

Electronic Supplementary Information (ESI) for

P-tert-butylthiacalix[4]arenes equipped with guanidinium fragments: aggregation, cytotoxicity, and DNA binding abilities

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RESULTS

- Figure S1. ¹H NMR spectrum of the compound **3b**.
- Figure S2. ¹³C NMR spectrum of the compound **3b**.
- Figure S3. NOESY 1H-1H NMR spectrum of the compound **3b**.
- Figure S4. MALDI MS of the compound **3b**.
- Figure S5. ¹H NMR spectrum of the compound **3c**.
- Figure S6. ¹³C NMR spectrum of the compound **3c**.
- Figure S7. MALDI MS of the compound **3c**.
- Figure S8. ¹H NMR spectrum of the compound **3d**.
- Figure S9. ¹³C NMR spectrum of the compound **3d**.
- Figure S10. NOESY 1H-1H NMR spectrum of the compound **3d**.
- Figure S11. MALDI MS of the compound **3d**.
- Figure S12. ¹H NMR spectrum of the compound **3**.
- Figure S13. ¹³C NMR spectrum of the compound **3**.
- Figure S14. MALDI MS of the compound **3**.

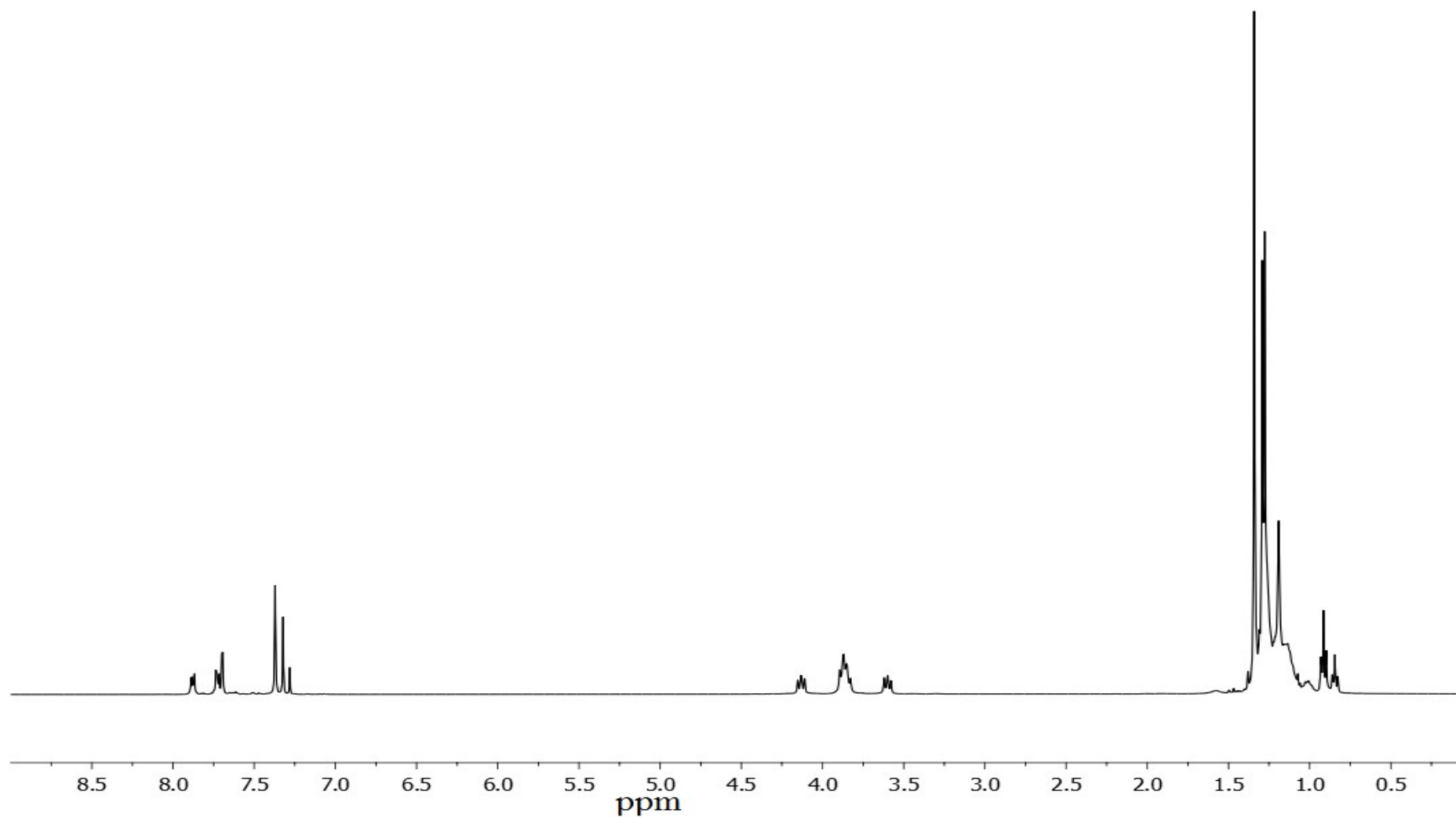


Figure S1. ^1H NMR spectrum of the compound 5,11,17,23-Tetra-*tert*-butyl-25,26,27-tridecyl-28-[2-phthalimidoethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-alternate) (**3b**). (CDCl_3 , 25°C , 400 MHz).

