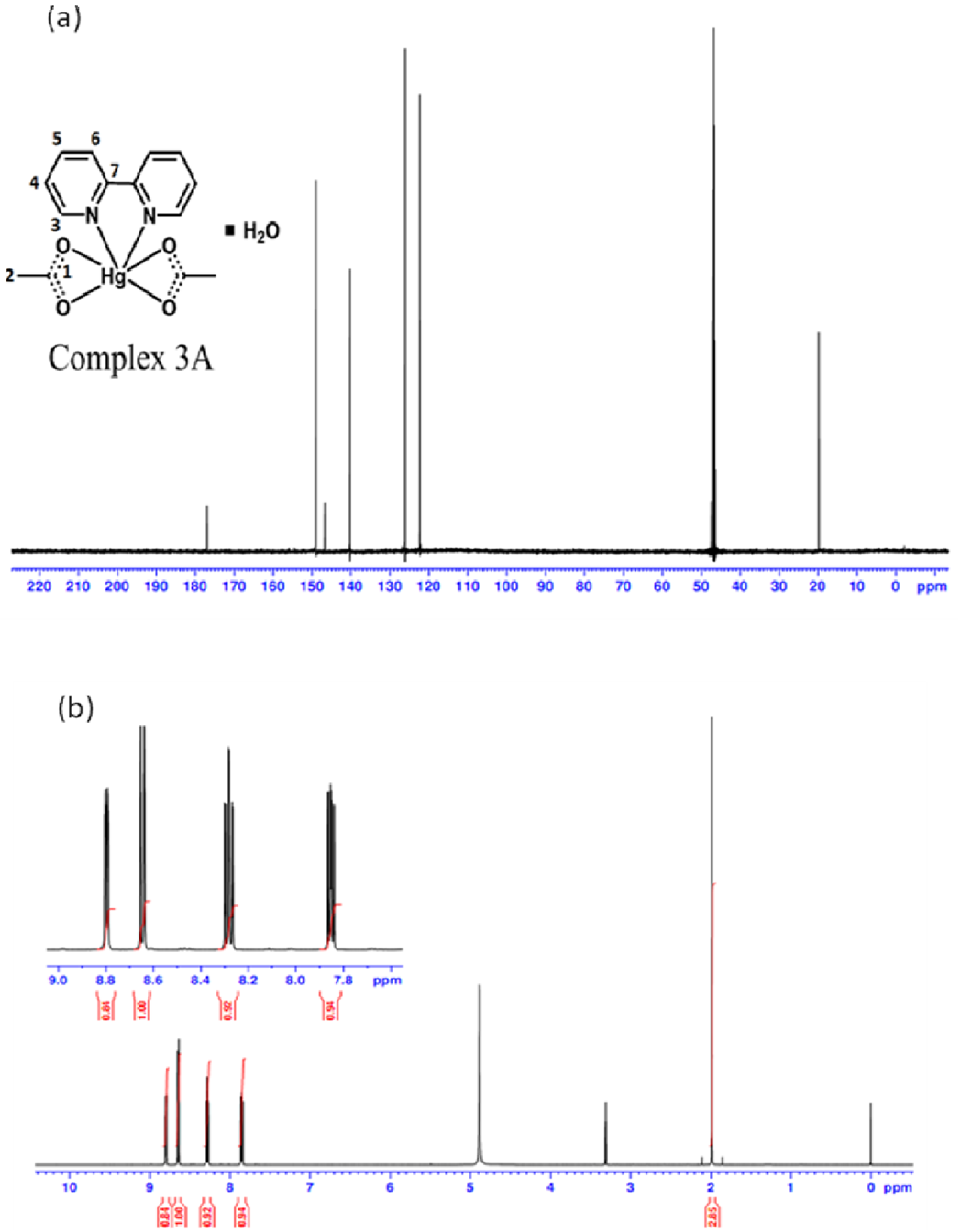


Figure S15. (a) ^{13}C NMR and (b) ^{1}H NMR spectra of **3A**. ^{1}H NMR (500 MHz, Methanol-d4) δ (ppm): 8.79 (dq, 1H, *J* 5.05; 0.83, H-3), 8.64 (dt, 1H, *J* 7.80; 0.83, H-6), 8.28 (td, 1H, *J* 7.80; 1.73, H-4), 7.75 (ddd, 1H, *J* 7.80; 5.12; 1.06, H-5), 1.98 (s, 3H, H-2). ^{13}C NMR (125 MHz, Methanol-d4) δ (ppm): 177.0 (C-1), 149.0 (C-7), 146.7 (C-5), 140.3 (C-3), 126.1 (C-4), 122.3 (C-6), 19.8 (C-2).

