Supplementary material

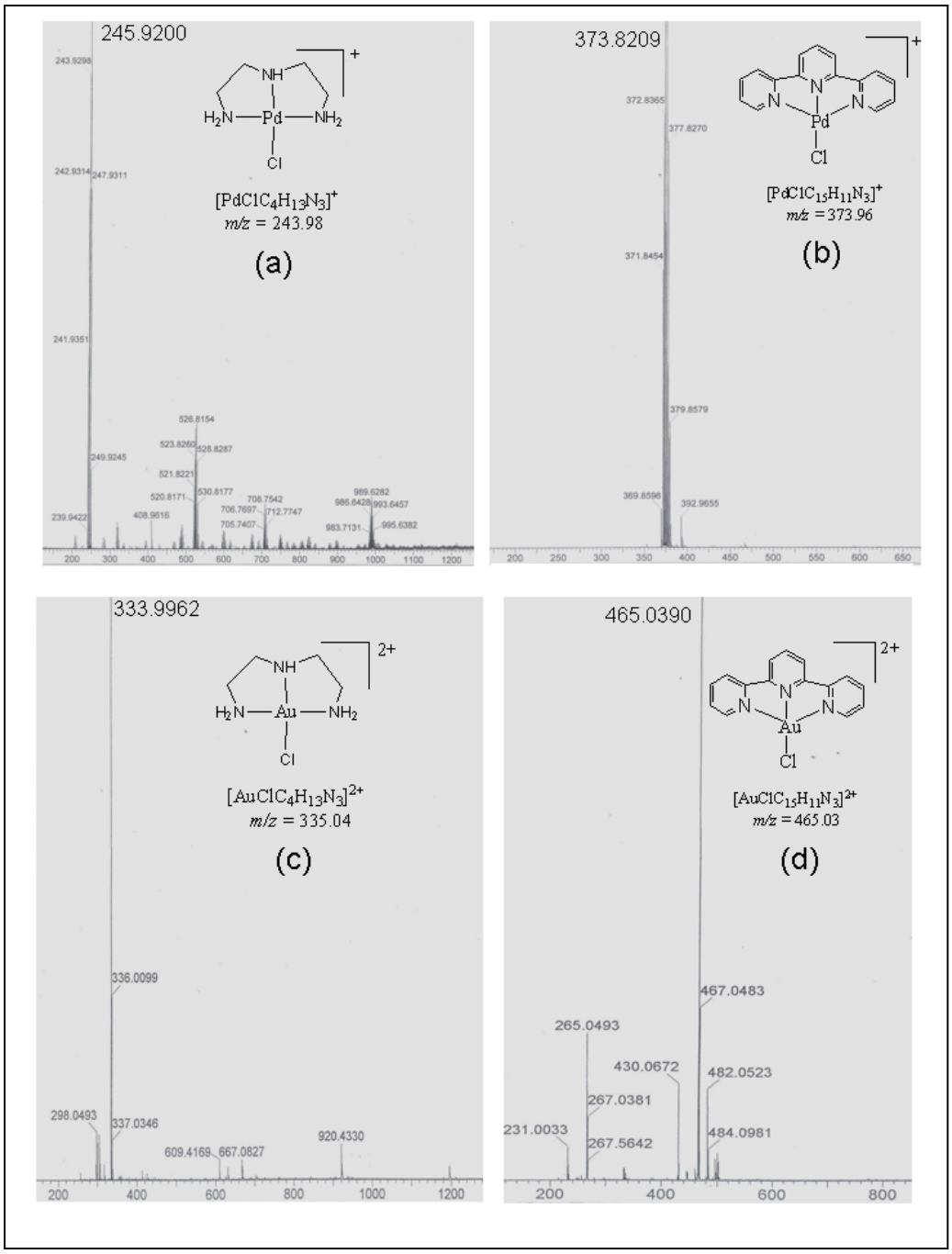

Figure S1: The ESI-MS full scan (positive mode) for the Pd(II) and Au(III) starting materials. (a) [PdCl(dien)]Cl compound; (b) [PdCl(terpy)]Cl; (c) [AuCl(dien)]Cl_2, and (d) [AuCl(terpy)]Cl_2.

