

Synthesis of Water-Soluble Amino Functionalized Multithiacalix[4]arene via Quaternization of Tertiary Amino Groups

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Figure 1S. NMR ^1H spectrum of macrocycle 1

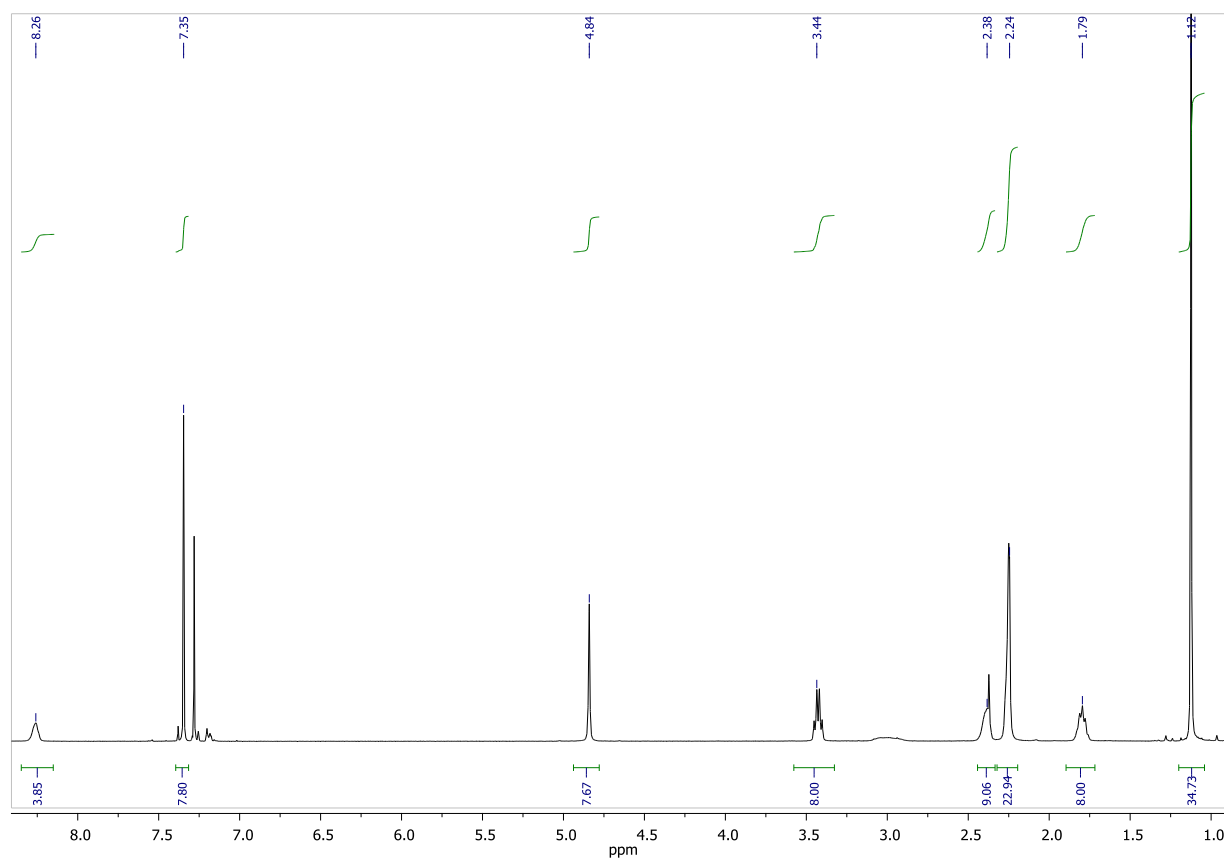


Figure 2S. IR spectrum of macrocycle 1

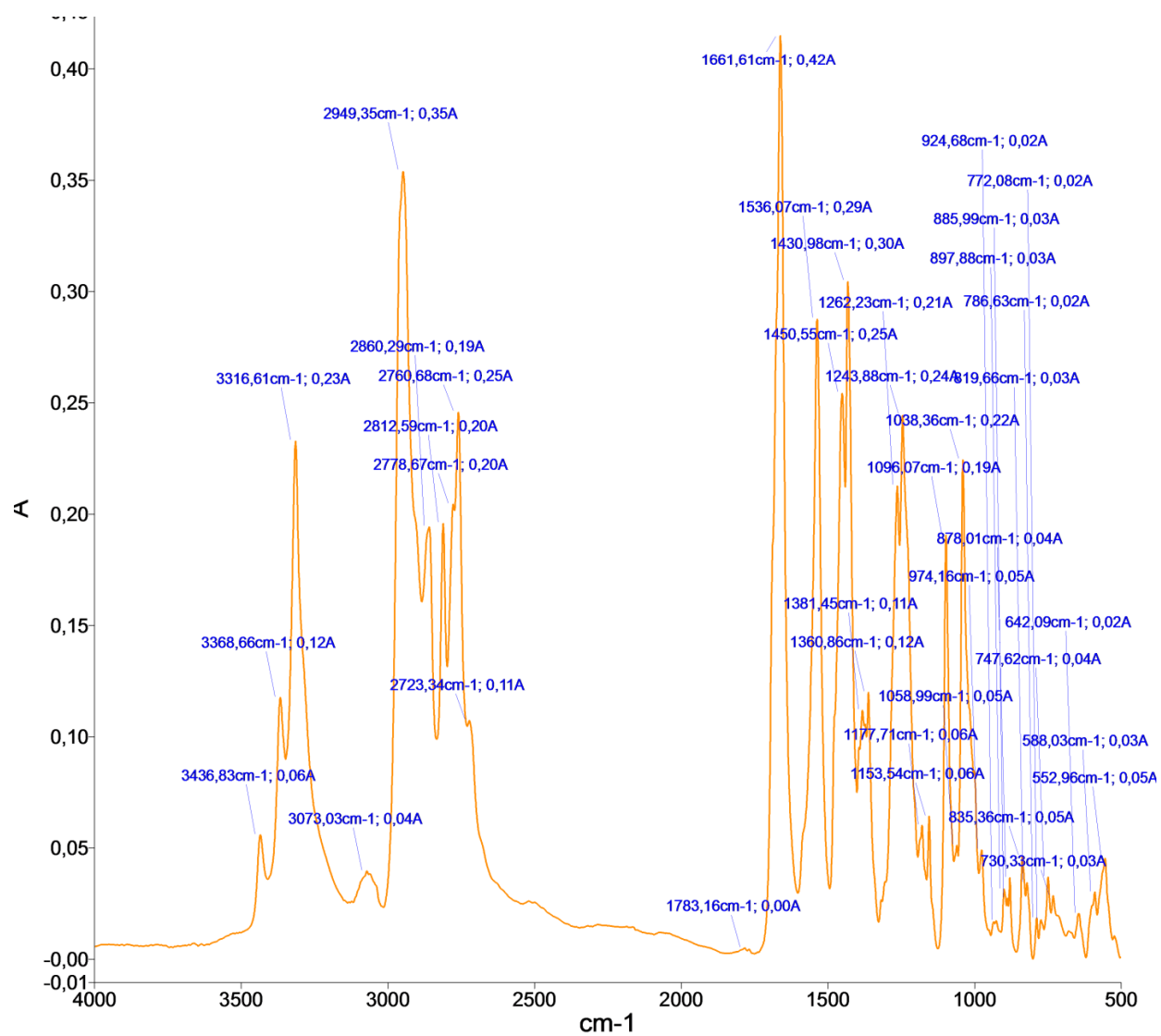


Figure 3S. NMR ^1H spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27-[3'-(N-phthalimido)propoxy]-28-[*tert*-butyl(2'-aminoethoxy)carbamate]-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*) **3**

