Supporting Information

SYNTHESIS, CONFORMATIONAL STUDY, AND BIOLOGICAL PROPERTIES OF PHOSPHONOMETHOXY DERIVATIVES OF NUCLEOBASES WITH LOCKED CONFORMATION VIA PYRROLIDINE RING

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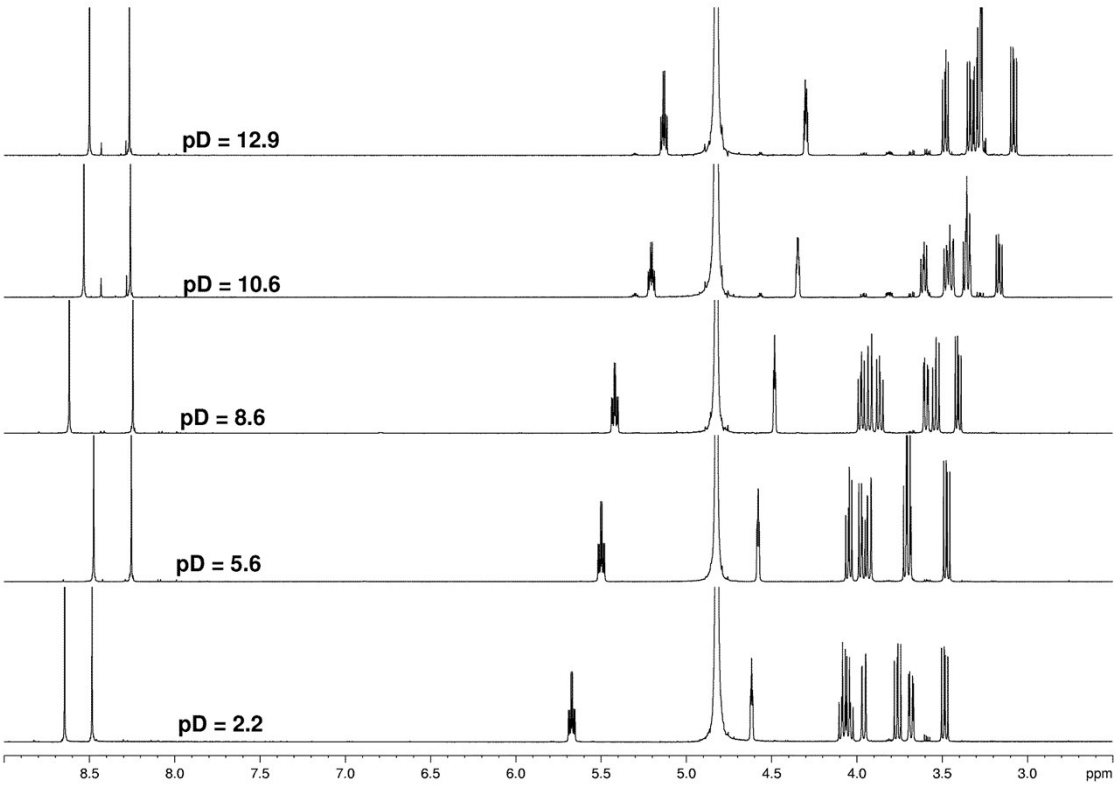
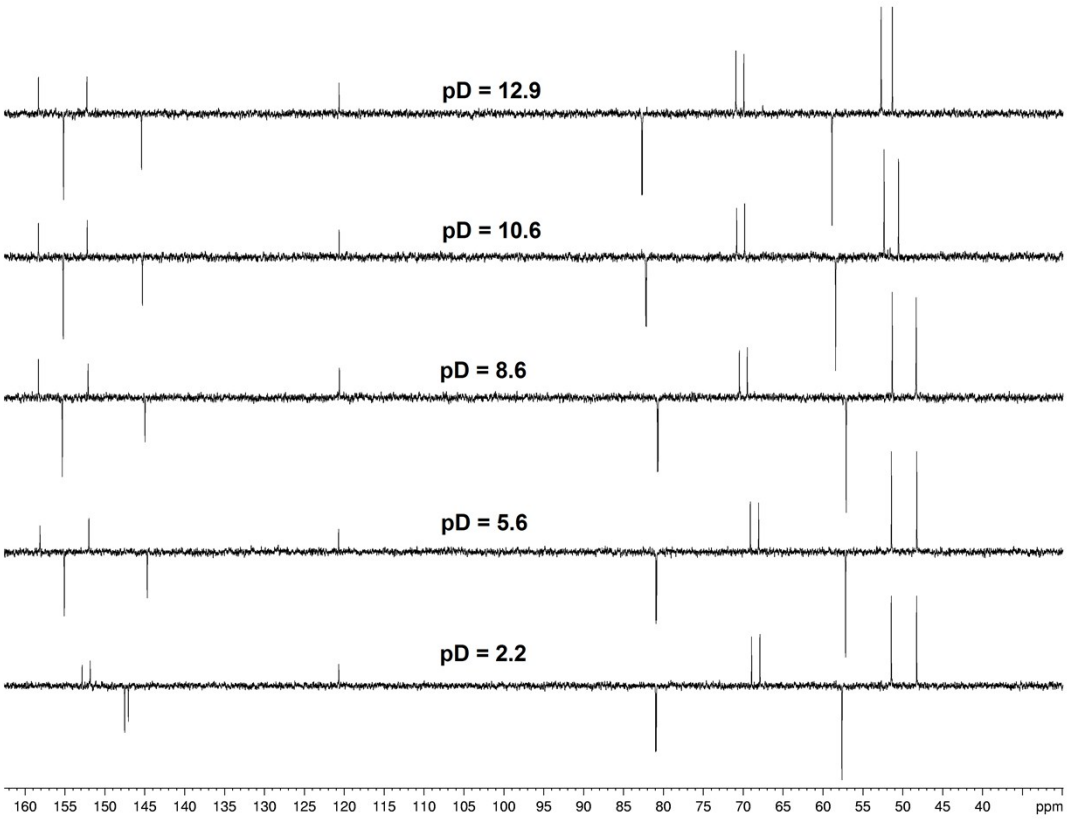
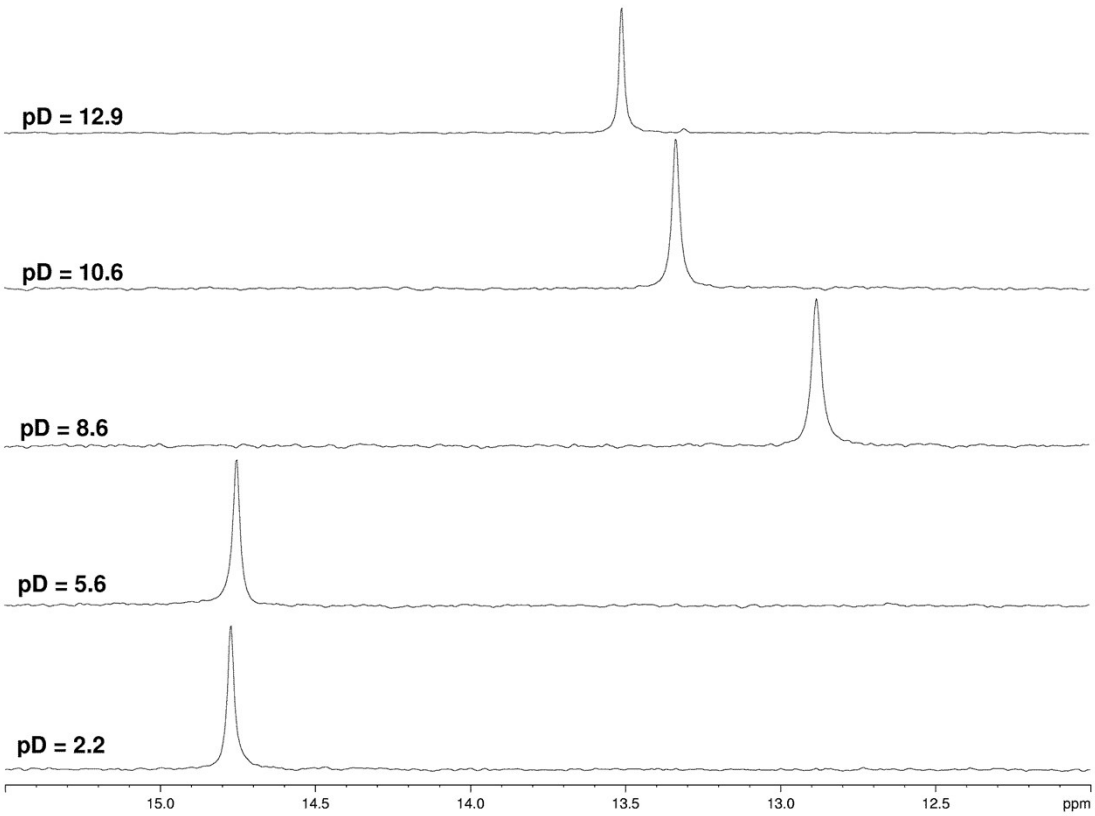
^{1}H NMR spectra of **15a** measured in D_2O at various pD values:



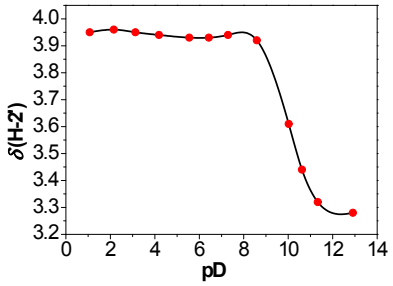
^{13}C NMR spectra of **15a** measured in D_2O at various pD values:

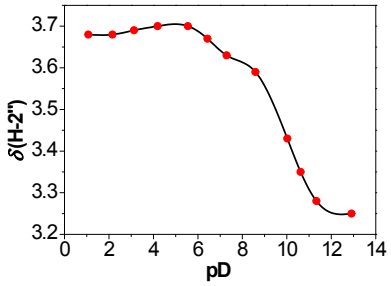


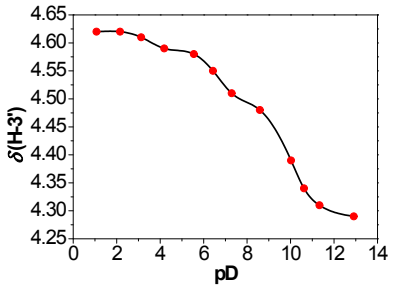
^{31}P NMR spectra of **15a** measured in D_2O at various pD values:

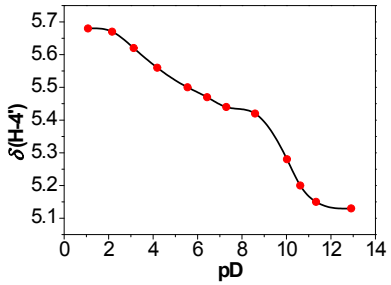


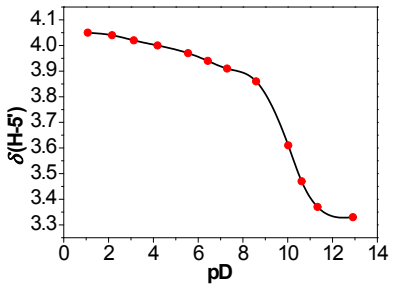
pD dependence of ^{1}H chemical shifts of pyrrolidine, phosphonate and adenine protons of **15a**:

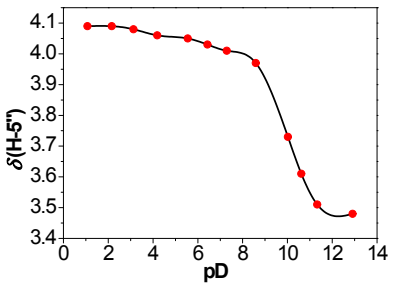


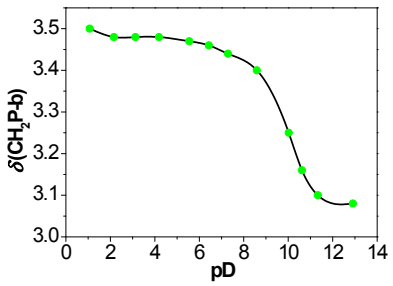


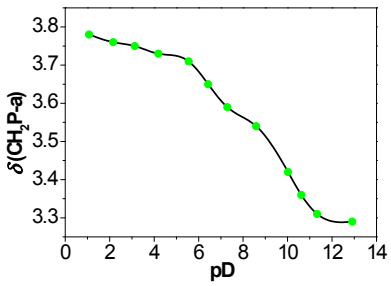


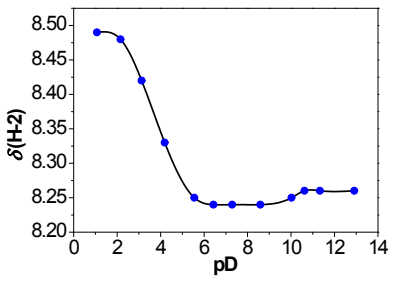


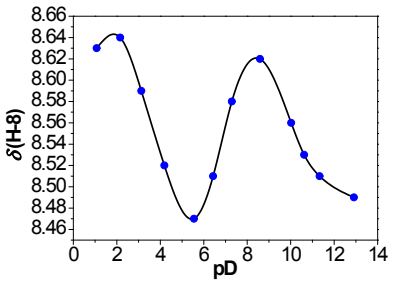




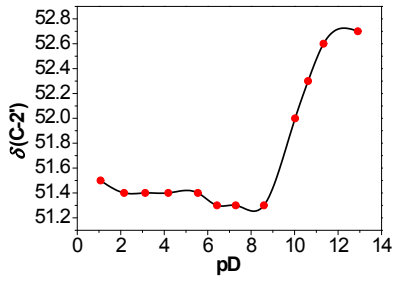


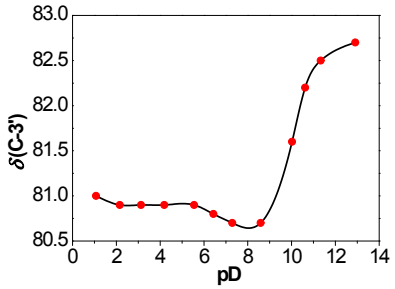


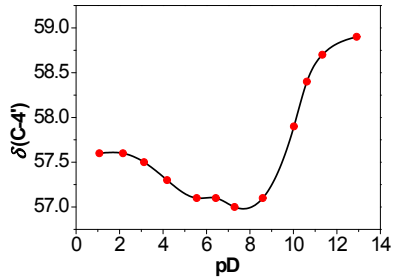


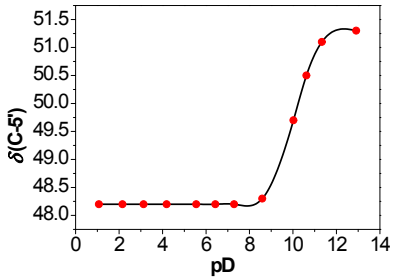


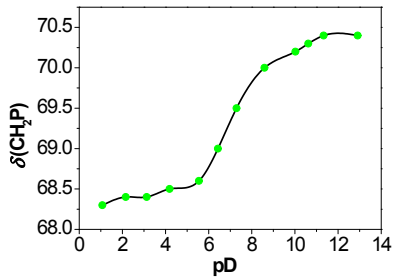
pD dependence of ^{13}C chemical shifts of pyrrolidine, phosphonate and adenine[a] carbons of **15a**:

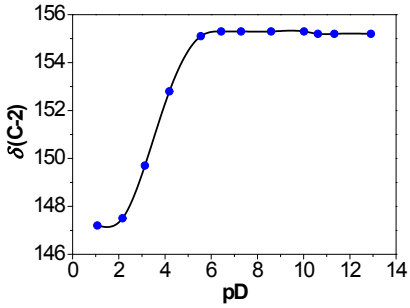


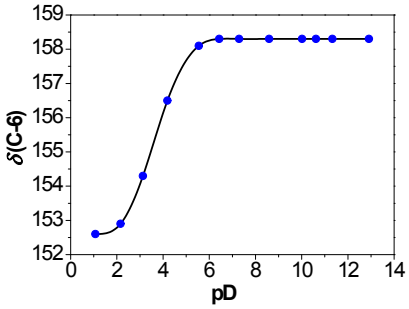


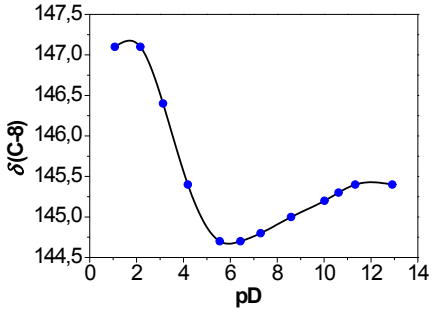






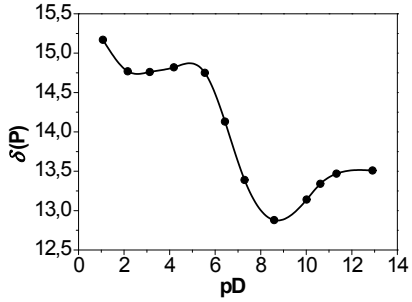




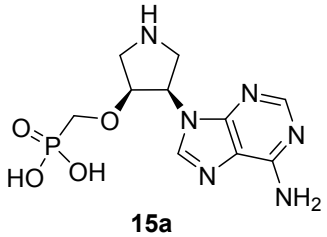


[a]C-4 and C-5 are not shown due to their negligible changes in their chemical shifts

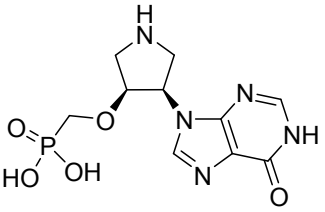
pD dependence of ^{31}P chemical shift of **15a**:



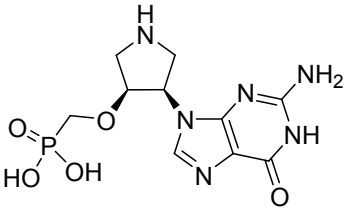
Copies of ^{1}H, ^{13}C and ^{31}P NMR spectra of **15a-e** and **16a-c**



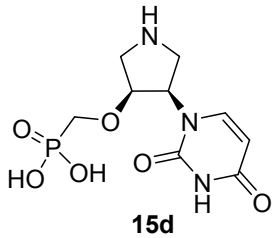
15a



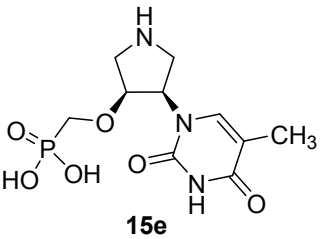
15b



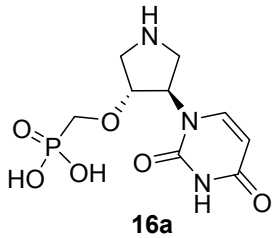
15c



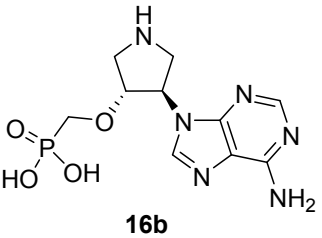
15d



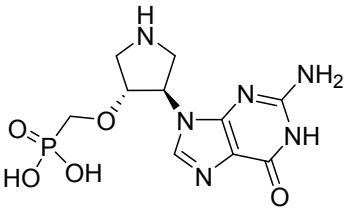
15e



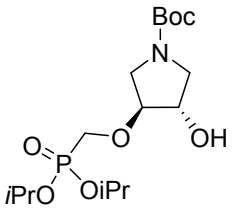
16a



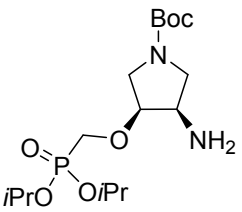
16b



16c

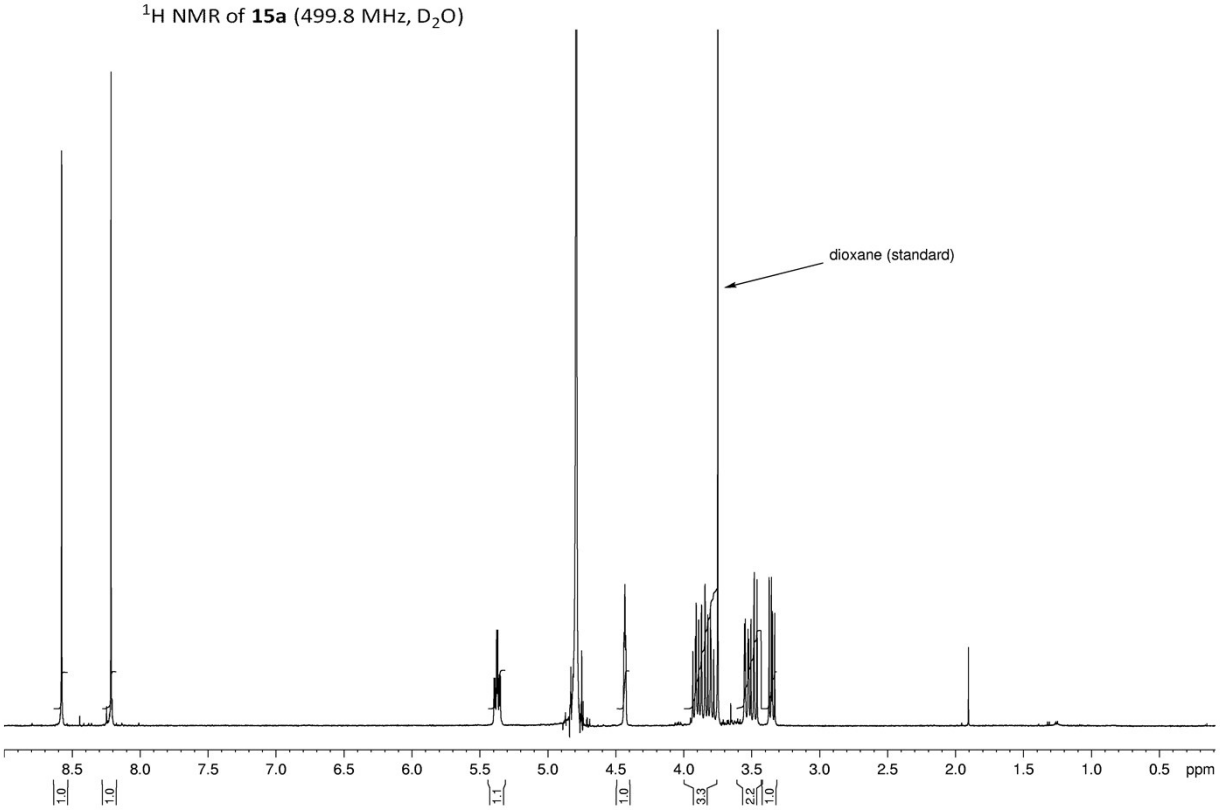


16a

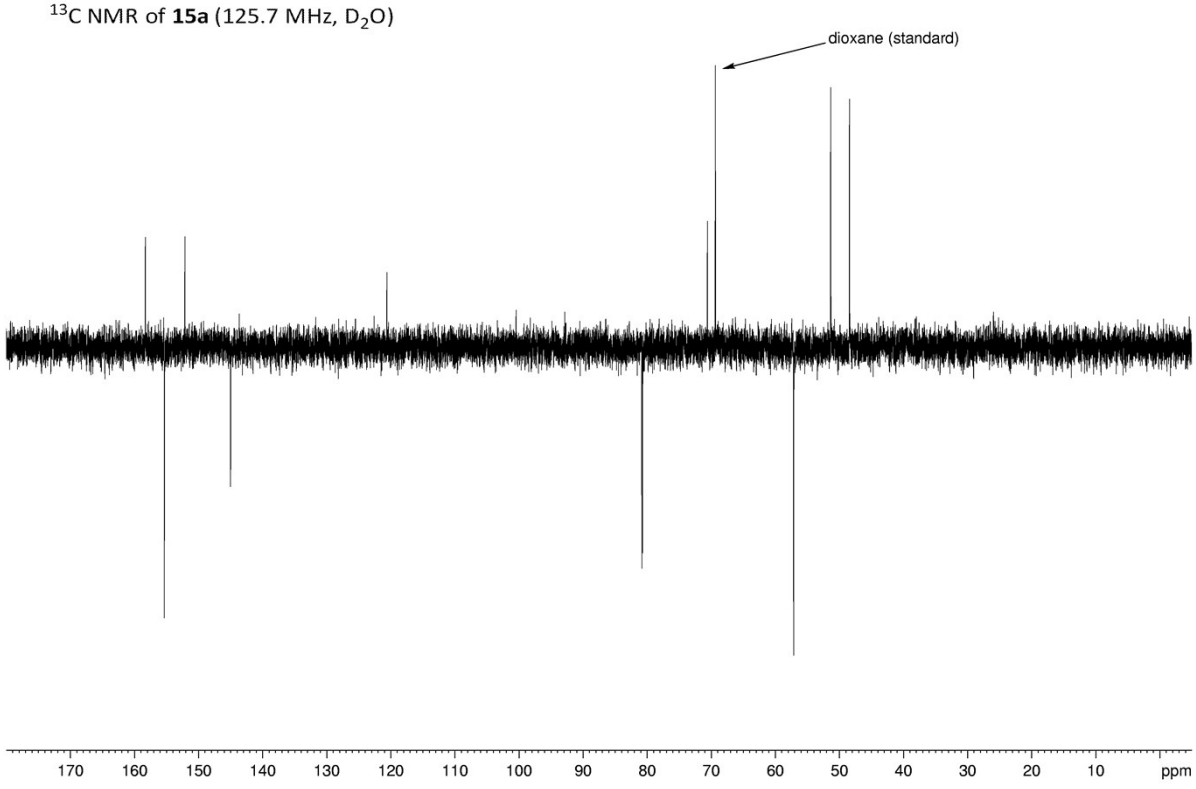


23

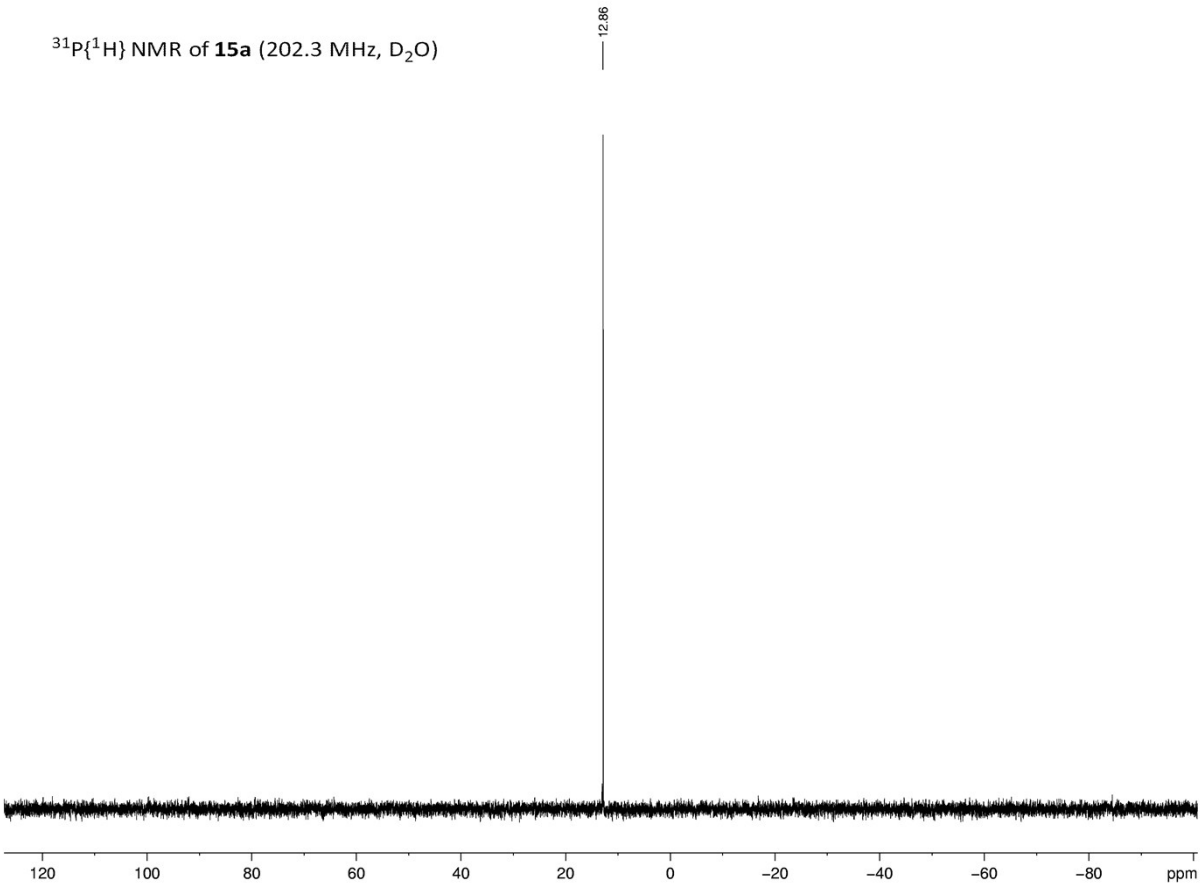
^{1}H NMR of **15a** (499.8 MHz, D_2O)



