Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

SUPPORTING INFORMATION

Cyclopeptoids: a Novel Class of Phase-Transfer Catalysts

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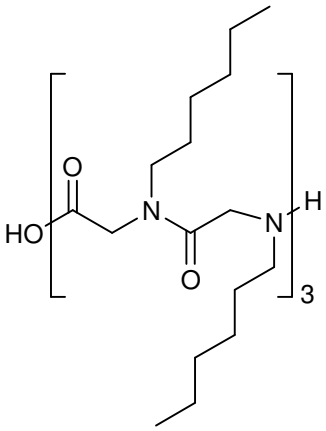
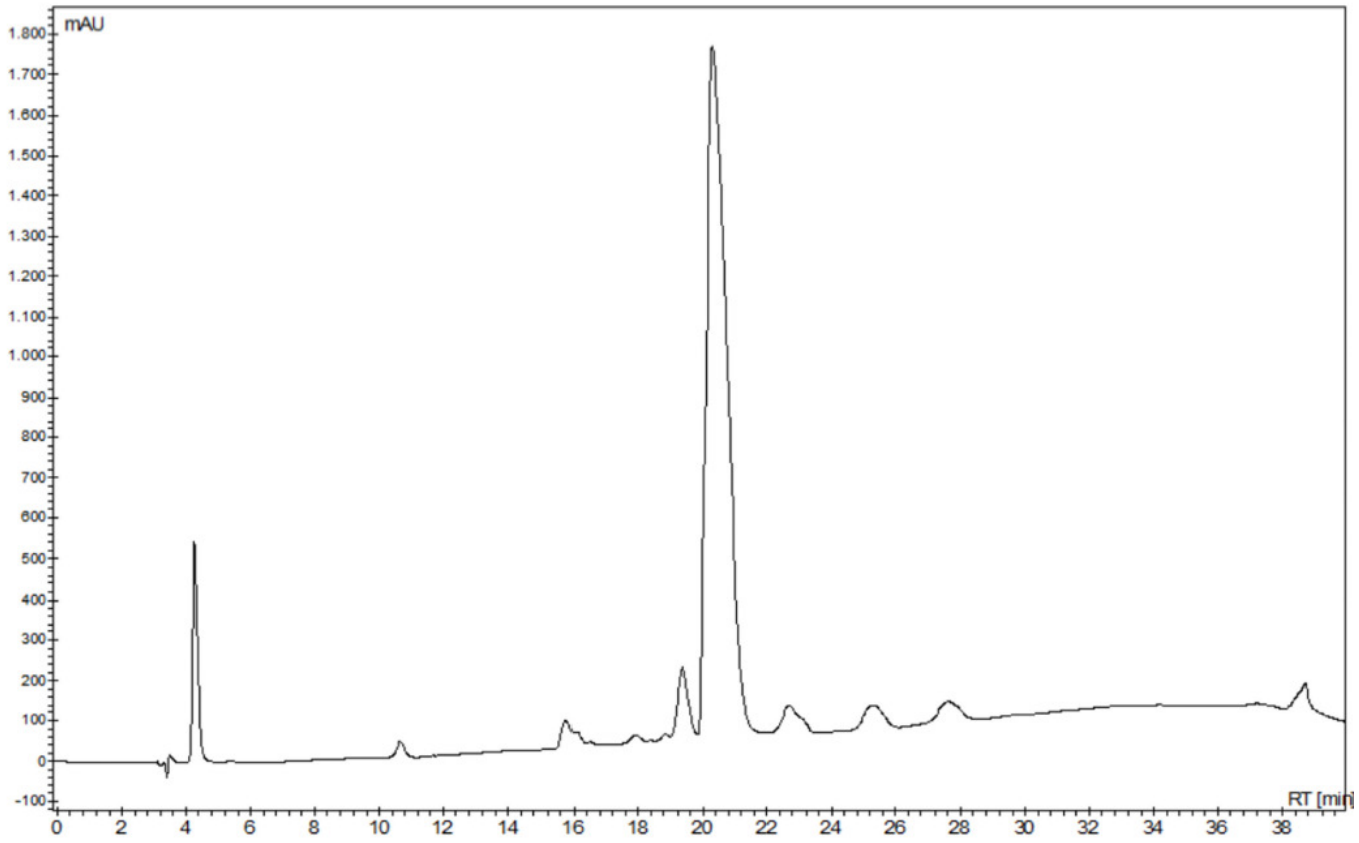
1. HPLC chromatograms of linear compounds 8-11.

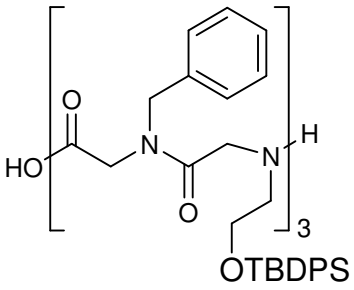
Compound 8

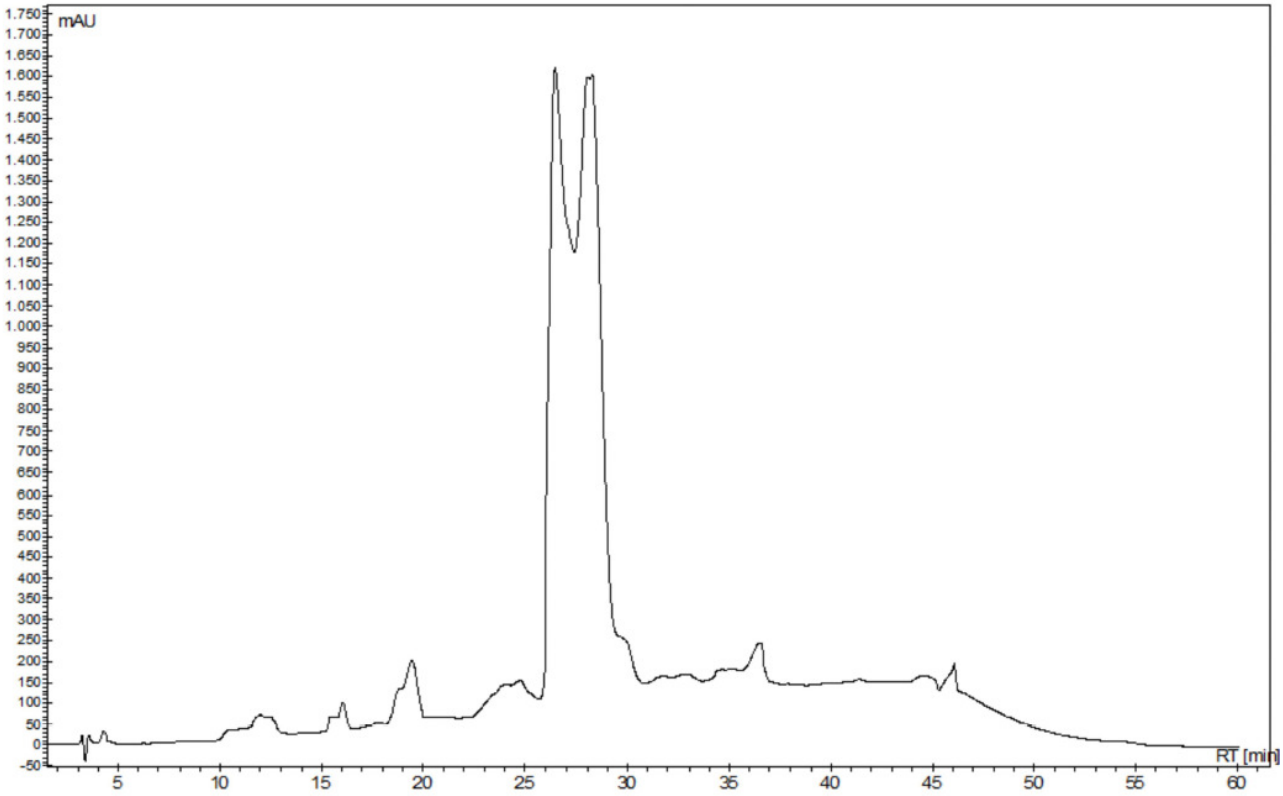




Yield: 61% (crude residue); **ES-MS:** 865.9 *m/z* [M + H^+] $\mathbf{t_R}$**:** 20.3 min; conditions: 5→100% B in 30 min ; (A, 0.1% TFA in water, B, 0.1% TFA in acetonitrile); flow: 1 mL/min, 220 nm].

