

Supporting Information

Insight into the conformational selectivity in cobalt(III) complexes with a tetradentate salen-type Schiff base ligand and their biorelevant catalysis: a combined experimental and theoretical study

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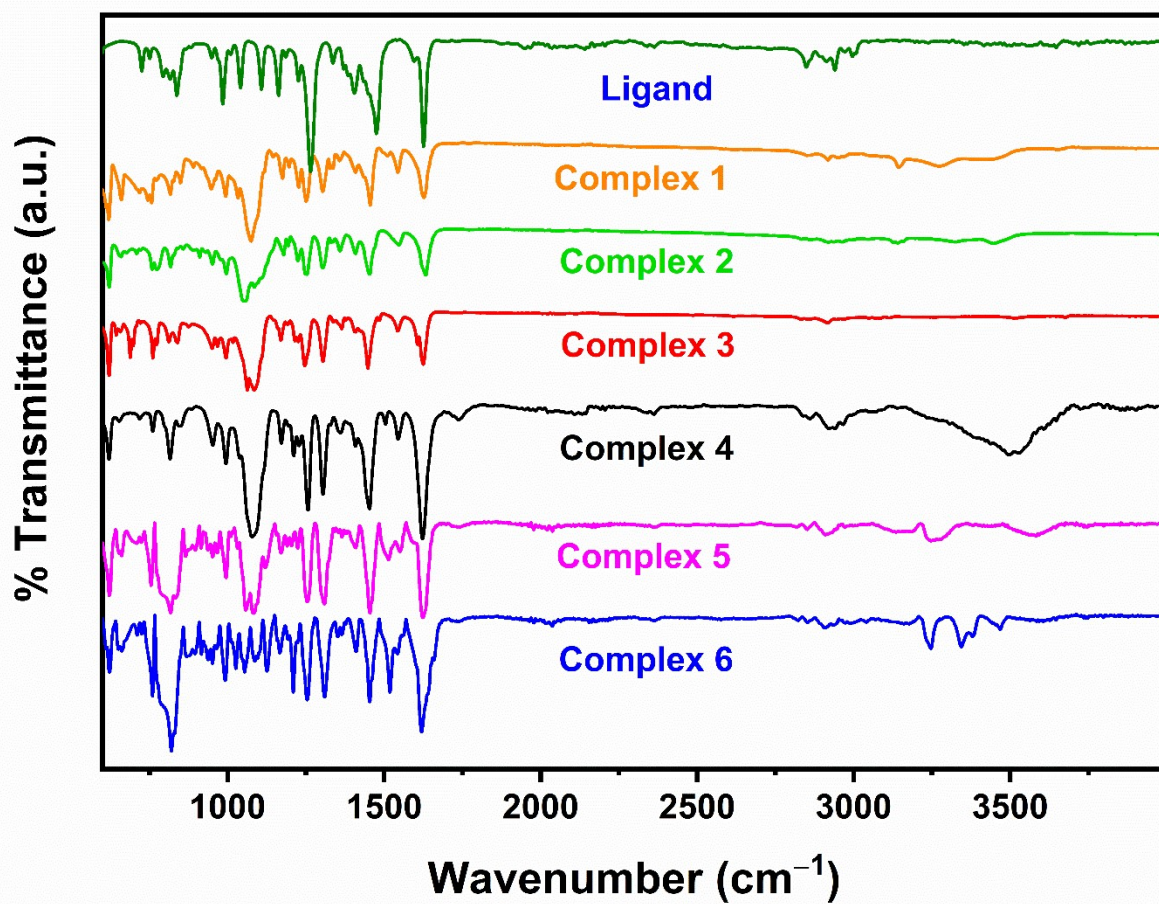


Fig. S1. IR spectra of the Ligand (H₂L) and all complexes.

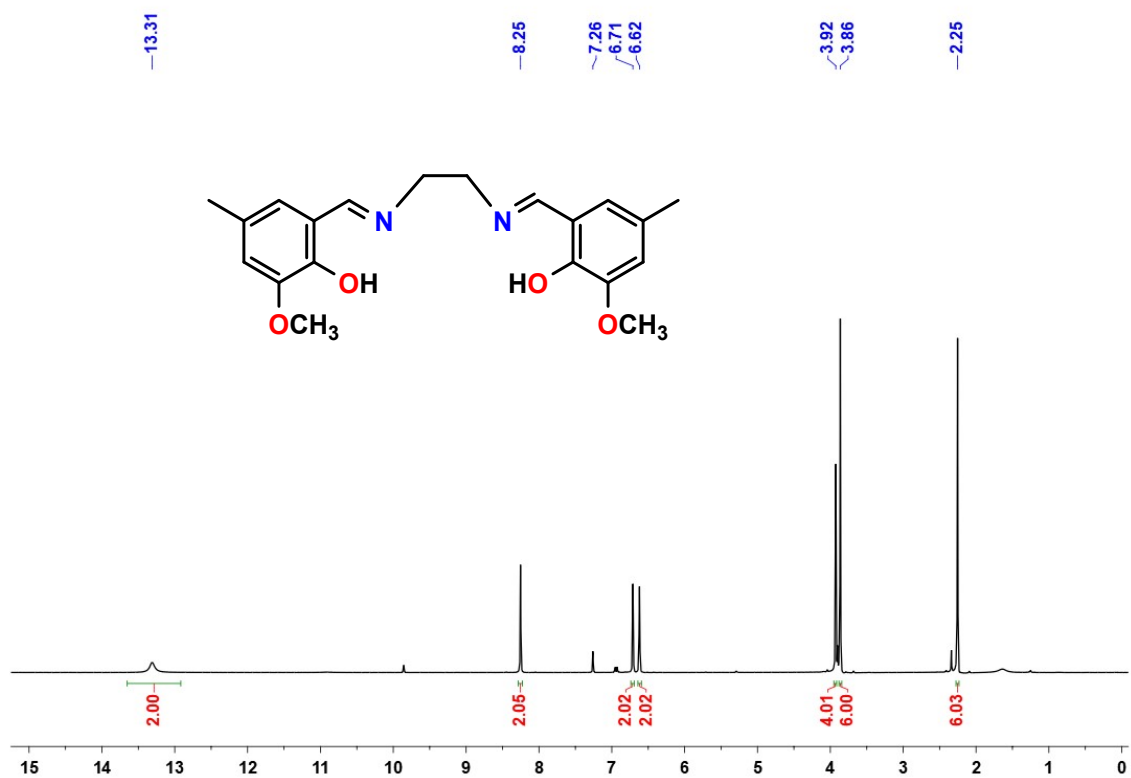


Fig. S2. ¹H NMR of *N,N'*-bis(3-methoxy-5-methylsalicylidene)-ethane-1,2-diamine in CDCl₃ at r.t.

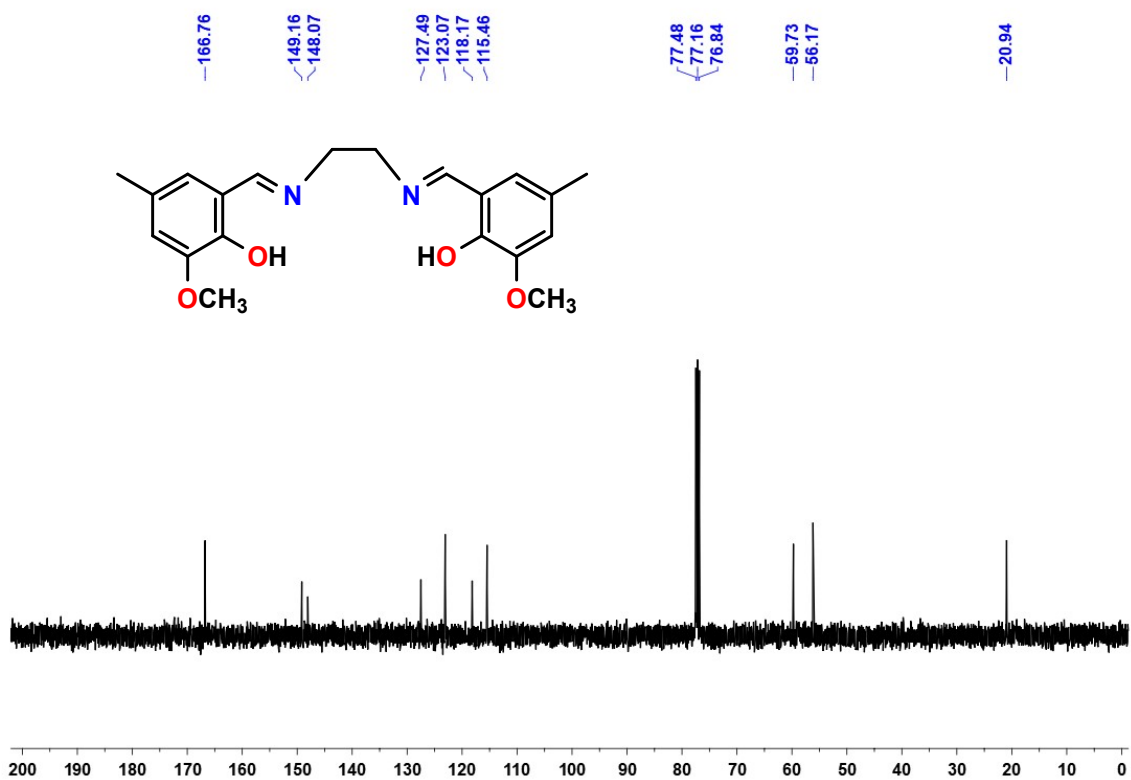


Fig. S3. ¹³C NMR of *N,N'*-bis(3-methoxy-5-methylsalicylidene)-ethane-1,2-diamine in CDCl₃ at r.t.

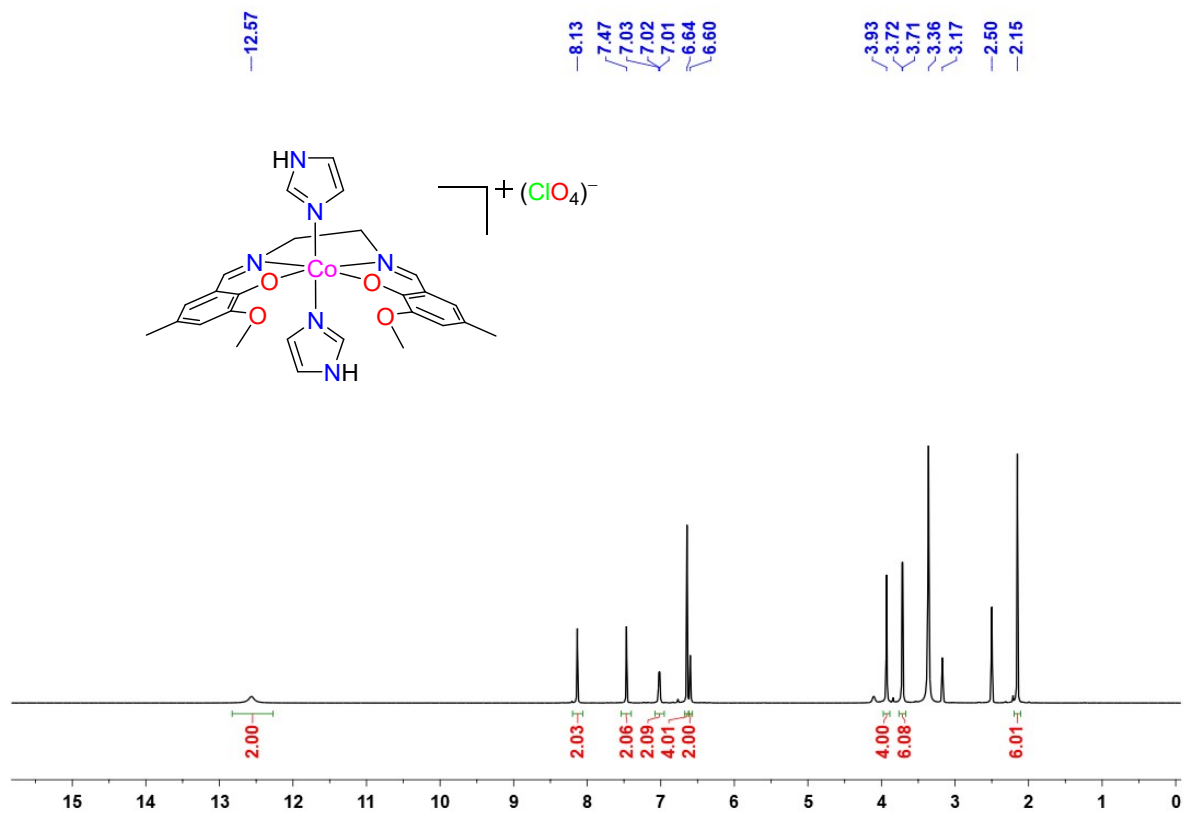


Fig. S4. ^1H NMR of complex 1 in DMSO-d_6 at r.t.

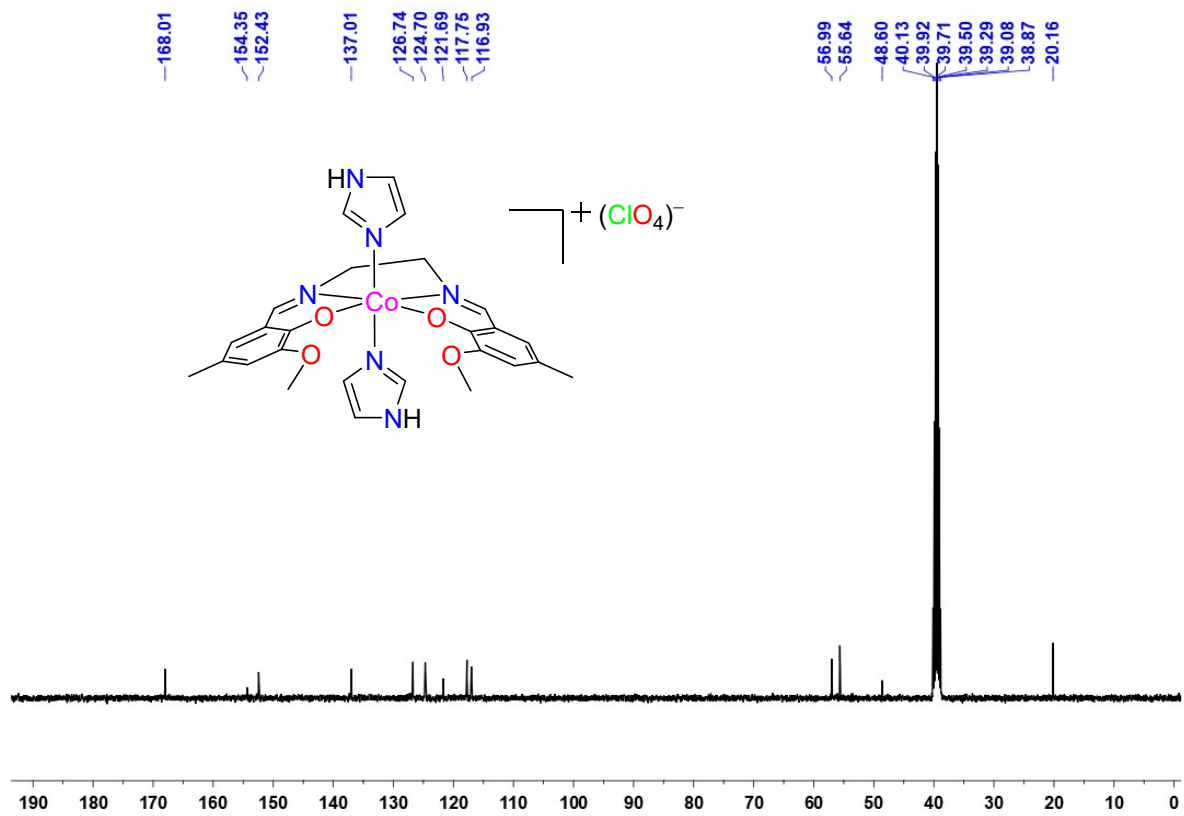


Fig. S5. ^{13}C NMR of Complex 1 in DMSO-d_6 at r.t.

