Supporting information for Haarr *et al*.

# 1,4-Dideoxy-1,4-imino-D-arabinitol (DAB) analogues possessing a hydrazide imide moiety as potent and selective α-mannosidase inhibitors

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$^{1}$H NMR, $^{13}$C NMR (some spectra are supported with HMBC), and IR

**Figure S1:** $^{1}H$ NMR, $CDCl_3$, 400 MHz: 2,3,5-Tri-*O*-benzyl-L-xylono-1,4-lactone (**8**)

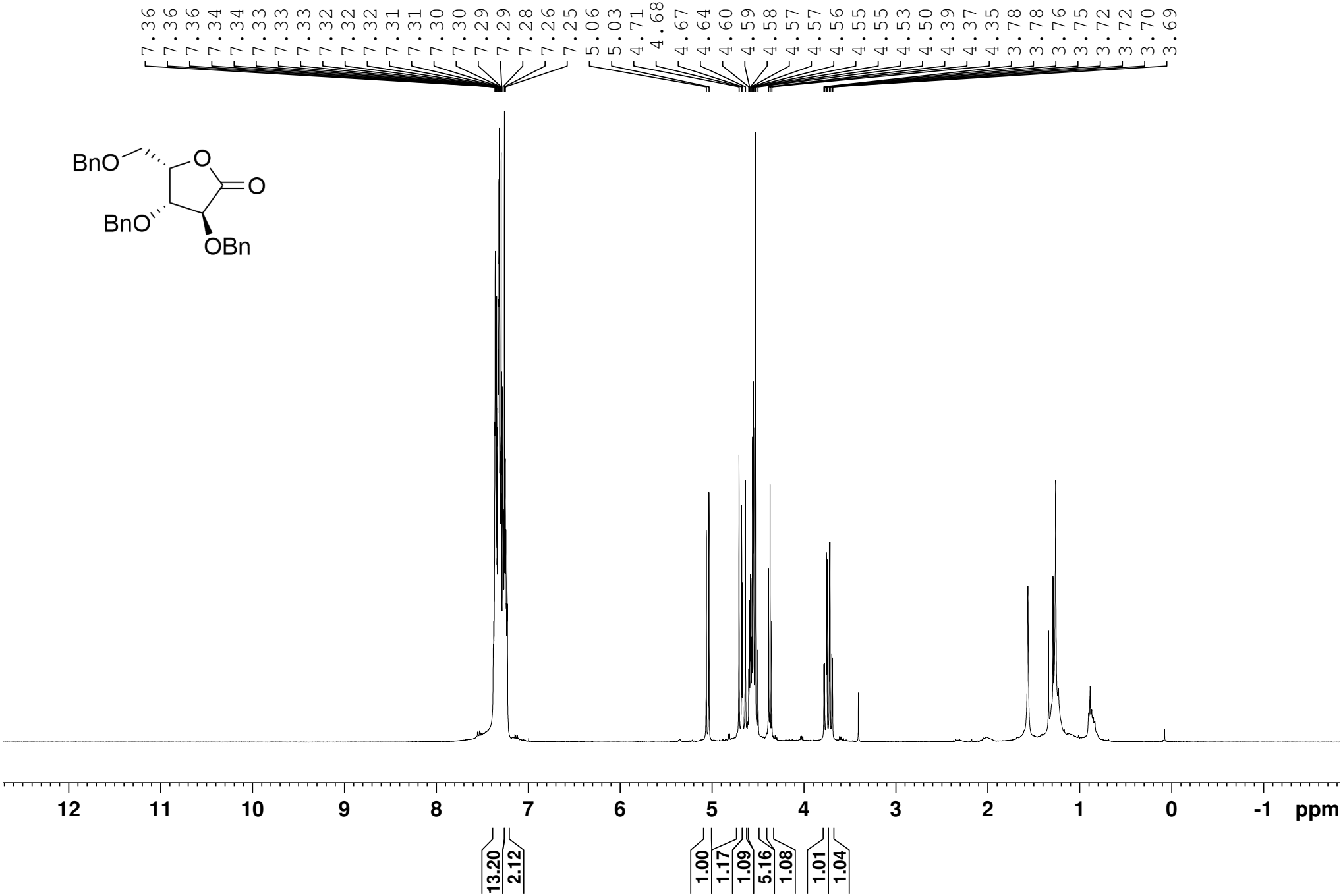


**Figure S2:** $^{13}C$ NMR, $CDCl_3$, 100 MHz: 2,3,5-Tri-O-benzyl-L-xylono-1,4-lactone (8)

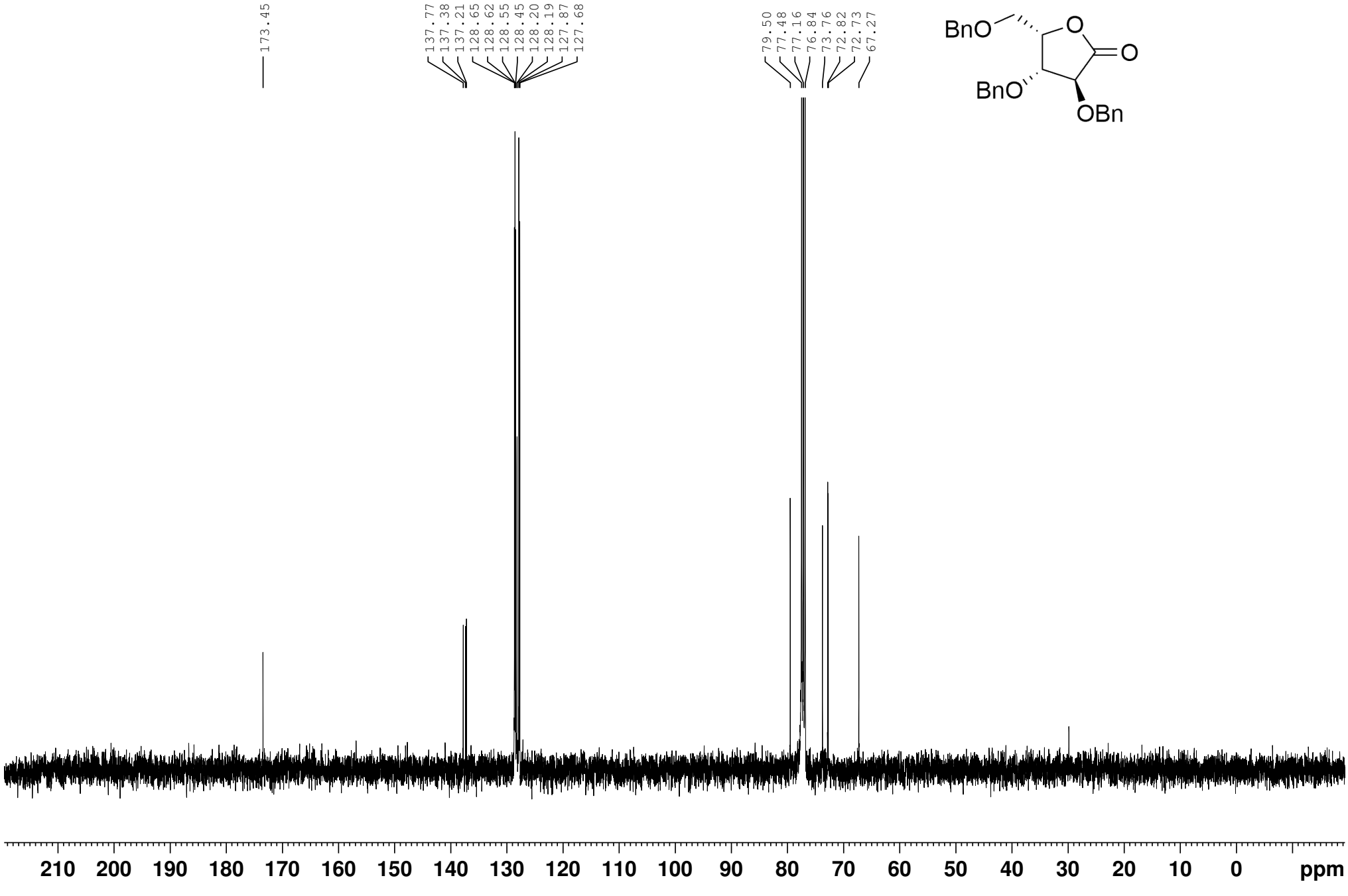