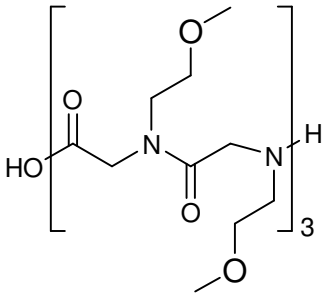
1.1 Compound 9

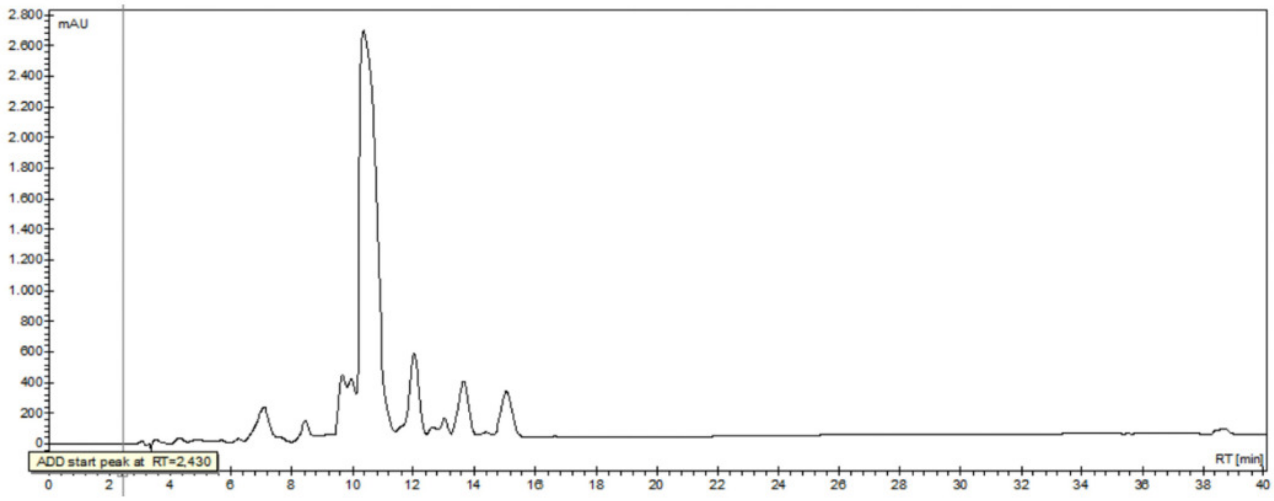




Yield: 76% (crude residue); **ES-MS:** 1499.7 *m/z* [M + H^+] $\mathbf{t_R}$**:** 26.4 min; ; conditions: 5→100% B in 30 min ; (A, 0.1% TFA in water, B, 0.1% TFA in acetonitrile); flow: 1 mL/min, 220 nm].

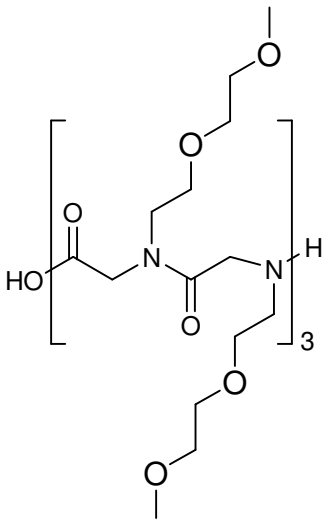
1.2 Compound 10

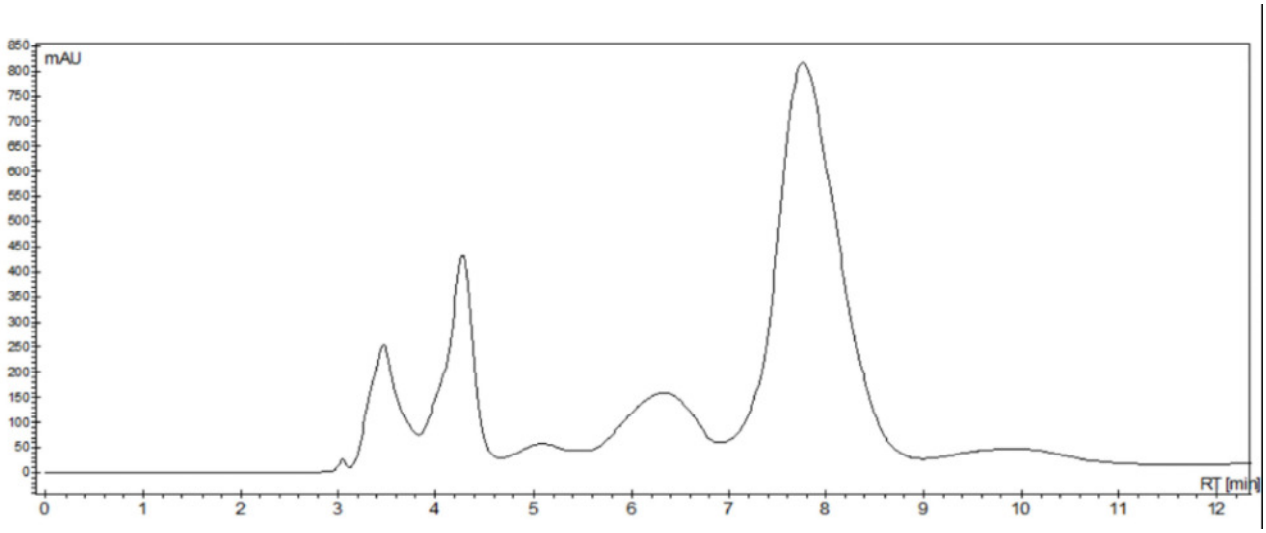




Yield: 65% (crude residue); **ES-MS:** 709.1 *m/z* [M + H^+] $\mathbf{t_R}$**:** 10.4 min; ; conditions: 5→100% B in 30 min ; (A, 0.1% TFA in water, B, 0.1% TFA in acetonitrile); flow: 1 mL/min, 220 nm].

1.3 Compound 11

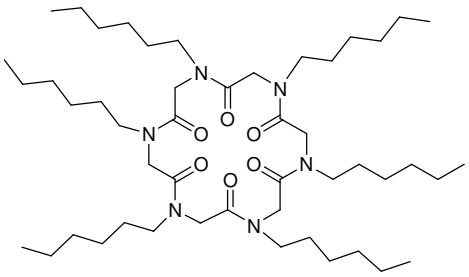




Yield: 69% (purified by RP-HPLC); **ES-MS:** 972.5 m/z [M + H^+] t_R: 7.8 min; conditions: 25→100% B in 30 min ; (A, 0.1% TFA in water, B, 0.1% TFA in acetonitrile); flow: 1 mL/min, 220 nm].

2 ^{1}H- and ^{13}C-NMR spectra of cyclopeptoids 3-6, 12 and 13.

