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Proposed Reporting Requirements for NMR-based Metabolomics

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1. Status of this document

This document is the outcome of three meetings involving Mark Viant, Christian Ludwig, John Easton and Ulrich Guenther from Birmingham, Denis Rubtsov from Cambridge and Helen Jenkins and Nigel Hardy (3rd meeting only) from Aberystwyth that were held at the Henry Wellcome Building for Biomolecular NMR Spectroscopy on the 25th of July 2005, the 18th of August 2005 and the 1st of December 2005. The aim of the first two meetings was to compare and merge the concepts (and their descriptions) encapsulated in the Cambridge and Aberystwyth (ArMet-compliant) NMR data models and the instrument parameters and data processing parameters models developed at Birmingham. The Cambridge model is based on experience from both Cambridge and Imperial College London (based upon the SMRS policy document), whilst the Aberystwyth model is based on requirements for the UK Centre for Plant and Microbial Metabolomics based at Rothamsted Research. The aim of the third meeting was to compare and devise a merging strategy for the two XML implementations of the standard that were produced at Aberystwyth and Cambridge.

Presentation of the proposed standard at MetaboMeeting2.0 in Cambridge on the 10th of January, 2006 elicited positive feedback from the community. This document represents the results of re-working the original document to produce a standalone representation of the standard suitable for distribution to interested parties for more detailed assessment.

2. Concepts addressed

The tables in this section represent the concepts that were discussed at the meetings and contain the data items that are required to describe them. A *Block* is a distinct subset of the data items for a concept. The *Domain* column indicates the data types for the data items. The *Units* column contains candidate units of measurement for numeric data items. The column headed *?* contains an indication of whether a data item is a required (*R*) or optional (*O*) element of its Block.

Following each table is a list of the association rules that describe how the blocks of data items for the concept are related. There is also a UML representation of the structure of the concept.

2.1. Analysis

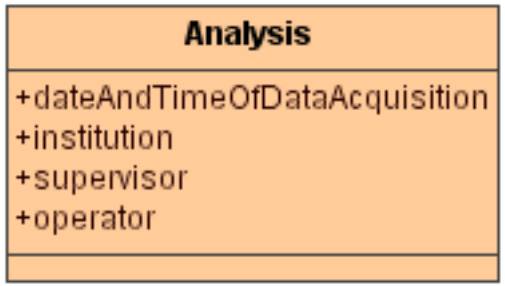
In this context an *Analysis* is NMR data acquisition for a single sample.

Block	**Field**				
	Name	**Definition**	**Domain**	**Units**	**?**
Analysis					
	dateAndTimeOfDataAcquisition	The date/time at which the analysis of a sample by NMR was performed.	ISO 8601		R

Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
	institution	The name of the institution at which the analysis was carried out.	string		R
	supervisor	The name of the supervisor who oversaw the analysis. by NMR.	string		R
	operator	The name of the operator who carried out the analysis.	string		R

Association rules. As there is only one data block for Analysis there are no association rules.

Figure 1. UML for the Analysis concept



2.2. Sample

Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
NMR Sample					
	originalBiologicalSampleReference	A reference to information on the provenance of the original biological source material.	URI		R
	originalBiologicalSamplepH	The pH value of the original biological sample material.	float	pH	O
	postBufferpH	The pH value of the sample after the buffer has been added.	float	pH	R
	concentrationOfSoluteInSample	The concentration of additional solute (e.g. buffer, chelating agent) within the sample.	float	('moles' | 'millimoles')	R
	concentrationOfChemShiftStdInSample	The concentration of chemical shift standard within the sample.	float	('moles' | 'millimoles')	O

Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
	concentrationOfSolventInSample	The concentration of a solvent within the sample.	float	('moles' | 'millimoles')	R
	concentrationOfConcentrationStdIn-Sample	The concentration of concentration standard compound within the sample.	float	('moles' | 'millimoles')	R
	concentrationStdType	An indication of the type of the concentration standard within the sample.	See §4.1		R
Field Frequency Lock					
	fieldFrequencyLockName	The name of a field frequency lock compound.	string		R
Additional Solute					
	soluteName	The name of a solute that is added to a sample, e.g. a buffer or chelating agent.	string		R
Chemical Shift Standard					
	chemicalShiftStdName	The name of a compound added to a sample to enable alignment of spectra.	string		R
Solvent					
	solventName	The name of a solvent.	string		R
Concentration Standard					
	concentrationStdName	The name of a concentration standard compound.	string		R

Association rules. The following association rules apply to the data blocks for the Sample concept:

- An NMR Sample is associated with one Field Frequency Lock
- An NMR Sample is associated with one Additional Solute
- An NMR Sample is optionally associated with one Chemical Shift Standard
- An NMR Sample is associated with at least one and possibly many Solvents
- An NMR Sample is associated with one Concentration Standard.