**Figure S3:** $^{1}H$-$^{13}C$ HSQC NMR ($CDCl_3$): 2,3,5-Tri-*O*-benzyl-L-xylono-1,4-lactone (**8**)

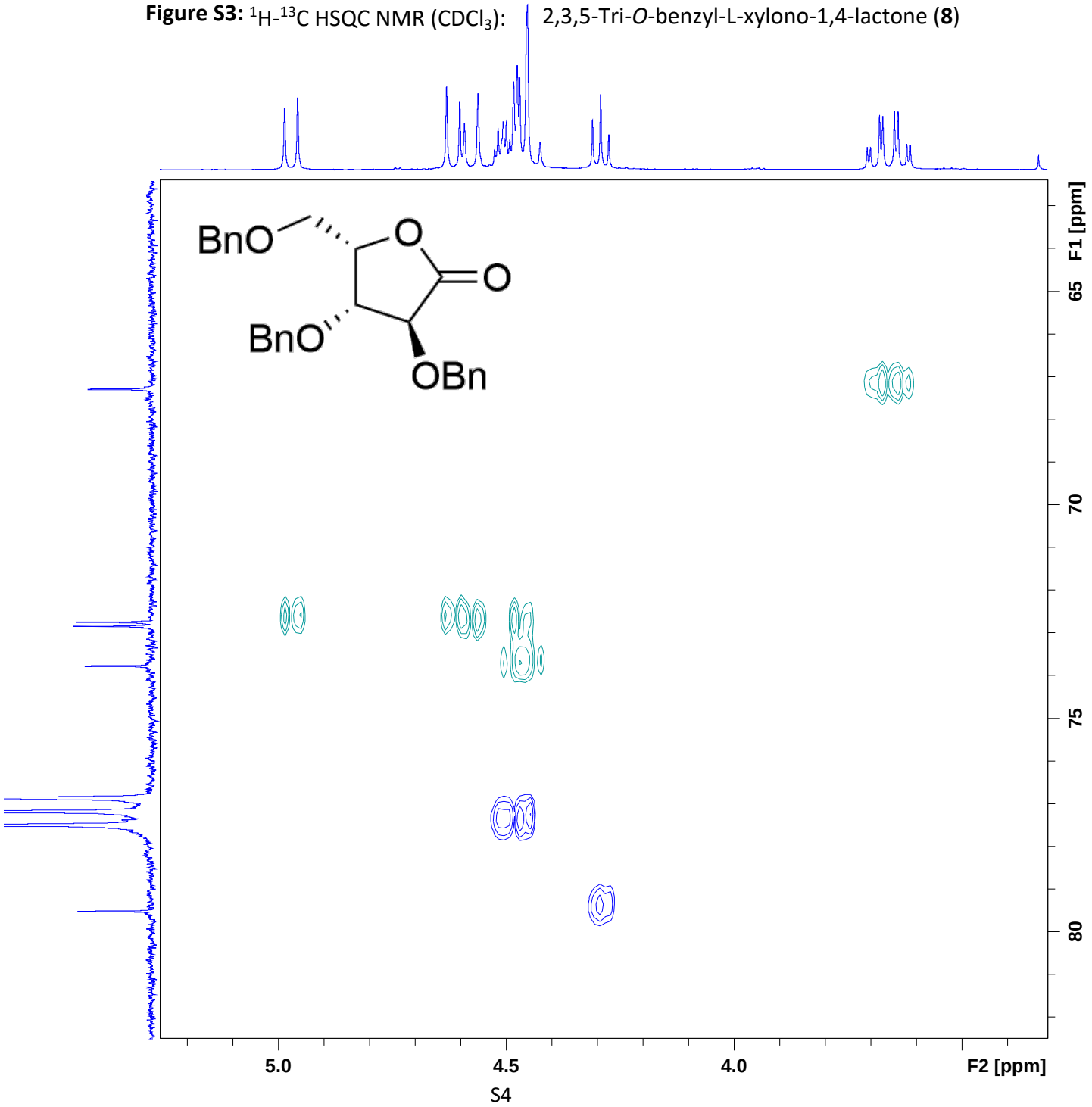


**Figure S4:** $^{1}H$ NMR, $CDCl_3$, 400 MHz: 2,3,5-Tris-*O*-benzyl-L-xylononitrile (**9**)

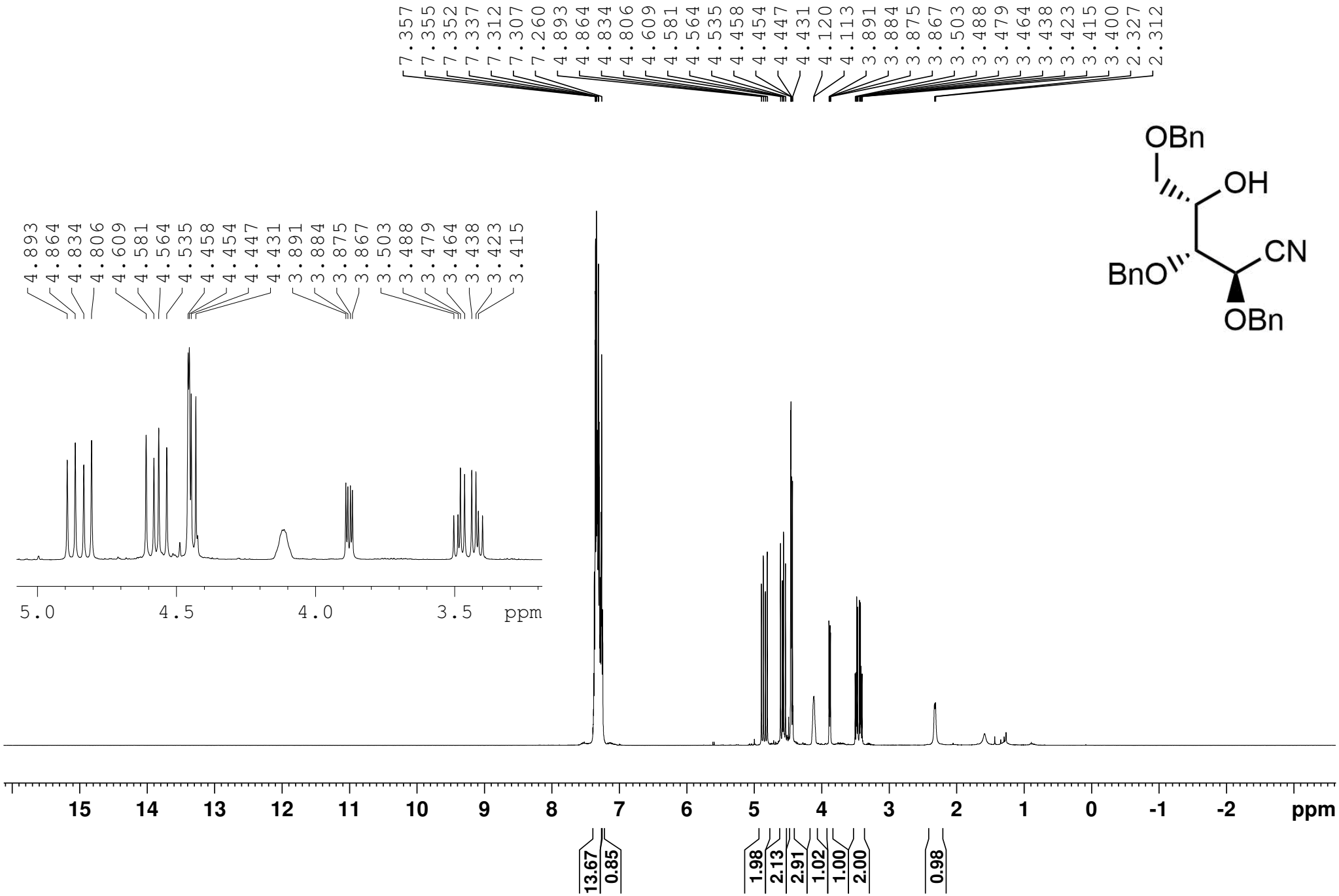


**Figure S5:** $^{13}C$ NMR, $CDCl_3$, 100 MHz: 2,3,5-Tris-*O*-benzyl-L-xylononitrile (**9**)

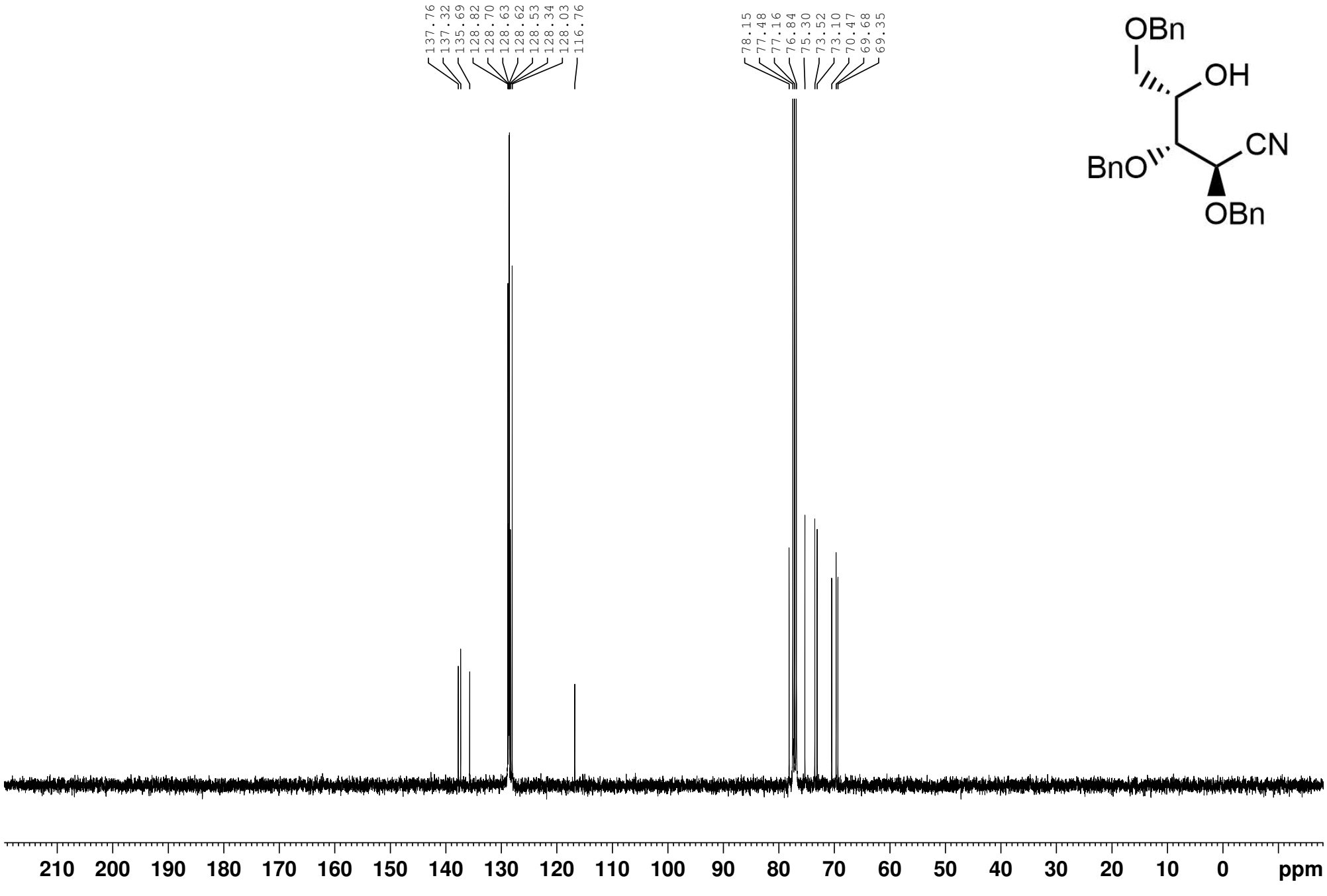


**Figure S6:** IR: 2,3,5-Tris-*O*-benzyl-L-xylononitrile (**9**)

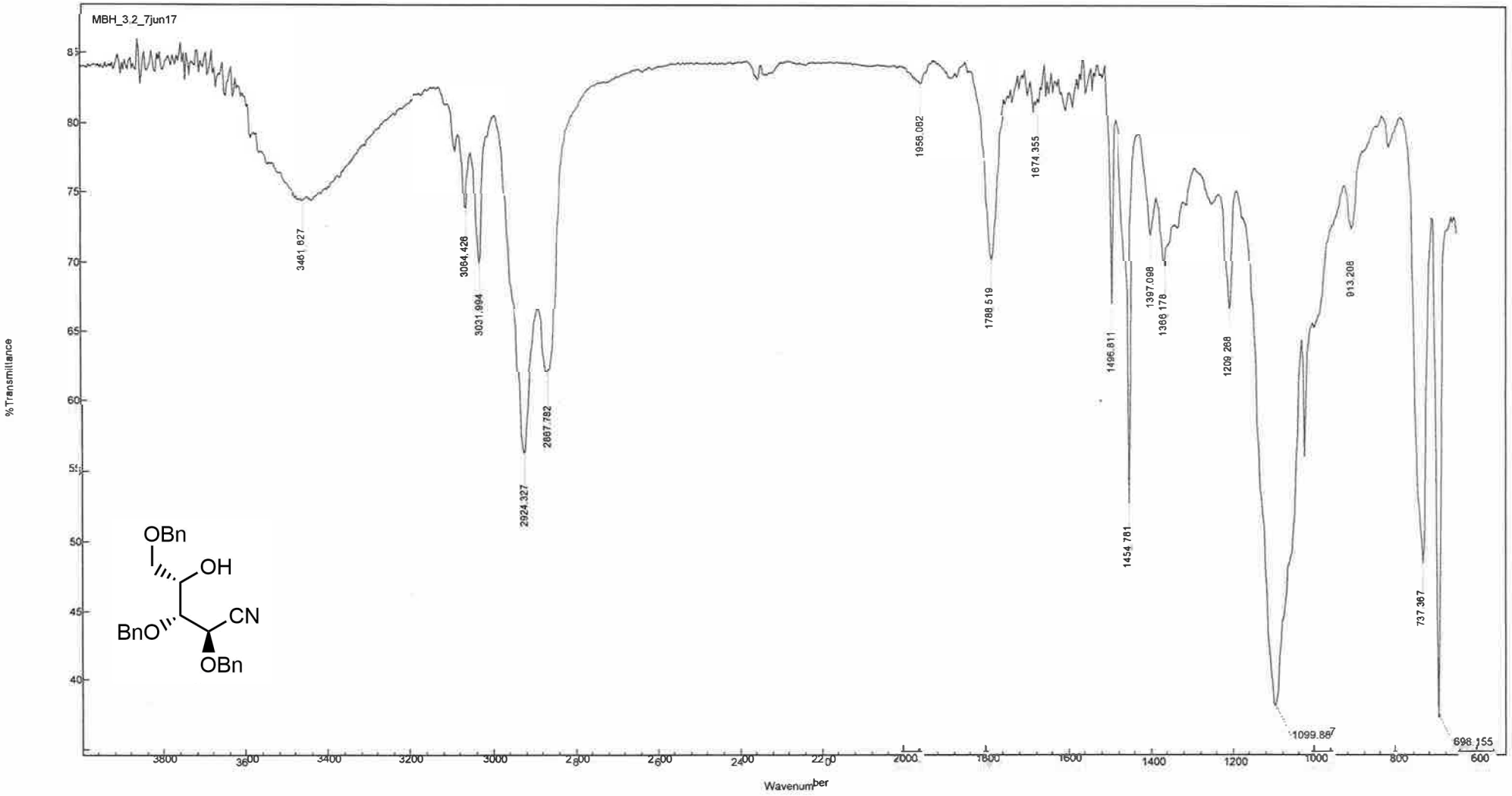


**Figure S7:** $^{1}$H NMR, $CDCl_3$, 400 MHz: 2,3,5-Tris-*O*-benzyl-4-(2-tert-butoxycarbonyl)hydrazinyl-4-deoxy-D-arabinonitrile (**10**)

