

**Glycosidic Bond Expanded Cyclic Oligosaccharides: Synthesis and Host-Guest Binding
Property of a Cyclic Pentasaccharide**

Gopal Ch Samanta,[§] Krishnagopal Maiti,[§] Narayanaswamy Jayaraman^{*§}

[§] Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560 012, India.

Supporting Information

Contents

Figures	Page No.
Figure S1. ^1H NMR spectrum of 3	S3
Figure S2. ^{13}C NMR spectrum of 3	S3
Figure S3. HRMS spectrum of 3	S4
Figure S4. ^1H NMR spectrum of 5	S4
Figure S5. ^{13}C NMR spectrum of 5	S5
Figure S6. HRMS spectrum of 5	S5
Figure S7. ^1H NMR spectrum of 6	S6
Figure S8. ^{13}C NMR spectrum of 6	S6
Figure S9. HRMS spectrum of 6	S7
Figure S10. MALDI spectrum of 7	S7
Figure S11. ^1H NMR spectrum of 7	S8
Figure S12. ^{13}C NMR spectrum of 7	S8
Figure S13. COSY NMR spectrum of 7	S9
Figure S14. HMQC NMR spectrum of 7	S10
Figure S15. Few more energy minimized structures of 7	S10
References	S11

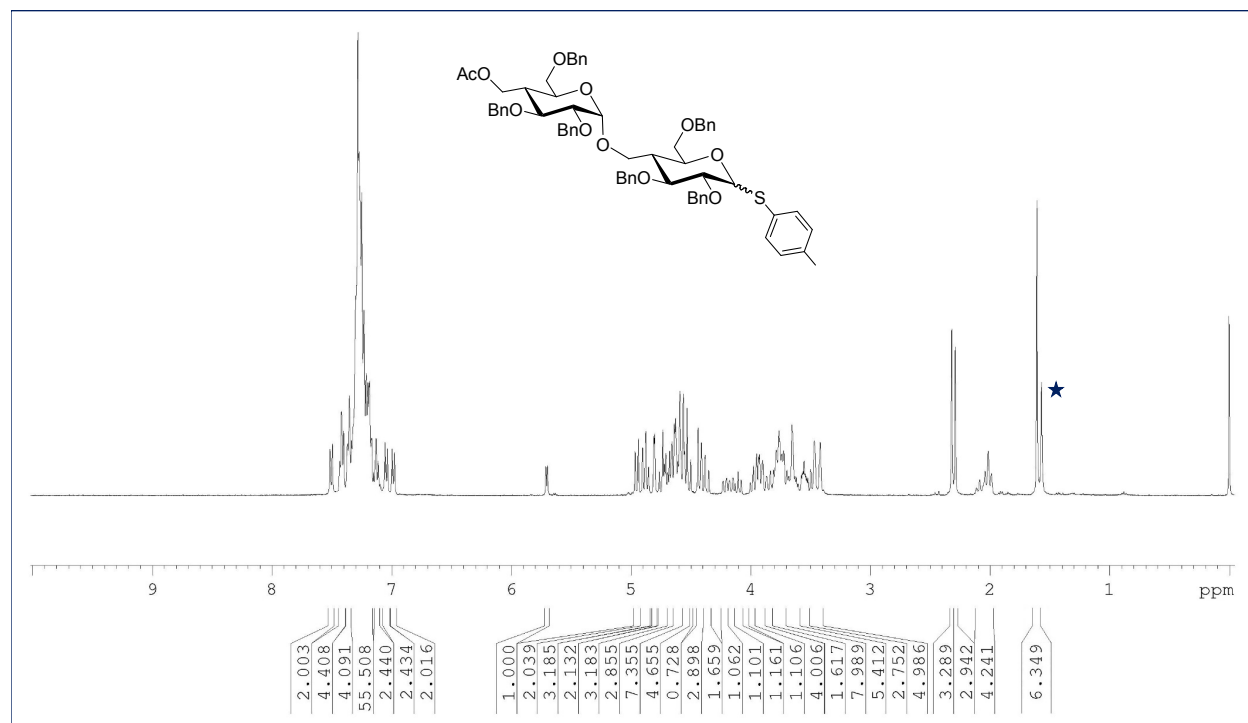


Figure S1. ¹H NMR spectrum of **3** (CDCl₃, 400 MHz).

