Appendix

to „Reasons for the single-source contract award regarding a cryogenic ion trap mass spectrometer for infrared laser spectroscopy for HFML-FELIX"

1. Demands of Specification

1.1 General description of the system and main requirements:

1. A new or fully refurbished computer-controlled high-resolution (>10000 at m/z 400) cryogenic ion trap mass spectrometer (hereafter "cryoMS") with robust computer controlled electrospray ionization source allowing versatile positive and negative ion detection with minimal adjustment and maintenance.
2. Accurate mass-determination possible in all MS modes over a wide mass range (m/z 50 – 10000)
3. Collision-induced dissociation MS/MS operation must be possible.
4. The instrument must have an onboard ion mobility separation (IMS) stage.
5. The instrument must have a neutral / ion separation stage before mass-selection.
6. Changing between different atmospheric pressure ionization sources (ESI, APCI) without the need to break the vacuum must be possible.
7. The instrument must be adaptable for the use of other ionization sources.
8. The instrument must be compatible with a commercially available (U)HPLC chromatographic separation platform. Software integration between MS and LC must be possible.
9. The ion storage device must be mounted on a two-stage helium cryocooler that reaches 4 K, and must be able to store ions for a duration of several seconds.
10. The ions in the cryogenic storage device must be accessible for a high intensity infrared laser beam. Software integration and synchronization between the laser control and the MS must be possible.

1.2 The mass spectrometer must include the following parts:

a) The MS must have a resolving power higher than 10 thousand at m/z 400, with accurate mass determination possible in all MS modes over a wide mass range (m/z 50 – 10000), with a duty cycle better than 40 ms / 25 Hz.
b) The MS must be modified for cryogenic infrared laser spectroscopy
   I. The vacuum housing must be modified to hold IR transparent optical window(s)
   II. Entrance of the laser beam into the instrument must be easily accessible.
   III. Optical access to the region where ions are stored is possible.
   IV. The storage device must be mounted on / being connected to a helium cryocooler that can reach 4 K, and be equipped with a resistive heater (at least 40 W), temperature read-out and cryo-shield.

V. The trapping region must have a software-controlled or externally synchronized pulsed valve that allows gas pulses (0.1-100 ms, up to 10^{-3} mbar) to reach the stored ions.
VI. The trapping region must have a continuous gas inlet allowing neutral gas admittance with controllable, low flow rates.
VII. The base pressure in the ion trap region should be better than 10^{-6} mbar

c) Synchronization of the MS acquisition sequence with external triggers must be possible.
d) The MS must produce a trigger signal at any point in the acquisition sequence with the highest flexibility and have an interface to configure and read out these signals.
e) All aspects of operation of the MS must be controllable by a highly flexible user command interface in addition to the general use software GUI. This must enable control of the instrument and data acquisition by laser scanning programs of the FELIX free electron laser.
f) The system must be equipped with a type of high-resolution ion mobility region.
g) The ion transfer system includes ion tunnel technology for high sensitivity in demanding analytical applications and enables simultaneous transfer of a broad m/z range that eliminates the necessity of compound-specific tuning.
h) The instrument inlet must incorporate a neutral-blocking mechanism to avoid contamination of the high-vacuum optics and ion trap without compromising ion sampling efficiency.
i) A lens system enabling switching from soft ion transfer to in-source CID experiments.
j) Comprehensive support/compatibility (hardware and software) with commercial (U)HPLC systems of different HPLC-Systems from vendors such as Thermo/Dionex (Ultimate 3000 nano, cap, micro und RSLC/RSLCnano-Systems), Waters (AcquityUPLC, Alliance HPLC), Agilent, VWR/Hitachi.
k) Possibility to integrate commercially available atmospheric pressure ion sources, as well as home-built ion sources.