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MDPI

# Supplementary Information

# Reaction with Proteins of a Five-Coordinate Platinum(II) Compound

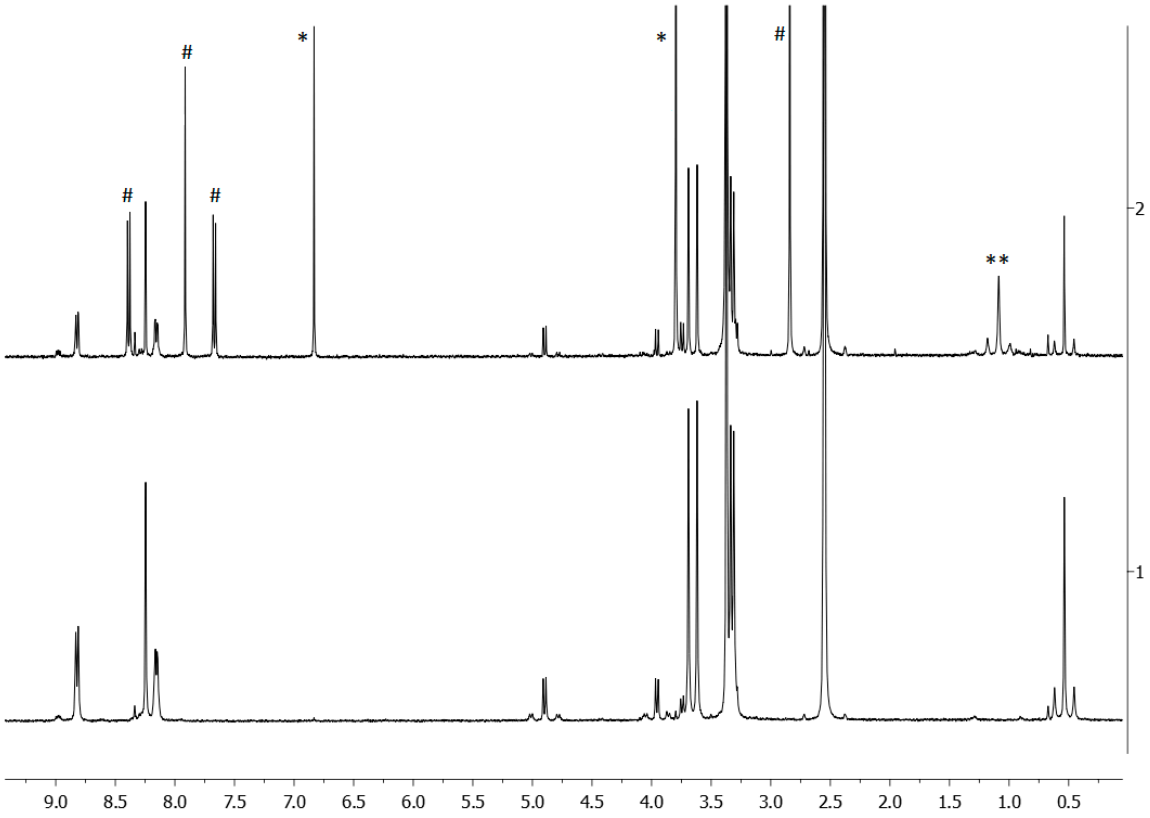



**Figure S1.** $^{1}$H NMR spectra at 400 MHz in DMSO-$d_6$ of [Pt(I)(Me)(dmphen)(dimethylfumarate)] after 5 minutes (trace 1) and after 18 hours (trace 2). Legend: *: free dimethylfumarate; #: free dmphen; **: Pt-Me in the square-planar product.

