Supplementary information

Chiral multidentate oxazoline ligands based on cyclophosphazene cores: Synthesis, characterization and complexation studies

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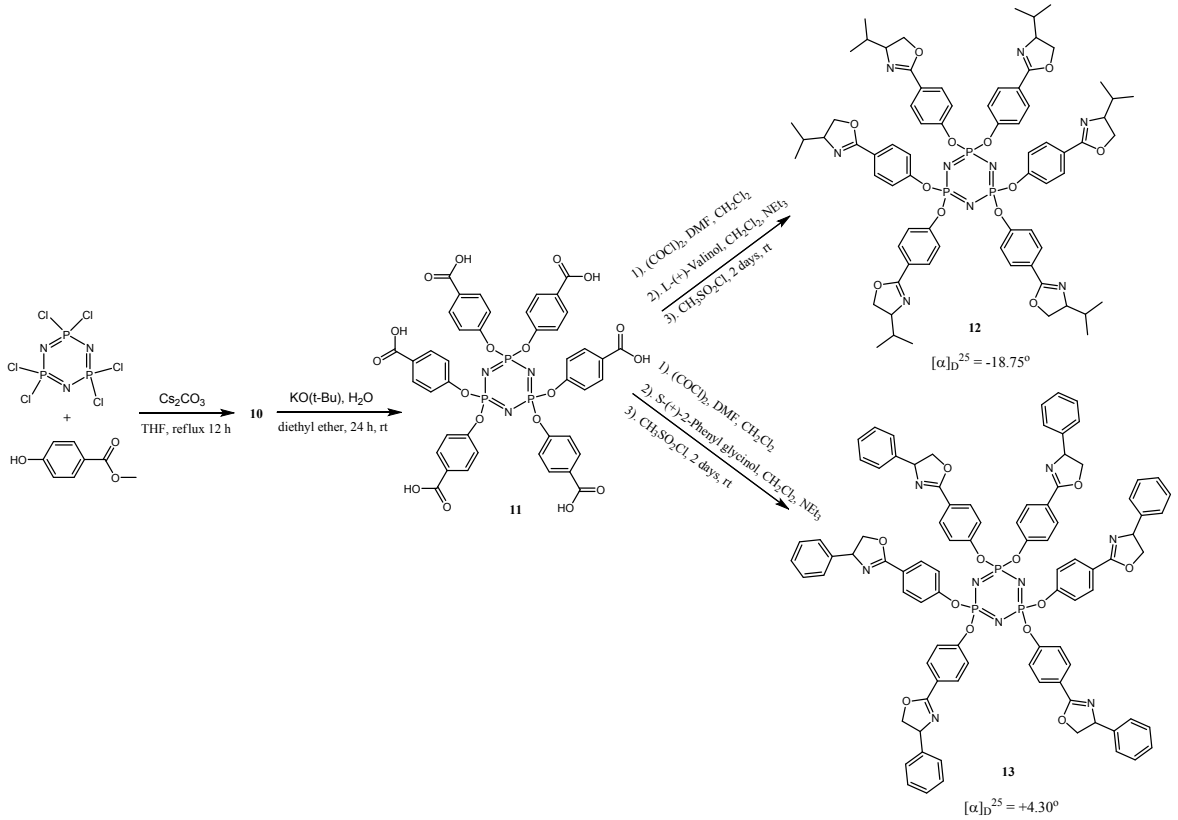
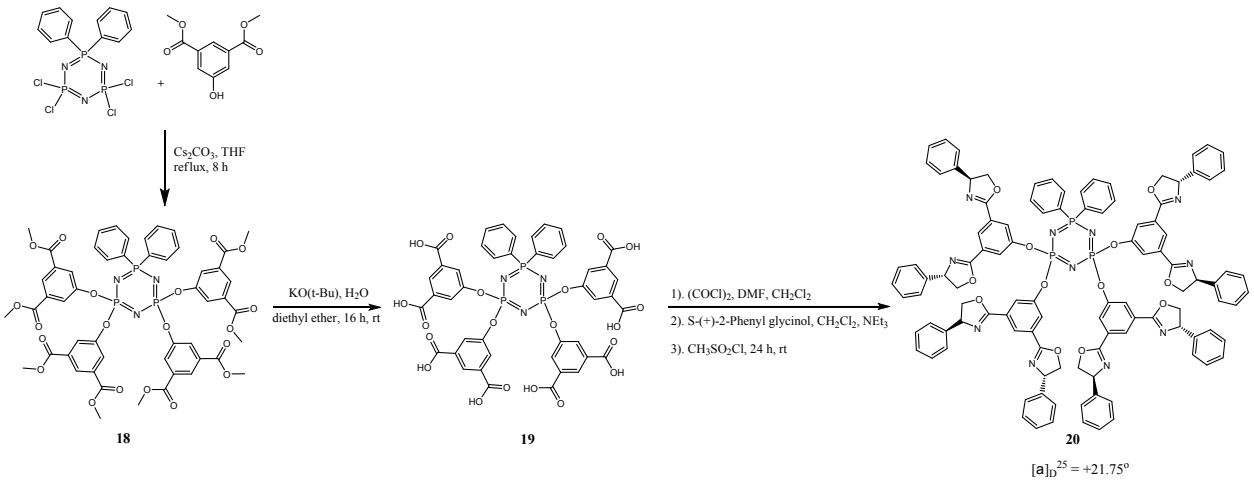
Reaction Schemes



Scheme A:



Scheme B:

Figures

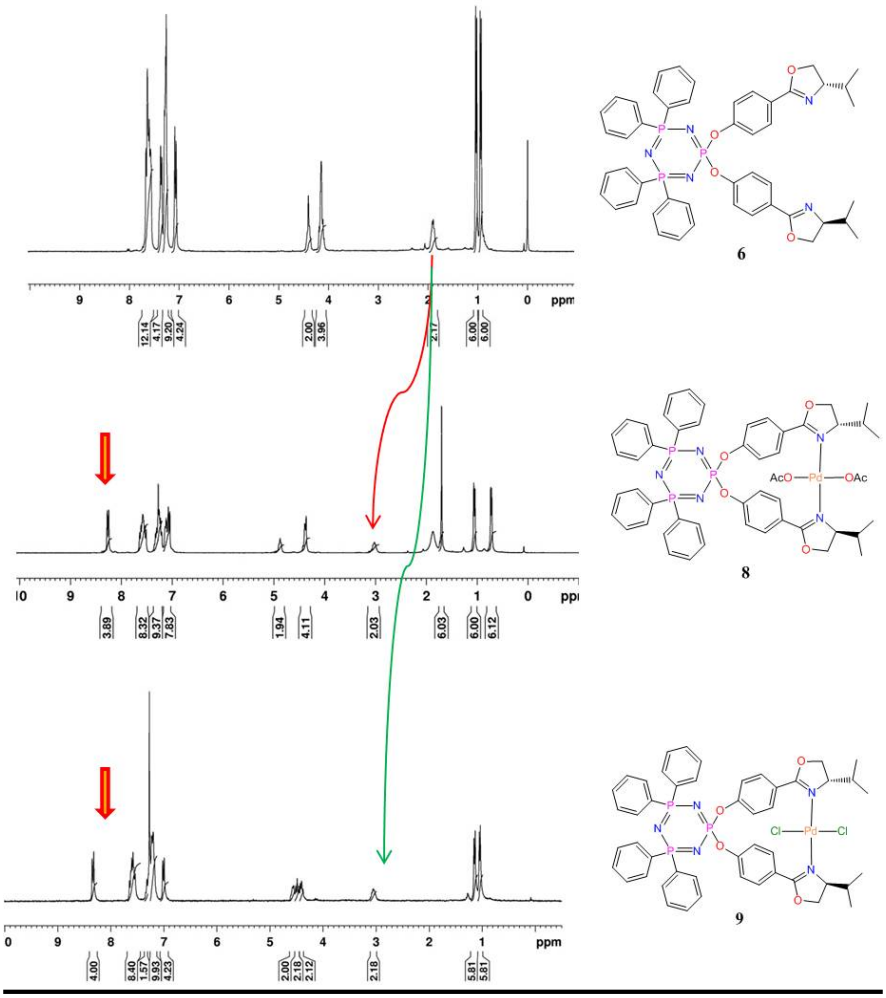


Fig. A Changes in the ^{1}H NMR of compound 6 after complexation

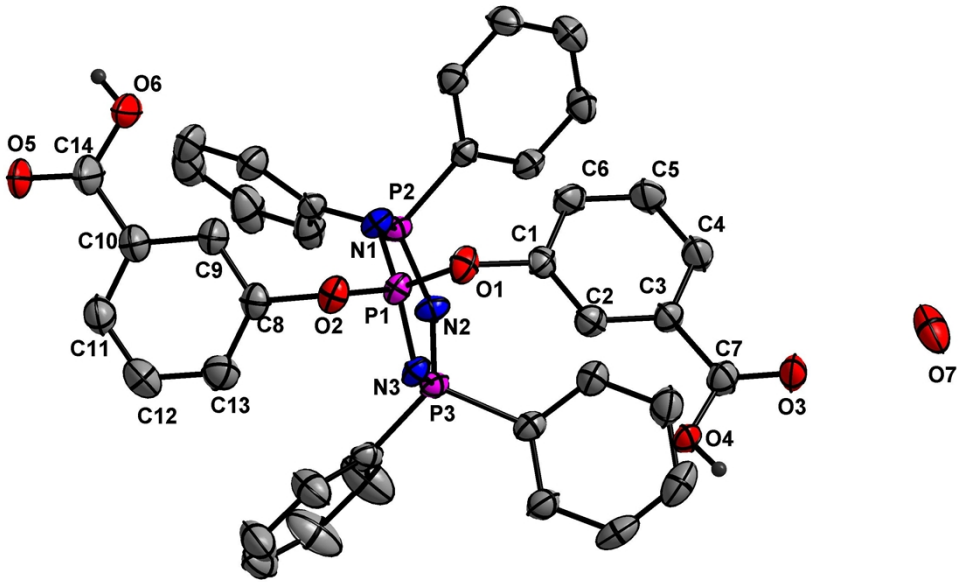


Fig. B ORTEP diagram of compound **2** with thermal ellipsoids at the 30% probability level (data was collected at 298 K).

