Supplementary Materials

Chain-branched Polyhydroxylated Octahydro-*1H*-indoles, as Potential Leads against Lysosomal Storage Diseases

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Figure S1. Single Crystal XRD- for compound **5**,
with thermal ellipsoids drawn at the 50% probability
level and **CCDC: 1885010**

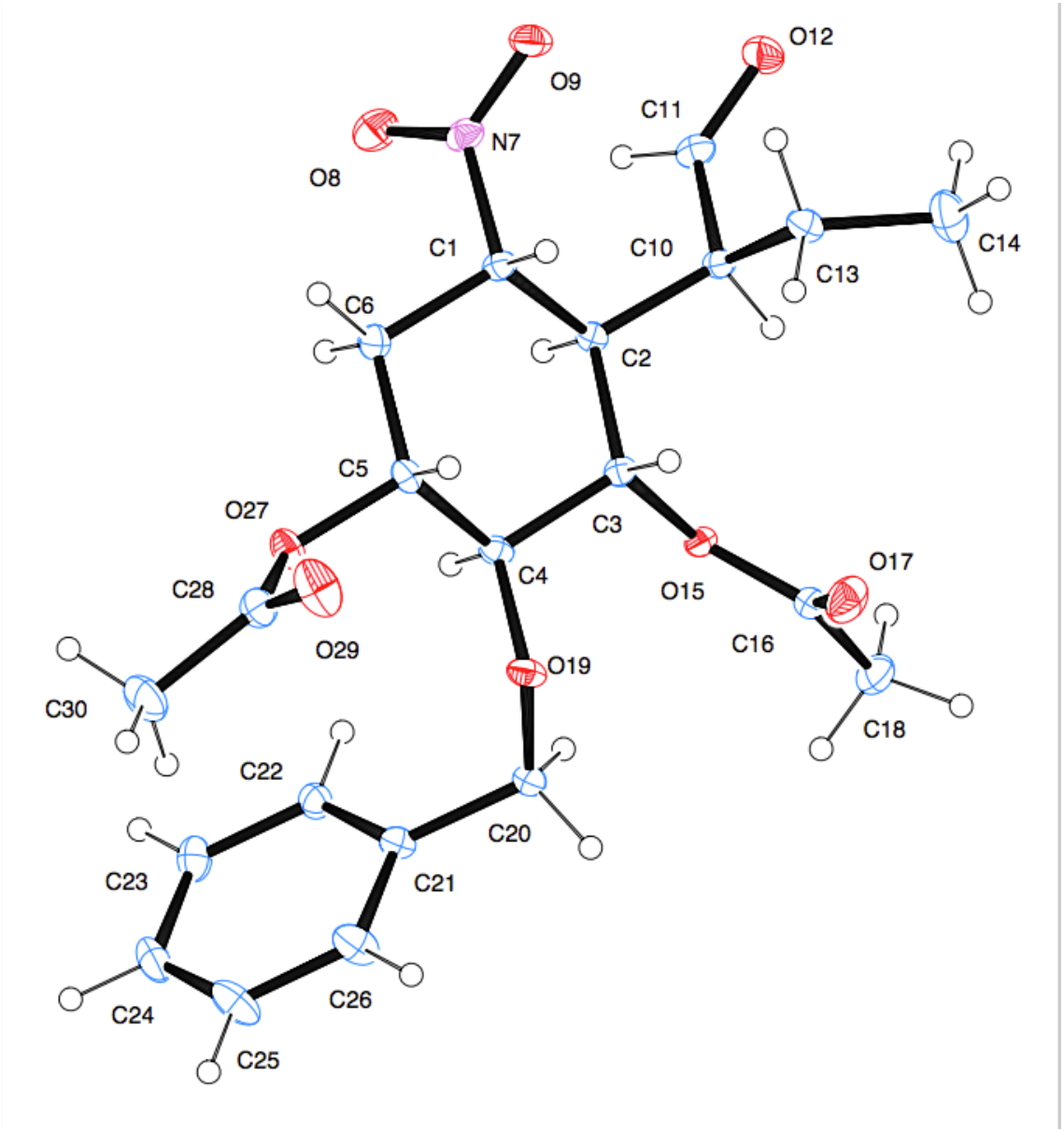


Table S1. Crystal data and structure refinement for compound **5**, and **CCDC: 1885010**

Experimental data **5** (2011re02mgc01)

Crystal data	
Chemical formula	$C_{21}H_{27}NO_8$
Temperature (K)	421.44
Crystal system, space group	Monoclinic $P2_1$
Temperature (K)	100(2) K
a,b,c(Å)	a = 10.4104(6) Å α= 90° b = 8.8682(5) Å β= 101.541(3)° c = 11.6487(6) Å γ= 90°
V(Å^3)	1053.68(10) Å^3
Z	2
Radiation type	*MoKa*
μ(mm–^{1})	0.102 mm^{-1}
Crystal size (mm)	0.42 x 0.14 x 0.09 mm^3
Data collection	
Diffractometer	BRUKER APPEX-II CCD
Absorption correction	Multi-scan BRUKER *SADABS*
Tmin, *Tmax*	0.9253-0.9853
No. of measured, independent and observed (I > 2σ(I)] reflections	18089, 2777, 2302
Rint	0.052
(sin(θ)/λ)$_{max}$ {Å^{-1})	0.667
Refinement	
R[F^2 > 2σ(F^2)], wR(F^2), S	0.0390, 0.0878, 1.038
No. of reflections	2777
No. of parameters	274
H-atom treatment	H atoms treated by constrained rcfinement
Δr$_{max}$, □Δ□$_{min}$ {e Å-3)	0.199, -0.193
Absolute structure	Absolute structure cannot be determined reliably.
Absolute structure parameter	N/A

Computer programs: APPEX2 (BRUKER AXS, 2005), *S/R97* (Giacovazzo *et ai.J*, 1999, *SHELXL97* (ShcJdrick, 1997), *ORTEP-3 for Windows* (Farrugia,1997), *WinGX* publication routines (Farrugia, 1999).

Figure S2. Single Crystal XRD- for compound **7**,
with thermal ellipsoids drawn at the 50% probability
level and **CCDC: 1885009**

