Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

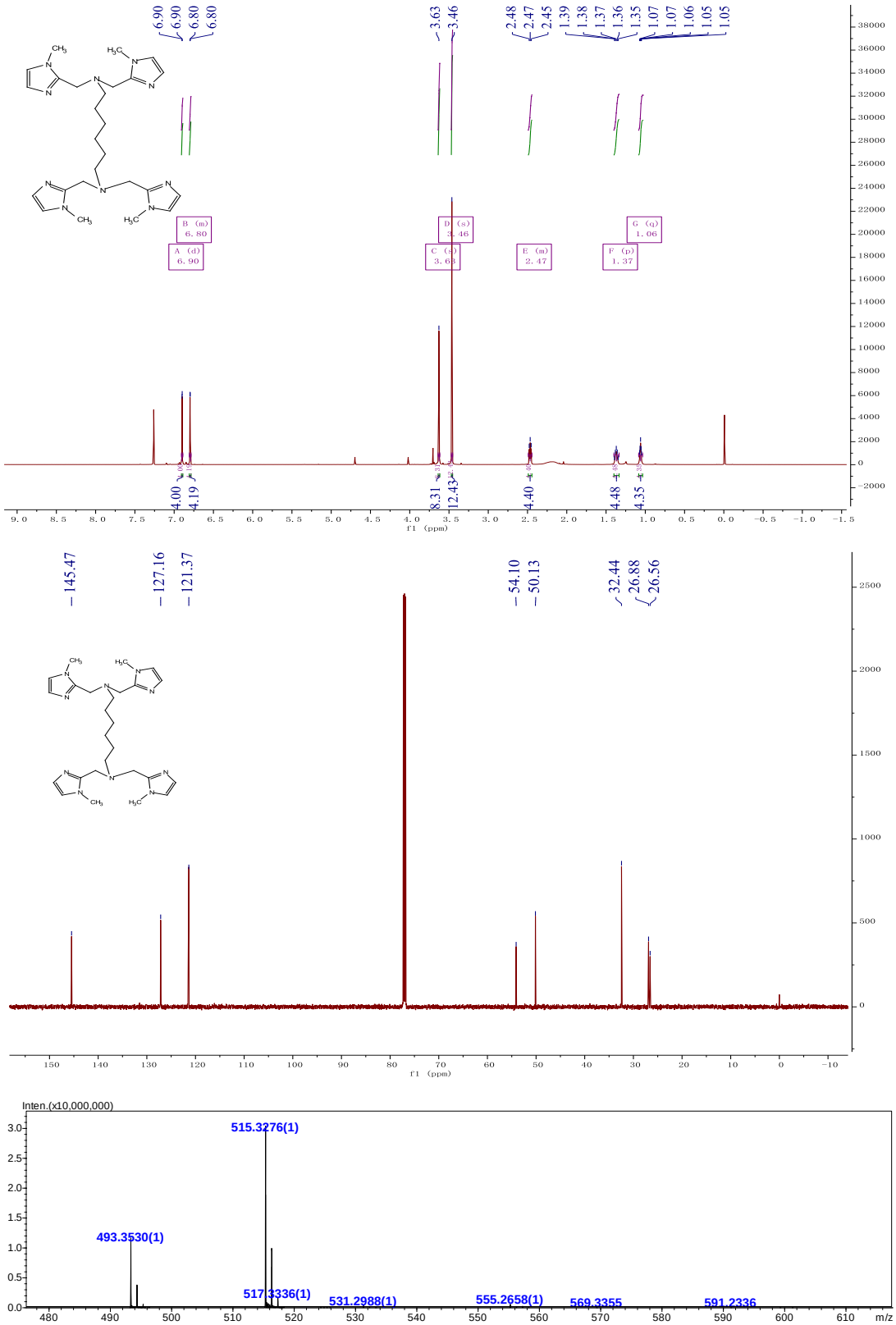

Figure S1. ^{1}H NMR (A), ^{31}C NMR (B) and ESI-MS (C) of hexadentate imidazole derivative (L) as the desired ligand for binuclear metal complexes.

