

# Supporting Information

## Efficient Synthesis of $\alpha$ -Branched Purine-Based Acyclic Nucleosides: Scopes and Limitations of the Method

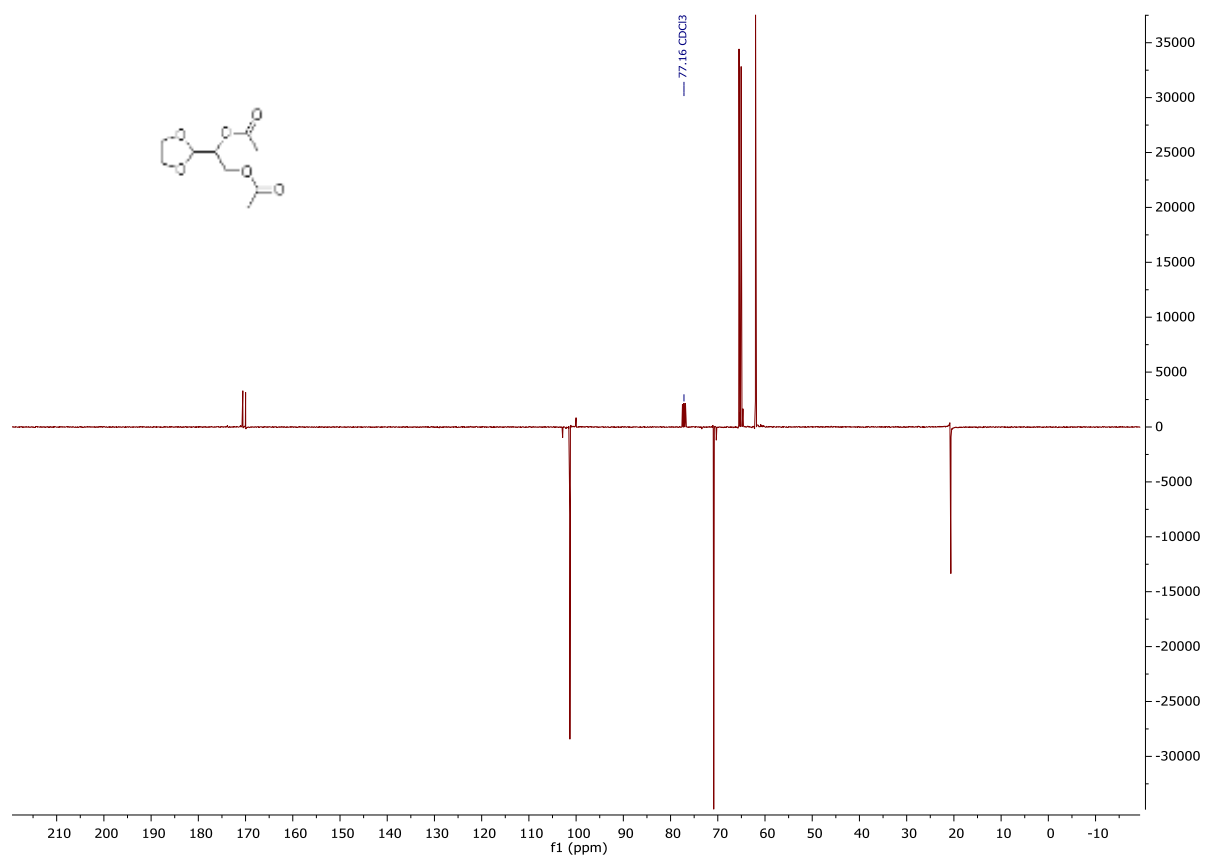
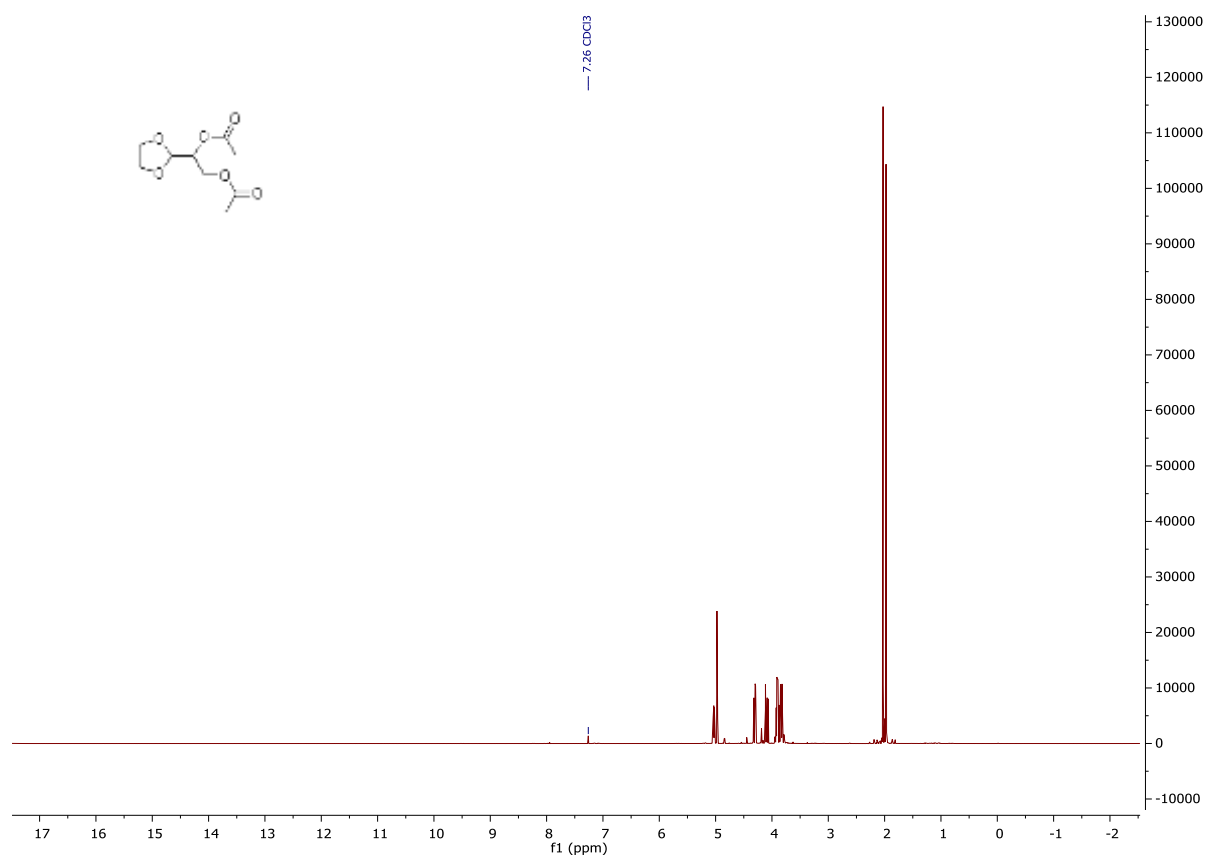
*Jan Frydrych, Lenka Poštová Slavětínská, Martin Dračínský, Zlatko Janeba\**

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Flemingovo nám. 2, CZ-16610, Prague 6, Czech Republic

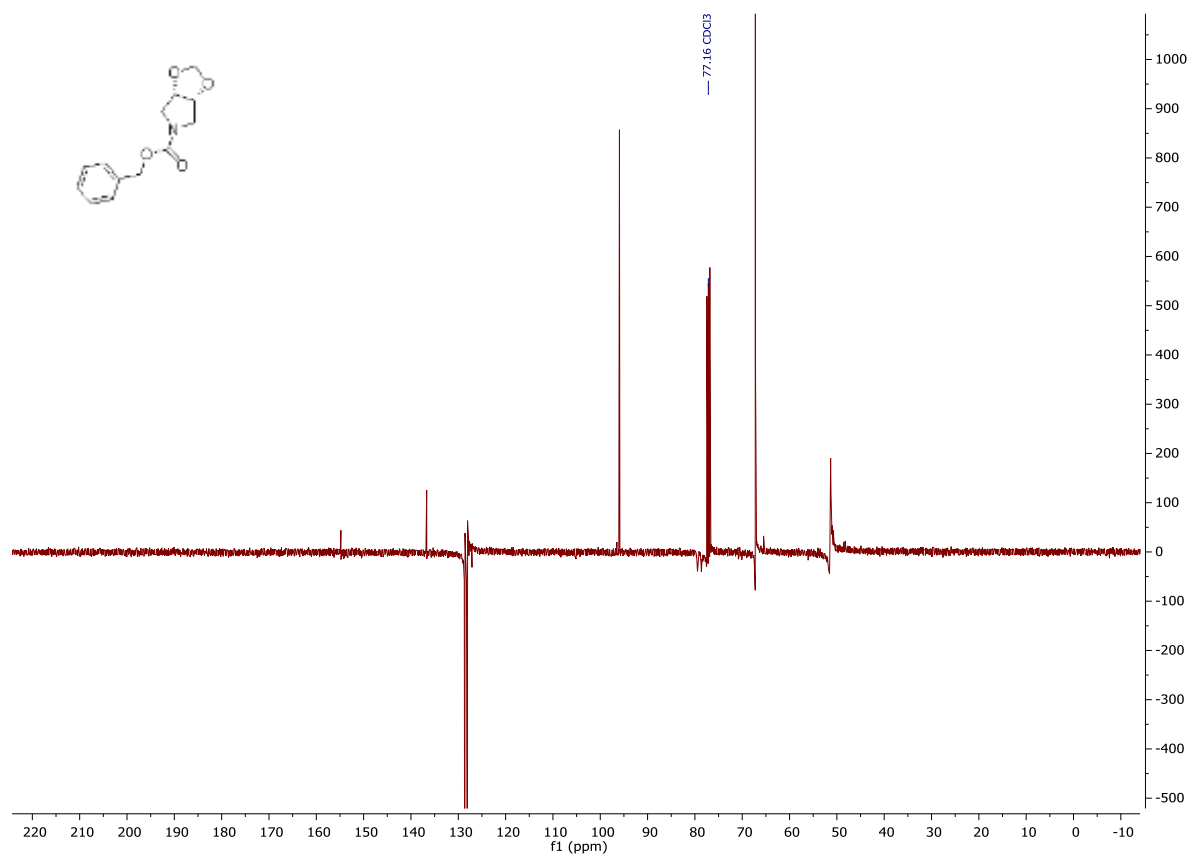
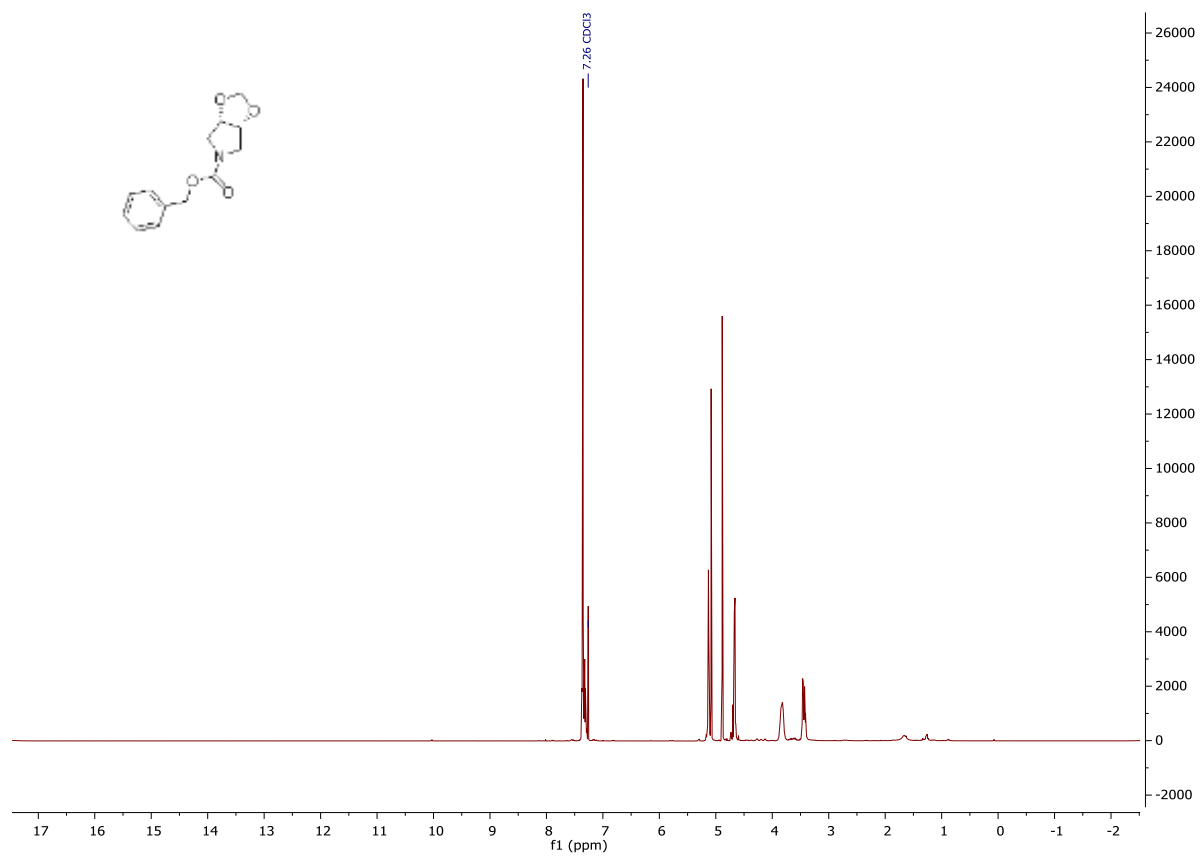
e-mail: janeba@uochb.cas.cz

1. Copies of  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra ..... S2-S42
2. HMBC spectra of compounds 22 and 42 ..... S43-S44

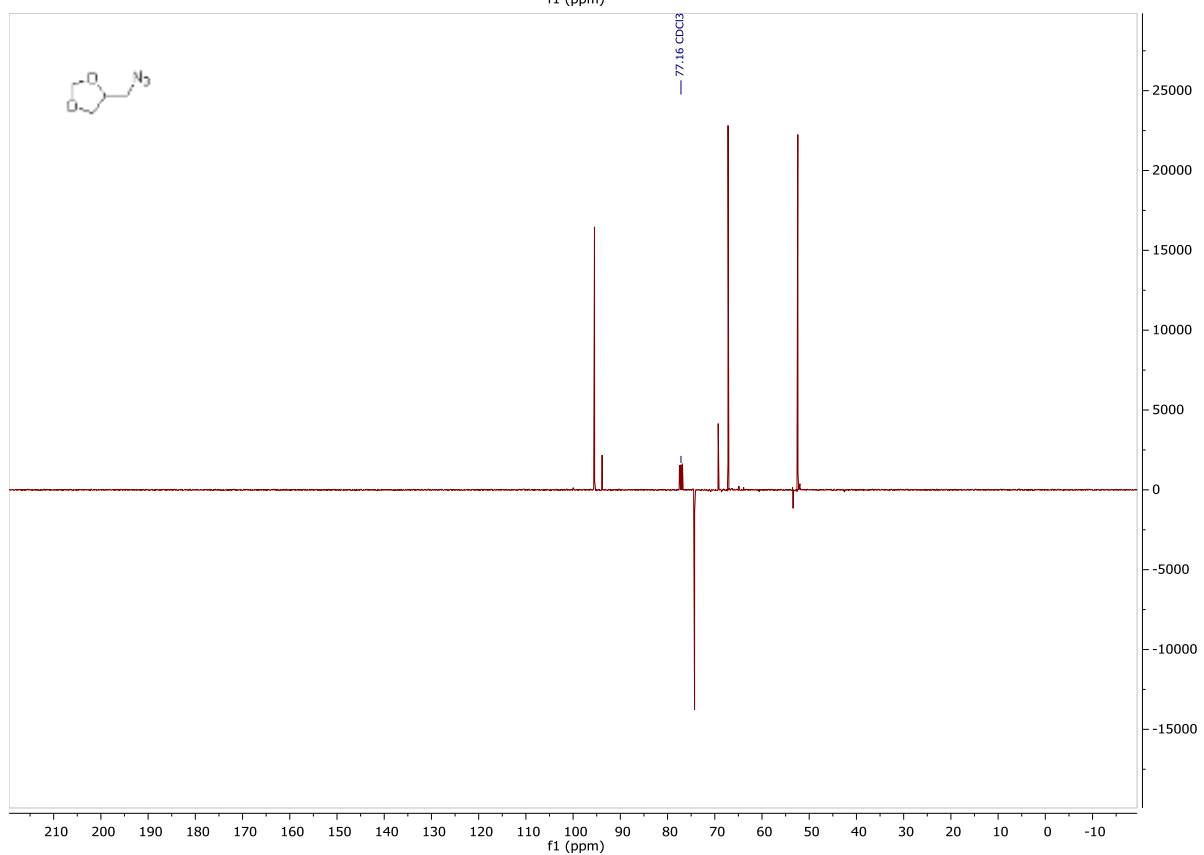
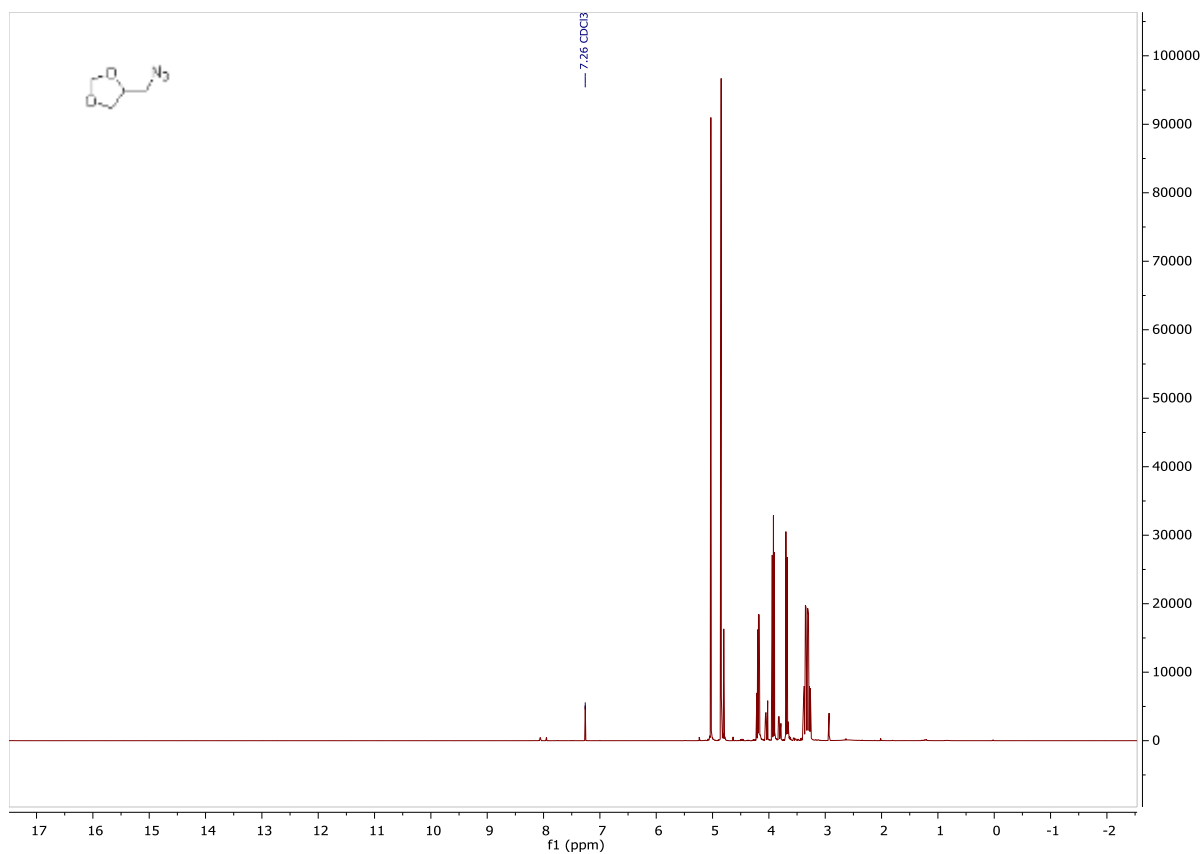
2-(1,2-Dihydroxyethyl)-1,3-dioxolane-1,3-diacetate (**2b**)



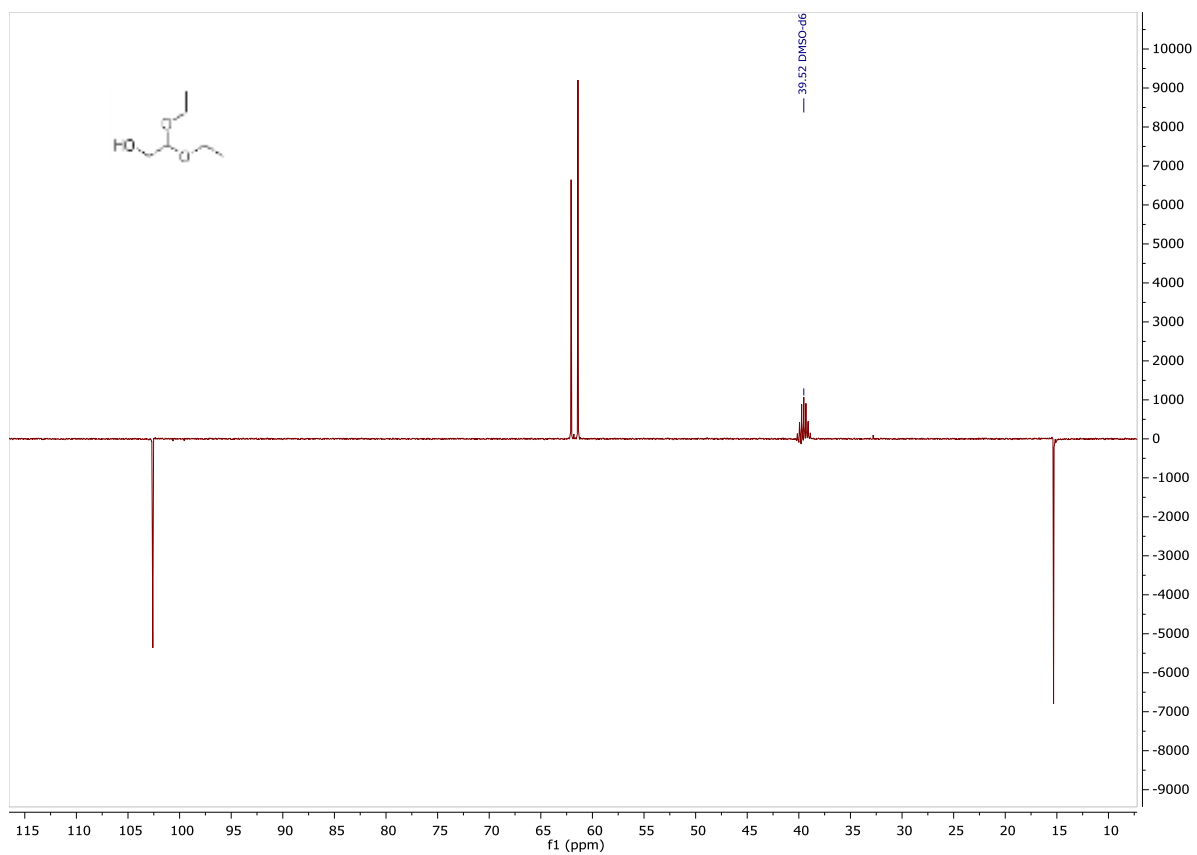
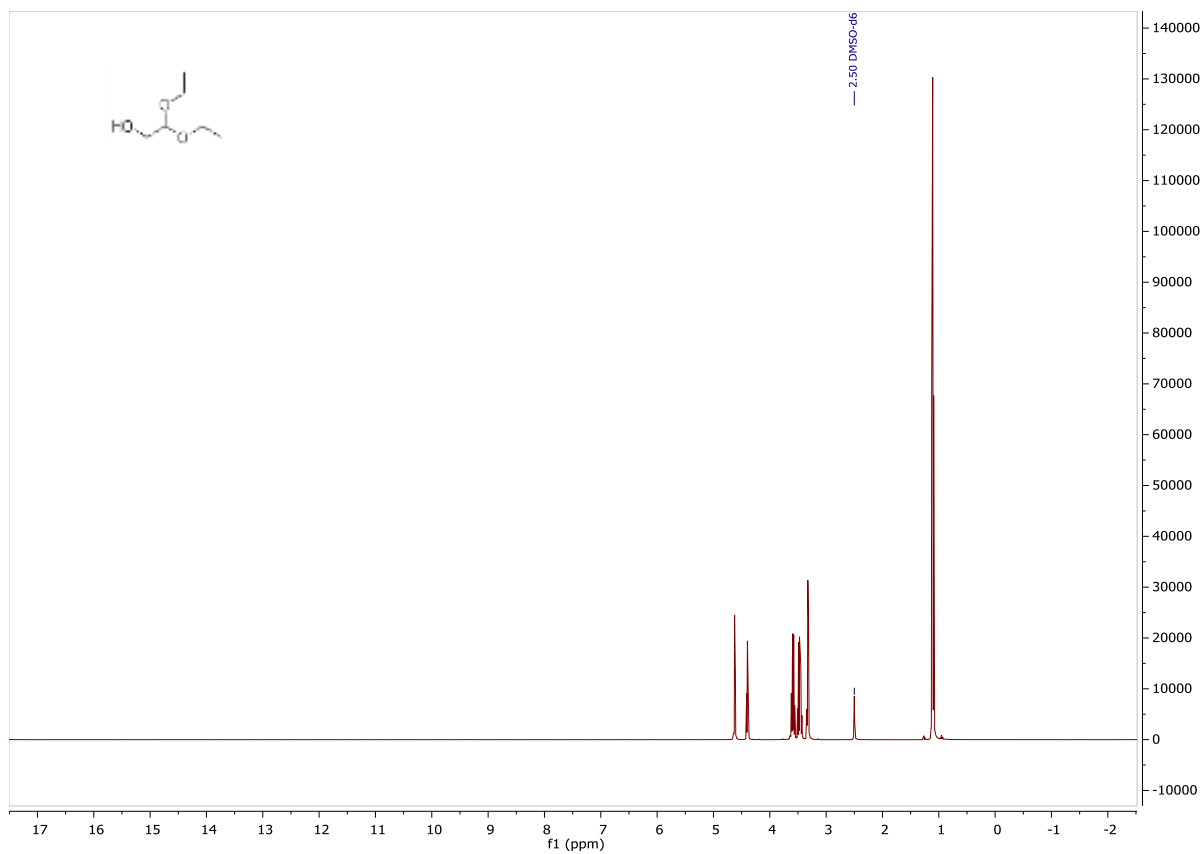
Phenylmethyl *syn*-tetrahydro-5*H*-[1,3]dioxolo[4,5-*c*]pyrrole-5-carboxylate (**2k**)



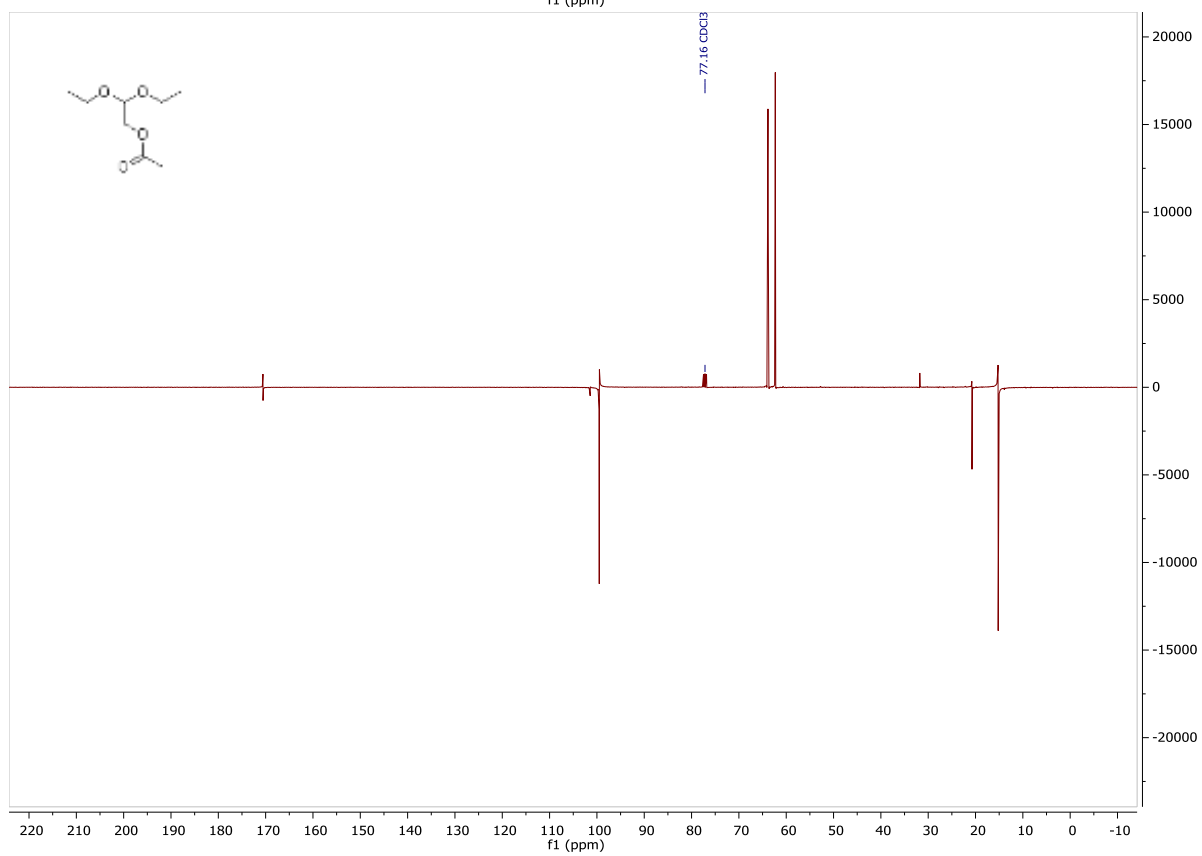
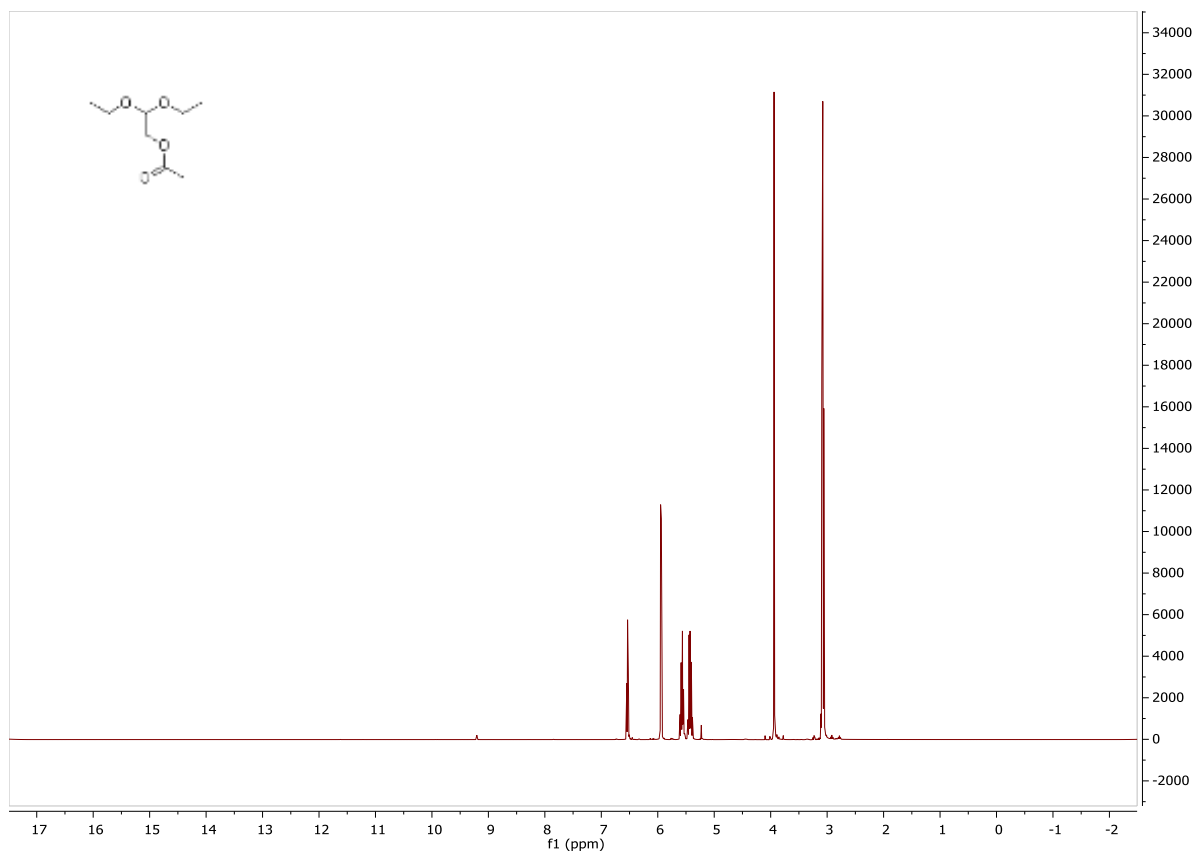
# 4-(Azidomethyl)-1,3-dioxolane (**2n**)