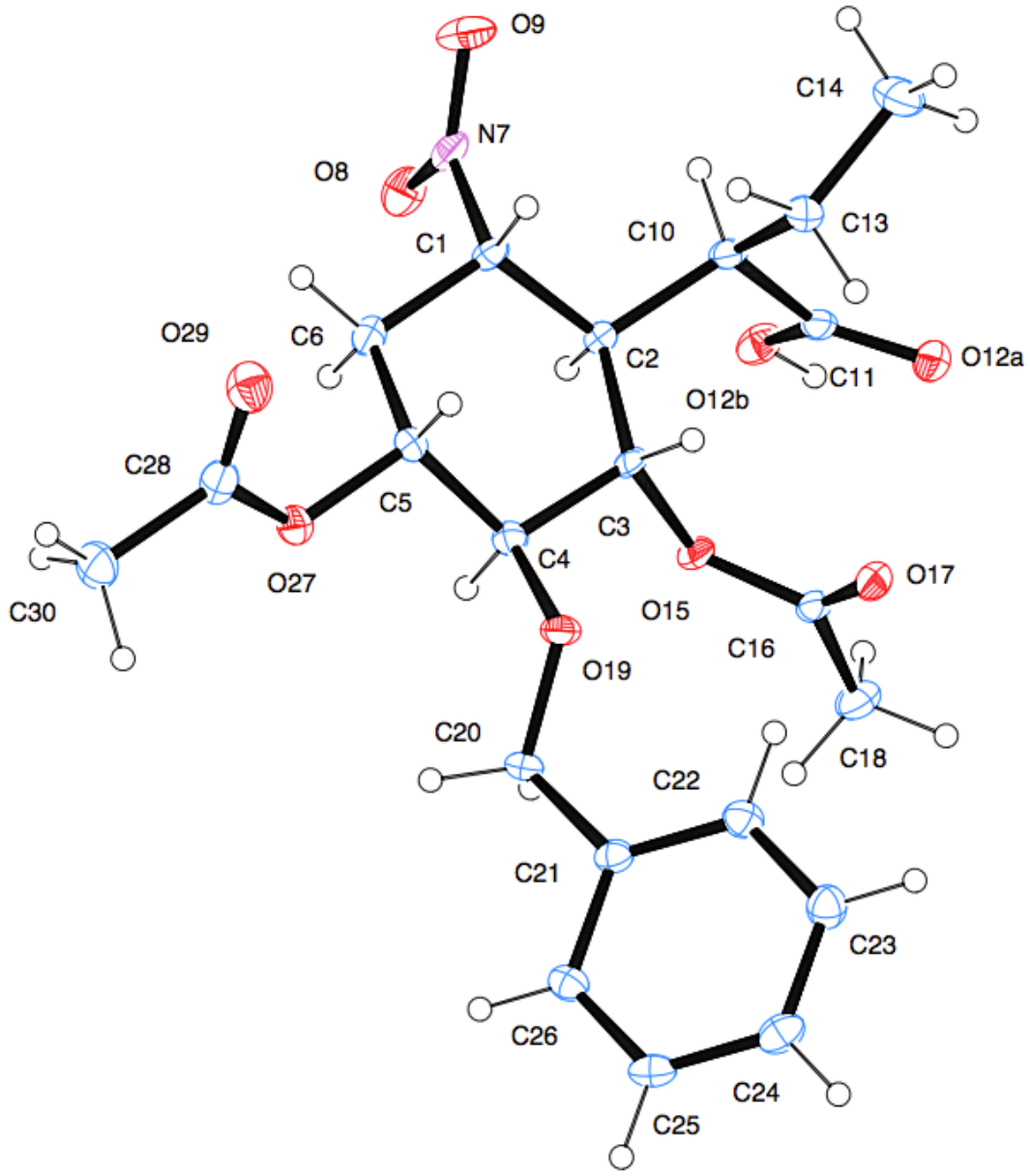


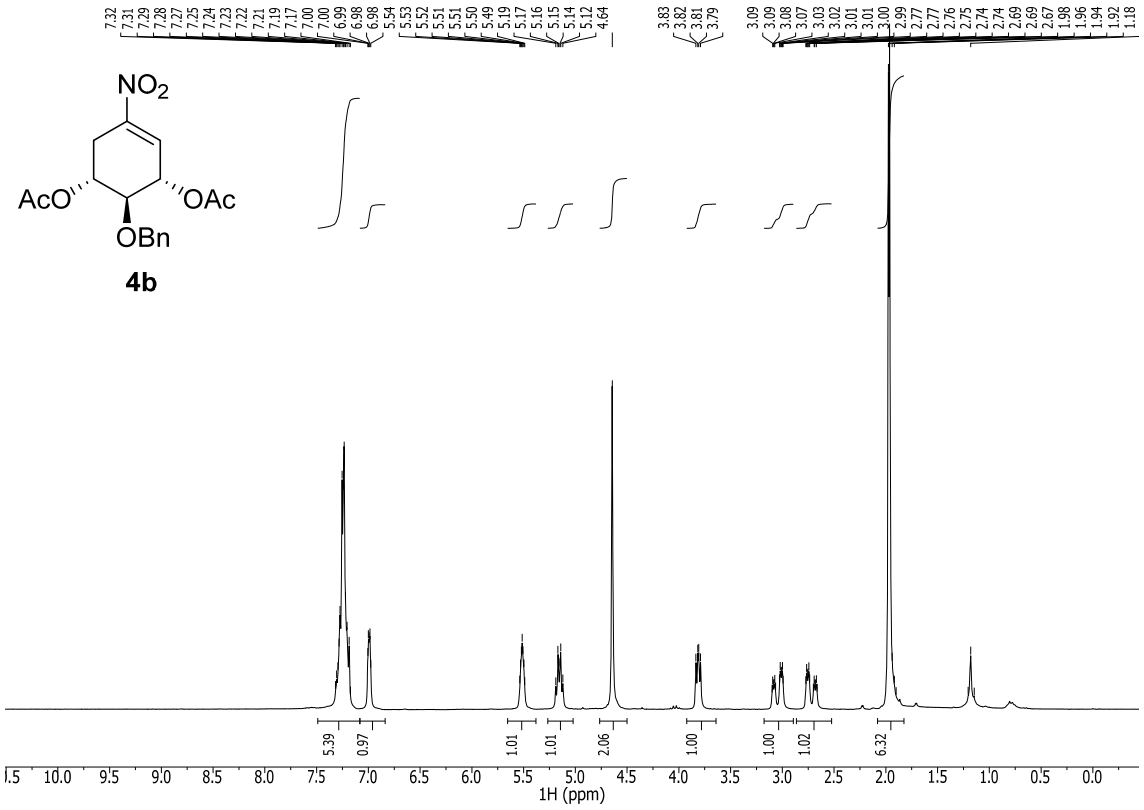
Table S2. Crystal data and structure refinement for compound **7**, and **CCDC: 1885009**

Experimental data 7 (2011re03mgc02)

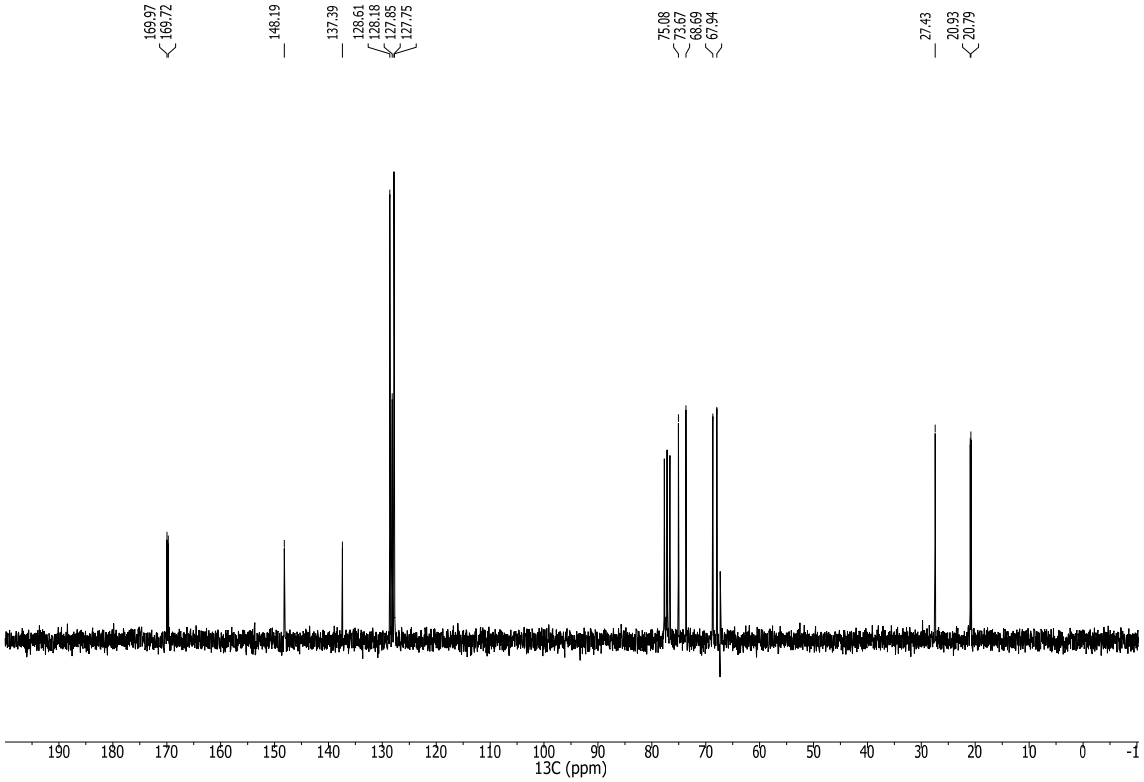
Crystal data	
Chemical formula	$C_{21}H_{27}NO_9$
Tcmperature (K)	437.44
Crystal system, space group	Monoclinic $P2_1$
Tcmpcrature (K)	100(2) K
a,b,c (Á)	a = 9.7916(13) Å α= 90° b = 9.2932(12) Å β= 99.230(8)° c = 12.3910(17) Å γ= 90°
V(Å^3)	1112.9(3)Å^3
Z	2
Radiation type	*MoKa*
μ(mm^{-1})	0.103 mm^{-1}
Crystal size (mm)	0.35 x 0.12 x 0.04 mm^3
Data collection	
Diffractometer	BRUKER APPEX-II CCD
Absorption correction	Multi-scan BRUKER *SADABS*
Tmin, Tmax	0.8784-0.9866
No. of measured, independent and observed ($I > 2\sigma(I)$] reflections	21663, 2417, 1945
Rint	0.0602
$(\sin(\theta)/\lambda)_{max}$ {Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.0384, 0.0913, 1.067
No. of reflections	2417
No. of parameters	287
H-atom treatment	H atoms treated by a mixture of indepcndent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ {e Å-3)	0.171, -0.205
Absolute structure	Absolute structure cannot be determined reliably.
Absolute structure parameter	N/A

Computer programs: APPEX2 (BRUKER AXS, 2005), *S/R97* (Giacovazzo *et ai.J*, 1999, *SHELXL97* (ShcJdrick, 1997), *ORTEP-3 for Windows* (Farrugia,1997), *WinGX* publication routines (Farrugia, 1999).

