**File: FTICRMS.xlsx**

**Description of data by row:**

|  |  |
| --- | --- |
| **Row(s)** | **Description** |
| 1 | Header (columns 16-74 report synoptic site codes) |
| 2+ | Data, sorted by measured ionic mass |

**Description of data by column (for rows 2+, where row 1 is a header):**

|  |  |
| --- | --- |
| **Column(s)** | **Description** |
| 1 | Measured Ionic Mass (m/z) |
| 2 | Number of known atoms of C in each molecule |
| 3 | Number of known atoms of H in each molecule |
| 4 | Number of known atoms of O in each molecule |
| 5 | Number of known atoms of N in each molecule |
| 6 | Number of known atoms of C13 in each molecule |
| 7 | Number of known atoms of S in each molecule |
| 8 | Number of known atoms of P in each molecule |
| 9 | Number of known atoms of Na in each molecule |
| 10 | Known functional group(s) present |
| 11 | Classification of molecule as lignin, sugar, etc. |
| 12 | Molecular mass if charge is balanced by adding protons or electrons to attain neutral charge |
| 13 | Mass error (ppm) calculated as:  Error = (expected molecular mass – measured molecular mass) / (expected molecular mass) \* 1e6 |
| 14 | Number of known molecules that this could represent |
| 15 - 74 | FTICRMS peak intensity for each molecule |
| 75 - 76 | FTICRMS peak intensity for laboratory standards |