



Supplementary Information

For

Macrocyclic Ionic Liquids with Amino Acid Residues: Synthesis and Influence of Thiacalix[4]arene Conformation on Thermal Stability

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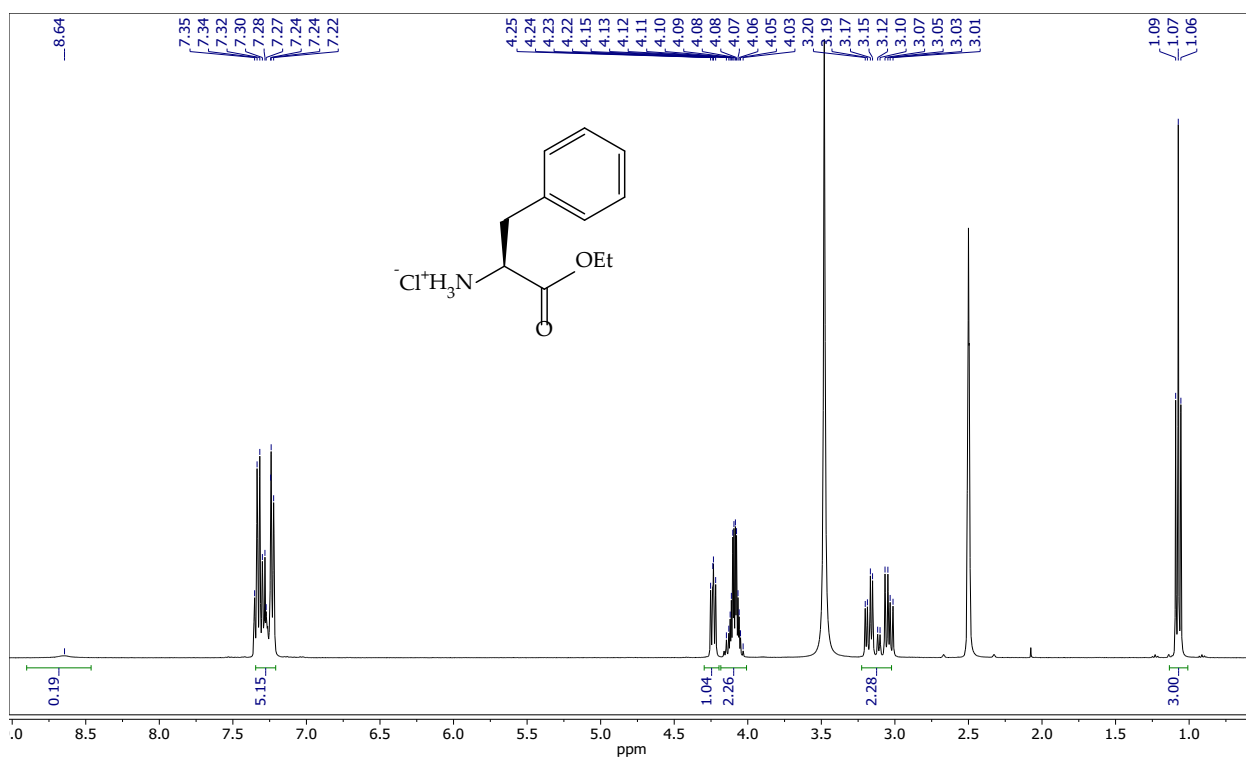


Figure S1. ¹H NMR spectrum of the compound **4**, DMSO-*d*₆, 298 K, 400 MHz.

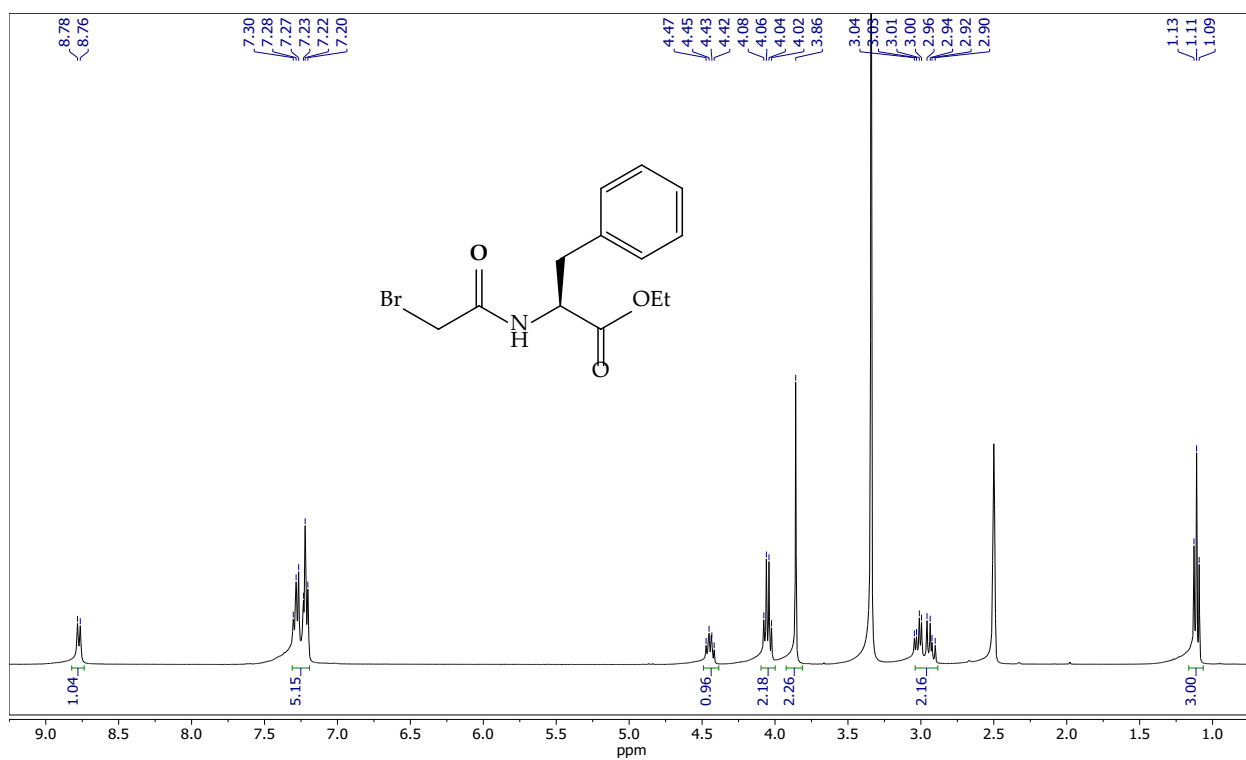


Figure S2. ¹H NMR spectrum of the compound **6**, DMSO-*d*₆, 298 K, 400 MHz.

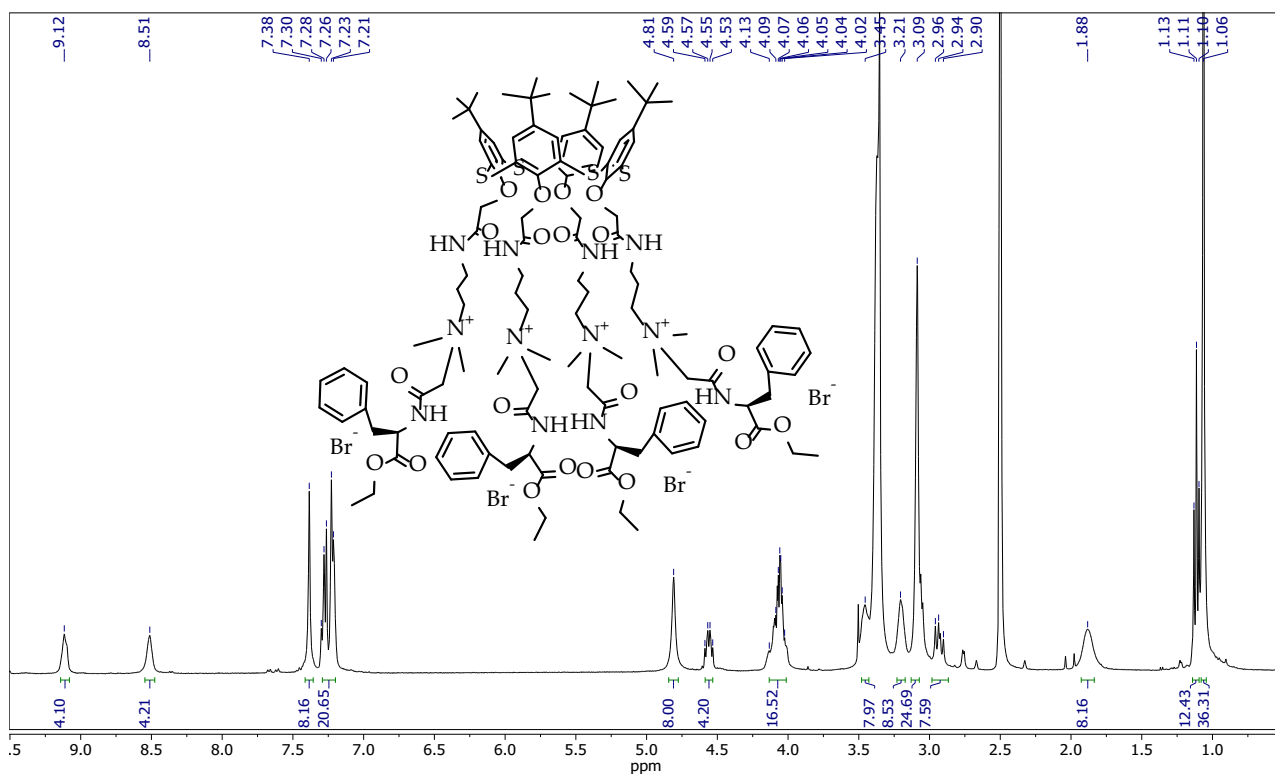


Figure S3. ^1H NMR spectrum of the compound **11** (*cone*), DMSO- d_6 , 298 K, 400 MHz.

