



Stability Diagram Demo

This tutorial demonstrates how to compute stability diagrams of quadrupole analysers by SIMAX software.

In the first example, we build an upper part of the stability triangle for a quadrupole mass filter with hyperbolic electrodes. Note that it takes approximately 2 hours to plot the diagram on an Intel Core *i7* (2.80 GHz) processor.

The analyser has the inscribed radius $r_0=5$ mm and 200 mm long hyperbolic electrodes. A sinusoidal RF voltage is applied to electrodes at the frequency of 2 MHz.

SIMAX offers a powerful **2D scan** tool to construct the stability diagram. The diagram is plotted in the DC offset-versus-the RF amplitude space. In simulations, we leave RF amplitude fixed and vary the DC offset through 50 values. Then RF amplitude is changed and the computations are repeated again.

To plot the stability diagram, a group of 100 ions of 609 Da starts from the centre of the trap and oscillates in the XY plane in the middle of the electrode system. We assume that ion trajectories are stable when the trapping time exceeds 200 μ s. The stability diagram is given by the frontier between stable and non-stable trajectories.

In the second example, we use **2D scan** to build a stability chart for a 3D ion trap.

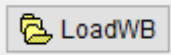
A sinusoidal RF voltage at 1 MHz is applied to the ring electrode of the ion trap with $r_0 = 7.07$ mm and $z_0 = 10$ mm. To plot the full stability zone, we scan RF amplitude from 0 to 9 kV and DC offset voltage in the range from -2100V to +500 V.

A computation of the diagram on an Intel Core *i7* (2.80 GHz) processor takes 1 hour.

In the third example, we examine a quadrupole mass filter with hyperbolic rods operated in the X-band mass selection mode.

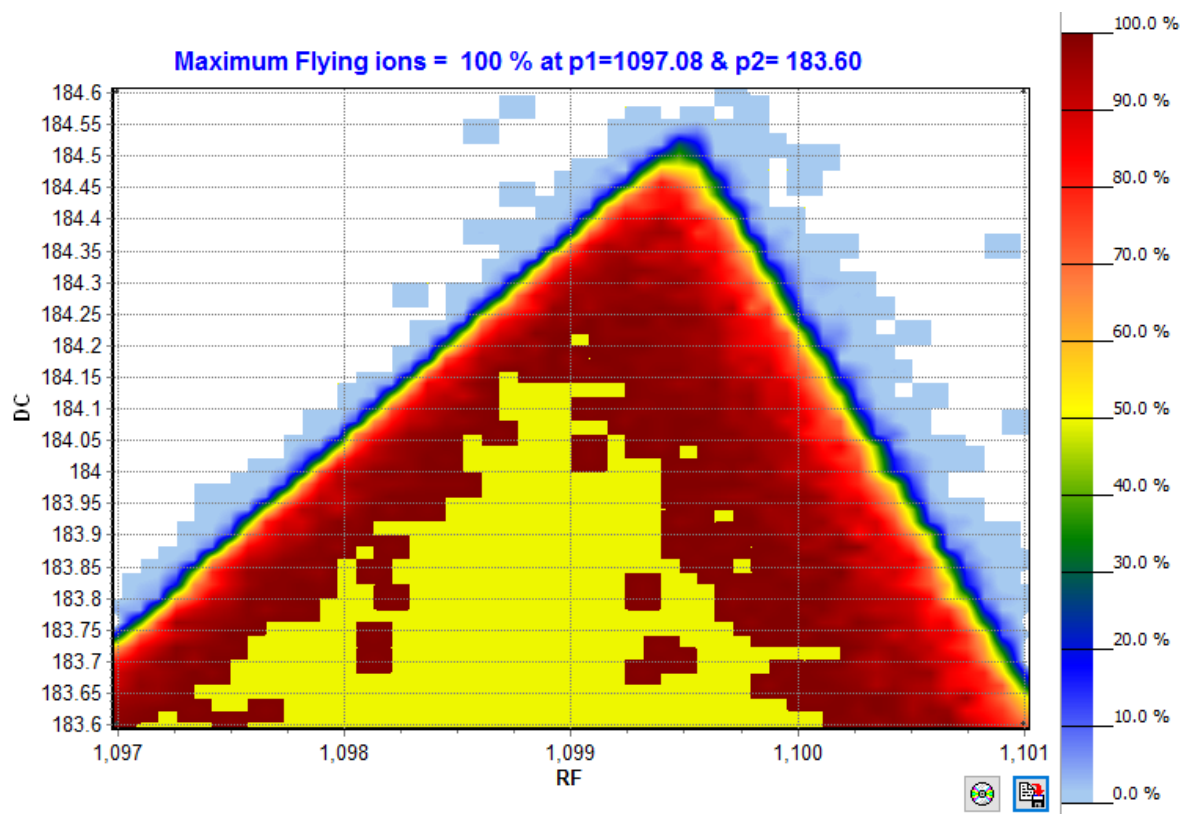
The fourth example demonstrates stability diagrams of the mass filter with circular rods.