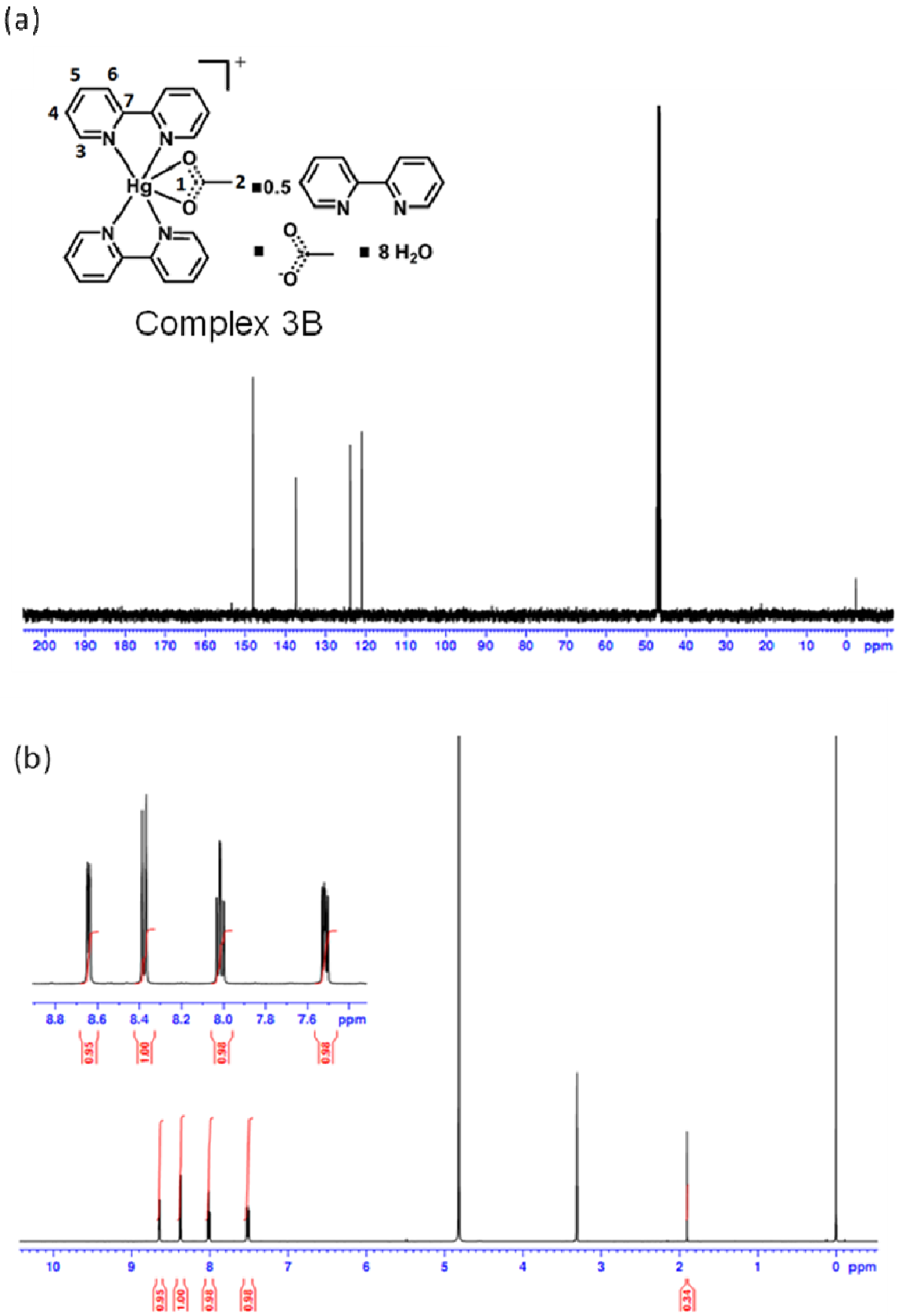


Figure S16. (a) ^{13}C NMR and (b) ^{1}H NMR spectra of **3B**. ^{1}H NMR (500 MHz, Methanol-d4) δ (ppm): 8.63 (dq, 1H, J 4.95; 0.84, H-3), 8.37 (dl, 1H, J 7.52, H-6), 8.01 (td, 1H, J 7.52; 1.76, H-4), 7.51 (ddd, 1H, J 7.52; 4.95; 0.84, H-5), 1.89 (s, 3H, H-2). ^{13}C NMR (125 MHz, Methanol-d4) δ (ppm): 155.6 (C-7), 150.3 (C-5), 139.4 (C-3), 125.9 (C-4), 123.05 (C-6).

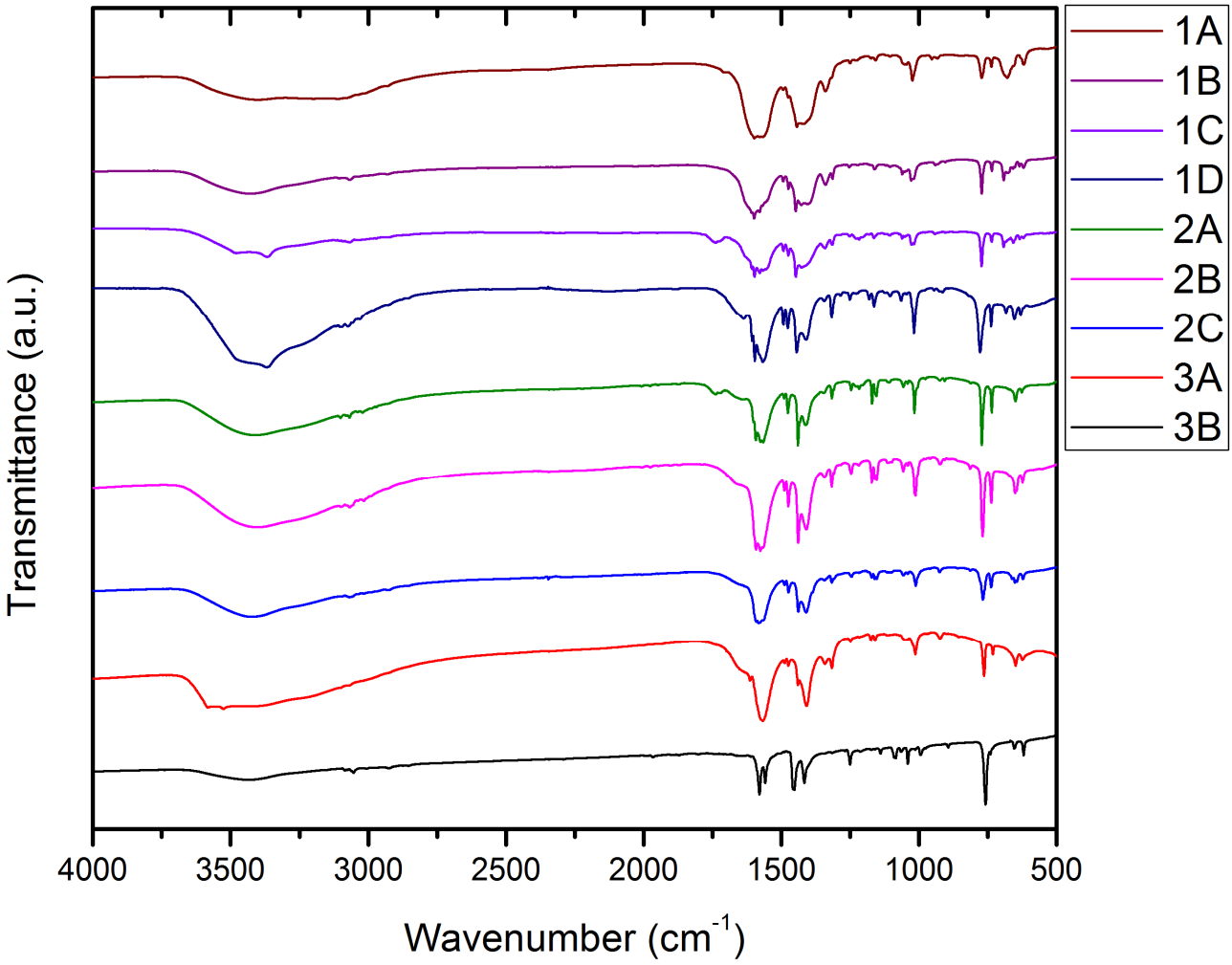
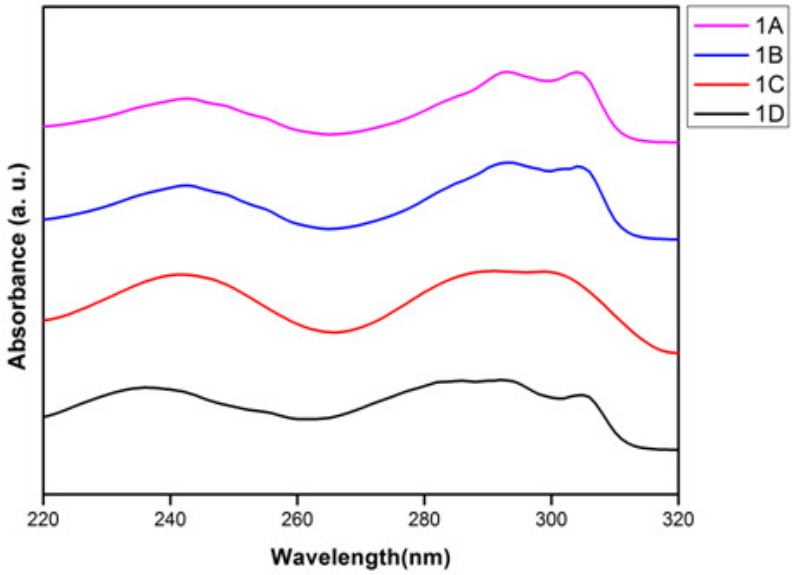
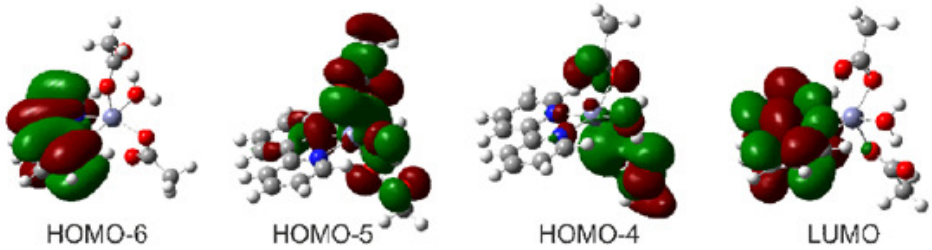


