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Supporting information available for

Stereoselectivity in Dehydrative Cyclic Trimerization of Substituted 4-Alkylaminobenzoic Acids

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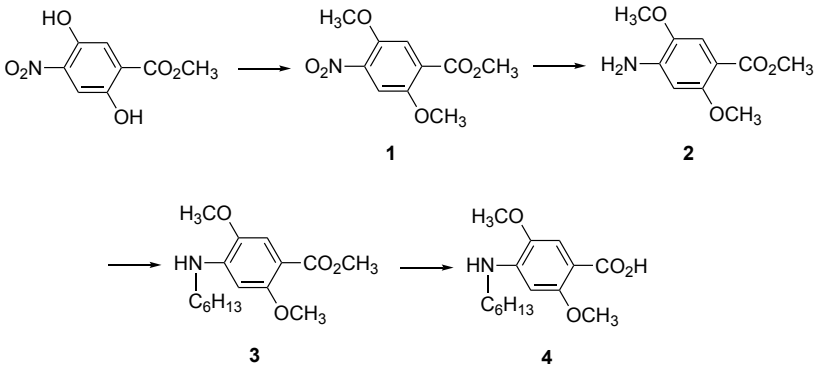
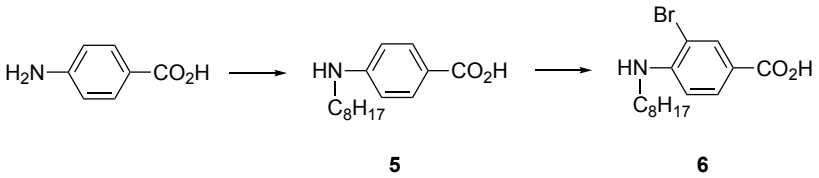


Scheme S1. Synthetic route to 2,5-dimethoxy monomer.



Scheme S2. Synthetic route to 3-bromo monomer.

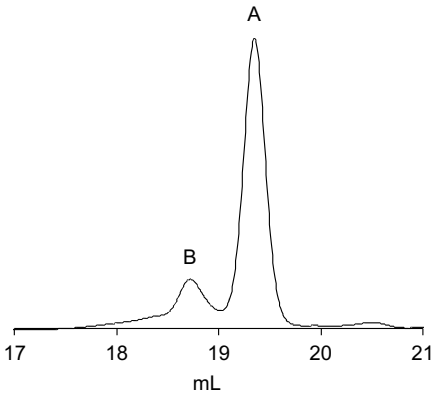


Figure S1. GPC profile of the product obtained after SiO_2 column chromatography in the cyclization of **4** using $SiCl_4$.

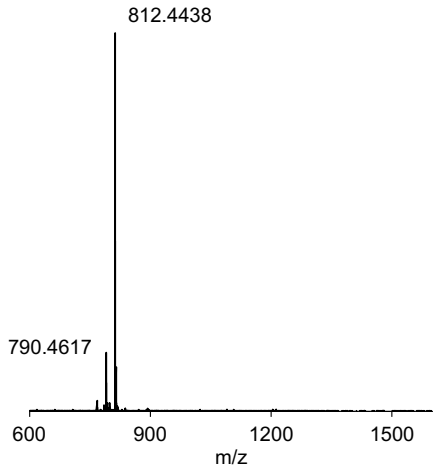


Figure S2. ESI-MS of isolated **DiMeO_C3A**.

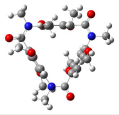
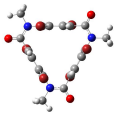
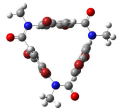
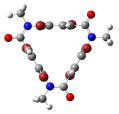
	Optimized structure	Energy/a.u.	ΔE/kcal·mol^{-1}
DiMeO_C3A-anti		-2003.6620	
DiMeO_C3A-syn		-2003.6734	-7.2
DiBr_C3A-anti		-16743.4225	
DiBr_C3A-syn		-16743.4316	-5.7

Figure S3. Optimized structure and energy of *anti*- and *syn*-stereoisomers of **DiMeO_C3A** and **DiBr_C3A**. The calculations were performed on Gaussian 09 (Revision E.01) package of programs using B3LYP/6-31G(d) level of theory. For saving the computational cost, the alkyl chain was replaced by the methyl group.

