

Supplement of Atmos. Meas. Tech., 13, 4111–4121, 2020
<https://doi.org/10.5194/amt-13-4111-2020-supplement>
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Supplement of

Development of an automatic linear calibration method for high-resolution single-particle mass spectrometry: improved chemical species identification for atmospheric aerosols

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Fig.S1 the location of the Fengxian and Fudan university

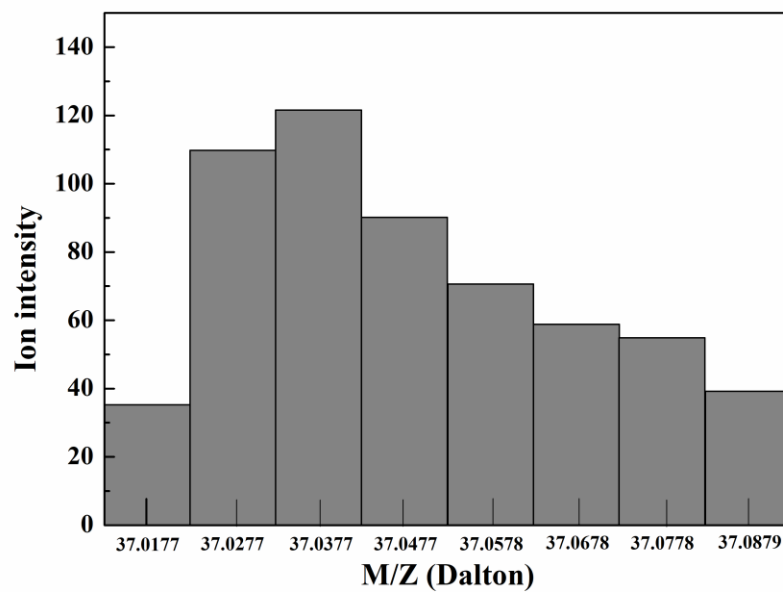
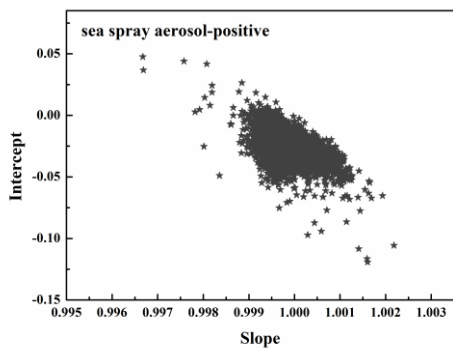
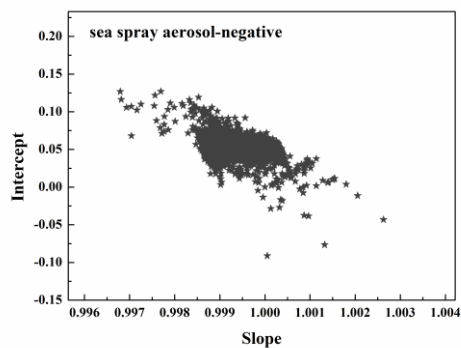


Fig.S2 partial enlarged detail in the single particle mass spectra for the explanation of the m/z bin value