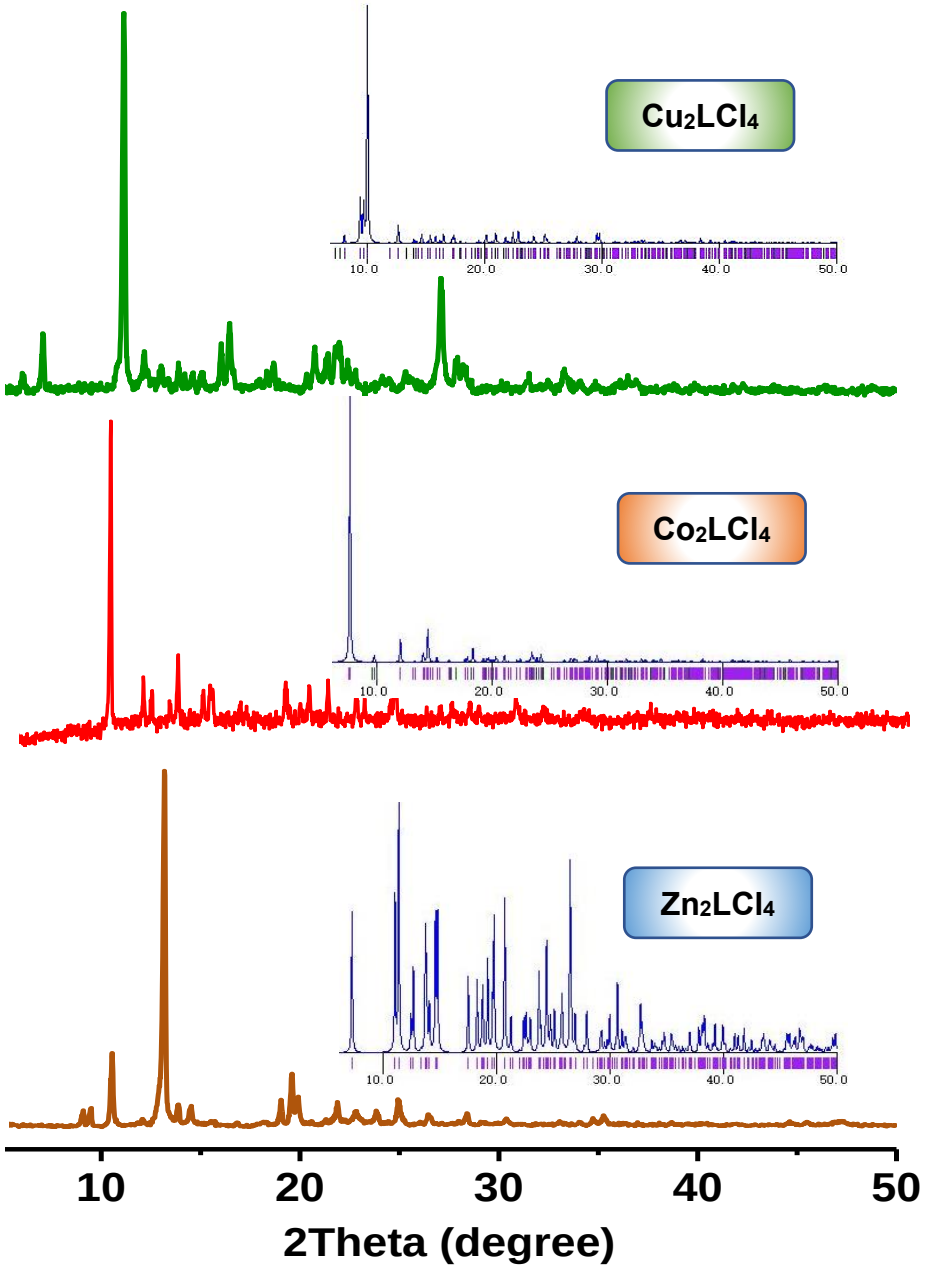

Figure S2. Collected PXRD patterns of three binuclear complexes (Cu_2LCl_4, Co_2LCl_4, Zn_2LCl_4). The inserts are the simulated PXRD patterns from single crystal data.