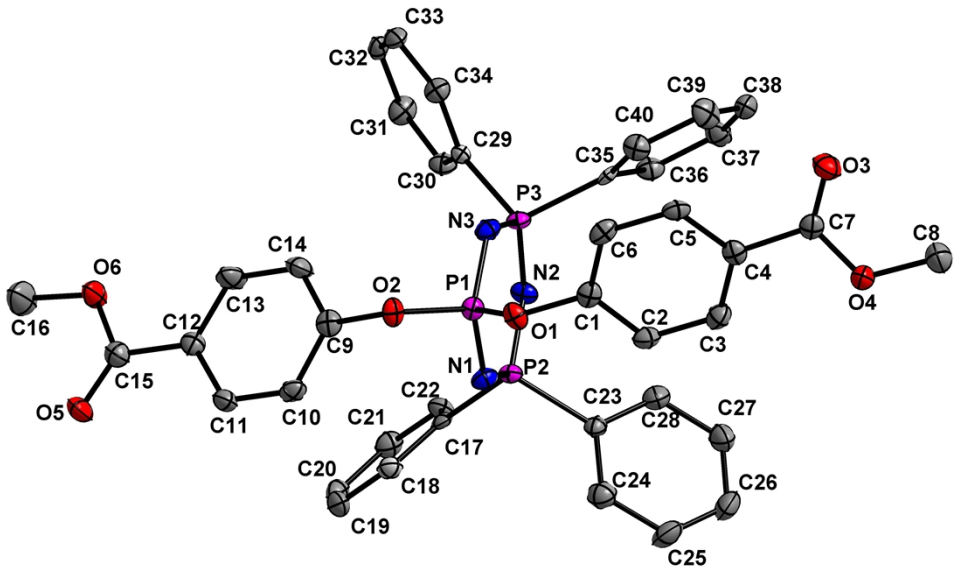


Fig. C ORTEP diagram of compound **4** with thermal ellipsoids at the 30% probability level (data was collected at 298 K).

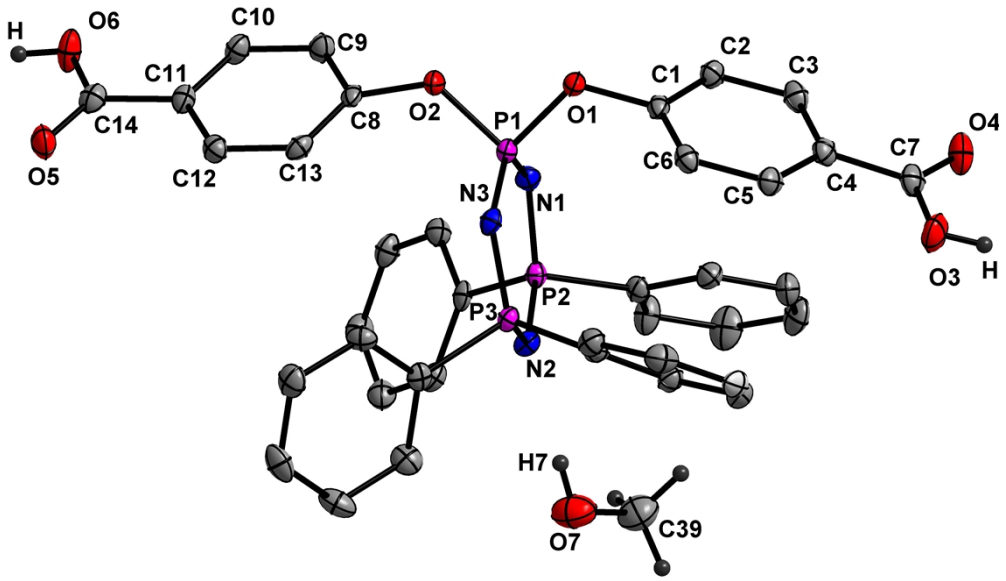


Fig. D ORTEP diagram of compound **5** with thermal ellipsoids at the 30% probability level (data was collected at 298 K).

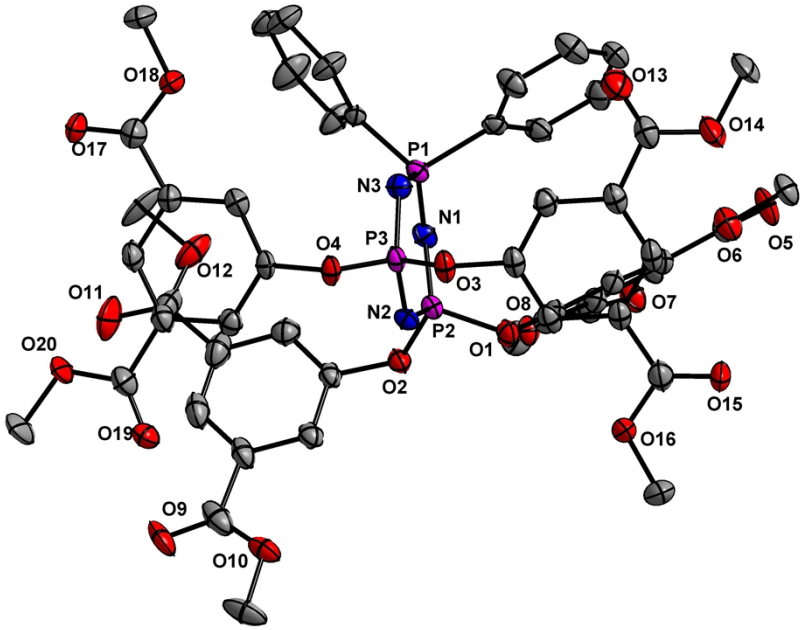


Fig. E ORTEP diagram of compound **18** with thermal ellipsoids at the 30% probability level (data was collected at 298 K).

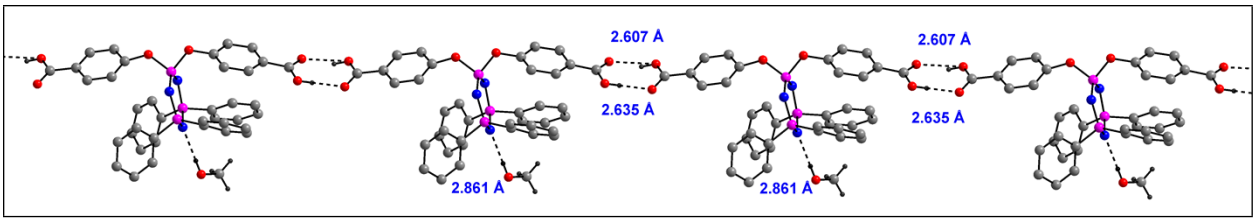


Fig. F Crystal structure of compound **5** showing intermolecular H-bonding.

