Supporting Information

An atmospheric pressure ion funnel with a slit entrance for enhancing signal and resolution in high resolution differential ion mobility mass spectrometry

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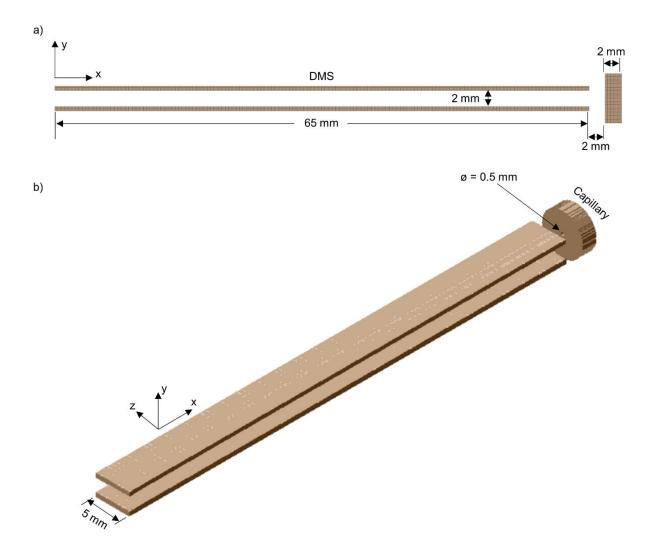


Figure S1: a) Cross-sectional and b) three dimensional views of a DMS-capillary interface.

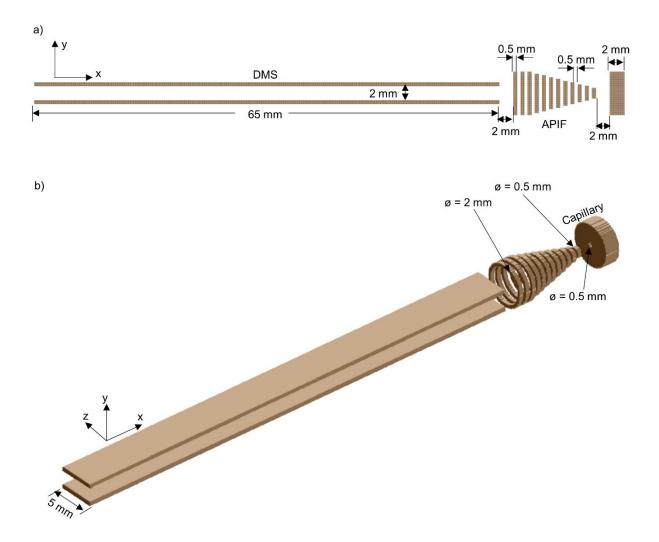


Figure S2: a) Cross-sectional and b) three dimensional views of a DMS-APIF interface.

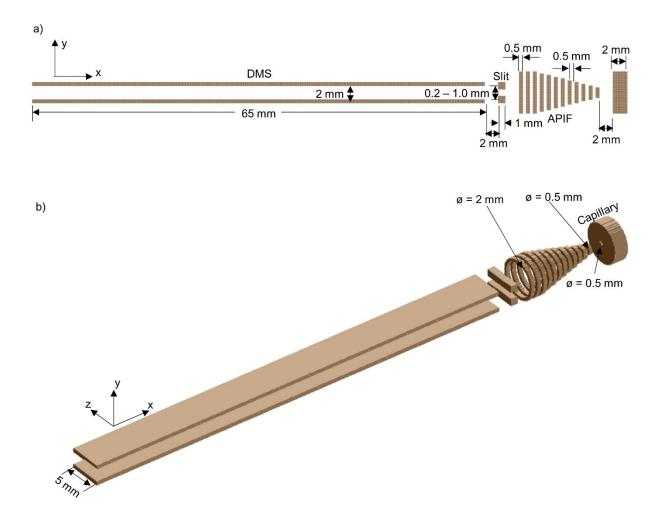


Figure S3: a) Cross-sectional and b) three dimensional views of a DMS-Slit-APIF interface.

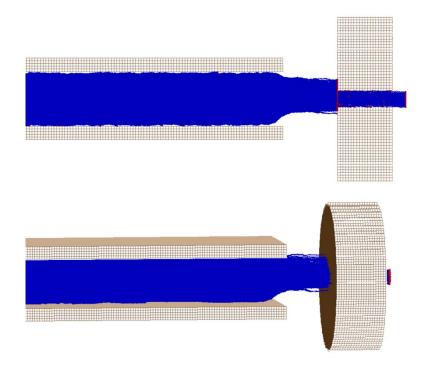


Figure S4: Magnified view of simulated ion trajectories in a DMS-capillary interface for [DMMP+H]+ at a CV of -19.3 V. A carrier gas flow rate, dispersion voltage and APIF RF amplitude of 4.0 L/min, 5.0 kV and 750 V were used.

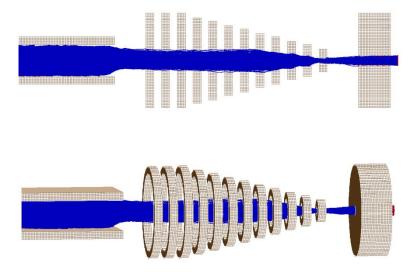


Figure S5: Magnified view of simulated ion trajectories in a DMS-APIF interface for [DMMP+H]+ at a CV of -19.3 V. A carrier gas flow rate, dispersion voltage and APIF RF amplitude of 4.0 L/min, 5.0 kV and 750 V were used.

