Supplementary information

Velocity Control of Protein Translocation through a Nanopore by Tuning the Fraction of Benzenoid Residues

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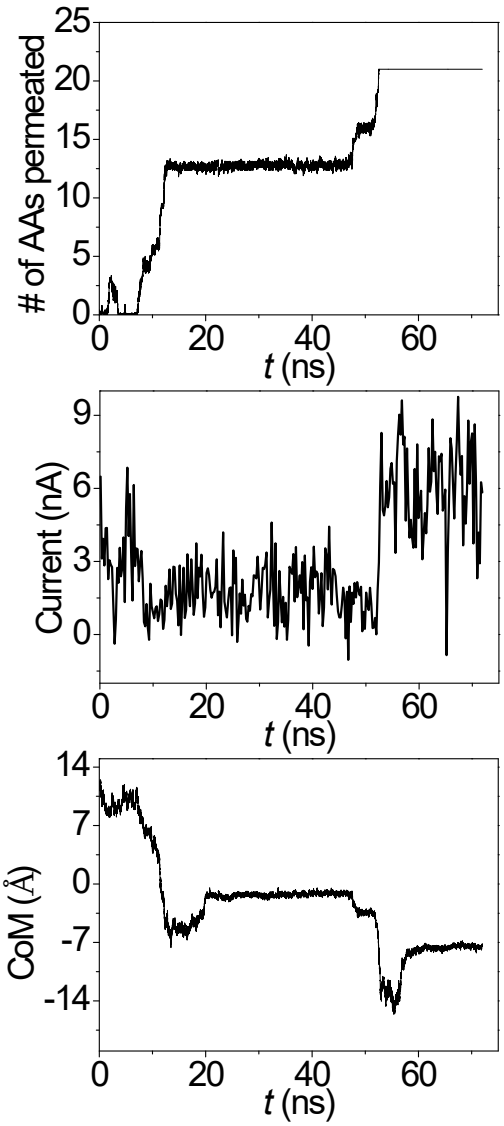

Figure S1. Independent molecular dynamics simulation of peptide (with sequence of EADVEIDLEFDAEVDIELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

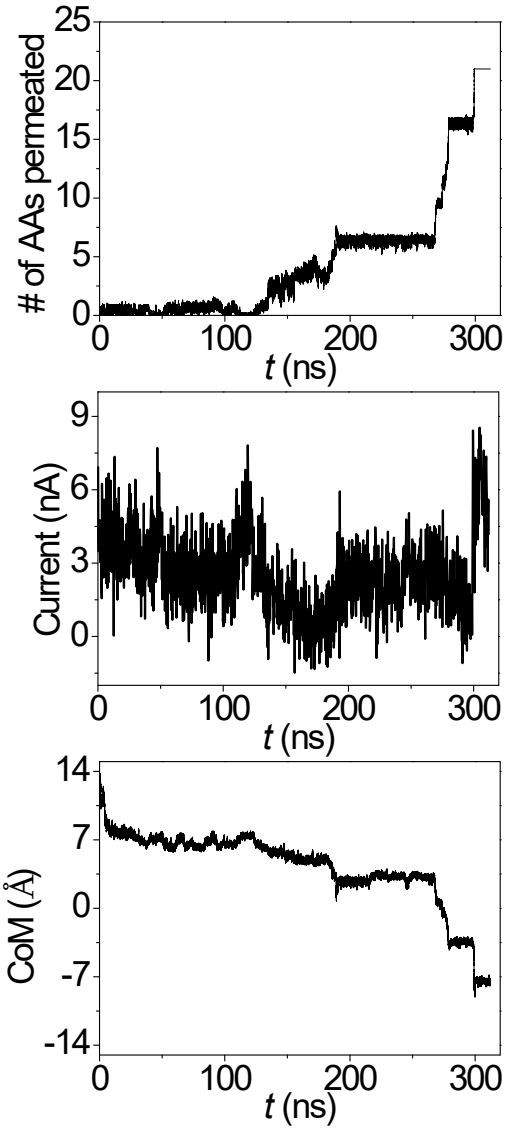

Figure S2. Independent molecular dynamics simulation of peptide (with sequence of EADVEIDLEFDAEVDIELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

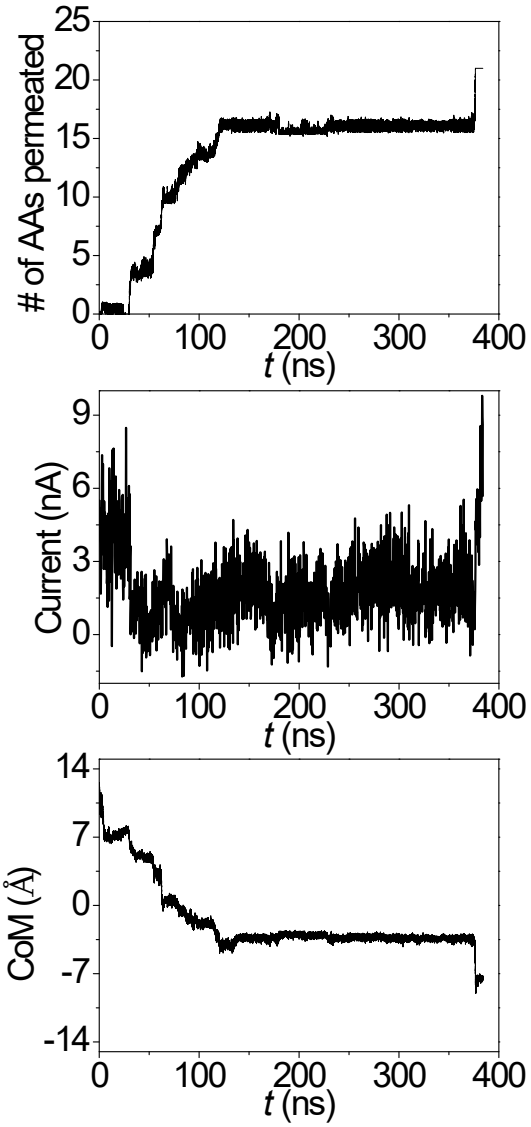

Figure S3. Independent molecular dynamics simulation of peptide (with sequence of EADVEIDLEFDAEVDIELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

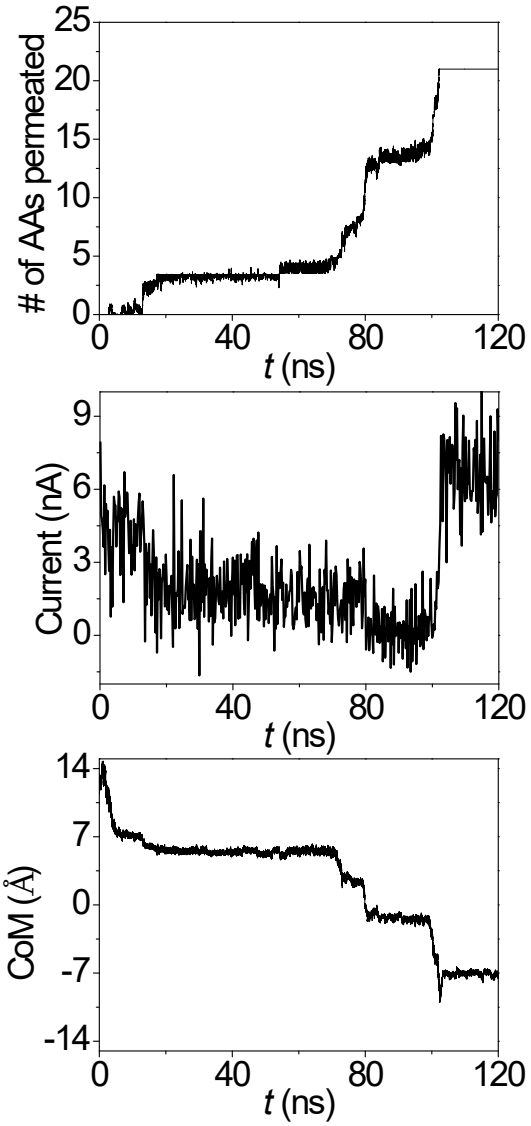

Figure S4. Independent molecular dynamics simulation of peptide (with sequence of EADVEIDLEFDAEVDIELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

