

NIST TANDEM MS LIBRARY

2017 Release

GREATLY EXPANDED COVERAGE

- 13,808 compounds, a 65% increase over NIST 14!
- 574,826 tandem spectra (3x increase) over a range of fragmentation conditions including positive and negative modes from ion-trap (up to MS⁴) and 'beam-type' collision cells (QTOF, HCD, and QqQ); new spectra acquired at high accuracy and resolution
- 118,082 precursor ions including in-source fragments
- 16,421 glycan spectra (3x increase)
- 1,904 biologically relevant peptides in an additional library

NIST 17 Tandem Library		Spectra	Precursor Ions	Compounds
Small Molecules	Ion Trap	163,532	114,925	12,992
	Collision Cell	411,294	34,517	12,728
Peptides	Ion Trap	13,062	6,422	1,828
	Collision Cell	77,182	5,637	1,814
Total		652,475	123,881	15,243

NEW COMPOUNDS

Human and plant metabolites, designer drugs, lipids, glycans, and much more

Amino Carnitine
E = 16 eV

Metabolites

JWH 302
IT/FT 35%

Designer
Drugs

18:0 Lyso PA
E = 21eV

Lipids

NGA4B
E = 50eV

Glycans

