JCAMP-DX Field Name	Contents [brief description of contents]	Notes on contents
##TITLE=	[first 8 characters assigned by MaSC]; [Sample name]	This must be the first line in any JCAMP-DX file. The name of the compound should be entered here, and will most often be the common or trivial name. Once accepted into the MaSC library, the editing committee will insert an 8 character indexing number.
##JCAMP-DX=	5.01 [Version number of JCAMP-DX used, invariant]	This must follow the ##TITLE= line. We are using the field definitions from JCAMP-DX version 5.01
##DATA TYPE=	MASS SPECTRUM	This is the designation for a single mass spectrum. This should remain as is.
##DATA CLASS=	XYDATA	This denotes a set of x,y data. This should remain as is.
##ORIGIN=	[Analyst name, Institution name, address, phone, fax, e-mail]	At minimum, the analyst name, institution name, and institution address should be entered here. Additional contact details are welcomed, however.
##OWNER=	COPYRIGHT (C) [Year] by [Institution Name]	Enter the year the spectrum was submitted as well as the institution's name. The submitting institution retains copyright over the spectrum.
##$LICENSE=	[a licensing statement to be determined at a later date]	This is a field defined by MaSC, and not by JCAMP-DX. This statement will include words to the effect of "user of this library agrees to abide by MaSC user's license, contributor agrees to abide by the MaSC contributor's license, any reference made to this spectrum oral or written should credit both the contributing individual/institution and MaSC."
##$INSTITUTION FILENAME=	[originating institution's filename]	Enter the filename, including extension, under which the data were originally saved by the analyst. This will serve as a reference if the original data need to be accessed at a later date. This is a field defined by MaSC, and not by JCAMP-DX.
##SAMPLE DESCRIPTION=	[composition or origin, collection date, state (solution/solid), etc.]	Enter a brief description of the sample analysed (include information such as source/supplier, age, physical state, or purity).
##SAMPLING PROCEDURE=	[no pretreatment, no derivatisation, derivatisation (diazomethane, BSTFA, Methprep I/II, TMAH, BF3, etc.)]	Enter a brief description of all sample preparation before introduction to any instrumental analysis. Include derivatising reagents, reaction times, solvent, etc. Sample quantitation, such as mass, volume, and/or concentration, can be included here. *No pretreatment* would be appropriate where online (in situ) pyrolysis/methylation is carried out as part of the instrumental analysis, or for direct insertion mass spectrometry with no prior sample pretreatment.
##TEXT=	YES [if the spectrum has been published]; NO [if the spectrum is unpublished]	Future plans: complete bibliographic information for published spectra available on www.mascgroup.org.
##LONG DATE=	[YYYY/MM/DD HH:MM:SS.SSSS ±UUUU]	The date YYYY/MM/DD is required. The precise time is optional. For example, 2004/06/28 09:55:49 or 2004/06/28 are acceptable.
$$ Equipment		

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##.INLET=	GC (gas chromatograph), LC (liquid chromatograph), DIRECT (direct insertion probe), BATCH (batch inlet), CZE (capillary zone electrophoresis system), PB (particle beam inlet), MOB (moving belt inlet), etc.	Enter the standard abbreviation for the instrument that introduces the sample into the mass spectrometer. The inlets named here are only a partial list.
##INSTRUMENTAL PARAMETERS=	[For GC: column brand, stationary phase, i.d., o.d., film thickness, column length, pressure/flow control, temperature program, carrier gas, flow rate, injection parameters (pyrolysis, split/splitless, on-column), etc.]	All instrumental components and parameters with reference to the INLET only. Mass spectrometer parameters are entered in subsequent fields. Mass spectrometer details may be entered here, if such information is not included in subsequent fields. If no GC, LC, pyrolysis equipment, etc. was used, leave this field blank.
##SPECTROMETER/DATA SYSTEM=	[Manufacturer and Model of Mass Spectrometer and of inlet system, software system(s)and version(s)]	The JCAMP-DX definition only includes the name of the mass spectrometer and data collection hardware/software. MaSC includes the name of the inlet system (GC, LC, etc.) to prevent defining an additional field.
##.SPECTROMETER TYPE=	Q (quadrupole), TRAP (ion trap), TOF (time-of-flight), B (magnetic sector field spectrometer), BE or EB (double-focussing spectrometer), etc.	Designation of the mass spectrometer type
##.SOURCE TEMPERATURE=	[temperature of ion source in °C]	Do not include units.
##.IONIZATION MODE=	EI+/– (electron impact), CI+/– (chemical ionisation), FAB+/– (fast-atom bombardment), TSP+/– (thermospray), ESI+/– (electrospray), APCI+/– (atmospheric pressure chemical ionisation), LD +/– (laser desorption)	Designation of the mass spectrometer ionization mode
##.IONIZATION ENERGY=	[ionization energy in eV]	
##.AQUISITION RANGE=	[lowest mass, highest mass in amu]	This refers to the acquisition range of the current spectrum only, and not to the range the mass spectrometer is capable of. Do not include units and separate values by a comma
##.SCAN RATE=	[scan rate in scans/sec, masses/second or seconds/decade with units defined]	Enter the scan rate, with units (scans/sec is defined by MaSC).
##RESOLUTION=	[mass resolution with units]	
##$THRESHOLD=	[threshold value for data acquisition]	Enter the threshold value for data acquisition if applicable.
$$ Compound Information		
##CAS NAME=	[if known]	Chemical Abstracts Service (CAS) name if known.