Table 1. Selected bond lengths and bond angles of compound **1**

Bond Lengths (Å)

P(1)-N(1)	1.571(3)	P(2)-N(1)	1.606(3)
P(1)-O(1)	1.626(2)	P(1)-O(2)	1.603(2)
O(1)-C(1)	1.343(4)	C(7)-O(4)	1.316(6)
C(7)-O(3)	1.193(6)	C(8)-O(4)	1.454(6)

Bond Angles (deg)

N(1)-P(1)-N(3)	118.8(1)	N(1)-P(2)-N(2)	116.5(2)
O(1)-P(1)-O(2)	97.3(1)	P(1)-O(1)-C(1)	119.7(2)
O(1)-C(1)-C(2)	116.9(3)	O(3)-C(7)-O(4)	122.5(6)
C(17)-P(2)-C(23)	107.3(2)	P(1)-N(1)-P(2)	120.8(2)

Table 2. Selected bond lengths and bond angles of compound **2**

Bond Lengths (Å)

P(1)-N(1)	1.561(3)	P(2)-N(1)	1.609(3)
P(1)-O(1)	1.596(3)	P(1)-O(2)	1.586(3)
O(1)-C(1)	1.403(5)	C(7)-O(4)	1.305(5)
C(7)-O(3)	1.217(5)	P(2)-C(15)	1.799(4)

Bond Angles (deg)

N(1)-P(1)-N(3)	117.3(2)	N(1)-P(2)-N(2)	116.6(2)
O(1)-P(1)-O(2)	93.2(2)	P(1)-O(1)-C(1)	121.3(3)
O(1)-C(1)-C(2)	118.8(4)	O(3)-C(7)-O(4)	123.3(4)
C(15)-P(2)-C(21)	104.7(2)	P(1)-N(1)-P(2)	122.3(2)

Table 3. Selected bond lengths and bond angles of compound **4**

Bond Lengths (Å)

P(1)-N(1)	1.570(3)	P(2)-N(1)	1.608(3)
P(1)-O(1)	1.604(2)	P(1)-O(2)	1.601(2)
O(1)-C(1)	1.389(4)	C(7)-O(4)	1.341(4)
C(7)-O(3)	1.205(4)	C(8)-O(4)	1.447(4)

Bond Angles (deg)

N(1)-P(1)-N(3)	118.6(1)	N(1)-P(2)-N(2)	117.3(1)
O(1)-P(1)-O(2)	92.7(1)	P(1)-O(1)-C(1)	122.0(2)
O(1)-C(1)-C(2)	120.8(3)	O(3)-C(7)-O(4)	123.4(3)
C(17)-P(2)-C(23)	106.6(1)	P(1)-N(1)-P(2)	122.5(2)

Table 4. Selected bond lengths and bond angles of compound **5**

Bond Lengths (Å)

P(1)-N(1)	1.572(2)	P(2)-N(1)	1.612(2)
P(1)-O(1)	1.607(2)	P(1)-O(2)	1.592(2)
O(1)-C(1)	1.398(3)	C(7)-O(4)	1.257(3)
C(7)-O(3)	1.284(3)	P(2)-C(15)	1.815(2)

Bond Angles (deg)

N(1)-P(1)-N(3)	117.8(1)	N(1)-P(2)-N(2)	116.3(1)
O(1)-P(1)-O(2)	91.6(9)	P(1)-O(1)-C(1)	118.8(2)
O(1)-C(1)-C(2)	118.1(2)	O(3)-C(7)-O(4)	123.5(2)
C(15)-P(2)-C(21)	104.7(1)	P(1)-N(1)-P(2)	123.2(1)

Table 5. Selected bond lengths and bond angles of compound **7**

Bond Lengths (Å)

P(1)-N(1)	1.568(8)	P(2)-N(1)	1.587(7)
P(1)-O(1)	1.585(5)	P(1)-O(2)	1.592(6)
O(1)-C(1)	1.404(1)	C(7)-O(3)	1.339(1)
C(7)-N(4)	1.269(1)	C(4)-C(7)	1.462(2)
O(3)-C(9)	1.457(1)	N(4)-C(8)	1.479(1)

Bond Angles (deg)

N(1)-P(1)-N(3)	119.0(3)	N(1)-P(2)-N(2)	117.5(4)
O(1)-P(1)-O(2)	97.3(3)	P(1)-O(1)-C(1)	121.8(6)
O(1)-C(1)-C(2)	120.1(8)	O(3)-C(7)-N(4)	116.7(1)
O(3)-C(9)-C(8)	105.1(9)	P(1)-N(1)-P(2)	121.3(5)

Table 6. Selected bond lengths and bond angles of compound **14**

Bond Lengths (Å)

P(1)-N(1)	1.567(3)	P(2)-N(1)	1.610(3)
P(1)-O(1)	1.595(3)	P(1)-O(2)	1.603(2)
O(1)-C(1)	1.400(4)	C(7)-O(4)	1.327(5)

C(7)-O(3)	1.199(5)	C(8)-O(4)	1.455(5)

Bond Angles (deg)

N(1)-P(1)-N(3)	118.6(2)	N(1)-P(2)-N(2)	116.8(2)
O(1)-P(1)-O(2)	92.1(1)	P(1)-O(1)-C(1)	118.7(2)
O(1)-C(1)-C(2)	118.5(3)	O(3)-C(7)-O(4)	123.3(4)
C(27)-P(2)-C(21)	103.8(2)	P(1)-N(1)-P(2)	122.0(2)

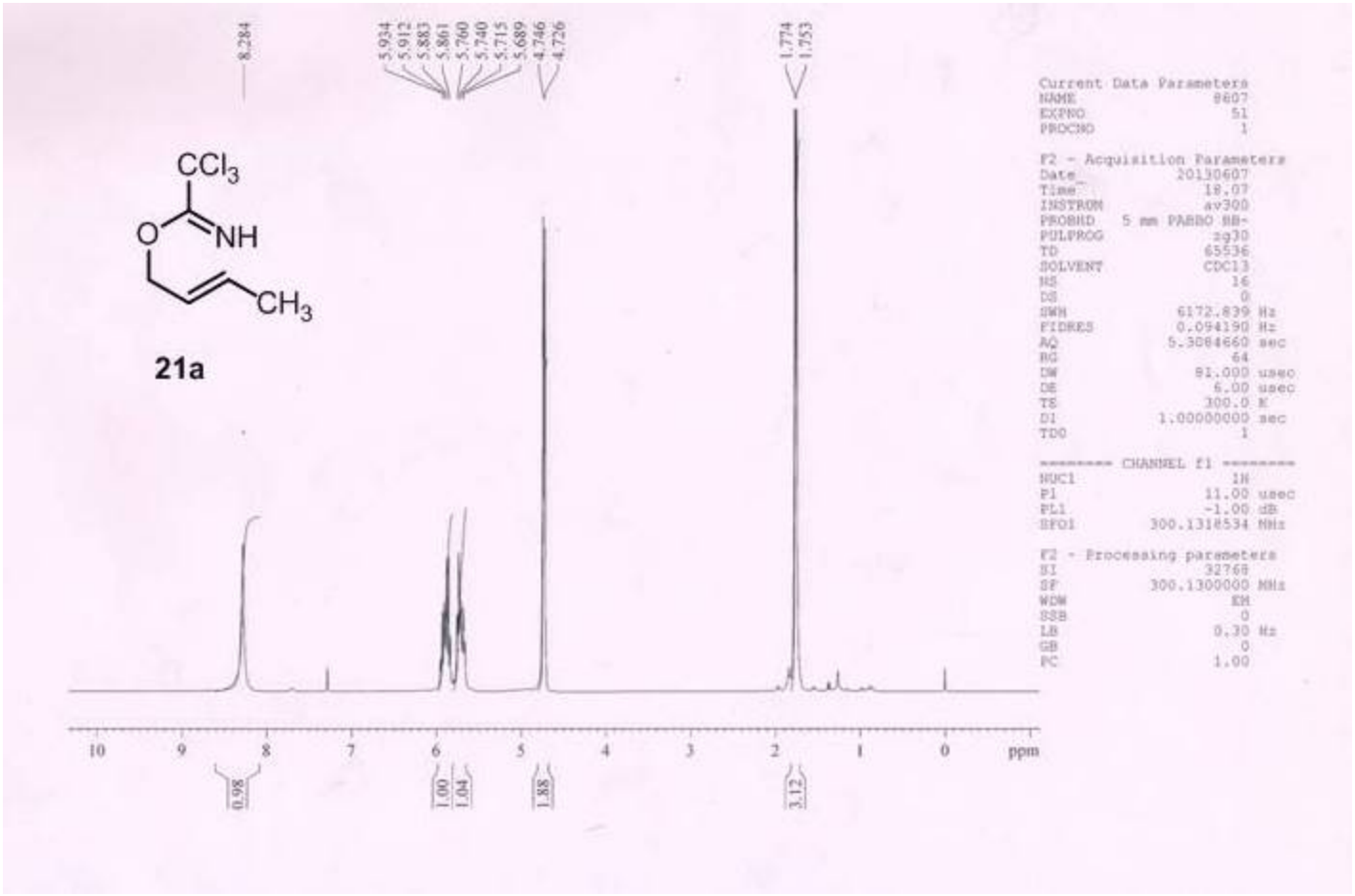
Table 7. Selected bond lengths and bond angles of compound **18**

Bond Lengths (Å)

