

Table S1. X-ray diffraction and structure refinement, related to Fig. 3, Fig. S1-S2.

Ligand	0.05 mM Tirofiban Mg/Ca*	0.1 mM Eptifibatide Mg/Ca*	1 mM Sibrafiban Mg/Ca	1 mM Sibrafiban Mn/Ca	1 mM Lamifiban Mg/Ca	1 mM Lamifiban Mn/Ca	1 mM Fradafiban Mg/Ca
Space group	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2
Unit cell (a, b, c) (Å)	256.6, 144.4, 104.3	260.3, 145.0, 104.9	257.8, 144.8, 104.8	258.4, 144.6, 104.9	259.4, 145.2, 105.3	257.9, 144.6, 105.1	258.3, 145.0, 105.0
(α , β , γ) (°)	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90
Wavelength (Å)	1.0332	0.97934	0.97934	0.97934	0.97934	0.97934	0.97934
Resolution (Å)	50.0-2.60/2.67-2.60 ^a	50.0-2.75/2.82-2.75 ^a	50-2.35/2.41-2.35 ^a	50-2.60/2.67-2.60 ^a	50-2.45/2.49-2.45 ^a	50-2.60/2.63-2.60 ^a	50-2.74/2.51-2.74 ^a
Number of reflections (total/unique)	692,763/119,442	549,631/103,704	526,330/154,446	793,424/119,874	572,007/146,004	407,101/219,139	340,129/101,407
Completeness (%)	99.8/99.1	99.9/99.0	99.1/99.2 ^a	99.3/97.6 ^a	99.2/96.2 ^a	93.8/93.8 ^a	97.5/94.8 ^a
I/ σ (I)	13.1/1.2	10.4/1.1	4.90/0.44 ^a	6.74/0.45 ^a	7.79/0.60 ^a	5.07/0.40 ^a	8.14/0.52 ^a
{R _{merge} ^b } or CC _{1/2} ^c	{0.10/1.26 ^a }	{0.114/1.63 ^a }	0.14 ^a	0.26 ^a	0.16 ^a	0.11 ^a	0.16 ^a
R _{work} /R _{free} ^d	0.182/0.210	0.189/0.222	0.203/0.245	0.214/0.239	0.221/0.247	0.223/0.242	0.225/0.253
RMSD: Bond (Å)	0.002	0.003	0.006	0.007	0.005	0.005	0.005
Angle (°)	0.539	0.548	0.640	0.603	0.561	0.607	0.530
Ramachandran plot ^e	96.0/3.9/0.1	95.2/4.6/0.2	94.7/4.8/0.5	94.9/4.9/0.2	94.6/5.1/0.3	94.7/5.1/0.2	95.5/4.4/0.1
Molecules/asymmetric unit	2	2	2	2	2	2	2
Conformational states ^f (molecule 1/molecule 2)	State 3/State 3	State 4/State 3	State 1/State 1	State 4/State 2	State 1/State 1	State 3/State 3	State 1/State 1
MolProbity score	1.23	1.34	1.29	1.50	1.61	1.44	1.11
Clash score	1.92	2.27	1.49	2.01	2.51	2.06	1.16
PDB code	7TD8	7THO	7L8P	7UKO	7UJK	7UK9	7UE0
SBCGrid Data Bank ID	-	950	933	934	935	936	937

Table S1 (cont'd)