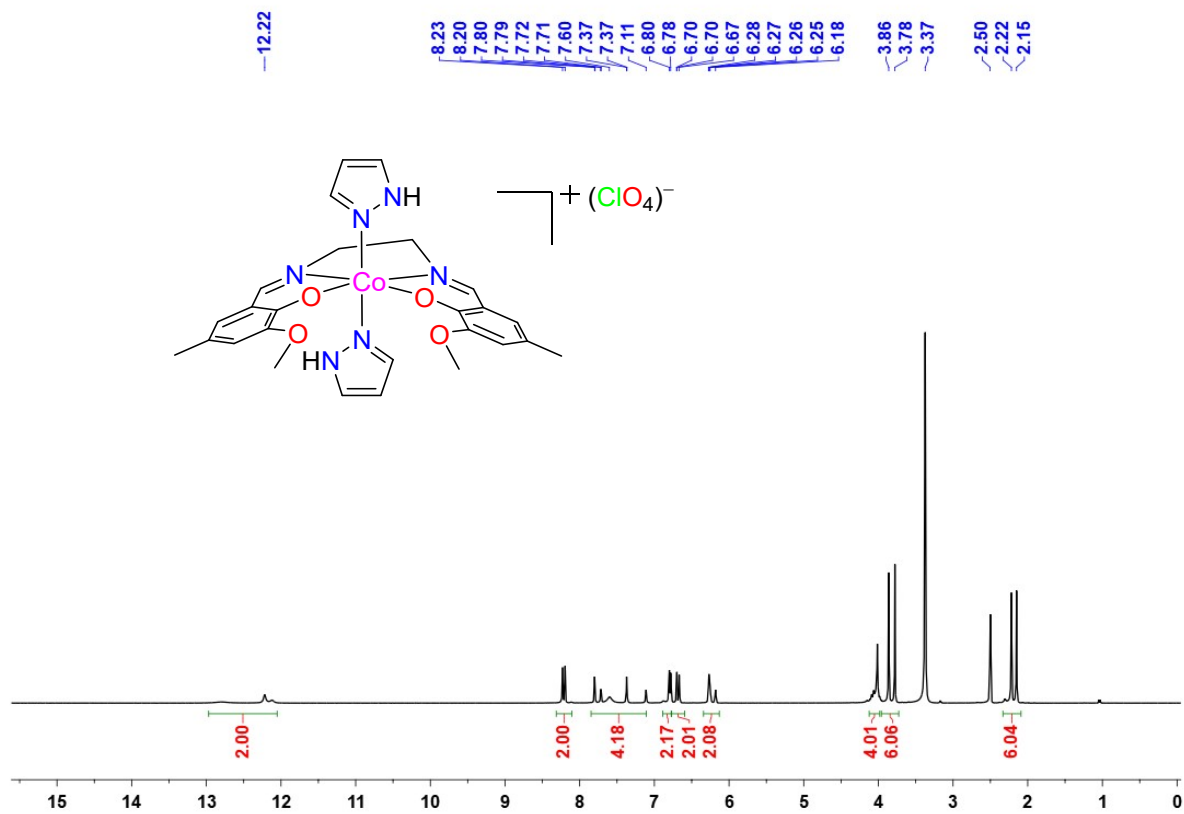


Fig. S6. ¹H NMR of Complex 2 in DMSO-d₆ at r.t.

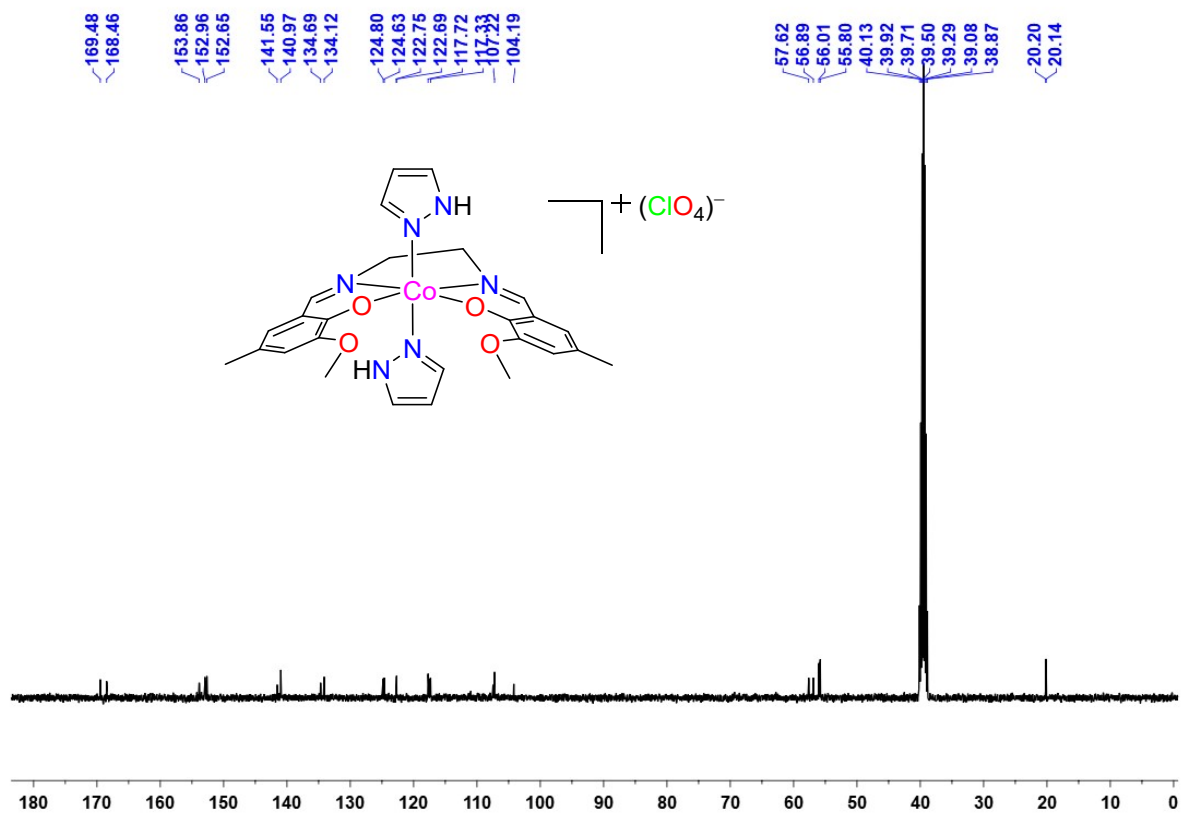


Fig. S7. ¹³C NMR of Complex 2 in DMSO-d₆ at r.t.

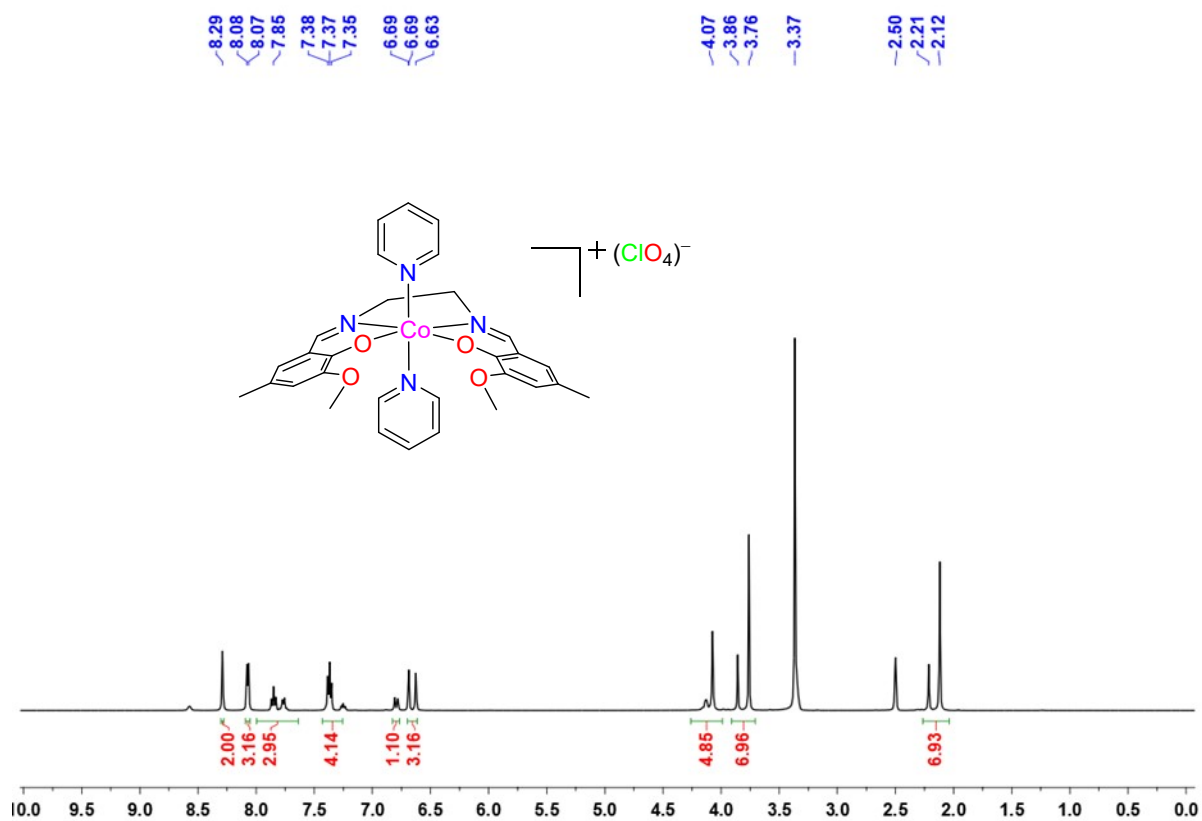


Fig. S8. $^1\text{H NMR}$ of Complex 3 in DMSO-d_6 at r.t.

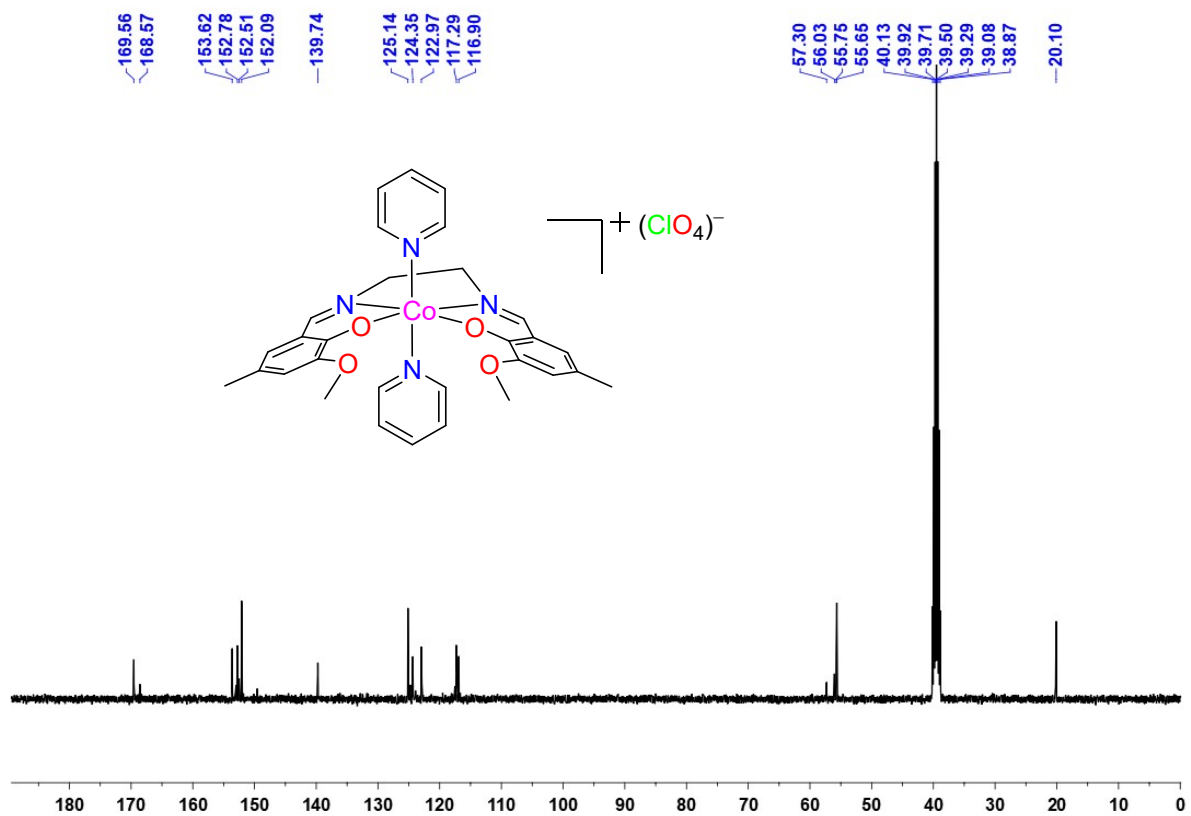


Fig. S9. $^{13}\text{C NMR}$ of Complex 3 in DMSO-d_6 at r.t.

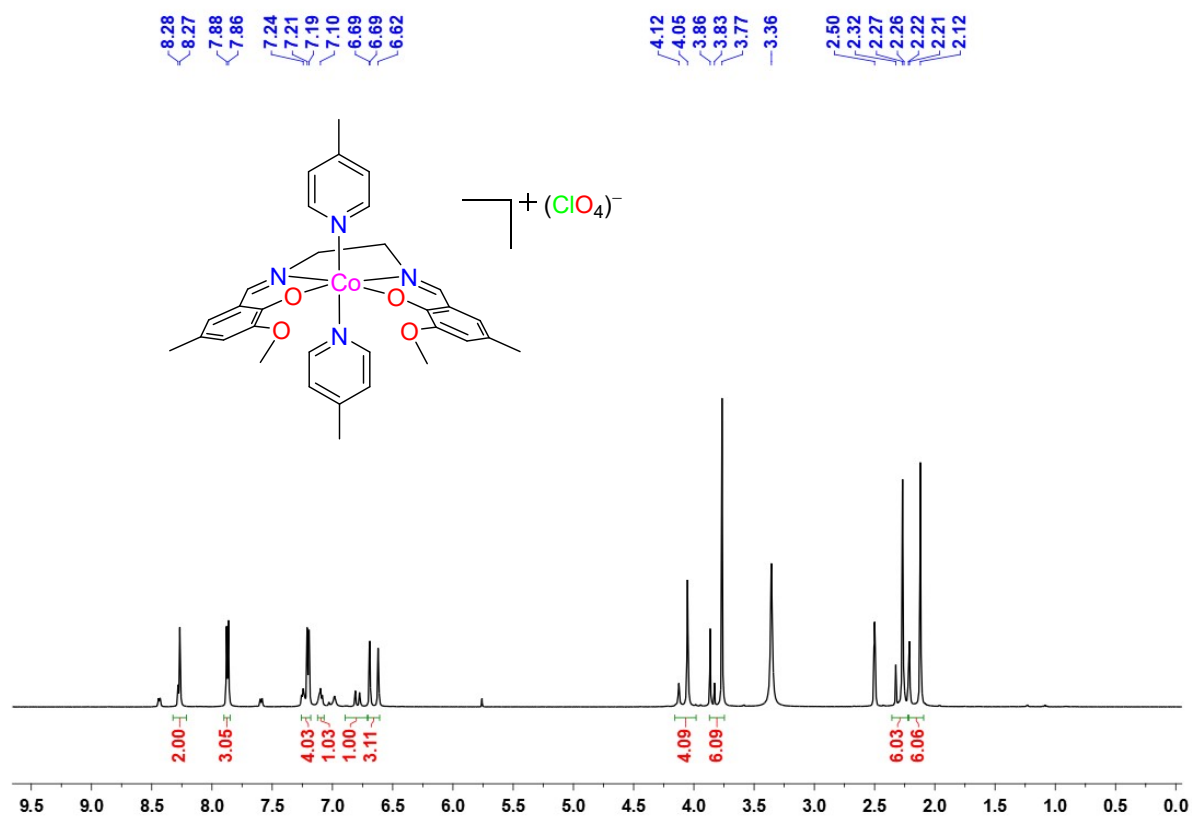


Fig. S10. ¹H NMR of Complex 4 in DMSO-d₆ at r.t.

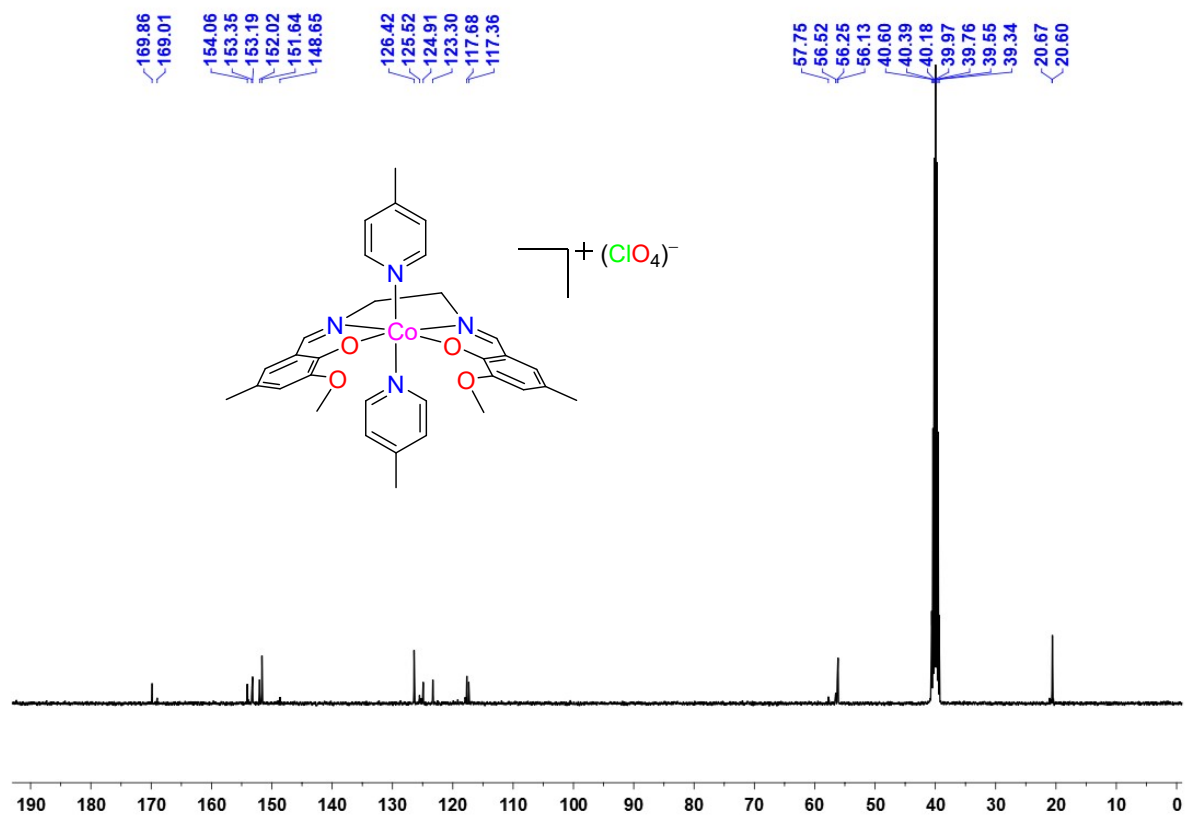


Fig. S11. ¹³C NMR of Complex 4 in DMSO-d₆ at r.t.