Figure S17. Infrared spectra of the complexes prepared in this study. Assignments of vibrational modes (KBr, cm^{-1}): 3110 [$\upsilon(C_{sp3}\text{-}H + C_{Ar}\text{-}H)$], 1597 and 1567 [$\upsilon(C{=}O)$], 1443 [$\upsilon(C{=}N)_{Ar}$], 1416 [$\upsilon(C{=}C)_{Ar}$], 1023 [in plane $\delta(C\text{-}H)_{Ar}$], 772 [out-of-plane $\delta(C\text{-}H)_{Ar}$], 680 (ring deformation) (**1A**); 3424 [$\upsilon(O\text{-}H)$], 1595, 1578 [$\upsilon(C{=}O)$], 1447 [$\upsilon(C{=}N)_{Ar}$], 1429 [$\upsilon(C{=}C)_{Ar}$], 1018 [in plane $\delta(C\text{-}H)_{Ar}$], 772 [out-of-plane $\delta(C\text{-}H)_{Ar}$], 692 (ring deformation) (**1B**); 3369 [$\upsilon(O\text{-}H)$], 1596, 1576 [$\upsilon(C{=}O)$], 1447 [$\upsilon(C{=}N)_{Ar}$], 1425 [$\upsilon(C{=}C)_{Ar}$], 1023 [in plane $\delta(C\text{-}H)_{Ar}$], 773 [out-of-plane $\delta(C\text{-}H)_{Ar}$], 692 (ring deformation) (**1C**); 3397 [$\upsilon(O\text{-}H)$], 1595, 1565 [$\upsilon(C{=}O)$], 1444 [$\upsilon(C{=}N)_{Ar}$], 1410 [$\upsilon(C{=}C)_{Ar}$], 1017 [in plane $\delta(C\text{-}H)_{Ar}$], 778 [out-of-plane $\delta(C\text{-}H)_{Ar}$], 650 (ring deformation) (**1D**); 3406 [$\upsilon(O\text{-}H)$], 1592, 1576 [$\upsilon(C{=}O)$], 1438 [$\upsilon(C{=}N)_{Ar}$], 1410 [$\upsilon(C{=}C)_{Ar}$], 1016 [in plane $\delta(C\text{-}H)_{Ar}$], 771 [out-of-plane $\delta(C\text{-}H)_{Ar}$], 649 (ring deformation) (**2A**); 3400 [$\upsilon(O\text{-}H)$], 1591, 1575 [$\upsilon(C{=}O)$], 1438 [$\upsilon(C{=}N)_{Ar}$], 1409 [$\upsilon(C{=}C)_{Ar}$], 1011 [in plane $\delta(C\text{-}H)_{Ar}$], 769 [out-of-plane $\delta(C\text{-}H)_{Ar}$], 650 (ring deformation) (**2B**); 3424 [$\upsilon(O\text{-}H)$], 1580 [$\upsilon(C{=}O)$], 1437 [$\upsilon(C{=}N)_{Ar}$], 1409 [$\upsilon(C{=}C)_{Ar}$], 1010 [in plane $\delta(C\text{-}H)_{Ar}$], 766 [out-of-plane $\delta(C\text{-}H)_{Ar}$], 650 (ring deformation) (**2C**); 3526 [$\upsilon(O\text{-}H)$], 1613, 1568 [$\upsilon(C{=}O)$], 1437 [$\upsilon(C{=}N)_{Ar}$], 1407 [$\upsilon(C{=}C)_{Ar}$], 1012 [in plane $\delta(C\text{-}H)_{Ar}$], 764 [out-of-plane $\delta(C\text{-}H)_{Ar}$], 648 (ring deformation) (**3A**); 3437 [$\upsilon(O\text{-}H)$], 1578, 1559 [$\upsilon(C{=}O)$], 1453 [$\upsilon(C{=}N)_{Ar}$], 1415 [$\upsilon(C{=}C)_{Ar}$], 1030 [in plane $\delta(C\text{-}H)_{Ar}$], 755 [out-of-plane $\delta(C\text{-}H)_{Ar}$], 619 (ring deformation) (**3B**).



(a)

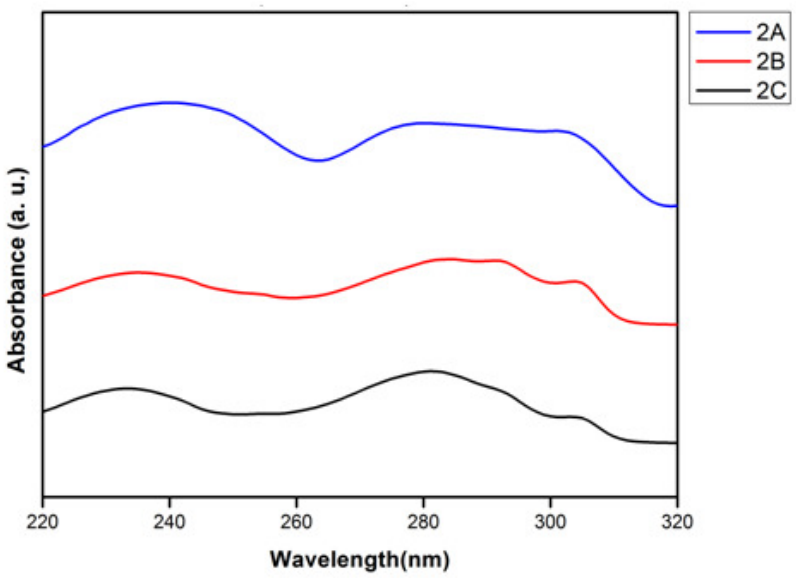
Main transitions computed for **1B**



Excited State	Main Transition (% contribution)	Wavelenght (nm)	f
S5	HOMO-4→LUMO (98%)	343.9	0.009
S7	HOMO-5→LUMO (97%)	321.9	0.007
S14	HOMO-6→LUMO (83%)	269.2	0.303

