

Supporting Information

Facile, cost effective synthesis and DFT based studies of substituted aryl hydrazones of β -diketones: A new selective Fluorescent Chemosensor for Co^{2+}

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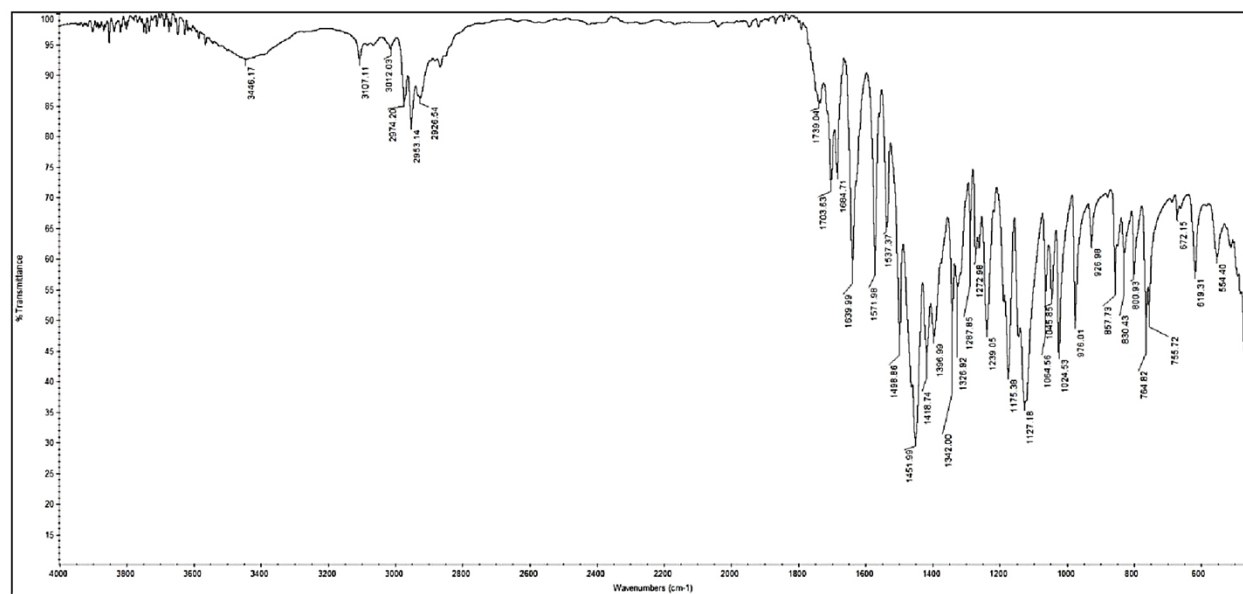