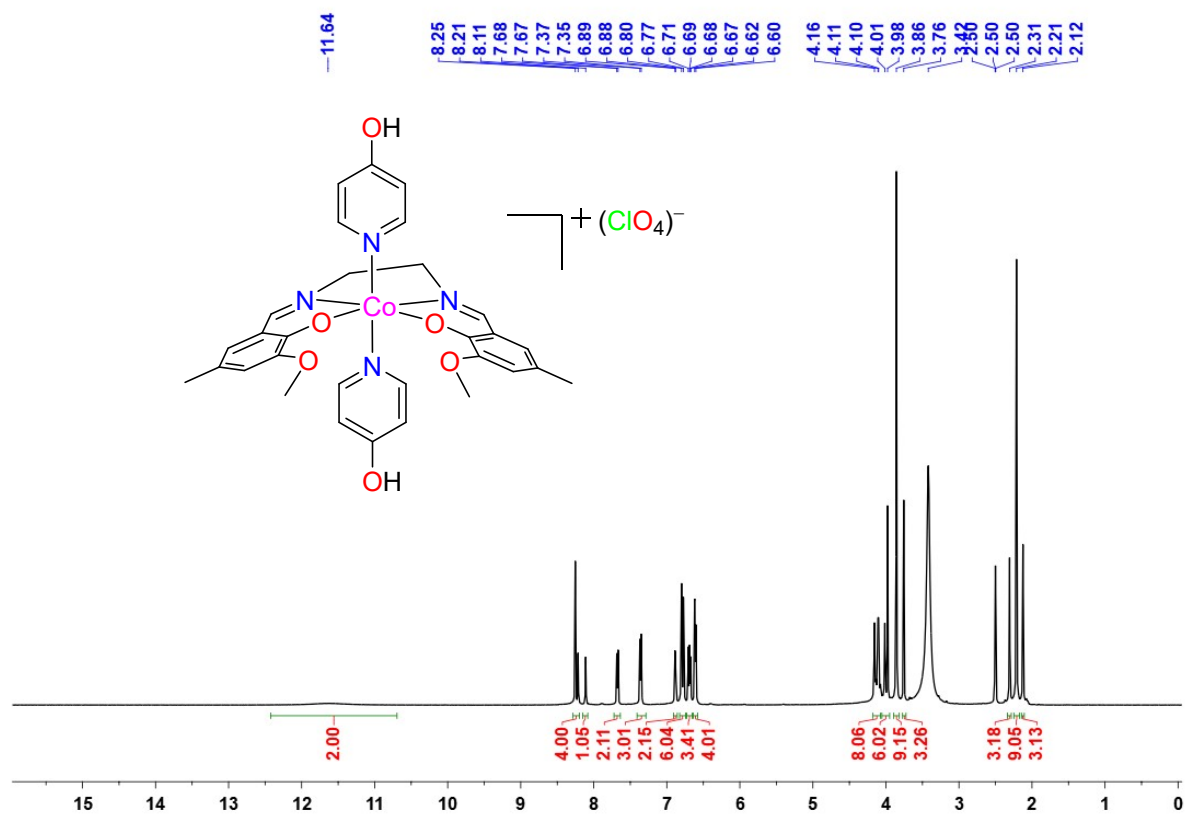


Fig. S12. $^1\text{H NMR}$ of Complex **5** in DMSO-d_6 at r.t.

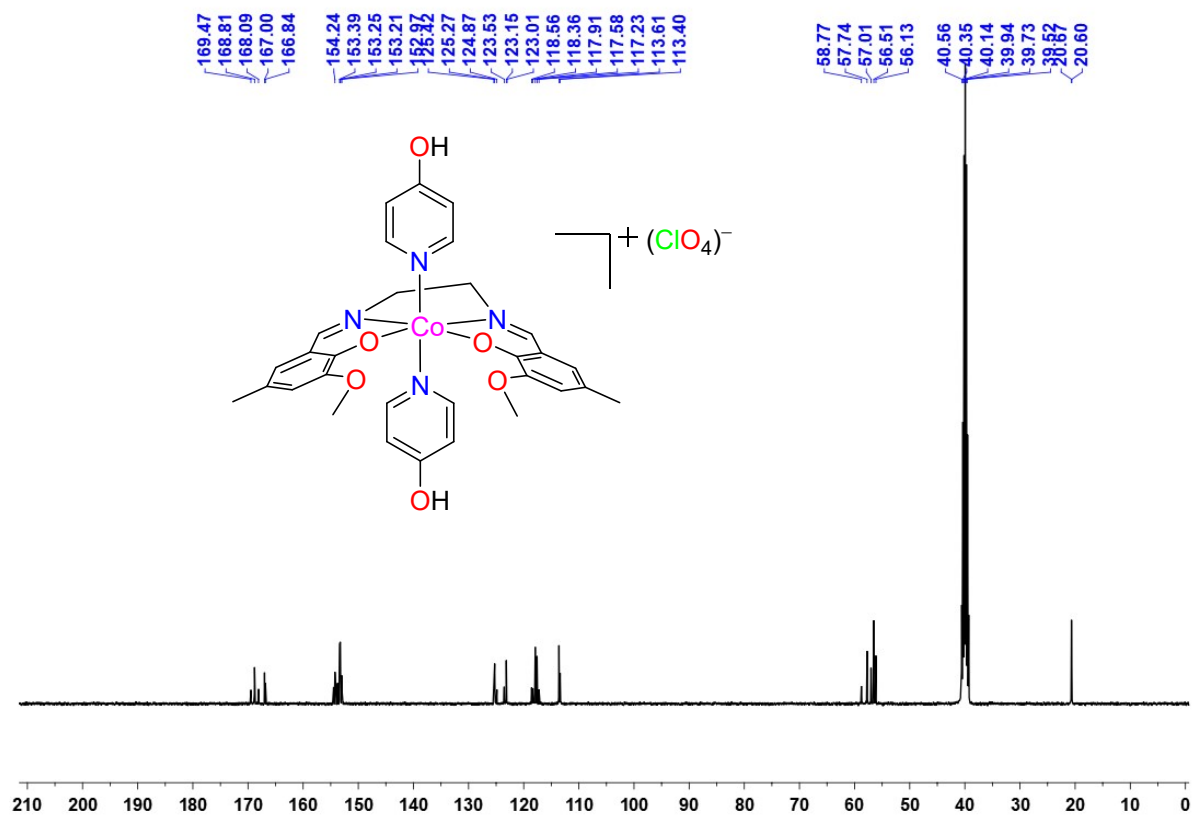


Fig. S13. $^{13}\text{C NMR}$ of Complex **5** in DMSO-d_6 at r.t.

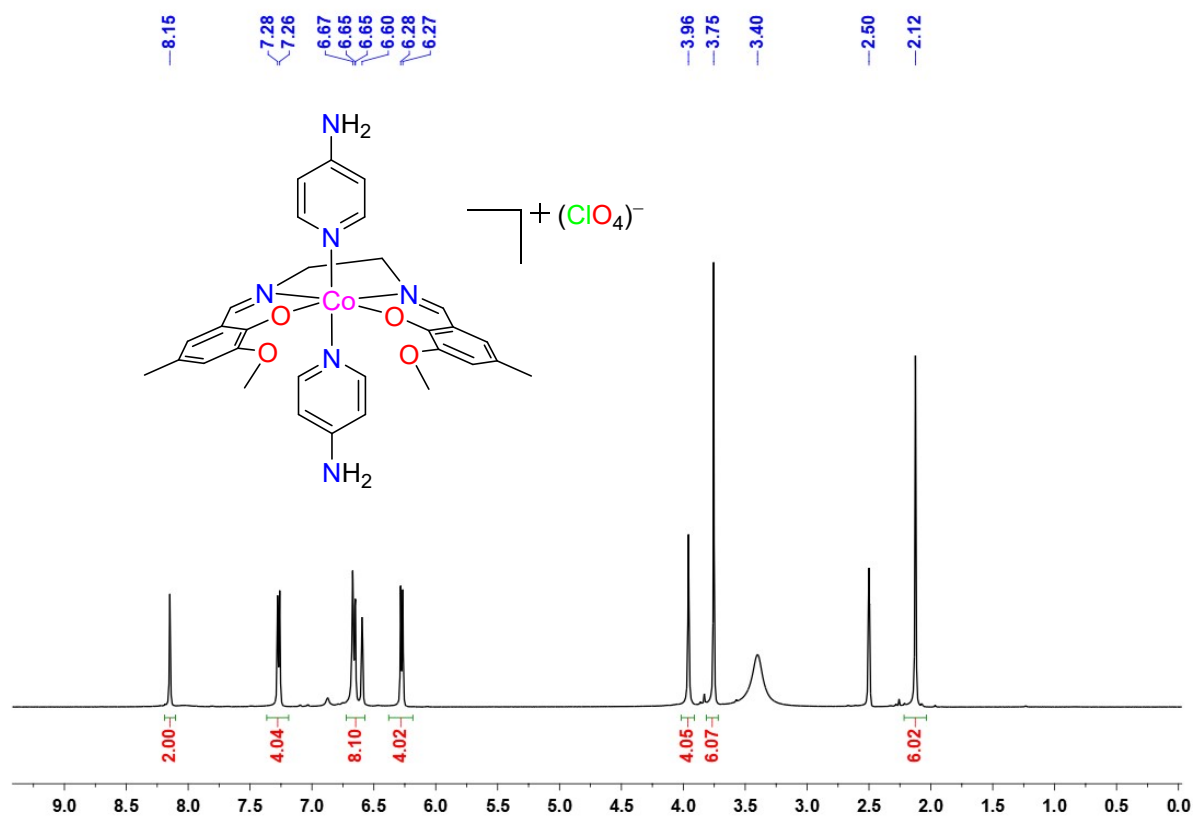


Fig. S14. $^1\text{H NMR}$ of Complex 6 in DMSO-d_6 at r.t.

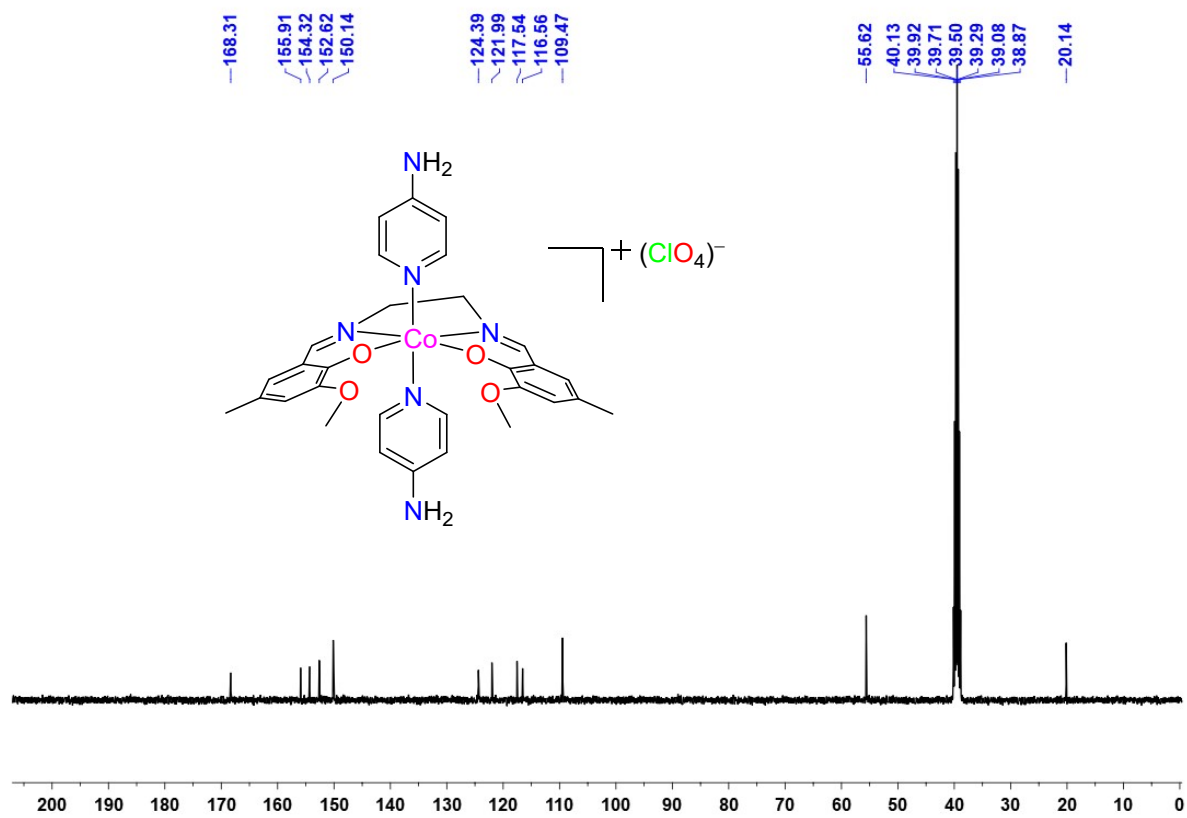


Fig. S15. $^{13}\text{C NMR}$ of Complex 6 in DMSO-d_6 at r.t.

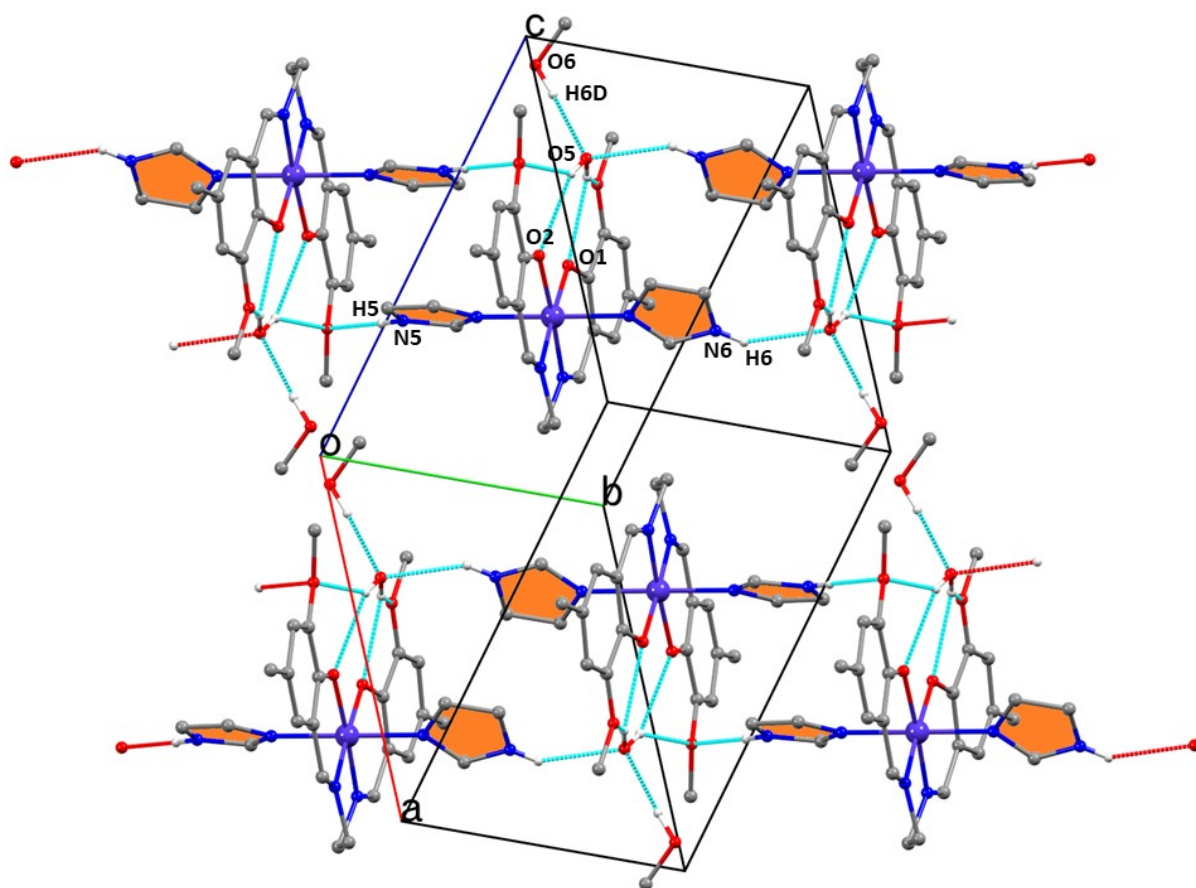


Fig. S16. A part of crystal packing showing hydrogen bonding interaction in 1.

