

Regioselective Synthesis of Isoxazole and 1,2,4-Oxadiazole-Derived Phosphonates via [3+2] Cycloaddition

Bohdan A. Chalyk,^{a,b} Alona S. Sosedko,^{a,c} Dmitriy M. Volochnyuk,^{a,b} Andrey A. Tolmachev,^a Konstantin S. Gavrilenko,^{a,c} Oleksandr S. Liashuk^{a,c} and Oleksandr O. Grygorenko^a

^aEnamine Ltd., Chervonotkatska Street 78, Kyiv 02094, Ukraine, www.enamine.net

^bInstitute of Organic Chemistry, National Academy of Sciences of Ukraine, Murmanska Street 5, Kyiv 02660, Ukraine

^cNational Taras Shevchenko University of Kyiv, Volodymyrska Street 64, Kyiv 01601, Ukraine.

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9012595s1.1.fid

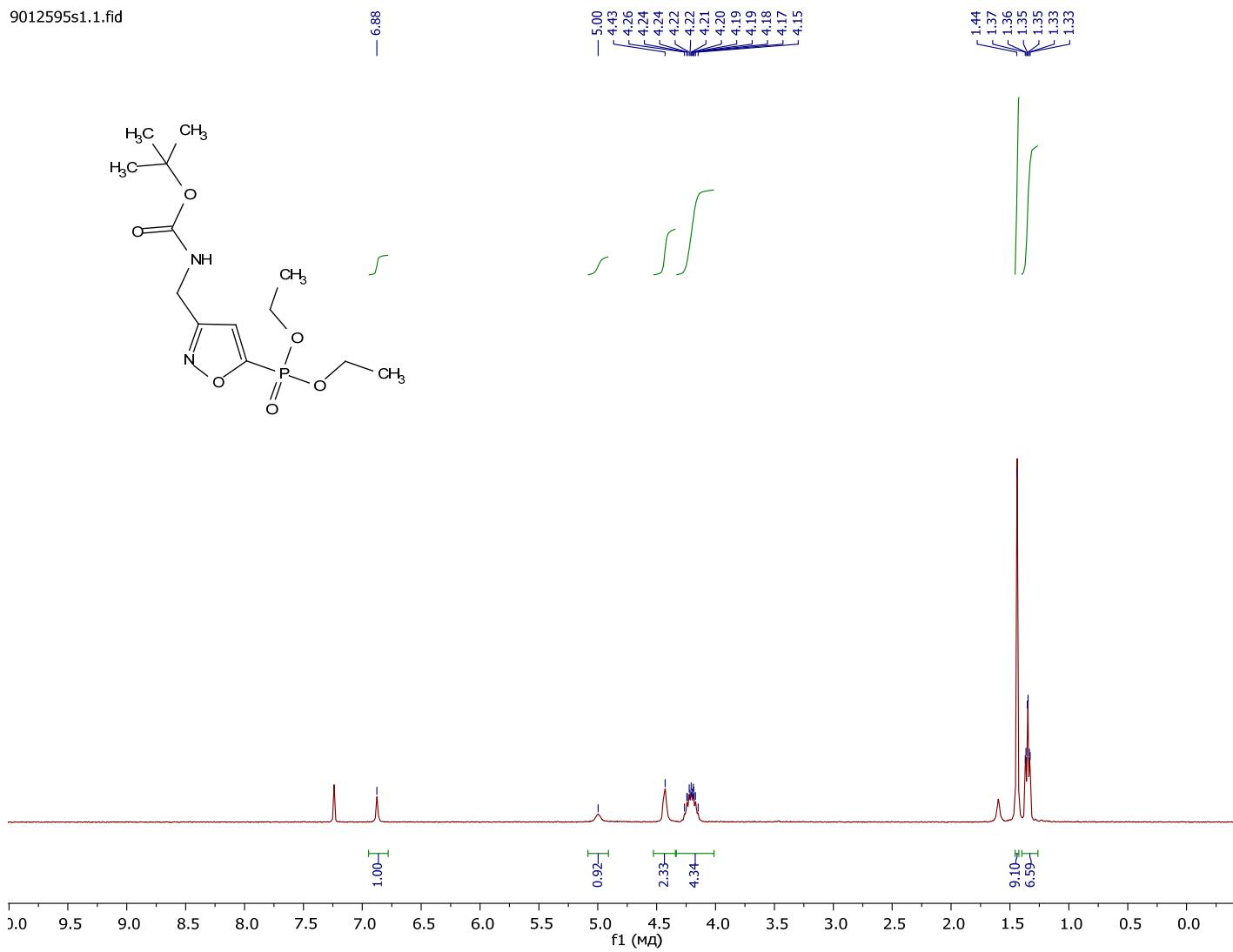


Figure 1 ^1H NMR spectrum of 1a

sklf6662_C13.1.fid

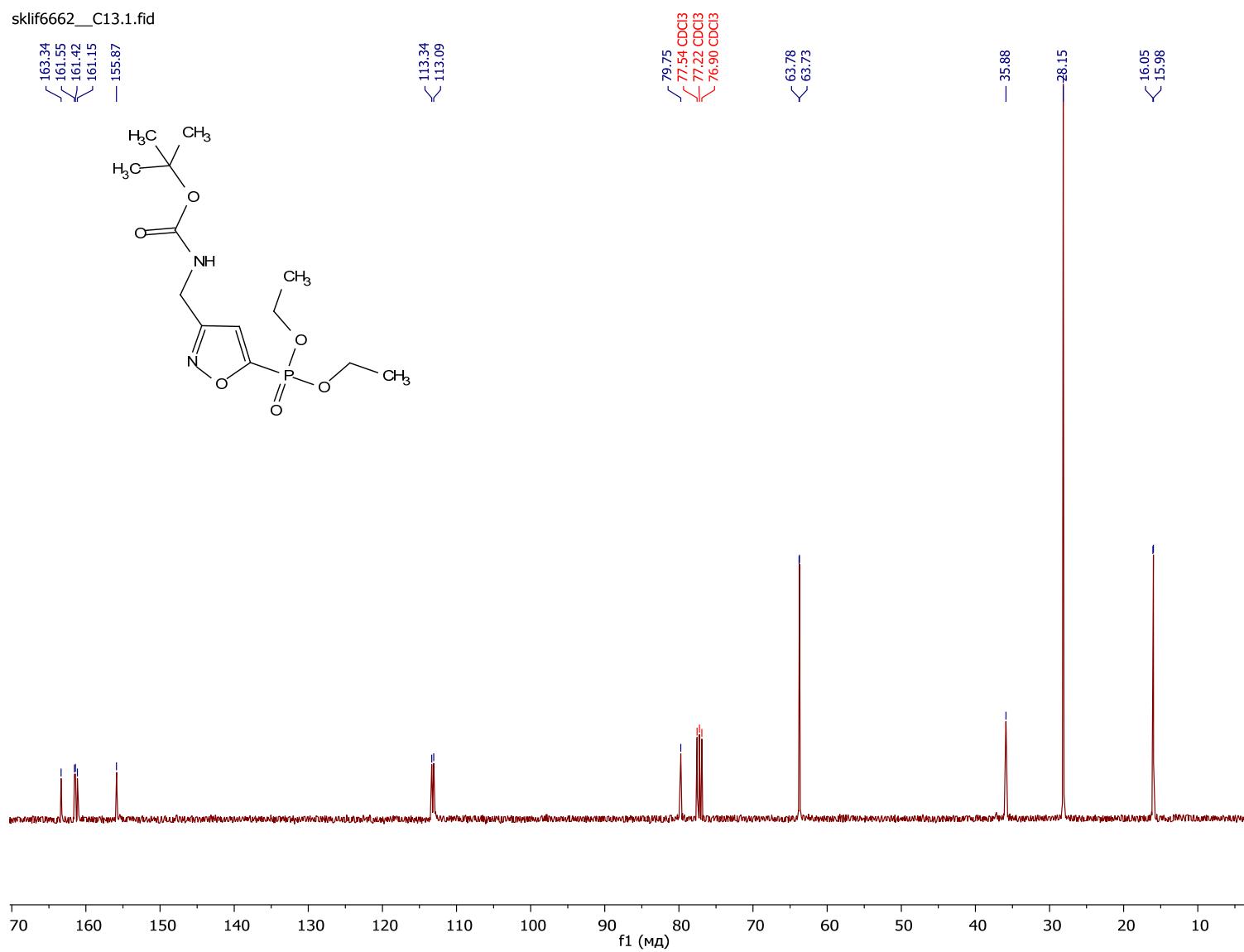


Figure 2 ^{13}C NMR spectrum of 1a

sklf6662_P31.1.fid

— 0.34

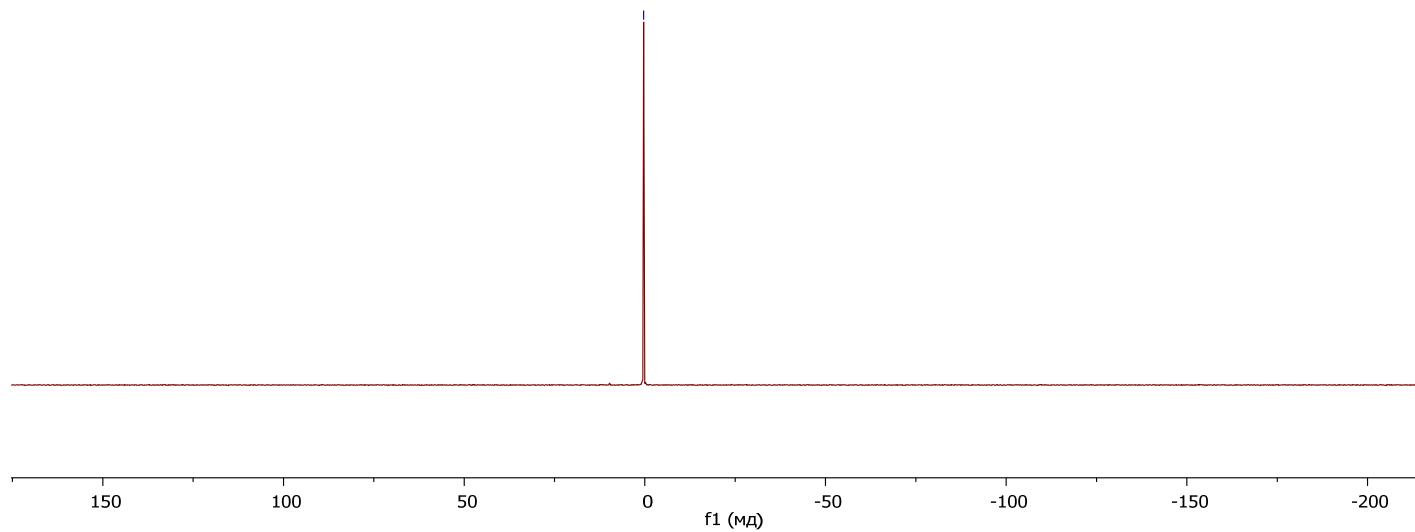
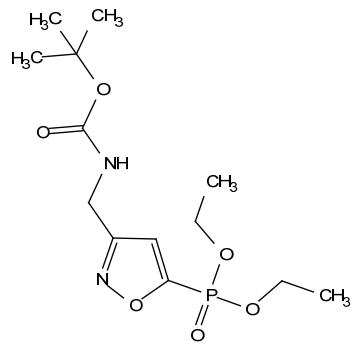


Figure 3 ³¹P NMR spectrum of 1a

9012610s1.1.fid

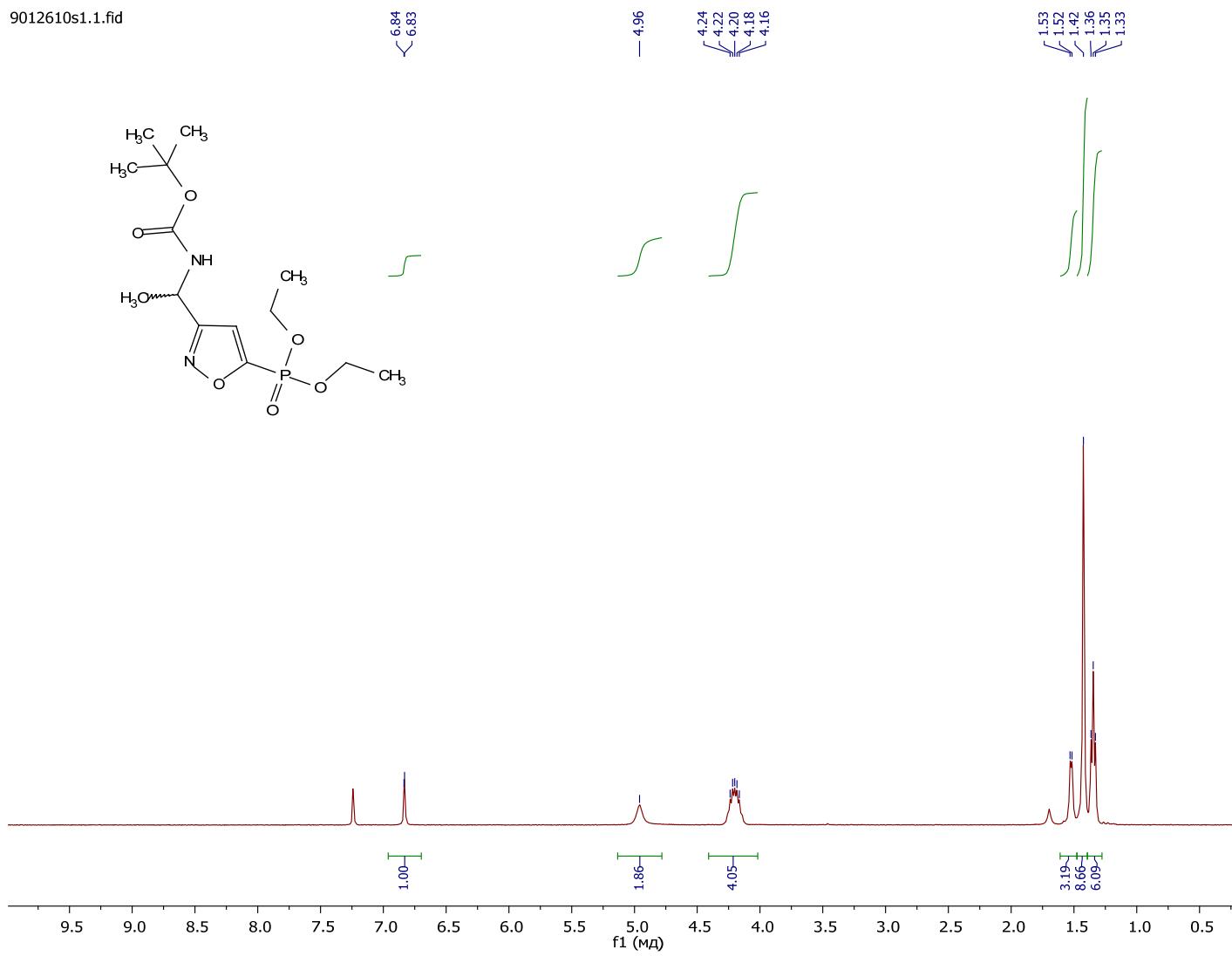


Figure 4 ¹H NMR spectrum of 1b and 1c (R-isomer)

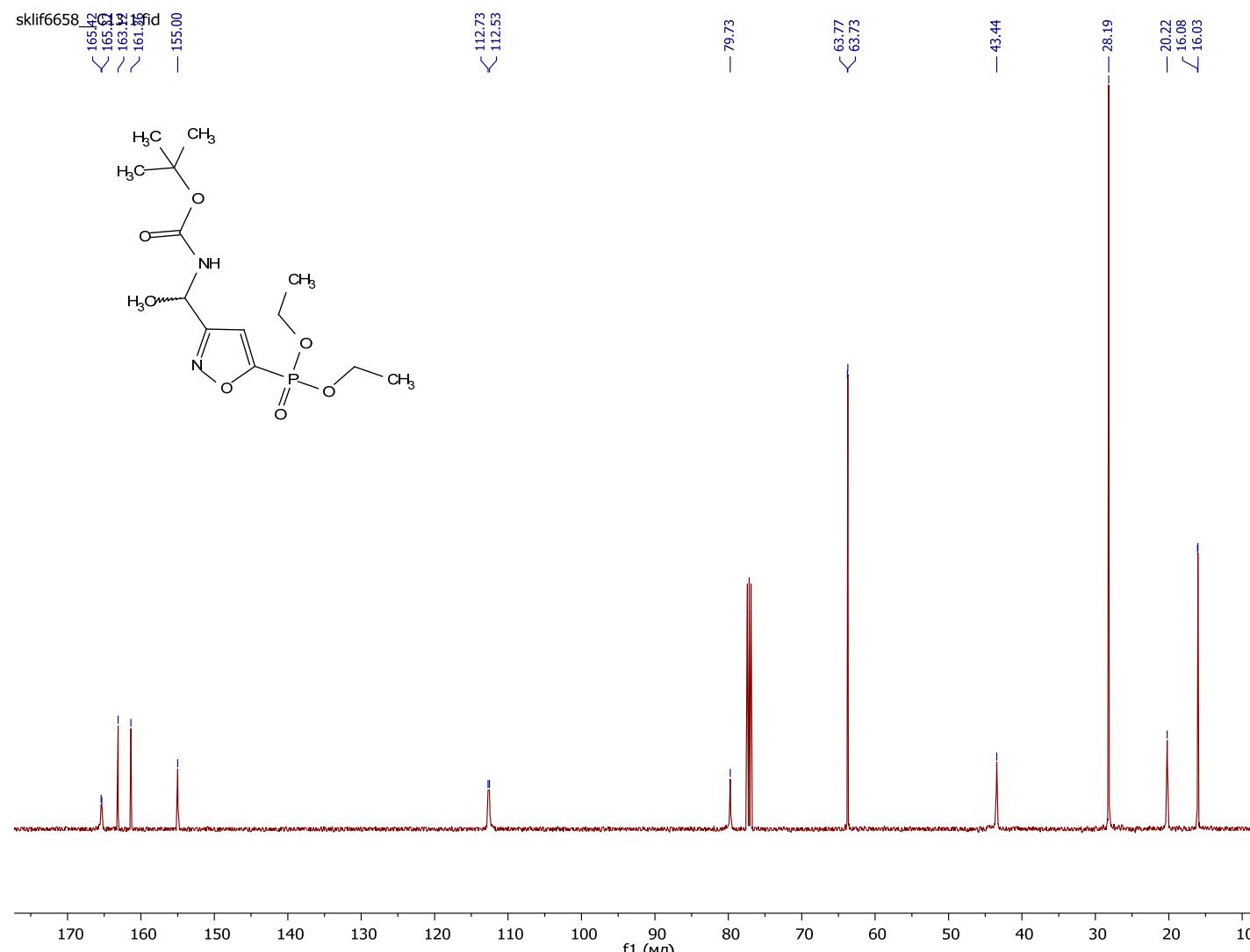


Figure 5 ^{13}C NMR spectrum of 1b and 1c (*R*-isomer)

sklf6658_P31.1.fid

— 0.31

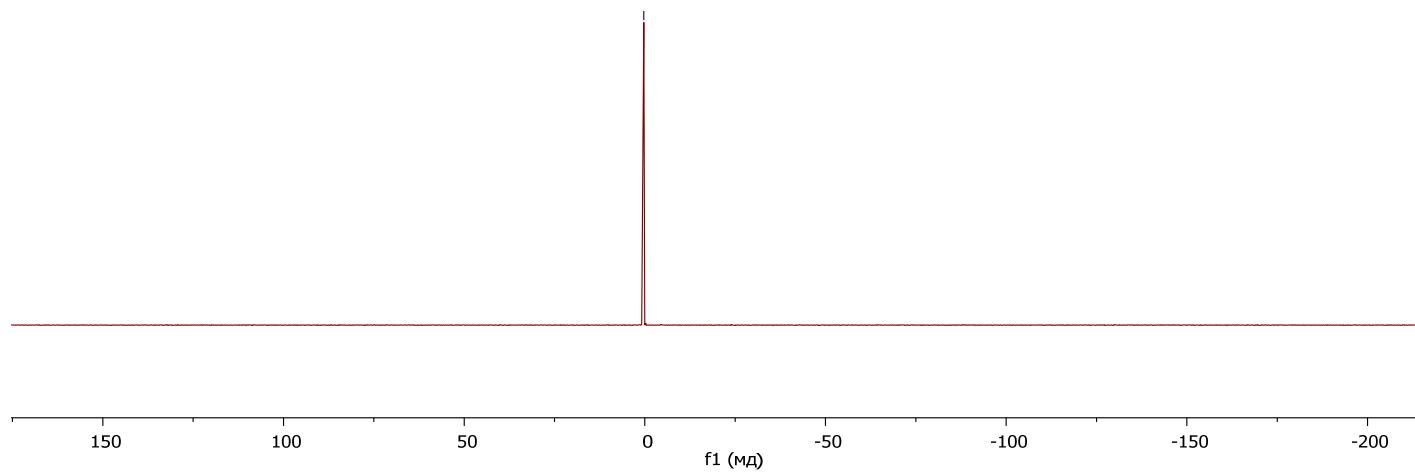
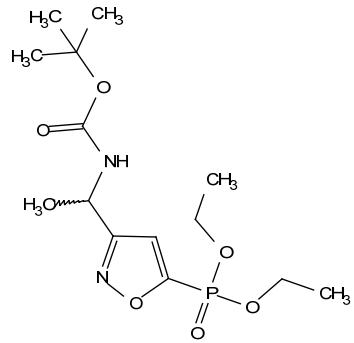


Figure 6 ^{31}P NMR spectrum of 1b and 1c (*R*-isomer)

AB6566-3.1.fid

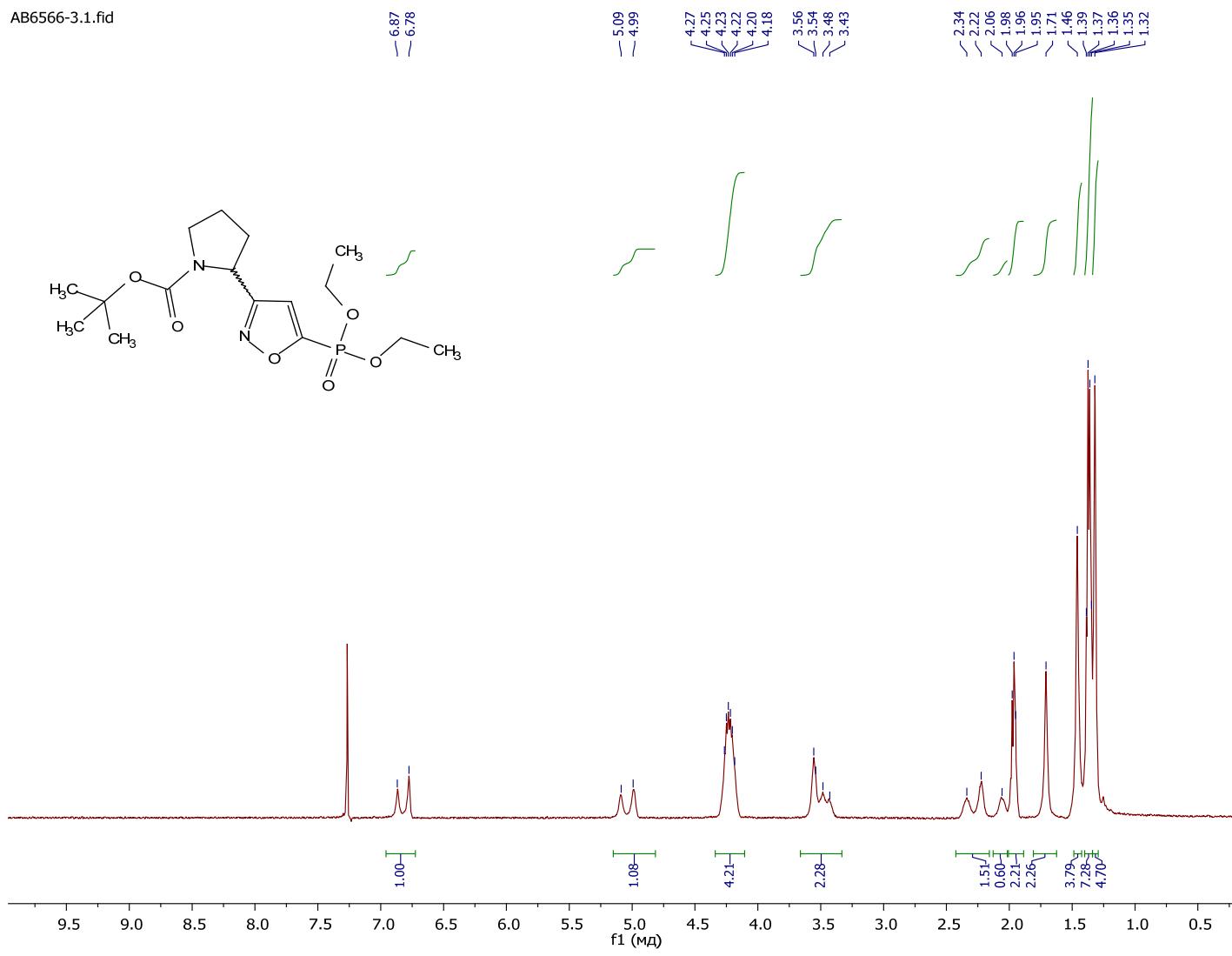


Figure 7 ¹H NMR spectrum of 1f and 1g (R-isomer)

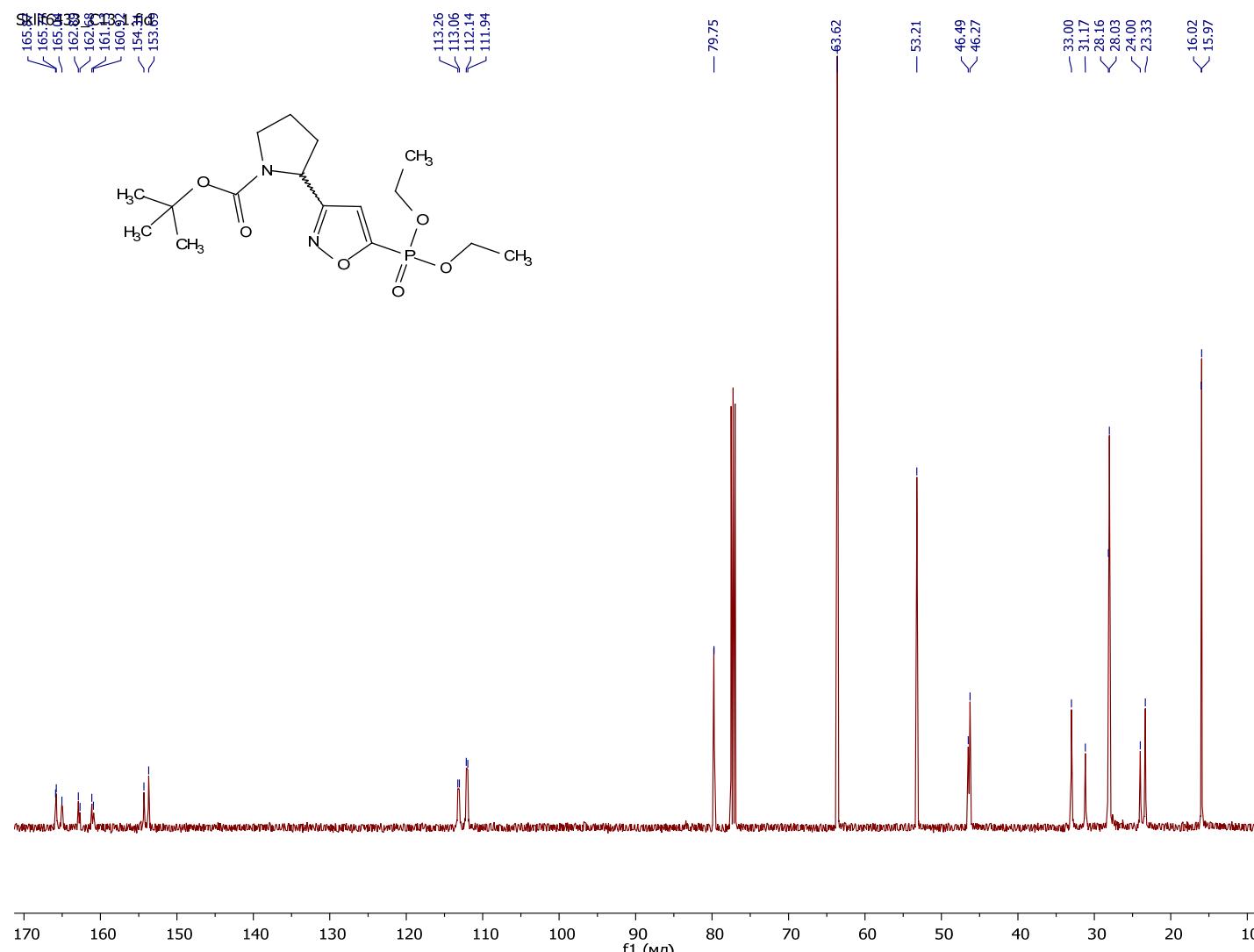


Figure 8 ^{13}C NMR spectrum of 1f and 1g (R-isomer)

Sklif6433_P31.1.fid
31P-{1H}

0.50
0.35

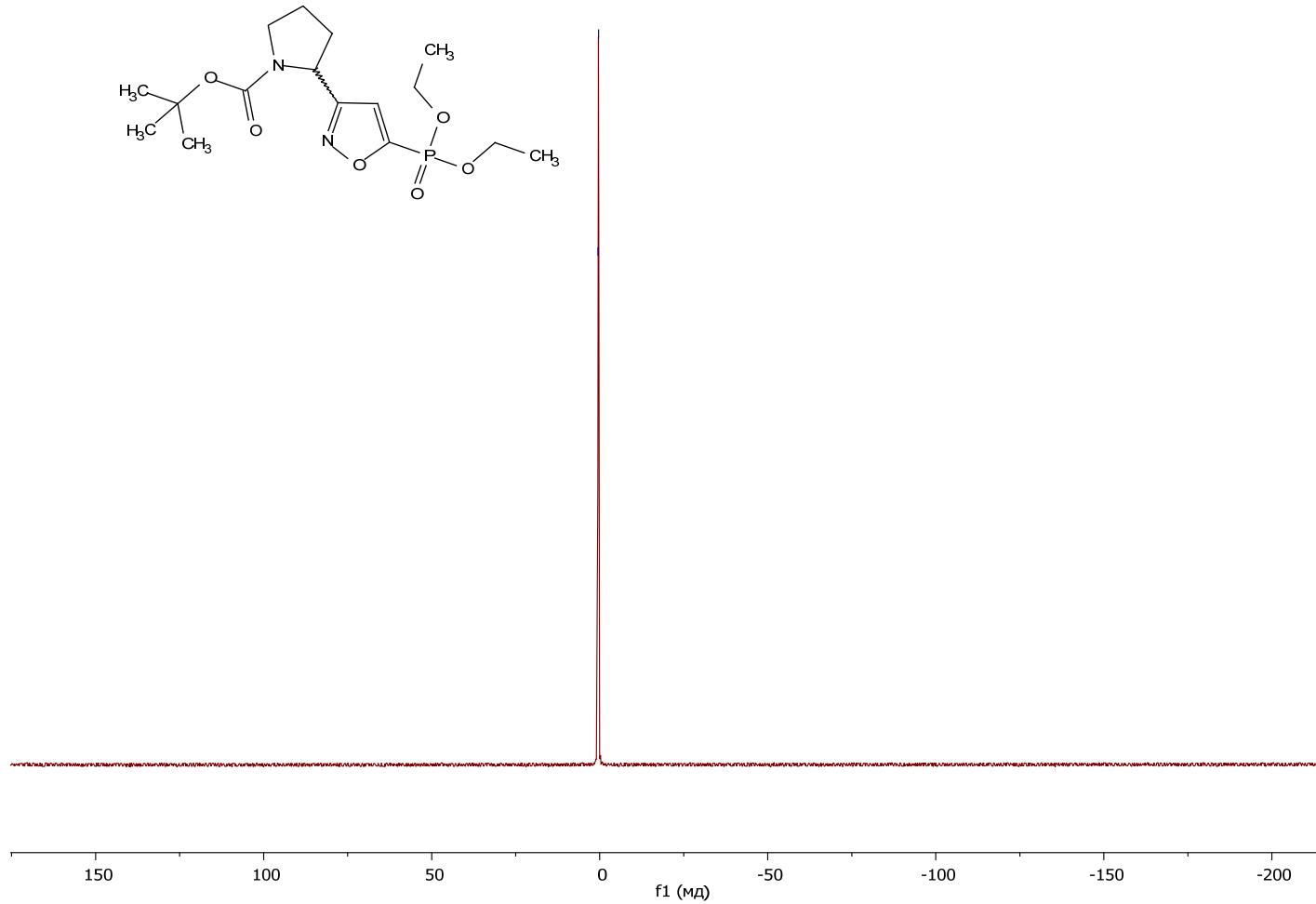


Figure 9 ^{31}P NMR spectrum of 1f and 1g (*R*-isomer)

9000692s2.1.fid

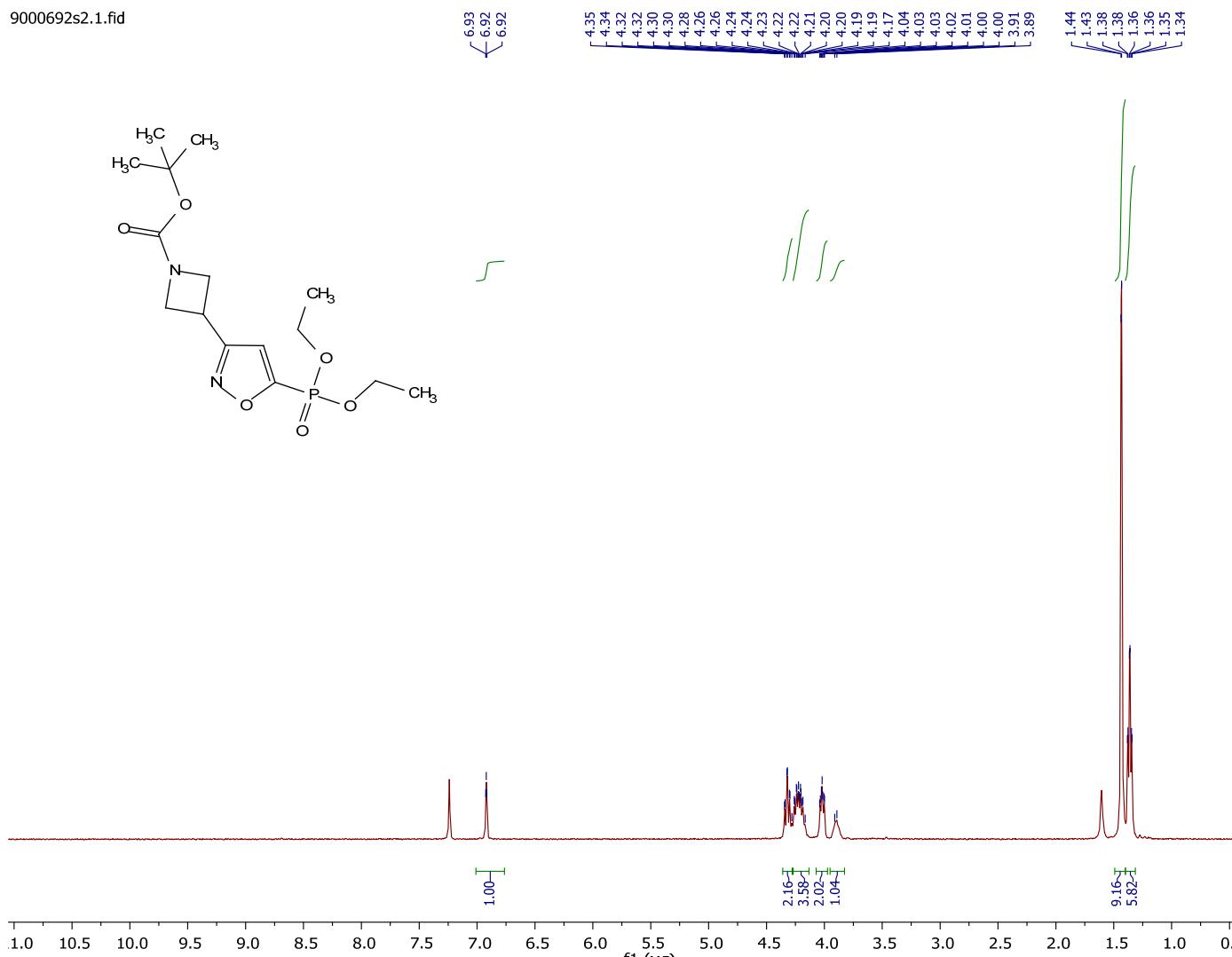


Figure 10 ^1H NMR spectrum of 1j

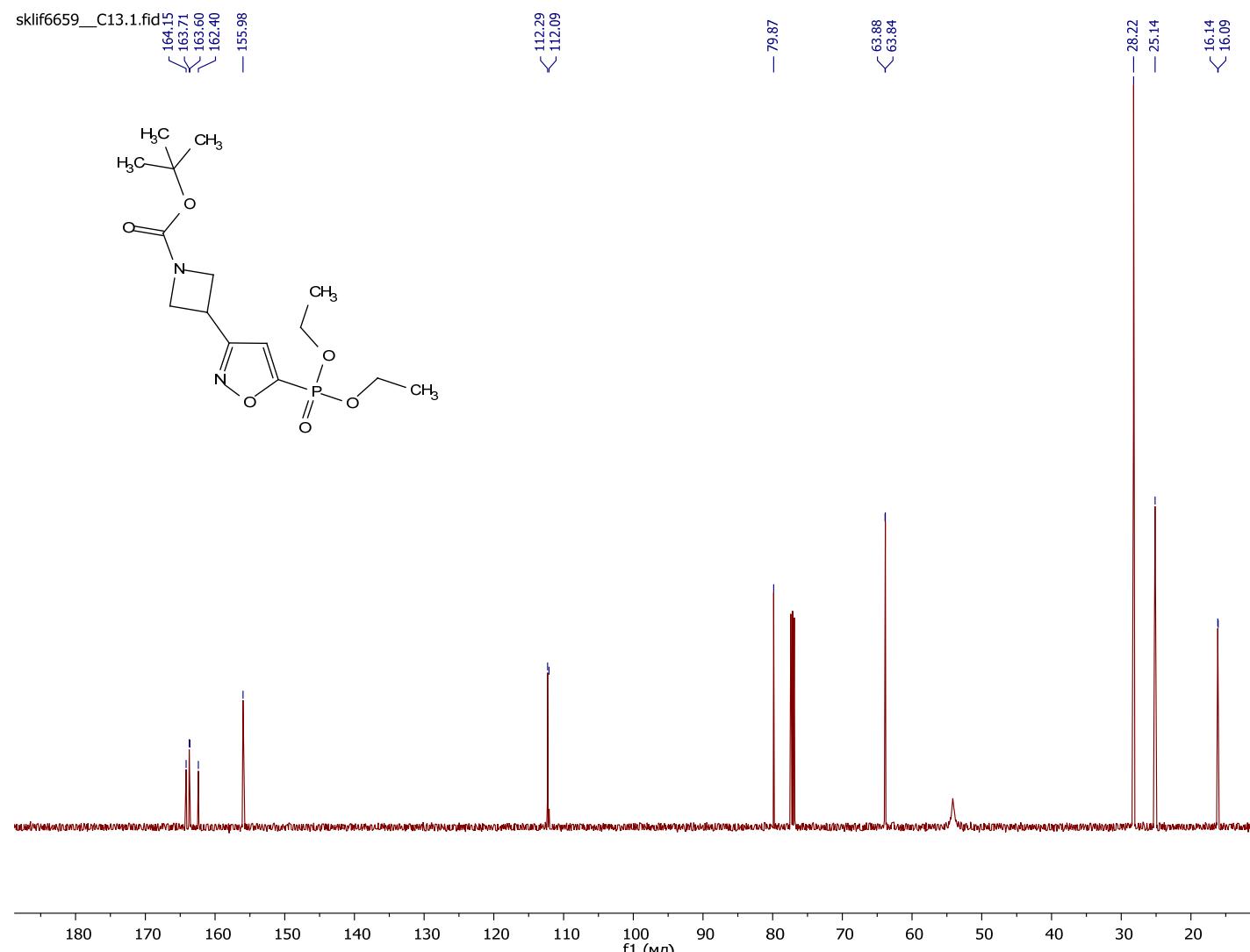


Figure 11 ^{13}C NMR spectrum of 1j

sklf6659_P31.1.fid

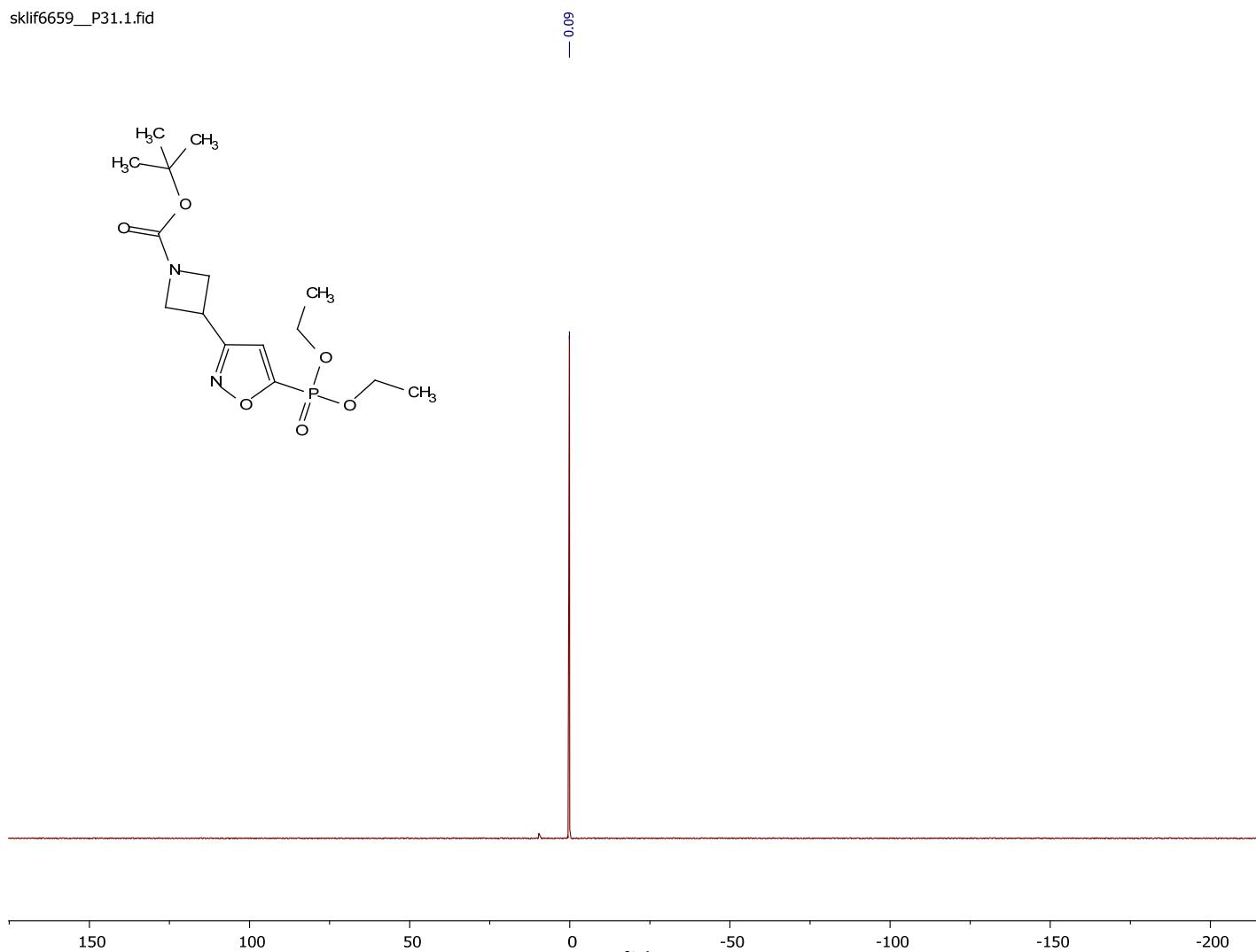


Figure 12 ^{31}P NMR spectrum of 1j

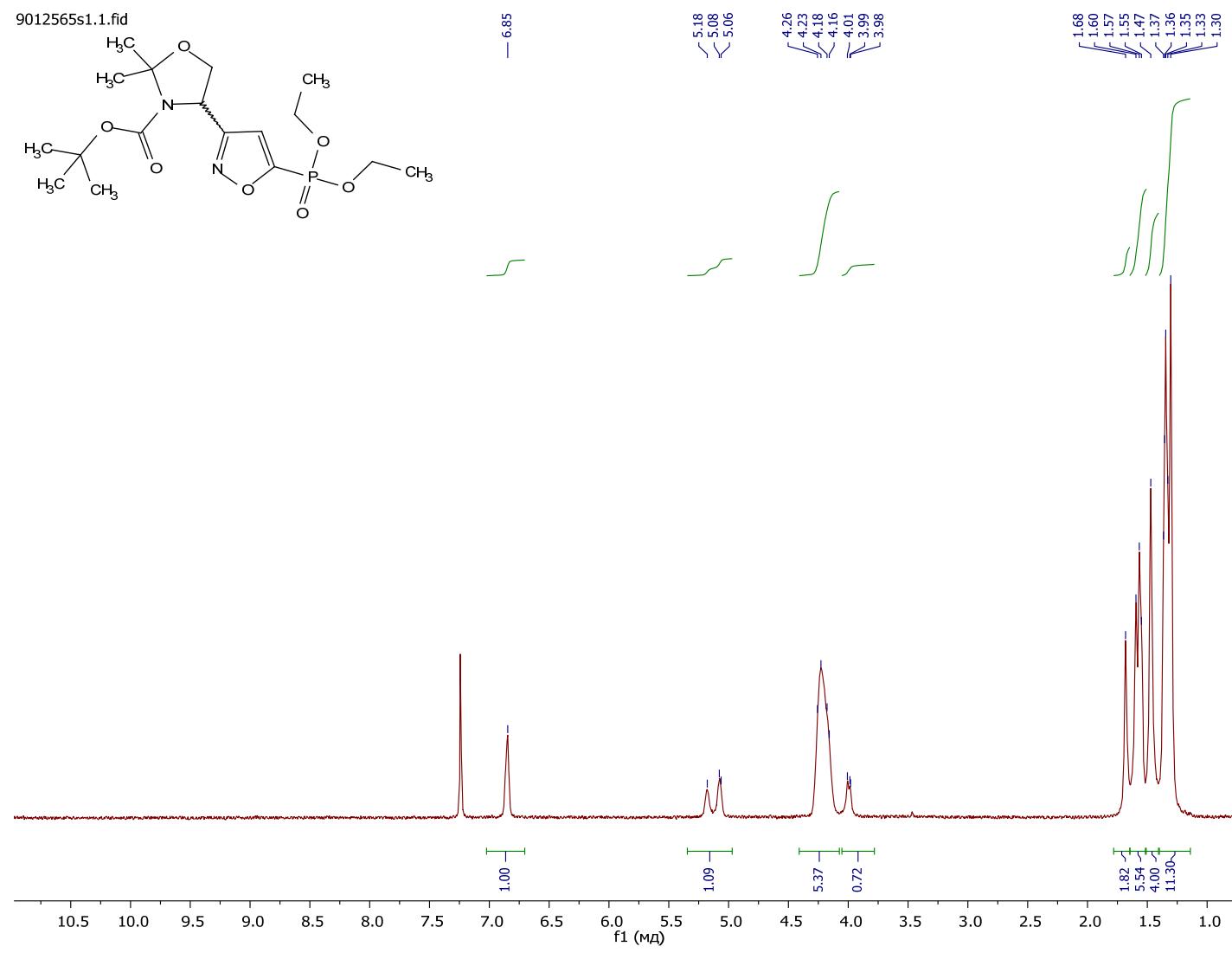


Figure 13 ¹H NMR spectrum of 1k and 1l (*R*-isomer)

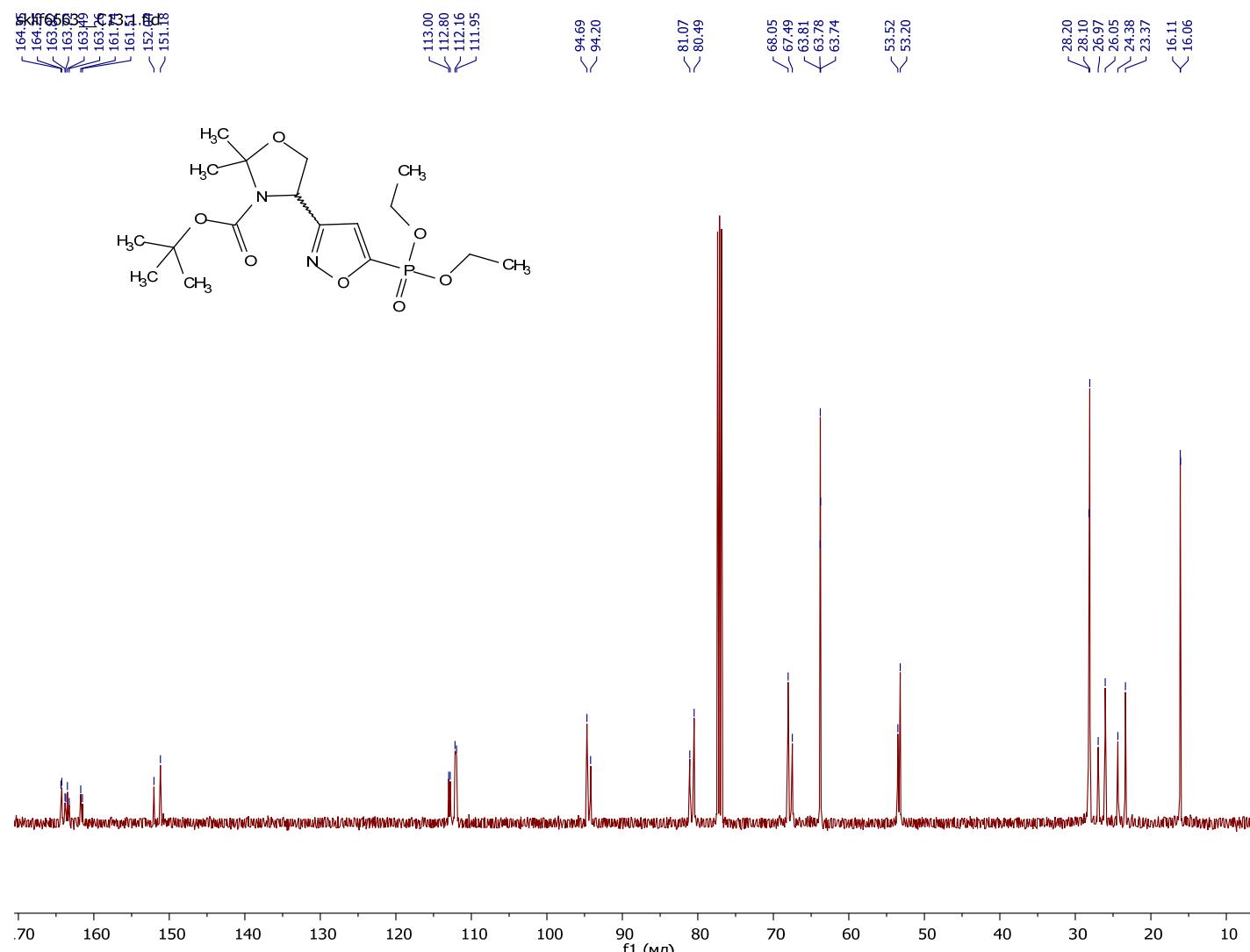


Figure 14 ^{13}C NMR spectrum of **1k** and **1l** (R-isomer)

sklf6663_P31.1.fid

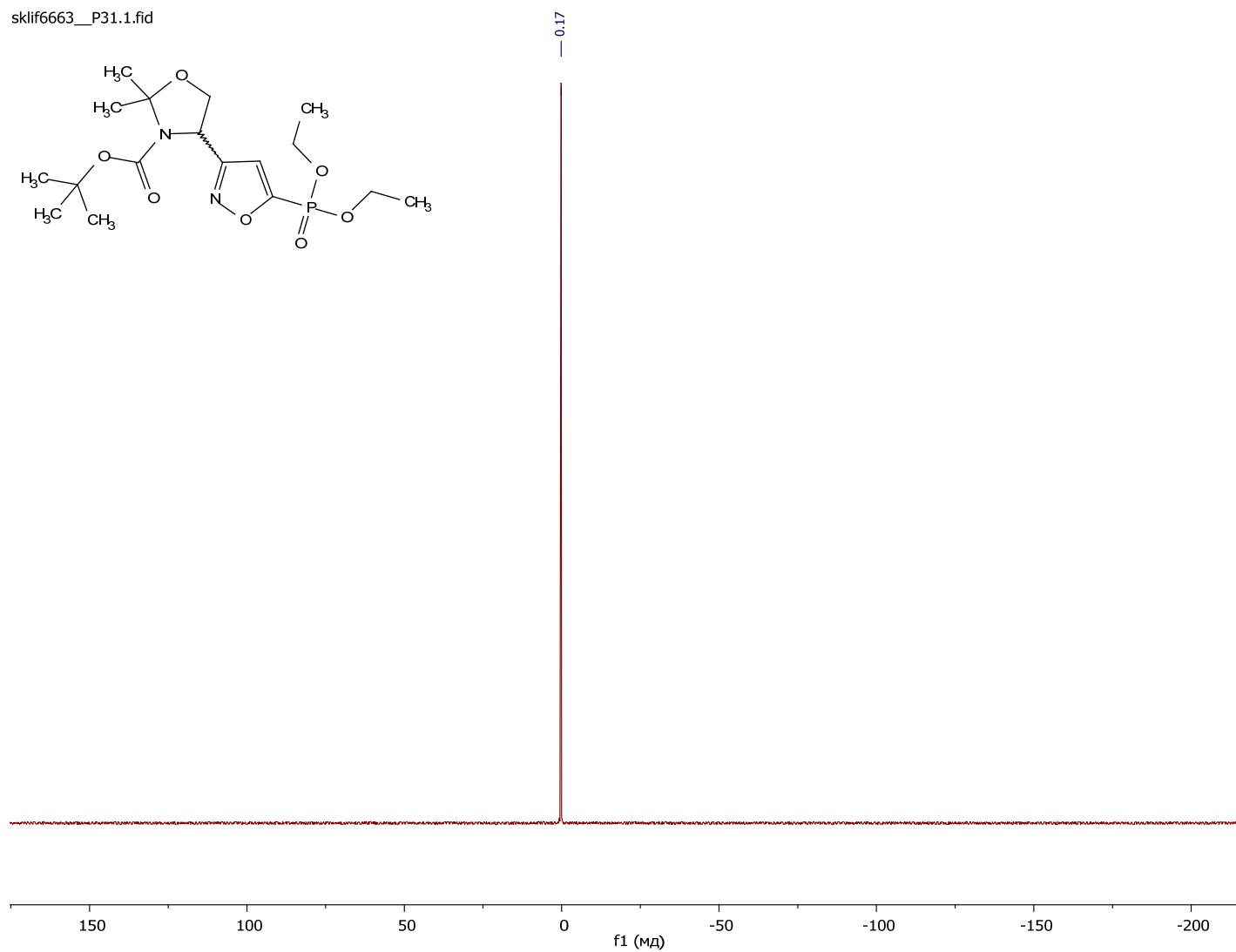
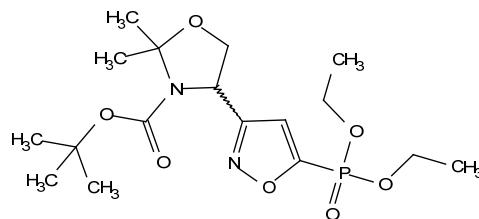


Figure 15 ³¹P NMR spectrum of 1k and 1l (*R*-isomer)

M024208s2

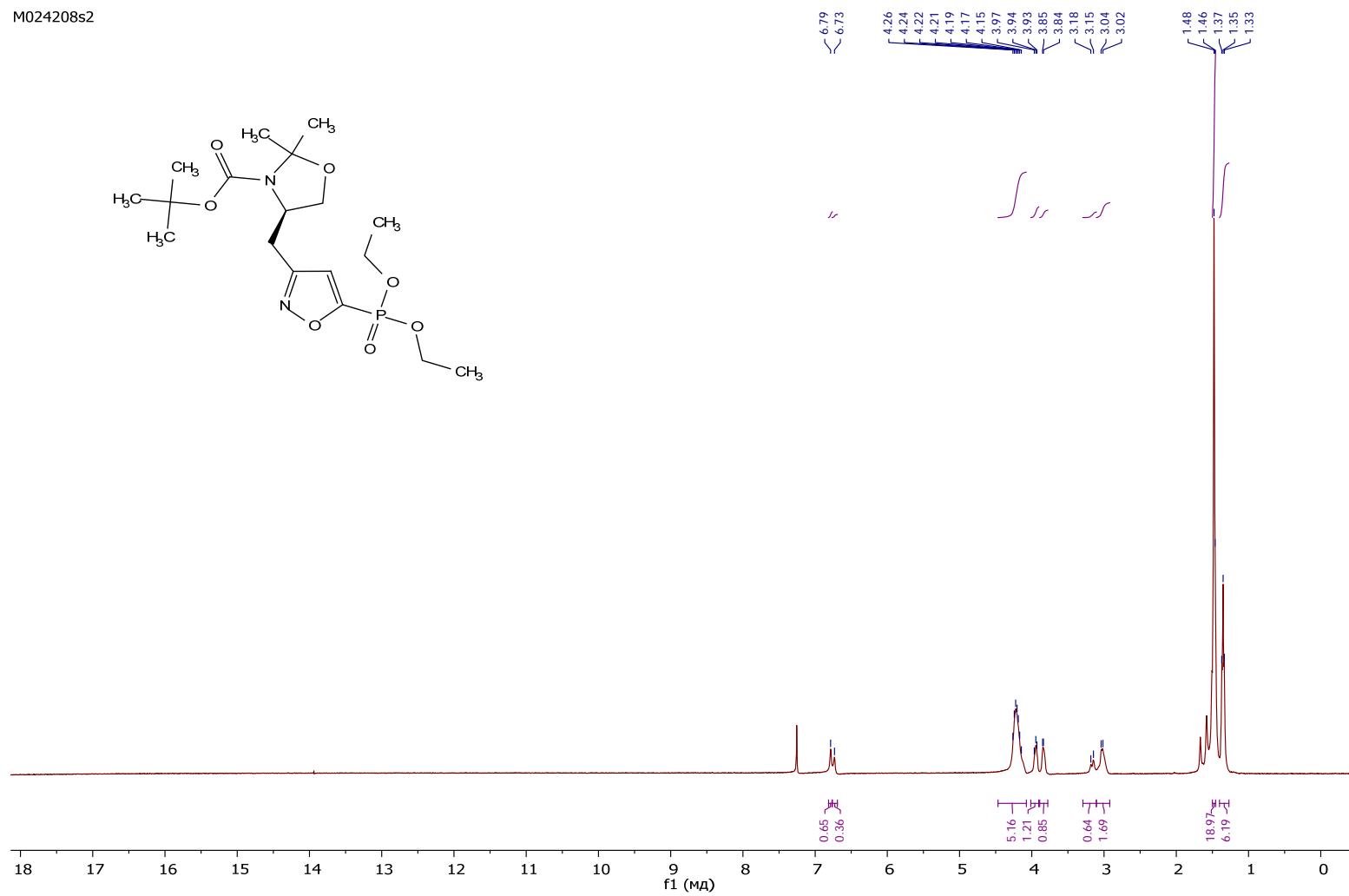
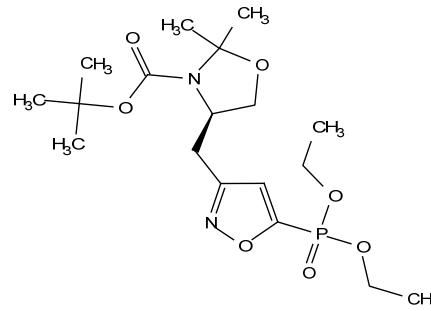


Figure 16. ^1H NMR spectrum of 1m and 1n (*R*-isomer)

sklif1868_13C.1.fid

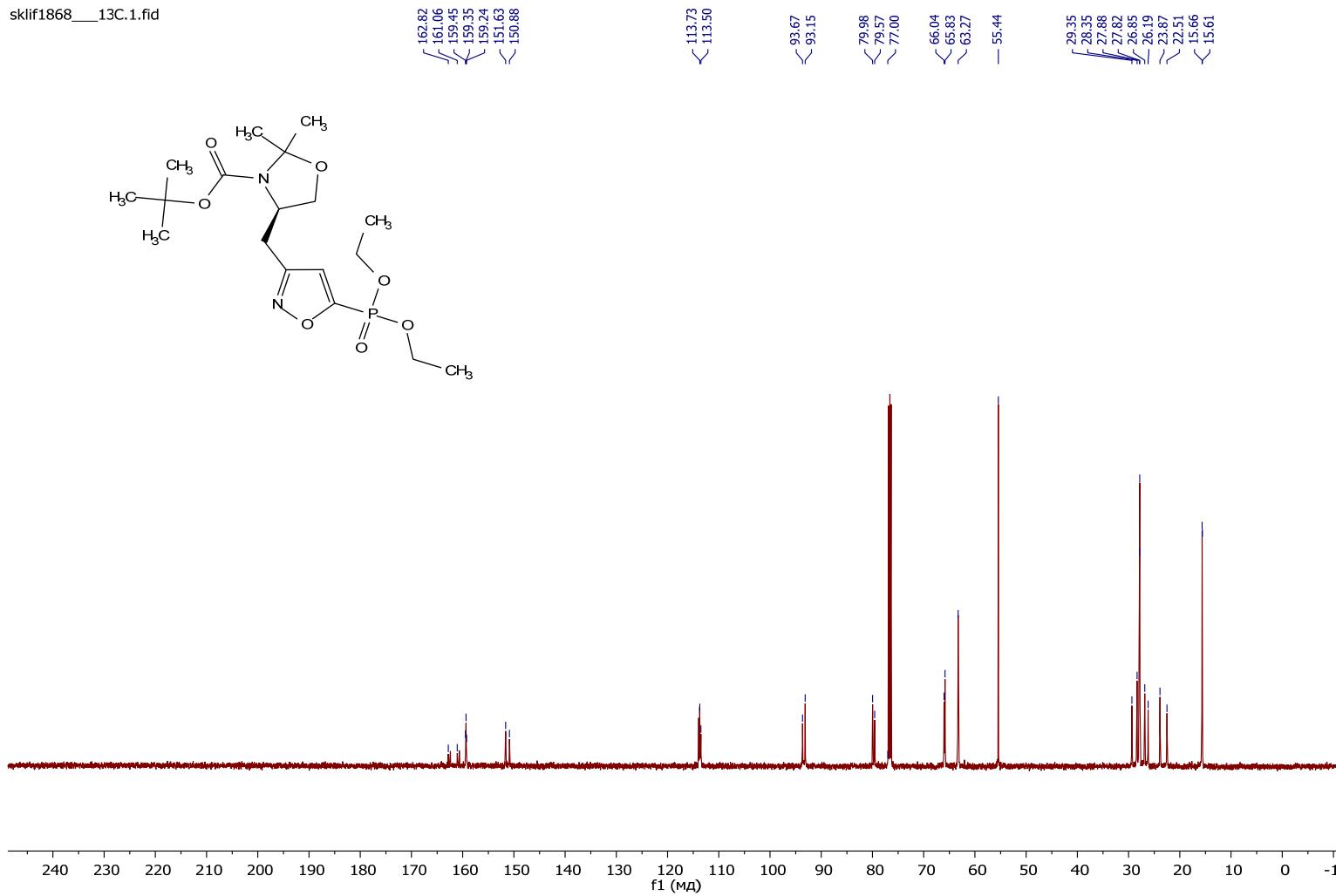


Figure 17. ^{13}C NMR spectrum of 1m and 1n (R-isomer)

sklif1858_31P.1.fid

0.07
0.03
0.01
-0.19
-0.23
-0.27

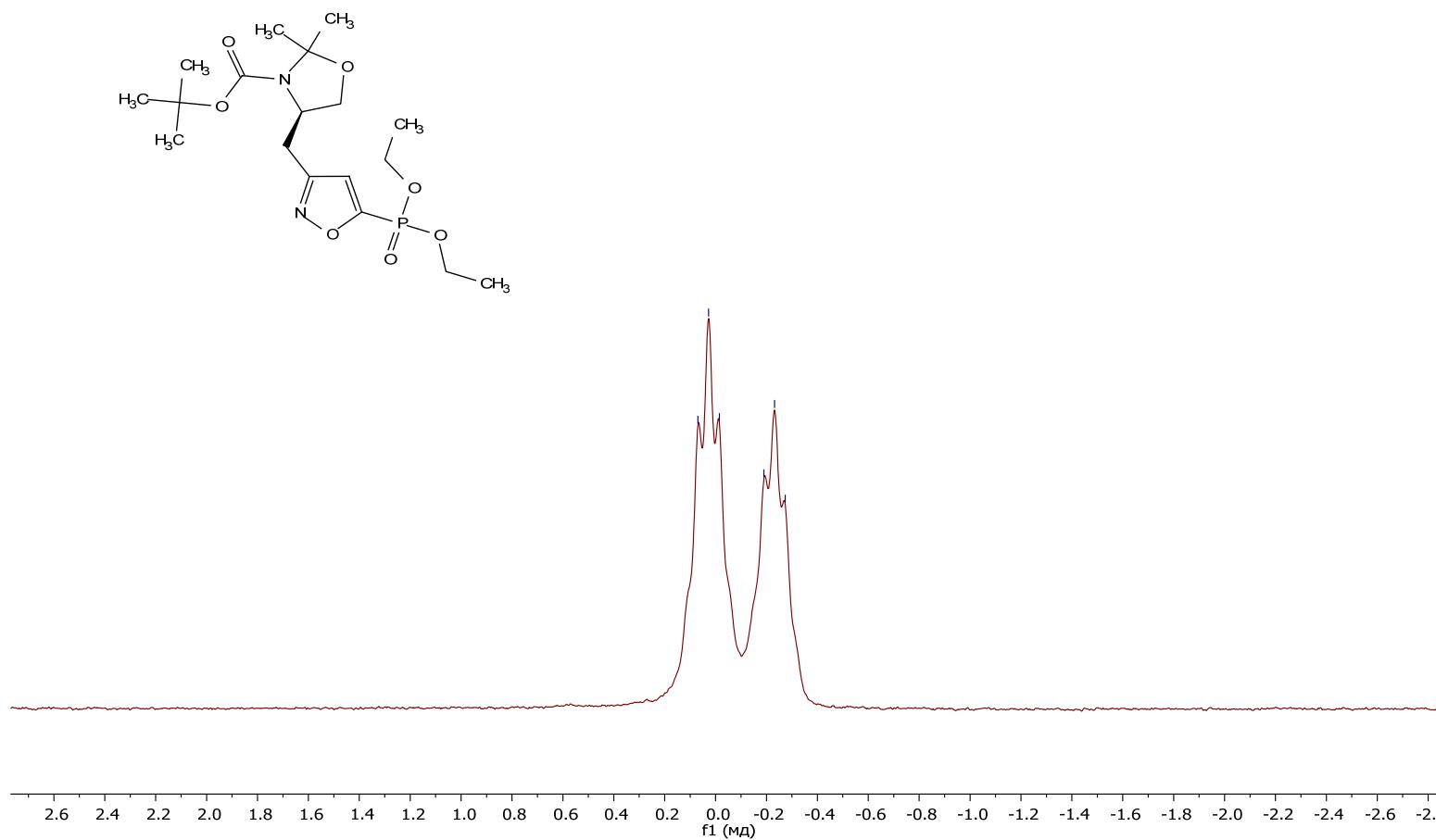


Figure 18. ^{31}P NMR spectrum of **1m** and **1n** (*R*-isomer)

