

Supporting Information

A novel bis-phosphonyl C-glycoside: First synthesis of C-(1,6-deoxy- β -D-glucopyranosyl)dimethylphosphonate, a stable bisphosphonate to probe the mechanism of β -phosphoglucomutase

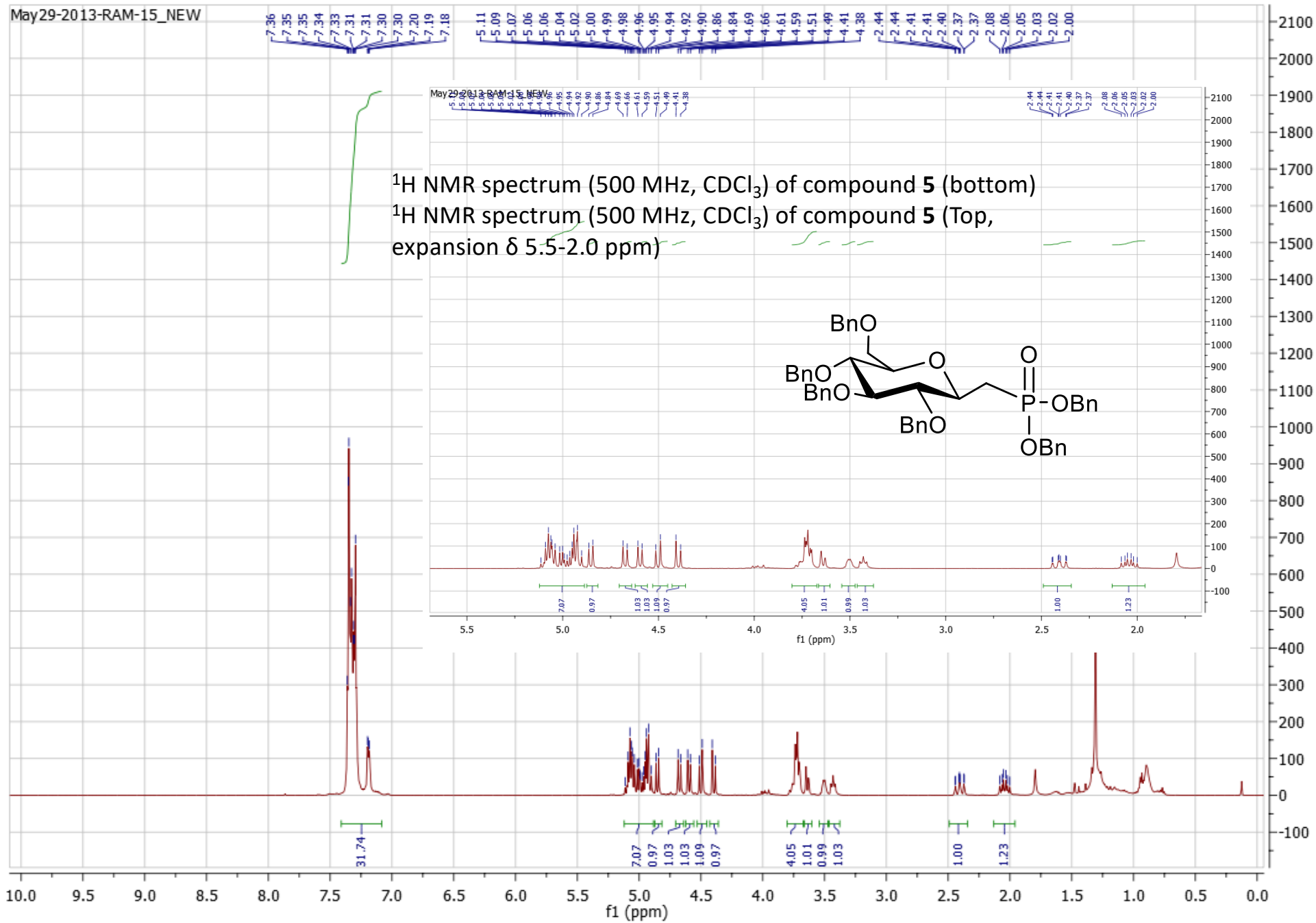
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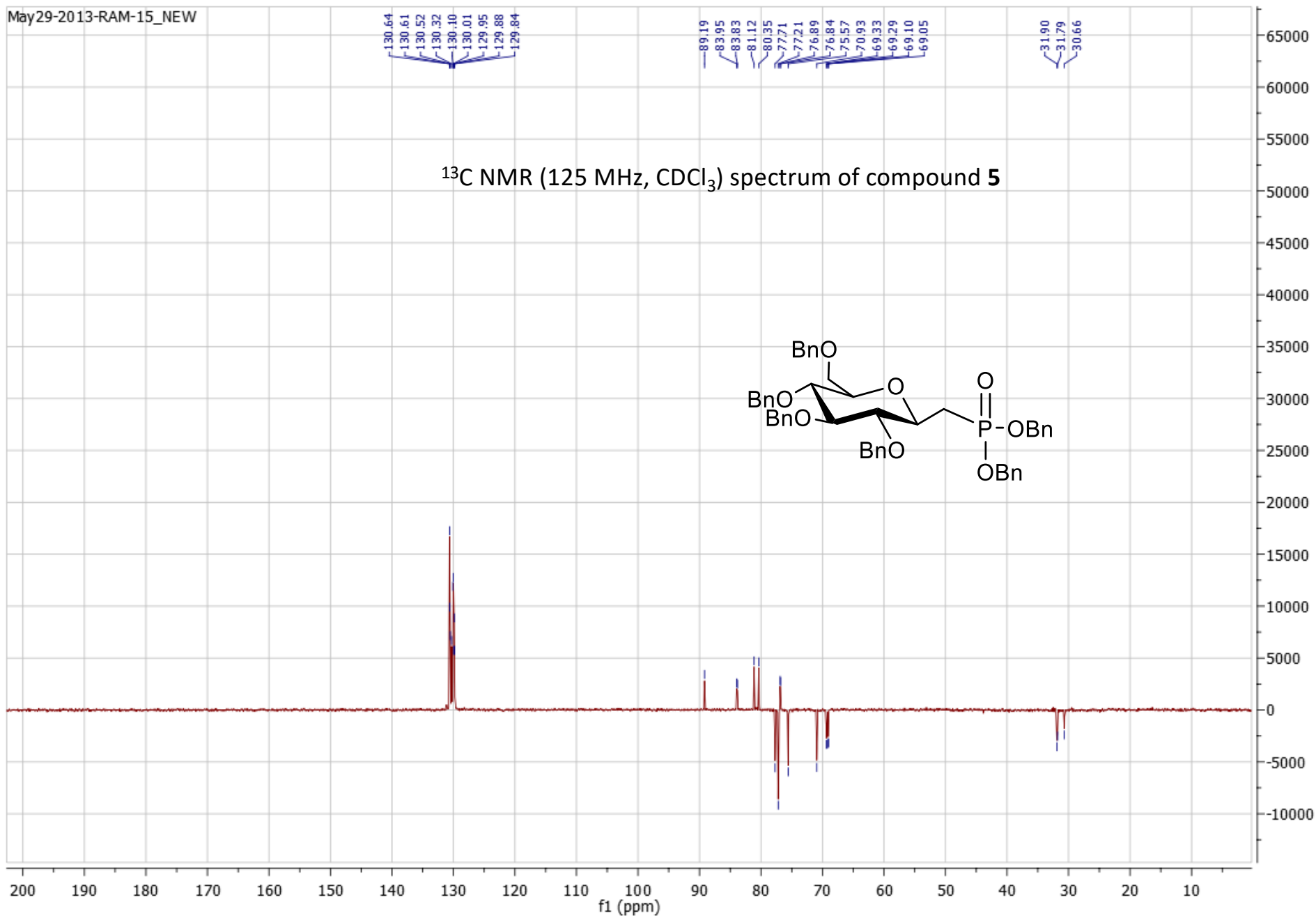
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Supporting Information

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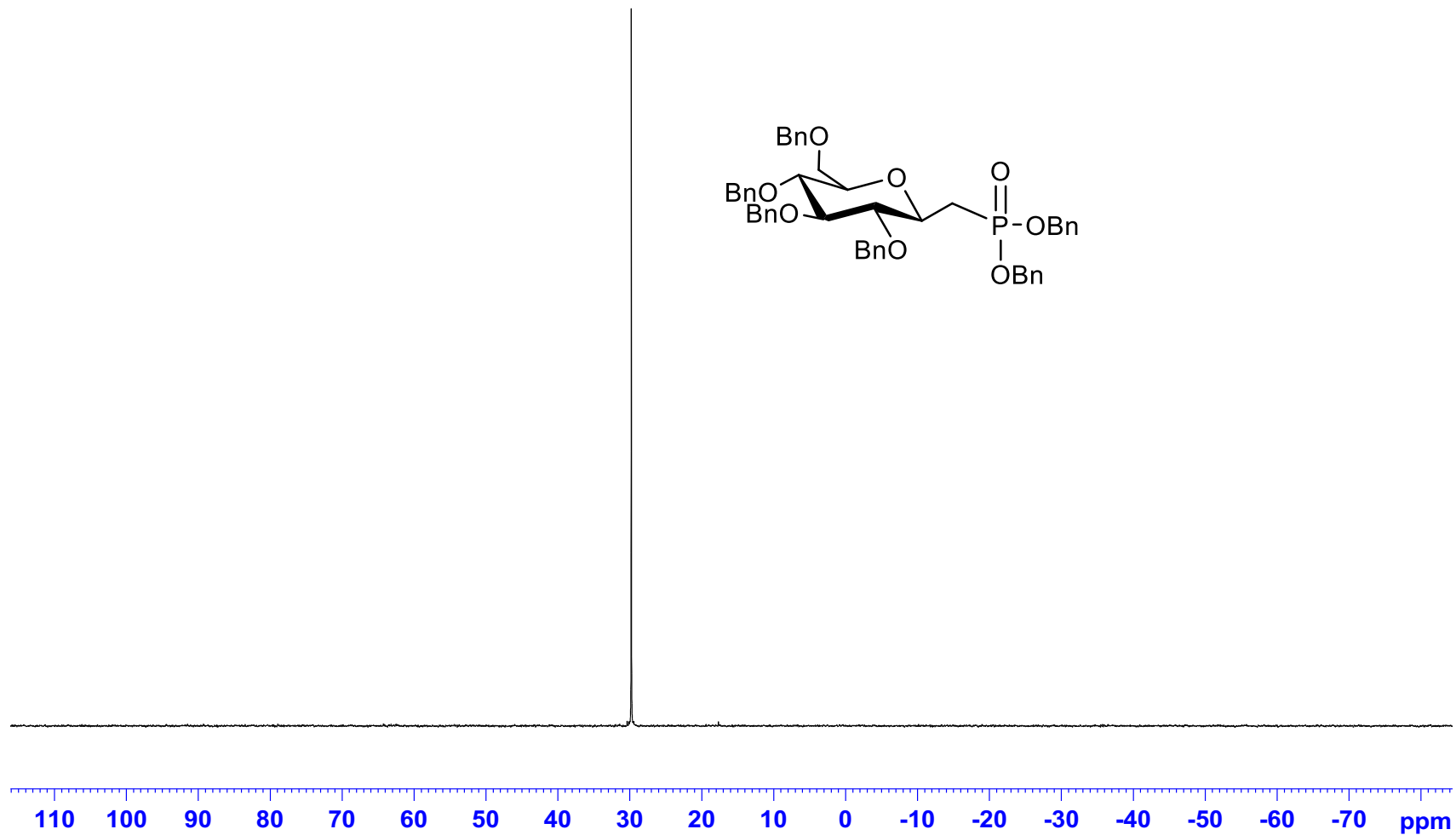
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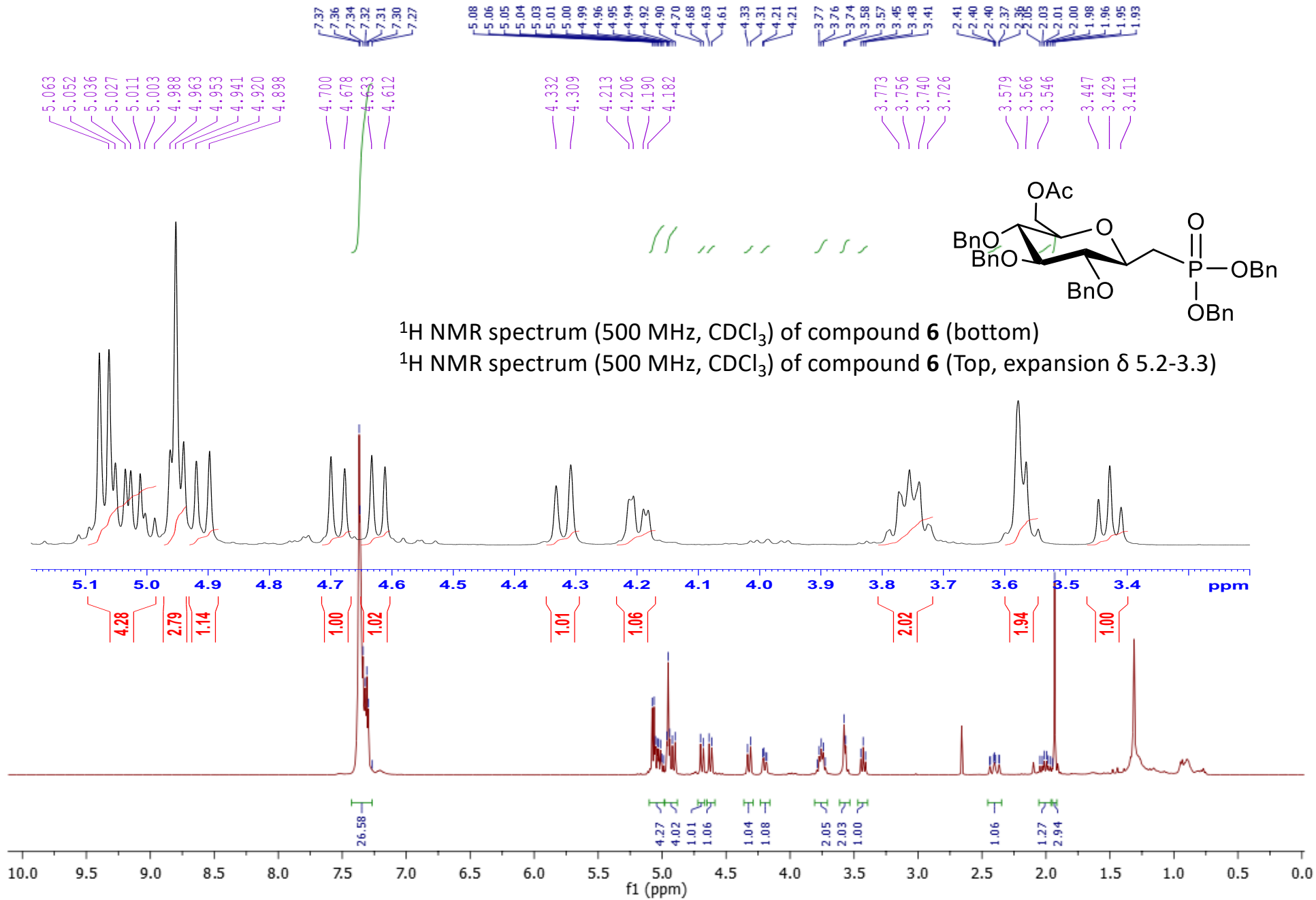