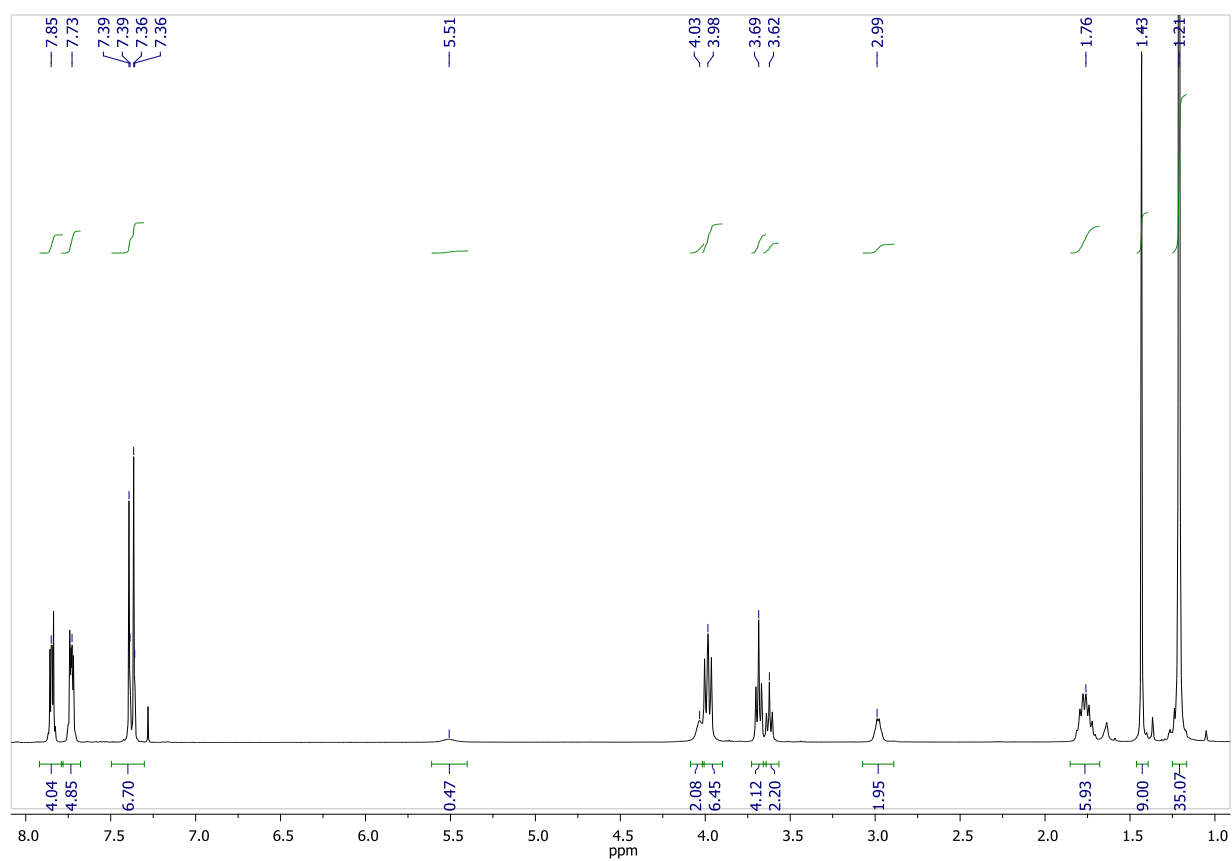


Figure 4S. NMR ^{13}C spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27-[3'-(N-phthalimido)propoxy]-28-[*tert*-butyl(2'-aminoethoxy)carbamate]-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*) 3

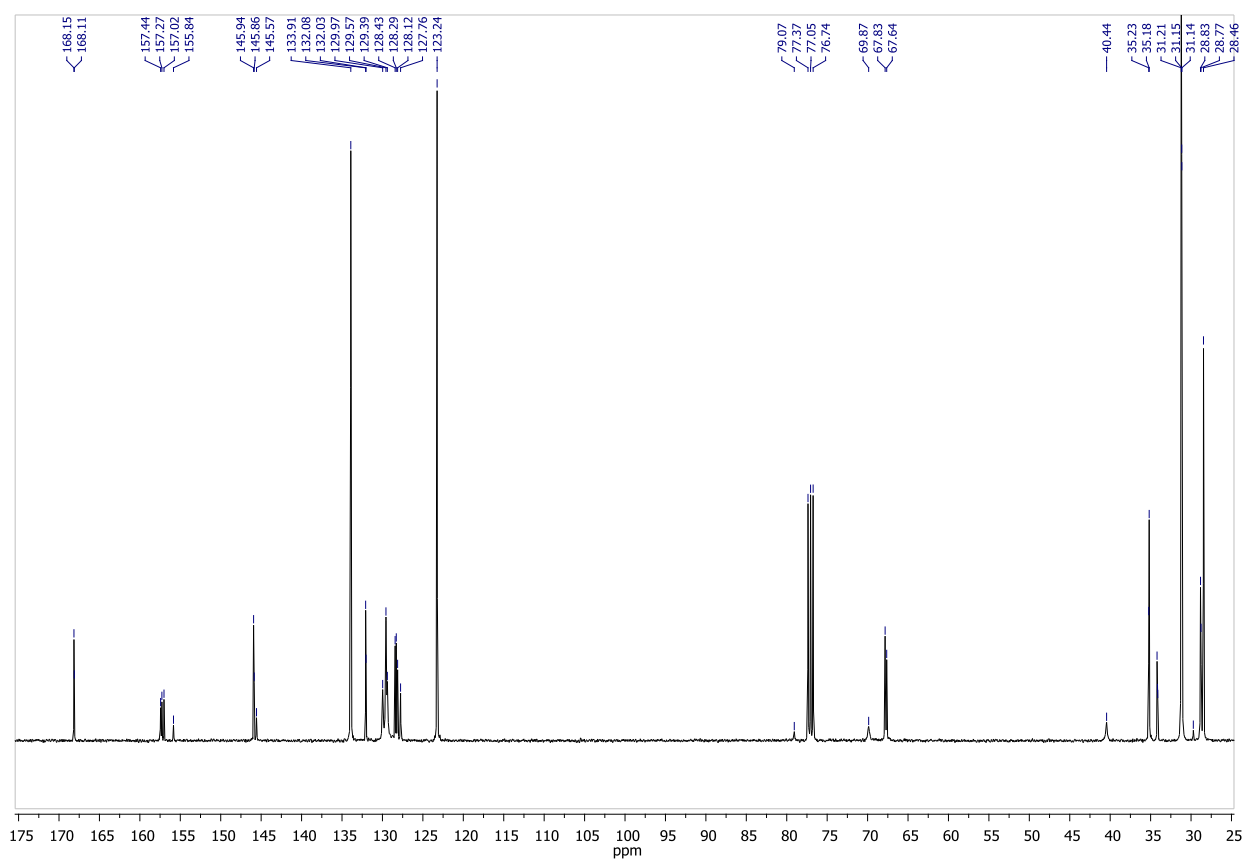


Figure 5S. NMR ^1H - ^1H NOESY spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27-[3'-(*N*-phthalimido)propoxy]-28-[*tert*-butyl(2'-aminoethoxy)carbamate]-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*) **3**

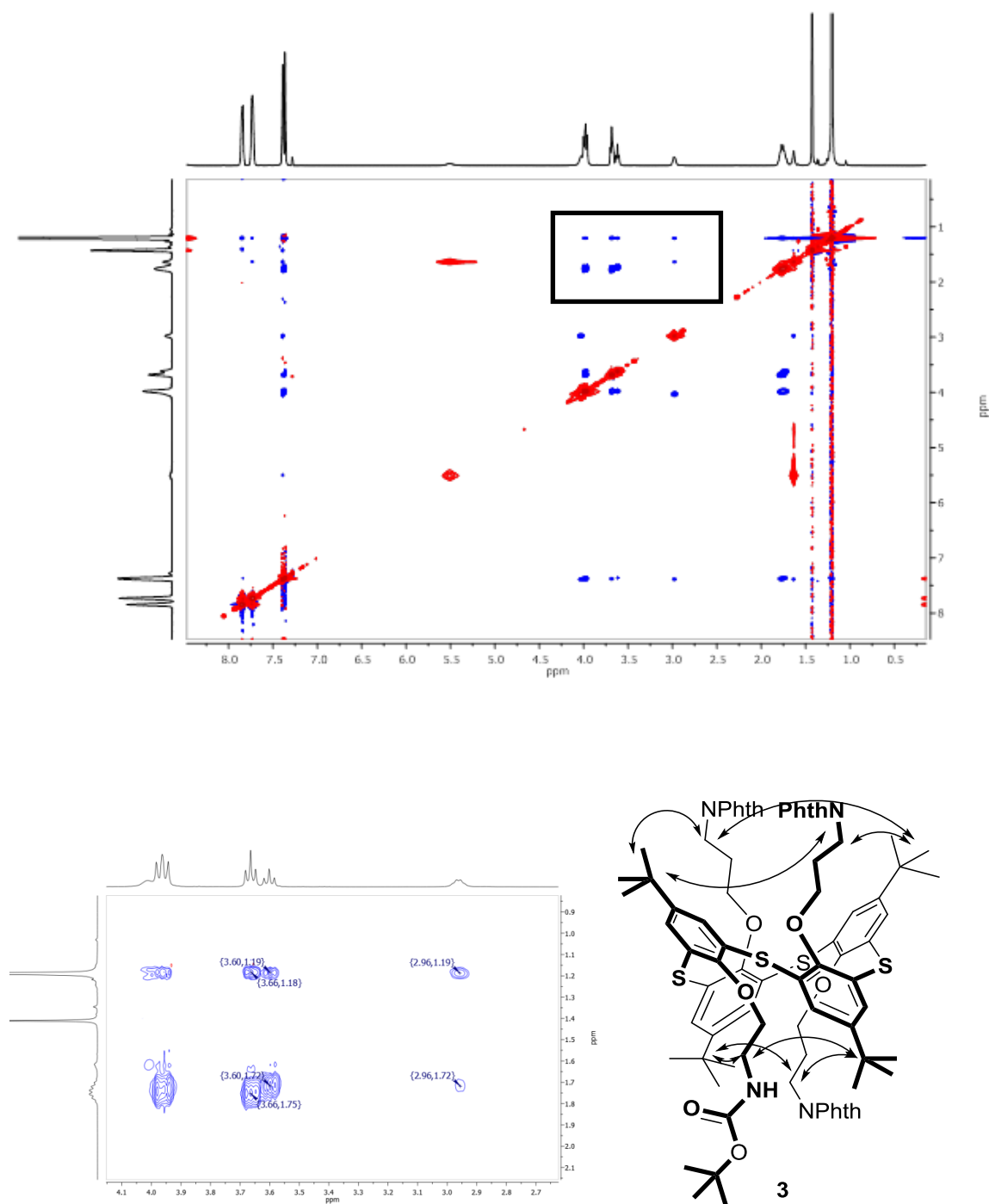


Figure 6S. MALDI TOF spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27-[3'-(N-phthalimido)propoxy]-28-[*tert*-butyl(2'-aminoethoxy)carbamate]-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*) **3**

