

Synthesis, Thermal Properties and Cytotoxicity Evaluation of Hydrocarbon and Fluorocarbon Alkyl β -D-xylopyranoside Surfactants

SUPPORTING MATERIAL

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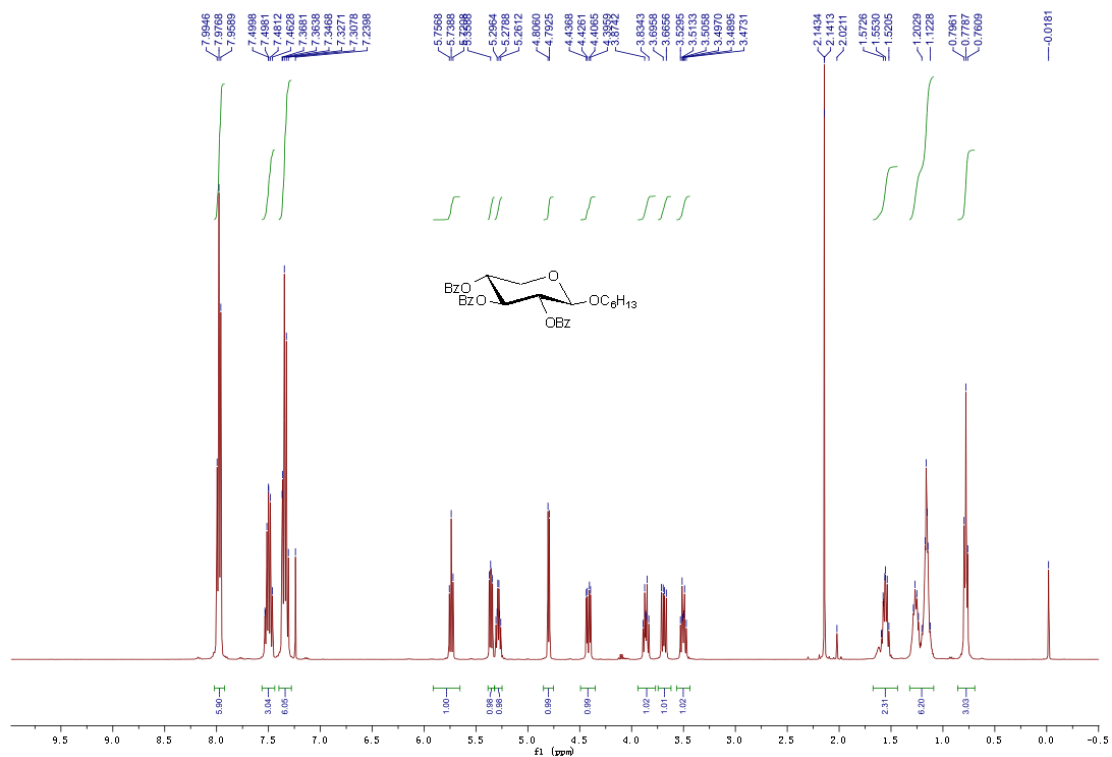


Figure S1. ¹H NMR spectrum (400 MHz) of compound **8a** in CDCl₃.

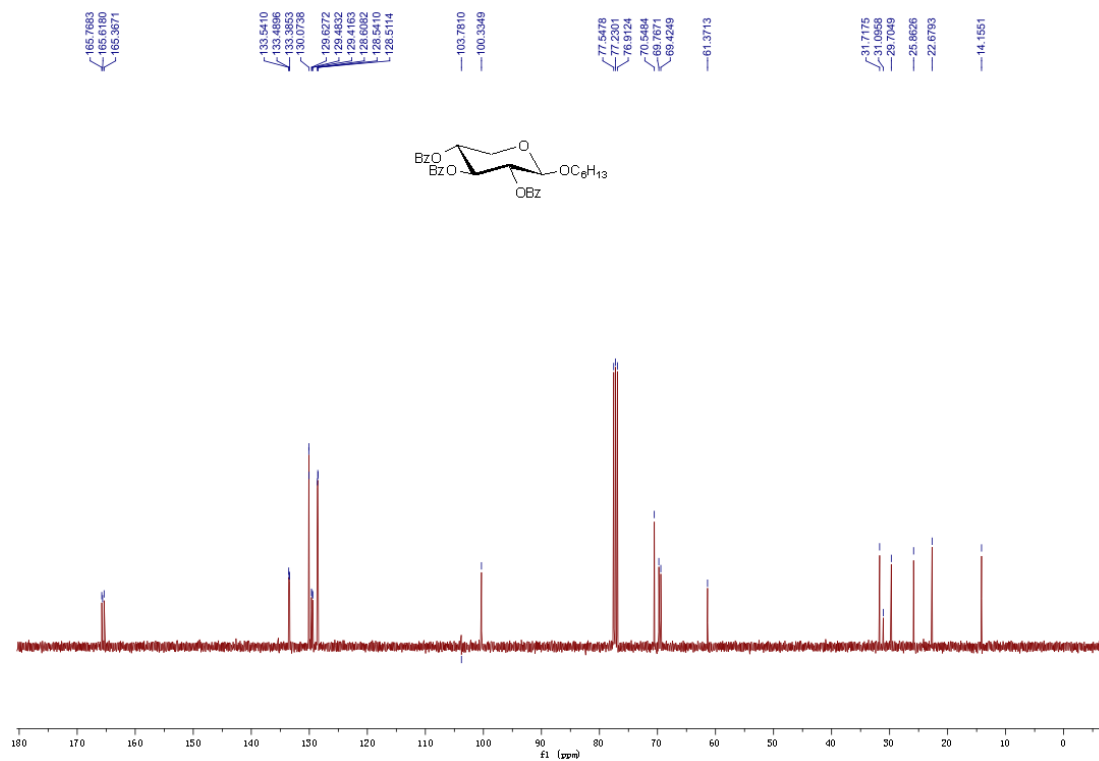


Figure S2. ¹³C NMR spectrum (100 MHz) of compound **8a** in CDCl₃.

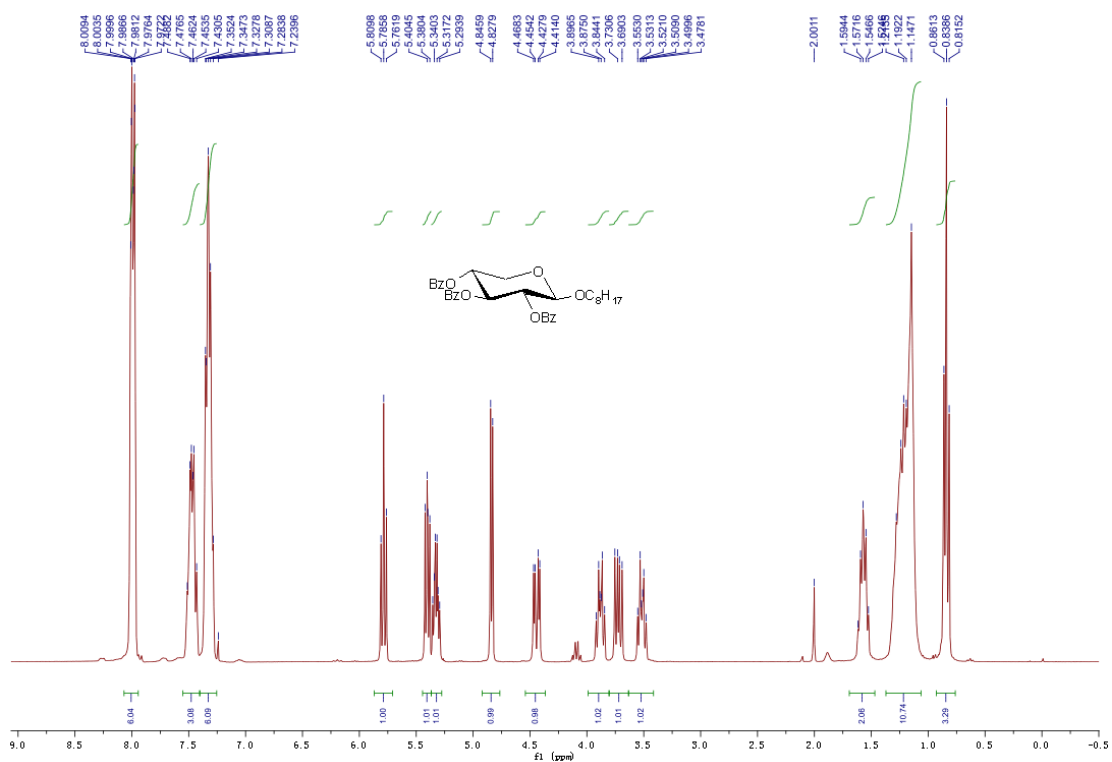


Figure S3. ¹H NMR spectrum (300 MHz) of compound **8b** in CDCl₃.

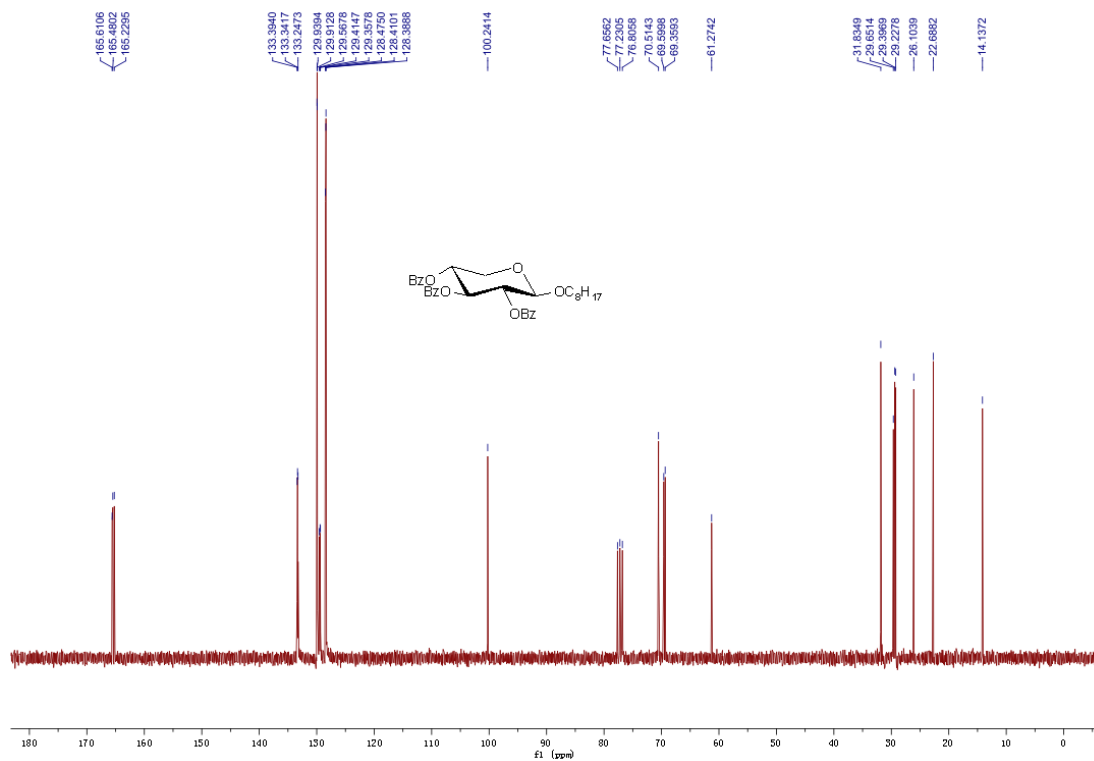


Figure S4. ¹³C NMR spectrum (75 MHz) of compound **8b** in CDCl₃.

