Table 2: The two datasets used in this study.

[a]number of compounds in the datasets; [b]alphabet of potential elements provided to the method for molecular ion and molecular formula identification; [c]average mass of all compound in Da

|  | #[a] | instrument | alphabet[b] | average mass[c] |
|---|---|---|---|---|
| **simulated data** | 22 | simulated |  | 187.6 |
| standard compounds | 20 |  | CHNOPS | 170.78 |
| chlorinated compounds | 2 |  | CHNOPSCl | 1338.1 |
| **measured data** | 50 | GC/TOF-MS |  | 212.98 |
| standard compounds | 35 |  | CHNOPS | 1202.0 |
| chlorinated compounds | 5 |  | CHNOPSCl | 153.233 |