Supplementary Information for

The Synthesis and Characterisation of Several Corroles

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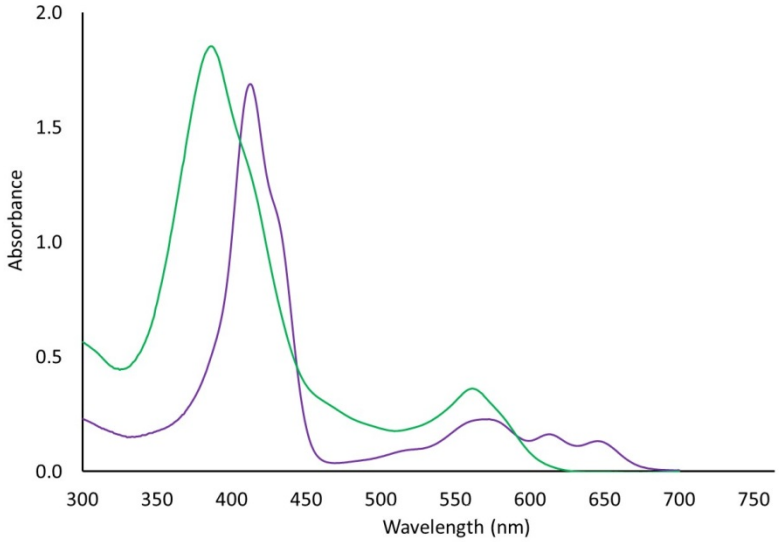

Figure S1. UV-vis spectrum of TPCrl (purple) amdCoTPCrl (green) in dichloromethane

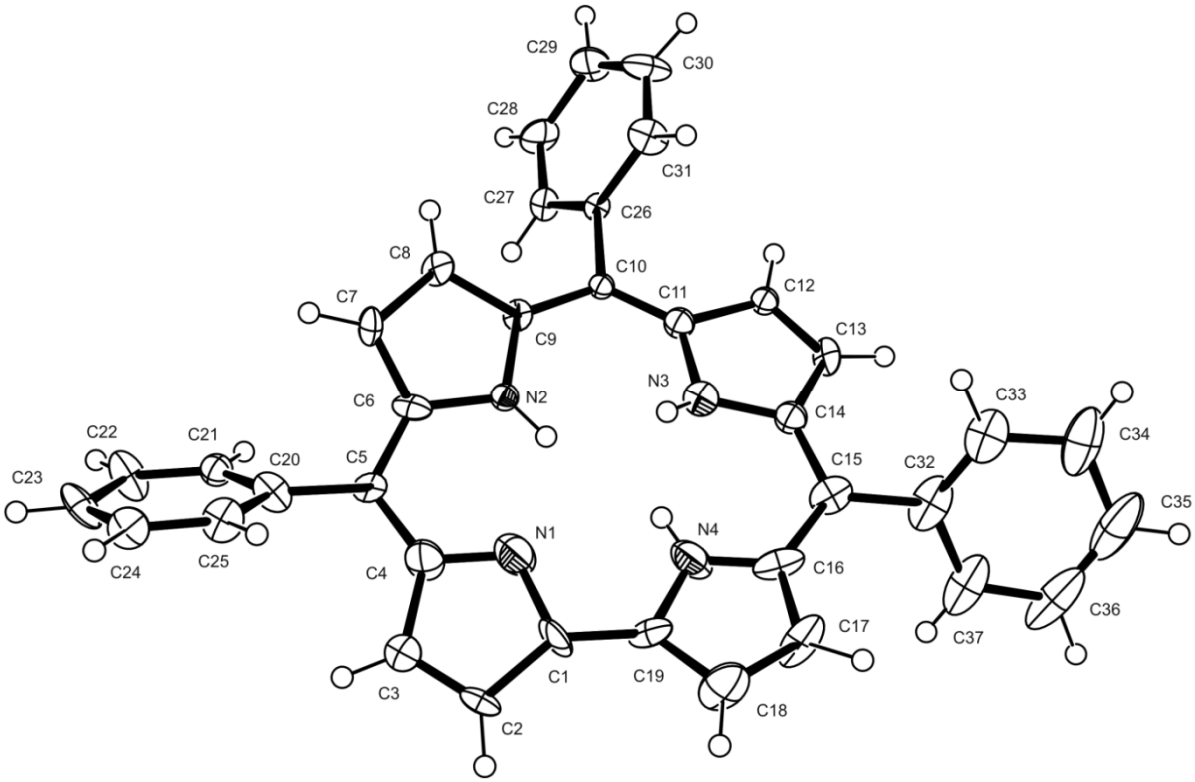

Figure S2. ORTEP diagram (50% probability contour level) of TPCrl.

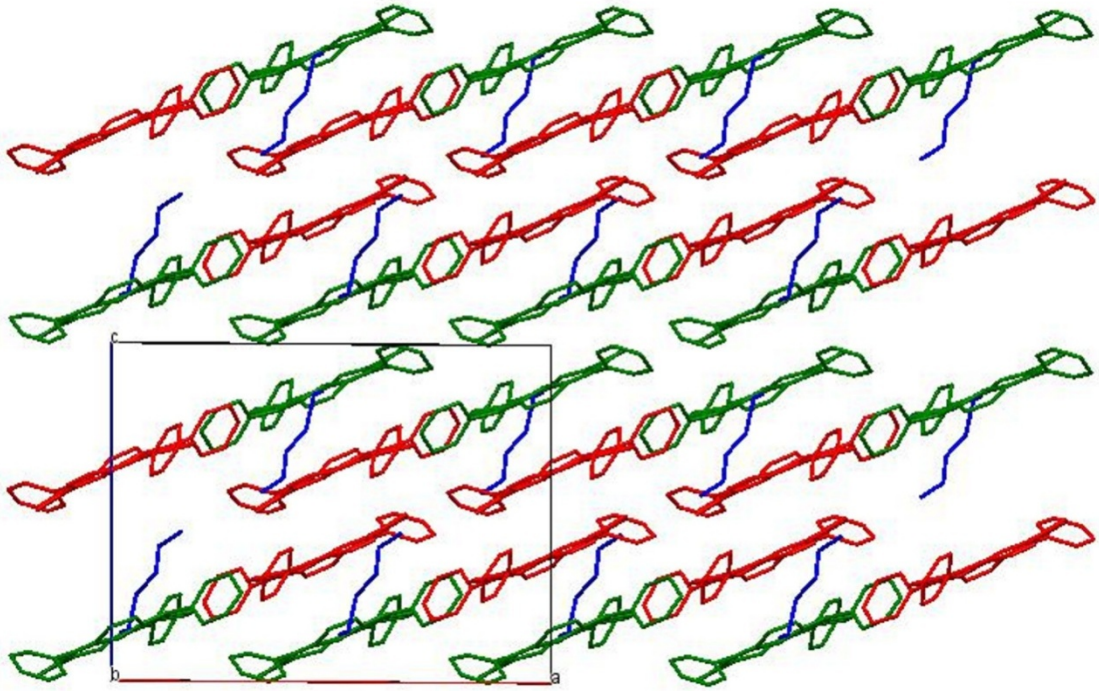

Figure S3 View down the crystallographic *b* axis of the packing in TPCrl.hexane. Nearest corrole neighbours are coloured green and red, respectively. Ordered hexane solvate in blue. Hydrogen atoms omitted for clarity.

