Supplementary Material (S1)

Table S1. Correlation between Hamada index *m* and FEB values (obtained after performing docking experiments) from the different carbon nanotuboes assayed. Values are expressed in terms of determination coefficient (R^2). No correlation was calculated for zig-zag SWCNT since *m* Hamada index = 0.

Functionalization	Structural geometry	R^2	p-value
Pristine	chiral	0.28	$p<0.05$
Hydroxyl	chiral	0.20	$p<0.05$
Carboxyl	chiral	0.02	$p>0.05$
Pristine	armchair	0.13	$p>0.05$
Hydroxyl	armchair	0.41	$p>0.05$
Carboxyl	armchair	0.01	$p>0.05$

Supplementary Material (S2)

Table S2a. Comparison between rigid and flexible docking simulations considering the cationic cluster formed by the arginine residues (Arg 79, Arg 187, Arg 231, Arg 234, and Arg 279) of the ANT-1 active site as flexible residues. Assays were conducted with zig-zag SWCNT, where the first number indicates *n* Hamada index and the second value is *m* Hamada index. **FEB**: free energy binding

Carbon nanotubes (SWCNT)	FEB rigid docking (kcal/mol)	FEB flexible docking (kcal/mol)	Simulation time of rigid docking (s)	Simulation time of flexible docking (s)
Zigzag (3, 0)	-11.0	-10.3	0 min:7.894 s	3 min: 56.226 s
Zigzag (6, 0)	-12.2	-12.0	0 min:14.738 s	5 min: 57.509 s
Zigzag (9, 0)	-11.9	-10.8	0 min:30.080 s	9 min:37.743 s

Table S2b. Comparison of free energy binding (FEB) in docking simulations using exhaustiveness values of 8 and 100, respectively. Assays were conducted with zig-zag SWCNT, where the first number indicates *n* Hamada index and the second value is *m* Hamada index.

Carbon nanotubes (SWCNT)	Exhaustiveness	Simulation time (s)	FEB (kcal/mol)
Zigzag (3, 0)	8	0 min:7.894 s	-11.0
Zigzag (3, 0)	100	0 min:59.963 s	-11.0
Zigzag (6, 0)	8	0 min:14.738 s	-12.2
Zigzag (6, 0)	100	2min:18.337s	-12.2
Zigzag (9, 0)	8	0 min:30.080 s	-11.9
Zigzag (9, 0)	100	5min:13.584 s	-11.9

Supplementary Material (S3)

Supplementary Material (S3) can be found in the compressed file and contains the results of the docking experiments

Supplementary Material (S4)