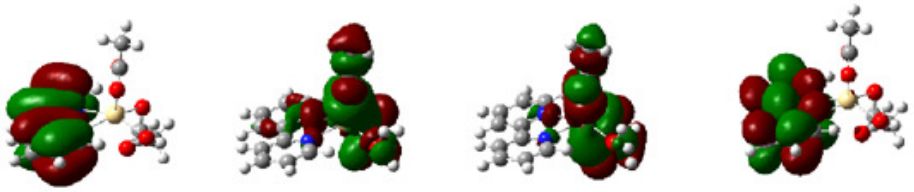
(b)

Figure S18. (a) UV spectra of Zn complexes prepared here (in water). Wavelengths of maximal absorptions: 305 nm, 294 nm, 242 nm (**1A**); 305 nm, 294 nm, 242 nm (**1B**); 303 nm, 285 nm, 242 nm (**1C**); and 305 nm, 294 nm, 236 nm (**1D**). The absorption spectra of the Zn complexes present mainly two bands regions. The strongest bands for complexes **1A**, **1B**, **1C** and **1D** are seen in the region of 270-310 nm, which can be attributed to metal to ligand charge transfer (MLCT) and ligand to metal charge transfer (LMCT). The other band observed in the region of 220-260 nm can be assigned to intraligand charge transfer (ILCT). These transitions were found at the B3LYP/LANLDZ&6-31G* level of theory for **1B** [panel (b)] and **1C** [Tables 1 and S5, Figures S23 and S25], taken as templates for calculating main transitions of Zn complexes. All these assignments are in good agreement with those described in literature for related complexes.[S1,S2]



(a)

Main transitions computed for **2A**

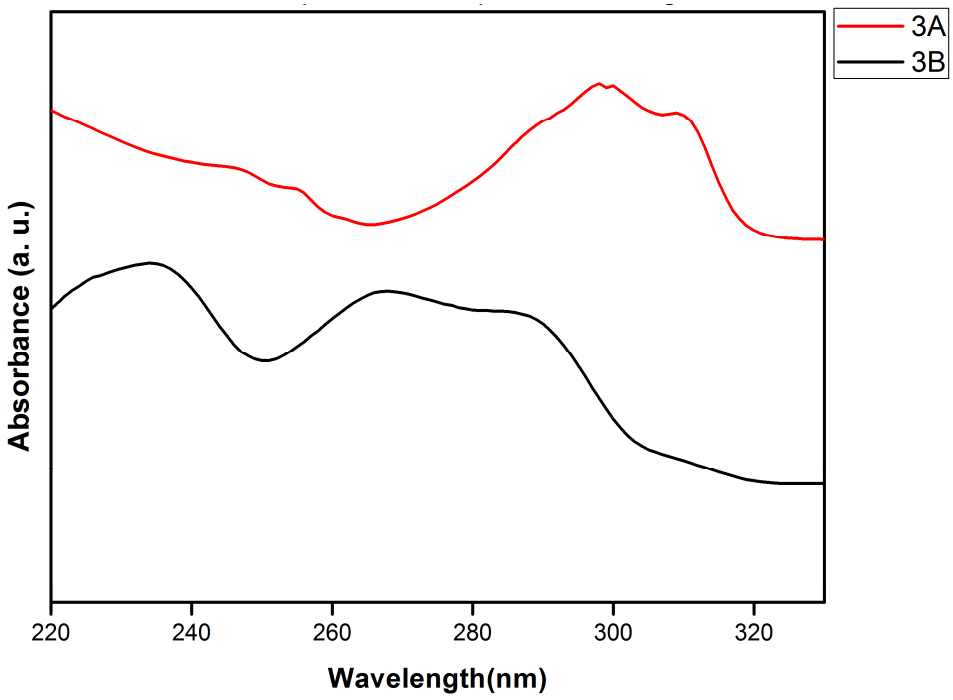


HOMO-6 HOMO-5 HOMO-4 LUMO

Excited State	Main Transition (% contribution)	Wavelenght (nm)	f
S5	HOMO-4→LUMO (98%)	348.9	0.014
S7	HOMO-5→LUMO (97%)	331.6	0.010
S14	HOMO-6→LUMO (85%)	271.2	0.342

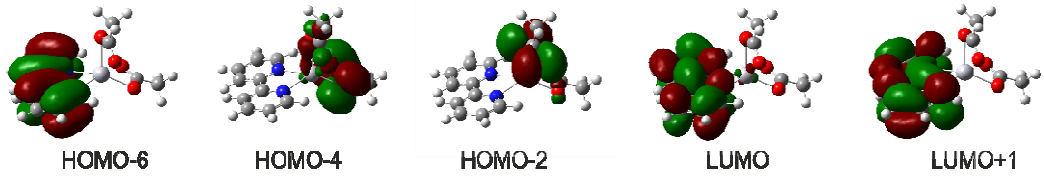
(b)

Figure S19. (a) UV spectra of Cd complexes prepared here (in water). Wavelengths of maximal absorptions: 303 nm, 280 nm, 240 nm (**2A**); 303 nm, 287 nm, 235 nm (**2B**); and 305 nm, 281 nm, 233 nm (**2C**). Their absorption spectra also consist of two main bands intervals. The bands found in the region of 270-310 nm are mainly due to MLCT and LMCT, as observed for complexes **1A**-**1D**. Likewise, the band in the region of 220-260 nm can be assigned to ILCT. These transitions were found at the B3LYP/LANLDZ&6-31G* level of theory for **2A** [panel (b)] and **2B** [Tables S4 and S6, Figures S24 and S26], taken as templates for calculating main transitions of Cd complexes. All these assignments are in good agreement with those described in literature for related complexes.[S1,S2]



(a)

Main transitions computed for **3A**



Excited State	Main Transition (% contribution)	Wavelenght (nm)	f
S7	HOMO-4→LUMO (98%)	353.4	0.003
S9	HOMO-2→LUMO+1 (96%)	326.6	0.03
S18	HOMO-6→LUMO (87%)	262.5	0.296

(b)

Figure S20. (a) UV spectra of Hg complexes prepared here (in water). Wavelengths of maximal absorptions: 309 nm, 298 nm, 253 nm, 245 nm (**3A**); and 290 nm, 268 nm, 235 nm (**3B**). Complex **3A** shows two absorption bands in the 270-320 nm range, which can also be attributed to MLCT and LMCT. In addition to these bands, two weaker bands have been seen in the higher energy region between 240-260 nm, which are mainly due to ILCT. The UV spectrum of **3B** exhibits two bands in the region of 250-300 nm that are predominantly due to MLCT and LMCT, while others bands have been seen in the region of 220-250 nm due to ILCT. These transitions were found at the B3LYP/LANLDZ&6-31G* level of theory for **3A** [panel (b)], taken as template for calculating main transitions of Hg complexes. All these assignments are in good agreement with those described in literature for related complexes.[S1,S2]