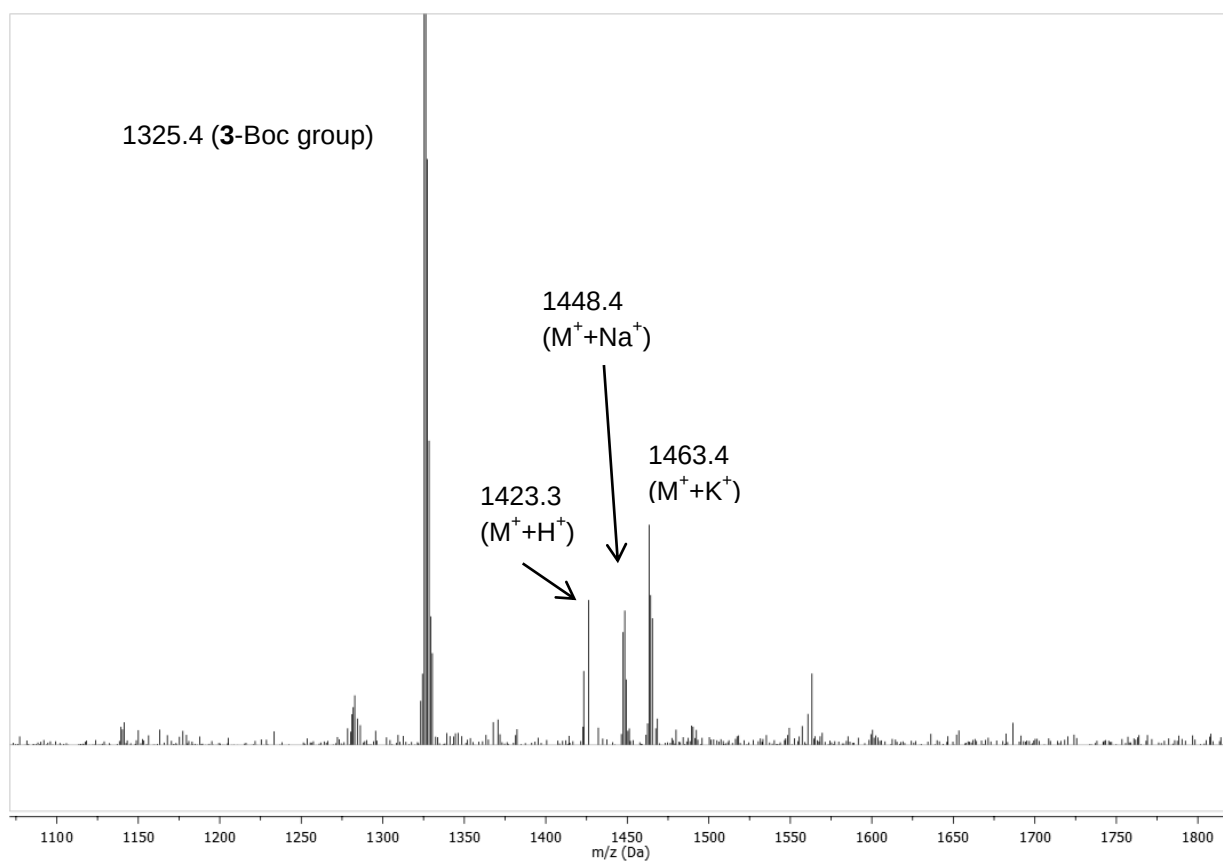


Figure 7S. NMR ^1H spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27-[3'-(N-phthalimido)propoxy]-28-[2'-aminoethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*) **4**

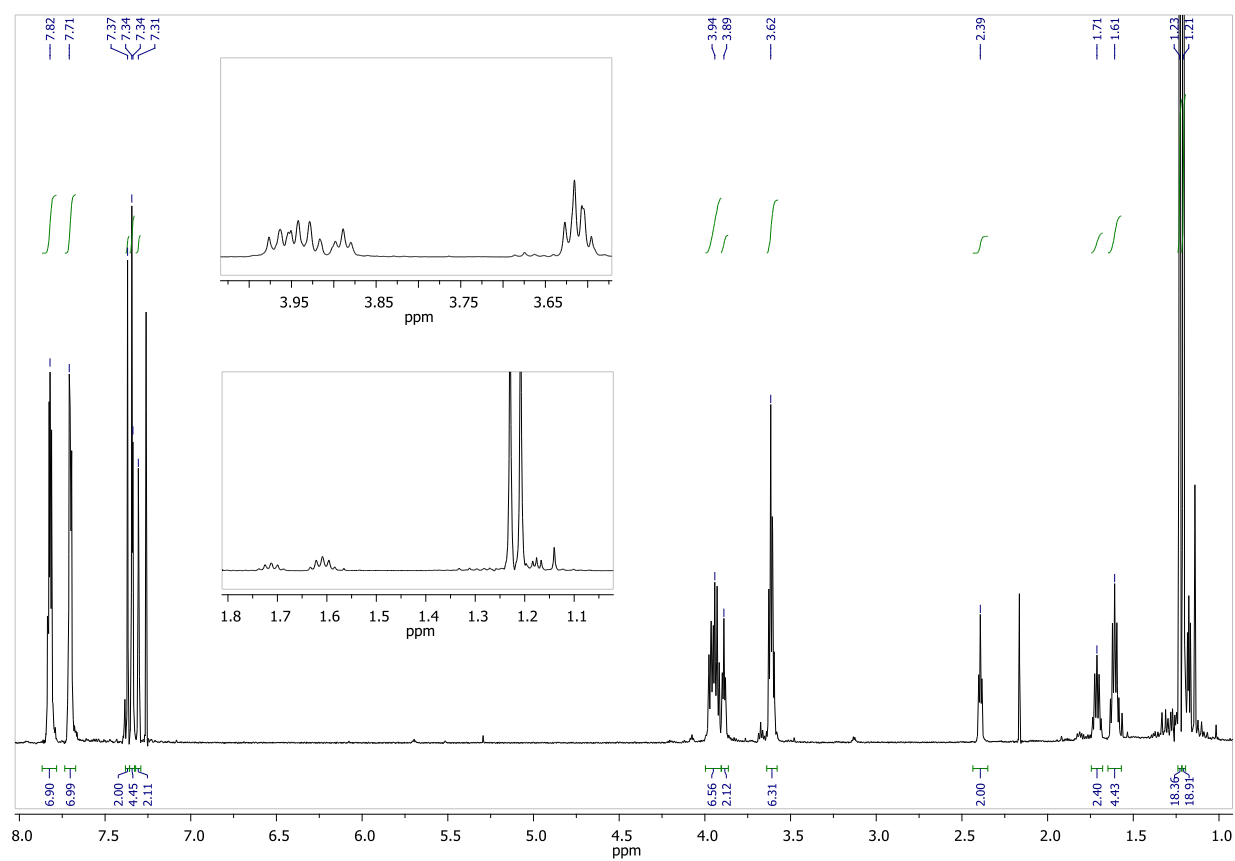


Figure 8S. NMR ^{13}C spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27-[3'-(N-phthalimido)propoxy]-28-[2'-aminoethoxy]-2,8,14,20-tetrathiacalix[4]arene 4

