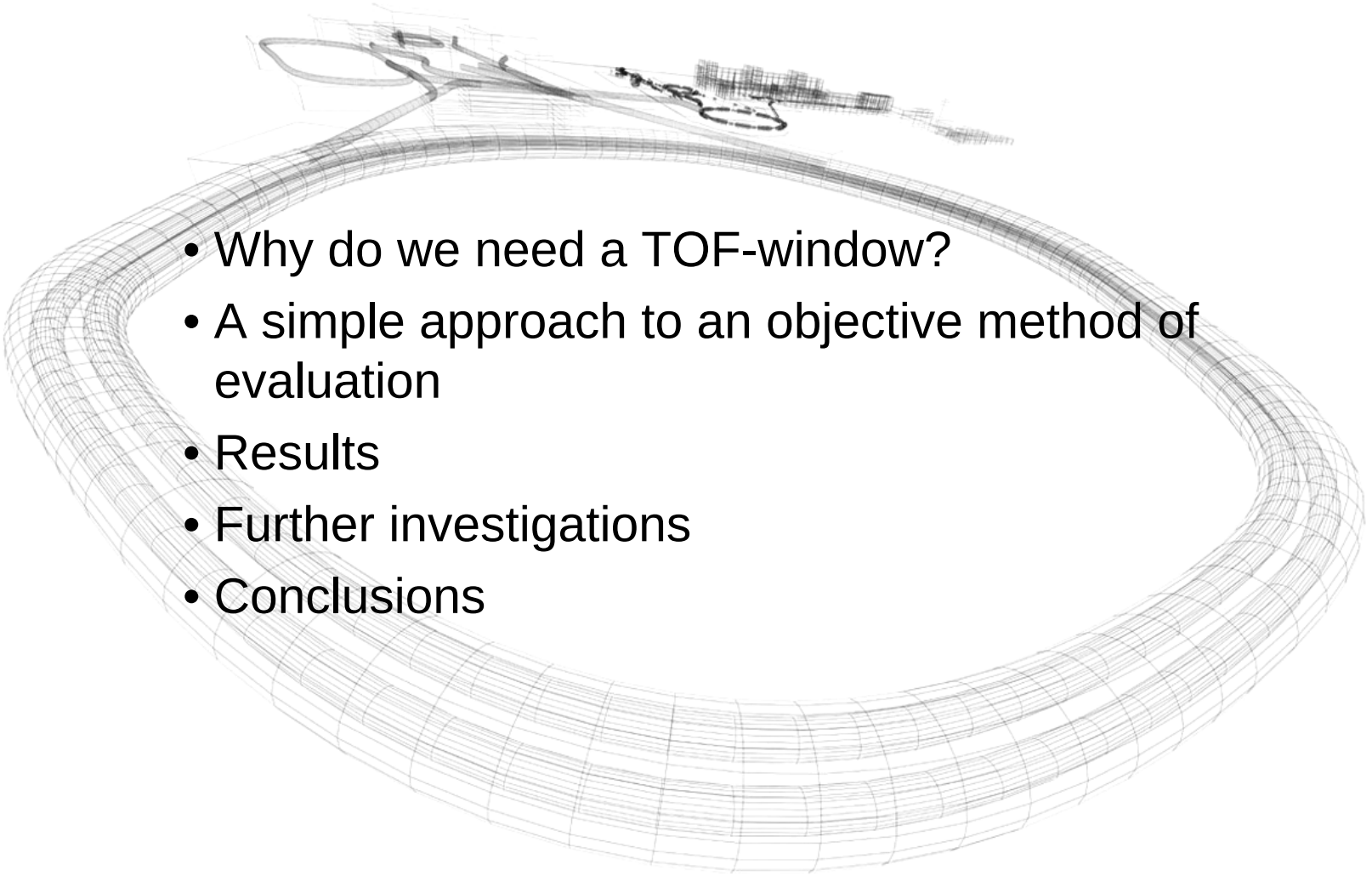
