

Fig. S1 The ESMS full scan (positive mode) of the complex $trans\text{-}[\text{Pt}(\text{pyr})_2(9\text{-EtGua})\text{Cl}]\text{NO}_3$ and the isotopic distribution of $[\text{Pt}(\text{pyr})_2(9\text{-EtGua})\text{Cl}]^+$ (a) experiment (b) calculated results

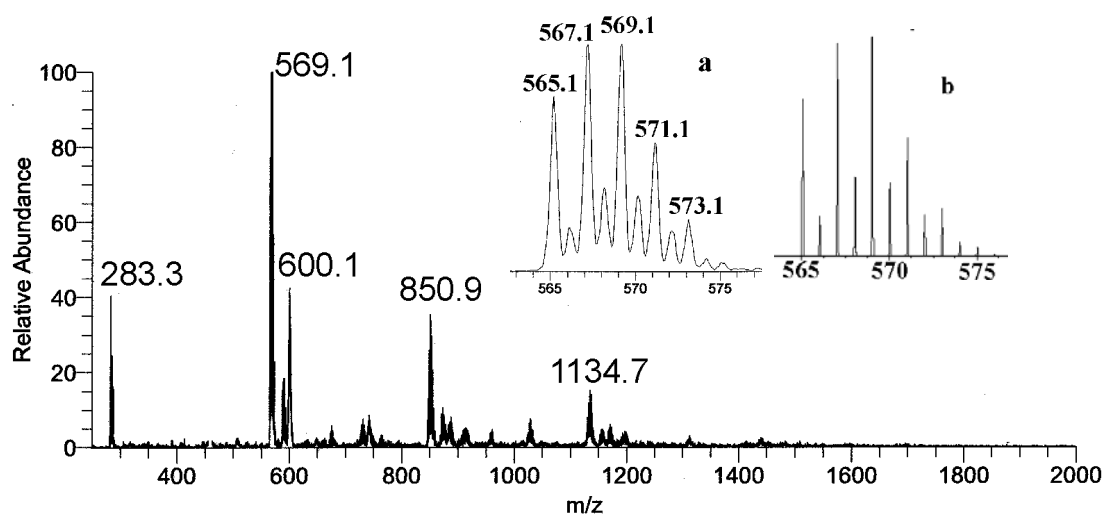


Fig. S2 The ESMS full scan (positive mode) of zinc finger model compound $[\text{Zn}(\text{bme-dach})]_2$ and the isotopic distribution of $[\text{Zn}(\text{bme-dach})]_2^+$ (a) experiment (b) calculated results.

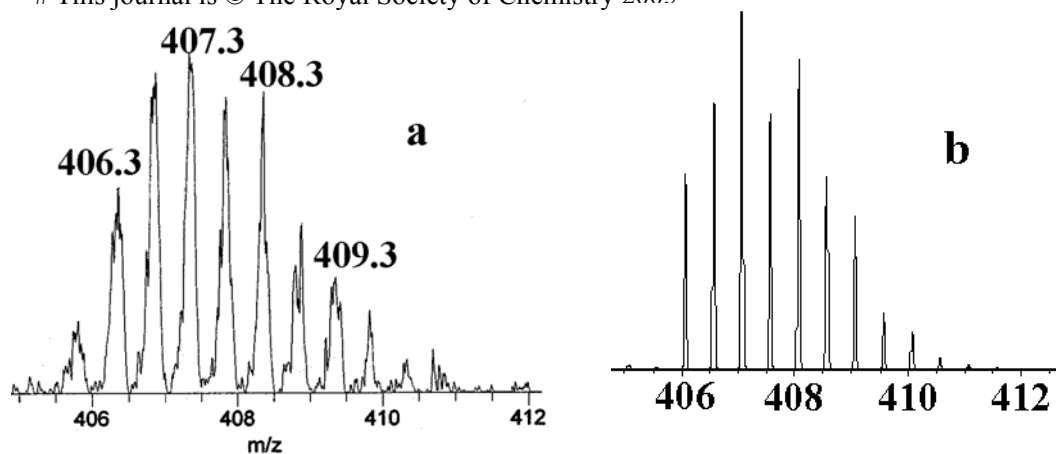


Fig S3. (a) The experiment isotopic distribution of peak 407.3 and (b) the calculation isotopic distribution of $[\text{Zn}(\text{bme-dach})\text{Pt}(\text{pyr})_2(9\text{-EtGua})]^{2+}$

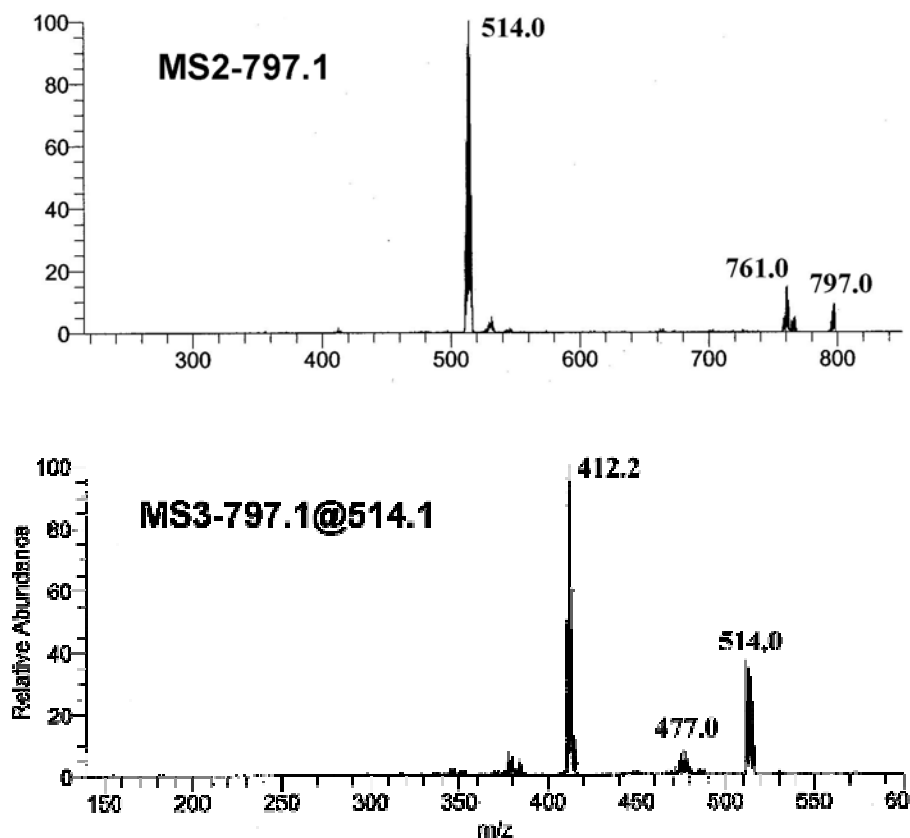


Fig S4. The MS2 of the peak 797.1 and MS3 of the peak 797.1 @ 514.0

Table S1 Assignment of the peaks observed in Figure S1 and S2.

Peak observed	Charge	Corresponding species	Calculated
565.1-573.1	+1	$\{[\text{Zn}(\text{bme-dach})]_2 + \text{H}^+\}^+$	568.2
600.1	+2	?	
846.8-858.8	+1	$\{[\text{Zn}(\text{bme-dach})]_3 + \text{H}^+\}^+$	851.8
1128.8-1142.8	+1	$\{[\text{Zn}(\text{bme-dach})]_4 + \text{H}^+\}^+$	1134.4
281.13-288.1	+1	$\{[\text{Zn}(\text{bme-dach})] + \text{H}^+\}^+$	284.6
566.1-572.1	+1	$[\text{Pt}(9\text{-EtGua})\text{Cl}(\text{Py})_2]^+$	567.5
354.8-356.8	+2	$[\text{Pt}(9\text{-EtGua})_2(\text{Py})_2]^{2+}$	355.5
1130.7-1139.8	+1	$\{[\text{Pt}(9\text{-EtGua})\text{Cl}(\text{Py})_2]_2^{2+} - \text{H}^+\}^+$	1134.0
487.2-491.2	+1	$[\text{Pt}(9\text{-EtGua})\text{Cl}(\text{Py})]^+$	488.5
451.3-455.3	+1	$\{[\text{Pt}(9\text{-EtGua})(\text{Py})]^{2+} - \text{H}^+\}^+$	452.0