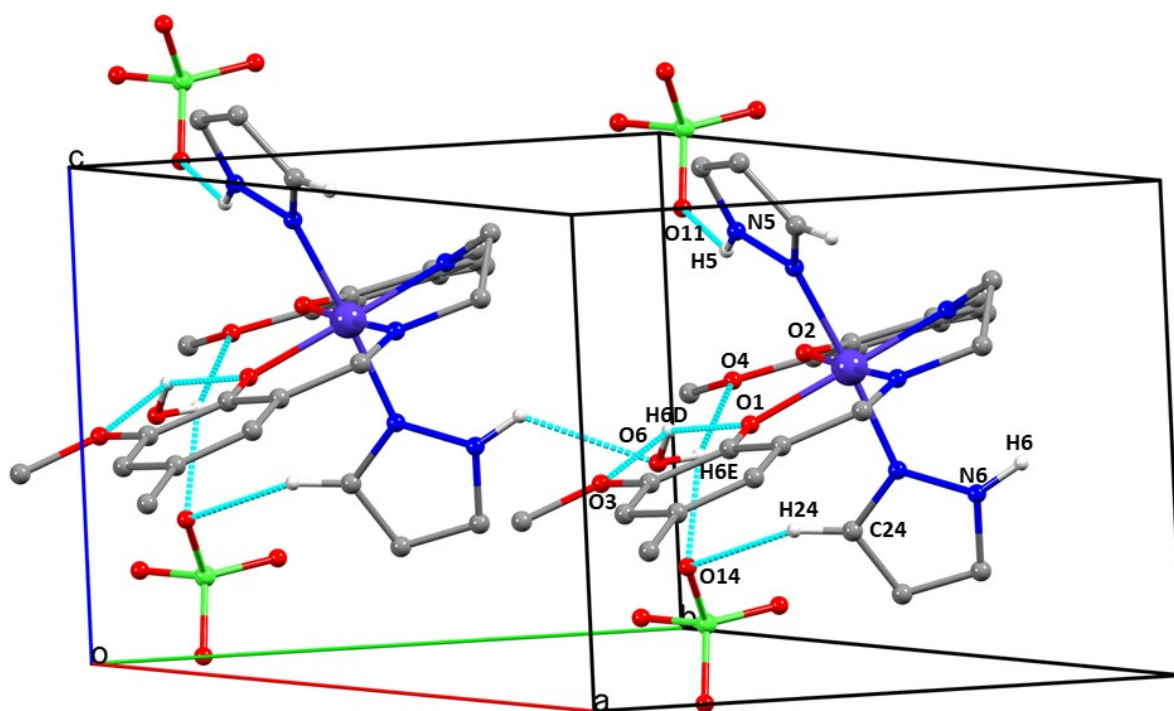


Fig. S17. A part of crystal packing showing hydrogen bonding interaction in 2.

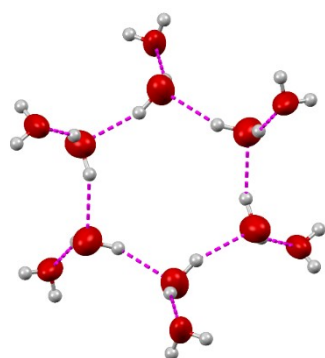
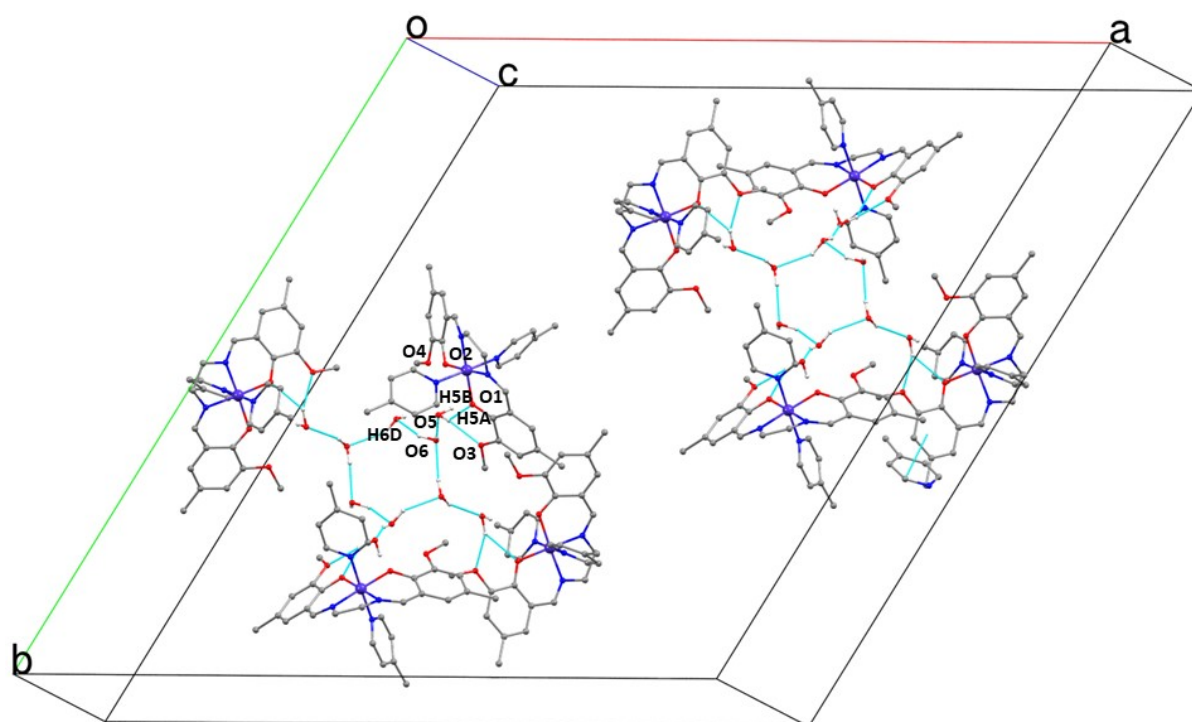


Fig. S18. Packing diagram of **4** showing inclusion of dodecameric water cluster.

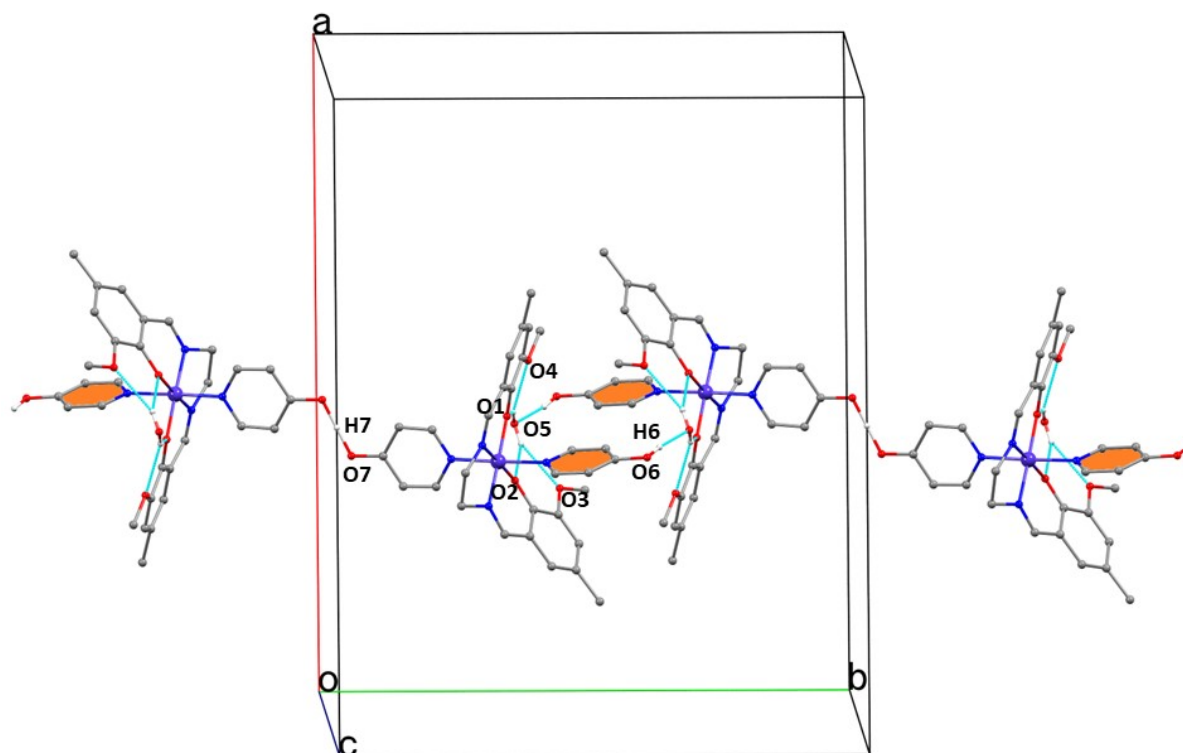


Fig. S19. A part of crystal packing showing hydrogen bonding interaction in **5**.

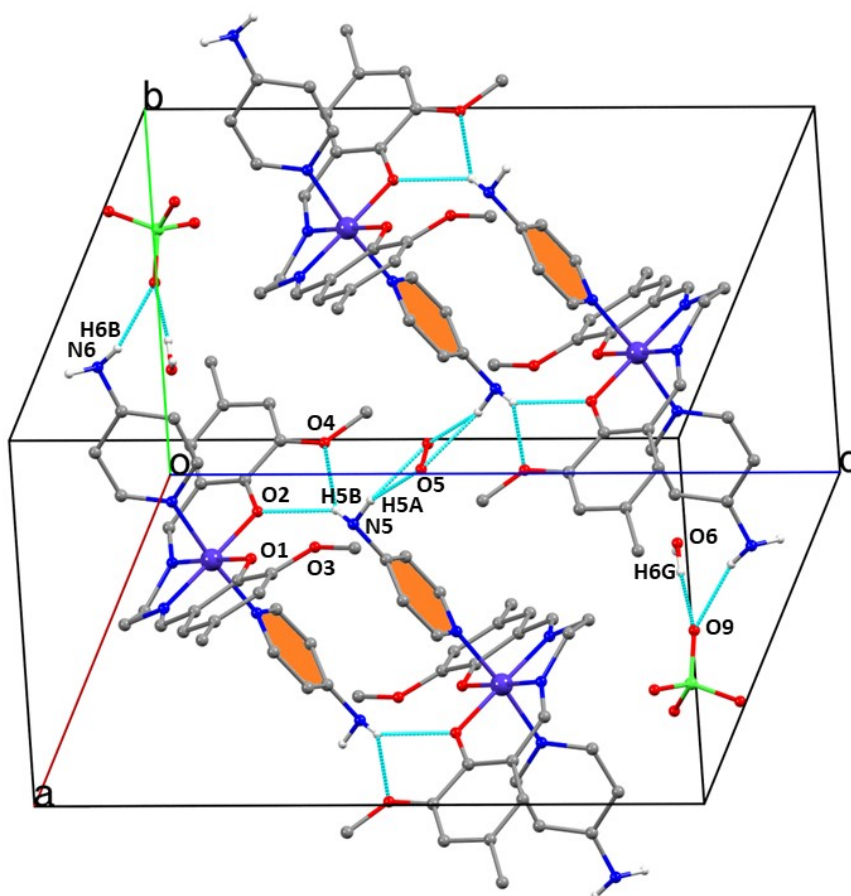


Fig. S20. A part of crystal packing showing hydrogen bonding interaction in **6**.

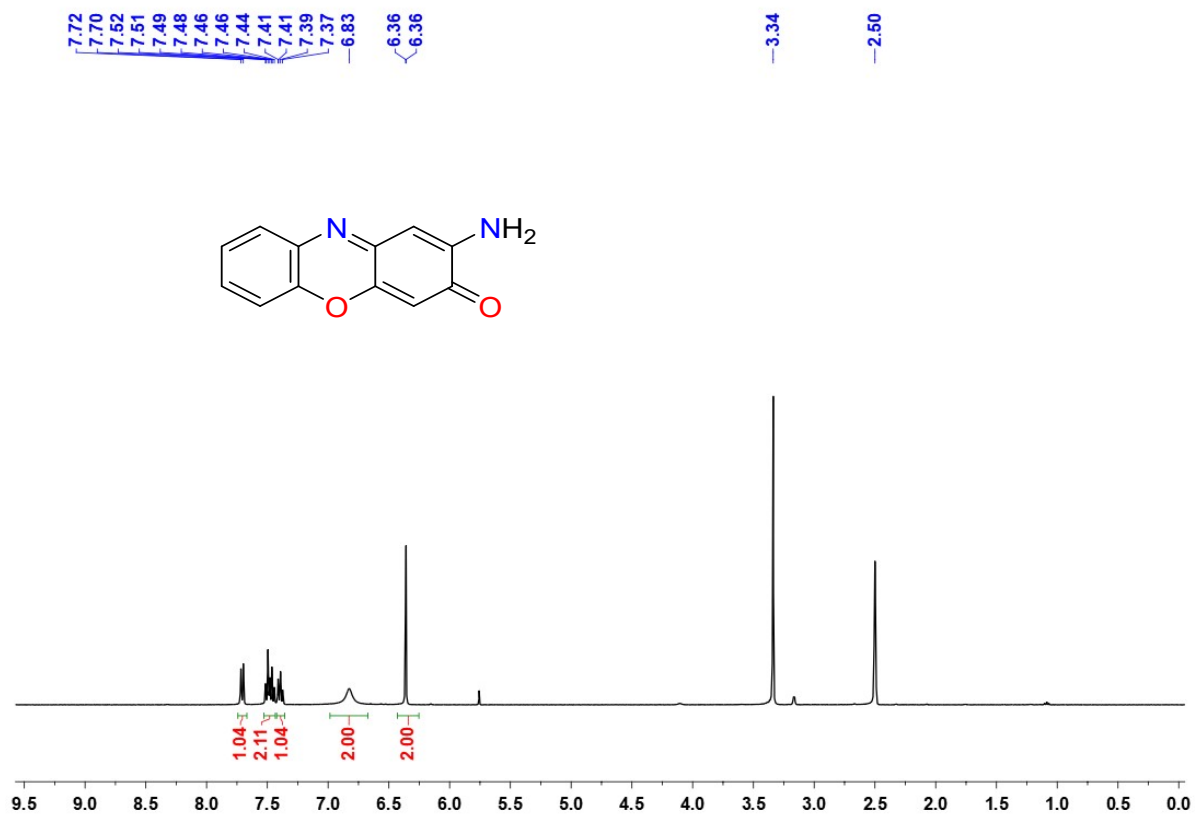


Fig. S21. ¹H NMR of the catalytic product PHX in DMSO-d₆ at r.t.

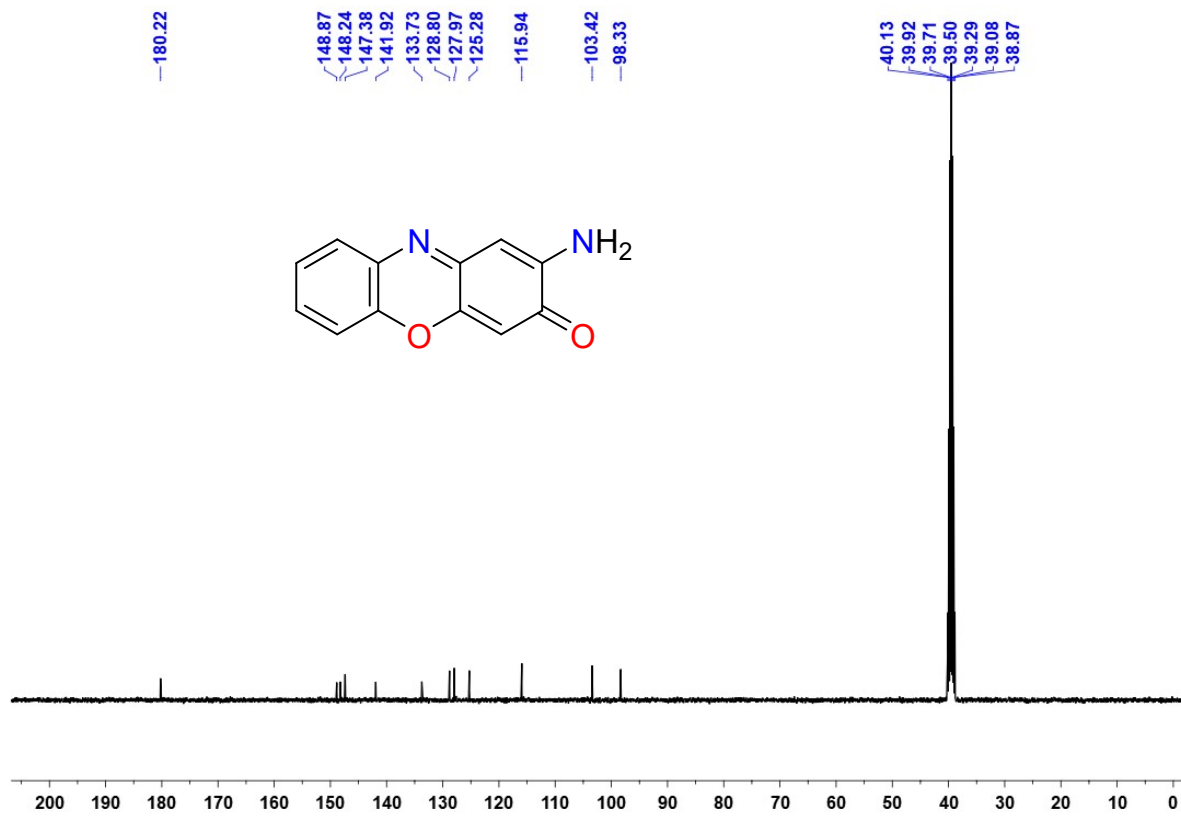


Fig. S22. ¹³C NMR of the catalytic product PHX in DMSO-d₆ at r.t.