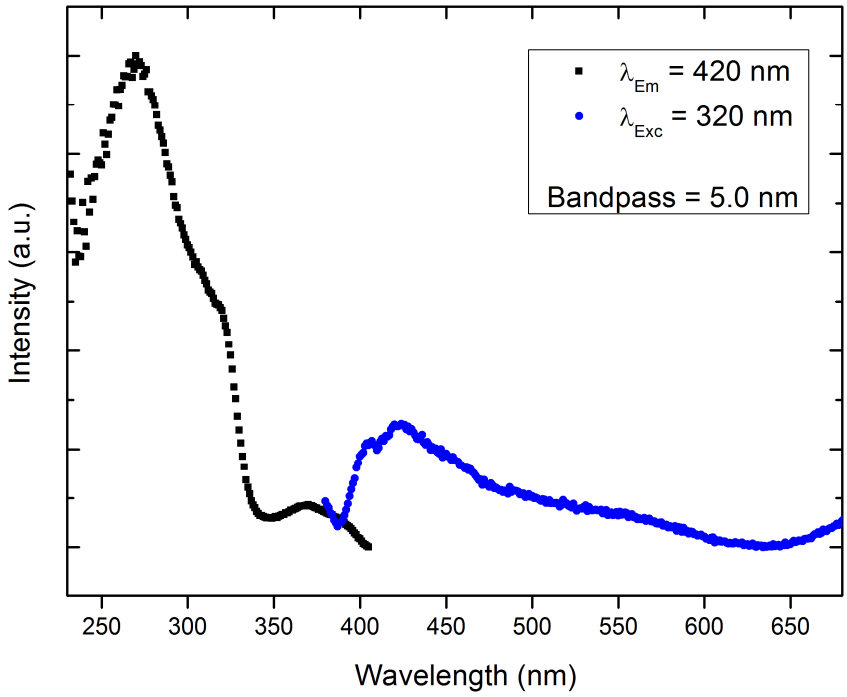


Figure S21. Photoluminescence excitation and emission spectra of **3A**.

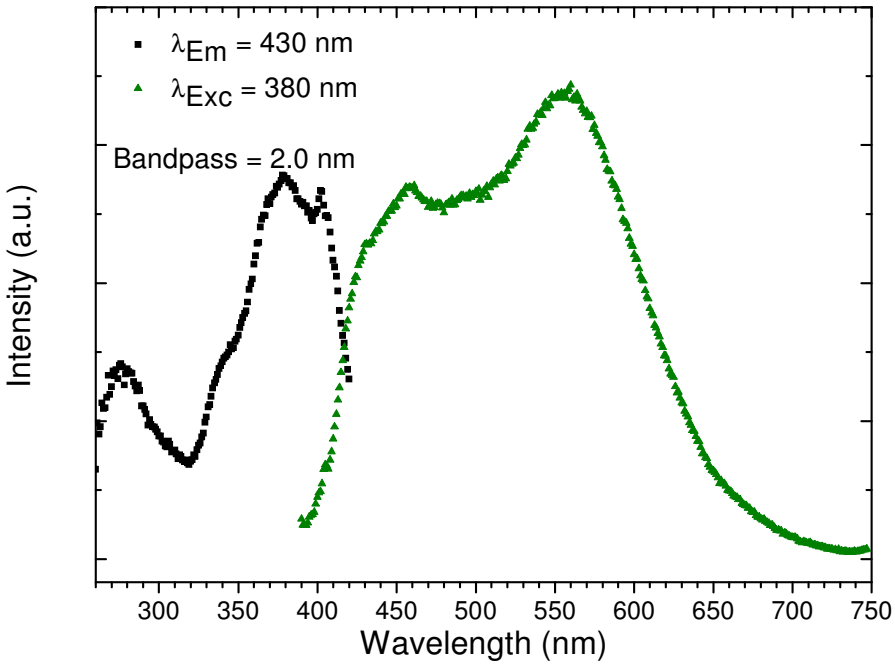


Figure S22. Photoluminescence excitation and emission spectra of **3B**.

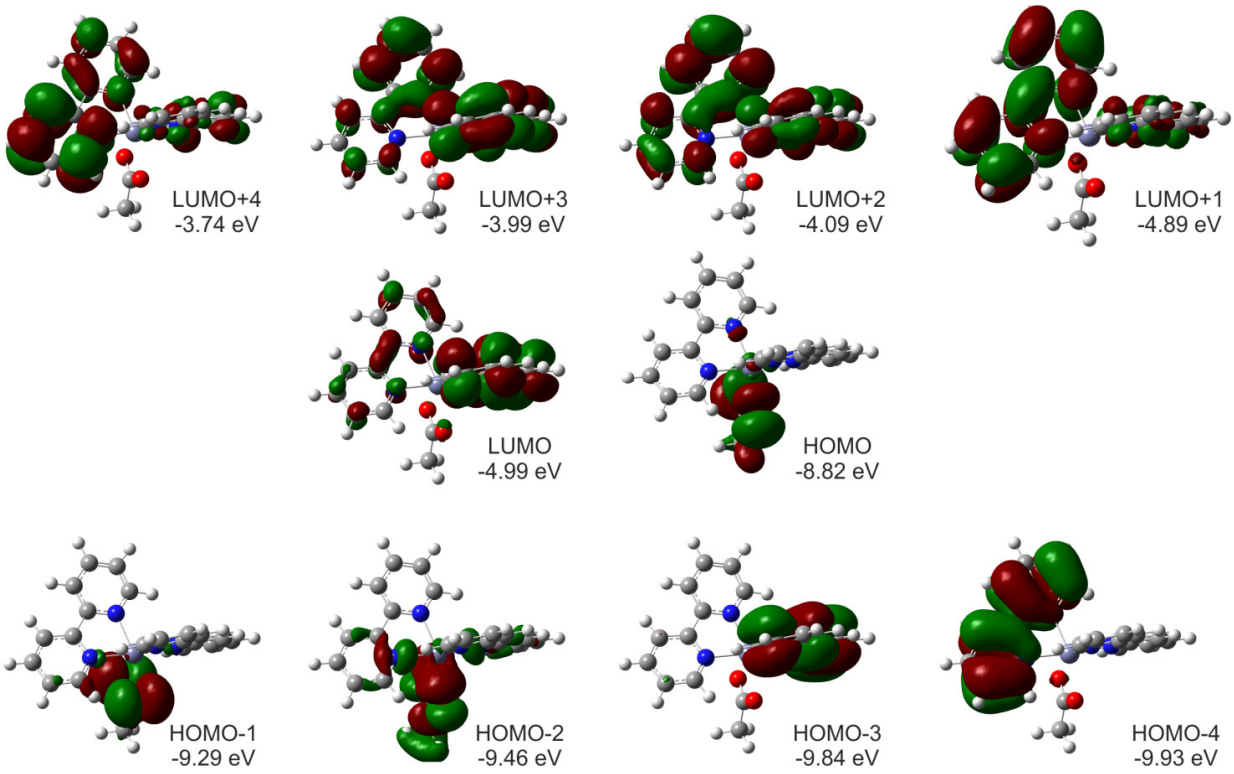


Figure S23. Molecular orbitals of **1C** (partially optimized geometry) calculated using the B3LYP functional, the 6-31G* basis set for all H, C, O and N atoms, and the Los Alamos effective core potential (LANLDZ) basis set for Zn.