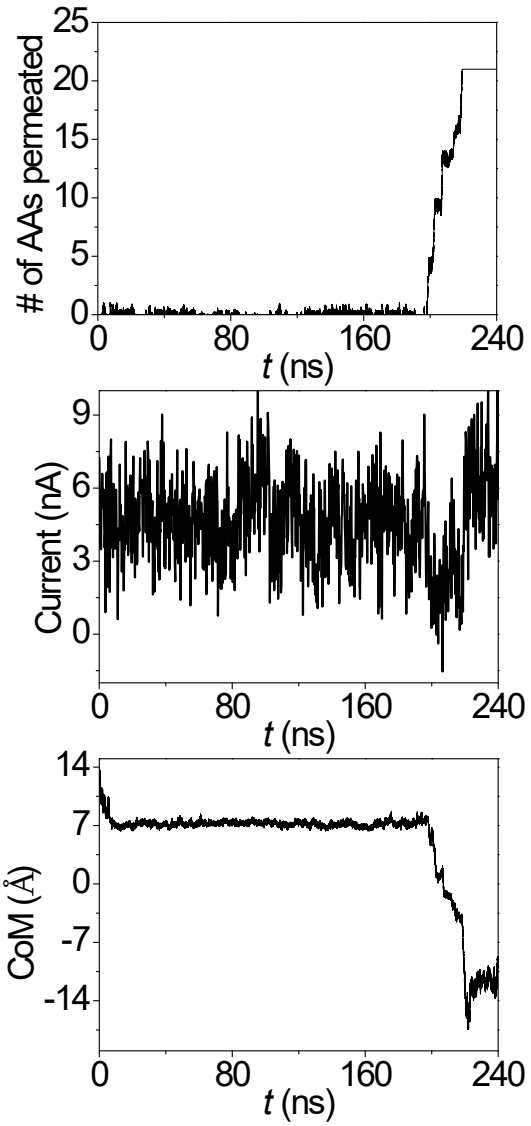

Figure S5. Independent molecular dynamics simulation of peptide (with sequence of ESDTENDQENDTESDTENDQE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

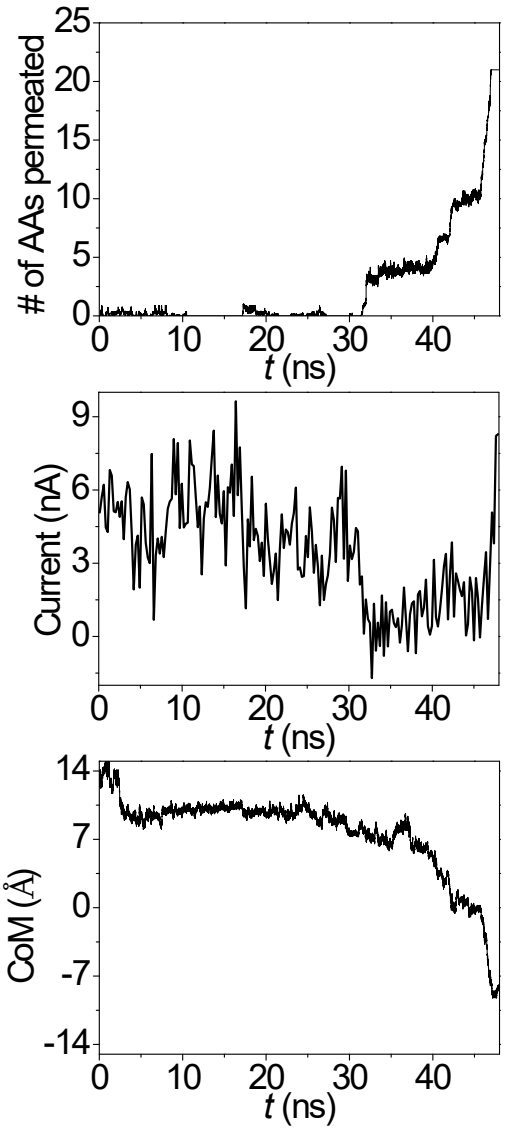

Figure S6. Independent molecular dynamics simulation of peptide (with sequence of ESDTENDQENDTESDTENDQE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

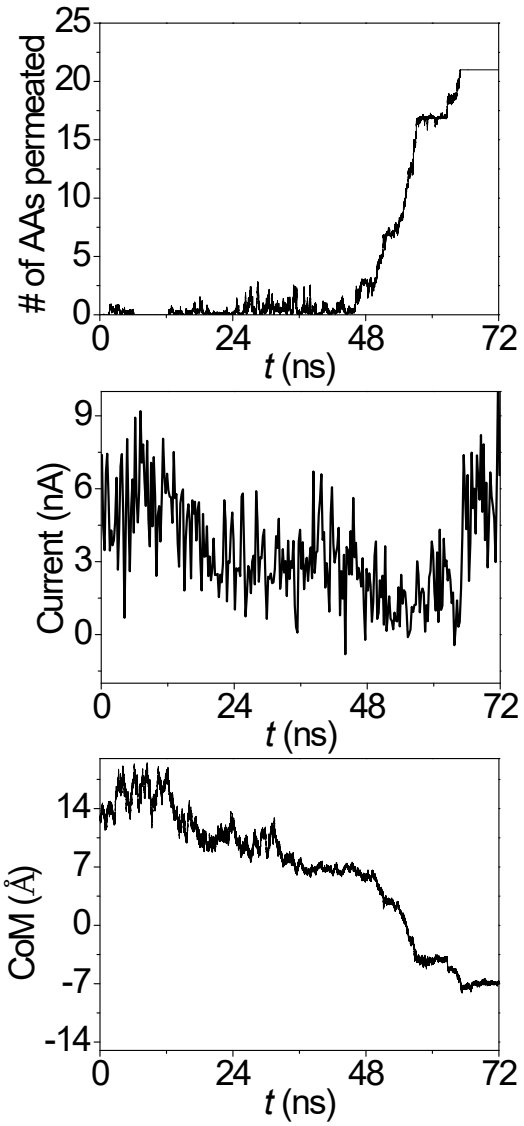

Figure S7. Independent molecular dynamics simulation of peptide (with sequence of ESDTENDQENDTESDTENDQE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

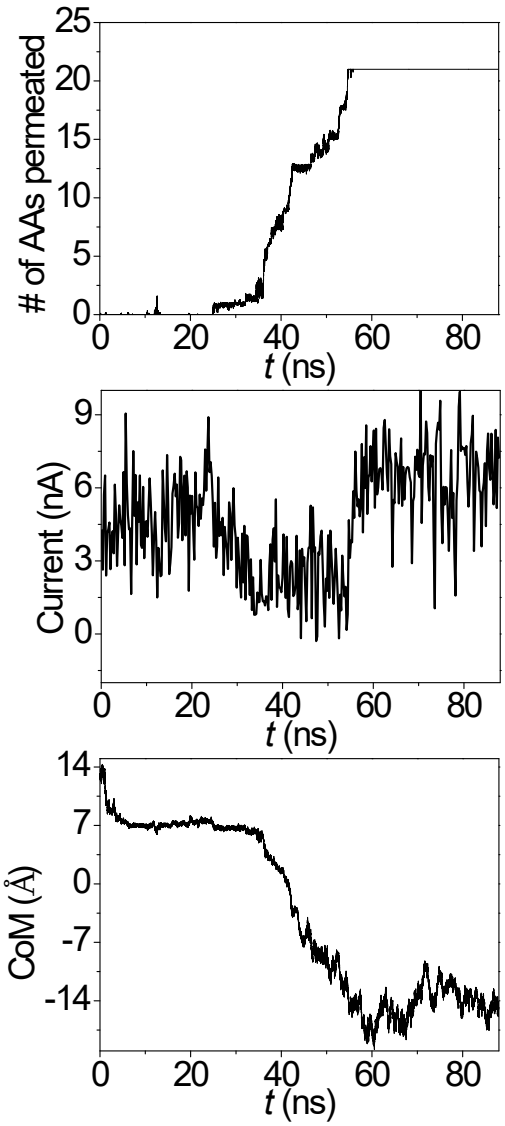

Figure S8. Independent molecular dynamics simulation of peptide (with sequence of ESDTENDQENDTESDTENDQE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