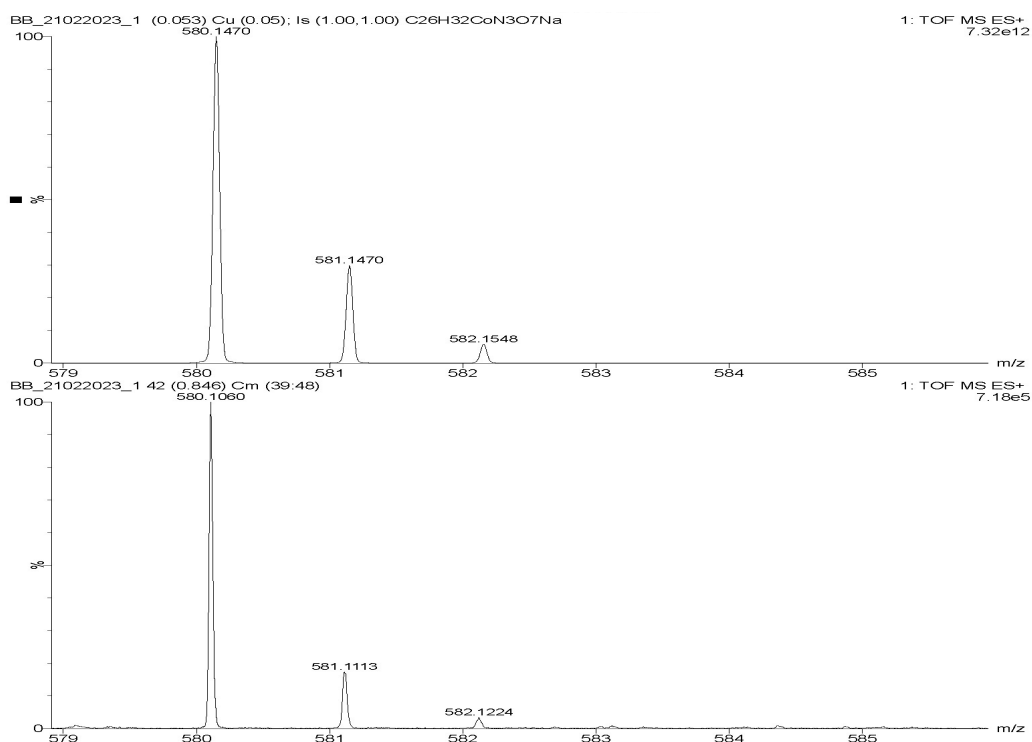


Fig. S23. HR-MS of the species B ($m/z = [M_B + 2H_2O + Na]^+ = 580.1470$); calculated $m/z = 580.1848$ for C₂₆H₃₂CoN₃O₇Na) which is a 1 : 1 complex–substrate aggregate of a monocationic species of composition [Co^{III}(L)(OAP)(H₂O)₂Na]⁺.

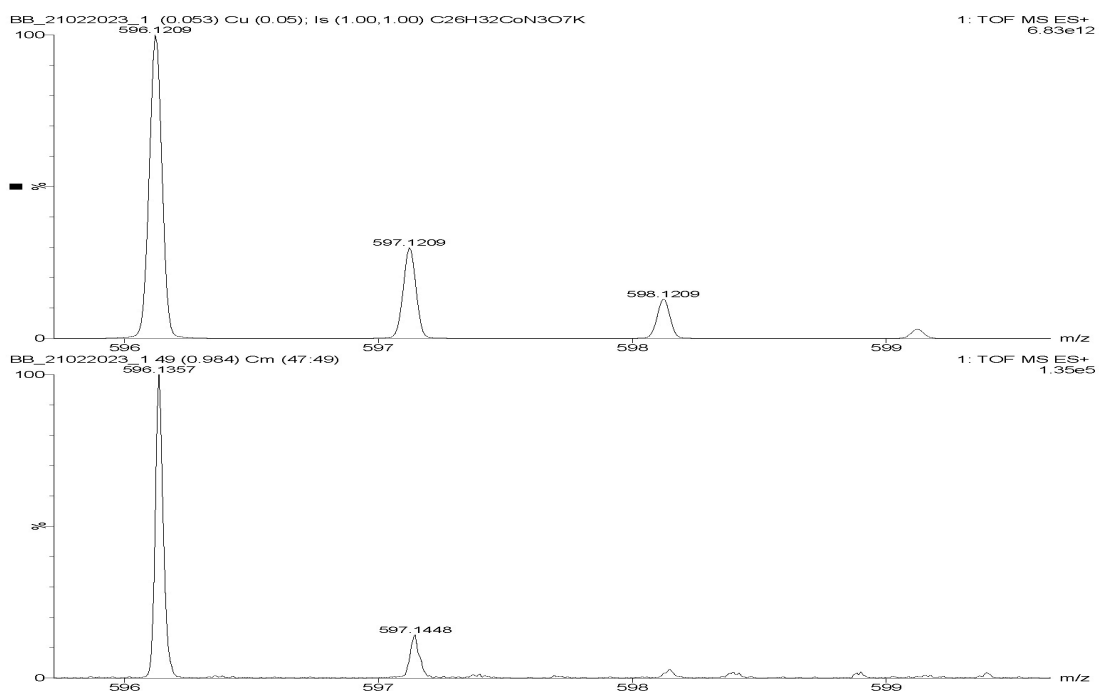


Fig. S24. HR-MS of the intermediate B ($m/z = [M_B + 2H_2O + K]^+ = 596.1357$); calculated $m/z = 596.1209$ for C₂₆H₃₂CoN₃O₇K) for the cationic species [Co^{III}(L)(OAP)(H₂O)₂K]⁺

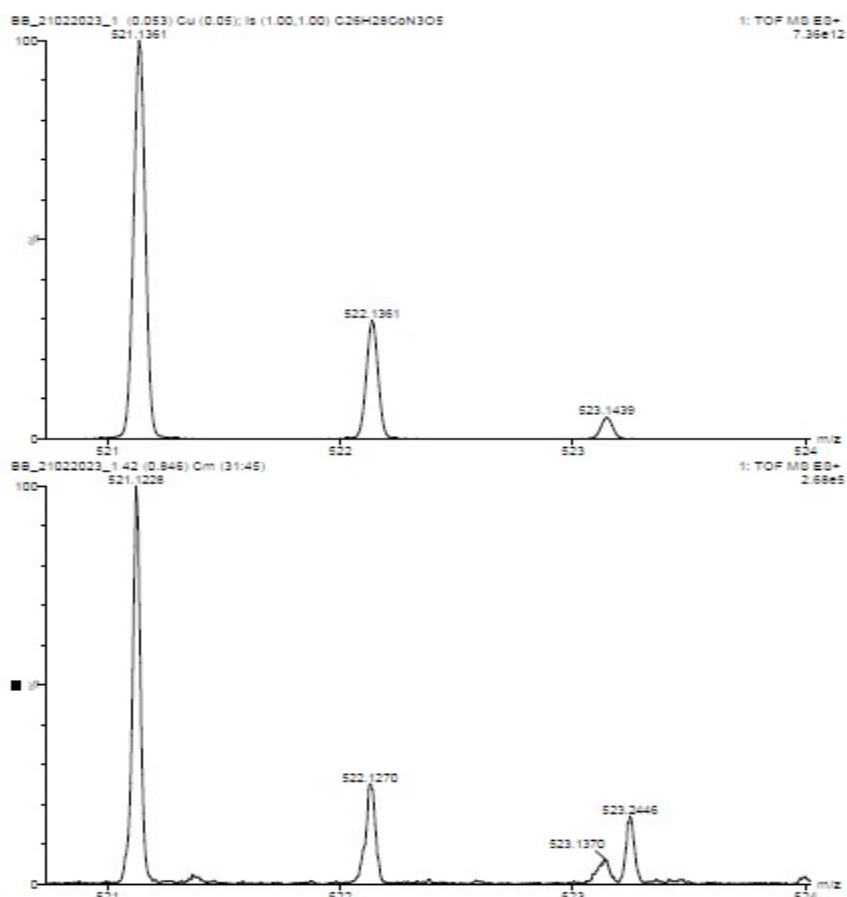


Fig. S25. HR-MS of the species C ($M_C - H_2O$)⁺ calculated $m/z = 520.1194$ for $C_{26}H_{27}CoN_3O_5$.

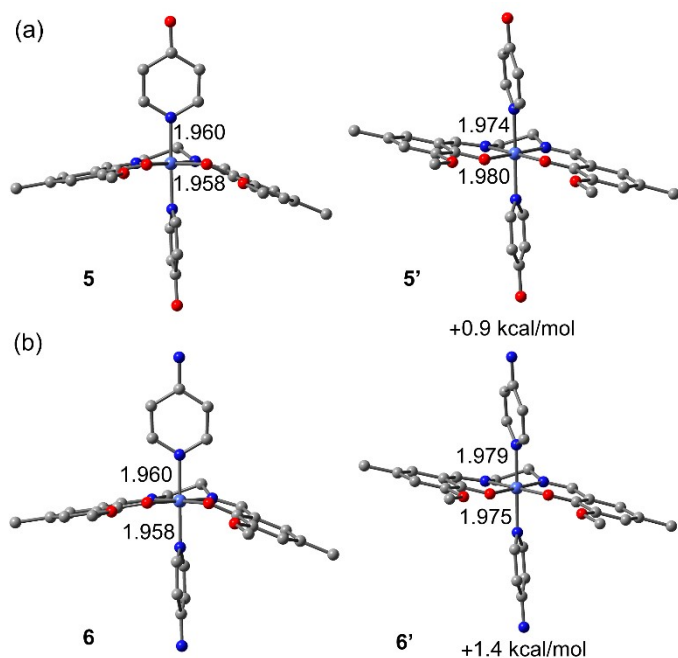


Fig. S26 Optimized structures of compounds **5** and **5'** (a) and **6** and **6'** (b) at the RI-BP86-D4/def2-TZVP level of theory. Distances in Å

Table S1: Selected bond distances (Å) for complexes 1–4

Bonds distances	1	2	3	4	5		6	
					Co1	Co1'		
Co–O1	1.9107(11)	1.899(2)	1.8982(13)	1.8960(2)	1.911(3)	1.901(3)	1.9026(17)	
Co–O2	1.9013(12)	1.906(2)	1.8900(14)	1.8992(2)	1.892(3)	1.901(3)	1.8958(16)	
Co–N1	1.8996(14)	1.884(3)	1.8818(17)	1.886(2)	1.889(4)	1.889(4)	1.900(2)	
Co–N2	1.8883(14)	1.897(3)	1.8928(17)	1.887(2)	1.887(4)	1.887(4)	1.8857(19)	
Co–N3	1.9546(14)	1.935(3)	1.9774(17)	1.962(2)	1.966(3)	1.996(3)	1.9543(19)	
Co–N4	1.9498(14)	1.933(3)	1.9632(17)	1.962(2)	1.976(3)	1.976(3)	1.9699(19)	
			Bond Angles					
	1	2	3	4	5		6	
					Co1	Co1'		
O1–Co–N3	90.98(6)	88.34(10)	88.48(6)	89.55(10)	89.71(13)	89.66(12)	87.47(16)	
O1–Co–N4	89.03(6)	89.19(10)	88.80(6)	89.34(9)	88.25(13)	89.66(12)	86.95(16)	
O2–Co–O1	86.01(5)	86.63(9)	87.21(6)	88.51(9)	88.15(11)	89.35(12)	88.46(14)	
O2–Co–N3	88.89(6)	89.57(10)	89.49(7)	89.34(10)	88.33(12)	88.95(13)	88.29(16)	
O2–Co–N4	90.78(6)	87.31(10)	88.40(7)	88.49(10)	88.82(12)	88.60(13)	88.26(16)	
N1–Co–O1	94.03(6)	93.13(11)	93.47(6)	93.94(10)	92.97(14)	92.09(13)	94.23(16)	
N1–Co–O2	177.60(6)	179.44(11)	179.15(7)	177.52(10)	178.79(14)	178.43(13)	177.28(17)	
N1–Co–N3	88.71(6)	90.93(11)	90.03(7)	91.09(11)	91.20(14)	90.44(14)	91.43(18)	
N1–Co–N4	91.63(6)	92.18(11)	92.11(7)	91.12(11)	91.68(13)	92.05(14)	92.28(18)	
N2–Co–O1	177.25(5)	177.70(11)	178.08(7)	178.11(10)	177.23(14)	176.39(14)	178.22(17)	
N2–Co–O2	94.69(6)	95.58(11)	94.69(7)	93.34(10)	94.33(13)	94.06(15)	93.31(17)	
N2–Co–N1	85.39(6)	84.66(12)	84.62(7)	84.21(11)	84.56(16)	84.50(16)	84.00(19)	
N2–Co–N3	91.70(6)	92.34(11)	90.95(7)	90.07(10)	91.59(13)	91.57(14)	92.75(19)	
N2–Co–N4	88.30(6)	90.25(11)	91.83(7)	91.11(10)	90.58(13)	89.93(14)	92.93(19)	
N3–Co–N4	179.66(6)	176.13(11)	176.64(7)	177.59(11)	176.54(13)	177.21(14)	173.52(17)	

Table S2: Hydrogen Bonds for complex-1.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N5	H5	O5 ¹	0.78(3)	2.21(3)	2.856(2)	141(3)
O6	H6D	O5	0.91(5)	1.89(5)	2.793(3)	174(4)
O5	H5A	O3	0.78(3)	2.18(3)	2.851(2)	144(3)
O5	H5B	O4	0.80(4)	2.13(4)	2.847(2)	150(3)

¹1-X,1-Y,2-Z

Table S3: Hydrogen Bonds for complex-2.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O6	H6D	O3	0.87	2.04	2.880(5)	161.1
O5	H5A	O2	0.87	2.10	2.816(4)	139.3
O5	H5B	O3	0.87	2.07	2.794(6)	139.7
O7	H7A	O9	0.87	1.69	2.289(11)	124.0
N5	H5	O6 ¹	0.916(10)	1.916(14)	2.818(5)	168(4)

¹1+X,+Y,+Z**Table S4:** Hydrogen Bonds for complex-3.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O5	H5A	O9 ¹	0.898(7)	1.945(3)	2.834(7)	170.4(5)

¹2-X,1-Y,-Z**Table S5:** Hydrogen Bonds for complex-4.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O5	H5A	O2	0.85	2.37	3.072(4)	140.9
O5	H5A	O4	0.85	2.12	2.873(4)	147.8
O6	H6D	O5	0.833(11)	2.330(5)	3.132(12)	161.7(6)
O6	H6E	O6 ⁵	0.918(9)	2.144(9)	2.919(10)	141.5(5)
O5	H5B	O1	0.960(4)	2.254(2)	3.071(5)	142.5(2)
O5	H5B	O3	0.960(4)	2.128(3)	2.870(5)	133.1(3)

¹1/3+Y,2/3-X+Y,2/3-Z; ²1/3-Y+X,-1/3+X,2/3-Z; ³4/3+Y-X,5/3-X,-1/3+Z; ⁴2/3+Y,4/3-X+Y,4/3-Z; ⁵1/3+Y,2/3-X+Y,5/3-Z**Table S6:** Hydrogen Bonds for complex-5.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O7	H7A	O2	0.85	2.08	2.805(5)	143.4
O7	H7B	O1	0.85	2.10	2.825(4)	143.0
O13	H13	O14	0.82	1.80	2.594(5)	161.0
O6	H6	O7 ¹	0.82	1.78	2.590(5)	171.8
O14	H14A	O8 ⁴	0.85	2.24	2.795(4)	123.3
O14	H14B	O9 ⁴	0.85	2.00	2.810(4)	157.7

¹1-X,1-Y,2-Z; ²1-X,-Y,2-Z; ³-X,-Y,2-Z; ⁴-X,1-Y,2-Z**Table S7:** Hydrogen Bonds for complex-6.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N5	H5A	O2 ¹	0.88	2.21	2.928(3)	138.6
N5	H5A	O4 ¹	0.88	2.24	3.023(3)	147.8
N5	H5B	O5 ²	0.88	2.15	2.996(16)	160.7
N5	H5B	O5 ¹	0.88	2.28	3.098(17)	154.9
N6	H6B	O9 ³	0.88	2.11	2.939(3)	157.2
O6	H6F	O10 ⁴	0.87	2.02	2.744(12)	139.9
O6	H6G	O9 ⁵	0.87	2.01	2.865(11)	168.2

¹2-X,1-Y,1-Z; ²1+X,+Y,+Z; ³-1+X,3/2-Y,-1/2+Z; ⁴+X,3/2-Y,-1/2+Z; ⁵2-X,-1/2+Y,1/2-Z

Cartesian coordinates

Geometries of 1-6 and 1'-6'