Fig. S1 IR spectra of CD1

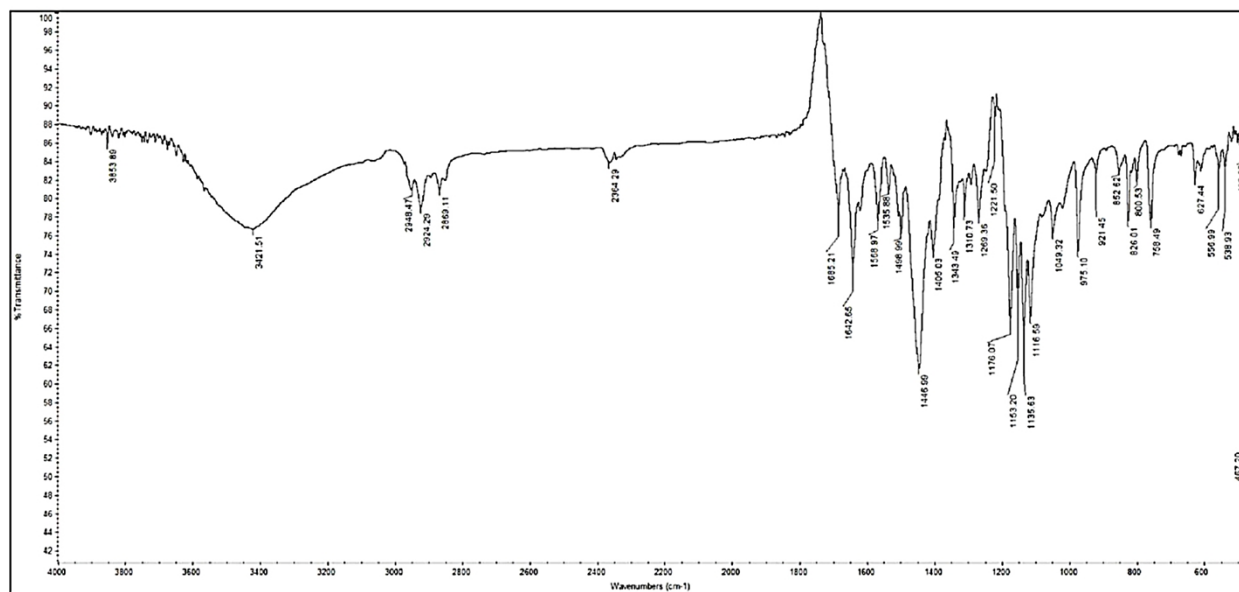


Fig. S2 IR spectra of CD2

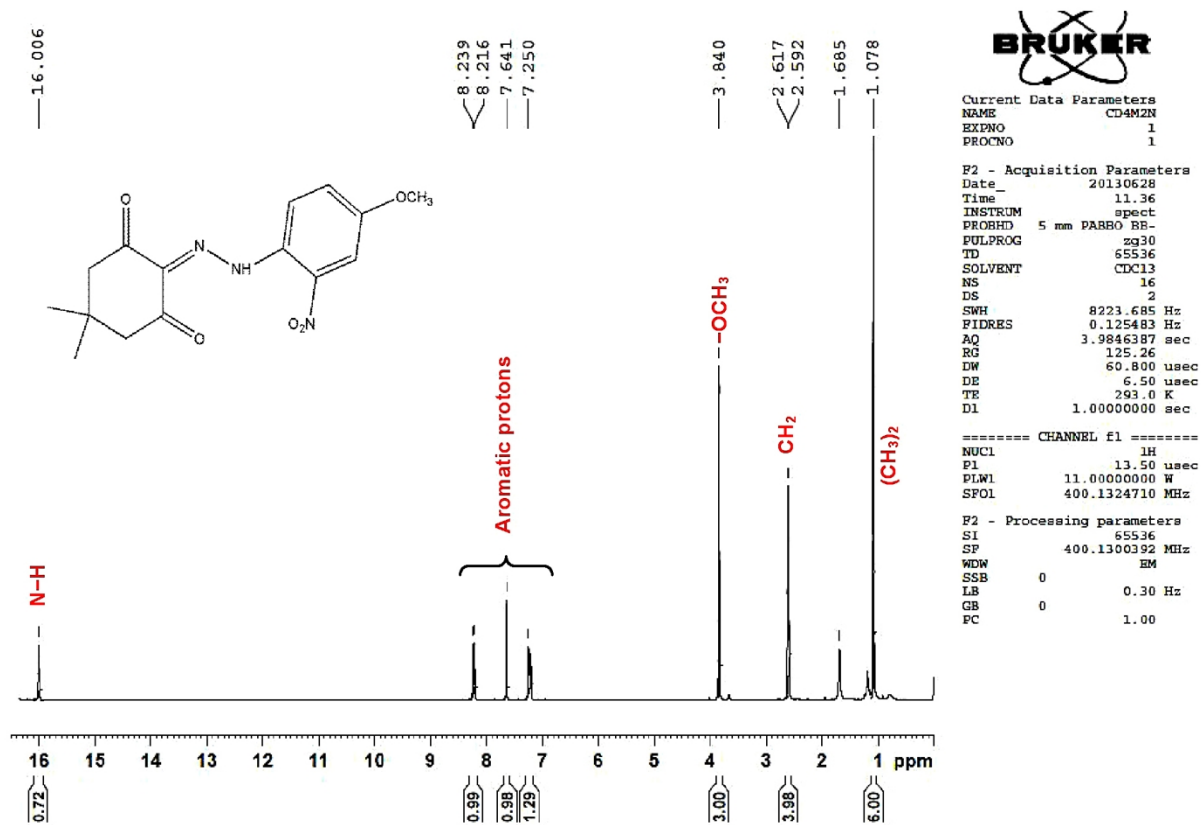


Fig. S3 ¹H NMR spectrum of CD1 in CDCl₃

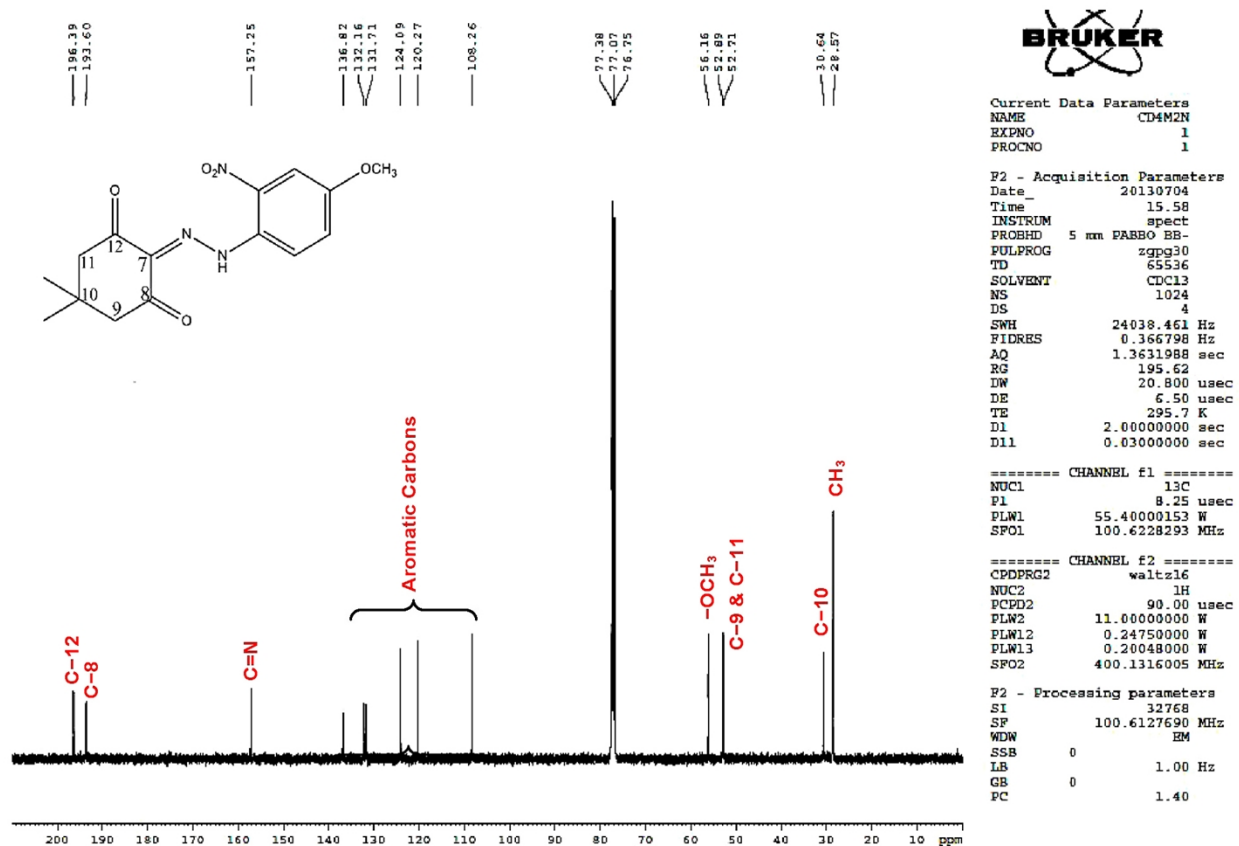


Fig. S4 ^{13}C NMR spectrum of CD1 in CDCl_3

