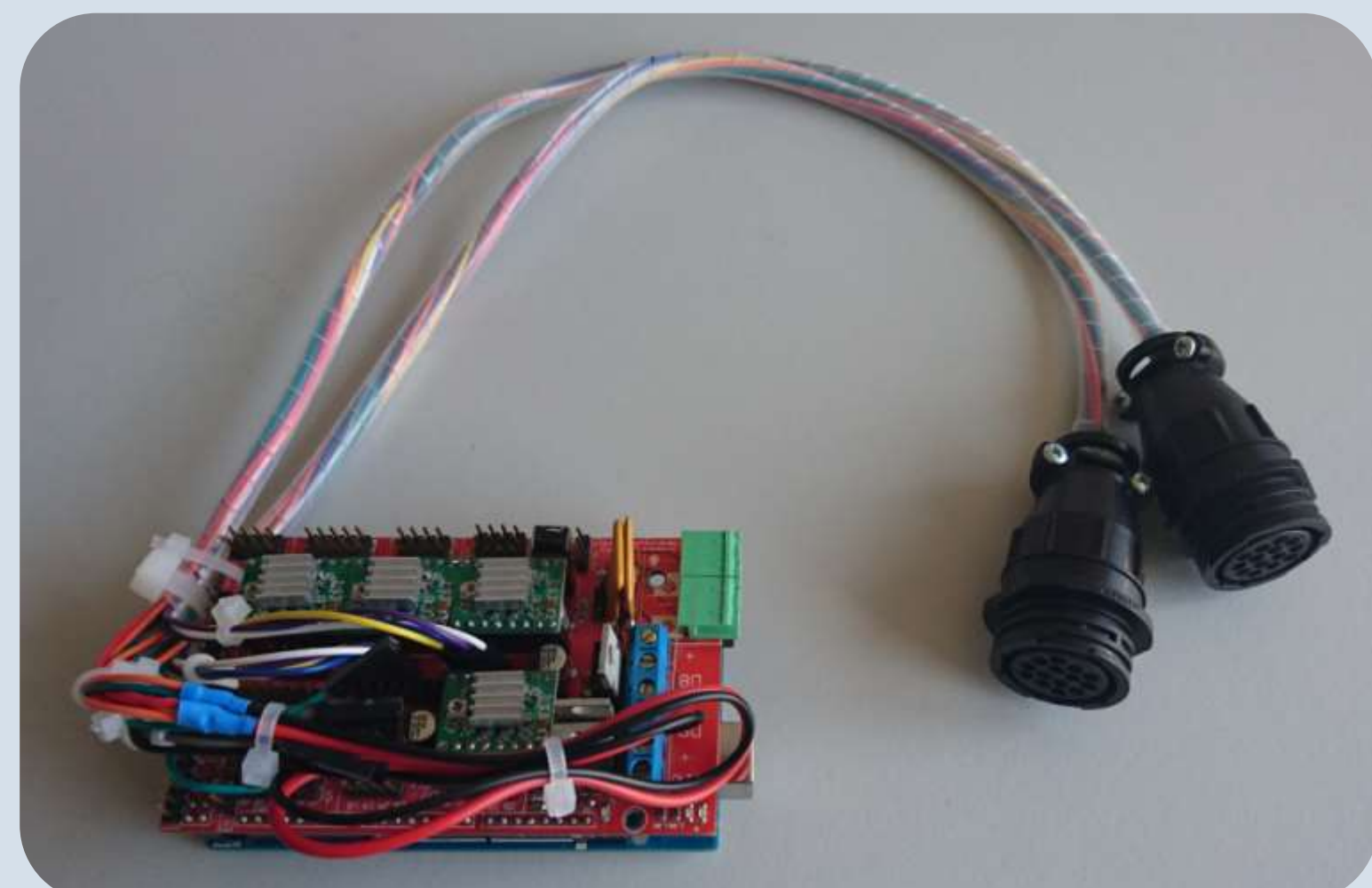


Automated hyphenation of HPTLC to DART-MS and ESI-MS