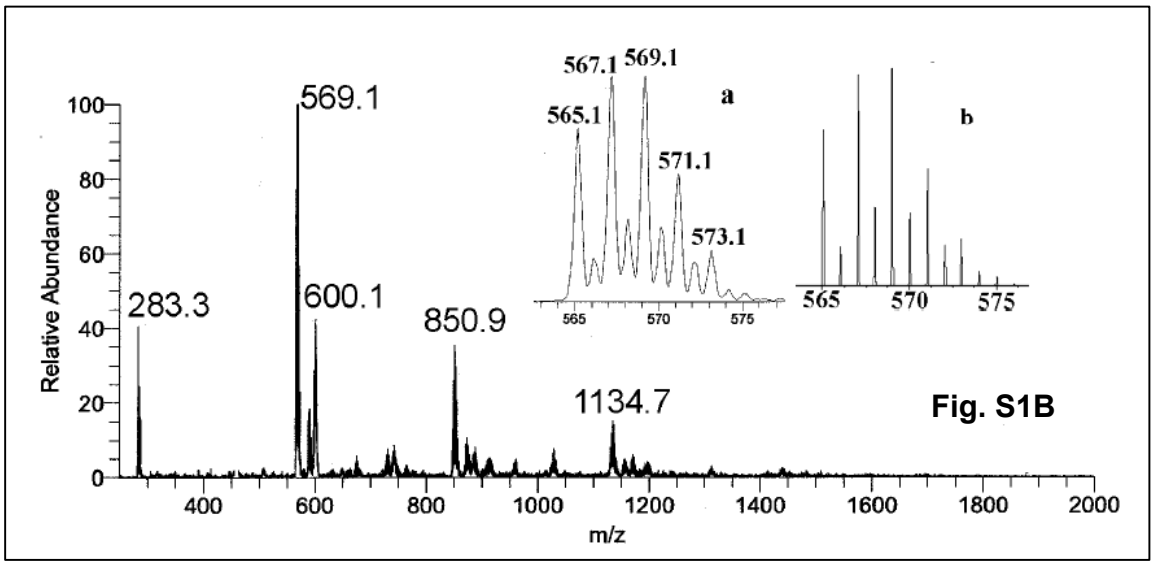

Figure S2: The ESI-MS full scan (positive mode) of zinc finger model compound [Zn(bme-dach)]$_2$ and the isotopic distribution of {[Zn(bme-dach)]$_2$]}$^+$ (a) experimental and (b) calculated results. Assignments: *m/z* = 569.1 corresponds to {[Zn(bme-dach)]$_2$]/H$^+$}$^+$, *m/z* = 850.9 corresponds to {[Zn(bme-dach)]$_3$]}$^+$, and *m/z* = 1134.7 corresponds to {[Zn(bme-dach)]$_4$]}$^+$.

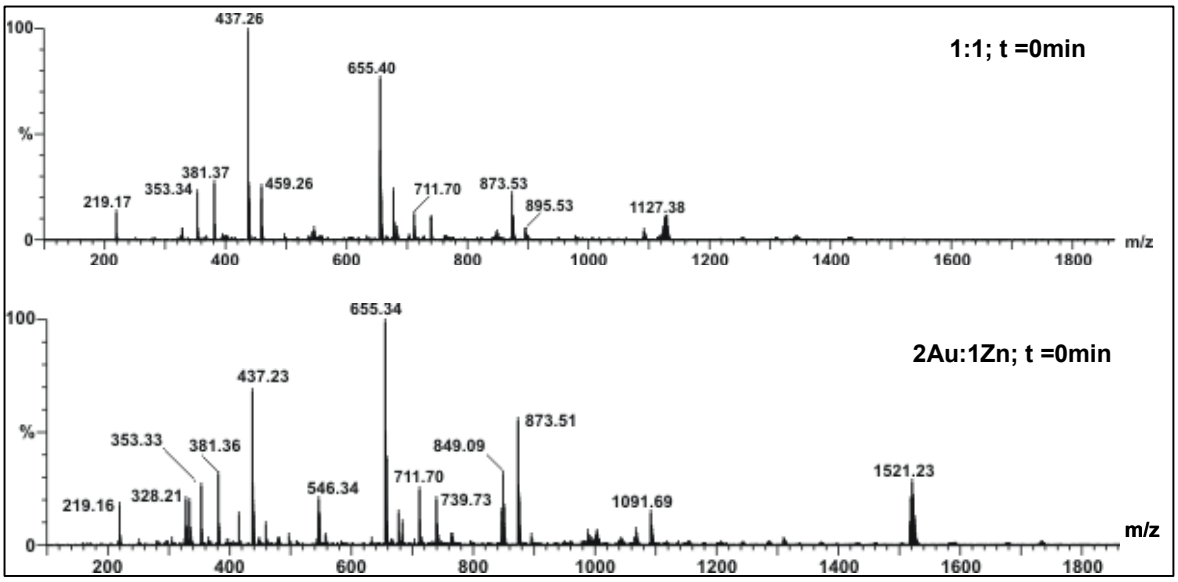

Figure S3. The ESI-MS full scan (positive mode) of the reaction between $[AuCl(dien)]Cl_2$ and $[Zn(bme\text{-}dach)]_2$ after immediately incubation at 37°.

