Design and Performance of New High Resolution MALDI-TOF Mass Spectrometers

Kevin Hayden and Marvin Vestal. Virgin Instruments, Sudbury, MA.

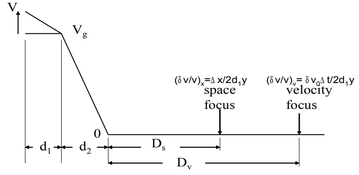
Introduction

In earlier work, theoretical techniques for optimizing the resolving power of MALDI TOF MS systems were presented, and validated for a single reflector instrument. In the work presented here, all of the known contributions to peak width are considered and ultimate limits with presently available technology are defined.

Objective

Establish the practical limits on performance of MALDI-TOF instruments and design and build instruments that test these limits.

Space and Velocity Focusing in MALDI-TOF Ion Source



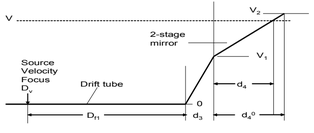
Contributions to Peak Width (dm/m):

$R_{s1}=2K^{-1}(\delta x/D_s)$ $R_{v1}=[4d_1y/D_{est}](\delta V_0/V_s)$

$R_m=R_{v1}[1-(m/m^*)^{1/2}]$ where m* = focused mass

$R_{v2}=2K^2(\delta V_0/V_s)^2$ $R_t=2\delta t/t=2\delta t V_s/D_v$

$R_{v3}=2K^3(\delta V_0/V_s)^3$ δt is width of single ion pulse



Voltage ratio w= V/(V-V$_1$) and $d_d=d_d{}^o(V-V_1)/(V_2-V_1)$

At first and second order focus

w=3/[1-(4d$_d$/D$_t$)], $V_1/V=(w-1)/w$ and

$V_2/V=V_1/V+(1-V_1/V)(d_d{}^o/d_d)$

$d_d/d_3=(D/4d_3)w^{3/2}+(w+w^{1/2})^{-1}=[w^{1/2}(w-3)]^{-1}+(w+w^{1/2})^{-1}$

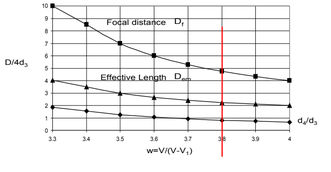
Effective length of the mirror

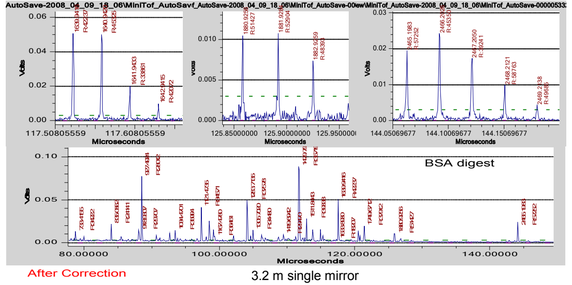
$D_{em}/4d_3=(w-3)^{-1}+1$

Total effective length of the analyzer

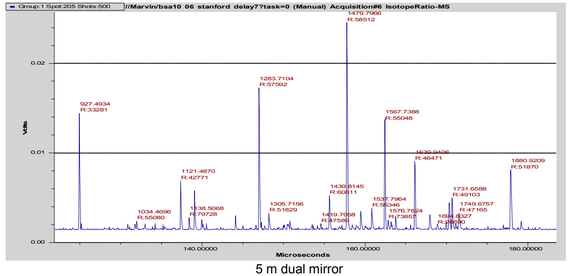
$D_e=D_{em}+D_f+D_d+D_{dm}$ where $D_{dm}=2d_1y^{1/2}[1+(d_2/d_1)/(y^{1/2}+1)]$

The principal benefit of the mirror is to increase D_e without increasing ion peak width.