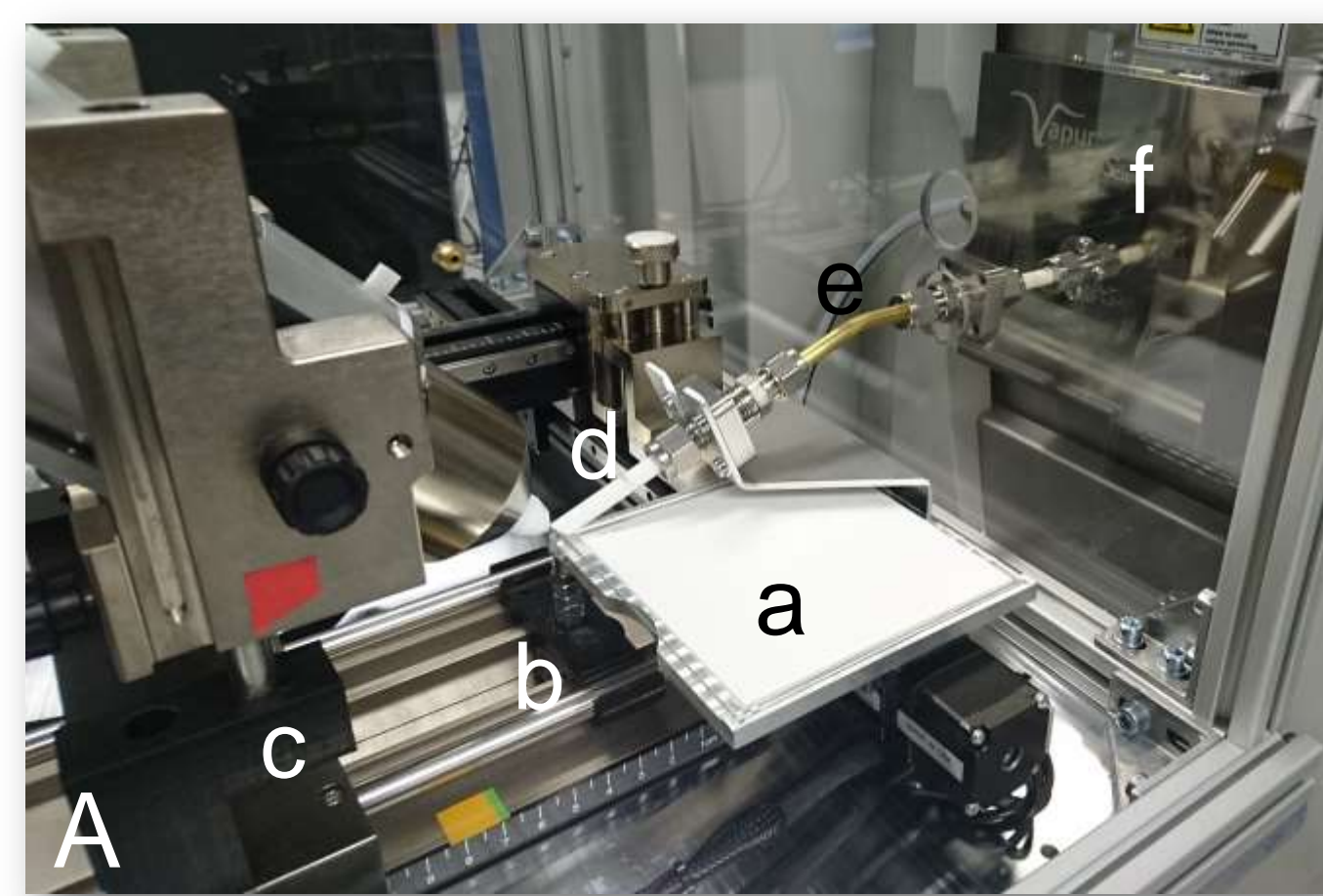
Arduino mega 2560 with RAMPS 1.4 for motor control used on both prototypes