29.82

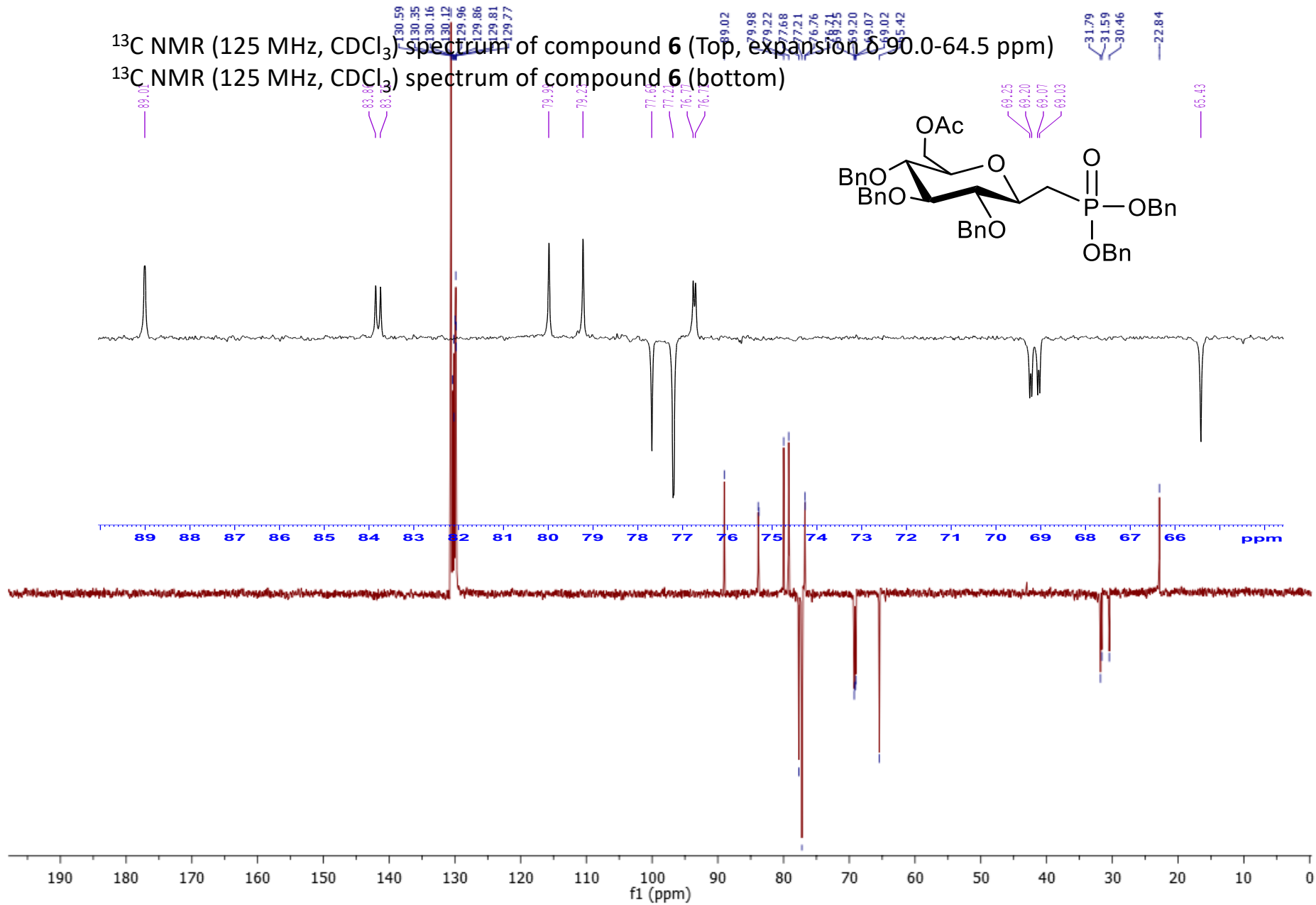
$^{31}\text{P}\{^1\text{H}\}$ NMR (202.5 MHz, CDCl_3) spectrum of compound **5**





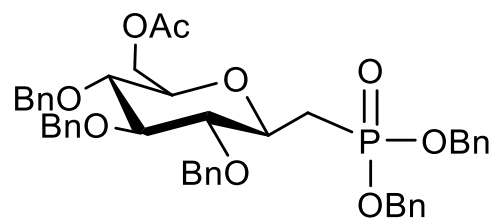
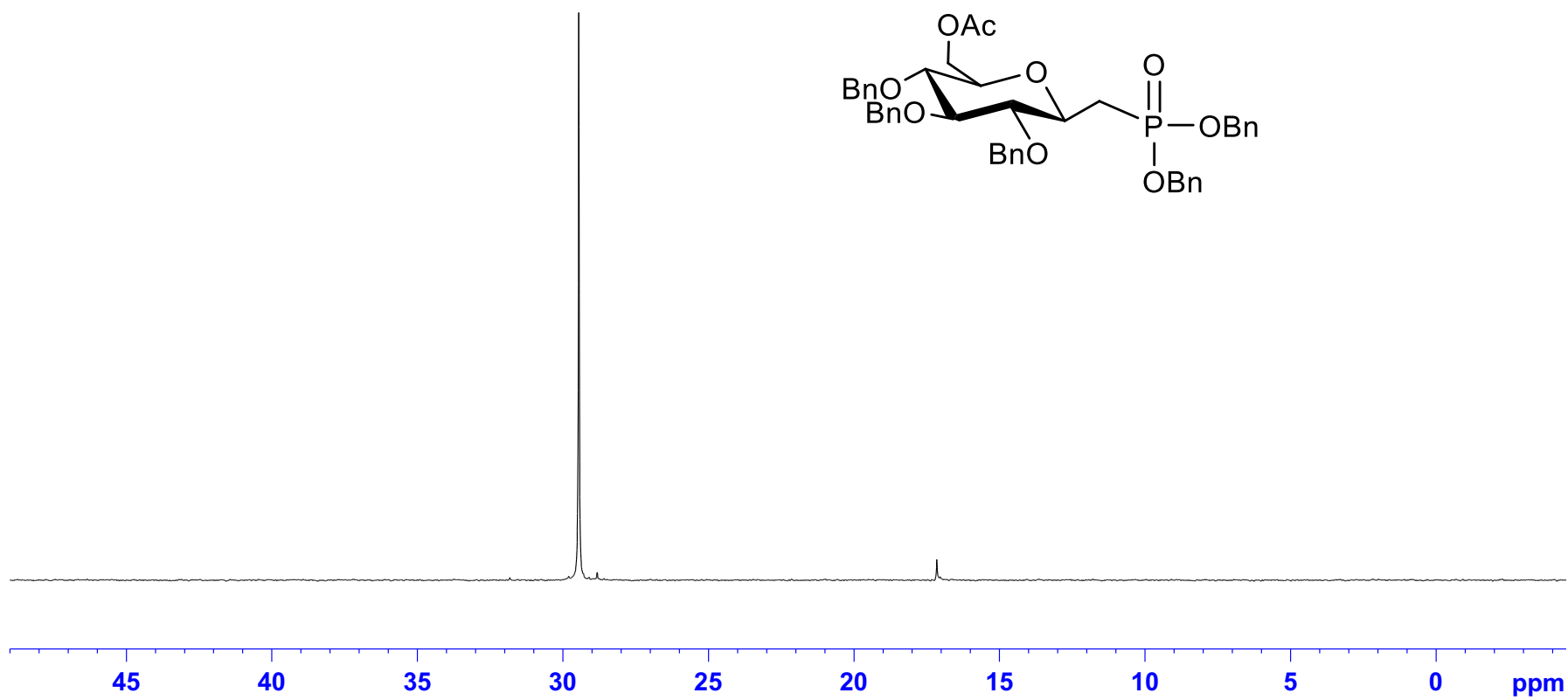
¹³C NMR (125 MHz, CDCl₃) spectrum of compound **6** (Top, expansion of 90.0-64.5 ppm)

¹³C NMR (125 MHz, CDCl₃) spectrum of compound **6** (bottom)

