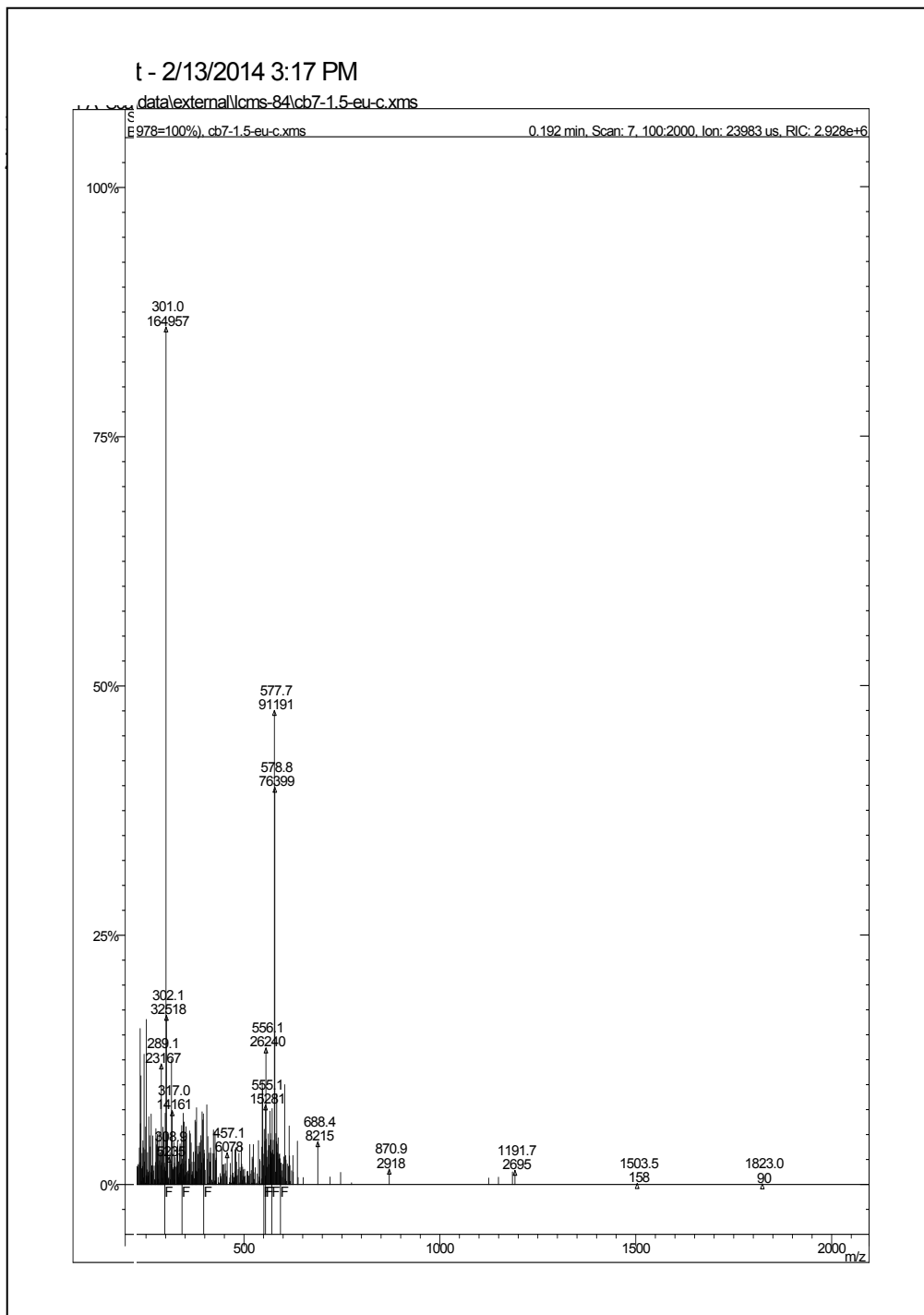
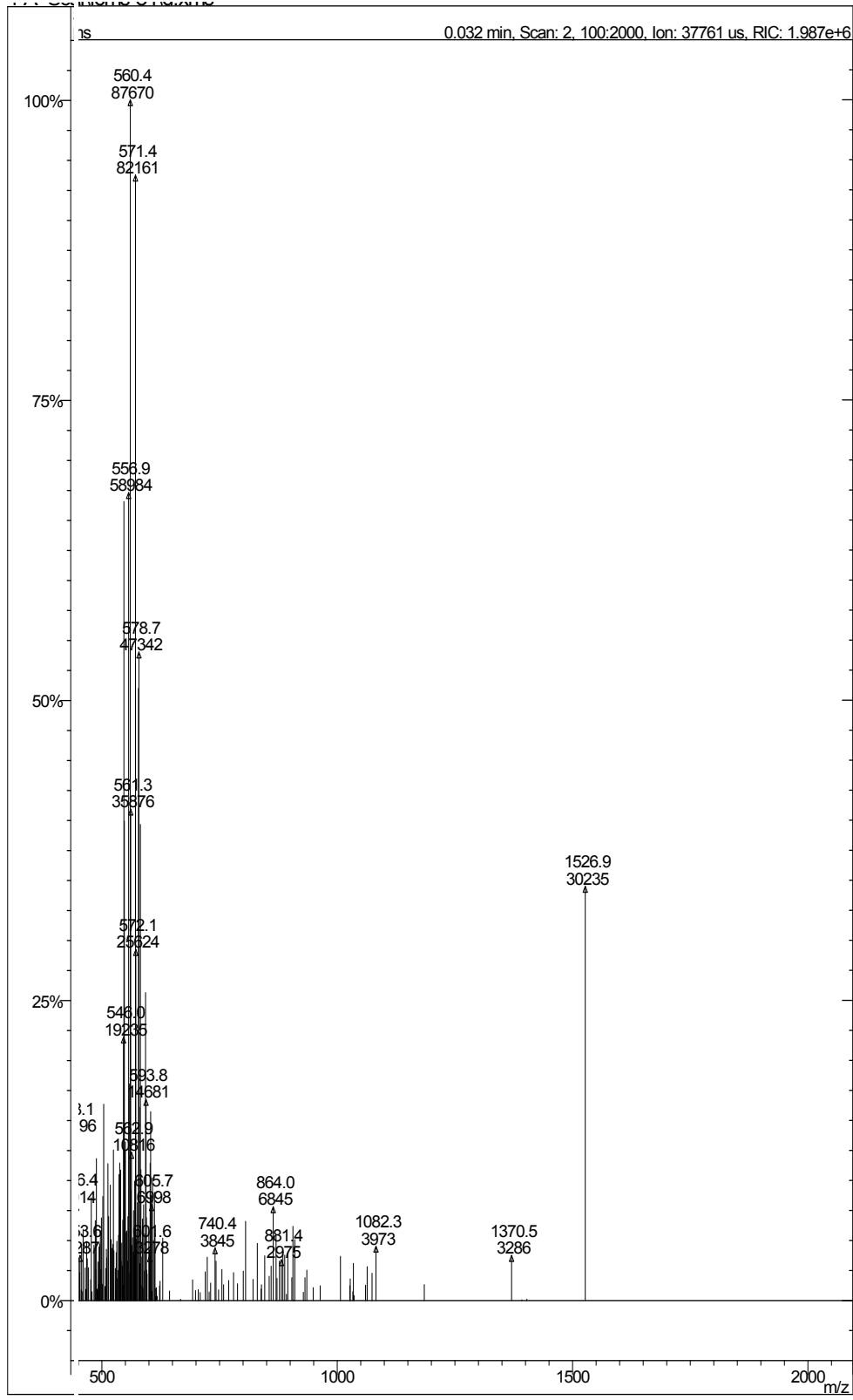


