

Supplementary Materials: Identification of Novel Human Breast Carcinoma (MDA-MB-231) Cell Growth Modulators from a Carbohydrate-Based Diversity Oriented Synthesis Library

Elena Lenci, Riccardo Innocenti, Alessio Biagioni, Gloria Menchi, Francesca Bianchini and Andrea Trabocchi

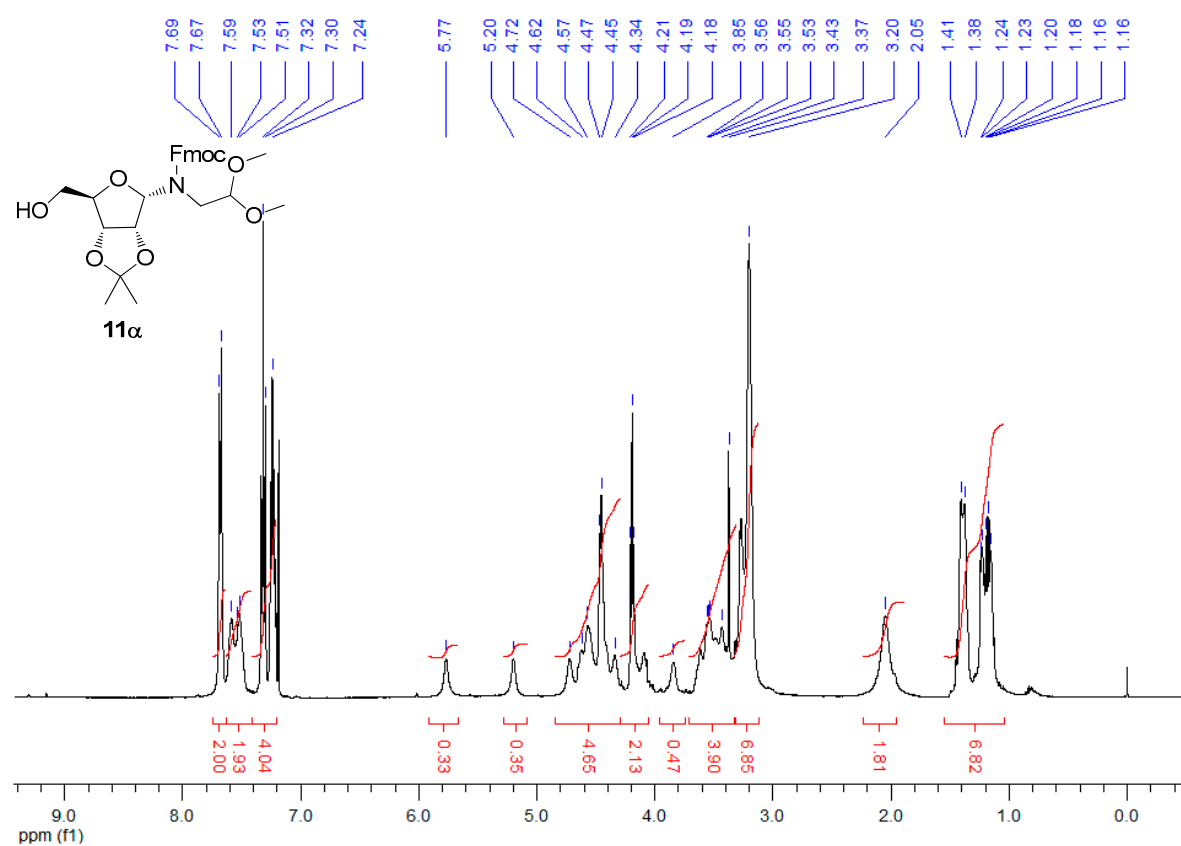
