Chemistry of Heterocyclic Compounds **2021**, *57*(1), 55–62

Synthesis of 2-triazolylpurine phosphonates

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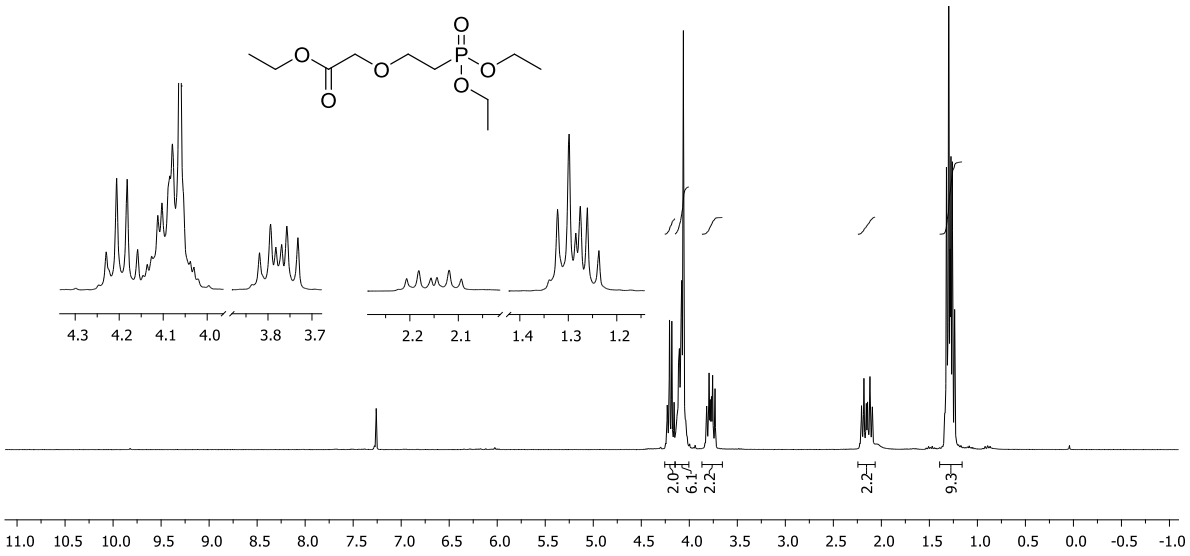
SUPPLEMENTARY INFORMATION

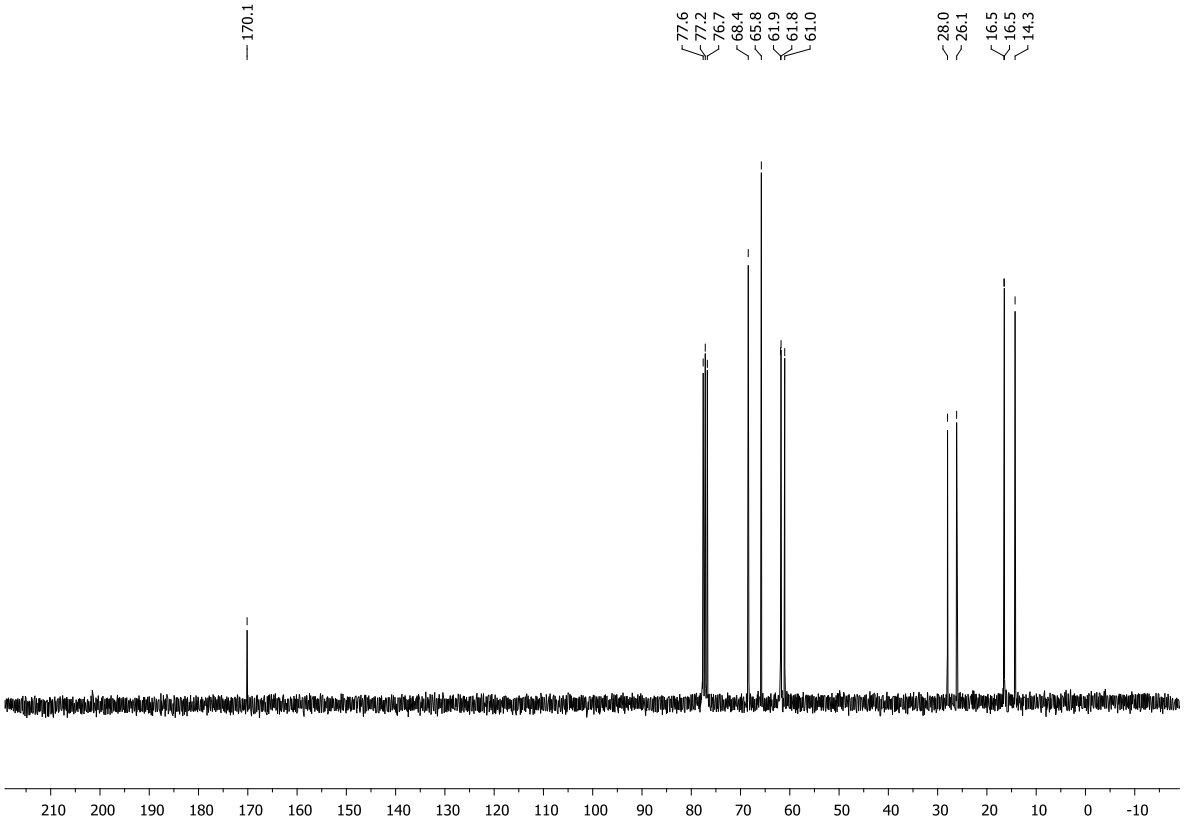
NMR SPECTRA OF COMPOUNDS

Ethyl 2-[2-(diethoxyphosphoryl)ethoxy]acetate (4)

^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 4:

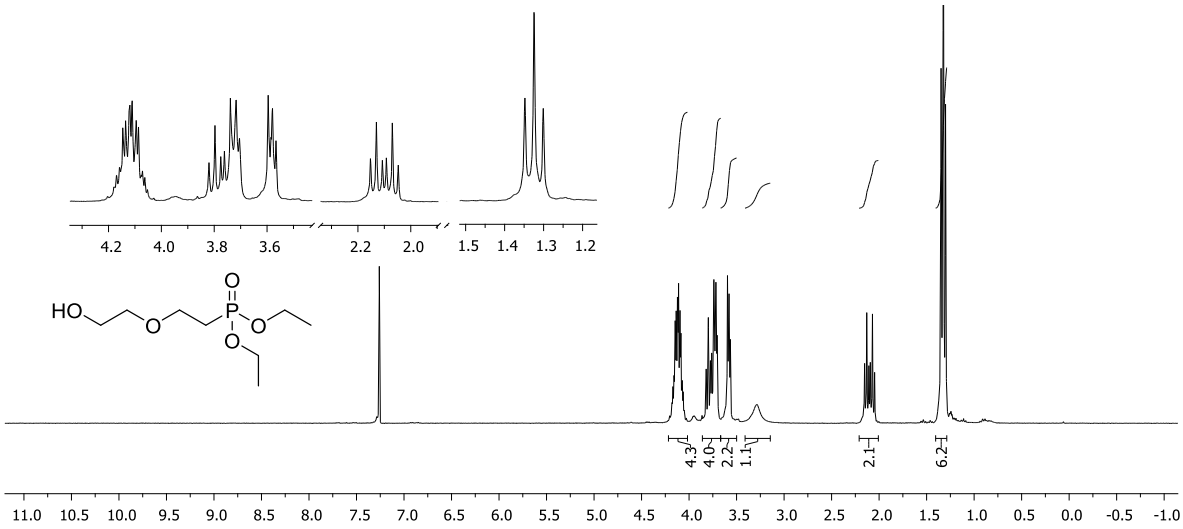


^{13}C-NMR (76 MHz, $CDCl_3$) spectrum of compound 4:

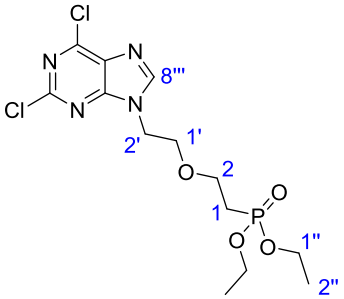


Diethyl [2-(2-hydroxyethoxy)ethyl]phosphonate (1)

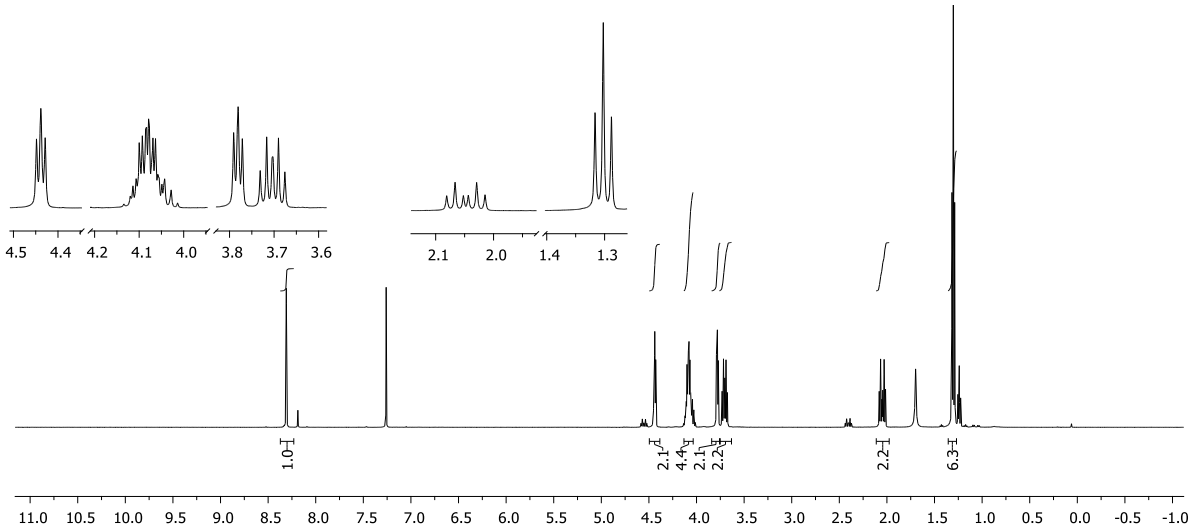
^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 1:



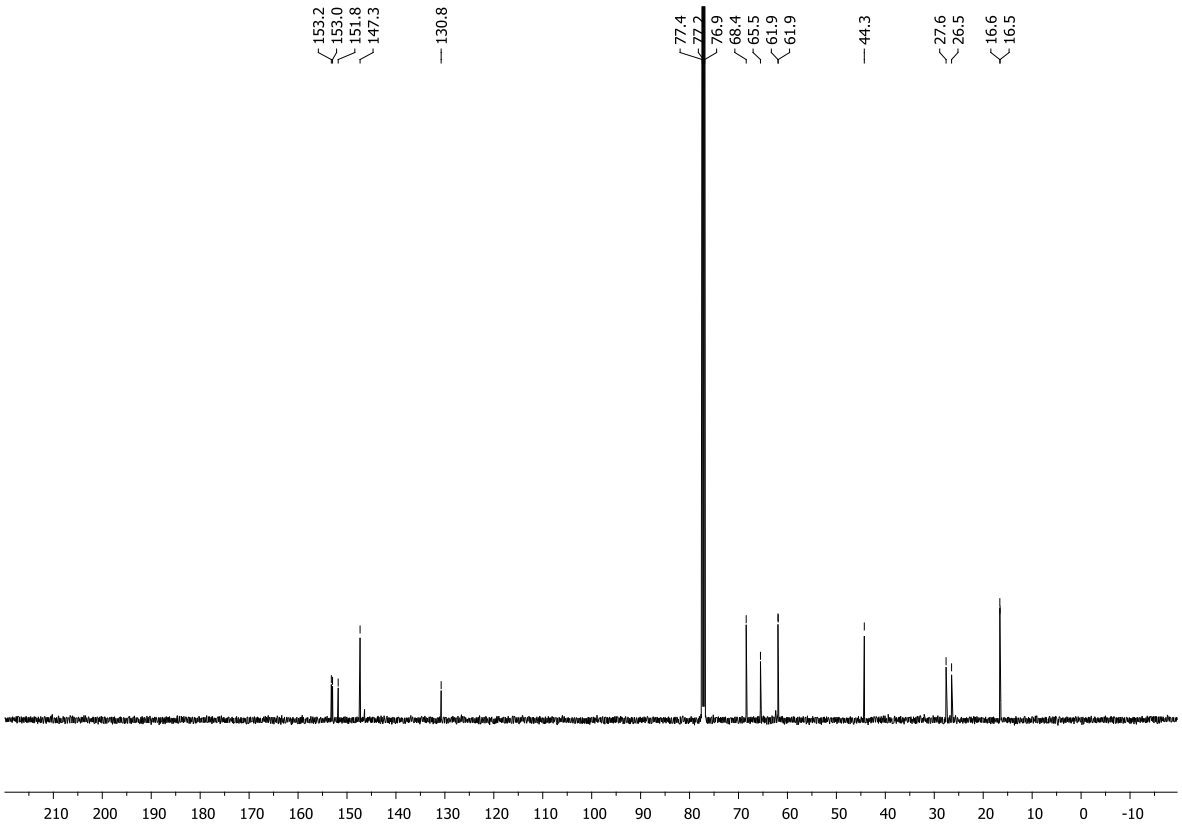
Diethyl {2-[2-(2,6-dichloro-9*H*-purin-9-yl)ethoxy]ethyl}phosphonate (A)



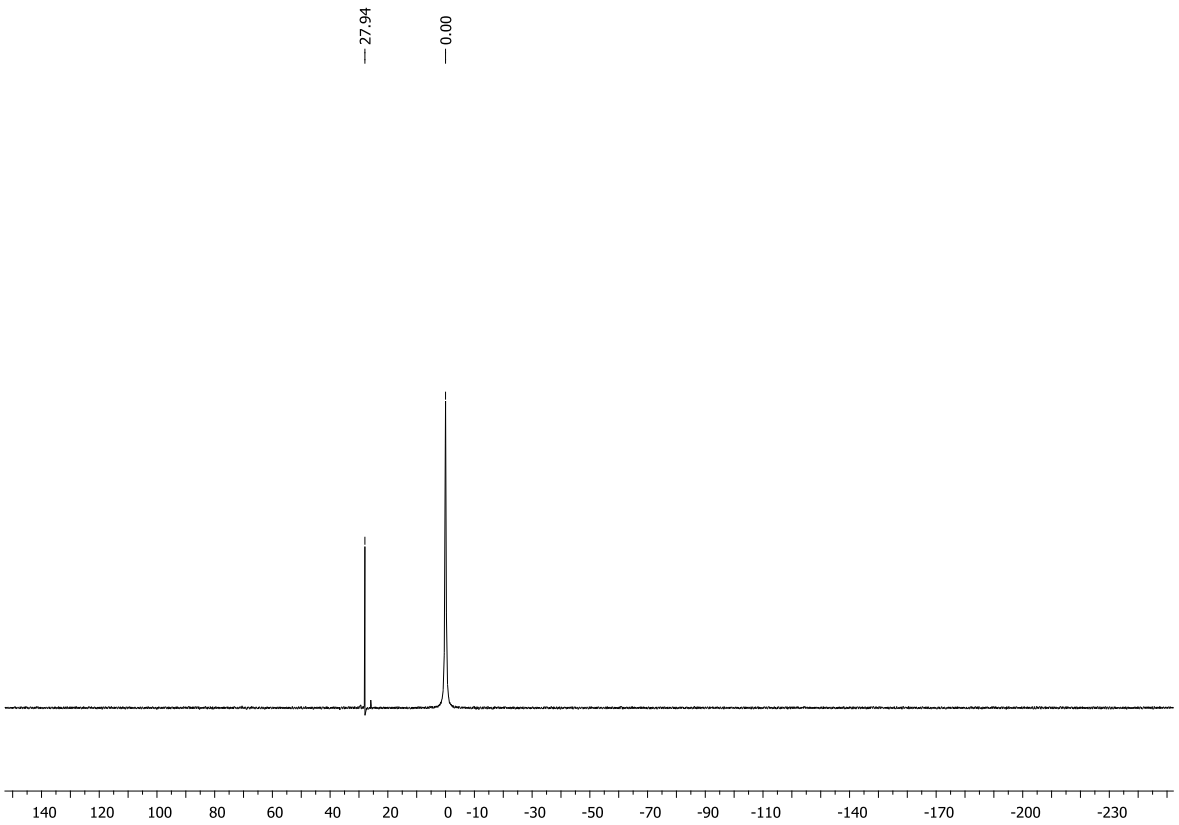
^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound A:



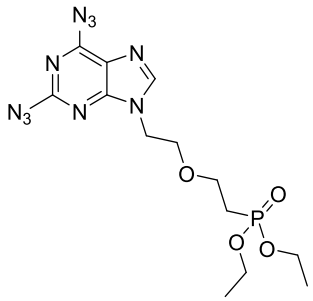
^{13}C-NMR (126 MHz, $CDCl_3$) spectrum of compound A:



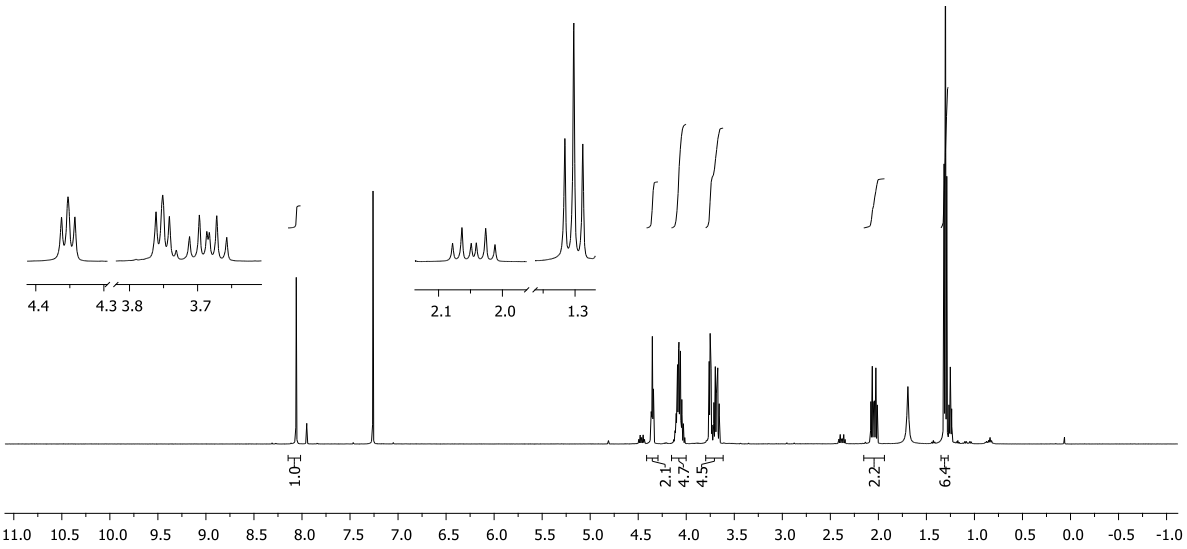
^{31}P-NMR (202 MHz, $CDCl_3$) spectrum of compound A:



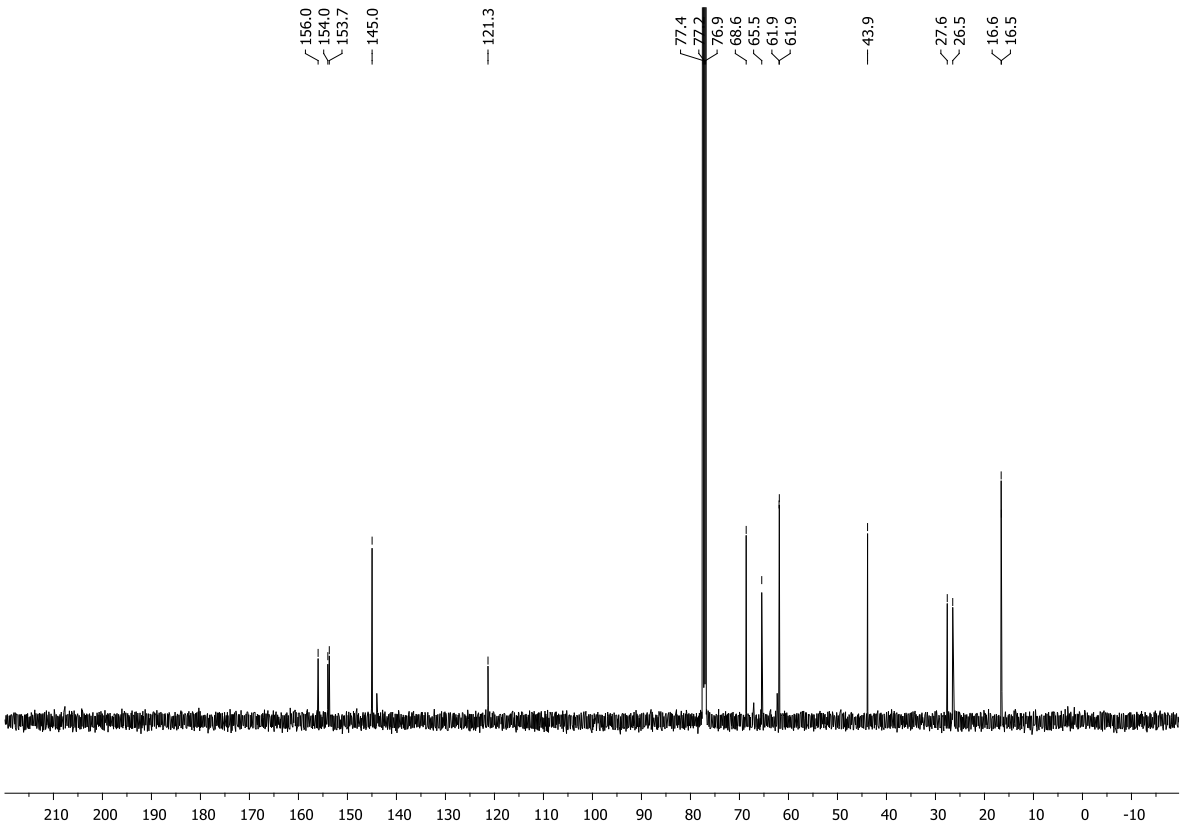
Diethyl {2-[2-(2,6-diazido-9*H*-purin-9-yl)ethoxy]ethyl}phosphonate (6)



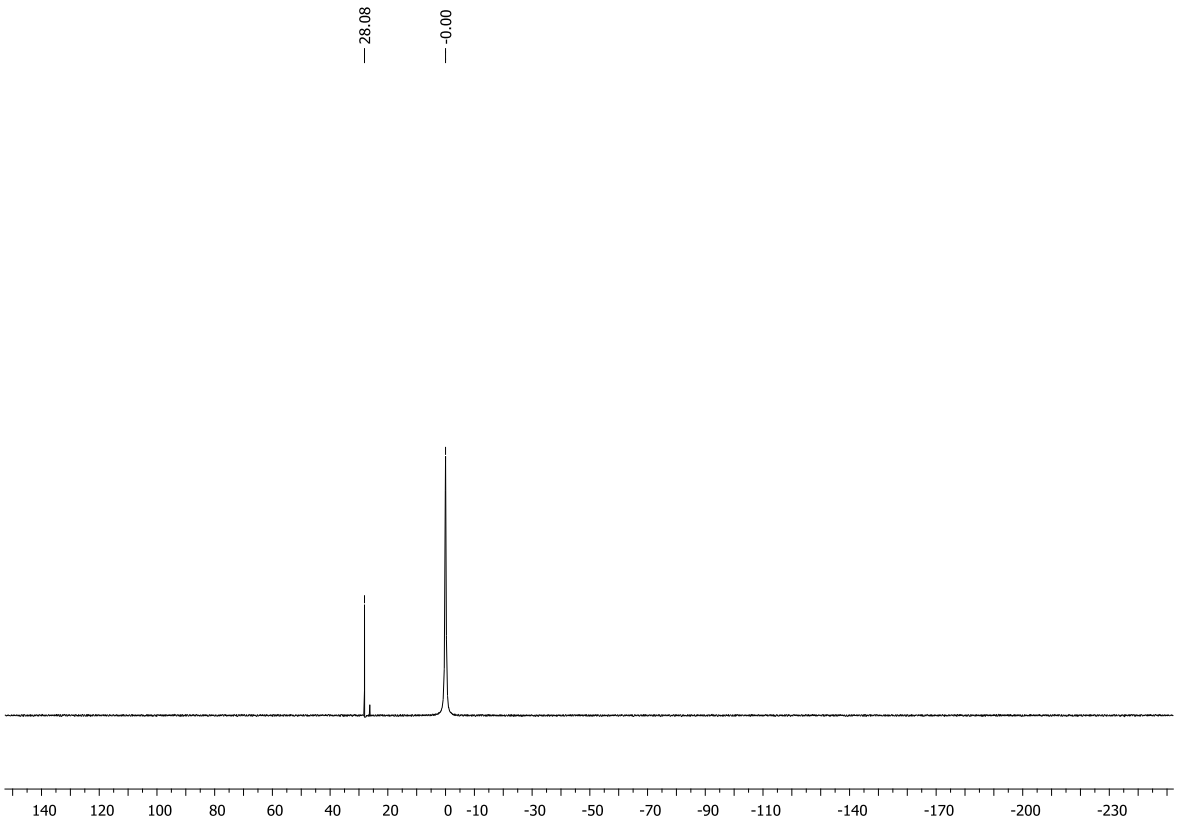
^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound 6:



^{13}C-NMR (126 MHz, $CDCl_3$) spectrum of compound 6:

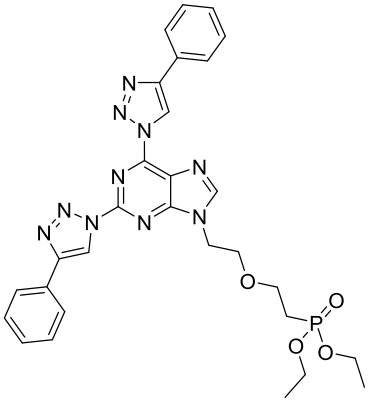


^{31}P-NMR (202 MHz, $CDCl_3$) spectrum of compound 6:

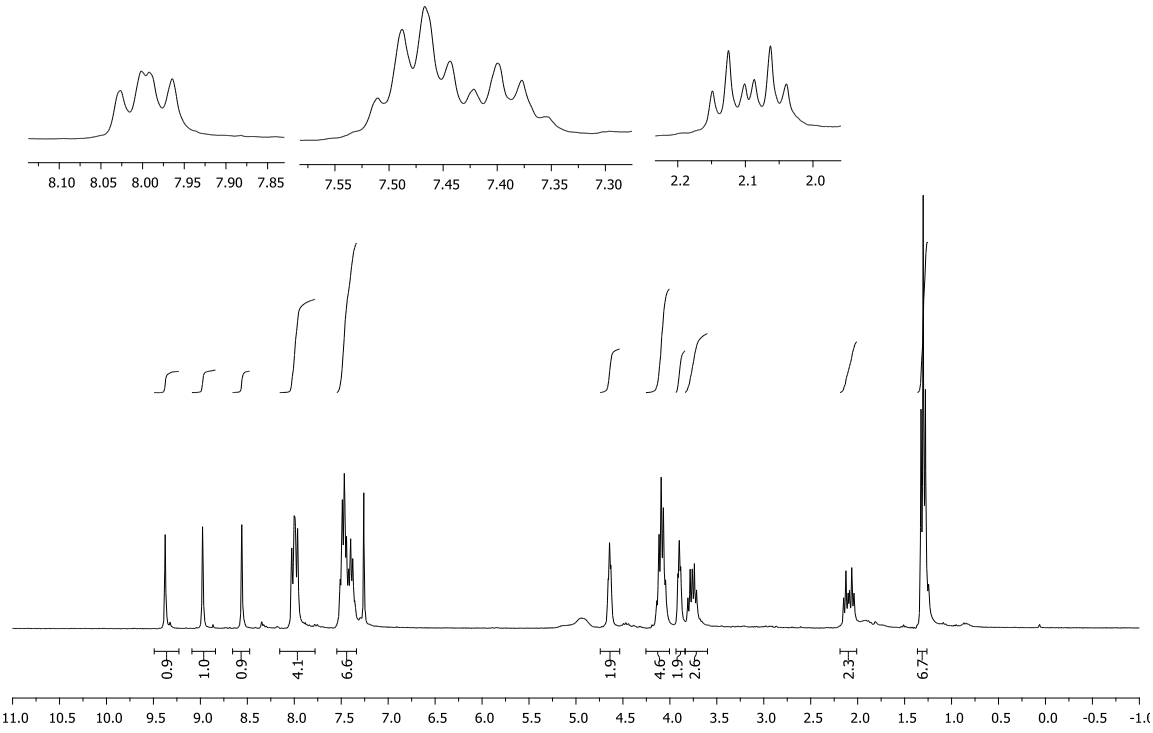


2,6-BISTRIAZOLYLPURINE DERIVATIVES 7

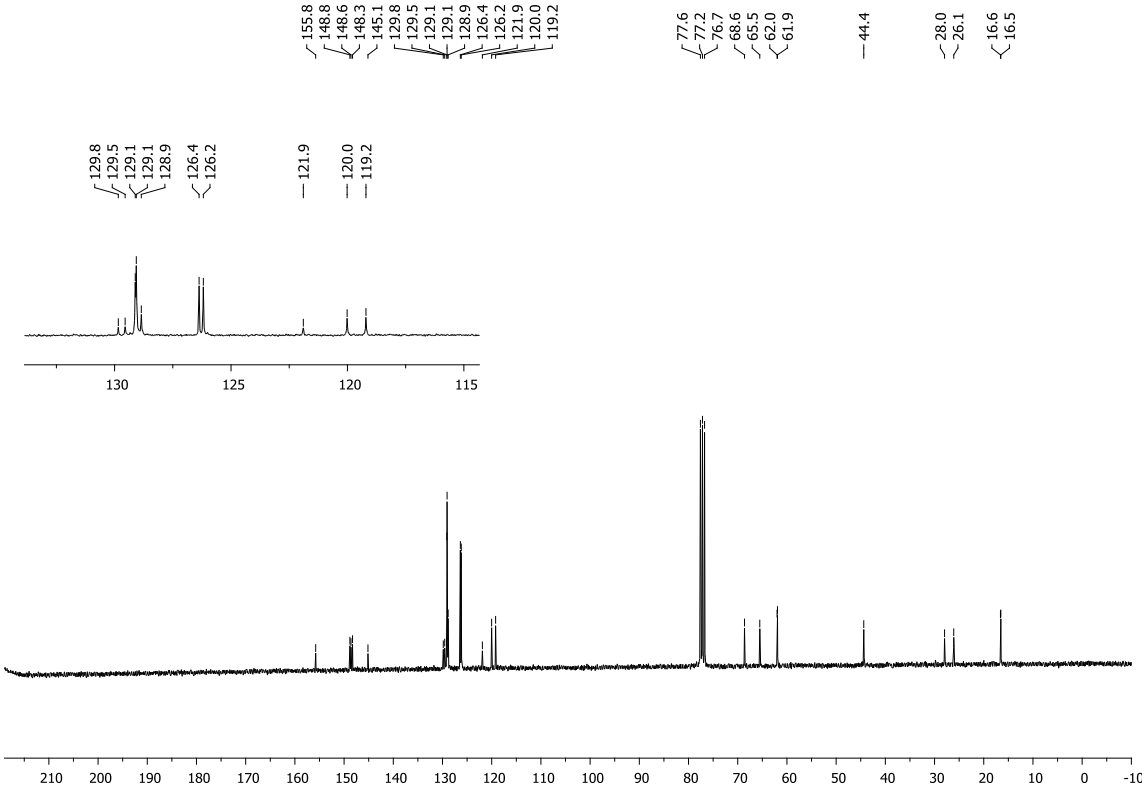
Diethyl (2-{2-[2,6-bis(4-phenyl-1*H*-1,2,3-triazol-1-yl)-9*H*-purin-9-yl]ethoxy}ethyl) phosphonate (7a)



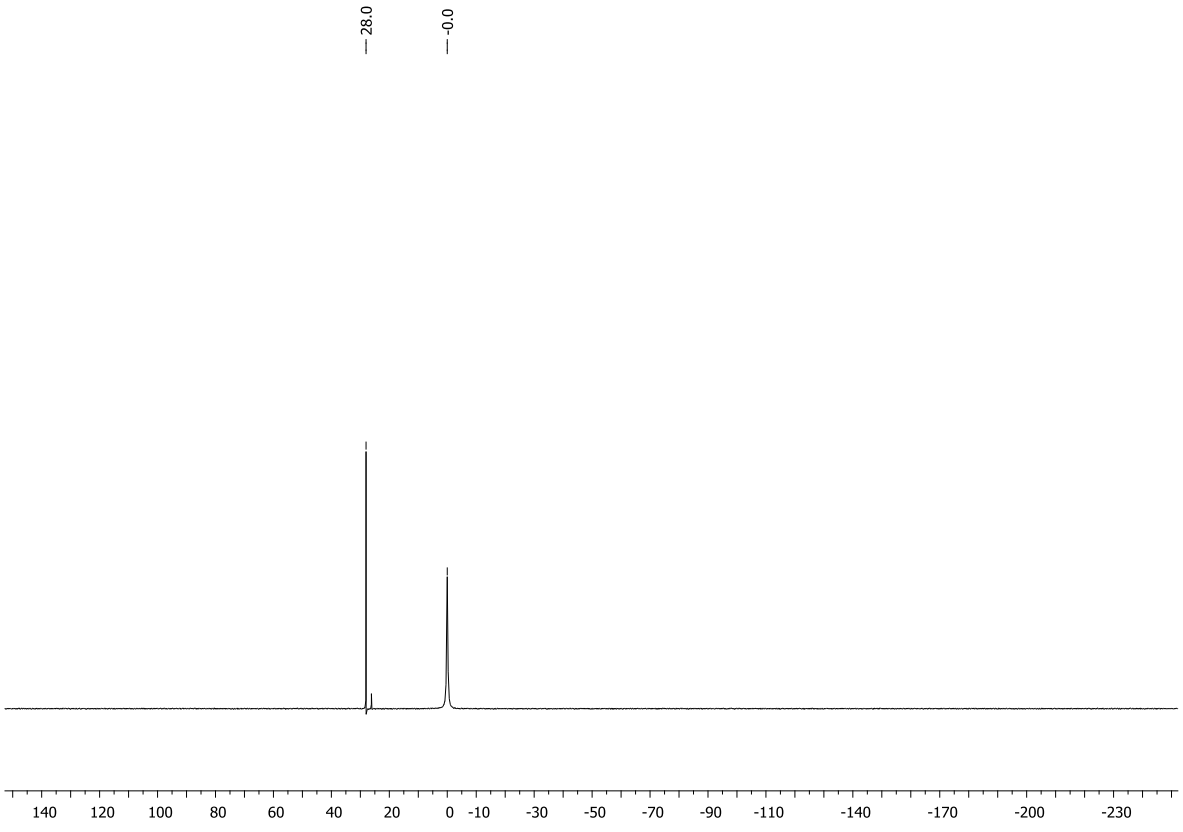
^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 7a:



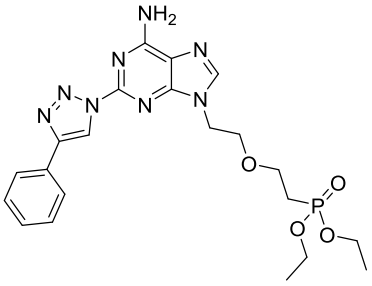
^{13}C-NMR (76 MHz, $CDCl_3$) spectrum of compound 7a:



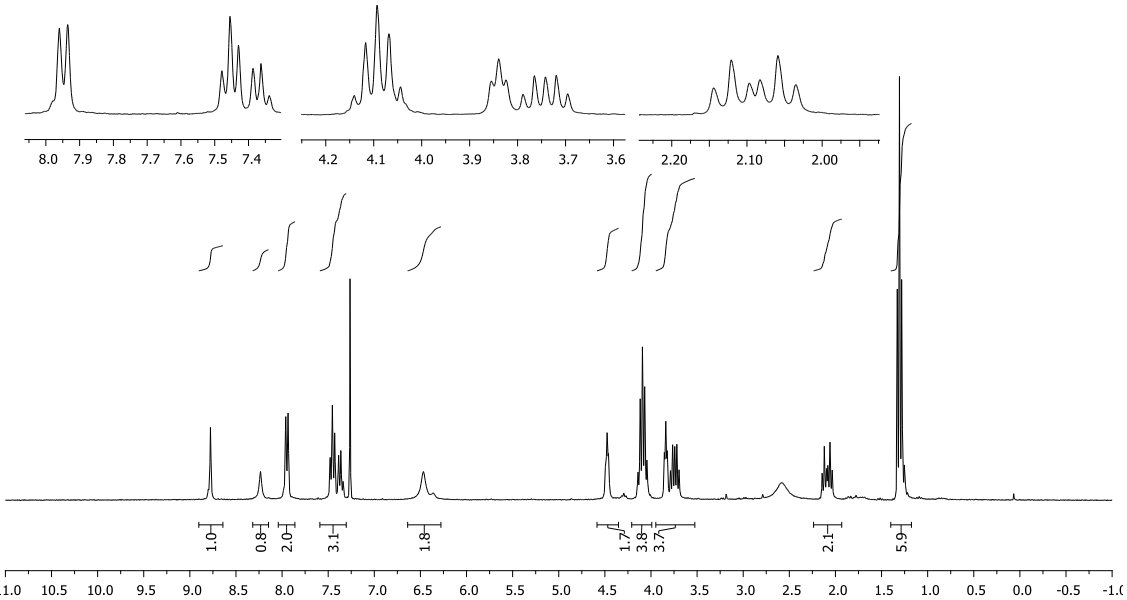
^{31}P-NMR (202 MHz, $CDCl_3$) spectrum of compound 7a:



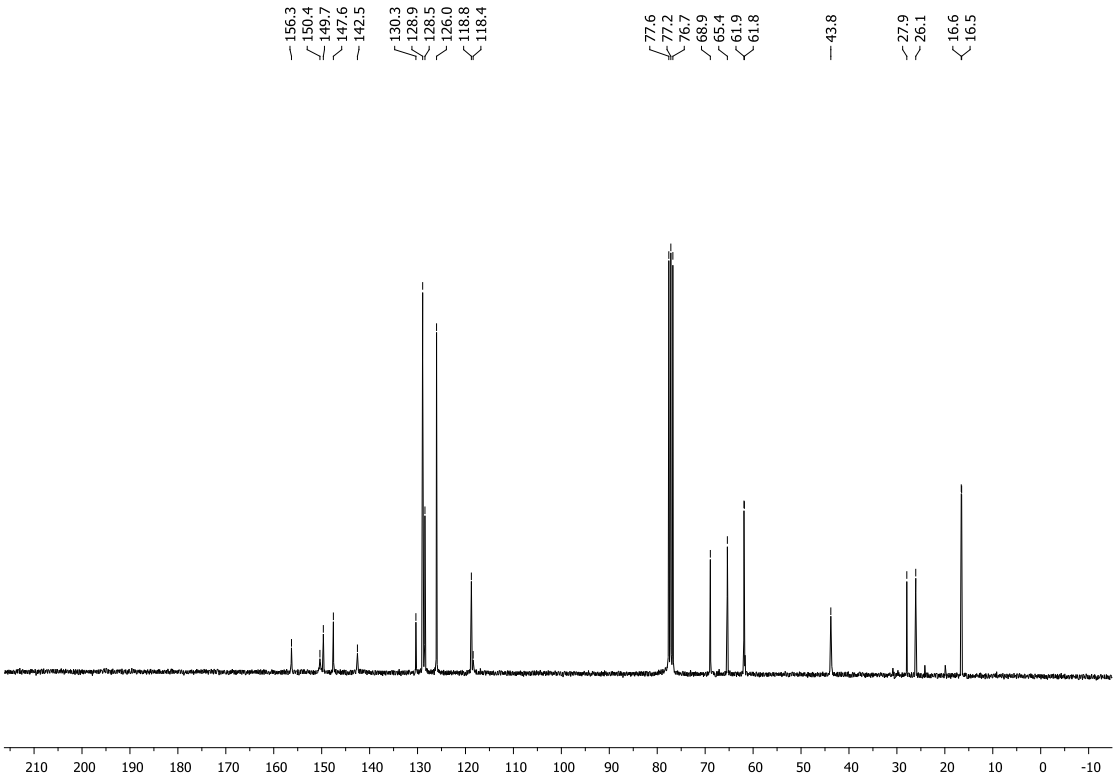
Diethyl (2-{2-[6-amino-2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-9*H*-purin-9-yl]ethoxy}ethyl)phosphonate (7a')