Ligand	1 mM Fradafiban Mn/Ca	1 mM Roxifiban Mn/Ca	1 mM Lotrafiban Mg/Ca	1 mM Gantofiban Mn/Ca	1 mM Gantofiban analog, Mn/Ca	0.1 mM EF-5154 Mg/Ca*	0.1 mM UR-2922 Mg/Ca*
Space group	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2
Unit cell (a, b, c) (Å)	259.9, 144.5, 104.7	258.7, 144.0, 104.8	258.7, 144.0, 104.8	258.6, 144.5, 105.1	259.2, 144.4, 104.8	260.2, 144.3, 104.3	259.2, 143.8, 104.9
(α , β , γ) (°)	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90
Wavelength (Å)	0.97934	0.97934	0.97934	0.97934	0.97934	0.97948	1.0332
Resolution (Å)	50-3.00 /3.07-3.00 ^a	50-2.75/2.80-2.75 ^a	50-2.80/2.84-2.80 ^a	50-2.35/2.38-2.35 ^a	50-2.80/2.87-2.80 ^a	50-2.60/2.69-2.60	50-2.50/2.57-2.50 ^a
Number of reflections (total/unique)	276,766/78,827	404,953/196,083	482,115/183,986	678,316/315,839	445,555/96,001	799,550/121,114	633,917/134,985
Completeness (%)	99.2/98.9 ^a	99.7/99.9 ^a	99.6/99.7 ^a	99.7/99.8 ^a	98.4/99.9 ^a	99.9/99.0	99.4/95.4
I/ σ (I)	7.56/0.66 ^a	4.47/0.55 ^a	4.66/0.50 ^a	3.78/0.43	7.26/0.49	11.0/1.8	14.6/1.6
{R _{merge} ^b } or CC _{1/2} ^c	0.13 ^a	0.11 ^a	0.14 ^a	0.11 ^a	0.15 ^a	{0.09/1.10 ^a }	{0.064/0.888 ^a }
R _{work} /R _{free} ^d	0.223/0.242	0.229/0.248	0.213/0.235	0.221/0.231	0.219/0.241	0.166/0.194	0.195/0.227
RMSD: Bond (Å)	0.007	0.006	0.006	0.007	0.006	0.003	0.004
Angle (°)	0.511	0.588	0.605	0.576	0.575	0.584	0.55
Ramachandran plot ^e	95.0/4.6/0.4	95.3/4.4/0.3	95.3/4.5/0.2	95.5/4.3/0.2	95.2/4.6/0.2	96.6/3.3/0.1	95.8/4.0/0.2
Molecules/asymmetric unit	2	2	2	2	2	2	2
Conformational states ^f (molecule 1/molecule 2)	State 3/State 3	State 6/State 3	State 6/State 3	State 1/State 1	State 3/State 3	State 3/State 3	State 1/State 1
MolProbity score	1.31	1.20	1.20	1.11	1.16	1.23	1.29
Clash score	1.94	1.40	1.40	0.99	1.14	1.80	2.22
PDB code	7UFH	7UH8	7UDG	7UCY	7UKP	7TPD	7TCT
SBGrid Data Bank ID	938	939	940	941	942	-	-

Table S1 (cont'd)