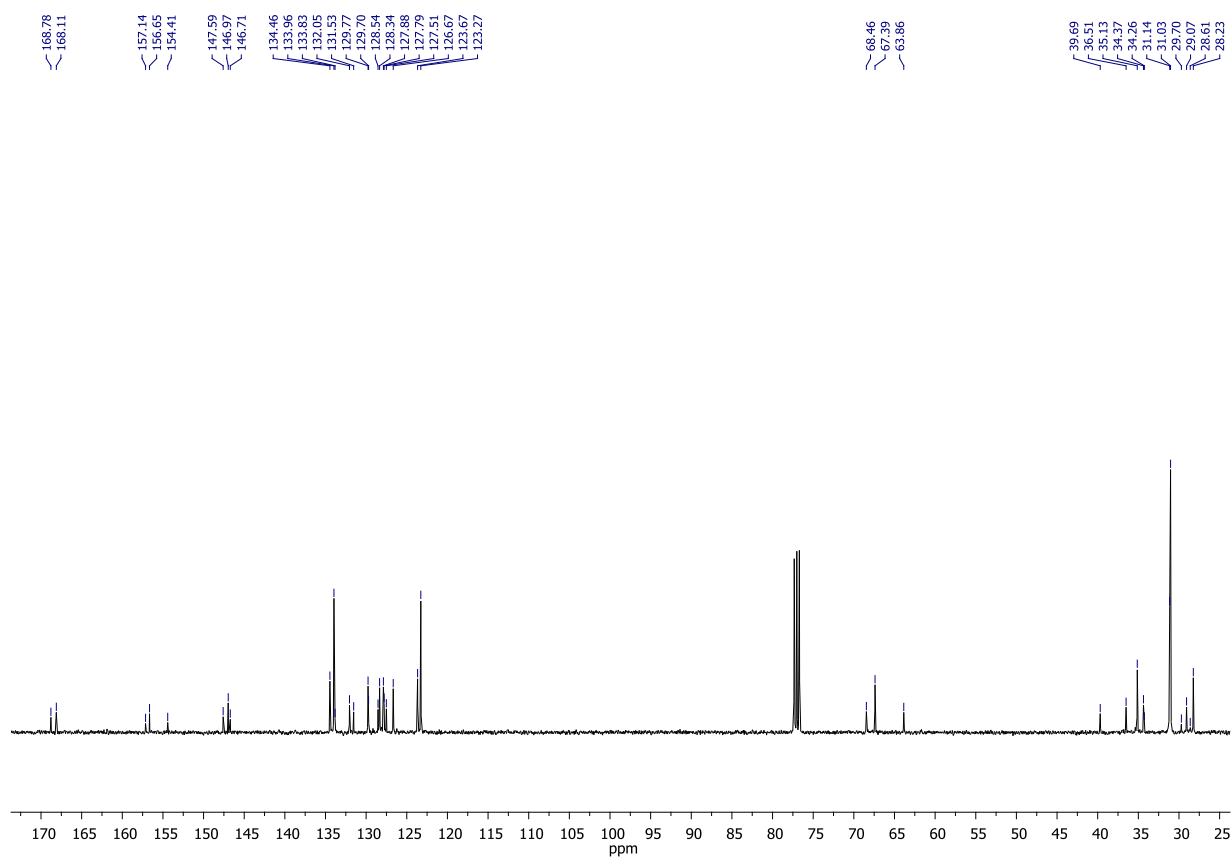


Figure 9S. MALDI-TOF mass spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27-[3'-(N-phthalimido)propoxy]-28-[2'-aminoethoxy]-2,8,14,20-tetrathiacalix[4]arene **4**

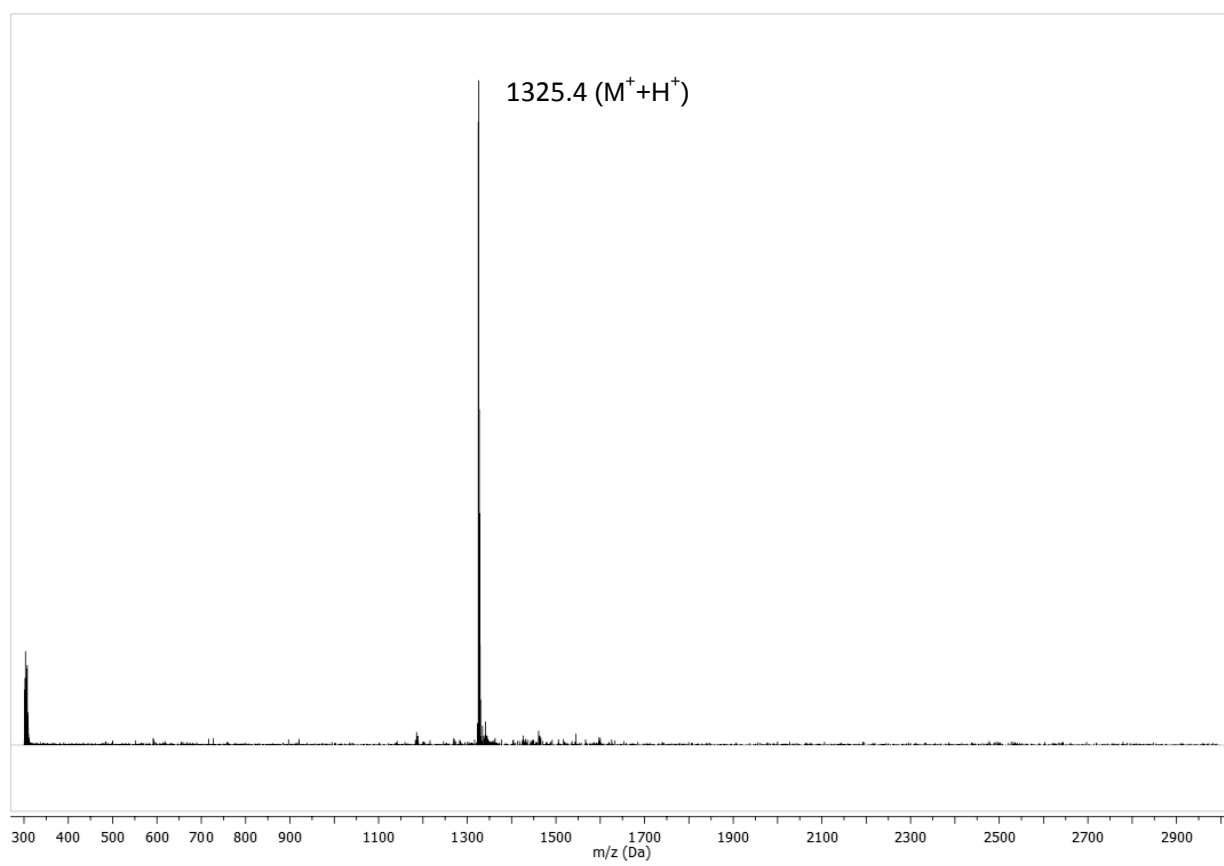


Figure 10S. NMR ^1H spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27-[3'-(N-phthalimido)propoxy]-28-[2'-bromoacetamidethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*) 5

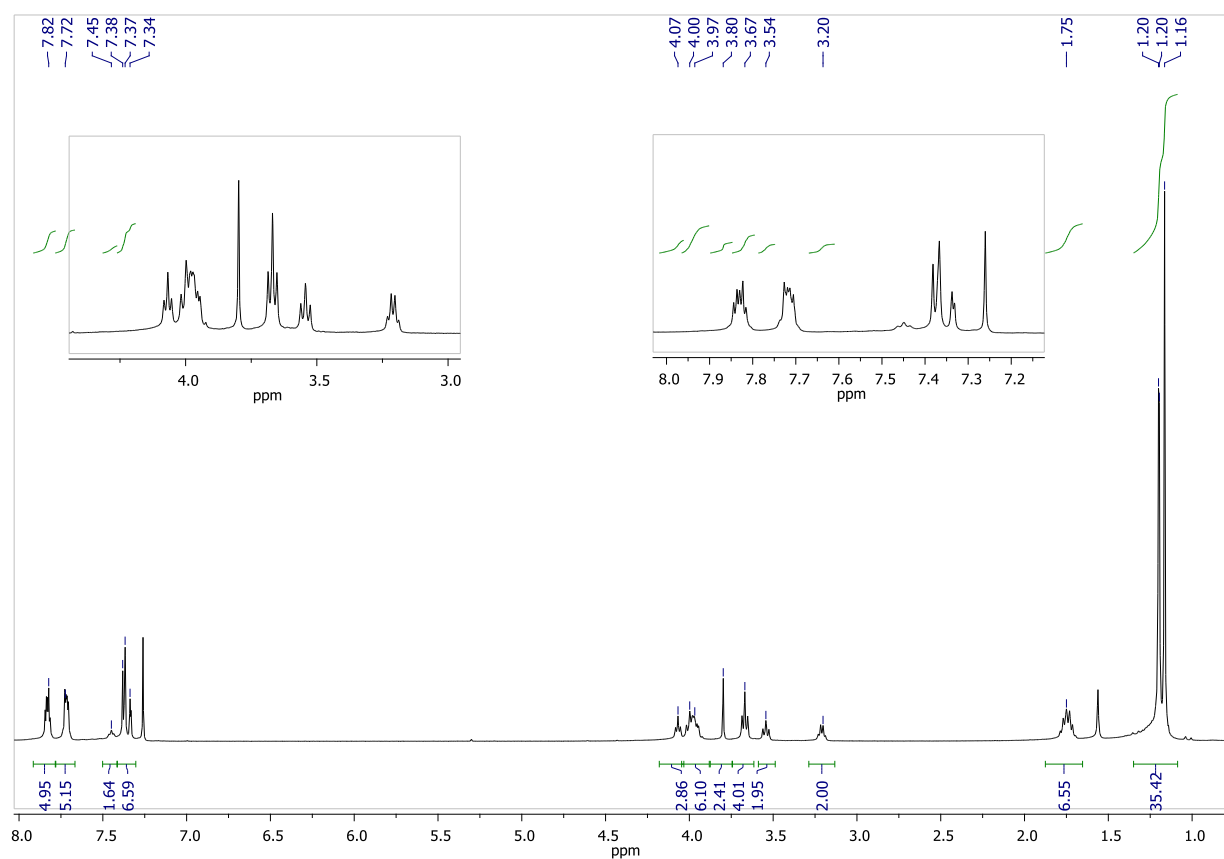


Figure 11S. NMR ^{13}C spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27-[3'-(N-phthalimido)propoxy]-28-[2'-bromoacetamidethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*) 5

