10.15 - 10.45 WP1. Theory, instrument overview and status
10.45 – 11.15 WP1. IMS Electronics & IMS Mechanical design

11.15 – 11.45 Coffee break

11.45 – 12.15 WP2. Implementation of CAD, ECD, HECD, UV, IR, PD, and EID MS/MS techniques in Omnitrap

12.15-12.45 WP3. Development and application of H-atom bombardment techniques

12.45-13.45 Lunch

13.45-14.15 WP4. Development and application of Coulomb explosion MS/MS technique

TopSpec

WP1 – Omnitrap & IMS development and testing

D1.1 – 2xOMNI & 1x IMS installed

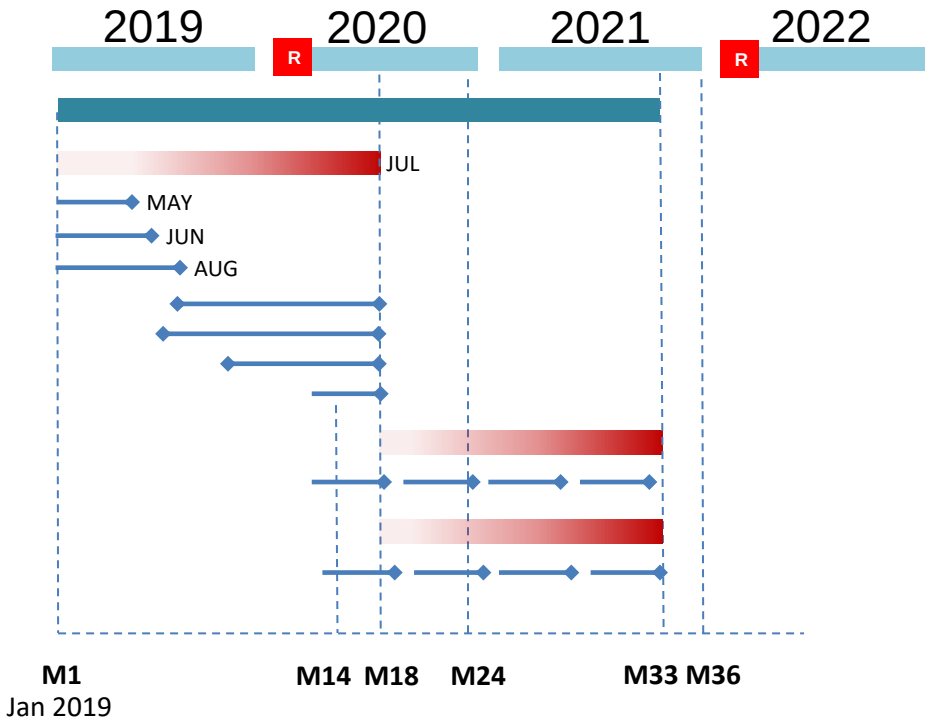
T1.1 – mech design & pulsed EI source
T1.2 – ion isolation simulation
T1.3 – rect RF Generator
T1.4 – assembly of omni's & ims
T1.5 – ctrl software
T1.6 – electronics testing and QE synch
T1.7 – installation

D1.2 – Modifications

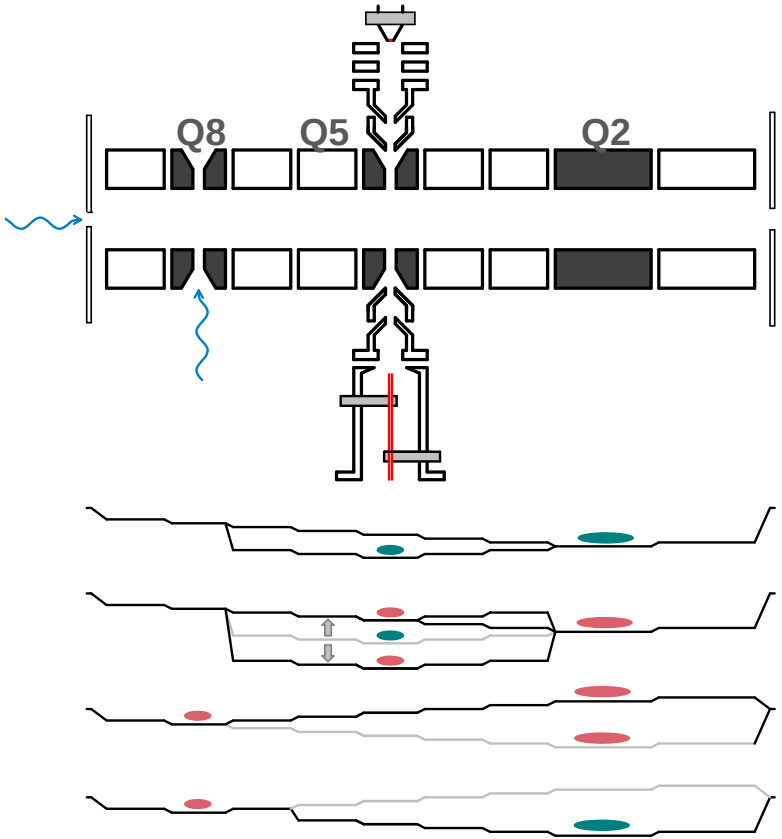
T1.8 – software modification & requests

D1.2 – Serviced Omni's

T1.8 – maintenance



The Omnitrap activation platform



functionality

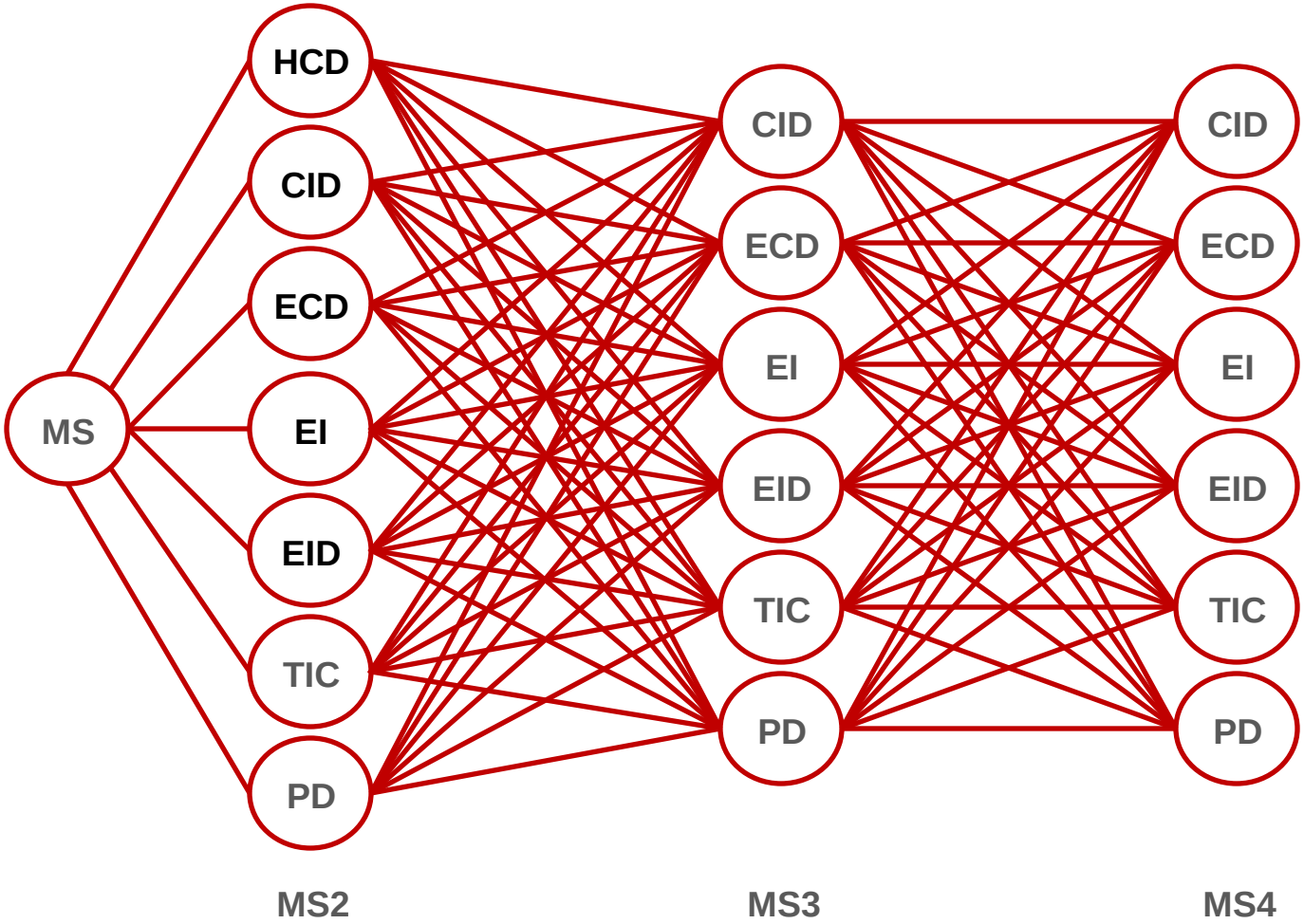
- **Trapping regions for processing ions:**
  - ►Q2: Resolving DC & duty cycle isolation
    dipolar excitation for CID, AC wave multi-notch isolation
  - ►Q5: external injection of electrons, ions and activated neutrals
    dipolar excitation for CID
  - ►Q8: optical access for photoionizagtion & accumulation

- **Rectangular RF employed for radial trapping:**
  - ►extended m/z range trapping
  - ►frequency jumps - fast q_z parking
  - ►external injection of charged particles

- **Multi-level switched DCs applied to segments:**
  - ►lossless axial ion transfer
  - ►multiple trapping regions for sequential or parallel processing
  - ►KE resolved external injection of electrons, neutrals & ions

- **Dynamic control of pressure:**
  - ►CID at elevated pressure – dipolar excitation sin wave
  - ►collision free ion isolation, ECD, EID
  - ►fast thermalization

Omnitrap Ion Activation Network



Extensions

HCD in omni ✓

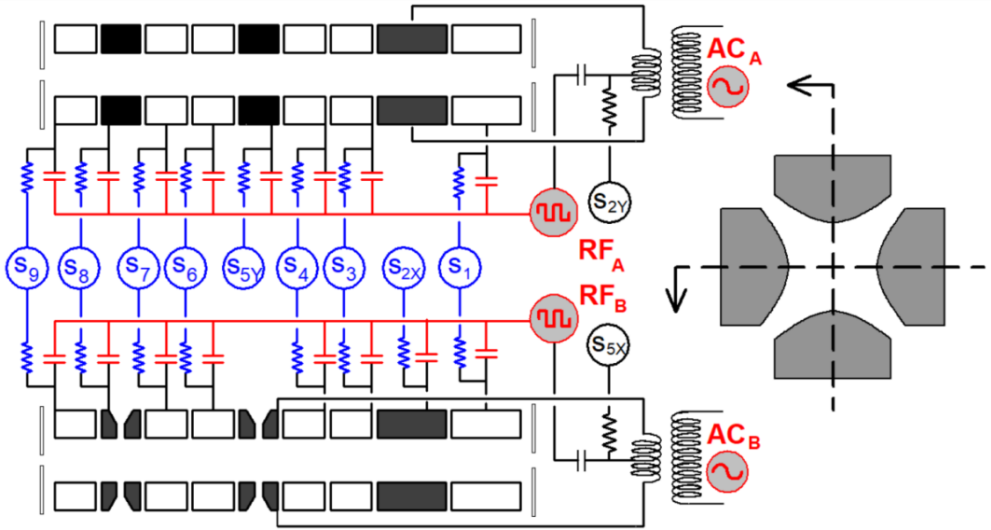
CA ExD ✓

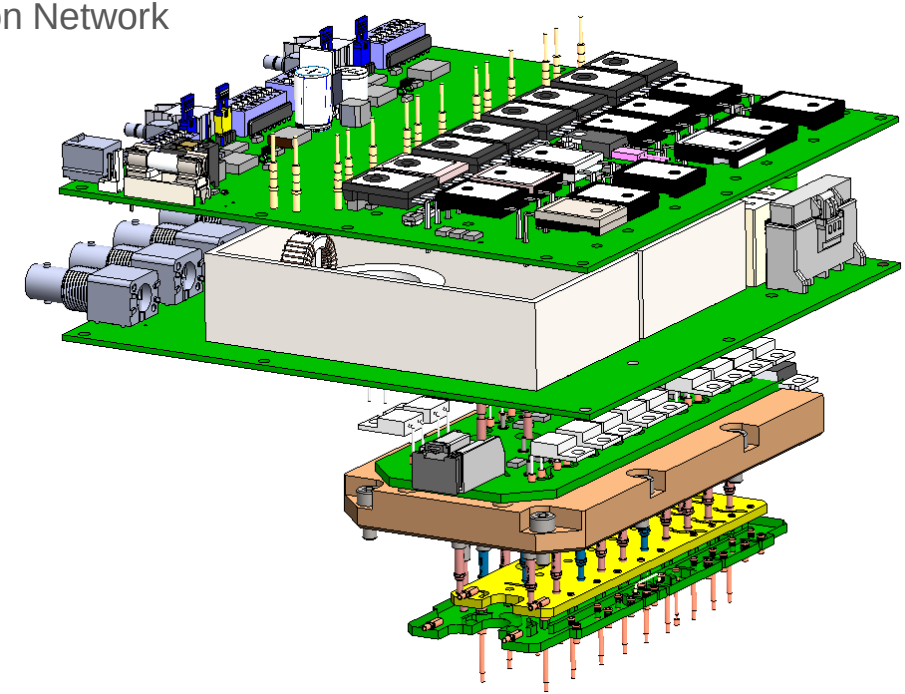
Hyperthermal H

SID

⋮

External RC Distribution Network



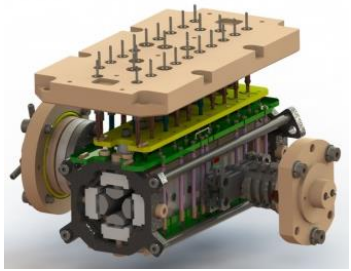


26 individual signals

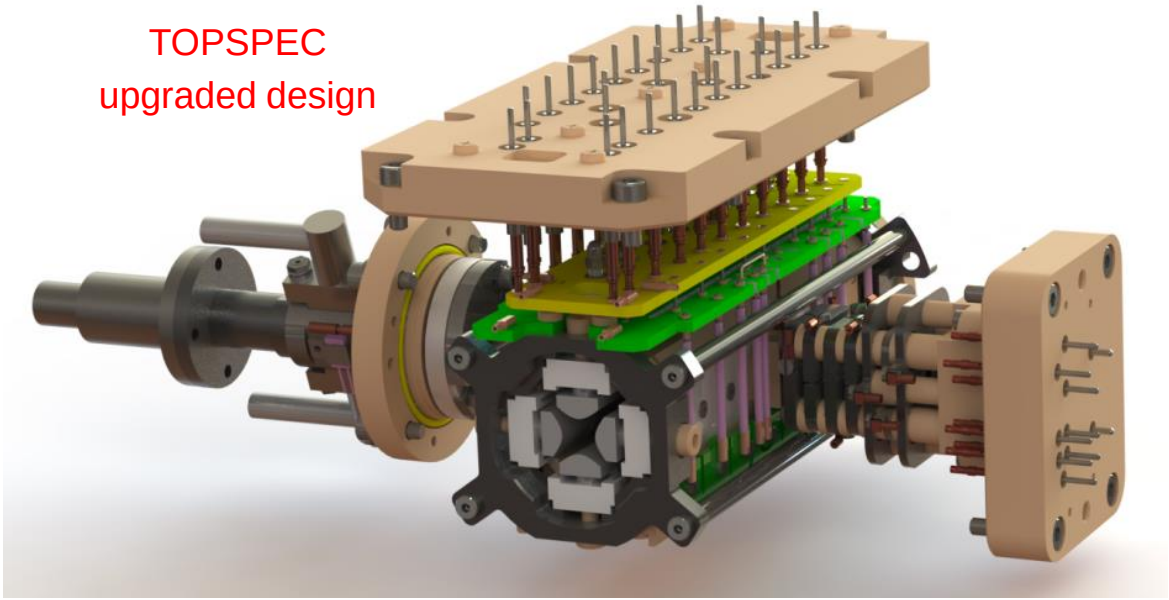
applied to trap electrodes

WP1 – Omnitrap & IMS development and testing

T1.1 – mech design & pulsed EI source



TOPSPEC
upgraded design



Omnitrap v2

$250V_{0p}$ Rectangular RF Generator ✓
Ext RC Distribution Network ✓
RF Amplitude Ctrl ✓

Sweep Isolation Resolution (83ms - 12.5MHz) ✓
RF Duty Cycle Isolation (35% @ 1MHz) ✓

Phase-Coherent Frequency Transitions ✓

Dipolar Excitation in Q5 (ECD-CID) ✓

Pulsed Electron Source (v2) ✓

Thermal (v3) & Hyperthermal H atom guns (v1)

Ion mobility drift cell / MSn-IMSn (v2)

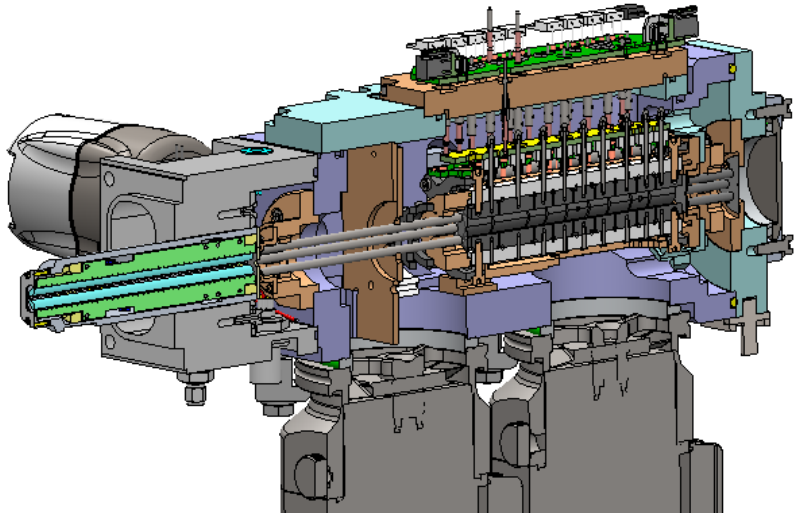
T1.1 – mech design & pulsed EI source

QExactive HF mass spectrometer used for developing and debugging the omnitrap platform in Athens

