

Supplementary Material

Exploration of Pyrido[3,4-*d*]pyrimidines as Antagonists of the Human Chemokine Receptor CXCR2

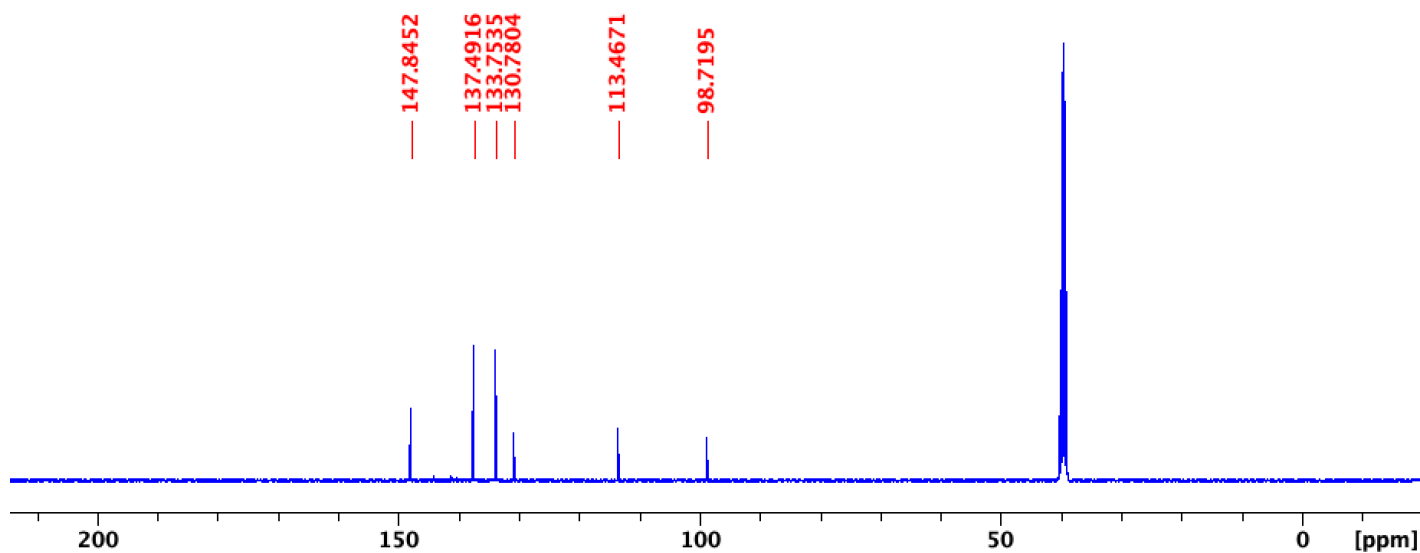
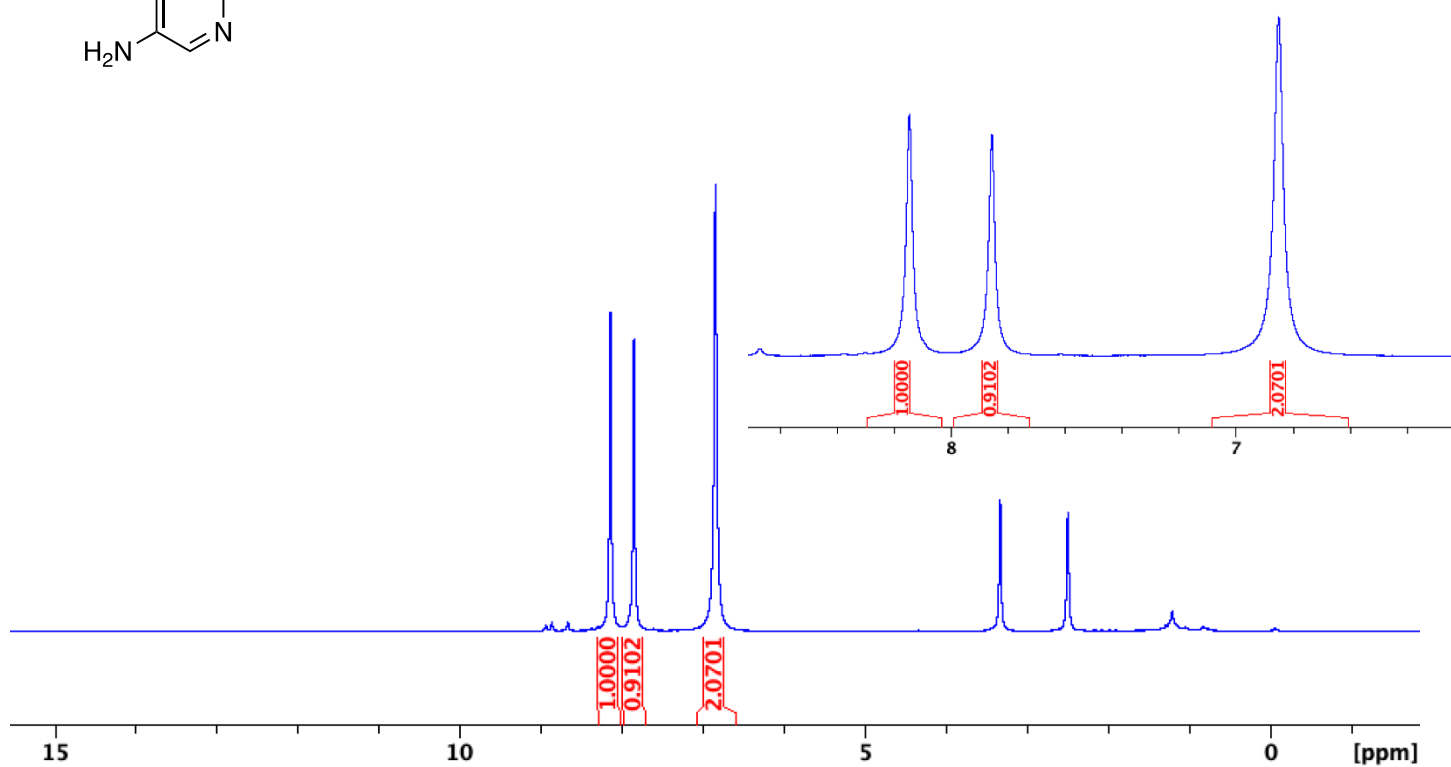
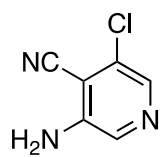
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¹ Molecular Design and Synthesis, Department of Chemistry, KU Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium

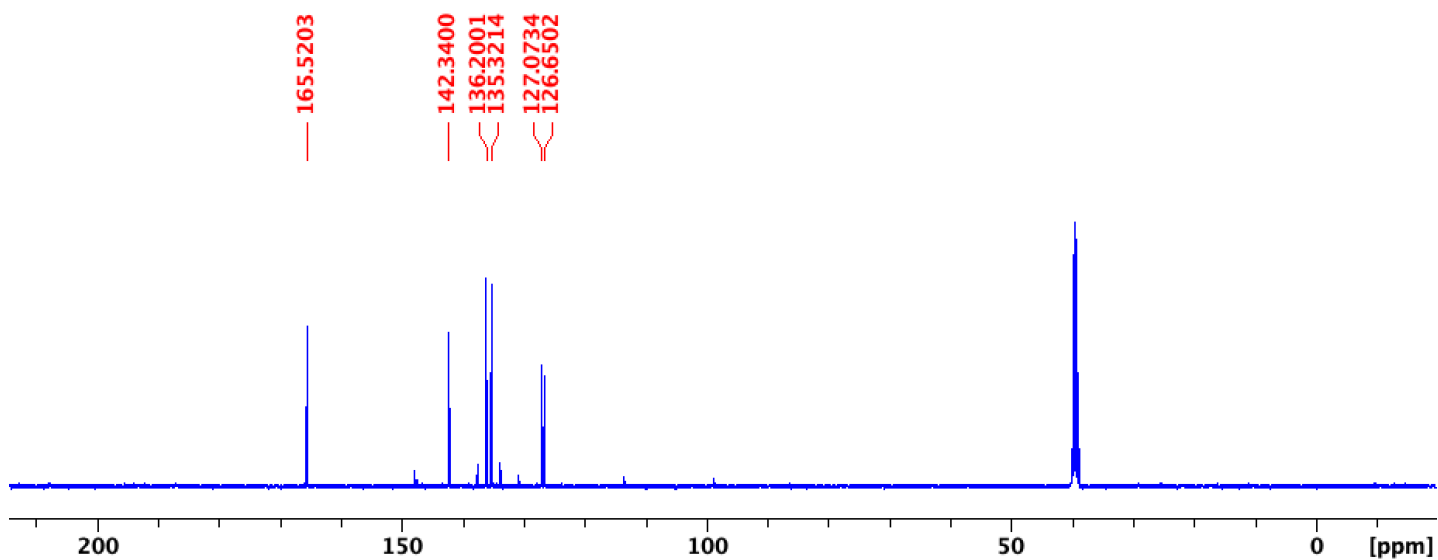
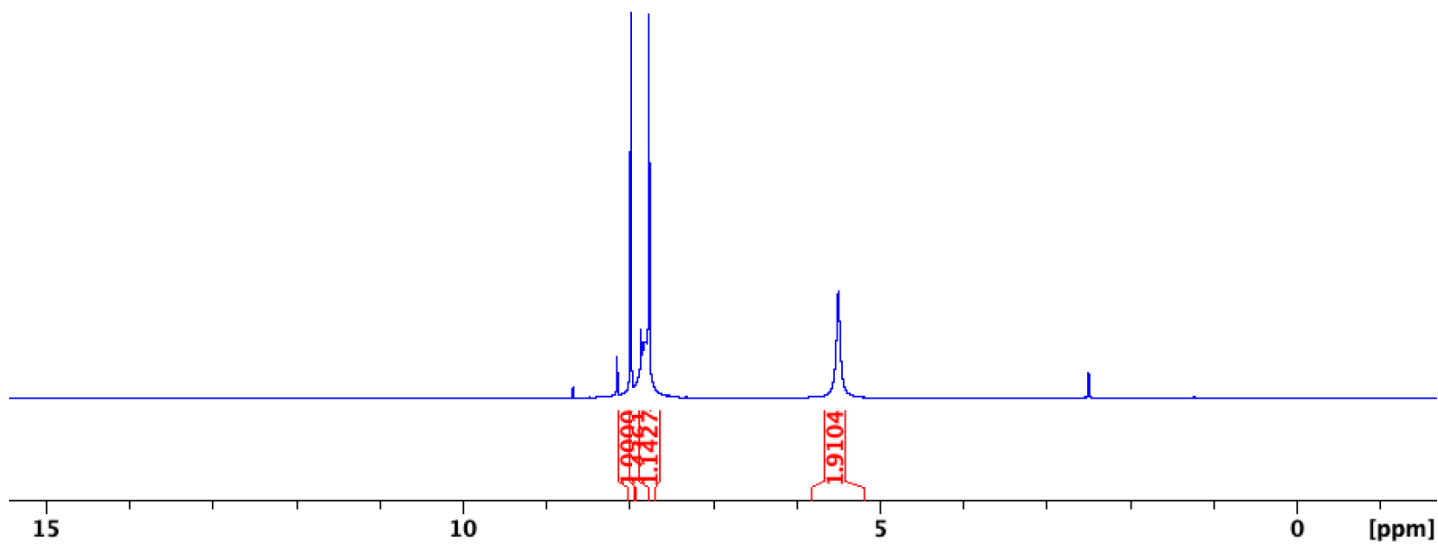
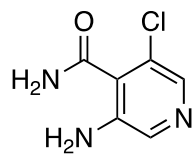
² Department of Microbiology, Immunology and Transplantation, Rega Institute for Medical Research, Laboratory of Virology and Chemotherapy, KU Leuven, Herestraat 49, B-3000 Leuven, Belgium

NMR Spectra

3-Amino-5-chloropyridine-4-carbonitrile (5)



3-Amino-5-chloropyridine-4-carboxamide (6)

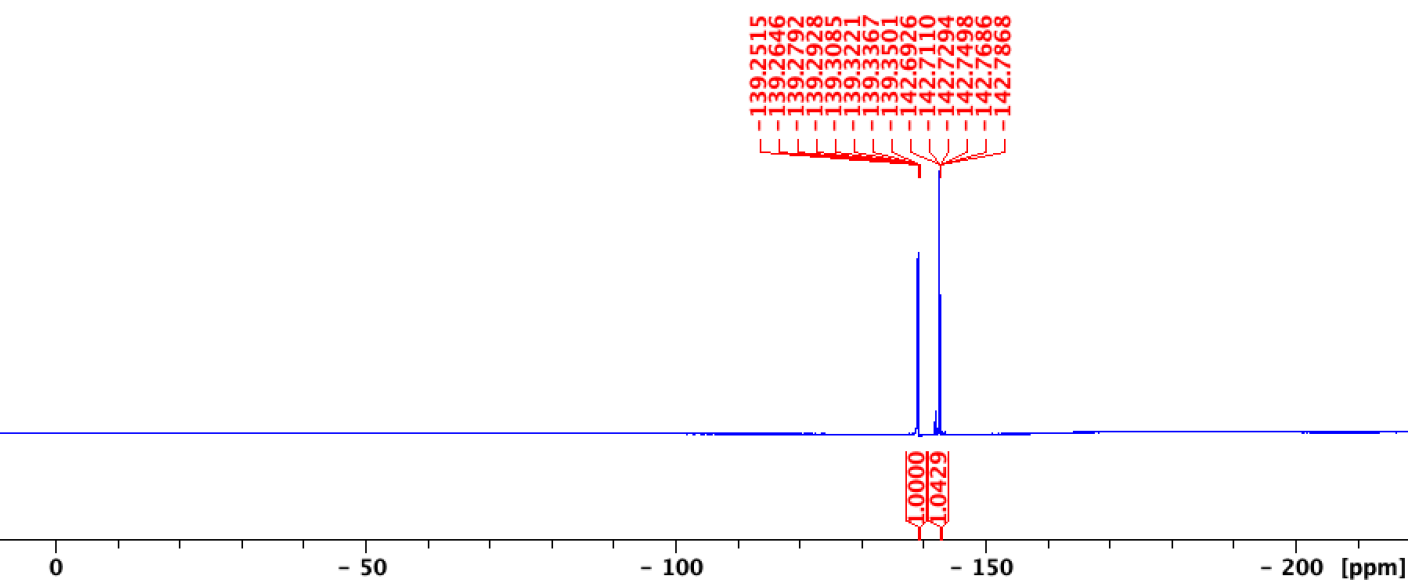
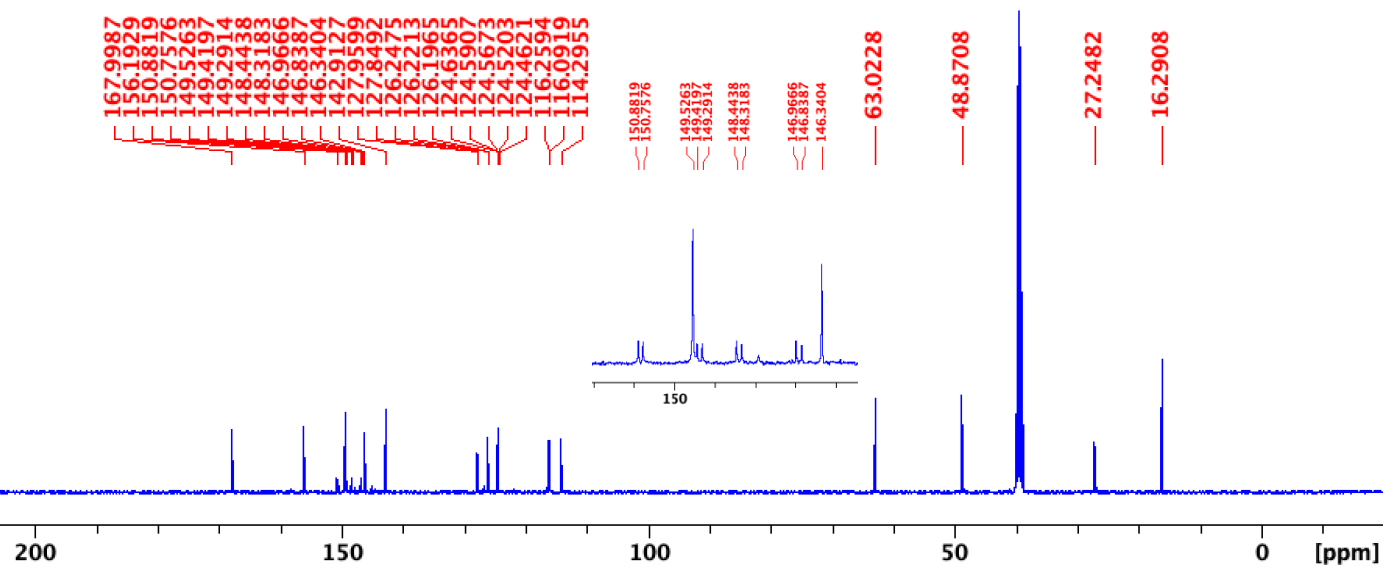


2-(2,3-Difluorobenzylmercapto)-5-chloropyrido[3,4-*d*]pyrimidine-4-one (8)

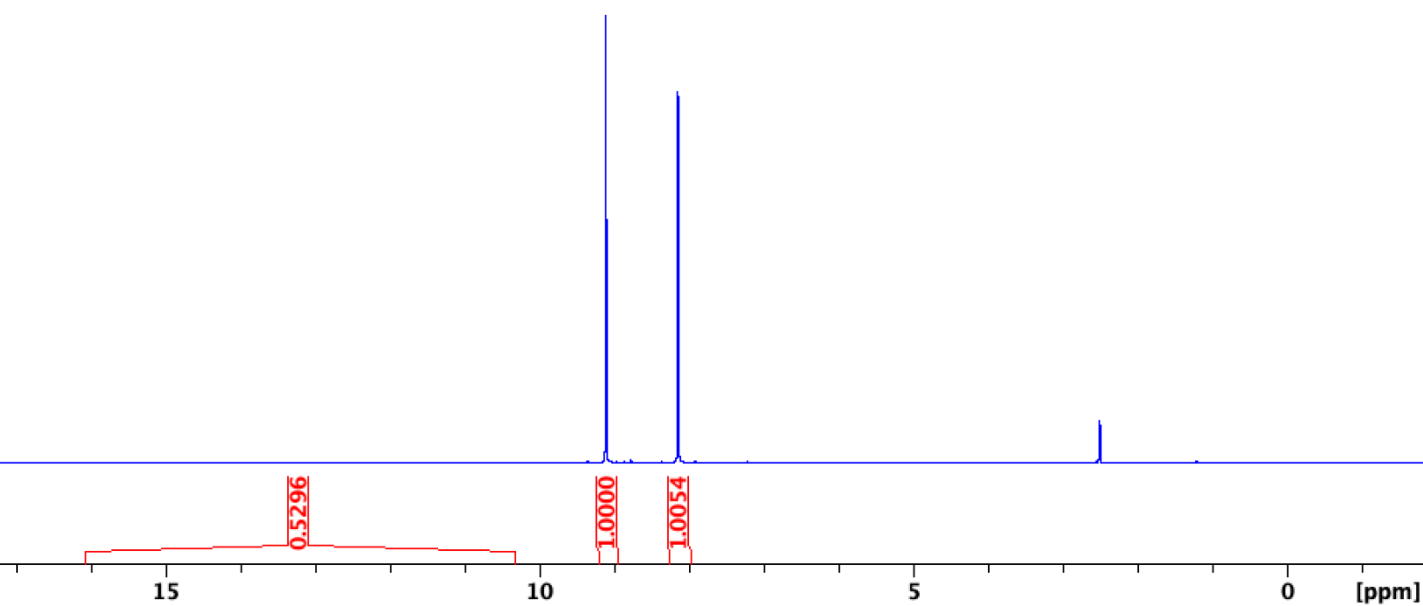
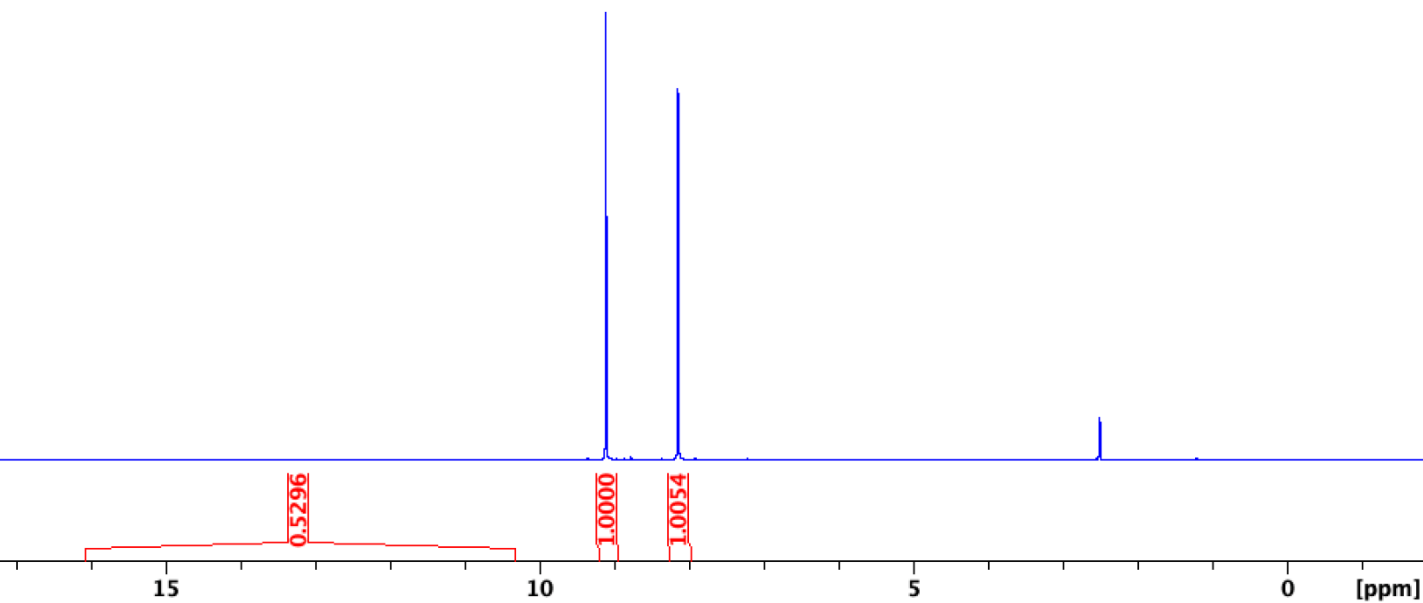


(2R)-2-[(5-Chloro-2-(2,3-difluorobenzylmercapto)-pyrido[3,4-*d*]pyrimidine-4-yl)amino]propanol (9)

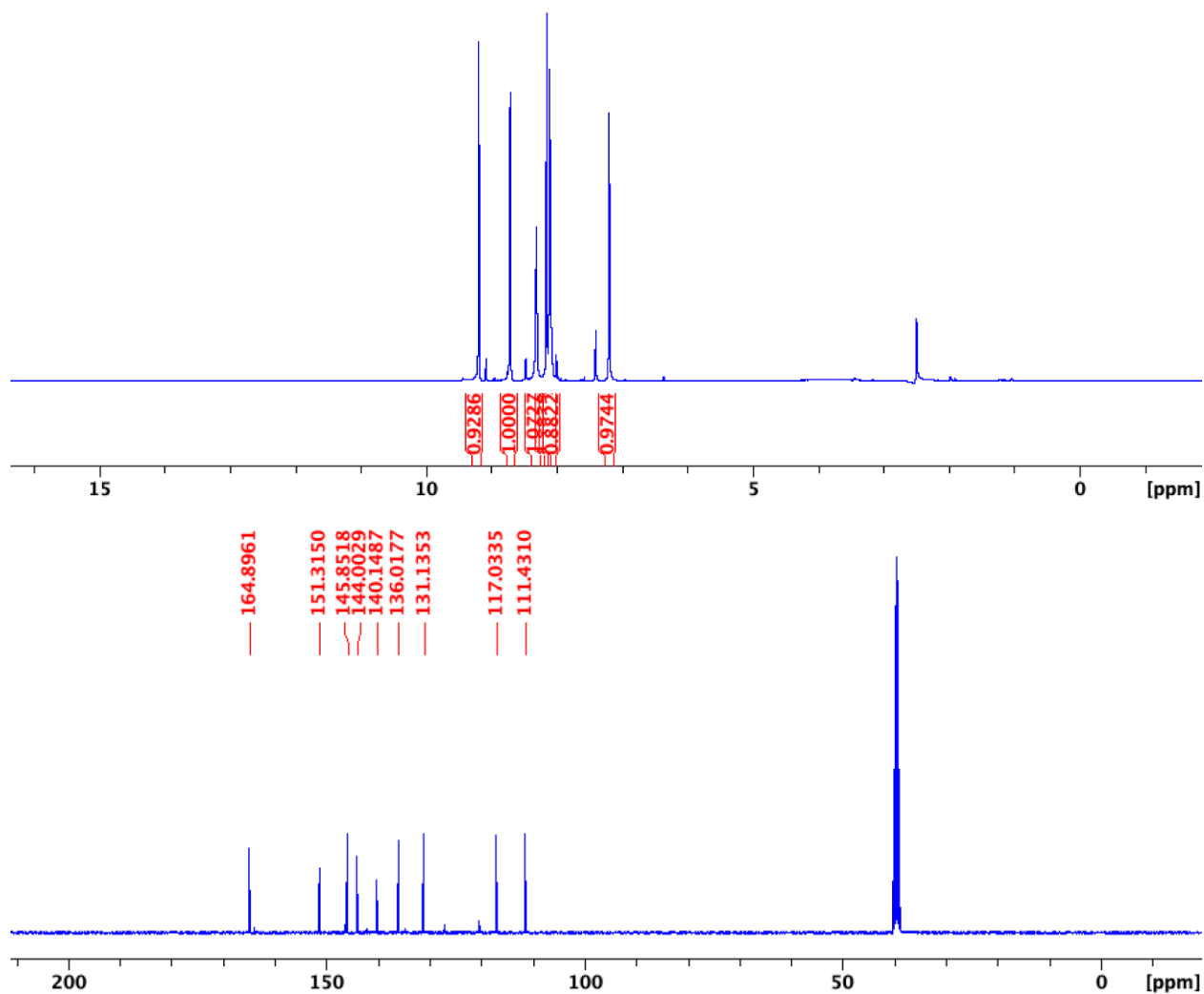
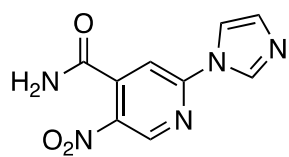