2.1 Compound 3



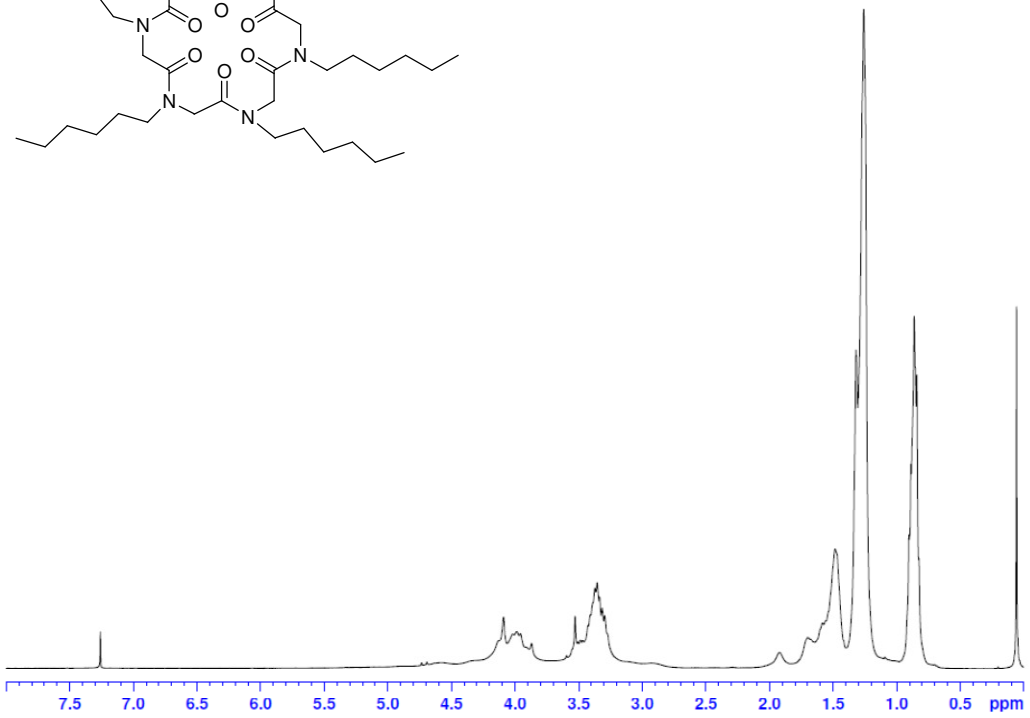


Figure S1. ^{1}H-NMR (400 MHz, $CDCl_3$, mixture of rotamers) of **3**.

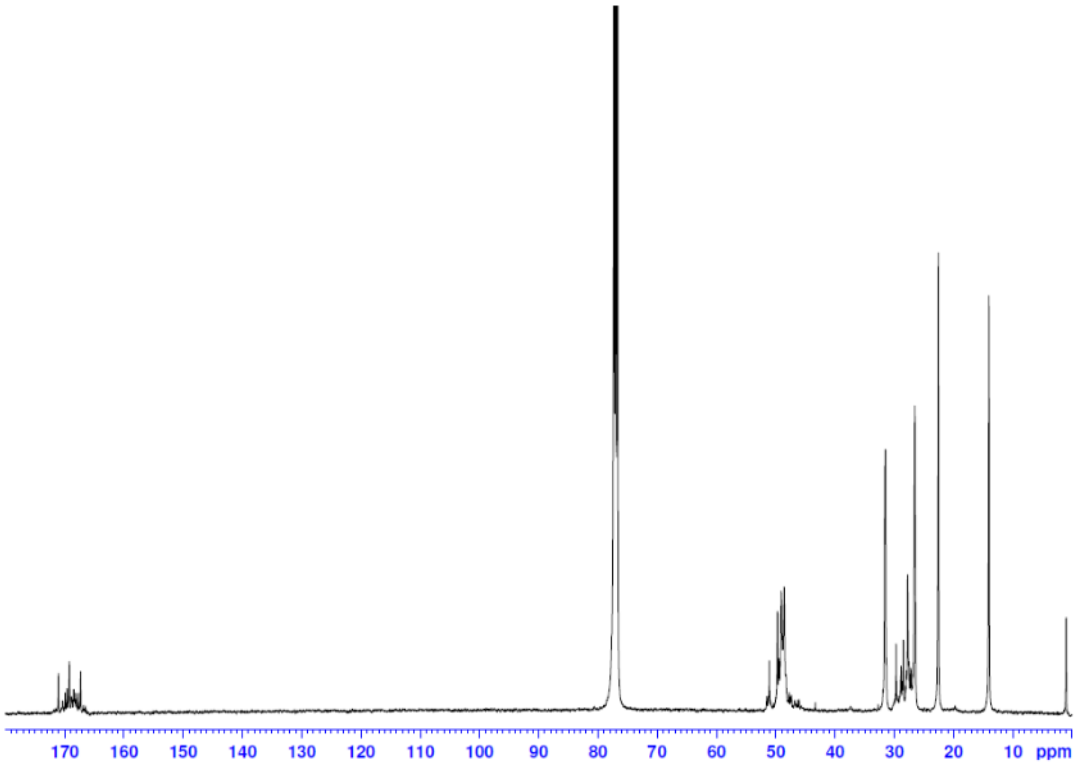


Figure S2. ^{13}C-NMR (100 MHz, $CDCl_3$, mixture of rotamers) of **3**.

2.2 Compound 4

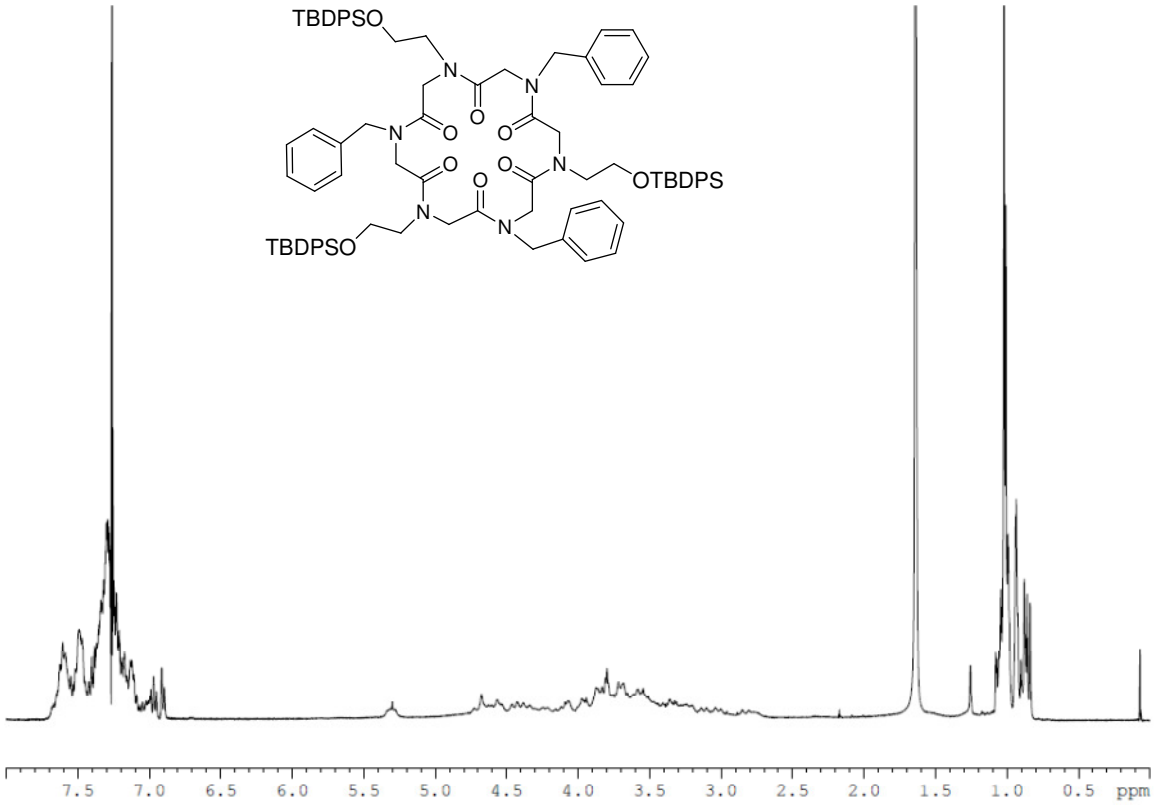


Figure S3. ^{1}H-NMR (400 MHz, $CDCl_3$, mixture of rotamers) of **4**.

