

## **Description of Additional Supplementary Files**

### Supplementary Data 1

Description: Heat map of statistically significant biochemicals between PDX and patients' primary tumours (PT).

### Supplementary Data 2

Description: Heat map of statistically significant biochemicals between HBCx-124 and HBCx-137 control and treated groups.

### Supplementary Data 3

Description: Chemical annotation, sample meta data and normalized metabolomics data.