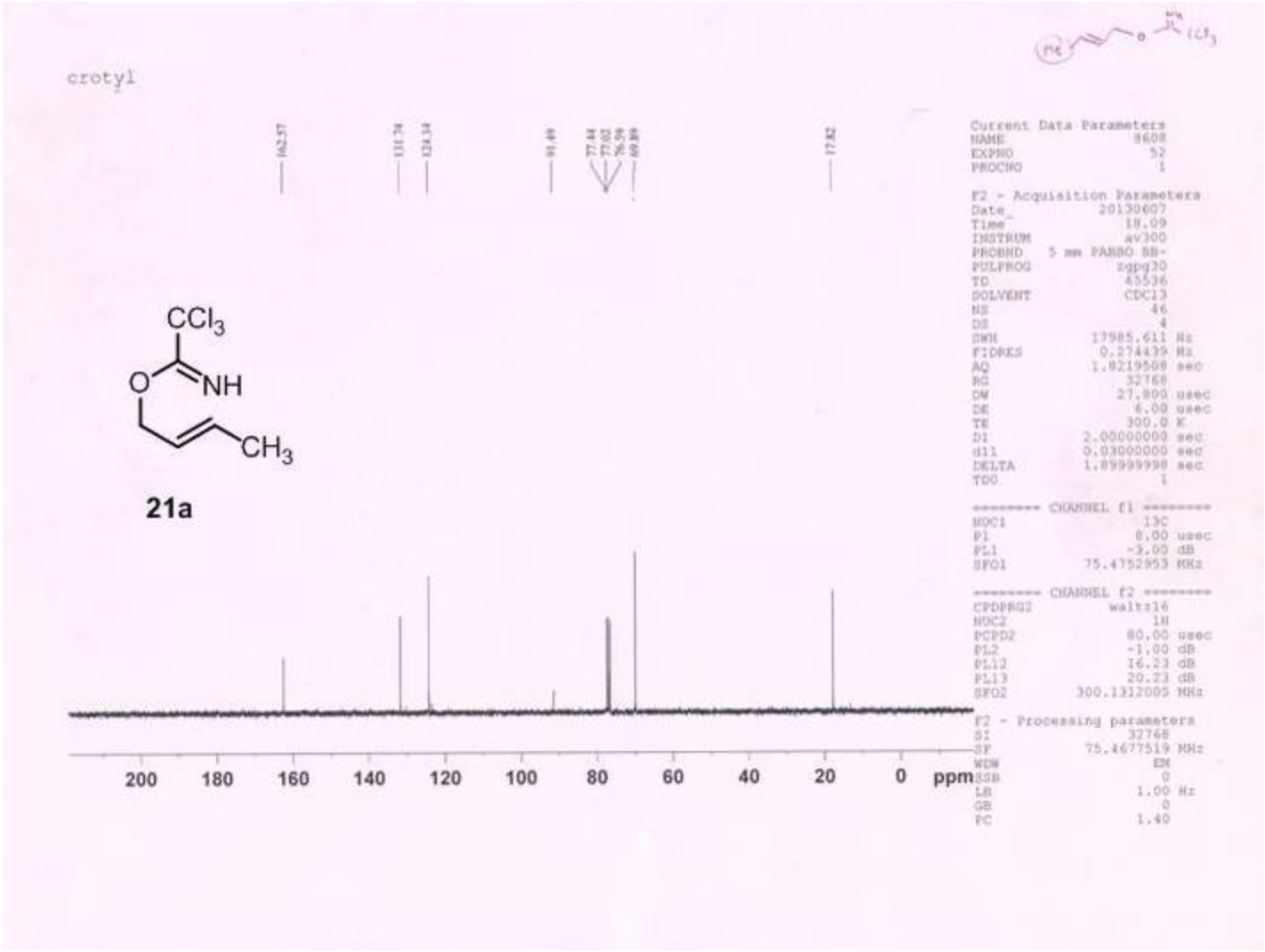
P(1)-N(1)	1.612(2)	P(2)-N(1)	1.565(2)
P(2)-O(1)	1.591(2)	P(2)-O(2)	1.586(2)
O(1)-C(13)	1.395(3)	C(19)-O(5)	1.194(3)
C(29)-O(9)	1.198(4)	P(1)-C(1)	1.801(3)

Bond Angles (deg)

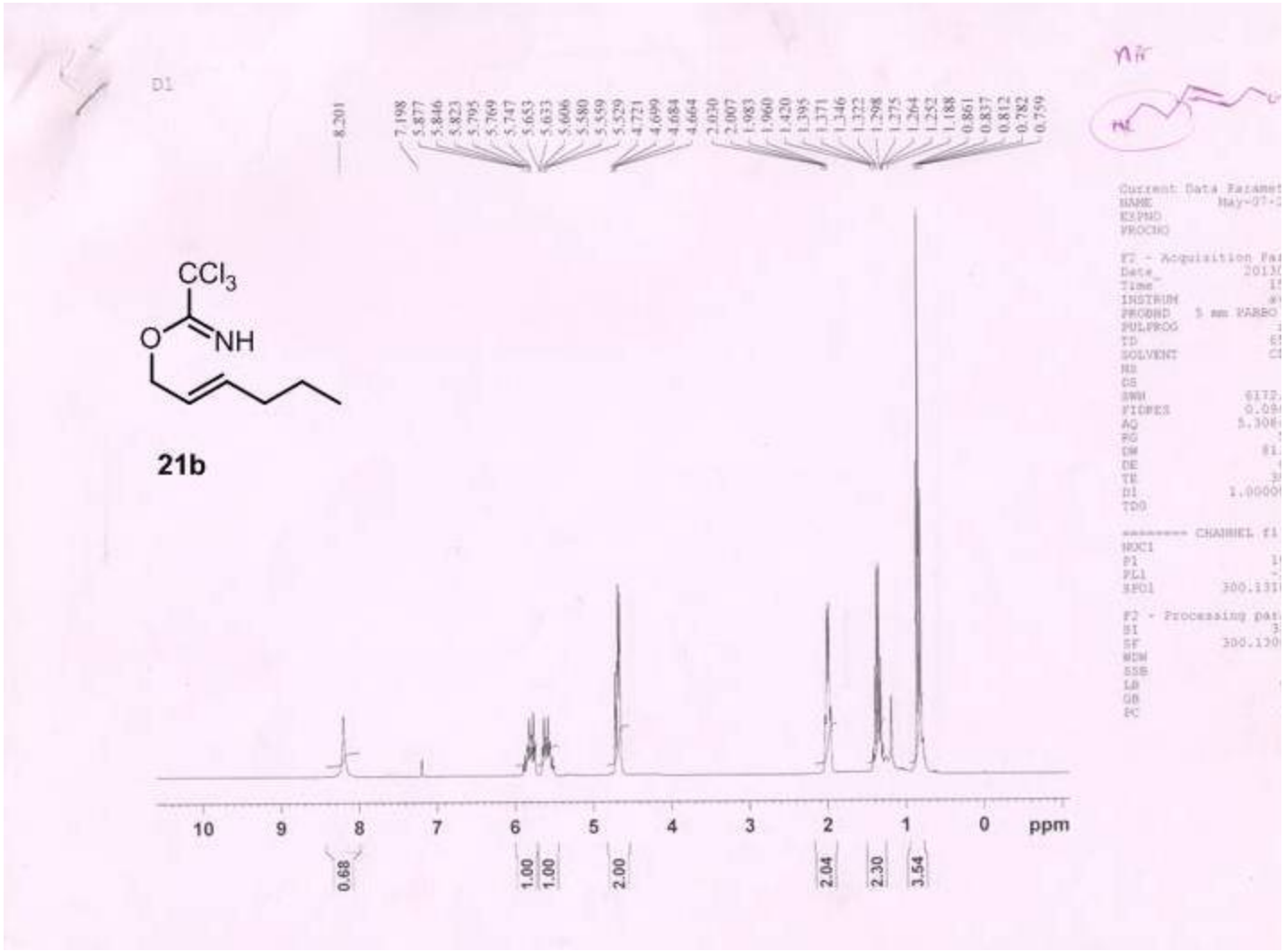
N(1)-P(1)-N(3)	116.2(1)	N(1)-P(2)-N(2)	118.5(1)
O(1)-P(2)-O(2)	98.2(1)	P(2)-O(1)-C(13)	124.4(2)
O(1)-C(13)-C(14)	116.9(3)	O(5)-C(19)-O(6)	123.4(3)
C(1)-P(1)-C(7)	105.5(1)	P(1)-N(1)-P(2)	120.0(1)