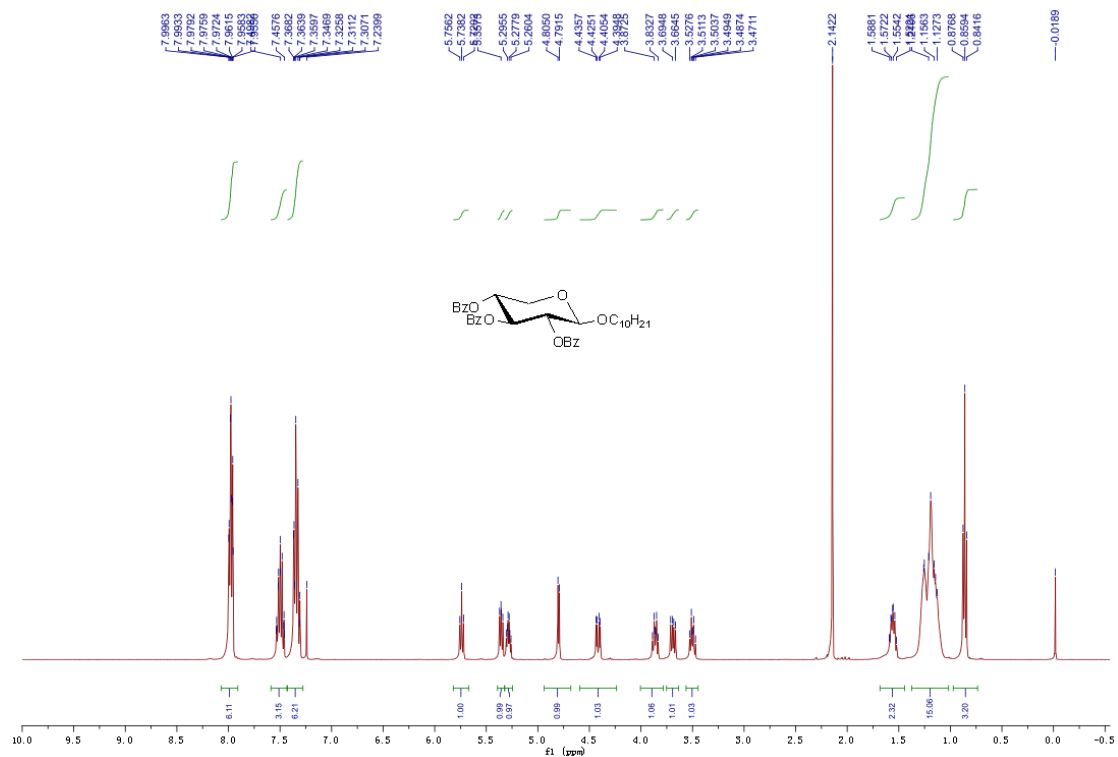


Figure S5. ¹H NMR spectrum (400 MHz) of compound **8c** in CDCl₃.

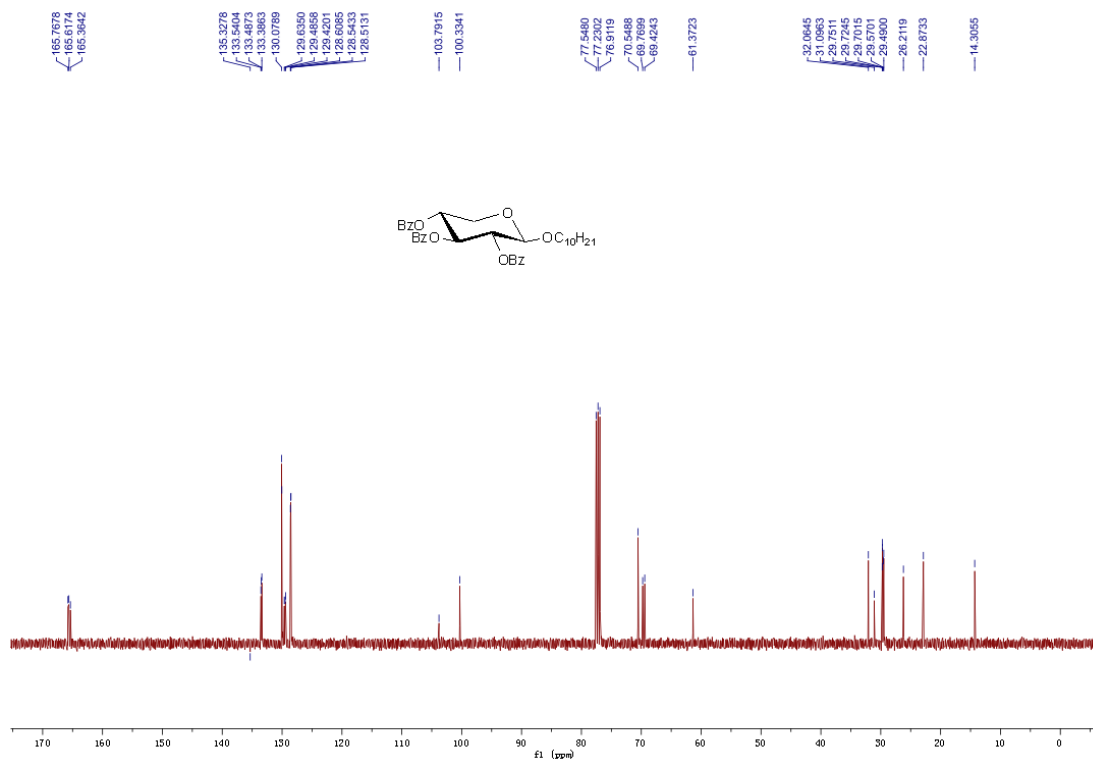


Figure S6. ¹³C NMR spectrum (100 MHz) of compound **8c** in CDCl₃.

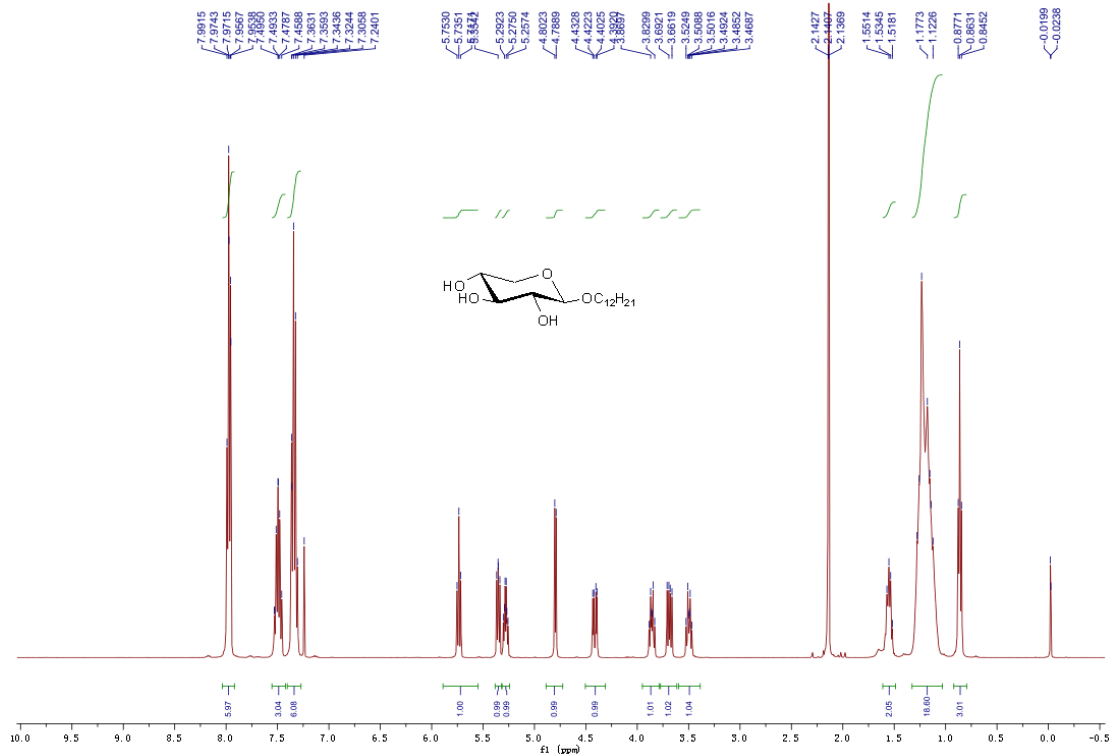


Figure S7. ^1H NMR spectrum (400 MHz) of compound **8d** in CDCl_3 .

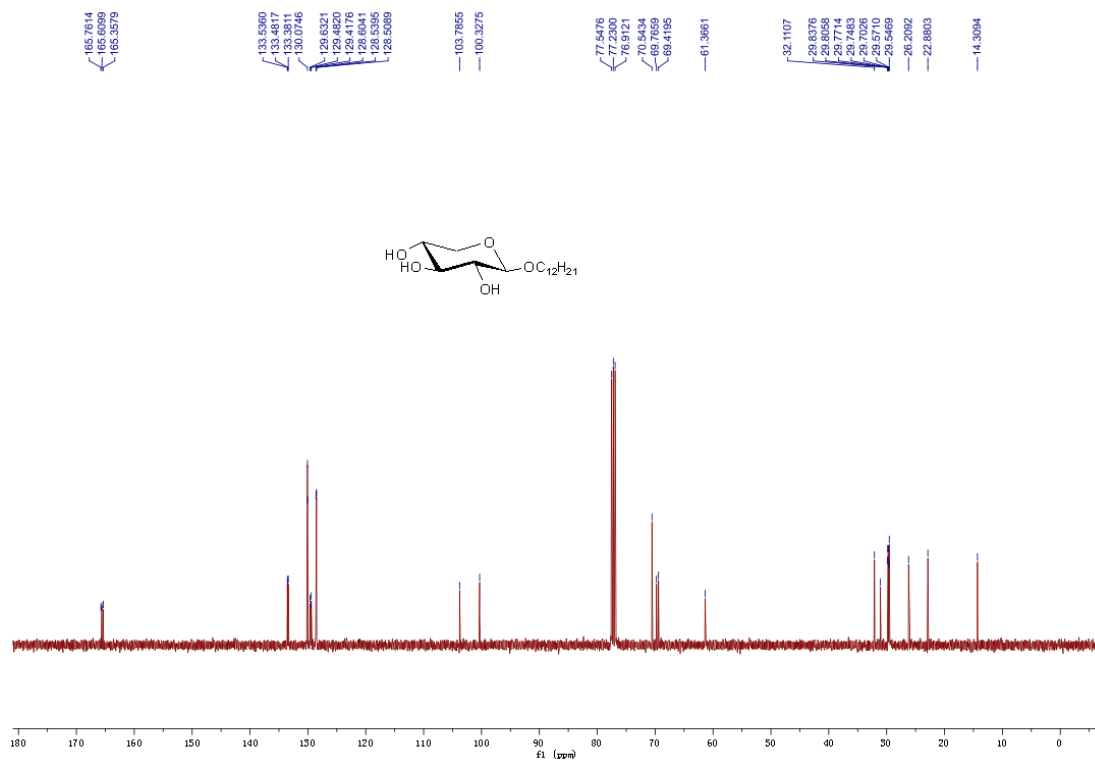


Figure S8. ^{13}C NMR spectrum (100 MHz) of compound **8d** in CDCl_3 .