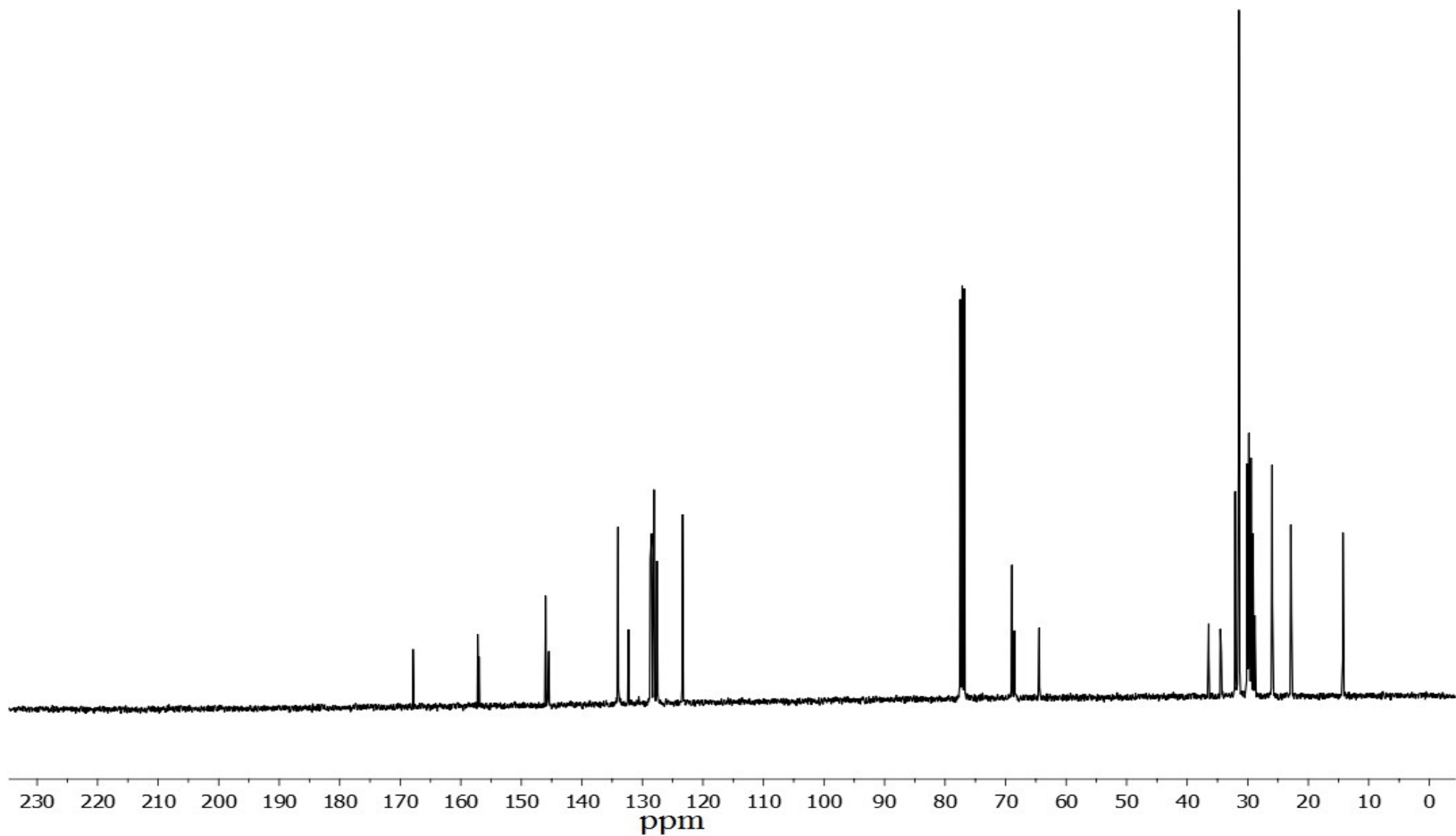


Figure S2. ^{13}C NMR spectrum of the compound 5,11,17,23-Tetra-*tert*-butyl-25,26,27-tridecyl-28-[2-phthalimidoethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-alternate) (**3b**). (CDCl_3 , 25°C , 400 MHz).

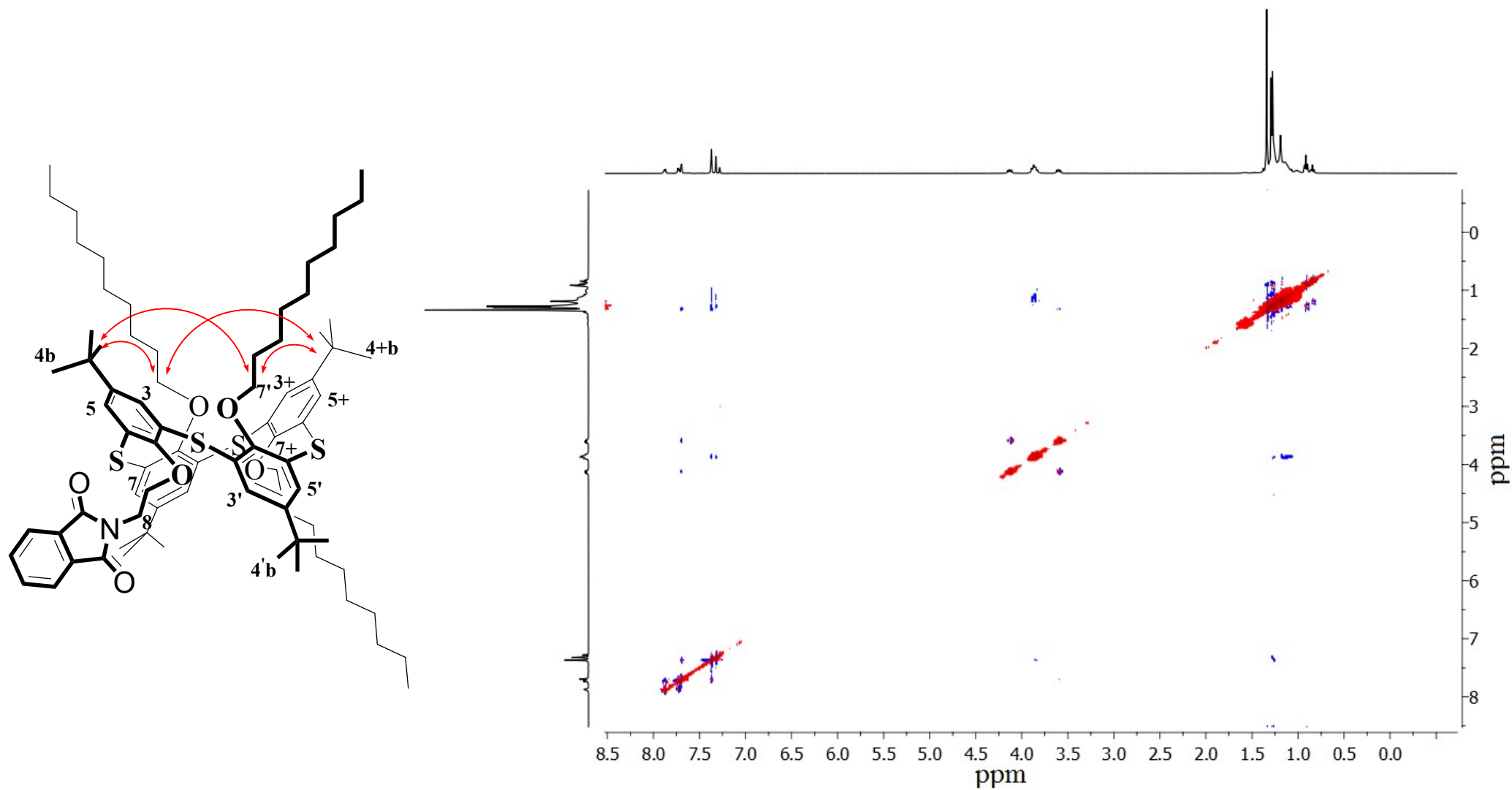


Figure S3. NOESY ^1H - ^1H NMR spectrum of the compound 5,11,17,23-Tetra-tert-butyl-25,26,27-tridecyl-28-[2-phthalimidoethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-alternate) (**3b**). (CDCl_3 , 25°C , 400 MHz).

