SPINE SAMPLE HOLDER & VIAL SPECIFICATIONS-L-R04

Revised November 15th 2004

Drawings:

DM16106A Cap, *DM16210A* Vial, *DM16100* Sample Holder (with Hampton™ pin), *DM16001A* Sample Holder + Vial (with Hampton™ pin), *DM16300* Goniometer mount

Terminology:

- **Cap:** support of the pin
- **Pin:** pin with mounted crystal support (loop…)
- **Sample holder:** Cap + pin
- **Sample Holder Length:** Distance from the base of the cap to the crystal (or beam position) Refer to drawing *DM16100*.
- **Vial:** sample holder reservoir
- **Goniometer mount**: Magnet or electromagnet that holds the Sample holder on the goniometer

Design rules:

1) Compatible with commercial <u>Sample changers</u> using HAMPTON Magnetic style Sample holders
   - Mar research
   - Rigaku – ACTOR
   - Bruker Nonius BruNo
2) Compatible with sample changers that are <u>under development</u> in academic institutes:
   - EMBL/ESRF Grenoble
   - EMBL Hamburg
   - CNRS Grenoble - ESRF FIP Beamline
   - LBNL Sample changer
3) Compatible with the HAMPTON Magnetic Sample holder and Vial system
4) Caps accept different pin types (customized mounting holes)
5) Identification with ECC200 DATA MATRIX codes + human readable code
6) Improved precision for robotised handling
7) Improved stability for use with micro crystals
8) Compatible with manual use
9) Public design for multiple manufacturing companies

Vials - *DM16210A*

- Rounded edges (or chamfers) on top and on the bottom of the vials to avoid potential blocking during transfers.
- Ferromagnetic disc at the bottom of the vials for "positive" vial manipulation with a magnet
- Polarity of the vial magnetic ring is specified
- Vent hole

Caps - *DM16106A*

- Rounded edges (or chamfers) to avoid potential blocking during transfers.
- Recommended material: Steel anticorrosion coated or ferromagnetic stainless steel (Stainless steel 430F or equivalent).
- Minimum material quantity to reduce the freezing/melting/drying cycle when the sample holder is transferred
- Pin' hole diameter and depth are not specified, they depends on the type of pin used. An example is given for 18 mm Hampton "Mounted Cryoloop™". (*DM16100*)
- DATA MATRIX code protection when a sample holder is mounted on a goniometer mount: A gap is maintained between the code and the mount. The surface of contact between the Cap and the Goniometer mount is the Cap Base (*DM16300*). The surface of the internal disc (Φ9.7mm) is reserved for labelling. The stability of the sample holder is improved when mounted on the Goniometer.
  The Sample holder remains compatible with existing goniometer mounts.

Sample holder length - *DM16100*

(Sample holder = Cap + pin + loop)

- The sample holder length is **22 mm** (from base of cap to crystal or beam position)
- A fixed Sample Holder length will ensure compatibility with all sample changers
- The pin should be stably attached to the cap

Example of cap design for 18 mm Hampton pin is shown in drawing *DM16100*

Sample Holder identification:

Sample holder's caps are identified with DATA MATRIX and human readable codes.

- **ECC200 DATA MATRIX** label on the top of the cap, printed or engraved on the magnet footprint face (Φ 9.7 mm).
- Readable code near the DATA MATRIX code and/or on the rim of the Cap.
- The data matrix should be well readable in LN2, cold and RT N2 environment.[1]

Each Sample Holder can be reused and the Sample (crystal) identifier in a database can be associated with the "**Sample Holder ID**" when it is mounted in the loop.
DATA MATRIX and readable codes can either be engraved or printed.

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[1] A LN2 layer or drops might impair readability. Grenoble is doing tests with cap options 1 and 2 *(DM106A)*. Extensive use of the data matrix will allow a better evaluation.

ID encoding scheme

A **Sample Holder ID** should be composed of a string of 10 alphanumerical characters**:**

MA12BC3456.

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The first letter identifies the manufacturer and ensures that different manufactures cannot produce the same ID.
Contact spine.sh.mid@spineurope.org for attribution of the Manufacturers IDs.
See Annex 1.

M**A12BC3456.**
The remaining 9 characters are organised for good human readability into 1 character, 2 numbers, 2 letters, followed by 4 numbers. These numbers and letters are random.

DATA MATRIX format

Allowed ECC200 DATA MATRIX codes are:

	Format Number	Numeric Capacity	Alphanumeric capacity	Correctable Errors/Erasures
14x14	2	16	10	5/7
16x16	3	24	16	6/9