Supporting Information

Genetic Algorithm Parallel Optimization of a New High Mass Resolution Planar Electrostatic Ion Trap Mass Analyzer

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Schematic View of angularly-precessing ion motion. Figure-S1a shows the voltage distribution and simulative ion trajectory in the PEIT-7 mass analyzer on the x-y plane in 0.29 ms. In Figure S-1b, the red line indicates the ion trajectory on the x-z plane, which is also one axial drift of the ion. Due to the symmetrical electrode structure, the ion also has a periodic oscillatory motion in the x-z plane (parallel to point focus).
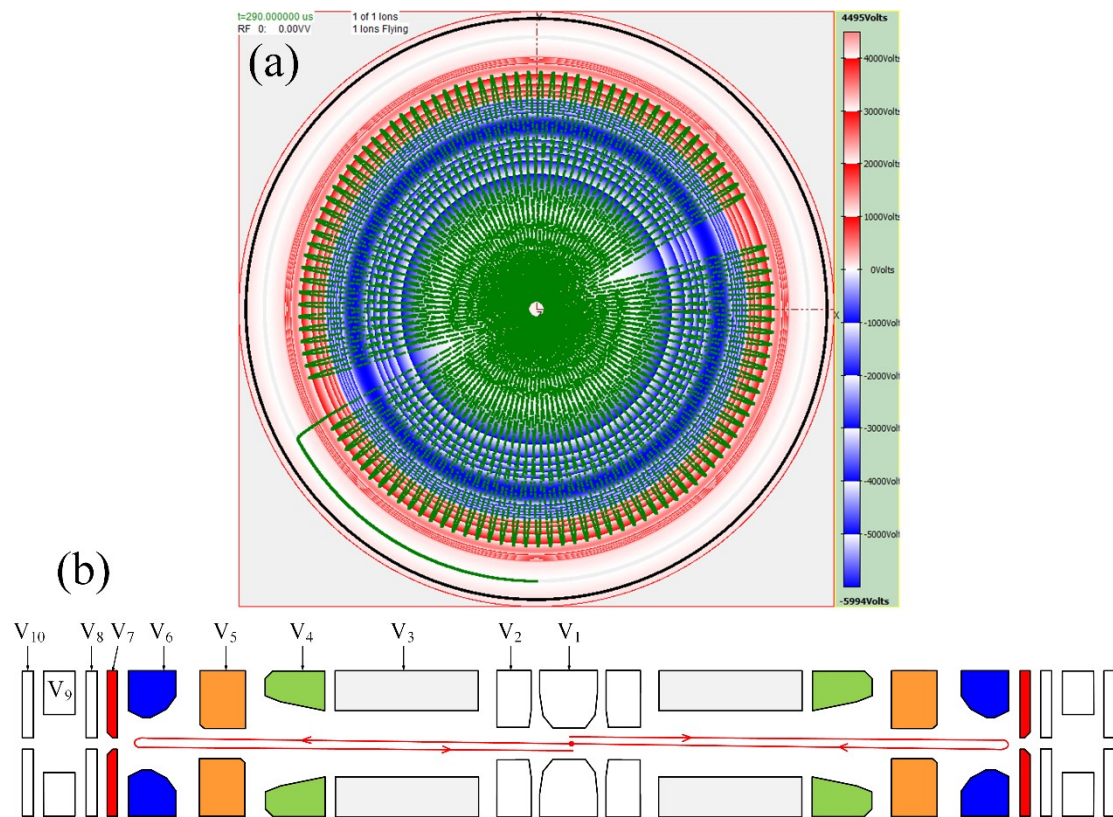

Figure S-1 (a) Simulative ion motion trajectory in the x-y plane within 0.29 ms and voltage distribution (b) Projection of the 3D ion motion trajectory schematic view on the x-z plane, showing the trajectory from parallel to point and then from point to parallel symmetrically.