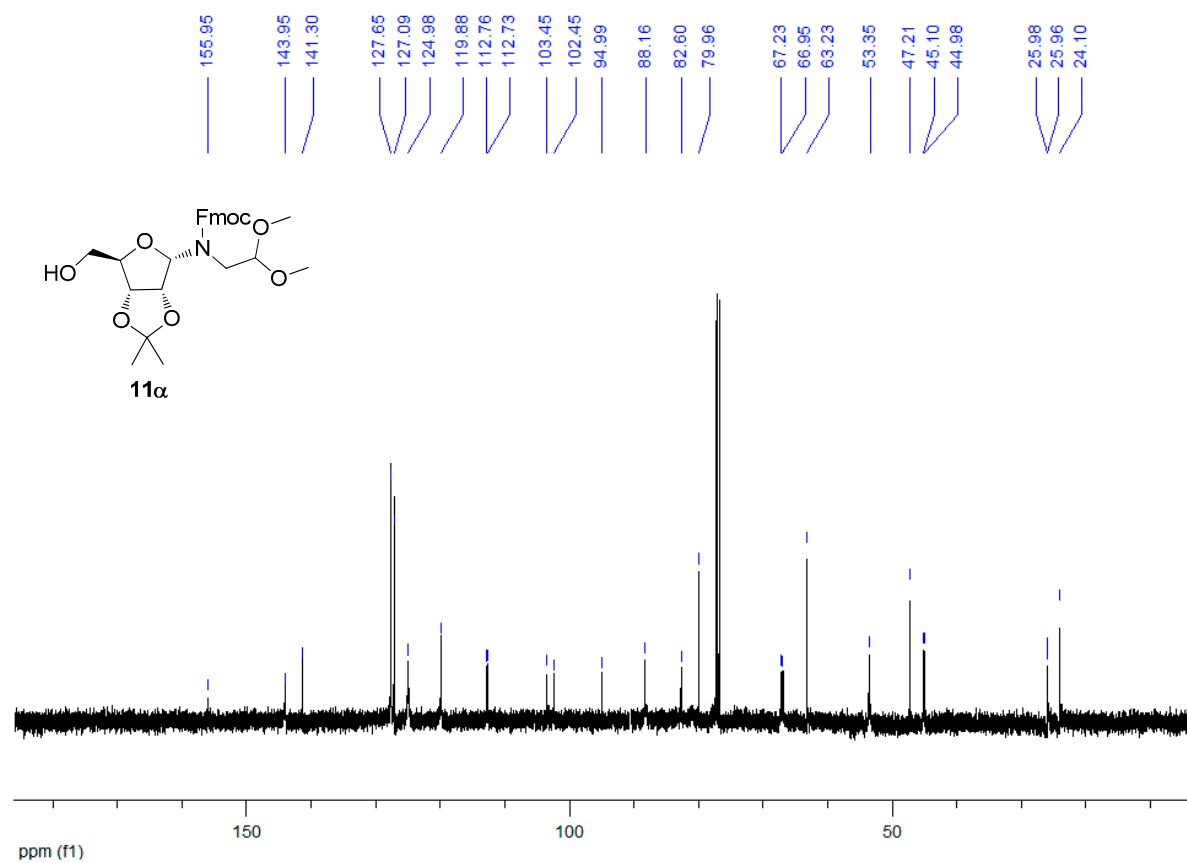
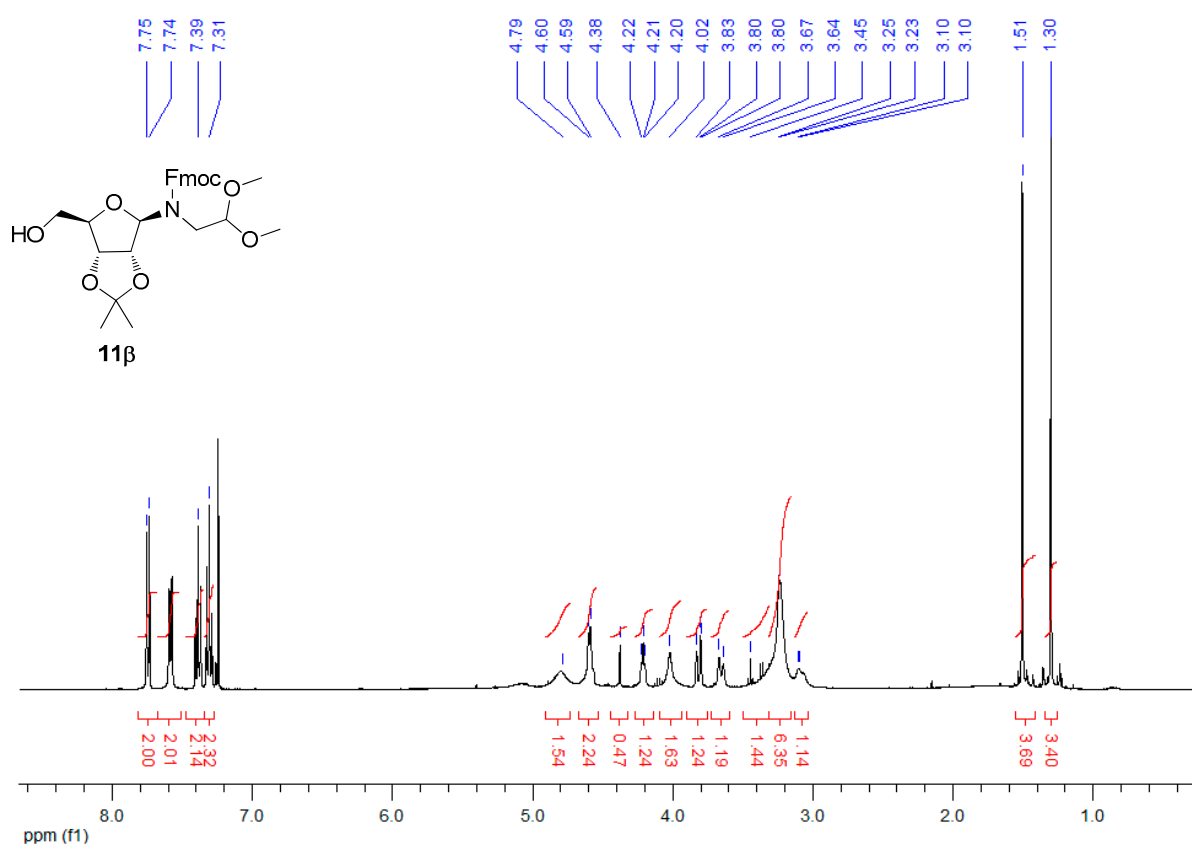
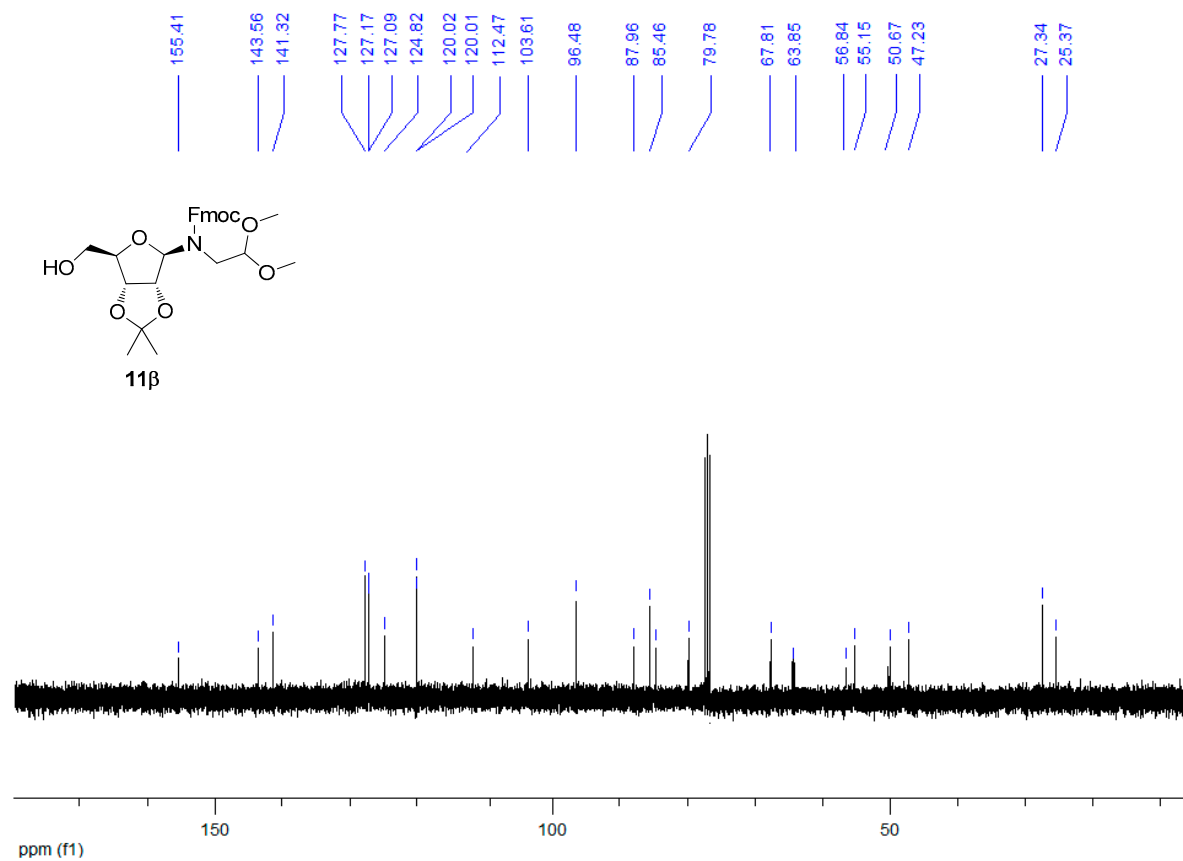
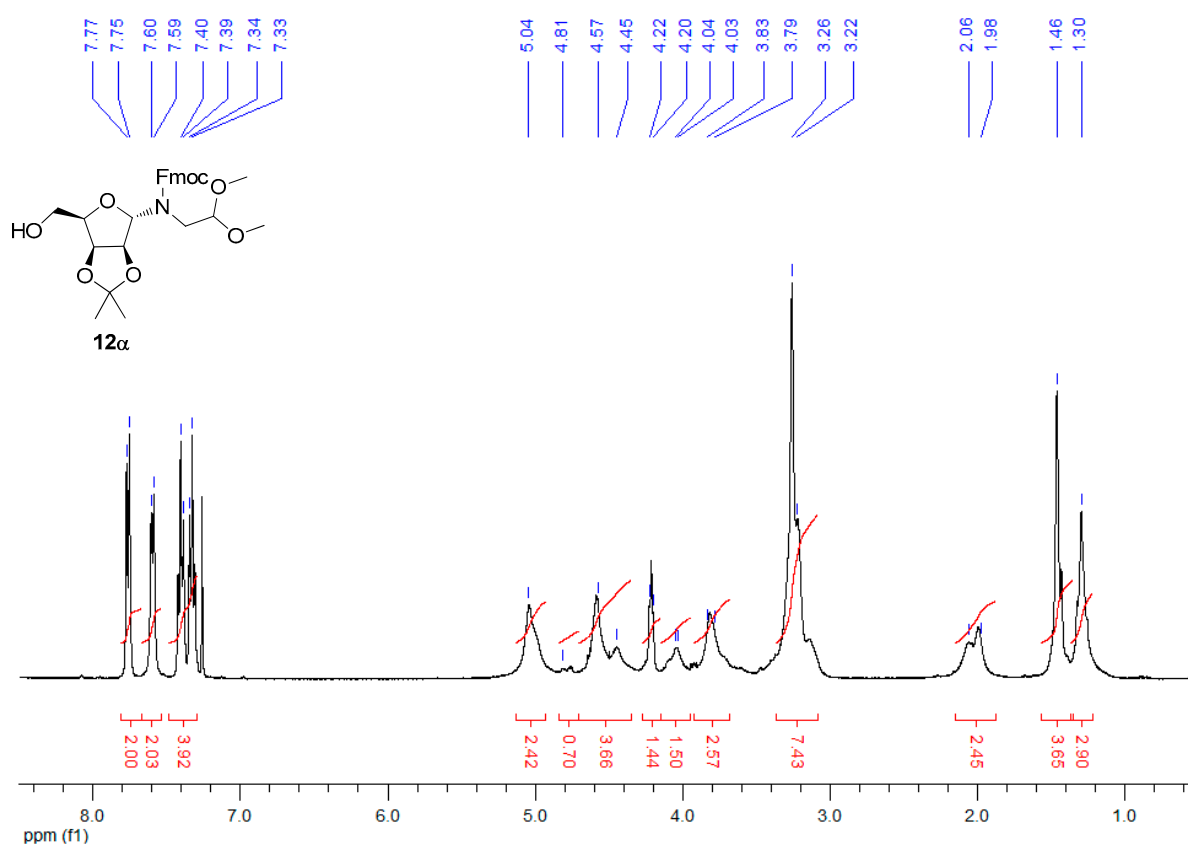
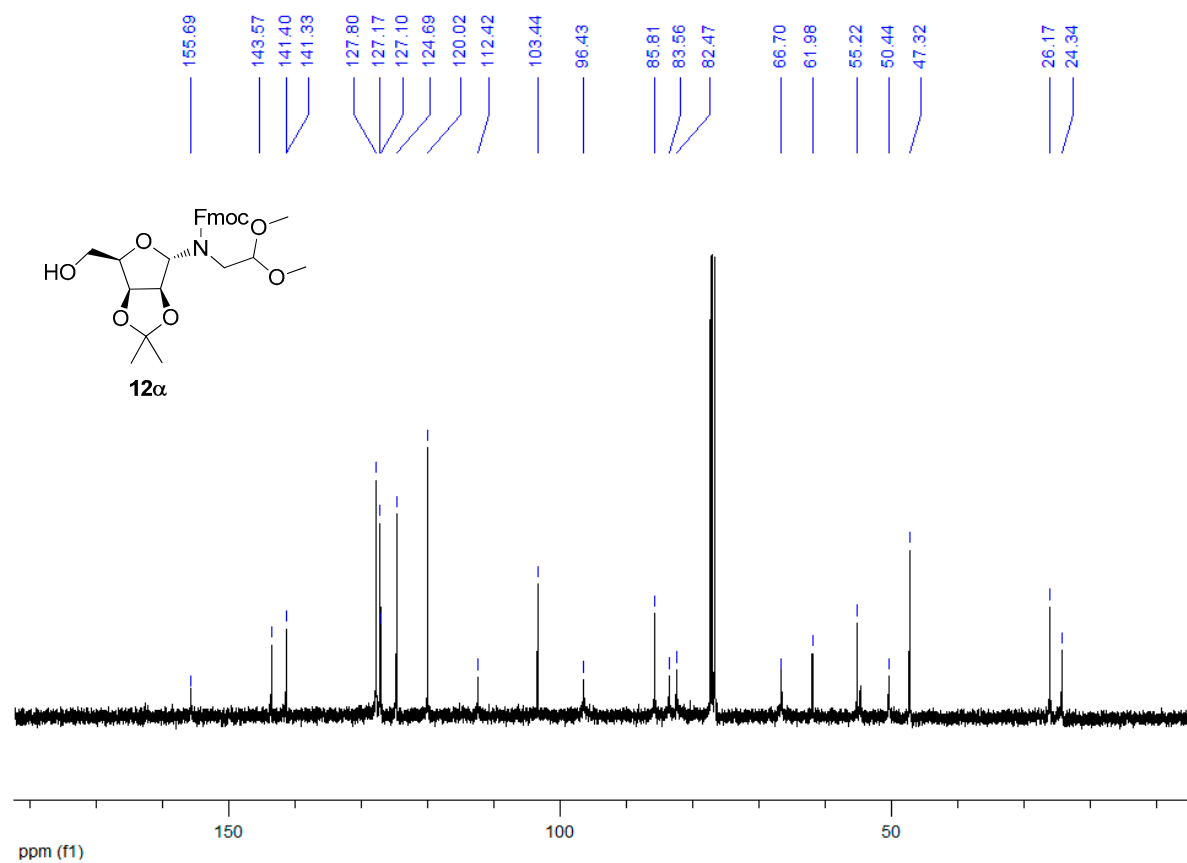
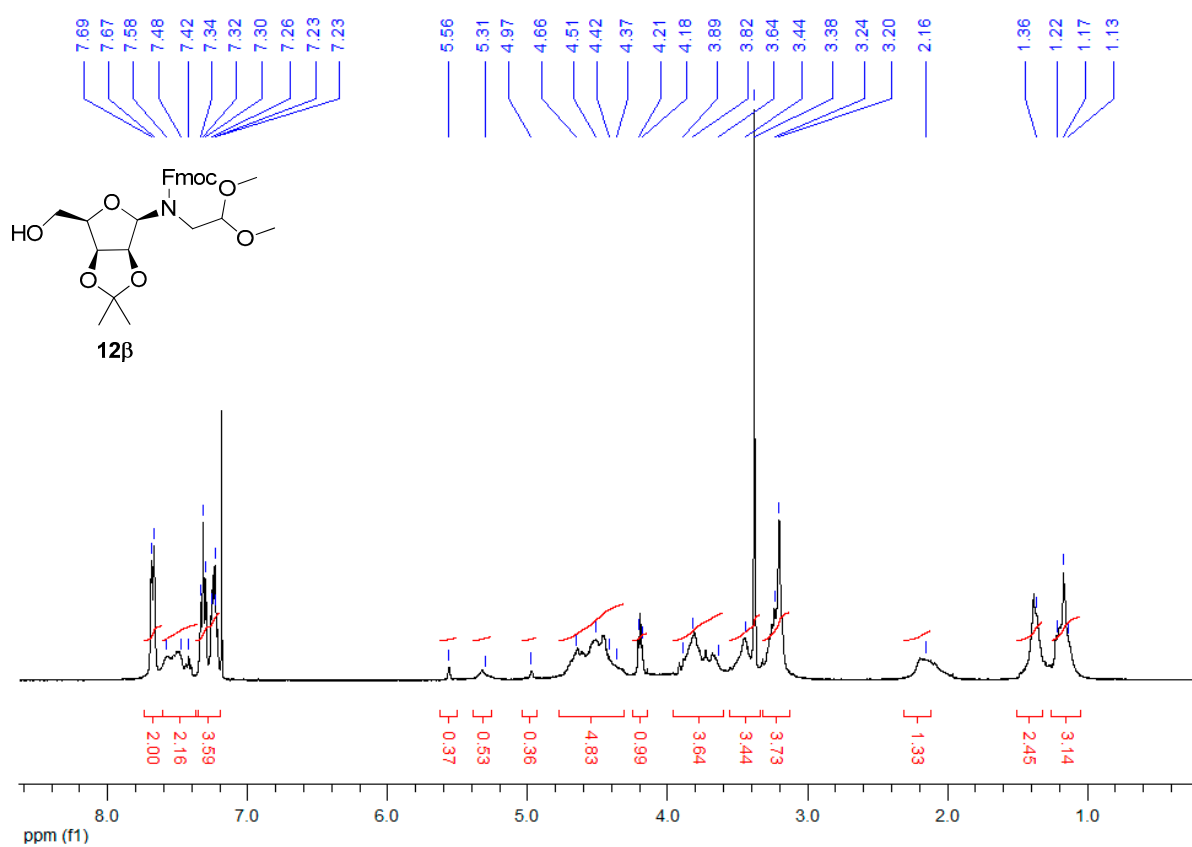
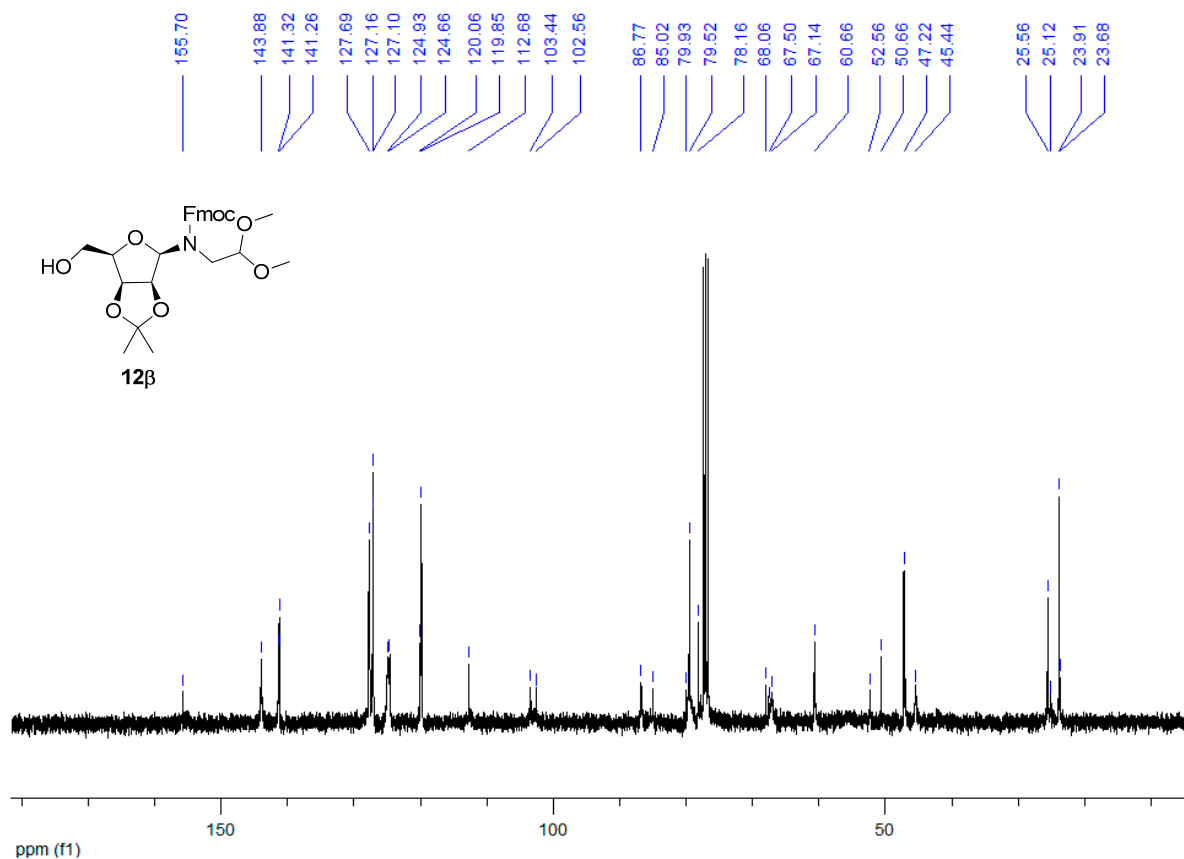
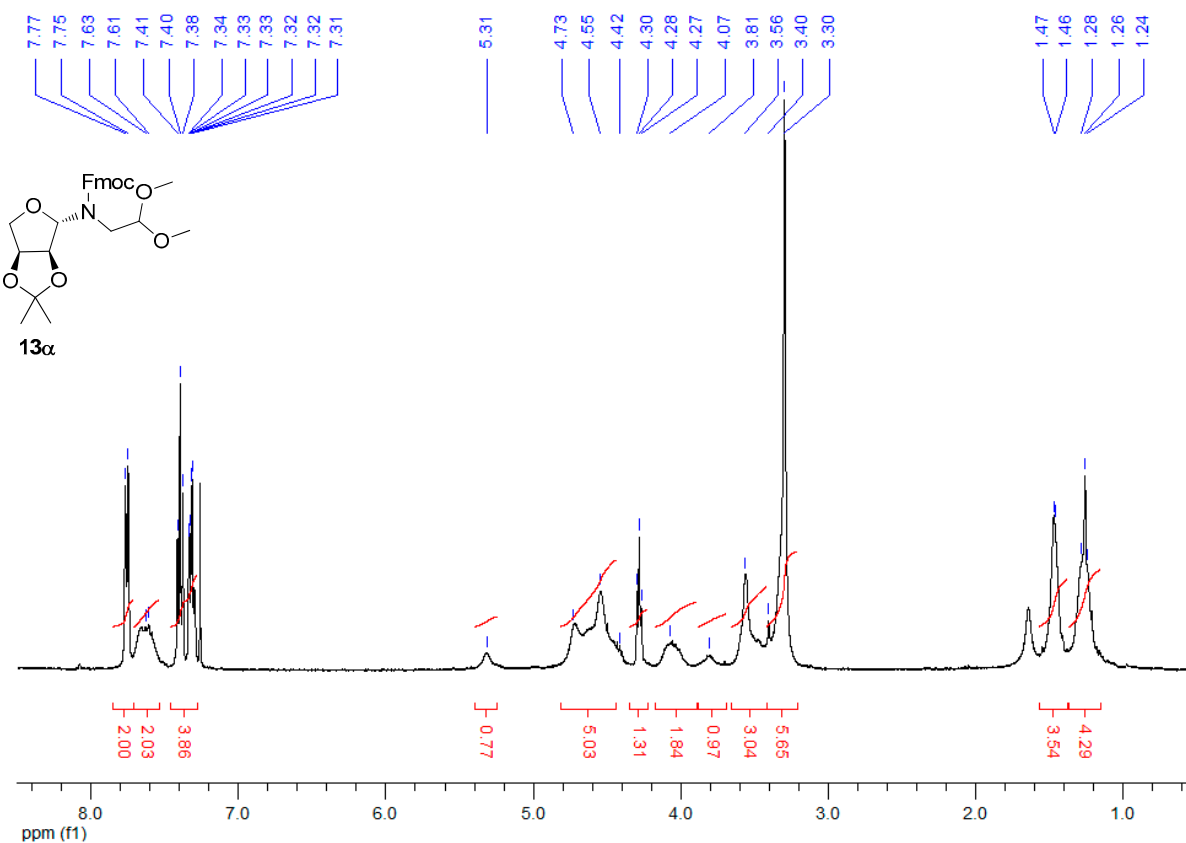


