Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

New Journal of Chemistry

Hybrid[4]arenes with anthracene units and tuneable cavities

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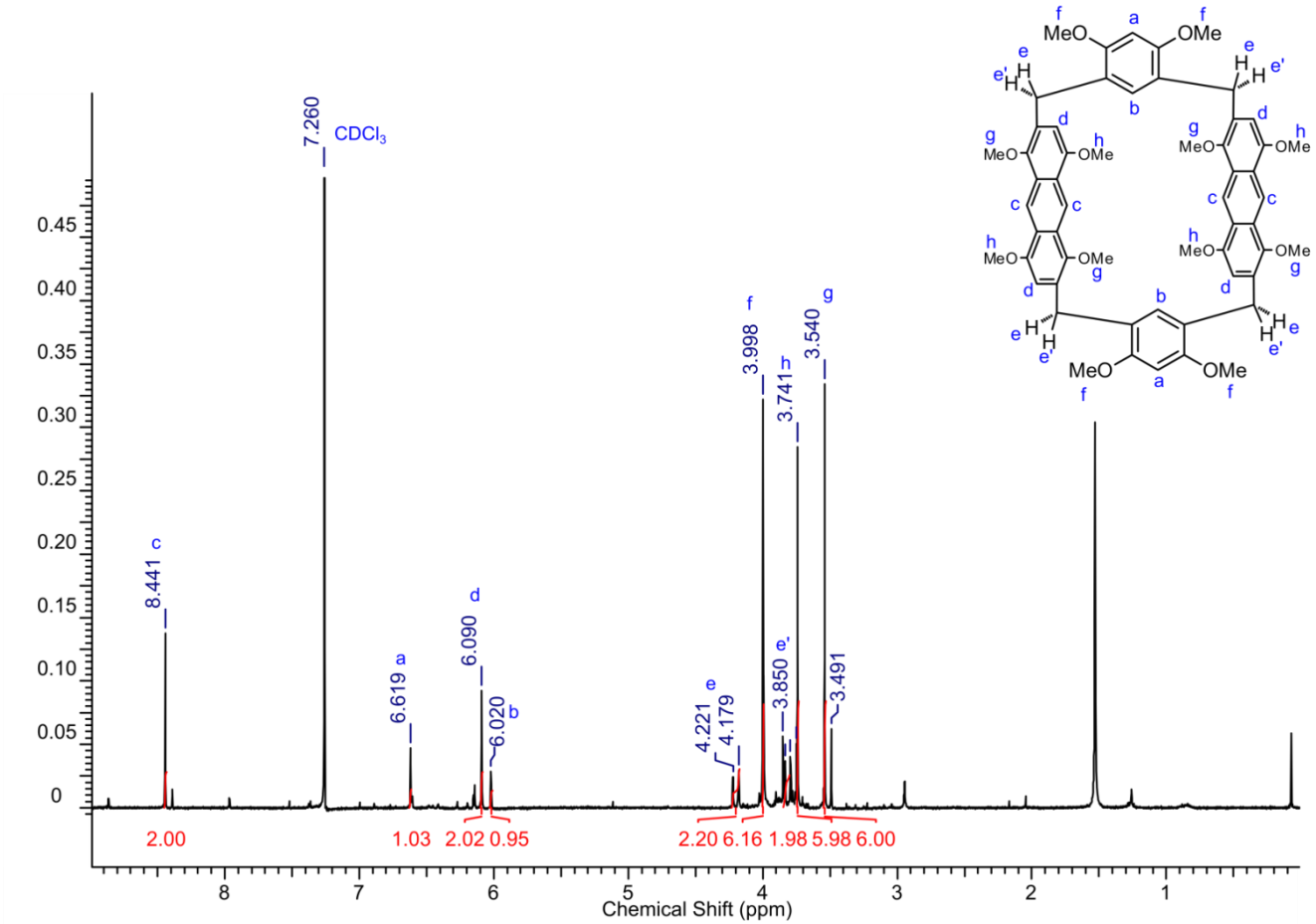


Figure 1: ^{1}H NMR spectrum of **4** ($CDCl_3$, 400MHz, 303K).

^{1}H NMR ($CDCl_3$, 400MHz, 303K): 8.44 (2H, s), 6.62 (1H, s), 6.09 (2H, s), 6.02 (2H,s), 4.20 (2H, d, J^2 = 16.1 Hz), 4.00 (6H, s), 3.83 (2H, d, J^2 = 16.1 Hz), 3.74 (6H, s), 3.54 (6H, s)

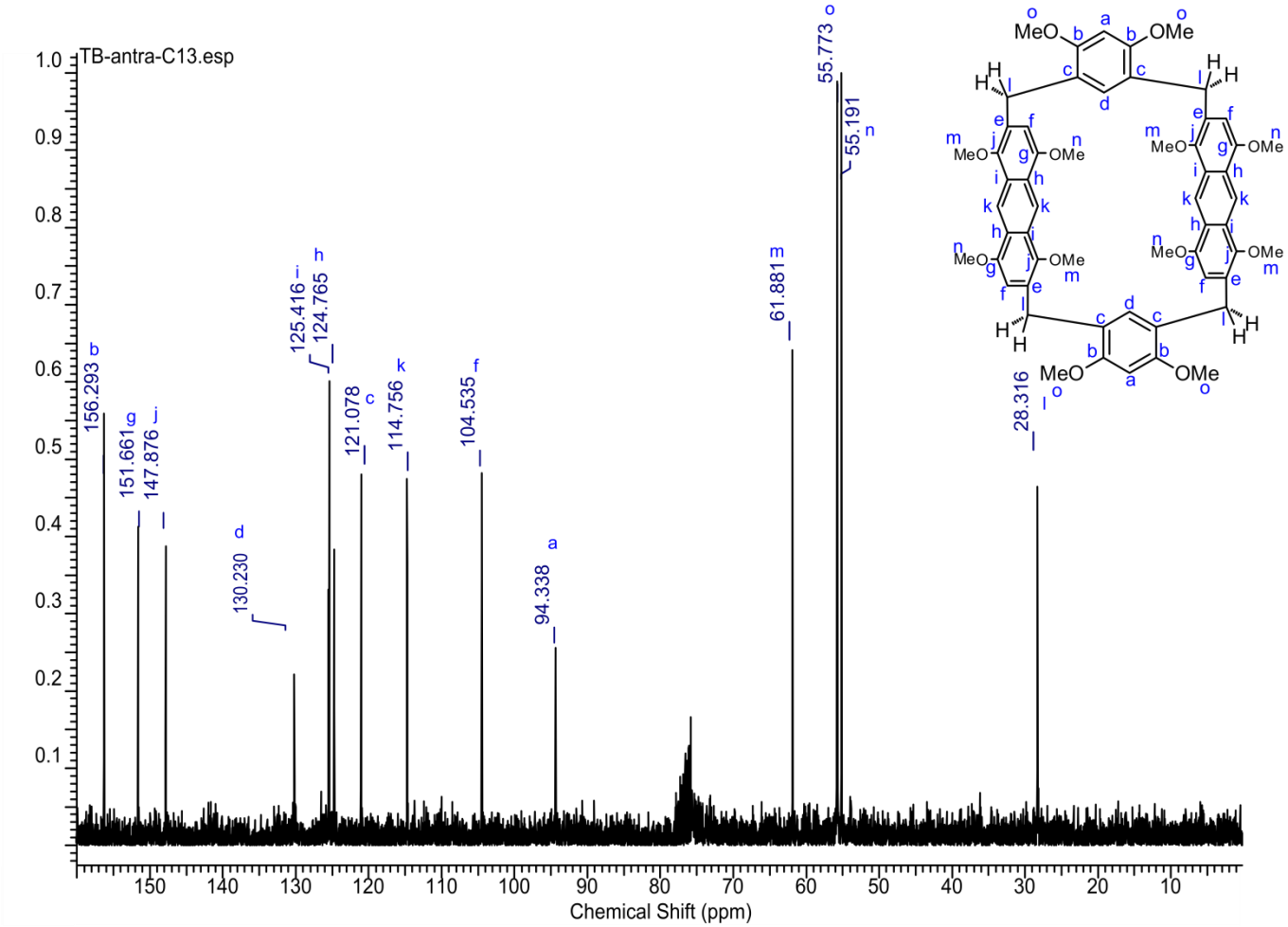


Figure 2: ^{13}C NMR spectrum of **3** ($CDCl_3$, 125MHz, 303K).