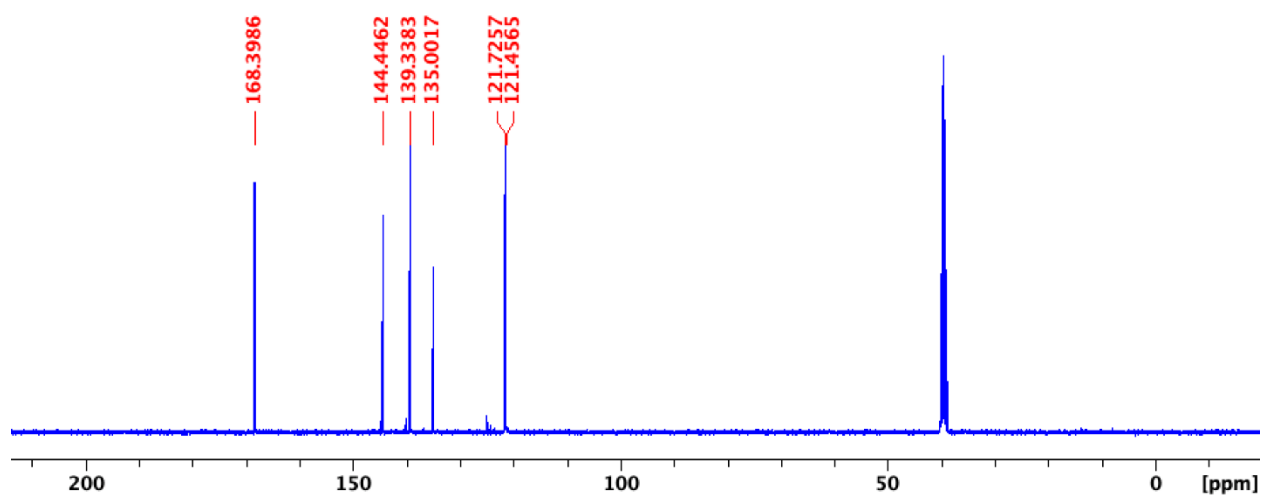
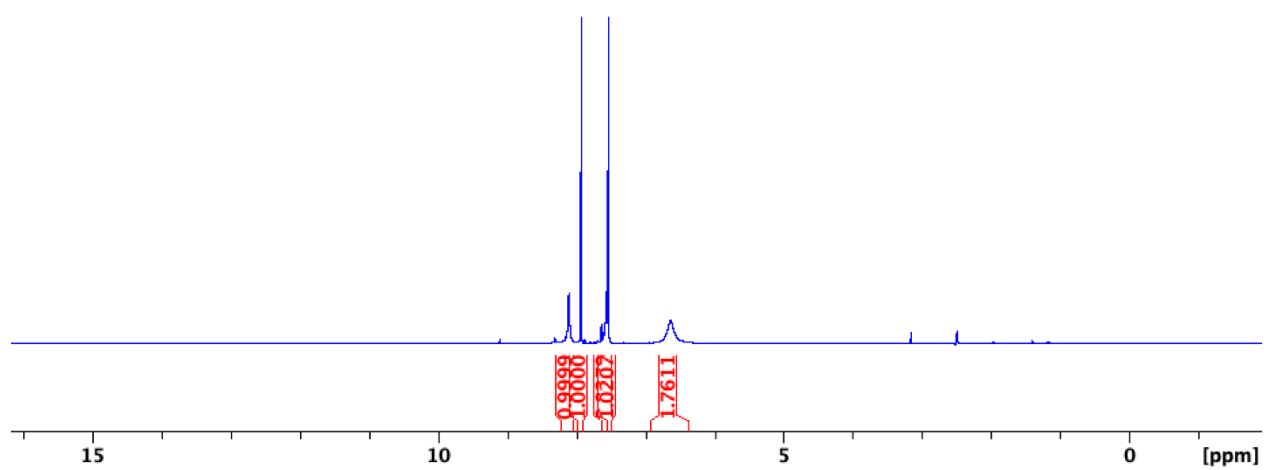
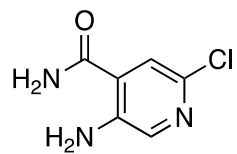
2-Bromo-5-nitropyridine-4-carboxylic acid (11)



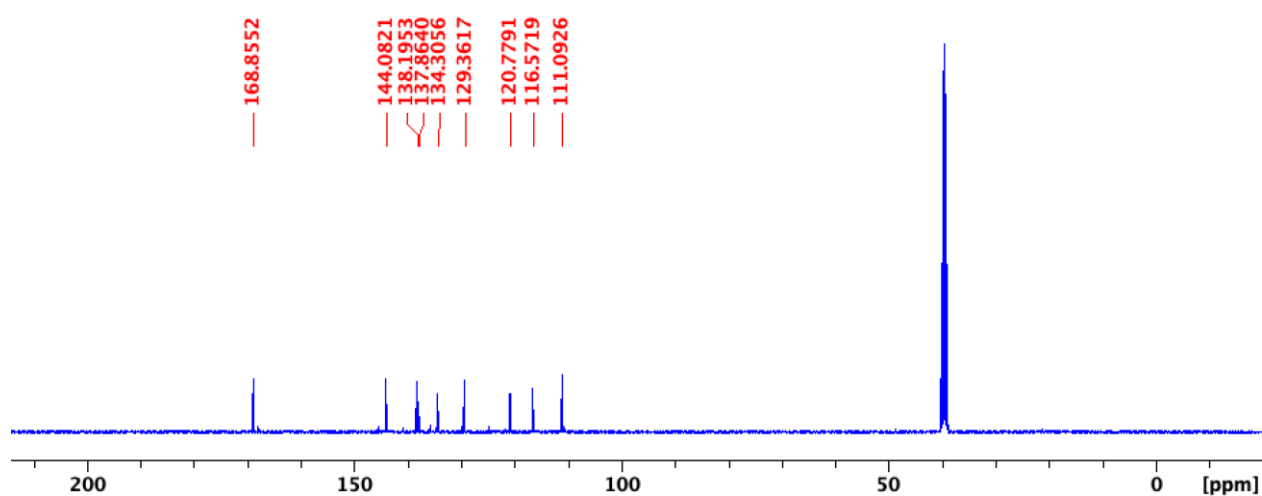
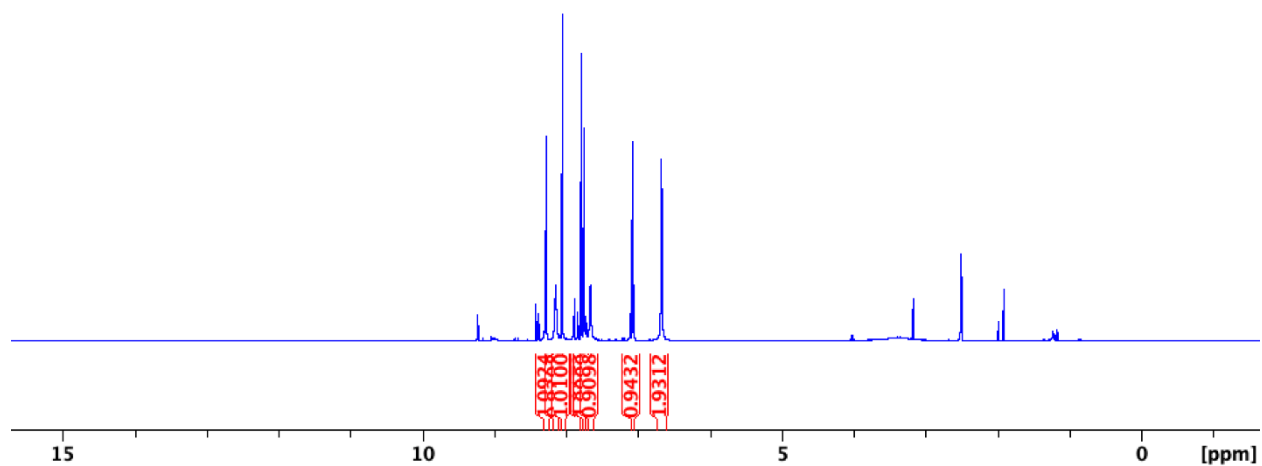
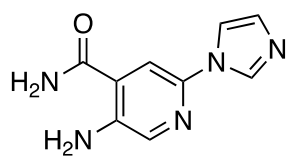
2-Imidazolyl-5-nitropyridine-4-carboxamide (12b)



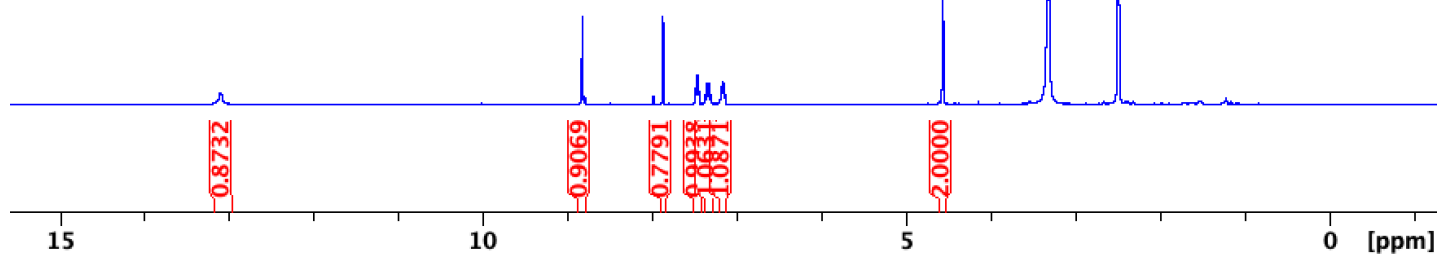
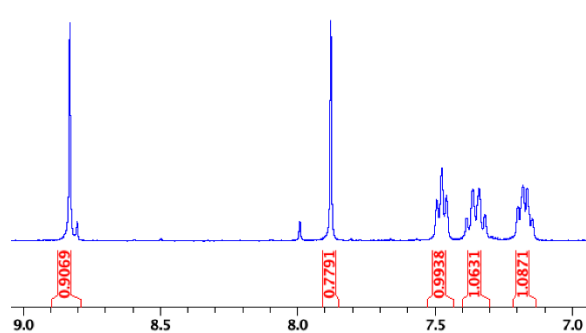
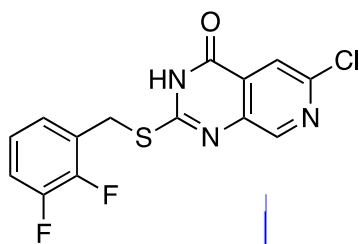
2-Chloro-5-aminopyridine-4-carboxamide (13a)



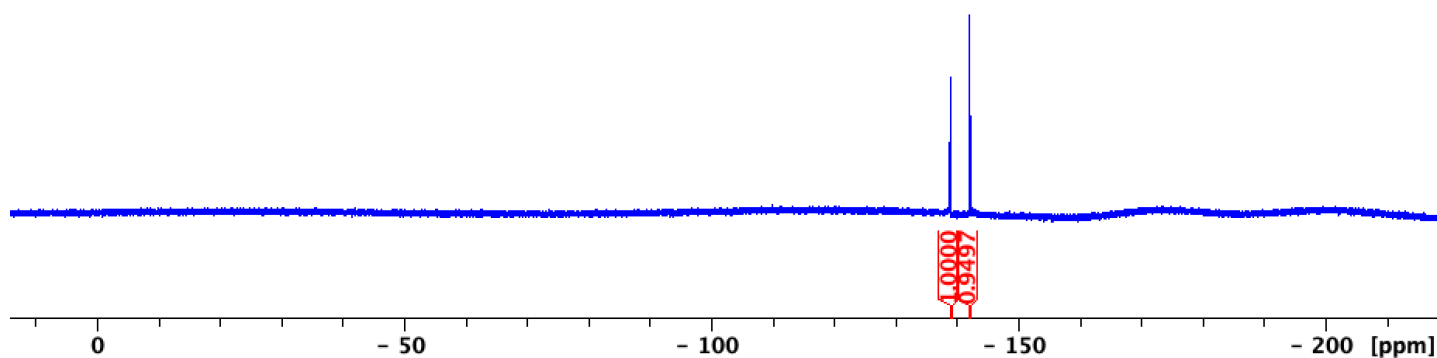
5-Amino-2-imidazolyl-pyridine-4-carboxamide (13b)



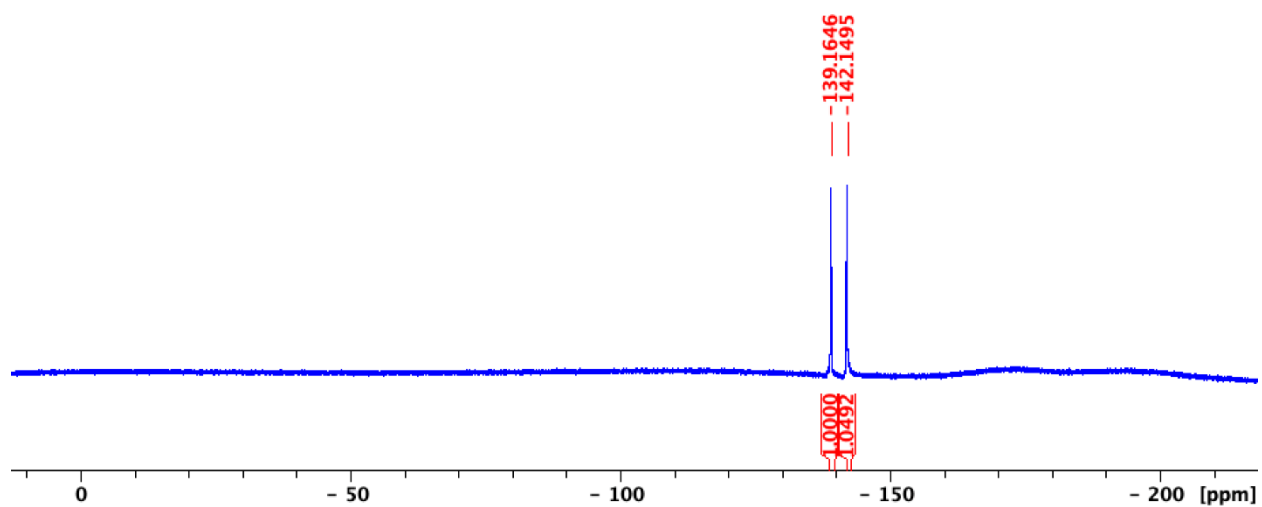
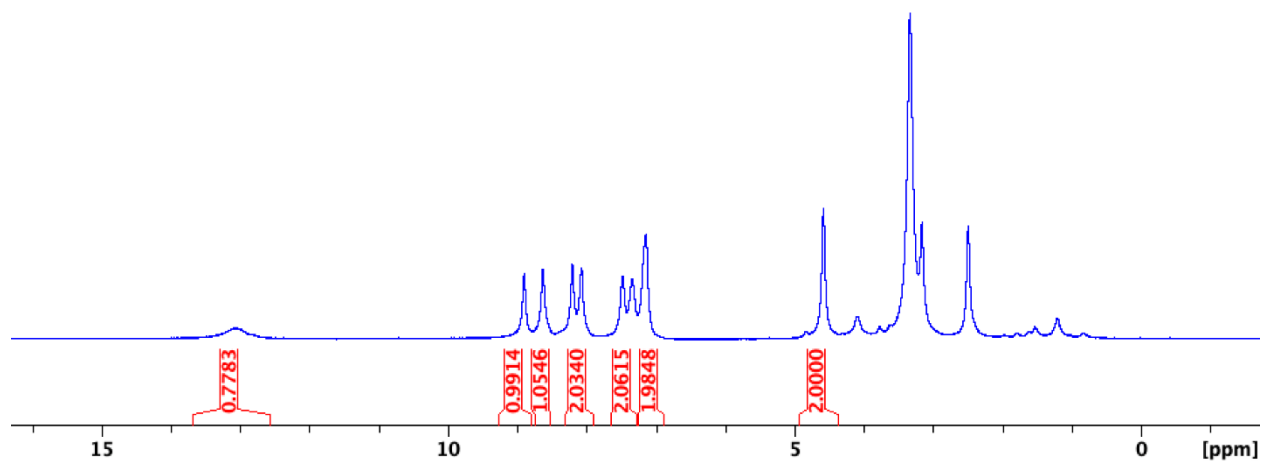
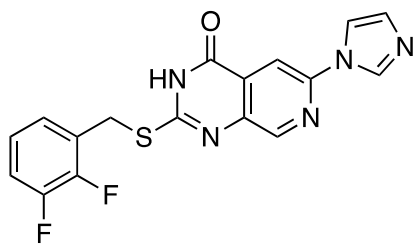
2-(2,3-Difluorobenzylmercapto)-6-chloropyrido[3,4-*d*]pyrimidine-4-one (15a)



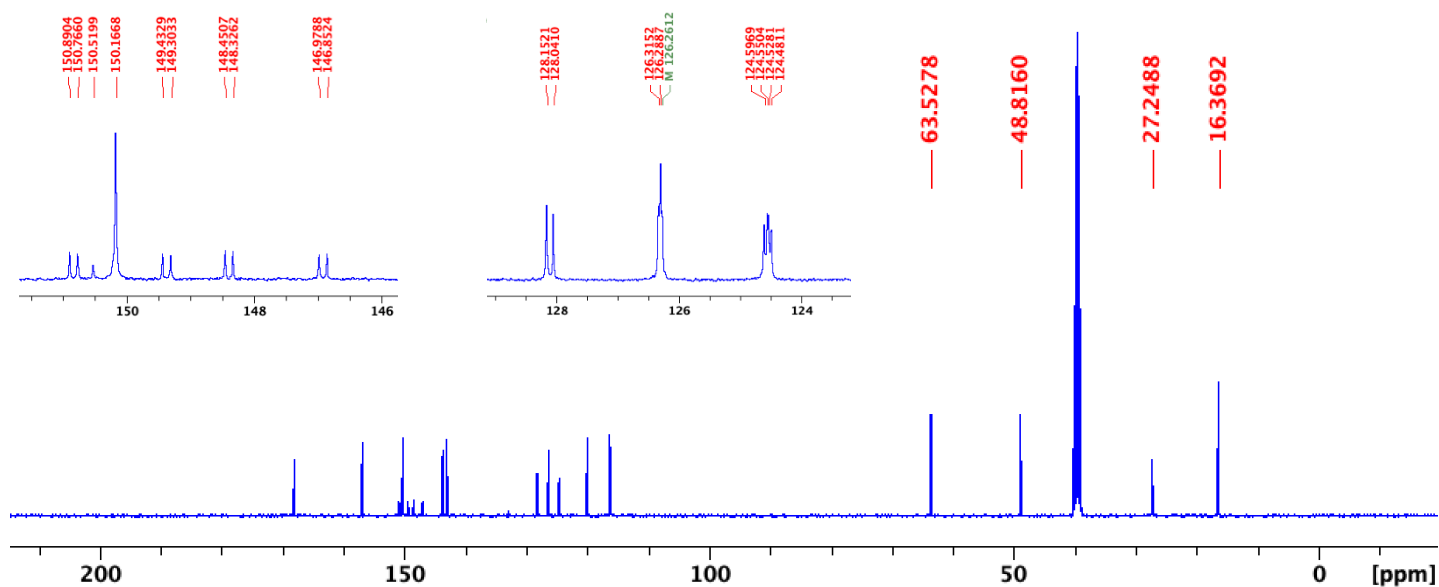
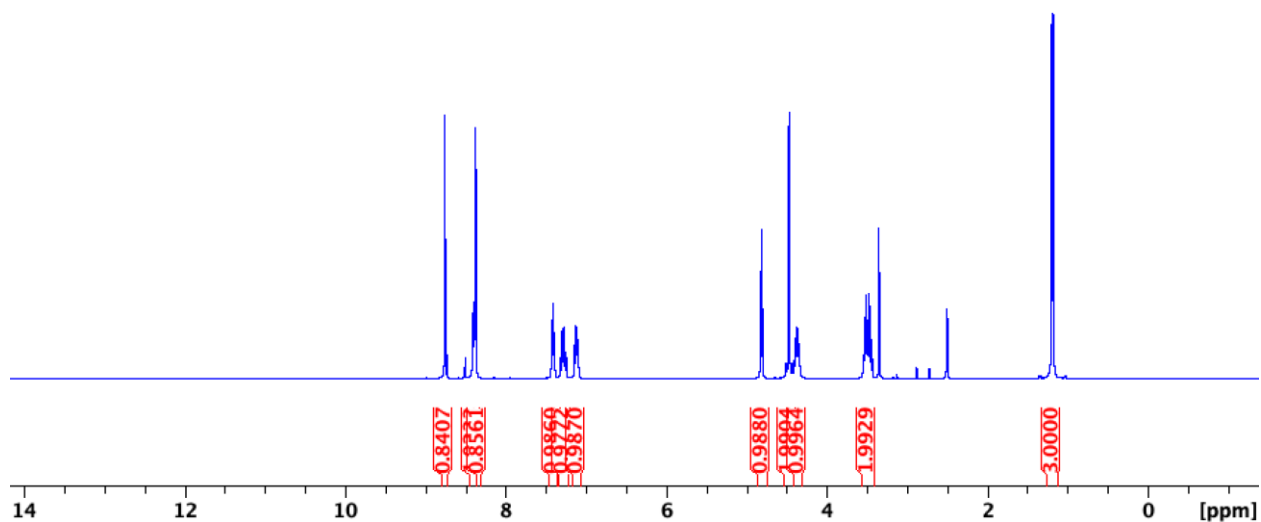
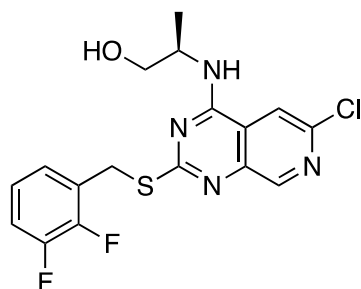
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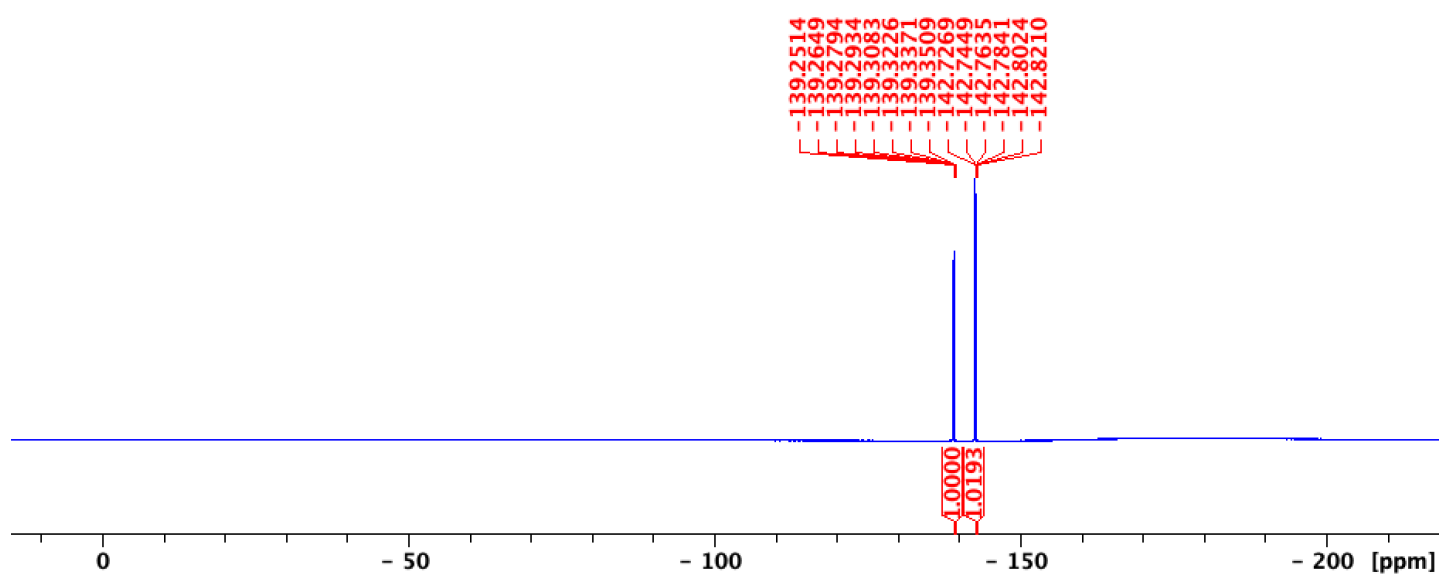