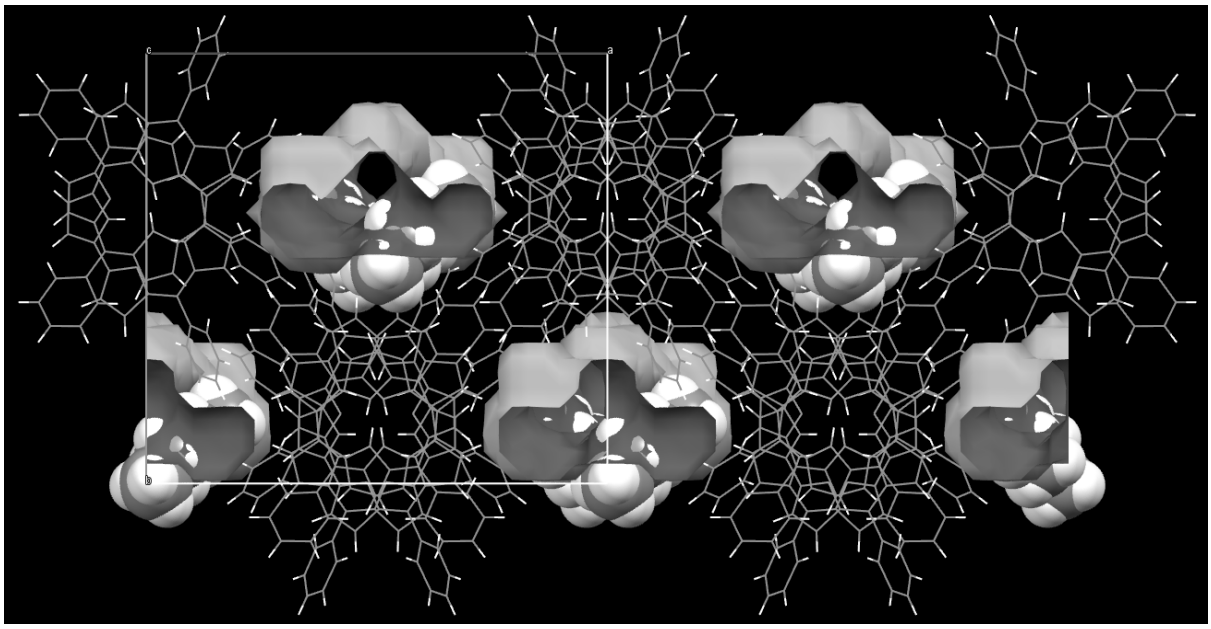

Figure S4. Projection down the *c* axis showing the hexane solvent channels filled with disordered and possibly partially present hexane in the structure of TPCrl. These are surrounded by the ordered hexane molecules shown using a space fill (CPK) representation, as well as the corrole molecules which are shown as wire frames.

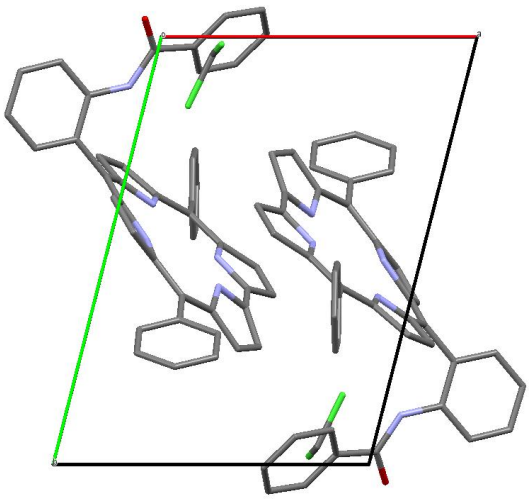

Figure S5. The unit cell, viewed down the crystallographic *c* axis, of DPAPCrl. Hydrogen atoms omitted for clarity.

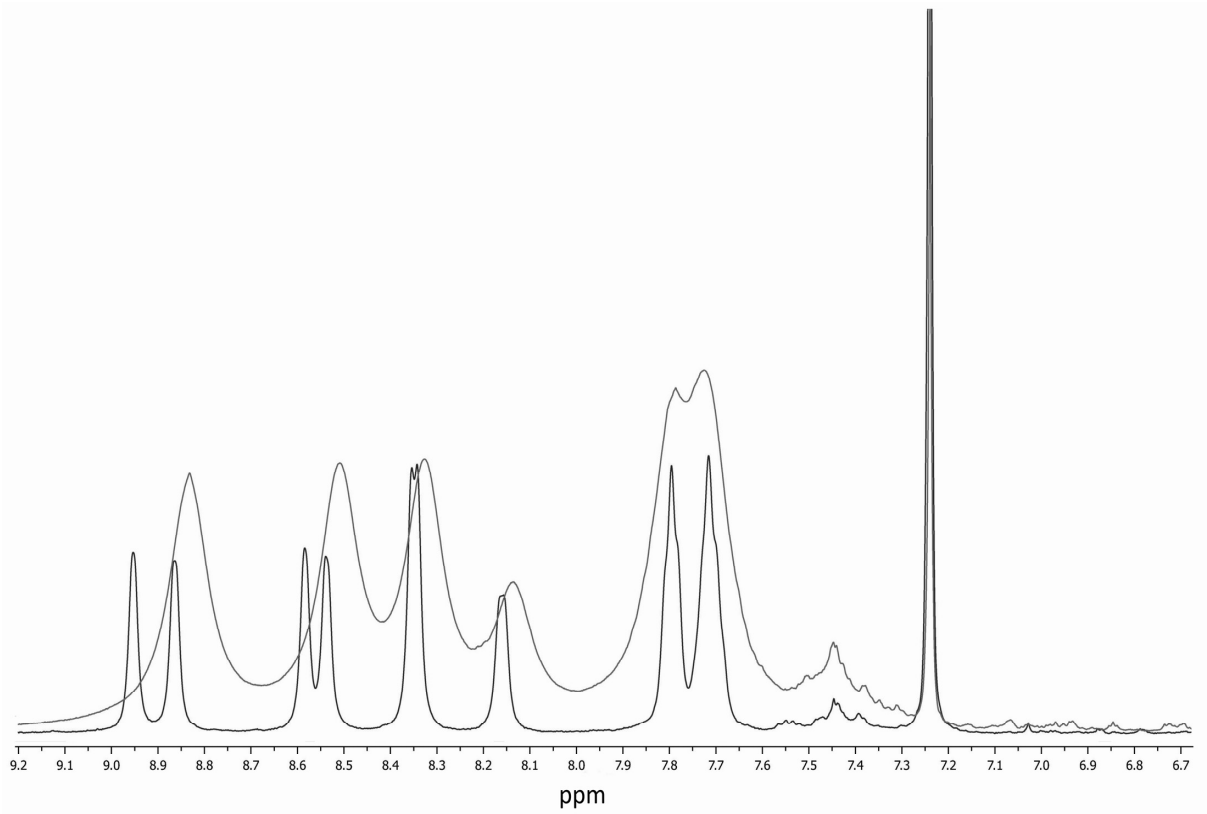

Fig S6. Part of the ^{1}H NMR spectrum of DPAPCrl and higher (5 mg ml^{-1}, blue) and lower (1 mg ml^{-1}, red) concentrations. Line broadening is attributed to aggregation in solution.

