Supporting Information

for

2D monomolecular nanosheets based on thiacalixarene derivatives: synthesis, solid state self-assembly and crystal polymorphism

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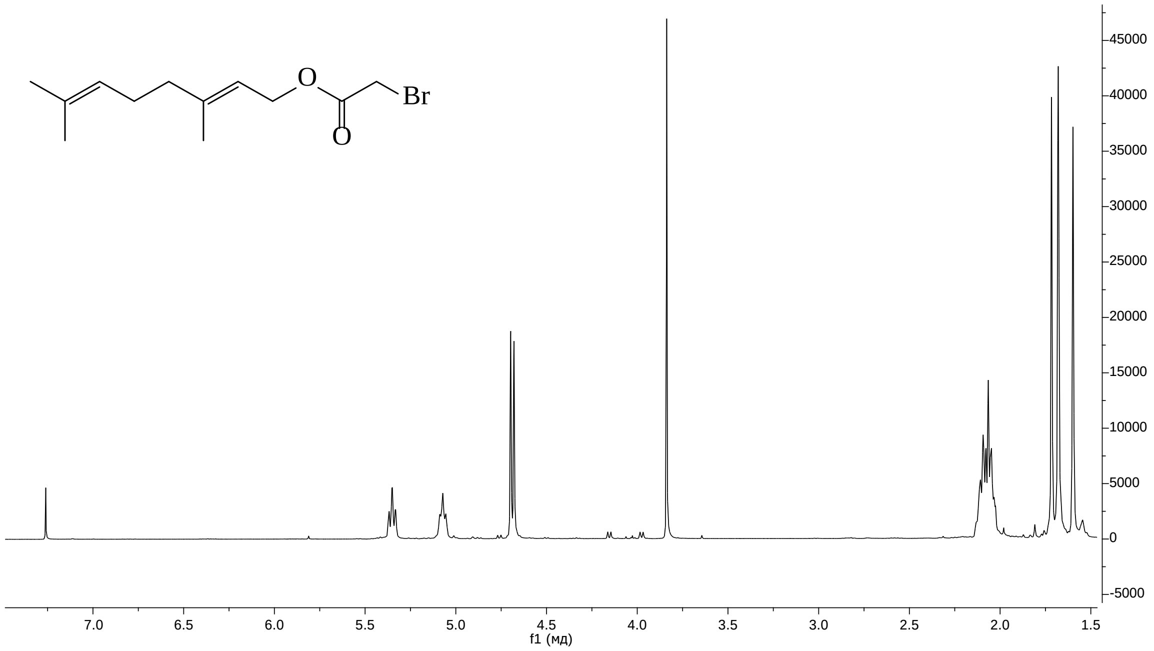

Figure S1. ^{1}H NMR spectrum of geranyl bromoacetate **2** ($CDCl_3$, 298 K, 400 MHz).

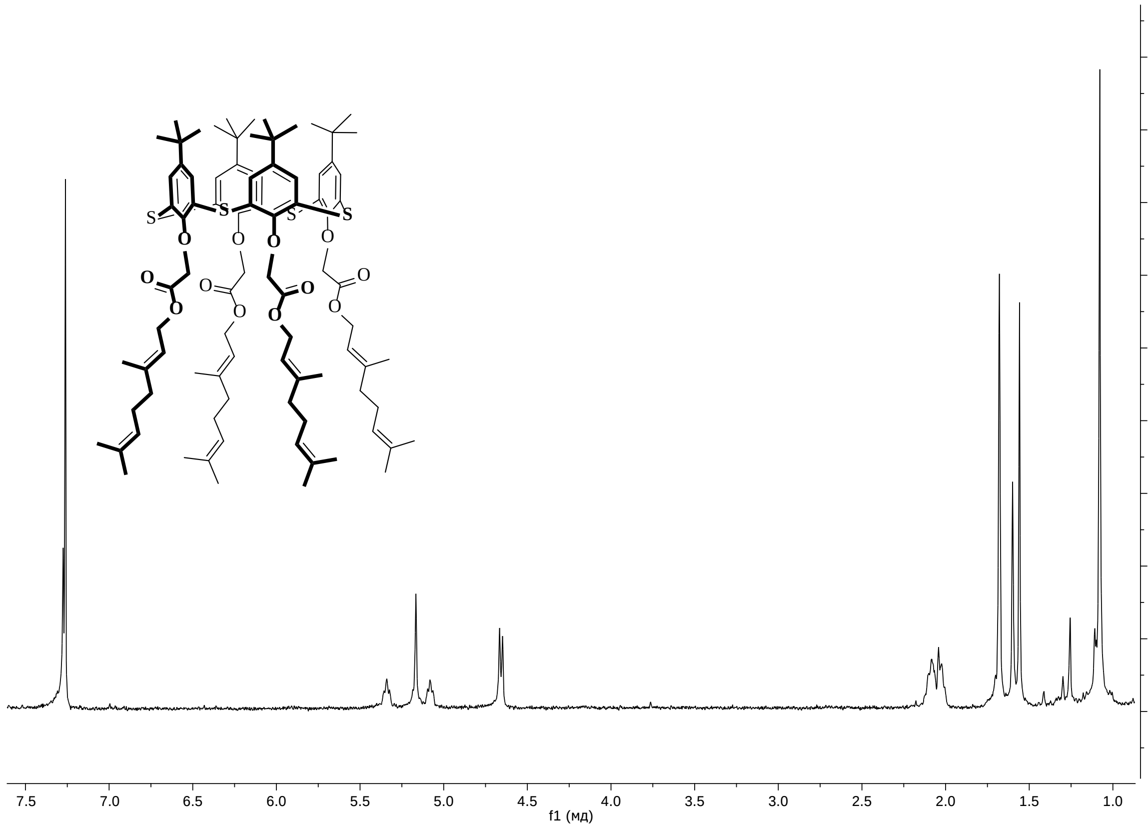

Figure S2. ^{1}H NMR spectrum of thiacalix[4]arene **4** in *cone* conformation ($CDCl_3$, 298 K, 400 MHz).

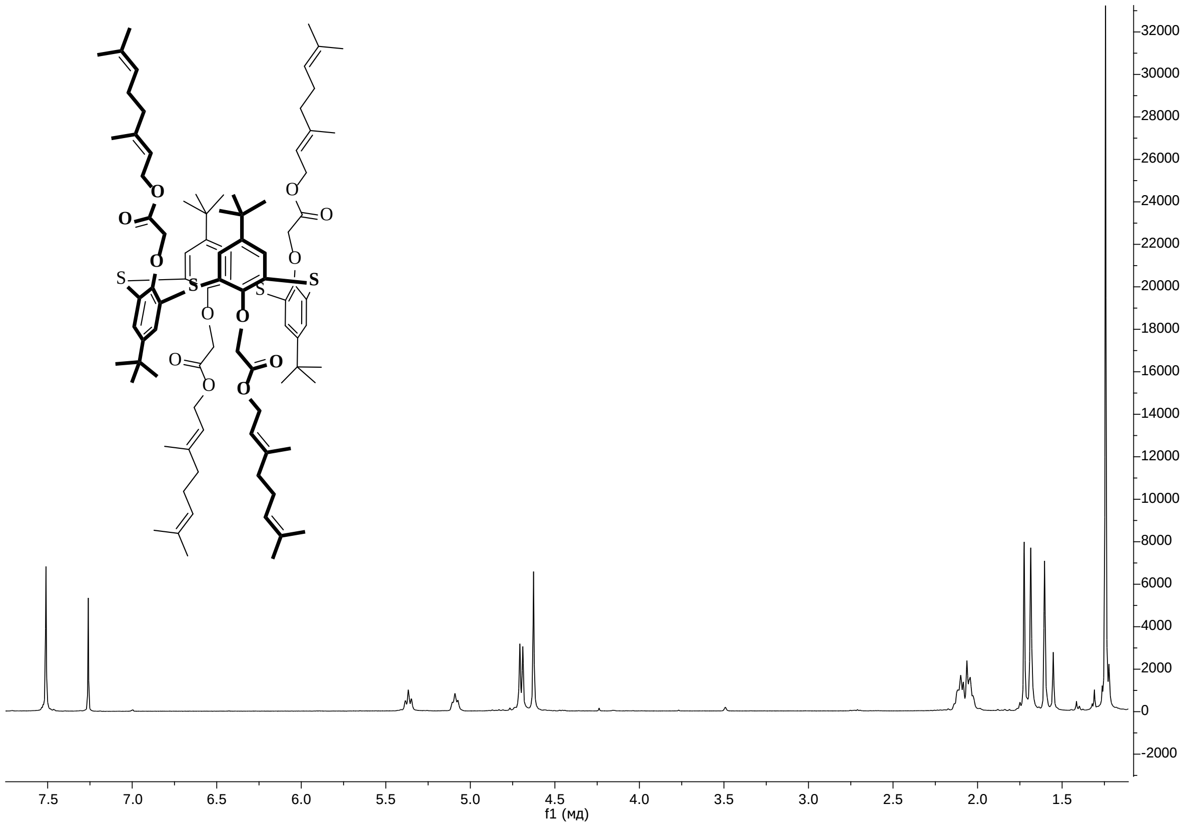

Figure S3. ^{1}H NMR spectrum of thiacalix[4]arene **5** in *1,3-alternate* conformation ($CDCl_3$, 298 K, 400 MHz).

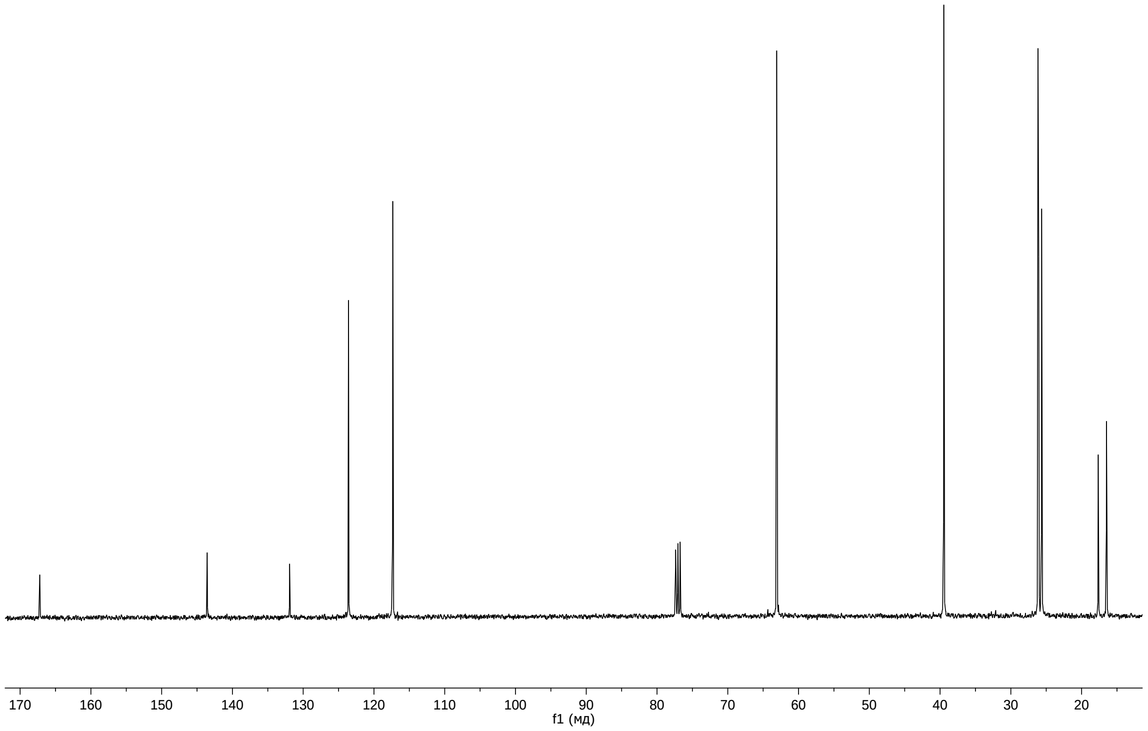

Figure S4. ^{13}C NMR spectrum of geranyl bromoacetate **2** ($CDCl_3$, 298 K, 100 MHz).

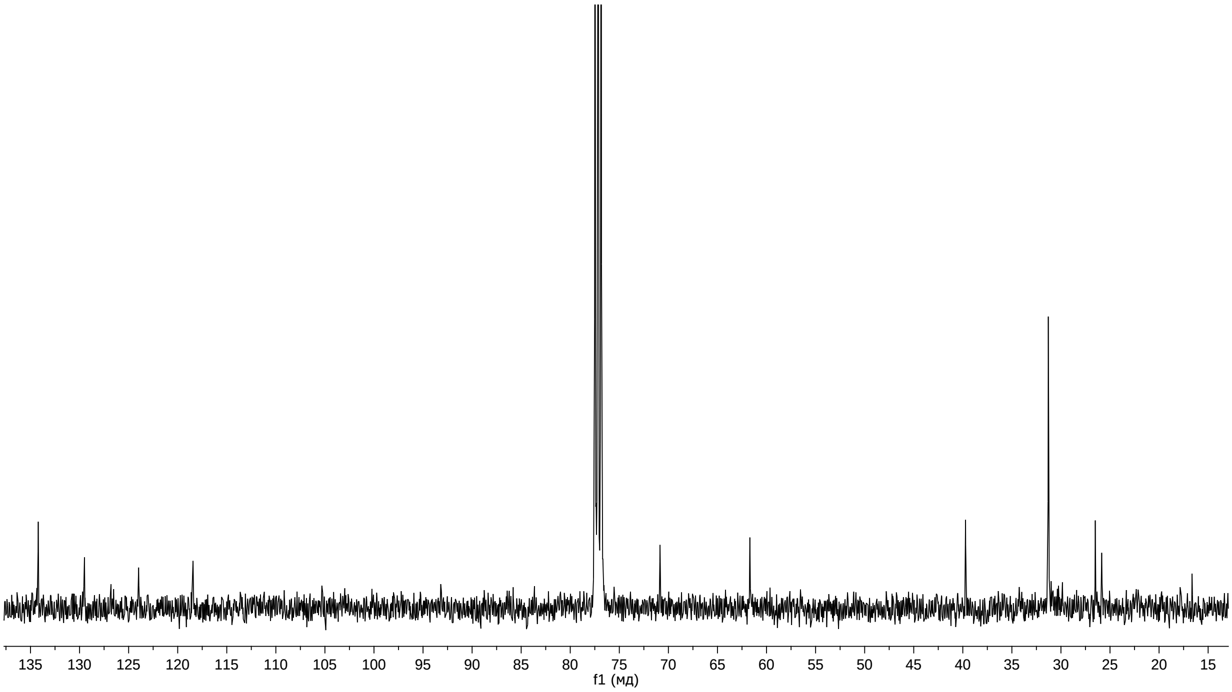

Figure S5. ^{13}C NMR spectrum of thiacalix[4]arene **4** in *cone* conformation (CDCl$_3$, 298 K, 100 MHz).

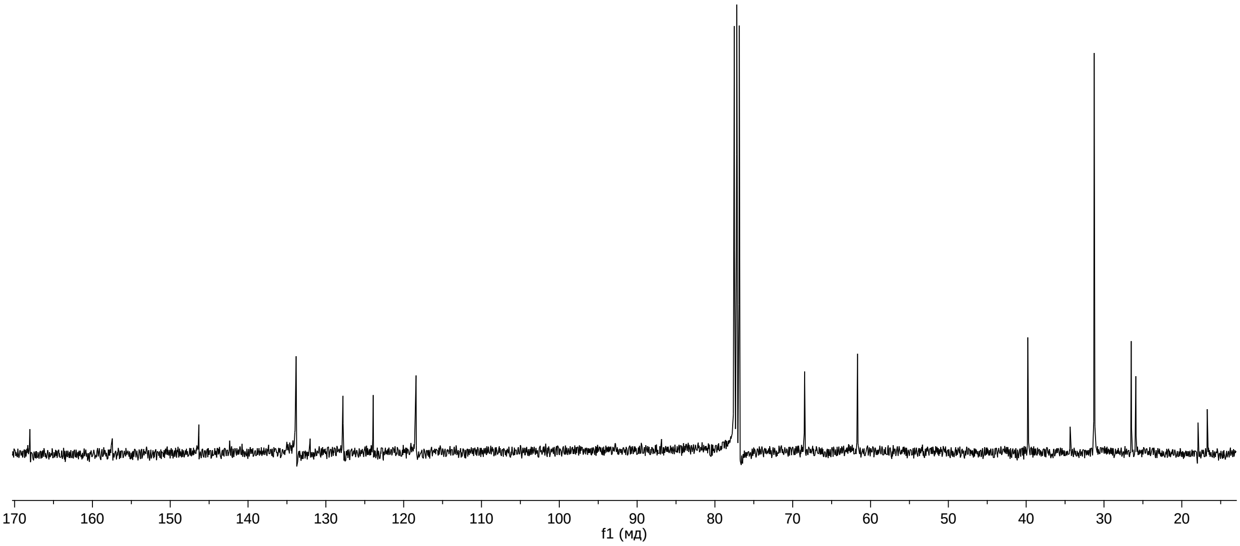

Figure S6. ^{13}C NMR spectrum of thiacalix[4]arene **5** in *1,3-alternate* conformation (CDCl$_3$, 298 K, 100 MHz).

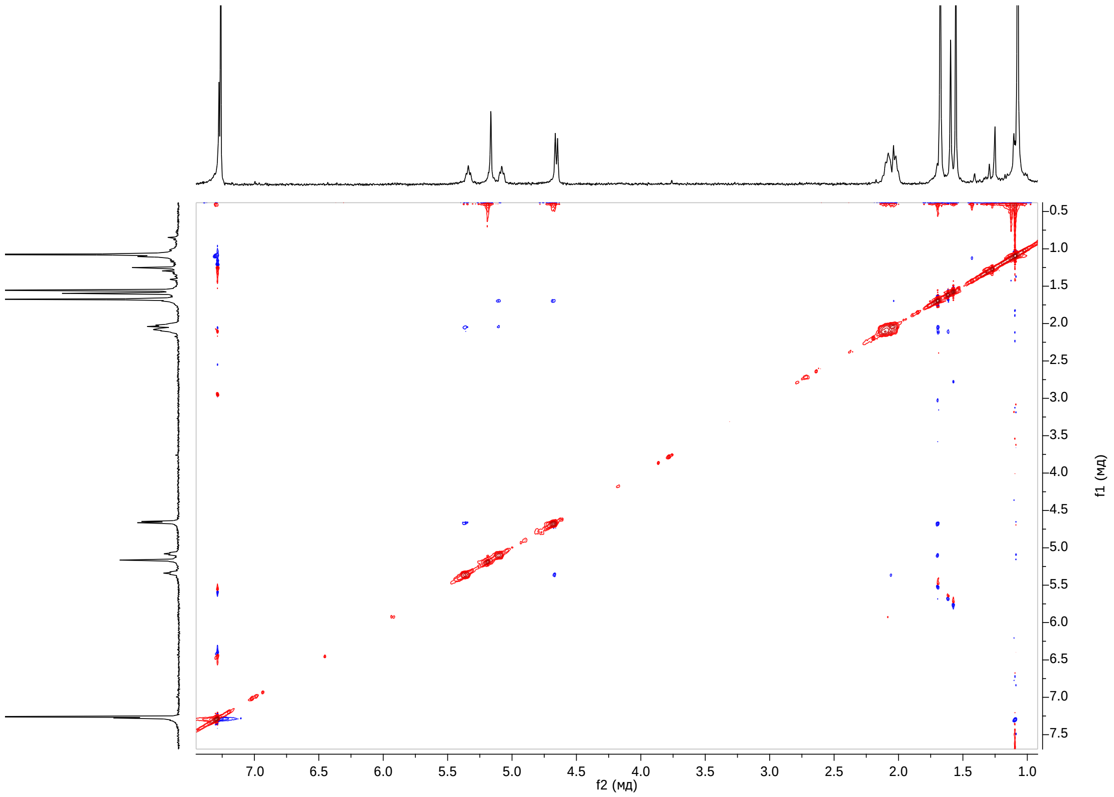

Figure S7. 2D NMR NOESY ^{1}H-^{1}H spectrum of thiacalix[4]arene **4** in *cone* conformation (CDCl$_3$, 298 K, 400 MHz).

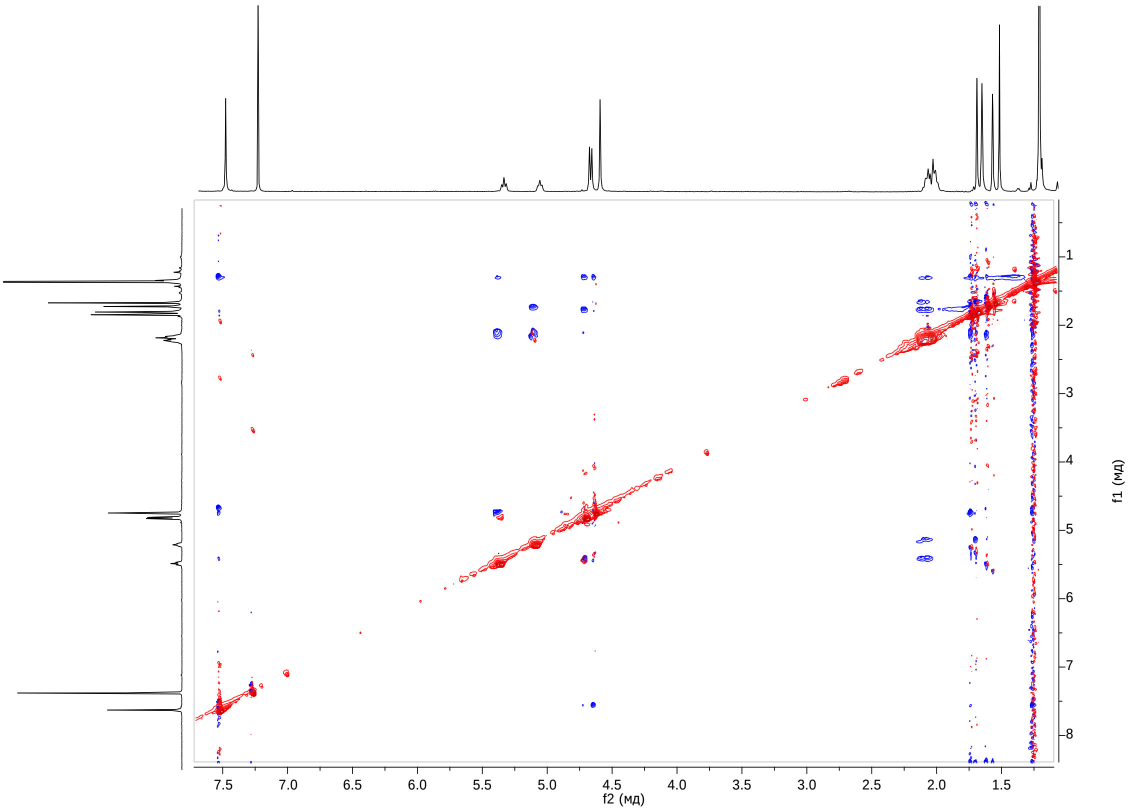

Figure S8. 2D NMR NOESY ^{1}H-^{1}H spectrum of thiacalix[4]arene **5** in *1,3-alternate* conformation (CDCl$_3$, 298 K, 400 MHz).

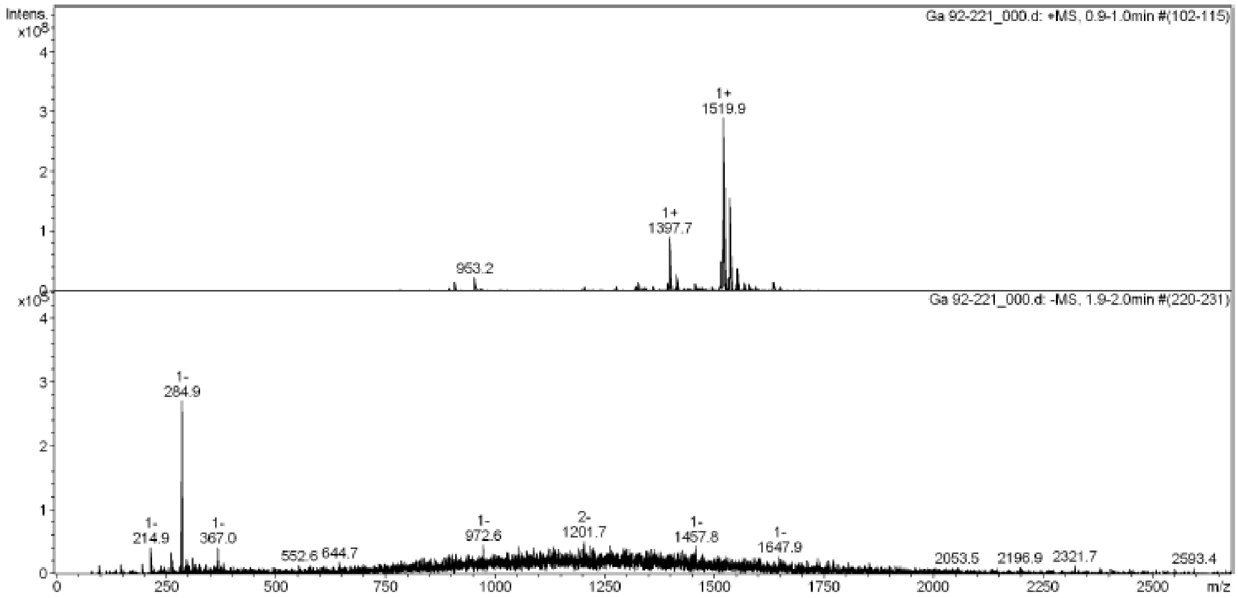

Figure S9. Mass spectrum ESI of thiacalix[4]arene **4** in *cone* conformation.

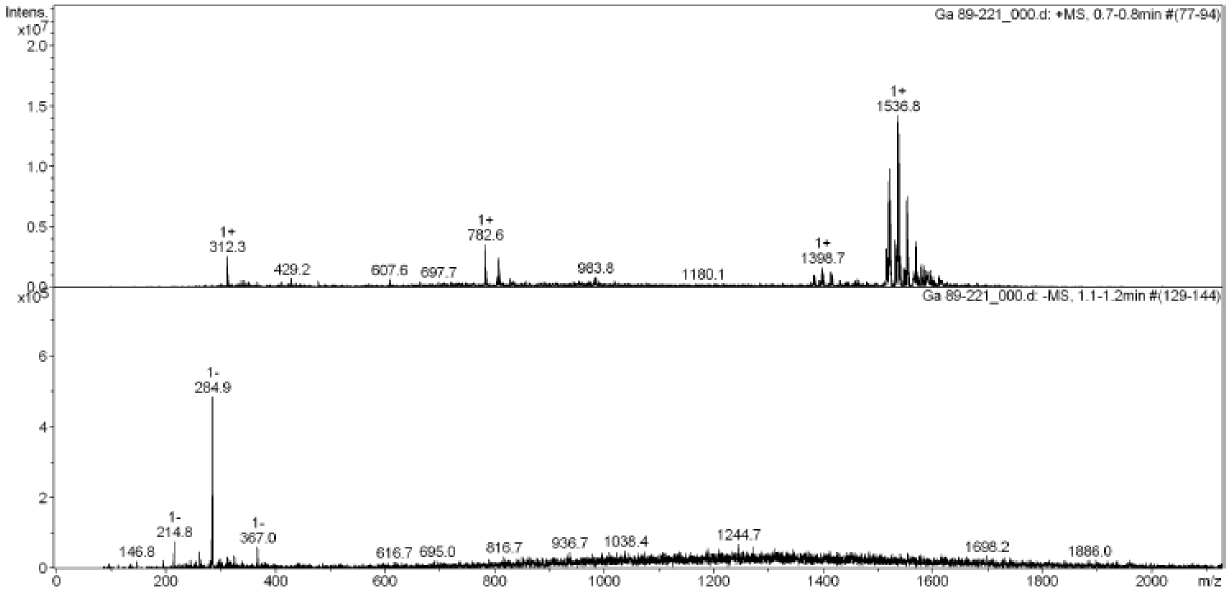

Figure S10. Mass spectrum ESI of thiacalix[4]arene **5** in *1,3-alternate* conformation.

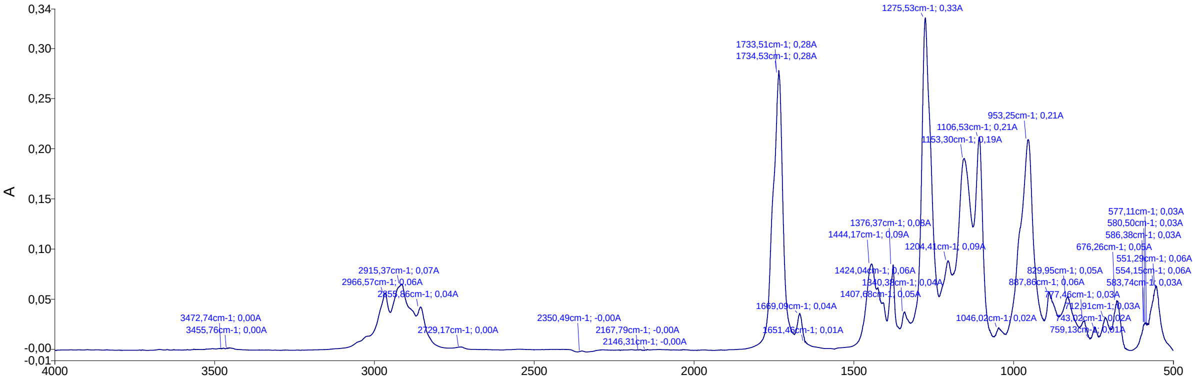

Figure S11. ATR FTIR spectrum of geranyl bromoacetate **2**.

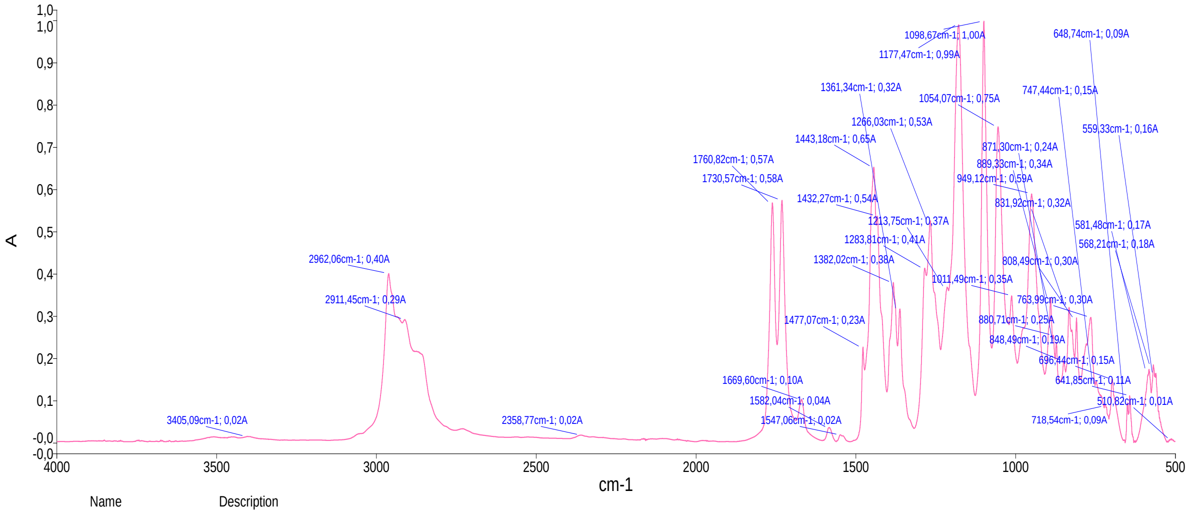

Figure S12. ATR FTIR spectrum of thiacalix[4]arene **4** in *cone* conformation.

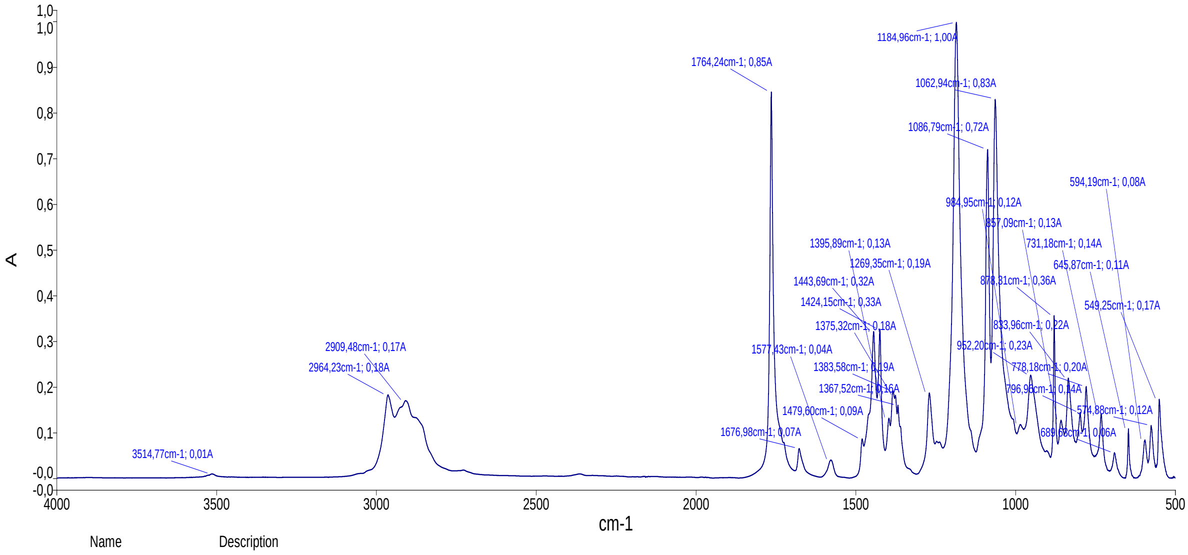

Figure S13. ATR FTIR spectrum of thiacalix[4]arene **5** in *1,3-alternate* conformation.

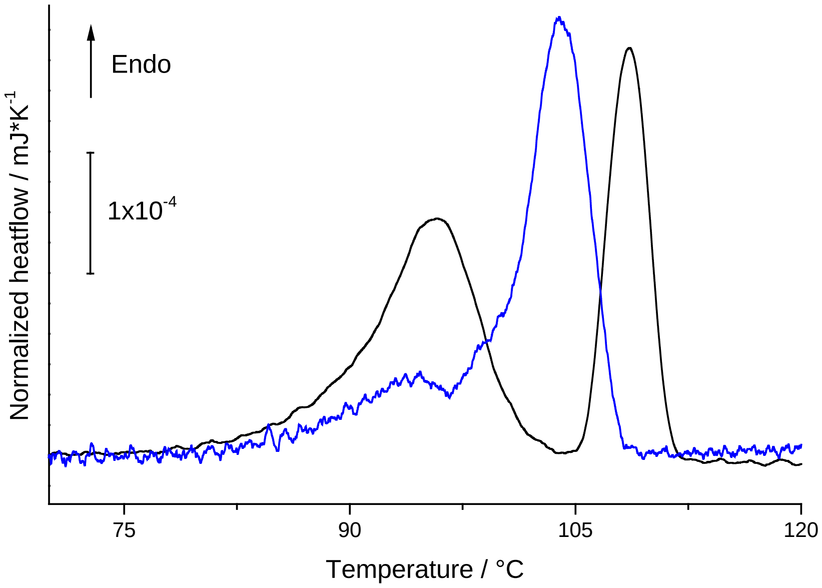

Figure S14. Data of FSC analysis: Heating scans of different samples of compound **5** crystallized on the chip-sensor. 100 K/s heating rate.

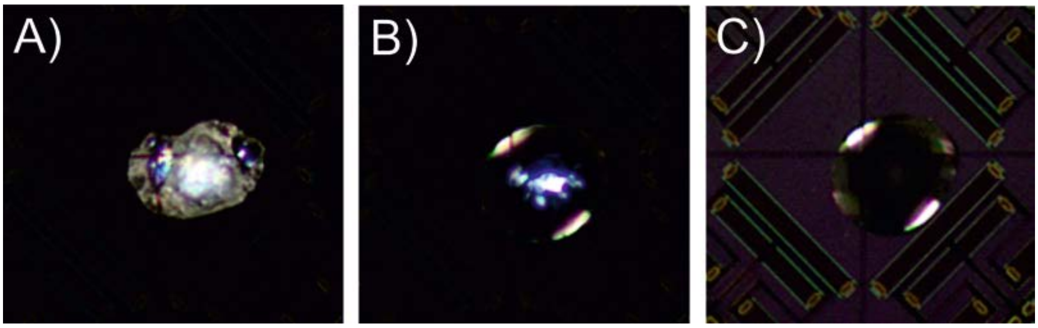

Figure S15. The images of microcrystalline sample **4** (*cone*) under polarized light at heating to 53°C (A), 60°C (B) and 63°C (C).

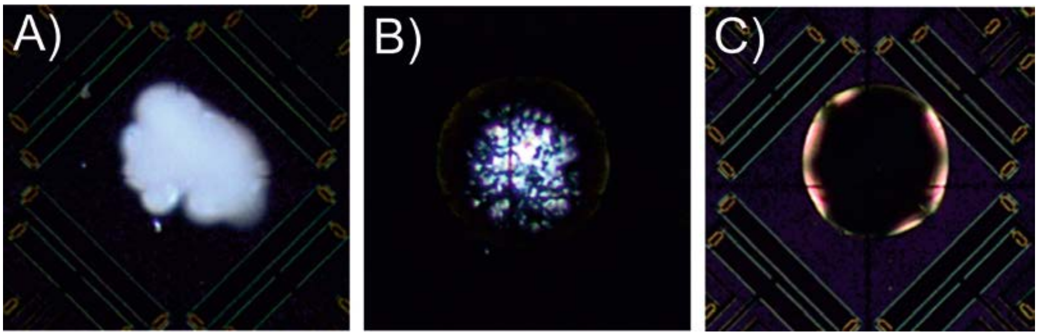

Figure S16. The images of microcrystalline sample **5** (*1,3-alternate*) under polarized light at heating to 95°C (A), 106°C (B) and 112°C (C).