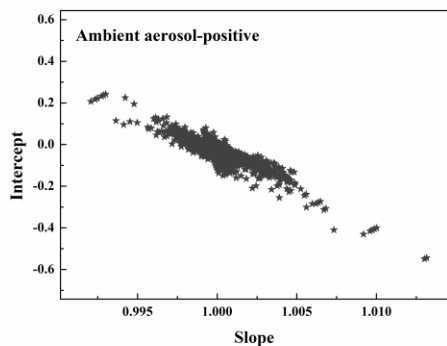


(a) positive ions

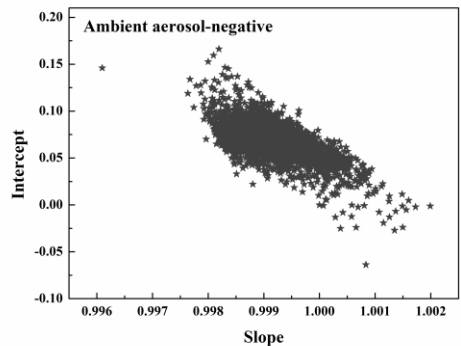


(b) negative ions

Fig.S3 slope-intercept of the sea spray aerosol calibration



(a) positive ions



(b) negative ions

Fig.S4 slope-intercept of the ambient aerosol calibration

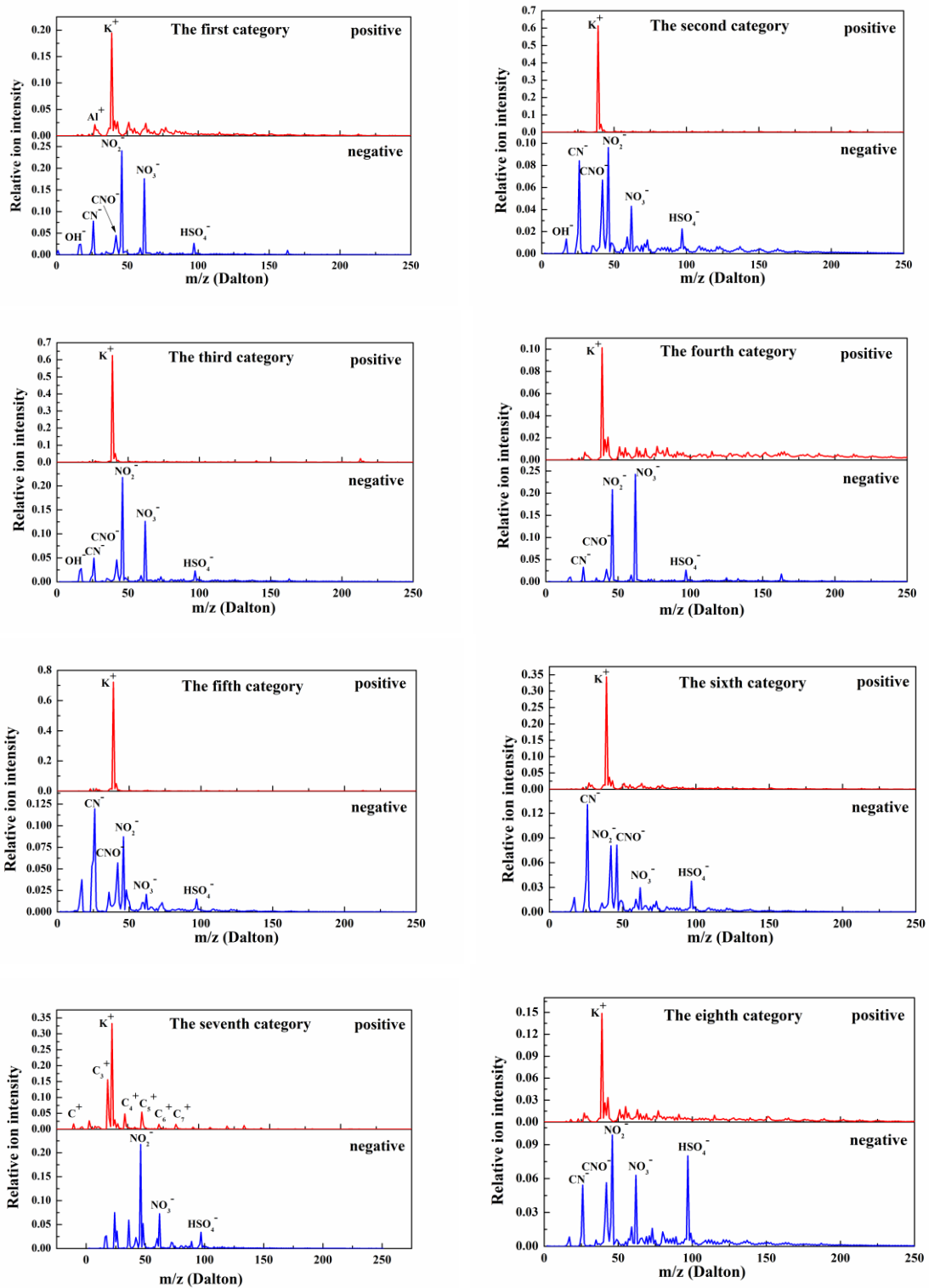