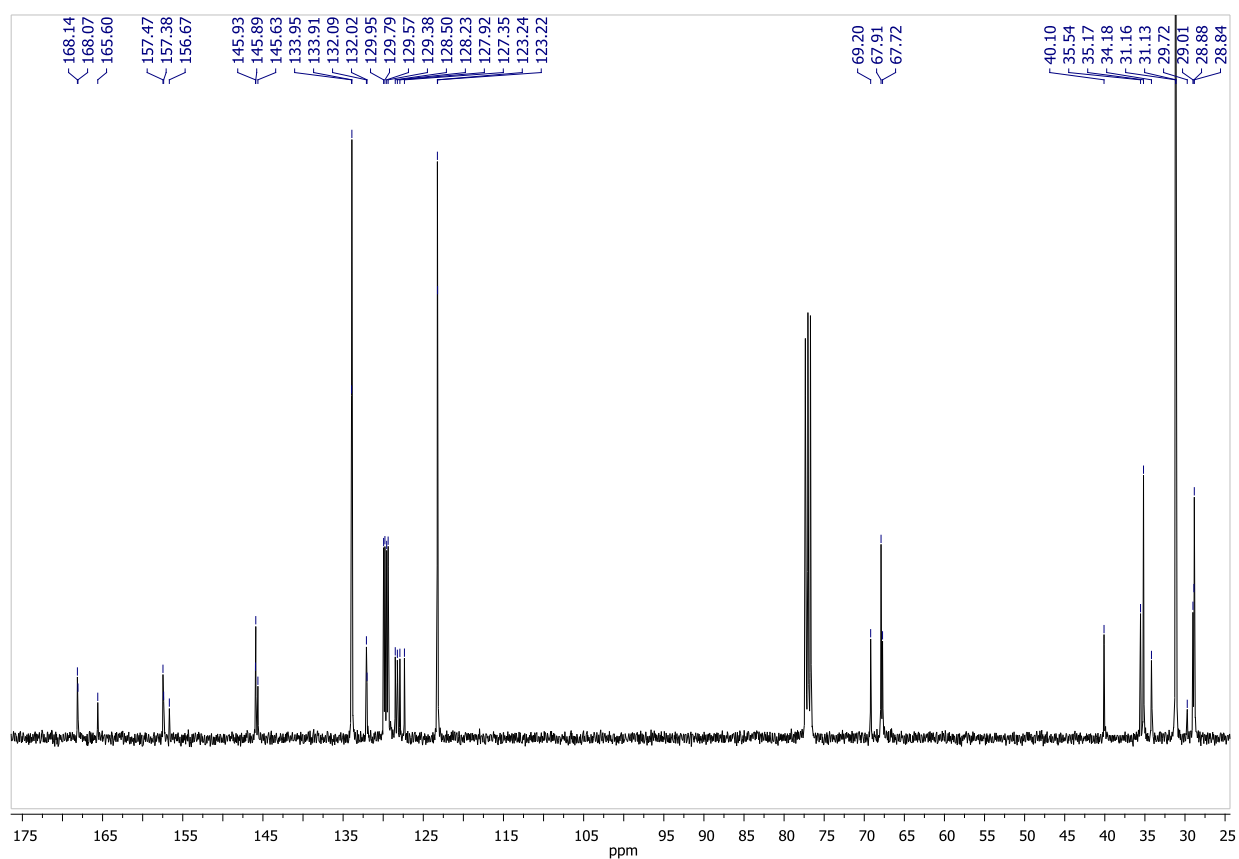


Figure 12S. NMR ^1H - ^1H NOESY spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27-[3'-(*N*-phthalimido)propoxy]-28-[2'-bromoacetamidethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*) **5**

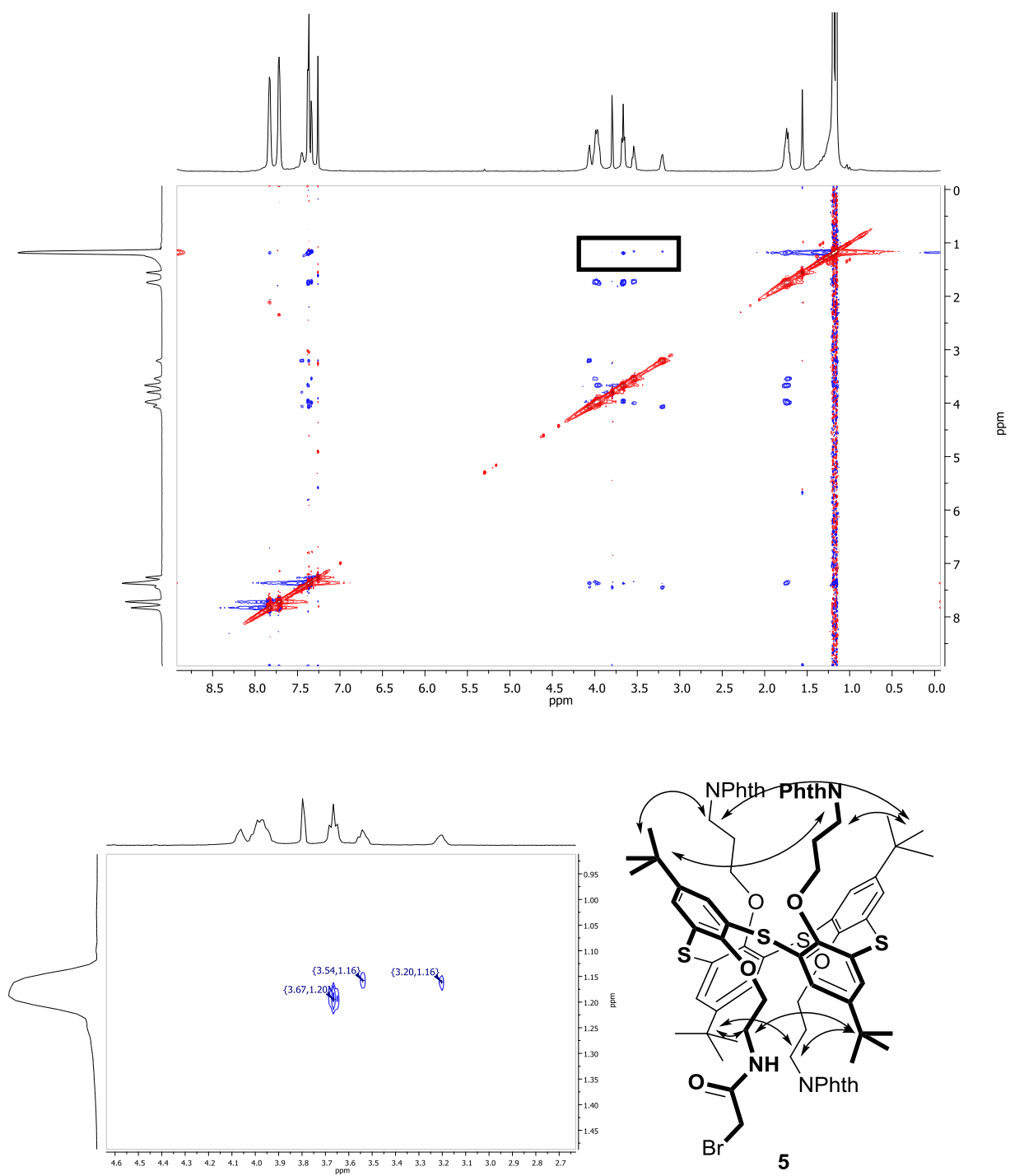


Figure 13S. MALDI TOF mass spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27-[3'-(N-phthalimido)propoxy]-28-[2'-bromoacetamidethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*) **5**