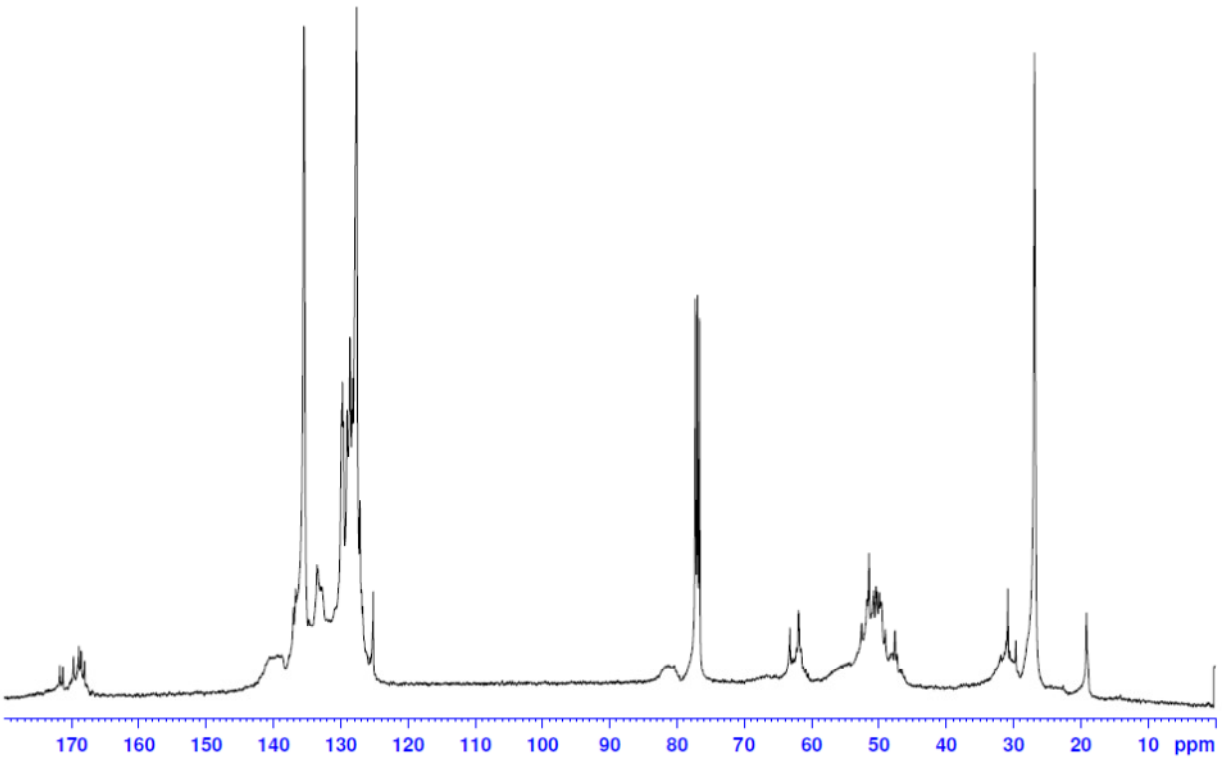


Figure S4. ^{13}C-NMR (100 MHz, $CDCl_3$, mixture of rotamers) of **4**.

2.3 Compound 5

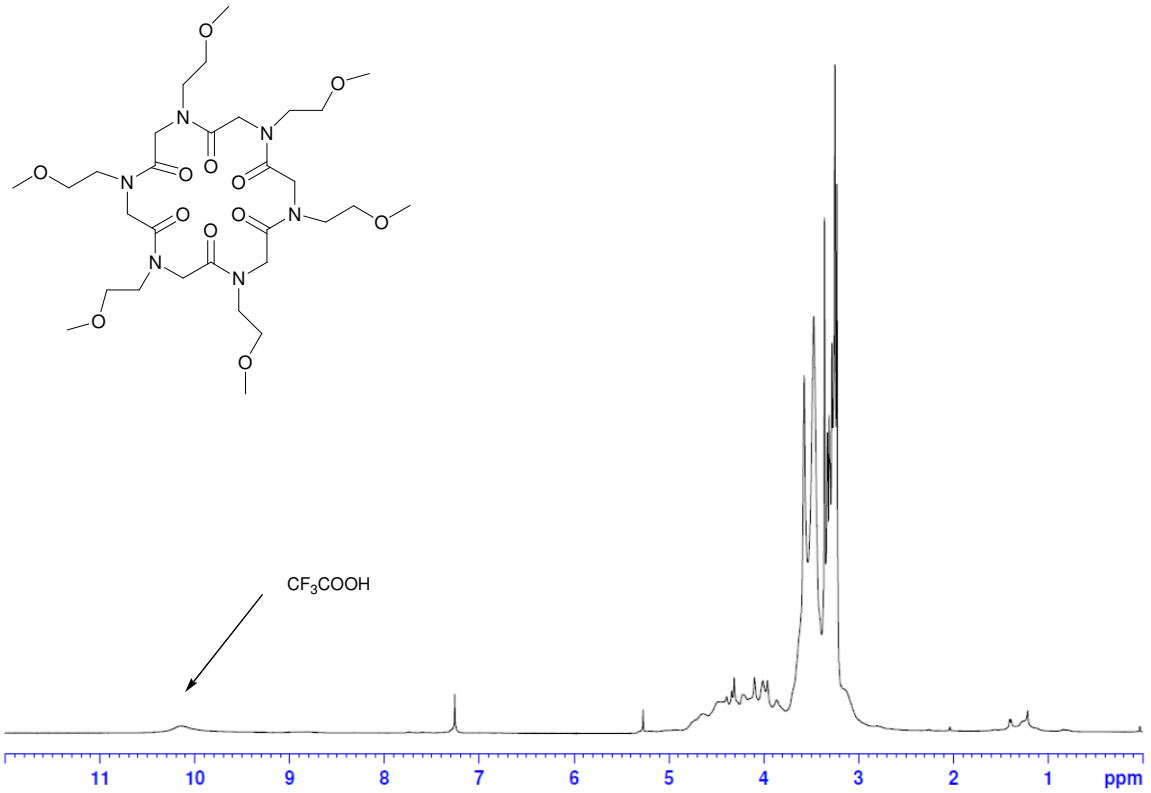


Figure S5. ^{1}H-NMR (400 MHz, $CDCl_3$, mixture of rotamers) of **5**.

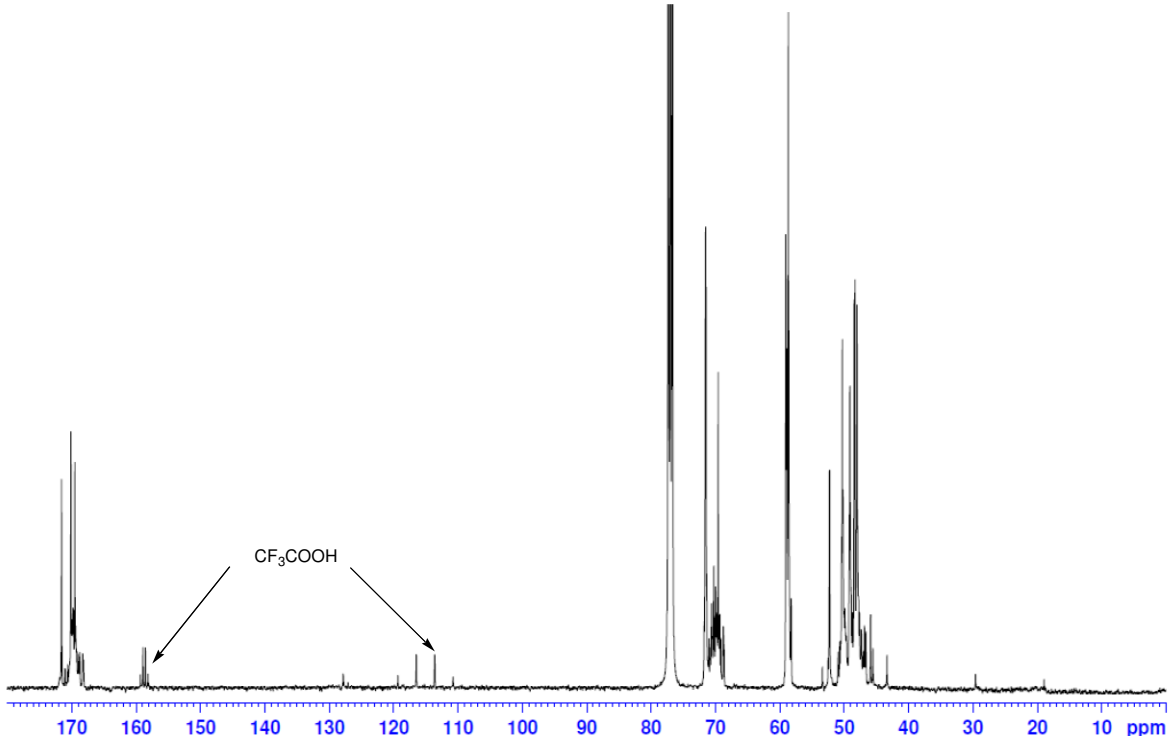


Figure S6. ^{13}C-NMR (100 MHz, $CDCl_3$, mixture of rotamers) of **5**.