Items evaluated experimentally and redesigned for further testing :

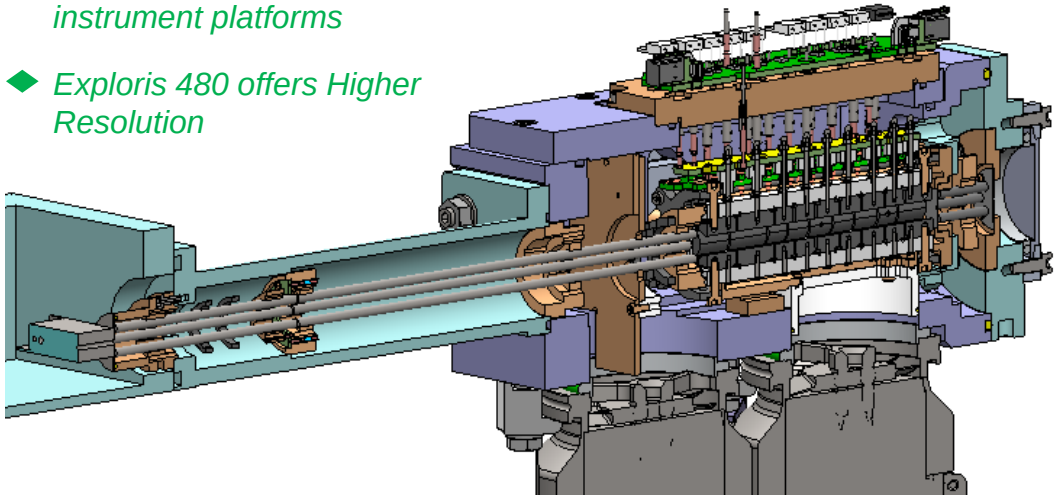
Electron source (v2)
Thermal H• source (v3)
Hyperthermal H• source (v1)
Ion Mobility Drift Cell (v2)
$400V_{0p}$ rect RF generator (v2)
FPGA (v2)

Omnitrap QExactive™ HF



Omnitrap Exploris™ 480

- *Target both existing and new instrument platforms*
- *Exploris 480 offers Higher Resolution*

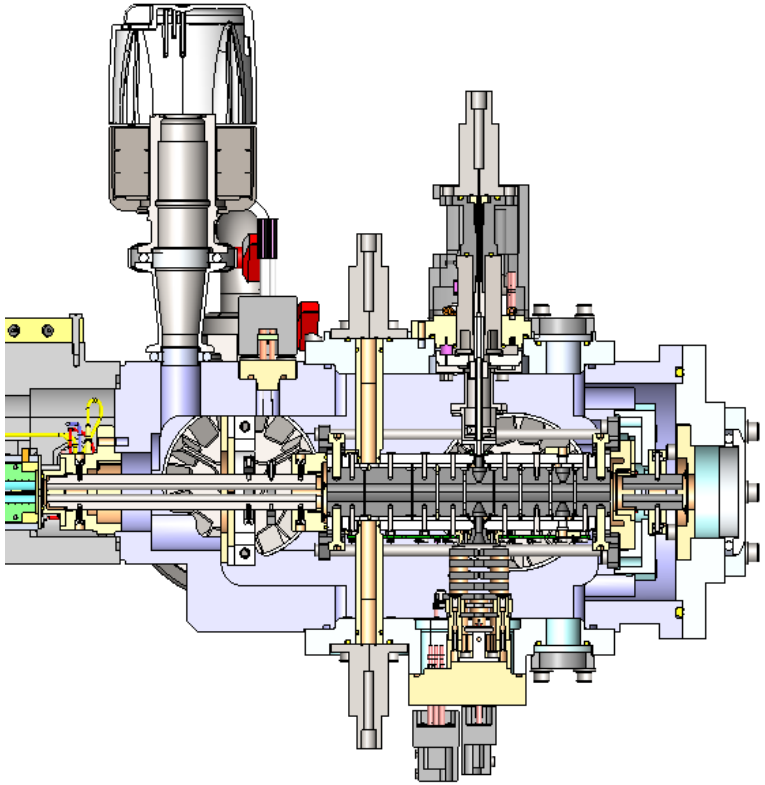


New features: Upgraded vacuum chamber design for enhanced pumping speed in RF hex bridge

New H_2 screen for minimizing gas load to orbitrap mass analyzer

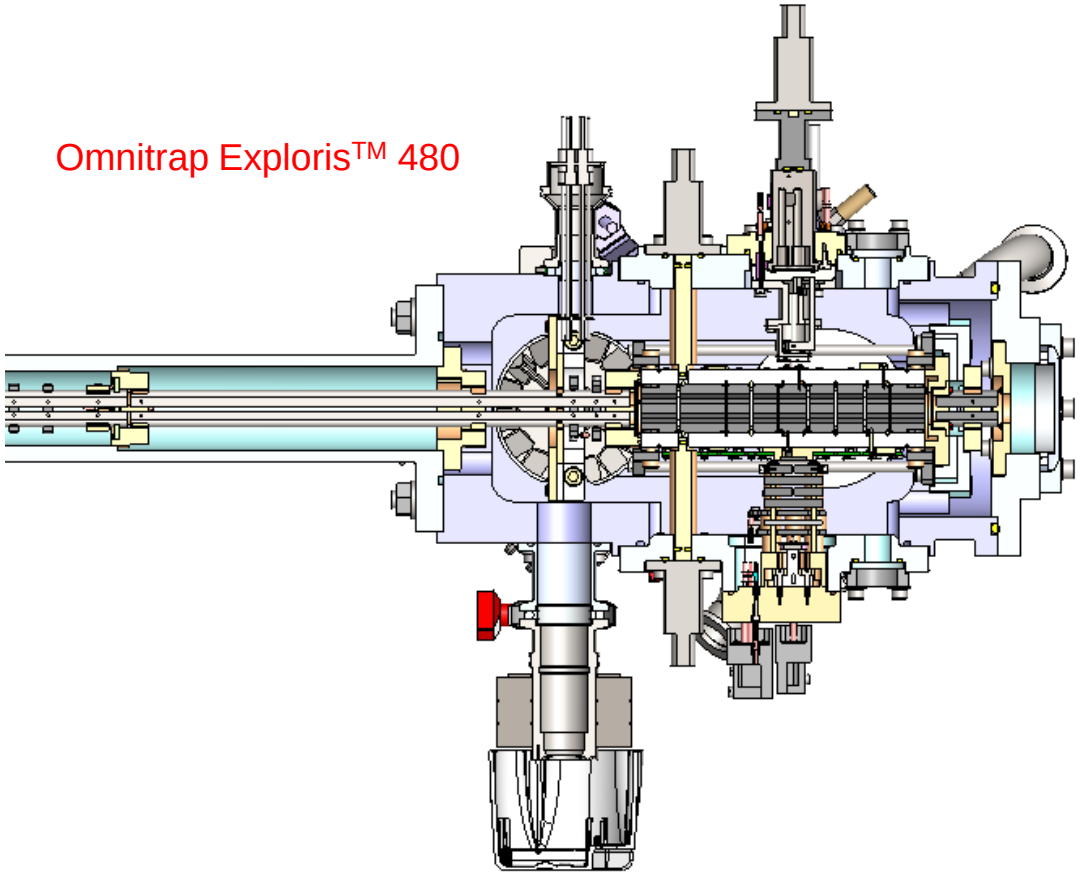
New multipin feedthru for driving segmented extended-length RF hex bridge (Exploris config)

T1.1 – mech design & pulsed EI source

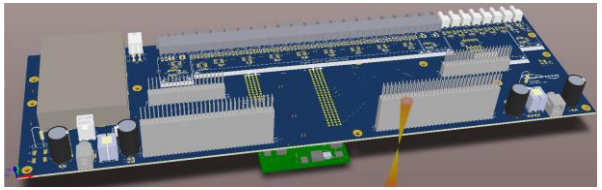


Omnitrap QExactive™ HF

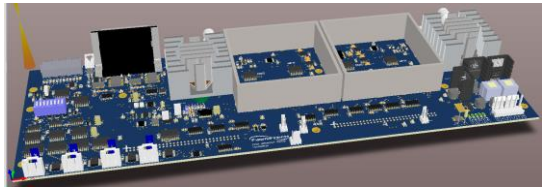
Omnitrap Exploris™ 480



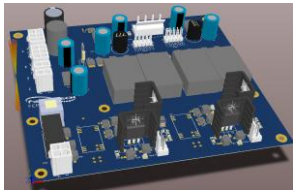
FPGA Board 1/3



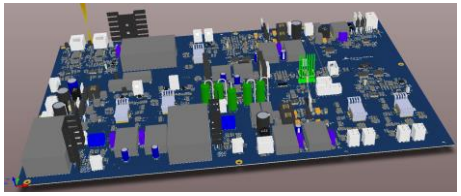
FPGA Board 2/3



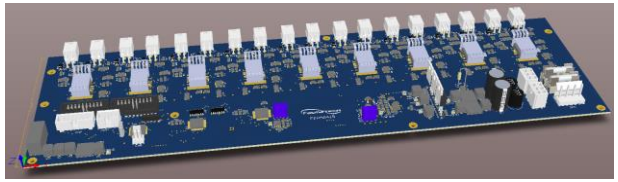
FPGA Board 3/3

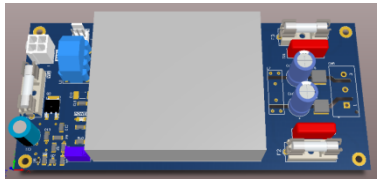


Electron Source Ctrl Unit

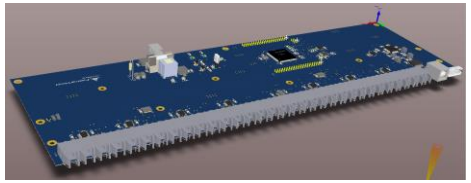


Multilevel DC Switch Unit & Rails Board

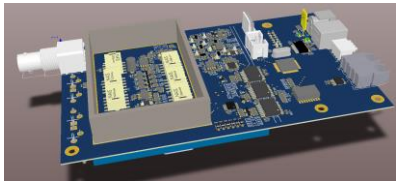




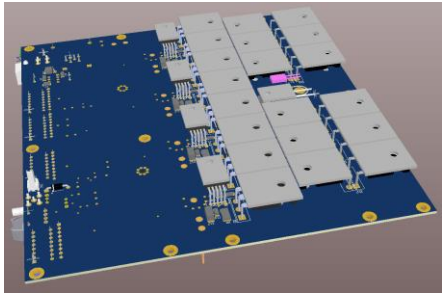
Uart Hub Communication Board

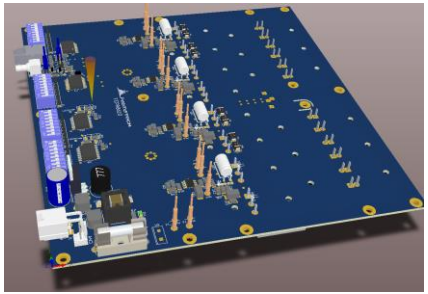


Electrometer

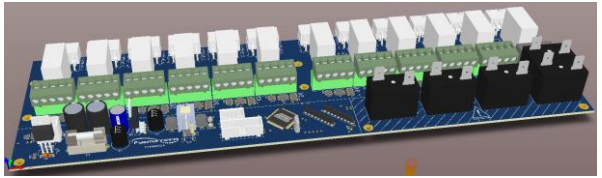


Rectangular RF Unit

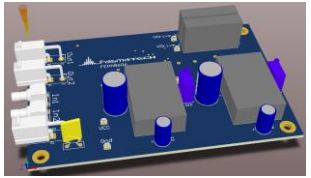




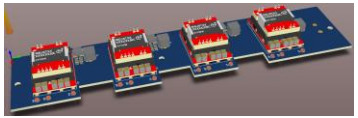
Power Board

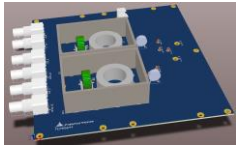


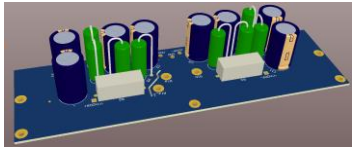
Pulse Valve



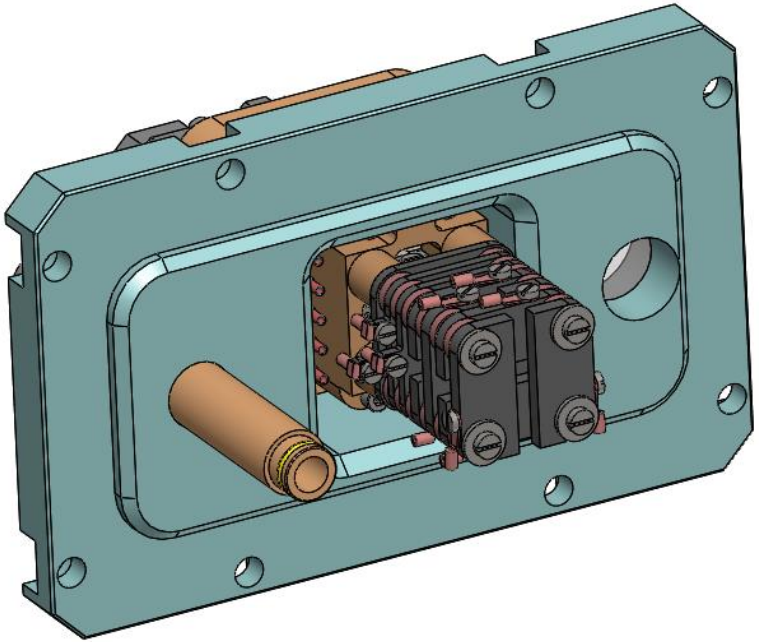
Rectangular RF Cards

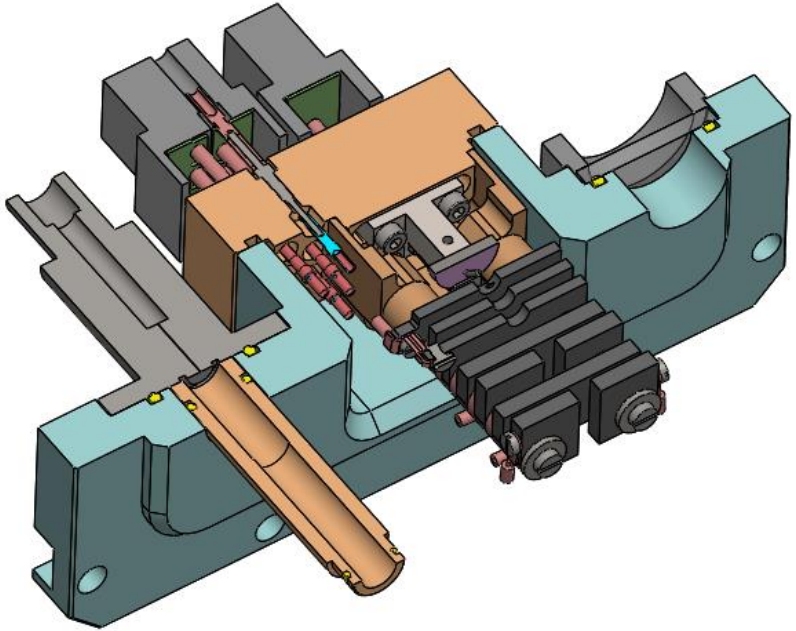






T1.1 – mech design & pulsed EI source

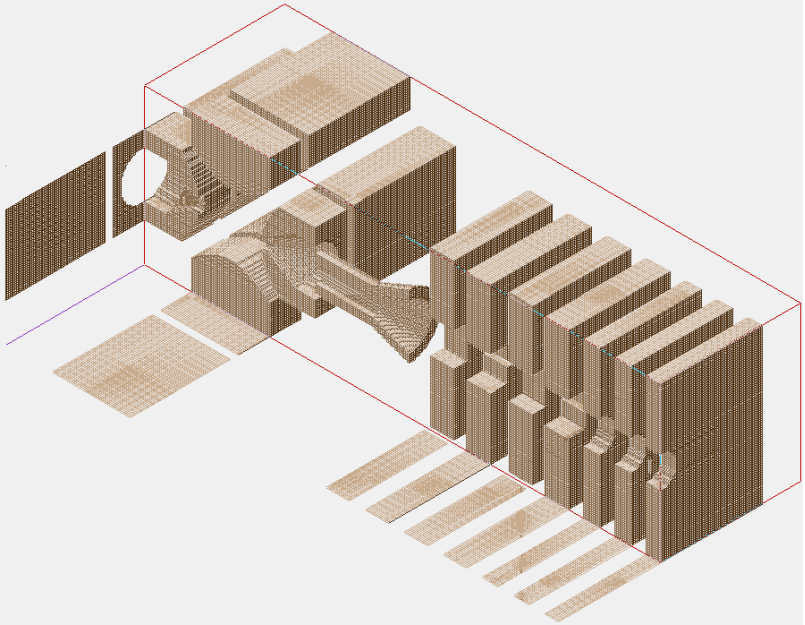


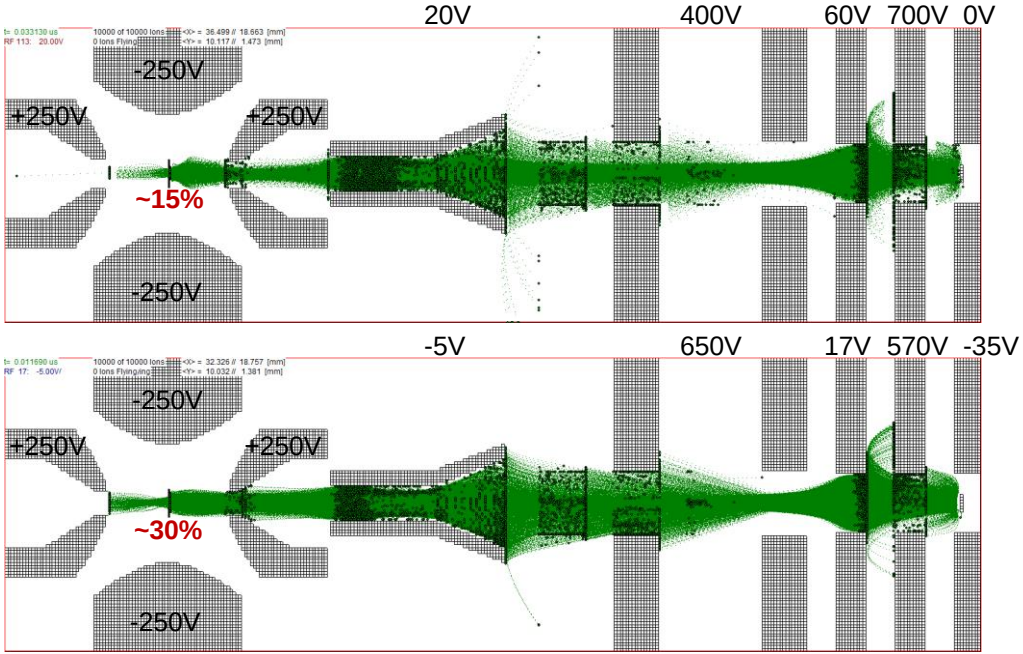


new electron source design with two-stage deflectors in both vertical and horizontal directions