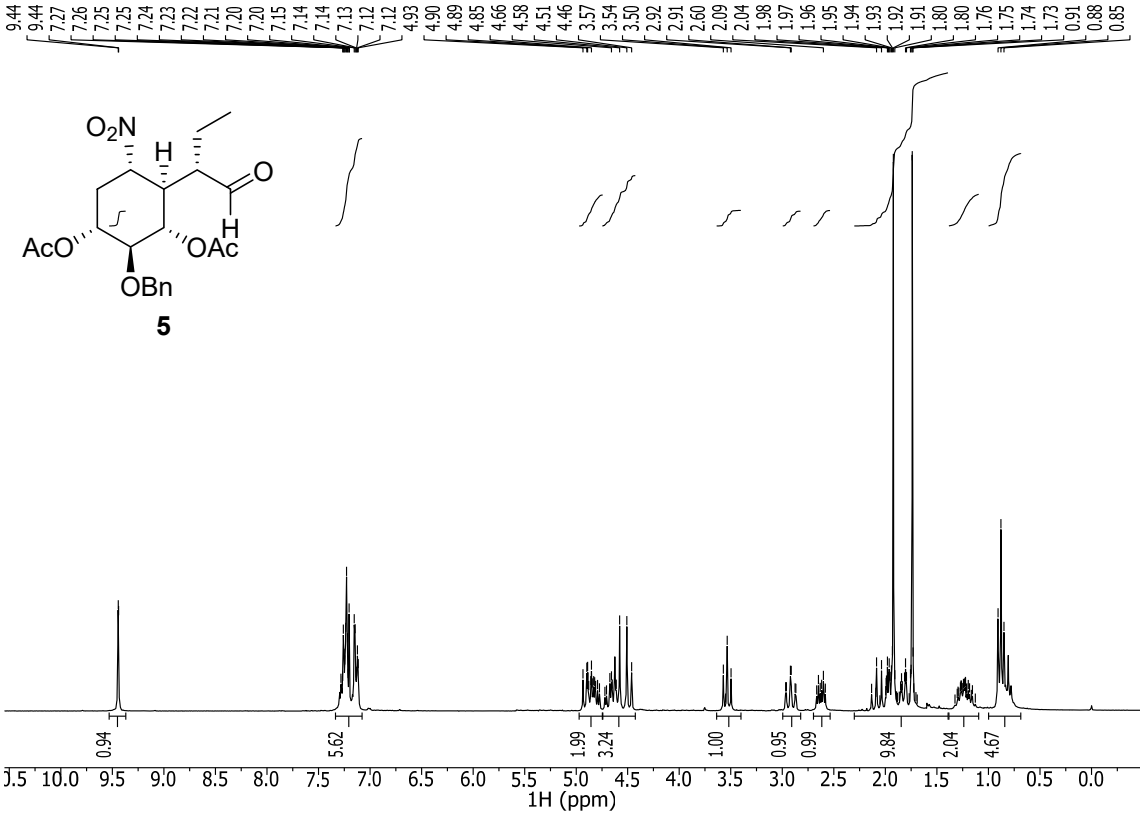
SI6. ^{1}H NMR (250 MHz, Cl_3CD, **4b**)



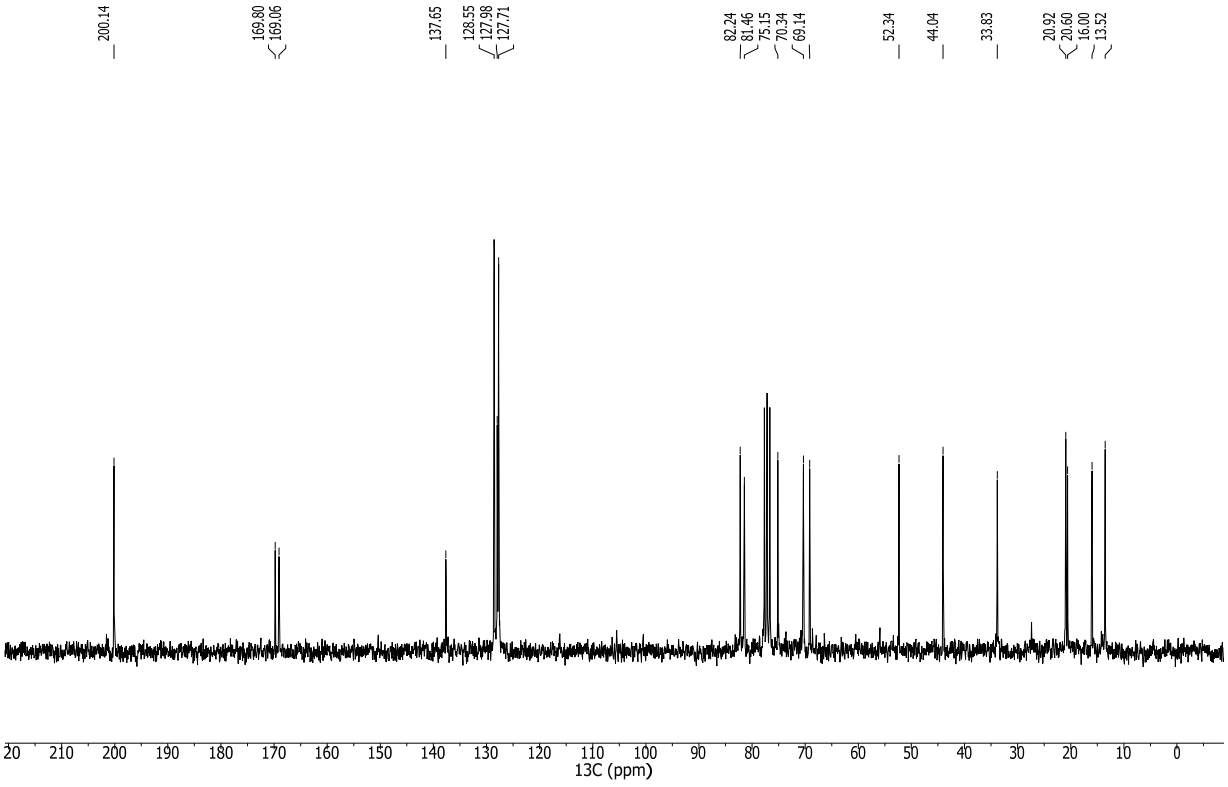
^{13}C NMR (62.5 MHz, Cl_3CD, **4b**)



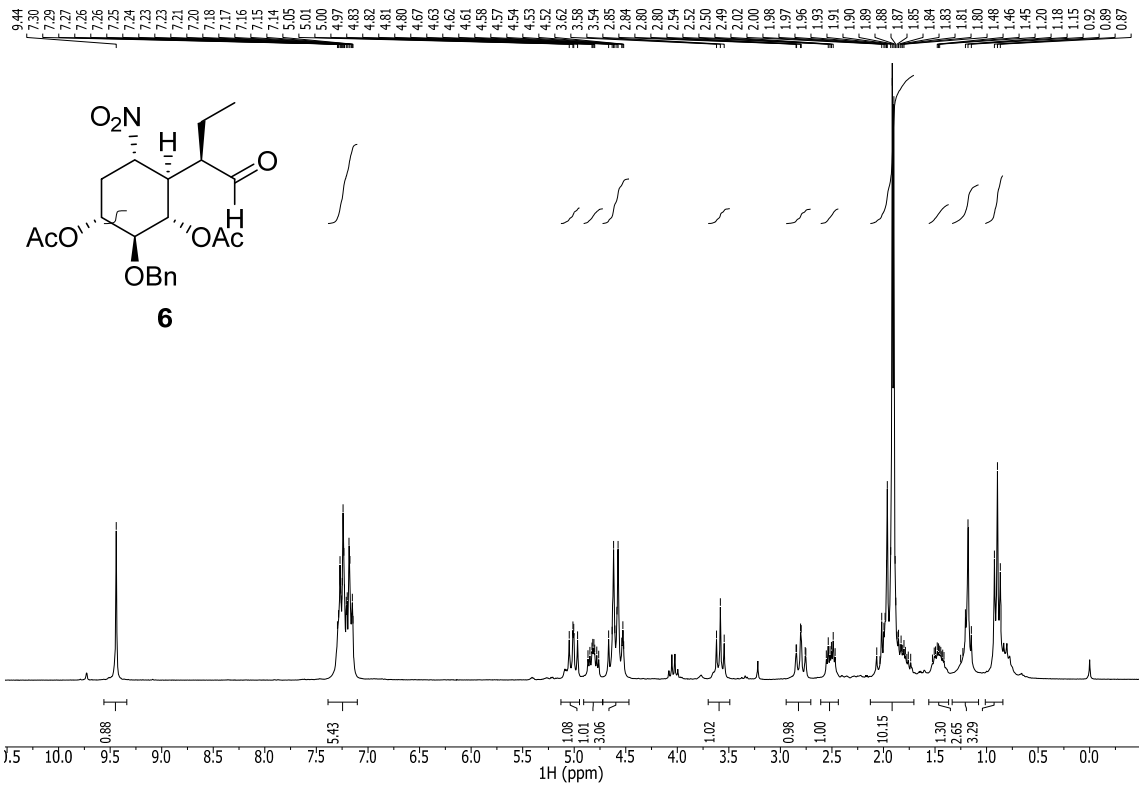
SI6. ^{1}H NMR (250 MHz, Cl_3CD, **5**)