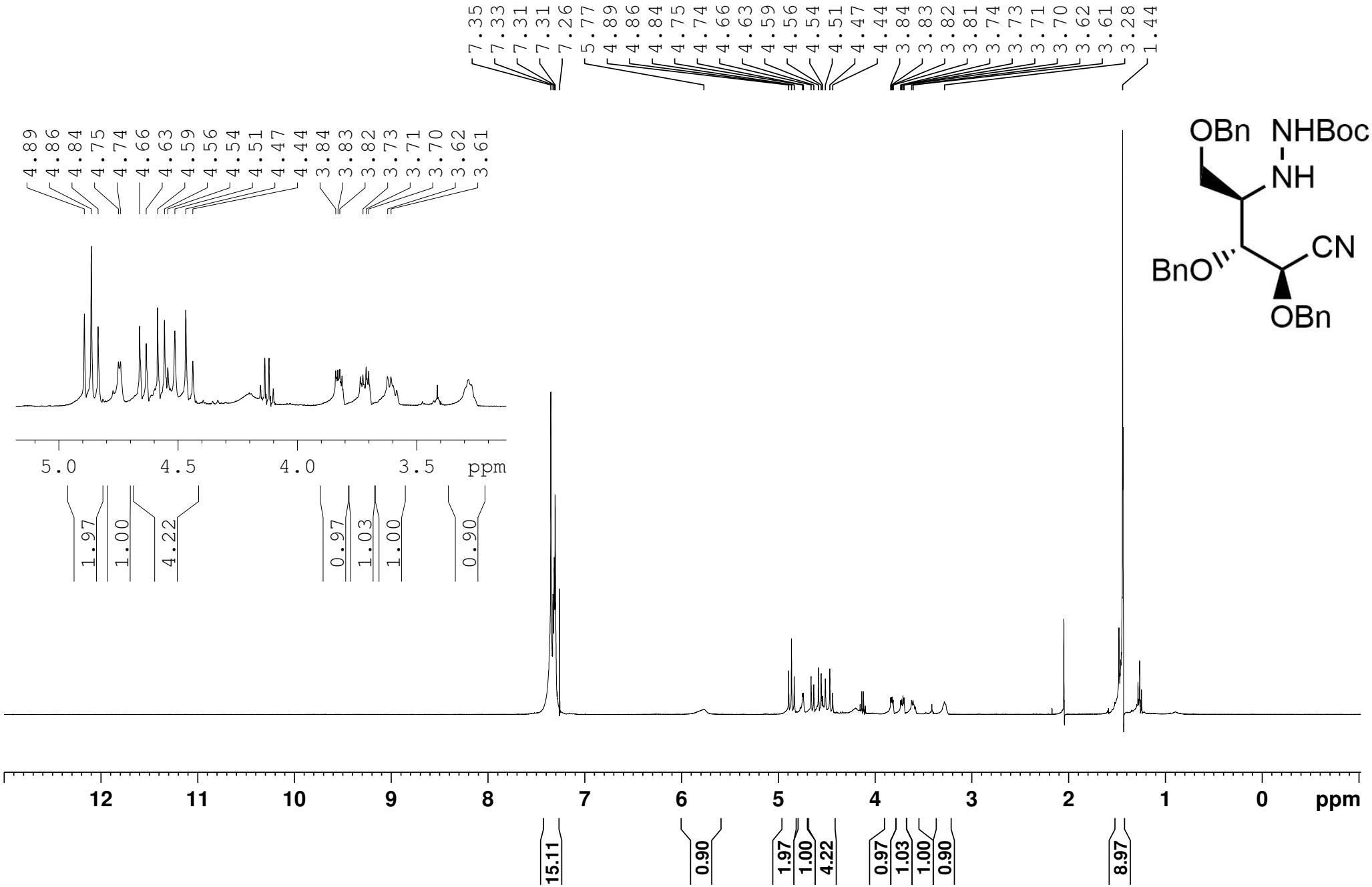


**Figure S8:** $^{13}C$ NMR, $CDCl_3$, 100 MHz: 2,3,5-Tris-*O*-benzyl-4-(2-tert-butoxycarbonyl)hydrazinyl-4-deoxy-D-arabinonitrile (**10**)

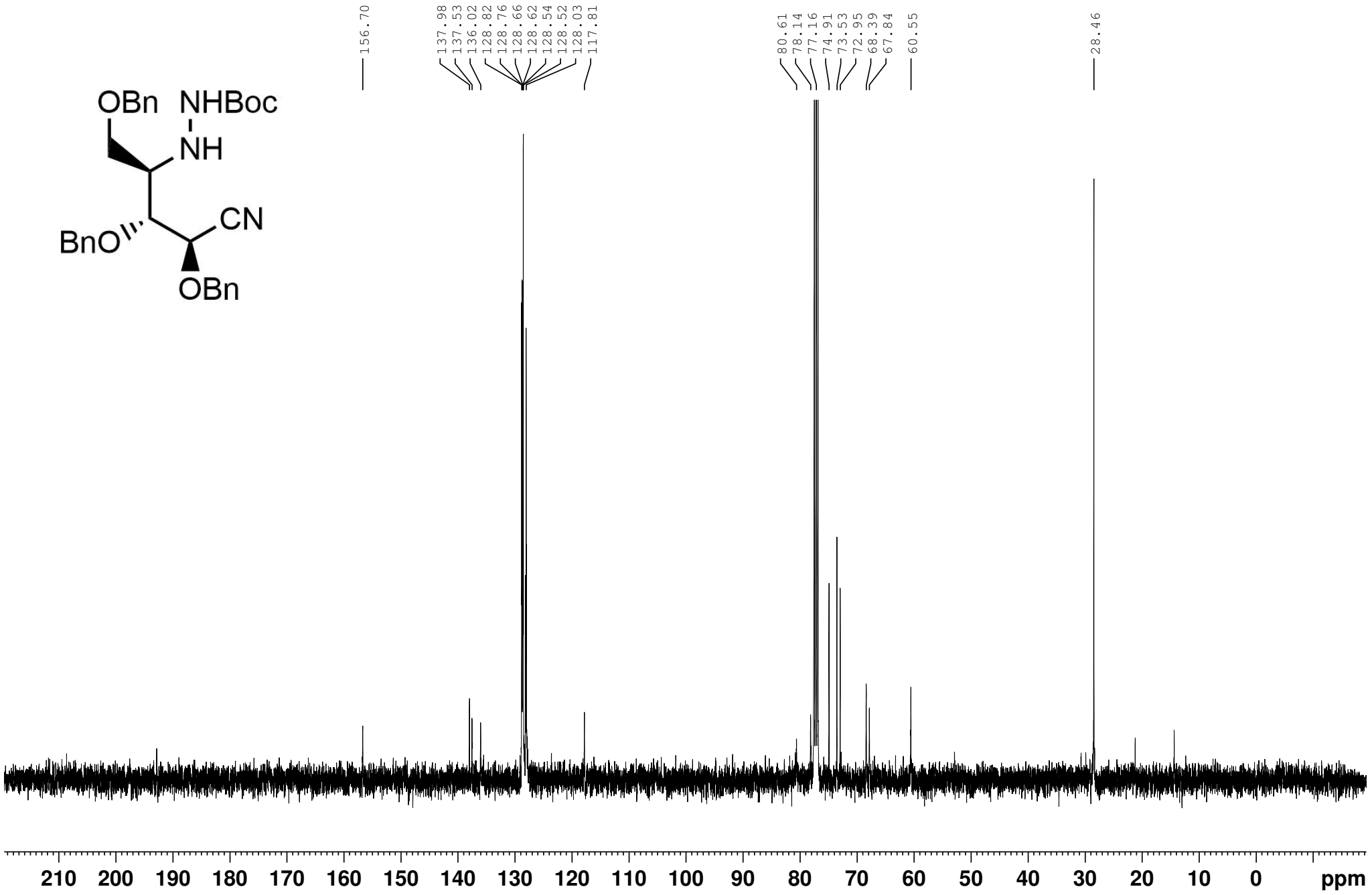


**Figure S9:** IR: 2,3,5-Tris-*O*-benzyl-4-(2-tert-butoxycarbonyl)hydrazinyl-4-deoxy-D-arabinonitrile (**10**)

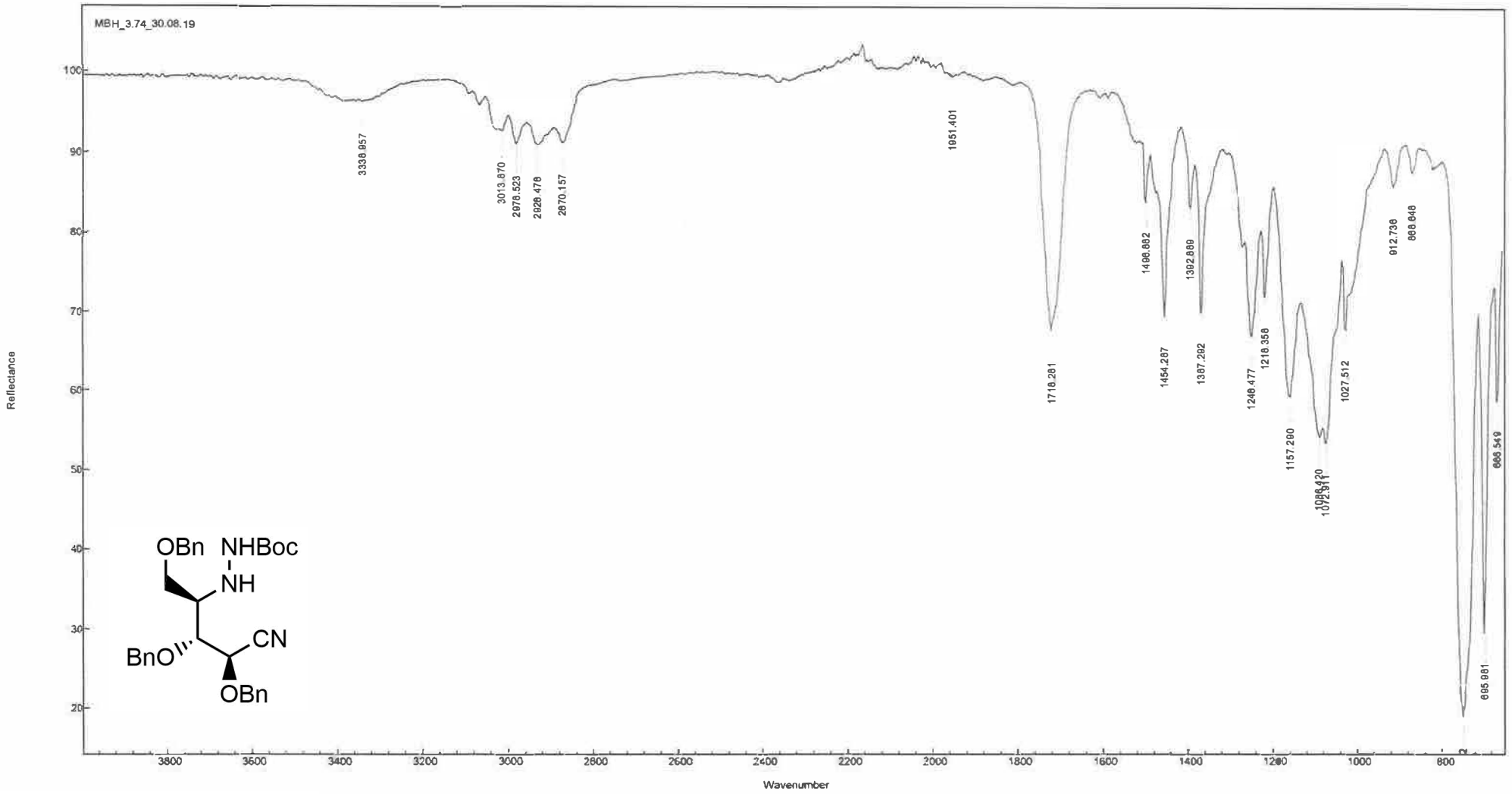


**Figure S10:** $^{1}$H NMR, MeOD, 400 MHz: (2*R*,3*R*,4*R*)-1-Amino-3,4-bis(benzyloxy)-2-((benzyloxy)methyl)-5-iminopyrrolidine hydrochloride (**11**)