2.3. Instrument

Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
Instrument					
	location	The geographical location of the instrument	string		R
Magnet					

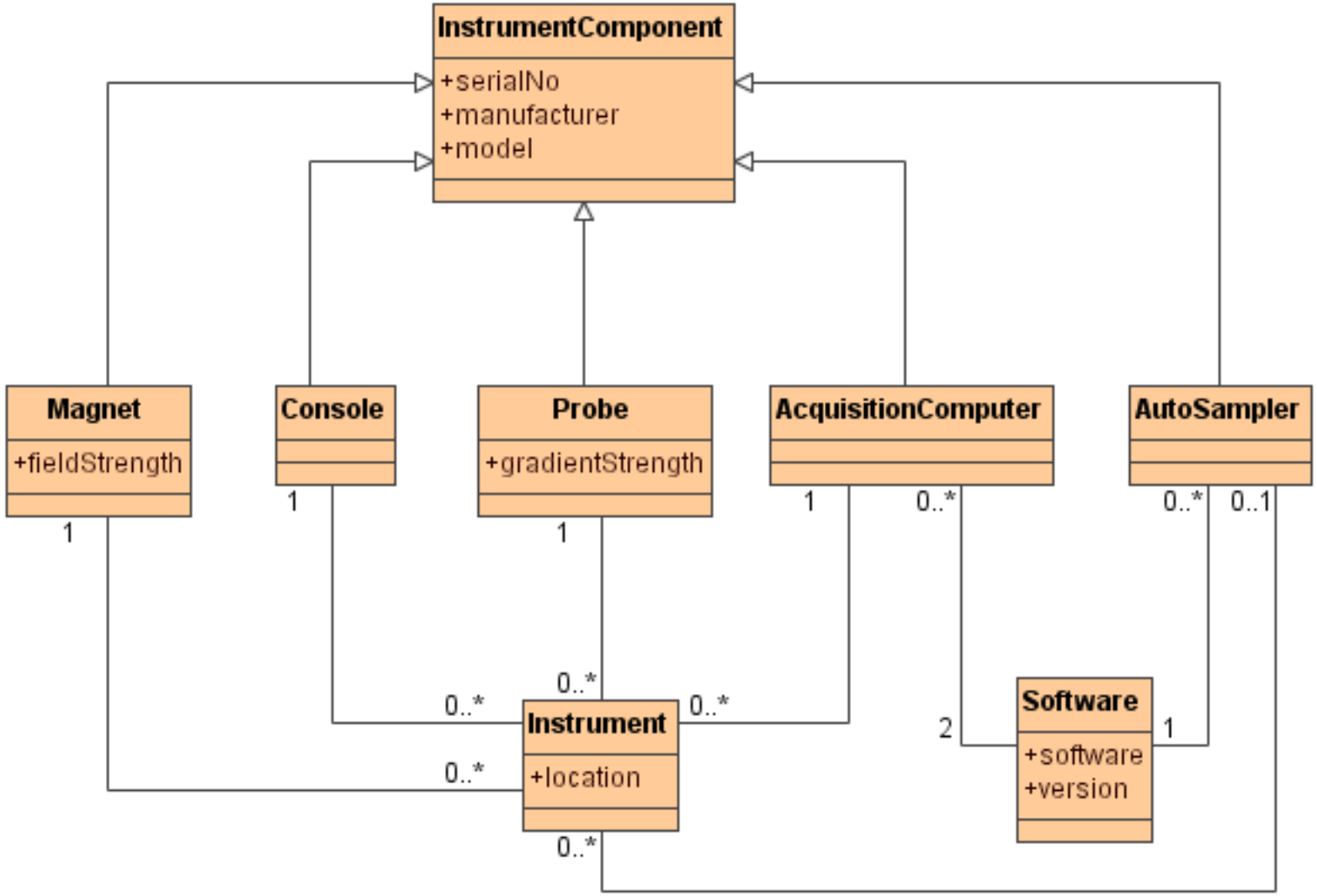
Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
	serialNo	The unique serial number for an NMR magnet.	string		O
	manufacturer	The manufacturer of an NMR magnet.	string		R
	model	The manufacturer's model identifier for an NMR magnet.	string		R
	fieldStrength	The strength of the magnetic field produced by an NMR magnet.	float	('gauss' | 'tesla')	R
Probe					
	serialNo	The unique serial number for an NMR probe.	string		O
	manufacturer	The manufacturer of an NMR probe (may be "custom made")	string		R
	model	The manufacturer's model identifier for an NMR probe.	string		R
	gradientStrength	The variation in magnetic field between the gradient coils in an NMR probe.	float	('gauss' | 'tesla')	O
Console					
	serialNo	The unique serial number for an NMR console.	string		O
	manufacturer	The manufacturer of an NMR console.	string		R
	model	The manufacturer's model identifier for an NMR console.	string		R
Acquisition Computer					
	serialNo	The unique serial for an NMR acquisition computer.	string		O
	manufacturer	The manufacturer of an NMR acquisition computer.	string		R
	model	The manufacturer's model identifier for an NMR acquisition computer.	string		R
	operatingSystemSoftware	The name of the operating system on an NMR acquisition computer.	string		R
	operatingSystemVersion	The version of the operating system on an NMR acquisition computer.	string		R
	applicationSoftware	The name of the software used for acquisition on an NMR acquisition computer.	string		R
	applicationSoftwareVersion	The version of the acquisition software on an NMR acquisition computer.	string		R
Autosampler					
	serialNo	The unique serial number for an NMR autosampler.	string		O
	manufacturer	The manufacturer of an NMR autosampler.	string		R
	model	The manufacturer's model identifier for an NMR autosampler.	string		R

Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
	applicationSoftware	The name of software used to control an NMR autosampler.	string		R
	applicationSoftwareVersion	The version of the software used to control an NMR autosampler.	string		R