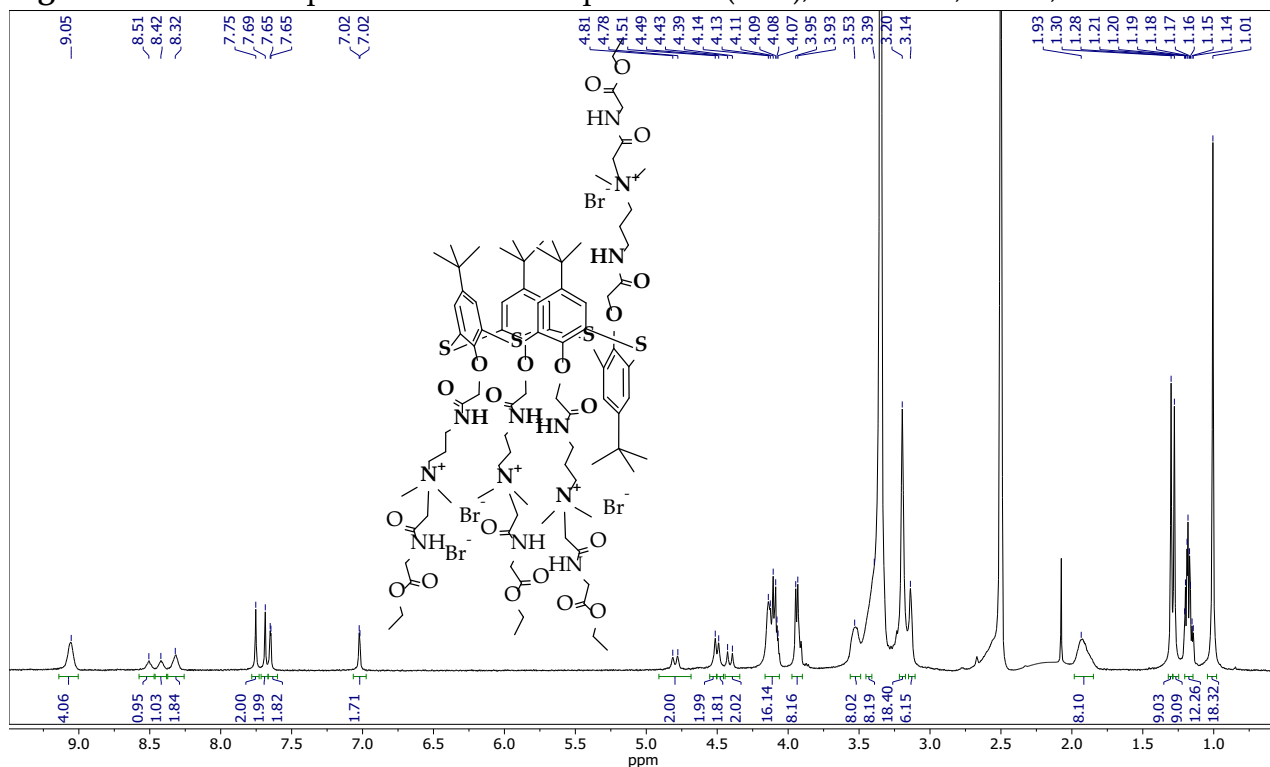
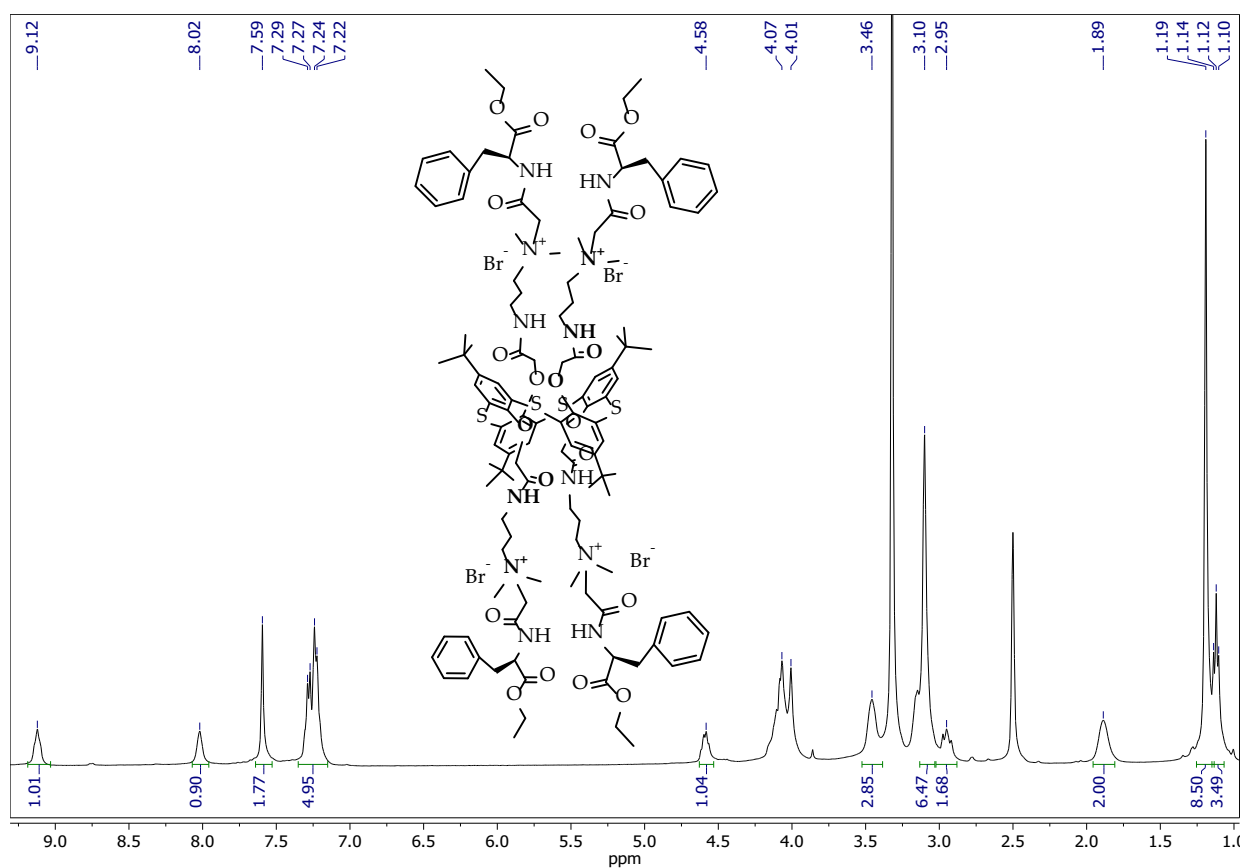
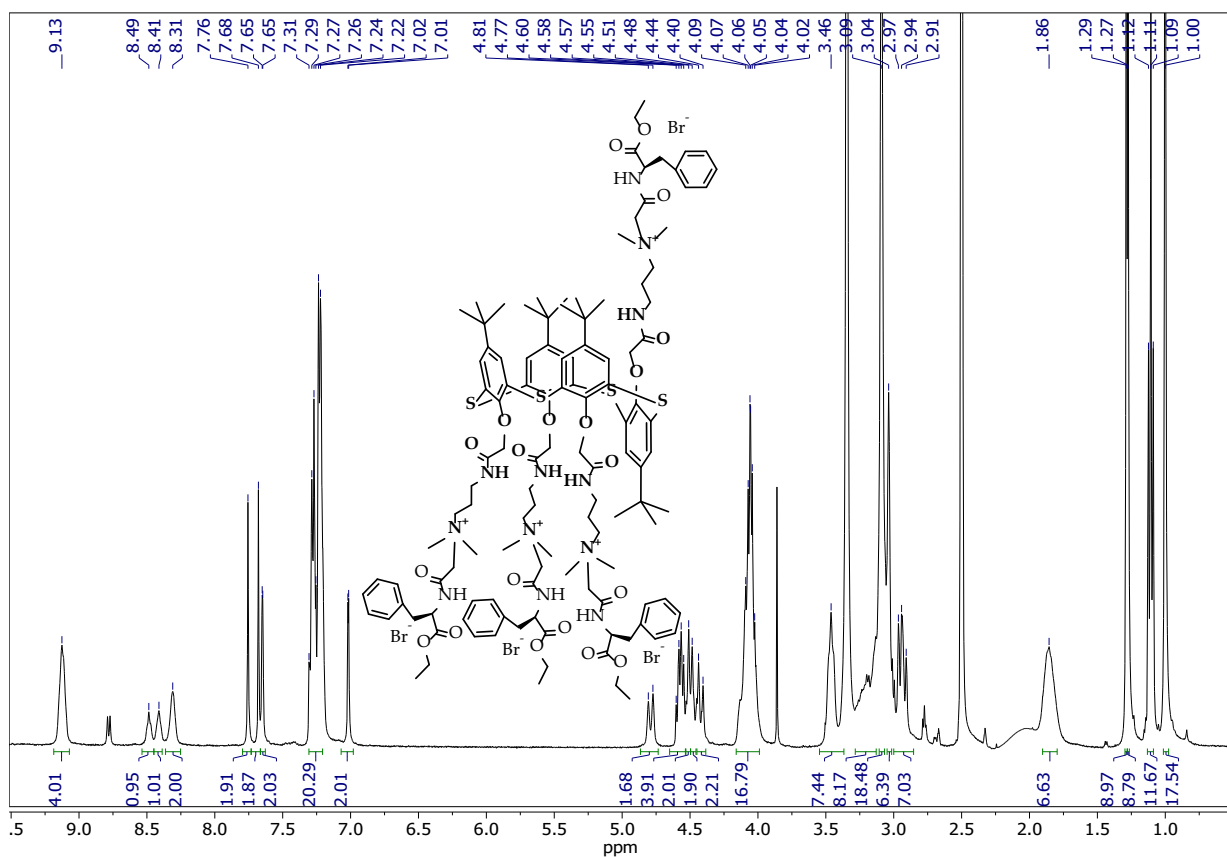


Figure S4. ^1H NMR spectrum of the compound **12** (*partial cone*), DMSO- d_6 , 298 K, 400 MHz.



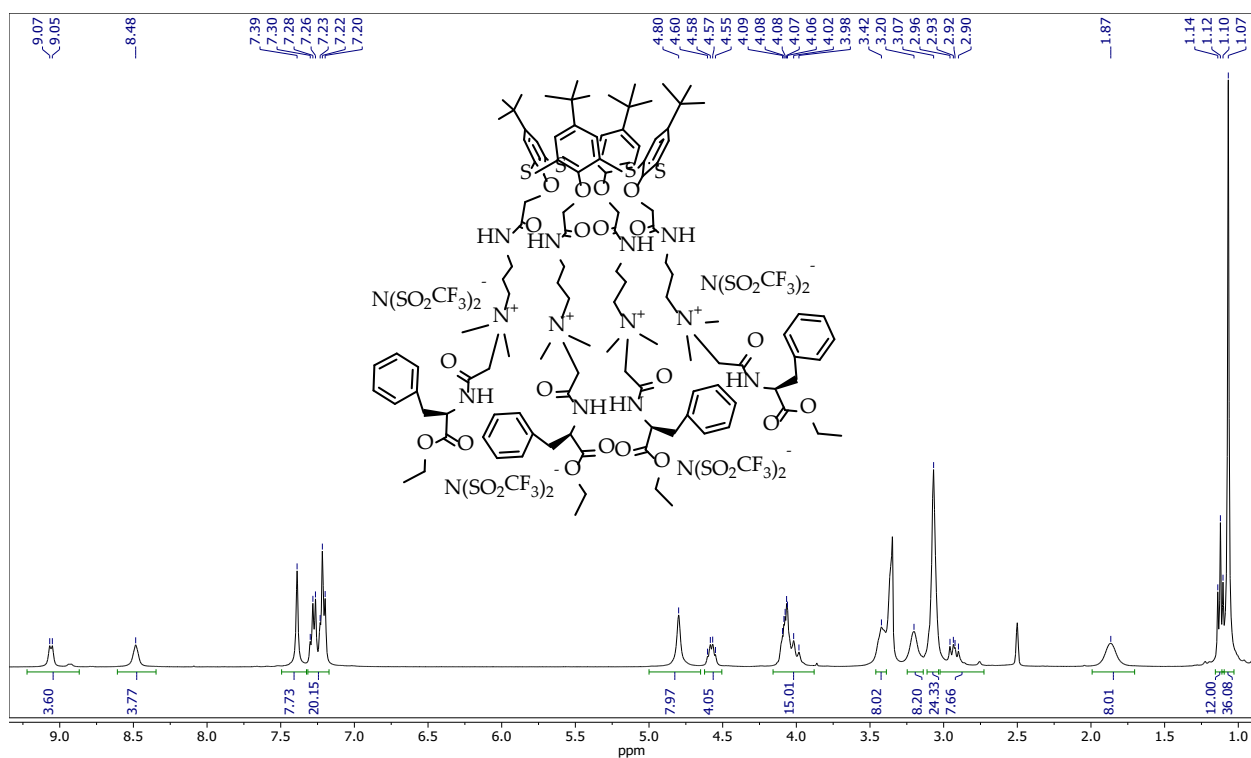


Figure S7. ¹H NMR spectrum of the compound **17** (cone), DMSO-*d*₆, 298 K, 400 MHz.

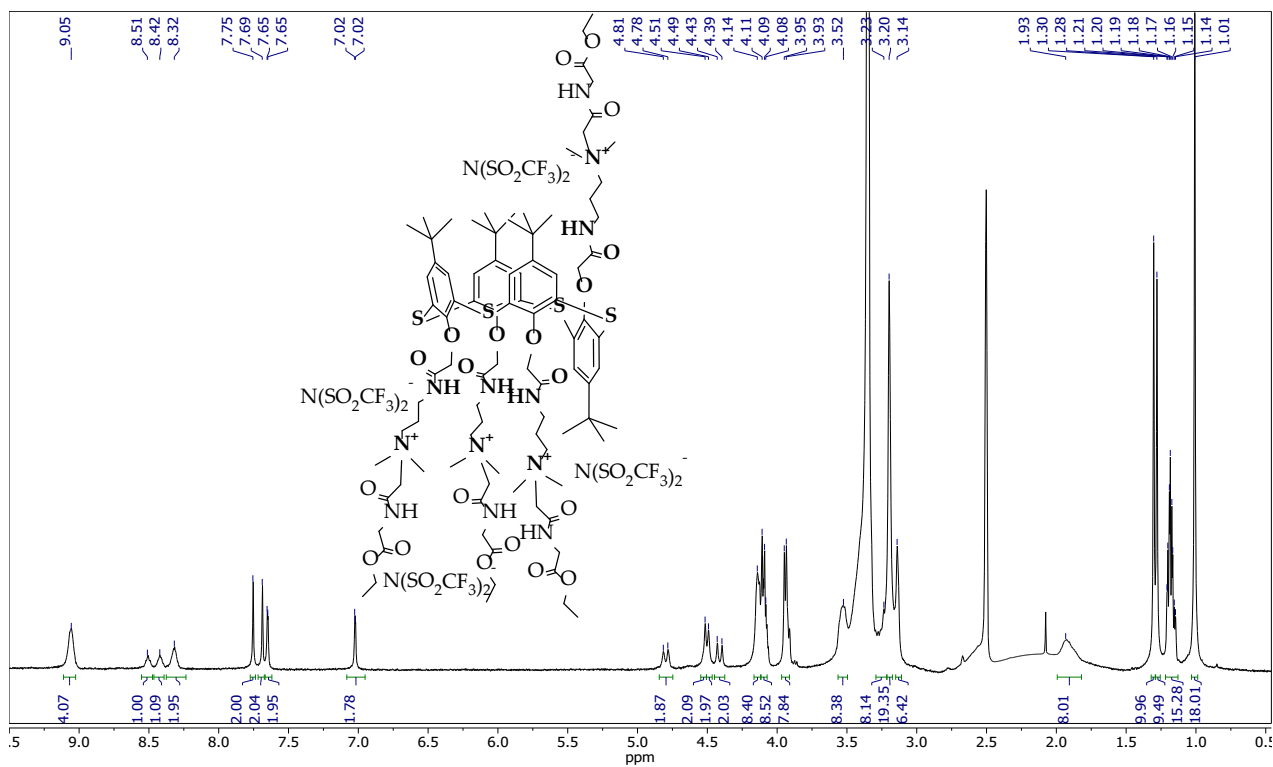


Figure S8. ¹H NMR spectrum of the compound **18** (partial cone), DMSO-*d*₆, 298 K, 400 MHz.