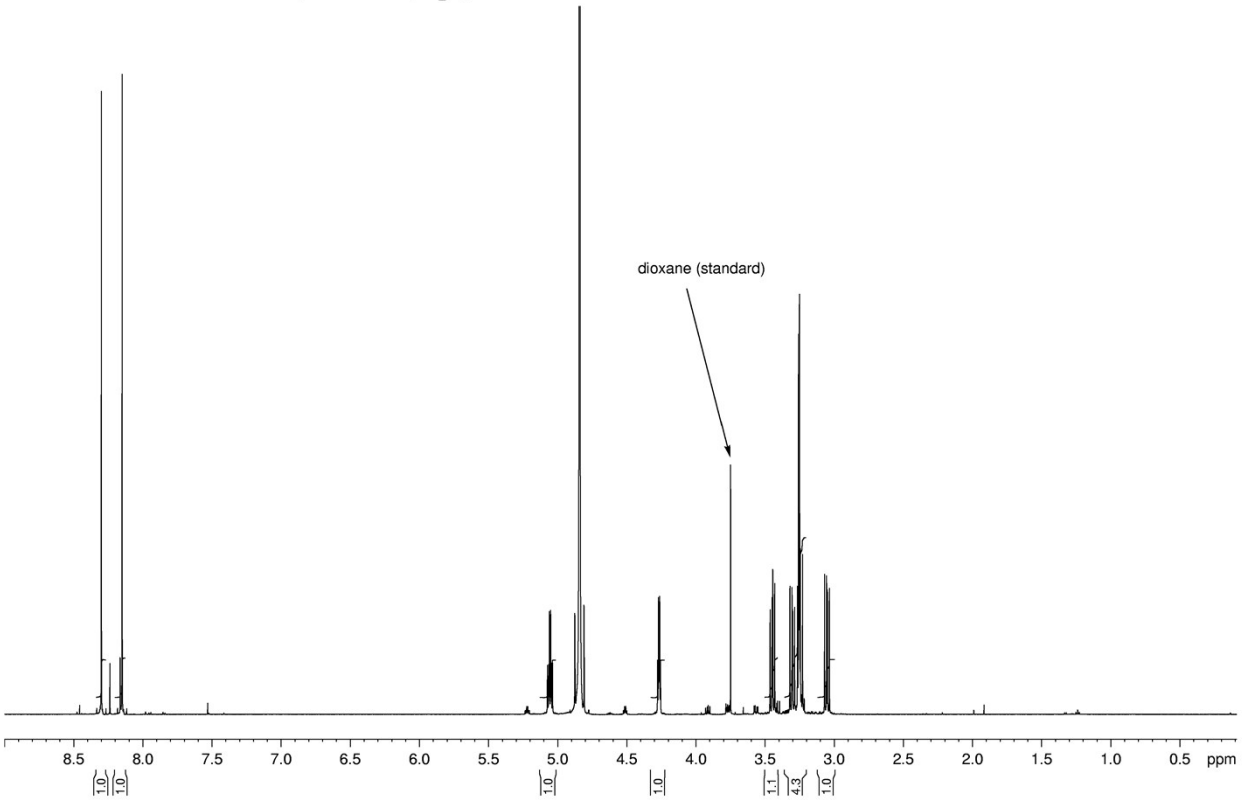
^{13}C NMR of **15a** (125.7 MHz, D_2O)

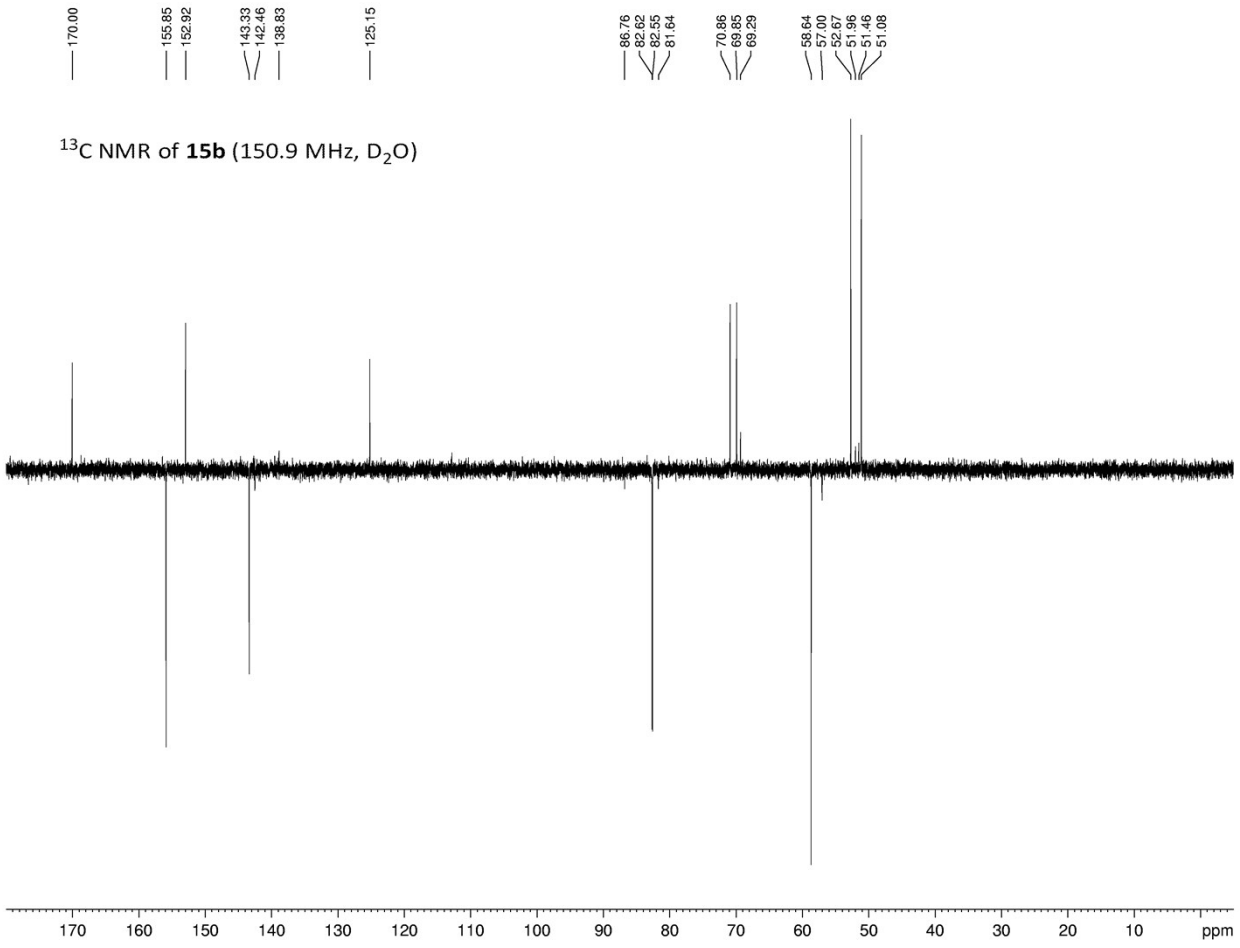


$^{31}P\{^{1}H\}$ NMR of **15a** (202.3 MHz, D_2O)

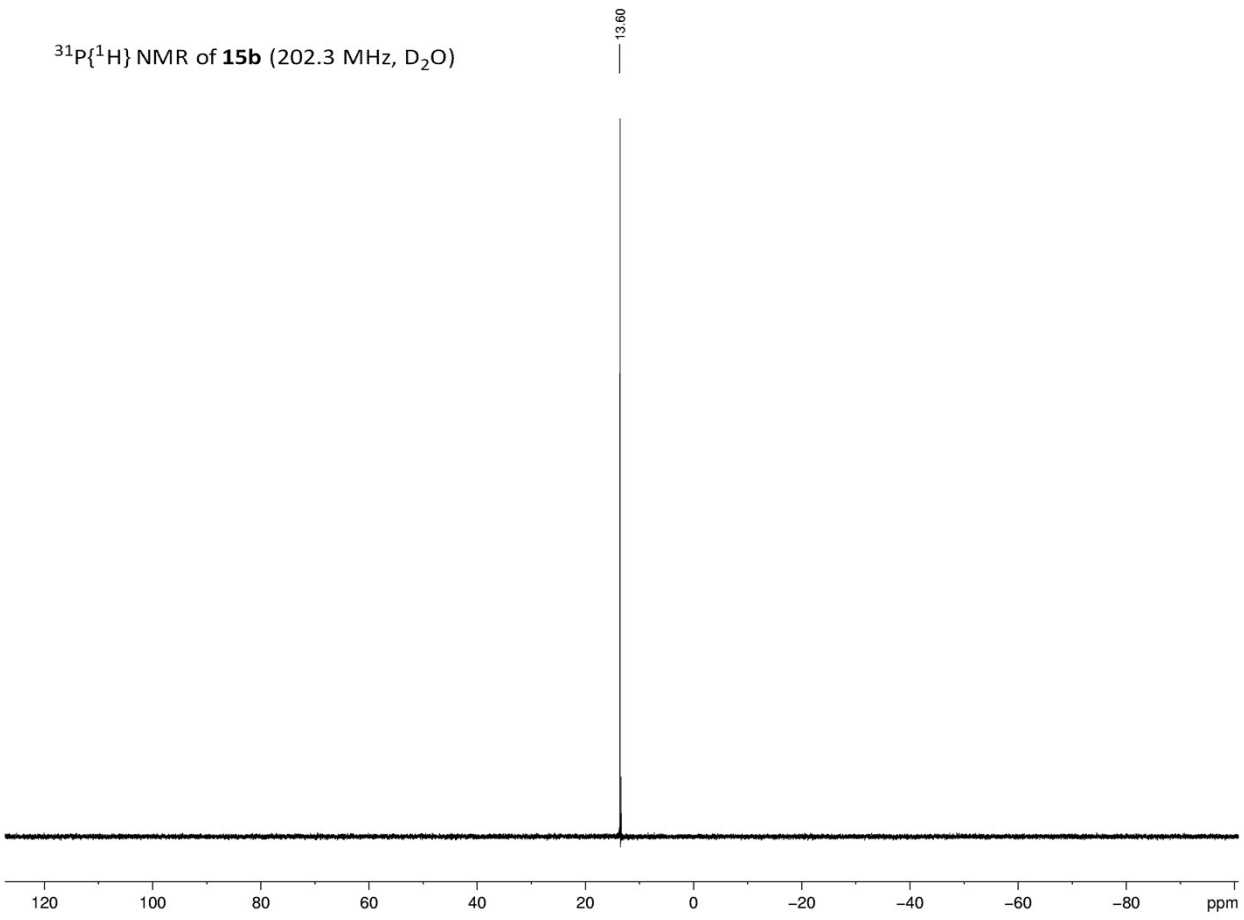


^{1}H NMR of **15b** (600.1 MHz, D_2O)

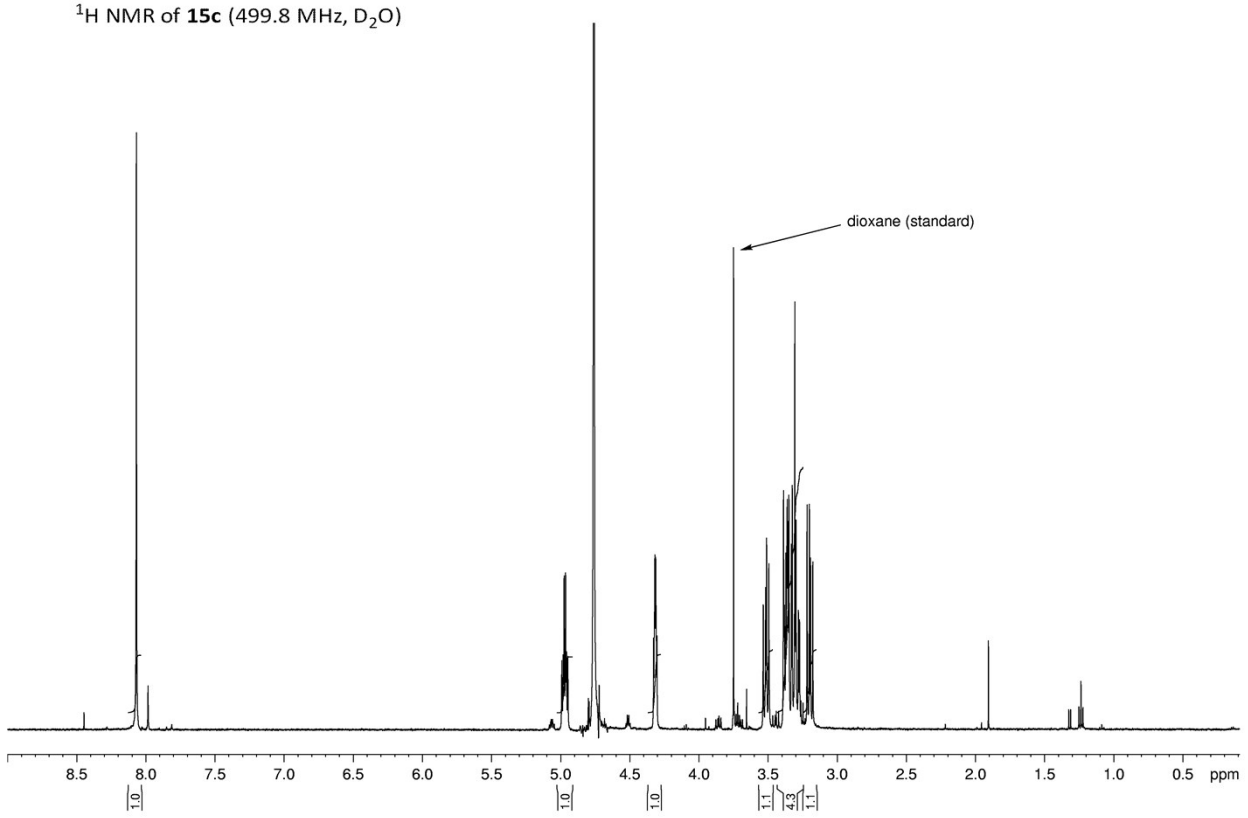


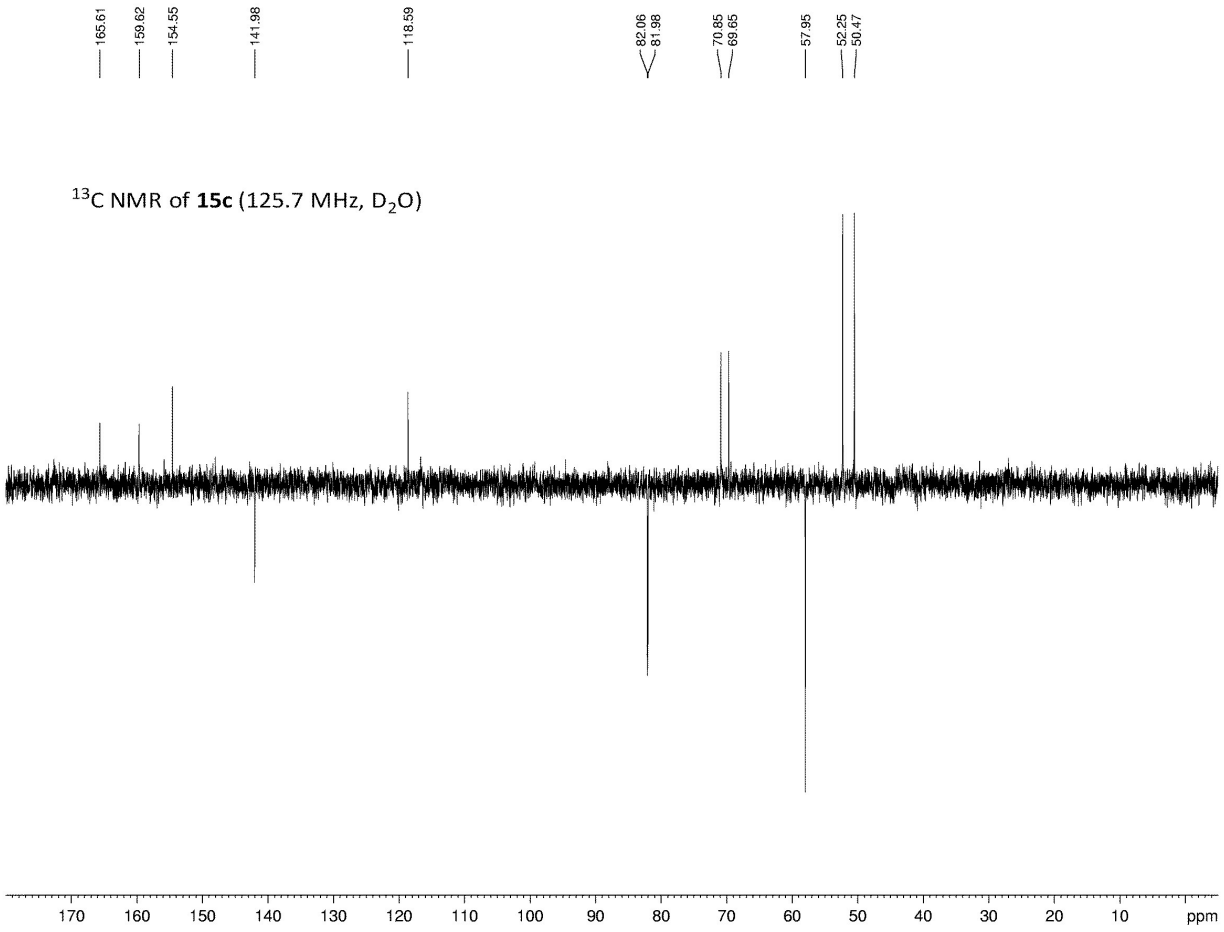

170.00
155.85
152.92
143.33
142.46
138.83
125.15
86.76
82.62
82.55
81.64
70.86
69.85
69.29
58.64
57.00
52.67
51.96
51.46
51.08
^{13}C NMR of **15b** (150.9 MHz, D_2O)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