K774890s2

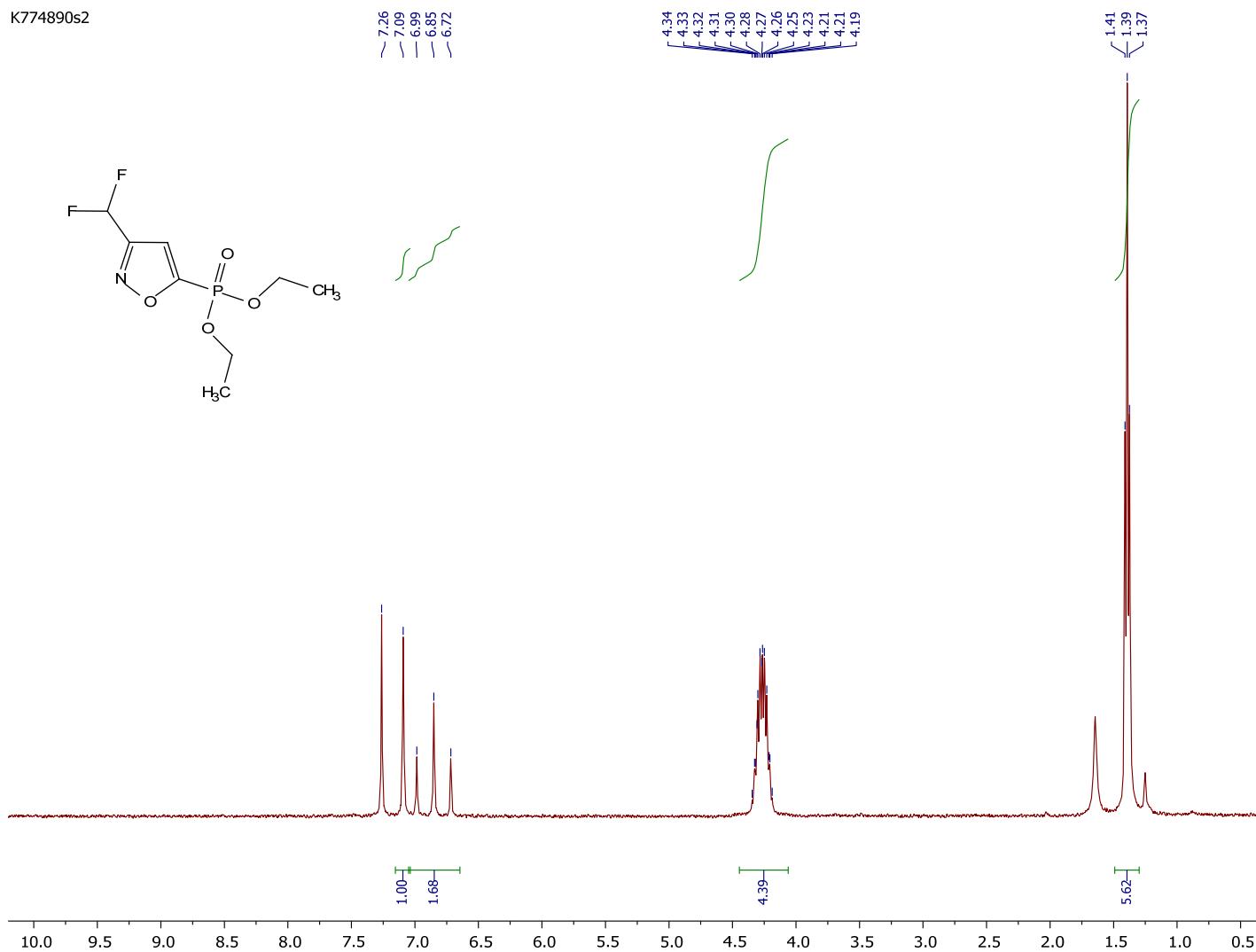


Figure 19 ¹H NMR spectrum of 1p

sklf3125_C13.1.fid

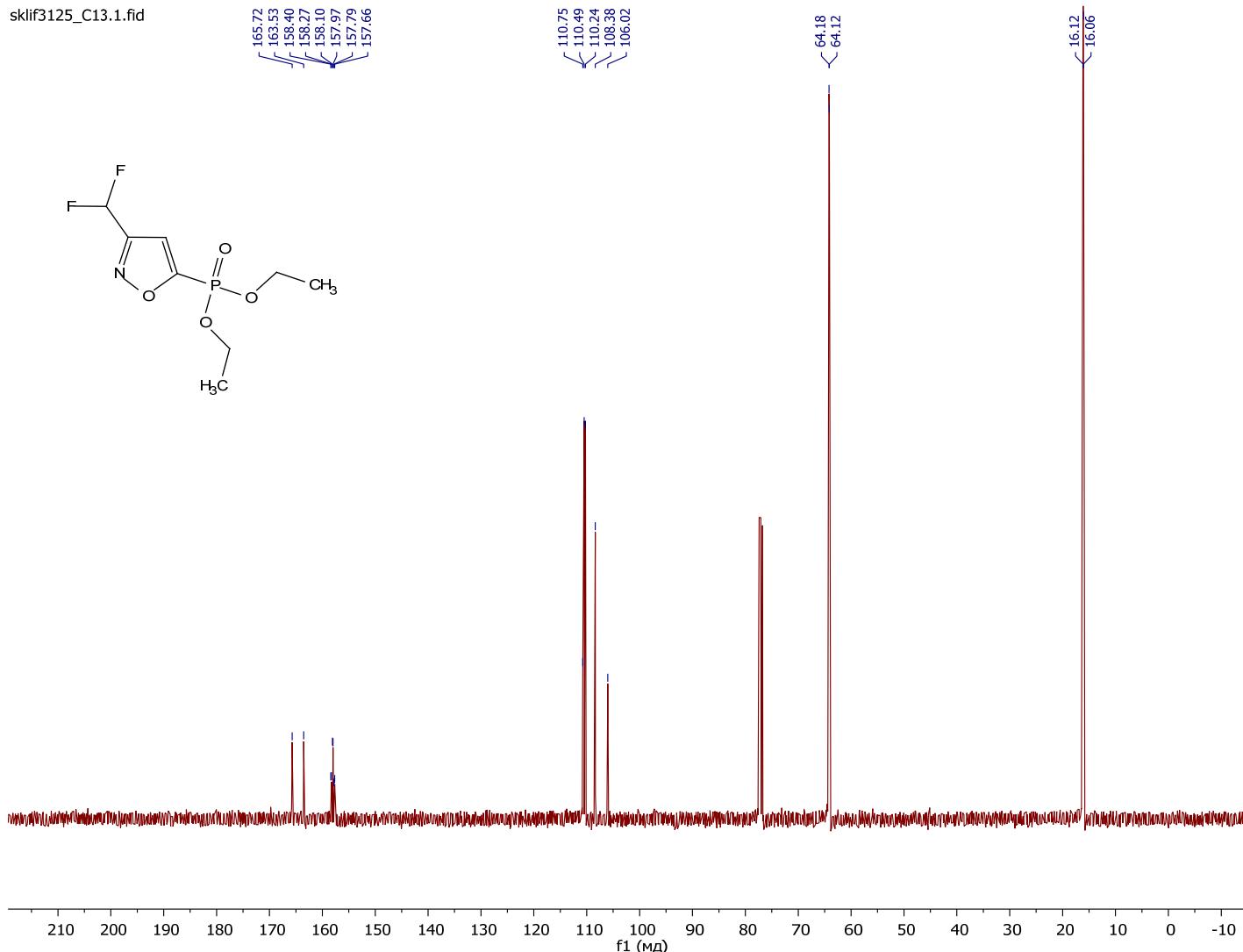


Figure 20 ^{13}C NMR spectrum of 1p

sklf3125 31P{1H}.1.fid

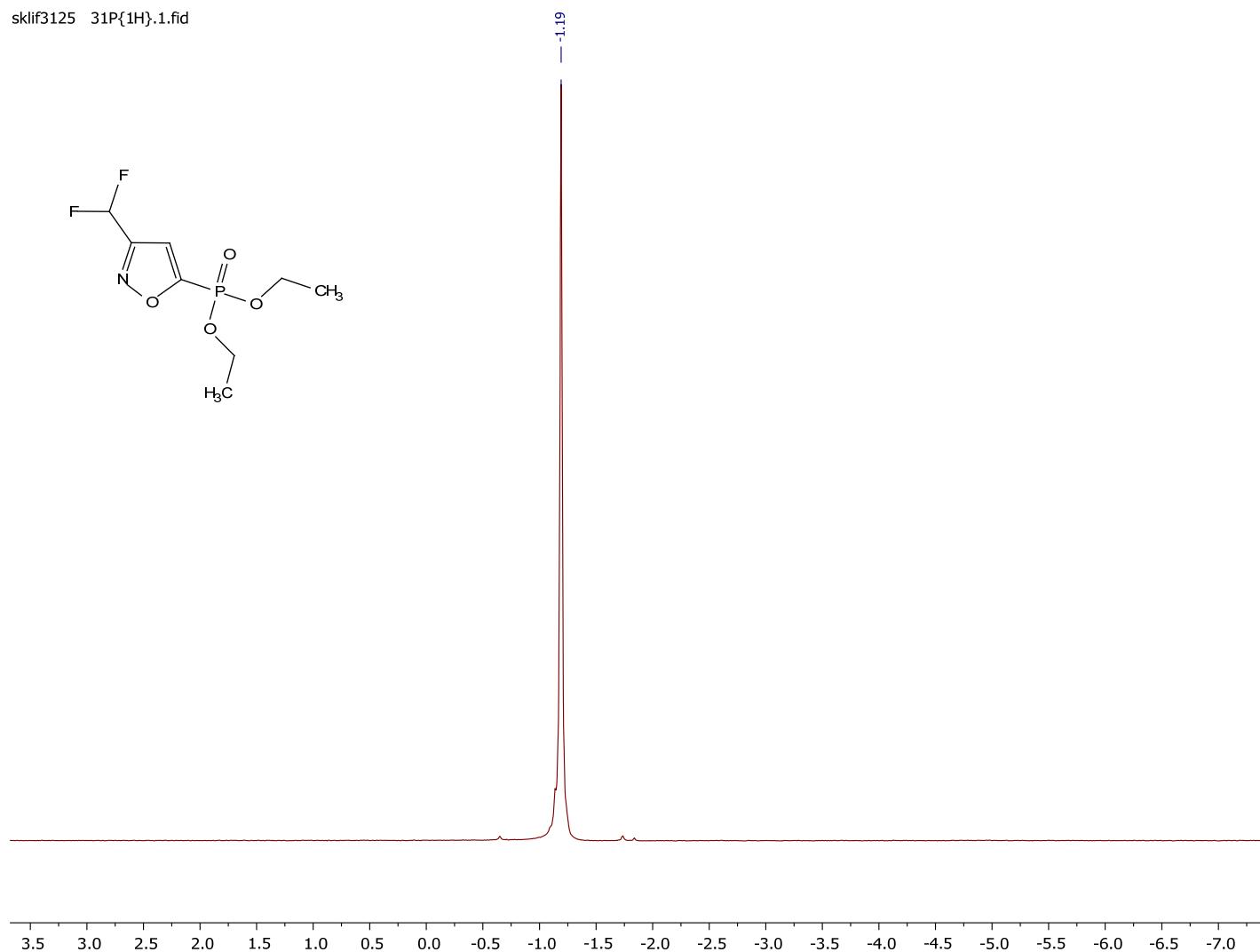


Figure 21 ^{31}P NMR spectrum of 1p

sklif3125_F19{H}.1.fid
19F-{1H}

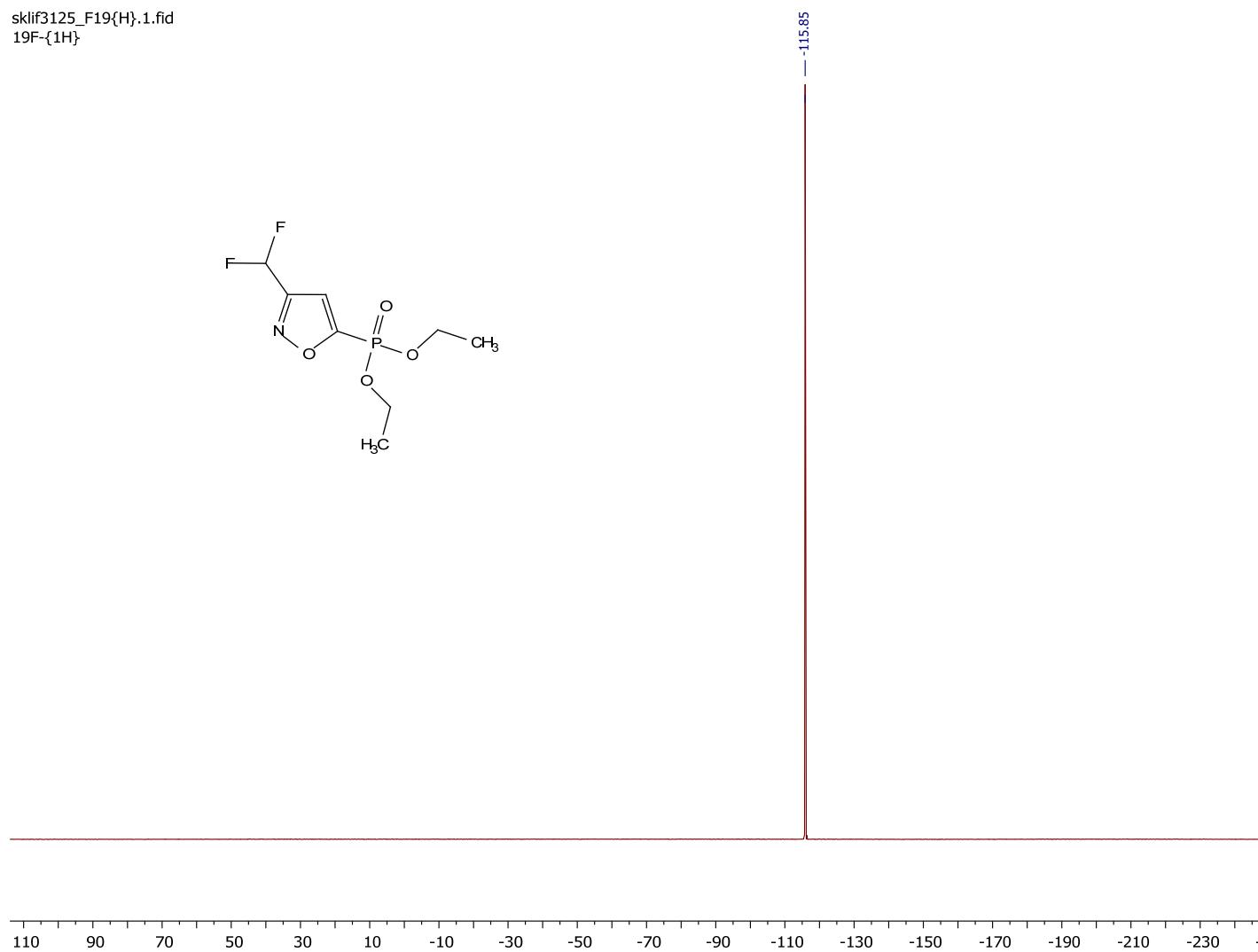
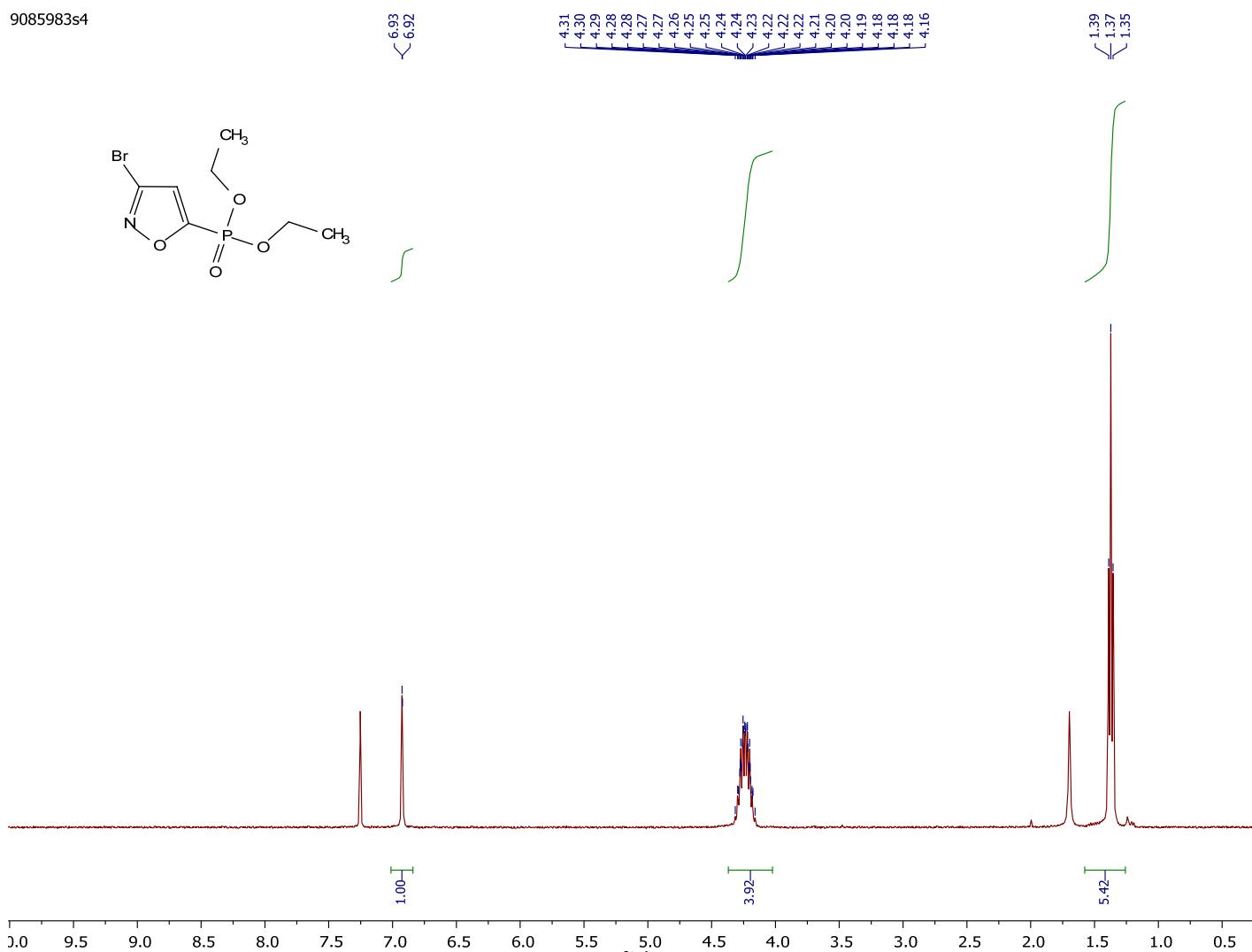


Figure 22 ^{19}F NMR spectrum of 1p

9085983s4

Figure 23 ^1H NMR spectrum of 1q

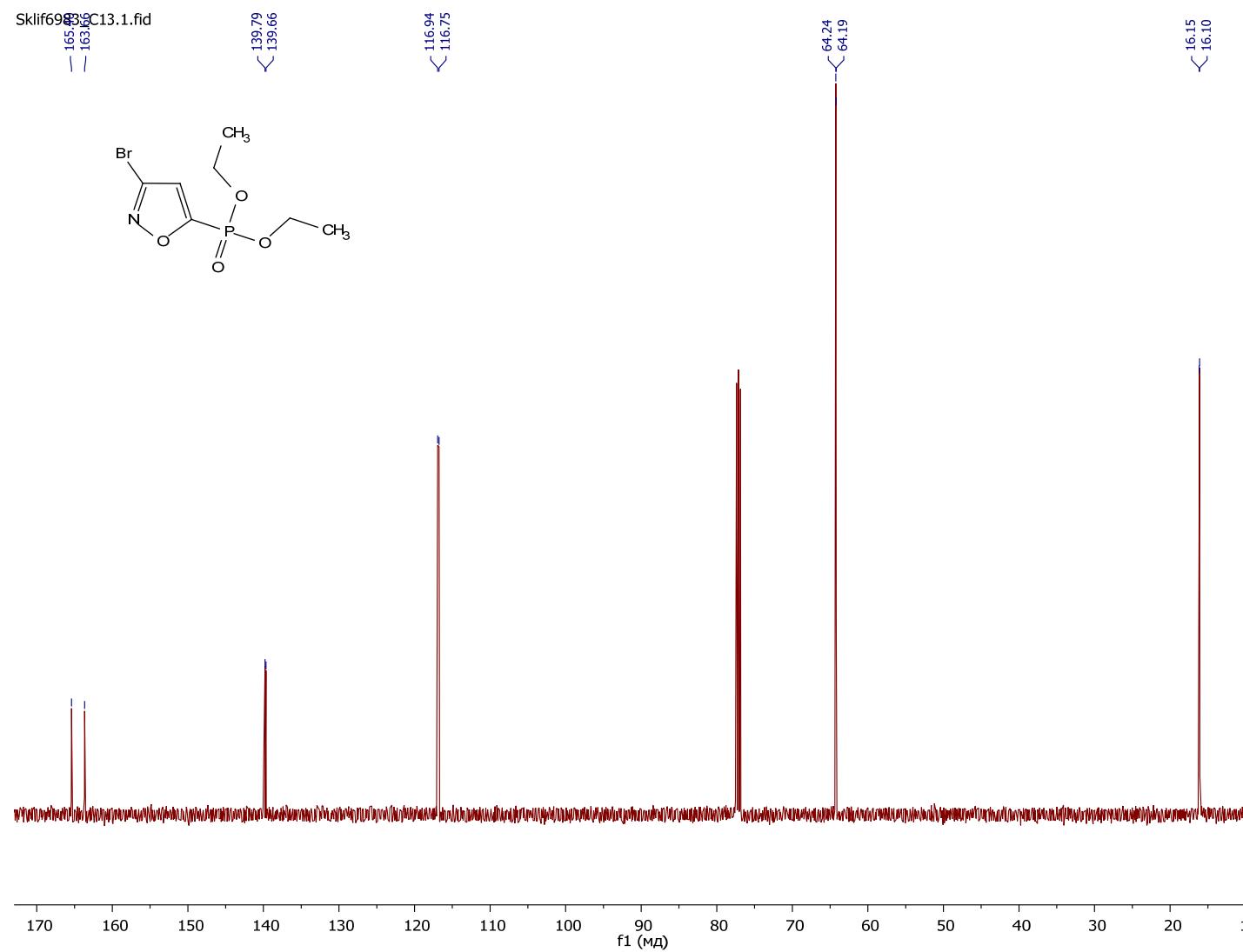


Figure 24 ^{13}C NMR spectrum of 1q

Sklif6983_P31.1.fid
31P-{1H}

-1.83

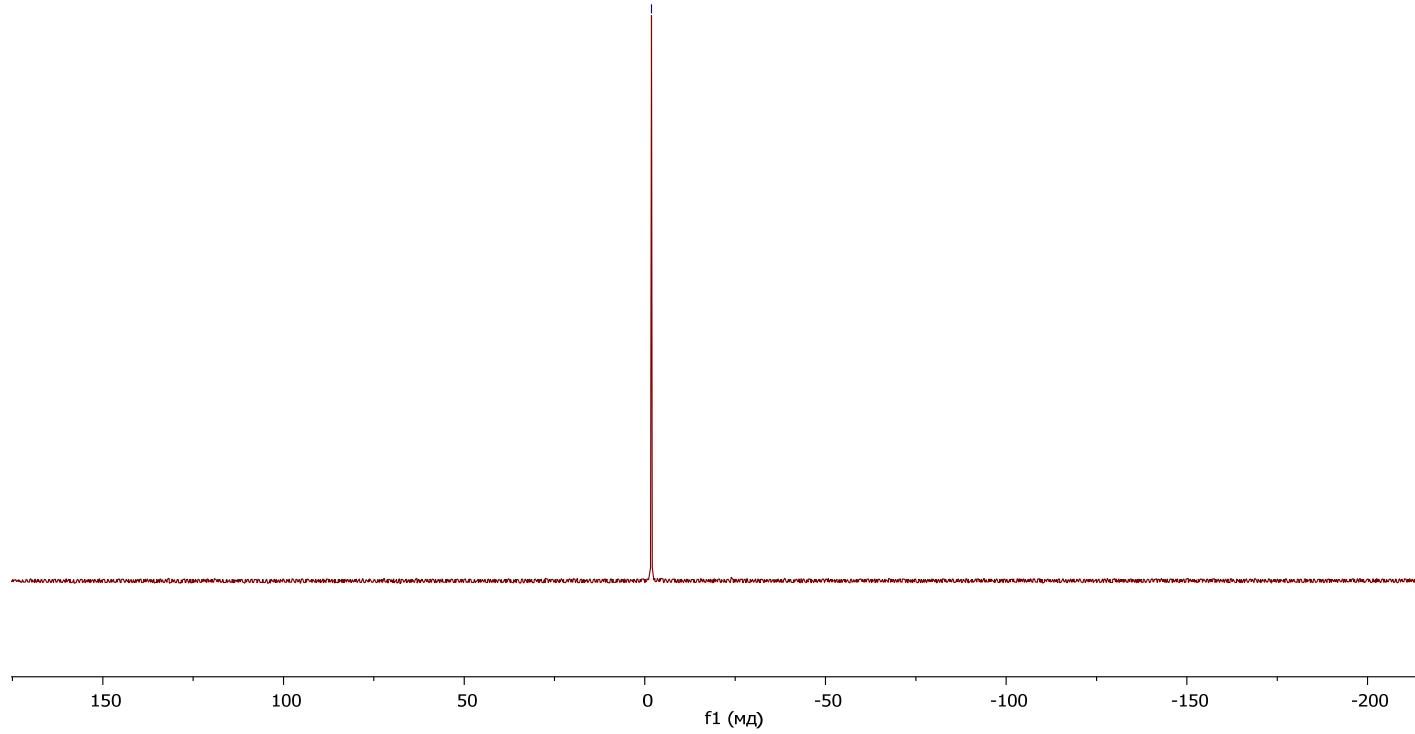
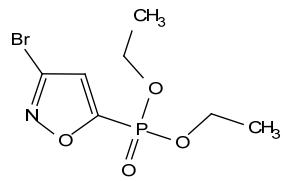


Figure 25 ${}^{31}\text{P}$ NMR spectrum of 1q

ab5985-31

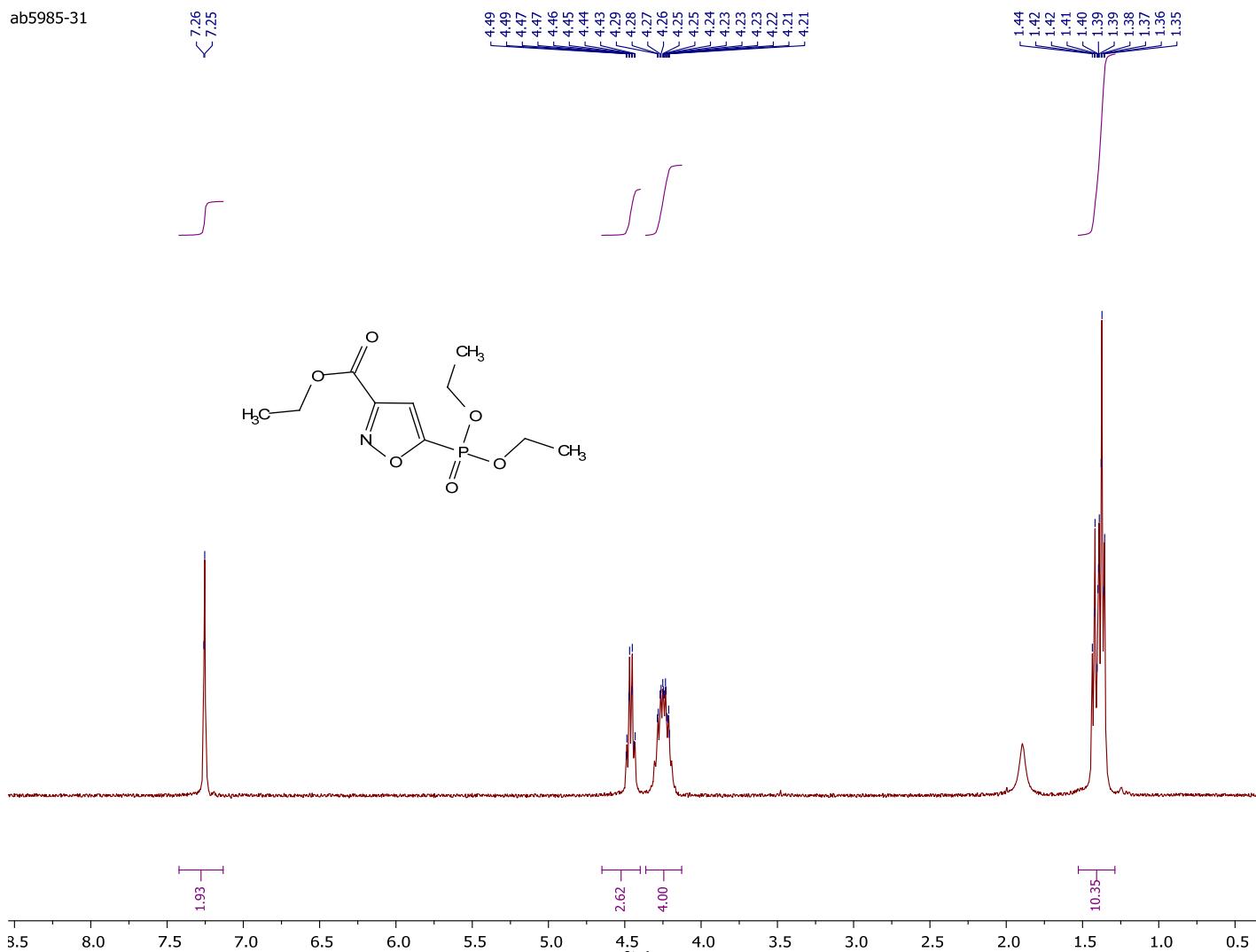


Figure 26 ¹H NMR spectrum of 1r

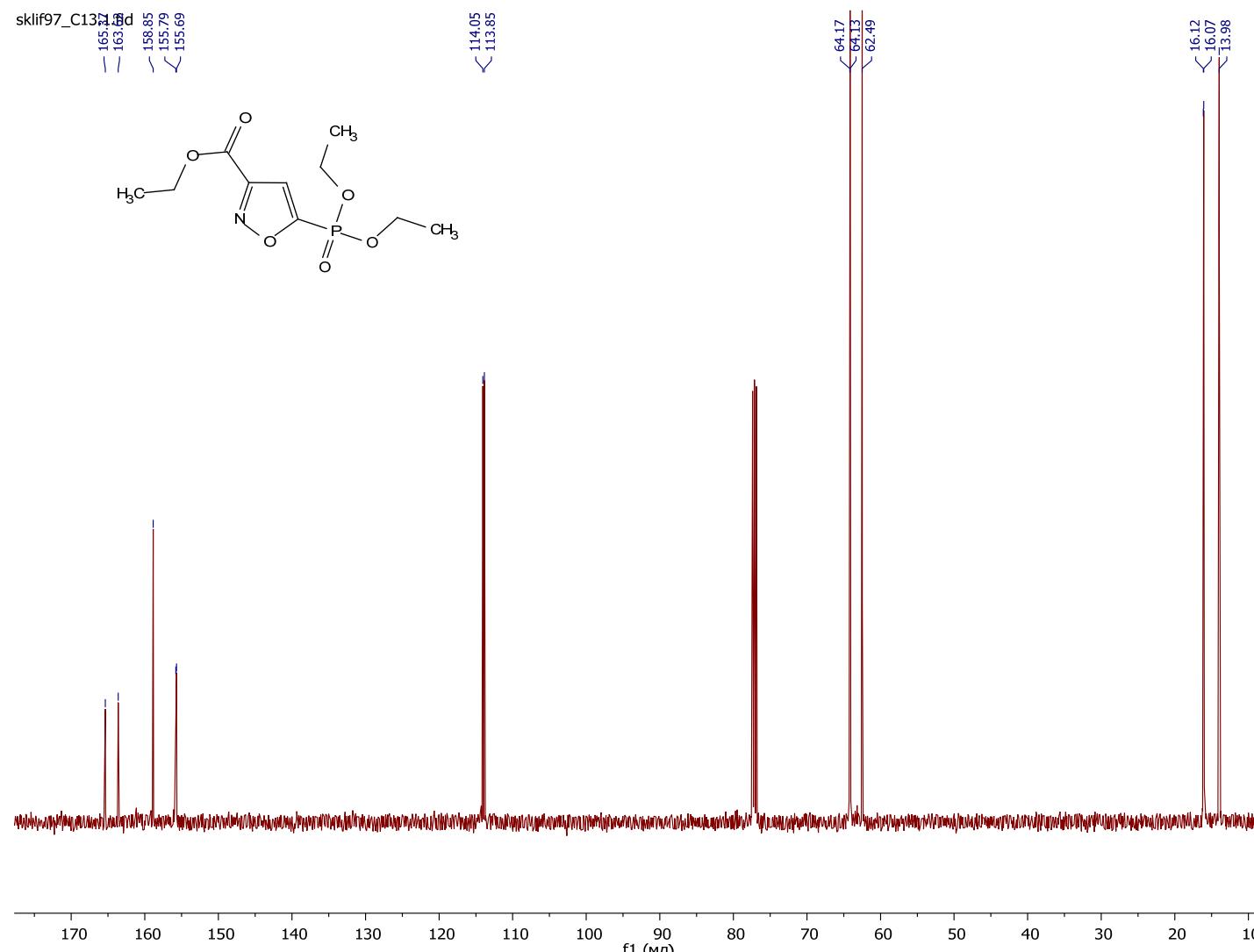
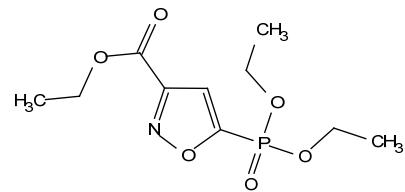


Figure 27 ^{13}C NMR spectrum of 1r

skrif97_P31{H}.1.fid



-1.16

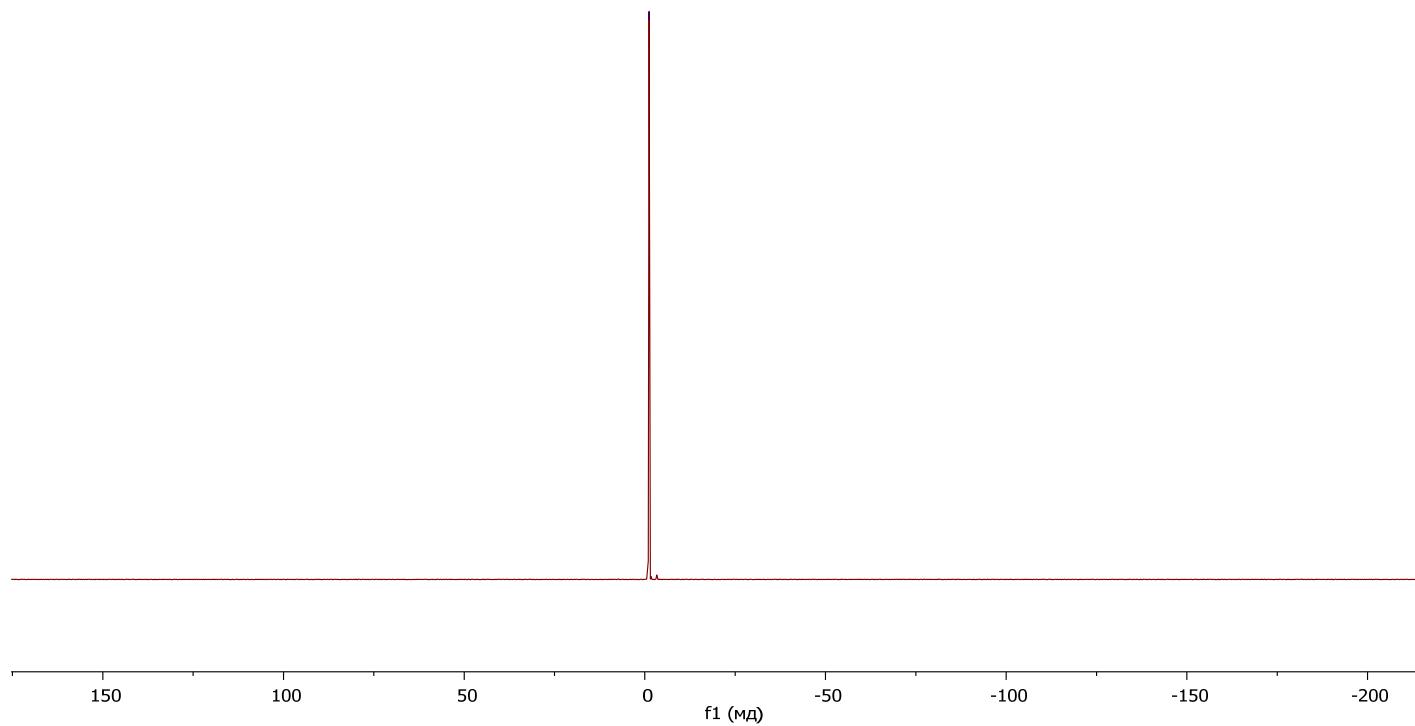


Figure 28 ${}^{31}\text{P}$ NMR spectrum of 1r

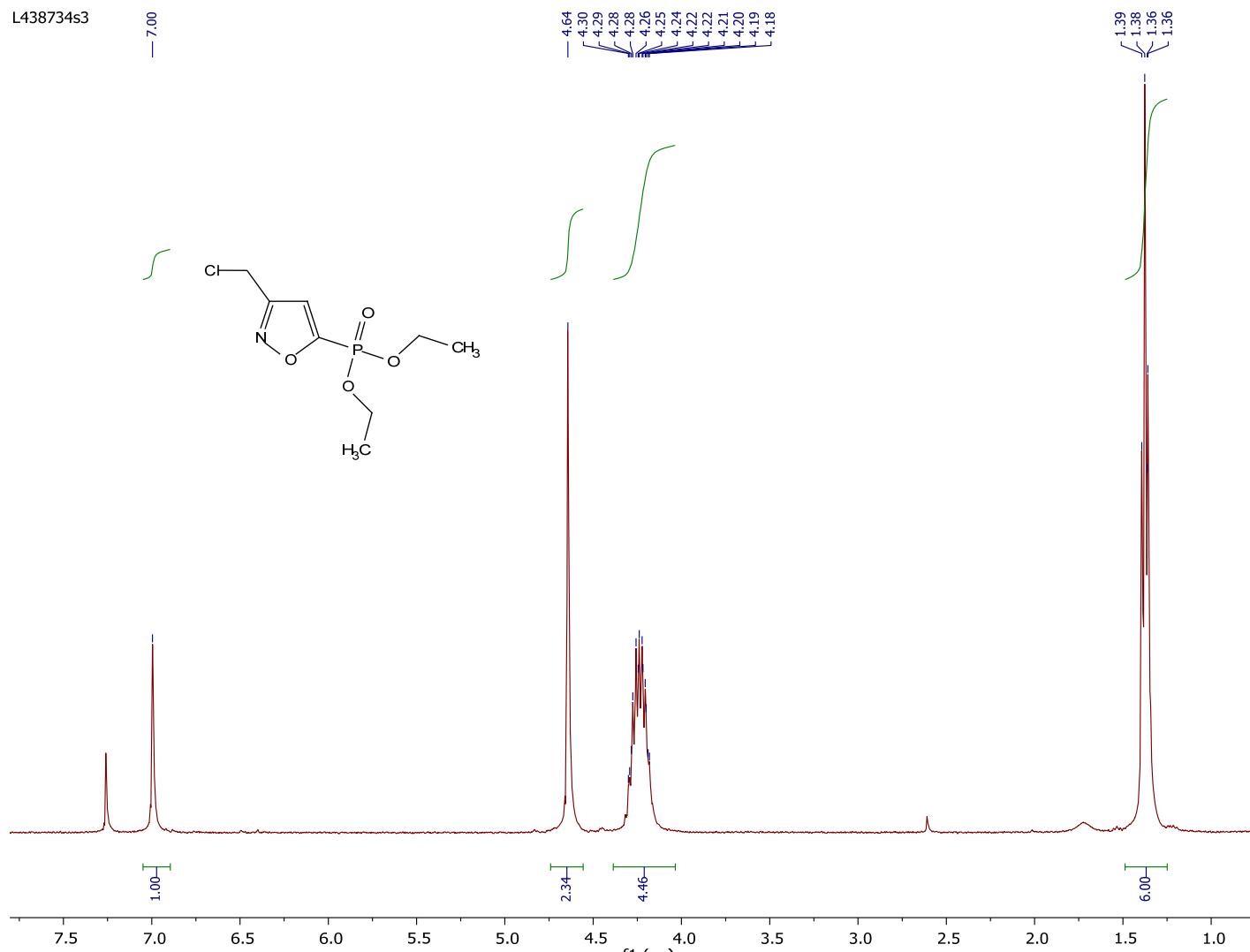


Figure 29 ¹H NMR spectrum of 1s

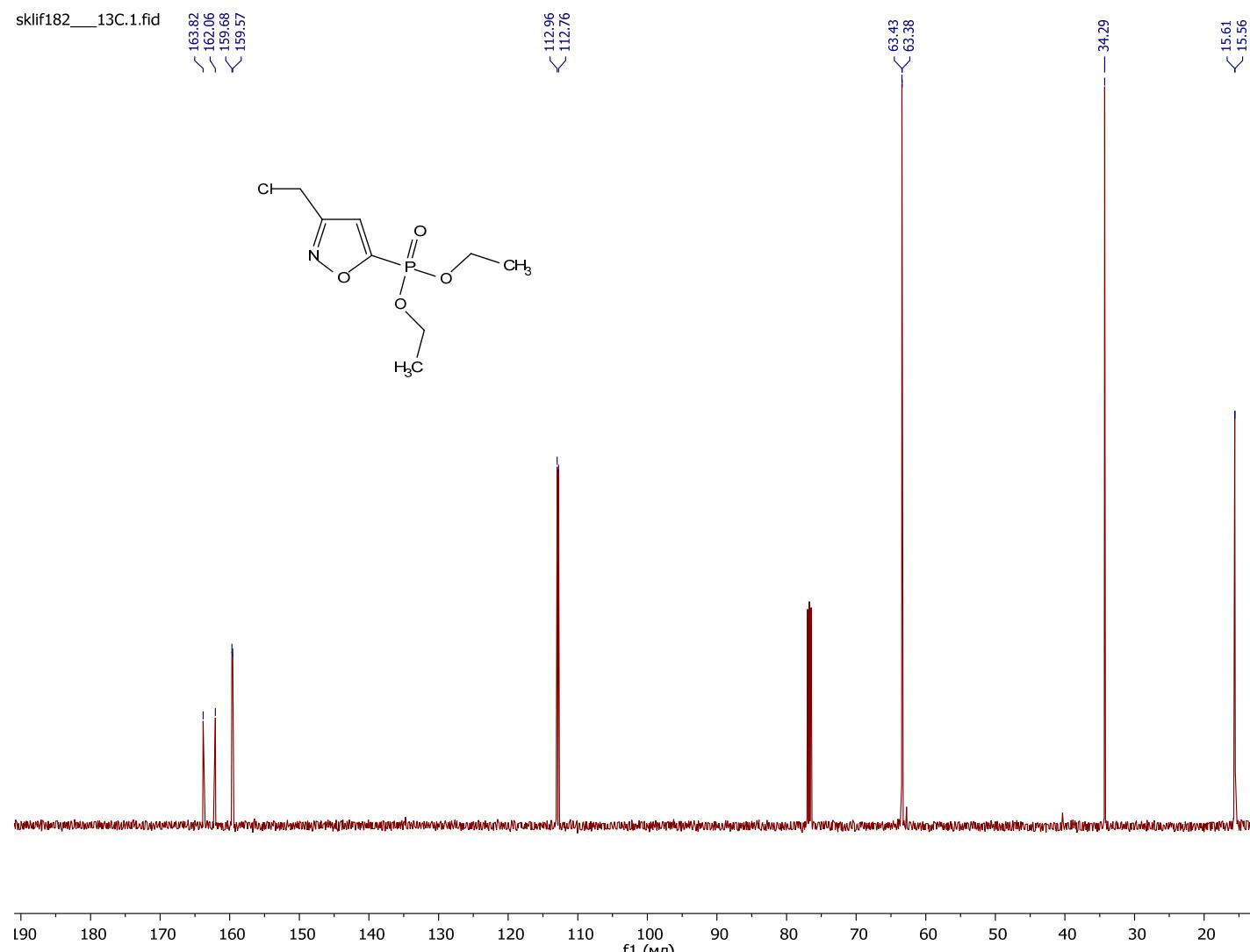


Figure 30 ^{13}C NMR spectrum of 1s

sklif182_P31{H}.1.fid

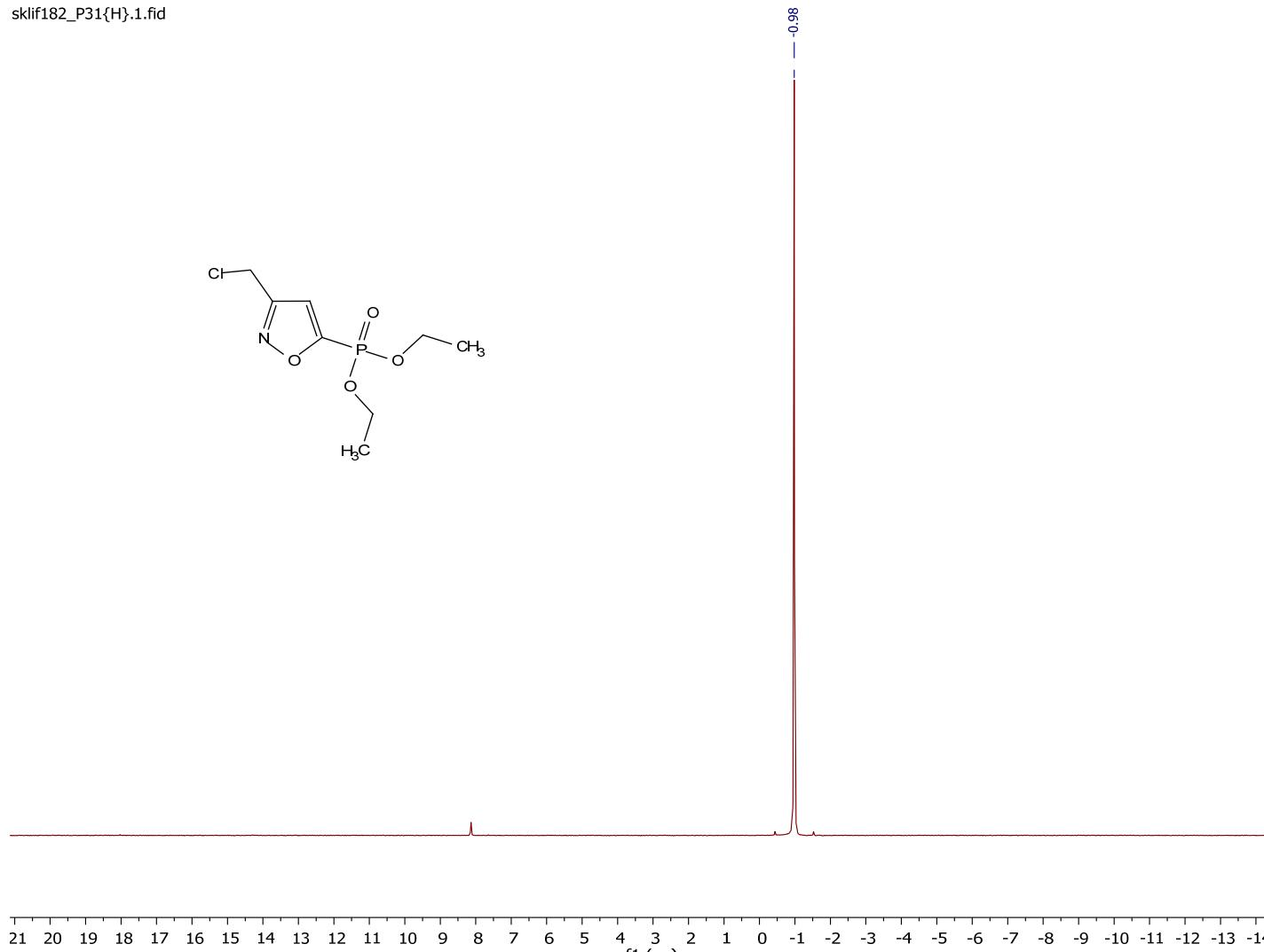


Figure 31 ^{31}P NMR spectrum of 1s

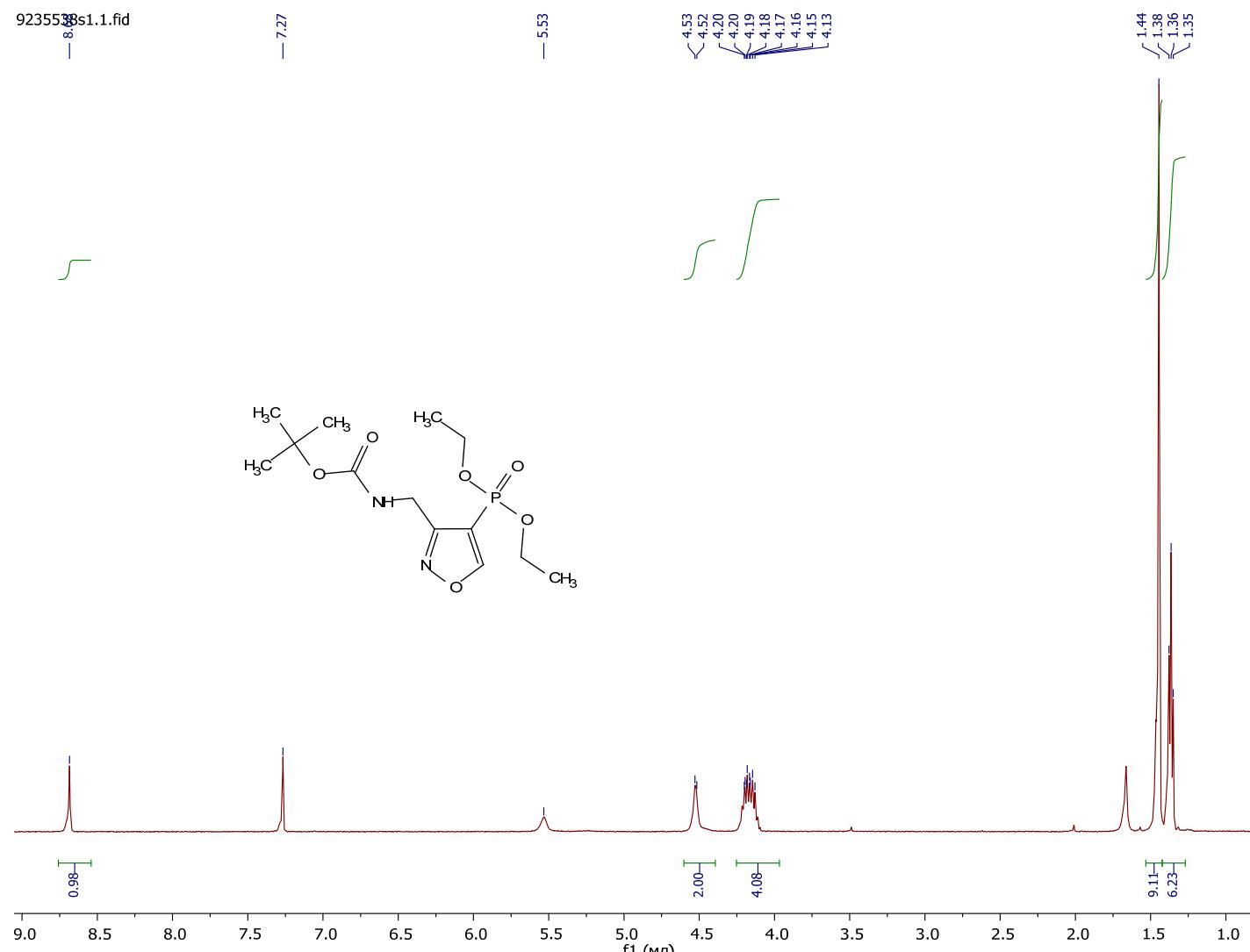


Figure 32 ^1H NMR spectrum of 2a

sklf379_C13.1.fid

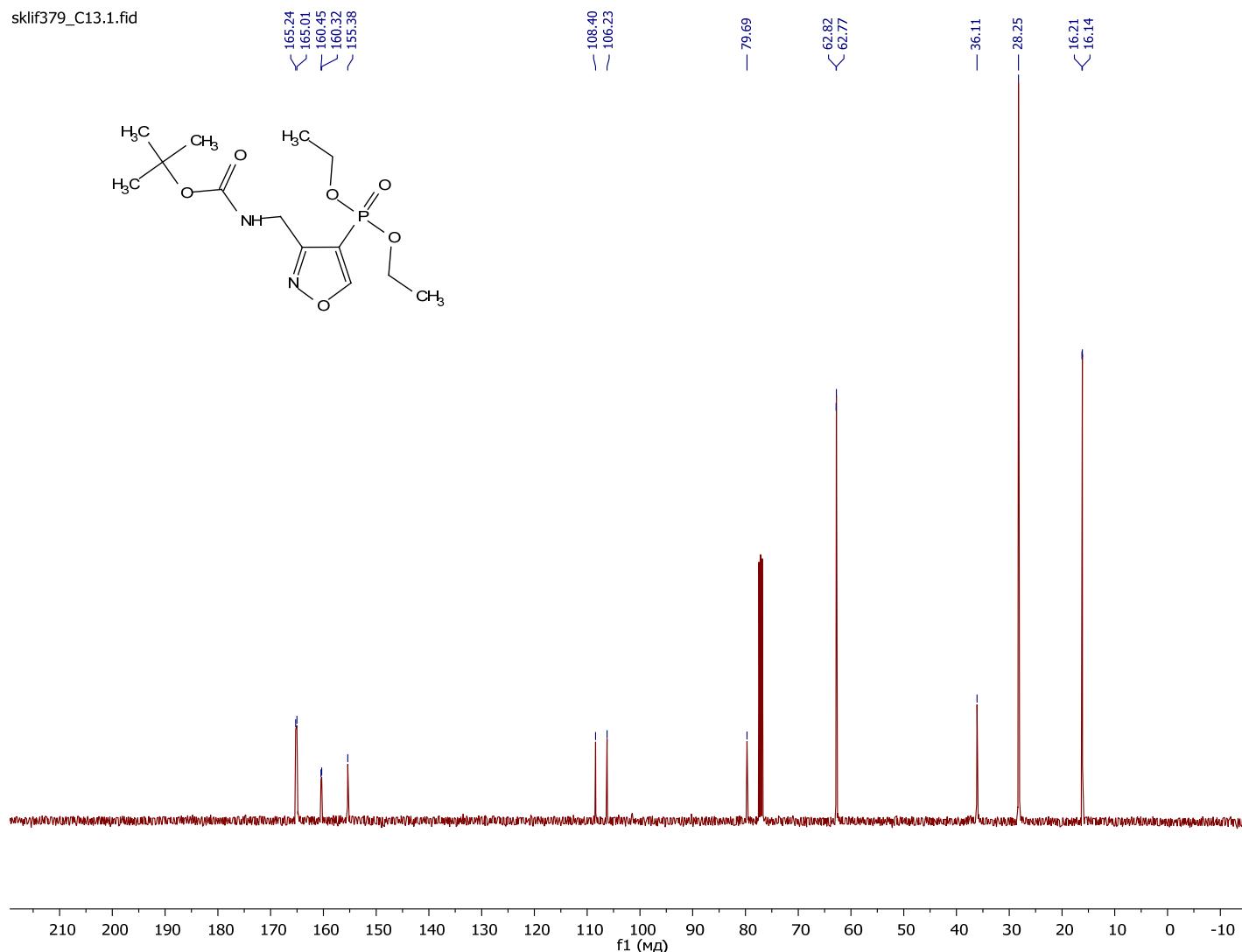


Figure 33 ^{13}C NMR spectrum of 2a

sklf379_P31{H}.1.fid

— 9.81 —

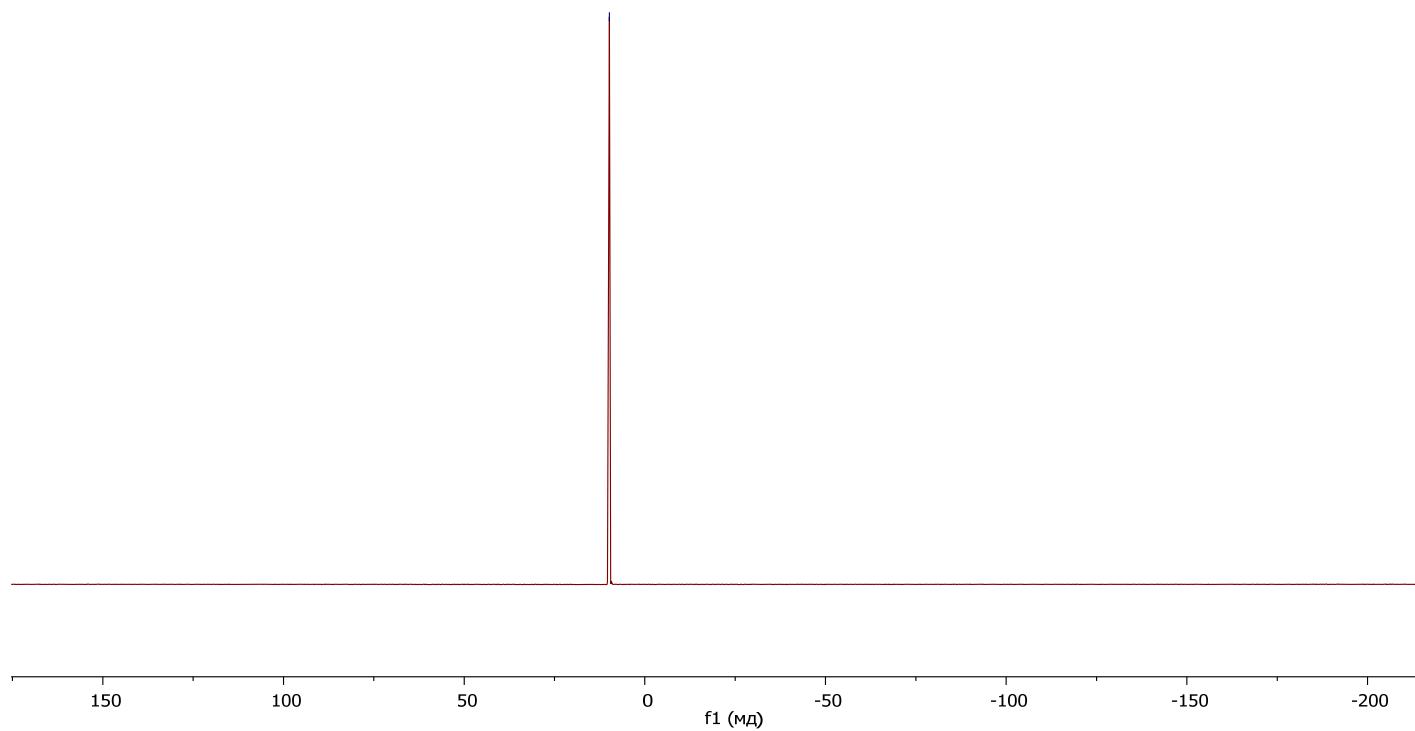
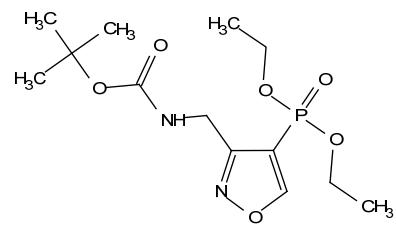