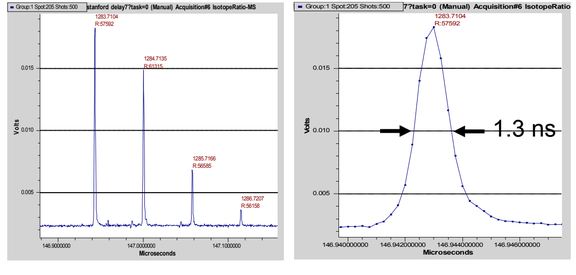




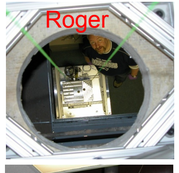
After Correction 3.2 m single mirror

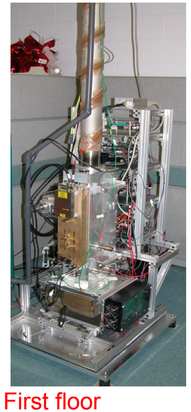


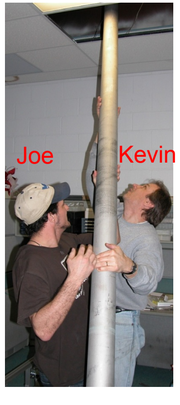
5 m dual mirror



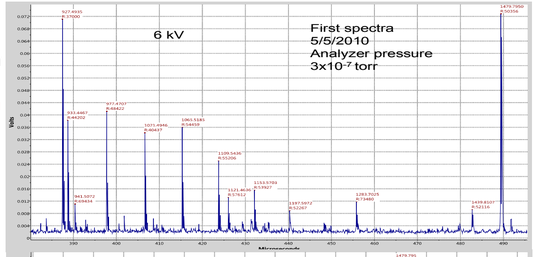
Two story MALDI MS
Physical Length 6m
Effective length 14.8 m
Goal is >200,000 RP
RMS mass error<1ppm

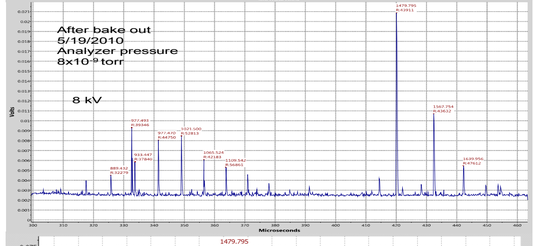


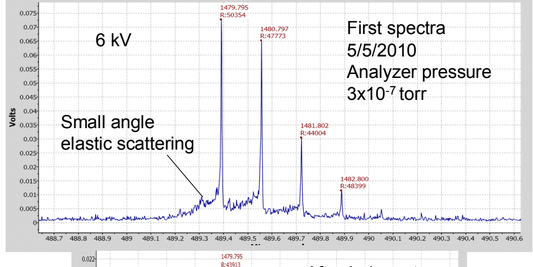


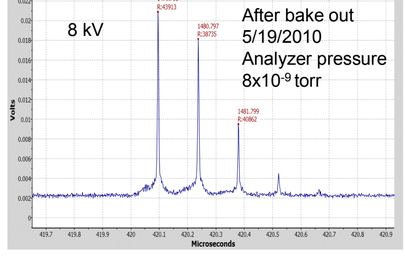


First floor

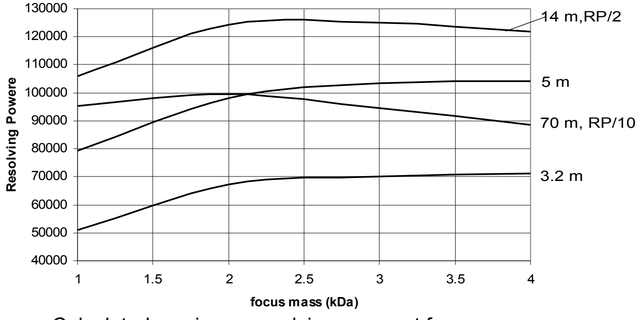








Poster Number TP673



Calculated maximum resolving power at focus mass

Present Status

Performance of 3.2 m single mirror system in good agreement with theory.

Resolving power of 5 m dual mirror system ca. 75% of theory.

- discrepancy appears to be due to combined trajectory error of 2 mirrors with relatively large deflection angle.

Initial results with 14.8 m vertical instrument off about factor of four from theoretical.

-appears to be due either to low frequency noise on HV or mechanical vibration.

Future work

1. Obtain theoretical performance from 14.8 m system.
   -If not; why not?
2. Build and test 1,000,000 resolving power instrument
   -basic design completed but delayed until 1. above is done.
   -requires analyzer pressure<10^{-10} torr and HV noise <1ppm

Acknowledgements

This work was supported by NIH National Center for Research Resources under grant RR025705 and by the staff of Virgin Instruments