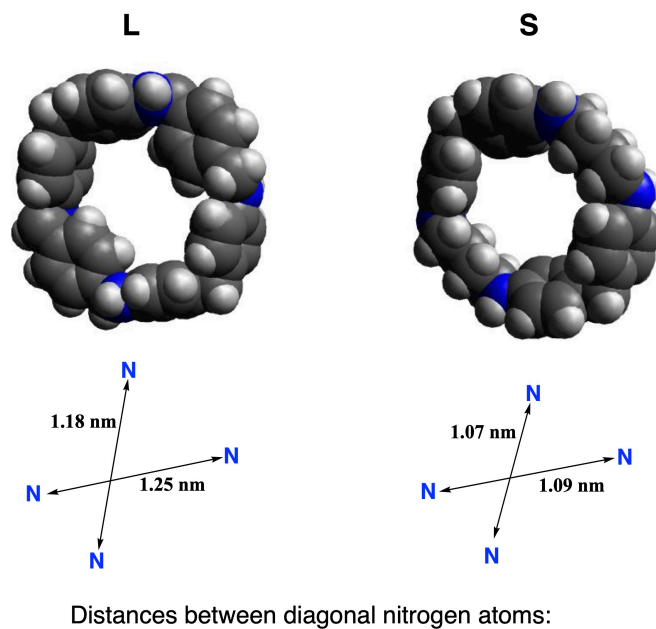


Supplementary information (SI)

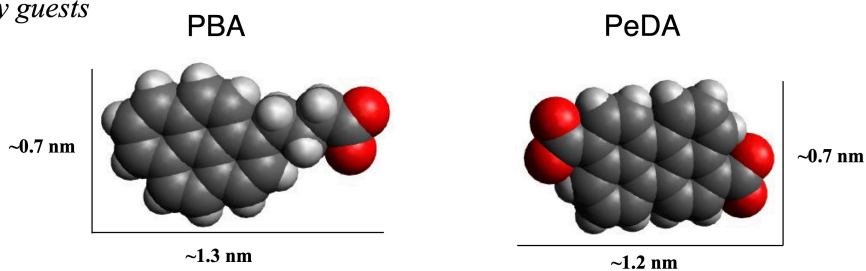
Homo- and heterotypic pentameric cyclophanes exhibiting fascinating
host-guest binding properties

*Osamu Hayashida**, *Hayato Saruwatari*, *Syota Minami*, and *Takaaki Miyazaki*
Department of Chemistry, Faculty of Science, Fukuoka University, 8-19-1 Nanakuma,
Fukuoka 814-0180, Japan

Table of Contents	Page:
Fig. S1. Computer-generated CPK models of L , S and guests	S3
Fig. S2. ^1H NMR spectrum of L1-Boc	S4
Fig. S3. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of L1-Boc	S5
Fig. S4. MALDI-TOF MS spectra of L1-Boc	S6
Fig. S5. ^1H NMR spectrum of L1	S7
Fig. S6. $^{13}\text{C}\{^1\text{H}\}$ spectrum of L1	S8
Fig. S7. MALDI-TOF MS spectra of L1	S9
Fig. S8. ^1H NMR spectrum of hetero5-Boc	S10
Fig. S9. $^{13}\text{C}\{^1\text{H}\}$ spectrum of hetero5-Boc	S11
Fig. S10. MALDI-TOF MS spectra of hetero5-Boc	S12
Fig. S11. ^1H NMR spectrum of hetero5	S13
Fig. S12. $^{13}\text{C}\{^1\text{H}\}$ spectrum of hetero5	S14
Fig. S13. MALDI-TOF MS spectra of hetero5	S15
Fig. S14. ^1H NMR spectrum of L5-Boc	S16
Fig. S15. $^{13}\text{C}\{^1\text{H}\}$ spectrum of L5-Boc	S17
Fig. S16. MALDI-TOF MS spectra of L5-Boc	S18
Fig. S17. ^1H NMR spectrum of L5	S19
Fig. S18. $^{13}\text{C}\{^1\text{H}\}$ spectrum of L5	S20
Fig. S19. MALDI-TOF MS spectra of L5	S21
Fig. S20. Fitting of fluorescence titration data (PBA)	S22
Fig. S21. Fitting of fluorescence titration data (PeDA)	S24
Fig. S22. Fitting of fluorescence titration data (TNS)	S26
Fig. S23. Fitting of fluorescence titration data (CDab)	S28
Fig. S24. Fluorescence spectral changes of PBA upon the addition of CDab in the absence (a) and presence of S1 (b), L1 (c) and L5 (d)	S30



Stocky guests



Elongated guests

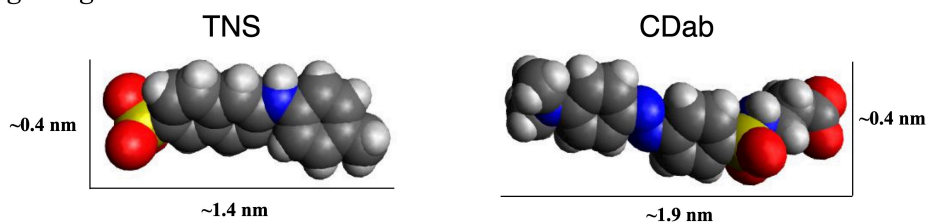


Fig. S1 Computer-generated CPK models of **L**, **S** and guests (PBA, PeDA, TNS and CDab) (Avogadro 1.2.0 software). Distances between diagonal nitrogen atoms are shown. Carbon, hydrogen, and nitrogen atoms are shown in gray, cloudy white, and blue, respectively.

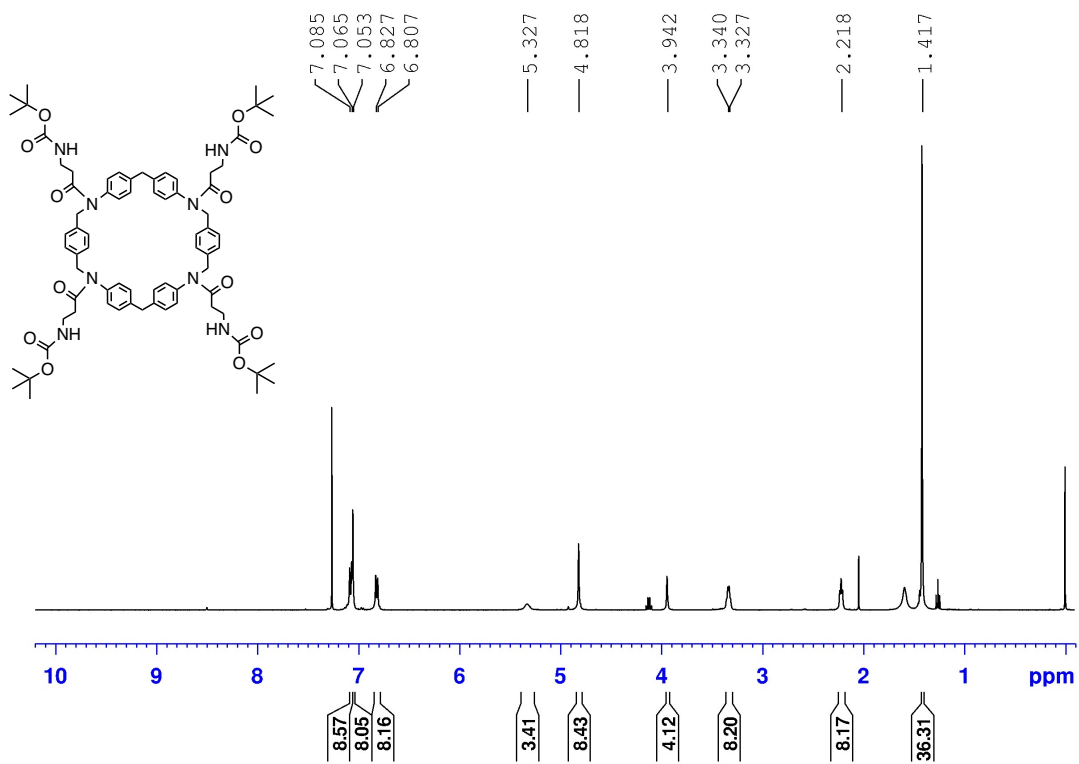


Fig. S2 ¹H NMR spectrum of **L1-Boc** (400 MHz, CDCl₃, 298K).