2-(2,3-Difluorobenzylthio)-6-imidazolyl-pyrido[3,4-*d*]pyrimidine-4-one (15b)

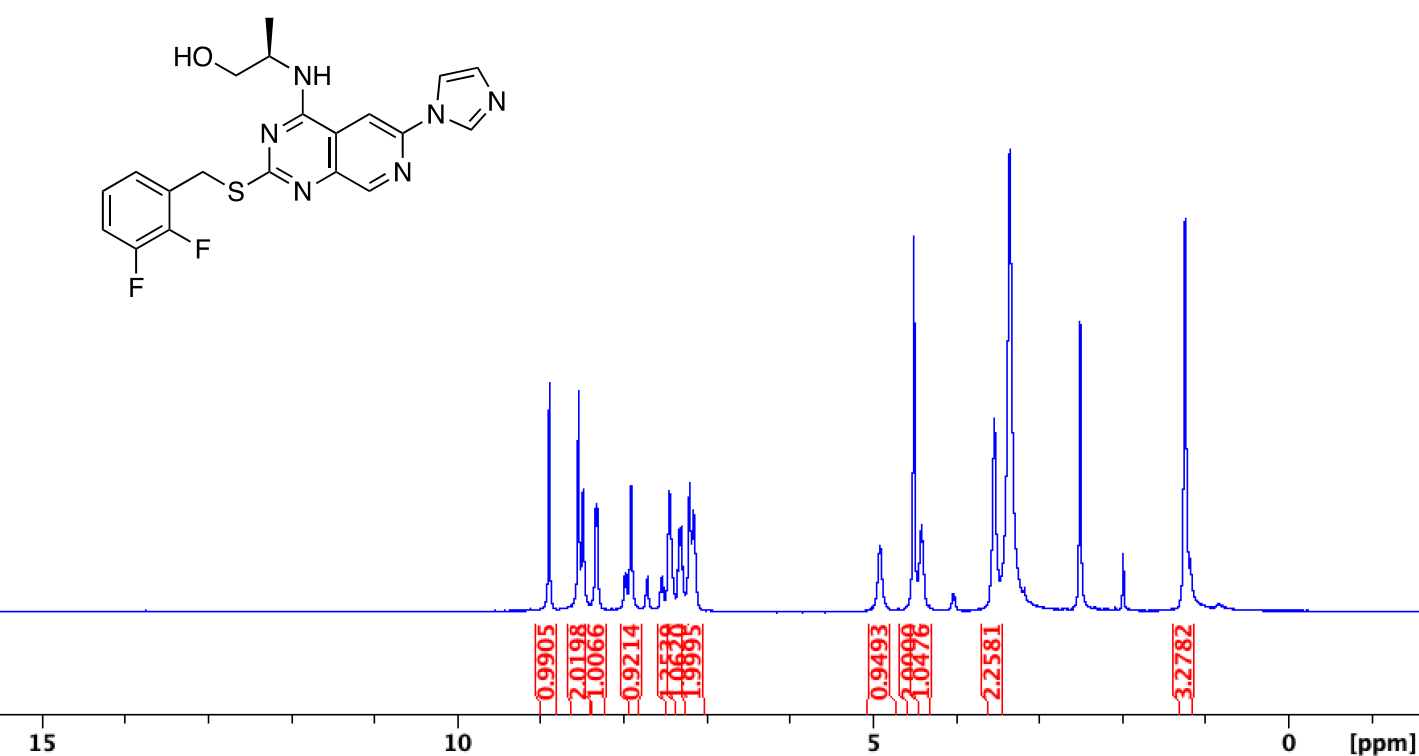


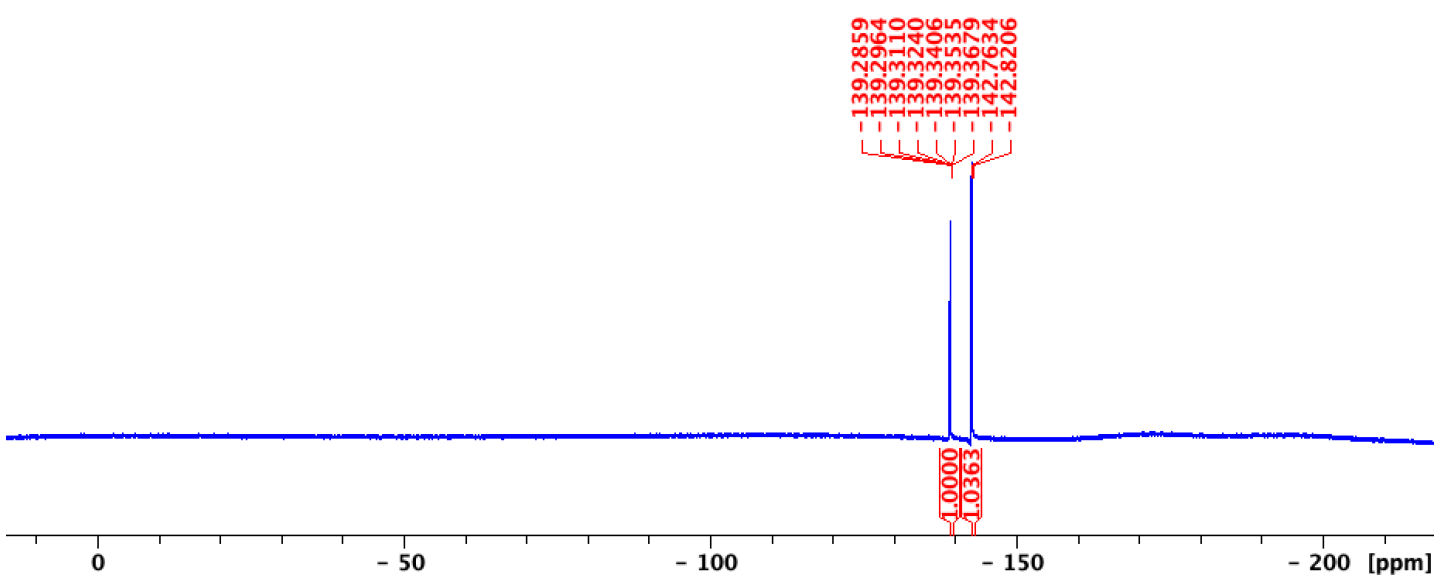
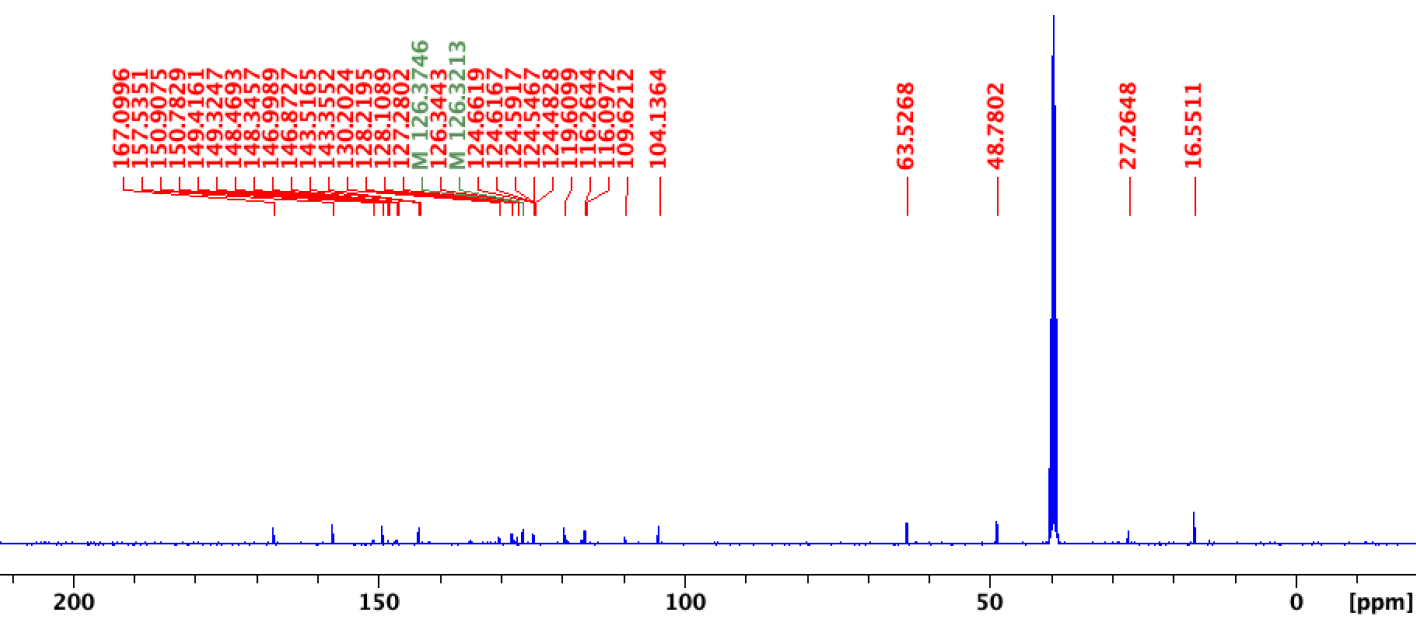
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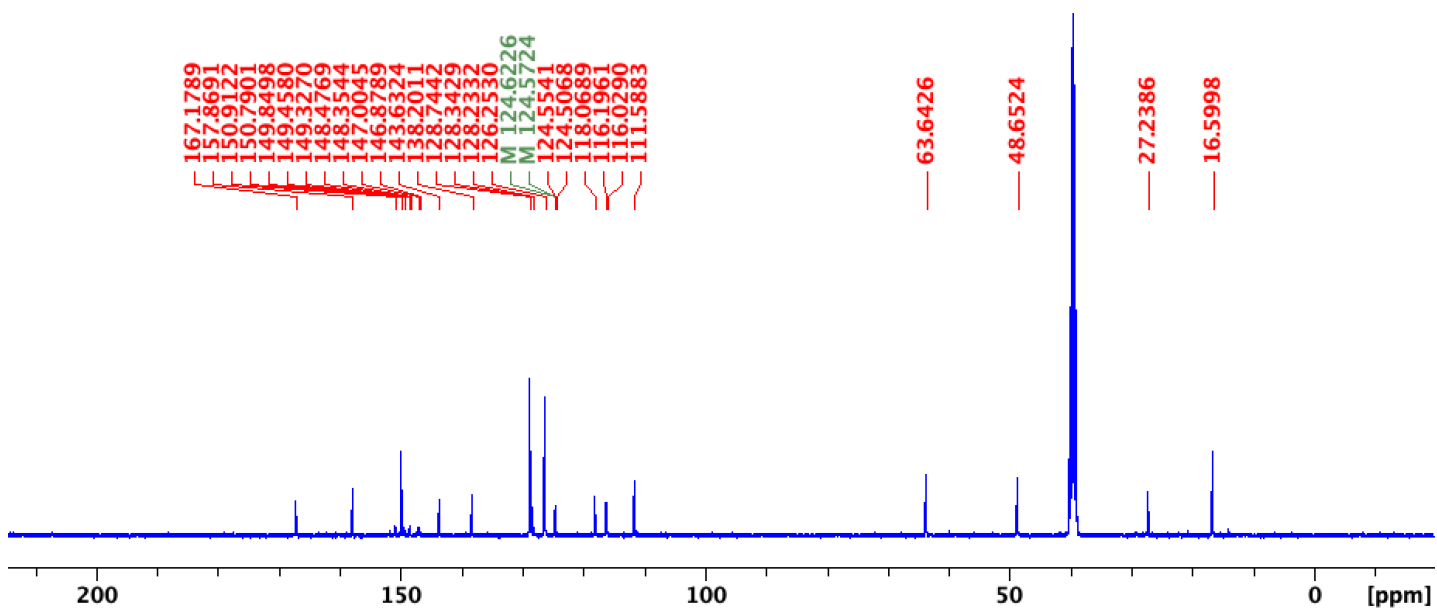
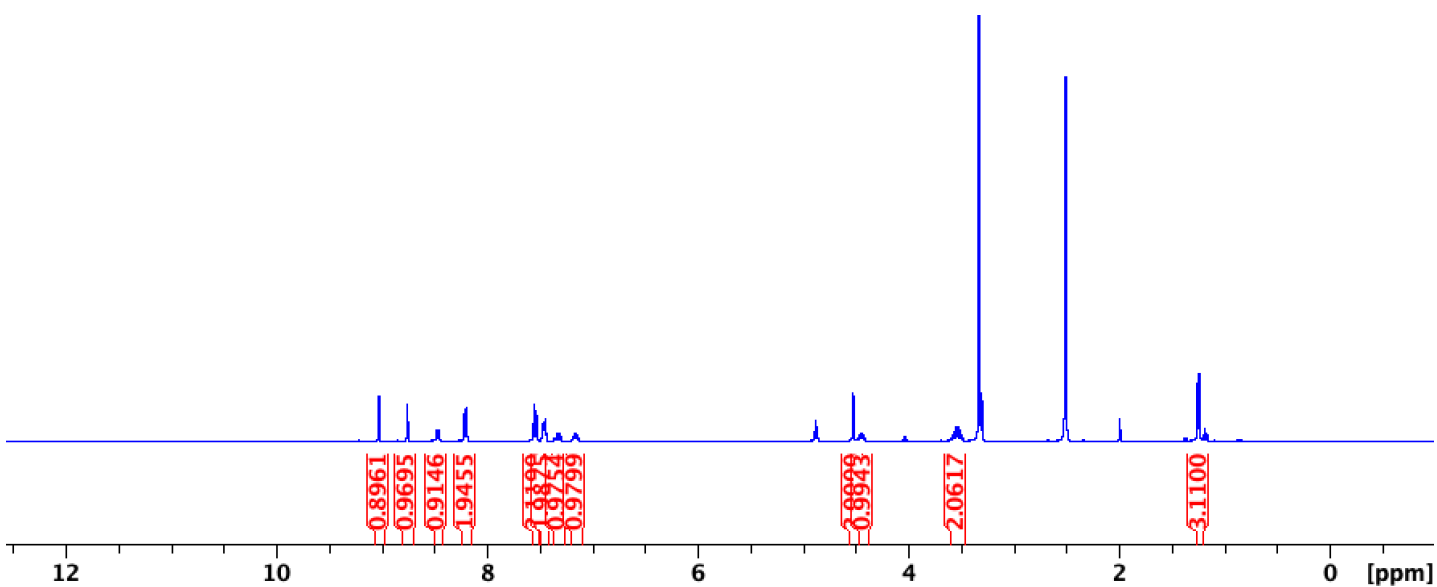
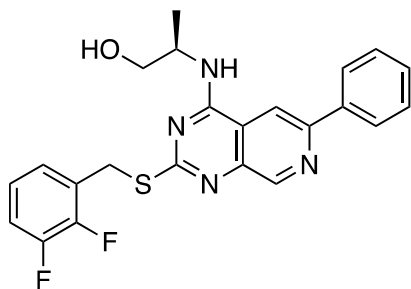


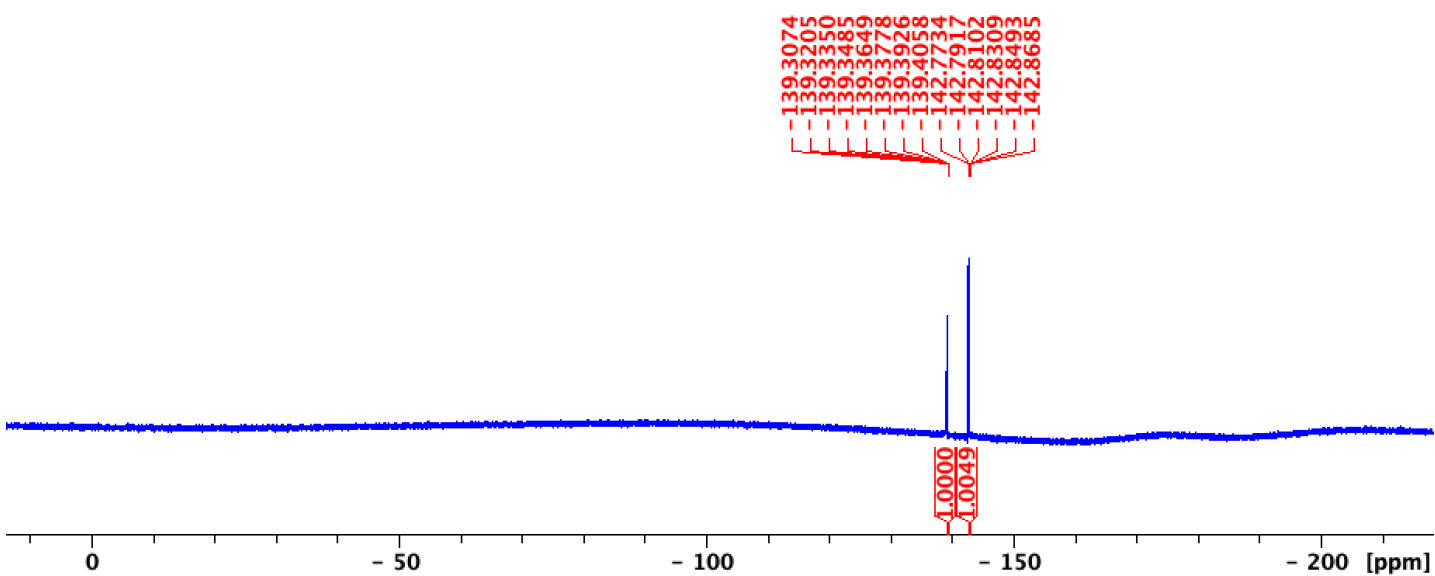
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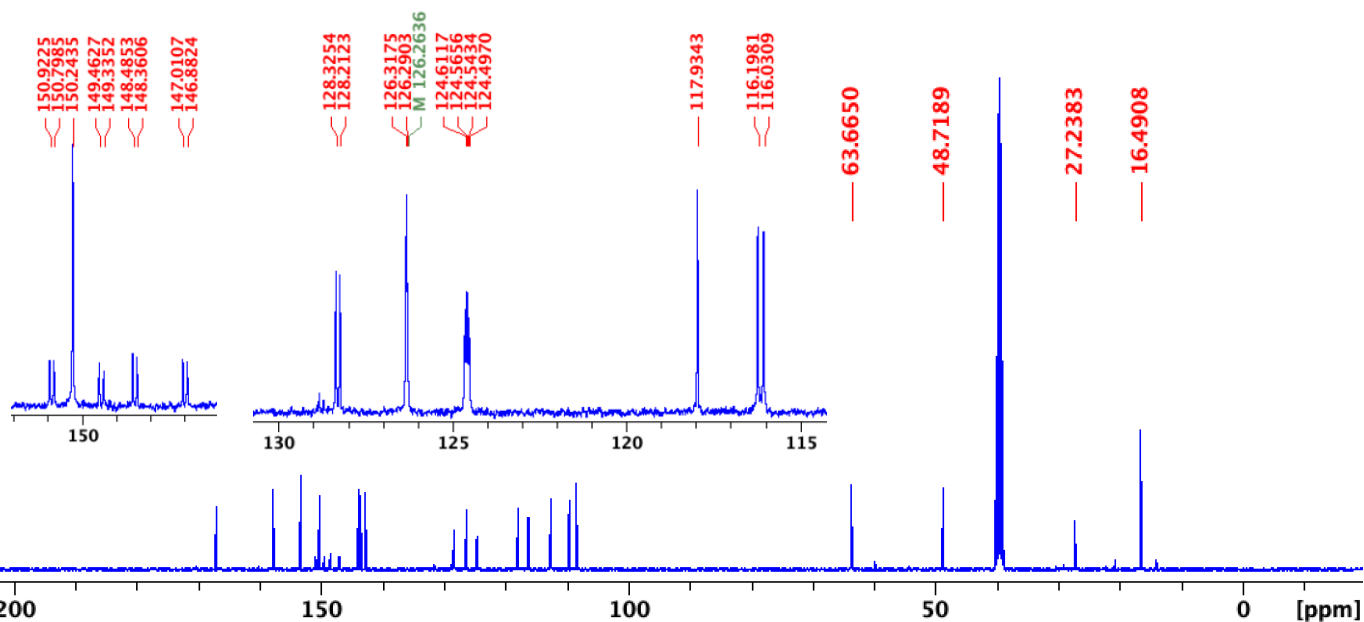
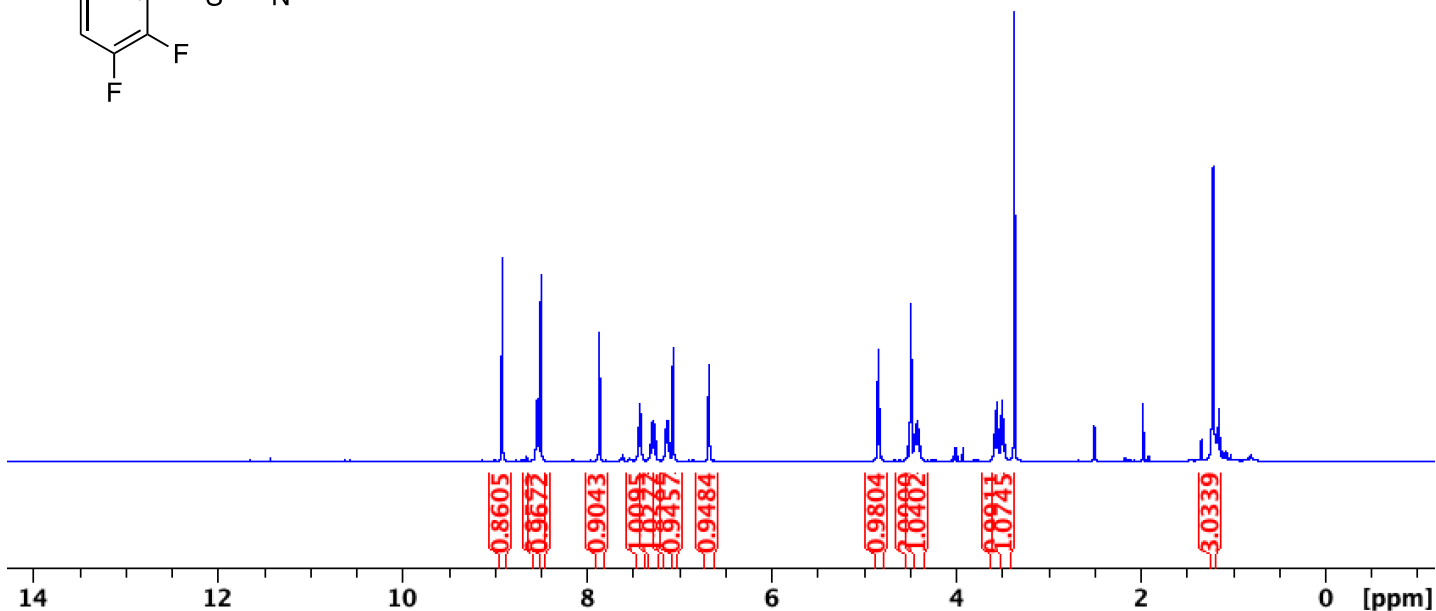
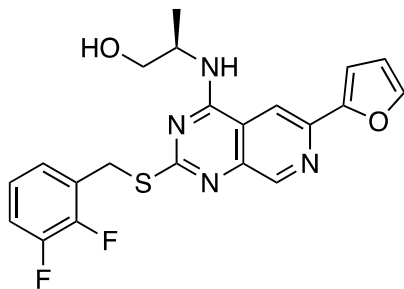