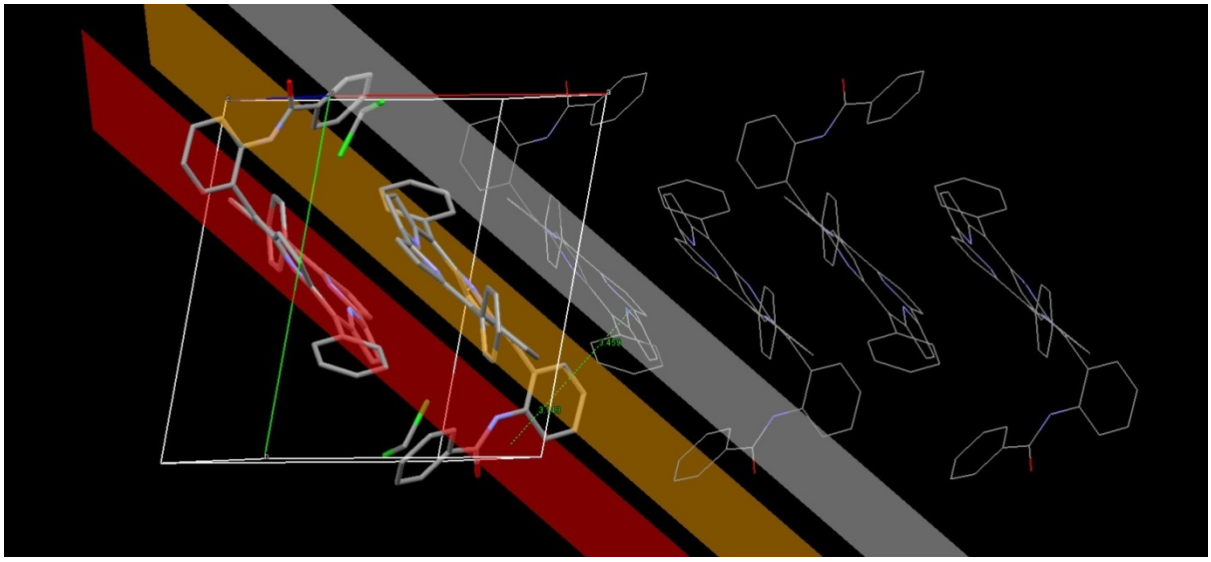

Figure S7. The mean planes (red, gold) through the corrin N atoms of DPAPCrl are parallel to each other at a distance of 3.14 Å. The planes are themselves parallel to the first plane of a neighbouring pair of molecules (grey) at a distance of 3.46 Å. Thus, the corroles stack along the *a* axis. Translation of these stacks along the *b* and *c* axis results in a layered structure.