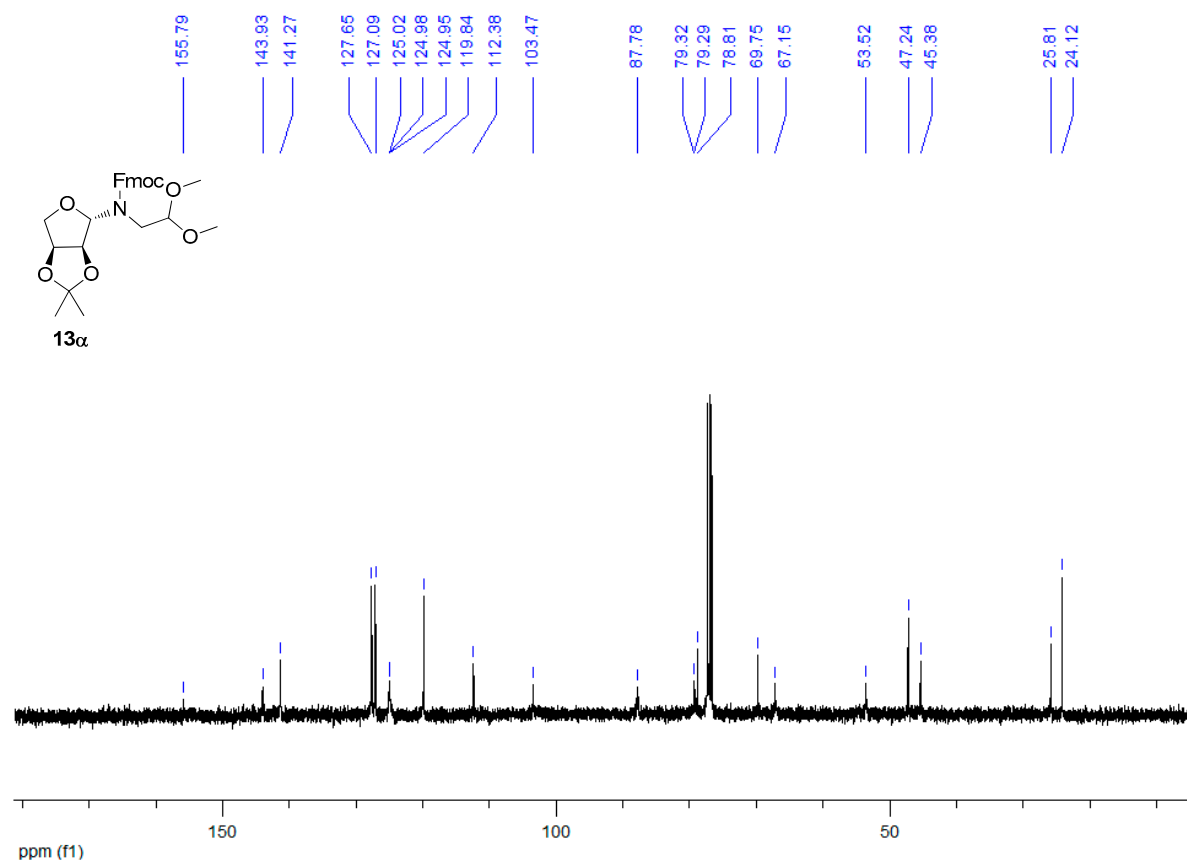
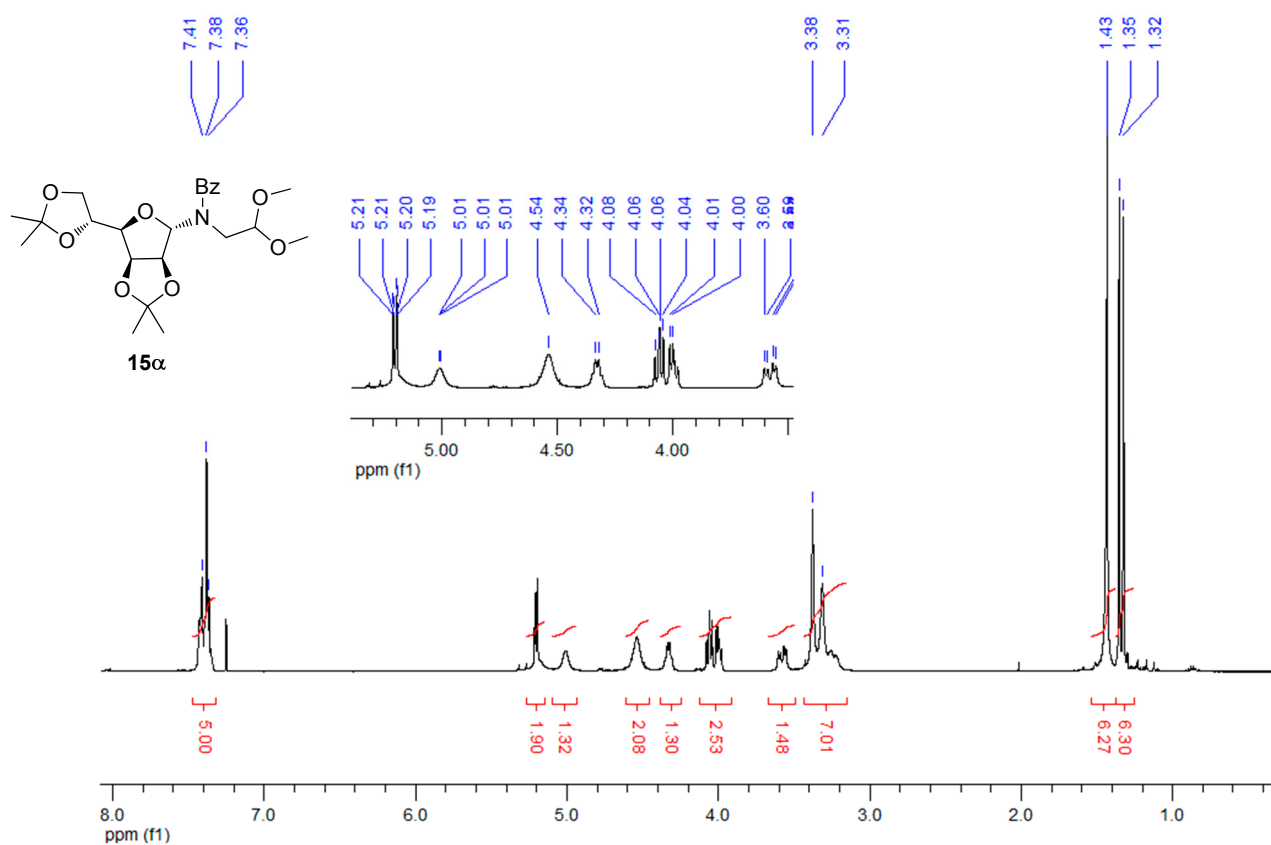
Figure S1. ¹H-NMR spectrum of compound **11α** (400 MHz, CDCl₃).

