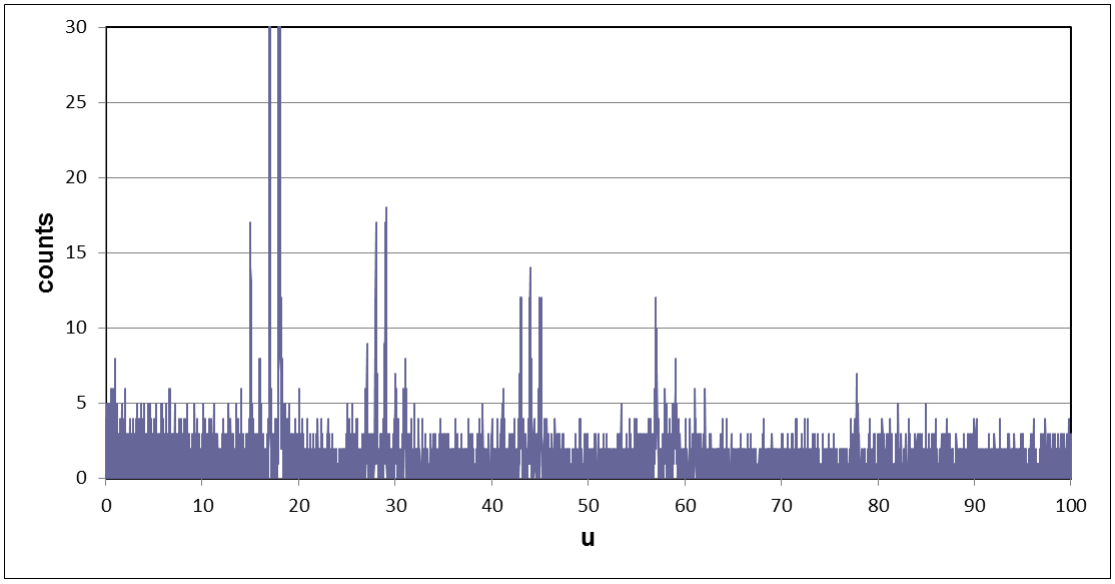
Refinement of mass calibration for COSAC as example:

For an initial evaluation one uses mass calibration given.



Mass spectrum plotted using the initial fit function

This usually allows for the identification of at least three peaks in every spectrum (18, 28, 44). In some spectra there will be more available (He in GC-MS, for example). The plot above is the one containing the highest number of recognizable peaks.

Then one looks into the level zero data containing the bin number and the ion count.

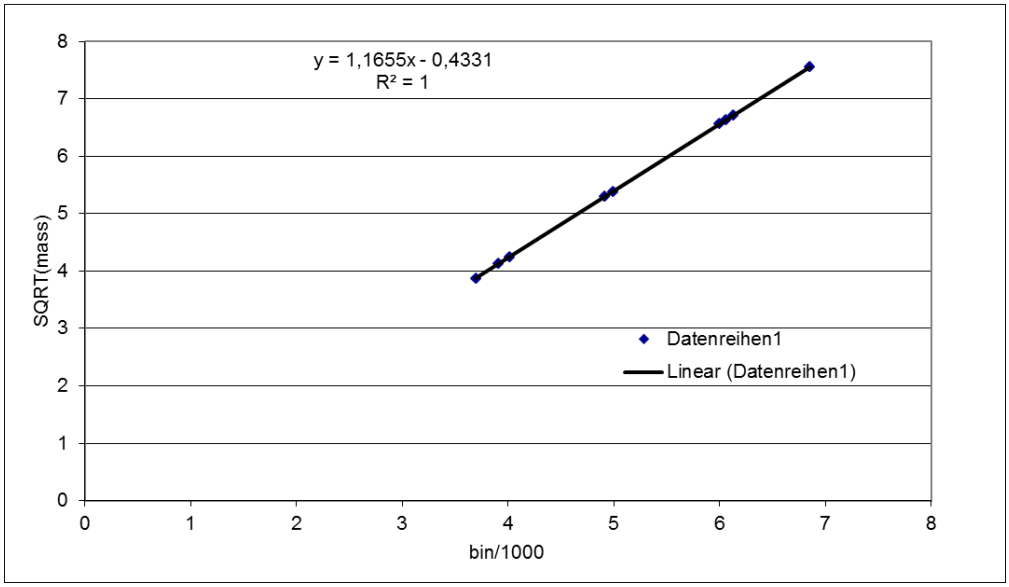
bin	counts
3997	3
3998	2
3999	3
4000	6
4001	7
4002	5
4003	11
4004	13
4005	30
4006	30
4007	87
4008	77
4009	174
4010	158
4011	266
4012	272
4013	305
4014	333
4015	218
4016	220
4017	118
4018	113
4019	29
4020	54
4021	29
4022	20
4023	13
4024	12
4025	11
4026	8
4027	7
4028	11
4029	5

X/Y pairs of bin and ion count; the example above corresponds to the m/z = 18 peak of the spectrum above.

For a better fit one picks some method of determining the peak maxima and the respective bin numbers. Example: This could be some shape fit or simply the largest value in the peak. That should give you a peak list:

mass	bin	bin/1000	SQRT(mass)
15	3695	3,695	3,8730
17	3909	3,909	4,1231
18	4013	4,013	4,2426
28	4912	4,912	5,2915
29	4991	4,991	5,3852
43	5998	5,998	6,5574
44	6061	6,061	6,6332
45	6128	6,128	6,7082
57	6851	6,851	7,5498

Then one performs a mathematical fit of the square root of mass vs bin number. Dividing the bins by 1000 looks a little silly but gives better precision in EXCEL; no idea, why.



The fit gives both, the parameters a and b, and the quality of the numerical fit.

Following this procedure should allow fitting the mass axes to the desired precision.