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Molecularly imprinted polymer nanogels targeting the HAV Motif in cadherins inhibit cell-cell adhesion and migration

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Supplementary Figures

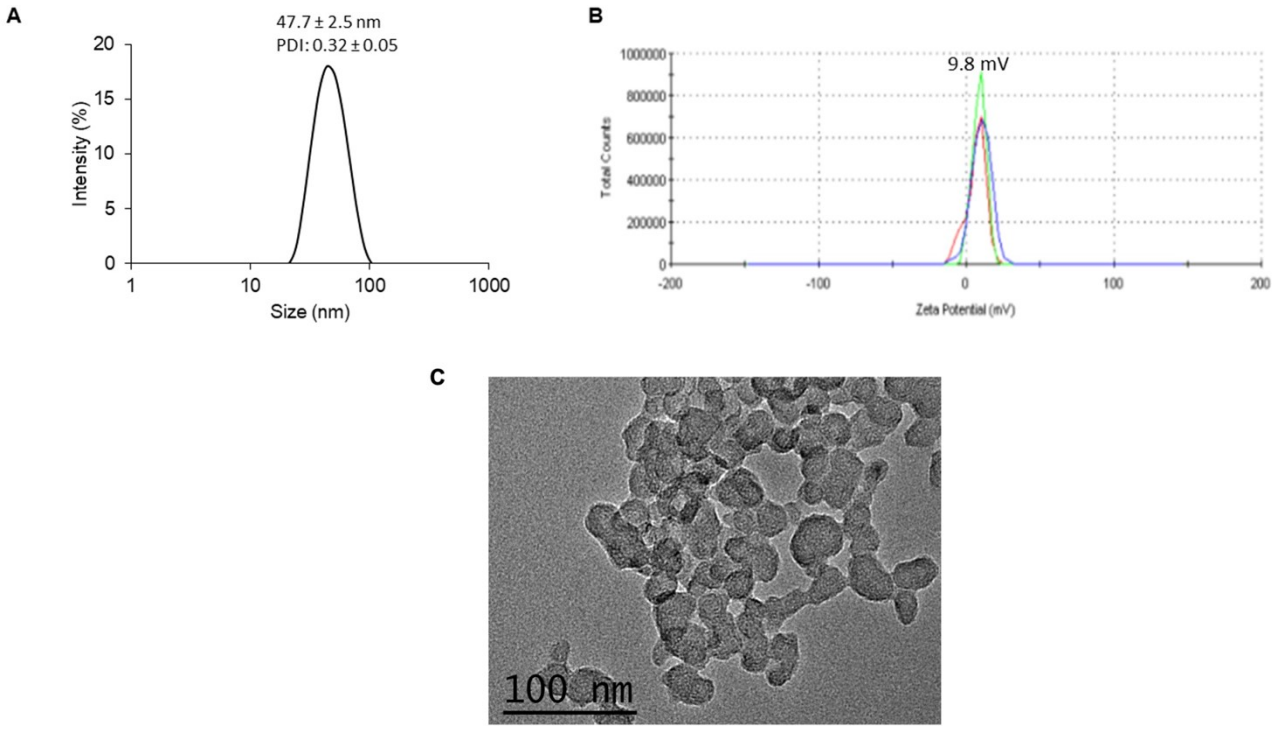

Fig. S1 (A) Size distribution measured by DLS (n=3 independent batches of polymers), (B) zeta potential and (C) TEM image, of MIP-NGs.