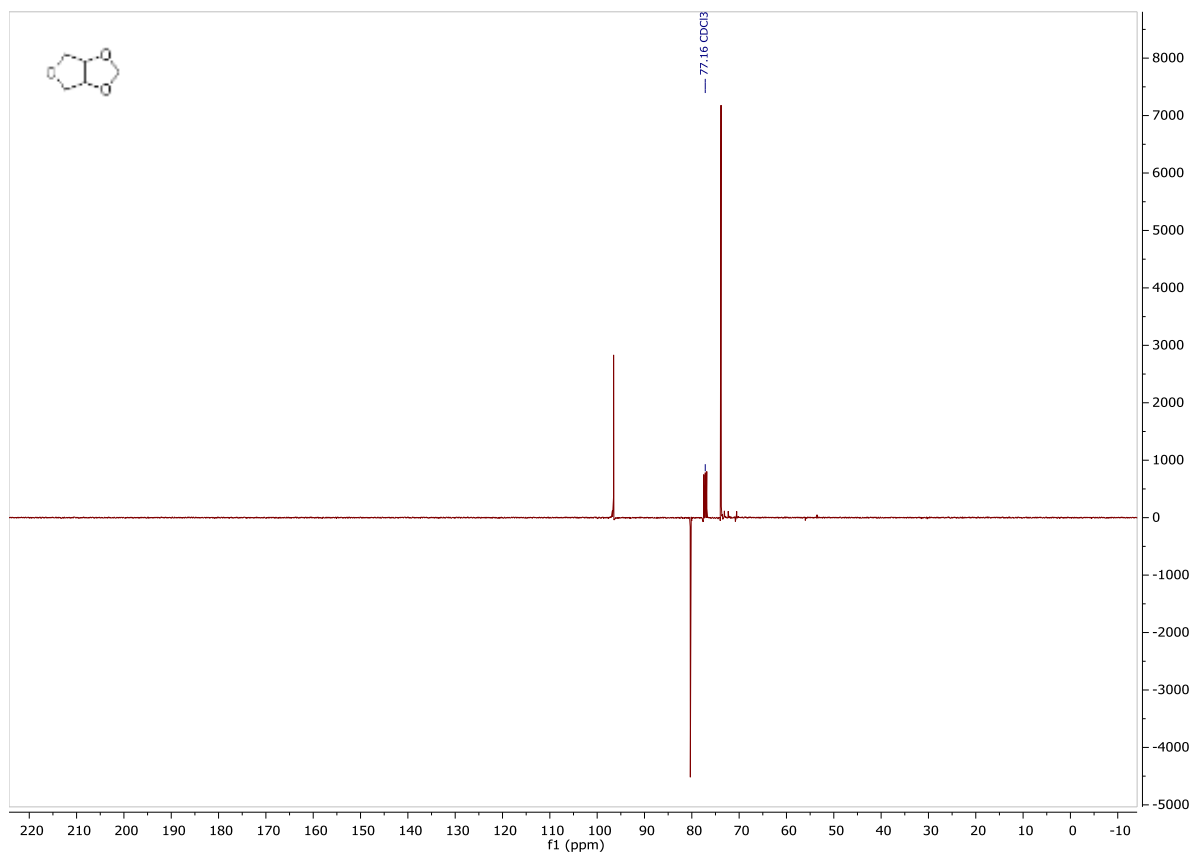
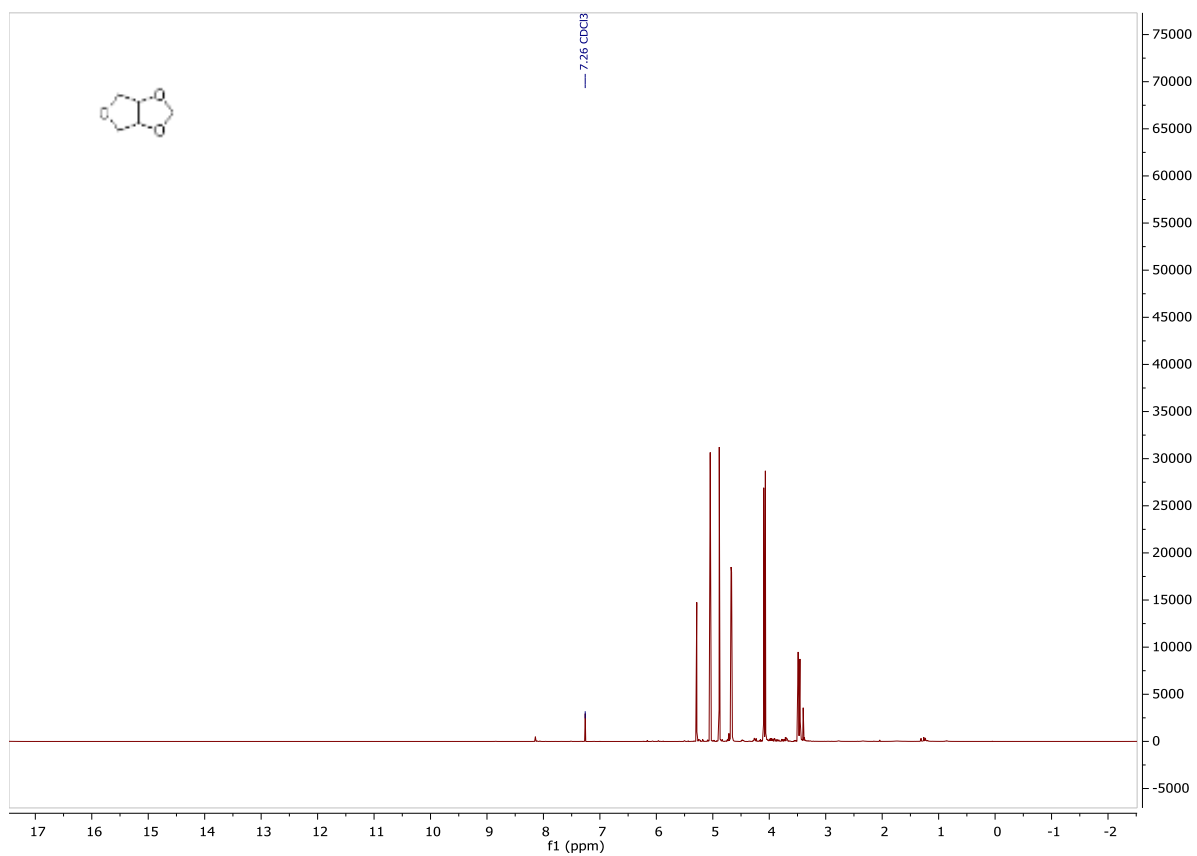
# 2,2-Diethoxyethan-1-ol (2q)



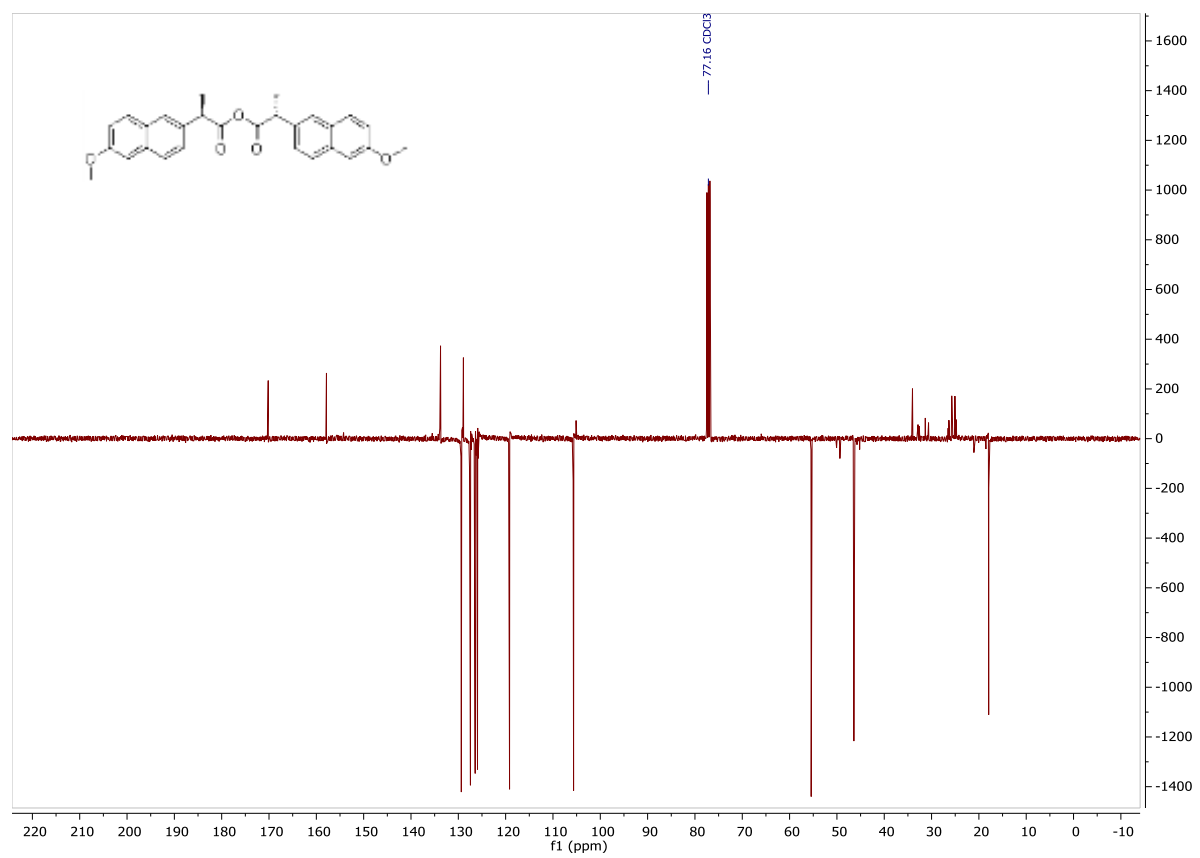
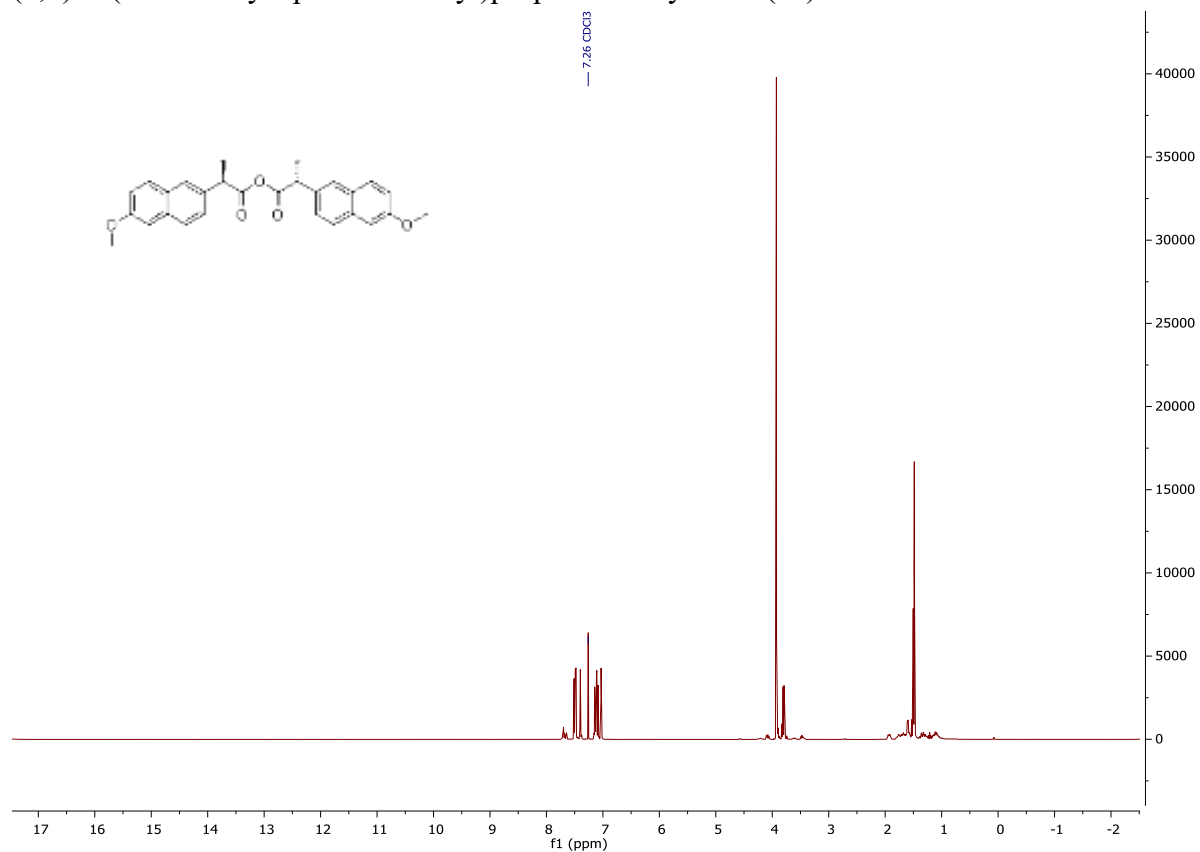
## 2,2-Diethoxyethyl acetate (2t)



Tetrahydrofuro[3,4-*d*][1,3]dioxole (**2v**)

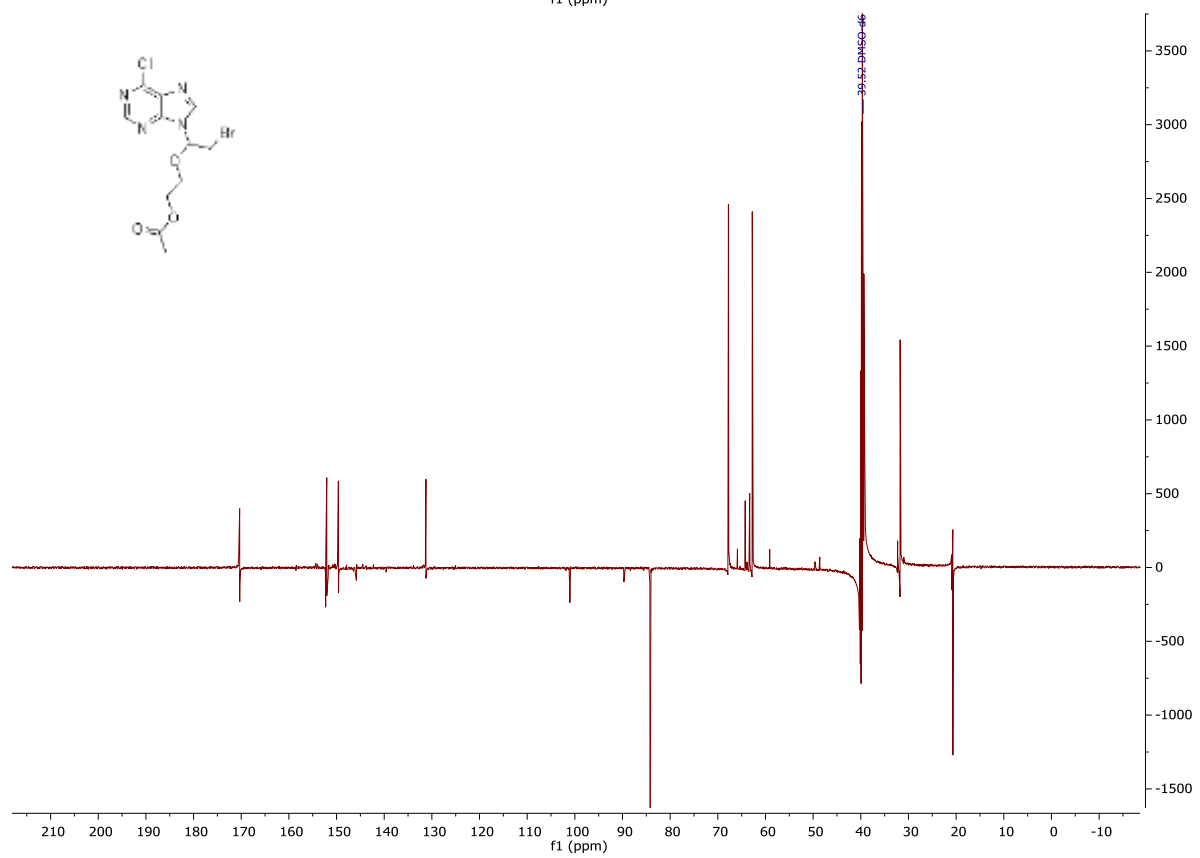
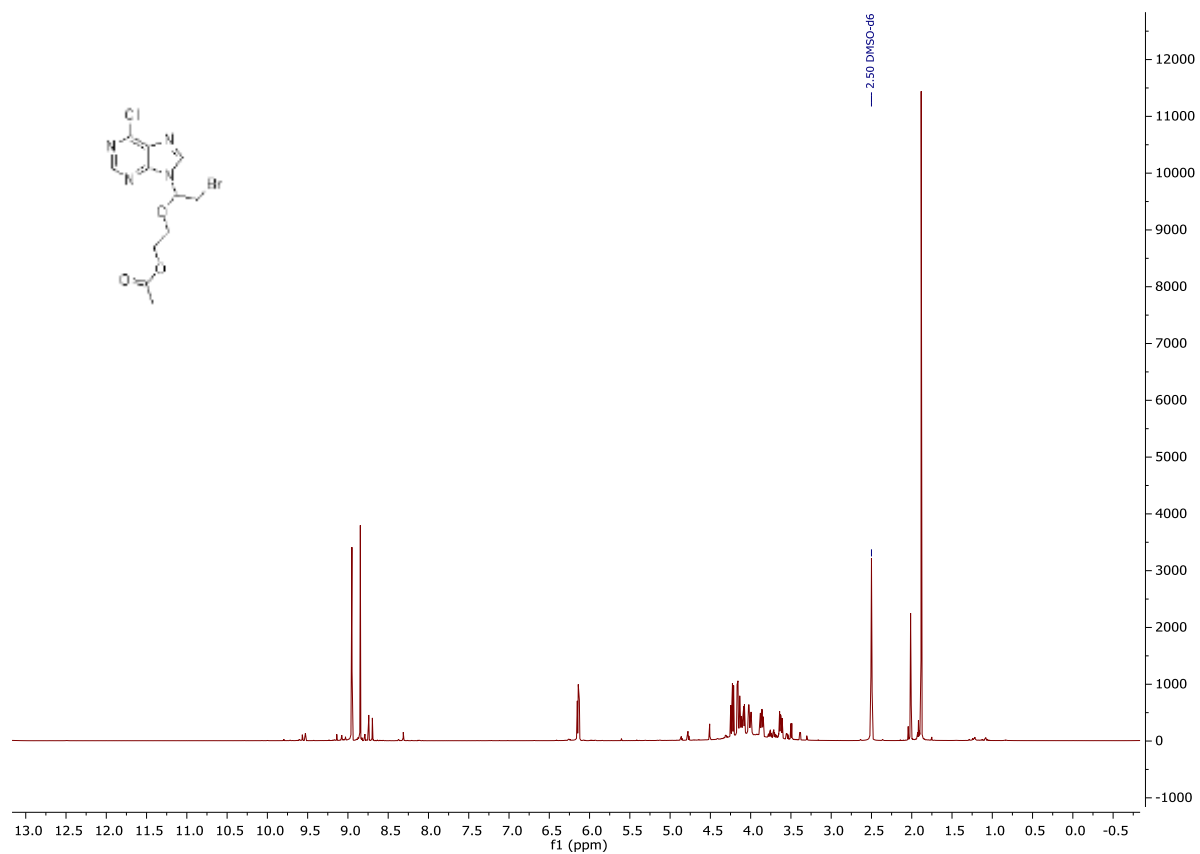


(*S,S*)-2-(6-Methoxynaphthalene-2-yl)propionic anhydride (**3e**)

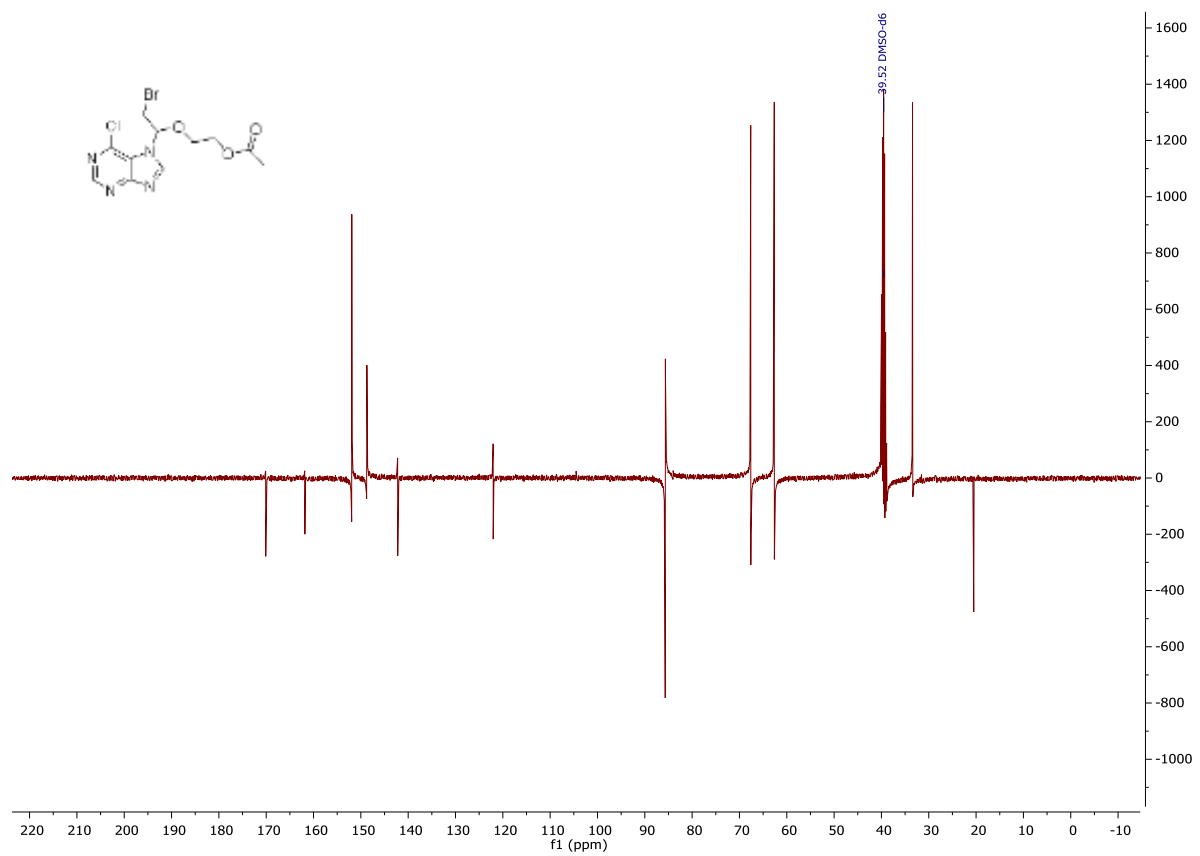
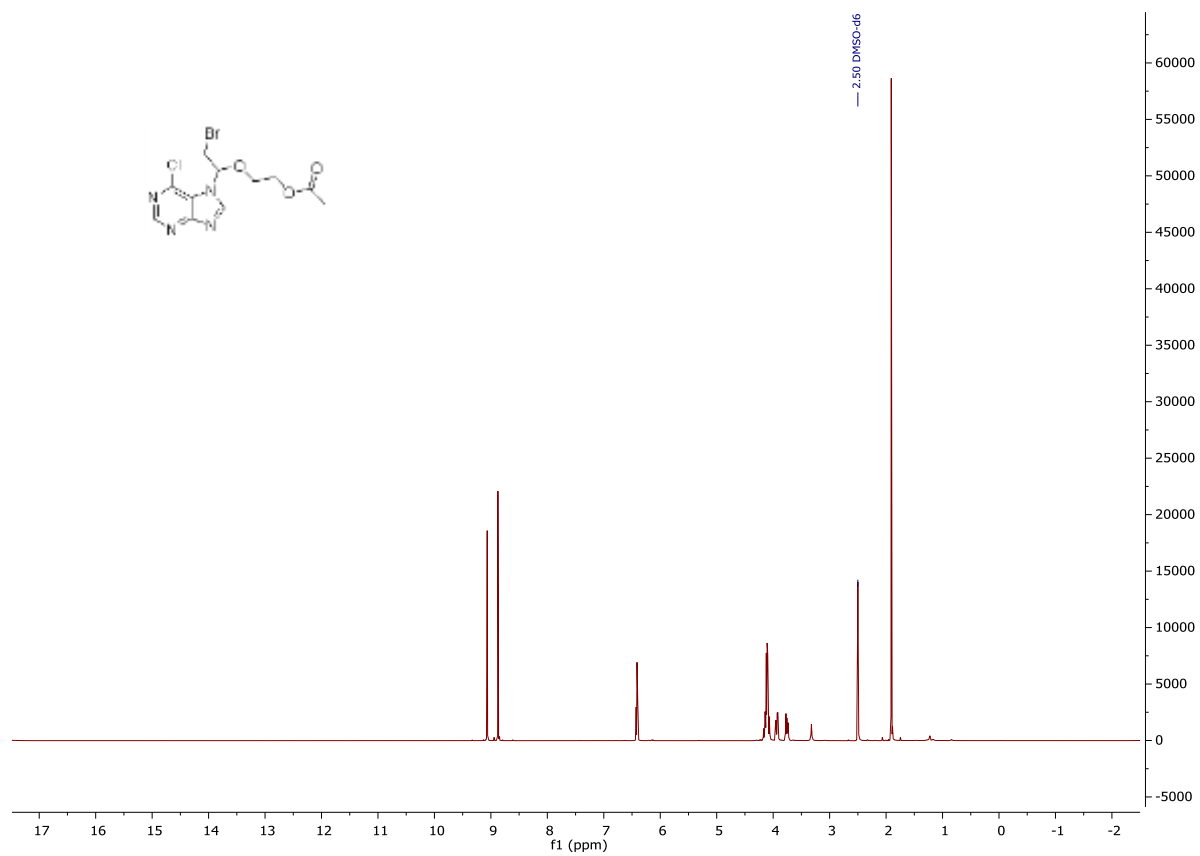




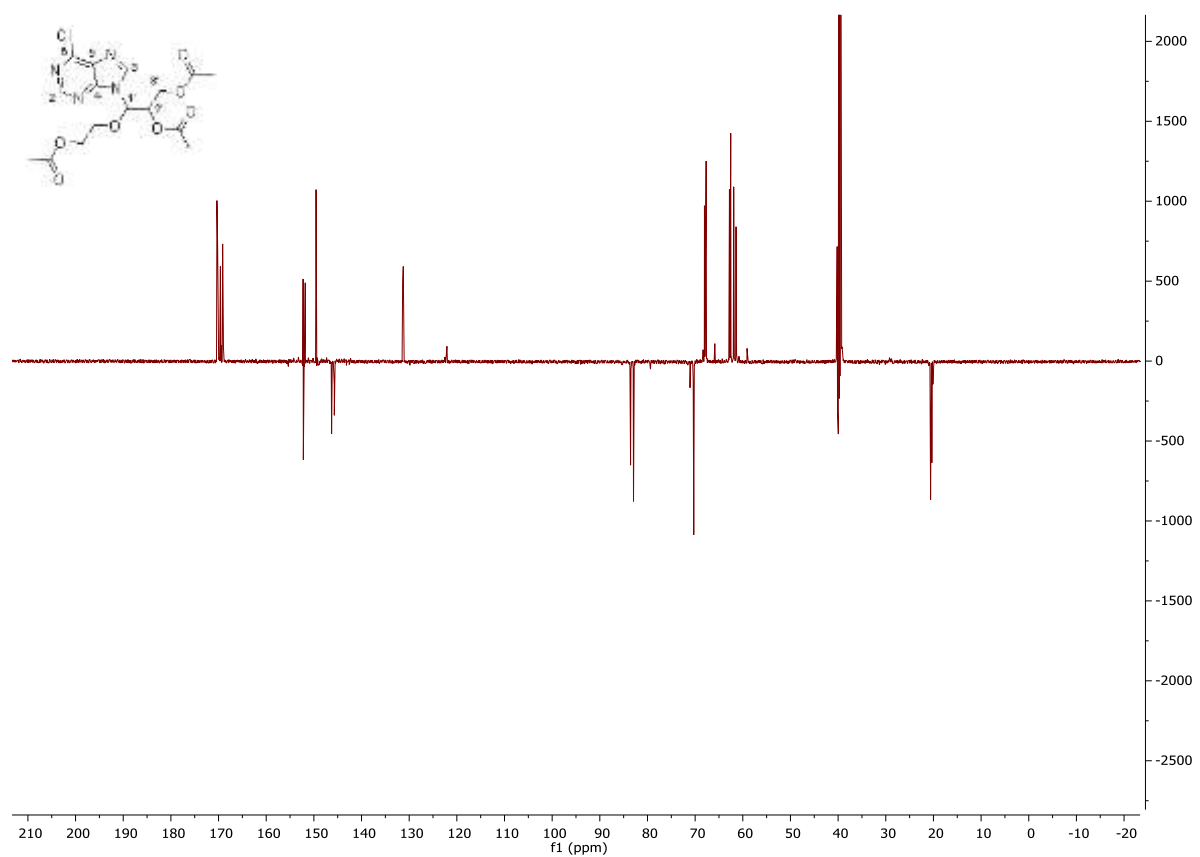
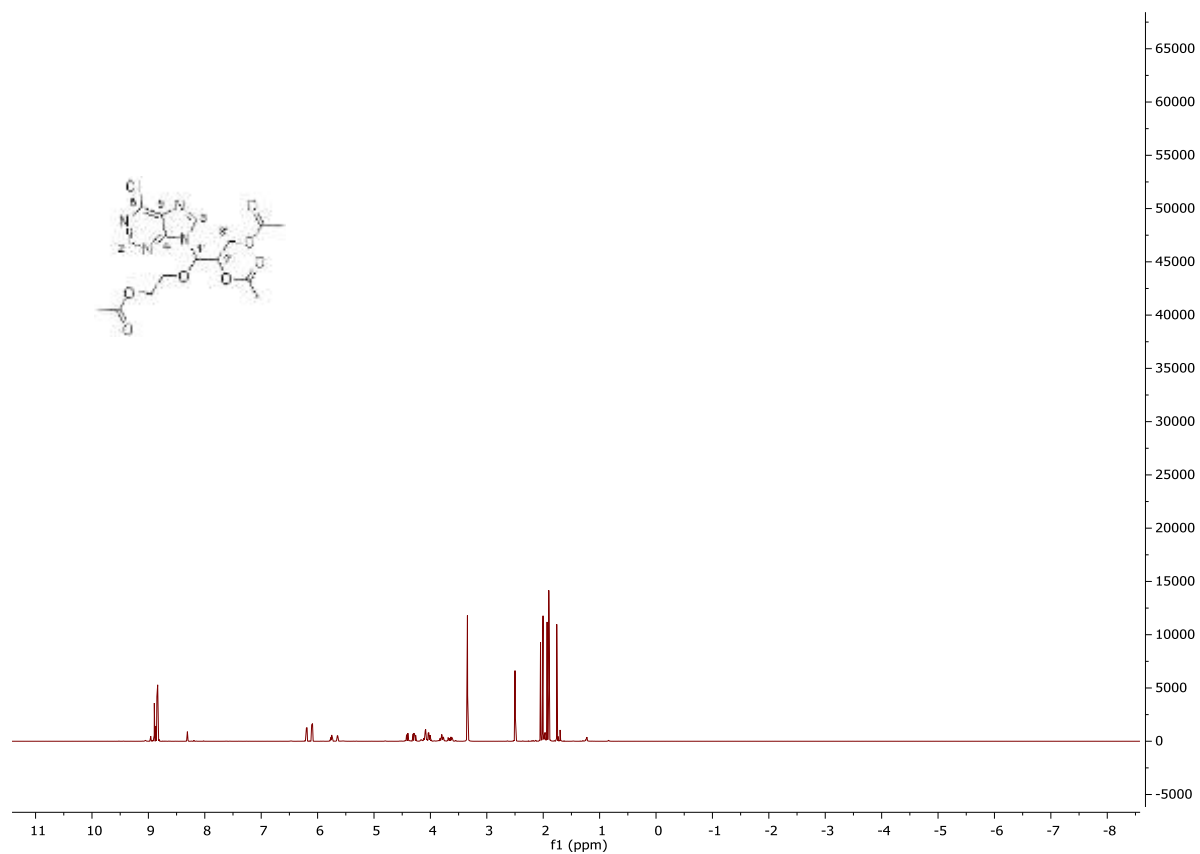
2-(2-Bromo-1-(6-chloro-9H-purin-7-yl)ethoxy)ethyl acetate (4)



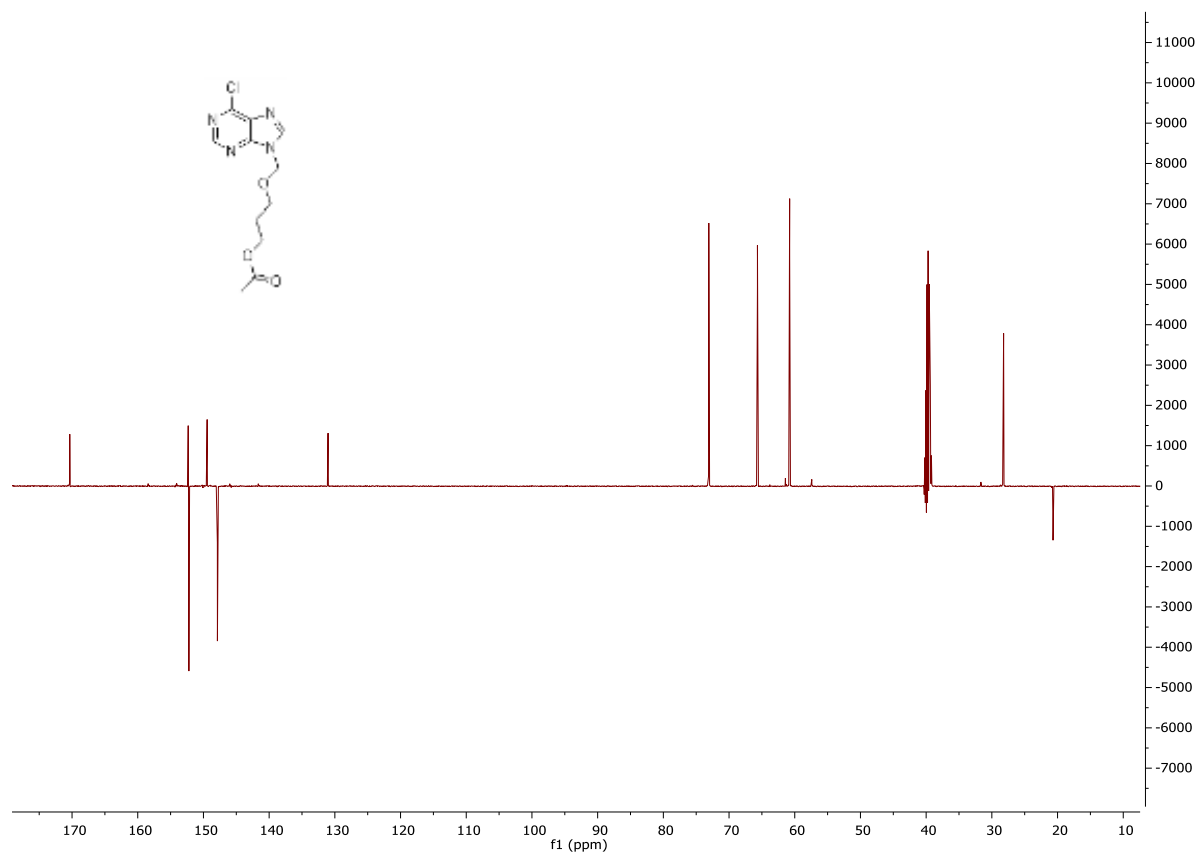
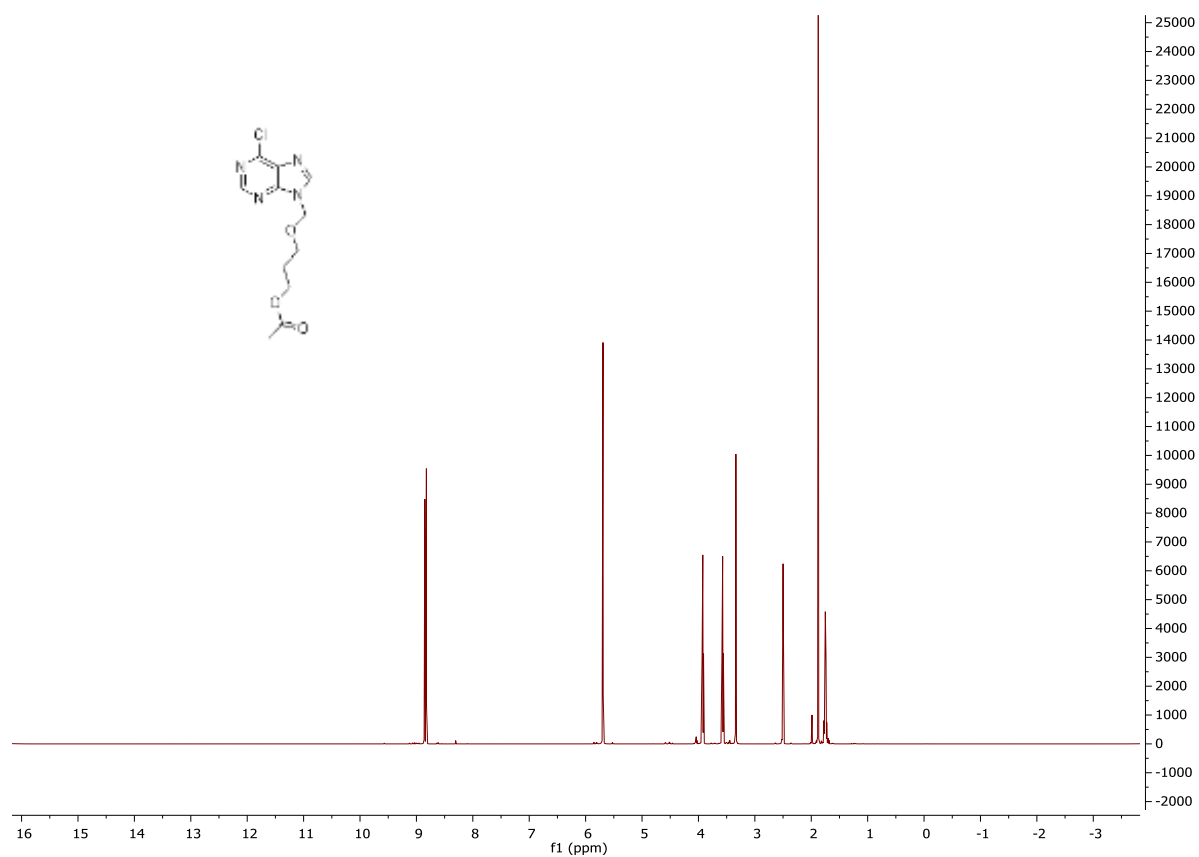
2-(2-Bromo-1-(6-chloro-7H-purin-7-yl)ethoxy)ethyl acetate (**5**)