Association rules. The following association rules apply to the data blocks for the Instrument concept:

- An Instrument is associated with one Magnet
- An Instrument is associated with one Probe
- An Instrument is associated with one Console
- An Instrument is associated with one Acquisition Computer
- An Instrument is optionally associated with one Autosampler

Figure 3. UML for the Instrument concept



2.4. Instrument Acquisition Parameters

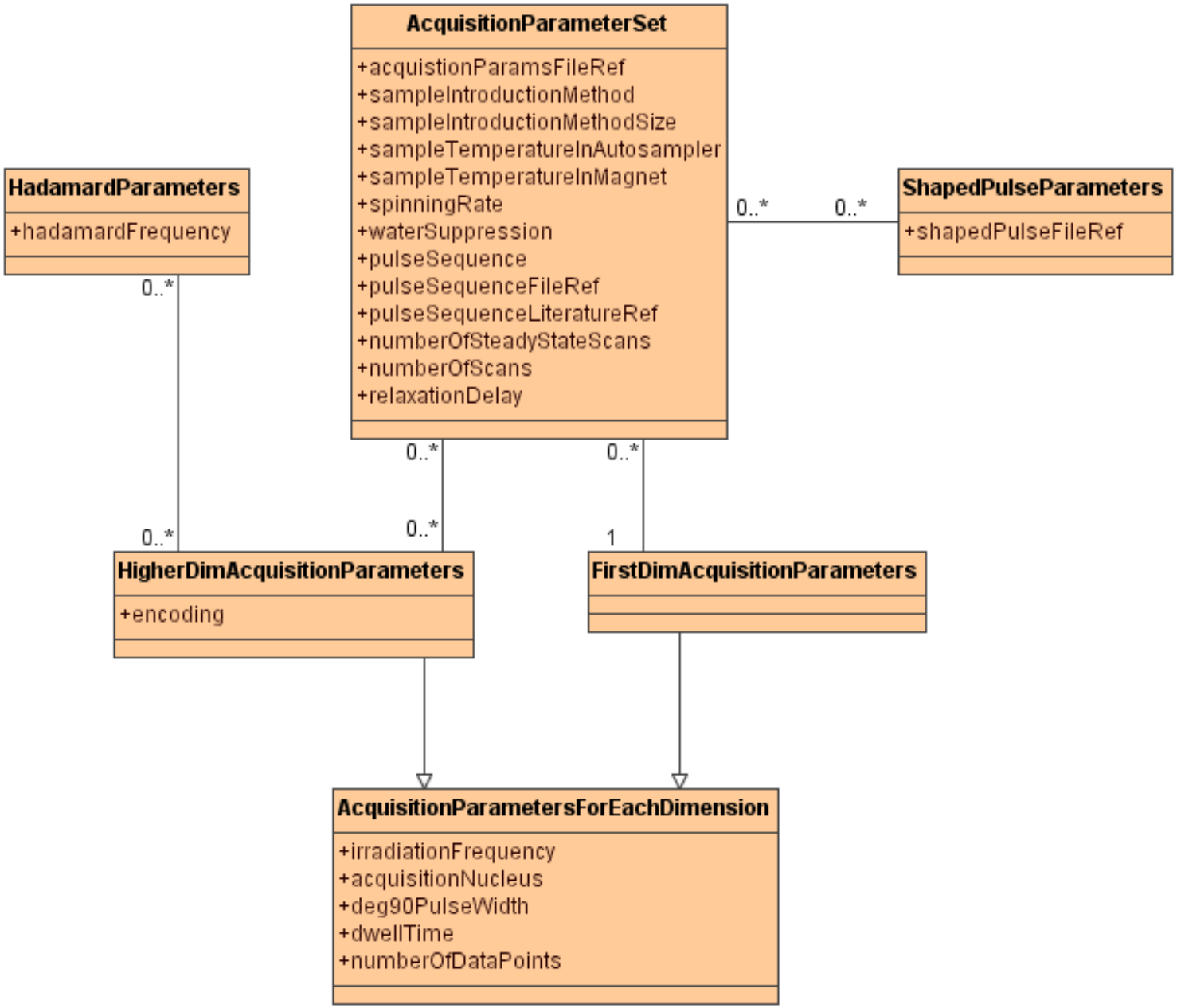
Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
Acquisition Parameter Set					
	acquisitionParamsFileRef	A reference to the file of acquisition parameters produced by the instrument	URI		R
	sampleIntroductionMethod	The method of introduction of the sample to the spectrometer	See §4.2		R
	sampleIntroductionMethodSize	The size of the tube or rotor or the active volume of the flow probe	float	('millilitres' | 'microlitres' | 'millimetres')	R
	sampleTemperatureInAutosampler	The temperature of the sample whilst in the autosampler if fitted	float	('centigrade' | 'kelvin' | 'fahrenheit')	O
	sampleTemperatureInMagnet	The temperature of the sample whilst in the magnet	float	('centigrade' | 'kelvin' | 'fahrenheit')	R
	spinningRate	The rate at which the sample is spun to improve resolution by partially averaging out inhomogeneities in the magnetic field	float	('hertz' | 'kilohertz' | 'megahertz')	R
	waterSuppression	The technique used to suppress the water peak in the spectrum	See §4.3		R
	pulseSequence	The pulse sequence name	See §4.4		R
	pulseSequenceFileRef	A reference to a file that specifies the pulse sequence	URI		R
	pulseSequenceLiteratureRef	A reference to a description of the pulse sequence in the literature	URI		R
	numberOfSteadyStateScans	The number of scans whose data is not summed to create the spectrum for a sample, but that are carried out to establish the steady-state of relaxation for the nuclei	integer		R
	numberOfScans	The number of repeat scans to be performed and summed to create the spectrum for a sample	integer		R
	relaxationDelay	The delay between repeat scans to allow the nuclei to relax back to their steady-state	float	('seconds' | 'milliseconds' | 'microseconds')	R
Acquisition Parameters Recorded For Each Dimension					
	irradiationFrequency	The frequency of RF radiation used to irradiate a sample	float	('hertz' | 'kilohertz' | 'megahertz')	R
	acquisitionNucleus	The nucleus being studied	string		R
	deg90PulseWidth	The 90 degree pulse width of acquisition nucleus	float	('seconds' | 'milliseconds' | 'microseconds')	R
	dwellTime	The digital sampling interval	float	('seconds' | 'milliseconds' | 'micro-	R

Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
				seconds')	
	noOfDataPoints	The number of data points acquired (should match the number of datapoints in the FID dataset(s) when describing the first dimension, or the additional axis of the 2D FID when describing the second dimension).	integer		R
Acquisition Parameters Recorded For Second and Higher Dimensions					
	encoding	The scheme for producing a numerical representation of the environment of an atom during an NMR experiment	See §4.5		R
Shaped Pulse Parameters					
	shapedPulseFileRef	A reference to a file containing a specification of the shape of an excitation pulse	URI		R
Hadamard Parameters					
	hadamardFrequency	A Hadamard frequency used during Hadamard encoding	float	('hertz' | 'kilohertz' | 'megahertz')	R

Association rules. The following association rules apply to the data blocks for the Instrument Acquisition Parameters concept:

- When describing a 1D NMR experiment an Acquisition Parameter Set is associated with:
  - One set of Acquisition Parameters Recorded for Each Dimension
  - Zero or many sets of Shaped Pulse Parameters
- When describing an NMR experiment with 2 or more dimensions an Acquisition Parameter Set is associated with:
  - A set of Acquisition Parameters Recorded for Each Dimension for the first dimension and for each additional dimension.
  - A set of Acquisition Parameters Recorded for the Second and Higher Dimensions for each additional dimension each of which is associated with:
    - One or more sets of Hadamard Parameters if, and only if, the second dimension *encoding* data item contains the value *Hadamard*
  - Zero or many sets of Shaped Pulse Parameters

Figure 4. UML for the Instrument Acquisition Parameters concept

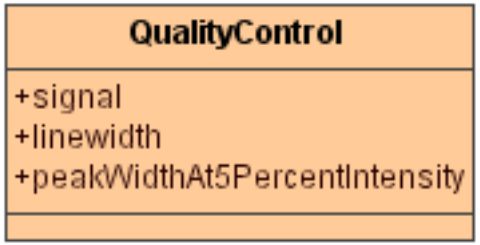

AcquisitionParameterSet
+acquistionParamsFileRef
+sampleIntroductionMethod
+sampleIntroductionMethodSize
+sampleTemperatureInAutosampler
+sampleTemperatureInMagnet
+spinningRate
+waterSuppression
+pulseSequence
+pulseSequenceFileRef
+pulseSequenceLiteratureRef
+numberOfSteadyStateScans
+numberOfScans
+relaxationDelay
HadamardParameters
+hadamardFrequency
ShapedPulseParameters
+shapedPulseFileRef
0..*
0..*
0..*
0..*
0..*
0..*
1
HigherDimAcquisitionParameters
+encoding
FirstDimAcquisitionParameters
AcquisitionParametersForEachDimension
+irradiationFrequency
+acquisitionNucleus
+deg90PulseWidth
+dwellTime
+numberOfDataPoints

2.5. Quality Control

Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
Quality Control					
	signal	The identity of signal used for checking	string		R
	linewidth	The linewidth (FWHM: full width at half maximum) measured for the chosen signal in the 1D data in absence of Window Function processing	float	('hertz' | 'kilohertz' | 'megahertz')	R
	peak-WidthAt5PercentIntensity	A measurement of the width of the peak at 5% of its total height.	float	percentage	R

Association rules. As there is only one data block for Quality Control there are no association rules.

Figure 5. UML for the Quality Control concept



2.6. Data Processing

Data processing has been split into two parts. This split is based on the datasets that are produced as a result of different levels of data processing (described below). 1D FID and multi-dimension FID data are as produced by the instrument. 1D Spectra, mutli-dimension Spectra and Projected Spectra are produced by FID and spectral processing (spectra generation from FID data). Bucketed Spectra and Peak-Picked Spectra are produced by spectral quantitation.

Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
FID & Spectral Processing Parameter Set					
	postAcquisitionWaterSuppression	The data processing technique used to suppress the water peak in the spectrum.	See §4.6		O
	transformationType	The method use to transform the time-based acquisition data into frequency-based	See §4.7		R

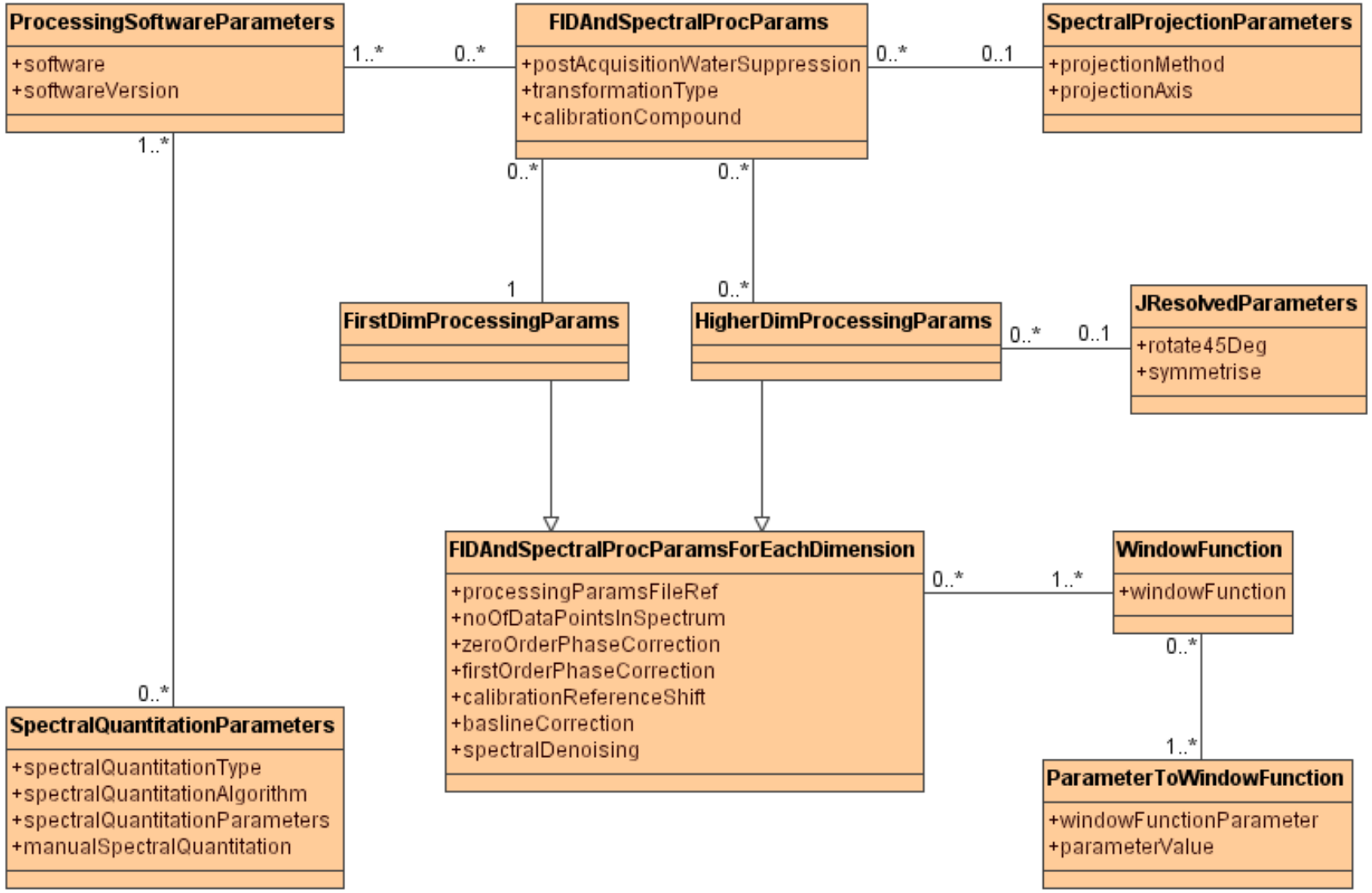
Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
		data.			
	calibrationCompound	The chemical identity used to reference the spectrum (default to Chemical Shift Standard where available)	string		R
Processing Parameters Recorded for Each Dimension					
	processingParamsFileRef	A reference to the file of processing parameters produced by the instrument	URI		O
	noOfDataPointsInSpectrum	The number of data points in the spectrum that results from data pre-processing (should match the number of datapoints in the spectrum when describing the first dimension, or the number of data points in the additional axis of the 2D spectrum when describing the second dimension)	integer		R
	zeroOrderPhaseCorrection	The number of degrees of the zero order phase adjustment.	float	degrees	O
	firstOrderPhaseCorrection	The number of degrees of the first order phase adjustment.	float	degrees	O
	calibrationReferenceShift	The parts-per-million value of the peak used to reference the spectrum.	integer	ppm	R
	baselineCorrection	A description of the approach to flattening the baseline of the spectrum that results from data pre-processing.	string		O
	spectralDenoising	A description of any processing carried out to eliminate or reduce the noise in a spectrum.	string		O
Window Function Parameters					
	windowFunction	A function applied to a FID to increase the SNR or the resolution.	See §4.8		R
Parameter to Window Function Parameters					
	windowFunctionParameter	The name of a parameter to a Window Function	See §4.9		R
	parameterValue	The value for a parameter to a Window Function	string		R
2D J-Resolved Processing Parameters					
	rotate45Deg	An indication of whether a data set resulting from 2D J-Resolved analysis was rotated as part of data pre-processing.	Boolean		R
	symmetrise	An indication of whether a data set resulting from 2D J-Resolved analysis was symmetrised about the horizontal axis as part of data pre-processing.	Boolean		R
Processing Software Parameters					
	software	The name of a software artifact used during data processing.	string		R
	softwareVersion	The version of a software artifact used during data processing.	string		R
Spectral Projection Parameters					
	projectionMethod	A method of spectral projection.	See §4.10		R

Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
	projectionAxis	The axis onto which a 2D spectrum was projected.	See §4.11		R
Spectral Quantitation Parameter Set					
	spectralQuantitationType	The approach to spectral quantitation.	See §4.12		R
	spectralQuantitationAlgorithm	A description of the approach to spectral quantitation.	string		R
	spectralQuantitationParameters	A description of the parameters used to govern spectral quantitation.	string		O
	manualSpectralQuantitation	A description of any manual manipulation or tidying of the data performed during spectral quantitation.	string		O

Association rules. The following association rules apply to the data blocks for the Data Processing concept:

- When describing FID and spectral processing in a 1D NMR experiment a FID & Spectral Processing Parameter Set is associated with:
  - One set of Processing Parameters Recorded for Each Dimension which is associated with:
    - One or more sets of Window Function Parameters each of which is associated with:
      - One of more sets of Parameter to Window Function Parameters
  - One or more sets of Processing Software Parameters
- When describing multi-dimensional FID and spectral processing without spectral projection a FID & Spectral Processing Parameter Set is associated with:
  - One set of Processing Parameters Recorded for Each Dimension to describe the first dimension which is associated with:
    - One or more sets of Window Function Parameters each of which is associated with:
      - One of more sets of Parameter to Window Function Parameters
  - A set of Processing Parameters Recorded for Each Dimension to describe each additional dimension each of which is associated with:
    - One or more sets of Window Function Parameters each of which is associated with:
      - One of more sets of Parameter to Window Function Parameters
    - Zero or one set of 2D J-Resolved Processing Parameters
  - One or more sets of Processing Software Parameters
- When describing multi-dimensional FID and spectral processing with spectral projection a FID & Spectral Processing Parameter Set is associated with:
  - One set of Processing Parameters Recorded for Each Dimension to describe the first dimension which is associated with:
    - One or more sets of Window Function Parameters each of which is associated with:
      - One of more sets of Parameter to Window Function Parameters
  - A set of Processing Parameters Recorded for Each Dimension to describe each additional dimension each of which is associated with:
    - One or more sets of Window Function Parameters each of which is associated with:
      - One of more sets of Parameter to Window Function Parameters
    - Zero or one set of 2D J-Resolved Processing Parameters
  - One or more sets of Processing Software Parameters
  - One set of Spectral Projection Parameters
- When describing spectral quantitation a Spectral Quantitation Parameter Set is associated with:
  - One or more sets of Processing Software Parameters

Figure 6. UML for the Data Processing concept



2.7. Data Sets

The content of the datasets described here is based on the JCAMP-DX format for NMR.

