Electronic Supplementary Information for:

Comparative study of interaction energies between $\alpha_{IIb}\beta_3$ integrin and the peptidic, peptidomimetic and non-peptidic ligands by quantum mechanics FMO-PIEDA calculations.

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Table S1. The most significant partial interaction energies ($\Delta E_{L:R\text{-}AA}$) between the peptidic ligand (GAKQAGDV-COO^-) and structural fragments of $\alpha_{IIb}\beta_3$ calculated at the MP2/6-31G(d) level. The energy terms of $\Delta E_{L:R\text{-}AA}$, the electrostatic energy ($\Delta E_{L:R\text{-}AA}^{els}$), the exchange repulsion energy ($\Delta E_{L:R\text{-}AA}^{exch}$), the charge transfer and higher order mixed term ($\Delta E_{L:R\text{-}AA}^{ct+mix}$), the dispersion energy ($\Delta E_{L:R\text{-}AA}^{disp}$) and solute-solvent solvation free energy ($\Delta G_{L:R\text{-}AA}^{sol}$) (in kcal mol^{-1}).

	$\Delta E_{L:R\text{-}AA}$	$\Delta E_{L:R\text{-}AA}^{els}$	$\Delta E_{L:R\text{-}AA}^{exch}$	$\Delta E_{L:R\text{-}AA}^{ct+mix}$	$\Delta E_{L:R\text{-}AA}^{disp}$	$\Delta G_{L:R\text{-}AA}^{sol}$
Mg^{2+}(MIDAS)	-350.2	-350.5	8.5	-13.8	-10.3	15.9
Ca^{2+}(ADMIDAS)	-158.9	-202.5	0.0	-5.6	28.1	21.1
Asp224A	-90.5	-96.5	23.7	-10.2	-7.7	0.2
Ca^{2+}(SYMBS)	-75.8	-116.7	0.00	-0.9	32.1	9.6
Asn215B	-55.3	-57.1	12.4	-6.3	-6.2	1.8
Asp159A	-52.1	-52.9	20.4	-9.7	-10.0	0.1
Lys125B	-49.2	-64.1	0.0	0.0	0.0	14.9
Arg214B	-43.7	-47.2	0.6	-1.9	-1.9	6.7
Tyr122B	-28.7	-26.8	5.0	-4.1	-6.2	3.5
Lys253B	-28.6	-37.3	0.0	0.0	0.0	8.8
Tyr190A	-28.5	-23.0	3.8	-2.5	-6.1	-0.7

Table S2. The most significant partial interaction energies ($\Delta E_{L:R\text{-}AA}$) between the peptidic ligand (AKQRGDV-COO^-) and structural fragments of $\alpha_{IIb}\beta_3$ calculated at the MP2/6-31G(d) level. The energy terms of $\Delta E_{L:R\text{-}AA}$, the electrostatic energy ($\Delta E_{L:R\text{-}AA}^{els}$), the exchange repulsion energy ($\Delta E_{L:R\text{-}AA}^{exch}$), the charge transfer and higher order mixed term ($\Delta E_{L:R\text{-}AA}^{ct+mix}$), the dispersion energy ($\Delta E_{L:R\text{-}AA}^{disp}$) and solute-solvent solvation free energy ($\Delta G_{L:R\text{-}AA}^{sol}$) (in kcal mol^{-1}).

	$\Delta E_{L:R\text{-}AA}$	$\Delta E_{L:R\text{-}AA}^{els}$	$\Delta E_{L:R\text{-}AA}^{exch}$	$\Delta E_{L:R\text{-}AA}^{ct+mix}$	$\Delta E_{L:R\text{-}AA}^{disp}$	$\Delta G_{L:R\text{-}AA}^{sol}$
Mg^{2+}(MIDAS)	-352.0	-343.3	9.4	-13.3	-10.2	5.4
Ca^{2+}(ADMIDAS)	-169.4	-200.1	0.0	-4.9	28.6	7.0
Ca^{2+}(SYMBS)	-75.6	-109.2	0.0	-0.6	32.1	2.1
Asp224A	-63.7	-70.8	16.6	-6.7	-5.1	2.4
Asn215B	-52.6	-51.9	8.6	-5.2	-5.5	1.5
Lys125B	-49.2	-58.7	0.0	0.0	0.0	9.5
Arg214B	-42.2	-41.3	-0.7	-1.5	-1.6	1.5
H_2O-312	-40.1	-50.6	28.0	-9.9	-8.1	0.5
Tyr122B	-35.4	-35.3	14.2	-6.9	-8.4	0.9
Lys253B	-33.8	-36.1	0.0	0.0	0.0	2.3
Tyr190A	-32.5	-28.9	12.2	-4.3	-10.9	-0.6

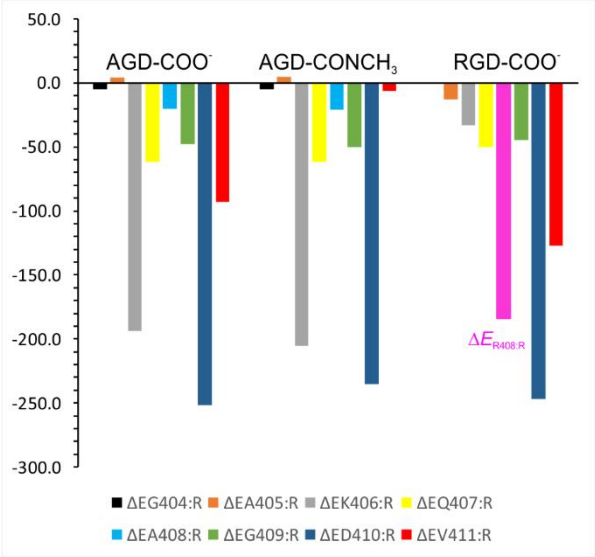

Figure S1. FMO-PIEDA interaction energies ($\Delta E_{\text{L-AA:R}}$, in kcal mol^{-1}) between the amino acid residues of the bound peptides and $\alpha_{\text{IIb}}\beta_3$ calculated at the *ab initio* MP2/6-31G(d) level (AGD-COO$^-$ and AGD-CONCH$_3$ are the peptides with the GAKQAGDV sequence, RGD-COO$^-$ is the peptide with the AKQRGDV sequence).