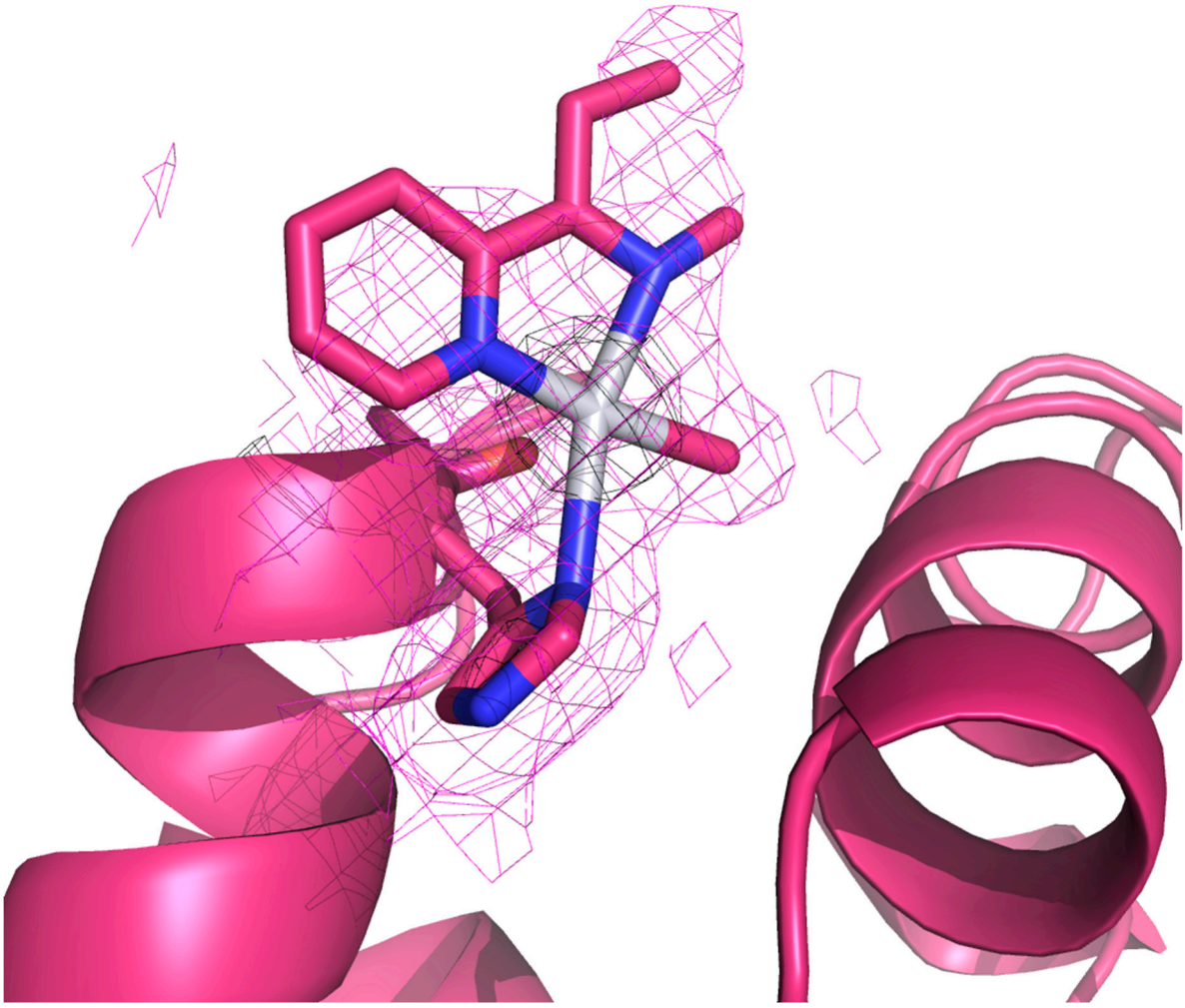


**Figure S2.** Details of the binding site of compound **I** fragment to HEWL. 2Fo-Fc electron density map is contoured at 3σ (dark grey), 0.3 σ (purple) level. Pt is in grey.

