**Supplemental Table 1.** Fragment ion, predicted formula, and the relative intensity for each ion for NPC1161B and metabolite. For ions with a predicted formula, the predicted fragment structure resulting from NPC1161B is shown in red.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Fragment *m/z*** | **Predicted Formula** | **% Rel. Int. NPC1161B (434.14 *m/z*)** | **% Rel. Int. Metabolite (520.13 *m/z*)** | **Predicted Fragment Structure** |
| 70.08 | [C5H10]+ | 11.1 | 16.3 |  |
| 80.95 |  | 0.9 | 2.3 |  |
| 84.08 | [C5H11N-H]+ | 17.7 | - |  |
| 86.10 | [C5H12N]+ | 8.0 | - |  |
| 175.09 | [C10H10N2O+H]+ | 8.6 | 6.23 |  |
| 187.06 | [C11H9NO2]+ | 3.8 | 2.2 |  |
| 203.08 | [C11H10N2O2+H]+ | 19.5 | 16.7 |  |
| 215.12 | [C13H14N2O+H]+ | 11.9 | 8.35 |  |
| 290.01 |  | 1.3 | 1.3 |  |
| 303.04 |  | 1.6 | 3.5 |  |
| 318.01 |  | 2.2 | 5.3 |  |
| 334.03 | [C17H12Cl2NO2+2H]+ | 4.1 | 1.9 |  |
| 345.06 | [C18H14Cl2N2O]+H]+ | 51.2 | 12.0 |  |
| 349.05 | [C17H13Cl2N2O2+2H]+ | 22.0 | 4.0 |  |
| 360.04 | [C18H14Cl2N2O2]+ | 22.0 | 13.5 |  |
| 372.05 |  | 1.0 | 2.5 |  |
| 375.07 | [C19H17Cl2N2O2]+ | 100 | 100 |  |