Figure.S5 Classification results of the LR-SPAMS by ART-2a

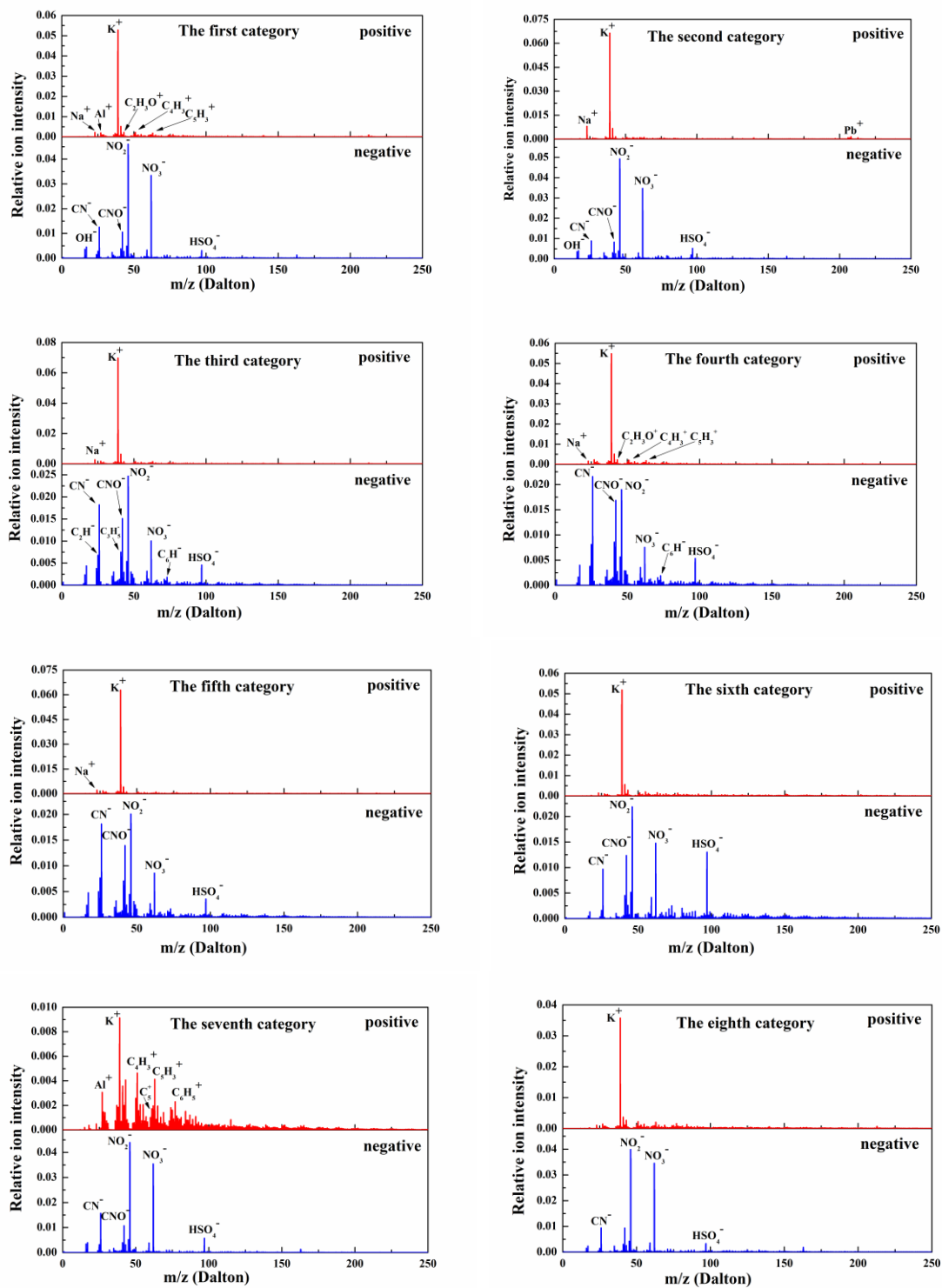


Figure.S6 Classification results of the HR-SPAMS by ART-2a

Table S1 deviation comparison between the averaged positive and negative mass spectra of calibration and non-calibration for sea spray aerosol