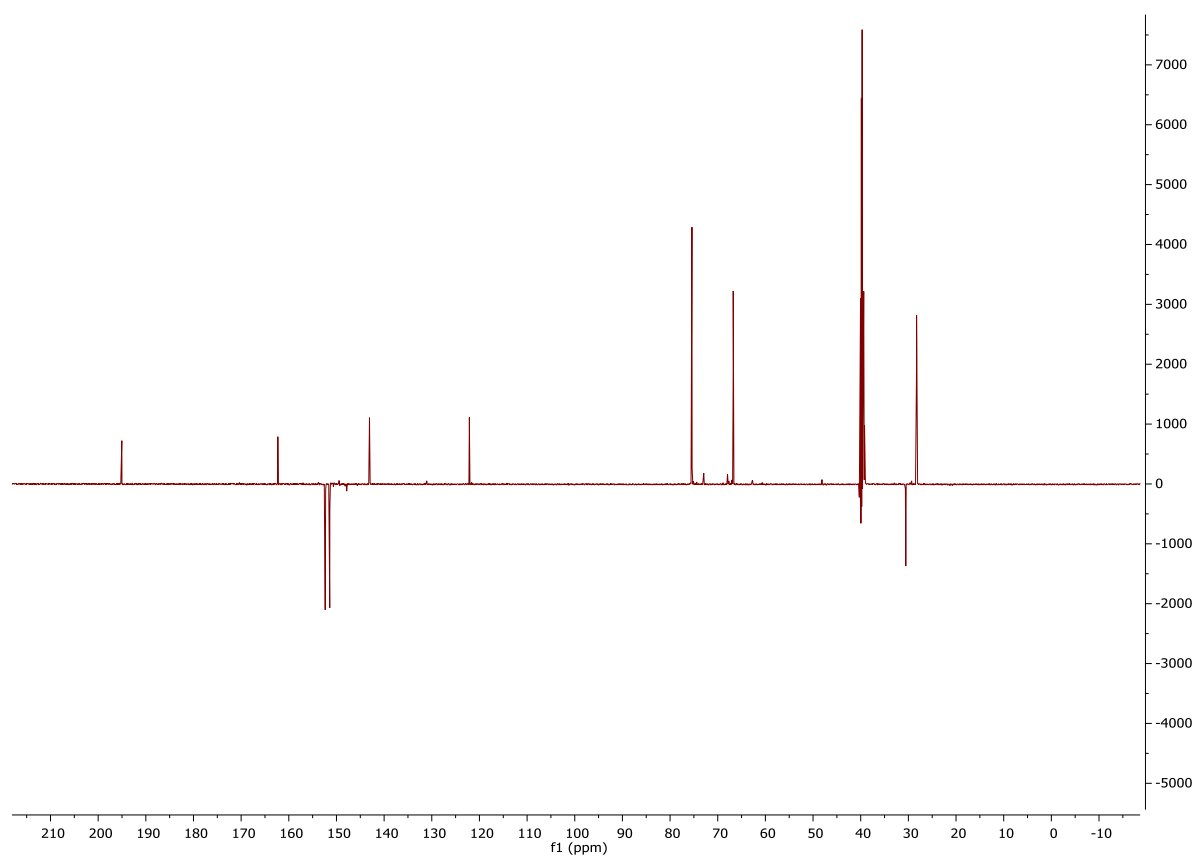
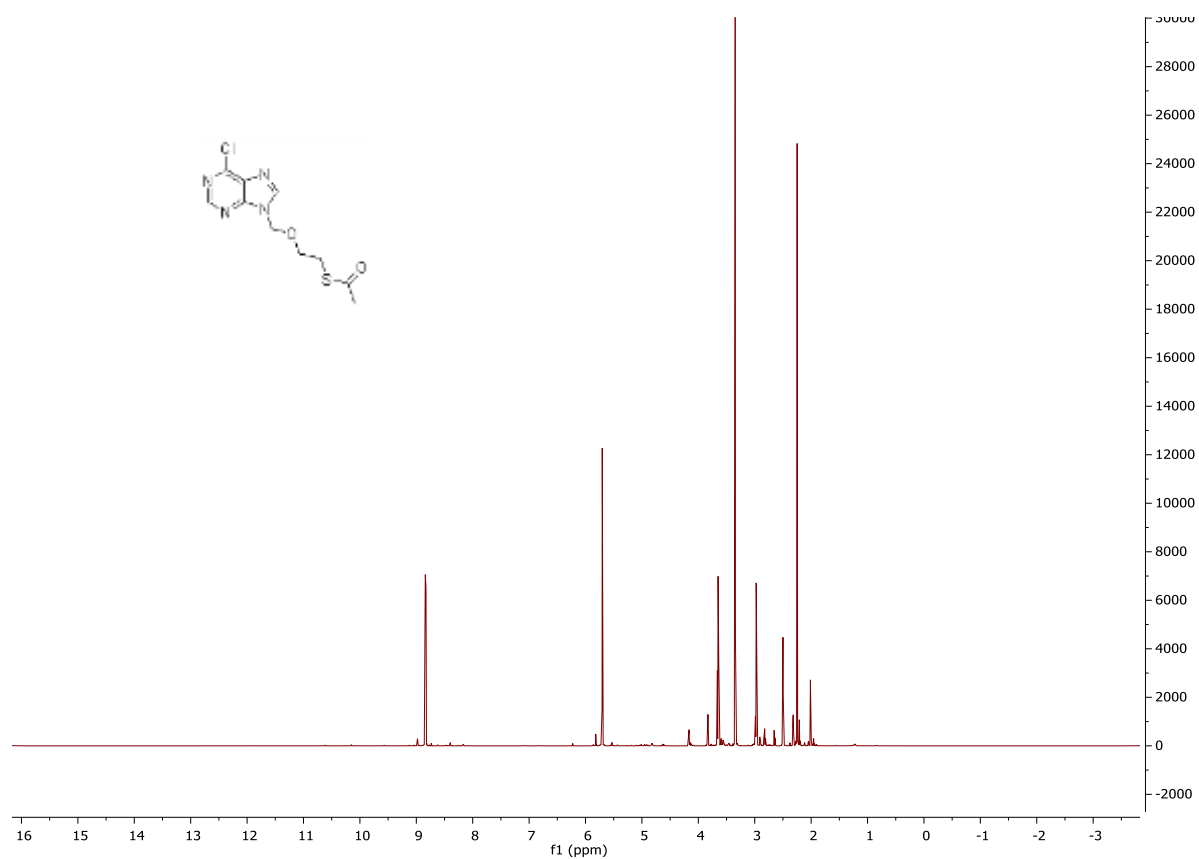
3-(2-Acetoxyethoxy)-3-(6-chloro-9H-purin-9-yl)propane-1,2-diyl diacetate (6)



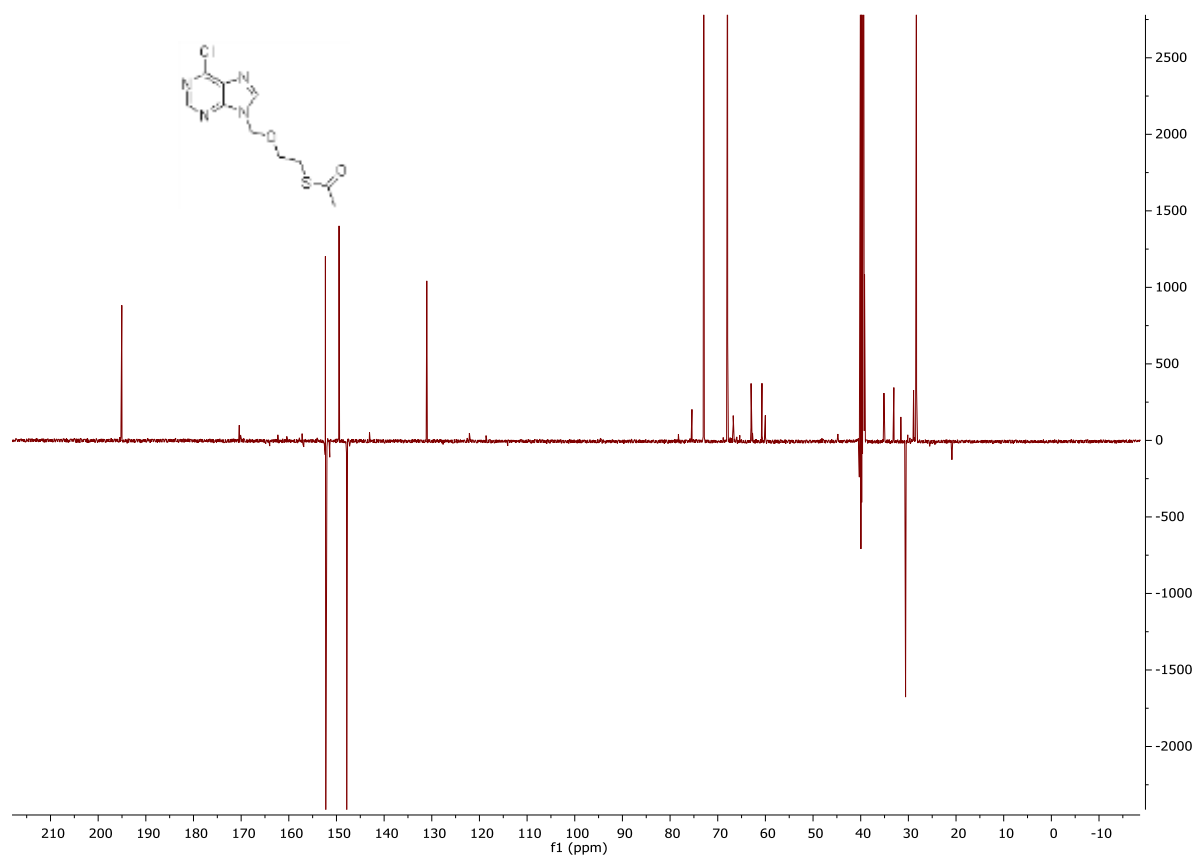
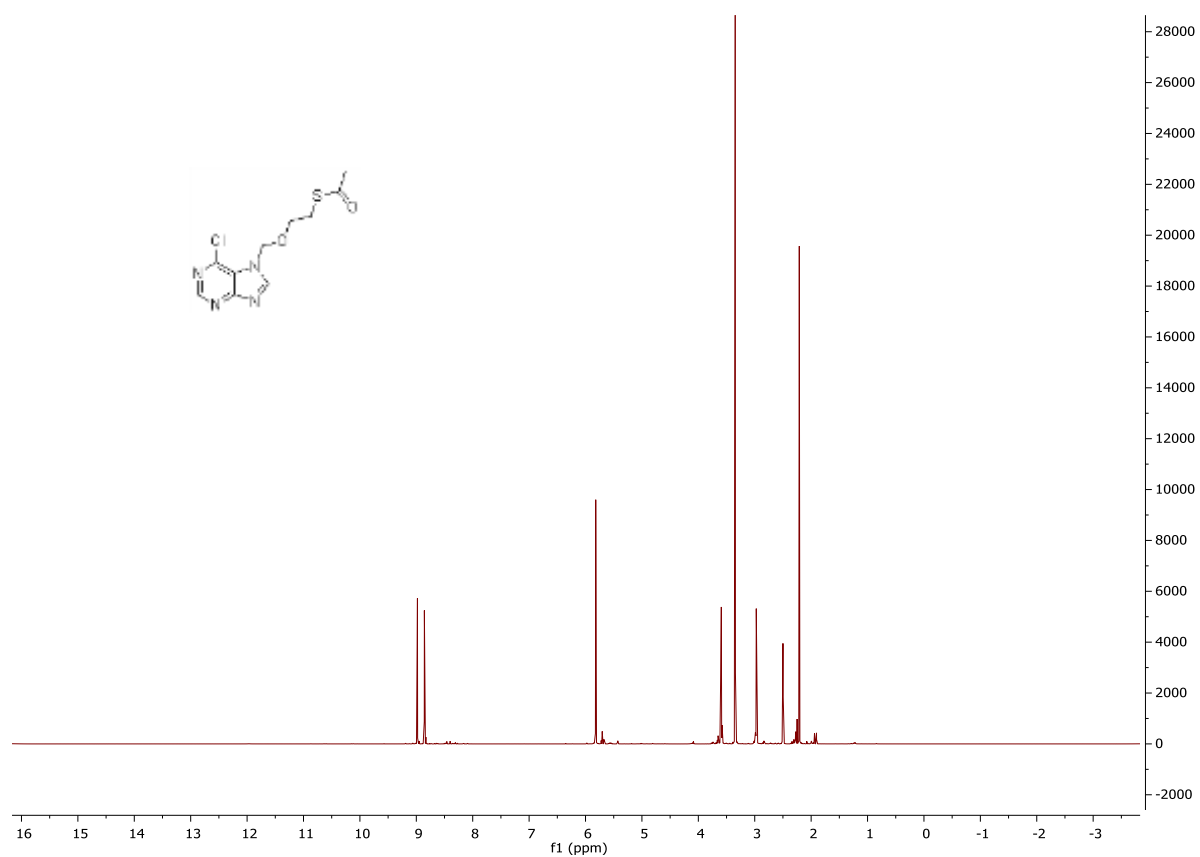
3-((6-Chloro-9H-purin-9-yl)methoxy)propyl acetate (7)



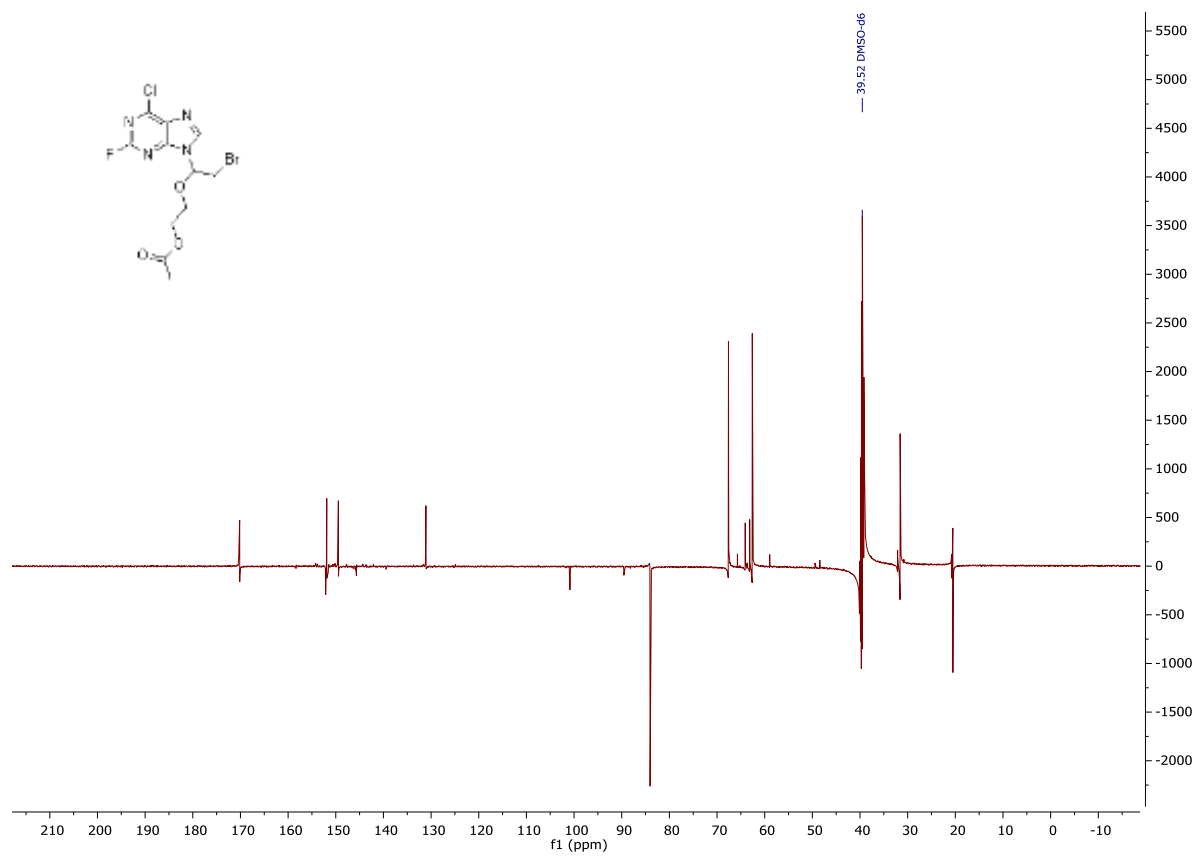
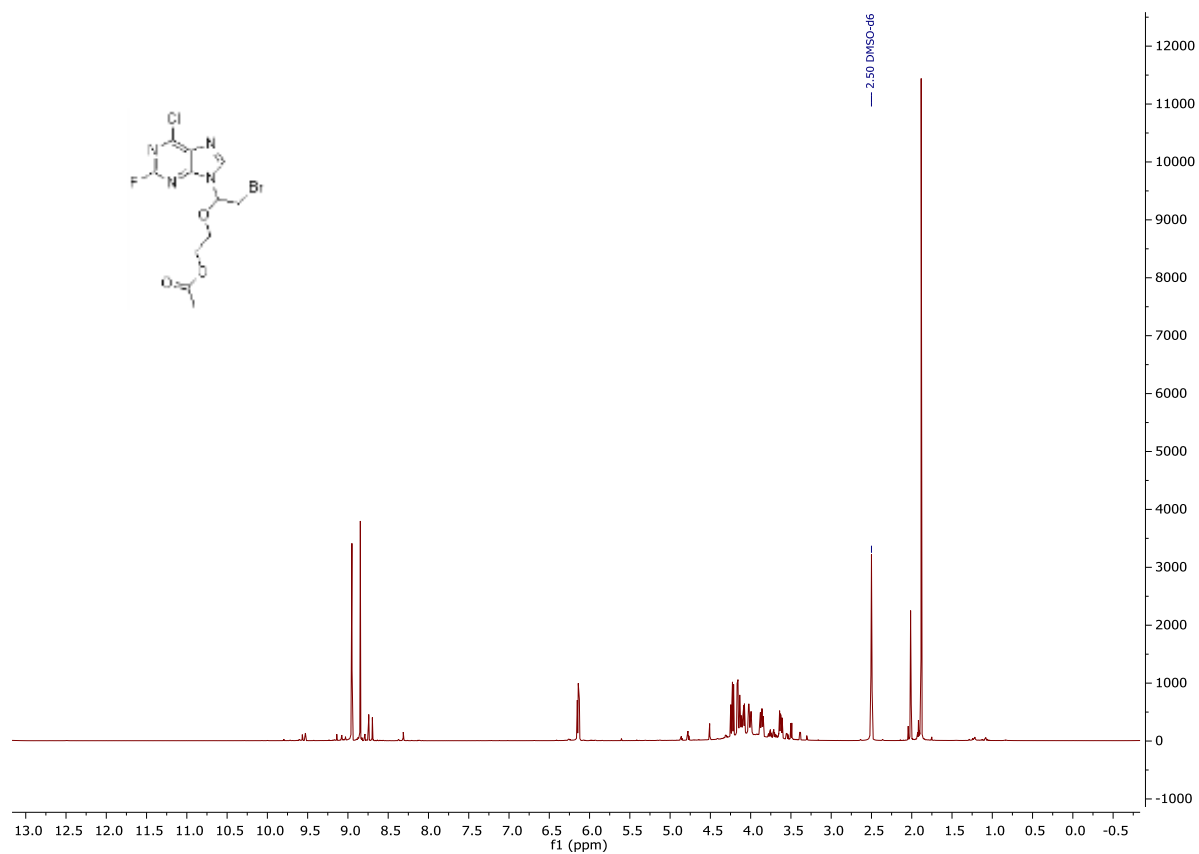
*S*-2-((6-Chloro-9*H*-purin-9-yl)methoxy)ethyl ethanethioate (**8**)



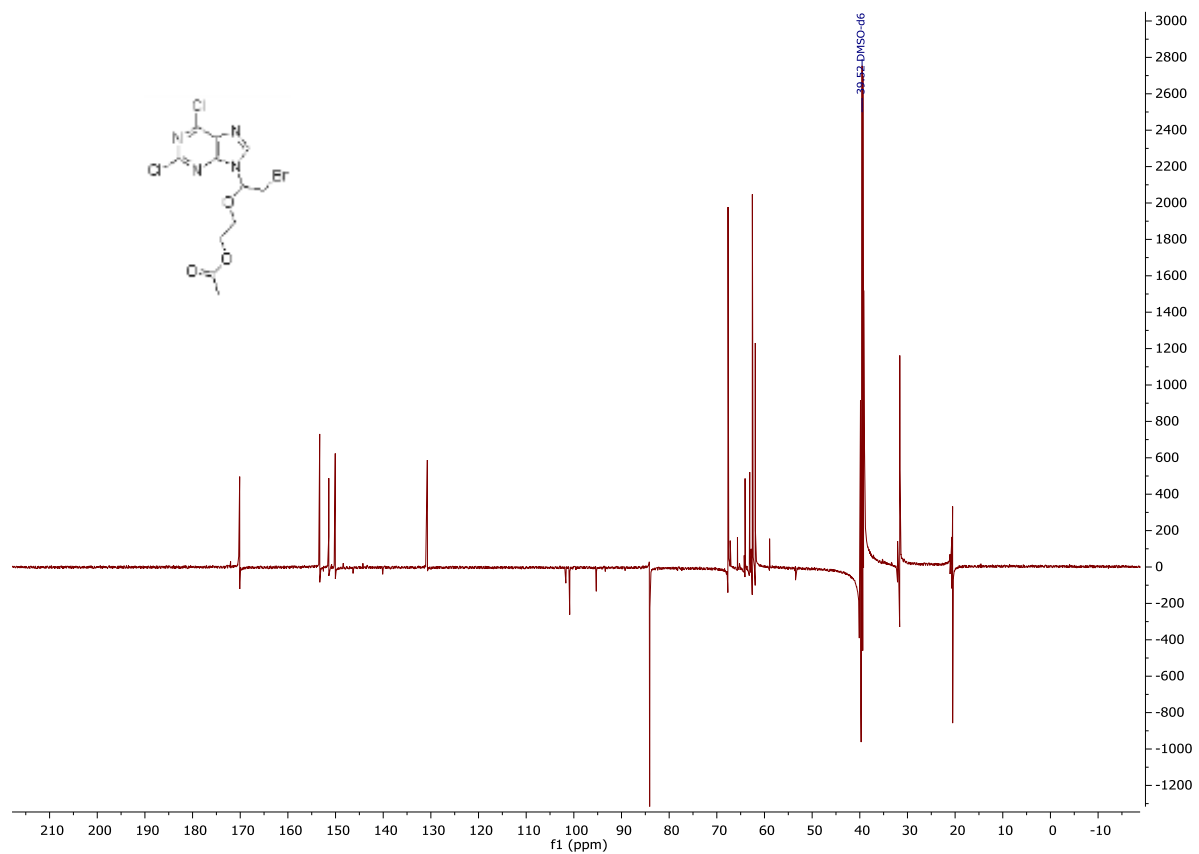
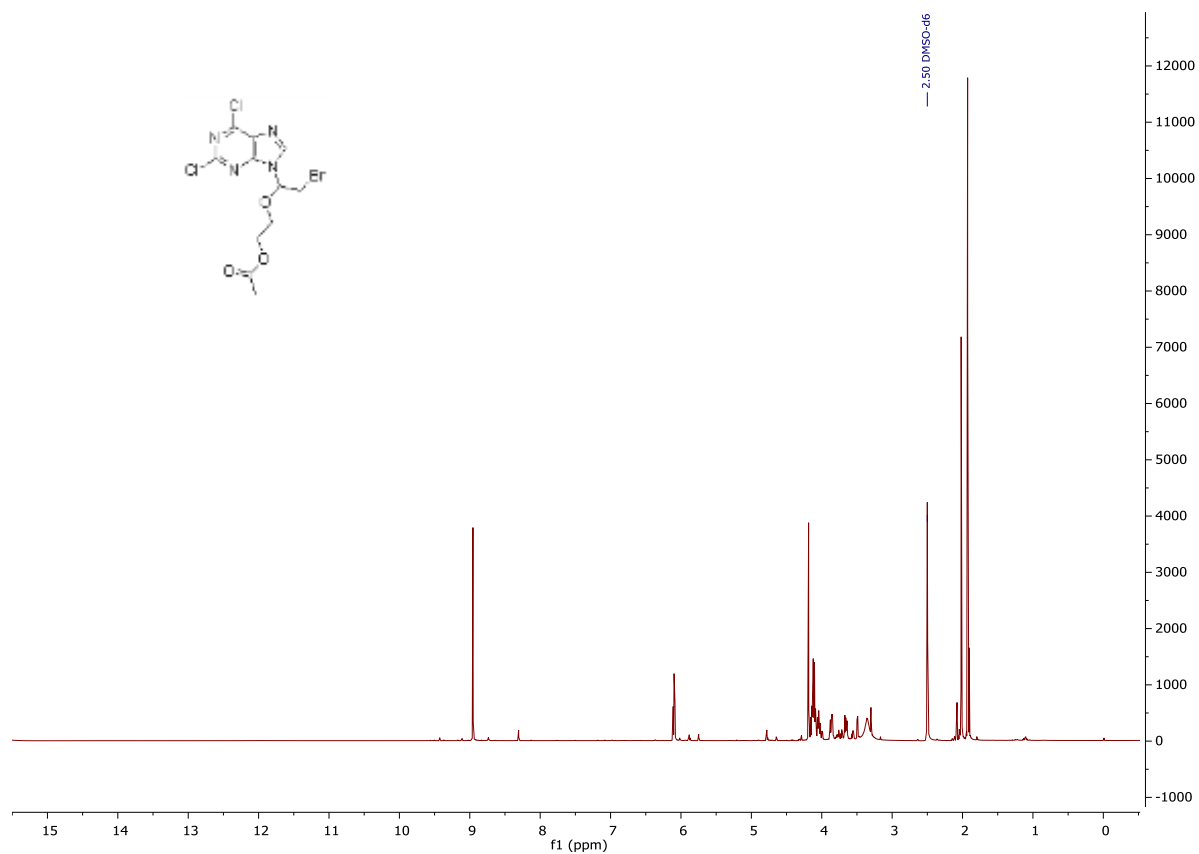
*S*-2-((6-Chloro-7*H*-purin-7-yl)methoxy)ethyl ethanethioate (**9**)



2-(2-Bromo-1-(6-chloro-2-fluoro-9H-purin-9-yl)ethoxy)ethyl acetate (**12**)

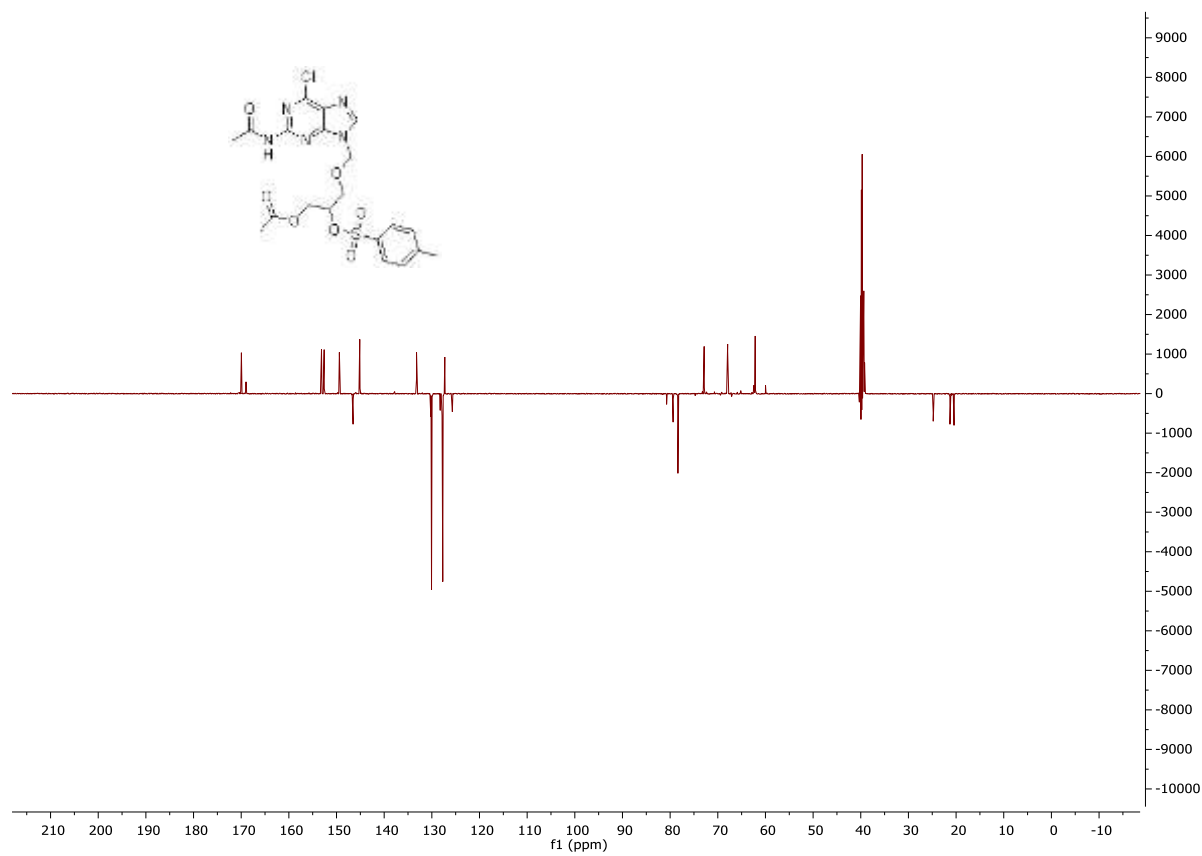
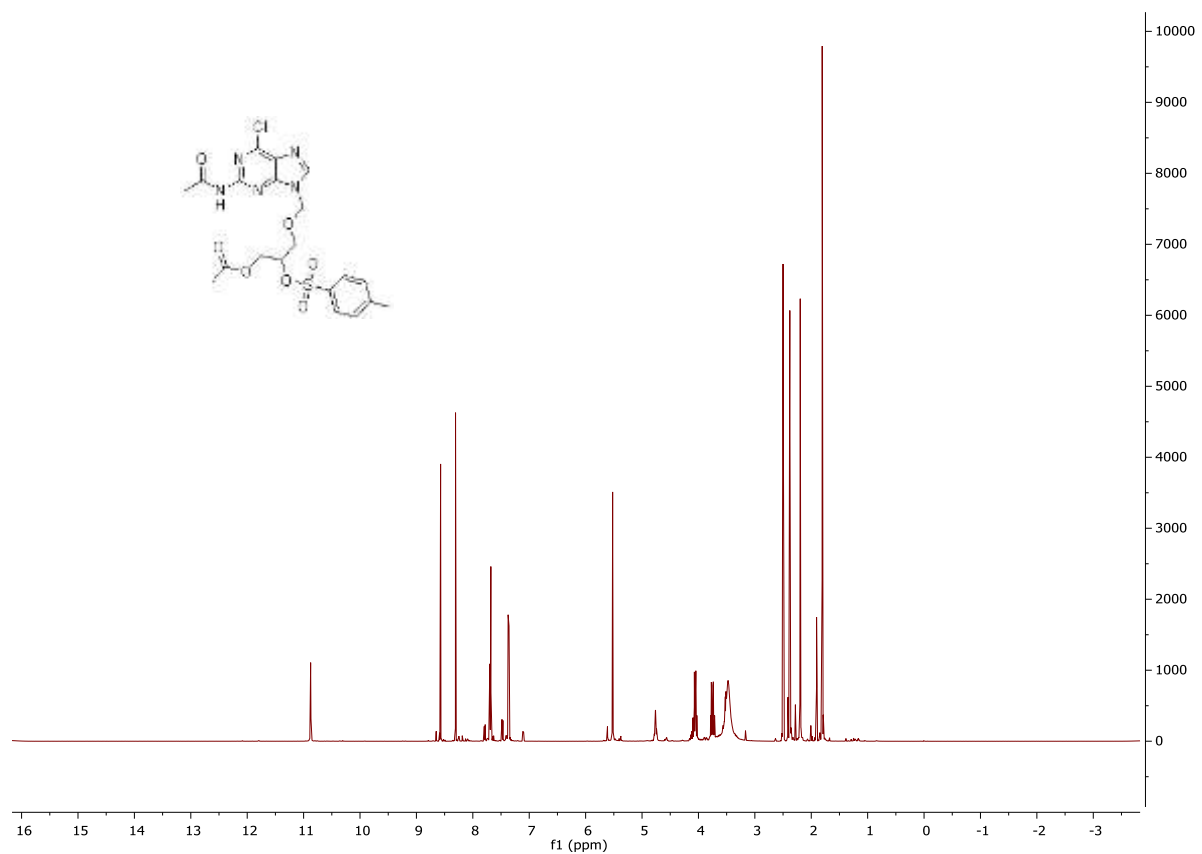