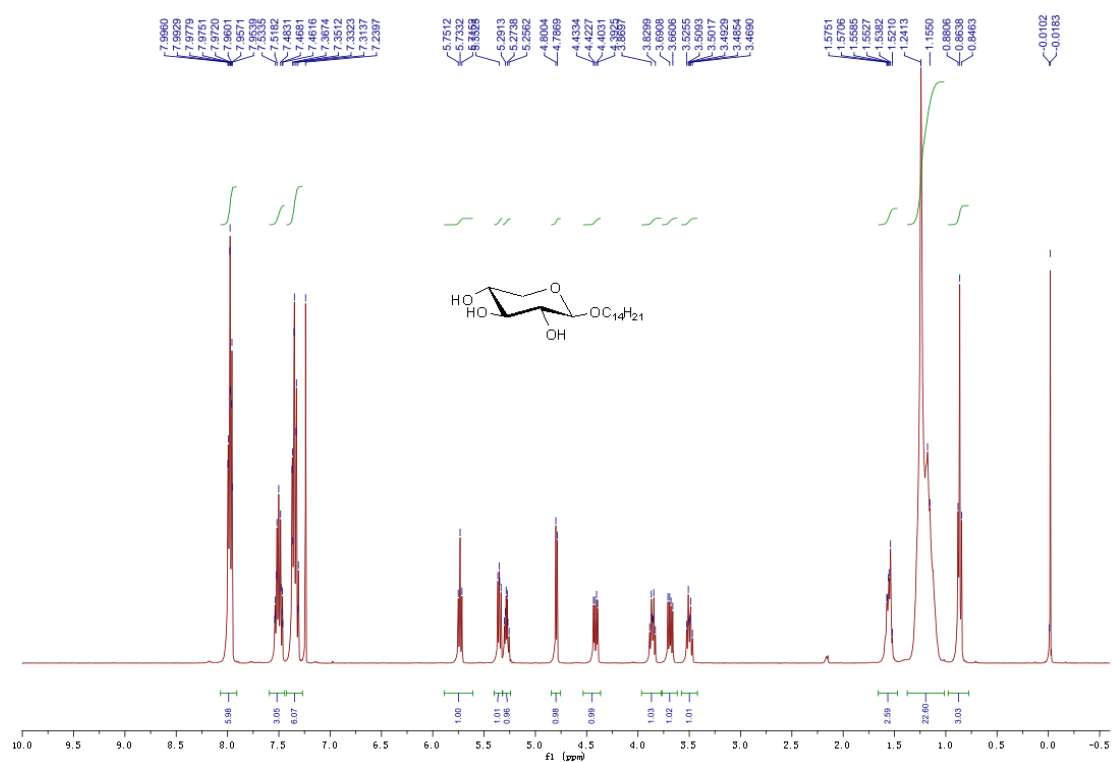


Figure S9. ^1H NMR spectrum (400 MHz) of compound **8e** in CDCl_3 .

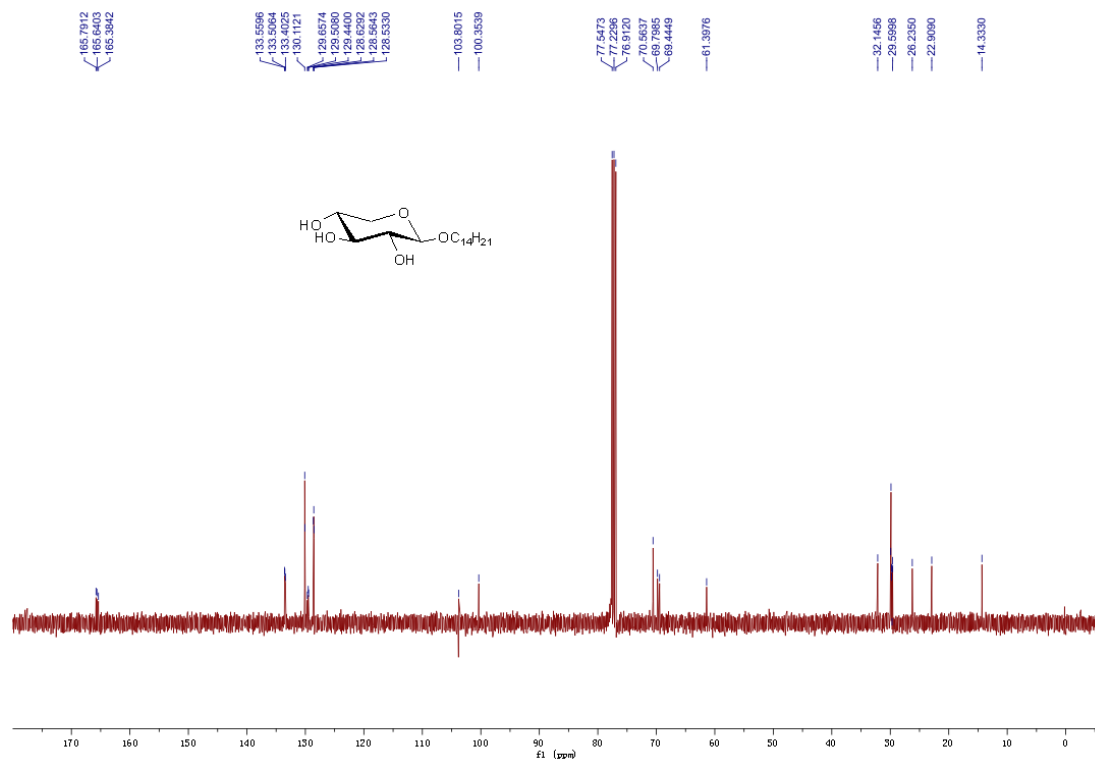


Figure S10. ^{13}C NMR spectrum (100 MHz) of compound **8e** in CDCl_3 .

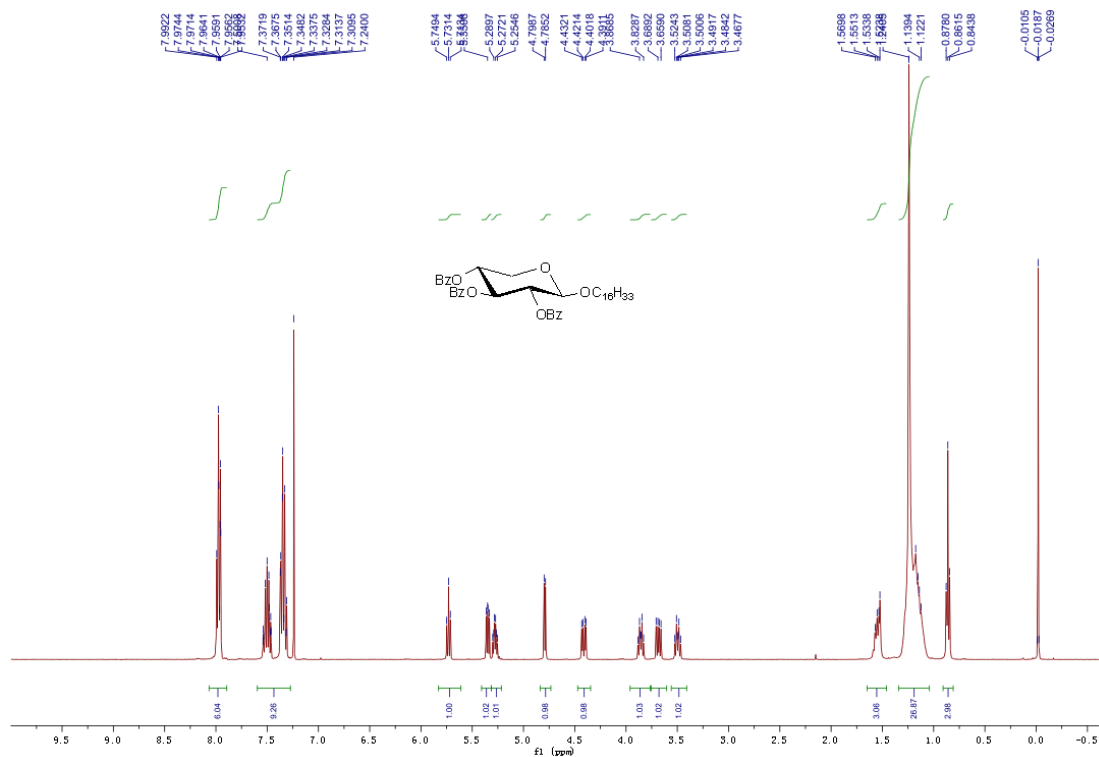


Figure S11. ^1H NMR spectrum (400 MHz) of compound **8f** in CDCl_3 .