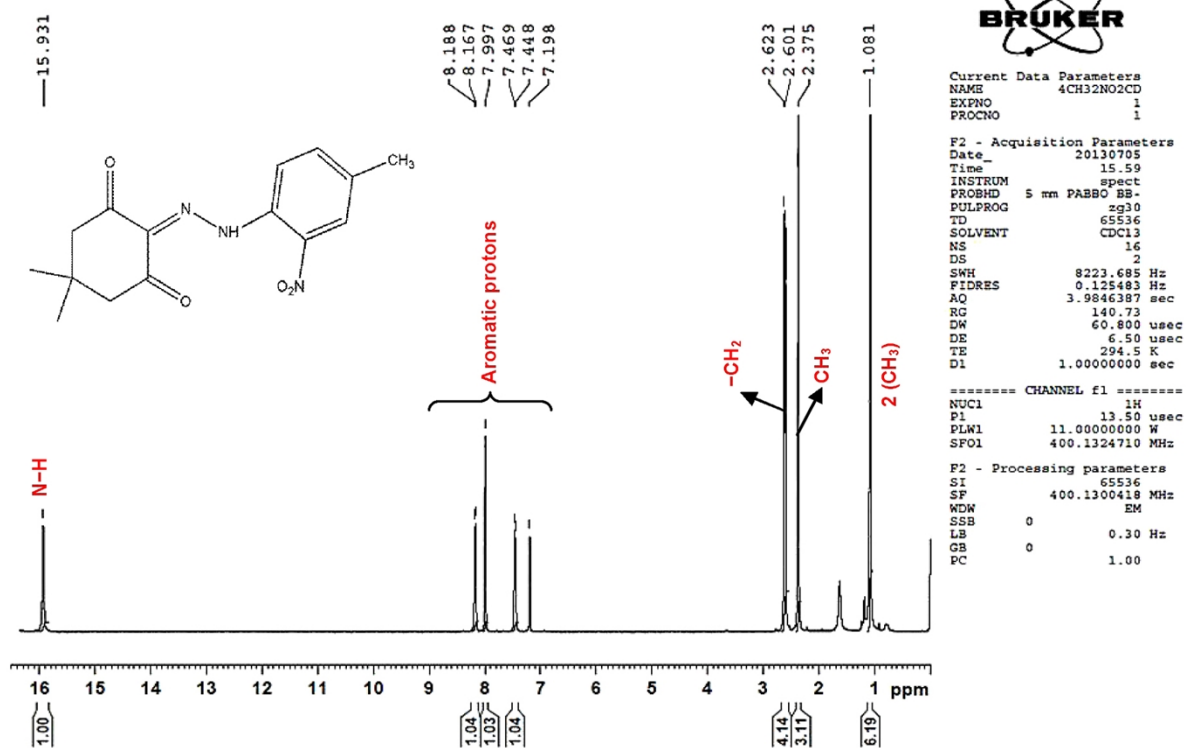


Fig. S5 ¹H NMR spectrum of CD2 in CDCl₃

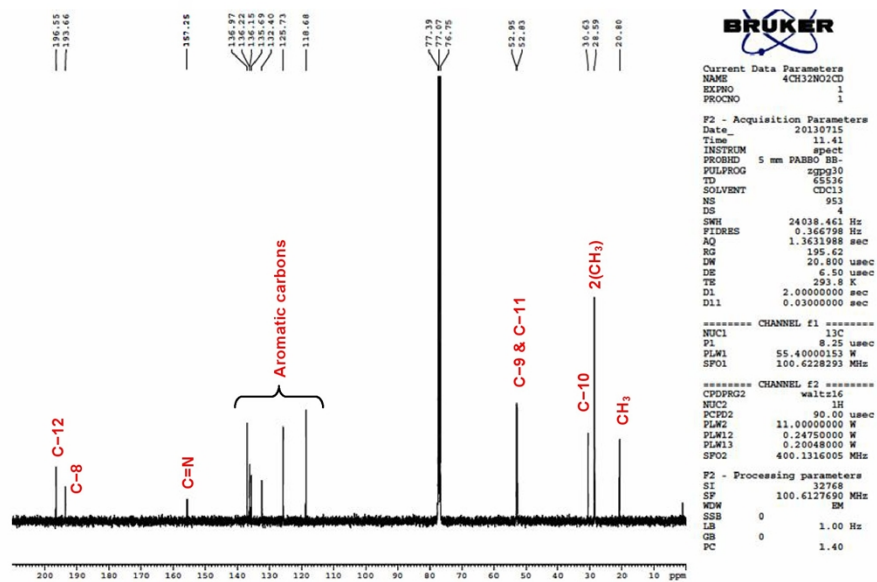


Fig. S6 ¹³C NMR spectrum of CD₂ in CDCl₃

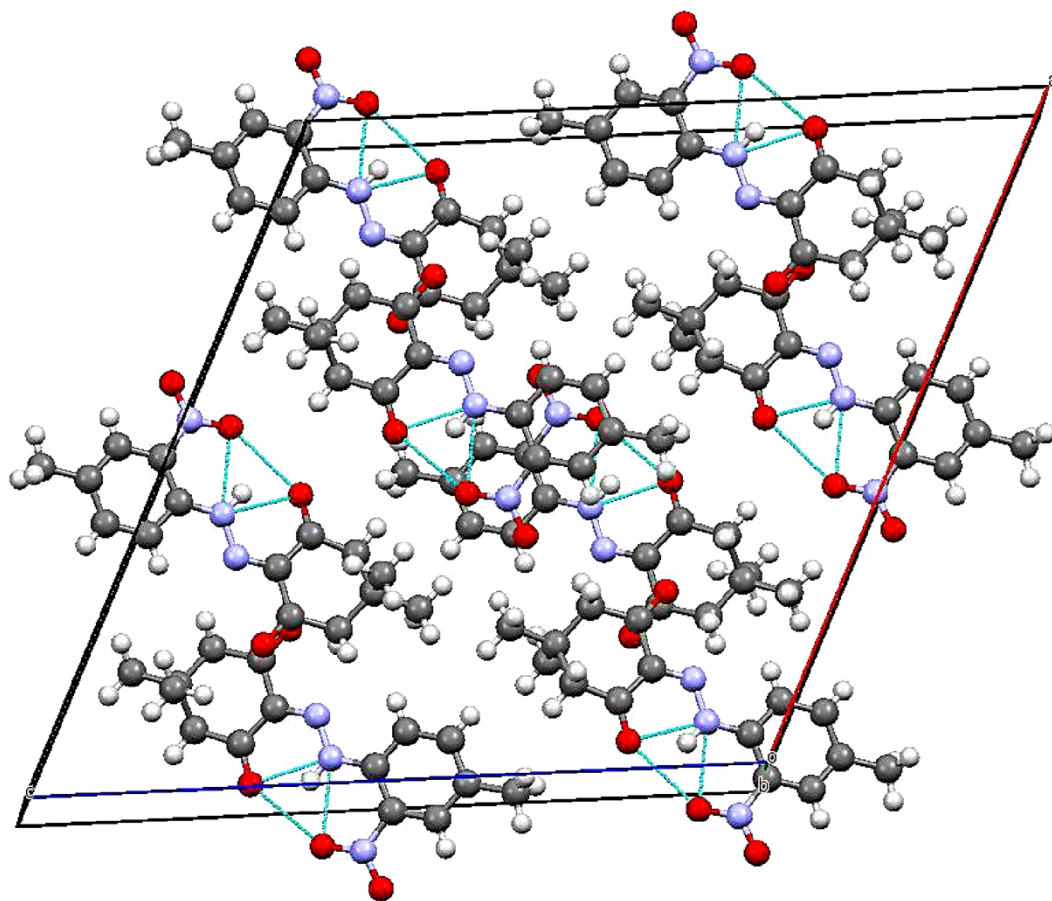
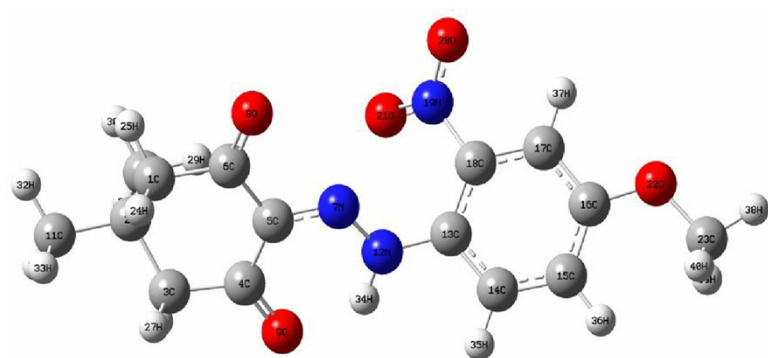
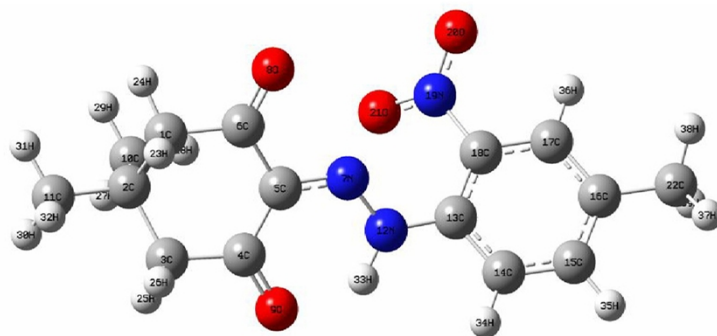