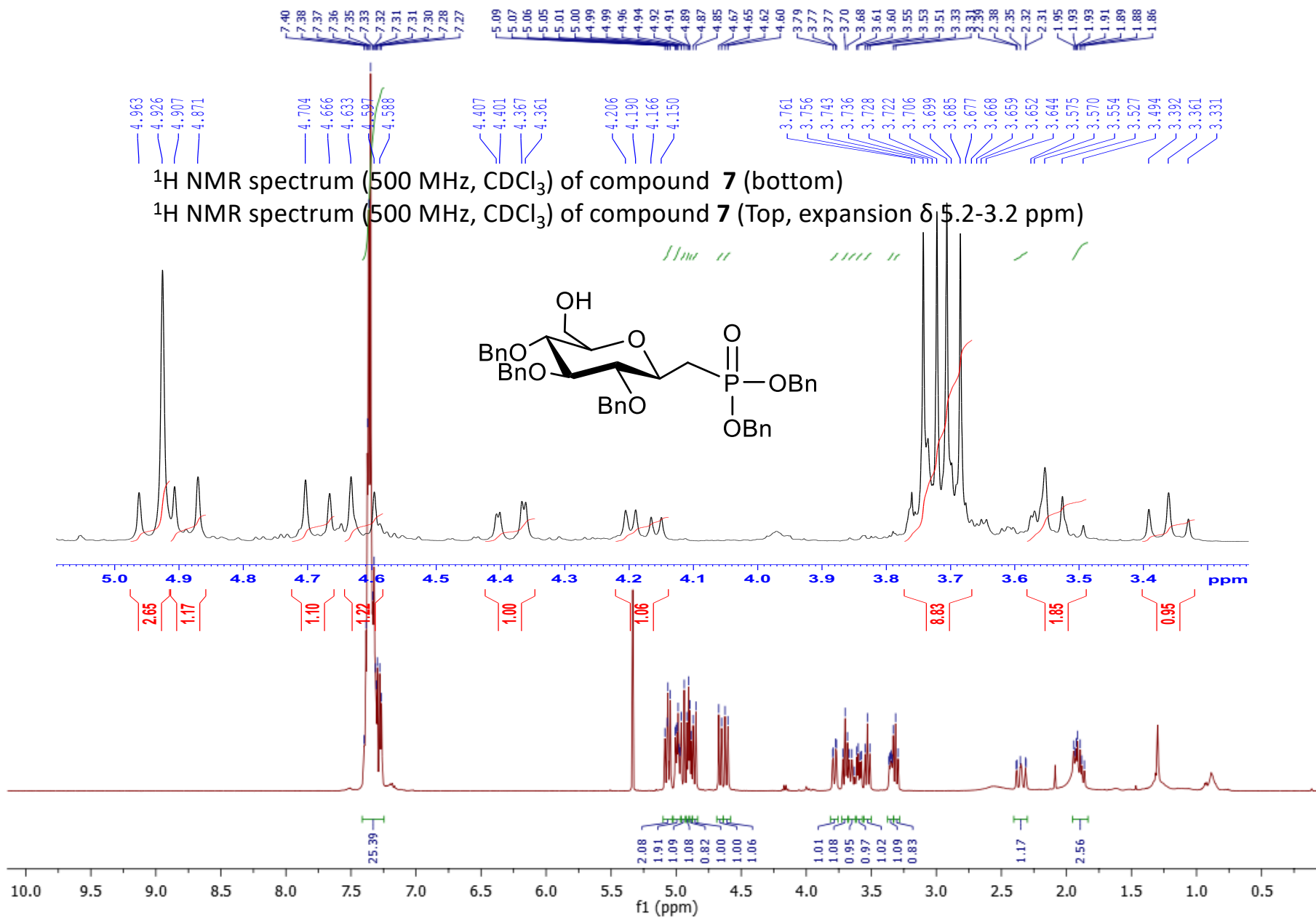


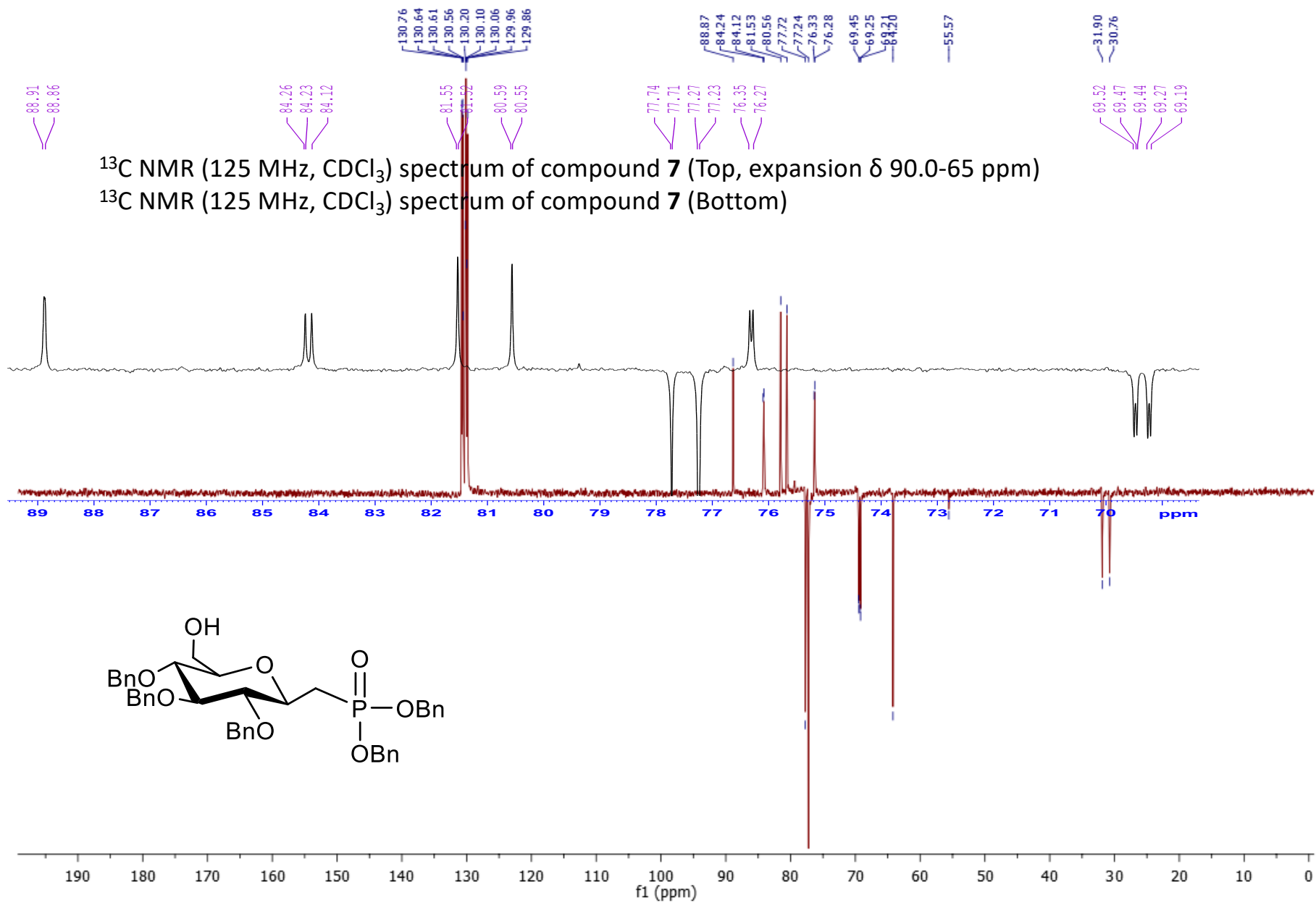
29.47

$^{31}\text{P}\{^1\text{H}\}$ NMR (202.5 MHz, CDCl_3) spectrum of compound **6**



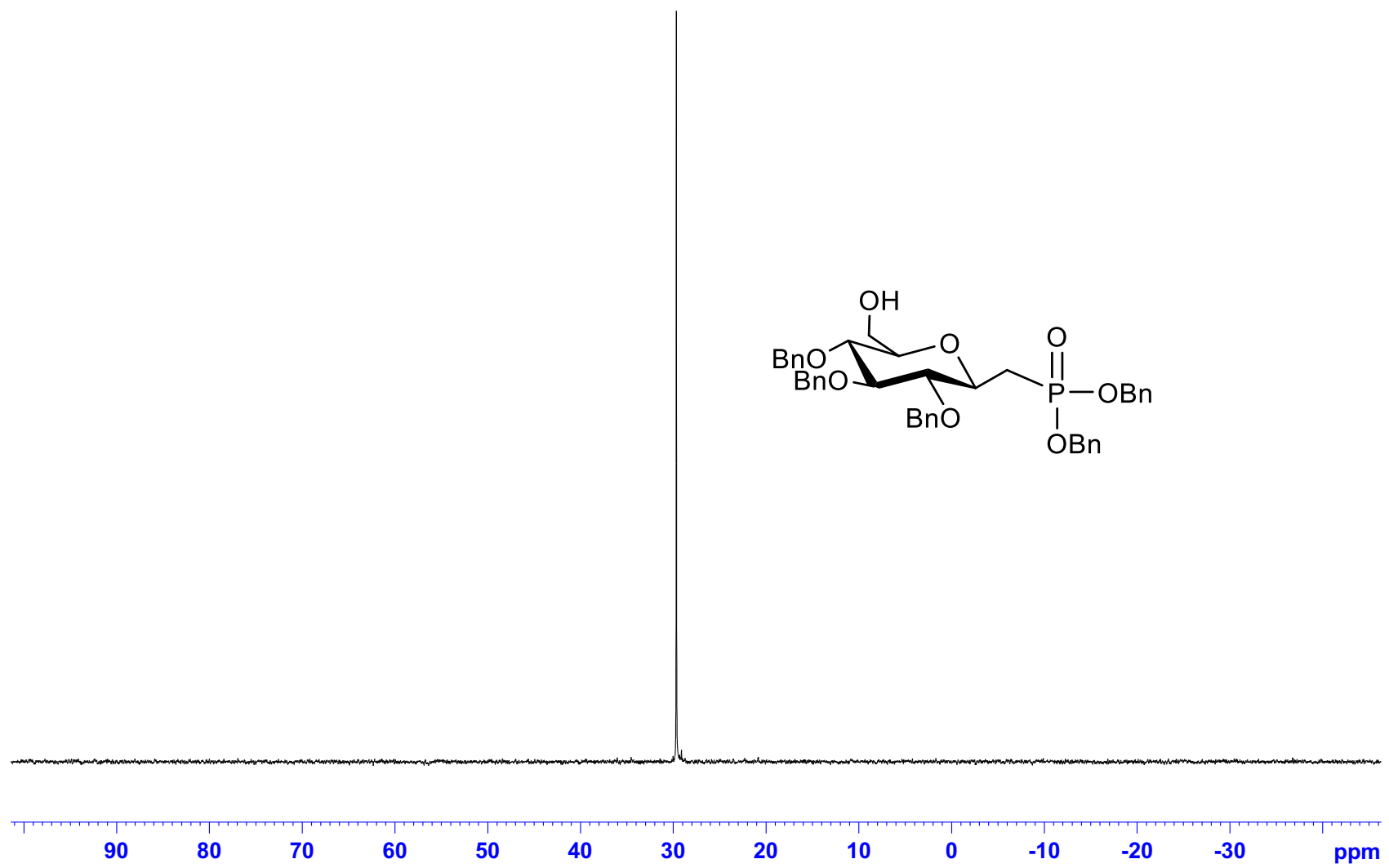
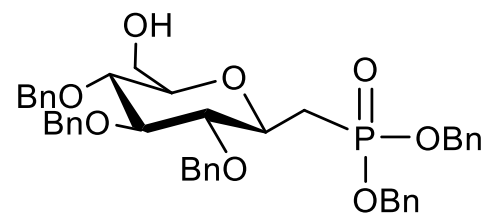
S8

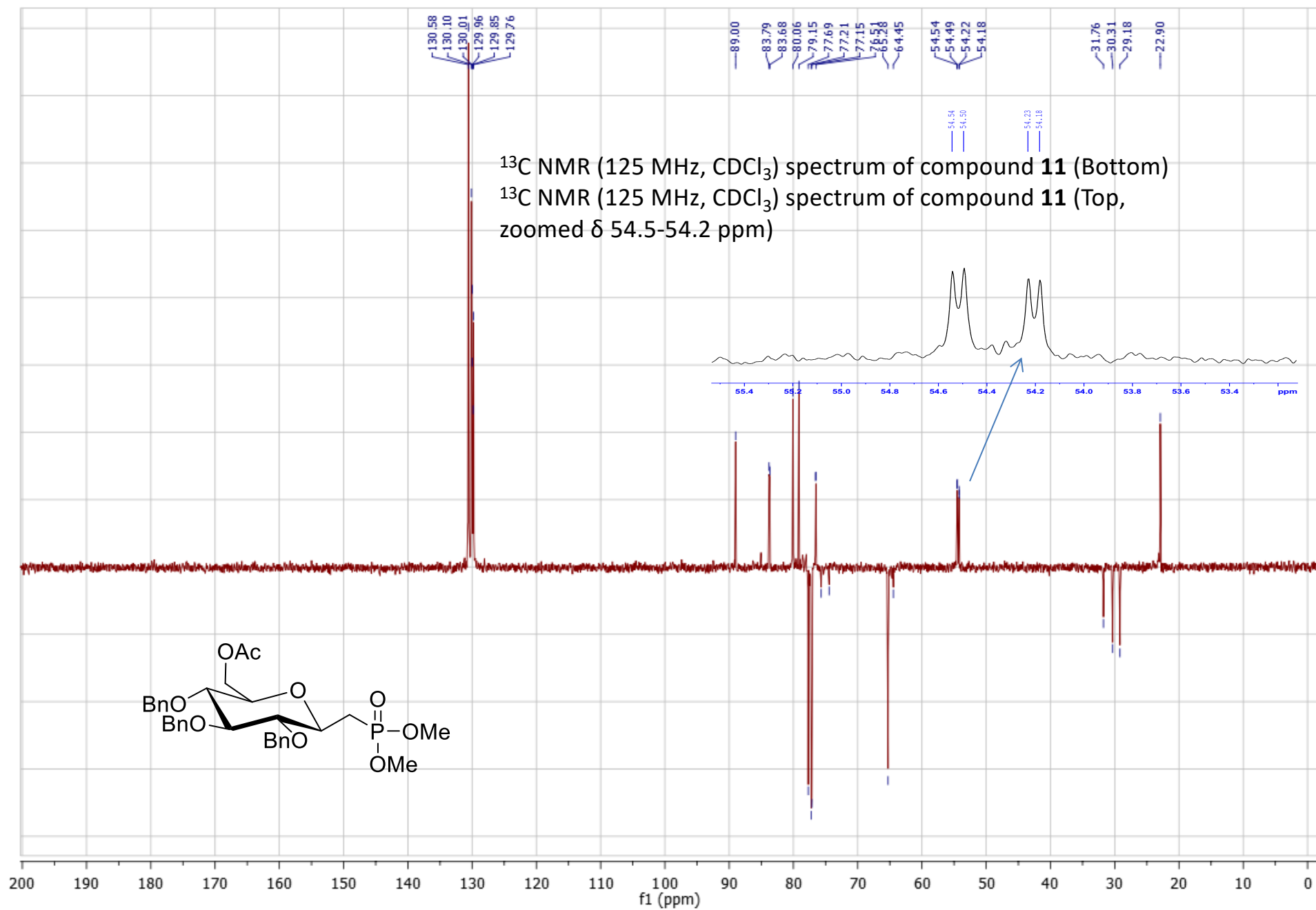




29.71

$^{31}\text{P}\{^1\text{H}\}$ NMR (202.5 MHz, CDCl_3) spectrum of compound **7**





89.01

83.79

83.68

80.07

79.15

77.69

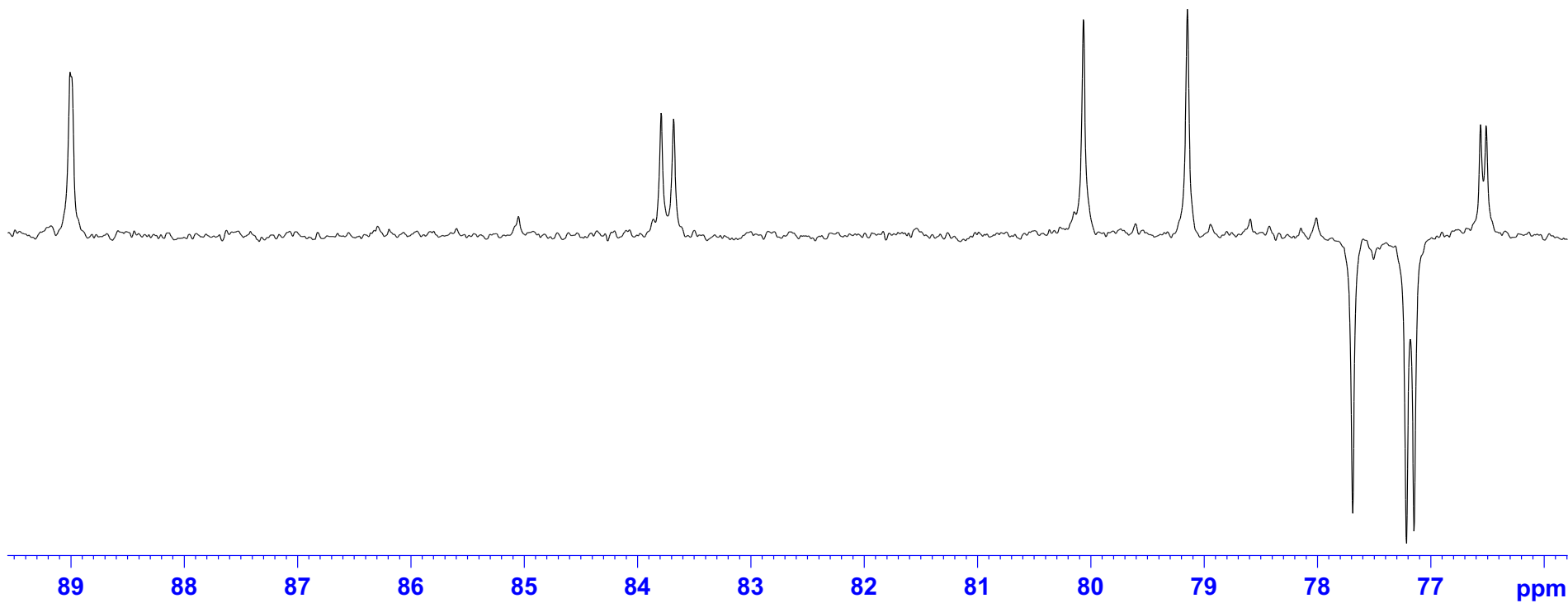
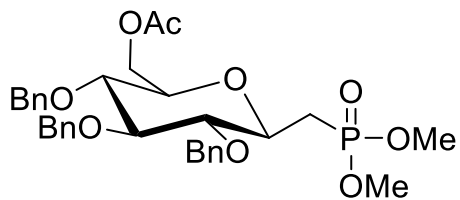
77.22