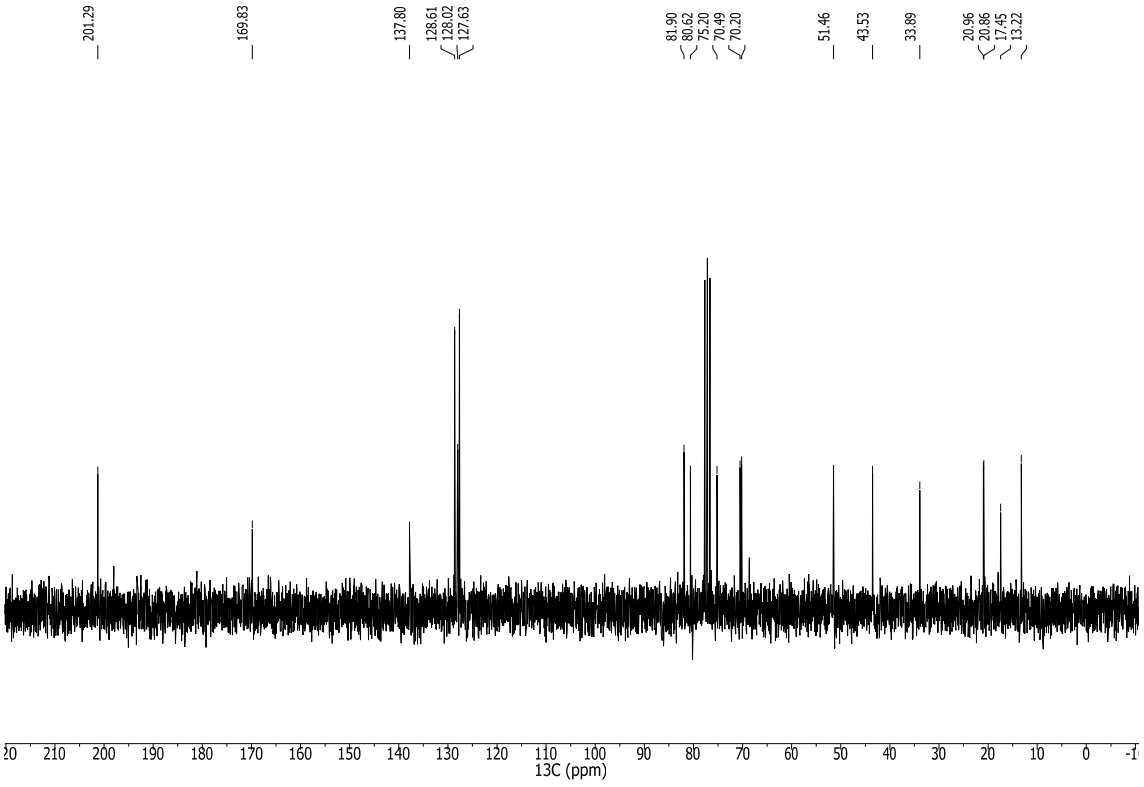
^{13}C NMR (62.5 MHz, Cl_3CD, **5**)



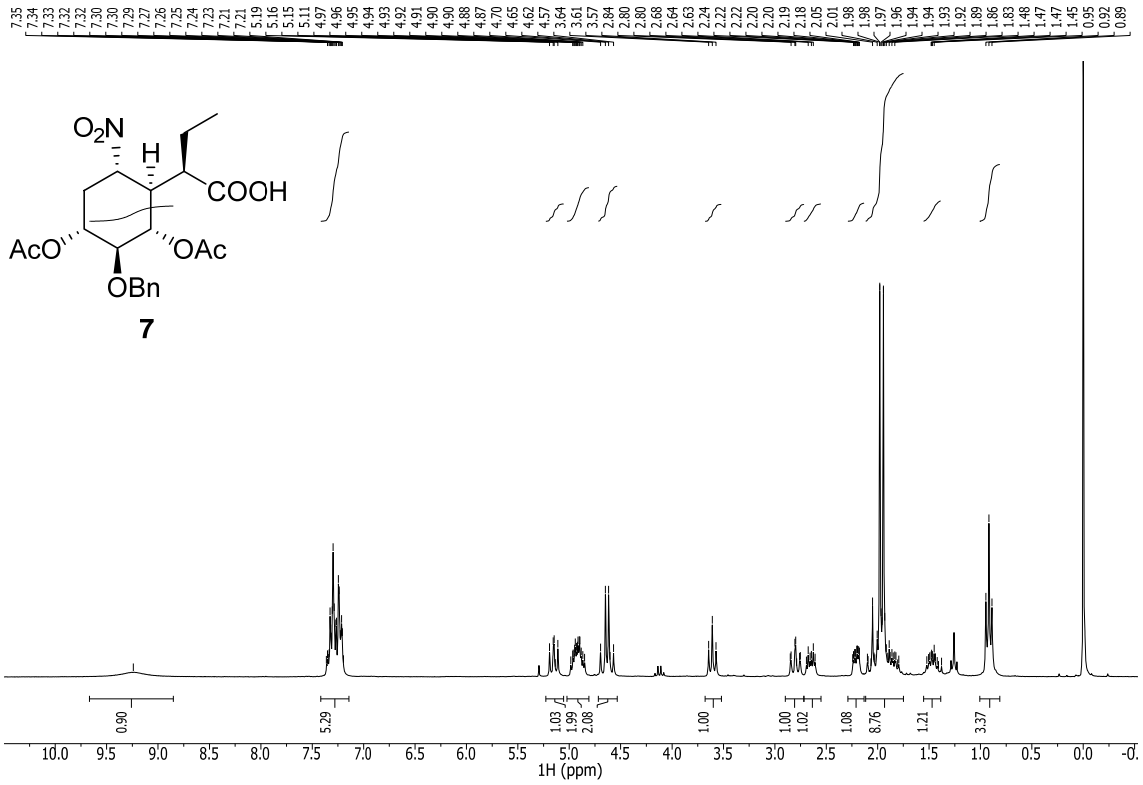
SI6. ^{1}H NMR (250 MHz, Cl_3CD, **6**)



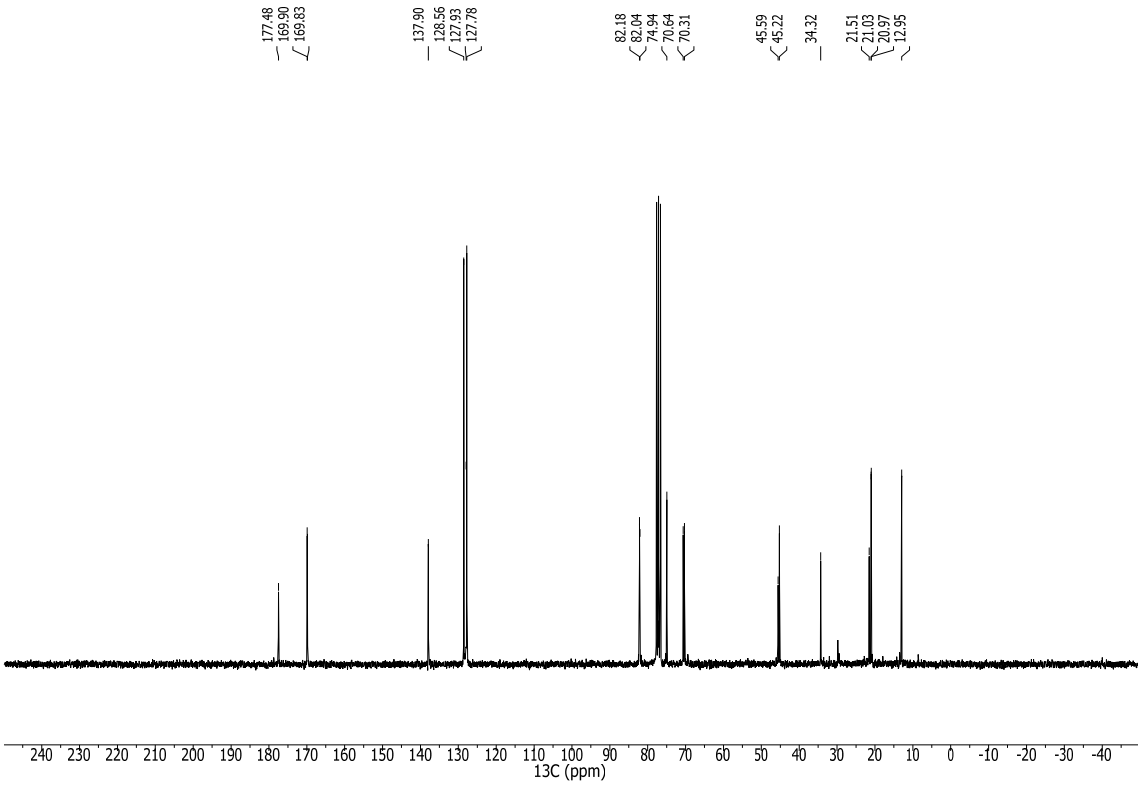
^{13}C NMR (62.5 MHz, Cl_3CD, **6**)