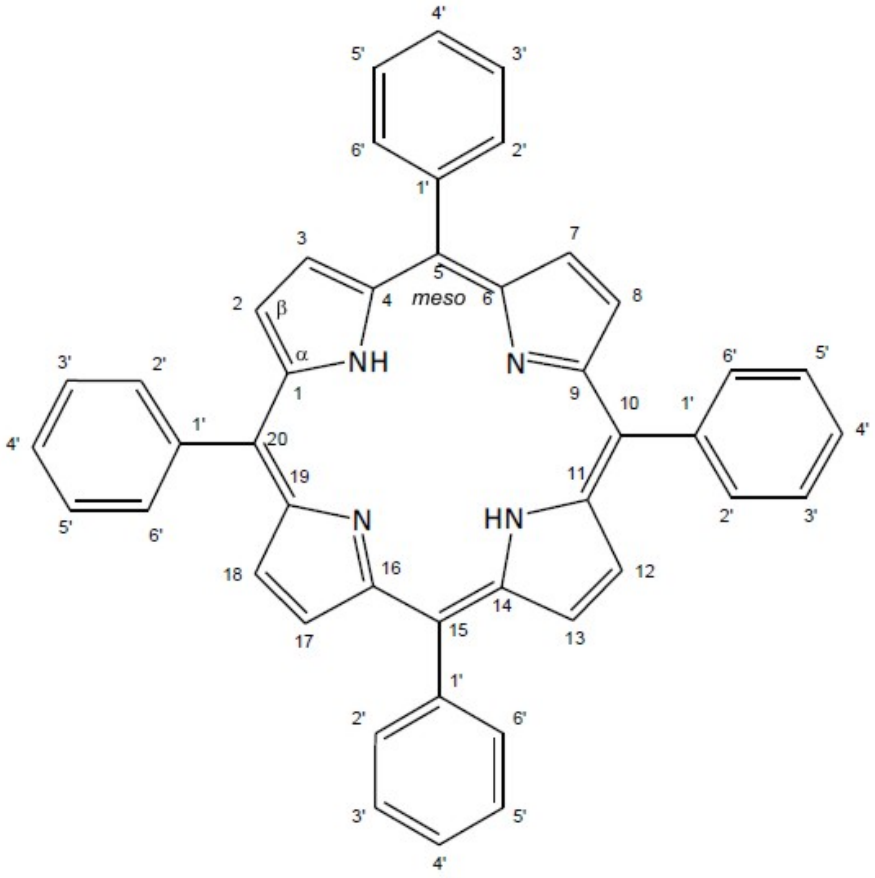

Figure S8. The standard numbering scheme of porphyrins

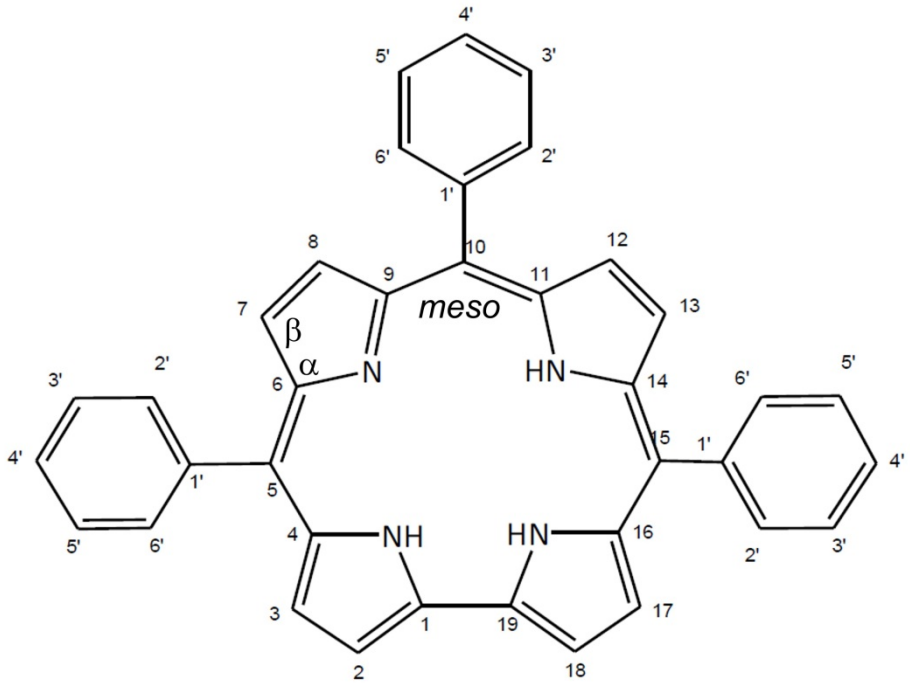

Figure S9. The standard numbering scheme of corroles

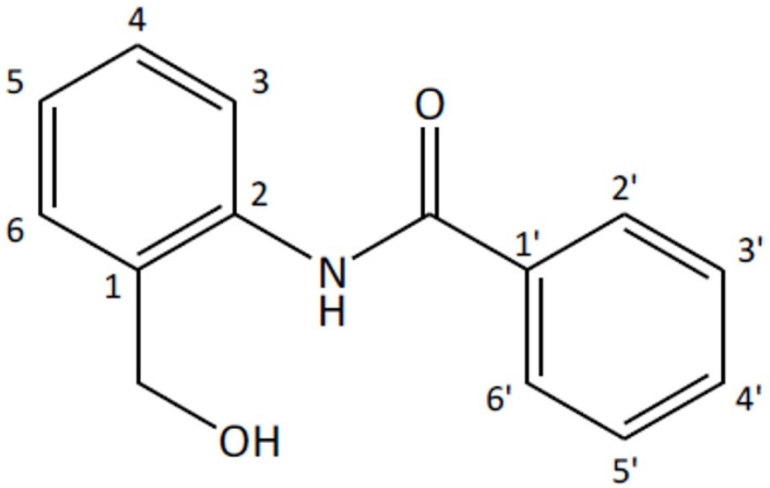

Figure S10. Numbering scheme for *N*-[2-(hydroxymethyl)phenyl]benzamide

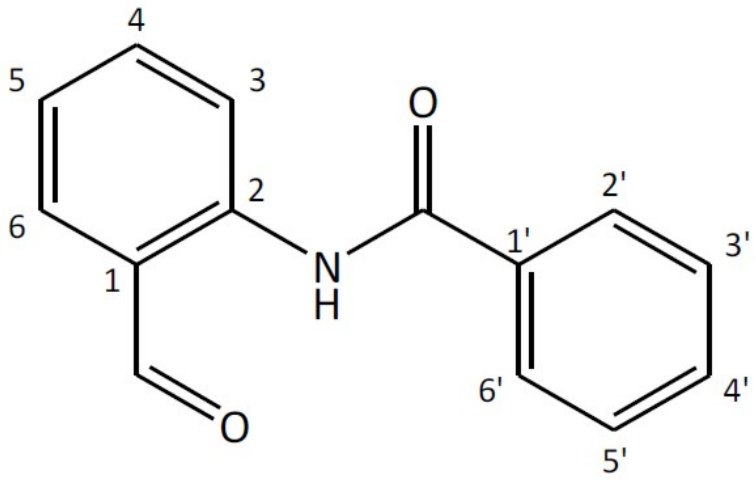

Figure S11. Numbering scheme for *N*-(2-formylphenyl)benzamide

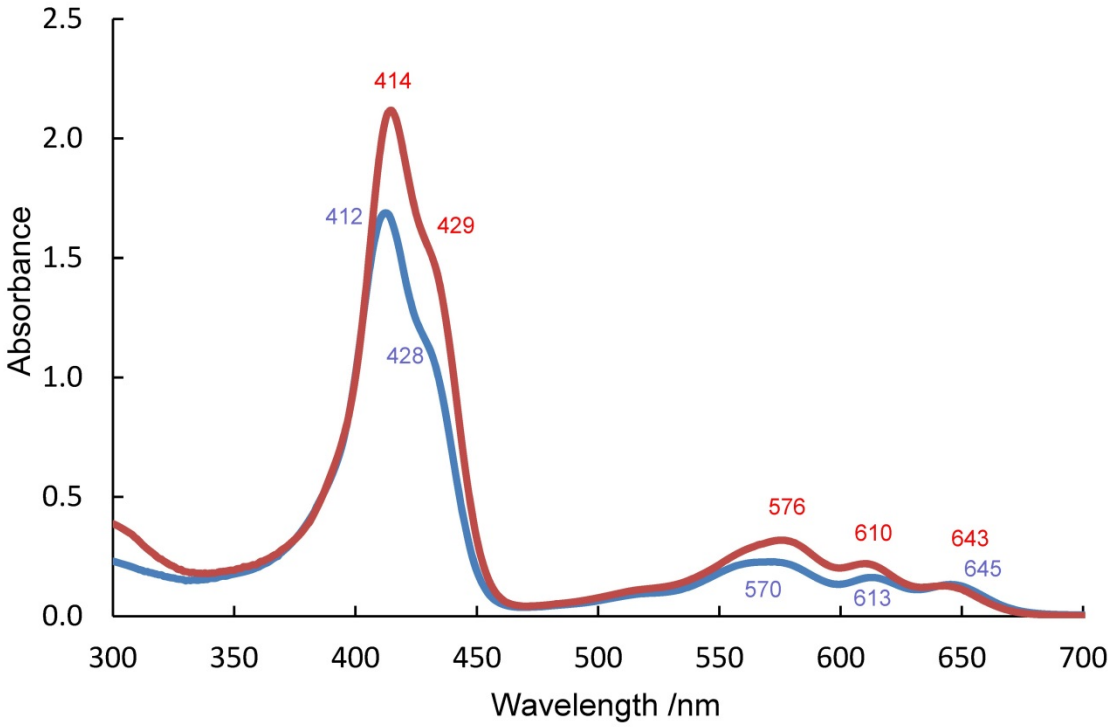

Figure S12. The UV-vis spectra of (blue) TPCrl and (red) DPAPCrl in methanol at 25 ^{o}C. The concentrations of the corrole in the two sample are only approximately equal.

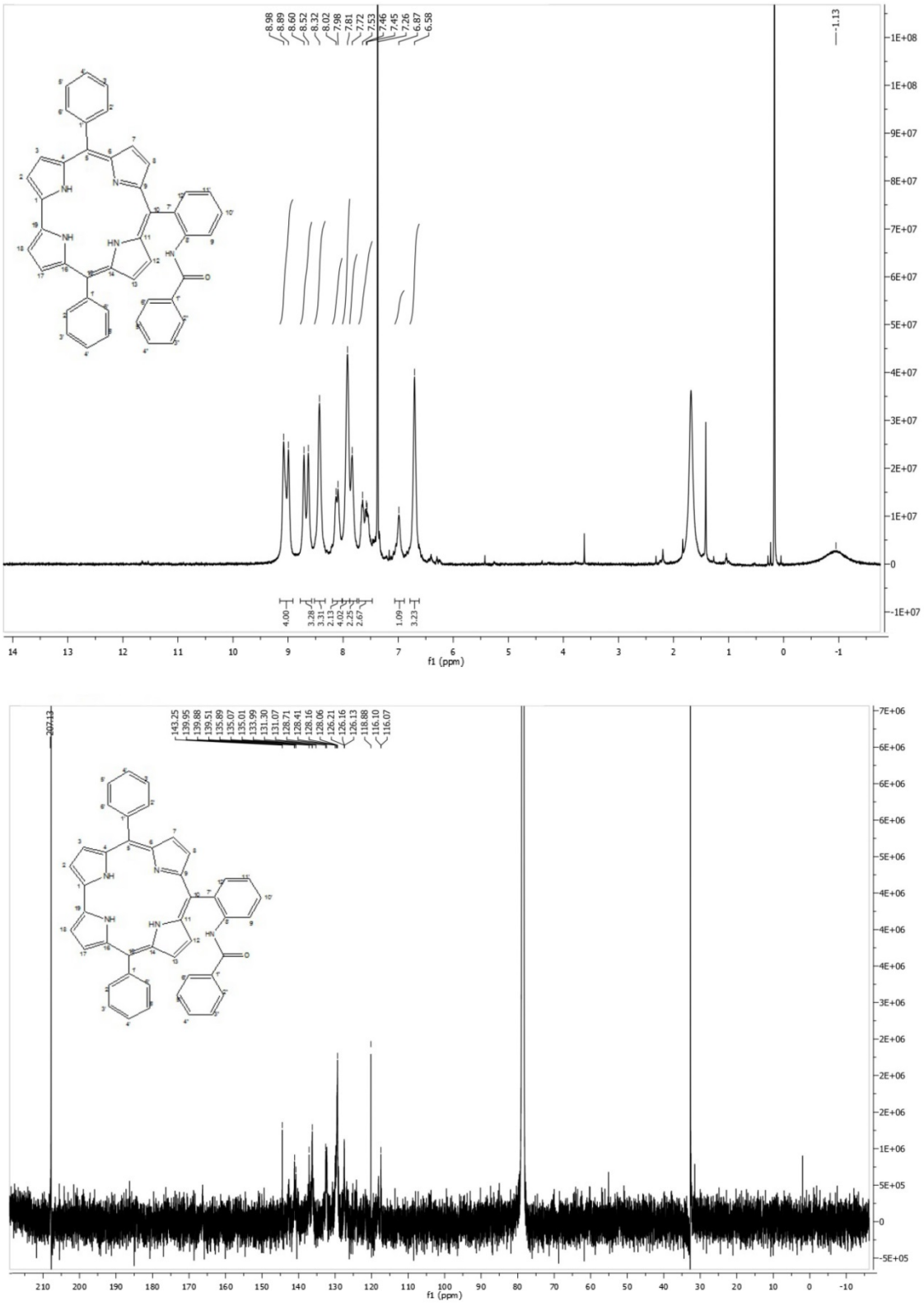

Figure S13. ^{1}H and ^{13}C NMR of DPAPCrl (1 mg ml^{-1})

