3.2. Analyses of Haloacetic Acids and Phenols

We also conducted the analyses of 3 haloacetic acids (monochloroacetic acid, dichloroacetic acid, trichloroacetic acid) and 4 phenols (phenol, 2-chlorophenol, 2,4-dichlorophenol, 2,4,6-trichlorophenol) by using the Nexera X2 UHPLC system (Shimadzu Corporation, Japan) coupled with the LCMS-8060NX to confirm the improvement of the sensitivity by applying the higher RF voltage to the ion guide at higher pressure vacuum region. The multiple reaction monitoring (MRM) transition of each compound was as shown in Table 1.

4. Result

4.1. Ion Trajectory Simulation

The examples of result of gas dynamics simulation and ion trajectory simulation considering gas dynamics are shown in Fig.3 and Fig.4 respectively. According to the results, it was found that in case of the analysis of the low-mass molecular ions (at m/z of 150 or smaller), the amplitude of the radio frequency (RF) voltage of the ion guide to converge ions sufficiently was higher than the theoretical value. This is because the low-mass molecular ions easily collide with gas molecules and diffuse at a higher pressure vacuum region, we think.

5. Conclusions

Improve the sensitivity of low-mass compounds (at m/z of 150 or smaller) by increasing ion transmission efficiency based on the ion trajectory simulation considering gas dynamics at the higher pressure vacuum region.

Table 1: MRM transitions of the target compounds

<table>
<thead>
<tr>
<th>Compound Type</th>
<th>Compound Name</th>
<th>MRM Transition</th>
</tr>
</thead>
<tbody>
<tr>
<td>haloacetic</td>
<td>monochloroacetic acid (MCIA)</td>
<td>93.0 &gt; 35.0</td>
</tr>
<tr>
<td></td>
<td>dichloroacetic acid (DCIA)</td>
<td>127.0 &gt; 82.9</td>
</tr>
<tr>
<td></td>
<td>trichloroacetic acid (TCIA)</td>
<td>161.0 &gt; 118.9</td>
</tr>
<tr>
<td>phenols</td>
<td>phenol</td>
<td>93.0 &gt; 65.0</td>
</tr>
<tr>
<td></td>
<td>2-chlorophenol</td>
<td>127.0 &gt; 35.1</td>
</tr>
<tr>
<td></td>
<td>2,4-dichlorophenol</td>
<td>161.0 &gt; 35.1</td>
</tr>
<tr>
<td></td>
<td>2,4,6-trichlorophenol</td>
<td>104.0 &gt; 35.1</td>
</tr>
</tbody>
</table>

Fig.2 The Nexera and the LCMS-8060NX LC-MS/MS system

Fig.3 An example of result of gas dynamics simulation at a higher vacuum region

Fig.4 An example of result of ion trajectory simulation at a higher vacuum region