77.15

76.56

76.51

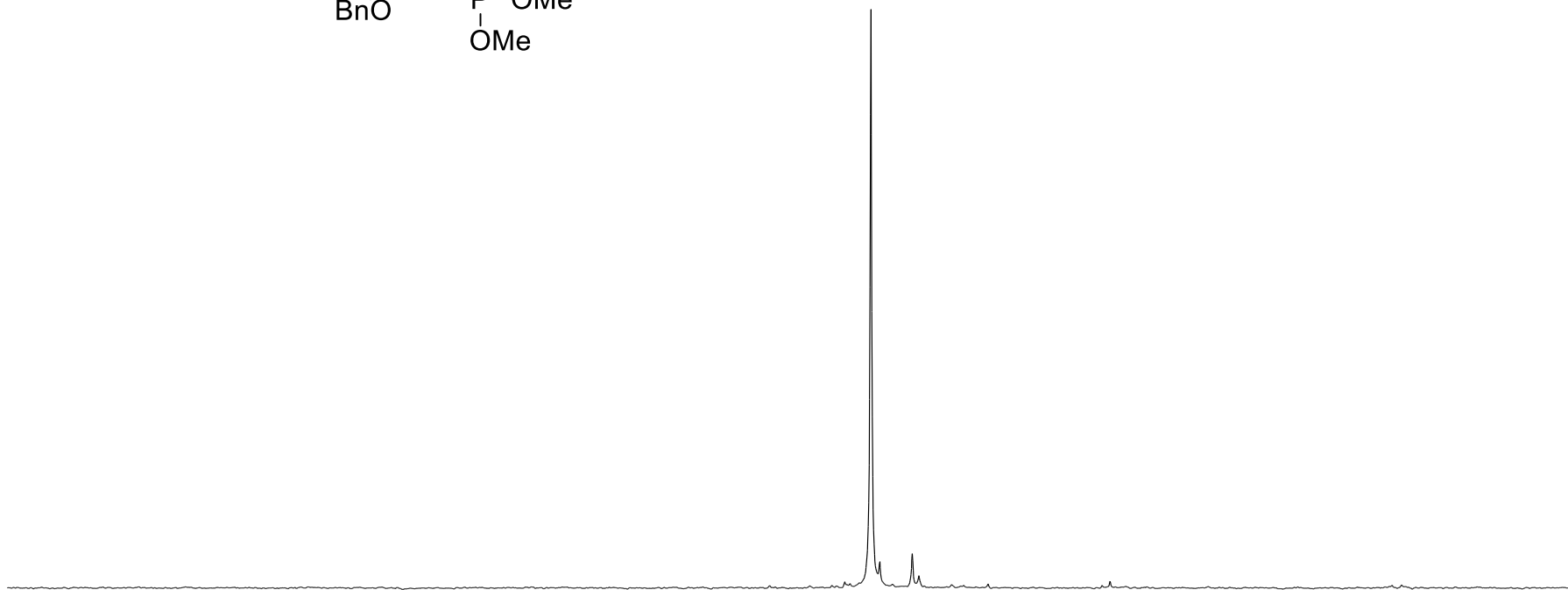
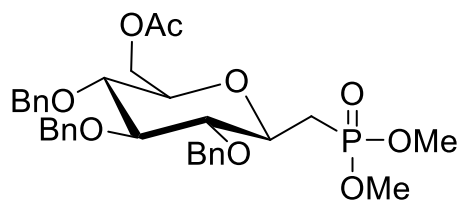
^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **11** (expansion δ 90-76 ppm)



S14

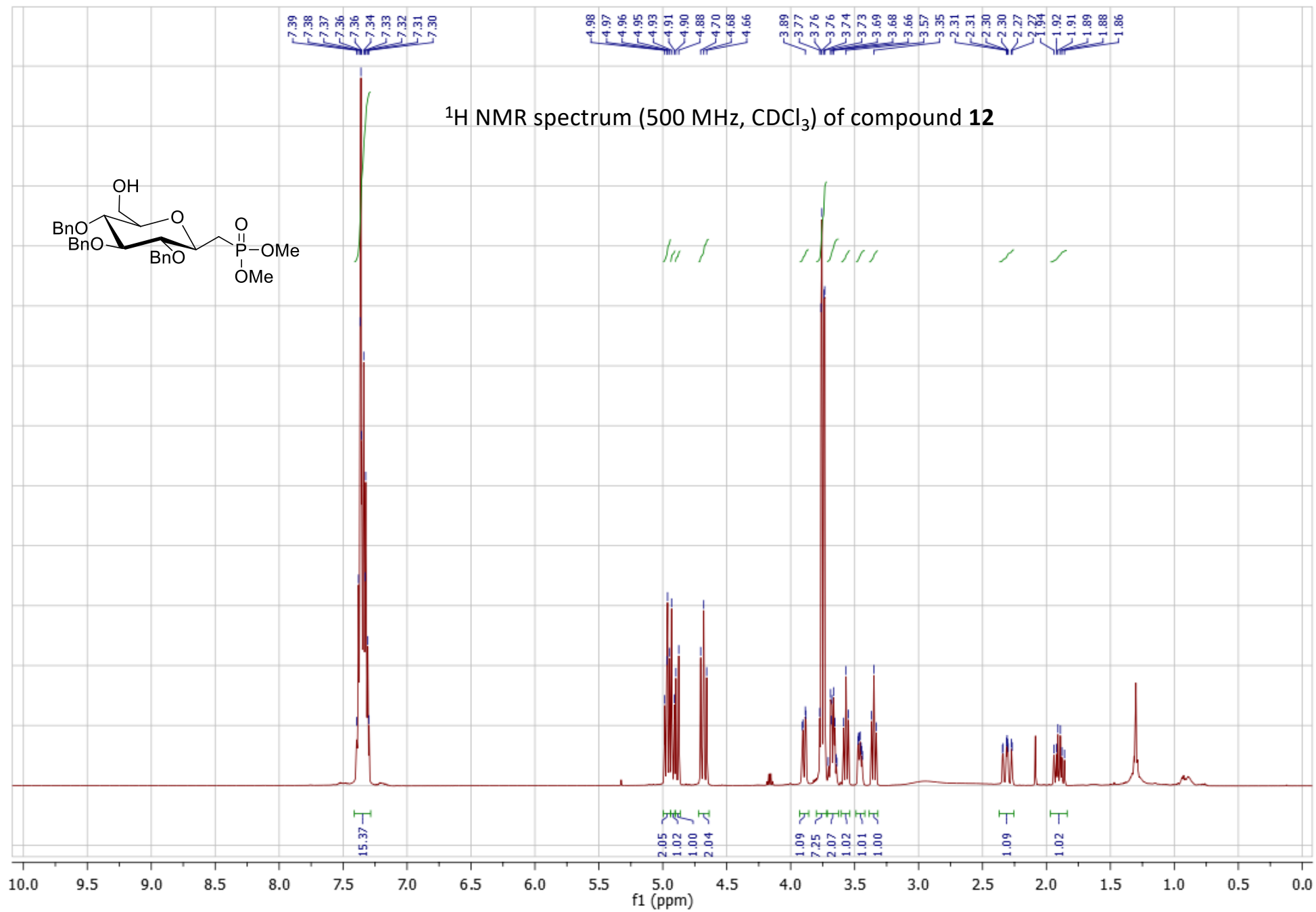
31.14

$^{31}\text{P}\{^1\text{H}\}$ NMR (202.5 MHz, CDCl_3) spectrum of compound **11**



45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24 23 22 21 ppm

S15

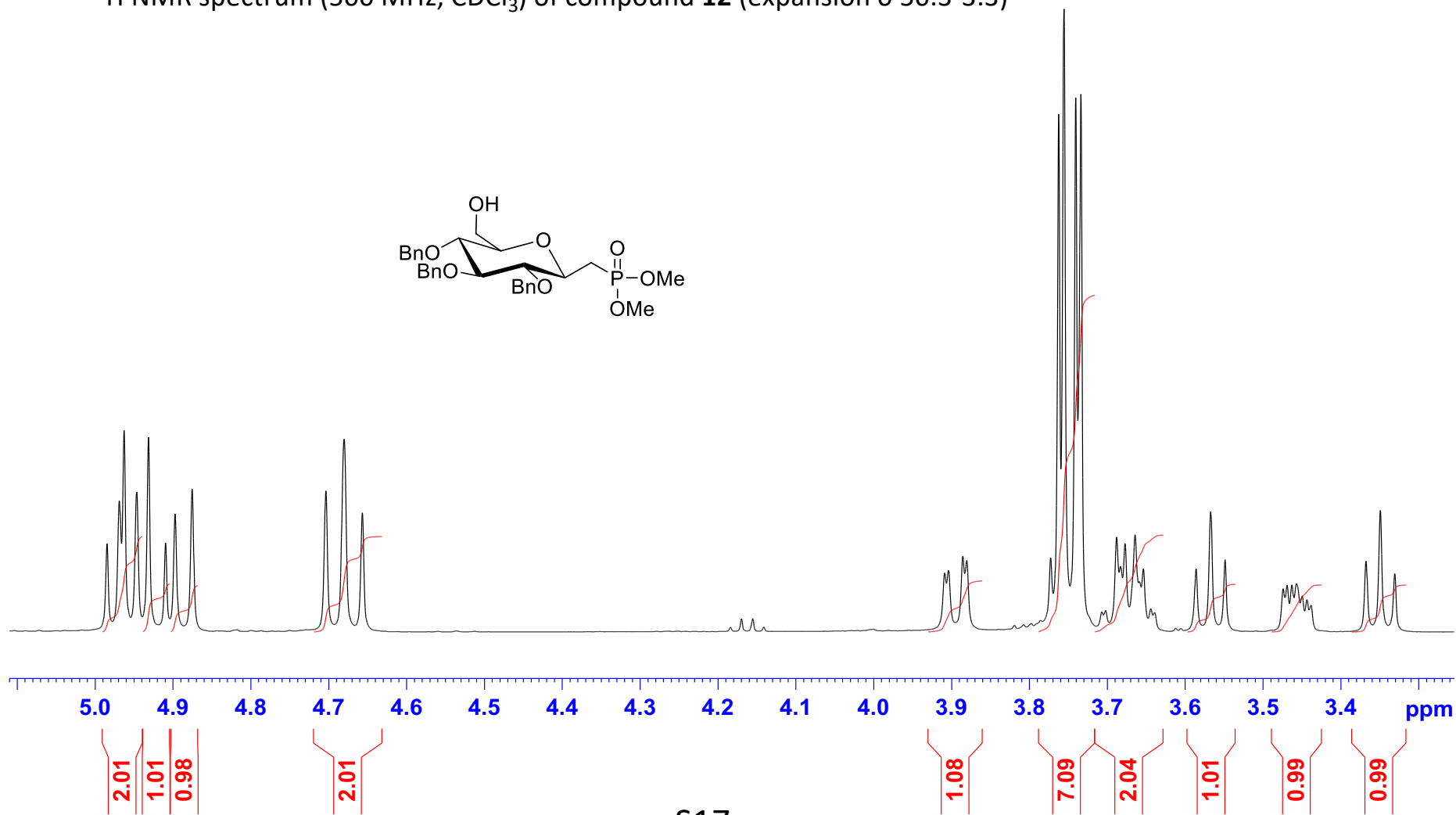


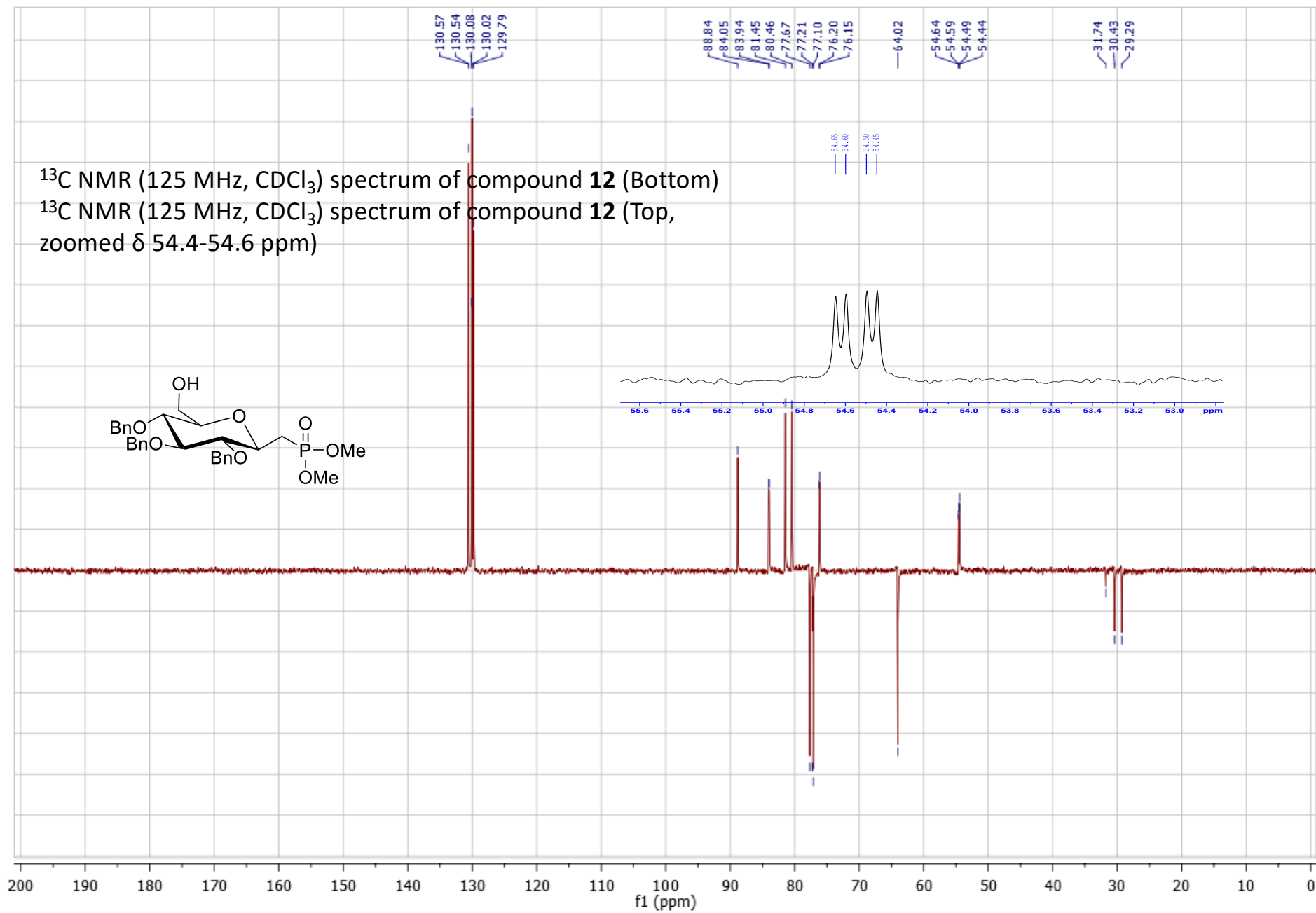
4.985
4.969
4.963
4.947
4.932
4.910
4.898
4.876