^{13}C NMR ($CDCl_3$, 125MHz, 303K): 156.3, 151.7, 147.9, 130.2, 125.4, 124.8, 121.1, 114.8, 104.5, 61.9, 55.8, 55.2, 28.3

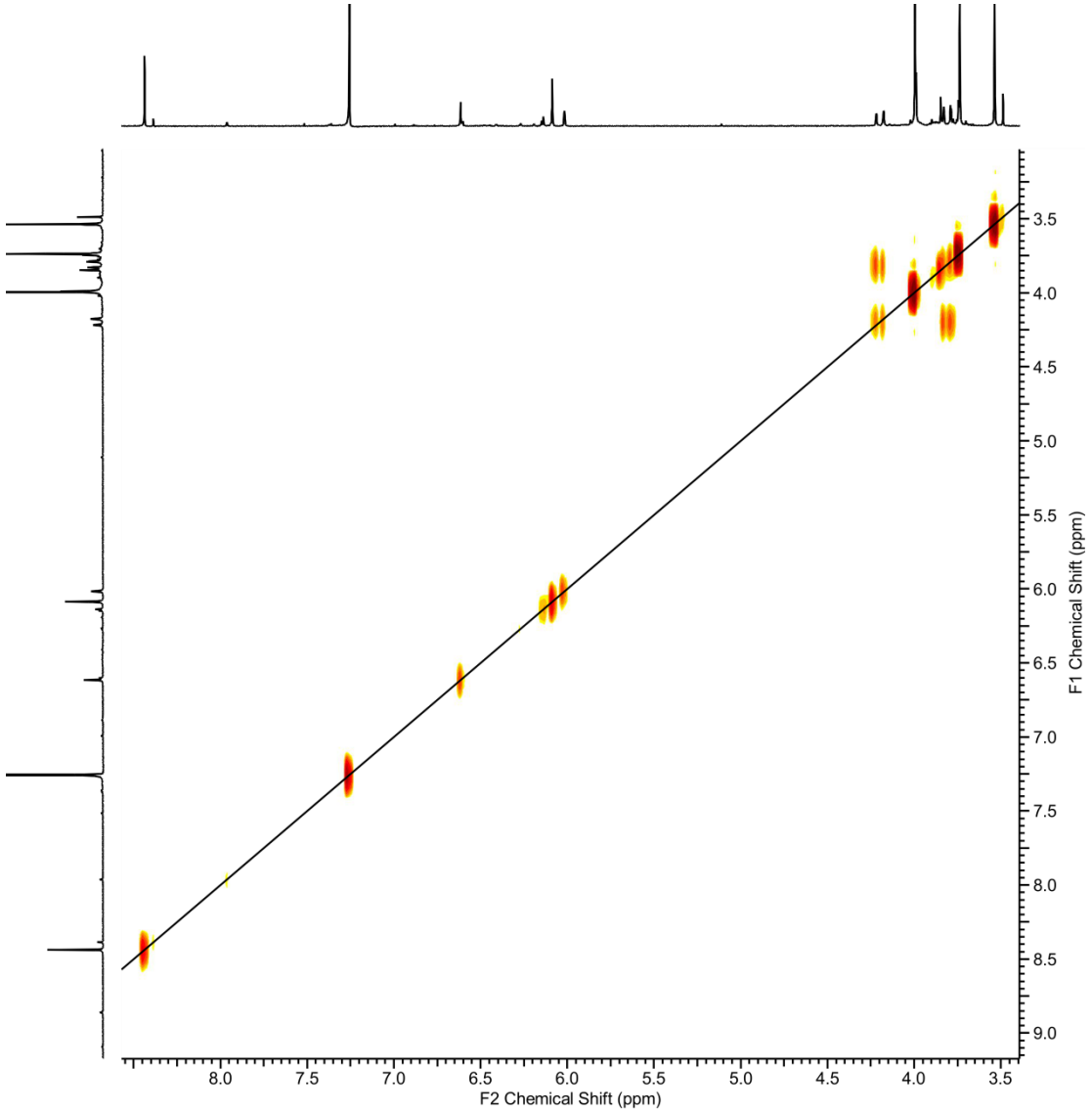


Figure 3: ^{1}H-^{1}H COSY spectrum of **3** ($CDCl_3$, 400MHz, 303K).

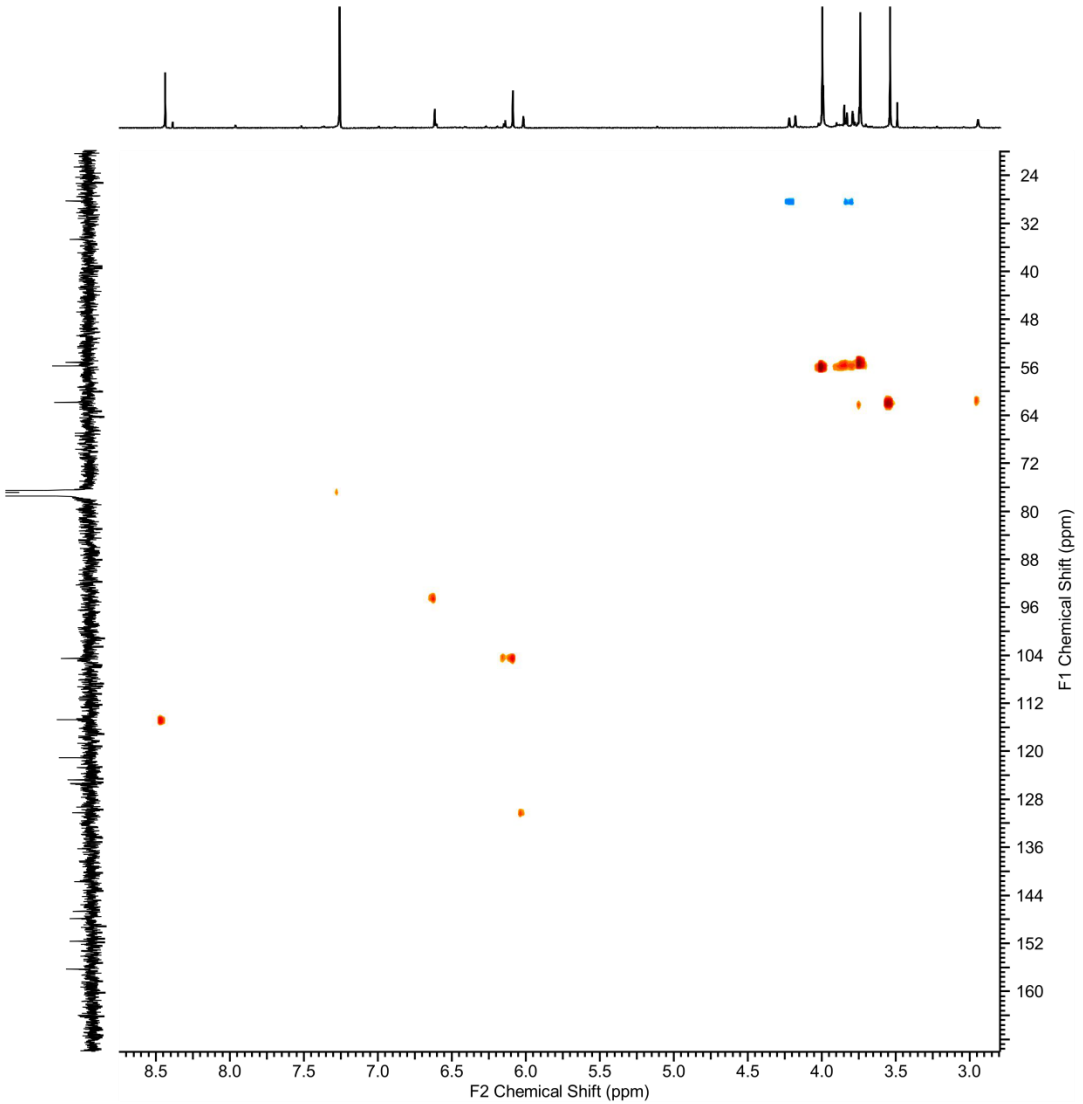


Figure 4: ^{1}H-^{13}C HSQC NMR spectrum of **3** ($CDCl_3$, 400MHz, 303K).

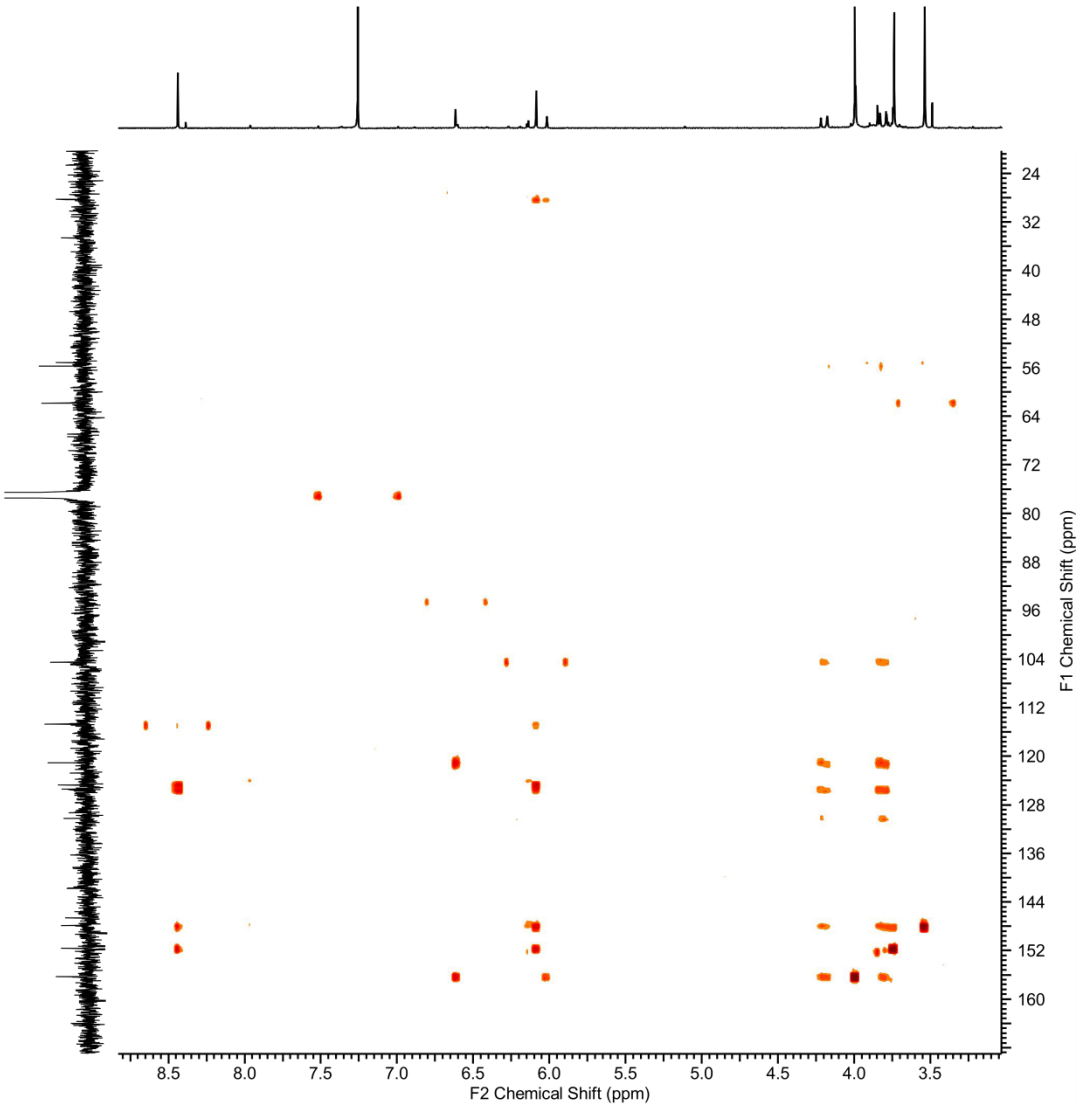


Figure 5: ^{1}H-^{13}C HMBC NMR spectrum of **3** ($CDCl_3$, 400MHz, 303K).