Figure 34 ³¹P NMR spectrum of 2a

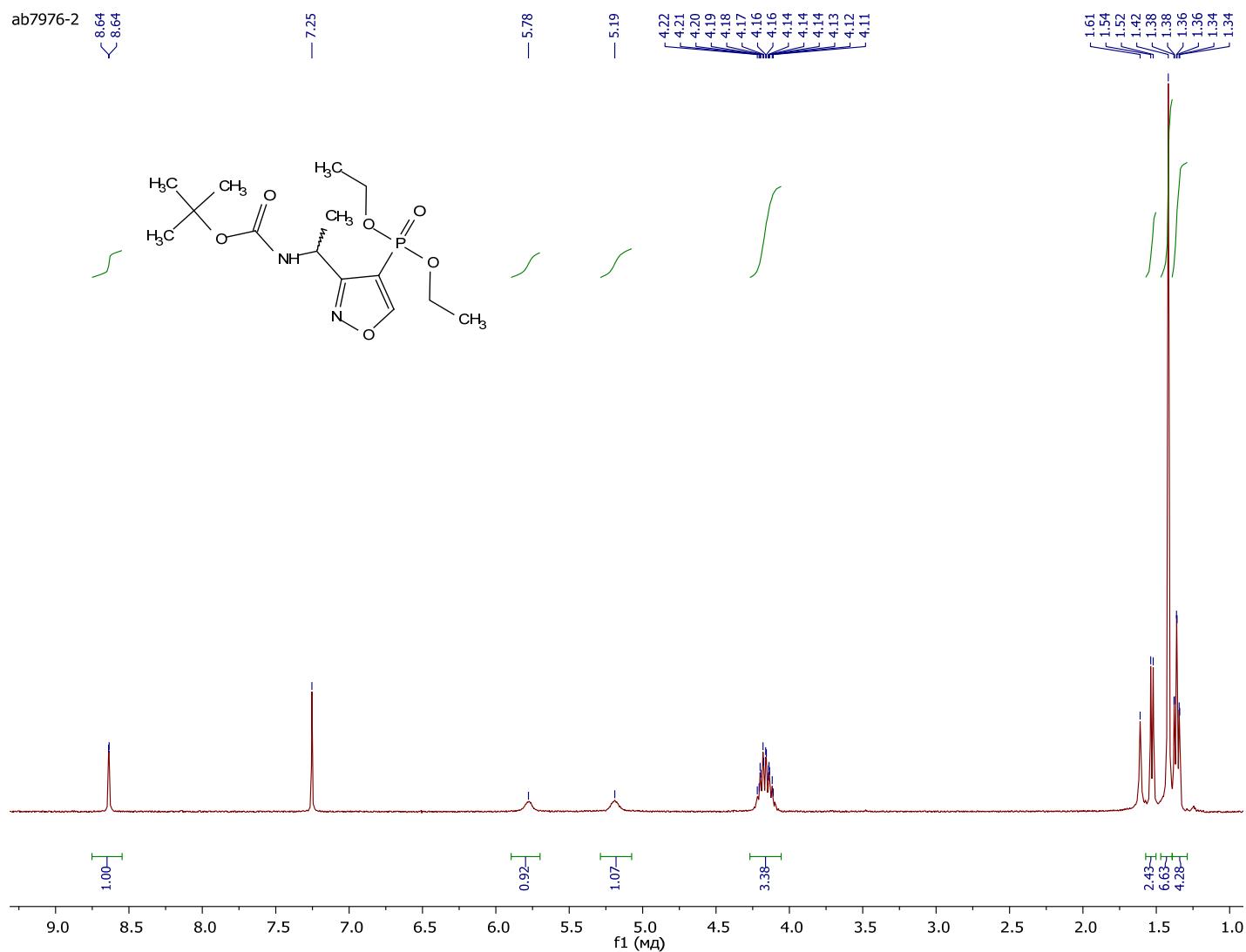


Figure 35 ¹H NMR spectrum of 2b and 2c (R-isomer)

sklf6319_C13.1.fid

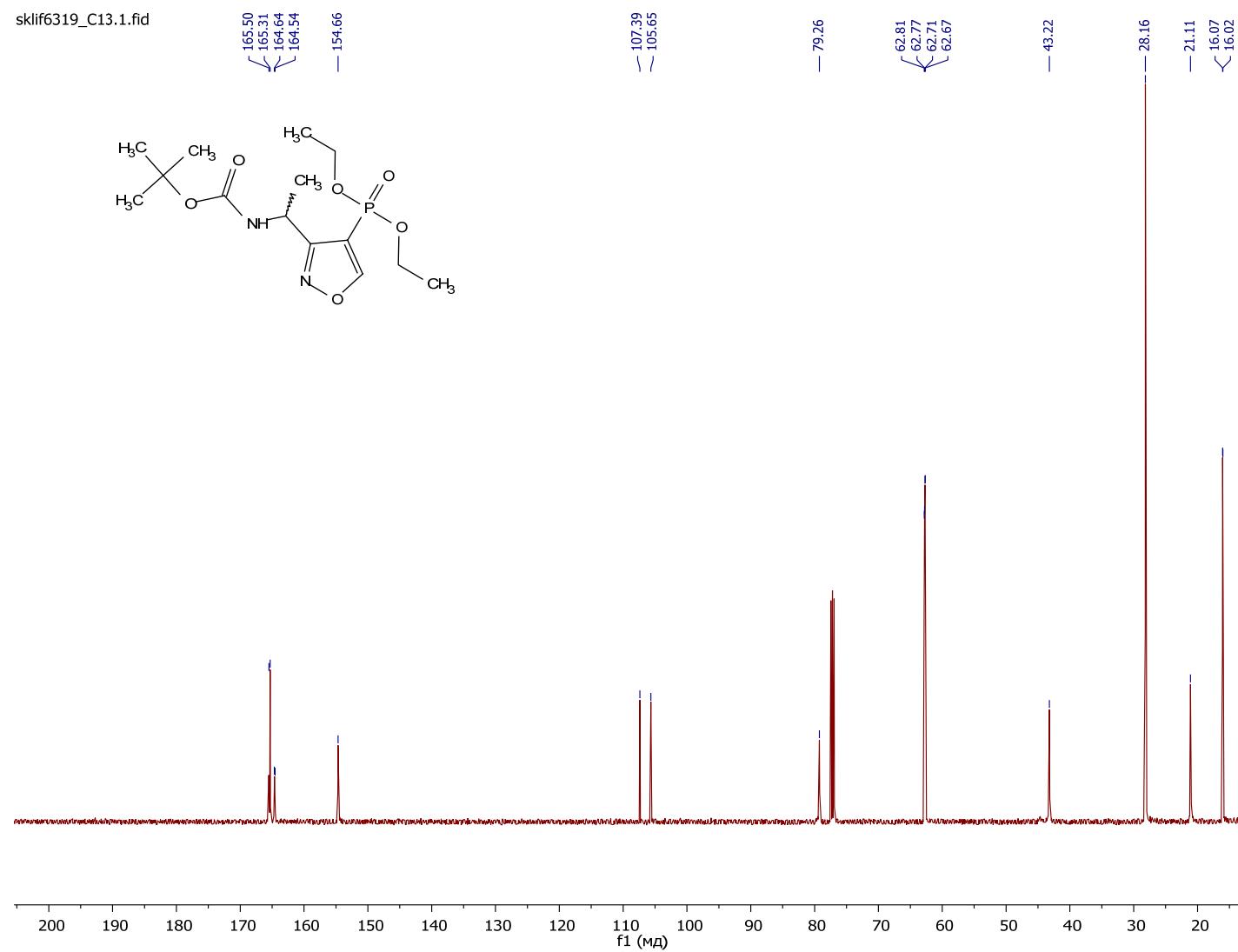


Figure 36 ^{13}C NMR spectrum of 2b and 2c (R-isomer)

sklf6319_P31.1.fid

—
10.21

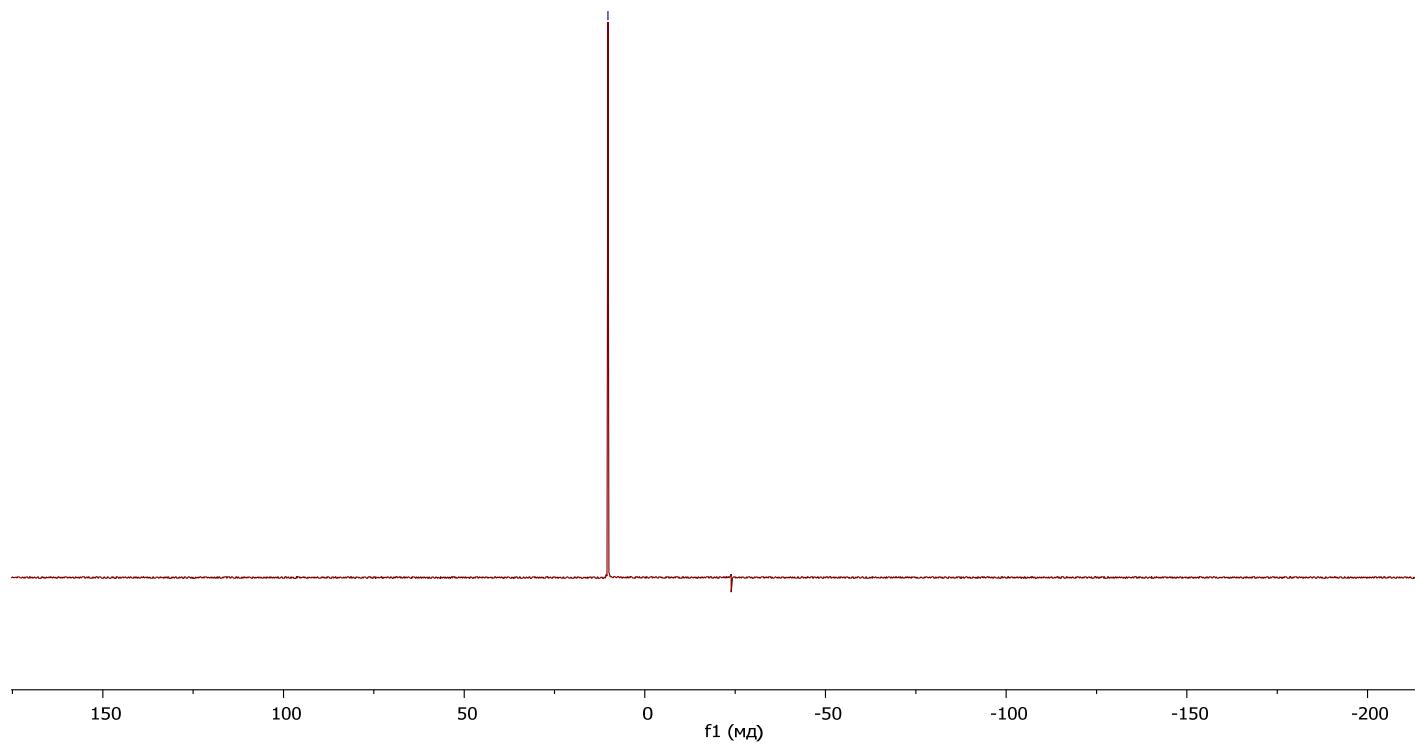
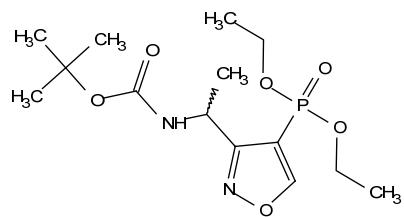


Figure 37 31P NMR spectrum of 2b and 2c (*R*-isomer)

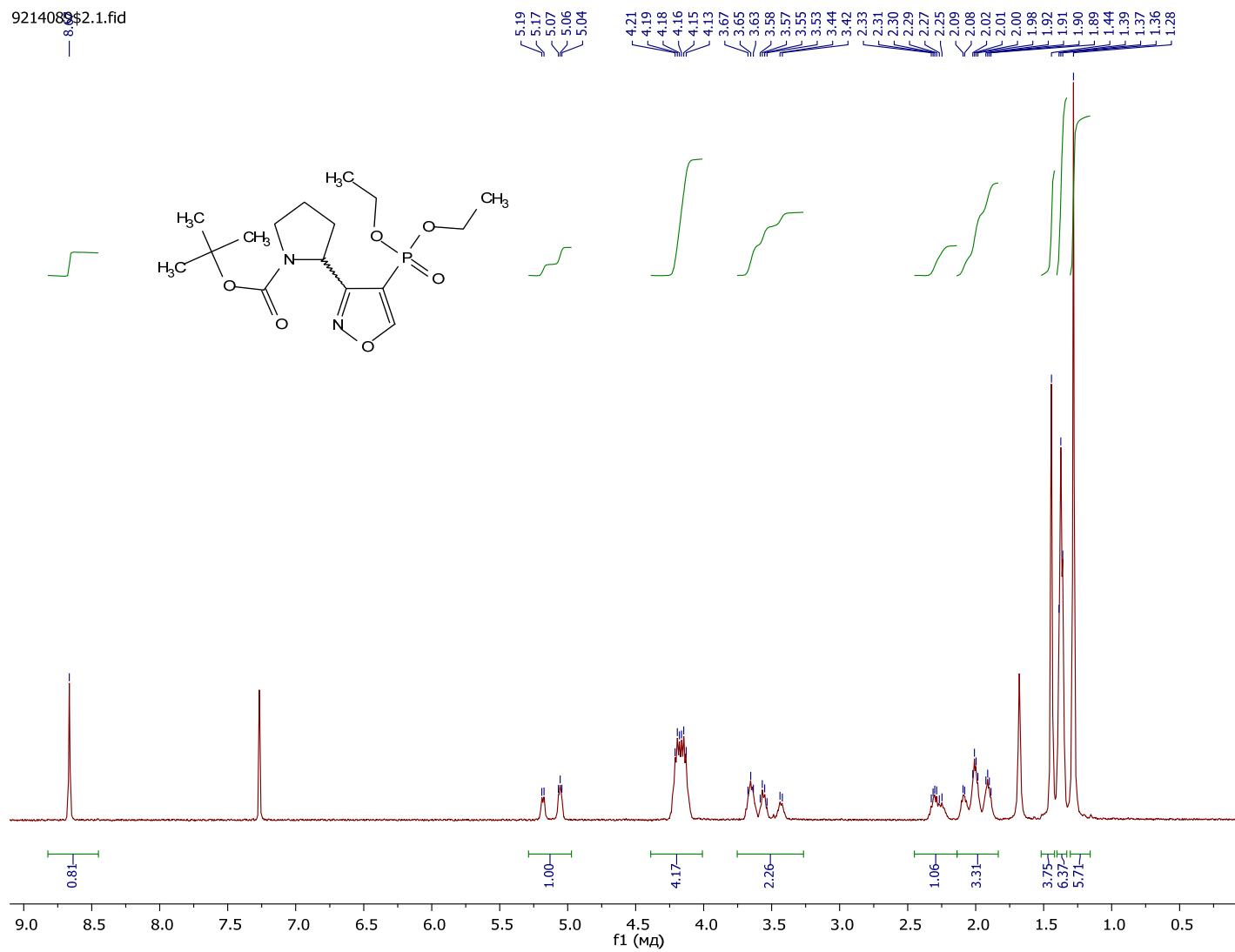


Figure 38 ^1H NMR spectrum of 2f and 2g (R-isomer)

sklf331 C13.1.fid

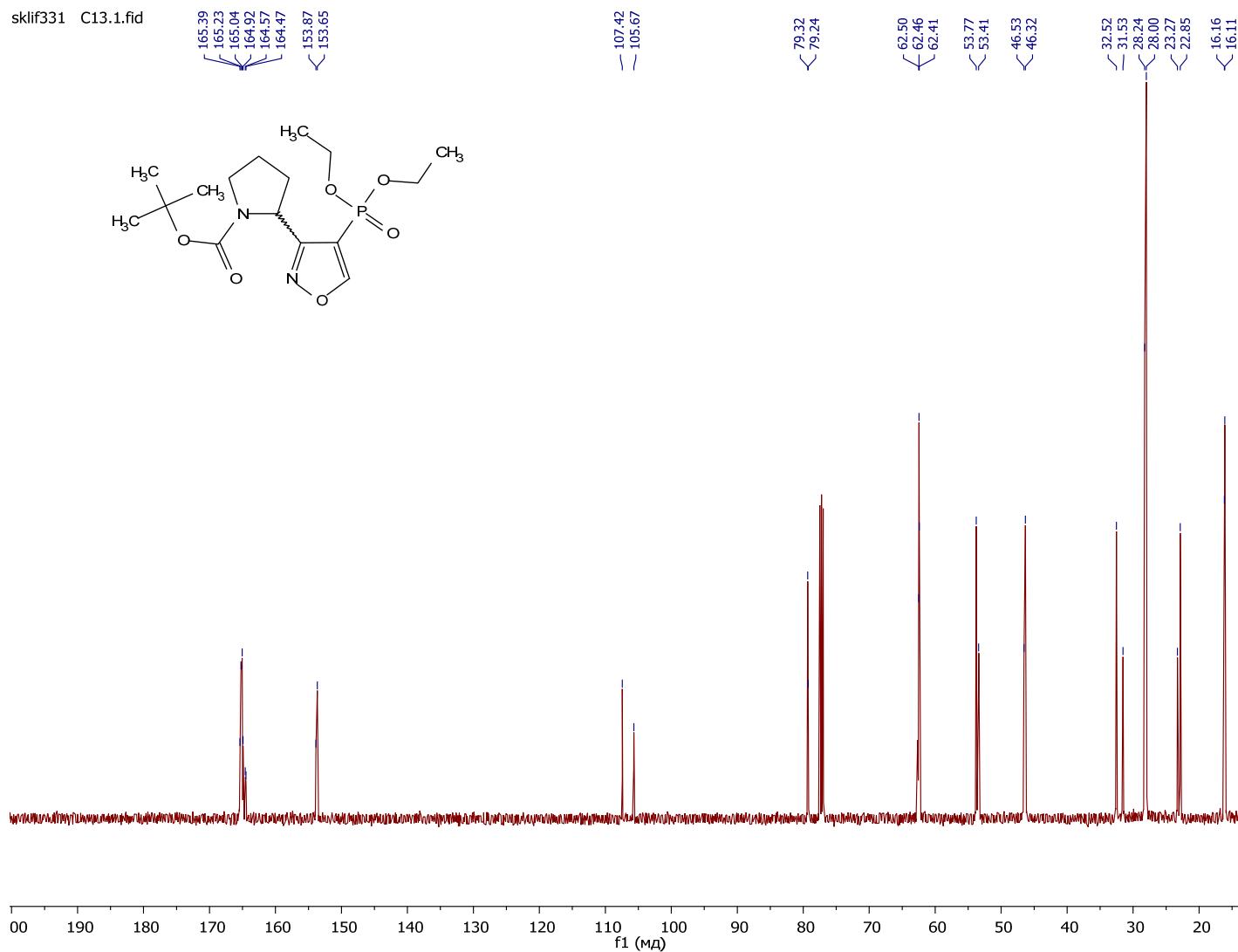


Figure 39 ^{13}C NMR spectrum of 2f and 2g (R-isomer)

SKLif331_P31.1.fid
31P-{1H}

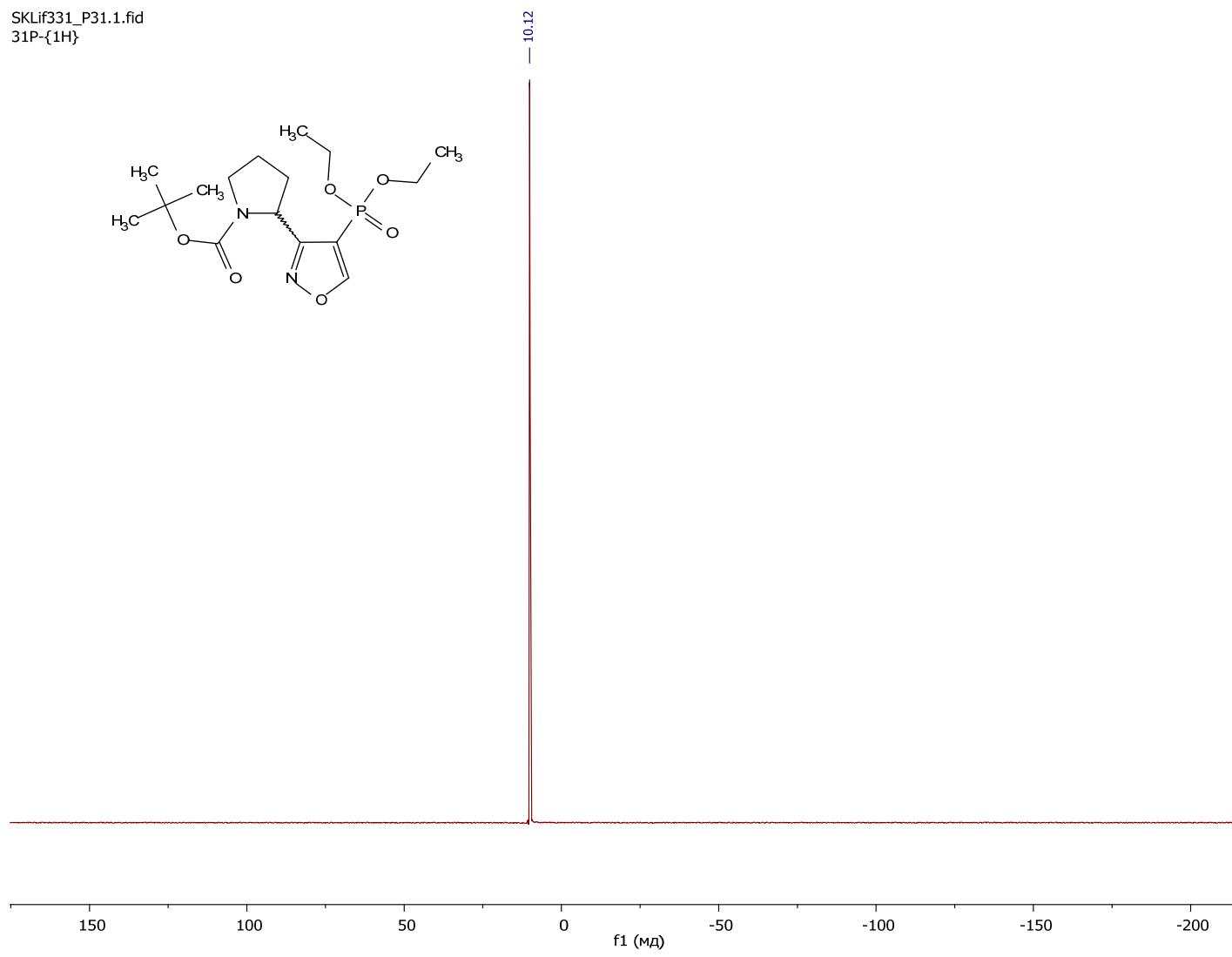


Figure 40 ^{31}P NMR spectrum of 2f and 2g (*R*-isomer)

ab3550-4

8.64
8.64

— 7.25 cdd3

4.18
4.16
4.14
4.13
4.12
4.12

3.09
3.08
3.06
3.04
2.85

2.01
1.98
1.79
1.78
1.76
1.75
1.46
1.36
1.35
1.33

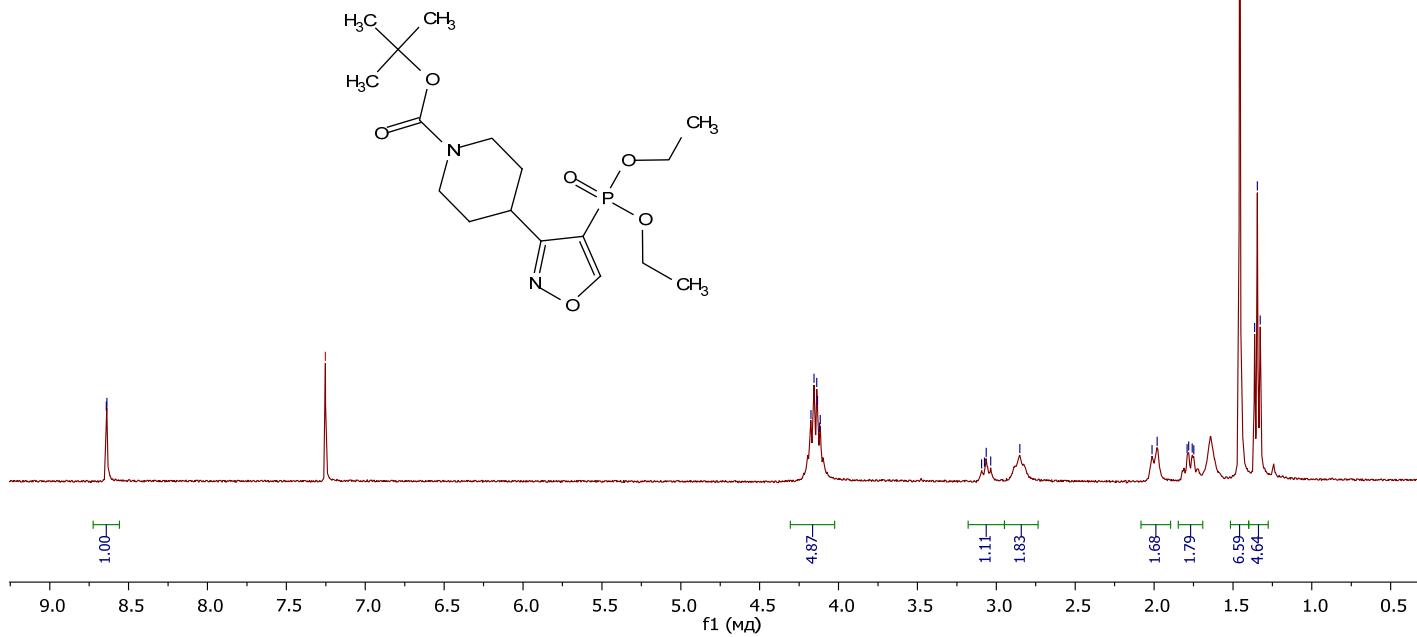
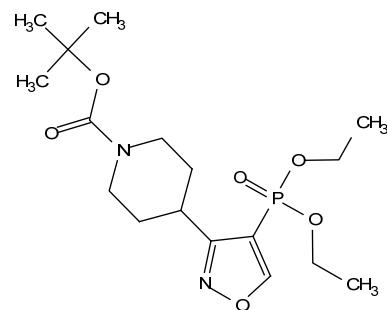


Figure 41 ^1H NMR spectrum of 2h

sklf6330_C13.1.fid

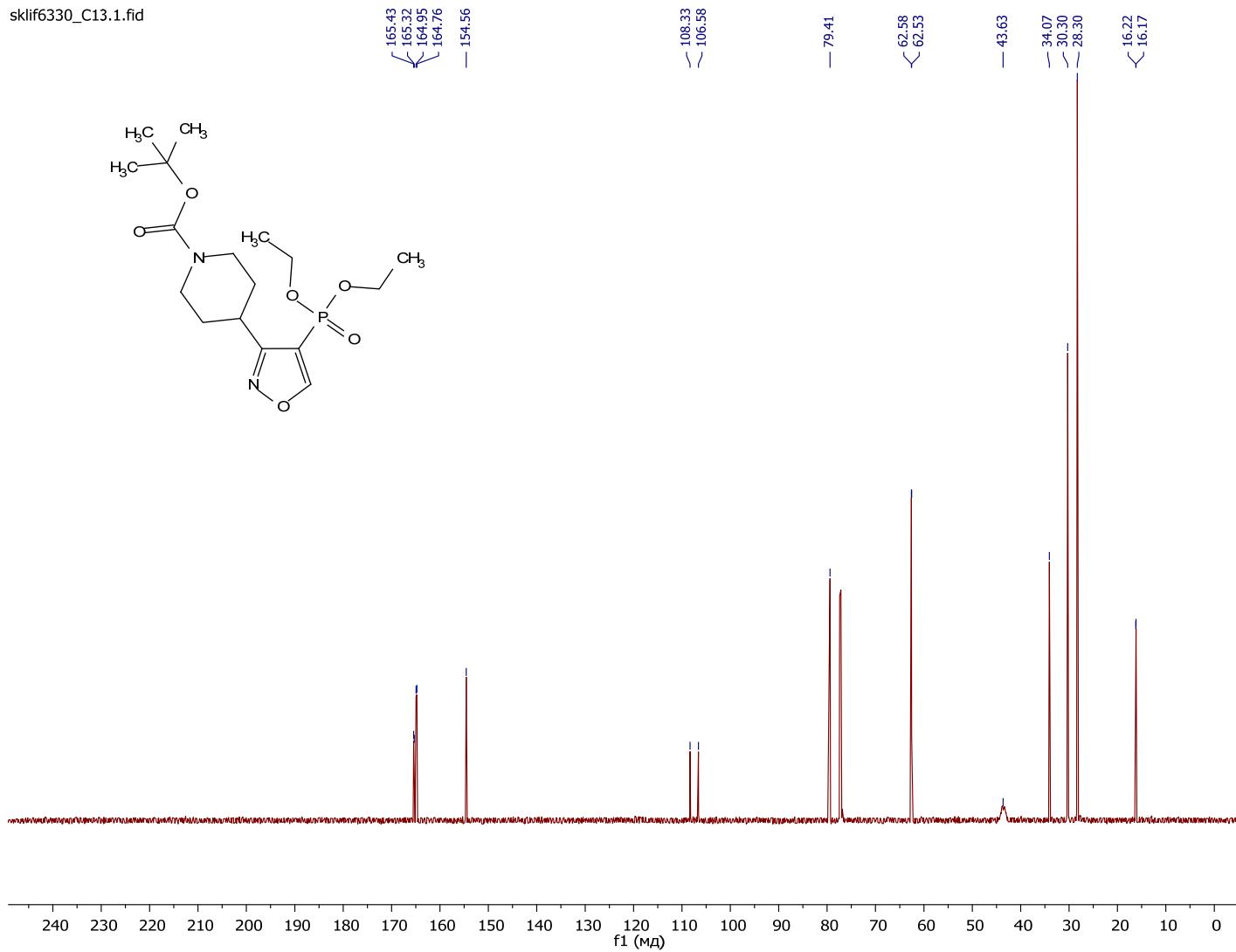


Figure 42 ^{13}C NMR spectrum of 2h

sklif6330_P31.1.fid

10.47
10.43
10.39

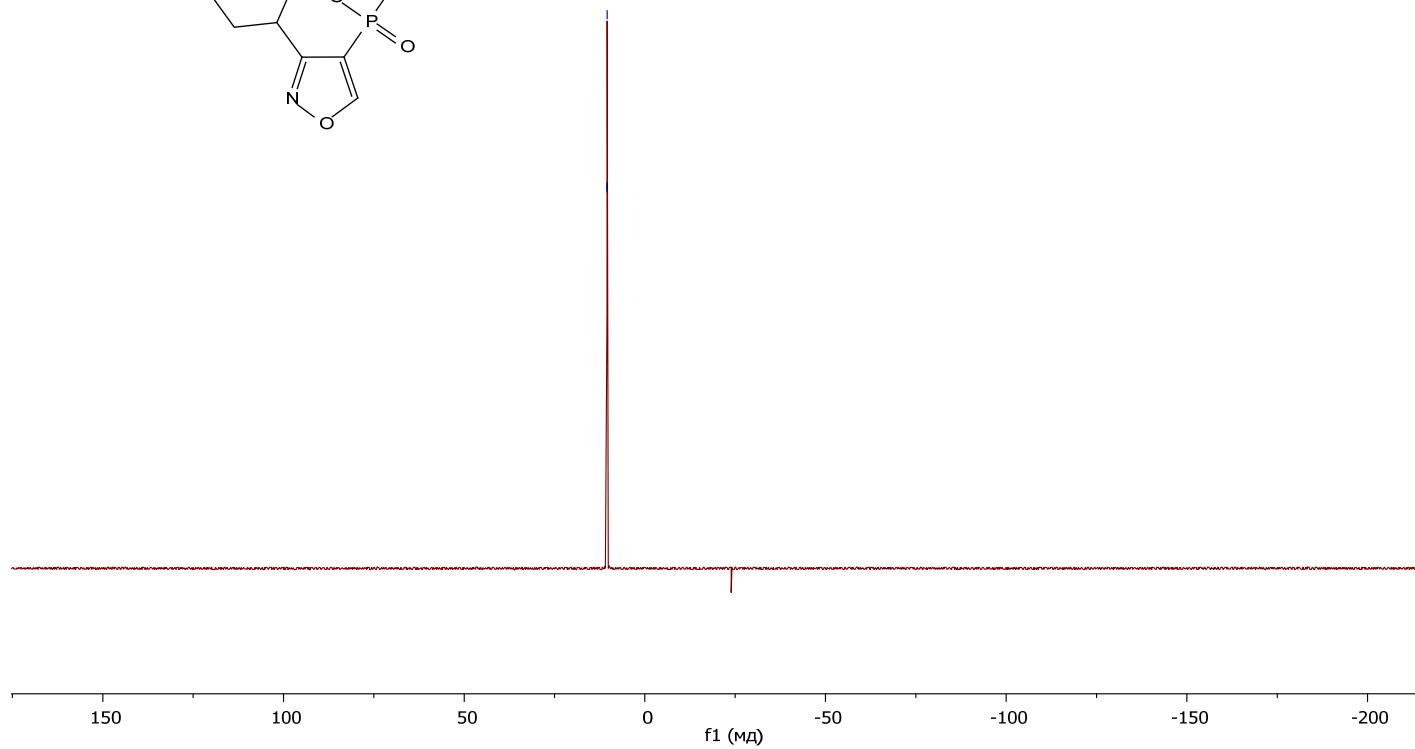
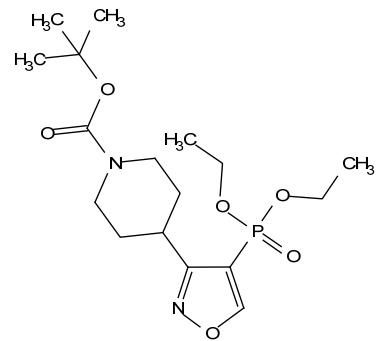


Figure 43 ³¹P NMR spectrum of 2h

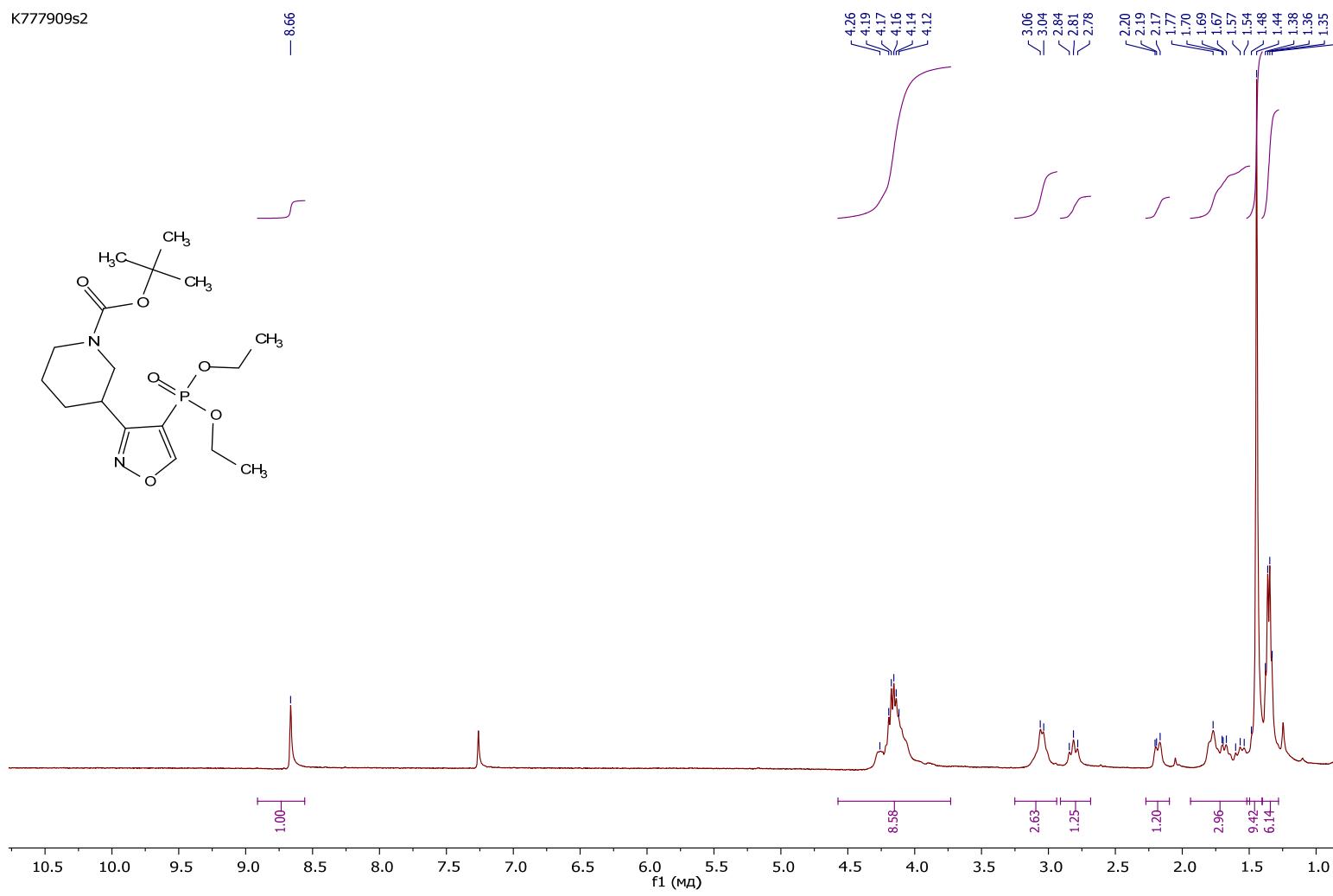


Figure 44. ¹H NMR spectrum of 2i

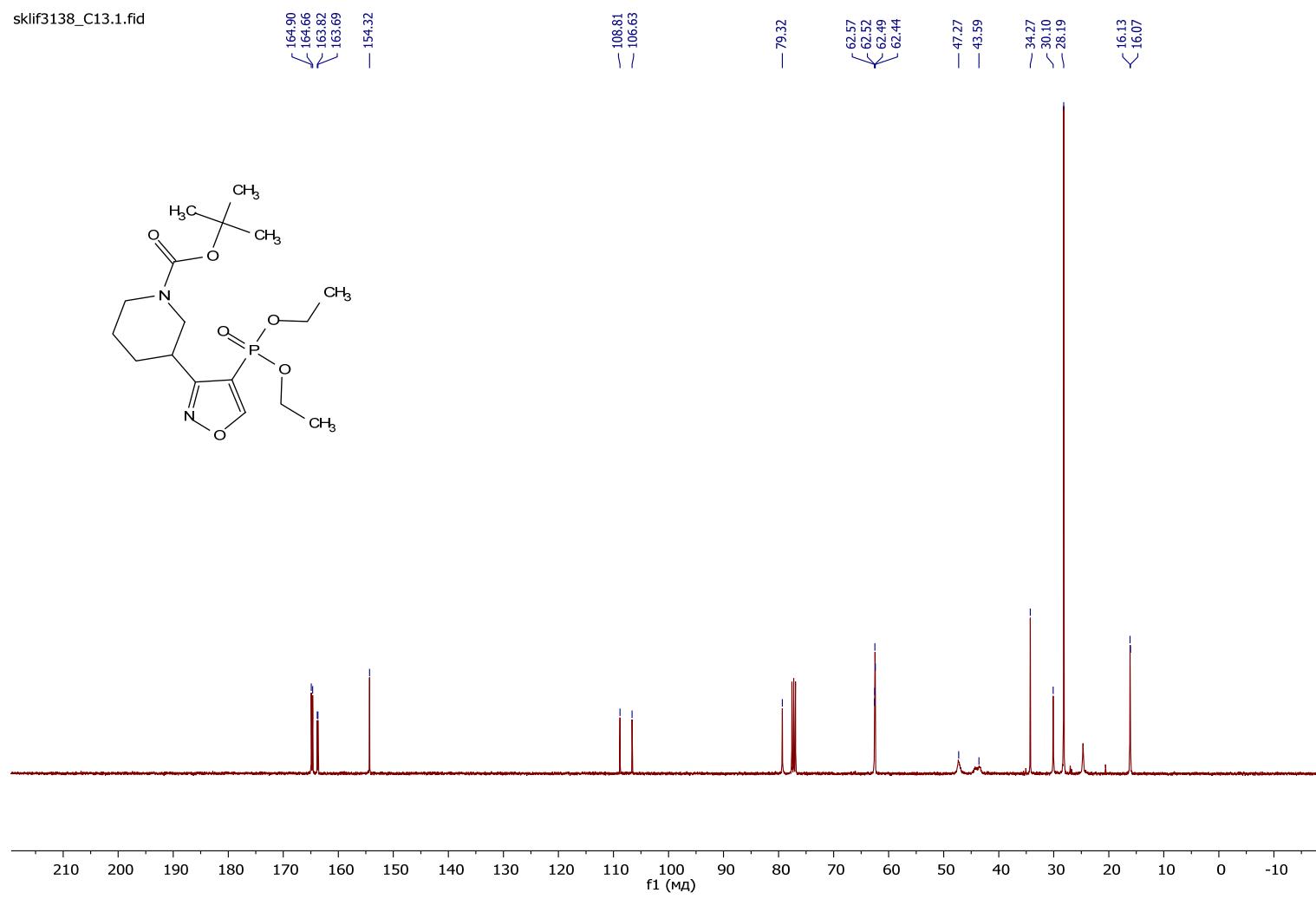


Figure 45. ¹³C NMR spectrum of 2i

sklf3138 31P{1H}.1.fid

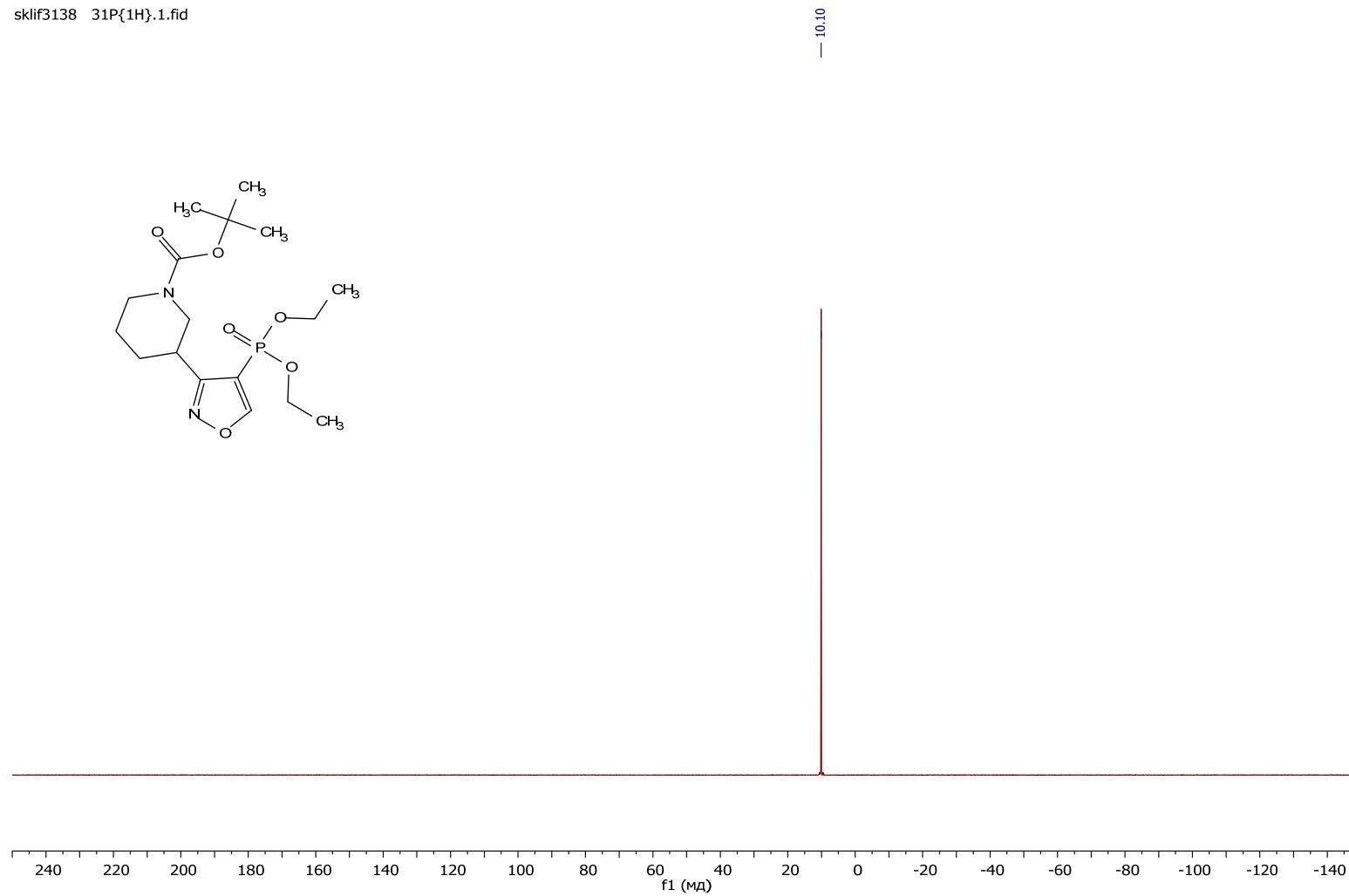


Figure 46. ^{31}P NMR spectrum of 2i

9231572s2.1.fid

8.72

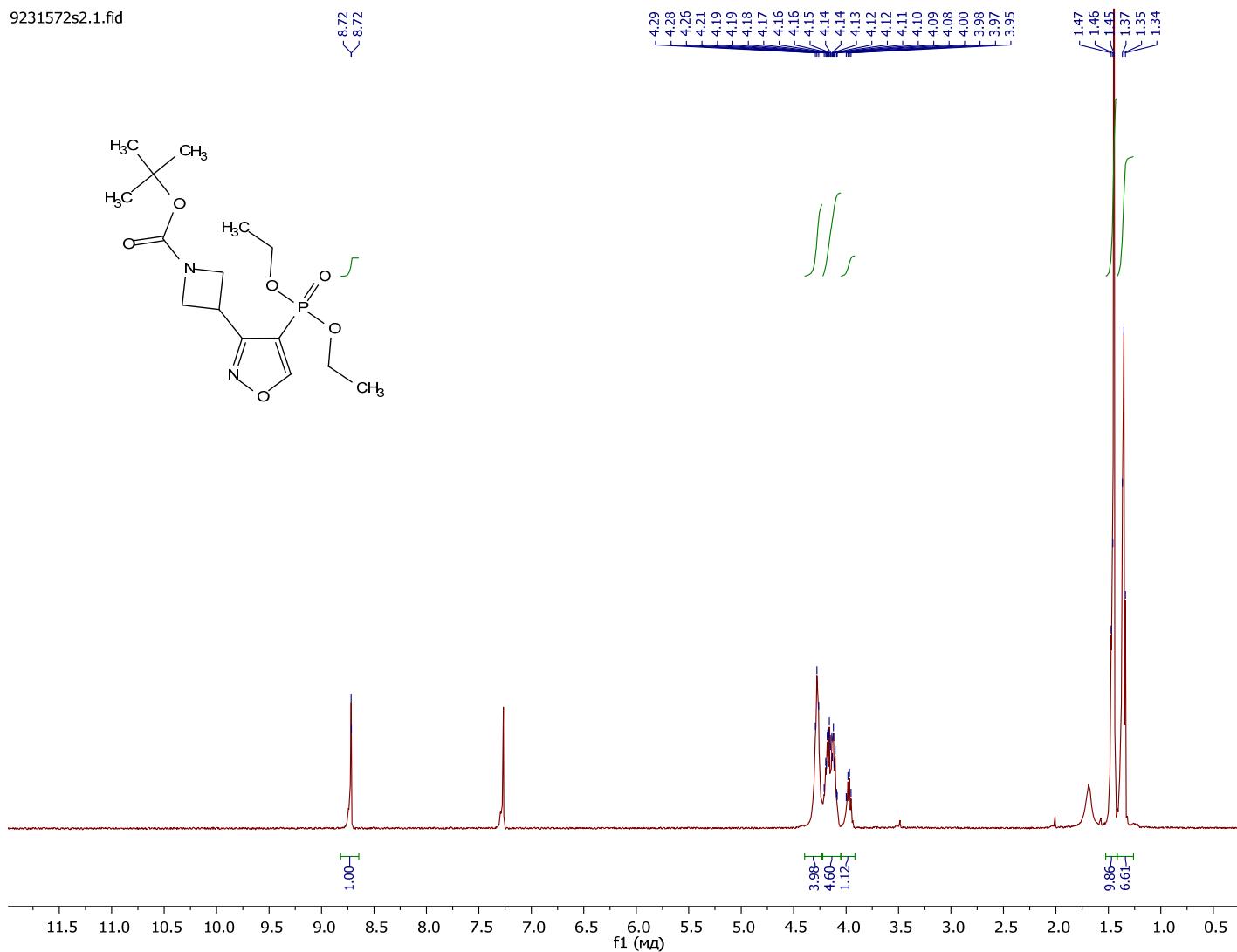
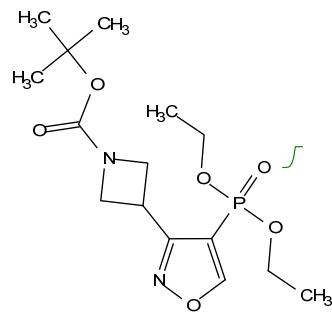


Figure 47 ¹H NMR spectrum of 2j

sklf378_C13.1.fid

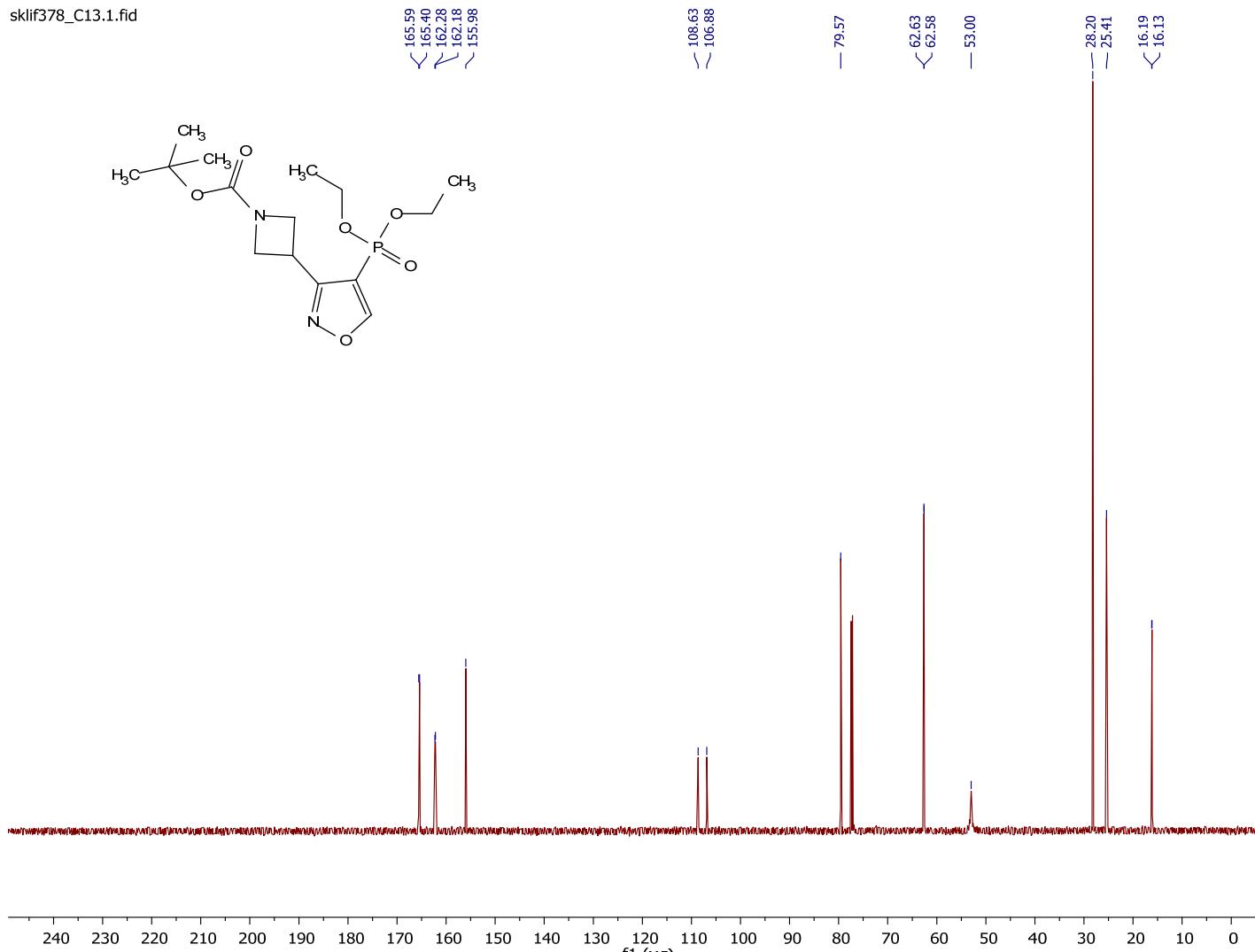


Figure 48 ^{13}C NMR spectrum of 2j

sklif378_P31.1.fid

-9.68

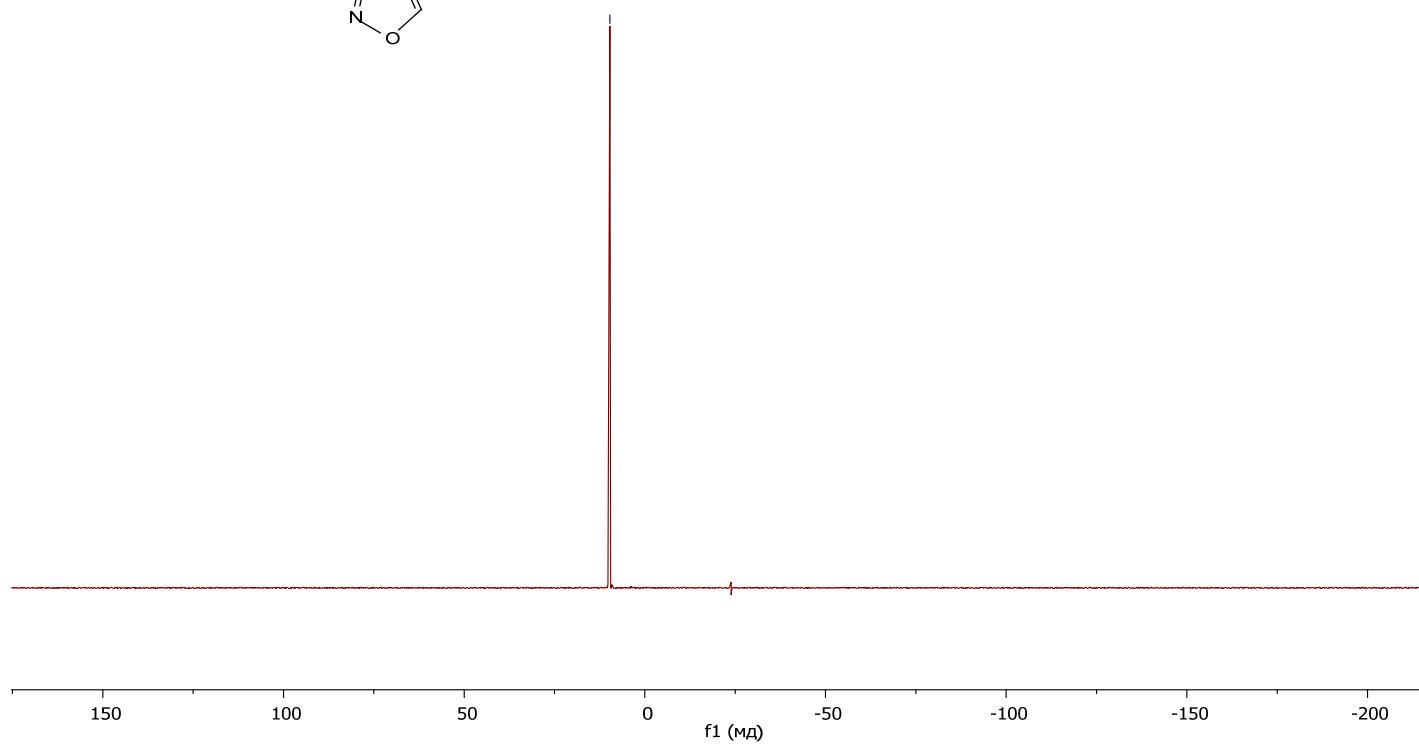
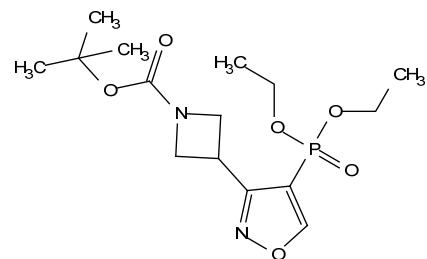
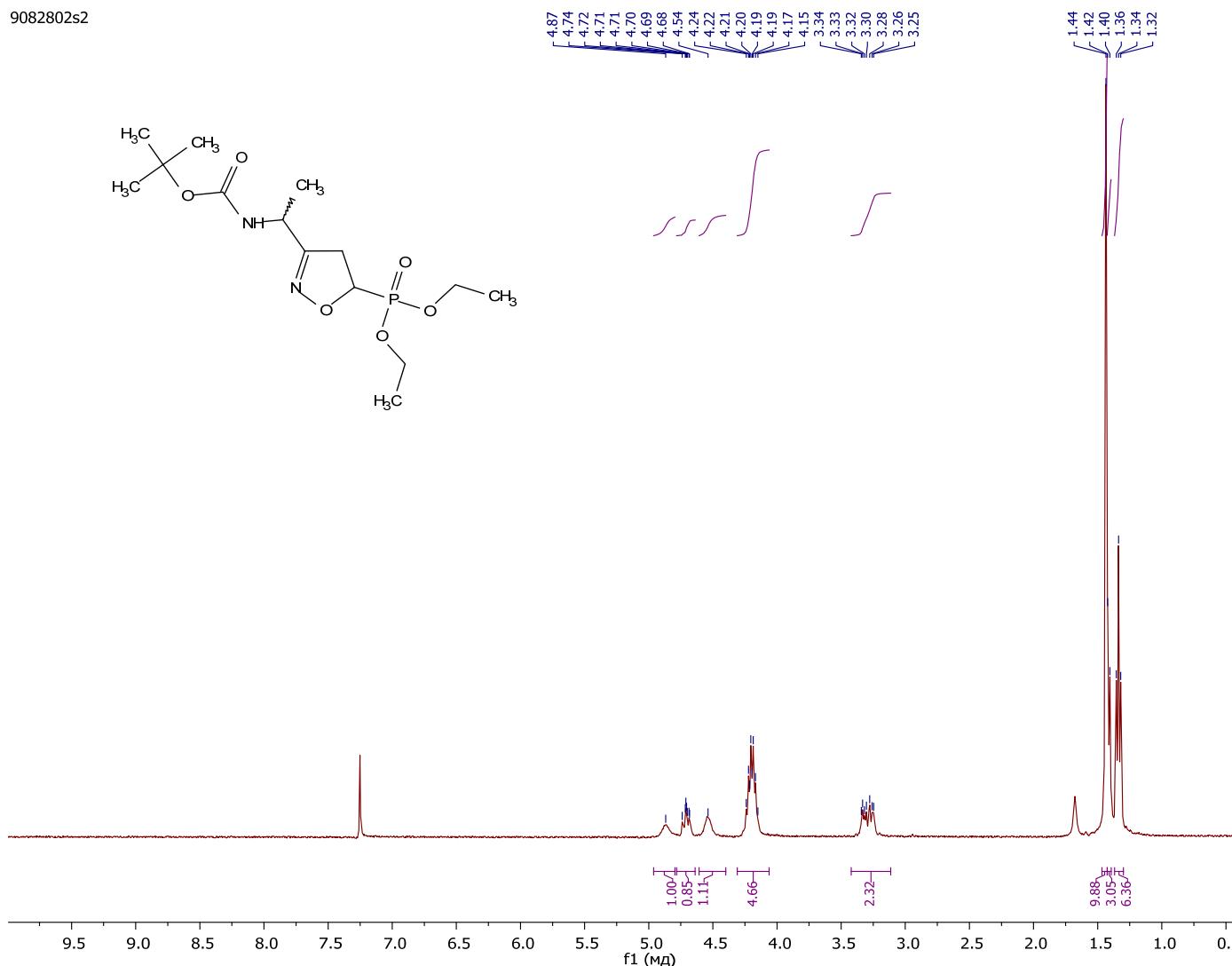


Figure 49 ³¹P NMR spectrum of 2j

9082802s2

Figure 50 ^1H NMR spectrum of 16b and 16c (R-isomer)

sklf6991_C13.1.fid

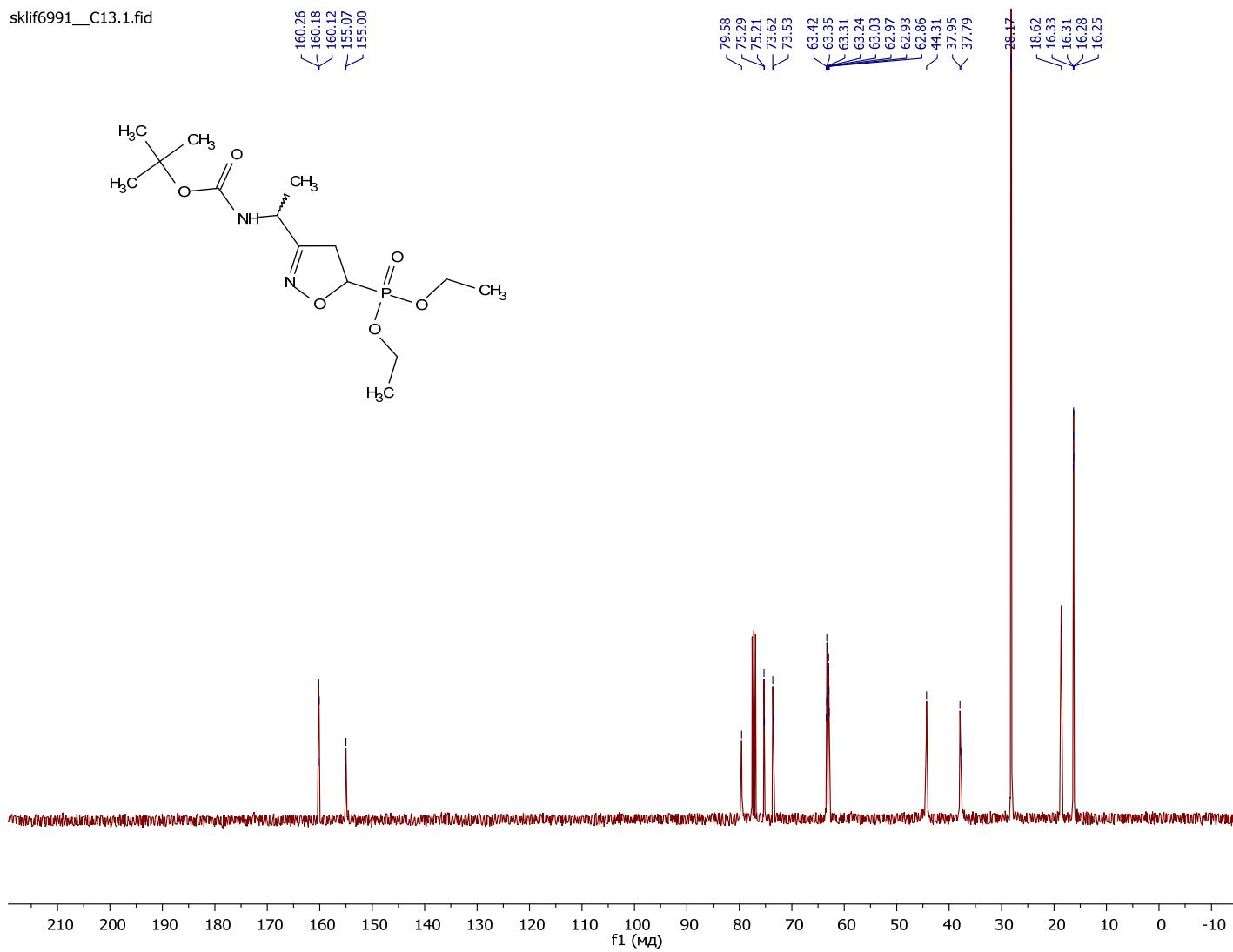


Figure 51 ^{13}C NMR spectrum of 16b and 16c (*R*-isomer)