2.4 Compound 6

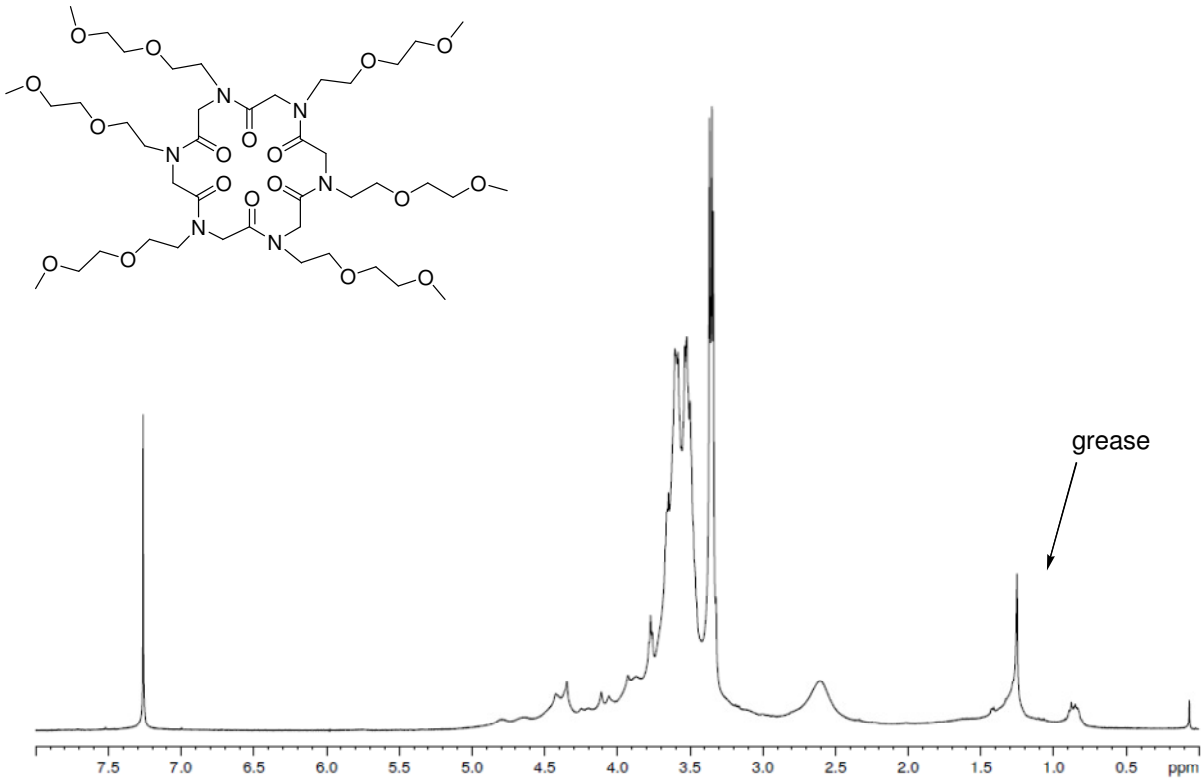


Figure S7. ^{1}H-NMR (400 MHz, $CDCl_3$, mixture of rotamers) of **6**.

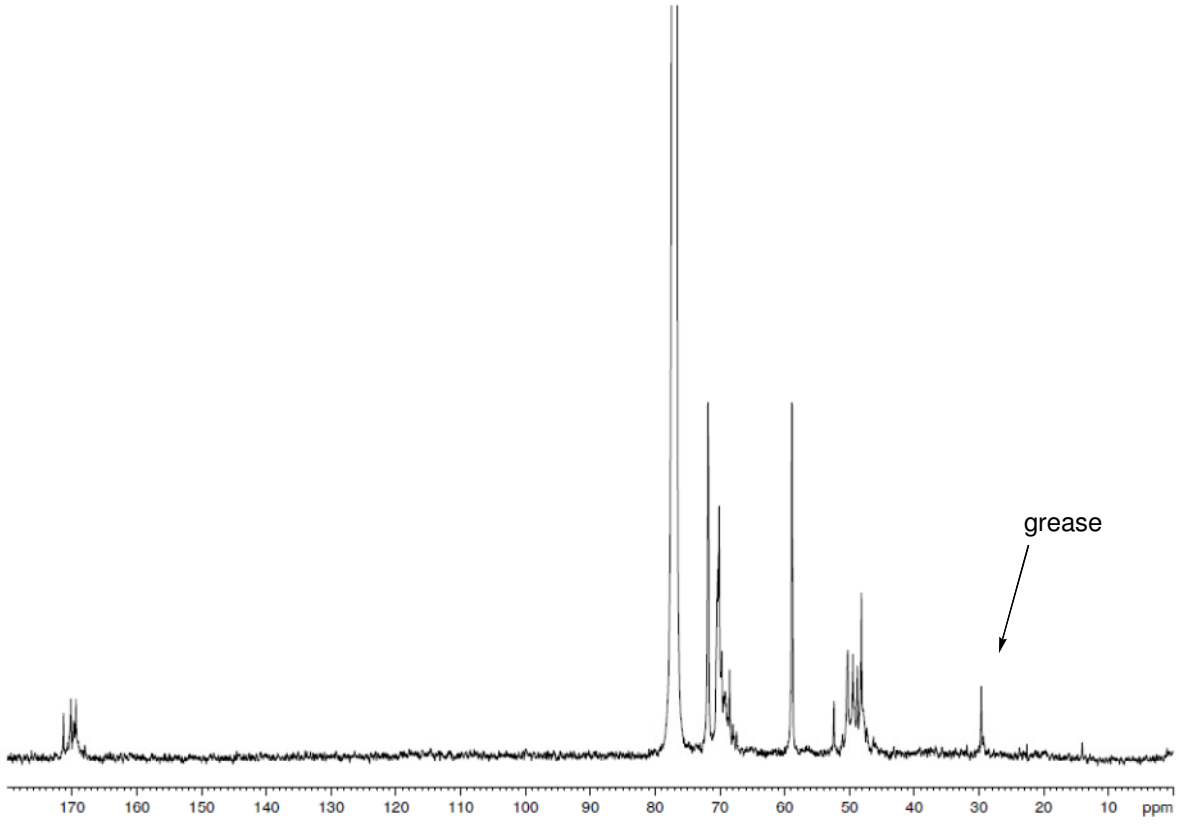


Figure S8. ^{13}C-NMR (100 MHz, $CDCl_3$, mixture of rotamers) of **6**.