$^{31}P\{^{1}H\}$ NMR of **15b** (202.3 MHz, D_2O)

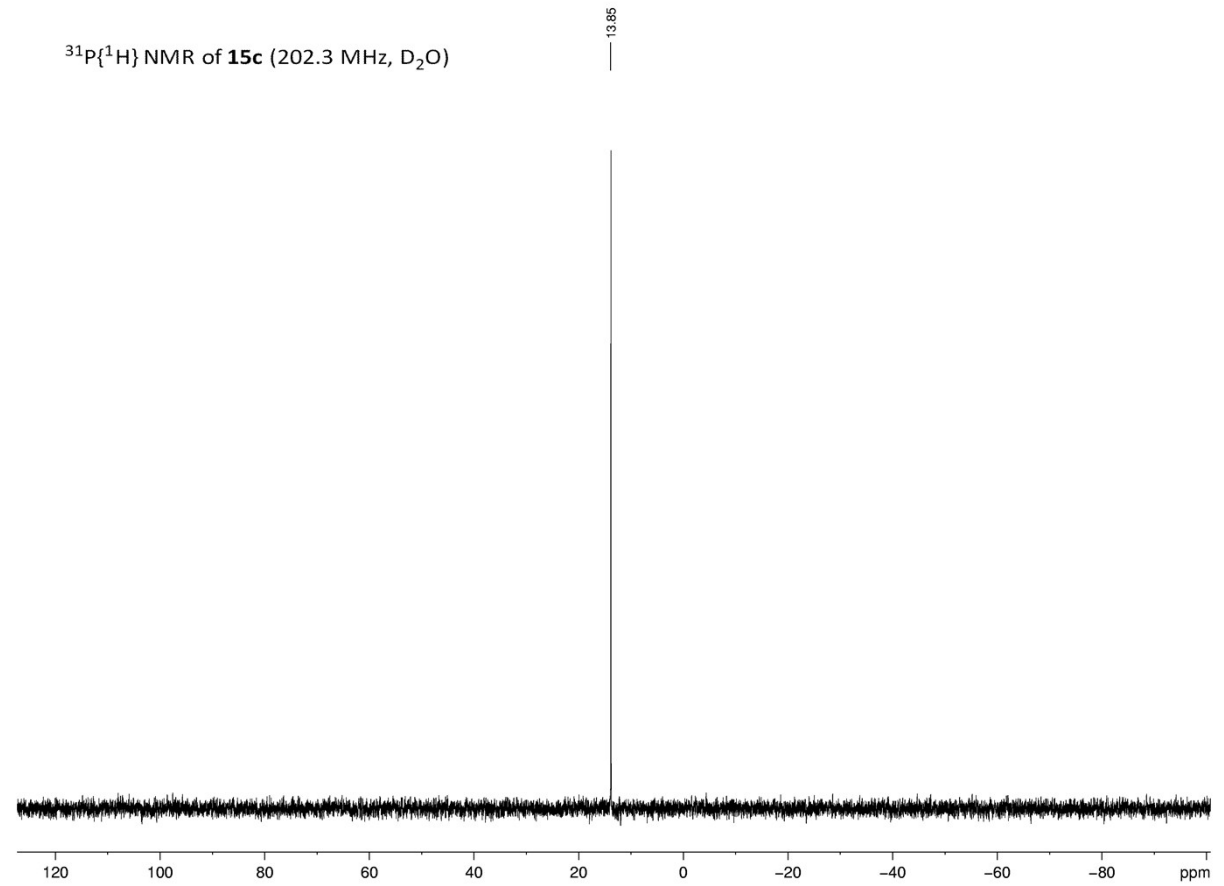


^{1}H NMR of **15c** (499.8 MHz, D_2O)



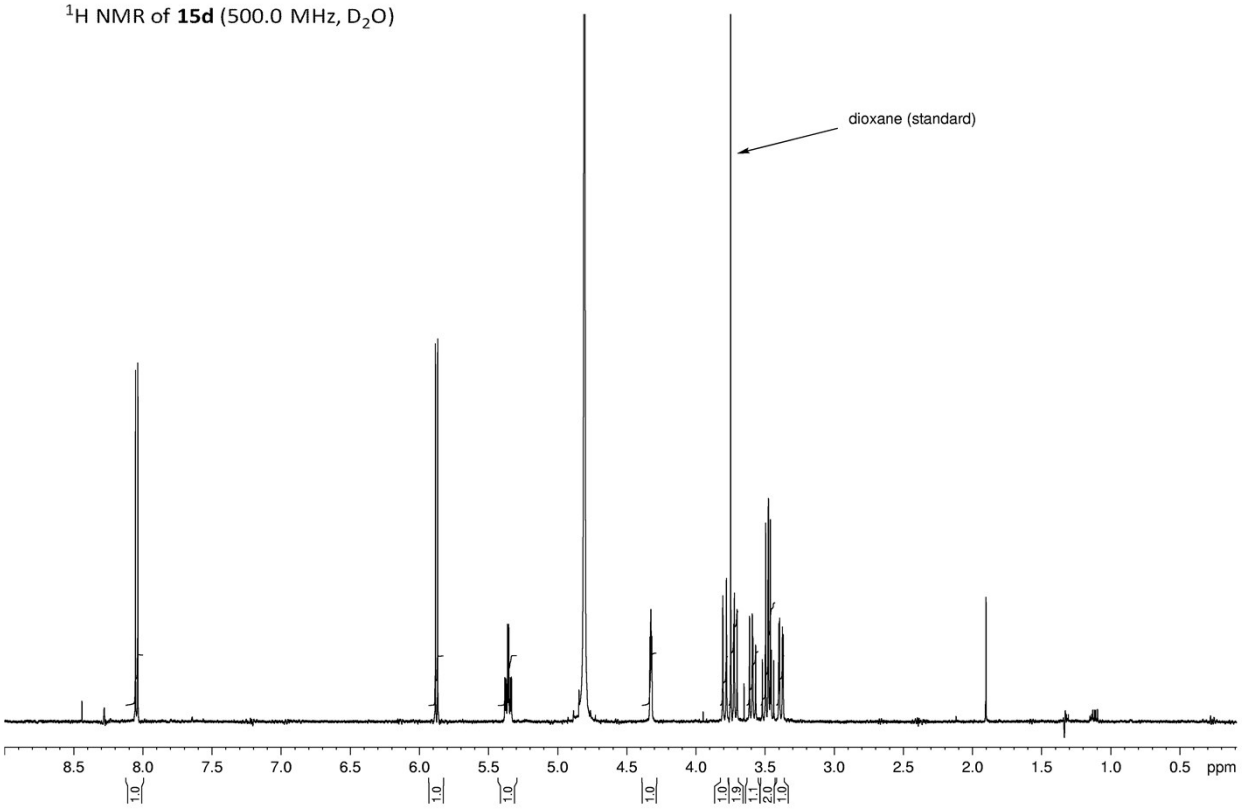


^{13}C NMR of **15c** (125.7 MHz, D_2O)

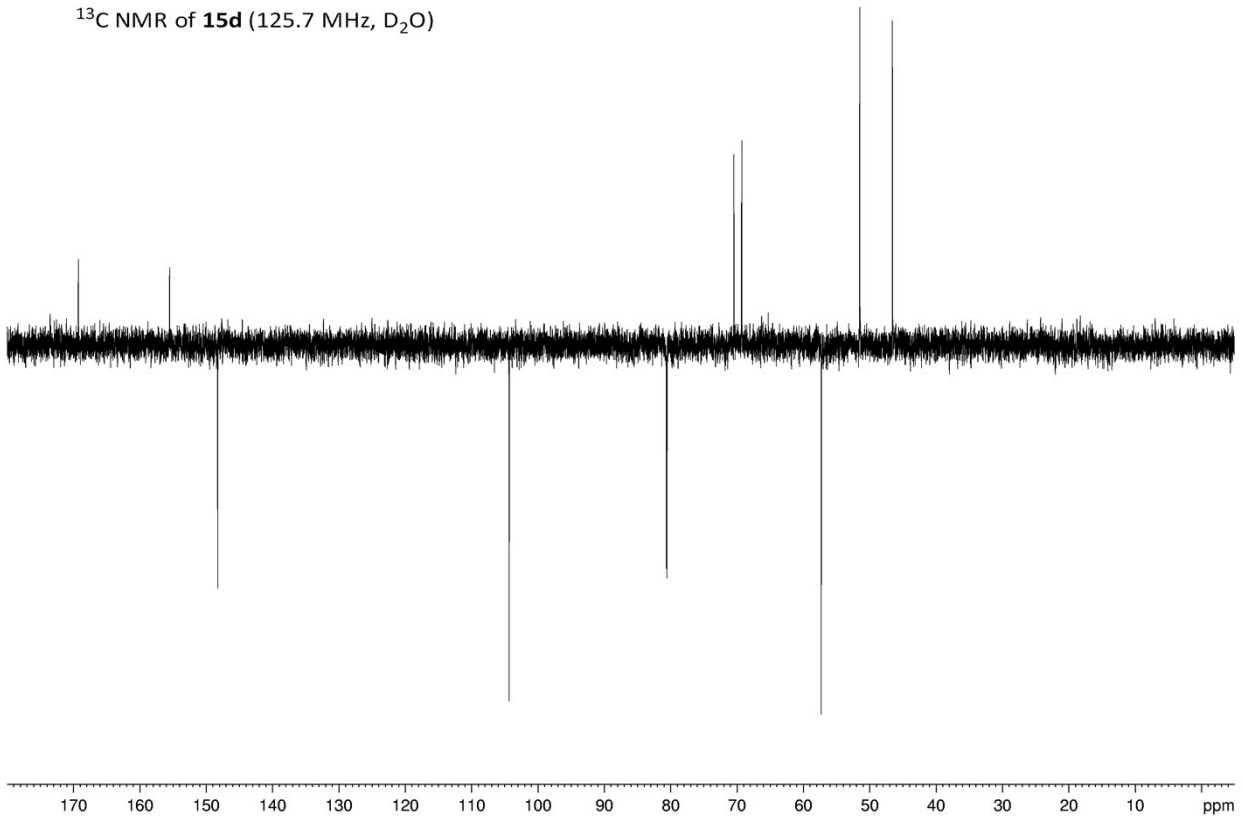


$^{31}P\{^1H\}$ NMR of **15c** (202.3 MHz, D_2O)

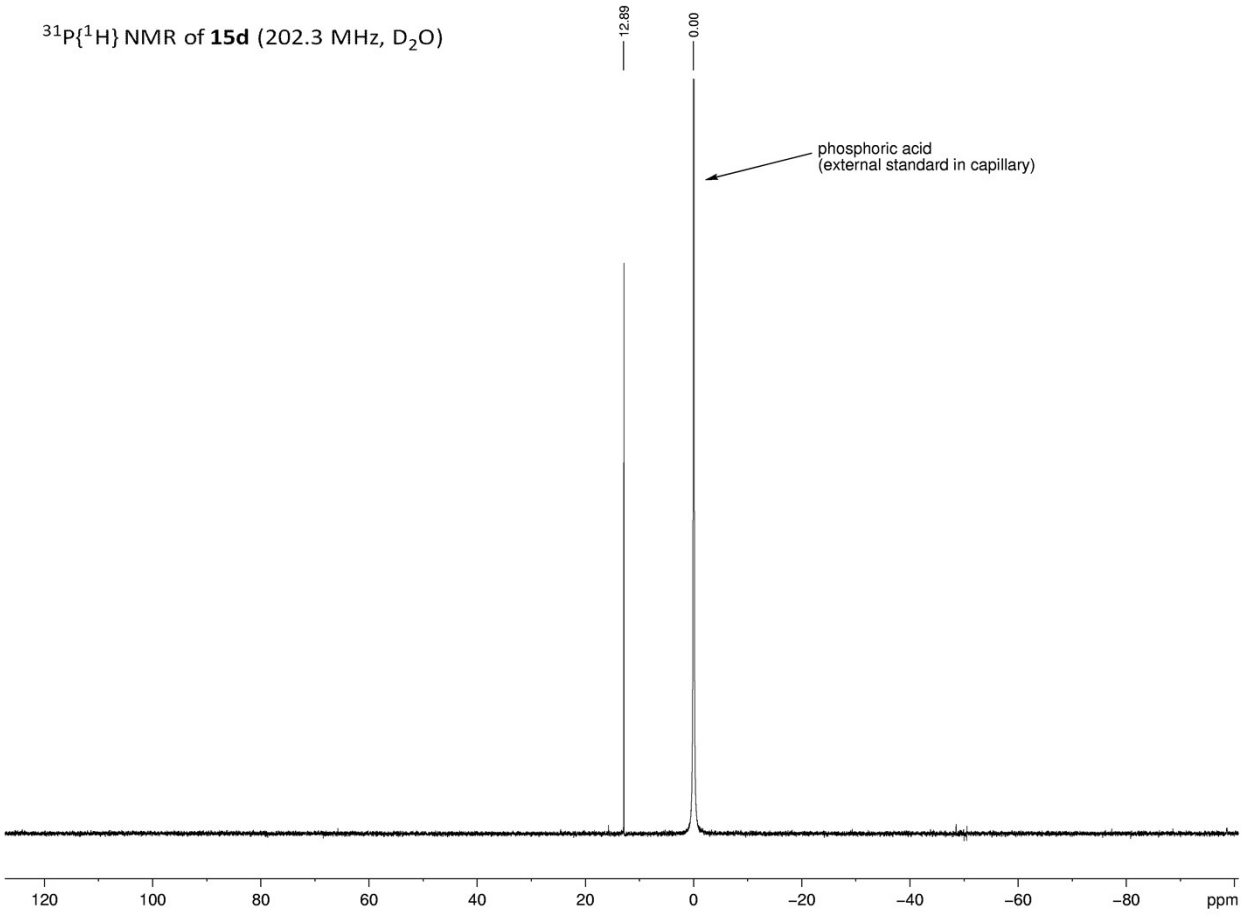
^{1}H NMR of **15d** (500.0 MHz, D_2O)