Sklif6991_P31.1.fid
31P-{1H}

< 19.57
< 19.34

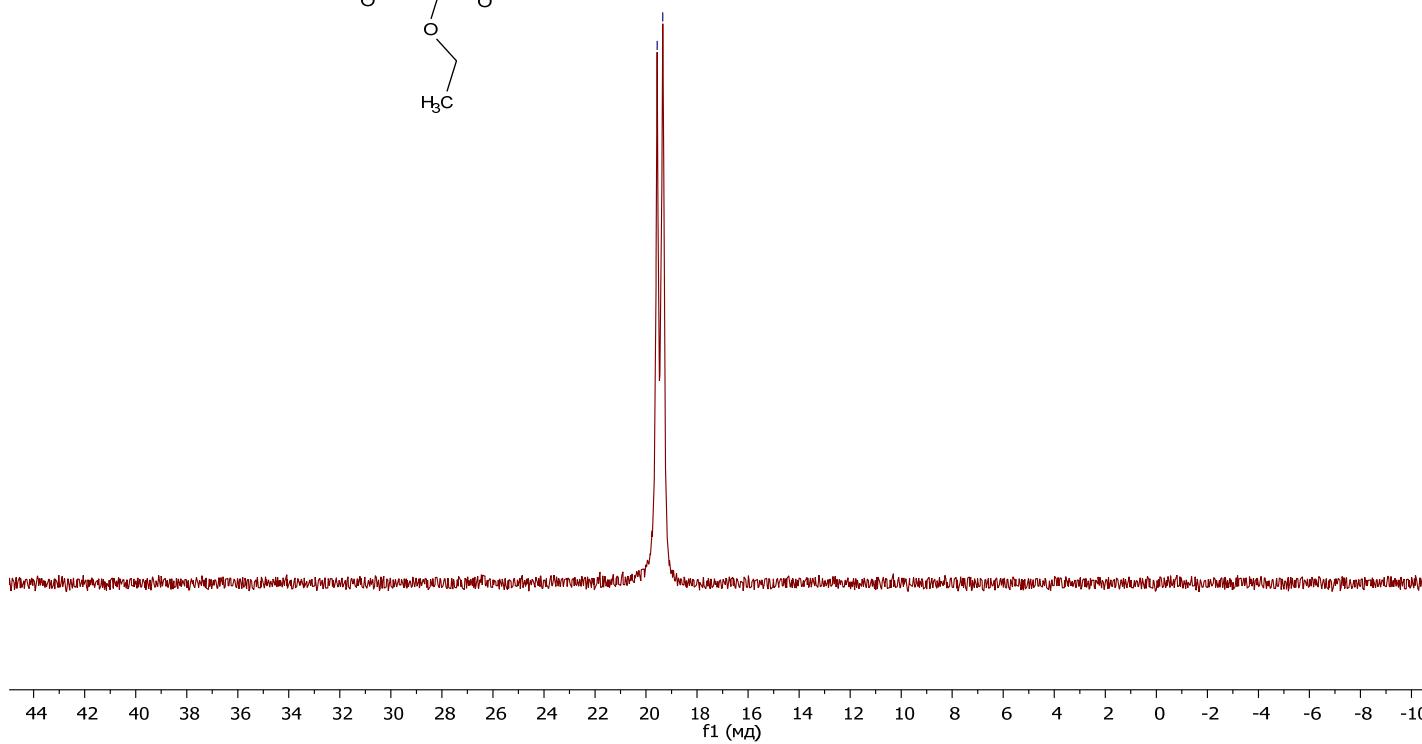
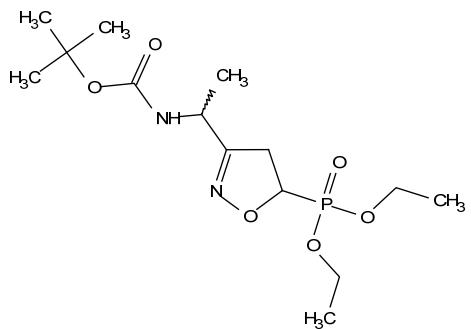


Figure 52 ^{31}P NMR spectrum of 16b and 16c (*R*-isomer)

9000690s1.1.fid

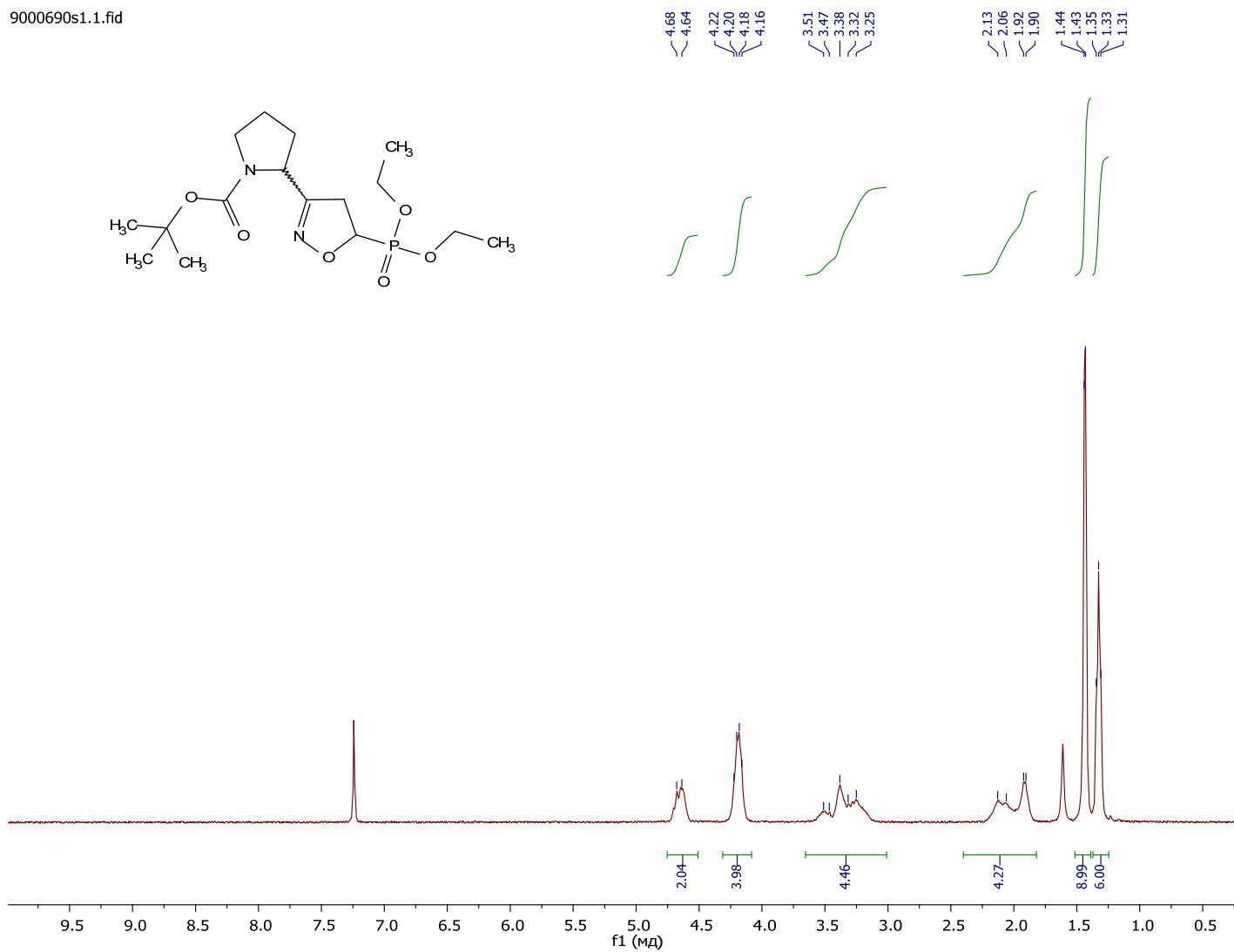


Figure 53 ^1H NMR spectrum of 16f and 16g (R-isomer)

sklf6660_C13.1.fid

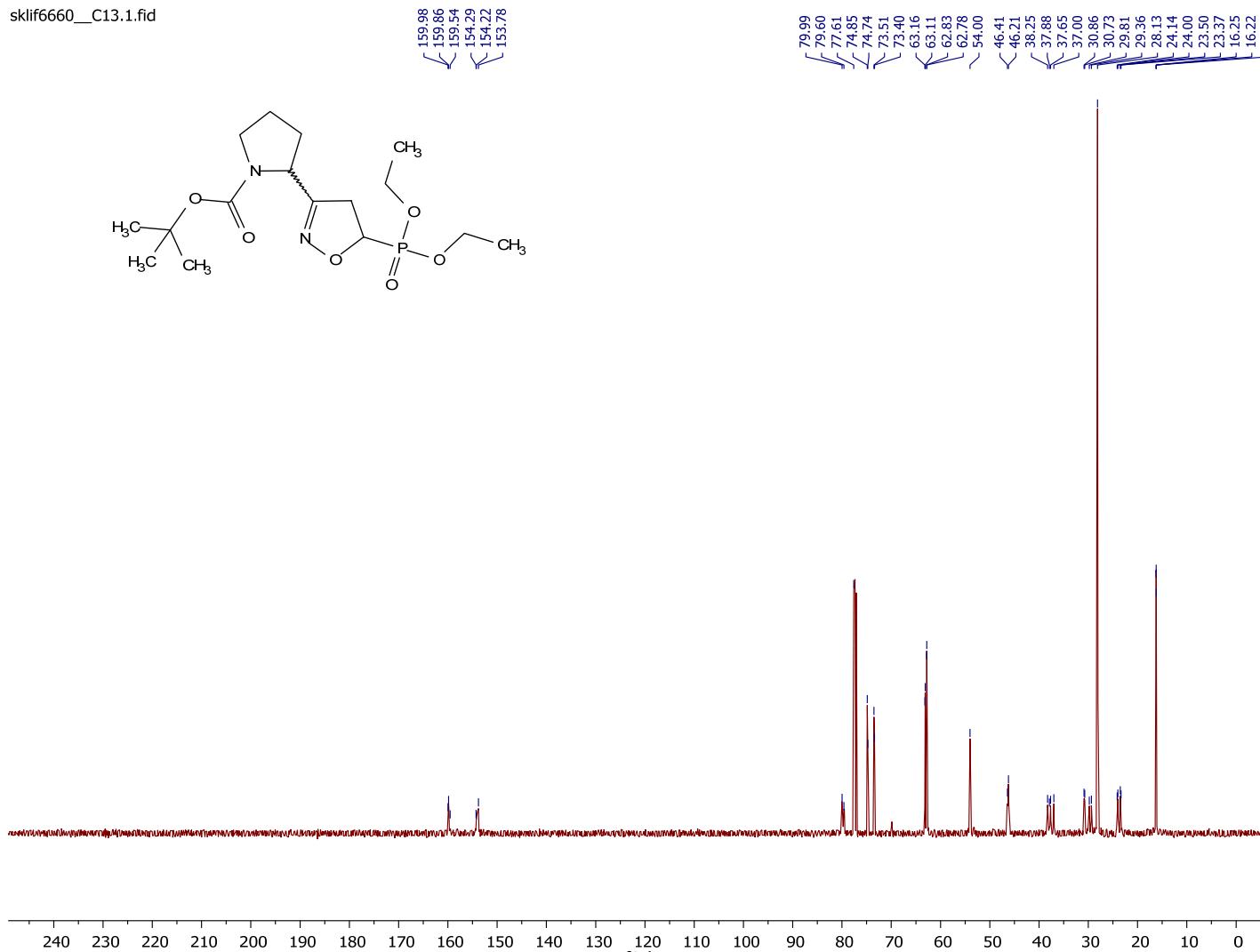


Figure 54 ^{13}C NMR spectrum of 16f and 16g (*R*-isomer)

sklf6660_P31.1.fid

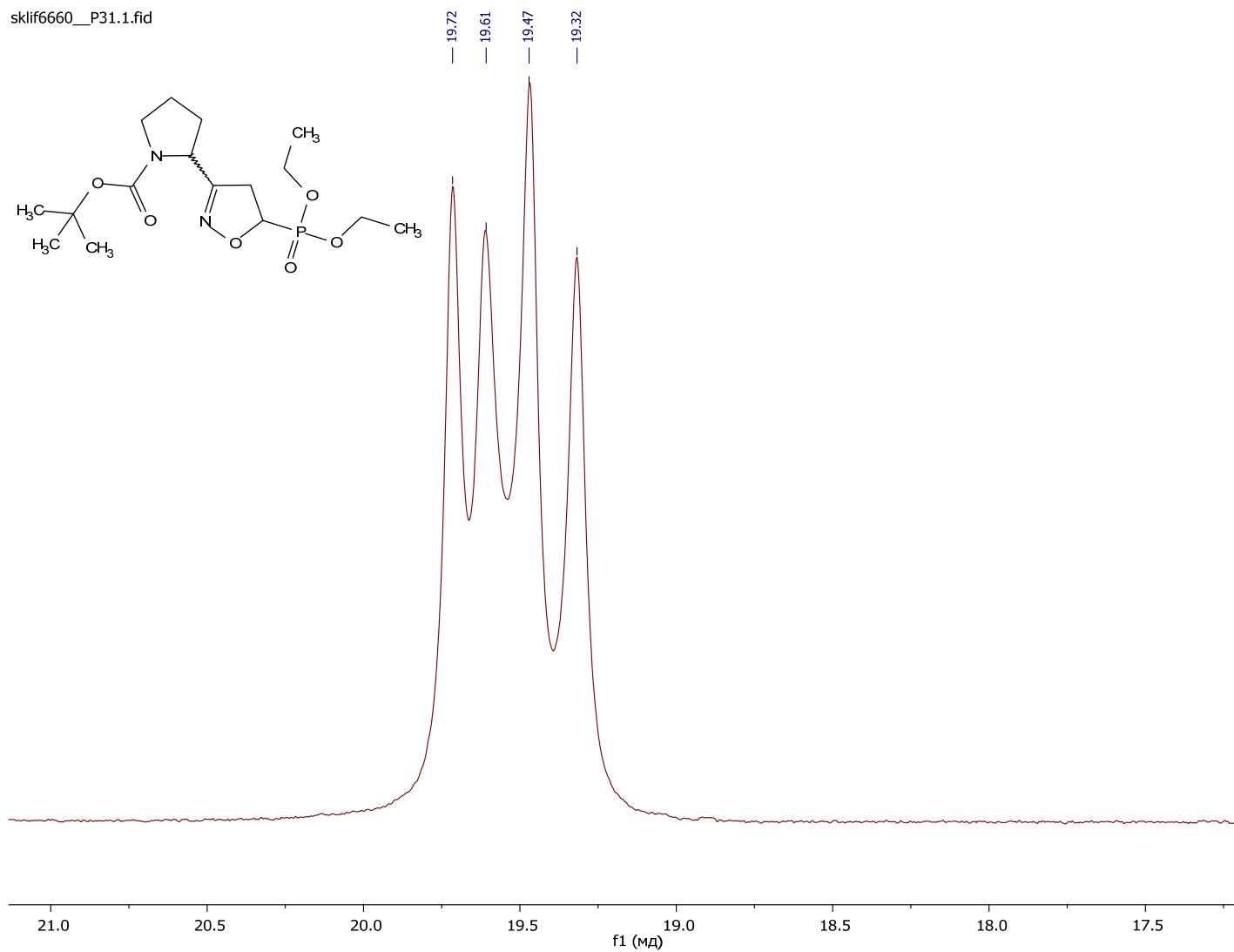


Figure 55 ^{31}P NMR spectrum of 16f and 16g (*R*-isomer)

ab0572-1

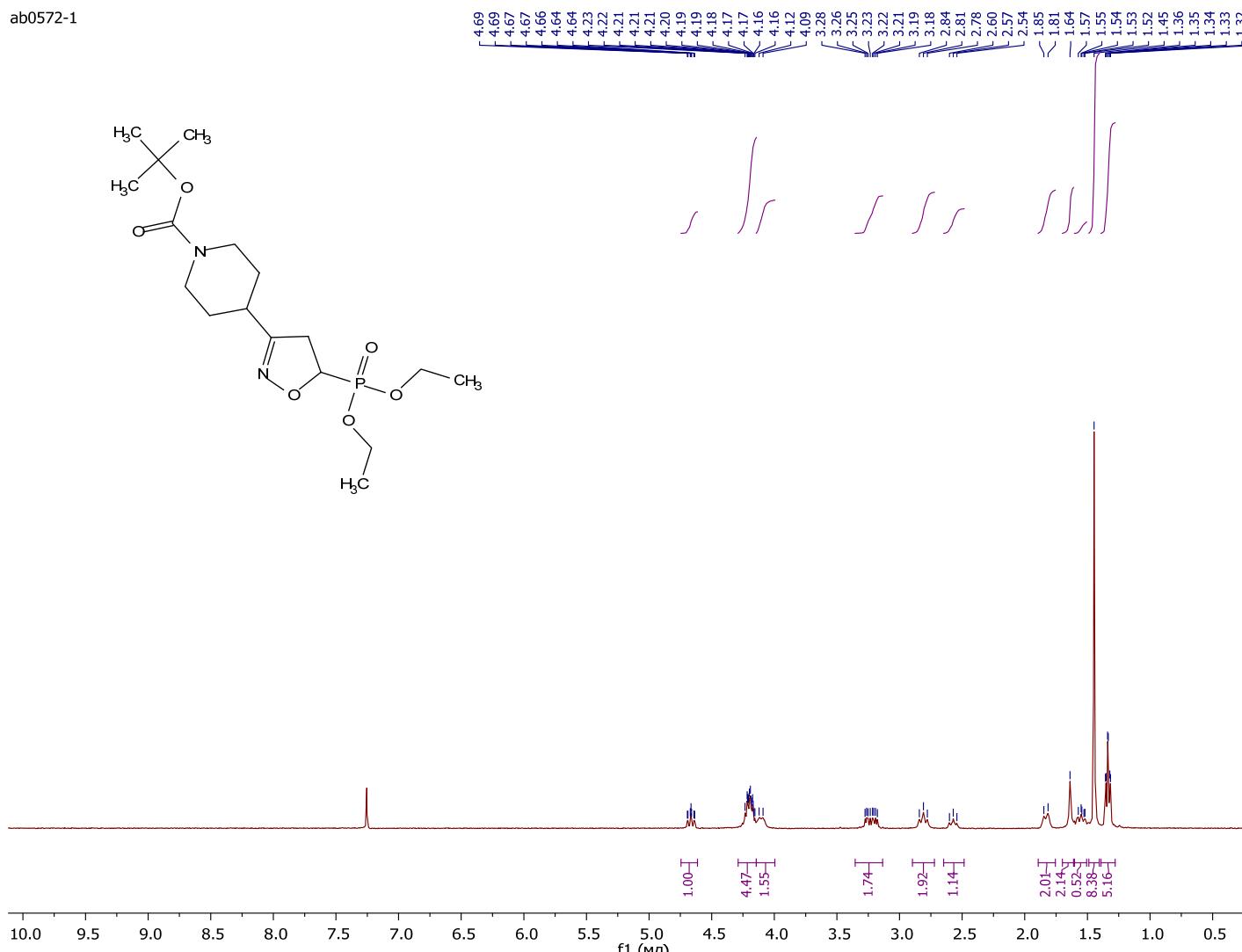


Figure 56 ¹H NMR spectrum of 16h

sklif6279_C13.1.fid

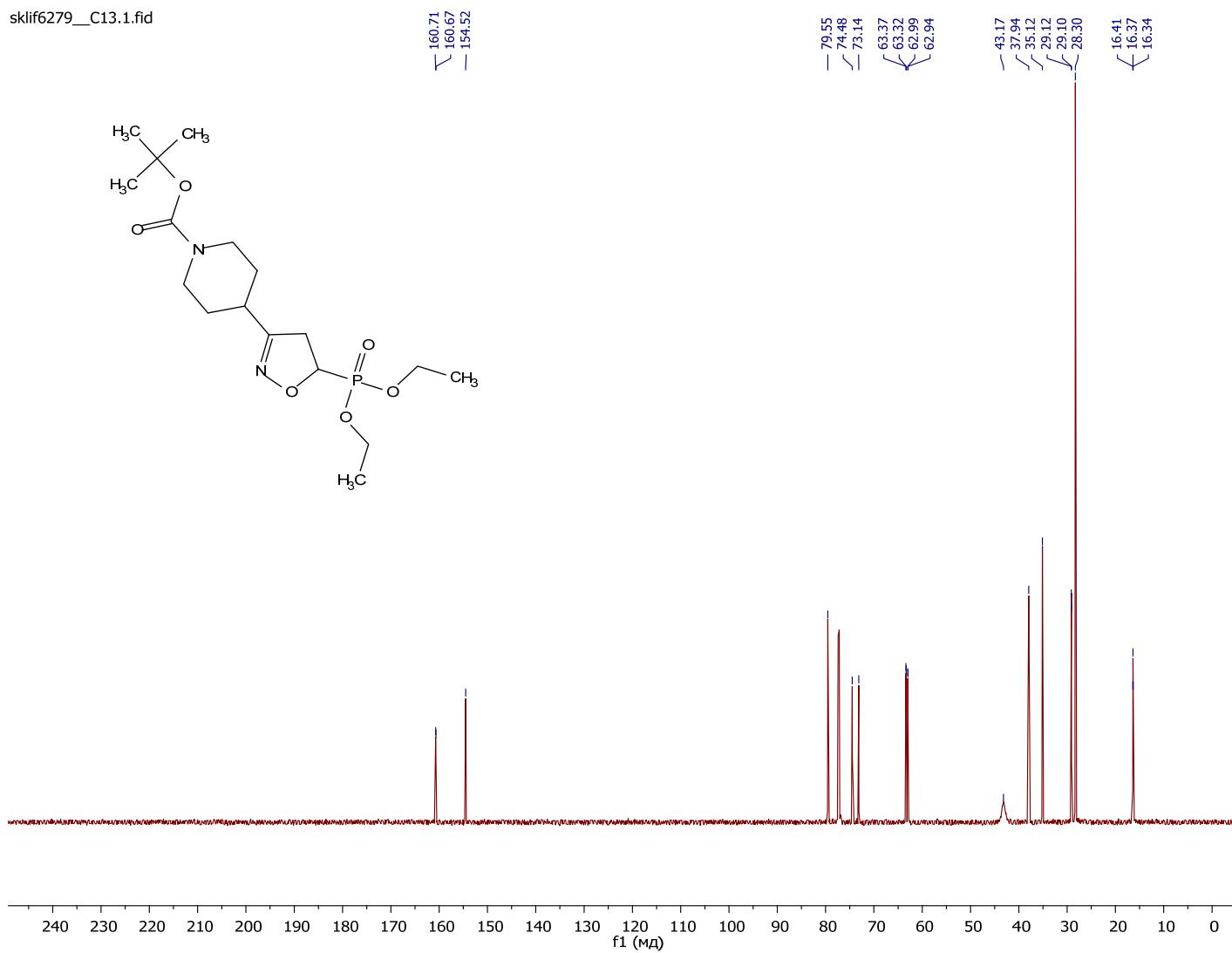


Figure 57 ^{13}C NMR spectrum of 16h

sklif6279_P31{H}.1.fid

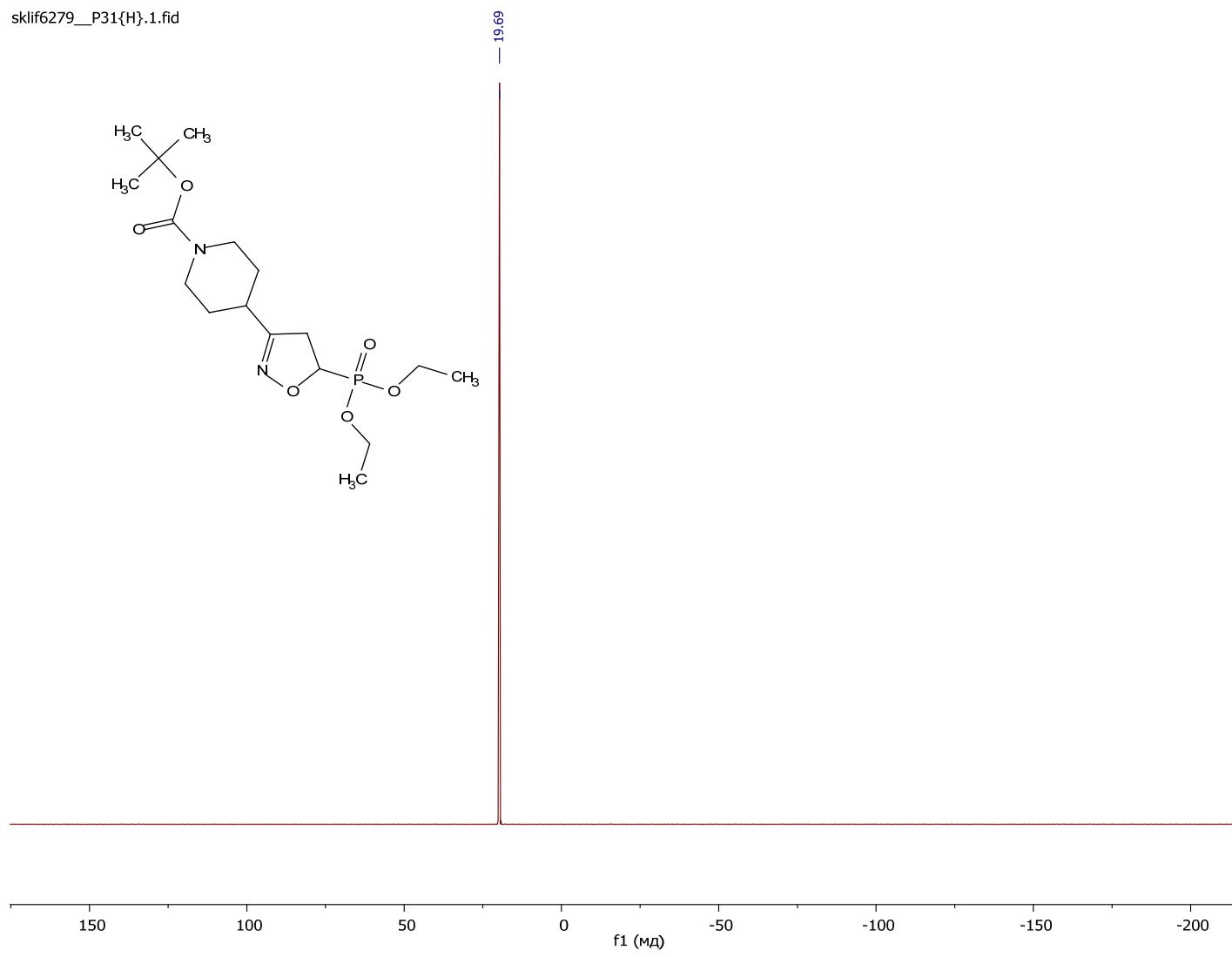


Figure 58 ^{31}P NMR spectrum of 16h

K788732s1

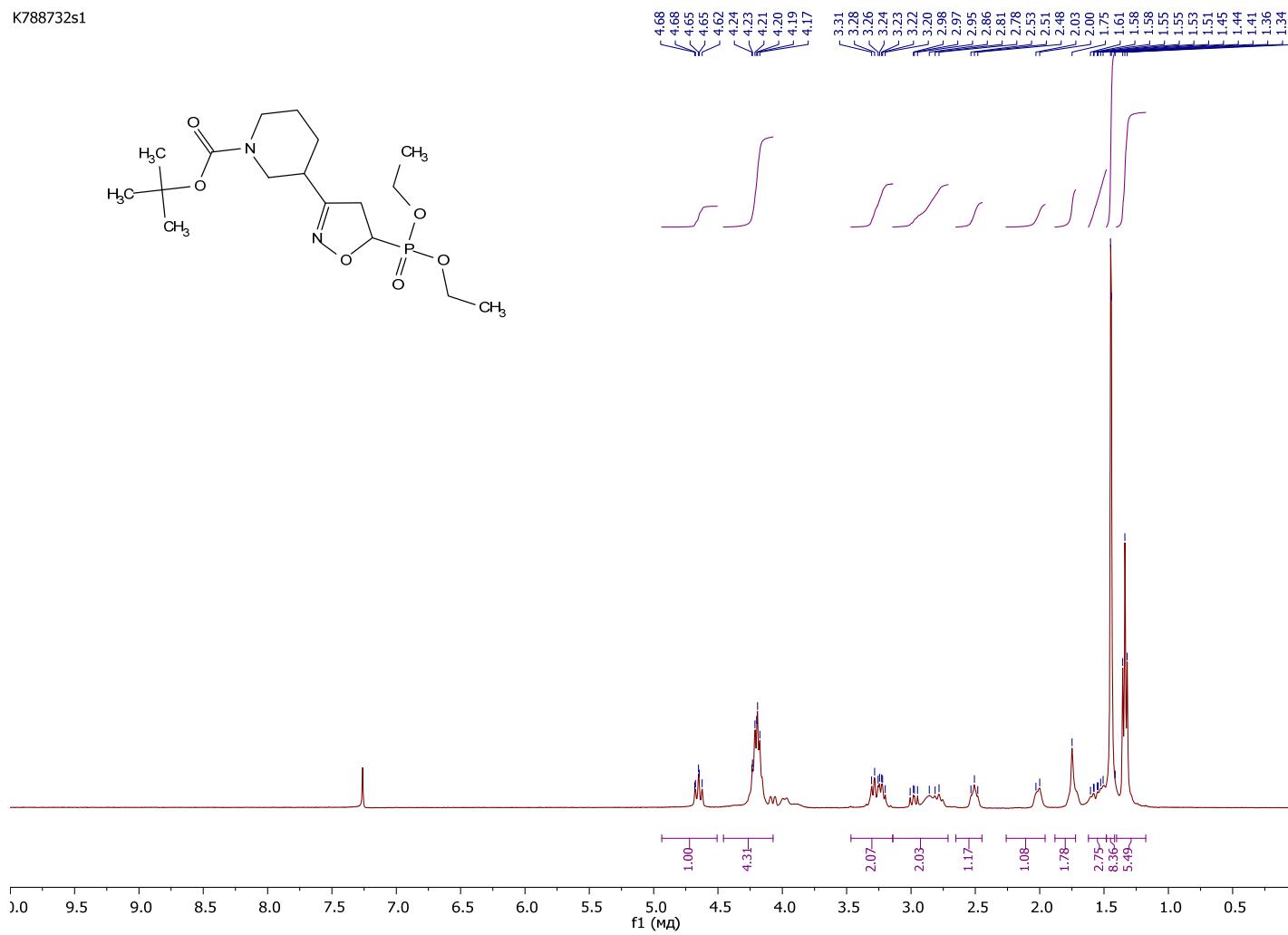


Figure 59. ¹H NMR spectrum of 16i

sklf3168_C13.1.fid

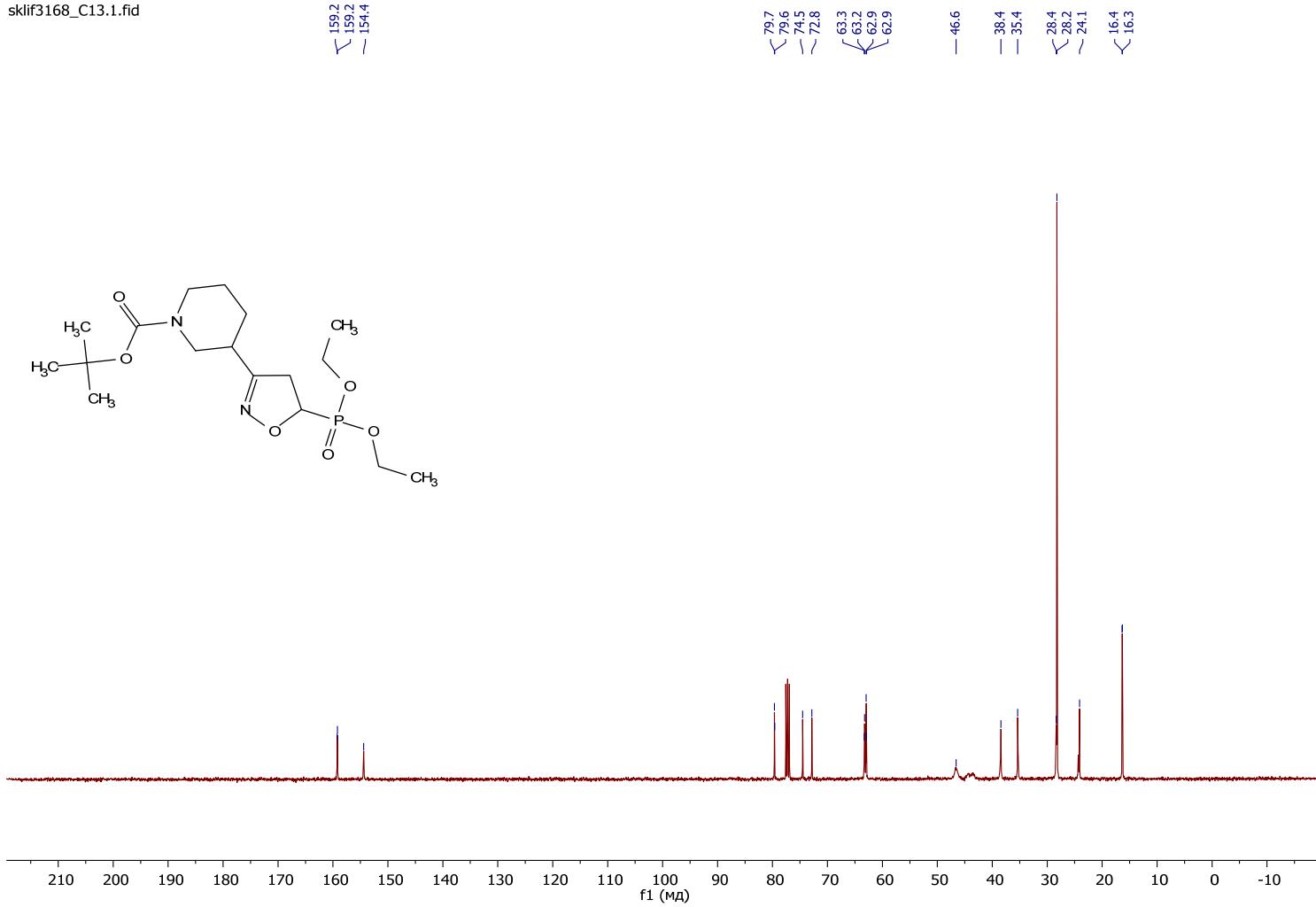


Figure 60. ^{13}C NMR spectrum of 16i

sklif3168_P31{H}.1.fid

19.65
19.53

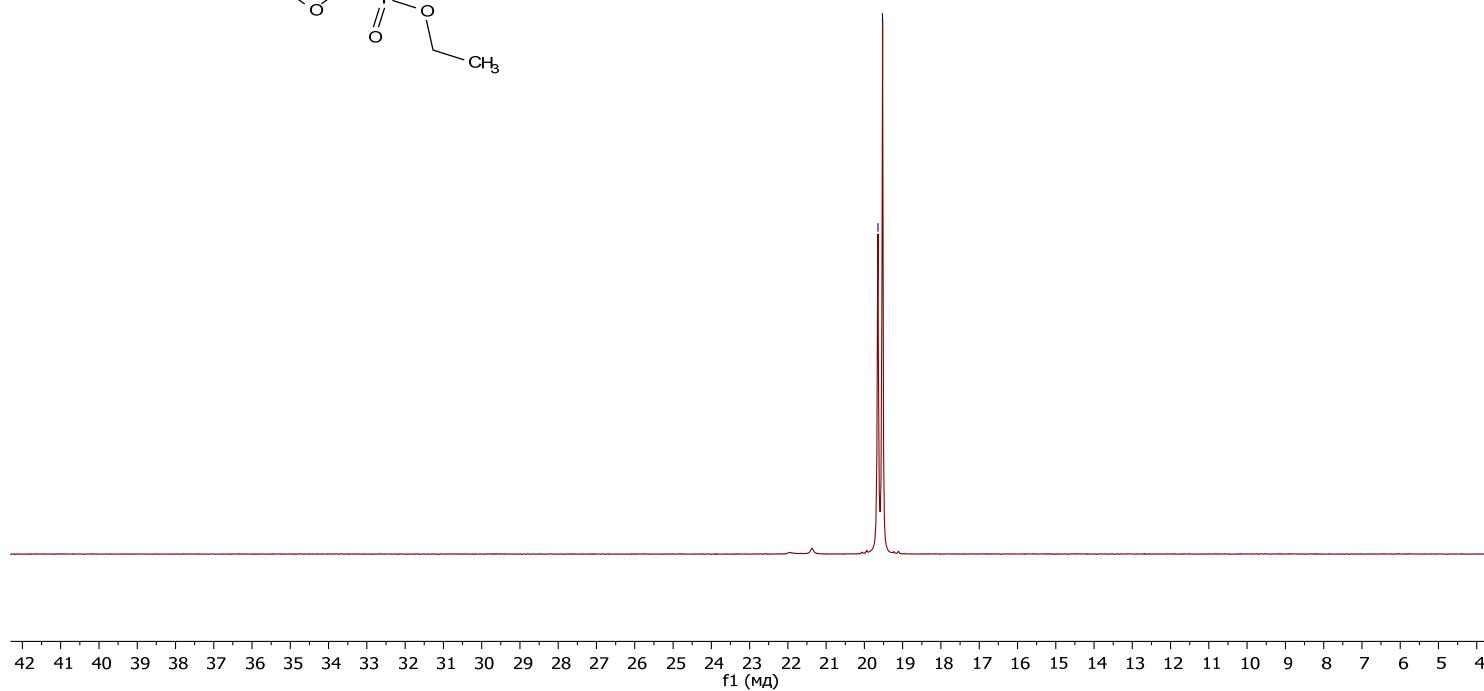
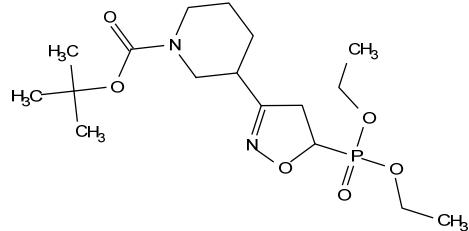