2.5 Compound 12

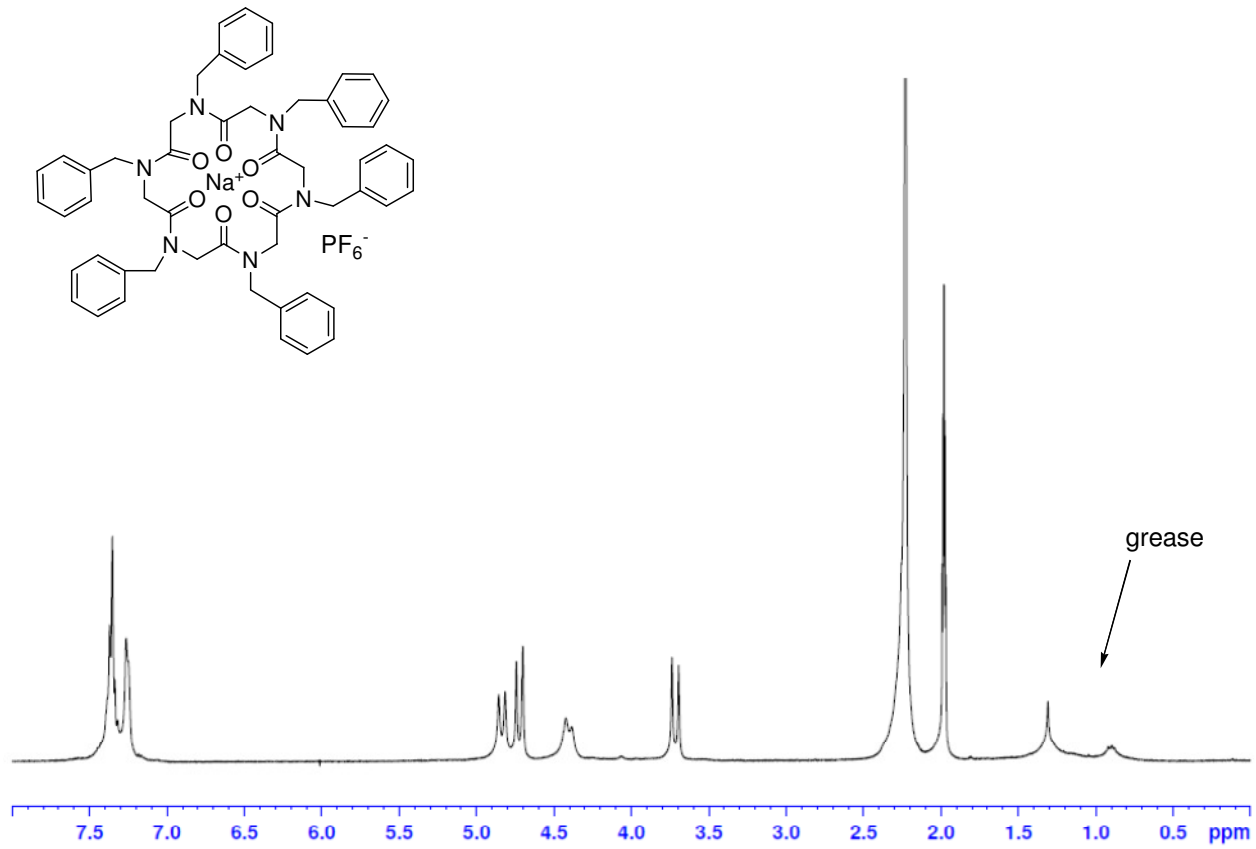


Figure S9. ^{1}H-NMR (400 MHz, CD_3CN) of 12, complex with $Na^+PF_6^-$.

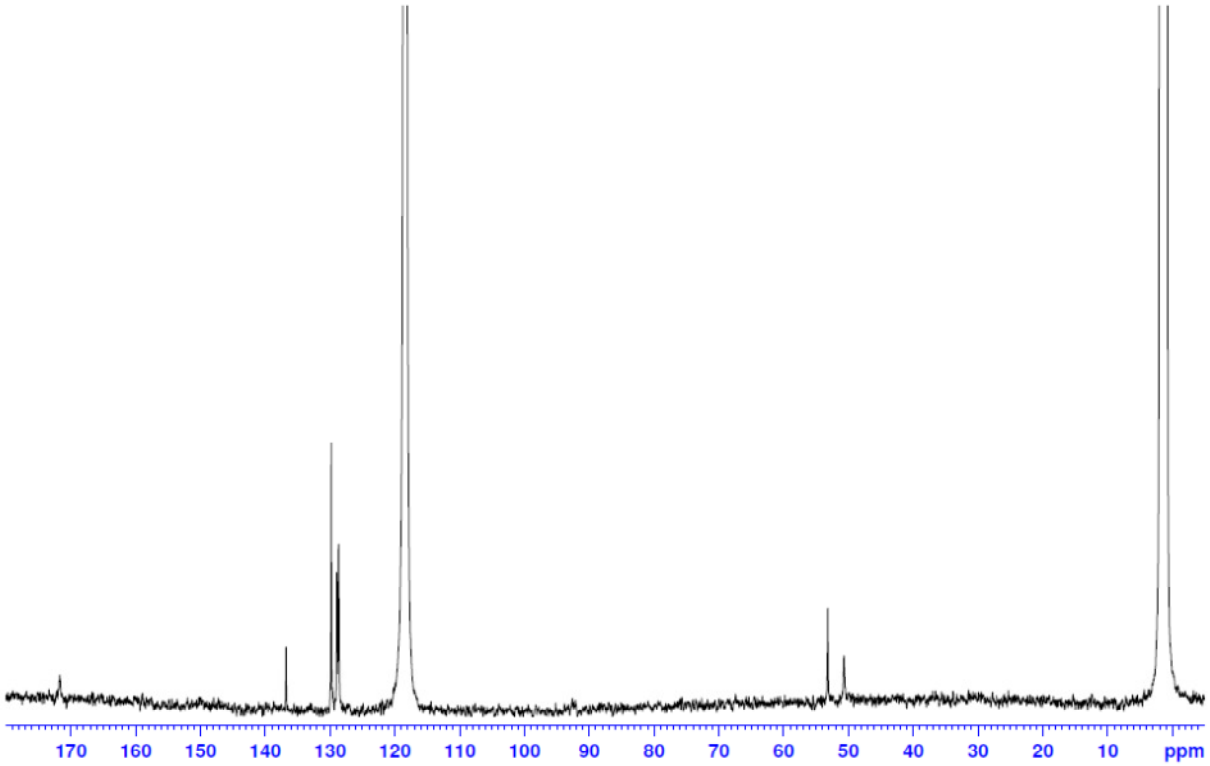


Figure S10. ^{13}C-NMR (100 MHz, CD_3CN)) of **12**, complex with $Na^+PF_6^-$.

2.6 Compound 13

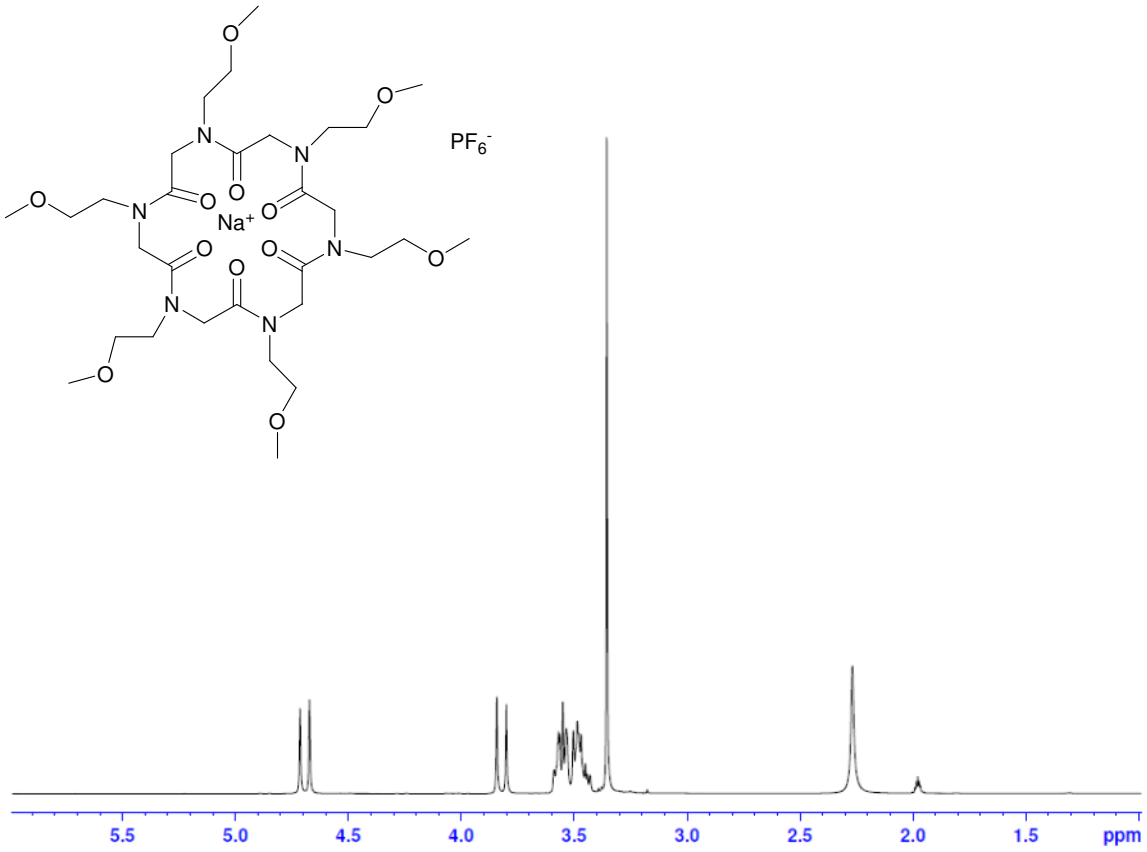


Figure S11. ^{1}H-NMR (400 MHz, CD_3CN) of 12, complex with $Na^+PF_6^-$.