4.704
4.681
4.657

3.909
3.904
3.886
3.881
3.773
3.763
3.756
3.741
3.734
3.707
3.703
3.688
3.683
3.678
3.665
3.659
3.654
3.644
3.640
3.586
3.567
3.549
3.474
3.470
3.463
3.457

^1H NMR spectrum (500 MHz, CDCl_3) of compound **12** (expansion δ 5.0-3.3)

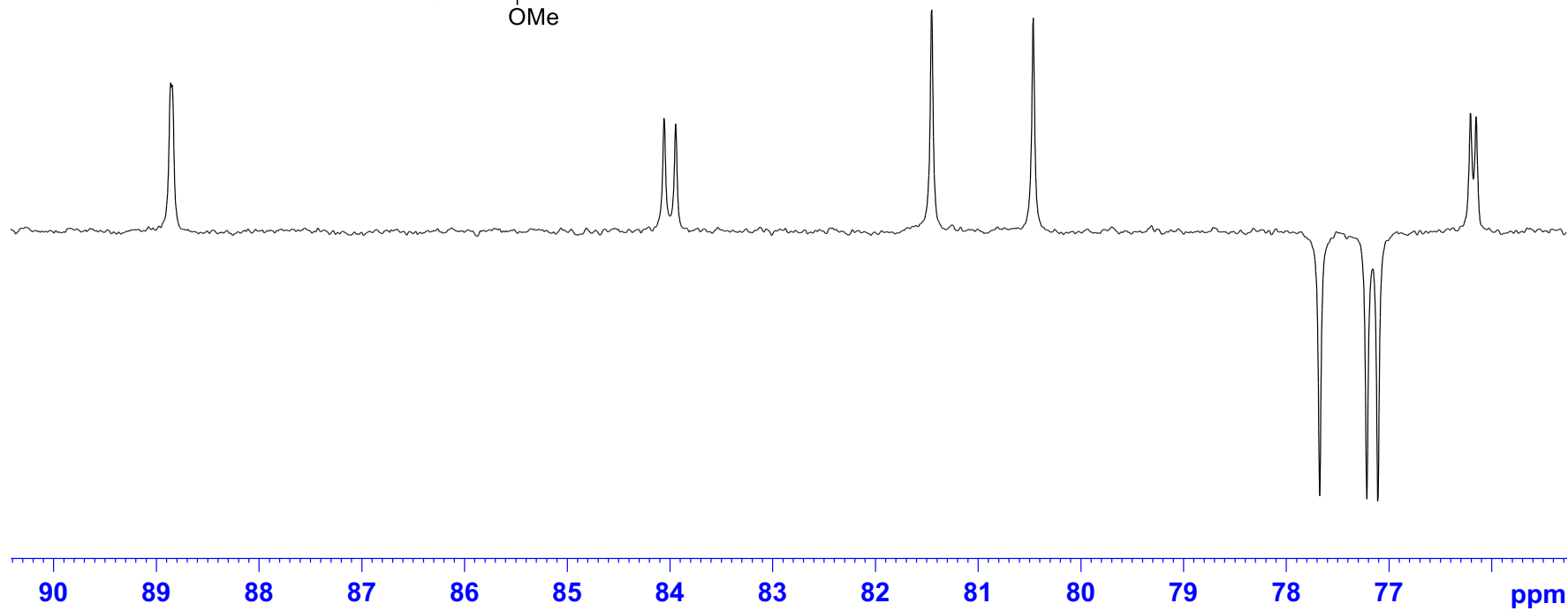
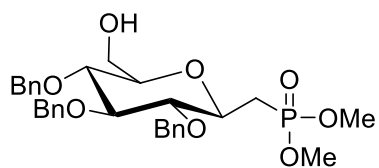






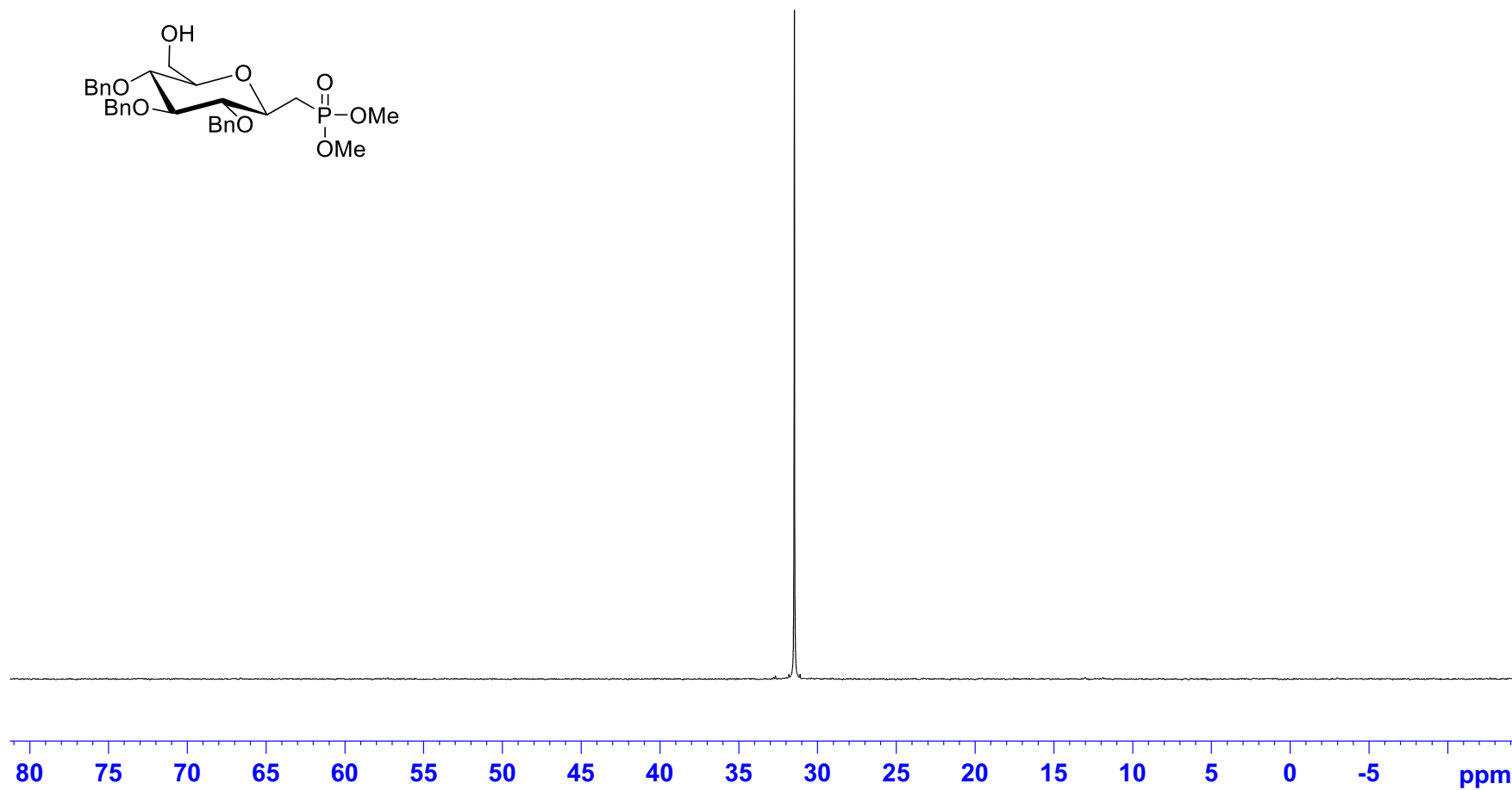
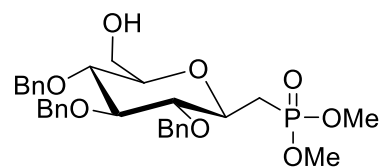
¹³C NMR (125 MHz, CDCl₃) spectrum of compound **12** (Bottom)

¹³C NMR (125 MHz, CDCl₃) spectrum of compound **12** (Top, zoomed δ 64.5-64.2 ppm)

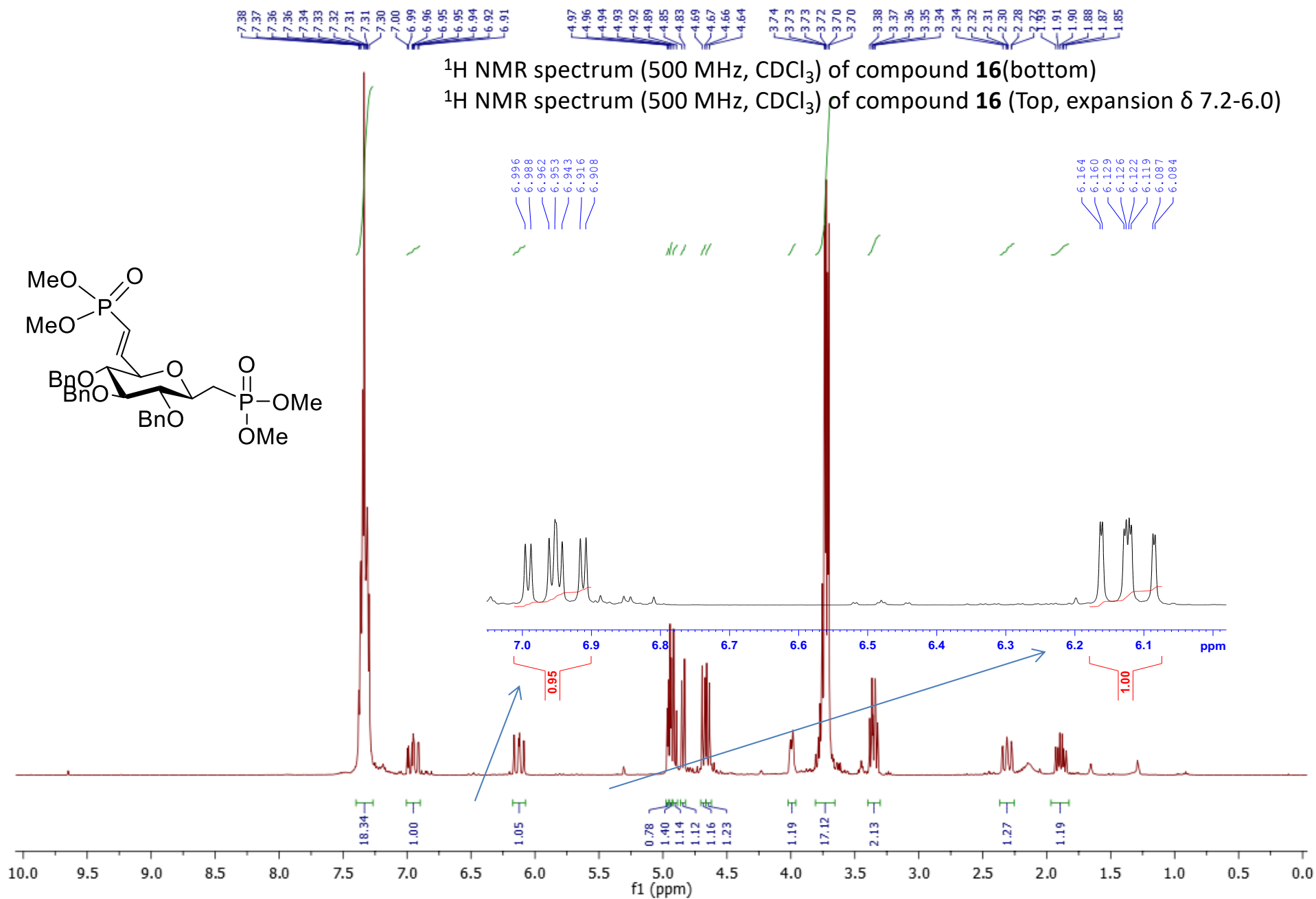


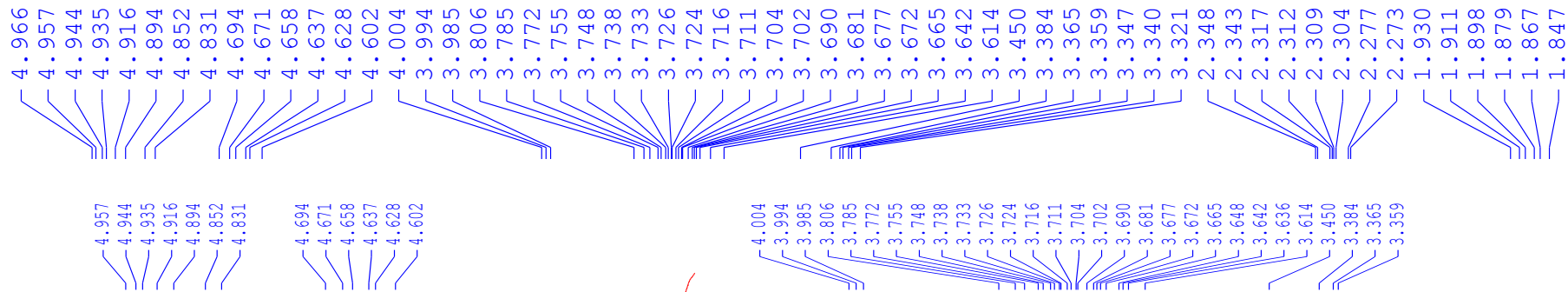
31.47

$^{31}\text{P}\{^1\text{H}\}$ NMR (202.5 MHz, CDCl_3) spectrum of compound **12**