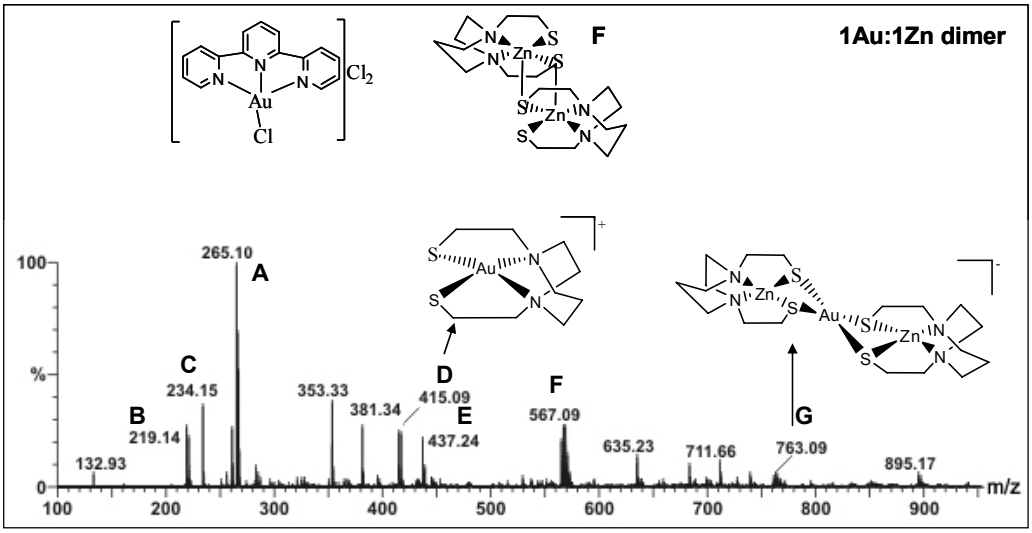

Figure S4: The ESI-MS full scan (positive mode) of the reaction between $[AuCl(terpy)]Cl_2$ and $[Zn(bme\text{-}dach)]_2$ after 5 min of the reaction.

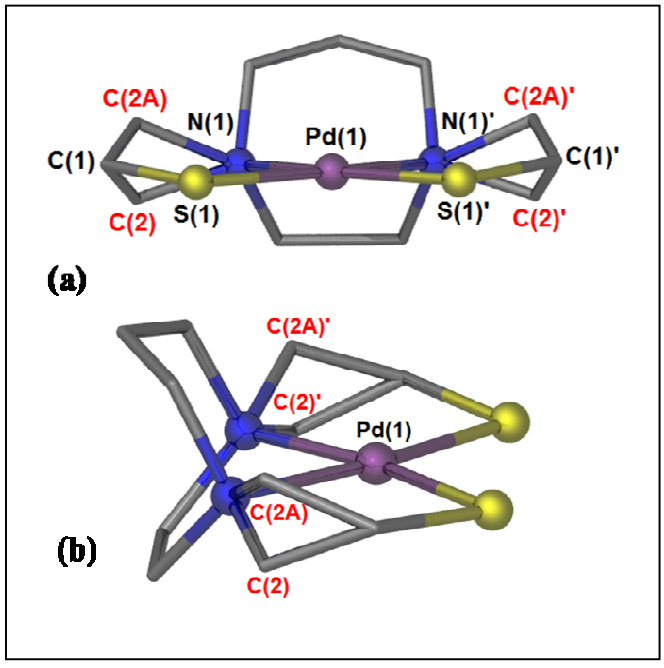

Figure S5. Ball and stick images of the [Pd(bme-dach)] structural disorder at C(2) (Occ = 0.69355) and C(2A) (Occ = 0.30645), labeled in red. (a) end-on view and (b) side view.