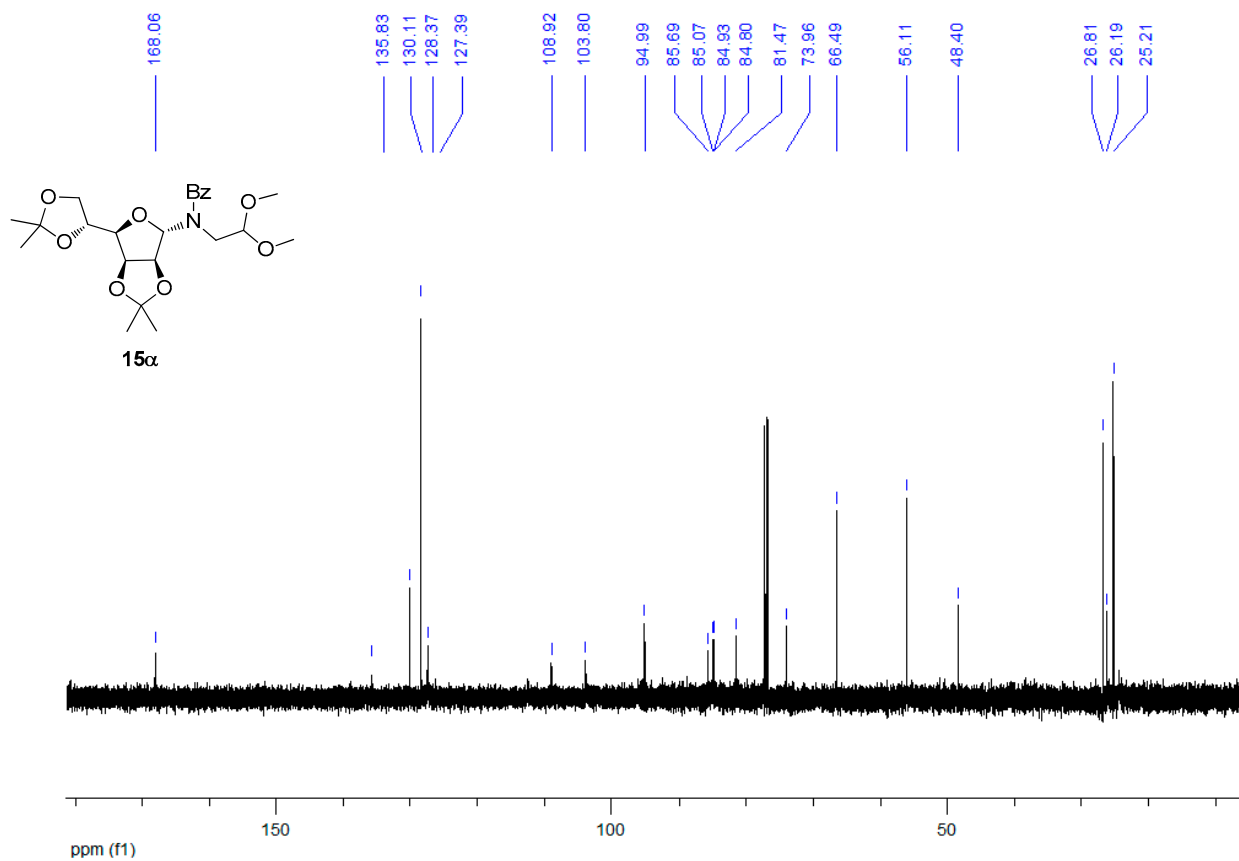
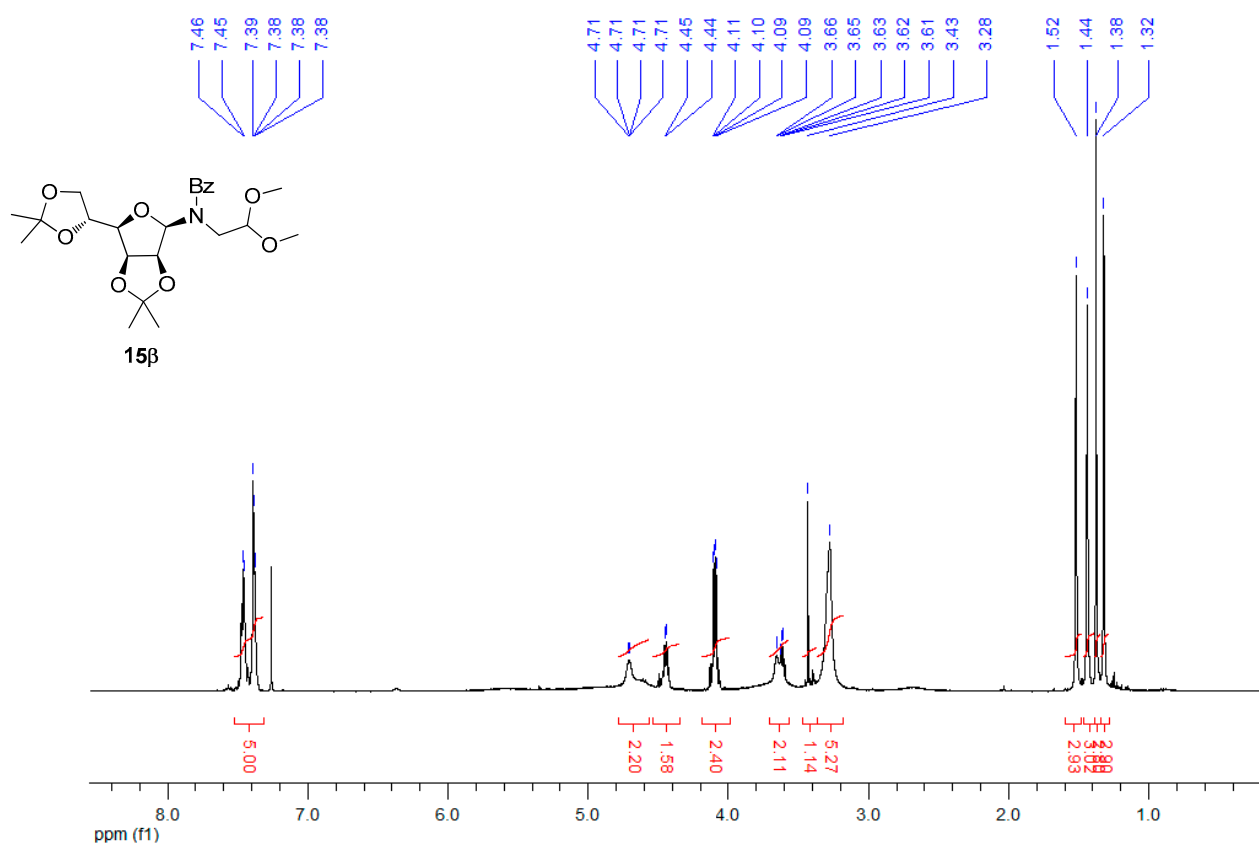
Figure S2. ¹³C-NMR spectrum of compound **11α** (50 MHz, CDCl₃).Figure S3. ¹H-NMR spectrum of compound **11β** (400 MHz, CDCl₃).