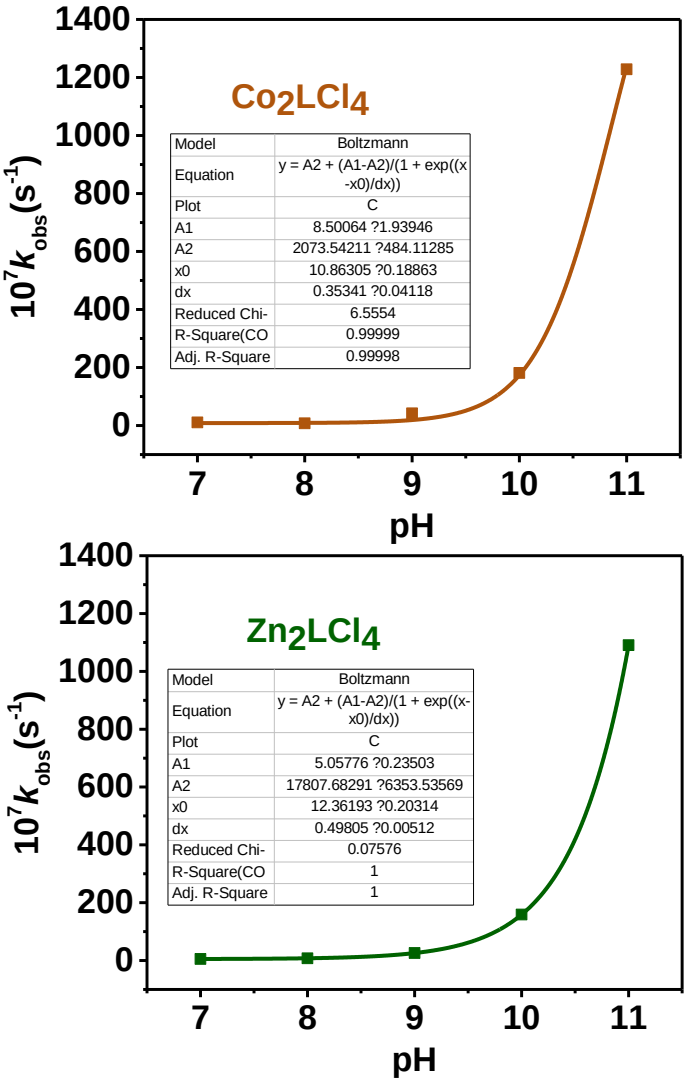

Figure S3. pH-Dependence of the transesterification rate of HPNP promoted by Co_2LCl_4 or Zn_2LCl_4. Conditions: 25°C, [HPNP]=1.0×10^{-4} mol/L, [complex]=5.0×10^{-5} mol/L.

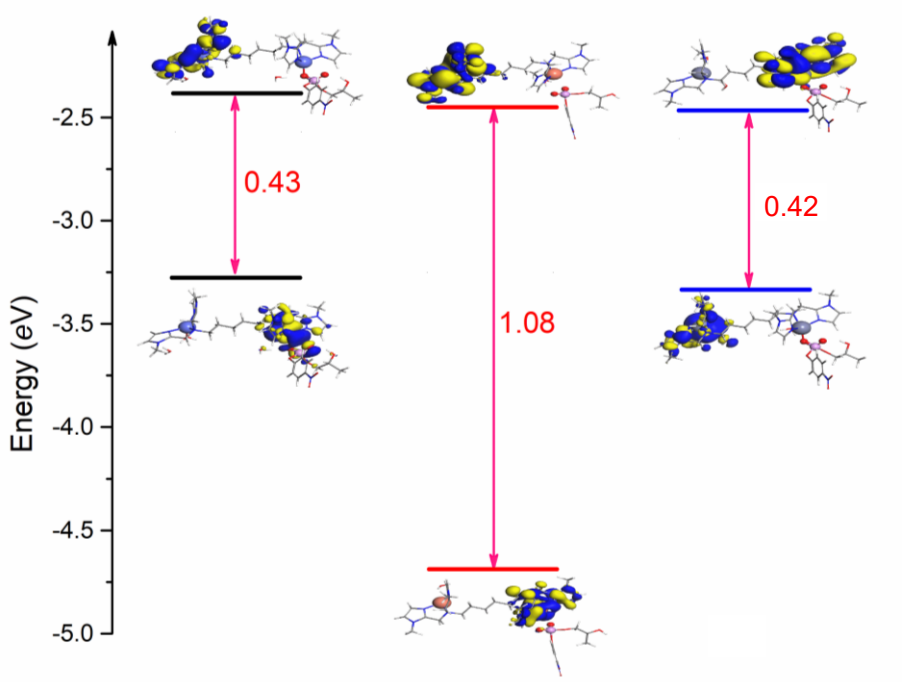

Figure S4. Calculated energies of HOMO, LUMO orbits of three HPNP-catalyst binary complexes (left to right: HPNP-Co_2LCl_4, HPNP-Cu_2LCl_4, HPNP-Zn_2LCl_4).