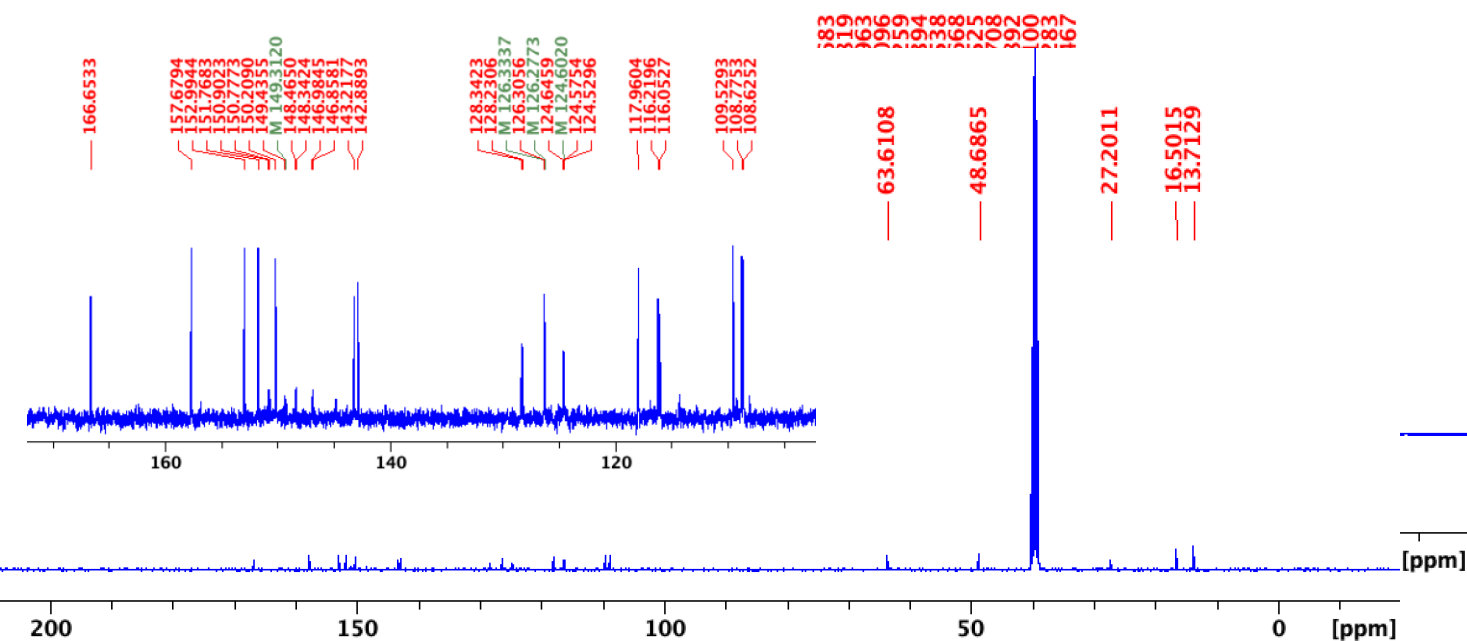
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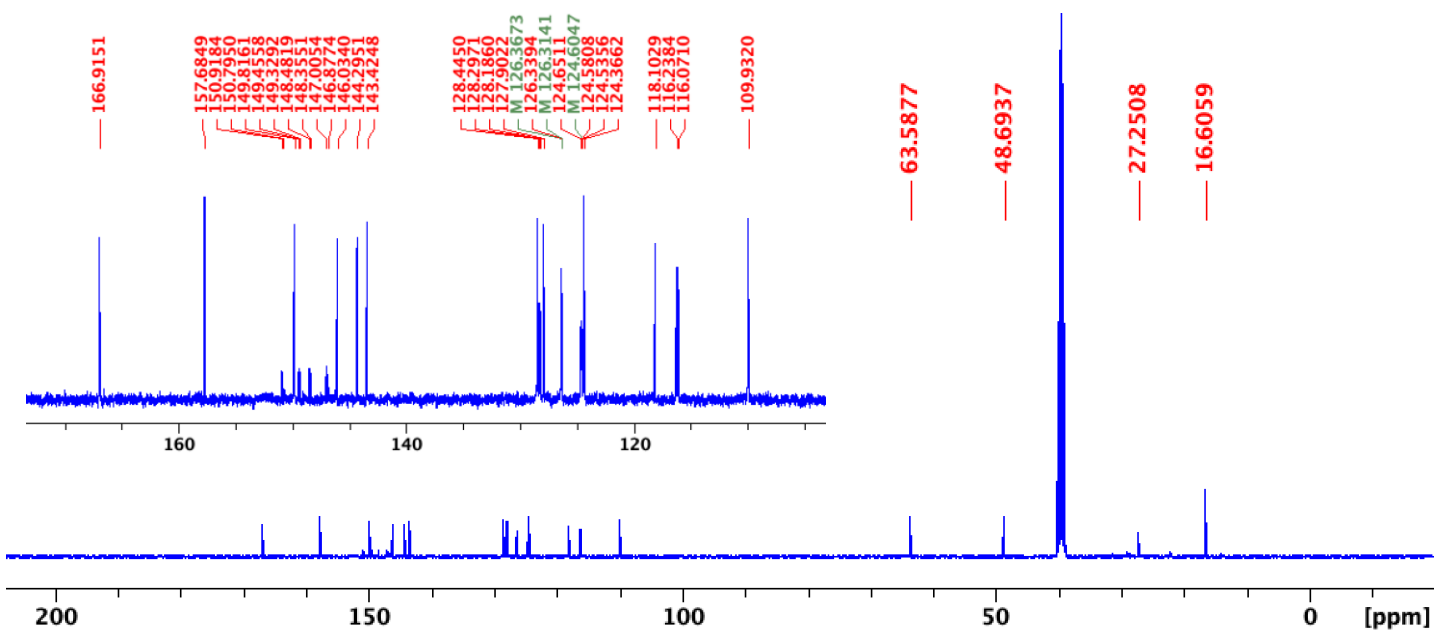
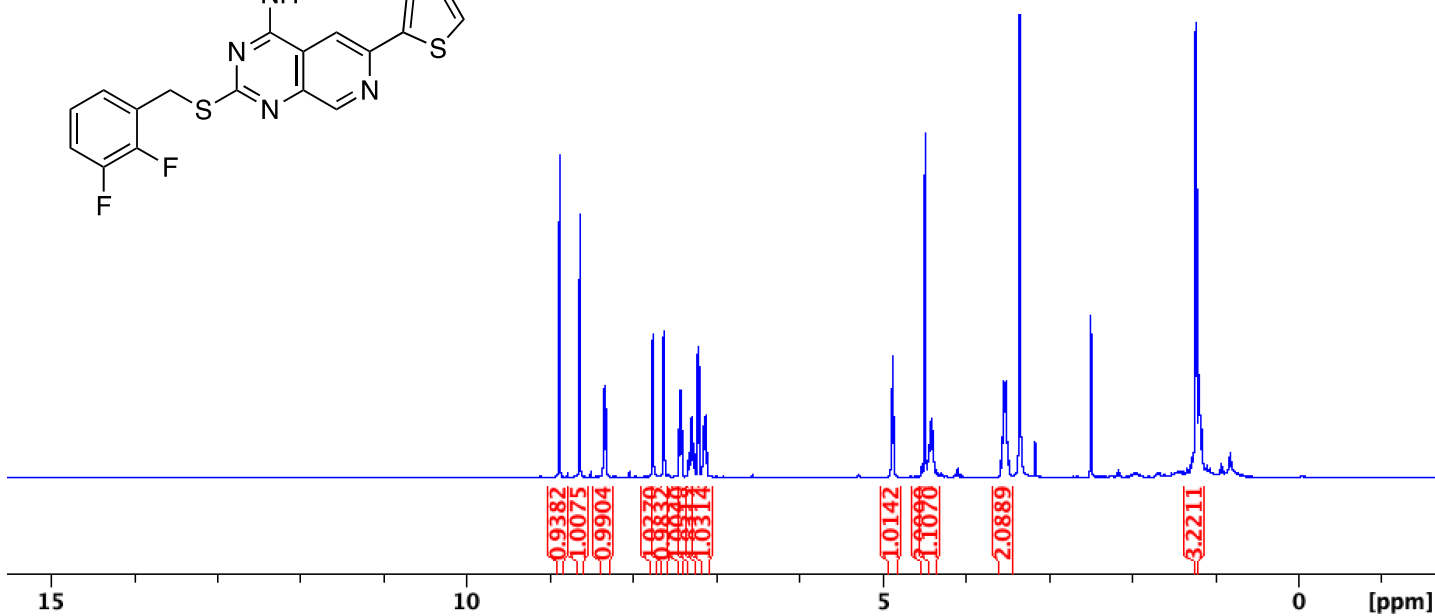
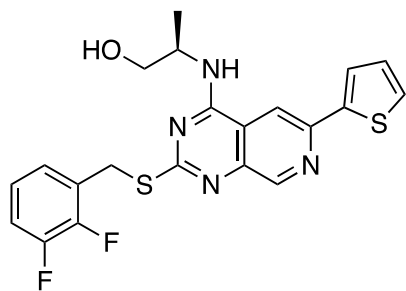


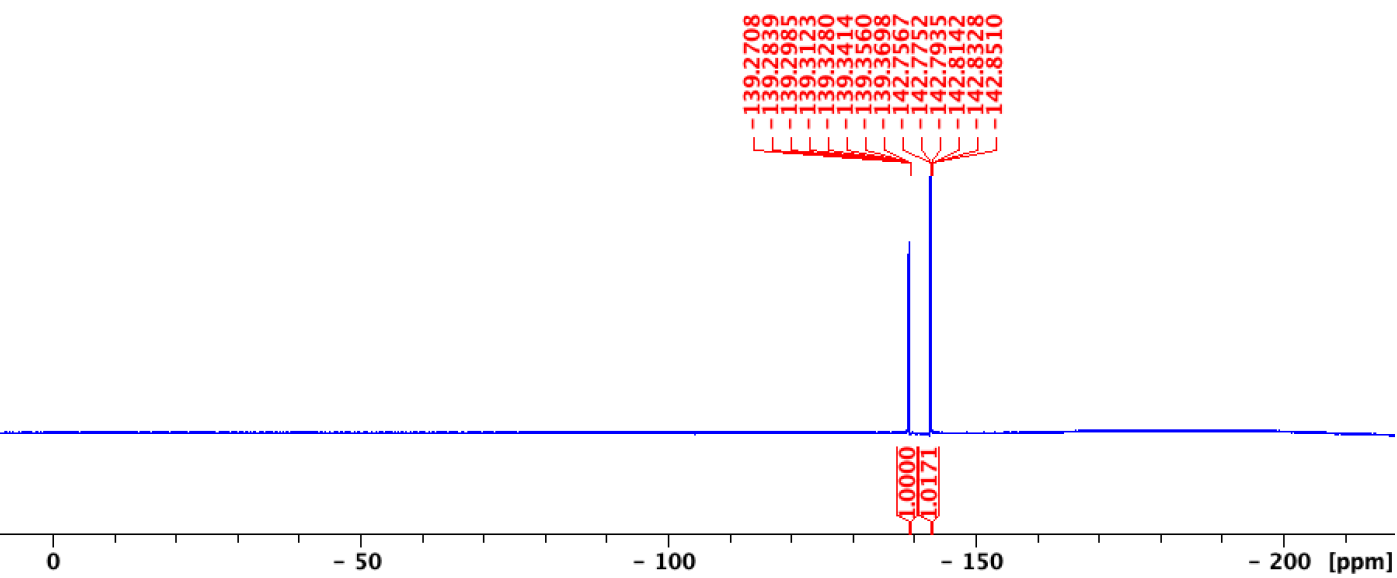
(2*R*)-2-[(2-(2,3-Difluorobenzylmercapto)-6-(2-furanyl)-pyrido[3,4-*d*]pyrimidine-4-yl)amino]propanol (17b)



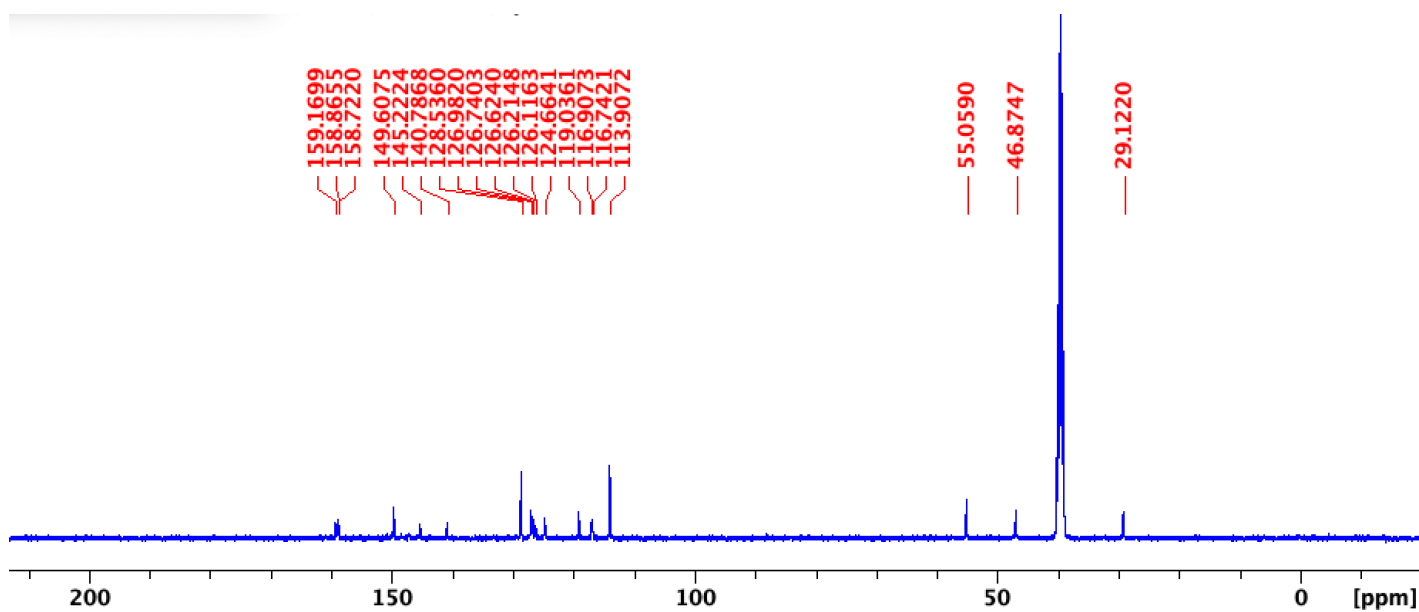
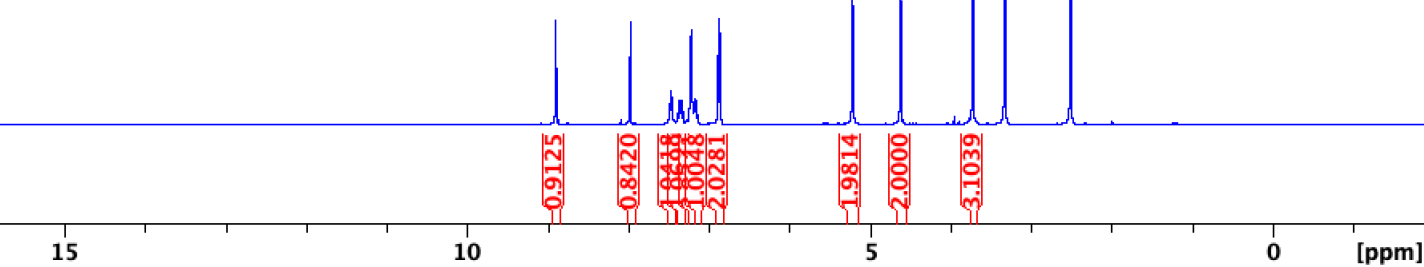
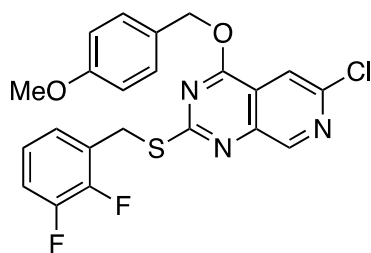


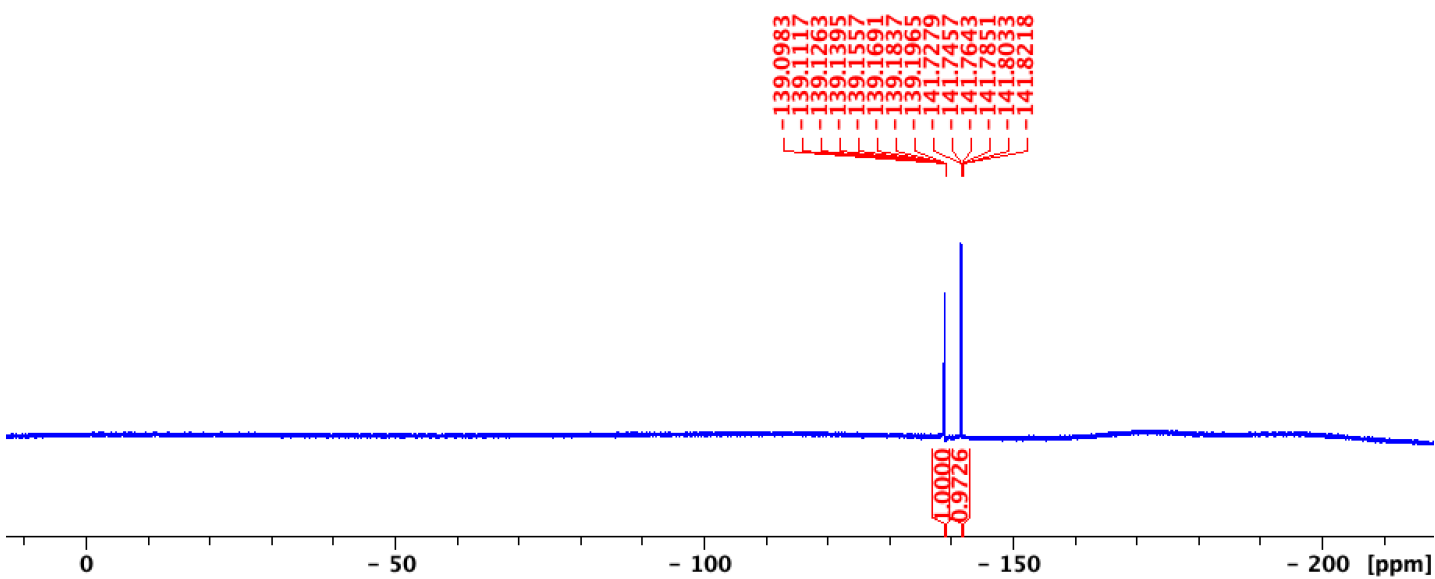
(2*R*)-2-[(2-(2,3-Difluorobenzylmercapto)-6-(2-thienyl)-pyrido[3,4-*d*]pyrimidine-4-yl)amino]propanol (17d)



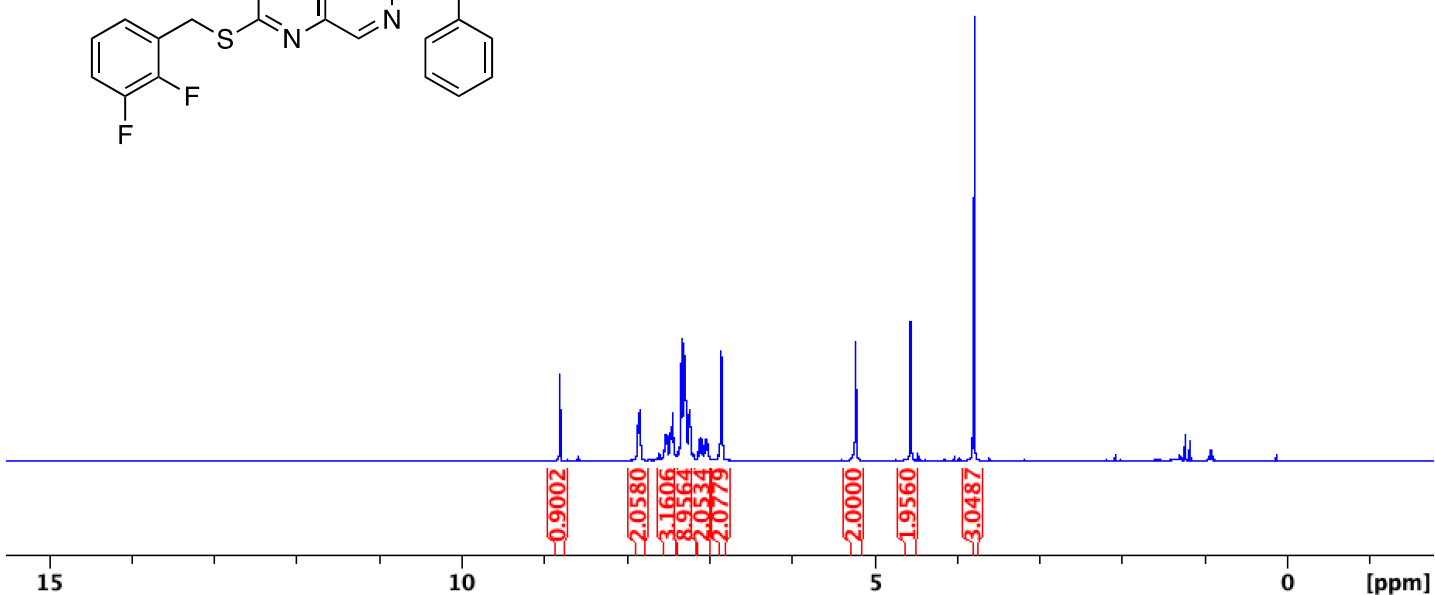
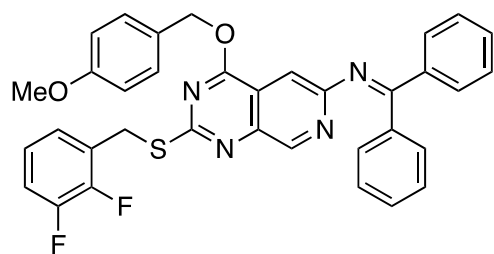


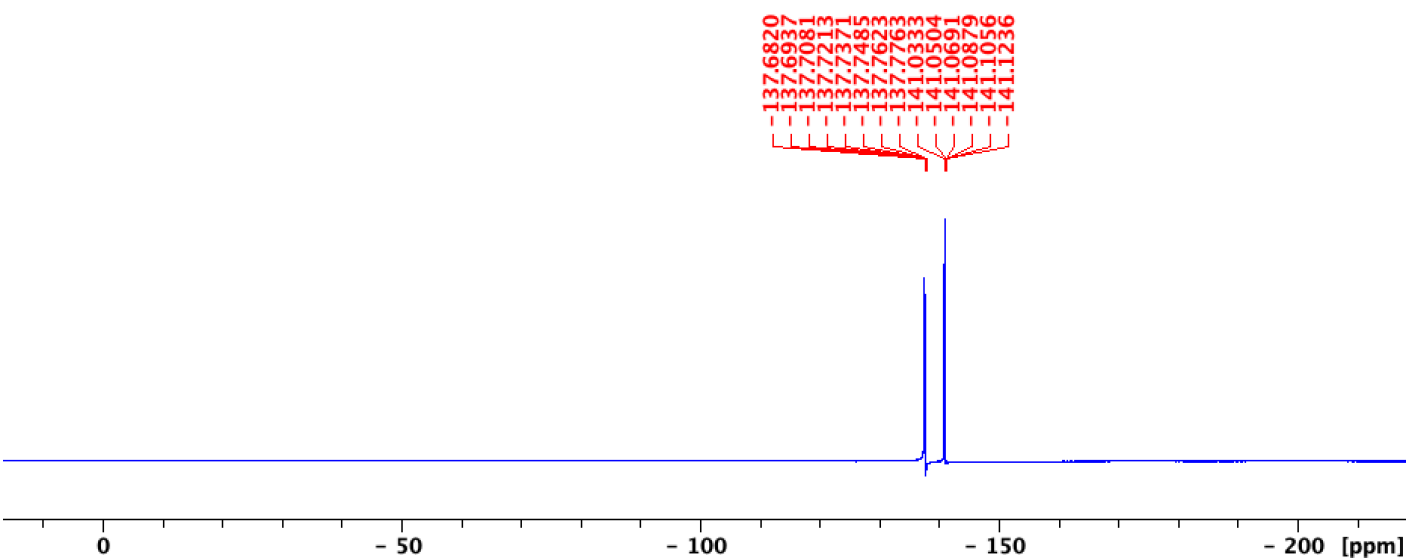
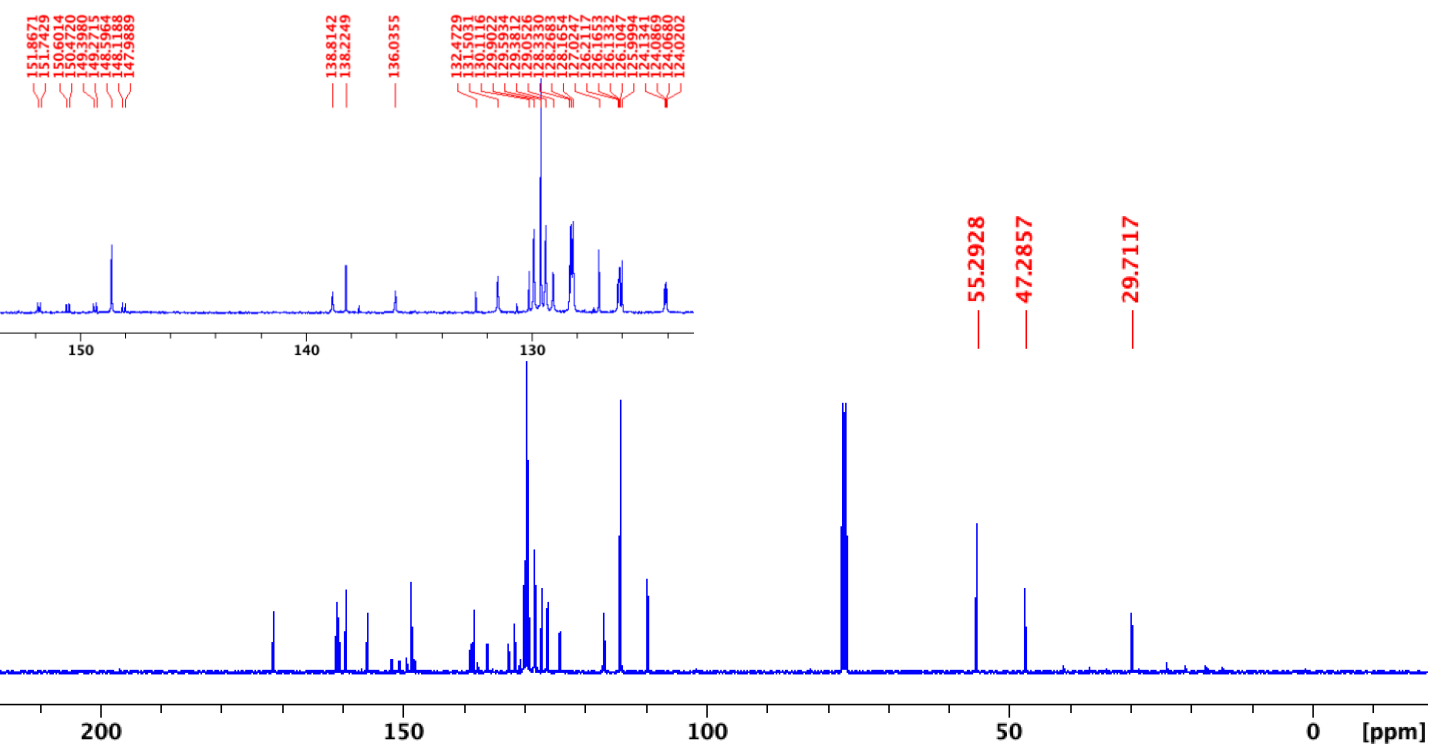
6-Chloro-2-(2,3-difluorobenzylmercapto)-4-(4-methoxybenzyl)-pyrido[3,4-*d*]pyrimidine (18)