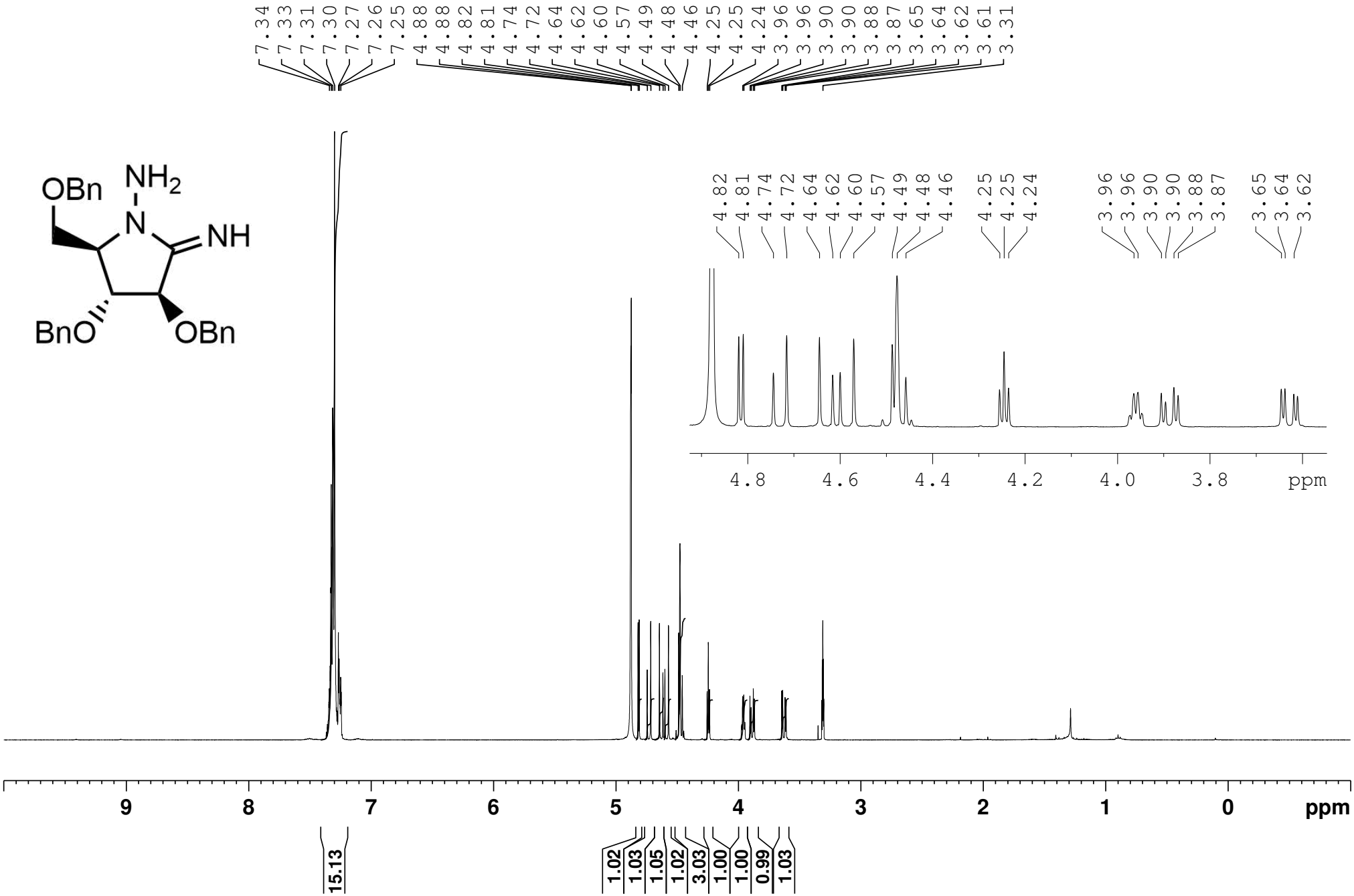


**Figure S11:** $^{13}$C NMR, MeOD, 100 MHz: (2*R*,3*R*,4*R*)-1-Amino-3,4-bis(benzyloxy)-2-((benzyloxy)methyl)-5-iminopyrrolidine hydrochloride (**11**)

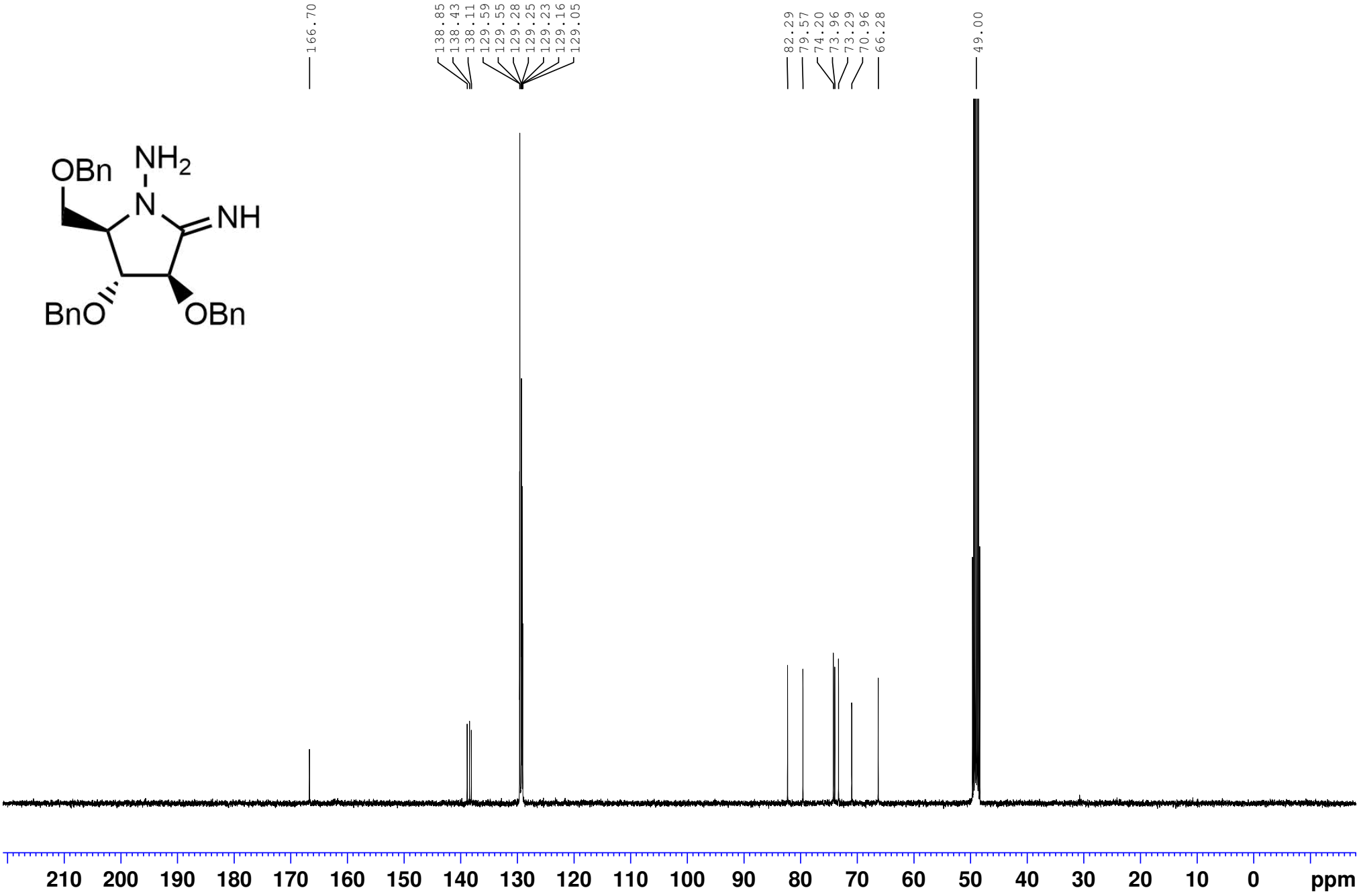


**Figure S12:** IR: (2*R*,3*R*,4*R*)-1-Amino-3,4-bis(benzyloxy)-2-((benzyloxy)methyl)-5-iminopyrrolidine hydrochloride (**11**)

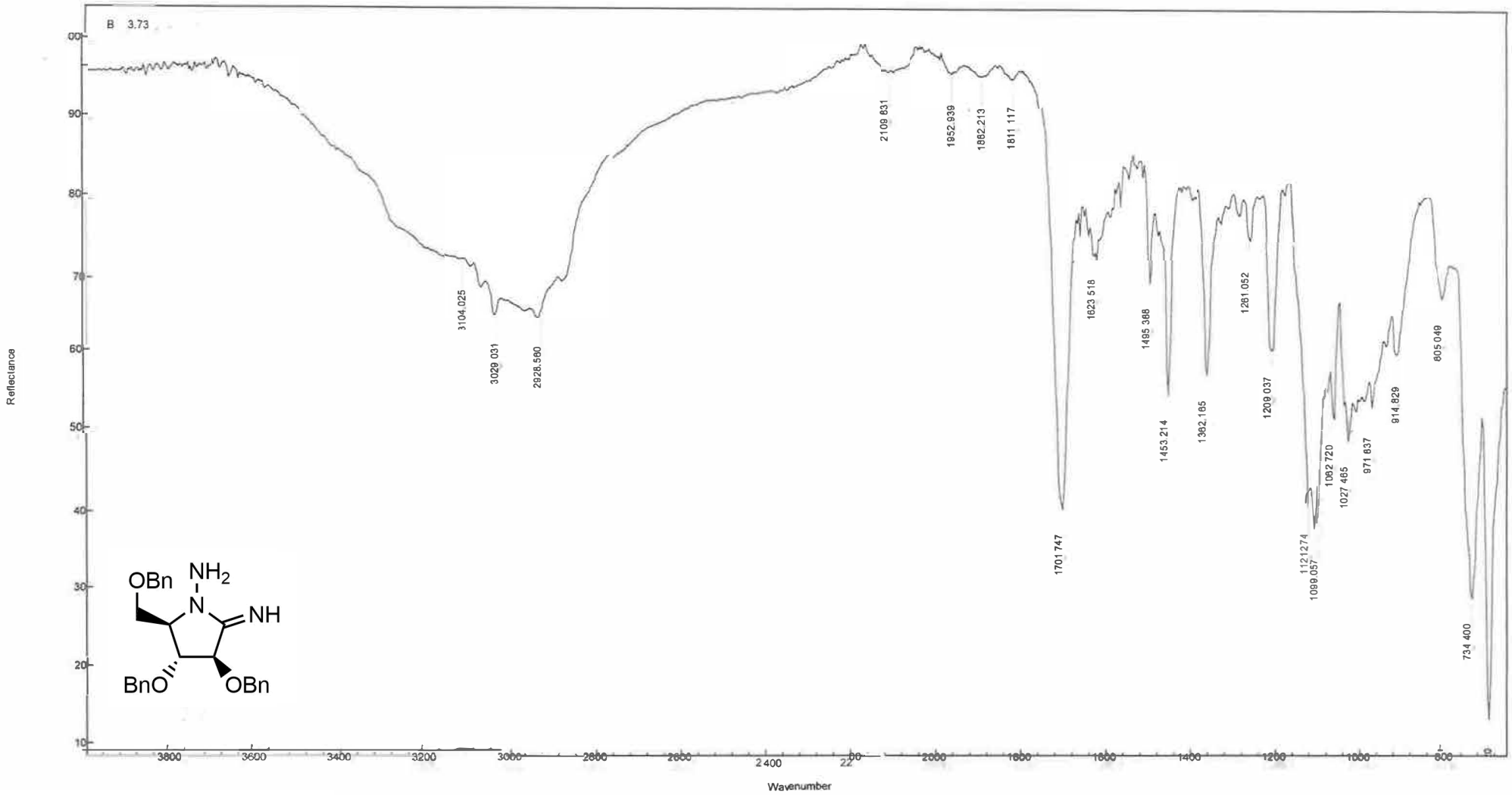


**Figure S13:** $^{1}H$ NMR, $D_2O$, 400 MHz: (2*R*,3*R*,4*R*)-1-Amino-3,4-dihydroxy-2-(hydroxymethyl)-5-iminopyrrolidine hydrochloride (**4Cl**)

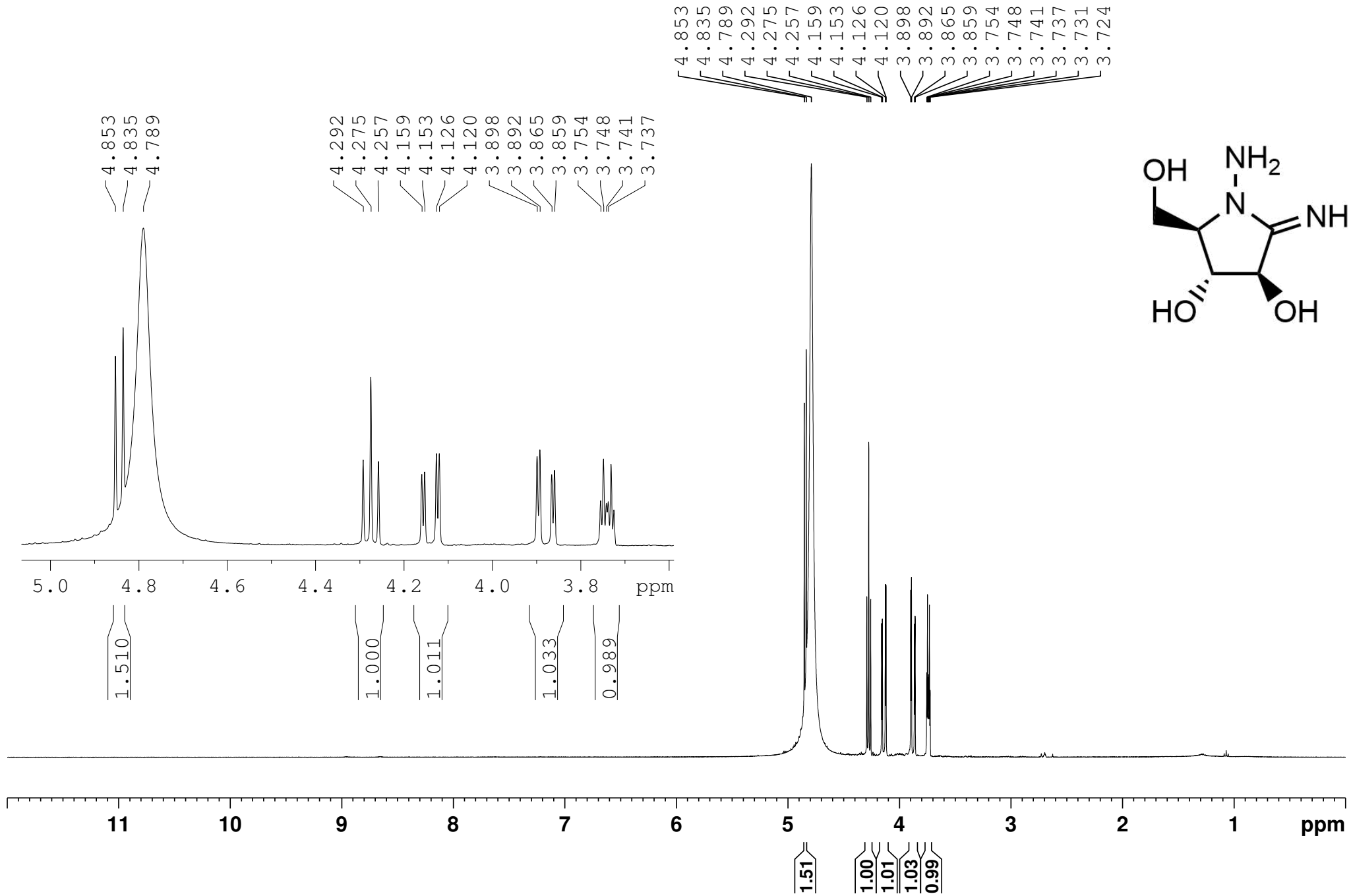


**Figure S14:** $^{13}C$ NMR, $D_2O$, 100 MHz: (2*R*,3*R*,4*R*)-1-Amino-3,4-dihydroxy-2-(hydroxymethyl)-5-iminopyrrolidine hydrochloride (**4Cl**)