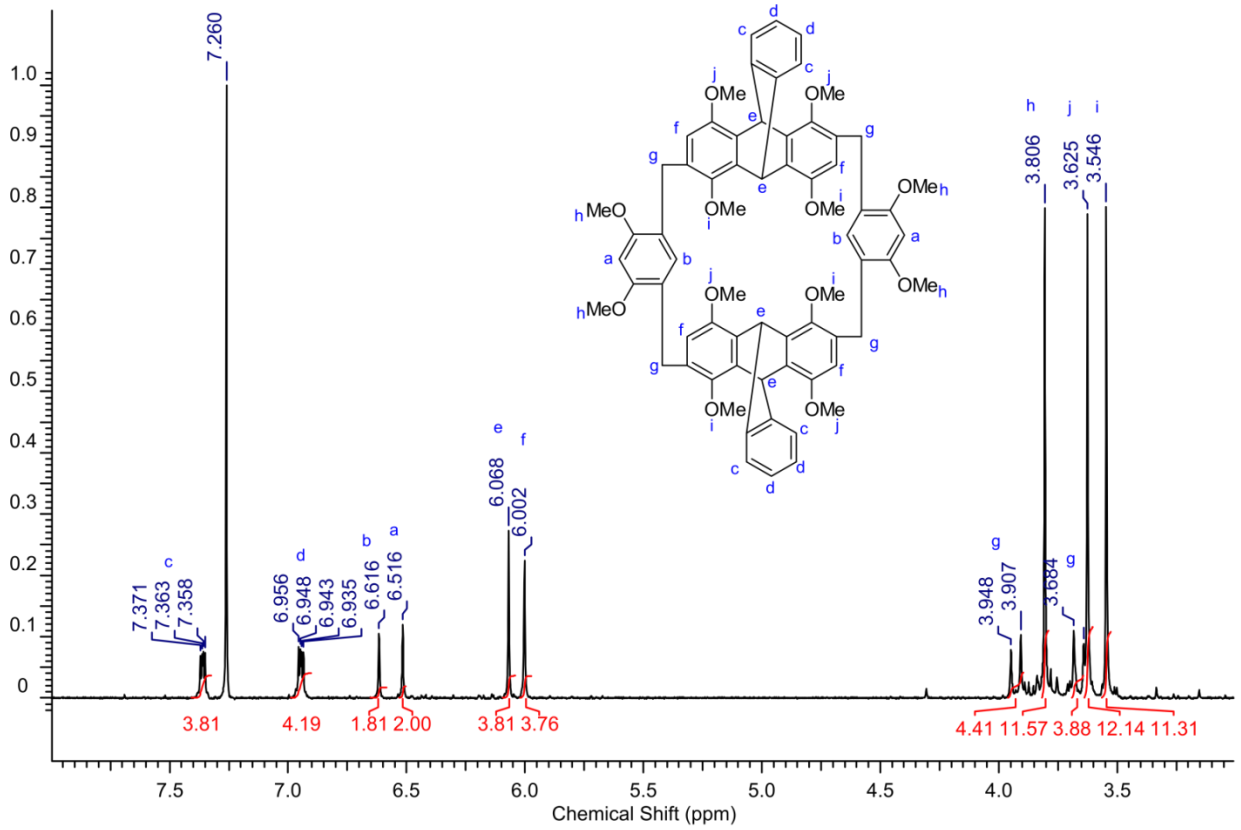


Figure 6: ^{1}H NMR spectrum of **5** ($CDCl_3$, 400MHz, 303K).

^{1}H NMR ($CDCl_3$, 400MHz, 303K): 7.33 (dd, 4H, J^3 = 5.4 Hz, J^4 = 3.2 Hz), 6.95 (dd, 4H, J^3=5.4 Hz, J^4= 3.2 Hz), 6.62 (s, 2H), 6.52 (s, 2H), 6.07 (s, 4H), 6.00 (s, 4H), 3.93 (d, 4H, J^2 = 16.6 Hz), 3.81 (s, 12H) 3.66 (d, 4H, J^2 = 16.6 Hz) 3.63 (s, 12H), 3.55 (s, 12H)

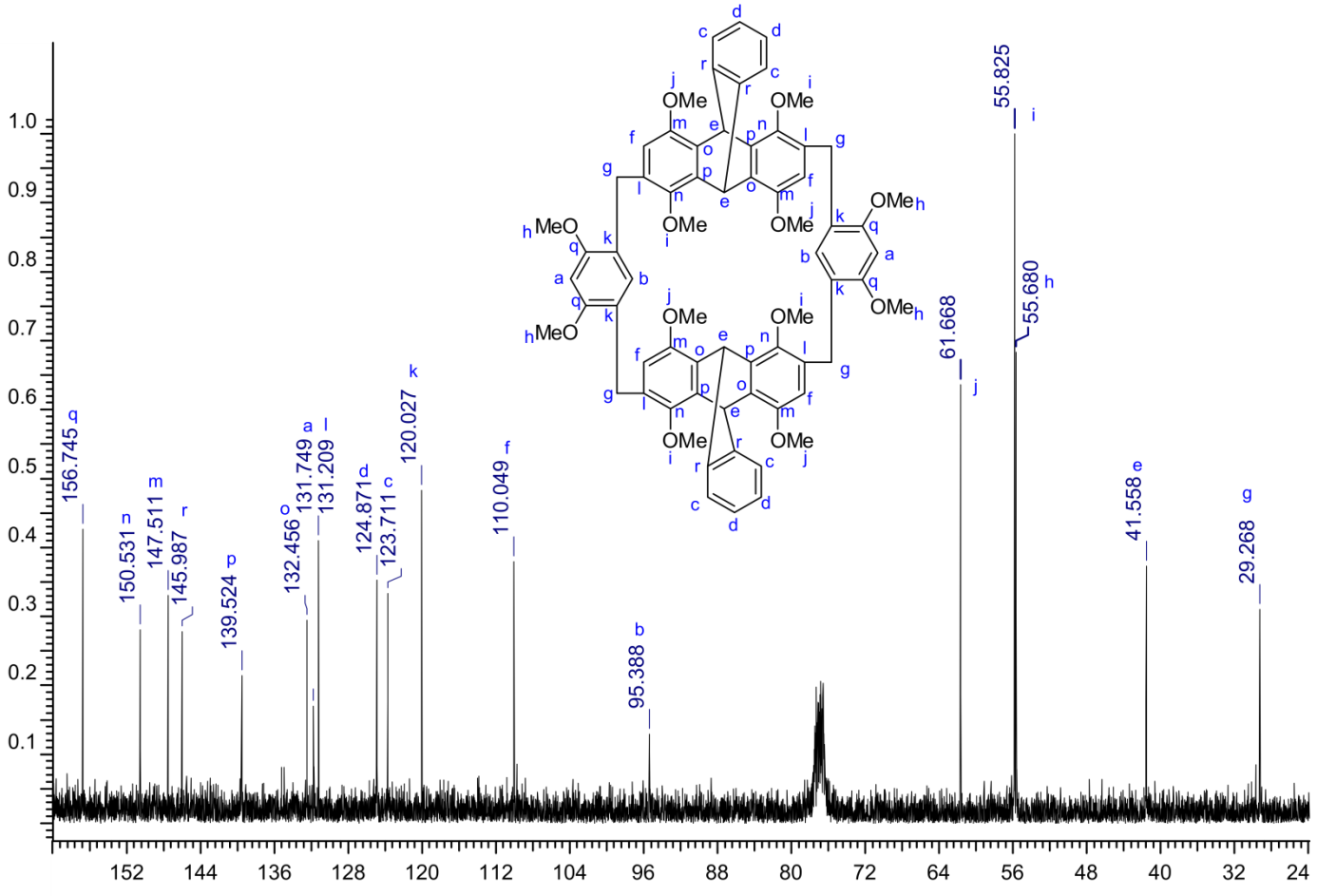


Figure 7: ^{13}C NMR spectrum of **5** ($CDCl_3$, 100MHz, 303K).