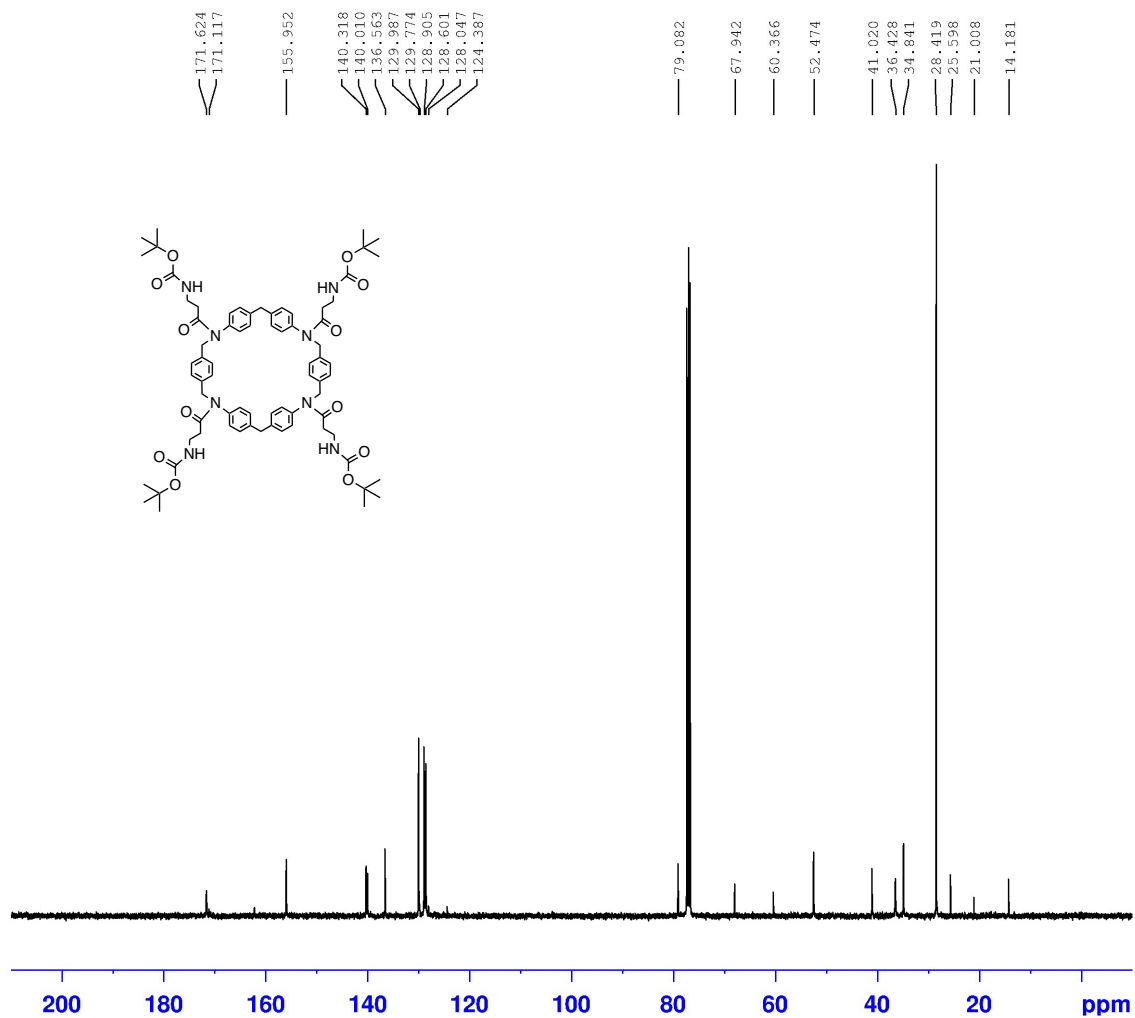


Fig. S3 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of L1-Boc (100 MHz, CDCl_3 , 298K).

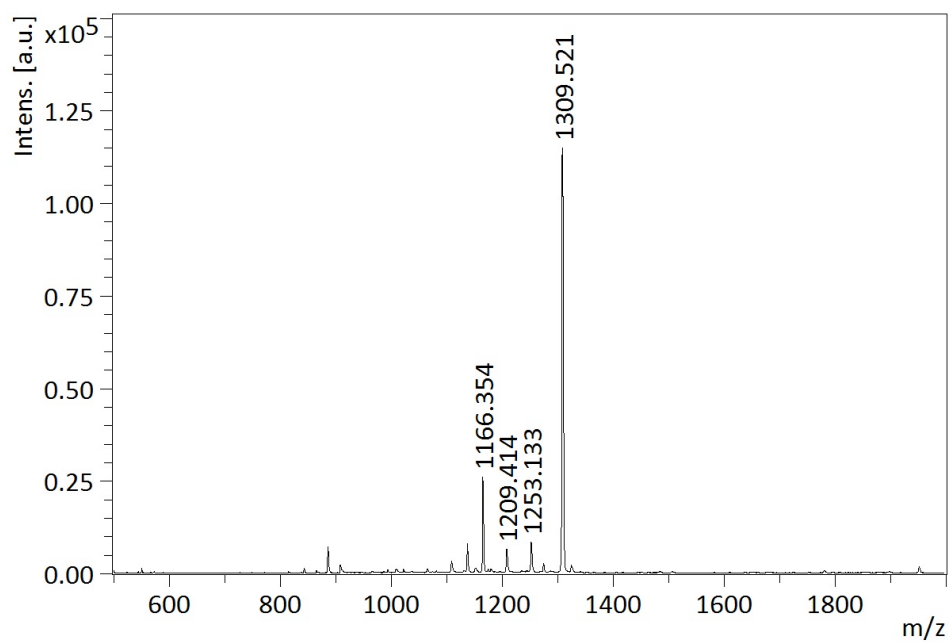


Fig. S4 MALDI-TOF MS spectra of **L1-Boc**.

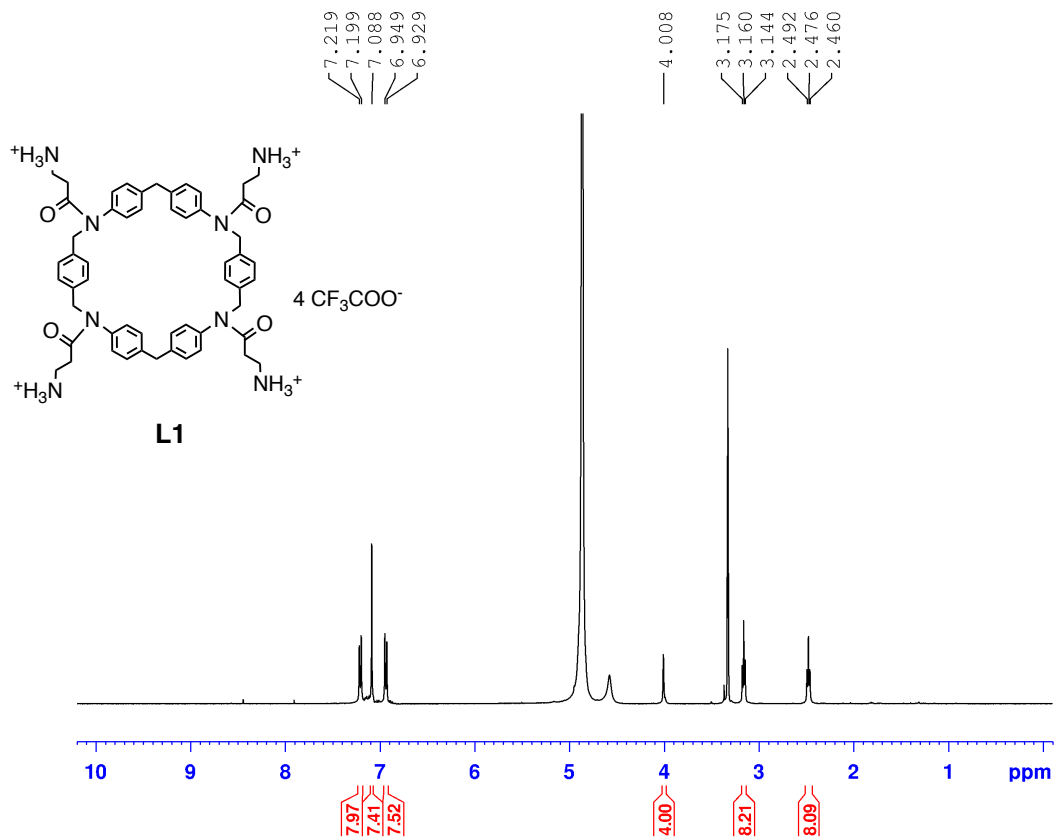


Fig. S5 ^1H NMR spectrum of **L1** (400 MHz, CD_3OD , 298K).

