Supporting Information

Table S1 The contribution of energy for important individual amino acid residues towards the binding free energies computed by the MM/GBSA method (energies are in kcal·mol⁻¹): (1) WT, (2) A252D, (3) A252D/D126A, (4) A252D/D127A, (5) A252D/D126A/D127A.

<table>
<thead>
<tr>
<th>Residue</th>
<th>Mg²⁺·Ca²⁺·Ca²⁺</th>
<th>Mn²⁺·Mn²⁺·Mn²⁺</th>
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<tr>
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<tr>
<td>Arg⁺</td>
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<td>Gly⁺</td>
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<td>Asp¹⁰⁹</td>
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<tr>
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<td>Tyr¹²²</td>
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<tr>
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<tr>
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<td>Glu²²⁰</td>
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<td>Asp¹¹³</td>
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<td>Met¹³⁵</td>
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* represents Ligand RGD