Genetic Algorithm. A schematic diagram of the operation of GA is shown in the fig. S-2. First, the population is initialized with m number of random set of voltages (chromosomes), which are composed of genes. Then, each chromosome is evaluated according to the fitness function. The best fit chromosomes are selected into the new population. The selected chromosomes are reproduced by reproduction, cross-over and mutation. Thereafter, the new population is exposed to new iteration. The GA stops when the maximum number of generations or termination conditions is reached. Three GA operators, namely reproduction, cross-over, and mutation, are used in the computational code to create the next generation of chromosomes. Reproduction is

operated based on the fitness of the members so that only the most fit members are selected into the mating pool. The cross-over operator selects any two members from the mating pool and randomly exchanges some portion of the genetic codes to create two new offspring. The mutation operator alters one or more genes of the new offspring with a probability equal to the random mutation rate.
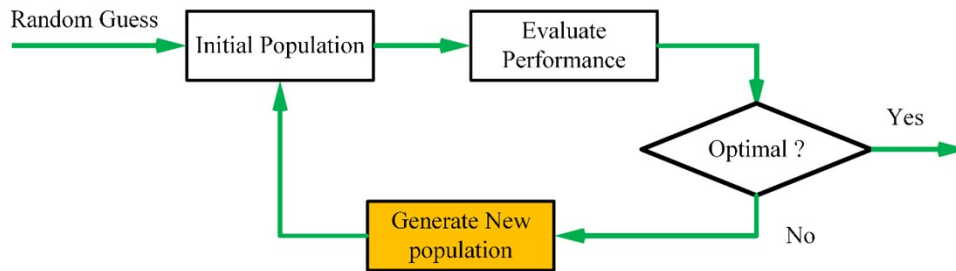
Figure S-2. Schematic diagram of GA operation

Table S1. V_n optimization process with GAPO method for HTD_{max}^p reduction

Iterations	Population	Chromosome				HTD_{max}^p (ns)
		$V_4{}^a$	$V_5{}^b$	$V_6{}^c$	$V_7{}^d$	
	Individual No. 1	-1179	-4340	4608	5712	0.26
	Individual No. 2	-1290	-4923	4088	5094	0.36
Generation 1	…		…			…
	Individual. m-1	-386	-5911	4355	4545	0.22
	Individual. m	-521	-5904	4331	4522	0.15
…	…		…			…
	Individual. 1	-852	-5949	3590	4513	0.009
	Individual. 2	-973	-6115	3540	4448	0.008
Generation n	…		…			…
	Individual. m-1	-765	-5856	3518	4418	0.005
	Individual. m	-710	-5859	3510	4406	0.005

a: operating voltage ranges is 500~-1500 V   b: operating voltage ranges is -4000~-7000 V

c: operating voltage ranges is 3000~6000 V   d: operating voltage ranges is 2500~5500 V

p: 1~m

Simulation Platform

In figure S-3b, it can be noticed that at the beginning, ion from starting point travels around CIG until the time of pulse injection. The ion injected from any part of CIG rapidly form a disc-shaped ion cloud that occupies the whole middle plane of mass analyzer.
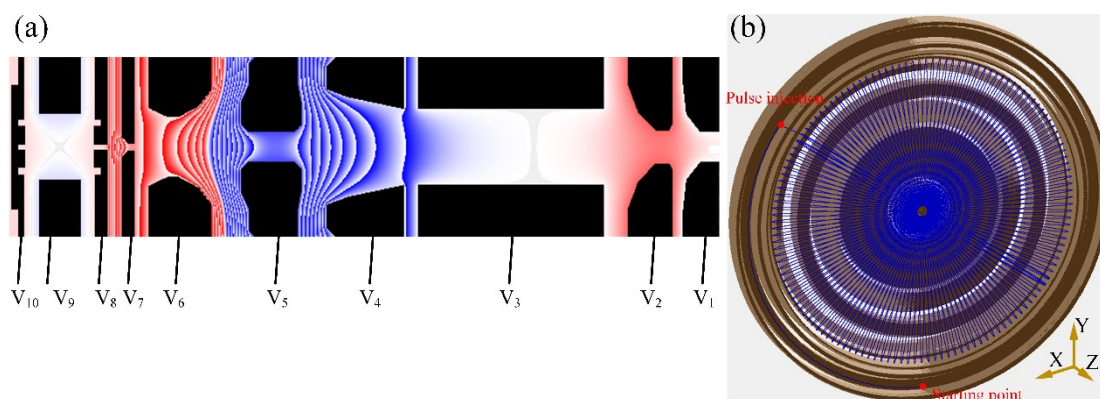

