

## Transferred-NOE NMR Experiments on Intact Human Platelets: Receptor-Bound Conformation of RGD-Peptide Mimics

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### Supplementary Information

The NOESY spectra of **1** and **2** in the free state (figure 1) show cross-peaks that are opposite in sign to those of the diagonal.

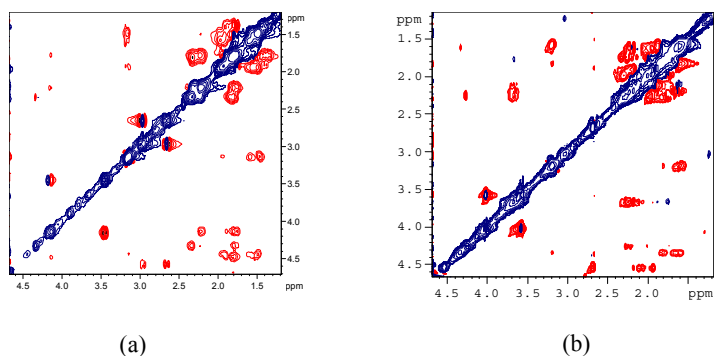


Figura 1. (a) NOESY spectrum ( $mt = 0.4$  s) in  $D_2O$  buffer solution of **1**. (b) NOESY spectrum ( $mt = 0.4$  s) in  $D_2O$  buffer solution of **2**

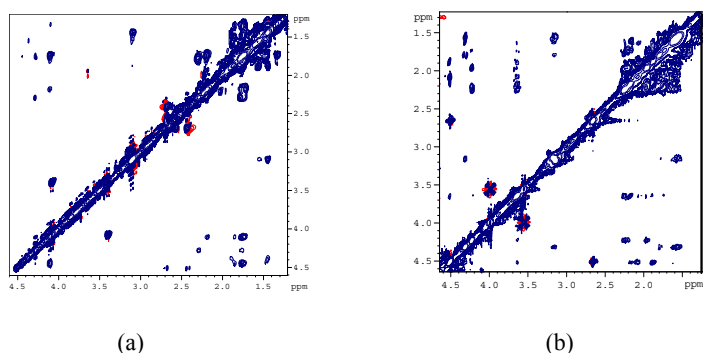


Figure 2. (a) TrNOESY spectrum ( $mt = 0.2$  s) in  $D_2O$  buffer solution of a platelet suspension with **1**. (b) TrNOESY spectrum ( $mt = 0.2$  s) in  $D_2O$  buffer solution of a platelet suspension with **2**.