Example 1. Tip of Stability triangle for a quadrupole mass filter

1. Start SIMAX. Press  button to load the model *TipOfStability.wb8* from the simulation folder.
2. Go to Scan2D tab in the main control window and press  button. SIMAX repeats simulations and counts ions remaining inside the quadrupole mass filter.

The theoretical computation predicts that the tip of the stability diagram for 609 Da ions appears at the RF amplitude of 1099.507 V and the DC offset voltage of 184.5452 V.

When Scan2D is completed you see the following stability chart:

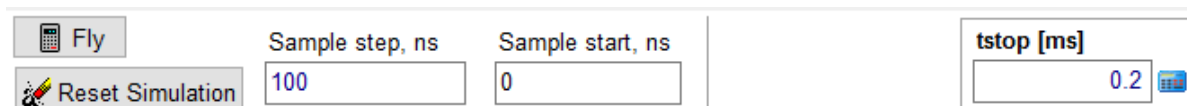


Example 2. Stability diagram for a 3D ion trap

In this example, a 3D ion trap with $r_0 = 7.07$ mm and $z_0 = 10$ mm is modelled. The electrodes of the trap are hyperboloids of revolution. Thus, the trap produces almost ideal quadrupole field. A sinusoidal RF voltage at 1 MHz is applied to the ring electrode of the trap.

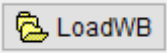
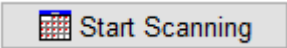
To plot the stability diagram, a group of 100 ions of 609 Da starts from the centre of the trap. We assume that ion trajectories are stable when the trapping time exceeds 200 us. The stability diagram is given by the frontier between stable and non-stable trajectories.

In your simulations, you can set any desired trapping time by entering a new value of *tstop* parameter (in msec), at the bottom of the “Fly” tab in the main control window.