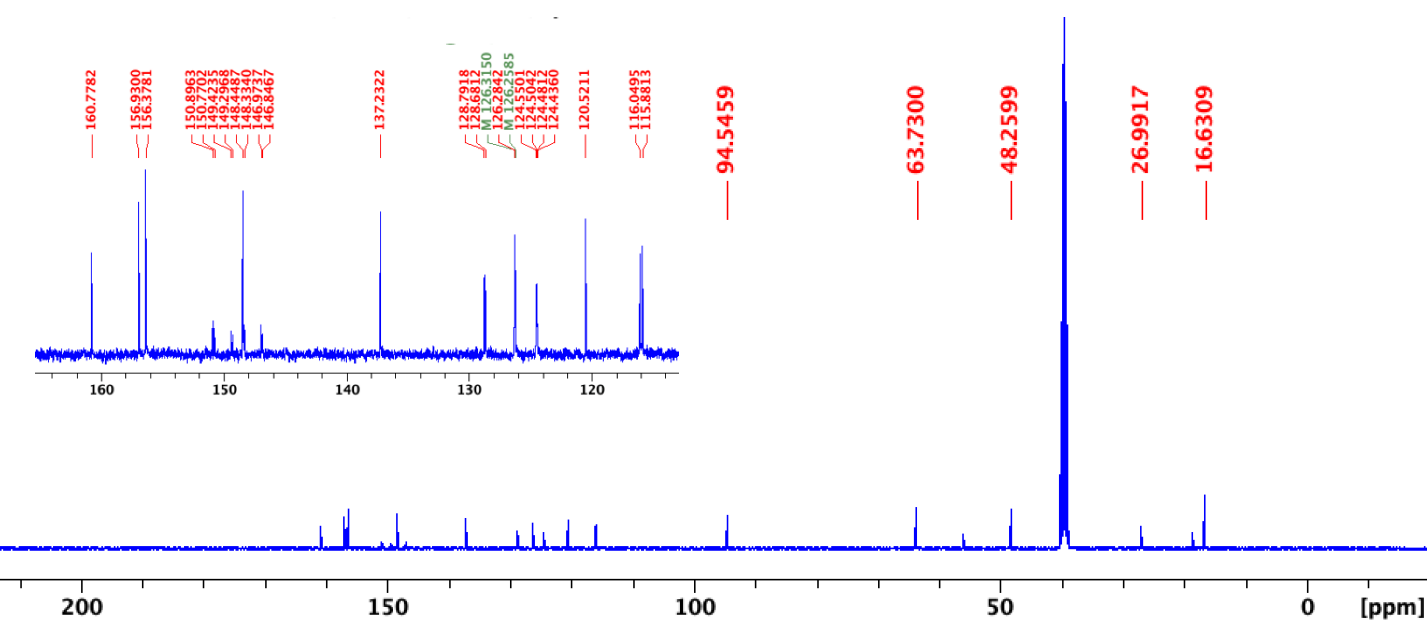
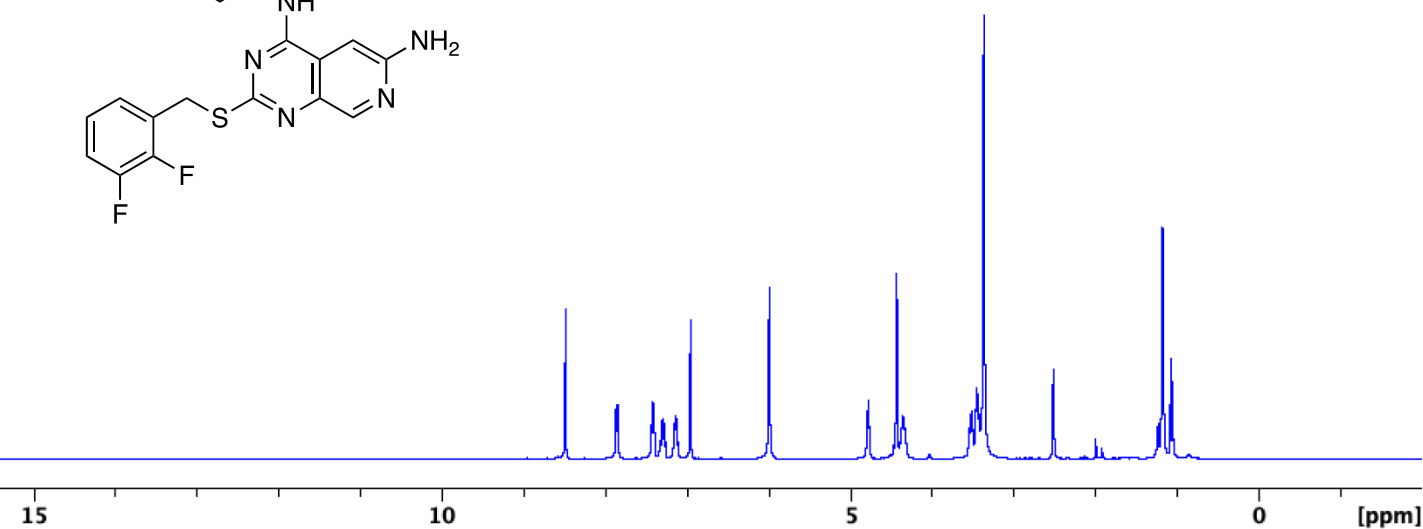
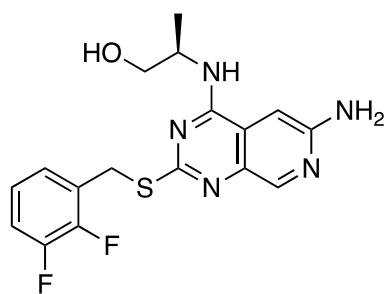


2-(2,3-Difluorobenzylmercapto)-4-(4-methoxybenzyl)-(N-diphenylmethylene)-pyrido[3,4-*d*]pyrimidine-6-amine (19)

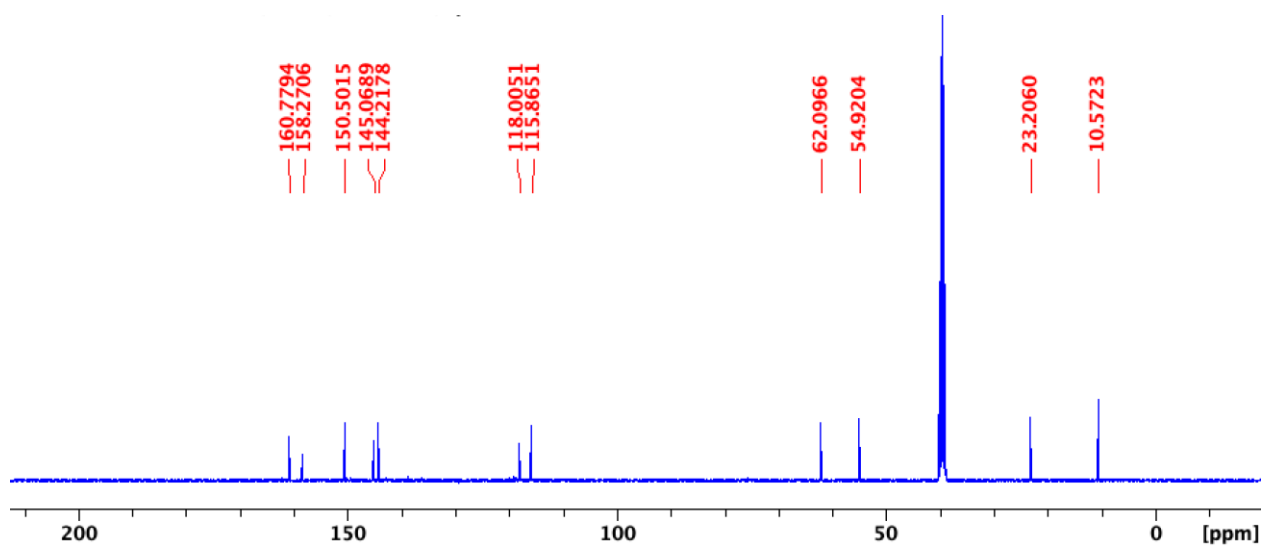
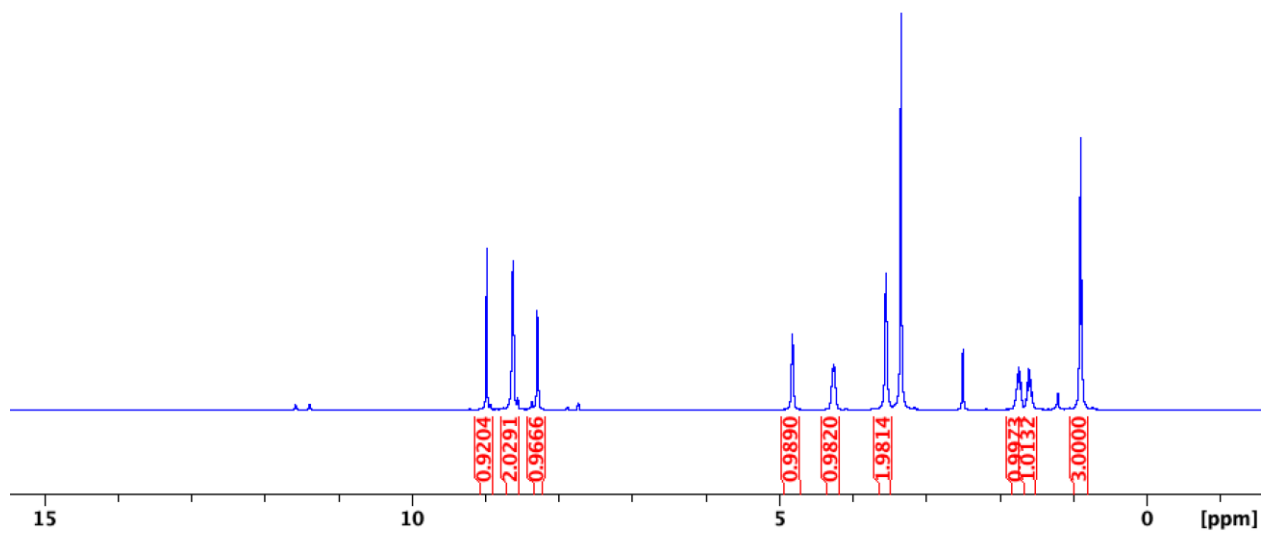
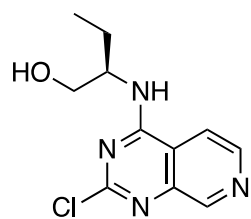




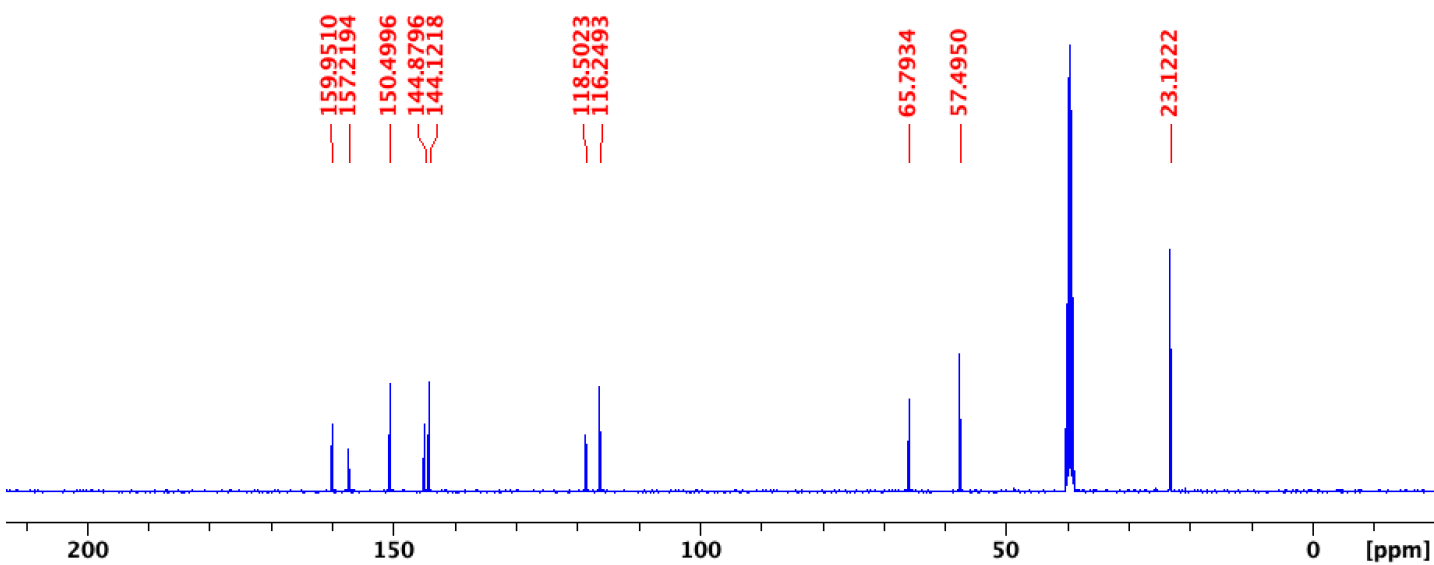
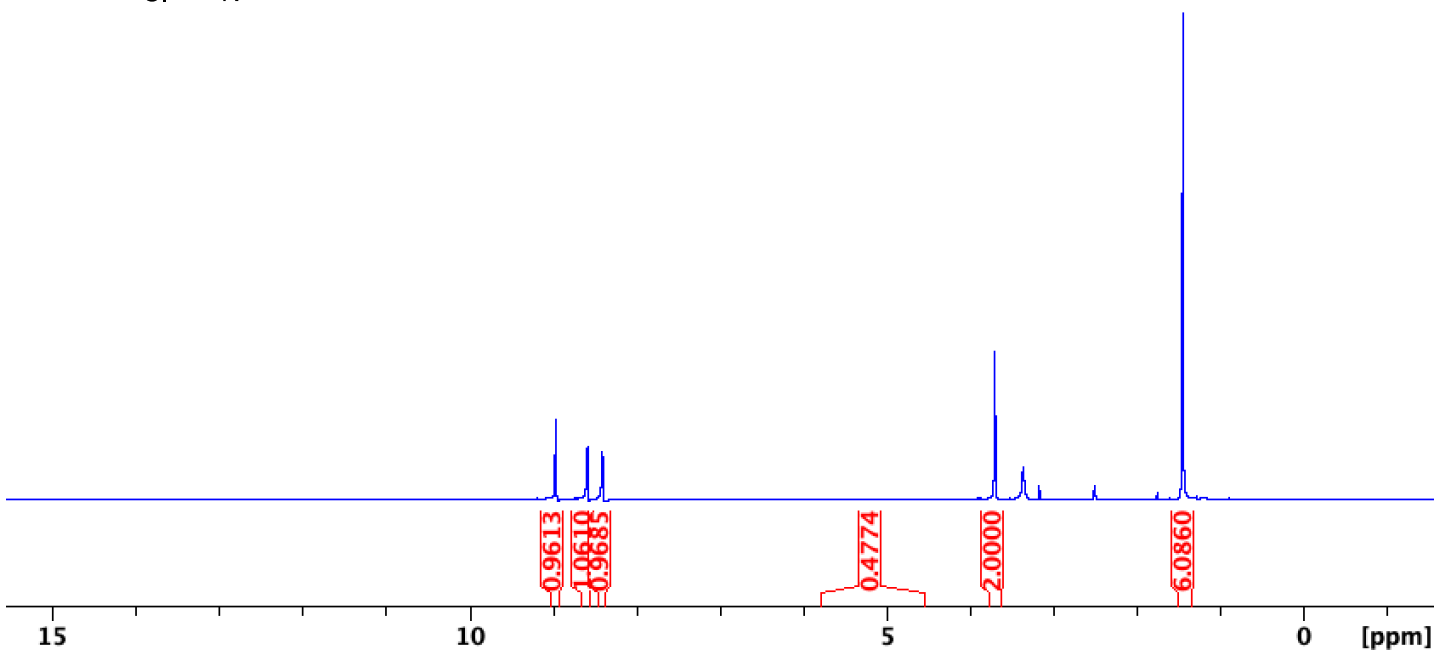
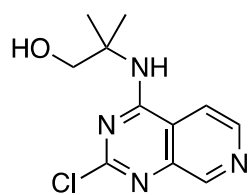
(2*R*)-2-[[6-Amino-2-(2,3-difluorobenzylmercapto)-pyrido[3,4-*d*]pyrimidine-4-yl]amino]propanol (21)