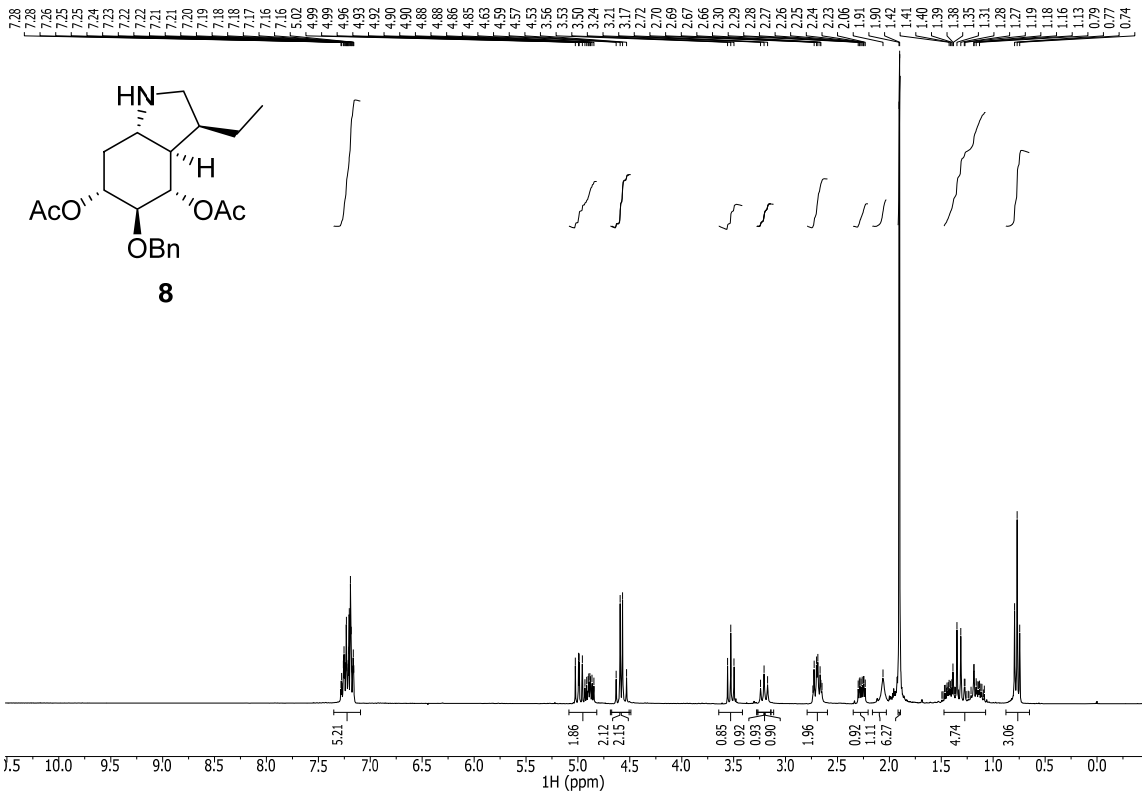
SI6. ^{1}H NMR (250 MHz, Cl_3CD, **7**)



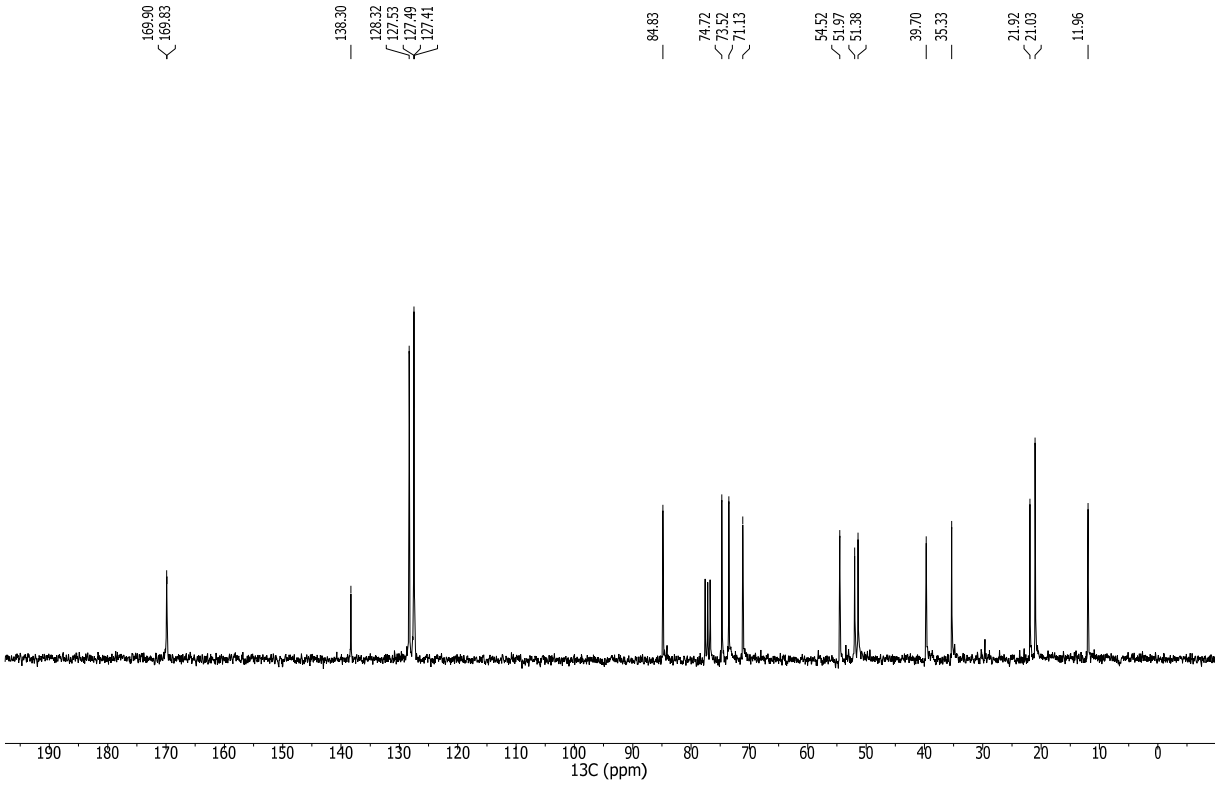
^{13}C NMR (62.5 MHz, Cl_3CD, **7**)



