**TABLE 1.** User defined modifications in Skyline for quantifying BS\(^3\) cross-linked peptides.

<table>
<thead>
<tr>
<th>Modification</th>
<th>Chemical formula</th>
<th>Amino acid</th>
<th>Variable modifications</th>
<th>Calculated mass by Skyline</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mod:BS3-OH(KSTY)</td>
<td>H(<em>{12})C(</em>{8})O(_{3})</td>
<td>K,S,T,Y</td>
<td>Yes</td>
<td>156.078644</td>
</tr>
<tr>
<td>Mod:BS3-NH(_{2}(KSTY))</td>
<td>H(<em>{13})C(</em>{8})O(_{2})N</td>
<td>K,S,T,Y</td>
<td>Yes</td>
<td>155.094629</td>
</tr>
<tr>
<td>Mod:BS3d4-OH(KSTY)*</td>
<td>H(<em>{8})C(</em>{8})O(<em>{3})H'(</em>{4})</td>
<td>K,S,T,Y</td>
<td>Yes</td>
<td>160.103751</td>
</tr>
<tr>
<td>Mod:BS3d4-NH(_{2}(KSTY))*</td>
<td>H(<em>{9})C(</em>{8})O(<em>{2})NH'(</em>{4})</td>
<td>K,S,T,Y</td>
<td>Yes</td>
<td>159.119736</td>
</tr>
<tr>
<td>LinkSite(KSTY)</td>
<td>H</td>
<td>K,S,T,Y</td>
<td>Yes</td>
<td>1.007828</td>
</tr>
<tr>
<td>Xlink:BS3-link</td>
<td>C(<em>{2})H(</em>{3})-N</td>
<td>E</td>
<td>Yes</td>
<td>25.020401</td>
</tr>
<tr>
<td>Xlink:BS3d4-link*</td>
<td>C(<em>{2})H'(</em>{4})-NH</td>
<td>E</td>
<td>Yes</td>
<td>29.040508</td>
</tr>
</tbody>
</table>

\[1\]. Modifications marked with “*” are only defined and applied when quantifying using isotope labelled cross-linkers.