Figure 61. ^{31}P NMR spectrum of 16i

9000691s1.1.fid

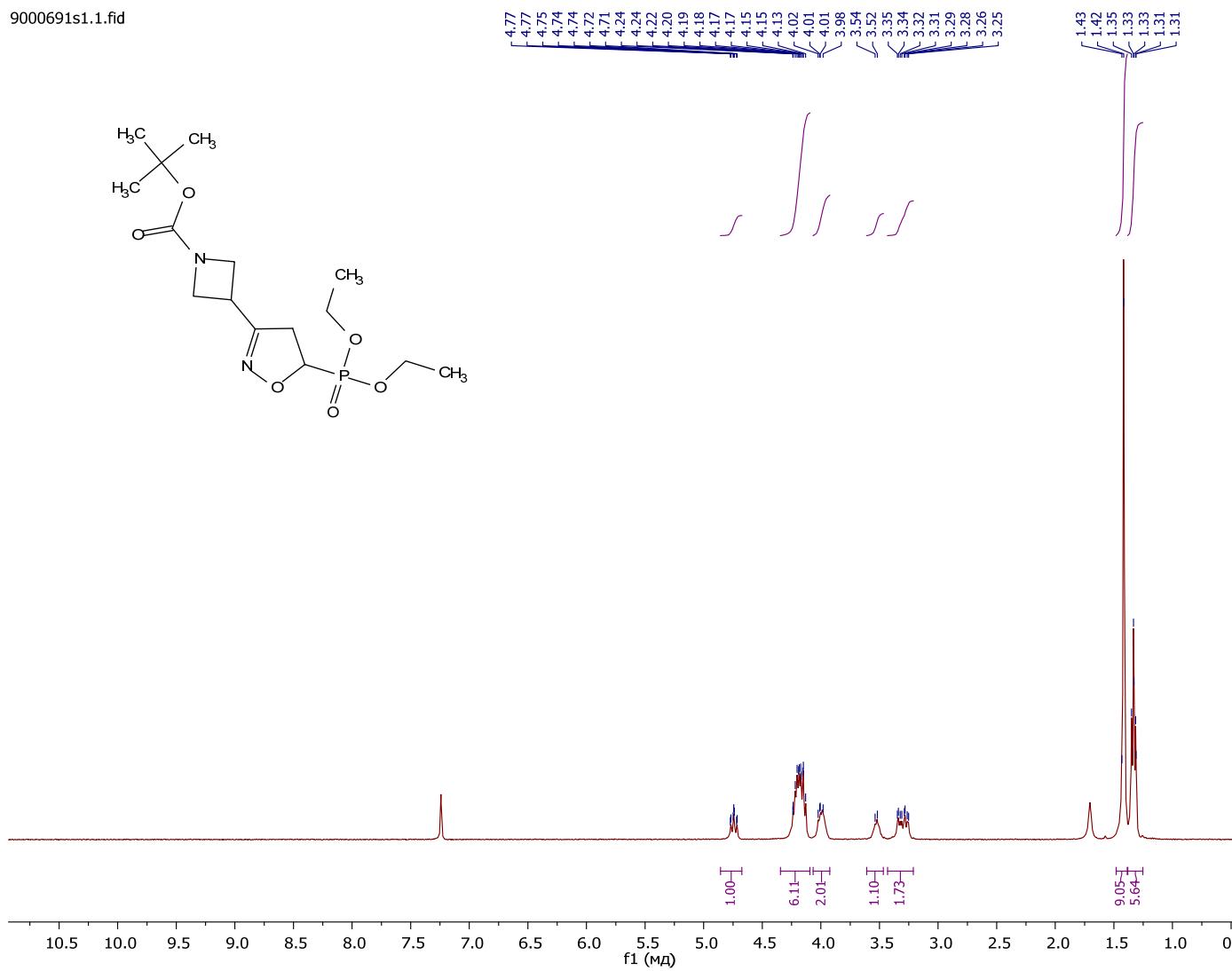


Figure 62 ^1H NMR spectrum of 16j

sklf6661_C13.1.fid

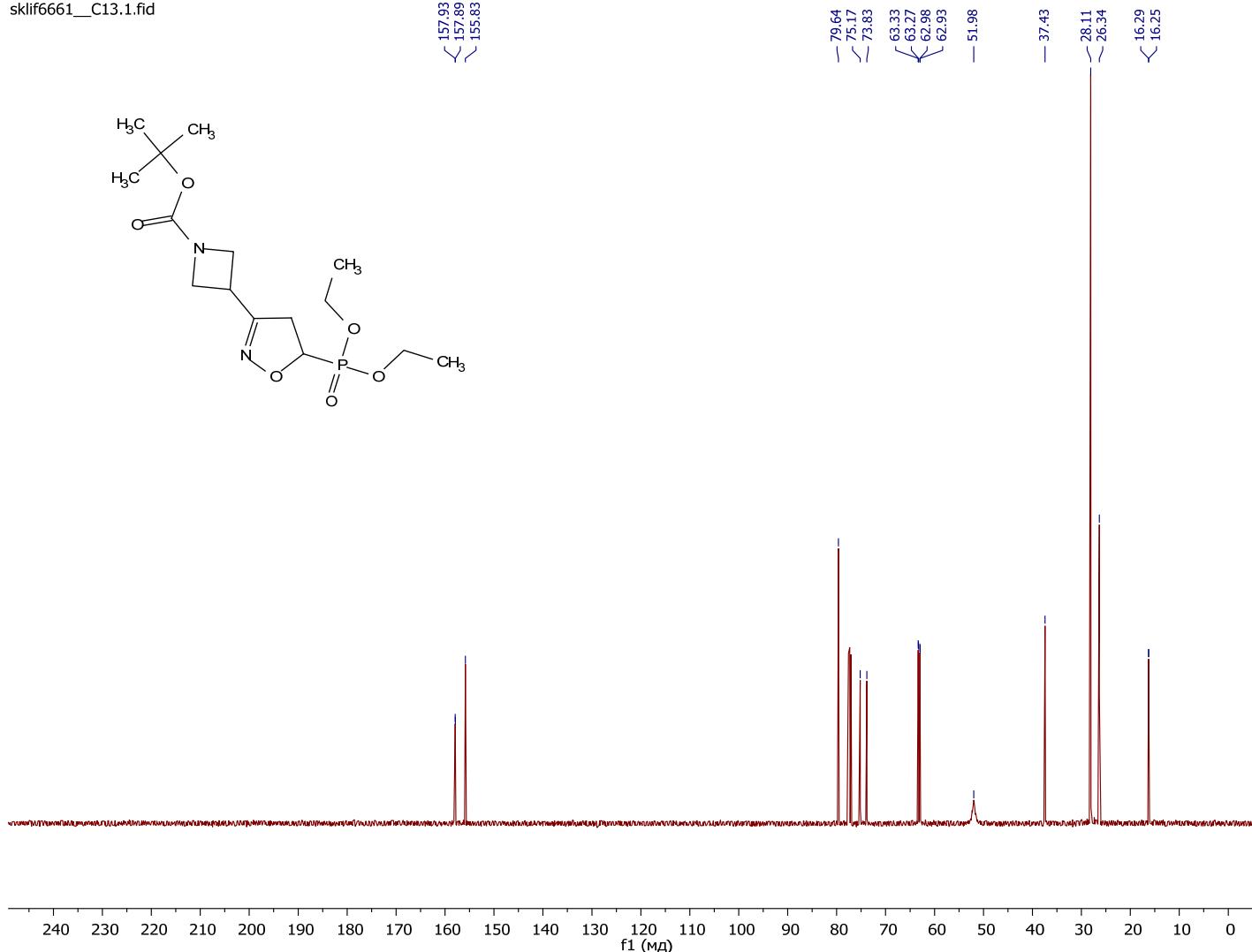


Figure 63 ^{13}C NMR spectrum of 16j

sklif6661_P31.1.fid

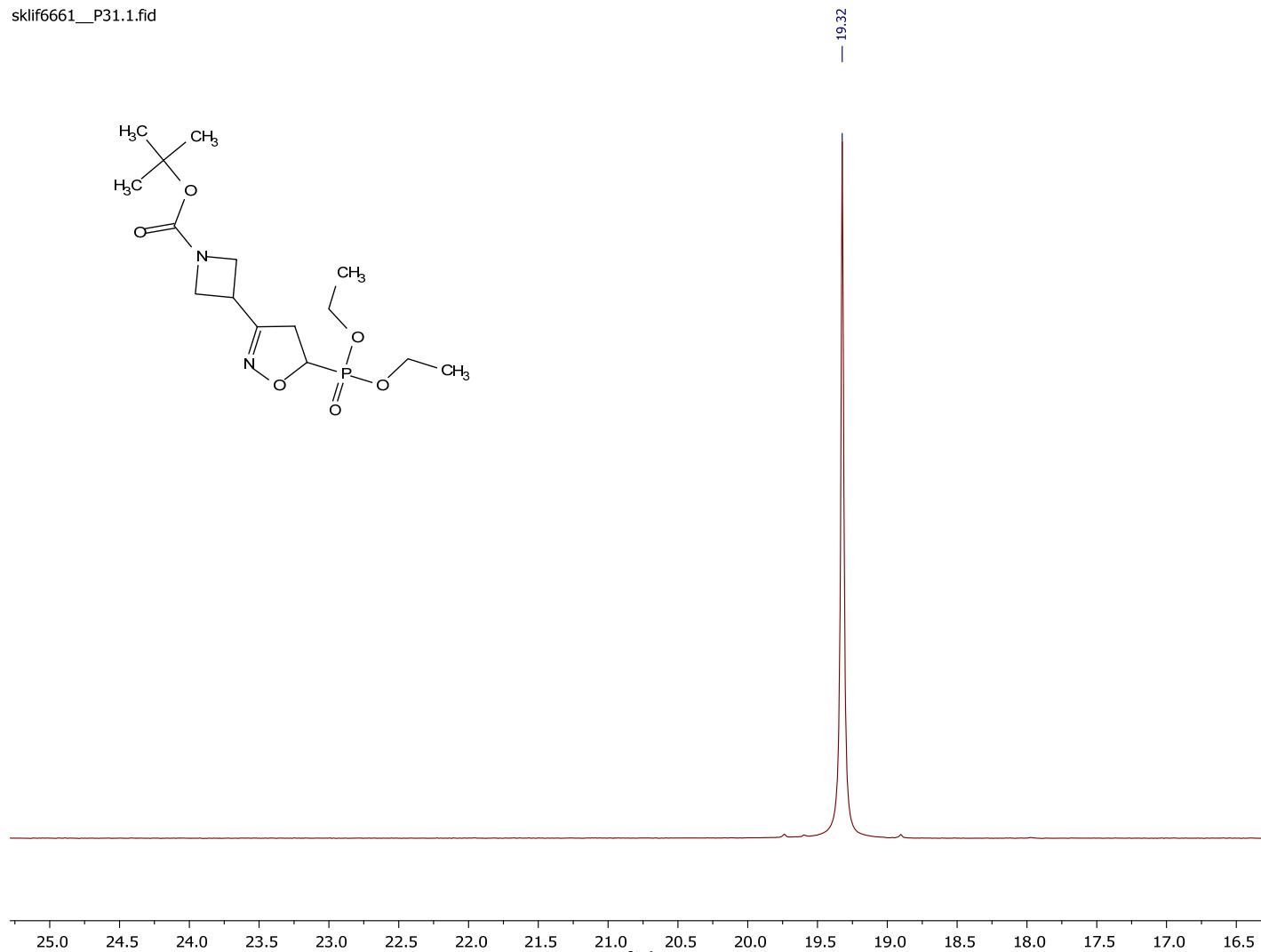


Figure 64. ^{31}P NMR spectrum of 16j

K846846s2

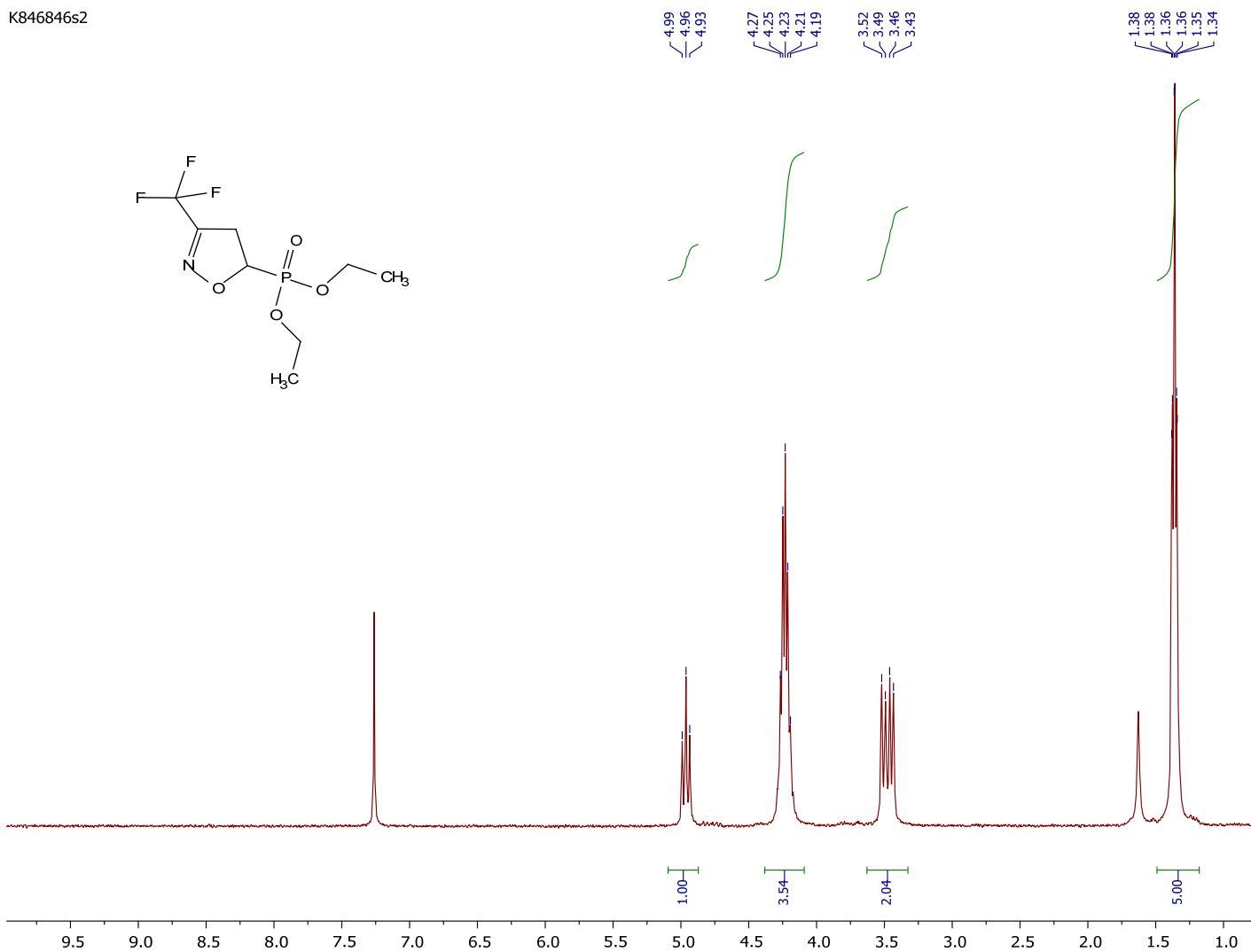


Figure 65. ^1H NMR spectrum of 160

sklf3475_C13.1.fid

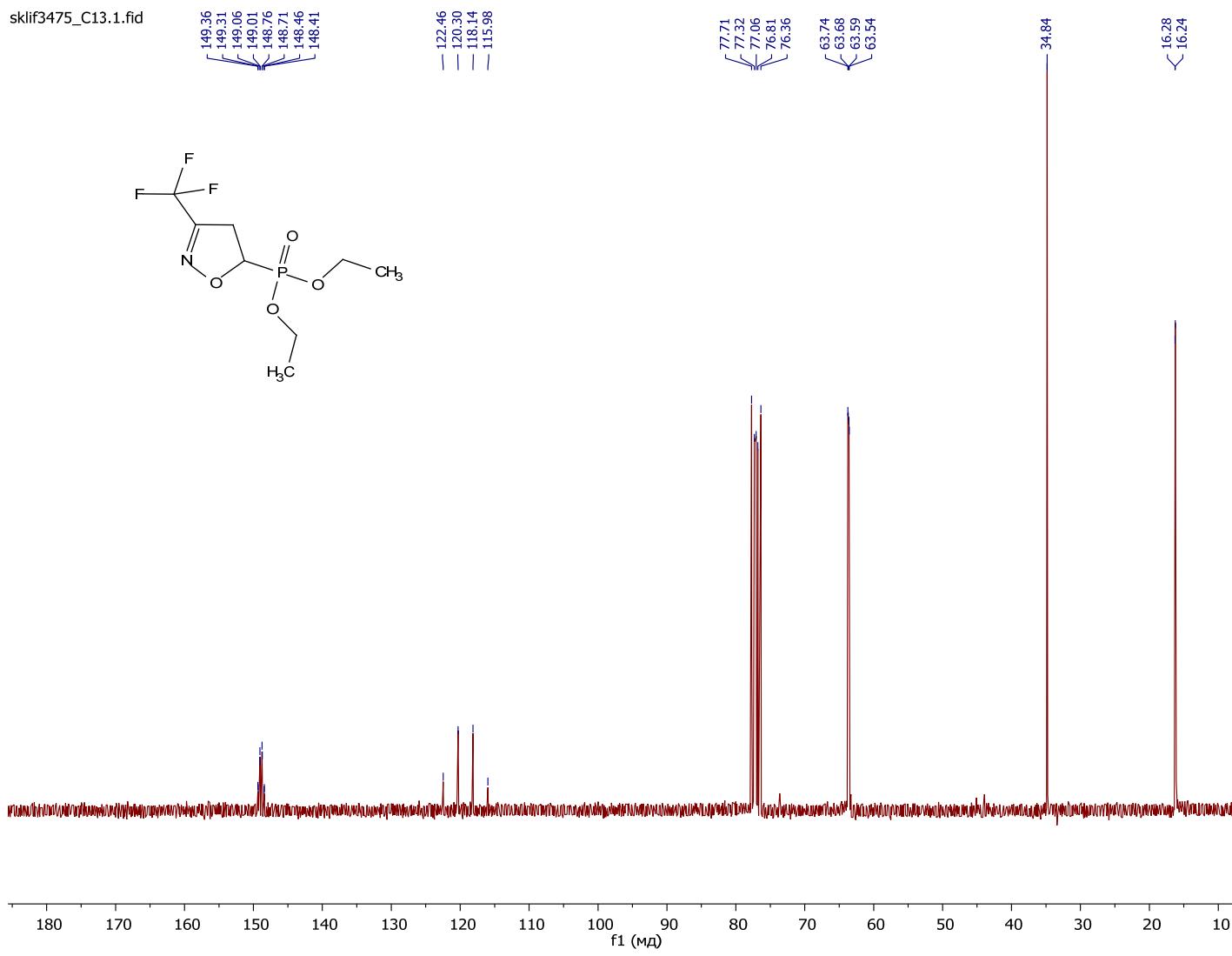


Figure 66. ^{13}C NMR spectrum of 160

SKLif3475_P31.1.fid
31P-{1H}

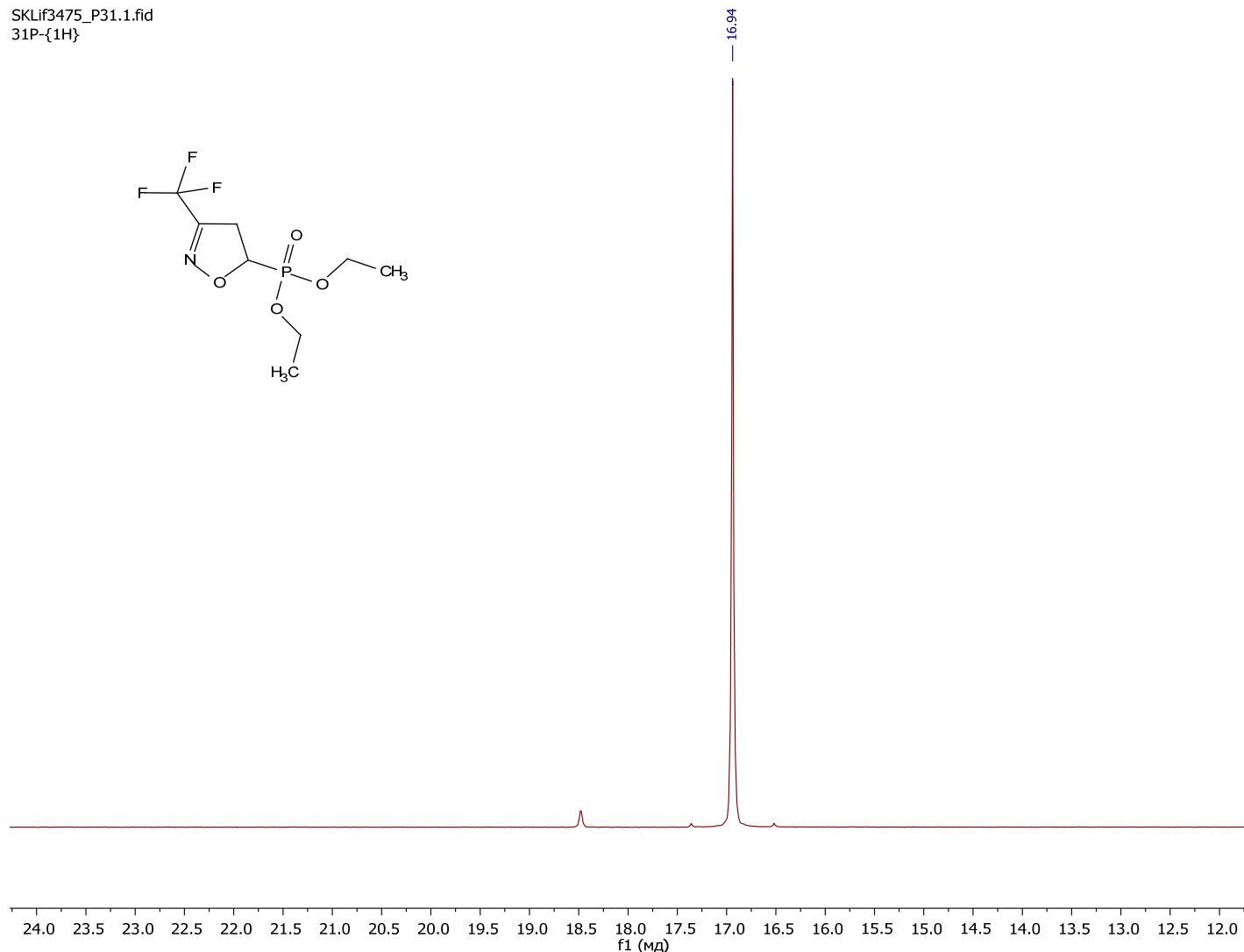


Figure 67. ^{31}P NMR spectrum of 160

sklf3475_F19{H}.1.fid

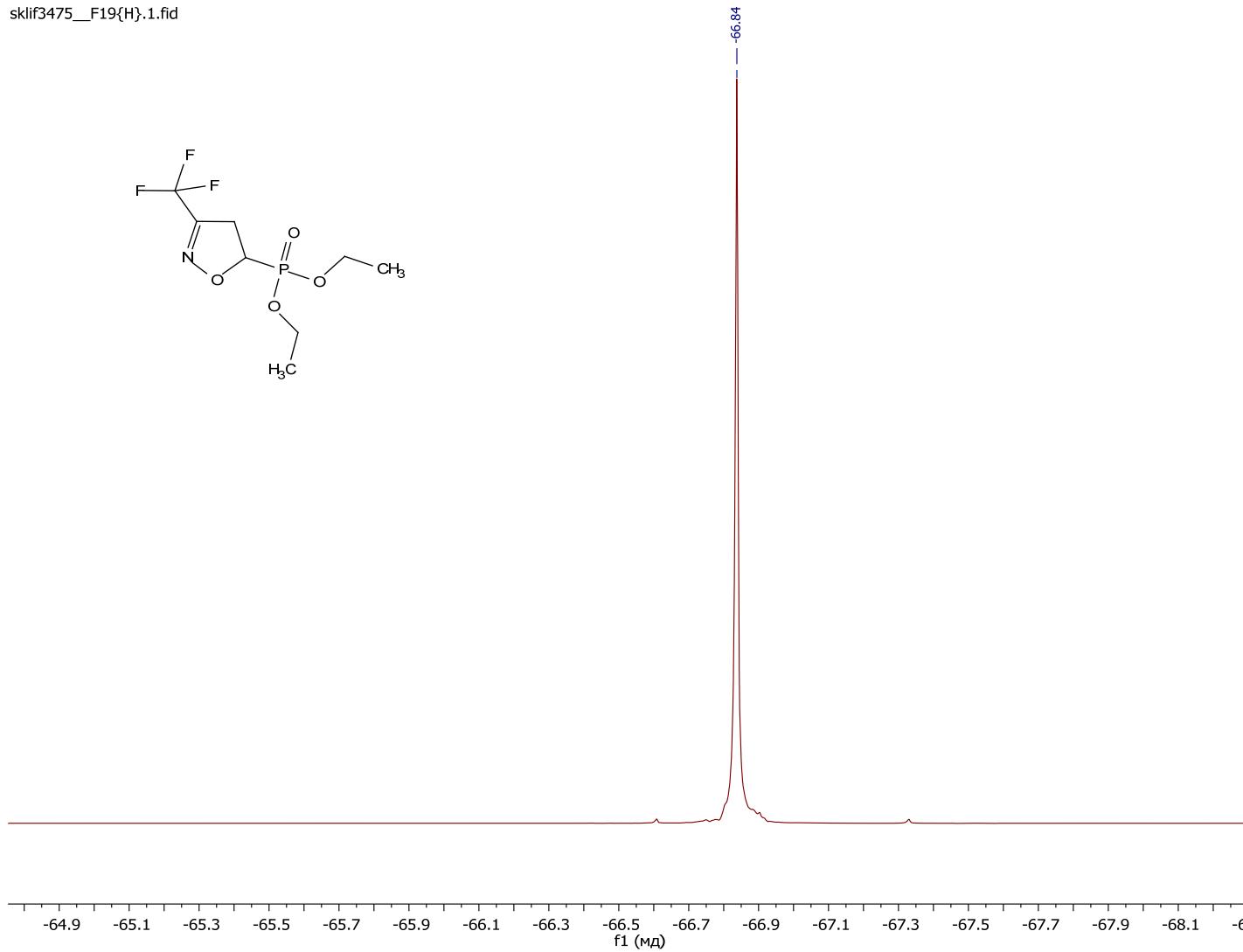


Figure 68. ^{19}F NMR spectrum of 160

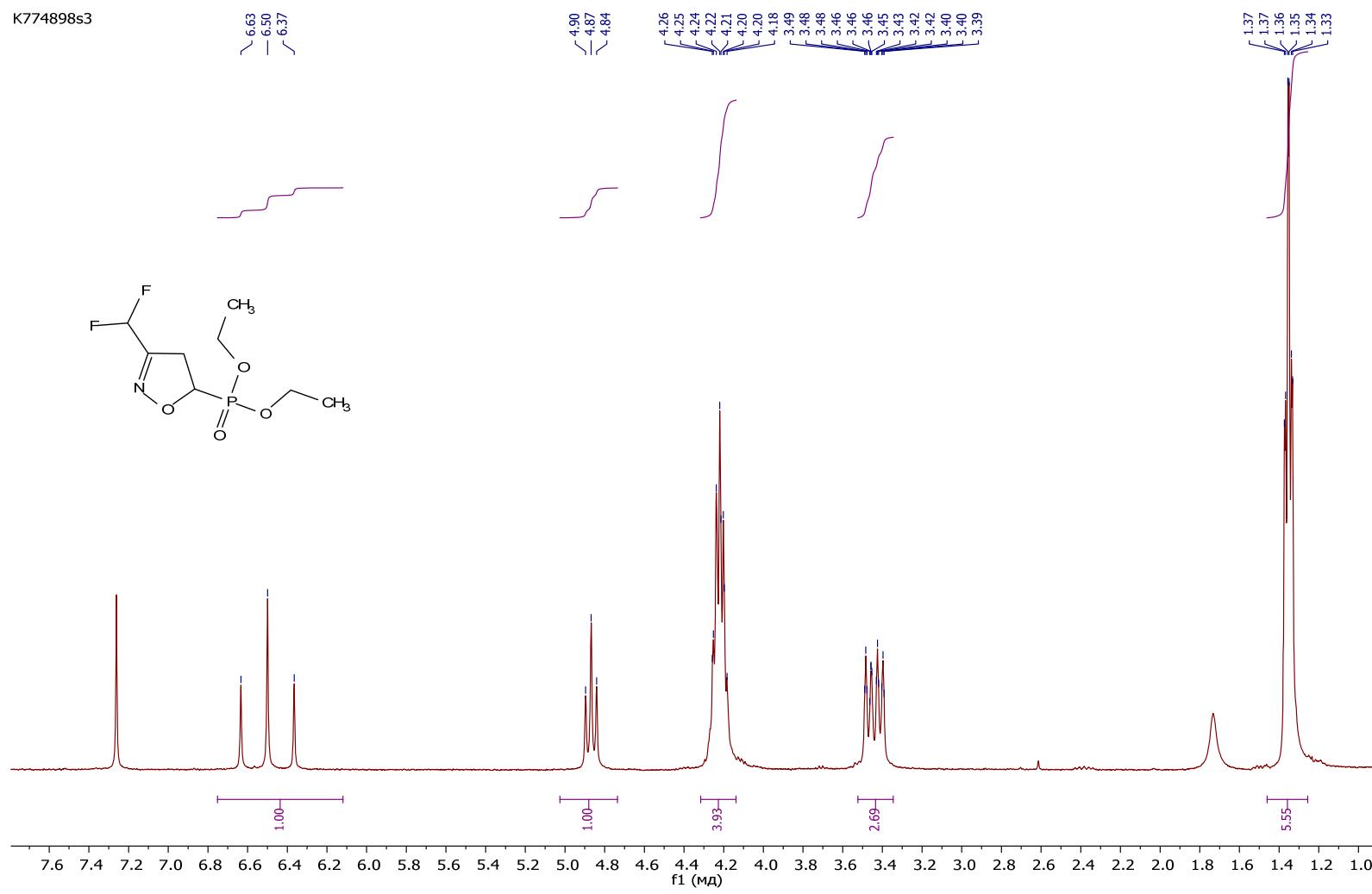


Figure 69. ^1H NMR spectrum of 16p

sklf3137_C13.1.fid

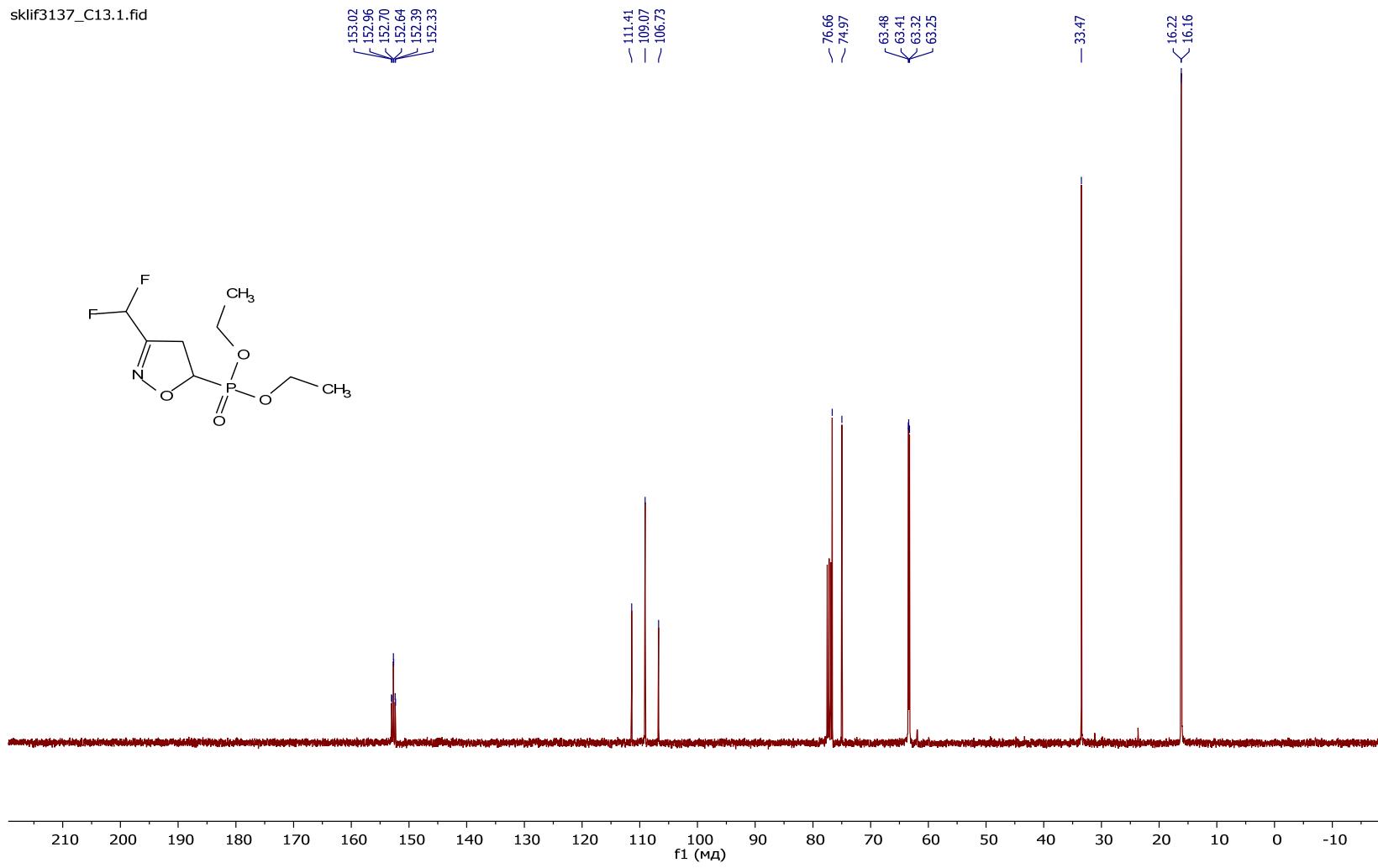


Figure 70. ^{13}C NMR spectrum of 16p

sklf3137 31P{1H}.1.fid

—17.76

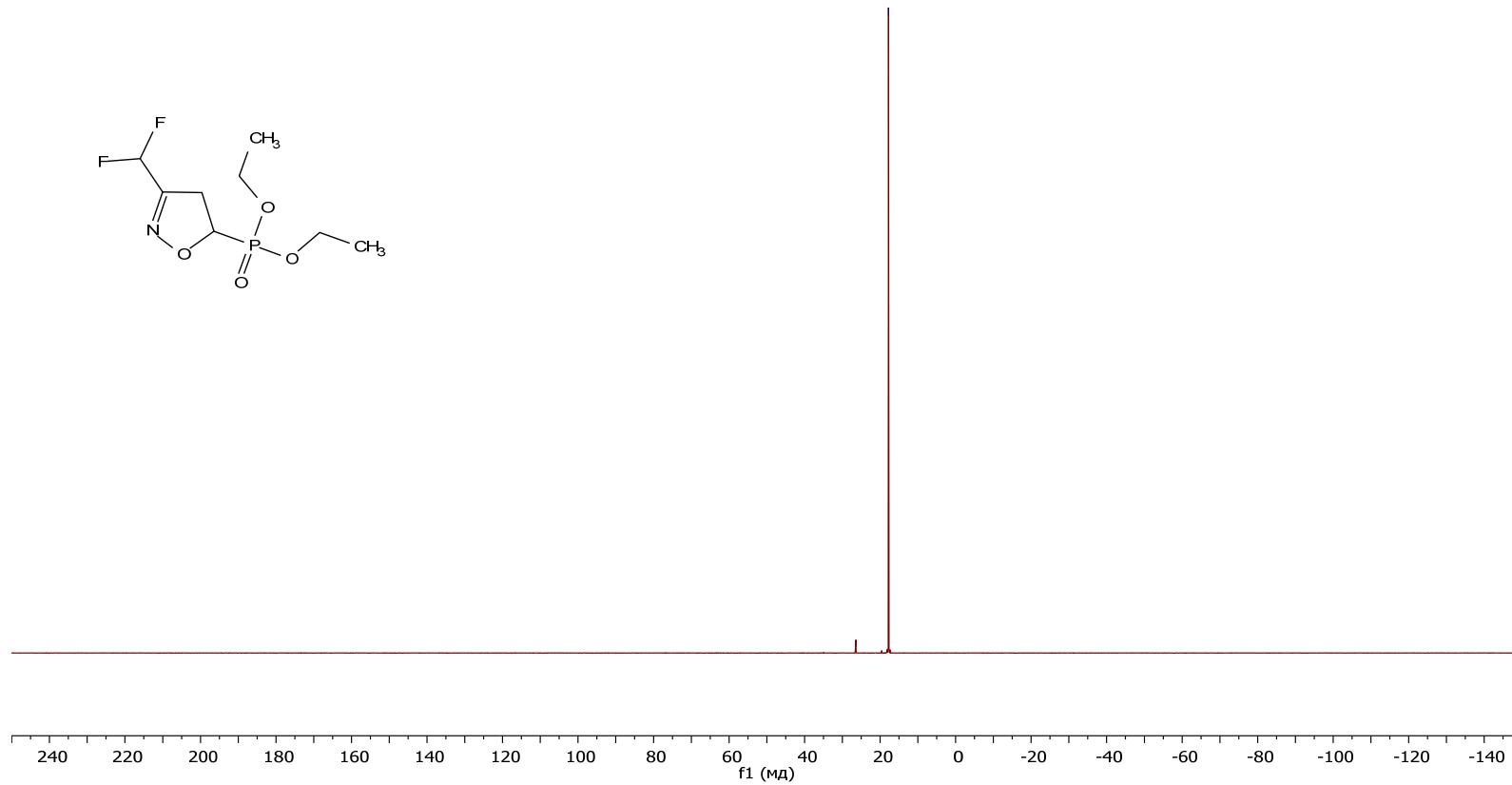
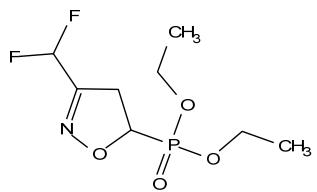


Figure 71. ^{31}P NMR spectrum of 16p

sklf3137_F19{H}.1.fid
19F-{1H}

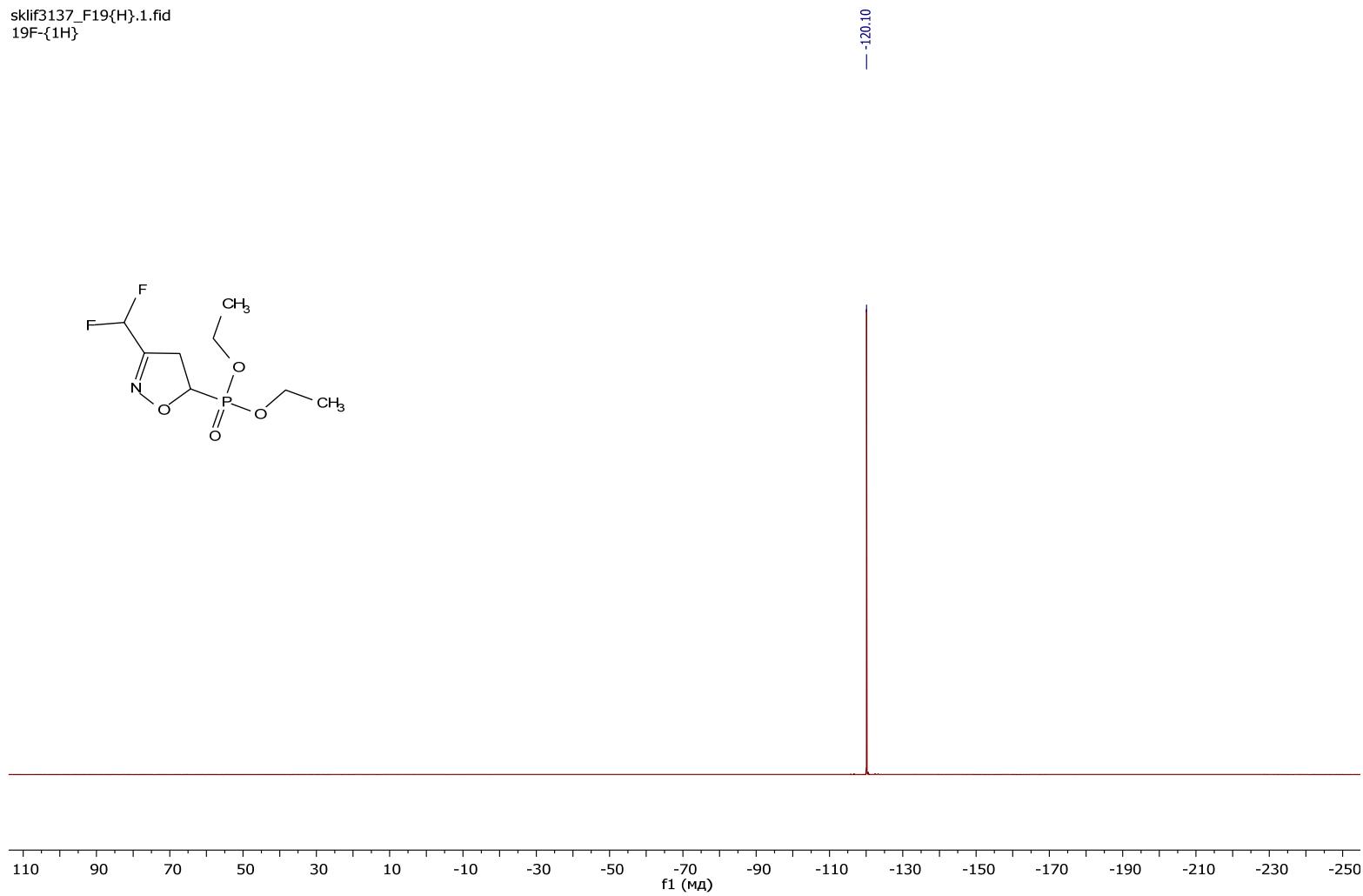


Figure 72. ¹⁹F NMR spectrum of 16p

9630994s2

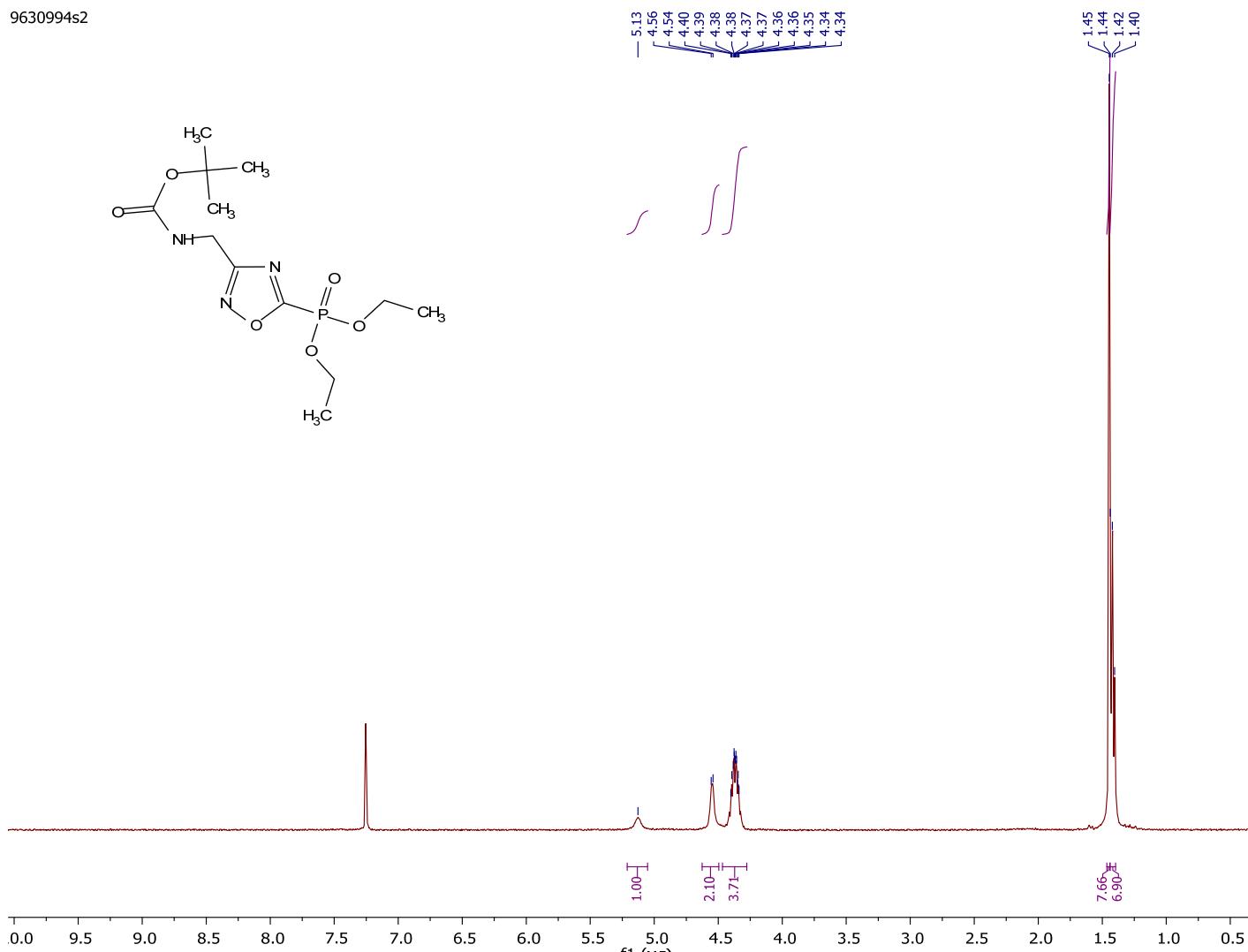


Figure 73 ¹H NMR spectrum of 3a

sklif1799 13C.1.fid

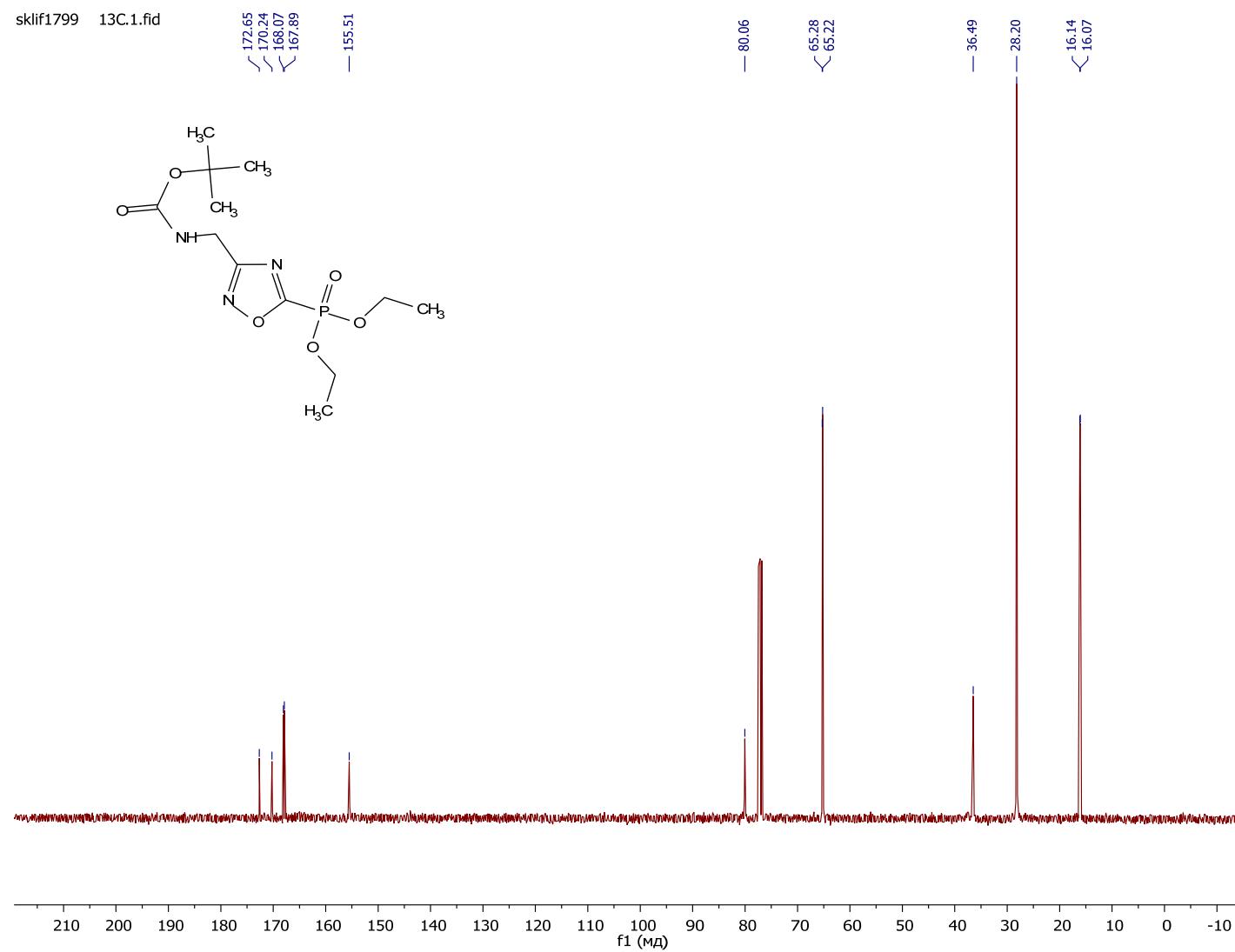
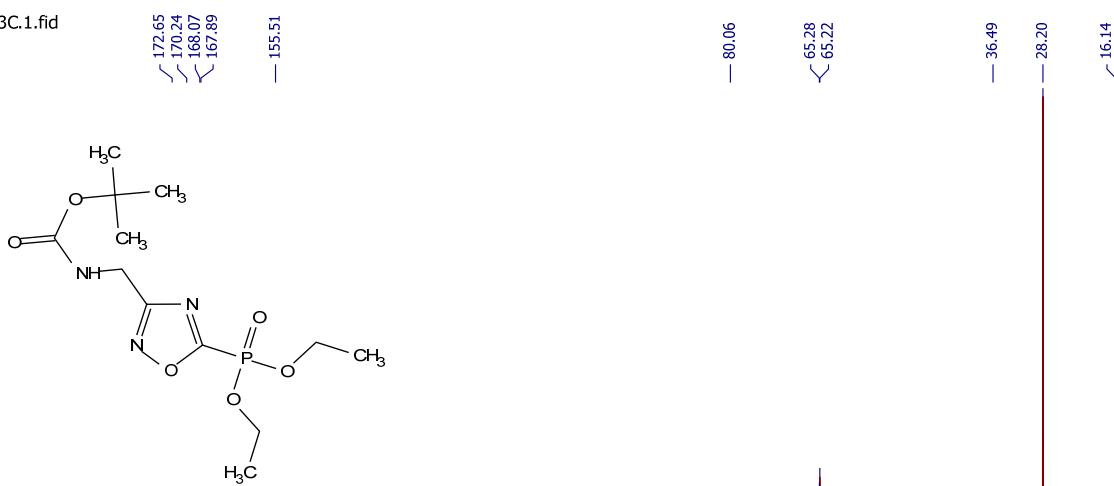


Figure 74 ¹³C NMR spectrum of 3a

sklif1799_P31.1.fid

4.74
4.77
4.82
4.86
4.90

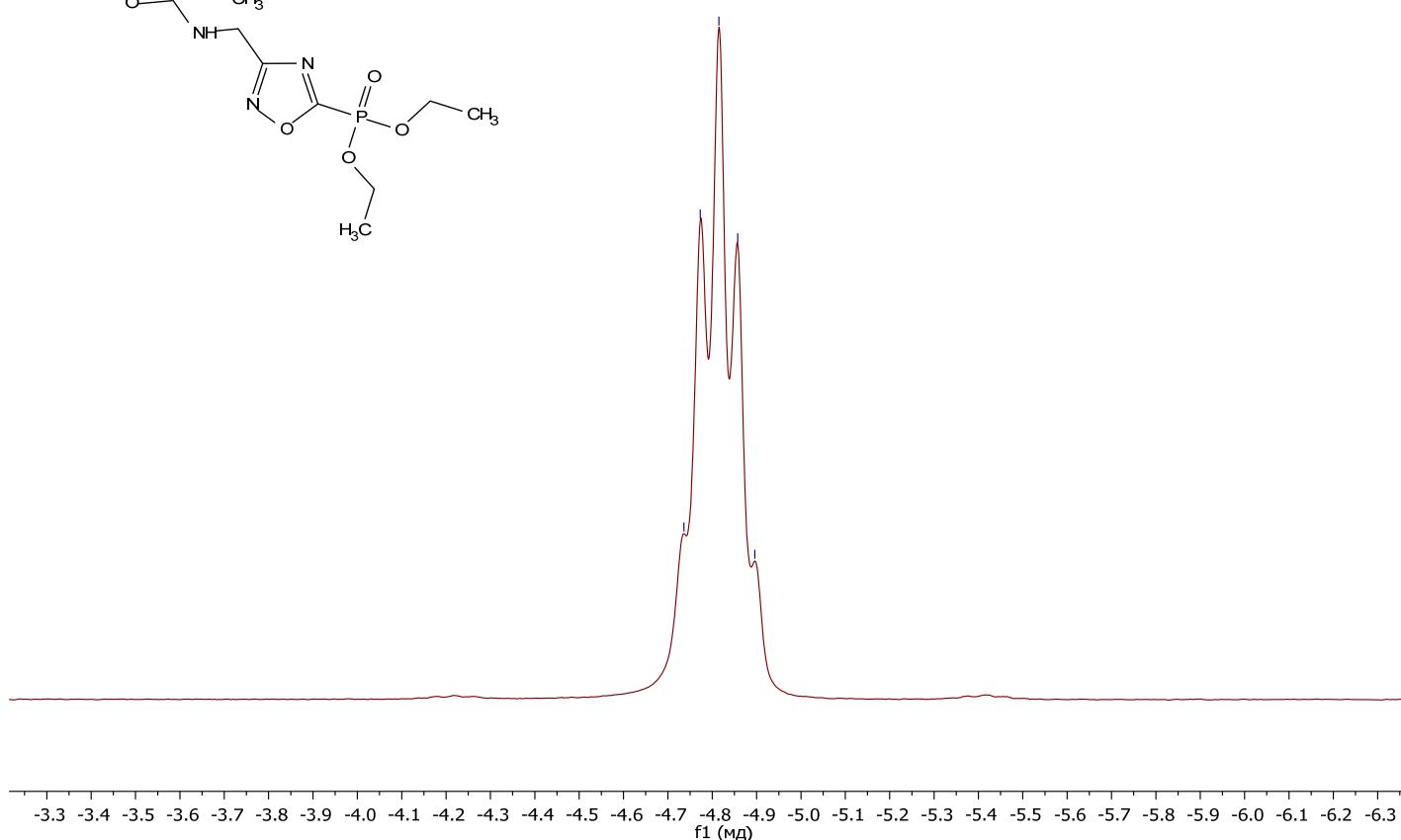
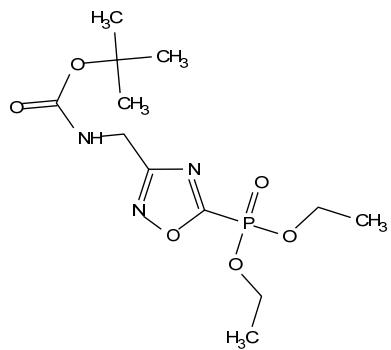
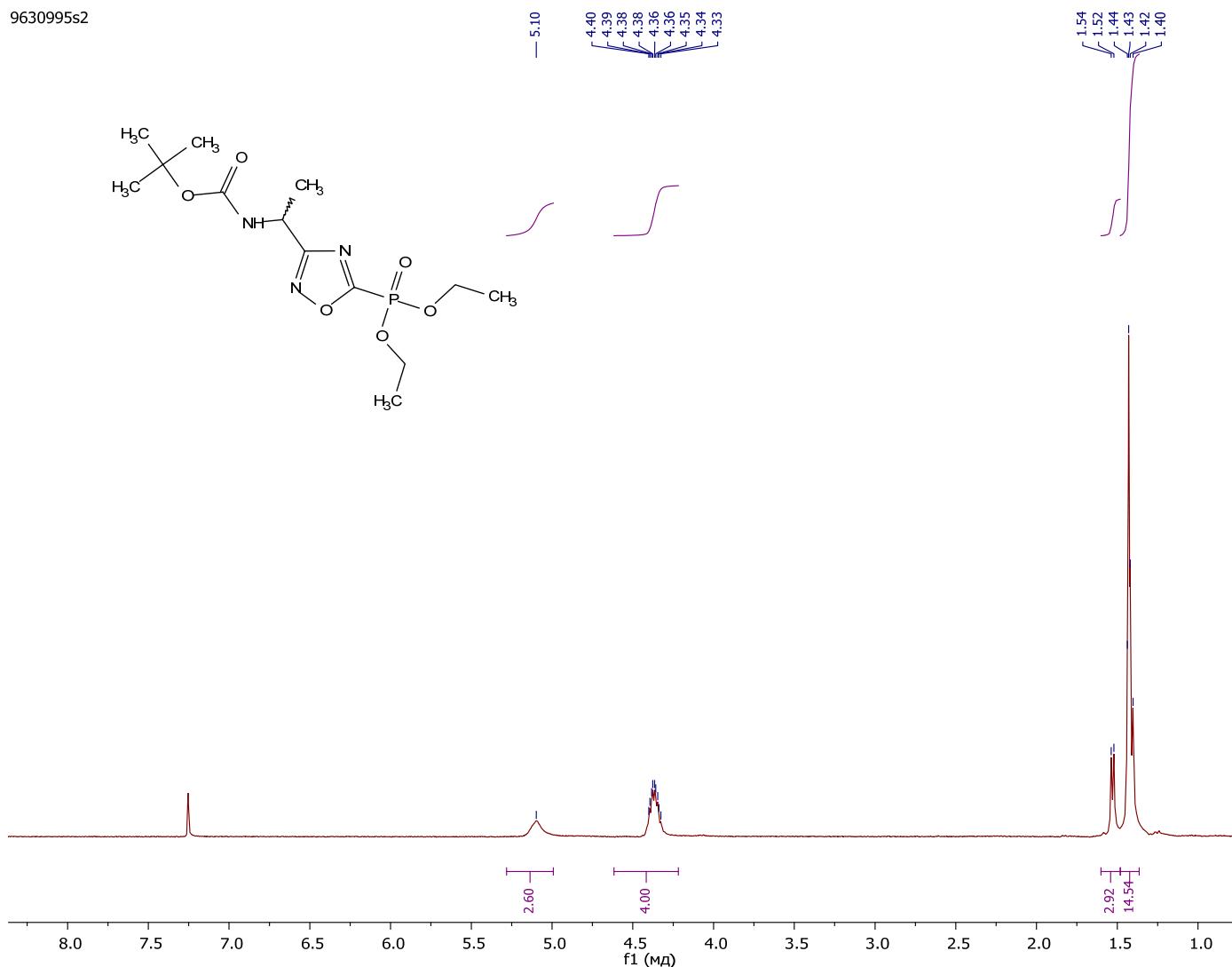


Figure 75 ³¹P NMR spectrum of 3a

9630995s2

Figure 76 ^1H NMR spectrum of 3b and 3c (R-isomer)

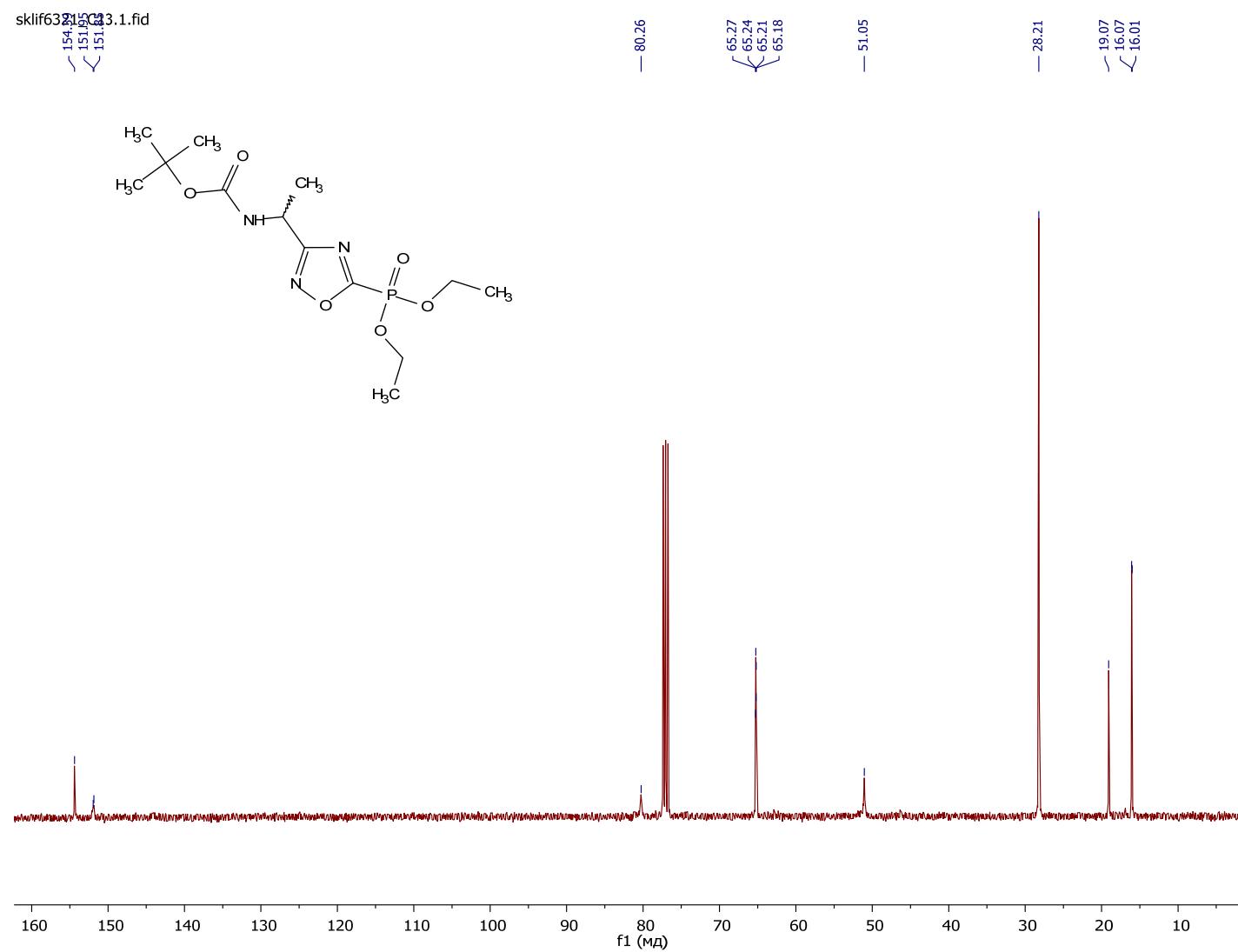


Figure 77 ^{13}C NMR spectrum of 3b and 3c (*R*-isomer)

sklf6321_P31.1.fid

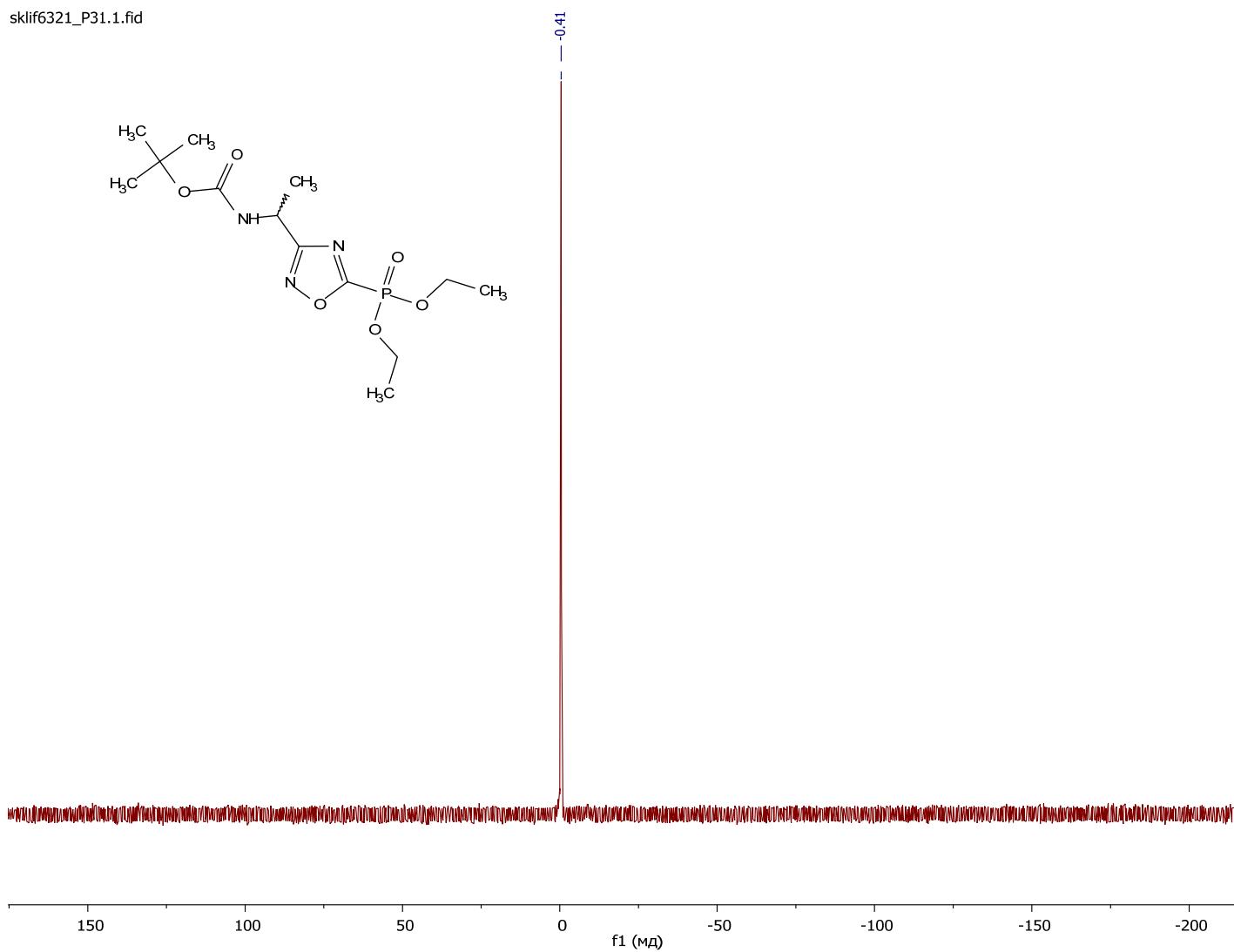
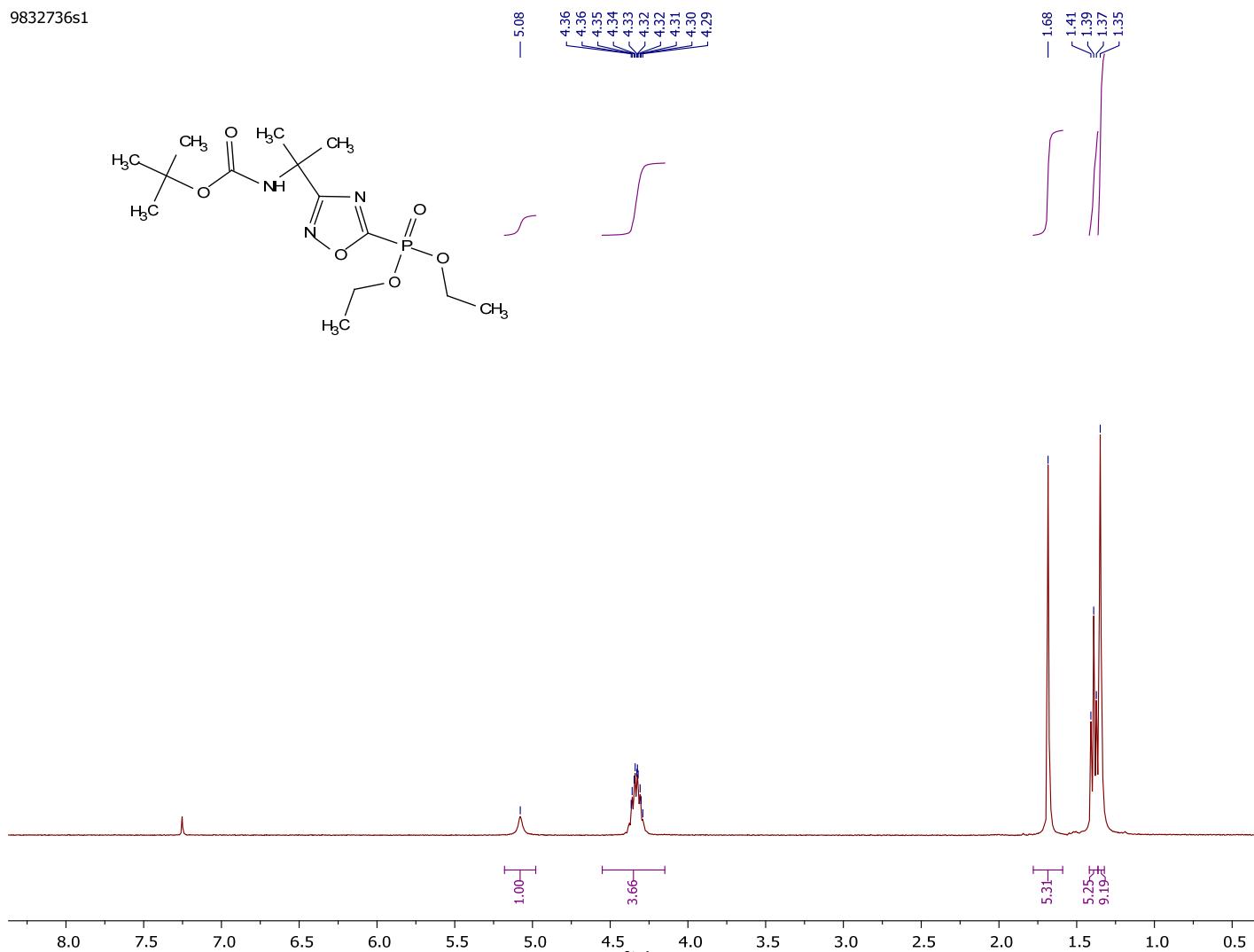


Figure 78 ^{31}P NMR spectrum of 3b and 3c (*R*-isomer)

9832736s1

Figure 79 ^1H NMR spectrum of 3d

sklf270_C13.1.fid

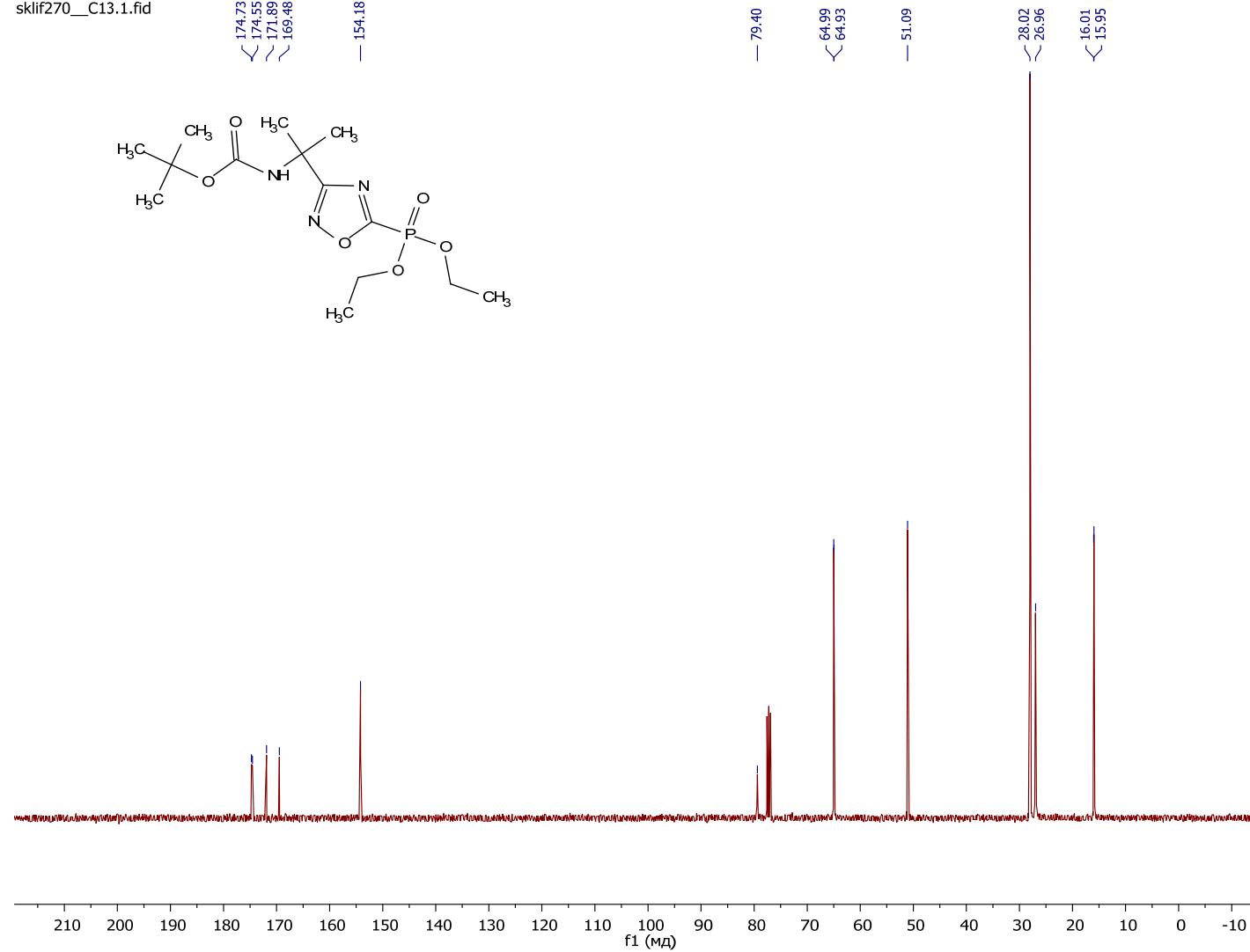
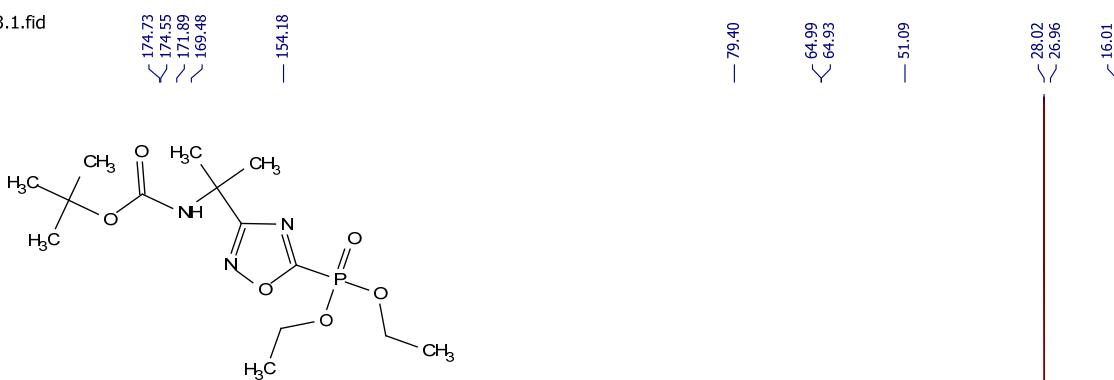


Figure 80 ^{13}C NMR spectrum of 3d

sklf270_P31{H}.1.fid

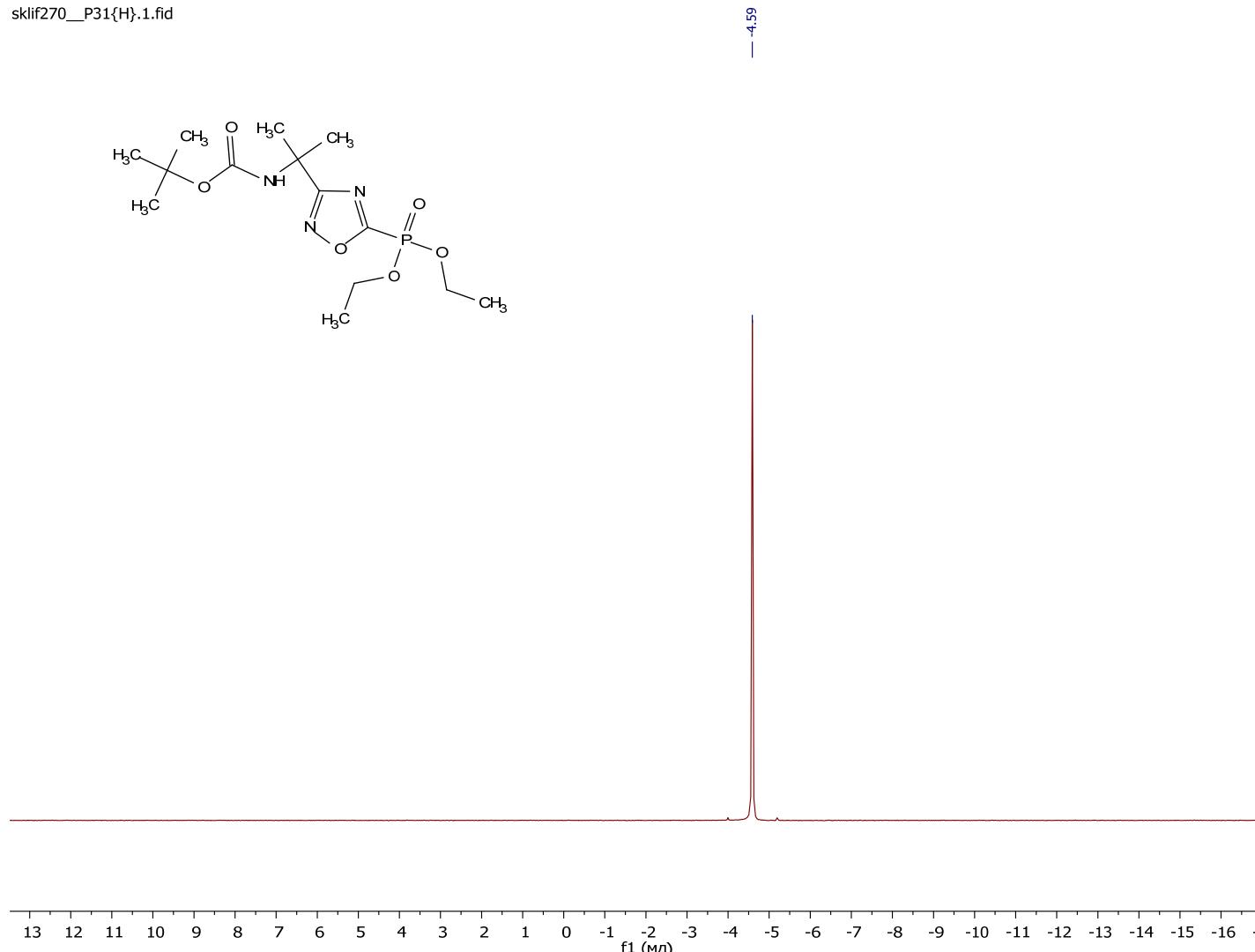
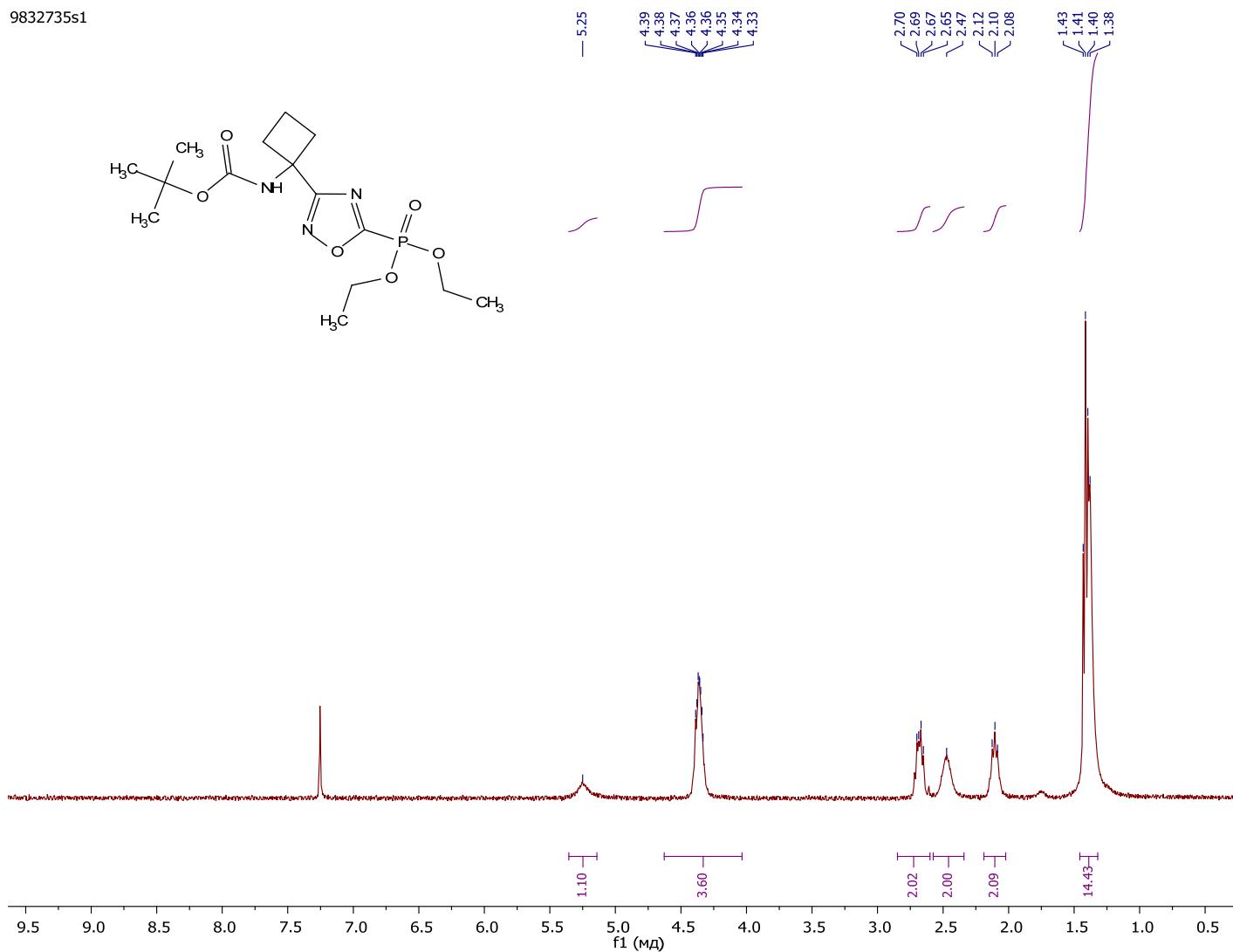


Figure 81 ³¹P NMR spectrum of 3d

9832735s1

Figure 82 ^1H NMR spectrum of 3e

sklf271_C13.1.fid

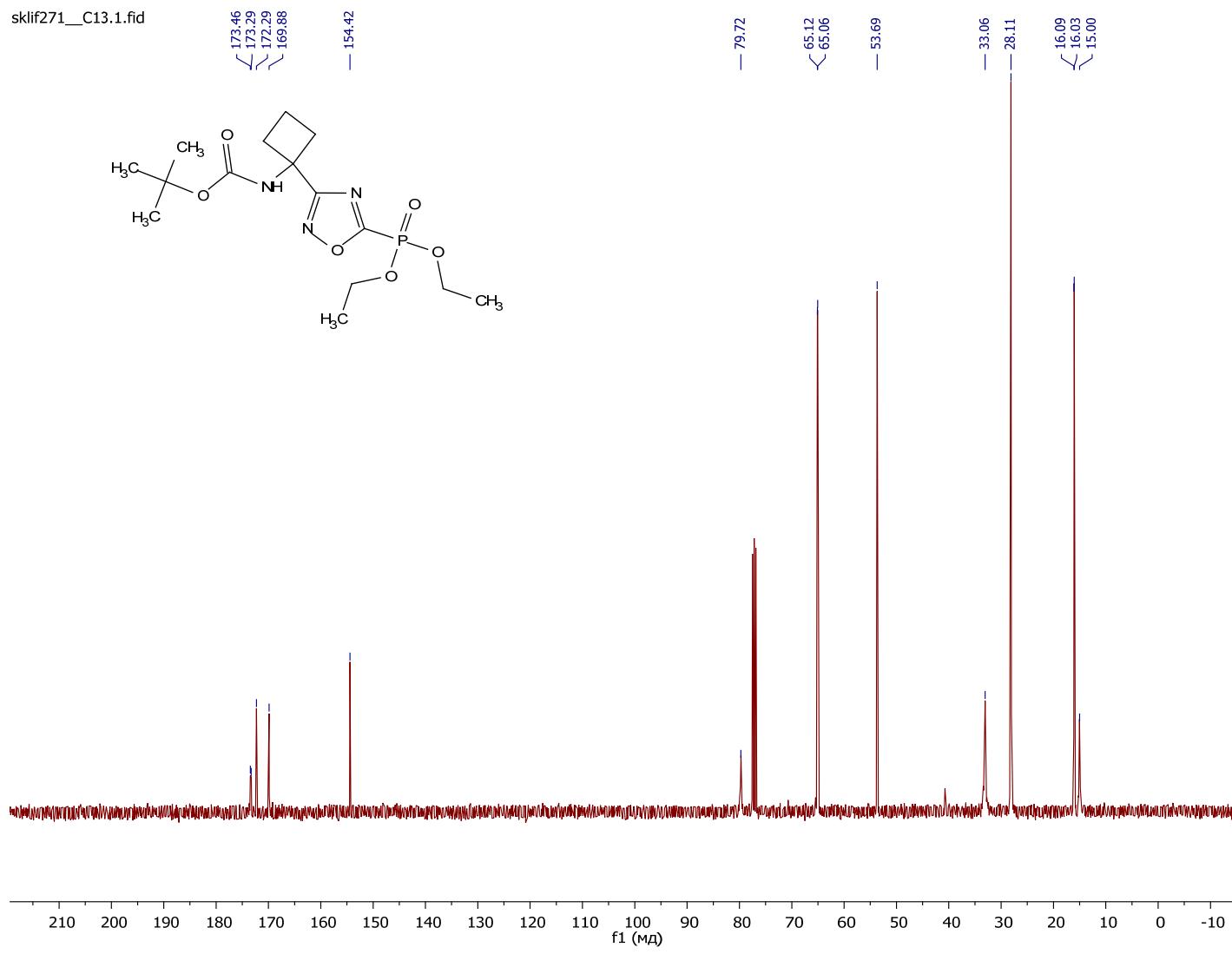


Figure 83 ^{13}C NMR spectrum of 3e

sklf271_P31{H}.1.fid

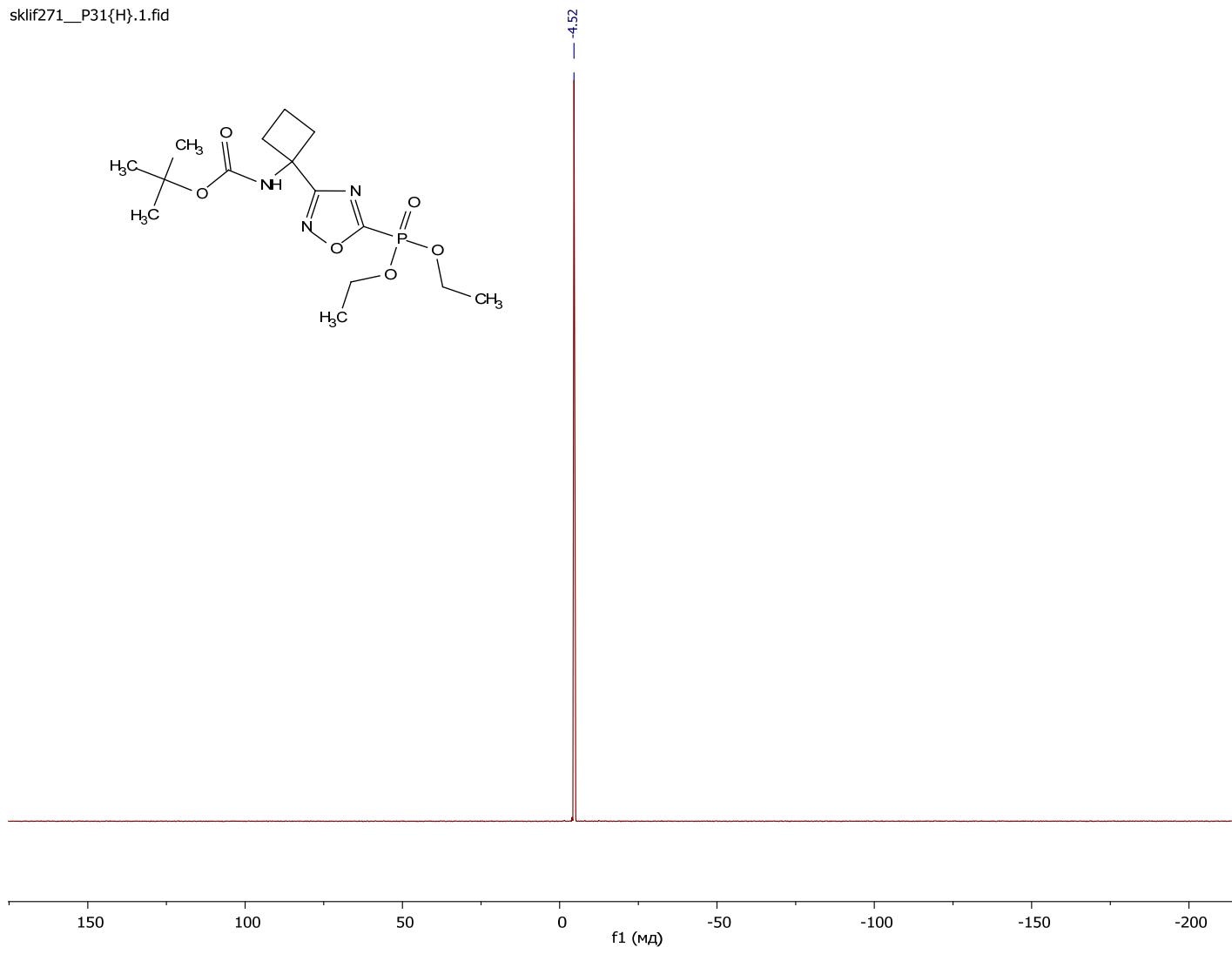
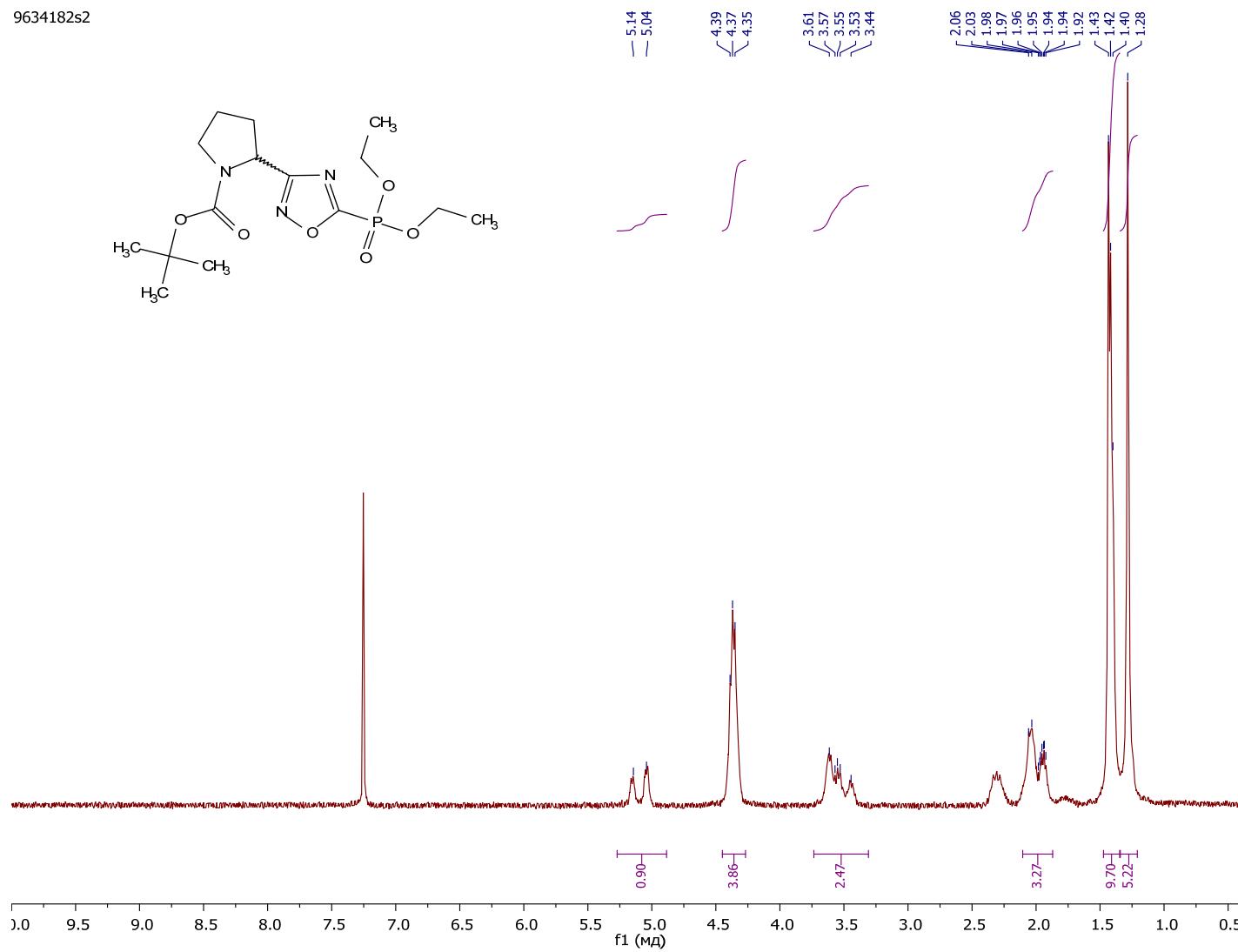