Table S1. Bond lengths [Å] and angles [°] TPCrl

C(1)-C(19)	1.386(11)
C(1)-N(1)	1.413(11)
C(1)-C(2)	1.449(10)
C(2)-C(3)	1.344(10)
C(2)-H(2)	0.9500
C(3)-C(4)	1.443(10)
C(3)-H(3)	0.9500
C(4)-N(1)	1.332(11)
C(4)-C(5)	1.417(10)
C(5)-C(20)	1.445(10)
C(5)-C(6)	1.446(10)
C(6)-C(7)	1.412(10)
C(6)-N(2)	1.416(9)
C(7)-C(8)	1.418(9)
C(7)-H(7)	0.9500
C(8)-C(9)	1.409(10)
C(8)-H(8)	0.9500
C(9)-N(2)	1.376(8)
C(9)-C(10)	1.456(9)
C(10)-C(11)	1.338(9)
C(10)-C(26)	1.477(9)
C(11)-N(3)	1.451(9)
C(11)-C(12)	1.485(10)
C(12)-C(13)	1.336(10)
C(12)-H(12)	0.9500
C(13)-C(14)	1.432(10)
C(13)-H(13)	0.9500
C(14)-N(3)	1.395(10)
C(14)-C(15)	1.419(10)
C(15)-C(16)	1.421(11)
C(15)-C(32)	1.491(12)
C(16)-N(4)	1.290(10)
C(16)-C(17)	1.397(10)
C(17)-C(18)	1.334(12)
C(17)-H(17)	0.9500

C(18)-C(19)	1.401(12)
C(18)-H(18)	0.9500
C(19)-N(4)	1.385(9)
C(20)-C(25)	1.430(9)
C(20)-C(21)	1.462(11)
C(21)-C(22)	1.318(10)
C(21)-H(21)	0.9500
C(22)-C(23)	1.396(10)
C(22)-H(22)	0.9500
C(23)-C(24)	1.358(12)
C(23)-H(23)	0.9500
C(24)-C(25)	1.351(11)
C(24)-H(24)	0.9500
C(25)-H(25)	0.9500
C(26)-C(31)	1.370(9)
C(26)-C(27)	1.376(9)
C(27)-C(28)	1.383(9)
C(27)-H(27)	0.9500
C(28)-C(29)	1.450(11)
C(28)-H(28)	0.9500
C(29)-C(30)	1.343(12)
C(29)-H(29)	0.9500
C(30)-C(31)	1.398(10)
C(30)-H(30)	0.9500
C(31)-H(31)	0.9500
C(32)-C(33)	1.315(12)
C(32)-C(37)	1.414(12)
C(33)-C(34)	1.426(12)
C(33)-H(33)	0.9500
C(34)-C(35)	1.444(15)
C(34)-H(34)	0.9500
C(35)-C(36)	1.443(17)
C(35)-H(35)	0.9500
C(36)-C(37)	1.360(12)
C(36)-H(36)	0.9500
C(37)-H(37)	0.9500
N(2)-H(2A)	0.8800
N(3)-H(3A)	0.8008

N(4)-H(4A)	0.8005
C(1')-N(1')	1.315(11)
C(1')-C(2')	1.380(15)
C(1')-C(19')	1.450(14)
C(2')-C(3')	1.416(15)
C(2')-H(2')	0.9500
C(3')-C(4')	1.382(16)
C(3')-H(3')	0.9500
C(4')-C(5')	1.406(14)
C(4')-N(1')	1.424(12)
C(5')-C(6')	1.348(15)
C(5')-C(20')	1.506(14)
C(6')-N(2')	1.384(13)
C(6')-C(7')	1.485(15)
C(7')-C(8')	1.299(14)
C(7')-H(7')	0.9500
C(8')-C(9')	1.461(15)
C(8')-H(8')	0.9500
C(9')-C(10')	1.288(17)
C(9')-N(2')	1.414(16)
C(10')-C(11')	1.483(14)
C(10')-C(26')	1.59(2)
C(11')-N(3')	1.288(13)
C(11')-C(12')	1.349(15)
C(12')-C(13')	1.379(14)
C(12')-H(12')	0.9500
C(13')-C(14')	1.370(15)
C(13')-H(13')	0.9500
C(14')-N(3')	1.379(13)
C(14')-C(15')	1.429(15)
C(15')-C(16')	1.405(13)
C(15')-C(32')	1.469(12)
C(16')-N(4')	1.410(10)
C(16')-C(17')	1.474(14)
C(17')-C(18')	1.420(14)
C(17')-H(17')	0.9500
C(18')-C(19')	1.344(14)
C(18')-H(18')	0.9500

C(19')-N(4')	1.322(12)
C(20')-C(25')	1.298(14)
C(20')-C(21')	1.332(15)
C(21')-C(22')	1.414(14)
C(21')-H(21')	0.9500
C(22')-C(23')	1.361(17)
C(22')-H(22')	0.9500
C(23')-C(24')	1.399(19)
C(23')-H(23')	0.9500
C(24')-C(25')	1.493(17)
C(24')-H(24')	0.9500
C(25')-H(25')	0.9500
C(26')-C(31')	1.44(2)
C(26')-C(27')	1.446(16)
C(27')-C(28')	1.376(15)
C(27')-H(27')	0.9500
C(28')-C(29')	1.39(2)
C(28')-H(28')	0.9500
C(29')-C(30')	1.26(2)
C(29')-H(29')	0.9500
C(30')-C(31')	1.41(2)
C(30')-H(30')	0.9500
C(31')-H(31')	0.9500
C(32')-C(37')	1.375(13)
C(32')-C(33')	1.440(11)
C(33')-C(34')	1.341(12)
C(33')-H(33')	0.9500
C(34')-C(35')	1.290(13)
C(34')-H(34')	0.9500
C(35')-C(36')	1.392(14)
C(35')-H(35')	0.9500
C(36')-C(37')	1.448(15)
C(36')-H(36')	0.9500
C(37')-H(37')	0.9500
N(1')-H(1B')	0.8800
N(2')-H(2B')	0.8004
N(3')-H(3B')	0.8001
C(38)-C(39)	1.518(5)

C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-C(40)	1.515(5)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(40)-C(41)	1.516(5)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-C(42)	1.523(5)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-C(43)	1.511(5)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800

C(19)-C(1)-N(1)	113.3(6)
C(19)-C(1)-C(2)	140.8(8)
N(1)-C(1)-C(2)	105.9(7)
C(3)-C(2)-C(1)	106.4(7)
C(3)-C(2)-H(2)	126.8
C(1)-C(2)-H(2)	126.8
C(2)-C(3)-C(4)	110.5(7)
C(2)-C(3)-H(3)	124.8
C(4)-C(3)-H(3)	124.8
N(1)-C(4)-C(5)	121.8(7)
N(1)-C(4)-C(3)	106.1(7)
C(5)-C(4)-C(3)	131.7(8)
C(4)-C(5)-C(20)	120.5(6)
C(4)-C(5)-C(6)	118.9(7)
C(20)-C(5)-C(6)	120.3(7)
C(7)-C(6)-N(2)	108.5(5)
C(7)-C(6)-C(5)	126.6(7)
N(2)-C(6)-C(5)	124.6(7)
C(6)-C(7)-C(8)	106.7(6)