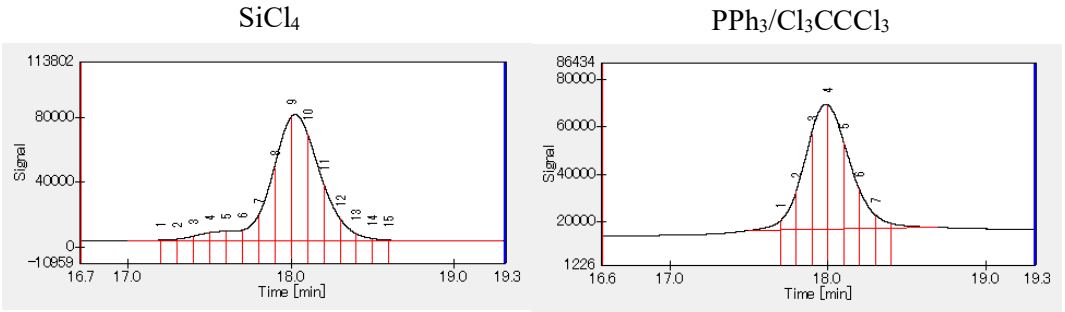


Figure S4. GPC profiles of the product obtained after SiO_2 column chromatography in the cyclization of **6** using $SiCl_4$ and PPh_3/Cl_3CCCl_3.

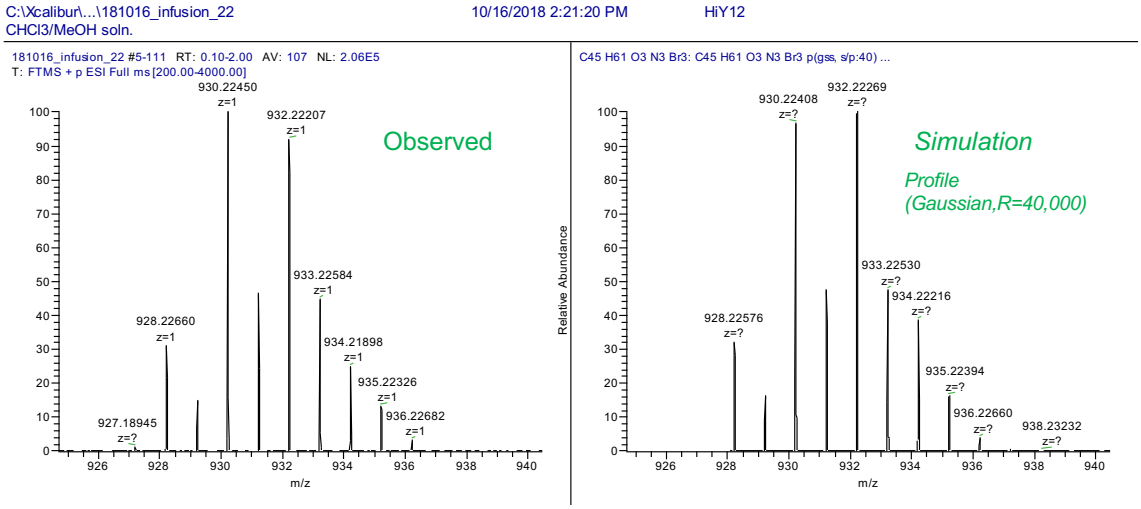


Figure S5. HR ESI-MS of **3Br_C3A** (left) and simulated pattern (right).

