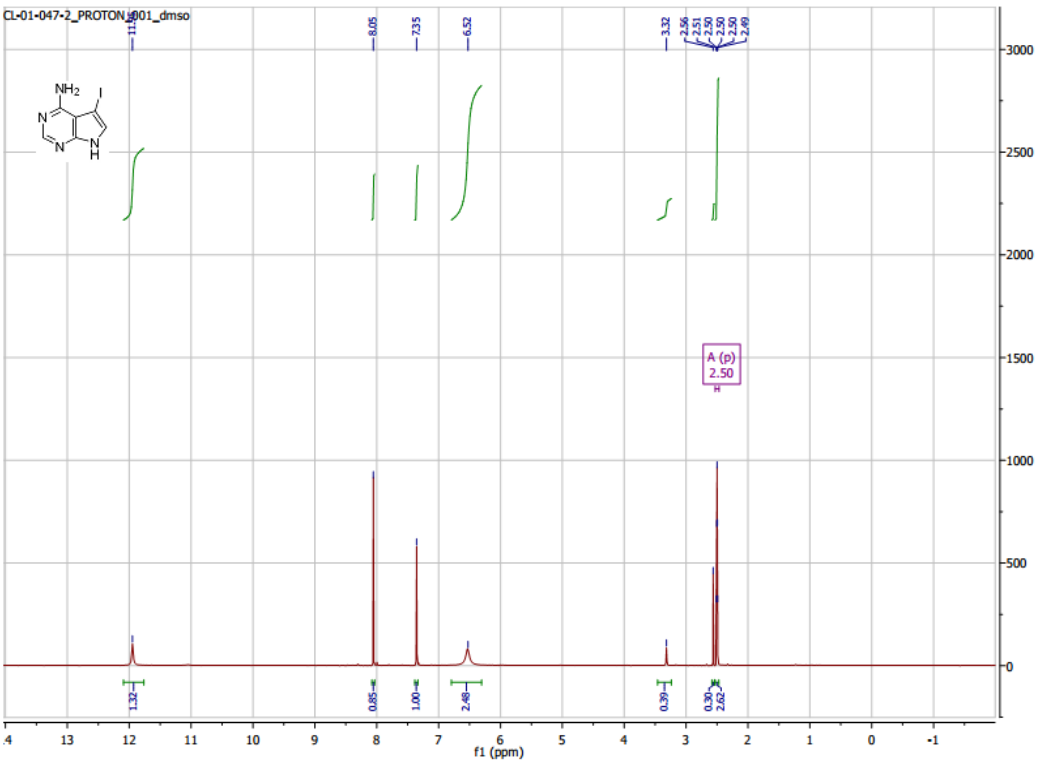
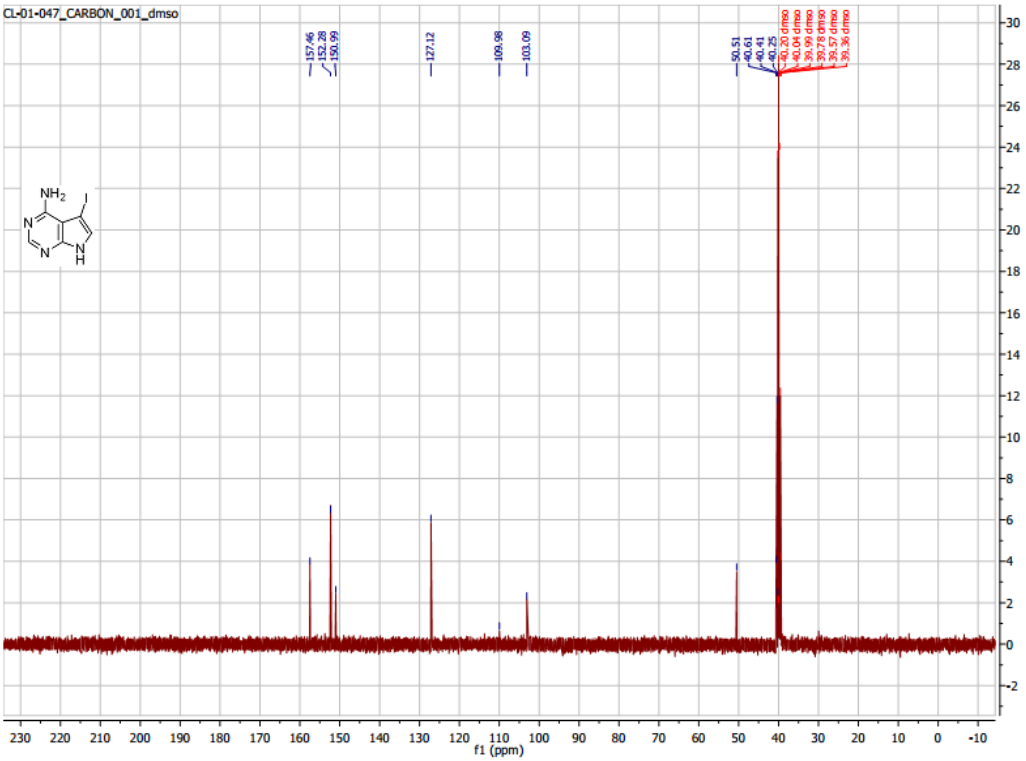
Supporting Information

Synthesis and photophysical characterization of new fluorescent triazole adenine analogues

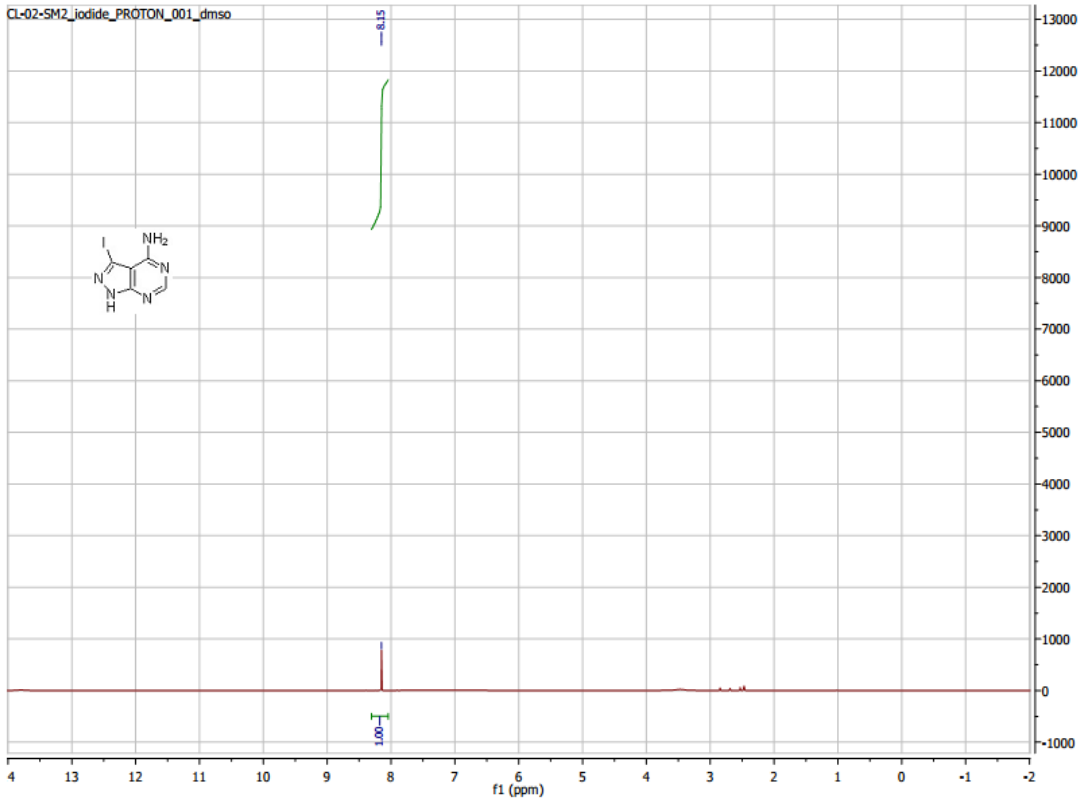
Christopher P. Lawson,[a†], Anke Dierckx,[b†], Francois-Alexandre Miannay,[b] Eric Wellner,[c] L. Marcus Wilhelmsson[b*] and Morten Grøtli[a*]

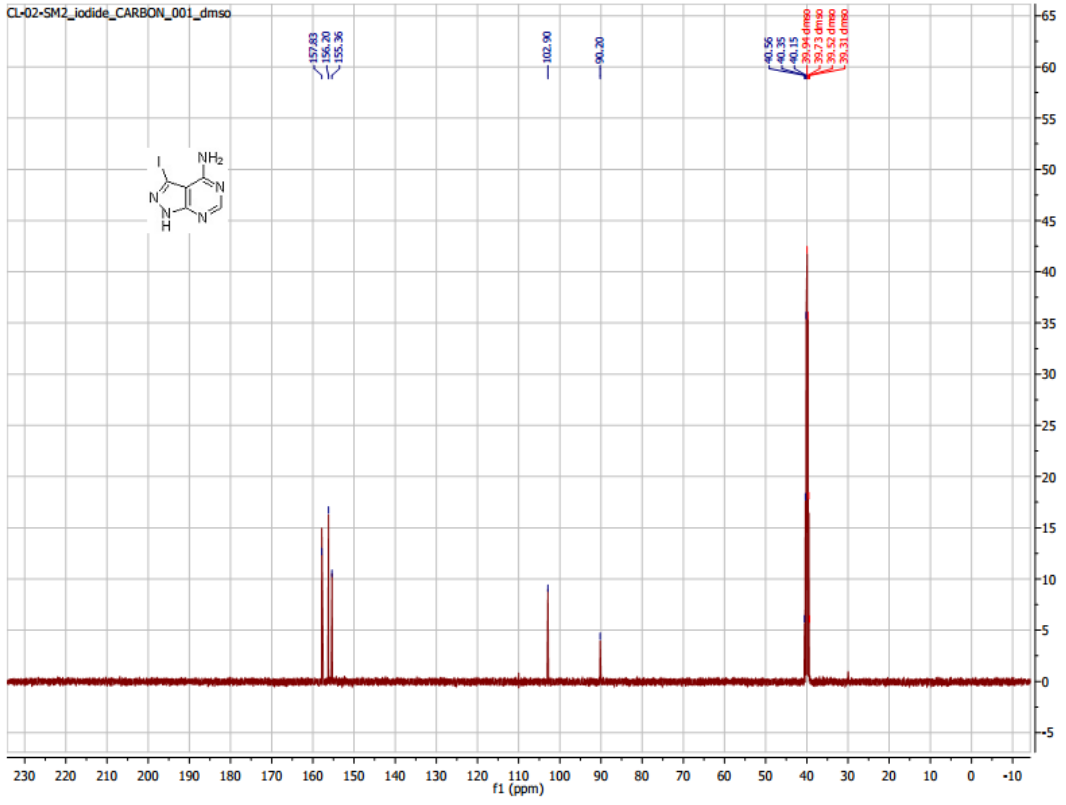
5-Iodo-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-amine (3)



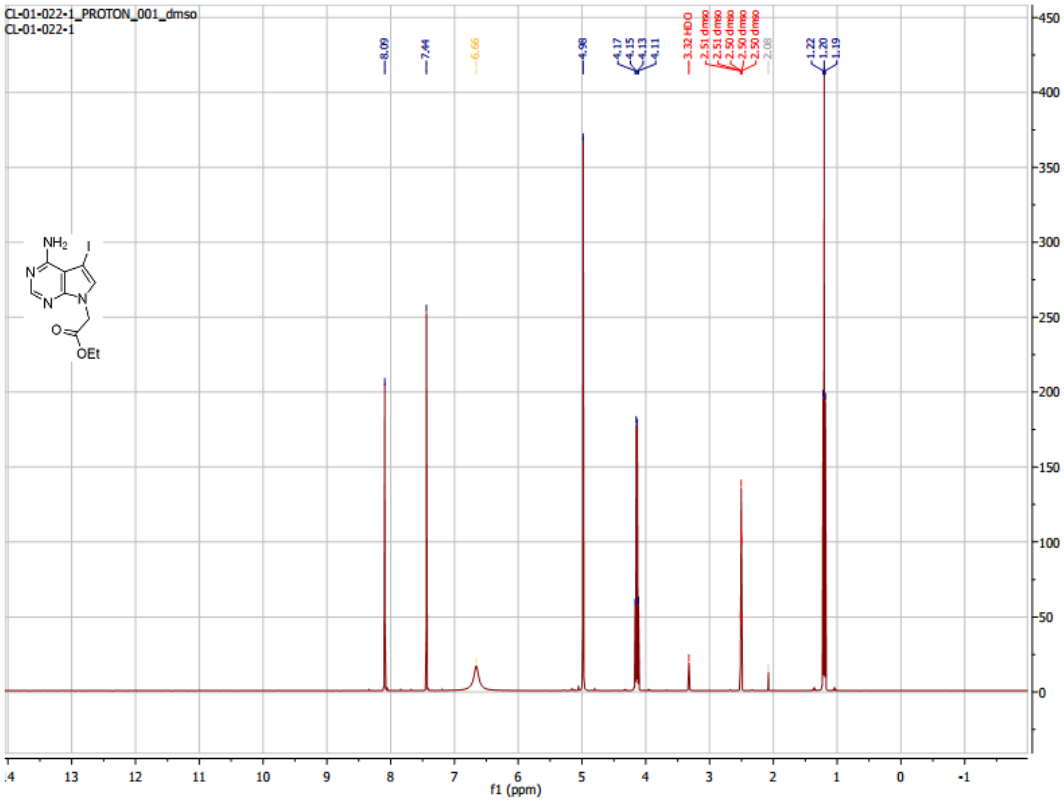


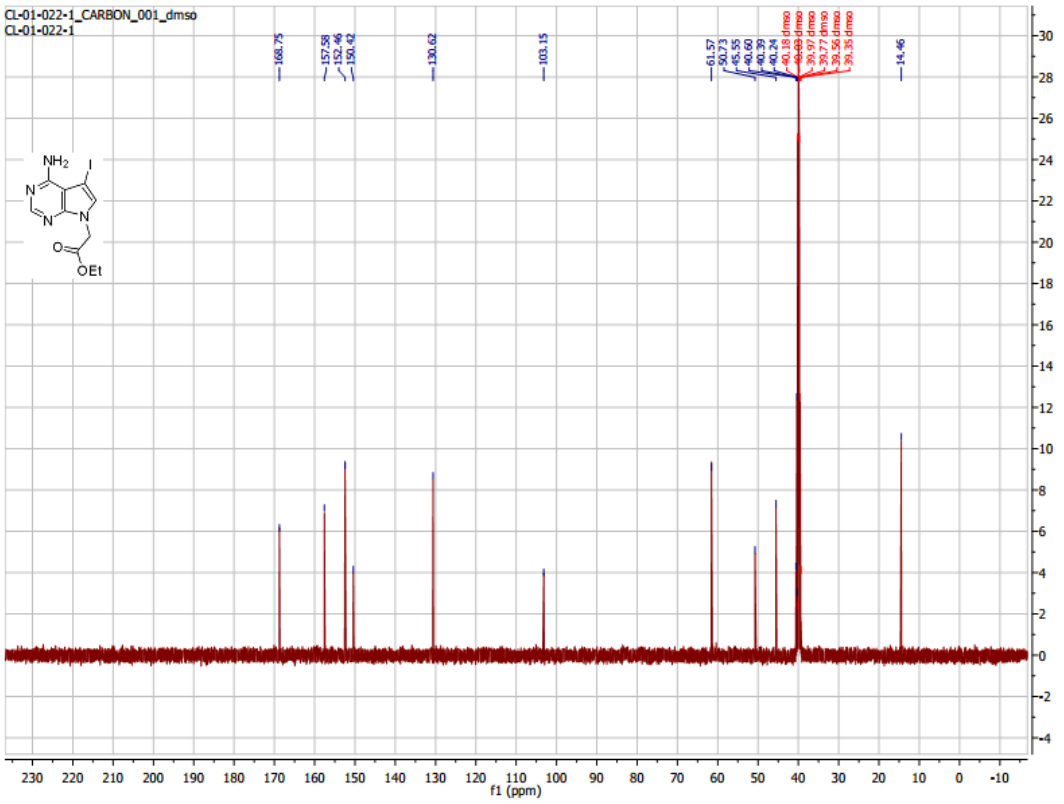
3-Iodo-1*H*-pyrazolo[3,4-*d*]pyrimidin-4-amine (4)



