

Figure S1. Viability of PC-3 cells treated with Aib-substituted Djeya1 analogues. PC-3 cells were seeded in Roswell Park Memorial Institute media-1640 with L-glutamine (RPMI-1640, Gibco, Life Technologies, USA) growth medium, supplemented with 10% (*v/v*) foetal bovine serum (FBS, Gibco, Life Technologies, USA) and 1% (*v/v*) penicillin/streptomycin mixture (Gibco, Life Technologies, USA) in 96-well plates (1.00×10^4 cells/well) and maintained in an incubator (MCO-170AICUV, Panasonic, Germany) at 37 °C, with a 5% CO₂ atmosphere under fully humidified conditions for 24 h. Then, the cells were incubated with 3, 10 and 25 µM of [Aib¹⁰]Djeya1, [Aib¹³]Djeya1 and [Aib¹⁶]Djeya1 in RPMI-1640 medium without FBS and incubated for 24 h. Untreated cells were also included in the assay and used as control (100% viability). One hour before the incubation time, 10 µL of PrestoBlue™ Cell Viability reagent, resazurin-based reagent (Thermo Fisher Scientific, USA) was added to each well and incubated for 1 h at 37 °C and 5% CO₂ atmosphere. After the incubation, 100 µL of the culture medium of each well were transferred to a black bottom 96-well plate and the fluorescence at $\lambda_{\text{abs}} = 560$ nm and $\lambda_{\text{em}} = 590$ nm was measured in the microplate reader Tecan Infinite® 200 PROseries, Mannedorf, Switzerland. Cell viability was expressed as the percentage of viable cells, considering untreated cells as 100% viability. Three independent experiments with five replicates for each condition were performed. These data confirm that Aib-substituted Djeya1 analogues do not impact upon the viability of PC-3 cells.

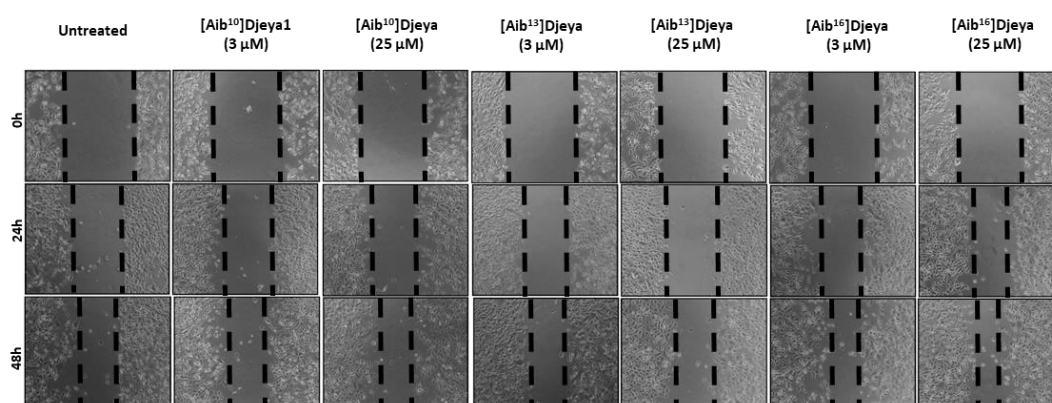


Figure S2. Impact of Aib-substituted Djeya1 peptides (3 µM and 25 µM) on prostate cancer (PC-3) cell migration. This is a representative experiment to evaluate the impact of peptides in the wound healing assay. Wound size was measured at 0, 24, and 48 h.

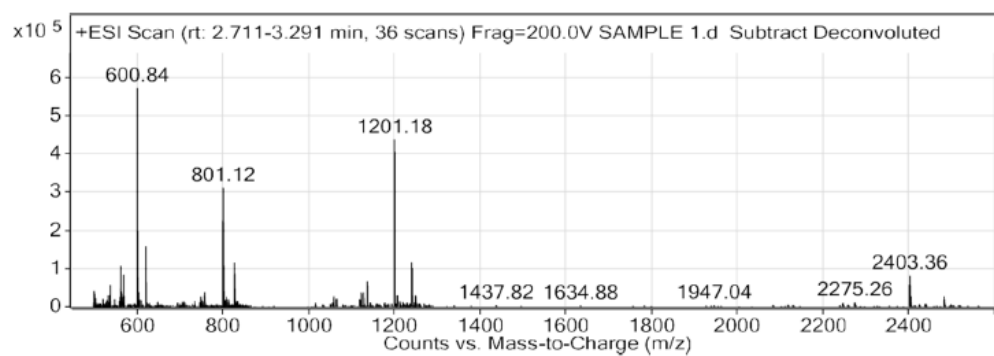


Figure S3. Identification of [Aib¹⁰]Djey 1 by mass spectrometry, Agilent 6200 TOF.

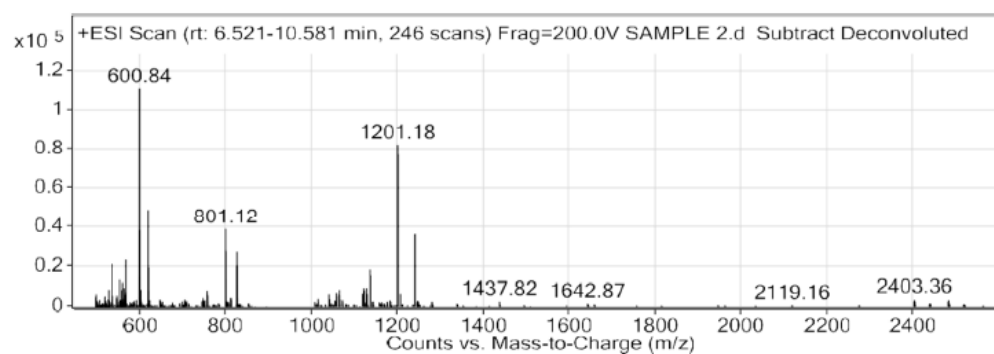


Figure S4. Identification of [Aib¹³]Djey 1 by mass spectrometry, Agilent 6200 TOF.

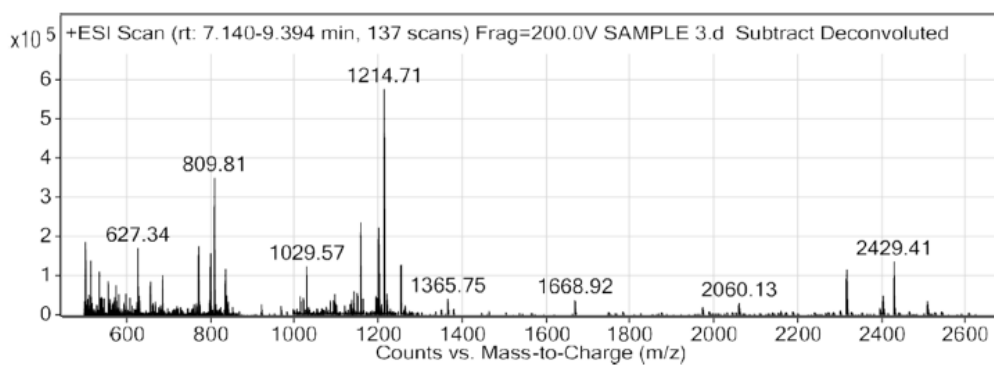


Figure S5. Identification of [Aib¹⁶]Djey 1 by mass spectrometry, Agilent 6200 TOF.