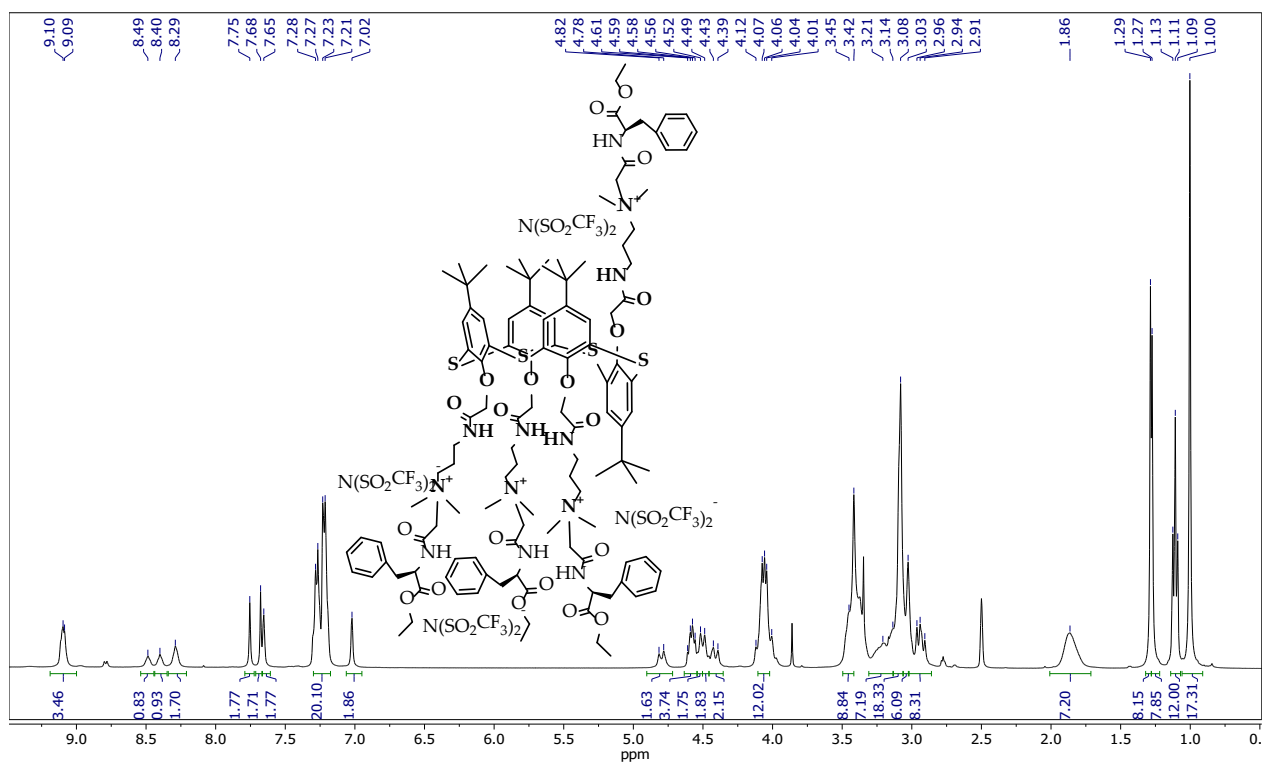


Figure S9. ^1H NMR spectrum of the compound **19** (*partial cone*), DMSO- d_6 , 298 K, 400 MHz.

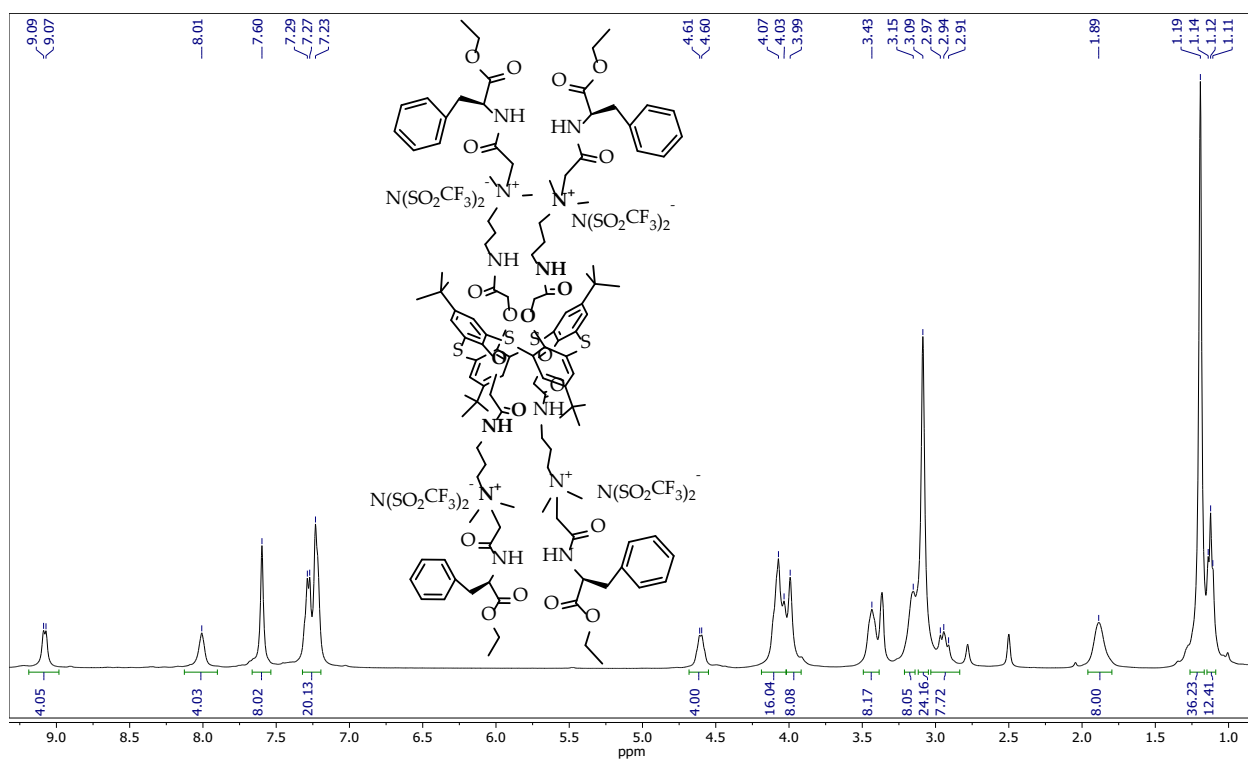
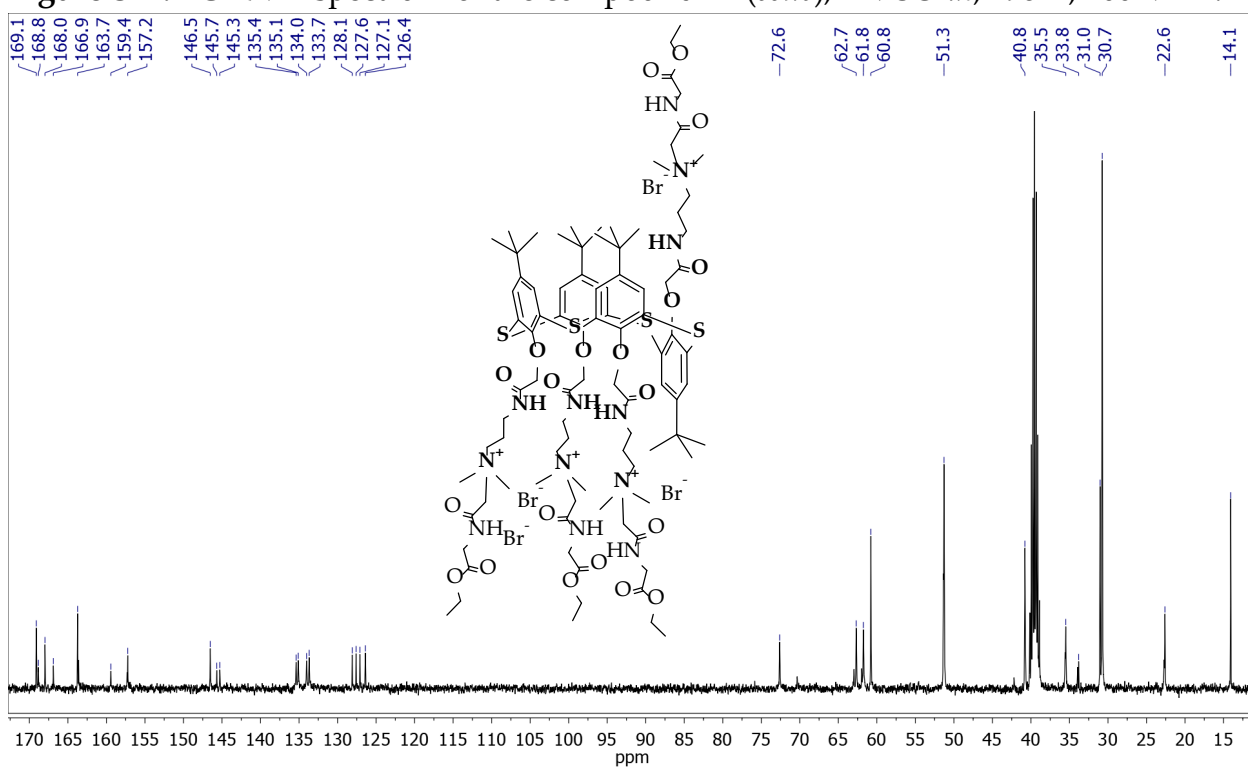
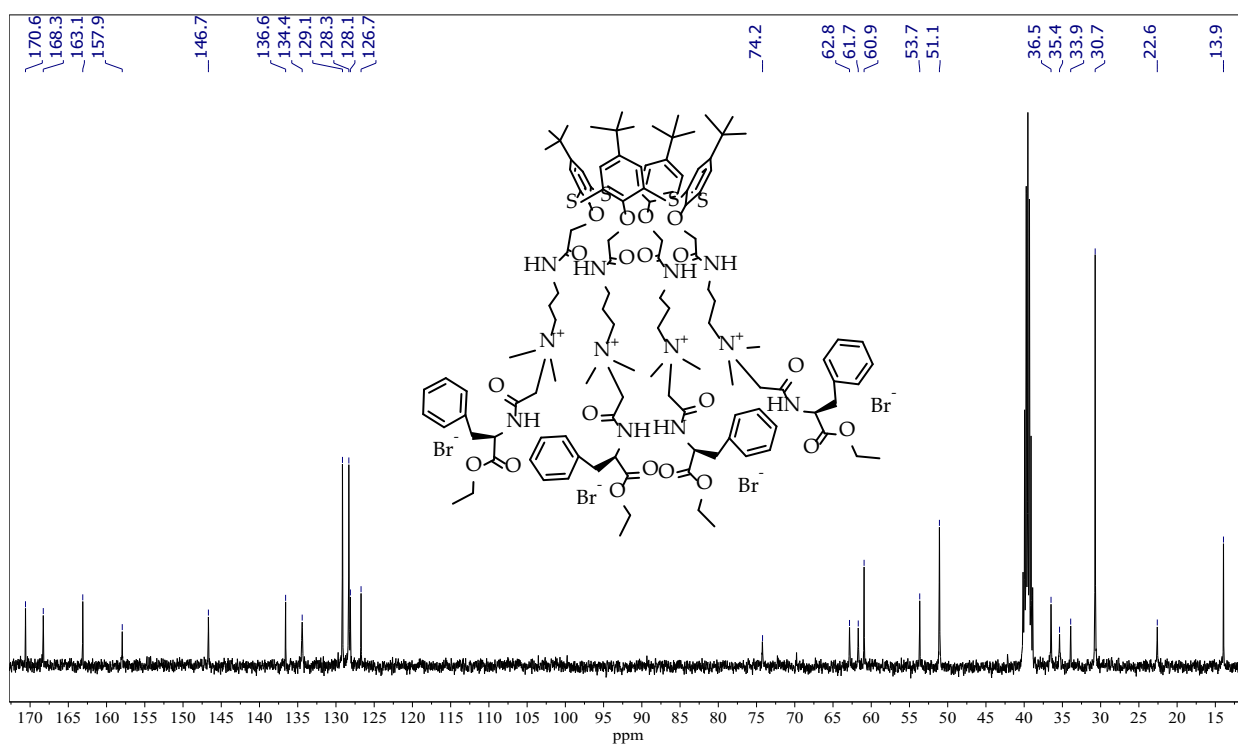


Figure S10. ^1H NMR spectrum of the compound **21** (*1,3-alternate*), DMSO- d_6 , 298 K, 400 MHz.



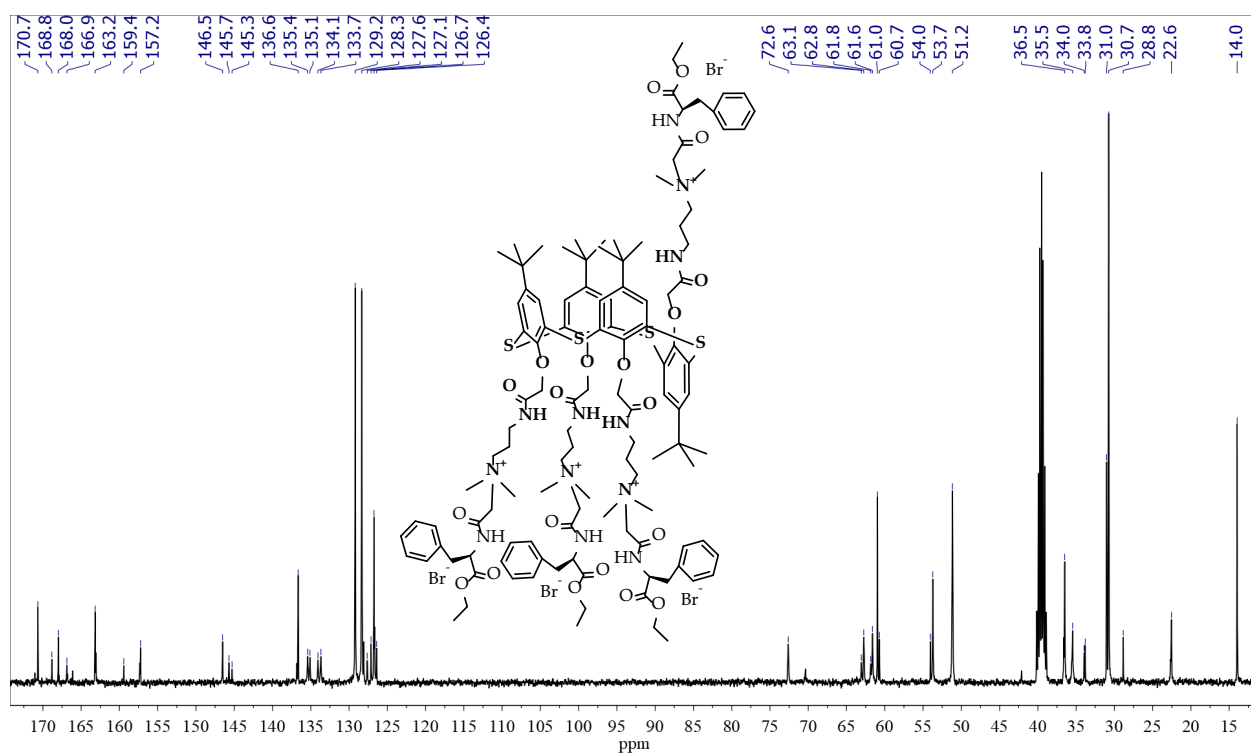


Figure S13. ^{13}C NMR spectrum of the compound **13** (*partial cone*), DMSO- d_6 , 298 K, 100 MHz.

