Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Electronic Supplementary Information for:

Glucosylthioureidocalix[4]arenes: synthesis, conformations and gas-phase recognition of amino acids

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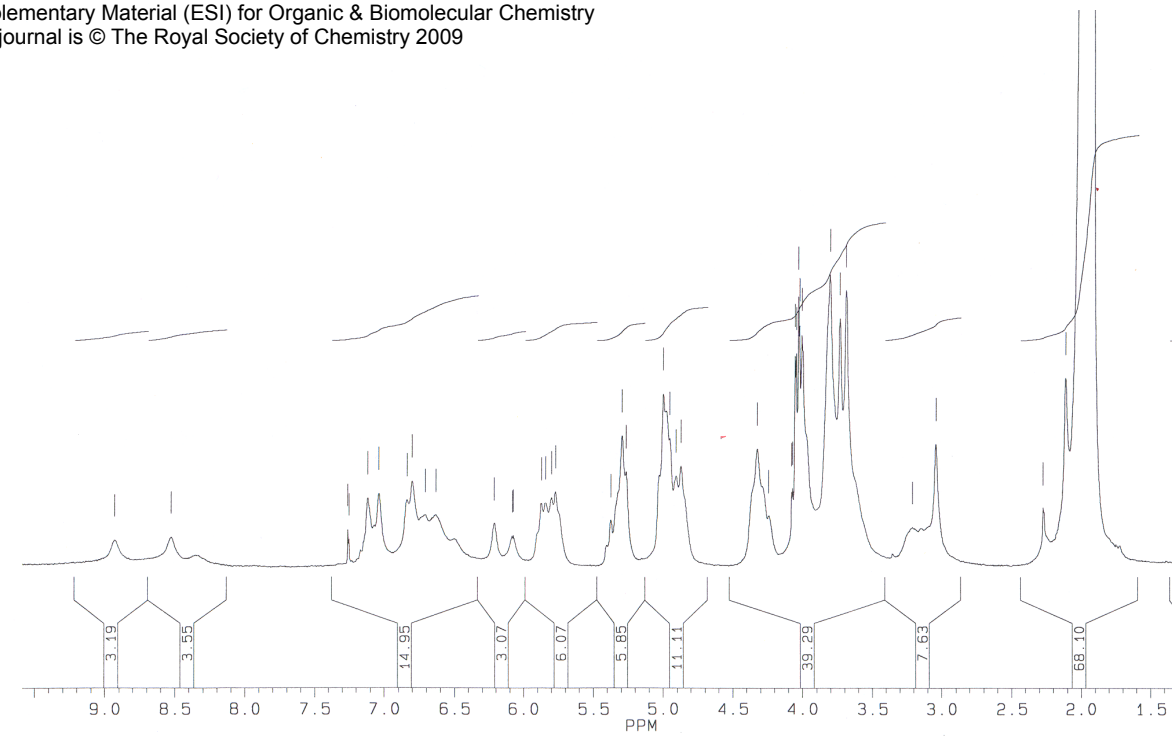


Figure ESI1. ^{1}H NMR ($CDCl_3$, 300 MHz, 298 K) of **6**.

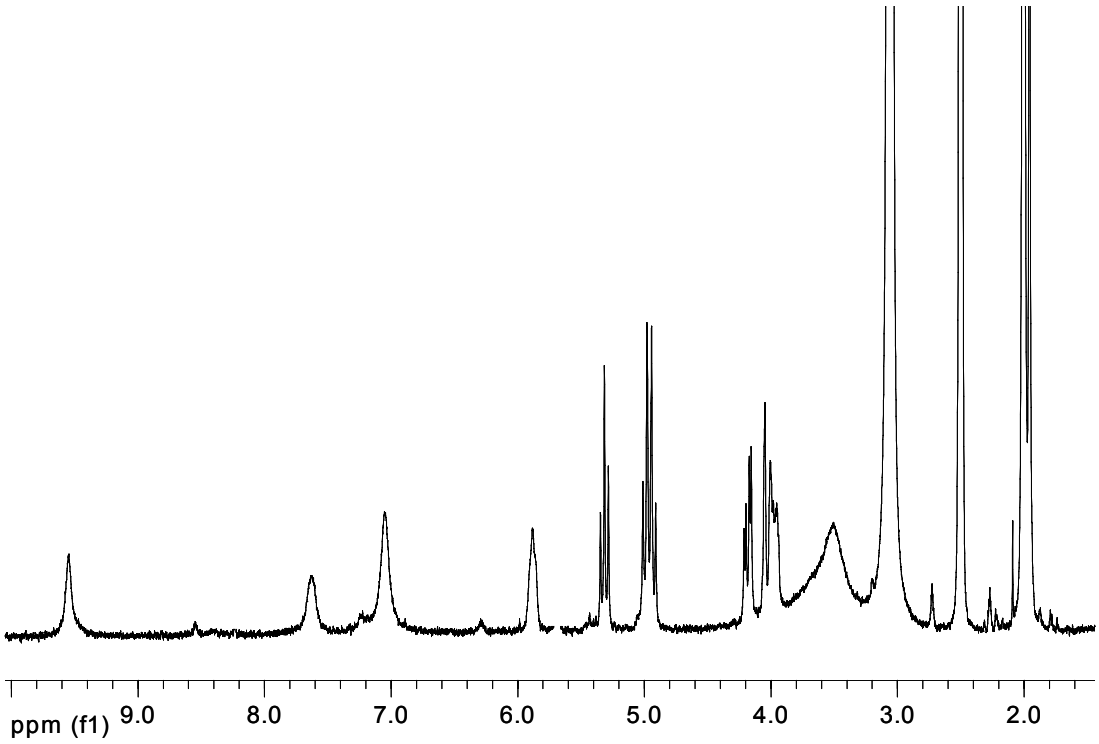


Figure ESI2. ^{1}H NMR (DMSO-d_6, 300 MHz, 363 K) of **6**.

