MSP creation for MALDI Biotyper

ID (culture collection number or similar)

Metadata (MSP-Metadata MBT Compass):

Organism					
Strain (e.g. ATCC nr./ ID/ …)					
Provided by (e.g. ATCC/DSMZ/ …)					
Determined by (sequenced/ type strain/ …)					
Conserved	☐	**Sample Preparation** ("Extraction Method")	☐ DT ☐ eDT ☐ EFex ☐ ……		
Matrix		HCCA			
Growing conditions		Agar	Temperature (°C)	Time (h)	Culture Conditions:
Comment					

Information of measured sample data:

Count of measured spectra		Date:	Time:	Acronym:
File directory of the raw data	☐ *D/Data /…*			

Spectra editing (flexAnalysis):

- Load the measured sample spectra and the BTS
- **WINDOWS EXPLORER: rename** …
  - ☐ file „BTS" → „BTS **raw**"
  - ☐ raw sample spectra file: e.g.: ID 1234 → ID 1234 ***raw 24sp***

Select all spectra → Assign Method Method → Open …	☐ **MBT_Standard.FAMSMethod**	☐ **Baseline Subtraction**	☐ **Smooth (1x)**

BTS check/ recalibration:

Check Mass Control List Calibrate → Internal …	☐ **Automatic-Assign**	☐ **Peaks manually assigned**
	Max. deviation (ppm):	
Recalibrate sample spectra	☐ **Copy calibration**	
Mass calibration constants BTS Select BTS spectrum → Properties …	**C0:**	
	C1:	
	C2:	
Mass calibration constants sample spectra	☐ **Check: same as BTS?**	

- Close and save the BTS spectrum

  ☐ **WINDOWS EXPLORER: rename** the newly created file (by flexAnalysis) „BTS" → „BTS **ed**"

Editing the sample spectra:

Conspicuous spectra (position\measurement): (Flat lines etc.)				☐ **removed**	
Remaining spectra: Peak accuracy (calculation Excel-worksheet, **+/- 500ppm**)					
m/z	≈ 3000	≈ 5000	≈ 6000	≈ 8000	≈ 10000
Minimum Mass (top of the peak(s))					
Maximum Mass (top of the peak(s))					
Removed spectra					
Count of remaining spectra					

- **Select removed spectra and close** (right click → „Close“) → **DO NOT SAVE THE SPECTRA!**
- **Close remaining spectra and SAVE THEM ALL!**

WINDOWS EXPLORER: rename the newly created file (by flexAnalysis): e.g. ID 1234 → ID 1234 ***ed 21sp***	**File name:**

MSP Creation with MBT Compass Explorer:

- Open MBT Compass Explorer
- Load and select all edited sample spectra
- Right click → „**Create MSP**“ → **assign MSP name**

MSP Name: e.g.: Streptobacillus hongkongensis DSM 26322 CVUAS / Escherichia coli CVUAS 5146 CVUAS

- Taxonomy tree: change the dropdown list to “Projects”, select the node where the MSP should be stored and start the Taxonomy Tree Editor (right click or button next to dropdown menu)

☐ Edited MSP **Metadata**

☐ **Added** MSP to “Projects” node: _____

☐ Verification of the MSP with an **independent spectrum** (date): _____

☐ Report printout

Preparation:
☐ DT
☐ eDT
☐ EFex
☐ ……

MSP created …: ☐ **own MSP library updated**

Comment:	

Date / acronym _____