Figure S-3. (a) Potential distribution over the quarter cross-section of the PEIT-7 mass analyzer (b) Simulative ion trajectory (blue line) in the PEIT-7 mass analyzer

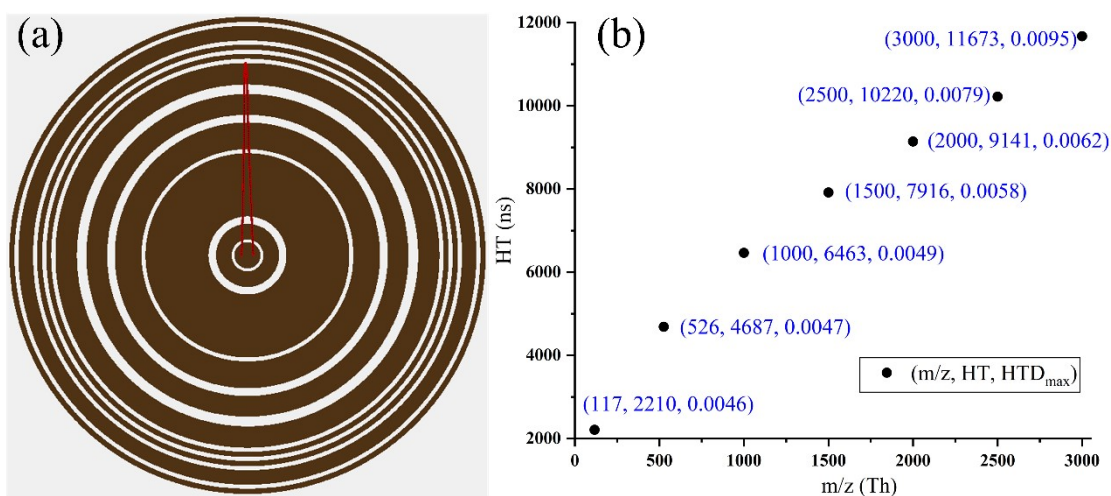## GAPO optimization ion trajectory and results

Figure S-4. (a) Half-turn ion trajectory in the x-y plane(b) Profiles of (HT, HTD_{max}) as a function for different m/z ion

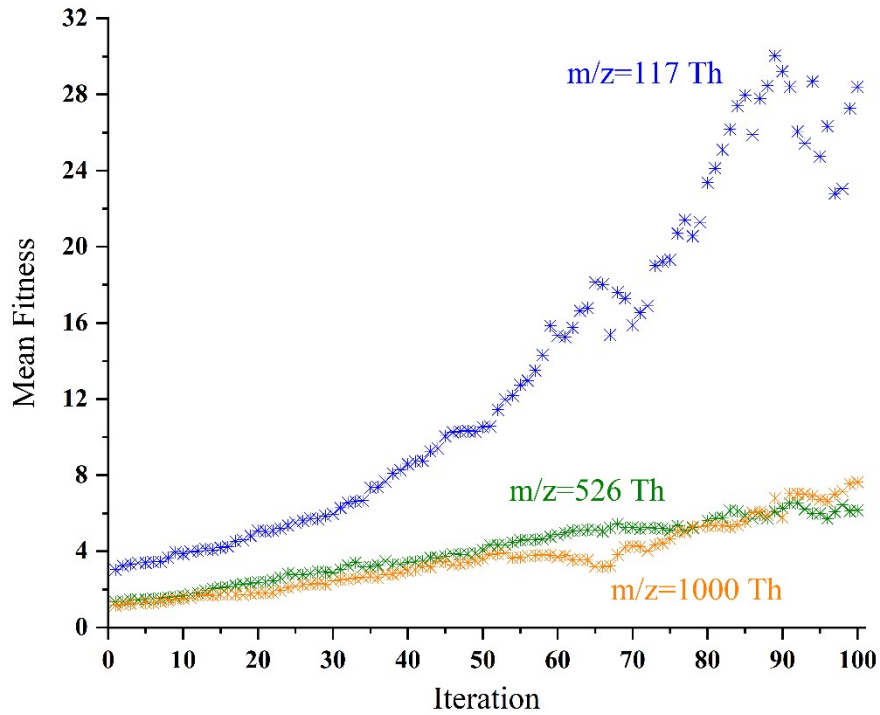## Mean fitness of the ions for different m/z over the iterations

