

Supporting Information

Paramagnetic phospholipid-based micelles targeting VCAM-1 receptors for the MRI visualization of inflammation

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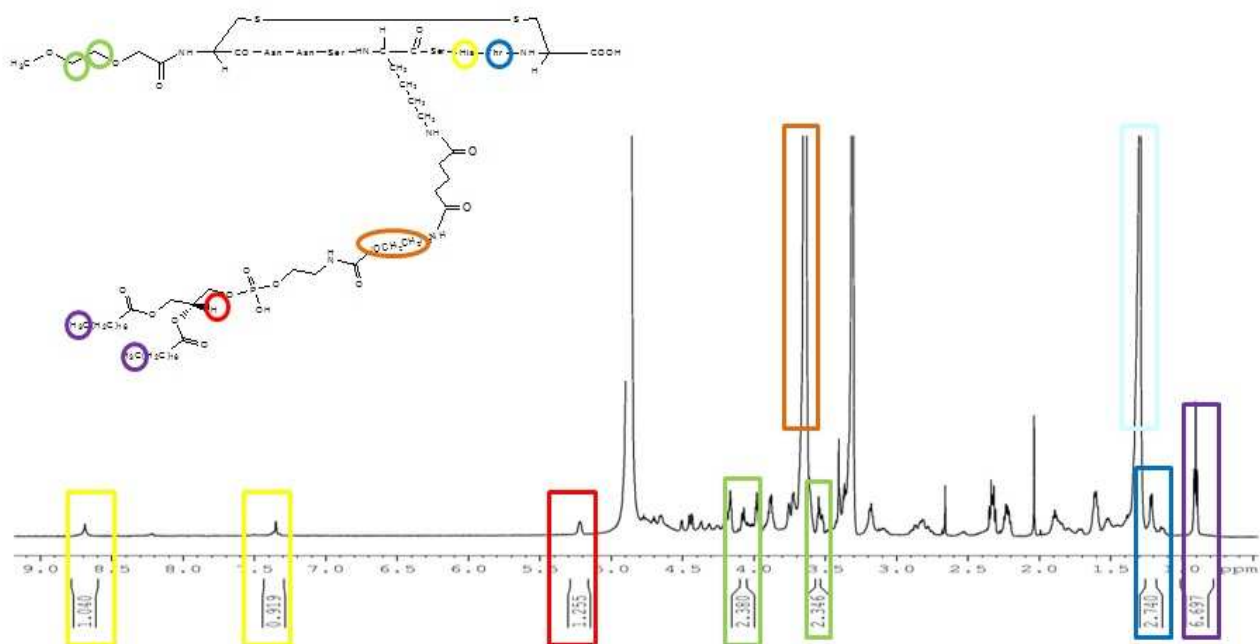


Figure S1. ^1H -NMR spectrum of DSPE-PEG2000-peptide. Assignment of the principal ^1H -NMR signals: CH groups of histidine (yellow), CH group of phospholipid (red), CH_2 groups of (methoxyethoxy)acetic acid (green), CH_2 groups of phospholipid (orange), CH_3 group of threonine (blue), CH_3 terminal groups of phospholipid (purple).