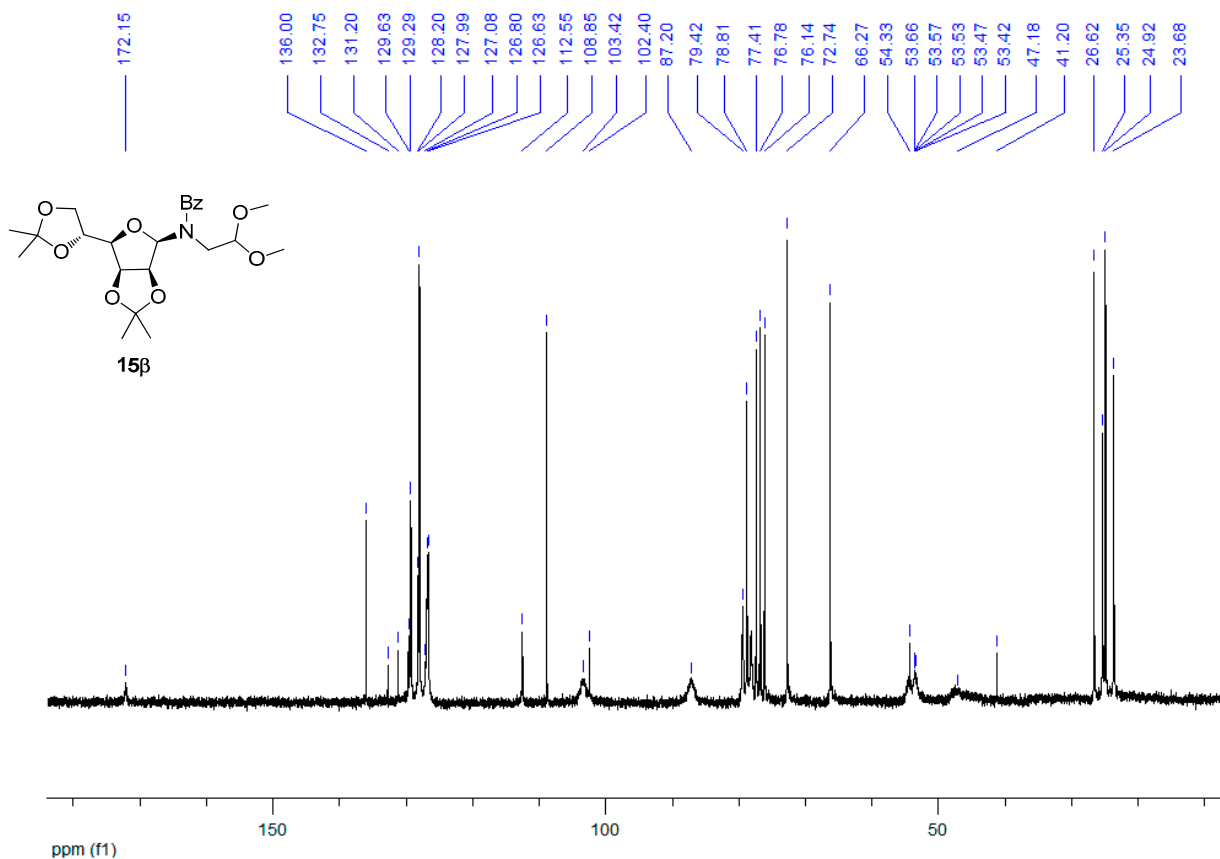
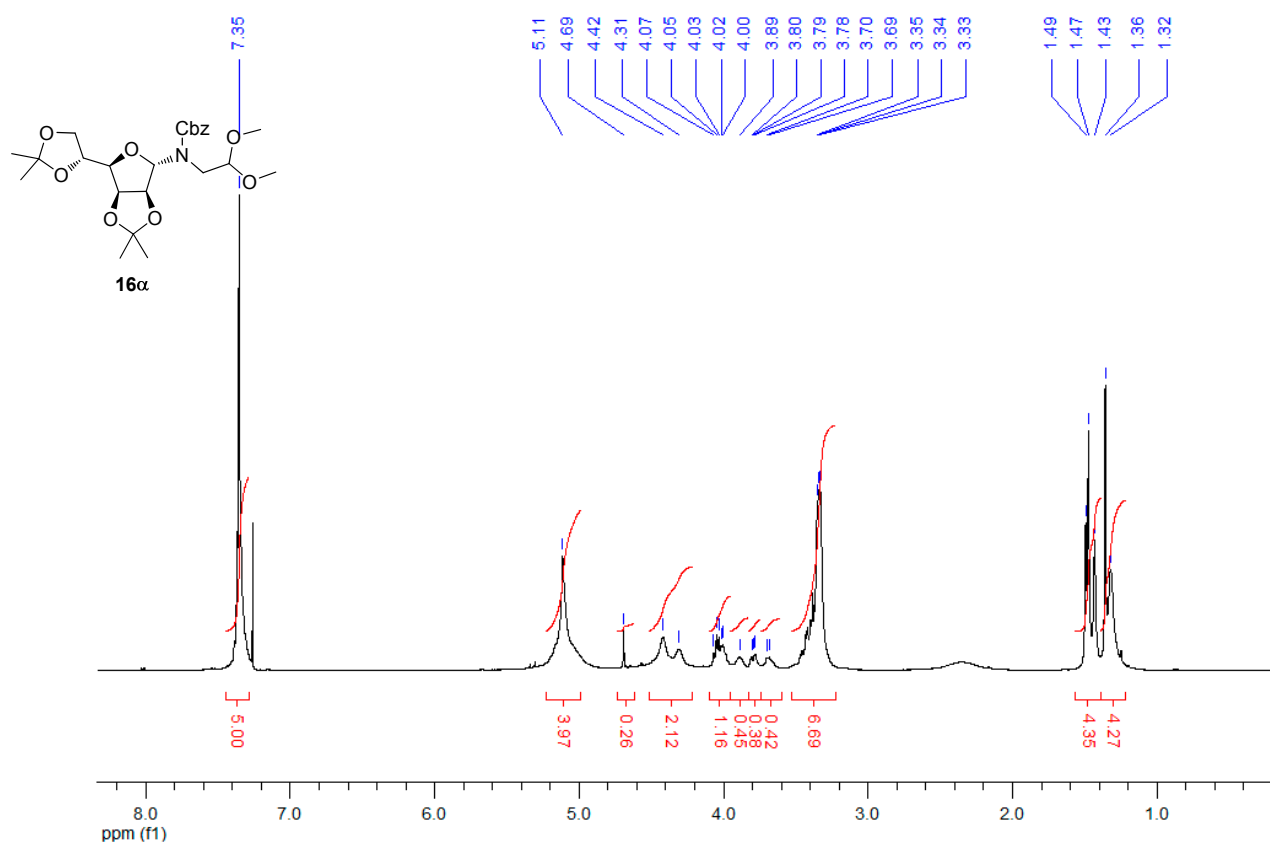
Figure S4. ^{13}C -NMR spectrum of compound **11β** (100 MHz, CDCl_3).Figure S5. ^1H -NMR spectrum of compound **12α** (400 MHz, CDCl_3).

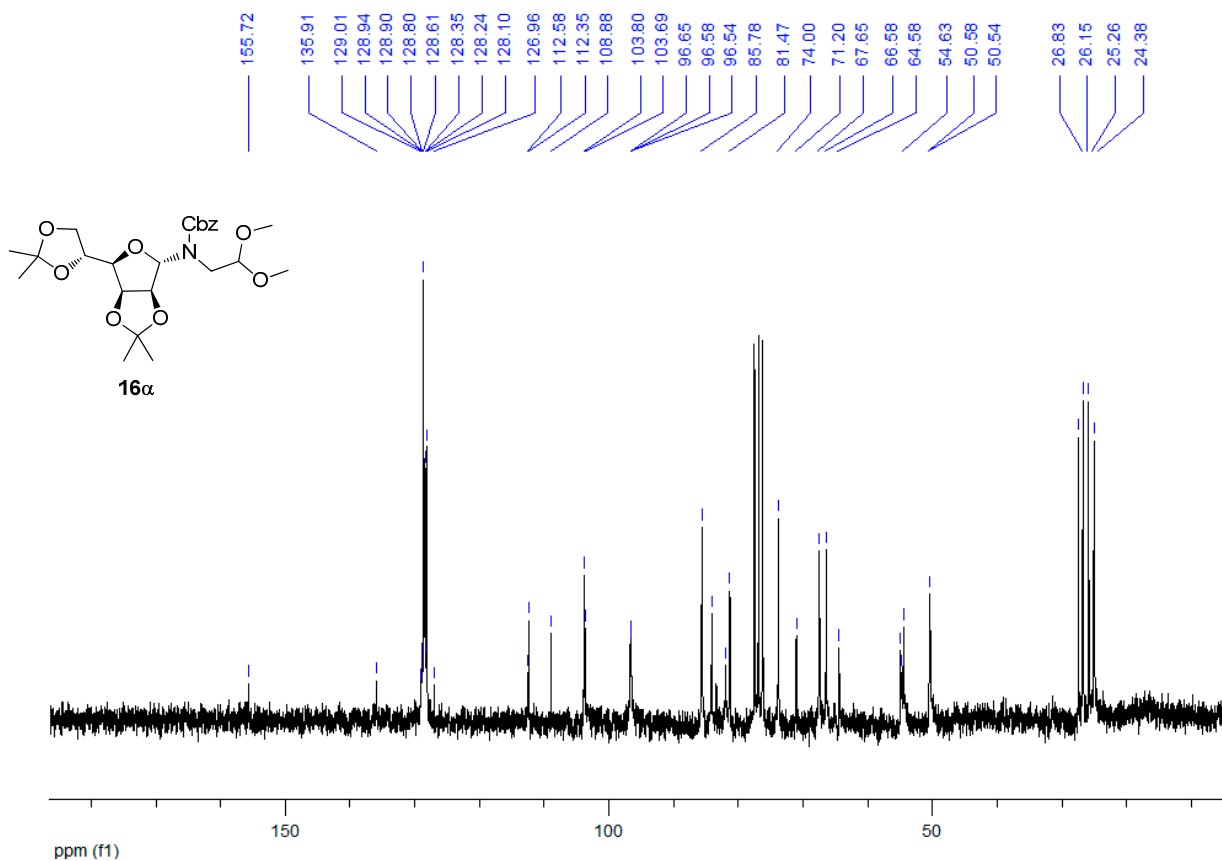
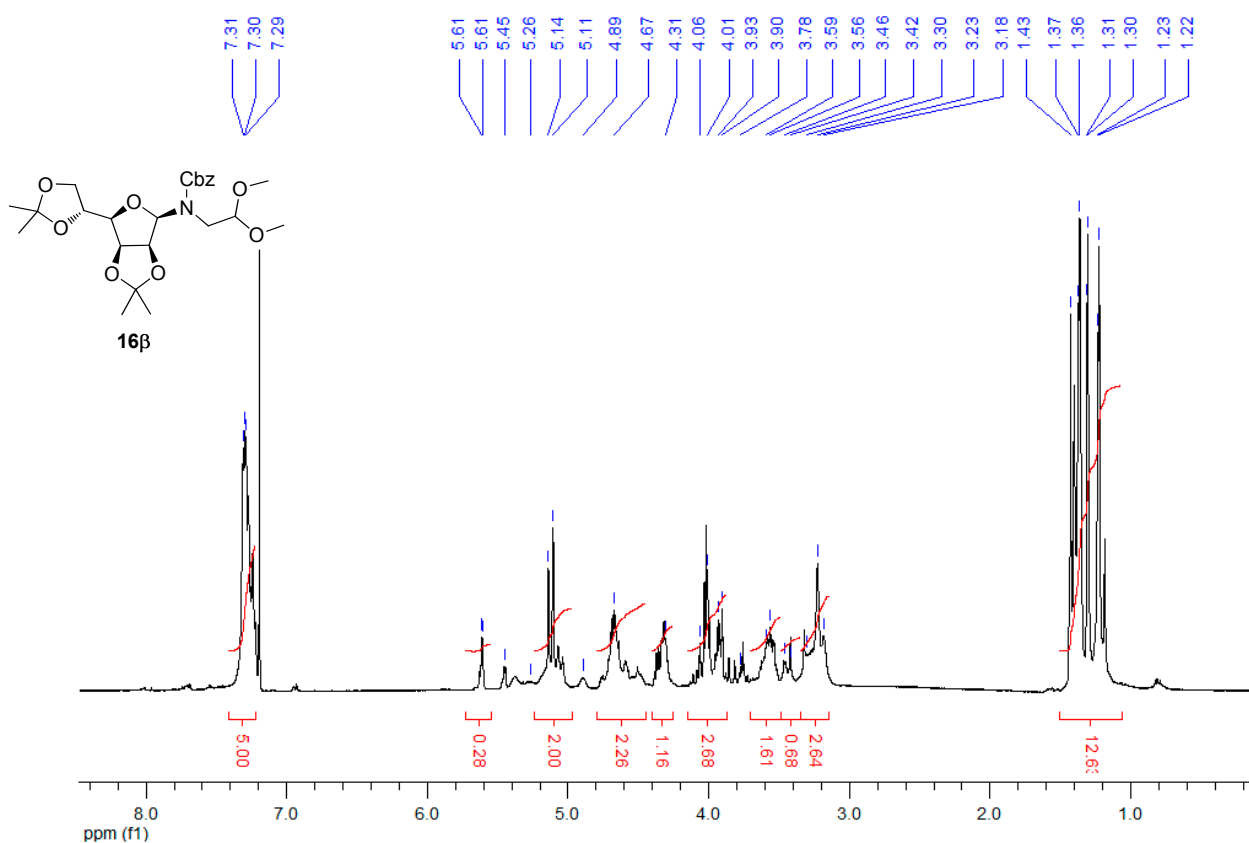
Figure S6. ¹³C-NMR spectrum of compound **12α** (50 MHz, CDCl₃).Figure S7. ¹H-NMR spectrum of compound **12β** (400 MHz, CDCl₃).