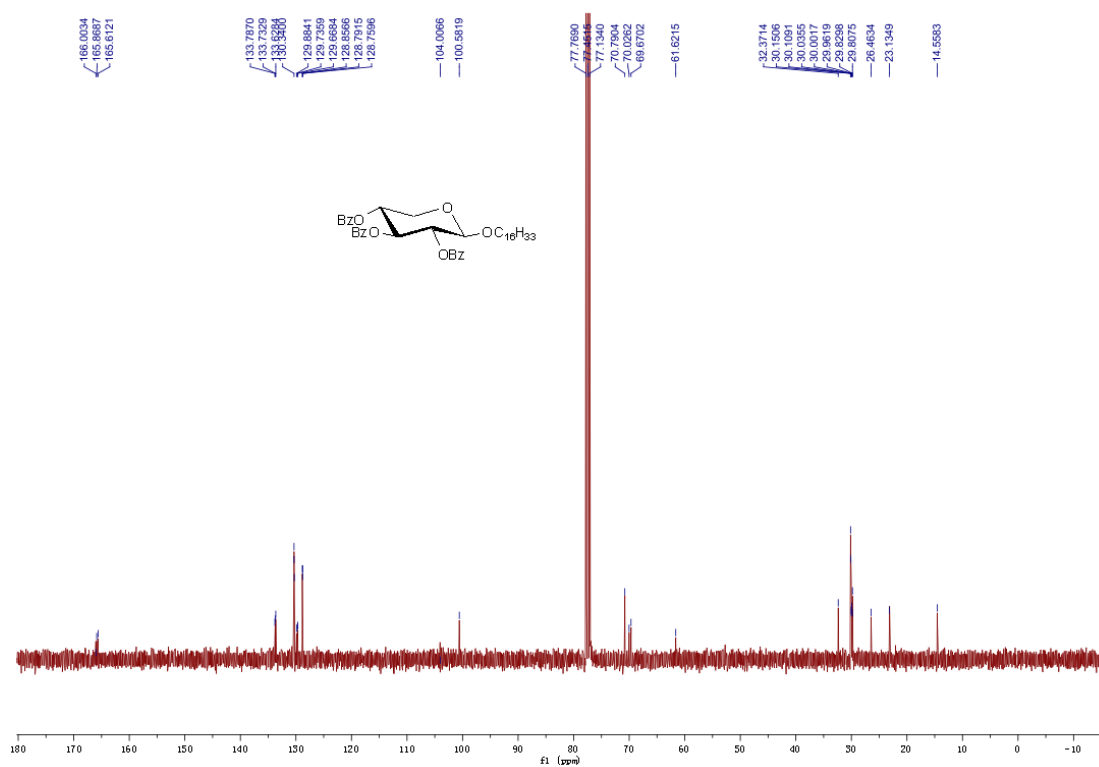


Figure S12. ^{13}C NMR spectrum (100 MHz) of compound **8f** in CDCl_3 .

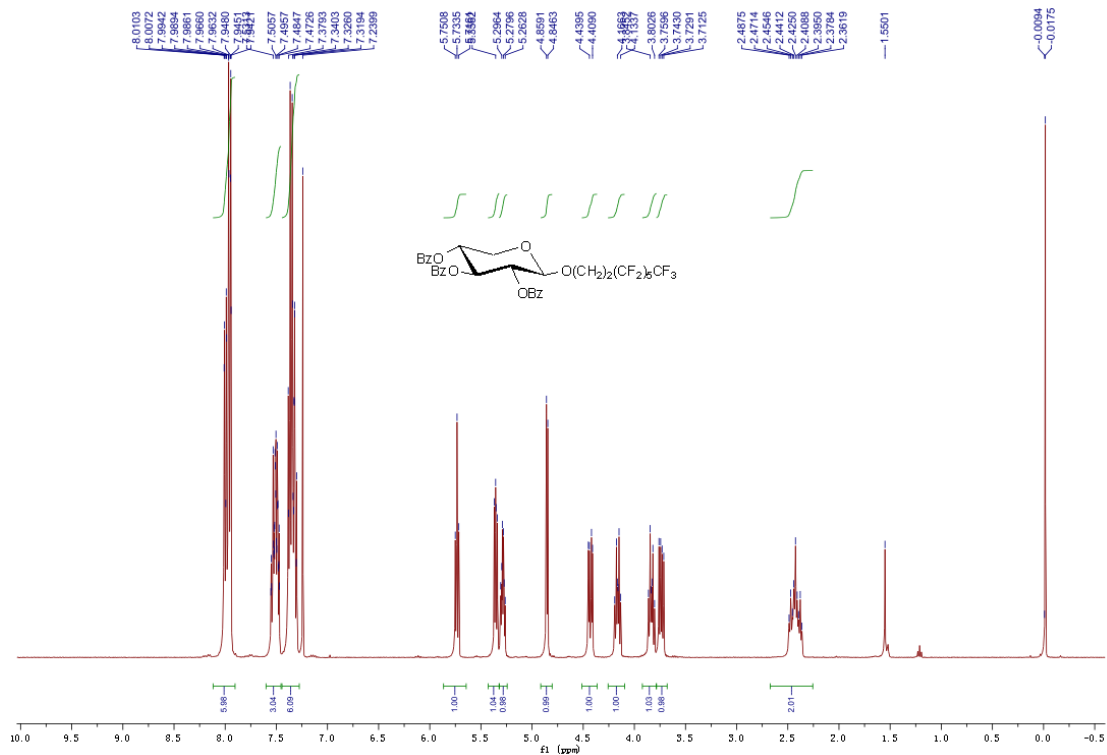


Figure S13. ¹H NMR spectrum (400 MHz) of compound **8g** in CDCl₃.

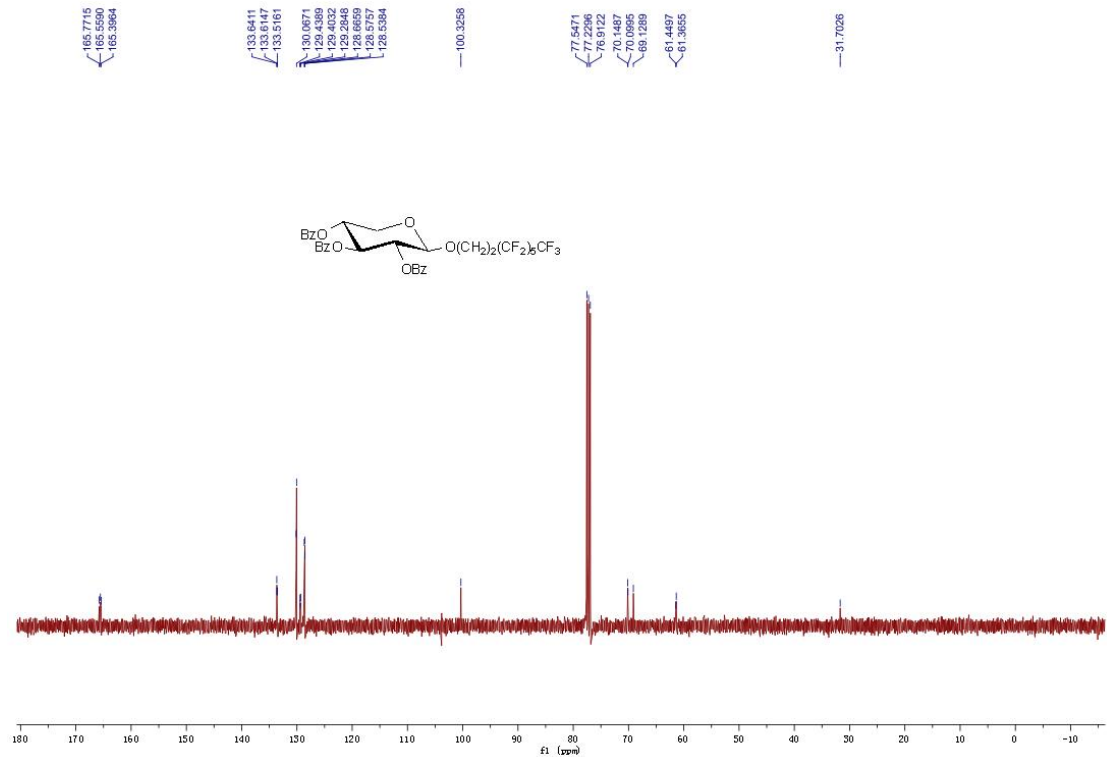


Figure S14. ¹³C NMR spectrum (100 MHz) of compound **8g** in CDCl₃.

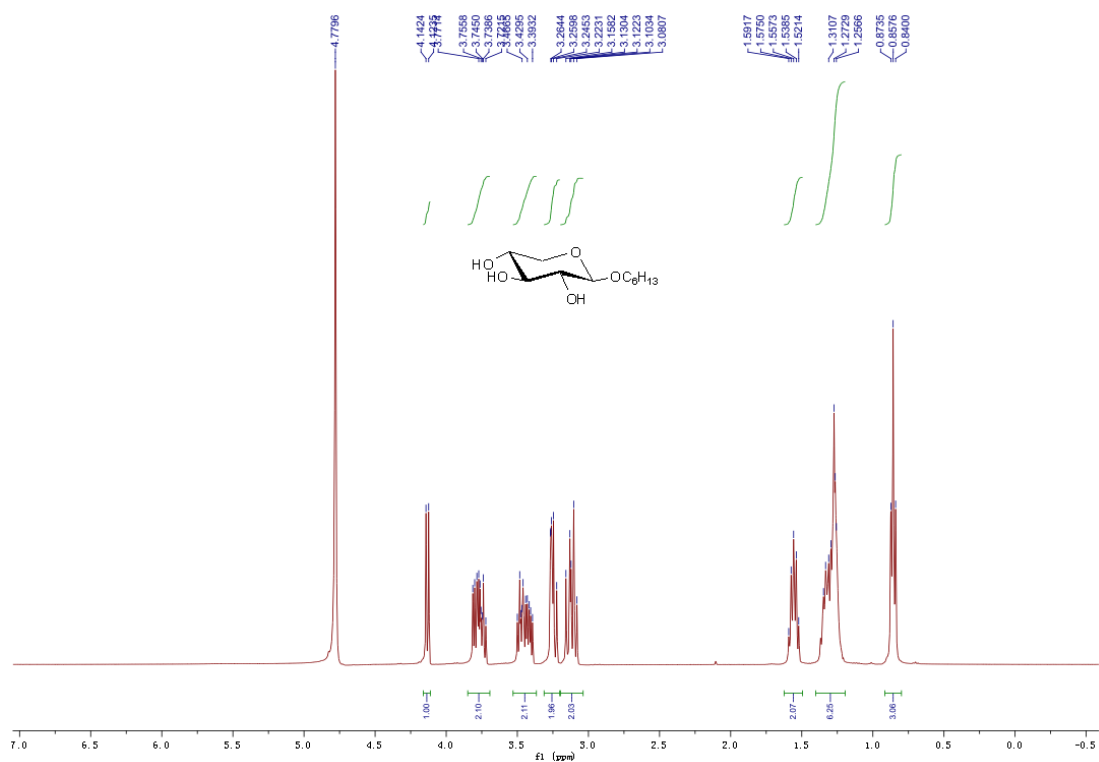


Figure S15. ^1H NMR spectrum (400 MHz) of compound **9a** in $\text{d}_4\text{-MeOH}$.