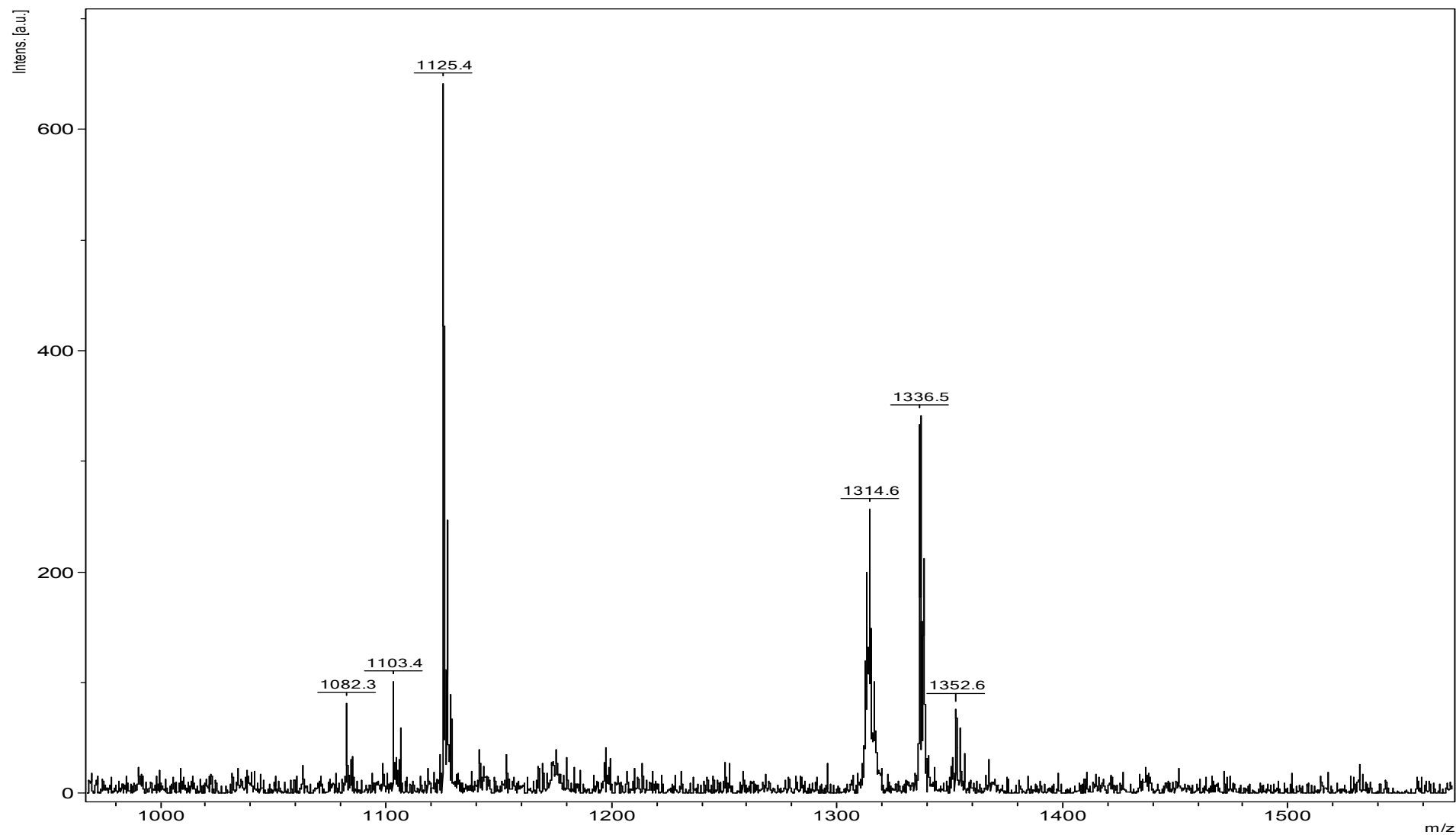


Figure S4. MALDI MS of 5,11,17,23-Tetra-tert-butyl-25,26,27-tridecyl-28-[2-phthalimidoethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-alternate) (**3b**). (*p*-nitroaniline matrix).

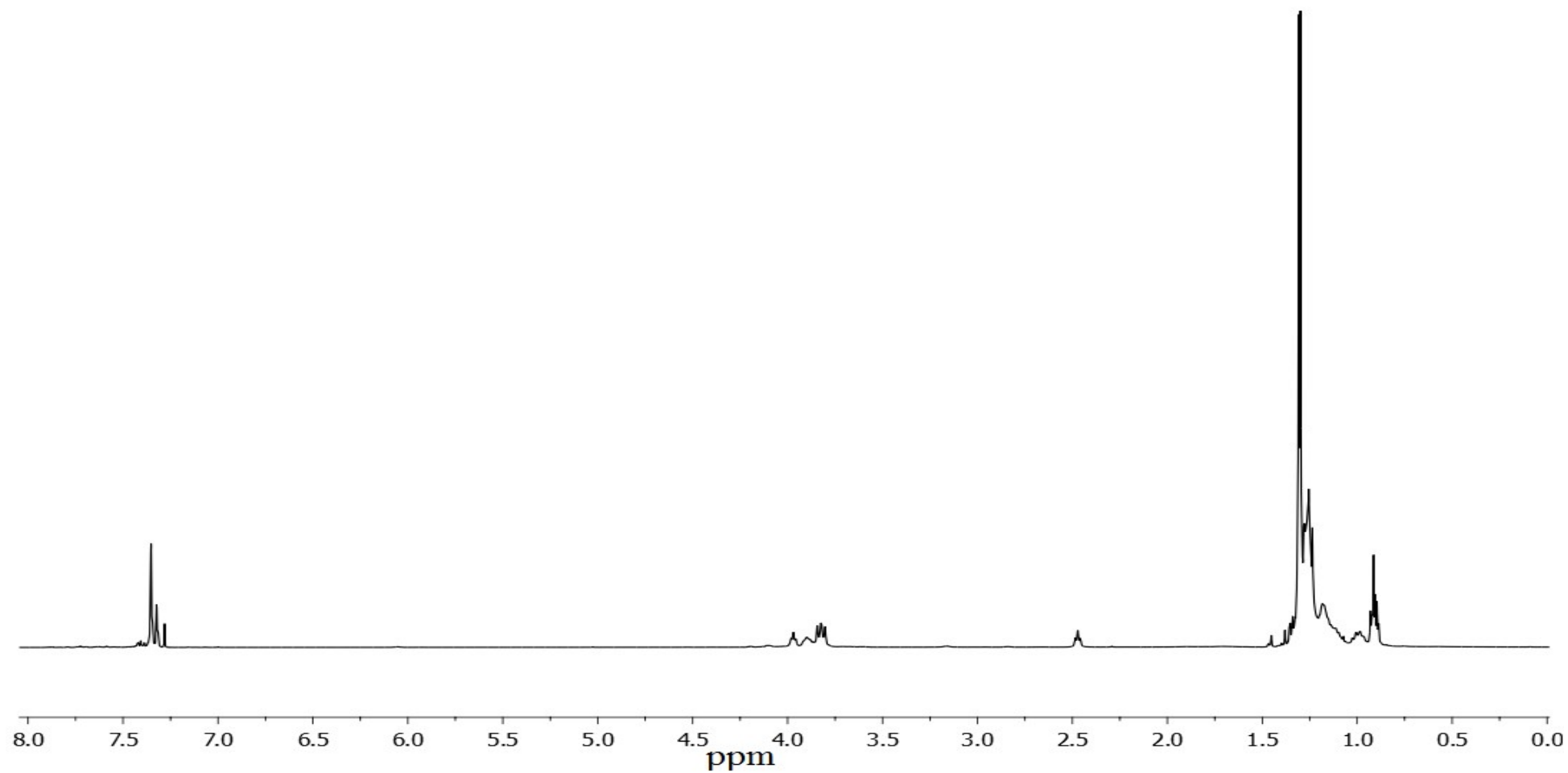


Figure S5. ^1H NMR spectrum of 5,11,17,23-Tetra-*tert*-butyl-25,26,27-tridecyl-28-[2-aminoethoxy]-2,8,14,20-tetrathiacalix[4]arene (**3c**).
(CDCl_3 , 25°C , 400 MHz).