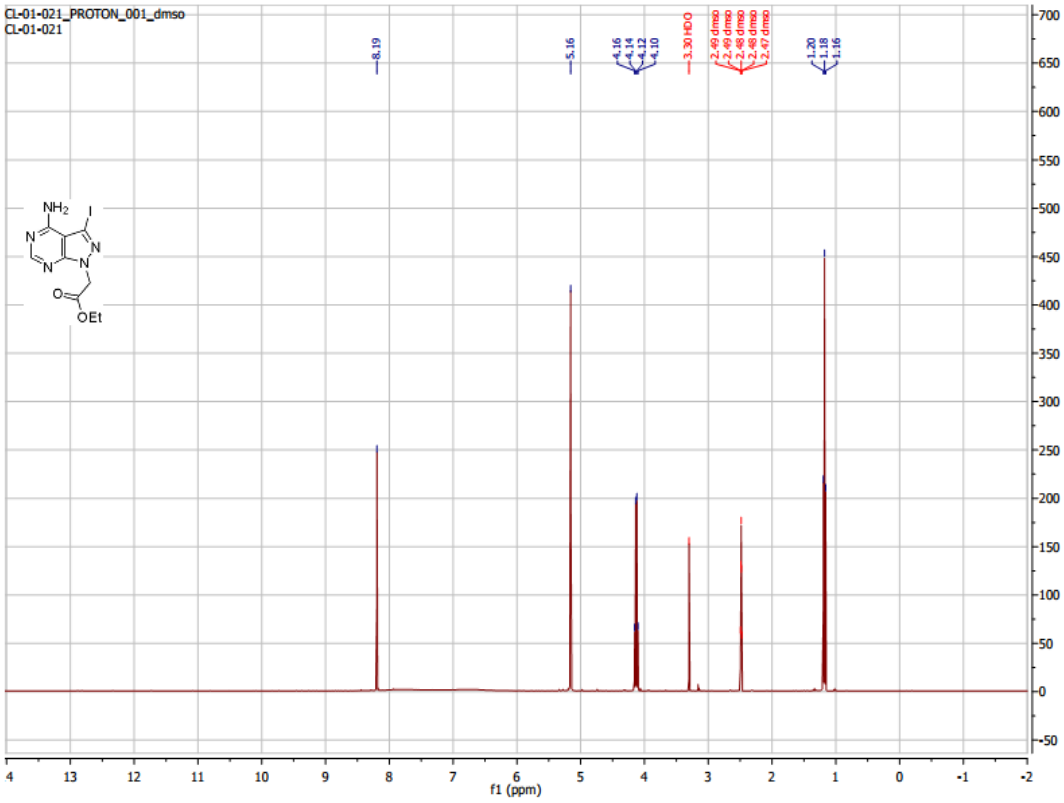


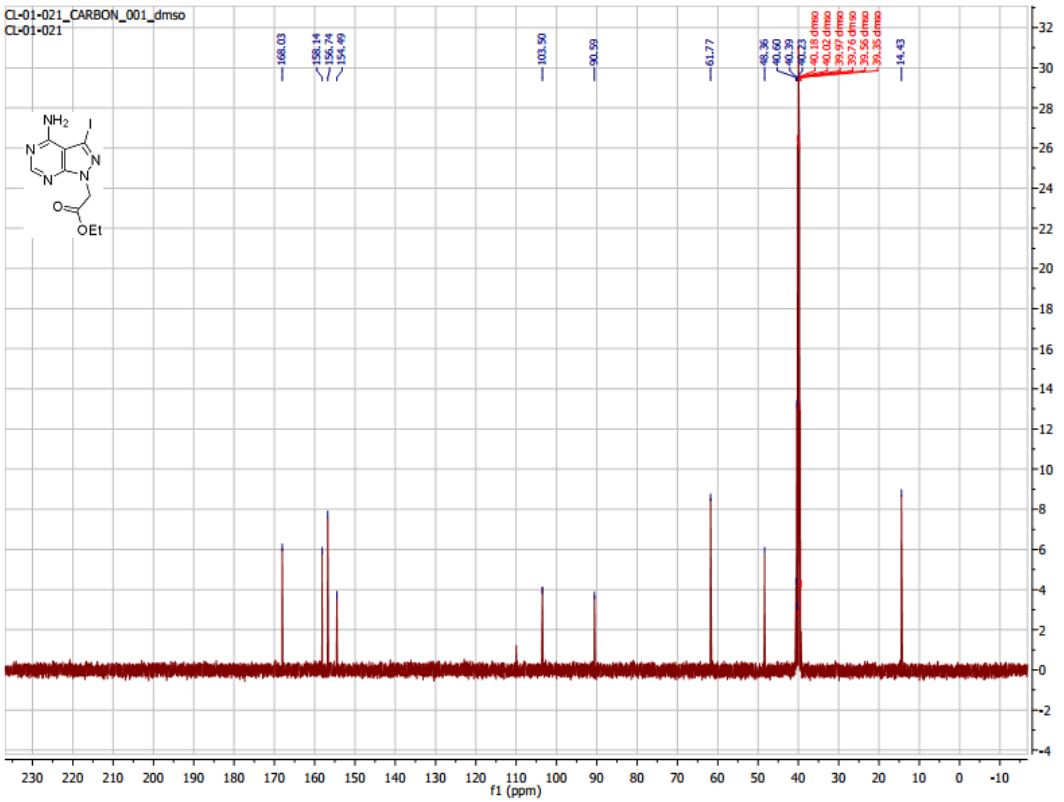
Ethyl 2-(4-amino-5-iodo-7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl)acetate (5)



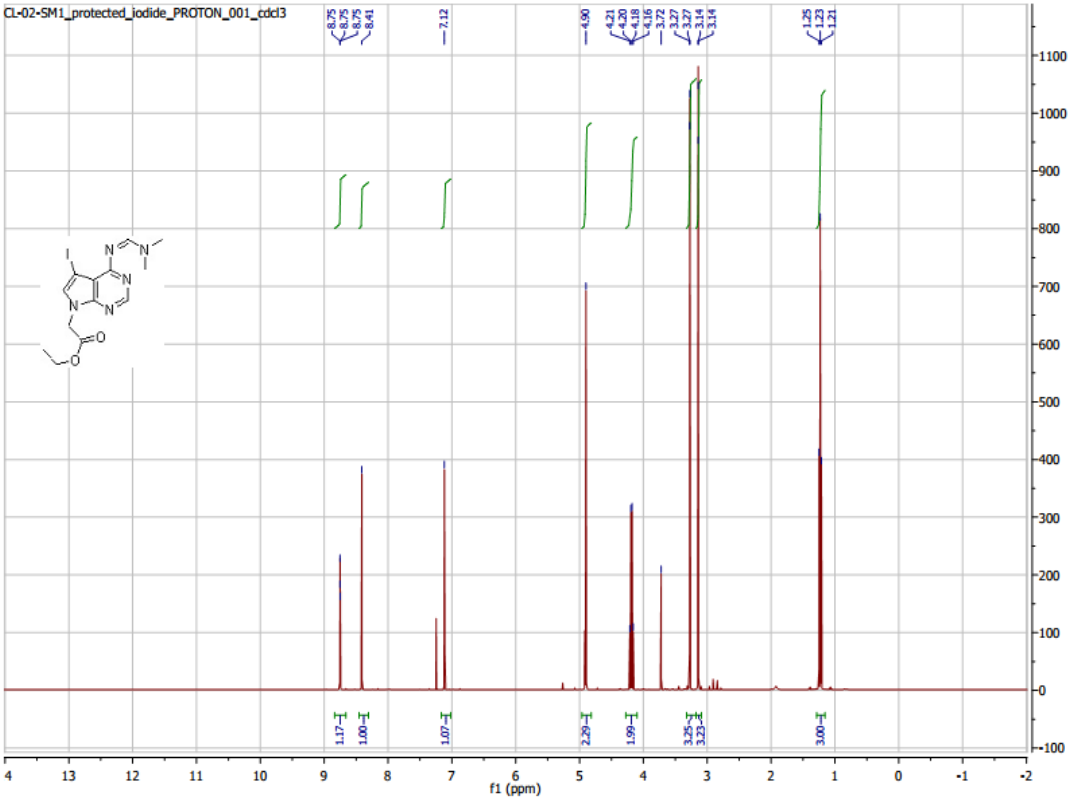


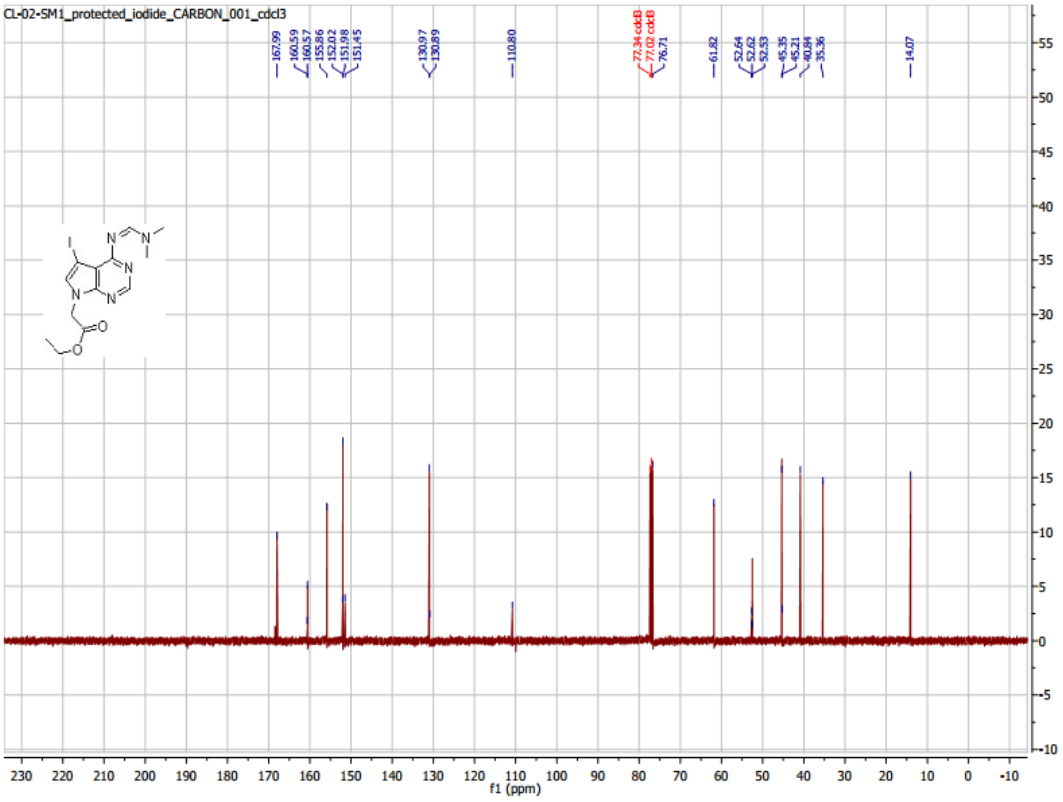
Ethyl 2-(4-amino-3-iodo-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl)acetate (6)



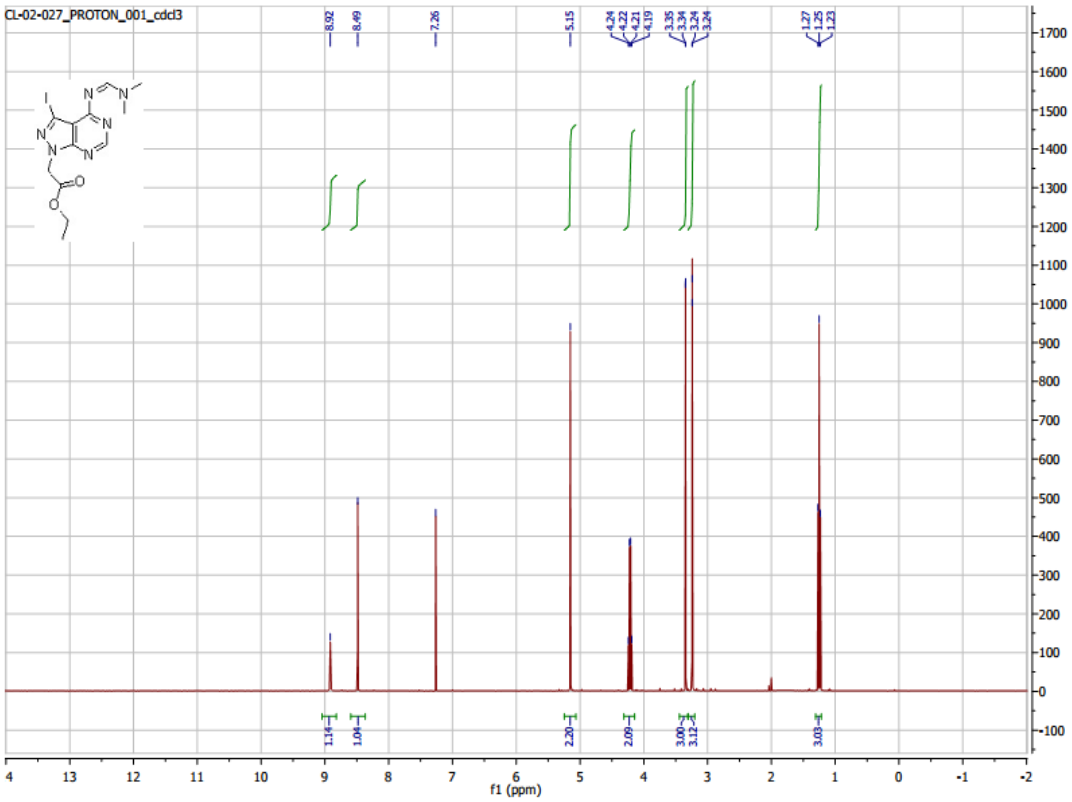


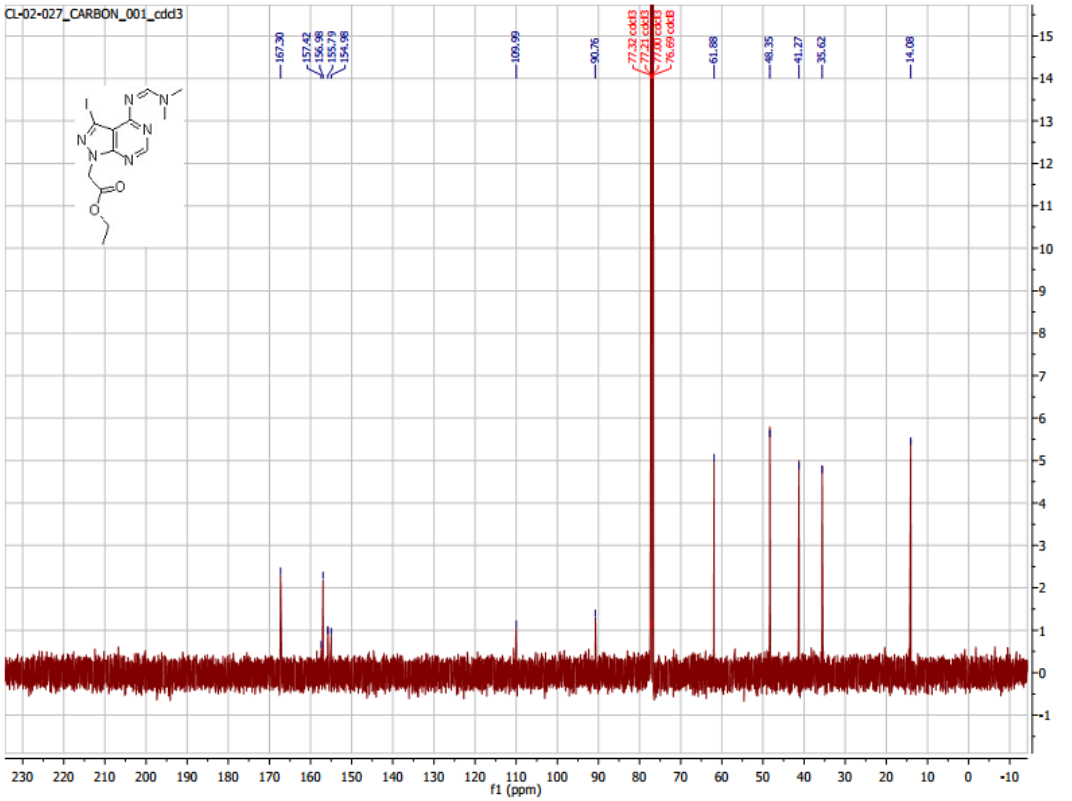
Ethyl (E)-2-(4-(((dimethylamino)methylene)amino)-5-iodo-7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl)acetate (15)