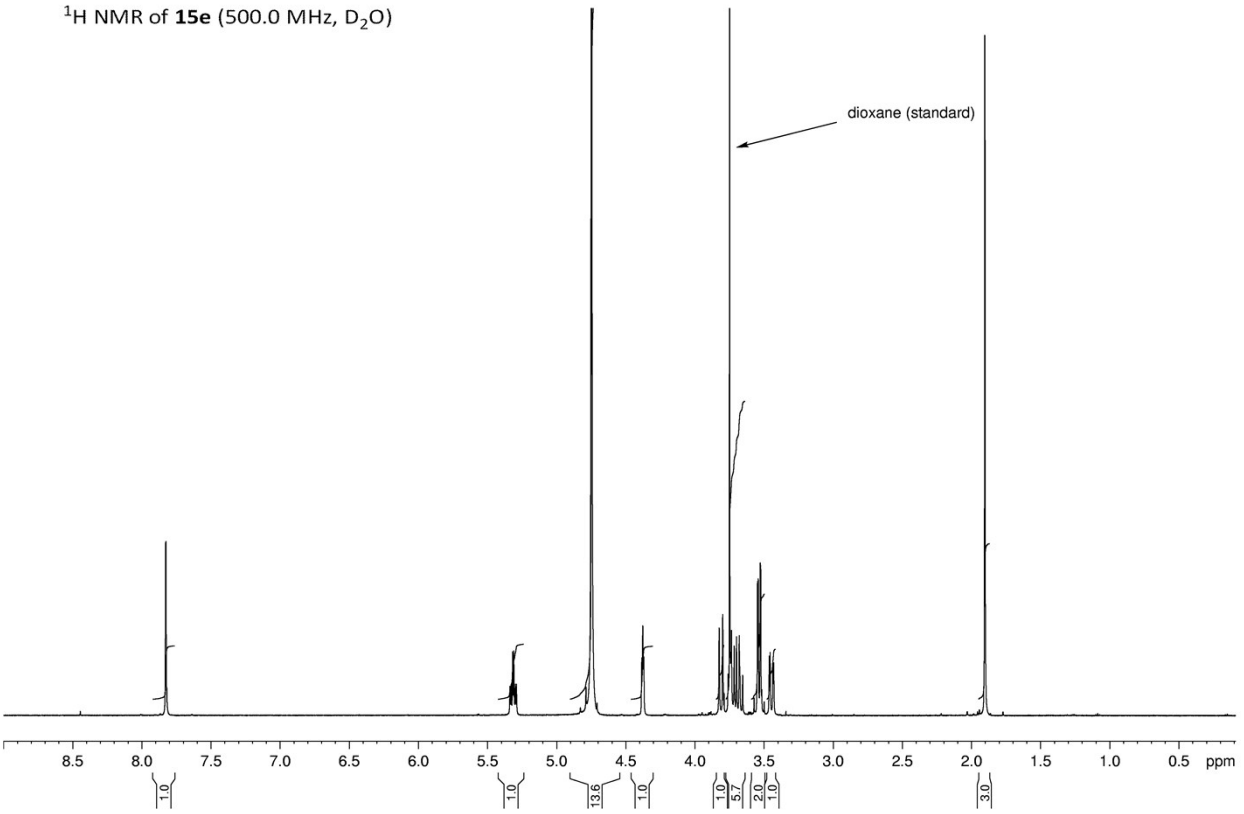
^{13}C NMR of **15d** (125.7 MHz, D_2O)

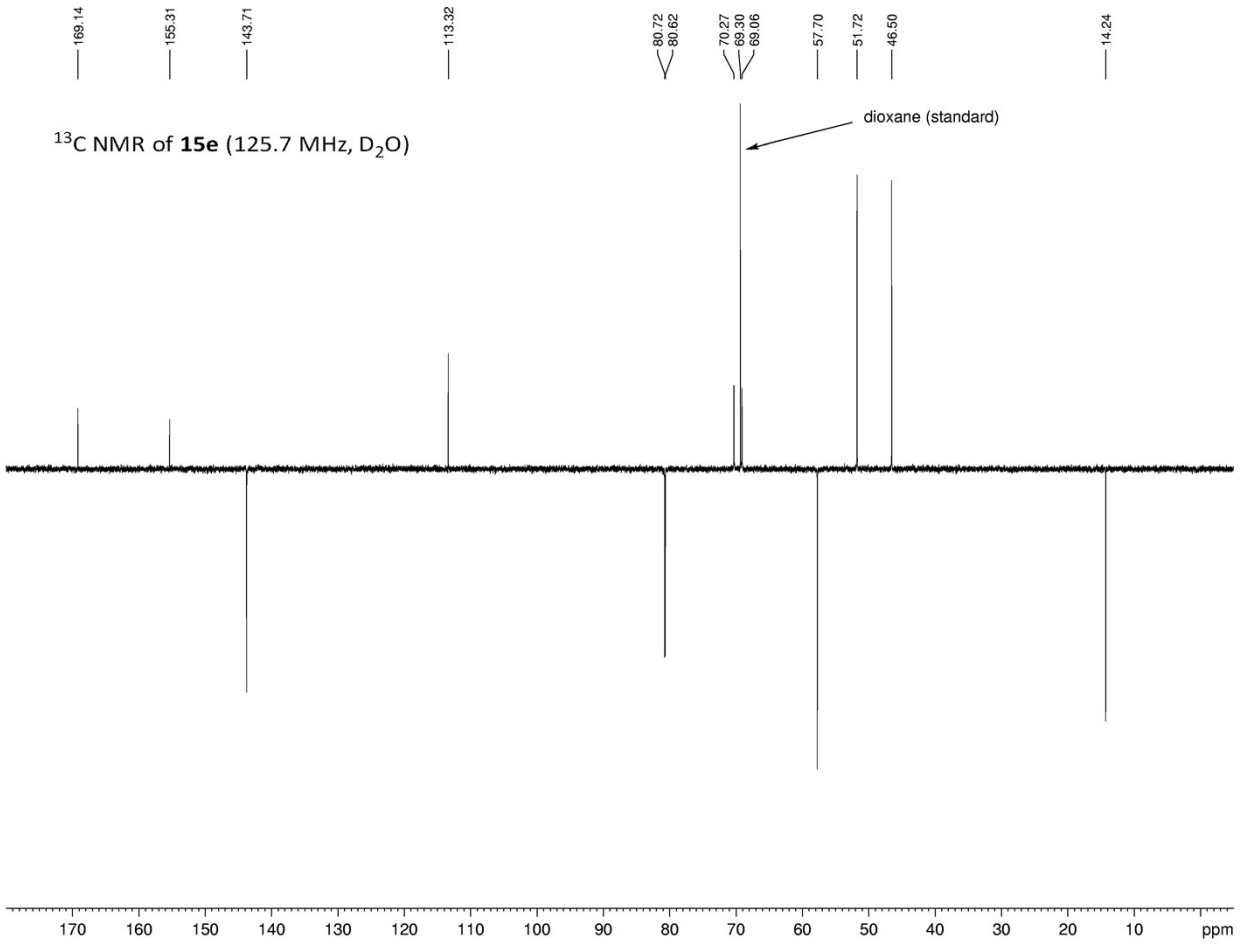


$^{31}P\{^{1}H\}$ NMR of **15d** (202.3 MHz, D_2O)

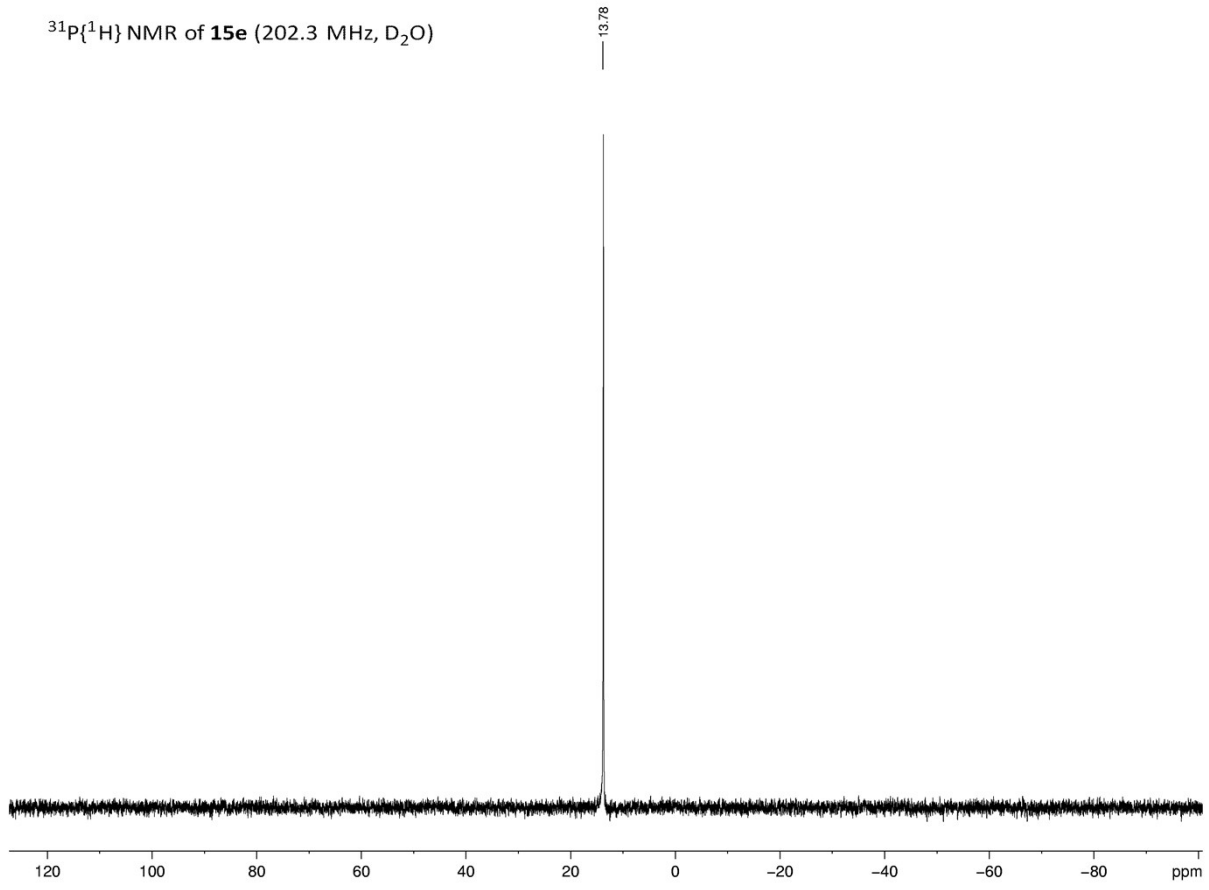


^{1}H NMR of **15e** (500.0 MHz, D_2O)

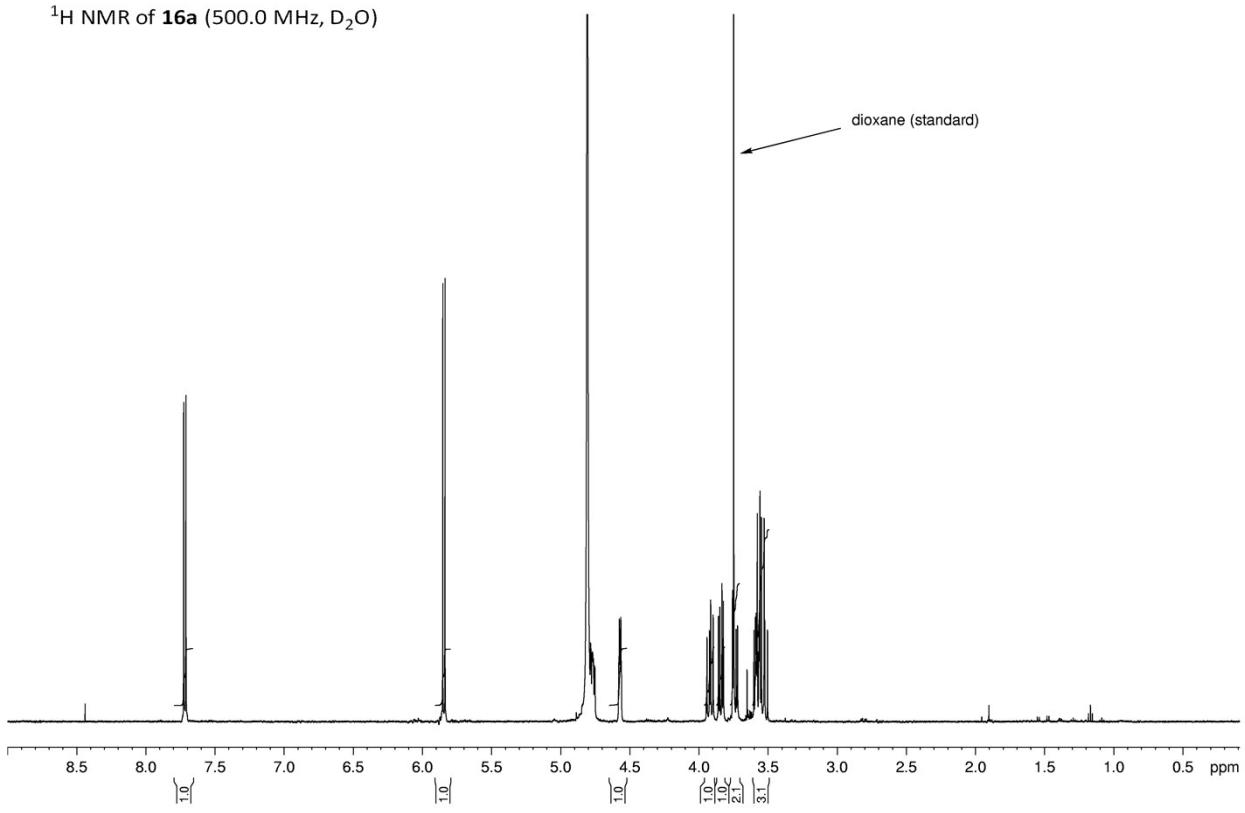


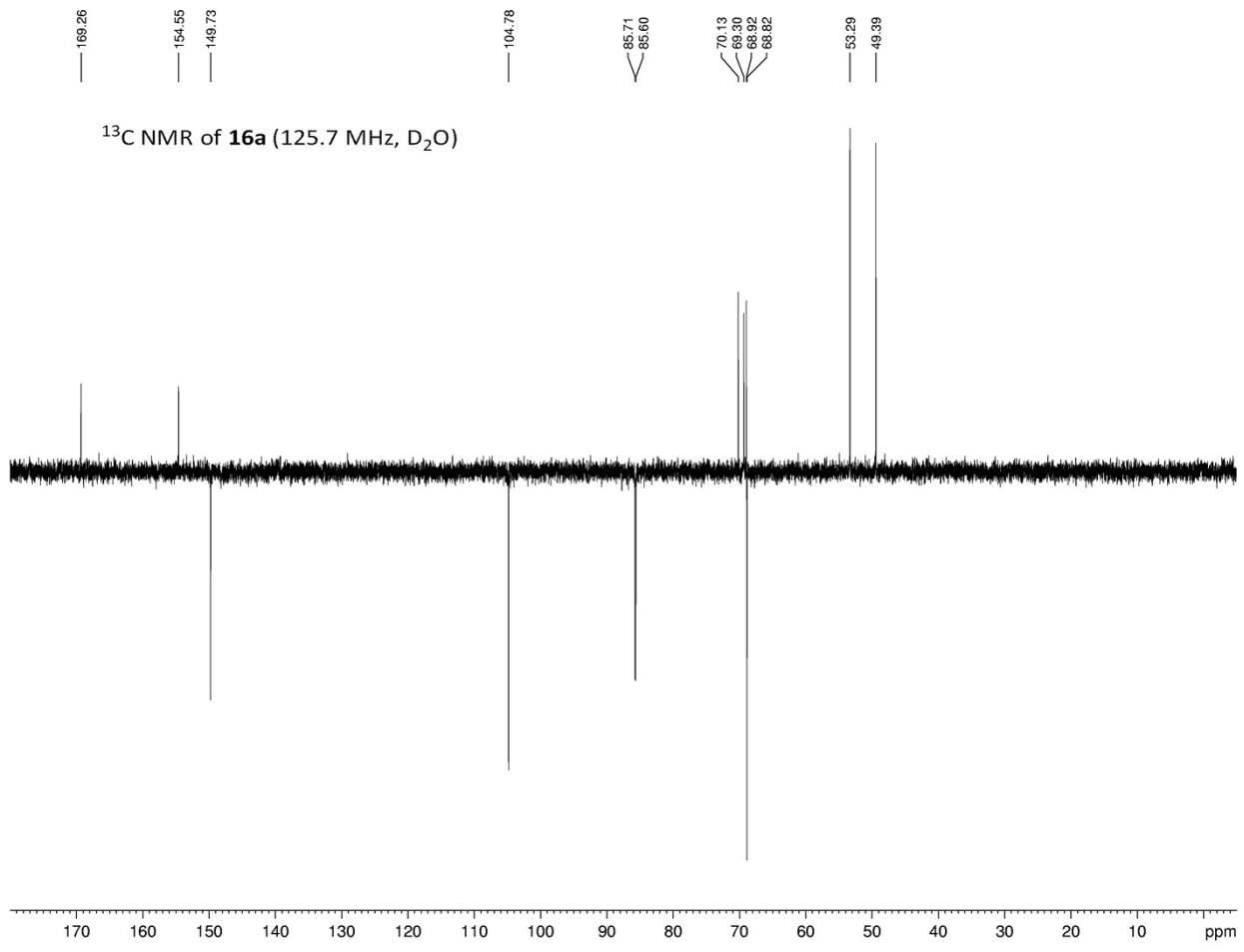


^{13}C NMR of **15e** (125.7 MHz, D_2O)