2-(2-Bromo-1-(2,6-dichloro-9*H*-purin-9-yl)ethoxy)ethyl acetate (**13**)

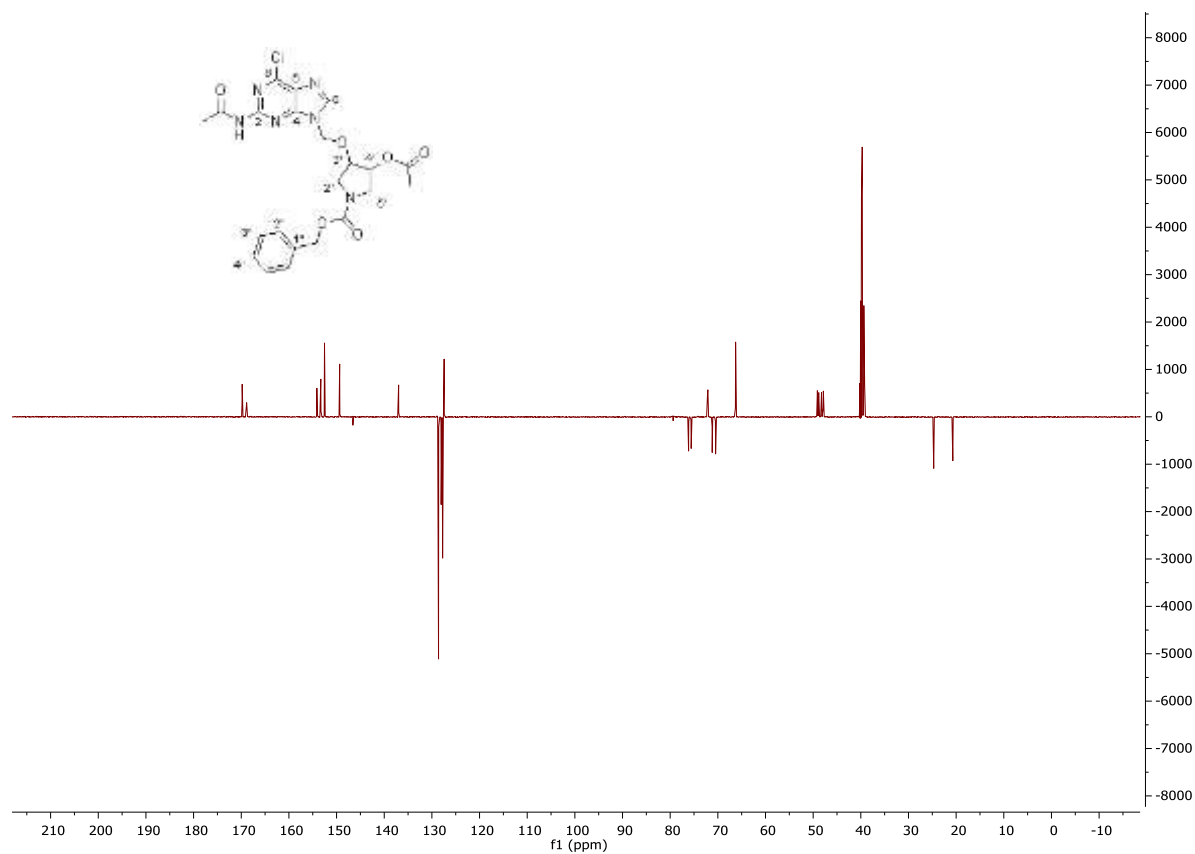
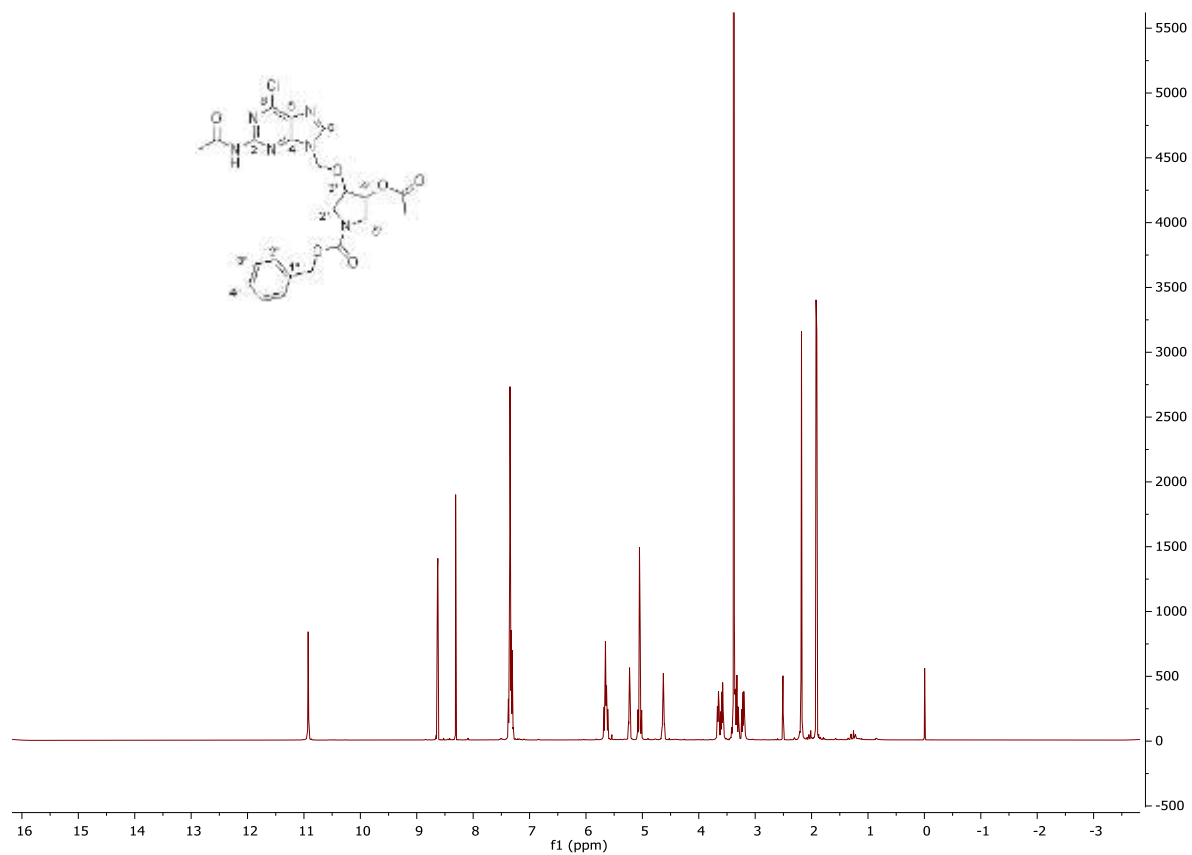




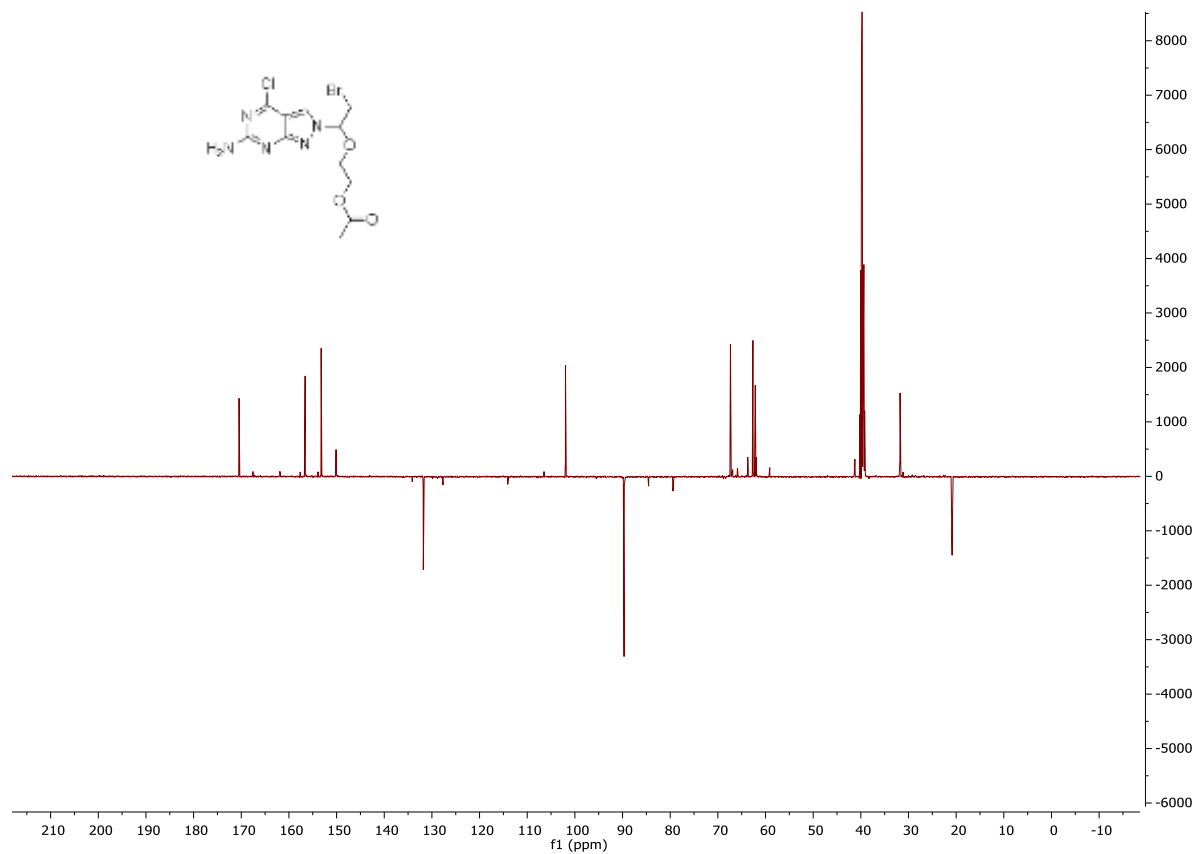
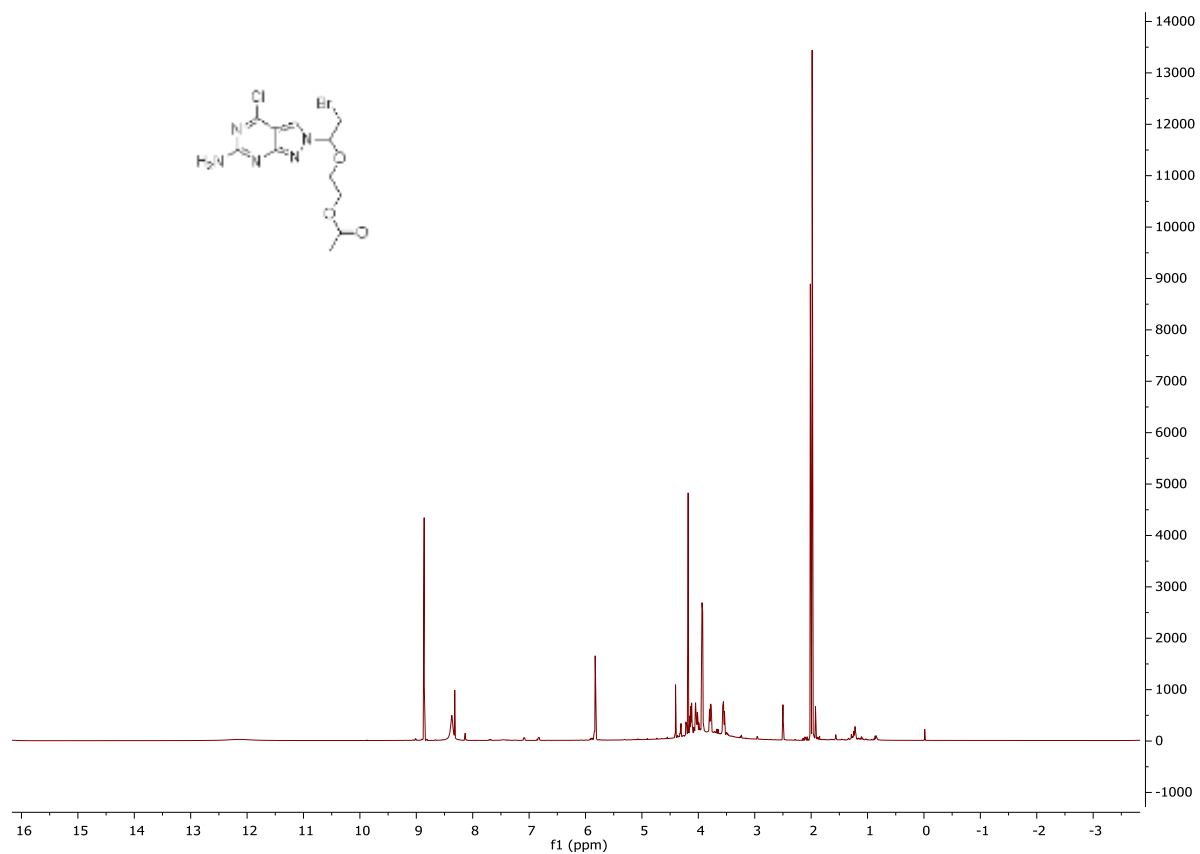
3-((2-Acetamido-6-chloro-9H-purin-9-yl)methoxy)-2-(tosyloxy)propyl acetate (**17**)



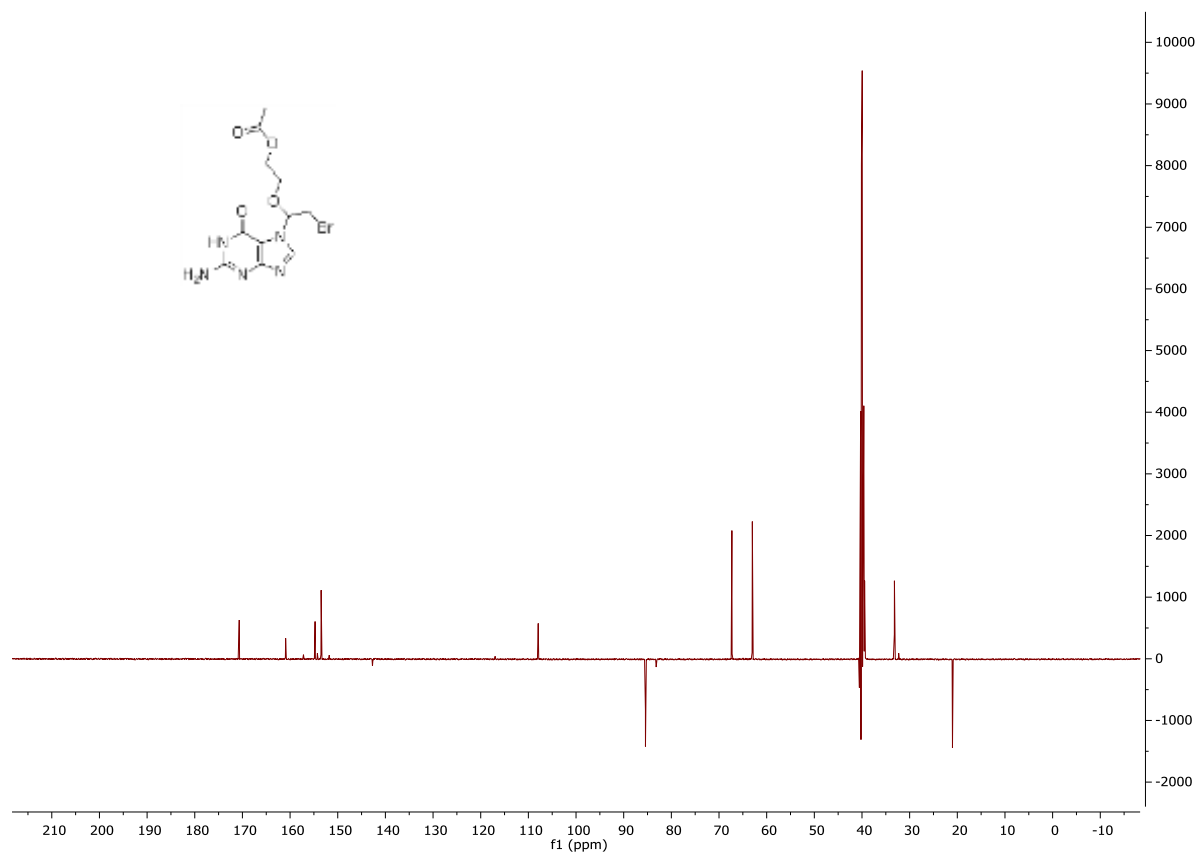
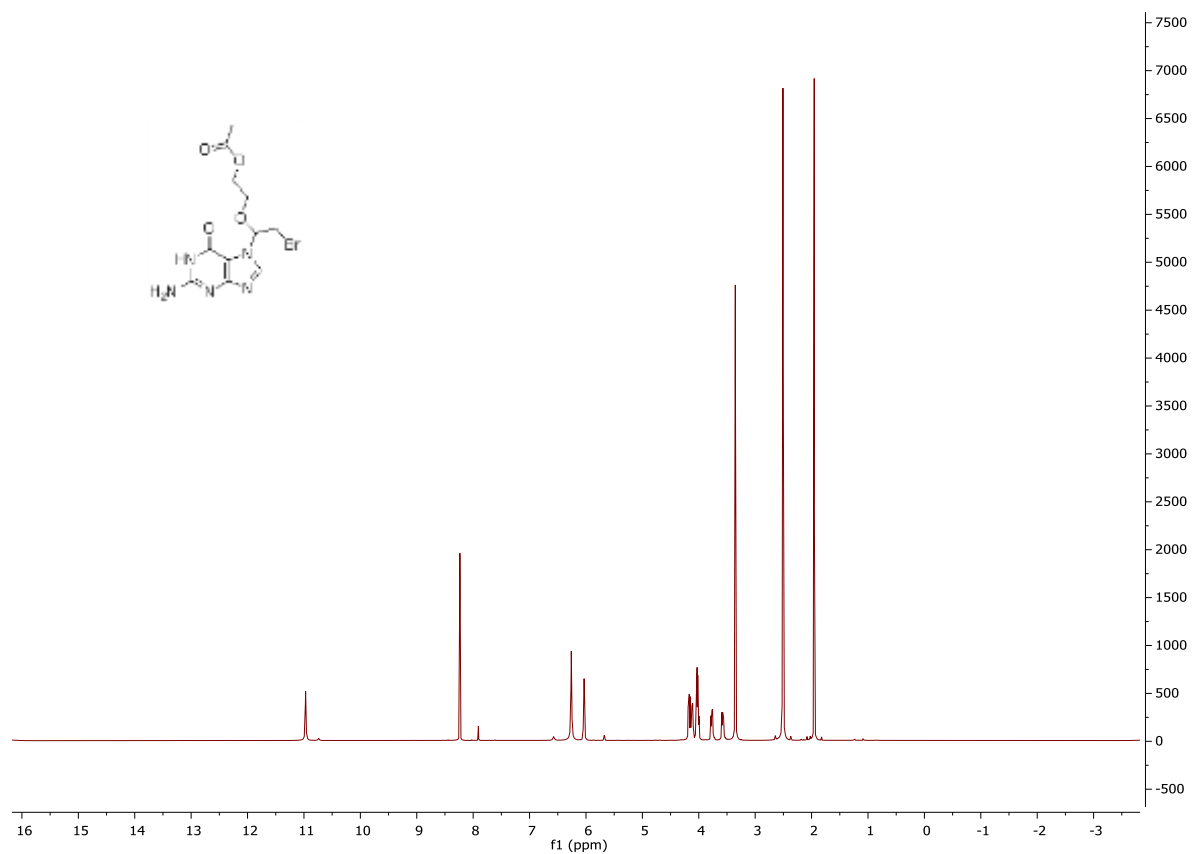
Benzyl 3-((2-acetamido-6-chloro-9*H*-purin-9-yl)methoxy)-4-acetoxypyrrolidine-1-carboxylate (**20**)



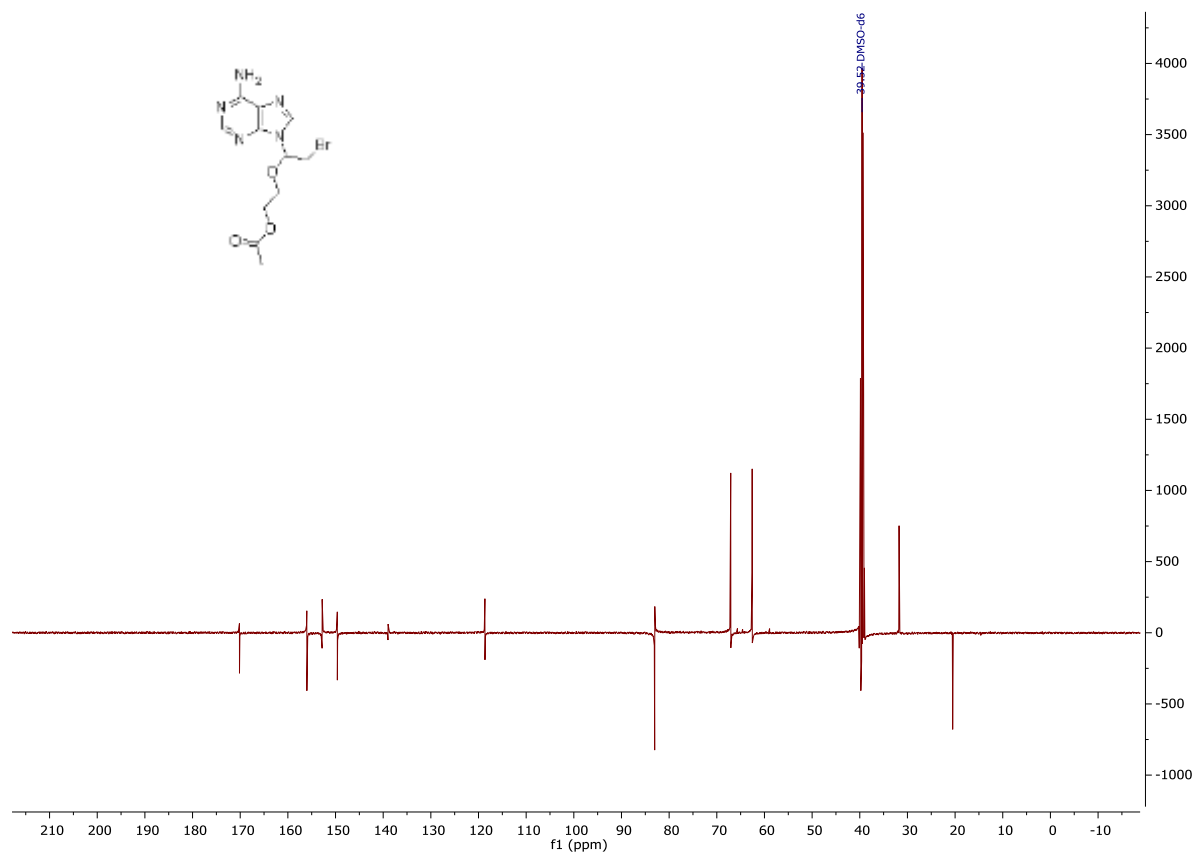
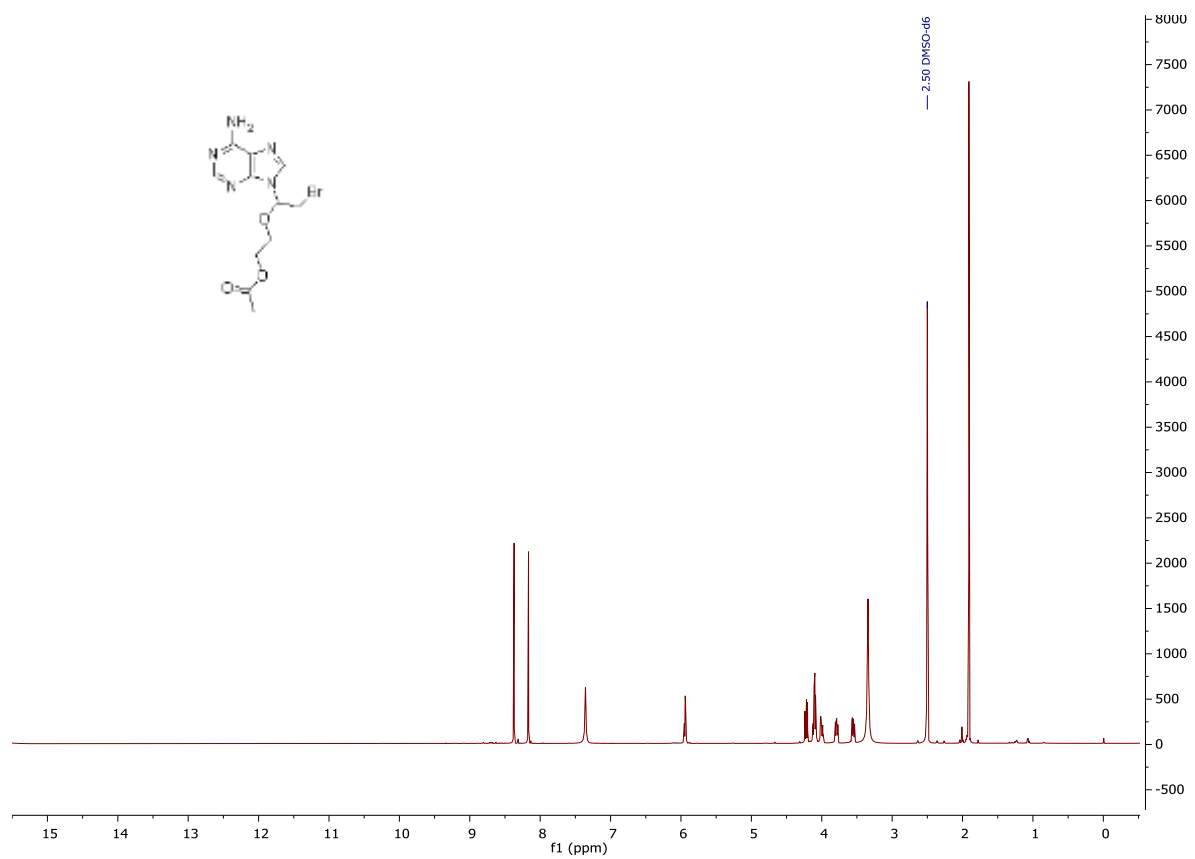
2-(1-(6-Amino-4-chloro-2*H*-pyrazolo[3,4-*d*]pyrimidin-2-yl)-2-bromoethoxy)ethyl acetate (**22**)



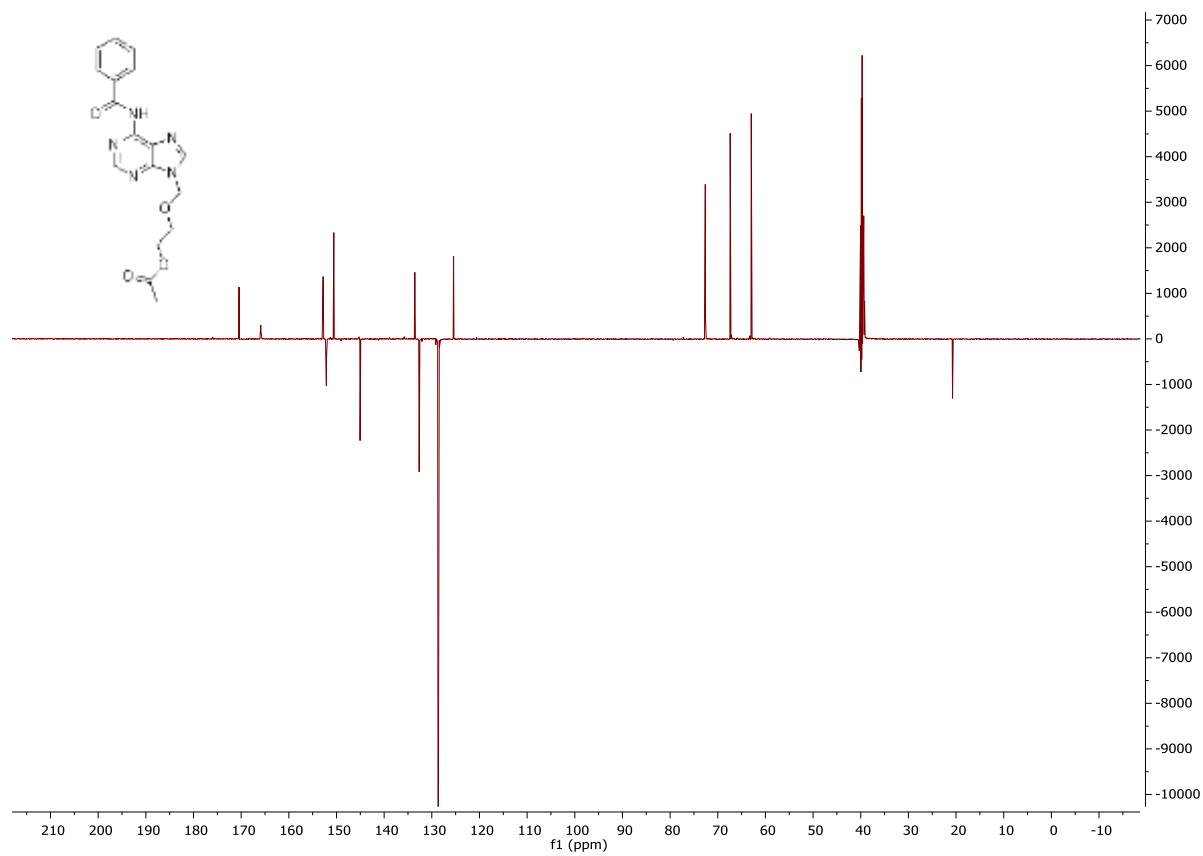
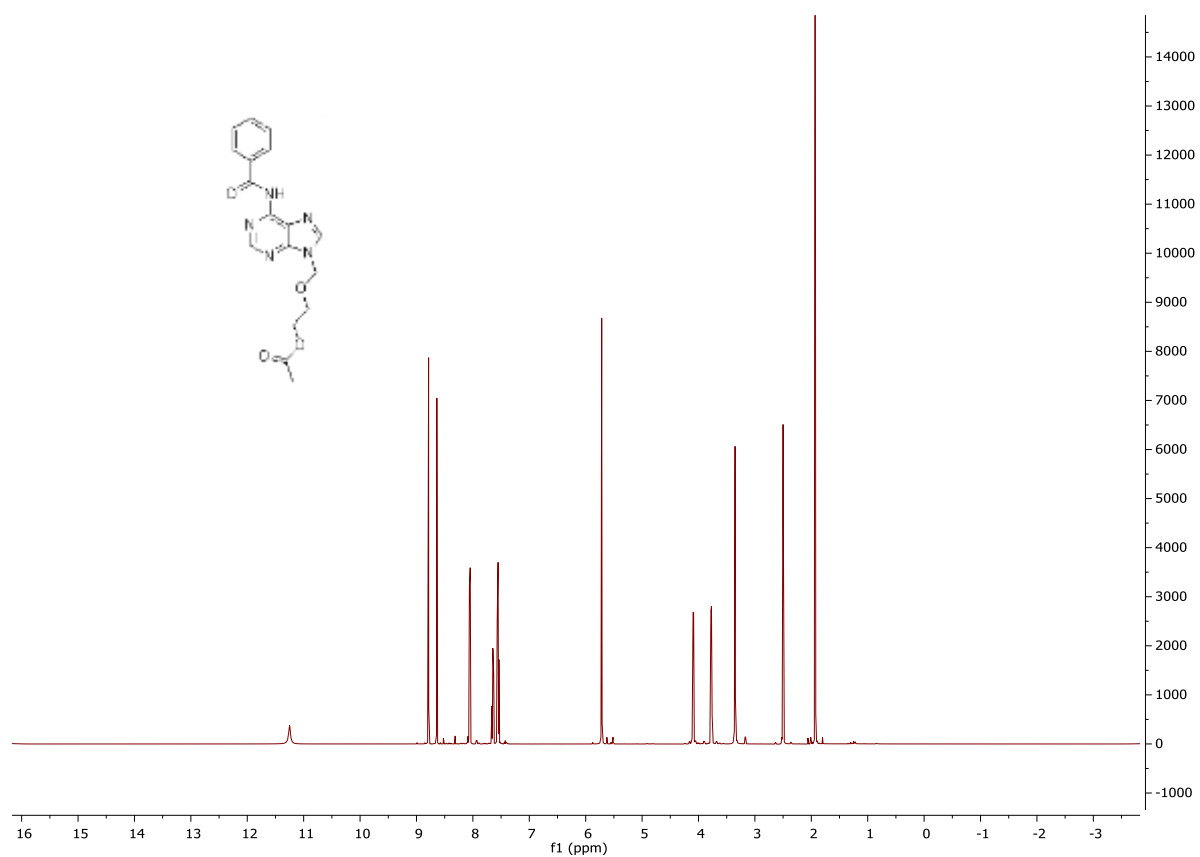
2-(1-(Guanine-7-yl)-2-bromoethoxy)ethyl acetate (**23**)



