

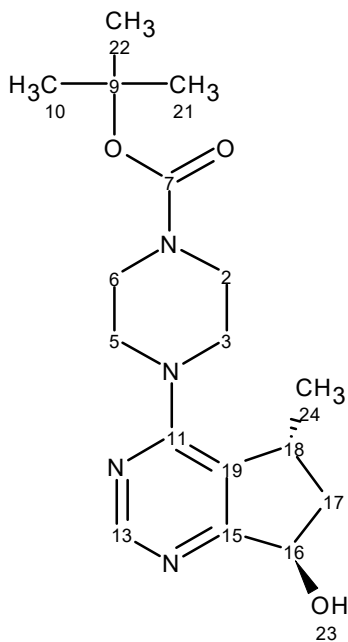
Structure Analytics, NMR & MS, non-GxP

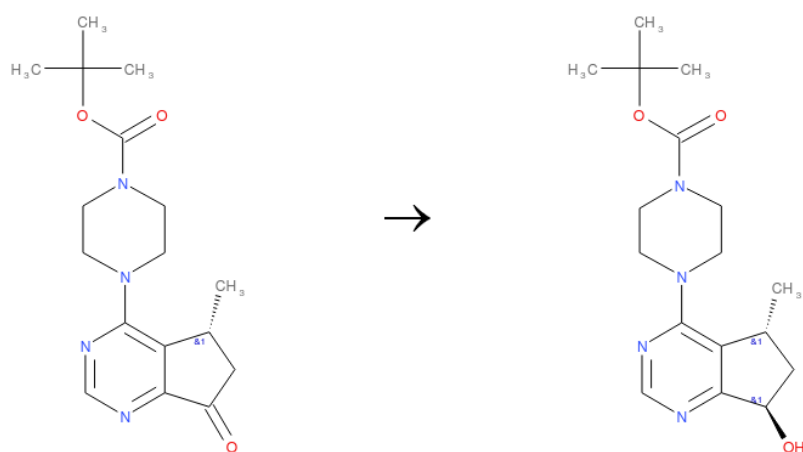
NMR spectra

Structural_id_nmr	stereochemistry determination of 2a (Batch 2021002020557)
Purity_1H_visual	>95%
Linebroadening_1H	no broad signals
Dynamics_1H	none
NMR_comment	NMRdata identical with 2a (Batch 2021002020556)
NMR_comment_2	Overlay plot shows: red : Batch 2021002020557 blue : Batch 2021002020556

Final structure

20.10.2021





C₁₇H₂₄N₄O₃ (332.1848) --> C₁₇H₂₆N₄O₃ (334.2005)

Reactants:

4-[rac-(5R)-7-keto-5-methyl-5,6-dihydrocyclopenta[d]pyrimidin-4-yl]piperazine-1-carboxylic acid tert-butyl ester // Ssal-KRED_M6 Iyo // NADP+

Solvents:

KPi 0.1 M, pH 7.2 // Isopropanol // MgCl₂ * 6 H₂O // water

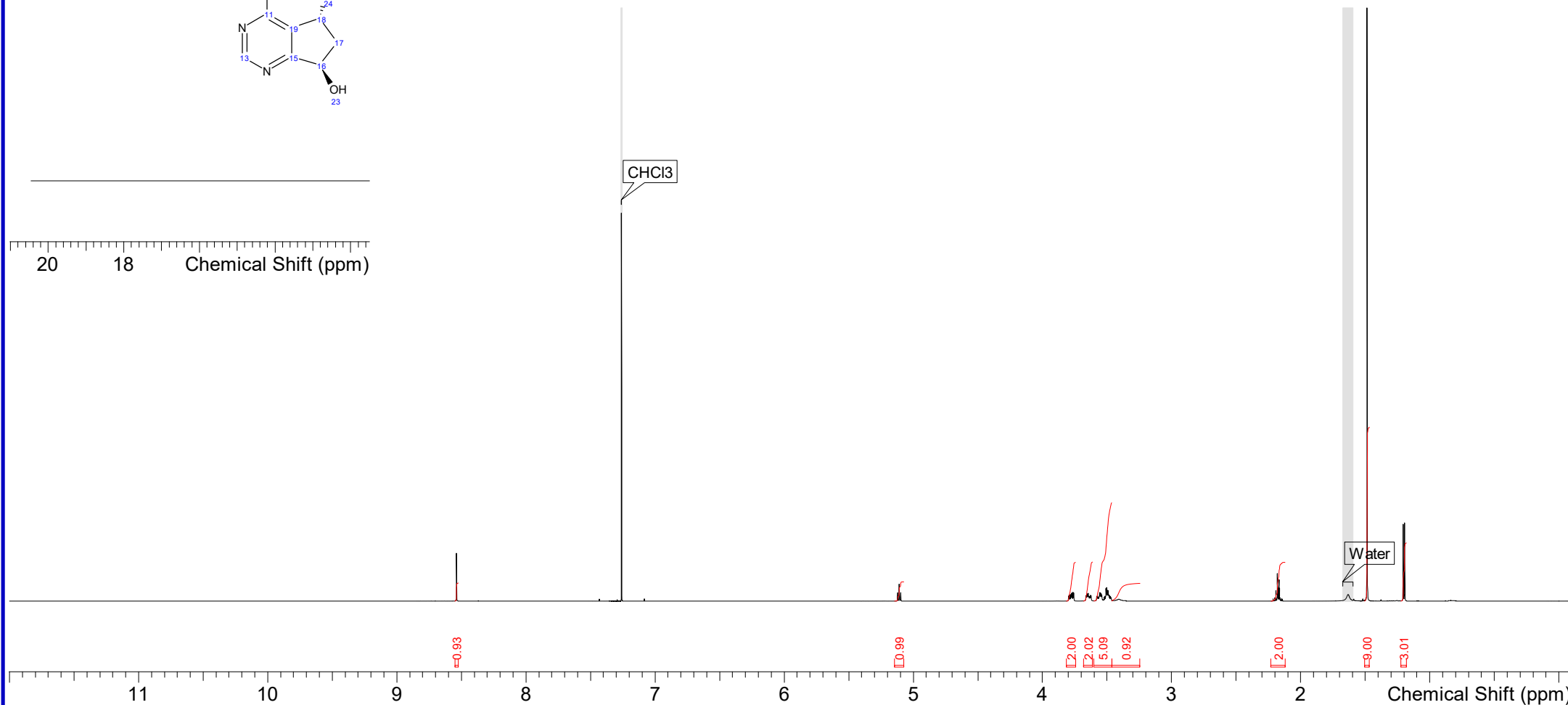
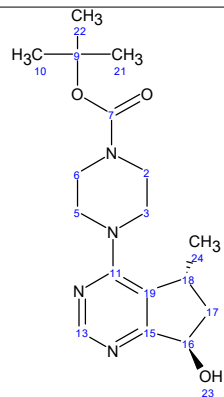
Method		Sample Preparation		Sample amount	Sample back
NMR&MS		CDCl ₃		1.9 mg	N
Structure ID	Ref Order ID1	Ref Order ID2	Ref Order ID3	Ref Order ID4	Ref Order ID5
E1	2013001251714				

1H-NMR spectrum - overview

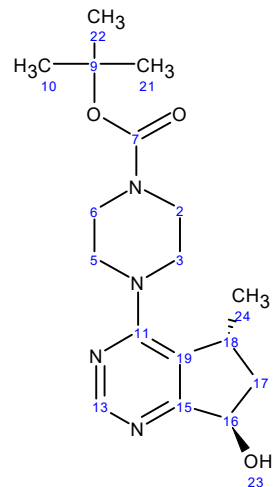
Comment Sample amount 1.9 mg - Topic 7728 IPATASERTIB