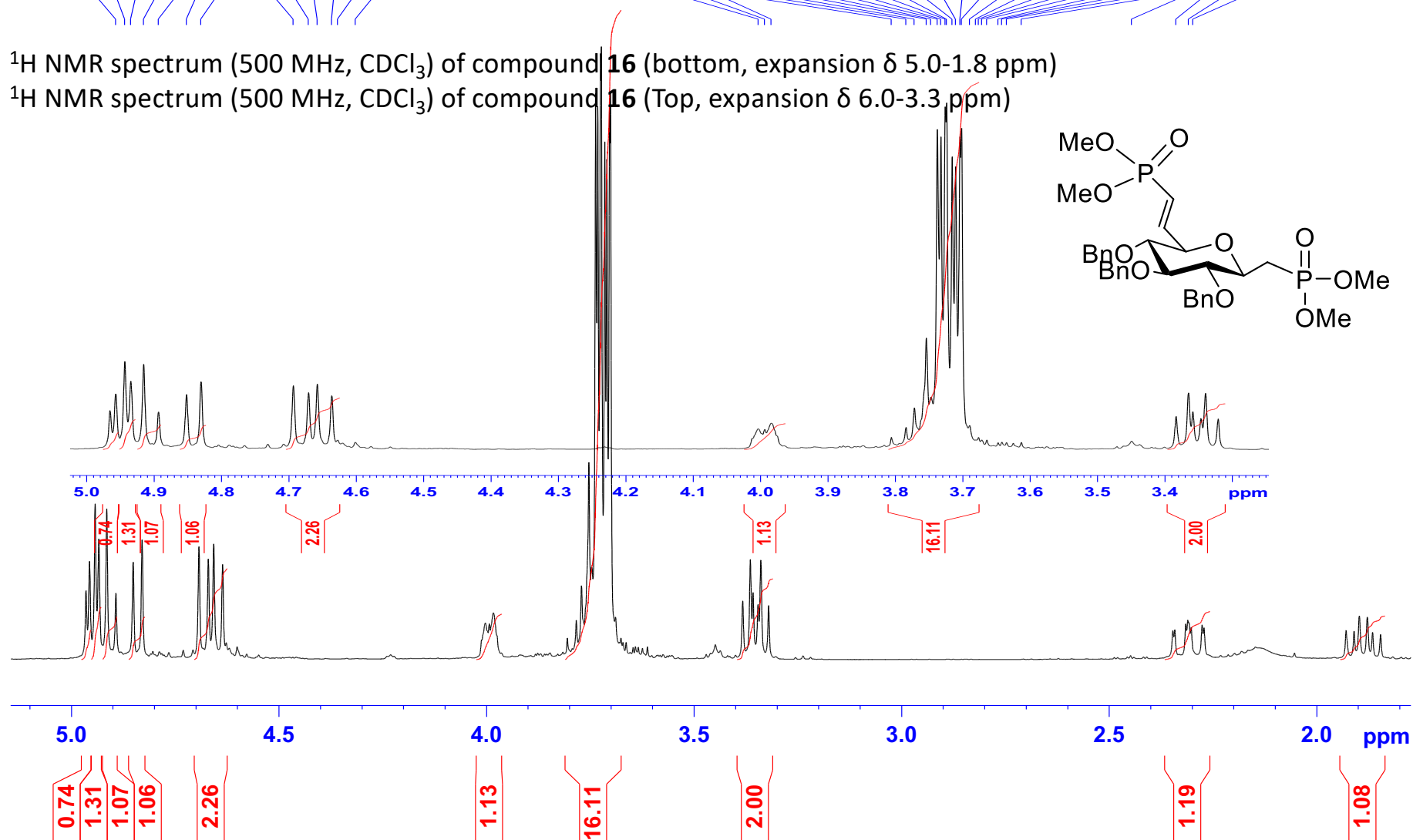
S20

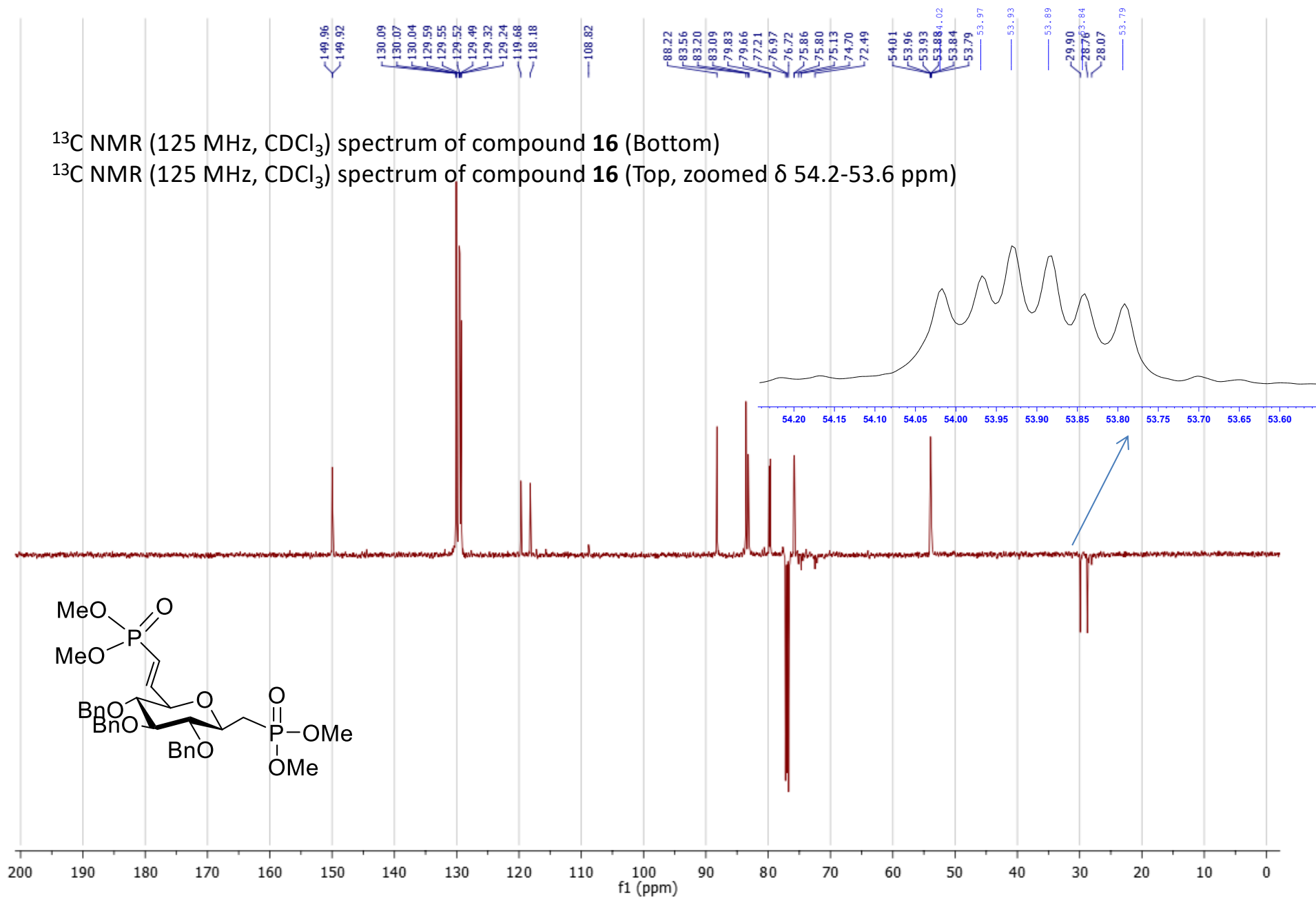


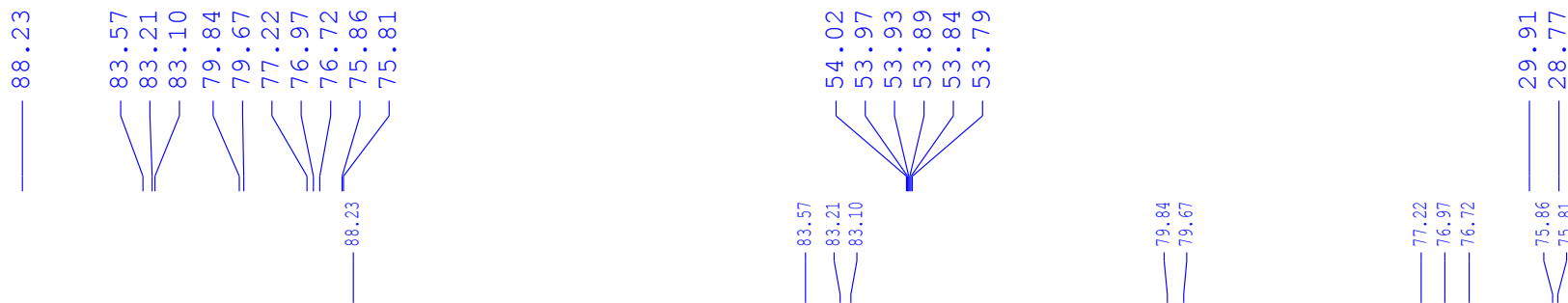


¹H NMR spectrum (500 MHz, CDCl₃) of compound **16** (bottom, expansion δ 5.0-1.8 ppm)

¹H NMR spectrum (500 MHz, CDCl₃) of compound **16** (Top, expansion δ 6.0-3.3 ppm)

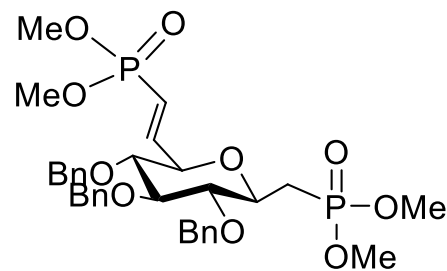
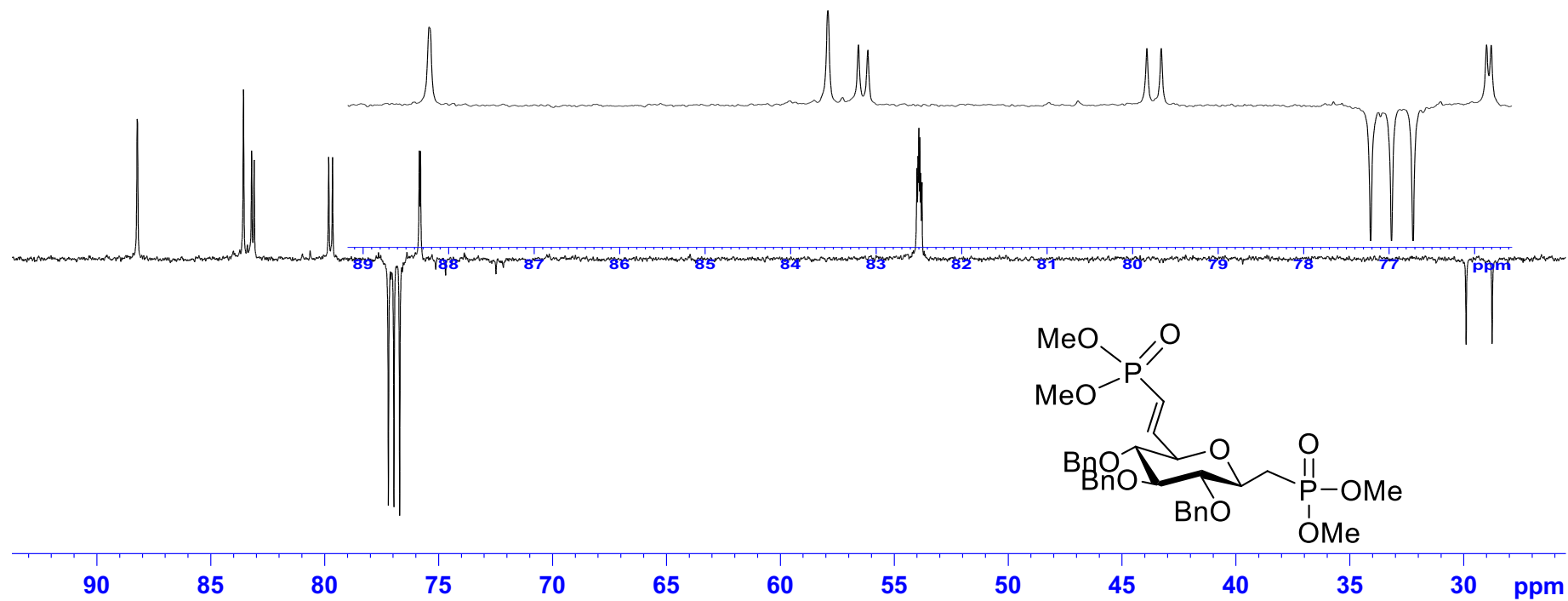






^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **16** (Bottom, expansion δ 90.0-28.0 ppm)

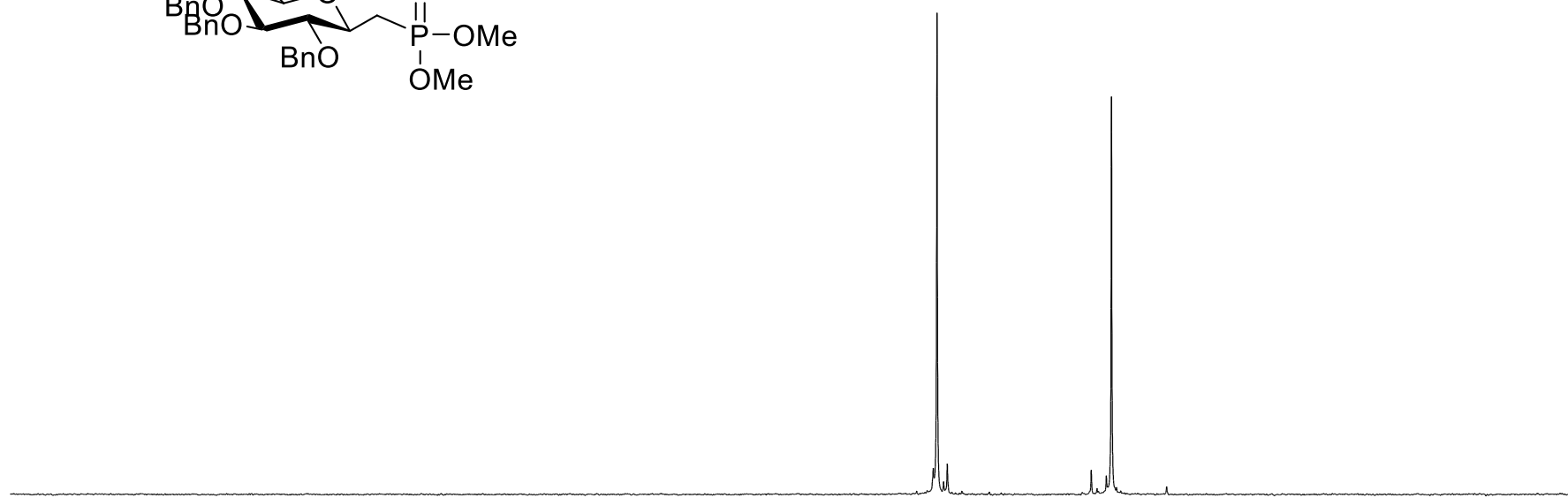
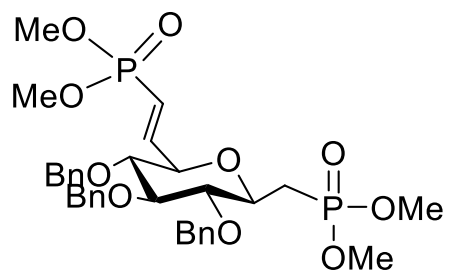
^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **16** (Top, zoomed δ 89.0-75.0 ppm)