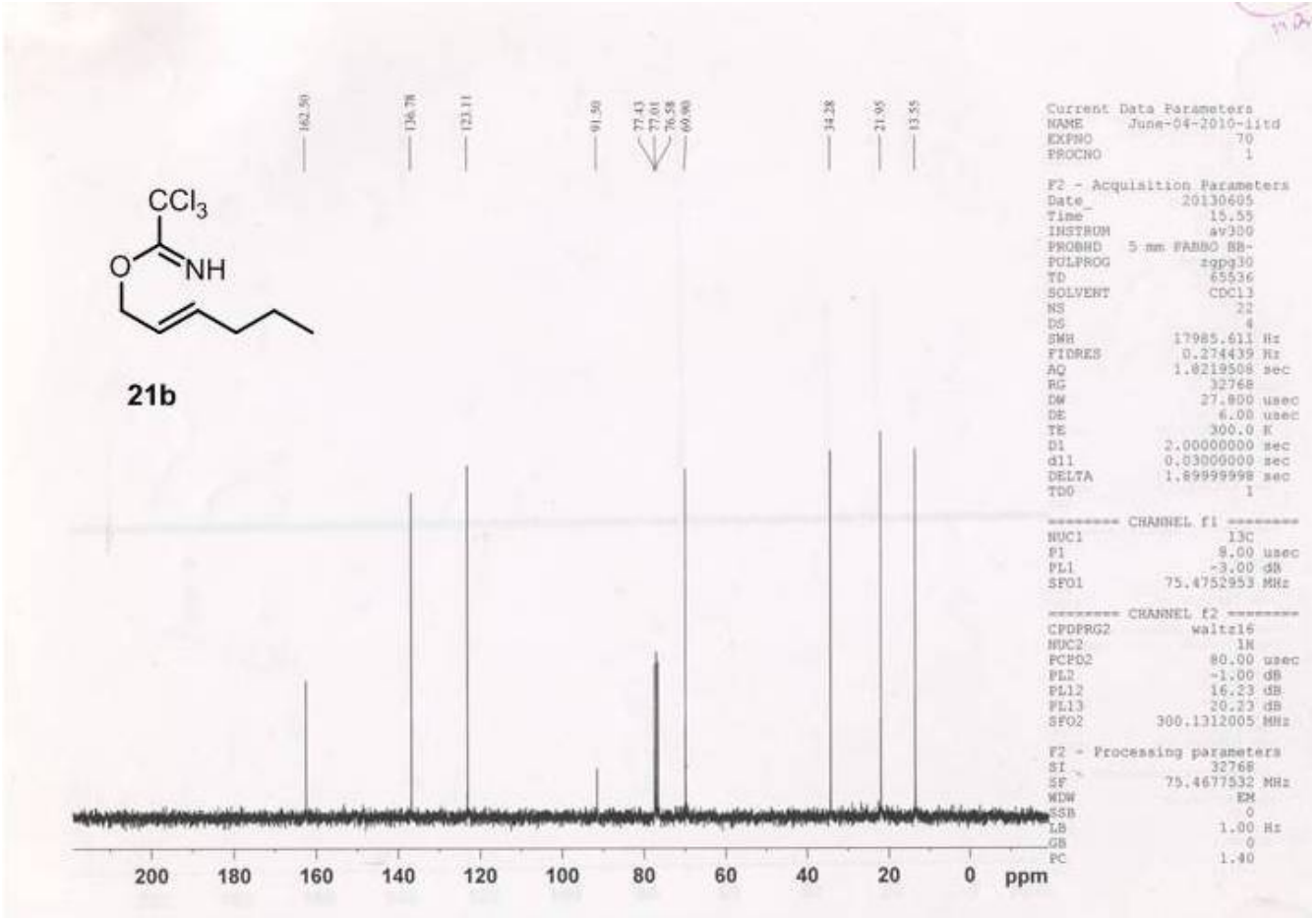
^{1}H NMR of compound 21a



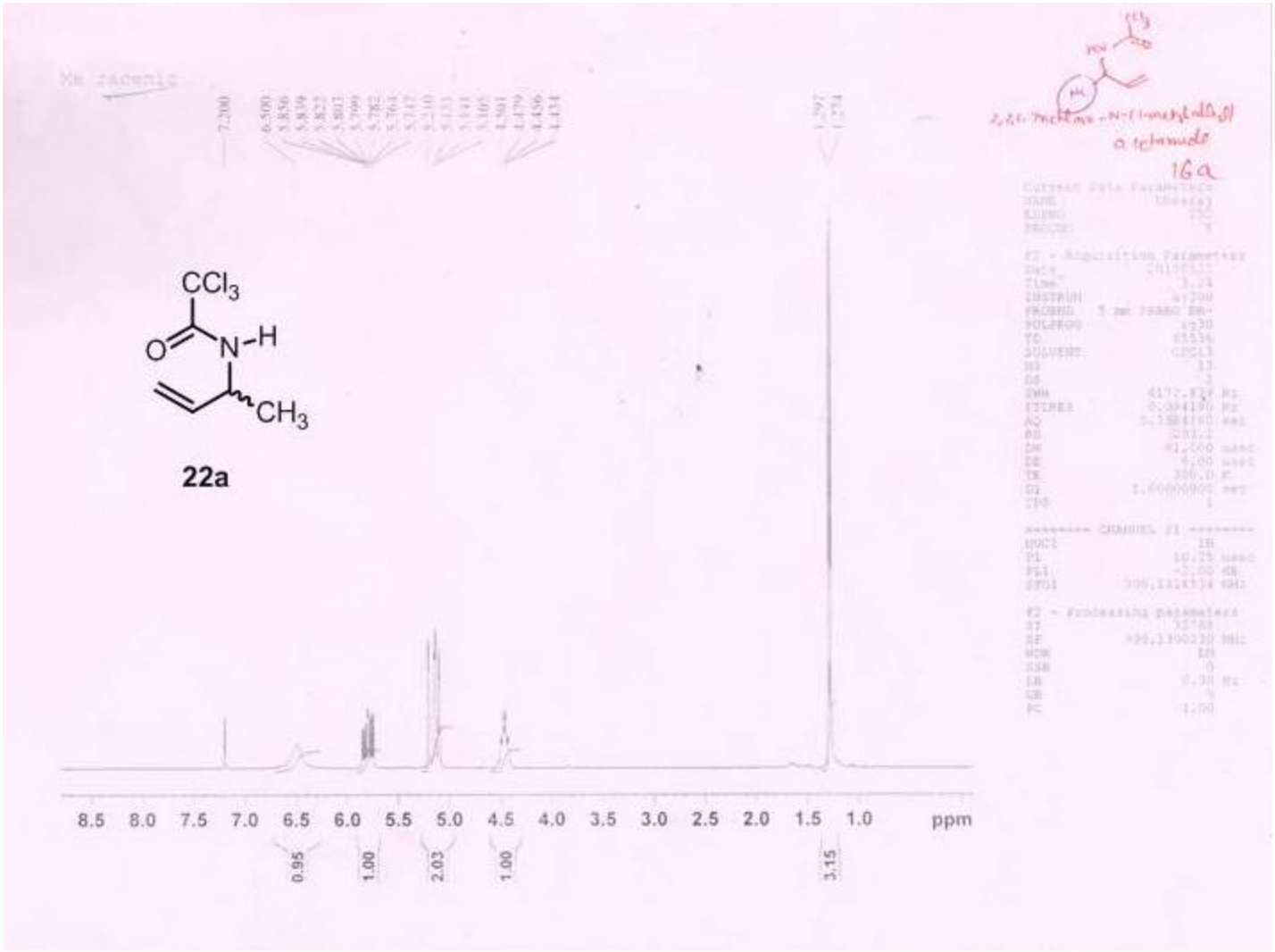
^{13}C NMR of compound 21a



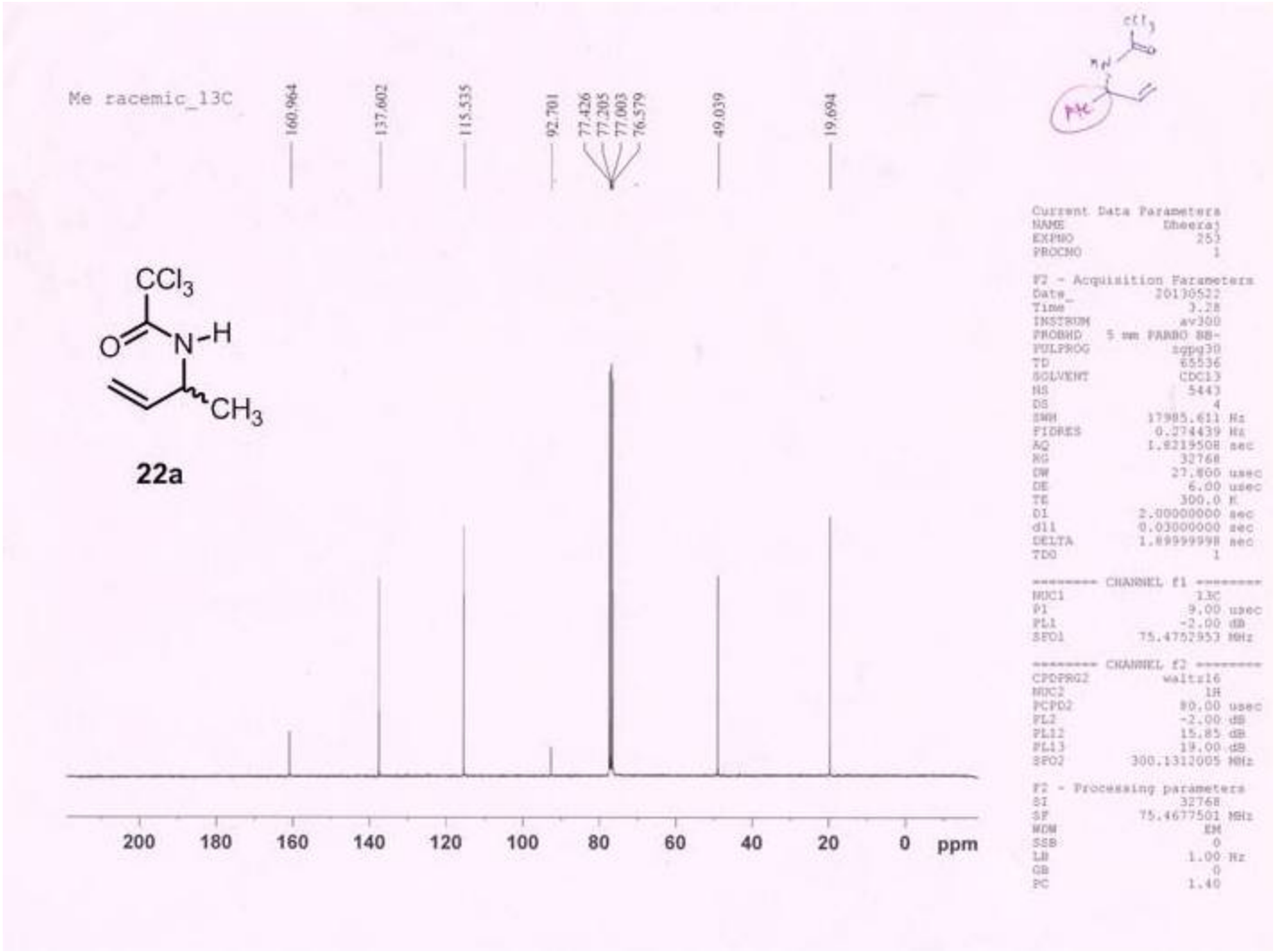
[1]H NMR of compound 21b



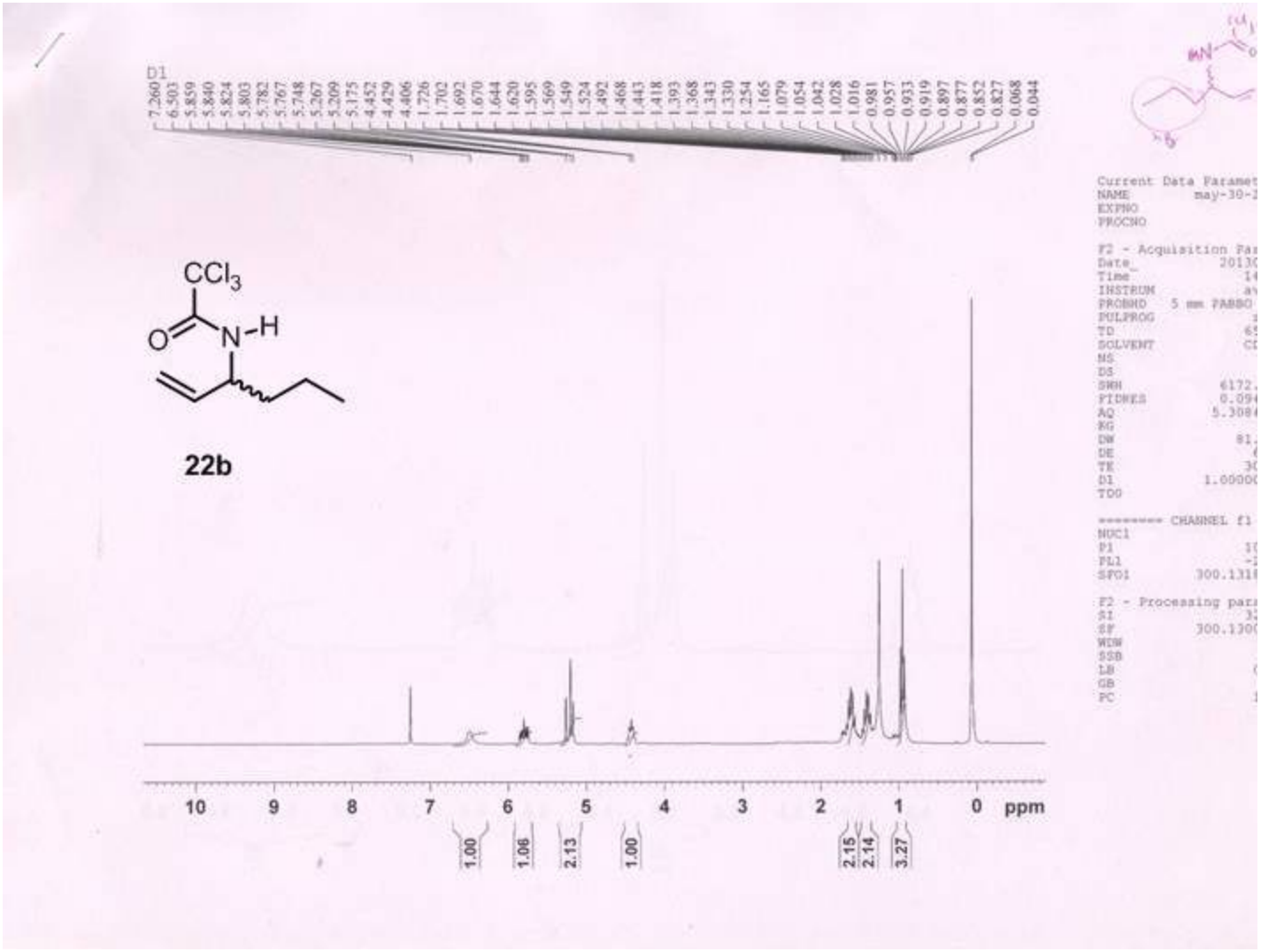
^{13}C NMR of compound 21b