Fig.S7 Packing diagram of compound CD2



CD1



CD2

Fig. S8 Optimized structure of CD1 and CD2

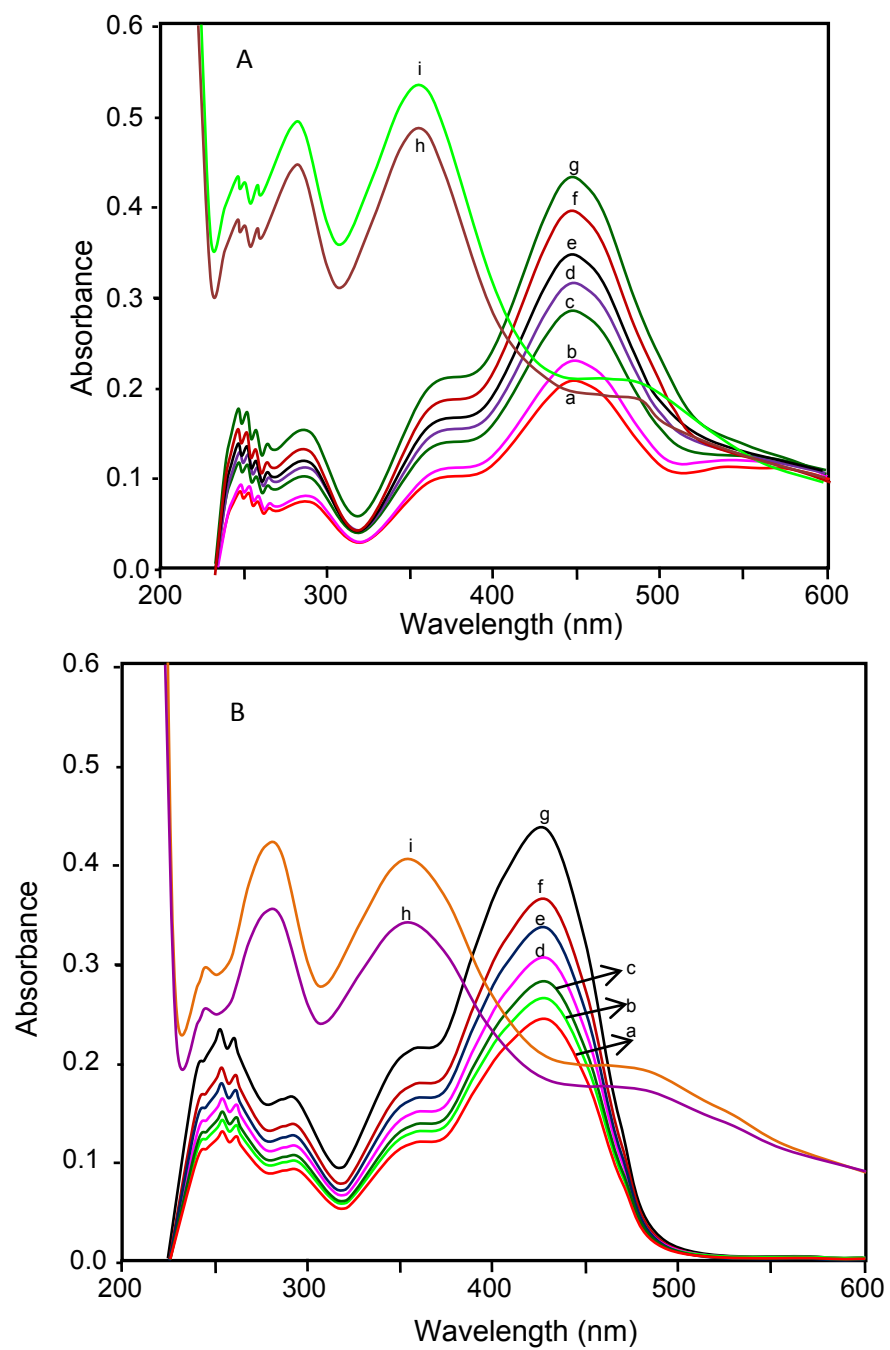


Fig. S9 Absorbance spectra of CD1(A) and CD2(B) in ethanol:H₂O with Co²⁺ Solution at different pH. (a-i) pH = 3 to pH = 11.

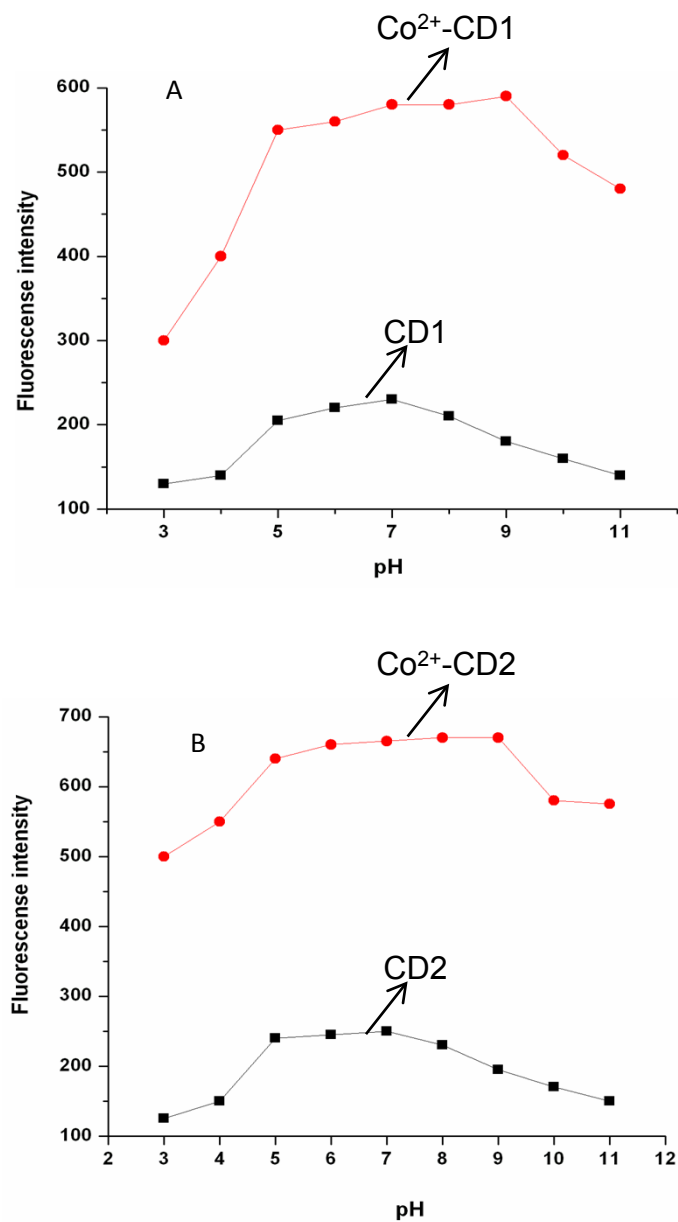


Fig.S10 Fluorescence intensities of CD1 (A), CD2 (B) and Co²⁺-CD1, Co²⁺-CD2 at various pH values at room temperature, HEPES buffer solution (10 mM, 8 mM NaCl, pH = 7.0) (CH₃-CH₂-OH /H₂O=4:1, v/v). [CD 1 and CD 2] =10.0 μmol/L, the concentration of Co²⁺ values ranging from 0 to 10.0 μmol/L.