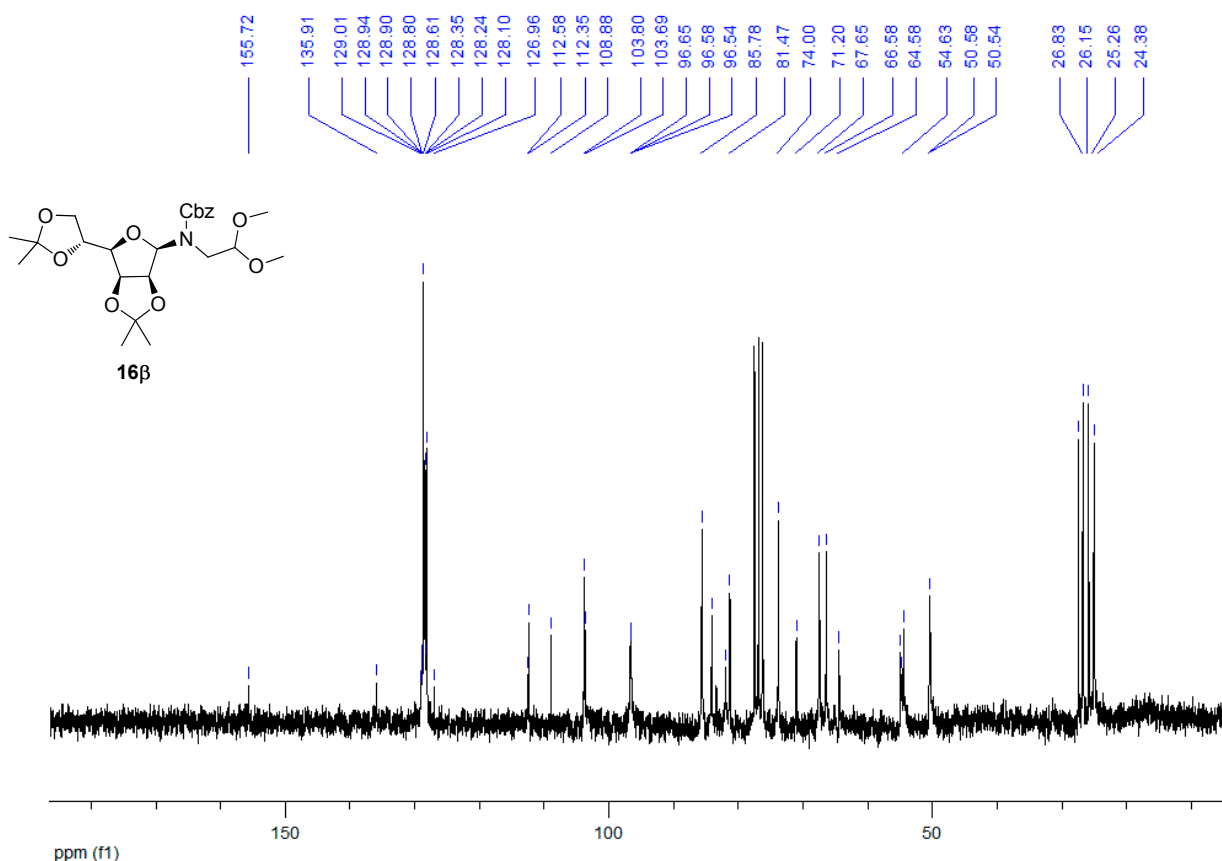
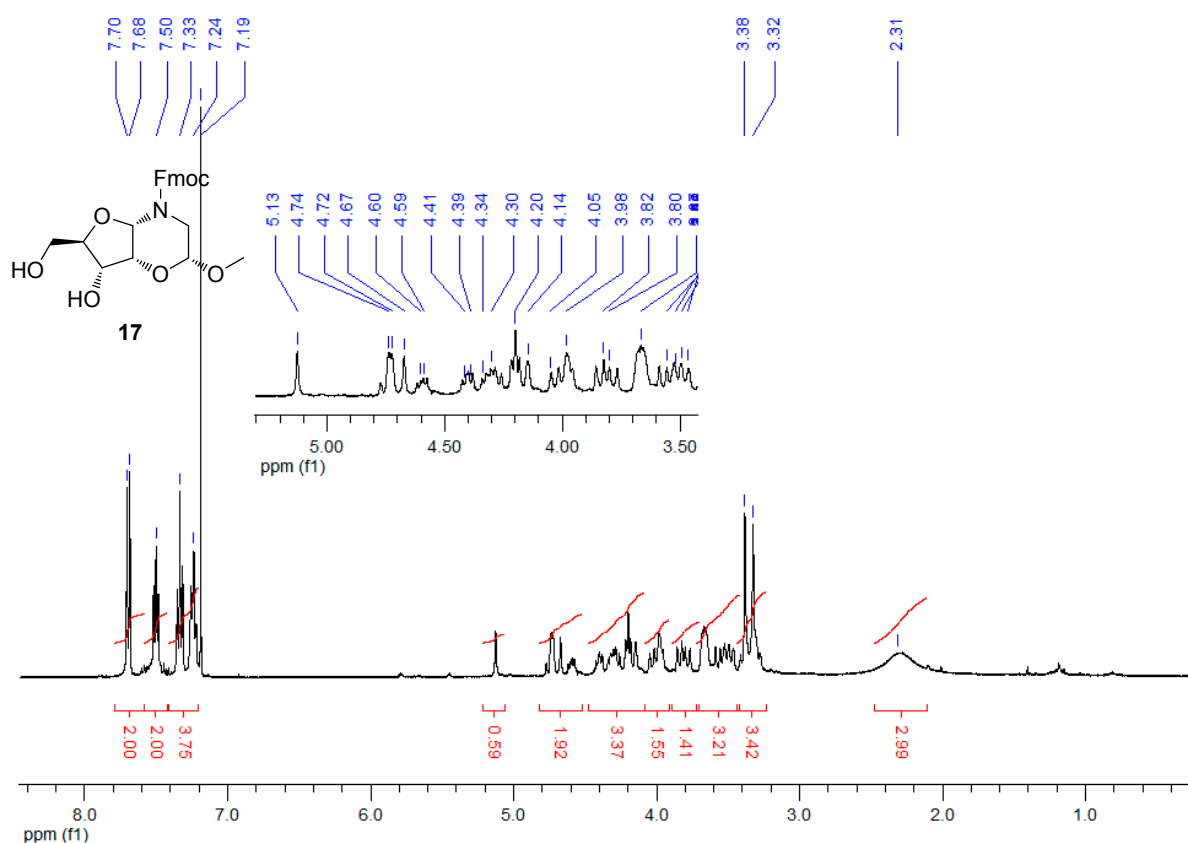
Figure S8. ¹³C-NMR spectrum of compound **12β** (100 MHz, CDCl₃).Figure S9. ¹H-NMR spectrum of compound **13α** (400 MHz, CDCl₃).

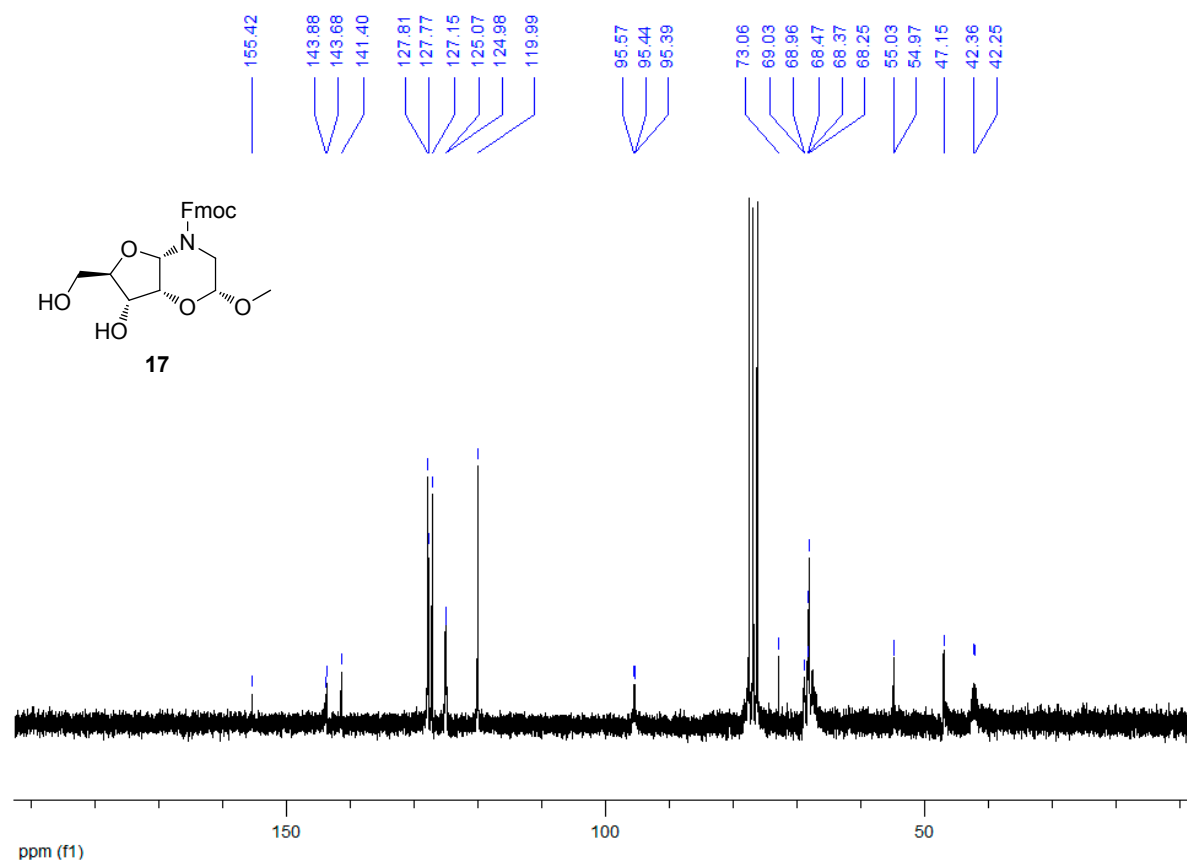
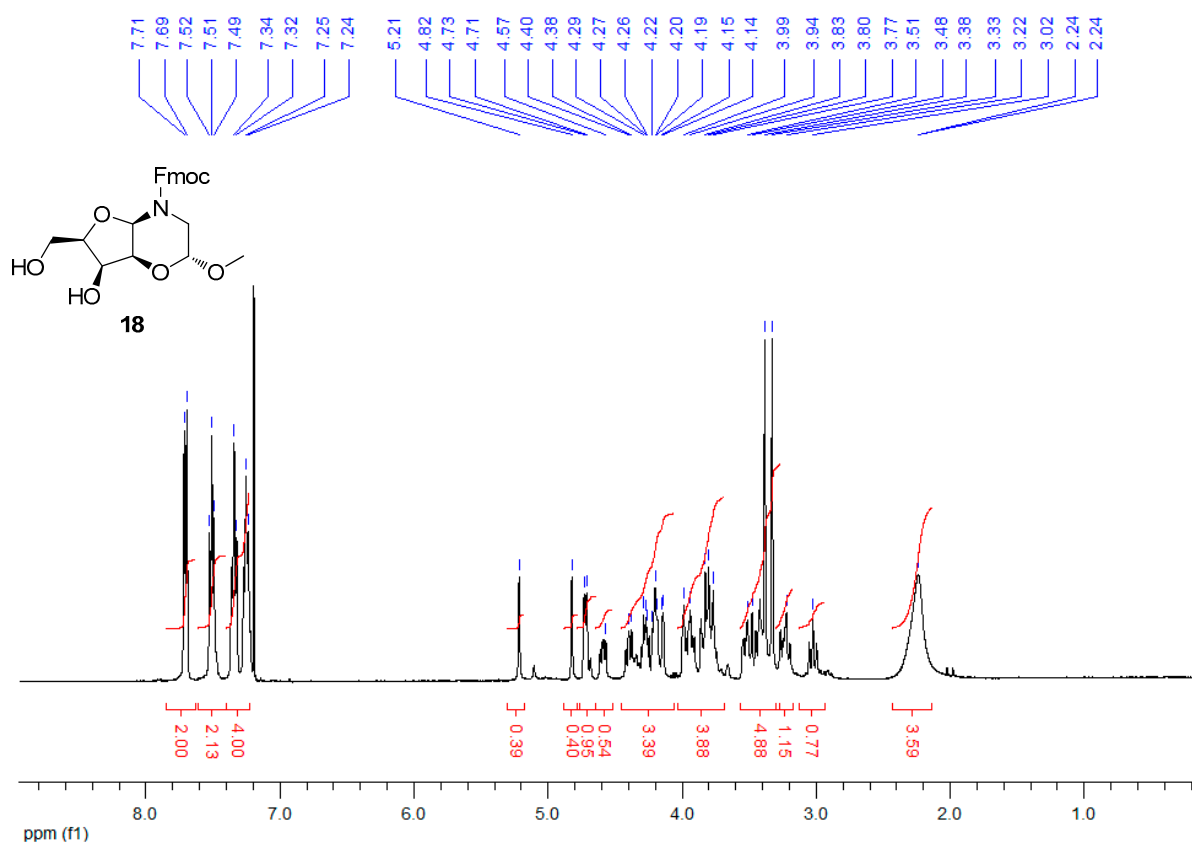
Figure S10. ^{13}C -NMR spectrum of compound **13α** (100 MHz, CDCl_3).Figure S11. ^1H -NMR spectrum of compound **15α** (400 MHz, CDCl_3).