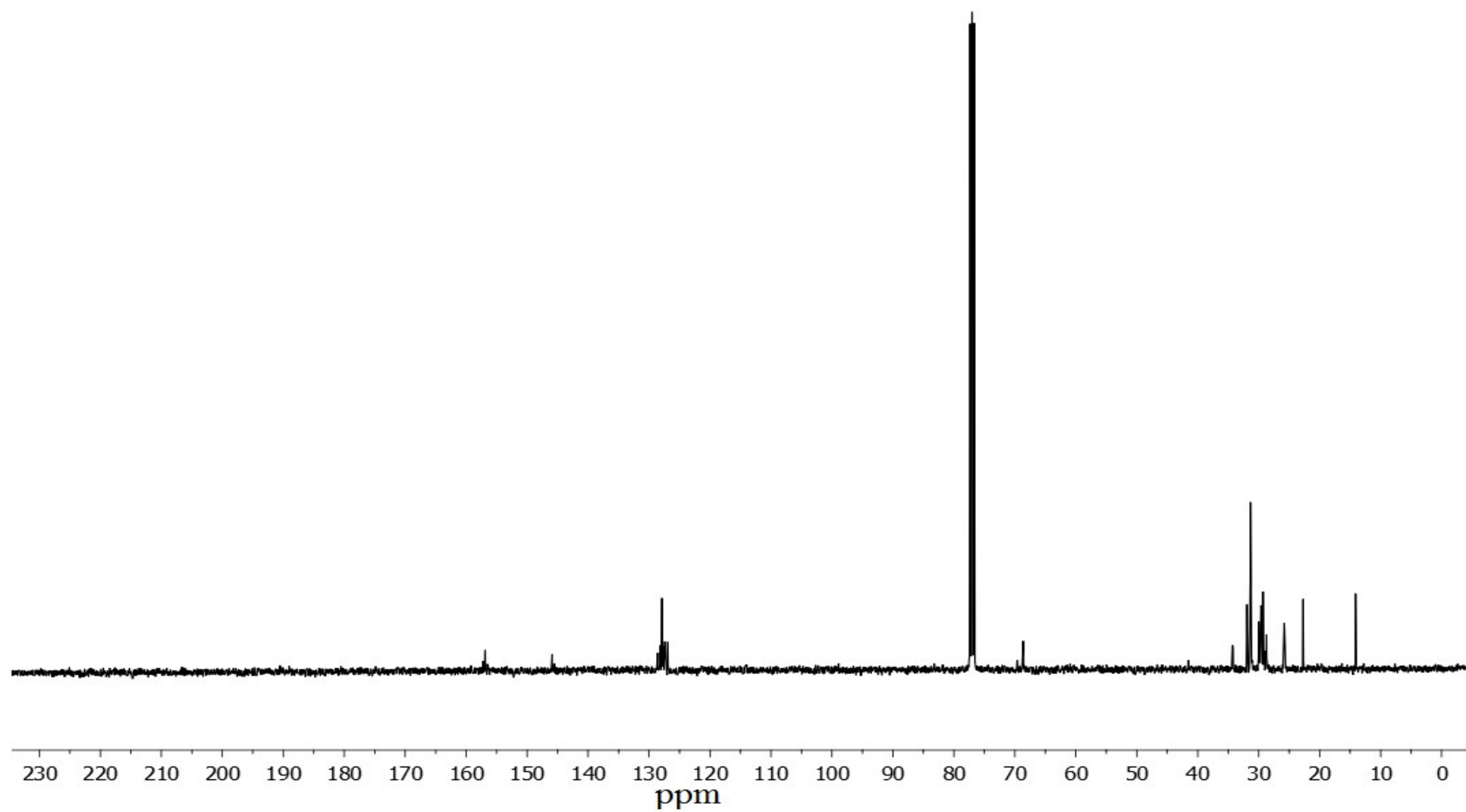


Figure S6. ^{13}C NMR spectrum of 5,11,17,23-Tetra-tert-butyl-25,26,27-tridecyl-28-[2-aminoethoxy]-2,8,14,20-tetrathiacalix[4]arene (**3c**). (CDCl_3 , 25°C , 400 MHz).

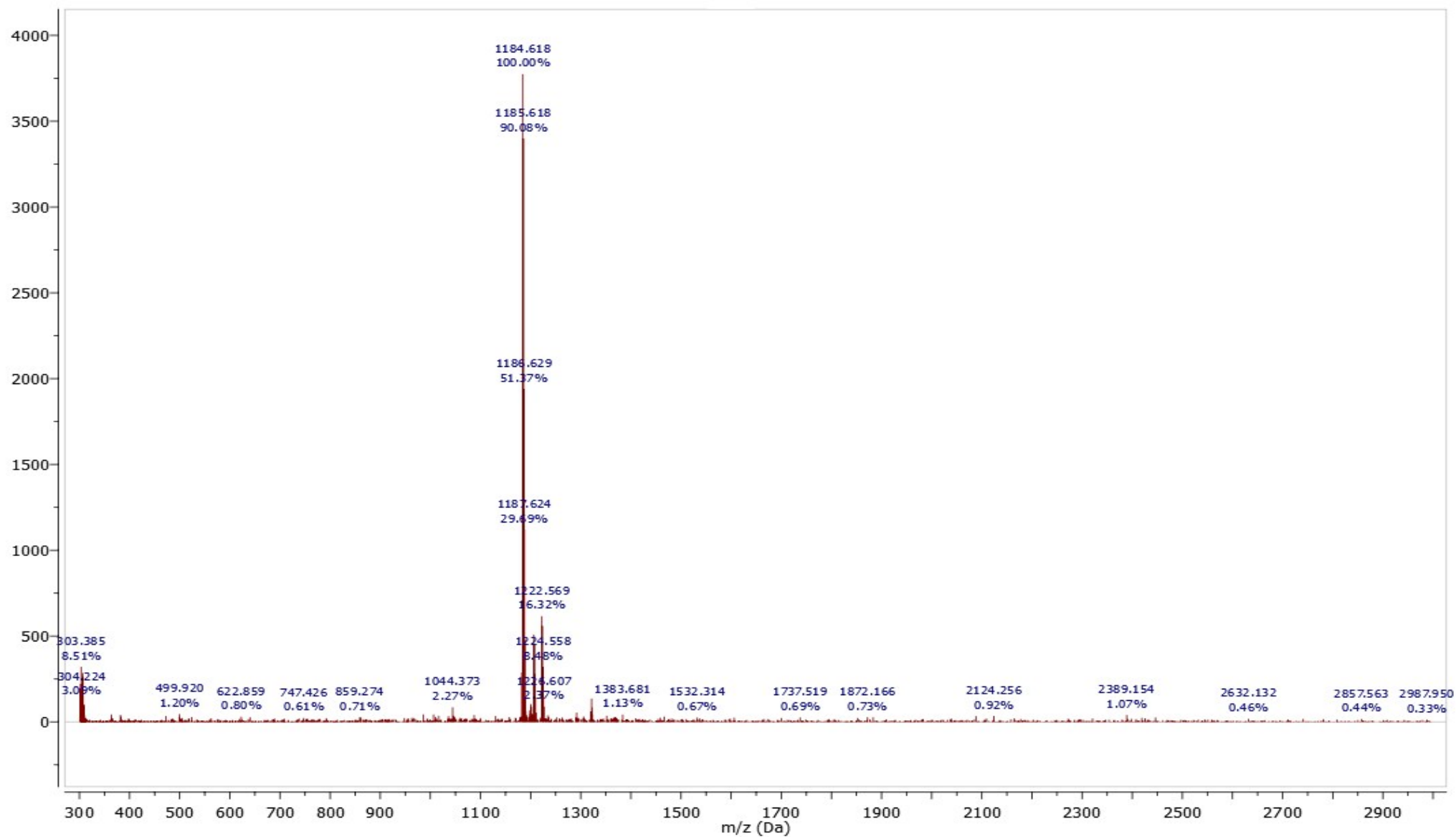


Figure S7. MALDI MS of 5,11,17,23-Tetra-*tert*-butyl-25,26,27-tridecyl-28-[2-aminoethoxy]-2,8,14,20-tetrathiacalix[4]arene (**3c**). (*p*-nitroaniline matrix).