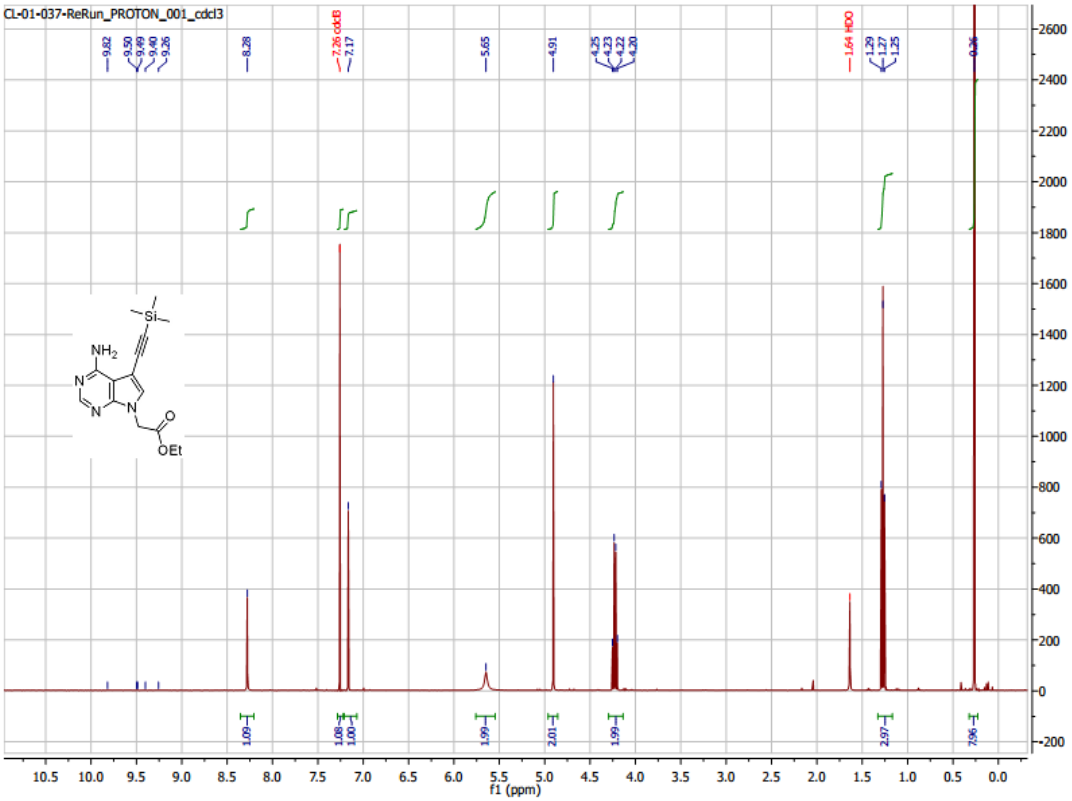


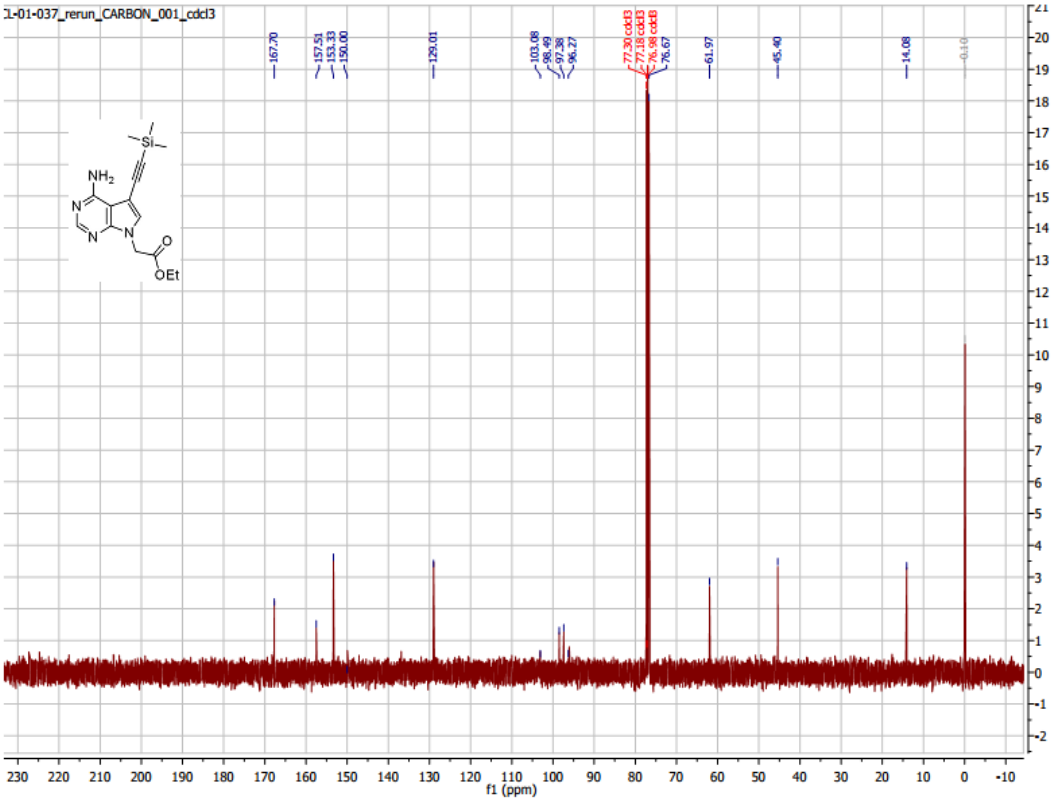
Ethyl (E)-2-(4-(((dimethylamino)methylene)amino)-3-iodo-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl)acetate (16)



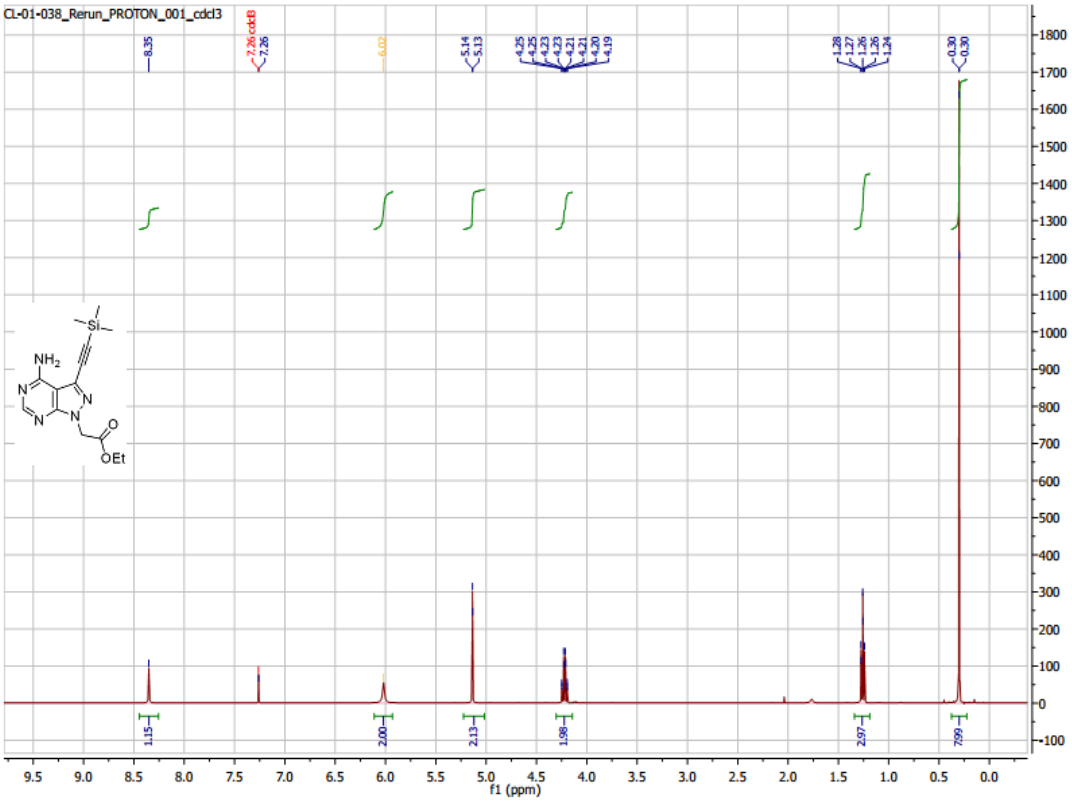


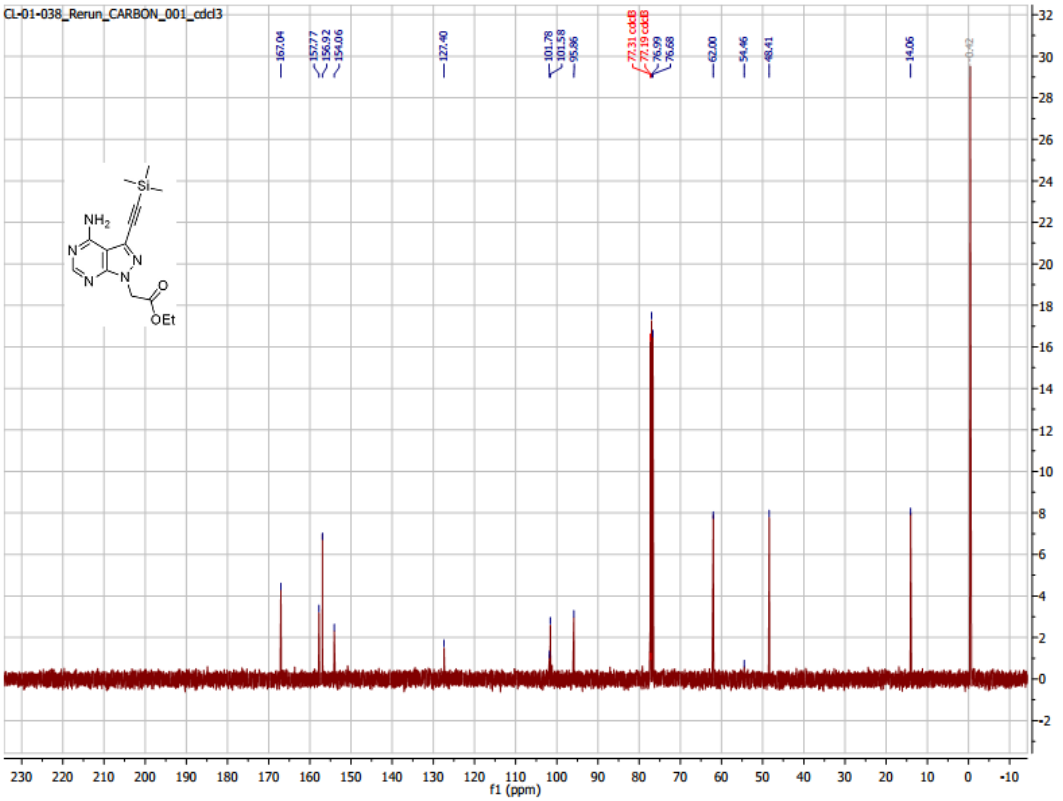
Ethyl 2-(4-amino-5-((trimethylsilyl)ethynyl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl)acetate (7)



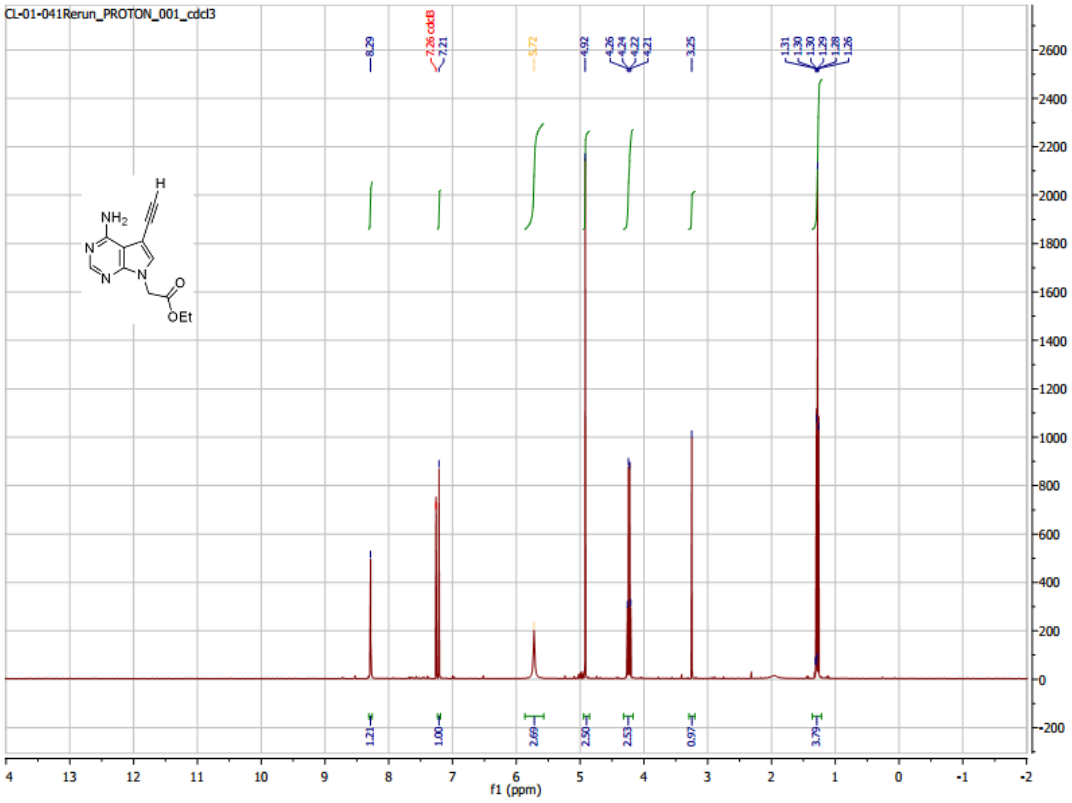


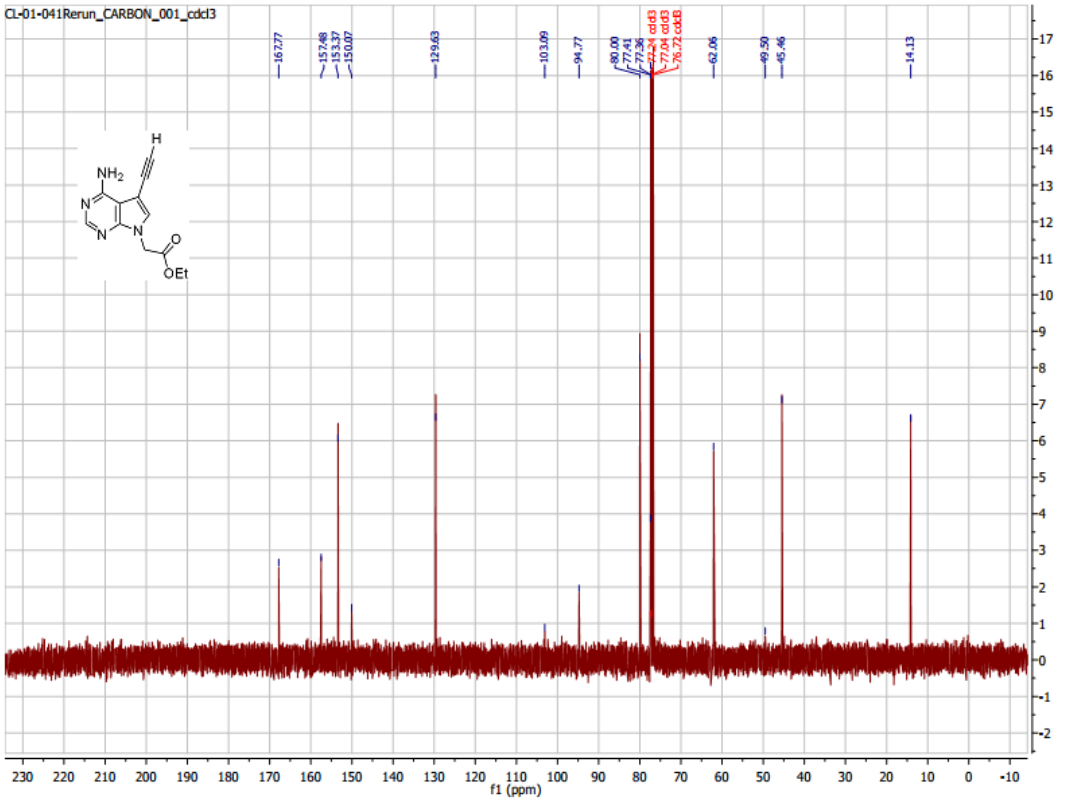
Ethyl 2-(4-amino-3-((trimethylsilyl)ethynyl)-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl)acetate (8)