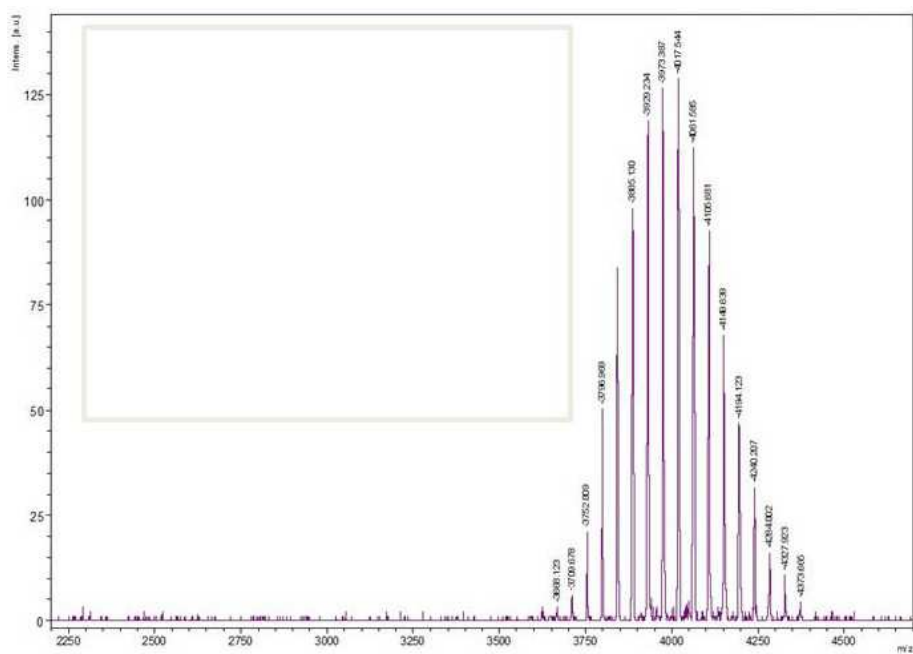


Figure S2. MALDI-MS (positive ion mode) of the phospholipid conjugated to the targeting peptide. The molecular mass of the product is 3973.387.

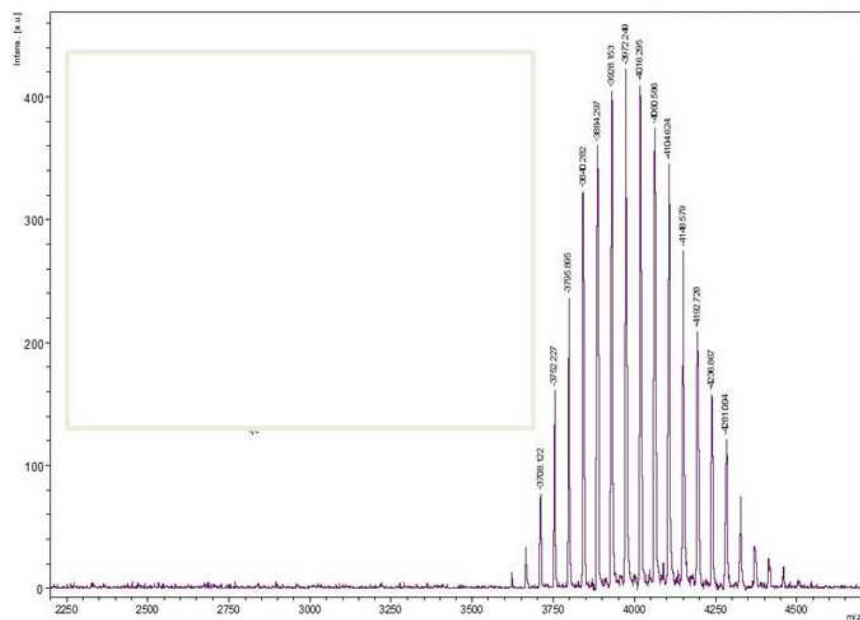


Figure S3. MALDI-MS (negative ion mode) of the phospholipid conjugated to the targeting peptide. The molecular mass of the product is 3972.249.

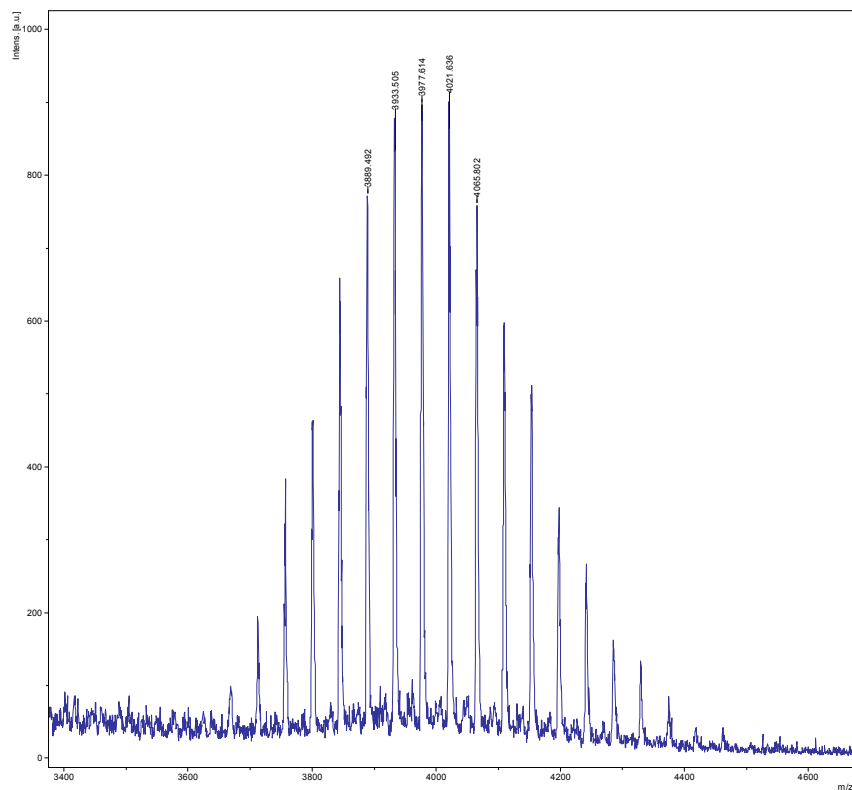


Figure S4. MALDI-MS (positive ion mode) of the phospholipid conjugated to the scrambled peptide. The molecular mass of the product is 3977.614.

