Supplementary data

The product of matrix metalloproteinase cleavage of doxorubicin conjugate for anticancer drug delivery. Calorimetric, spectroscopic and molecular dynamics studies on peptide–doxorubicin binding to DNA

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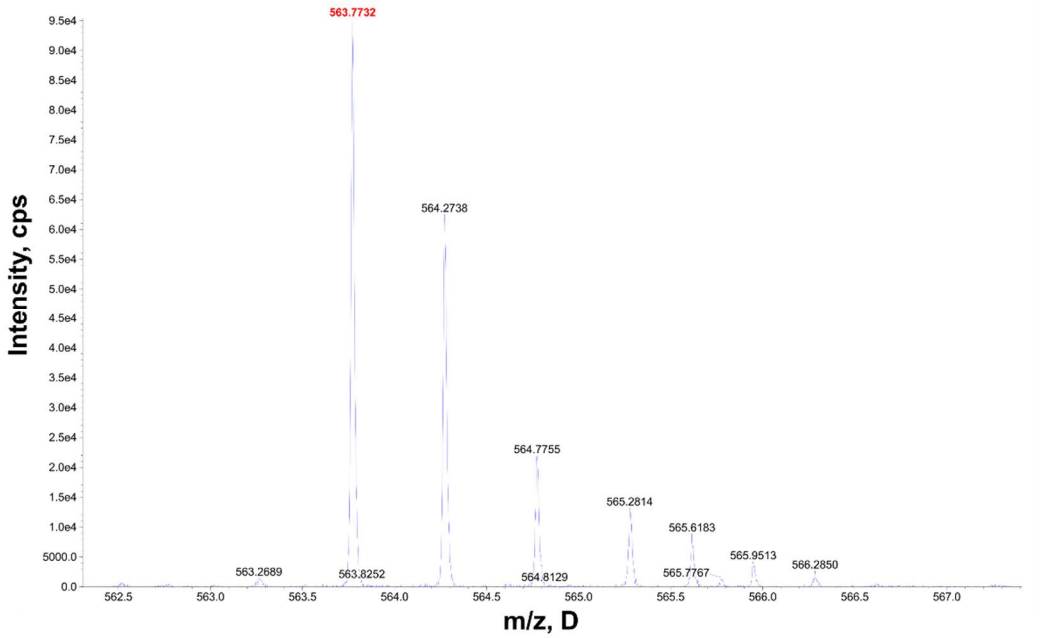

Figure S1. MALDI-TOF mass spectrum of Fmoc–Gly–Pro–Leu–Gly in a positive mode (m/z 563.7732).