^{13}C NMR ($CDCl_3$, 100MHz, 303K): 156.7, 150.5, 147.5, 146.0, 139.5, 132.5, 131.7, 131.2, 124.9, 123.7, 120.0, 110.0, 95.4, 61.7, 55.8, 55.7, 41.6, 29.3

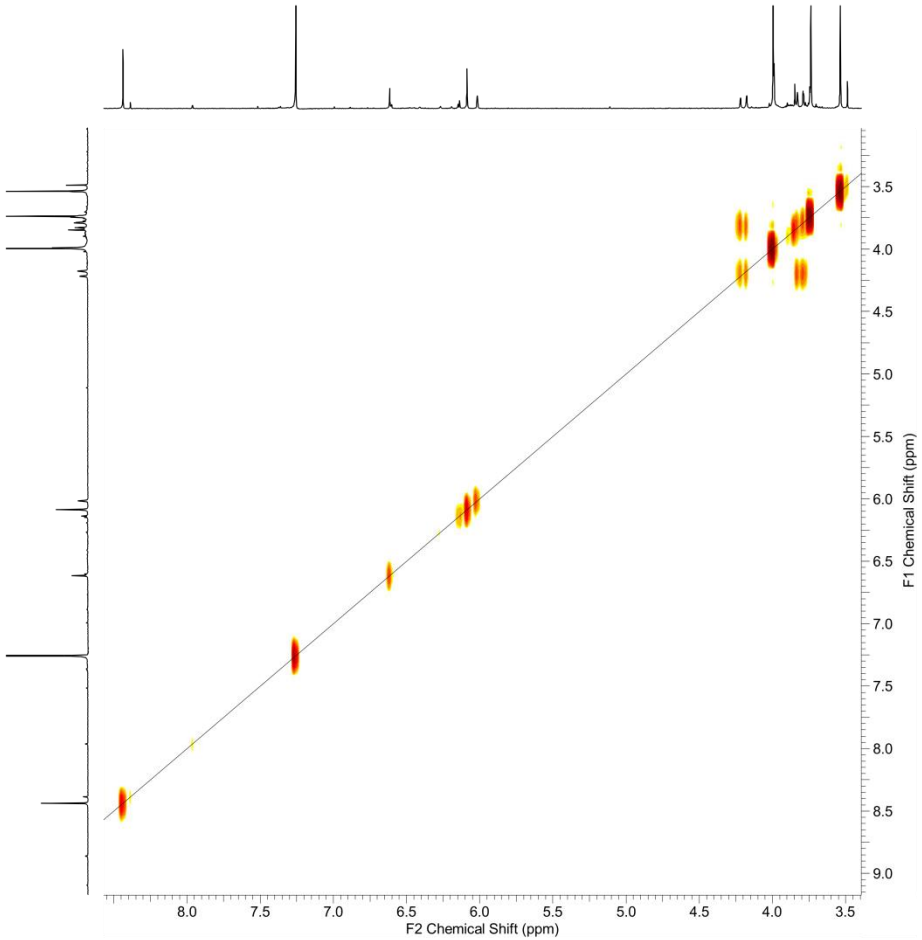


Figure 8: ^{1}H-^{1}H COSY spectrum of **5** ($CDCl_3$, 400MHz, 303K).

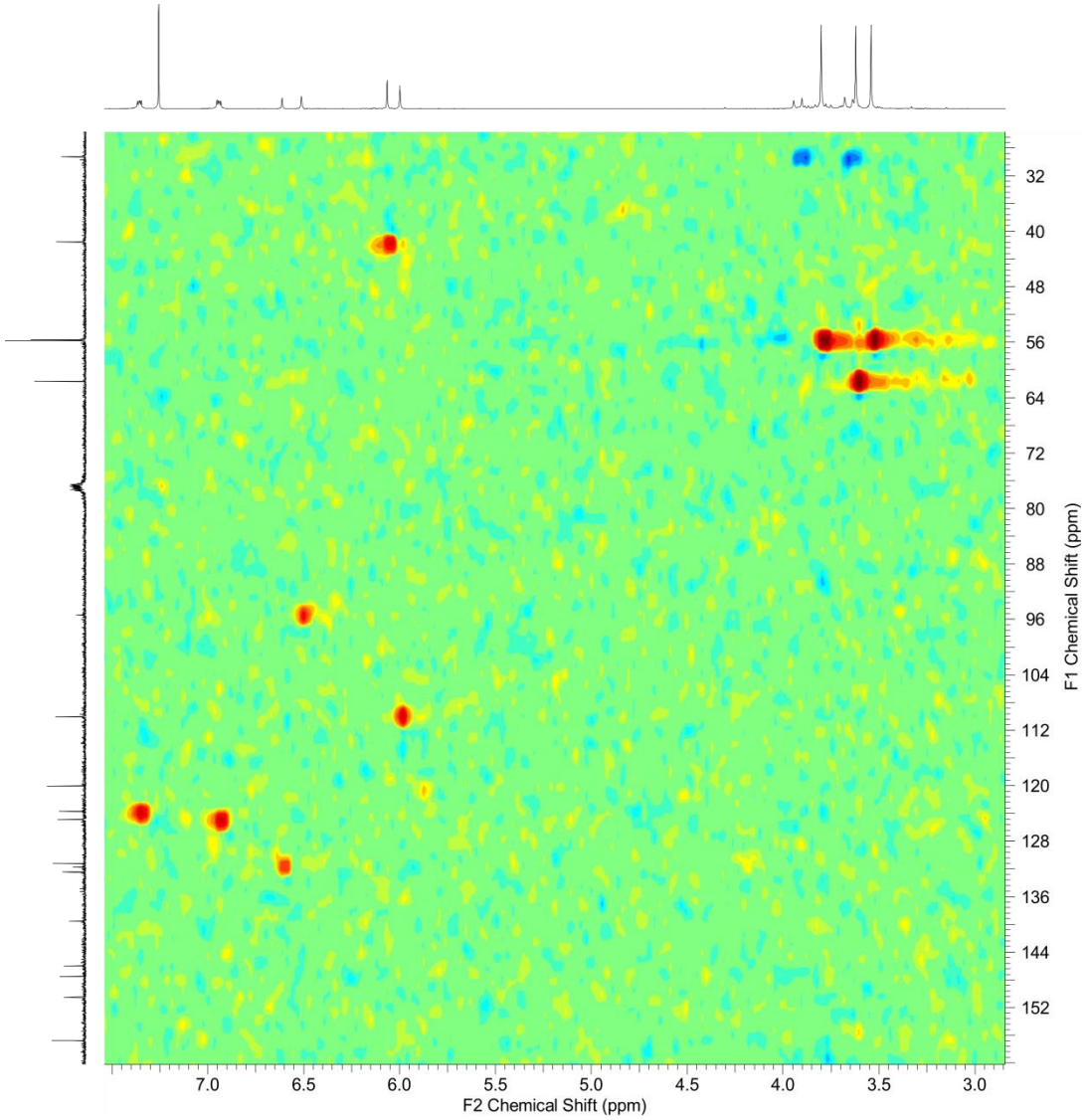


Figure 9: ^{1}H-^{13}C HSQC NMR spectrum of **5** ($CDCl_3$, 400MHz, 303K).

