Journal Name

ARTICLE

Supporting Information

Controlled manipulation of the Co-Alq_3 interface by rational design of Alq_3 derivatives

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NMR Spectra

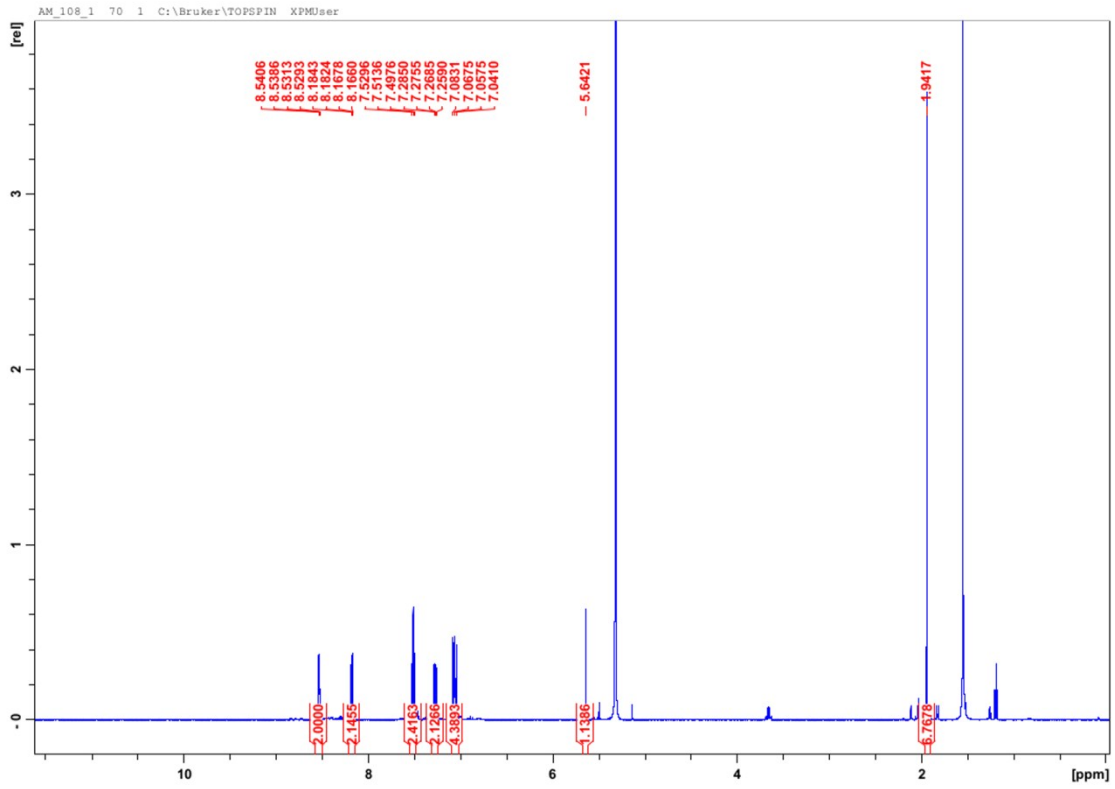

Figure 1. ^{1}H-NMR of **1**

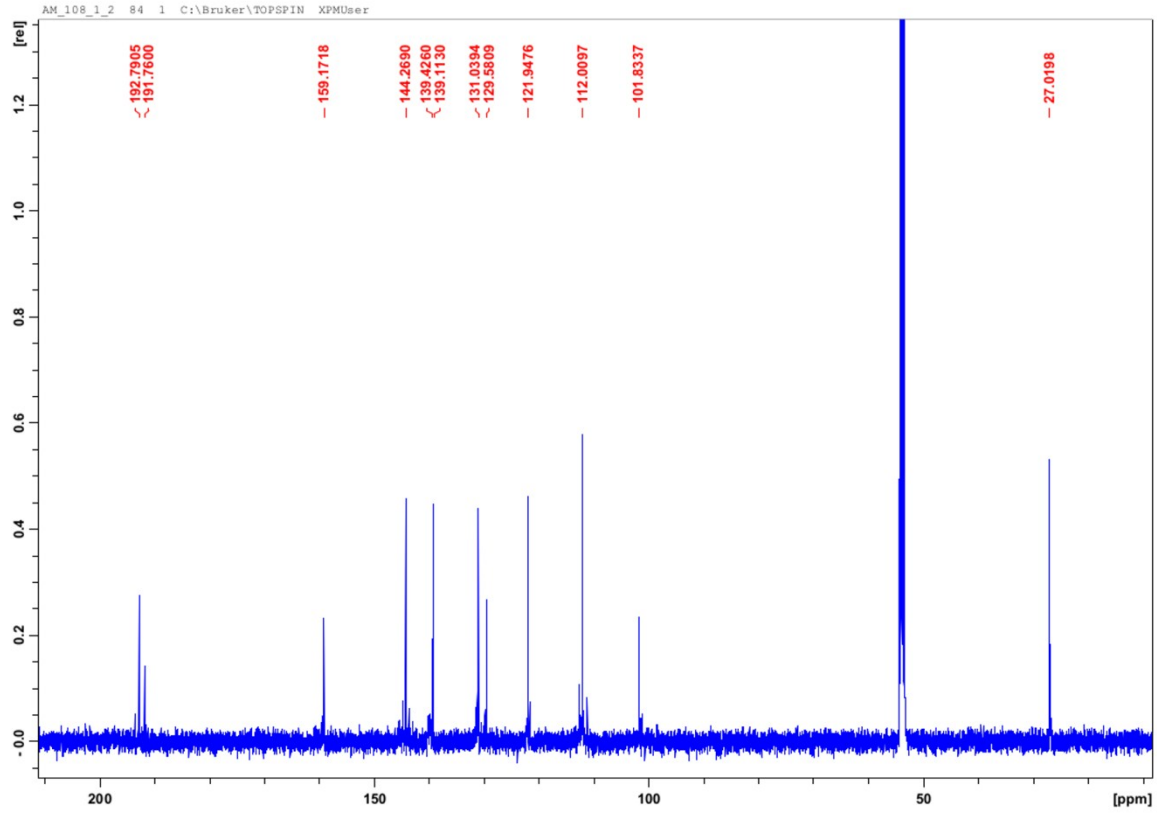

Figure 2. ^{13}C-NMR of **1**

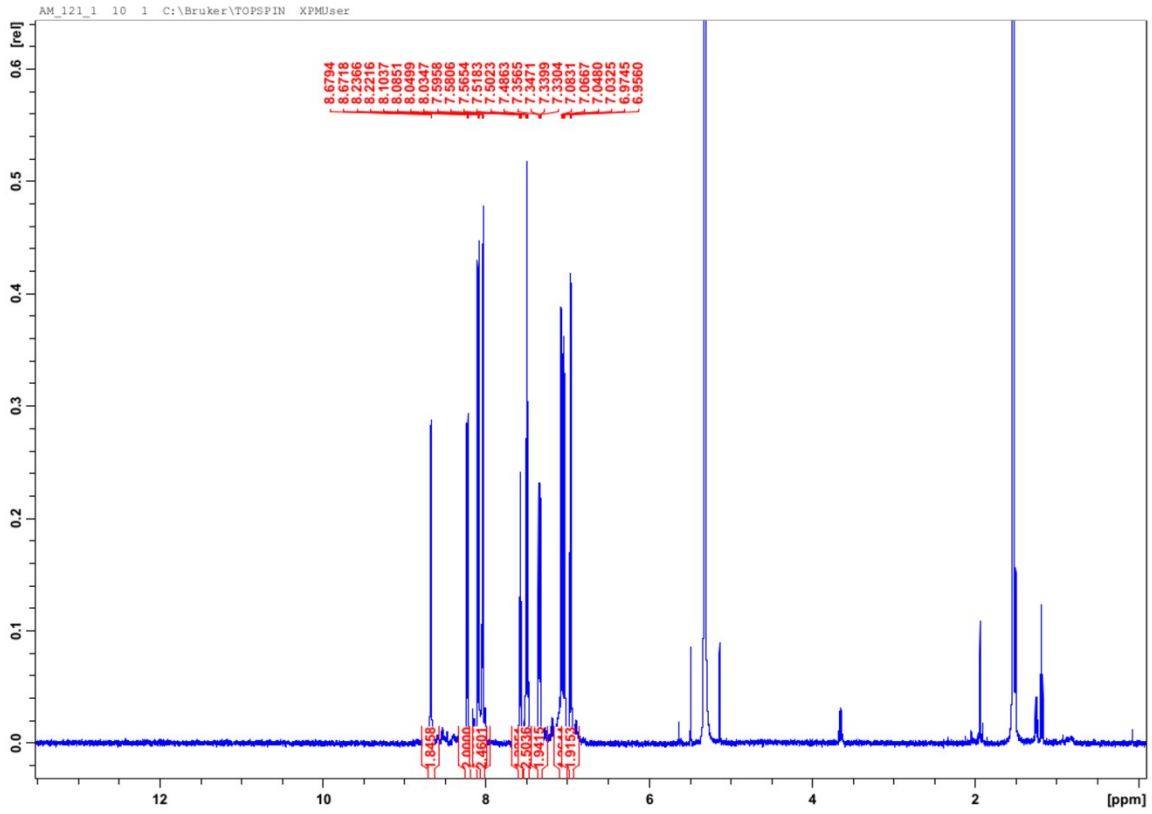

Figure 3. ^{1}H-NMR of **2**