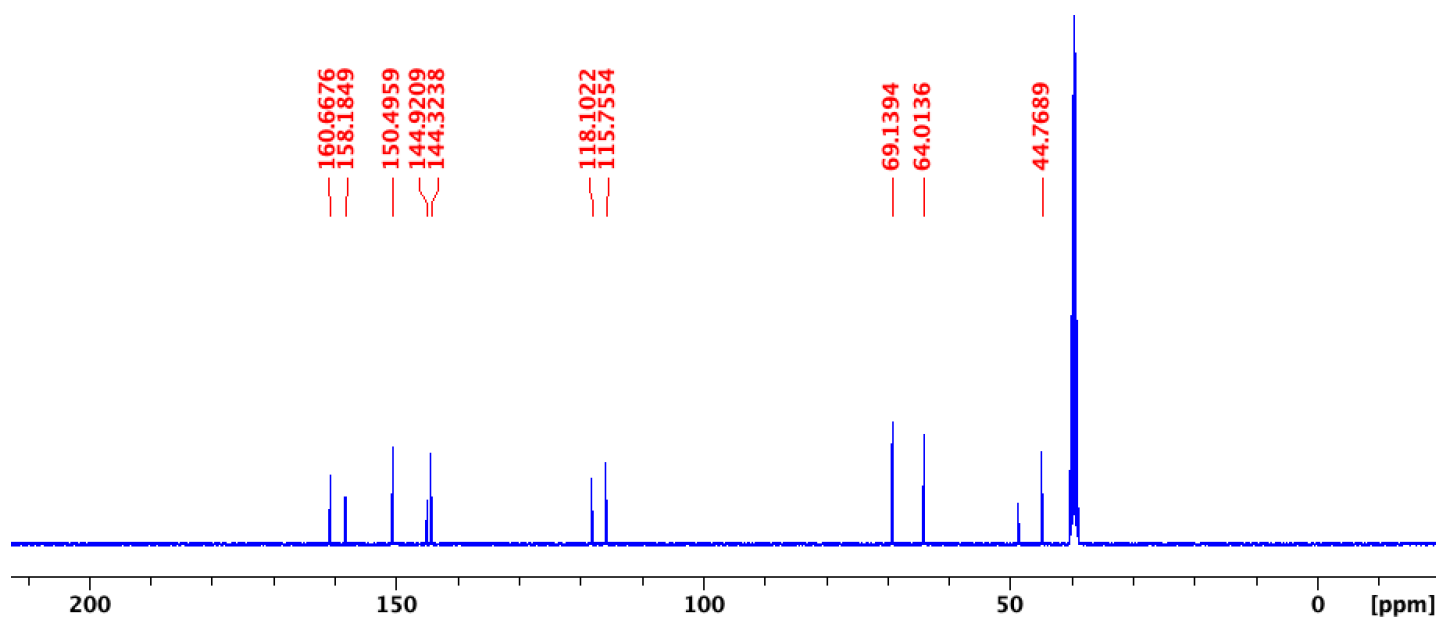
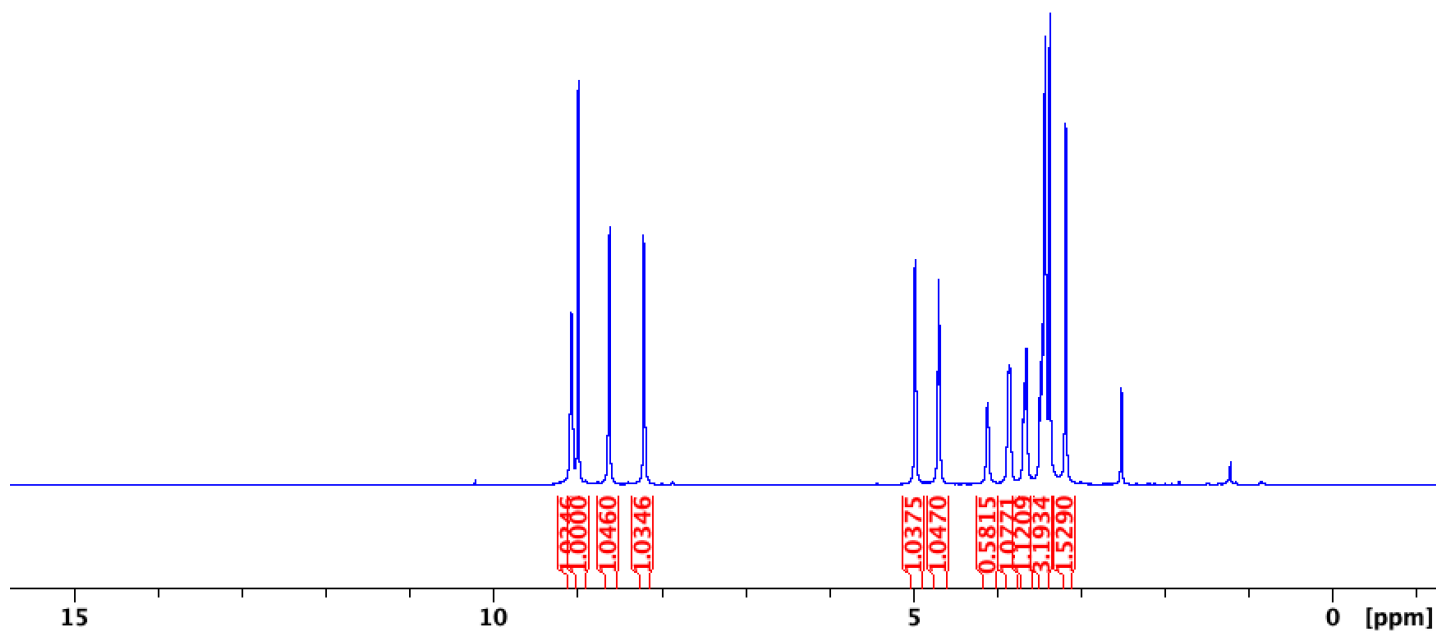
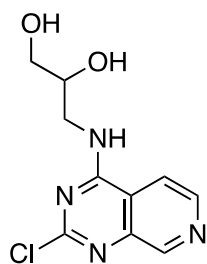
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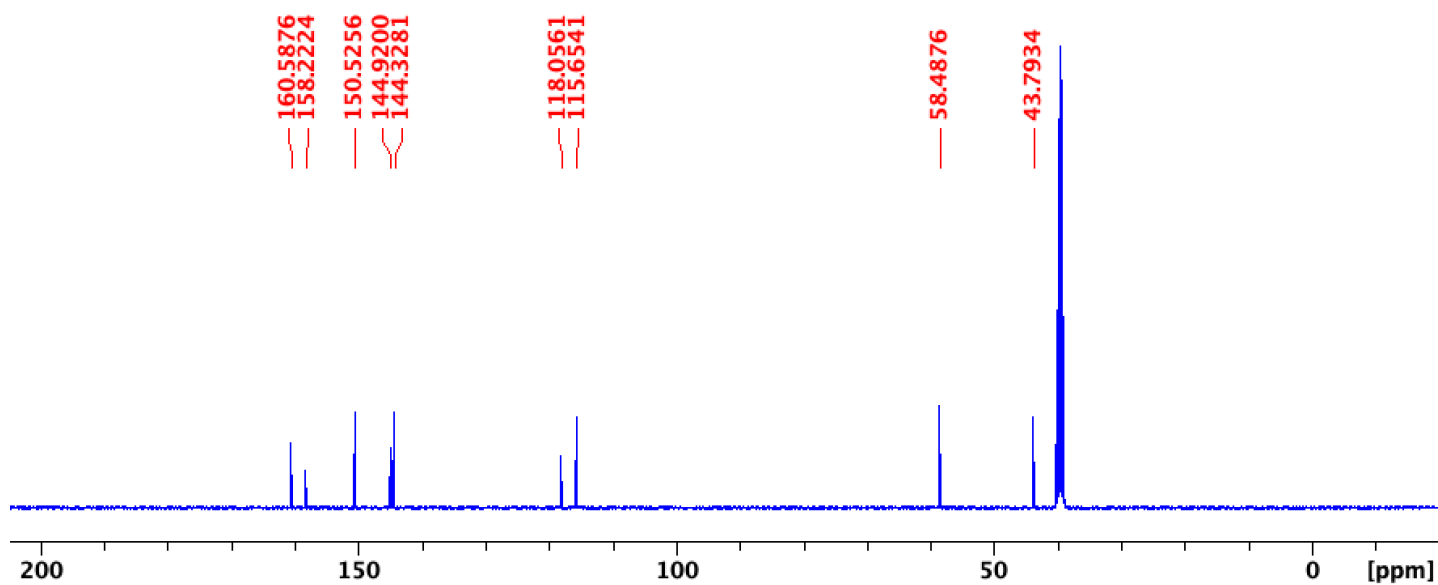
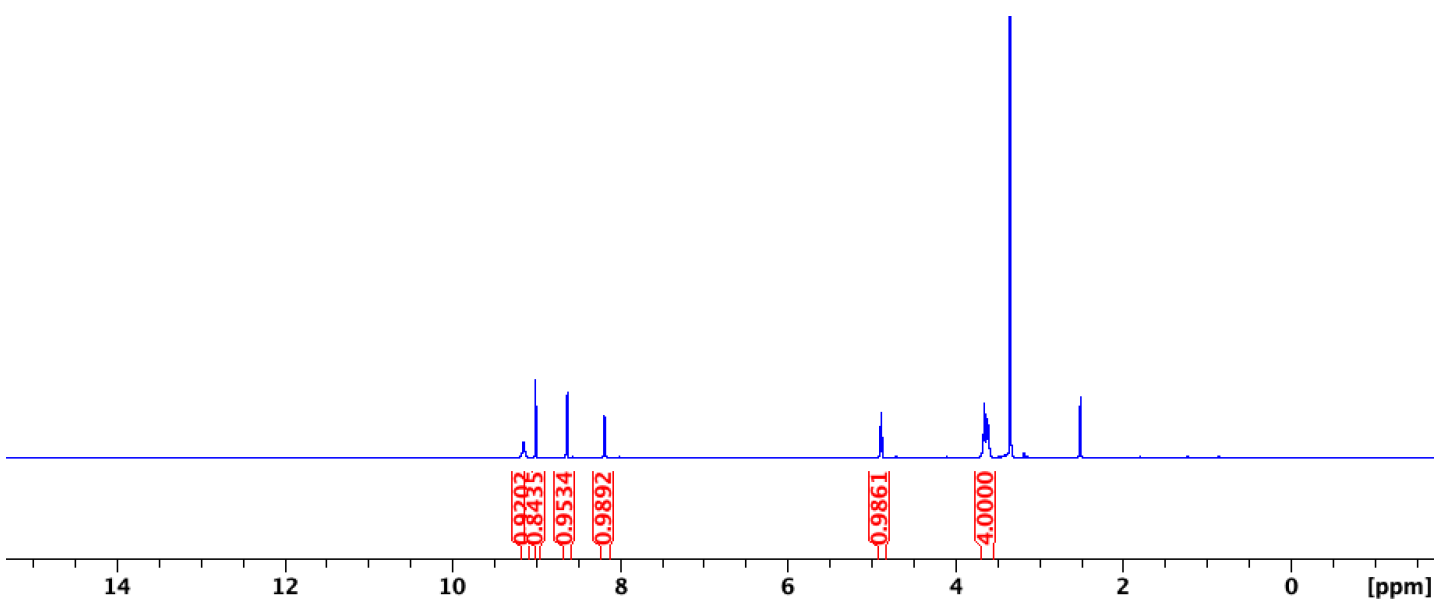
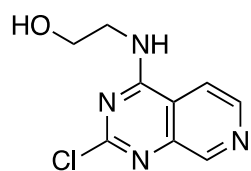
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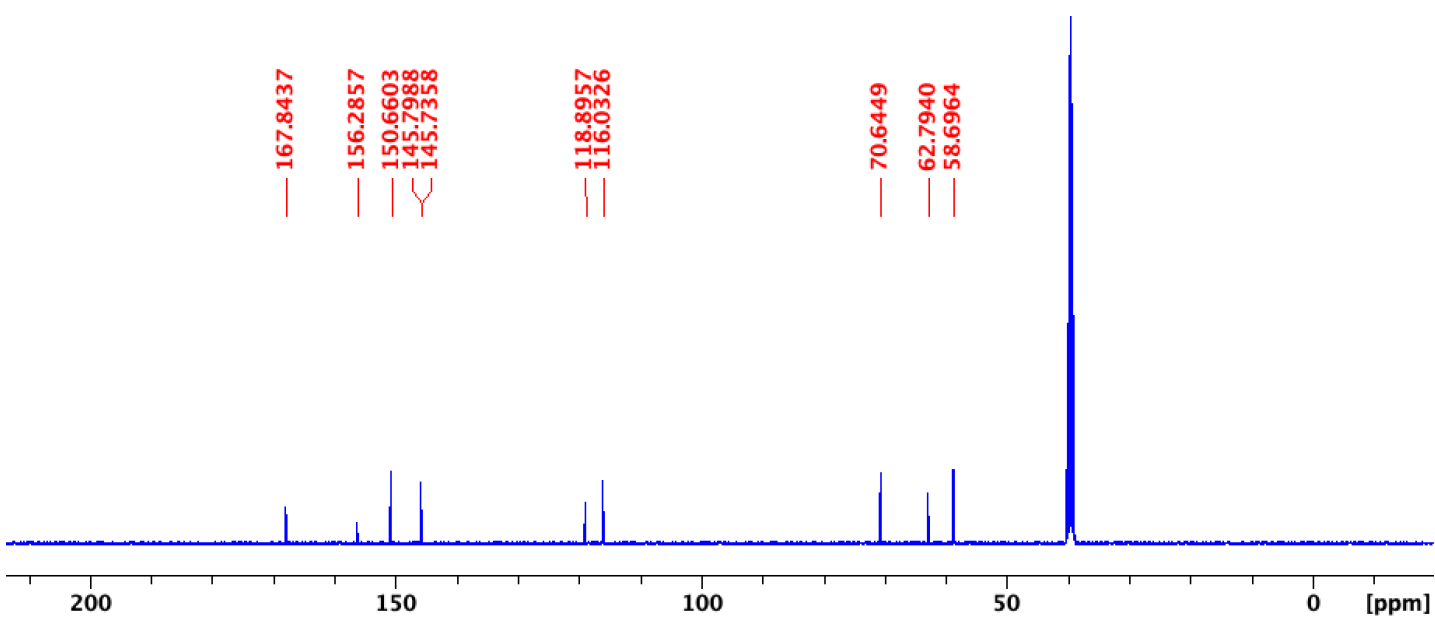
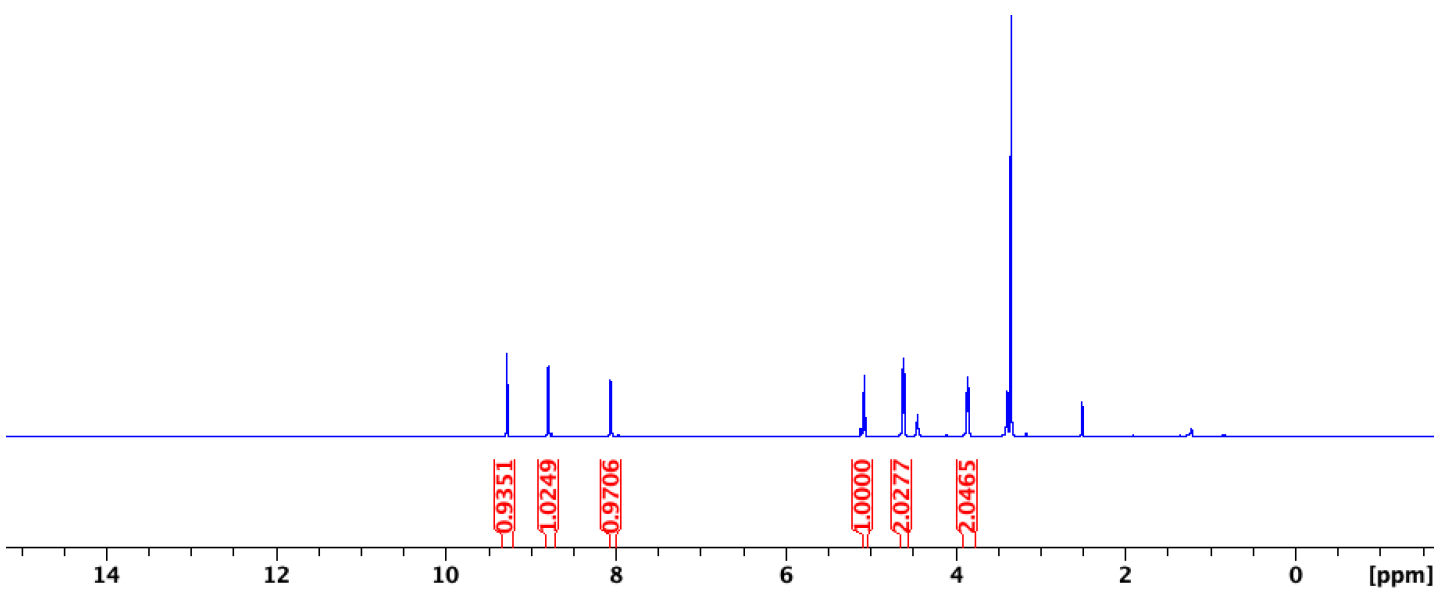
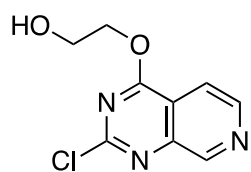
3-[(2-Chloro-pyrido[3,4-*d*]pyrimidine-4-yl)amino]propan-1,2-diol (23c)



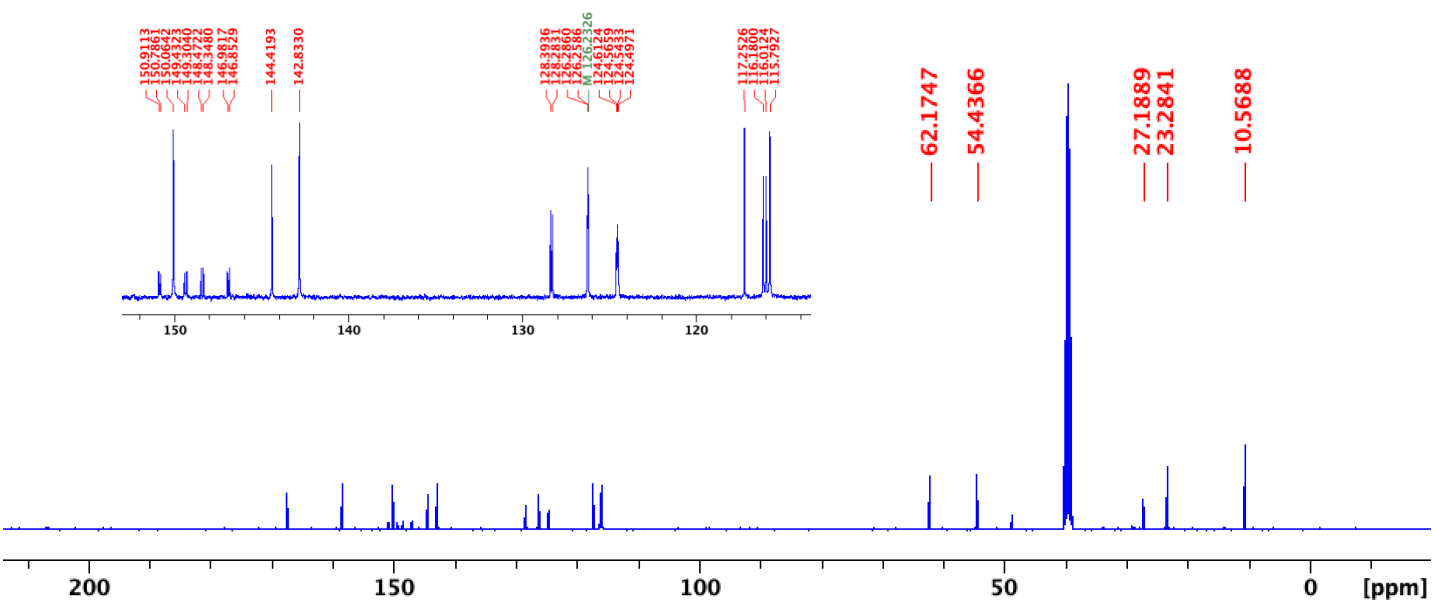
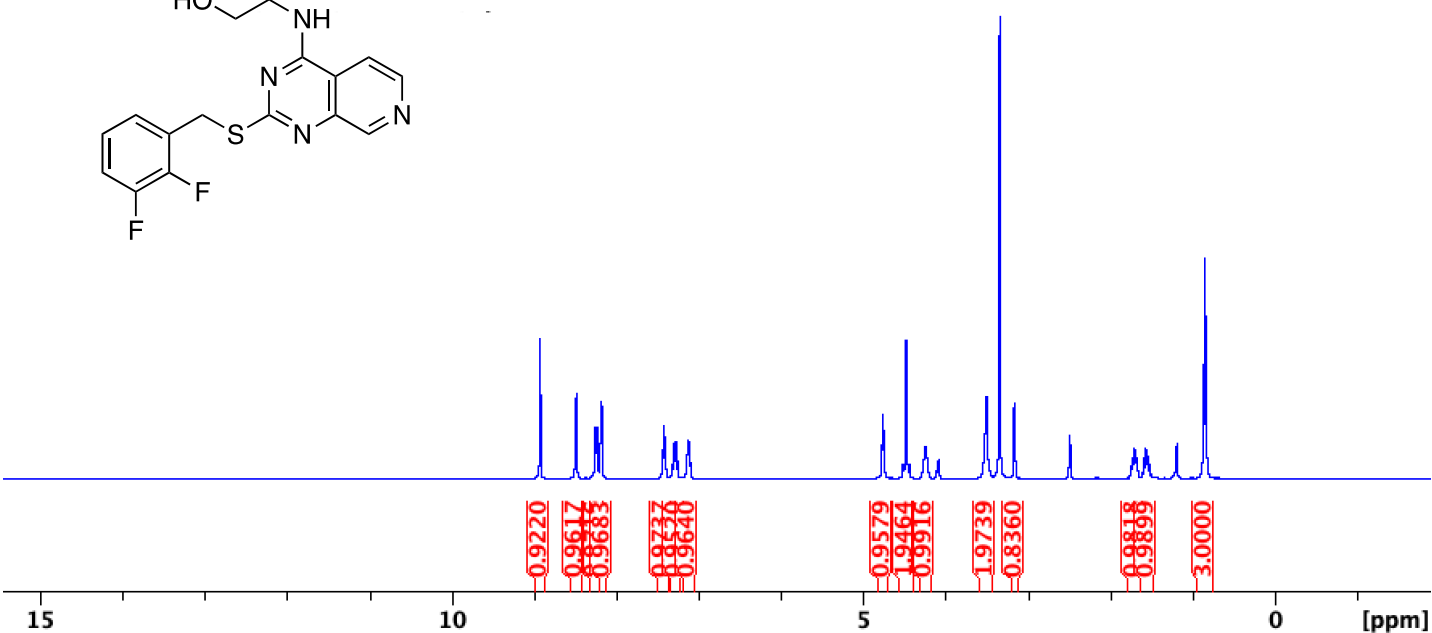
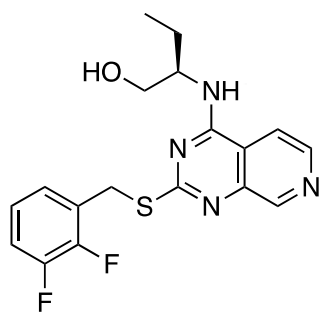
2-[(2-Chloro-pyrido[3,4-*d*]pyrimidine-4-yl)amino]ethanol (23d)

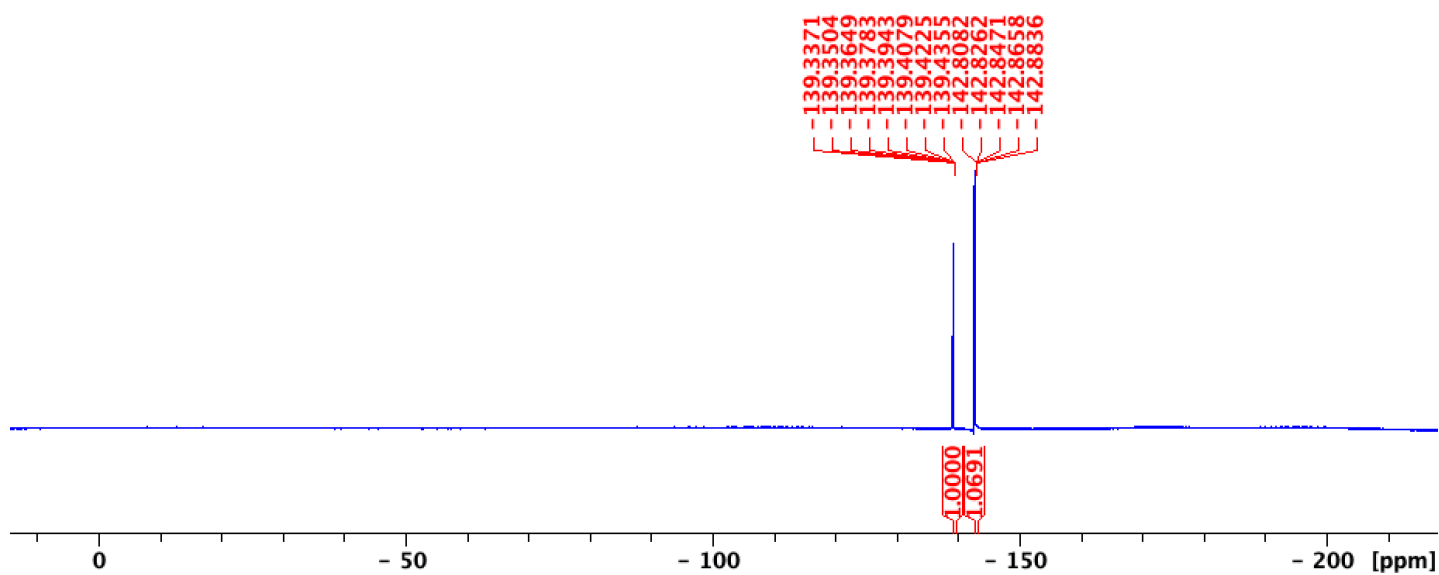


3-[(2-(2,3-Difluorobenzylmercapto)-pyrido[3,4-*d*]pyrimidine-4-yl)oxy]ethanol (23e)

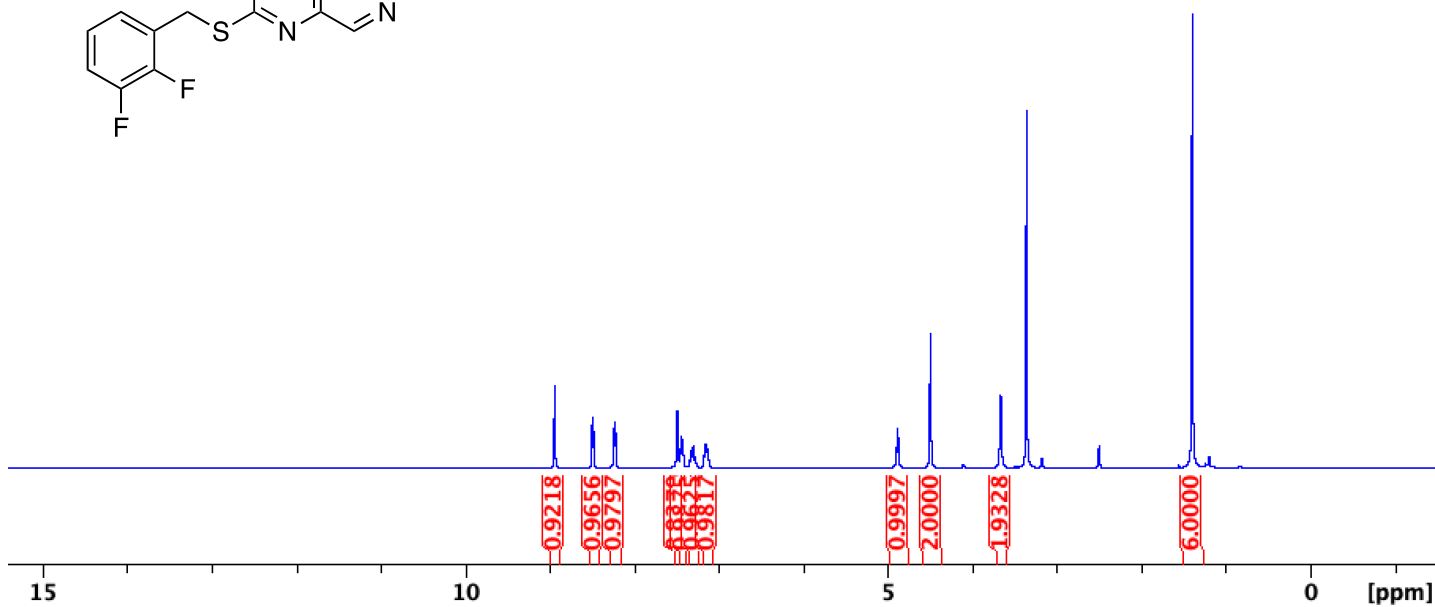
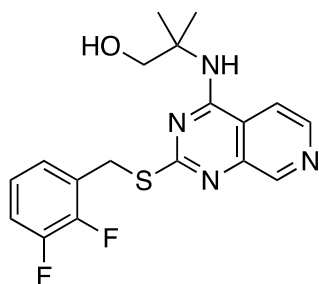