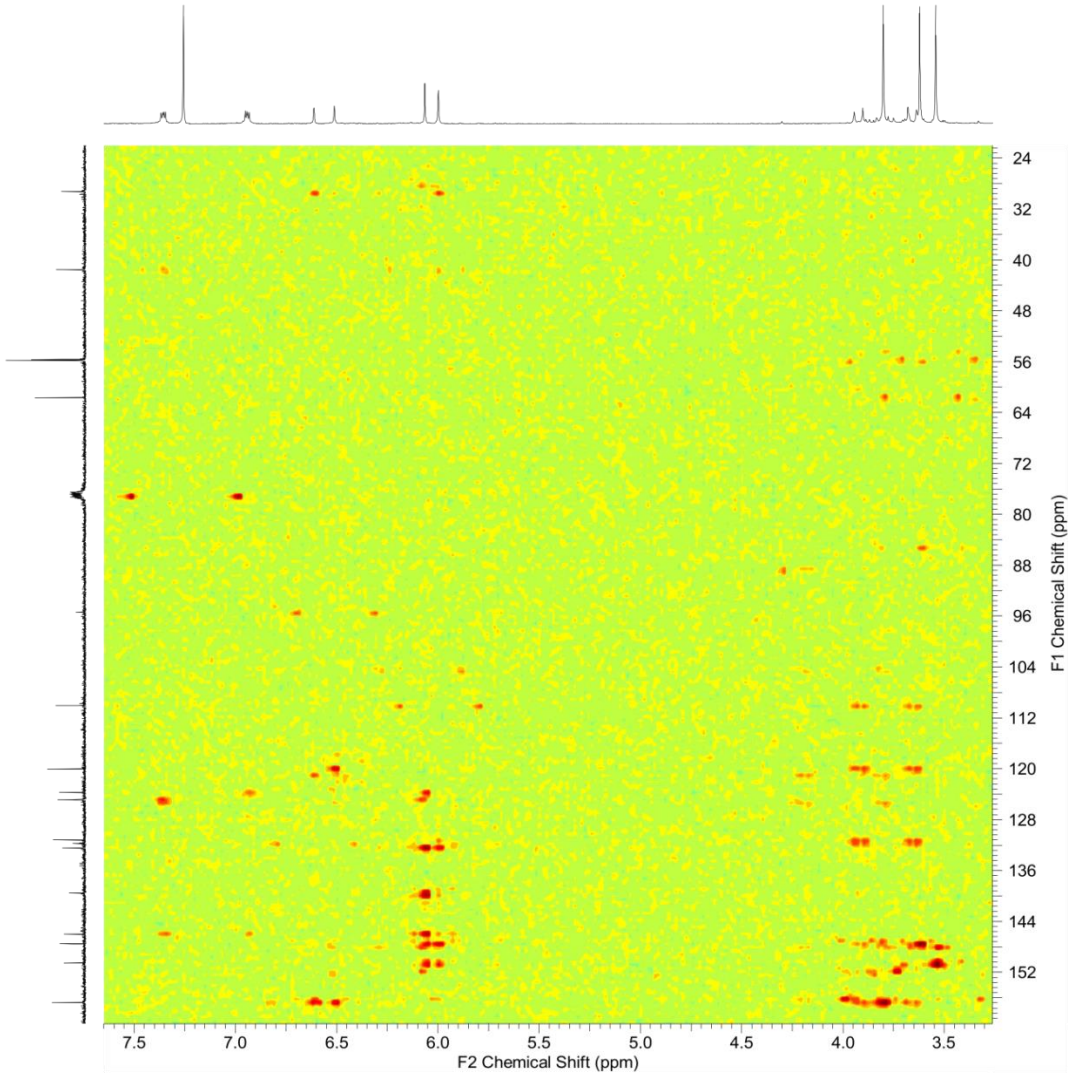
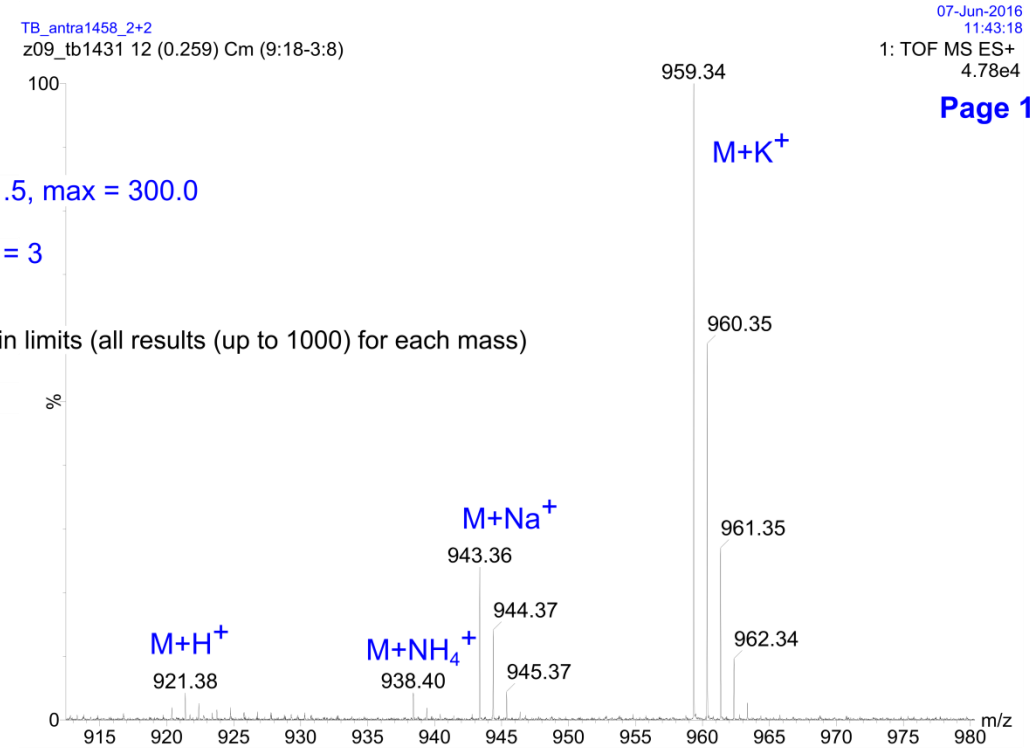


Figure 10: ^{1}H-^{13}C HMBC NMR spectrum of **5** ($CDCl_3$, 400MHz, 303K).



Elemental Composition Report **Page 1**

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 300.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
285 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-120 O: 0-13 Na: 0-1

Minimum:				-1.5				
Maximum:		20.0	5.0	300.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
943.3665	943.3669	-0.4	-0.4	28.5	439.1	0.020	98.01	C56 H56 O12 Na
	943.3694	-2.9	-3.1	31.5	443.0	3.940	1.94	C58 H55 O12
	943.3635	3.0	3.2	40.5	446.7	7.674	0.05	C65 H51 O7

Figure 11: HR MS of **3**.

Elemental Composition Report **Page 1**

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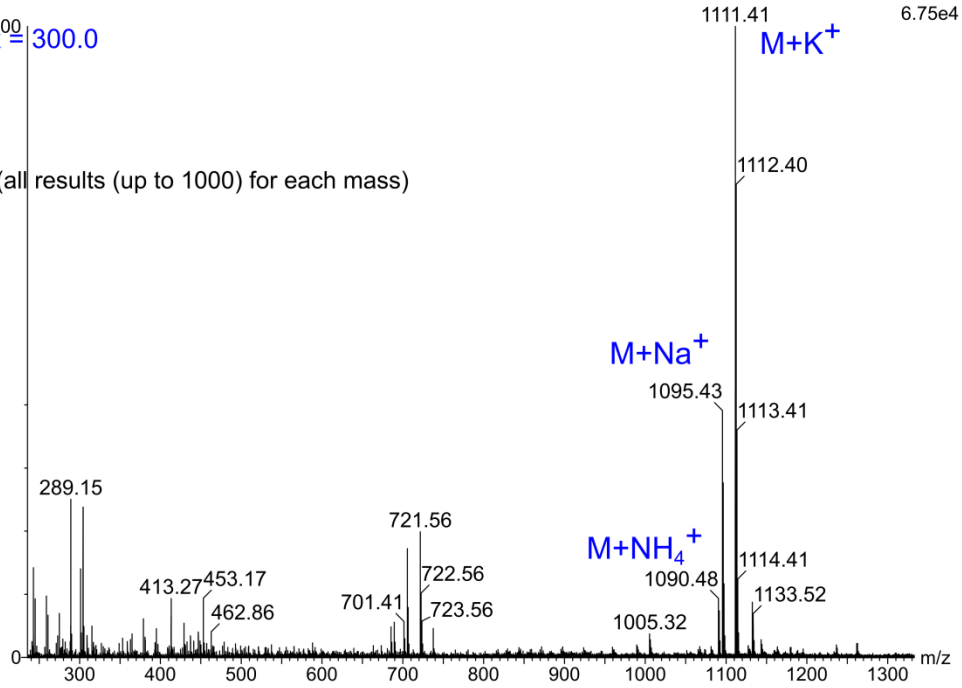
Single Mass Analysis

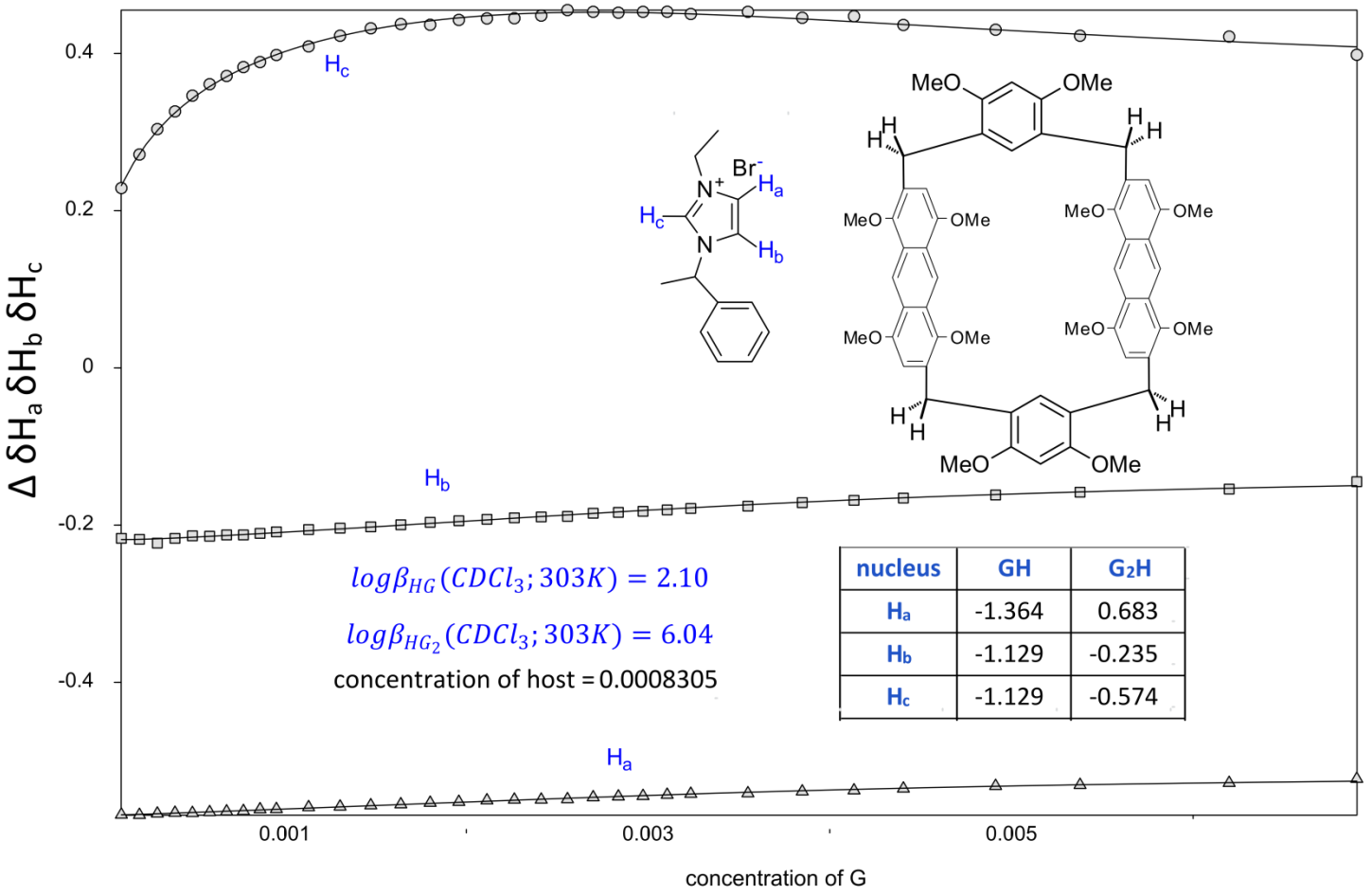
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 300.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
332 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-200 O: 0-12 Na: 0-1