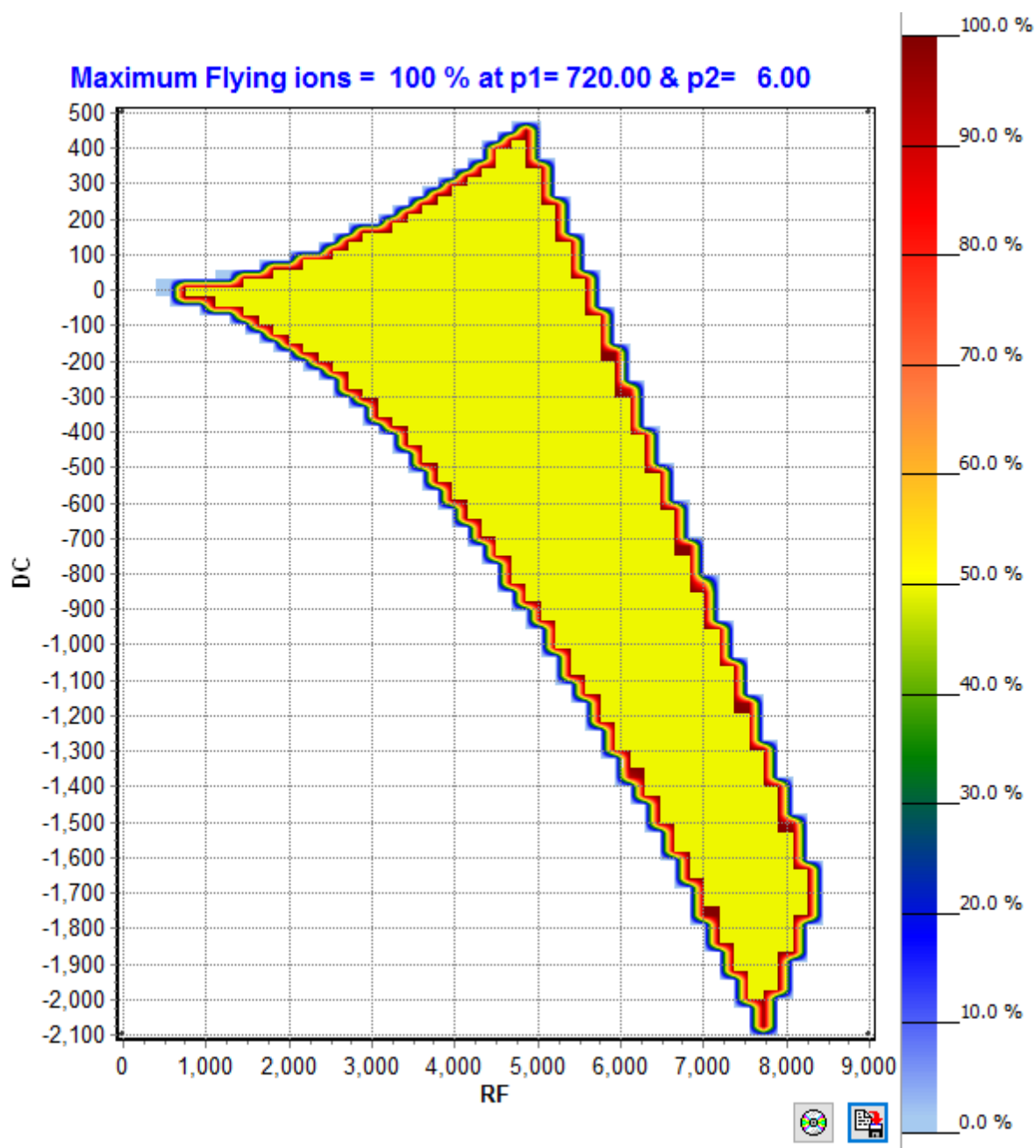


The screenshot shows the 'Fly' tab in the SIMAX main control window. It contains a 'Reset Simulation' button with a pencil icon, two input fields: 'Sample step, ns' with the value '100' and 'Sample start, ns' with the value '0', and a 'tstop [ms]' field with the value '0.2' next to a 'Start Scanning' button with a grid icon.

In this example, we use Scan2D tool to build the first stability zone completely.

1. Start SIMAX. Press  button to load the model *StabilityDiagram_3Dtrap.wb8* from the simulation folder.
2. Open Scan2D tab in the main control window and press  button. SIMAX starts the simulation and counts ions trapped inside the ion trap.

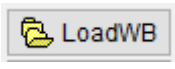
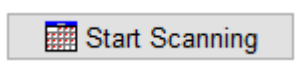
When 2D scan is completed, you can see the following stability chart:



Example 3. Stability diagram for the QMF with hyperbolic electrodes operated in the X-band mass selection mode.

This example relates to a new mode of quadrupole mass filter operation described in details in *M. Sudakov, E. Mamontov, F. Xu, Ch. Xu, Chuan-Fan Ding, Possibility of operating of quadrupole mass filter at high resolution, Int. J. of Mass Spectrometry, v.408 (2016), pp.9-19.*

SIMAX computes the stability diagram directly by 2D scan tool.