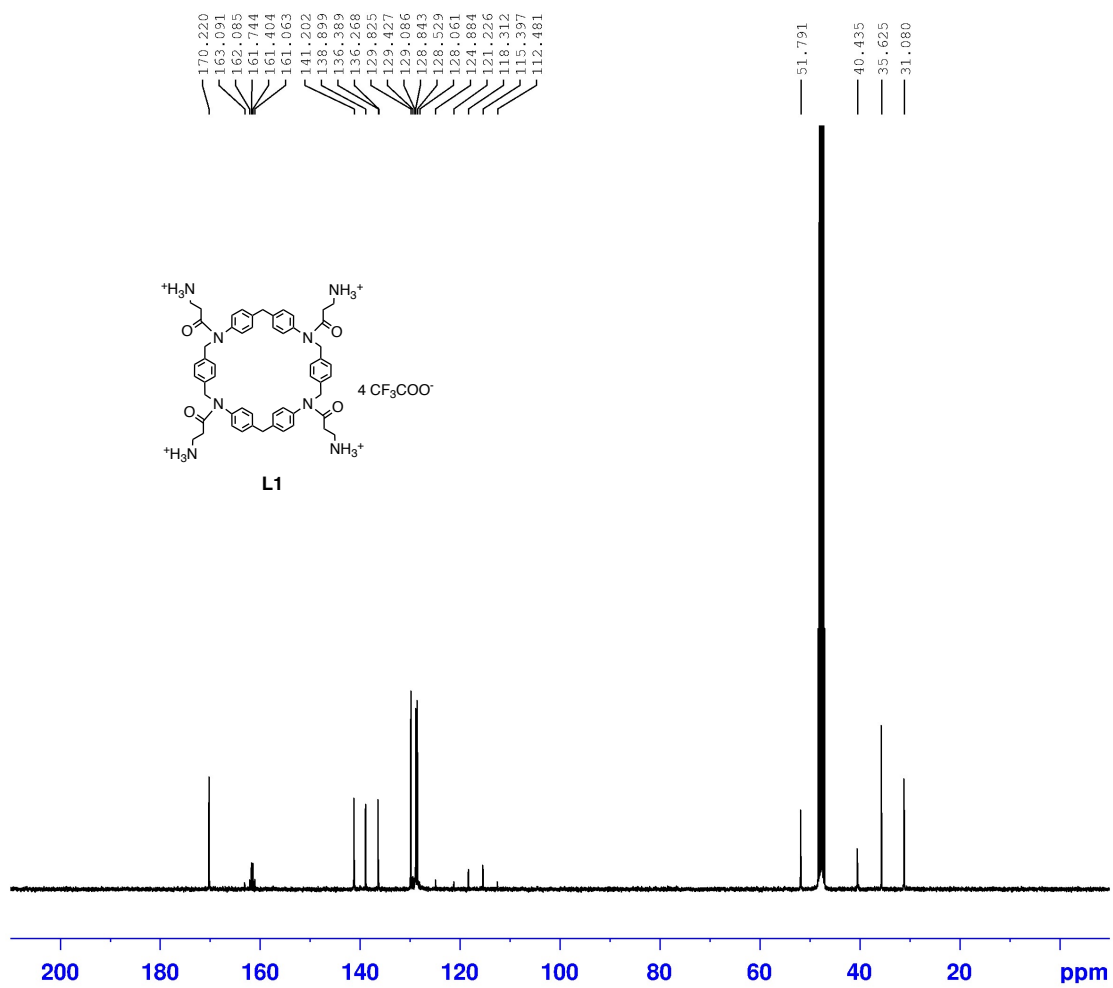


Fig. S6 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of L1 (100 MHz, CD_3OD , 298K).

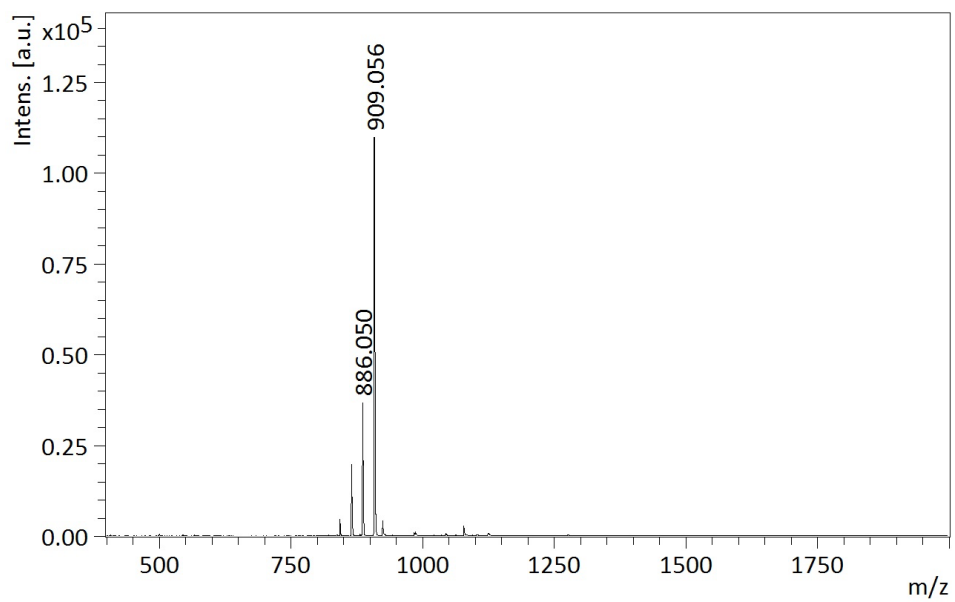


Fig. S7 MALDI-TOF MS spectra of **L1**.

]]

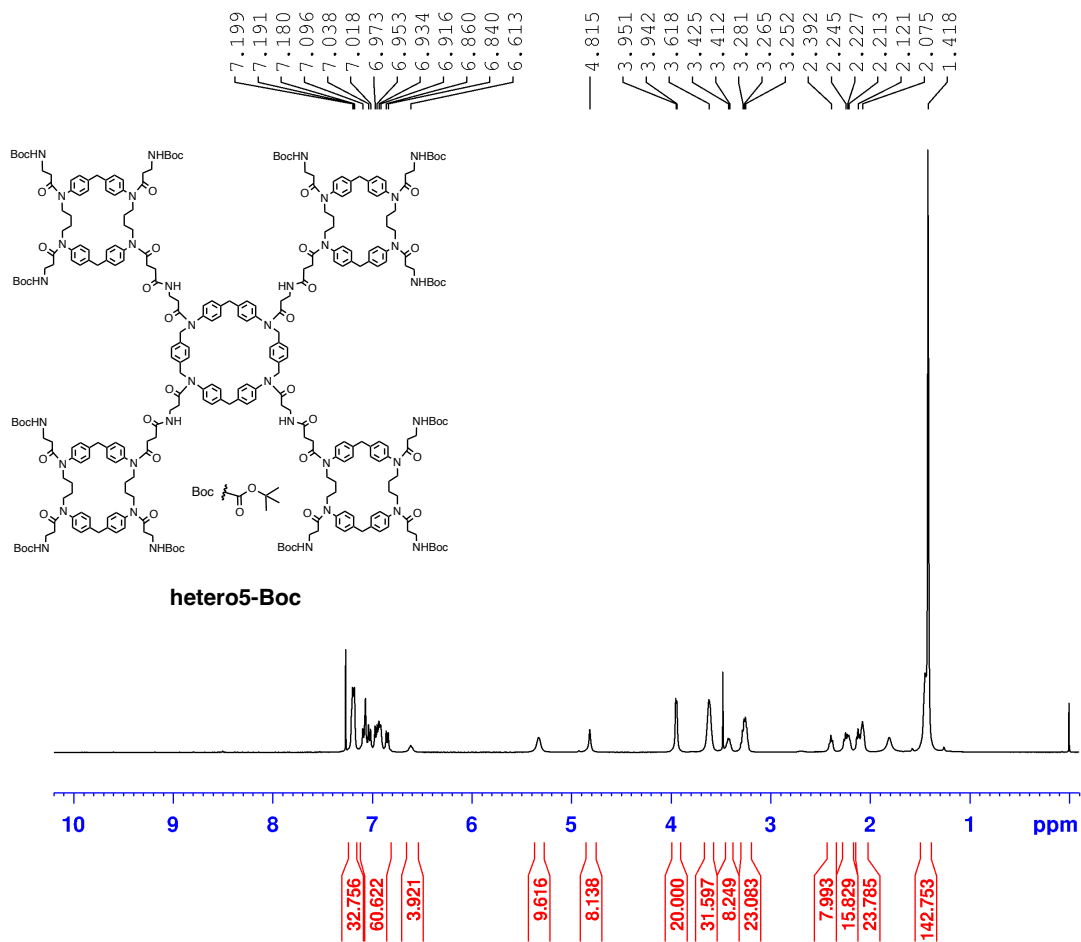


Fig. S8 ^1H NMR spectrum of **hetero5-Boc** (400 MHz, CDCl_3 , 298K).

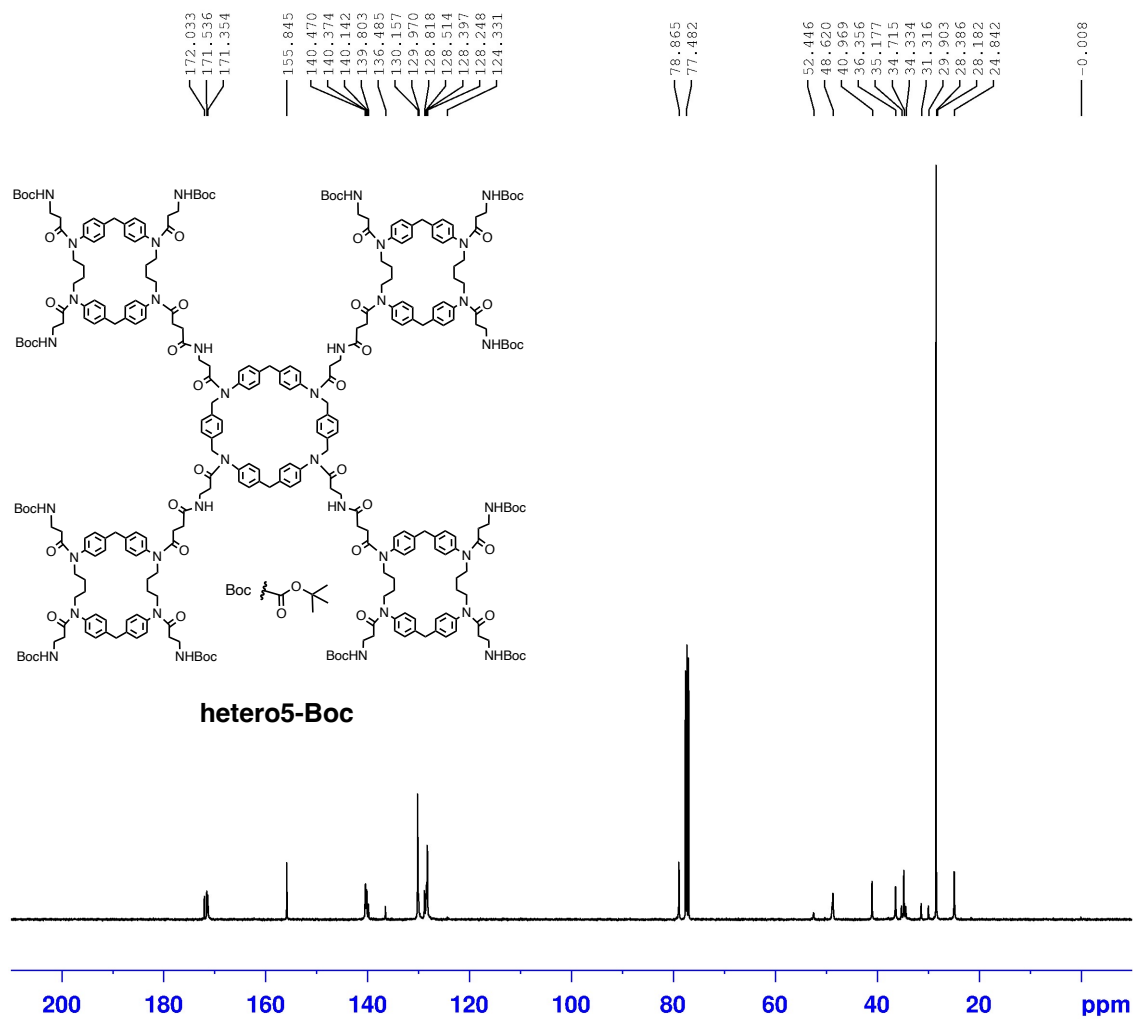


Fig. S9 ¹³C{¹H} NMR spectrum of **hetero5-Boc** (100 MHz, CDCl₃, 298K).