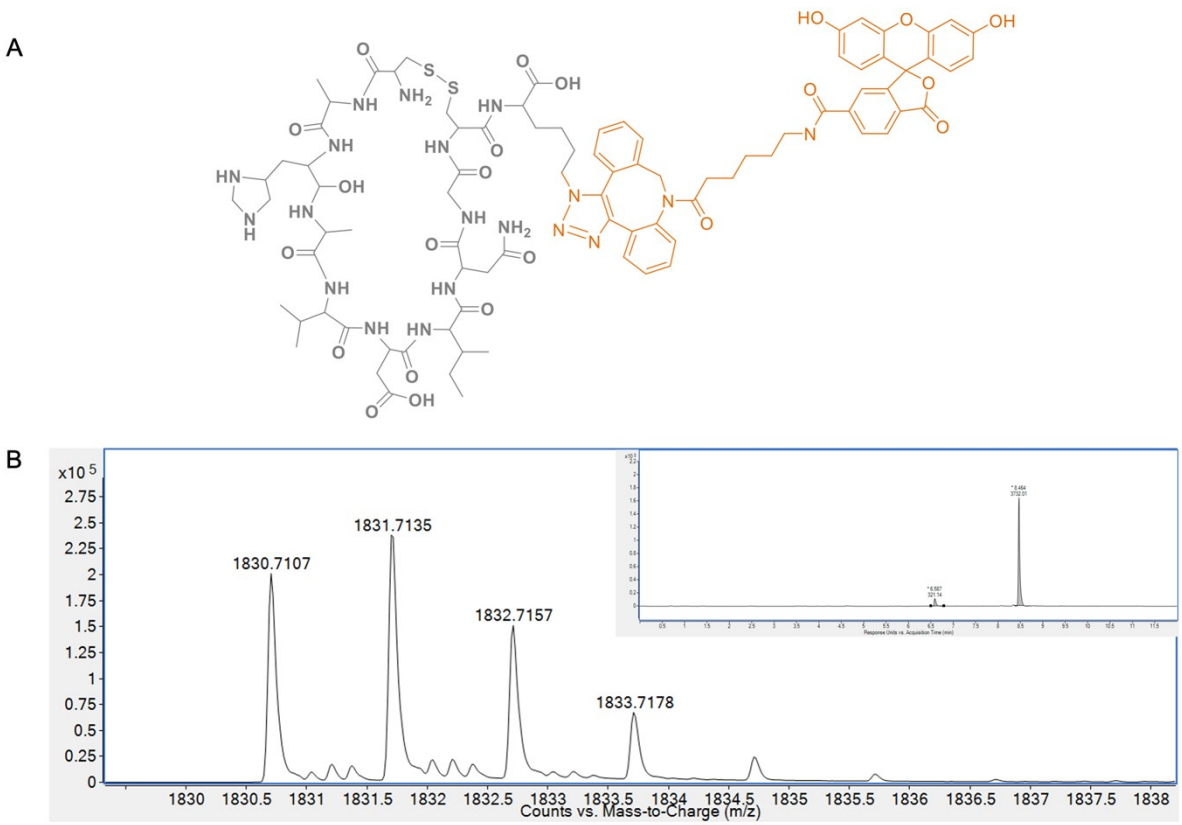

Fig. S2 (A) Chemical structure and (B) HPLC-ESI-HRMS, of the fluorescein-labelled cyclic peptide. ESI$^+$ at 6.66 min showing the characteristic isotopic mass ratio of the compound. Theoretical value: $[M+H]^+$ 1830.7040 u and measured value: $[M+H]^+$ 1830.7107 u. (Inset) UV_{280nm} chromatogram before semi-preparative purification.