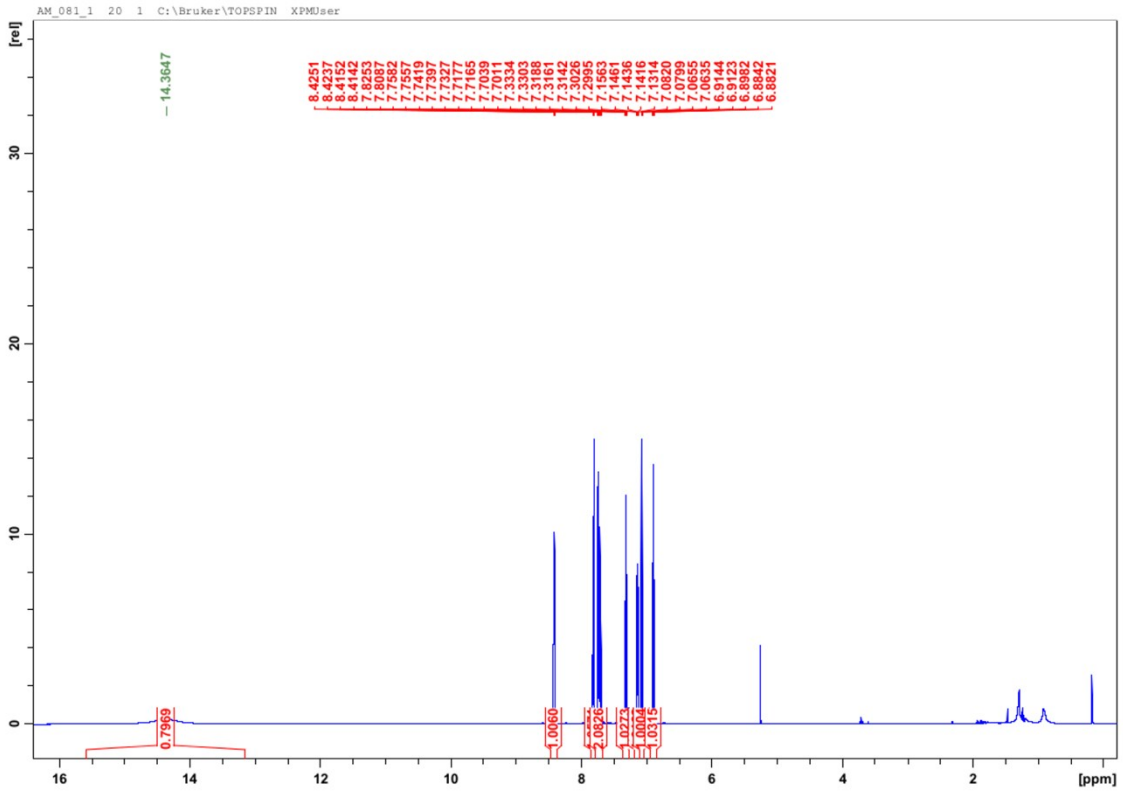

Figure 4. ^{1}H-NMR of HPP

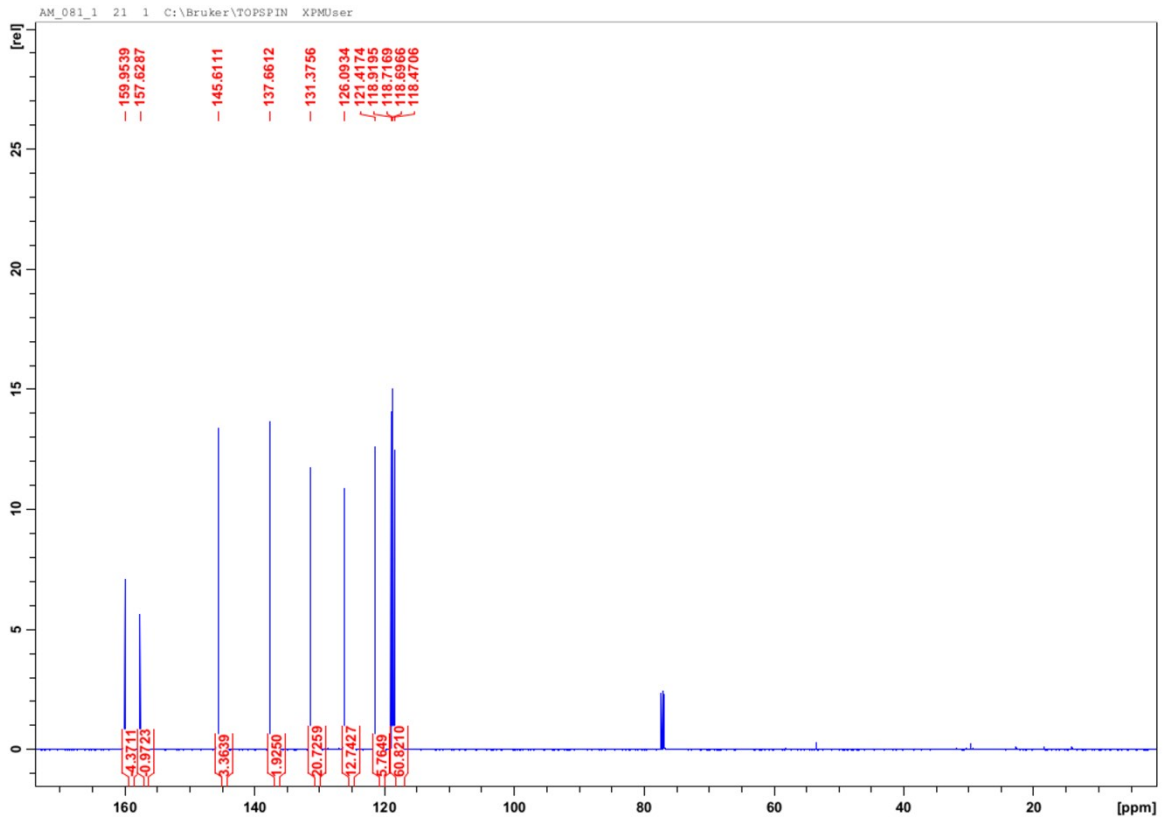

Figure 5. ^{13}C-NMR of HPP

MS Spectra

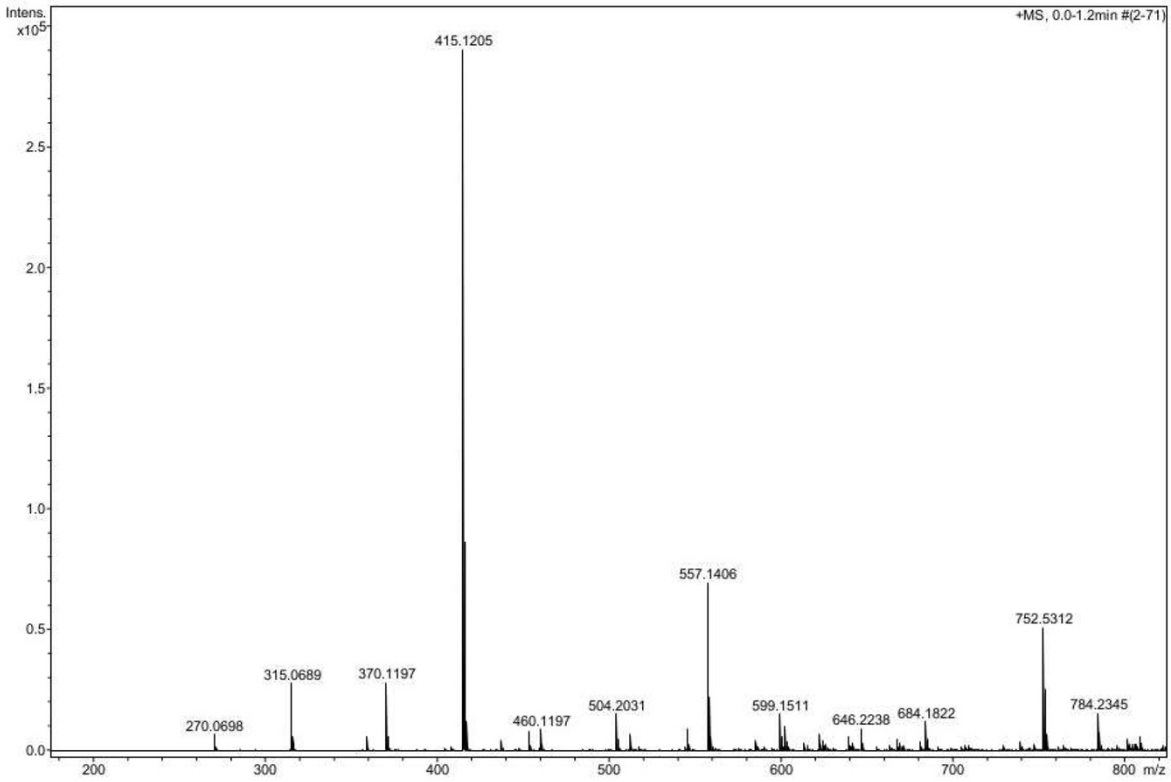