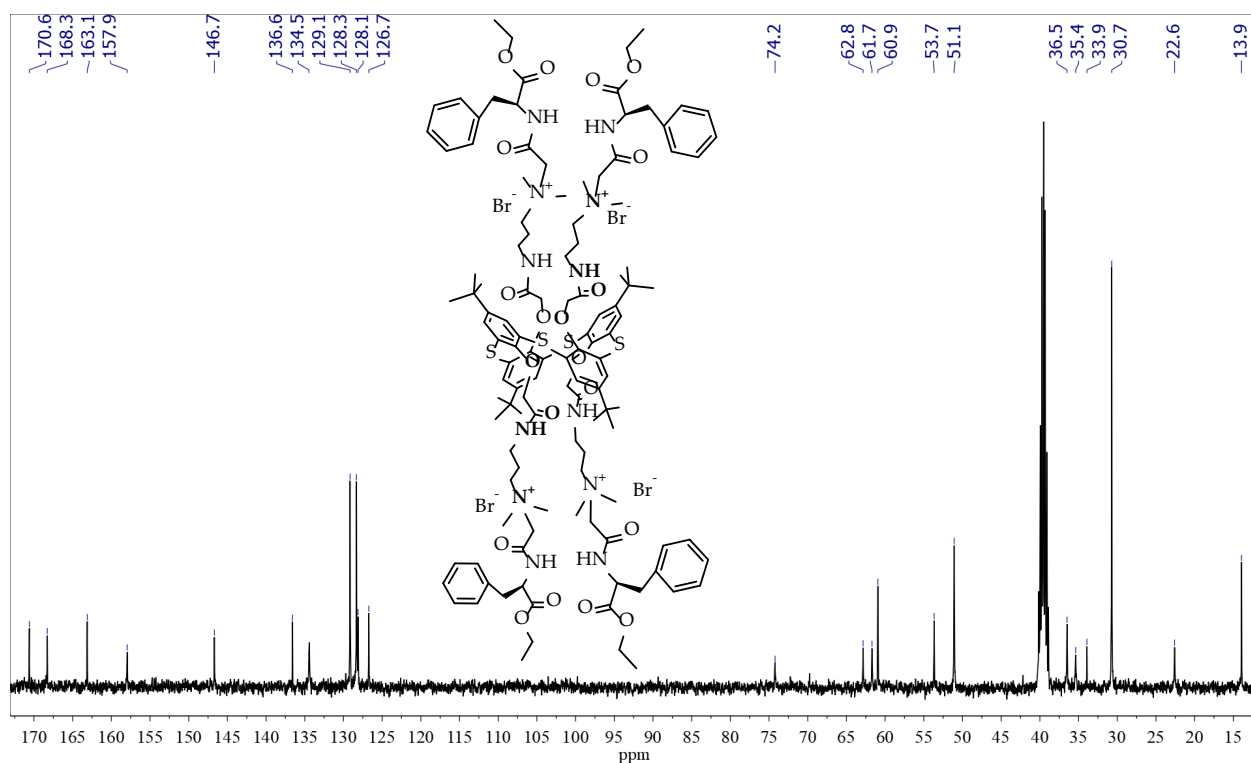
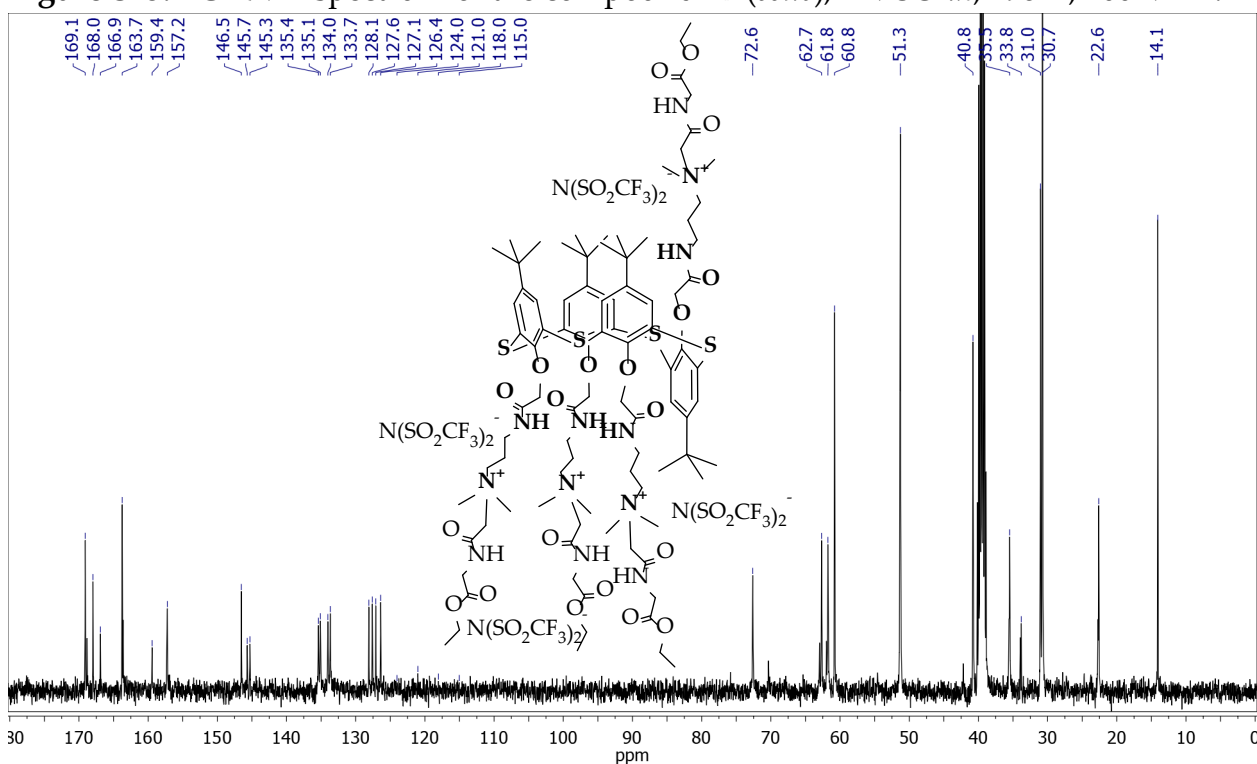
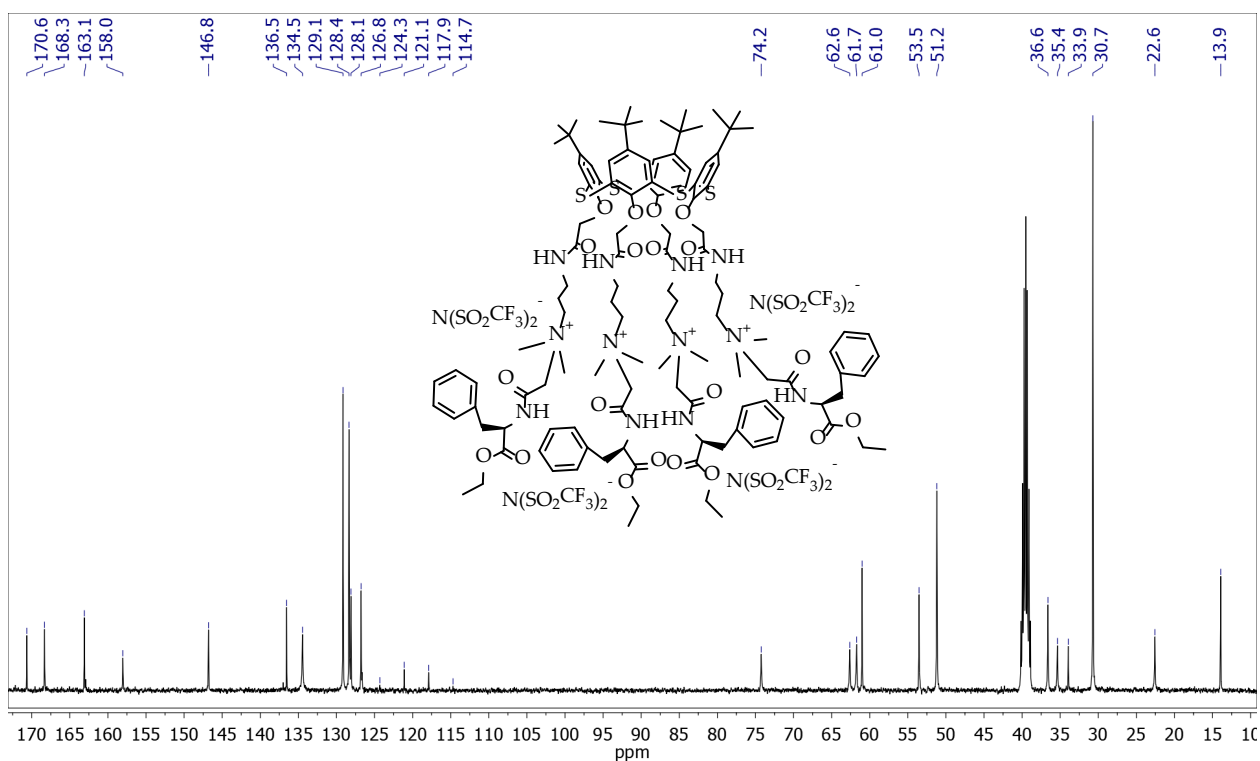


Figure S14. ^{13}C NMR spectrum of the compound **15** (*1,3-alternate*), DMSO- d_6 , 298 K, 100 MHz.



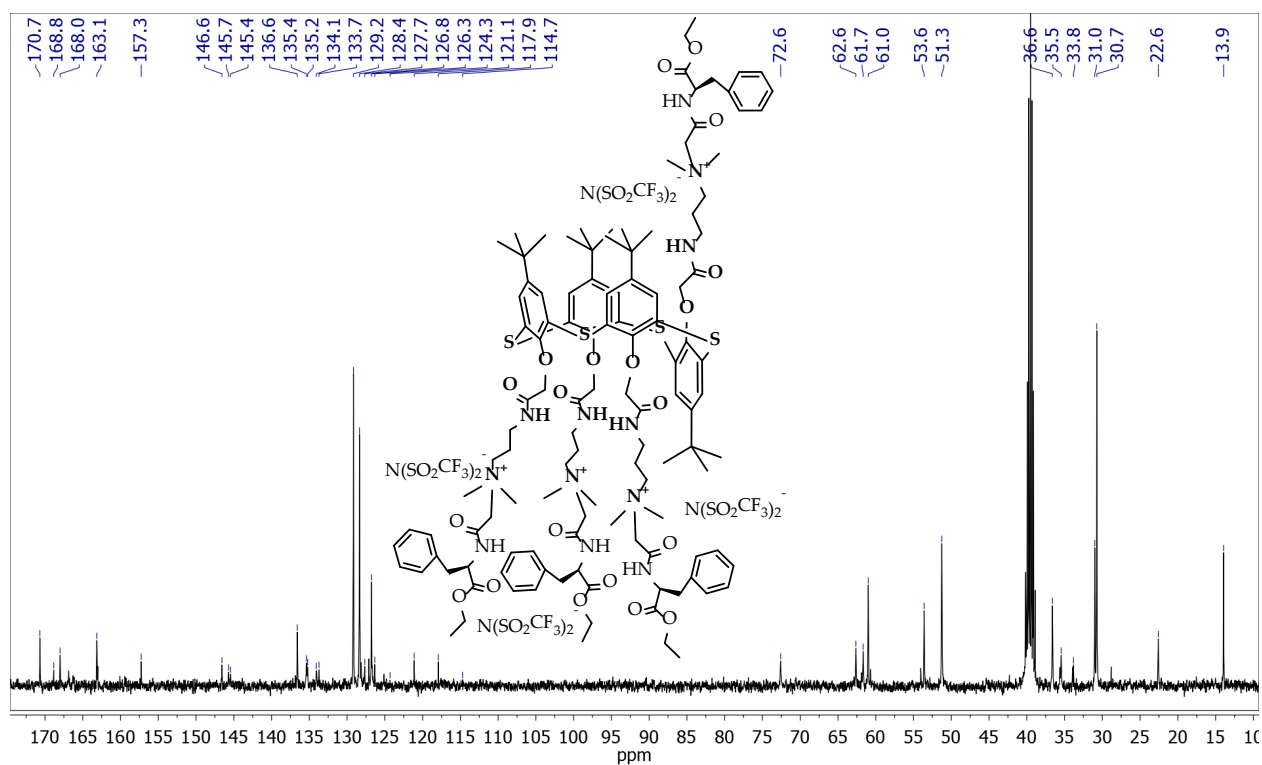


Figure S17. ¹³C NMR spectrum of the compound **19** (*partial cone*), DMSO-*d*₆, 298 K, 100 MHz.