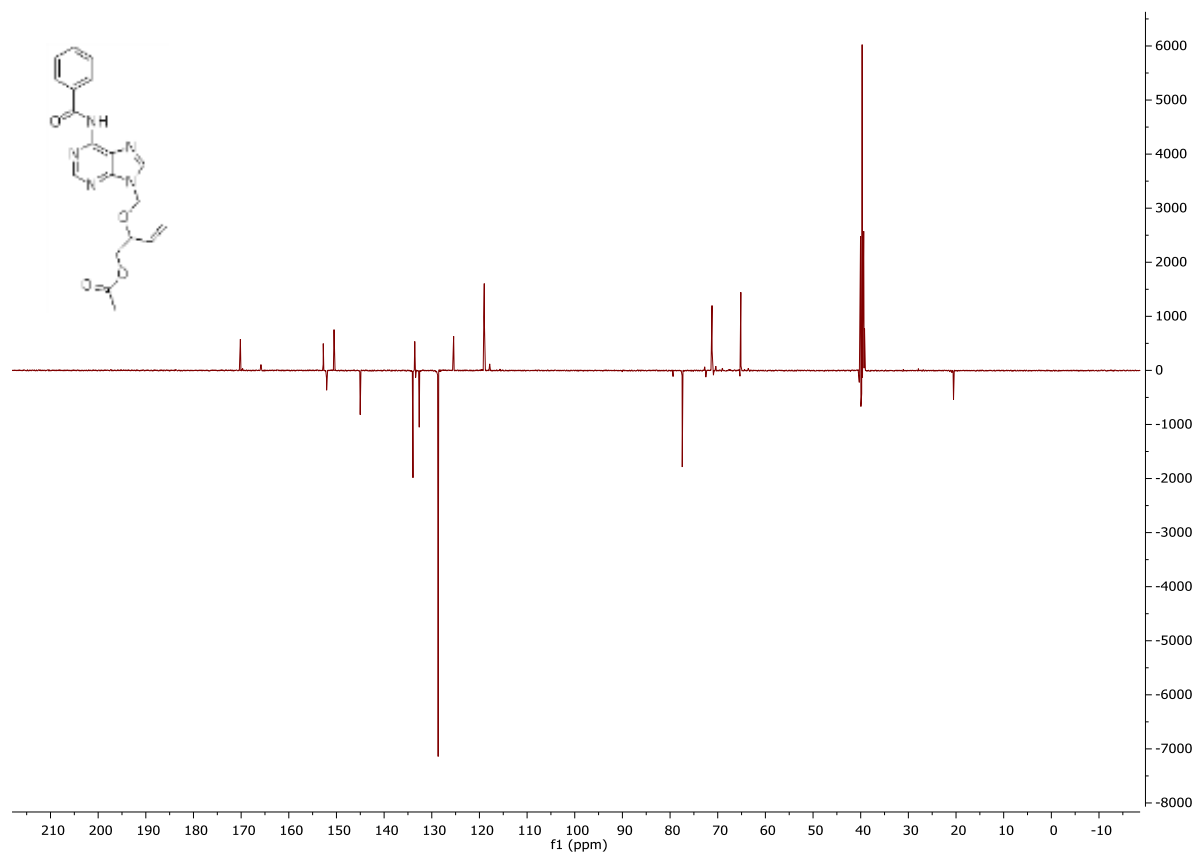
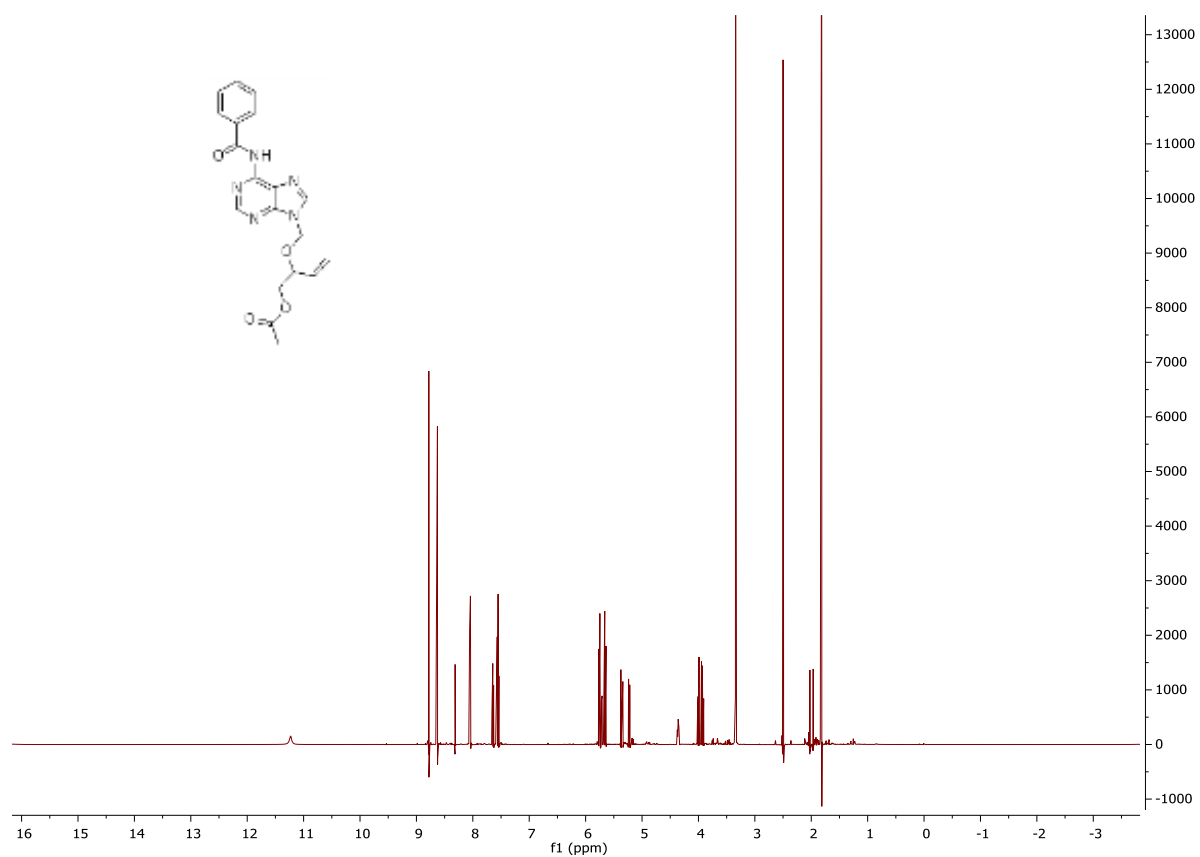
2-(1-(Adenin-9-yl)-2-bromoethoxy)ethyl acetate (**24**)



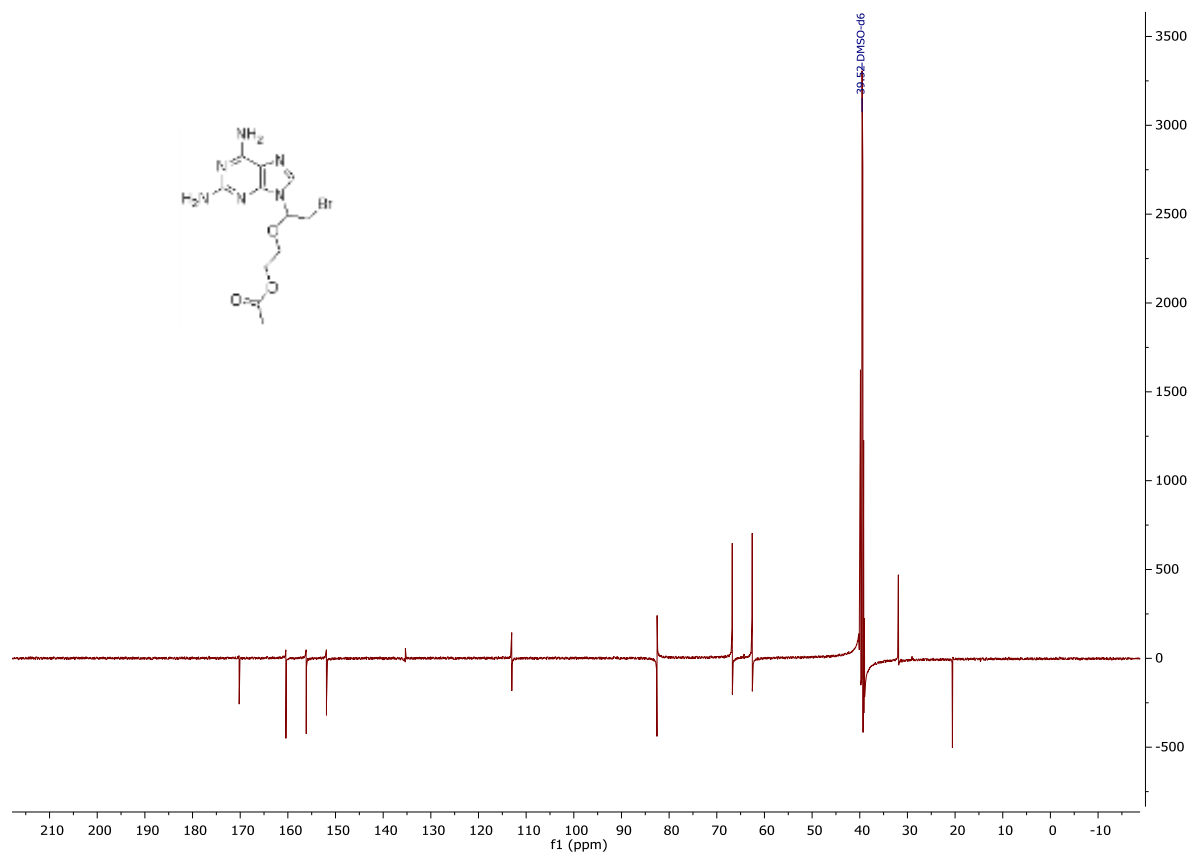
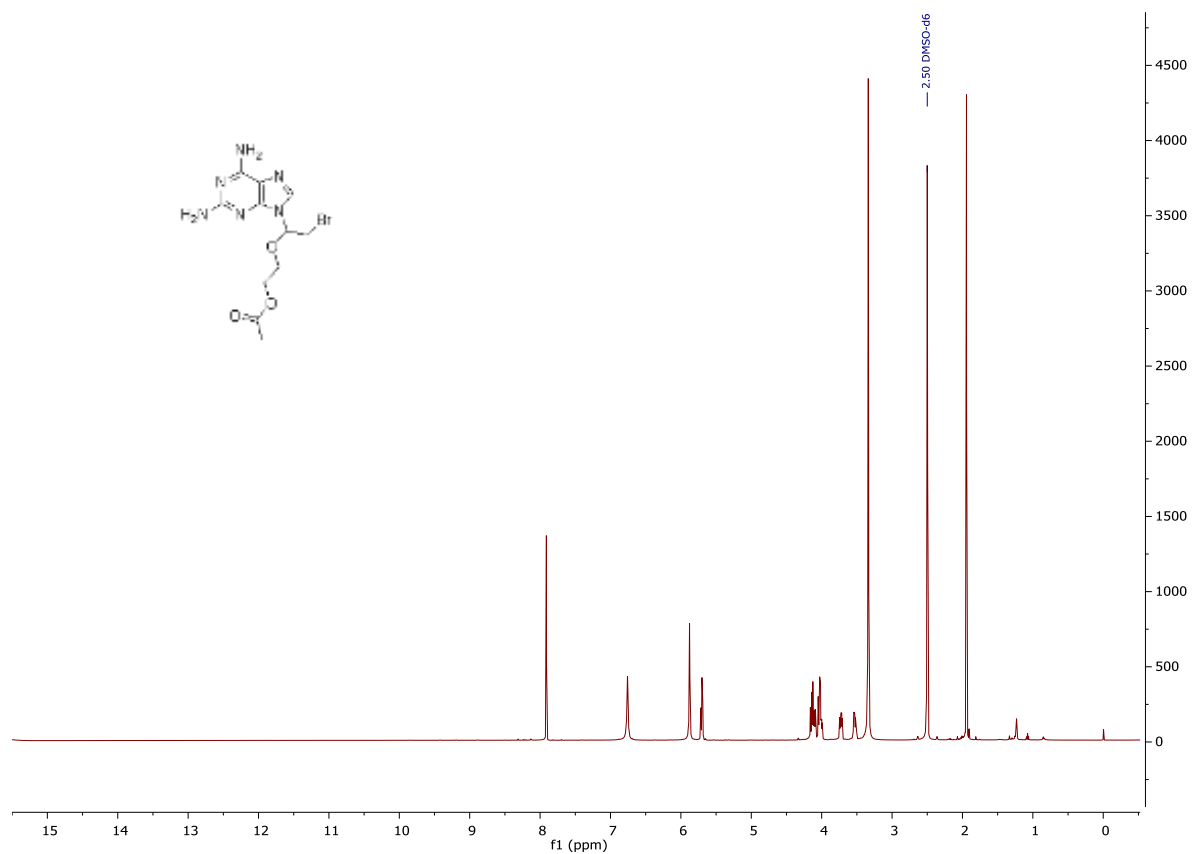
2-((6-Benzamido-9H-purin-9-yl)methoxy)ethyl acetate (**25**)



2-((6-Benzamido-9H-purin-9-yl)methoxy)but-3-en-1-yl acetate (**26**)

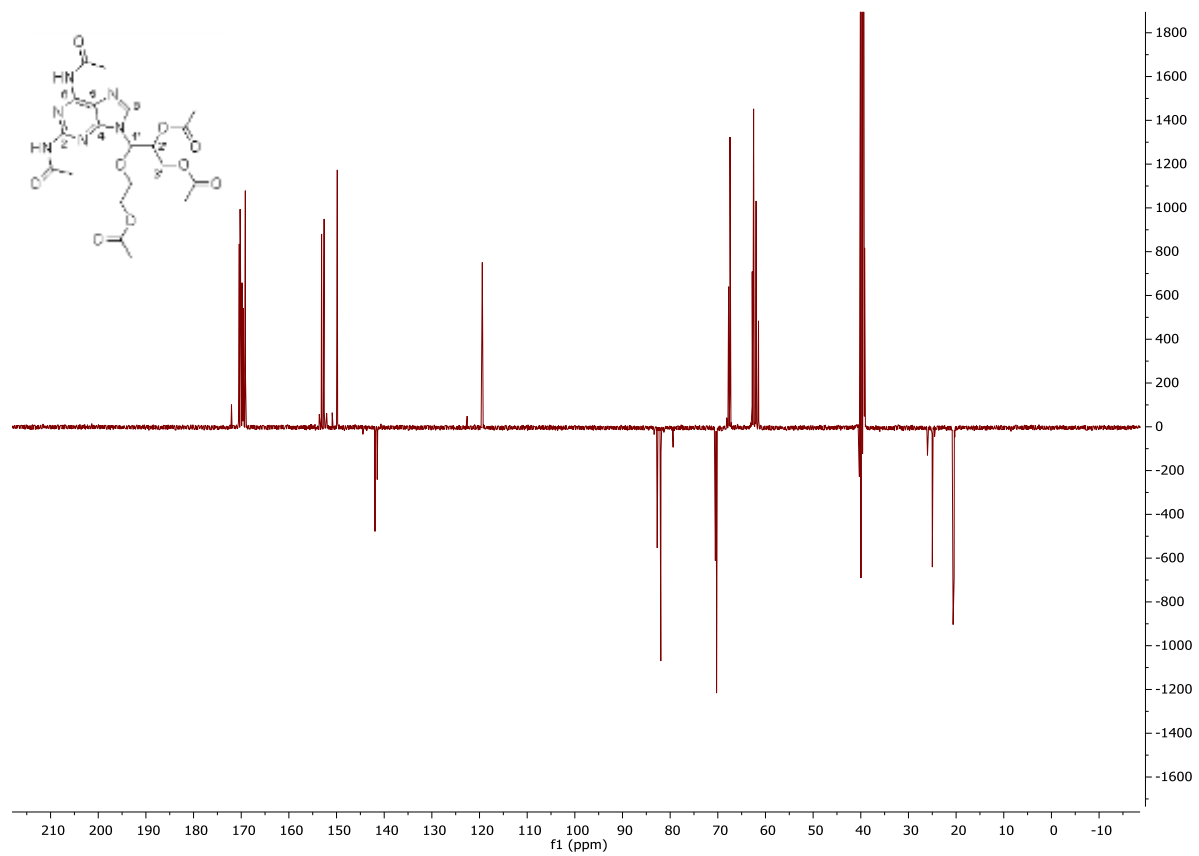
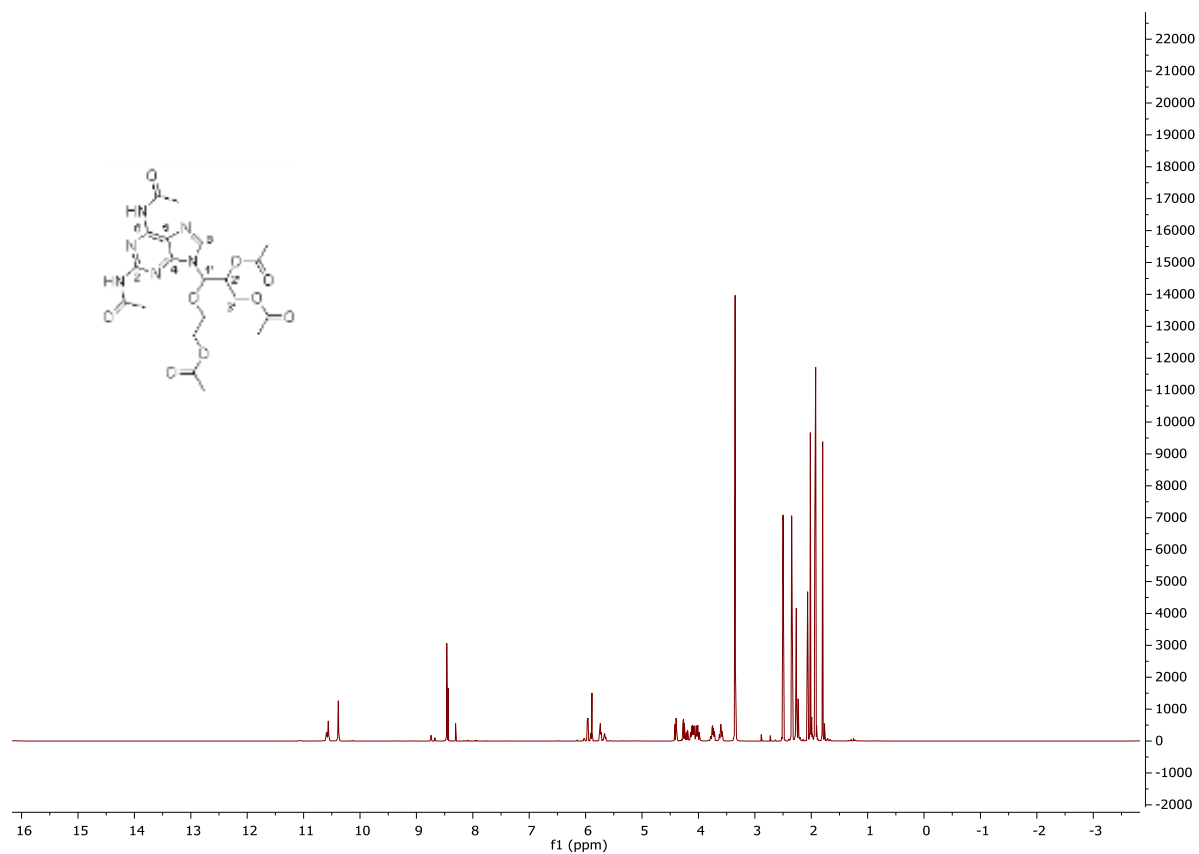


2-(2-Bromo-1-(2,6-diamino-9H-purin-9-yl)ethoxy)ethyl acetate (**29**)

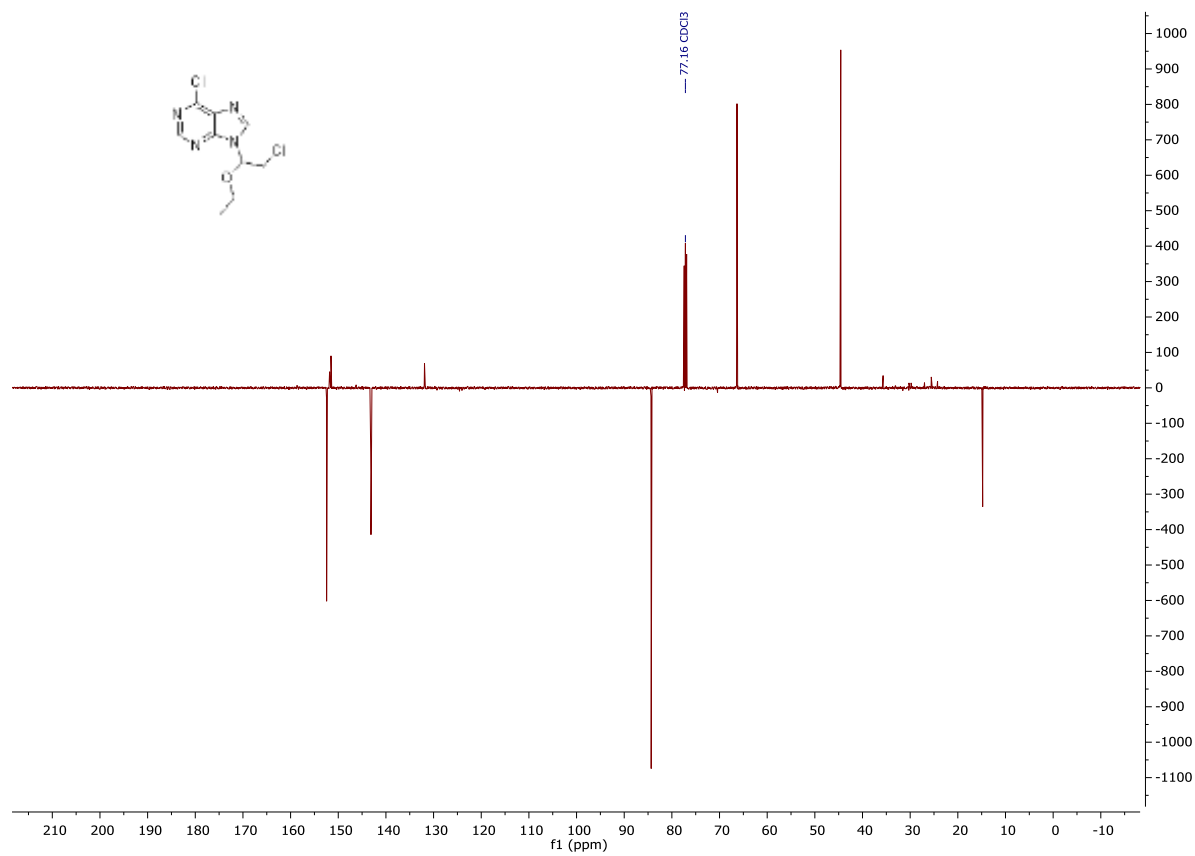
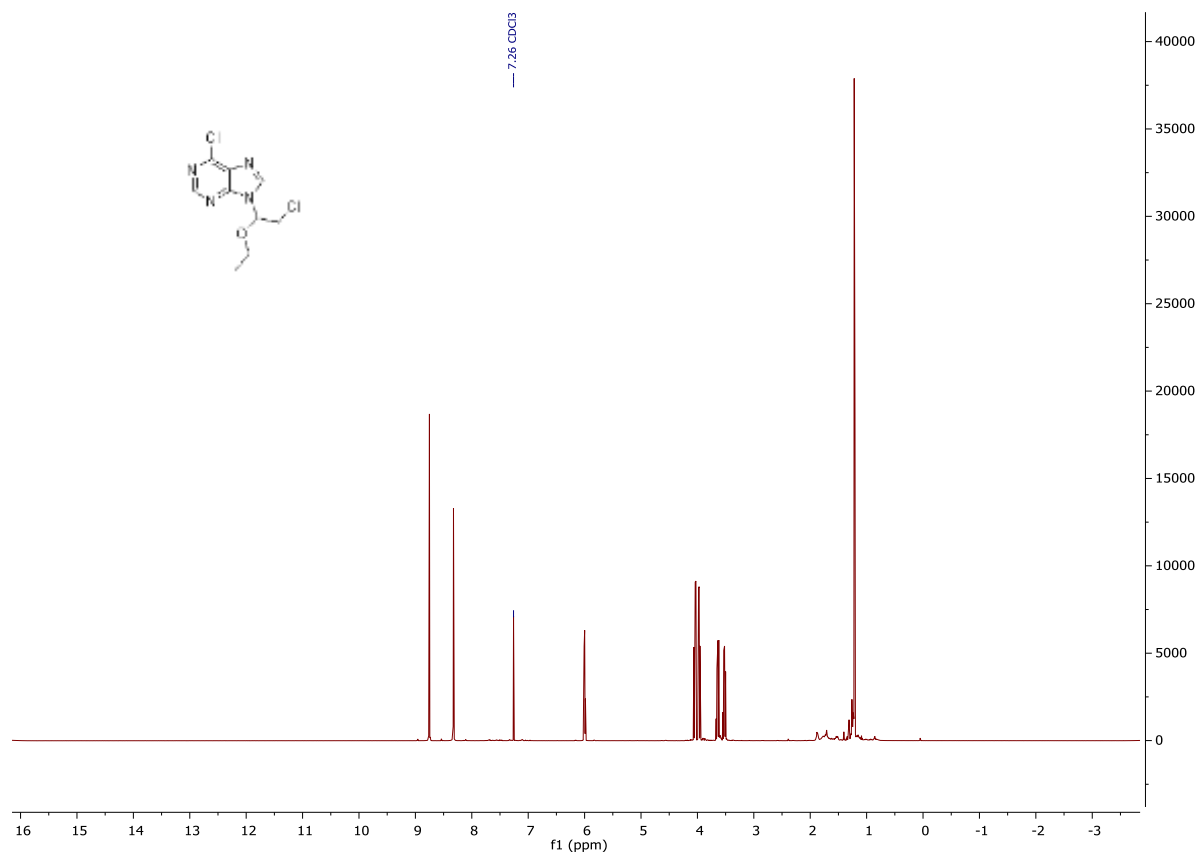




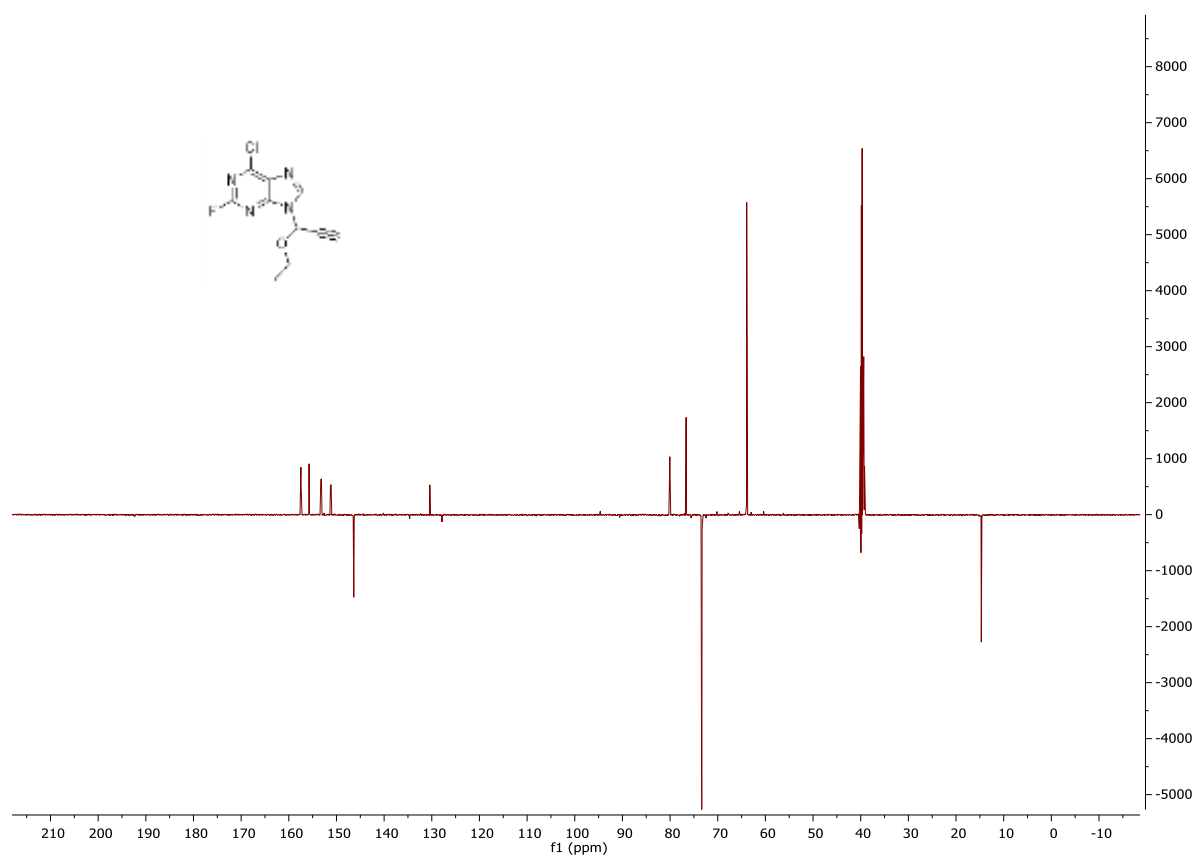
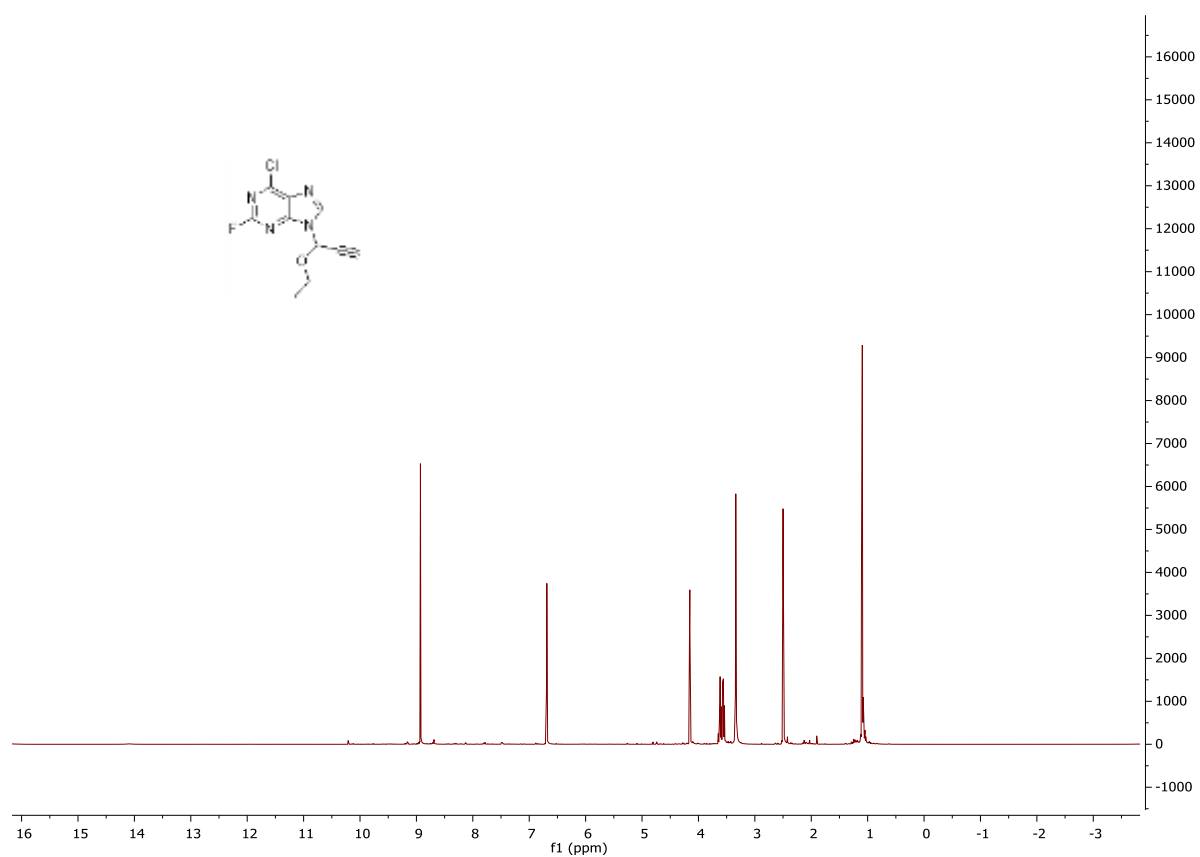
3-(2-Acetoxyethoxy)-3-(2,6-diacetamido-9H-purin-9-yl)propane-1,2-diyl diacetate (**30**)