C(6)-C(7)-H(7)	126.6
C(8)-C(7)-H(7)	126.6
C(9)-C(8)-C(7)	107.7(7)
C(9)-C(8)-H(8)	126.2
C(7)-C(8)-H(8)	126.2
N(2)-C(9)-C(8)	109.3(6)
N(2)-C(9)-C(10)	122.9(6)
C(8)-C(9)-C(10)	127.9(6)
C(11)-C(10)-C(9)	126.8(6)
C(11)-C(10)-C(26)	118.8(6)
C(9)-C(10)-C(26)	114.3(6)
C(10)-C(11)-N(3)	127.8(7)
C(10)-C(11)-C(12)	130.9(7)
N(3)-C(11)-C(12)	101.3(6)
C(13)-C(12)-C(11)	112.0(6)
C(13)-C(12)-H(12)	124.0
C(11)-C(12)-H(12)	124.0
C(12)-C(13)-C(14)	108.3(6)
C(12)-C(13)-H(13)	125.9
C(14)-C(13)-H(13)	125.9
N(3)-C(14)-C(15)	123.0(6)
N(3)-C(14)-C(13)	107.4(6)
C(15)-C(14)-C(13)	129.0(7)
C(14)-C(15)-C(16)	121.2(7)
C(14)-C(15)-C(32)	117.9(7)
C(16)-C(15)-C(32)	120.9(7)
N(4)-C(16)-C(17)	106.2(7)
N(4)-C(16)-C(15)	120.7(7)
C(17)-C(16)-C(15)	132.9(8)
C(18)-C(17)-C(16)	109.5(8)
C(18)-C(17)-H(17)	125.2
C(16)-C(17)-H(17)	125.2
C(17)-C(18)-C(19)	107.3(8)
C(17)-C(18)-H(18)	126.3
C(19)-C(18)-H(18)	126.3
C(1)-C(19)-N(4)	117.9(7)
C(1)-C(19)-C(18)	137.5(7)
N(4)-C(19)-C(18)	104.6(7)

C(25)-C(20)-C(5)	123.1(7)
C(25)-C(20)-C(21)	115.4(7)
C(5)-C(20)-C(21)	121.4(6)
C(22)-C(21)-C(20)	120.9(7)
C(22)-C(21)-H(21)	119.6
C(20)-C(21)-H(21)	119.6
C(21)-C(22)-C(23)	121.1(8)
C(21)-C(22)-H(22)	119.4
C(23)-C(22)-H(22)	119.4
C(24)-C(23)-C(22)	120.4(7)
C(24)-C(23)-H(23)	119.8
C(22)-C(23)-H(23)	119.8
C(25)-C(24)-C(23)	120.8(7)
C(25)-C(24)-H(24)	119.6
C(23)-C(24)-H(24)	119.6
C(24)-C(25)-C(20)	121.3(7)
C(24)-C(25)-H(25)	119.4
C(20)-C(25)-H(25)	119.4
C(31)-C(26)-C(27)	118.5(6)
C(31)-C(26)-C(10)	121.6(6)
C(27)-C(26)-C(10)	119.9(6)
C(26)-C(27)-C(28)	122.9(7)
C(26)-C(27)-H(27)	118.5
C(28)-C(27)-H(27)	118.5
C(27)-C(28)-C(29)	117.4(7)
C(27)-C(28)-H(28)	121.3
C(29)-C(28)-H(28)	121.3
C(30)-C(29)-C(28)	118.4(7)
C(30)-C(29)-H(29)	120.8
C(28)-C(29)-H(29)	120.8
C(29)-C(30)-C(31)	122.1(7)
C(29)-C(30)-H(30)	119.0
C(31)-C(30)-H(30)	119.0
C(26)-C(31)-C(30)	120.1(7)
C(26)-C(31)-H(31)	119.9
C(30)-C(31)-H(31)	119.9
C(33)-C(32)-C(37)	118.1(9)
C(33)-C(32)-C(15)	123.6(8)

C(37)-C(32)-C(15)	118.2(8)
C(32)-C(33)-C(34)	125.2(10)
C(32)-C(33)-H(33)	117.4
C(34)-C(33)-H(33)	117.4
C(33)-C(34)-C(35)	115.7(10)
C(33)-C(34)-H(34)	122.1
C(35)-C(34)-H(34)	122.1
C(36)-C(35)-C(34)	119.4(10)
C(36)-C(35)-H(35)	120.3
C(34)-C(35)-H(35)	120.3
C(37)-C(36)-C(35)	118.6(10)
C(37)-C(36)-H(36)	120.7
C(35)-C(36)-H(36)	120.7
C(36)-C(37)-C(32)	122.9(11)
C(36)-C(37)-H(37)	118.5
C(32)-C(37)-H(37)	118.5
C(4)-N(1)-C(1)	110.8(7)
C(9)-N(2)-C(6)	107.5(6)
C(9)-N(2)-H(2A)	126.2
C(6)-N(2)-H(2A)	126.2
C(14)-N(3)-C(11)	110.8(6)
C(14)-N(3)-H(3A)	128.0
C(11)-N(3)-H(3A)	117.2
C(16)-N(4)-C(19)	112.2(7)
C(16)-N(4)-H(4A)	127.3
C(19)-N(4)-H(4A)	119.2
N(1')-C(1')-C(2')	108.0(10)
N(1')-C(1')-C(19')	115.8(9)
C(2')-C(1')-C(19')	136.2(11)
C(1')-C(2')-C(3')	108.9(12)
C(1')-C(2')-H(2')	125.5
C(3')-C(2')-H(2')	125.5
C(4')-C(3')-C(2')	105.6(12)
C(4')-C(3')-H(3')	127.2
C(2')-C(3')-H(3')	127.2
C(3')-C(4')-C(5')	136.1(11)
C(3')-C(4')-N(1')	106.8(10)
C(5')-C(4')-N(1')	117.1(9)

C(6')-C(5')-C(4')	124.8(10)
C(6')-C(5')-C(20')	118.0(10)
C(4')-C(5')-C(20')	117.0(10)
C(5')-C(6')-N(2')	125.7(10)
C(5')-C(6')-C(7')	133.2(10)
N(2')-C(6')-C(7')	100.8(10)
C(8')-C(7')-C(6')	110.7(11)
C(8')-C(7')-H(7')	124.7
C(6')-C(7')-H(7')	124.7
C(7')-C(8')-C(9')	112.1(13)
C(7')-C(8')-H(8')	124.0
C(9')-C(8')-H(8')	124.0
C(10')-C(9')-N(2')	130.8(12)
C(10')-C(9')-C(8')	128.2(13)
N(2')-C(9')-C(8')	100.4(12)
C(9')-C(10')-C(11')	129.3(13)
C(9')-C(10')-C(26')	117.8(12)
C(11')-C(10')-C(26')	111.4(11)
N(3')-C(11')-C(12')	108.6(11)
N(3')-C(11')-C(10')	123.5(12)
C(12')-C(11')-C(10')	127.9(13)
C(11')-C(12')-C(13')	106.1(11)
C(11')-C(12')-H(12')	126.9
C(13')-C(12')-H(12')	126.9
C(14')-C(13')-C(12')	109.8(11)
C(14')-C(13')-H(13')	125.1
C(12')-C(13')-H(13')	125.1
C(13')-C(14')-N(3')	102.6(10)
C(13')-C(14')-C(15')	131.3(10)
N(3')-C(14')-C(15')	126.2(10)
C(16')-C(15')-C(14')	121.7(9)
C(16')-C(15')-C(32')	119.3(9)
C(14')-C(15')-C(32')	118.7(9)
C(15')-C(16')-N(4')	121.9(9)
C(15')-C(16')-C(17')	132.4(8)
N(4')-C(16')-C(17')	105.6(8)
C(18')-C(17')-C(16')	103.7(9)
C(18')-C(17')-H(17')	128.2