Figure 84 ^{31}P NMR spectrum of 3e

9634182s2

Figure 85 ^1H NMR spectrum of 3f and 3g (R-isomer)

sklif1774_C13.1.fid

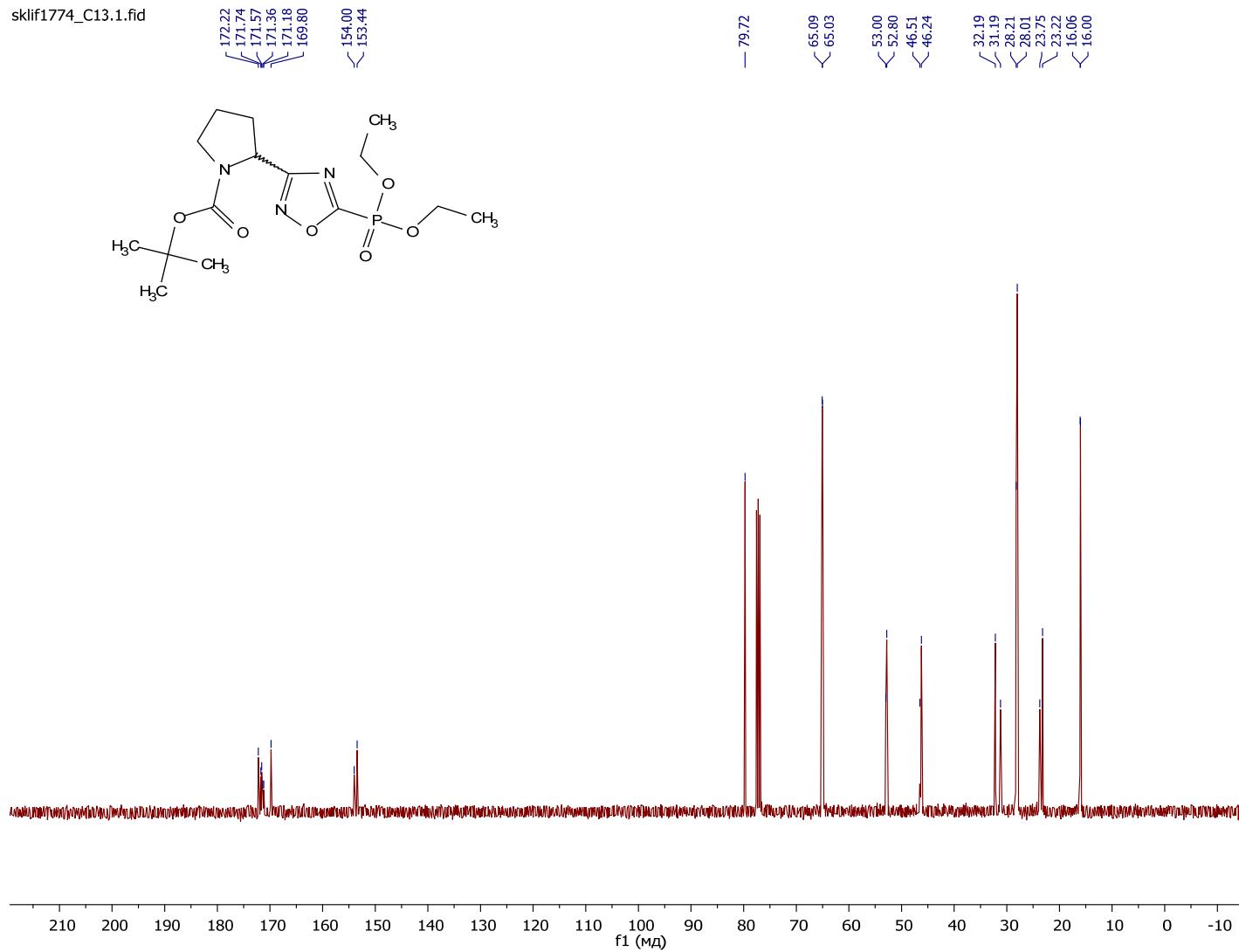


Figure 86. ^{13}C NMR spectrum of 3f and 3g (R-isomer)

sklif1774_P31.1.fid

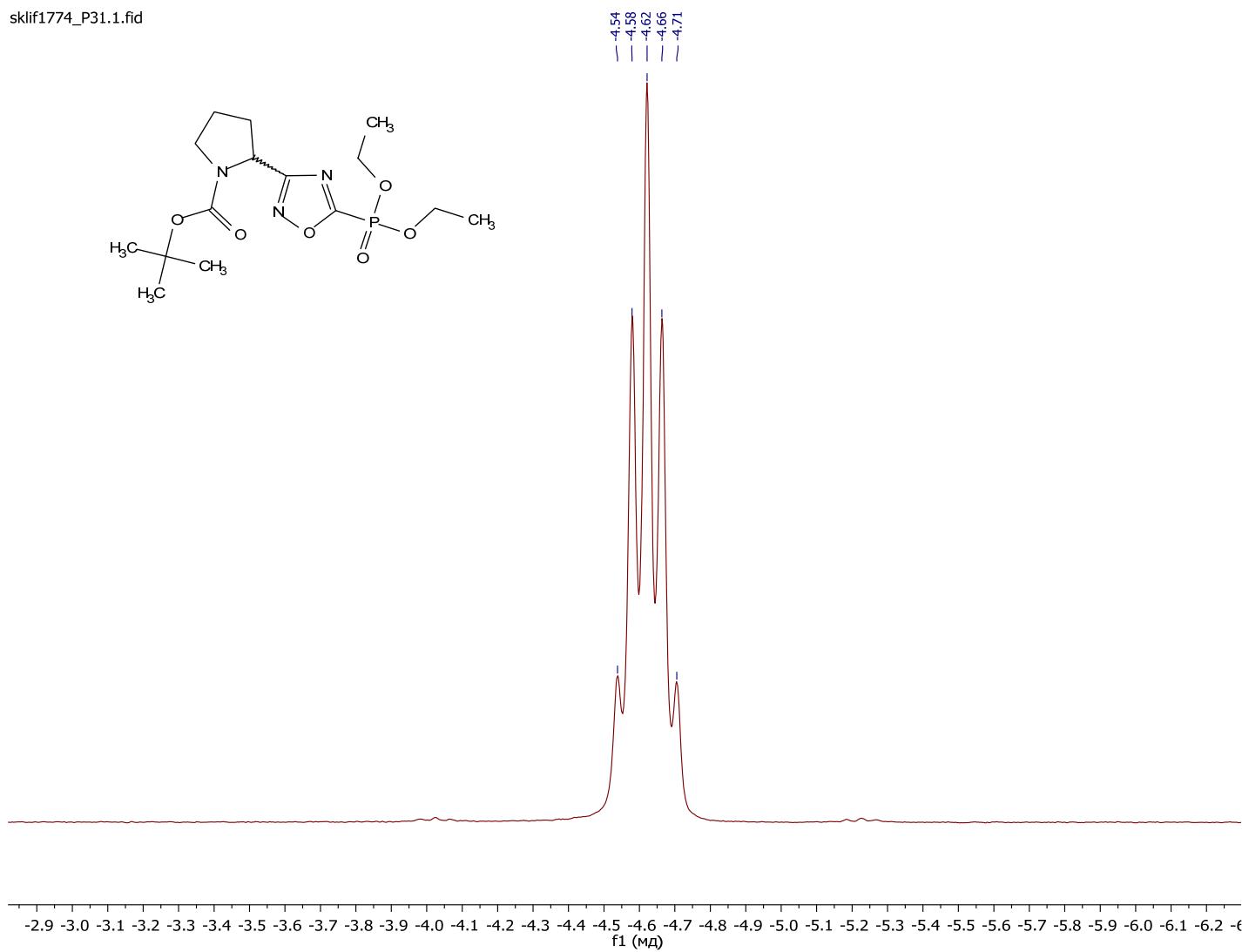
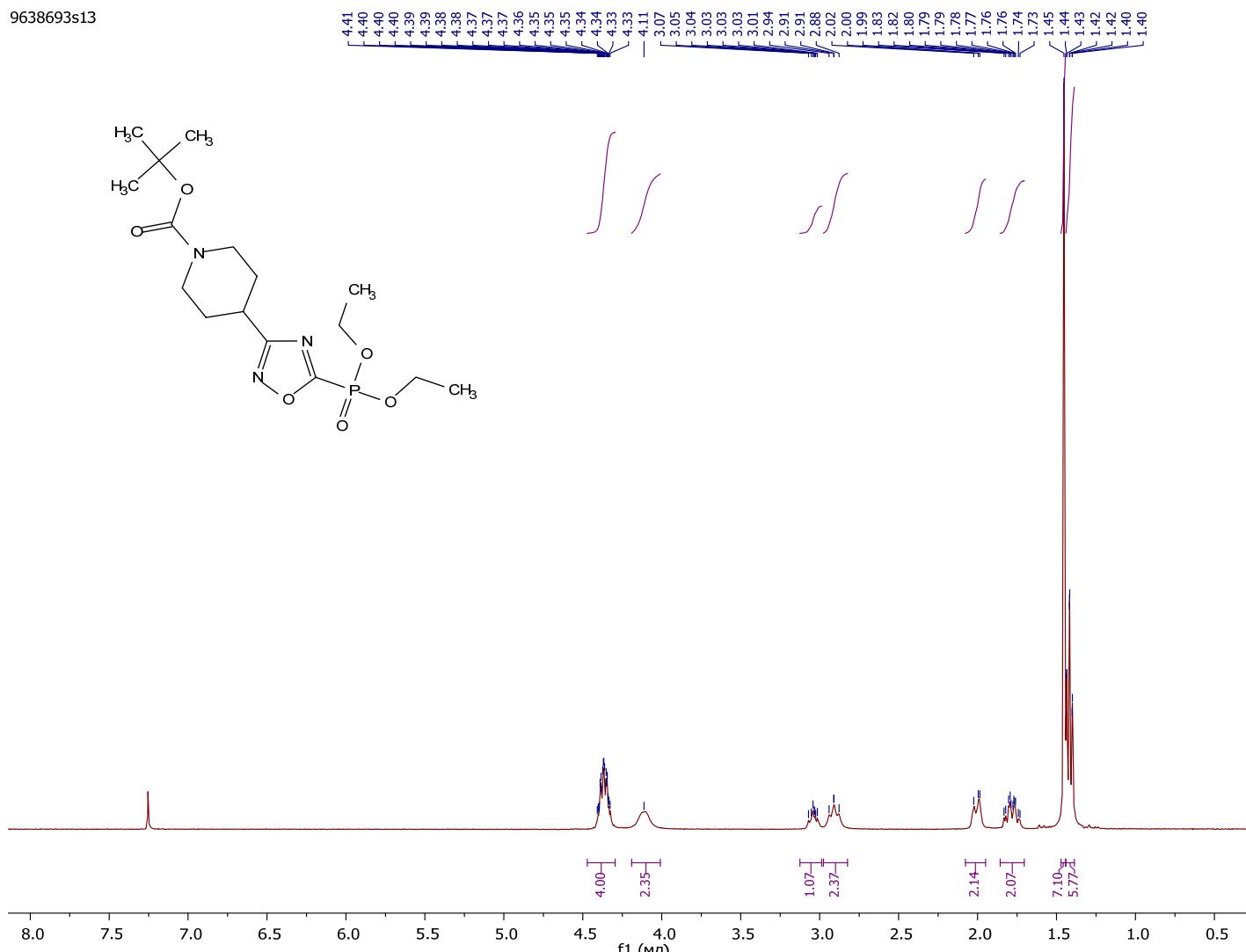


Figure 87. ^{31}P NMR spectrum of 3f and 3g (*R*-isomer)

9638693s13

Figure 88 ^1H NMR spectrum of 3h

sklf1964 13C.1.fid

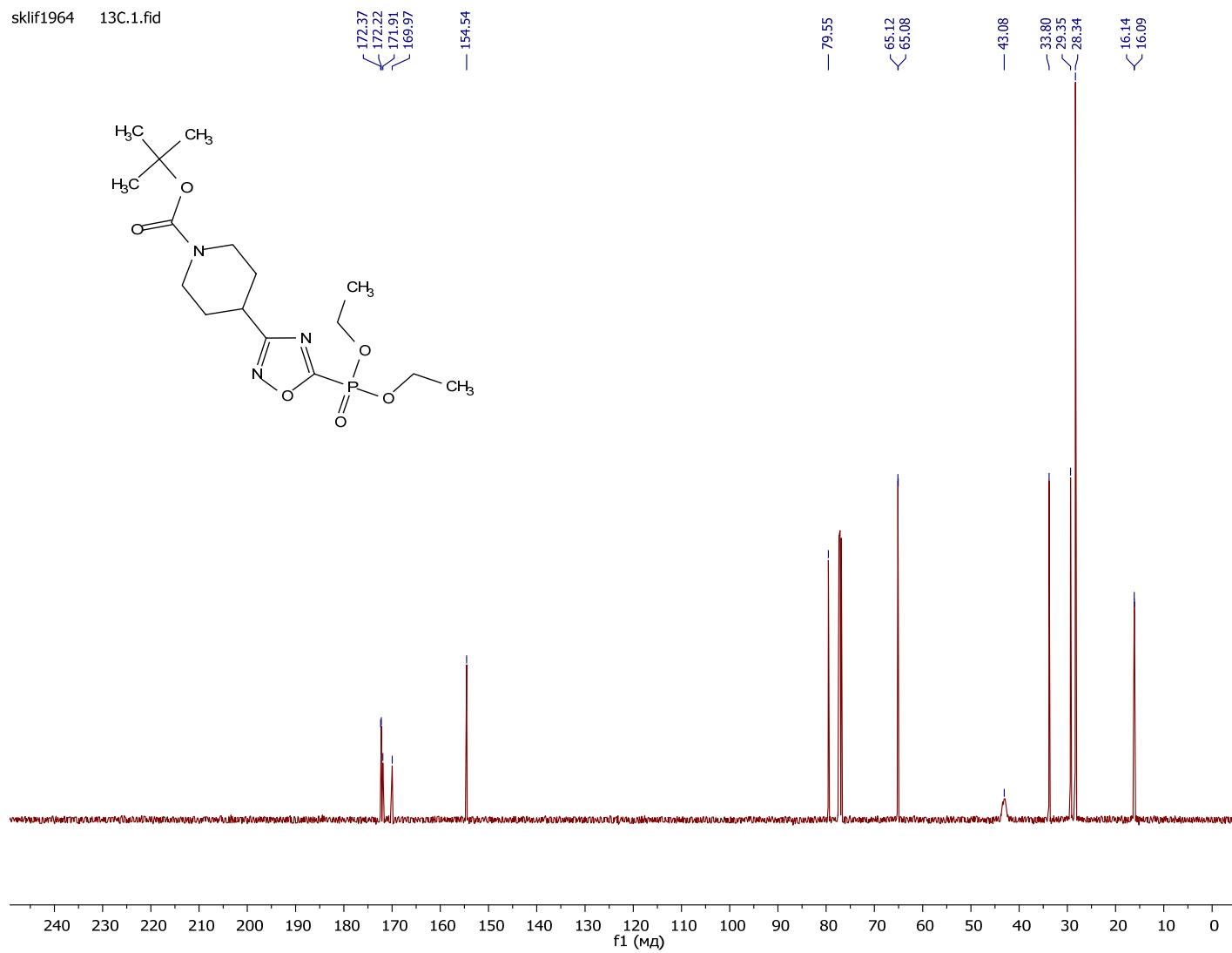


Figure 89 ^{13}C NMR spectrum of 3h

sklf1964_P31.1.fid

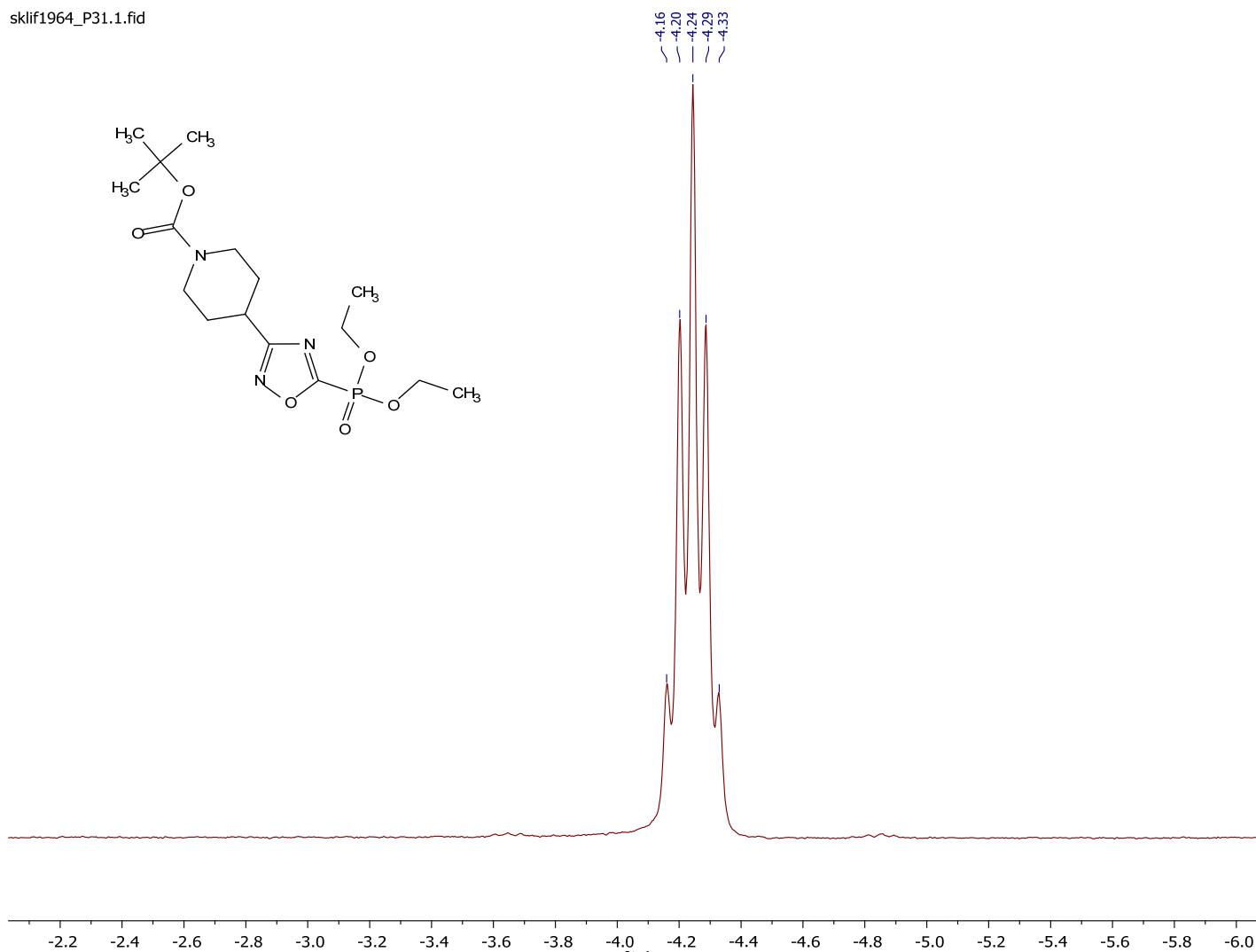


Figure 90 ^{31}P NMR spectrum of 3h

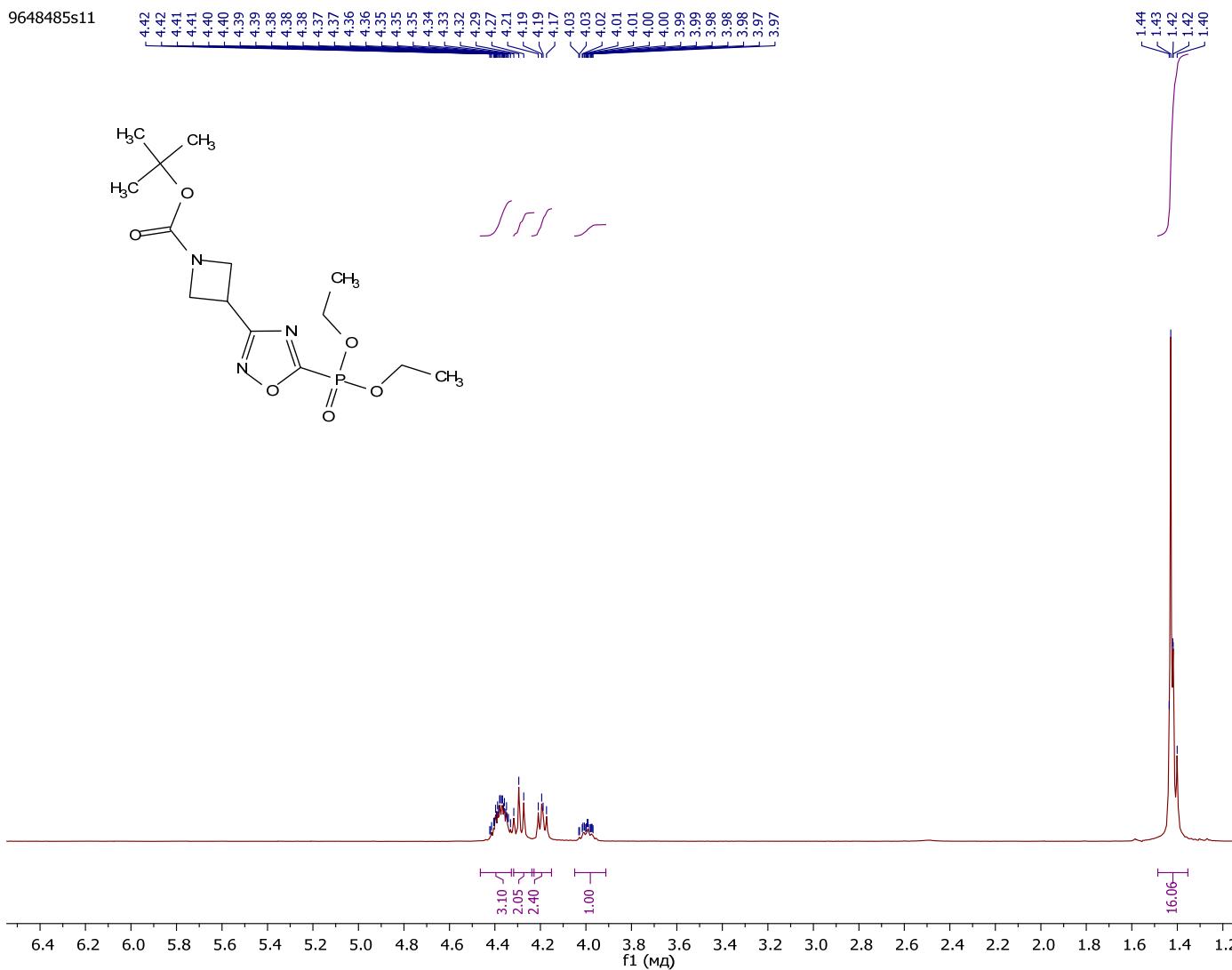


Figure 91 ^1H NMR spectrum of 3j

sklif1965 13C.1.fid

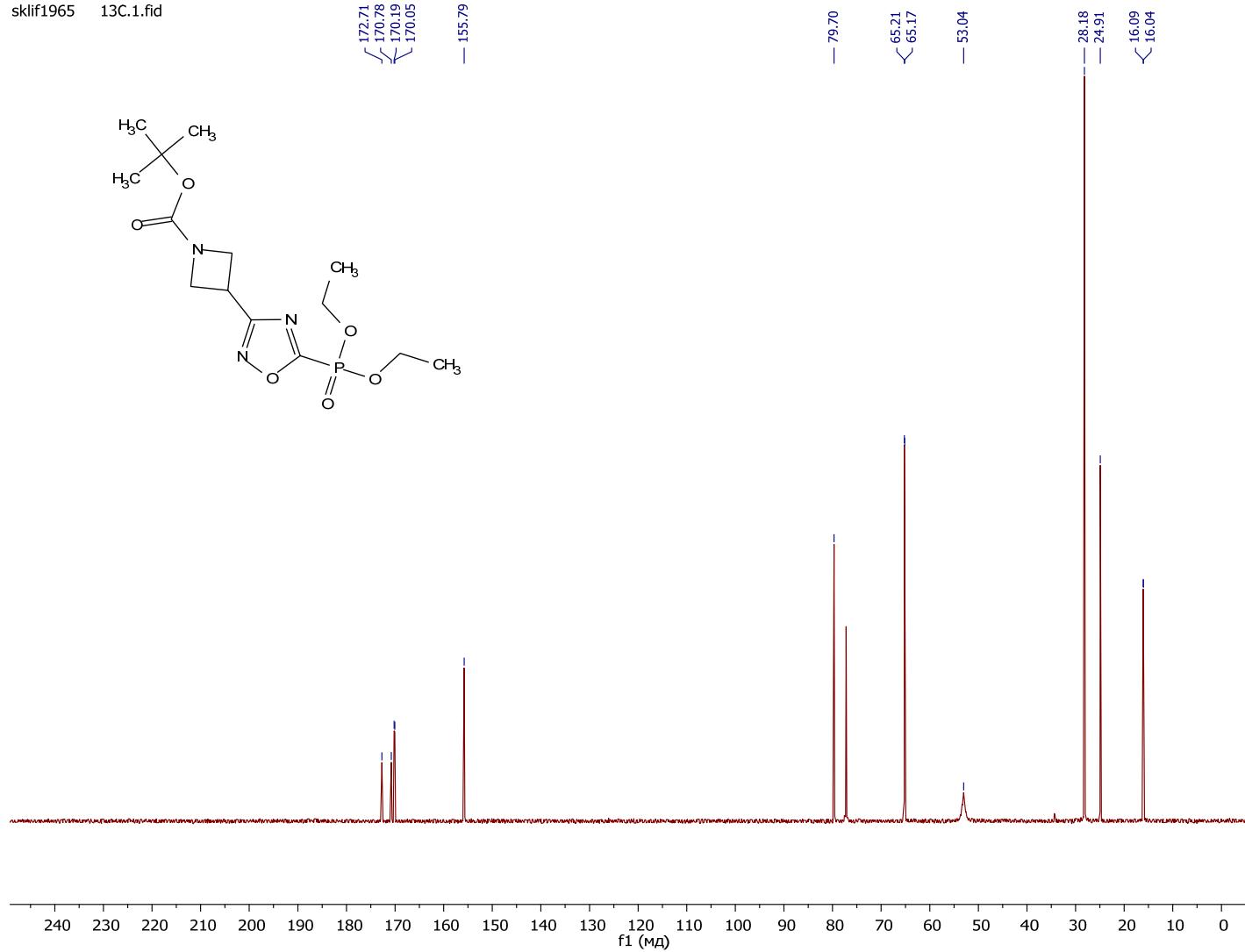


Figure 92 ^{13}C NMR spectrum of 3j

sklif1965_P31.1.fid

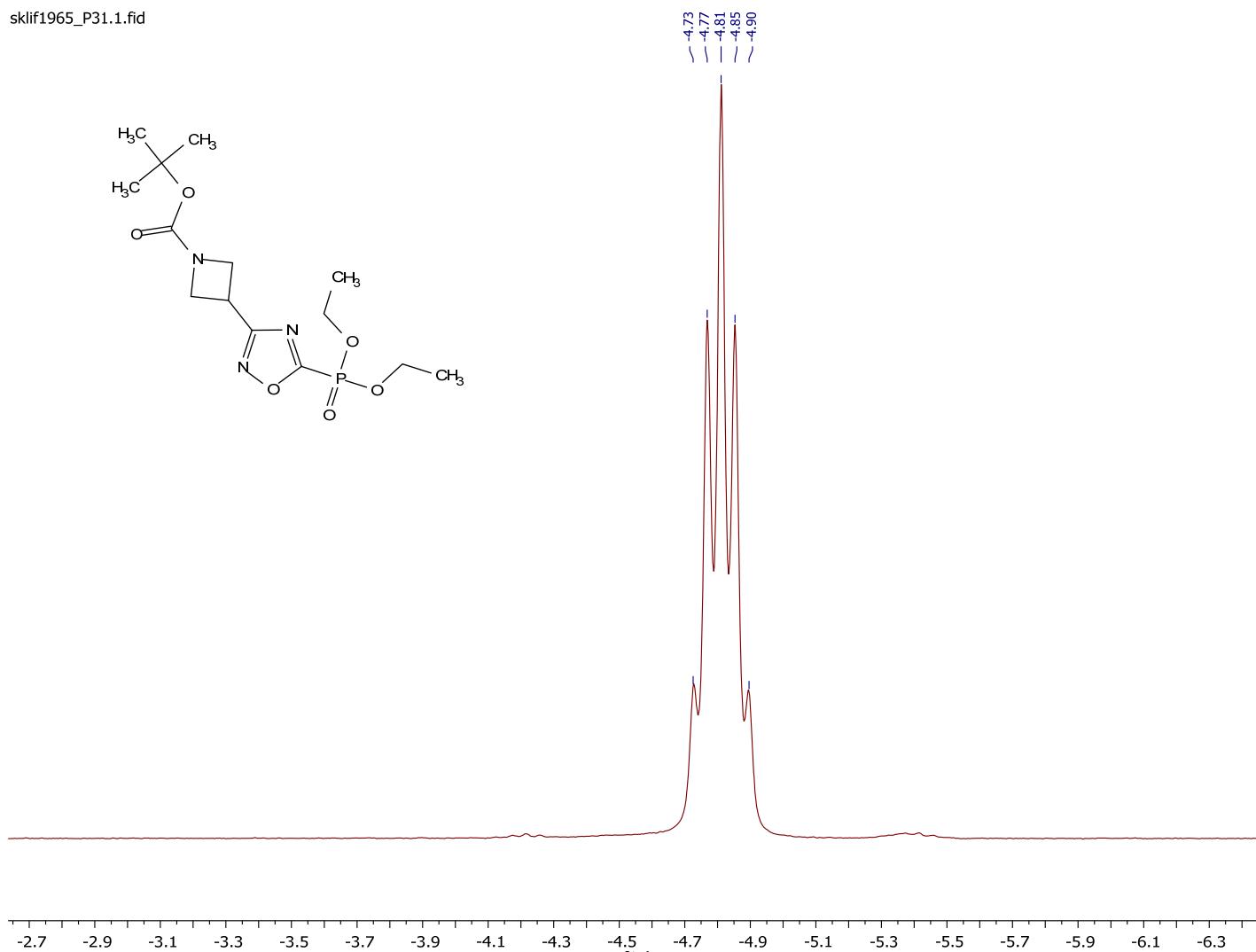
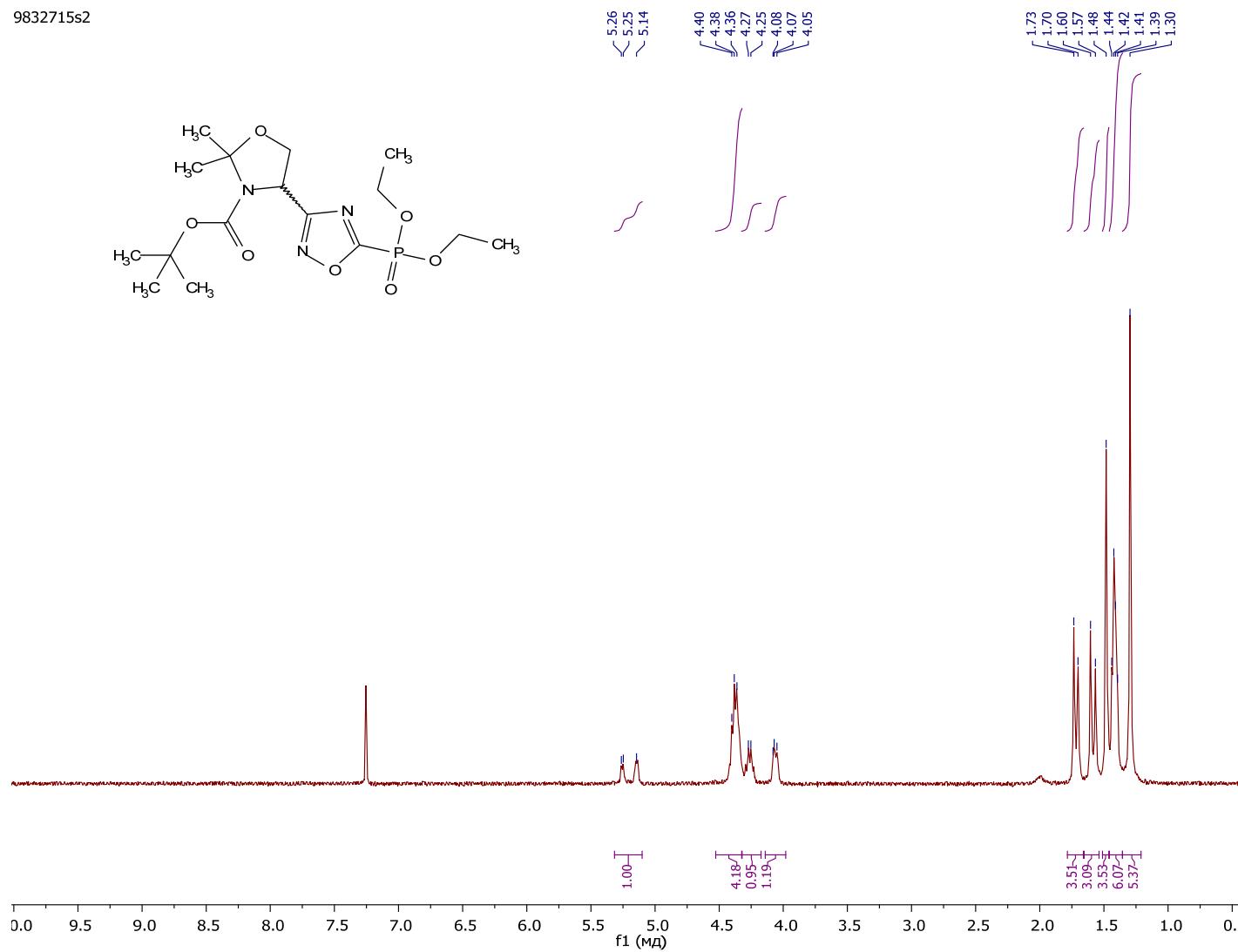


Figure 93 ^{31}P NMR spectrum of 3j

9832715s2

Figure 94 ^1H NMR spectrum of 3k and 3l (R-isomer)

sklf1966 13C.1.fid

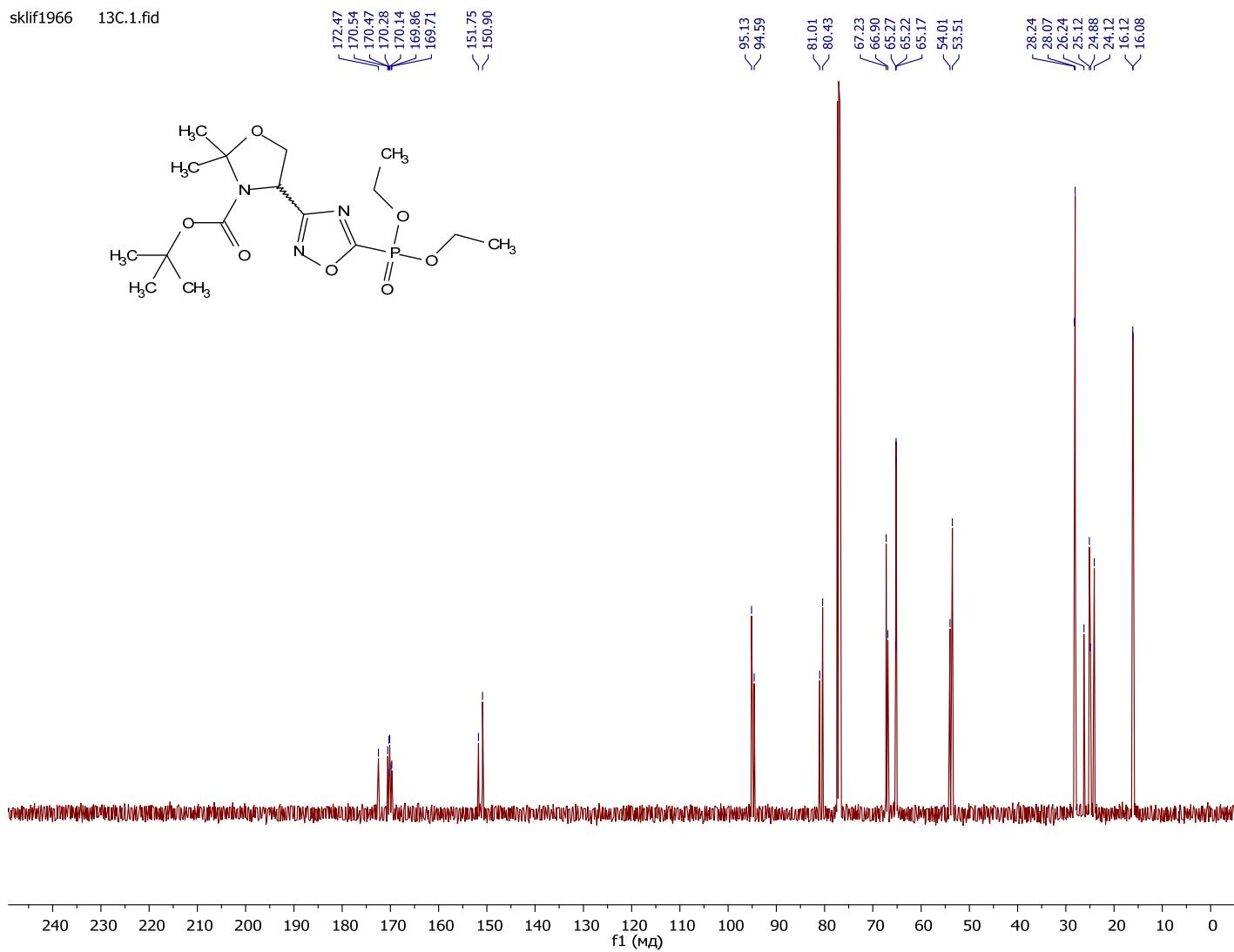


Figure 95 ^{13}C NMR spectrum of 3k and 3l (R-isomer)

sklif1966_P31.1.fid

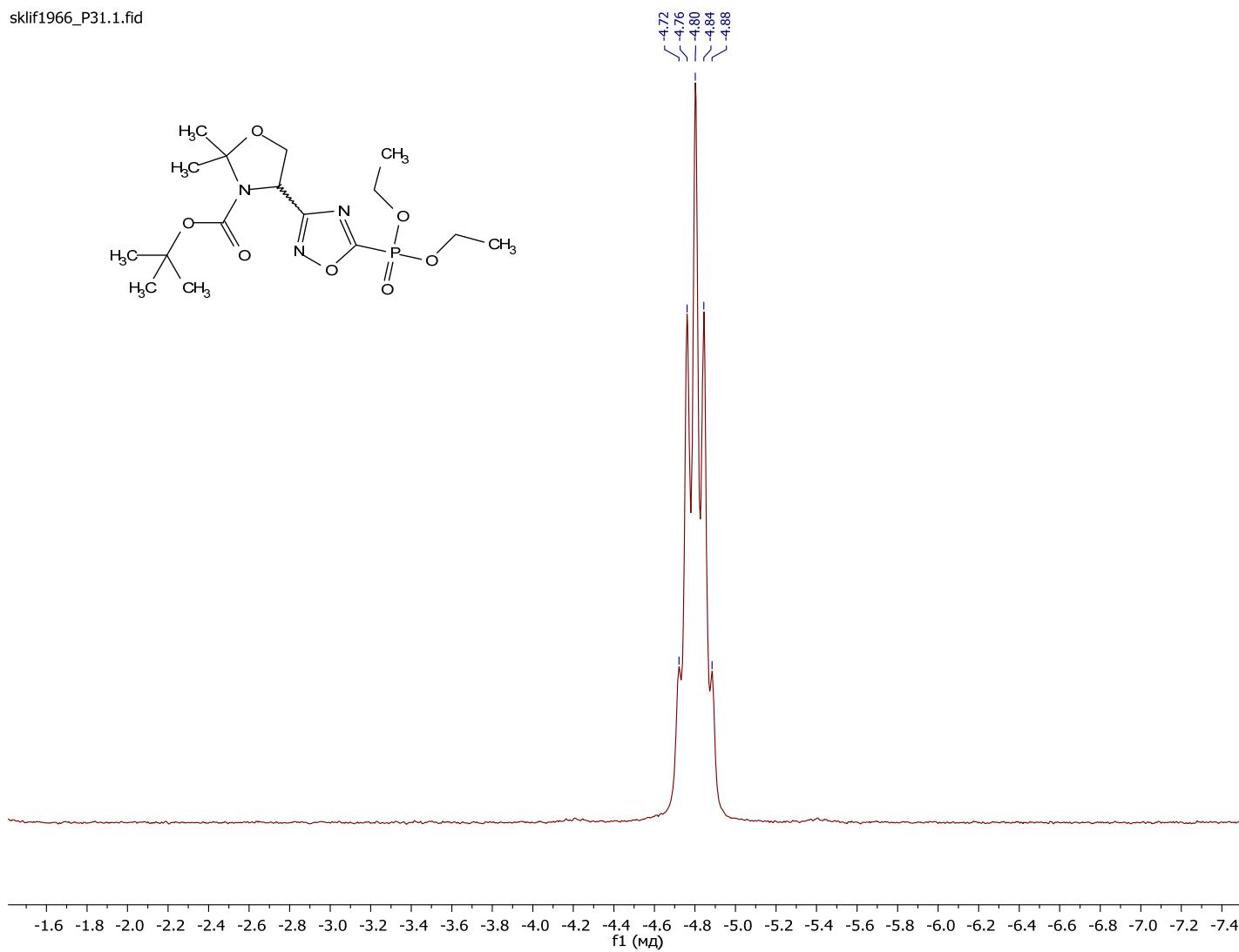


Figure 96 ^{31}P NMR spectrum of 3k and 3l (*R*-isomer)

sklf577.1.fid

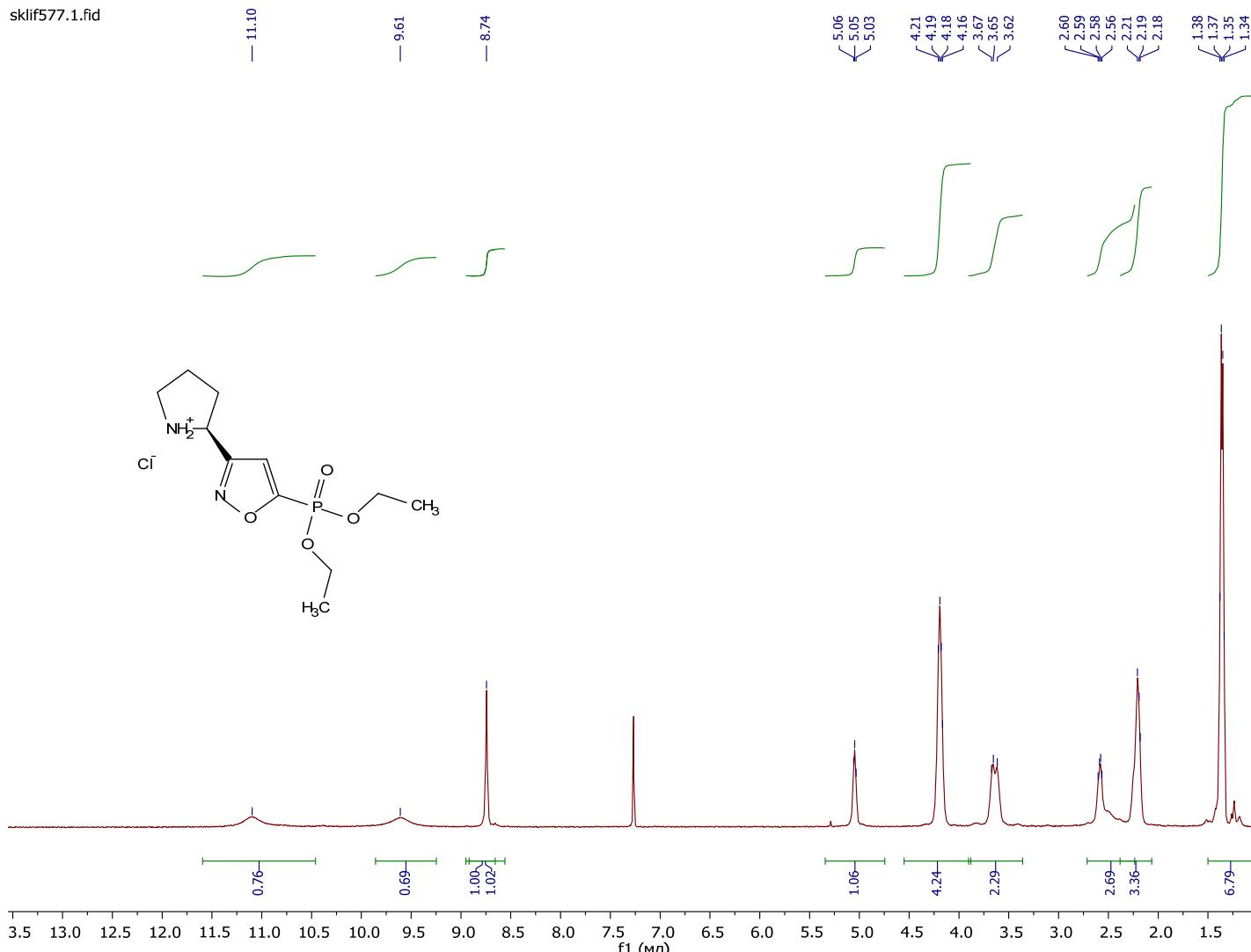


Figure 97 ^1H NMR spectrum of 19a·HCl and 19b·HCl (S-isomer)

sklf577_C13.1.fid

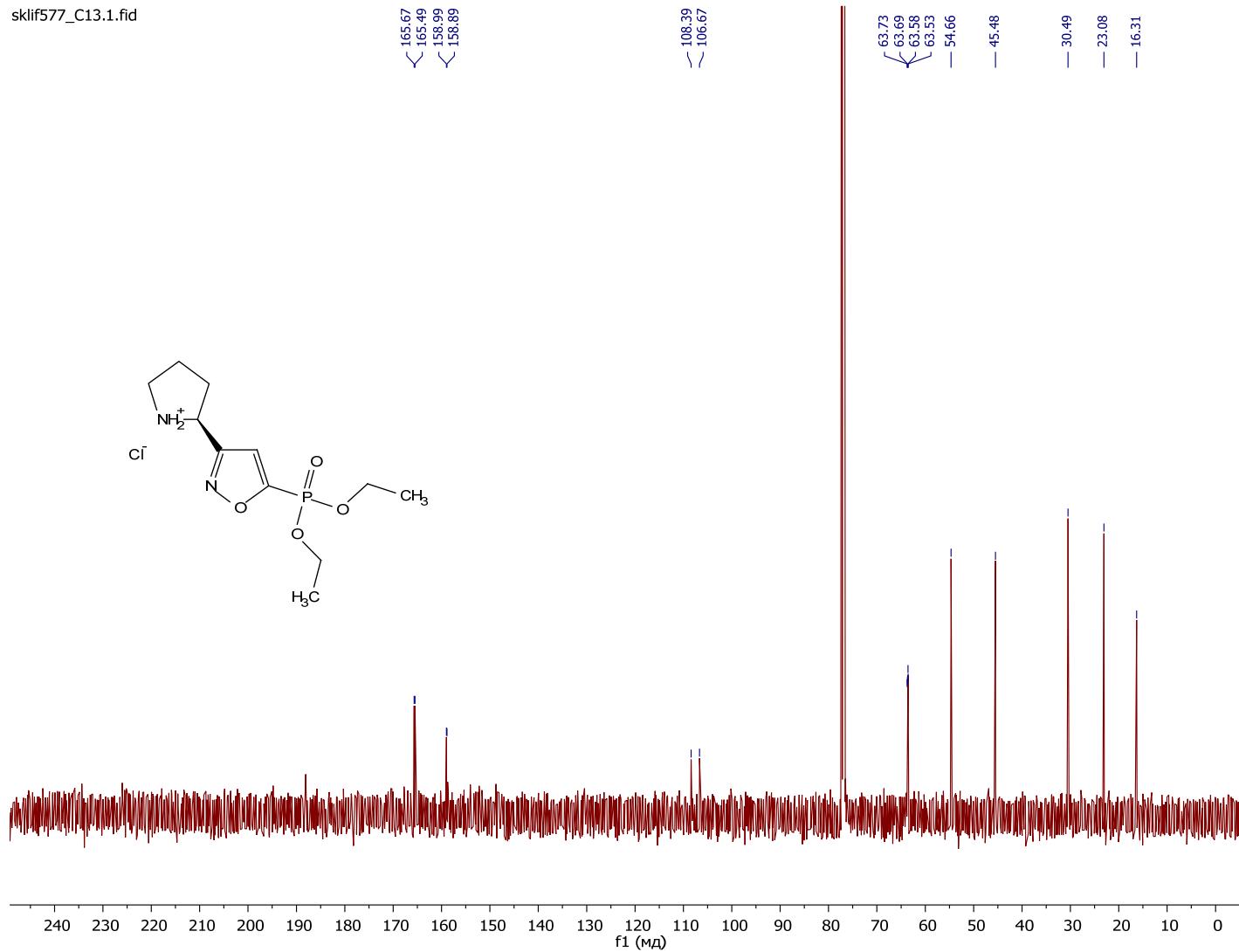


Figure 98 ^{13}C NMR spectrum of 19a·HCl and 19b·HCl (S-isomer)

sklif577_P31{H}.1.fid

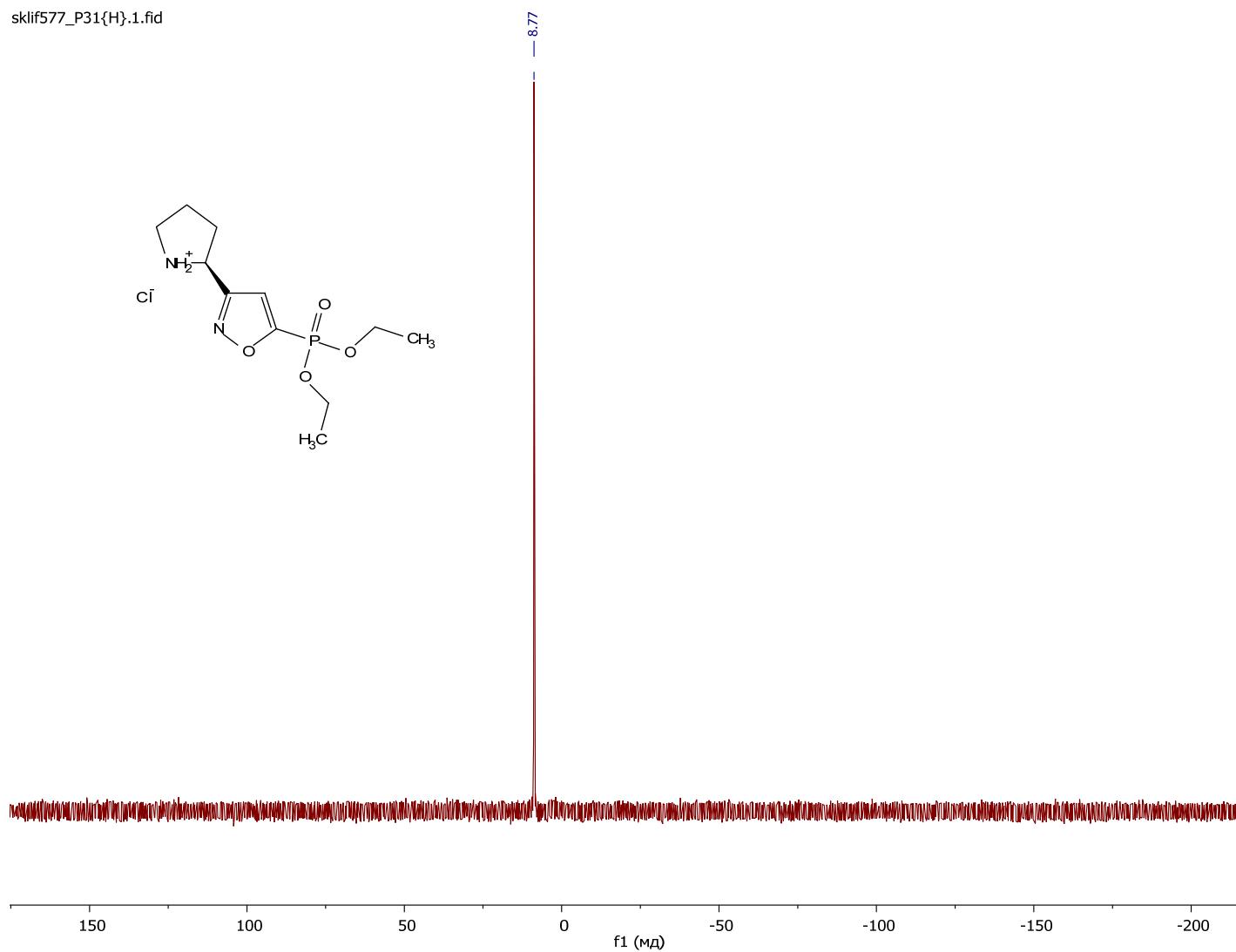


Figure 99 ^{31}P NMR spectrum of 19a·HCl and 19b·HCl (*S*-isomer)

sklf454.1.fid

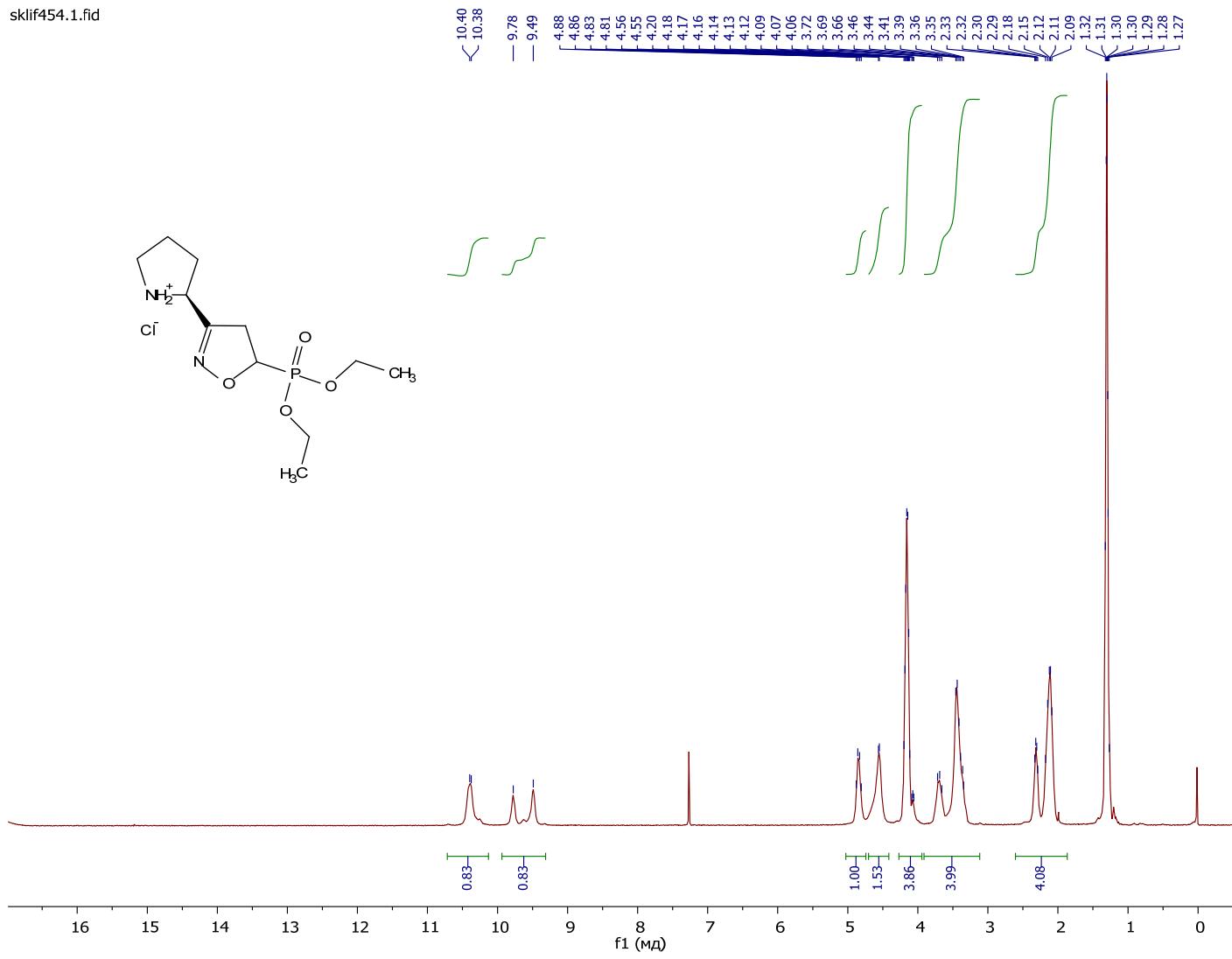


Figure 100 ^1H NMR spectrum of 19c·HCl and 19d·HCl (S-isomer)

sklf454 C13.1.fid

— 154.83

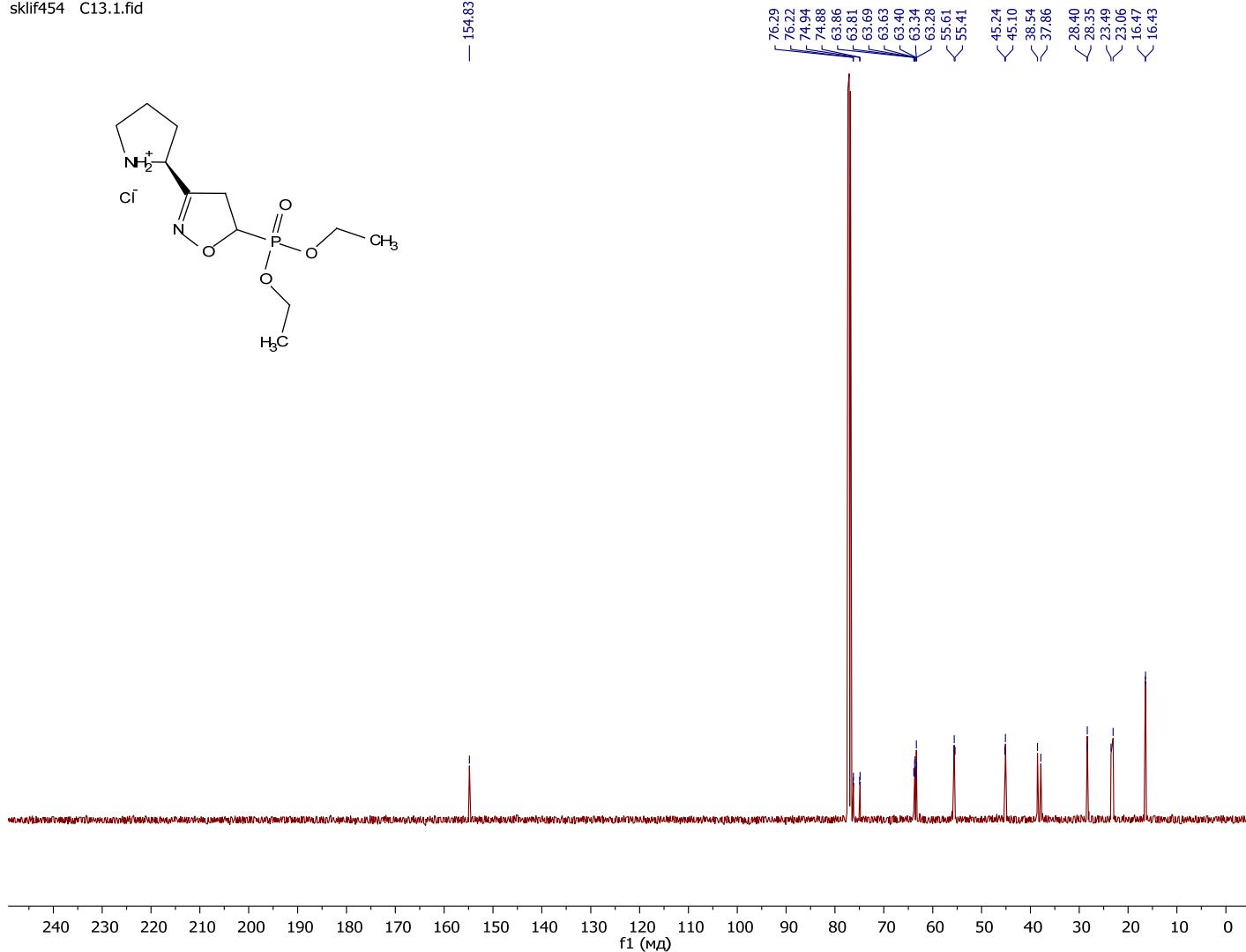
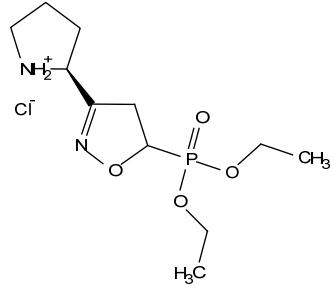


Figure 101 ^{13}C NMR spectrum of 19c·HCl and 19d·HCl (*S*-isomer)