**Table of chemical shifts**

Compound 1	<sup>1</sup> H-free D <sub>2</sub> O/H <sub>2</sub> O	<sup>1</sup> H-free D <sub>2</sub> O/buffer	<sup>13</sup> C D <sub>2</sub> O/buf	<sup>1</sup> H-bound D <sub>2</sub> O/buffer	Compound 2	<sup>1</sup> H-free D <sub>2</sub> O/buffer	<sup>1</sup> H-free H <sub>2</sub> O/D <sub>2</sub> O	<sup>13</sup> C D <sub>2</sub> O/buffer	<sup>1</sup> H-bound D <sub>2</sub> O/buffer
Arg-NH	8.22				Arg-NH	-	6.97	-	-
Arg-H $\alpha$	4.42	4.42	52.7	4.42	Arg-H $\alpha$	4.33	4.32	52.3	4.33
Arg-H $\beta$	1.96-1.65	1.96-1.65	27	1.96-1.65	Arg-H $\beta$	1.83-1.64	1.78	30.3	1.83-1.64
Arg-H $\gamma$	1.55	1.55	25	1.55	Arg-H $\gamma$	1.55-1.62	1.56-1.62	24.4	1.55-1.62
Arg-H $\delta$	3.11	3.11	40.5	3.11	Arg-H $\delta$	3.20	3.13	40.9	3.20
Gly-NH	7.65	7.65			Gly-NH	-	9.02	-	-
Gly-H $\alpha$	4.15-3.47	4.15-3.47	44	4.10-3.39	Gly-H $\alpha$	4.03-3.58	3.98-3.56	45.3	4.03-3.58
Asp-NH	8.92	8.92			Asp-NH	-	8.69	-	-
Asp-H $\alpha$	4.58	4.58	52	4.52	Asp-H $\alpha$	4.55	4.59	52.6	4.55
Asp-H $\beta$	2.96-2.62	2.96-2.62	36.8	2.70-2.41	Asp-H $\beta$	2.69	2.75	38.5	2.69
Lact-NH	7.95	7.95			Lact-NH	-	7.97	-	-
Lact-H $\alpha$	4.49	4.49	54.2	4.49	Lact-H $\alpha$	4.55	4.53	52.6	4.55
Lact-H $\beta$	1.90-1.55	1.90-1.55	30.5	1.90-1.55	Lact-H $\beta$	2.12-1.91	2.12-1.91	29.2	2.12-1.91
Lact-H $\gamma$	1.85	1.85	26.8	1.85	Lact-H $\gamma$	2.21-1.63	2.21-1.60	25.8	2.21-1.63
Lact-H $\delta$	1.45-1.78	1.45-1.78	34	1.45-1.78	Lact-H $\delta$	-	-	-	-
Pro-H $\alpha$	4.35	4.35	63.6	4.35	Pro-H $\alpha$	4.26	4.24	62.2	4.26
Pro-H $\beta$	2.28-1.78	2.28-1.78	28.3	2.28-1.78	Pro-H $\beta$	2.25-2.00	2.25	27.7	2.25-2.00
Pro-H $\gamma$	2.21-1.75	2.21-1.75	32.6	2.21-1.75	Pro-H $\gamma$	2.3-1.76	2.08-2.17	31.7	2.3-1.76
Pro-H $\delta$	4.14	4.14	60.5	4.10	Pro-H $\delta$	3.68	3.66	61.2	3.68

As a control, mannose was added to a platelets suspension containing compound **2** and a NOESY spectrum was recorded under the same conditions. (Figure 3) The platelet membrane does not contain mannose receptors and, as expected, the NOESY spectrum showed negative cross peaks (trNOEs) for compound **2** and positive cross peaks for mannose

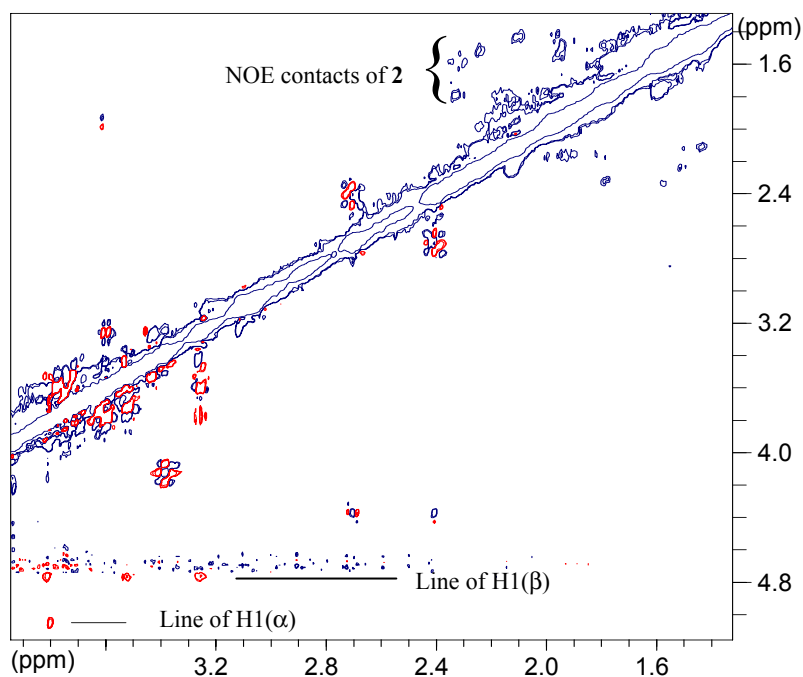


Figure 3. NOESY (200 ms) spectrum of compound **2** and mannose in the presence of platelets suspension in D<sub>2</sub>O buffer