new electronics for pulsed operation at high voltage

T1.1 – mech design & pulsed EI source



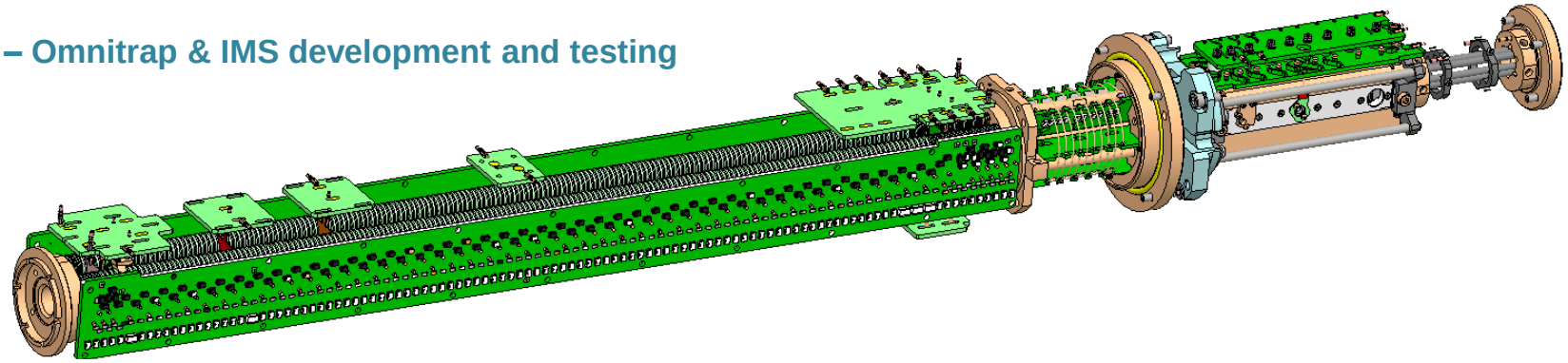


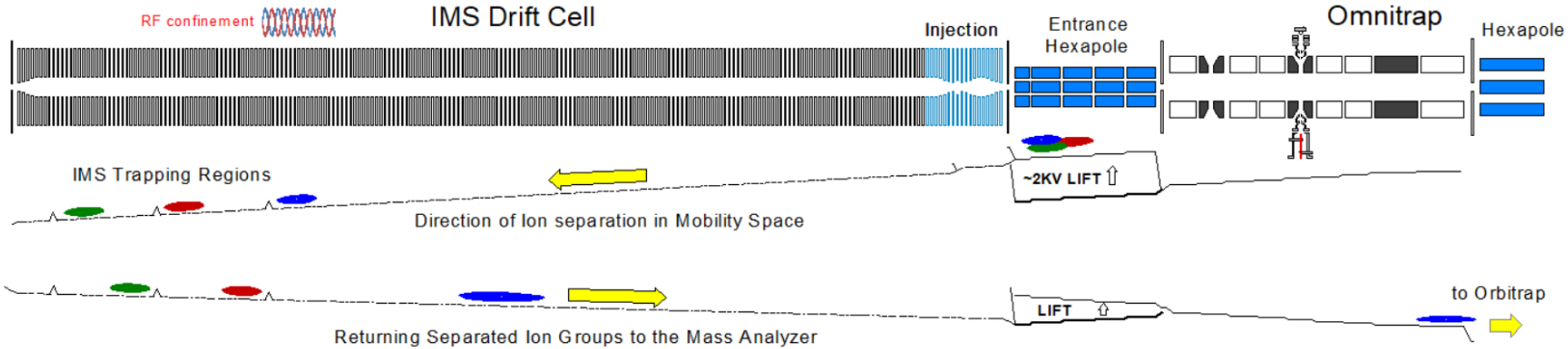
electron optics simulations are performed for dense electron beams

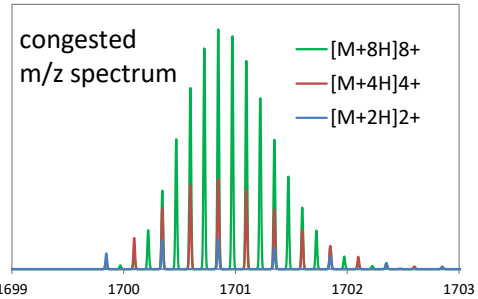
space charge effects are taken into account for an electron current of 40µA

electrode geometry was optimized for focusing electrons over an extended kinetic energy range

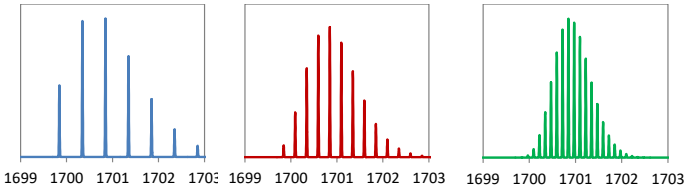
WP1 – Omnitrap & IMS development and testing





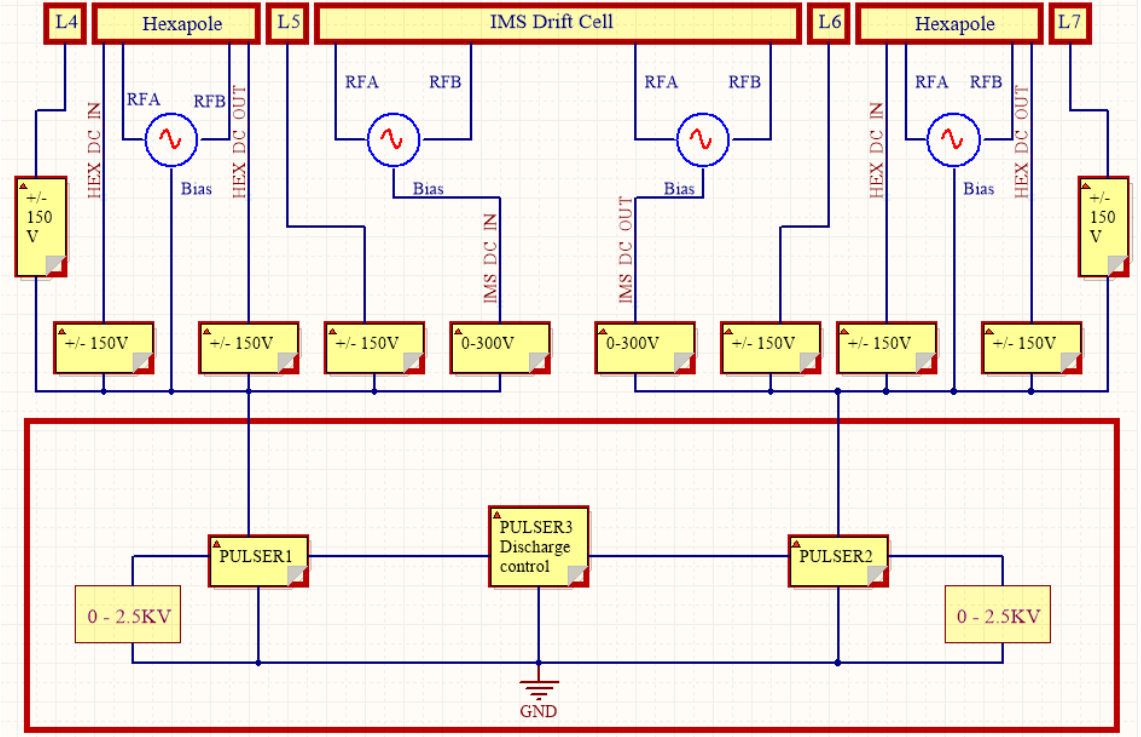


mobility separated isotopic distributions

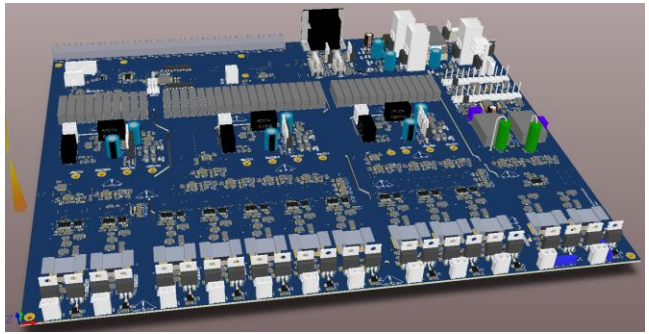


Top-Down
Spectral Complexity
Reduction

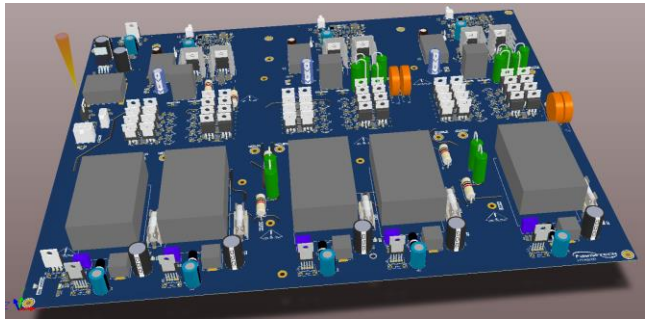
T1.1 – mech design & pulsed EI source



IMS Main Ctrl Board



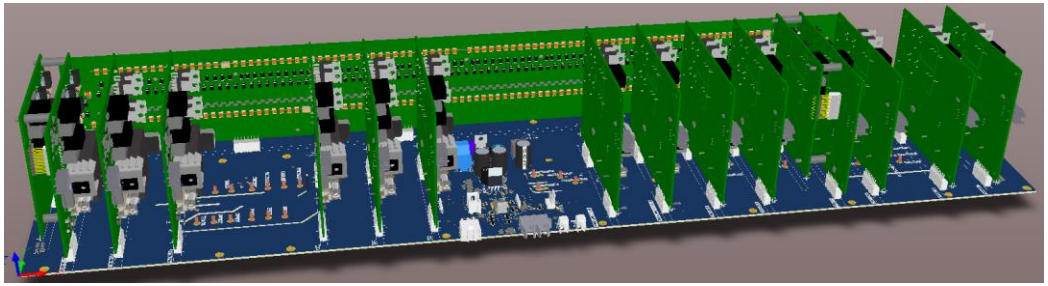
IMS HV Pulsing Board



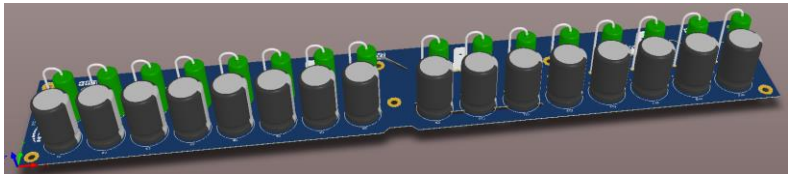
WP1 – Omnitrap & IMS development and testing

T1.1 – mech design & pulsed EI source

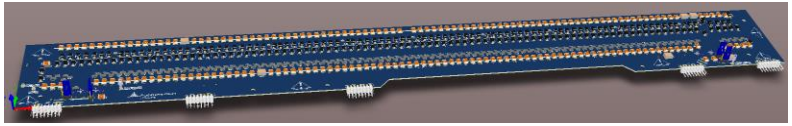
IMS Switch Board & Floating Switch Cards