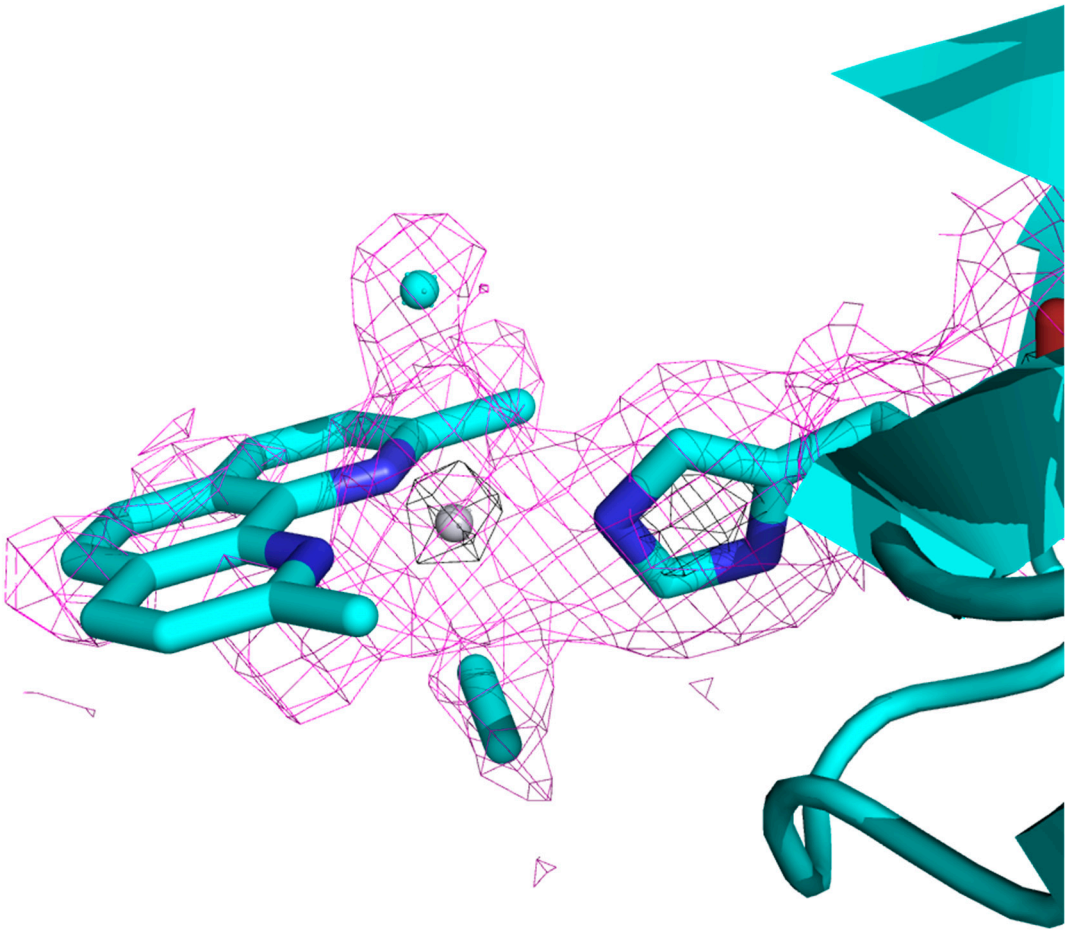
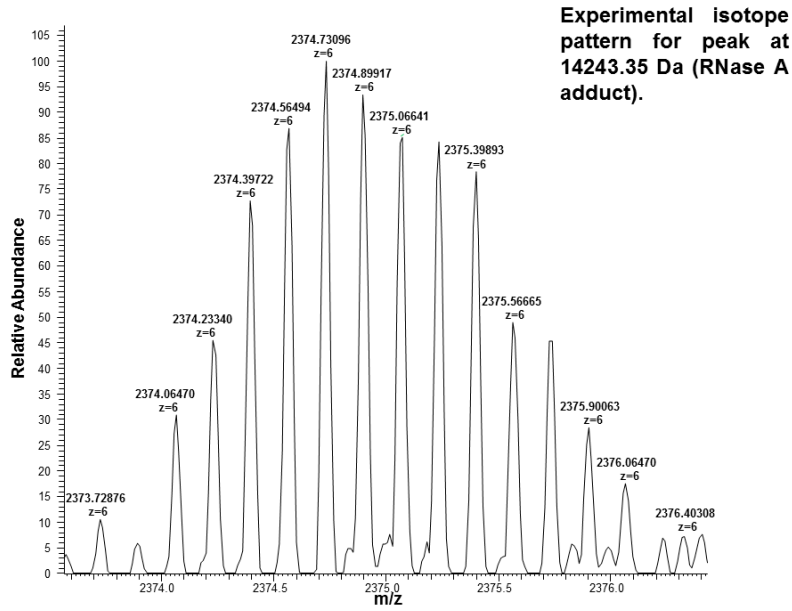
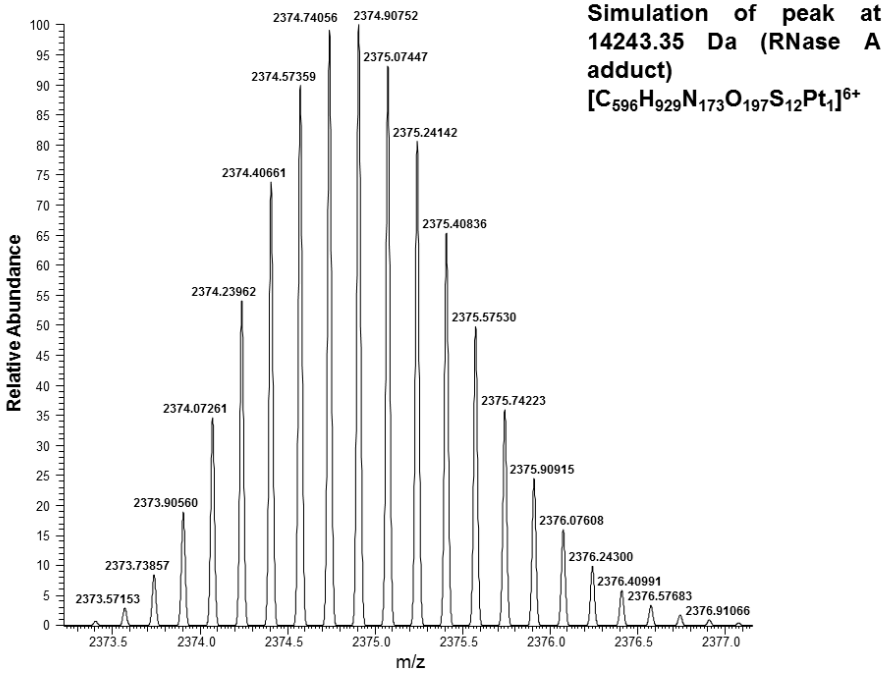