Figure S-5. Mean fitness of the ions for different m/z over the iterations

V_n optimization with GAPO method to reduce HZ_{max}

Finally, based on the minimum HZ_{max}, the chromosome generated at the (100 th iteration, 15 th individual, 17.03 nm) was selected as the optimal chromosome.
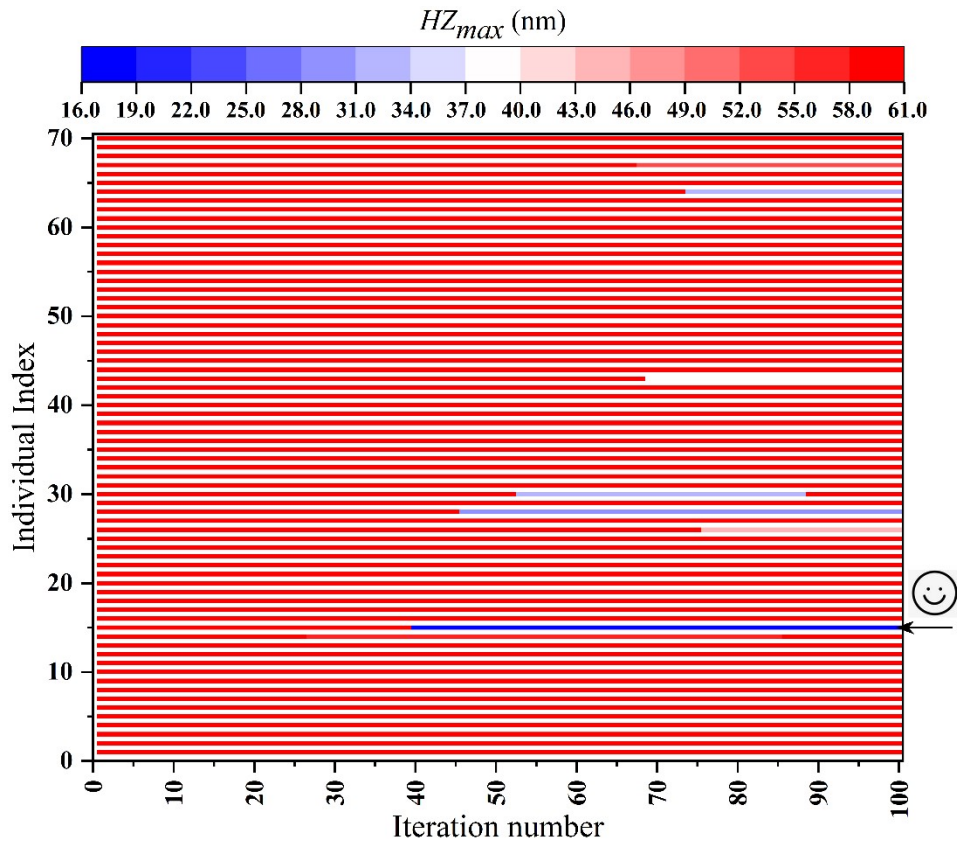
Figure S-6. Contour plot of Vn optimization process for HZ_{max} reduction