| positive species | Theo (m/z) | Theo-bin(m/z) | Noncal-bin(m/z) | $\Delta m/z$ | Cal-bin(m/z) | $\Delta m/z$ | negative species | Theo (m/z) | Theo-bin(m/z) | Noncal-bin(m/z) | $\Delta m/z$ | Cal-bin(m/z) | $\Delta m/z$ |
|---------------------------------|------------|---------------|-----------------|--------------|--------------|--------------|--------------------------------|------------|---------------|-----------------|--------------|--------------|--------------|
| Na ⁺ | 22.98977 | 22.993 | 23.0167 | 0.0237 | 22.993 | 0 | CN ⁻ | 26.00307 | 25.9994 | 25.9658 | - | 26.0078 | 0.0084 |
| Mg ⁺ | 23.98505 | 23.9829 | 24.0072 | 0.0243 | 23.9829 | 0 | Cl ⁻ | 34.96885 | 34.9641 | 34.9349 | - | 34.9641 | 0 |
| K ⁺ | 38.96371 | 38.9672 | 38.998 | 0.0288 | 38.9672 | 0 | Cl ⁻ | 36.9659 | 36.9622 | 36.9321 | - | 36.9622 | 0 |
| Na ₂ Cl ⁺ | 80.94839 | 80.9438 | 80.9883 | 0.0445 | 80.9438 | 0 | CNO ⁻ | 41.99799 | 41.9971 | 41.965 | - | 41.9864 | 0.0107 |
| Na ₂ Cl ⁺ | 82.94544 | 82.9421 | 82.9871 | 0.045 | 82.9421 | 0 | NaCl ⁻ | 57.95862 | 57.9574 | 57.9448 | - | 57.9574 | 0 |
| K ₂ Cl ⁺ | 112.89627 | 112.898 | 112.951 | 0.053 | 112.898 | 0 | MgCl ₃ ⁻ | 128.89161 | 128.883 | 128.939 | 0.056 | 128.901 | 0.018 |
| K ₂ Cl ⁺ | 114.89332 | 114.885 | 114.938 | 0.053 | 114.885 | 0 | MgCl ₃ ⁻ | 130.88866 | 130.894 | 130.932 | 0.038 | 130.894 | 0 |
| | | | | | | | MgCl ₃ ⁻ | 132.88571 | 132.884 | 132.941 | 0.057 | 132.884 | 0 |

Table S2 deviation comparison between the averaged positive and negative mass spectra of calibration and non-calibration for ambient aerosol