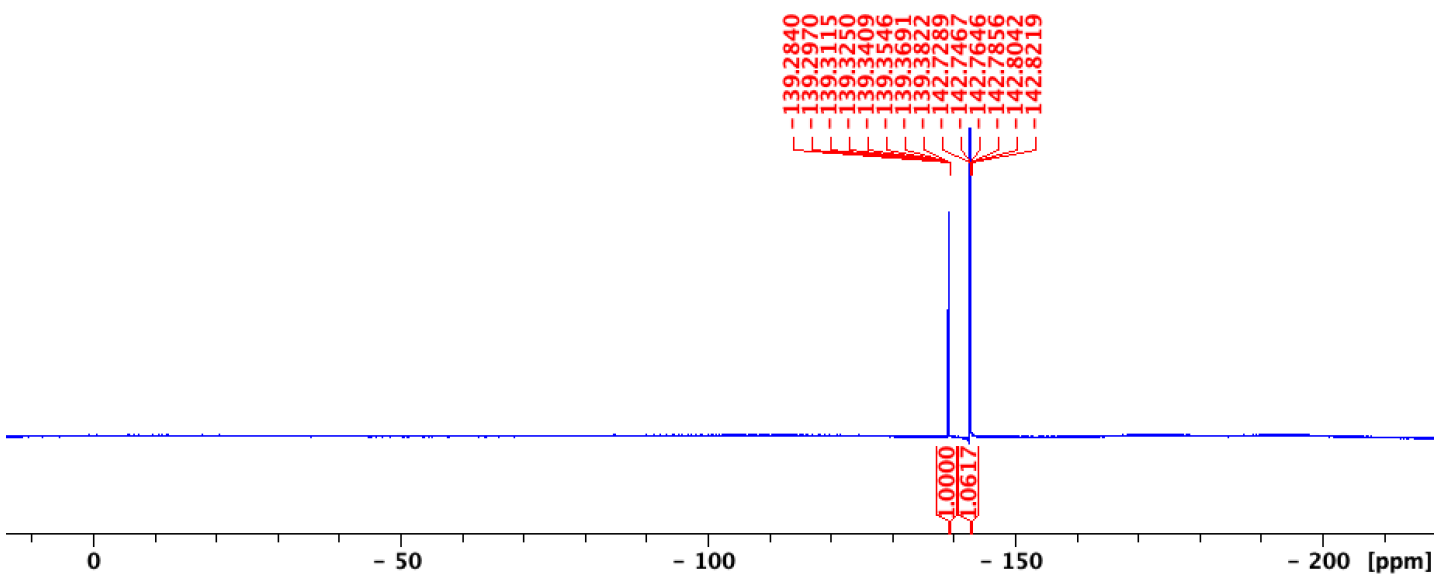
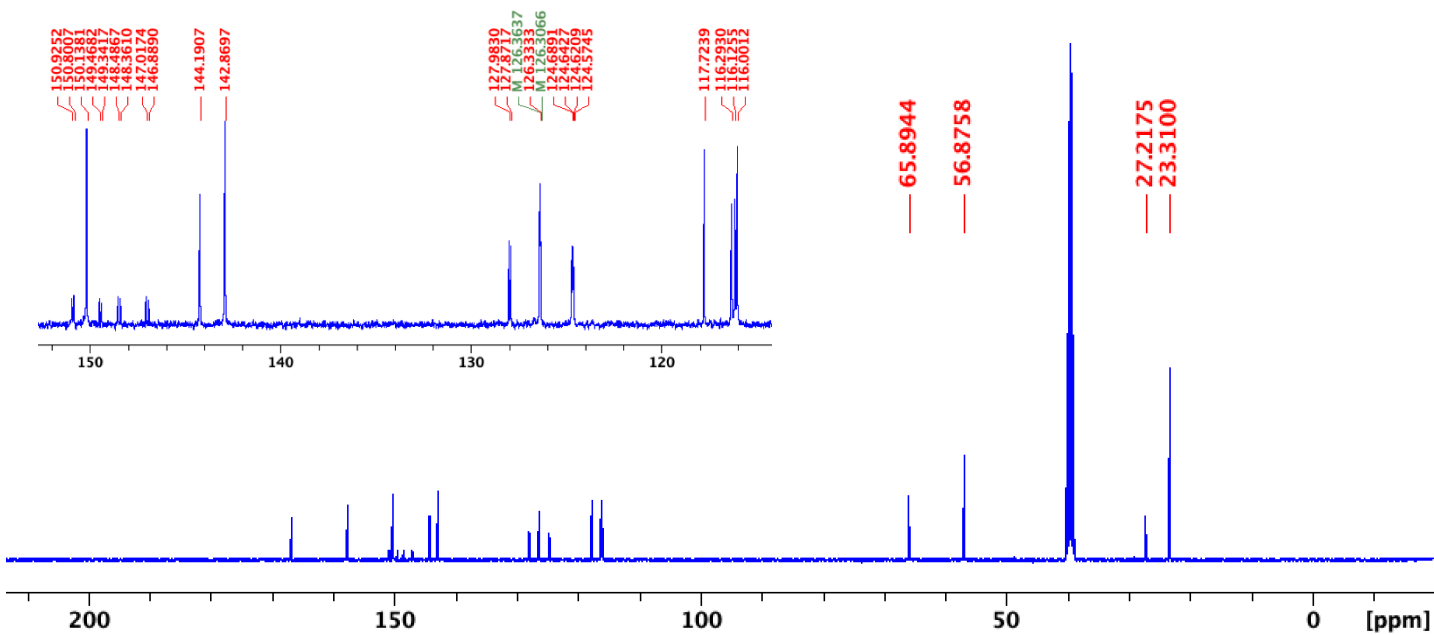
(2R)-2-[(2-(2,3-Difluorobenzylmercapto)-pyrido[3,4-d]pyrimidine-4-yl)amino]butanol (24a)



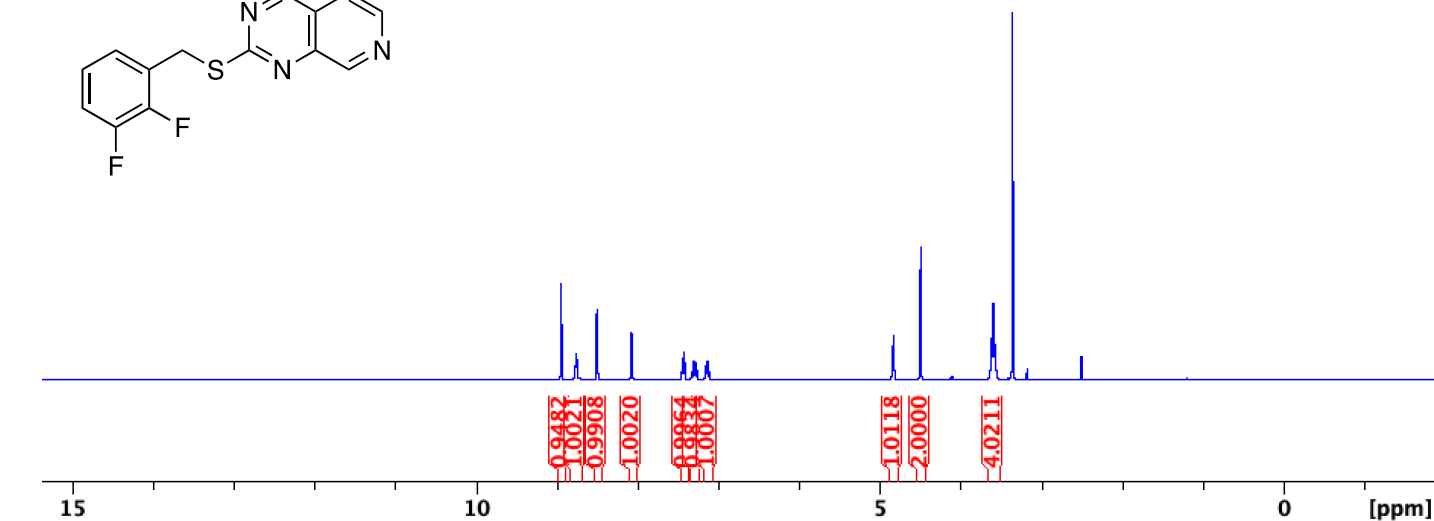
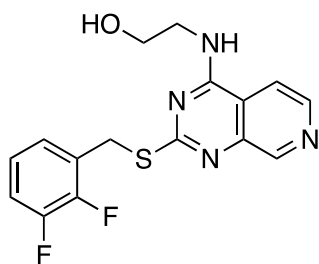
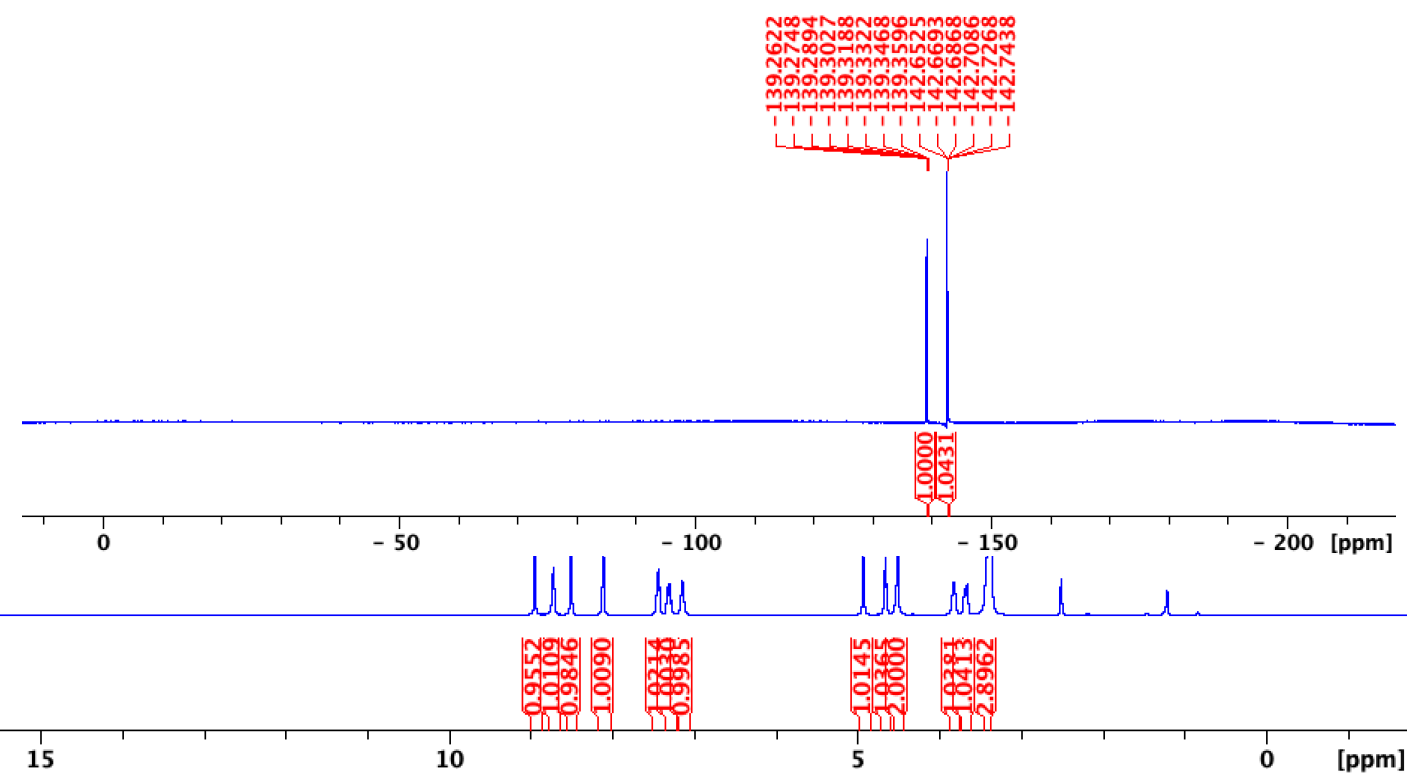


2-[(2-(2,3-Difluorobenzylmercapto)-pyrido[3,4-d]pyrimidine-4-yl)amino]-2-methyl-propan-1-ol (24b)

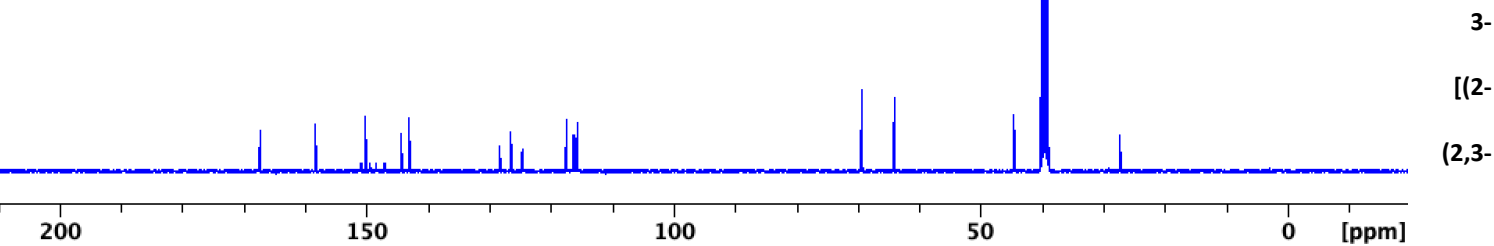


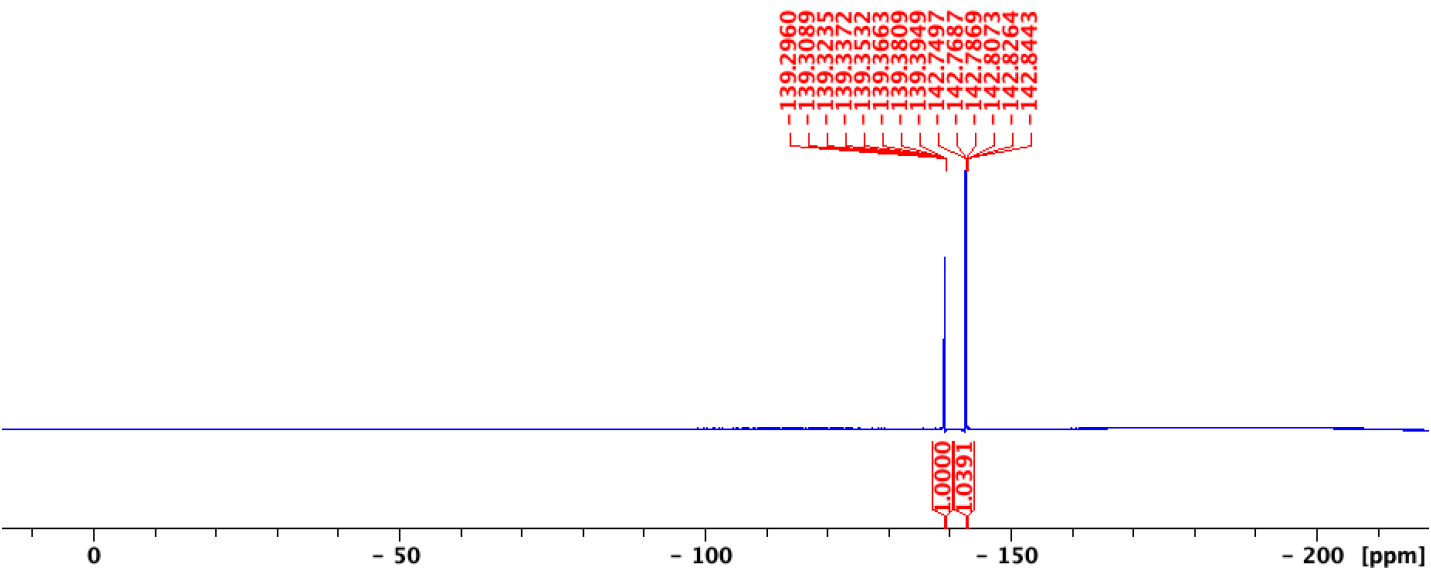
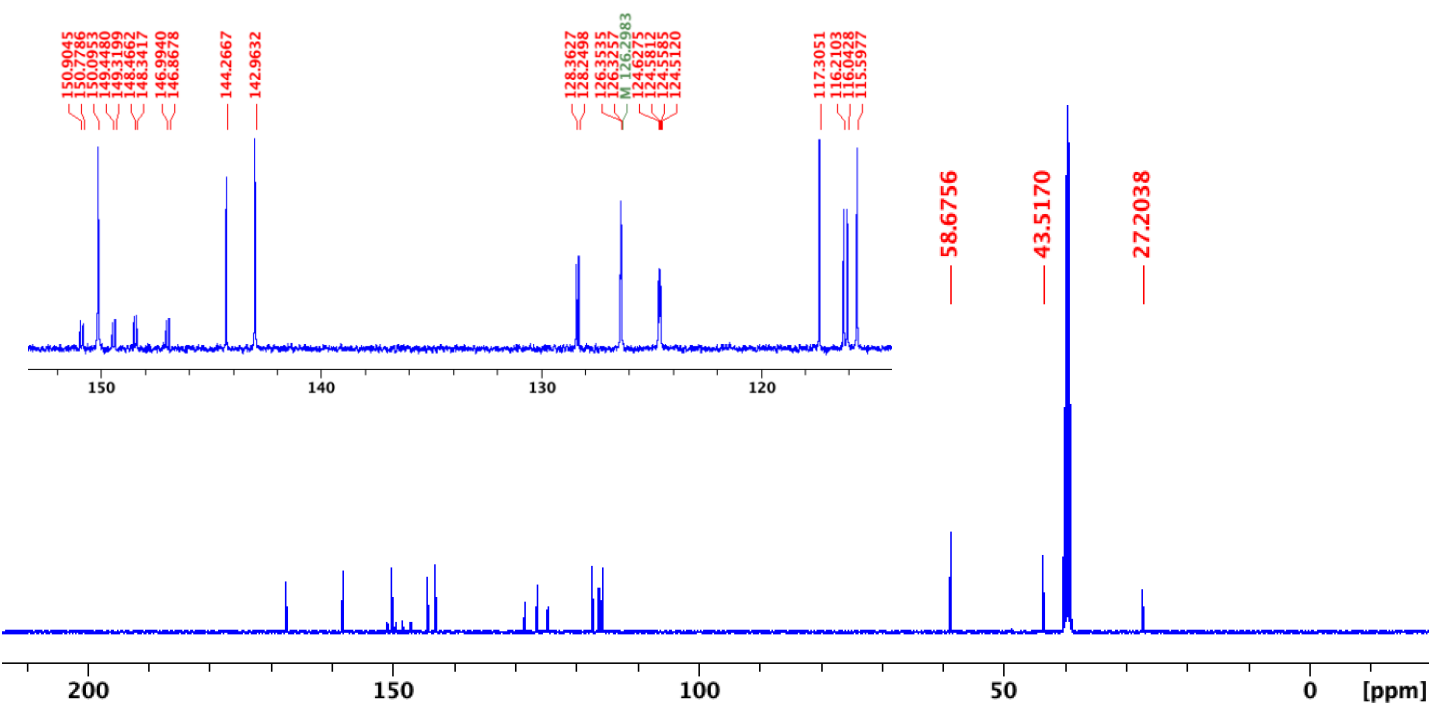


3-[(2-(2,3-Difluorobenzylmercapto)-pyrido[3,4-*d*]pyrimidine-4-yl)amino]propan-1,2-diol (24c)

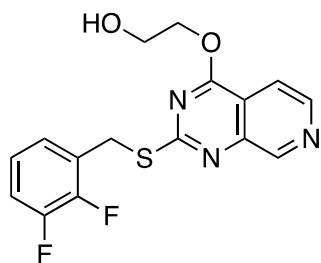
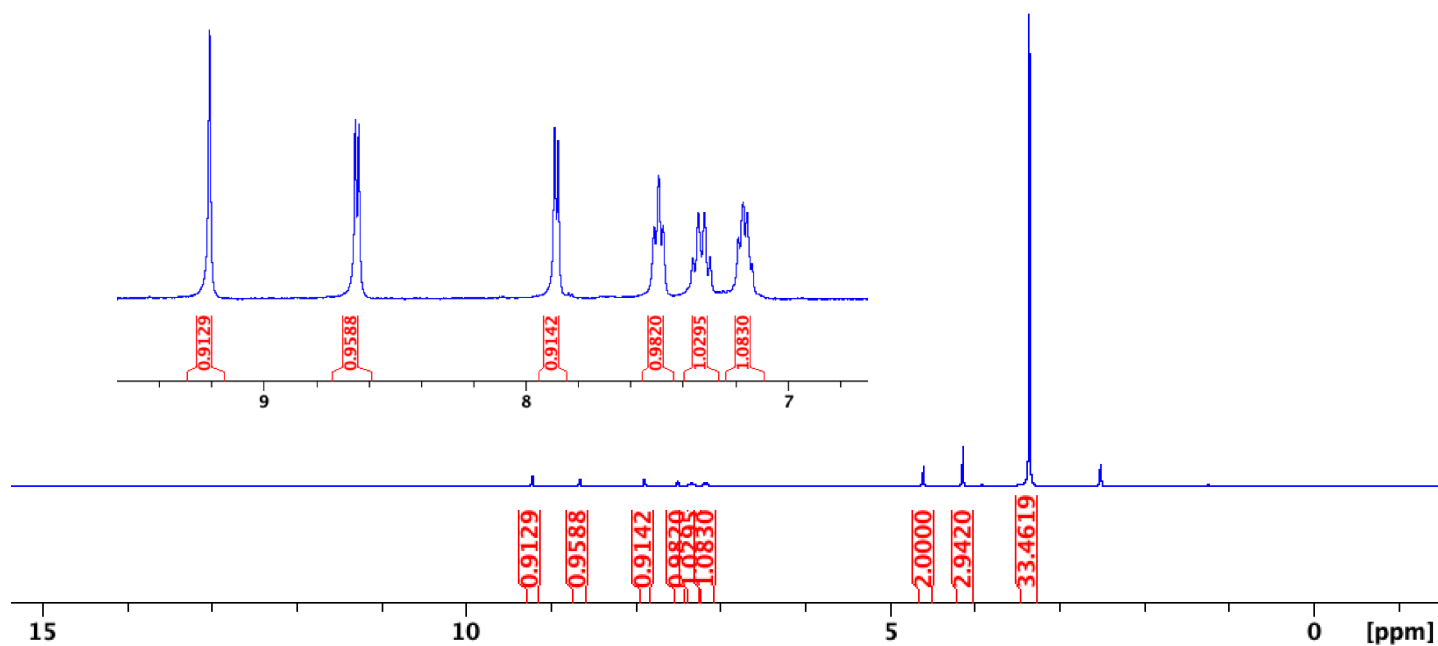


Difluorobenzylmercapto)-pyrido[3,4-*d*]pyrimidine-4-yl)amino]ethanol (24d)



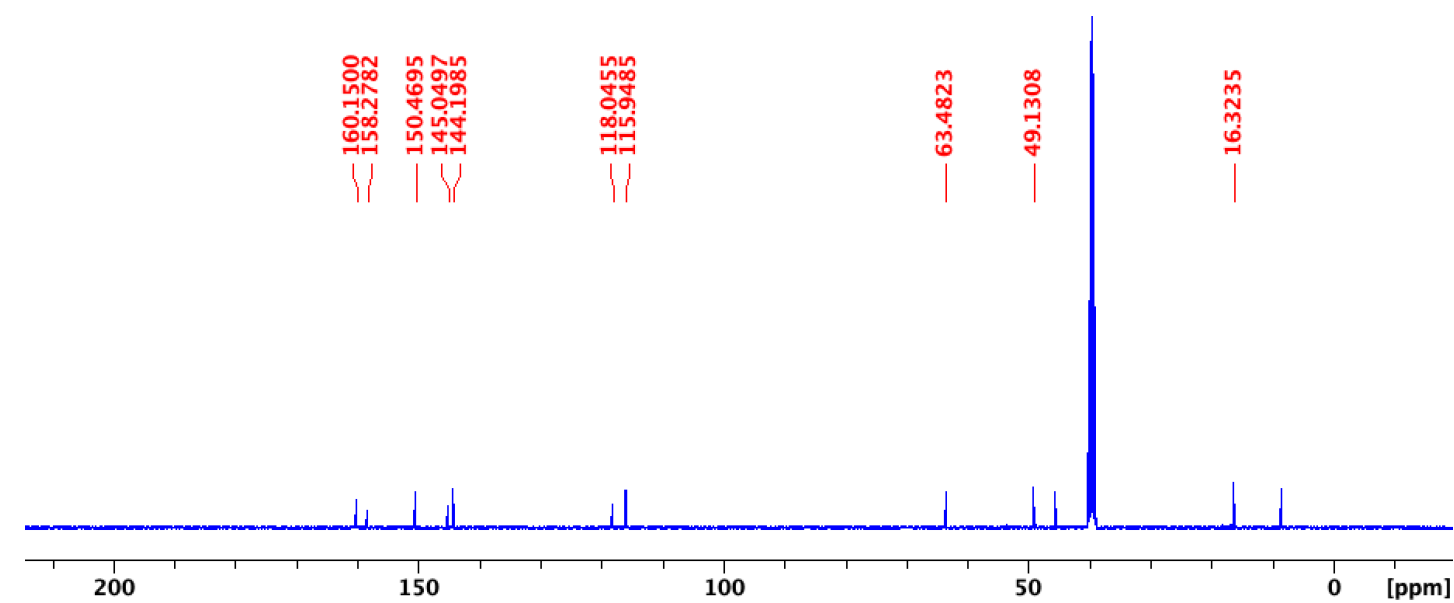
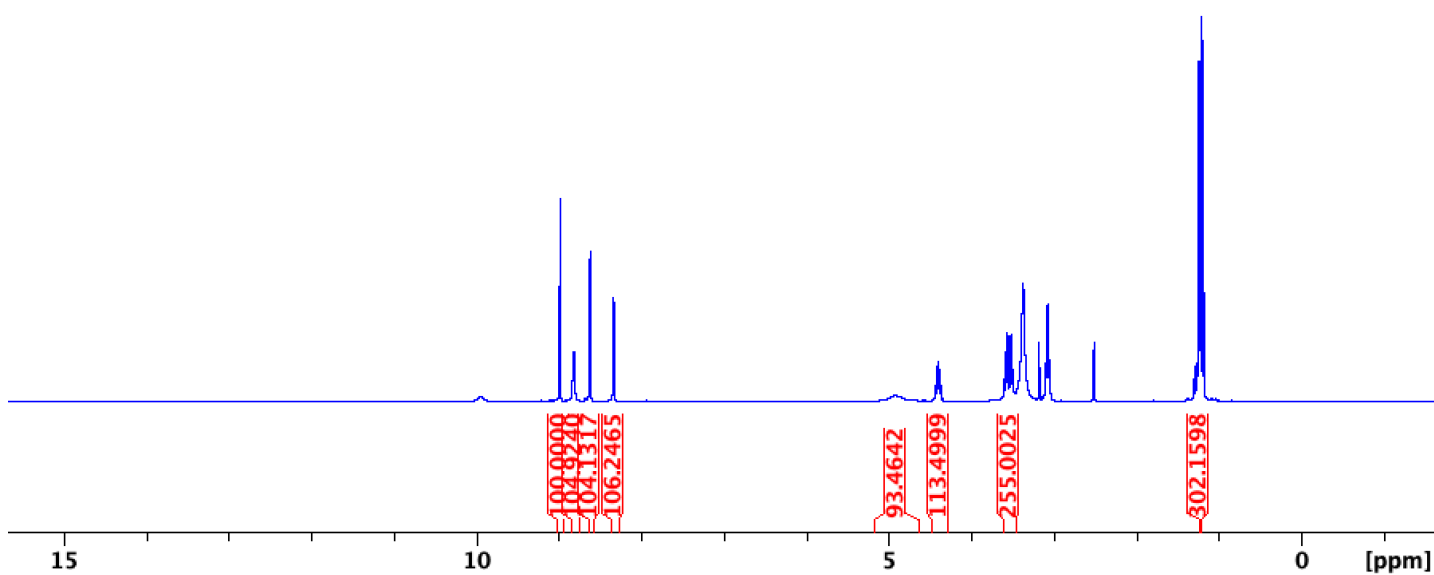
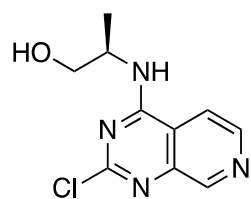