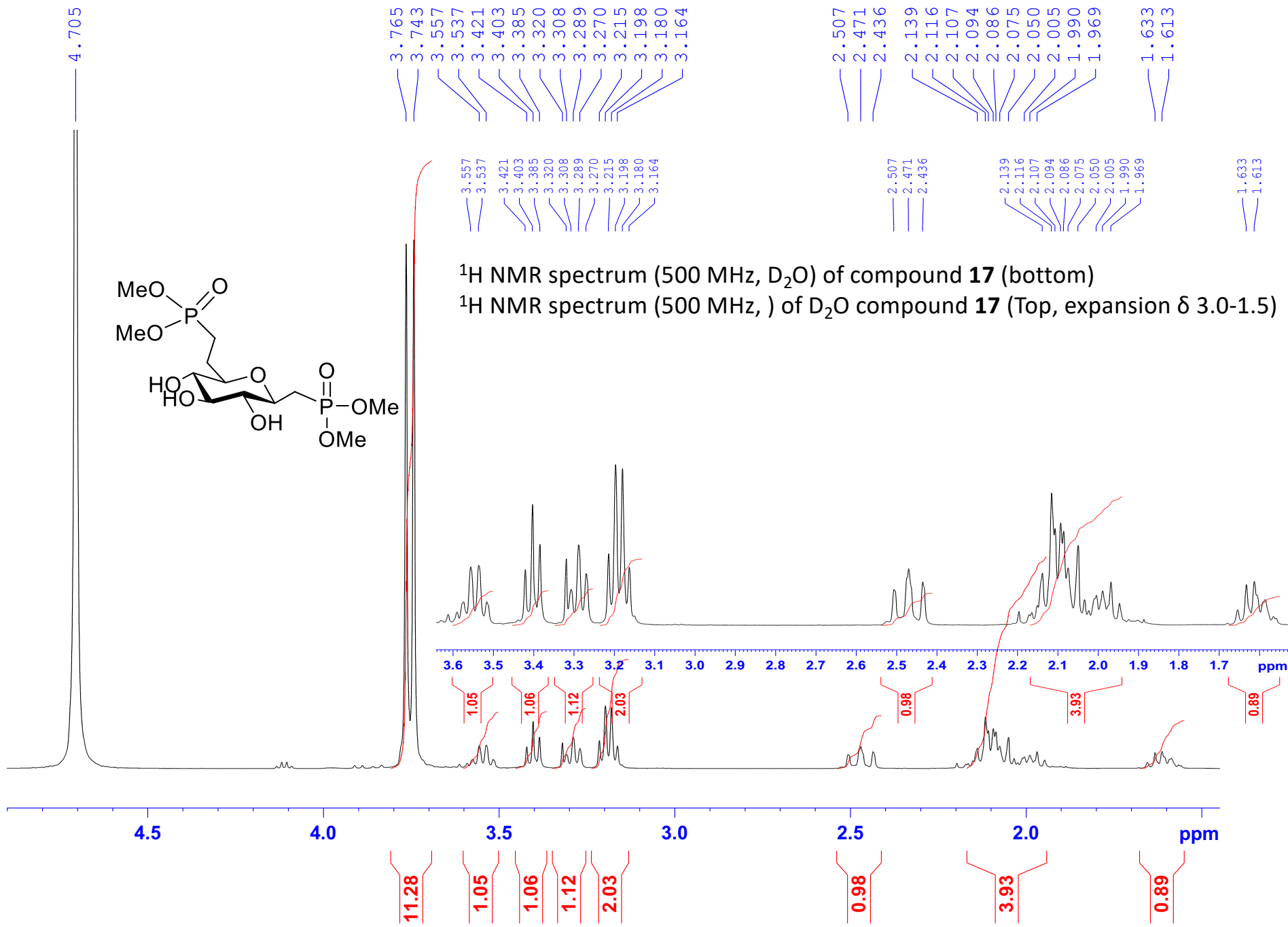
30.99

20.55

$^{31}\text{P}\{^1\text{H}\}$ NMR (202.5 MHz, CDCl_3) spectrum of compound **16**



85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 ppm



78.78
78.65

76.95

78.78
78.65
76.95
74.45
74.39
74.19
74.06
73.38

53.12
53.09
53.04

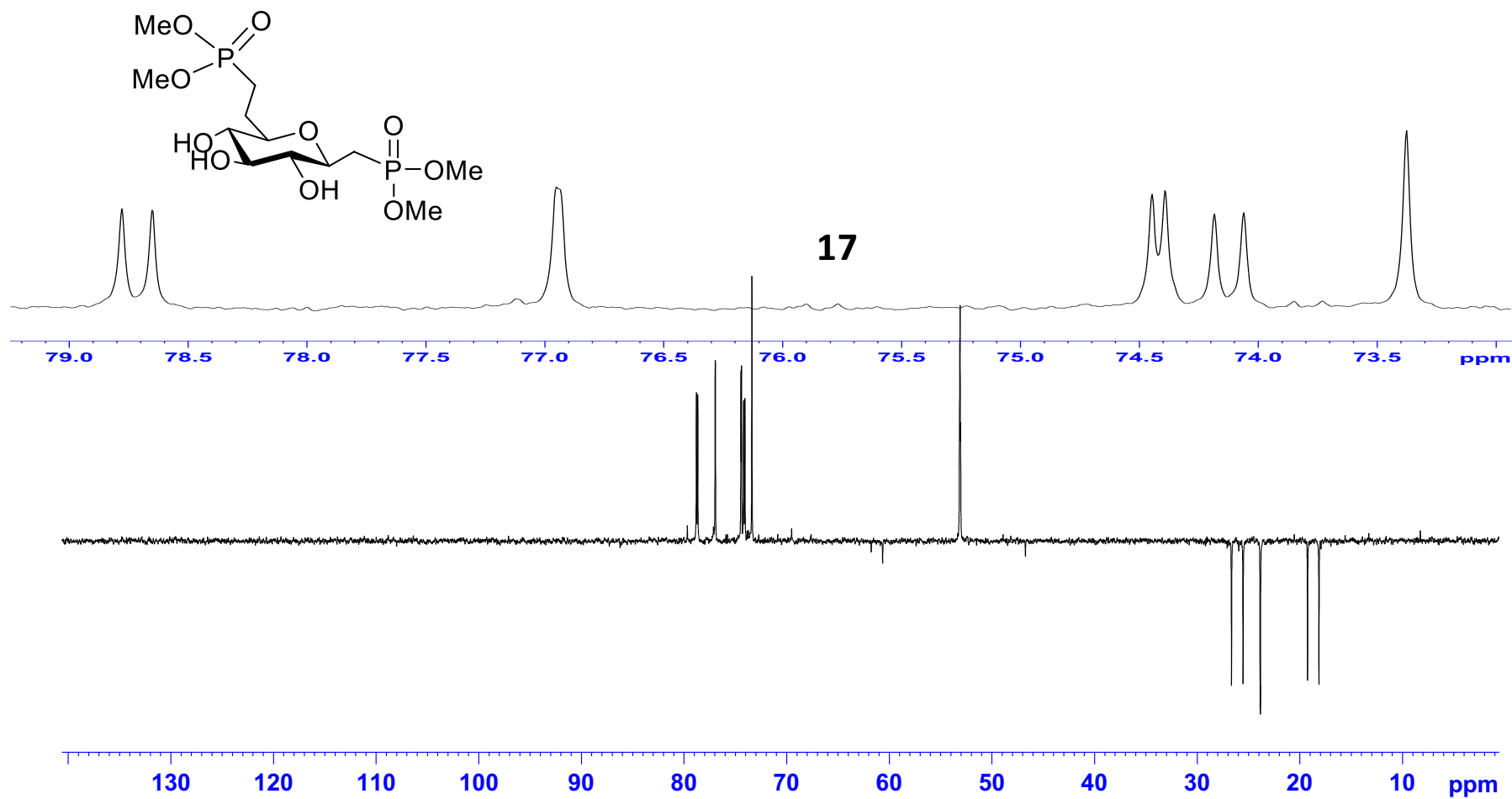
74.45
74.39

74.19
6.67
25.55
23.89
23.86
19.26
18.15

73.38

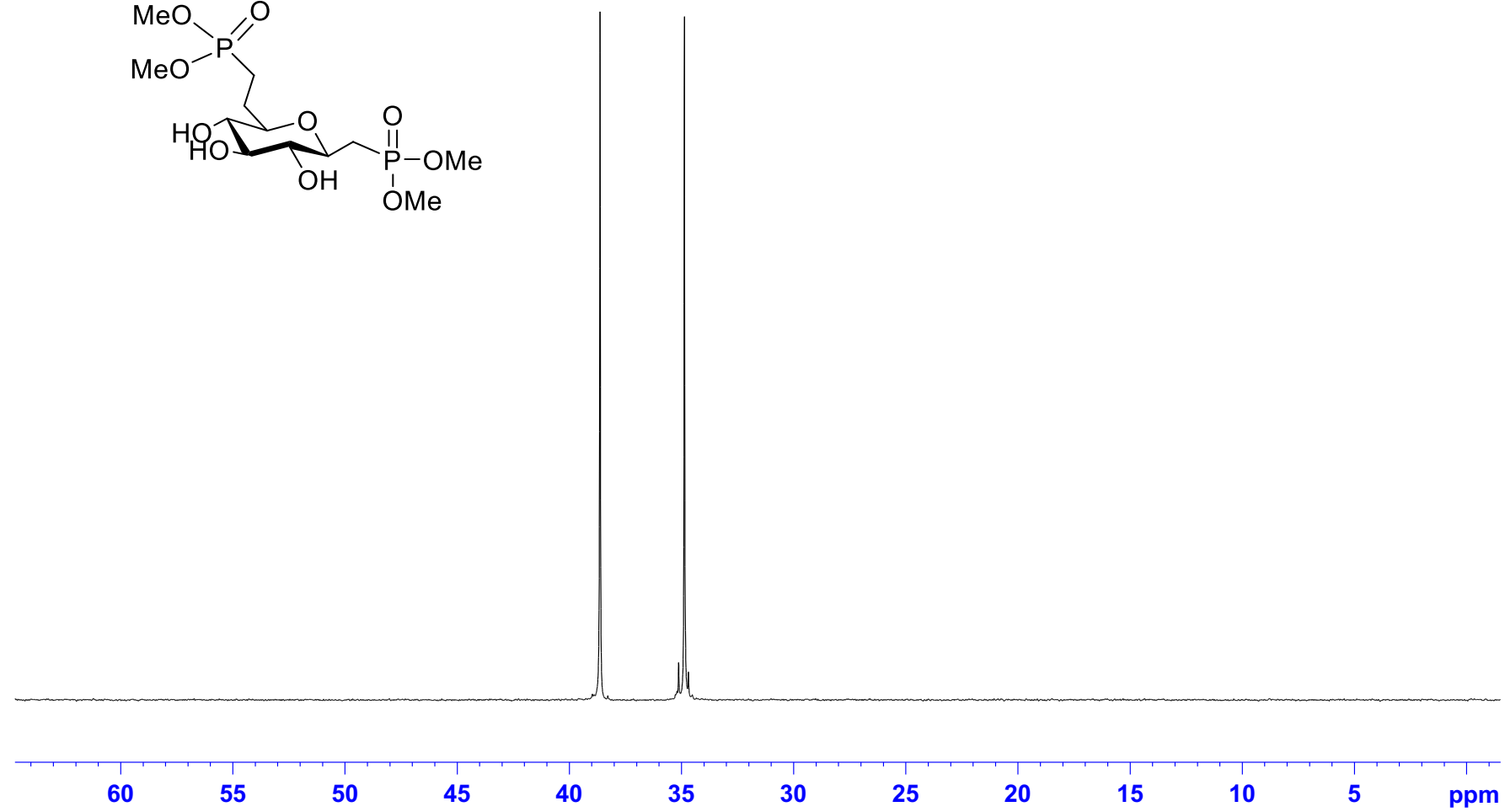
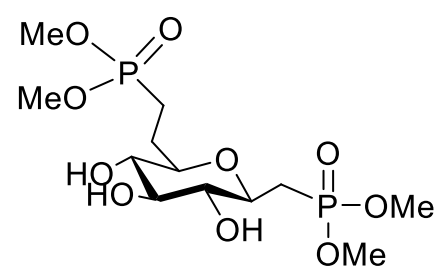
^{13}C NMR (125 MHz, D_2O) spectrum of compound **17** (Bottom)