1. Start SIMAX. Using button  load the model *hQuad_Xband_I_1.wb8* or *hQuad_Xband_I_2.wb8* from the simulation folder.
2. Go to Scan2D tab in the main control window and press  button. SIMAX repeats simulations and counts ions remaining inside the quadrupole mass filter.

After Scan2D is completed (2 hours on an Intel Core i7 (2.80 GHz) processor), you see the following stability charts (depending on the selected model).

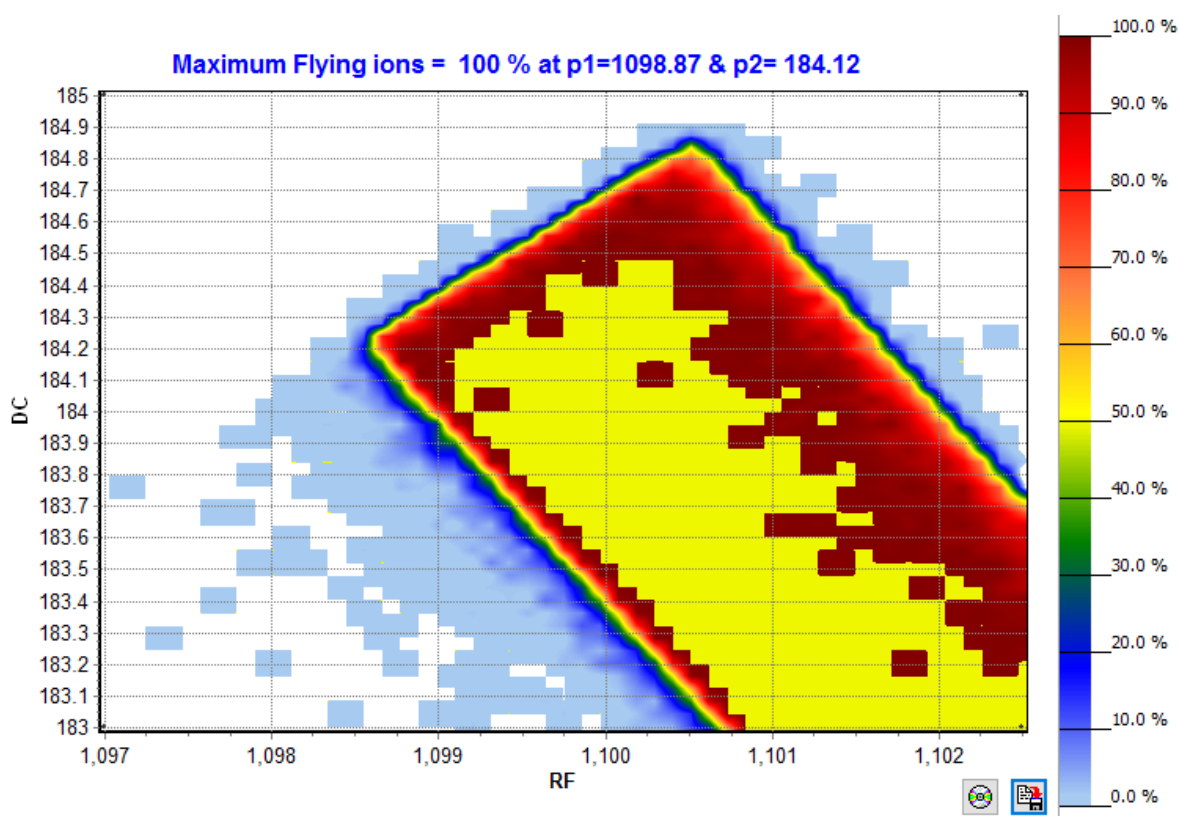


Fig.4. The X-band-I obtained for reserpine ions (609Da). The quadrupole mass filter with $r_0=5\text{mm}$ operates at the main RF frequency of 1MHz with AC1= 1.87755V and AC2= 5.51995V.