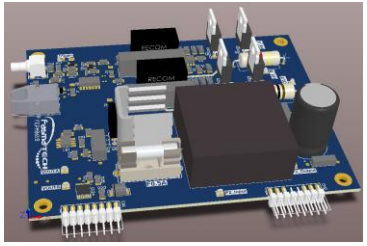
Capacitor Bank



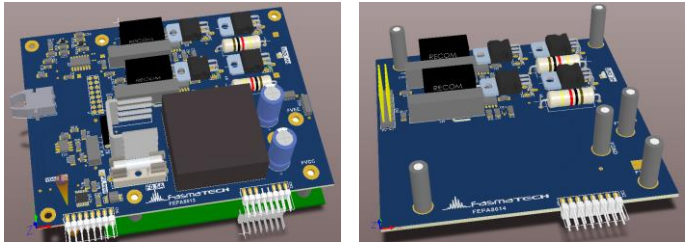
BN Gate Resistor Chain



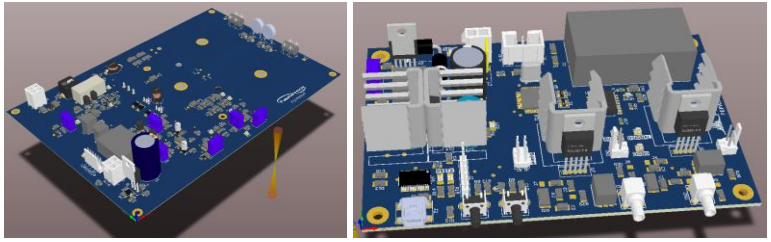
Bipolar Switch Cards



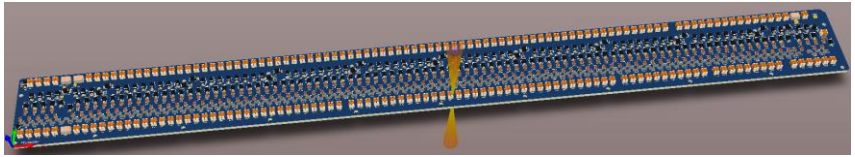
Bipolar Switch Cards for BN Gate



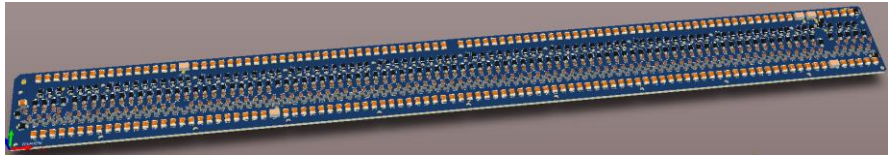
RF PSU & RF synch Unit

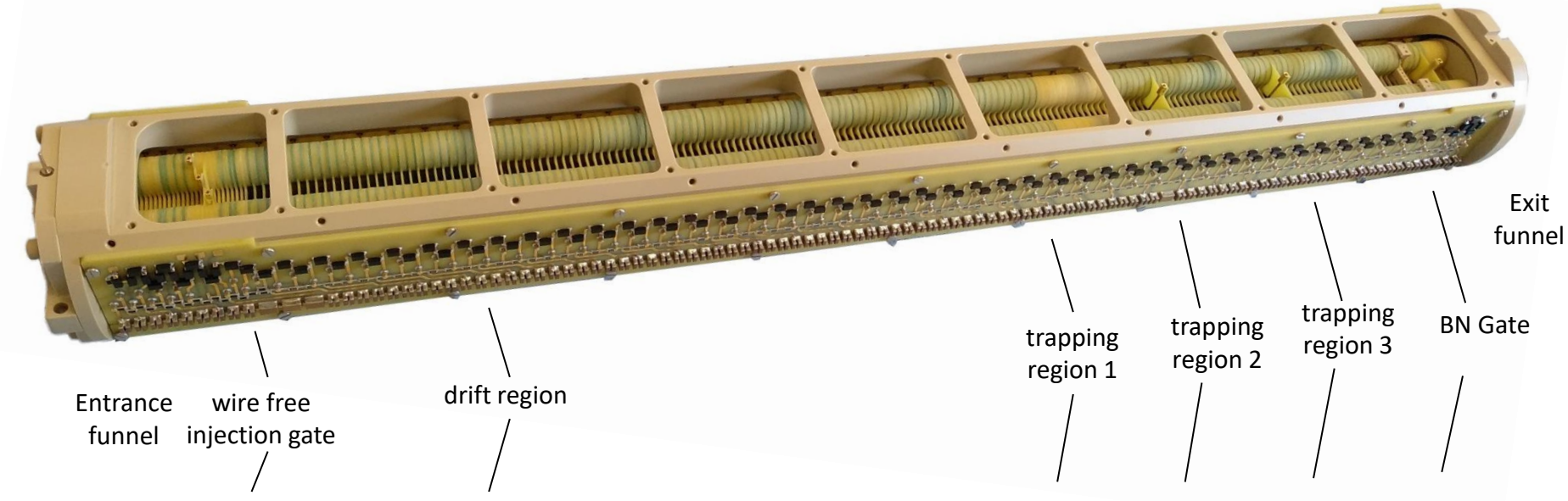


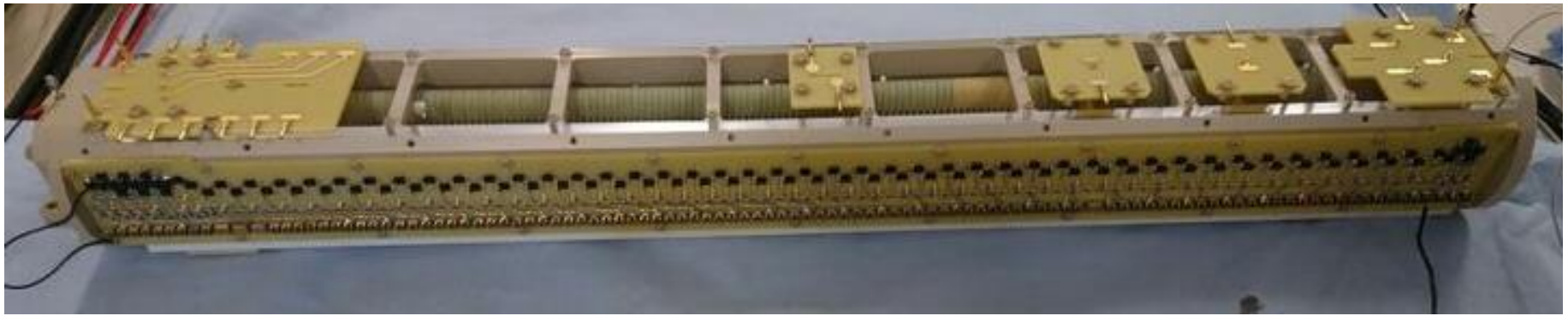
IMS Left RF-DC Distribution Unit



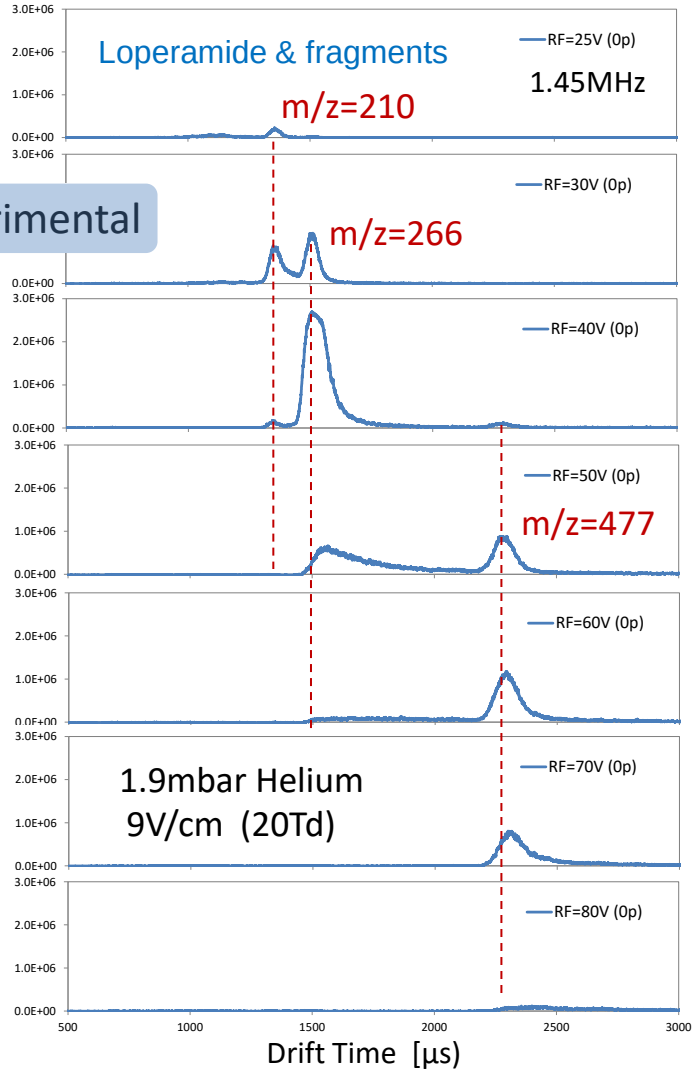
IMS Right RF-DC Distribution Unit



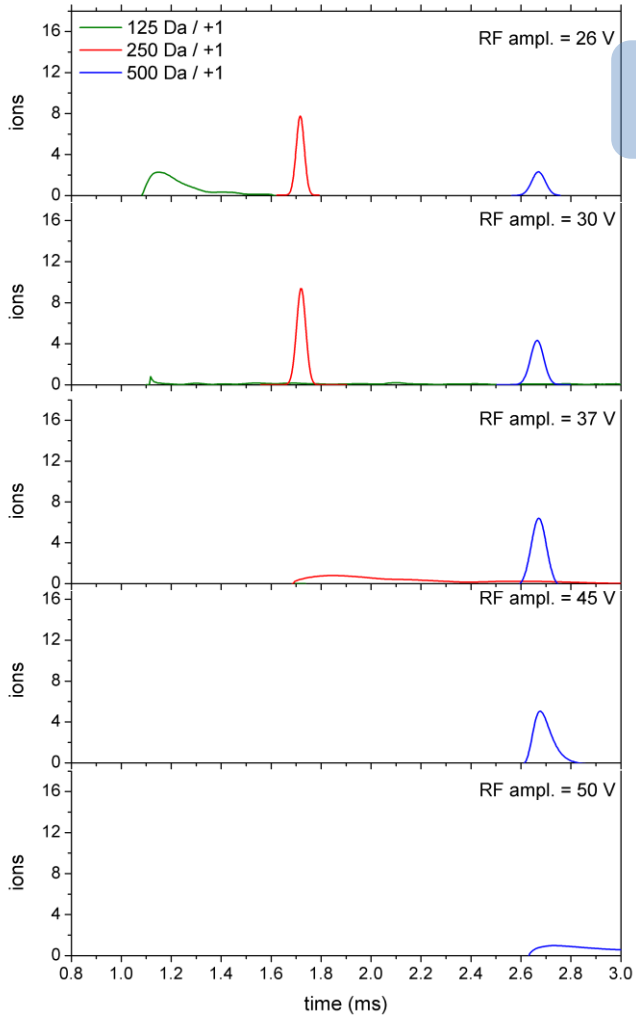

Entrance funnel
wire free injection gate
drift region
trapping region 1
trapping region 2
trapping region 3
BN Gate
Exit funnel



Experimental

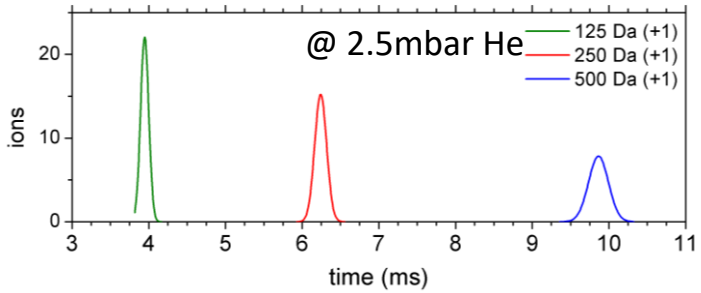


Ion Optics Simulations

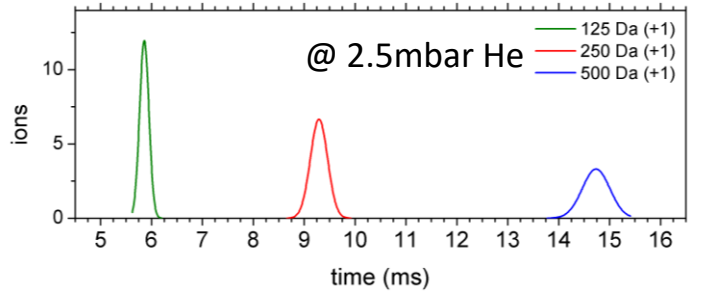


Variable DC Grad Across Drift Cell and Exit Funnel

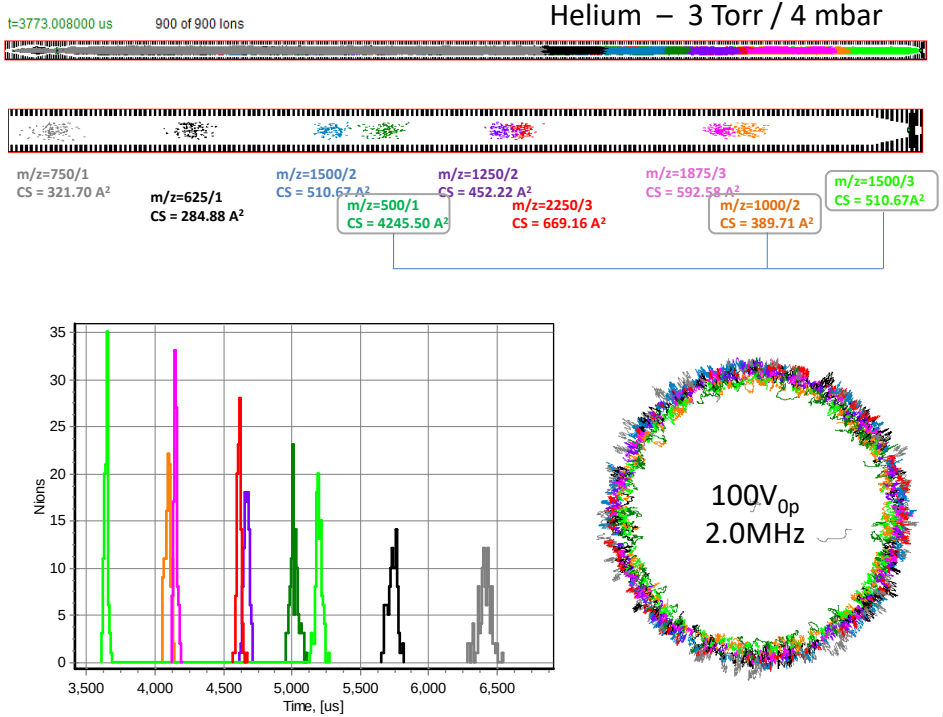
IM:300V - F:100V RF:100V_{0p} @ 1.5MHz 9.9 Td