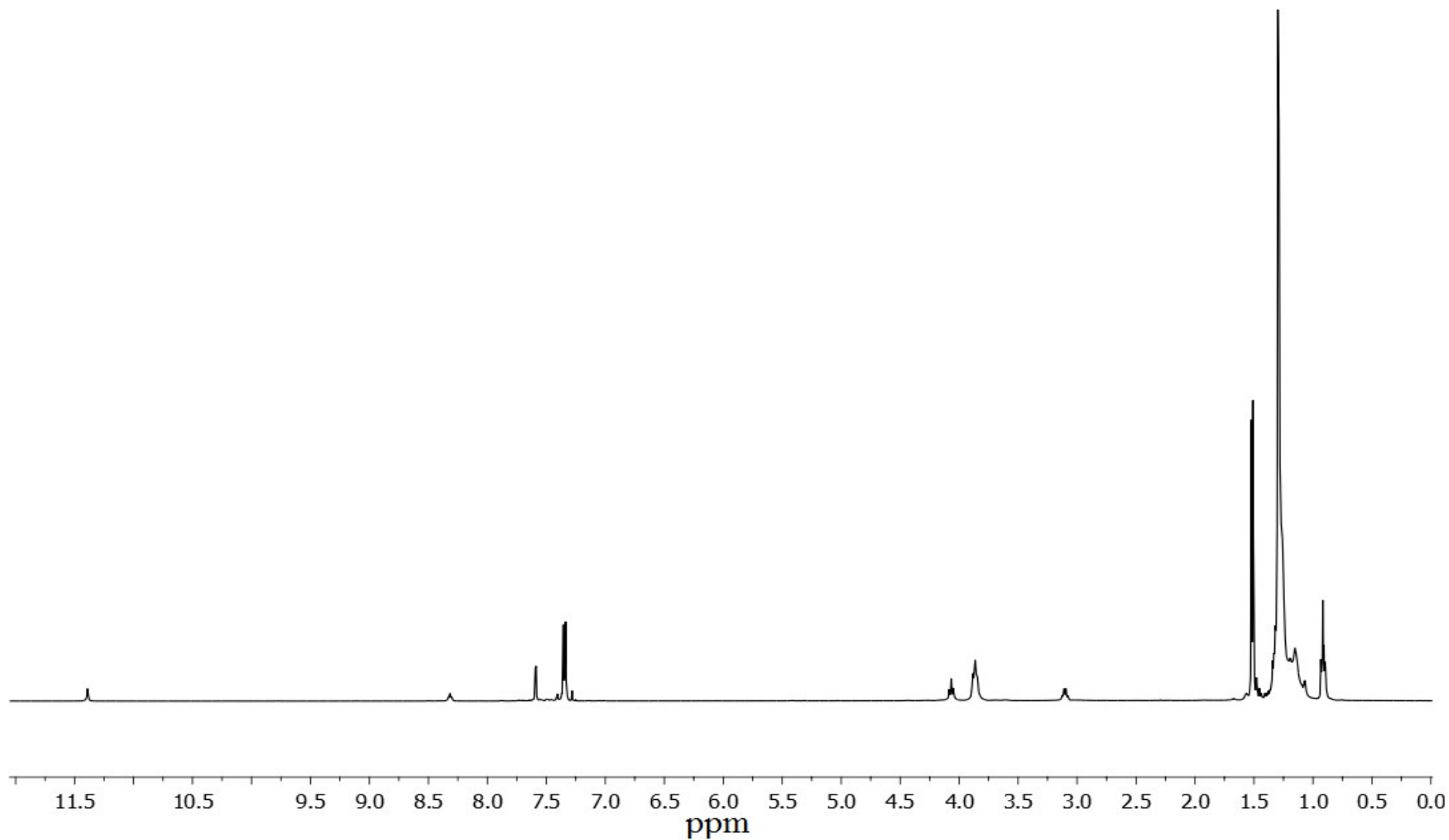


Figure S8. ^1H NMR spectrum of 5,11,17,23-Tetra-tert-butyl-25,26,27-tridecyl-28-[2-(bis-tert-butoxycarbonyl-guanidine)ethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-alternate) (**3d**). (CDCl_3 , 25°C , 400 MHz).

