Supplemental Material for “Effect of Sequence Pattern on Conformation of DOPA-Peptide Conjugate Aggregates: A Discontinuous Molecular Dynamics Simulation Study”

Supplemental Material

# S1. Trial Results for Design Set 1 (Effect of Varying the DOPA percentage)

Table

Description automatically generated

# S2. Trial Results for Design Set 2 (Effect of Varying the DOPA pattern)

Table

Description automatically generated

A screenshot of a computer

Description automatically generated with medium confidence

# S3. Contact Maps for Design Set 2 Sequences

|  |  |
| --- | --- |
| **A) KLVFFAE-G-YYYYGGGG** | **B) KLVFFAE-G-GGGGYYYY** |
| Chart  Description automatically generated with low confidence | Chart  Description automatically generated |
|  |  |
| **C) KLVFFAE-G-YYGGYYGG** | **D) KLVFFAE-G-GGYYGGYY** |
| Chart  Description automatically generated | Chart  Description automatically generated |
|  |  |
| **E) KLVFFAE-G-YYYGYYY** | **F) KLVFFAE-G-GYYYGYYY** |
| Chart  Description automatically generated with medium confidence | Chart, surface chart  Description automatically generated |
| **Figure S3: Design Set 2. Contact maps comparing the distances between the amino acid residues of two sample chains for designs varying in DOPA tail pattern** | |

# S4. Trial Results for Design Set 3 (Effect of Adding K to DOPA Tail to Impart Stiffness)

A picture containing chart

Description automatically generated

# S5. Contact Maps for Design Set 3 Sequences

|  |  |
| --- | --- |
| **A) KLVFFAE-G-KYKYKYKY** | **B) KLVFFAE-G-KYKYGYGY** |
| Chart  Description automatically generated | Chart  Description automatically generated |
| **Figure S5: Design Set 3. Contact maps comparing the distances between the amino acid residues of two sample chains for designs including K in the tail for stiffness** | |

# S6. Trial Results for Design Set 4 (Effect of Linker Sequence in Design)

A picture containing table

Description automatically generated

# S7. Contact Maps for Design Set 4 Sequences

|  |  |
| --- | --- |
| **A) KLVFFAE-K-YYGYYGYY** | **B) KLVFFAE-GG-YYGYYGYY** |
| Chart  Description automatically generated | Graphical user interface  Description automatically generated with medium confidence |
| **C) KLVFFAE-KK-YYGYYGYY** |  |
| Chart  Description automatically generated |  |
| **Figure S7: Design Set 4. Contact maps comparing the distances between the amino acid residues of two sample chains for designs varying in linker type** | |

Note that for the GG and KK linker sequences, the contact maps include 17 amino acid residues in each of the two chains, so the indices go up to 17 on each of the axes.