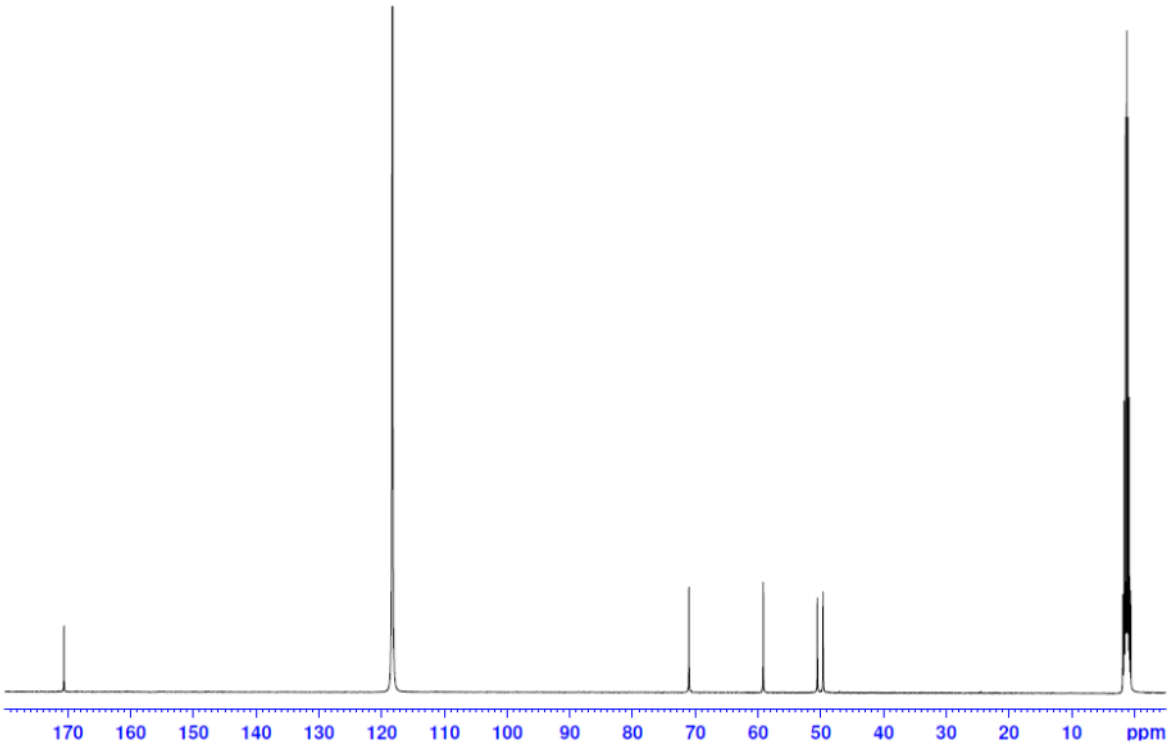
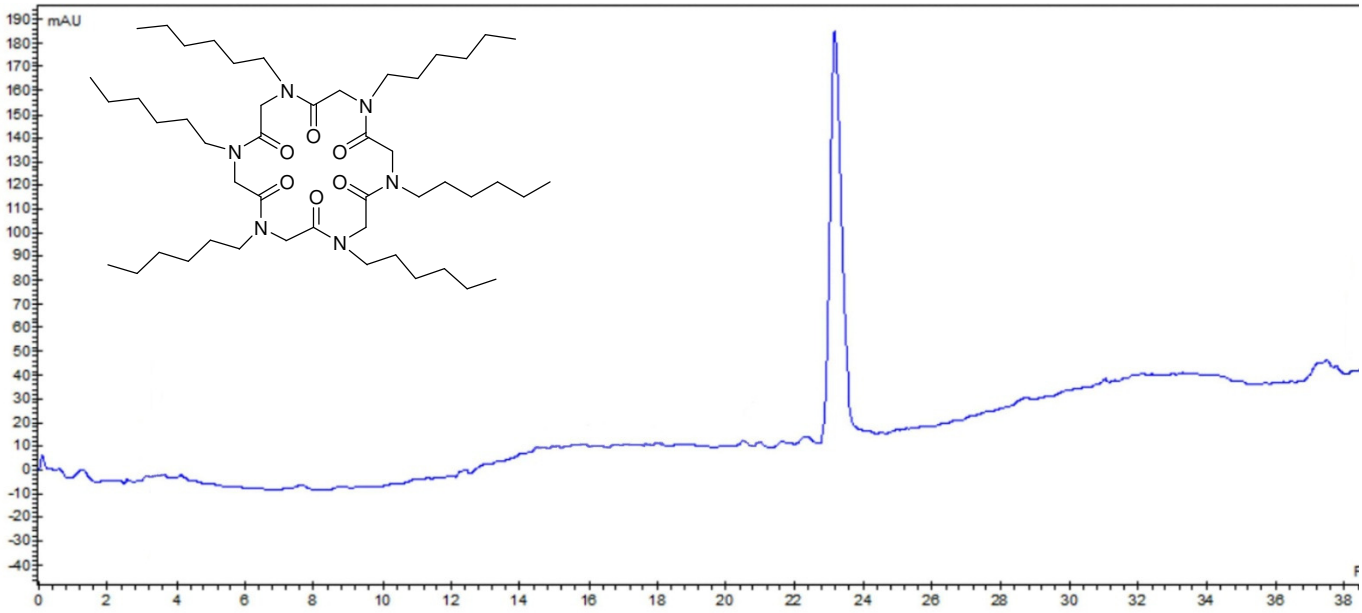


Figure S12. ^{13}C-NMR (100 MHz, CD_3CN) of **12**, complex with $Na^+PF_6^-$.

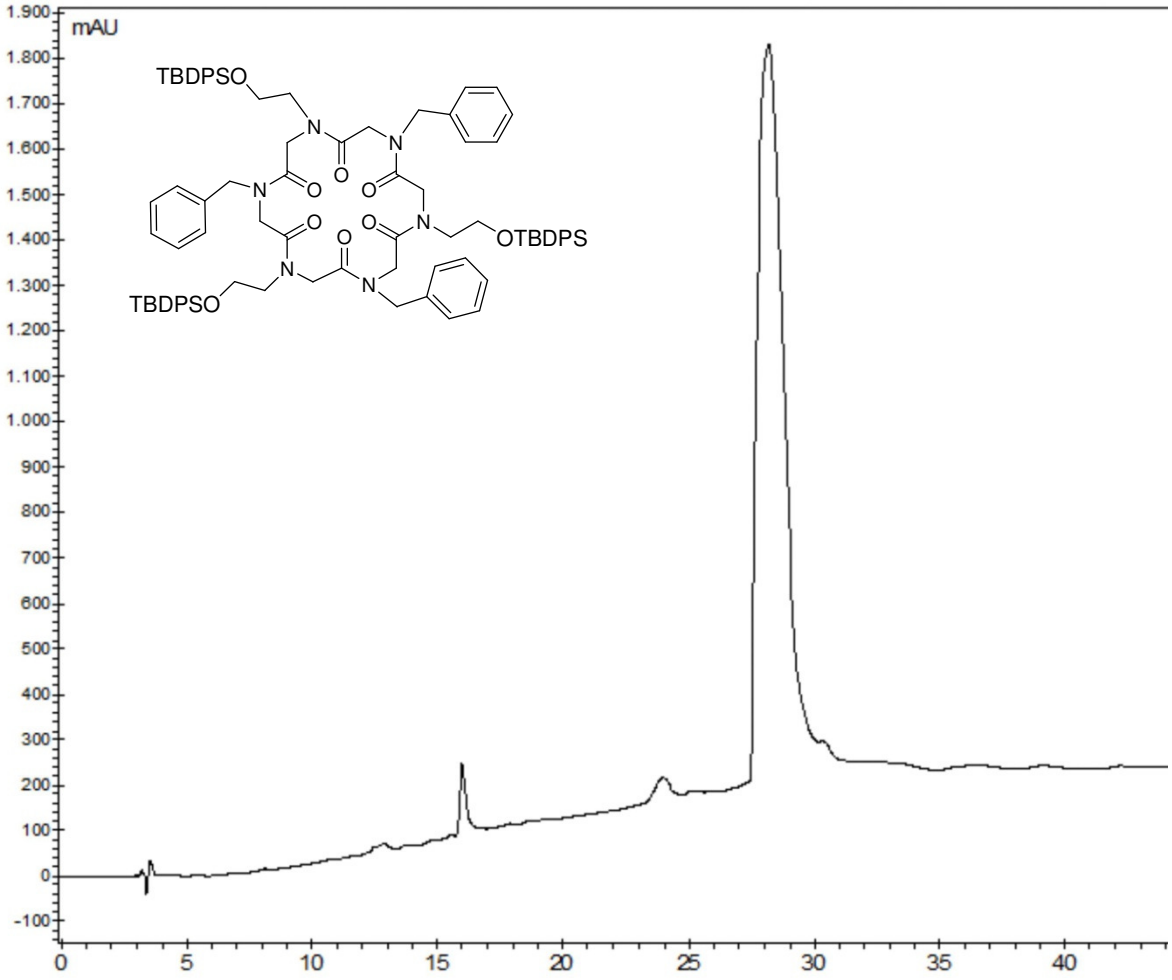
3. HPLC chromatograms of cyclic compounds 3-6.