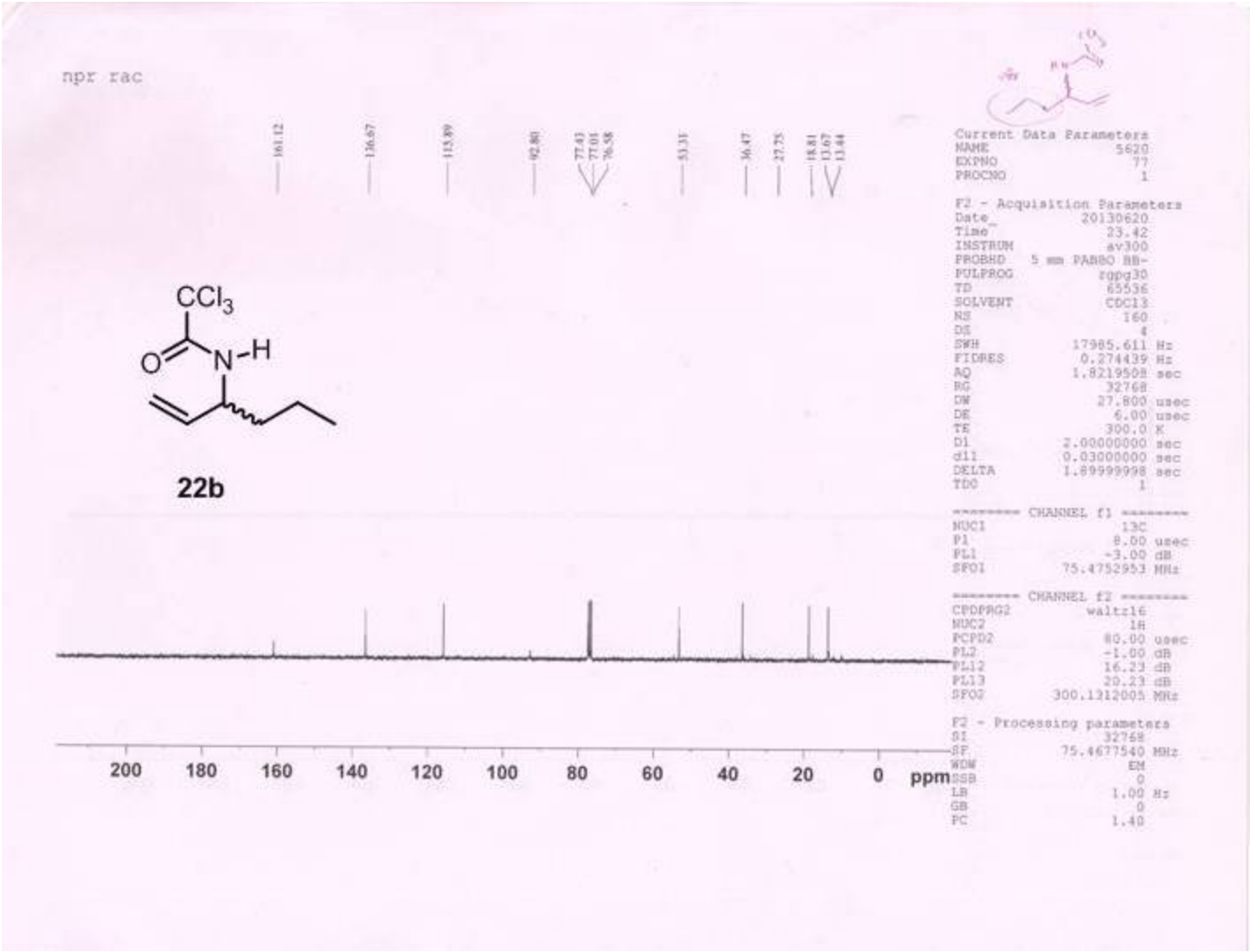
^{1}H NMR of compound 22a



^{13}C NMR of compound 22a



^{1}H NMR of compound 22b



^{13}C NMR of compound 22b

CD Spectra

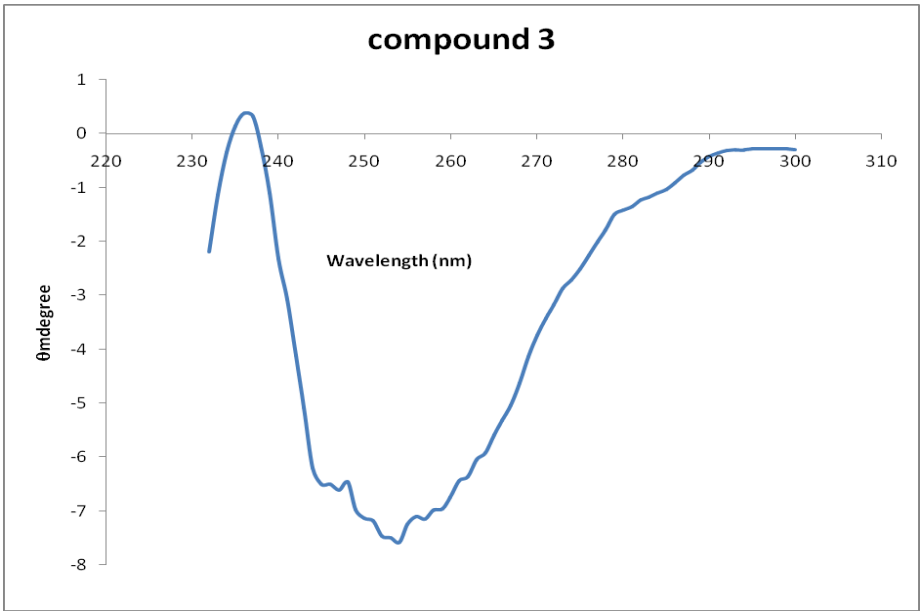


Figure 1: CD spectra of compound **3**

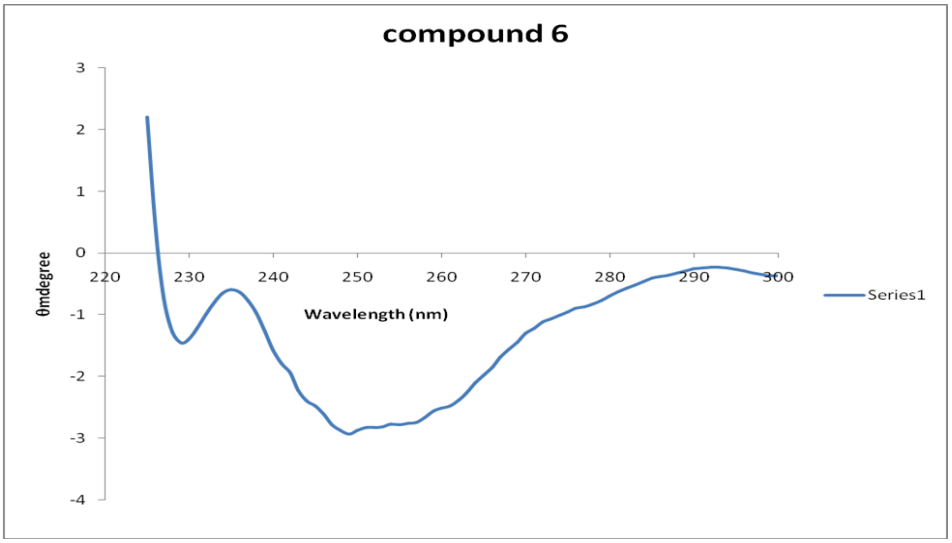


