

Supplementary Information

Synthesis, structural characterization and anion binding studies of palladium macrocycles with hydrogen-bonding ligands

Pilar Diaz,¹ Jorge A. Tovilla,^{1,2} Pablo Ballester,^{2,3} Jordi Benet-Buchholz,² Ramón
Vilar^{1,2*}

*Corresponding author: r.vilar@imperial.ac.uk

JTC293

060524QT3727SH 50 (2.154) Cm (9:50)

TOF MS ES+
2.62e5

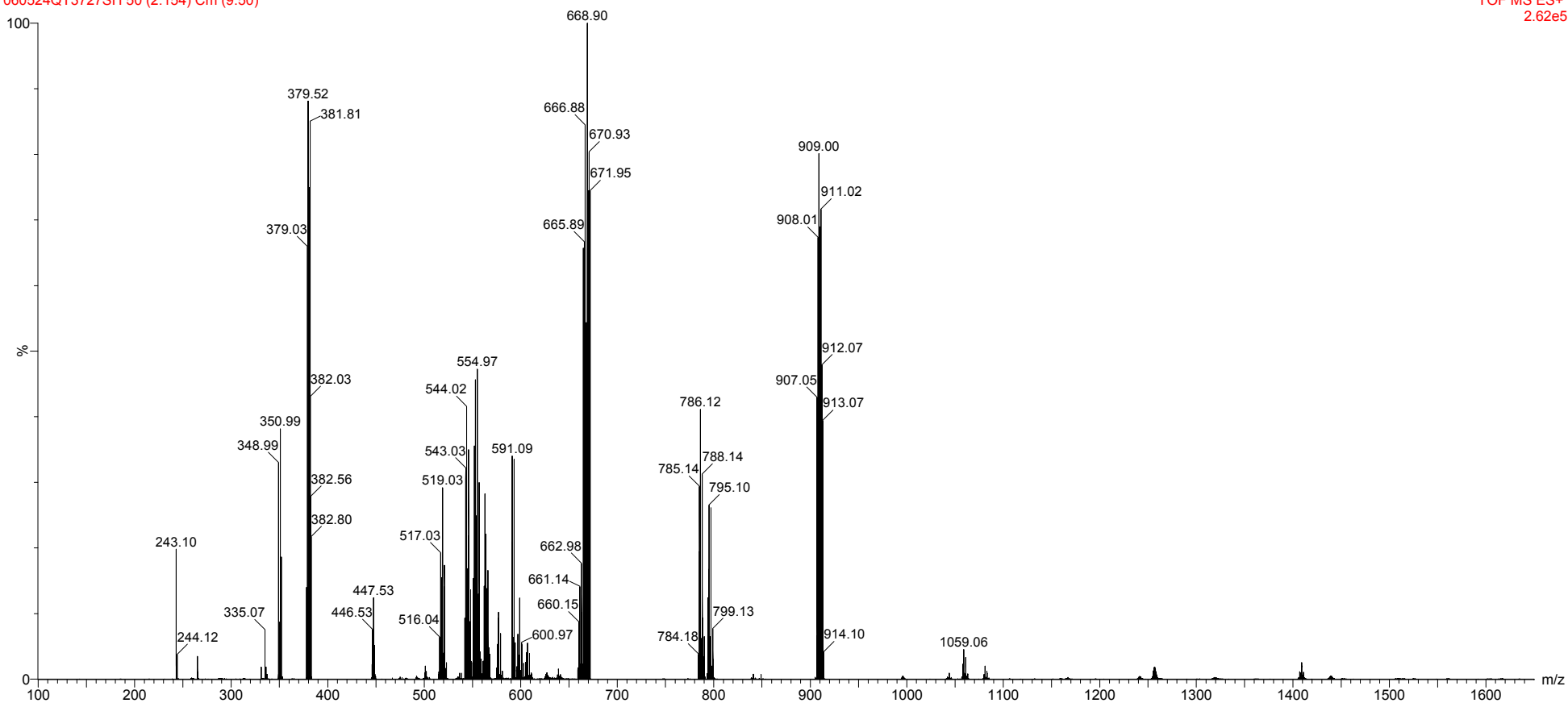


Figure S1 – ESI(+) mass spectrum of 1 in MeCN

JTC293

060524QT3727SH 50 (2.154) Cm (9:50)