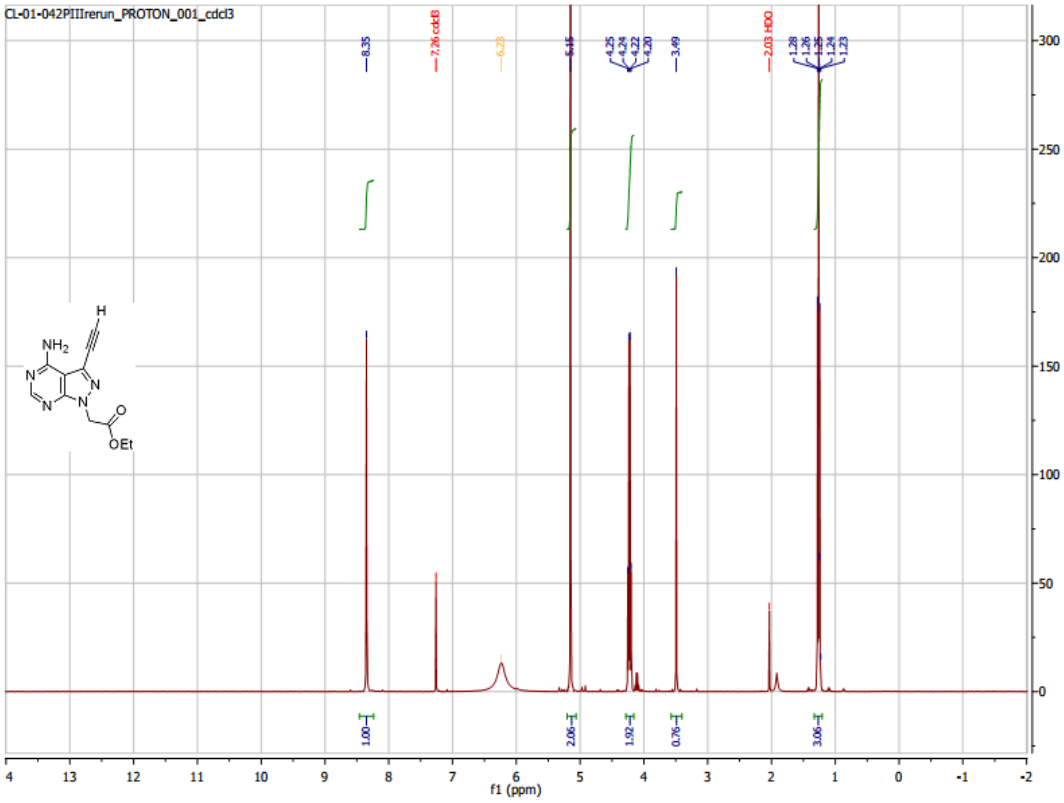


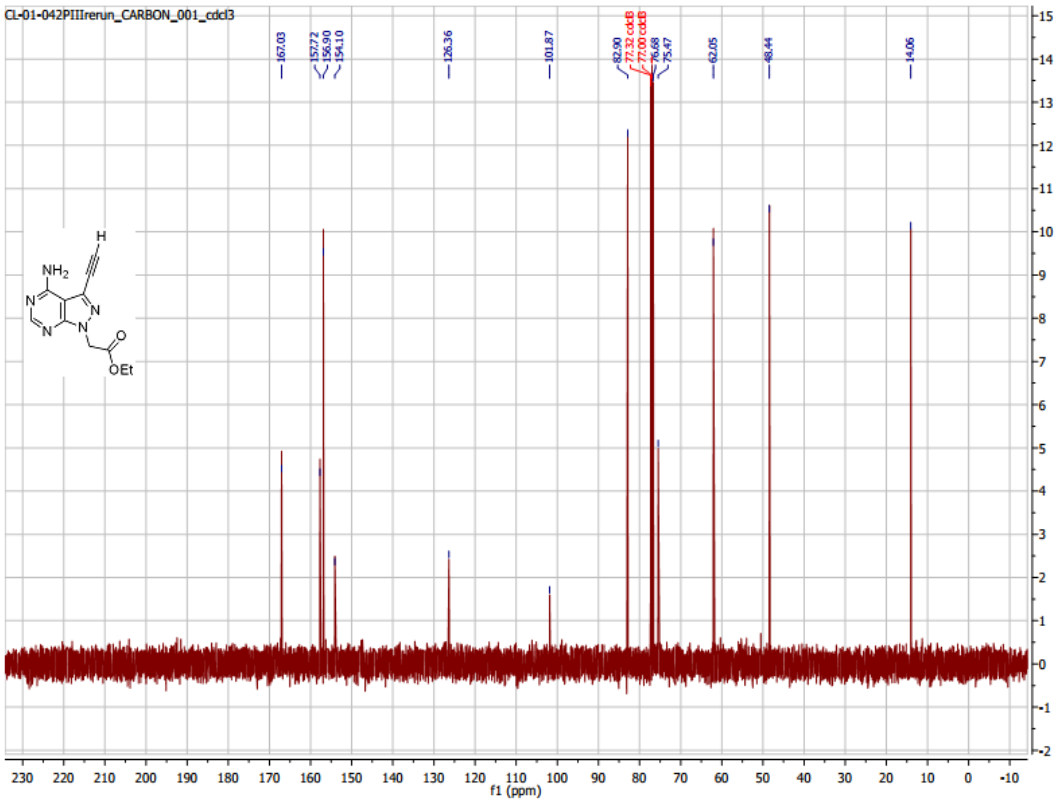
Ethyl 2-(4-amino-5-ethynyl-7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl)acetate (9)



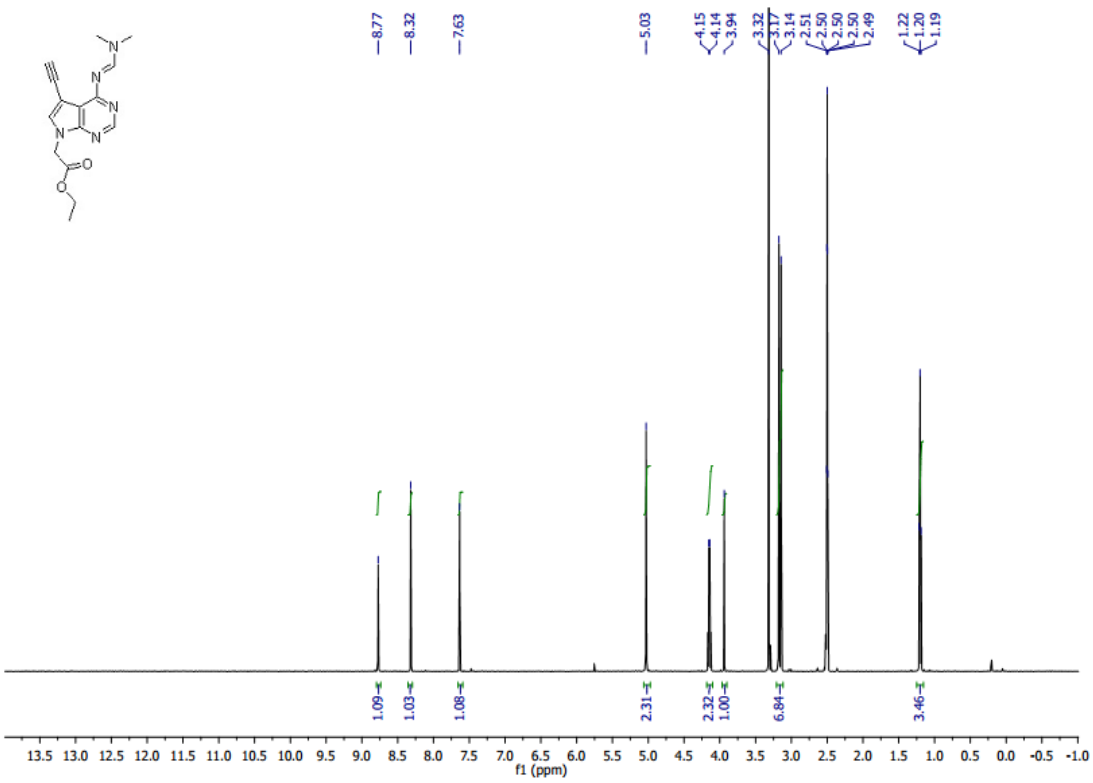


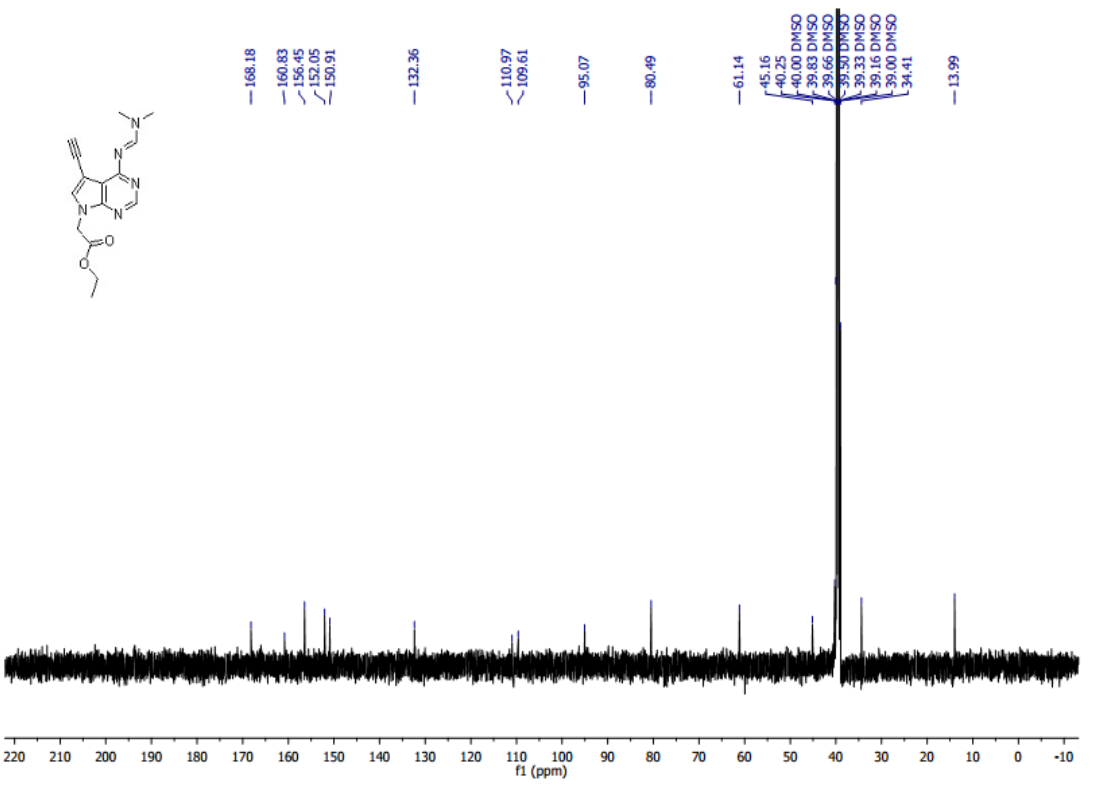
Ethyl 2-(4-amino-3-ethynyl-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl)acetate (10)



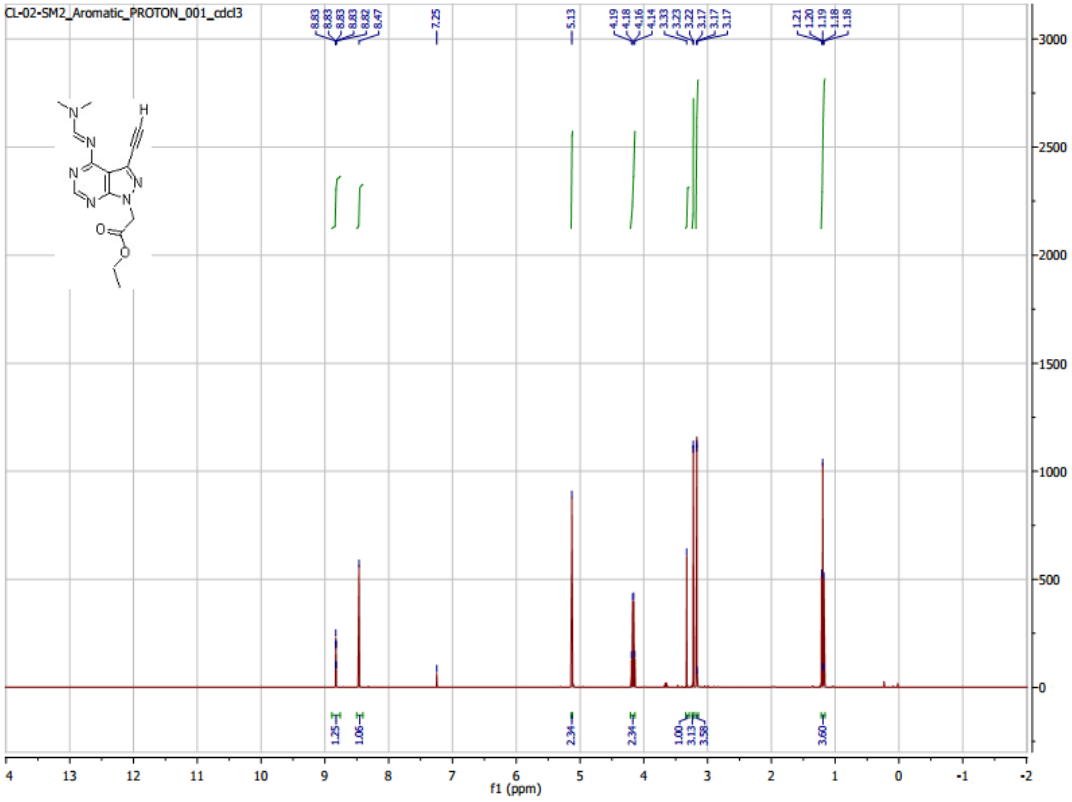


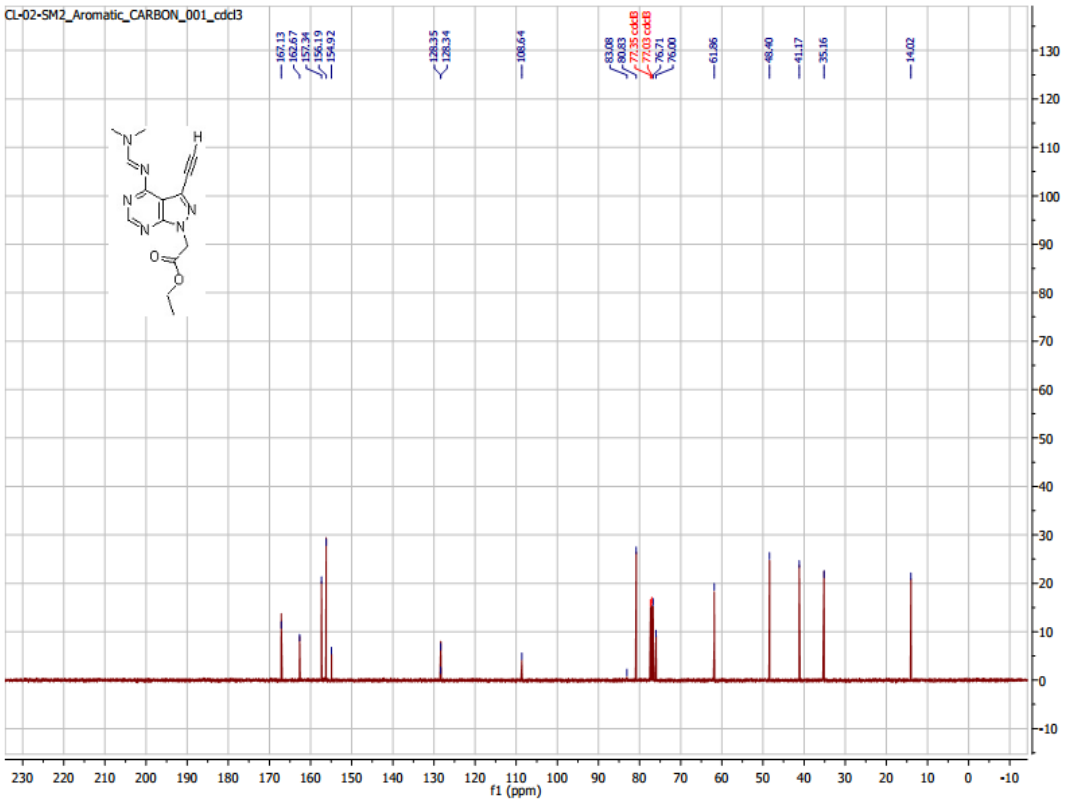
Ethyl (E) 2-(4-(((dimethylamino)methylene)amino)-5-ethynyl-7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl)acetate (17)