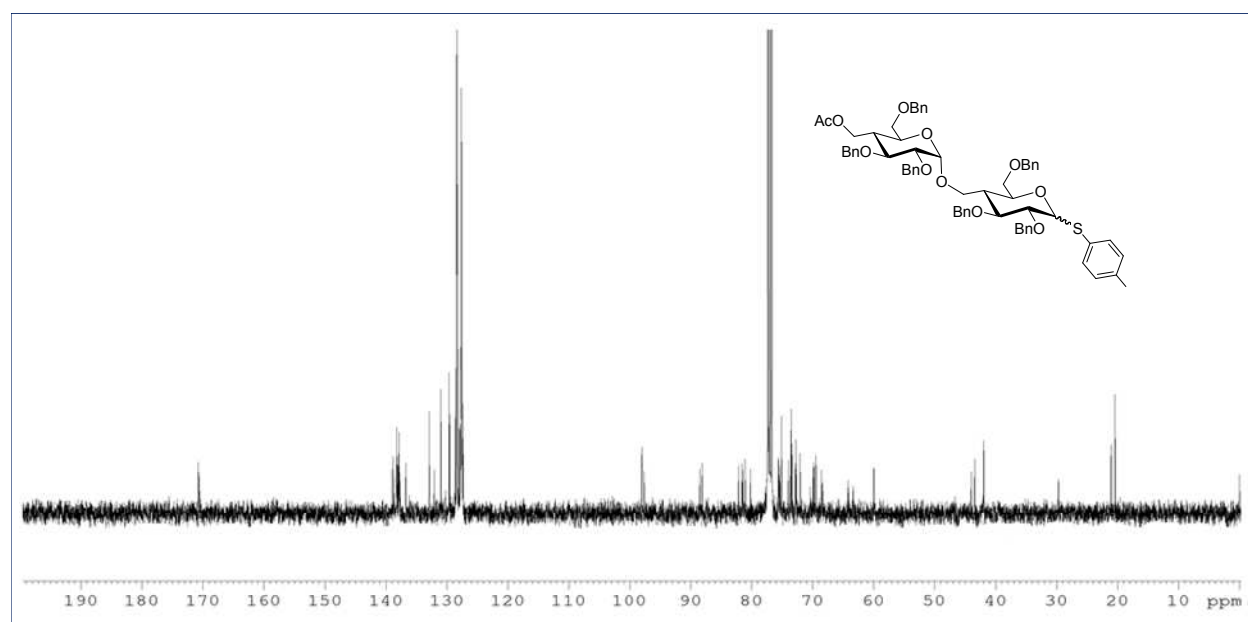


Figure S2. ¹³C NMR spectrum of **3** (CDCl₃, 100 MHz).

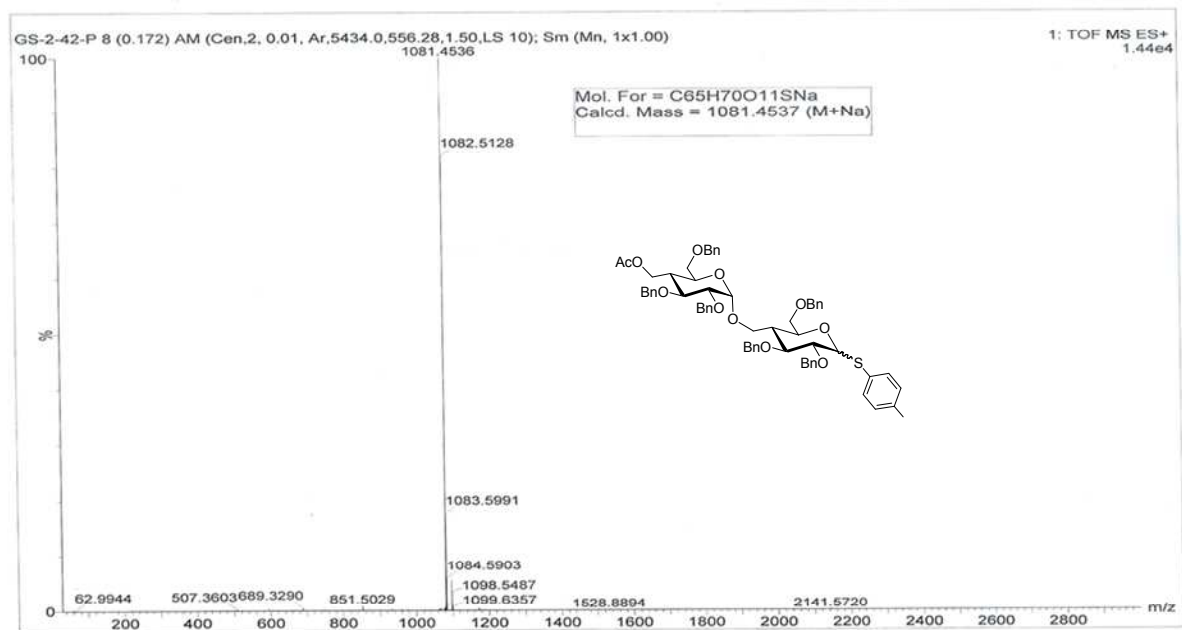


Figure S3. HRMS spectrum of **3**.