C(16')-C(17')-H(17')	128.2
C(19')-C(18')-C(17')	109.9(11)
C(19')-C(18')-H(18')	125.0
C(17')-C(18')-H(18')	125.0
N(4')-C(19')-C(18')	110.6(10)
N(4')-C(19')-C(1')	112.1(9)
C(18')-C(19')-C(1')	135.4(10)
C(25')-C(20')-C(21')	119.5(11)
C(25')-C(20')-C(5')	122.7(10)
C(21')-C(20')-C(5')	117.6(11)
C(20')-C(21')-C(22')	121.4(12)
C(20')-C(21')-H(21')	119.3
C(22')-C(21')-H(21')	119.3
C(23')-C(22')-C(21')	120.9(13)
C(23')-C(22')-H(22')	119.6
C(21')-C(22')-H(22')	119.6
C(22')-C(23')-C(24')	119.4(13)
C(22')-C(23')-H(23')	120.3
C(24')-C(23')-H(23')	120.3
C(23')-C(24')-C(25')	115.3(13)
C(23')-C(24')-H(24')	122.3
C(25')-C(24')-H(24')	122.3
C(20')-C(25')-C(24')	123.2(13)
C(20')-C(25')-H(25')	118.4
C(24')-C(25')-H(25')	118.4
C(31')-C(26')-C(27')	115.2(14)
C(31')-C(26')-C(10')	124.9(13)
C(27')-C(26')-C(10')	119.4(13)
C(28')-C(27')-C(26')	120.4(12)
C(28')-C(27')-H(27')	119.8
C(26')-C(27')-H(27')	119.8
C(27')-C(28')-C(29')	121.4(14)
C(27')-C(28')-H(28')	119.3
C(29')-C(28')-H(28')	119.3
C(30')-C(29')-C(28')	117.8(19)
C(30')-C(29')-H(29')	121.1
C(28')-C(29')-H(29')	121.1
C(29')-C(30')-C(31')	126.6(18)

C(29')-C(30')-H(30')	116.7
C(31')-C(30')-H(30')	116.7
C(30')-C(31')-C(26')	117.4(14)
C(30')-C(31')-H(31')	121.3
C(26')-C(31')-H(31')	121.3
C(37')-C(32')-C(33')	119.1(9)
C(37')-C(32')-C(15')	120.1(8)
C(33')-C(32')-C(15')	120.8(8)
C(34')-C(33')-C(32')	119.0(9)
C(34')-C(33')-H(33')	120.5
C(32')-C(33')-H(33')	120.5
C(35')-C(34')-C(33')	124.9(9)
C(35')-C(34')-H(34')	117.5
C(33')-C(34')-H(34')	117.5
C(34')-C(35')-C(36')	119.2(10)
C(34')-C(35')-H(35')	120.4
C(36')-C(35')-H(35')	120.4
C(35')-C(36')-C(37')	120.5(10)
C(35')-C(36')-H(36')	119.7
C(37')-C(36')-H(36')	119.7
C(32')-C(37')-C(36')	117.3(9)
C(32')-C(37')-H(37')	121.4
C(36')-C(37')-H(37')	121.4
C(1')-N(1')-C(4')	110.0(8)
C(1')-N(1')-H(1B')	125.0
C(4')-N(1')-H(1B')	125.0
C(6')-N(2')-C(9')	116.0(10)
C(6')-N(2')-H(2B')	137.5
C(9')-N(2')-H(2B')	105.2
C(11')-N(3')-C(14')	112.7(10)
C(11')-N(3')-H(3B')	128.1
C(14')-N(3')-H(3B')	110.8
C(19')-N(4')-C(16')	109.9(9)
C(39)-C(38)-H(38A)	109.5
C(39)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(39)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5

H(38B)-C(38)-H(38C)	109.5
C(40)-C(39)-C(38)	109.7(6)
C(40)-C(39)-H(39A)	109.7
C(38)-C(39)-H(39A)	109.7
C(40)-C(39)-H(39B)	109.7
C(38)-C(39)-H(39B)	109.7
H(39A)-C(39)-H(39B)	108.2
C(39)-C(40)-C(41)	109.7(6)
C(39)-C(40)-H(40A)	109.7
C(41)-C(40)-H(40A)	109.7
C(39)-C(40)-H(40B)	109.7
C(41)-C(40)-H(40B)	109.7
H(40A)-C(40)-H(40B)	108.2
C(40)-C(41)-C(42)	109.4(6)
C(40)-C(41)-H(41A)	109.8
C(42)-C(41)-H(41A)	109.8
C(40)-C(41)-H(41B)	109.8
C(42)-C(41)-H(41B)	109.8
H(41A)-C(41)-H(41B)	108.2
C(43)-C(42)-C(41)	109.3(6)
C(43)-C(42)-H(42A)	109.8
C(41)-C(42)-H(42A)	109.8
C(43)-C(42)-H(42B)	109.8
C(41)-C(42)-H(42B)	109.8
H(42A)-C(42)-H(42B)	108.3
C(42)-C(43)-H(43A)	109.5
C(42)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(42)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5

Table S2. Bond lengths [Å] and angles [°] for DPAPCrl

C(1)-N(1)	1.360(3)
C(1)-C(2)	1.404(3)
C(1)-C(19)	1.427(3)
C(2)-C(3)	1.384(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.416(3)
C(3)-H(3)	0.9500
C(4)-N(1)	1.372(3)
C(4)-C(5)	1.415(3)
C(5)-C(6)	1.410(3)
C(5)-C(20)	1.481(3)
C(6)-N(2)	1.399(3)
C(6)-C(7)	1.417(3)
C(7)-C(8)	1.364(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.425(3)
C(8)-H(8)	0.9500
C(9)-N(2)	1.387(3)
C(9)-C(10)	1.400(3)
C(10)-C(11)	1.425(3)
C(10)-C(26)	1.493(3)
C(11)-N(3)	1.367(3)
C(11)-C(12)	1.438(3)
C(12)-C(13)	1.363(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.434(3)
C(13)-H(13)	0.9500
C(14)-N(3)	1.388(3)
C(14)-C(15)	1.411(3)
C(15)-C(16)	1.413(3)
C(15)-C(32)	1.489(3)
C(16)-N(4)	1.363(3)
C(16)-C(17)	1.429(3)
C(17)-C(18)	1.376(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.418(3)

C(18)-H(18)	0.9500
C(19)-N(4)	1.353(3)
C(20)-C(25)	1.398(3)
C(20)-C(21)	1.406(3)
C(21)-C(22)	1.390(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.390(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.388(4)
C(23)-H(23)	0.9500
C(24)-C(25)	1.389(3)
C(24)-H(24)	0.9500
C(25)-H(25)	0.9500
C(26)-C(27)	1.396(3)
C(26)-C(31)	1.412(3)
C(27)-C(28)	1.380(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.392(4)
C(28)-H(28)	0.9500
C(29)-C(30)	1.377(4)
C(29)-H(29)	0.9500
C(30)-C(31)	1.394(3)
C(30)-H(30)	0.9500
C(31)-N(5)	1.412(3)
C(32)-C(37)	1.397(3)
C(32)-C(33)	1.400(3)
C(33)-C(34)	1.391(3)
C(33)-H(33)	0.9500
C(34)-C(35)	1.384(3)
C(34)-H(34)	0.9500
C(35)-C(36)	1.386(4)
C(35)-H(35)	0.9500
C(36)-C(37)	1.389(3)
C(36)-H(36)	0.9500
C(37)-H(37)	0.9500
C(38)-O(1)	1.228(3)
C(38)-N(5)	1.357(3)
C(38)-C(39)	1.497(4)

C(39)-C(44)	1.389(4)
C(39)-C(40)	1.399(4)
C(40)-C(41)	1.390(5)
C(40)-H(40)	0.9500
C(41)-C(42)	1.372(6)
C(41)-H(41)	0.9500
C(42)-C(43)	1.379(5)
C(42)-H(42)	0.9500
C(43)-C(44)	1.392(4)
C(43)-H(43)	0.9500
C(44)-H(44)	0.9500
C(45)-Cl(2)	1.755(3)
C(45)-Cl(1)	1.765(4)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
N(1)-H(1N)	0.8800
N(2)-H(2N)	0.8800
N(4)-H(4N)	0.8800
N(5)-H(5)	0.8800