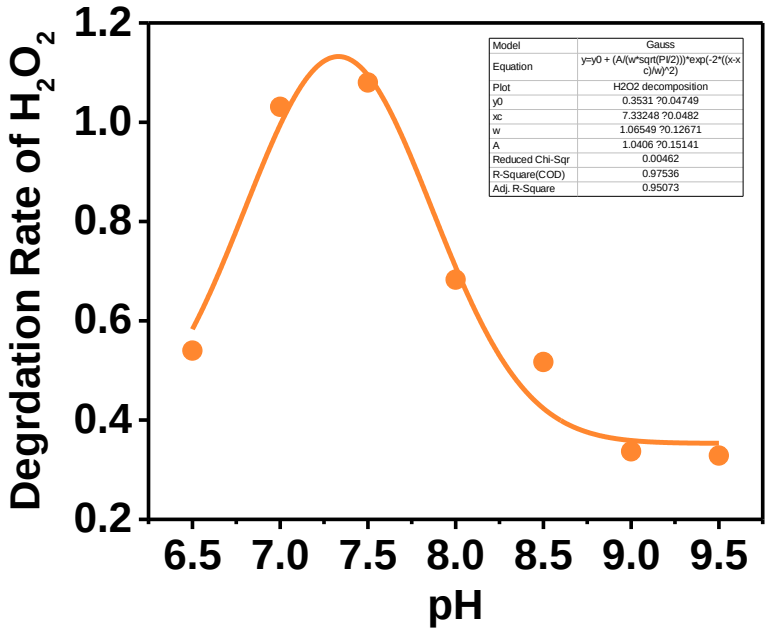

Figure S5. pH-dependent decomposition rate of H_2O_2 catalyzed by Cu_2LCl_4.

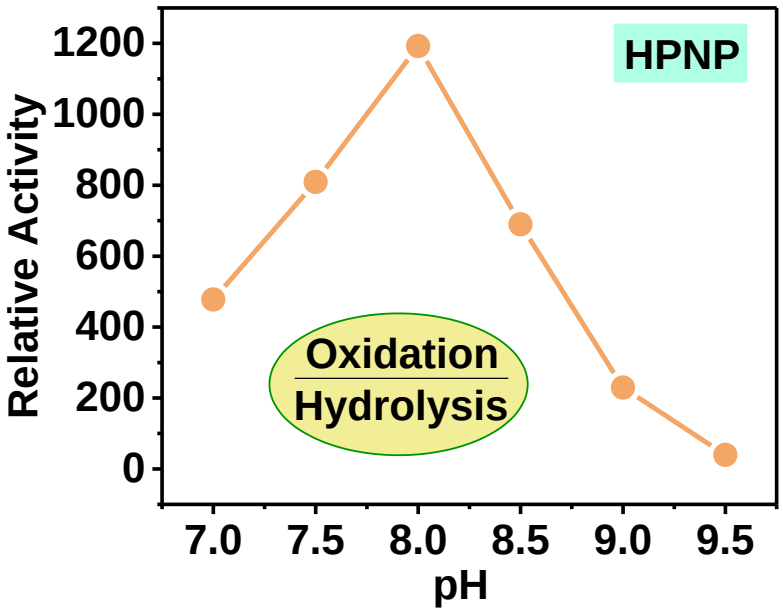

Figure S6. pH-Dependent relative rate of the oxidative cleavage to the hydrolytic one of HPNP promoted by Cu_2LCl_4.