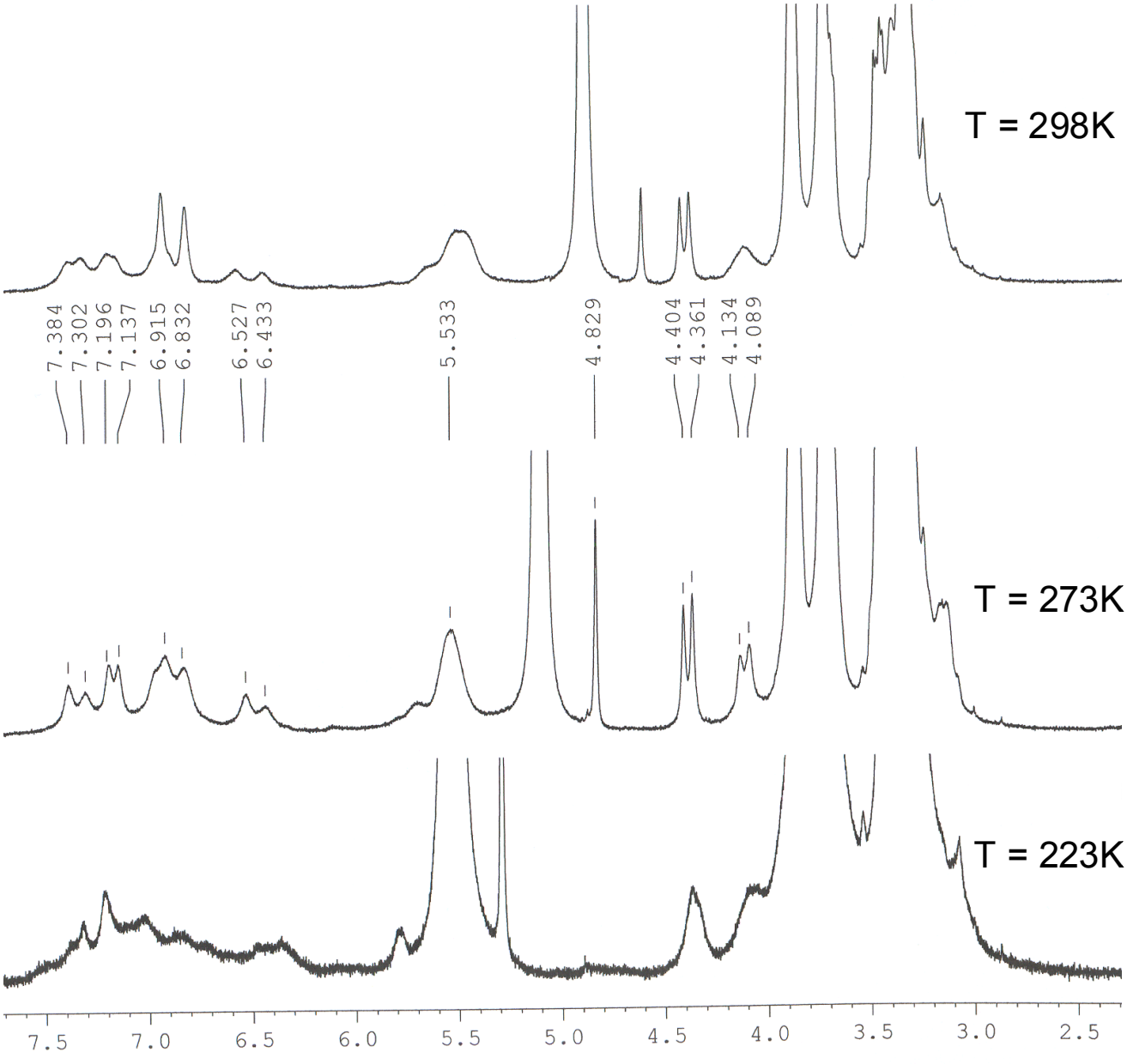
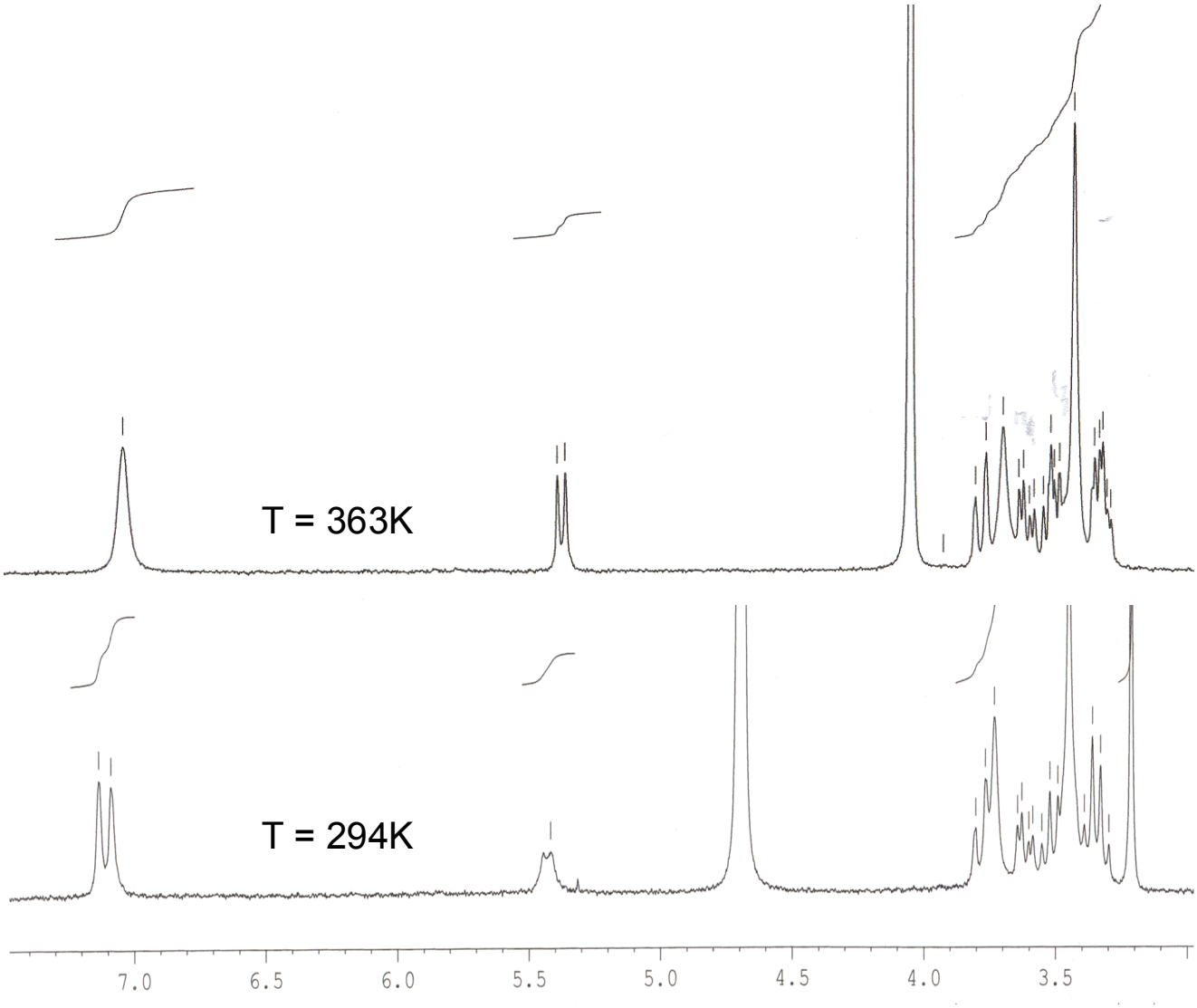