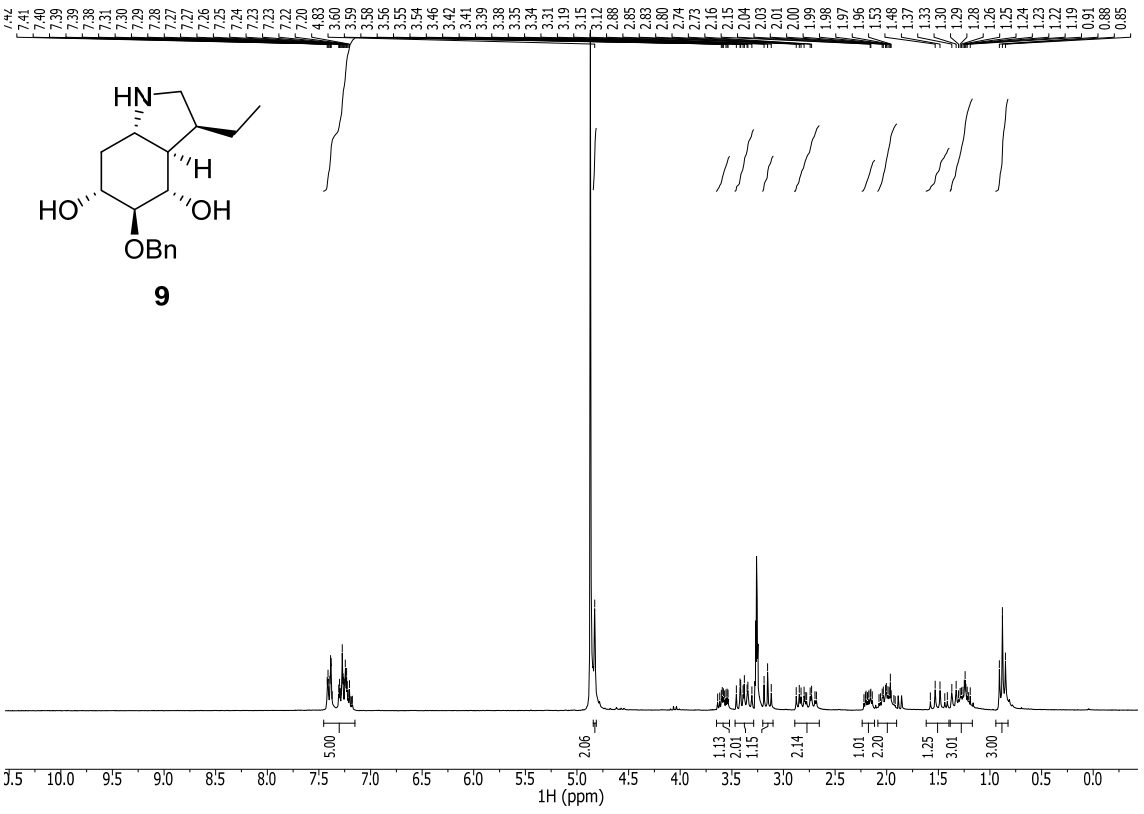
SI6. ^{1}H NMR (250 MHz, Cl_3CD, **8**)



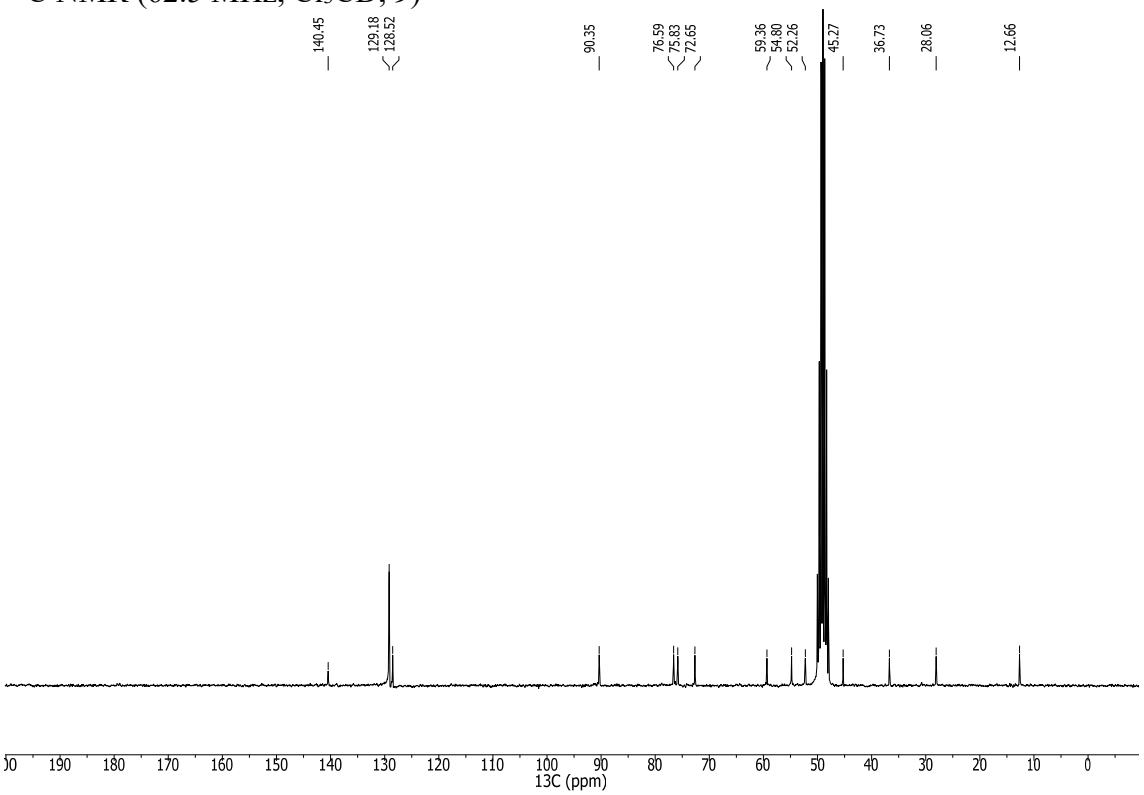
^{13}C NMR (62.5 MHz, Cl_3CD, **8**)



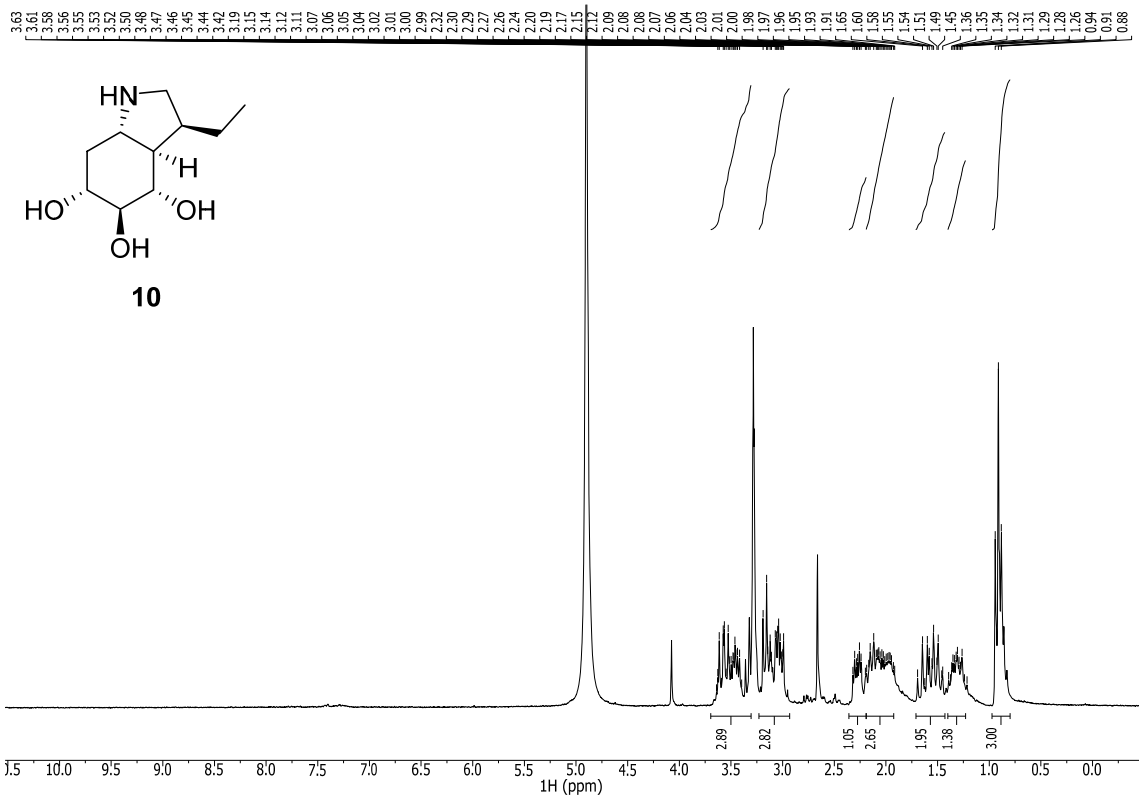
SI6. ^{1}H NMR (250 MHz, CD_3OD, **9**)