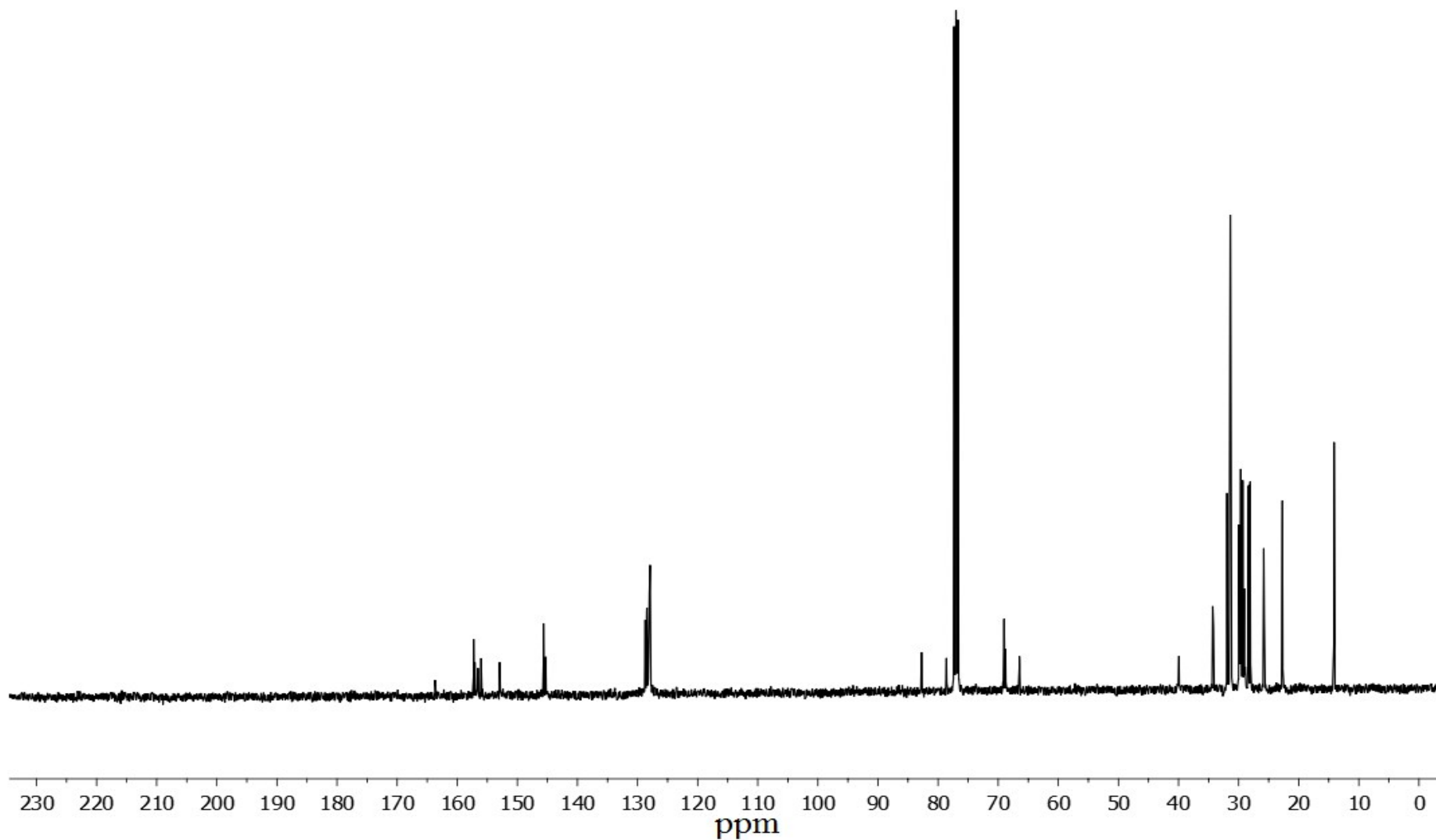


Figure S9. ^{13}C NMR spectrum of 5,11,17,23-Tetra-tert-butyl-25,26,27-tridecyl-28-[2-(bis-tert-butoxycarbonyl-guanidine)ethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-alternate) (**3d**). (CDCl_3 , 25°C , 400 MHz).

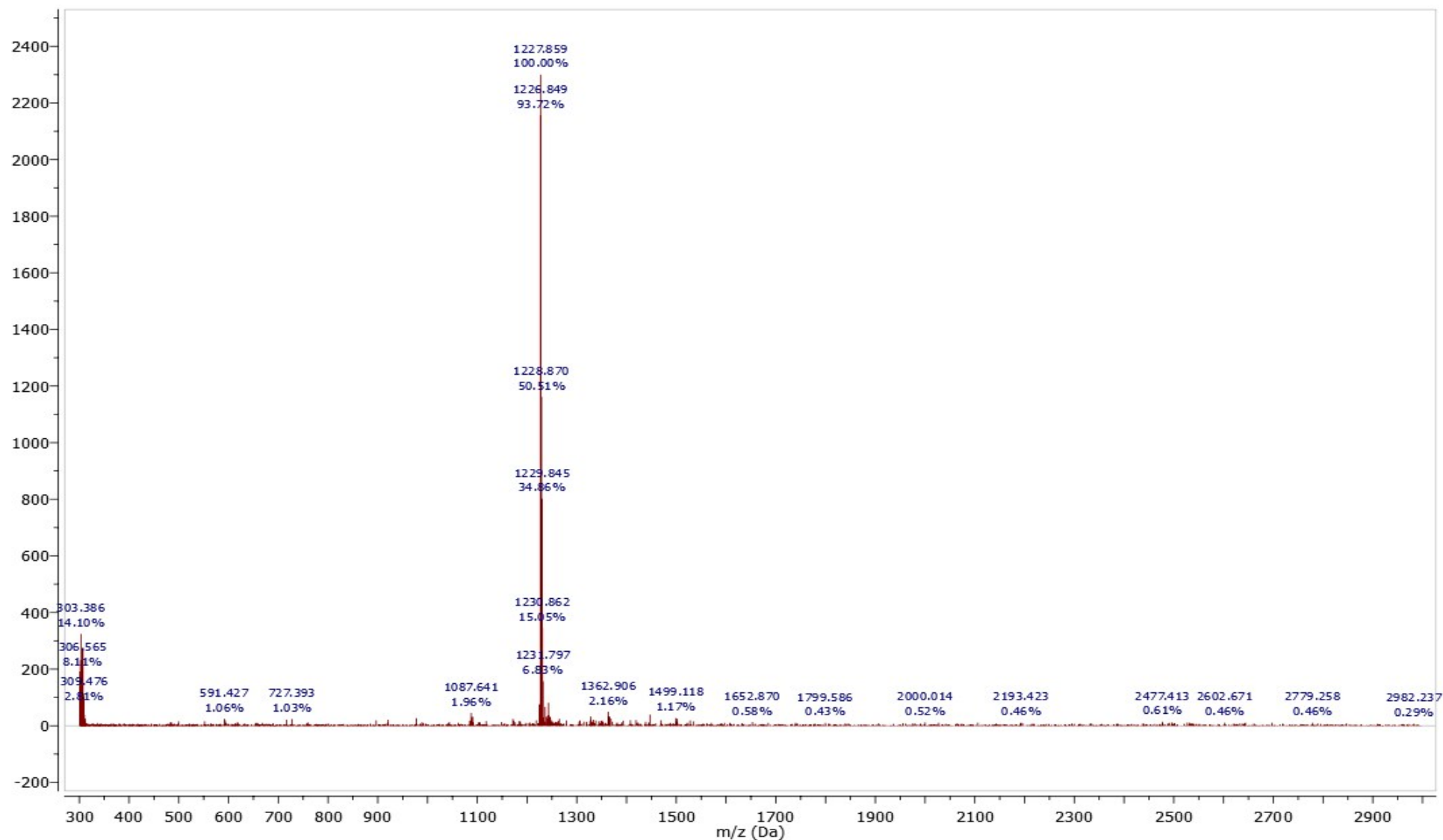


Figure S10. MALDI MS of 5,11,17,23-Tetra-tert-butyl-25,26,27-tridecyl-28-[2-(bis-tert-butoxycarbonyl-guanidine)ethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-alternate) (**3d**). (*p*-nitroaniline matrix).