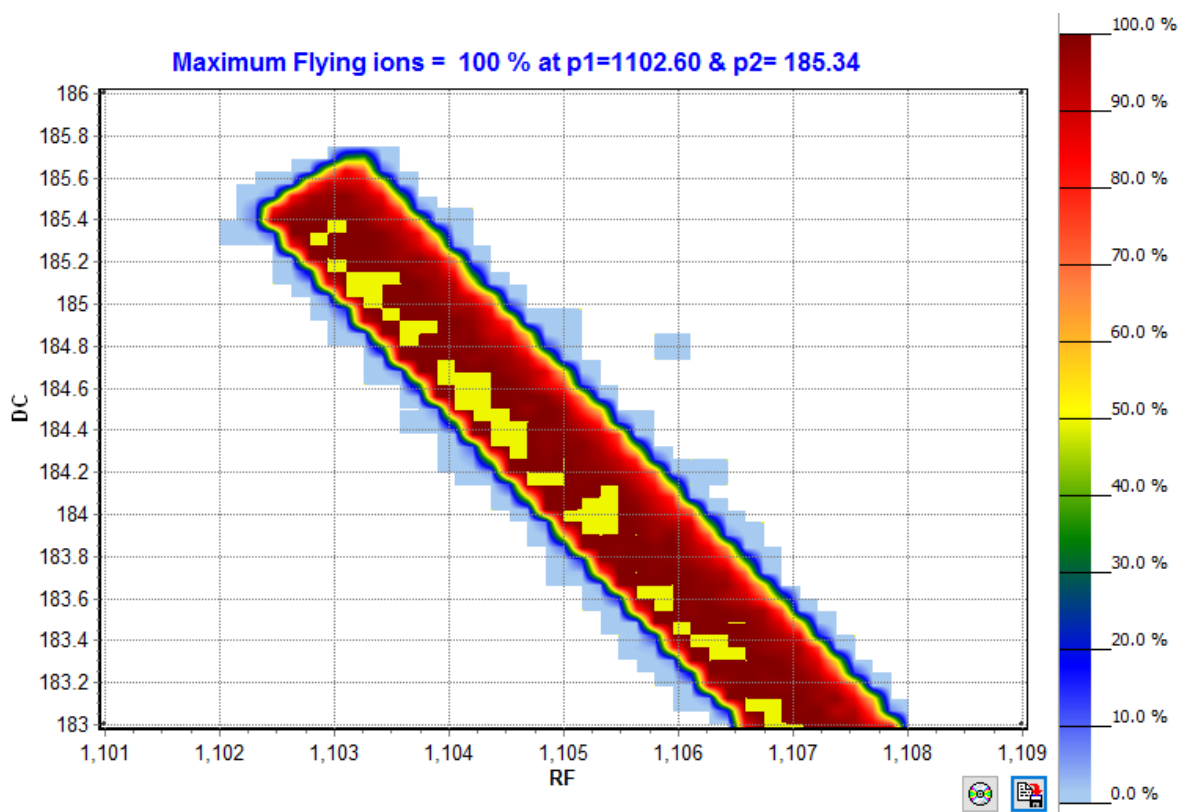


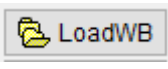
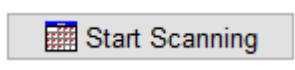
Fig.5. The X-band-I for reserpine ions (609Da) in the quadrupole mass filter with hyperbolic rods, $r_0=5$ mm operated at the main RF frequency of 1MHz with AC1= 3.7551V and AC2= 11.0399V.

Example 4. Stability diagram for a quadrupole mass filter with cylindrical rods

Here we present one more exciting exercise for a quadrupole mass filter with cylindrical rods. The electric field in such analysers deviates from the ideal quadrupole field and suffers from some nonlinear distortions.

