| | Construct 1 | Construct 2 |
|--|---------------------------|--------------------------|
| | Alpha helix: 22.46% | Alpha helix: 23.92% |
| Secondary structure | Extended strand: 26.84% | Extended strand: 26.16% |
| | Random coil: 50.7% | Random coil: 49.91% |
| Ramachandran plot | Favored regions: 81.2% | Favored regions: 4.2% |
| Kamachanuran piot | Disallowed regions: 82.2% | Disallowed regions: 1.6% |
| QMEAN scores | 0.74 | 0.74 |
| ERRAT Overall Quality Factor | 86.5731 | 89.4212 |
| VERIFY 3D averaged 3D-1D score of >= 0.1 | 73.84% | 73.84% |

Appendix 1. The quality scores for predicted secondary and tertiary structures of the Construct 1

and construct 2.

Appendix 2. Physicochemical properties of the Construct 1 and construct 2.

| | Construct 1 | Construct 2 |
|---------------------------|---|---|
| Molecular weight | 62246.31 Da | 63524.67 Da |
| Pi | 9.07 | 8.97 |
| Extinction coefficient | 77615 M ⁻¹ cm ⁻¹ | 77615 M ⁻¹ cm ⁻¹ |
| | mammalian reticulocytes, in vitro: 30 hours | mammalian reticulocytes, in vitro: 30 hours |
| Estimated half-life | yeast, in vivo: >20 hours | yeast, in vivo: >20 hours |
| | Escherichia coli, in vivo: >10 hours | Escherichia coli, in vivo: >10 hours |
| Instability index | 39.33 meaning as a stable protein | 38.65 meaning as a stable protein |

Appendix 3. Docking results and binding affinity assessment of the Construct 1 and construct 2.

| | Construct 1 and EphA2 | Construct 2 and EphA2 |
|--------------------------|-----------------------------|-----------------------------|
| HADDOCK score | 914.6 +/- 47.0 | 926.1 +/- 47.1 |
| Prodigy binding affinity | ΔG : -19.1 kcal/mol | ΔG : -20.9 kcal/mol |
| | Kd: 9.2e-15M | Kd: 4.6e-16M |

Appendix 4. allergencity and antigenicity results of the Construct 1 and construct 2.

| | Construct 1 | Construct 2 |
|--------------|------------------|-------------------|
| Allergencity | -1.29 | -1.32 |
| antigenicity | probable antigen | probable antigens |



Appendix 5. The energy plot of predicting mRNA structures of the Construct 1 (a) and construct 2 (b).