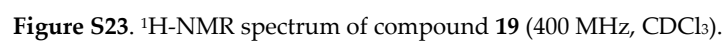
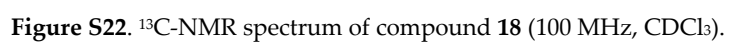
Figure S12. ^{13}C -NMR spectrum of compound **15α** (100 MHz, CDCl_3).Figure S13. ^1H -NMR spectrum of compound **15β** (400 MHz, CDCl_3).

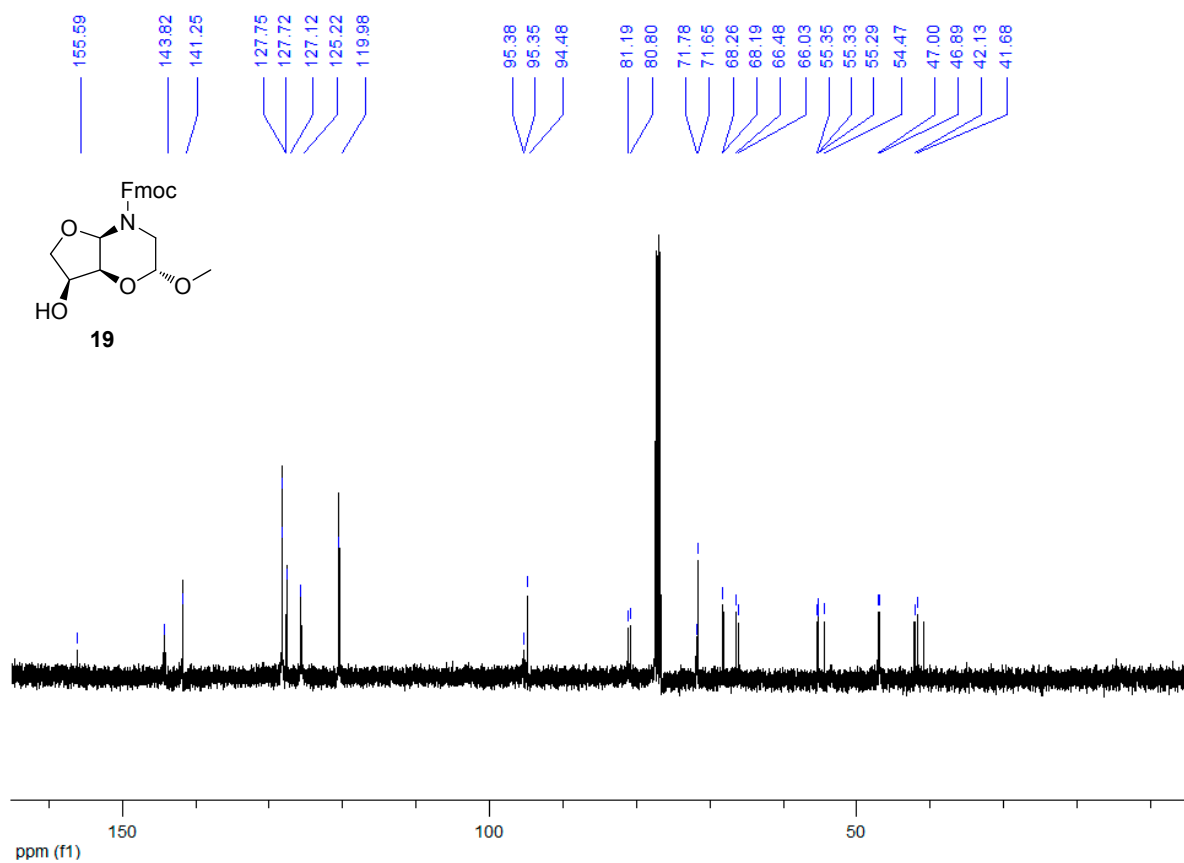
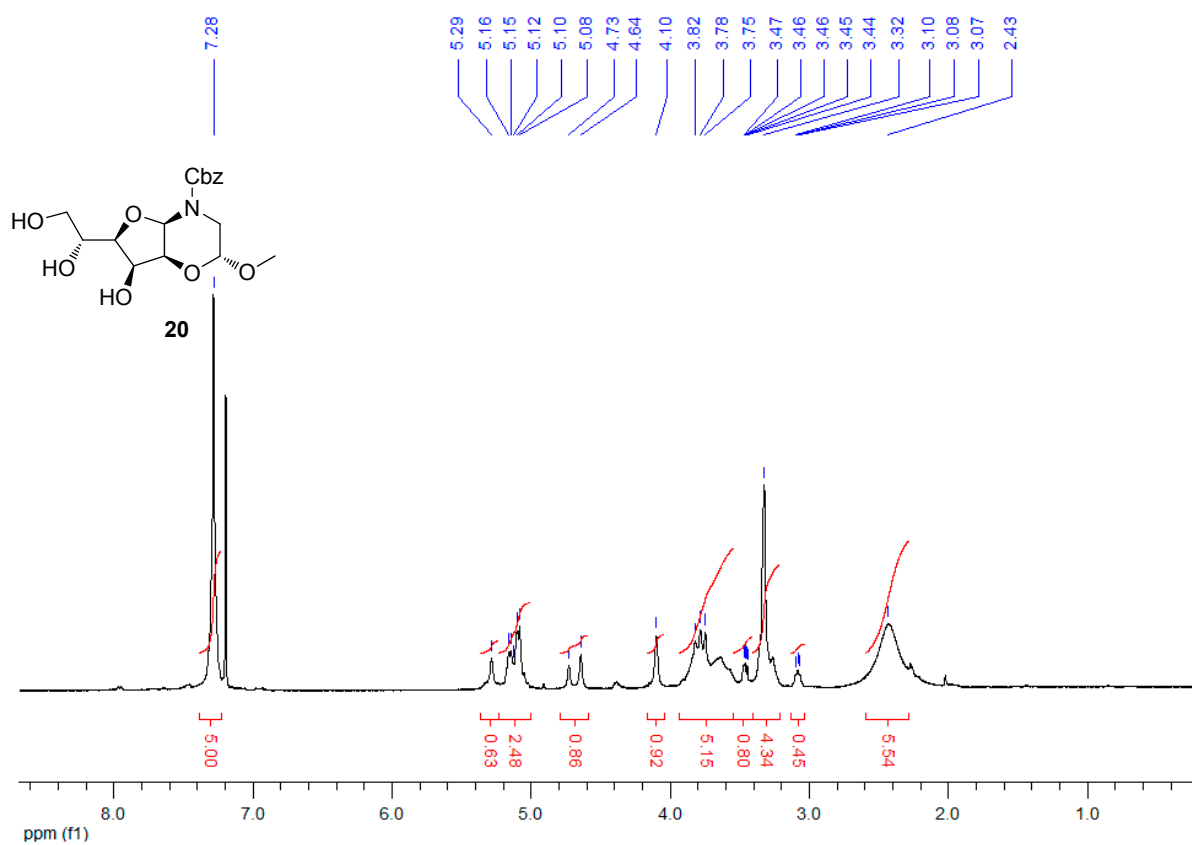
Figure S14. ¹³C-NMR spectrum of compound **15β** (100 MHz, CDCl₃).Figure S15. ¹H-NMR spectrum of compound **16α** (400 MHz, CDCl₃).

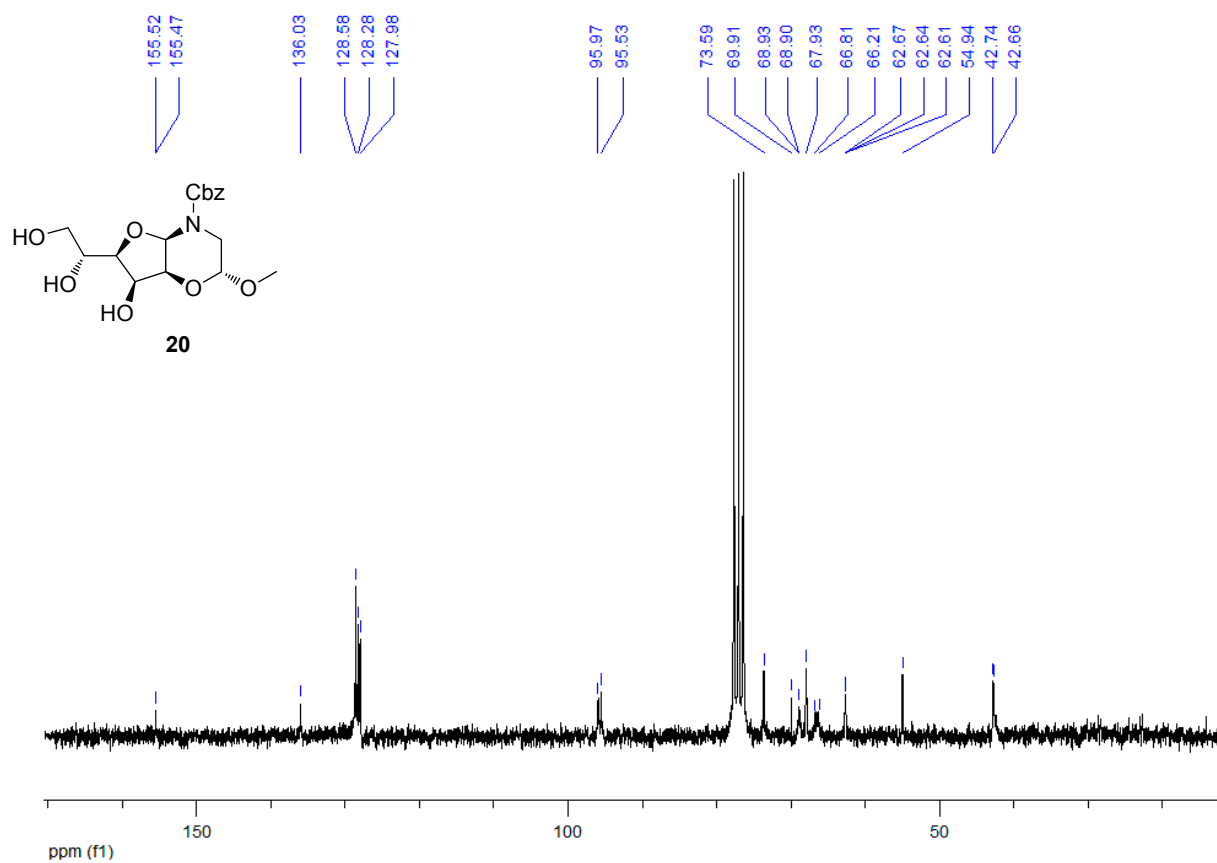
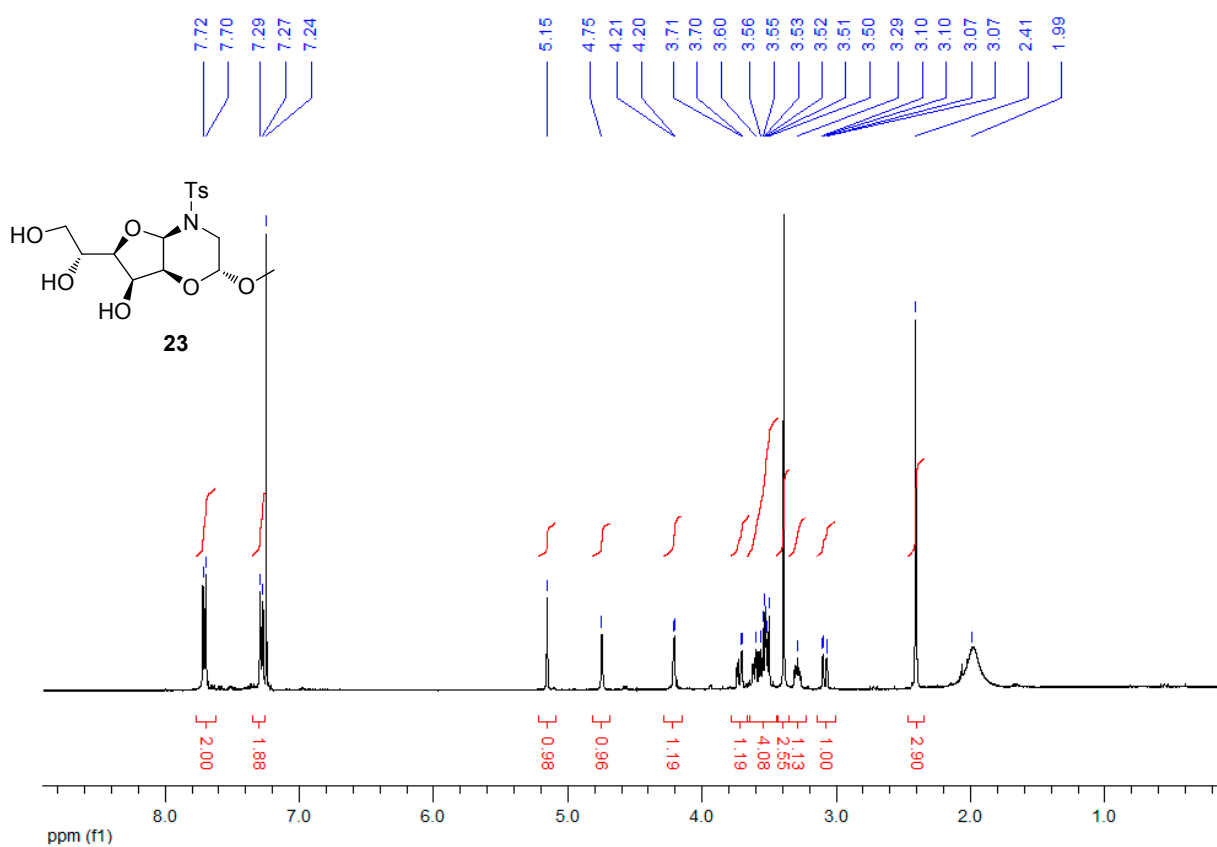
Figure S16. ¹³C-NMR spectrum of compound **16α** (50 MHz, CDCl₃).Figure S17. ¹H-NMR spectrum of compound **16β** (400 MHz, CDCl₃).