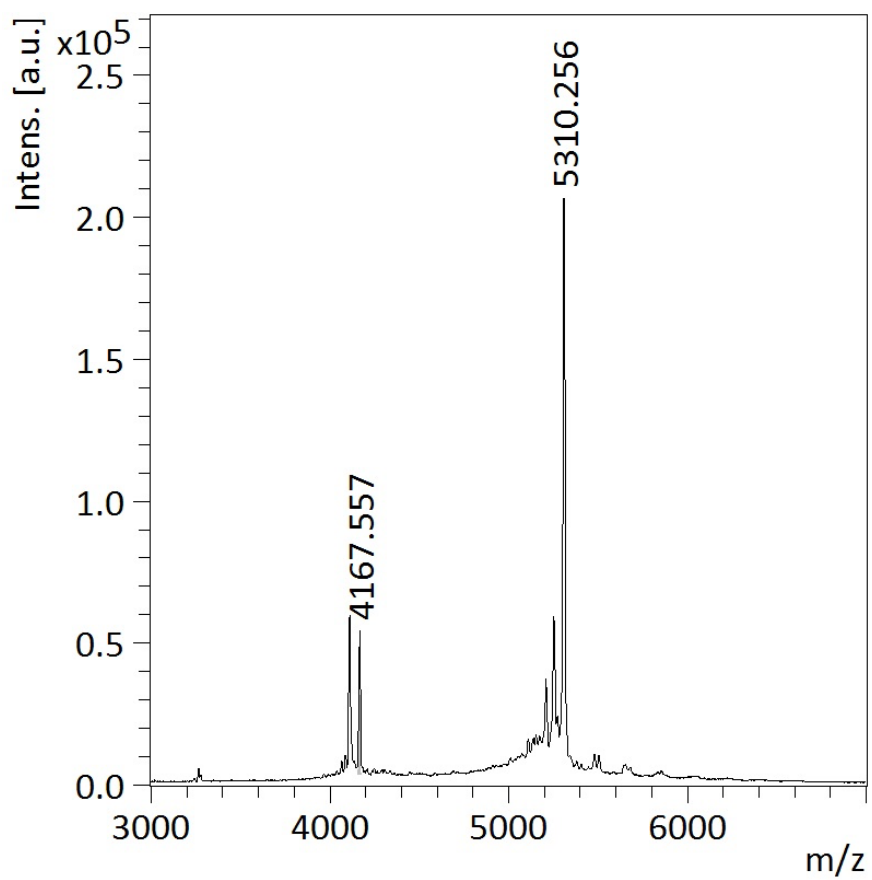


Fig. S10 MALDI-TOF MS spectra of **hetero5-Boc**.

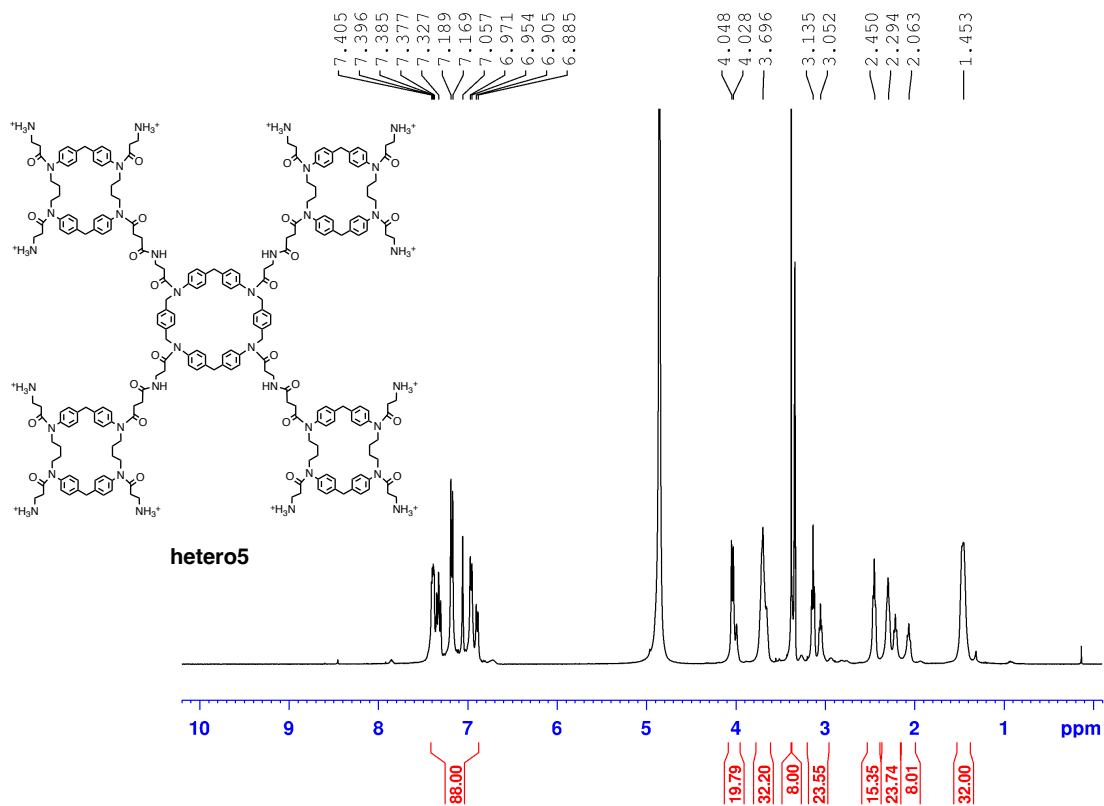


Fig. S11 ^1H NMR spectrum of **hetero5** (400 MHz, CD_3OD , 298K).

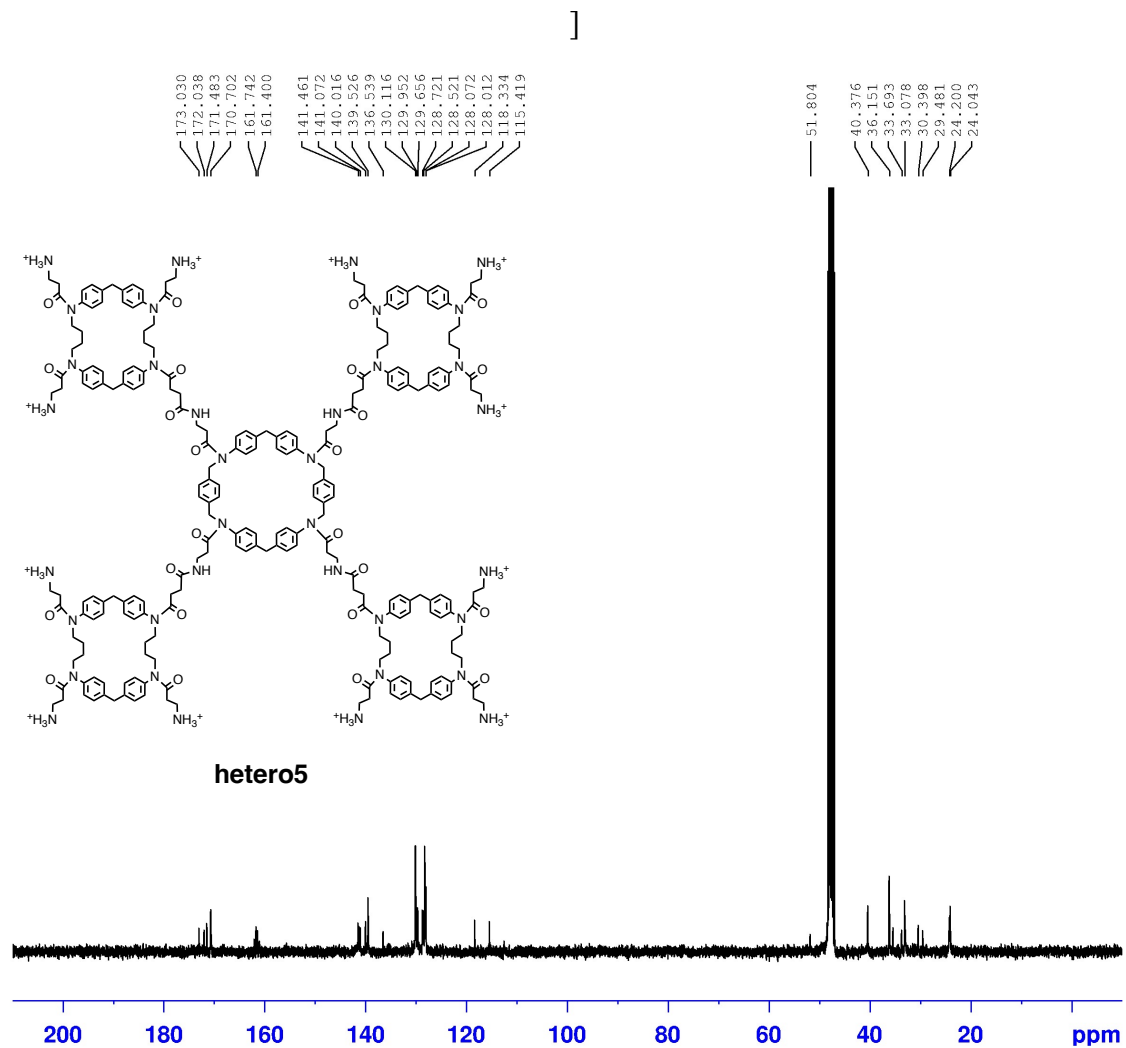


Fig. S12 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **hetero5** (100 MHz, CD_3OD , 298K).