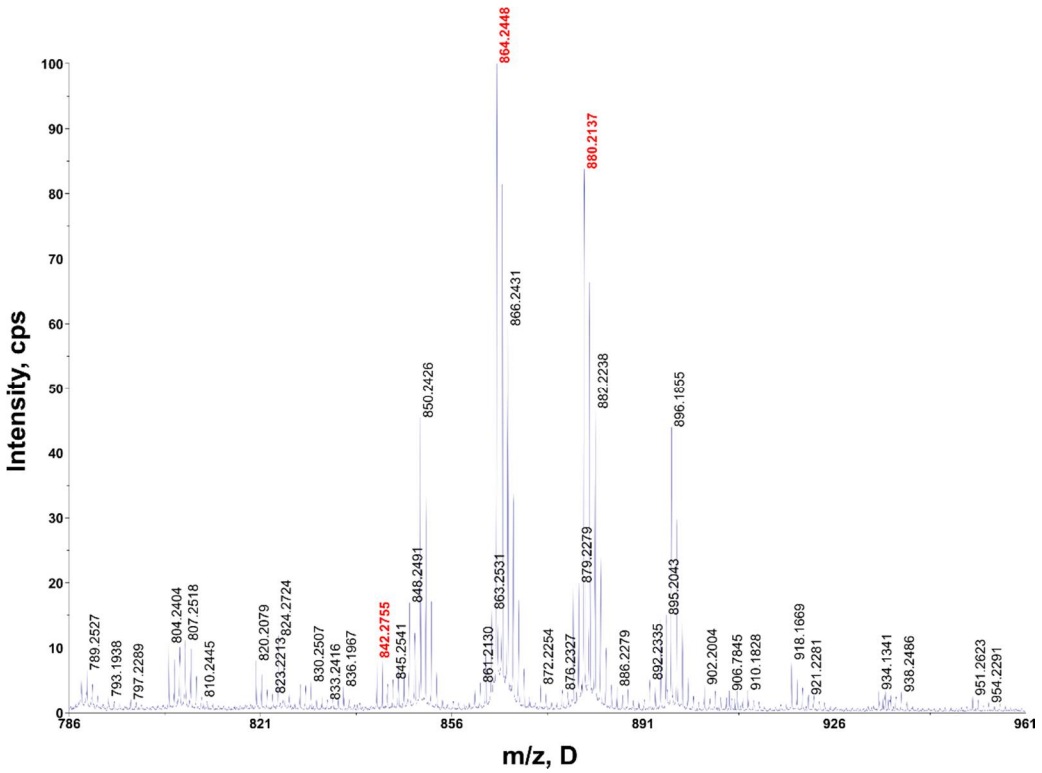

Figure S2. MALDI-TOF spectrum of Leu–Ala–Gly–Gly–DOX in a positive mode [(Leu–Ala–Gly–Gly–DOX + H^+) m/z 842.2755; (Leu–Ala–Gly–Gly–DOX + Na^+) m/z 864.2448; (Leu–Ala–Gly–Gly–DOX + K^+) m/z 880.2137].

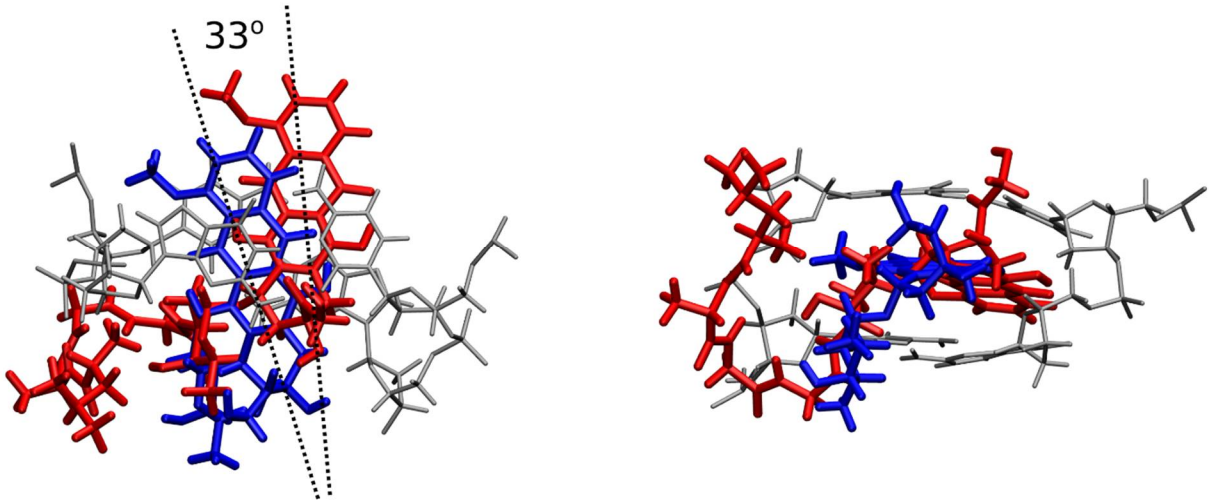

Figure S3. Comparison of the minor groove intercalation modes of DOX (blue) and 4-pep-DOX (red) -- top view (left), side view (right). When intercalated from the minor groove, 4-pep-DOX is rotated by ca. 33deg with respect to the flanking base pairs, compared to DOX.