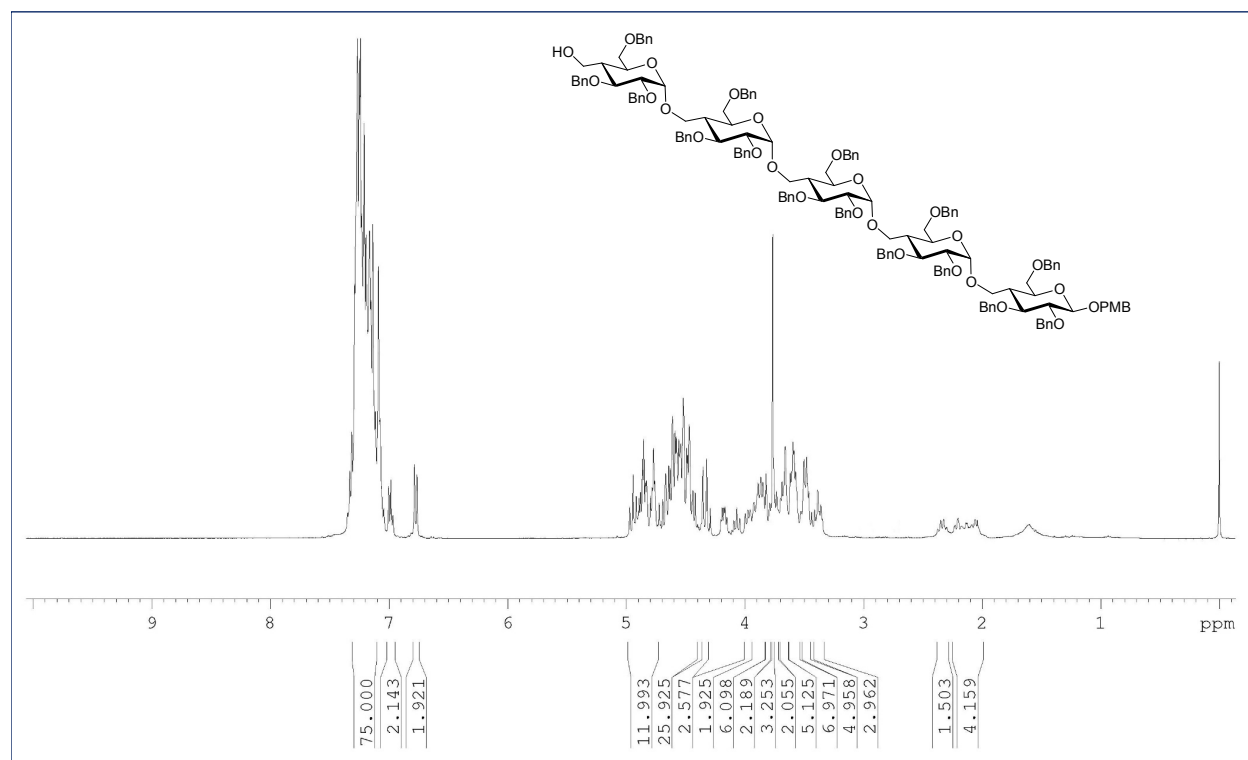
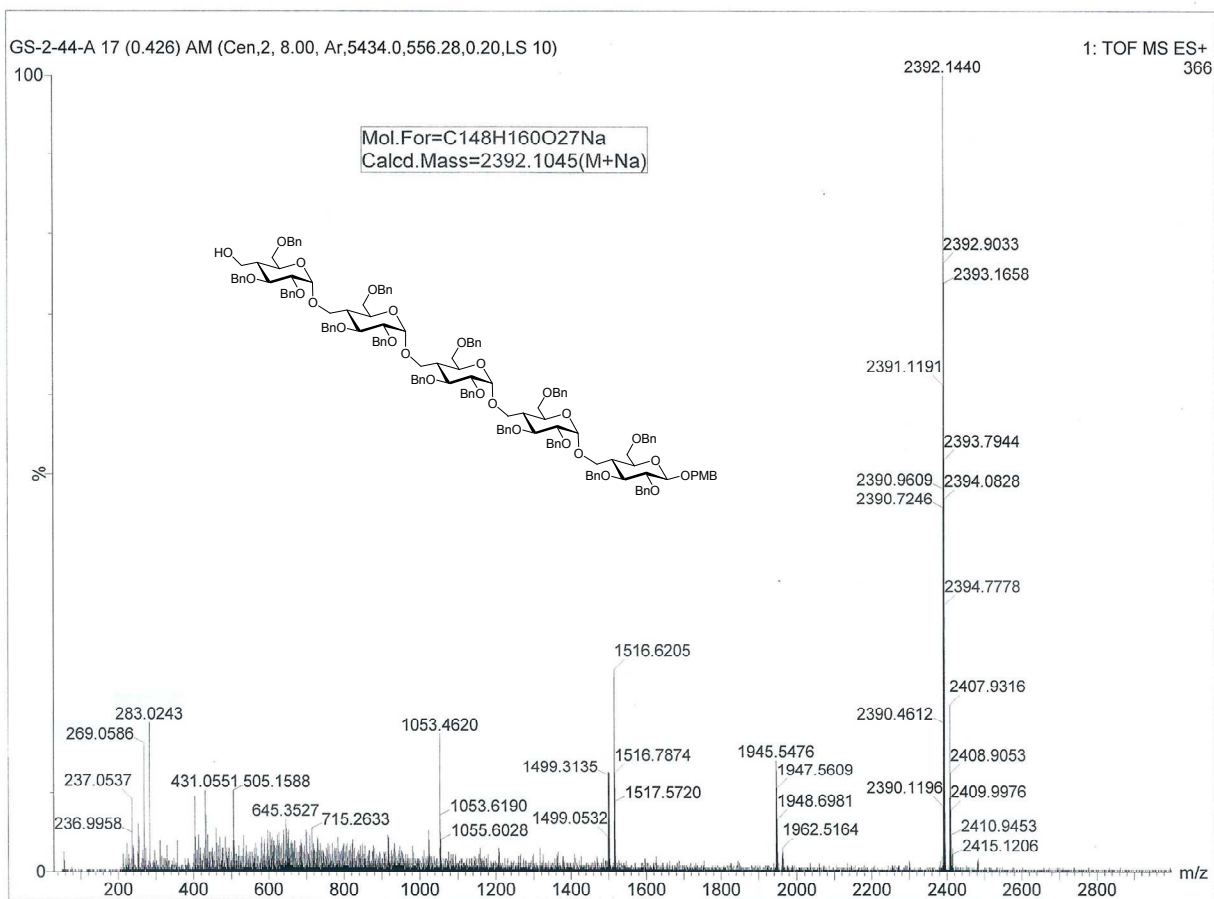
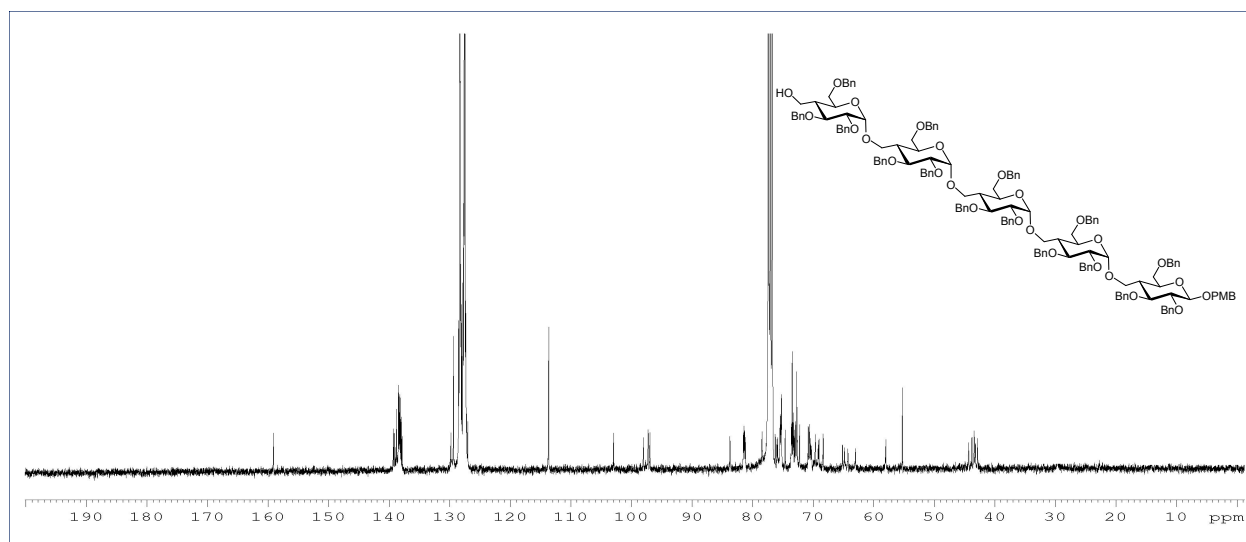