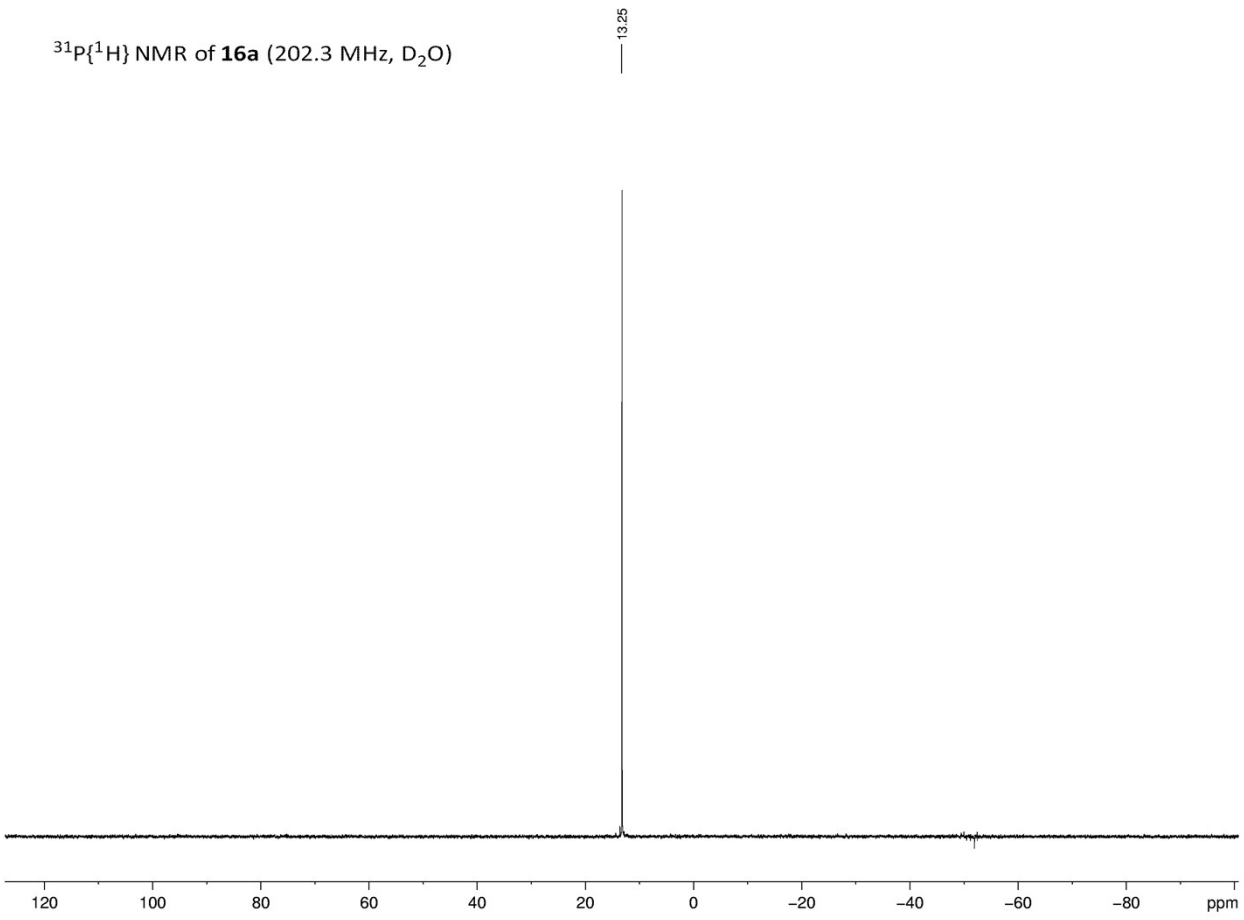


$^{31}P\{^1H\}$ NMR of **15e** (202.3 MHz, D_2O)

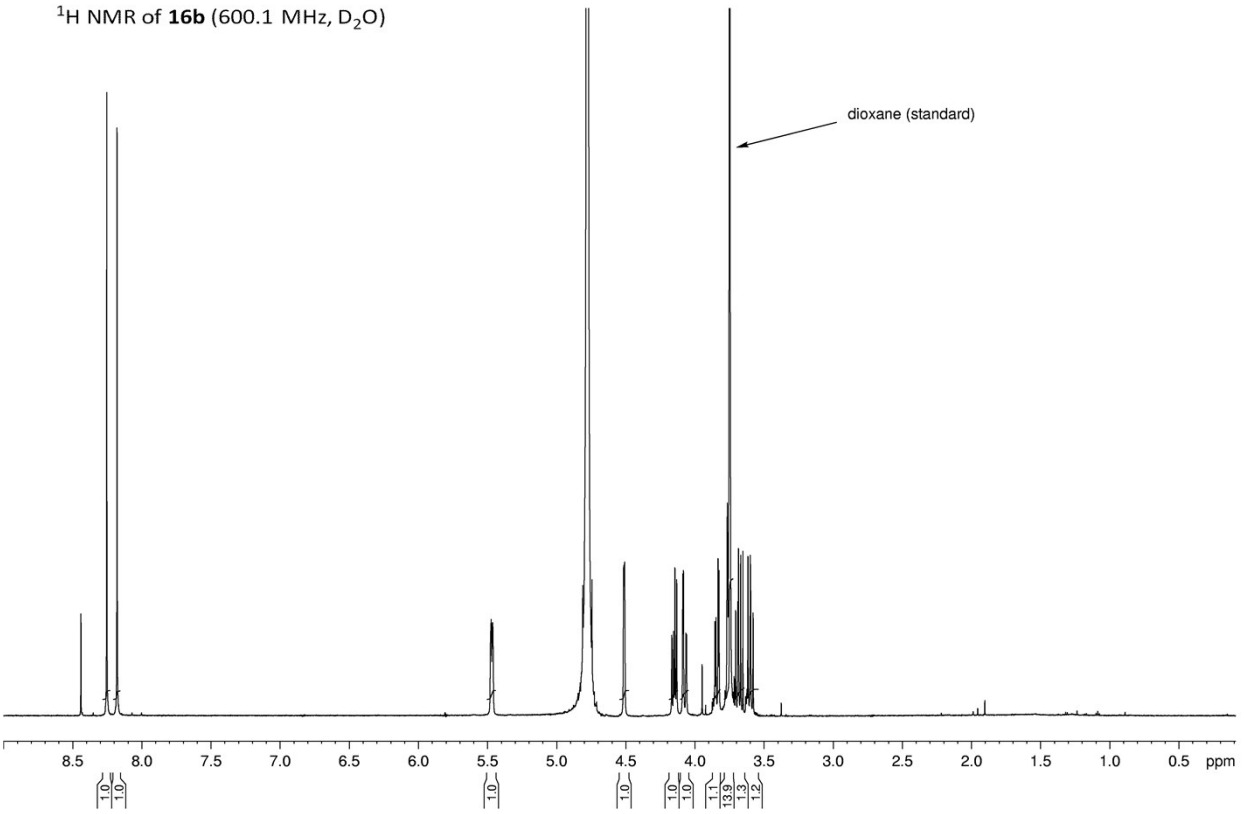

^{1}H NMR of **16a** (500.0 MHz, D_2O)
dioxane (standard)
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.0 1.0 1.0 1.0 1.0 2.1 3.1

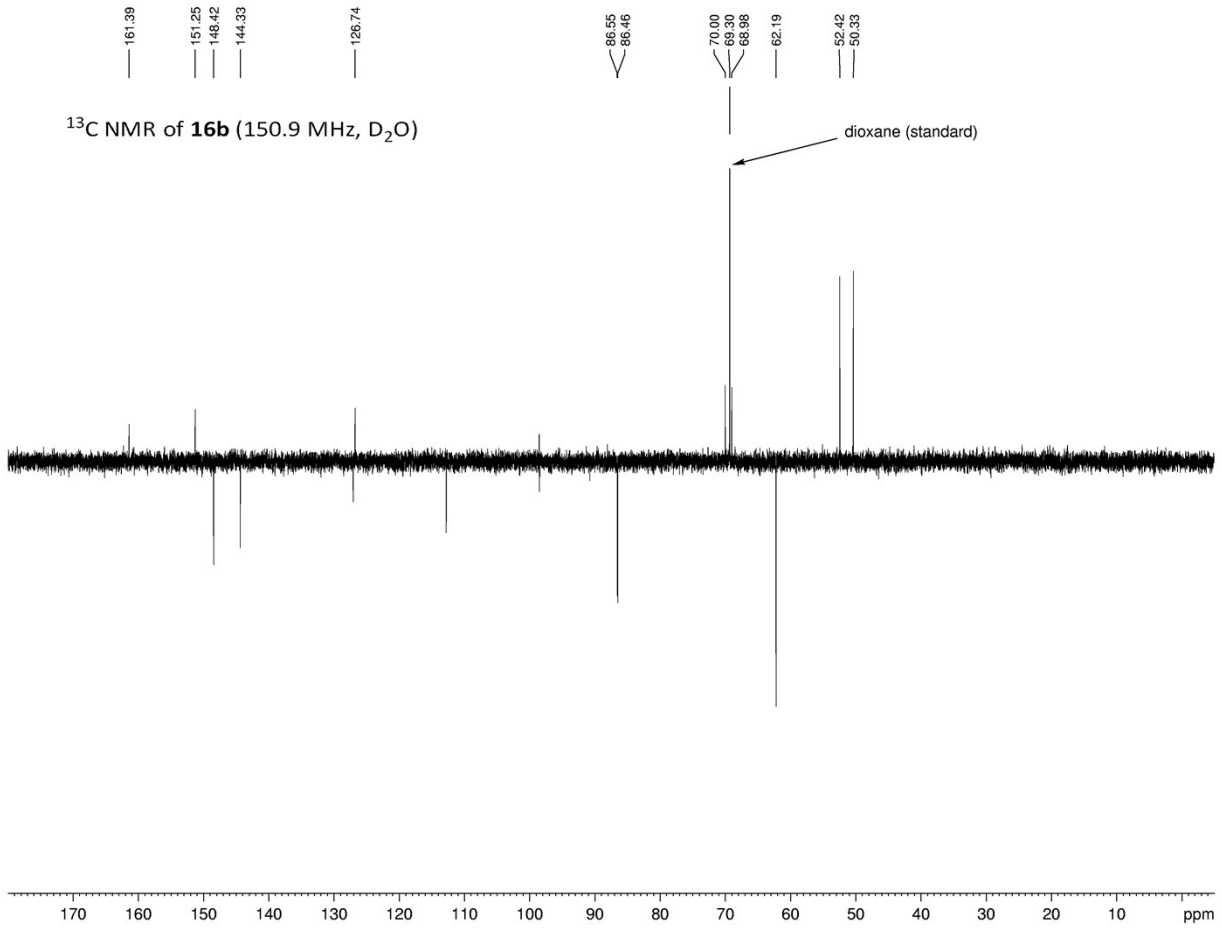

169.26
154.55
149.73
104.78
85.71
85.60
70.13
69.30
68.92
68.82
53.29
49.39
^{13}C NMR of **16a** (125.7 MHz, D_2O)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

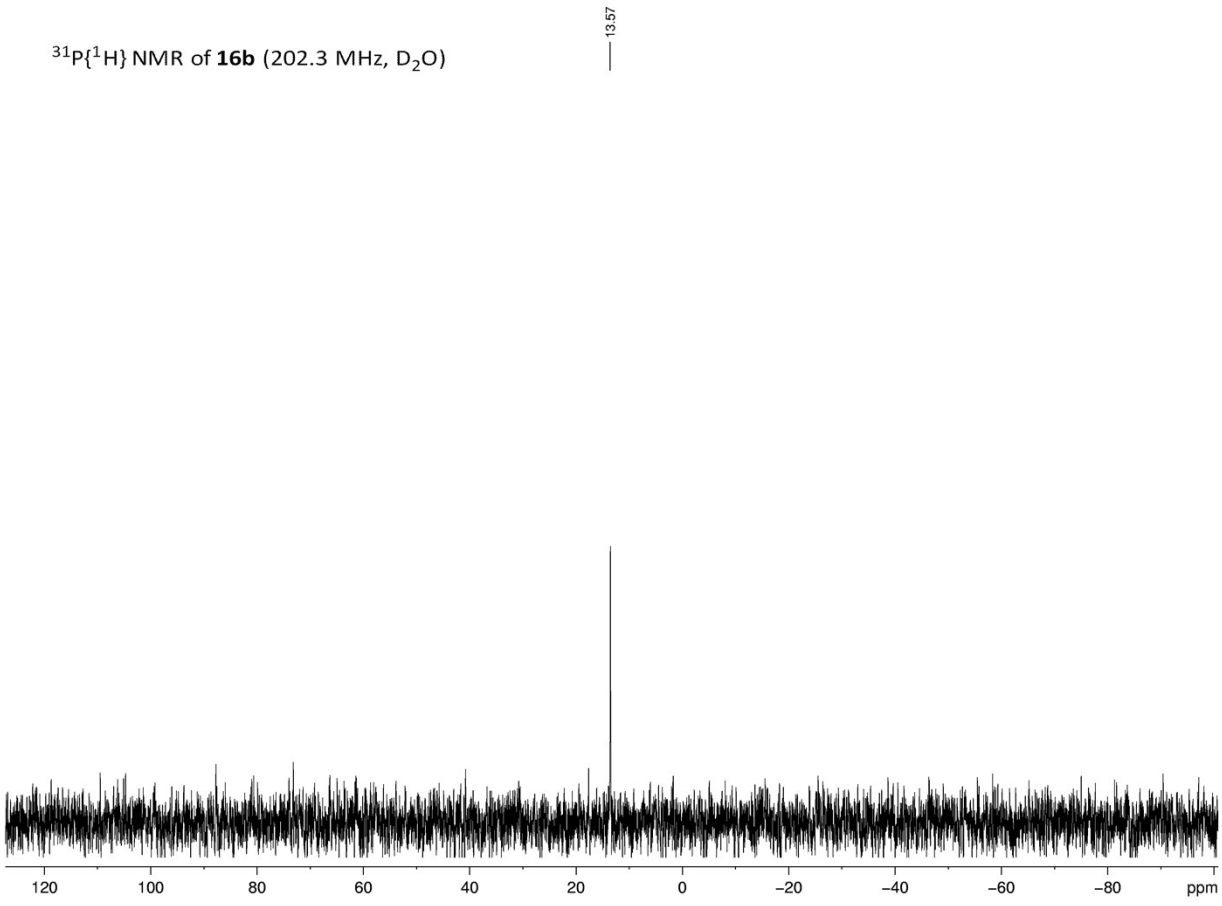
$^{31}P\{^{1}H\}$ NMR of **16a** (202.3 MHz, D_2O)