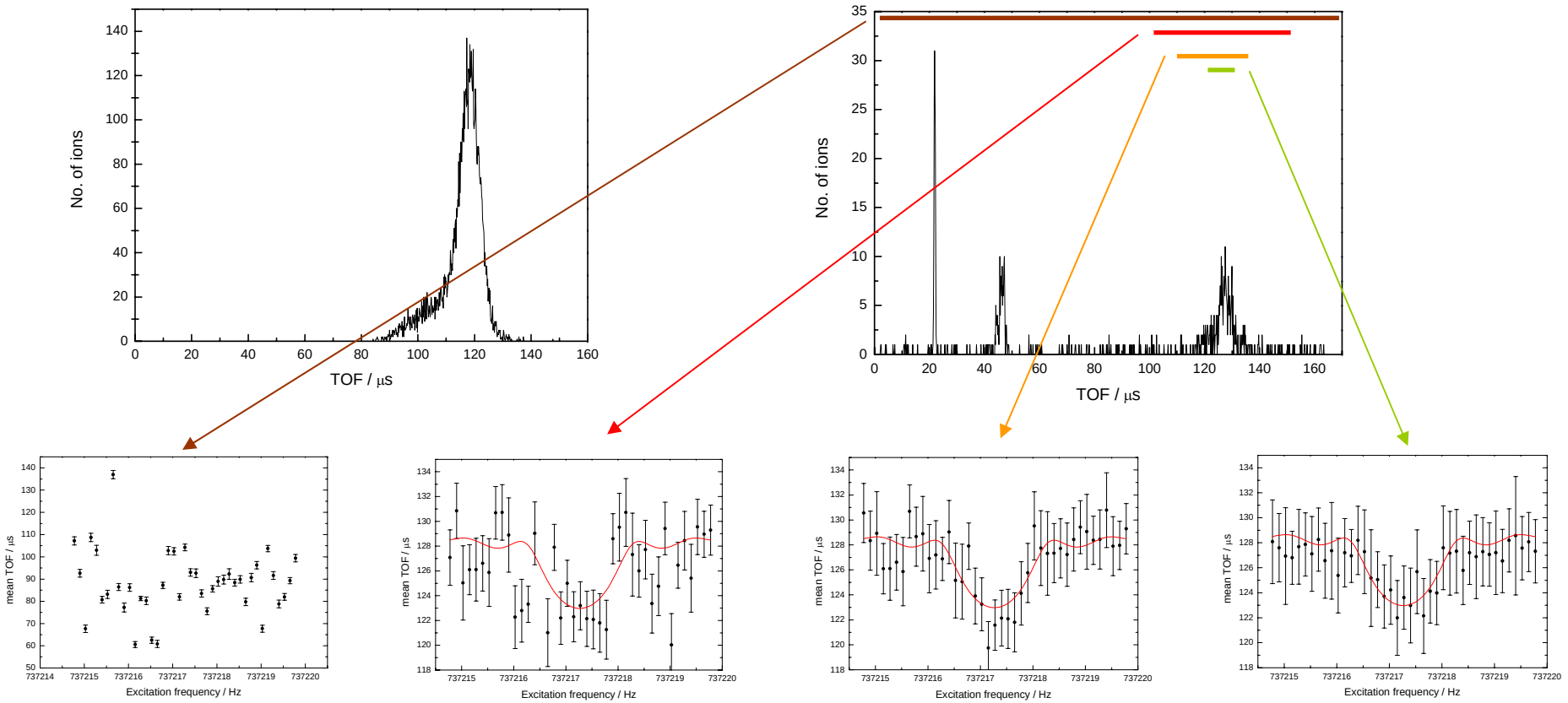
A new way to set the TOF-window?!