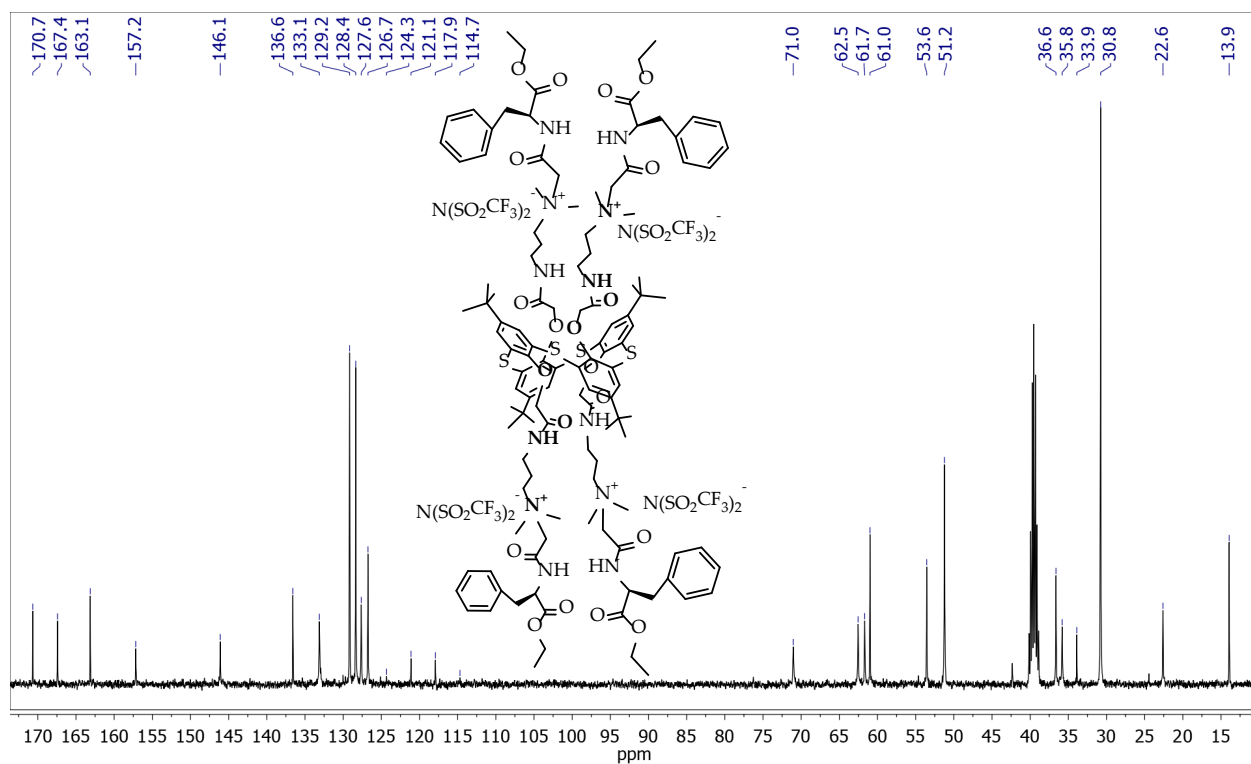


Figure S18. ¹³C NMR spectrum of the compound **21** (*1,3-alternate*), DMSO-*d*₆, 298 K, 100 MHz.

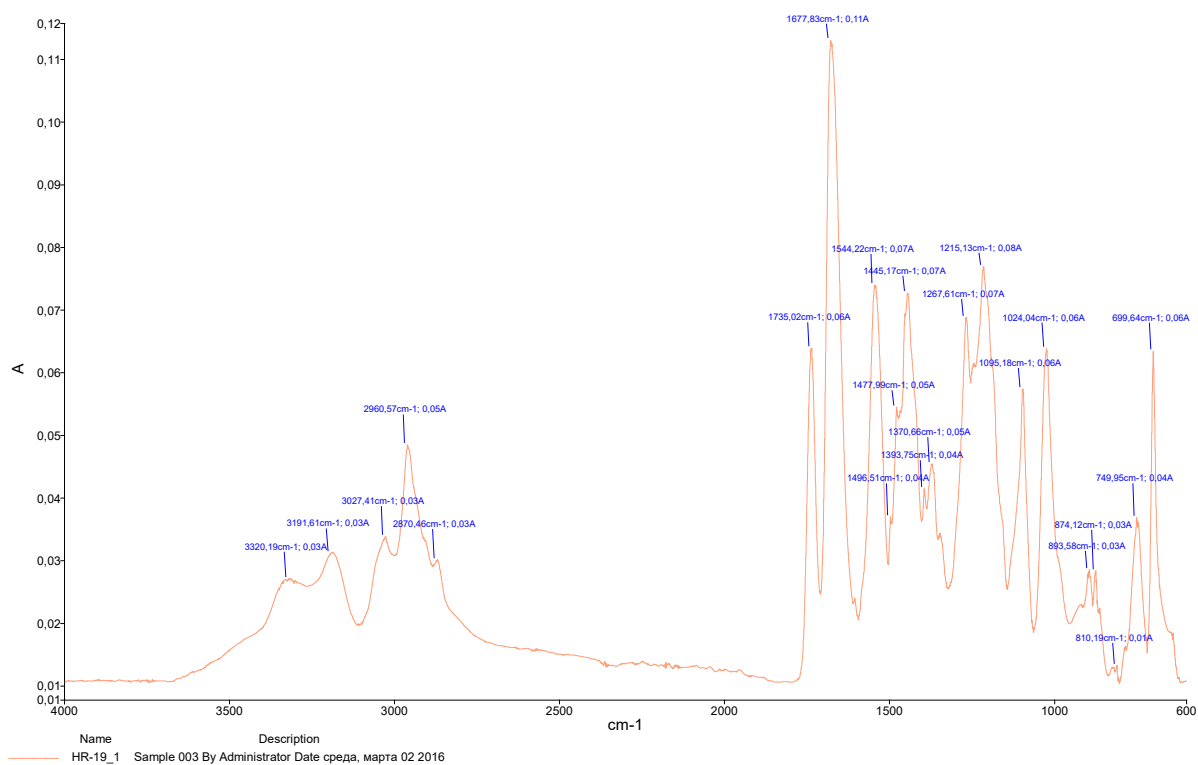


Figure S19. IR spectrum of the compound **11** (*cone*).

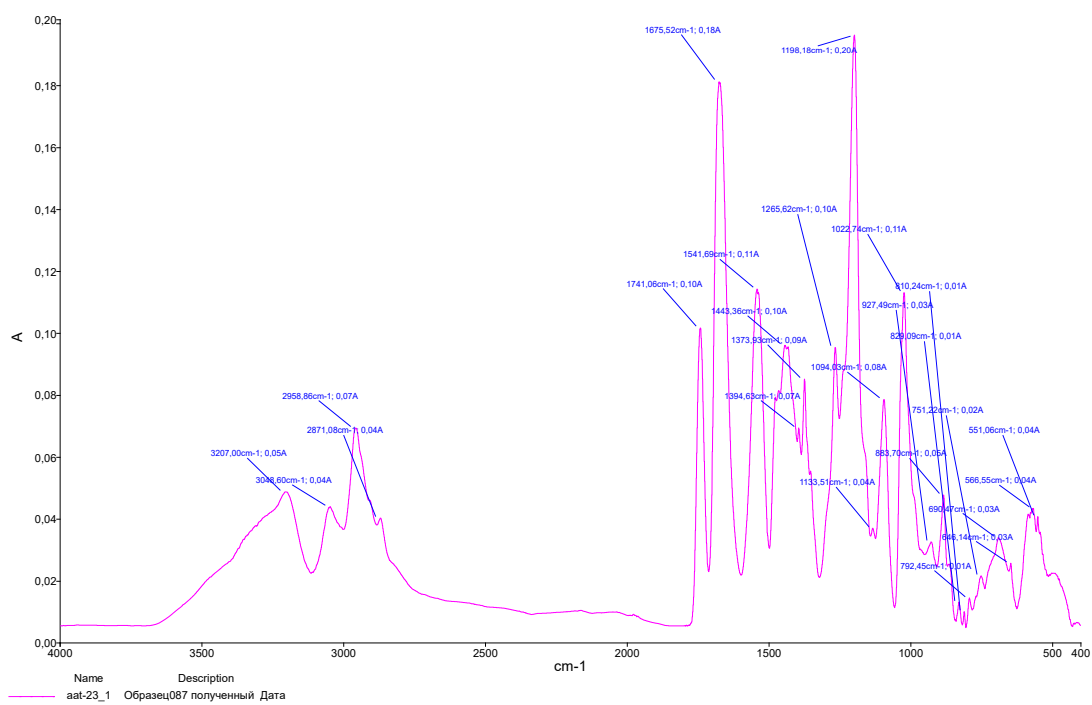


Figure S20. IR spectrum of the compound **12** (*partial cone*).

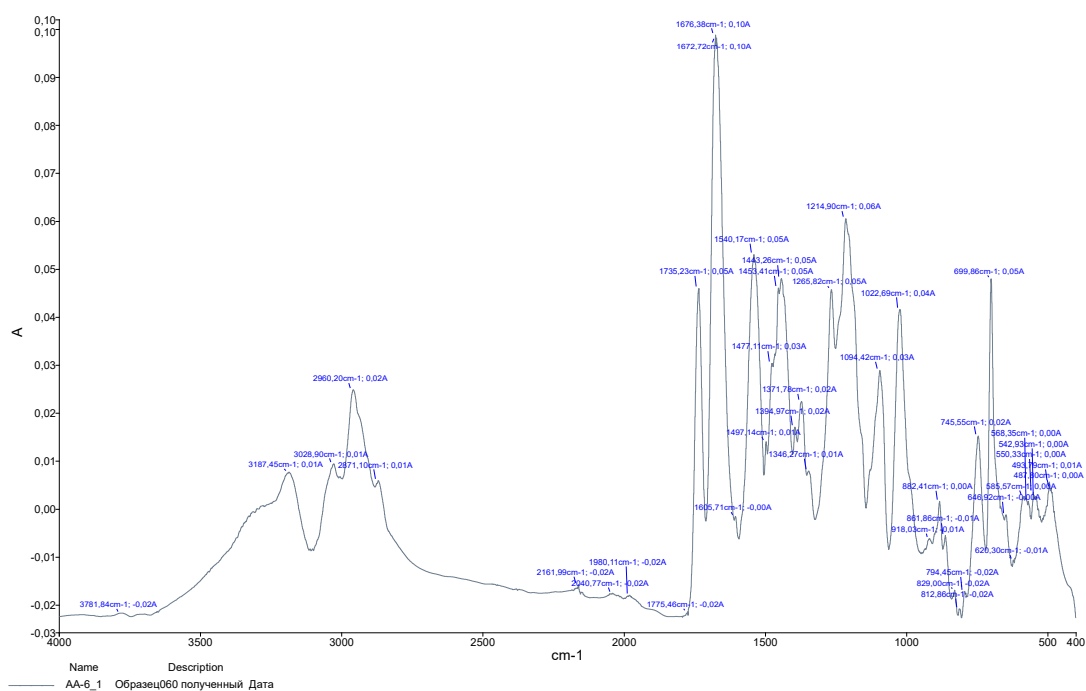


Figure S21. IR spectrum of the compound **13** (*partial cone*).

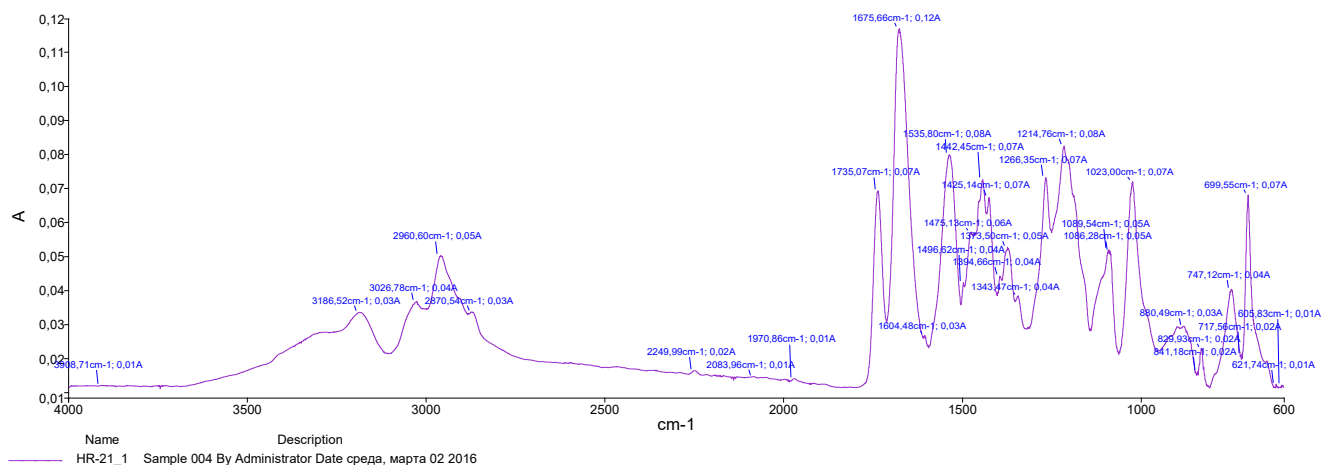


Figure S22. IR spectrum of the compound **15** (*1,3-alternate*).

