

## Supplementary Information

### Exploring the Interaction of Cisplatin with $\beta$ 2-Microglobulin: New Insights into a Chemotherapeutic Drug

Ningbo Zhang, Meng Cui\*, Yonggang Du, Zhiqiang Liu and Shuying Liu

Table S-1. Platinum species with charge state 10+ observed during reaction of  $\beta$ 2M and cisplatin at molar ratio of 1:15 by ESI-FT-ICR-MS.

| ions<br>(z = 10+)  | Experimental<br>m/z | error<br>(ppm) |
|--|---------------------|----------------|
| $[\beta$ 2M+10H] $^{10+}$  | 1173.8845           | -1.53          |
| [Met99-oxidated $\beta$ 2M+10H] $^{10+}$   | 1175.4880           | 1.87           |
| $[\beta$ 2M+Pt+8H] $^{10+}$  | 1193.1835           | +1.93          |
| $[\beta$ 2M+Pt(NH <sub>3</sub> )+8H] $^{10+}$  | 1194.8854           | +1.34          |
| $[\beta$ 2M+Pt(NH <sub>3</sub> )(H <sub>2</sub> O)+8H] $^{10+}$                                  | 1196.6837           | -1.00          |
| $[\beta$ 2M+Pt(NH <sub>3</sub> )Cl+9H] $^{10+}$  | 1198.4807           | -0.50          |
| $[\beta$ 2M+Pt(NH <sub>3</sub> ) <sub>2</sub> +8H] $^{10+}$                                      | 1196.5849           | -1.34          |
| [Met99-oxidated<br>$\beta$ 2M+Pt(NH <sub>3</sub> ) <sub>2</sub> +8H] $^{10+}$                    | 1198.1846           | -1.17          |
| $[\beta$ 2M+Pt(NH <sub>3</sub> )+Pt(NH <sub>3</sub> ) <sub>2</sub> +6H] $^{10+}$                 | 1217.5846           | +0.49          |
| $[\beta$ 2M+Pt(NH <sub>3</sub> )+{Pt(NH <sub>3</sub> ) <sub>2</sub> } <sub>2</sub> +4H] $^{10+}$ | 1240.2862           | +1.69          |

Table S-2. Tryptic peptide ions of platinated  $\beta$ 2M observed by ESI-FT-ICR-MS.

| ions                                      | experimental<br>m/z | error<br>(ppm) |
|---|---------------------|----------------|
| $[(4-6)+H]^+$                             | 345.2132            | 0              |
| $[(92-94)+H]^+$                           | 359.2652            | -0.28          |
| $[(13-19)+2H]^{2+}$                       | 376.6880            | +0.27          |
| $[(46-48)+H]^+$                           | 389.2394            | -0.26          |
| $[(1-3)+H]^+$                             | 416.2618            | +0.48          |
| $[(42-45)+H]^+$                           | 475.2259            | 0              |
| $[(82-91)+2H]^{2+}$                       | 561.8182            | +2.31          |
| $[(49-58)+2H]^{2+}$                       | 574.7835            | +1.39          |
| $[(82-91)+Pt(NH_3)_2]^{2+}$               | 675.3179            | -0.44          |
| $[(49-58)+Pt(NH_3)]^{2+}$                 | 679.7702            | -0.74          |
| $[(49-58)+Pt(NH_3)_2]^{2+}$               | 688.2843            | +0.44          |
| $[(13-19)+H]^+$                           | 752.3688            | +0.27          |
| $[(46-58)+2H]^{2+}$                       | 759.8944            | +1.05          |
| $[(7-12)+H]^+$                            | 765.4275            | +2.74          |
| $[(46-58)+Pt(NH_3)_2]^{2+}$               | 873.8943            | -1.49          |
| $[(95-99)+Pt(NH_3)-H]^+$                  | 932.2674            | -0.97          |
| $[(20-41)-s-s-(76-81)+3H]^{3+}$           | 1084.4989           | -0.83          |
| $[(59-75)+2H]^{2+}$                       | 1102.5159           | -2.54          |
| $[(82-91)+H]^+$                           | 1122.6282           | +1.43          |
| $[(49-58)+H]^+$                           | 1148.5582           | 0              |
| $[(20-41)-s-s-(76-81)+Pt(NH_3)_2+H]^{3+}$ | 1160.5006           | -0.43          |
| $[(20-41)-s-s-(59-81)+4H]^{4+}$           | 1360.1283           | -1.47          |
| $[(49-58)+Pt(NH_3)_2-H]^+$                | 1375.5629           | 1.60           |

Table S-3. Fragment ions observed in SORI CID mass spectrum of the platinated peptide [(95-99)+Pt(NH<sub>3</sub>)-H]<sup>+</sup>.

| ions                                 | experimental<br>m/z | error<br>(ppm) |
|--------------------------------------|---------------------|----------------|
| [y <sub>3</sub> +Pt-2H] <sup>+</sup> | 614.1361            | +0.81          |
| [(95-99)+Pt-H] <sup>+</sup>          | 915.2430            | +1.20          |

Table S-4. Fragment ions observed in SORI CID mass spectrum of the platinated peptide [(49-58)+Pt(NH<sub>3</sub>)<sub>2</sub>]<sup>2+</sup>

| ions  | experimental m/z | error (ppm) |
|---|------------------|-------------|
| y <sub>2</sub> <sup>+</sup>                                 | 234.1448         | 0           |
| y <sub>4</sub> <sup>+</sup>                                 | 468.2457         | +0.85       |
| [a <sub>3</sub> +Pt-2H] <sup>+</sup>                        | 531.1306         | -1.69       |
| [b <sub>3</sub> +Pt-2H] <sup>+</sup>                        | 559.1261         | -0.54       |
| y <sub>5</sub> <sup>+</sup>                                 | 581.3283         | -1.72       |
| [(49-58)+Pt-(H <sub>2</sub> O)] <sup>2+</sup>               | 662.2516         | -0.91       |
| [(49-58)+Pt] <sup>2+</sup>                                  | 671.2564         | -1.34       |
| [(49-58)+Pt+(NH <sub>3</sub> ) <sub>2</sub> ] <sup>2+</sup> | 679.7696         | -1.62       |
| y <sub>7</sub> <sup>+</sup>                                 | 783.3866         | -2.17       |
| [b <sub>8</sub> +Pt-2H] <sup>+</sup>                        | 1108.3670        | -2.8        |
| [c <sub>8</sub> +Pt-2H] <sup>+</sup>                        | 1125.3966        | 0           |