**Table S1:** Composition of PCL and PCL-G nanocomposites

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **S.No.** | **Coding Name** | **PCL** **(%w/w)** | **Graphene (G) concentrations (mg/ml)** | **G filler (%w/v of PCL solution)** |
| 1 | PCL | 15 | 0.0 | 0.0 |
| 2 | PCL-G0.01 | ~15 (14.99) | 0.1 | 0.01% |
| 3 | PCL-G0.05 | ~15 (14.95) | 0.5 | 0.05% |
| 4 | PCL-G0.1 | ~15 (14.9) | 1.0 | 0.1% |

Table S2: F-actin (UniportKB: P60709) protein displays the PDB ID with the method of 3D structure elucidation, resolution, and information of chains, sequence length and reason to choose the 3D structure which was used for docking. Table reproduced from [1], licensed with CC BY 4.0.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **PDB ID** | **Experimental****Method** | **Resolution (Å)** | **Chains** | **Sequence length** | **Reason to choose for simulations** |
| 3BYH | Electron microscopy | 12.00 | A | 2-375 | Facing problem while performing the equilibration step |
| 3D2U | X-ray | 2.21 | C/G | 170-178 | Do not have the whole structure |
| 3J82 | electron microscopy | 7.70 | B/C/D | 2-375 | Proceed with this structure but have a lower resolution than 6ANU |
| 3LUE | electron microscopy | 15.00 | A/B/C/D/E/F/G/H/I/J | 2-375 | Poor resolution |
| 6ANU | electron microscopy | 7.00 | A/B/C/D/E/F | 1-375 | Best resolution |
| 6ICT | X-ray | 1.95 | E/G/H/I | 66-88 | 23aa only |
| 6ICV | X-ray | 2.15 | C/D | 66-88 | 23aa |
| 6MBJ | X-ray | 1.78 | Y/Z | 66-80 | 15aa |
| 6MBK | X-ray | 1.69 | Y/Z | 66-80 | 15aa |
| 6MBL | X-ray | 2.20 | Y | 66-80 | 15aa |

**References:**

1. The UniProt Consortium, UniProt: the universal protein knowledgebase in 2021, *Nucleic Acids Res*, 49(D1), D480–D489 (2021).