Figure 6. ESI-TOF of **1**

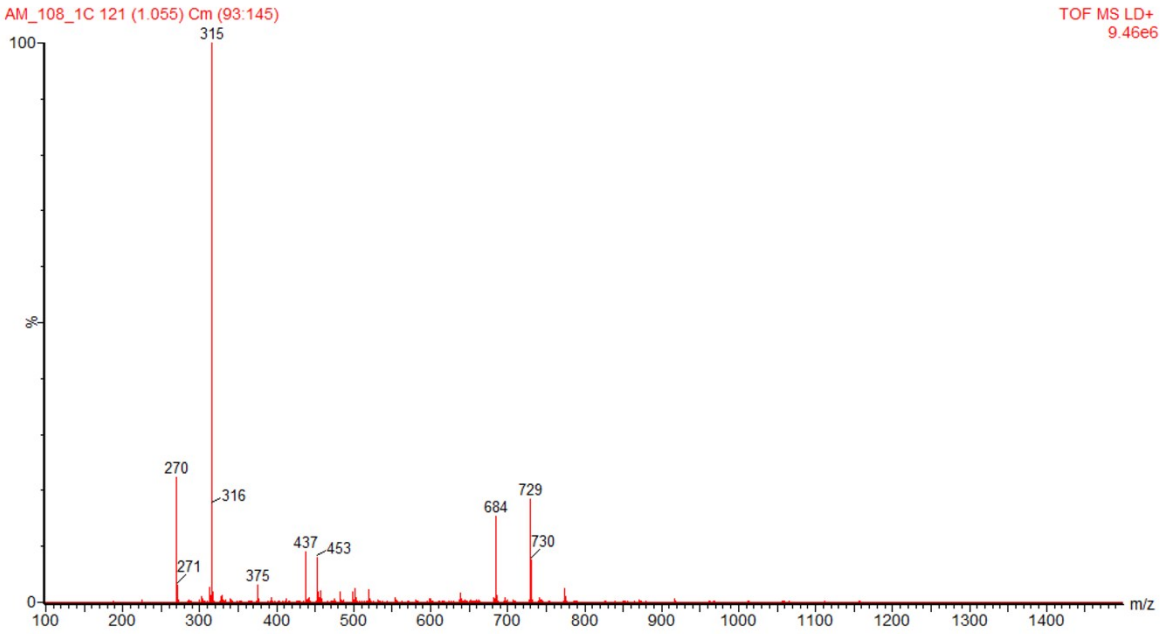

Figure 7. MALDI-TOF of **1**

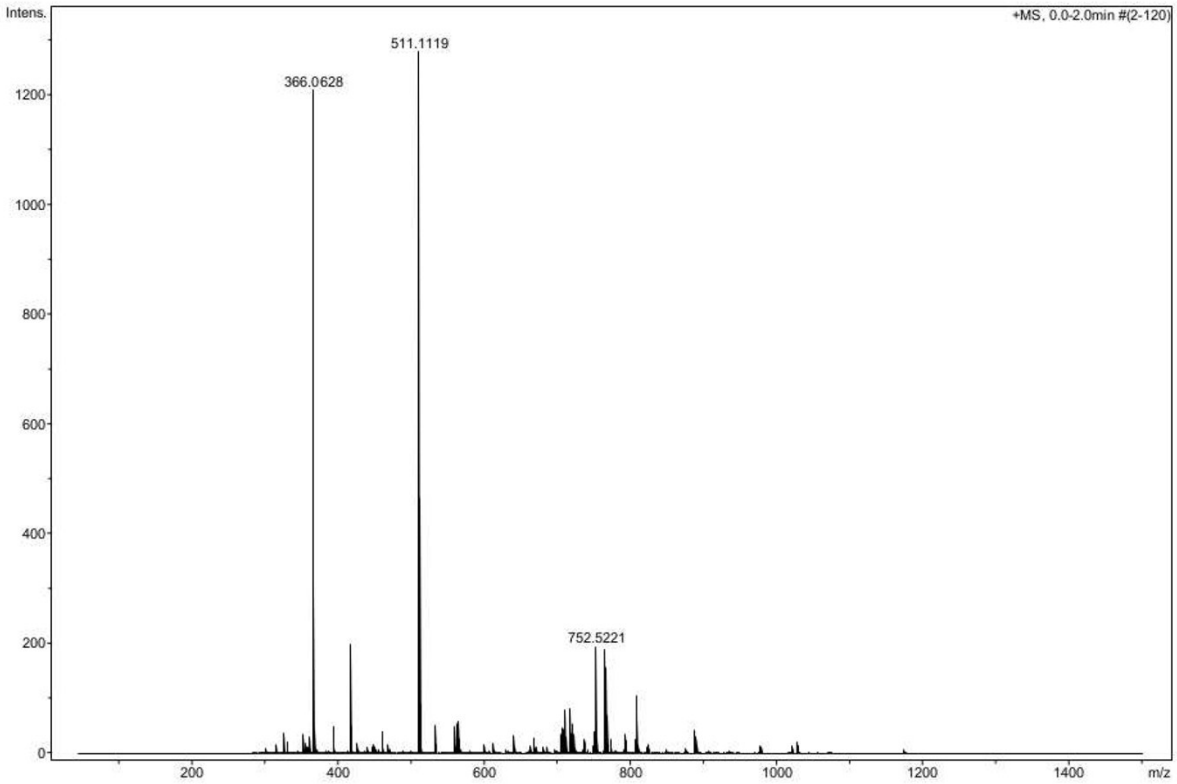

Figure 8. ESI-TOF of **2**

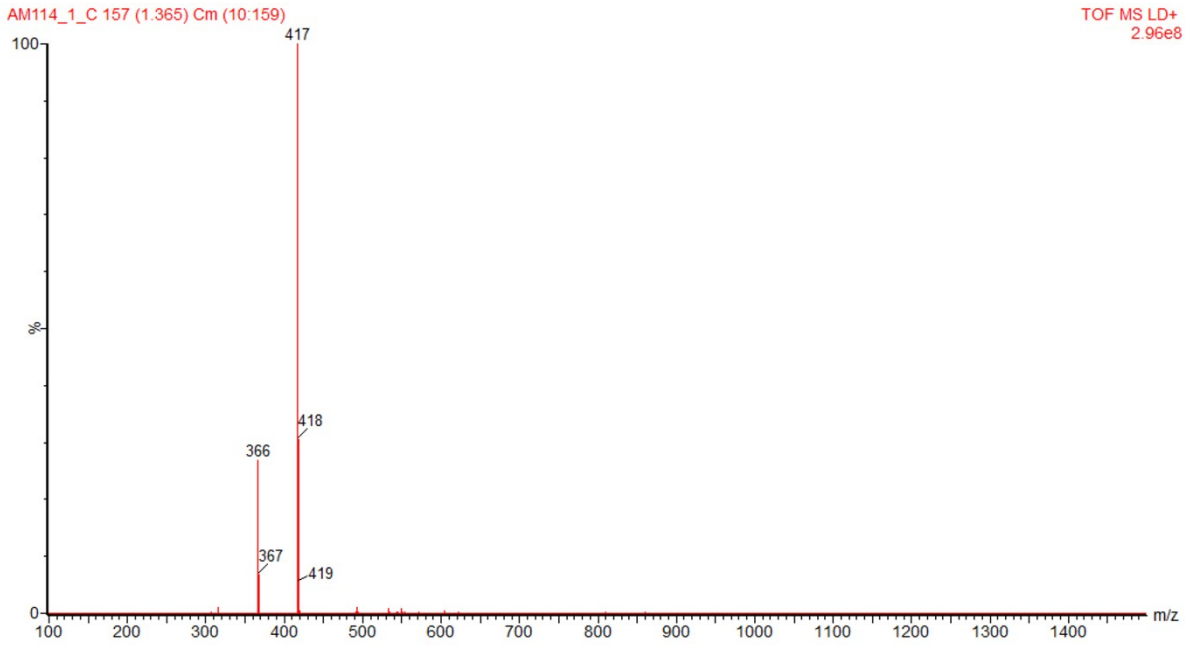