1

Co	0.47865350	-0.81867950	8.11040930
O	-0.33683520	-2.16359600	9.18010830
O	-1.92055210	-3.85613500	10.33666150
O	-1.22051600	0.04970030	8.17826460
O	-3.51523350	1.01011260	8.91032070
N	2.17006310	-1.66420870	8.04166460
N	1.27620950	0.52005950	7.03653360
N	0.88659890	0.15489740	9.74358400
N	1.59185690	1.59086570	11.24026230
H	2.13029300	2.33481810	11.67052610
N	-0.15998930	-1.83662520	6.58040380
N	-1.65382180	-2.84268100	5.33923880
H	-2.55710820	-3.12985920	4.97819390
C	0.17354430	-3.34331260	9.40102650
C	-0.66910030	-4.31196190	10.04852680
C	-2.80745360	-4.75875730	10.99722080
H	-3.00127670	-5.65311900	10.38275660
H	-3.74120210	-4.20559970	11.14206810
H	-2.40764520	-5.06972290	11.97586680
C	-0.19630020	-5.58227400	10.33327610
H	-0.85330870	-6.30226660	10.82131500
C	1.12613270	-5.98709910	10.01075200
C	1.58539290	-7.38019010	10.34948720
H	2.62484910	-7.54312090	10.03749500
H	0.96168950	-8.14004330	9.85452770
H	1.52508620	-7.56918050	11.43198830
C	1.94992130	-5.07142450	9.39585320
H	2.97486380	-5.34593730	9.13698980
C	1.50276800	-3.75536690	9.08078570
C	2.42752400	-2.86974390	8.46425830
H	3.45154550	-3.24479670	8.32709120
C	3.21791880	-0.82349980	7.46252430
H	4.00843240	-1.43373620	6.99986530
H	3.68554310	-0.22277160	8.26057190
C	2.54296380	0.09414030	6.44487620
H	3.17598300	0.95779850	6.18904890
H	2.33667570	-0.45980930	5.51470330
C	0.78643130	1.70758010	6.82206070
H	1.38807720	2.40261980	6.21956790
C	-0.46229780	2.19090510	7.30395390
C	-1.39667800	1.32204240	7.94403210
C	-2.65561550	1.89522850	8.33370380
C	-4.78529450	1.51084770	9.32812570
H	-4.67408300	2.29937190	10.09001030
H	-5.31399940	0.65580280	9.76175180
H	-5.36074980	1.90695660	8.47549360
C	-2.91867700	3.23798320	8.11547720
H	-3.87569910	3.65499710	8.42942020
C	-1.98020850	4.10029970	7.49073410
C	-2.32299090	5.55069540	7.27799970
H	-2.53100920	6.05836700	8.23230580
H	-3.22106480	5.66202580	6.65180800
H	-1.50144350	6.08531070	6.78458860
C	-0.77683730	3.56344050	7.08932020
H	-0.03594610	4.19420500	6.59308390
C	0.50184070	-2.61725260	5.65335860
H	1.57941030	-2.69802280	5.62568450
C	-0.42409070	-3.24954350	4.86474320
H	-0.31560800	-3.93616760	4.03498110
C	-1.46488810	-1.99515690	6.37630510
H	-2.24263870	-1.52662850	6.96701590
C	1.76110690	1.12882980	9.97892130
H	2.48350260	1.52970250	9.28114110
C	0.56089980	0.88718930	11.82938970
H	0.23389640	1.07843300	12.84342790
C	0.12552520	-0.00452700	10.88516780
H	-0.67003670	-0.73750910	10.91937930

1'

Co	9.30823530	13.47771200	3.66427680
O	9.65558230	12.49902580	5.26184560
O	9.18694370	11.11515690	7.40978520
O	8.02230470	14.43766830	4.68367280
O	6.35065010	15.41241480	6.39779220
N	10.59845450	12.52766270	2.66288670
N	8.98324710	14.42575560	2.05100900
C	10.09307660	11.27025840	5.24860820
C	9.87379850	10.47488350	6.42676910
C	8.94725250	10.39416990	8.61786720
H	8.33849190	9.49348370	8.43499620
H	8.39804910	11.08144530	9.26933650
H	9.89227010	10.10263820	9.10405780
C	10.33870520	9.17119920	6.49438060
H	10.15215640	8.58140170	7.39223210
C	11.05411120	8.56550040	5.42828450
C	11.53610320	7.14610610	5.56439860
H	12.08885300	6.82639450	4.67197930
H	10.69595130	6.44972090	5.70888640
H	12.20152080	7.03066510	6.43316110
C	11.28352840	9.31330610	4.29461560
H	11.83485510	8.88152580	3.45625180
C	10.80735230	10.65017970	4.17609000
C	11.09791370	11.36749430	2.98210040
H	11.79937330	10.90346800	2.27411680
C	11.00951430	13.25521960	1.46642220
H	11.47593650	12.58392230	0.72906860
H	11.74855810	14.02081690	1.75194970
C	9.75812430	13.93001750	0.90934010
H	10.01263960	14.74604640	0.21686180
H	9.15265020	13.19605830	0.35044610
C	8.12024760	15.38994490	1.89727880
H	8.04250640	15.84567040	0.90008490
C	7.26268950	15.91653420	2.90304240
C	7.25830440	15.39069260	4.23241780
C	6.32334640	15.97384340	5.15910330
C	5.44504160	15.93073390	7.37187510
H	5.63956660	16.99681870	7.57306690
H	5.62363550	15.34894650	8.28176320
H	4.39758090	15.80488960	7.05251250
C	5.48991800	17.00679390	4.76562460
H	4.78813060	17.43190770	5.48362790
C	5.50973630	17.53593200	3.44717690
C	4.58089910	18.66240790	3.08038590
H	4.70868060	18.95825580	2.03128250
H	4.76079280	19.55032640	3.70558370
H	3.52773520	18.37661110	3.22388990
C	6.38786540	16.98449970	2.54264020
H	6.42151890	17.35813560	1.51667070
C	12.45040780	15.62276470	5.22163100
C	11.83742620	14.45415820	4.85064550
C	10.52191720	16.08329730	4.21915090
N	11.60535120	16.63530840	4.81502930
H	11.75452460	17.62894130	4.95335670
H	13.38427200	15.81561300	5.73381710
H	12.15200980	13.43154640	5.01030270
H	9.68209420	16.64549010	3.82786920
N	10.64459070	14.75963020	4.22739430
C	6.96792180	11.86119260	4.25608670
C	6.20346440	10.82657180	3.78539760
C	7.76273760	11.32875720	2.28819310
N	7.92925000	12.16190700	3.31043380
H	6.92278470	12.40662130	5.18991810
H	5.35998610	10.30158350	4.21501410
H	8.36772240	11.27825200	1.39296070
N	6.71821600	10.50648250	2.54496170
H	6.37957710	9.77636540	1.92791150

2

Co	0.5575904	-0.7568393	8.3079765
O	-0.2550553	-2.0813162	9.3980570
O	-1.9581641	-3.8070435	10.3280251
O	-1.1417446	0.1287416	8.3773073
O	-3.5397410	1.0145628	8.7930387
N	2.2253433	-1.6336597	8.2259792
N	1.3663478	0.5669210	7.2089181
N	1.0942497	0.1554805	9.9218642

N	-0.1298291	-1.7587172	6.8037577
C	0.1728978	-3.3132803	9.4709941
C	-0.7306484	-4.2952668	10.0050674
C	-2.8972677	-4.7216587	10.8950724
H	-3.1348737	-5.5390972	10.1949209
H	-3.7999087	-4.1347051	11.0933143
H	-2.5200674	-5.1466909	11.8389293
C	-0.3295767	-5.6137821	10.1520764
H	-1.0312795	-6.3442904	10.5545687
C	0.9699499	-6.0572663	9.7907679
C	1.3445937	-7.5032984	9.9760254
H	2.3754105	-7.6922650	9.6509527
H	0.6817492	-8.1660098	9.3992041
H	1.2634648	-7.8049204	11.0311336
C	1.8493802	-5.1314306	9.2757323
H	2.8562431	-5.4363414	8.9829335
C	1.4762717	-3.7675458	9.0999953
C	2.4431589	-2.8722956	8.5680597
H	3.4612642	-3.2614033	8.4293420
C	3.2947053	-0.7516986	7.7642052
H	4.1425379	-1.3282543	7.3649910
H	3.6538353	-0.1478880	8.6134826
C	2.6813420	0.1613198	6.7070131
H	3.3166348	1.0356006	6.5019219
H	2.5441864	-0.3917818	5.7635410
C	0.8567188	1.7218456	6.9047374
H	1.4672606	2.4055672	6.2991464
C	-0.4380096	2.1933252	7.2887655
C	-1.3738007	1.3499937	7.9612619
C	-2.6834536	1.8883022	8.2013884
C	-4.8610042	1.4811572	9.0808728
H	-4.8377540	2.3368637	9.7738855
H	-5.3747456	0.6395146	9.5556956
H	-5.3930068	1.7682390	8.1596002
C	-2.9895823	3.1894243	7.8328441
H	-3.9857639	3.5827615	8.0354399
C	-2.0480090	4.0347902	7.1909647
C	-2.4368157	5.4397690	6.8164107
H	-2.7067216	6.0304201	7.7049685
H	-3.3101943	5.4473929	6.1475270
H	-1.6158498	5.9573334	6.3047618
C	-0.7971600	3.5234908	6.9210529
H	-0.0548083	4.1370129	6.4065763
C	0.3775086	-2.5408632	5.8376632
H	1.4482239	-2.6145328	5.6931905
C	-0.6626985	-3.1882884	5.1543956
H	-0.5768323	-3.8768846	4.3229275
C	1.7545111	0.6650004	12.0102644
H	2.1462412	0.5700226	13.0154087
C	1.6225025	-0.3477867	11.0467617
H	1.8620891	-1.4027495	11.1106504
C	-1.8299874	-2.7578718	5.7743157
H	-2.8722434	-2.9900303	5.5879644
C	1.2662125	1.8136457	11.4049815
H	1.1584676	2.8307509	11.7642901
N	-1.4669360	-1.9069728	6.7550018
N	0.8878359	1.4702746	10.1520117
H	-2.0037590	-1.3725232	7.4471198
H	0.4161364	2.0368180	9.4453831
2'			
Co	9.0644640	13.3130184	3.6116014
O	9.3669284	12.2926352	5.1907598
O	9.1948066	10.9905917	7.4269624
O	7.7400017	14.2351509	4.6208684
O	6.2520198	15.3463061	6.4283884
N	10.3979882	12.4100980	2.6073616
N	8.7560251	14.3135174	2.0287246
C	10.0417244	11.1808395	5.2467410
C	9.9714626	10.4238364	6.4726913
C	9.0696030	10.2989068	8.6715835
H	8.6169391	9.3039301	8.5311135
H	8.4102583	10.9180376	9.2876470
H	10.0470365	10.1916899	9.1686372
C	10.6581223	9.2272065	6.5999547
H	10.5851824	8.6677039	7.5325913
C	11.4620492	8.6935669	5.5562519
C	12.1863158	7.3911766	5.7647918

H	12.7648684	7.1105985	4.8759646
H	11.4839309	6.5730650	5.9843015
H	12.8822227	7.4541485	6.6149094
C	11.5513860	9.4023368	4.3803895
H	12.1651607	9.0282451	3.5584585
C	10.8538610	10.6353137	4.1982693
C	11.0267498	11.3284011	2.9637999
H	11.7535531	10.9066755	2.2556468
C	10.7087832	13.0990317	1.3550106
H	11.1397769	12.4069850	0.6165984
H	11.4441911	13.8937125	1.5614792
C	9.4072056	13.7184240	0.8615035
H	9.5820550	14.4690968	0.0770831
H	8.7518783	12.9313437	0.4531061
C	8.0181734	15.3808188	1.9269551
H	7.9608437	15.8667039	0.9432715
C	7.2707724	15.9789782	2.9838729
C	7.1611187	15.3449173	4.2654597
C	6.3269097	15.9988638	5.2437936
C	5.4284443	15.9195428	7.4463208
H	5.7901991	16.9187665	7.7373533
H	5.5007804	15.2399850	8.3010700
H	4.3791943	15.9896617	7.1172693
C	5.6849521	17.1872805	4.9373915
H	5.0630574	17.6672555	5.6934313
C	5.8020235	17.8125470	3.6661880
C	5.0727564	19.1014847	3.3998900
H	5.2526811	19.4575545	2.3778601
H	5.3916152	19.8927321	4.0952327
H	3.9868999	18.9787603	3.5286677
C	6.5837353	17.2019044	2.7133005
H	6.6893201	17.6475923	1.7219153
C	12.1854475	15.5465600	5.1847369
C	11.5912264	14.3346217	4.7990164
H	13.1475425	15.6853524	5.6620267
H	11.9542988	13.3195885	4.9078511
N	10.3940172	14.5675563	4.2409600
C	6.4373518	12.2891014	2.6703746
C	5.7658351	11.0735479	2.4652905
N	7.6941590	12.0563744	3.0776746
H	6.0785960	13.3055144	2.5597442
H	4.7430075	10.9337606	2.1381270
N	10.2171346	15.9062366	4.2634836
N	7.8338272	10.7143227	3.1337189
C	11.2728301	16.5305745	4.8340194
H	11.2928682	17.6085973	4.9461607
C	6.6888648	10.0870229	2.7797444
H	6.6193489	9.0051844	2.7799120
H	9.3280713	16.3011898	3.9508976
H	8.7020972	10.3137601	3.4946100

3

Co	9.38257490	13.56979930	3.72650620
O	9.69815880	12.56107660	5.30970160
O	9.14729250	11.14686070	7.41891270
O	8.12976710	14.56607810	4.74701490
O	6.38411160	15.47453400	6.42851120
N	10.65513050	12.60279250	2.72024510
N	9.08728100	14.52397710	2.11029380
N	7.93974060	12.30288340	3.34989040
N	10.75779420	14.83259900	4.32017200
C	10.08927970	11.31237930	5.27487340
C	9.82825440	10.50415320	6.43266040
C	8.86266240	10.40840300	8.60770850
H	8.23162650	9.53049660	8.39348950
H	8.32103540	11.09849390	9.26246980
H	9.78909400	10.07925240	9.10505890
C	10.24841960	9.18373830	6.47949380
H	10.03371890	8.58410610	7.36433740
C	10.95054760	8.57393480	5.40812450
C	11.38289100	7.13669470	5.52061290
H	11.92007330	6.81080460	4.62115040
H	10.51942350	6.46840430	5.65892810
H	12.04769550	6.98587380	6.38431630
C	11.21219480	9.33416720	4.28908230
H	11.75005040	8.89822520	3.44444670
C	10.78506610	10.68858530	4.19434800
C	11.11317810	11.42042030	3.01798950

H	11.81140000	10.95099430	2.31090930
C	11.14363620	13.36071830	1.57136380
H	11.60279000	12.69765830	0.82249200
H	11.91525070	14.06609560	1.91877510
C	9.95983550	14.13362650	0.99228650
H	10.30130010	15.01782940	0.43396450
H	9.39681190	13.49898380	0.28793080
C	8.13242010	15.39153150	1.91903510
H	8.04120900	15.83164120	0.91629020
C	7.19516430	15.83769200	2.89131810
C	7.25549560	15.39806910	4.24943760
C	6.27381310	15.93401690	5.15322010
C	5.45914450	15.98396610	7.39022280
H	5.54196470	17.07896390	7.48320670
H	5.73187210	15.51487570	8.34102030
H	4.42195660	15.71690840	7.13025750
C	5.31568520	16.82734790	4.70353690
H	4.57344590	17.21339460	5.40260620
C	5.25840010	17.26063820	3.35235400
C	4.18921950	18.22943540	2.92321150
H	4.27423220	18.46814410	1.85552400
H	4.25273620	19.17242040	3.48675000
H	3.18344730	17.81753440	3.09728050
C	6.19590790	16.76631240	2.47454820
H	6.18258250	17.07797680	1.42784580
C	7.75852010	11.69509840	2.16276150
H	8.46407700	11.94334860	1.37502940
C	6.73505450	10.78117660	1.94692910
H	6.62954520	10.31627000	0.96781130
C	5.86665350	10.47933770	2.99542070
H	5.05507880	9.76510750	2.85598360
C	6.06048670	11.10888370	4.22332450
H	5.41136470	10.90625210	5.07394220
C	7.10399960	12.01545150	4.37113450
H	7.30528970	12.53349130	5.30624590
C	10.54973650	16.16173070	4.24335060
H	9.62159700	16.48744500	3.78077430
C	11.46627350	17.08015330	4.74260570
H	11.25115940	18.14466920	4.66153580
C	12.63572040	16.61652430	5.34342080
H	13.36914520	17.31478090	5.74649270
C	12.84251690	15.24015800	5.42514150
H	13.73460230	14.82569030	5.89237370
C	11.88226610	14.37784320	4.90860710
H	11.99243150	13.29868190	4.97339010

3'

Co	0.66031460	-0.78984270	8.09044030
O	-0.16266130	-2.15647670	9.12306650
O	-1.76661330	-3.86031770	10.23454310
O	-1.02528450	0.08848210	8.17367980
O	-3.32855860	1.02976380	8.89534860
N	2.34785510	-1.64589580	8.00859780
N	1.47717830	0.56953060	7.05534390
N	1.03870370	0.16930610	9.77458690
C	0.33446030	-3.34895250	9.31821510
C	-0.52038030	-4.32240490	9.93753390
C	-2.67010190	-4.77370370	10.85854980
H	-2.86598630	-5.64615990	10.21453800
H	-3.59952290	-4.21529560	11.00998380
H	-2.28343200	-5.11753240	11.83126100
C	-0.06089980	-5.60575340	10.18671150
H	-0.72582970	-6.33274560	10.65309920
C	1.25682430	-6.01523890	9.85229050
C	1.70157800	-7.42223590	10.15032290
H	2.73524900	-7.59005450	9.82233670
H	1.06229300	-8.16103200	9.64376320
H	1.65139970	-7.63742310	11.22831760
C	2.09121640	-5.09205460	9.26251440
H	3.11219780	-5.37136950	8.99376840
C	1.65800900	-3.76290120	8.98579400
C	2.59029420	-2.86832350	8.39394760
H	3.60836680	-3.25281840	8.24114780
C	3.41962880	-0.81975740	7.44241770
H	4.16095530	-1.44304780	6.91966320
H	3.95027990	-0.30099190	8.25649690
C	2.77741140	0.19376740	6.49332020
H	3.41774360	1.07876770	6.35803770