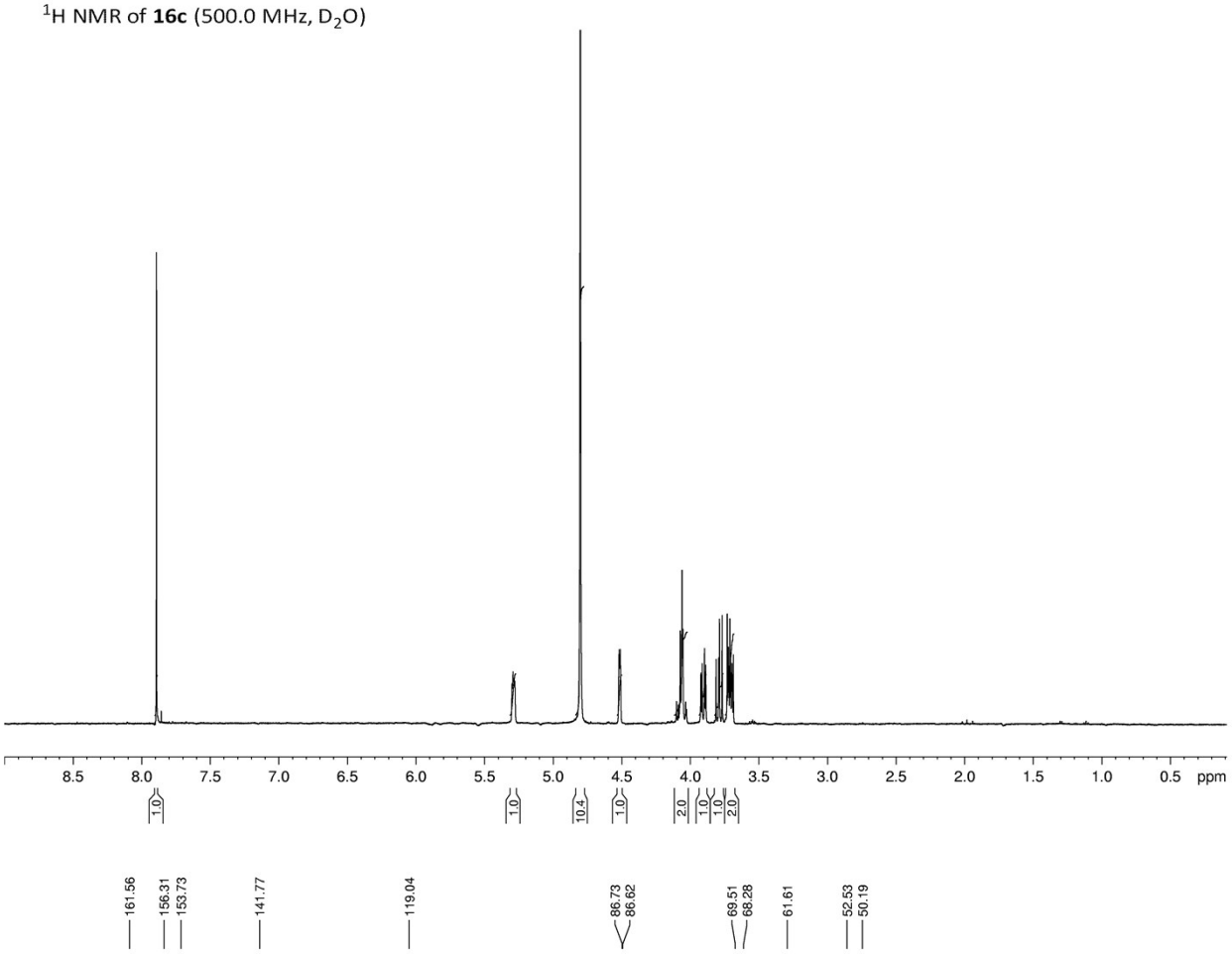
^{1}H NMR of **16b** (600.1 MHz, D_2O)



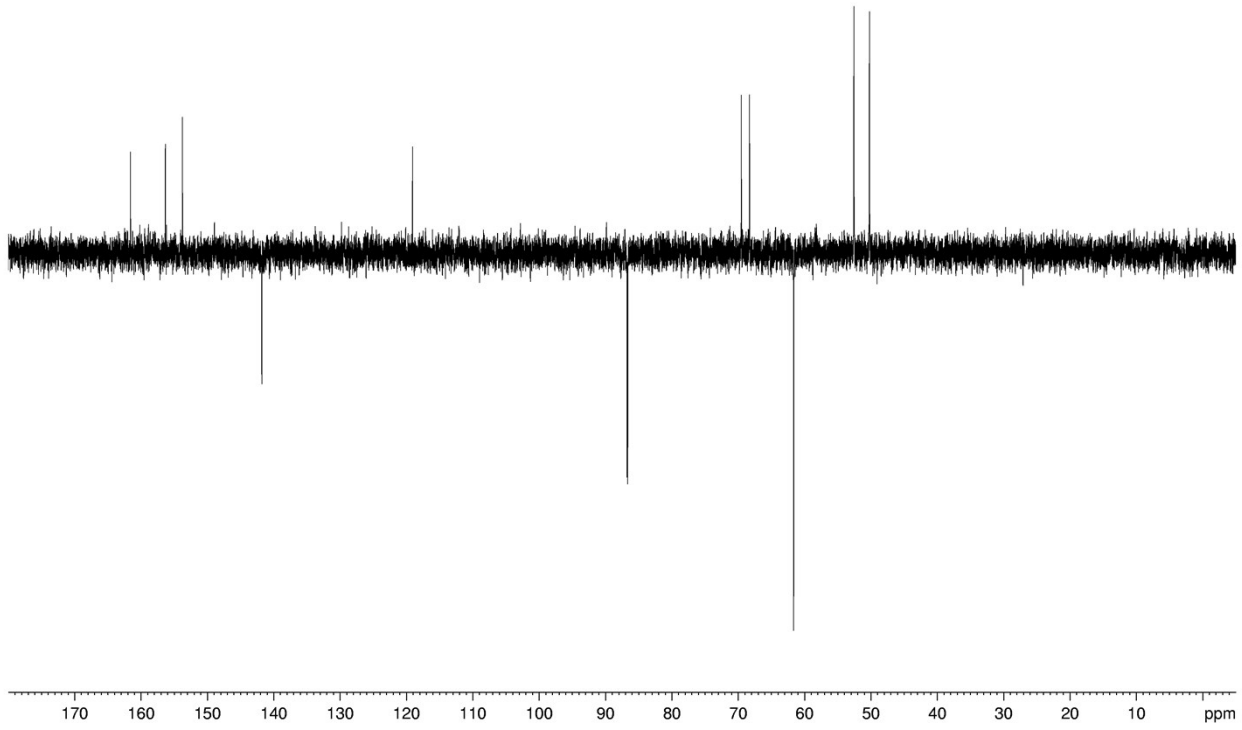

161.39
151.25
148.42
144.33
126.74
86.55
86.46
70.00
69.30
68.98
62.19
52.42
50.33
^{13}C NMR of **16b** (150.9 MHz, D_2O)
dioxane (standard)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


13.57
^{31}P{^{1}H} NMR of **16b** (202.3 MHz, D_2O)
120 100 80 60 40 20 0 −20 −40 −60 −80 ppm

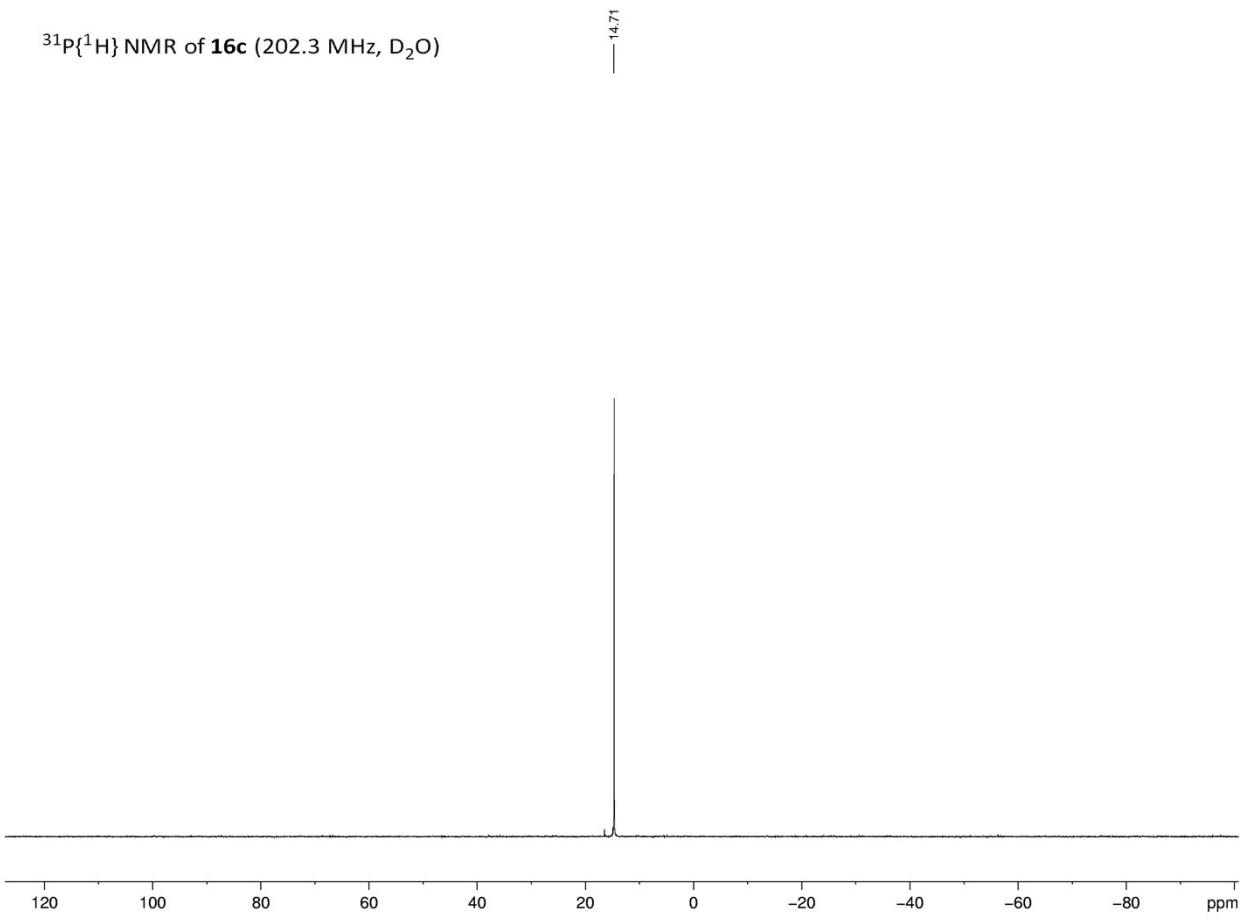
^{1}H NMR of **16c** (500.0 MHz, D_2O)



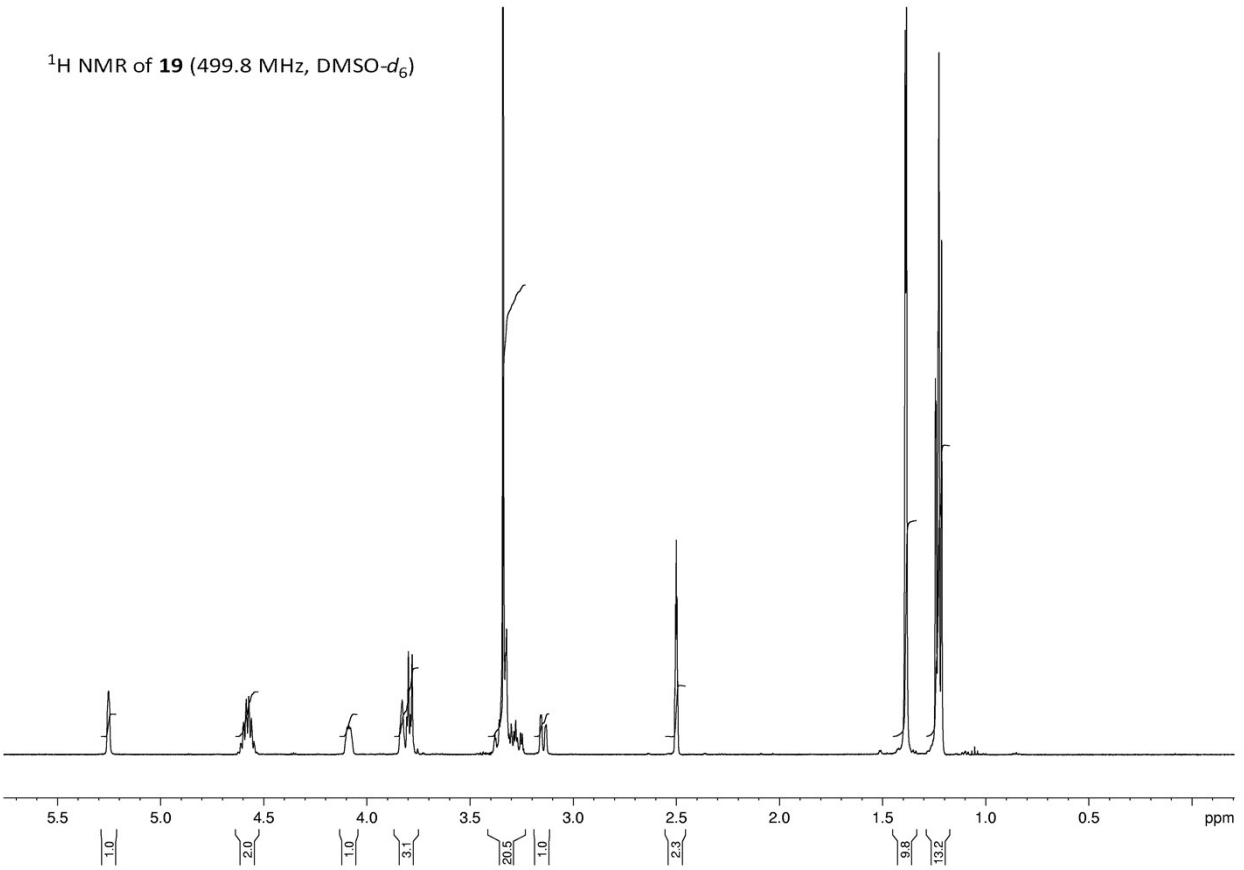
^{13}C NMR of **16c** (125.7 MHz, D_2O)