Date	18 Oct 2021 18:54:44 (GMT+02:00)
Frequency (MHz)	600.1300
Nucleus	1H
Number of Transients	8
Solvent	CHLOROFORM-d
Temperature (degree C)	25.027
File Name	NMR\nmrfs_u\data\actual\nmr\2021002020557\1000\PDATA\1\1r

^1H NMR (600 MHz, CHLOROFORM-*d*) δ ppm 8.54 (s, 1 H), 5.11 (t, $J=7.2$ Hz, 1 H), 3.78 (ddd, $J=13.1, 7.3, 3.3$ Hz, 2 H), 3.64 (ddd, $J=13.0, 6.9, 3.3$ Hz, 2 H), 3.46 - 3.60 (m, 5 H), 3.24 - 3.46 (m, 1 H), 2.12 - 2.23 (m, 2 H), 1.49 (s, 9 H), 1.20 (d, $J=7.1$ Hz, 3 H)

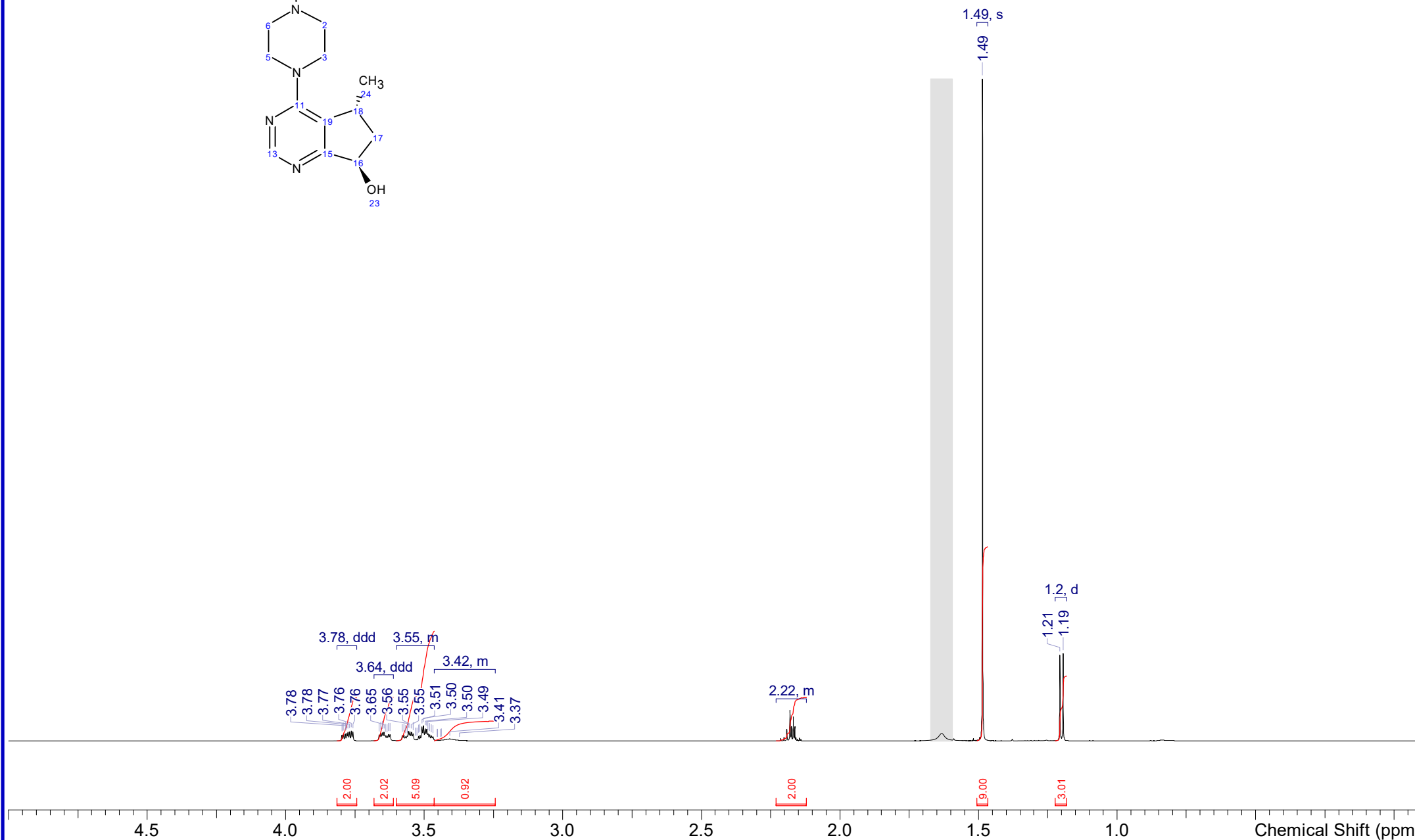


1H-NMR spectrum - expansion region 1

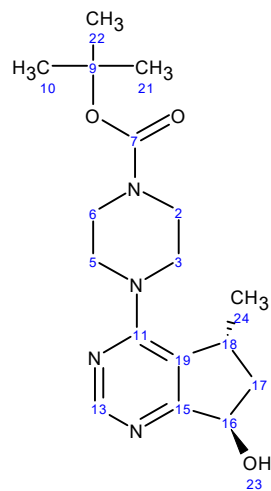


File Name	NMR\nmrfs_u\data\actual\nmr\20 21002020557\1000\PDATA\1\1r
Frequency (MHz)	600.1300
Nucleus	1H
Solvent	CHLOROFORM-d
Temperature (degree C)	25.027