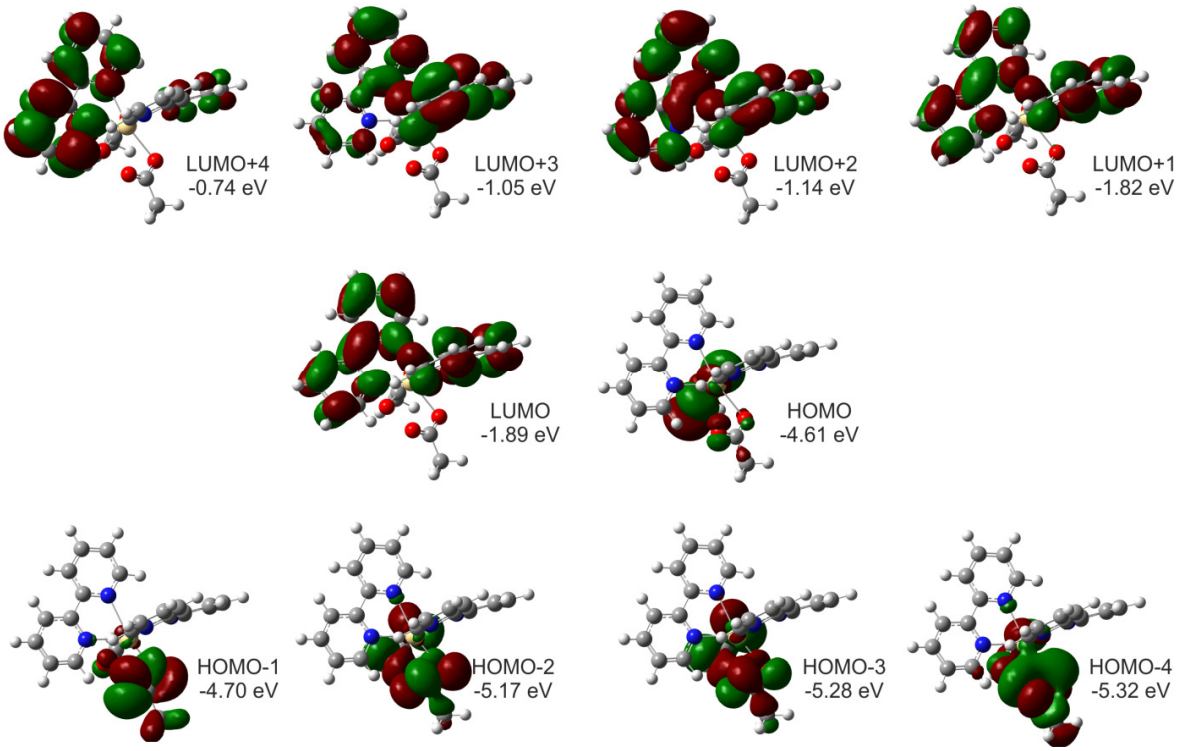


Figure S24. Molecular orbitals of **2B** (partially optimized geometry) calculated using the B3LYP functional, the 6-31G* basis set for all H, C, O and N atoms, and the Los Alamos effective core potential (LANLDZ) basis set for Cd.

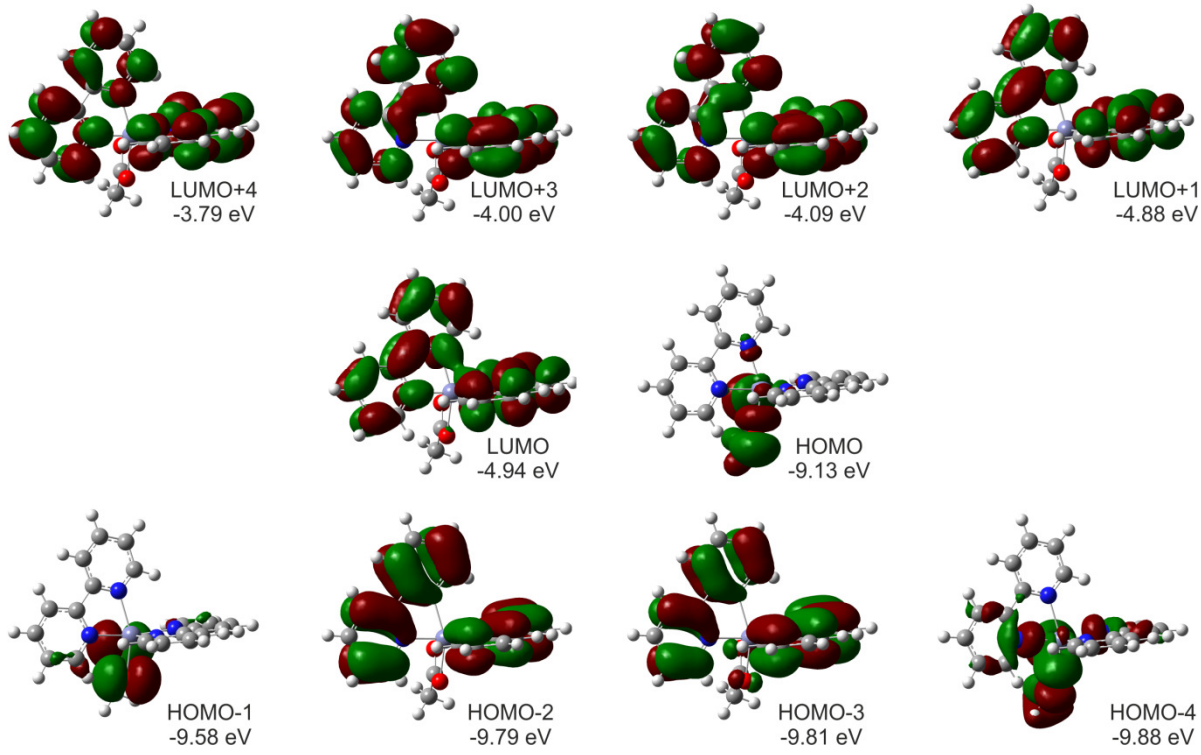


Figure S25. Molecular orbitals of **1C** (fully optimized geometry) calculated using the B3LYP functional, the 6-31G* basis set for all H, C, O and N atoms, and the Los Alamos effective core potential (LANLDZ) basis set for Zn.