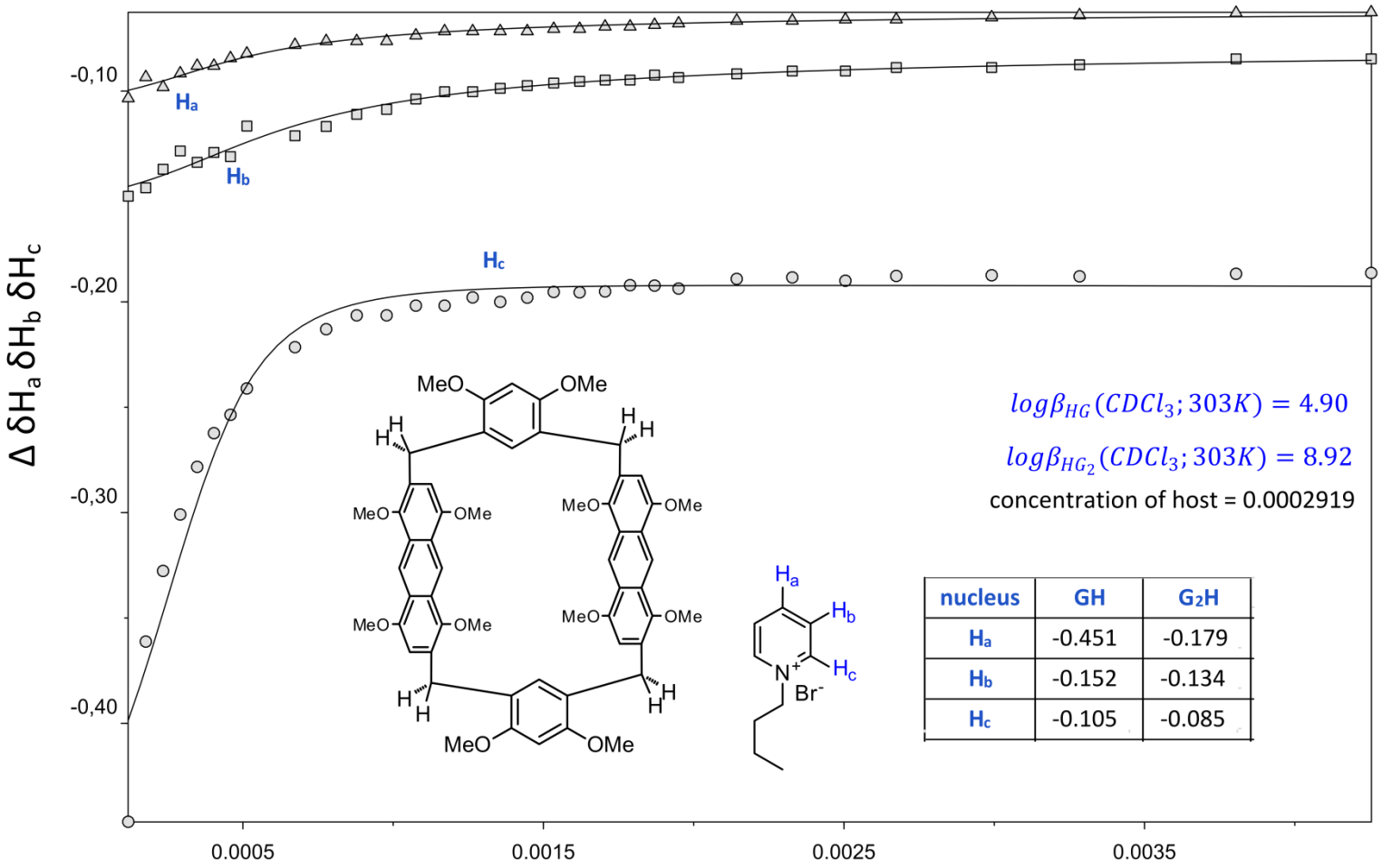
Minimum:				-1.5				
Maximum:		10.0	3.0	300.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
1095.4291	1095.4295	-0.4	-0.4	36.5	397.9	0.126	88.18	C68 H64 O12 Na
	1095.4320	-2.9	-2.6	39.5	399.9	2.143	11.73	C70 H63 O12
	1095.4261	3.0	2.7	48.5	404.8	7.044	0.09	C77 H59 O7

Figure 12: HR MS of **5**.



nucleus	GH	G₂H
H_a	-1.364	0.683
H_b	-1.129	-0.235
H_c	-1.129	-0.574

Figure 13: Complexation of *rac*-**6** by **3** in $CDCl_3$ (303K).



nucleus	GH	G_2H
H_a	-0.451	-0.179
H_b	-0.152	-0.134
H_c	-0.105	-0.085

Figure 14: Complexation of **7** by **3** in $CDCl_3$ (303K).

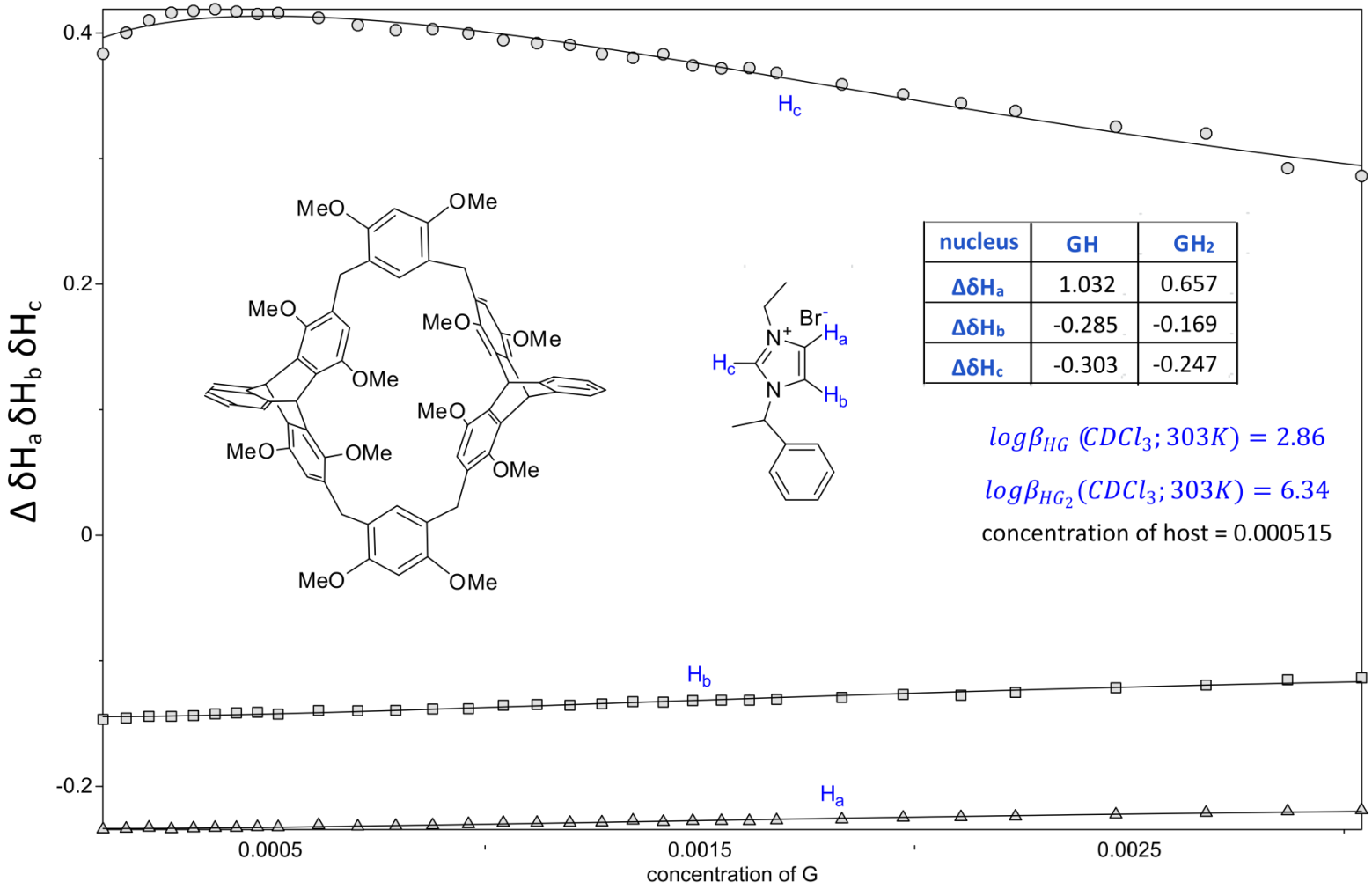
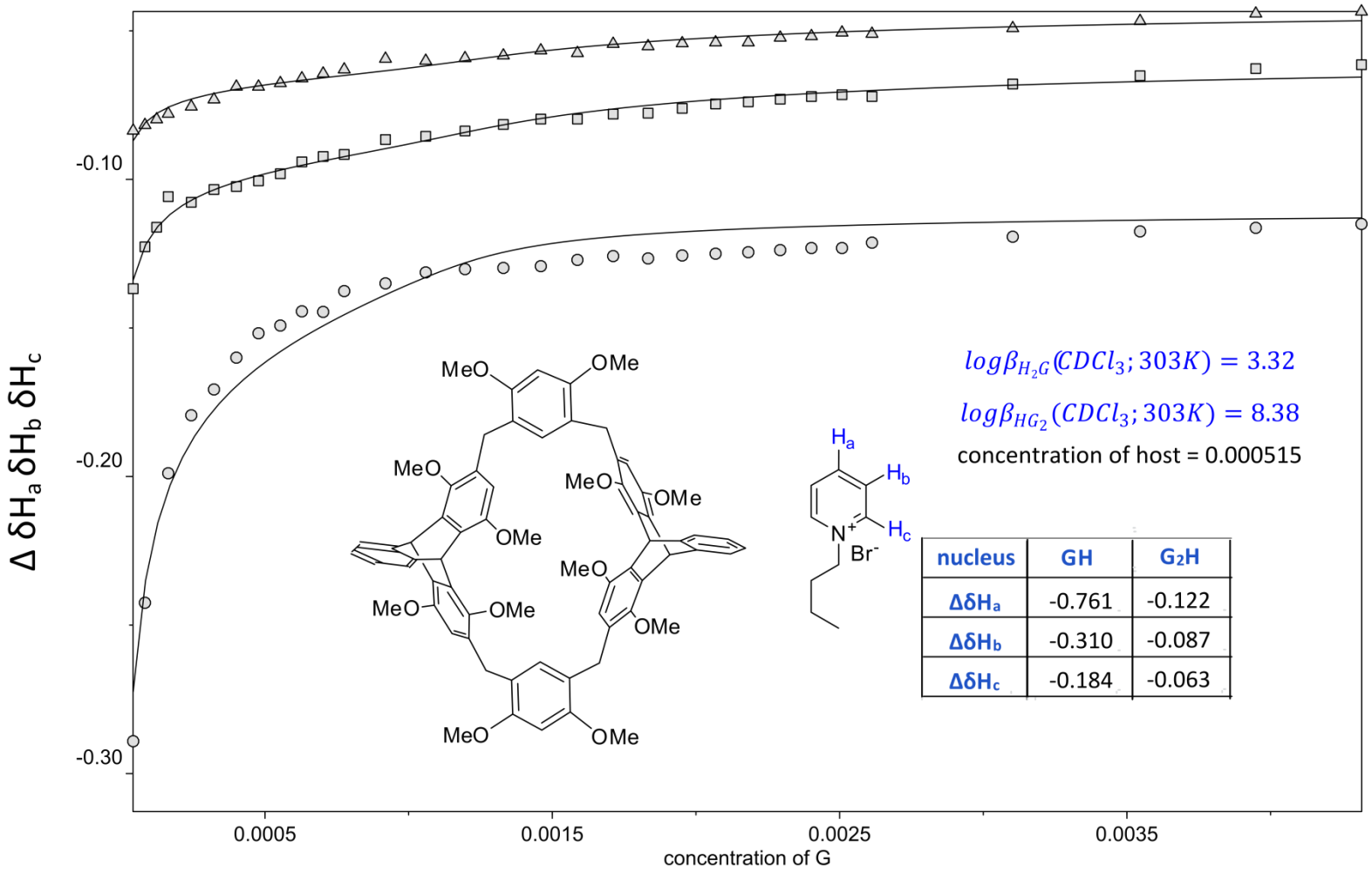


