**In silico** Studies of Parasporin Proteins: Structural and Functional Insights and Proposed Cancer Cell Killing Mechanism for Parasporin 5 and 6

Nasima Aktar\(^{a,b}\), Muhammad Manjurul Karim\(^a\), Shakila Nargis Khan\(^a\), Mustafizur Rahman\(^c\), Anowara Begum\(^a\), Md. Mozammel Hoq\(^a\)*

Supplementary Information
S. Figure 1: Ligand-receptor domain binding orientation of different parasporin protein. Endotoxin_N (4ARX) domain of class 1 and 6 acts as ligand to bind with 2RH1, 5GLI, 1EDN, 3RZE, 3TYF, 4DAJ and 4XNV receptor molecule of HeLa cells (1-7). Moreover, class 1 interacts with 1NKG domain (8-14); Class 5 interacts with HeLa cells through ETX-MTX2 (1UYJ) ligand (15-21); Class 2 parasporin interacts with 2MPM, 2LNL, 3ODU, 4JL7, 4NY9 and 5X33 receptor of HL-60 cells through ETX-MTX2 (1UYJ) domain (22-27); Aerolysin (2PRE) domain (28-33) and Duf916 (1QLE) domain (34-39); 4ARX, 4ION and 4OWL ligand of Class 3 interacts with 2MPM, 2LNL, 3ODU, 4JL7, 4NY9 and 5X33 receptor of HL-60 cells (40-57); Class 4 ETX-MTX2 ligand molecule (1UYJ) and binds with 1XXZ receptor of CACO-2 cells (58).
Supplementary Tables

S. Table 1: *Physico-chemical parameters of different parasporin proteins*

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https://doi.org/10.25163/microbbioacts.21007A0621280219
| PS2Aa1 | 338 | Bacterial cytoplasm | 0.567 | Soluble | None | 316 | -80.18 (8.001545e-01) | 5.35 | 63.11 | 34.26 Stable | -0.433 | 0.161 | 146-163 (I to O) | 356 |
| PS2Aa2 | 338 | Bacterial cytoplasm | 0.531 | Soluble | None | 316 | -80.03 (7.981347e-01) | 5.21 | 62.54 | 34.09 Stable | -0.441 | 0.164 | 146-163 (I to O) | 356 |
| PS2Ab1 | 304 | Bacterial cytoplasm | 0.320 | Soluble | None | 287 | -34.04 (7.962966e-02) | 5.12 | 75 | 39.99 Stable | -0.258 | 0.126 | 254-276 (I to O) | 109 |
| PS3Aa1 | 825 | Bacterial membrane | 0.183 | Soluble | None | 802 | -66.14 (5.584945e-01) | 6.18 | 76.22 | 30.98 Stable | -0.496 | 0.183 | 75-99 (I to O) | 1655 |
| PS3Ab1 | 829 | Bacterial membrane | 0.183 | Soluble | None | 806 | -66.14 (5.584945e-01) | 6.19 | 75.16 | 31.41 Stable | -0.508 | 0.167 | 75-99 (I to O) | 1655 |
| PS4Aa1 | 275 | Bacterial cytoplasm | 0.286 | Soluble | None | 261 | -40.05 (1.280721e-01) | 6.09 | 81.16 | 29.03 Stable | -0.171 | 0.201 | 17-37 (I to O) | 204 |
| PS5Aa1 | 305 | Bacterial cytoplasm | 0.602 | Soluble | None | 276 | -59.46 (4.238438e-01) | 5.99 | 72.85 | 35.57 Stable | -0.439 | 0.126 | 158-176 (I to O) | 392 |
| PS6Aa1 | 753 | Bacterial Cytoplasm | 0.450 | Soluble | None | 736 | -52.36 (2.919484e-01) | 5.75 | 94.79 | 33.39 Stable | -0.226 | 0.205 | 96-116 (I to O) | 240 |

https://doi.org/10.25163/microbbioacts.21007A0621280219
S. Table 2: **3D structural properties of parasporin proteins**

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S. Table 4: Domain Information of parasporin proteins

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Domain | PR | Location | Database Used | E-value | Biological Function | Family | Domain | Clan | Location | Database | E-value |