- Why do we need a TOF-window?
- A simple approach to an objective method of evaluation
- Results
- Further investigations
- Conclusions

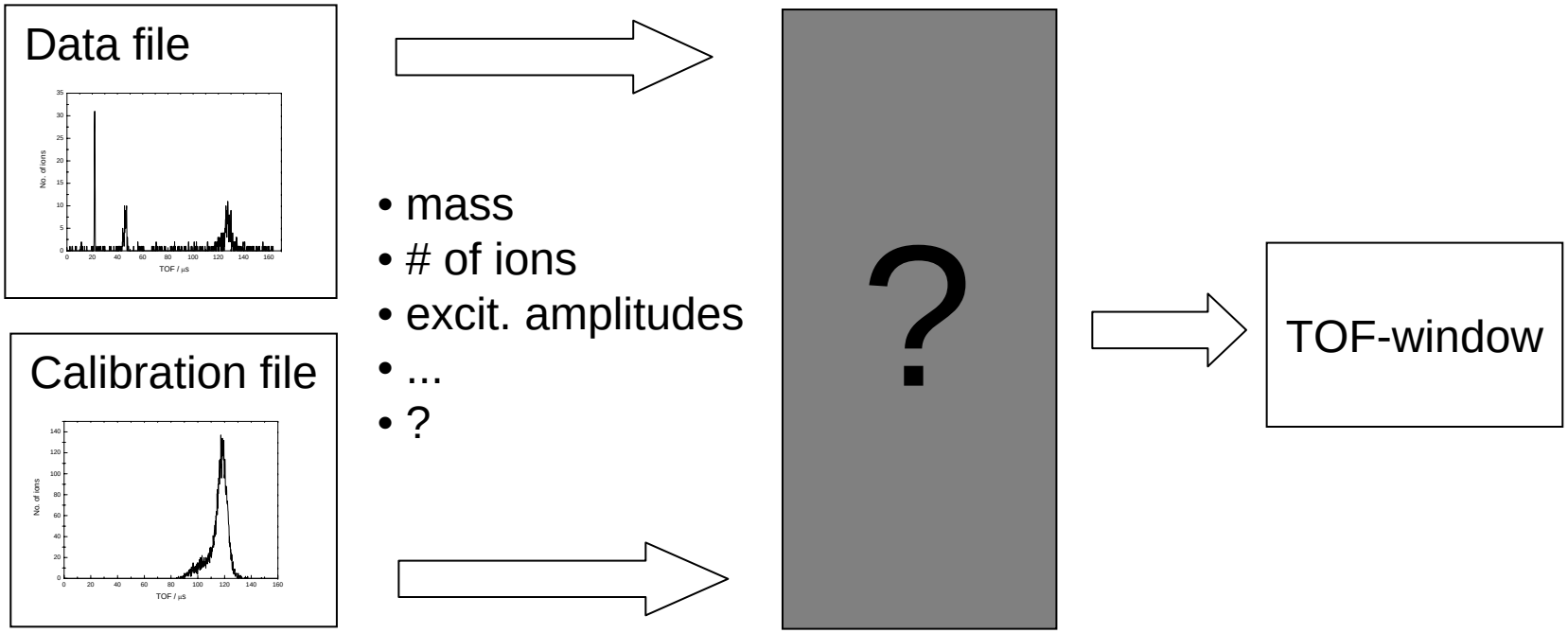
Why do we need a TOF-window?

In files with a high background, the shape or even the existence of a resonance depends on the time-of-flight (TOF) window. By selecting the correct range, the background is discriminated and the signal-to-noise ratio improved.



The Black Box

Is there a (simple) procedure to calculate the TOF-window for a given spectrum from a calibration file, where the TOF-window is known, and some data from this file?

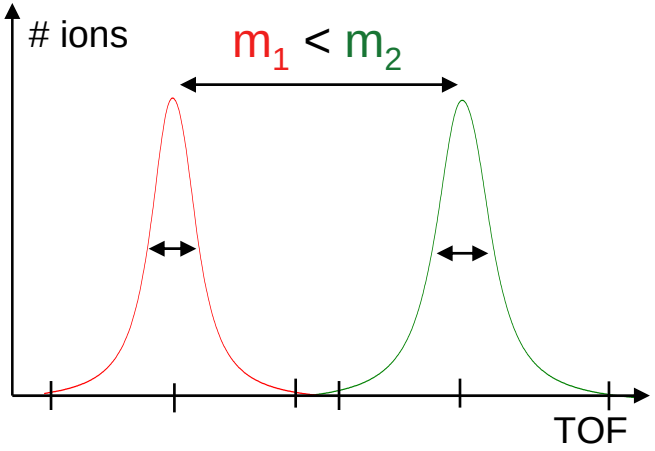


Parameters of the TOF-window

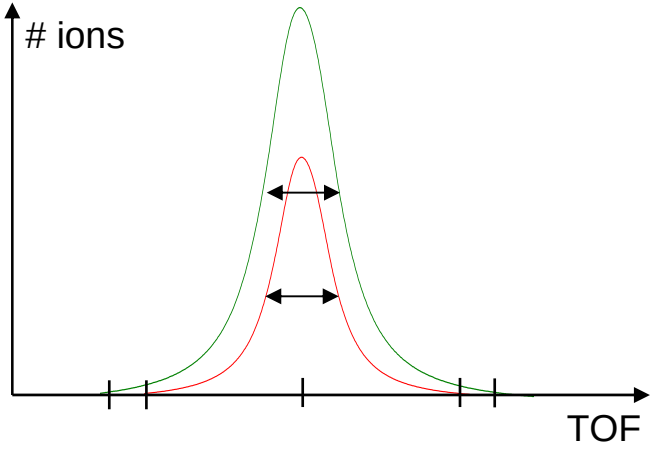
The TOF-window depends primary on:

- the mass

$$t \propto \sqrt{m}$$

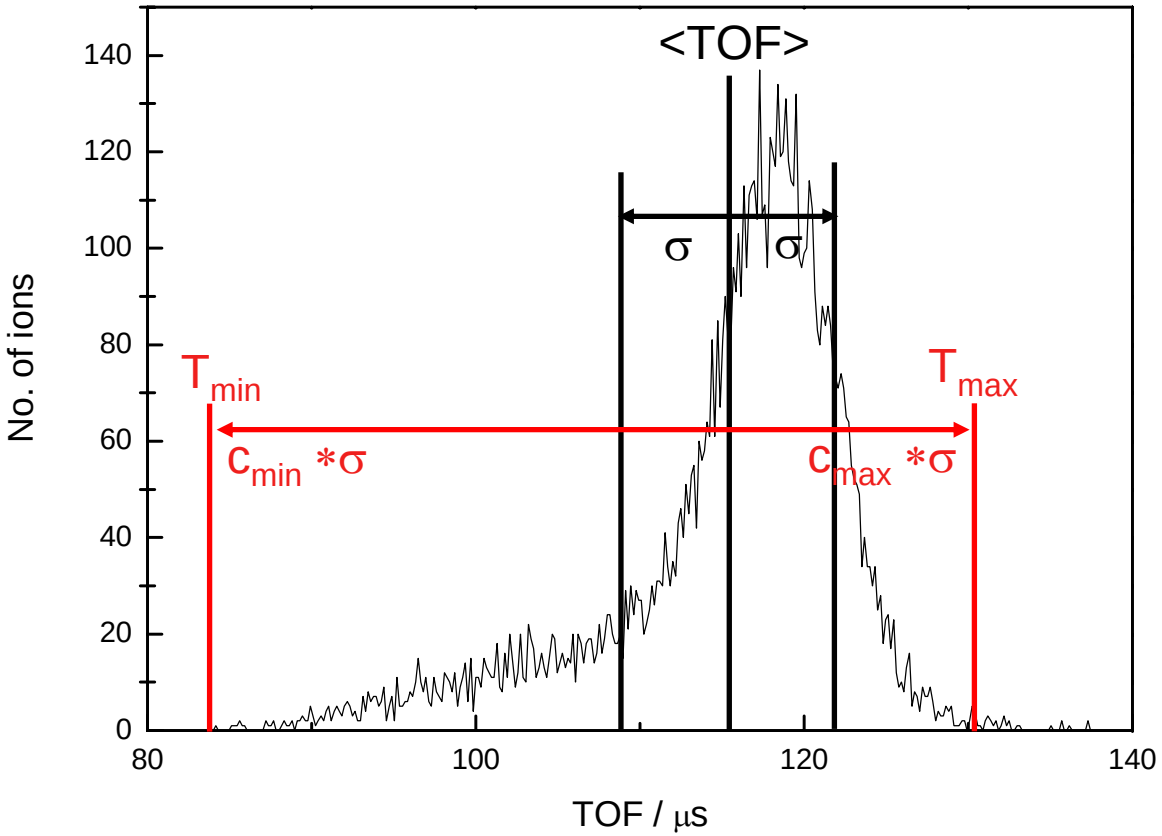


- the number of ions in the peak



Simple statistical model

Model independent statistical approach:



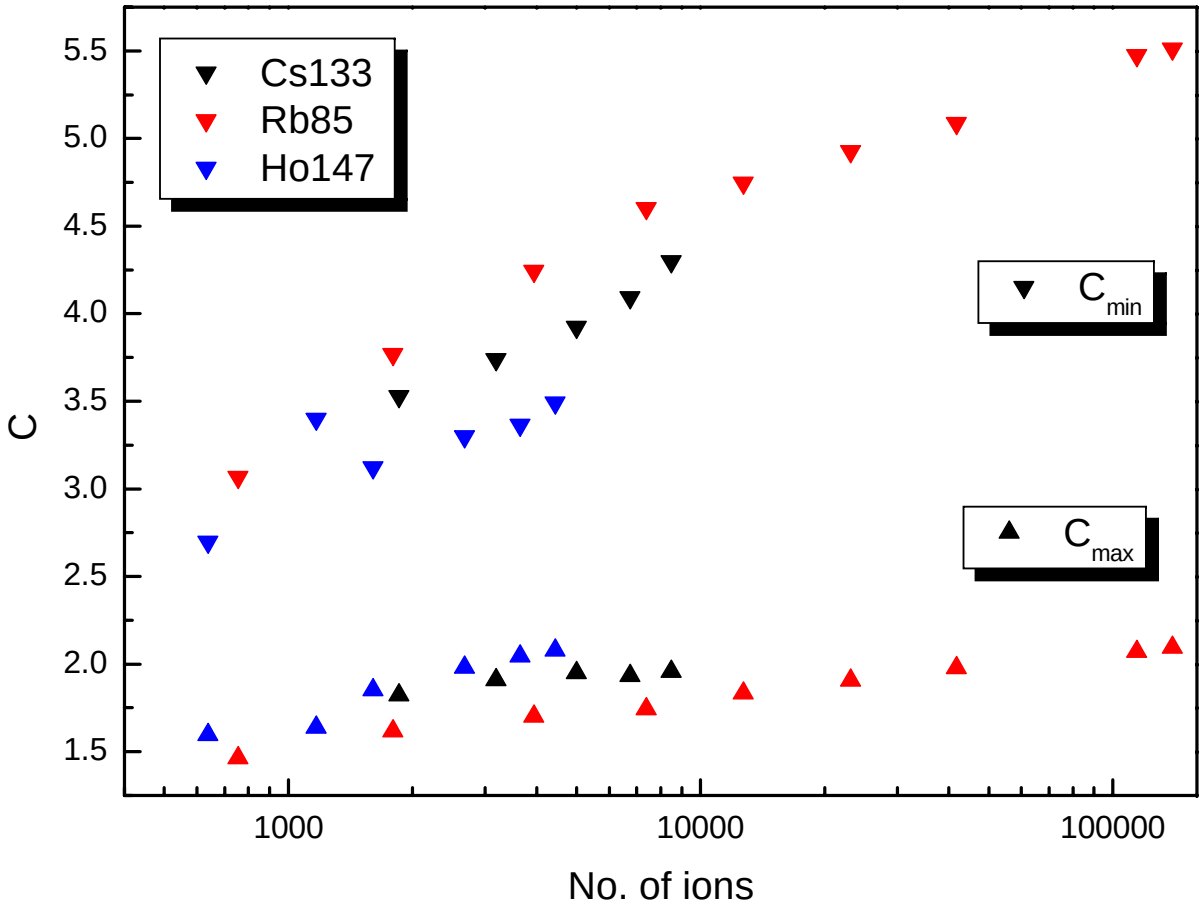
- Calculate mean time-of-flight <TOF> and standard devitation σ
- Estimate T_{min} and T_{max} and calculate C_{min} and C_{max}