3-[(2-(2,3-Difluorobenzylmercapto)-pyrido[3,4-*d*]pyrimidine-4-yl)oxy]ethanol (24e)

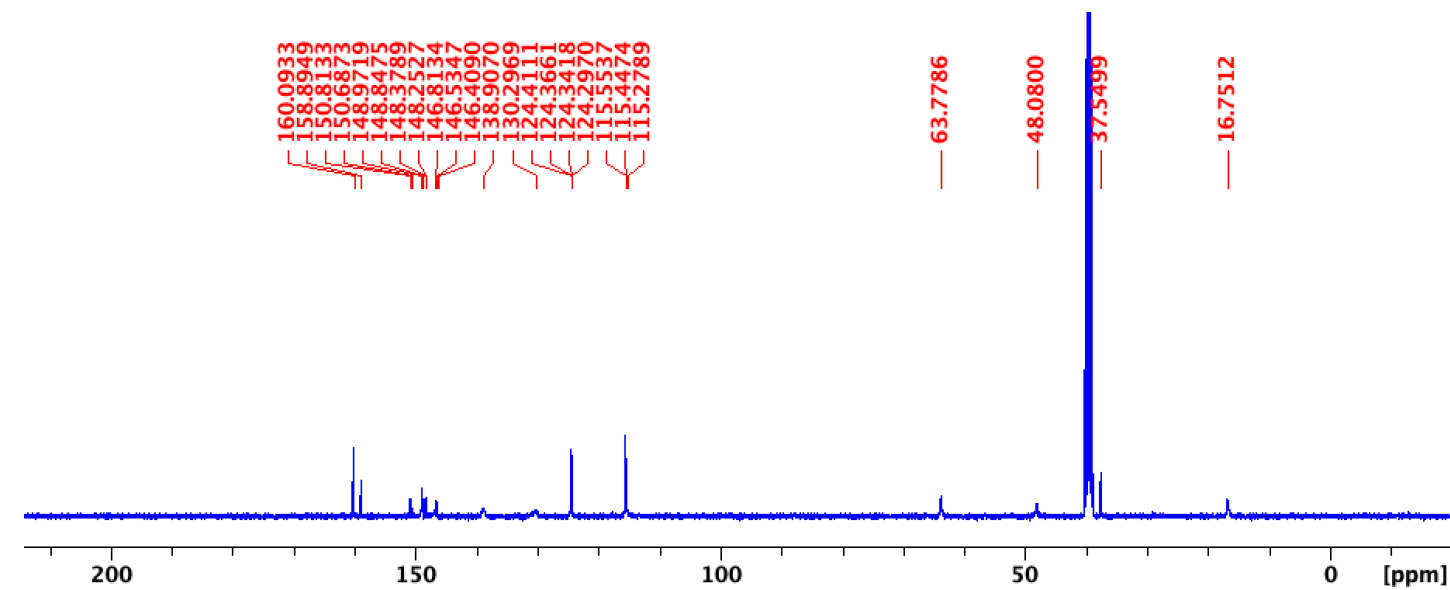
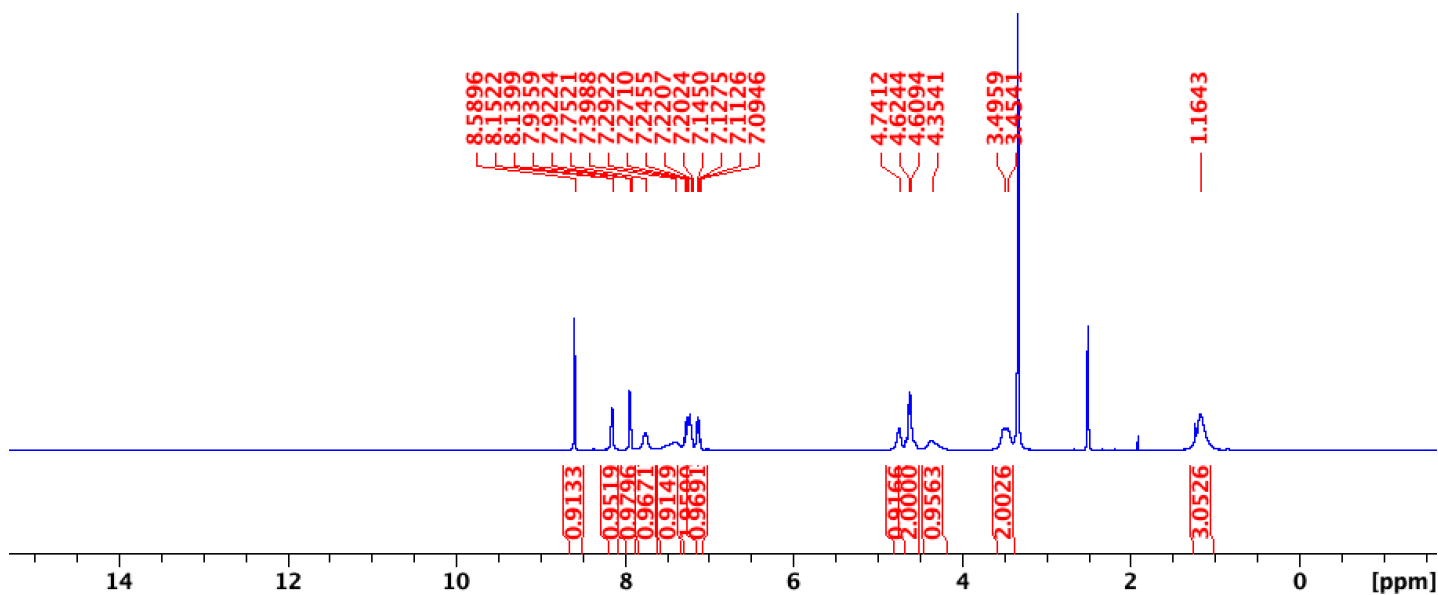
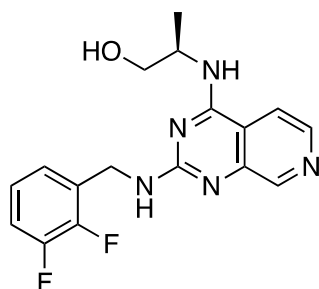


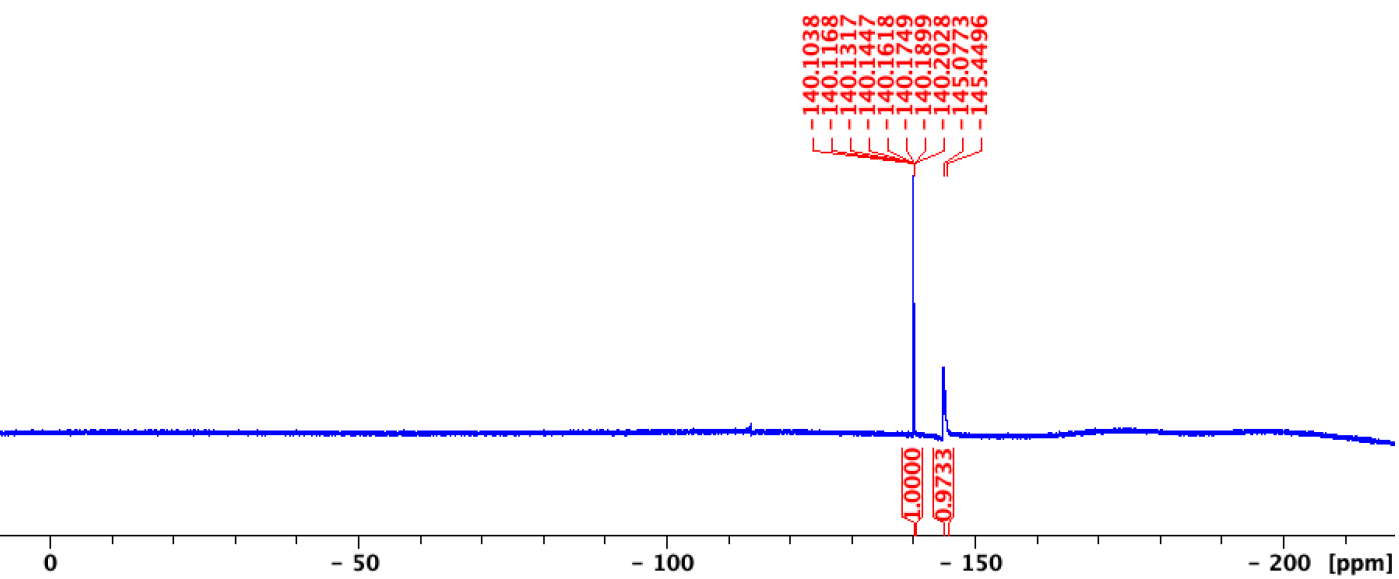


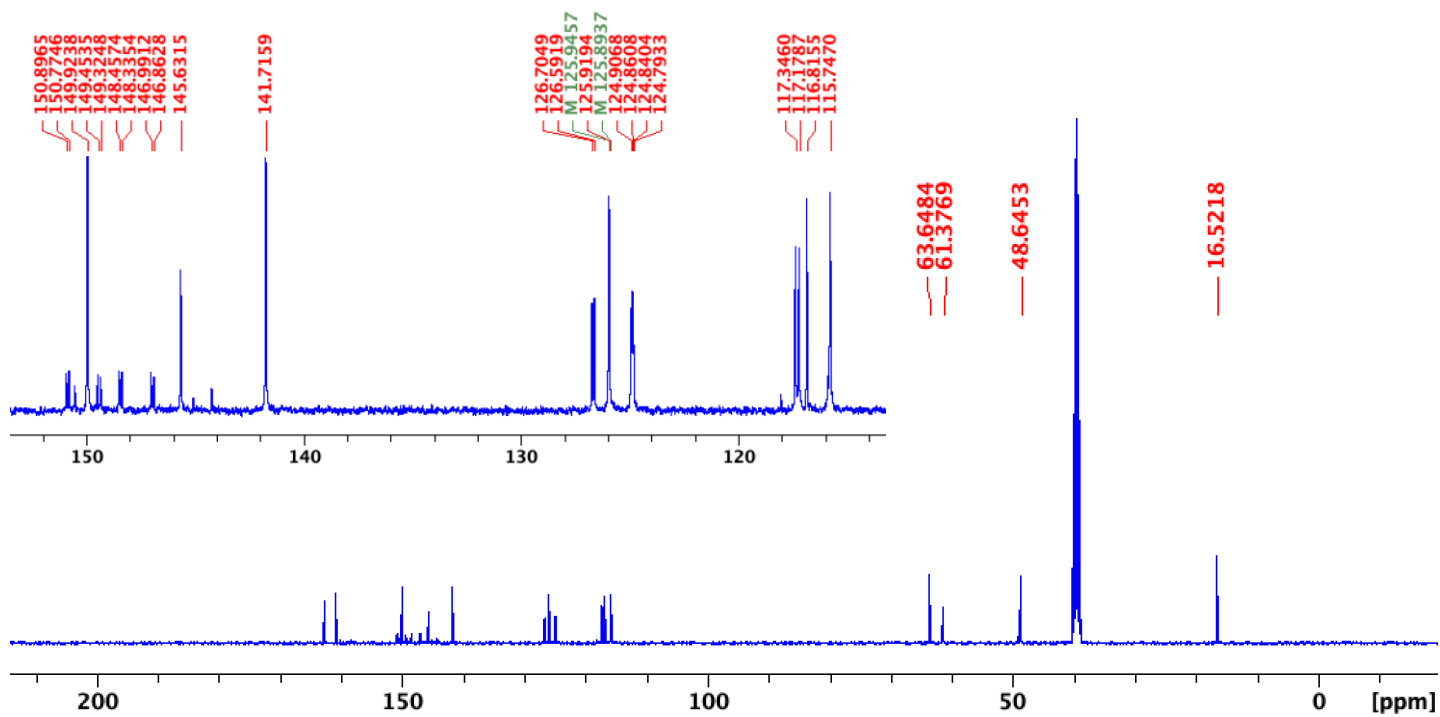
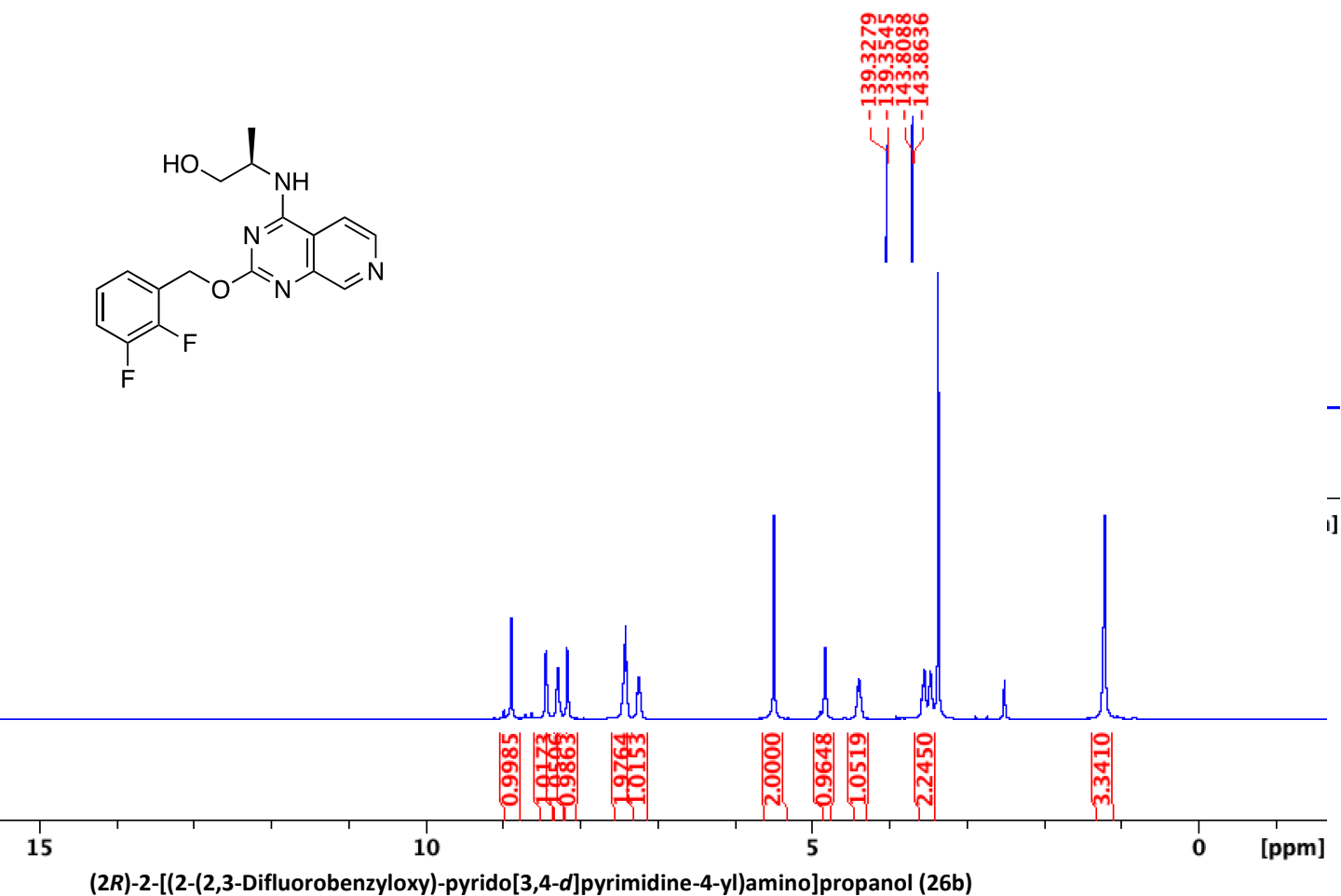
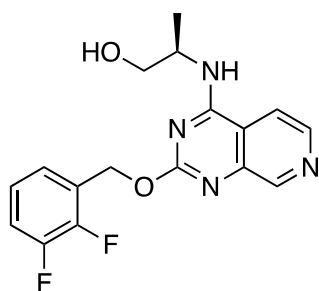
(2*R*)-2-[(6-Chloro-2-pyrido[3,4-*d*]pyrimidine-4-yl)amino]propanol (25)



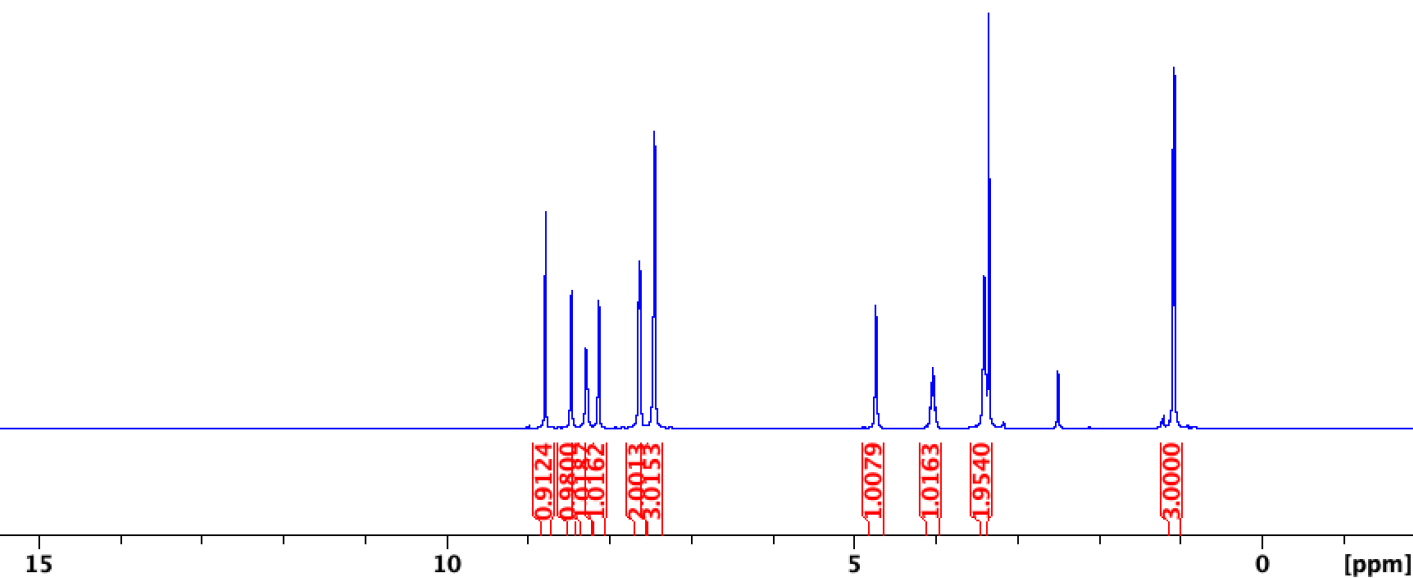
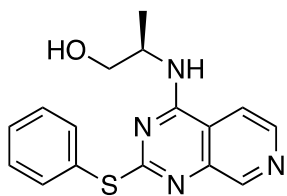
(2R)-2-[(2-(2,3-Difluorobenzylamino)-pyrido[3,4-d]pyrimidine-4-yl)amino]propanol (26a)



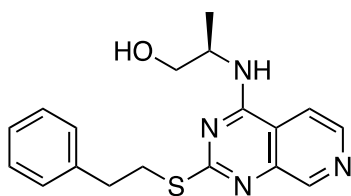
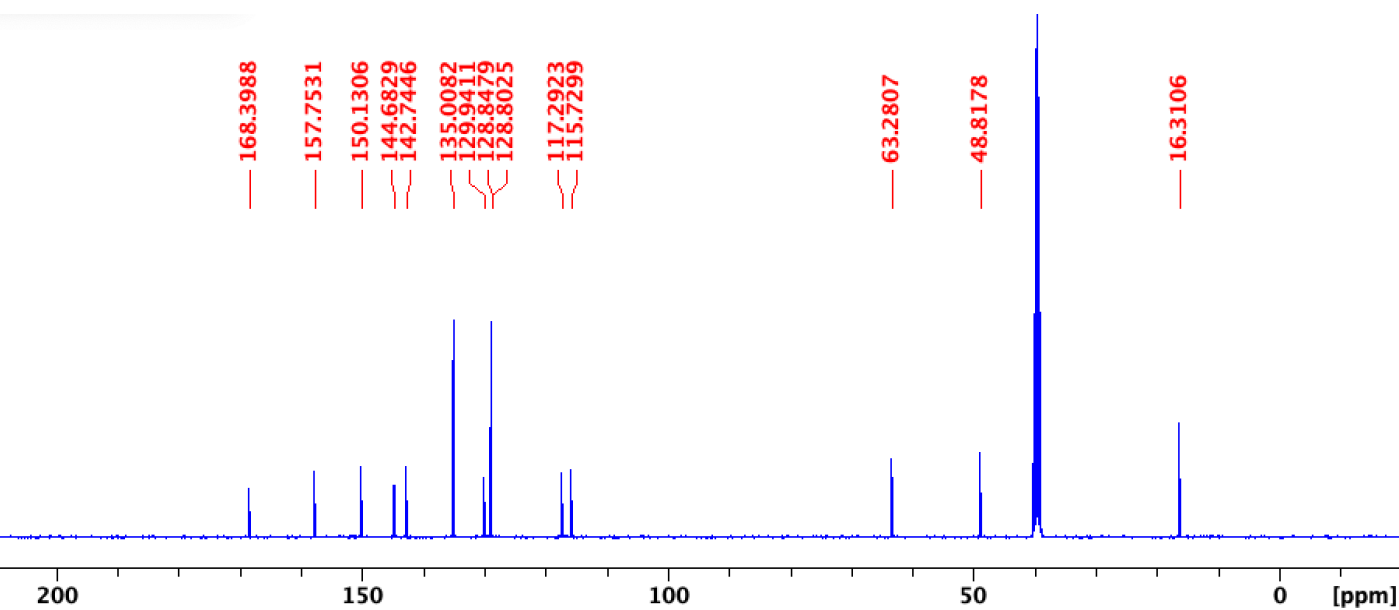


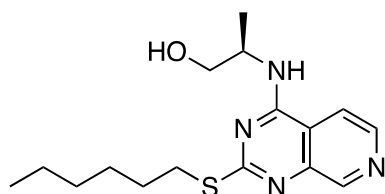


(2R)-2-[(2-(Phenylmercapto)-pyrido[3,4-*d*]pyrimidine-4-yl)amino]propanol (26c)



(2R)-2-[(2-(Phenylethylmercapto)-pyrido[3,4-*d*]pyrimidine-4-yl)amino]propanol (26d)





(2*R*)-2-[(2-(Hexylmercapto)-pyrido[3,4-*d*]pyrimidine-4-yl)amino]propanol (26e)