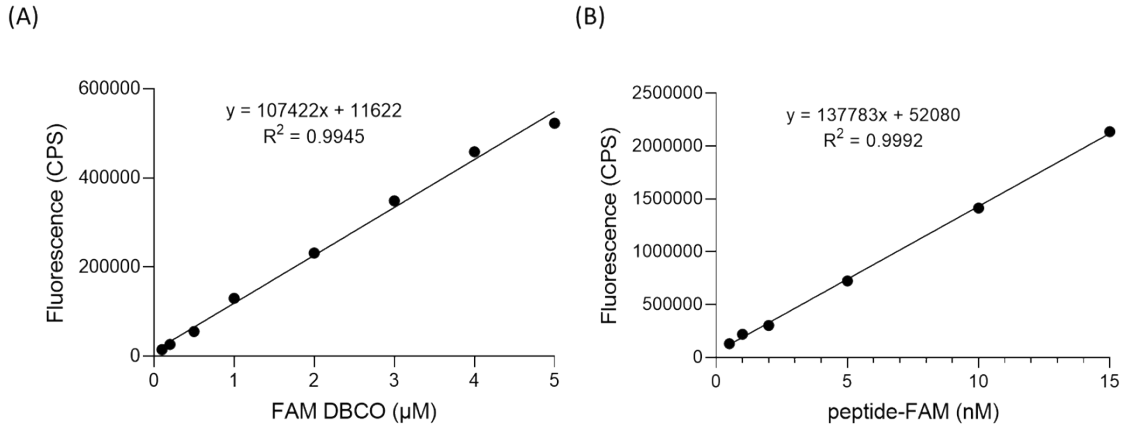

Fig. S3 Representative calibration curves (n =2) at λ_{ex} 494 nm and λ_{em} 500-560 nm of (A) FAM DBCO, slit 1 nm and (B) FAM-labelled cyclic template peptide, slit 4 nm, in 25 mM sodium phosphate buffer pH 7.0.

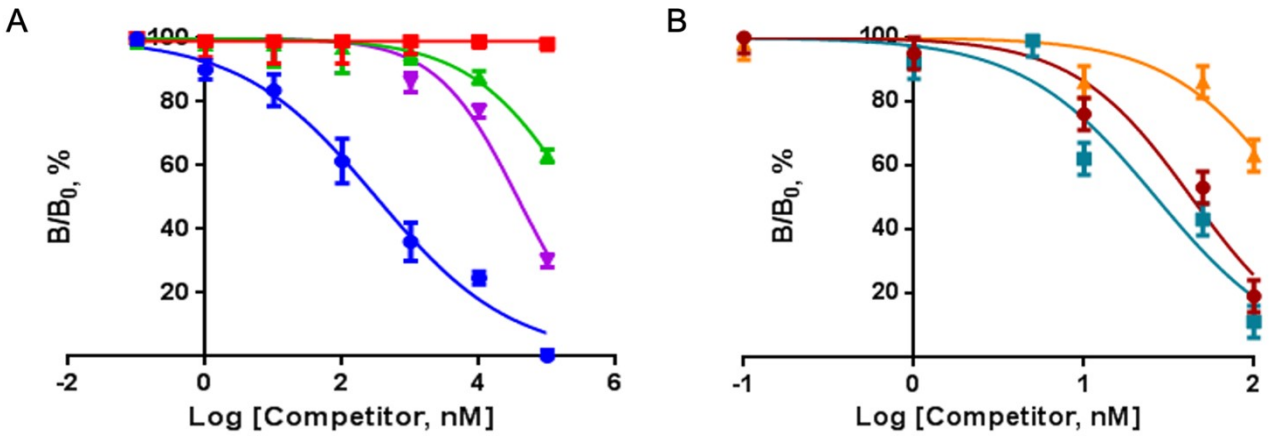

Fig. S4 Inhibition of binding of 10 nM fluorescent template peptide to 200 μg/mL of MIP-NGs by competing (A) peptides: CAHAVDINGC-K(N_3) (blue), CHAVDINC-K(N_3) (violet), HAVDI linear peptide (green) and DWVIPPI linear peptide (red) and (B) recombinant proteins: N-cadherin (blue), E-cadherin (red) and P-cadherin (orange). B/B_0 is the ratio of the amount of fluorescent peptide bound in the presence and absence of displacing ligands.

Table S1. IC_{50} values of MIP-NGs with various competitors, as determined by competitive binding assays with the fluorescently labelled template peptide epitope.

Competitor	**IC_{50} (nM)**
Template peptide CAHAVDINGC-K(N_3)	300
Short cyclic peptide CHAVDINC-K(N_3)	36,400
HAVDI linear peptide	>100,000
DWVIPPI linear peptide	No binding
N-cadherin	25
E-cadherin	41
P-cadherin	200