Normally, stability diagrams are computed for the ideal quadrupole field. However, SIMAX software offers a unique opportunity to compute the trapping efficiency as a function of operating parameters (amplitude of the RF supply and DC voltage) for any arbitrary electrode system with a non-perfect field, for example, for a quadrupole mass analyser with cylindrical rods. In this example, the filter with $r/r_0=1.125$ is examined (this is a commonly used value for quadrupole mass filters with cylindrical rods).

A computation of the diagram on an Intel Core i7 (2.80 GHz) processor takes 1 hour.

1. Start SIMAX. Using  button to load the model *cQuad_Xband_I_0.wb8* from the simulation folder.
2. Go to Scan2D tab in the main control window and press  button. The program repeats simulations and counts ions trapped inside the quadrupole mass filter.

When 2D-scan is completed (1 hour on an Intel Core i7 (2.80 GHz) processor), you can see the following chart:

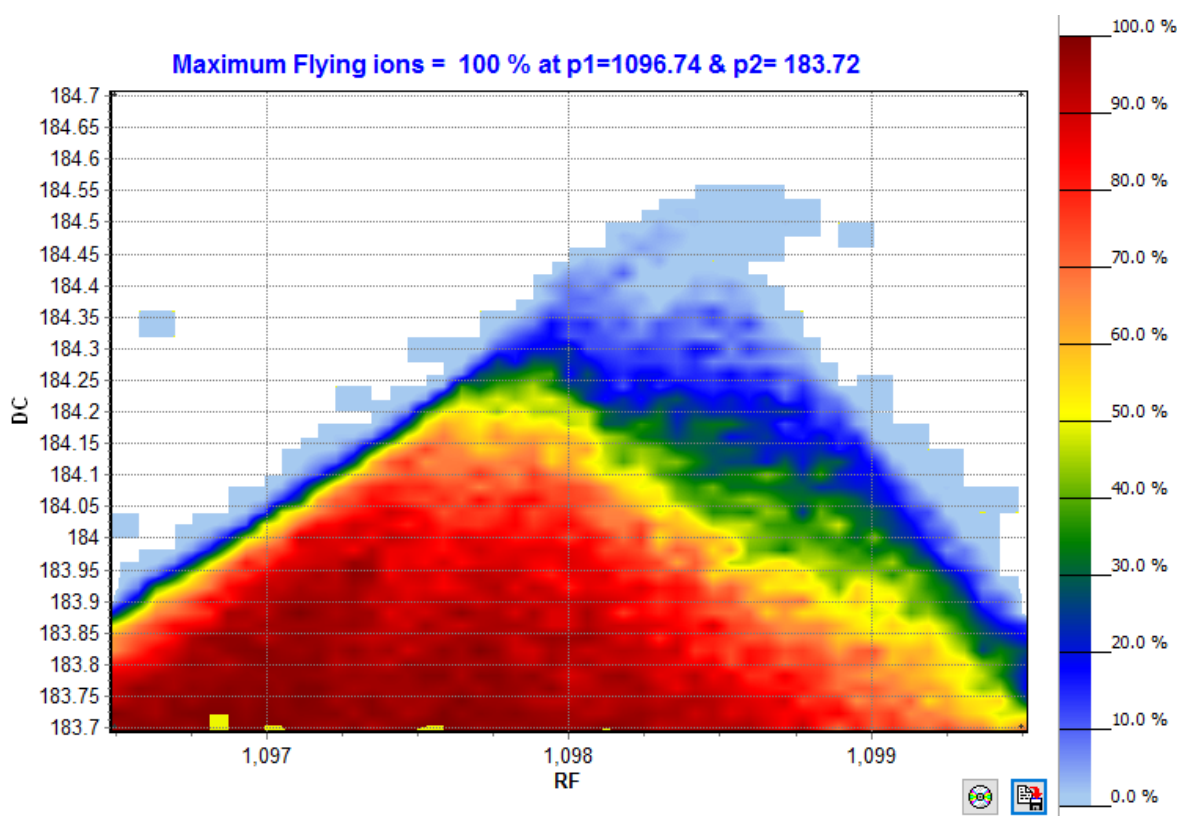


Fig.6. The trapping efficiency for a quadrupole mass filter with cylindrical rods in a normal mode of operation for reserpine ions (609 Da) computed for the quadrupole mass filter with $r_o=5\text{mm}$, $r/r_o=1.125$. The mass filter is driven by a sine wave RF voltage at 1MHz. Note, that the nonlinear field completely destroys the tip of the stability triangle. There is no more clear Y boundary (on the right side of the diagram) since it is also distorted by the field imperfections. This affects the stability in the Y direction substantially.

3. Another model *cQuad_Xband_I_1.wb8* gives the following stability chart:

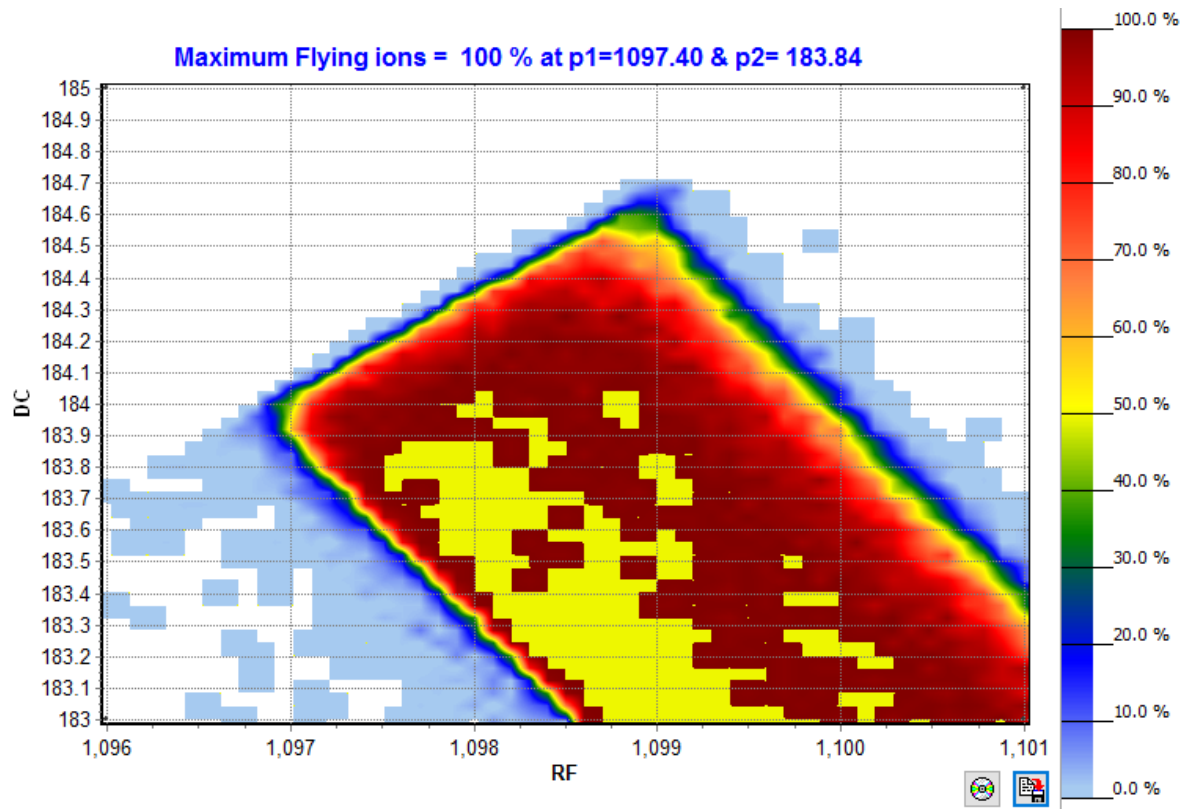


Fig.7. The X-band-I with AC1= 1.87755 V and AC2= 5.51995 V for reserpine ions (609Da) in the mass filter with cylindrical rods with $r_o=5\text{mm}$ ($r/r_o=1.125$) operated at the main frequency of 1MHz