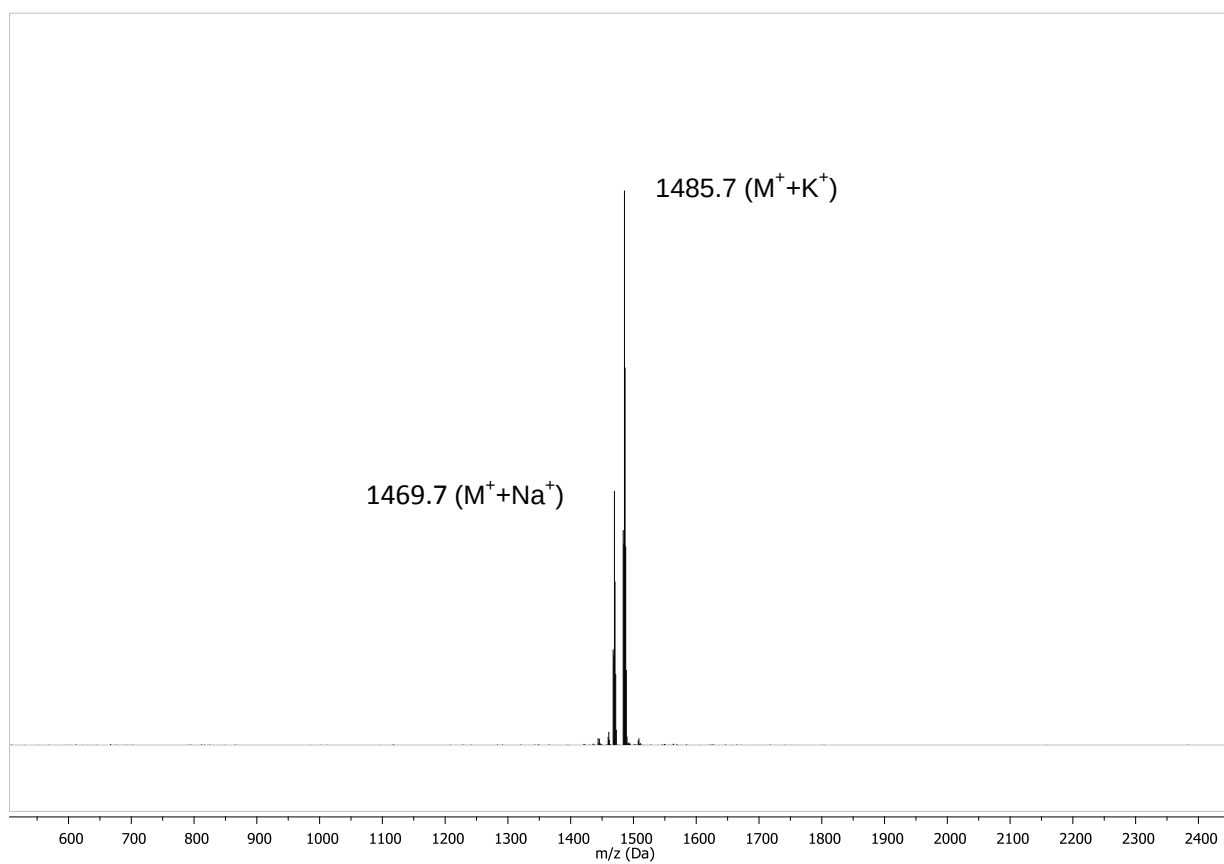


Figure 14S. IR spectrum of 5,11,17,23-tetra-*tert*-butyl-25,26,27-[3'-(N-phthalimido)propoxy]-28-[2'-bromoacetamidethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-*alternate*) 5