TOF MS ES+
2.10e5

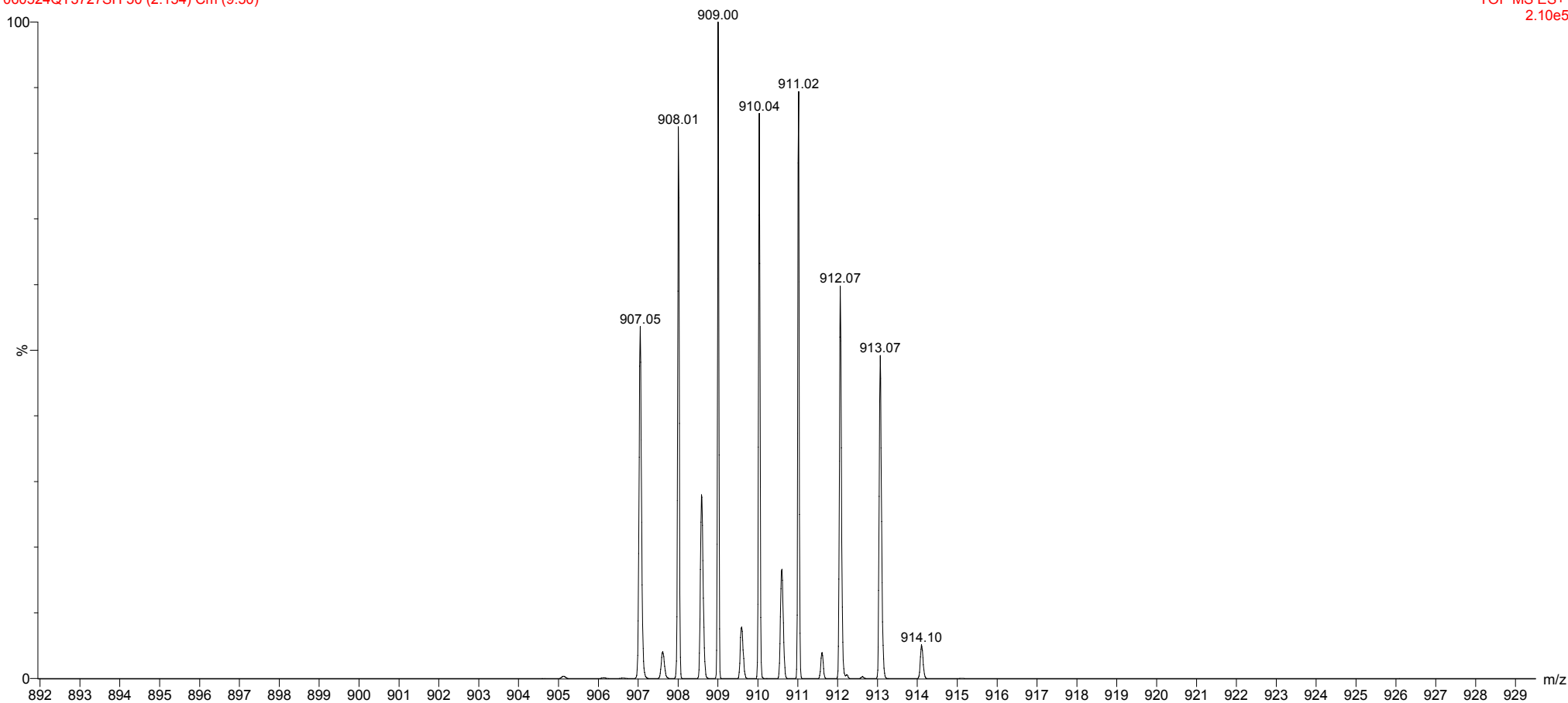


Figure S2 – Amplification of the area corresponding to $[\text{Pd}(\text{dppp})(\text{L}^1)(\text{OTf})]^+$. The smaller peaks at fractional a.m.u. correspond to the doubly charged species $[\text{Pd}_2(\text{dppp})_2(\text{L}^1)_2(\text{OTf})_2]^{2+}$.