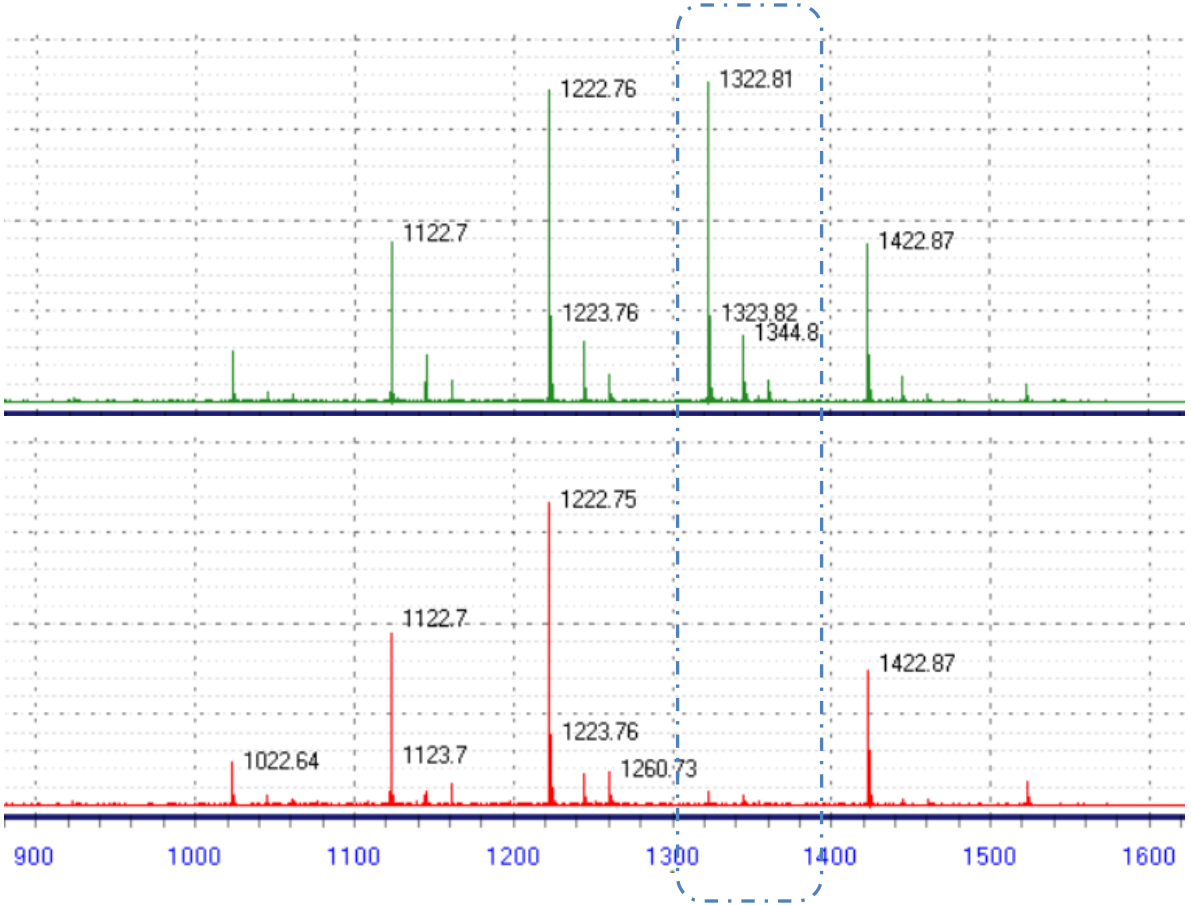


IM:200V - F:100V RF:100V_{0p} @ 1.5MHz 6.6 Td

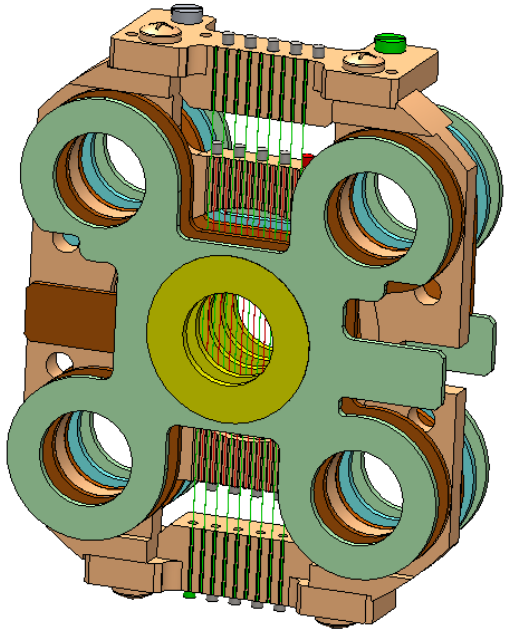


Mobility Separation of Ions with Coinciding m/z values



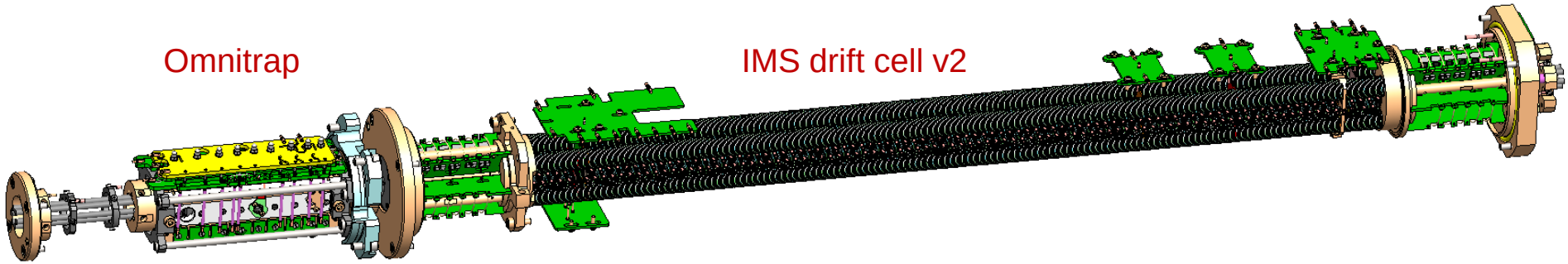


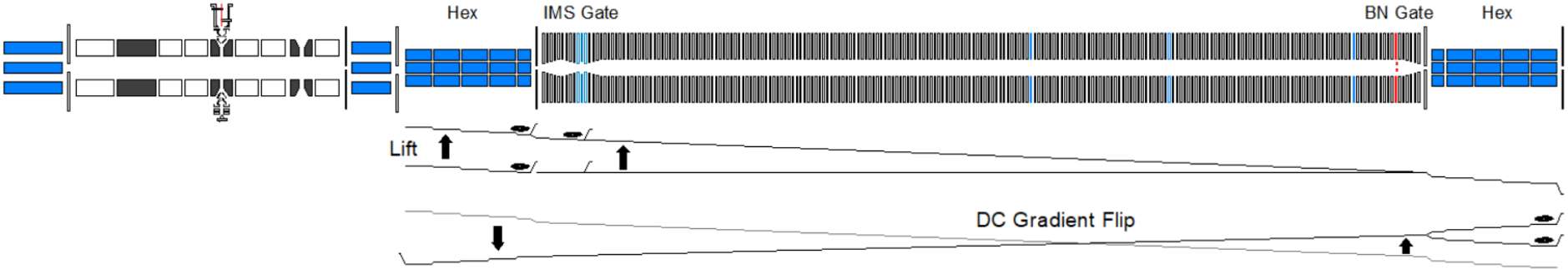
BN Gate Selection of Ion Bands

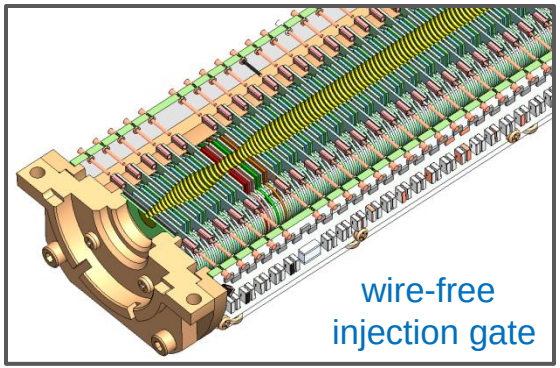


Omnitrap

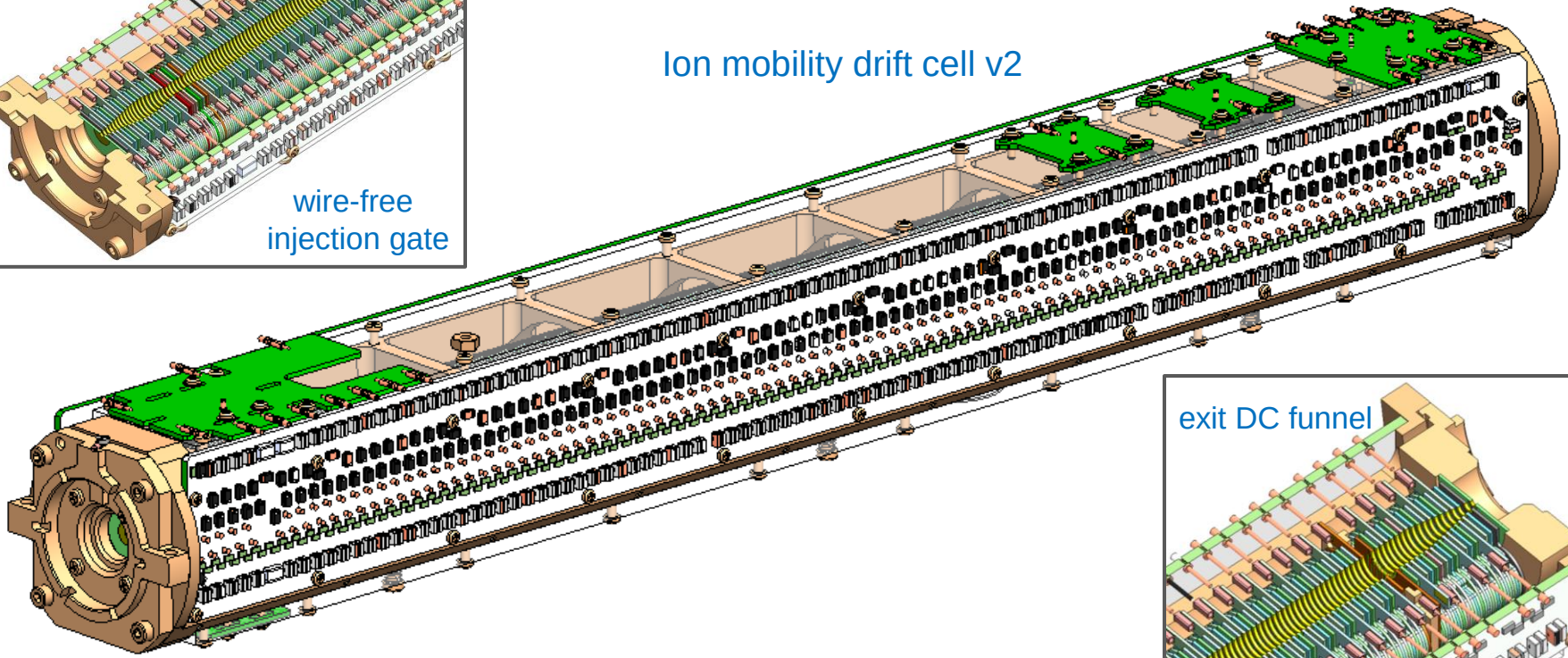
IMS drift cell v2

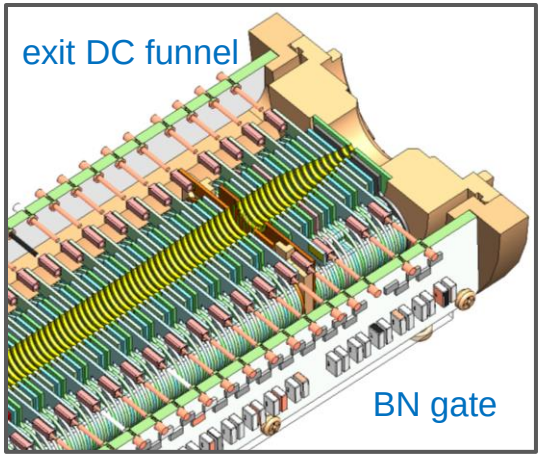




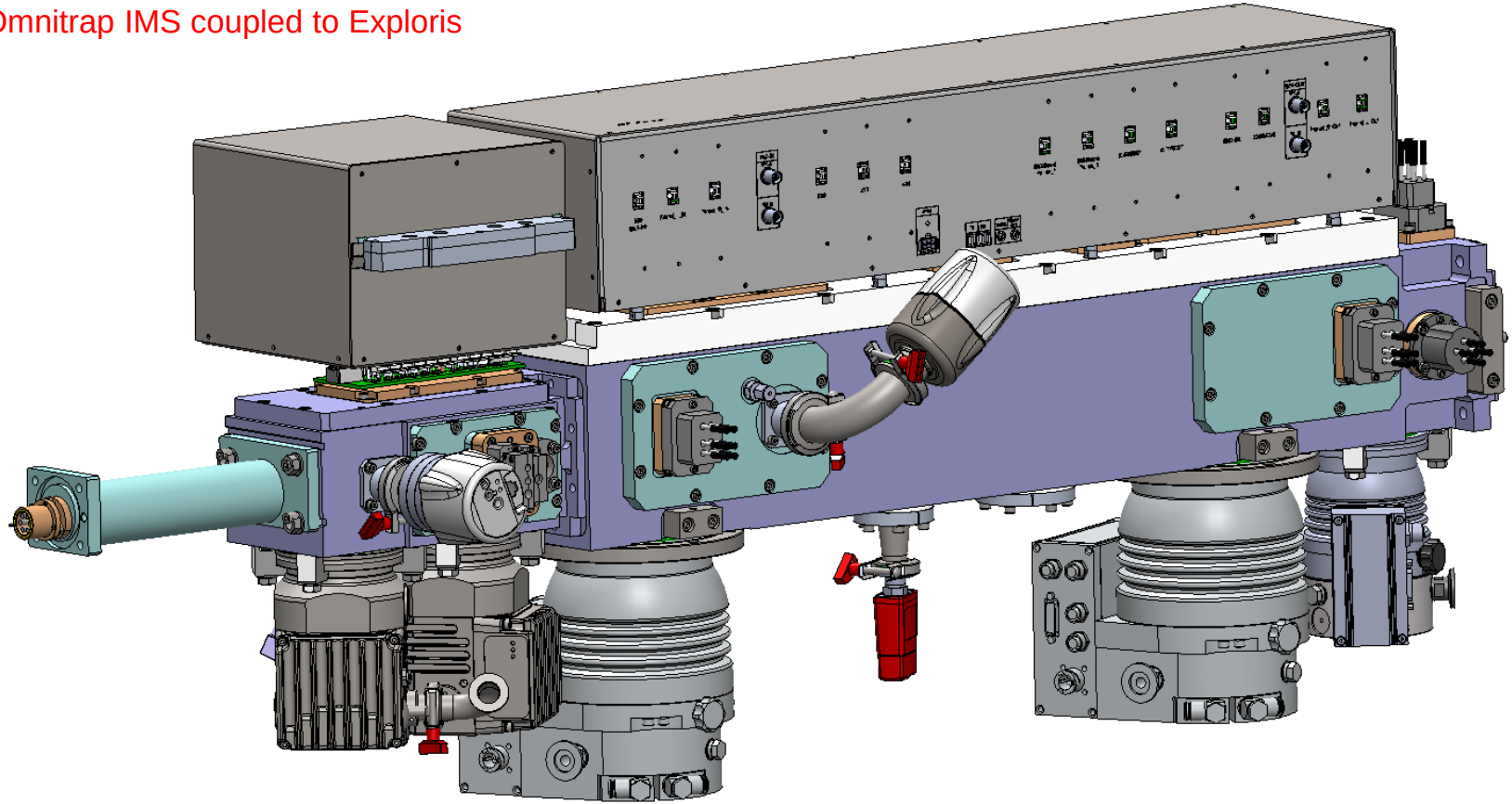


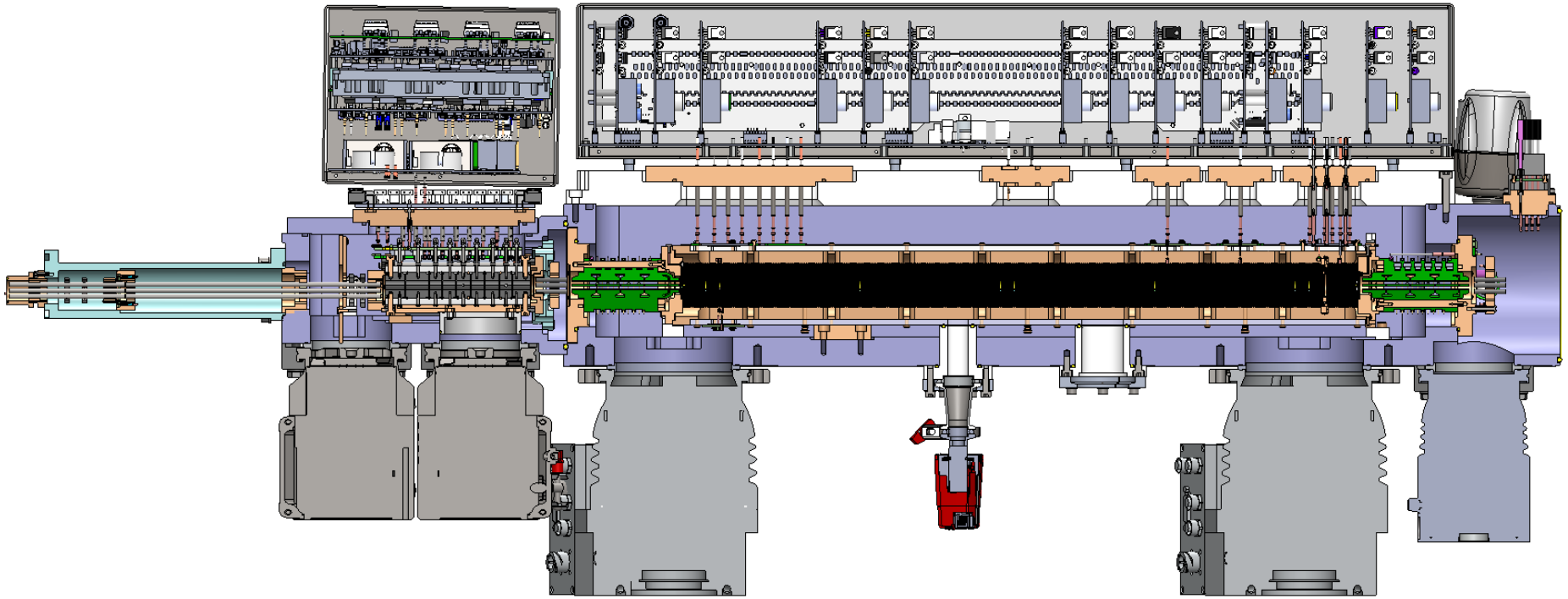
Ion mobility drift cell v2





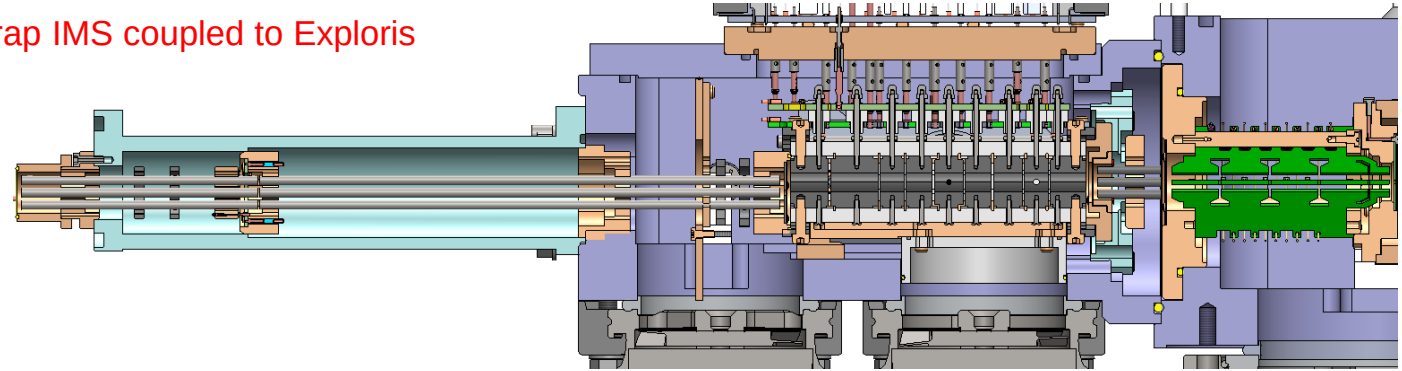
Omnitrap IMS coupled to Exploris

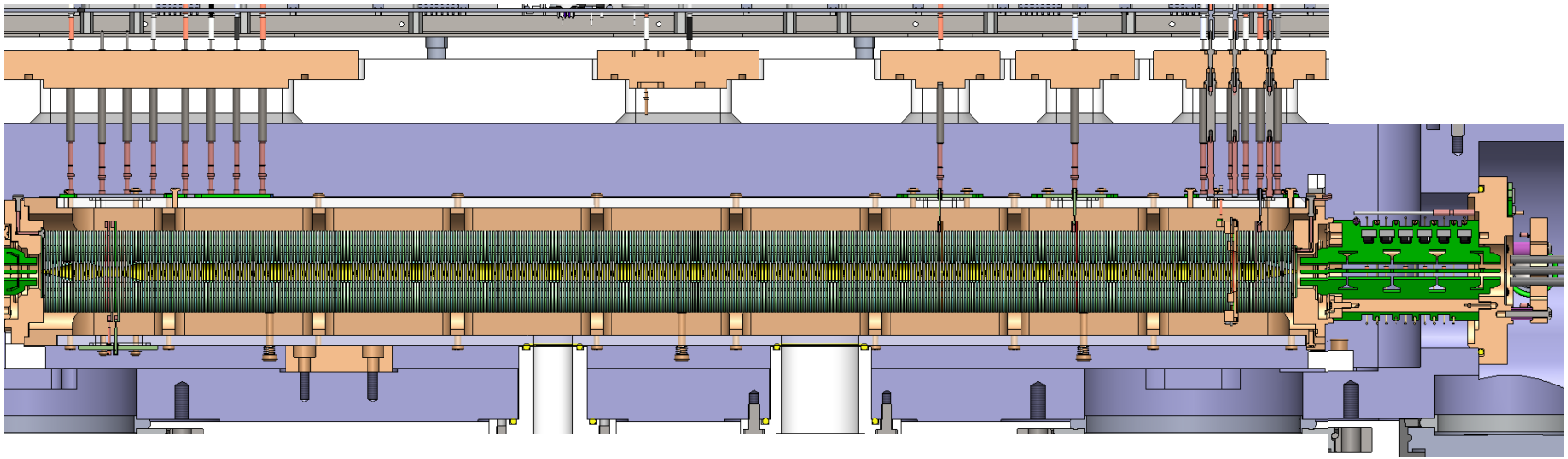




Omnitrap IMS coupled to Exploris

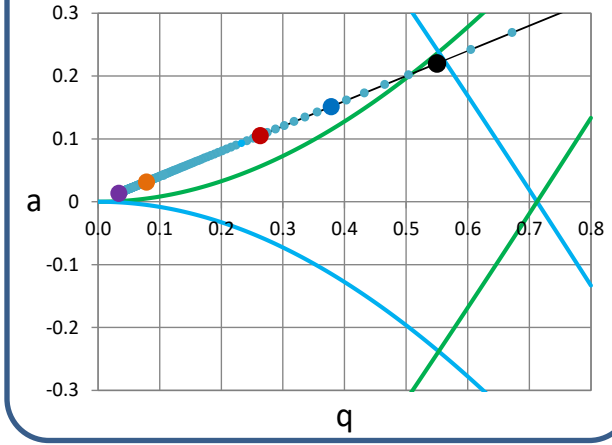
Omnitrap IMS coupled to Exploris



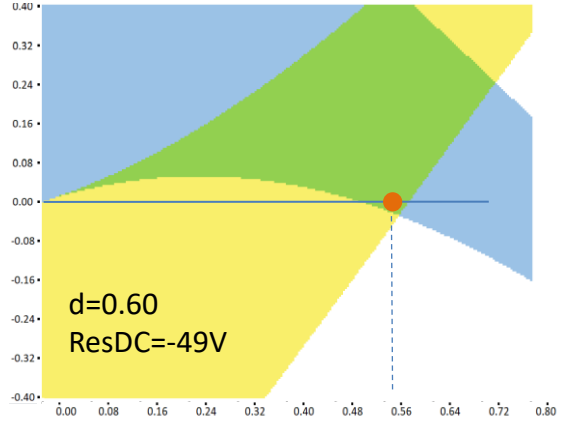


T1.2 – ion isolation simulation

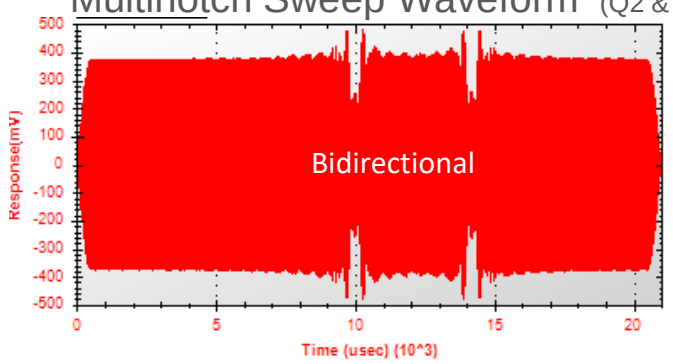
Resolving DC (Q2 & Q5)

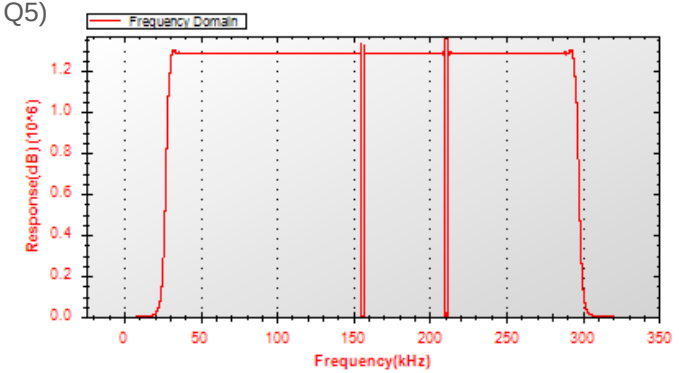


Duty Cycle (Q2 – Q9)