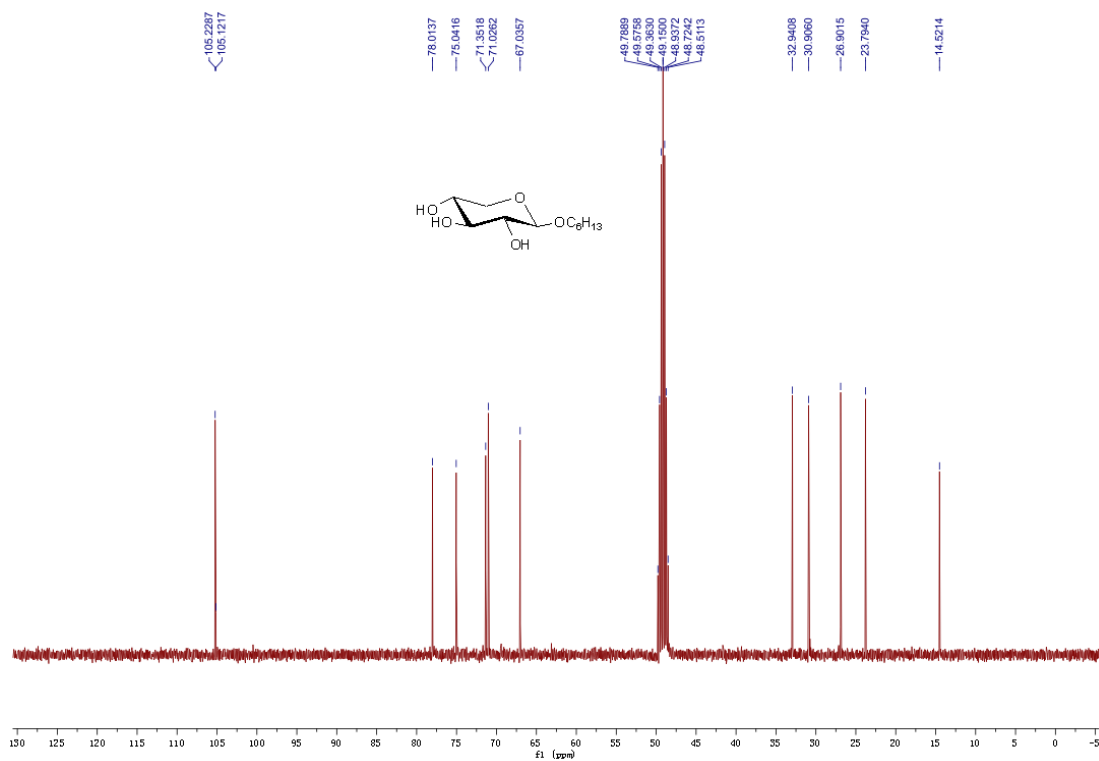


Figure S16. ^{13}C NMR spectrum (400 MHz) of compound **9a** in $\text{d}_4\text{-MeOH}$.

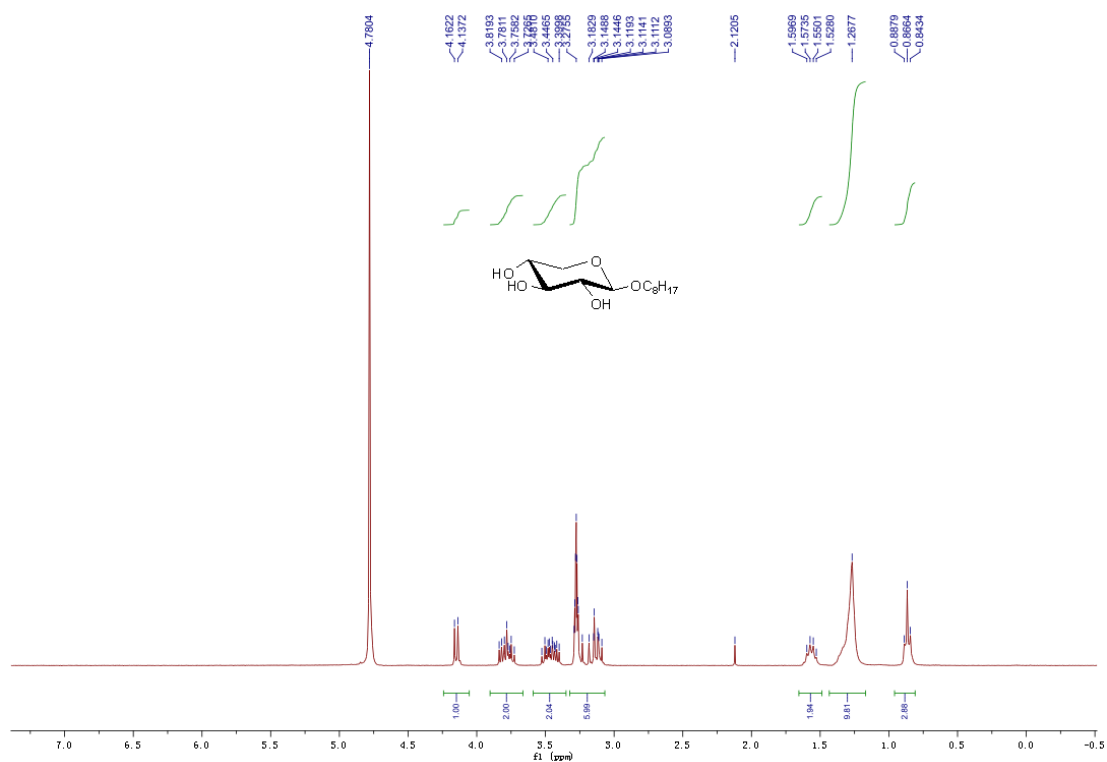


Figure S17. ¹H NMR spectrum (300 MHz) of compound **9b** in d₄-MeOH.

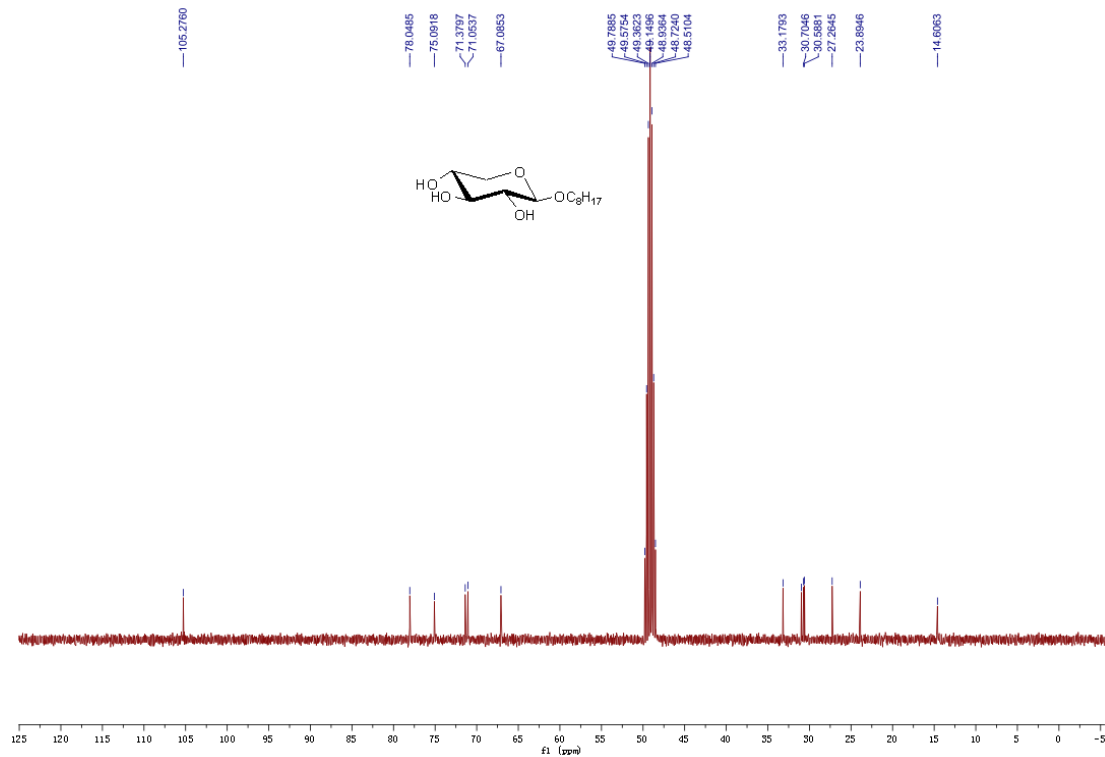


Figure S18. ¹³C NMR spectrum (100 MHz) of compound **9b** in d₄-MeOH.

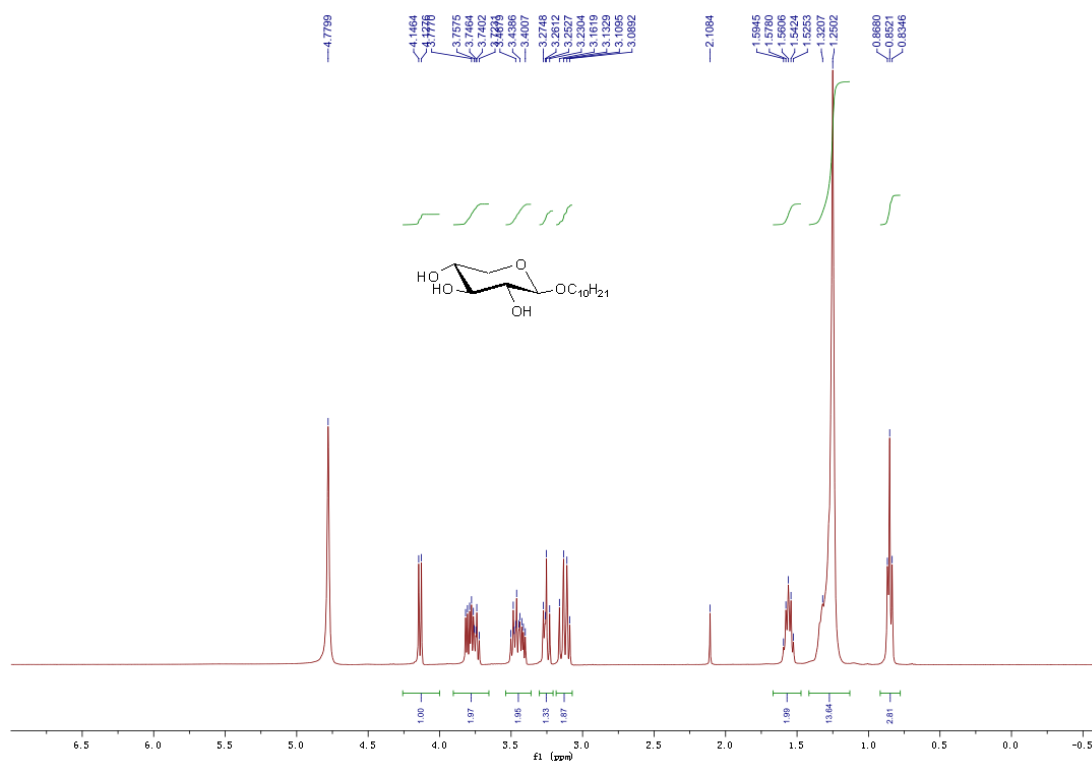


Figure S19. ¹H NMR spectrum (400 MHz) of compound **9c** in d₄-MeOH.