JTC293

060524QT3727SH 50 (2.154) Cm (9:50)

TOF MS ES+
6.66e3

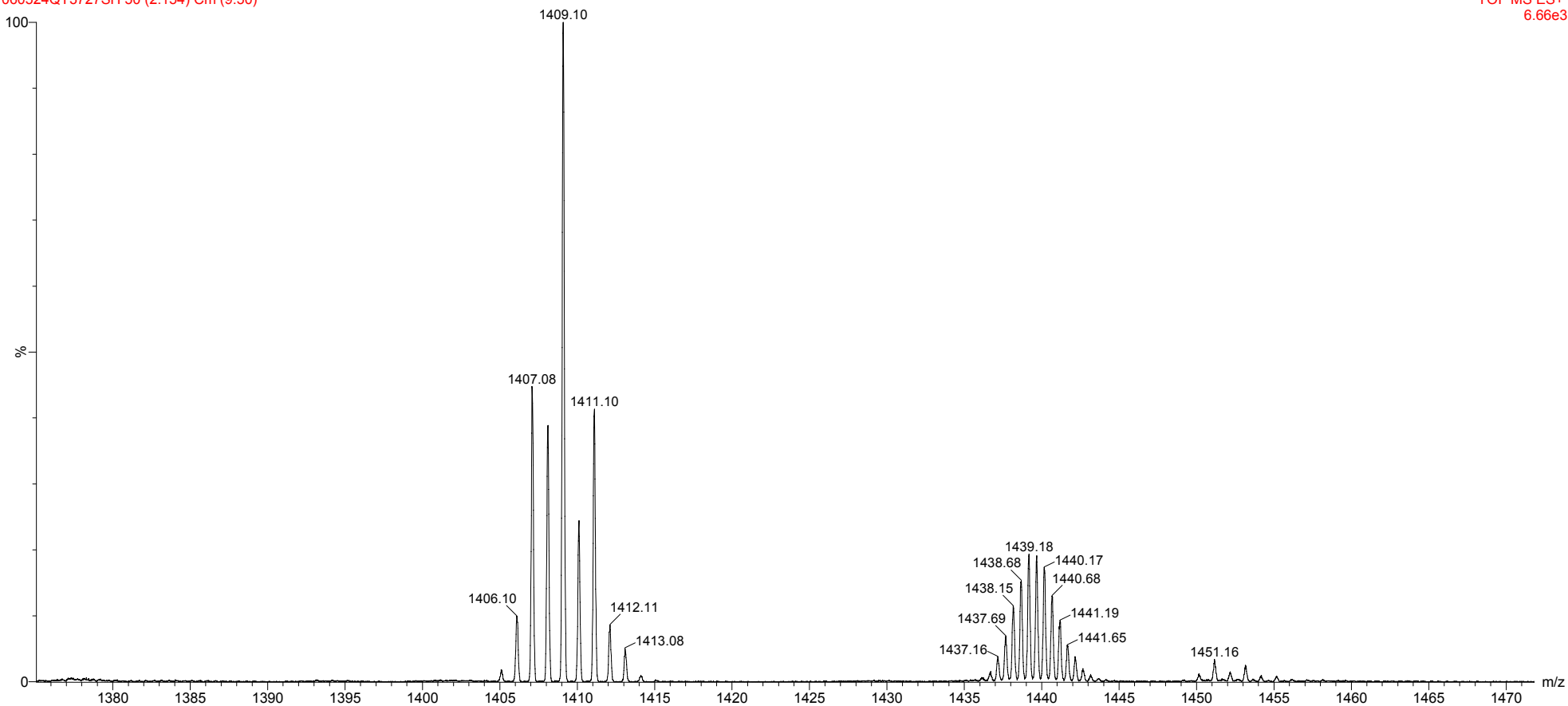


Figure S3 – Amplification of the area corresponding to the doubly charged species (peak on the right) $[\text{Pd}_3(\text{dppp})_3(\text{L}^1)_3(\text{OTf})_4]^{2+}$.