H	2.62736680	-0.25312120	5.49790600
C	0.98560930	1.76000360	6.85274050
H	1.60253850	2.47128960	6.28655810
C	-0.27737340	2.23184380	7.30426440
C	-1.21316210	1.35976590	7.93219580
C	-2.47791590	1.92014030	8.31369430
C	-4.61423940	1.51372940	9.28629270
H	-4.52913050	2.31204500	10.04120560
H	-5.13628260	0.65430640	9.71929930
H	-5.18049980	1.88994310	8.41901360
C	-2.75109630	3.25965180	8.08610500
H	-3.71377330	3.67005710	8.39108560
C	-1.81414390	4.12737030	7.46674330
C	-2.16628960	5.57423140	7.24575590
H	-2.38187030	6.08457500	6.19687130
H	-3.06224930	5.67600470	6.61520430
H	-1.34623160	6.11211710	6.75361590
C	-0.60025310	3.60118980	7.08277020
H	0.14240730	4.23787390	6.59741380
C	2.07428870	1.00503080	9.97783090
H	2.77486440	1.12668520	9.15748570
C	0.75416460	-2.36669930	5.57579720
C	0.22965970	-3.16249910	4.56459960
C	-1.14054090	-3.41859730	4.54799360
C	-1.92954670	-2.86544710	5.55398190
C	-1.33801650	-2.07581430	6.53426570
N	-0.01253460	-1.82063600	6.53860570
H	-1.58138120	-4.04366340	3.77129790
H	1.82108200	-2.17647520	5.63215150
H	0.89688460	-3.57829580	3.81097190
H	-3.00333740	-3.04178430	5.59542800
H	-1.90801730	-1.62650890	7.34358780
C	2.24342120	1.70872830	11.16380910
C	1.30098540	1.55719440	12.17958760
C	0.22217440	0.70343600	11.96103820
C	0.11773400	0.02589600	10.75107550
H	1.40373910	2.09916260	13.11967680
H	3.10187420	2.36947270	11.27591580
H	-0.54766250	0.55584400	12.71707110
H	-0.70562400	-0.64839460	10.52945160
4			
Co	9.3823256	13.5706133	3.7267776
O	9.6957357	12.5603893	5.3100738
O	9.1473309	11.1468739	7.4201937
O	8.1290232	14.5666752	4.7469313
O	6.3835316	15.4739363	6.4280844
N	10.6545886	12.6038290	2.7214271
N	9.0872939	14.5248249	2.1114274
N	7.9391486	12.3048611	3.3478606
N	10.7570086	14.8323200	4.3214194
C	10.0878166	11.3129530	5.2752027
C	9.8276858	10.5039662	6.4331809
C	8.8633730	10.4081855	8.6083223
H	8.2311942	9.5308885	8.3944063
H	8.3232414	11.0982952	9.2644186
H	9.7899697	10.0773596	9.1045035
C	10.2475033	9.1836599	6.4800446
H	10.0324482	8.5838012	7.3646932
C	10.9504291	8.5744721	5.4086999
C	11.3836559	7.1372728	5.5201609
H	11.9199261	6.8127295	4.6195765
H	10.5206220	6.4683005	5.6583835
H	12.0497448	6.9852461	6.3828088
C	11.2119839	9.3352461	4.2900158
H	11.7509705	8.8997783	3.4457930
C	10.7839843	10.6892334	4.1947862
C	11.1123284	11.4214678	3.0185170
H	11.8104940	10.9522145	2.3112350
C	11.1429010	13.3615359	1.5726353
H	11.6034580	12.6988679	0.8241502
H	11.9127542	14.0685744	1.9205976
C	9.9582021	14.1324648	0.9931871
H	10.2985753	15.0153864	0.4320710
H	9.3939528	13.4955190	0.2919278
C	8.1323948	15.3915369	1.9191251
H	8.0402213	15.8300613	0.9156809
C	7.1947102	15.8376711	2.8911684

C	7.2553887	15.3977795	4.2492158
C	6.2731723	15.9338951	5.1526430
C	5.4578625	15.9825591	7.3885851
H	5.5413555	17.0774376	7.4832073
H	5.7281565	15.5118392	8.3393089
H	4.4206852	15.7172653	7.1264444
C	5.3155134	16.8277485	4.7036727
H	4.5737713	17.2144504	5.4028701
C	5.2584016	17.2612240	3.3524723
C	4.1900902	18.2313325	2.9239760
H	4.2751117	18.4709422	1.8564378
H	4.2545760	19.1738706	3.4882370
H	3.1838436	17.8203591	3.0976074
C	6.1954268	16.7661434	2.4746411
H	6.1822911	17.0779192	1.4279217
C	7.7514968	11.6897252	2.1644262
H	8.4528711	11.9331464	1.3709043
C	6.7310677	10.7758690	1.9563779
H	6.6292077	10.3083544	0.9764884
C	5.8479362	10.4581429	2.9990766
C	6.0628095	11.1060883	4.2201957
H	5.4187360	10.9054844	5.0765621
C	7.1025057	12.0146111	4.3659640
H	7.2995063	12.5319733	5.3025151
C	10.5559609	16.1623177	4.2454104
H	9.6270233	16.4934292	3.7876947
C	11.4773258	17.0773186	4.7352115
H	11.2608606	18.1422811	4.6465810
C	12.6619882	16.6350580	5.3383105
C	12.8464200	15.2478912	5.4139101
H	13.7409623	14.8291431	5.8756392
C	11.8848707	14.3845043	4.9087817
H	11.9986861	13.3058913	4.9803775
C	13.6660127	17.5952864	5.9031703
H	13.4555807	17.7790616	6.9687991
H	14.6859822	17.1955484	5.8375226
H	13.6299951	18.5642632	5.3900120
C	4.7297662	9.4777372	2.8032183
H	3.9887547	9.8740011	2.0923833
H	5.1037994	8.5338813	2.3820882
H	4.2135029	9.2589748	3.7454641
4'			
Co	0.6603979	-0.7899166	8.0906590
O	-0.1616485	-2.1553414	9.1265897
O	-1.7670618	-3.8608345	10.2344622
O	-1.0267680	0.0872439	8.1720565
O	-3.3300769	1.0301676	8.8953777
N	2.3476766	-1.6448294	8.0103687
N	1.4762021	0.5683779	7.0545499
N	1.0395126	0.1726431	9.7712235
C	0.3346690	-3.3474152	9.3195925
C	-0.5203150	-4.3222652	9.9374275
C	-2.6696484	-4.7743428	10.8584567
H	-2.8662045	-5.6468330	10.2144119
H	-3.5991391	-4.2162269	11.0111074
H	-2.2824042	-5.1187837	11.8308461
C	-0.0615617	-5.6058688	10.1852235
H	-0.7268963	-6.3327753	10.6510786
C	1.2562727	-6.0151920	9.8508165
C	1.7003292	-7.4223781	10.1493056
H	2.7341223	-7.5911181	9.8221254
H	1.0610431	-8.1609803	9.6423635
H	1.6491596	-7.6375048	11.2273512
C	2.0907988	-5.0914118	9.2622824
H	3.1124728	-5.3698015	8.9950455
C	1.6580197	-3.7620451	8.9863500
C	2.5902902	-2.8672994	8.3942867
H	3.6081128	-3.2520054	8.2401134
C	3.4188992	-0.8186560	7.4440811
H	4.1613890	-1.4419922	6.9230034
H	3.9474981	-0.2974778	8.2579505
C	2.7763333	0.1926926	6.4930865
H	3.4165640	1.0776544	6.3565914
H	2.6258694	-0.2565308	5.4987750
C	0.9854254	1.7589440	6.8525290
H	1.6033057	2.4708145	6.2880037
C	-0.2781060	2.2304250	7.3034784

C	-1.2139984	1.3577876	7.9311310
C	-2.4785424	1.9196247	8.3130911
C	-4.6144611	1.5158614	9.2866934
H	-4.5286884	2.3142812	10.0416411
H	-5.1374593	0.6572692	9.7202620
H	-5.1806753	1.8933538	8.4197725
C	-2.7516558	3.2589936	8.0858713
H	-3.7145091	3.6693836	8.3904628
C	-1.8144376	4.1264416	7.4665170
C	-2.1670830	5.5731218	7.2451683
H	-2.3829208	6.0834727	8.1962684
H	-3.0630486	5.6745479	6.6143906
H	-1.3470549	6.1113982	6.7533527
C	-0.6008569	3.5998190	7.0824097
H	0.1418230	4.2362560	6.5966073
C	2.0739668	1.0077865	9.9823091
H	2.7766847	1.1364498	9.1643227
C	0.7515846	-2.3698368	5.5738829
C	0.2232247	-3.1547955	4.5596194
C	-1.1517601	-3.4211343	4.5200971
C	-1.9237254	-2.8604304	5.5444070
C	-1.3342043	-2.0806975	6.5298268
N	-0.0091373	-1.8232282	6.5410844
H	1.8203908	-2.1865491	5.6271052
H	0.8933315	-3.5630576	3.8026098
H	-3.0001361	-3.0289918	5.5854530
H	-1.9092016	-1.6374747	7.3390773
C	2.2448362	1.7010279	11.1712861
C	1.3132547	1.5591482	12.2080369
C	0.2352920	0.7002622	11.9634894
C	0.1233793	0.0315704	10.7524352
H	3.1085848	2.3572386	11.2821317
H	-0.5339221	0.5433788	12.7200753
H	-0.7047781	-0.6381319	10.5346098
C	1.4484216	2.3124739	13.4979317
H	2.5015402	2.4788002	13.7584610
H	0.9723662	3.3019753	13.4111793
H	0.9579550	1.7840926	14.3249948
C	-1.7576180	-4.2889418	3.4573092
H	-1.2059862	-4.2129027	2.5116359
H	-1.7296742	-5.3452463	3.7686191
H	-2.8081767	-4.0284740	3.2770993
5			
Co	9.3796958	13.5831829	3.7008415
O	9.7065266	12.5829214	5.2877343
O	9.1656345	11.1798525	7.4060336
O	8.1391976	14.5861238	4.7281541
O	6.3843573	15.4648053	6.4126346
N	10.6410191	12.6095764	2.6892465
N	9.0683431	14.5283901	2.0836420
N	7.9290913	12.3172867	3.3471126
N	10.7658123	14.8458343	4.2712898
C	10.0967908	11.3349017	5.2566839
C	9.8418102	10.5316676	6.4198468
C	8.8785093	10.4461445	8.5967445
H	8.2420262	9.5714221	8.3856916
H	8.3417766	11.1410797	9.2505366
H	9.8034179	10.1127109	9.0942513
C	10.2622737	9.2116664	6.4712665
H	10.0505702	8.6157588	7.3593526
C	10.9612222	8.5979712	5.3998114
C	11.3974746	7.1620844	5.5162641
H	11.9301988	6.8344212	4.6146804
H	10.5361960	6.4924401	5.6614741
H	12.0677890	7.0151831	6.3765527
C	11.2161823	9.3528075	4.2756143
H	11.7508852	8.9132719	3.4307323
C	10.7863468	10.7057909	4.1750784
C	11.1040631	11.4304081	2.9909817
H	11.7974168	10.9573469	2.2813397
C	11.1164890	13.3601997	1.5304247
H	11.5716615	12.6934974	0.7821803
H	11.8870301	14.0725682	1.8654784
C	9.9234619	14.1235376	0.9581417
H	10.2546999	14.9991998	0.3804310
H	9.3504336	13.4768296	0.2728423
C	8.1172253	15.4014542	1.8982045

H	8.0181623	15.8376374	0.8943622
C	7.1909261	15.8543572	2.8777077
C	7.2587385	15.4125424	4.2348376
C	6.2744047	15.9379078	5.1420994
C	5.4450934	15.9467769	7.3738525
H	5.5189873	17.0399410	7.4921469
H	5.7095817	15.4585640	8.3173661
H	4.4129891	15.6785975	7.0953592
C	5.3150014	16.8334032	4.7002575
H	4.5730181	17.2137054	5.4026960
C	5.2560923	17.2758225	3.3518930
C	4.1874710	18.2490257	2.9312590
H	4.2661858	18.4892265	1.8633899
H	4.2577927	19.1910831	3.4956835
H	3.1815301	17.8402046	3.1111250
C	6.1902651	16.7849182	2.4686678
H	6.1730707	17.1011372	1.4233353
C	7.7250418	11.6961459	2.1718917
H	8.4201187	11.9269873	1.3691195
C	6.6974726	10.7899786	1.9685951
H	6.5788560	10.3173942	0.9927661
C	5.8316600	10.5014390	3.0334320
C	6.0486826	11.1439321	4.2594953
H	5.3982542	10.9408111	5.1083434
C	7.0965085	12.0372787	4.3778776
H	7.3071381	12.5593521	5.3086844
C	10.5753349	16.1796630	4.1794734
H	9.6518904	16.5109045	3.7111189
C	11.4874423	17.1003793	4.6619709
H	11.2979863	18.1687896	4.5745313
C	12.6572961	16.6364062	5.2798890
C	12.8516077	15.2515858	5.3814190
H	13.7381296	14.8351873	5.8614625
C	11.8857739	14.3983203	4.8730847
H	11.9936281	13.3201442	4.9584867
O	13.5299078	17.5533911	5.7461734
H	14.2925973	17.1138558	6.1659724
O	4.7994380	9.6363071	2.9477063
H	4.7483318	9.2559204	2.0513514
5'			
Co	0.6828569	-0.7855652	8.0907820
O	-0.1486764	-2.1599114	9.1085629
O	-1.7535659	-3.8687822	10.2175546
O	-1.0000486	0.0984164	8.1941806
O	-3.3056695	1.0441743	8.9117507
N	2.3654650	-1.6466465	7.9997207
N	1.5020710	0.5774217	7.0650617
N	1.0775915	0.1517963	9.7827323
C	0.3471663	-3.3529926	9.2987275
C	-0.5068165	-4.3292485	9.9155925
C	-2.6539253	-4.7861885	10.8389196
H	-2.8514965	-5.6555008	10.1908392
H	-3.5836202	-4.2298727	10.9973031
H	-2.2639529	-5.1361481	11.8082645
C	-0.0485718	-5.6138185	10.1591025
H	-0.7138727	-6.3413669	10.6239776
C	1.2681842	-6.0233436	9.8215195
C	1.7108501	-7.4325069	10.1121689
H	2.7478435	-7.5974085	9.7933662
H	1.0771972	-8.1668537	9.5921044
H	1.6494981	-7.6573535	11.1876273
C	2.1024719	-5.0979045	9.2352609
H	3.1237003	-5.3760444	8.9662179
C	1.6702743	-3.7675055	8.9641380
C	2.6047319	-2.8716876	8.3767551
H	3.6217582	-3.2577776	8.2212366
C	3.4400948	-0.8182541	7.4429965
H	4.1825815	-1.4386742	6.9185781
H	3.9676313	-0.3052377	8.2627379
C	2.8009692	0.2018937	6.4997062
H	3.4435939	1.0858998	6.3687277
H	2.6481072	-0.2398128	5.5023193
C	1.0087345	1.7660943	6.8594937
H	1.6254330	2.4775317	6.2932122
C	-0.2567629	2.2363344	7.3064541
C	-1.1901180	1.3666122	7.9421235
C	-2.4558735	1.9293304	8.3186901

C	-4.5859520	1.5357962	9.3086626
H	-4.4923236	2.3427414	10.0536135
H	-5.1065482	0.6830028	9.7564375
H	-5.1596974	1.9048513	8.4429937
C	-2.7338269	3.2649240	8.0761509
H	-3.6986352	3.6747487	8.3751233
C	-1.7997546	4.1289998	7.4476613
C	-2.1576730	5.5718228	7.2104624
H	-2.3737886	6.0915926	8.1563389
H	-3.0548421	5.6632823	6.5798732
H	-1.3402971	6.1076118	6.7116361
C	-0.5838308	3.6023697	7.0712219
H	0.1574000	4.2361603	6.5798287
C	2.1081426	0.9957993	9.9931507
H	2.7993825	1.1403180	9.1684012
C	0.7674029	-2.3421780	5.5567622
C	0.2491283	-3.1103230	4.5306127
C	-1.1326979	-3.3422350	4.4941983
C	-1.9228661	-2.7888110	5.5100571
C	-1.3216808	-2.0295260	6.5004678
N	0.0070762	-1.7897279	6.5243495
H	1.8381510	-2.1761653	5.6207791
H	0.9003114	-3.5367709	3.7697958
H	-3.0016315	-2.9482146	5.5410467
H	-1.8965429	-1.5864338	7.3102347
C	2.2966745	1.6810201	11.1790053
C	1.3677416	1.5049532	12.2135542
C	0.2850658	0.6441366	11.9911805
C	0.1735745	-0.0063591	10.7733616
H	3.1441963	2.3519677	11.3066094
H	-0.4748769	0.4779626	12.7561662
H	-0.6523569	-0.6799240	10.5576850
O	1.5686849	2.1825006	13.3628738
H	0.8589048	1.9818653	14.0007943
O	-1.6191401	-4.0950391	3.4856778
H	-2.5867345	-4.1848540	3.5679840
6			
Co	9.3856309	13.5564490	3.7043969
O	9.6901703	12.5472531	5.2914843
O	9.1561922	11.1439978	7.4125152
O	8.1297506	14.5555469	4.7220876
O	6.3720545	15.4578298	6.3969658
N	10.6549717	12.5855471	2.7036962
N	9.0962111	14.5128355	2.0916523
N	7.9416749	12.2915320	3.3182804
N	10.7708636	14.8124206	4.2913356
C	10.0885532	11.3035785	5.2624562
C	9.8359744	10.4983320	6.4258061
C	8.8687238	10.4062044	8.5990465
H	8.2390941	9.5272564	8.3832096
H	8.3245029	11.0954798	9.2528705
H	9.7931665	10.0762677	9.1002885
C	10.2602313	9.1801232	6.4788116
H	10.0504657	8.5838479	7.3672015
C	10.9622231	8.5681875	5.4081686
C	11.4004294	7.1328288	5.5250669
H	11.9334893	6.8059263	4.6233069
H	10.5401707	6.4615708	5.6703868
H	12.0713483	6.9866845	6.3851531
C	11.2182963	9.3245164	4.2855388
H	11.7573828	8.8868615	3.4423485
C	10.7855667	10.6764869	4.1839208
C	11.1122507	11.4042575	3.0042272
H	11.8103737	10.9320737	2.2986280
C	11.1453644	13.3404229	1.5544243
H	11.6066920	12.6764221	0.8074140
H	11.9135200	14.0485792	1.9035188
C	9.9615220	14.1108669	0.9734050
H	10.3021828	14.9885162	0.4041255
H	9.3924701	13.4698698	0.2797422
C	8.1563384	15.3956404	1.9005063
H	8.0744600	15.8401741	0.8987603
C	7.2226410	15.8522419	2.8719622
C	7.2690727	15.3986314	4.2264863
C	6.2831491	15.9370721	5.1260823
C	5.4363681	15.9583224	7.3505091
H	5.5301176	17.0502693	7.4690807