Figure 15: Complexation of *rac*-**6** by **5** in $CDCl_3$ (303K).



nucleus	GH	G$_2$H
ΔδH_a	-0.761	-0.122
ΔδH_b	-0.310	-0.087
ΔδH_c	-0.184	-0.063

Figure 16: Complexation of **7** by **5** in $CDCl_3$ (303K)

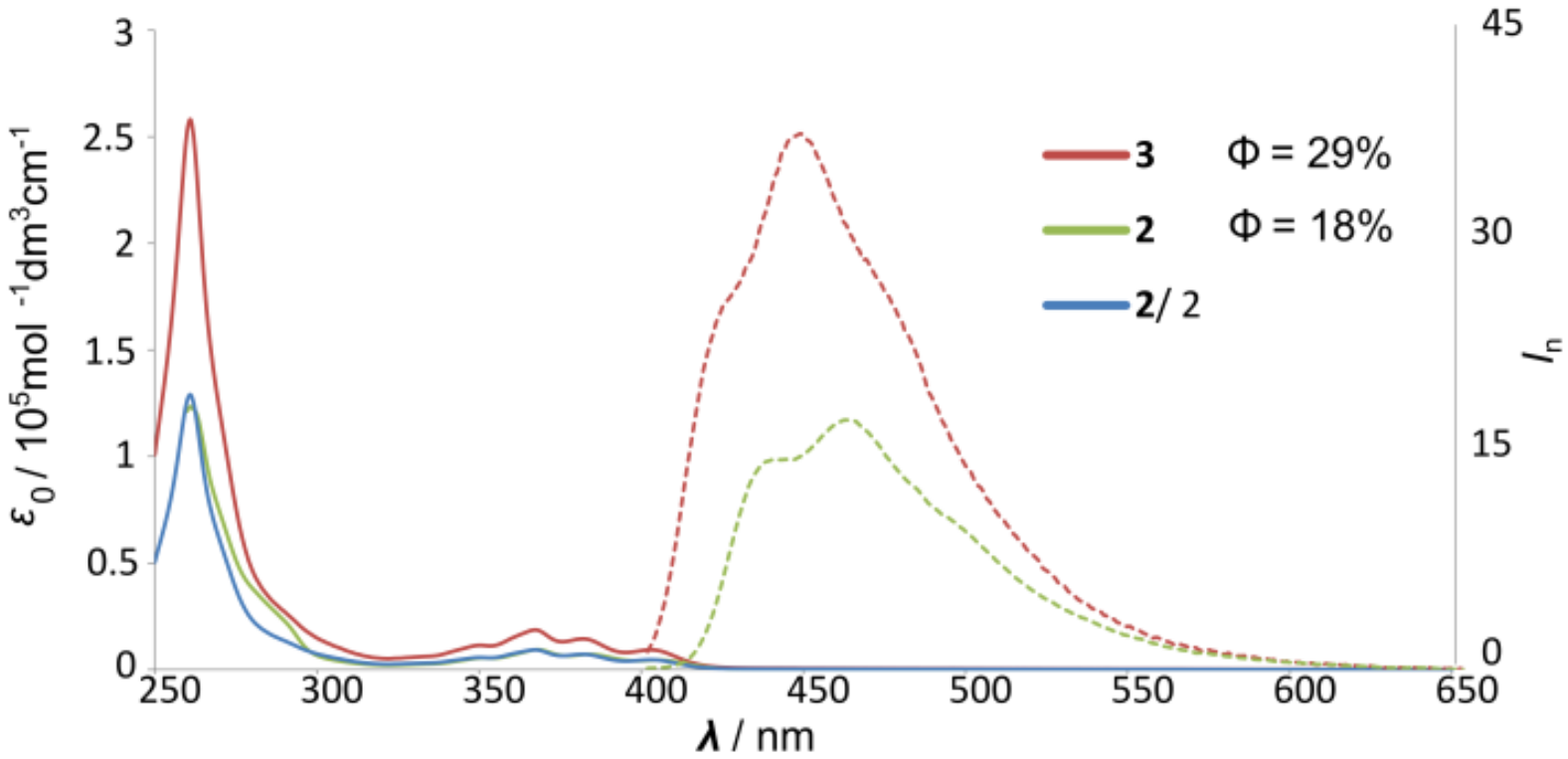


Figure 17: UV-Vis and fluorescence spectra of monomer **2** and macrocycle **3** in chloroform.