| positive species | Theo (m/z) | Theo-bin(m/z) | Noncal-bin(m/z) | $\Delta m/z$ | Cal-bin(m/z) | $\Delta m/z$ | negative species | Theo (m/z) | Theo-bin(m/z) | Noncal-bin(m/z) | $\Delta m/z$ | Cal-bin(m/z) | $\Delta m/z$ |
|-----------------------------|------------|---------------|-----------------|--------------|--------------|--------------|-------------------------------|------------|---------------|-----------------|--------------|--------------|--------------|
| C ⁺ | 12 | 11.9991 | 12.0105 | 0.0114 | 12.0048 | 0.0057 | | | | | - | | |
| Na ⁺ | 22.98977 | 22.993 | 23.0167 | 0.0237 | 22.993 | 0 | CN ⁻ | 26.00307 | 25.9994 | 25.9658 | 0.0336 | 26.0078 | 0.0084 |
| C ₃ ⁺ | 36 | 36.0023 | 36.032 | 0.0297 | 35.9925 | - | Cl ⁻ | 34.96885 | 34.9641 | 34.9349 | - | 34.9641 | 0 |
| | | | | | | 0.0098 | | | | | 0.0292 | | |
| K ⁺ | 38.9672 | 38.9672 | 38.998 | 0.0308 | 38.9672 | 0 | NO ₂ ⁻ | 45.99291 | 45.9897 | 45.9673 | - | 45.9897 | 0 |
| Fe ⁺ | 55.93494 | 55.932 | 55.9813 | 0.0493 | 55.9443 | 0.0123 | | | | | 0.0224 | | |
| Pb ⁺ | 207.97664 | 207.967 | 208.014 | 0.047 | 207.967 | 0 | NO ₃ ⁺ | 61.98783 | 61.9938 | 61.9678 | -0.026 | 61.9808 | -0.013 |
| Pb ⁺ | 205.97446 | 205.976 | 206.023 | 0.047 | 205.976 | 0 | SO ₄ ⁻ | 95.95175 | 95.9502 | 96.031 | 0.0808 | 95.9663 | 0.0161 |
| Pb ⁺ | 206.97589 | 206.97 | 207.018 | 0.048 | 206.994 | 0.024 | HSO ₄ ⁻ | 96.95958 | 96.9546 | 96.9709 | 0.0163 | 96.9546 | 0 |

Table S3 deviation comparison between the averaged positive and negative mass spectra of calibration and non-calibration for ambient aerosol with additional marker ions

| positive species | Theo (m/z) | Theo-bin(m/z) | Noncal-bin(m/z) | $\Delta m/z$ | Cal-bin(m/z) | $\Delta m/z$ | negative species | Theo (m/z) | Theo-bin(m/z) | Noncal-bin(m/z) | $\Delta m/z$ | Cal-bin(m/z) | $\Delta m/z$ |
|-----------------------------|------------|---------------|-----------------|--------------|--------------|--------------|-------------------------------|------------|---------------|-----------------|--------------|--------------|--------------|
| C ⁺ | 12 | 11.9991 | 12.0105 | 0.0114 | 11.9877 | - | CN ⁻ | 26.00307 | 25.9994 | 25.9658 | - | 26.0078 | 0.0084 |
| Na ⁺ | 22.98977 | 22.993 | 23.0167 | 0.0237 | 22.993 | 0 | Cl ⁻ | 34.96885 | 34.9641 | 34.9349 | - | 34.9641 | 0 |
| C ₃ ⁺ | 36 | 36.0023 | 36.032 | 0.0207 | 36.0023 | 0 | NO ₂ ⁻ | 45.99291 | 45.9897 | 45.9673 | - | 45.9897 | 0 |
| K ⁺ | 38.9672 | 38.9672 | 38.998 | 0.0308 | 38.9672 | 0 | NO ₃ ⁺ | 61.98783 | 61.9938 | 61.9678 | -0.026 | 61.9808 | -0.013 |
| Fe ⁺ | 55.93494 | 55.932 | 55.9813 | 0.0493 | 55.9566 | 0.0246 | SO ₄ ⁻ | 95.95175 | 95.9502 | 96.0148 | 0.0646 | 95.9663 | 0.0161 |
| Pb ⁺ | 207.97664 | 207.967 | 208.038 | 0.071 | 207.967 | 0 | HSO ₄ ⁻ | 96.95958 | 96.9546 | 96.9709 | 0.0163 | 96.9546 | 0 |
| Pb ⁺ | 205.97446 | 205.976 | 206.047 | 0.071 | 205.976 | 0 | | | | | | | |
| Pb ⁺ | 206.97589 | 206.97 | 207.041 | 0.071 | 206.994 | 0.024 | | | | | | | |

Notes: Theo(m/z): Theoretical m/z value; Theo-bin(m/z): Theoretical m/z bin value;
 Noncal-bin(m/z): Non-calibration m/z bin value. Cal bin(m/z): Calibration m/z bin value.