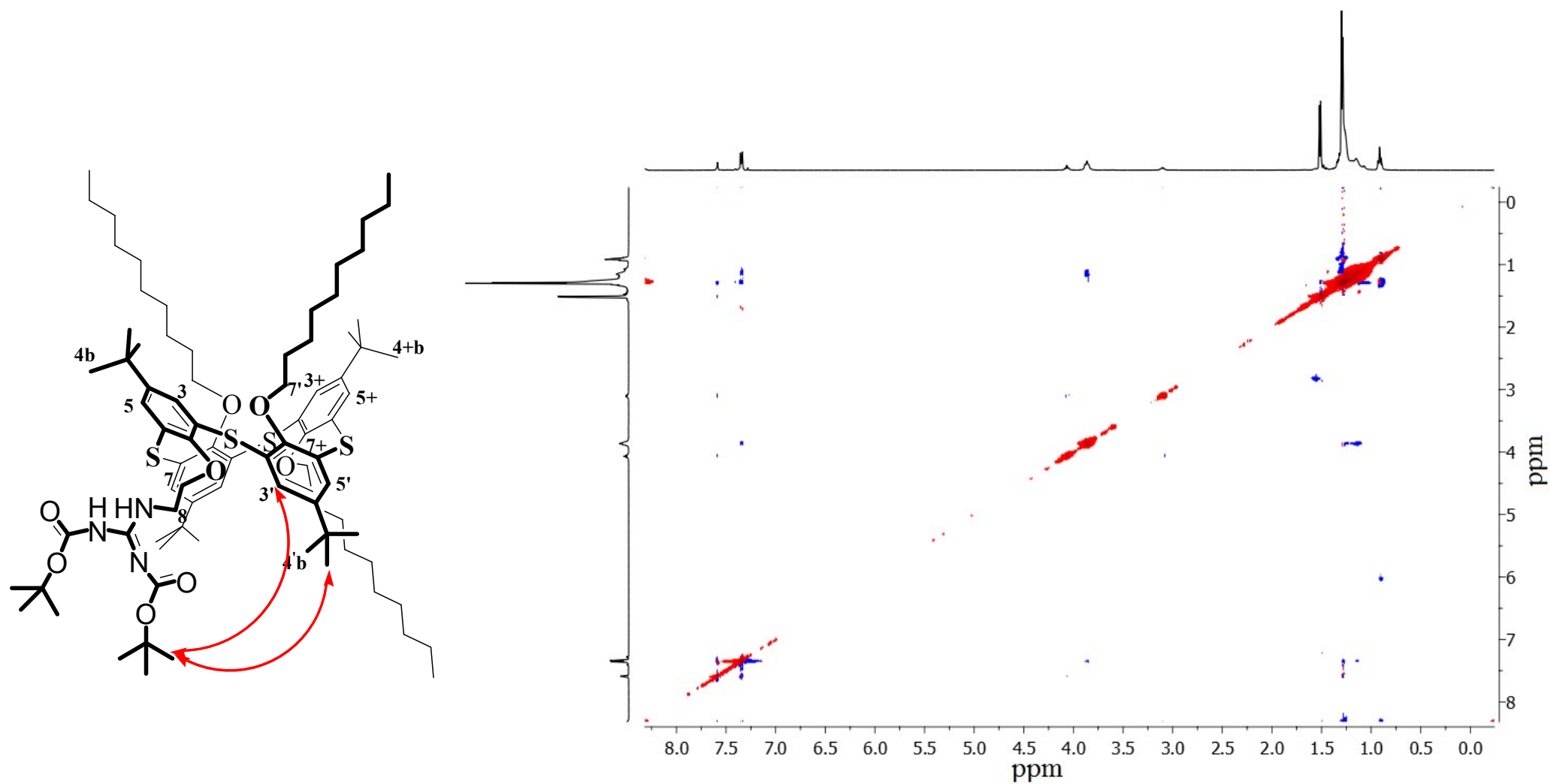


Figure S11. NOESY ^1H - ^1H NMR spectrum of the compound 5,11,17,23-Tetra-tert-butyl-25,26,27-tridecyl-28-[2-(bis-tert-butoxycarbonyl-guanidine)ethoxy]-2,8,14,20-tetrathiacalix[4]arene (1,3-alternate) (**3d**). (CDCl_3 , 25°C , 400 MHz).

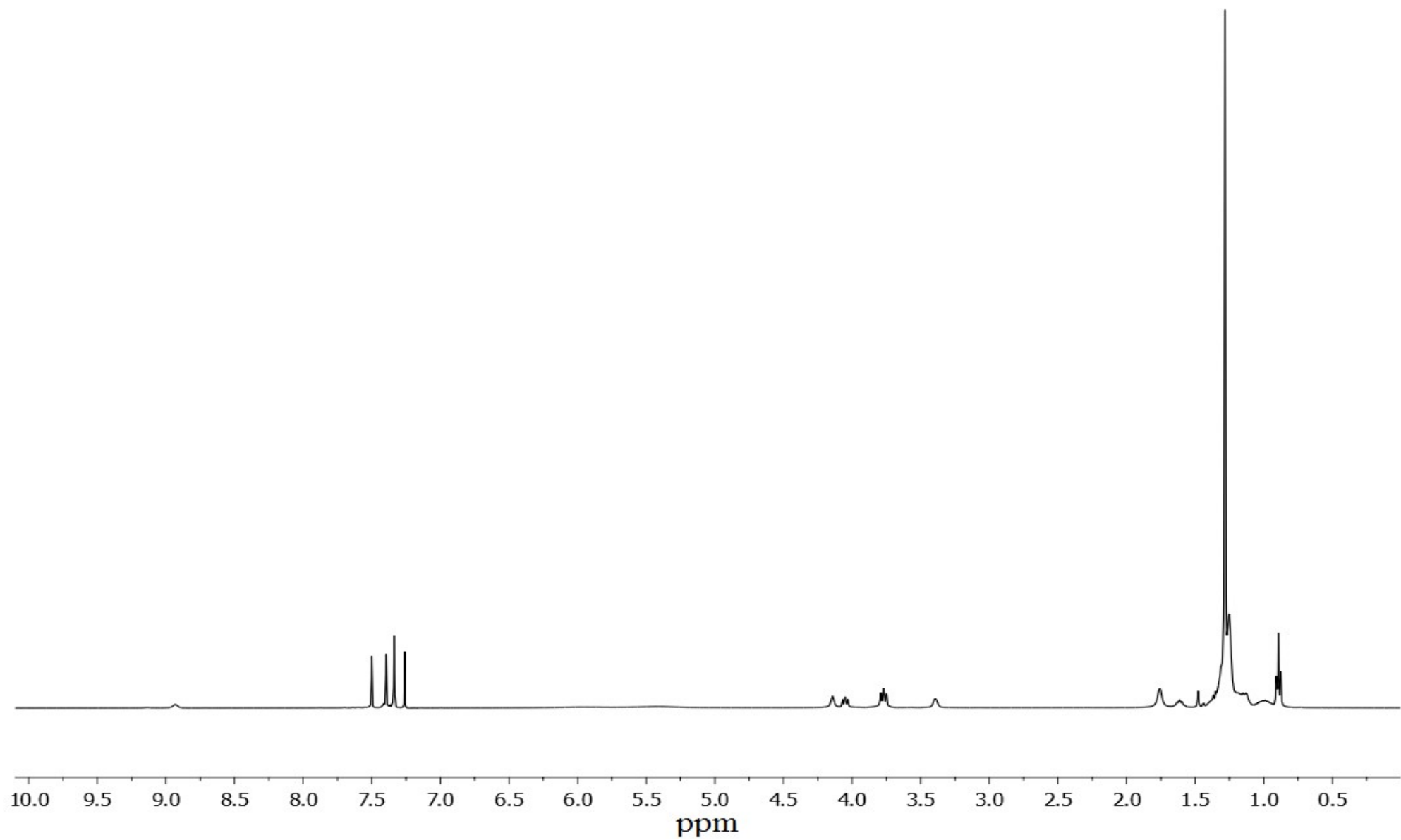


Figure S12. ^1H NMR spectrum of the compound 5,11,17,23-Tetra-*tert*-butyl-25,26,27-tridecyl-28-[2-guanidiniumethoxy]-2,8,14,20-tetrathiacalix[4]arene chloride (1,3-alternate) (**3**). (CDCl_3 , 25°C , 400 MHz).