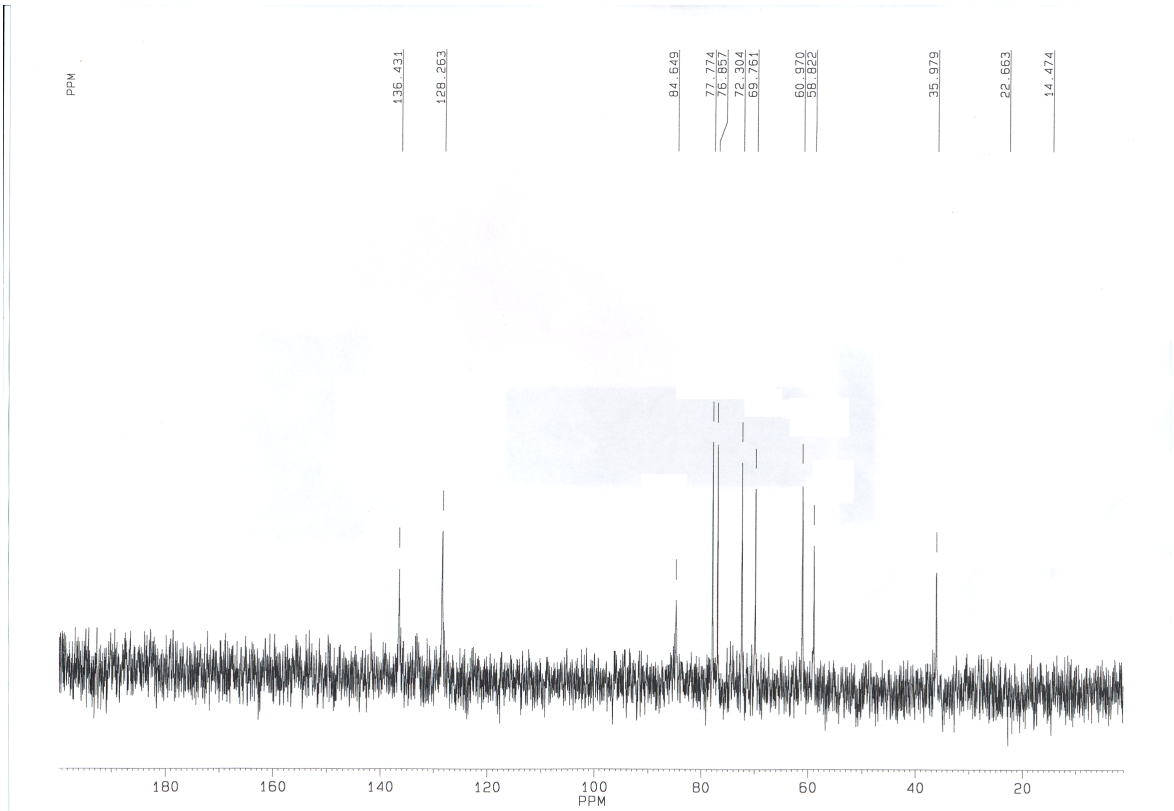