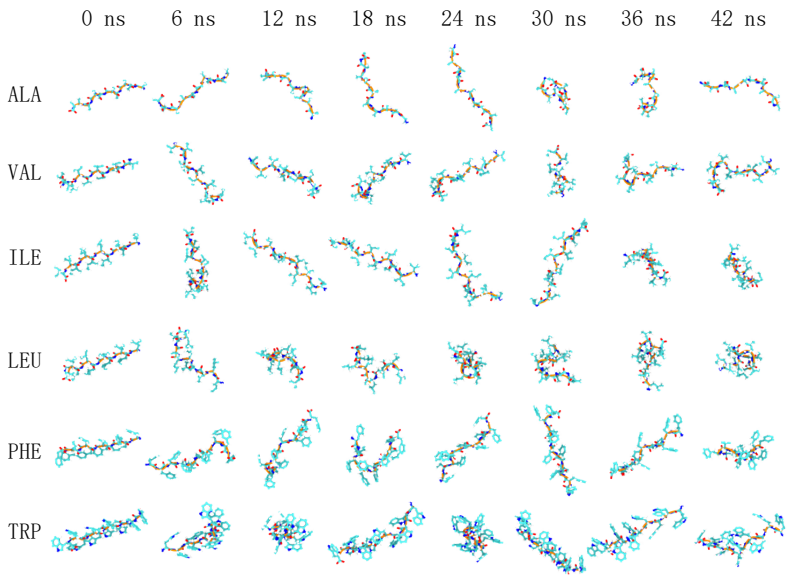

Figure S9. Microscopic configurations realized for the six homogeneous hydrophobic peptides in bulk MD simulations. Each amino acid is shown in licorice representation and the backbone of the peptide is shown in orange NewCartoon representation.

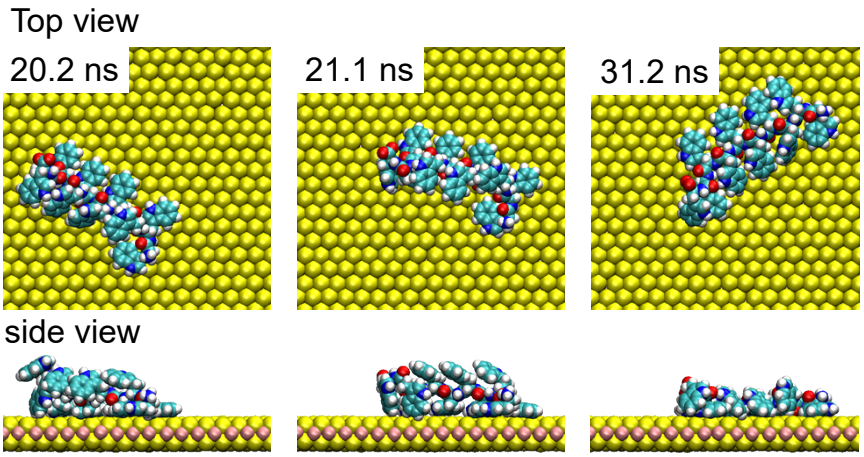

Figure S10. The typical snapshots illustrating microscopic configurations of homogeneous peptide containing 10 tryptophans interacting with the MoS_2 membrane. Top view (above) and side view (below) of the snapshots are shown. Sulfur and molybdenum atoms of the solid-state membrane are shown as yellow and pink spheres, respectively. The peptide is represented by vdW spheres and colored by the atom type (white, red, blue, and green indicate hydrogen, oxygen, nitride, and carbon atoms, respectively). Water molecules, potassium and chloride ions are not shown for clarity.

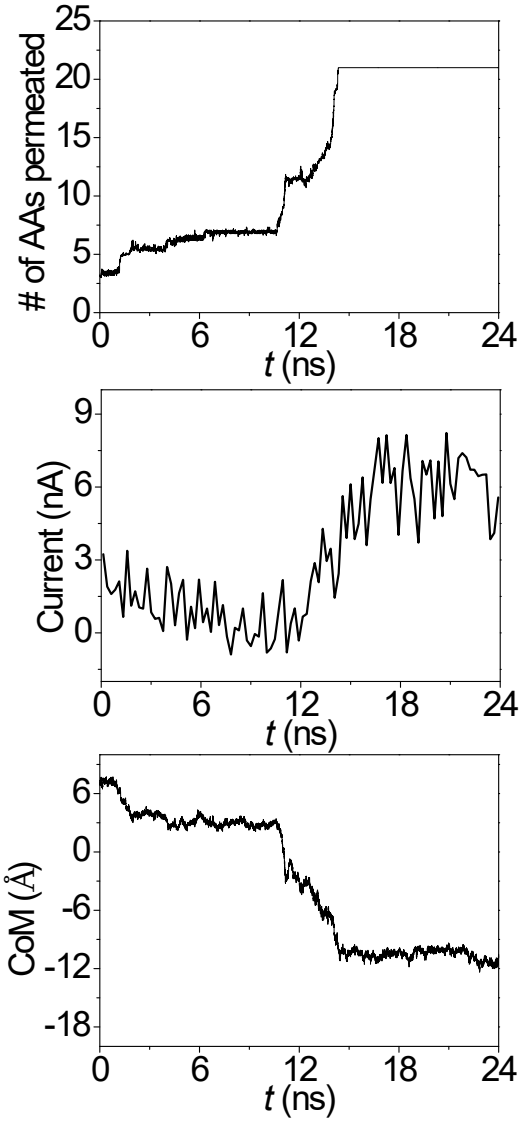

Figure S11. Independent molecular dynamics simulation of peptide (with sequence of EADVEIDLEIDVEADVEIDLE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

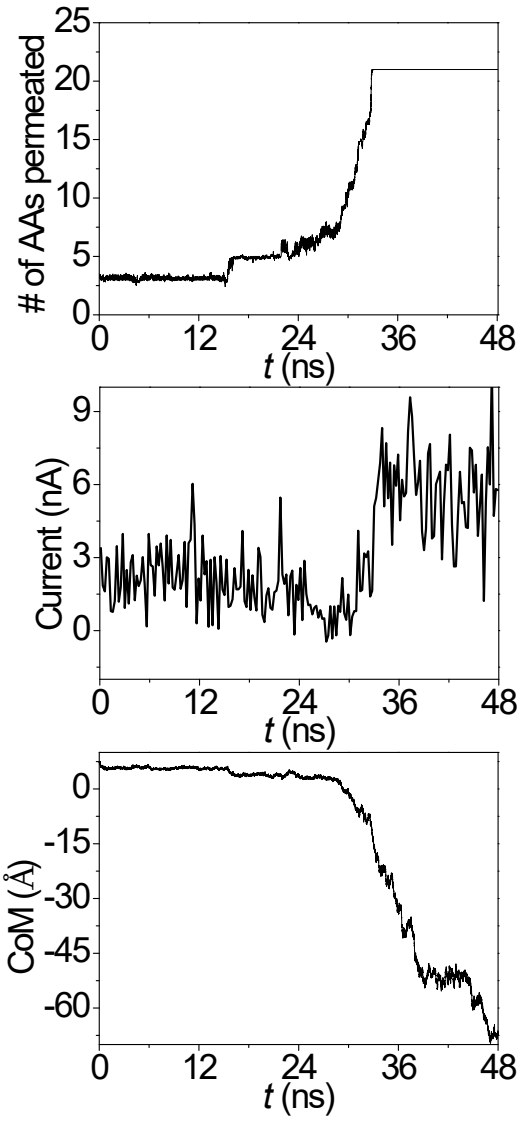

Figure S12. Independent molecular dynamics simulation of peptide (with sequence of EADVEIDLEIDVEADVEIDLE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