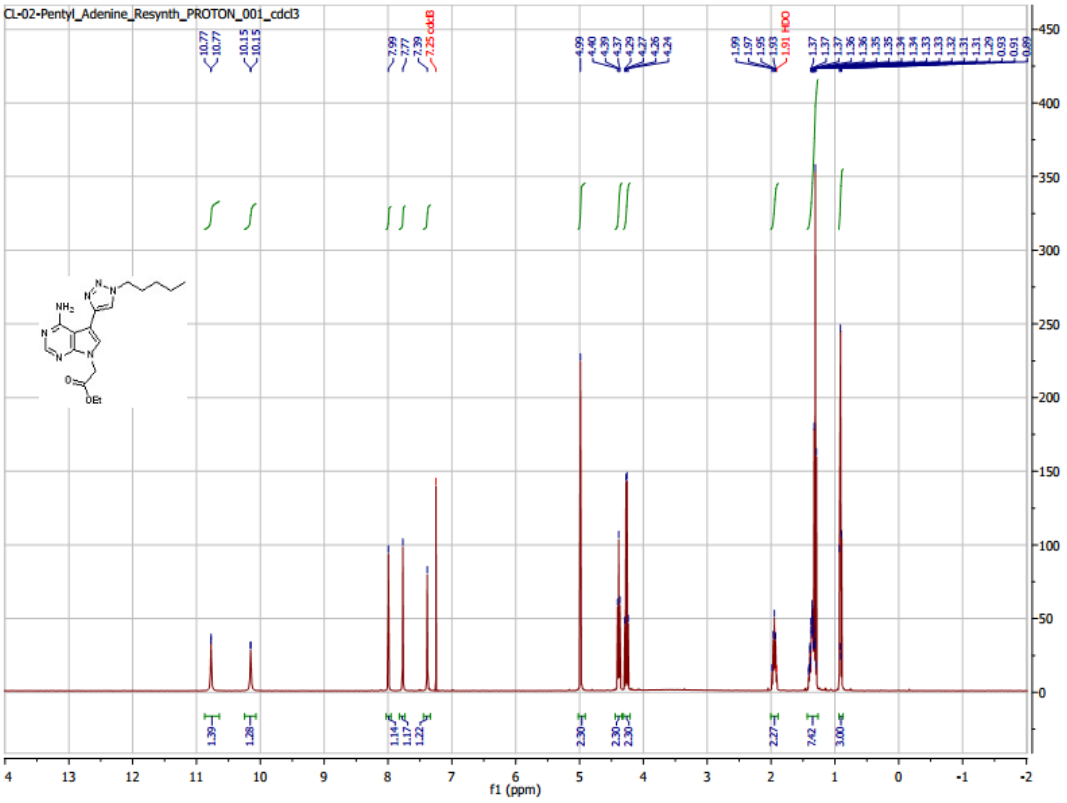


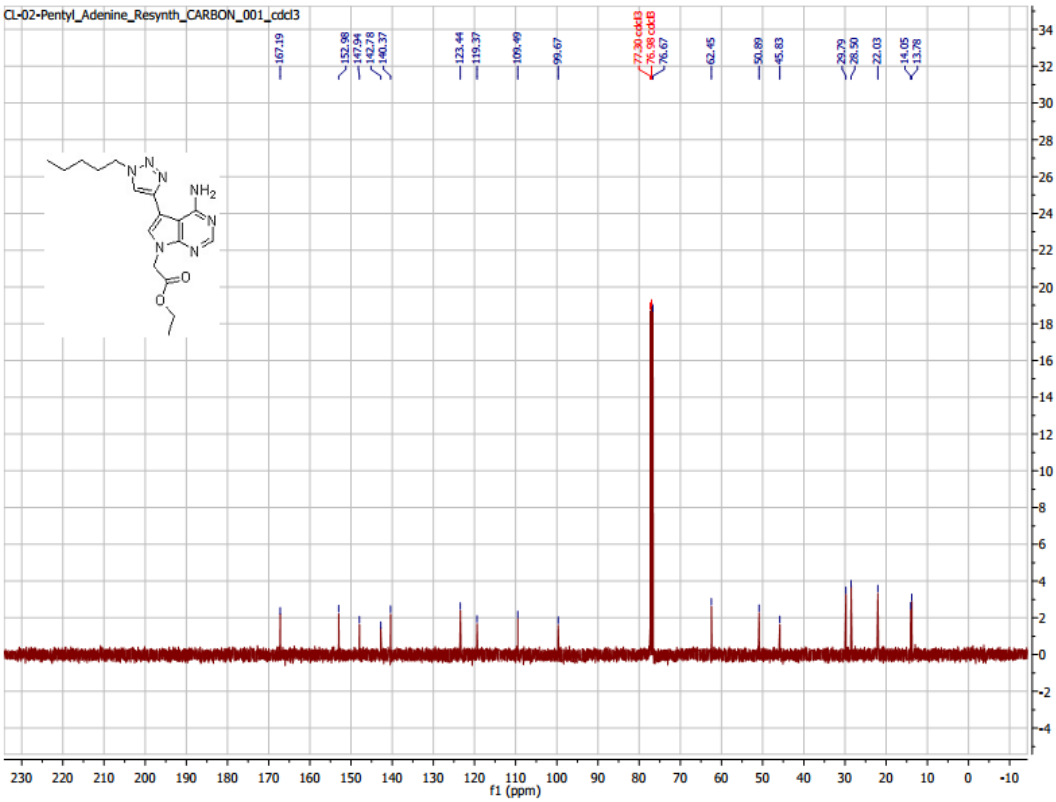
Ethyl (E)-2-(4-(((dimethylamino)methylene)amino)-3-ethynyl-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl)acetate (18)



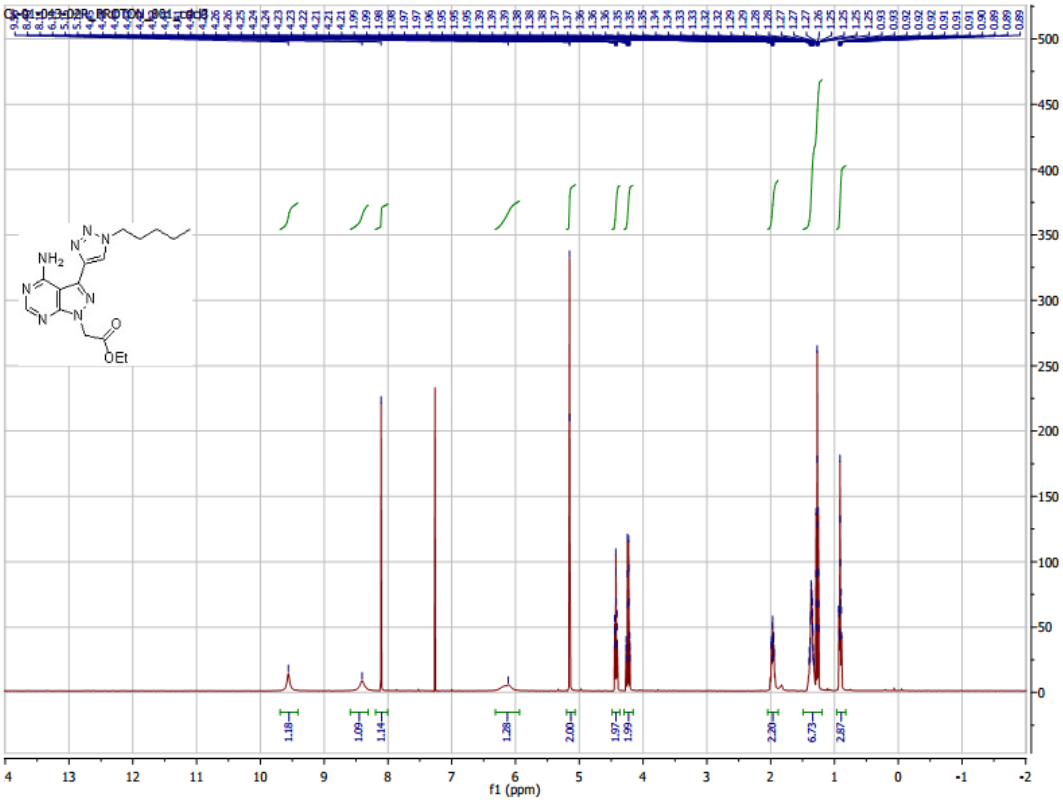


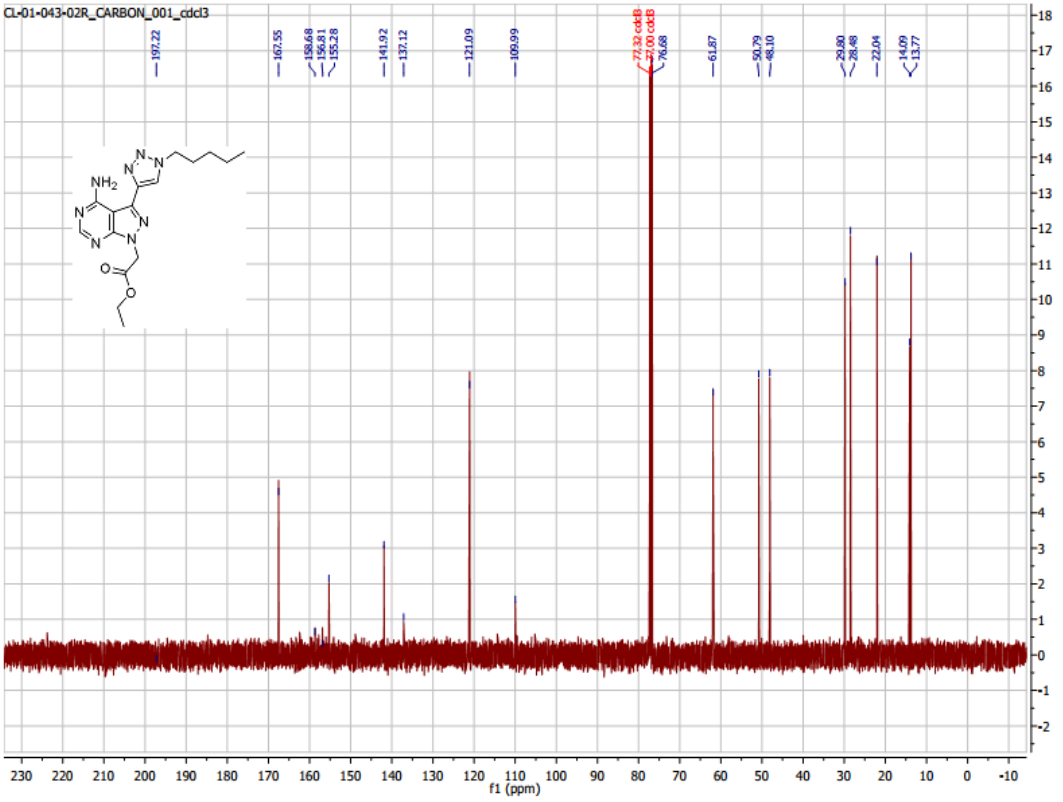
Ethyl 2-(4-amino-5-(1-pentyl-1*H*-1,2,3-triazol-4-yl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl)acetate (11a)



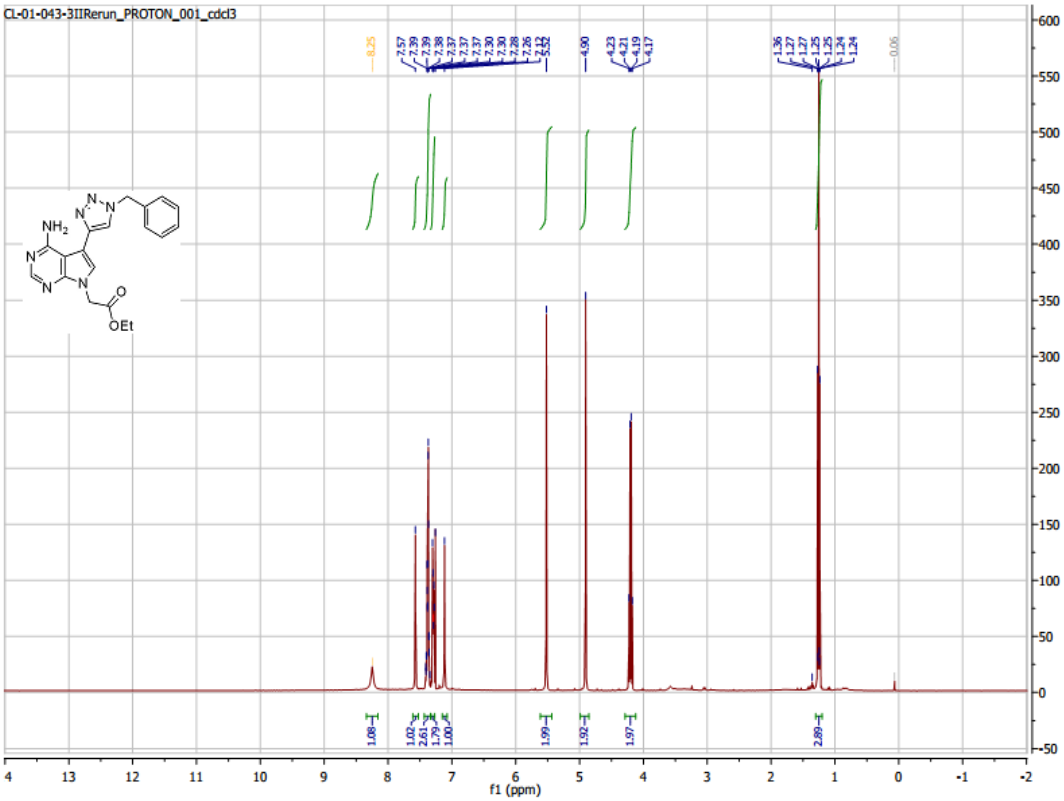


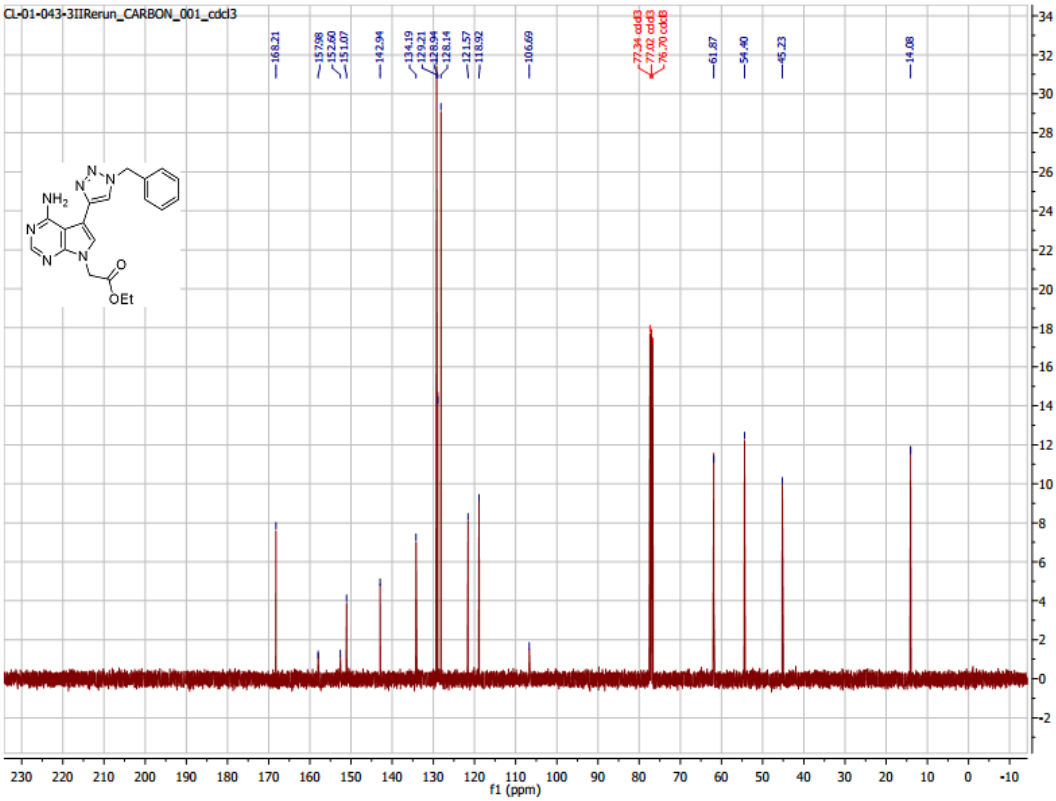
Ethyl 2-(4-amino-3-(1-pentyl-1*H*-1,2,3-triazol-4-yl)-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl)acetate (12a)