4. Finally, the model *cQuad_Xband_I_2.wb8* generates the following result

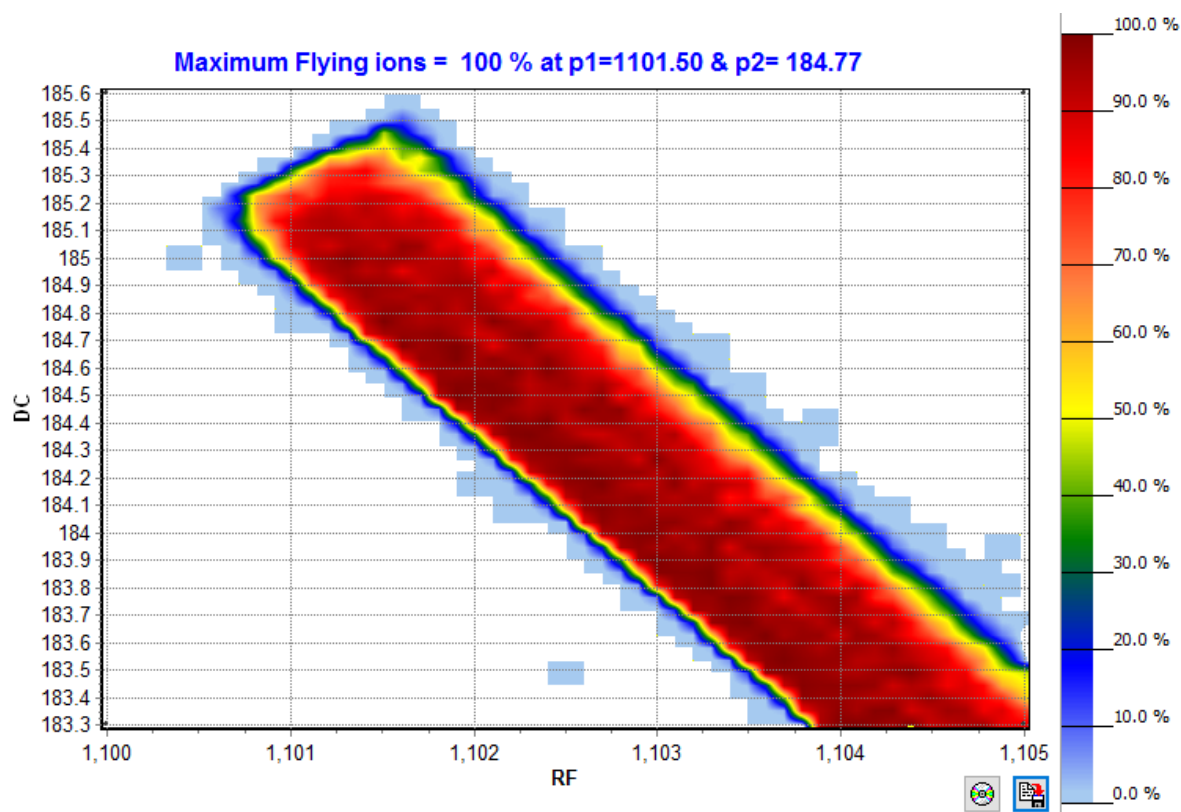


Fig.8. The X-band-I obtained with AC1= 3.7551 V and AC2= 11.0399 V for reserpine ions (609 Da) for the quadrupole mass filter with cylindrical rods with $r_o=5\text{mm}$ ($r/r_o=1.125$) operated at the main frequency of 1MHz.

Note, that the boundaries of the X-bands are not affected by nonlinear field distortions!