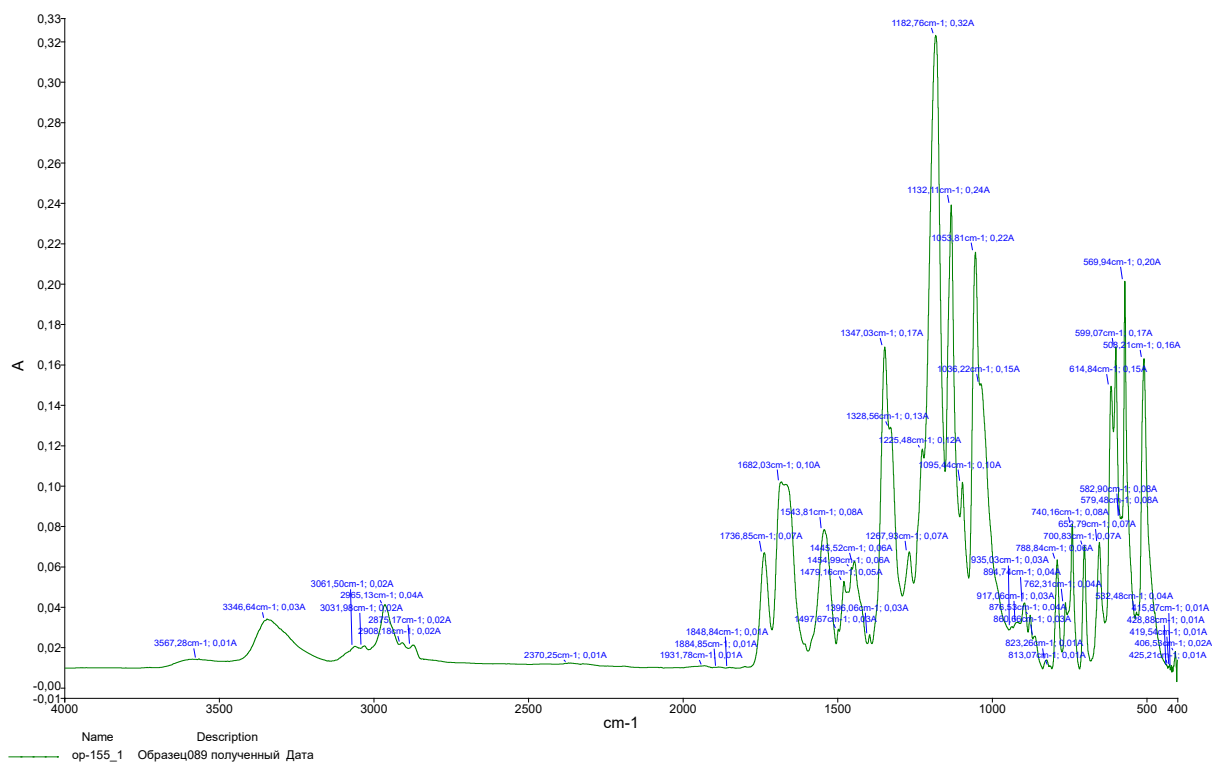


Figure S23. IR spectrum of the compound 17 (*cone*).

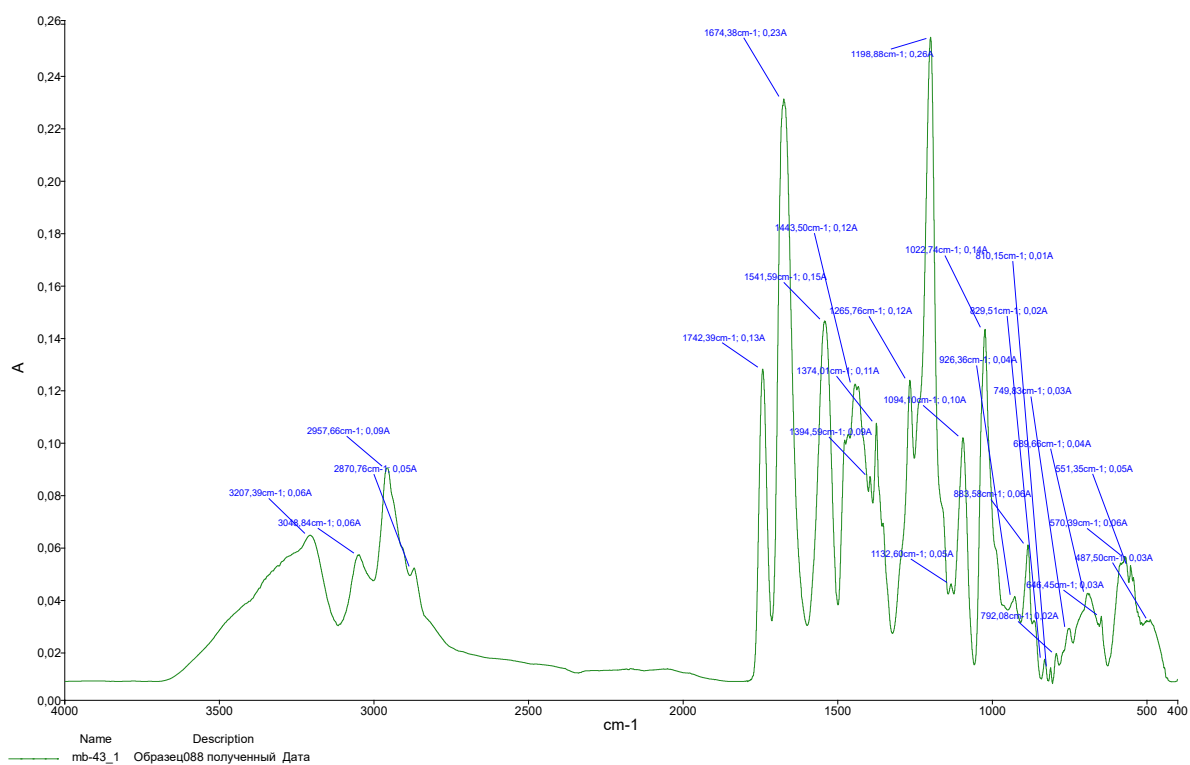


Figure S24. IR spectrum of the compound 18 (*partial cone*).

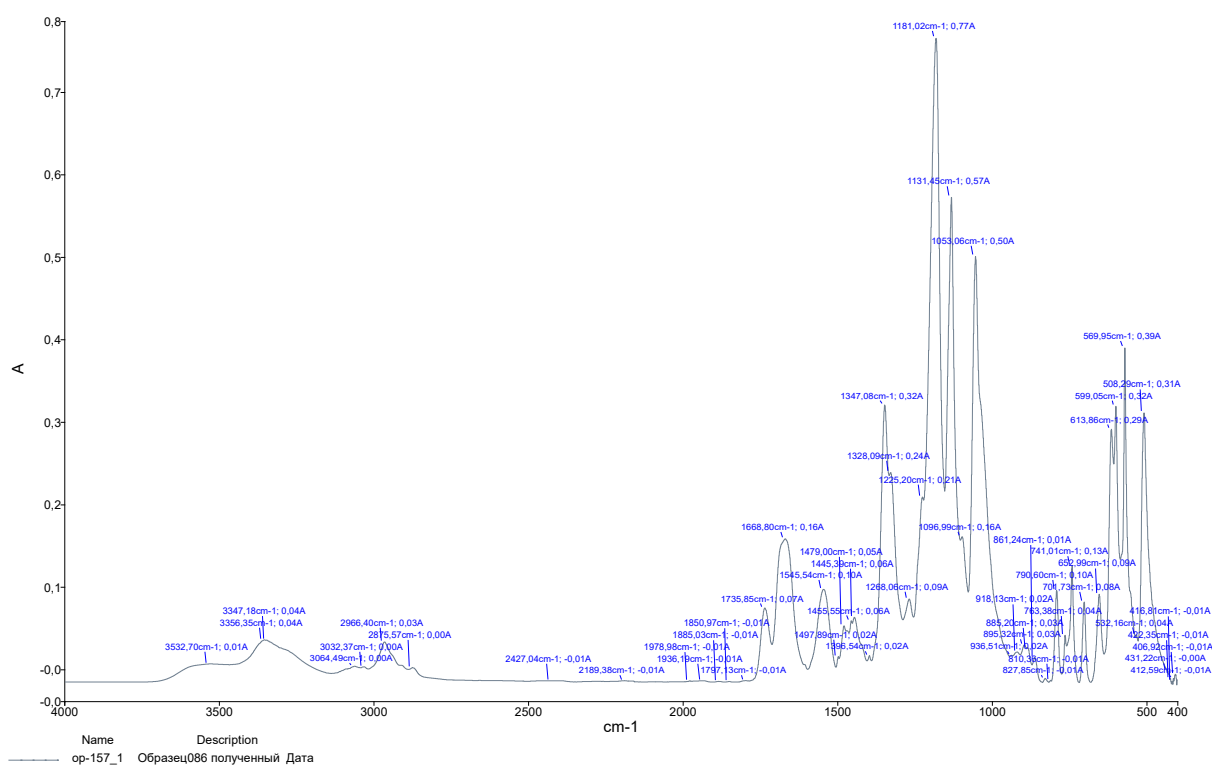


Figure S25. IR spectrum of the compound 19 (*partial cone*).

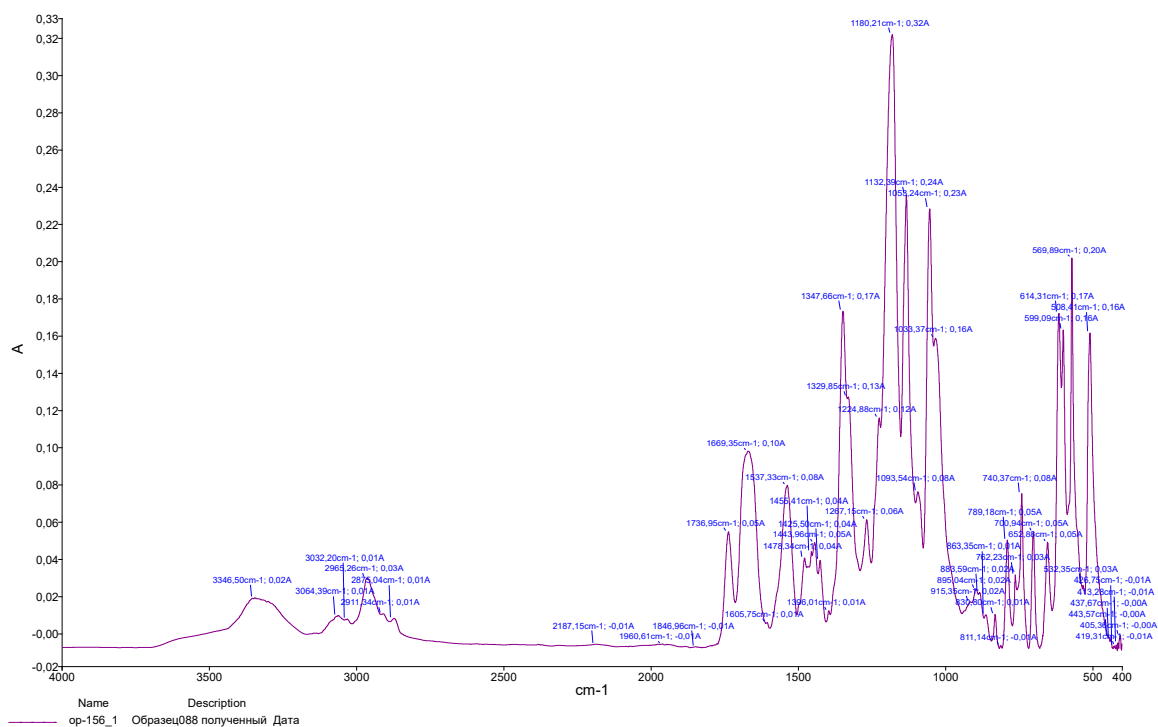


Figure S26. IR spectrum of the compound 21 (*1,3-alternate*).

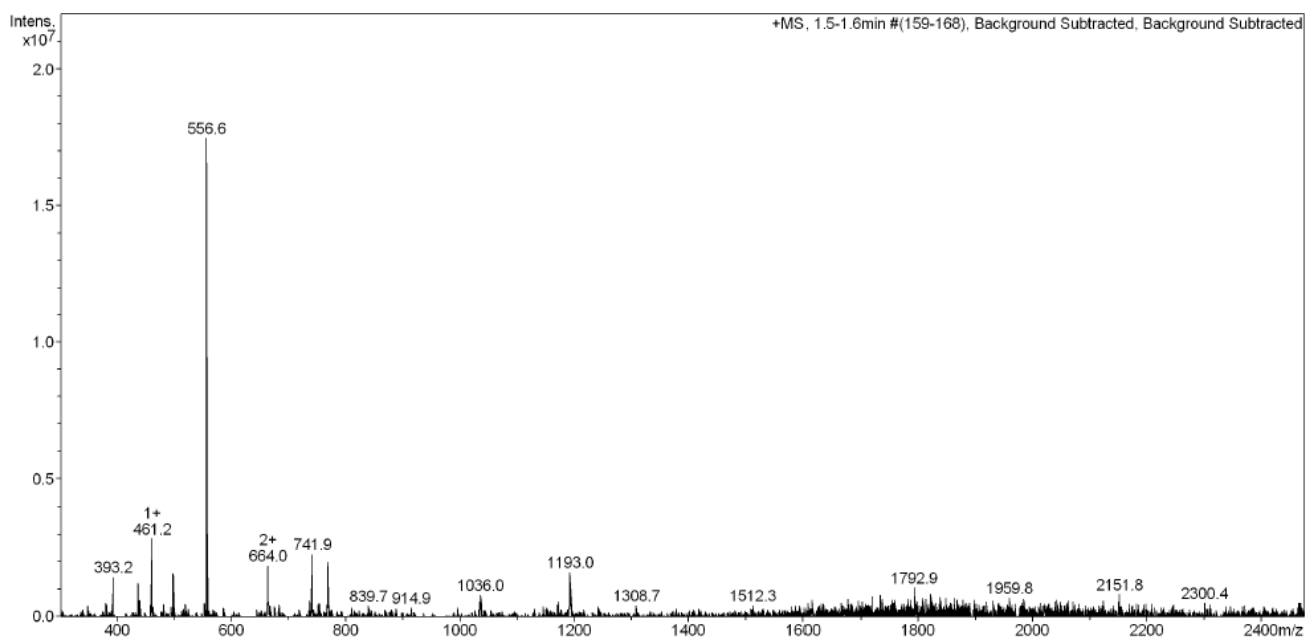


Figure S27. Mass spectrum (ESI) of the compound **11** (*cone*).