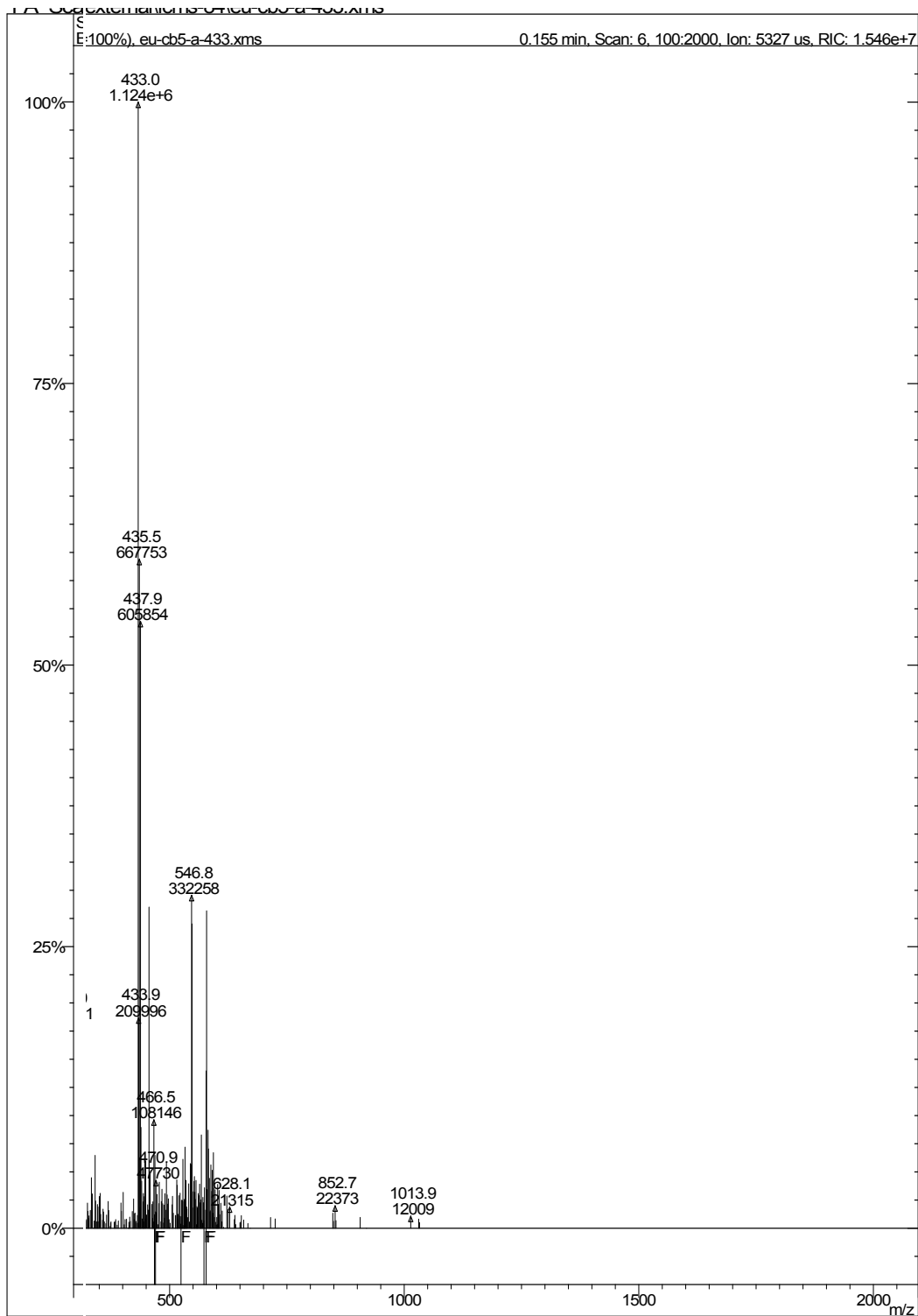
1. ESI-MS spectra of Eu-CB7 at ligand to metal ratio 1.