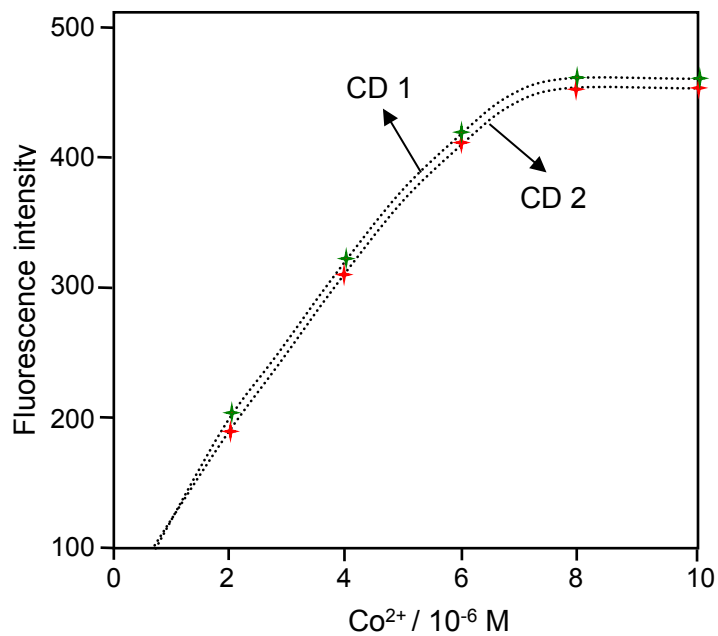


Fig. S11 Fluorescence intensity of CD1 and CD2 versus the Co²⁺ concentration at 548 nm and 490 nm respectively.

Table S1. Bond lengths [Å] and angles [deg] for CD 1

O(1)-C(12)	1.351(4)
O(1)-C(15)	1.426(5)
N(1)-C(6)	1.315(4)
N(1)-N(2)	1.316(4)
C(1)-C(3)	1.526(5)
C(1)-H(020)	0.95(5)
C(1)-H(26)	0.96(6)
C(1)-H(34)	0.99(5)
O(2)-C(17)	1.353(4)
O(2)-C(16)	1.427(6)
N(2)-C(9)	1.393(4)
N(2)-H(017)	0.94(4)
C(2)-C(3)	1.519(5)
C(2)-H(009)	0.95(5)
C(2)-H(012)	0.95(5)
C(2)-H(25)	0.97(4)
O(3)-C(24)	1.214(4)
N(3)-O(10)	1.215(4)
N(3)-O(6)	1.221(4)
N(3)-C(14)	1.455(4)
C(3)-C(4)	1.521(5)
C(3)-C(8)	1.536(5)
O(4)-C(28)	1.222(4)
N(4)-O(7)	1.219(4)
N(4)-O(11)	1.221(4)
N(4)-C(21)	1.460(4)
C(4)-C(5)	1.503(5)
C(4)-H(003)	0.95(4)
C(4)-H(008)	1.01(4)
O(5)-C(7)	1.231(4)
N(5)-N(6)	1.317(4)
N(5)-C(20)	1.393(4)
N(5)-H(015)	0.91(4)
C(5)-O(8)	1.211(4)
C(5)-C(6)	1.493(5)

N(6)-C(23)	1.314(4)
C(6)-C(7)	1.472(5)
C(7)-C(8)	1.499(5)
C(8)-H(24)	0.99(4)
C(8)-H(28)	1.00(4)
C(9)-C(14)	1.395(4)
C(9)-C(10)	1.405(5)
C(10)-C(11)	1.354(5)
C(10)-H(30)	0.95(4)
C(11)-C(12)	1.405(5)
C(11)-H(006)	1.06(4)
C(12)-C(13)	1.378(5)
C(13)-C(14)	1.393(5)
C(13)-H(21)	0.97(4)
C(15)-H(002)	1.03(4)
C(15)-H(29)	0.96(5)
C(15)-H(32)	1.01(4)
C(16)-H(004)	1.04(5)
C(16)-H(010)	1.02(4)
C(16)-H(31)	0.89(6)
C(17)-C(22)	1.372(5)
C(17)-C(18)	1.391(5)
C(19)-C(18)	1.361(5)
C(19)-C(20)	1.401(4)
C(19)-H(019)	0.97(4)
C(18)-H(016)	0.91(4)
C(20)-C(21)	1.397(5)
C(25)-C(24)	1.505(5)
C(25)-C(26)	1.513(5)
C(25)-H(005)	0.95(4)
C(25)-H(007)	1.00(4)
C(24)-C(23)	1.493(4)
C(23)-C(28)	1.466(5)
C(22)-C(21)	1.393(5)
C(22)-H(011)	0.97(4)
C(26)-C(30)	1.515(5)
C(26)-C(29)	1.529(5)
C(26)-C(27)	1.529(5)
C(28)-C(27)	1.508(5)
C(27)-H(001)	0.95(4)
C(27)-H(018)	0.99(4)

C(29)-H(22)	1.01(5)
C(29)-H(23)	1.01(4)
C(29)-H(27)	0.89(5)
C(30)-H(013)	0.98(5)
C(30)-H(014)	0.98(5)
C(30)-H(33)	0.94(6)
C(12)-O(1)-C(15)	117.7(3)
C(6)-N(1)-N(2)	119.0(3)
C(3)-C(1)-H(020)	108(3)
C(3)-C(1)-H(26)	108(3)
H(020)-C(1)-H(26)	105(4)
C(3)-C(1)-H(34)	107(3)
H(020)-C(1)-H(34)	119(4)
H(26)-C(1)-H(34)	110(4)
C(17)-O(2)-C(16)	117.5(3)
N(1)-N(2)-C(9)	119.3(3)
N(1)-N(2)-H(017)	123(2)
C(9)-N(2)-H(017)	118(2)
C(3)-C(2)-H(009)	108(2)
C(3)-C(2)-H(012)	109(3)
H(009)-C(2)-H(012)	110(4)
C(3)-C(2)-H(25)	112(3)
H(009)-C(2)-H(25)	106(3)
H(012)-C(2)-H(25)	112(4)
O(10)-N(3)-O(6)	121.6(3)
O(10)-N(3)-C(14)	119.0(3)
O(6)-N(3)-C(14)	119.4(3)
C(2)-C(3)-C(4)	111.0(3)
C(2)-C(3)-C(1)	109.1(4)
C(4)-C(3)-C(1)	110.2(3)
C(2)-C(3)-C(8)	109.7(3)
C(4)-C(3)-C(8)	107.6(3)
C(1)-C(3)-C(8)	109.3(3)
O(7)-N(4)-O(11)	121.8(3)
O(7)-N(4)-C(21)	118.5(3)
O(11)-N(4)-C(21)	119.6(3)
C(5)-C(4)-C(3)	116.2(3)
C(5)-C(4)-H(003)	108(2)
C(3)-C(4)-H(003)	110(2)
C(5)-C(4)-H(008)	107(2)