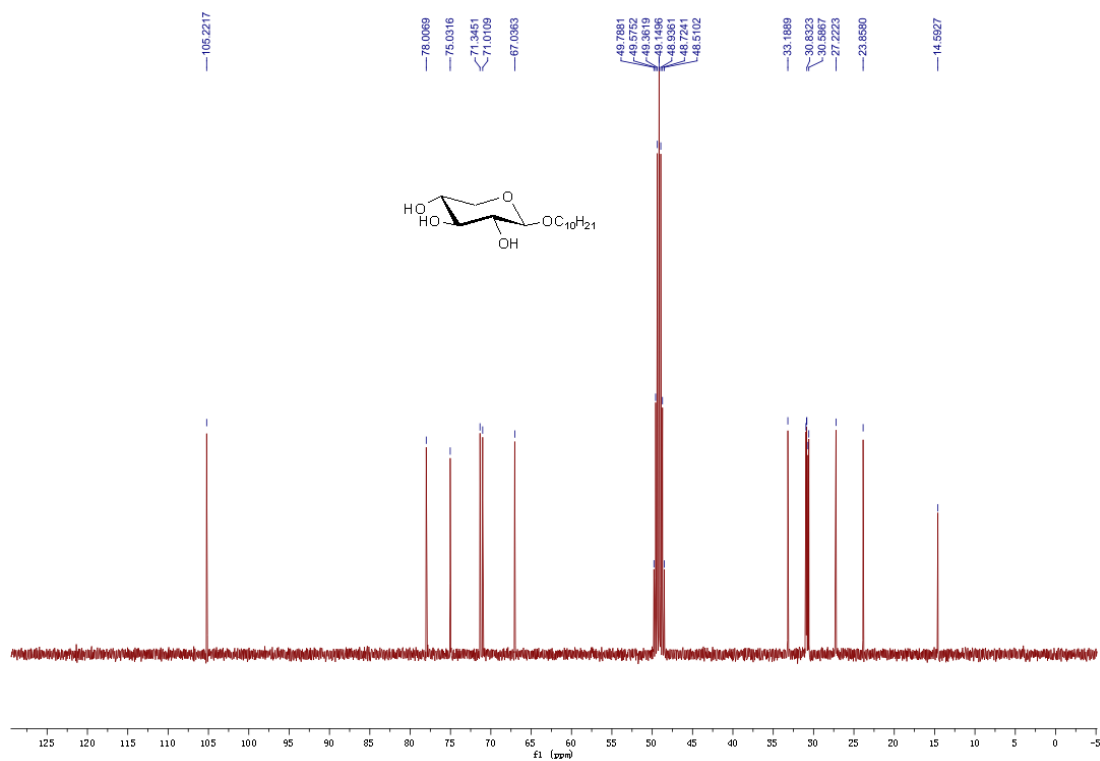


Figure S20. ¹³C NMR spectrum (100 MHz) of compound **9c** in d₄-MeOH.

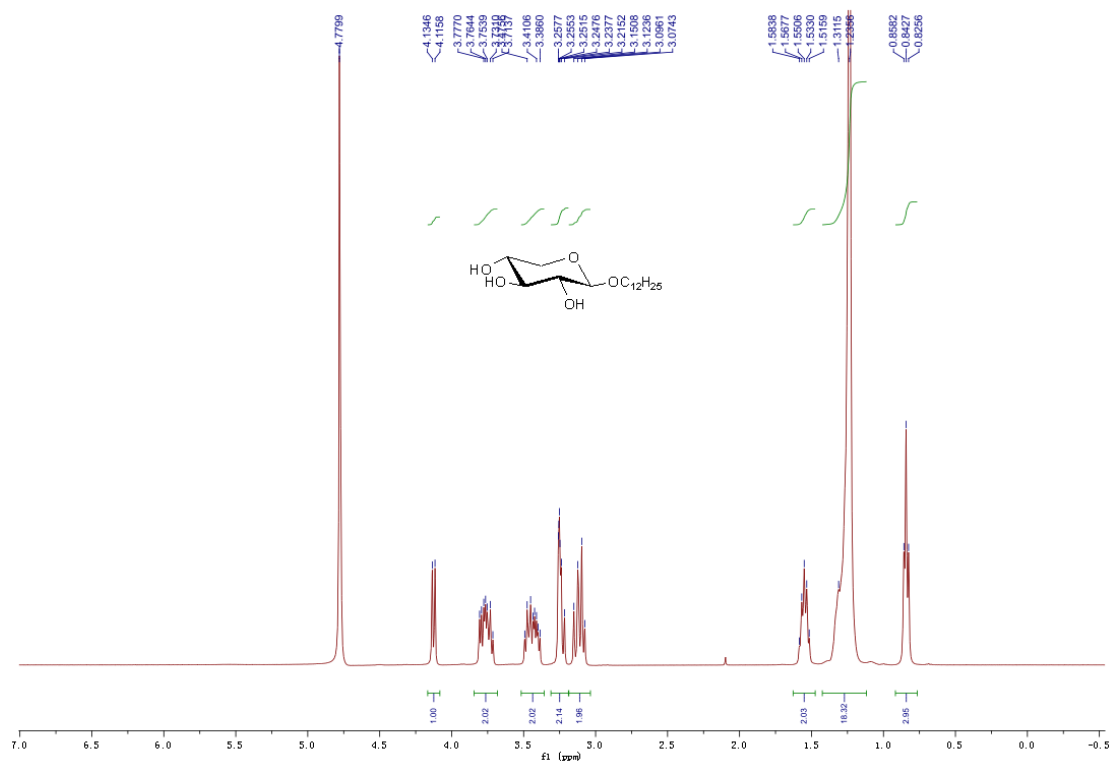


Figure S21. ^1H NMR spectrum (400 MHz) of compound **9d** in $\text{d}_4\text{-MeOH}$.

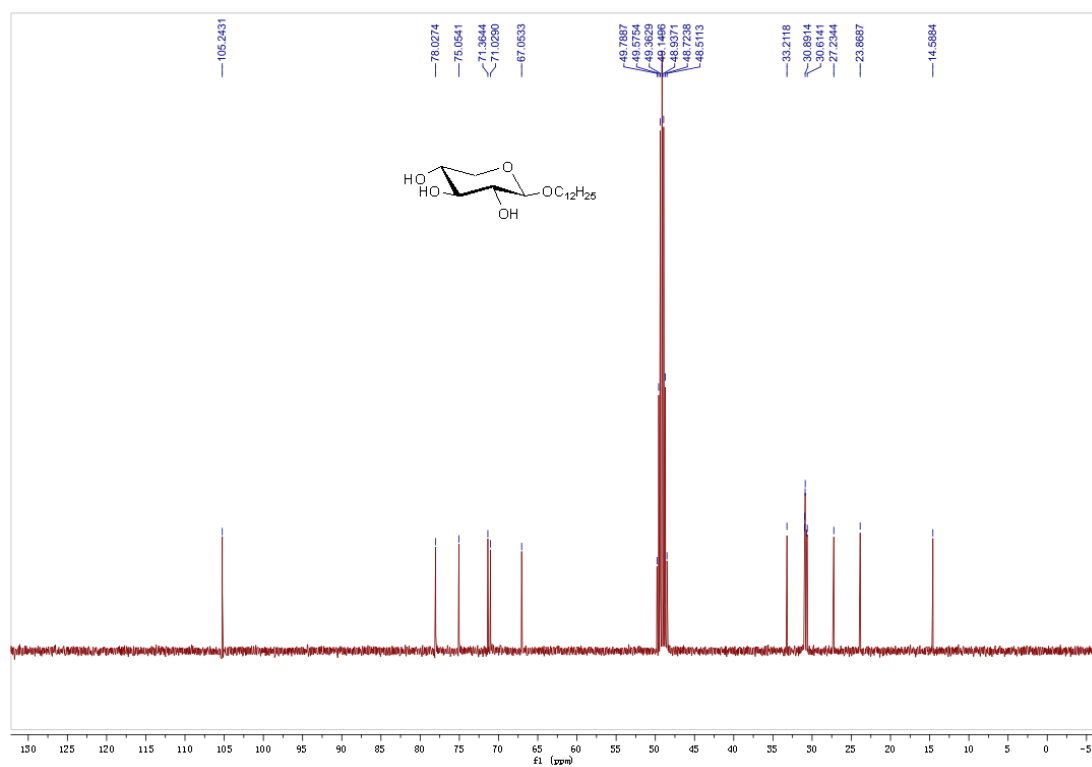


Figure S22. ^{13}C NMR spectrum (100 MHz) of compound **9d** in $\text{d}_4\text{-MeOH}$.

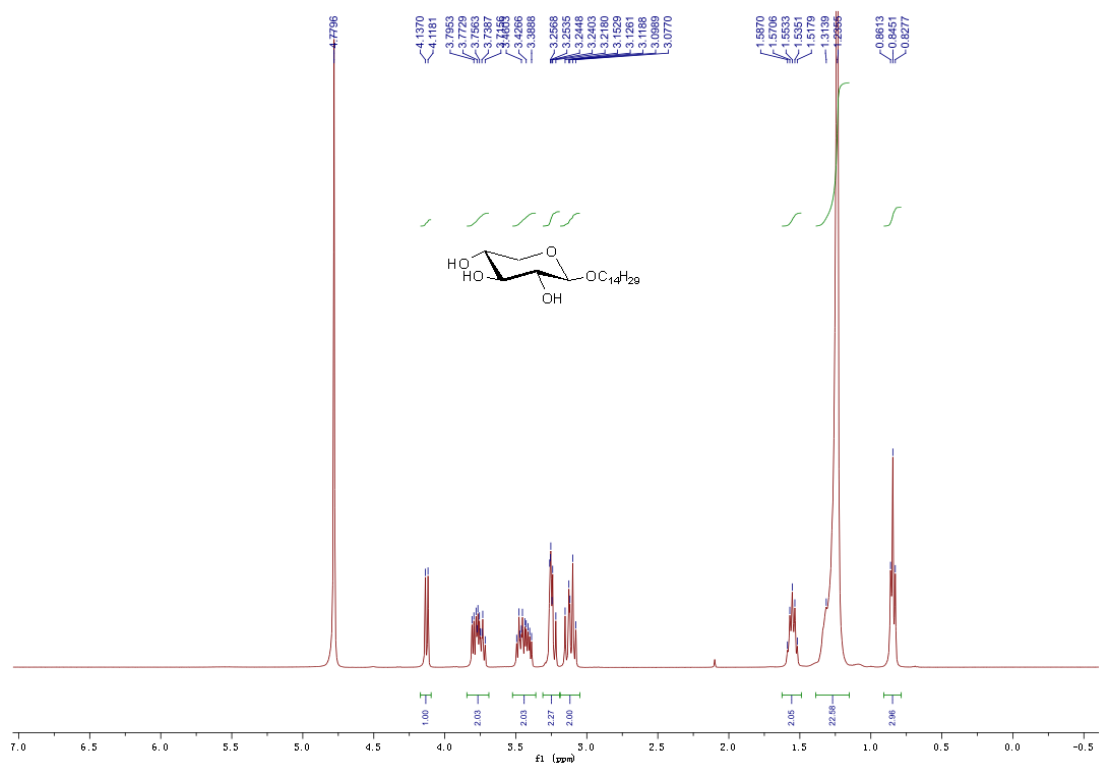


Figure S23. ^1H NMR spectrum (400 MHz) of compound **9e** in $\text{d}_4\text{-MeOH}$.