Sklif454_P31.1.fid
31P-{1H}

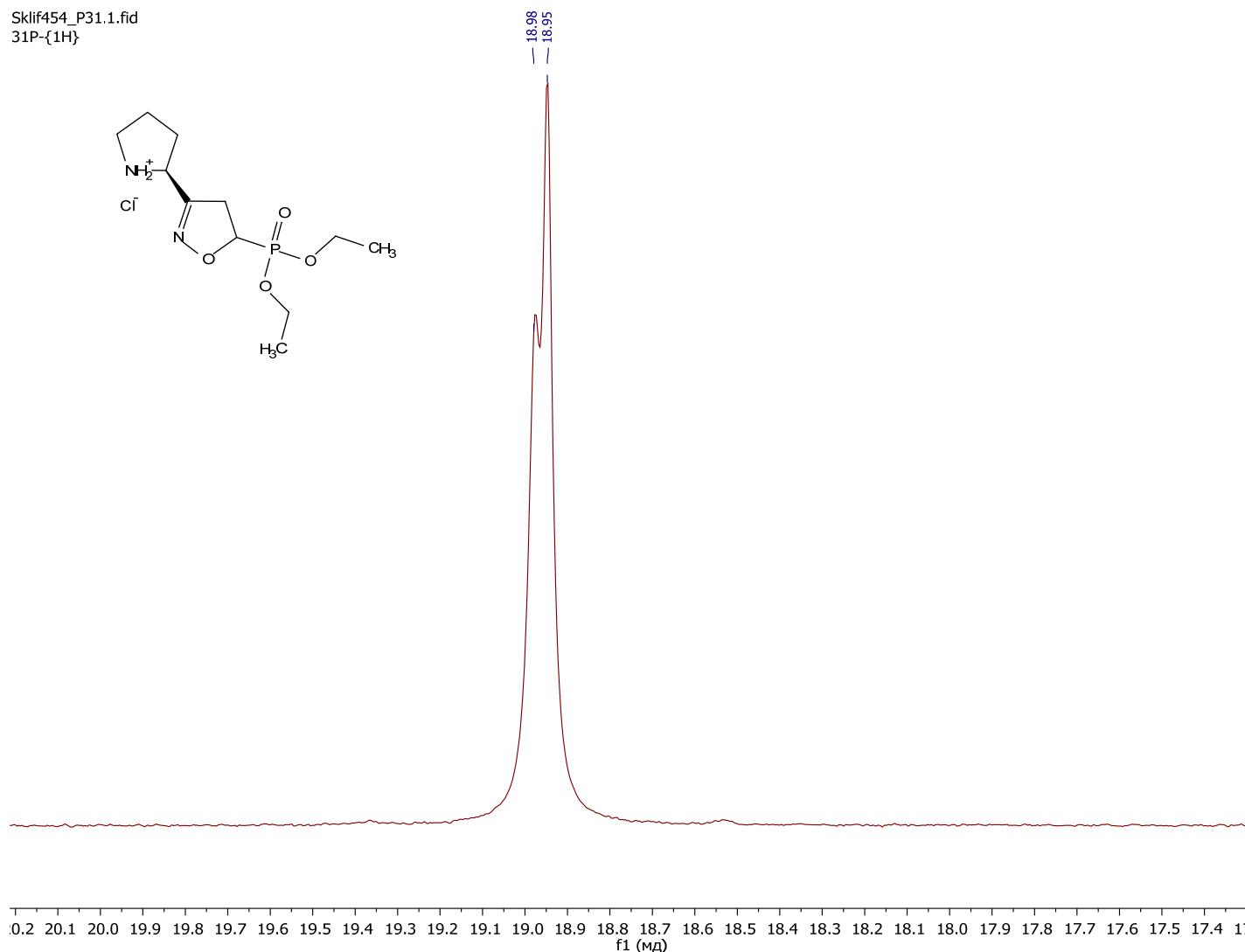


Figure 102 ^{31}P NMR spectrum of 19c·HCl and 19d·HCl (*S*-isomer)