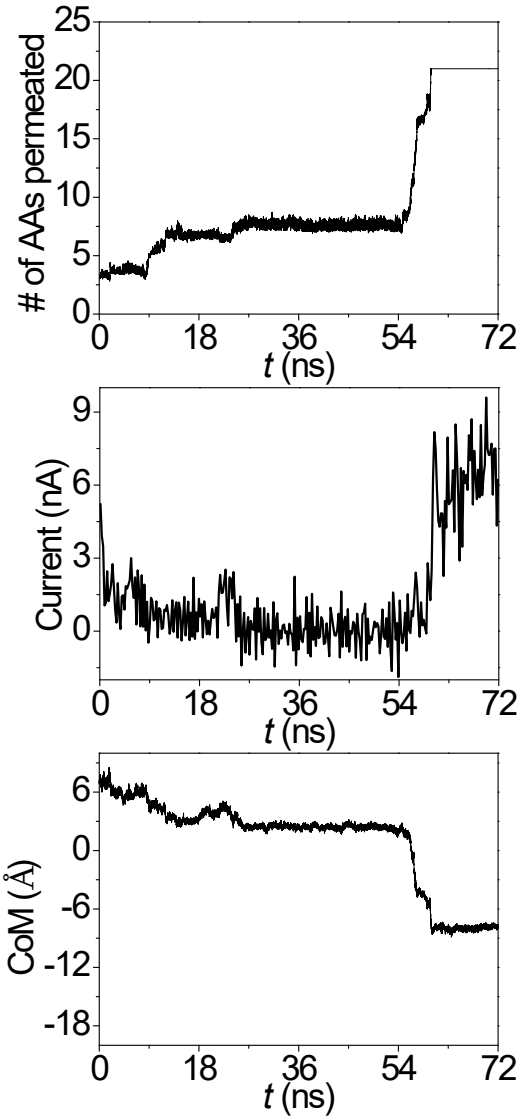

Figure S13. Independent molecular dynamics simulation of peptide (with sequence of EADVEIDLEIDVEADVEIDLE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

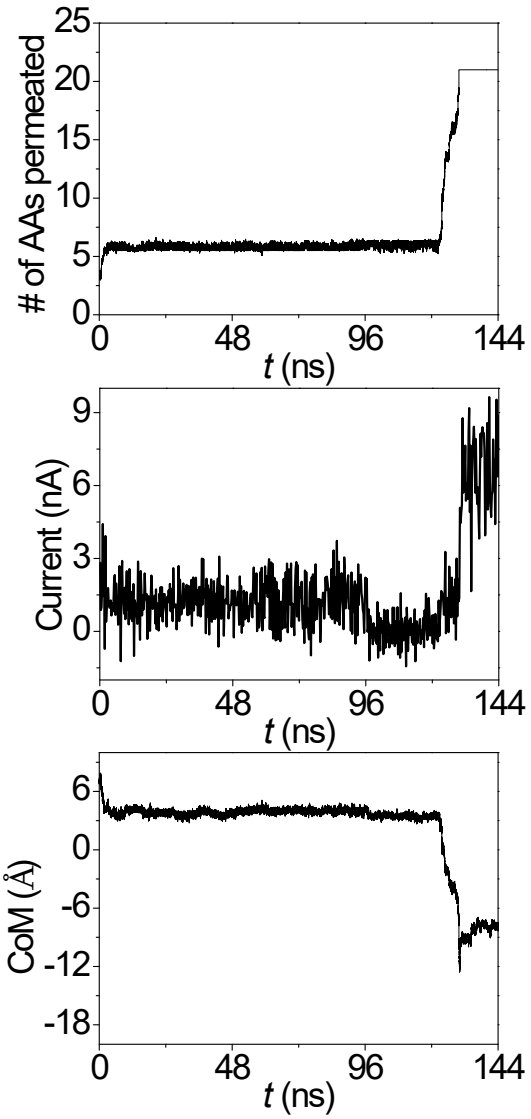

Figure S14. Independent molecular dynamics simulation of peptide (with sequence of EADVEIDLEIDVEADVEIDLE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

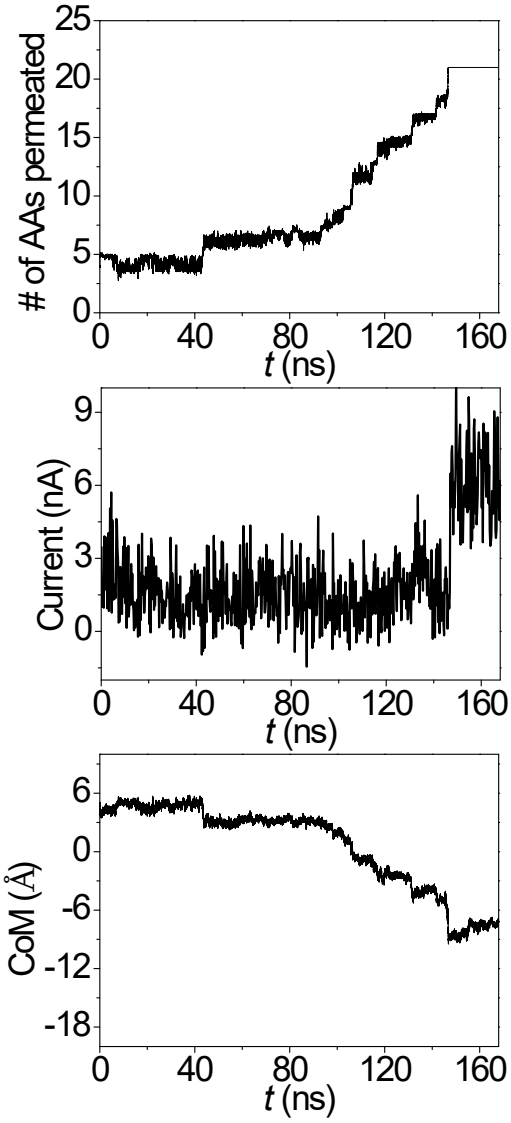

Figure S15. Independent molecular dynamics simulation of peptide (with sequence of EADVEIDLEFDAEVDIELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

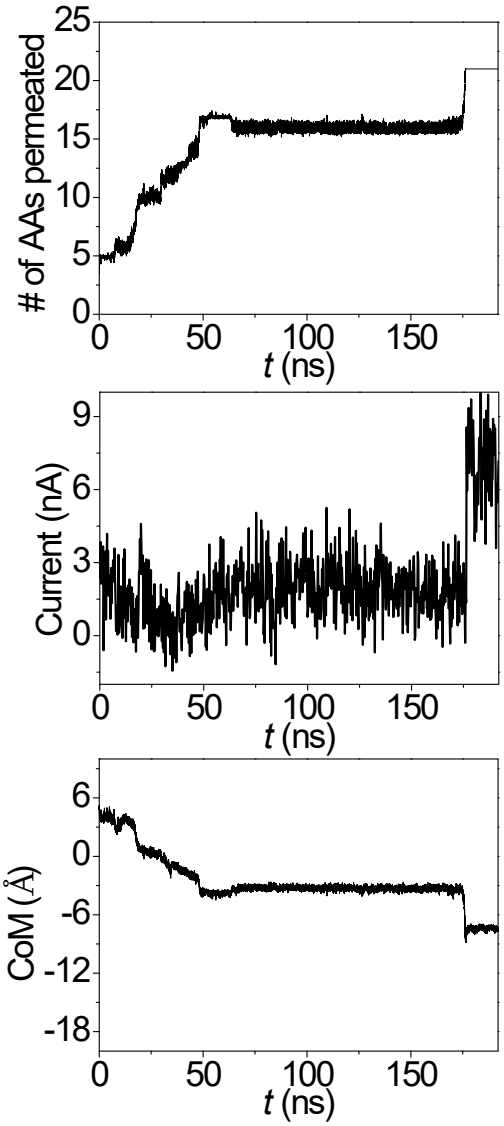

Figure S16. Independent molecular dynamics simulation of peptide (with sequence of EADVEIDLEFDAEVDIELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