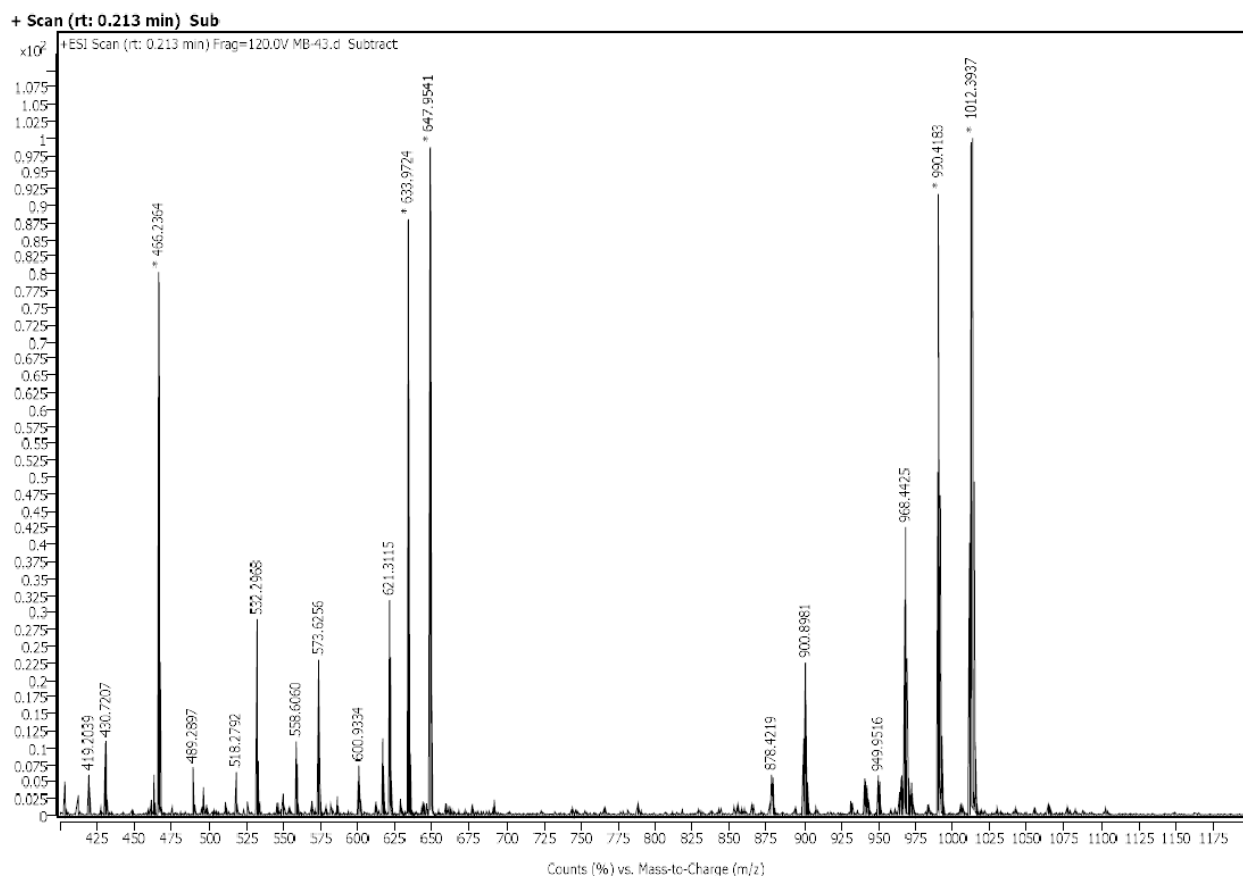


Figure S28. HR Mass spectrum (ESI) of the compound **12** (*partial cone*).

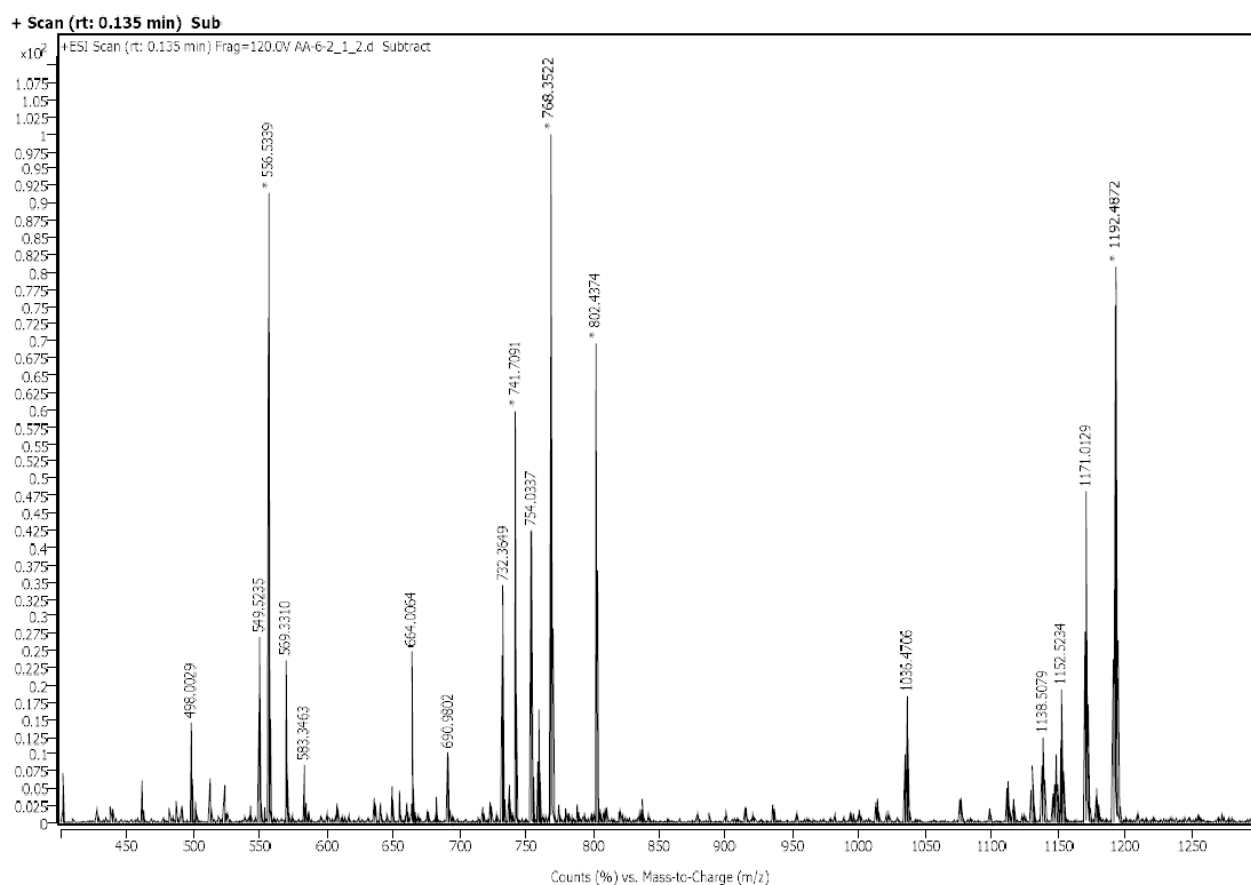


Figure S29. HR Mass spectrum (ESI) of the compound **13** (*partial cone*).

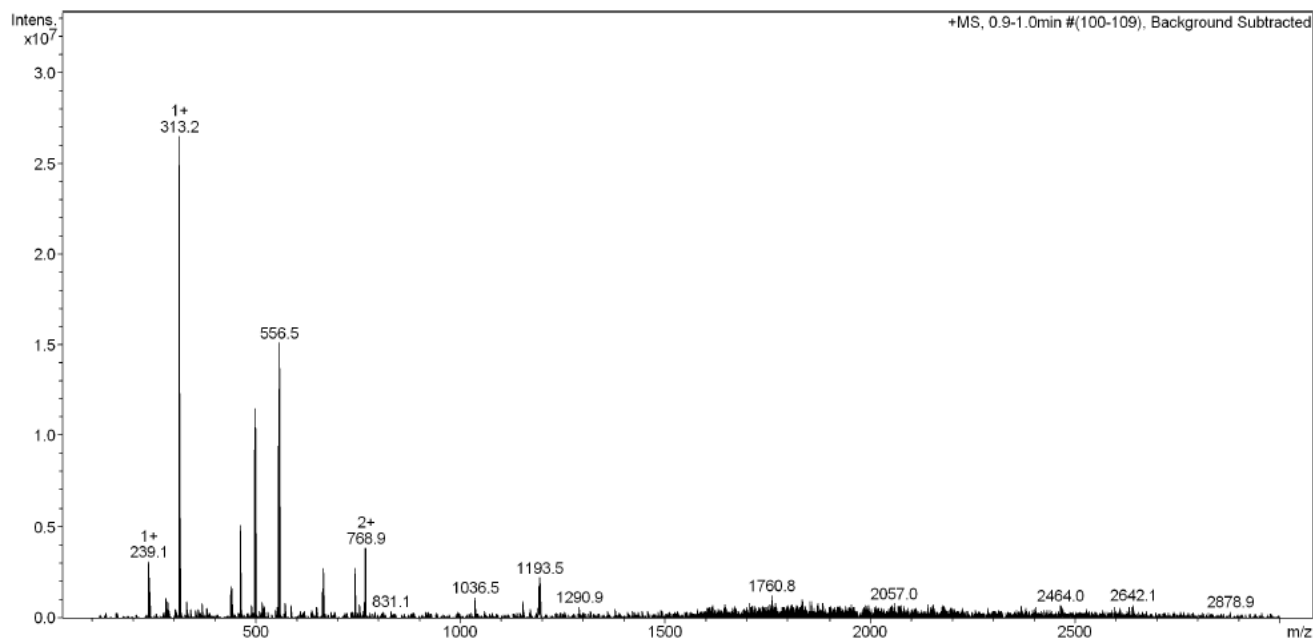


Figure S30a. Mass spectrum (ESI) of the compound **15** (*1,3-alternate*).

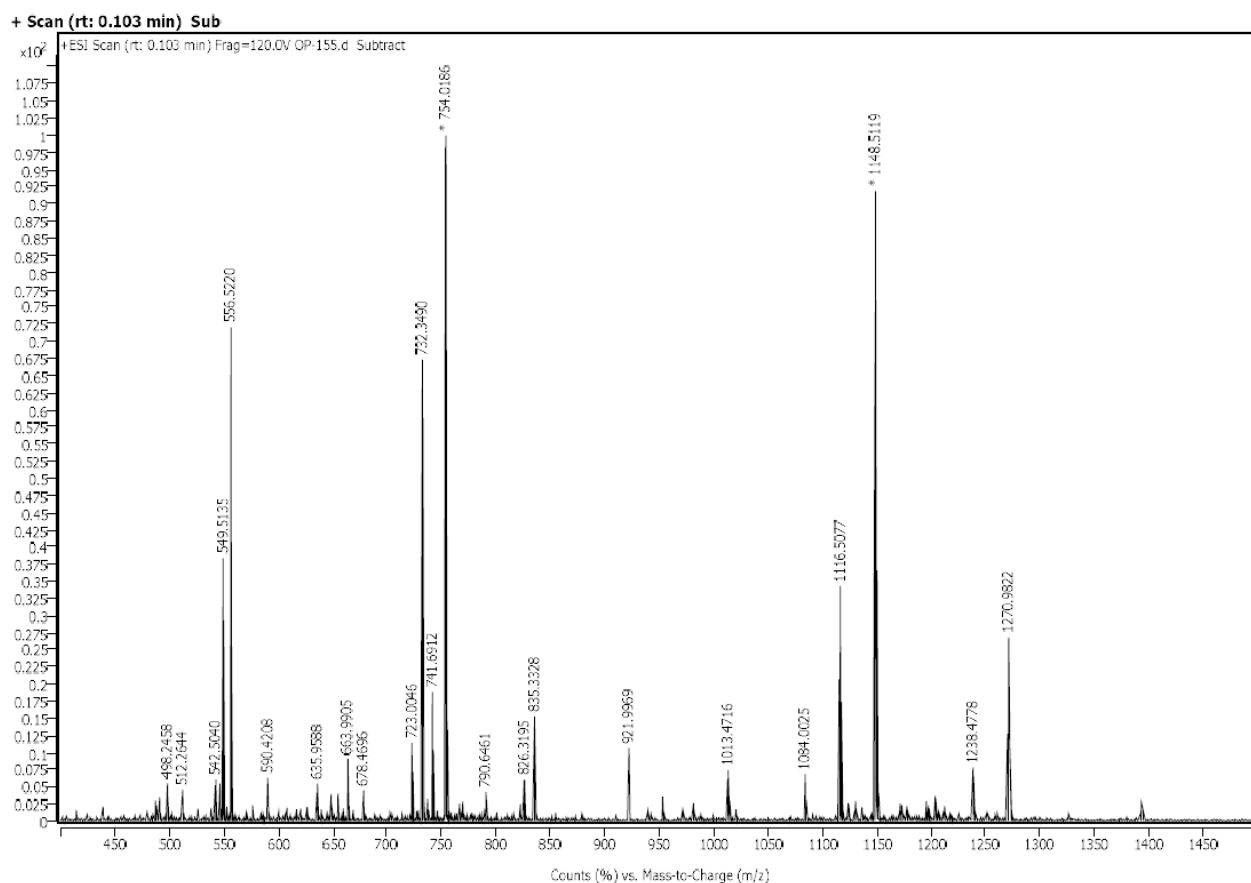


Figure S30b. HR Mass spectrum (ESI) of the compound **17** (*cone*).