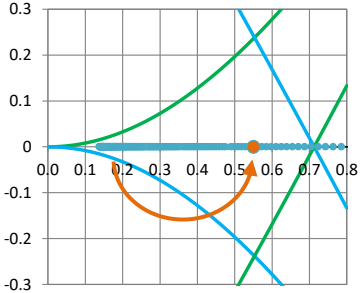
Multinotch Sweep Waveform (Q2 & Q5)



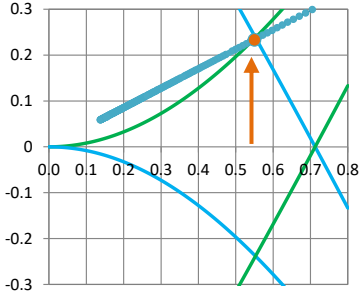


T1.2 – ion isolation simulation

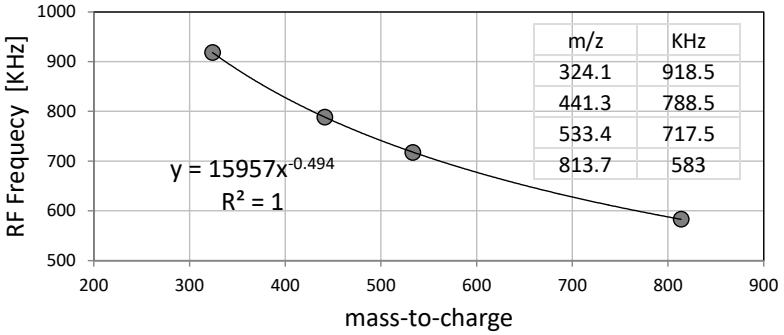
Resolving DC Isolation

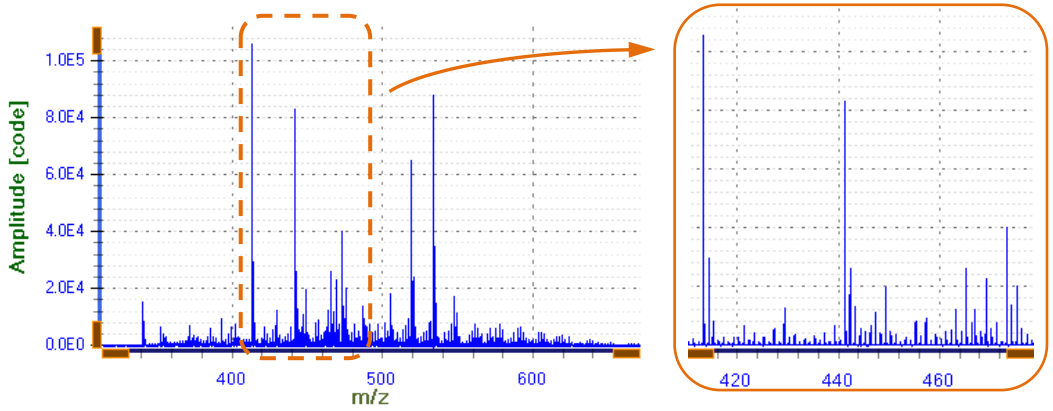


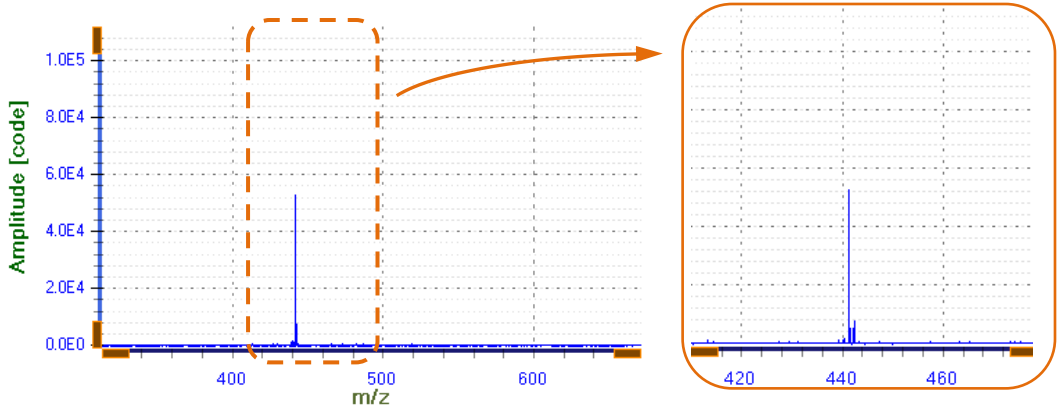
$250V_{0p}$
0.73MHz
DC_{res}=0V



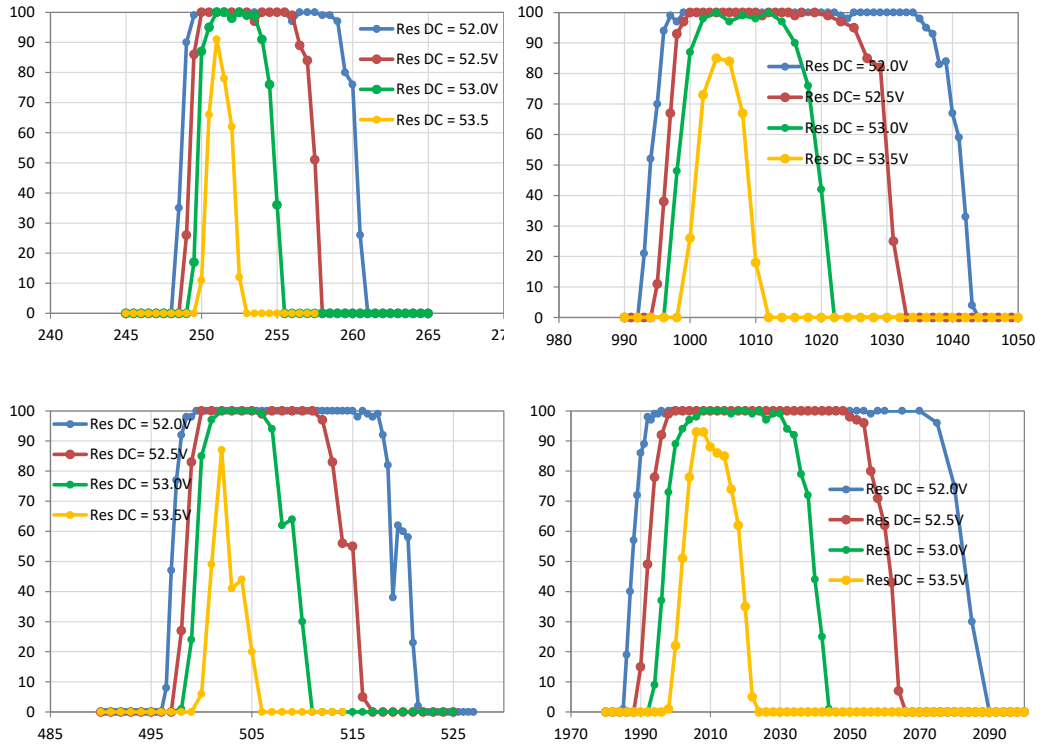
$250V_{0p}$
0.73MHz
DC_{res}=±53V

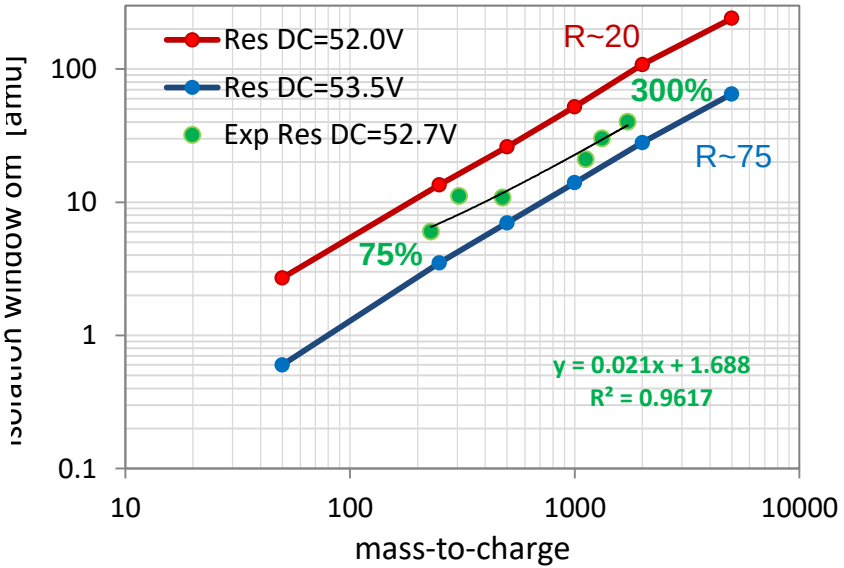






T1.2 – ion isolation simulation



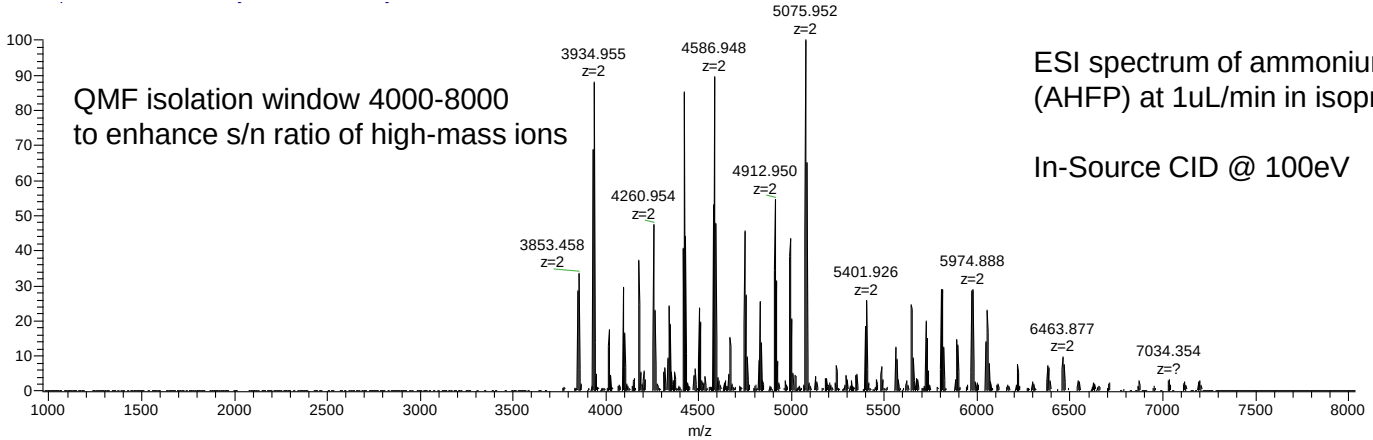


T1.2 – ion isolation simulation

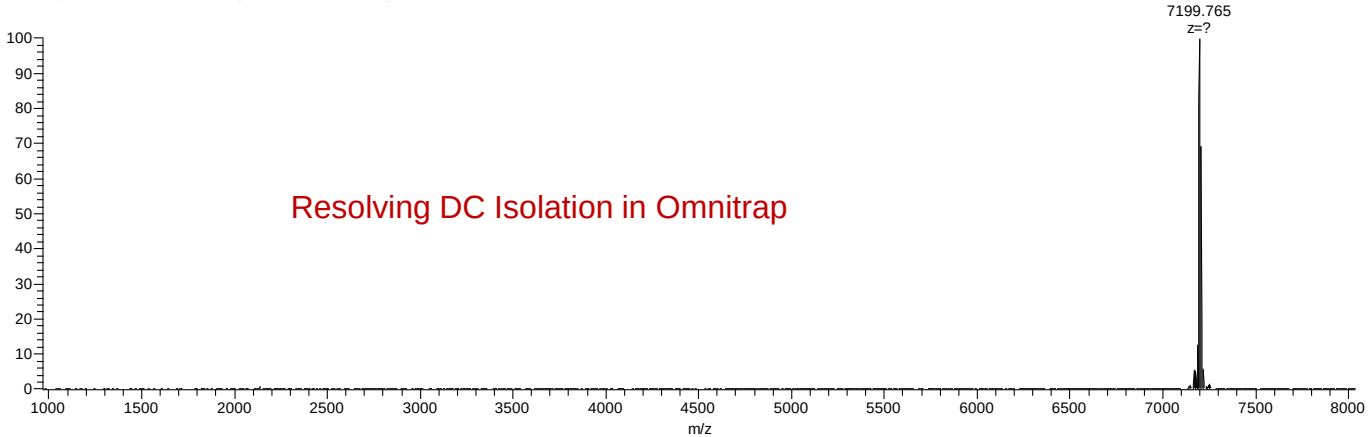
QMF isolation window 4000-8000
to enhance s/n ratio of high-mass ions

ESI spectrum of ammonium hexafluorophosphate (AHFP) at 1uL/min in isopropanol/water 50/50%

