

NIST 11

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This release contains

- o 243,893 EI spectra for 212,961 compounds; 212,958 compounds have structures
- o MS/MS libraries (nist\_msms and nist\_msms2) with 95,409 spectra of 12,568 ions
- o GC Method/Retention index library (nist\_ri) with 70,835 compounds;  
38,648 compounds in the Main library have GC method/retention index data.

History of the releases:

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Release Year	Number of spectra (EI)	Number of compounds (EI)	Number of spectra (MS/MS)	Number of Ions (MS/MS)	Number of compounds (RI)	Data-points (RI)	EI compounds that have RI	RI literature references
1993	74,828	62,235	-	-	-	-	-	-
1998	129,136	107,866	-	-	-	-	-	-
2002	174,948	147,198	-	-	-	-	-	-
2005	190,825	163,198	5,191	1,920	25,728	121,112	12,433	2,177
2008	220,460	192,108	14,802	5,308	44,008	293,247	21,940	4,632
2011	243,893	212,961	95,409	12,568	70,835	346,757	38,648	5,368

1. NIST 11 EI Spectra

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	#spectra	#compounds
NIST11	243,893	212,961
Increase from NIST08	23,433	20,853

Number of spectra in Mainlib: 212,961  
 Number of chemical structures: 212,958  
 Number of spectra in Replib: 30,932

NIST11 RI	2011	2008
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Number of species: 70,835 44,008  
 Number of species also in EI database: 38,648 21,940  
 Total number of GC Methods/RI data points: 346,757 293,247  
 Total number of references cited: 5,368 4,632

2. MS/MS library (small molecules, di and tri peptides)

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	#spectra	#compounds	#ions
collision cell	55,640	3,368	5,272
Ion Trap	8,871	4,277	8,012
Total	64,511	5,216	10,205

3. MS/MS peptide library

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	#spectra	#compounds	#ions
collision cell	29,704	509	1,900
Ion Trap	1,194	351	1,182
Total	30,898	627	2,363

4. MS/MS combined

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	#spectra	#compounds	#ions
collision cell	85,344	3,877	7,172
Ion Trap	10,065	4,628	9,194
Total	95,409	5,843	12,568