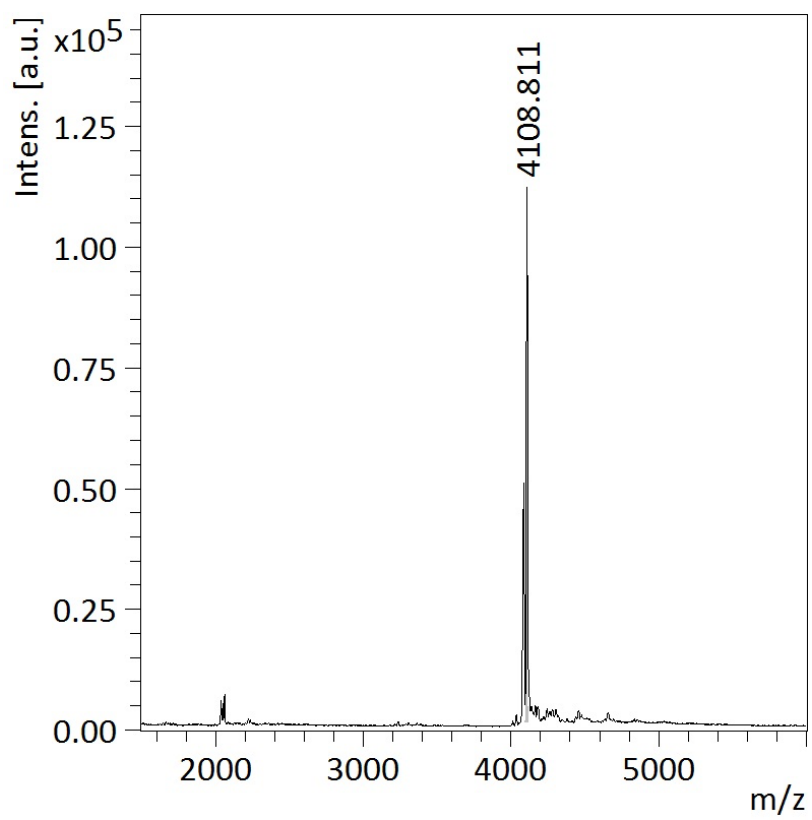


Fig. S13 MALDI-TOF MS spectra of **hetero5**.

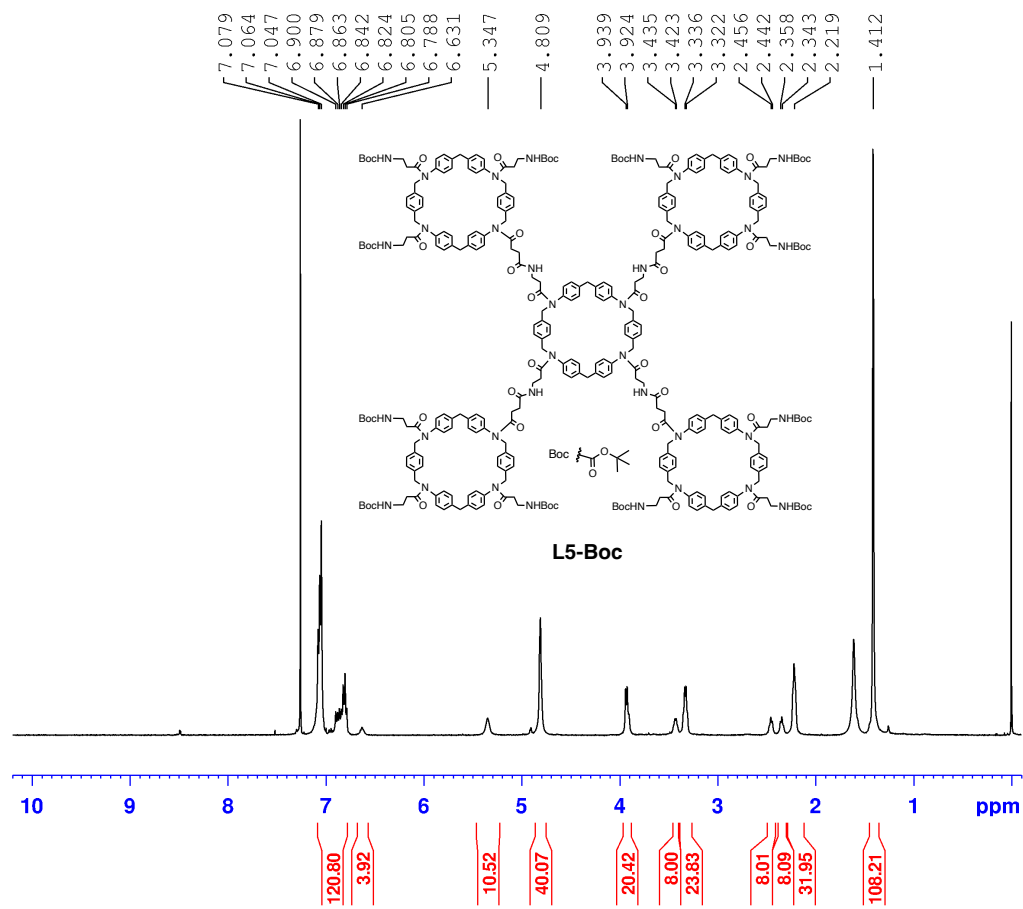


Fig. S14 ¹H NMR spectrum of L5-Boc (400 MHz, CDCl₃, 298K).

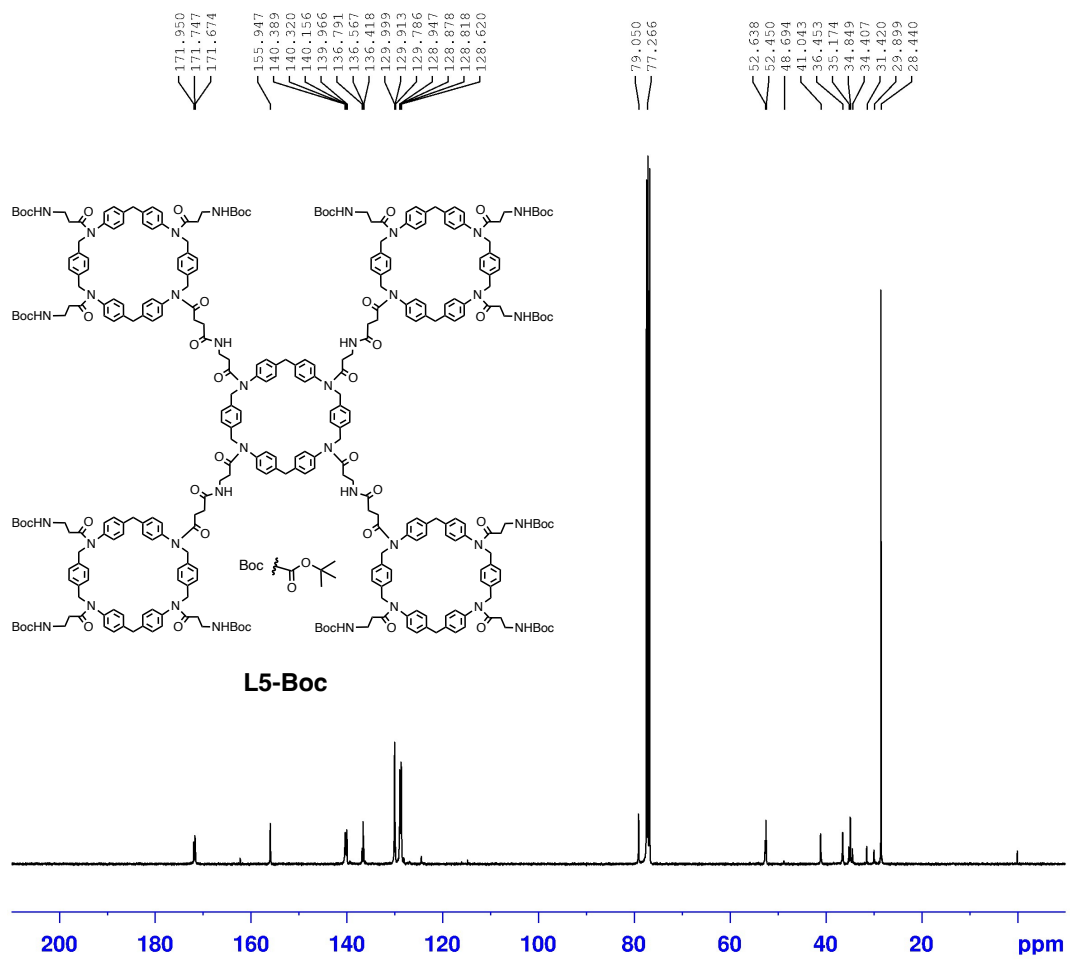


Fig. S15 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **L5-Boc** (100 MHz, CDCl_3 , 298K).