$$T_{\pm} = < TOF > \pm C_{\pm} \cdot \sigma$$

Data analysis

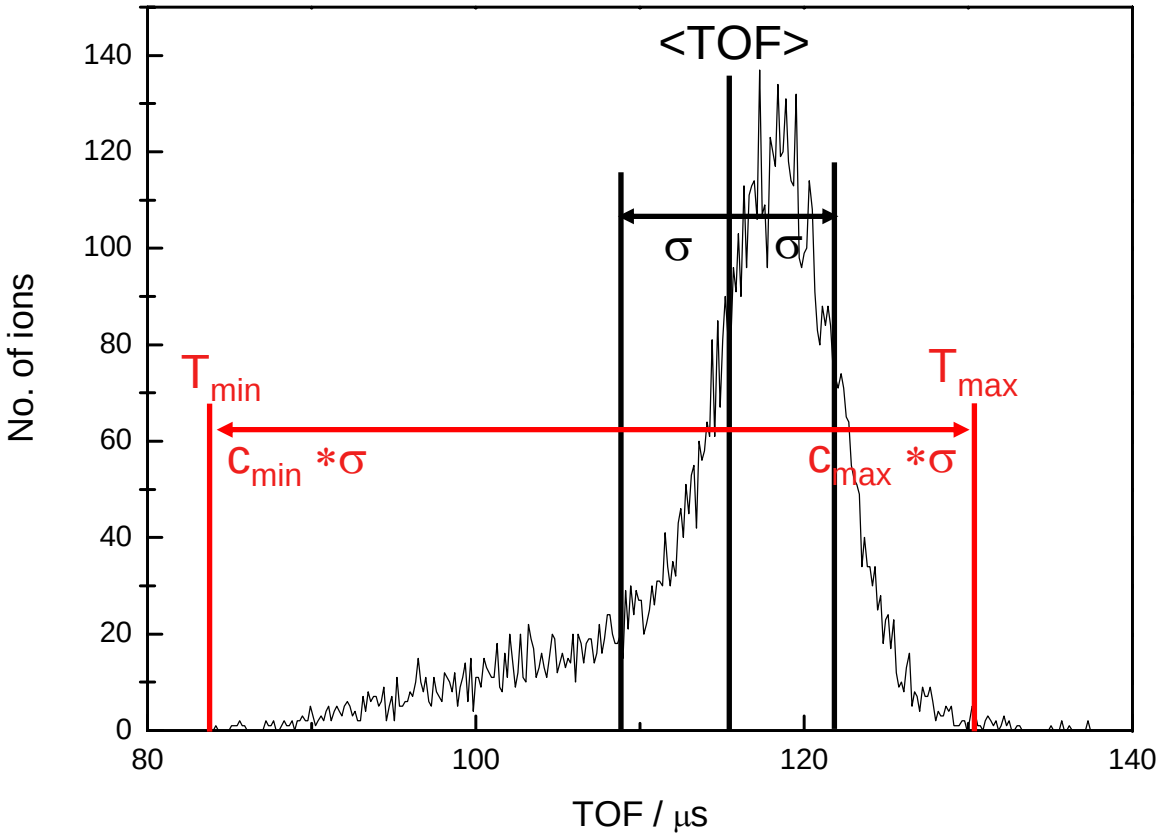
#scans	#ions	<TOF>	σ_{TOF}	TOF_{min}	TOF_{max}	C_{min}	C_{max}	D_{min}	D_{max}
Cs									
6	1856	114.9548578	6.902167712	90.59160317	127.5276285	3.52979755	1.82156841	0.838402108	1.046534887
12	3188	115.1312798	6.990414742	88.9870487	128.4876121	3.74001144	1.91066379	0.822880866	1.052127655
18	5000	115.2645269	7.180864556	87.08319409	129.2695143	3.92450416	1.95032051	0.805701733	1.05573197
24	6750	115.3978533	7.248093582	85.72432856	129.4051372	4.09397649	1.93254734	0.792644651	1.055111405
30	8500	115.54065	7.289476824	84.19943814	129.8135229	4.29951458	1.9580106	0.777815479	1.056854098
Avg		115.2578336	7.122203483						
Rb									
5	756	94.45687003	6.923053143	73.21802318	104.5947529	3.06784397	1.46436588	0.836454136	1.031710714
10	1794	94.42163861	6.764695518	68.93141958	105.3508583	3.76812511	1.61562625	0.786377178	1.041156982
20	3938	94.4156998	6.690447695	66.01674177	105.7940905	4.2447022	1.70069198	0.752539778	1.046366548
40	7375	94.43048137	6.723088693	63.48797771	106.1571089	4.60242384	1.74423217	0.723861191	1.049464778
100	12688	94.37585528	6.755398991	62.30561822	106.7662283	4.74734906	1.83414377	0.711085297	1.055719412
200	23125	94.33150379	6.760594323	61.02955427	107.2207154	4.92589082	1.90652049	0.696915844	1.060624098
400	41813	94.36162823	6.780415714	59.8565601	107.7760401	5.08893106	1.97840551	0.683440642	1.065590884
1000	114250	94.35841574	6.820821146	57.0016164	108.4828161	5.47687713	2.07077712	0.651167269	1.072184565
1184	139375	94.33063082	6.825059929	56.69978976	108.6304358	5.51362793	2.09519113	0.647956344	1.073893471
Avg		94.3869693	6.782619461						
CalcCs		92.14124891	5.69374509						
Ho									
10	638	125.756302	5.82047354	110.0545187	135.0428996	2.69768142	1.59550551	0.917611693	1.026342978
20	1169	125.8612881	5.678262977	106.5592366	135.1601168	3.39928805	1.63761854	0.886641325	1.027524541
30	1606	125.9111602	5.638130664	108.3071319	136.3536655	3.12231648	1.8521219	0.900510549	1.036521479
40	2675	125.87107	5.737773907	106.9421407	137.2288701	3.2990023	1.97947851	0.890195676	1.042702497
50	3644	125.7082008	5.765024213	106.3009326	137.4862555	3.36638104	2.04301913	0.886260775	1.04573578
60	4438	125.6602436	5.796201851	105.4136526	137.7003597	3.49307902	2.07724238	0.879443501	1.04749797
Avg		125.7947108	5.739311192						
CalcCs		121.1722854	7.487679113						
calcRb		124.1255672	8.919626234						