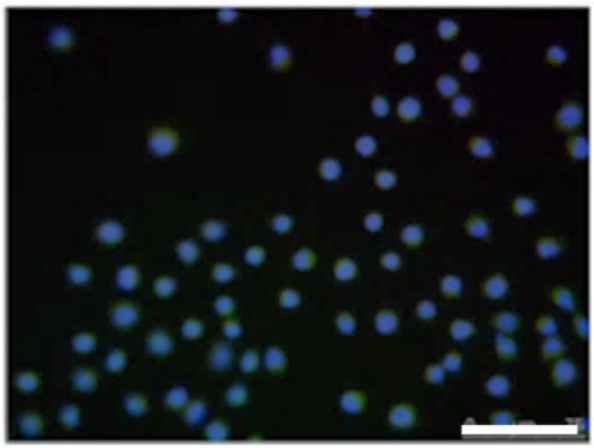

Fig. S5 Epifluorescence micrograph of L929 cells (no expression of cadherins), stained with rhodamine MIP-NGs (red), Hoechst (nucleus, blue) and DiO (cell membrane, green). Scale bar: 75 µm.

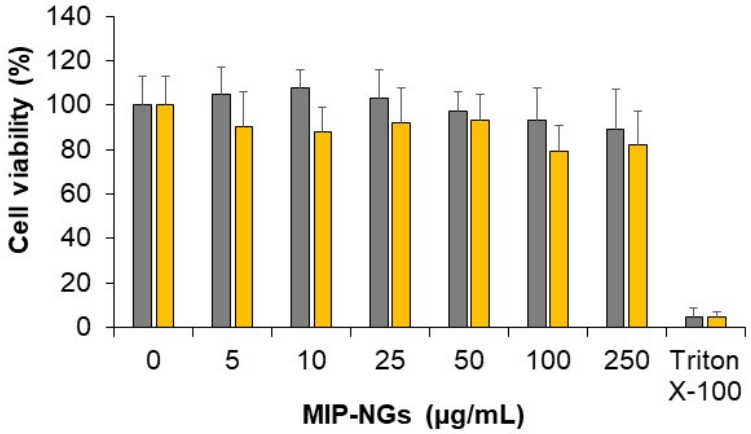

Fig. S6 Cell viability, as determined by MTT assay of HeLa (grey) and MCF-7 (yellow) cells in presence of MIP-NGs. Positive control: 1 % Triton X-100. Data are mean values ± s.e.m. (n=5 repetitions).

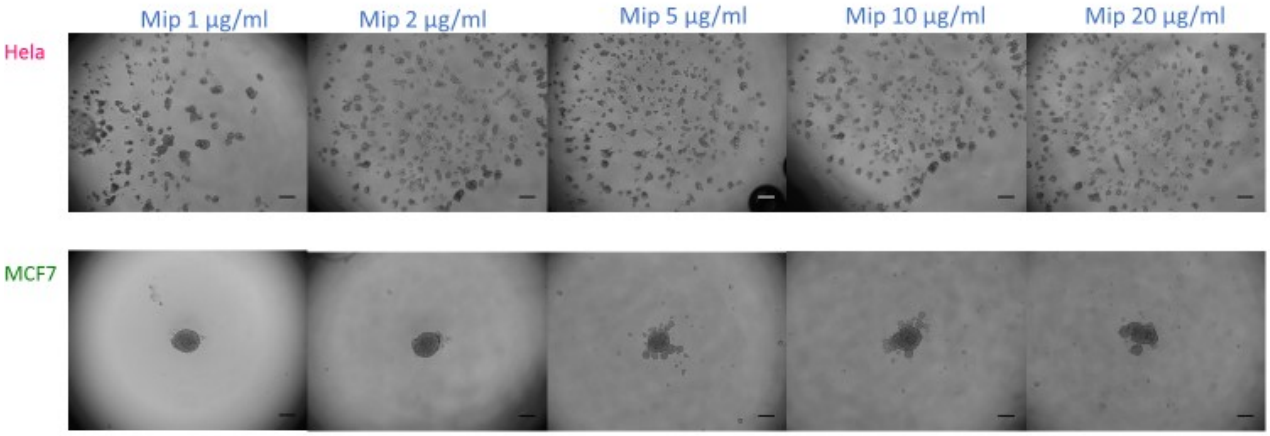

Fig. S7 Cell aggregation of HeLa and MCF-7 in presence of 1, 2, 5, 10 and 20 µg/mL of MIP-NGs. Scale bar: 250 µm.