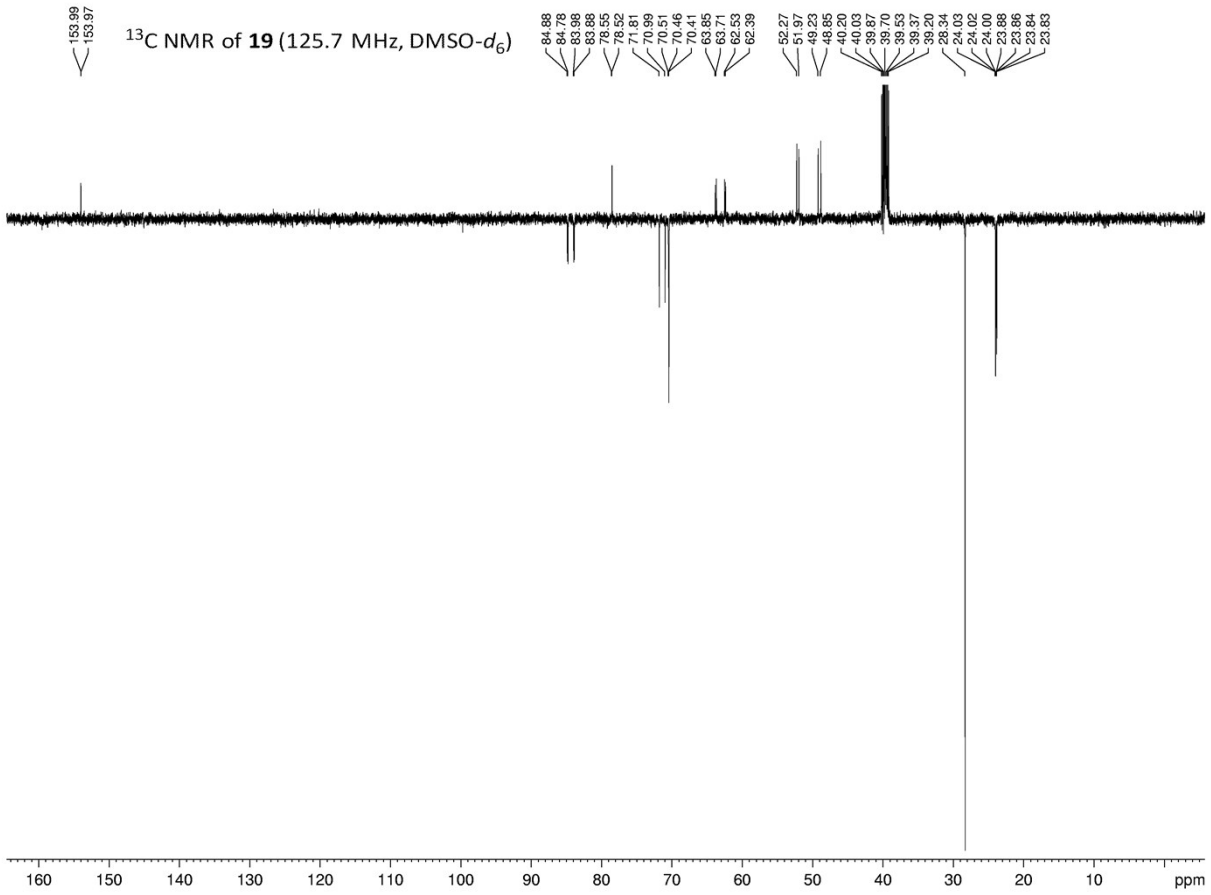


$^{31}P\{^{1}H\}$ NMR of **16c** (202.3 MHz, D_2O)

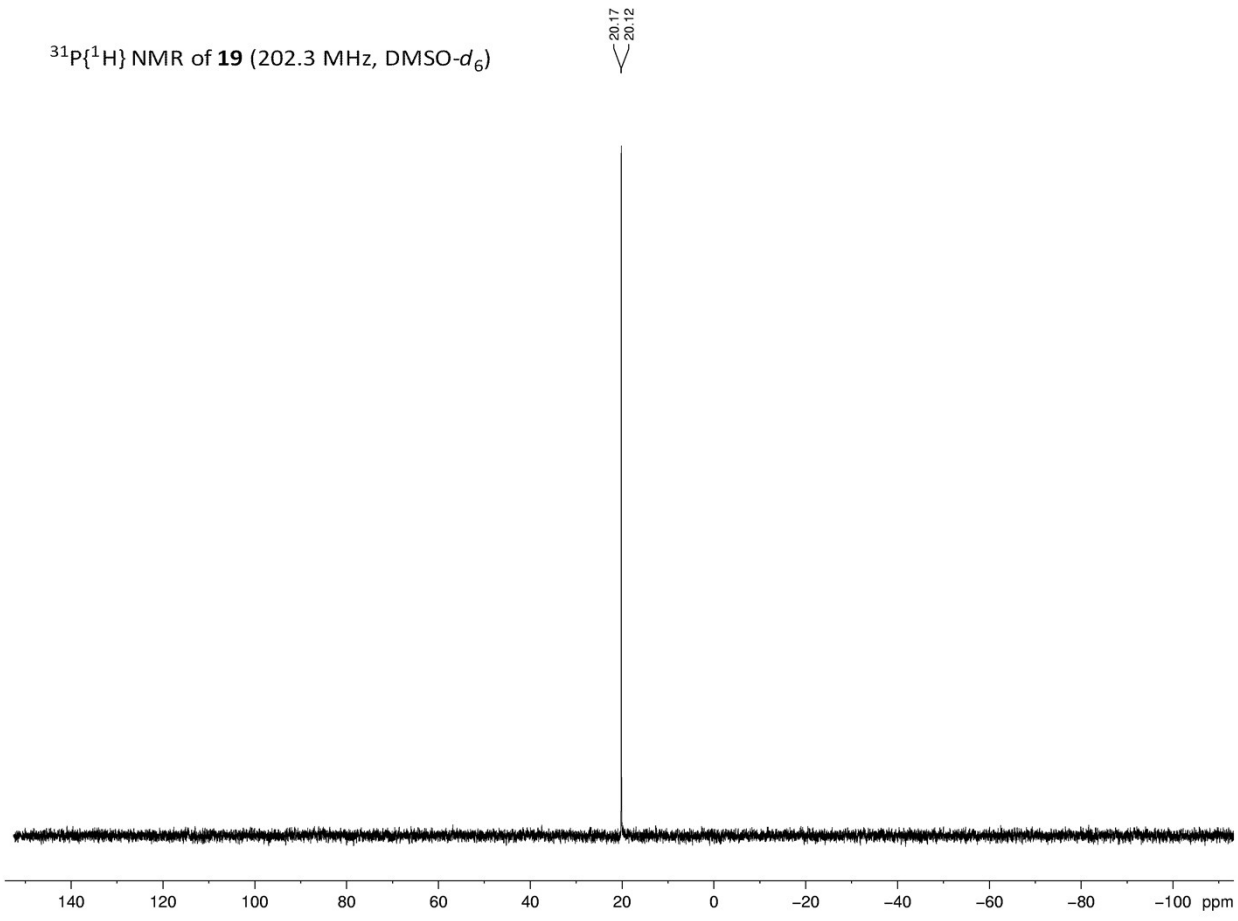


^{1}H NMR of **19** (499.8 MHz, DMSO-d_6)



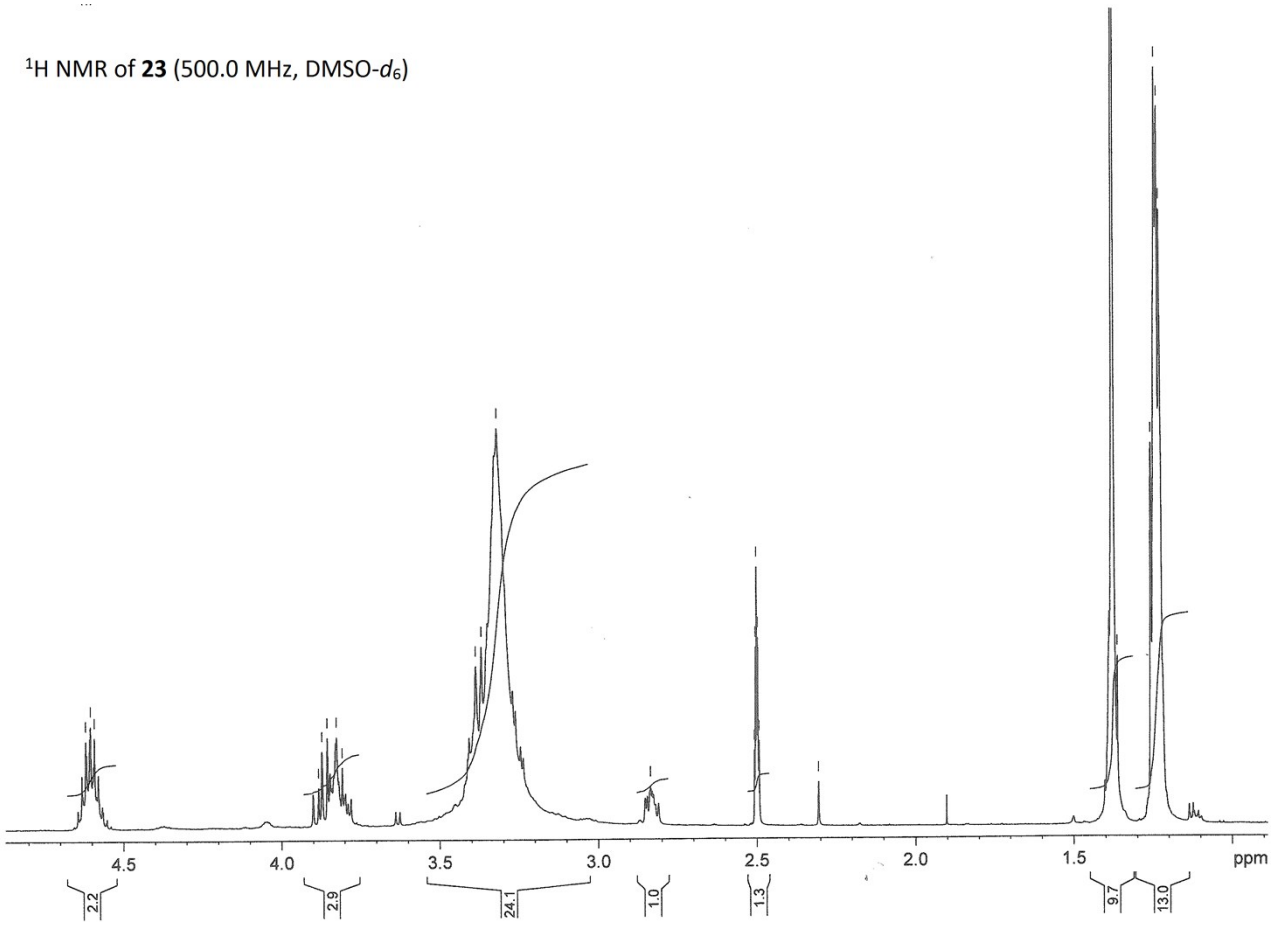


^{13}C NMR of **19** (125.7 MHz, DMSO-d_6)

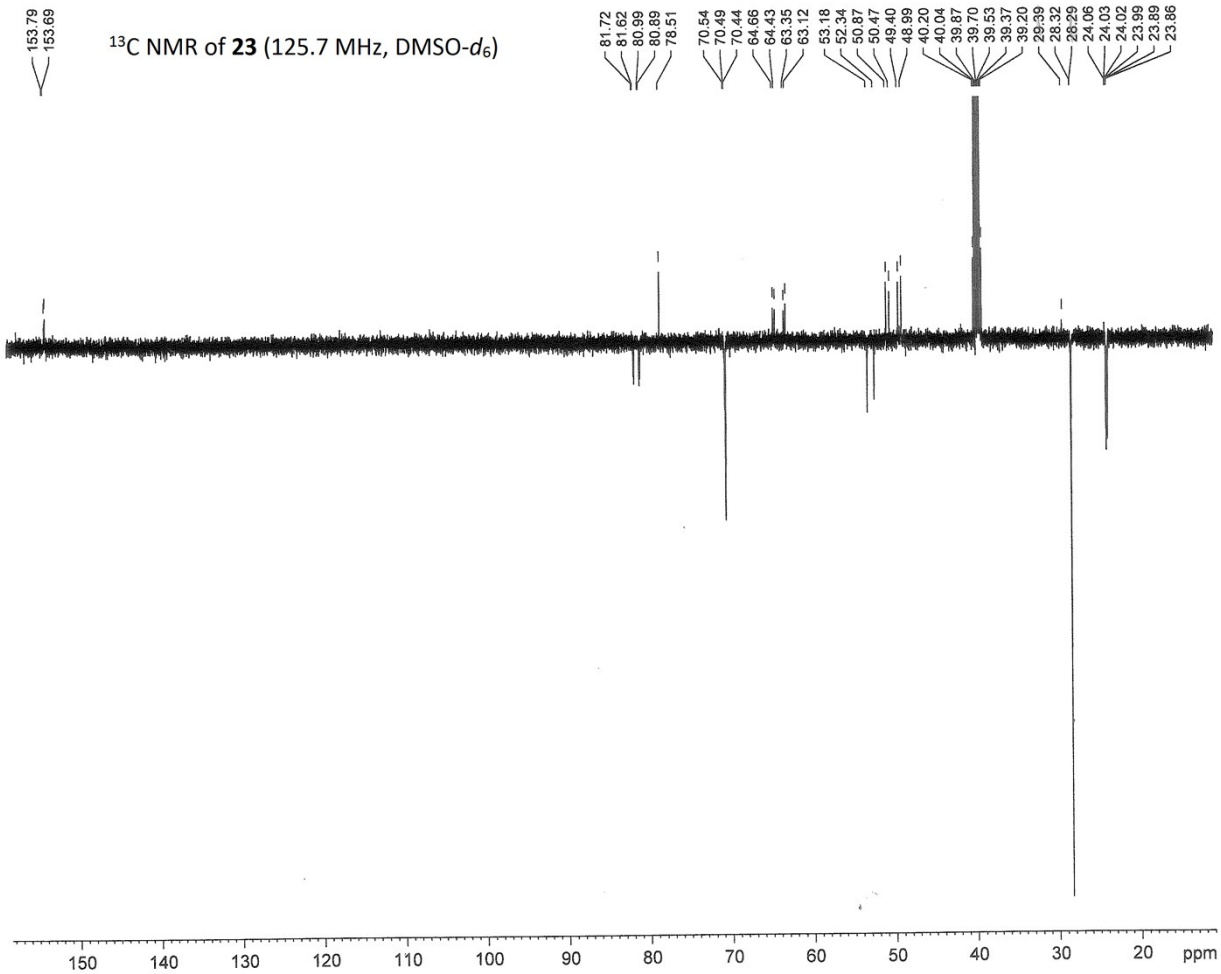


^{31}P{^{1}H} NMR of **19** (202.3 MHz, DMSO-d_6)

^{1}H NMR of **23** (500.0 MHz, DMSO-d_6)



^{13}C NMR of **23** (125.7 MHz, DMSO-d_6)



$^{31}P\{^{1}H\}$ NMR of **23** (202.3 MHz, DMSO-d_6)