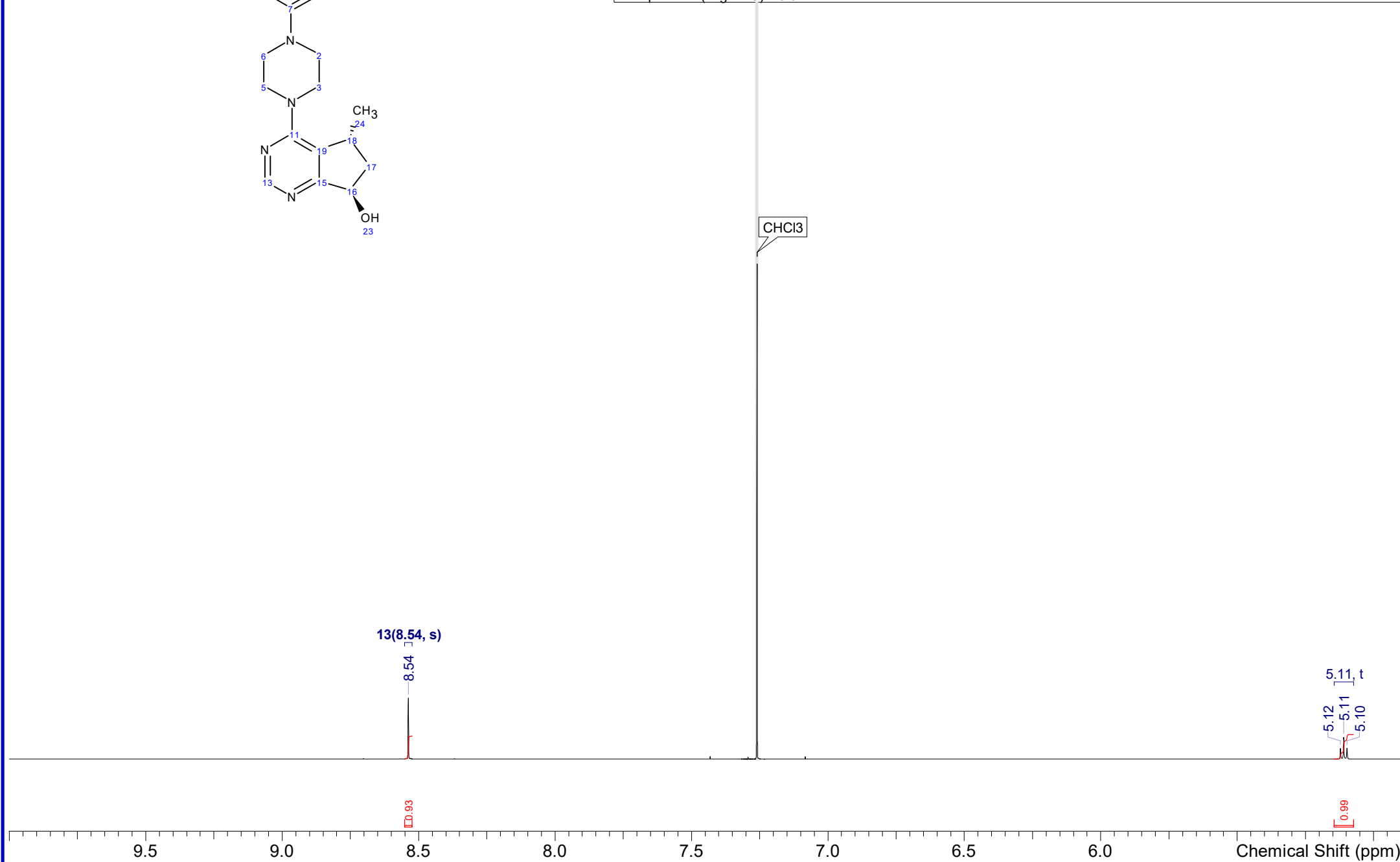
Water



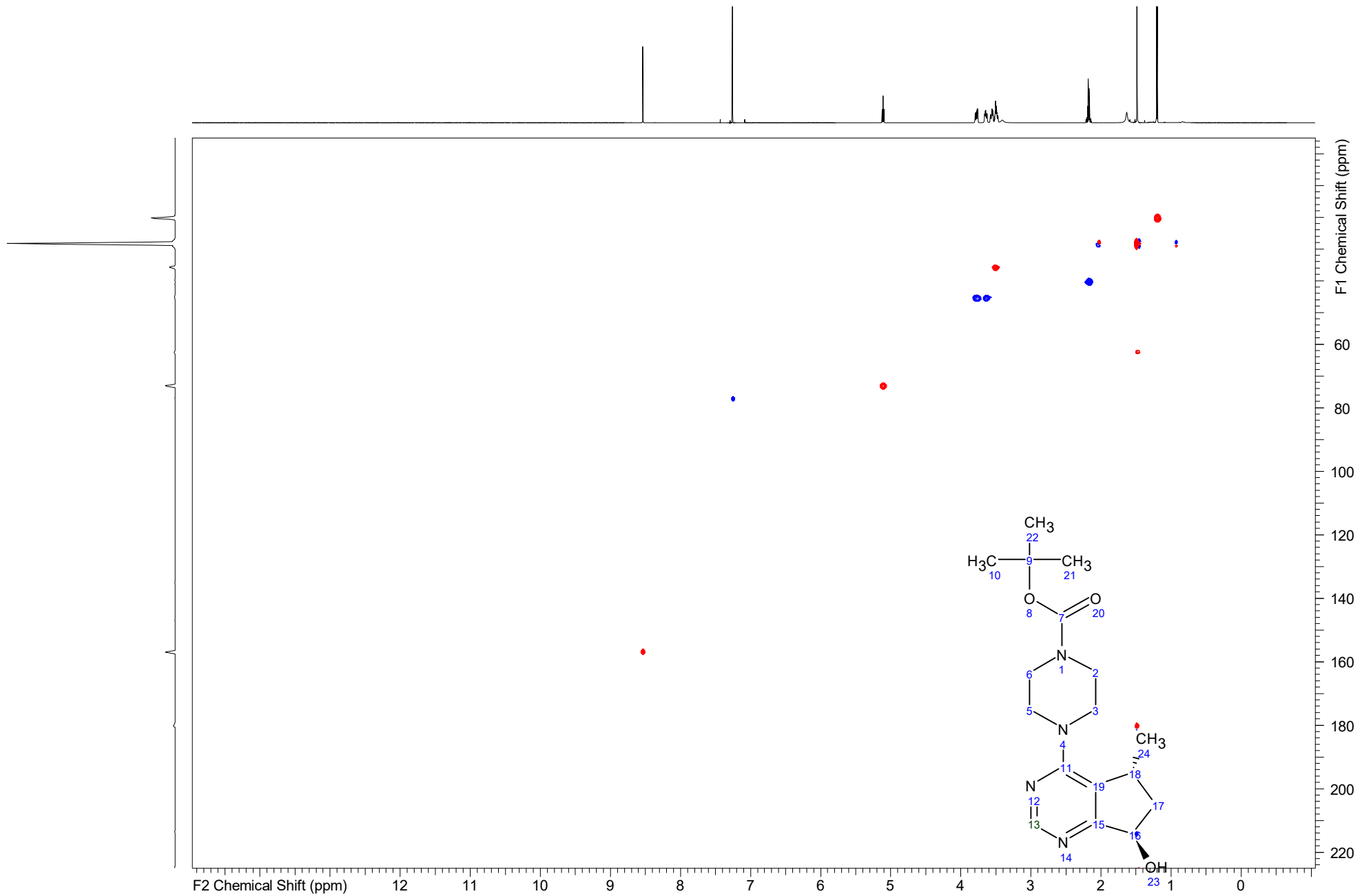
1H-NMR spectrum - expansion region 2



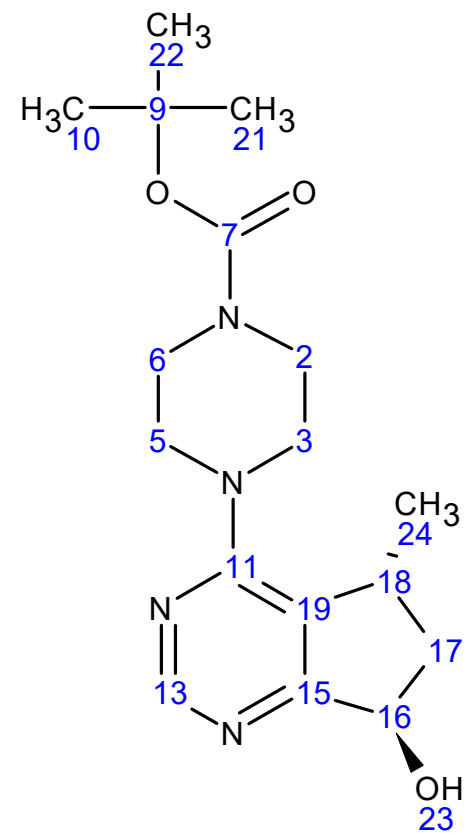
File Name	NMR\nmrfs_u\data\actual\nmr\20 21002020557\1000\PDATA\1\1r
Frequency (MHz)	600.1300
Nucleus	1H
Solvent	CHLOROFORM-d
Temperature (degree C)	25.027



Date	18 Oct 2021 19:28:40	File Name	NMR\nmrfs_u\data\actual\nmr\2021002020557\1022\pdata\1\2rr		
Frequency (MHz)	(600.1300, 150.9028)	Nucleus	(1H, 13C)	Solvent	CHLOROFORM-d
Spectrum Type	HSQC-DEPT				



Date	18 Oct 2021 19:28:40	File Name	NMR\nmrfs_u\data\actual\nmr\2021002020557\1022\pdata\1\2rr		
Frequency (MHz)	(600.1300, 150.9028)	Nucleus	(1H, 13C)	Solvent	CHLOROFORM-d
Spectrum Type	HSQC-DEPT				



2021002020556 1000 1 Q:\data\actual\nmr