C(3)-C(4)-H(008)	108(2)
H(003)-C(4)-H(008)	107(3)
N(6)-N(5)-C(20)	118.4(3)
N(6)-N(5)-H(015)	122(2)
C(20)-N(5)-H(015)	120(2)
O(8)-C(5)-C(6)	121.7(3)
O(8)-C(5)-C(4)	121.5(3)
C(6)-C(5)-C(4)	116.8(3)
C(23)-N(6)-N(5)	119.6(3)
N(1)-C(6)-C(7)	124.8(3)
N(1)-C(6)-C(5)	114.7(3)
C(7)-C(6)-C(5)	120.5(3)
O(5)-C(7)-C(6)	121.1(3)
O(5)-C(7)-C(8)	120.5(3)
C(6)-C(7)-C(8)	118.3(3)
C(7)-C(8)-C(3)	113.3(3)
C(7)-C(8)-H(24)	106(2)
C(3)-C(8)-H(24)	107(2)
C(7)-C(8)-H(28)	106(2)
C(3)-C(8)-H(28)	111(2)
H(24)-C(8)-H(28)	114(3)
N(2)-C(9)-C(14)	123.0(3)
N(2)-C(9)-C(10)	120.7(3)
C(14)-C(9)-C(10)	116.4(3)
C(11)-C(10)-C(9)	122.1(3)
C(11)-C(10)-H(30)	122(2)
C(9)-C(10)-H(30)	116(2)
C(10)-C(11)-C(12)	120.5(3)
C(10)-C(11)-H(006)	121(2)
C(12)-C(11)-H(006)	119(2)
O(1)-C(12)-C(13)	124.8(3)
O(1)-C(12)-C(11)	115.9(3)
C(13)-C(12)-C(11)	119.3(3)
C(12)-C(13)-C(14)	119.3(3)
C(12)-C(13)-H(21)	120(2)
C(14)-C(13)-H(21)	120(2)
C(13)-C(14)-C(9)	122.4(3)
C(13)-C(14)-N(3)	115.2(3)
C(9)-C(14)-N(3)	122.5(3)
O(1)-C(15)-H(002)	113(2)
O(1)-C(15)-H(29)	113(3)

H(002)-C(15)-H(29)	96(4)
O(1)-C(15)-H(32)	104(3)
H(002)-C(15)-H(32)	112(3)
H(29)-C(15)-H(32)	119(4)
O(2)-C(16)-H(004)	111(2)
O(2)-C(16)-H(010)	110(2)
H(004)-C(16)-H(010)	109(3)
O(2)-C(16)-H(31)	107(4)
H(004)-C(16)-H(31)	113(4)
H(010)-C(16)-H(31)	107(4)
O(2)-C(17)-C(22)	124.2(3)
O(2)-C(17)-C(18)	115.7(3)
C(22)-C(17)-C(18)	120.1(3)
C(18)-C(19)-C(20)	121.8(3)
C(18)-C(19)-H(019)	117(2)
C(20)-C(19)-H(019)	121(2)
C(19)-C(18)-C(17)	120.4(4)
C(19)-C(18)-H(016)	121(2)
C(17)-C(18)-H(016)	119(2)
N(5)-C(20)-C(21)	123.4(3)
N(5)-C(20)-C(19)	120.1(3)
C(21)-C(20)-C(19)	116.4(3)
C(24)-C(25)-C(26)	114.9(3)
C(24)-C(25)-H(005)	109(2)
C(26)-C(25)-H(005)	114(2)
C(24)-C(25)-H(007)	107(2)
C(26)-C(25)-H(007)	108(2)
H(005)-C(25)-H(007)	102(3)
O(3)-C(24)-C(23)	122.0(3)
O(3)-C(24)-C(25)	121.5(3)
C(23)-C(24)-C(25)	116.4(3)
N(6)-C(23)-C(28)	124.6(3)
N(6)-C(23)-C(24)	114.2(3)
C(28)-C(23)-C(24)	121.2(3)
C(17)-C(22)-C(21)	118.9(3)
C(17)-C(22)-H(011)	122(2)
C(21)-C(22)-H(011)	119(2)
C(22)-C(21)-C(20)	122.4(3)
C(22)-C(21)-N(4)	115.7(3)
C(20)-C(21)-N(4)	122.0(3)
C(25)-C(26)-C(30)	110.7(3)

C(25)-C(26)-C(29)	109.5(3)
C(30)-C(26)-C(29)	109.4(3)
C(25)-C(26)-C(27)	108.1(3)
C(30)-C(26)-C(27)	110.5(3)
C(29)-C(26)-C(27)	108.8(3)
O(4)-C(28)-C(23)	122.2(3)
O(4)-C(28)-C(27)	119.9(3)
C(23)-C(28)-C(27)	117.9(3)
C(28)-C(27)-C(26)	114.0(3)
C(28)-C(27)-H(001)	112(2)
C(26)-C(27)-H(001)	108(2)
C(28)-C(27)-H(018)	107(2)
C(26)-C(27)-H(018)	105(2)
H(001)-C(27)-H(018)	111(3)
C(26)-C(29)-H(22)	114(3)
C(26)-C(29)-H(23)	115(2)
H(22)-C(29)-H(23)	112(4)
C(26)-C(29)-H(27)	111(3)
H(22)-C(29)-H(27)	104(4)
H(23)-C(29)-H(27)	99(4)
C(26)-C(30)-H(013)	114(2)
C(26)-C(30)-H(014)	114(2)
H(013)-C(30)-H(014)	101(3)
C(26)-C(30)-H(33)	116(3)
H(013)-C(30)-H(33)	98(4)
H(014)-C(30)-H(33)	111(4)

Table S2. Hydrogen bonds for CD1

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(16)-H(004)...O(5)#1	1.04(5)	2.57(4)	3.230(6)	121(3)
C(11)-H(006)...O(7)#2	1.06(4)	2.59(4)	3.427(5)	136(2)
N(5)-H(015)...O(4)	0.91(4)	1.92(4)	2.602(4)	130(3)
N(5)-H(015)...O(11)	0.91(4)	2.00(4)	2.628(4)	125(3)
N(2)-H(017)...O(5)	0.94(4)	1.88(4)	2.579(4)	129(3)
N(2)-H(017)...O(6)	0.94(4)	1.94(4)	2.622(4)	127(3)
C(15)-H(29)...O(3)#3	0.96(5)	2.62(5)	3.189(6)	118(3)
C(16)-H(004)...O(5)#1	1.04(5)	2.57(4)	3.230(6)	121(3)
C(25)-H(005)...O(6)#4	0.95(4)	2.65(4)	3.469(5)	144(3)
C(11)-H(006)...O(7)#2	1.06(4)	2.59(4)	3.427(5)	136(2)
N(5)-H(015)...O(4)	0.91(4)	1.92(4)	2.602(4)	130(3)
N(5)-H(015)...O(11)	0.91(4)	2.00(4)	2.628(4)	125(3)
N(2)-H(017)...O(5)	0.94(4)	1.88(4)	2.579(4)	129(3)
N(2)-H(017)...O(6)	0.94(4)	1.94(4)	2.622(4)	127(3)
C(15)-H(29)...O(3)#3	0.96(5)	2.62(5)	3.189(6)	118(3)