Figure ESI3. VT-NMR spectra of **1** in CD_3OD.



a)

b)



c)

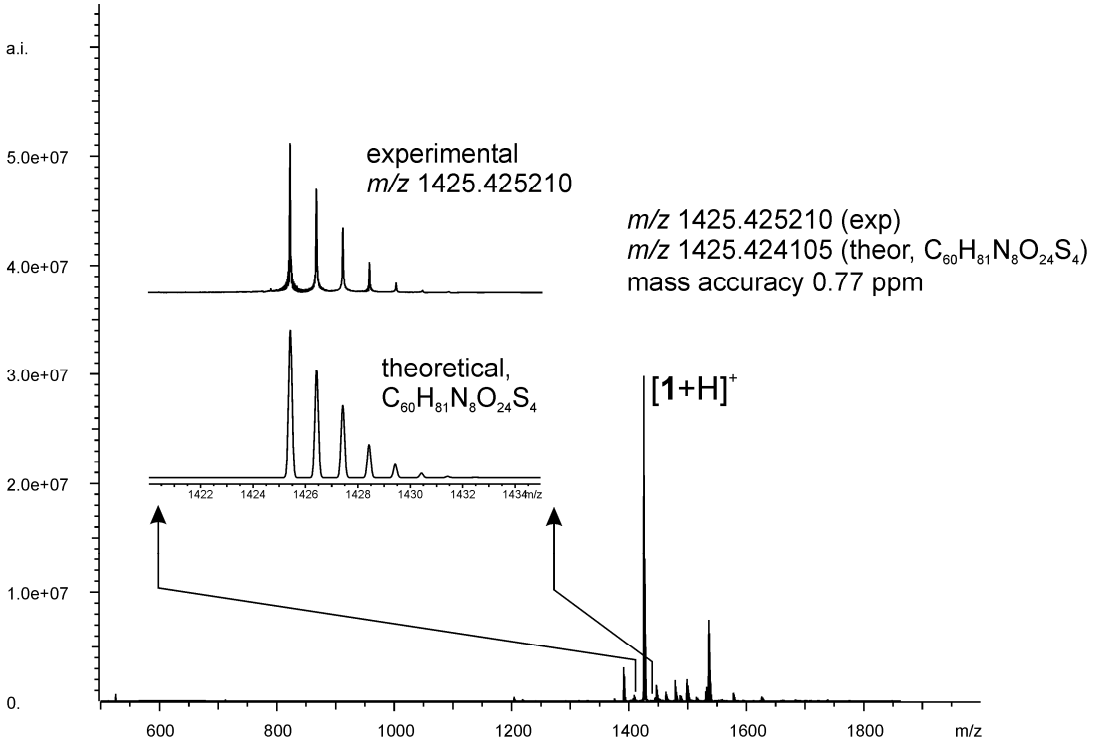


Figure ESI4. a) VT-NMR spectra of **1** in D_2O, b) ^{13}C NMR spectrum of **1** in D_2O 298K and c) exact mass measurement and comparison of isotopic distribution for **1**