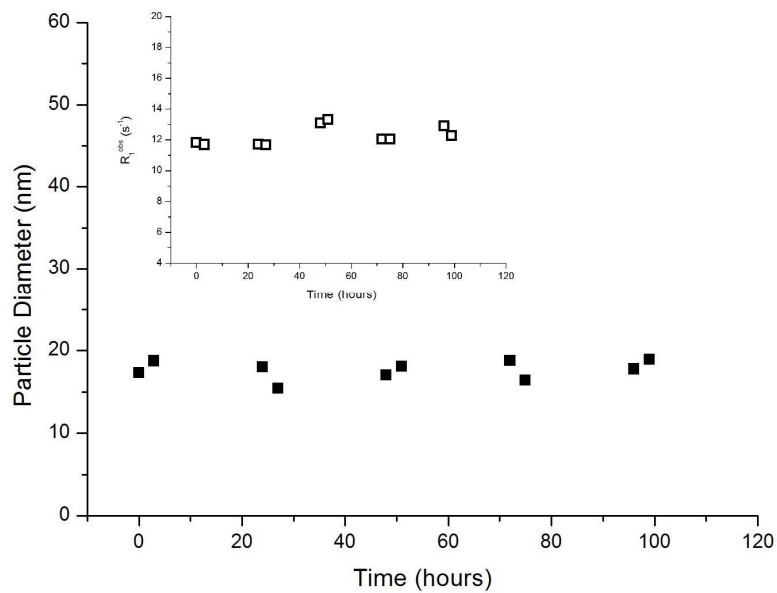


Figure S5. *In vitro* stability of the micelles targeting VCAM-1 receptors. DLS and relaxometric measurements over time of the Gd-loaded micelles targeting VCAM-1 receptors incubated at 37 °C with human serum.