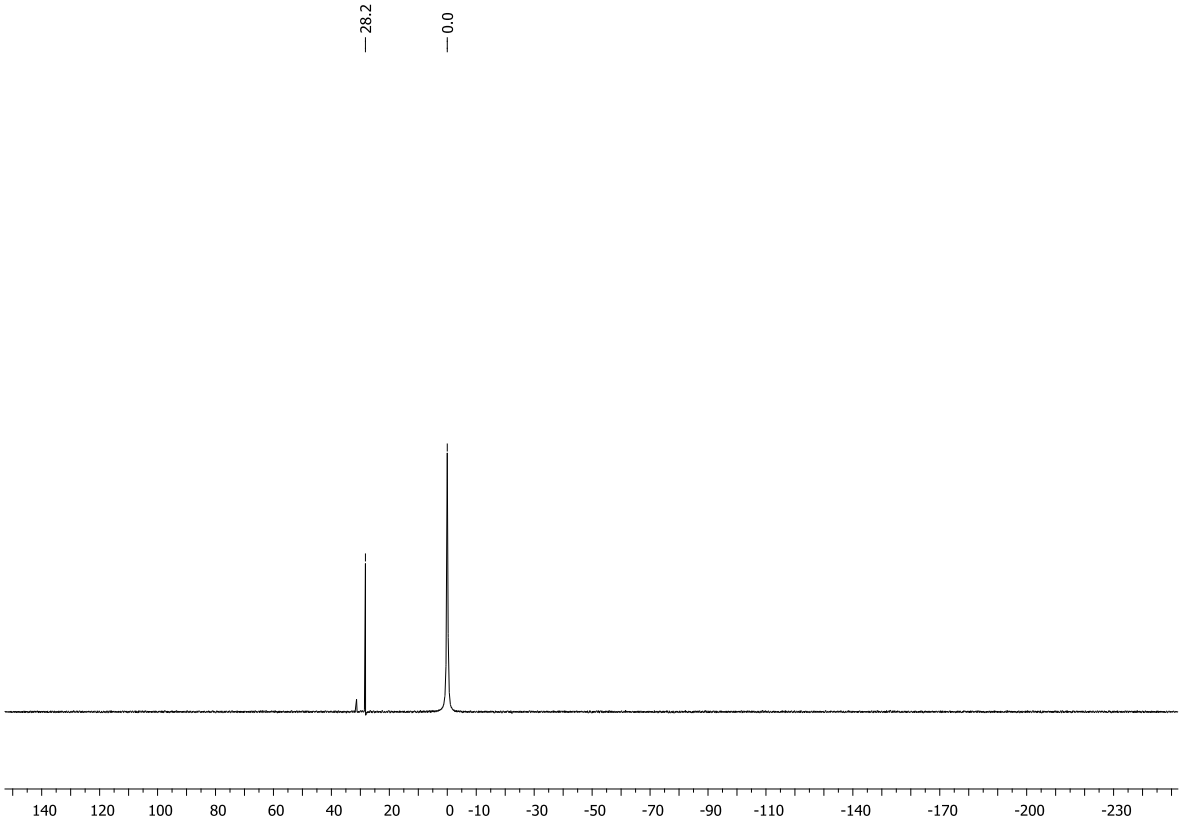
^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 7a':



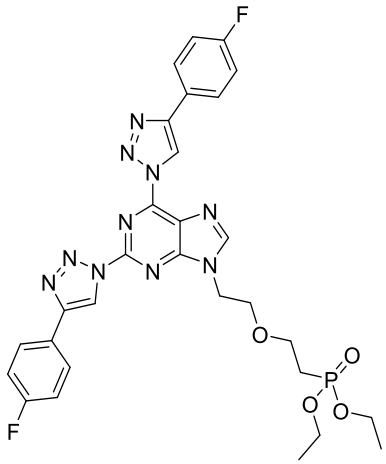
^{13}C-NMR (76 MHz, $CDCl_3$) spectrum of compound 7a':



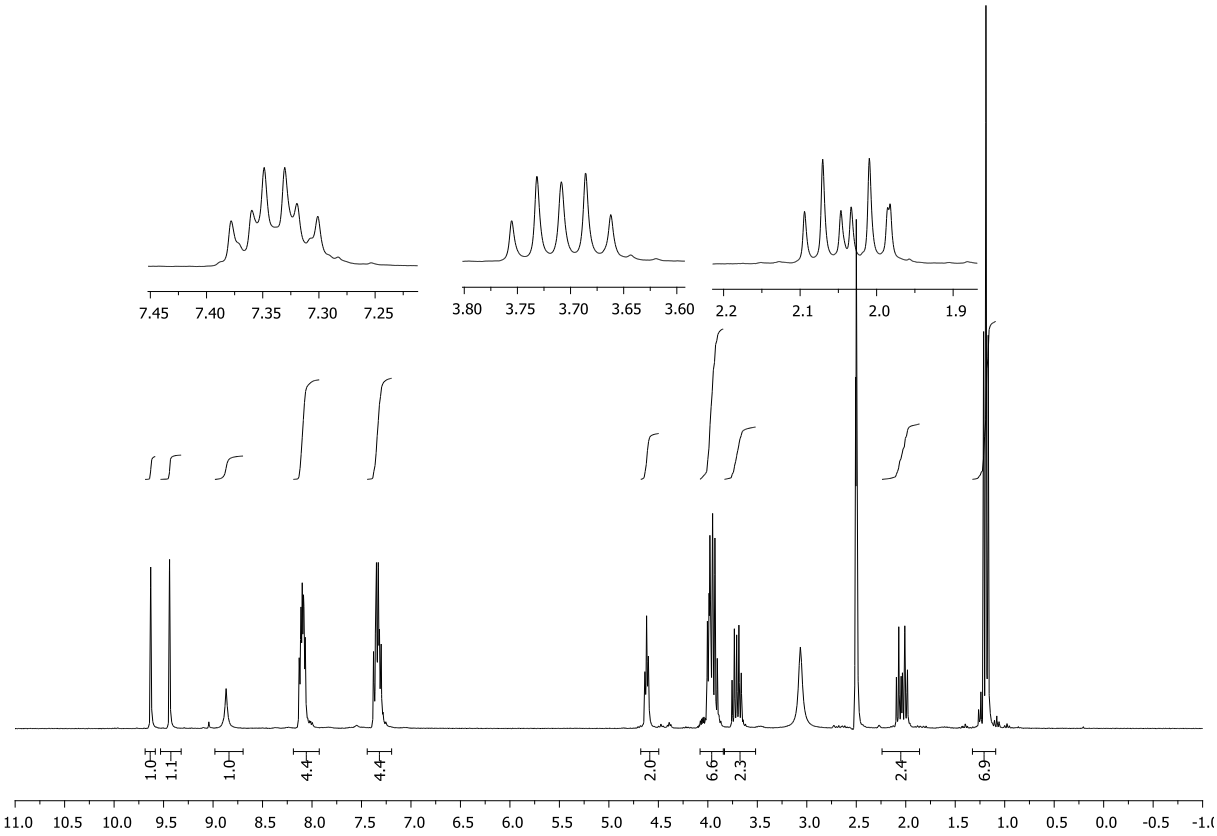
^{31}P-NMR (202 MHz, $CDCl_3$) spectrum of compound 7a':



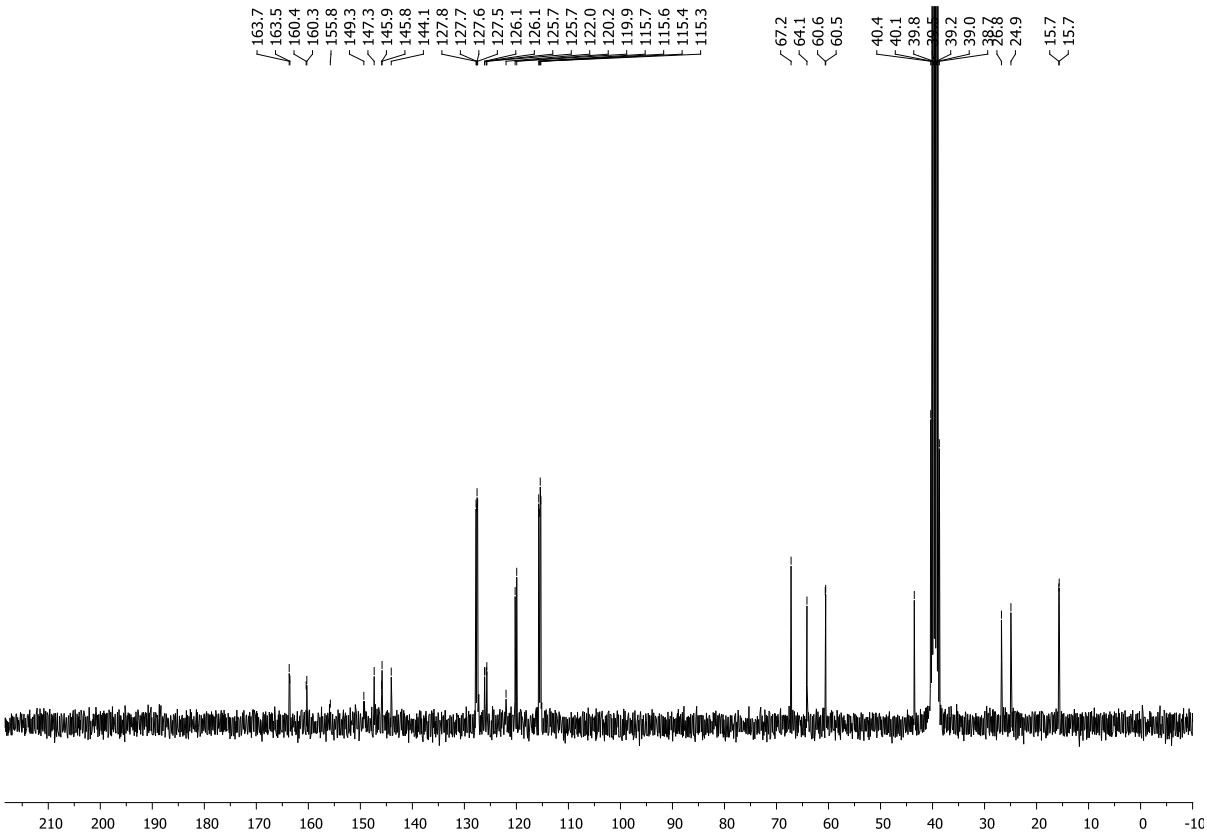
Diethyl [2-(2-{2,6-bis[4-(4-fluorophenyl)-1*H*-1,2,3-triazol-1-yl]-9*H*-purin-9-yl}ethoxy) ethyl]phosphonate (7b)



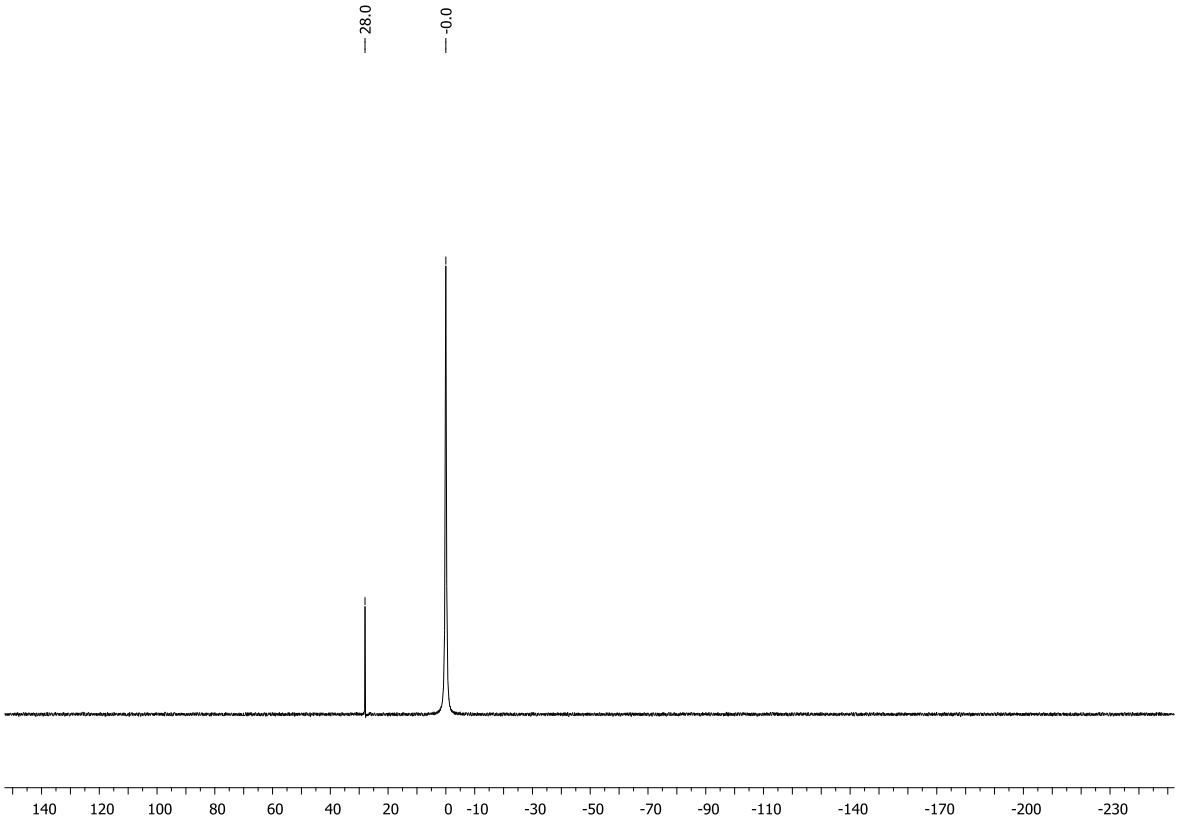
^{1}H-NMR (300 MHz, DMSO-d$_6$, 70 ^{o}C) spectrum of compound 7b:



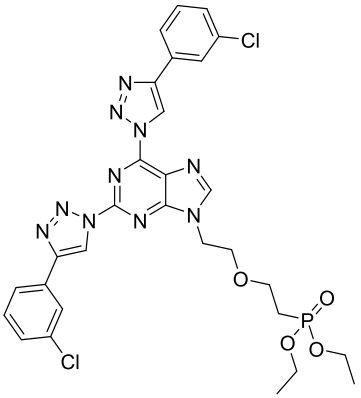
^{13}C-NMR (76 MHz, DMSO-d_6, 70 ^{o}C) spectrum of compound 7b:



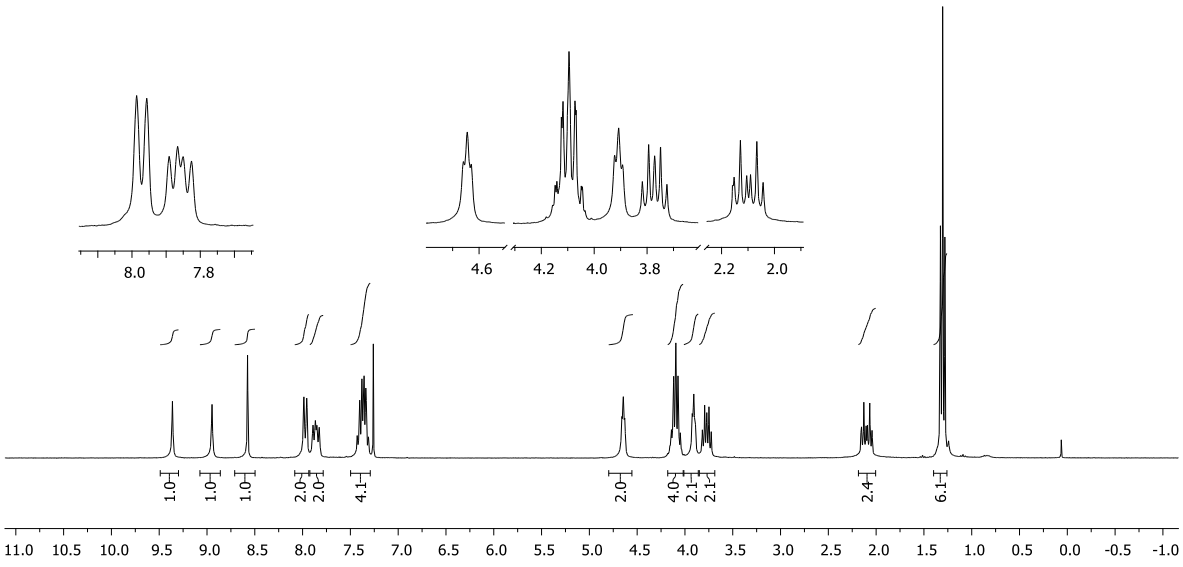
^{31}P-NMR (202 MHz, $CDCl_3$) δ (ppm) spectrum of compound 7b:



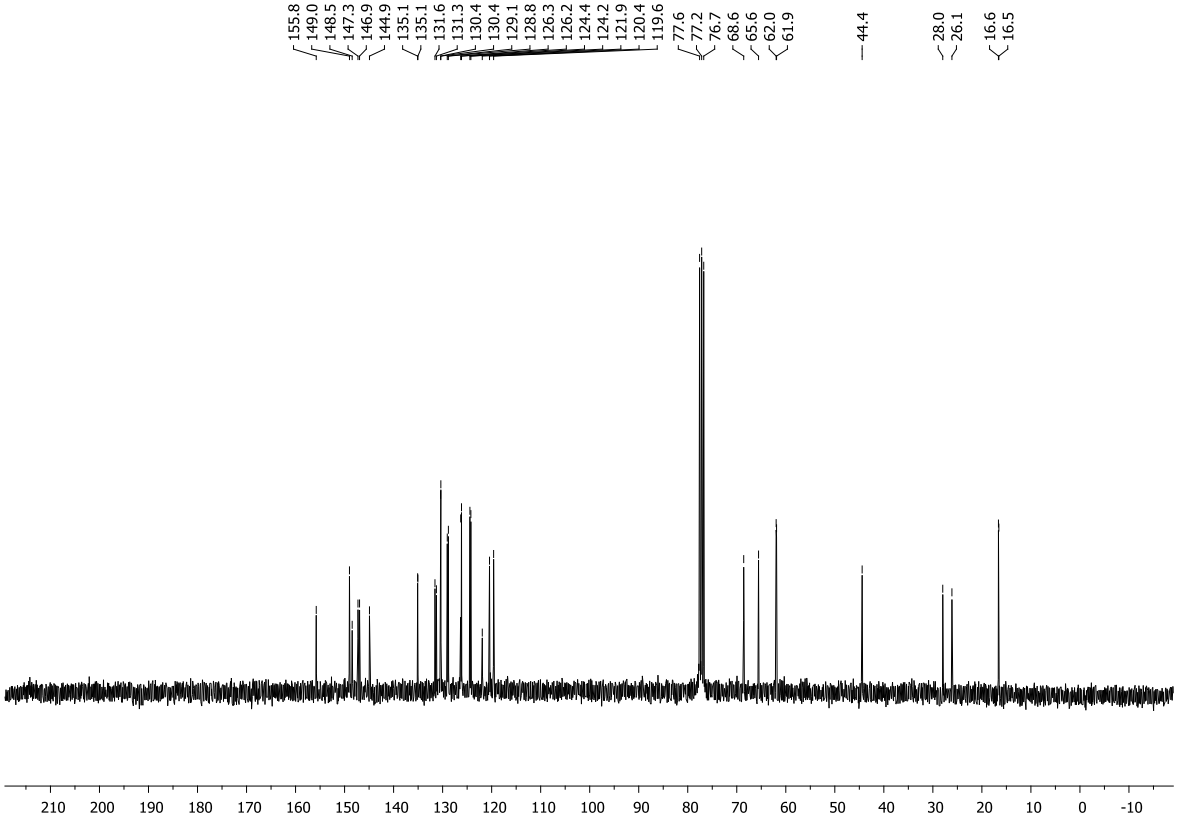
Diethyl [2-(2-{2,6-bis[4-(3-chlorophenyl)-1*H*-1,2,3-triazol-1-yl]-9*H*-purin-9-yl}ethoxy) ethyl]phosphonate (7c)