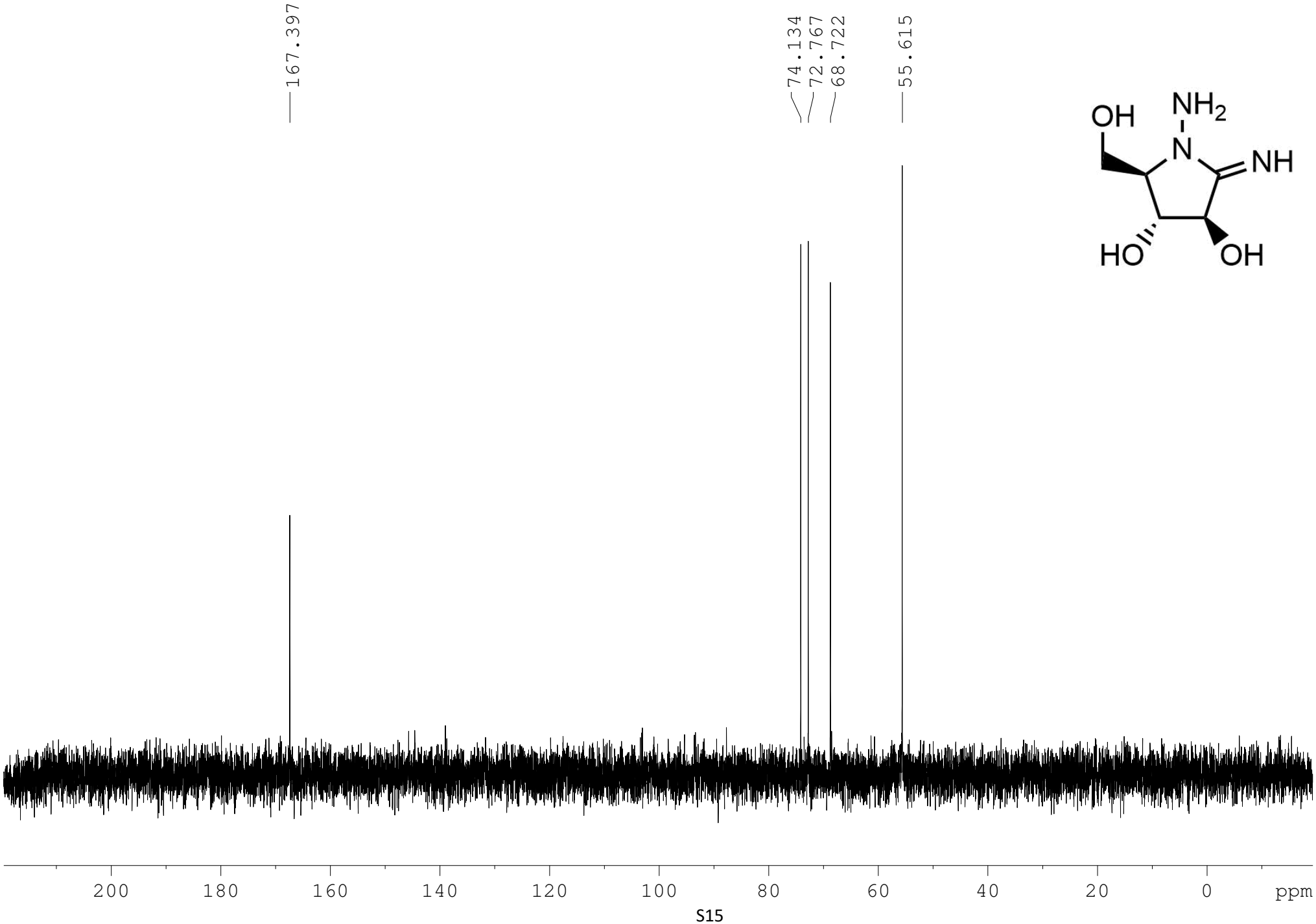
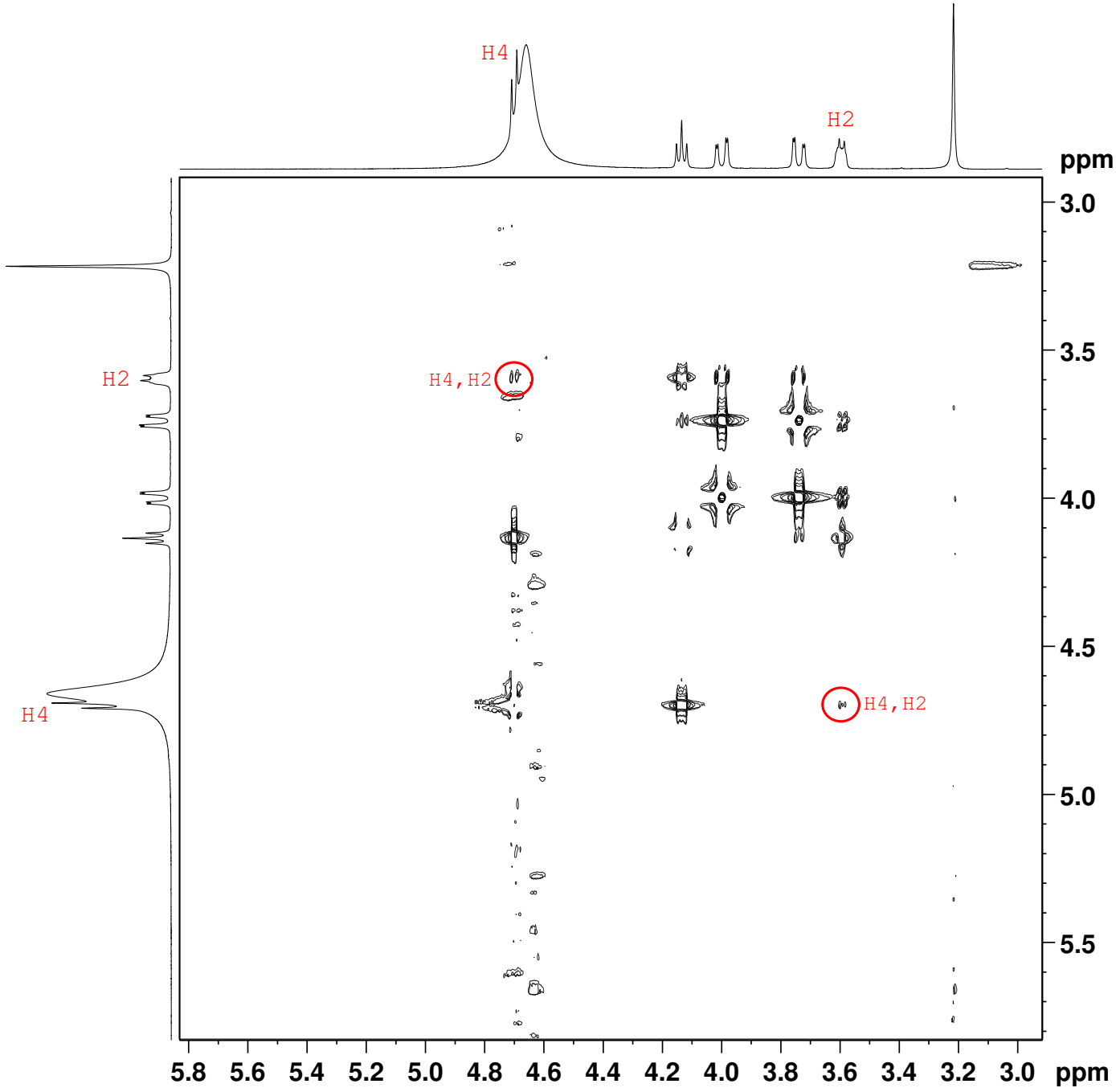


**Figure S15:** NOESY NMR, $D_2O$: (2*R*,3*R*,4*R*)-1-Amino-3,4-dihydroxy-2-(hydroxymethyl)-5-iminopyrrolidine hydrochloride (**4Cl**)



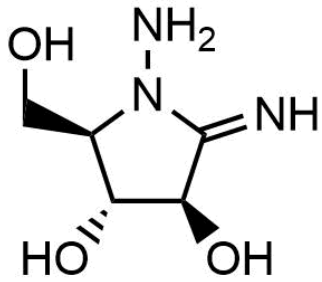



**Figure S16:** IR: (2*R*,3*R*,4*R*)-1-Amino-3,4-dihydroxy-2-(hydroxymethyl)-5-iminopyrrolidine hydrochloride (**4Cl**)

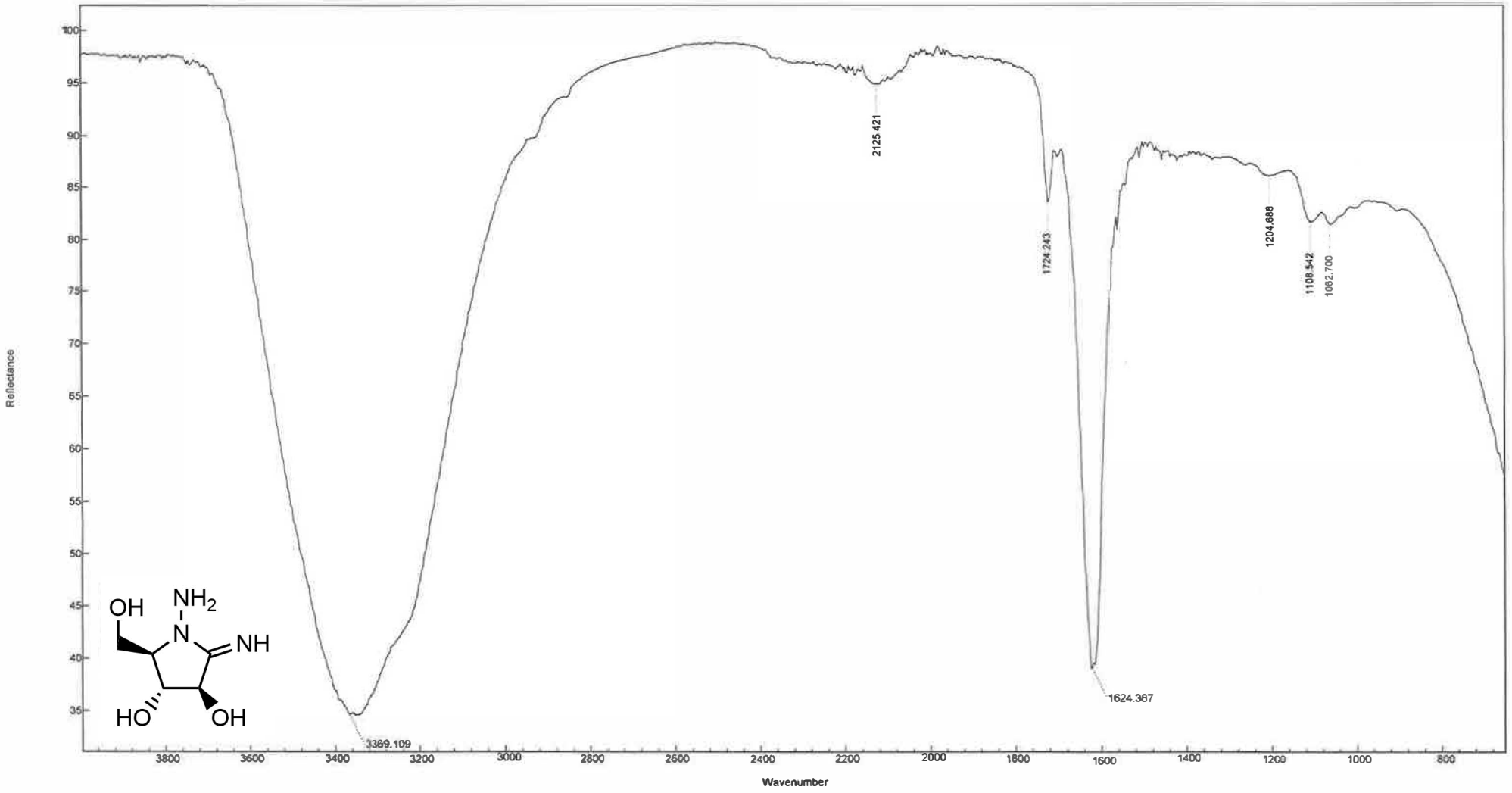


**Figure S17:** $^{1}H$ NMR, $D_2O$, 400 MHz: (2*R*,3*R*,4*R*)-1-(Ethylamino)-3,4-dihydroxy-2-(hydroxymethyl)-5-iminopyrrolidine hydrochloride (**5Cl**)

