Supporting Information for the manuscript

Probing molecular basis of single-walled carbon nanotube degradation and nondegradation by enzymes based on manganese peroxidase and lignin peroxidase

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Keywords: carbon nanotube, biodegradation, enzyme, interaction, environmental remediation.

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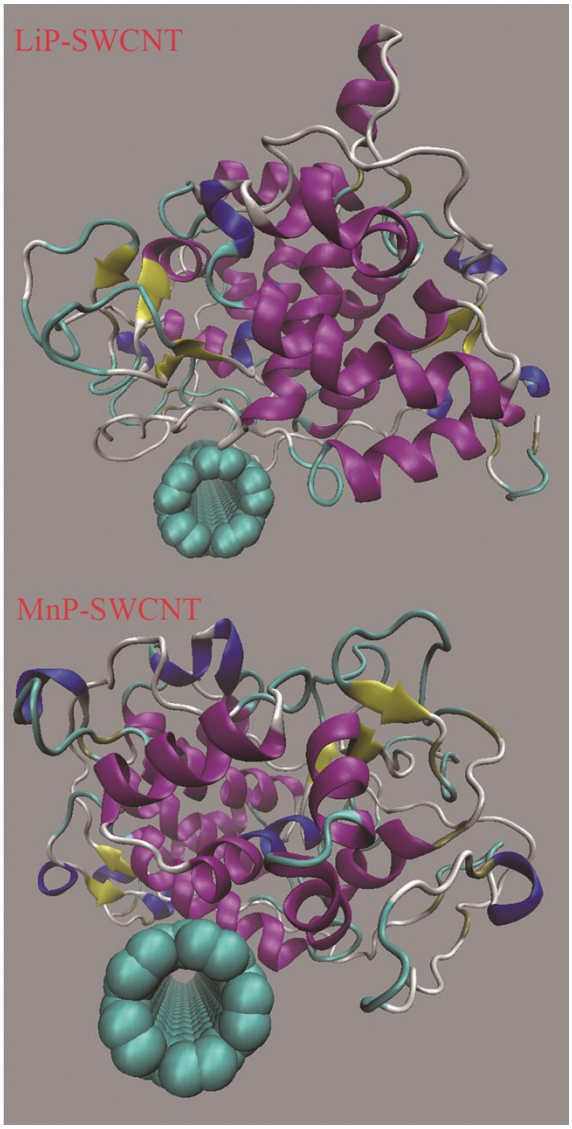

Figure S1. Initial configurations of LiP-SWCNT and MnP-SWCNT in water.

Table S1. Residues of LiP within 3 Å of SWCNT during the simulation

Time (ns)	Residues
0	HIS30, PRO296, GLY297, ASN298, GLY299, PRO300, LEU328, PRO329, ILE338, PRO339, HIS341, LYS342
10	GLN33, GLY35, THR196, ILE199, PRO296, GLY297, GLY299, PHE303, LEU328, PRO329, ALA336, ILE338
20	HIS30, GLN33, GLY35, THR196, ILE199, PRO296, GLY297, ASN298, GLY299, PHE303, LEU328, PRO329, ALA336, ILE338, PRO339
30	HIS30, GLN33, THR196, PRO197, ILE199, PRO296, GLY297, PRO300, PHE303, LEU328, PRO329, PRO339

Table S2. Residues of MnP within 3 Å of SWCNT during the simulation

Time (ns)	Residues
0	ARG8, ARG122, PHE264, ALA267, ARG270, ALA271
10	ARG8, ARG122, PRO249, ILE254, PHE264, ALA267, SER321, GLU322
20	ARG8, ARG122, ARG250, CYS253, ILE254, PHE264, ALA267, ARG270, SER321
30	ARG8, PHE164, CYS253, ILE254, PHE264, ALA267, SER321