H	5.6841140	15.4655950	8.2963771
H	4.4004248	15.7112186	7.0656172
C	5.3439280	16.8514872	4.6803918
H	4.6021592	17.2419928	5.3775944
C	5.3061137	17.3026774	3.3340969
C	4.2584700	18.2970168	2.9088878
H	4.3558404	18.5475473	1.8447621
H	4.3351499	19.2321981	3.4841282
H	3.2433320	17.9028831	3.0701338
C	6.2415534	16.8010746	2.4582686
H	6.2414175	17.1241728	1.4147177
C	7.7534924	11.6714691	2.1364857
H	8.4603551	11.9064649	1.3451319
C	6.7364696	10.7666862	1.9097750
H	6.6414852	10.3020043	0.9284376
C	5.8371367	10.4537023	2.9527016
C	6.0487151	11.1050163	4.1871563
H	5.3970273	10.9105730	5.0390446
C	7.0893431	11.9990698	4.3291489
H	7.2787958	12.5143370	5.2684402
C	10.5840231	16.1479635	4.2235751
H	9.6596490	16.4900780	3.7644382
C	11.4957154	17.0600255	4.7162850
H	11.2812532	18.1256392	4.6343157
C	12.6836102	16.6043777	5.3288896
C	12.8634122	15.2054359	5.3988485
H	13.7503512	14.7776315	5.8663166
C	11.8984247	14.3631887	4.8847099
H	12.0104433	13.2842198	4.9552219
N	13.6154682	17.4685232	5.8099125
H	14.4034605	17.1289015	6.3463864
H	13.4214334	18.4606526	5.8555077
N	4.8304257	9.5586667	2.7804033
H	4.1542026	9.3906280	3.5136899
H	4.6481892	9.1463477	1.8749553
6'			
Co	0.6470525	-0.7913012	8.1138072
O	-0.1799815	-2.1590579	9.1426390
O	-1.7900449	-3.8567570	10.2512974
O	-1.0393783	0.0860382	8.2100106
O	-3.3526243	1.0190976	8.9118730
N	2.3277424	-1.6532736	8.0254191
N	1.4623105	0.5685768	7.0837403
N	1.0418345	0.1621907	9.7981551
C	0.3077867	-3.3548529	9.3211752
C	-0.5502992	-4.3284799	9.9382843
C	-2.6937552	-4.7637159	10.8804104
H	-2.9080076	-5.6306318	10.2341734
H	-3.6156602	-4.1969165	11.0476141
H	-2.2989039	-5.1185780	11.8462513
C	-0.1024965	-5.6182605	10.1704961
H	-0.7705272	-6.3437094	10.6350636
C	1.2092236	-6.0356977	9.8211657
C	1.6432582	-7.4491167	10.1046748
H	2.6745832	-7.6229325	9.7722137
H	0.9965324	-8.1787980	9.5940145
H	1.5948281	-7.6735950	11.1809609
C	2.0475788	-5.1137821	9.2348283
H	3.0650422	-5.3990194	8.9582397
C	1.6255345	-3.7778389	8.9750341
C	2.5634226	-2.8820115	8.3920245
H	3.5785771	-3.2714808	8.2315815
C	3.4014845	-0.8222868	7.4734796
H	4.1505809	-1.4398680	6.9545647
H	3.9197884	-0.3042842	8.2960115
C	2.7632573	0.1939862	6.5242139
H	3.4052834	1.0785634	6.3923036
H	2.6144649	-0.2525748	5.5282894
C	0.9689426	1.7575029	6.8803570
H	1.5855626	2.4715017	6.3168350
C	-0.2980711	2.2252353	7.3269444
C	-1.2318376	1.3514306	7.9574747
C	-2.5021907	1.9100307	8.3284622
C	-4.6398832	1.5010732	9.2941400
H	-4.5616684	2.3049530	10.0443812
H	-5.1613877	0.6431392	9.7311024
H	-5.2048059	1.8710499	8.4228439

C	-2.7825453	3.2454228	8.0906895
H	-3.7494697	3.6525627	8.3870081
C	-1.8466188	4.1136174	7.4698813
C	-2.2078520	5.5561631	7.2353361
H	-2.4359168	6.0719940	8.1806884
H	-3.0990288	5.6468461	6.5959815
H	-1.3876336	6.0971204	6.7466858
C	-0.6282246	3.5912995	7.0957541
H	0.1129662	4.2289768	6.6089833
C	2.0605698	1.0214092	10.0031076
H	2.7541440	1.1650031	9.1795816
C	0.7317696	-2.3614367	5.5831346
C	0.2170253	-3.1457028	4.5702032
C	-1.1691015	-3.4111866	4.5294703
C	-1.9475011	-2.8464270	5.5623902
C	-1.3516685	-2.0704187	6.5350281
N	-0.0235971	-1.8071469	6.5532098
H	1.8017586	-2.1829820	5.6331787
H	0.8896855	-3.5584520	3.8184098
H	-3.0229813	-3.0183957	5.6079965
H	-1.9296860	-1.6289647	7.3431598
C	2.2390722	1.7260228	11.1766309
C	1.3136021	1.5701992	12.2312909
C	0.2399572	0.6836788	11.9995848
C	0.1393089	0.0154795	10.7967460
H	3.0890667	2.4019403	11.2706459
H	-0.5226235	0.5192748	12.7612012
H	-0.6816825	-0.6675822	10.5929232
N	1.4433843	2.2463673	13.4009598
H	0.7806726	2.1175398	14.1539858
H	2.2213028	2.8720282	13.5624996
N	-1.7229964	-4.1718140	3.5512601
H	-2.7137590	-4.3749620	3.5472741
H	-1.1538816	-4.5975426	2.8318497

Geometries of A-C

A			
Co	0.5281937	-0.7776869	8.0988543
O	-0.1882720	-2.0035790	9.3547020
O	-1.8162073	-3.6863765	10.5078044
O	-1.2006840	0.0005096	7.9695600
O	-3.5007643	0.9629795	8.7589048
N	2.2330300	-1.5979712	8.0955033
N	1.2991233	0.5108316	6.9488290
C	0.2485134	-3.2442378	9.4847768
C	-0.6182276	-4.1906963	10.1224231
C	-2.7262773	-4.5729464	11.1670452
H	-3.0035463	-5.4168177	10.5155675
H	-3.6145843	-3.9725603	11.3861876
H	-2.2978502	-4.9560370	12.1063725
C	-0.2001795	-5.5031911	10.3131971
H	-0.8721100	-6.2124942	10.7960699
C	1.0745848	-5.9573714	9.8995360
C	1.4714699	-7.3902854	10.1305290
H	2.4882387	-7.5862803	9.7685237
H	0.7888449	-8.0810081	9.6132683
H	1.4382619	-7.6439673	11.2002839
C	1.9233023	-5.0516876	9.2913662
H	2.9148957	-5.3680744	8.9622781
C	1.5344929	-3.7032296	9.0746334
C	2.4816560	-2.8155012	8.4741700
H	3.4989100	-3.2012770	8.3232866
C	3.2638271	-0.7345617	7.5170495
H	4.1110774	-1.3236280	7.1366007
H	3.6317675	-0.0519403	8.2992040
C	2.5846829	0.0686223	6.4079014
H	3.1981265	0.9224653	6.0846640
H	2.3962267	-0.5802213	5.5383886
C	0.8249861	1.7007100	6.7340422
H	1.4312058	2.3949976	6.1369276
C	-0.4310028	2.1850274	7.2216939
C	-1.3798058	1.3004918	7.8143056
C	-2.6324994	1.8585963	8.2303596
C	-4.7830947	1.4463930	9.1735082
H	-4.6872485	2.1967371	9.9741356

H	-5.3174324	0.5705832	9.5541393
H	-5.3377340	1.8788796	8.3260956
C	-2.8808139	3.2173756	8.0657107
H	-3.8341836	3.6293306	8.3962623
C	-1.9349727	4.0927776	7.4830201
C	-2.2588426	5.5545878	7.3342972
H	-2.4372978	6.0241367	8.3134292
H	-3.1700931	5.7002707	6.7357010
H	-1.4415516	6.0972407	6.8437654
C	-0.7279859	3.5636632	7.0635445
H	0.0226995	4.2109165	6.6061422
O	-0.1331767	-1.8750448	6.5897810
H	-1.0423814	-1.4858852	6.6089461
O	0.9231233	0.2757649	9.7280245
H	0.3792118	1.0918936	9.6935395
H	-0.2328966	-2.7951168	6.9137147
H	0.4440197	-0.3405187	10.3352427
B			
Co	0.44539700	-1.02685780	8.12928810
O	-0.11239000	-2.19614360	9.54868050
O	-1.61529140	-3.80068940	10.97030830
O	-1.20529820	-0.07563260	8.38853620
O	-3.49469440	0.93157150	9.11693220
N	2.10954690	-1.87303770	7.98574860
N	1.12138480	0.21235330	6.89057800
C	0.27395840	-3.44332510	9.61528890
C	-0.51692930	-4.35979120	10.38603870
C	-2.45794360	-4.66122350	11.72552300
H	-2.87483740	-5.46933870	11.10055660
H	-3.27345890	-4.03041050	12.09619950
H	-1.92076250	-5.10735500	12.58026520
C	-0.15357590	-5.69443530	10.49588980
H	-0.78052330	-6.37811330	11.06891180
C	1.01379620	-6.20657960	9.87865000
C	1.35920070	-7.66603480	10.01796920
H	2.31239440	-7.89546530	9.52317140
H	0.58597510	-8.30875870	9.56821850
H	1.44915030	-7.96147080	11.07490430
C	1.80492250	-5.33219380	9.16116060
H	2.71915190	-5.69182000	8.68252080
C	1.45766930	-3.96457140	9.01468520
C	2.35999410	-3.10225960	8.31971770
H	3.34940080	-3.51068040	8.06872440
C	3.12248260	-1.02341920	7.36495420
H	3.93782890	-1.62426200	6.93201730
H	3.54476380	-0.36158600	8.13866350
C	2.40437860	-0.19213750	6.30822330
H	2.99603810	0.68558180	6.00593770
H	2.20169350	-0.80910070	5.41847460
C	0.57482550	1.33466930	6.52849790
H	1.12418490	1.96133270	5.81276830
C	-0.68472970	1.83595240	6.97756110
C	-1.49610760	1.09656930	7.88730290
C	-2.75442080	1.68904700	8.25620200
C	-4.76050850	1.44561520	9.51193890
H	-4.65884670	2.40584520	10.04611490
H	-5.18943830	0.69605250	10.18583210
H	-5.42864050	1.58549690	8.64508940
C	-3.14419390	2.91769650	7.74518660
H	-4.10417610	3.34325250	8.03881300
C	-2.32779600	3.64565220	6.84330200
C	-2.79001280	4.98001880	6.31872950
H	-2.92868730	5.70853960	7.13312870
H	-3.75462850	4.89753180	5.79380560
H	-2.06043900	5.40120330	5.61424220
C	-1.11783300	3.09375910	6.47781470
H	-0.46481100	3.62567160	5.78149910
O	-0.32403770	-2.28666120	6.90603930
O	1.08708580	0.10116420	9.88722170
H	0.32488140	0.71318340	9.91371310
H	0.74667050	-0.69323640	10.36850310
C	-0.26063520	-2.11435100	5.59481800
C	-1.30337130	-1.37367150	4.94092310
C	0.76331260	-2.68025220	4.80713600
C	-1.22564750	-1.16330480	3.55245570
C	0.80797780	-2.48825830	3.42825040
H	1.51519090	-3.28292710	5.31905870

C	-0.18043920	-1.70736970	2.80965930
H	-2.00557830	-0.58110800	3.05598950
H	1.60145940	-2.94215040	2.83330890
H	-0.14492530	-1.53760810	1.73244970
N	-2.35489950	-0.94747170	5.70582790
H	-2.91821690	-0.17457590	5.37314600
H	-2.21659180	-1.01236000	6.71513110
O	-2.49186323	-1.29850997	10.13327775
H	-2.30044777	-0.38390639	9.81028311
H	-1.67750178	-1.76637263	10.44221120
H	-3.21416855	-1.31544253	10.80814502

C

Co	0.6862491	-0.9210548	8.5499780
O	0.1184952	-2.4082697	10.1203701
O	-1.6420705	-4.2595628	10.7852210
O	-0.7306188	0.4804705	8.7370547
O	-3.1528407	1.4689383	8.8580635
N	2.4729644	-1.8868779	8.6285168
N	1.6541506	0.2330762	7.2359220
C	0.4538575	-3.7193649	9.9231613
C	-0.4554337	-4.7270342	10.3013363
C	-2.6382747	-5.2232815	11.1446602
H	-2.9157259	-5.8445682	10.2793657
H	-3.5067403	-4.6448813	11.4749344
H	-2.2889551	-5.8648193	11.9681956
C	-0.1043234	-6.0690157	10.1756185
H	-0.8106799	-6.8426248	10.4750461
C	1.1583677	-6.4494727	9.6826749
C	1.5190651	-7.9069902	9.5739149
H	2.5351211	-8.0380004	9.1821354
H	0.8276004	-8.4394237	8.9042066
H	1.4681669	-8.4035449	10.5540298
C	2.0429356	-5.4484710	9.3064675
H	3.0244031	-5.7156011	8.9102460
C	1.7080558	-4.0764799	9.3940410
C	2.6855520	-3.1335836	8.8853045
H	3.6802686	-3.5587838	8.6729773
C	3.5407728	-1.0300807	8.1220644
H	4.4381065	-1.6064291	7.8430904
H	3.8116142	-0.3301127	8.9280103
C	3.0041539	-0.2391806	6.9231752
H	3.6801506	0.5927143	6.6713772
H	2.9477881	-0.9049591	6.0447804
C	1.1128303	1.1733152	6.5273069
H	1.6980324	1.6373118	5.7178581
C	-0.2331302	1.6584456	6.6748824
C	-1.0848923	1.2850342	7.7596364
C	-2.3994124	1.8574121	7.7877127
C	-4.4632533	2.0291308	8.9757494
H	-4.4198121	3.1267147	9.0496838
H	-4.8851135	1.6171572	9.8981193
H	-5.0985621	1.7462179	8.1211539
C	-2.8335023	2.7060749	6.7812296
H	-3.8427682	3.1164292	6.8115128
C	-1.9916228	3.0610405	5.7039450
C	-2.4991928	3.9722061	4.6211309
H	-2.8573860	4.9265554	5.0351924
H	-3.3458973	3.5174890	4.0842204
H	-1.7153177	4.1942254	3.8870376
C	-0.7065261	2.5440835	5.6813755
H	-0.0322677	2.8116306	4.8653865
O	-0.5243923	-2.0762837	7.4930332
O	1.3882918	0.1036494	10.4409249
H	0.7042637	0.7975106	10.5070530
H	1.1756643	-0.5494935	11.1335630
C	-0.9404637	-1.6032472	6.3430233
C	-2.3405814	-1.2443715	6.2142325
C	-0.1016233	-1.4322986	5.2169599
C	-2.7999616	-0.6619582	5.0132019
C	-0.5847568	-0.8852941	4.0423524
H	0.9305588	-1.7712754	5.3007721
C	-1.9350168	-0.4756411	3.9508577
H	-3.8478248	-0.3680469	4.9316965
H	0.0703367	-0.7804968	3.1775091
H	-2.3032114	-0.0301484	3.0270114
N	-3.1553682	-1.4802809	7.2676742

H	-2.7637746	-1.7584479	8.1677365
O	-2.2172753	-1.2478584	10.1370476
H	-1.8891641	-0.4021160	9.7147118
H	-4.1182428	-1.1700510	7.2438029
H	-0.8722309	-2.2693891	10.2721109
H	-2.8006902	-0.9987946	10.8712579