**Figure S3.** Details of the binding site of compound **I** fragment to molecule B of RNase A-compound **I** adduct. 2Fo-Fc electron density maps are contoured at 3σ (dark grey) and 0.3σ (purple) level. Pt is in grey.

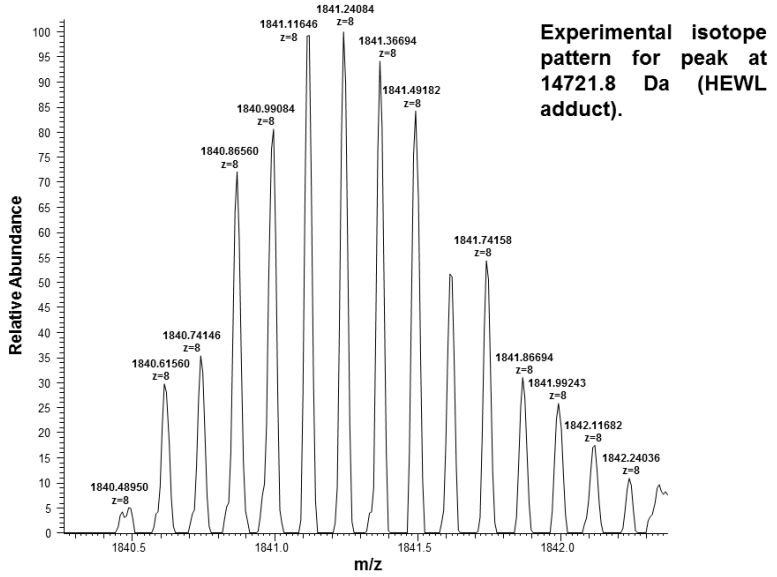



(a)