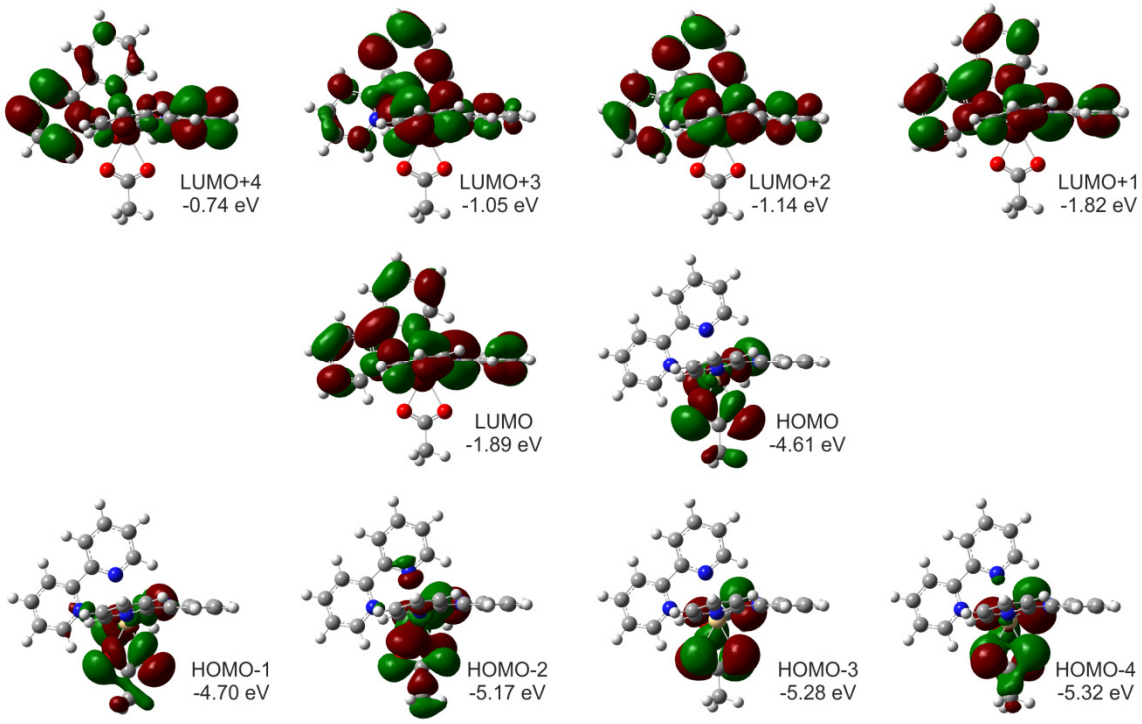


Figure S26. Molecular orbitals of **2B** (fully optimized geometry) calculated using the B3LYP functional, the 6-31G* basis set for all H, C, O and N atoms, and the Los Alamos effective core potential (LANLDZ) basis set for Cd.

B3LYP/LANLDZ&6-31G* partially optimized geometry of **1C**

N 0	-1.953840	-0.589696	-0.164853
C 0	-2.480328	-1.637917	0.388645
C 0	-3.844702	-1.801281	0.588515
C 0	-4.682754	-0.801959	0.150131
C 0	-4.139906	0.335176	-0.426229
C 0	-2.770992	0.422954	-0.550151
C 0	-2.094234	1.611614	-1.141706
C 0	-2.745879	2.793870	-1.401283
C 0	-2.020675	3.865656	-1.917657
C 0	-0.711275	3.707308	-2.136360
C 0	-0.120813	2.537609	-1.856618
N 0	-0.759185	1.491567	-1.372359
H 0	-1.784752	-2.429202	0.660930
H 0	-4.223285	-2.704911	1.053298
H 0	-5.760000	-0.895264	0.254521
H 0	-4.789717	1.125794	-0.781102
H 0	-3.803869	2.907298	-1.198312
H 0	-2.523903	4.804917	-2.127585
H 0	-0.111519	4.520553	-2.536130
H 0	0.943554	2.398734	-2.029747
Zn 0	0.072448	-0.399640	-0.866270
N 0	2.046746	-0.022977	-1.560083
N 0	1.112118	-0.015910	0.925369
C 0	0.584356	0.013333	2.147325
C 0	1.330191	0.263257	3.296997
C 0	2.667277	0.519955	3.115632
C 0	3.242694	0.495078	1.907677
C 0	2.434446	0.225188	0.774787
C 0	2.950827	0.158560	-0.633874
C 0	2.417744	-0.094212	-2.852336
C 0	3.771135	0.042020	-3.228483
C 0	4.707366	0.225718	-2.228161
C 0	4.306871	0.313112	-0.962366
H 0	-0.481800	-0.186806	2.206485
H 0	0.862281	0.269692	4.274305
H 0	3.283172	0.734074	3.987138
H 0	4.301603	0.692713	1.791575
H 0	1.624652	-0.284033	-3.567862
H 0	4.050432	-0.023844	-4.274305
H 0	5.760000	0.319520	-2.482118
H 0	5.033600	0.462008	-0.170873
O 0	0.317694	-2.612321	-0.844643
O 0	-0.430528	-1.587232	-2.646031
C 0	-0.136372	-2.643116	-2.021863
C 0	-0.365074	-3.980538	-2.723980
H 0	0.069288	-4.804917	-2.155866
H 0	-1.442499	-4.146464	-2.836508
H 0	0.062162	-3.948653	-3.730425

SCF Energy = -1284.75889664

B3LYP/LANLDZ&6-31G* partially optimized geometry of **2B**

Cd 0	-0.017404	0.469974	-0.191297
O 0	-1.256053	2.673515	0.406628
O 0	-0.007020	1.674733	1.855127
C 0	-0.674696	2.658787	1.507611
C 0	-0.794727	3.824759	2.412178
H 0	-0.963898	3.504553	3.446841
H 0	-1.600234	4.491132	2.095464
H 0	0.143767	4.394712	2.408288
N 0	-1.100439	-1.235663	1.190840
C 0	-2.392821	-1.508078	0.973789
N 0	-2.225316	-0.066922	-0.946927
C 0	-2.996798	-0.889748	-0.233373
C 0	-4.297202	-1.149177	-0.618277
C 0	-4.803823	-0.567390	-1.754140
C 0	-4.026381	0.244275	-2.490206
C 0	-2.753088	0.488647	-2.050140
C 0	-0.518593	-1.811301	2.250241
C 0	-1.173039	-2.652329	3.115874
C 0	-2.496380	-2.894279	2.897055
C 0	-3.121323	-2.314798	1.828967
H 0	-4.928362	-1.813718	-0.040257
H 0	-5.828765	-0.781915	-2.049340
H 0	-4.382240	0.723142	-3.397265
H 0	-2.067689	1.152597	-2.575341
H 0	0.527706	-1.558781	2.394534
H 0	-0.641055	-3.091861	3.953918
H 0	-3.059711	-3.537532	3.569050
H 0	-4.175197	-2.498439	1.660201
O 0	1.443328	2.092429	-1.035464
O 0	0.087566	1.646771	-2.654193
C 0	0.969250	2.331893	-2.153261
C 0	1.548615	3.485027	-2.917533
H 0	2.643307	3.445472	-2.896867
H 0	1.257251	4.427483	-2.437585
H 0	1.200382	3.498732	-3.953918
N 0	0.828615	-1.411740	-1.484628
N 0	2.127560	-0.343844	0.630613
C 0	0.129227	-1.987323	-2.462769
C 0	0.563937	-3.090036	-3.154103
C 0	1.777048	-3.617562	-2.840779
C 0	2.526749	-3.047540	-1.839001
C 0	2.025865	-1.930304	-1.179336
C 0	2.793535	-1.256098	-0.100471
C 0	2.789040	0.287218	1.606166
C 0	4.108149	0.044697	1.903454
C 0	4.777037	-0.872533	1.142081
C 0	4.137863	-1.518039	0.138041
H 0	-0.824004	-1.521165	-2.690836
H 0	-0.053745	-3.512515	-3.941009
H 0	2.154598	-4.491132	-3.367001
H 0	3.484795	-3.473158	-1.566456
H 0	2.191580	1.024938	2.138792
H 0	4.594044	0.585099	2.709515
H 0	5.828765	-1.077890	1.330416
H 0	4.681430	-2.221385	-0.483097