https://doi.org/10.25163/microbioacts.21007A0621280219
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- Pfam domains are listed with their respective E-values.
- GO:0009405 pathway is associated with pathogenesis.
- Endotoxin_N and Delta endotoxin, N-terminal domain are identified.
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<td>N/a</td>
<td>327 – 530</td>
<td>Pfam 9.5e-11</td>
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<td>333 – 421 GENE3 D 2.0E-8</td>
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<td>Delta endotoxin, central domain, subgroup 1</td>
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<td>Pfam 9.5E-11</td>
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<td>Endotoxin_C delta endotoxin</td>
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<td>540 – 681</td>
<td>Pfam 7.2e-37</td>
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<td>Galactose-binding domain-like</td>
<td>IPR0 513 – 685</td>
<td>GENE3 D 1.2E-51</td>
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<td>RicinB_lectin_2 Ricin-type beta-trefoil lectin domain-like</td>
<td>CL0 202</td>
<td>715 – 816</td>
<td>Pfam 1.6e-15</td>
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<td>532 – 681 SUPER FAMIL Y 4.89E-37</td>
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<tr>
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<td>Delta endotoxin, C-terminal</td>
<td>IPR0 540 – 681</td>
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<td>PS4Aa1</td>
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<td>IPR0 39 – 186</td>
<td>GENE3D</td>
<td>1.2E-24</td>
<td>-</td>
<td>Clostridium epsilon toxin ETX/Bacillus mosquitocidal toxin MTX2</td>
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<td>33–252</td>
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<td>ETX_MTX2</td>
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<td>Cl0 13–276</td>
<td>Pfam 5.4e-27</td>
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<td>IPR0</td>
<td>128 – 355</td>
<td>Gene3 D</td>
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<td>GO:0009405 pathogenesis</td>
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S. Table 5: *Parasporin protein and their probable ligand identification*

<table>
<thead>
<tr>
<th>PS Proteins</th>
<th>Domain</th>
<th>Ligand (PDB)</th>
<th>Ligand present (PDB)</th>
<th>Ligand present (RaptorX)</th>
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<tr>
<td>PS1Aa1</td>
<td>Endotoxin</td>
<td>4ARX</td>
<td>GOL, 13D</td>
<td>BR, NGA, 13D, SO₄</td>
</tr>
<tr>
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<td>Endotoxin</td>
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<td>GOL, 13D</td>
<td>BR, NGA, 13D, SO₄</td>
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<td>GOL, 13D</td>
<td>BR, NGA, 13D, SO₄, DOC, ZN, C2E, CL</td>
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<td>BR, NGA, 13D, SO₄, GUN, ZEA, NA, NEU</td>
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<td>GOL, 13D</td>
<td>BR, NGA, 13D, SO₄</td>
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<td>PS1Ac1</td>
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<td>BR, NGA, 13D, SO₄</td>
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<td>BR, NGA, 13D, SO₄</td>
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https://doi.org/10.25163/microbioacts.21007A0621280219
### Table 6: Parasporin class showing higher toxicity cancer cell lines, their receptors with PDB ID and probable ligands with which they tend to bind/interact

<table>
<thead>
<tr>
<th>Parasporin Protein</th>
<th>Cell Line</th>
<th>Receptors</th>
<th>PDB ID of Receptors</th>
<th>Binding site for Residue</th>
<th>Ligand with whom they Bind</th>
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<tr>
<td>PS 1, 5 and 6</td>
<td>Hela</td>
<td>1. Adrenergic β2</td>
<td>2RH1</td>
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<td>CLR</td>
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<td>SO4</td>
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<td>2RH1_A_BC2_5_412</td>
<td>CLR</td>
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<td>BU1</td>
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<td>Compounds</td>
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<td>Source</td>
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<td>2RH1_A_AC1_9_401</td>
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<td>2. Endothelin Type-B</td>
<td>5GLI</td>
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<td>Endothelin-1</td>
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<td>3. Histamine H1</td>
<td>3RZE</td>
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<td>4. Lysophospholipid</td>
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<td>5. Muscarinic</td>
<td>4DAJ</td>
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| 6. Purinoceptor | 4XNV   | 4XNV_A_AC9_4_1109 | OLC  |
|                |        | 4XNV_A_AD2_5_1111 | OLC  |
|                |        | 4XNV_A_AC1_10_1101| BUR  |
|                |        | 4XNV_A_AC5_7_1105 | Y01  |
|                |        | 4XNV_A_AC4_5_1104 | Y01  |
|                |        | 4XNV_A_AD1_6_1110 | OLC  |
|                |        | 4XNV_A_AC8_3_1108 | OLC  |
|                |        | 4XNV_A_AC7_5_1107 | OLC  |
|                |        | 4XNV_A_AC2_4_1102 | CLR  |
|                |        | 4XNV_A_AD3_5_1112 | OLC  |
|                |        | 4XNV_A_AD4_6_1113 | OLC  |
|                |        | 4XNV_A_AC3_4_1103 | Y01  |
|                |        | 4XNV_A_AD6_4_1115 | ZN   |

<p>| PS 2, 3 &amp; 4    | HL-60  | Chemokine CCR1   | 4NY9 | 4NY9_A_AC2_7_502 | GOL|
|                |        |                 |      | 4NY9_A_AC1_9_501 | 2Q4|
|                |        | Chemokine CCR3   | 2MPM | N/A               |
|                |        | Chemokine CXCR1  | 2LNL | N/A               |
|                |        | Chemokine CXCR2  | 4JL7 | N/A               |
|                |        | Chemokine CXCR4  | 3ODU | N/A               |</p>
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<tr>
<th>PS 4</th>
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