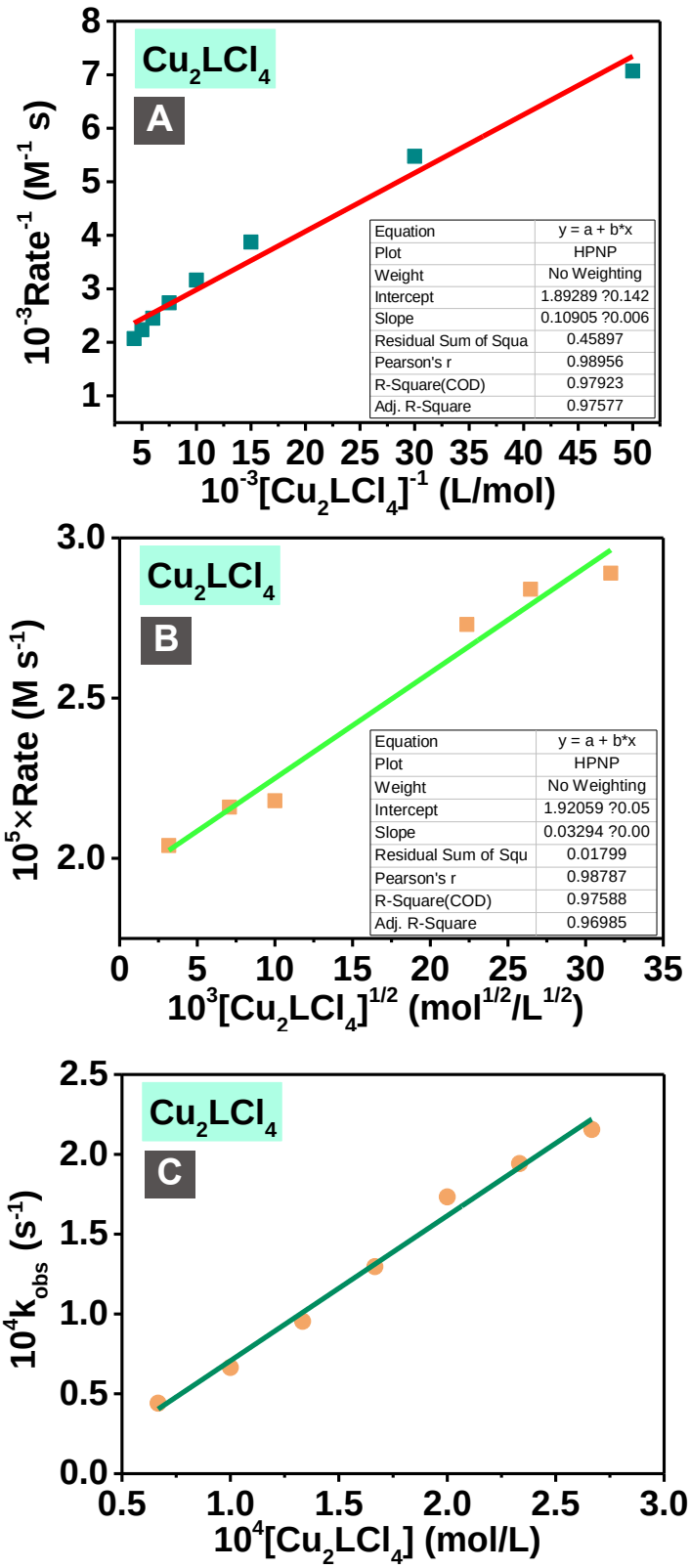

Figure S7. The linear $rate^{-1}_{oxid}$ -$[Cu_2LCl_4]^{-1}$ of the HPNP oxidative cleavage (A), dependence of the transesterification rate of HPNP on the $[Cu_2LCl_4]^{1/2}$ (B) and k_{obs}-$[Cu_2LCl_4]$ plot of the oxidative cleavage of BNPP (C).

