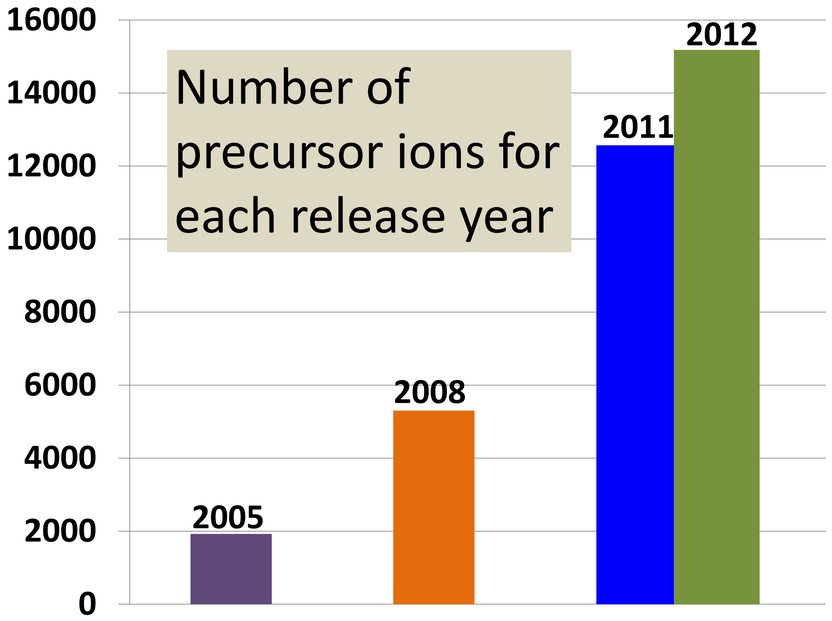
NIST Tandem Mass Spectral Library 2012



6,999 Compounds
15,180 Precursor Ions
121,586 Spectra
~90% Positive Ion Spectra
~10% Negative Ion Spectra

Instrument Type	Precursor Ions
Ion Trap	12,047
Collision Cell (QTOF, QQQ, HCD)	9,232

Compound Types: metabolites, drugs, sugars, phospholipids, peptides, surfactants, etc.

Precursor types:
$[M+H]^+$, $[M+2H]^{2+}$, $[M-H]^-$,
$[M+Na]^+$, $[M+NH_4]^+$, $[Cat]^+$, $[An]^-$,
$[p-H_2O]$, $[p-NH_3]$, etc.

New Software Features:

- Search for the exact or isotopic precursor mass in libraries.
- Search for exact fragment ion mass values in NIST EI and MS/MS libraries.
- Import spectra from instrument data system using standard formats including mzXML, mzData, mgf, msp, dta, pkl, JCAMP, etc.
- Full compatibility with most recent NIST Peptide MS/MS Libraries.
- Provides a variety of new methods for identifying target compounds or compound classes – even in the presence of noise.

New Tandem MS Search Algorithm for Small Molecules

- Improved ability to identify compounds with a few dominant peaks – a common situation for Tandem MS.
- More robust scoring for spectra acquired on imperfectly-tuned instruments.