Figure S4. ¹H NMR spectrum of **5** (CDCl₃, 400 MHz).



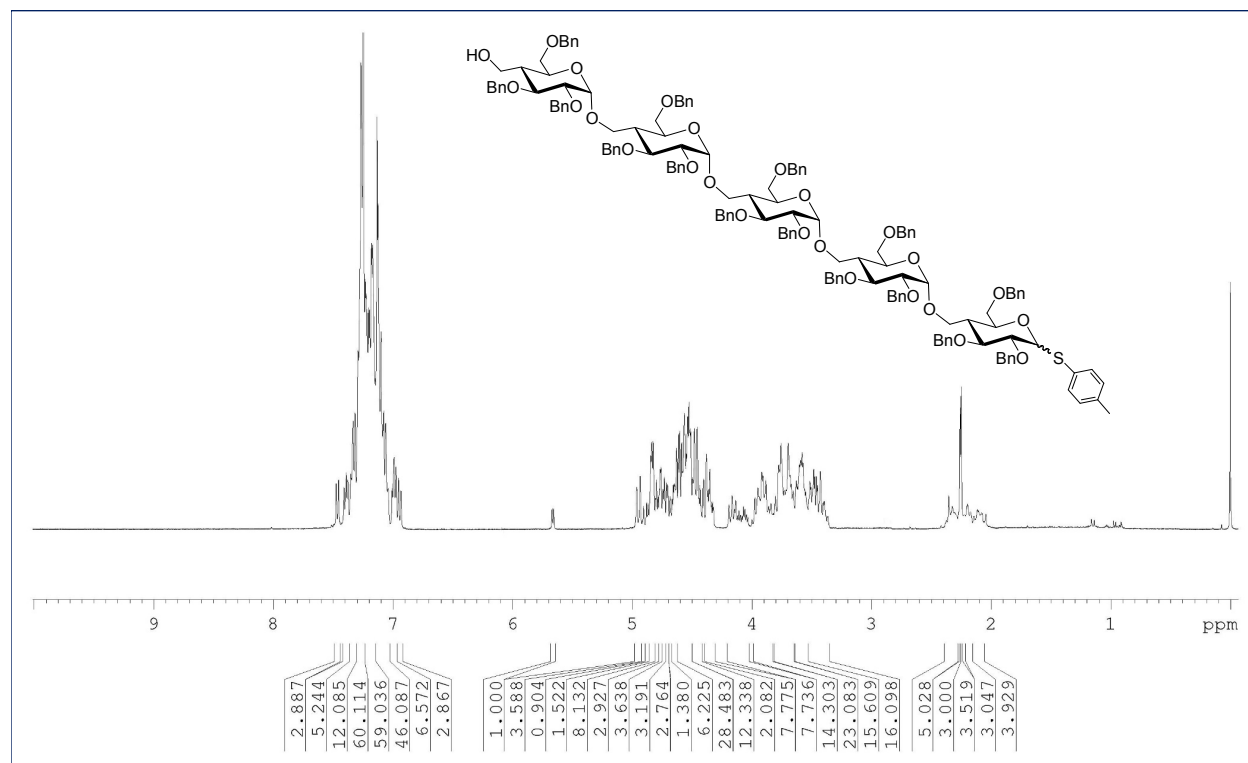


Figure S7. ^1H NMR spectrum of **6** (CDCl_3 , 400 MHz).