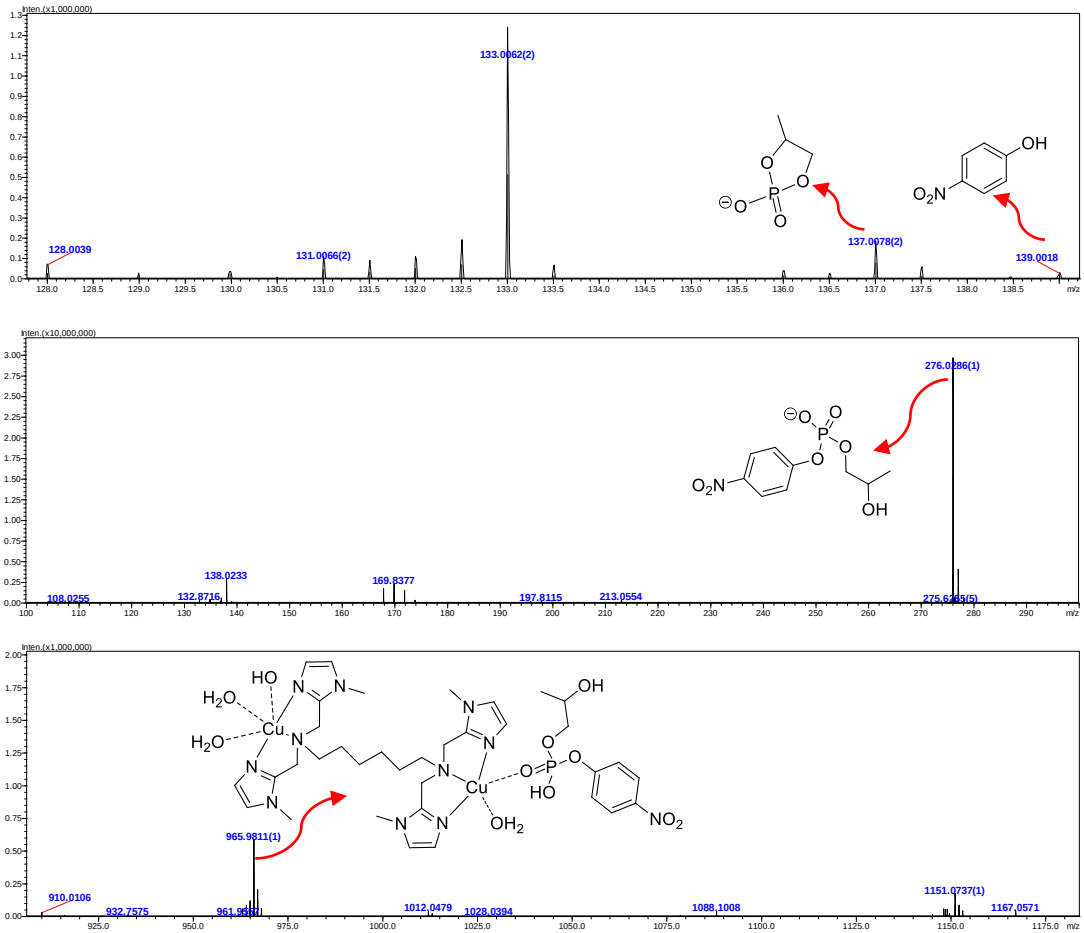

Figure S8. Selected ESI-MS spectra of the mixture for the hydrolytic cleavage of HPNP by Cu_2LCl_4.

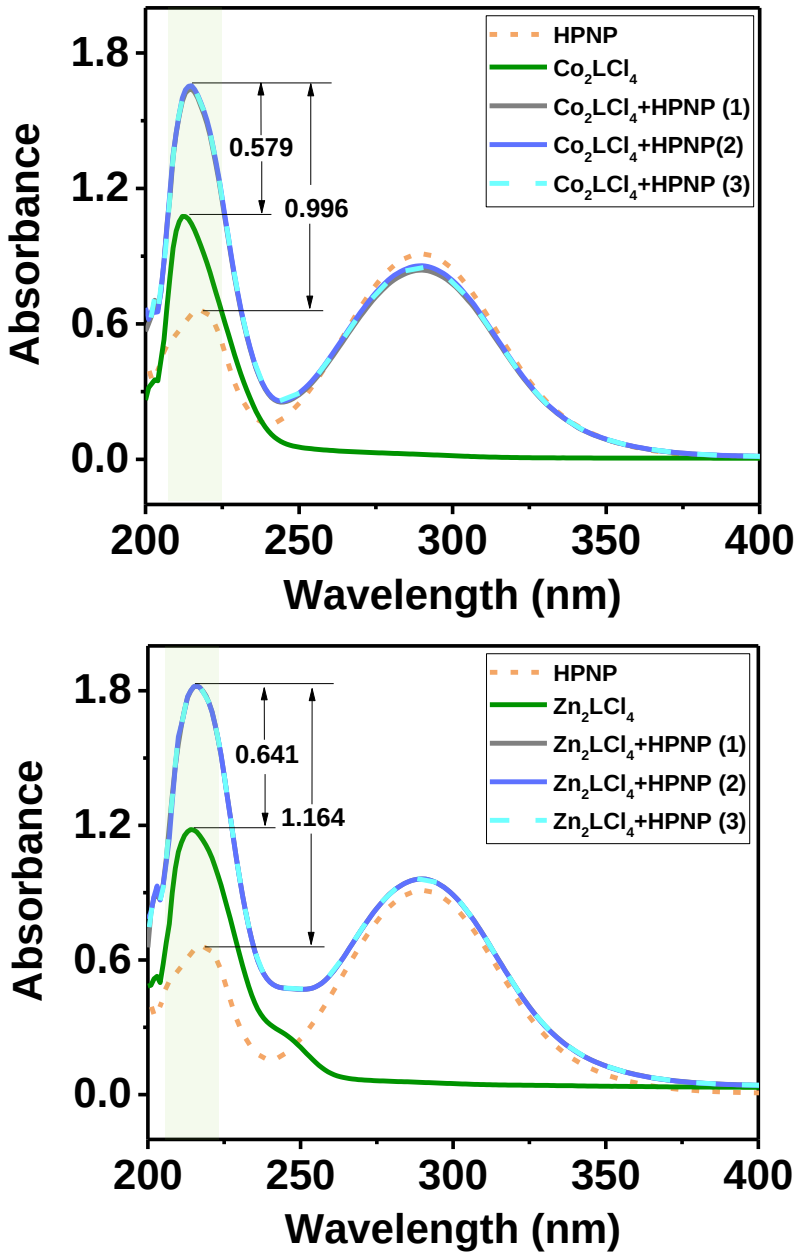

Figure S9. UV-vis spectra of the transesterification of HPNP in the presence of Co_2LCl_4 (Top) or Zn_2LCl_4 (Low). Numbers (1)-(3) shown in legend indicate different scans for three runs. Conditions: 25 °C, pH 7.00, [HPNP]= 1.0×10^{-4} mol/L, [complex]= 5.0×10^{-5} mol/L.

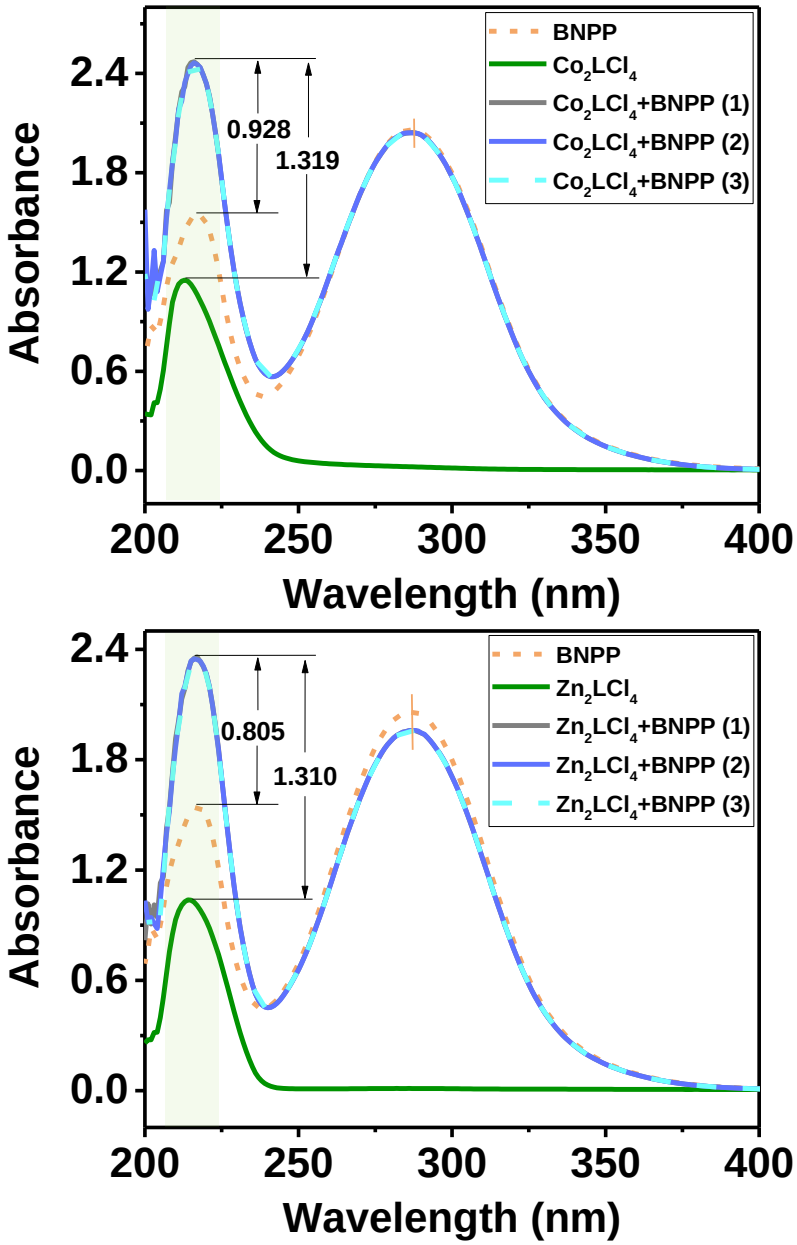

Figure S10. UV-vis spectra of the hydrolysis of BNPP in the presence of Co_2LCl_4 (Top) or Zn_2LCl_4 (Low). Numbers (1)-(3) shown in legend indicate different scans for three runs. Conditions: 25 °C, pH 7.00, [BNPP]= 1.0×10^{-4} mol/L, [complex]= 5.0×10^{-5} mol/L.