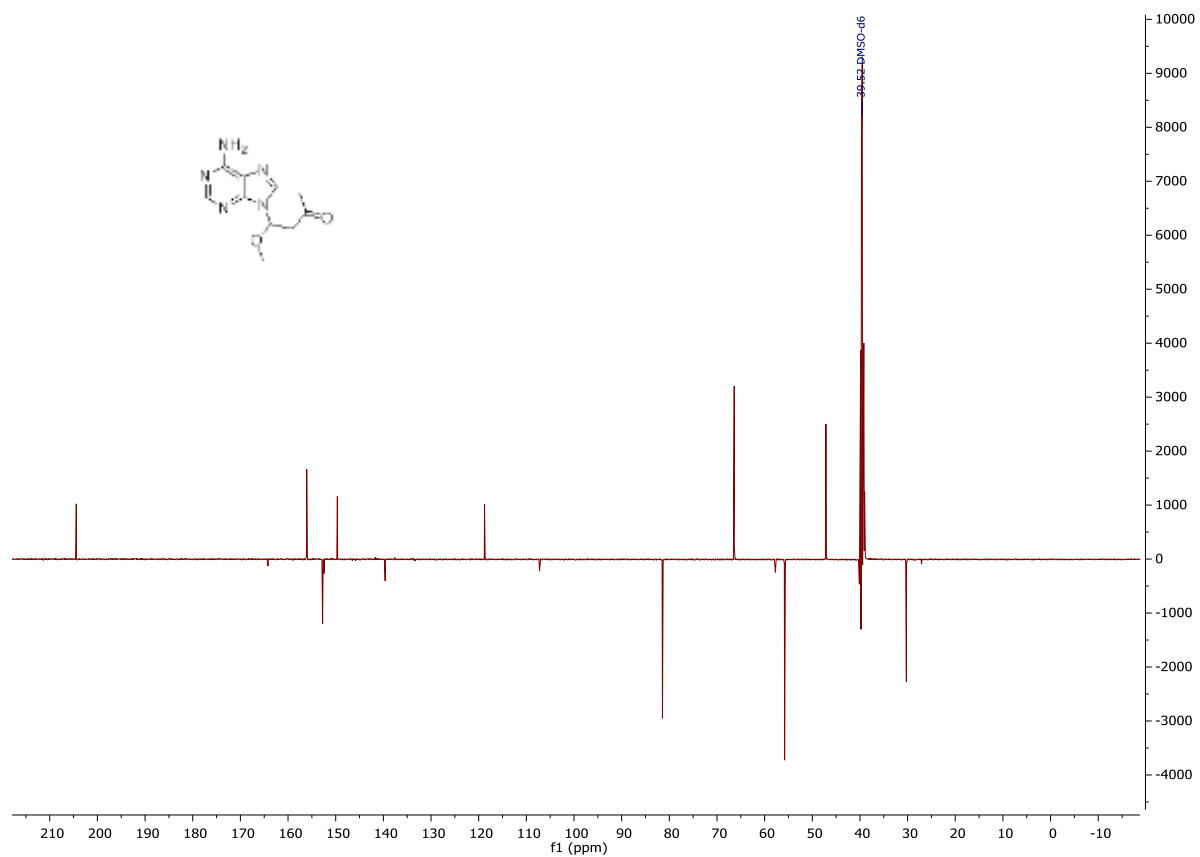
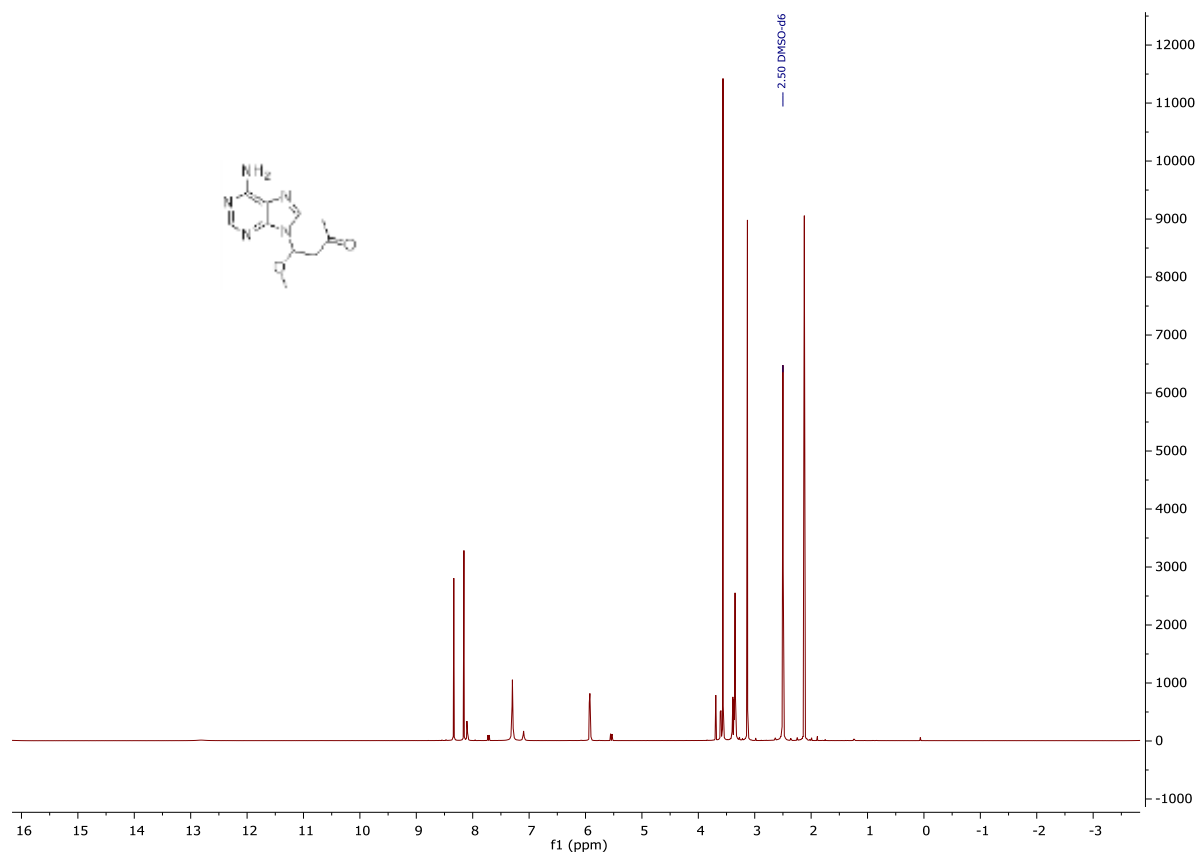
6-Chloro-9-(2-chloro-1-ethoxyethyl)-9H-purine (31)



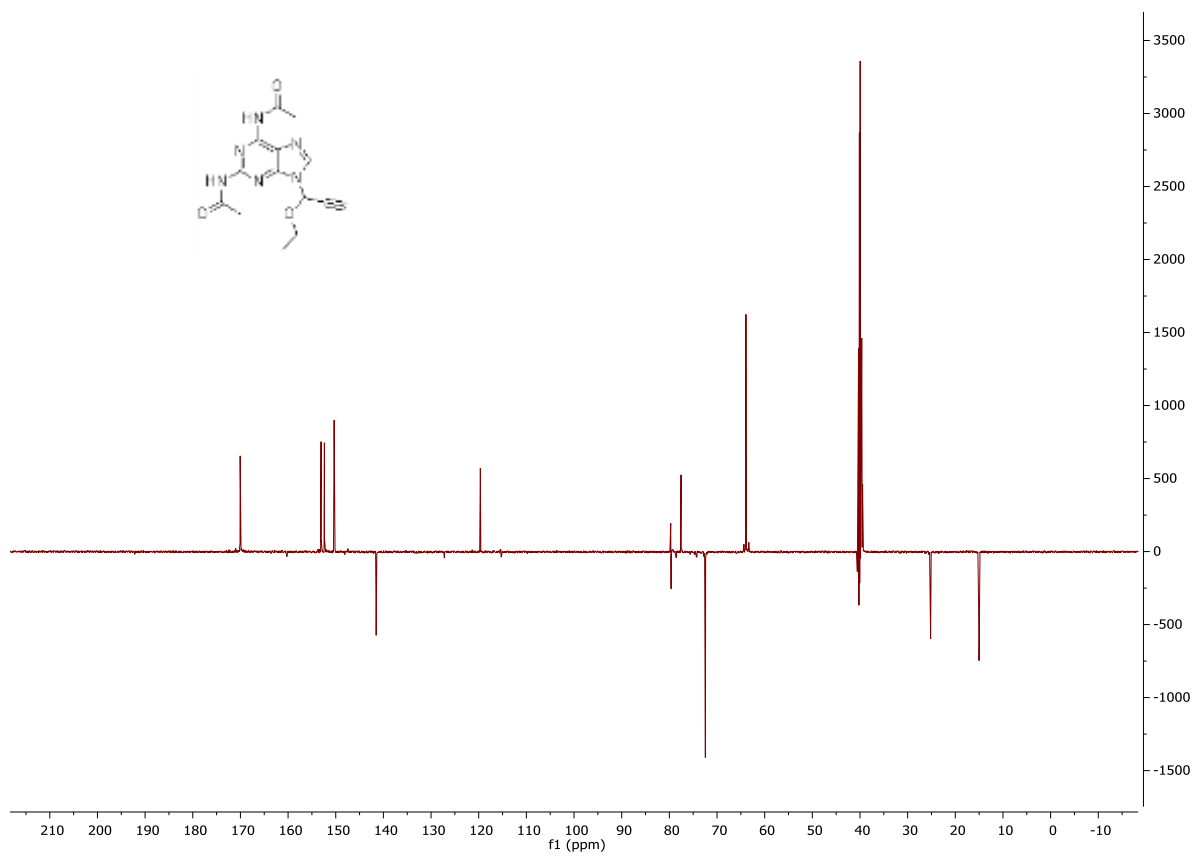
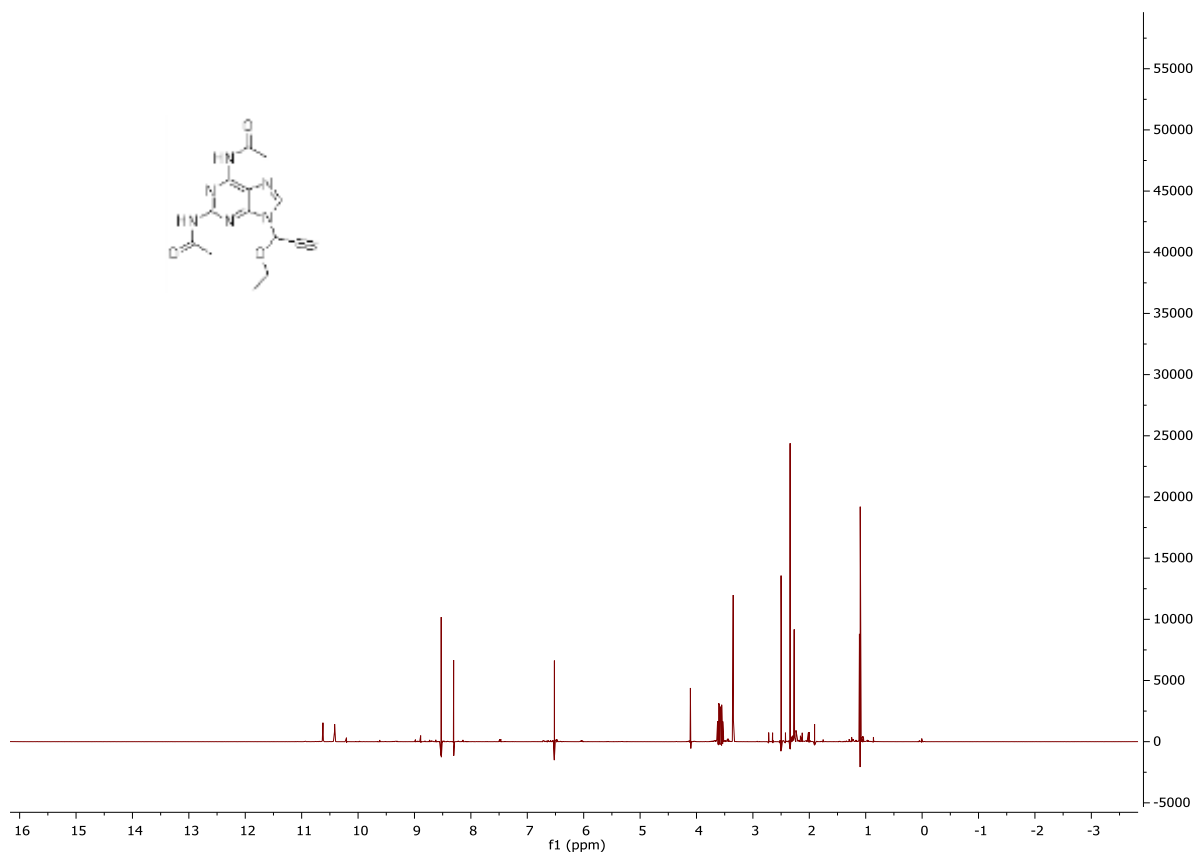
6-Chloro-9-(1-ethoxyprop-2-yn-1-yl)-2-fluoro-9H-purine (**34**)



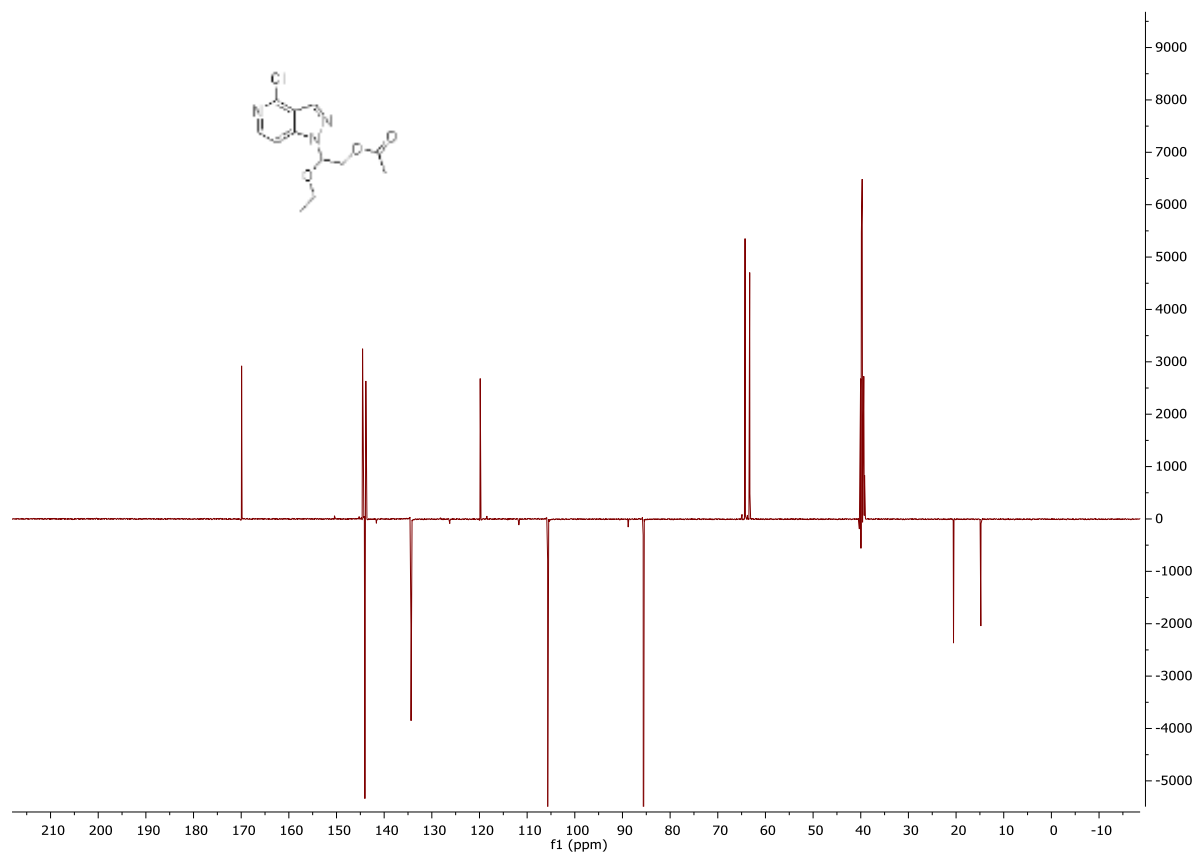
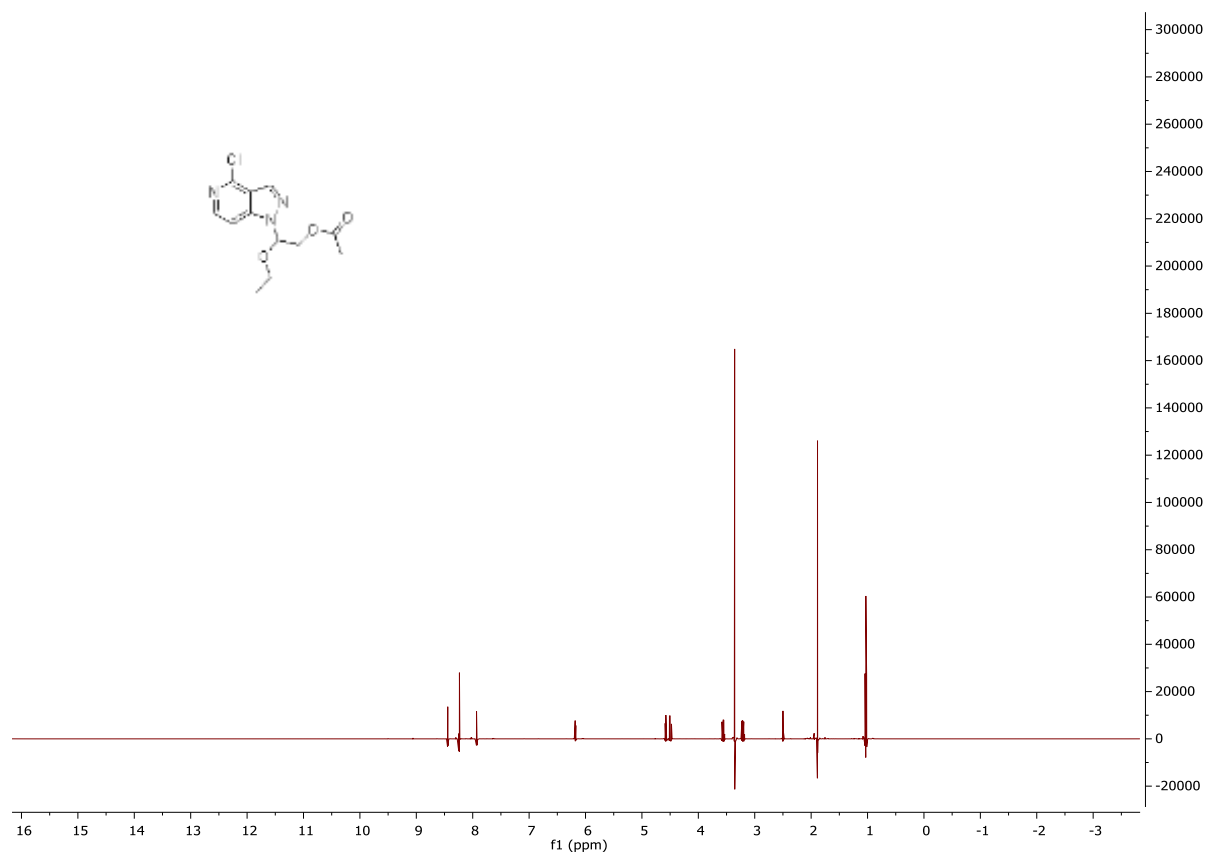
4-(Adenine-9-yl)-4-methoxybutan-2-one (35)



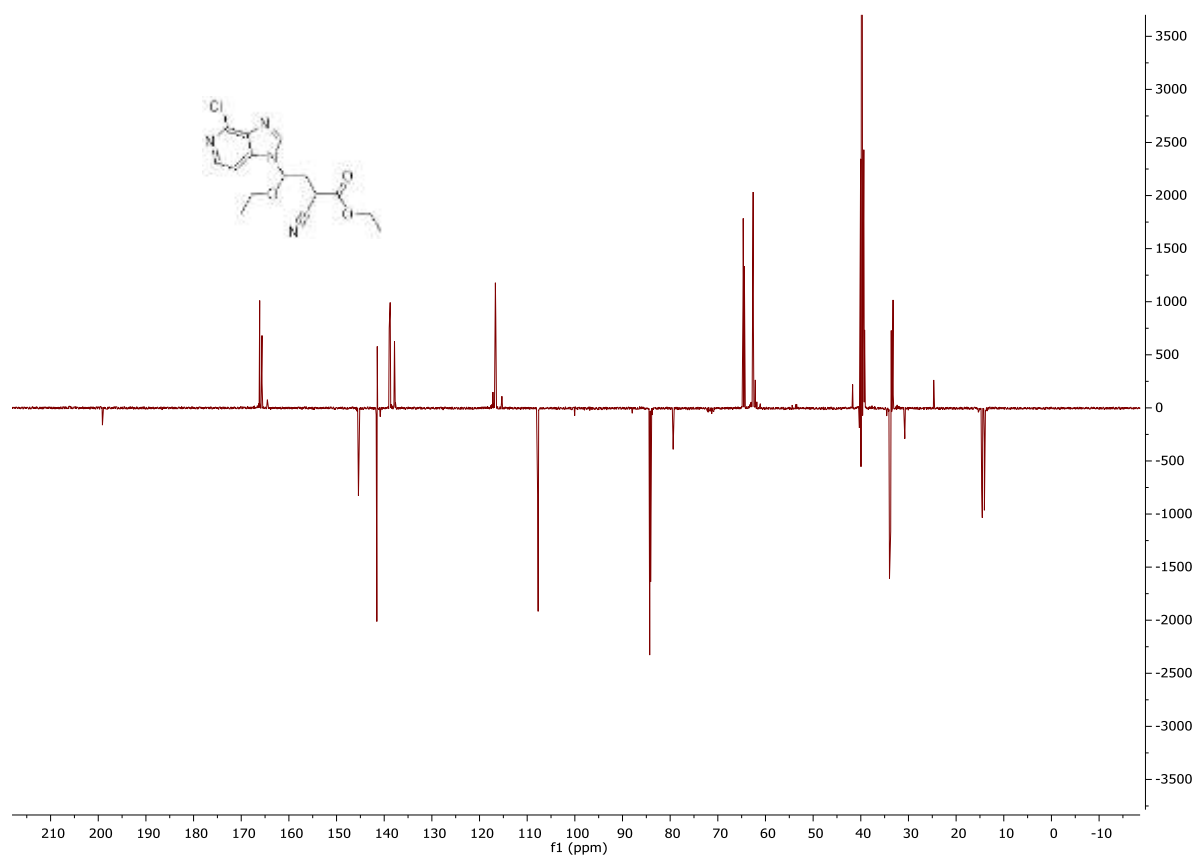
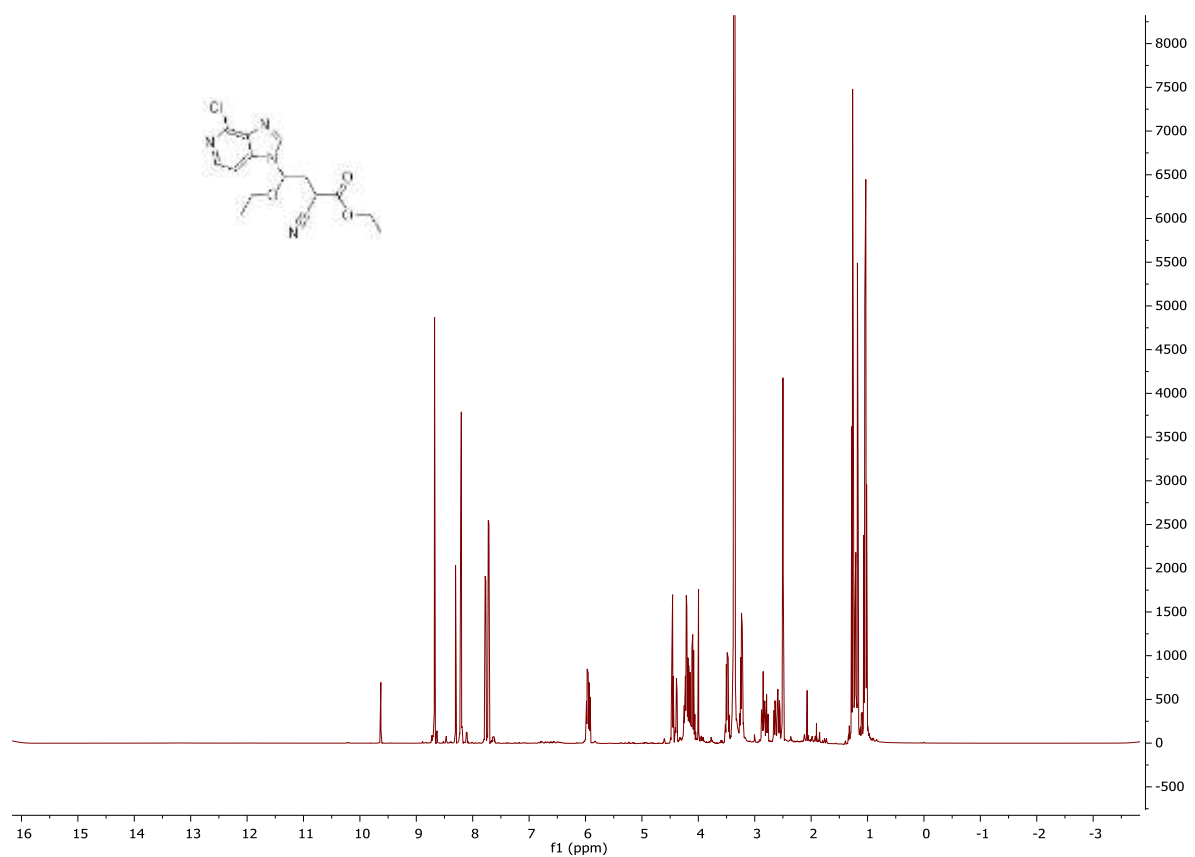
*N,N'*-(9-(1-Ethoxyprop-2-yn-1-yl)-9*H*-purine-2,6-diyl)diacetamide (**36**)



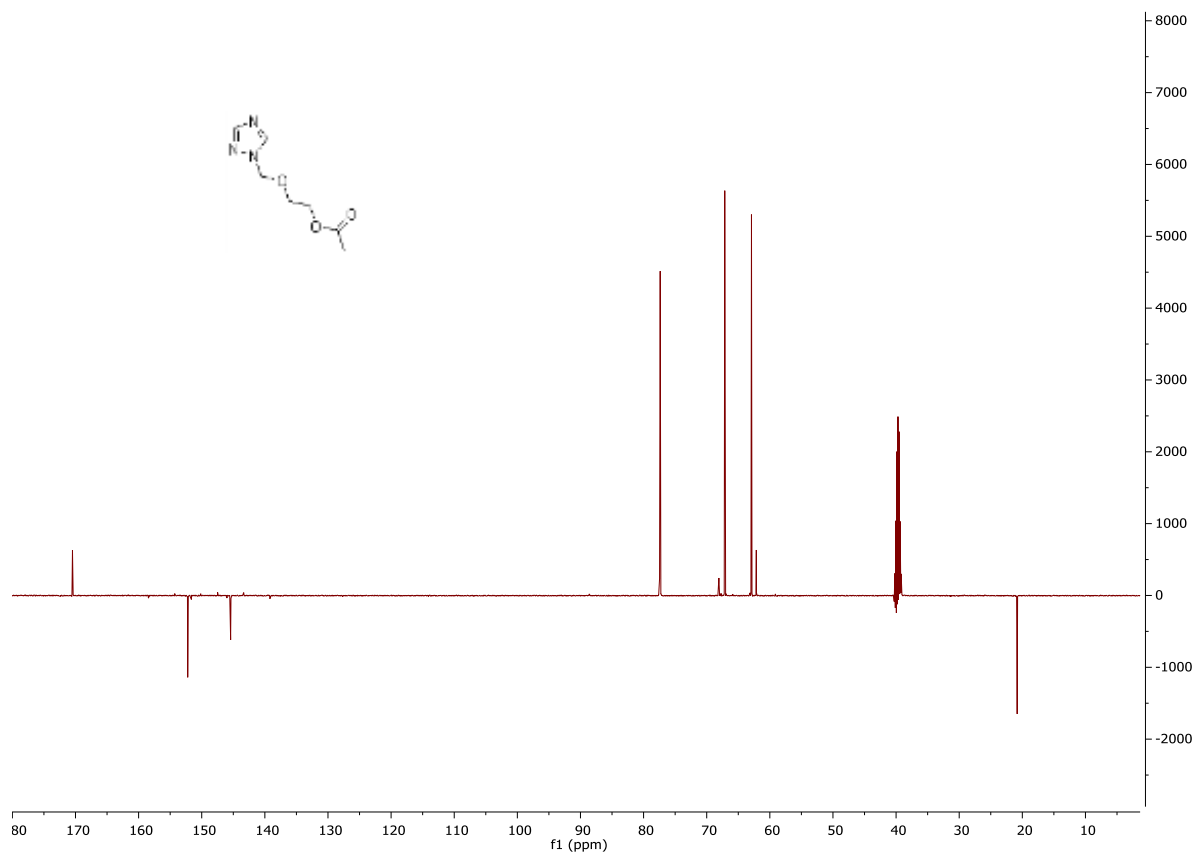
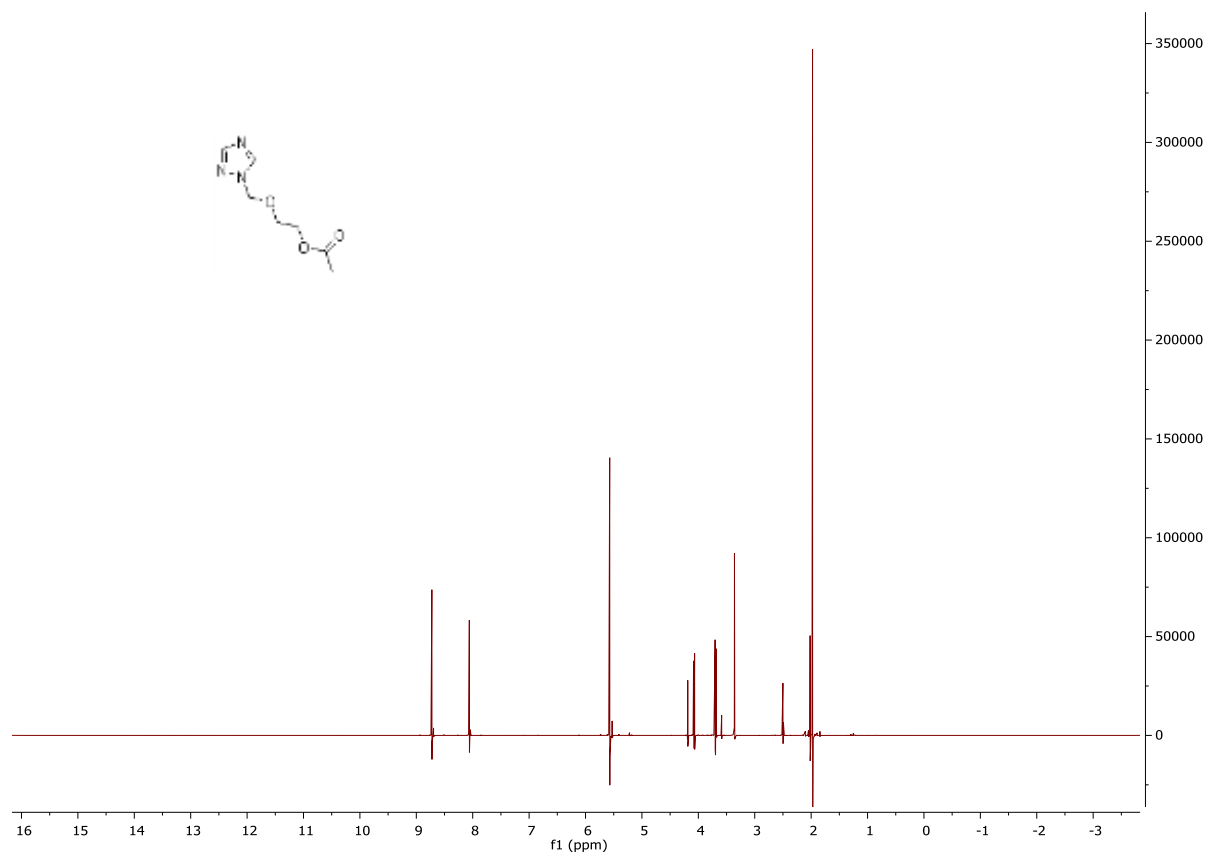
2-(4-Chloro-1*H*-pyrazolo[4,3-*c*]pyridin-1-yl)-2-ethoxyethyl acetate (**37**)



Ethyl 4-(4-chloro-1*H*-imidazo[4,5-*c*]pyridin-1-yl)-2-cyano-4-ethoxybutanoate (**38**)

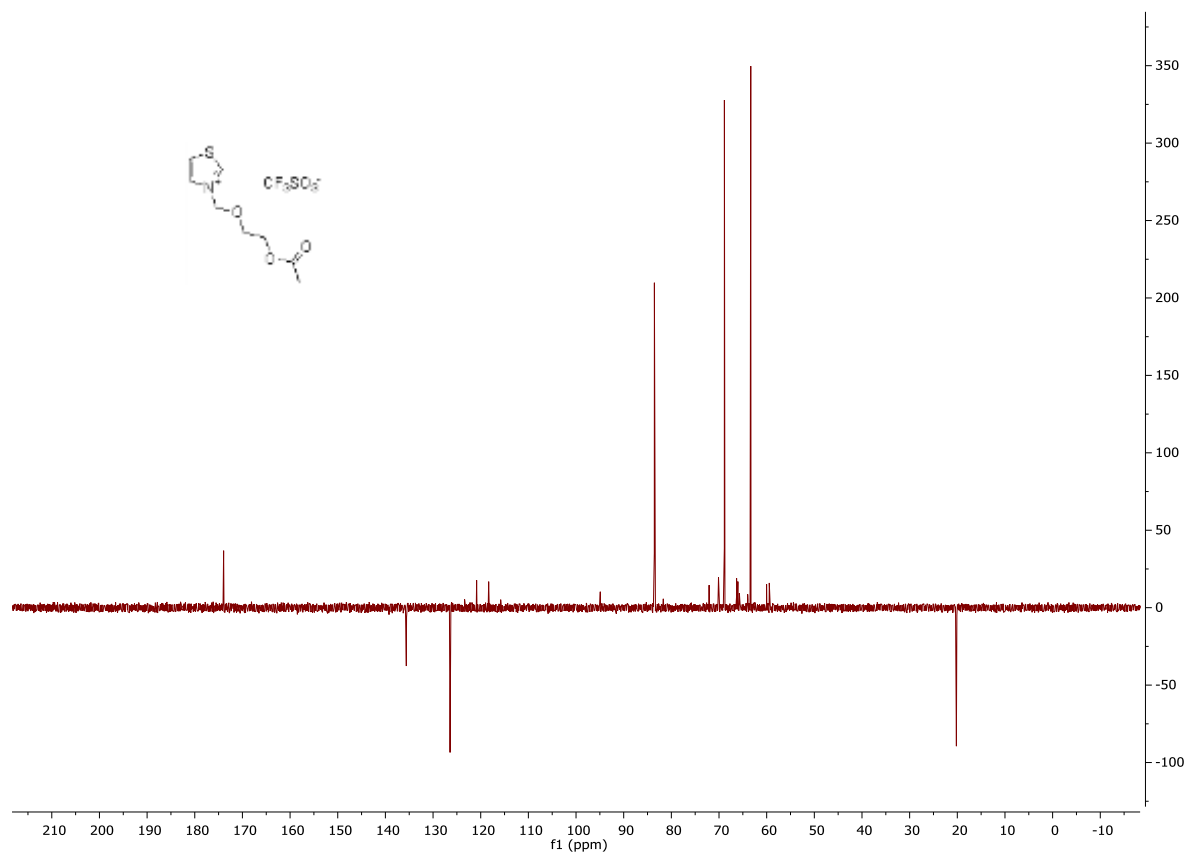
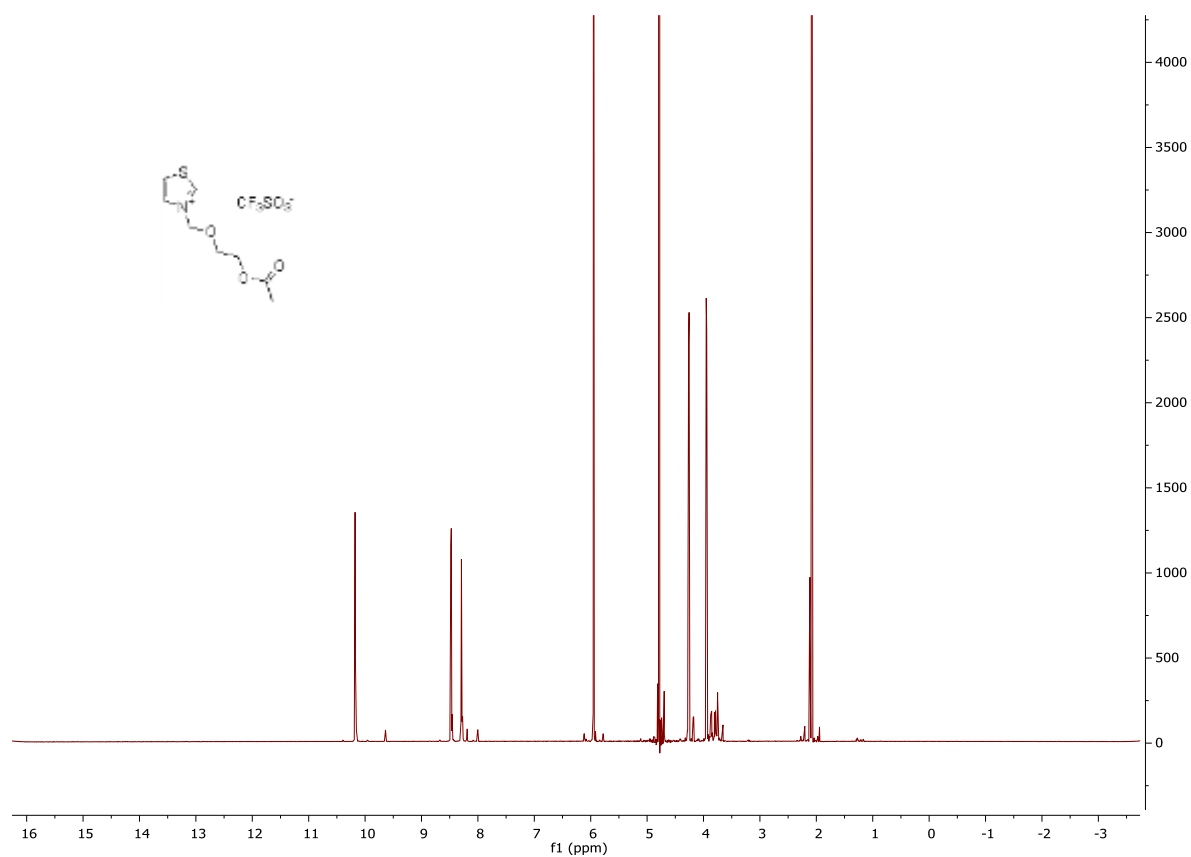