Highlights

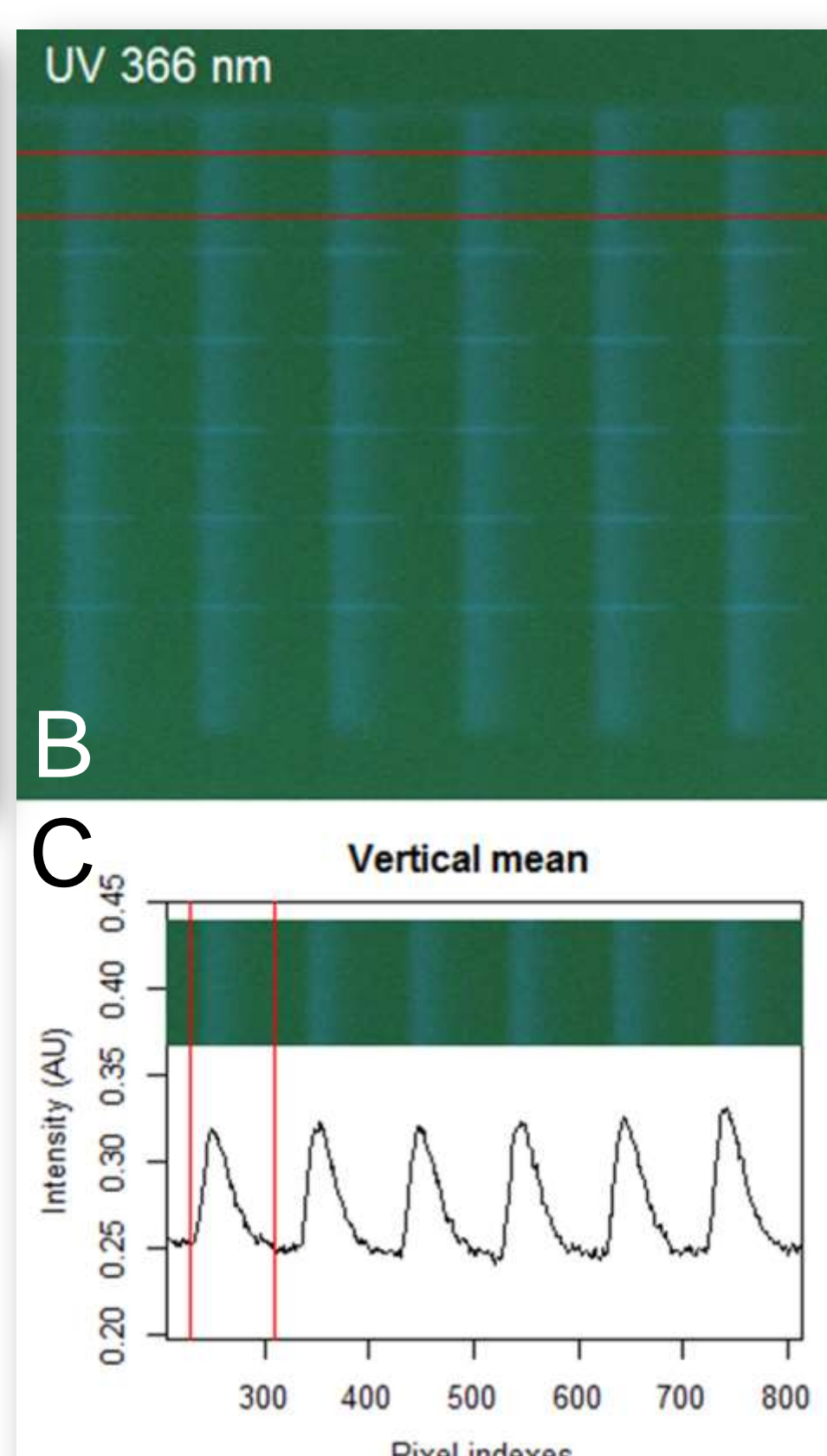
- ✓ Automated HPTLC plate alignment and batch processing of
 - multiple tracks for desorption-based DART-MS (10 x 10 cm)
 - multiple zones for elution-based ESI-MS (20 x 10 cm)
- ✓ High accuracy of positioning at a given high sample throughput
- ✓ 3D printer mechanics and electronics used for interface modifications
- ✓ Rapid prototyping by fused deposition modeling (FDM)

Inspection Box for automated HPTLC-DART-MS

- Automated scanning of multiple scan tracks
- Homogenous desorption/ionization
- Standardized gas phase in the enclosure
- Advanced ion transfer by tethered DART
- High-throughput scanning of tracks or substance windows