DQF-COSY

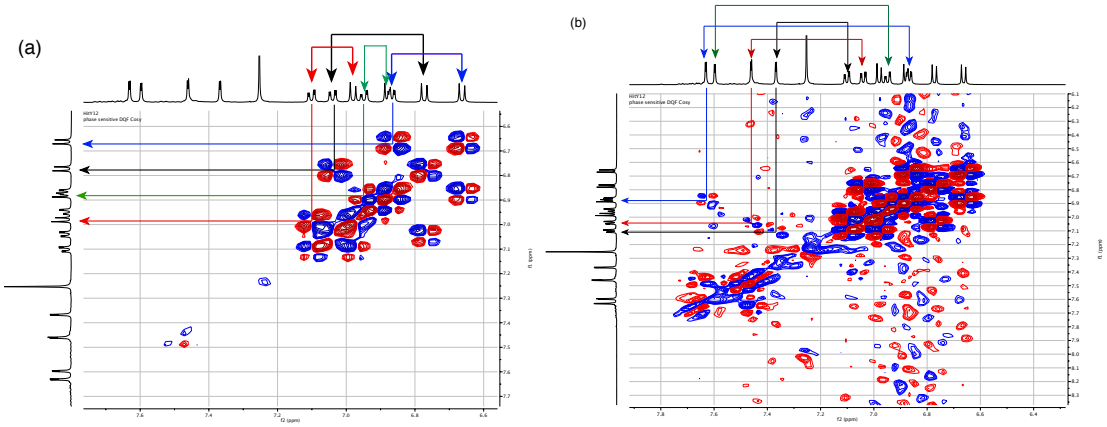


Figure S6. DQF-COSY charts of **3Br_C3A**.

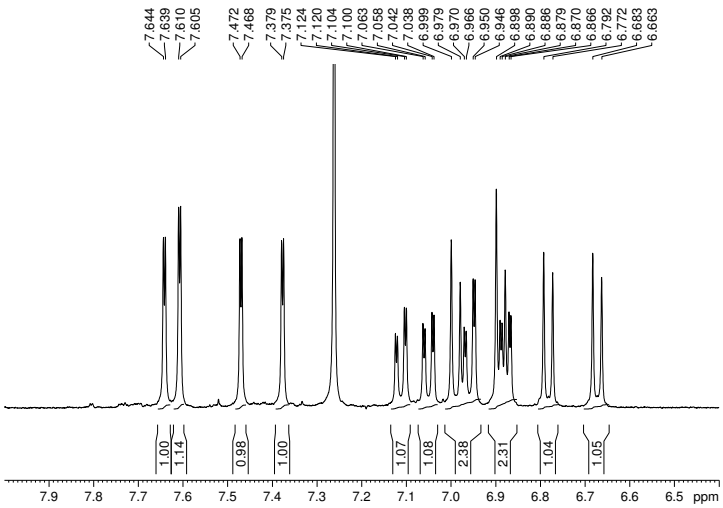


Figure S7. Expanded ^{1}H-NMR spectrum of **3Br_C3A** obtained at 100 °C in $CDCl_3$.

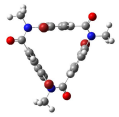
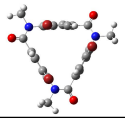
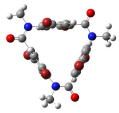
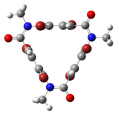
	Optimized structure	Energy/a.u.	ΔE/kcal·mol^{-1}
3Br_C3A-anti		-9030.0923	-1.1
3Br_C3A-syn		-9030.0906	
DiBr_C3A-anti		-16743.4225	
DiBr_C3A-syn		-16743.4316	-5.7

Figure S8. Optimized structure and energy of *anti*- and *syn*-stereoisomers of **3Br_C3A** and **DiBr_C3A**. The calculations were performed on Gaussian 09 (Revision E.01) package of programs using B3LYP/6-31G(d) level of theory. For saving the computational cost, the alkyl chain was replaced by the methyl group.