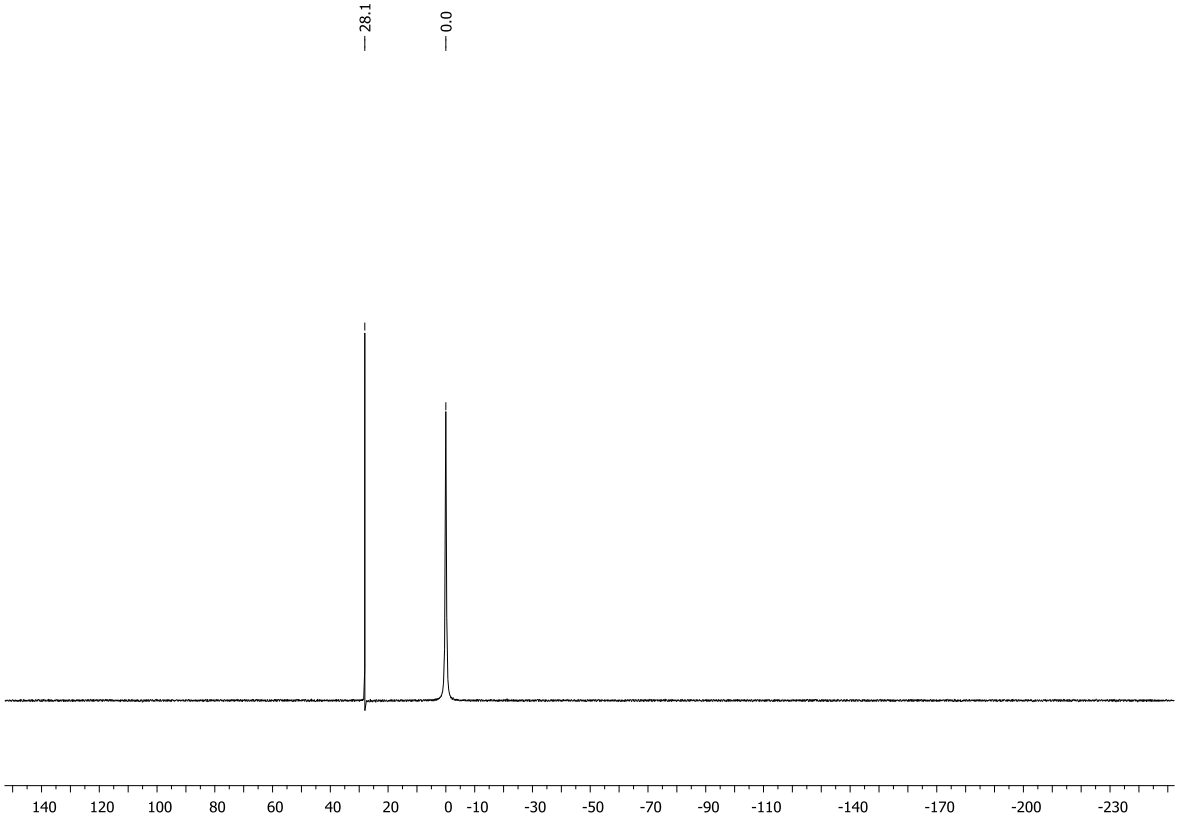
^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 7c:



^{13}C-NMR (75.5 MHz, $CDCl_3$) spectrum of compound 7c:

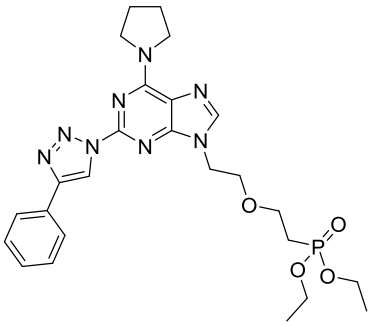


^{31}P-NMR (202 MHz, $CDCl_3$) spectrum of compound 7c:

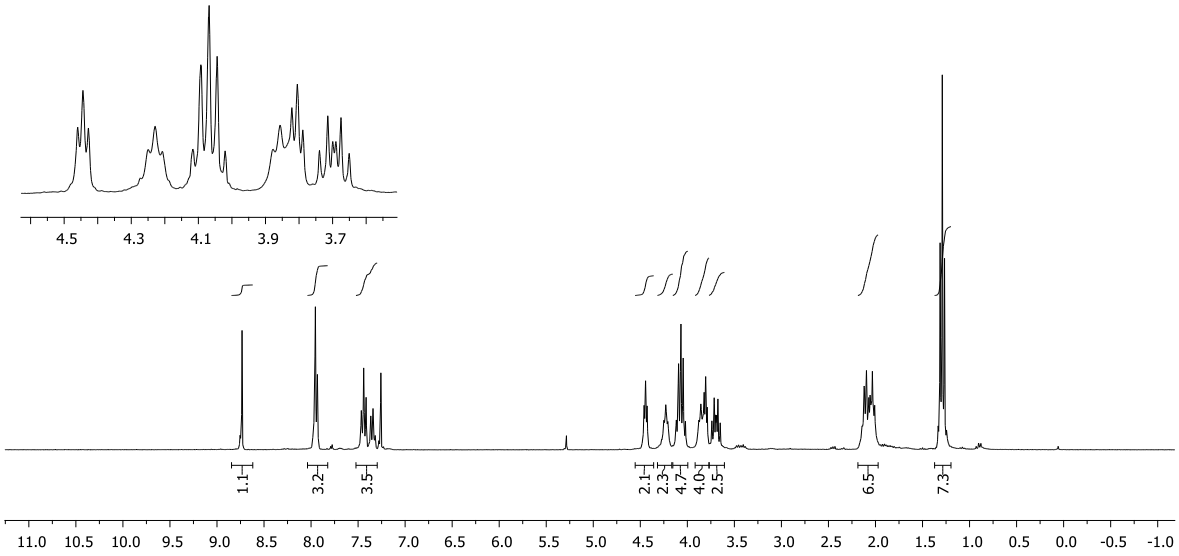


6-*N*-SUBSTITUTED 2-TRIAZOLYLPURINE DERIVATIVES

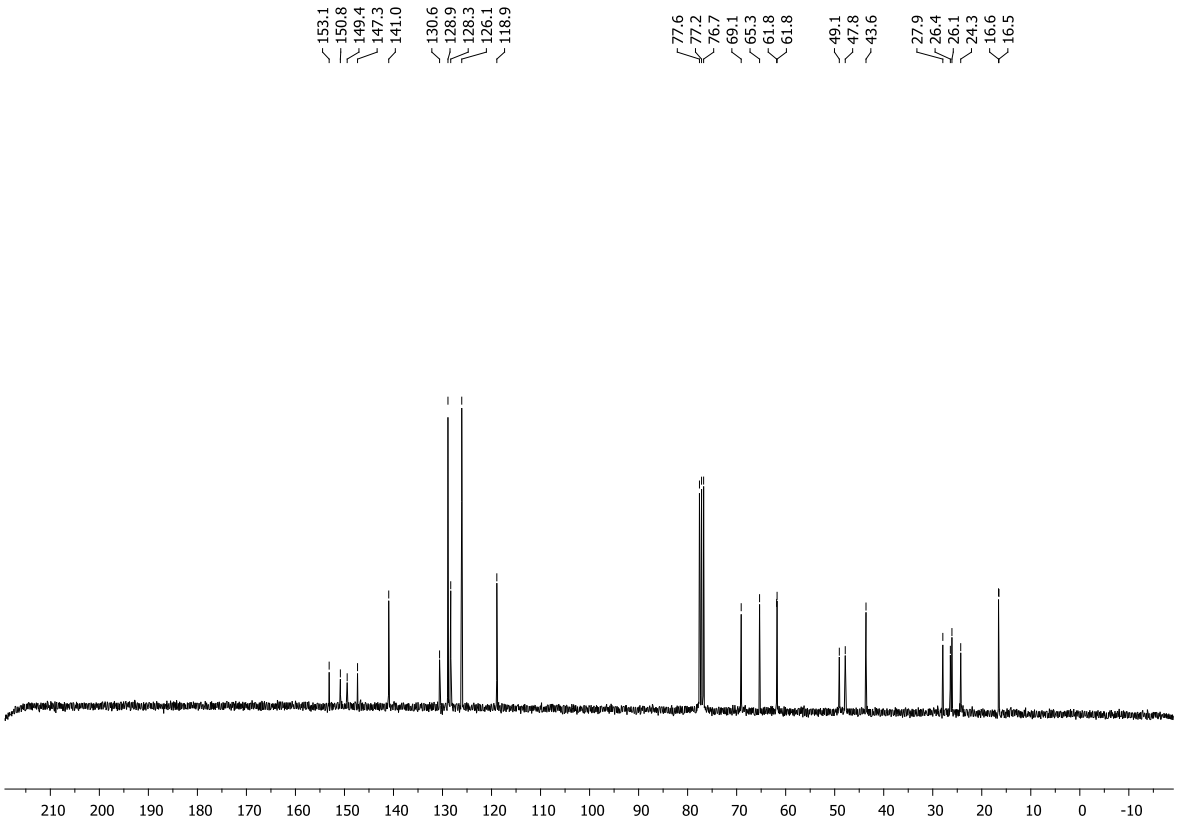
Diethyl (2-{2-[2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-6-(pyrrolidin-1-yl)-9*H*-purin-9-yl]ethoxy}ethyl)phosphonate (8a)



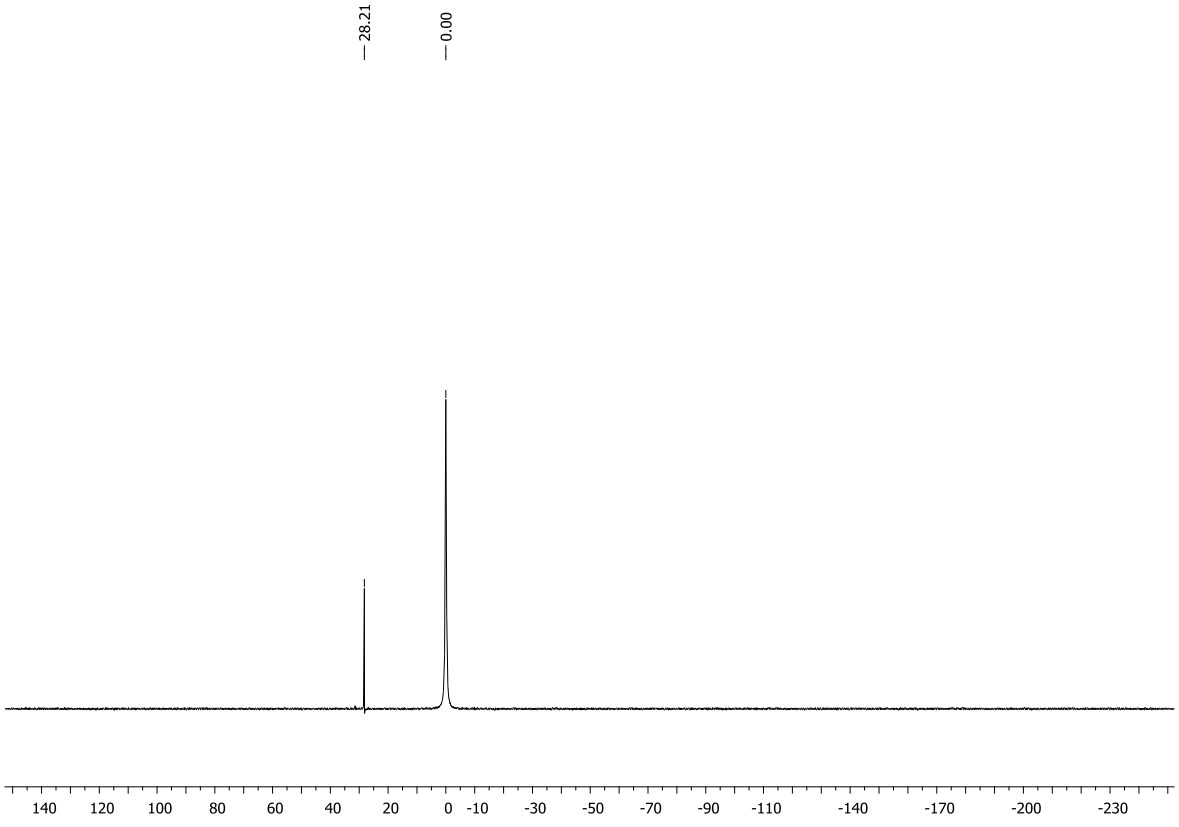
^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 8a:



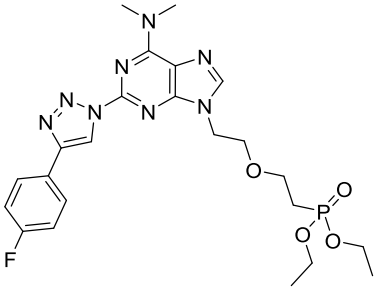
^{13}C-NMR (76 MHz, $CDCl_3$) spectrum of compound 8a:



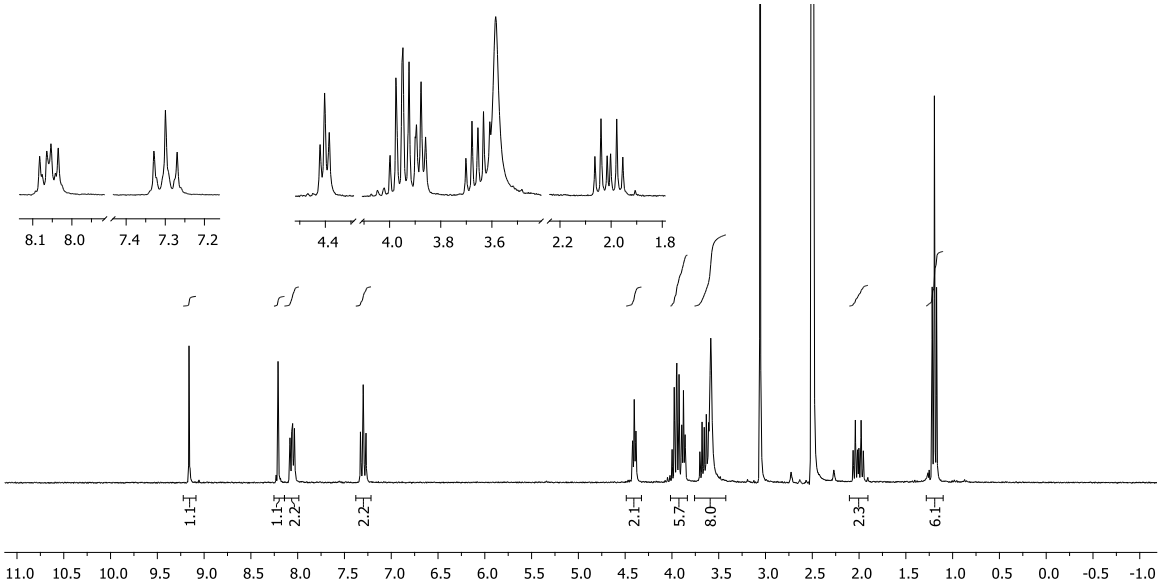
^{31}P-NMR (202 MHz, $CDCl_3$) spectrum of compound 8a:



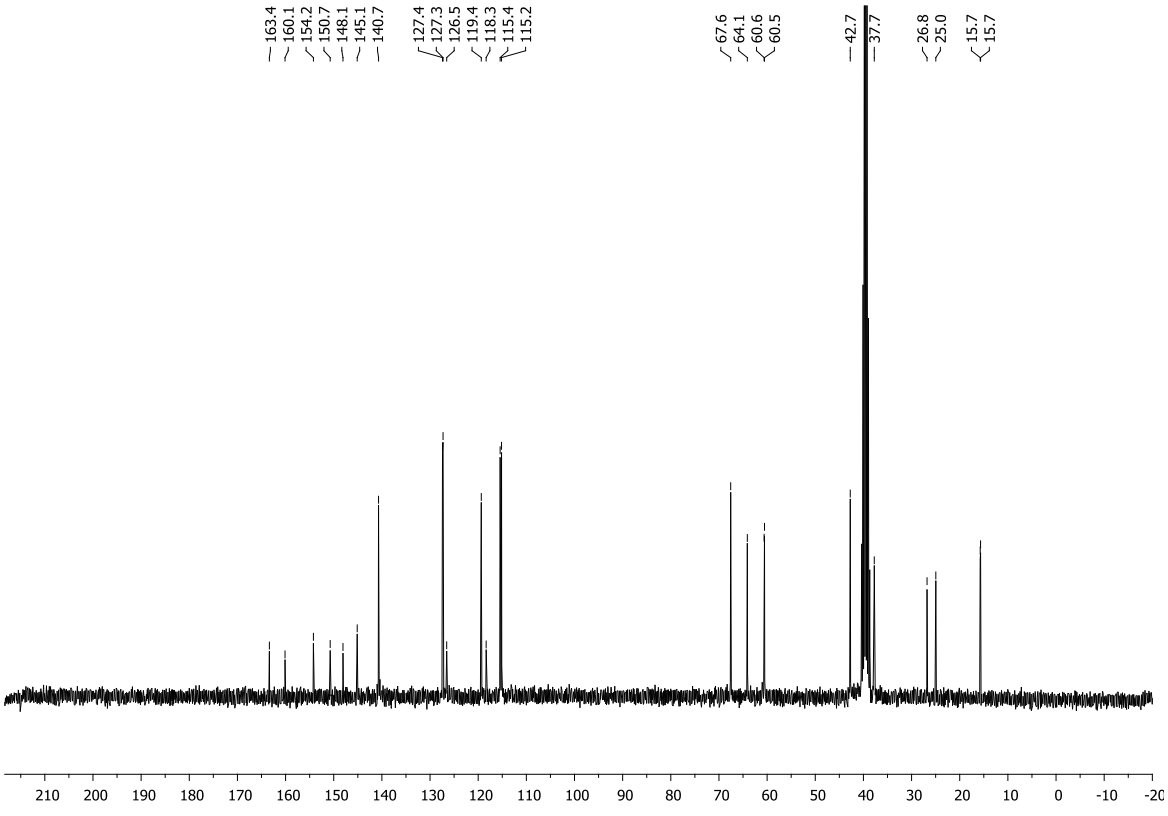
Diethyl [2-(2-{6-(dimethylamino)-2-[4-(4-fluorophenyl)-1*H*-1,2,3-triazol-1-yl]-9*H*-purin-9-yl}ethoxy)ethyl]phosphonate (8b)



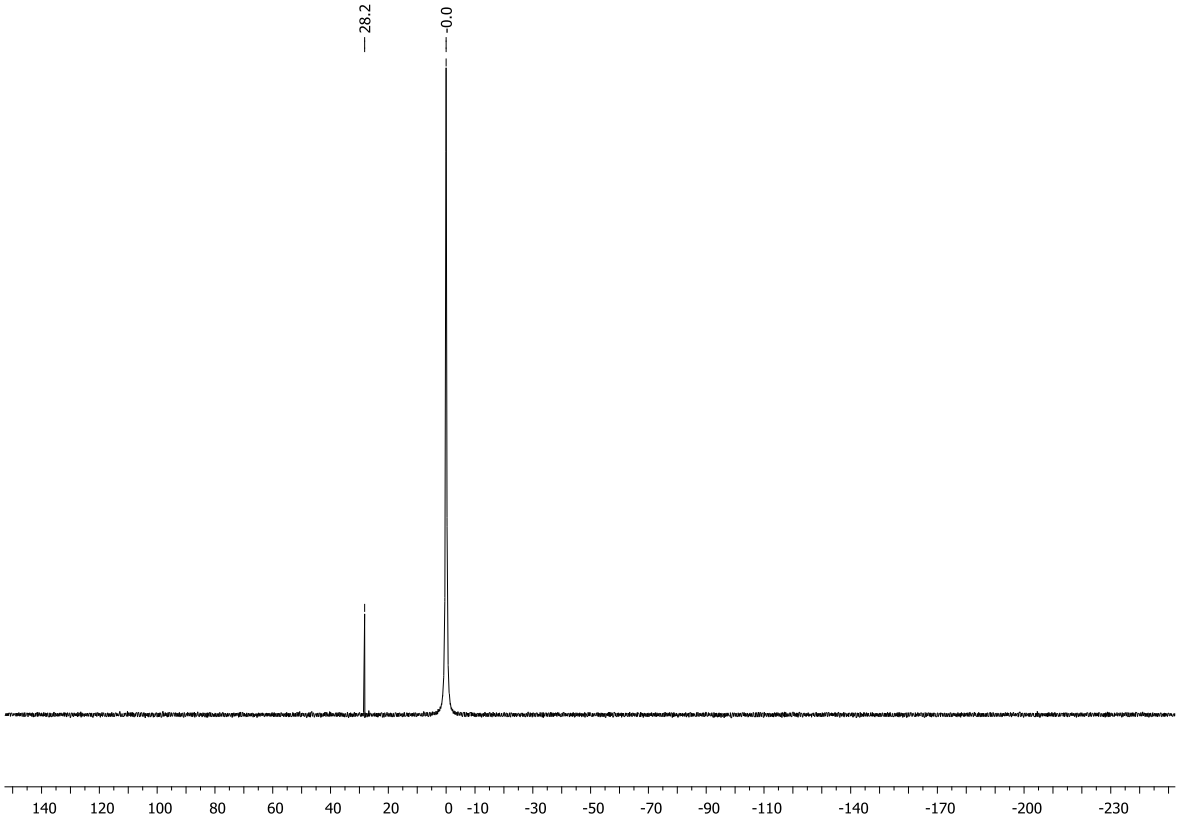
^{1}H-NMR (300 MHz, DMSO-d$_6$) spectrum of compound 8b:



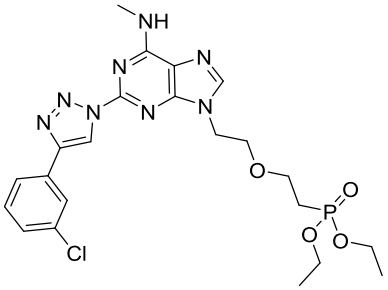
^{13}C-NMR (76 MHz, DMSO-d$_6$) spectrum of compound 8b:



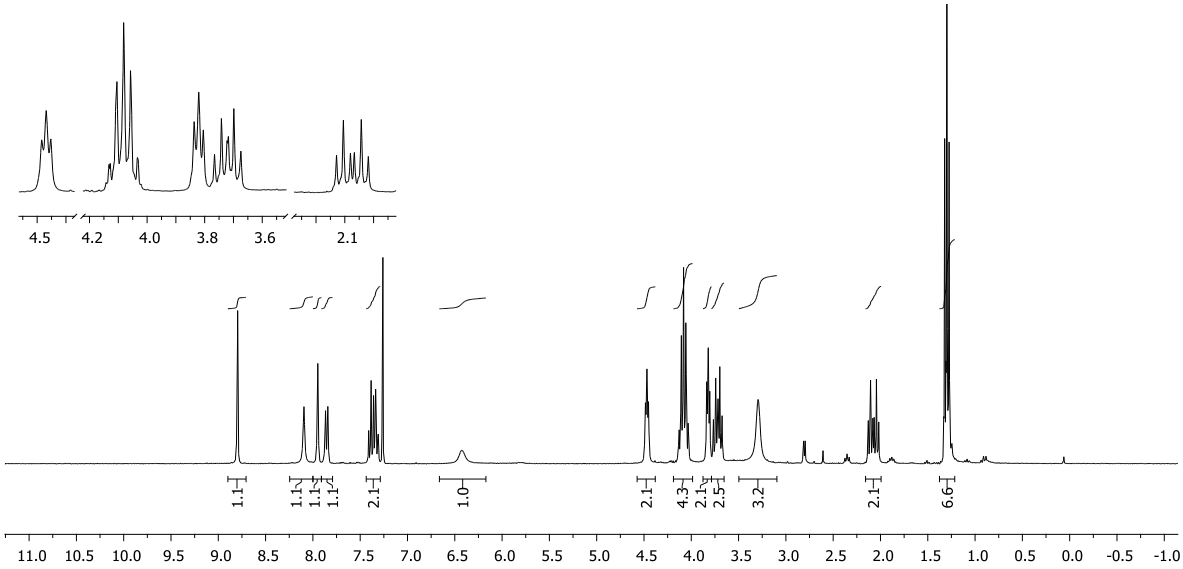
^{31}P-NMR (202 MHz, DMSO-d_6) spectrum of compound 8b:



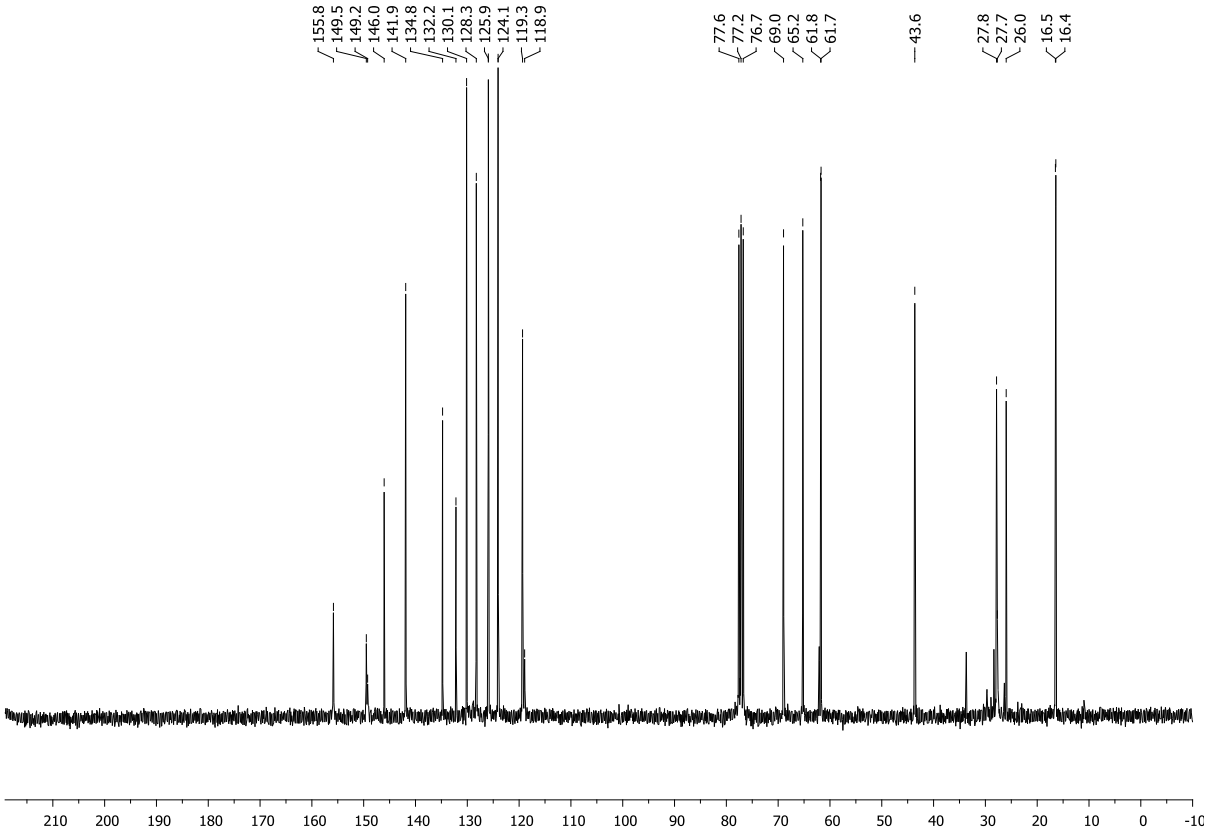
Diethyl [2-(2-{2-[4-(3-chlorophenyl)-1*H*-1,2,3-triazol-1-yl]-6-(methylamino)-9*H*-purin-9-yl}ethoxy)ethyl]phosphonate (8c)



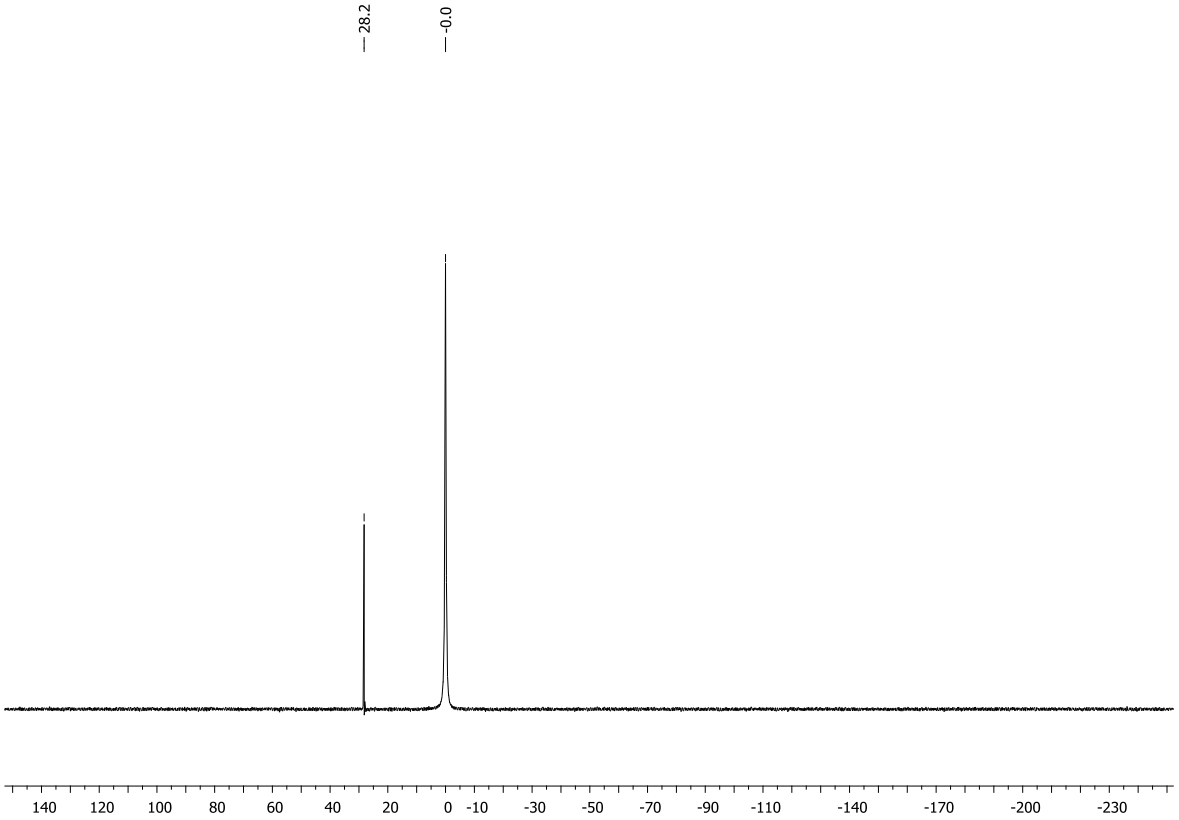
^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 8c:



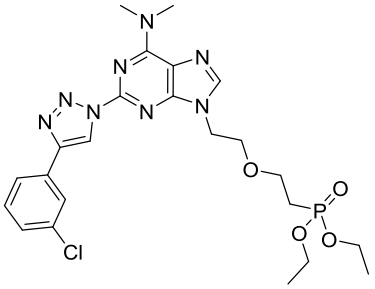
^{13}C-NMR (76 MHz, $CDCl_3$) spectrum of compound 8c:



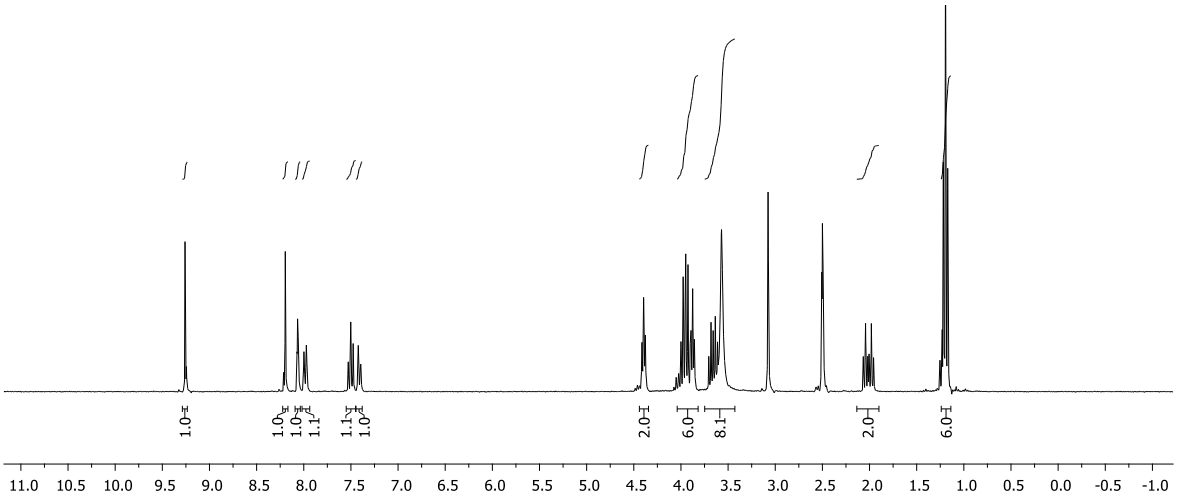
^{31}P-NMR (202 MHz, $CDCl_3$) spectrum of compound 8c:



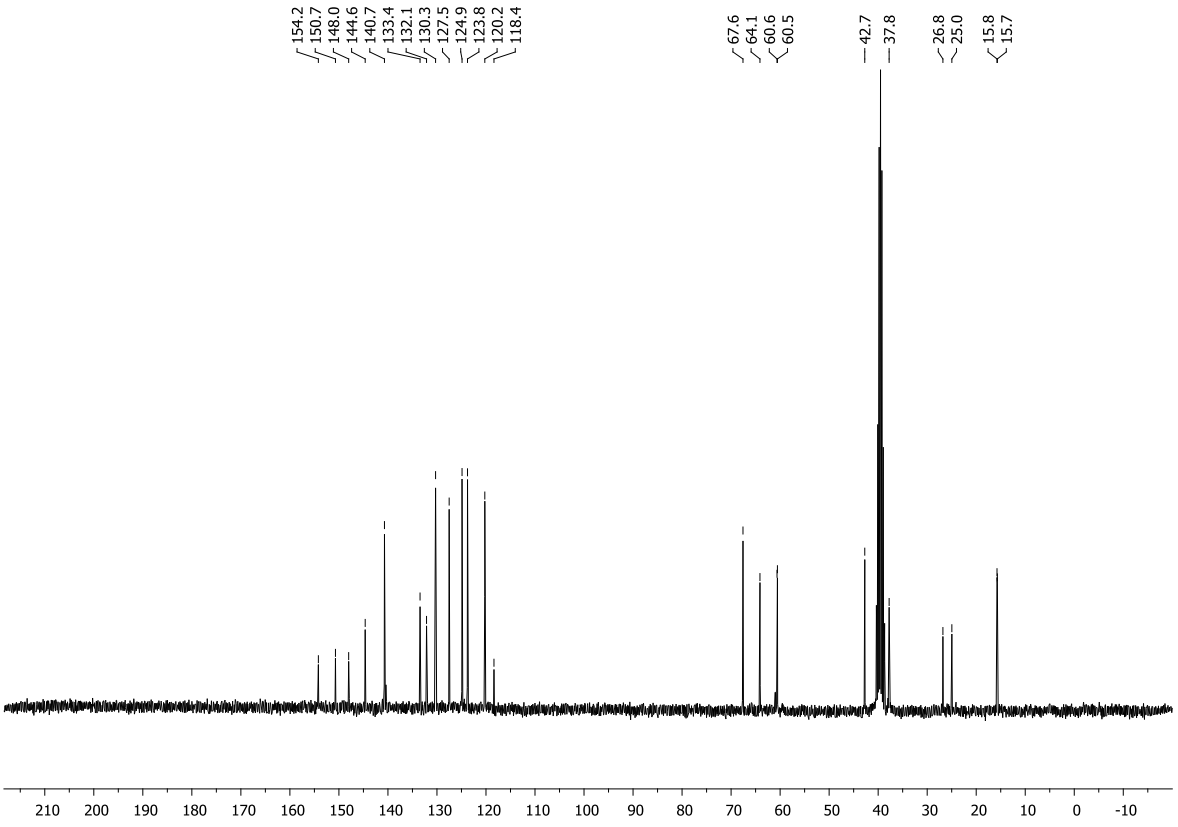
Diethyl [2-(2-{2-[4-(3-chlorophenyl)-1*H*-1,2,3-triazol-1-yl]-6-(dimethylamino)-9*H*-purin-9-yl}ethoxy)ethyl]phosphonate (8d)



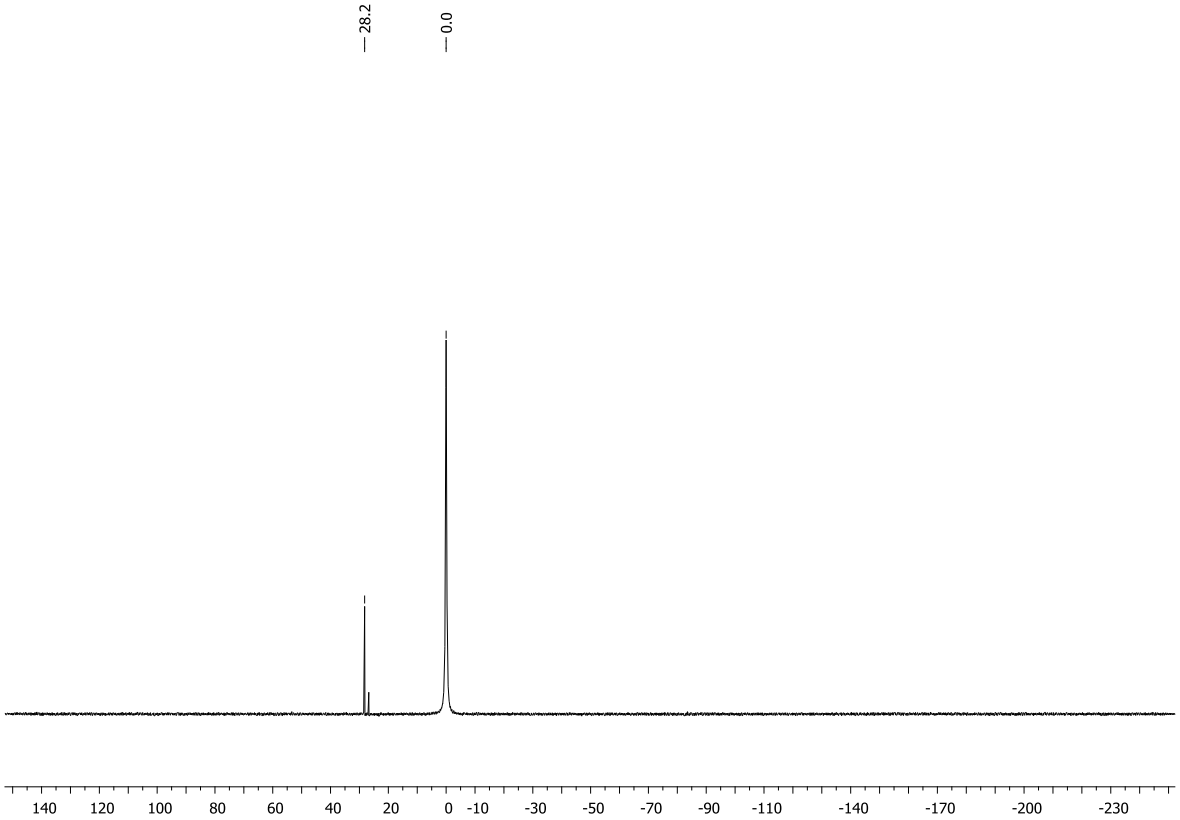
^{1}H-NMR (300 MHz, DMSO-d_6) spectrum of compound 8d:



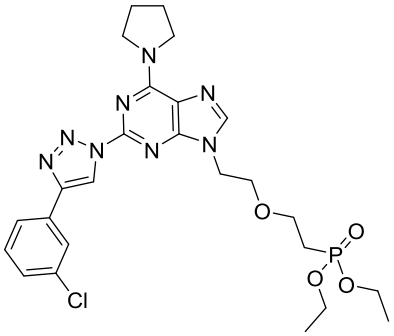
^{13}C-NMR (76 MHz, DMSO-d_6) spectrum of compound 8d:



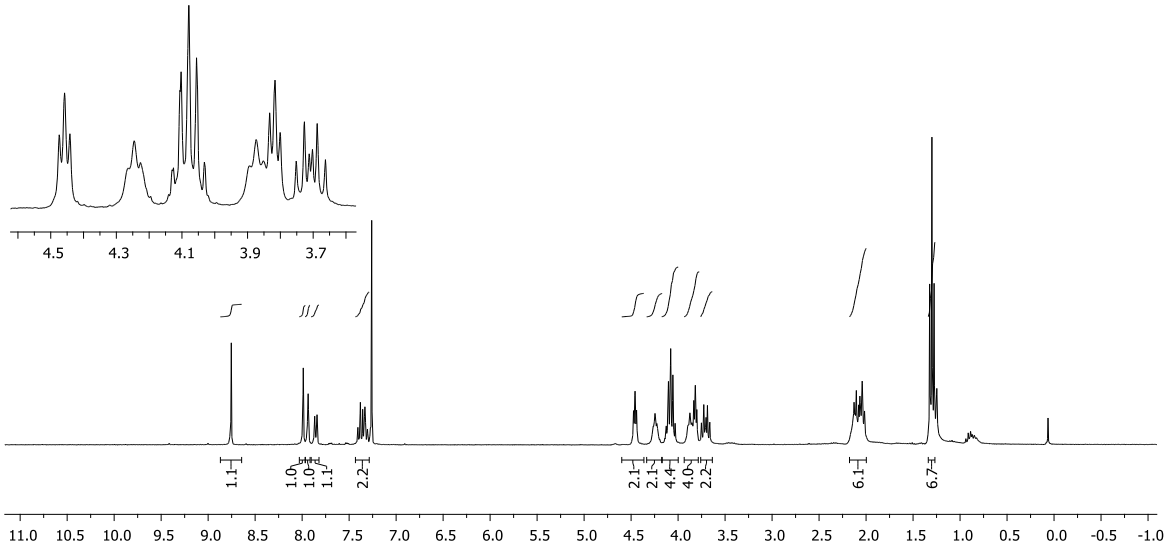
^{31}P-NMR (202 MHz, DMSO-d_6) spectrum of compound 8d:



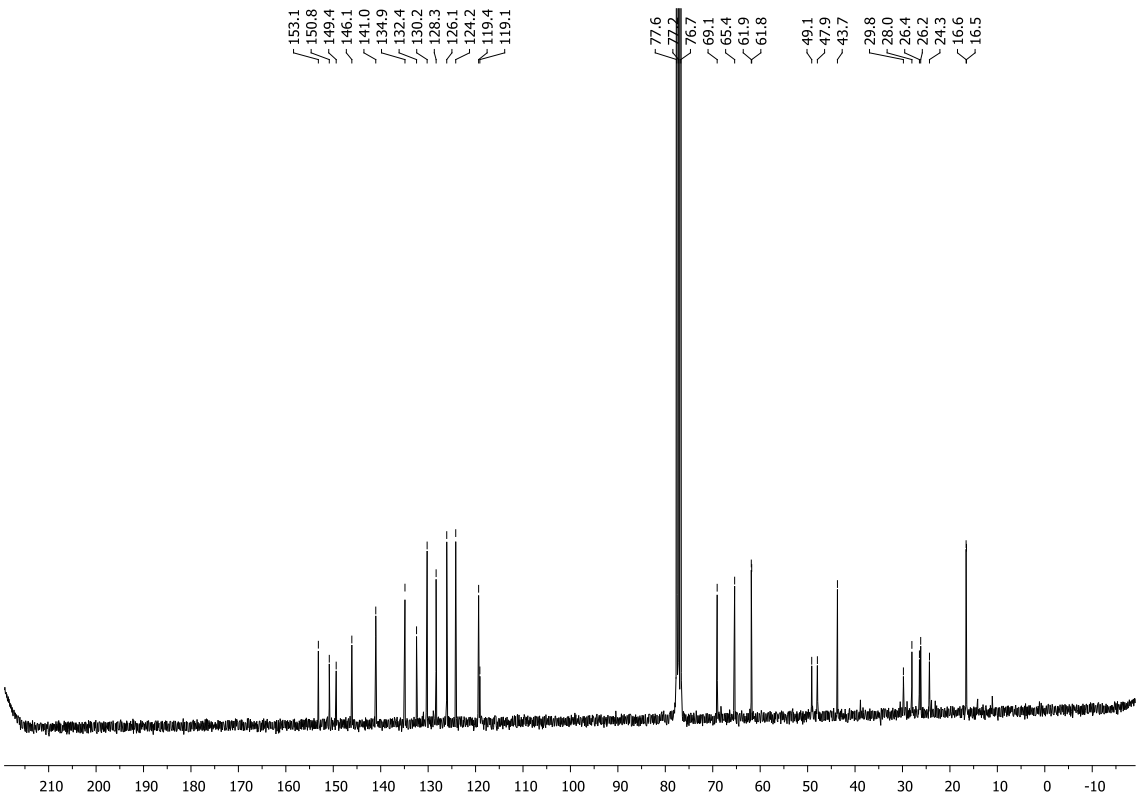
Diethyl [2-(2-{2-[4-(3-chlorophenyl)-1*H*-1,2,3-triazol-1-yl]-6-(pyrrolidin-1-yl)-9*H*-purin-9-yl}ethoxy)ethyl]phosphonate (8e)



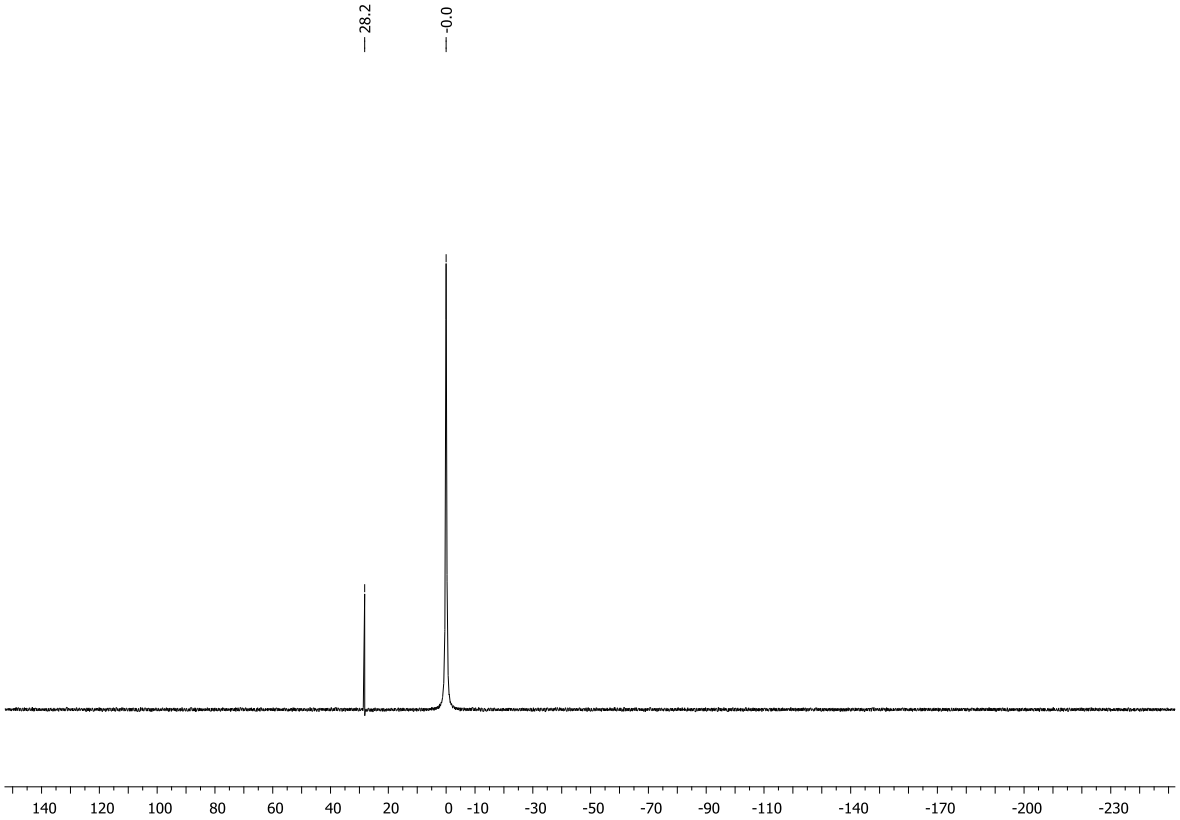
^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 8e:



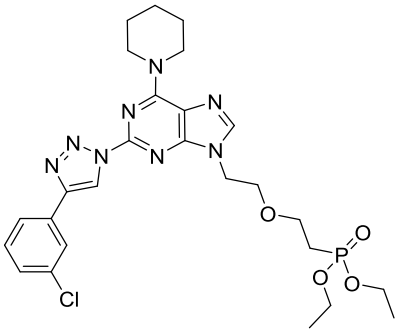
^{13}C-NMR (76 MHz, $CDCl_3$) spectrum of compound 8e:



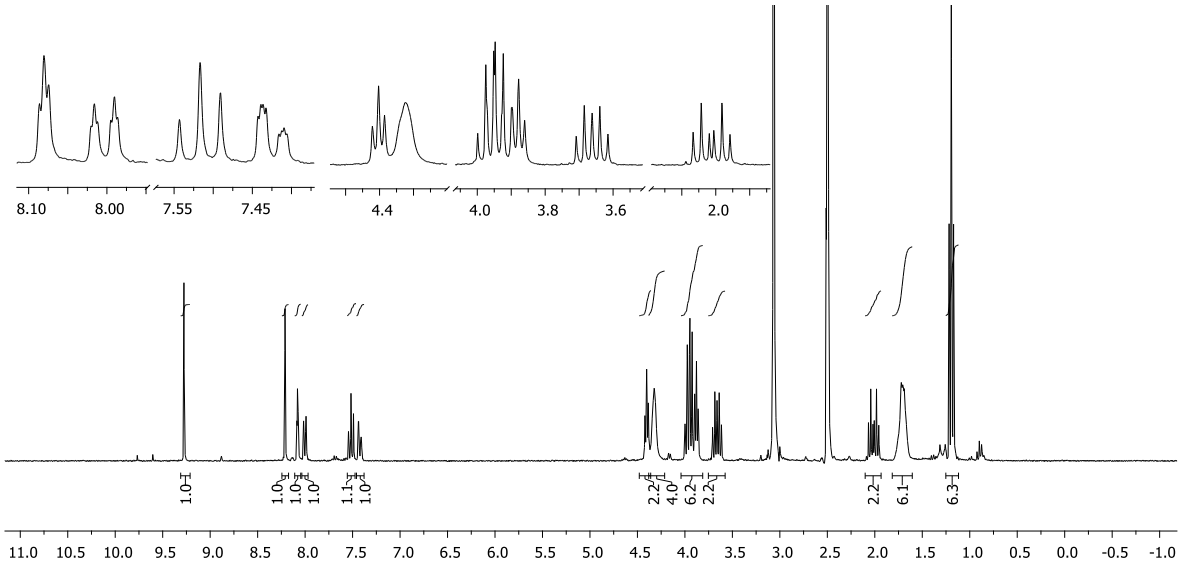
^{31}P-NMR (202 MHz, $CDCl_3$) spectrum of compound 8e:



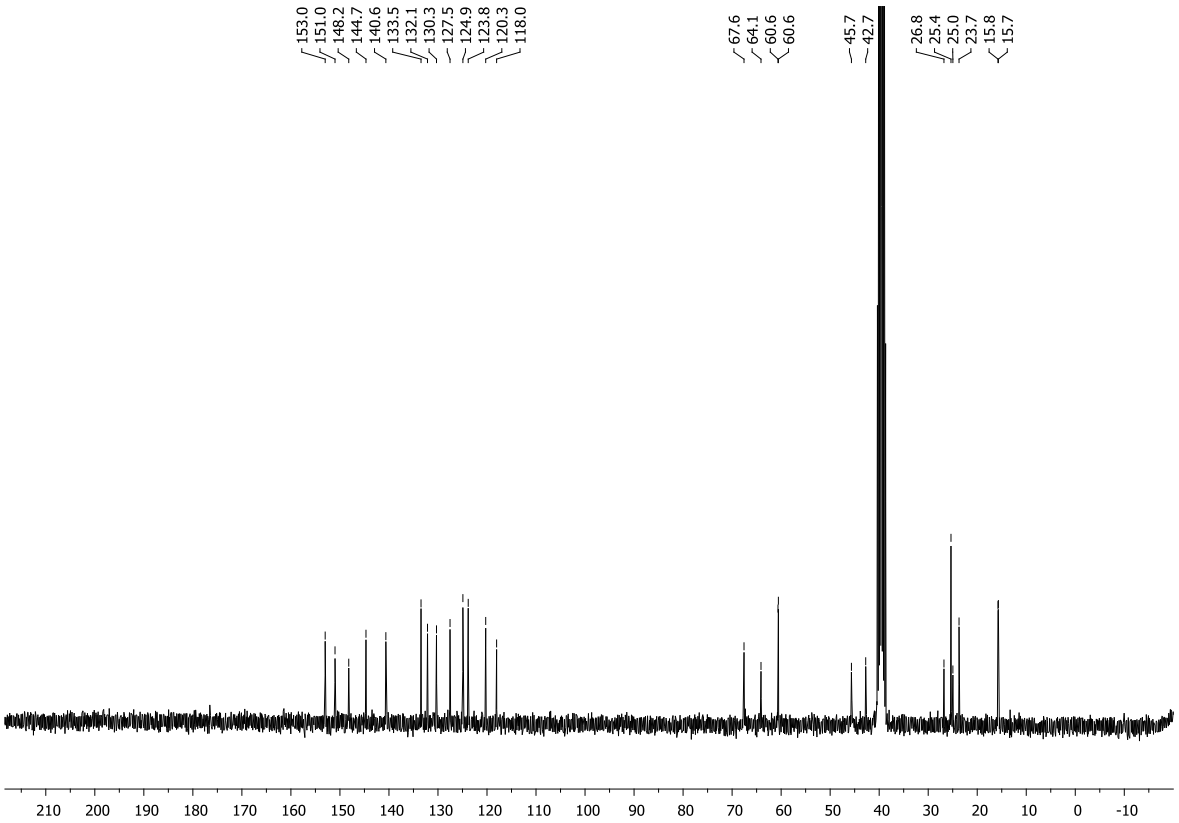
Diethyl [2-(2-{2-[4-(3-chlorophenyl)-1*H*-1,2,3-triazol-1-yl]-6-(piperidin-1-yl)-9*H*-purin-9-yl}ethoxy)ethyl]phosphonate (8f)



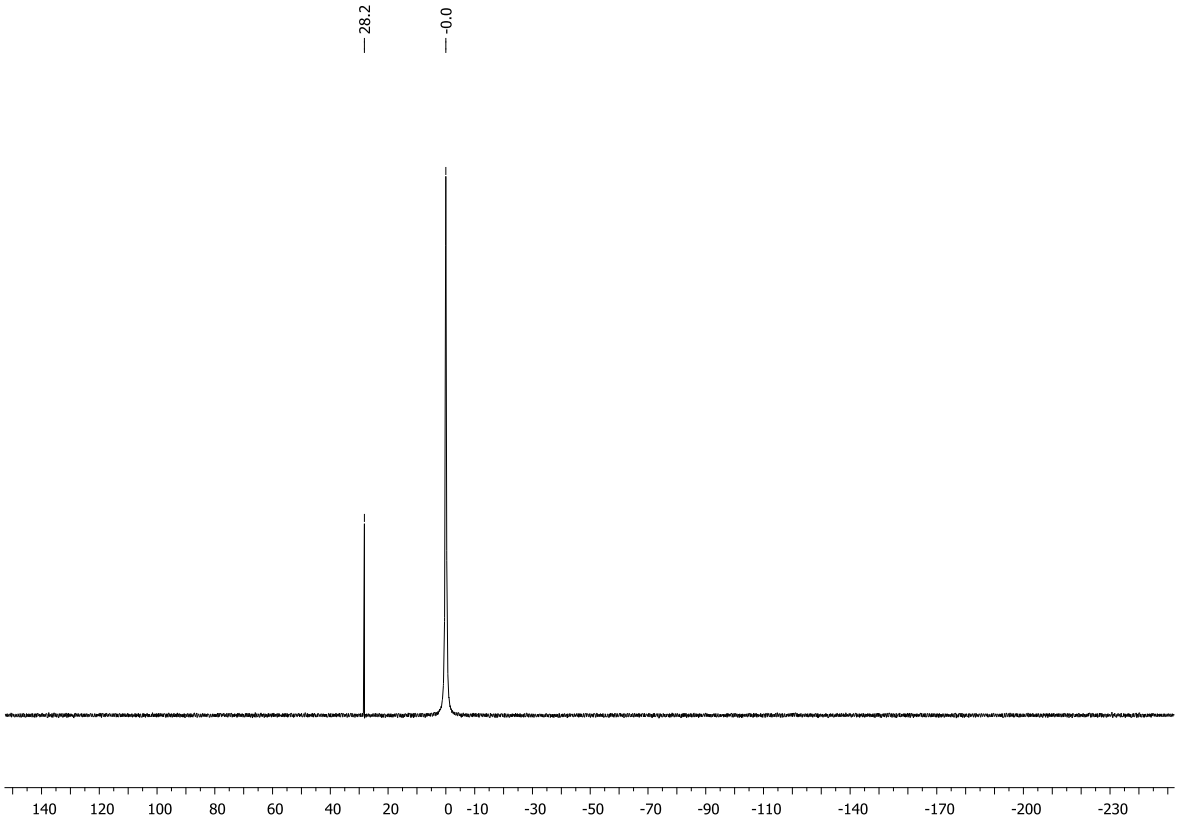
^{1}H-NMR (300 MHz, 70 °C, DMSO-d$_6$) spectrum of compound 8f:



^{13}C-NMR (76 MHz, 70 °C, DMSO-d_6) spectrum of compound 8f:

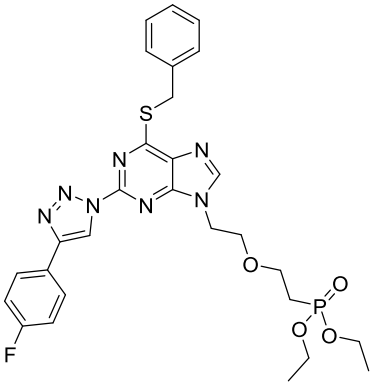


^{31}P-NMR (202 MHz, 70 °C, DMSO-d_6) spectrum of compound 8f:

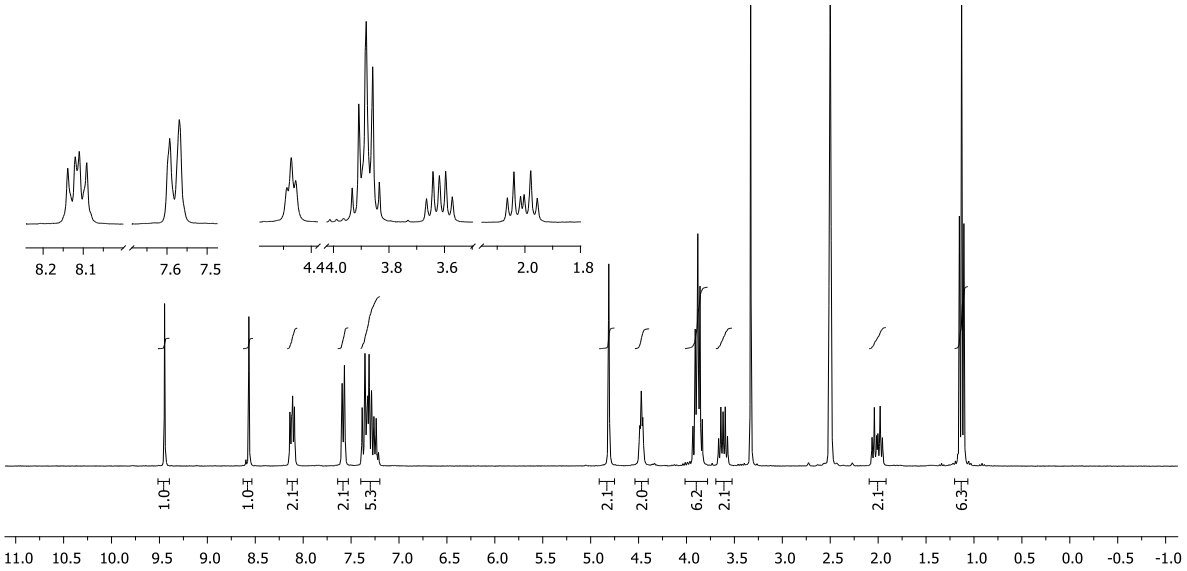


6-S-SUBSTITUTED 2-TRIAZOLYLPURINE DERIVATIVES

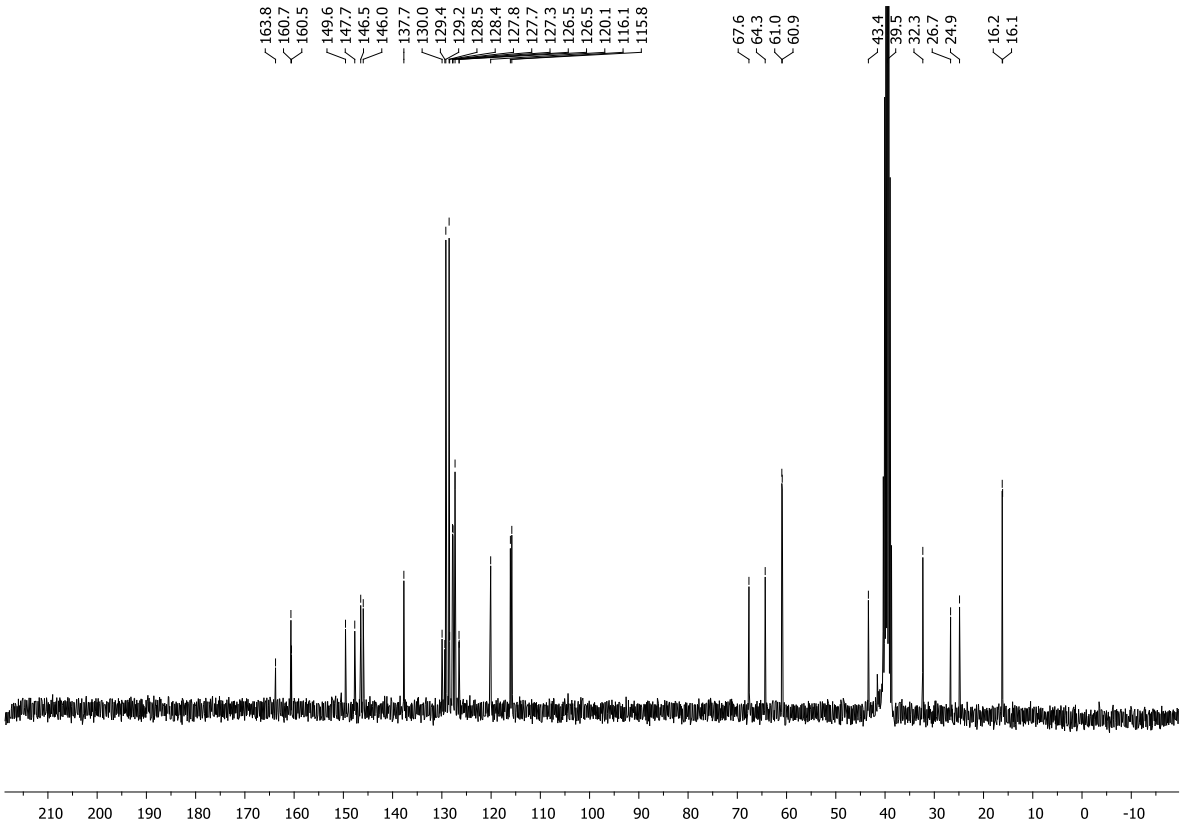
Diethyl [2-(2-{6-(benzylsulfanyl)-2-[4-(4-fluorophenyl)-1*H*-1,2,3-triazol-1-yl]-9*H*-purin-9-yl}ethoxy)ethyl]phosphonate (8g)



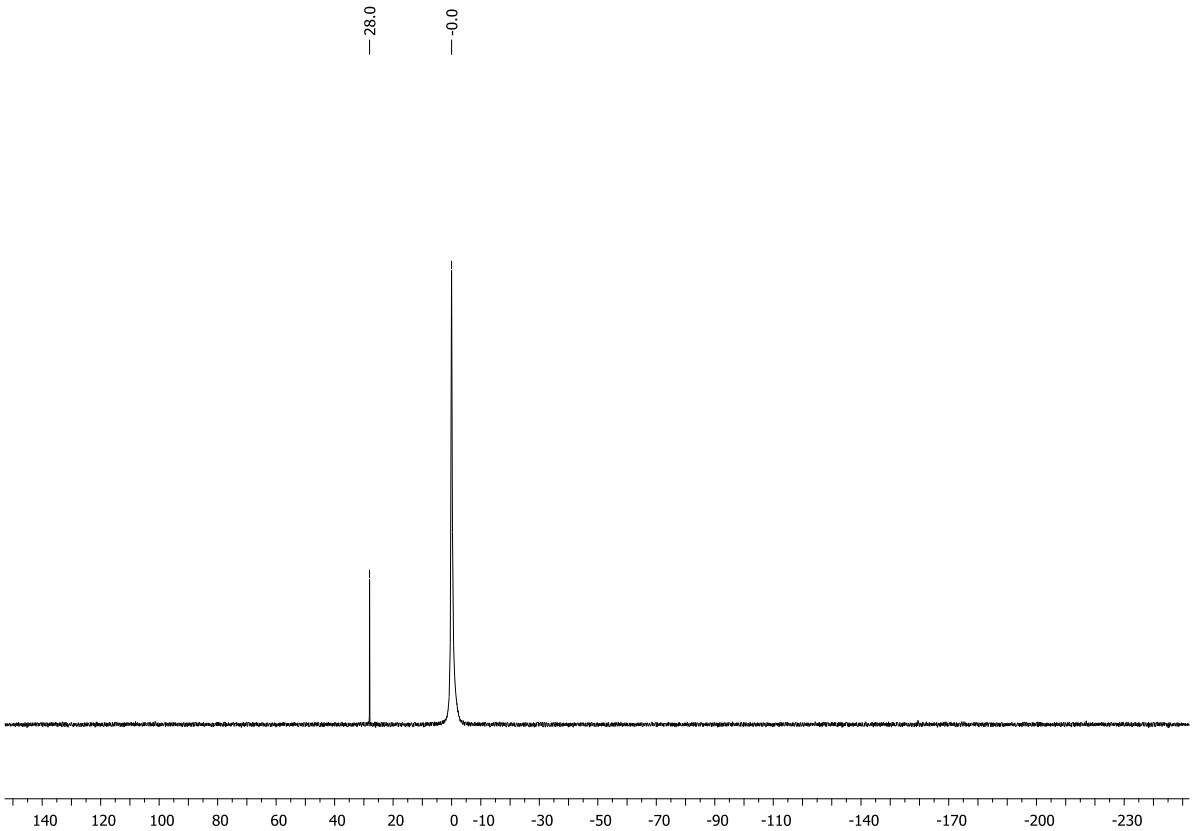
^{1}H-NMR (300 MHz, DMSO-d$_6$) spectrum of compound 8g:



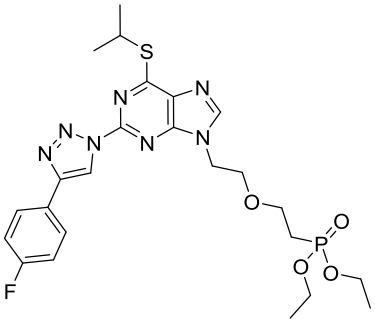
^{13}C-NMR (76 MHz, DMSO-d_6) spectrum of compound 8g:



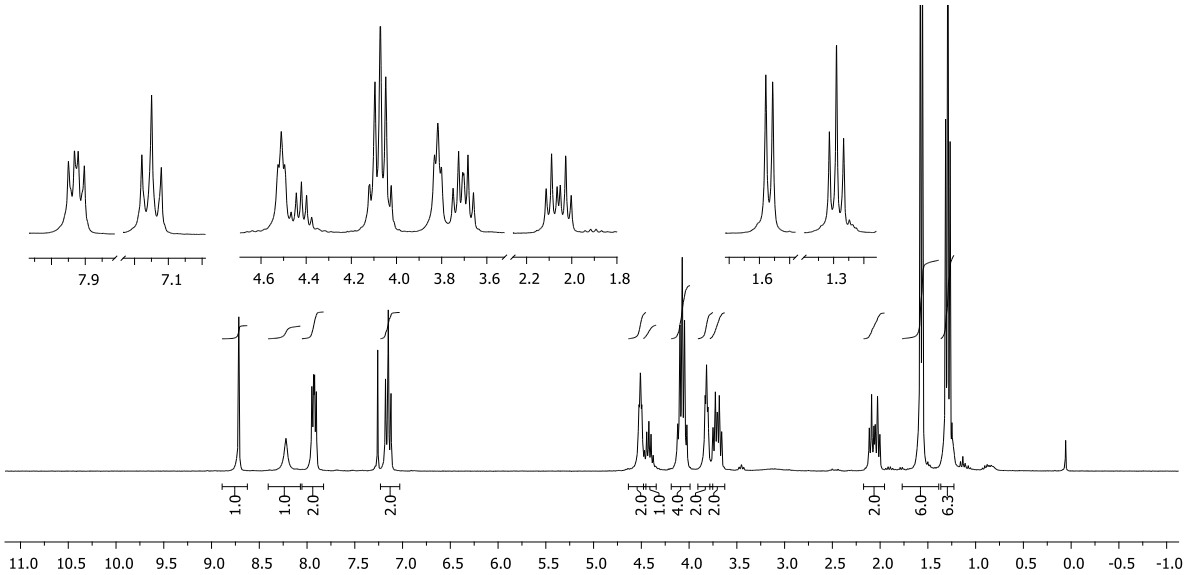
^{31}P-NMR (202 MHz, DMSO-d_6) spectrum of compound 8g:



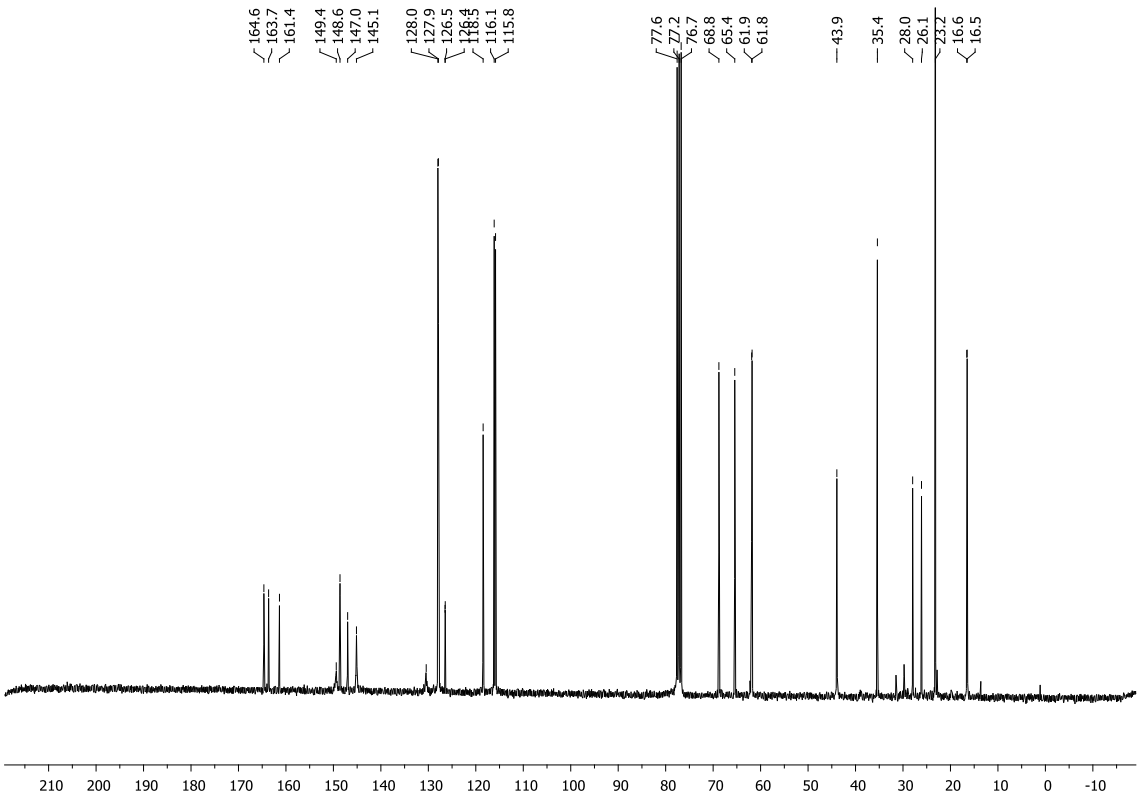
Diethyl [2-(2-{2-[4-(4-fluorophenyl)-1*H*-1,2,3-triazol-1-yl]-6-(isopropylsulfanyl)-9*H*-purin-9-yl}ethoxy)ethyl]phosphonate (8h)



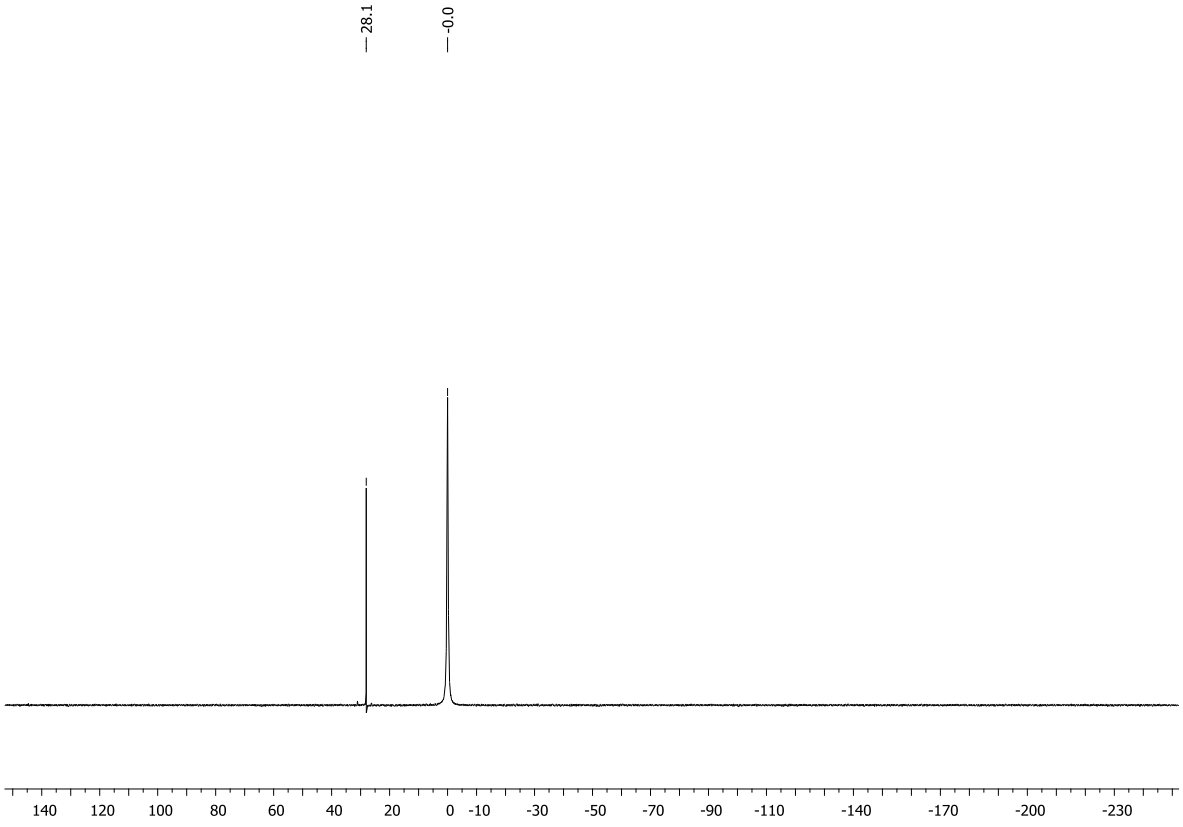
^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 8h:



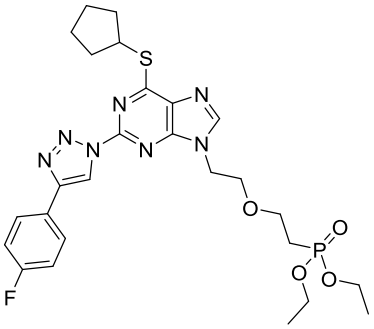
^{13}C-NMR (76 MHz, $CDCl_3$) spectrum of compound 8h:



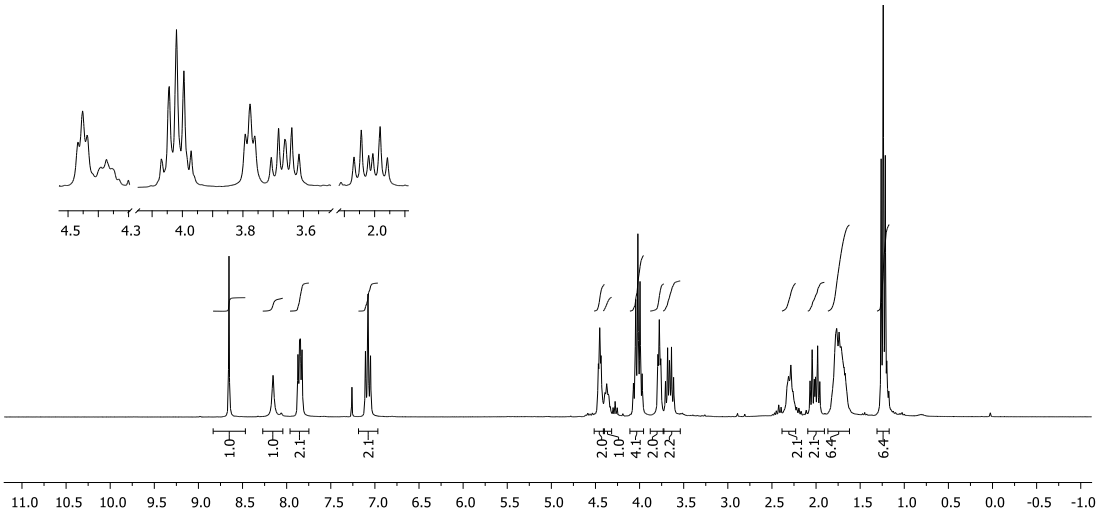
^{31}P-NMR (202 MHz, $CDCl_3$) spectrum of compound 8h:



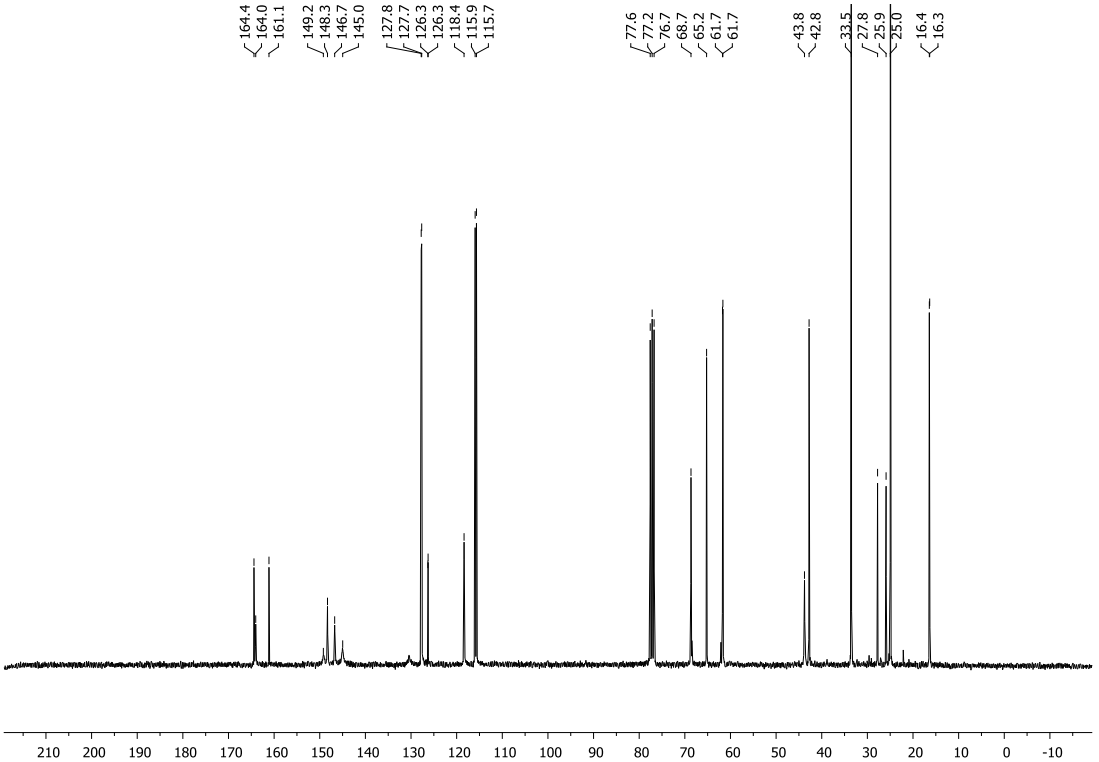
Diethyl [2-(2-{6-(cyclopentylsulfanyl)-2-[4-(4-fluorophenyl)-1*H*-1,2,3-triazol-1-yl]-9*H*-purin-9-yl}ethoxy)ethyl]phosphonate (8i)