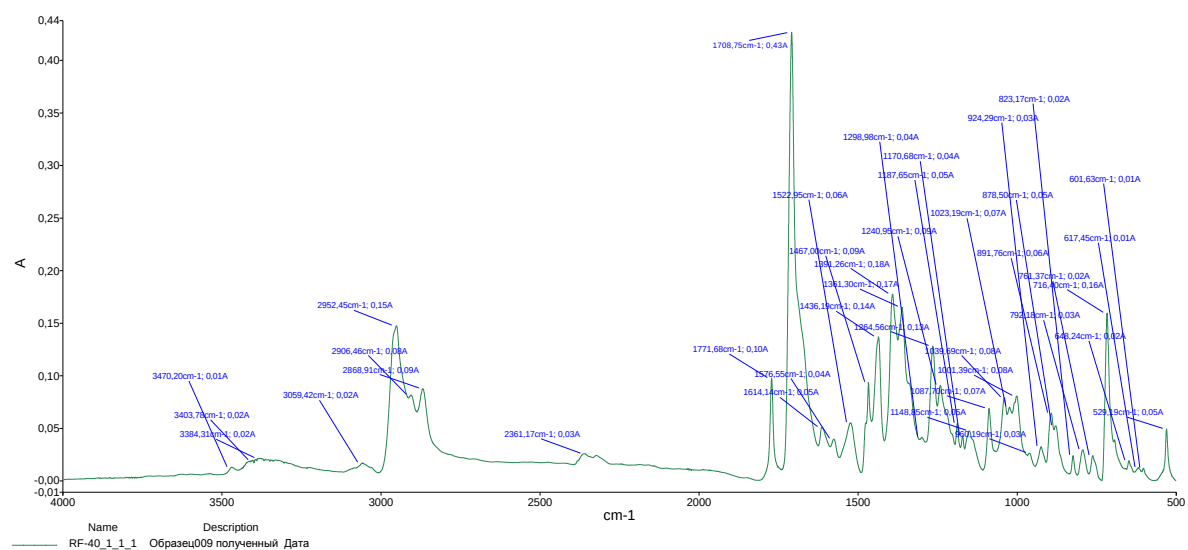


Figure 15S. NMR ^1H spectrum of multithiacalix[4]arene 6

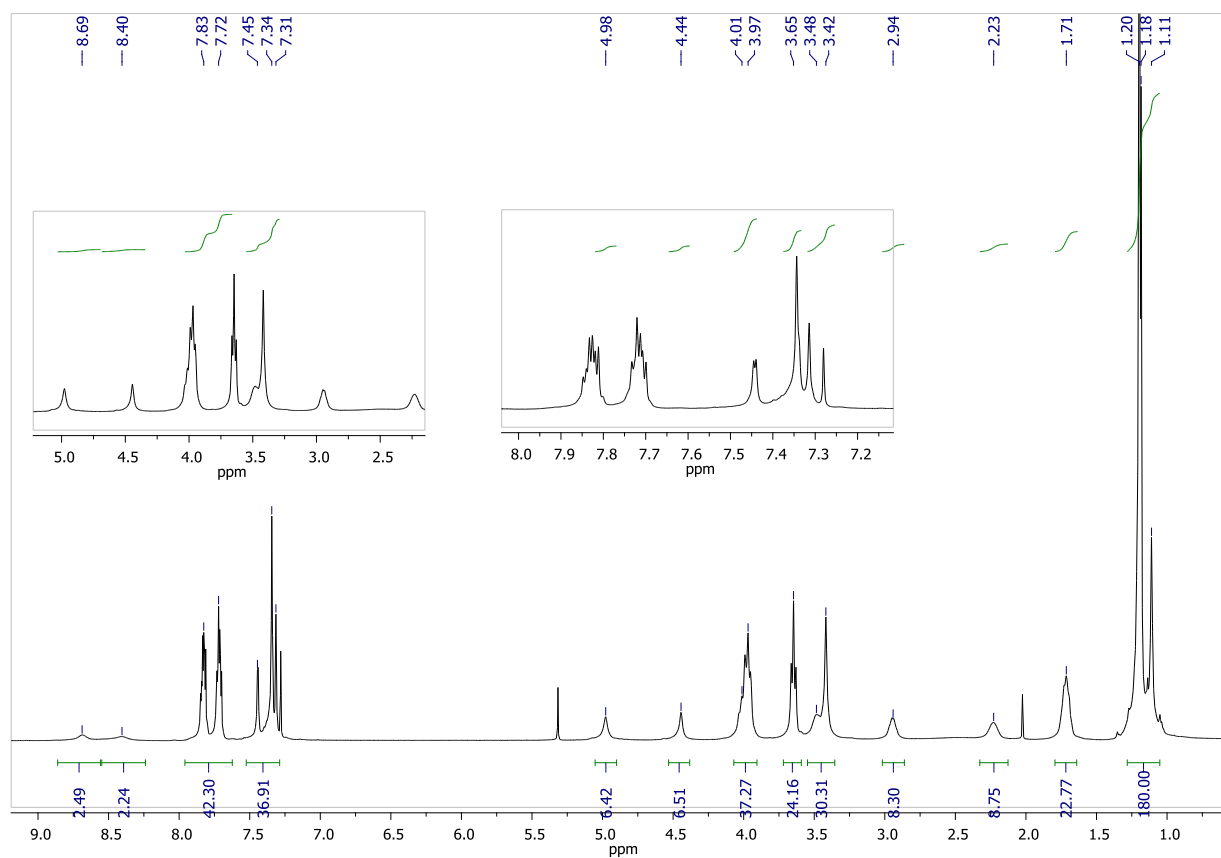


Figure 16S. NMR ^{13}C spectrum of multithiacalix[4]arene 6

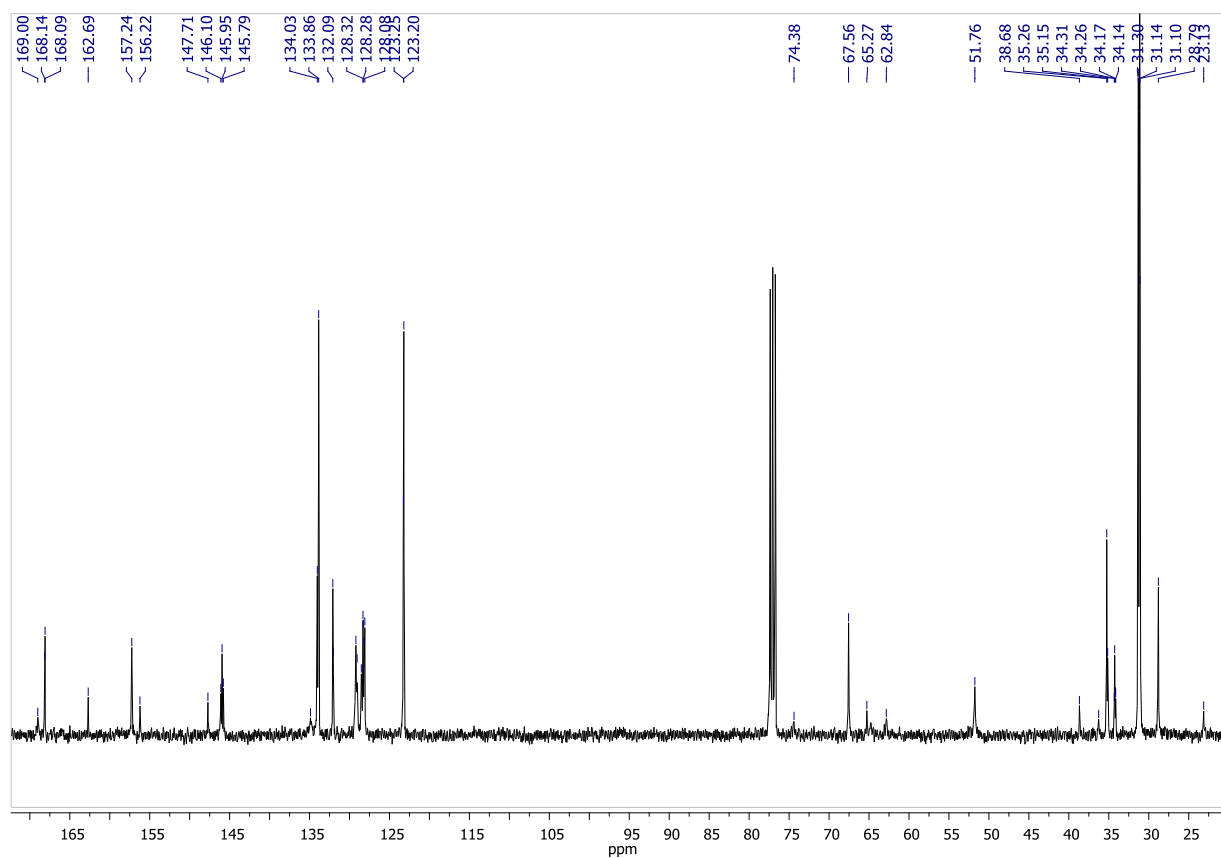


Figure 17S. MALDI TOF mass spectrum of multithiacalix[4]arene 6

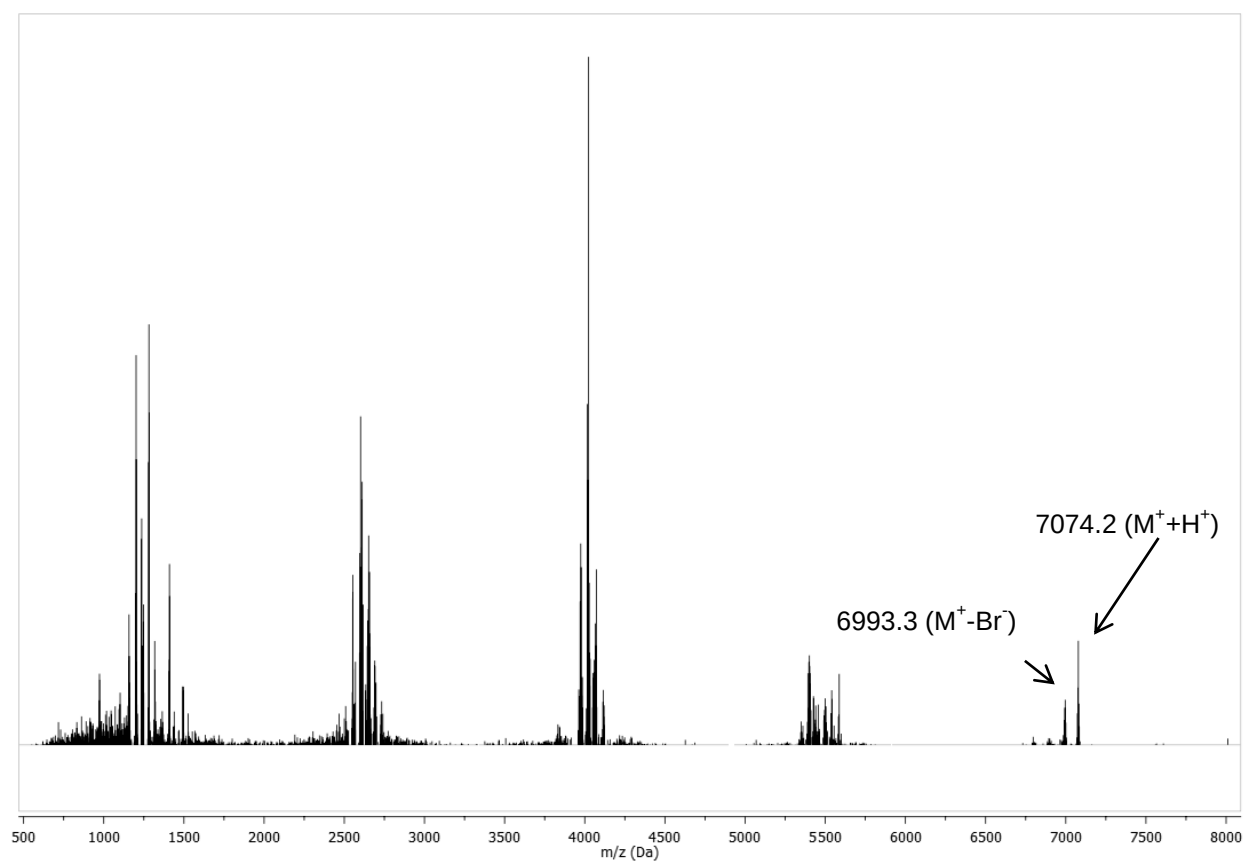


Figure 18S. IR spectrum of multithiacalix[4]arene 6