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##NAMES=	[common names]	Include synonyms, common or trivial names or other chemical names
##MOLFORM=	[molecular formula]	The molecular formula should be given in Hill Order, i.e. for organic compounds, C is listed first, followed by H, followed by the remaining elements in alphabetical order, e.g. palmitic acid, trimethylsilyl ester = C19H40O2Si
##CAS REGISTRY NO=	[CAS number]	Chemical Abstracts Service (CAS) registry number if known
##MW=	[molecular weight, to two decimal places]	Molecular weight is defined as the relative molecular mass averaged over all isotopes and can be easily calculated using various free web-based calculators such as http://www.ch.cam.ac.uk/magnus/MolWeight.html or http://medlib.med.utah.edu/masspec/mole.htm
##.MONOISOTOPIC MASS=	[accurate weight of the most common isotope peak, to two decimal places]	Monoisotopic mass (also referred to as the HRMS (high resolution mass spectrometry) mass) is the accurate mass of the molecule/ion containing only the most common elemental isotopes. It is obtained by summing up the masses of the most abundant isotopes of all elements in the molecule/ion. The monoisotopic mass can be easily calculated using various free web-based calculators such as http://www.ch.cam.ac.uk/magnus/MolWeight.html or http://medlib.med.utah.edu/masspec/mole.htm.
##.NOMINAL MASS=	[nominal mass, integer value]	Nominal mass is the sum of the integer atomic masses of the most common isotopes of the elements in the molecule, that is H=1, C=12, N=14, O=16, F=19, Si = 28, P = 31, S = 32 etc. See http://www.cem.msu.edu/~reusch/OrgPage/mass.htm for table of nominal masses. The calculator at www.ch.cam.ac.uk shows the nominal mass as the first integer value in the table giving the “molecular ion isotope pattern.” A nice example of the different values for these three masses is given by Ubiquitin (C378H630N105O118S) where MW = 8565.89, monoisotopic mass = 8560.62 and nominal mass = 8556.
$$ Spectrum		
##.SCAN NUMBER=	[scan number(s) of spectrum]	Enter scan number of submitted spectrum
##.RETENTION TIME=	[retention time in seconds]	Convert retention times in minutes:seconds to seconds and do not include the units.

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##$KOVATS INDEX=	[Kovats Index]	Kovats Retention Index is a logarithmic scale on which the adjusted retention time of a peak on a non-polar column is compared with those of linear n-alkanes as reference compounds. For polar phases a modified version of this is used with linear n-FAMEs as the reference, partly due to the poor peak shape of alkanes on these polar phases. See http://www.chromtech.net.au/kovats_ri.cfm for a more detailed definition.
##.BASE PEAK=	[m/z value of base peak]	Mass peak in the spectrum that has the greatest intensity.
##.BASE PEAK INTENSITY=	[unscaled Y-value of the base peak] COUNTS	
##.RIC=	[relative ion count or reconstructed ion current as recorded by instrument software]	
##DATA PROCESSING=	[average, background subtraction, etc.]	
##$SPECTRUM REMARKS=	[additional remarks on the mass spectral data]	This field is included for additional comments on the mass spectral data. Examples of useful comments might include tentative identification, suspected contamination, or high background. This field is defined by MaSC.
##XUNITS=	m/z	Invariant field. This should remain as is.
##YUNITS=	Relative Abundance	Invariant field. This should remain as is.
##NPOINTS=	[Total number of x,y data pairs]	
##XYDATA=	(XY..XY)	Invariant field. JCAMP field name for the type of data in the file.
x1 y1 x2 y2 etc.	[Mass spectral data where x is the m/z value and y is the relative intensity of the peak at that m/z value.]	x-values are separated from y-values by a space or a tab. The intensity of the base peak is set to 9999 and all other y-values are scaled to the base peak and rounded to the nearest whole number. Scaled y-values can be calculated using the MaSC-Mass Spectrum Template in MS Excel format.
##END=	[This remains blank.]	JCAMP definition for the end of the data.