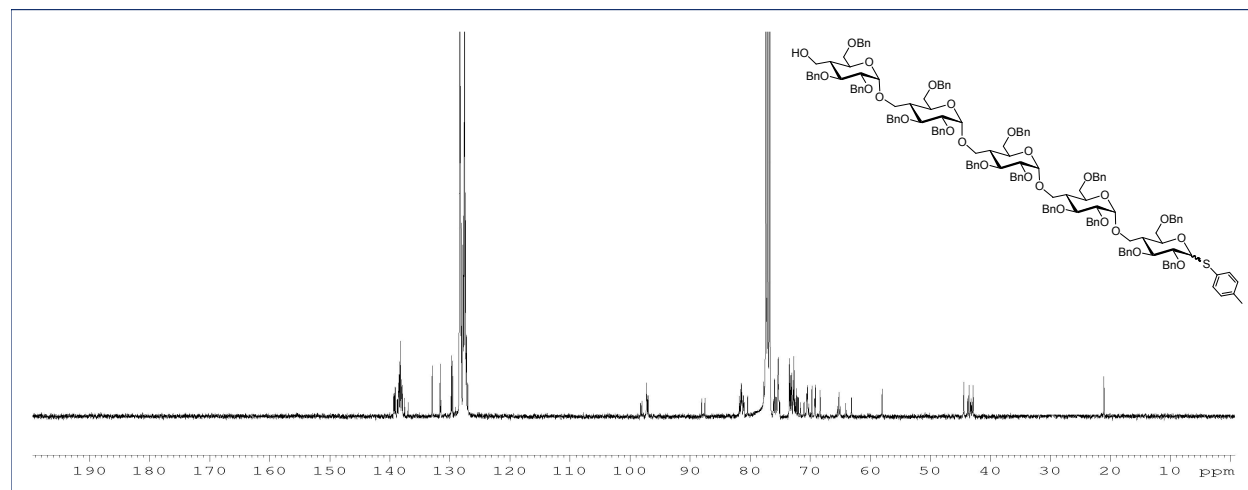


Figure S8. ^{13}C NMR spectrum of **6** (CDCl_3 , 100 MHz).

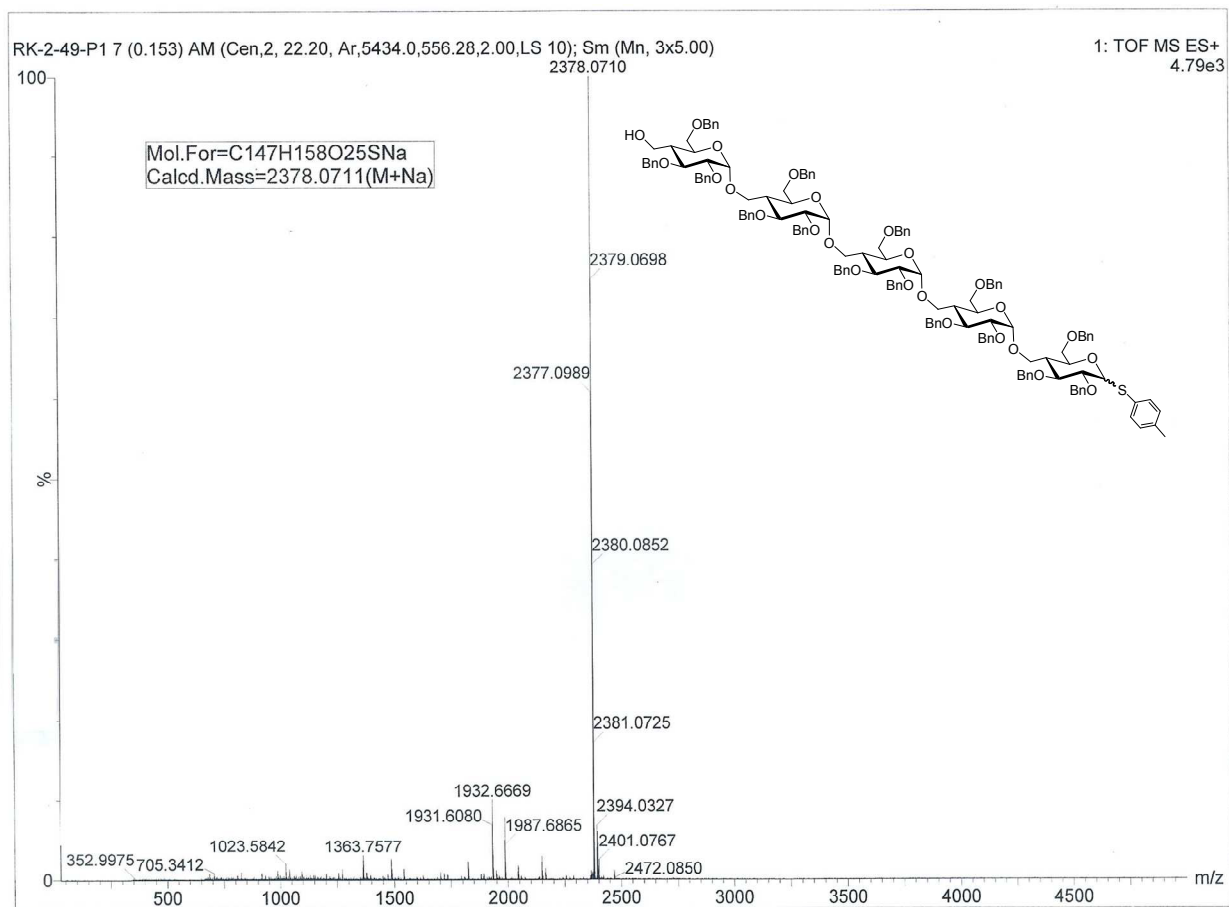


Figure S9. HRMS spectrum of **6**.