3.1 Compound 3



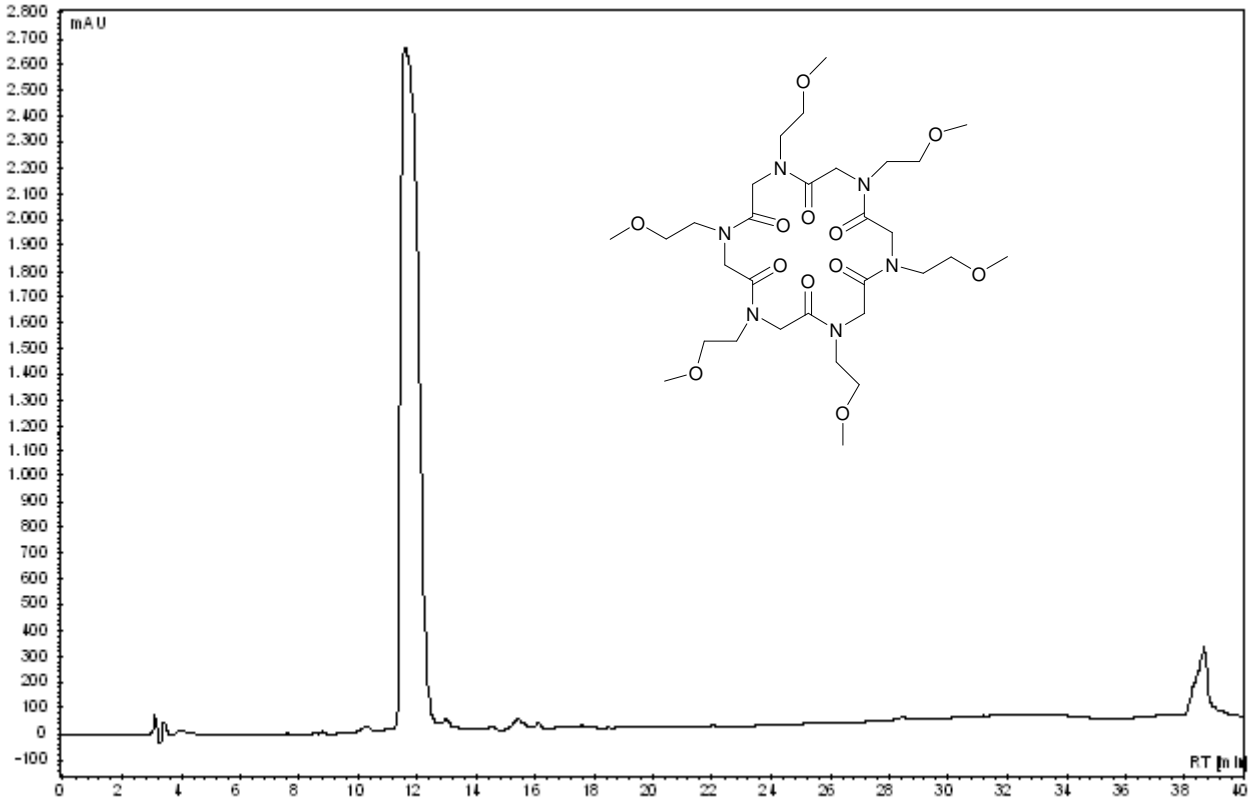
t_R: 23.2 min; ; conditions: 5→100% B in 30 min ; (A, 0.1% TFA in water, B, 0.1% TFA in acetonitrile); flow: 1 mL/min, 220 nm].

3.2 Compound 4



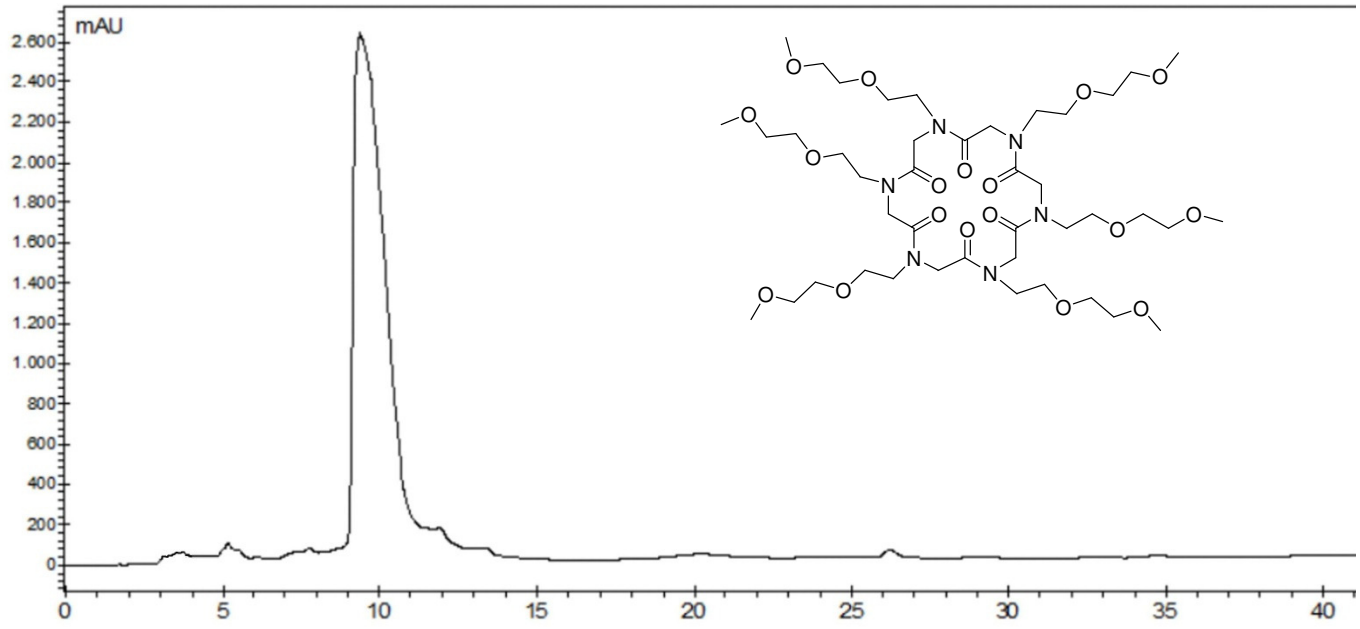
t_R: 28.2 min; ; conditions: 5→100% B in 30 min ; (A, 0.1% TFA in water, B, 0.1% TFA in acetonitrile); flow: 1 mL/min, 220 nm].

3.3 Compound 5



t_R: 11.8 min; ; conditions: 5→100% B in 30 min ; (A, 0.1% TFA in water, B, 0.1% TFA in acetonitrile); flow: 1 mL/min, 220 nm].

3.4 Compound 6



t_R: 10.6 min; ; conditions: 5→100% B in 30 min ; (A, 0.1% TFA in water, B, 0.1% TFA in acetonitrile); flow: 1 mL/min, 220 nm].