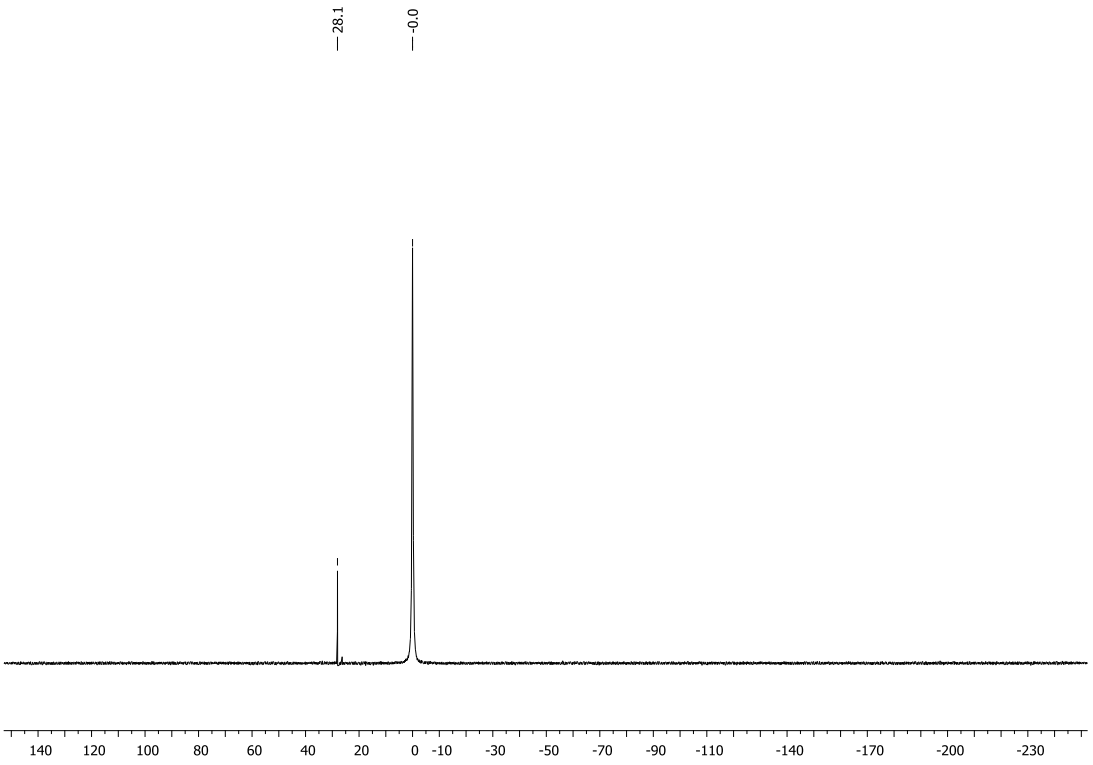
^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 8i:



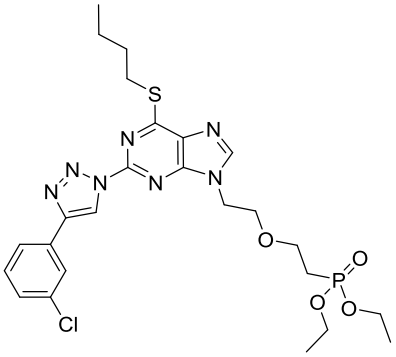
^{13}C-NMR (76 MHz, $CDCl_3$) spectrum of compound 8i:



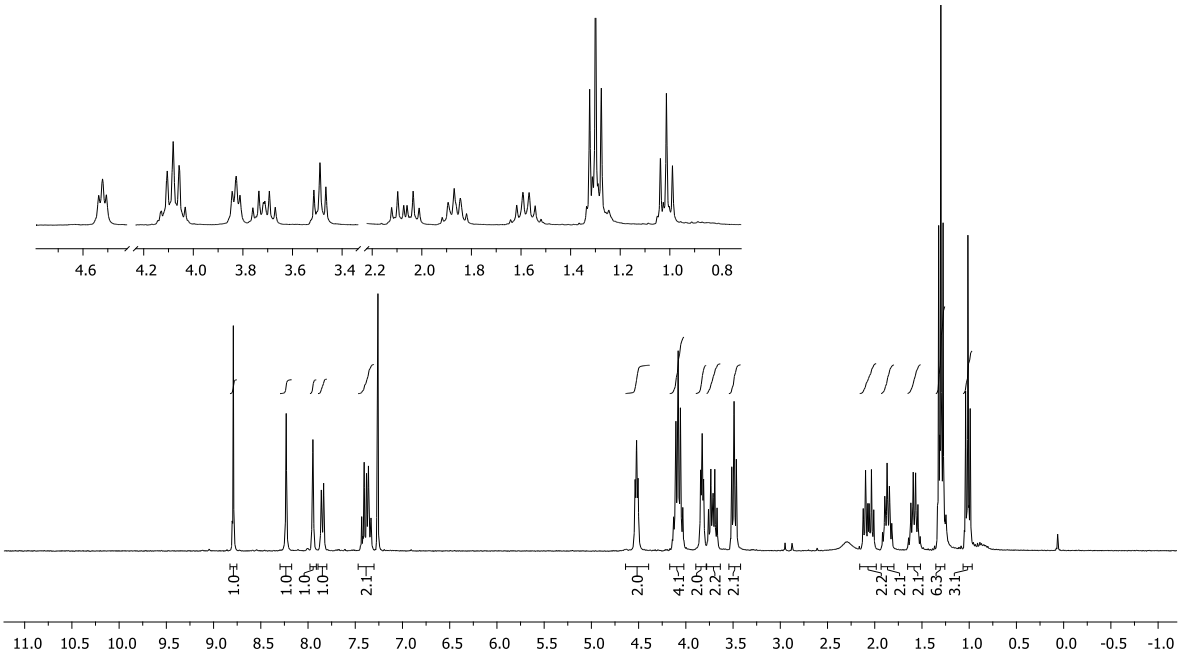
^{31}P-NMR (202 MHz, $CDCl_3$) spectrum of compound 8i:



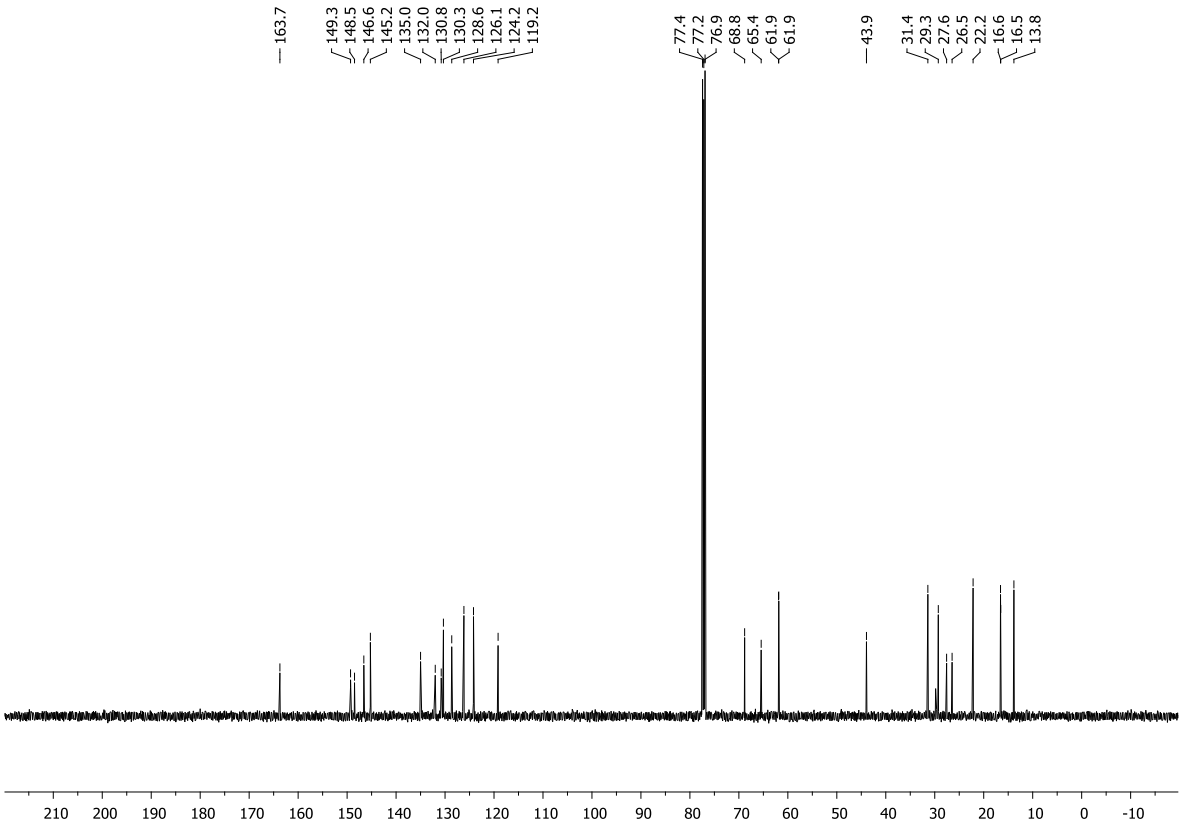
Diethyl [2-(2-{6-(butylsulfanyl)-2-[4-(3-chlorophenyl)-1*H*-1,2,3-triazol-1-yl]-9*H*-purin-9-yl}ethoxy)ethyl]phosphonate (8j)



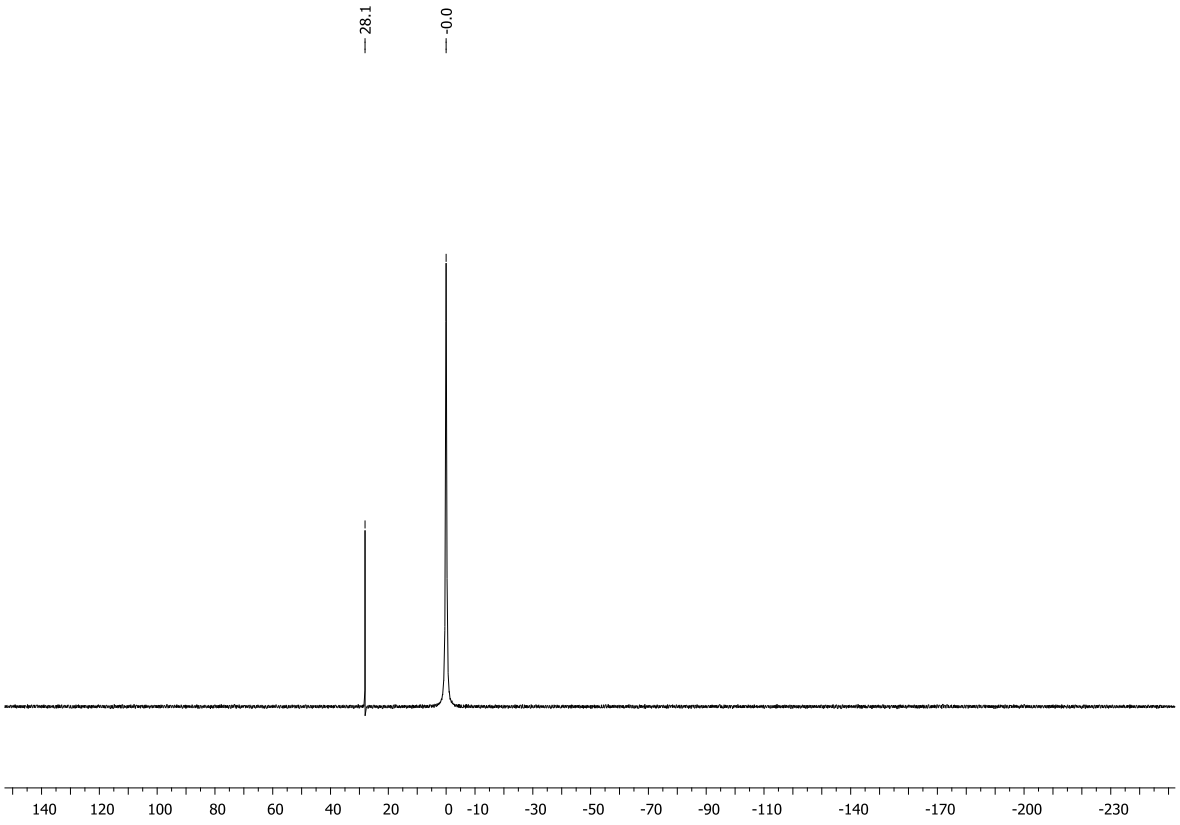
^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of compound 8j:



^{13}C-NMR (76 MHz, $CDCl_3$) spectrum of compound 8j:

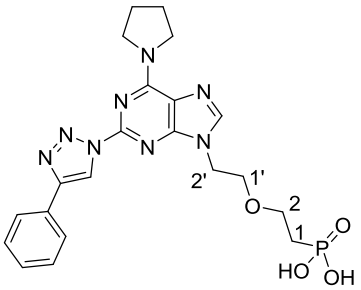


^{31}P-NMR (202 MHz, $CDCl_3$) spectrum of compound 8j:

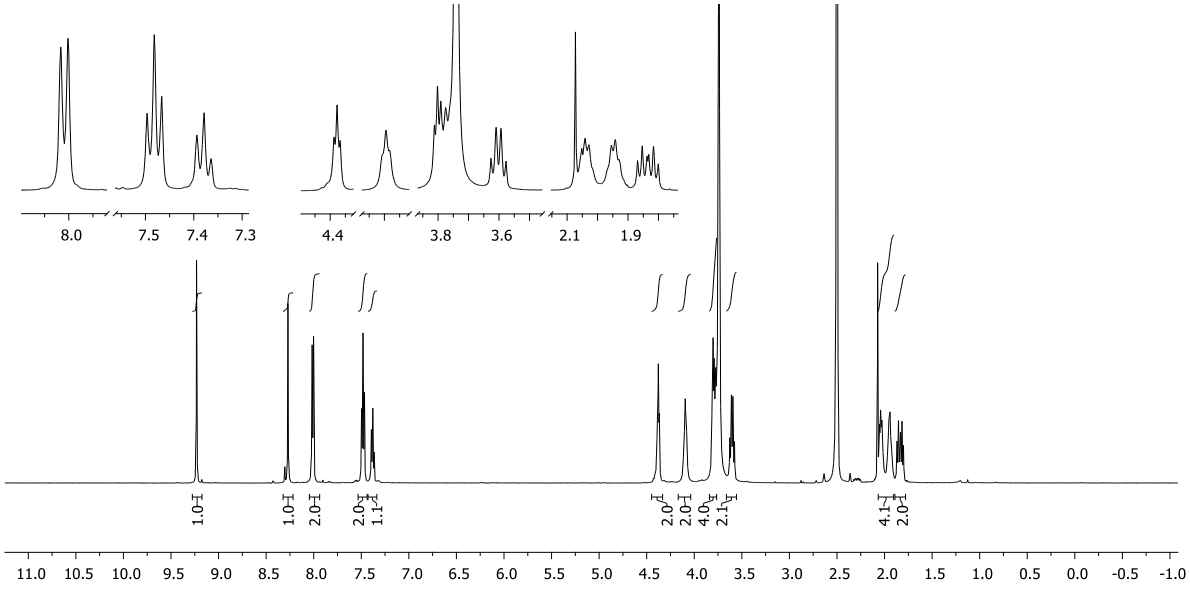


6-*N*-SUBSTITUTED 2-TRIAZOLYLPURINE PHOSPHONIC ACID

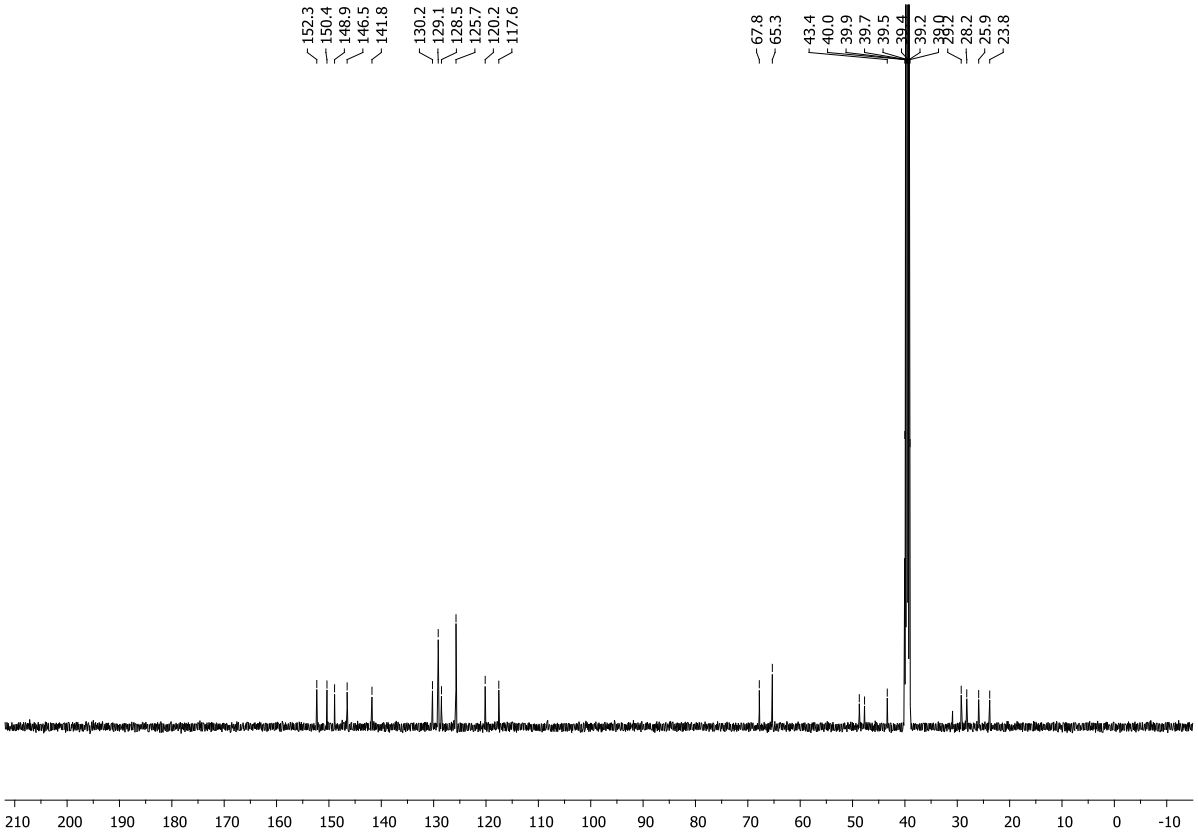
(2-{2-[2-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)-6-(pyrrolidin-1-yl)-9*H*-purin-9-yl]ethoxy}ethyl) phosphonic acid (10)



^{1}H-NMR (500 MHz, DMSO-d$_6$ + D$_2$O) spectrum of compound 10:



^{13}C-NMR (125.7 MHz, DMSO-d_6 + D_2O) spectrum of compound 10:



^{31}P-NMR (202 MHz, DMSO-d_6 + D_2O) spectrum of compound 10: