Supporting Information

Insight into the antitumor actions of the sterically hindered platinum(II) complex by combination of STD NMR and LCMS techniques

Zhimei Wang,[a] Lei Fang, [a] Jian Zhao*, [a] Shaohua Gou*,[a]

[a] Pharmaceutical Research Center and School of Chemistry and Chemical Engineering and Jiangsu Province Hi-Tech Key Laboratory for Biomedical Research, Southeast University, Nanjing 211189, China

E-mail: zhaojianzhaokuan@163.com； *sgou@seu.edu.cn.*

Content of Supplementary Information

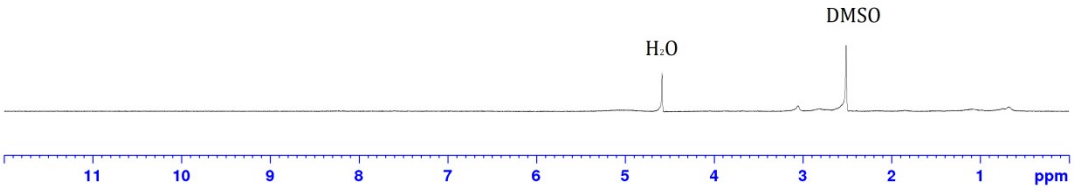

Fig. S1 STD spectrum of a sample containing 10 μM HSA in 0.05 uL DMSO-d_6 and 0.45uL D_2O at 298 K.

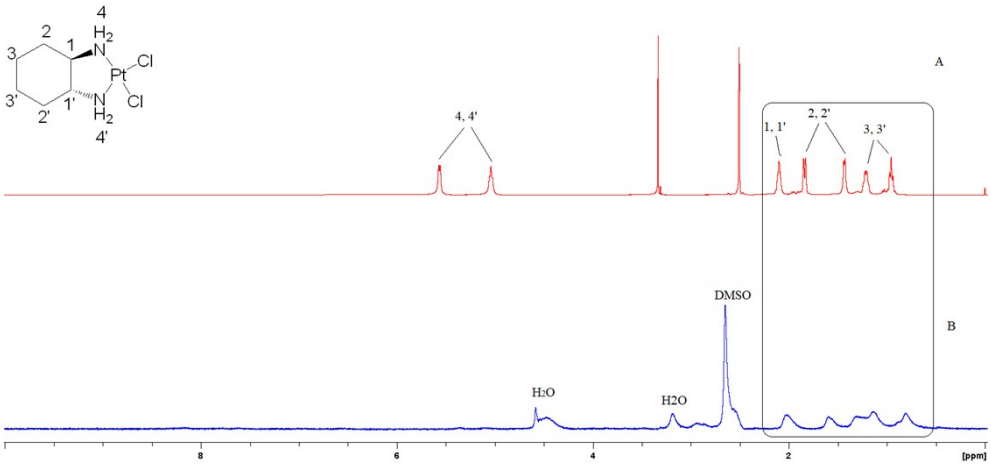

Fig. S2 (A) ^{1}H NMR reference spectrum of Pt(DACH)Cl_2 (1 mM) at 298 K. (B) STD spectrum of a sample containing 1 mM Pt(DACH)Cl_2 and 10 μM HSA at 298 K.

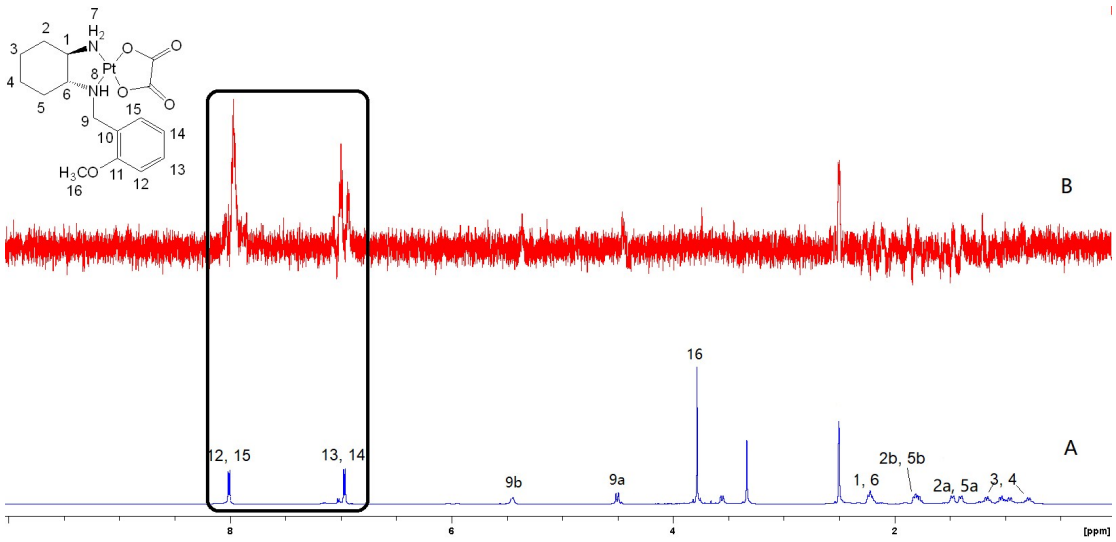

Fig. S3 (A) ^{1}H NMR reference spectrum of complex **2** (1 mM) at 298 K. (B) STD spectrum of a sample containing 1 mM complex **2** and 10 μM HSA at 298 K.

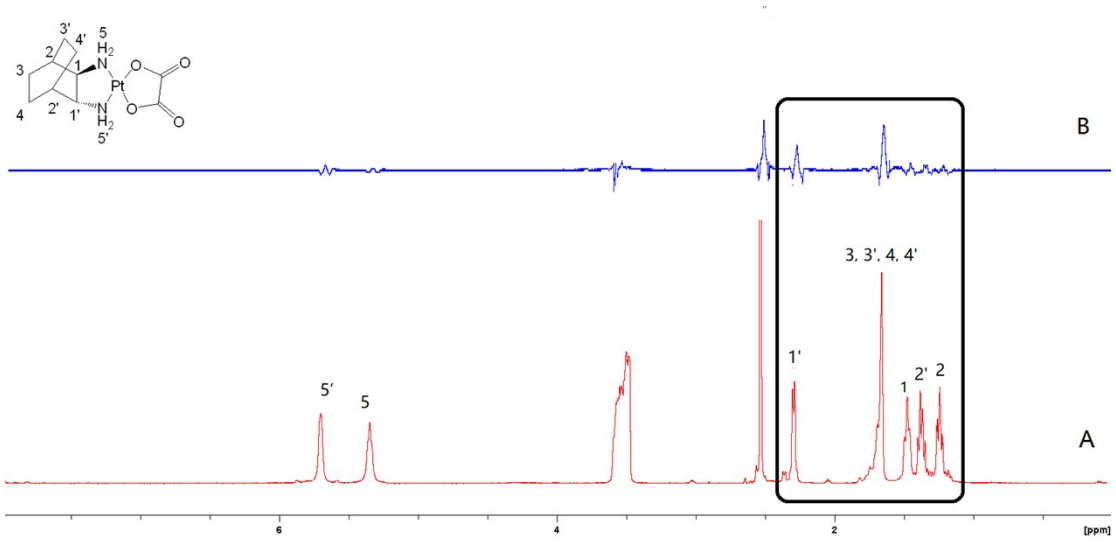

Fig. S4. (A) ^{1}H NMR reference spectrum of complex **3** (1 mM) at 298 K. (B) STD spectrum of a sample containing 1 mM complex **3** and 10 μM HSA at 298 K.

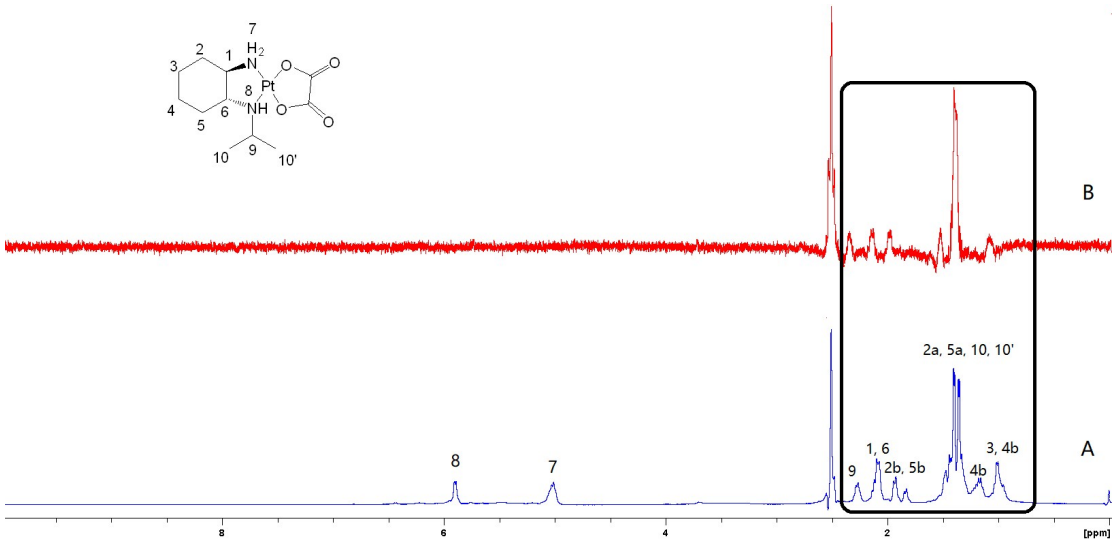

Fig. S5. (A) ^{1}H NMR reference spectrum of complex **4** (1mM) at 298 K. (B) STD spectrum of a sample containing 1 mM complex **4** and 10 µM HSA at 298 K.

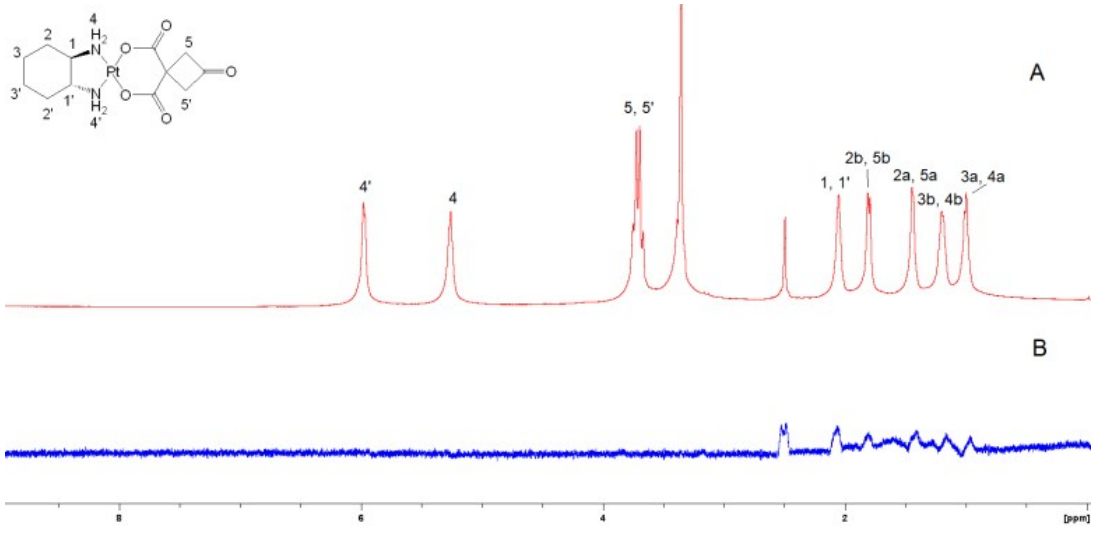

Fig. S6. (A) ^{1}H NMR reference spectrum of DN603 (1 mM) at 298 K. (B) STD spectrum of a sample containing 1 mM DN603 and 10 µM HSA at 298 K.

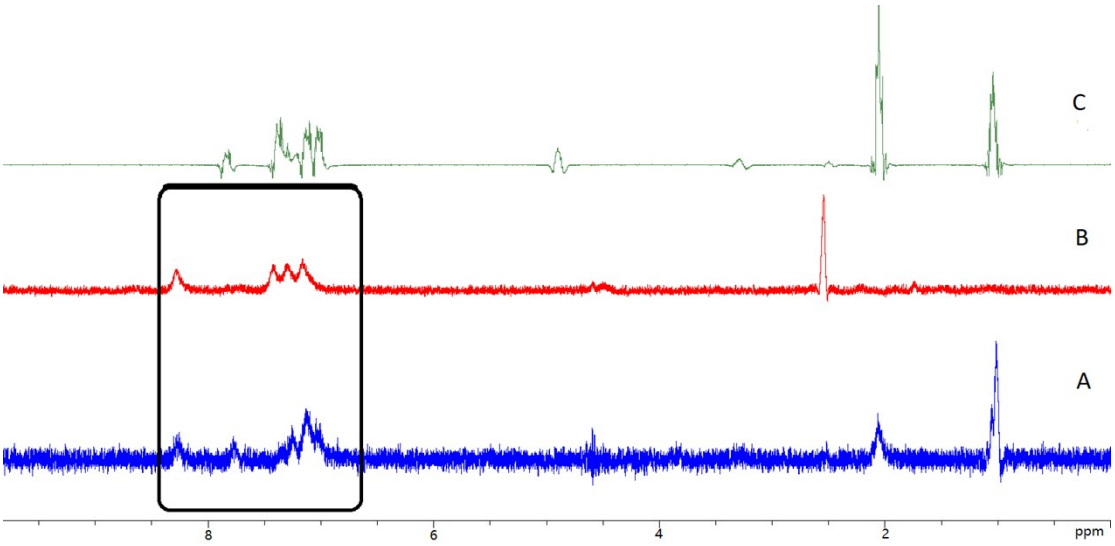

Fig. S7. (A) STD spectrum of complex **1** (0.5 mM) in the presence of HSA (1 μM) and warfarin(0.5 mM) at 298 K. (B)STD spectrum of complex **1** (1 mM) in the presence of HSA at 298 K. (C) STD spectrum of warfarin (1 mM) in the presence of HSA (1 μM) at 298 K.

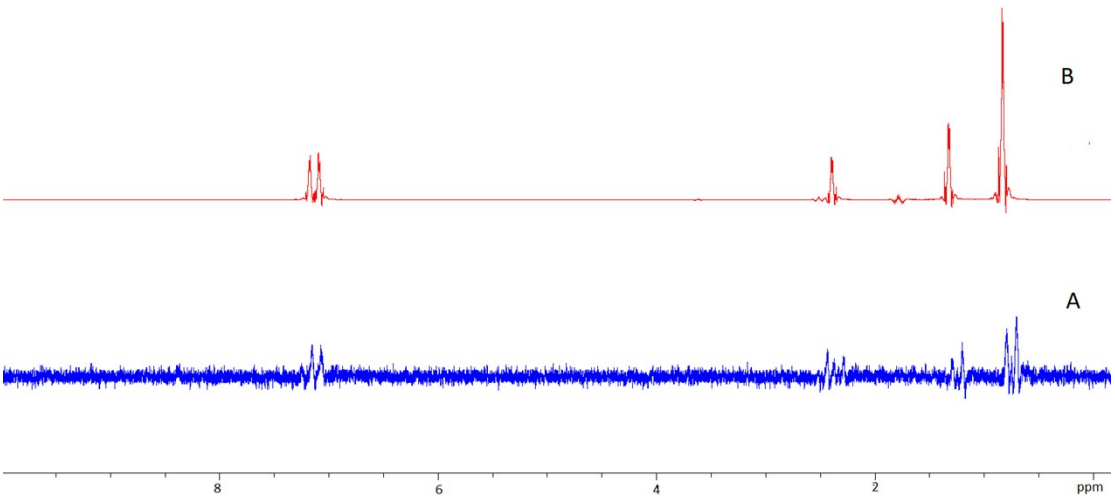

Fig. S8. (A) STD spectrum of a sample containing complex **1** and HSA in addition of ibuprofen at 298 K. (B) STD spectrum of a sample containing ibuprofen and HSA in addition of complex **1** at 298 K.

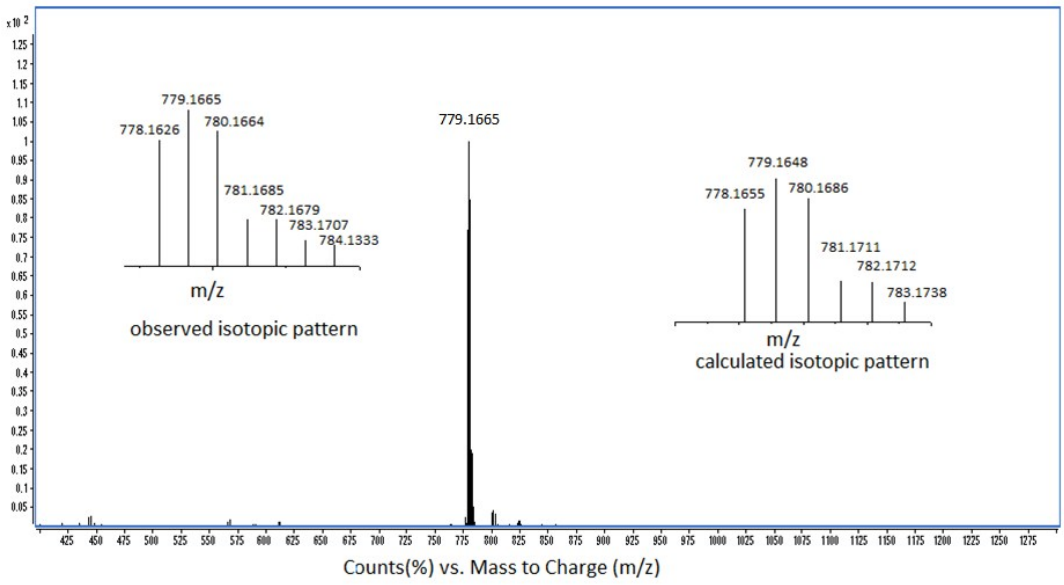

Fig. S9. MS spectra of adduct **1-I** and its calculated isotope pattern.

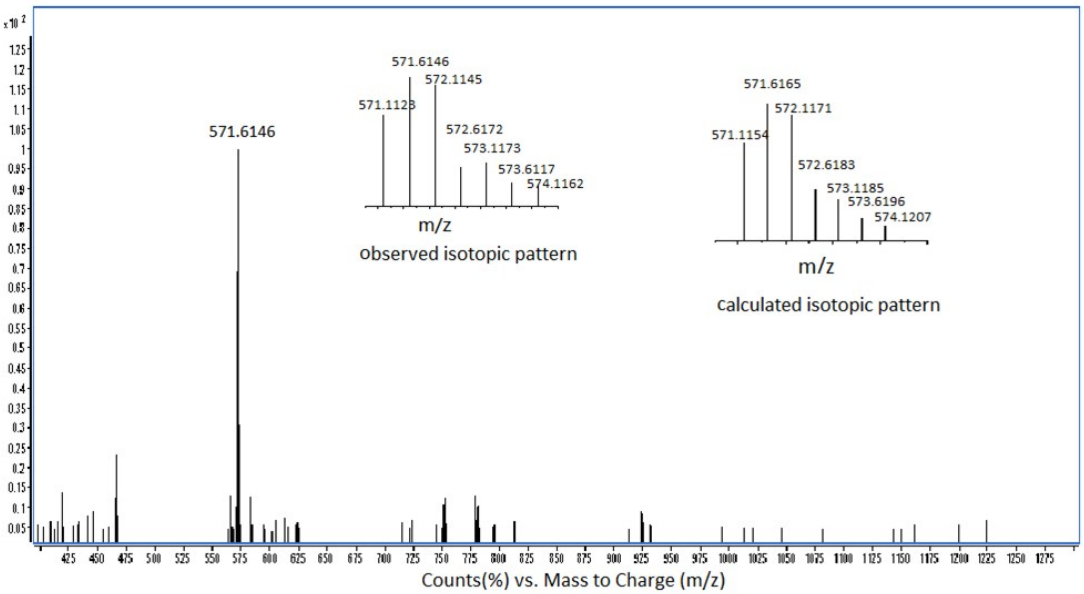

Fig. S10. MS spectra of adduct **1-II** and its calculated isotope pattern.

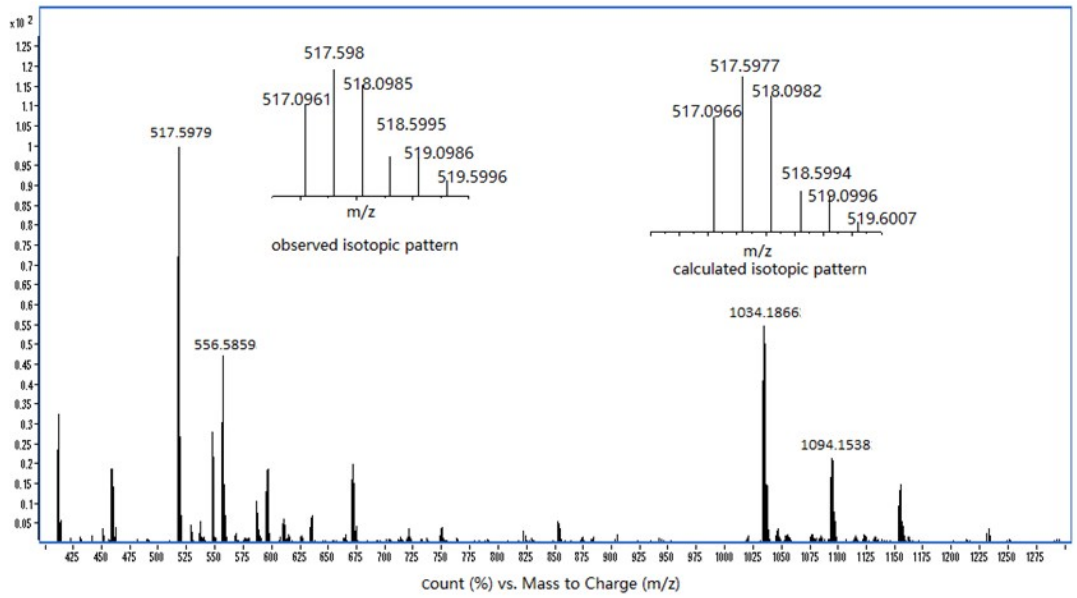

Fig. S11. MS spectra of adduct **R-I** and its calculated isotope pattern.

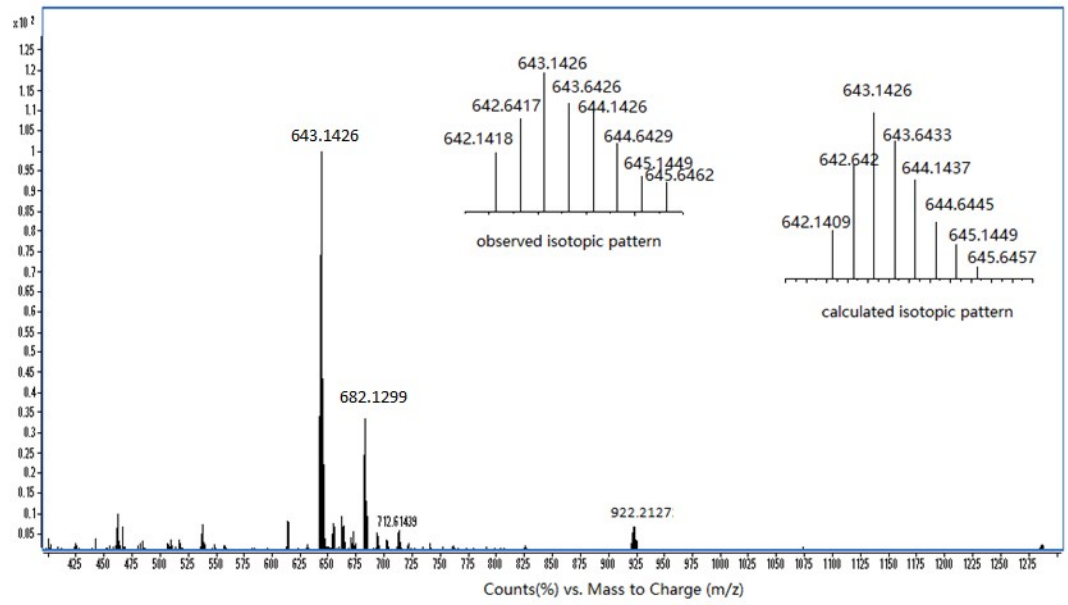

Fig. S12. MS spectra of adduct **R-II** and its calculated isotope pattern.

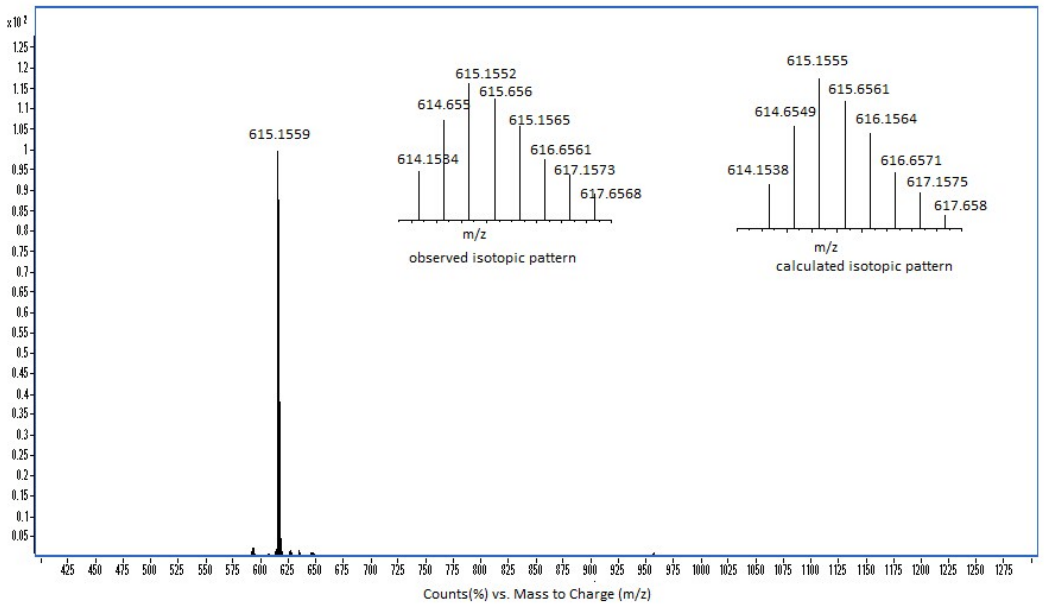

Fig. S13. MS spectra of adduct **R-III** and its calculated isotope pattern.

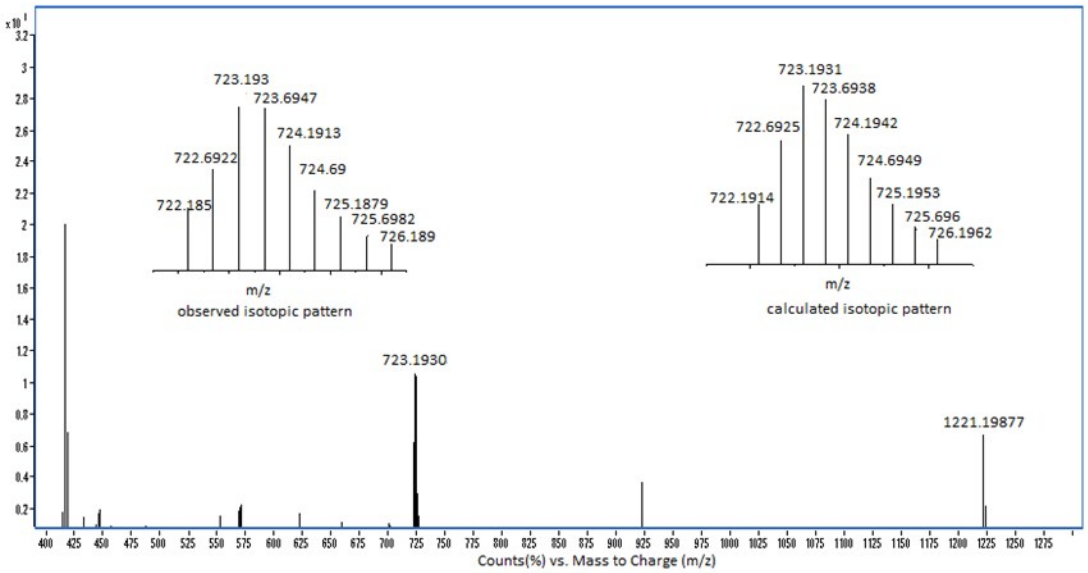

Fig. S14. MS spectra of adduct **1-III** and its calculated isotope pattern.

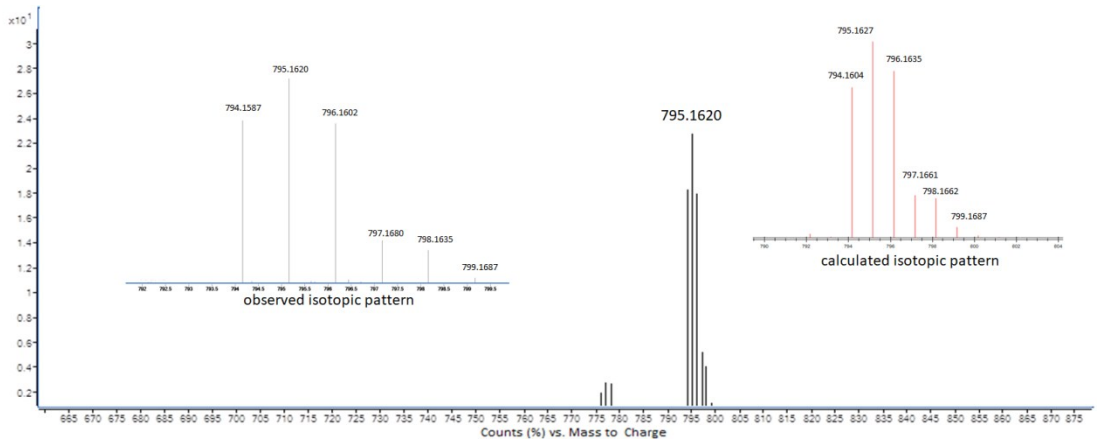

Fig. S15. MS spectra of adduct $[C_{23}H_{32}FN_7O_9PPt]^+$ and its calculated isotope pattern.