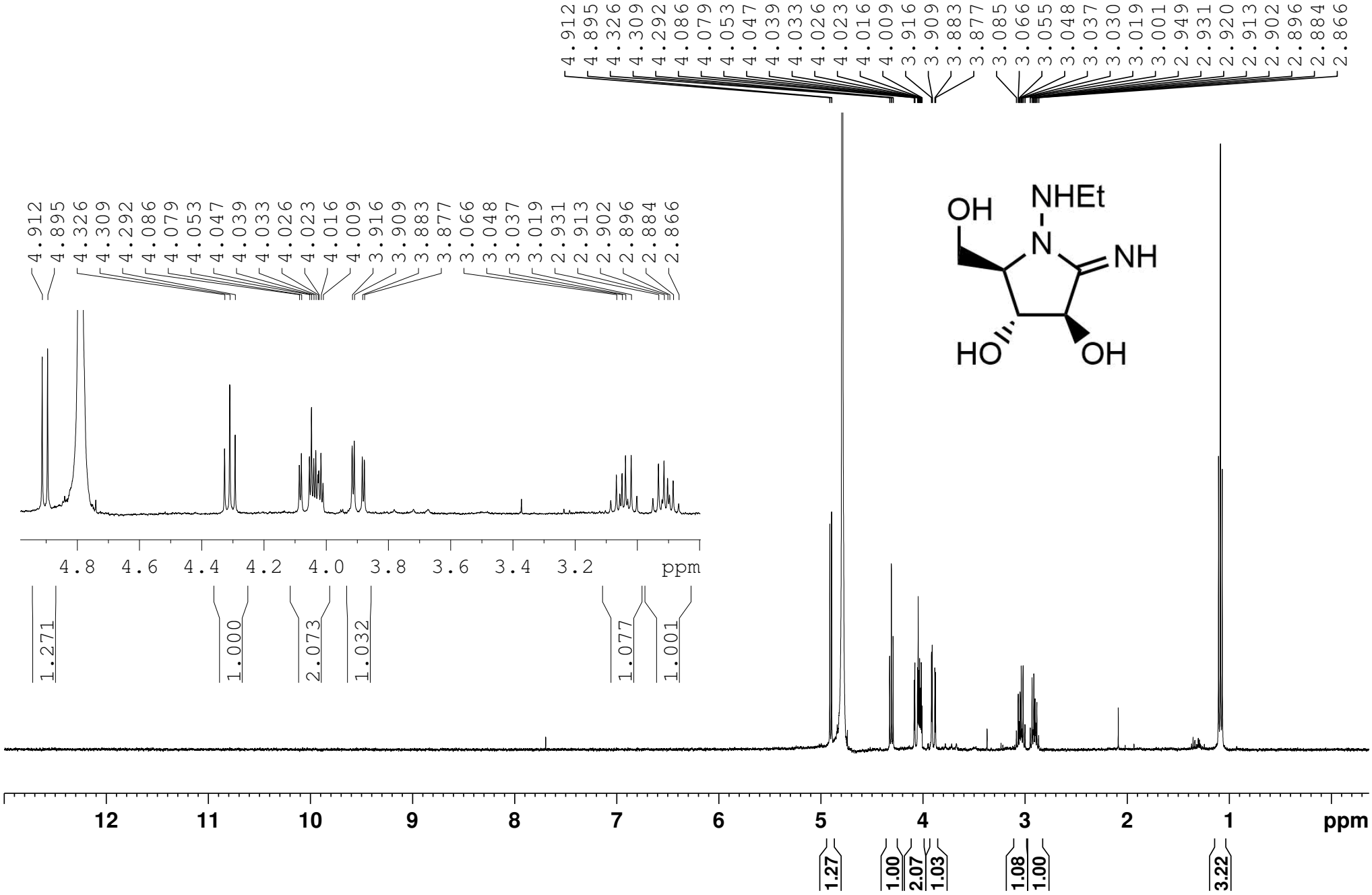


**Figure S18:** $^{13}C$ NMR, $D_2O$, 100 MHz: (2*R*,3*R*,4*R*)-1-(Ethylamino)-3,4-dihydroxy-2-(hydroxymethyl)-5-iminopyrrolidine hydrochloride (**5Cl**)

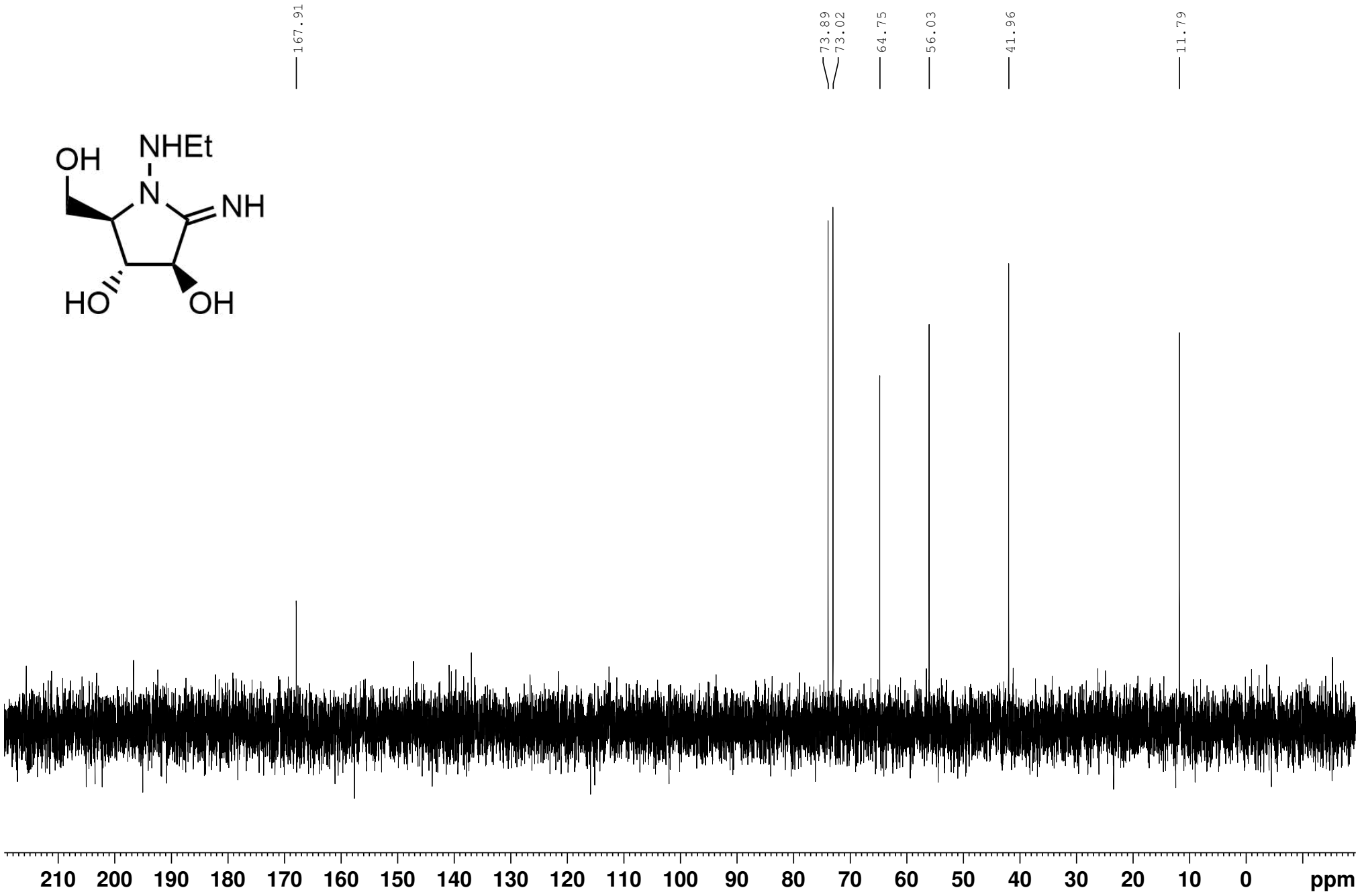


**Figure S19:** IR: (2*R*,3*R*,4*R*)-1-(Ethylamino)-3,4-dihydroxy-2-(hydroxymethyl)-5-iminopyrrolidine hydrochloride (**5Cl**)

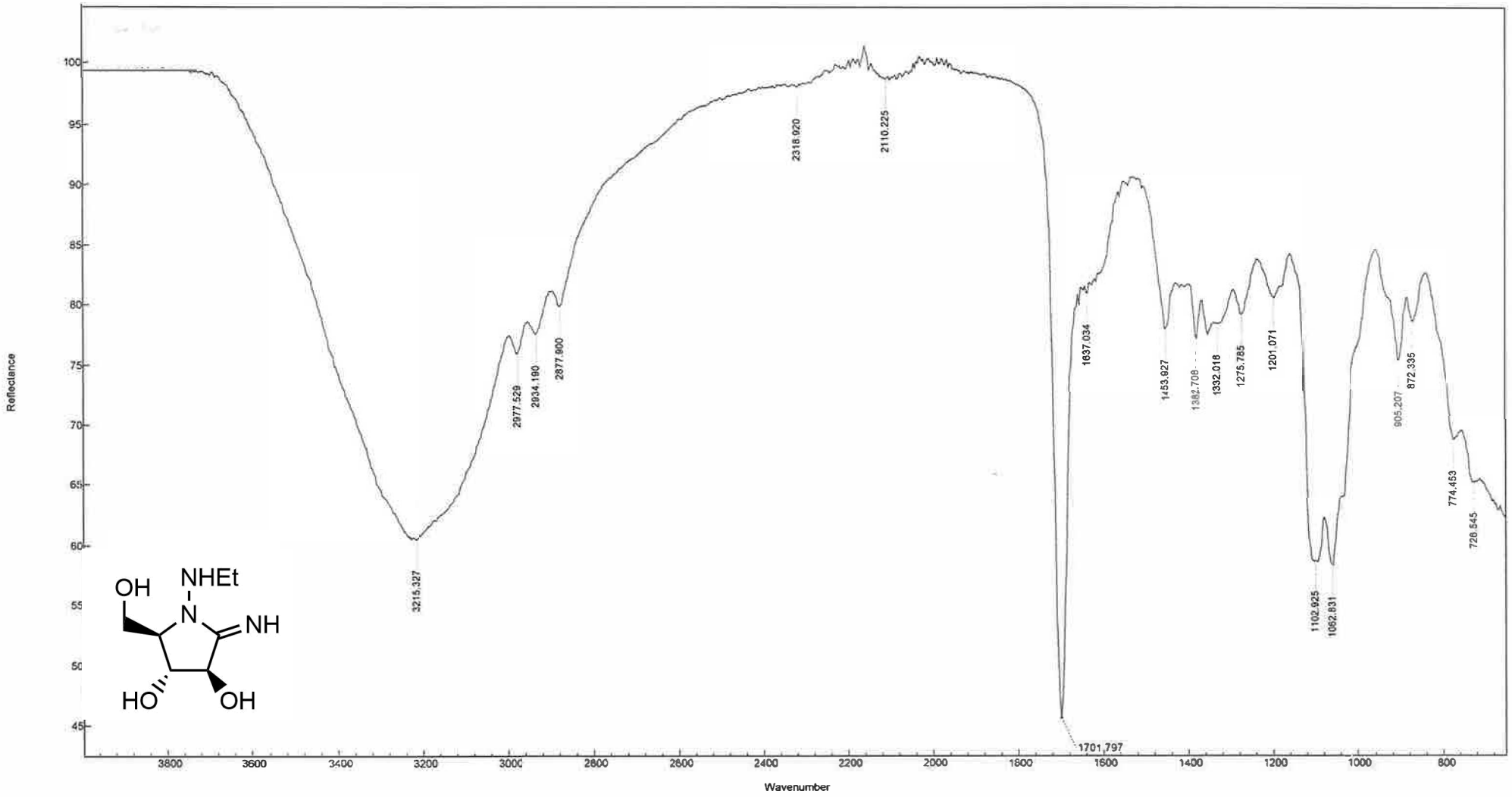


**Figure S20:** $^{1}H$ NMR, $D_2O$, 400 MHz: (2*R*,3*R*,4*R*)-1-Amino-3,4-dihydroxy-5-(hydroxymethyl)-2-pyrrolidinone hydrochloride (**5Cl**)