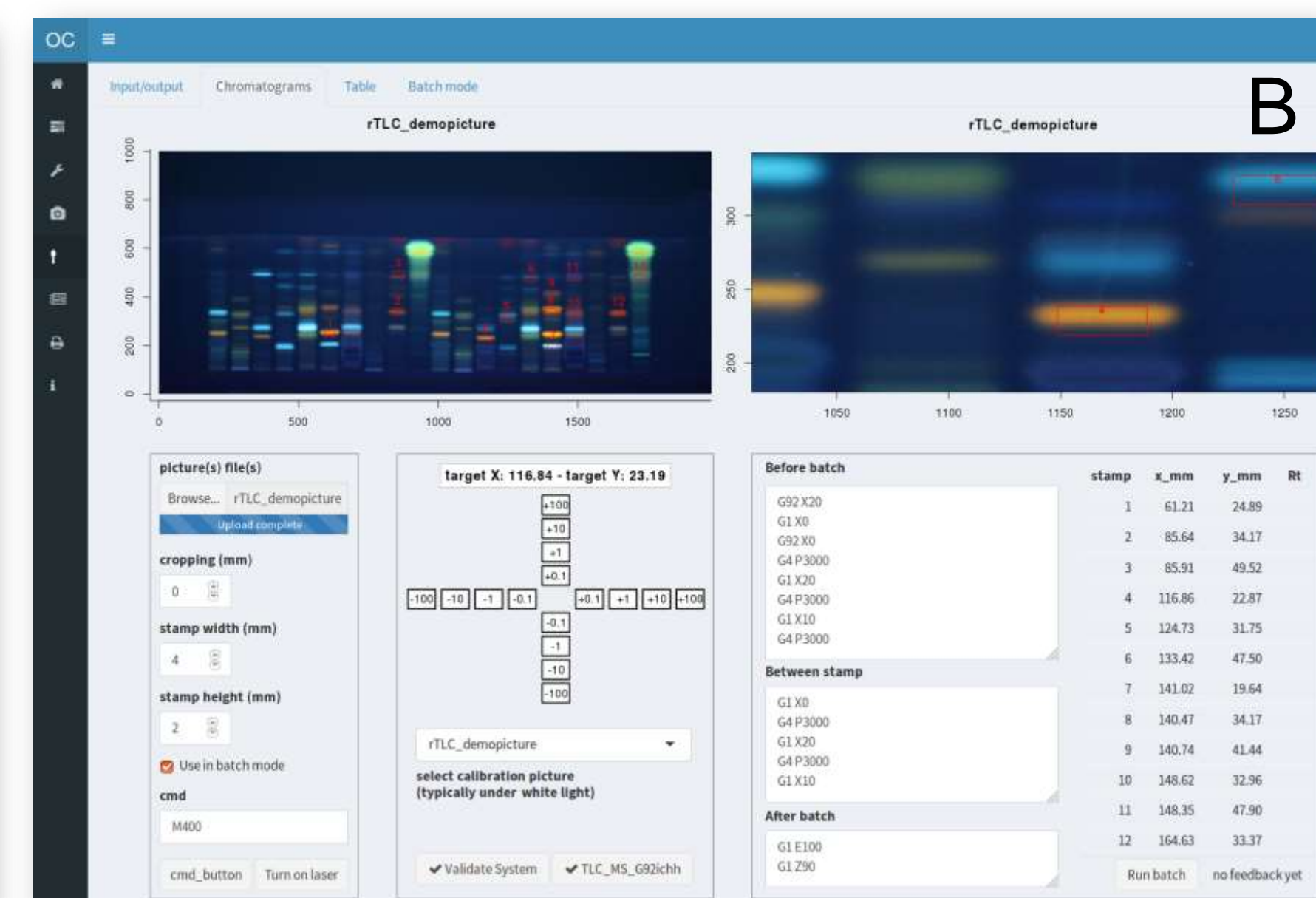