2-((1*H*-1,2,4-Triazol-1-yl)methoxy)ethyl acetate (**39**)

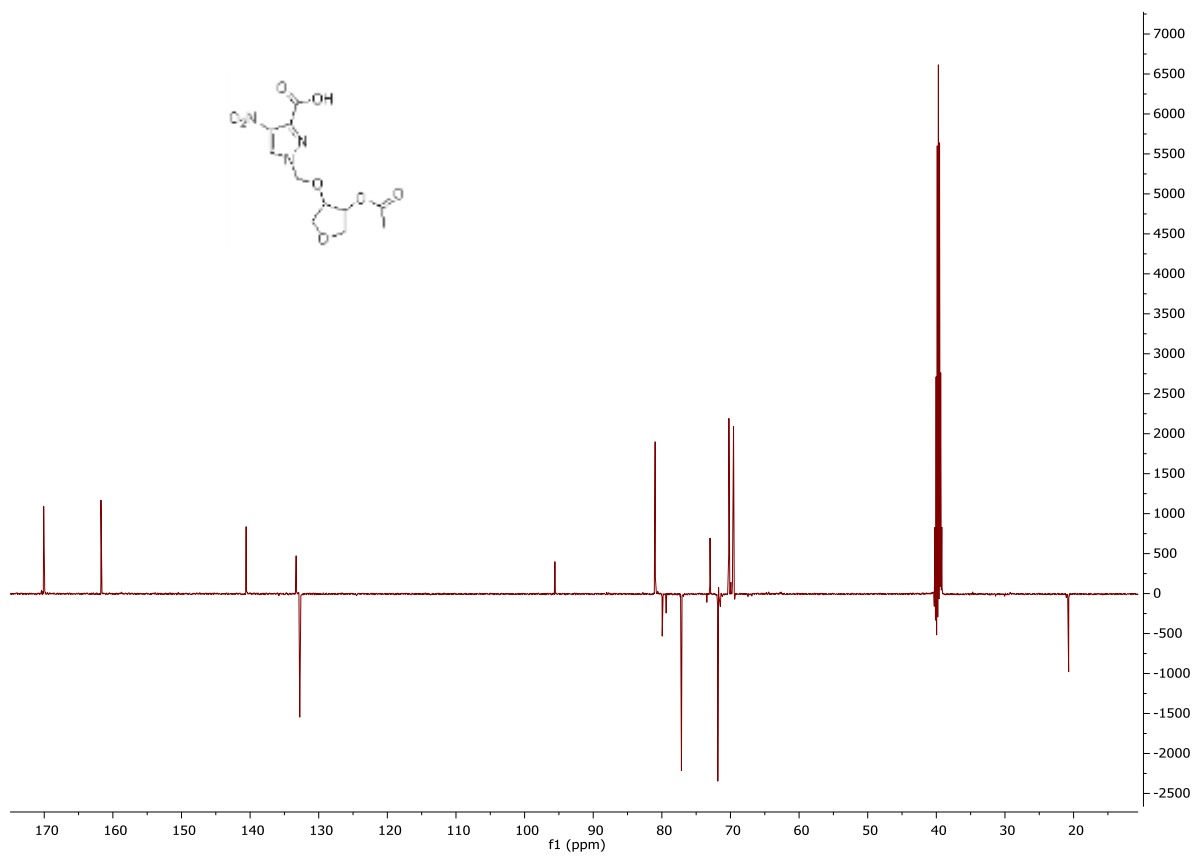
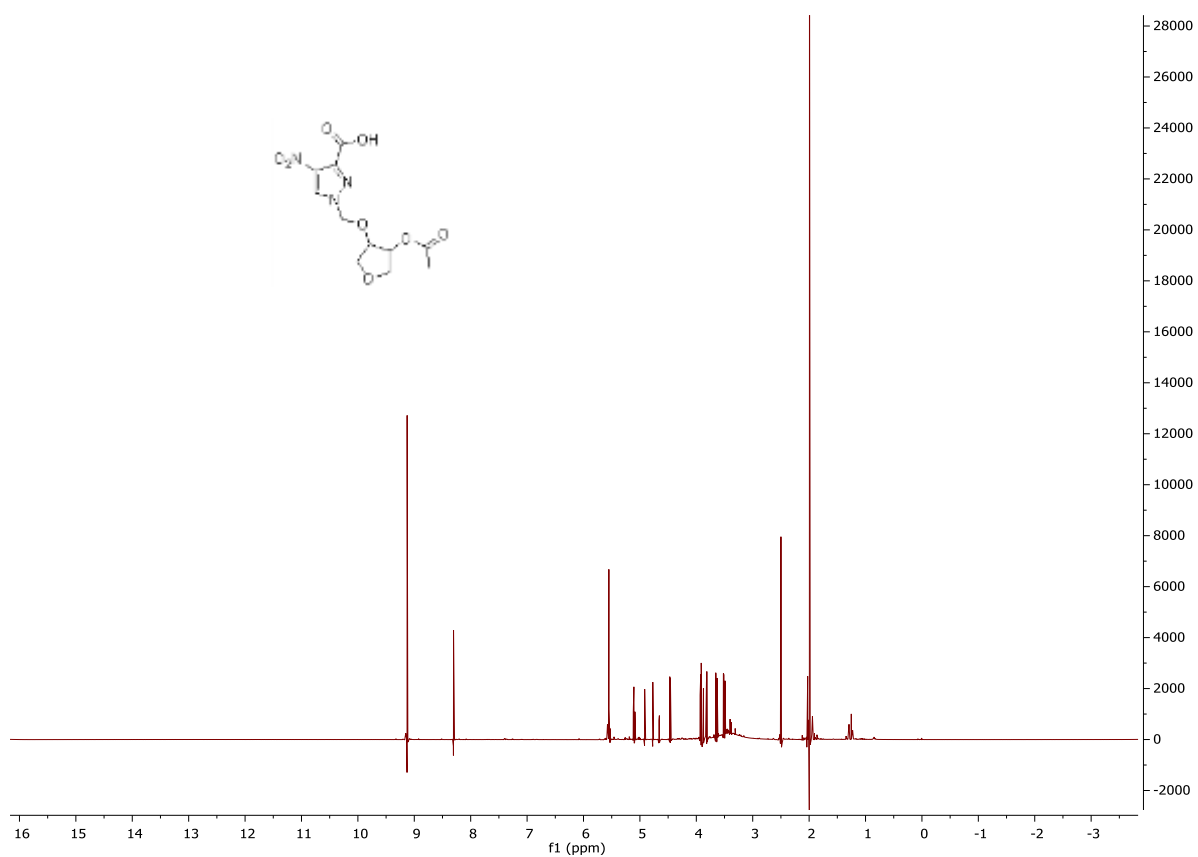




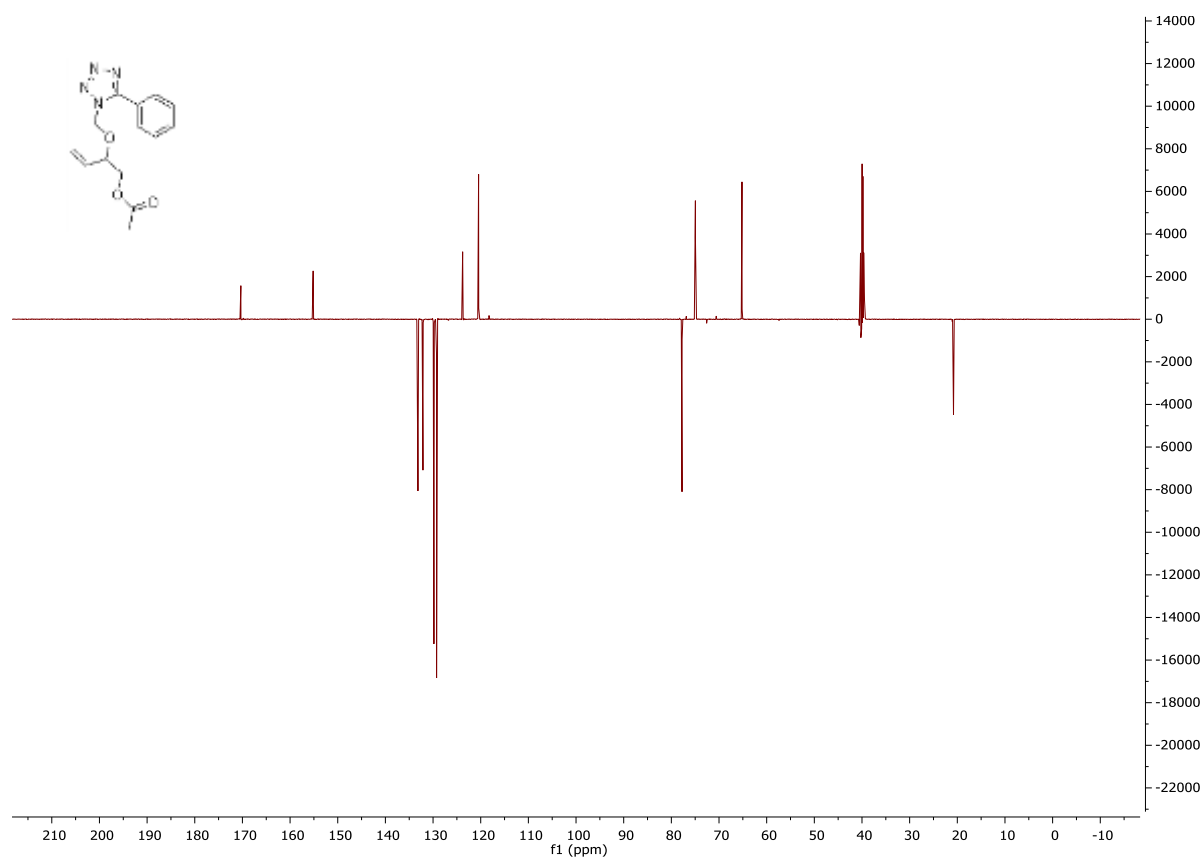
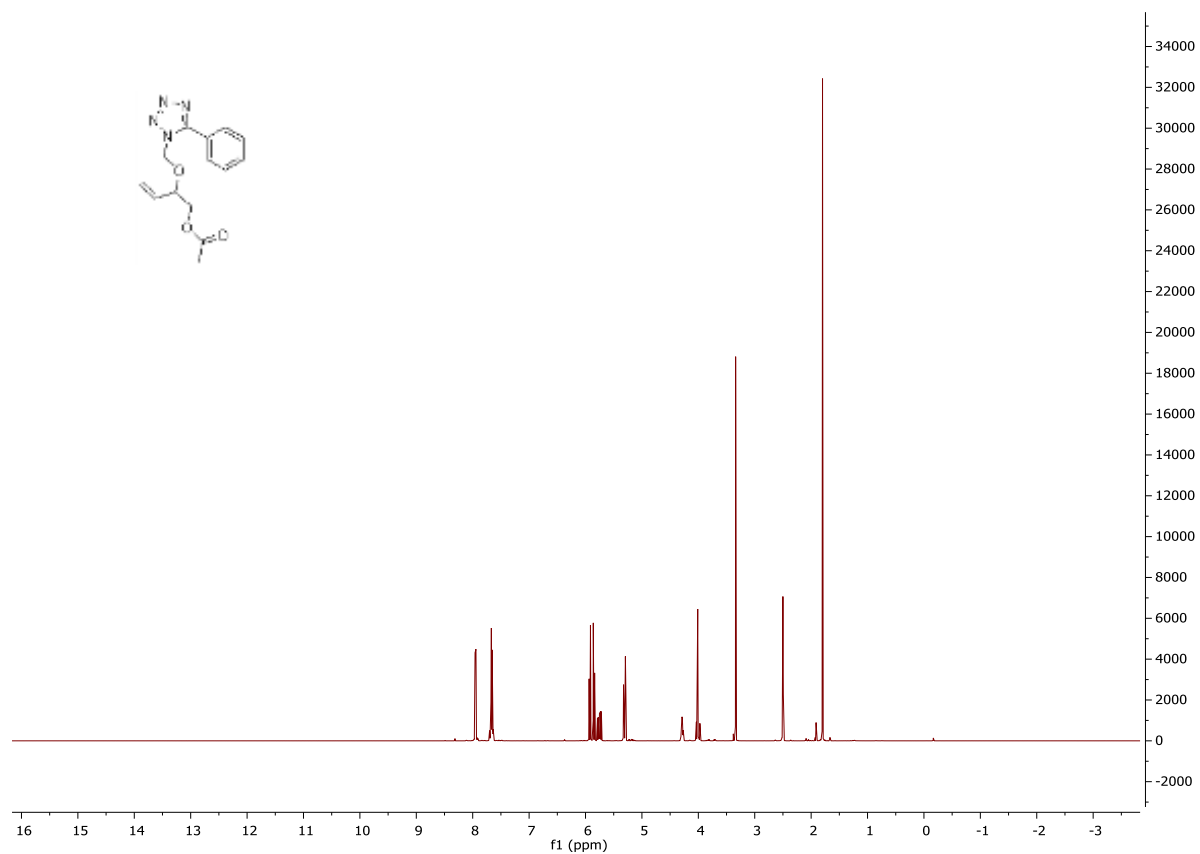
3-((2-Acetoxyethoxy)methyl)thiazol-3-ium trifluoromethanesulfonate (**40**)



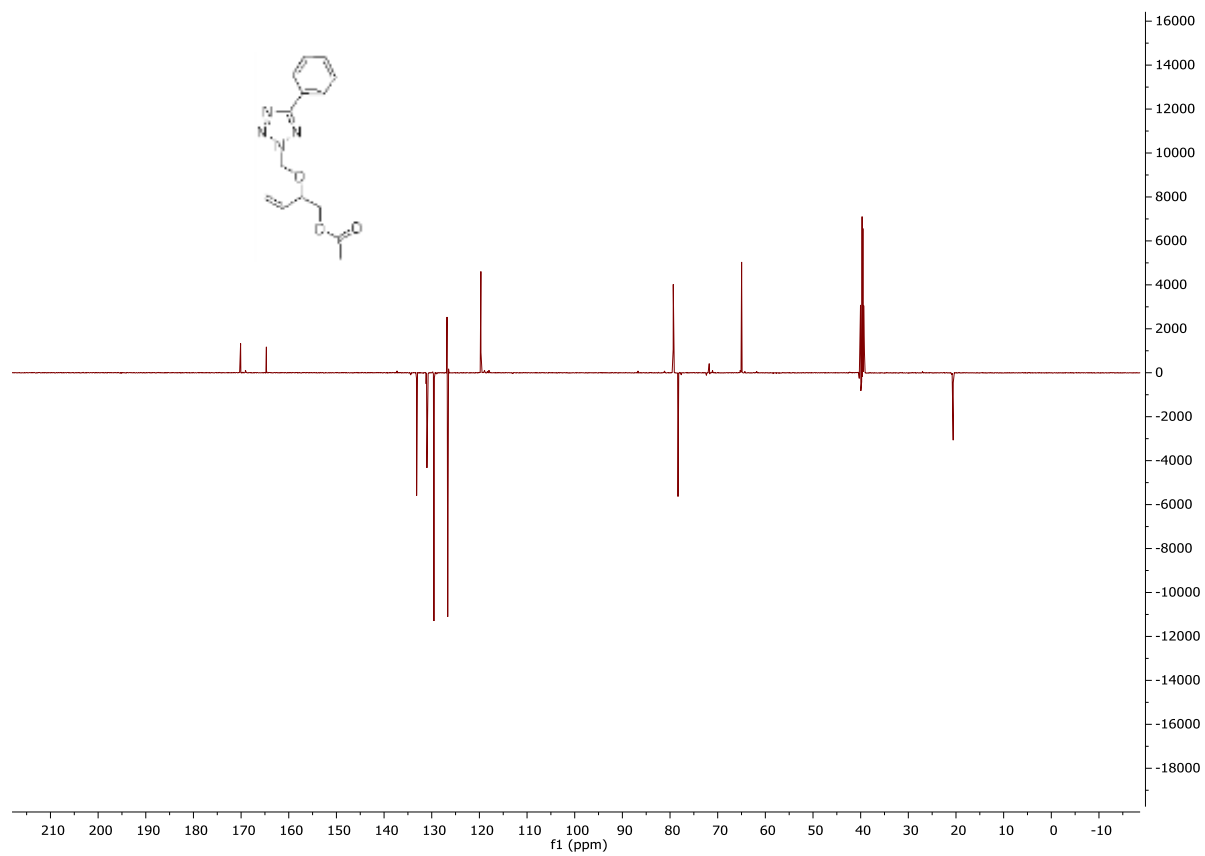
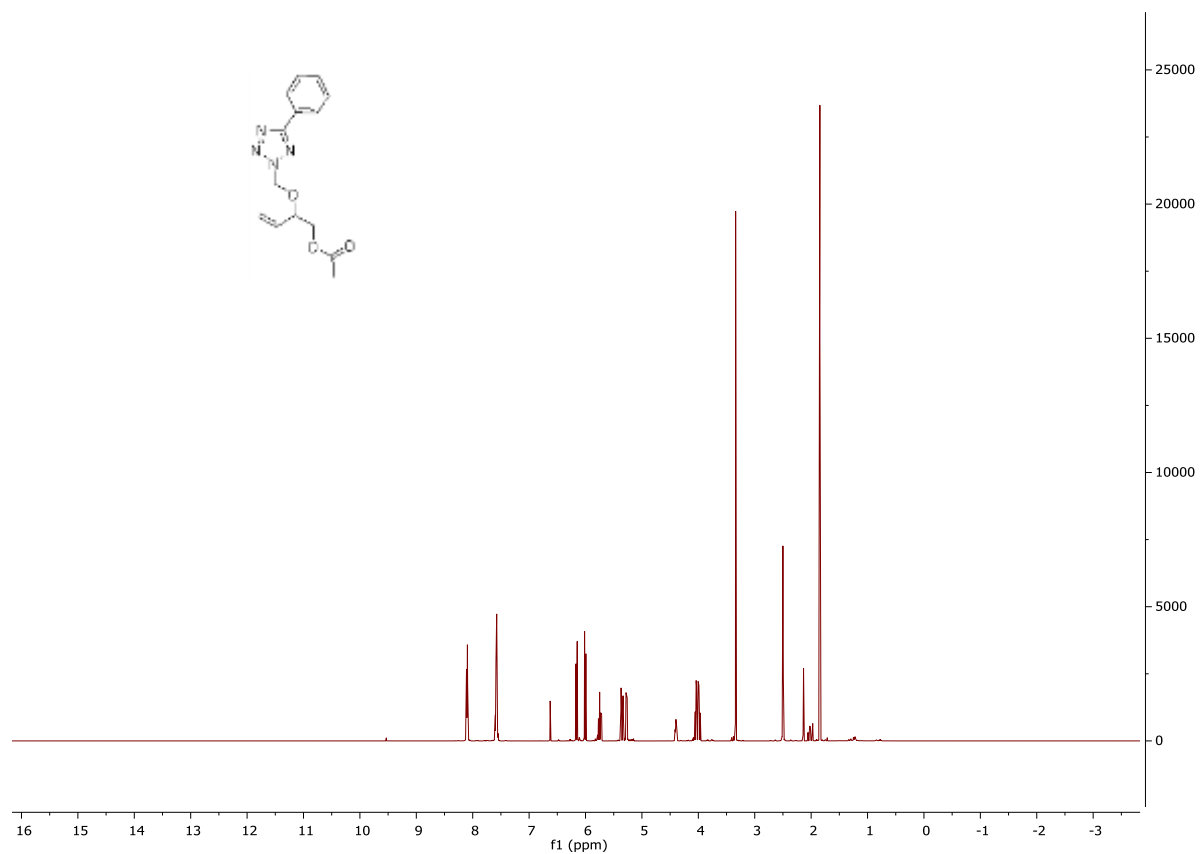
1-(((4-Acetoxytetrahydrofuran-3-yl)oxy)methyl)-4-nitro-1H-pyrazole-3-carboxylic acid (**41**)



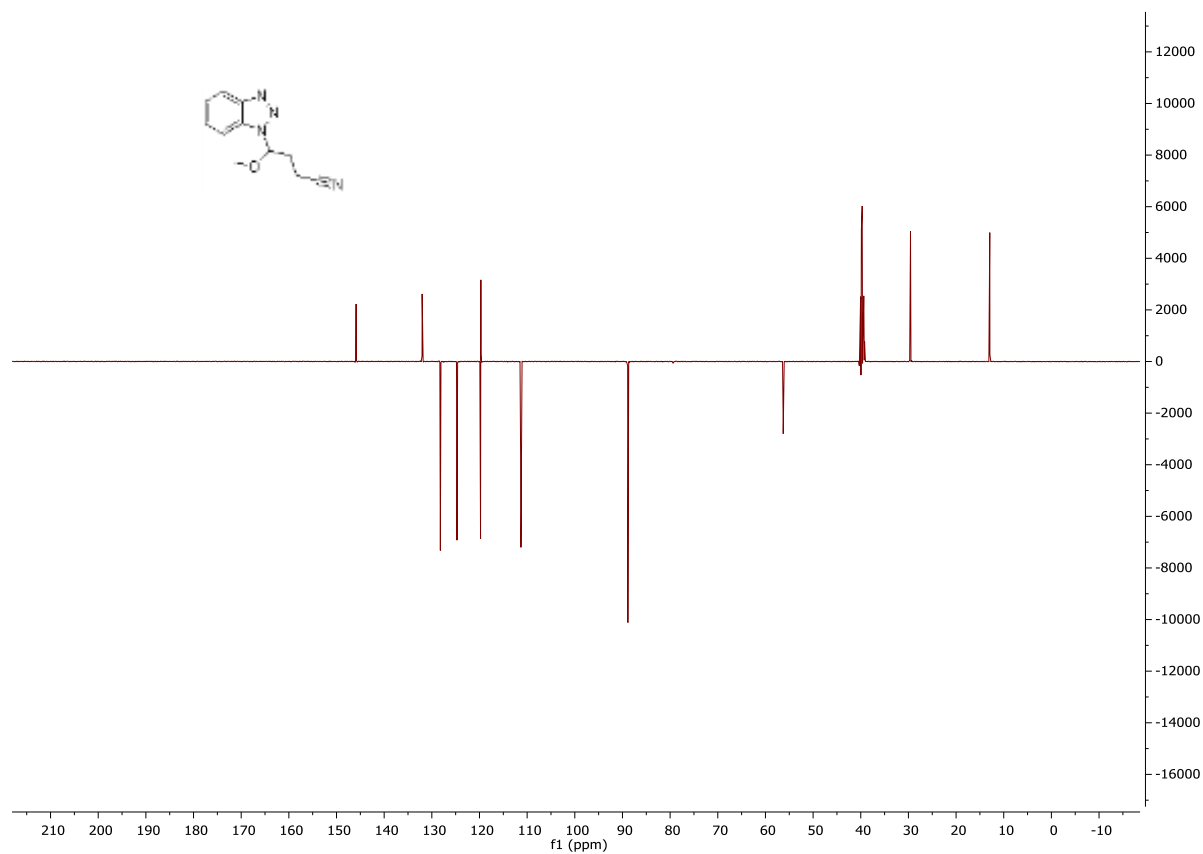
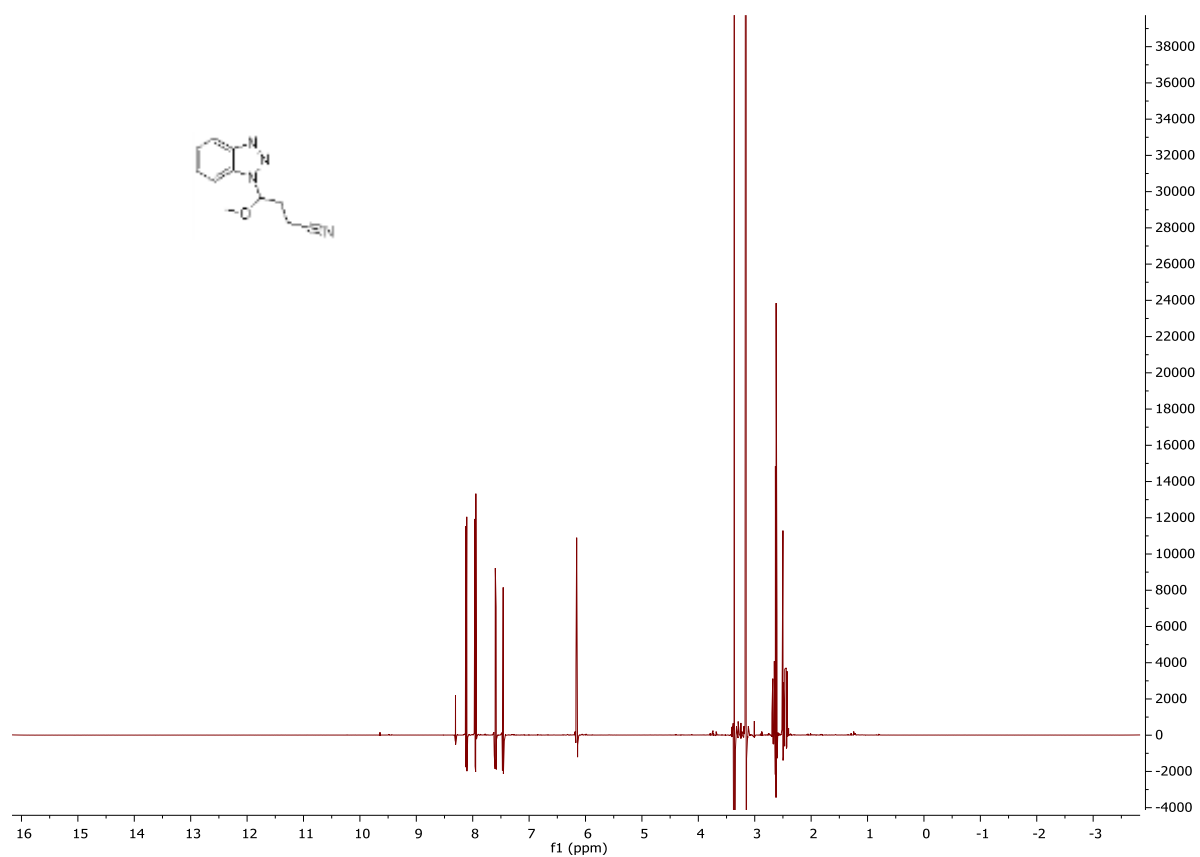
2-((5-Phenyl-1*H*-tetrazol-1-yl)methoxy)but-3-en-1-yl acetate (**42**)



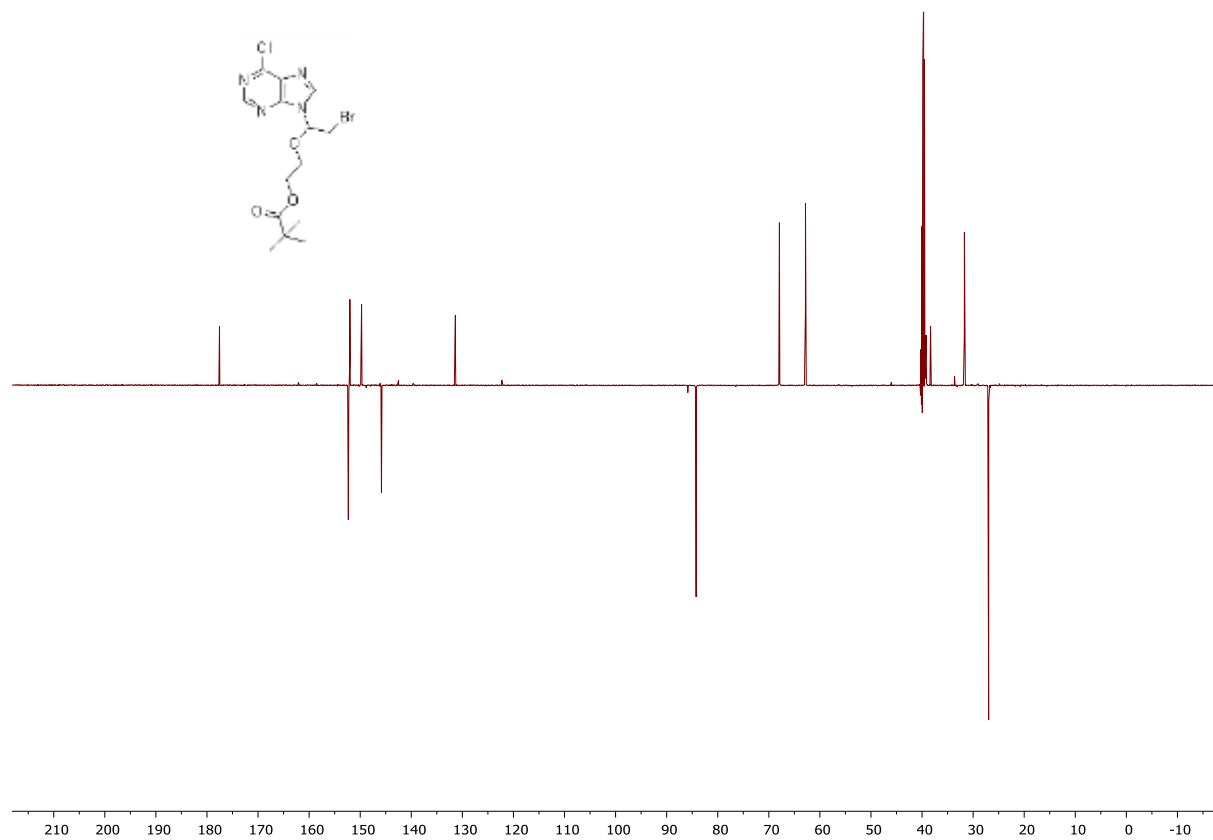
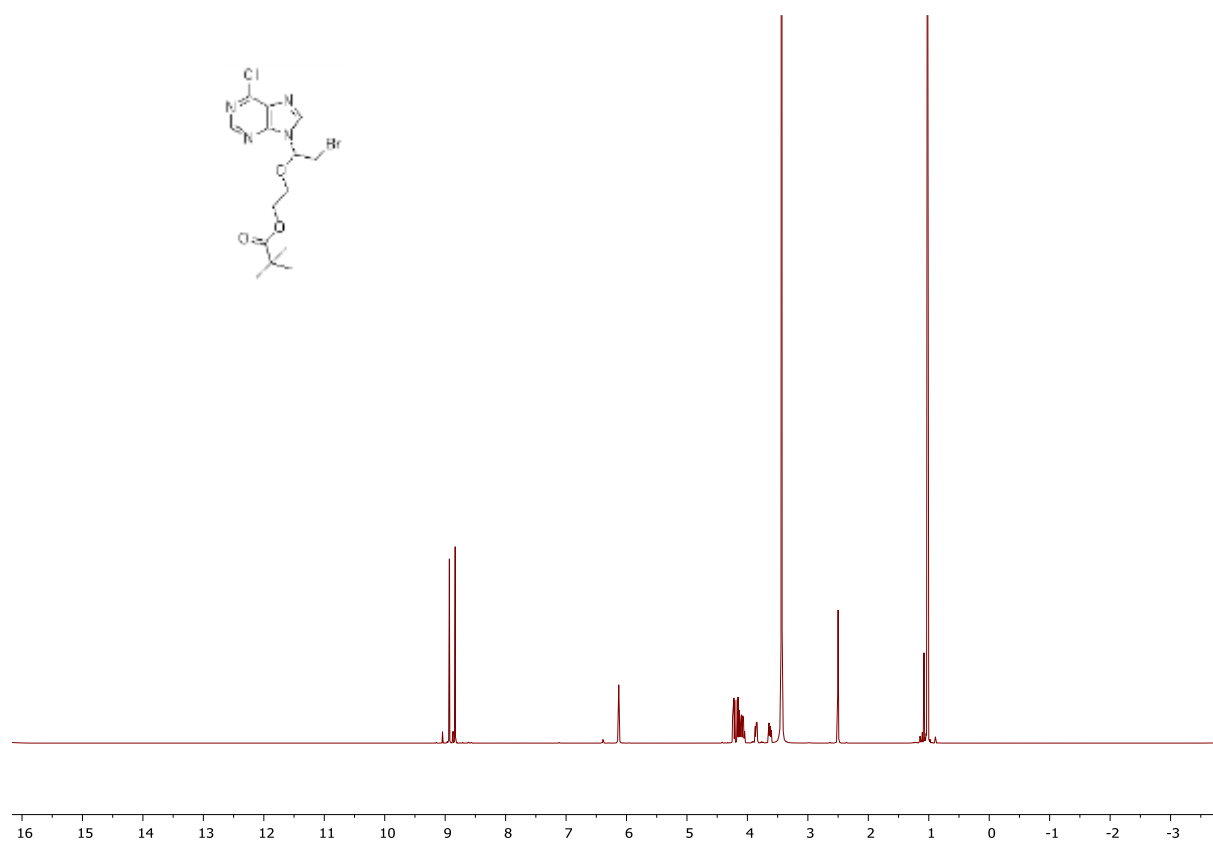
2-((5-Phenyl-2H-tetrazol-2-yl)methoxy)but-3-en-1-yl acetate (**43**)