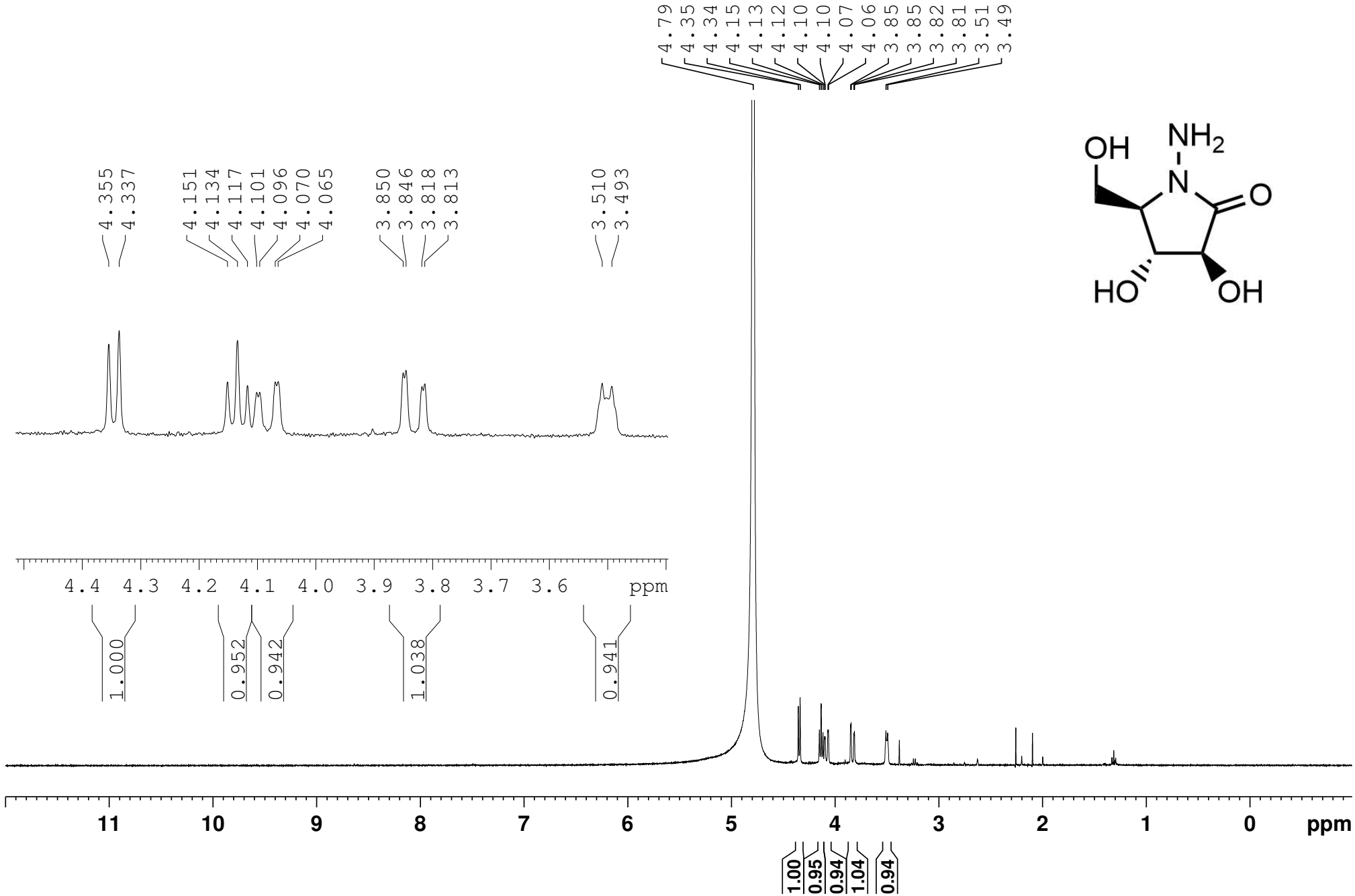


**Figure S21:** $^{13}C$ NMR, $D_2O$, 100 MHz: (2*R*,3*R*,4*R*)-1-Amino-3,4-dihydroxy-5-(hydroxymethyl)-2-pyrrolidinone hydrochloride (**5Cl**)

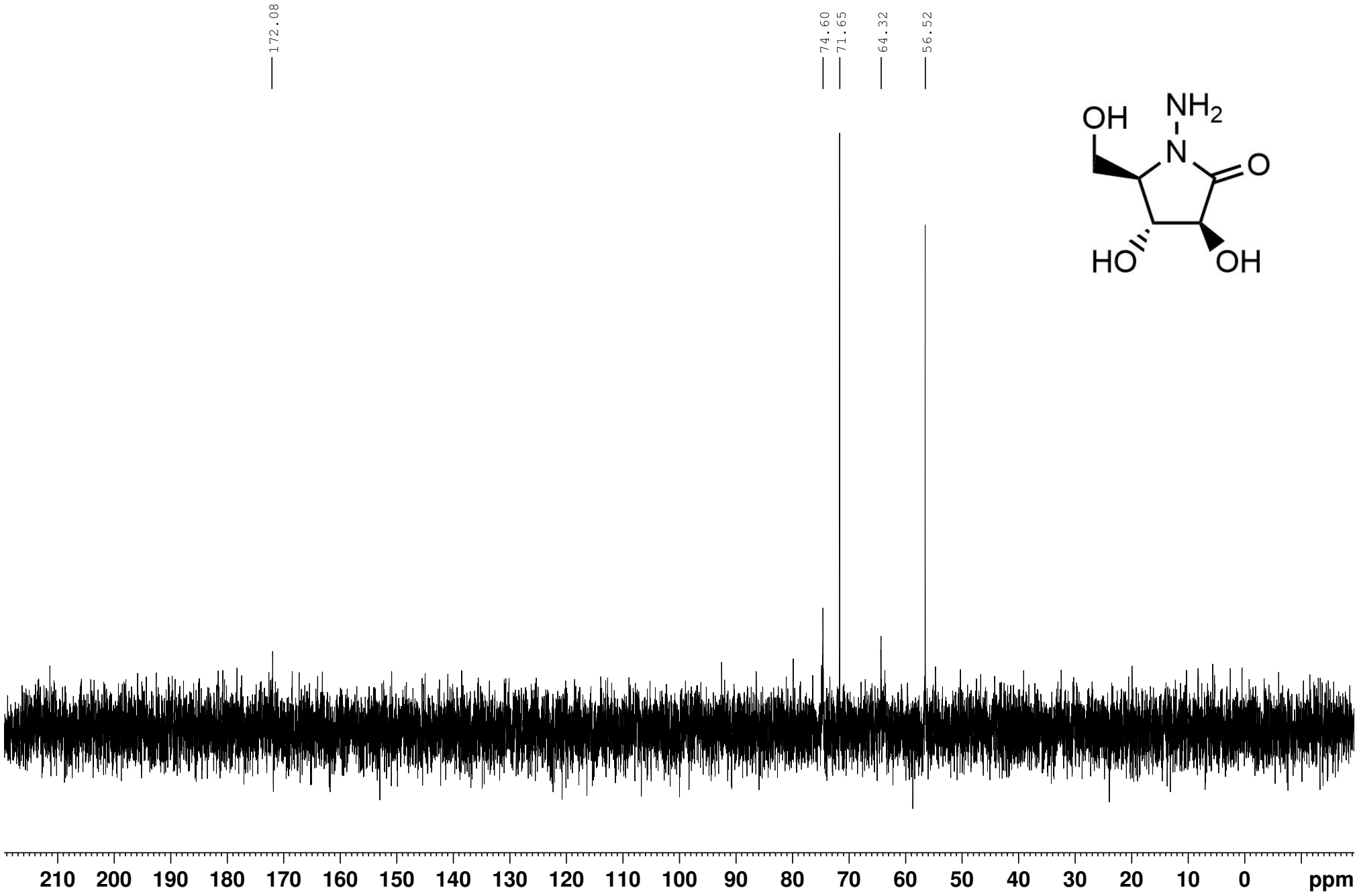
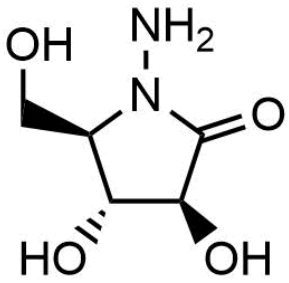


**Figure S22:** $^{1}H$ -$^{13}C$ HMBC NMR, $D_2O$: (2*R*,3*R*,4*R*)-1-Amino-3,4-dihydroxy-5-(hydroxymethyl)-2-pyrrolidinone hydrochloride (**5Cl**)