Table S3. Torsion angles [deg] for CD1

C(6)-N(1)-N(2)-C(9)	-178.5(3)
C(2)-C(3)-C(4)-C(5)	65.9(4)
C(1)-C(3)-C(4)-C(5)	-173.2(4)
C(8)-C(3)-C(4)-C(5)	-54.1(4)
C(3)-C(4)-C(5)-O(8)	-156.4(3)
C(3)-C(4)-C(5)-C(6)	23.5(5)
C(20)-N(5)-N(6)-C(23)	-175.2(3)
N(2)-N(1)-C(6)-C(7)	0.1(4)
N(2)-N(1)-C(6)-C(5)	178.9(3)
O(8)-C(5)-C(6)-N(1)	7.0(4)
C(4)-C(5)-C(6)-N(1)	-172.9(3)
O(8)-C(5)-C(6)-C(7)	-174.1(3)
C(4)-C(5)-C(6)-C(7)	6.0(4)
N(1)-C(6)-C(7)-O(5)	-3.2(5)
C(5)-C(6)-C(7)-O(5)	178.0(3)
N(1)-C(6)-C(7)-C(8)	177.1(3)
C(5)-C(6)-C(7)-C(8)	-1.7(4)
O(5)-C(7)-C(8)-C(3)	149.1(3)
C(6)-C(7)-C(8)-C(3)	-31.1(5)
C(2)-C(3)-C(8)-C(7)	-63.5(4)
C(4)-C(3)-C(8)-C(7)	57.3(4)
C(1)-C(3)-C(8)-C(7)	176.9(4)
N(1)-N(2)-C(9)-C(14)	169.6(3)
N(1)-N(2)-C(9)-C(10)	-10.8(4)
N(2)-C(9)-C(10)-C(11)	179.3(3)
C(14)-C(9)-C(10)-C(11)	-1.1(4)
C(9)-C(10)-C(11)-C(12)	0.6(5)
C(15)-O(1)-C(12)-C(13)	4.3(5)
C(15)-O(1)-C(12)-C(11)	-177.9(3)
C(10)-C(11)-C(12)-O(1)	-177.8(3)
C(10)-C(11)-C(12)-C(13)	0.1(5)
O(1)-C(12)-C(13)-C(14)	177.4(3)
C(11)-C(12)-C(13)-C(14)	-0.3(4)
C(12)-C(13)-C(14)-C(9)	-0.3(4)
C(12)-C(13)-C(14)-N(3)	180.0(3)
N(2)-C(9)-C(14)-C(13)	-179.5(3)
C(10)-C(9)-C(14)-C(13)	0.9(4)
N(2)-C(9)-C(14)-N(3)	0.3(4)
C(10)-C(9)-C(14)-N(3)	-179.3(3)
O(10)-N(3)-C(14)-C(13)	4.3(4)

O(6)-N(3)-C(14)-C(13)	-174.5(3)
O(10)-N(3)-C(14)-C(9)	-175.4(3)
O(6)-N(3)-C(14)-C(9)	5.8(5)
C(16)-O(2)-C(17)-C(22)	0.2(5)
C(16)-O(2)-C(17)-C(18)	-179.9(3)
C(20)-C(19)-C(18)-C(17)	0.6(5)
O(2)-C(17)-C(18)-C(19)	179.6(3)
C(22)-C(17)-C(18)-C(19)	-0.5(5)
N(6)-N(5)-C(20)-C(21)	-172.0(3)
N(6)-N(5)-C(20)-C(19)	8.4(4)
C(18)-C(19)-C(20)-N(5)	178.9(3)
C(18)-C(19)-C(20)-C(21)	-0.6(4)
C(26)-C(25)-C(24)-O(3)	-152.8(3)
C(26)-C(25)-C(24)-C(23)	28.7(4)
N(5)-N(6)-C(23)-C(28)	2.1(5)
N(5)-N(6)-C(23)-C(24)	-178.7(3)
O(3)-C(24)-C(23)-N(6)	5.0(5)
C(25)-C(24)-C(23)-N(6)	-176.6(3)
O(3)-C(24)-C(23)-C(28)	-175.7(3)
C(25)-C(24)-C(23)-C(28)	2.7(4)
O(2)-C(17)-C(22)-C(21)	-179.6(3)
C(18)-C(17)-C(22)-C(21)	0.4(5)
C(17)-C(22)-C(21)-C(20)	-0.5(5)
C(17)-C(22)-C(21)-N(4)	178.3(3)
N(5)-C(20)-C(21)-C(22)	-179.0(3)
C(19)-C(20)-C(21)-C(22)	0.6(4)
N(5)-C(20)-C(21)-N(4)	2.3(4)
C(19)-C(20)-C(21)-N(4)	-178.2(3)
O(7)-N(4)-C(21)-C(22)	-5.2(5)
O(11)-N(4)-C(21)-C(22)	173.5(3)
O(7)-N(4)-C(21)-C(20)	173.6(3)
O(11)-N(4)-C(21)-C(20)	-7.7(5)
C(24)-C(25)-C(26)-C(30)	64.0(4)
C(24)-C(25)-C(26)-C(29)	-175.4(3)
C(24)-C(25)-C(26)-C(27)	-57.0(4)
N(6)-C(23)-C(28)-O(4)	-3.6(5)
C(24)-C(23)-C(28)-O(4)	177.2(3)
N(6)-C(23)-C(28)-C(27)	175.8(3)
C(24)-C(23)-C(28)-C(27)	-3.4(5)
O(4)-C(28)-C(27)-C(26)	152.5(3)
C(23)-C(28)-C(27)-C(26)	-26.9(5)

C(25)-C(26)-C(27)-C(28)	55.7(4)
C(30)-C(26)-C(27)-C(28)	-65.4(4)
C(29)-C(26)-C(27)-C(28)	174.5(3)

Table S4. Bond lengths [Å] and angles [deg] for CD2

Bond Length	Bond Angle
O(1)-C(9)	1.225(3)
O(2)-C(13)	1.210(2)
O(3)-N(3)	1.221(2)
O(4)-N(3)	1.218(2)
N(1)-N(2)	1.318(2)
N(1)-C(2)	1.384(2)
N(1)-H(11)	0.92(2)
N(2)-C(8)	1.310(2)
N(3)-C(1)	1.453(3)
C(15)-C(11)	1.523(3)
C(15)-H(3)	0.99(3)
C(15)-H(1)	1.00(3)
C(15)-H(2)	0.98(3)
C(11)-C(12)	1.514(3)
C(11)-C(14)	1.517(3)
C(11)-C(10)	1.523(3)
C(14)-H(4)	0.92(3)
C(14)-H(5)	1.01(3)
C(14)-H(6)	1.01(3)
C(10)-C(9)	1.490(3)
C(10)-H(10)	0.97(2)
C(10)-H(9)	0.99(2)
C(7)-C(5)	1.500(3)
C(7)-H(15)	0.94(4)
C(7)-H(16)	0.95(3)
C(7)-H(17)	0.95(3)
C(12)-C(13)	1.496(3)
C(12)-H(8)	0.96(3)
C(12)-H(7)	1.05(3)
C(9)-C(8)	1.462(3)
C(8)-C(13)	1.497(3)
C(4)-C(3)	1.368(3)
C(4)-C(5)	1.392(3)
C(4)-H(13)	0.93(2)
C(5)-C(6)	1.358(3)
C(1)-C(6)	1.389(3)
C(1)-C(2)	1.398(3)
C(2)-C(3)	1.389(3)
C(3)-H(12)	0.92(2)