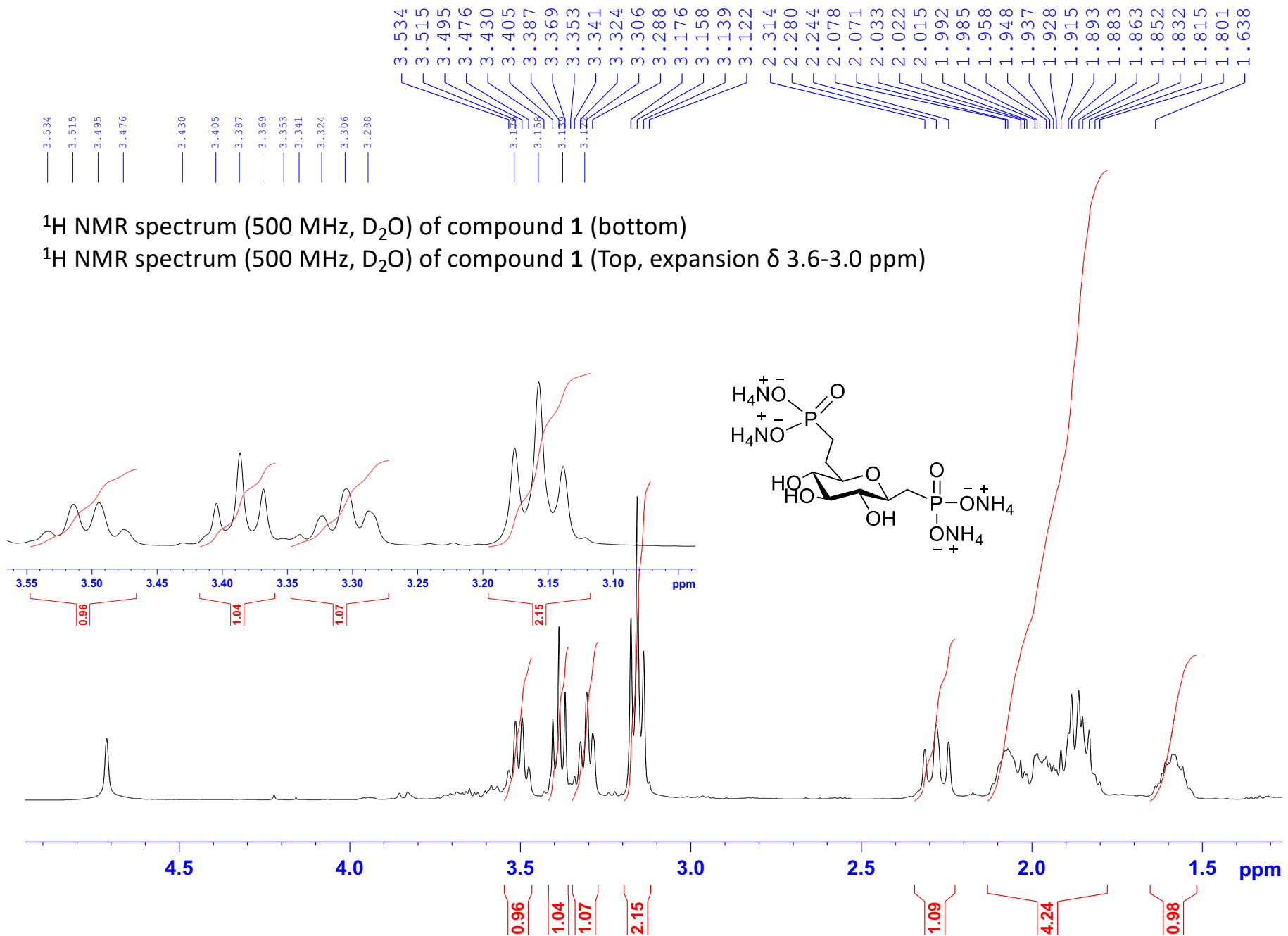
^{13}C NMR (125 MHz, D_2O) spectrum of compound **17** (Top, expansion δ 79.0-73.0 ppm)



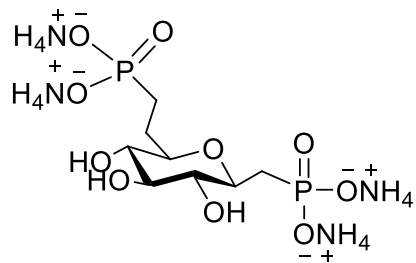
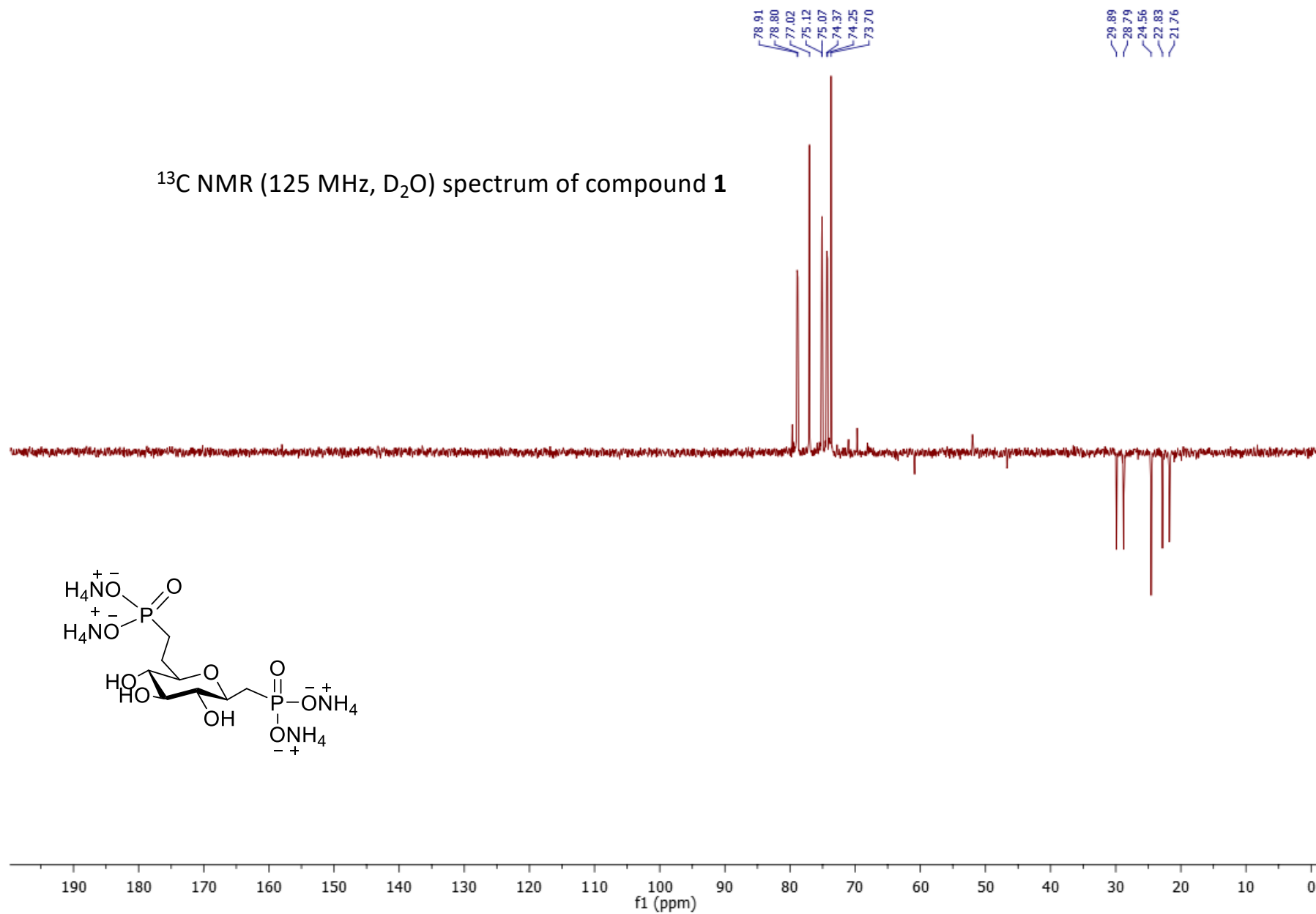
38.64
34.88

$^{31}\text{P}\{^1\text{H}\}$ NMR (202.5 MHz, D_2O) spectrum of compound **17**





^{13}C NMR (125 MHz, D_2O) spectrum of compound **1**



78.92
78.80

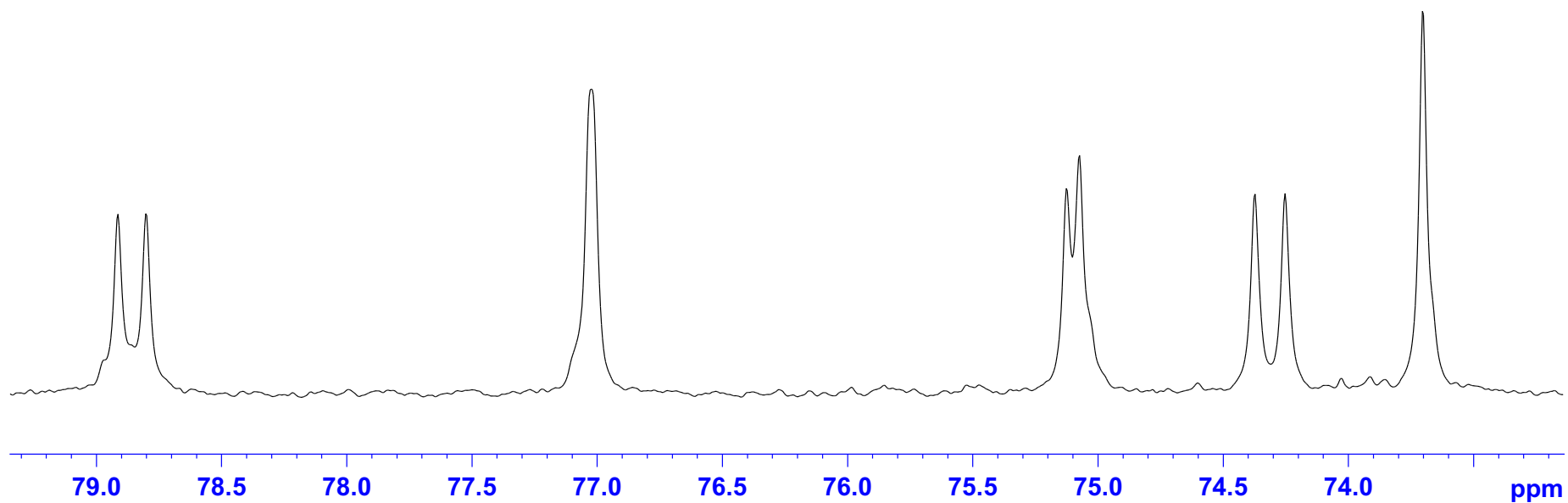
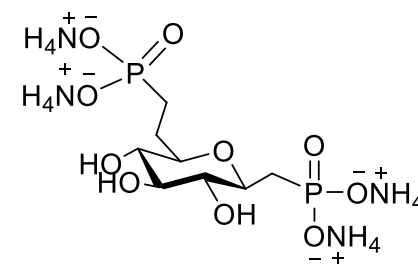
77.03

75.13
75.08

74.38
74.26

73.71

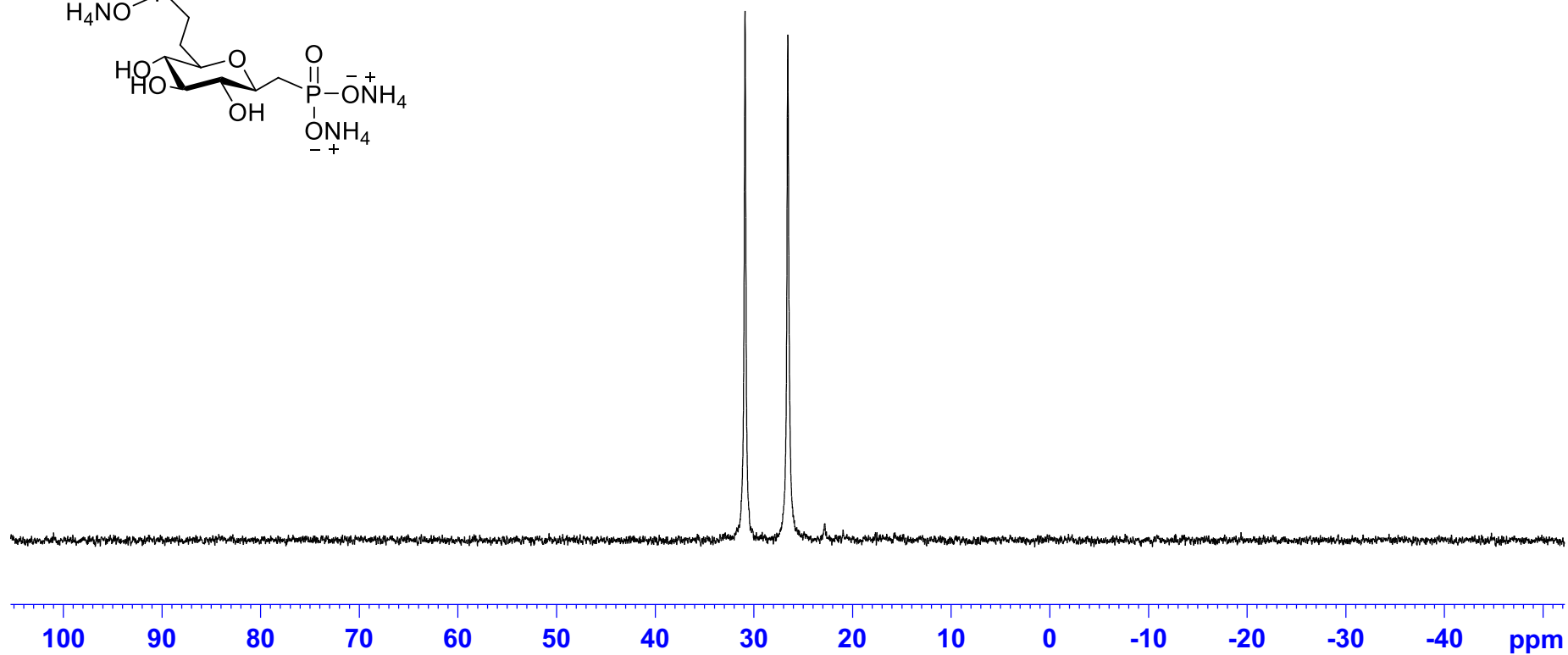
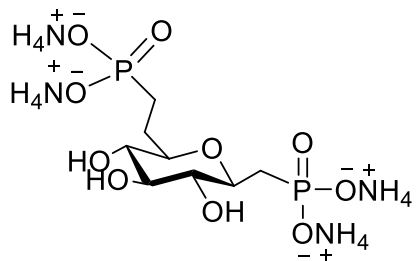
^{13}C NMR (125 MHz, D_2O) spectrum of compound **1** (expansion δ 80-73 ppm)



S31

30.88
26.55

$^{31}\text{P}\{^1\text{H}\}$ NMR (202.5 MHz, D_2O) spectrum of compound **1**



S32