Supporting Information

Non-polar modifier assisted analysis of aromatic compounds by means of planar differential ion mobility spectrometry with ^{63}Ni ionization source

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Description: Contains 3 Figures.

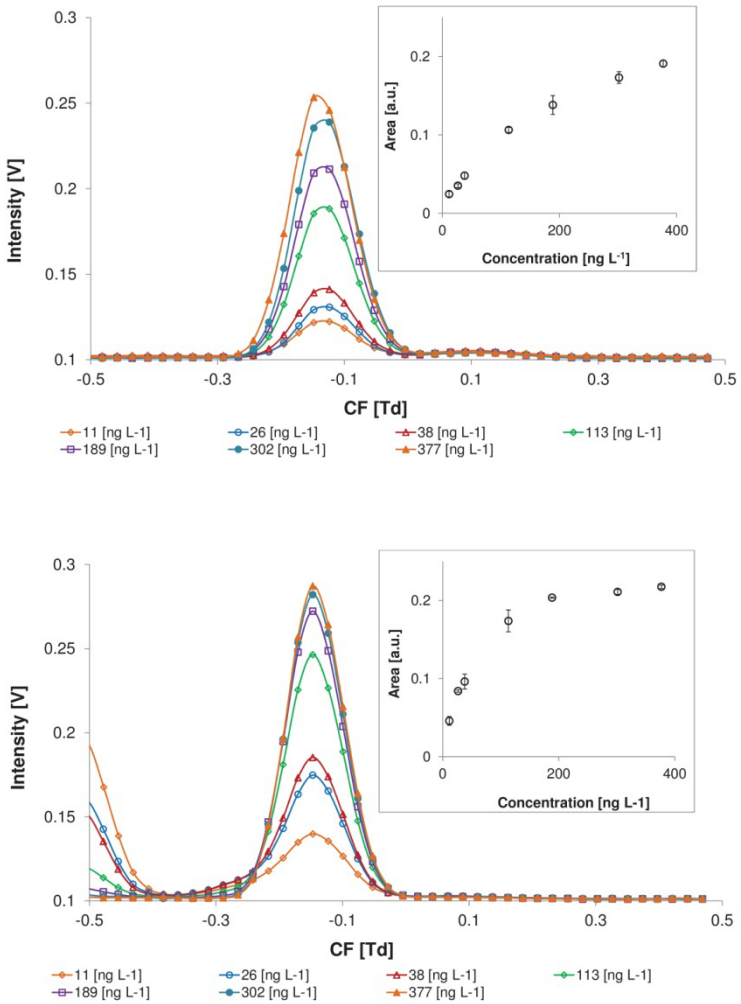

Fig. S-1: Differential mobility spectra of 1,2,4-trimethylbenzene at different concentrations without modifier (top) and with 0.015 % of benzene (bottom) in the carrier gas.

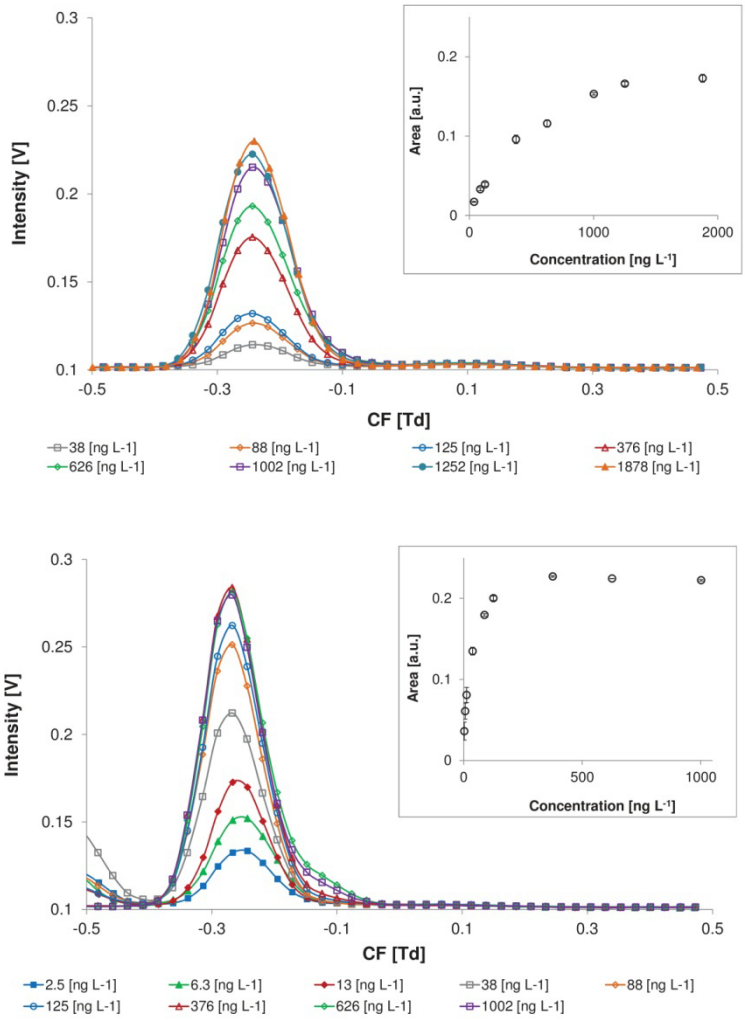

Fig. S-2: Differential mobility spectra of *p*-xylene at different concentrations without modifier (top) and with 0.015 % of benzene (bottom) in the carrier gas.