Figure 9. MALDI-TOF of **3**

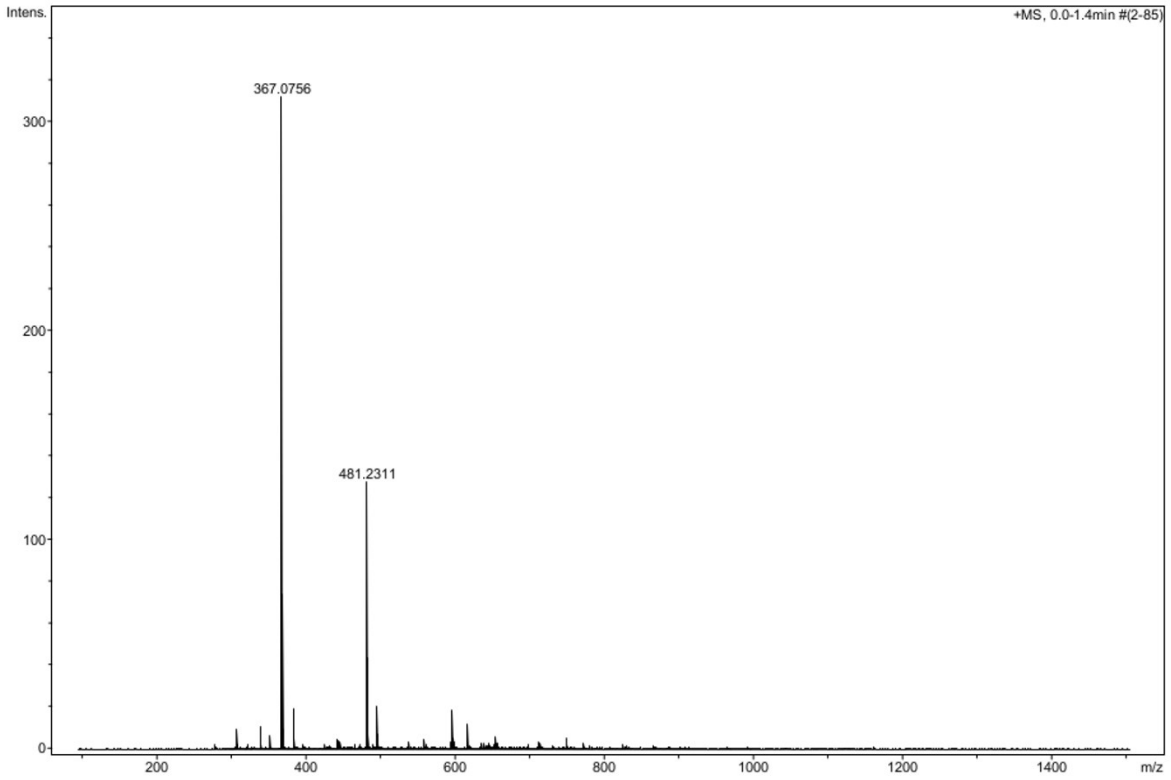

Figure 10. ESI-TOF of **4**

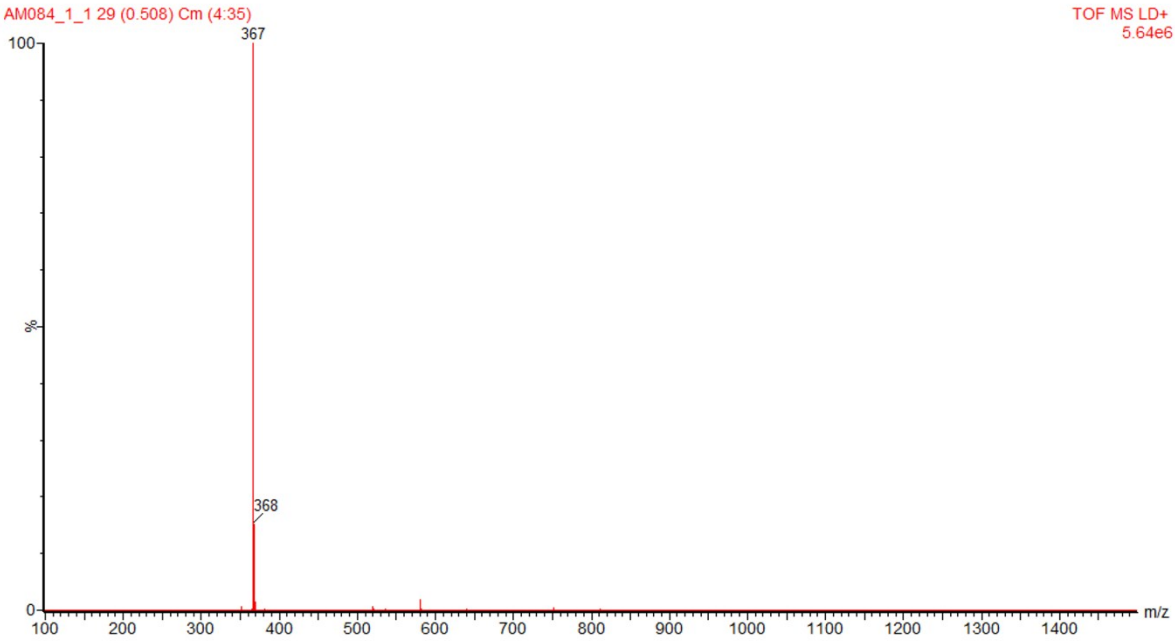

Figure 11. MALDI-TOF of **4**

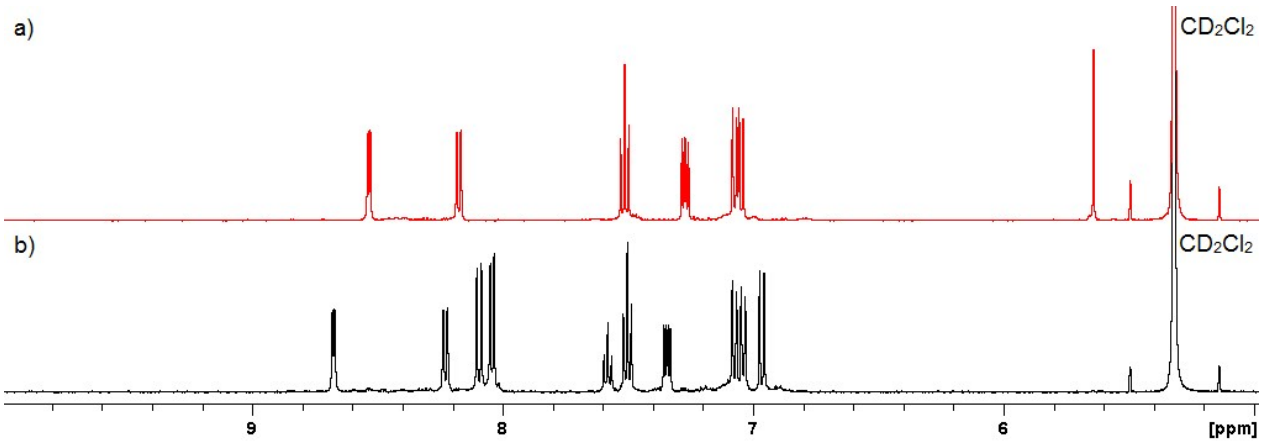