Pareto Frontier Points Table

Table S2. The V_n and the obtained HTD_{max} and HZ_{max} with GAPO method

Points	HTD_{max}	HZ_{max}	V4	V5	V6	V7
1	0.06049	0.0889	3274.02073	4183.62594	-5807.10824	-986.82178
2	0.00679	0.17002	3508.48317	4410.44112	-5793.06832	-895.03516
3	0.10082	0.10006	3453.836	4364.699	-5875.23	-1061.88
4	0.00868	0.43176	3537.59658	4448.08745	-5845.72354	-904.4052
5[B]	0.04345	0.08137	3545.80541	4466.96053	-5913.92718	-939.06309
6	0.05295	0.082	3400.41568	4293.687	-5763.90608	-1005.38607
7[C]	0.00744	0.09831	3527.96288	4436.30871	-5846.47683	-937.28815
8	0.09297	0.10999	3449.45244	4354.65705	-5797.66103	-910.46304
9	0.08049	0.08781	3551.374	4478.573	-5905.92	-843.294
10	0.00671	0.14816	3497.56801	4397.13965	-5770.54017	-872.46818
11	0.11769	0.10182	3543.065	4435.152	-5764.5	-894.198
12	0.00626	0.15525	3508.10925	4409.23958	-5785.23003	-881.37266
13	0.03413	0.1085	3540.46187	4446.21458	-5831.77995	-912.4277
14	0.08691	0.10786	3546.05642	4444.06985	-5809.66183	-944.5356
15	0.02273	0.10519	3533.0398	4439.34964	-5830.8203	-910.59604
16	0.11253	0.09908	3557.77565	4453.3296	-5779.47551	-874.57526
17	0.0988	0.09477	3553.6104	4452.33858	-5795.9671	-881.52393
18	0.00774	0.11187	3492.80962	4392.25853	-5793.22782	-939.90754
19	0.01571	0.09855	3515.11641	4422.34685	-5831.99026	-922.15519
20	0.00784	0.26	3510.36117	4414.34019	-5810.34853	-914.6527
21[A]	0.00614	0.13757	3529.93715	4436.72206	-5813.46056	-866.81464
22	0.06595	0.09174	3552.39096	4456.1419	-5822.48982	-894.07774
23	0.08223	0.10074	3539.67085	4437.57538	-5815.45626	-970.94429
24	0.03916	0.09663	3539.67339	4446.01536	-5854.69009	-968.34711
25	0.07437	0.09421	3544.8953	4445.26258	-5795.99703	-872.68352
26	0.05593	0.08753	3482.91226	4389.32793	-5828.20391	-957.81353
27	0.05061	0.08753	3511.99915	4422.60022	-5827.72397	-877.15929
28	0.02696	0.1237	3559.1313	4473.84289	-5881.24276	-909.23621
29	0.04811	0.08573	3533.59323	4437.19934	-5840.1967	-971.39944
30	0.06049	0.0889	3274.02073	4183.62594	-5807.10824	-986.82178

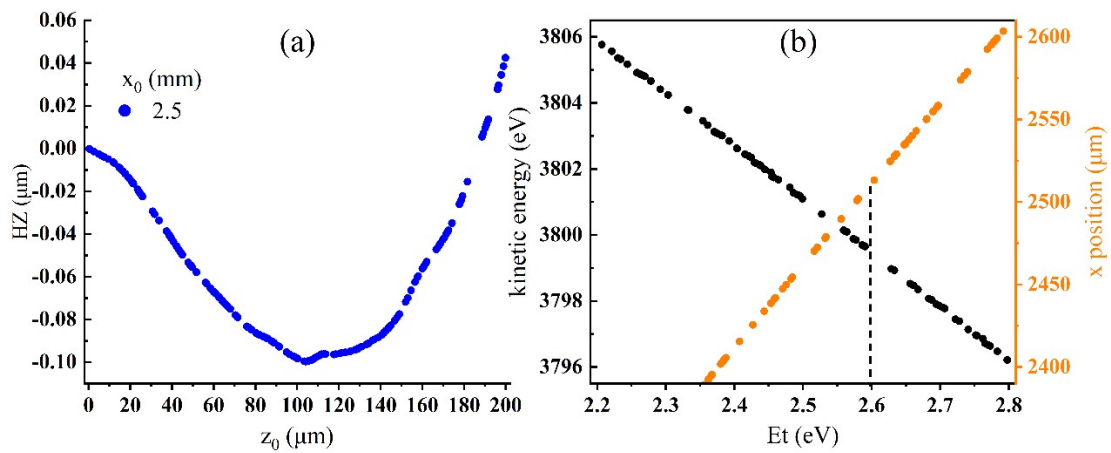## Iso-coordinate property for z_0 spread and kinetic energy and x position as function of E_t