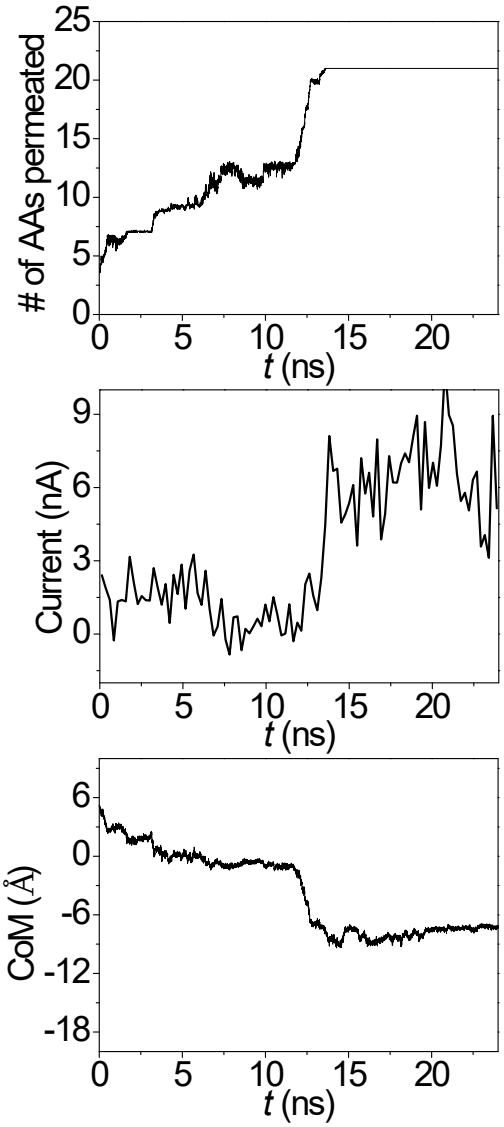

Figure S17. Independent molecular dynamics simulation of peptide (with sequence of EADVEIDLEFDAEVDIELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

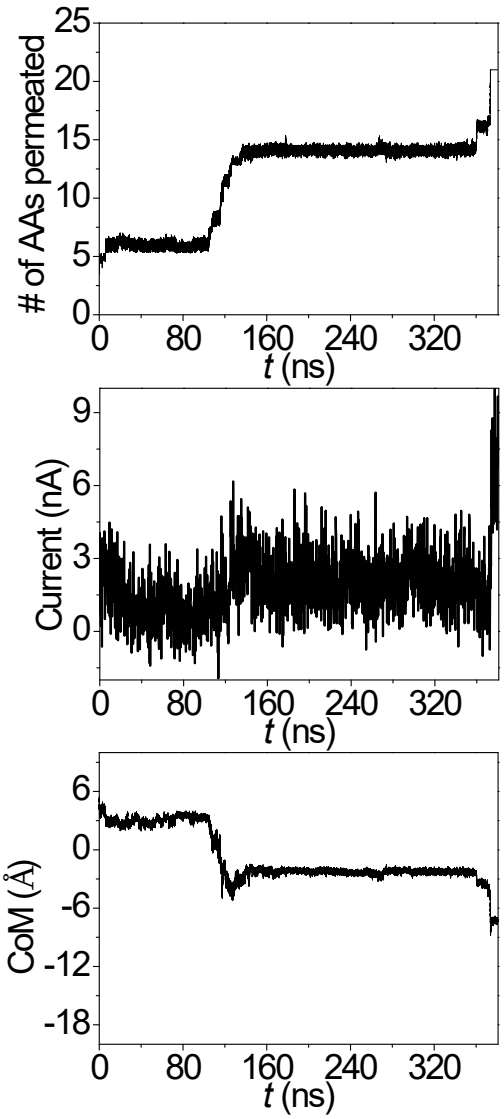

Figure S18. Independent molecular dynamics simulation of peptide (with sequence of EADVEIDLEFDAEVDIELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

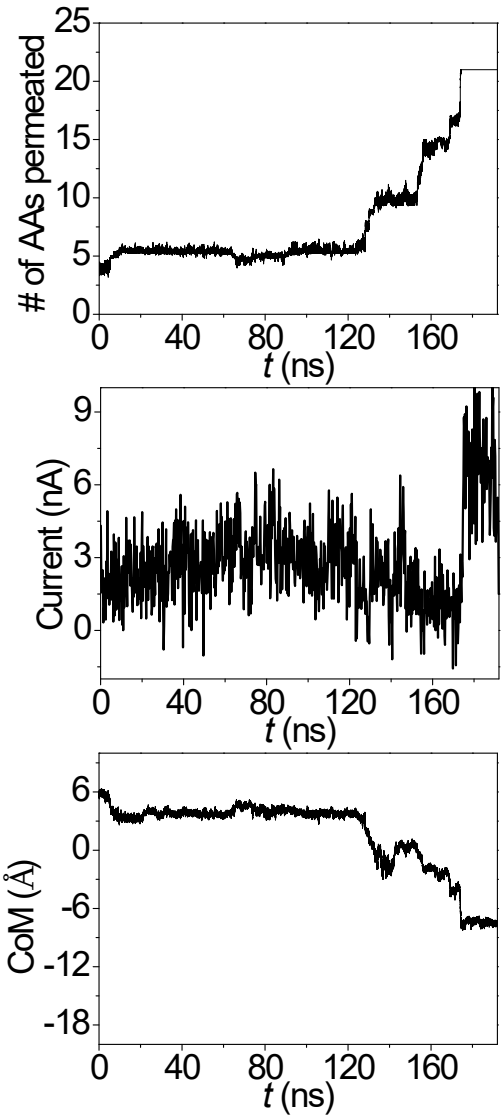

Figure S19. Independent molecular dynamics simulation of peptide (with sequence of : EADVEWDLEFDAEVDFELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

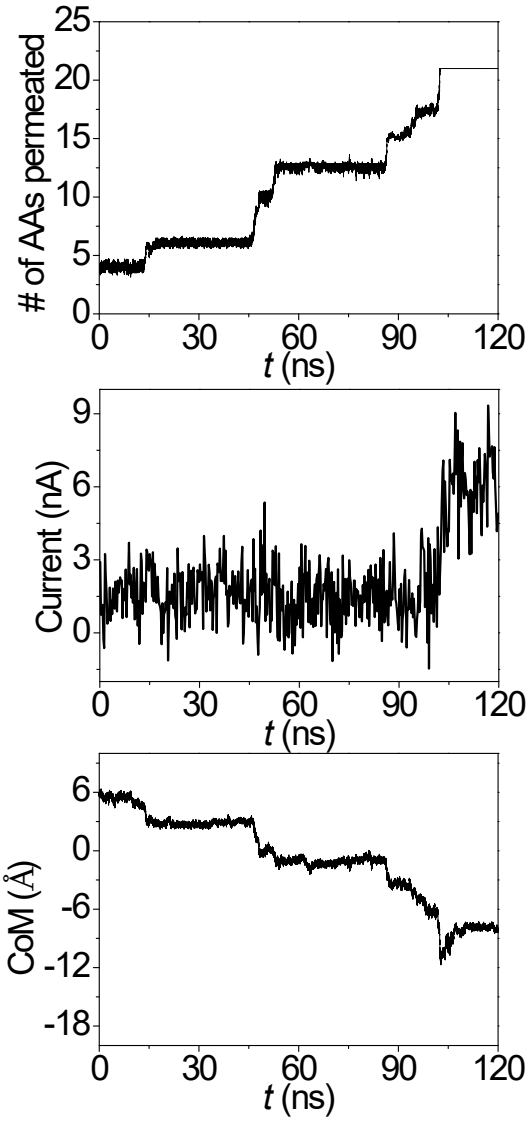

Figure S20. Independent molecular dynamics simulation of peptide (with sequence of : EADVEWDLEFDAEVDFELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