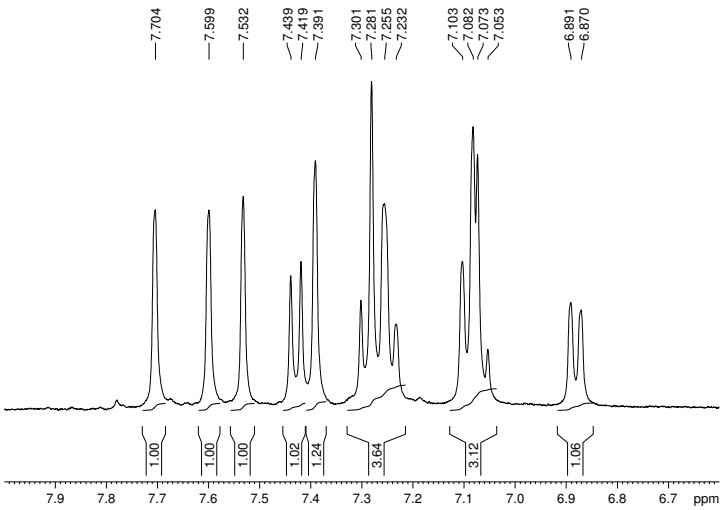


Figure S9. Expanded ^{1}H-NMR spectrum of **3Br_C3A** in DMSO-d_6. Because of the insufficient solubility of compound, well-resolved coupling pattern of signals were lost.

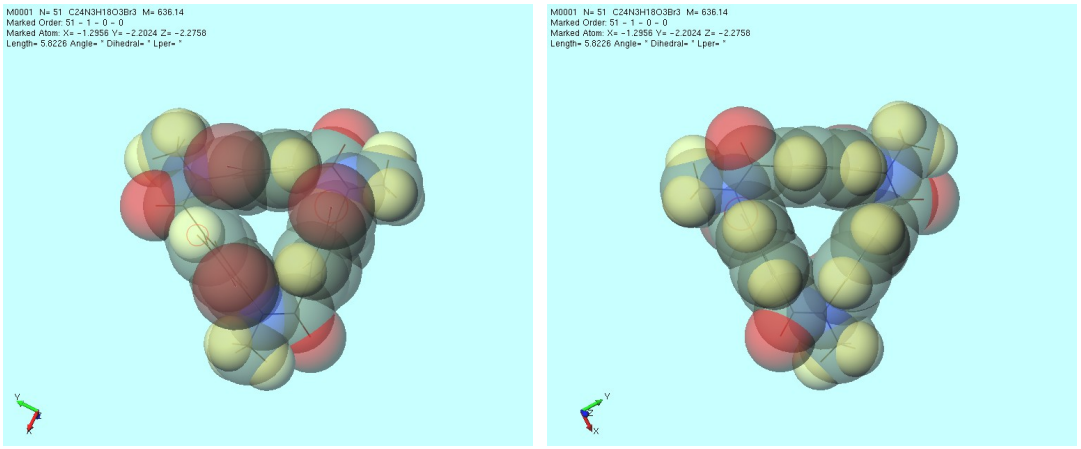


Figure S10. Space-filling model of the optimized structure of *syn*-stereoisomer of **3Br_C3A**. The octyl chains are replaced by the methyl groups for saving the computation cost.