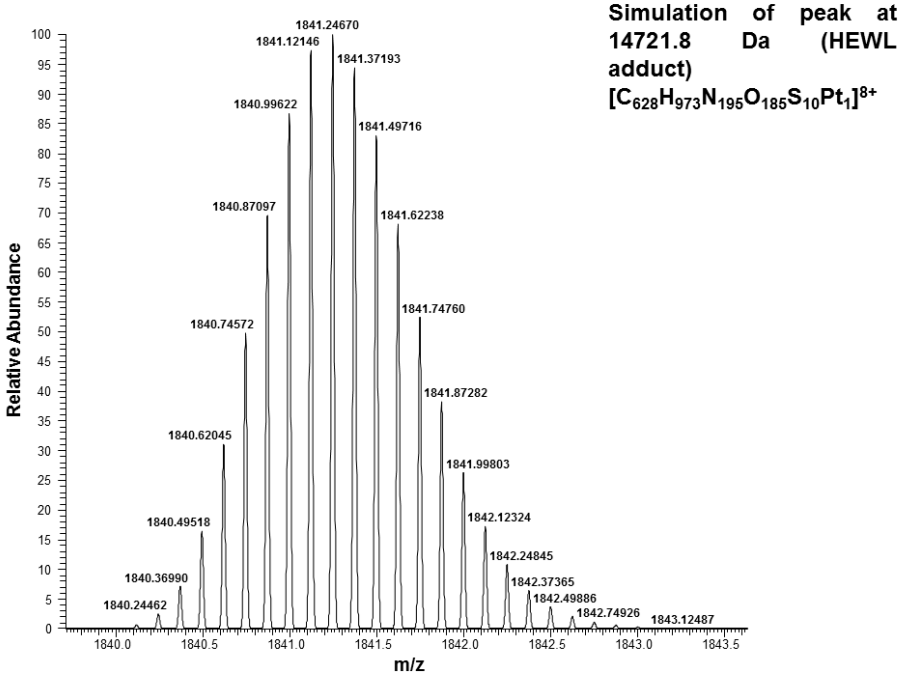



(b)

**Figure S4.** Experimental isotope (a) and theoretical simulation (b) pattern for the peak at 14243.35 Da obtained when RNase A was incubated with complex **I** (RNase A adduct)




(a)




(b)

**Figure S5.** Experimental isotope (a) and theoretical simulation (b) pattern for the peak at 14721.8 Da obtained when HEWL was incubated with complex **I** ( (HEWL adduct)

**Table S1.** Data collection and refinement statistics

| | HEWL-Compound **I** | RNase A-Compound **I** |
|---|---|---|
| PDB code | 6QEA | 6QE9 |
| Data-collection | | |
| Space group | $P4_32_12$ | C2 |
| Unit cell parameters | | |
| a,b,c (Å); β | 78.36, 78.36, 37.35; 90.0 | 99.00, 30.66, 68.68; 93.0 |
| Molecules per asymmetric unit | 1 | 2 |
| Observed reflections | 58658 | 36001 |
| Unique reflections | 8815 | 12949 |
| Resolution (Å) | 55.41-1.96 (1.99-1.96) | 50.00-2.03 (2.07-2.03) |
| Rmerge† | 0.099 (0.597) | 0.085 (0.528) |
| Completeness (%) | 99.9 (100.0) | 94.8 (92.3) |
| I/σ(I) | 13.3 (2.9) | 8.9 (2.3) |
| Multiplicity | 6.7 (5.0) | 2.8 (2.8) |
| Refinement | | |
| Resolution (Å) | 55.41-1.96 | 22.89-2.03 |
| number of reflections in working set | 8367 | 12313 |
| number of reflections in test set | 417 | 636 |
| R factor/Rfree (%) | 0.168 (0.204) | 0.176 (0.254) |
| Number of non-hydrogen atoms | 1178 | 2088 |
| Occupancy of Pt ion | 0.50 | 0.60, 0.40 |
| B-factor of Pt ion ($Å^2$) | 49.9 | 40.0, 74.7 |
| Overall B-factor ($Å^2$) | 23.0 | 30.8 |
| Ramachandran values (%) | | |
| Most favoured/ Additional allowed | 96.5/ 3.5 | 94.9/3.0 |
| Generously allowed/ Disallowed | 0.0 | 2.1* |
| R.m.s.d. bonds (Å) | 0.009 | 0.008 |
| R.m.s.d. angles (Å) | 1.62 | 1.52 |

*Outliers are Gln60B, residues of the molecule A hinge peptide (residues 18, 19 and 23), which is disordered in many structures of RNase A including RNase A-compound I, and Ser90B.