Figure 2: CD spectra of compound **6**

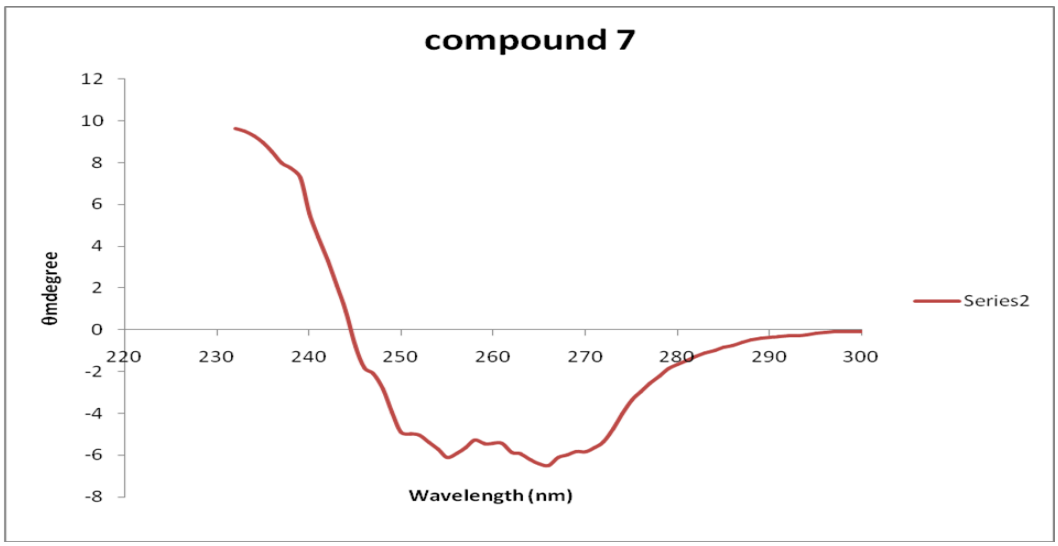


Figure 3: CD spectra of compound **7**

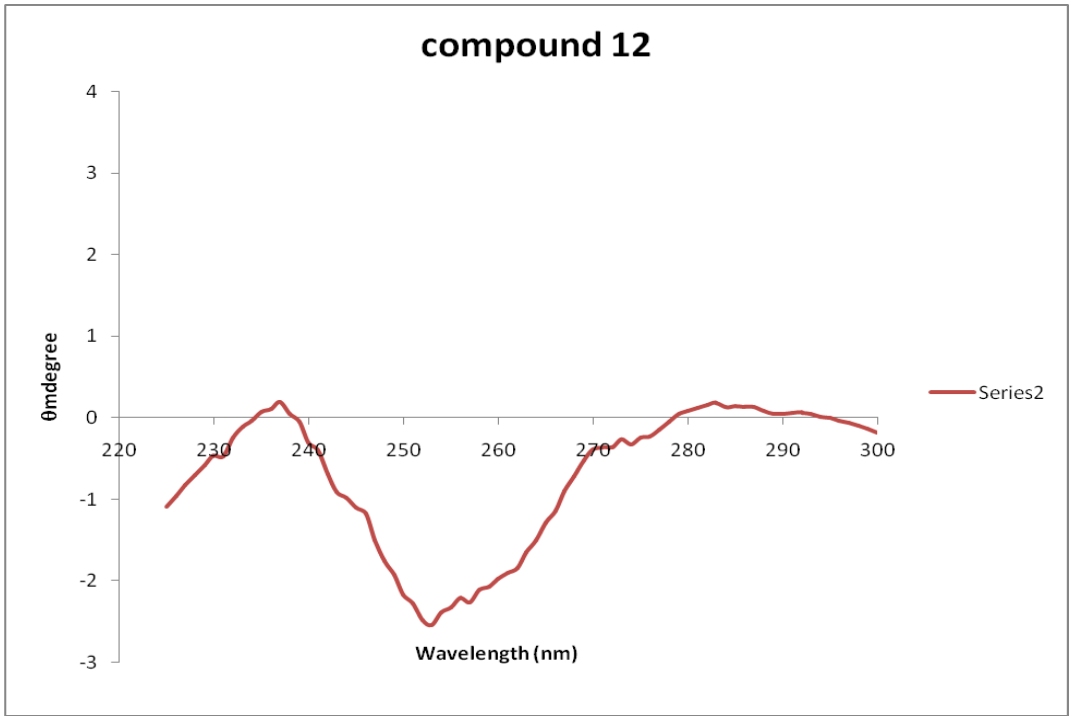


Figure 4: CD spectra of compound **12**

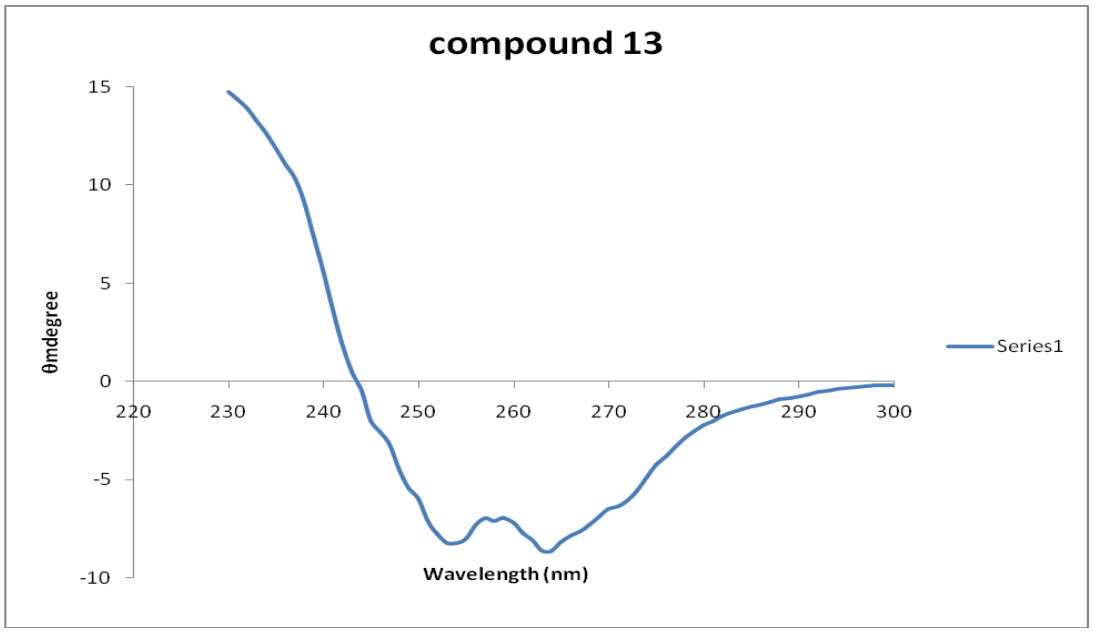