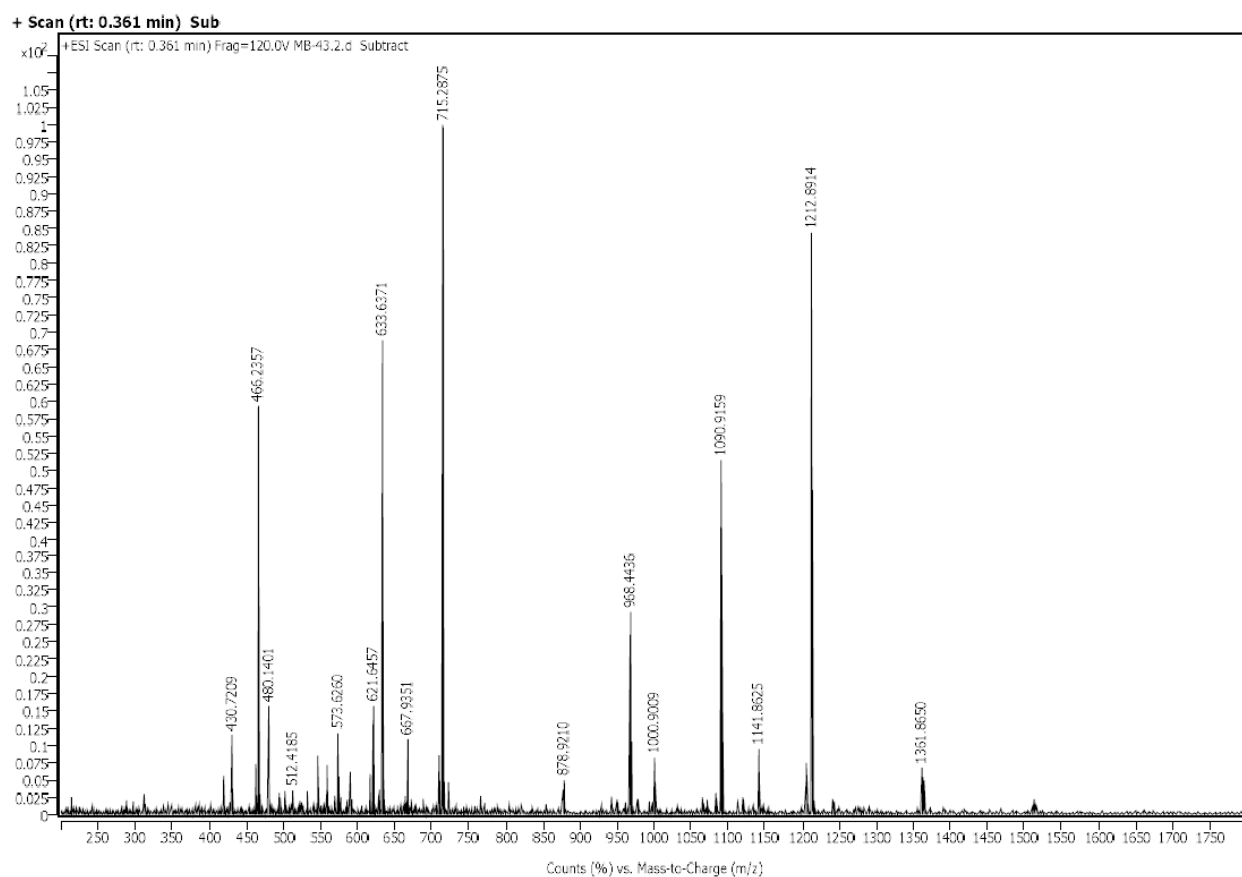


Figure S31. HR Mass spectrum (ESI) of the compound **18** (*partial cone*).

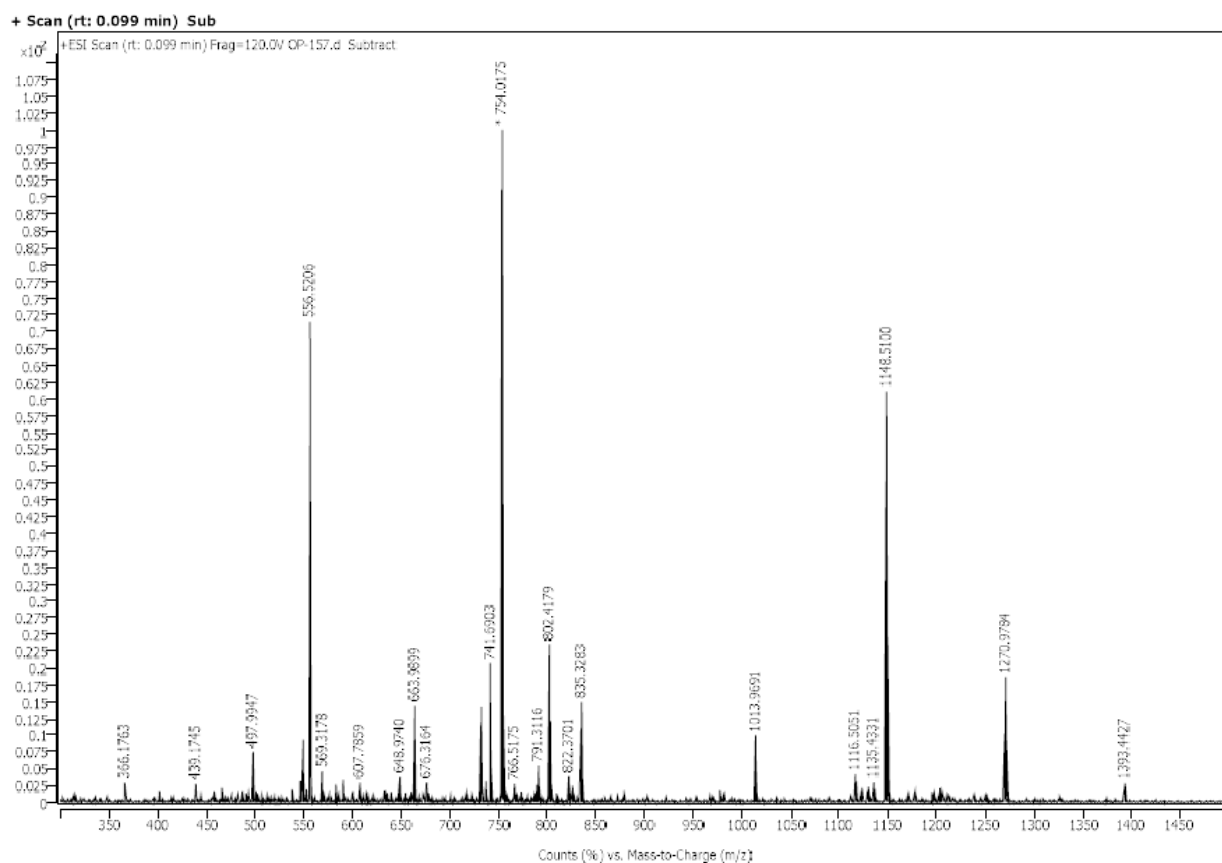


Figure S32. HR Mass spectrum (ESI) of the compound **19** (*partial cone*).

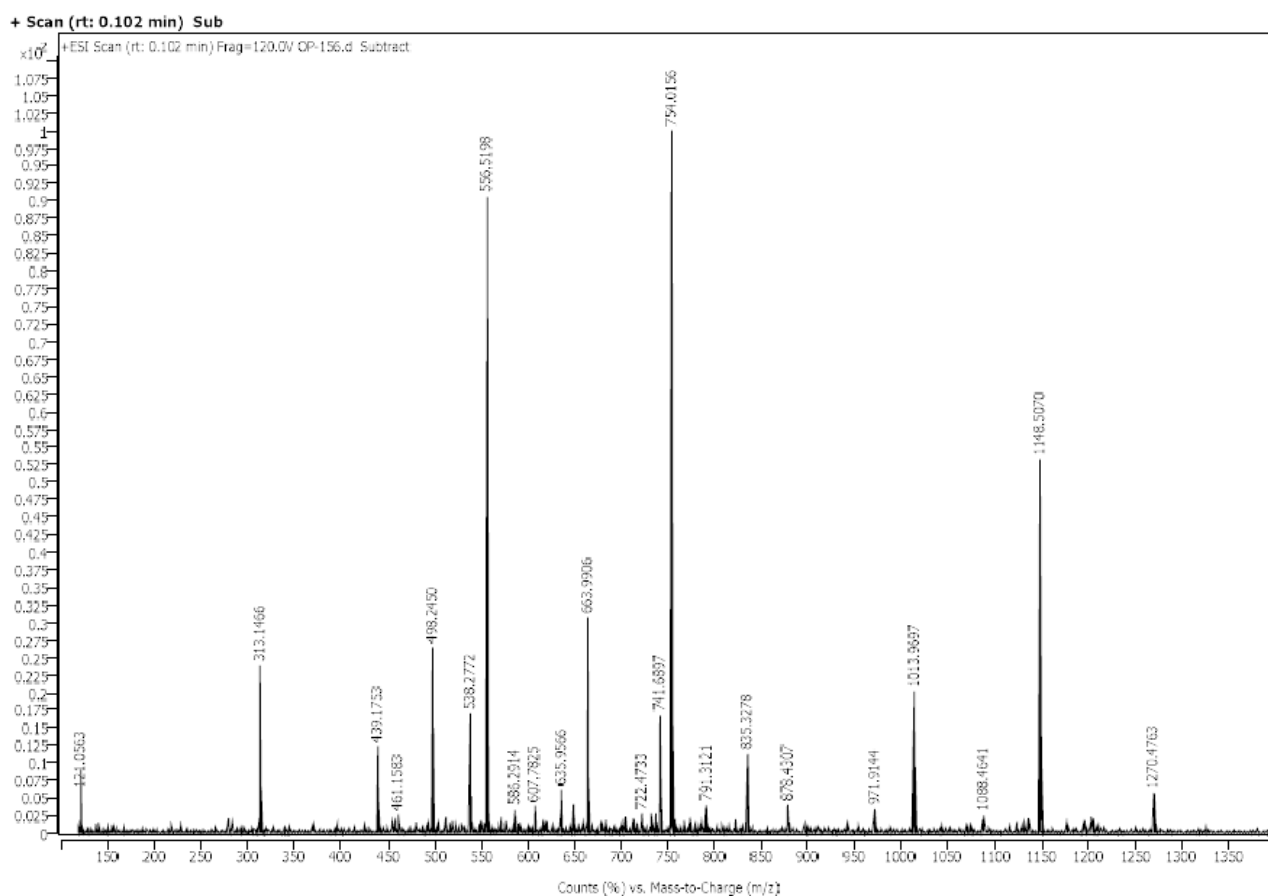


Figure S33. HR Mass spectrum (ESI) of the compound **21** (*1,3-alternate*).

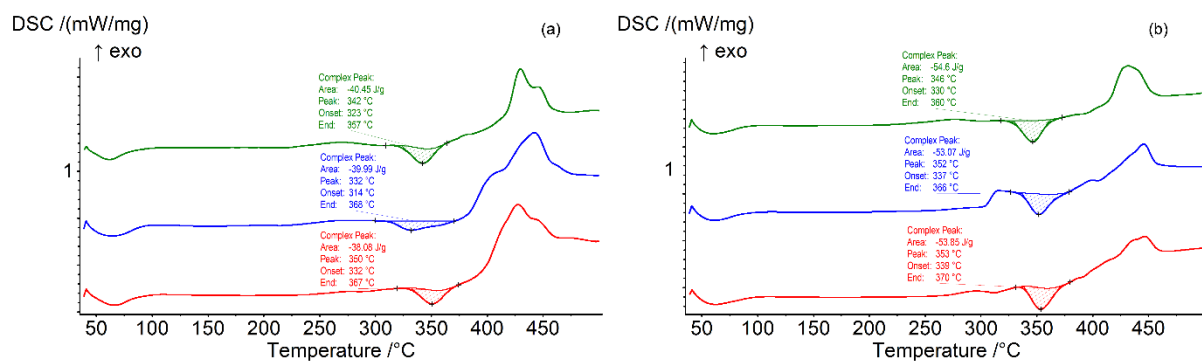


Figure S34. DSC curves of the compounds with Gly (a) **16** (green), **18** (blue), **20** (red), and *L*-Phe (b) **17** (green), **19** (blue), **21** (red) fragments (dynamic argon atmosphere of 75 ml/min in the temperature range from 40 to 500 °C).