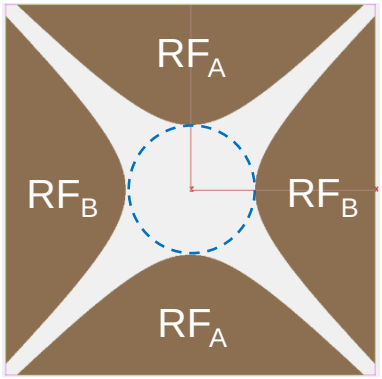
In-Source CID @ 100eV

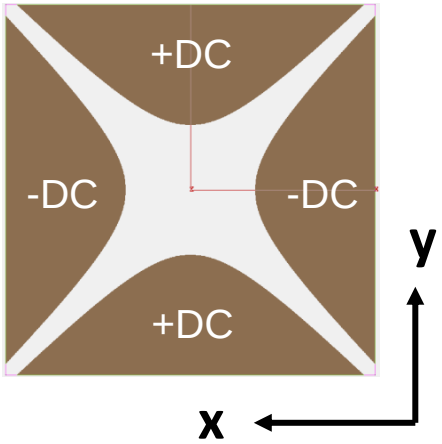


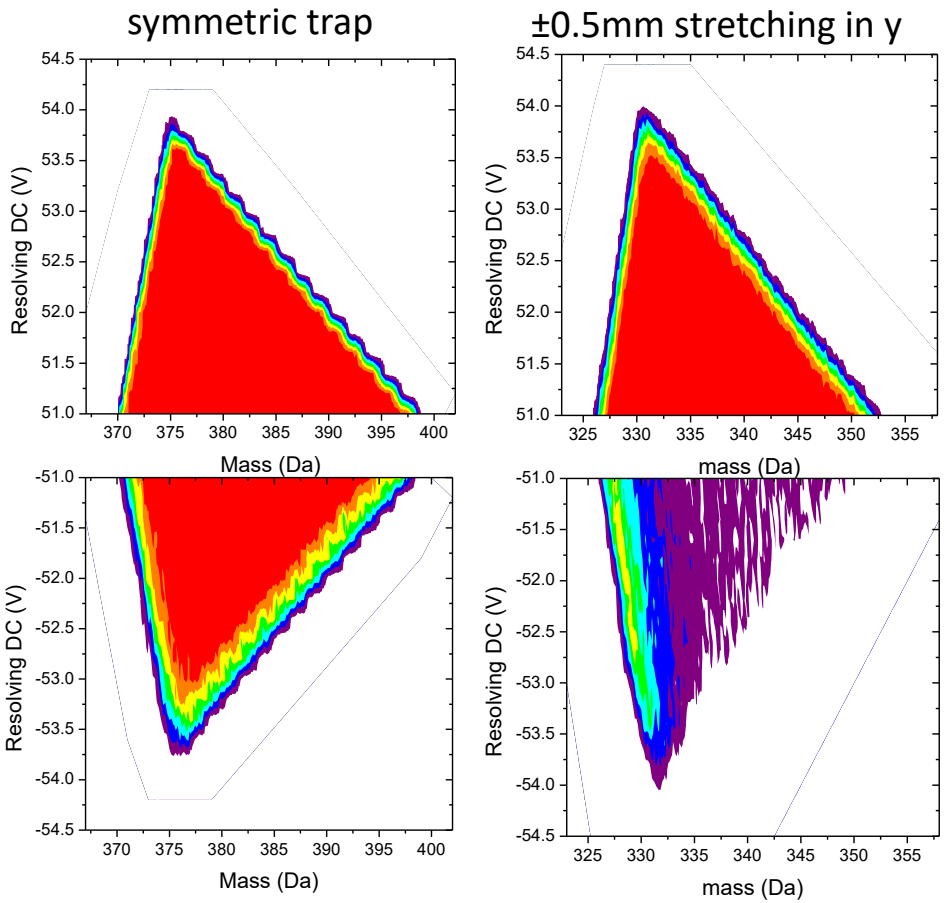
Resolving DC Isolation in Omnitrap



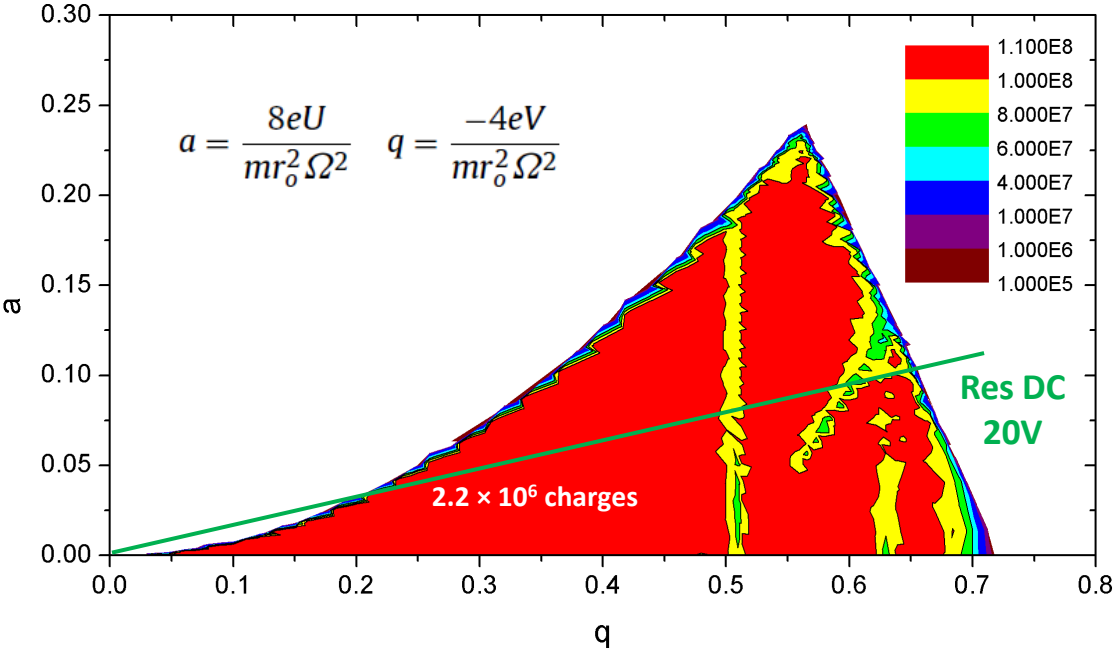
T1.2 – ion isolation simulation



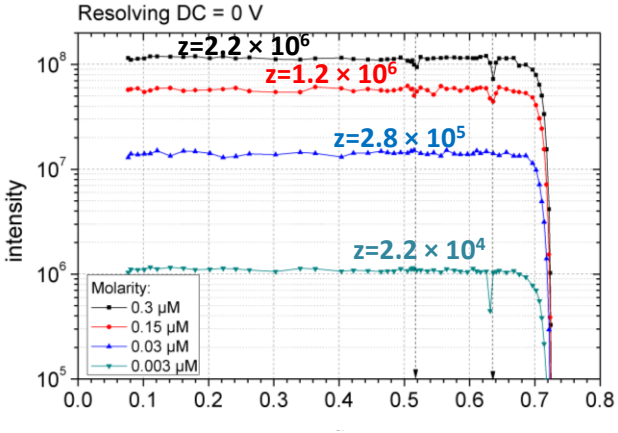


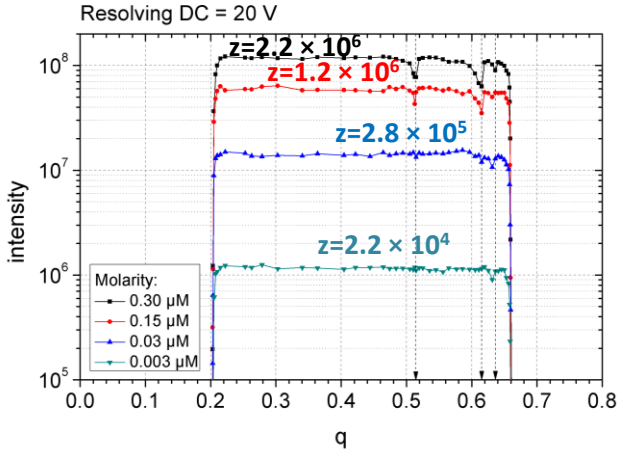


T1.2 – ion isolation simulation



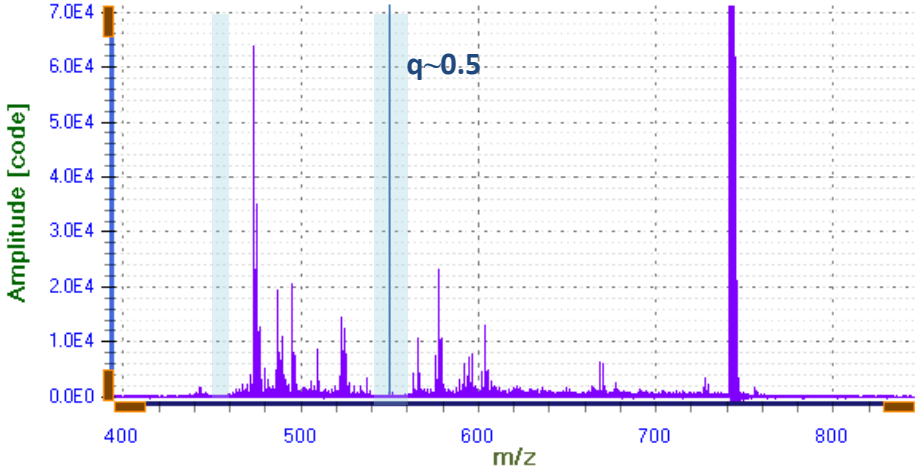
number of charges z =
= NL × Injection Time





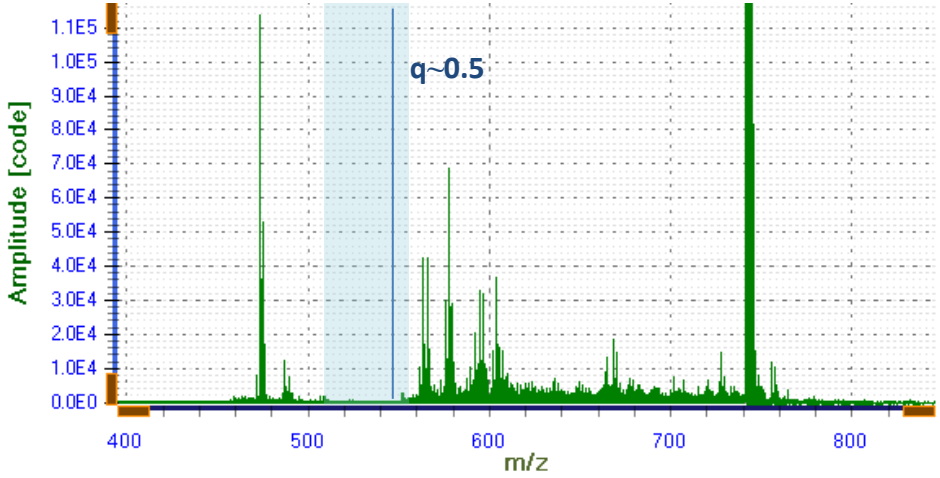
m/z-340.15

RF: 725KHz – 250V_{0p}
LMCO=388.5 r_o=4.1mm



25ms injection window

100pA – 15M charges

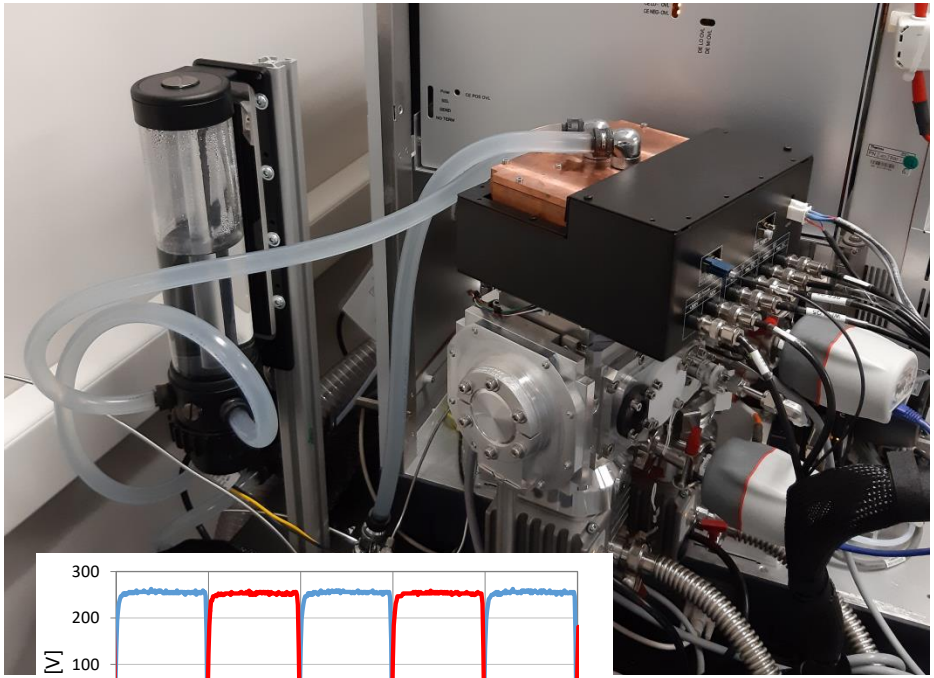


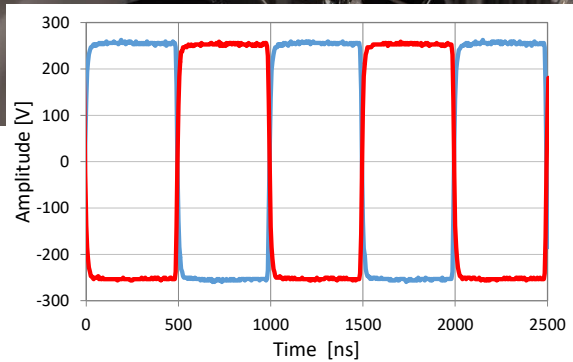
50ms injection window

100pA – 30M charges

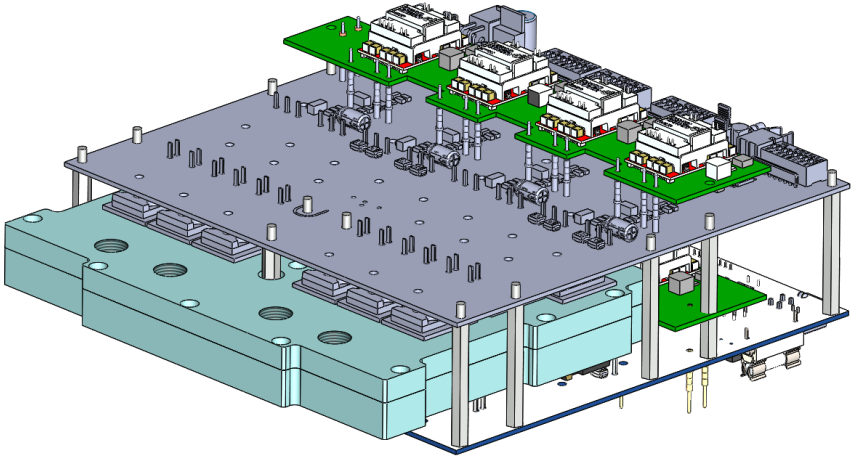
WP1 – Omnitrap & IMS development and testing

T1.3 – rect RF Generator



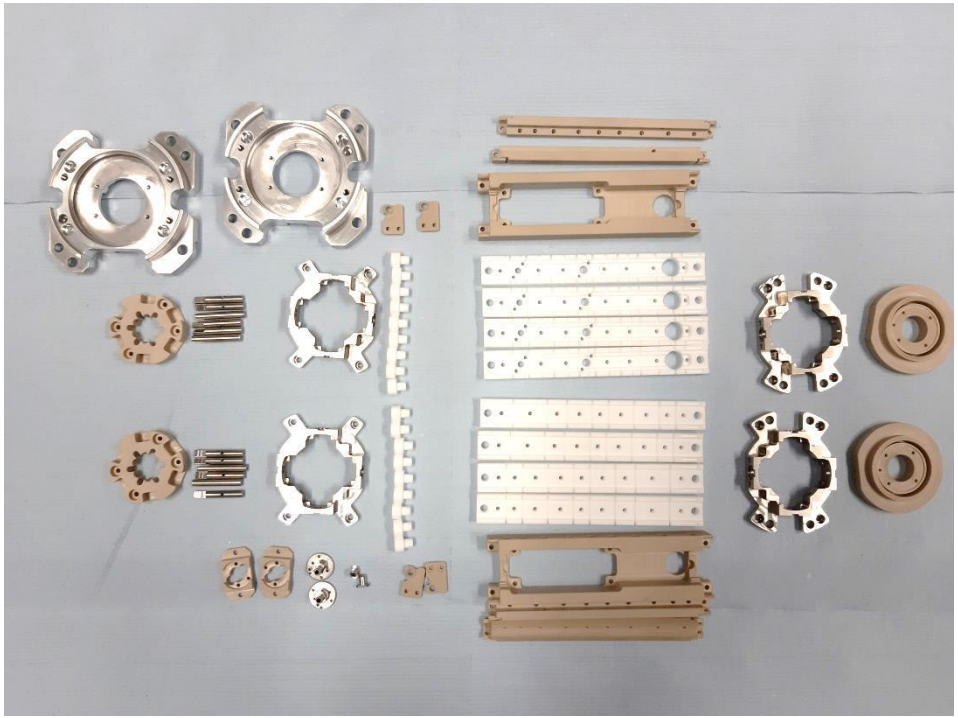


$250V_{0p}$
1000KHz

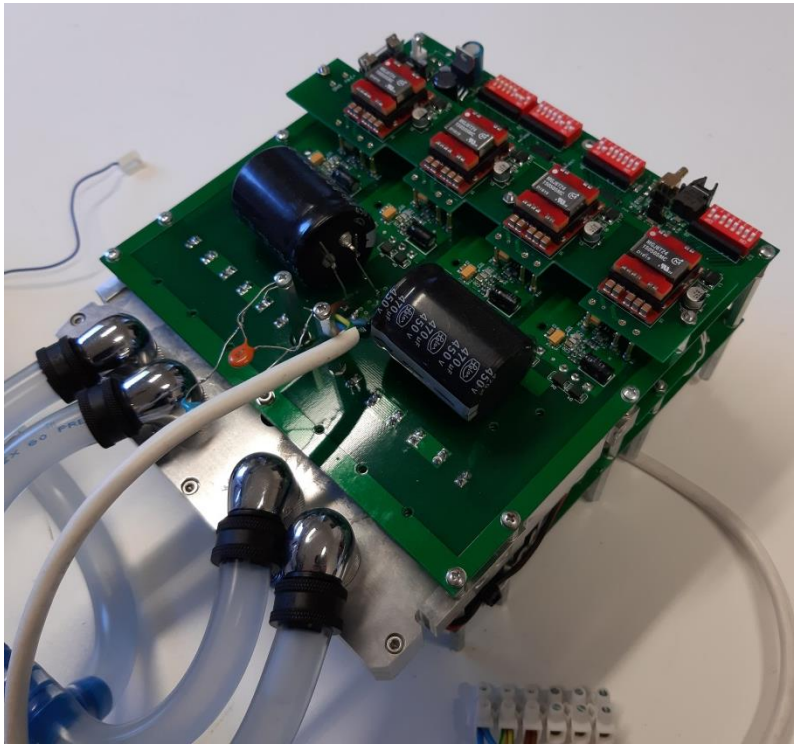


$400V_{0p}$ rectangular RF generator v3

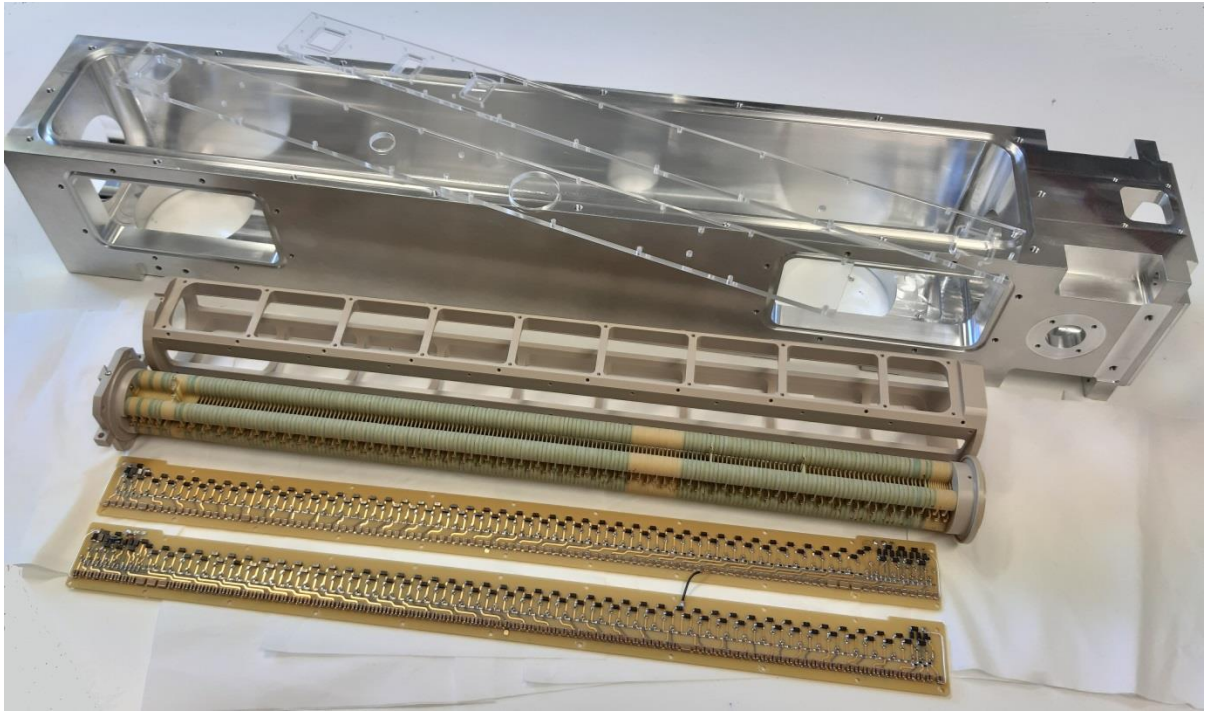
T1.4 – assembly of omni's & ims

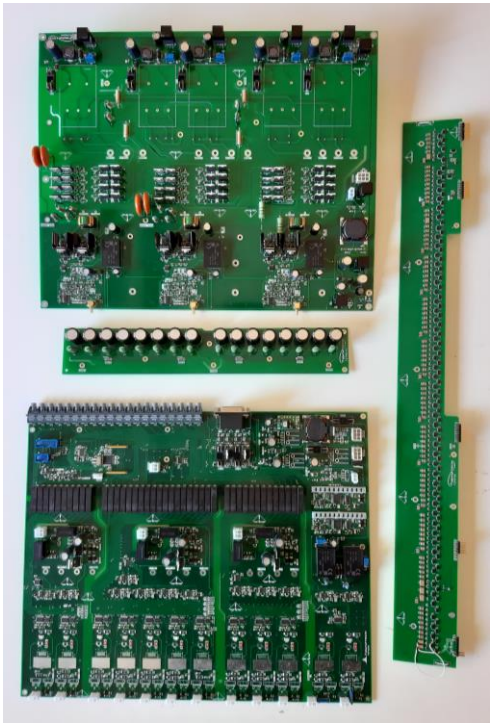


omnitrap parts received
assembly scheduled for February-end
ordering is still underway