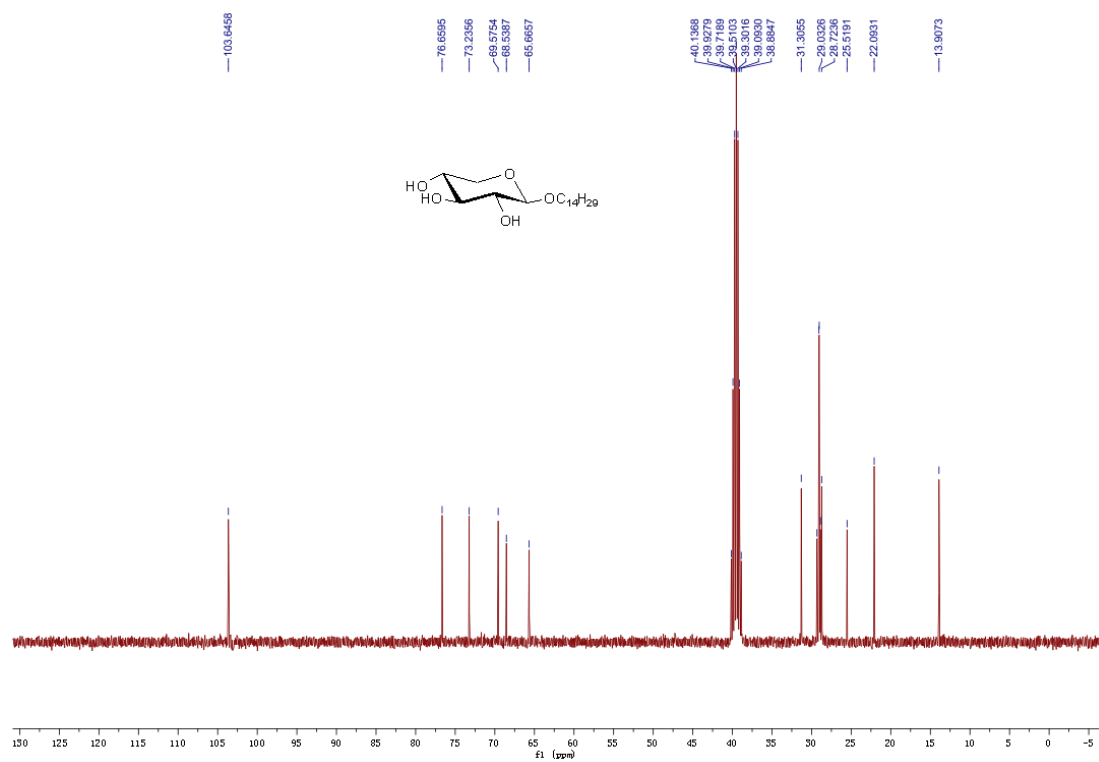


Figure S24. ^{13}C NMR spectrum (100 MHz) of compound **9e** in $\text{d}_4\text{-MeOH}$.

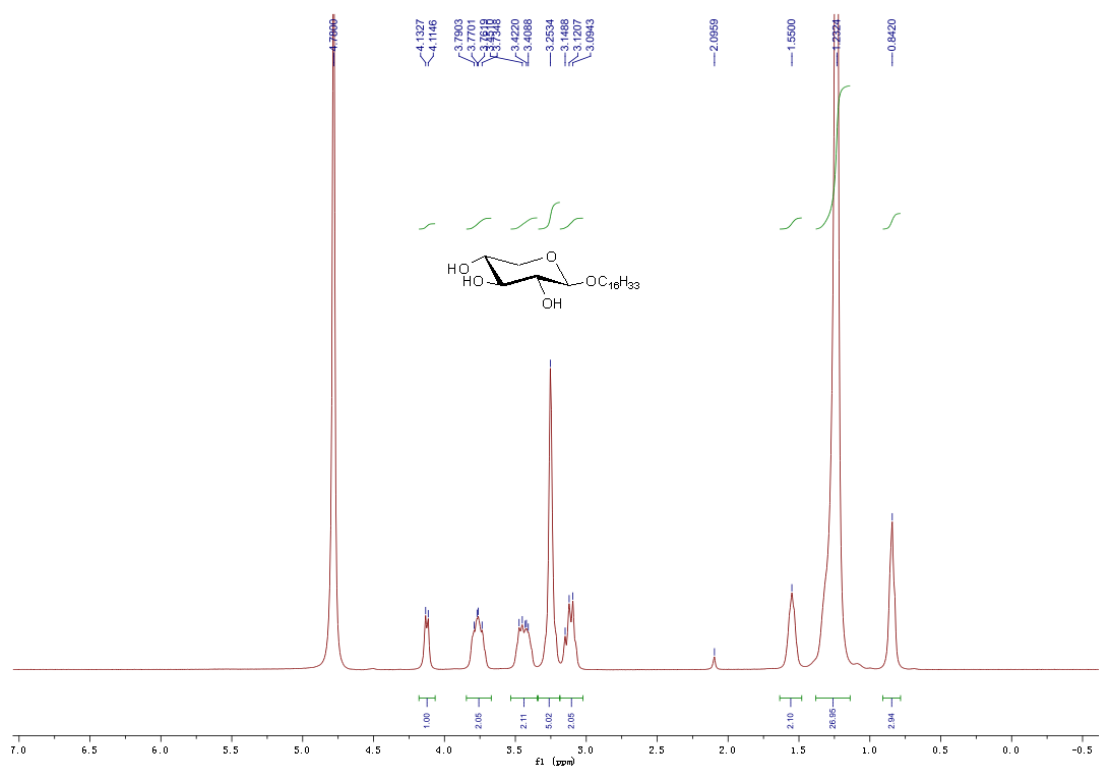


Figure S25. ^1H NMR spectrum (400 MHz) of compound **9f** in $\text{d}_4\text{-MeOH}$.

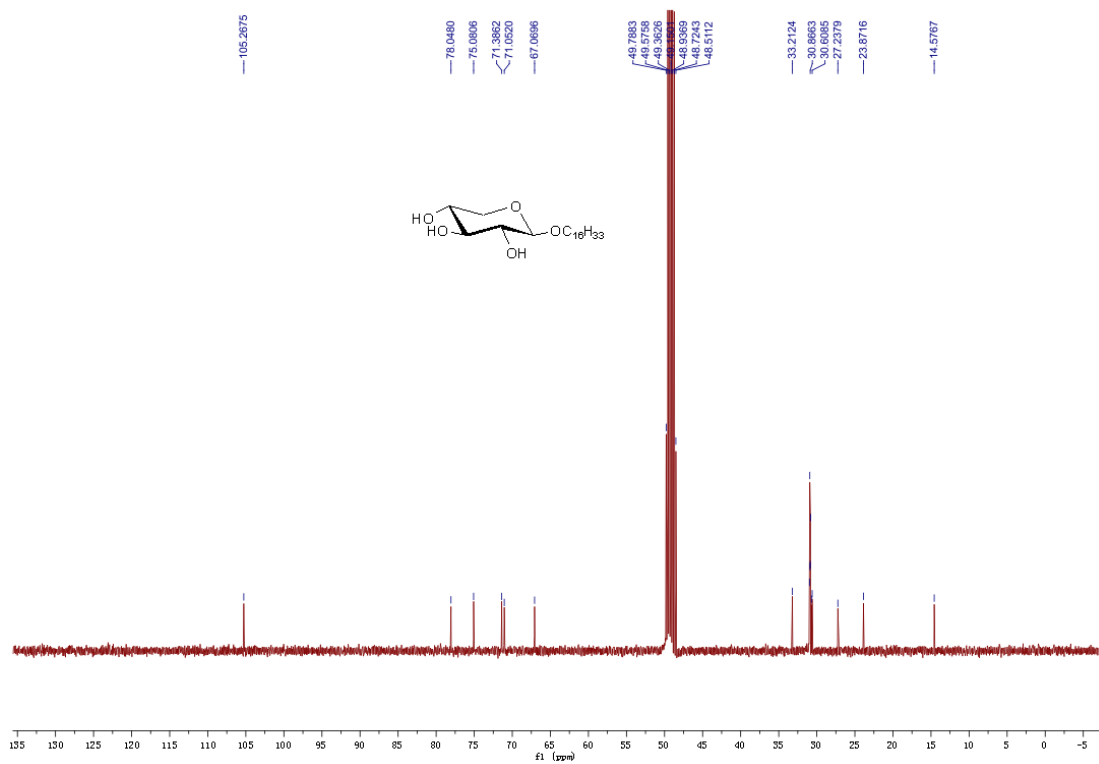


Figure S26. ^{13}C NMR spectrum (100 MHz) of compound **9f** in $\text{d}_4\text{-MeOH}$.

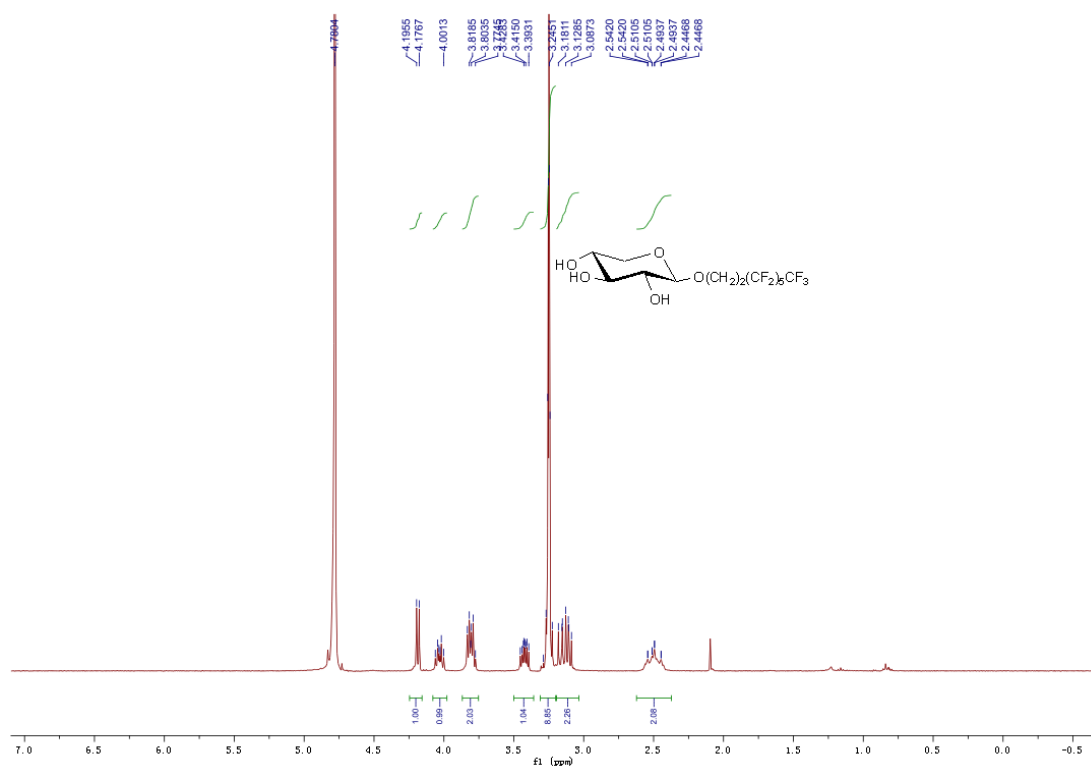


Figure S27. ^1H NMR spectrum (400 MHz) of compound **9g** in $\text{d}_4\text{-MeOH}$.