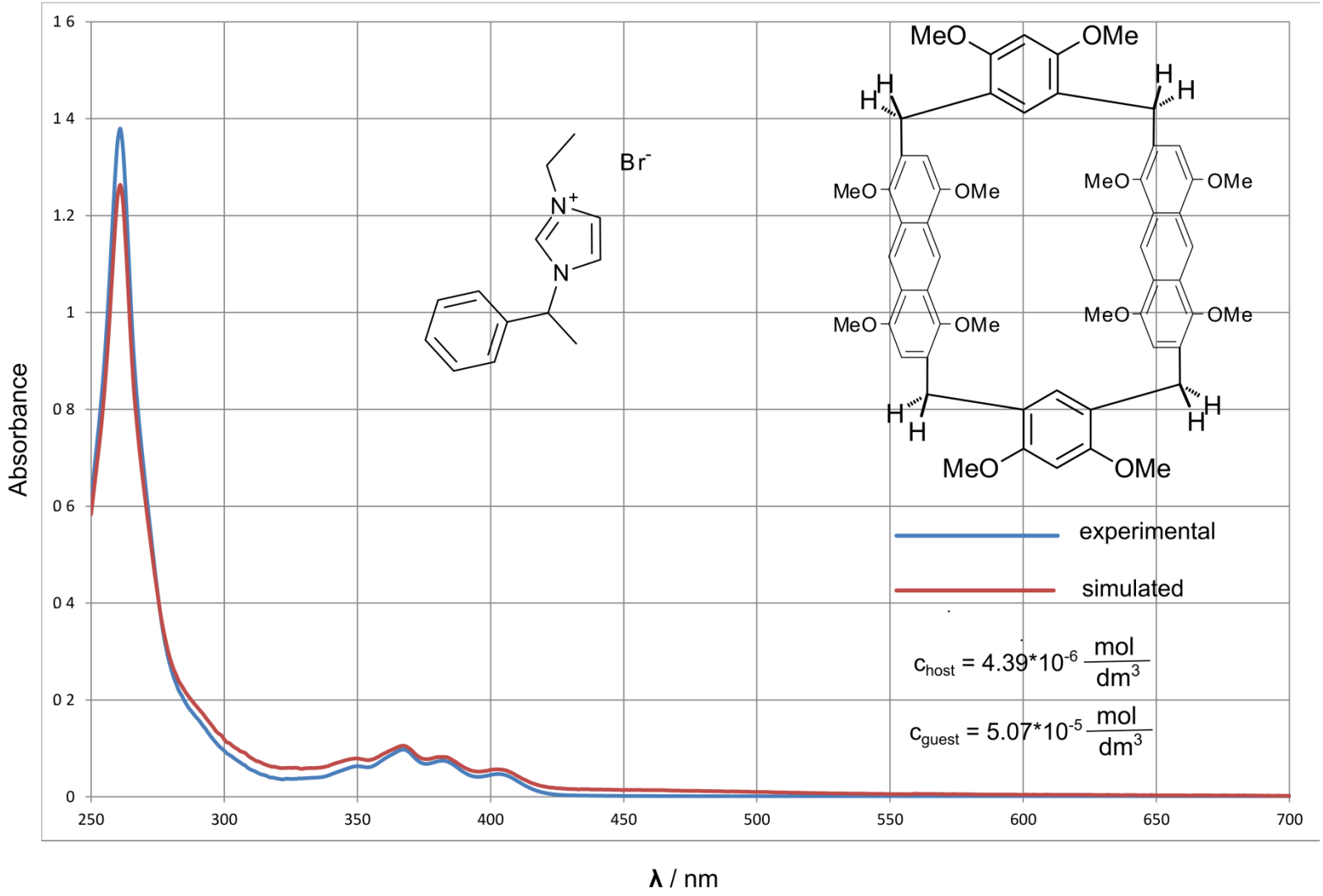


Figure 18: UV-vis spectra of **3** and *rac*-**6**.

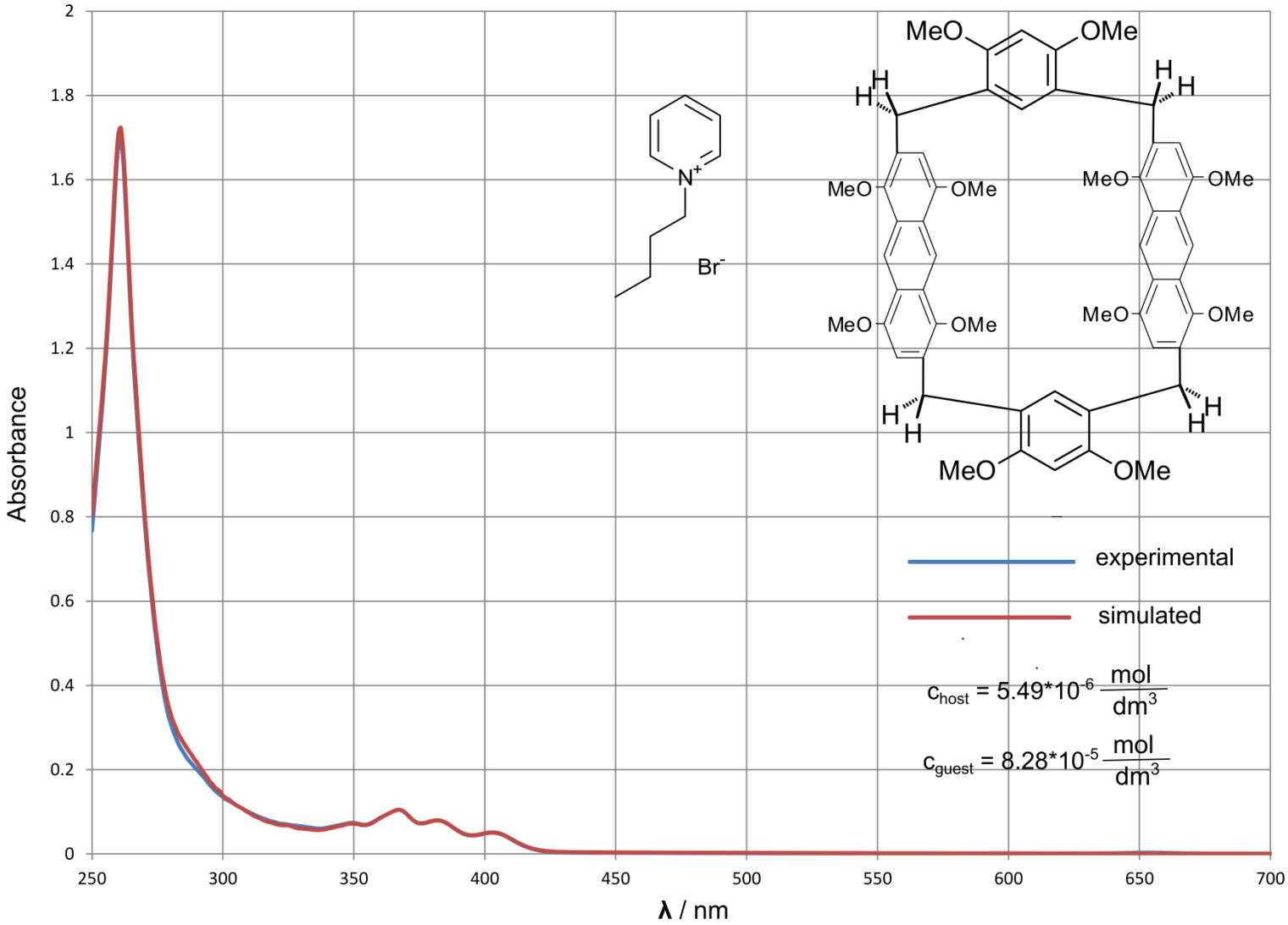


Figure 19: UV-Vis spectra of **3** and **7**.

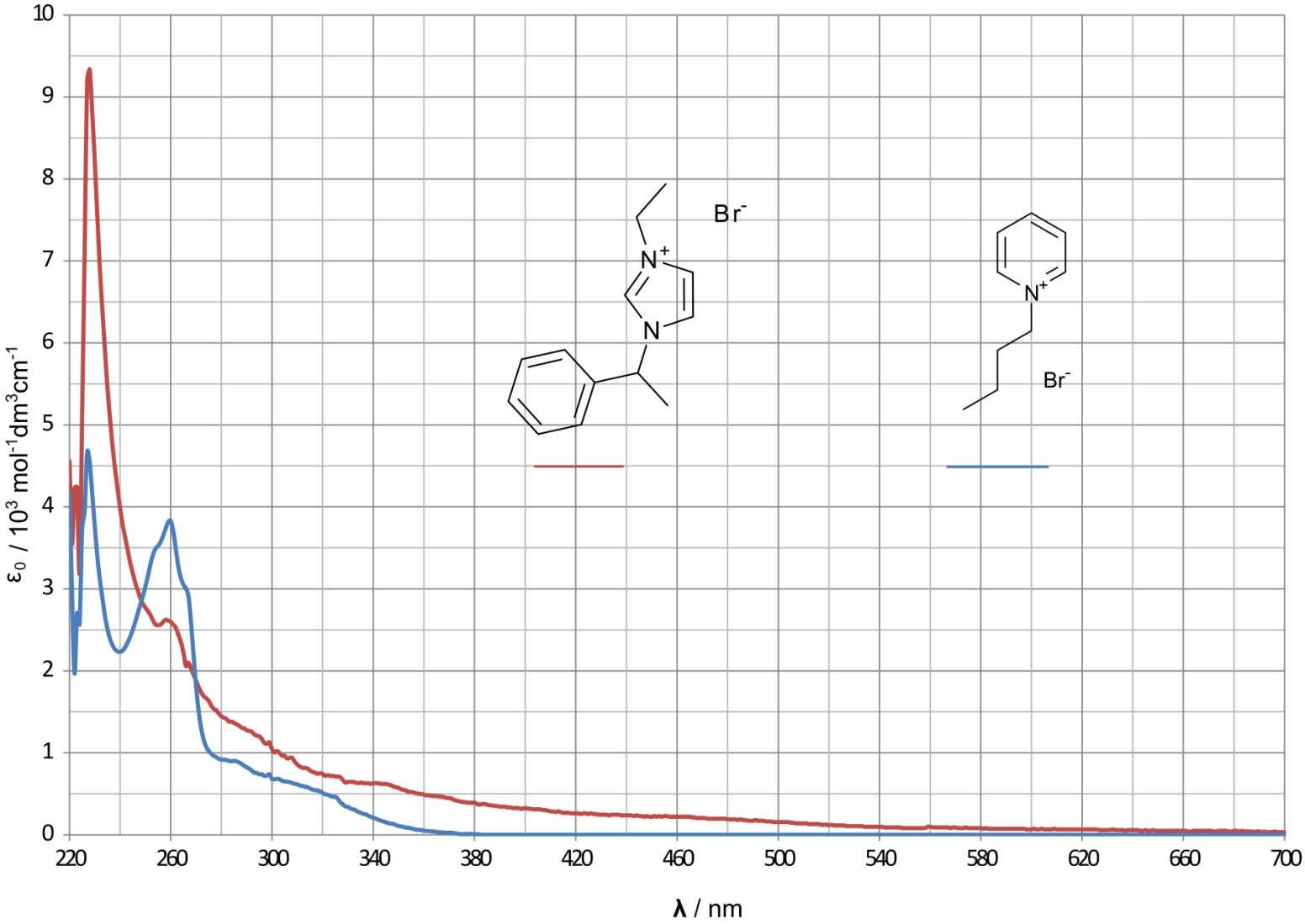


Figure 20: UV-Vis spectra of guests *rac*-**6** and **7**.