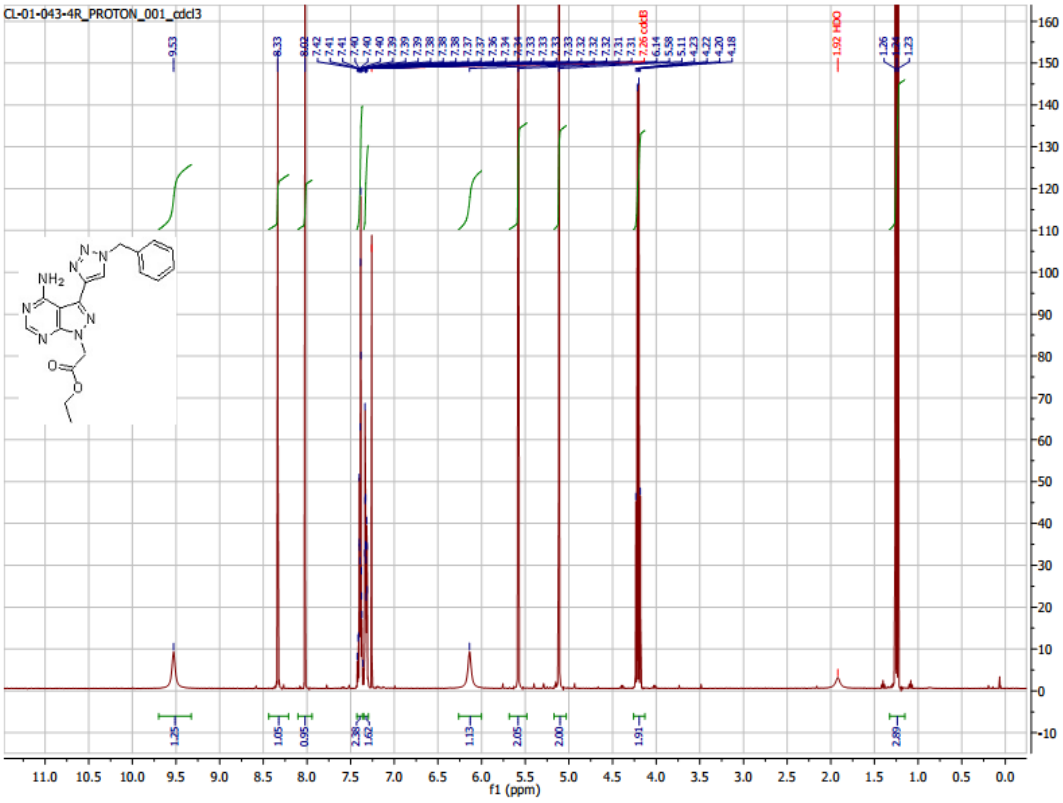


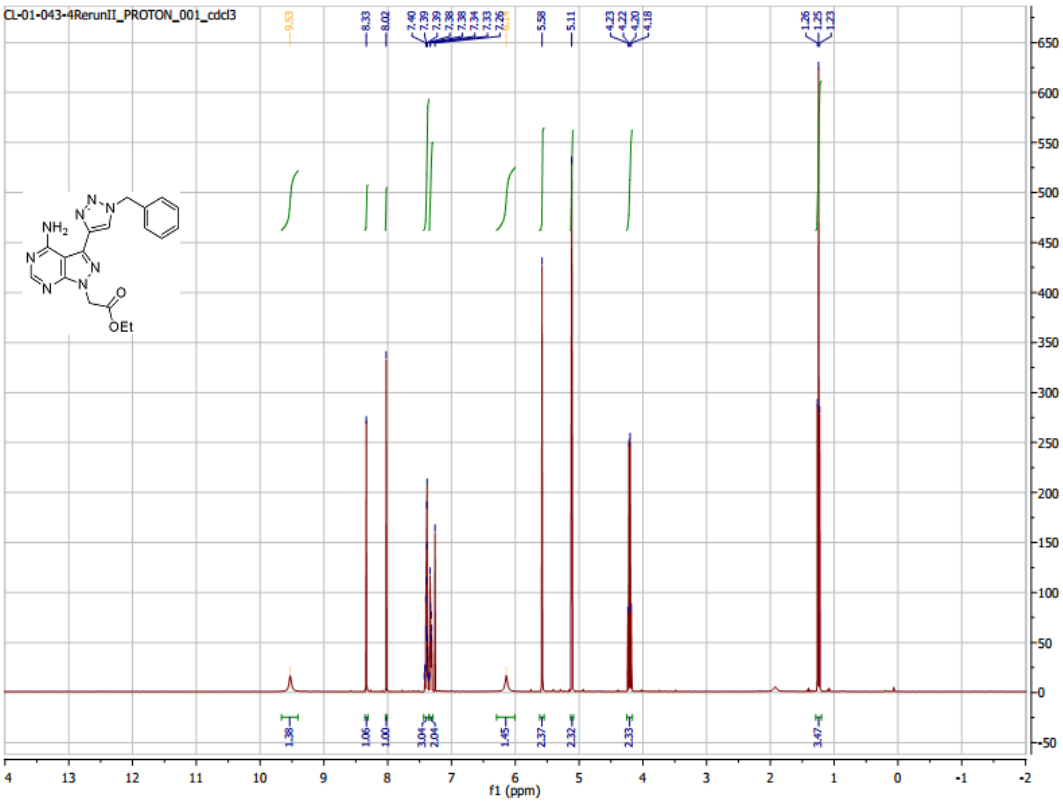
Ethyl 2-(4-amino-5-(1-benzyl-1*H*-1,2,3-triazol-4-yl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl)acetate (11b)



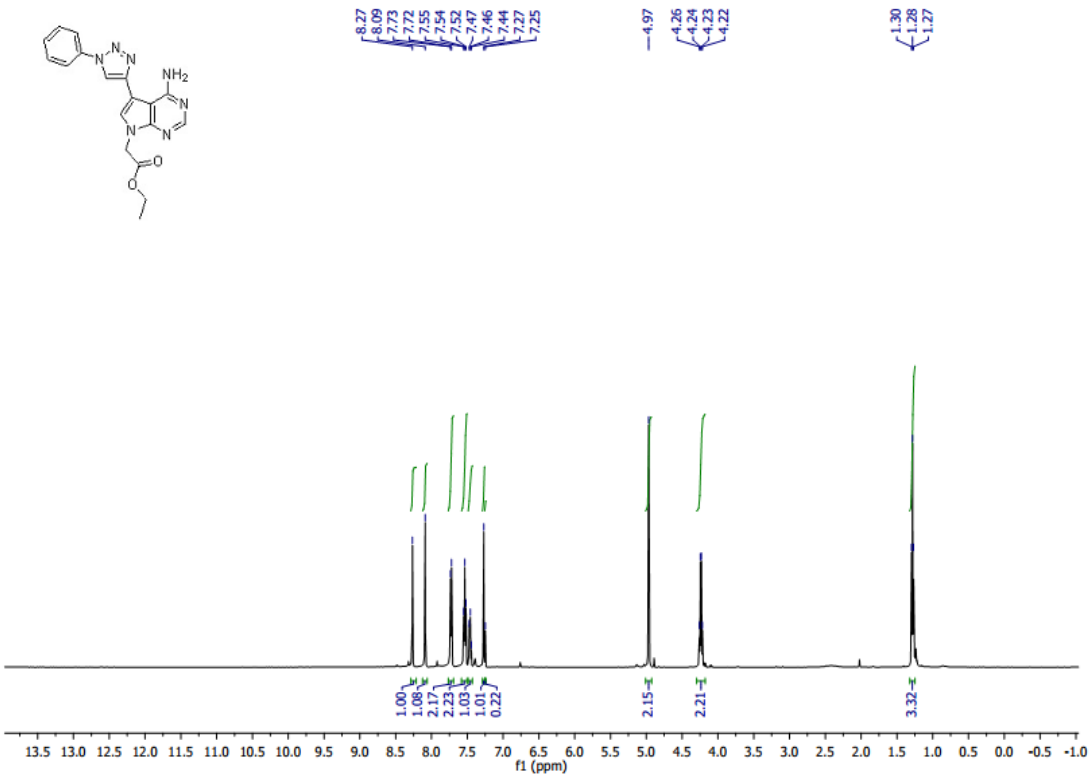


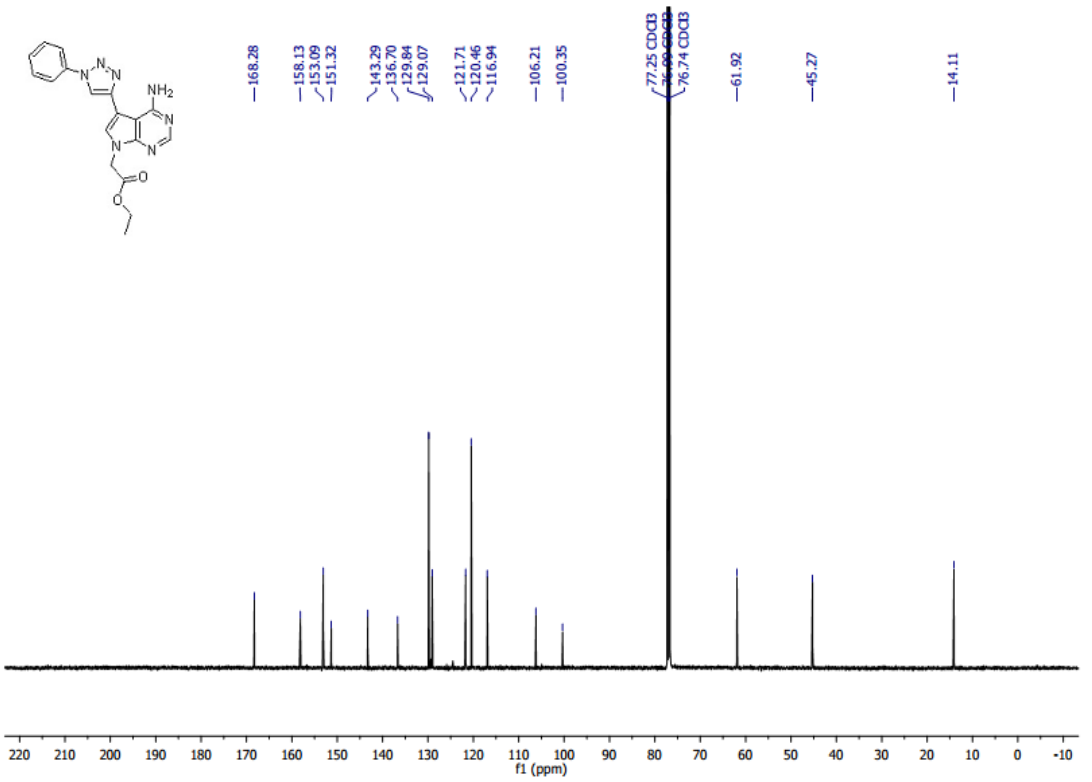
Ethyl 2-(4-amino-3-(1-benzyl-1*H*-1,2,3-triazol-4-yl)-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl)acetate (12b)