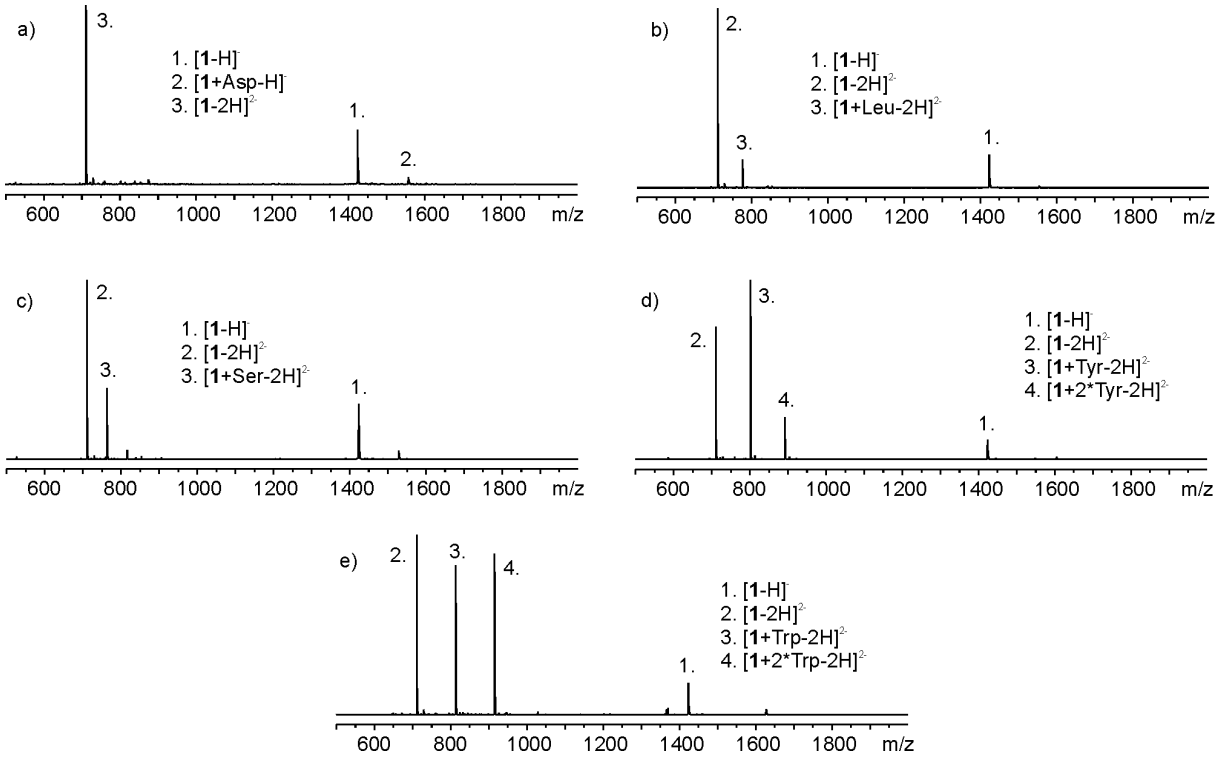


Figure ESI5. Profile spectra measured from samples containing **1** in the presence of a) Asp b) Leu c) Ser d) Tyr and e) Trp.

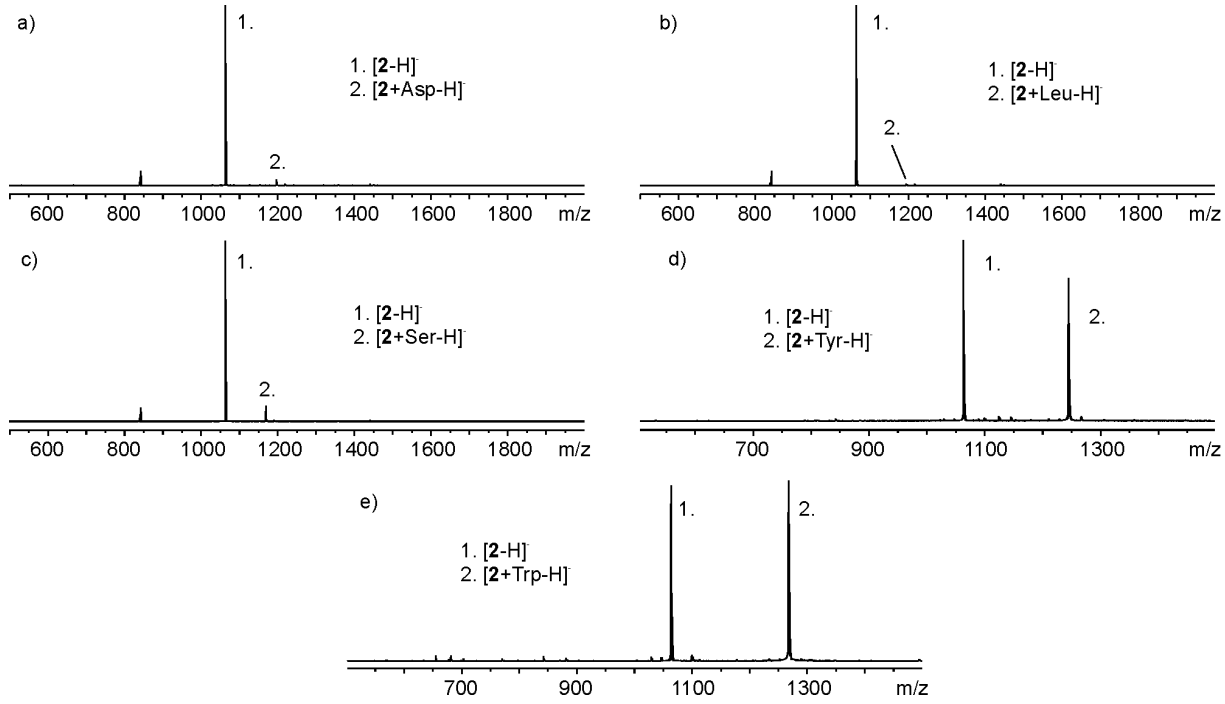


Figure ESI6. Profile spectra measured from samples containing **2** in the presence of a) Asp b) Leu c) Ser d) Tyr and e) Trp.