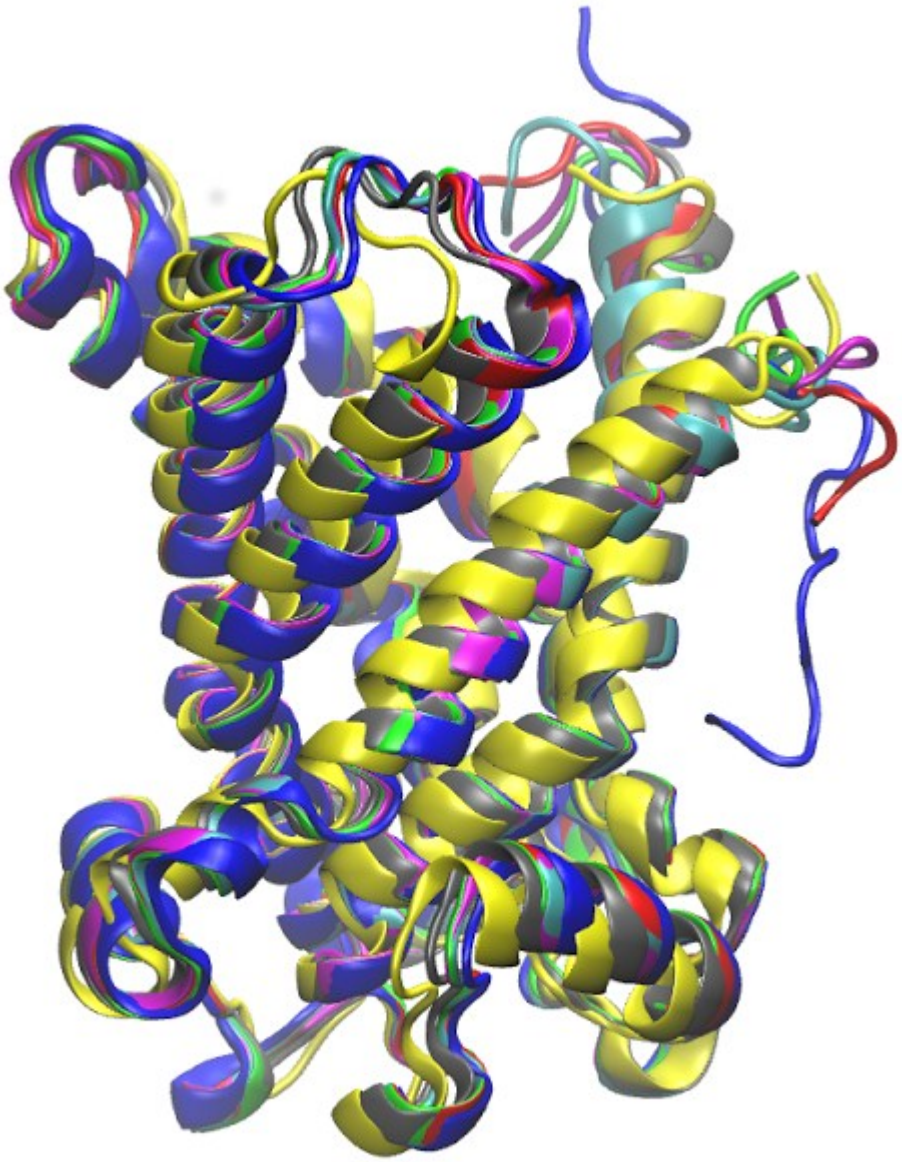

Figure S4. Structural alignment of protein ANT-1 from shrimp *Litopenaeus vannamei* (in blue), salmon louse *Lepeophtheirus salmonis* (in yellow), zebrafish *Danio rerio* (in red), rat *Rattus rattus* (in violet), mouse *Mus musculus* (in cyan), human *Homo sapiens* (in green) and in bovine *Bos taurus* (in grey).

Table S4a. Structural comparison of ANT-1 protein from different species. **RMSD**: **root-mean-square deviation of atomic positions (RMSD)**

Model	Label used in Figure S4	RMSD
Reference model: ANT-1 *Bos taurus* (PDB ID: 1OKC)	Grey	0
ANT-1 *Litopenaeus vannamei*	Blue	6.93
ANT-1 *Lepeophtheirus salmonis*	Yellow	5.75
ANT-1 *Danio rerio*	Red	5.05
ANT-1 *Rattus norvegicus*	Violet	5.05
ANT-1 *Mus musculus*	Cyan	5.07
ANT-1 *Homo sapiens*	Green	5.07

Table S4b. Comparison of free energy binding (FEB, in kcal/mol) in docking simulations using ANT-1 models from the different species compared in **Figure S4** and **Table S4a**. Assays were conducted with zig-zag SWCNT, where the first number indicates *n* Hamada index and the second value in *m* Hamada index. ANT-1 from *Bos taurus* was the reference model (PDB ID: 1OKC)

Species	Zig-zag (3, 0)	Zig-zag (6, 0)	Zig-zag (9, 0)
Bos taurus (PDB ID: 1OKC)	-11.0	-12.2	-11.9
Litopenaeus vannamei	-11.0	-13.5	-16.4
Lepeophtheirus salmonis	-11.9	-12.3	-13.5
Danio rerio	-11.0	-12.6	-13.9
Rattus norvegicus	-11.1	-15.4	-14.2
Mus musculus	-10.7	-13.0	-14.1
Homo sapiens	-11.0	-12.7	-15.0