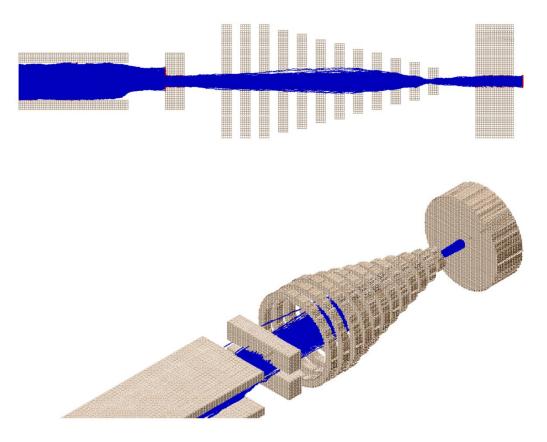


Figure S6: Magnified view of simulated ion trajectories in a DMS-Slit-APIF interface for [DMMP+H]+ at a CV of -19.3 V. A carrier gas flow rate, dispersion voltage and APIF RF amplitude of 4.0 L/min, 5.0 kV and 750 V were used.

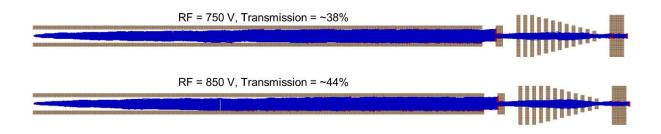


Figure S7: Simulated ion trajectories in a DMS-Slit-APIF interface for [ubiquitin+12H]¹²⁺ at a CV of 13.5 V using different APIF RF amplitudes of 750 and 850 V. A carrier gas flow rate and dispersion voltage of 4.0 L/min and 5.0 kV were used.

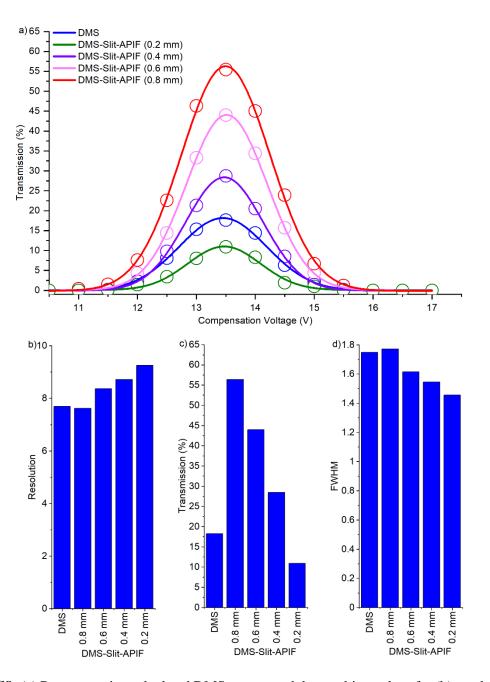


Figure S8: (a) Representative calculated DMS spectra and the resulting values for (b) resolving power, (c) ion transmission efficiency, and (d) FWHM for [ubiquitin+12H]¹²⁺ in a DMS-Slit-APIF interface with different slit gap widths. A carrier gas flow rate, dispersion voltage and APIF RF amplitude of 4.0 L/min, 5.0 kV and 850 V were used.

| Component Parameter | | Value | |
|---------------------|--------------------------|-----------------------------|--|
| | Dispersion voltage | 4-5 kV | |
| DMS | Wave period | 1 µs | |
| | Duty cycle | 0.33 | |
| | | 60 V (DMS model) | |
| | DC biasing voltage | 125 V (DMS-APIF model) | |
| | | 135 V (DMS-Slit-APIF model) | |
| APIF | RF amplitude | 150 to 950 V | |
| | RF frequency | 0.7 MHz | |
| | DC gradient | 5 V/mm | |
| Slit | DC biasing voltage 125 V | | |
| Capillary | DC biasing voltage 50 V | | |

Table S1: Electrical parameters used for simulations

| Parameter | Value | | |
|--------------|--|--|--|
| Pressure | 760 Torr | | |
| Temperature | 298.15 K | | |
| Gas velocity | 3.33 to 6.66 m/s | | |
| Gas mass | 28.94515 amu (N ₂), 4.00 amu (He) | | |
| Collision | 0.366 nm (N ₂), | | |
| gas diameter | 0.260 nm (He) | | |

Table S2: Environmental parameters used for simulations

| Analyte | Mass (u) | Diameter (nm) | Reduced mobility (k ₀) (10 ⁻⁴ m ² V ⁻¹ s ⁻¹) | Mobility constant, α (Td ⁻²) | Mobility constant, β (Td ⁻⁴) |
|--------------------------------|-------------|------------------|---|--|--|
| [DMMP+H] ⁺ | 125.1 | 0.54 | 2.05 | 5.09E-6 | -1.58E-10 |
| [Tryptophan+H] ⁺ | 205.236 | 0.60 | 2.28 | 1.27E-6 | 1.8E-12 |
| $[(2-dodecanone)_2+2H]^+$ | 368.6 | 0.68 | 1.39 | -2.16E-6 | -0.84E-10 |
| [Ubiquitin+12H] ¹²⁺ | 8600 | 0.76 | 1.31 | -2.34E-6 | -1.6E-12 |

Table S3: Ion mobility parameters of simulated ions