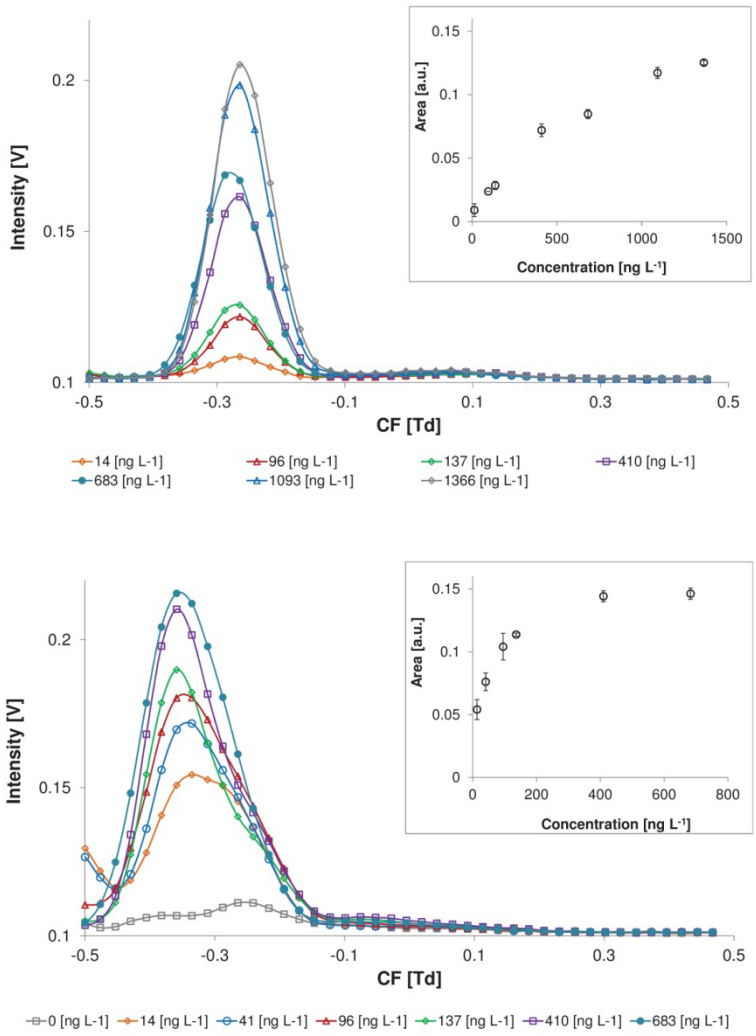

Fig. S-3: Differential mobility spectra of ethylbenzene at different concentrations without modifier (top) and with 0.015 % of benzene (bottom) in the carrier gas.

The relevant equations for the non linear calibration.

The coefficients $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$ for the calibration function $\boldsymbol{y = a + bx + cx^2}$ can be calculated as follows:

$Q_{xx} = \sum_{i=1}^{n} x_i^2 - \frac{(\sum_{i=1}^{n} x_i)^2}{n}$;

$Q_{xy} = \sum_{i=1}^{n} (x_i y_i) - \frac{(\sum_{i=1}^{n} x_i)(\sum_{i=1}^{n} y_i)}{n}$;

$Q_{xx^2} = \sum_{i=1}^{n} x_i^3 - \frac{(\sum_{i=1}^{n} x_i)(\sum_{i=1}^{n} x_i^2)}{n}$;

$Q_{x^2y} = \sum_{i=1}^{n} (x_i^2 y_i) - \frac{(\sum_{i=1}^{n} x_i^2)(\sum_{i=1}^{n} y_i)}{n}$;

$Q_{x^2x^2} = \sum_{i=1}^{n} x_i^4 - \frac{(\sum_{i=1}^{n} x_i^2)^2}{n}$;

$c = \frac{Q_{x^2y} Q_{xx} - Q_{xy} Q_{xx^2}}{Q_{xx} Q_{x^2x^2} - (Q_{xx^2})^2}$;

$b = \frac{Q_{xy} Q_{x^2x^2} - Q_{x^2y} Q_{xx^2}}{Q_{xx} Q_{x^2x^2} - (Q_{xx^2})^2}$;

$a = \overline{y} - b\overline{x} - \frac{c \sum_{i=1}^{n} x_i^2}{n}$;

The residual standard deviation:

$s_y = \sqrt{\frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{n-3}}$;

Limit of detection:

$y_{lod} = a + 3s_y$;

$LOD = \frac{-b + \sqrt{b^2 - 4c(a - y_{lod})}}{2c}$;

y_i = individual values for each dependent variable (peak area);

x_i = individual values for each independent variable (concentration);

n = number of points;

$\overline{x}$ and $\overline{y}$ = average of the x and y values;

$\hat{y} = a + bx_i + cx_i^2$;