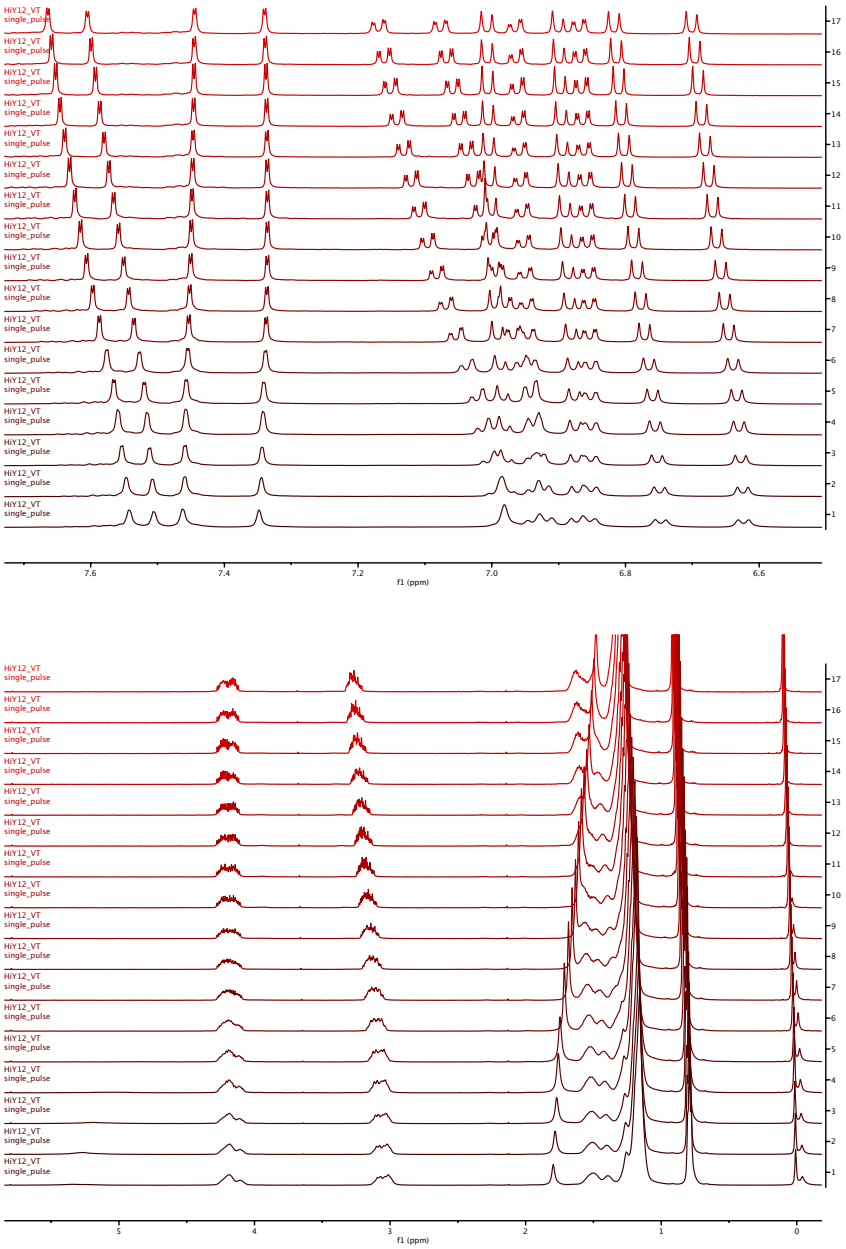


Figure S11. VT-NMR spectra of **3Br_C3A** at 100, 90, 80, 70, 60, 50, 40, 30, 20, 10, 0, –10, –20, –25, –30, –35, –40 °C (from top to bottom) on cooling. The spectra were recorded in 1,1,2,2-tetrachloroethane-d_2.