N(1)-C(1)-C(2)	106.50(19)
N(1)-C(1)-C(19)	115.09(19)
C(2)-C(1)-C(19)	137.5(2)
C(3)-C(2)-C(1)	107.6(2)
C(3)-C(2)-H(2)	126.2
C(1)-C(2)-H(2)	126.2
C(2)-C(3)-C(4)	108.9(2)
C(2)-C(3)-H(3)	125.5
C(4)-C(3)-H(3)	125.5
N(1)-C(4)-C(5)	120.87(19)
N(1)-C(4)-C(3)	104.74(18)
C(5)-C(4)-C(3)	134.3(2)
C(6)-C(5)-C(4)	121.55(19)
C(6)-C(5)-C(20)	119.19(18)
C(4)-C(5)-C(20)	119.26(18)
N(2)-C(6)-C(5)	124.99(18)
N(2)-C(6)-C(7)	105.40(18)
C(5)-C(6)-C(7)	129.27(19)

C(8)-C(7)-C(6)	109.32(18)
C(8)-C(7)-H(7)	125.3
C(6)-C(7)-H(7)	125.3
C(7)-C(8)-C(9)	108.79(18)
C(7)-C(8)-H(8)	125.6
C(9)-C(8)-H(8)	125.6
N(2)-C(9)-C(10)	125.60(18)
N(2)-C(9)-C(8)	105.67(18)
C(10)-C(9)-C(8)	128.73(19)
C(9)-C(10)-C(11)	125.68(18)
C(9)-C(10)-C(26)	116.51(17)
C(11)-C(10)-C(26)	117.74(18)
N(3)-C(11)-C(10)	126.02(19)
N(3)-C(11)-C(12)	108.58(17)
C(10)-C(11)-C(12)	125.24(19)
C(13)-C(12)-C(11)	107.50(18)
C(13)-C(12)-H(12)	126.3
C(11)-C(12)-H(12)	126.3
C(12)-C(13)-C(14)	107.69(18)
C(12)-C(13)-H(13)	126.2
C(14)-C(13)-H(13)	126.2
N(3)-C(14)-C(15)	123.40(19)
N(3)-C(14)-C(13)	108.01(18)
C(15)-C(14)-C(13)	128.59(19)
C(14)-C(15)-C(16)	121.53(19)
C(14)-C(15)-C(32)	120.36(19)
C(16)-C(15)-C(32)	118.08(18)
N(4)-C(16)-C(15)	119.63(18)
N(4)-C(16)-C(17)	106.99(19)
C(15)-C(16)-C(17)	133.3(2)
C(18)-C(17)-C(16)	107.63(19)
C(18)-C(17)-H(17)	126.2
C(16)-C(17)-H(17)	126.2
C(17)-C(18)-C(19)	107.10(19)
C(17)-C(18)-H(18)	126.4
C(19)-C(18)-H(18)	126.5
N(4)-C(19)-C(18)	108.15(19)
N(4)-C(19)-C(1)	115.52(19)

C(18)-C(19)-C(1)	136.3(2)
C(25)-C(20)-C(21)	118.0(2)
C(25)-C(20)-C(5)	121.12(19)
C(21)-C(20)-C(5)	120.87(19)
C(22)-C(21)-C(20)	120.6(2)
C(22)-C(21)-H(21)	119.7
C(20)-C(21)-H(21)	119.7
C(21)-C(22)-C(23)	120.5(2)
C(21)-C(22)-H(22)	119.7
C(23)-C(22)-H(22)	119.7
C(24)-C(23)-C(22)	119.4(2)
C(24)-C(23)-H(23)	120.3
C(22)-C(23)-H(23)	120.3
C(23)-C(24)-C(25)	120.3(2)
C(23)-C(24)-H(24)	119.9
C(25)-C(24)-H(24)	119.9
C(24)-C(25)-C(20)	121.2(2)
C(24)-C(25)-H(25)	119.4
C(20)-C(25)-H(25)	119.4
C(27)-C(26)-C(31)	118.12(19)
C(27)-C(26)-C(10)	120.36(19)
C(31)-C(26)-C(10)	121.47(18)
C(28)-C(27)-C(26)	121.8(2)
C(28)-C(27)-H(27)	119.1
C(26)-C(27)-H(27)	119.1
C(27)-C(28)-C(29)	119.2(2)
C(27)-C(28)-H(28)	120.4
C(29)-C(28)-H(28)	120.4
C(30)-C(29)-C(28)	120.5(2)
C(30)-C(29)-H(29)	119.8
C(28)-C(29)-H(29)	119.8
C(29)-C(30)-C(31)	120.5(2)
C(29)-C(30)-H(30)	119.7
C(31)-C(30)-H(30)	119.7
C(30)-C(31)-C(26)	119.8(2)
C(30)-C(31)-N(5)	121.6(2)
C(26)-C(31)-N(5)	118.56(18)
C(37)-C(32)-C(33)	118.50(19)

C(37)-C(32)-C(15)	119.80(19)
C(33)-C(32)-C(15)	121.70(18)
C(34)-C(33)-C(32)	120.6(2)
C(34)-C(33)-H(33)	119.7
C(32)-C(33)-H(33)	119.7
C(35)-C(34)-C(33)	120.1(2)
C(35)-C(34)-H(34)	120.0
C(33)-C(34)-H(34)	120.0
C(34)-C(35)-C(36)	120.0(2)
C(34)-C(35)-H(35)	120.0
C(36)-C(35)-H(35)	120.0
C(35)-C(36)-C(37)	120.1(2)
C(35)-C(36)-H(36)	119.9
C(37)-C(36)-H(36)	119.9
C(36)-C(37)-C(32)	120.7(2)
C(36)-C(37)-H(37)	119.7
C(32)-C(37)-H(37)	119.7
O(1)-C(38)-N(5)	123.1(2)
O(1)-C(38)-C(39)	120.9(2)
N(5)-C(38)-C(39)	116.1(2)
C(44)-C(39)-C(40)	119.4(3)
C(44)-C(39)-C(38)	123.6(2)
C(40)-C(39)-C(38)	116.9(3)
C(41)-C(40)-C(39)	119.3(3)
C(41)-C(40)-H(40)	120.3
C(39)-C(40)-H(40)	120.3
C(42)-C(41)-C(40)	120.9(3)
C(42)-C(41)-H(41)	119.5
C(40)-C(41)-H(41)	119.5
C(41)-C(42)-C(43)	120.1(3)
C(41)-C(42)-H(42)	120.0
C(43)-C(42)-H(42)	120.0
C(42)-C(43)-C(44)	120.0(3)
C(42)-C(43)-H(43)	120.0
C(44)-C(43)-H(43)	120.0
C(39)-C(44)-C(43)	120.3(3)
C(39)-C(44)-H(44)	119.9
C(43)-C(44)-H(44)	119.9

Cl(2)-C(45)-Cl(1)	112.0(2)
Cl(2)-C(45)-H(45A)	109.2
Cl(1)-C(45)-H(45A)	109.2
Cl(2)-C(45)-H(45B)	109.2
Cl(1)-C(45)-H(45B)	109.2
H(45A)-C(45)-H(45B)	107.9
C(1)-N(1)-C(4)	112.21(18)
C(1)-N(1)-H(1N)	123.9
C(4)-N(1)-H(1N)	123.9
C(9)-N(2)-C(6)	110.77(17)
C(9)-N(2)-H(2N)	124.6
C(6)-N(2)-H(2N)	124.6
C(11)-N(3)-C(14)	108.18(17)
C(19)-N(4)-C(16)	110.07(18)
C(19)-N(4)-H(4N)	125.0
C(16)-N(4)-H(4N)	125.0
C(38)-N(5)-C(31)	127.90(19)
C(38)-N(5)-H(5)	116.0
C(31)-N(5)-H(5)	116.0