Supplementary Materials

Table S1. Integrin/Skelemin tertiary complex: data used for docking.

	Sk45[b]	β_3[c]	α_{IIb}[d]
Active Residues[a] used in HADDOCK to define binary interfaces.	E1368 H1370 V1372 Y1374 V1382 D1383 I1411	K716* H722* R724* K725*	
	K1361 A1363 T1394		V990* F992* F993 K994 R995* N996 R997*

[a] Active residues are chosen based upon chemical shifts perturbation data. For Sk45, data is acquired in this study. For integrin subunits, our previously published data (*1*) is used. Integrin residues, shown to be involved in in complex with skelemin by mutagenesis studies (*2, 3*), are marked by star (*).

[b] The fold of tandem Ig domains 4 and 5 is determined as described in Structure Calculations (PDB ID: 4V10). The ensemble representative with the lowest energy is used for docking.

[c] β_3 conformer from its binary complex with α_{IIb} (PDB ID 1M80) is used for docking.

[d] α_{IIb} conformer, used for docking, is calculated in this study based upon trNOEs reported previously (*1*). These data resulted in total of 207 distance restrains (142 unambiguous and 65 ambiguous).

Figure S1.

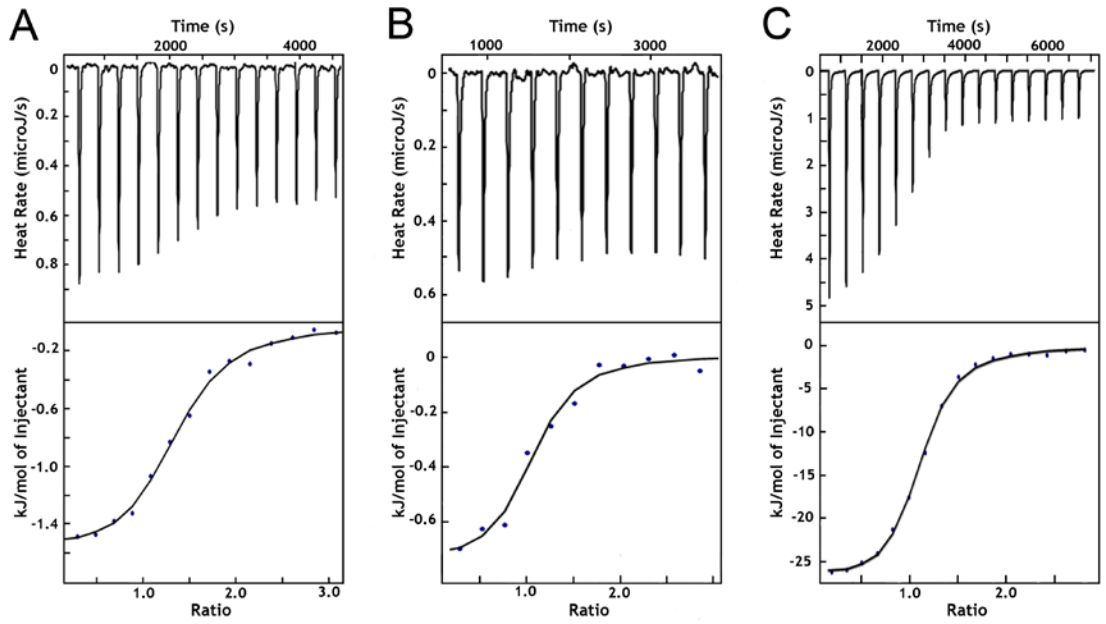

Figure S1. Thermograms and binding curves. **A:** C-terminal β_3 and Sk4, **B:** α_{IIb} and Sk45, and **C:** α_{IIb} and β_3. Note that N-terminal β_3 and Sk45 binding data is not shown as it contained high amounts of noise. The titration of β_3 with α_{IIb} is shown to compare the binding between the integrin subunits and integrin to skelemin. K_d of α_{IIb} and β_3 interaction appears to be 5.7 ± 0.7 μM.

Figure S2.

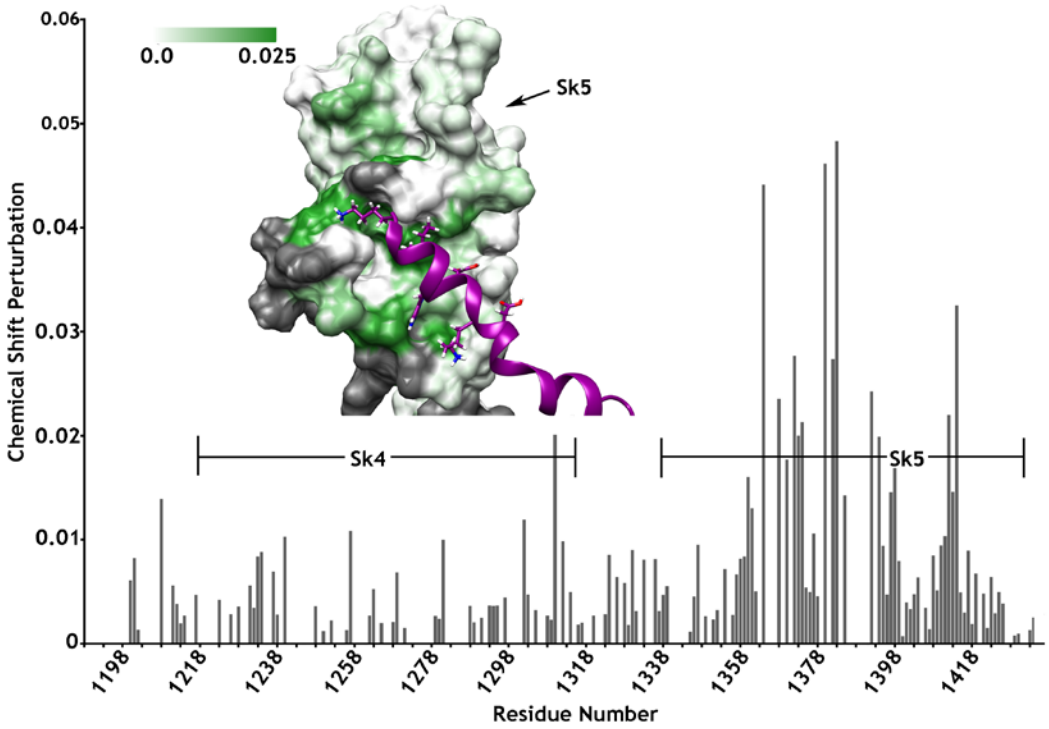

Figure S2. The chemical shift perturbations of Sk45 titrated with N-terminal β_3 peptide (at 1:3 ratio) is presented. The residues belonging to Sk4 or Sk5 are marked on the graph. The structure displayed in inset is of Sk5 with bound β_3 (purple). The surface of Sk5 is colored based on the magnitude of the chemical shift perturbation (according to the shown scale). The residues with no data available are colored gray.