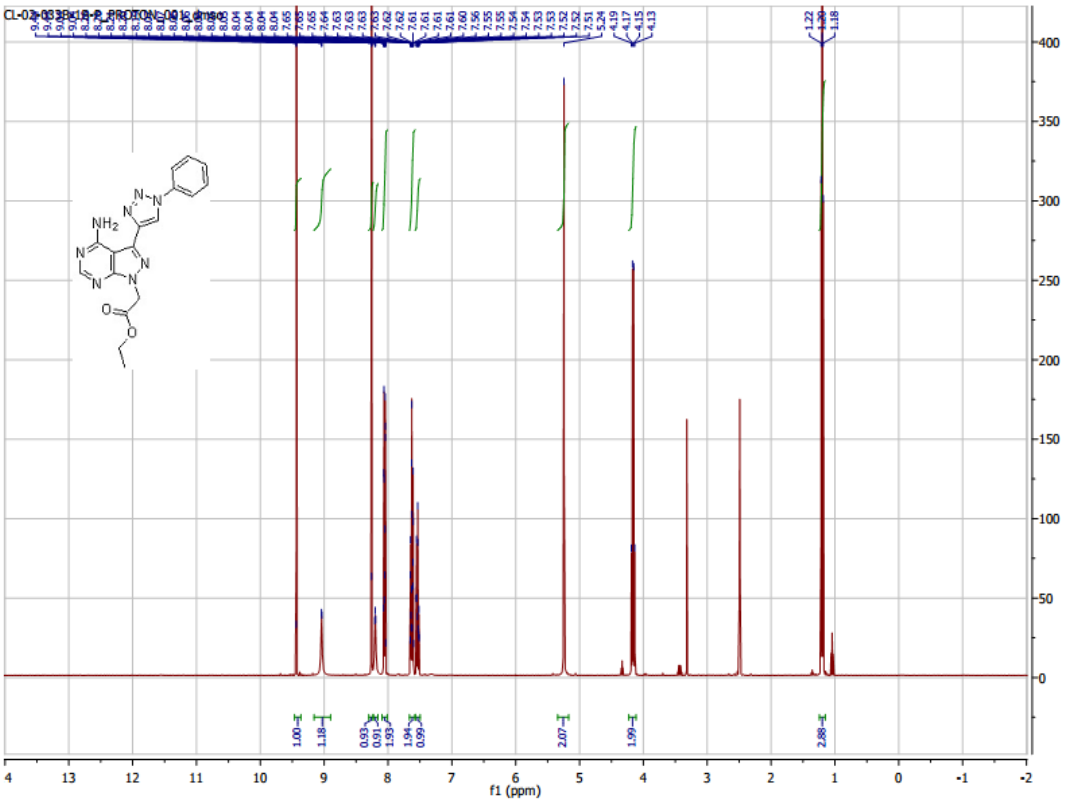


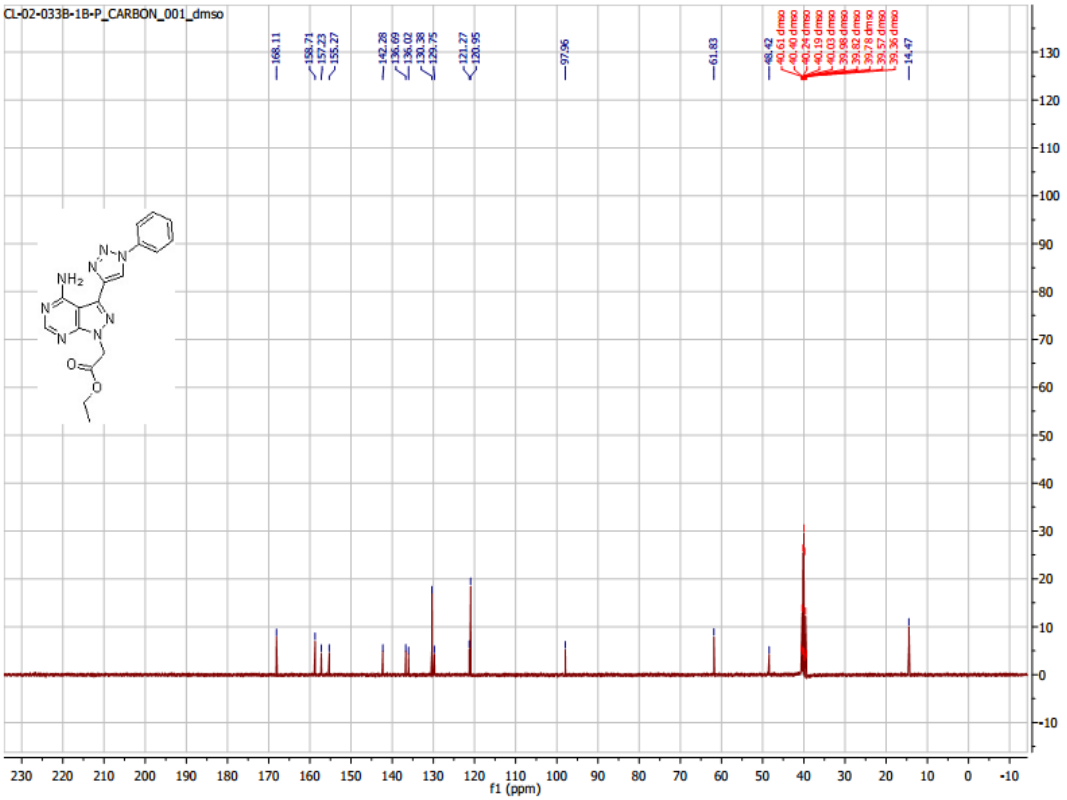
Ethyl 2-(4-amino-3-(1-phenyl-1*H*-1,2,3-triazol-4-yl)-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl)acetate(19)



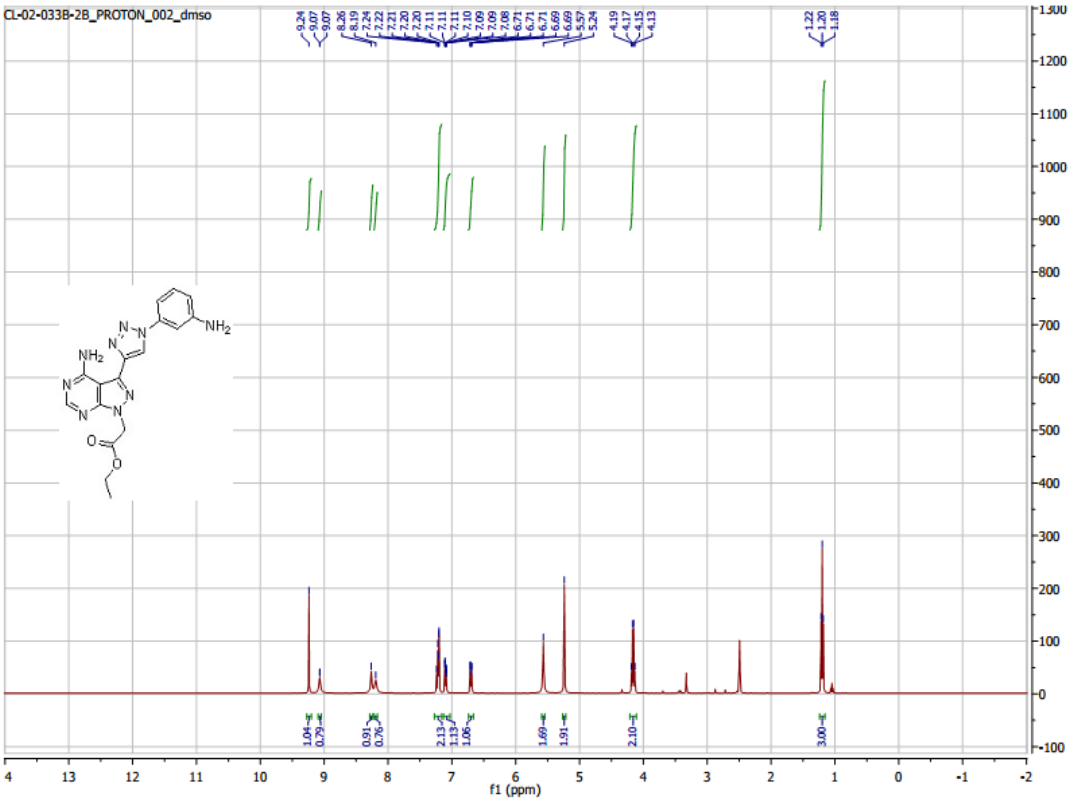


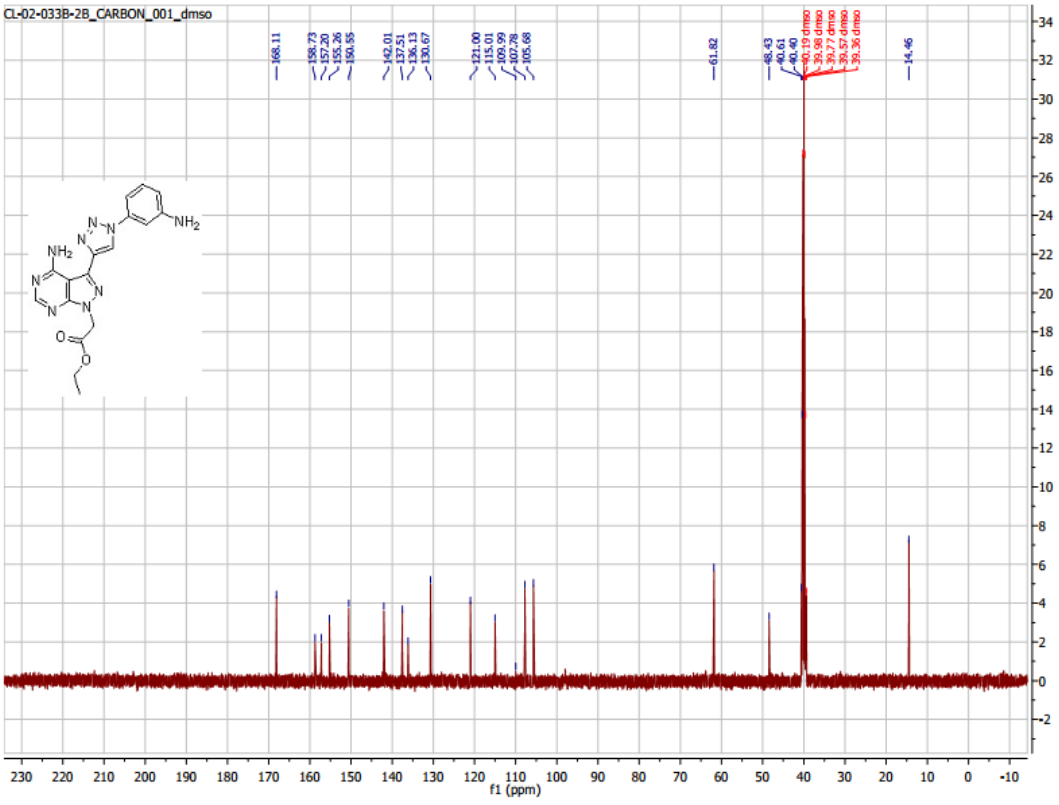
Ethyl 2-(4-amino-3-(1-phenyl-1*H*-1,2,3-triazol-4-yl)-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl)acetate (20a)



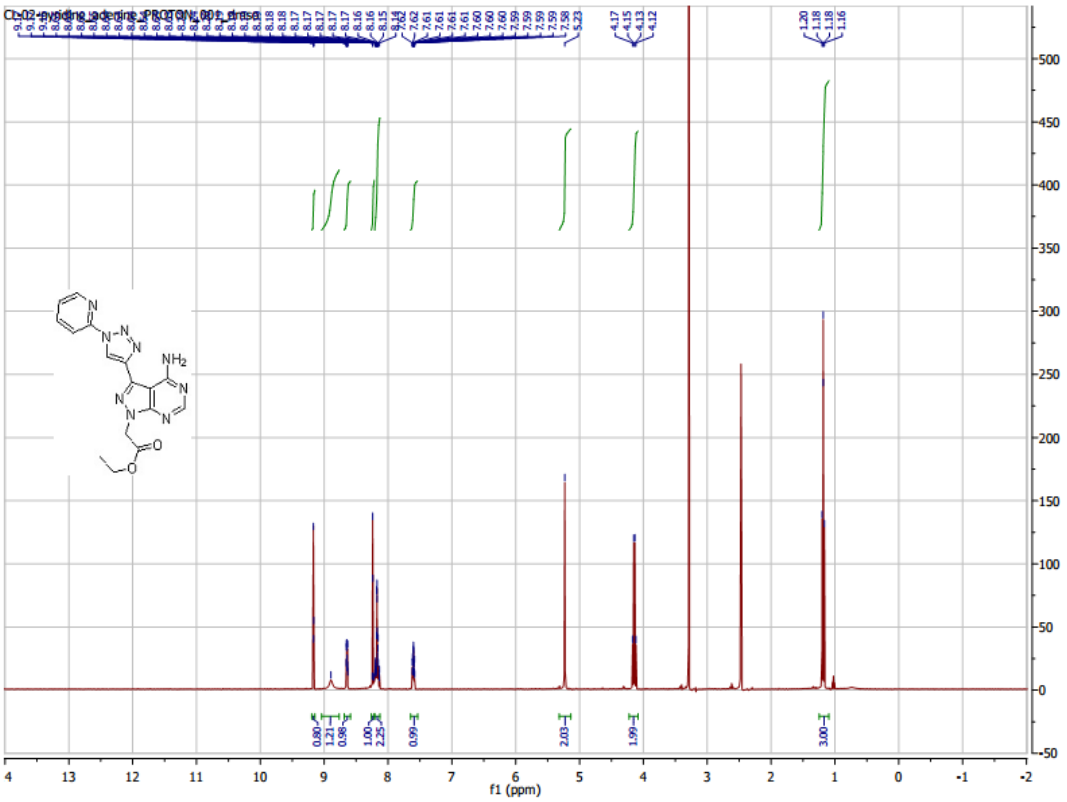


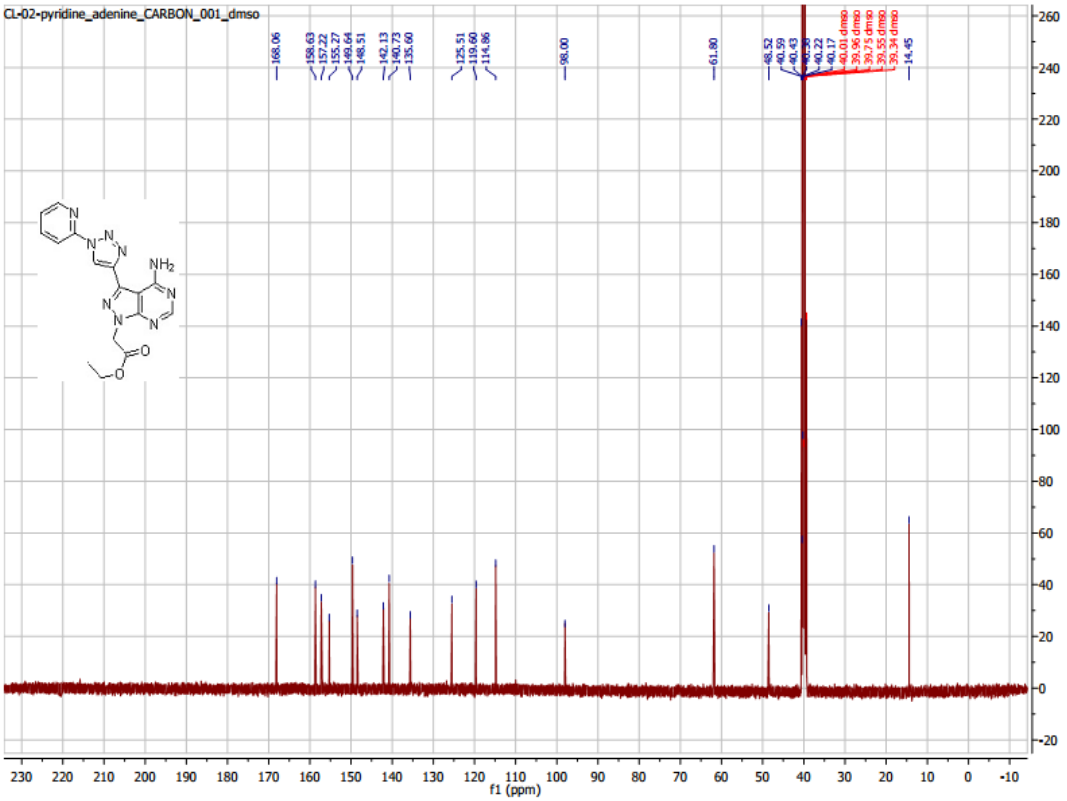
Ethyl-2-(4-amino-3-(1-(3-aminophenyl)-1*H*-1,2,3-triazol-4-yl)-1*H*-pyrazolo[3,4-d]pyrimidin-1-yl)acetate (20b))



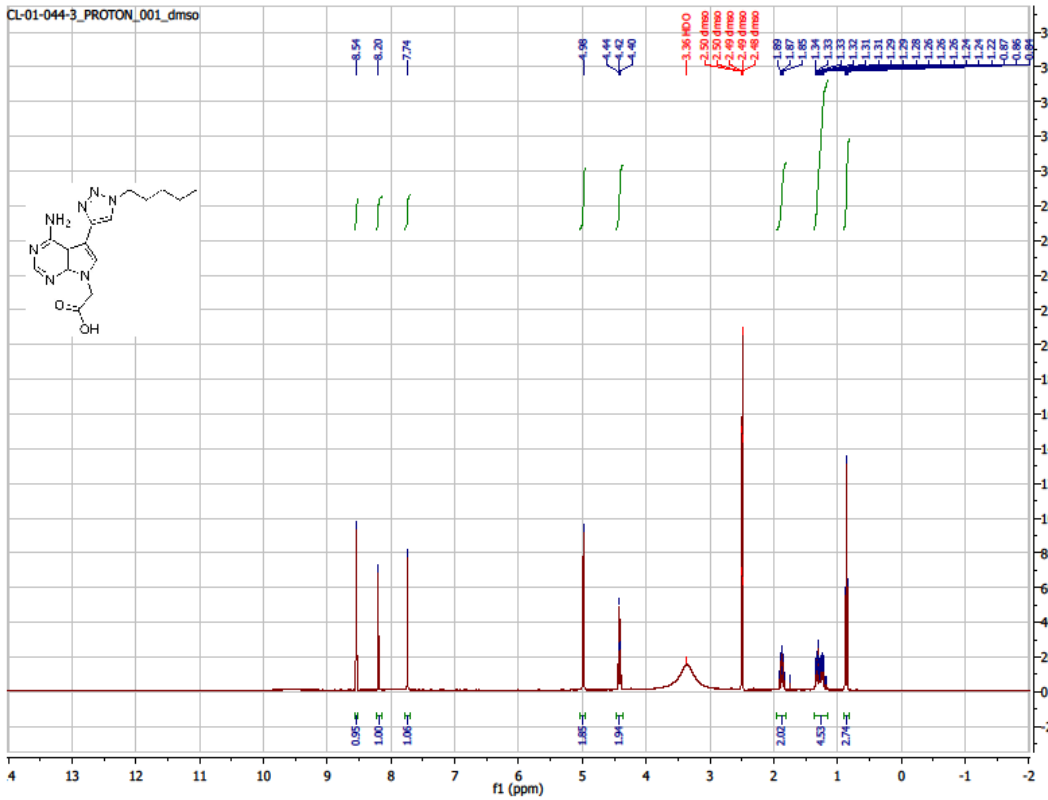


Ethyl 2-(4-amino-3-(1-(pyridin-2-yl)-1*H*-1,2,3-triazol-4-yl)-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl)acetate (20c)