Figure 12. ^{1}H NMR spectra of complex **1** (a) and **2** (b) after sublimation in high vacuum (10^{-6} mbar, ≈250 °C).

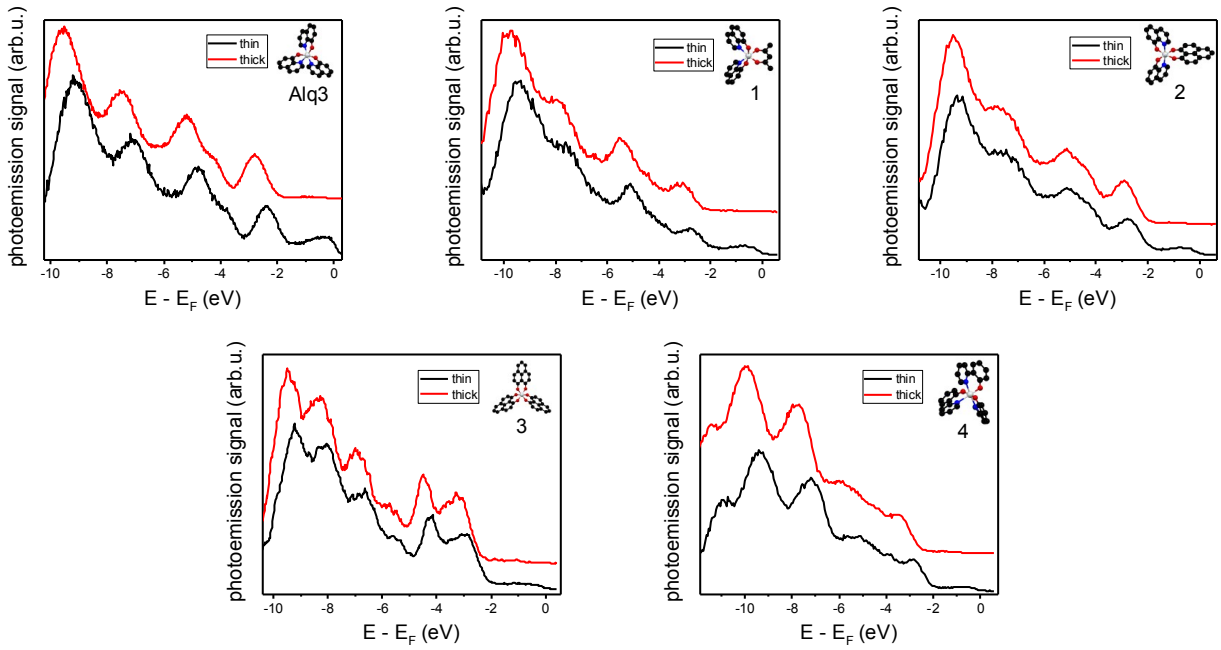

Figure 13. Comparison between the UPS spectra recorded from 1ML molecules on cobalt (black curves, "thin") and the UPS spectra recorded from 4ML molecules on cobalt (red curves, "thick"). The UPS spectra show identical spectral features, that can be reproduced using the eigenvalues from DFT calculations (see Figure 2 in the main article). We take this fact as a strong indication that the molecules in both thin and thick molecular layers on cobalt are intact.