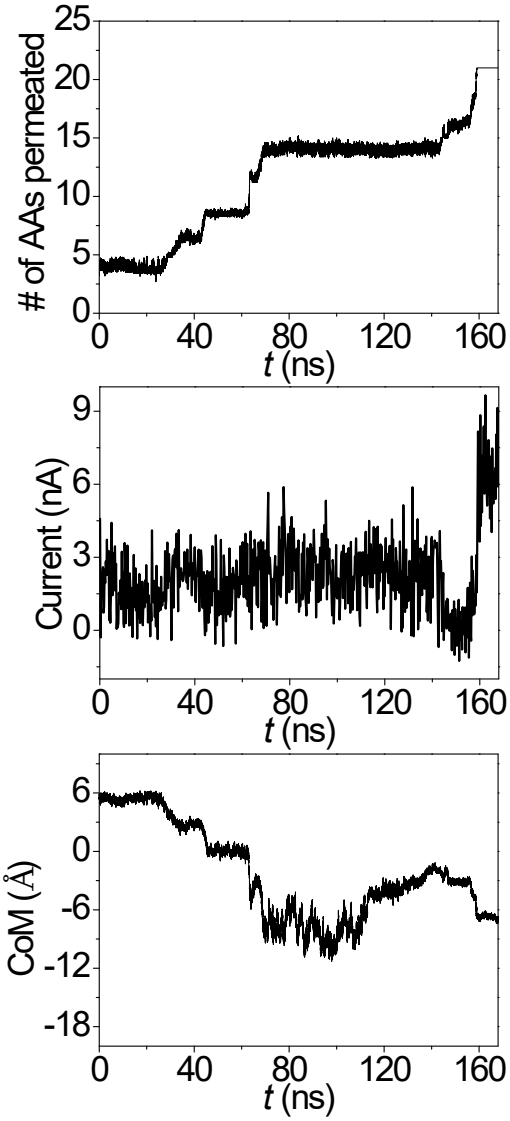

Figure S21. Independent molecular dynamics simulation of peptide (with sequence of : EADVEWDLEFDAEVDFELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

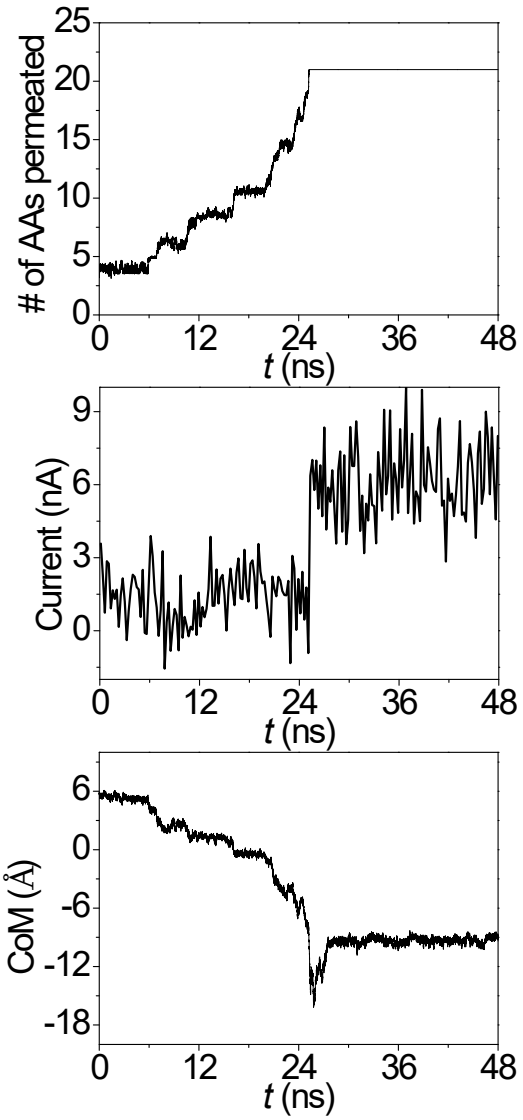

Figure S22. Independent molecular dynamics simulation of peptide (with sequence of : EADVEWDLEFDAEVDFELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

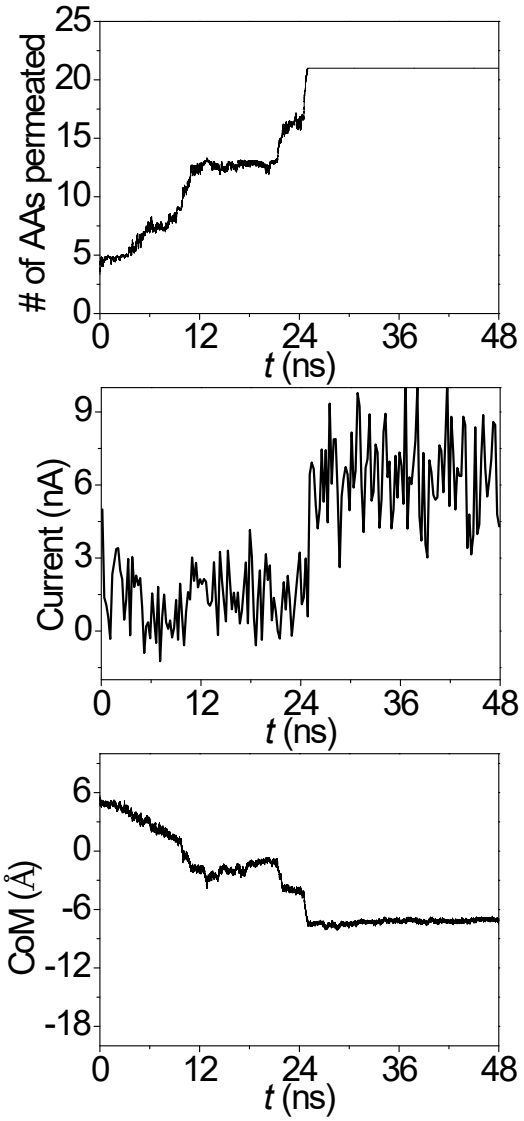

Figure S23. Independent molecular dynamics simulation of peptide (with sequence of : EADFEWDLEFDAEWDFELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

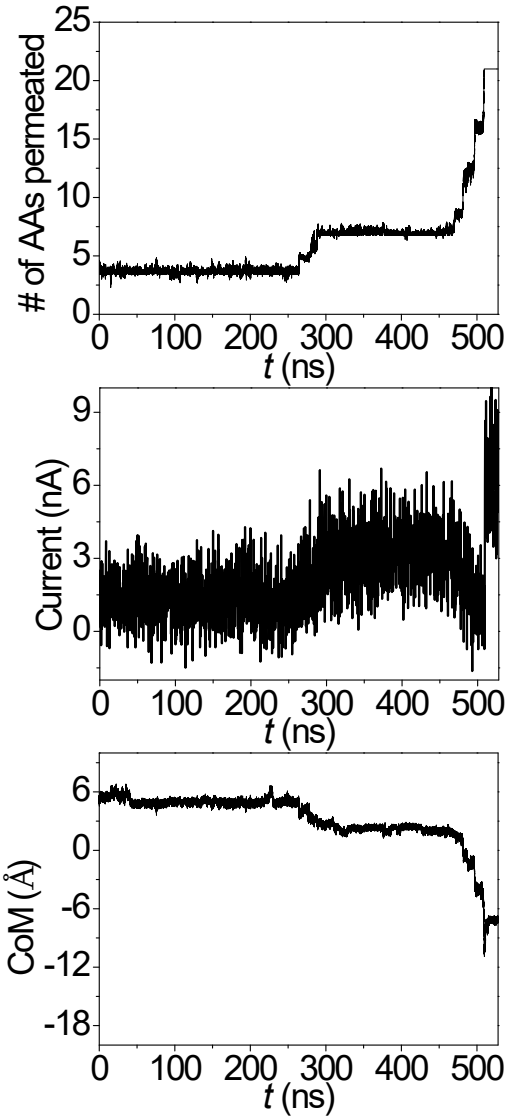

Figure S24. Independent molecular dynamics simulation of peptide (with sequence of : EADFEWDLEFDAEWDFELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