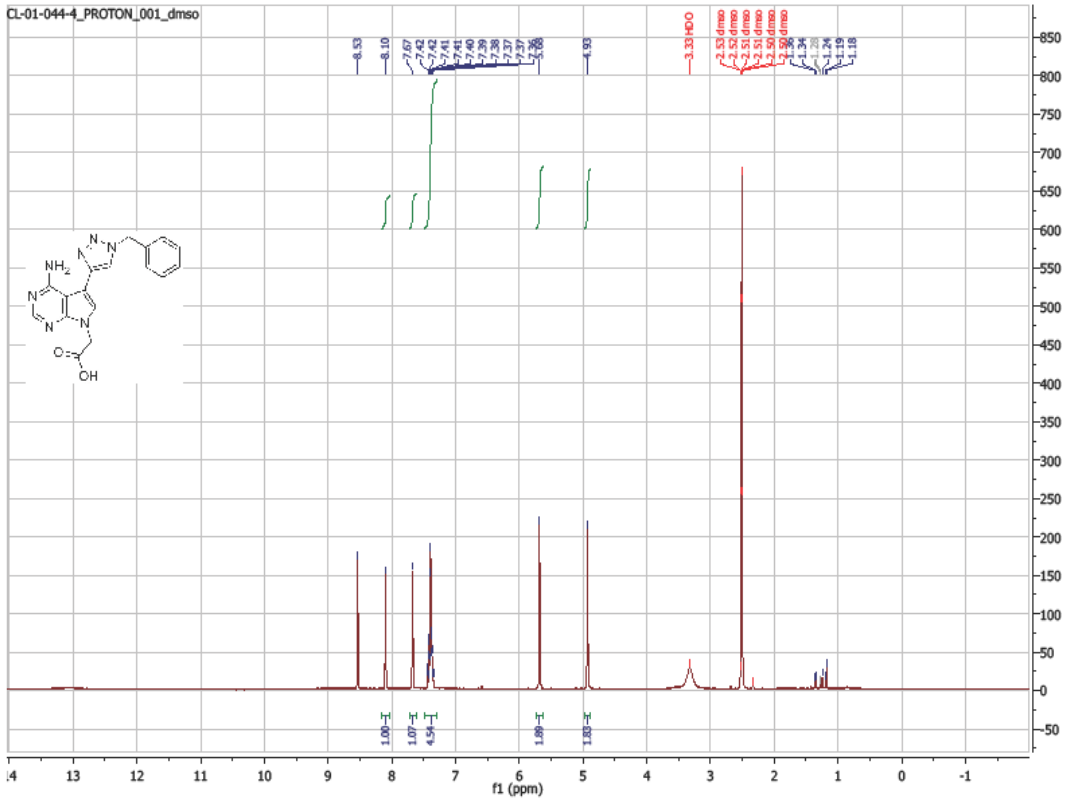




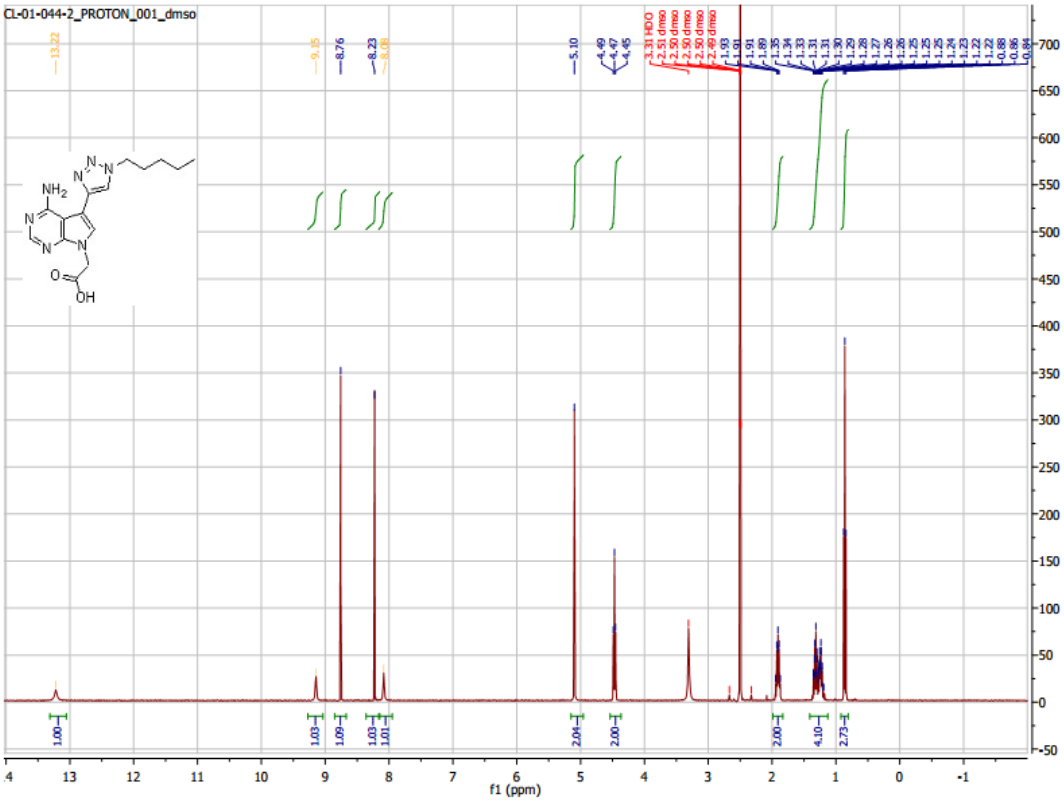
2-(4-amino-5-(1-pentyl-1*H*-1,2,3-triazol-4-yl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl)acetic acid (13a)



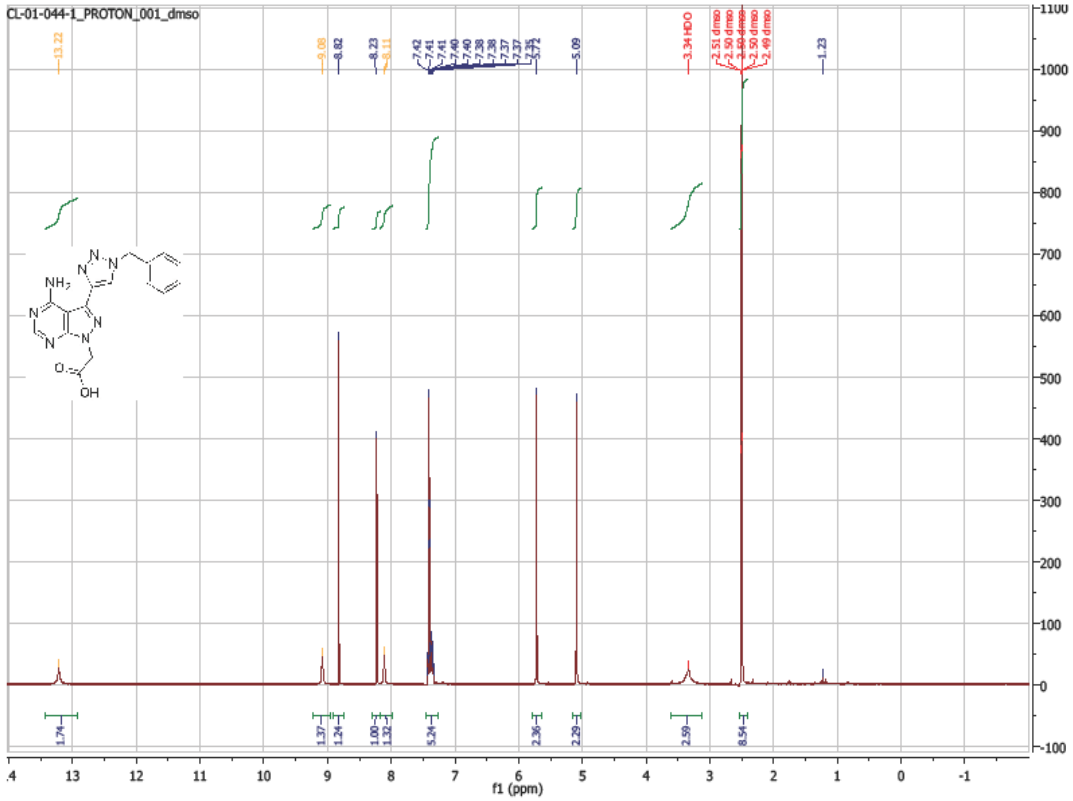
2-(4-amino-5-(1-benzyl-1*H*-1,2,3-triazol-4-yl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl)acetic acid (13b)



2-(4-amino-3-(1-pentyl-1*H*-1,2,3-triazol-4-yl)-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl)acetic acid (14a)



2-(4-amino-3-(1-benzyl-1*H*-1,2,3-triazol-4-yl)-1*H*-pyrazolo[3,4-*d*]pyrimidin-1-yl)acetic acid (14b)



Photophysical characterization

Absorption spectra of compounds **19** and **20b** were recorded in methanol at different concentrations (Figure S1-S2, respectively) and varying temperatures (Figure S3-S4, respectively) to investigate the influence on the long absorption tail.

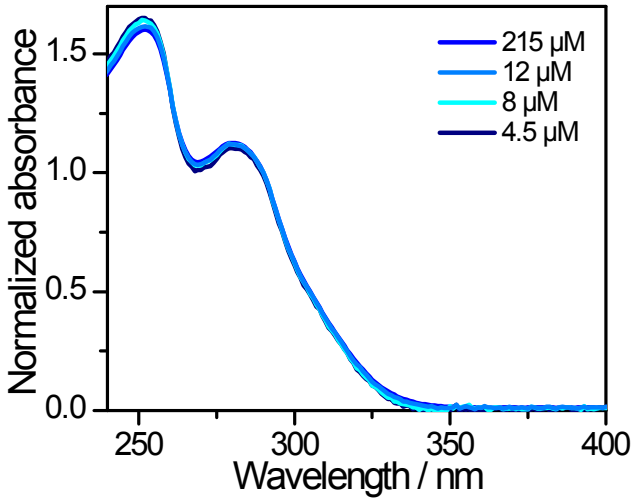


Figure S1. Normalized absorption spectra of solutions of varying concentrations of compound **19** in methanol.

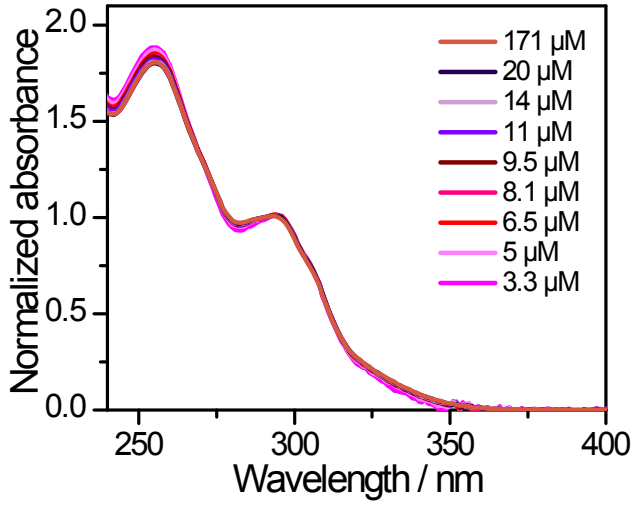


Figure S2. Normalized absorption spectra of solutions of varying concentrations of compound **20b** in methanol.

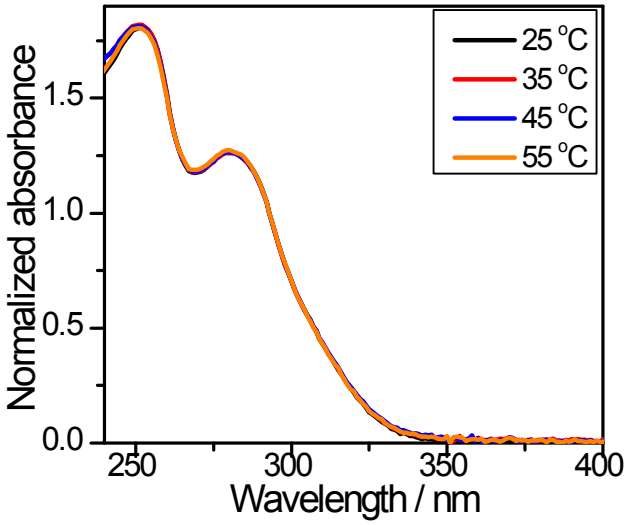


Figure S3. Normalized absorption spectra of compound **19** in methanol at varying temperatures.

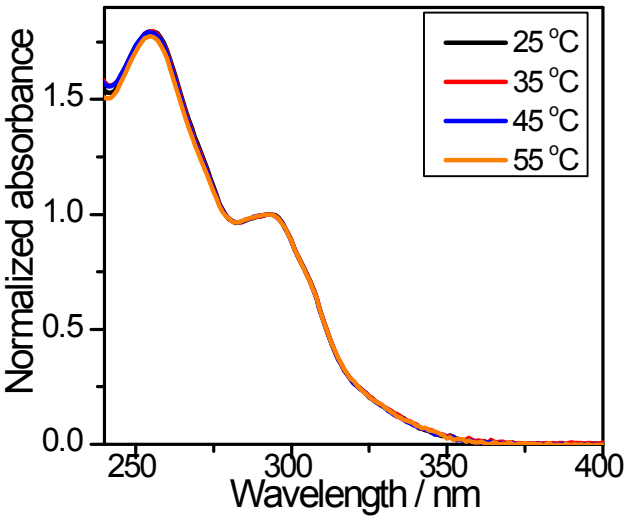


Figure S4. Normalized absorption spectra of compound **20b** in methanol at varying temperatures.

Due to a suspected excited state charge transfer process, the emission of **20b** was recorded in solvents with varying polarity and protic character.

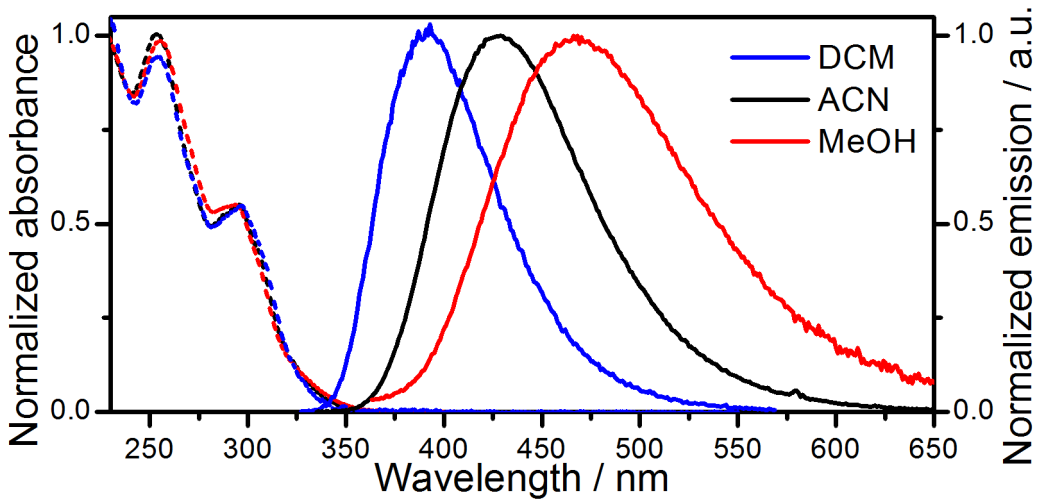


Figure S5. Normalized absorption (dashed line) and emission spectra (solid line) of **20b** in dichloromethane (DCM), acetonitrile (ACN) and methanol (MeOH).