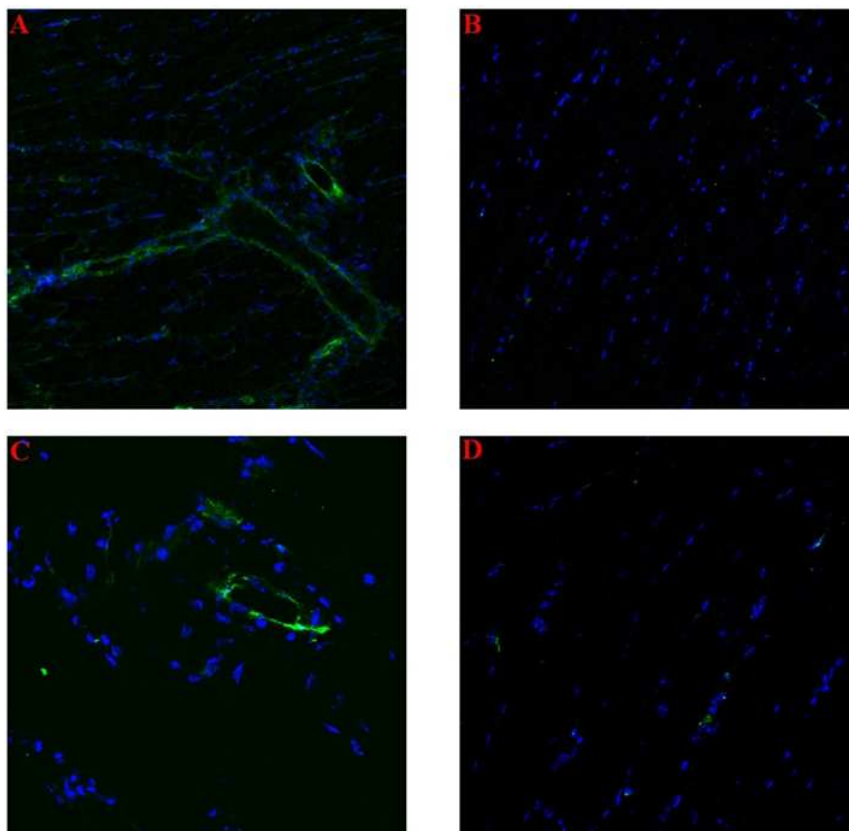


Figure S6. Effect of LPS over the vascular cell adhesion molecule-1 (VCAM-1) expression in leg muscles. Immunofluorescence was used to examine VCAM-1 overexpression in LPS-treated mice muscles in comparison with non treated healthy muscles. A and C represent respectively 20x and 40x confocal microscope images of stained inflamed tissue whereas B and D represent, at the same magnifications, stained healthy tissue (green: VCAM-1, blue: nuclei). As displayed in the images VCAM-1 is abundantly expressed in the inflamed endothelium, whereas a negligible basal expression is detectable in the healthy tissue.

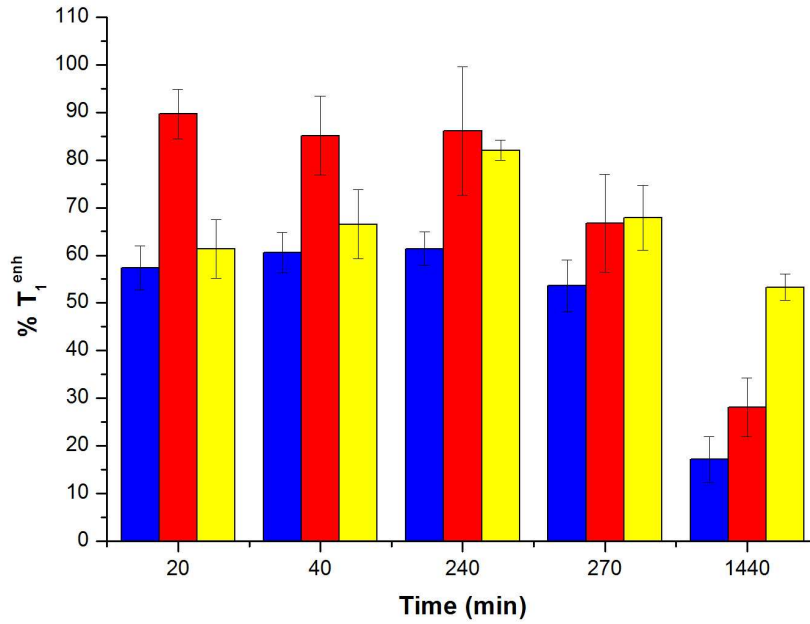


Figure S7. MRI contrast measured in some organs at different time points after the injection of the micelles targeting VCAM-1 receptors. Blue bars refer to kidneys, red bars to spleen and yellow bars to liver. Error bars represent SE of the mean.

Spin	Shift	Label	Assign.
1	0.900	HG1	T8
2	3.950	HB	T8
3	4.206	HA	T8
4	7.843	H	T8
5	4.417	HA	H7
6	3.071	HB	H7
7	2.972	HB2	H7
8	7.955	H	H7
9	8.201	HB	
10	6.972	HB2	
11	8.225	H	K5
12	1.155	HG	K5
13	1.198	HG2	K5
14	1.374	HD	K5
15	1.416	HD2	K5
16	1.528	HB	K5
17	1.617	HB2	K5
18	2.696	HE	K5
19	2.733	HE2	K5
20	3.984	HA	K5
21	4.183	HA	C9
22	8.002	H	C9
23	2.974	HB	C9
24	2.766	HB2	C9
25	7.370	HA	

Spin	Shift	Label	Assign.
26	6.690	HB	
27	8.185	H	N3
28	2.506	HB	N3
29	2.601	HB2	N3
30	4.470	HA	N3
31	3.459	HA	
32	3.370	HB	
33	8.036	H	S4
34	4.184	HA	S4
35	3.734	HB	S4
36	3.610	HB2	S4
37	3.851	II	
38	3.108	H	
39	7.798	H	S6
40	4.140	HA	S6
41	3.599	HB	S6
42	3.524	HB2	S6
43	8.492	H	N2
44	2.484	HB2	N2
45	2.518	HB	N2
46	4.437	HA	N2
47	8.199	H	C1
48	4.409	HA	C1
49	2.800	HB2	C1
50	2.887	HB	C1

Table S1. Complete assignment of the 2D-NMR TOCSY spectrum of the peptide targeting VCAM-1 receptors. The chemical shift and label of each proton are reported in the first and second column, respectively. In the third column the corresponding aminoacids are reported.