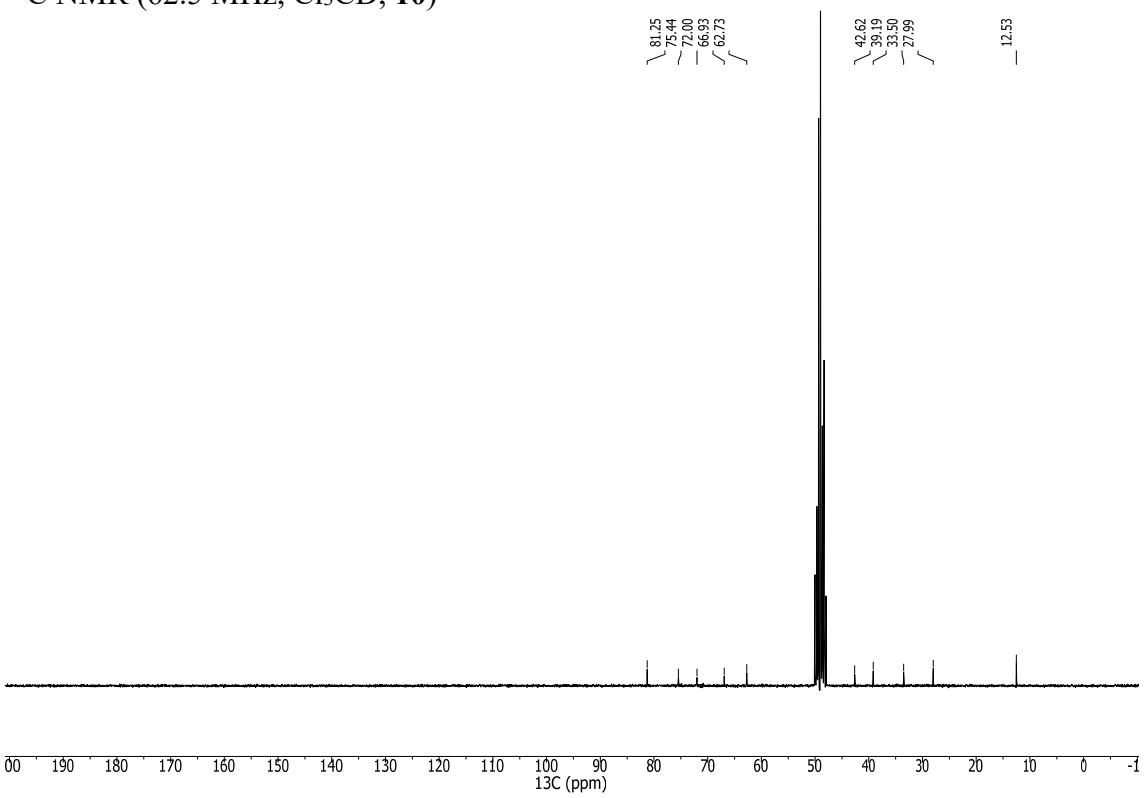
^{13}C NMR (62.5 MHz, Cl_3CD, **9**)



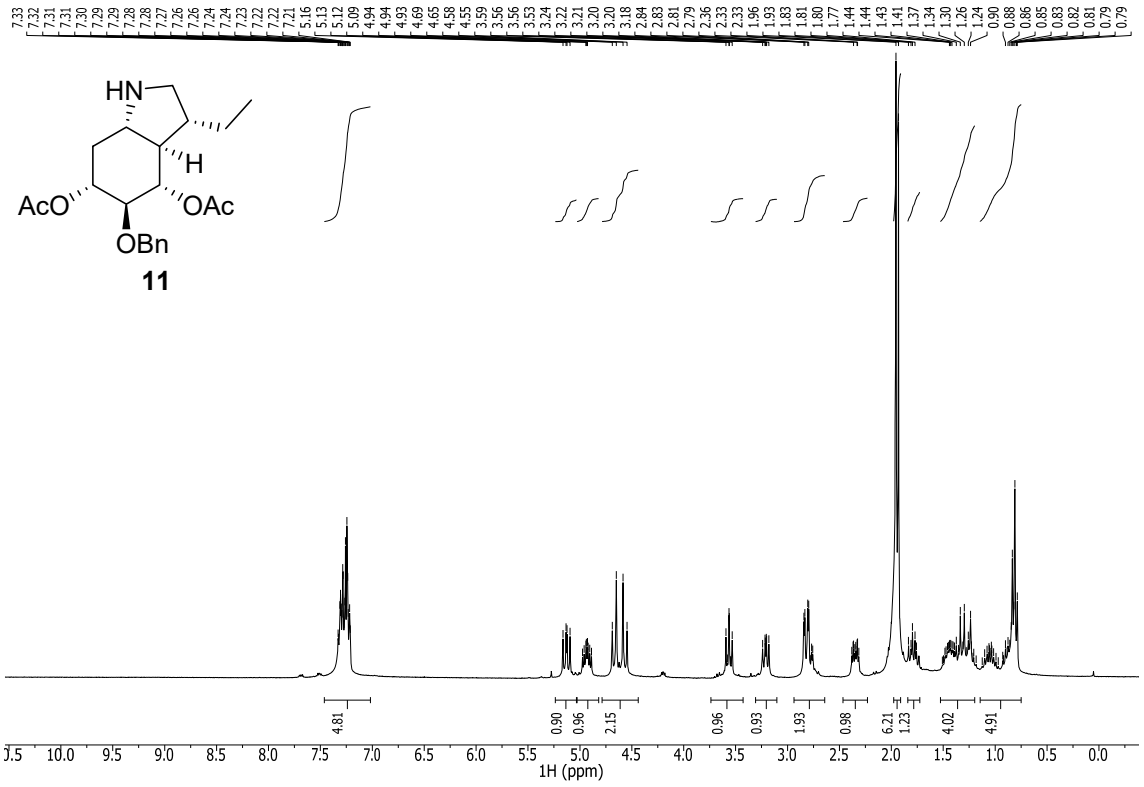
SI6. ^{1}H NMR (250 MHz, CD_3OD, **10**)



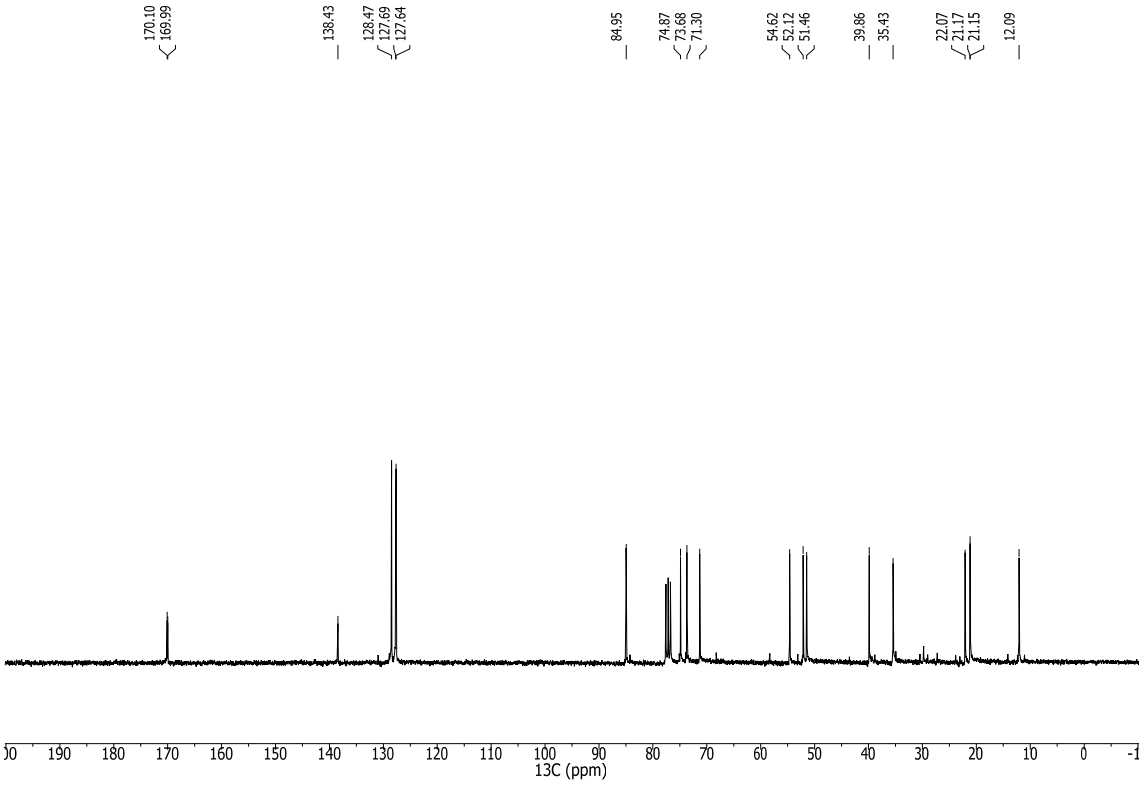
^{13}C NMR (62.5 MHz, Cl_3CD, **10**)