C(6)-H(14)	0.92(2)
N(2)-N(1)-C(2)	120.21(18)
N(2)-N(1)-H(11)	118.8(15)
C(2)-N(1)-H(11)	121.0(15)
C(8)-N(2)-N(1)	118.78(17)
O(4)-N(3)-O(3)	122.26(19)
O(4)-N(3)-C(1)	118.63(18)
O(3)-N(3)-C(1)	119.11(17)
C(11)-C(15)-H(3)	112.2(15)
C(11)-C(15)-H(1)	113.0(15)
H(3)-C(15)-H(1)	101(2)
C(11)-C(15)-H(2)	111.0(15)
H(3)-C(15)-H(2)	109(2)
H(1)-C(15)-H(2)	110(2)
C(12)-C(11)-C(14)	111.0(2)
C(12)-C(11)-C(15)	109.47(19)
C(14)-C(11)-C(15)	109.3(2)
C(12)-C(11)-C(10)	107.47(18)
C(14)-C(11)-C(10)	110.1(2)
C(15)-C(11)-C(10)	109.3(2)
C(11)-C(14)-H(4)	110.0(15)
C(11)-C(14)-H(5)	110.0(15)
H(4)-C(14)-H(5)	110(2)
C(11)-C(14)-H(6)	111.8(14)
H(4)-C(14)-H(6)	112(2)
H(5)-C(14)-H(6)	103(2)
C(9)-C(10)-C(11)	114.09(18)
C(9)-C(10)-H(10)	108.5(13)
C(11)-C(10)-H(10)	113.7(13)
C(9)-C(10)-H(9)	105.2(13)
C(11)-C(10)-H(9)	109.3(14)
H(10)-C(10)-H(9)	105.4(19)
C(5)-C(7)-H(15)	110(2)
C(5)-C(7)-H(16)	111.6(17)
H(15)-C(7)-H(16)	101(3)
C(5)-C(7)-H(17)	113.8(18)
H(15)-C(7)-H(17)	100(3)
H(16)-C(7)-H(17)	119(3)
C(13)-C(12)-C(11)	116.67(19)
C(13)-C(12)-H(8)	107.5(14)
C(11)-C(12)-H(8)	110.8(15)

C(13)-C(12)-H(7)	104.6(13)
C(11)-C(12)-H(7)	109.6(13)
H(8)-C(12)-H(7)	107(2)
O(1)-C(9)-C(8)	120.5(2)
O(1)-C(9)-C(10)	121.1(2)
C(8)-C(9)-C(10)	118.33(19)
N(2)-C(8)-C(9)	125.02(18)
N(2)-C(8)-C(13)	115.51(17)
C(9)-C(8)-C(13)	119.46(18)
C(3)-C(4)-C(5)	122.5(2)
C(3)-C(4)-H(13)	119.9(14)
C(5)-C(4)-H(13)	117.6(14)
C(6)-C(5)-C(4)	117.1(2)
C(6)-C(5)-C(7)	121.6(2)
C(4)-C(5)-C(7)	121.2(2)
O(2)-C(13)-C(8)	121.22(19)
O(2)-C(13)-C(12)	120.9(2)
C(8)-C(13)-C(12)	117.85(18)
C(6)-C(1)-C(2)	121.9(2)
C(6)-C(1)-N(3)	116.34(19)
C(2)-C(1)-N(3)	121.77(18)
N(1)-C(2)-C(3)	120.4(2)
N(1)-C(2)-C(1)	123.30(18)
C(3)-C(2)-C(1)	116.24(19)
C(4)-C(3)-C(2)	121.0(2)
C(4)-C(3)-H(12)	121.7(13)
C(2)-C(3)-H(12)	117.3(13)
C(5)-C(6)-C(1)	121.2(2)
C(5)-C(6)-H(14)	122.3(12)
C(1)-C(6)-H(14)	116.4(12)

Table 5. Torsion angles [deg] for CD2

C(2)-N(1)-N(2)-C(8)	179.06(16)
C(12)-C(11)-C(10)-C(9)	57.4(3)
C(14)-C(11)-C(10)-C(9)	-63.7(3)
C(15)-C(11)-C(10)-C(9)	176.1(2)
C(14)-C(11)-C(12)-C(13)	69.5(3)
C(15)-C(11)-C(12)-C(13)	-169.7(2)
C(10)-C(11)-C(12)-C(13)	-51.1(3)
C(11)-C(10)-C(9)-O(1)	146.2(2)
C(11)-C(10)-C(9)-C(8)	-34.9(3)
N(1)-N(2)-C(8)-C(9)	-0.3(3)
N(1)-N(2)-C(8)-C(13)	178.49(17)
O(1)-C(9)-C(8)-N(2)	0.5(3)
C(10)-C(9)-C(8)-N(2)	-178.49(19)
O(1)-C(9)-C(8)-C(13)	-178.3(2)
C(10)-C(9)-C(8)-C(13)	2.7(3)
C(3)-C(4)-C(5)-C(6)	0.6(3)
C(3)-C(4)-C(5)-C(7)	-179.7(2)
N(2)-C(8)-C(13)-O(2)	6.7(3)
C(9)-C(8)-C(13)-O(2)	-174.43(18)
N(2)-C(8)-C(13)-C(12)	-174.81(19)
C(9)-C(8)-C(13)-C(12)	4.1(3)
C(11)-C(12)-C(13)-O(2)	-159.7(2)
C(11)-C(12)-C(13)-C(8)	21.8(3)
O(4)-N(3)-C(1)-C(6)	-7.8(3)
O(3)-N(3)-C(1)-C(6)	172.82(18)
O(4)-N(3)-C(1)-C(2)	172.46(18)
O(3)-N(3)-C(1)-C(2)	-6.9(3)
N(2)-N(1)-C(2)-C(3)	-1.1(3)
N(2)-N(1)-C(2)-C(1)	-179.81(18)
C(6)-C(1)-C(2)-N(1)	179.62(17)
N(3)-C(1)-C(2)-N(1)	-0.7(3)
C(6)-C(1)-C(2)-C(3)	0.8(3)
N(3)-C(1)-C(2)-C(3)	-179.46(16)
C(5)-C(4)-C(3)-C(2)	0.1(3)
N(1)-C(2)-C(3)-C(4)	-179.63(18)
C(1)-C(2)-C(3)-C(4)	-0.8(3)

C(4)-C(5)-C(6)-C(1)	-0.6(3)
C(7)-C(5)-C(6)-C(1)	179.7(2)
C(2)-C(1)-C(6)-C(5)	-0.1(3)
N(3)-C(1)-C(6)-C(5)	-179.88(18)