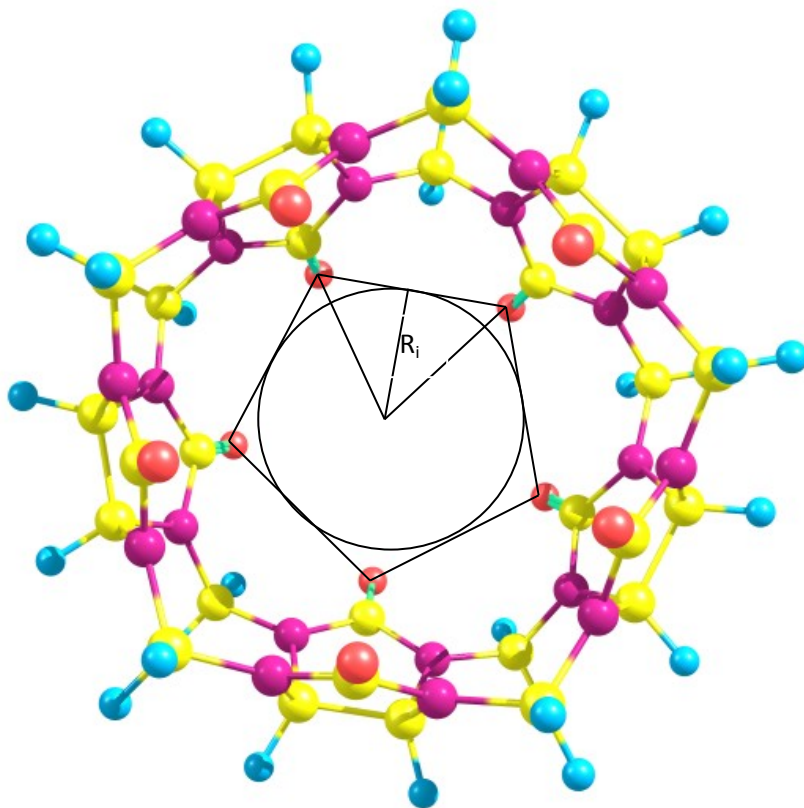
2. ESI-MS spectra of Eu-CB7 at ligand to metal ratio 5