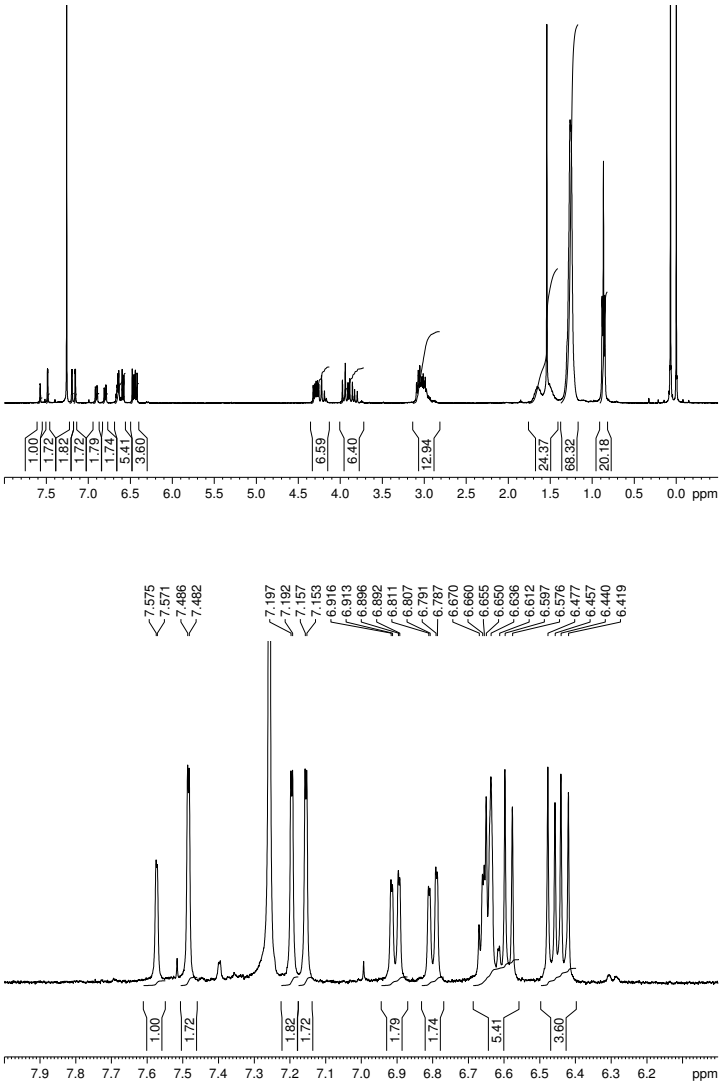


Figure S12. Full (top) and expanded (bottom) ^{1}H-NMR spectra of **3Br_C3Ared** in $CDCl_3$.

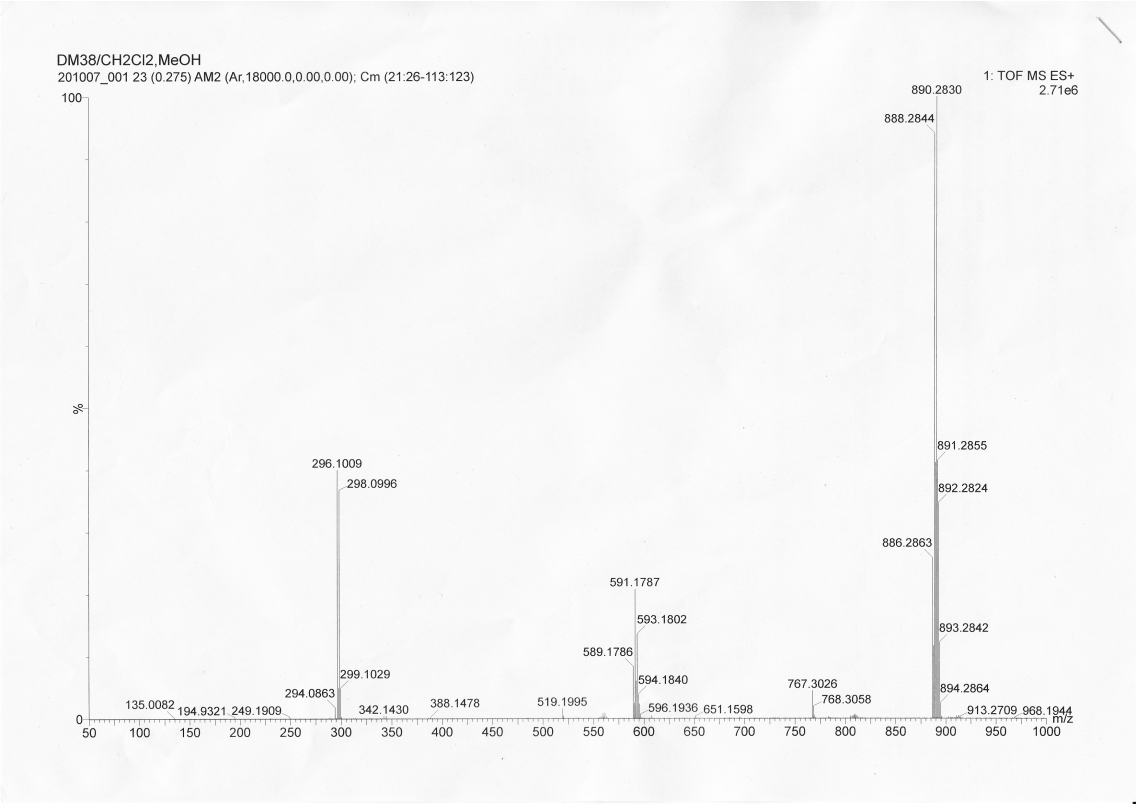


Figure S13. HR ESI-MS of **3Br_C3Ared**.