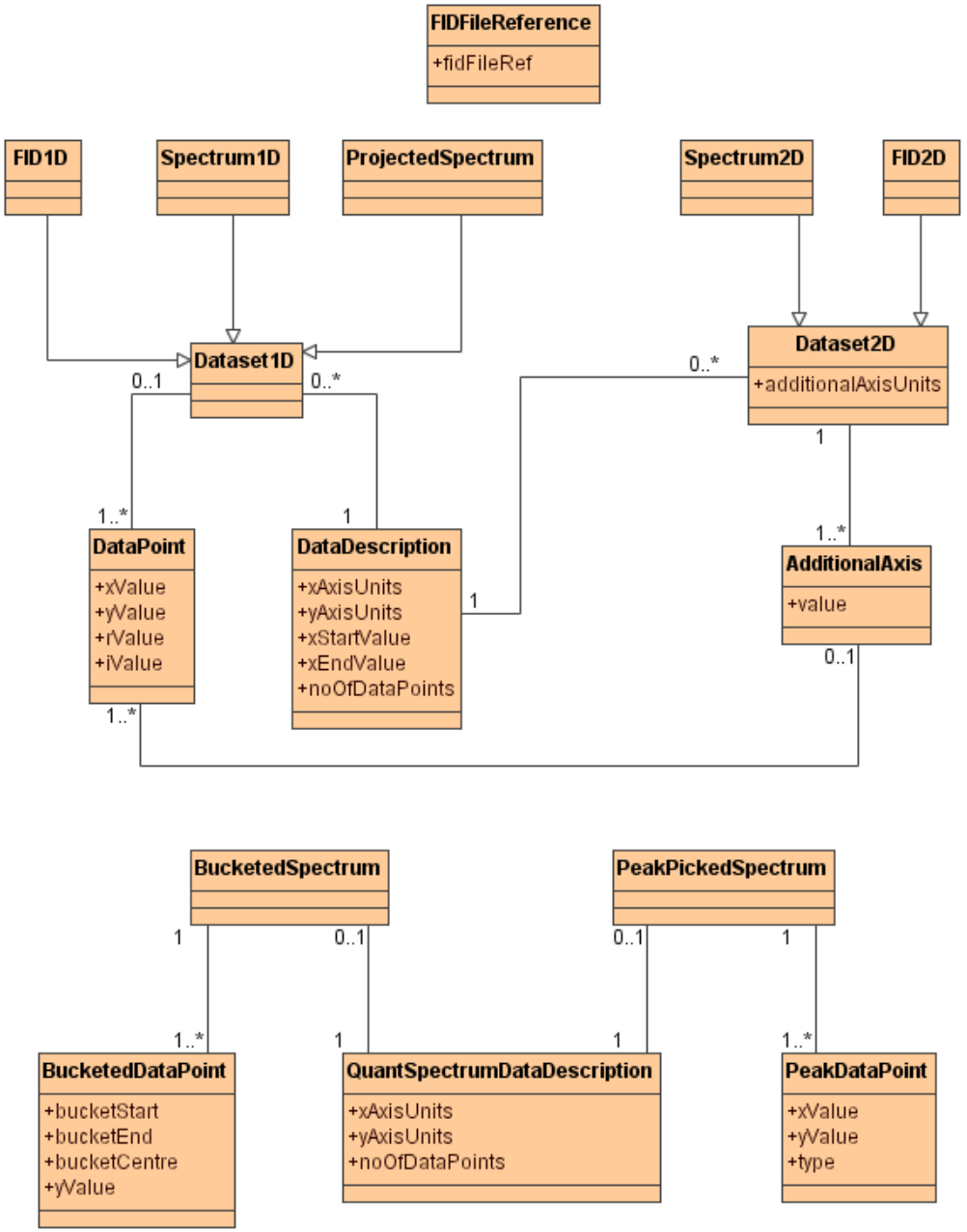
Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
1D FID Data Set					
	xAxisUnits	The units of measurement on the x-axis	string	('second' | 'millisecond' | 'microsecond')	R
	yAxisUnits	The type of y-axis values	See §4.13		R
	xStartValue	The starting x-axis value.	float		R
	xEndValue	The final x-axis value.	float		R
	numberofDataPoints	The number of data points on the x-axis.	integer		R
	data matrix	The data matrix for the FID represented as either a set of y-axis values at equal x-axis intervals or a set of (x,y) pairs			R
FID File Reference					
	fidFileRef	A reference to a file that contains FID data.	URI		R
2D FID Data Set					
	additionalAxisUnits	The units of measurement on the second dimension axis.	string	('second' | 'millisecond' | 'microsecond' | 'hertz' | 'kilohertz' | 'megahertz')	R
	xAxisUnits	The units of measurement on the first dimension x-axis	string	('second' | 'millisecond' | 'microsecond')	R
	yAxisUnits	The type of values on the first dimension y-axis	See §4.13		R
	xStartValue	The starting value for the first dimension x-axis	float		R
	xEndValue	The final value on the first dimension x-axis	float		R
	numberofDataPoints	The number of data points on the x-axis in the first dimension.	integer		R
	data matrix	The data matrix for the FID which comprises multiple 1D FIDs each annotated with a value for the second dimension axis. Each 1D FID is represented as either a set of y-axis values at equal x-axis intervals or a set of (x,y) pairs			R
1D Spectrum					
	xAxisUnits	The units of measurement on the x-axis	string	('hertz' | 'kilohertz' | 'megahertz')	R
	yAxisUnits	The type of y-axis values	See §4.13		R
	xStartValue	The starting x-axis value.	float		R

Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
	xEndValue	The final x-axis value.	float		R
	numberofDataPoints	The number of data points on the x-axis.	integer		R
	data matrix	The data matrix for the spectrum represented as either a set of y-axis values at equal x-axis intervals or a set of (x,y) pairs			R
2D Spectrum					
	additionalAxisUnits	The units of measurement on the second dimension axis.	string	('hertz' | 'kilohertz' | 'megahertz')	R
	xAxisUnits	The units of measurement on the first dimension x-axis	string	('hertz' | 'kilohertz' | 'megahertz')	R
	yAxisUnits	The type of values on the first dimension y-axis	See §4.13		R
	xStartValue	The starting value for the first dimension x-axis	float		R
	xEndValue	The final value on the first dimension x-axis	float		R
	numberofDataPoints	The number of data points on the x-axis in the first dimension.	integer		R
	data matrix	The data matrix for the spectrum which comprises multiple 1D spectra each annotated with a value for the second dimension axis. Each 1D spectrum is represented as either a set of y-axis values at equal x-axis intervals or a set of (x,y) pairs			R
2D Projected Spectrum					
	xAxisUnits	The units of measurement on the x-axis	string	('hertz' | 'kilohertz' | 'megahertz')	R
	yAxisUnits	The type of y-axis values	See §4.13		R
	xStartValue	The starting x-axis value.	float		R
	xEndValue	The final x-axis value.	float		R
	numberofDataPoints	The number of data points on the x-axis.	integer		R
	data matrix	The data matrix for the spectrum represented as either a set of y-axis values at equal x-axis intervals or a set of (x,y) pairs			R
Bucketed Spectrum					
	xAxisUnits	The units of measurement on the x-axis	string	('hertz' | 'kilohertz' | 'megahertz' | 'ppm')	R
	yAxisUnits	The type of y-axis values	See §4.13		R
	numberofDataPoints	The number of buckets in the spectrum.	integer		R
	data matrix	The data matrix for the spectrum. The points in the data matrix comprise (the			R