Figure 5: CD spectra of compound **13**

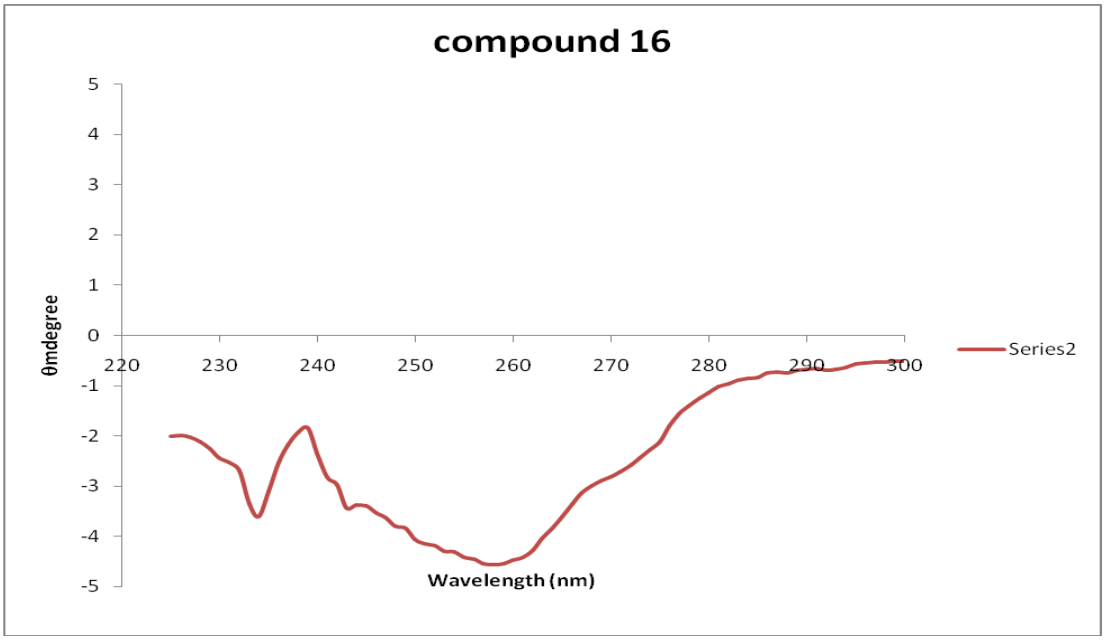


Figure 6: CD spectra of compound **16**

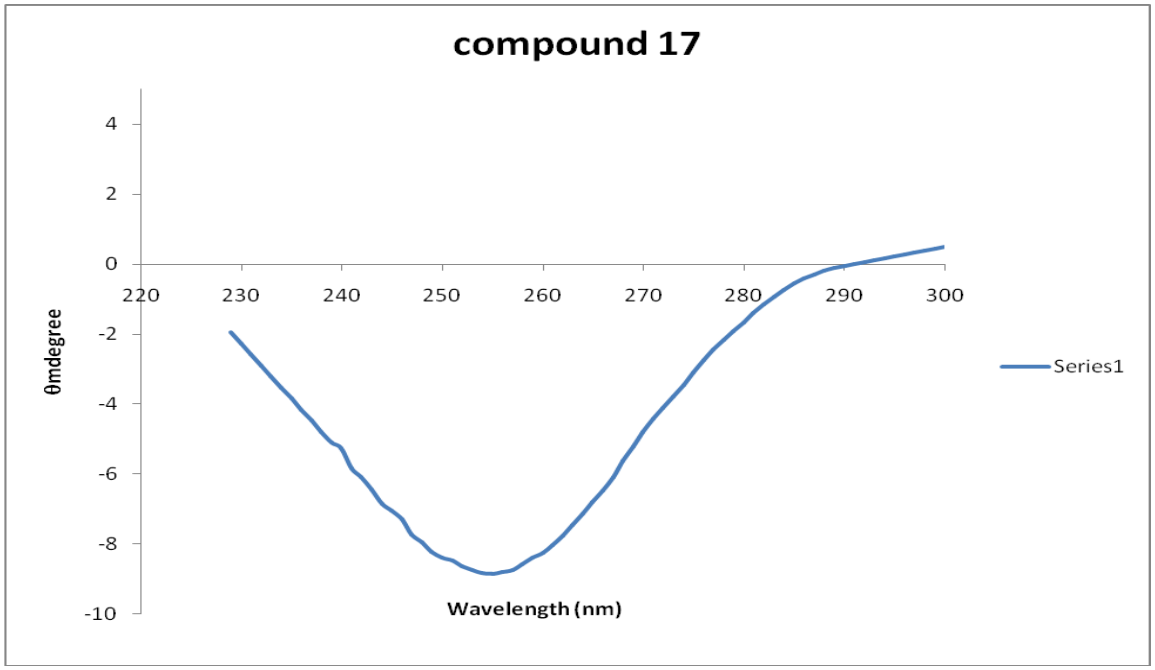


Figure 7: CD spectra of compound **17**

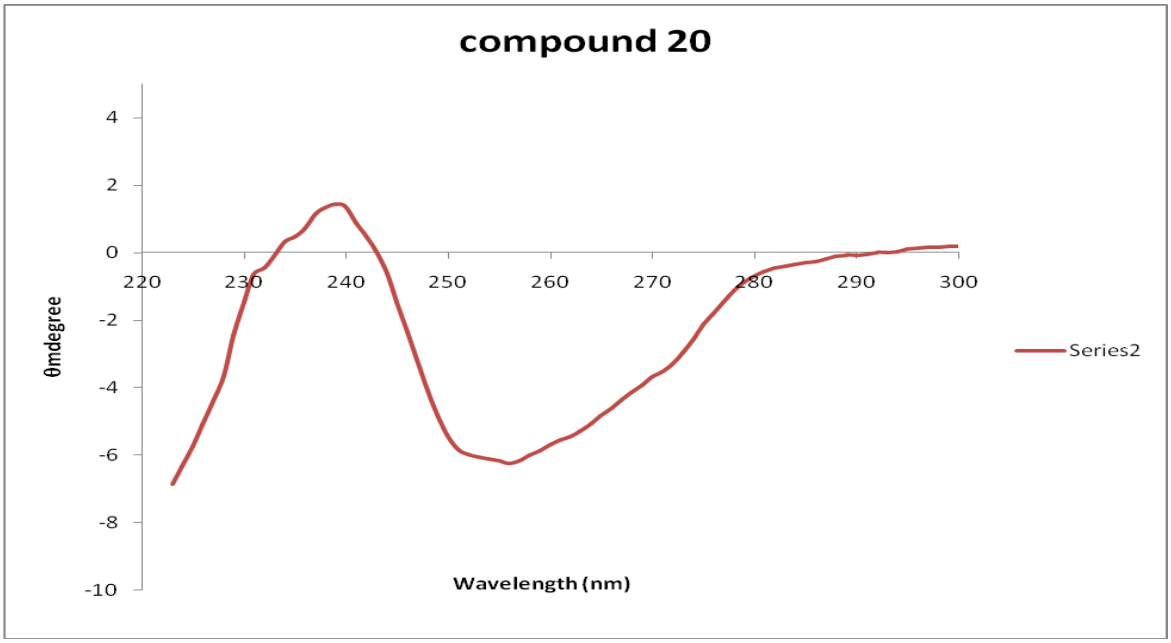


Figure 8: CD spectra of compound **20**