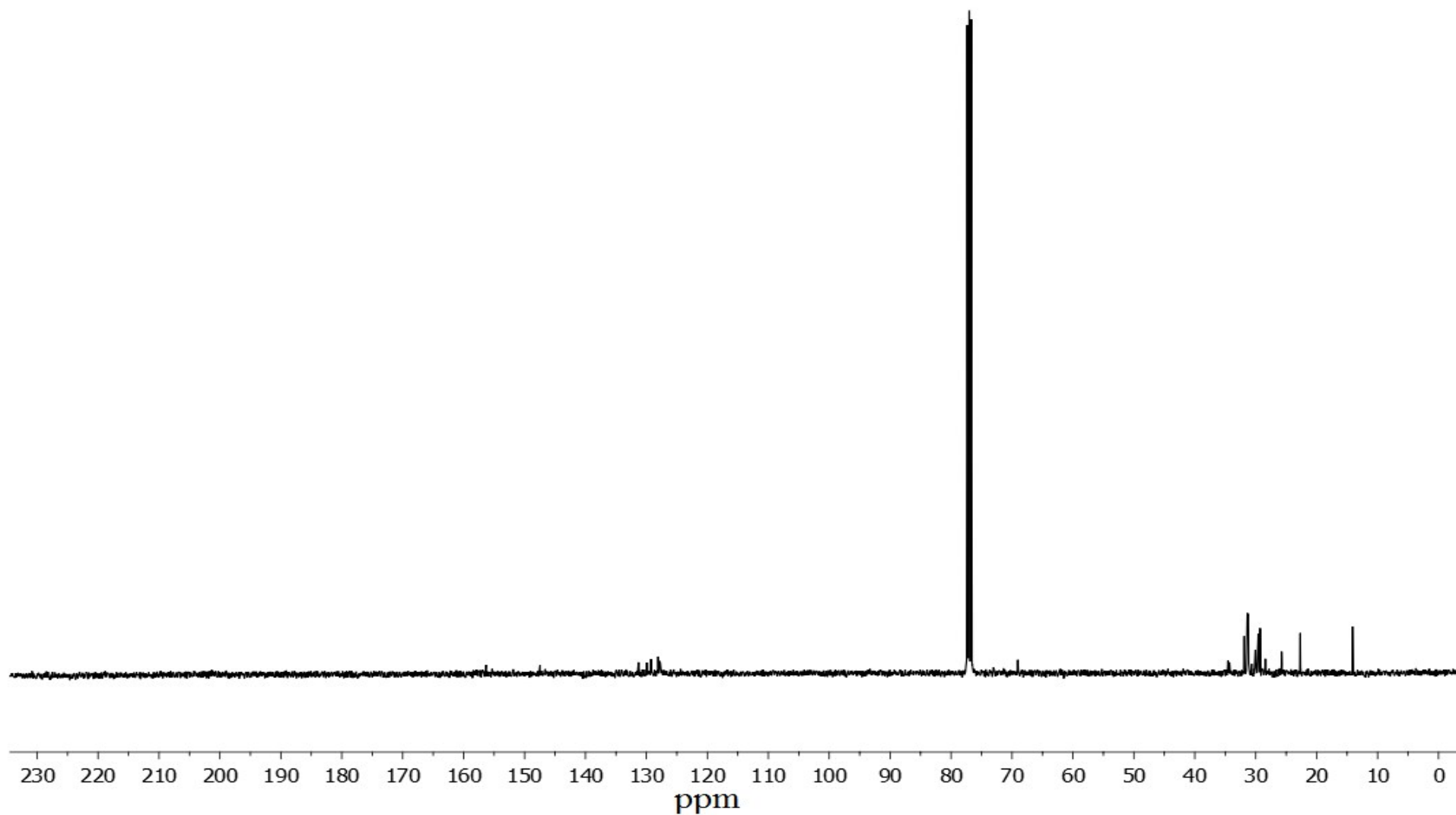


Figure S13. ^{13}C NMR spectrum of the compound 5,11,17,23-Tetra-*tert*-butyl-25,26,27-tridecyl-28-[2-guanidiniumethoxy]-2,8,14,20-tetrathiacalix[4]arene chloride (1,3-alternate) (**3**). (CDCl_3 , 25°C, 400 MHz).

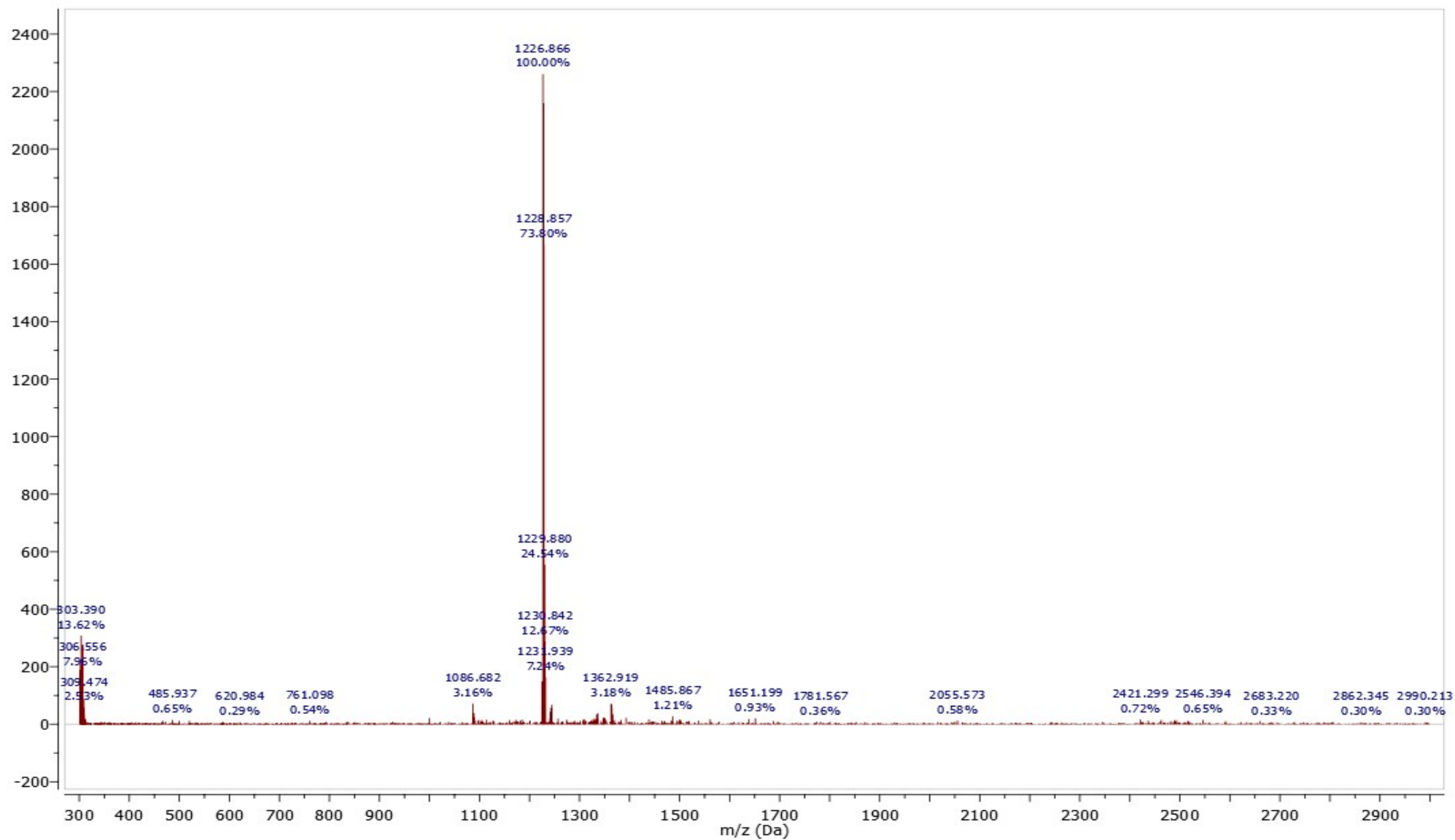


Figure S14. MALDI MS of 5,11,17,23-Tetra-*tert*-butyl-25,26,27-tridecyl-28-[2-guanidiniumethoxy]-2,8,14,20-tetrathiacalix[4]arene chloride (1,3-alternate) (**3**). (*p*-nitroaniline matrix).