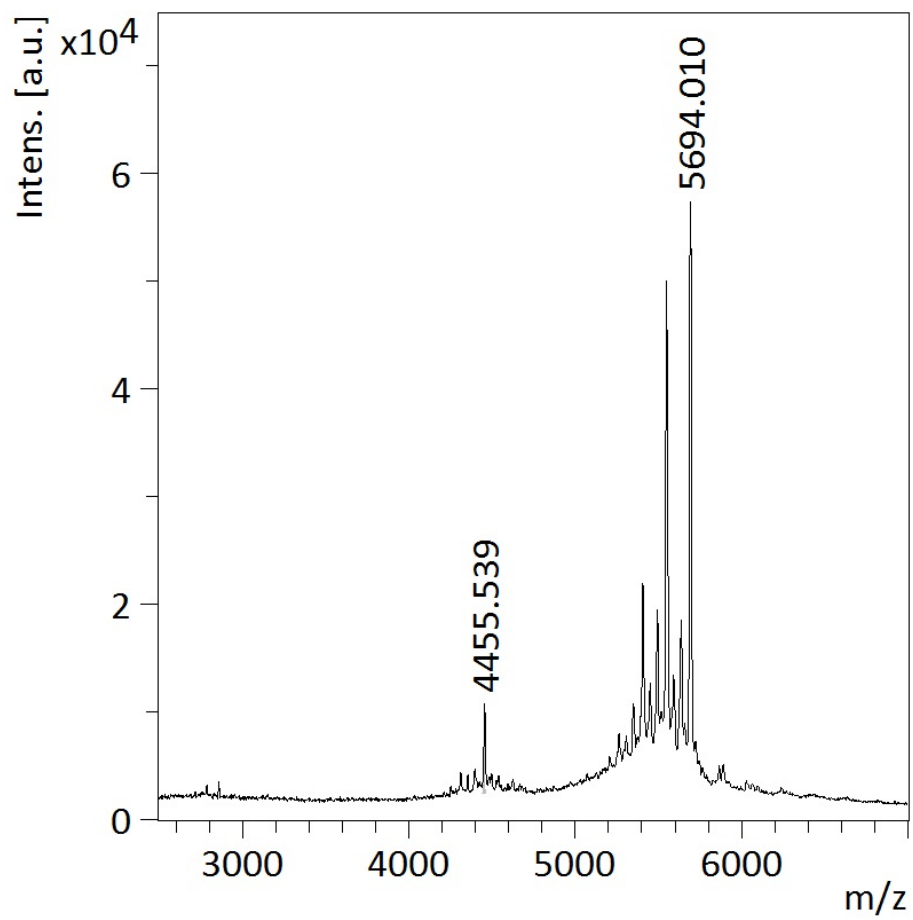


Fig. S16 MALDI-TOF MS spectra of **L5-Boc**

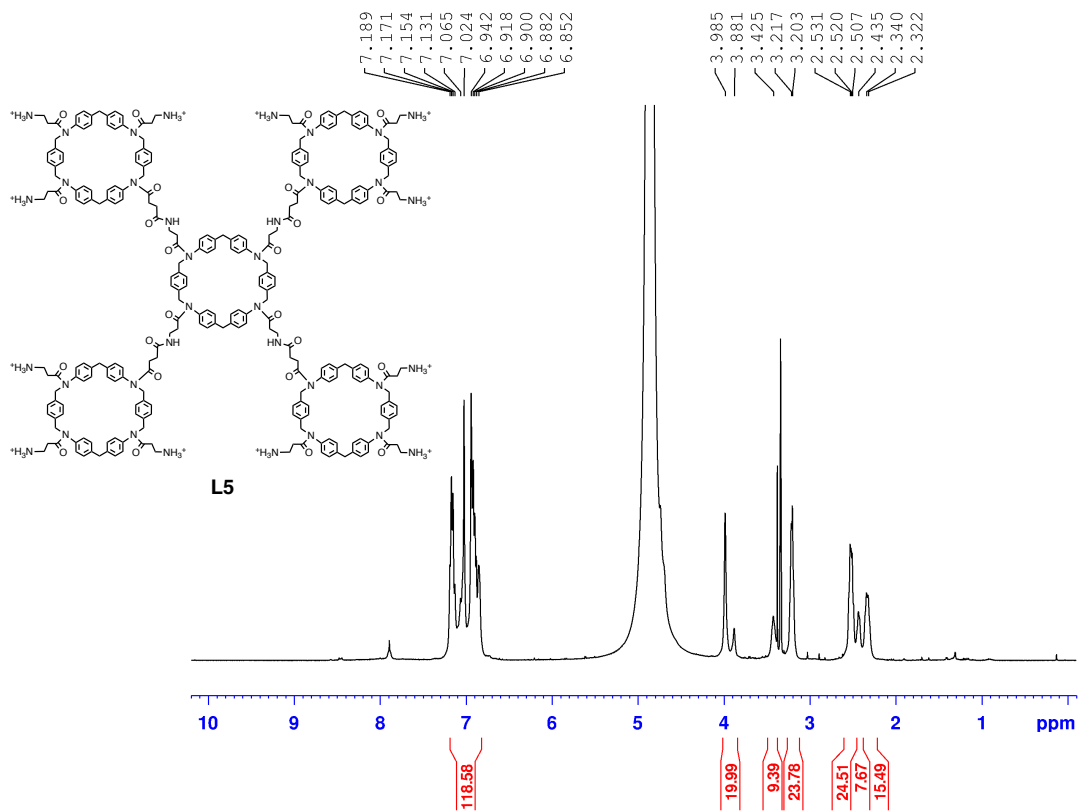


Fig. S17 ^1H NMR spectrum of **L5** (400 MHz, CD_3OD , 298K)

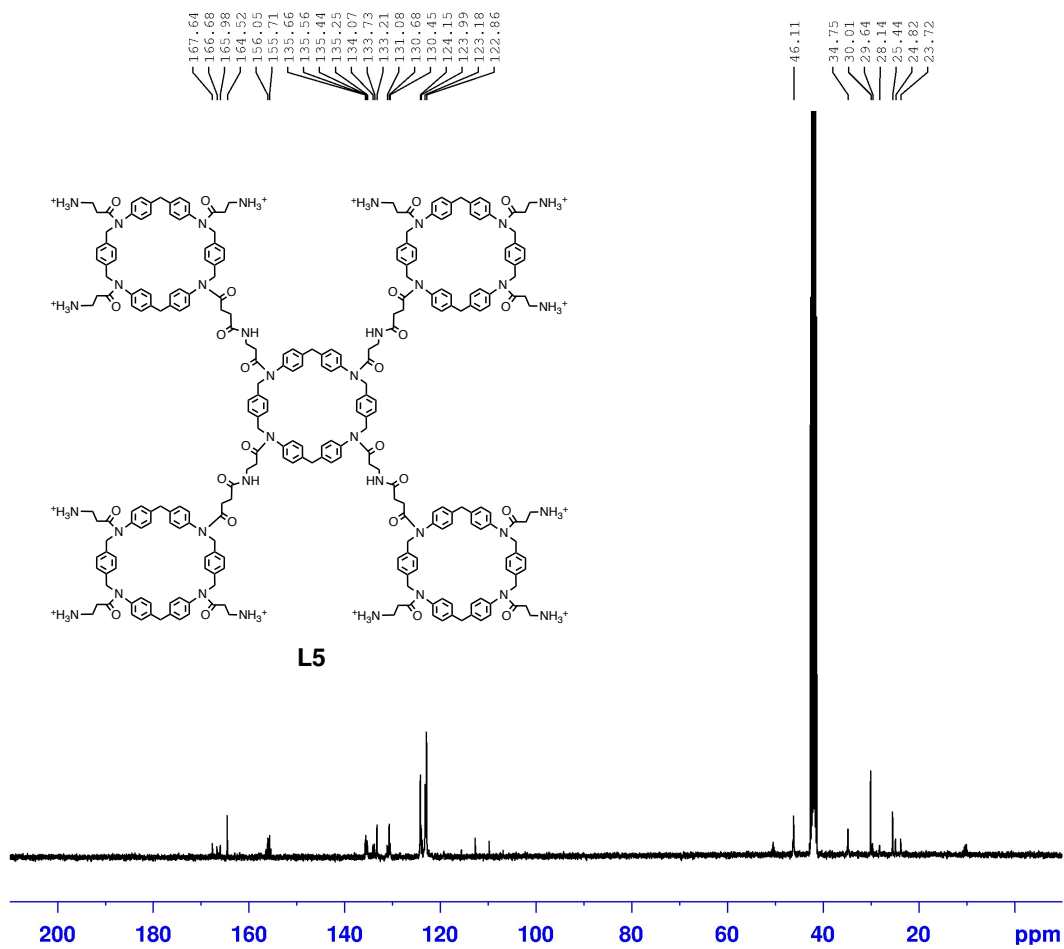


Fig. S18 $^{13}\text{C}\{^1\text{H}\}$ spectrum of L5 (100 MHz, CD₃OD, 298K)