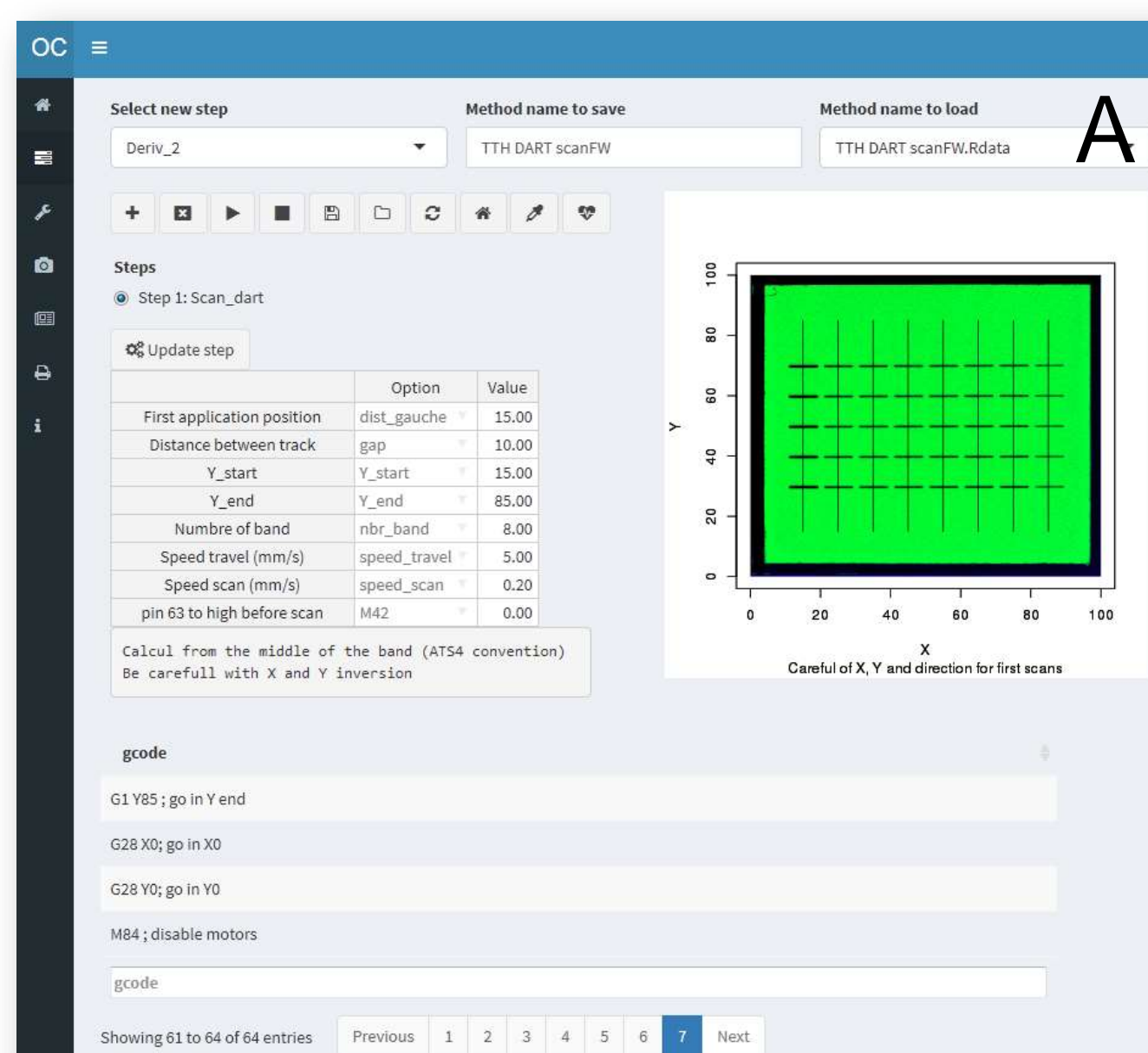