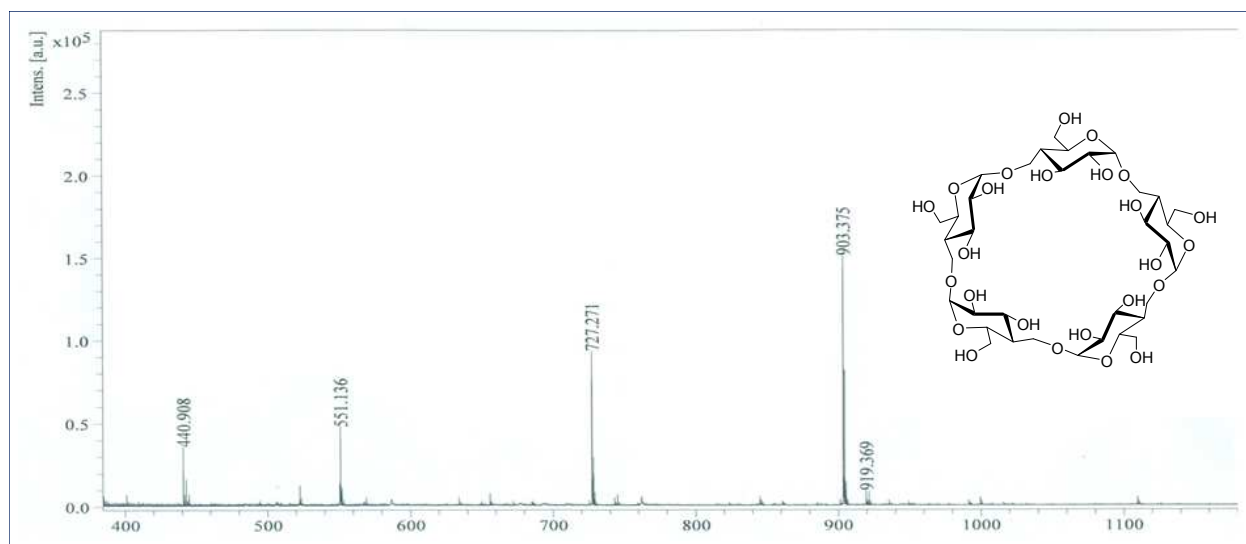


Figure S10. MALDI-TOF mass spectrum of **7**.

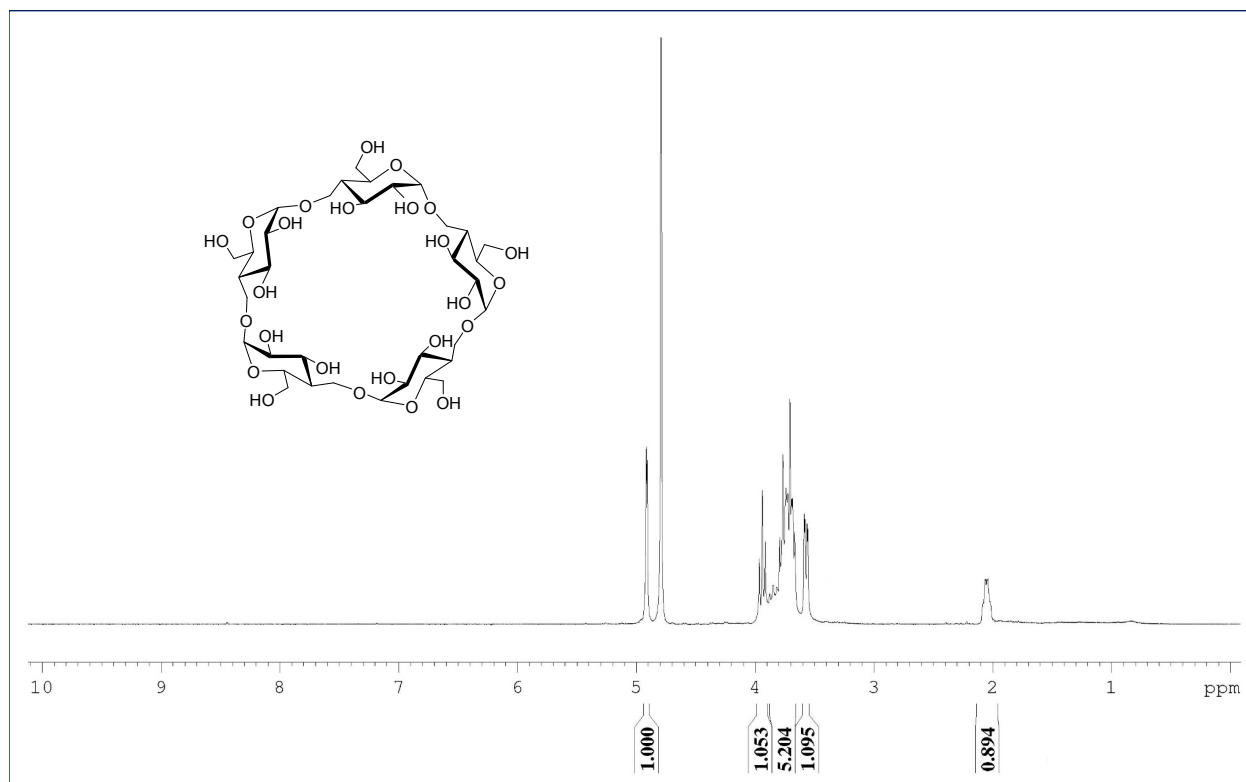


Figure S11. ^1H NMR spectrum of 7 (D_2O , 400 MHz).