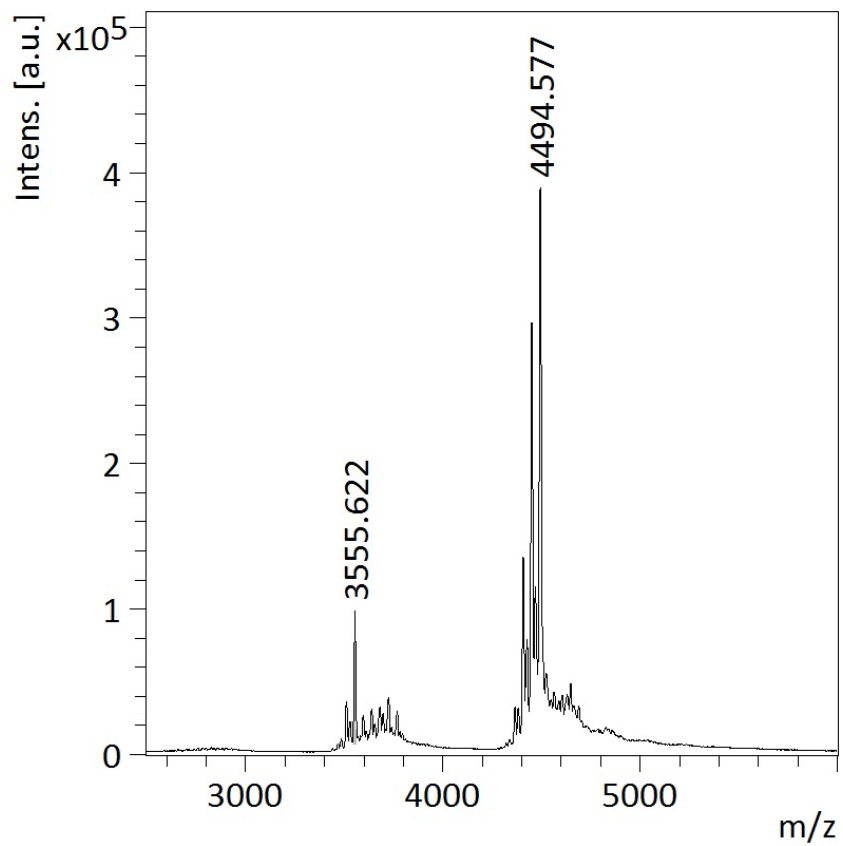


Fig. S19 MALDI-TOF MS spectra of **L5**

Fitter: UV 1:1 Fit Summary Save

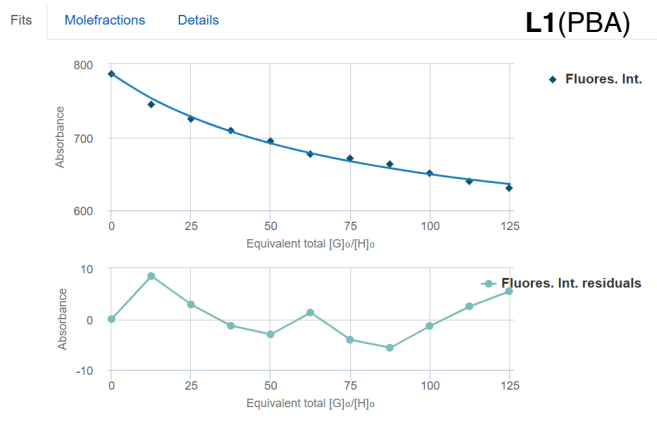
Details

Time to fit: 0.1185 s
 SSR: 178.4639
 Fitted datapoints: 11
 Fitted params: 2

Parameters

Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	63043.63 M ⁻¹	± 6.0849 %	10000.00 M ⁻¹

Back Next



Fitter: UV 1:1 Fit Summary Save

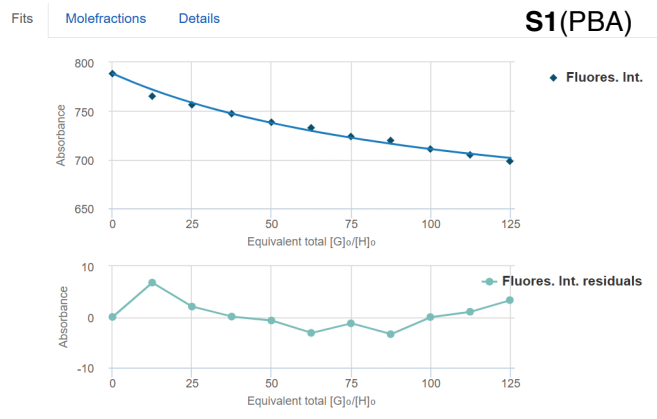
Details

Time to fit: 0.1213 s
 SSR: 85.3308
 Fitted datapoints: 11
 Fitted params: 2

Parameters

Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	44644.13 M ⁻¹	± 6.5820 %	10000.00 M ⁻¹

Back Next



Fitter: UV 1:1 Fit Summary Save

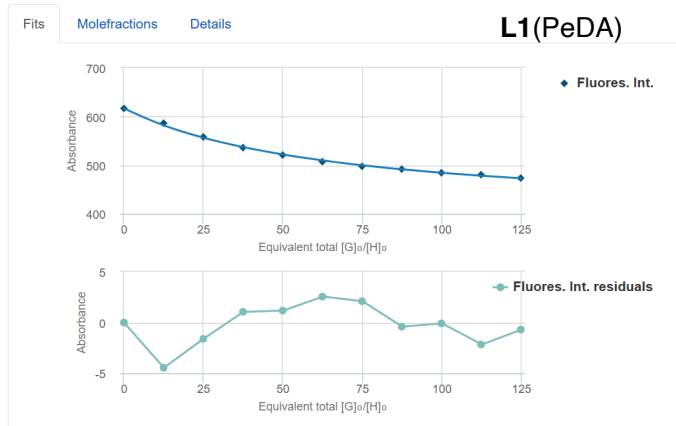
Details

Time to fit: 0.1220 s
 SSR: 41.0400
 Fitted datapoints: 11
 Fitted params: 2

Parameters

Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	76856.43 M ⁻¹	± 3.2679 %	10000.00 M ⁻¹

Back Next



Fitter: UV 1:1 Fit Summary Save

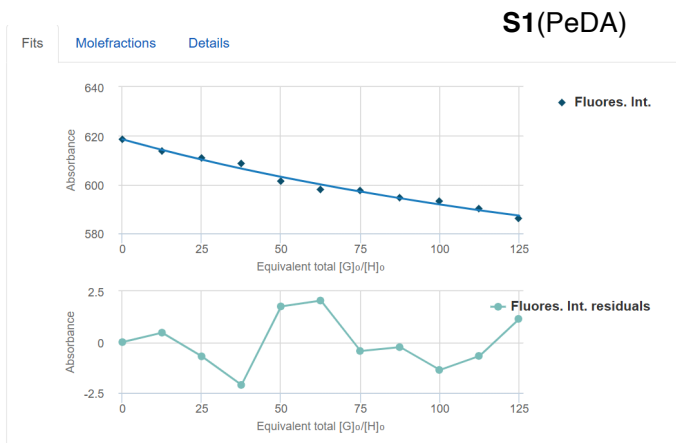
Details

Time to fit: 0.1169 s
 SSR: 16.2641
 Fitted datapoints: 11
 Fitted params: 2

Parameters

Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	18145.66 M ⁻¹	± 6.4854 %	10000.00 M ⁻¹

Back Next



Fitter: UV 1:1 Fit Summary Save

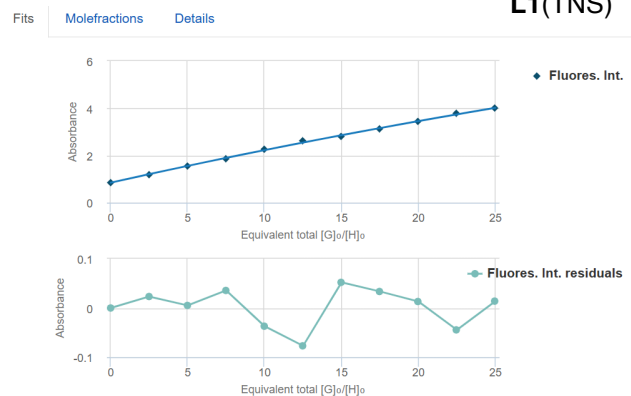
Details

Time to fit: 0.1214 s
 SSR: 1.5267e-2
 Fitted datapoints: 11
 Fitted params: 2

Parameters

Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	6172.46 M ⁻¹	± 1.7303 %	10000.00 M ⁻¹

Back Next



Fitter: UV 1:1 Fit Summary Save

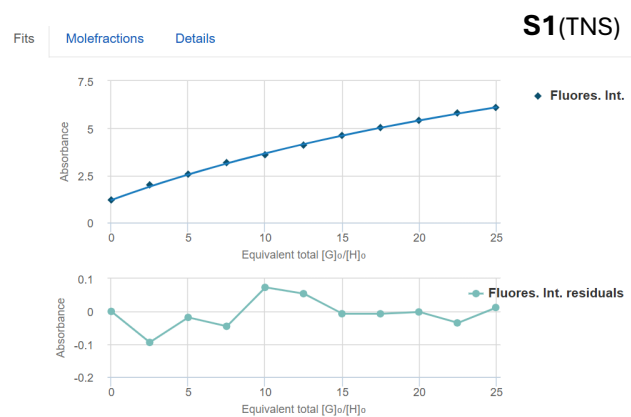
Details

Time to fit: 0.1203 s
 SSR: 2.1074e-2
 Fitted datapoints: 11
 Fitted params: 2

Parameters

Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	21391.35 M ⁻¹	± 1.5460 %	10000.00 M ⁻¹