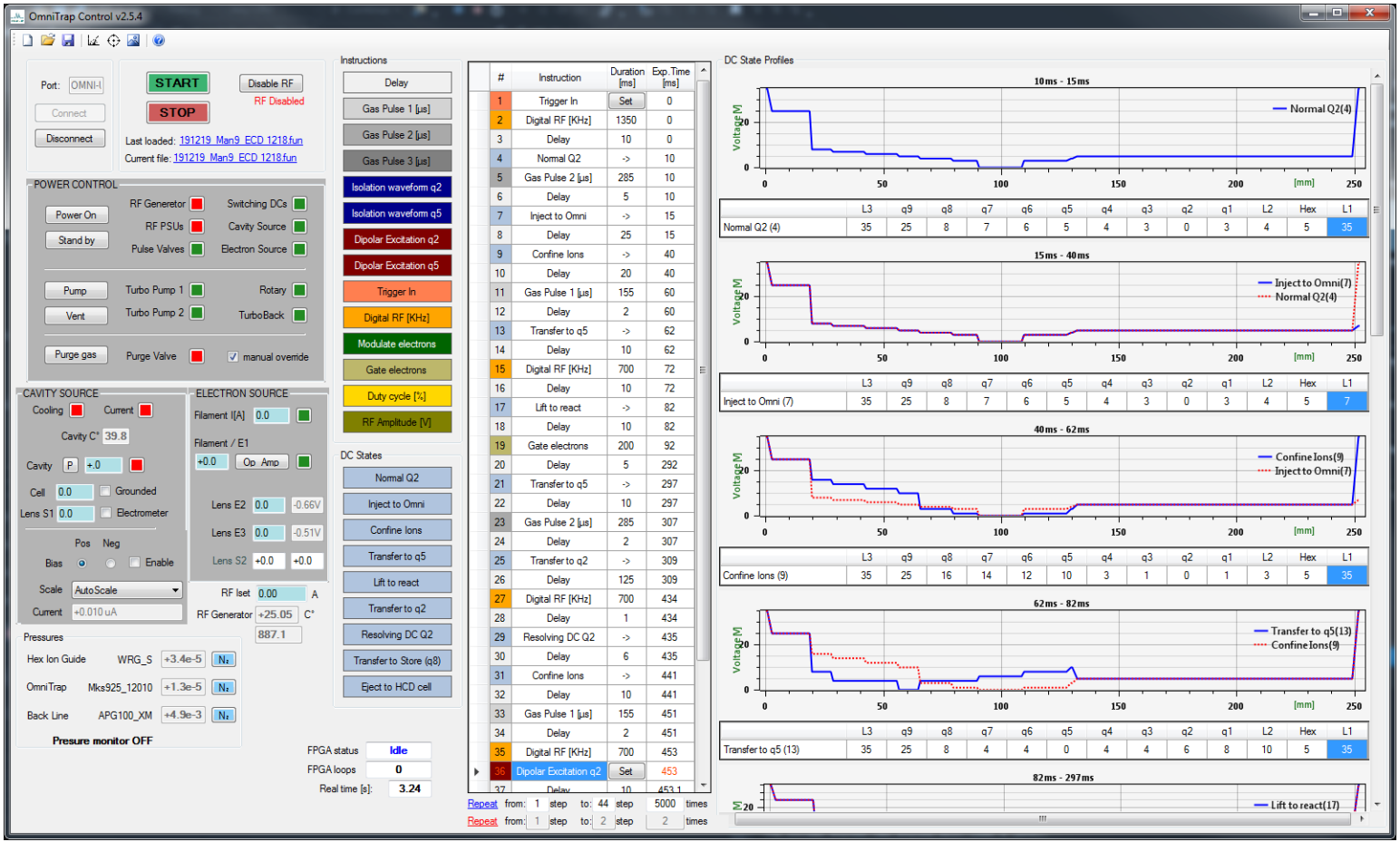


$400V_{0p}$ rectangular RF generator v3



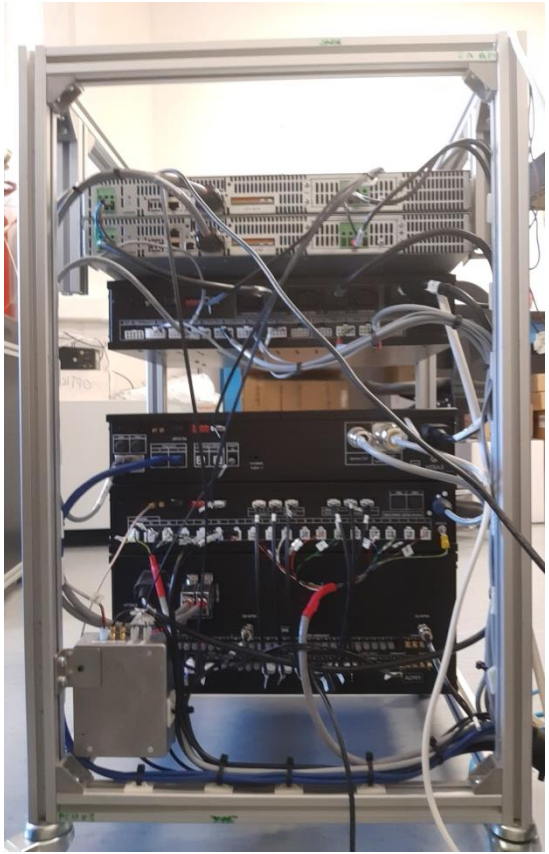


IMS outer & inner housing, drift pcb-electrode assembly, vacuum pcb’s and electronics circuitries


OmniTrap Control v2.5.4
Port: OMNI-1
Connect
Disconnect
START
STOP
Disable RF
RF Disabled
Last loaded: 191219_Man9_ECD_1218.fun
Current file: 191219_Man9_ECD_1218.fun
POWER CONTROL
Power On
Stand by
RF Generetor
RF PSUs
Pulse Valves
Switching DCs
Cavity Source
Electron Source
Pump
Vent
Turbo Pump 1
Turbo Pump 2
Rotary
TurboBack
Purge gas
Purge Valve
manual override
CAVITY SOURCE
Cooling
Current
Cavity C°
Cavity
Cell
Grounded
Lens S1
Electrometer
Bias
Pos
Neg
Enable
Scale
AutoScale
Current
ELECTRON SOURCE
Filament I[A]
Filament / E1
Op Amp
Lens E2
Lens E3
Lens S2
RF Iset
RF Generator
Pressures
Hex Ion Guide
WRG_S
OmniTrap
Mks925_12010
Back Line
APG100_XM
Presure monitor OFF
Instructions
Delay
Gas Pulse 1 [µs]
Gas Pulse 2 [µs]
Gas Pulse 3 [µs]
Isolation waveform q2
Isolation waveform q5
Dipolar Excitation q2
Dipolar Excitation q5
Trigger In
Digital RF [KHz]
Modulate electrons
Gate electrons
Duty cycle [%]
RF Amplitude [V]
DC States
Normal Q2
Inject to Omni
Confine Ions
Transfer to q5
Lift to react
Transfer to q2
Resolving DC Q2
Transfer to Store (q8)
Eject to HCD cell
FPGA status
Idle
FPGA loops
Real time [s]:
3.24
Instruction Duration [ms] Exp.Time [ms]
1 Trigger In Set 0
2 Digital RF [KHz] 1350 0
3 Delay 10 0
4 Normal Q2 -> 10
5 Gas Pulse 2 [µs] 285 10
6 Delay 5 10
7 Inject to Omni -> 15
8 Delay 25 15
9 Confine Ions -> 40
10 Delay 20 40
11 Gas Pulse 1 [µs] 155 60
12 Delay 2 60
13 Transfer to q5 -> 62
14 Delay 10 62
15 Digital RF [KHz] 700 72
16 Delay 10 72
17 Lift to react -> 82
18 Delay 10 82
19 Gate electrons 200 92
20 Delay 5 292
21 Transfer to q5 -> 297
22 Delay 10 297
23 Gas Pulse 2 [µs] 285 307
24 Delay 2 307
25 Transfer to q2 -> 309
26 Delay 125 309
27 Digital RF [KHz] 700 434
28 Delay 1 434
29 Resolving DC Q2 -> 435
30 Delay 6 435
31 Confine Ions -> 441
32 Delay 10 441
33 Gas Pulse 1 [µs] 155 451
34 Delay 2 451
35 Digital RF [KHz] 700 453
36 Dipolar Excitation q2 Set 453
Repeat from: 1 step to: 44 step 5000 times
Repeat from: 1 step to: 2 step 2 times
DC State Profiles
10ms - 15ms
Normal Q2(4)
Voltage M
[mm]
L3 q9 q8 q7 q6 q5 q4 q3 q2 q1 L2 Hex L1
Normal Q2 (4) 35 25 8 7 6 5 4 3 0 3 4 5 35
15ms - 40ms
Inject to Omni(7)
Normal Q2(4)
Inject to Omni (7) 35 25 8 7 6 5 4 3 0 3 4 5 7
40ms - 62ms
Confine Ions(9)
Inject to Omni(7)
Confine Ions (9) 35 25 16 14 12 10 3 1 0 1 3 5 35
62ms - 82ms
Transfer to q5(13)
Confine Ions(9)
Transfer to q5 (13) 35 25 8 4 4 0 4 4 6 8 10 5 35
82ms - 297ms
Lift to react(17)

T1.6 – electronics testing and QE synch

JUL ‘20



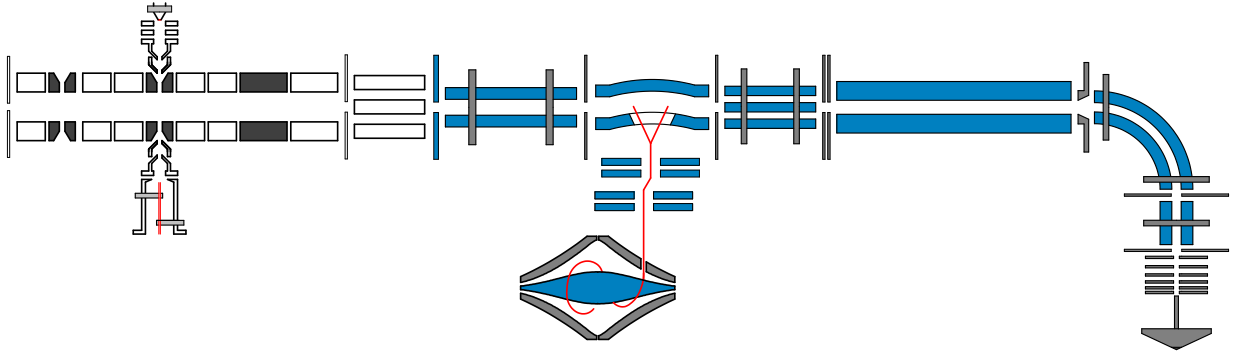
Omnitrap

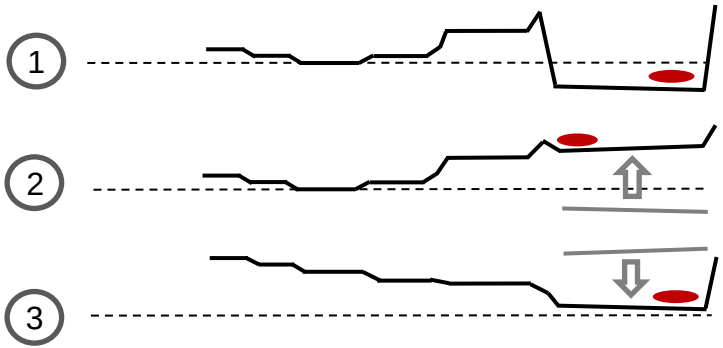
- $250V_{0p}$ Rectangular RF Generator ✓
- FPGA Unit ✓
- Multi-level DC Switch ✓
- Uart Hub (PC-electr comm) ✓
- Electron Source Unit ✓
- Hydrogen Atom Source Unit ✓
- Pulse Valves ✓
- High Voltage PSUs ✓

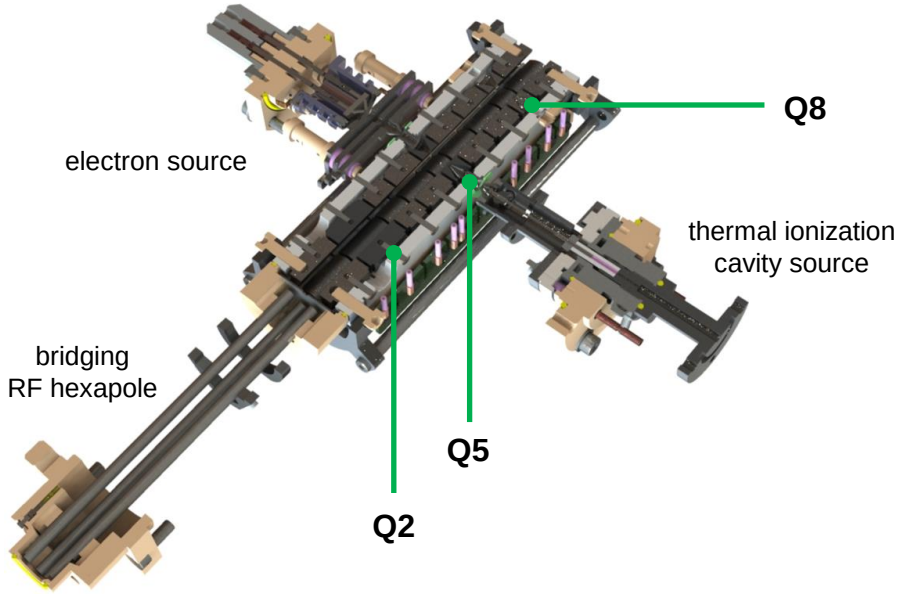
Power Unit ✓

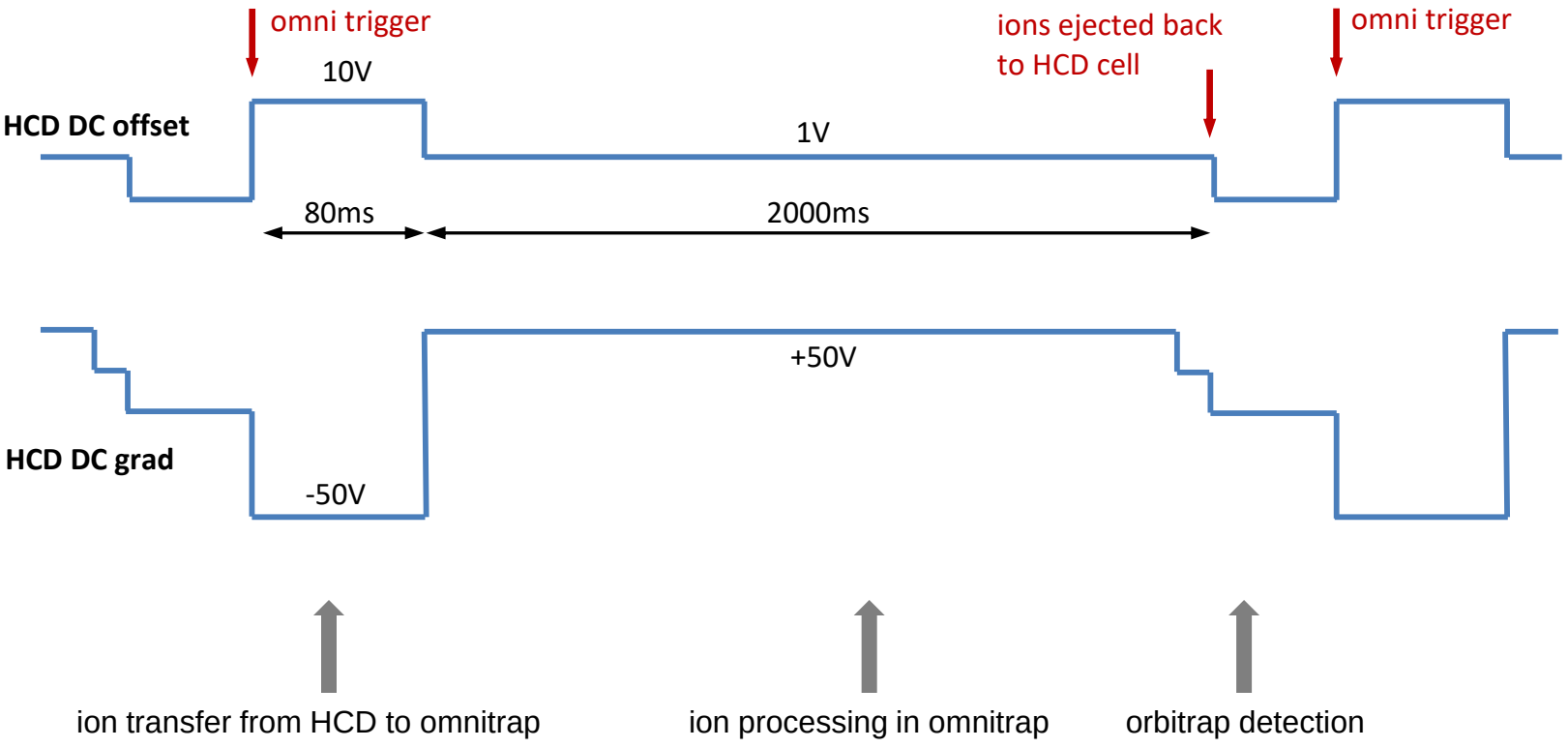
IMS Drift Cell

- IMS DC Pulsing & Floating DCs ✓
- Floating DC Switch Array Unit ✓
- Sin RG Generator & RF Driver synch ✓




1
2
3


Q8
electron source
thermal ionization
cavity source
bridging
RF hexapole
Q5
Q2


omni trigger
10V
ions ejected back
to HCD cell
omni trigger
HCD DC offset
1V
80ms
2000ms
+50V
HCD DC grad
-50V
ion transfer from HCD to omnitrap
ion processing in omnitrap
orbitrap detection

Omnitrap Instrumentation Development Overview