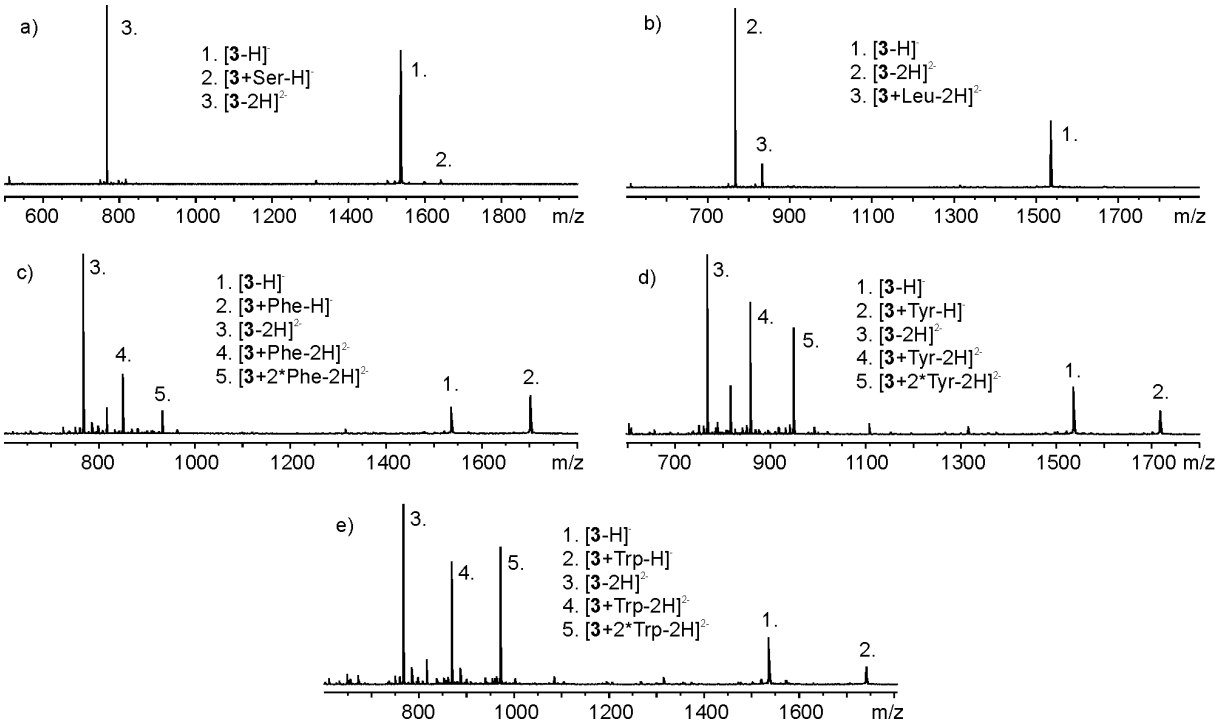


Figure ESI7. Profile spectra measured from samples containing **3** in the presence of a) Ser b) Leu c) Phe d) Tyr and e) Trp.

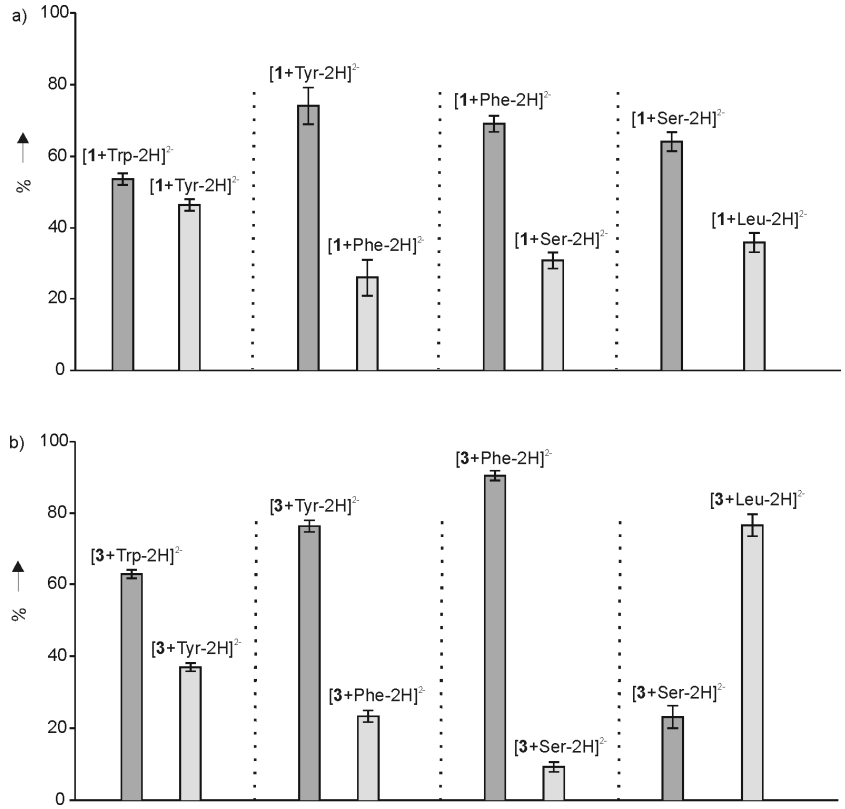


Figure ESI8. Competitive complexation of amino acids in the presence of a) **1** and b) **3**.