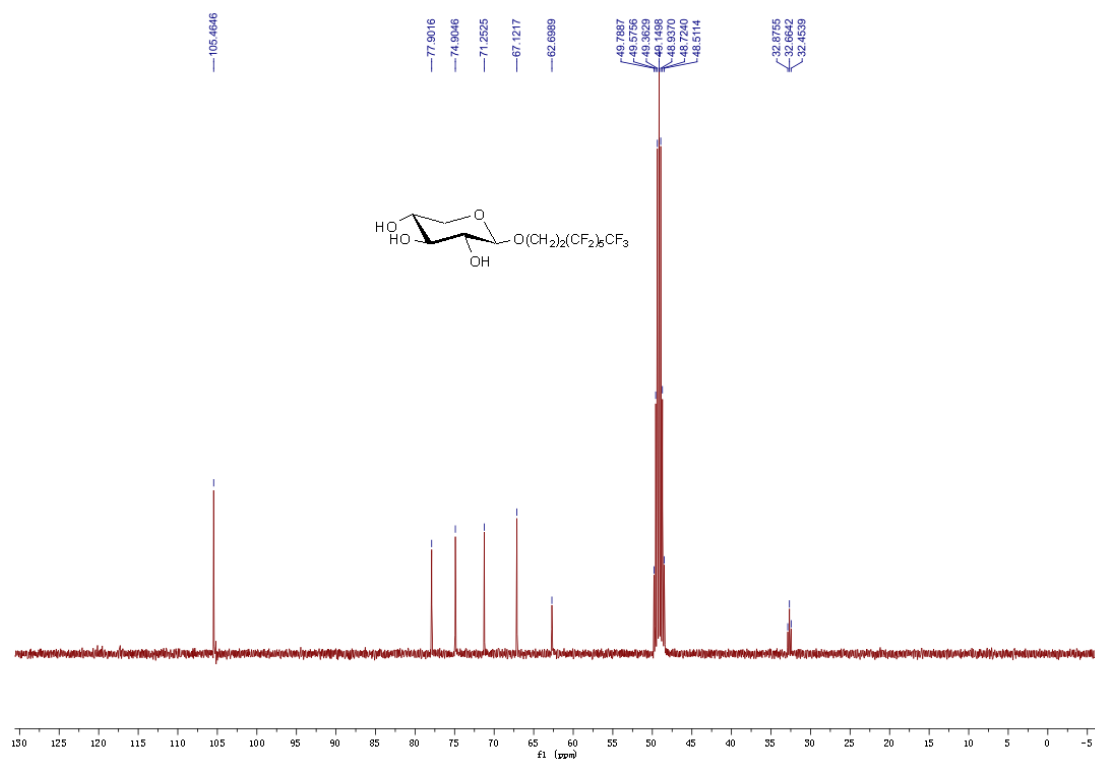


Figure S28. ^{13}C NMR spectrum (100 MHz) of compound **9g** in $\text{d}_4\text{-MeOH}$.

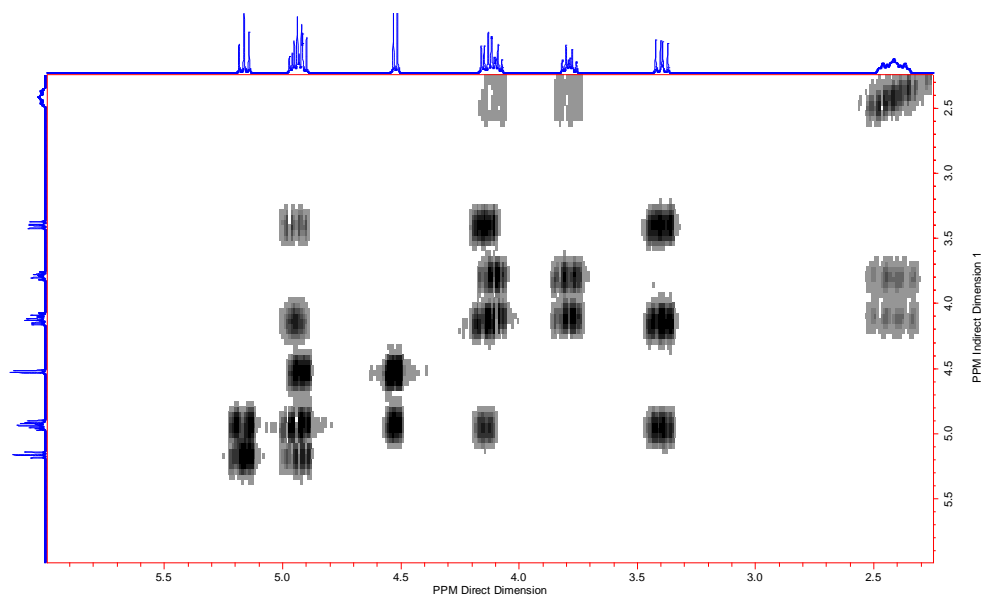


Figure S29. COSY spectrum of **10** in CDCl_3

Table S1. Crystal data and structure refinement for decyl β -D-xylopyranoside **9c**.

Empirical formula	C ₁₅ H ₃₀ O ₅
Formula weight	290.40
Temperature	90.0(2) K
Wavelength	0.71070 Å
Crystal system	Monoclinic
Space group	C2
Unit cell dimensions:	
<i>A</i>	13.2154(6) Å
<i>B</i>	4.3040(2) Å
<i>C</i>	29.9491(16) Å
Volume	1662.03(14) Å ³
Z, calculated density	2, 1.197 mg/m ³
Absorption coefficient	0.089 mm ⁻¹
<i>F</i> (000)	660
Crystal size	0.3×0.3×0.04 mm
Theta range for data collection	2.09- 27.41°
Limiting indices	-16 < <i>h</i> < 16, -5 < <i>k</i> < 5, -38 < <i>l</i> < 38
Reflections collected/unique	2131/ 1625 [<i>R</i> (int) = 0.0535]
Completeness to $\theta = 27.41$	99.5%
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data/restraints/parameters	2131/1/193
Goodness-of-fit on <i>F</i> ²	1.017
Final <i>R</i> indices [<i>I</i> > 2 Σ (<i>I</i>)]	<i>R</i> 1 = 0.0479, <i>wR</i> 2 = 0.0990
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0738, <i>wR</i> 2 = 0.1127
Largest diff. peak and hole	0.275 and -0.206 e Å ⁻³

Table S2. Selected bond lengths and angles for decyl β -D-xylopyranoside **9c**.

Atoms	Bond lengths (Å)	Atoms	Bond angles (°)
O1-C5	1.432(3)	O1- C5-C4	109.8(2)
C1-C2	1.505(4)	O5- C5-O1	108.5(2)
O2-C2	1.425(3)	O5-C5-C4	107.8(2)
C2-C3	1.519(3)	C1-O1-C5	110.3(2)
O3-C3	1.432(3)	O1-C1-C2	110.8(2)
C3-C4	1.506(3)	O2-C2-C1	108.0(2)
O4-C4	1.422(3)	O2- C2-C3	109.2(2)
C4 -C5	1.515(4)	C1-C2-C3	110.4(2)
O5-C5	1.385(3)	O3-C3 C4	109.1(2)
O5 -C6	1.433(3)	O5-C6-C7	106.3(2)
C6-C7	1.518(3)	C6-C7-C8	114.8(2)
		O3-C3-C2	111.2(2)
		C4-C3-C2	112.7(2)
		O4-C4-C3	107.7(2)
		O4-C4-C5	110.5(2)
		C3-C4-C5	110.1(2)
		C5-O5-C6	115.6(2)

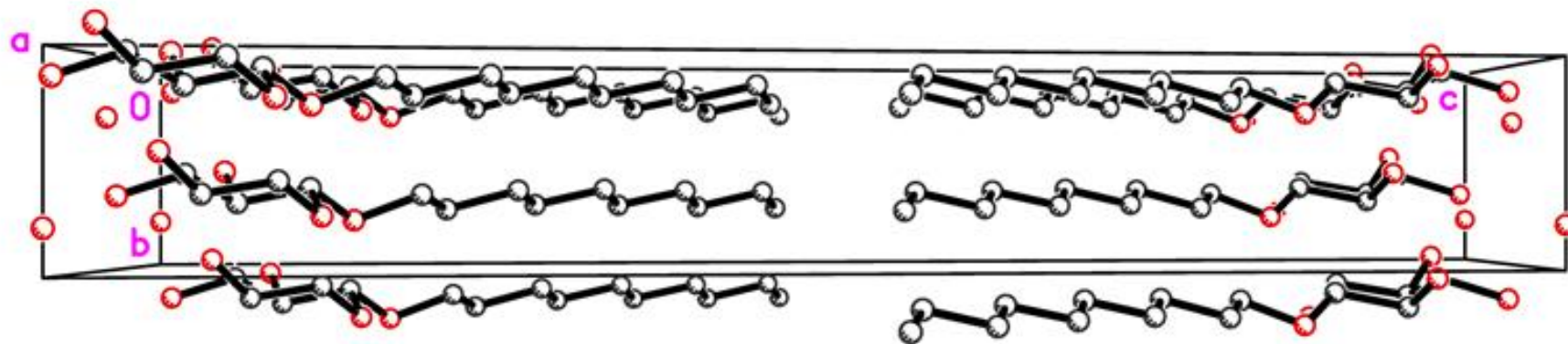


Figure S30. Alternating bilayers of hydrophilic xyloside groups and hydrophobic decyl groups formed parallel to the a-b plane by decyl β -D-xylopyranoside (**9c**).