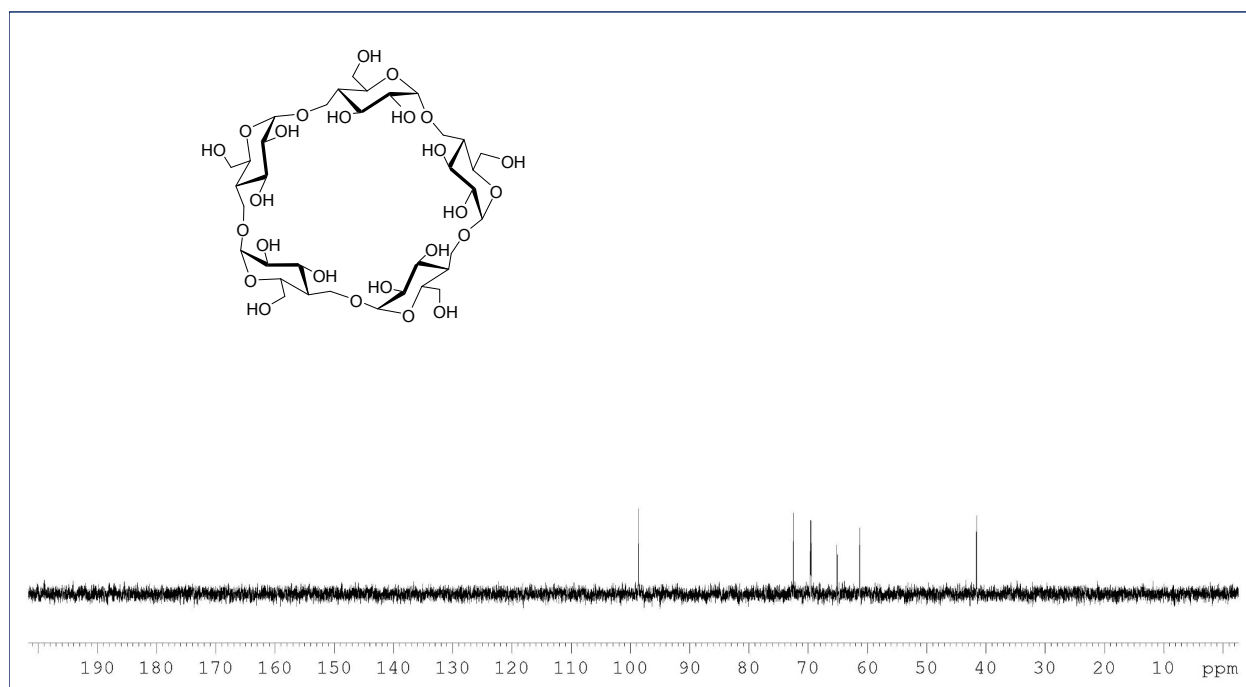


Figure S12. ^{13}C NMR spectrum of 7 (D_2O , 100 MHz).

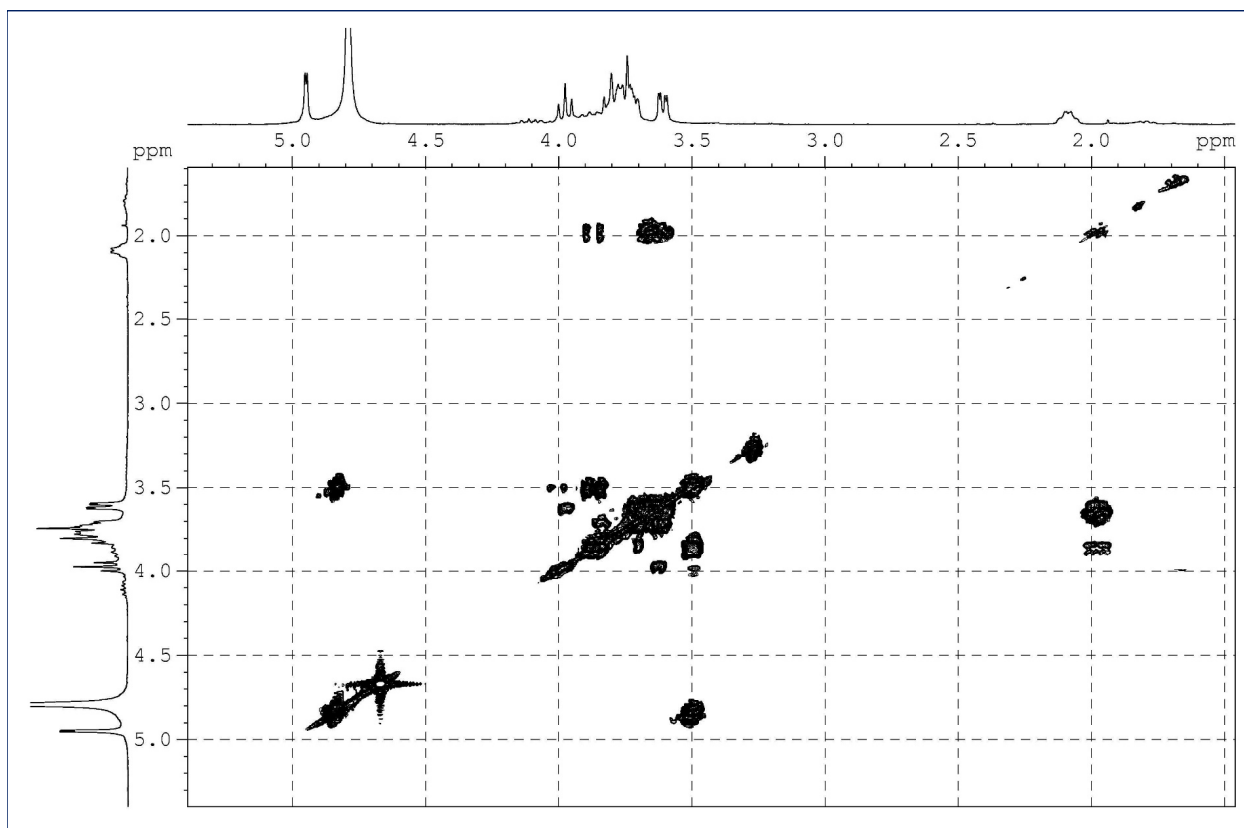


Figure S13. COSY NMR spectrum of **7** (D₂O, 400 MHz).