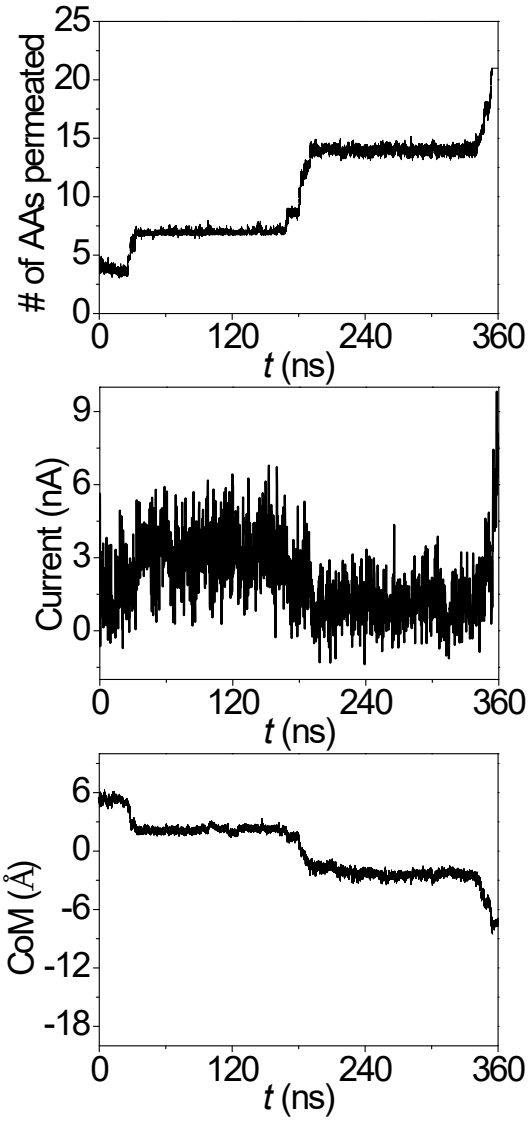

Figure S25. Independent molecular dynamics simulation of peptide (with sequence of : EADFEWDLEFDAEWDFELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

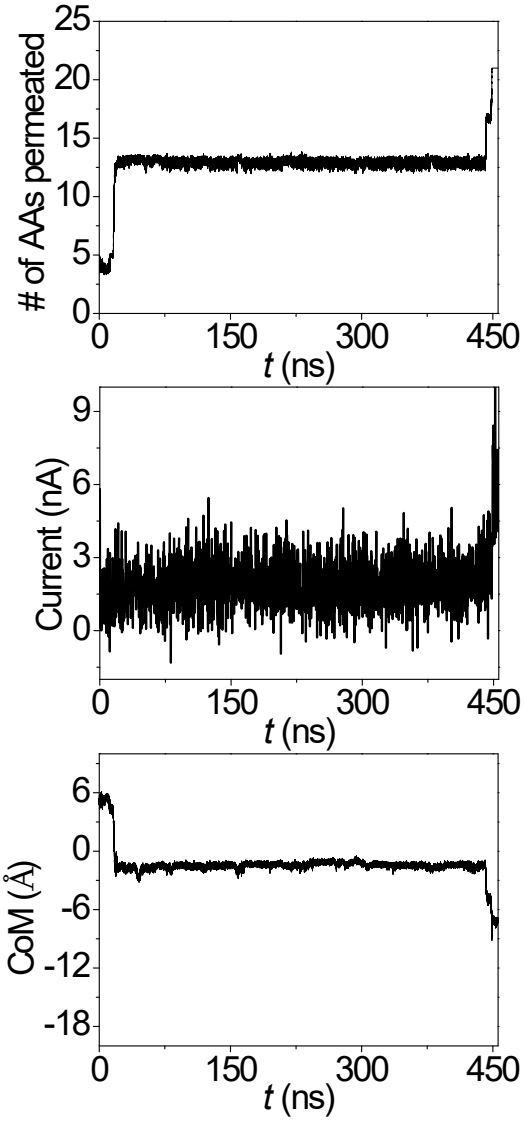

Figure S26. Independent molecular dynamics simulation of peptide (with sequence of : EADFEWDLEFDAEWDFELDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

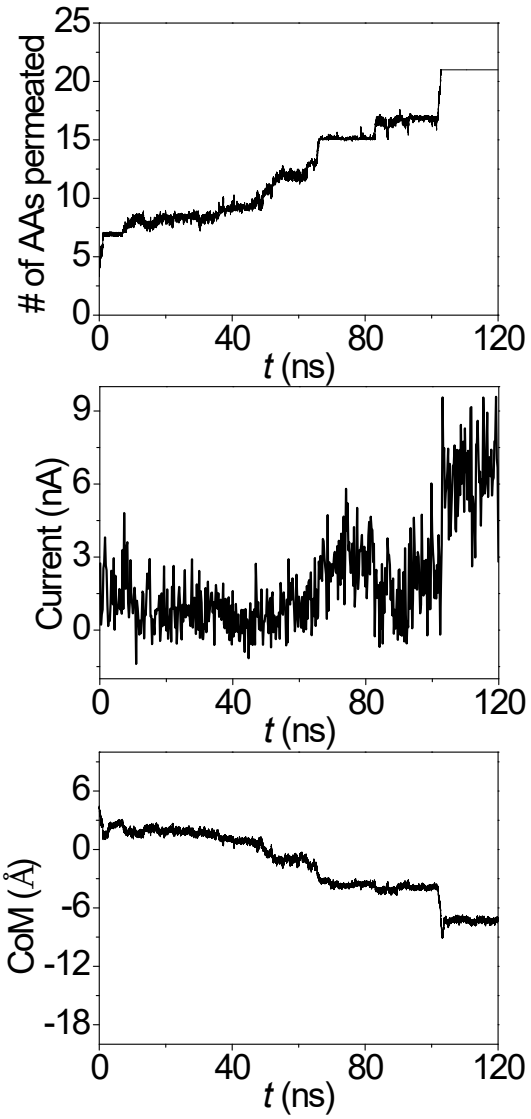

Figure S27. Independent molecular dynamics simulation of peptide (with sequence of : EFDWEFDWEFDWEFDWEFDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

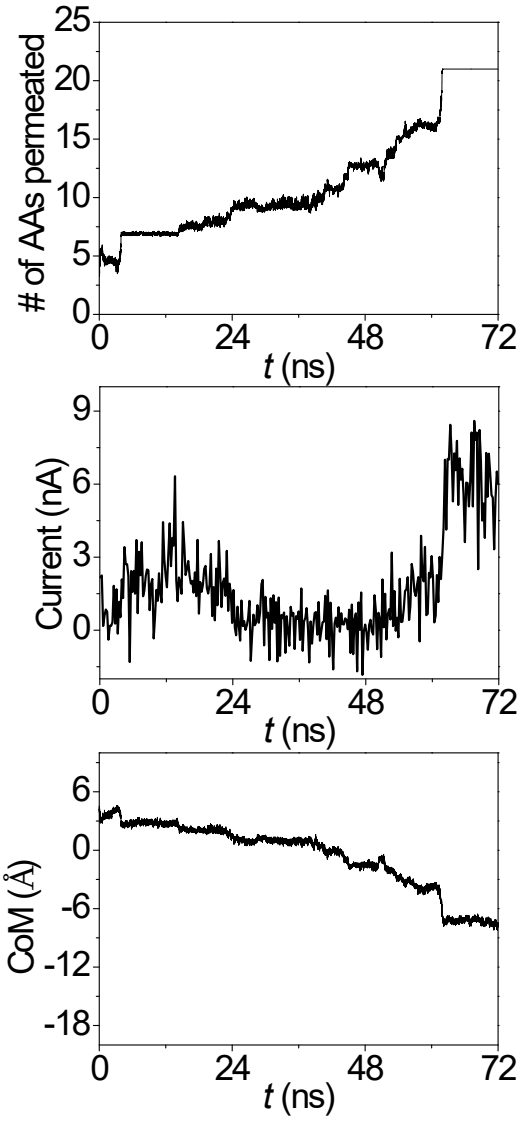

Figure S28. Independent molecular dynamics simulation of peptide (with sequence of : EFDWEFDWEFDWEFDWEFDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