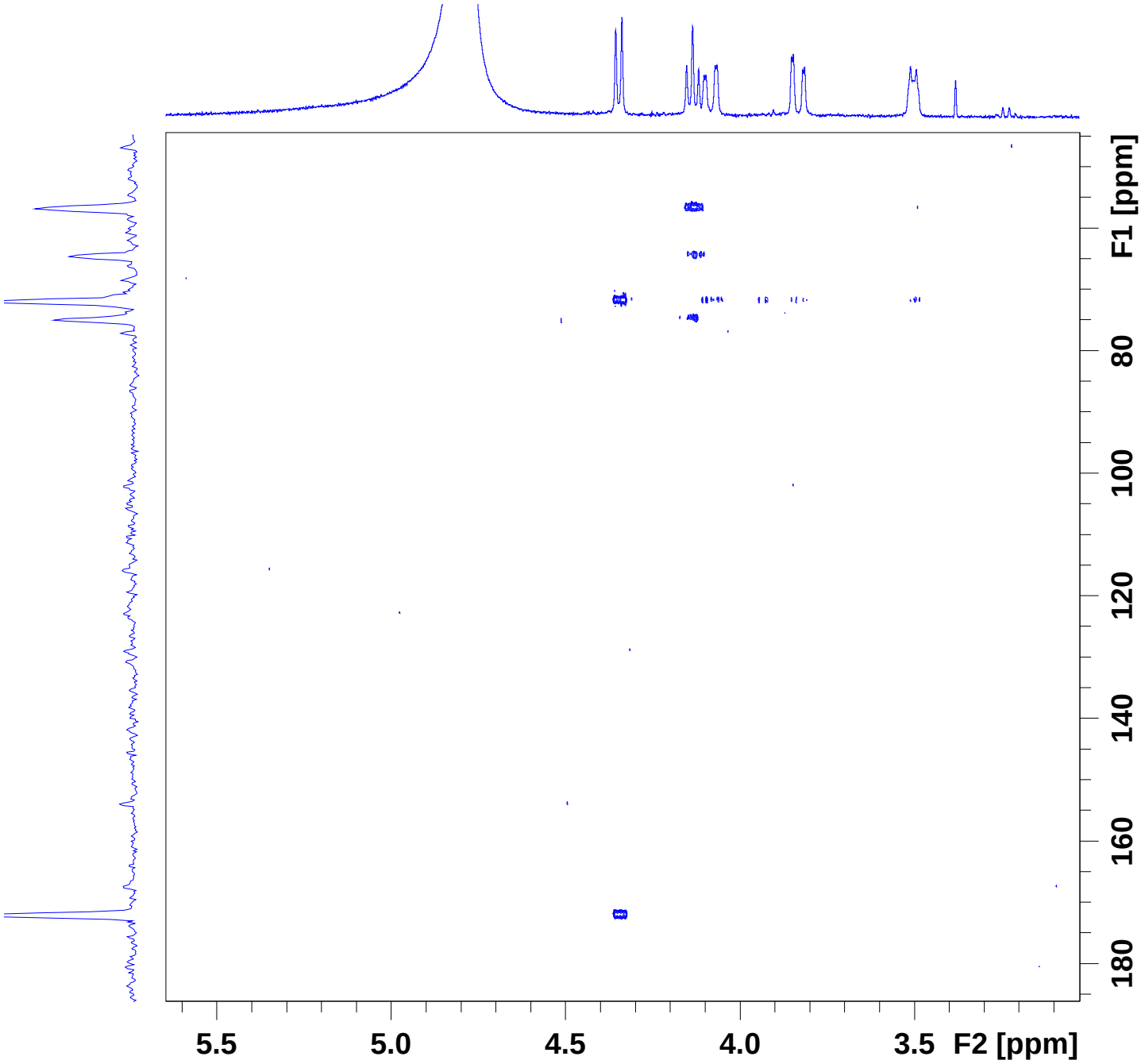



**Figure S23:** IR: (2*R*,3*R*,4*R*)-1-Amino-3,4-dihydroxy-5-(hydroxymethyl)-2-pyrrolidinone hydrochloride (**5Cl**)

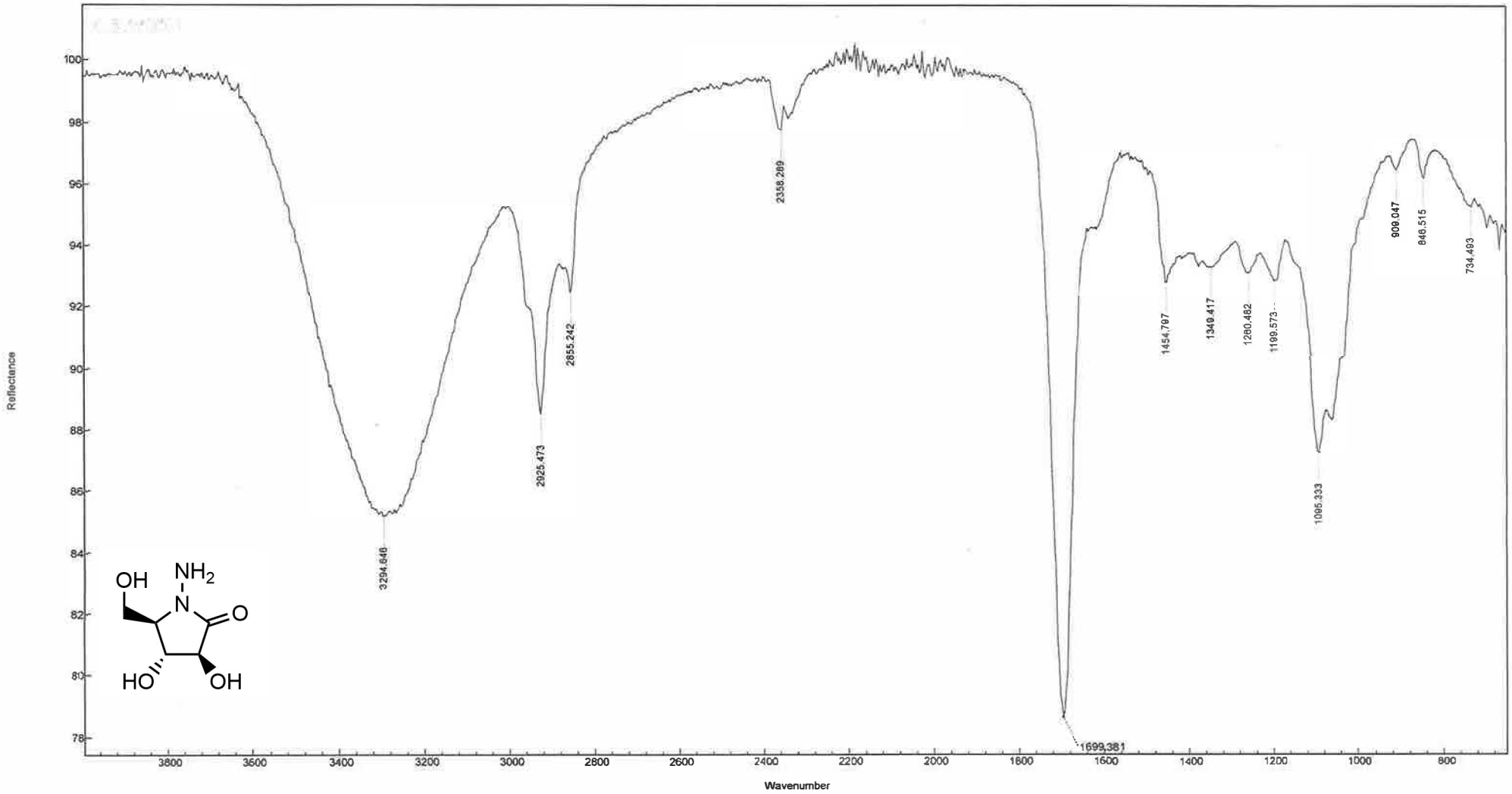


**Figure S24:** $^{1}H$ NMR, $CDCl_3$, 400 MHz: 2,3,5-Tris-*O*-benzyl-4-(1-*N*-benzyl-(2-tert-butoxycarbonyl)hydrazinyl)-4-deoxy-D-arabinonitrile (**13**)

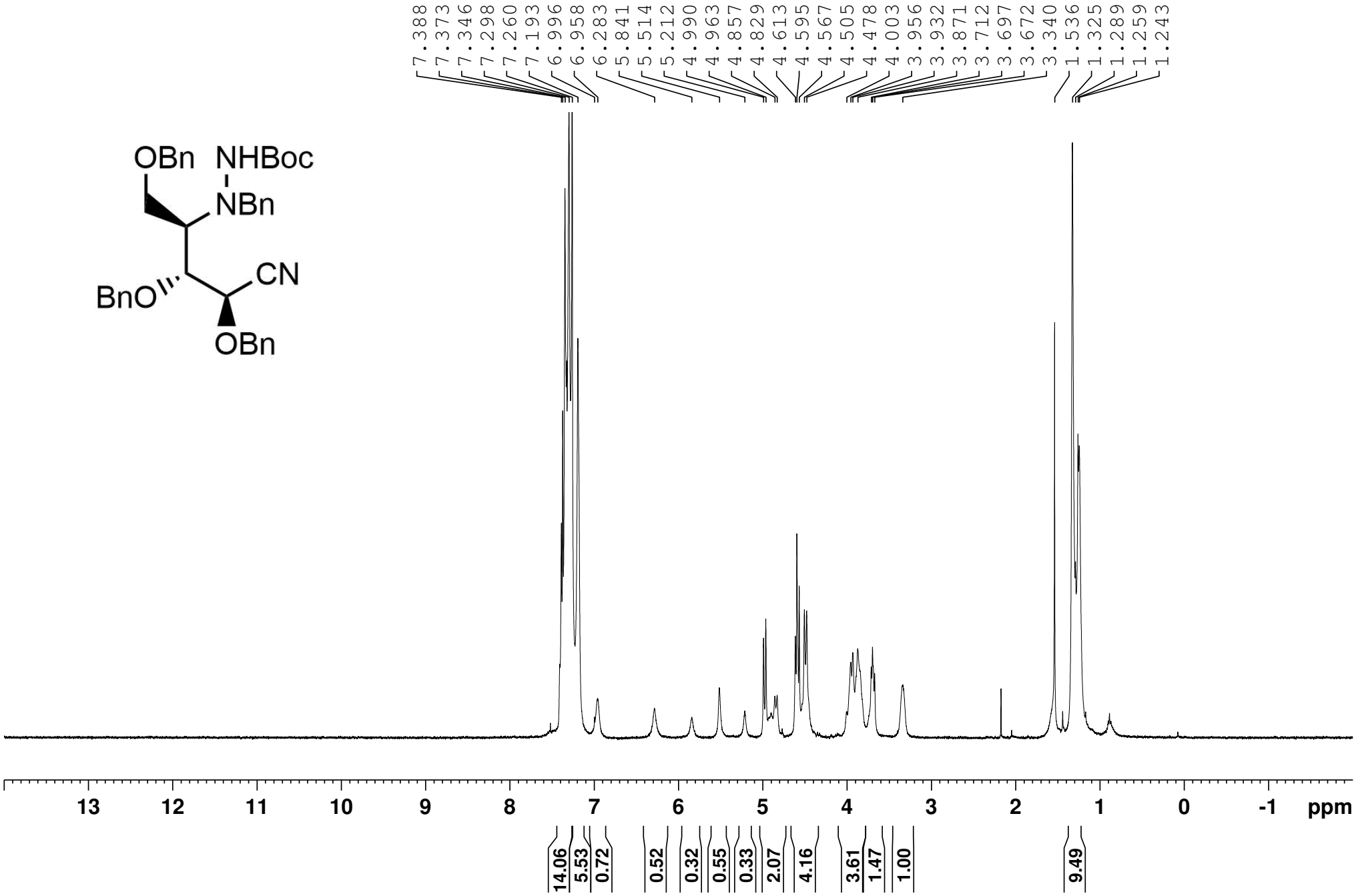


**Figure S25:** $^{13}C$ NMR, $CDCl_3$, 100 MHz: 2,3,5-Tris-*O*-benzyl-4-(1-*N*-benzyl-(2-tert-butoxycarbonyl)hydrazinyl)-4-deoxy-D-arabinonitrile (**13**)

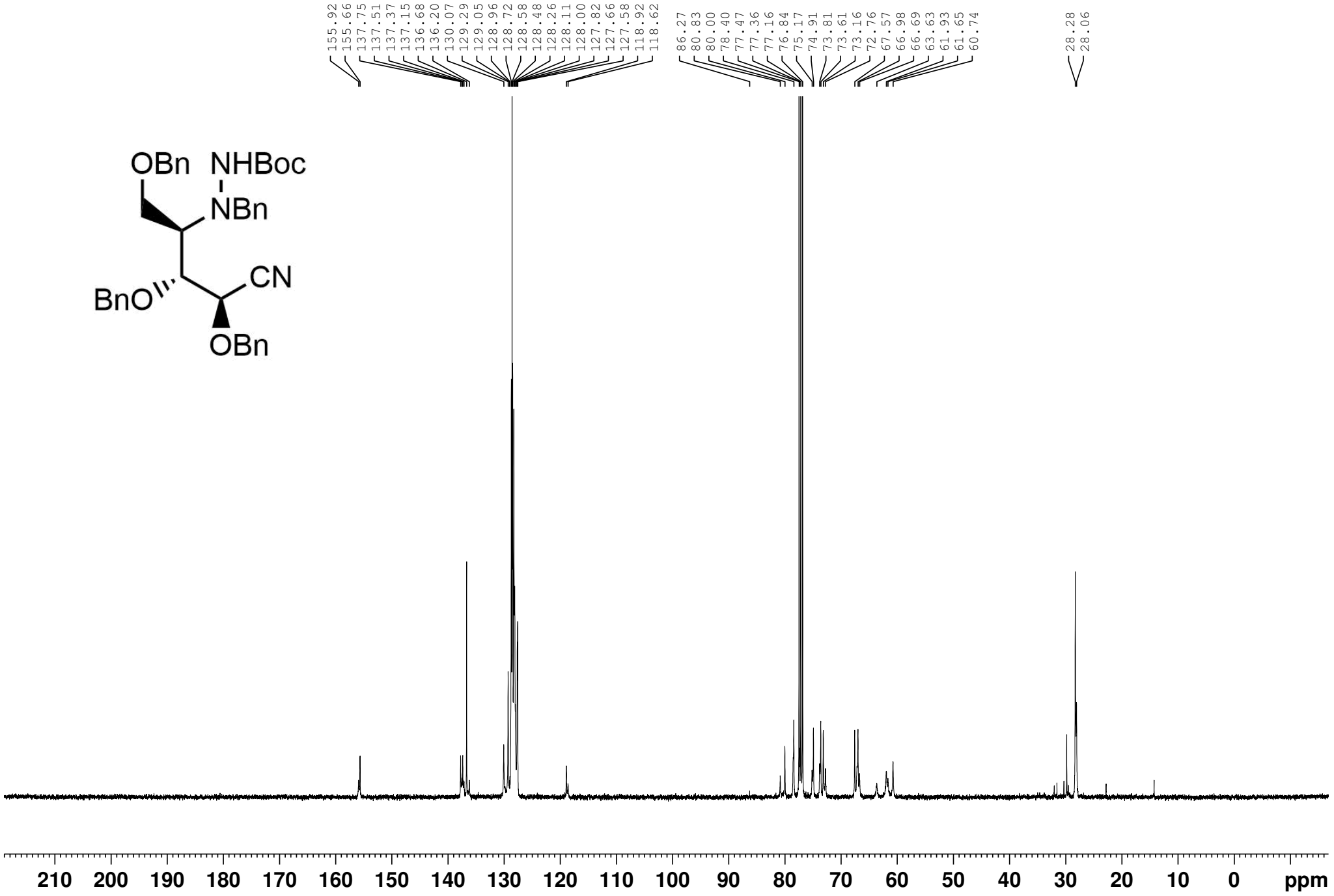


**Figure S26:** IR: 2,3,5-Tris-*O*-benzyl-4-(1-*N*-benzyl-(2-tert-butoxycarbonyl)hydrazinyl)-4-deoxy-D-arabinonitrile (**13**)