Block	Field				
	Name	**Definition**	**Domain**	**Units**	**?**
		starting x-axis value for the bucket, the ending x-axis value for the bucket, the x-axis value at the centre of the bucket, the y-axis value)			
Peak-picked Spectrum					
	xAxisUnits	The units of measurement on the x-axis	string	('hertz' | 'kilohertz' | 'megahertz' | 'ppm')	R
	yAxisUnits	The type of y-axis values	See §4.13		R
	numberofDataPoints	The number of peaks in the spectrum.	integer		R
	data matrix	The data matrix for the spectrum. The points in the data matrix comprise (the x-axis value for the peak, the y-axis value for the peak, the type of the peak). For values for the type of a peak see §4.14			R

Association rules. There are no associations between the data blocks for the Data Sets concept.

Figure 7. UML for the Data Sets concept


FIDFileReference
+fidFileRef
FID1D
Spectrum1D
ProjectedSpectrum
Spectrum2D
FID2D
Dataset1D
Dataset2D
+additionalAxisUnits
0..1
0..*
0..*
1
1..*
1
1..*
DataPoint
+xValue
+yValue
+rValue
+iValue
DataDescription
+xAxisUnits
+yAxisUnits
+xStartValue
+xEndValue
+noOfDataPoints
1
AdditionalAxis
+value
0..1
1..*
BucketedSpectrum
PeakPickedSpectrum
1
0..1
0..1
1
1..*
1
1
1..*
BucketedDataPoint
+bucketStart
+bucketEnd
+bucketCentre
+yValue
QuantSpectrumDataDescription
+xAxisUnits
+yAxisUnits
+noOfDataPoints
PeakDataPoint
+xValue
+yValue
+type

3. Generating a Complete Description of an NMR Analysis

Using the data items in the tables above descriptions of various aspects of an NMR analysis can be created. To generate a complete description of an NMR analysis that is compliant with the reporting requirements, descriptions of the various concepts, in the terms described above, must be combined as described below:

- An Analysis must be associated with:
  - One NMR Sample
  - One Instrument
  - One Acquisition Parameter Set (of appropriate dimensions)
  - One Quality Control description
  - One or more of:
    - One FID Data Set which may be either:
      - A 1D FID Data Set
      - A 2D FID Data Set
      - A FID File Reference
    - Zero or many spectra which may be either:
      - A 1D Spectrum which is associated with:
        - A FID & Spectral Processing Parameter Set (for 1D NMR)
      - A 2D Spectrum which is associated with:
        - A FID & Spectral Processing Parameter Set (for multi-dimensional NMR without spectral projection). Note that if the Acquisition Parameter Set *pulseSequence* data item contains the value *2D J-Resolved* then the FID & Spectral Processing Parameter Set must be associated with a set of 2D J-Resolved Processing Parameters.
      - A 2D Projected Spectrum which is associated with:
        - A FID & Spectral Processing Parameter Set (for multi-dimensional NMR with spectral projection). Note that if the Acquisition Parameter Set *pulseSequence* data item contains the value *2D J-Resolved* then the FID & Spectral Processing Parameter Set must be associated with a set of 2D J-Resolved Processing Parameters.
    - Zero or many spectra resulting from spectral quantitation which may be either:
      - A Bucketed Spectrum which is associated with:
        - A FID & Spectral Processing Parameter Set
        - A Spectral Quantitation Parameter Set in which the *spectralQuantitationType* data item contains the value *bucketing*
      - A Peak-Picked Spectrum which is associated with:
        - A FID & Spectral Processing Parameter Set
        - A Spectral Quantitation Parameter Set in which the *spectralQuantitationType* data item contains the value *peak-picking*

4. Controlled Vocabularies

Some data items in the tables above are restricted to values from controlled vocabularies. These vocabularies are currently defined as follows. Extension of these vocabularies would represent a development of the standard.

4.1. Concentration standard type

- internal
- external

4.2. Sample introduction methods

- tube
- MAS
- flow probe

4.3. Water suppression

- Presat
- NOESY-Presat
- Watergate
- WET
- excitation sculpting

4.4. Pulse sequence name

- 1D
- 1D CPMG
- 2D J-resolved
- 2D TOCSY
- 2D Hadamard TOCSY
- 1D Diffusion Edited

4.5. Encoding

- TPPI
- States
- States-TPPI
- Quadrature filter
- Hadamard
- Radon
- GFT
- Frydman
- Echo/Anti-Echo

4.6. Post acquisition water suppression

- convolution
- polynomial fitting
- WaveWat
- HSVD

4.7. Transformation type

- fourier transformation
- non-fourier transformation

4.8. Window function

- exponential multiplication
- gaussian broadening
- sine
- $sine^2$

4.9. Window Function Parameter

- line broadening
- line sharpening
- sine bell length
- sine bell shift

4.10. Method of spectral projection

- maximum intensity
- summation

4.11. Spectral projection axis

- f1
- f2

4.12. Spectral Quantitation type

- peak picking
- bucketing

4.13. Y-axis value type

- power
- magnitude
- real
- imaginary
- complex

4.14. Peak-picked data point type

- singlet

- doublet
- triplet
- quadruplet
- multiplet
- unassigned