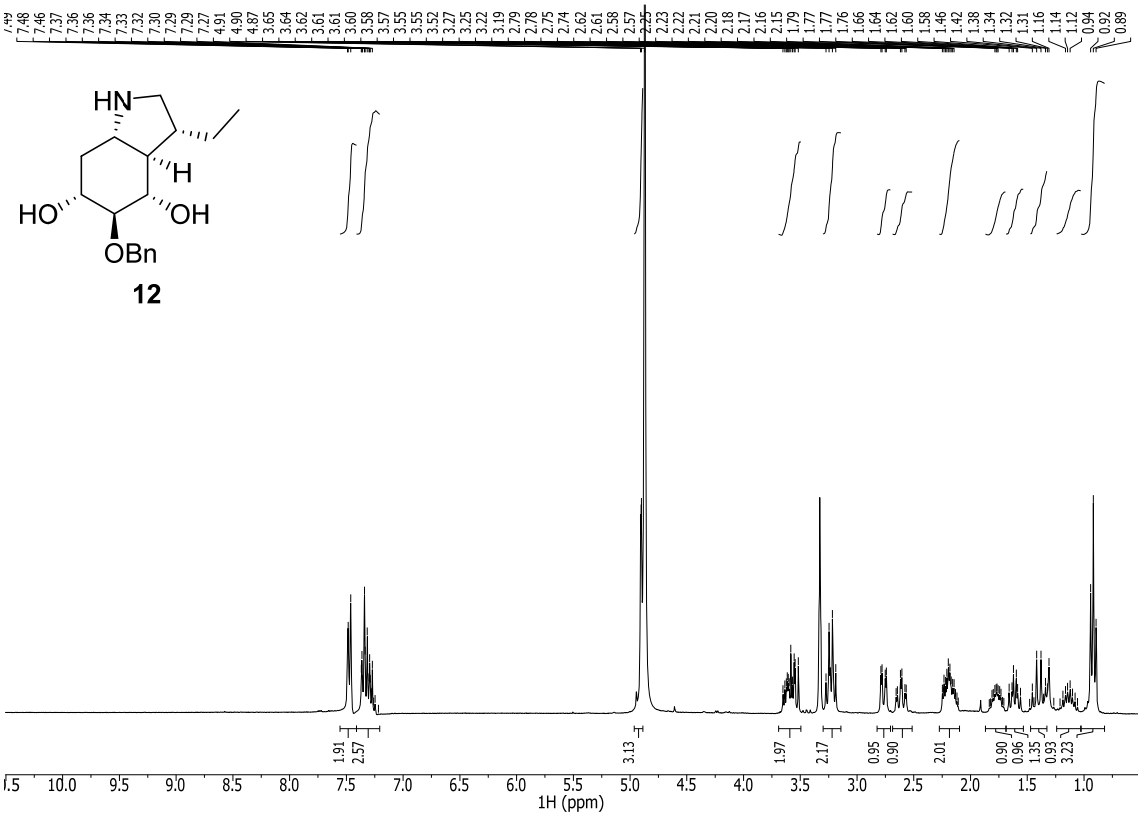
SI6. ^{1}H NMR (250 MHz, Cl_3CD, **11**)



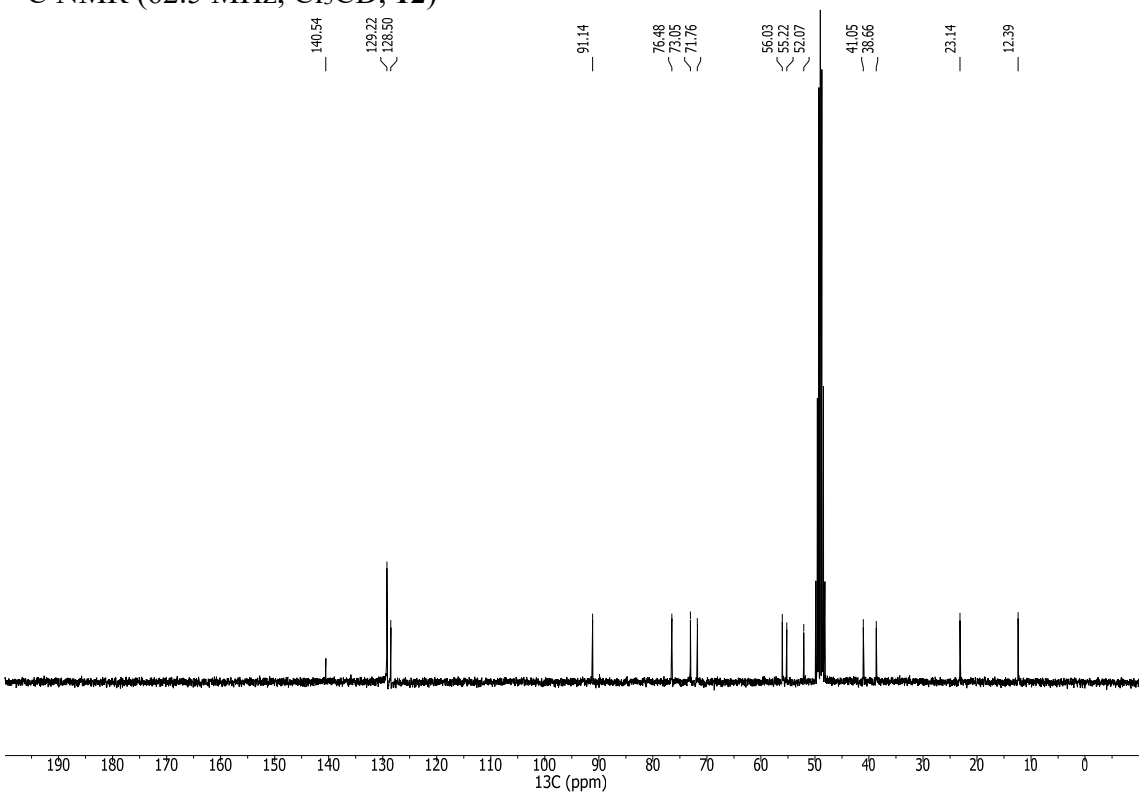
^{13}C NMR (62.5 MHz, Cl_3CD, **11**)



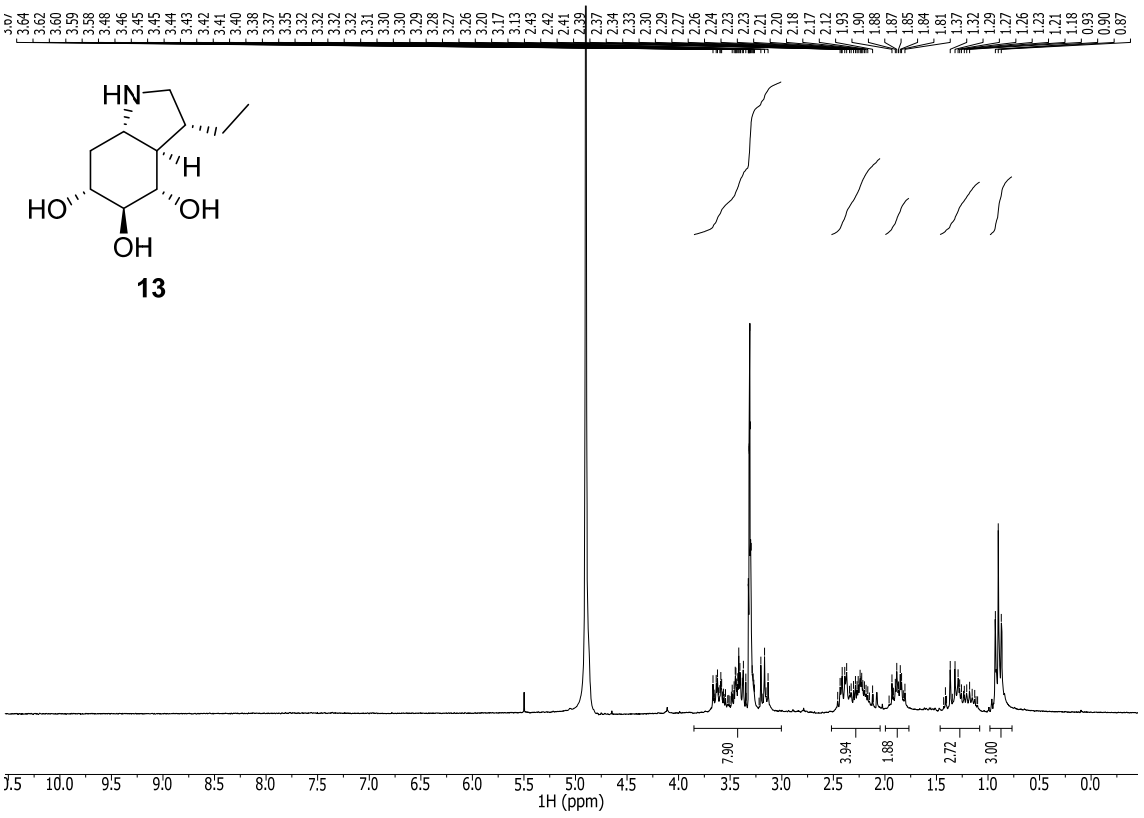
SI6. ^{1}H NMR (250 MHz, CD_3OD, **12**)



^{13}C NMR (62.5 MHz, Cl_3CD, **12**)



SI6. ^{1}H NMR (250 MHz, CD_3OD, **13**)



^{13}C NMR (62.5 MHz, Cl_3CD, **13**)