SCF Energy = -1495.85944760

B3LYP/LANLDZ&6-31G* fully optimized geometry of **1C**

N 0	2.109079	-0.439421	0.684670
C 0	2.630226	0.259930	1.703136
C 0	3.984607	0.208033	2.028251
C 0	4.819634	-0.590349	1.248967
C 0	4.280351	-1.302430	0.178532
C 0	2.908773	-1.208610	-0.083080
C 0	2.243399	-1.914169	-1.216143
C 0	2.920811	-2.803460	-2.058646
C 0	2.235633	-3.408338	-3.110033
C 0	0.886563	-3.116045	-3.298878
C 0	0.278343	-2.228228	-2.414656
N 0	0.932204	-1.644411	-1.402217
H 0	1.928173	0.887092	2.244161
H 0	4.368501	0.786439	2.861589
H 0	5.882481	-0.653432	1.461806
H 0	4.928496	-1.907717	-0.443402
H 0	3.968766	-3.028250	-1.902534
H 0	2.752136	-4.097567	-3.771029
H 0	0.315987	-3.560617	-4.106974
H 0	-0.770496	-1.967050	-2.515789
Zn 0	-0.001013	-0.197569	0.036572
O 0	-0.132945	1.628216	1.149677
O 0	0.119529	1.649648	-1.046266
C 0	-0.009804	2.274778	0.057288
C 0	-0.050282	3.785171	0.069698
H 0	-1.096547	4.112721	0.038125
H 0	0.388801	4.172272	0.992025
H 0	0.463163	4.193870	-0.802738
N 0	-2.111287	-0.436040	-0.614919
N 0	-0.925959	-1.680356	1.444001
C 0	-0.268335	-2.281978	2.443517
C 0	-0.871112	-3.191949	3.308735
C 0	-2.218579	-3.487795	3.114173
C 0	-2.907678	-2.864480	2.076194
C 0	-2.235670	-1.953593	1.252645
C 0	-2.905654	-1.227837	0.135161
C 0	-2.637029	0.281929	-1.617986
C 0	-3.990829	0.227227	-1.945116
C 0	-4.820298	-0.594502	-1.184328
C 0	-4.276400	-1.325910	-0.129393
H 0	0.779027	-2.017021	2.549877
H 0	-0.297652	-3.650404	4.106974
H 0	-2.730843	-4.193870	3.760527
H 0	-3.954443	-3.091779	1.915813
H 0	-1.939144	0.925987	-2.144456
H 0	-4.378568	0.820869	-2.765871
H 0	-5.882481	-0.660982	-1.399460
H 0	-4.920373	-1.949688	0.478443

SCF Energy = -1284.78574885

Sum of electronic and zero-point Energies= -1284.412378

Sum of electronic and thermal Energies= -1284.386299

Sum of electronic and thermal Enthalpies= -1284.385355

Sum of electronic and thermal Free Energies= -1284.472331

Number of Imaginary Frequencies= 0

B3LYP/LANLDZ&6-31G* fully optimized geometry of **2B**

Cd 0	0.002060	-0.814151	-0.031292
O 0	-1.563603	-2.187982	-1.130335
O 0	0.056052	-1.338102	-2.398216
C 0	-0.971795	-2.066103	-2.242647
C 0	-1.493611	-2.849102	-3.441250
H 0	-1.388624	-2.262250	-4.358479
H 0	-2.535691	-3.142444	-3.294529
H 0	-0.892249	-3.758768	-3.559449
N 0	-1.092538	1.301267	-1.061904
C 0	-2.295534	1.746218	-0.655051
N 0	-2.266657	0.006062	1.015289
C 0	-3.008601	0.912768	0.356653
C 0	-4.384881	1.041505	0.589645
C 0	-4.991170	0.216119	1.534343
C 0	-4.214145	-0.718471	2.214141
C 0	-2.852271	-0.793293	1.914489
C 0	-0.436372	1.971288	-2.013171
C 0	-0.924877	3.140952	-2.595784
C 0	-2.152964	3.629810	-2.155152
C 0	-2.848332	2.926013	-1.175443
H 0	-4.981461	1.750123	0.026153
H 0	-6.058156	0.296488	1.723673
H 0	-4.647972	-1.386903	2.951061
H 0	-2.188320	-1.509570	2.389999
H 0	0.513573	1.542082	-2.313657
H 0	-0.354430	3.649155	-3.366655
H 0	-2.567384	4.546035	-2.566781
H 0	-3.799779	3.298153	-0.812603
O 0	1.536320	-2.439136	0.703090
O 0	-0.073417	-1.903654	2.144191
C 0	0.944718	-2.584530	1.812907
C 0	1.456043	-3.643267	2.782464
H 0	2.493799	-3.906274	2.564701
H 0	0.841865	-4.546035	2.677970
H 0	1.359814	-3.296293	3.815479
N 0	1.140323	0.934872	1.499961
N 0	2.277260	0.215275	-0.854878
C 0	0.502984	1.331142	2.605048
C 0	1.012528	2.298363	3.471616
C 0	2.241329	2.876507	3.160033
C 0	2.917590	2.453550	2.018661
C 0	2.344351	1.460738	1.209886
C 0	3.035762	0.918604	0.003411
C 0	2.842854	-0.325903	-1.940206
C 0	4.200199	-0.179318	-2.233976
C 0	4.994051	0.546673	-1.349714
C 0	4.408730	1.100740	-0.213064
H 0	-0.447100	0.843005	2.794856
H 0	0.457458	2.587008	4.358479
H 0	2.671436	3.645813	3.795503
H 0	3.869858	2.900042	1.755747
H 0	2.166509	-0.893643	-2.572878
H 0	4.617524	-0.635642	-3.125981
H 0	6.058156	0.671836	-1.530737
H 0	5.019330	1.639147	0.503101

SCF Energy = -1495.89462579
Sum of electronic and zero-point Energies= -1495.472794
Sum of electronic and thermal Energies= -1495.439933
Sum of electronic and thermal Enthalpies= -1495.438989
Sum of electronic and thermal Free Energies= -1495.543995
Number of Imaginary Frequencies= 0

Supplementary References

S1. M. Shukla, N. Srivastava, S. Saha, T.R. Rao and S. Sunkari, *Polyhedron*, 2011, **30**, 754–763.

S2. G. H. Eom, H. M. Park, M. Y. Hyun, S. P. Jang, C. Kim, J. H. Lee, S. J. Lee, S.-J. Kim and Y. Kim, *Polyhedron*, 2011, **30**, 1555–1564.