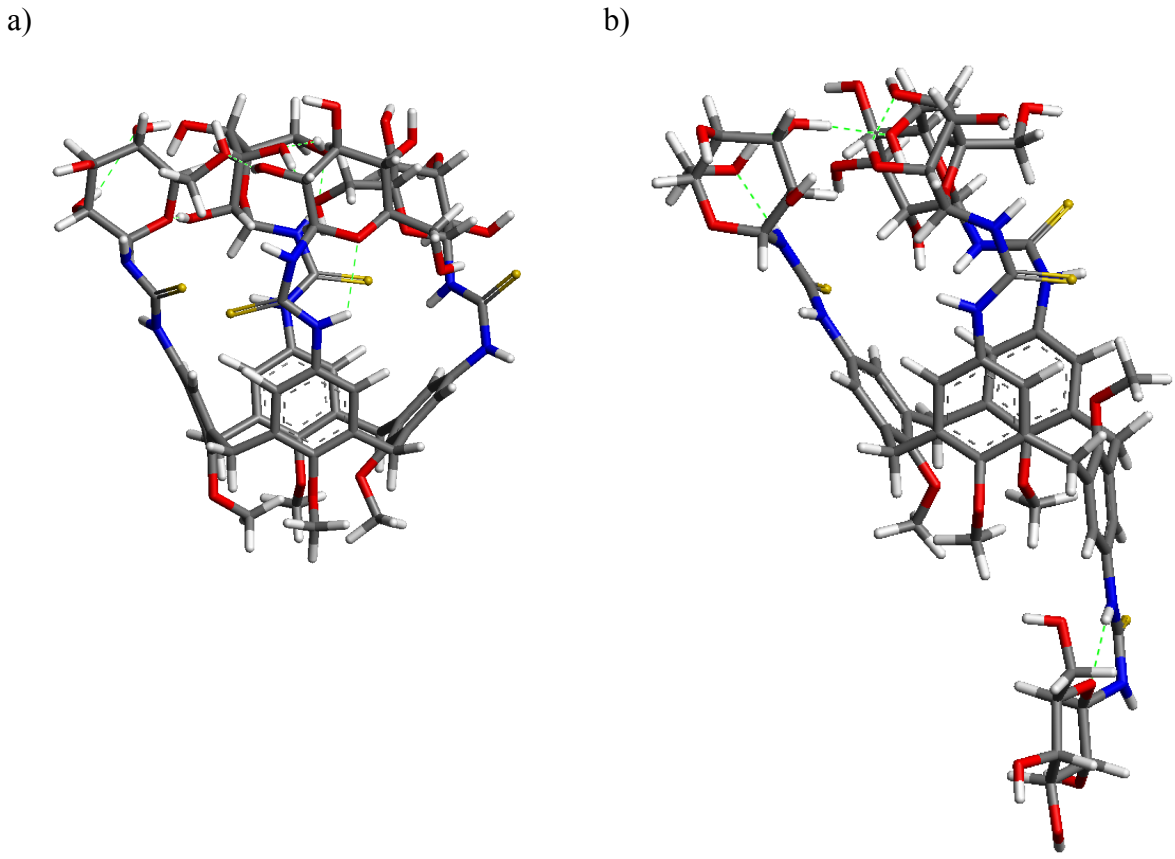


Figure ESI9. Molecular modelling of tetraglucocalixarene **1** carried out using *semi*-empirical methods at PM3 level: the more stable *cone* conformer a) is 123 kJ/mol more stable than the *partial cone* conformer b).

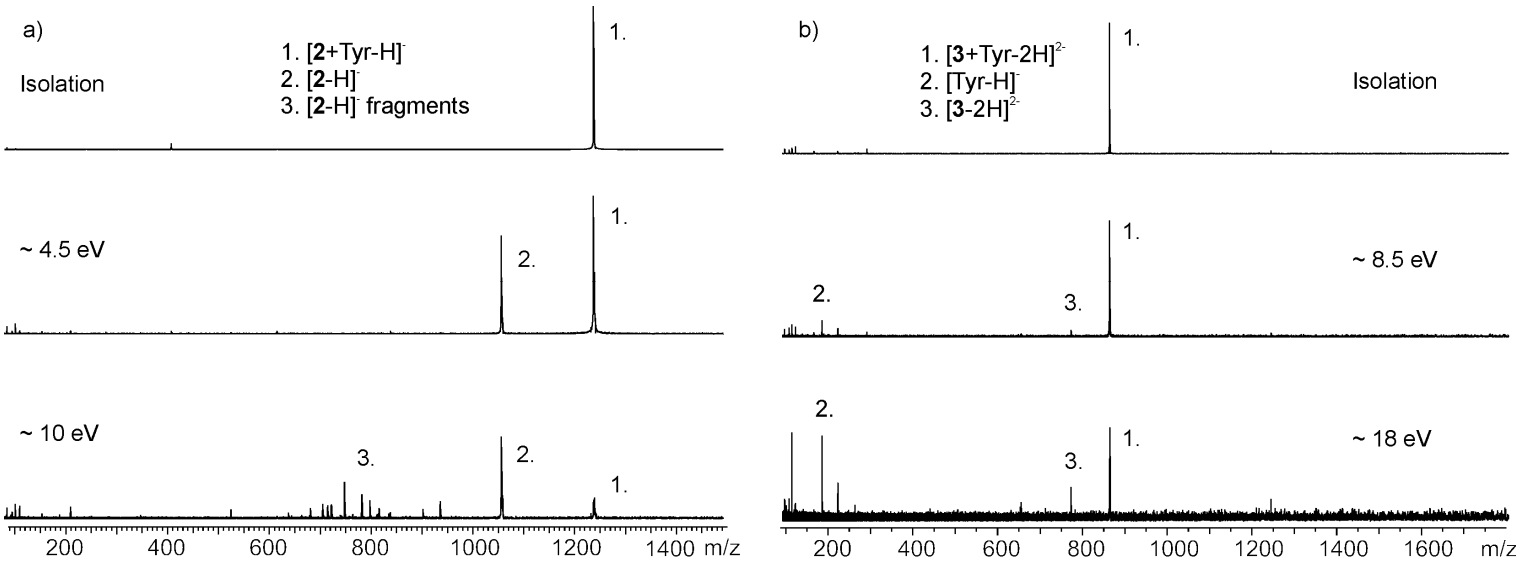


Figure ESI10. Examples of isolation and CID spectra for a) [**2**+Tyr–H]$^-$ and b) [**3**+Tyr–2H]$^{2-}$.