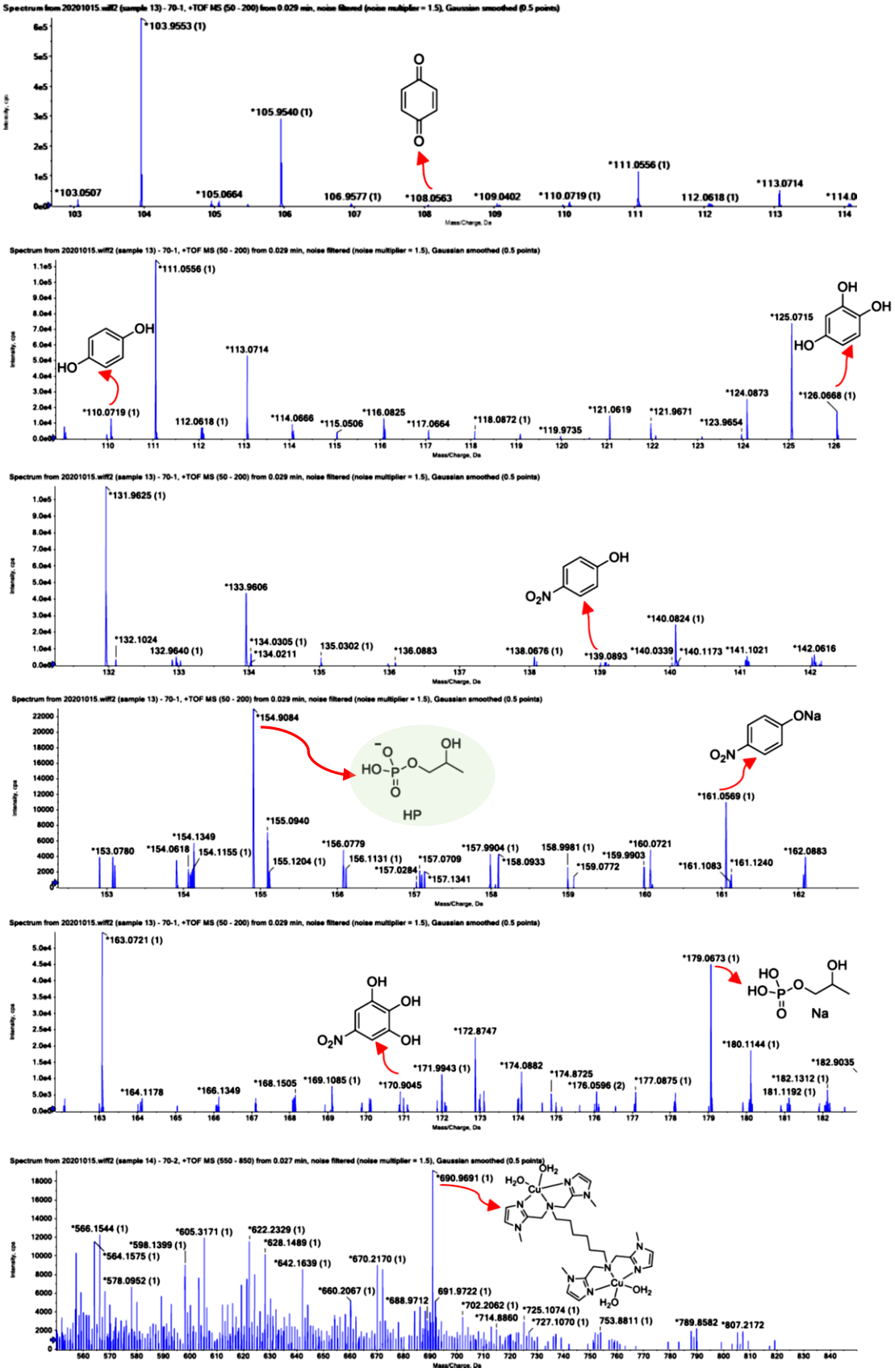

Figure S11. Selected ESI-MS spectra of the mixture for the oxidative cleavage of HPNP by Cu_2LCl_4 in the presence of H_2O_2.