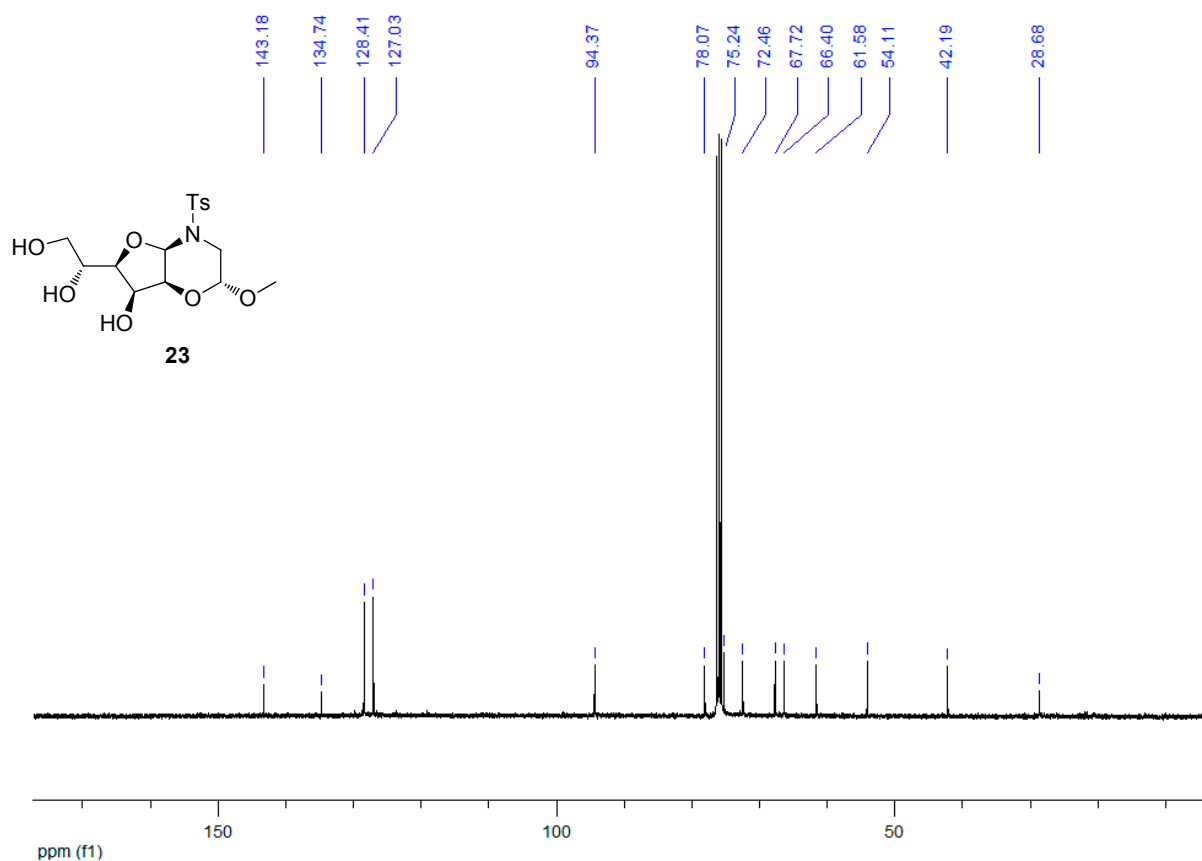
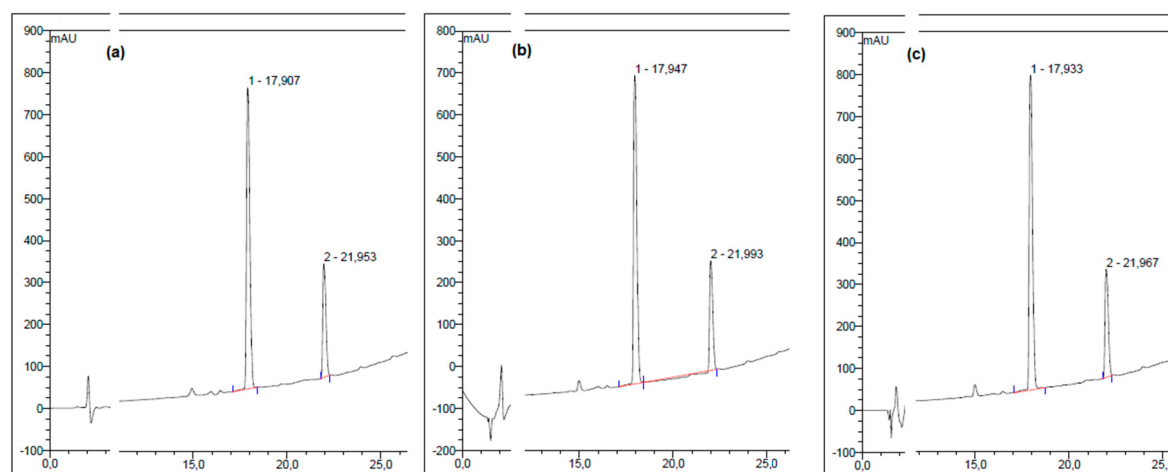
Figure S18. ¹³C-NMR spectrum of compound **16β** (50 MHz, CDCl₃).Figure S19. ¹H-NMR spectrum of compound **17** (400 MHz, CDCl₃).

Figure S20. ¹³C-NMR spectrum of compound 17 (100 MHz, CDCl₃).Figure S21. ¹H-NMR spectrum of compound 18 (400 MHz, CDCl₃).



Figure S24. ¹³C-NMR spectrum of compound 19 (100 MHz, CDCl₃).Figure S25. ¹H-NMR spectrum of compound 20 (400 MHz, CDCl₃).

Figure S26. ¹³C-NMR spectrum of compound **20** (50 MHz, CDCl₃).Figure S27. ¹H-NMR spectrum of compound **23** (400 MHz, CDCl₃).

Figure S28. ¹³C-NMR spectrum of compound 23 (100 MHz, CDCl₃).Figure S29. HPLC runs of compound 18 (0.5 mg/mL, final conc.) after 1h incubation in (a) CH₃CN; (b) 1:1 mixture of CH₃CN and HCl 1M; (c) 1:1 mixture of MeOH and HCl 1M. A 0.1 mg/mL quantity (final conc.) of benzophenone (rt = 22 min) was used as an internal standard.

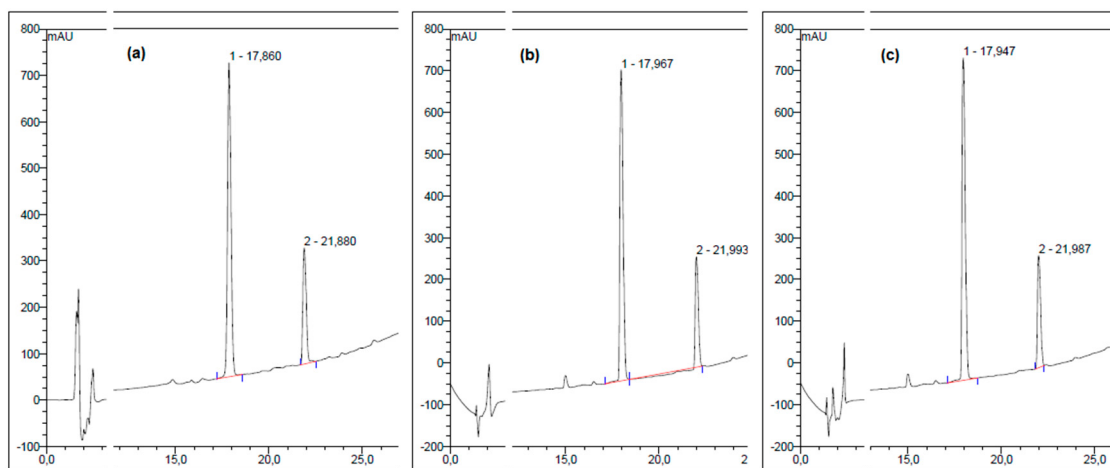


Figure S30. HPLC runs of compound **18** (0.5 mg/mL, final conc.) after 24h incubation in (a) CH₃CN; (b) 1:1 mixture of CH₃CN and HCl 1M; (c) 1:1 mixture of MeOH and HCl 1M. A 0.1 mg/mL quantity (final conc.) of benzophenone (rt = 22 min) was used as an internal standard.