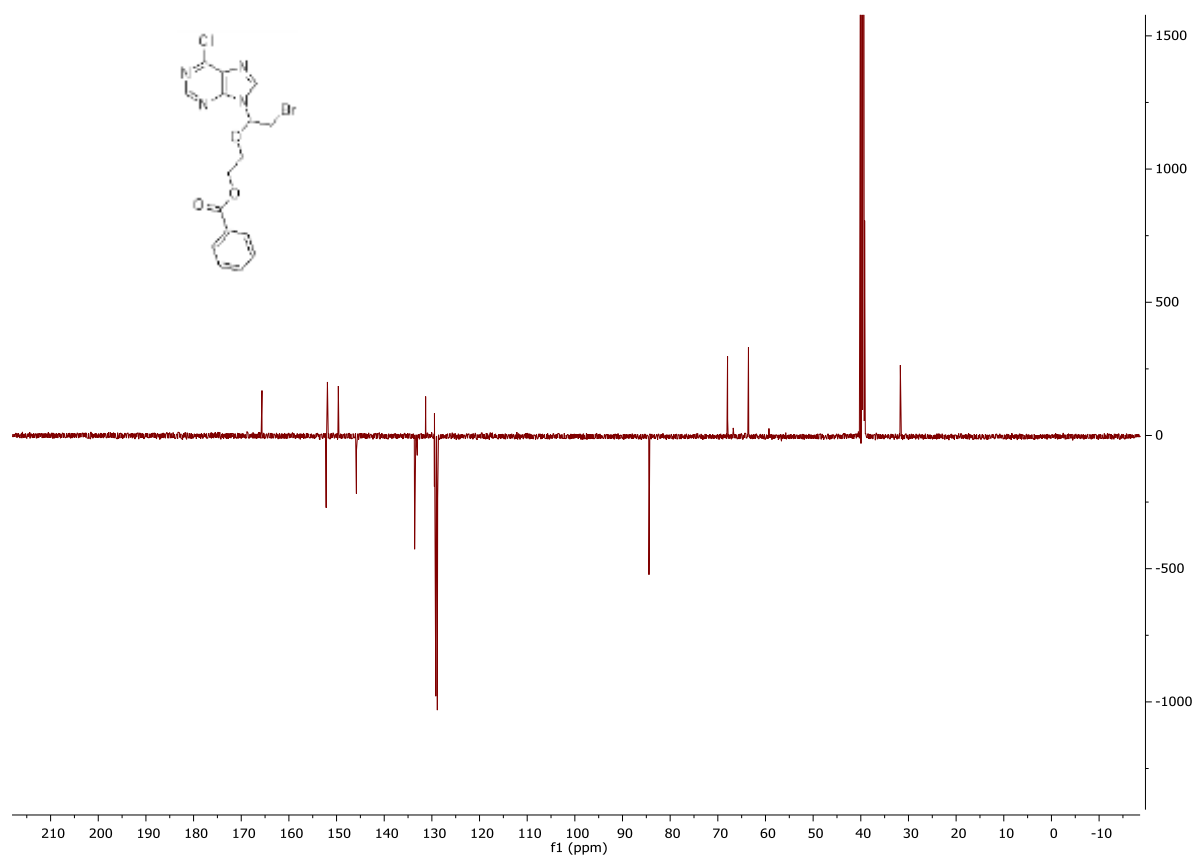
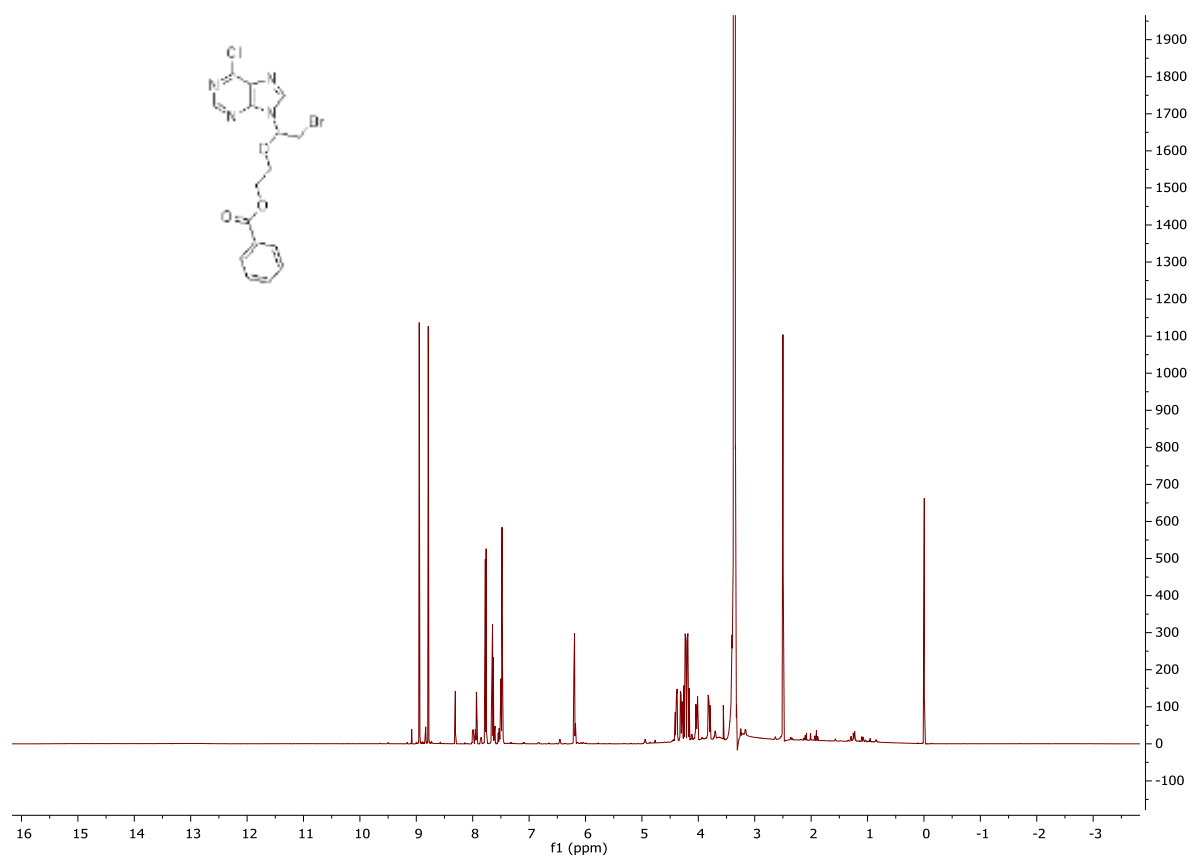
4-(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)-4-methoxybutanenitrile (**45**)



2-(2-Bromo-1-(6-chloro-9H-purin-9-yl)ethoxy)ethyl pivalate (**46**)

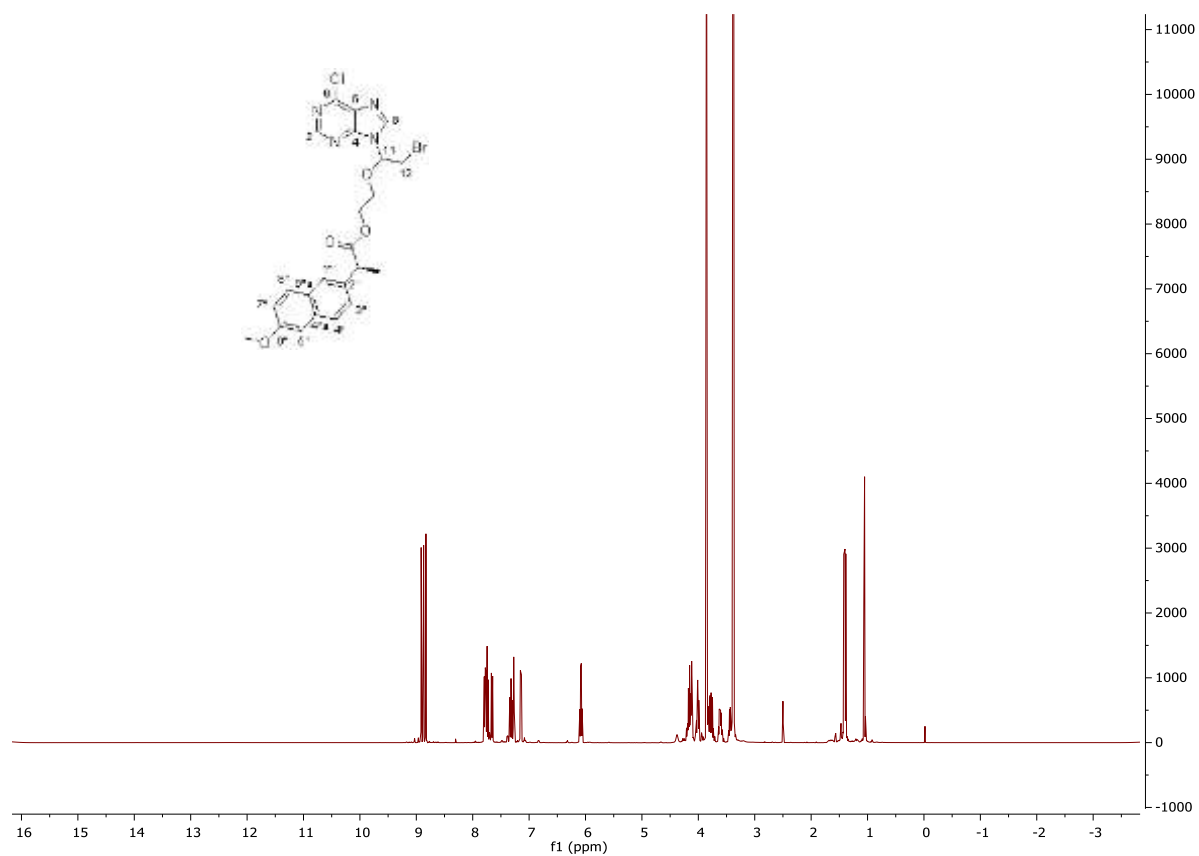
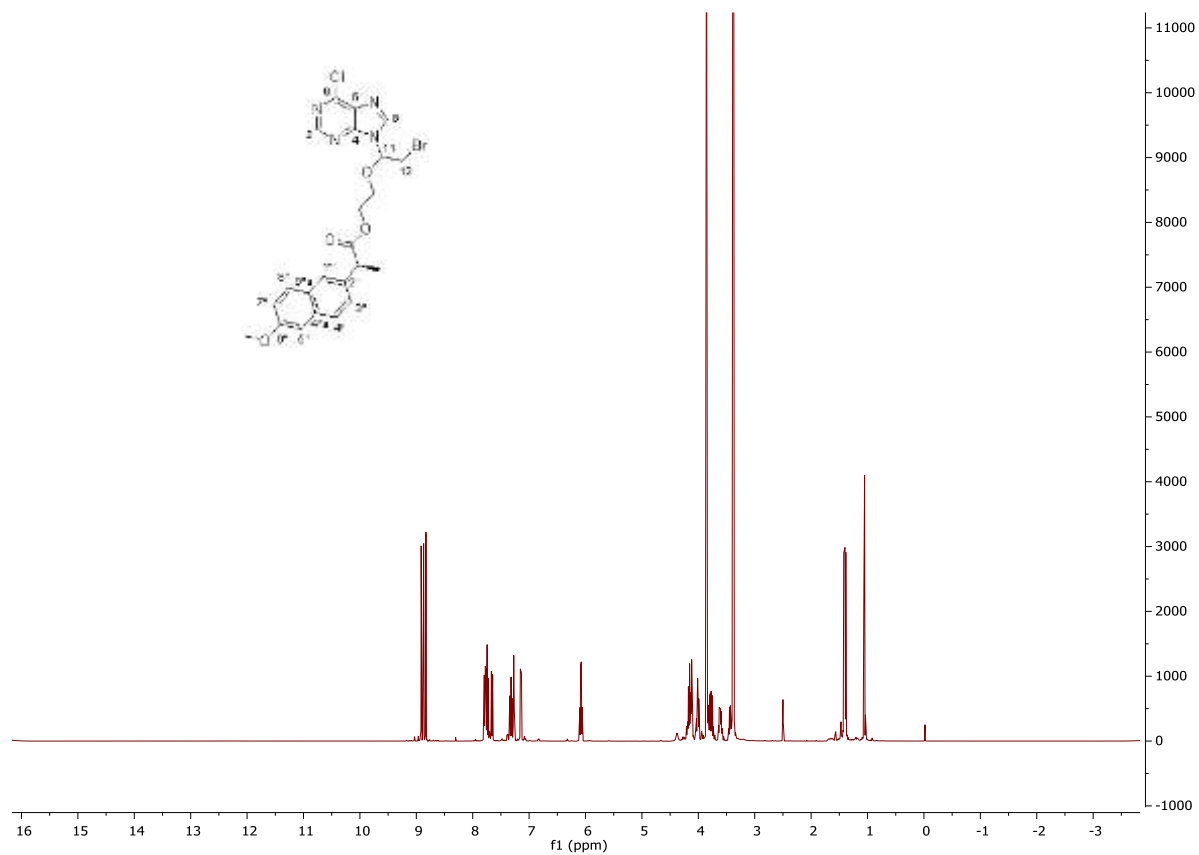


2-(2-Bromo-1-(6-chloro-9H-purin-9-yl)ethoxy)ethyl benzoate (47)



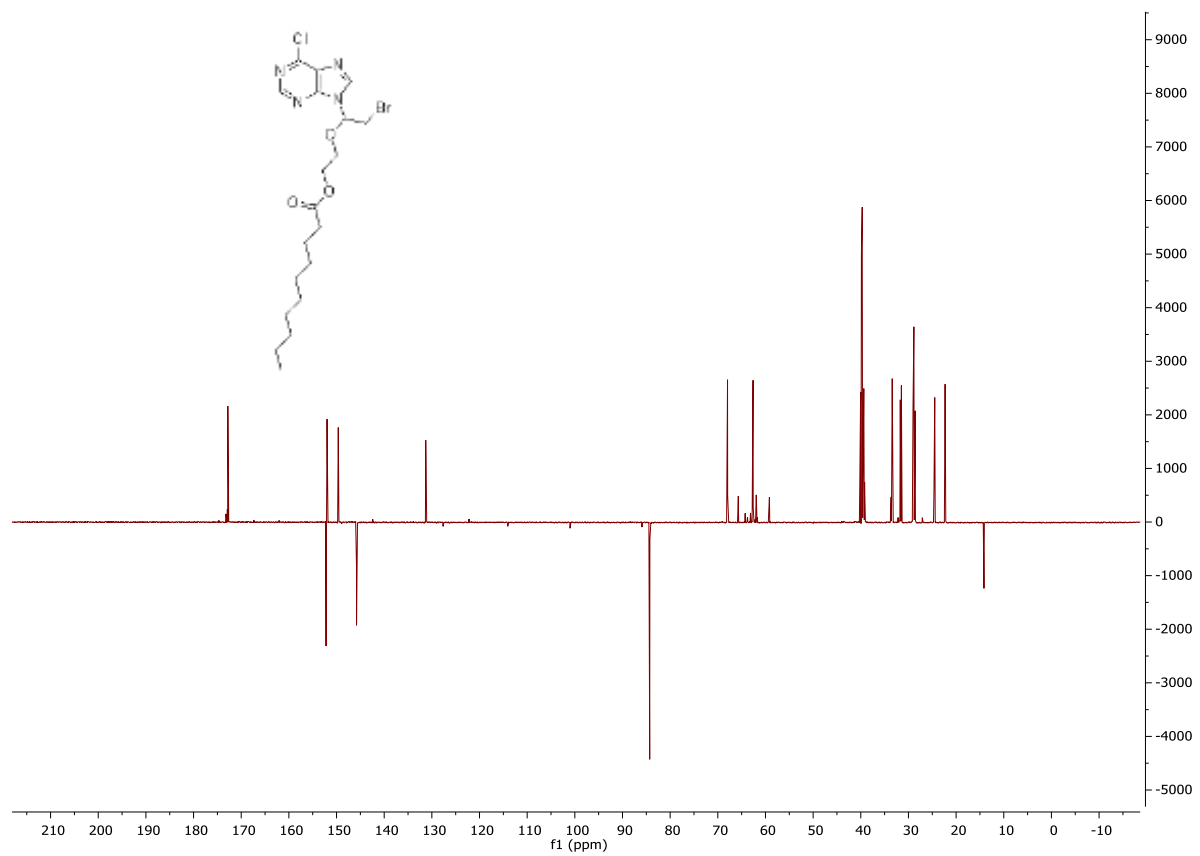
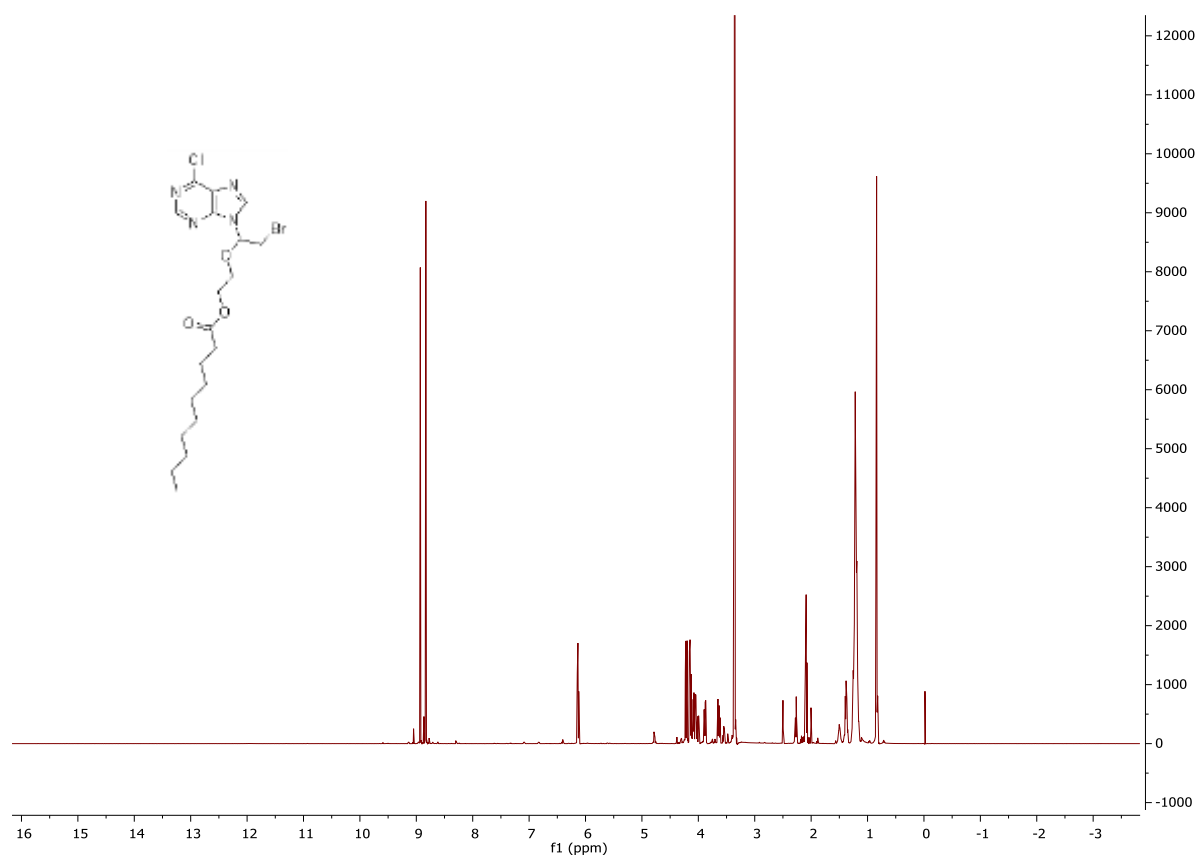
2-(2-Bromo-1-(6-chloro-9H-purin-9-yl)ethoxy)ethyl propanoate (49)

(2S)-2-(6-methoxynaphthalen-2-yl)-

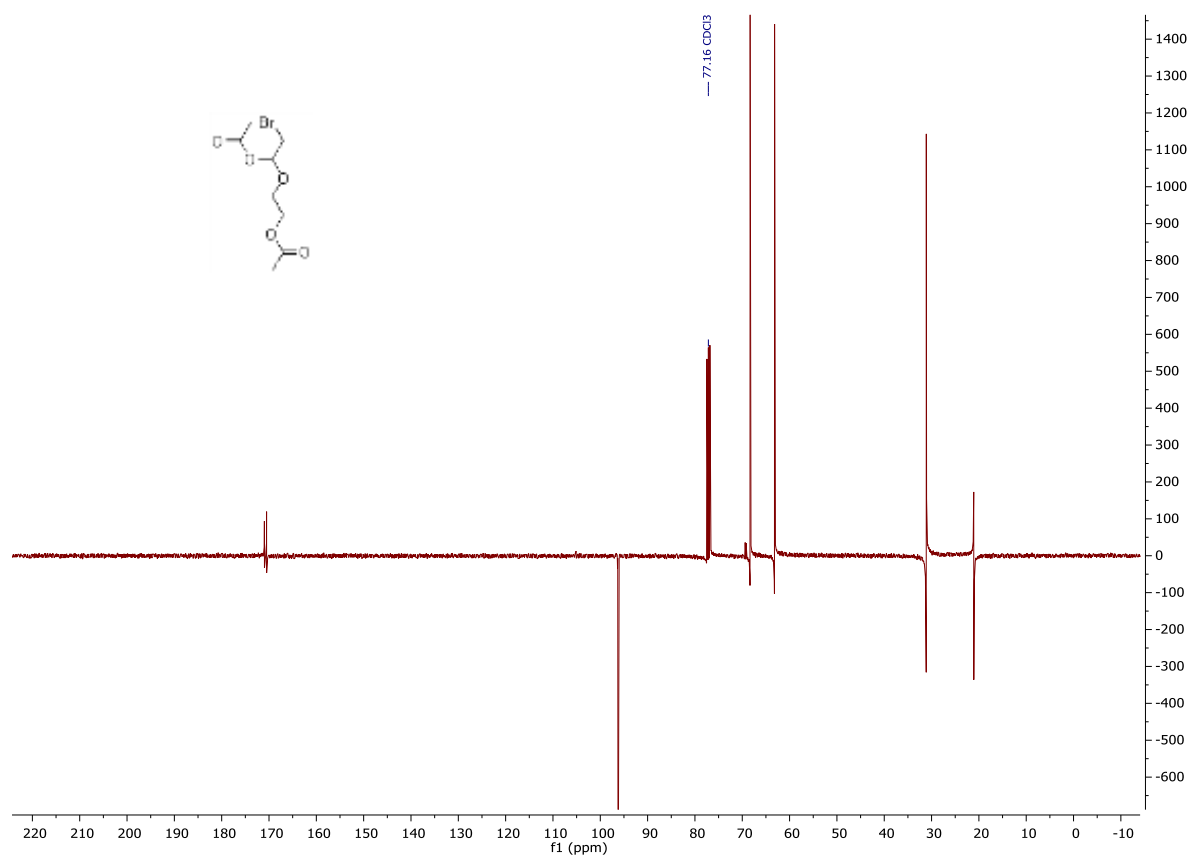
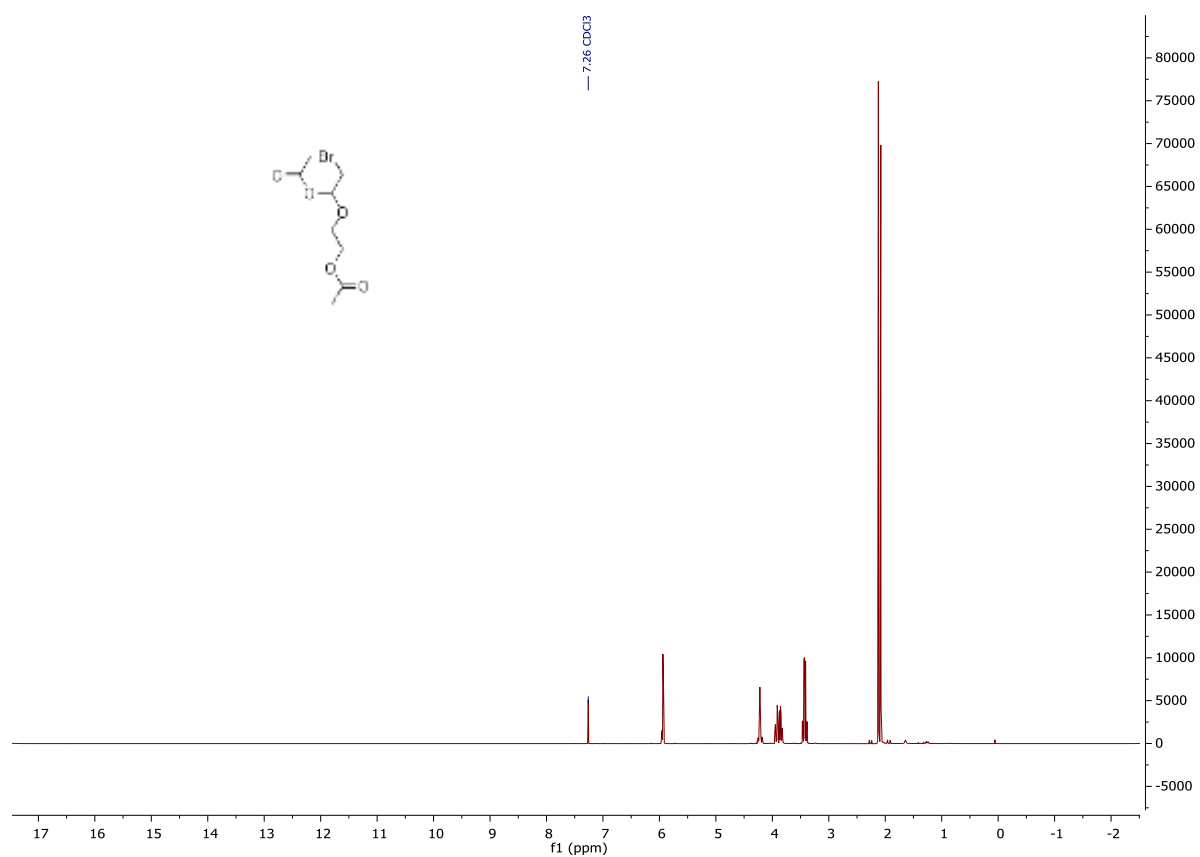




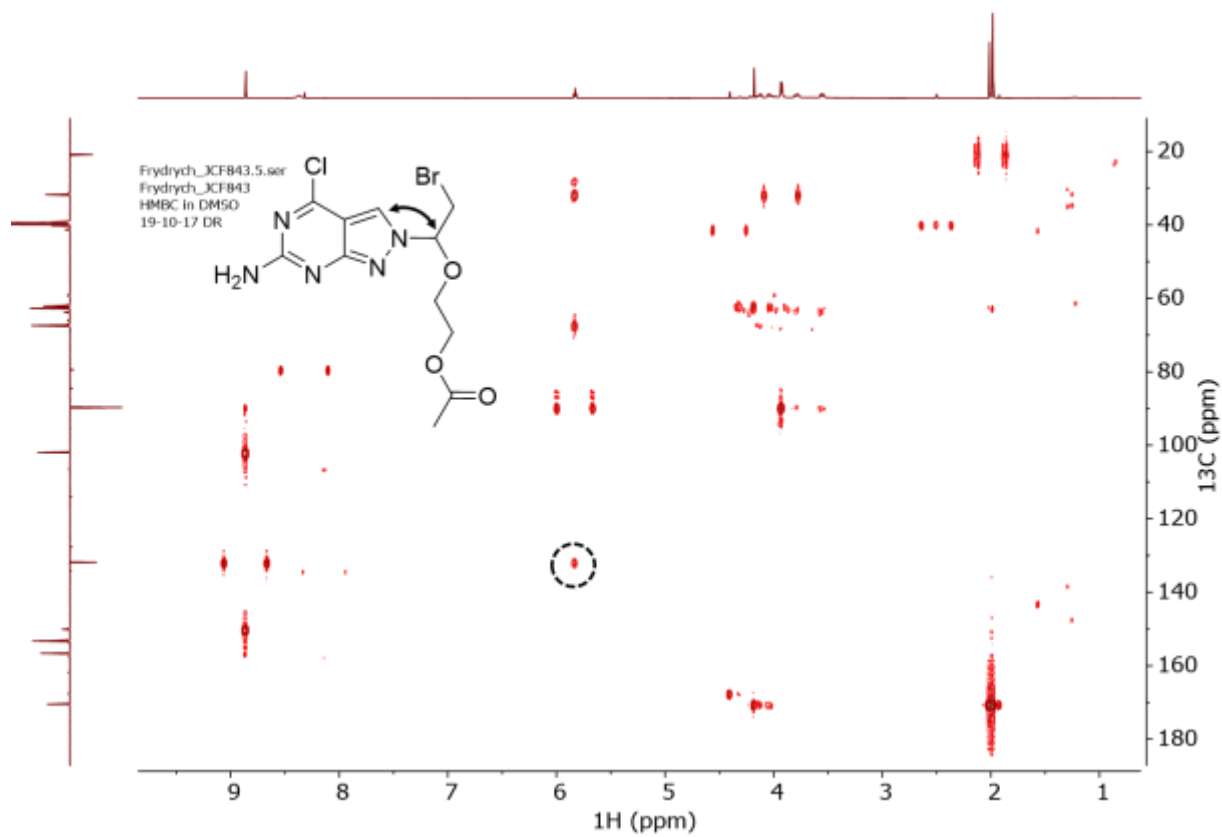
2-(2-Bromo-1-(6-chloro-9H-purin-9-yl)ethoxy)ethyl decanoate (**51**)



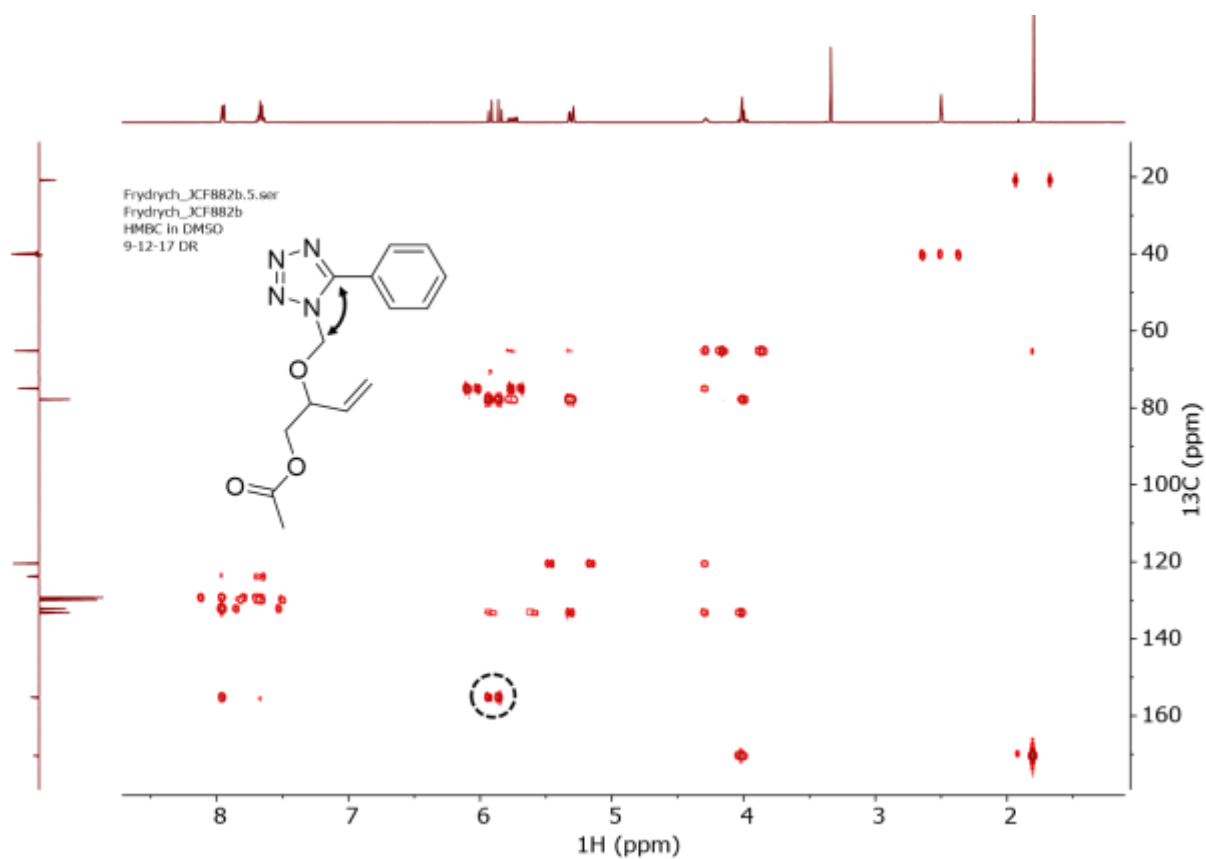
# 2-(1-Acetoxy-2-bromoethoxy)ethyl acetate (**52**)



## HMBC spectra of compounds 22 and 42:



**Figure S1.** HMBC spectrum of compound **22** showing a three-bond correlation crucial for the stereochemical assignment.



**Figure S2.** HMBC spectrum of compound **42** showing a three-bond correlation crucial for the stereochemical assignment.