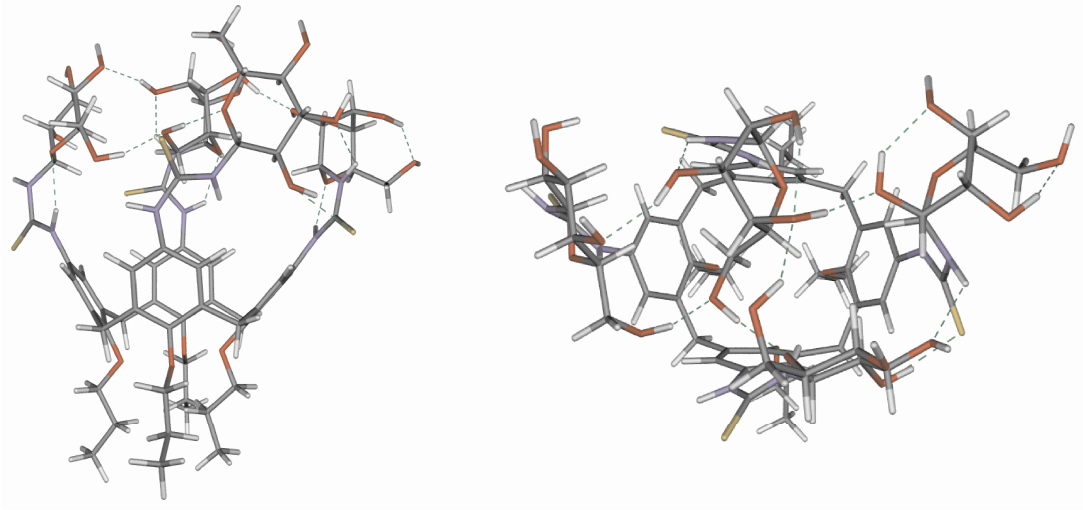


Figure ESI11. Optimized structure of **3** (lateral and apical views, possible H-bonds marked with green dotted lines).

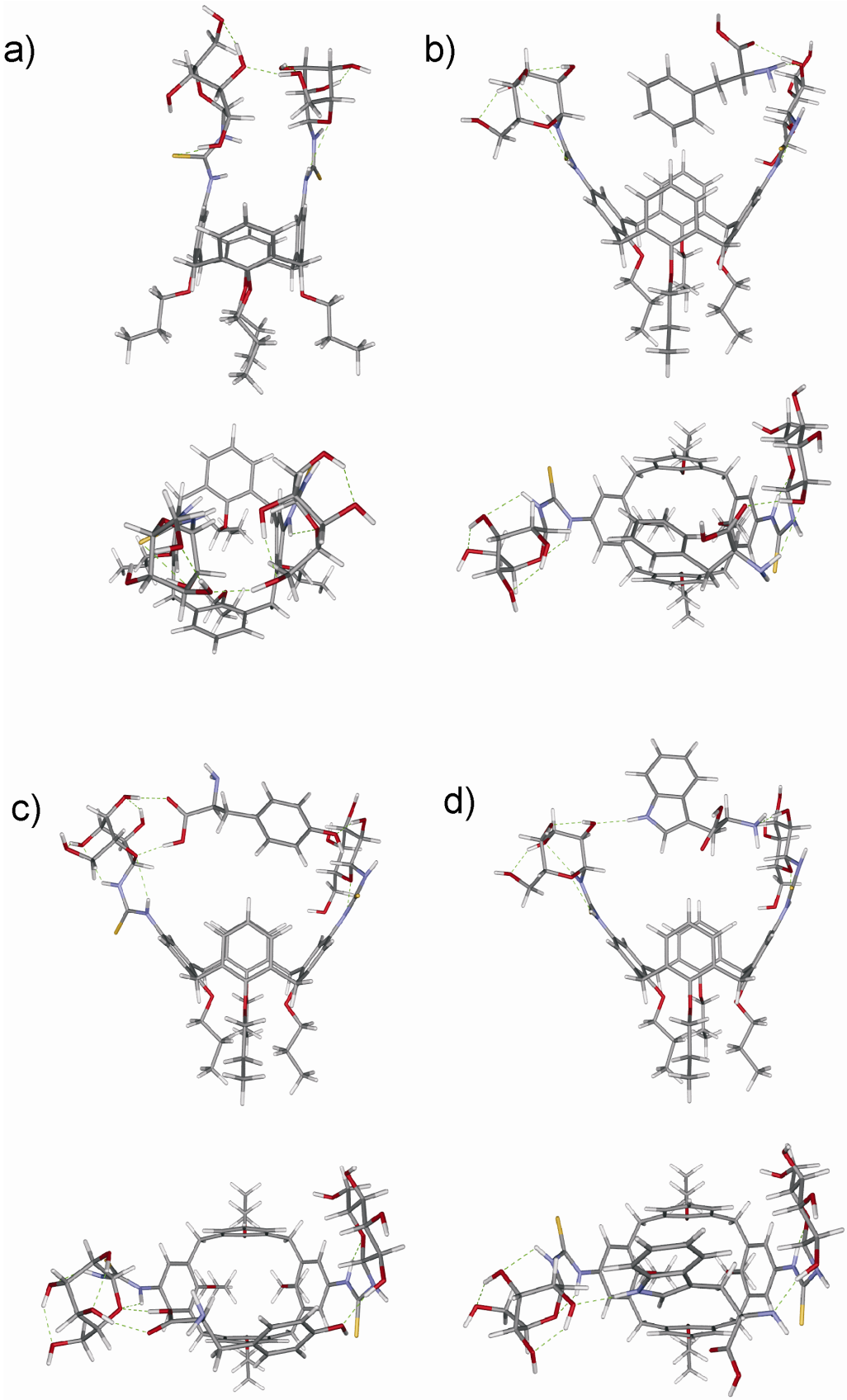


Figure ESI12. Optimized structures (density functional BP86) for a) **2**, b) **2** with Phe, c) **2** with Tyr and d) **2** with Trp (lateral and apical views, possible H-bonds marked with green dotted lines).