Supporting Information

Table S1. Structures by group using the clustering tool of Gromacs and % of structures collected in the first five groups.

<table>
<thead>
<tr>
<th>Group</th>
<th>Non-phosphorylated peptide</th>
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</thead>
<tbody>
<tr>
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<td>Free</td>
<td>N1</td>
<td>N2</td>
<td>N3</td>
<td>N4</td>
<td>N5</td>
<td>N6</td>
</tr>
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<td>234</td>
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<td>135</td>
<td>94</td>
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<td>128</td>
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<tr>
<td>% Structures</td>
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<td>62.7</td>
<td>54.5</td>
<td>62.2</td>
<td>61.3</td>
<td>99.9</td>
<td>97.8</td>
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<table>
<thead>
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<th>Group</th>
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<td>P3</td>
<td>P4</td>
<td>P5</td>
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<td>142</td>
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<td>52.7</td>
<td>50.0</td>
<td>94.3</td>
<td>64.0</td>
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</tbody>
</table>

Note S1

The geometry optimizations of the aluminum complexes with the phosphorylated derivative displayed some proton transfer from water molecules to the closer carboxyl group; in the P1 went to E2, in P2 went to E4, in P3 double proton transfer to \( \text{PO}_4 \), and in P4 and P5 none proton transfer.