Back Next



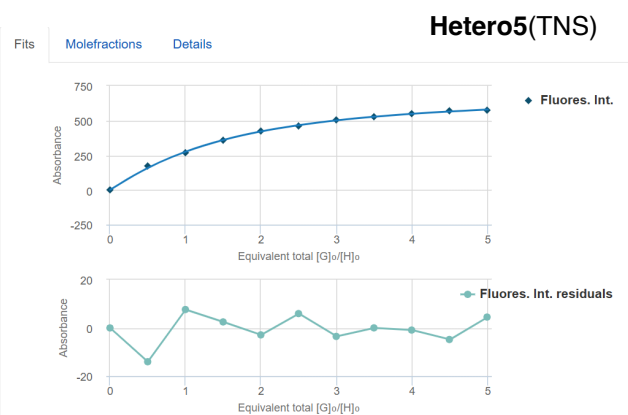
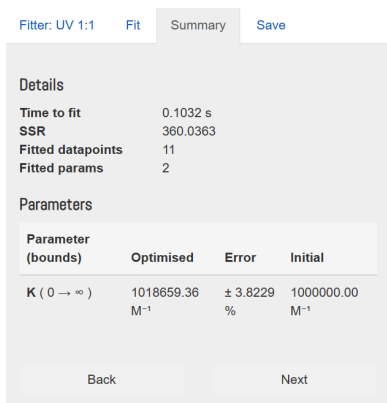
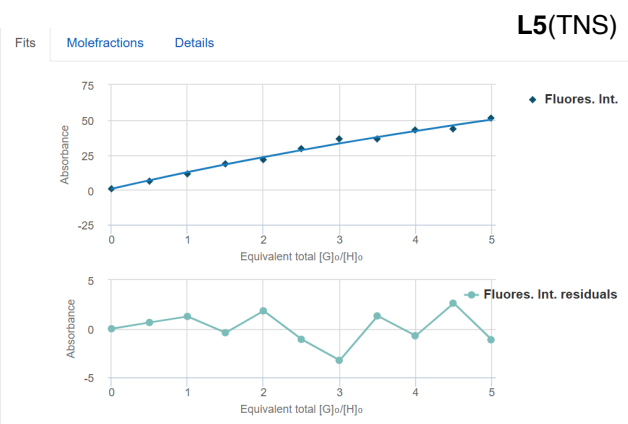
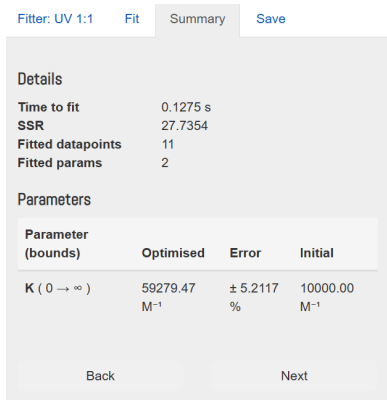


Fig. S22 Fitting of fluorescence titration data of each host with TNS into 1:1 host-guest model in BindFit software. Screenshots taken from the website supramolecular.org.

Fitter: UV 1:1 Fit Summary Save

Details

Time to fit 0.1222 s
 SSR 1.3817e-7
 Fitted datapoints 11
 Fitted params 2

Parameters

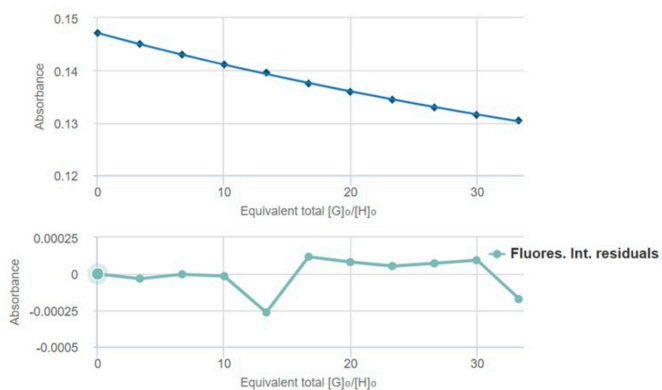
Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	301.58 M ⁻¹	± 1.0485 %	100.00 M ⁻¹

Back

Next

L1(C-Dab)

Fits Molefractions Details



Fitter: UV 1:1 Fit Summary Save

Details

Time to fit 0.1297 s
 SSR 2.8240e-7
 Fitted datapoints 11
 Fitted params 2

Parameters

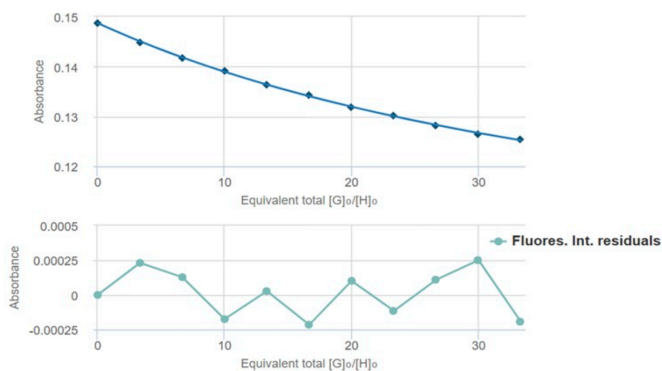
Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	673.53 M ⁻¹	± 1.2375 %	100.00 M ⁻¹

Back

Next

S1(C-Dab)

Fits Molefractions Details



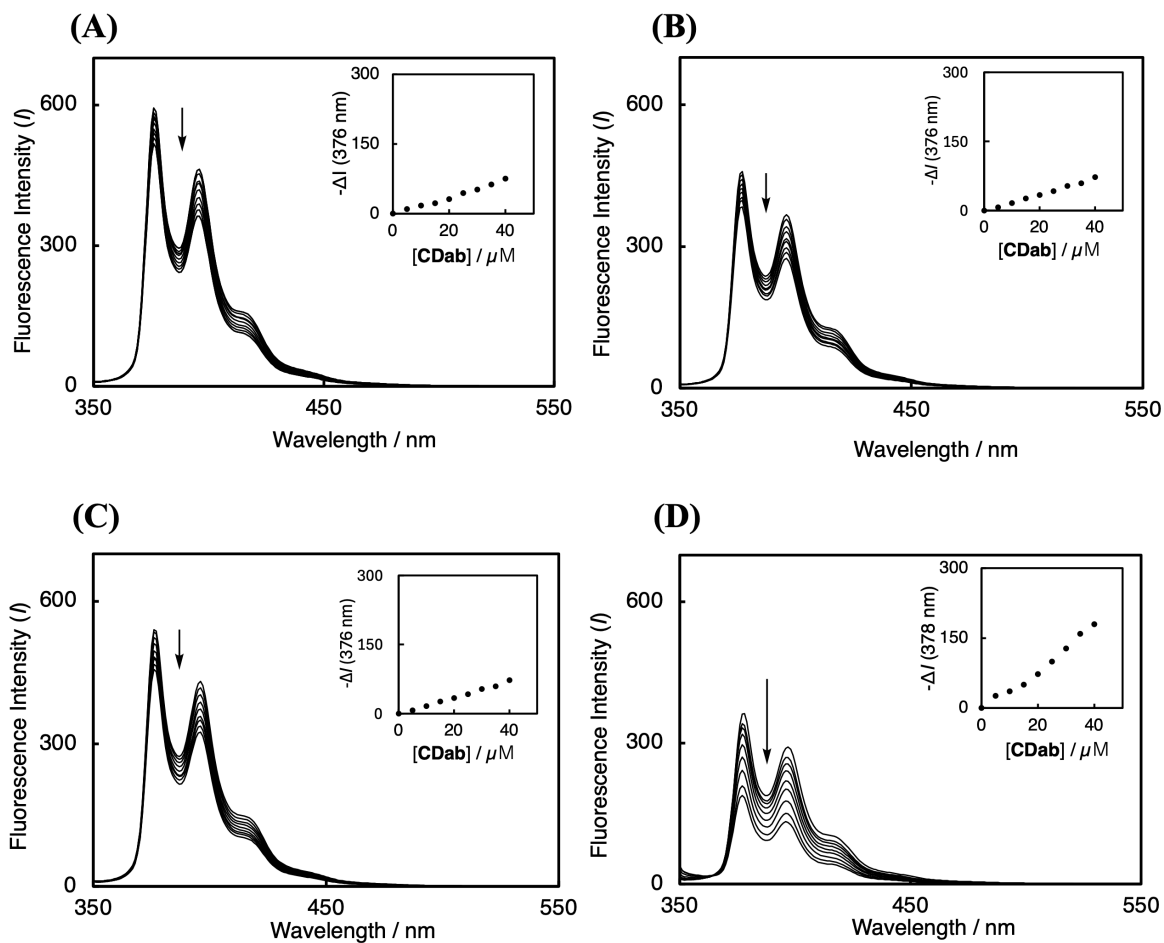


Fig. S24 Fluorescence spectral changes of PBA (0.5 μM) upon the addition of CDab in the (A) absence and presence of (B) L1 (50 μM), (C) S1 (50 μM) and (D) L5 (10 μM) in aqueous HEPES buffer (0.01 M, pH 7.4, 0.15 M with NaCl) at 298K. The corresponding titration curves. Ex 341 nm.