Ligand	0.5 mM UR-2922 Mn/Ca	0.5 mM BMS4 Mg/Ca	0.5 mM BMS4 Mn/Ca	0.5 mM BMS4.1 Mn/Ca	0.5 mM BMS4.2 Mn/Ca	0.5 mM BMS4.3 Mn/Ca	0.5 mM GR144053 Mn/Ca	0.1 mM cyclic RGDfV Mn/Ca
Space group	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2	P2 ₁ 2 ₁ 2
Unit cell (a, b, c) (Å)	259.6, 143.7, 105.2	258.9, 144.2, 105.1	259.4, 144.3, 104.9	257.8, 143.9, 104.7	259.8, 144.4, 105.0	258.3, 144.7, 105.1	257.9, 144.4, 104.8	260.9, 145.8, 105.2
(α , β , γ) (°)	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90
Wavelength (Å)	1.0332	0.97934	0.97934	0.97934	0.97934	0.97934	0.97934	0.97948
Resolution (Å)	50-2.50/2.56-2.50 ^a	50-2.20/2.23-2.20 ^a	50-2.70/2.77-2.70 ^a	50-2.25/2.31-2.25 ^a	50-2.37/2.40-2.37 ^a	50-2.00/2.05-2.00 ^a	50-2.05/2.08-2.05 ^a	50.0-2.55/2.62-2.55 ^a
Number of reflections (total/unique)	496,940/135,646	676,692/367,043	557,762/107,262	798,704/411,025	782,364/303,081	1,419,534/258,061	817,157/455,572	764,339/129,549
Completeness (%)	99.4/100.0 ^a	95.1/96.2 ^a	98.4/99.8 ^a	99.2/93.8 ^a	99.7/99.7 ^a	97.4/79.0	96.0/88.1 ^a	98.8/98.5
I/ σ (I)	7.42/0.80 ^a	4.03/0.36 ^a	5.50/0.81 ^a	10.3/0.65 ^a	9.04/0.4 ^a	8.34/0.38	4.71/0.41 ^a	11.4/1.2
{R _{merge} ^b } or CC _{1/2} ^c	{0.116/1.63 ^a }	{0.125/2.1 ^a }	{0.100/0.995 ^a }	0.27 ^a	0.10 ^a	0.09 ^a	0.12 ^a	{0.11/0.90 ^a }
R _{work} /R _{free} ^d	0.209/0.239	0.214/0.241	0.217/0.237	0.203/0.226	0.194/0.218	0.185/0.214	0.209/0.223	0.189/0.225
RMSD: Bond (Å)	0.006	0.006	0.006	0.006	0.006	0.007	0.007	0.002
Angle (°)	0.511	1.112	0.53	0.544	0.508	0.639	1.104	0.593
Ramachandran plot ^e	95.8/3.9/0.3	95.8/4.1/0.1	95.6/4.2/0.2	96.0/3.8/0.2	95.7/4.1/0.2	96.0/3.8/0.2	95.2/4.6/0.2	96.2/3.6/0.2
Molecules/asymmetric unit	2	2	2	2	2	2	2	2
Conformational states ^f (molecule 1/molecule 2)	State 1/State 1	State 1/State 1	State 1/State 1	State 1/State 1	State 2/State 2	State 1/State 1	State 1/State 1	State 3/State 1
MolProbity score	1.22	0.94	1.24	1.03	1.01	1.21	0.88	1.33
Clash score	1.69	0.41	1.72	0.82	0.65	1.72	0.12	2.17
PDB code	7UJE	7TMZ	7U9F	7U9V	7UKT	7UDH	7UBR	7U60
SBGrid Data Bank ID	943	944	945	946	947	948	949	-

^aNumbers correspond to the last resolution shell.

^b $R_{\text{merge}} = \sum_h \sum_i |I_i(h) - \langle I(h) \rangle| / \sum_h \sum_i I_i(h)$, where $I_i(h)$ and $\langle I(h) \rangle$ are the i th and mean measurement of the intensity of reflection h .

^cCC_{1/2} = correlation coefficient between two random half datasets (Karplus et al., 2012).

No I/ σ cutoff was applied.

^d $R_{\text{work}} = \sum_h ||F_{\text{obs}}(h) - F_{\text{calc}}(h)|| / \sum_h |F_{\text{obs}}(h)|$, where $F_{\text{obs}}(h)$ and $F_{\text{calc}}(h)$ are the observed and calculated structure factors, respectively; R_{free} is the R value obtained for a test set of reflections consisting of a randomly selected 1 % subset of data excluded from refinement.

^eResidues in favorable, allowed, and outlier regions of the Ramachandran plot as reported by MOLPROBITY.

^fConformational states are assigned by superimposing β I domain of the structure of interest with 8 discrete crystallographic snapshots observed by Zhu et al., 2013, state 1 being the closed, unliganded control, and state 8 the RGD-occupied fully open. There are 6 intermediate states in between states 1 and 8.

Mg/Ca: 1mM MgCl₂, 1mM CaCl₂

Mg/Ca*: 5mM MgCl₂, 1mM CaCl₂;

Mn/Ca: 2mM MnCl₂, 0.1mM CaCl₂