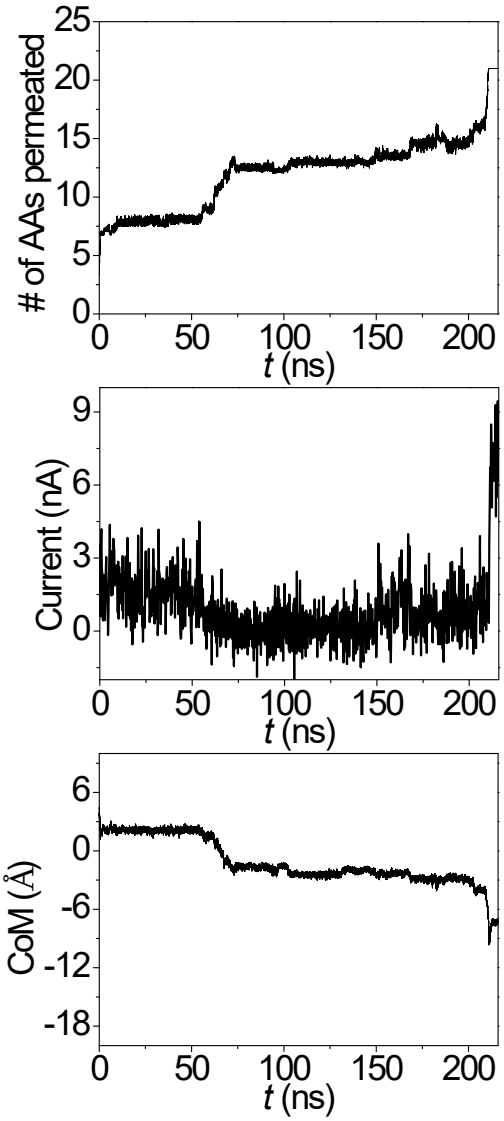

Figure S29. Independent molecular dynamics simulation of peptide (with sequence of : EFDWEFDWEFDWEFDWEFDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

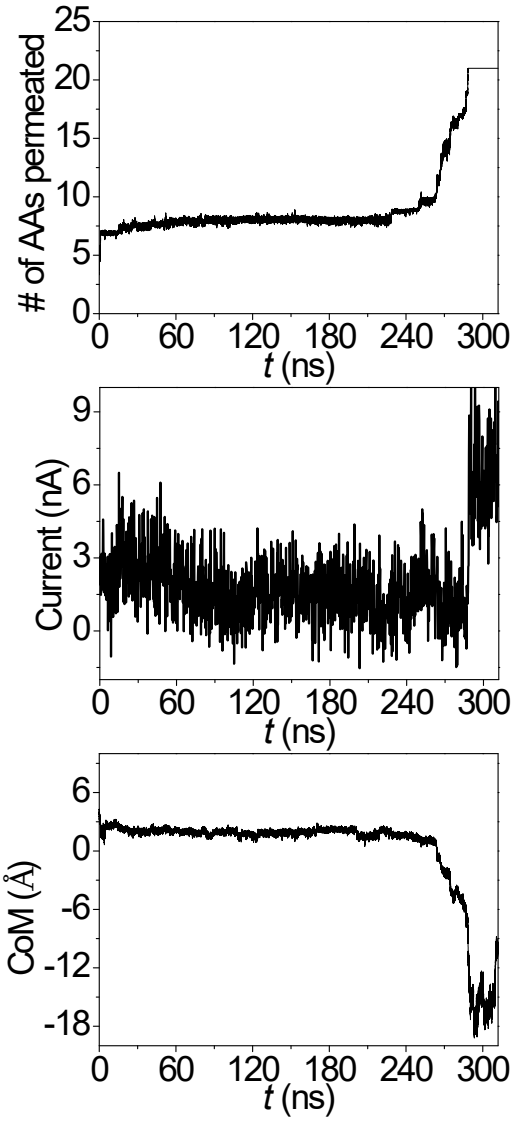

Figure S30. Independent molecular dynamics simulation of peptide (with sequence of : EFDWEFDWEFDWEFDWEFDWE) translocation through a MoS_2 nanopore. The number of translocated amino acids (above), ionic current trace (middle) and CoM (along *z* axis) of the peptide (below) *versus* time are shown in one column. The number of permeated residues, ionic current and CoM of the peptides were all sampled at 2.4 ps intervals, and the ionic currents were also block averaged in 0.24 ns blocks.

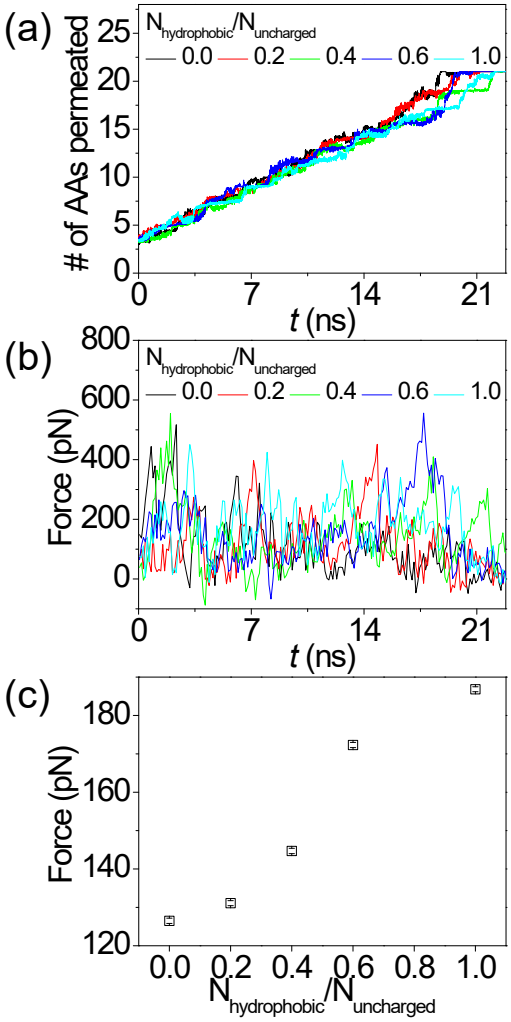

Figure S31. Constant velocity steered molecular dynamics simulations of peptides with different fraction of benzenoid residues pulled though the MoS2 nanopore. (a) The number of translocated amino acids versus time. (b) The SMD pulling forces exerted on the peptides versus simulation time. (c) The average pulling forces exerted on the peptides that have different fraction of benzenoid residues.

Table S1. The correlation between the size of the peptides with their translocation velocity.

Sequence	$N_{benzenoid}/N_{hydrophobic}$	Molecular weight (kDa)	Velocity (AAs/ns)
EADVEIDLEIDVEADVEIDLE	0.0	2.36	0.63±0.20
EADVEIDLEFDAEVDIELDWE	0.2	2.48	0.41±0.23
EADVEWDLEFDAEVDFELDWE	0.4	2.59	0.30±0.11
EADFEWDLEFDAEWDFELDWE	0.6	2.73	0.24±0.13
EFDWEFDWEFDWEFDWEFDWE	1.0	3.02	0.15±0.04

Table S2. The correlation between the fraction of prolines of the peptides with their translocation velocity.

Sequence	$N_{proline}/N_{hydrophobic}$	Molecular weight (kDa)	Velocity (AAs/ns)
EAEAEAEAEAEAEAEAEAEAE	0.0	2.14	1.03±0.31
EAEAEAEAEAEAEAEPEAEPE	0.2	2.19	0.62±0.22
EAEAEAEPEAEPEAEPEAEPE	0.4	2.24	0.65±0.23
EAEAEAEPEPEPEAEPEPEPE	0.6	2.29	0.29±0.10
EPEPEPEPEPEPEPEPEPEPE	1.0	2.40	2.63±0.67