3. ESI-MS spectra of Eu-CB5 at ligand to metal ratio 5

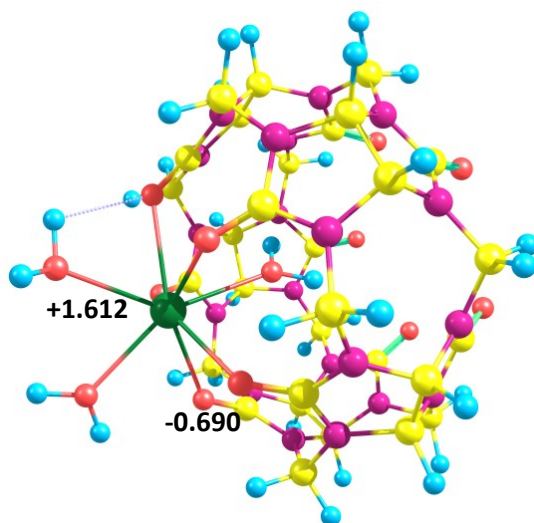


4. Optimised structure of CB5 describing R_i (Europium atom (green), Oxygen atom (red), Hydrogen atom (blue), Nitrogen atom (purple) and Carbon (yellow))



5. **Optimized structure of Eu(III)CB5(H₂O)₃ in two different geometries (Europium atom (green), Oxygen atom (red), Hydrogen atom (blue), Nitrogen atom (purple) and Carbon (yellow))**

- i) Out of three water molecules coordinated to Eu(III), one water molecule encapsulated in the cavity and two water molecules are coordinated from outside (Eu-CB5 A)



- ii) All the three water molecules are coordinated to Eu(III) from outside (Eu-CB5 B)