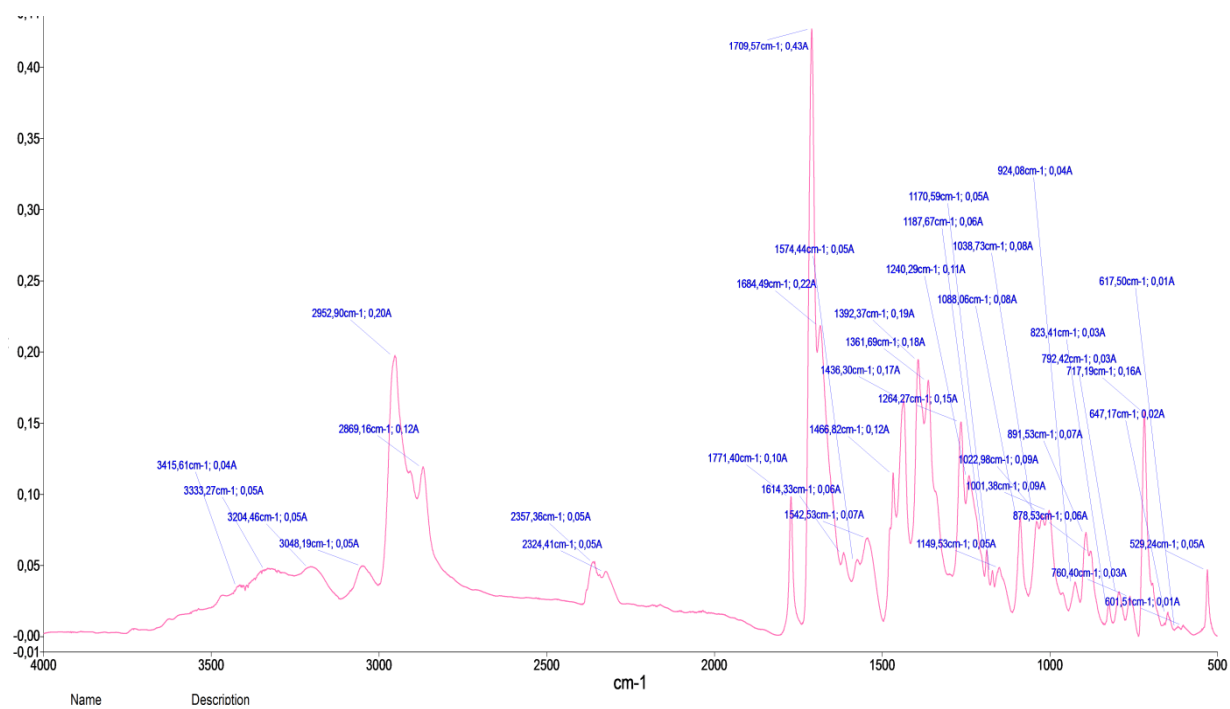


Figure 19S. NMR ^1H spectrum of multithiacalix[4]arene 7

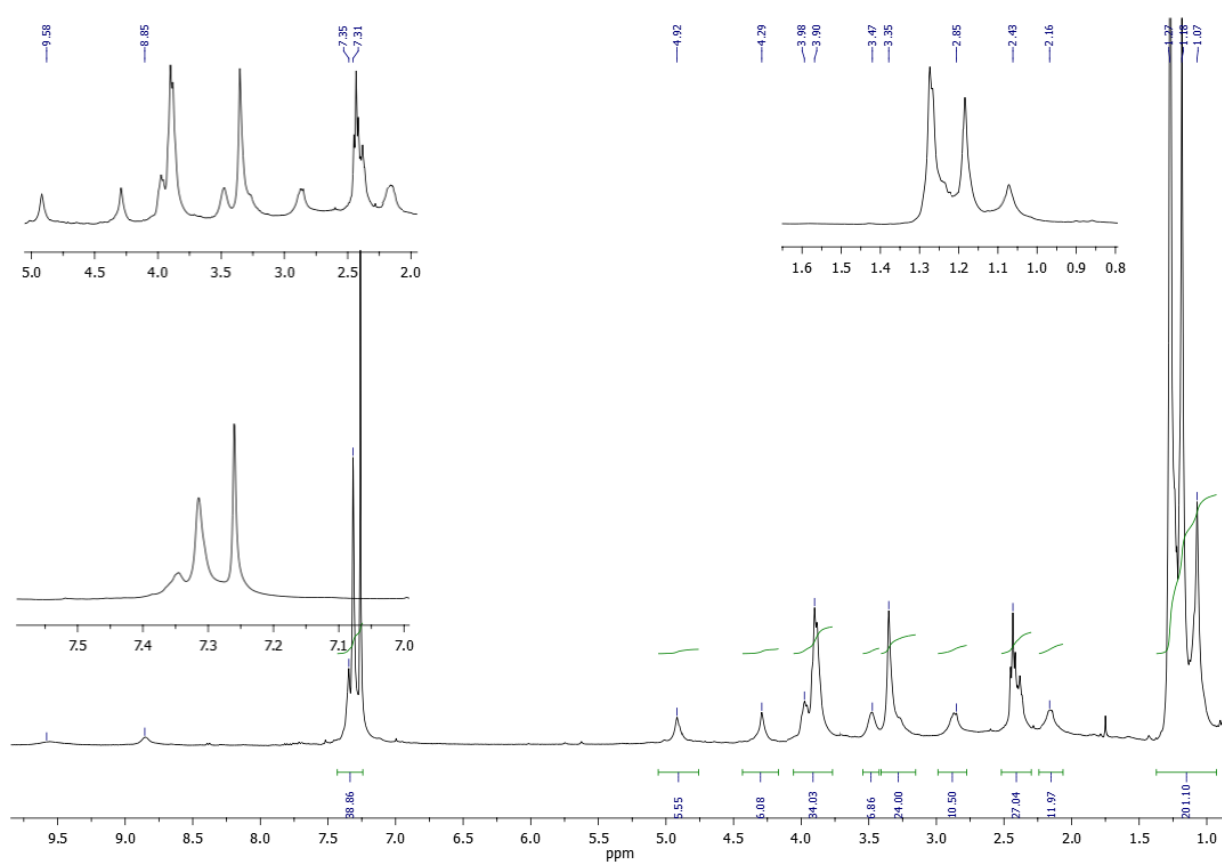


Figure 20S. NMR ^{13}C spectrum of multithiacalix[4]arene 7

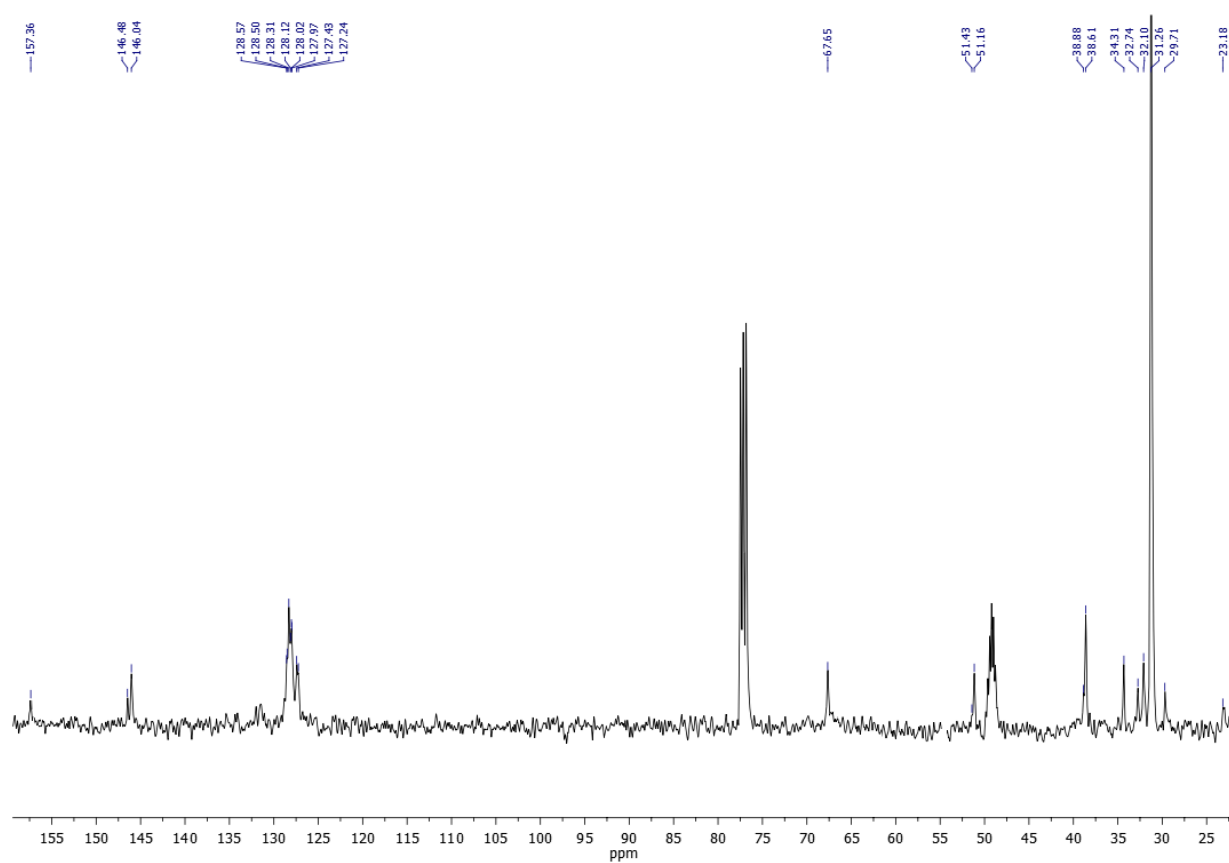


Figure 21S. IR spectrum of multithiacalix[4]arene 7

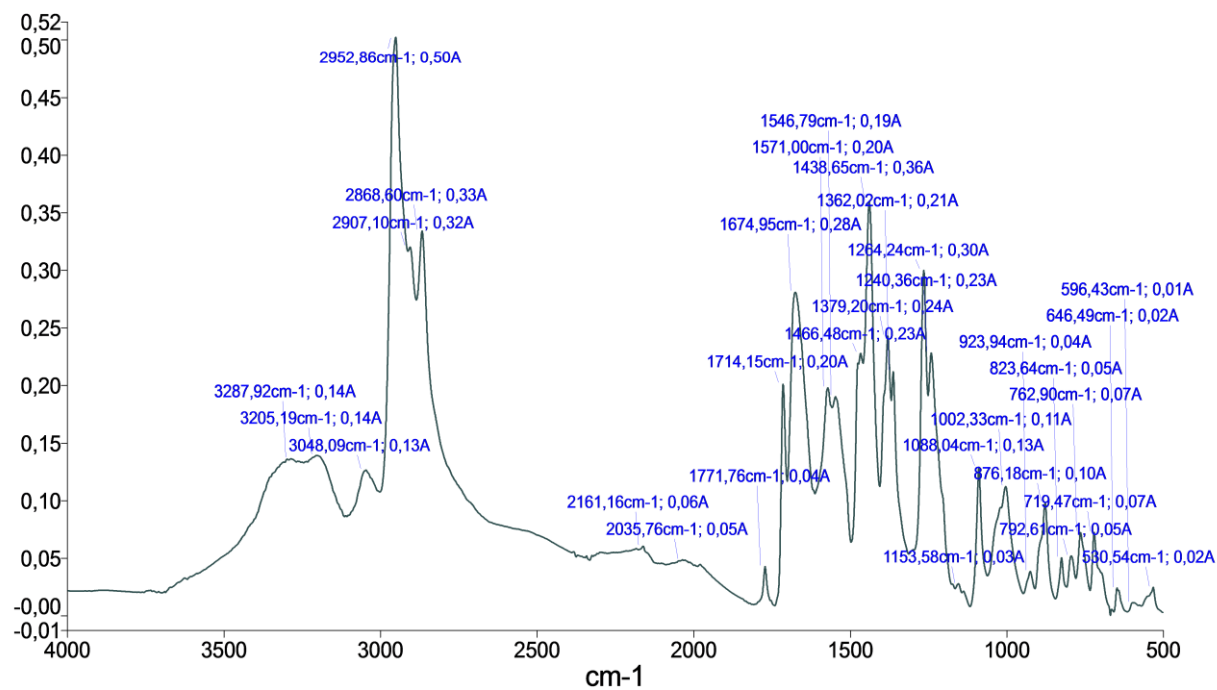


Figure 22S. MALDI TOF mass spectrum of multithiacalix[4]arene **7**