Results I


Cs133
Rb85
Ho147
C_min
C_max
C
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1000
10000
100000
No. of ions

Simple statistical model

Model independent statistical approach:

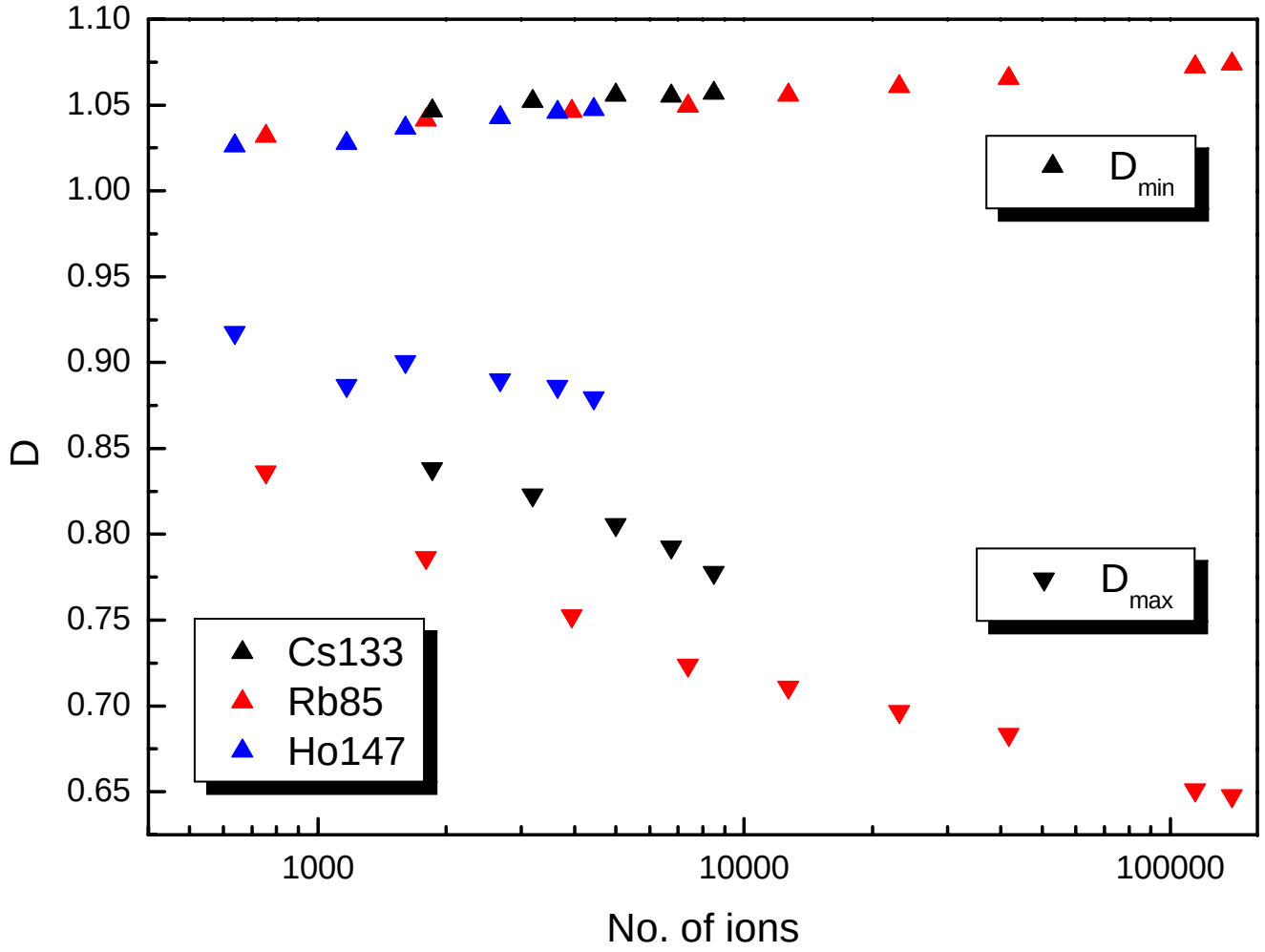


- Calculate mean time-of-flight <TOF> and standard devitation σ
- Estimate T_{min} and T_{max} and calculate C_{min} and C_{max}

$$T_{\pm} = <TOF> \pm C_{\pm} \cdot \sigma$$

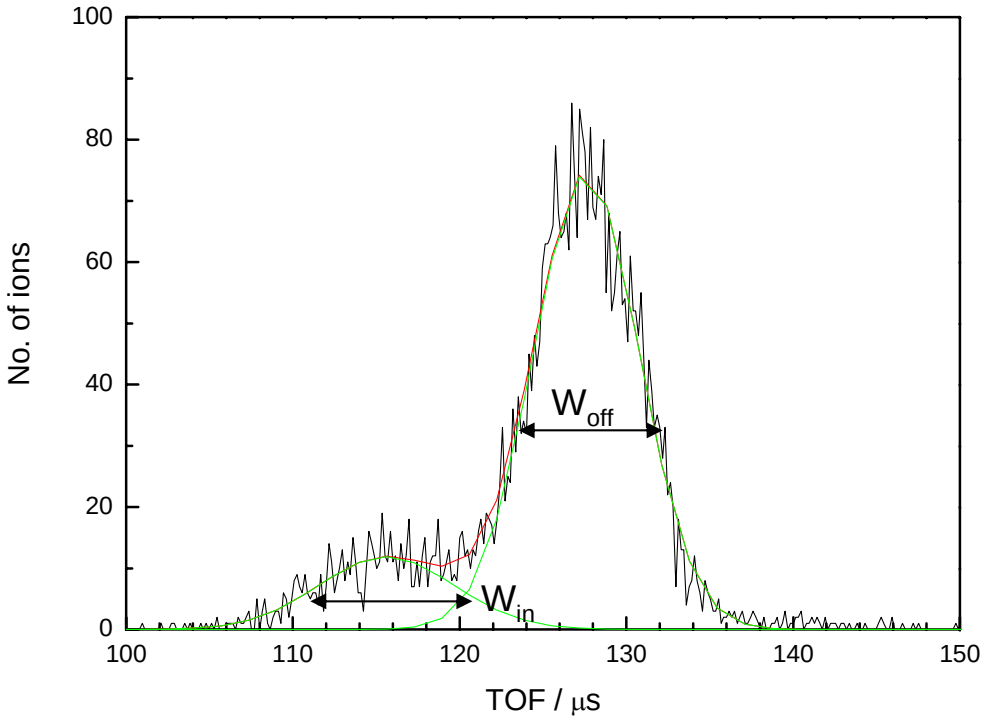
$$T_{\pm} = D_{\pm} \cdot \left(<TOF> \pm \sigma\right)$$

Results II


1.10
1.05
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
D
1000
10000
100000
No. of ions
Cs133
Rb85
Ho147
D min
D max

Further investigations

Fit with two Gaussians shows a independent mass dependence of the width of the "in-resonant" and "off-resonant" peak.



	W_{in}	W_{off}
^{85}Rb	16.8	5.6
^{133}Cs	17.3	7.1
^{147}Ho	9.1	6.1

Outlook

- A simple, model independent, statistical approach is not enough to describe the behavior of the TOF distribution.
- More input parameters than the mass and the number of ions are needed.

- Further investigations/simulations to investigate in these dependent parameters are necessary.