Figure S-7. (a) HZ plot at x_0=2.50 mm **(b)** kinetic energy and x position on the first perihelion as function of E_t

Simulated mass spectra for six groups of ions separated by 0.0005 Th (m/z = 117.0000 Th to 117.0025 Th)
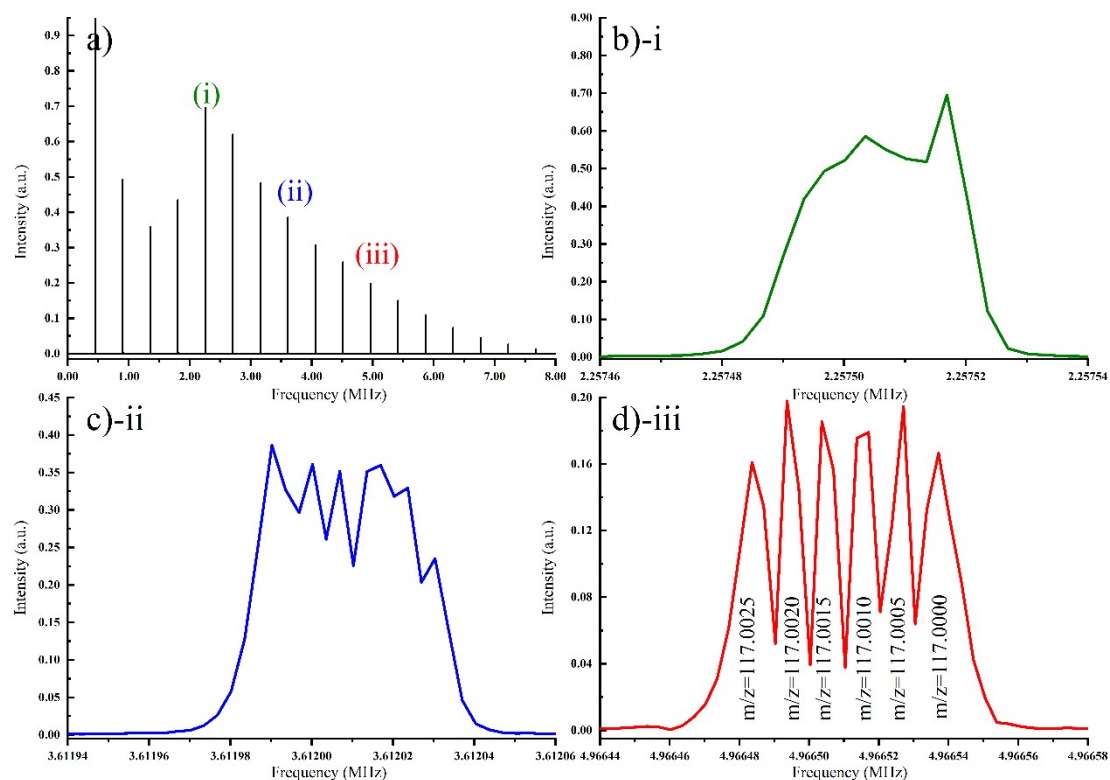

Figure S-8. (a) Simulated mass spectra after FFT with 200 ms from frequency 1~8 MHz, (b) Enlarged mass spectra from frequency 2.25746~2.25754 MHz (c) Enlarged mass spectra from frequency 3.61194~3.61206 MHz (d) Enlarged mass spectra from frequency 4.96644~4.96638 MHz