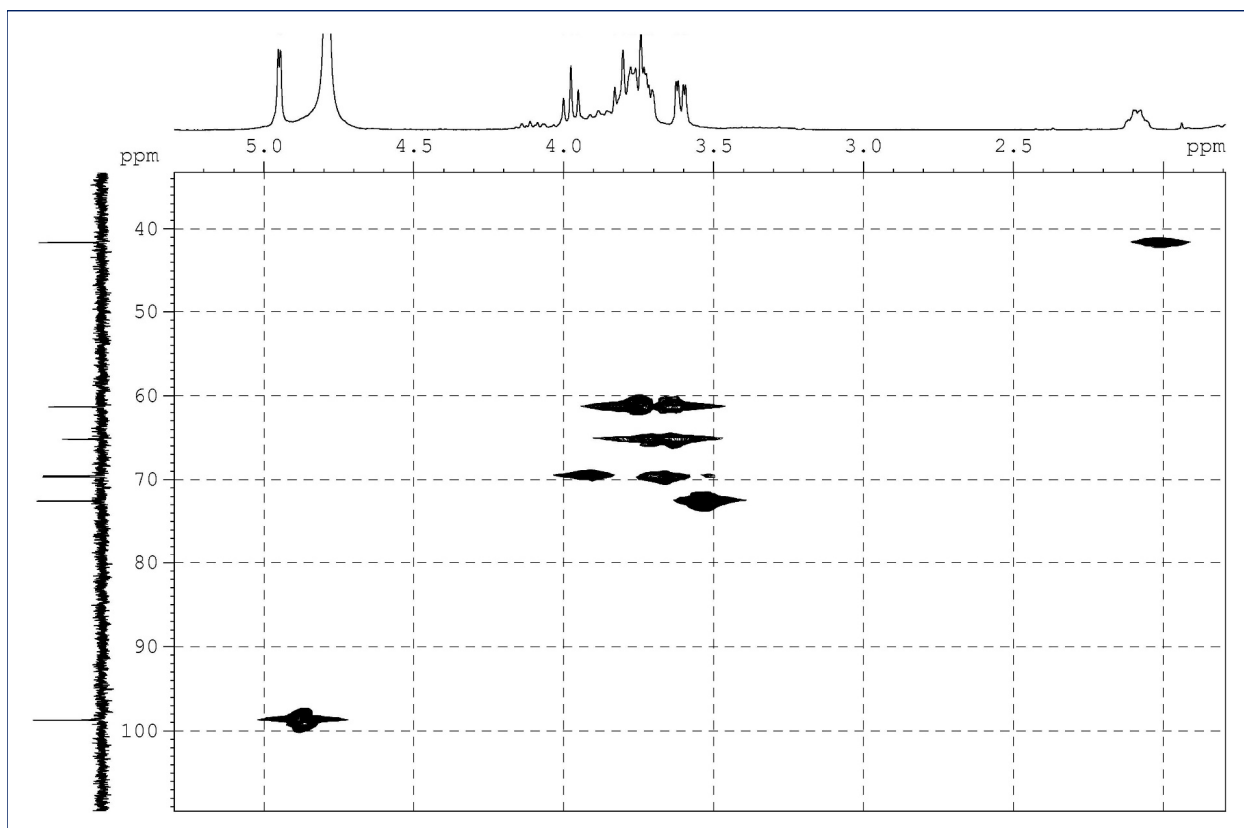


Figure S14. HMQC NMR spectrum of **7** (D₂O, 100 MHz).

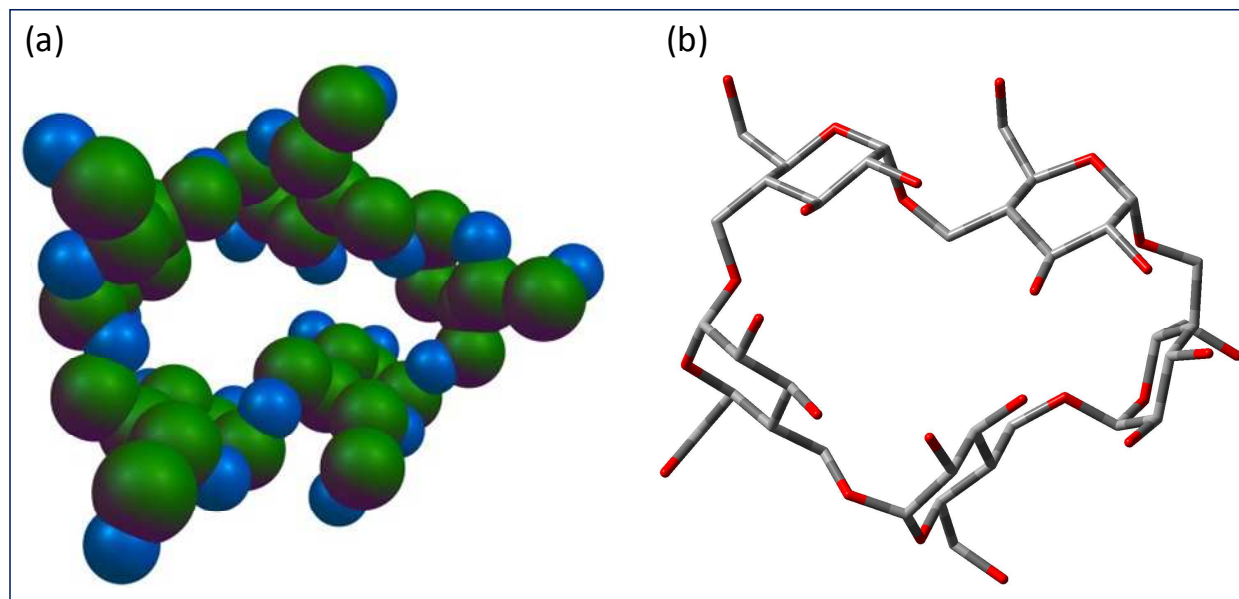


Figure S15. Energy minimized structures of **7** derived by using Gaussian 09 software¹: (a) view from wider rim (as CPK model); (b) view from narrower rim (as tube model).

Reference

1. Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.