Sklif809.1.fid

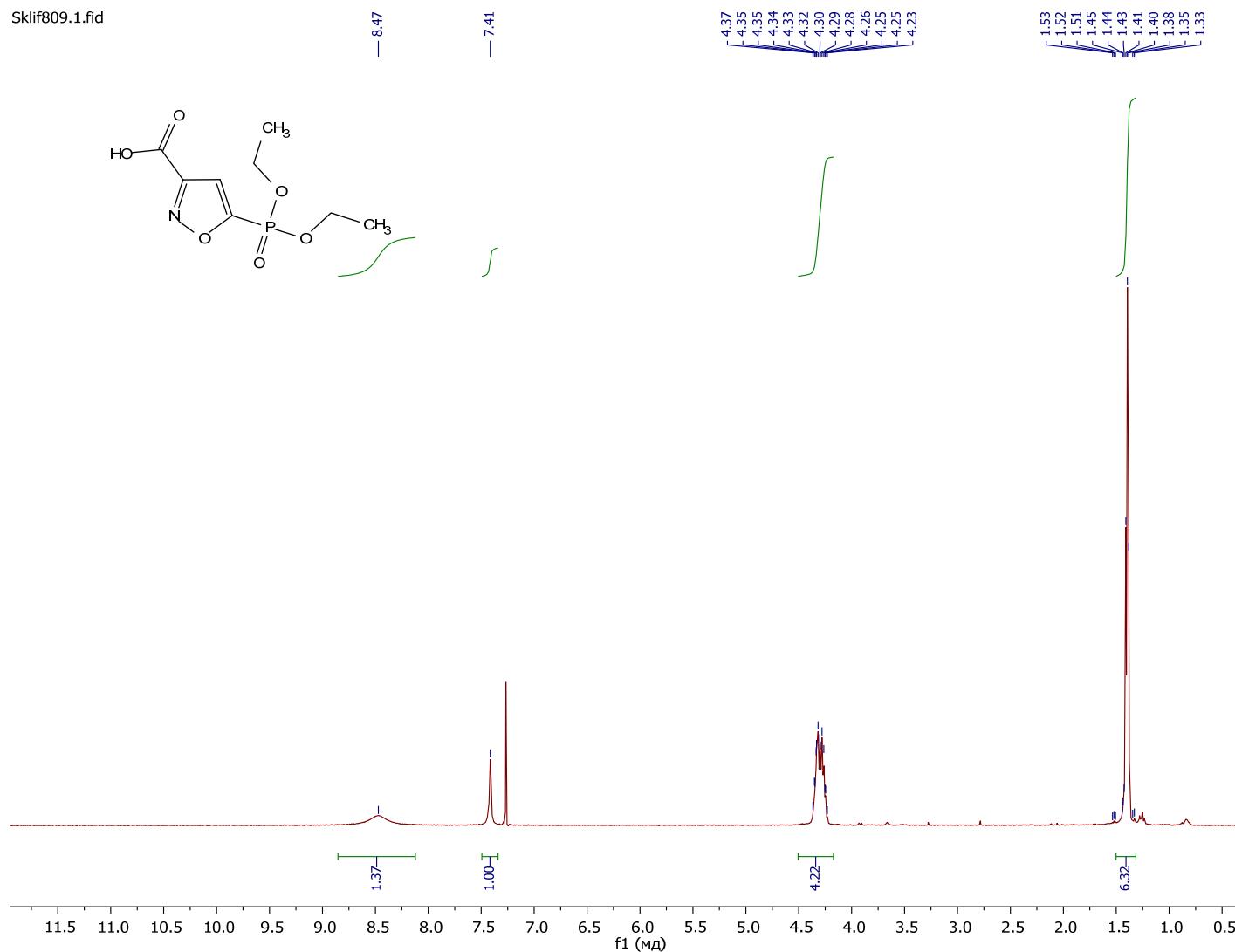


Figure 103 ^1H NMR spectrum of 20

Sklif809_C13.1.fid

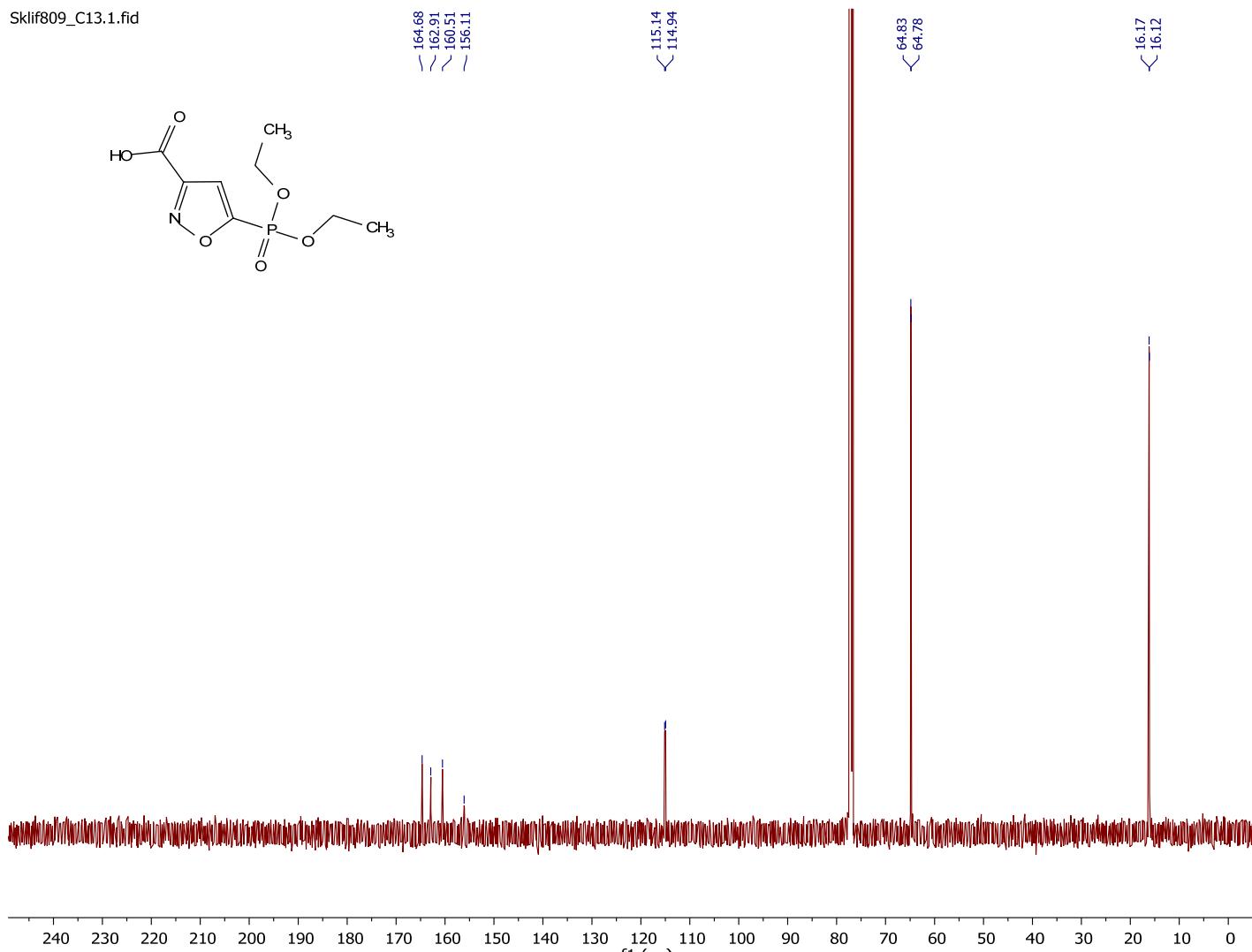


Figure 104 ^{13}C NMR spectrum of 20

Sklif809_P31.1.fid
31P-{1H}

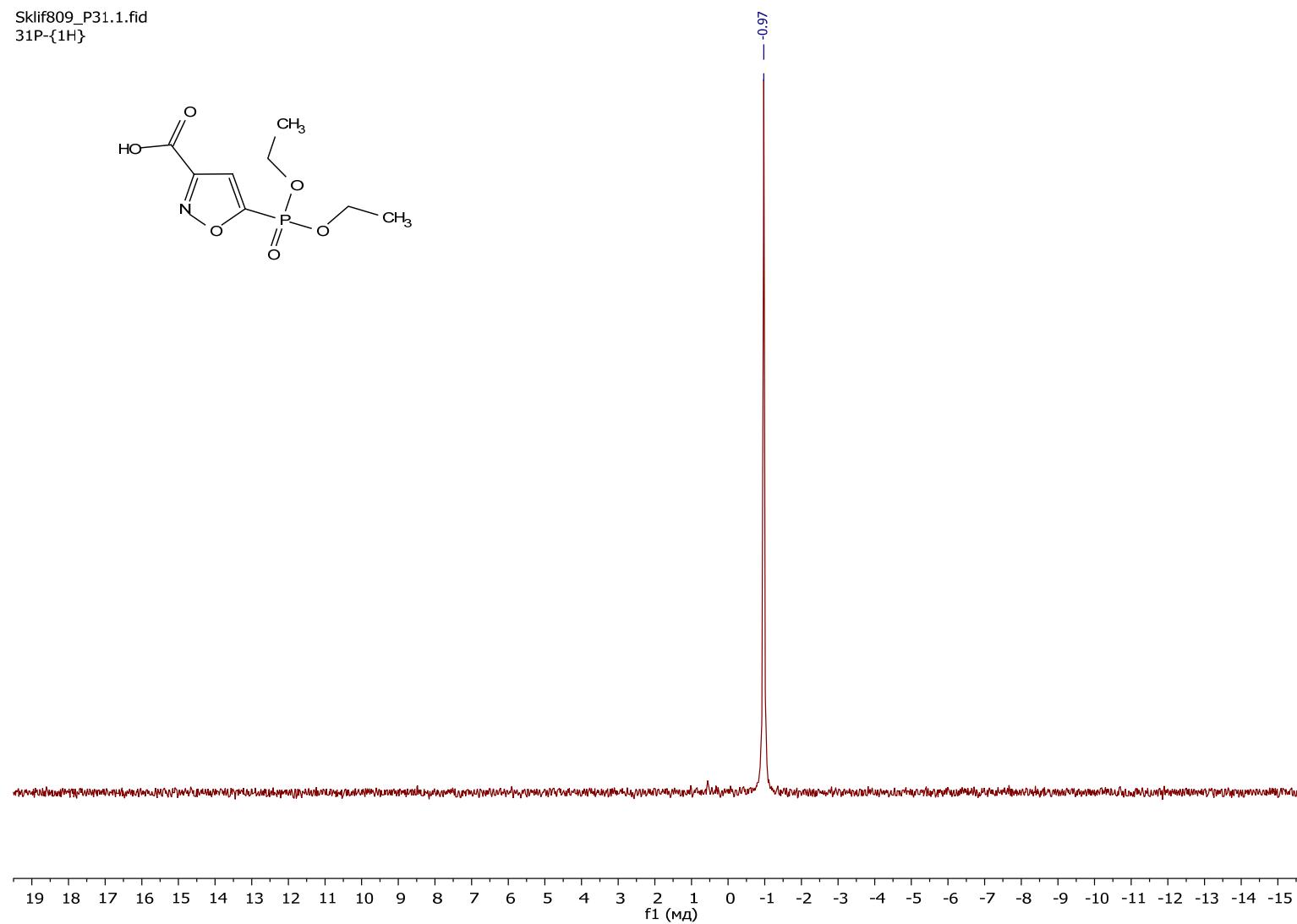


Figure 105 ^{31}P NMR spectrum of 20

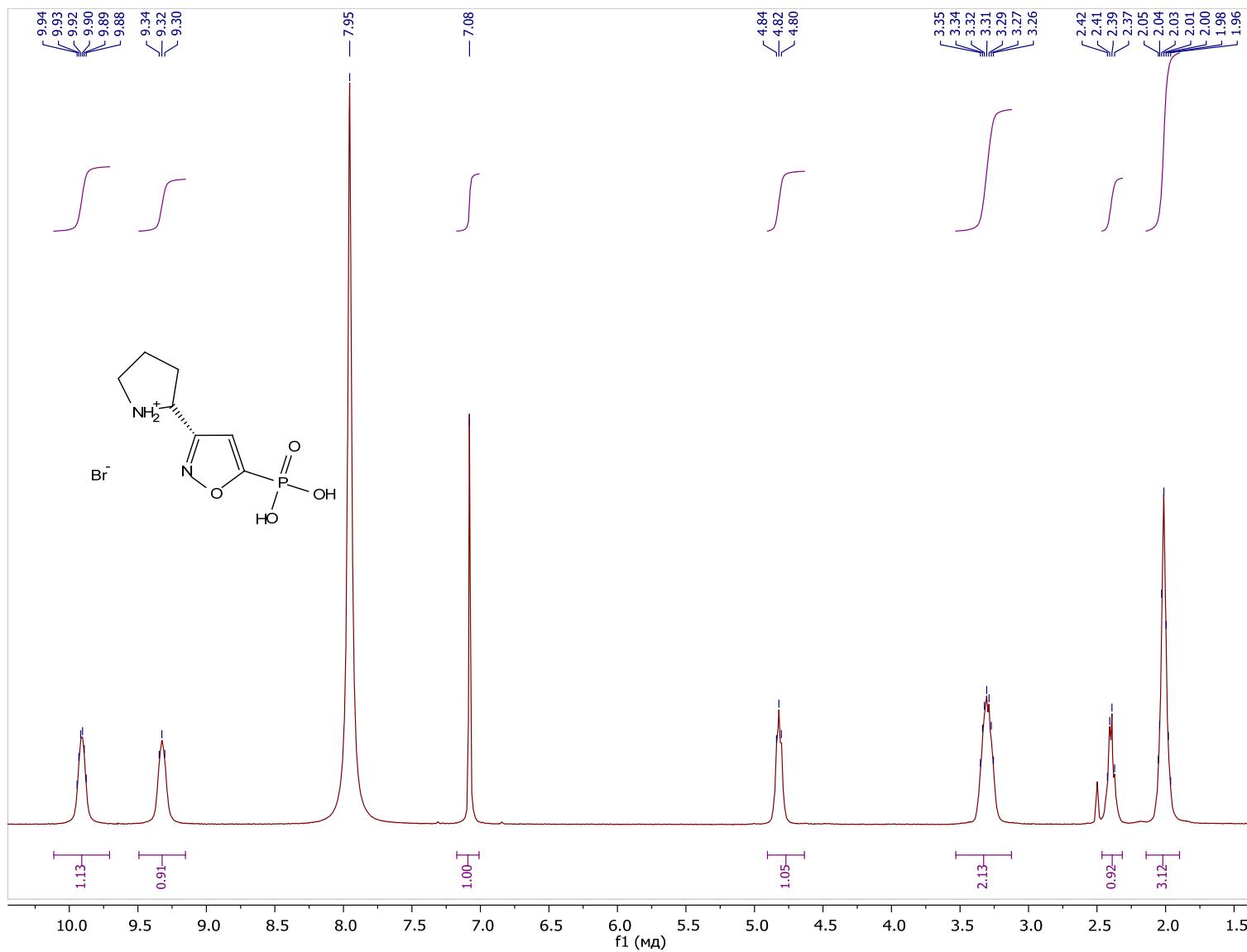


Figure 106. ^1H NMR spectrum of 21a and 21b

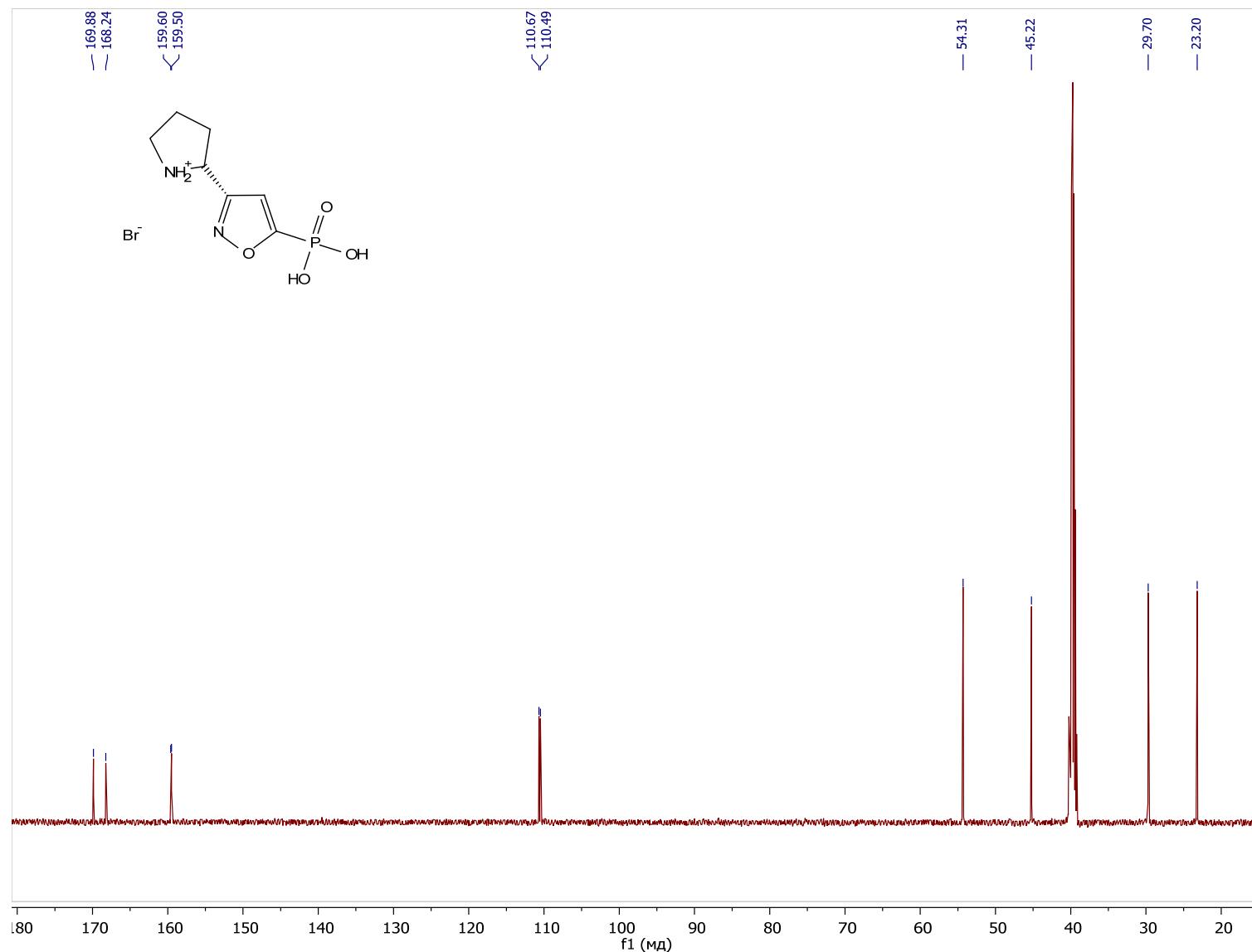


Figure 107. ^{13}C NMR spectrum of 21a and 21b

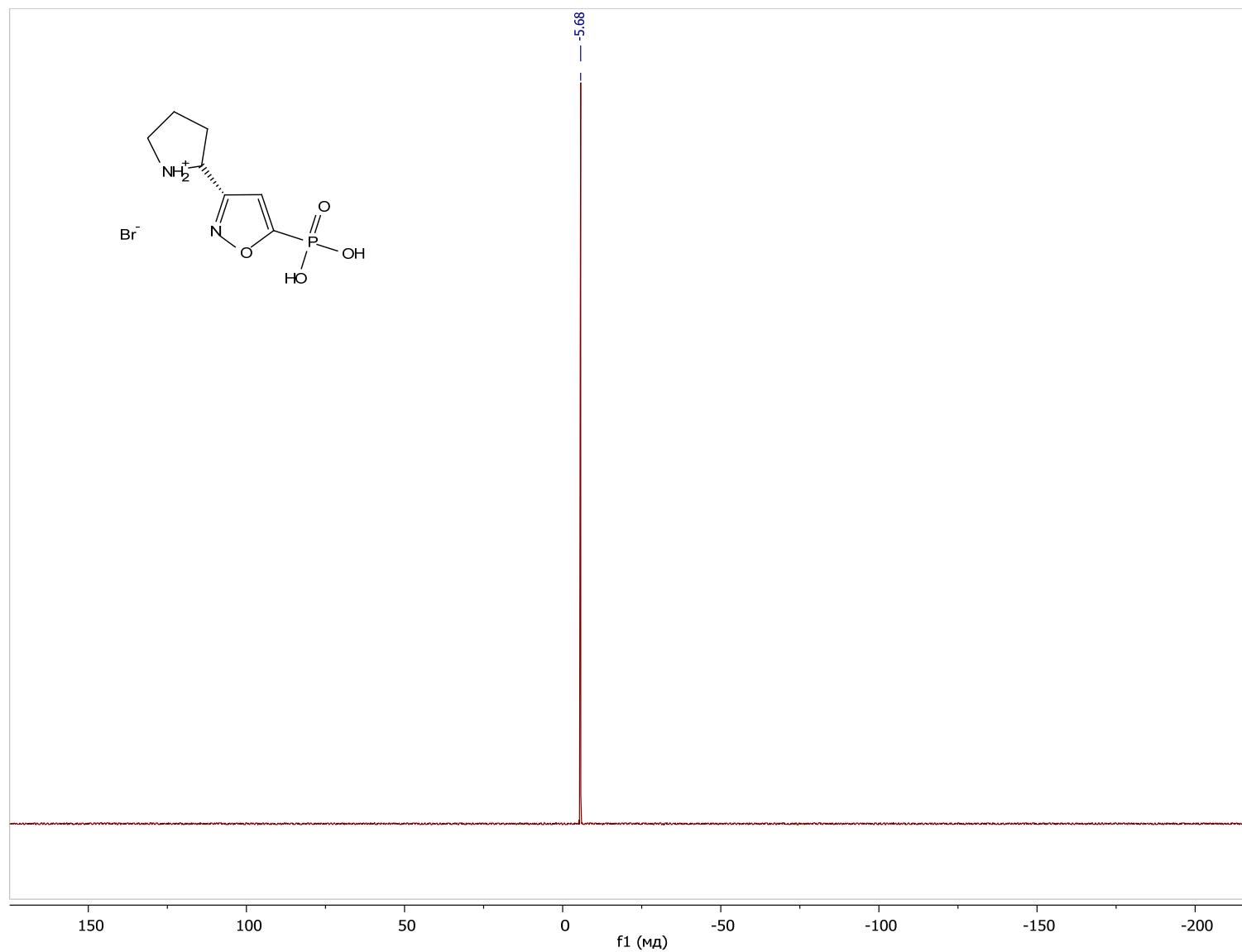


Figure 108. ^{31}P NMR spectrum of 21a and 21b

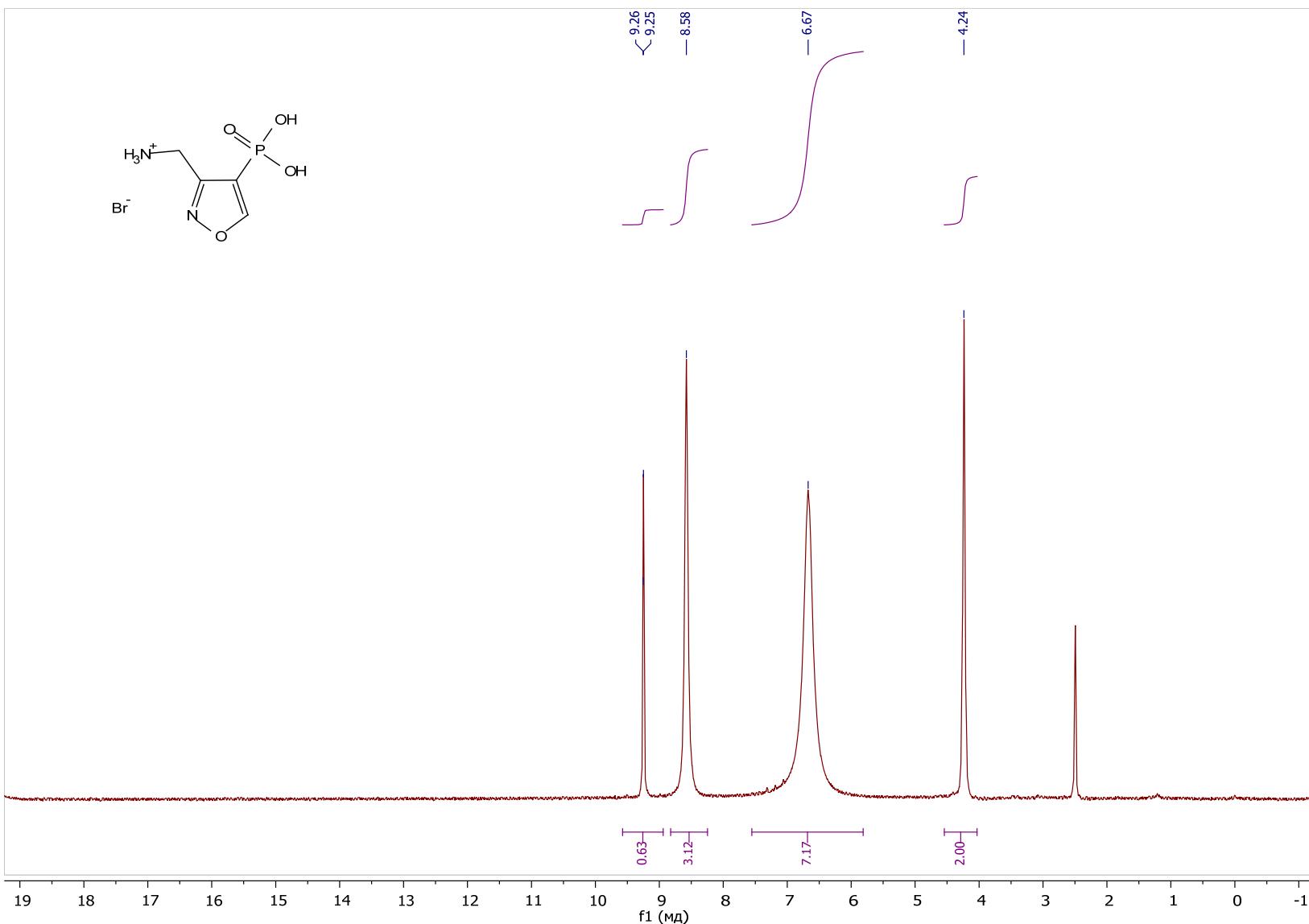


Figure 109. ^1H NMR spectrum of 21c

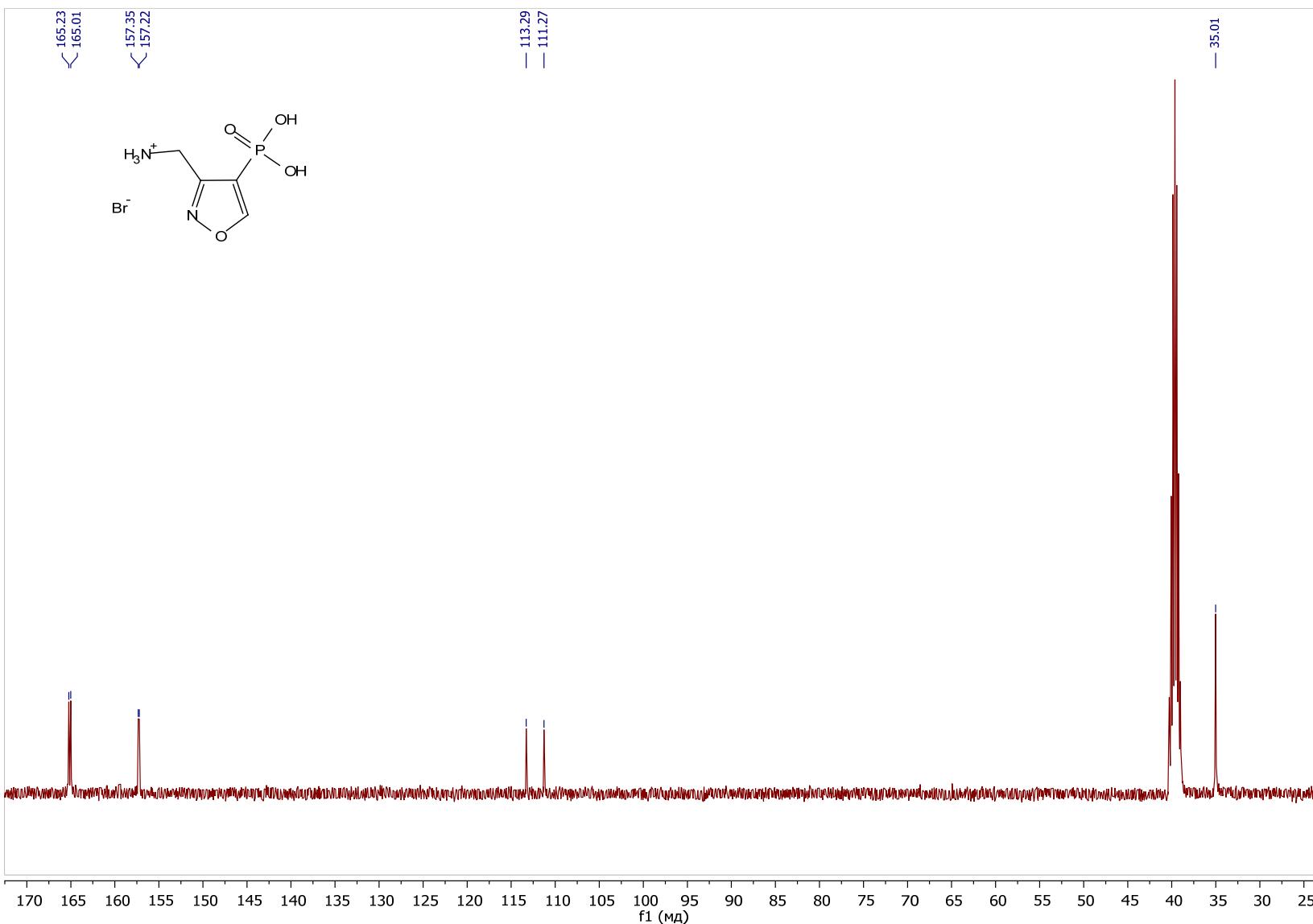


Figure 110. ^{13}C NMR spectrum of 21c

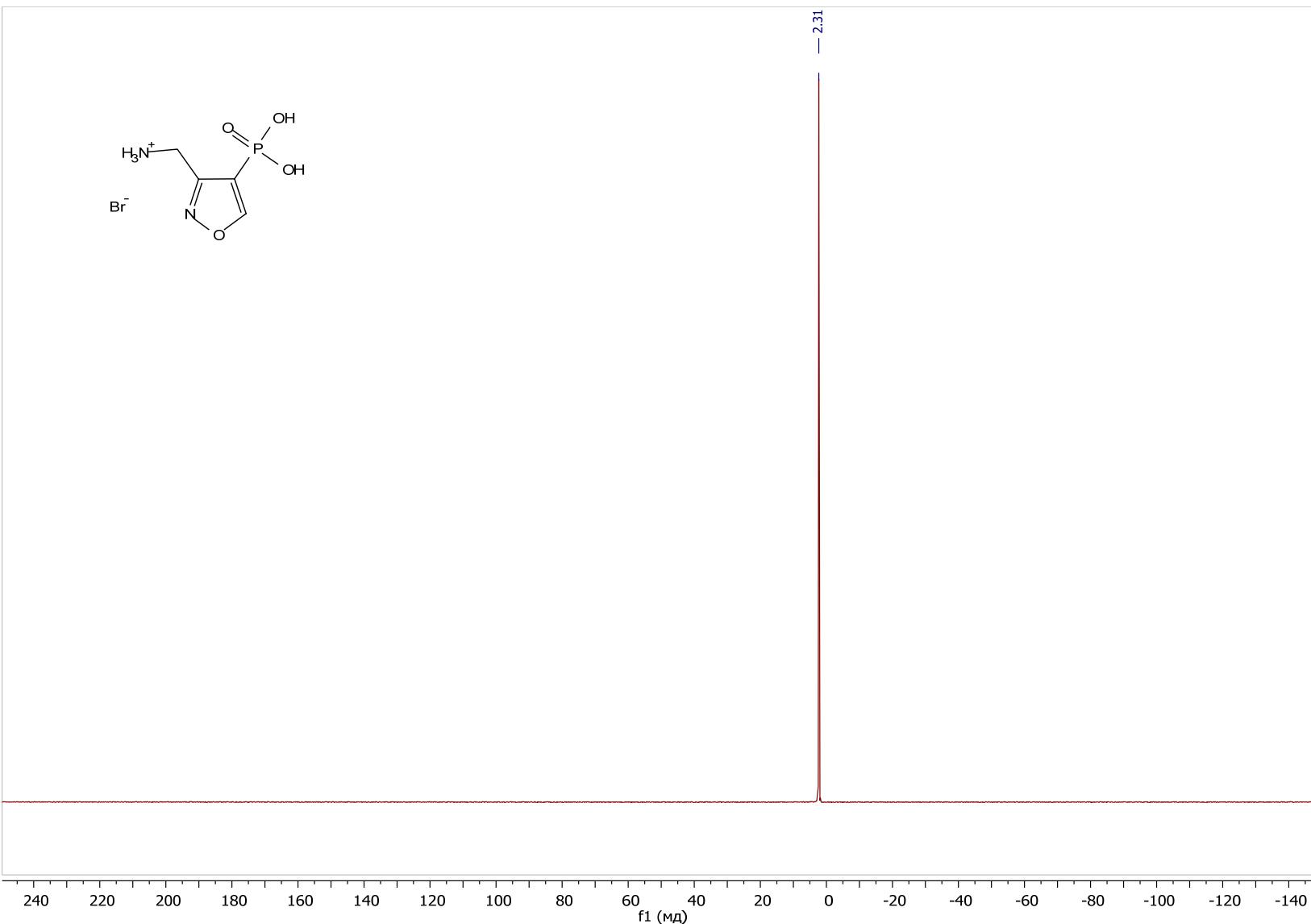


Figure 111. ^{31}P NMR spectrum of 21c

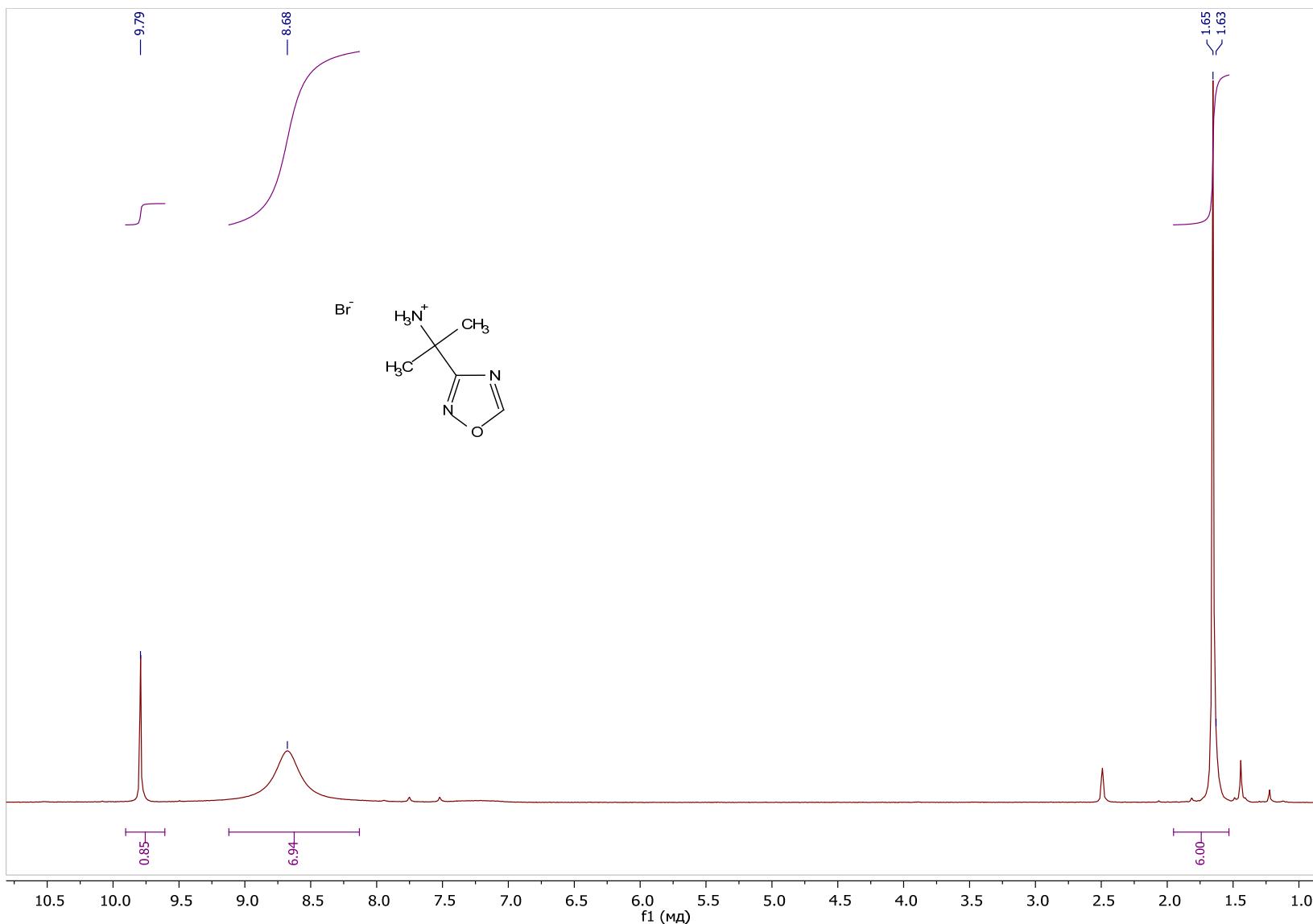


Figure 112. ^1H NMR spectrum of 21d

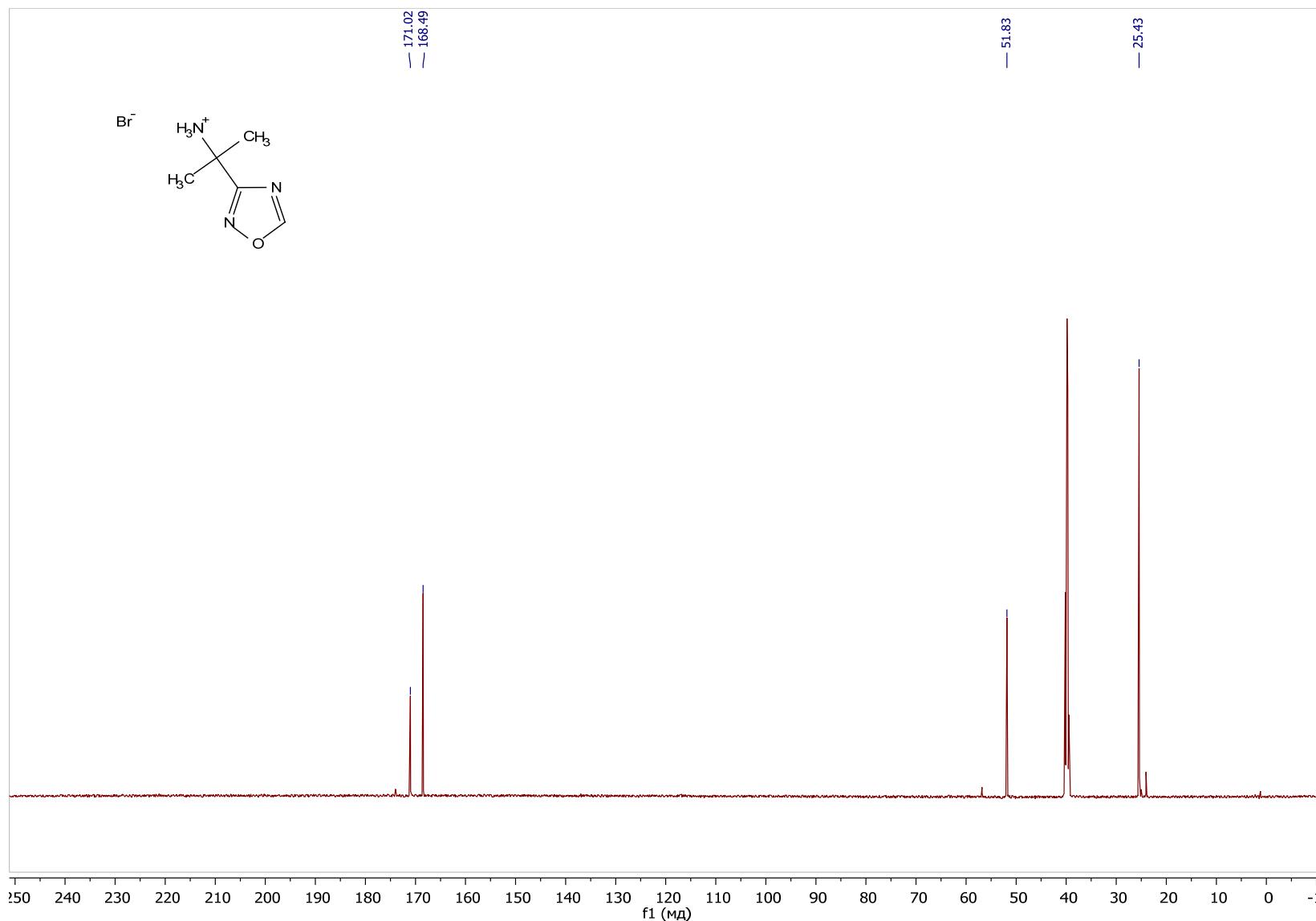


Figure 113. ^{13}C NMR spectrum of 21d

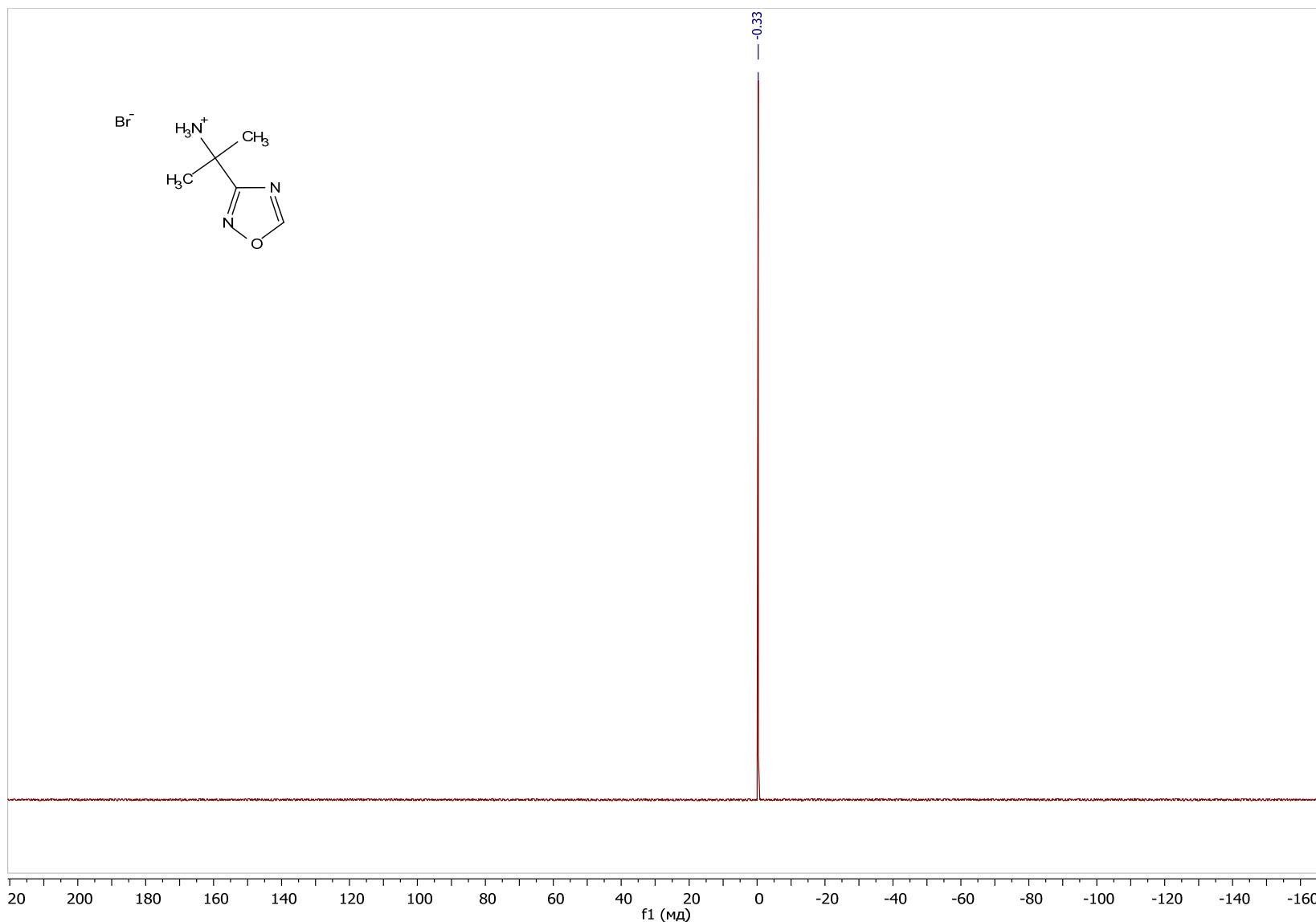


Figure 114. ^{31}P NMR spectrum of 21d

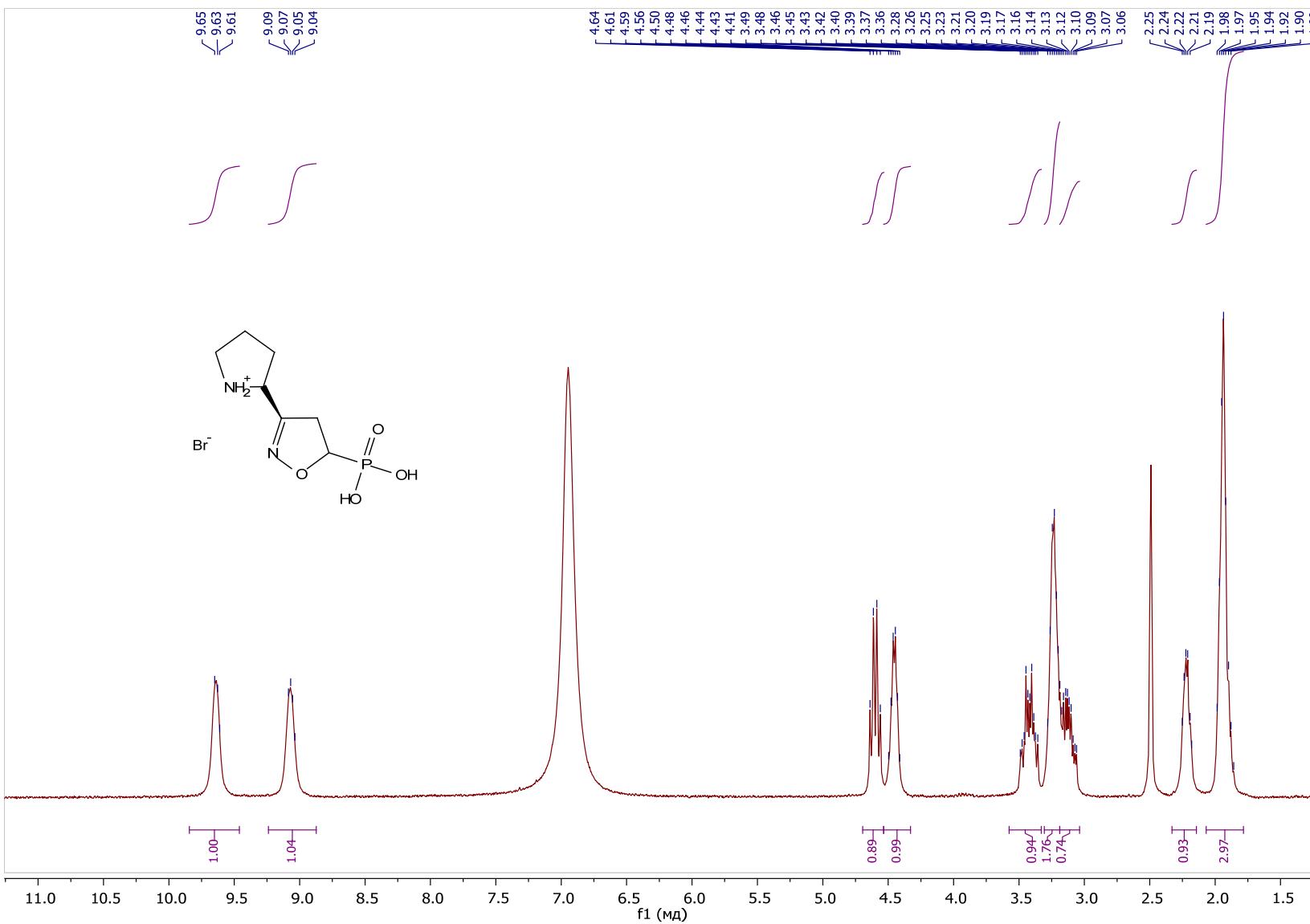


Figure 115. ¹H NMR spectrum of 21e and 21f

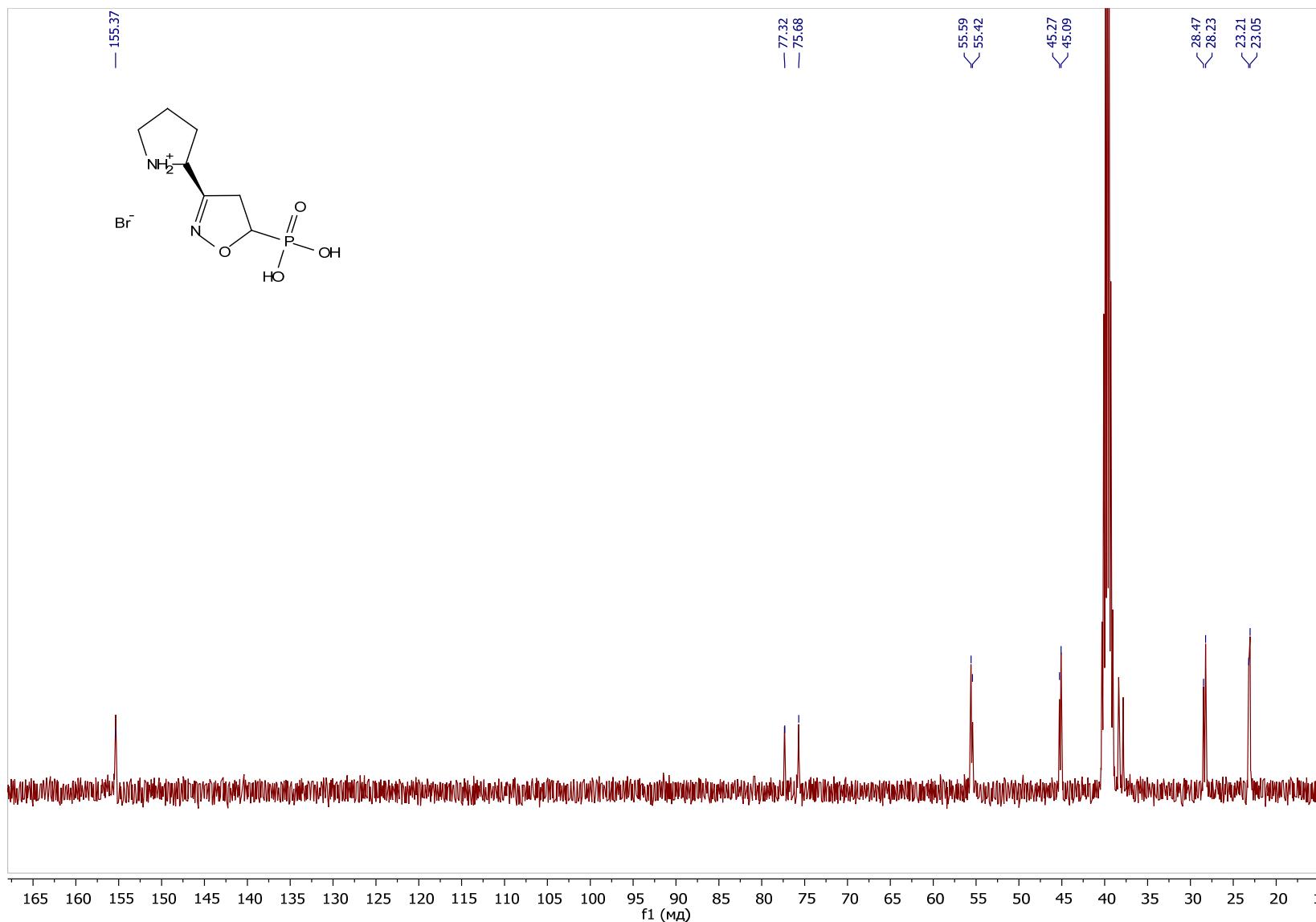


Figure 116. ^{13}C NMR spectrum of 21e and 21f

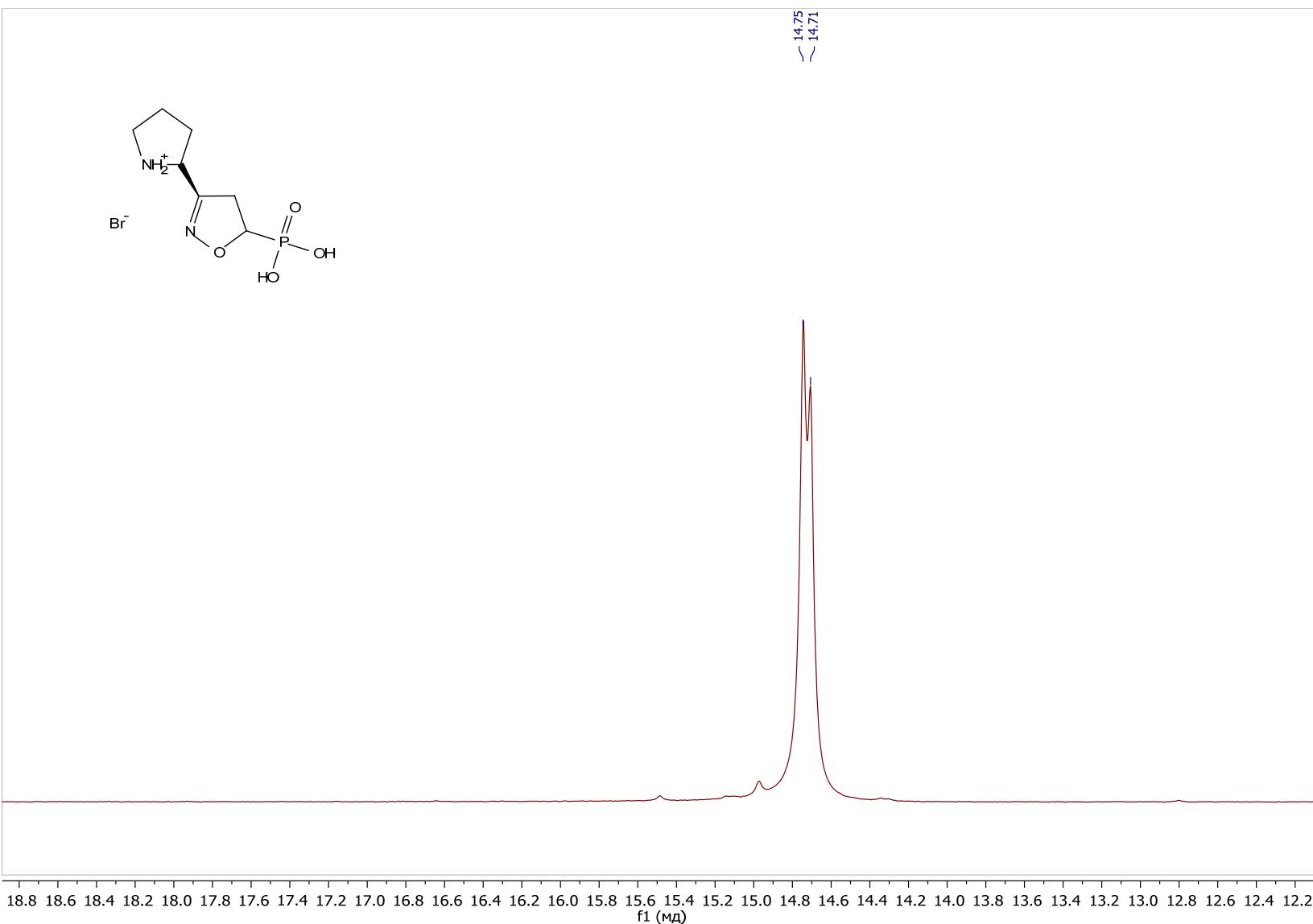


Figure 117. ^{31}P NMR spectrum of 21e and 21f

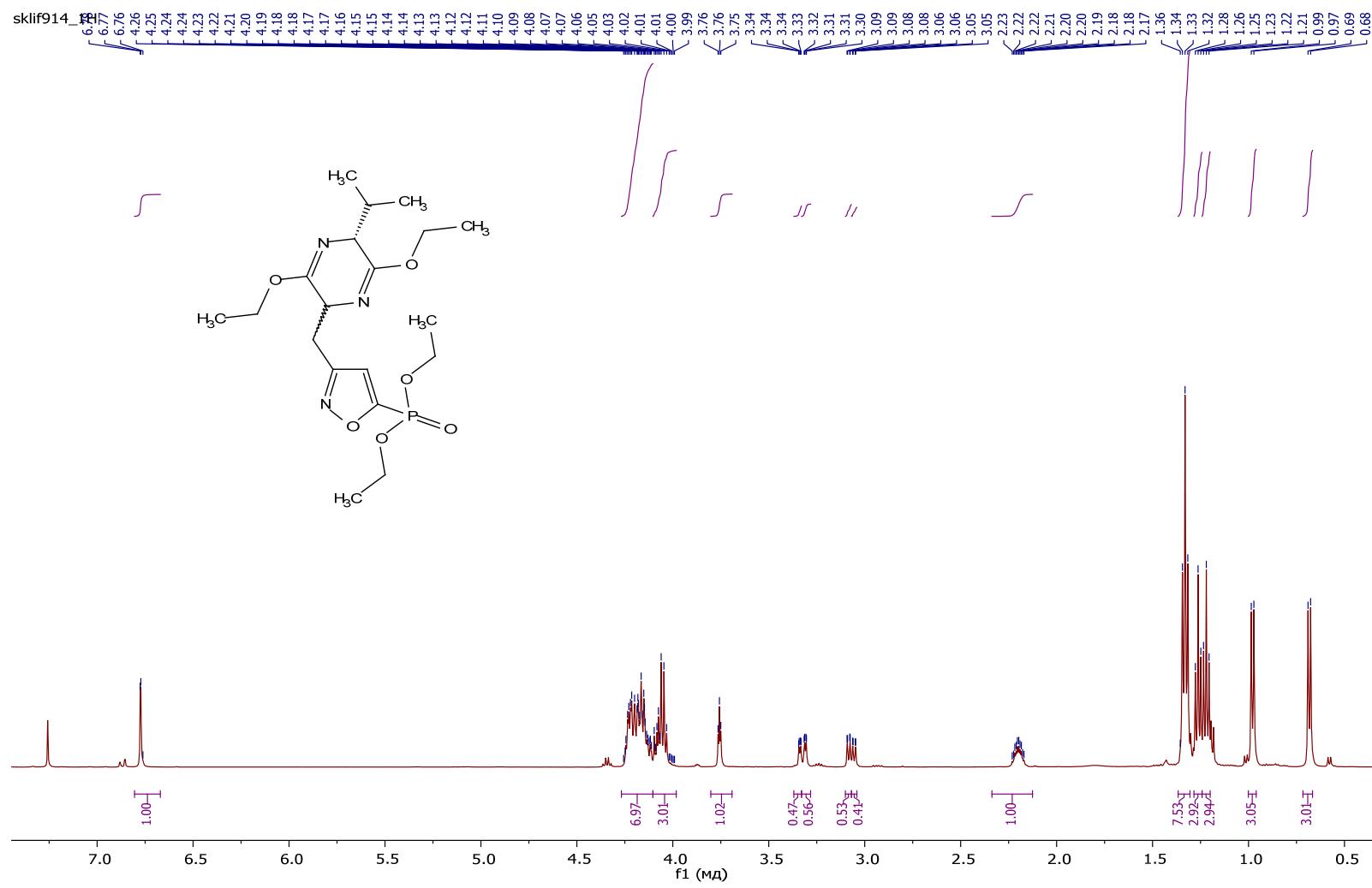


Figure 118. ¹H NMR spectrum of 23

sklf914_C13
Automated Probe tuning parameter

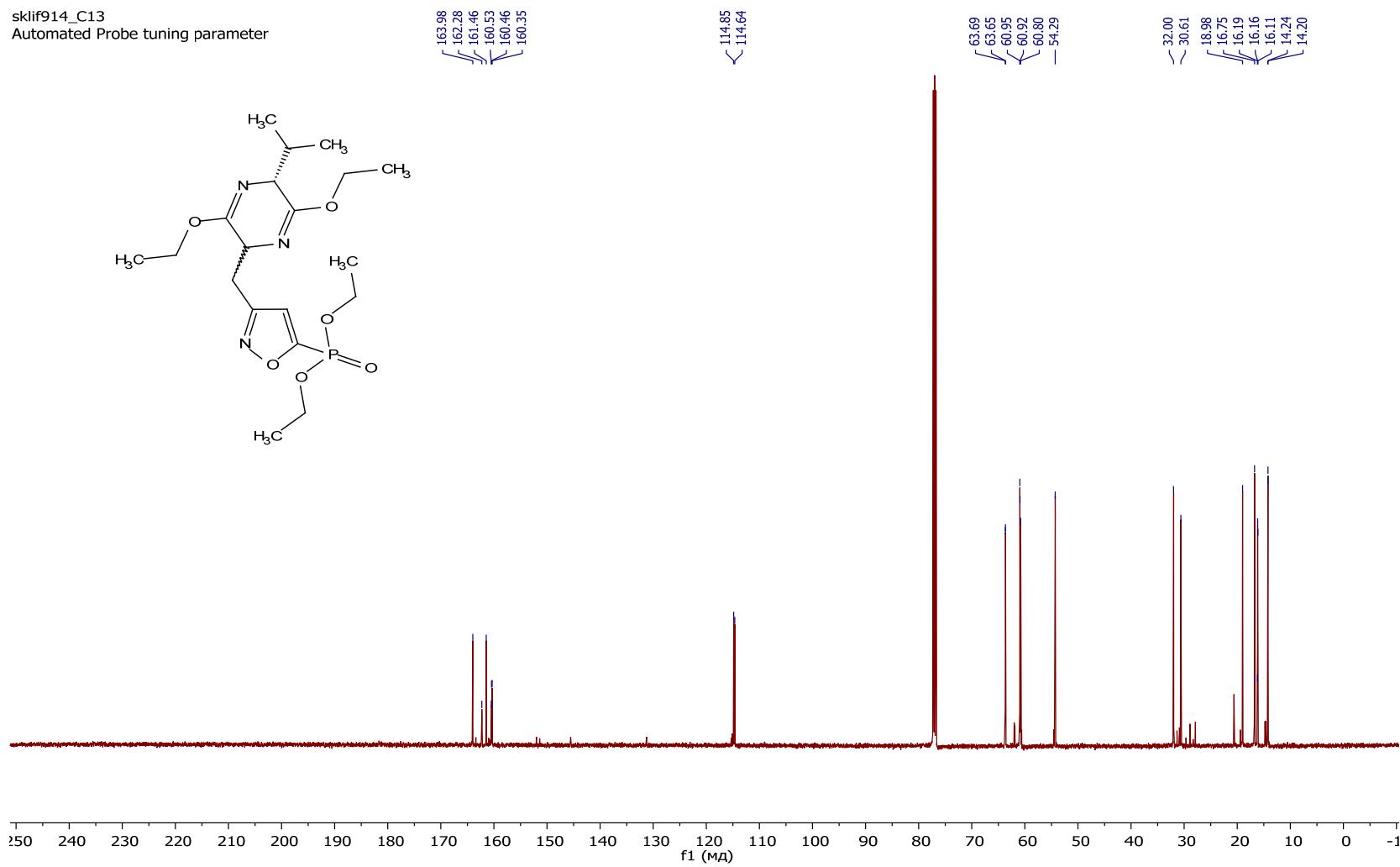


Figure 119. ^{13}C NMR spectrum of 23

sklf702_P31.1.fid

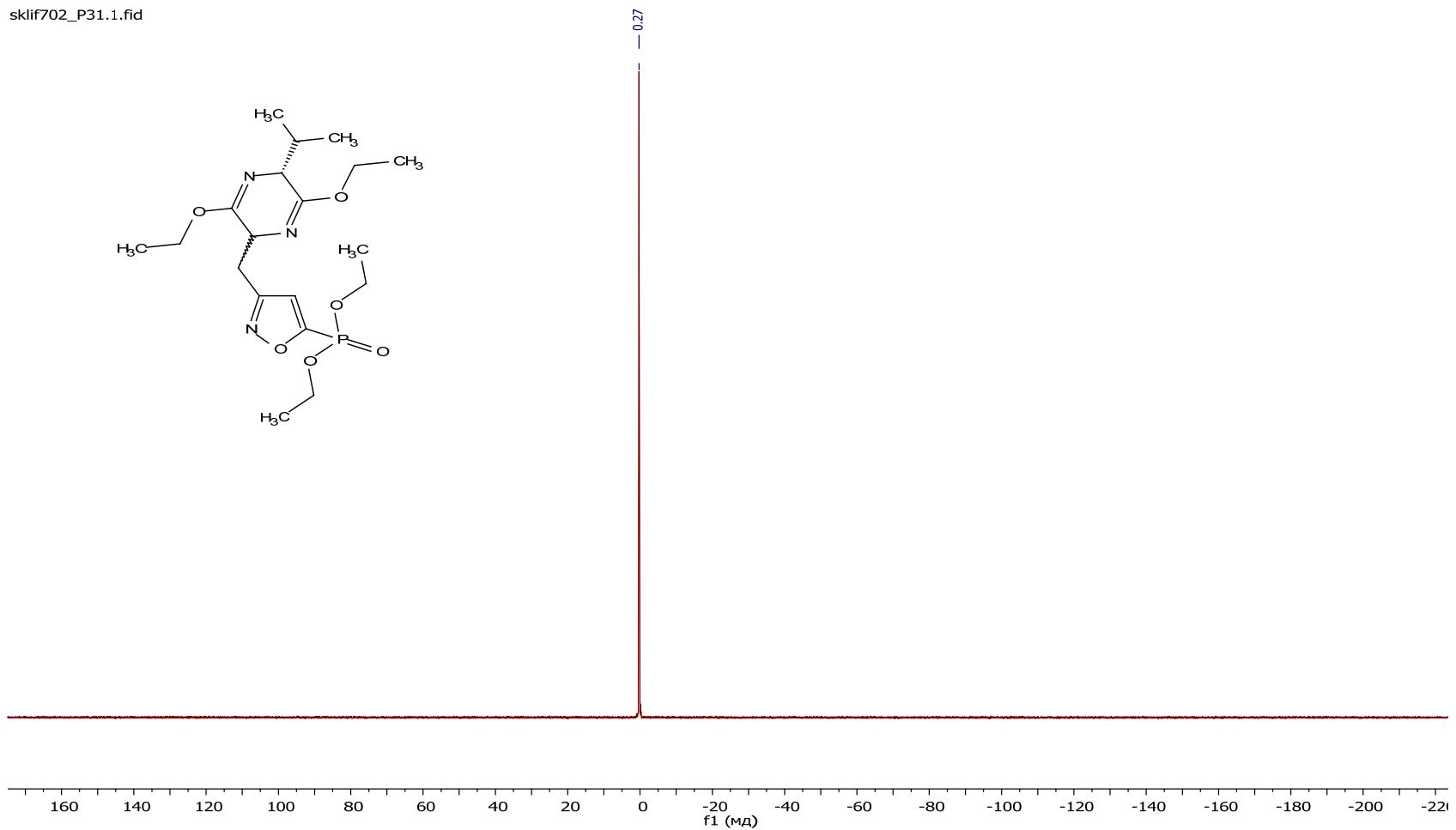


Figure 120. ^{31}P NMR spectrum of 23

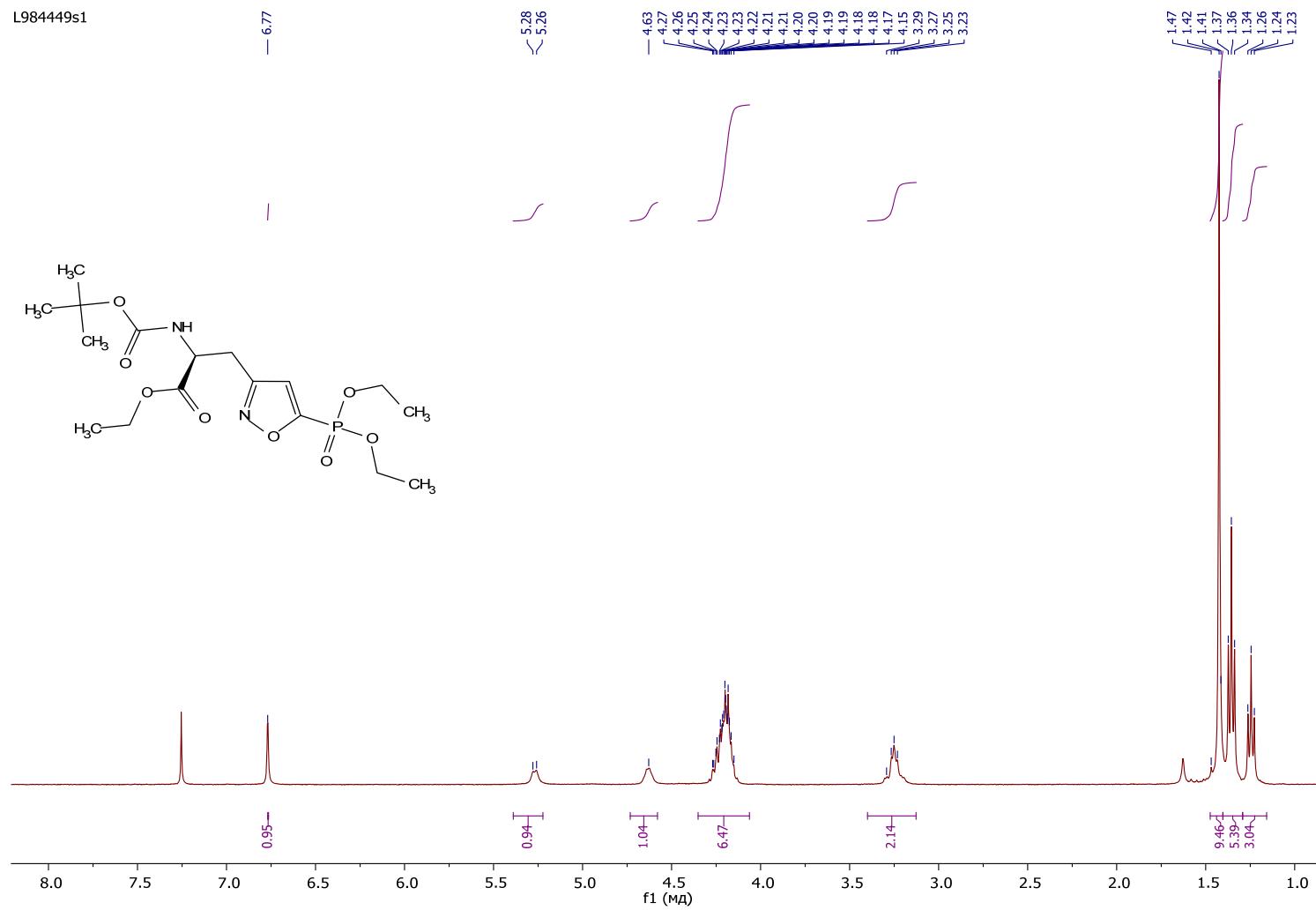


Figure 121. ^1H NMR spectrum of 24

sklf1869_13C.1.fid

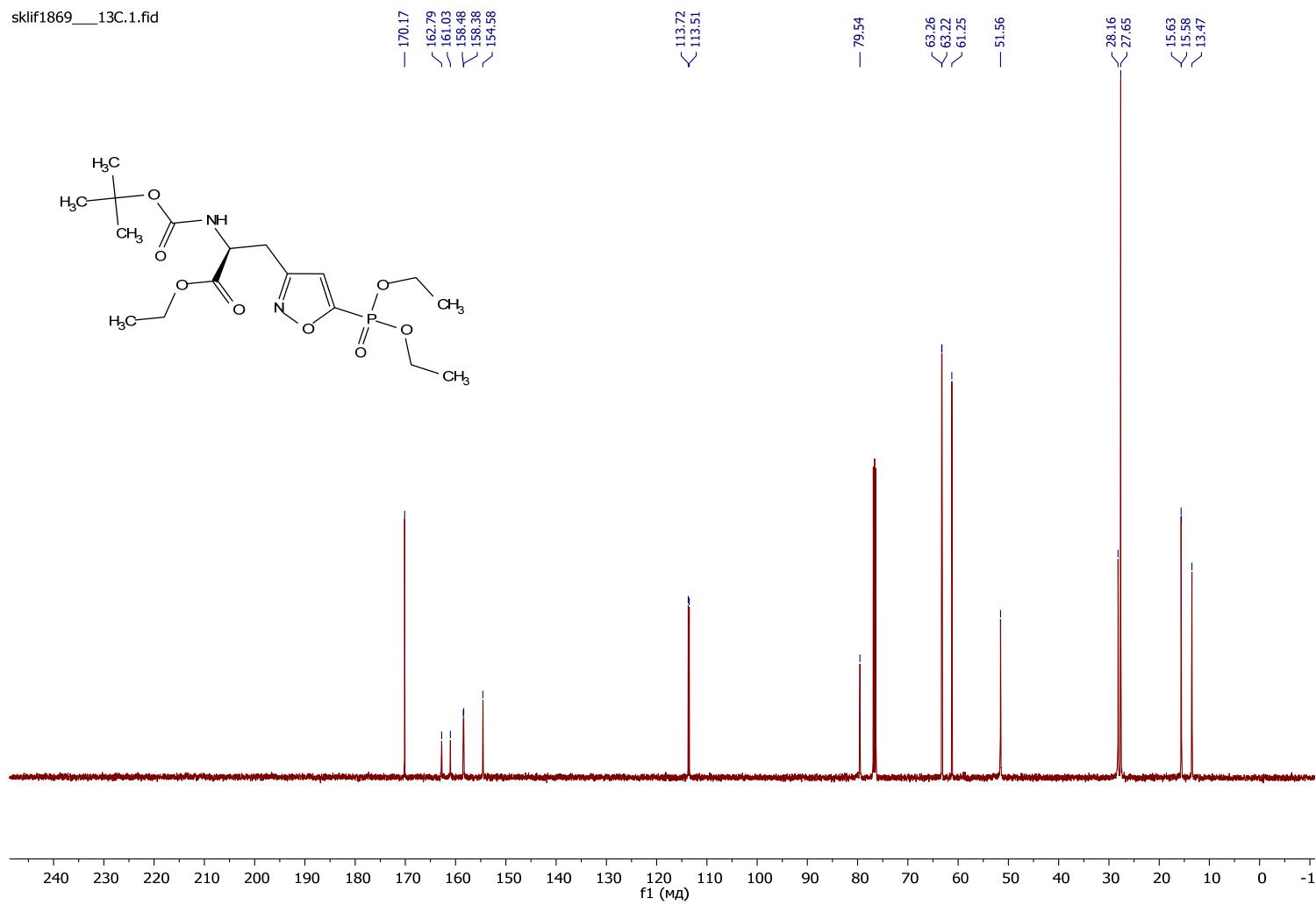


Figure 122. ^{13}C NMR spectrum of 24

sklif1869____31P.1.fid

-0.27

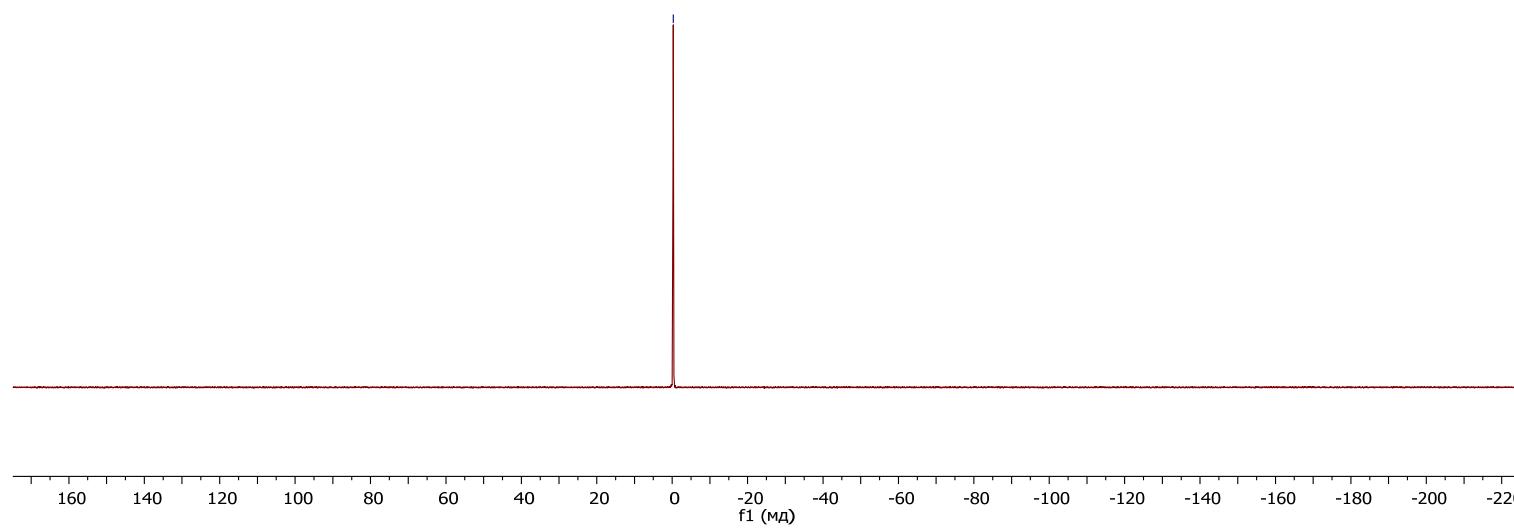
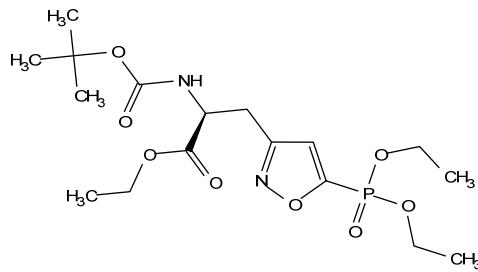


Figure 123. ^{31}P NMR spectrum of 24

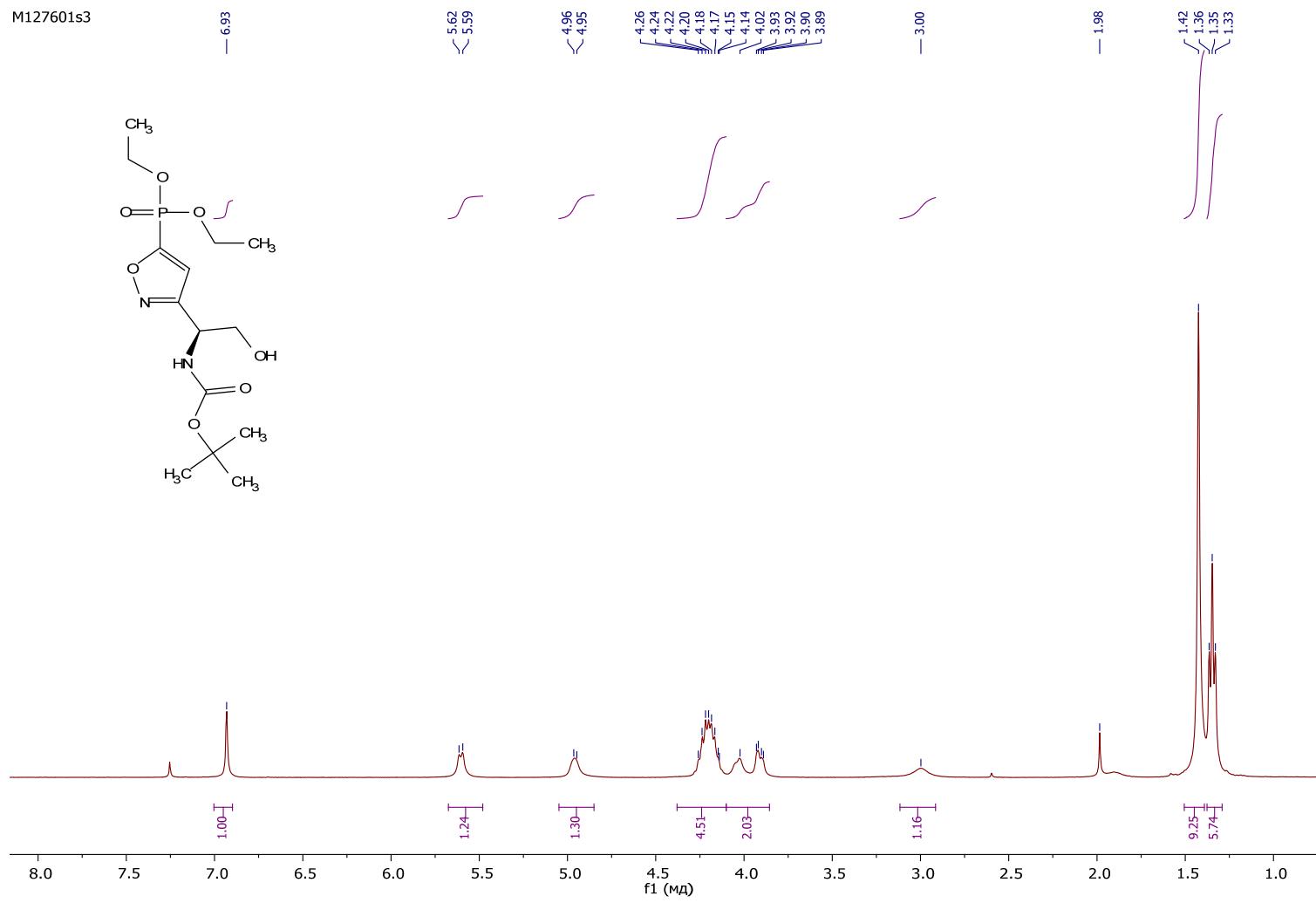


Figure 124. ¹H NMR spectrum of 25 and 26 (*S*-isomer)

sklf2024_C13.1.fid

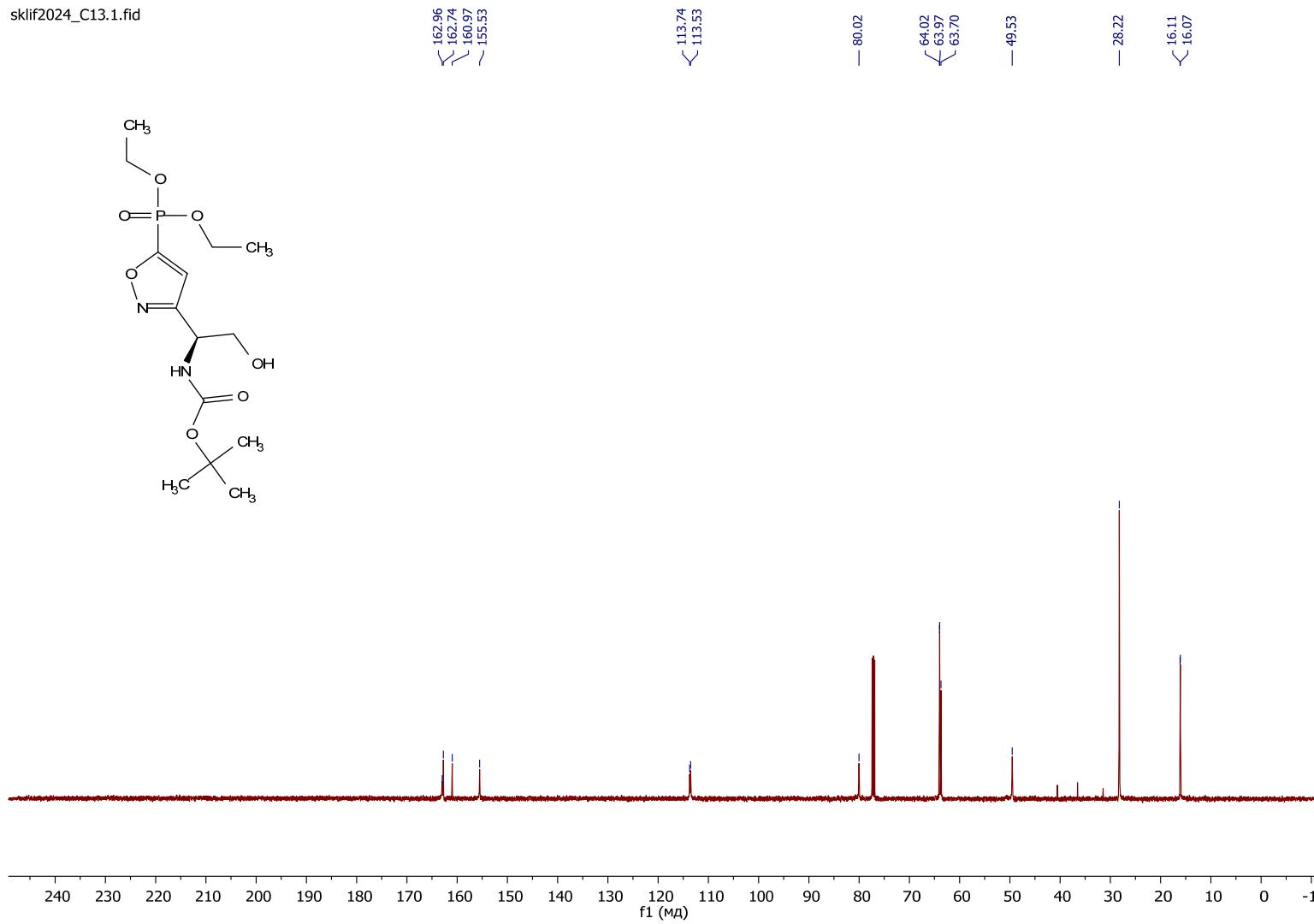


Figure 125. ^{13}C NMR spectrum of 25 and 26 (*S*-isomer)

sklf2024_P31.1.fid
31P-{1H}

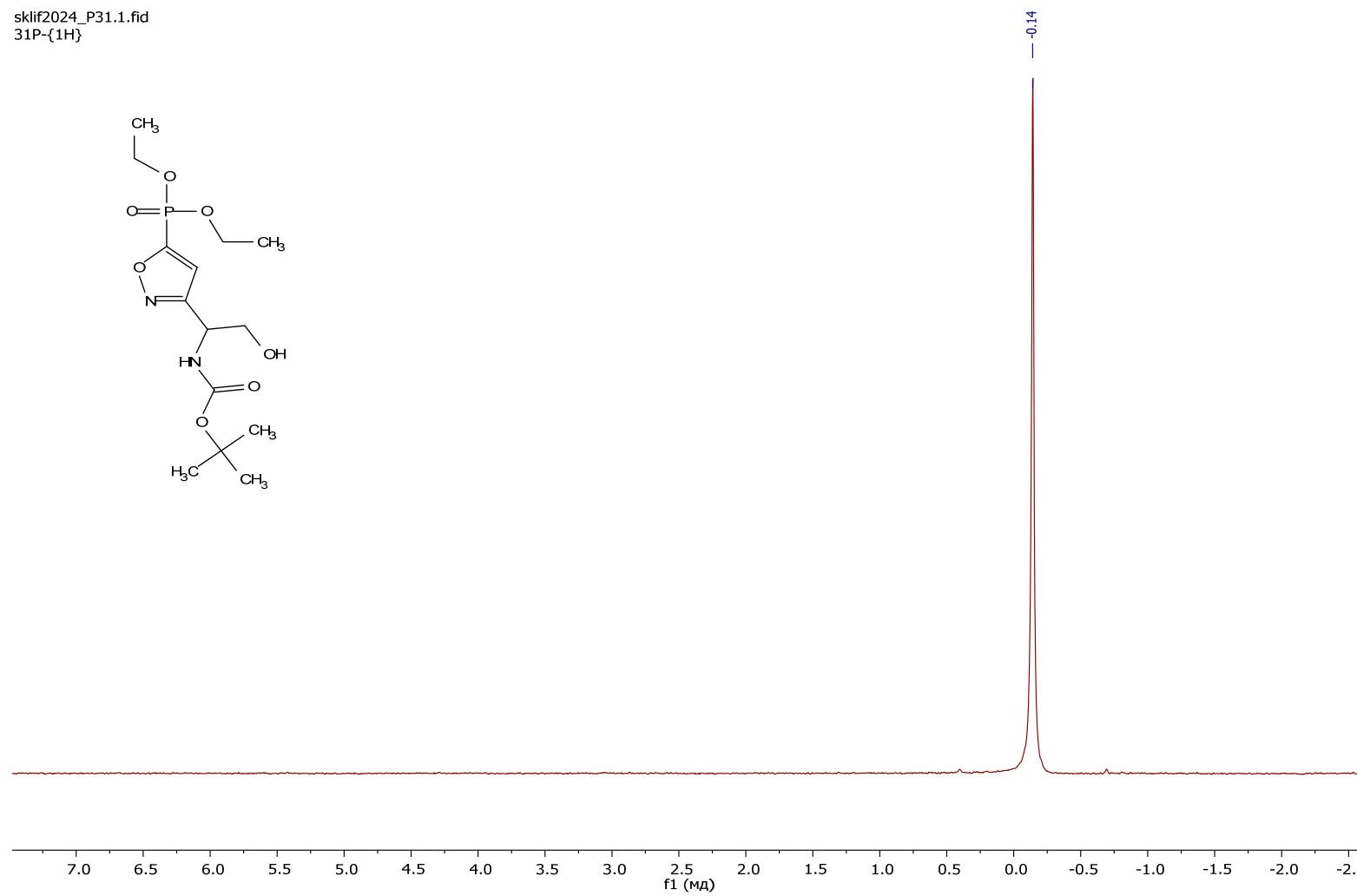


Figure 126. ^{31}P NMR spectrum of 25 and 26 (*S*-isomer)

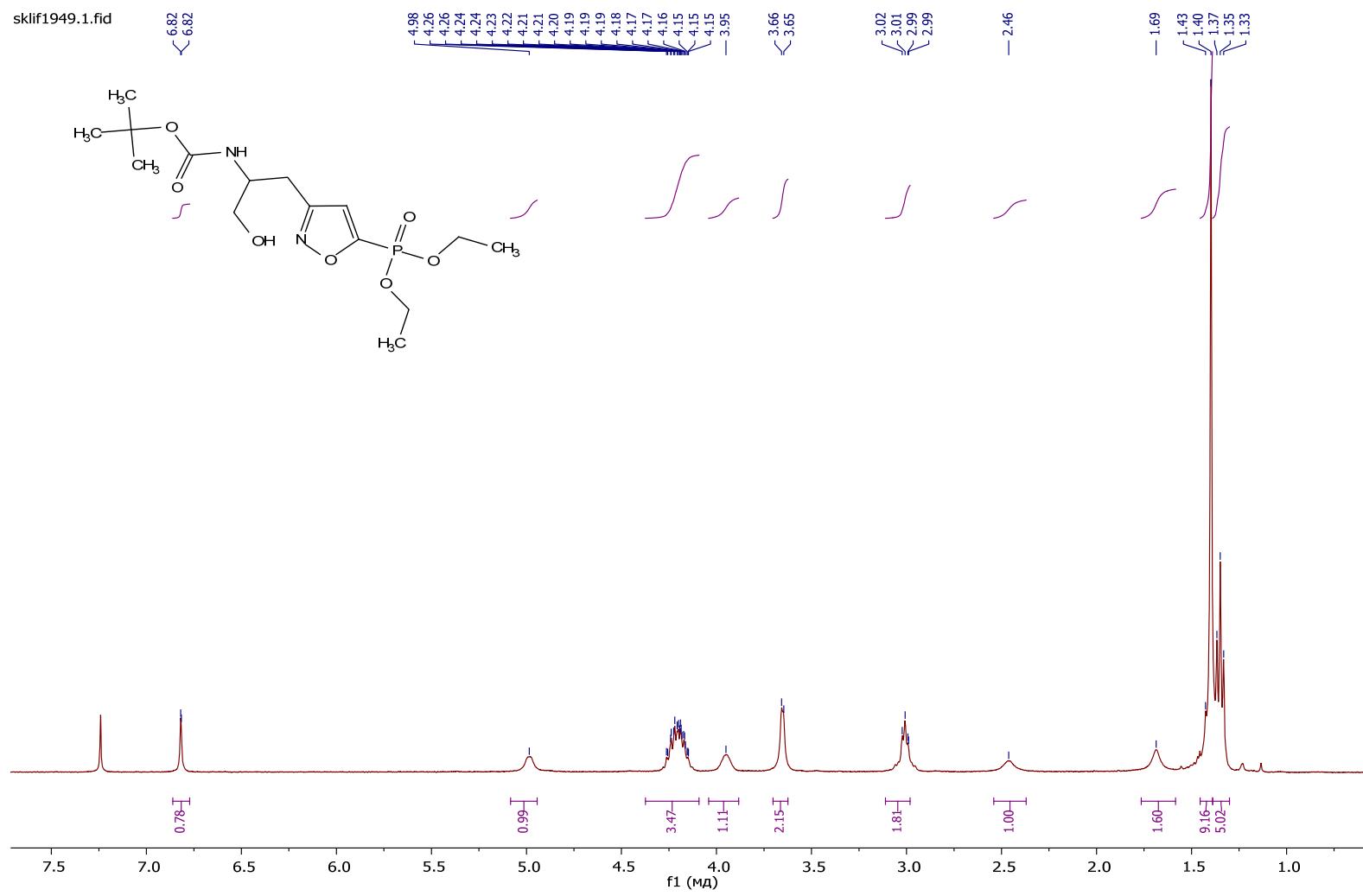


Figure 127. ^1H NMR spectrum of 27 and 28 (*S*-isomer)

sklif1939_C13.1.fid

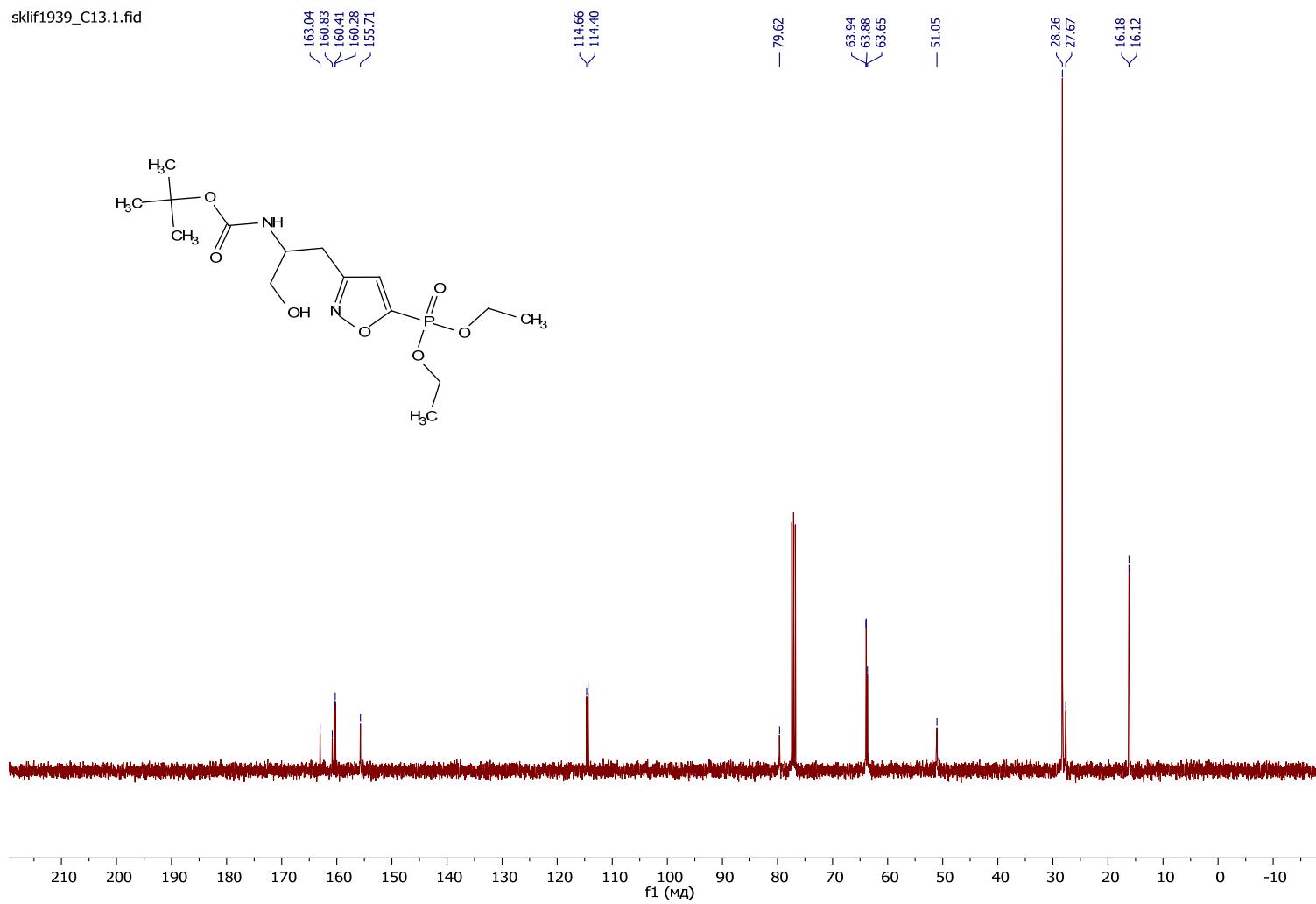


Figure 128. ^{13}C NMR spectrum of 27 and 28 (*S*-isomer)

sklf1939_P31.1.fid
31P-{1H}

— 0.12

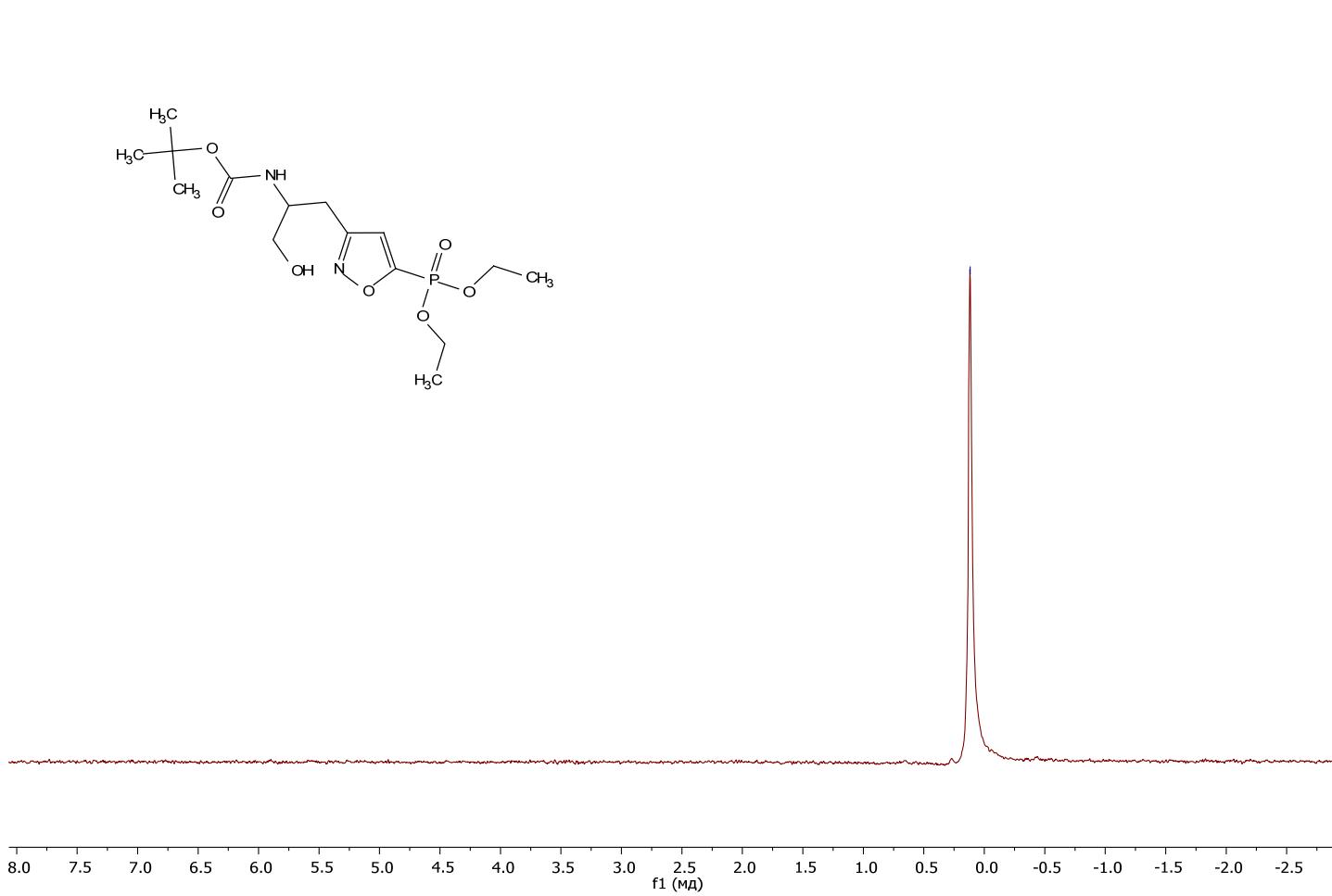
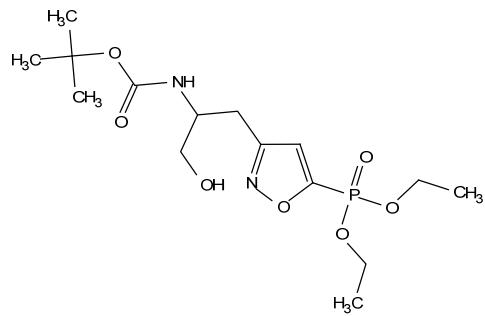


Figure 129. ³¹P NMR spectrum of 27 and 28 (*S*-isomer)

M158553s1

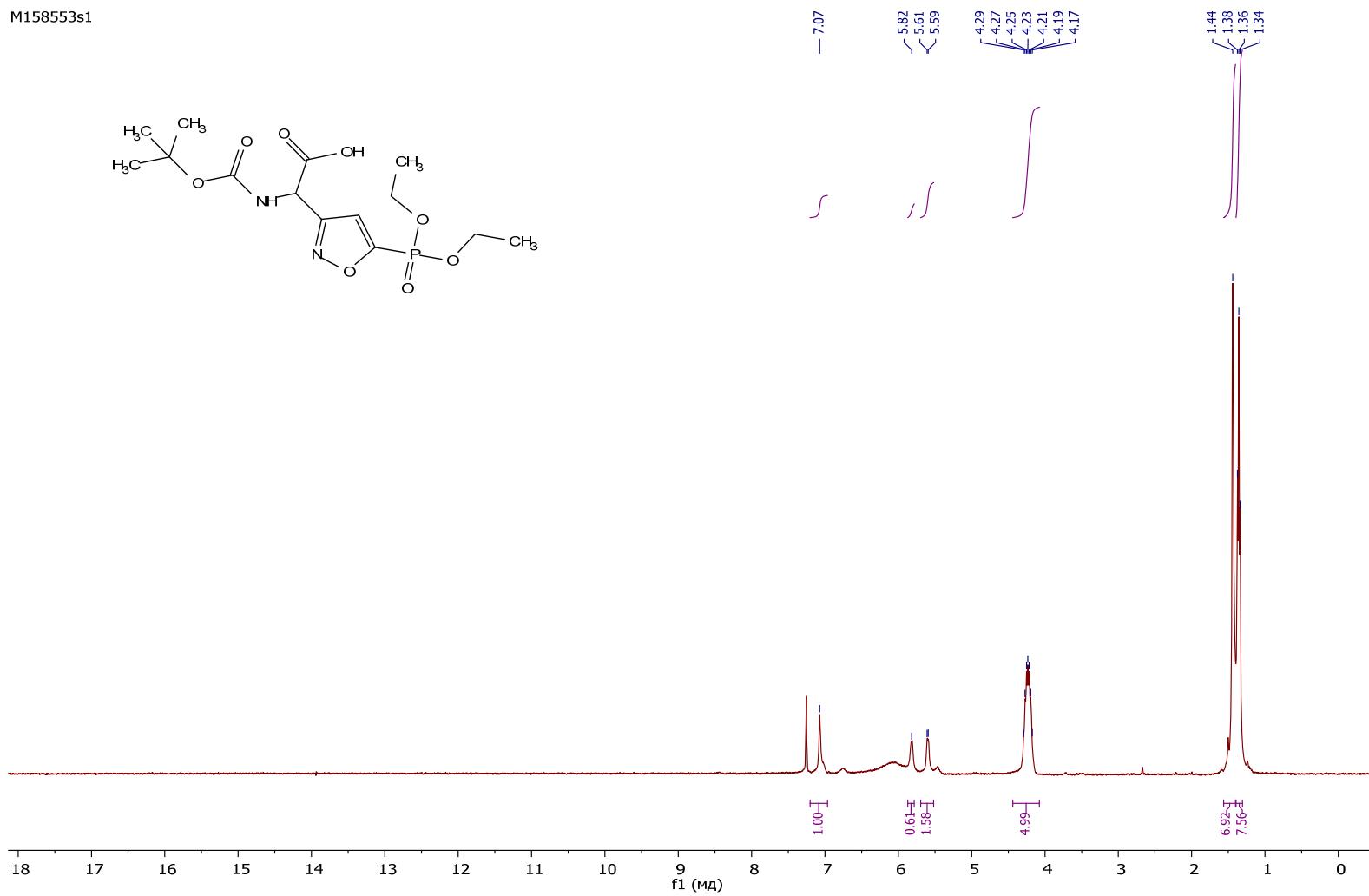


Figure 130. ¹H NMR spectrum of 29 and 30 (*S*-isomer)

sklf2155_C13.1.fid

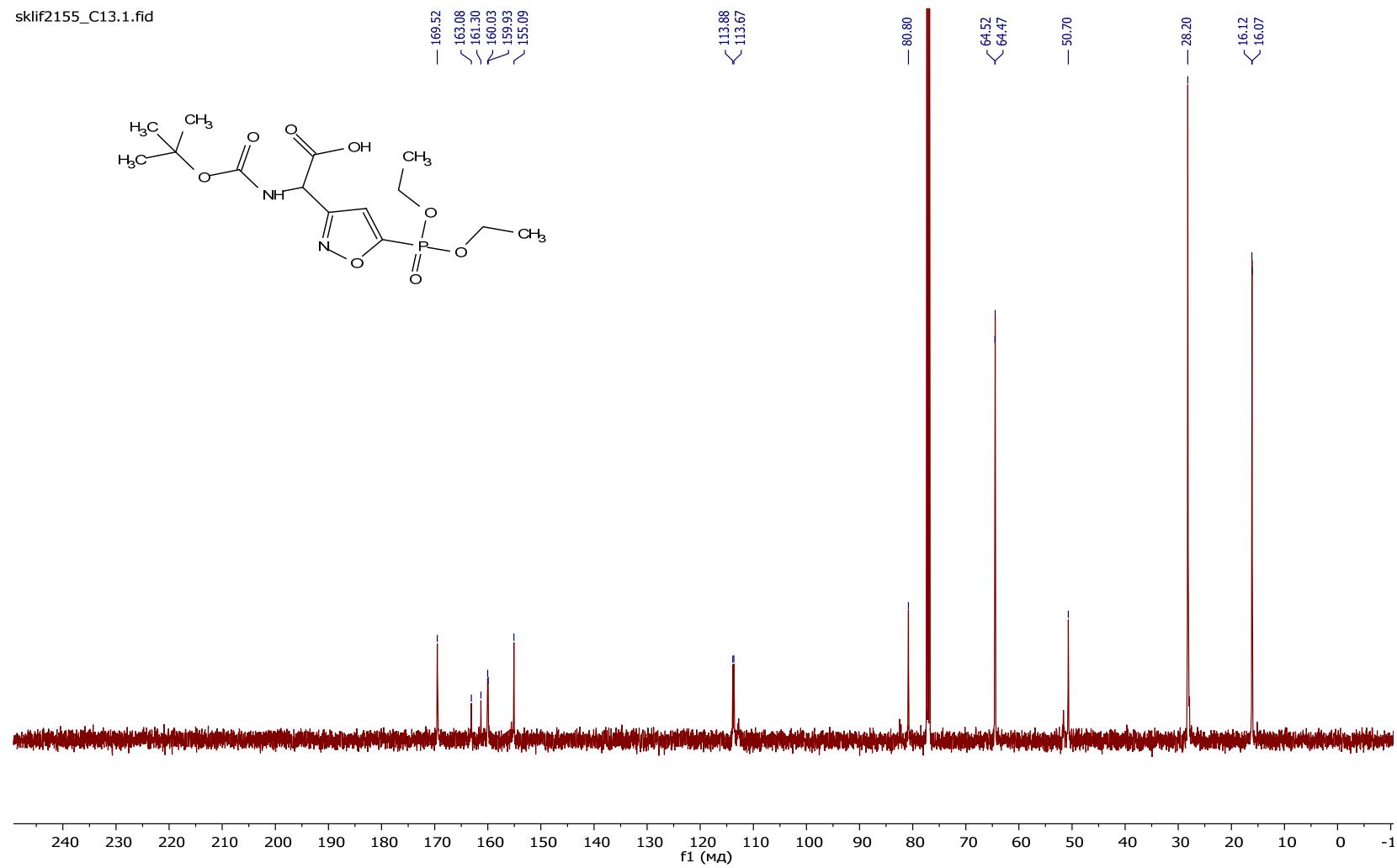


Figure 131. ^{13}C NMR spectrum of 29 and 30 (*S*-isomer)

sklf2155_P31{H}.1.fid

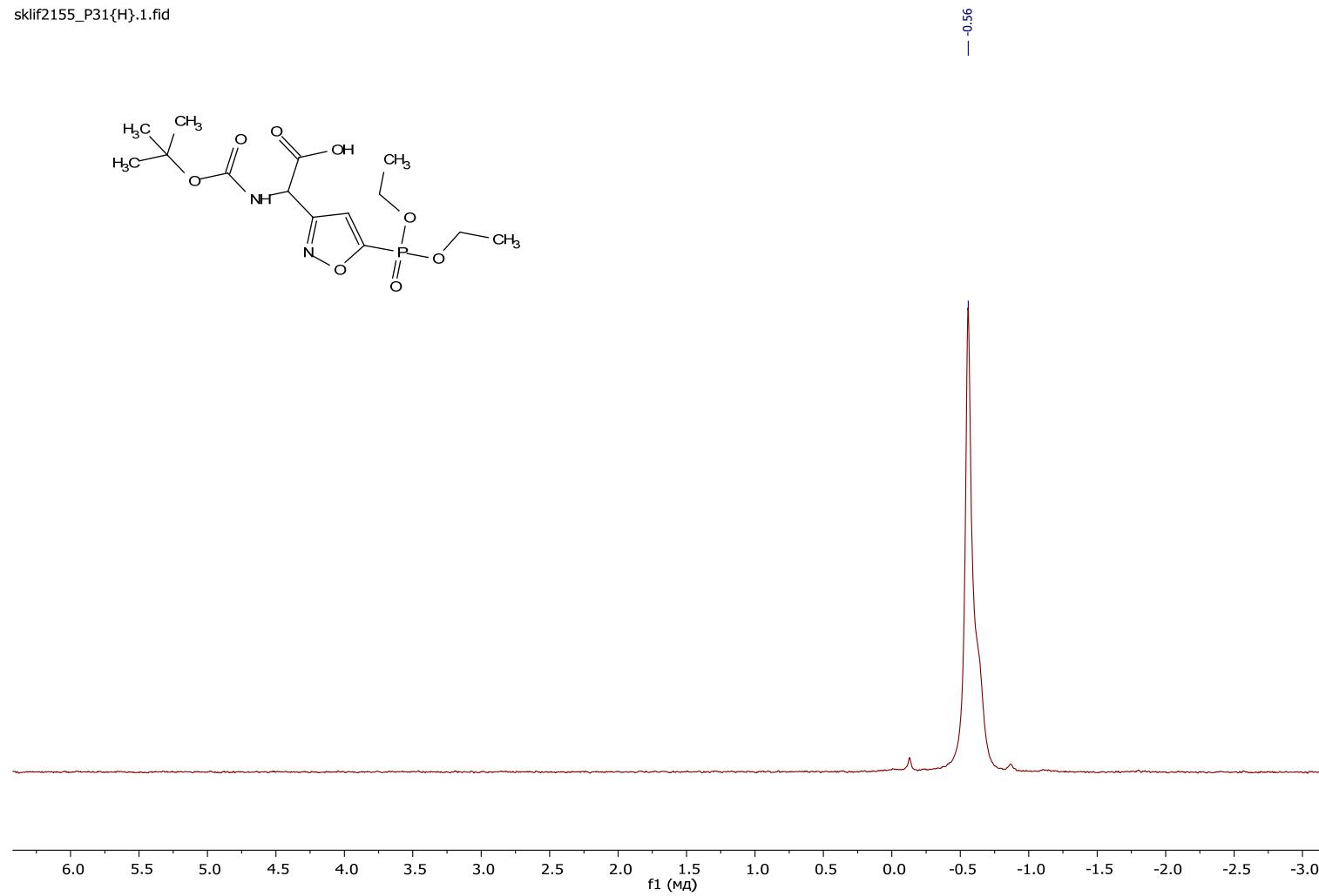


Figure 132. ^{31}P NMR spectrum of 29 and 30 (*S*-isomer)

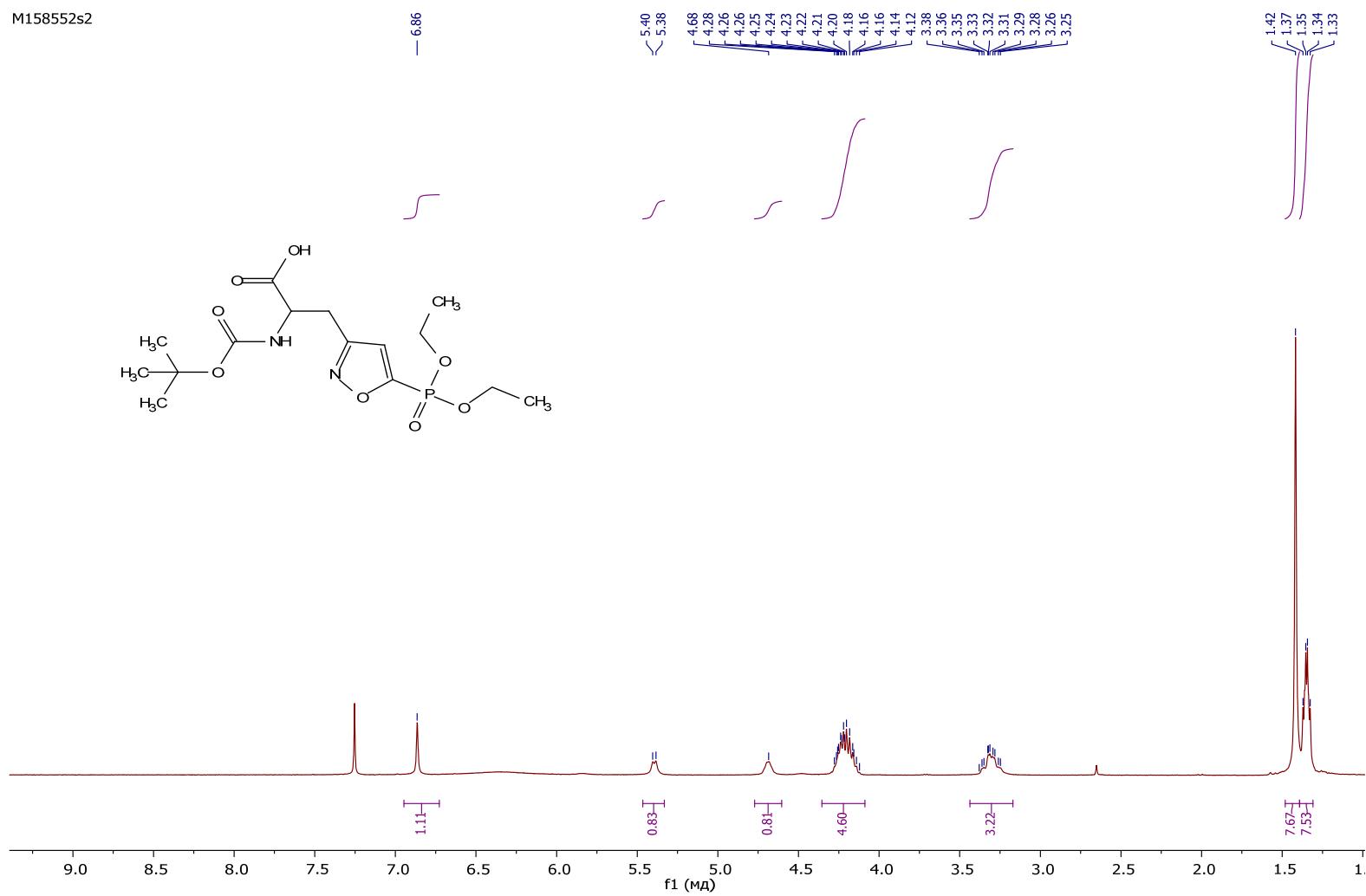


Figure 133. ^1H NMR spectrum of 31 and 32 (*S*-isomer)

sklf2285_C13
Automated Probe tuning parameter

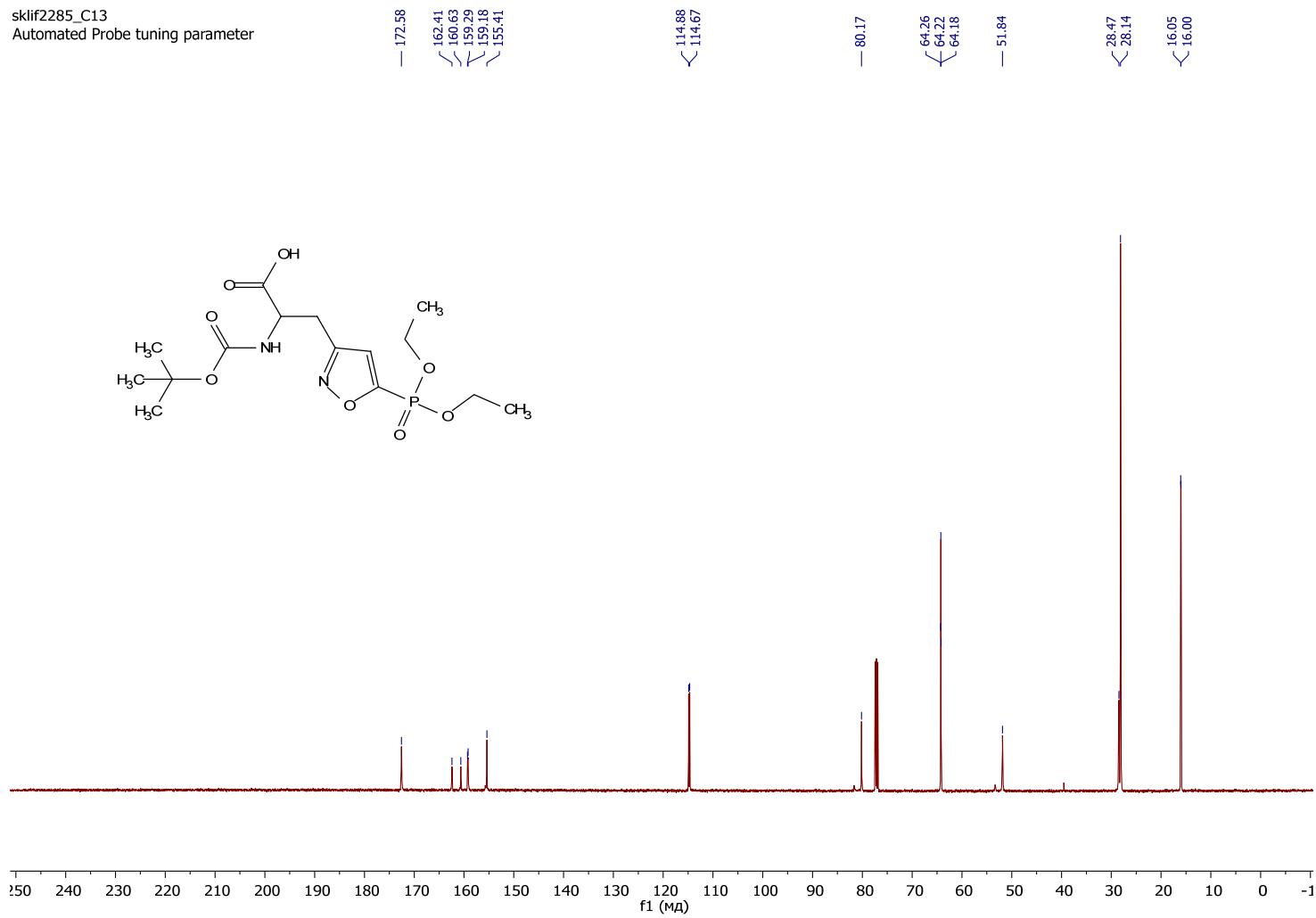


Figure 134. ^{13}C NMR spectrum of 31 and 32 (*S*-isomer)

sklif2285_31P.1.fid

—
0.07

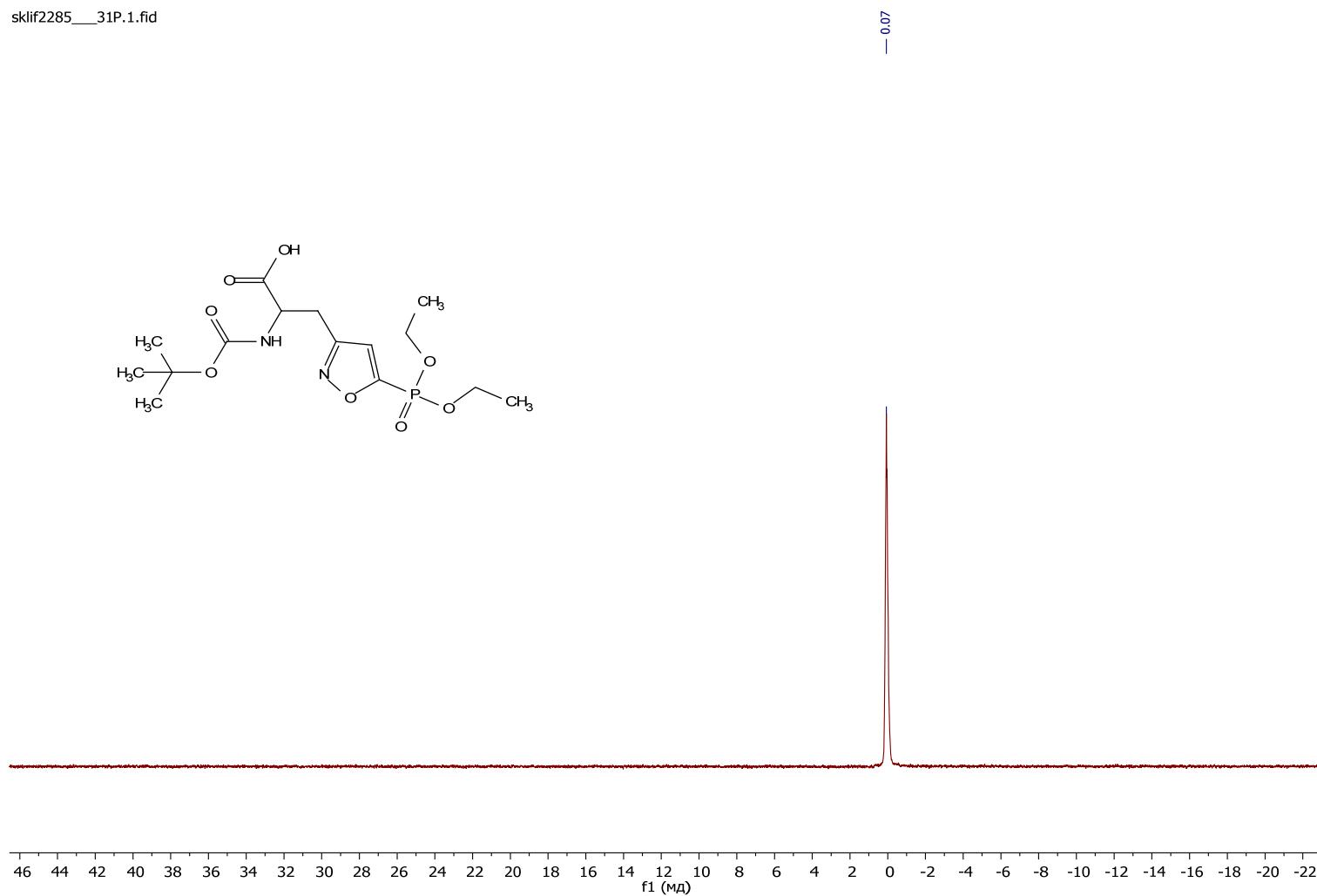
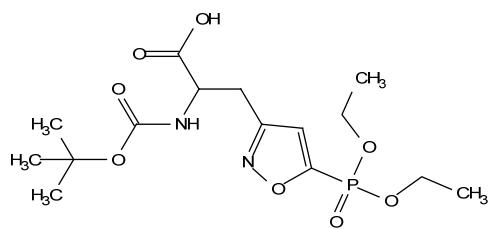


Figure 135. ^{31}P NMR spectrum of 31 and 32 (*S*-isomer)