A: Inspection Box with plate carrier (a), vertical stabilizer (b), notched source base (c), advanced ion transfer tube (d) and brass tether (e) towards the MS system (f)
B: Plate afterglow at UV 366 nm after scanning of applied butyl paraben bands (6 tracks x 5 bands of 120 ng each)
C: Homogeneity and width of the plate afterglow (8 mm) evaluated via video densitometry



OC Manager user interface

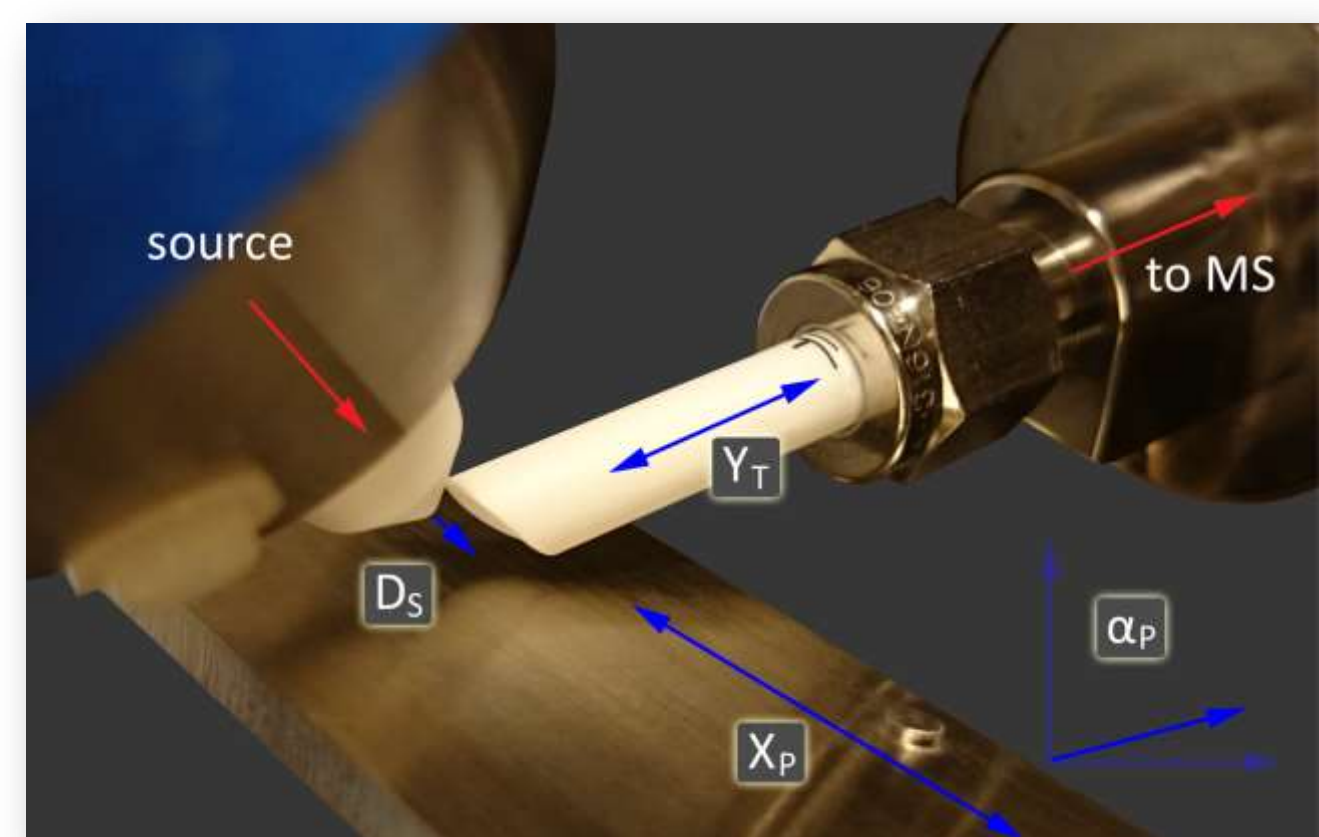
- Edit parameters of positioning for desorption scanning or targeted elution
- Visual feedback for scan track alignment
- Image-based target zone selection
- Multiple scan tracks and target zones in batch mode
- Outlook: Combining HPTLC and MS results in one software platform



Custom made OC Manager platform as user interface to control DART-MS (A) and ESI-MS (B) procedures

Base model for HPTLC-DART-MS

DART SVPA-3DS (IonSense) previously modified for quantitative HPTLC scanning (2 x 10 cm) at improved detectability [1]



- Modified DART SVPA-3DS with:
- shortened source cap
 - reduced distances (D_S)
 - movable (X_P) and angled (α_P) plate carrier
 - modified transfer tube (Y_T)

Modifications

- Enclosed stand-alone device with gas phase inlet
- Aluminum plate carrier (10 x 10 cm)
- Vertical stabilizer (FDM based)
- Notched source base (FDM based) for table movement
- Advanced ion transfer tube for „tethered DART“
- Temperature measurement to avoid heat stress
- Motor control by Arduino mega 2560 with RAMPS 1.4
- GCODE based input for Marlin Firmware

Automated HPTLC-ESI-MS interface

- Zone targeting based on UV/Vis images
- Automated stamping of multiple target zones
- Automated cleaning cycles
- Accurate elution times for quantification
- Easy documentation and assignment of zones
- Synchronization of stamping and MS data acquisition
- Touchscreen (Raspberry Pi) for digital control
- High-throughput stamping



Base model for HPTLC-ESI-MS

TLC-MS Interface 2 (CAMAG), unmodified

Modifications

- Plate frame (10 x 10 cm and 20 x 10 cm)
- Motorized X-Y rails to move the plate frame
- Motorized mechanic for pneumatic and purge system
- Motorized 6-port valve mechanic
- Touchscreen for digital control
- Motor control by Arduino mega 2560 with RAMPS 1.4
- GCODE based input for Marlin Firmware

