
Multivalent RGD synthetic peptides as potent $\alpha_v\beta_3$ integrin ligands

Elisabeth Garanger,^{a,b} Didier Boturyn,^a Jean-Luc Coll,^b Marie-Christine Favrot^b and Pascal Dumy^{a,*}

^a *Ingénierie Moléculaire et Chimie Bioorganique, LEDSS, CNRS UMR 5616, ICMG FR 2607, Université Joseph Fourier, BP 53, 38041 Grenoble Cedex 9, France. Fax: (+33) 476-514-946; Tel: (+33) 476-635-545; E-mail: Pascal.Dumy@ujf-grenoble.fr*

^b *Groupe de Recherche sur le Cancer du Poumon, INSERM U578, Institut Albert Bonniot IFR 73, Domaine de la Merci, 38706 La Tronche Cedex, France.*

SUPPORTING INFORMATION.

RP-HPLC chromatograms and ESI-MS spectra of purified peptides and conjugated compounds.

RP-HPLC were performed using UV monitoring at 214 nm. Solvent A consisted in 0.09% TFA in water and solvent B in 0.09% TFA/9.91% H₂O in 90% acetonitrile. Gradient conditions were :

- **Conditions A** : Analytical column (Macherey-Nagel Nucleosil 120 Å 3 µm C₁₈ particles, 30x4.6 mm); flow rate, 1.3 mL.min⁻¹; linear gradient, 20 to 35% of B in 15 min.

- **Conditions B** : Analytical column (Macherey-Nagel Nucleosil 120 Å 3 µm C₁₈ particles, 30x4.6 mm); flow rate, 1.3 mL.min⁻¹; linear gradient, 5 to 40% of B in 15 min.

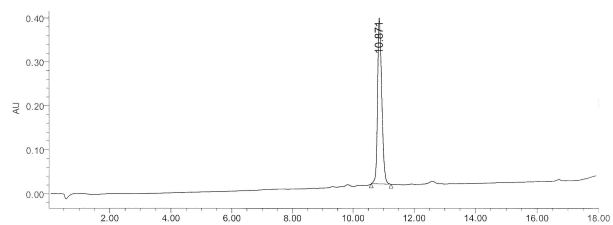
- **Conditions C** : Analytical column (Macherey-Nagel Nucleosil 100 Å 5 µm C₁₈ particles, 250x4.6 mm); flow rate, 1.0 mL.min⁻¹; linear gradient, 5 to 100% of B in 30 min.

- **Conditions D** : Analytical column (Macherey-Nagel Nucleosil 120 Å 3 µm C₁₈ particles, 30x4.6 mm); flow rate, 1.3 mL.min⁻¹; linear gradient, 5 to 60% of B in 15 min.

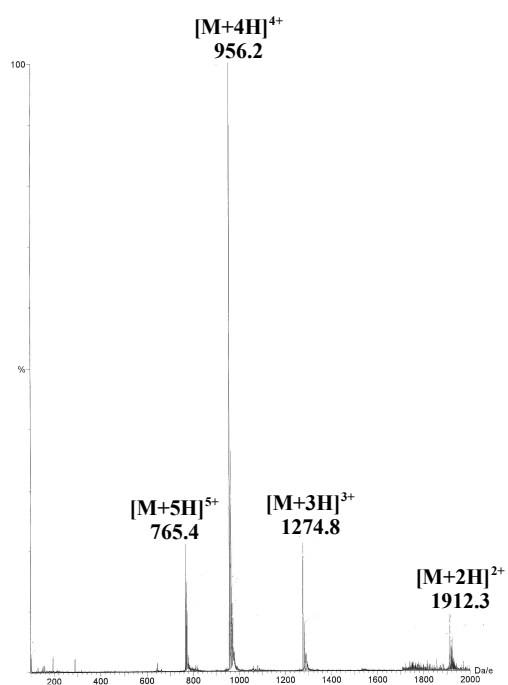
Electron Spray Ionization Mass Spectra (ESI-MS) were measured either on a VG Platform II (Micromass) or on an Esquire 3000 (Bruker). Analyses were performed in the positive mode using aqueous acetonitrile as eluent.

RAFT(c[-RGDfK-])₄: **1**.

RP-HPLC: Conditions A, 214 nm: **RT = 10.9 min**



ESI-MS: calcd 3822.2, **found 3821.7**

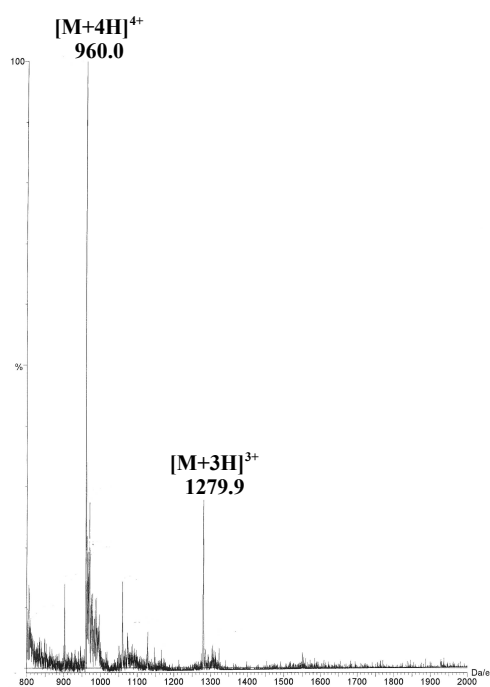


RAFT(c[-RGDfK-])₃,(c[-RβADfK-]) : **2**.

RP-HPLC: Conditions B, 214 nm: **RT = 14.6 min**

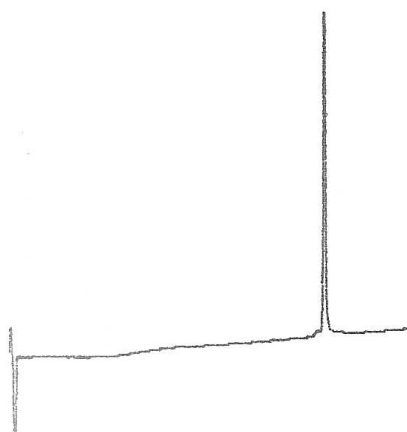


ESI-MS: calcd 3836.2, **found 3837.2**

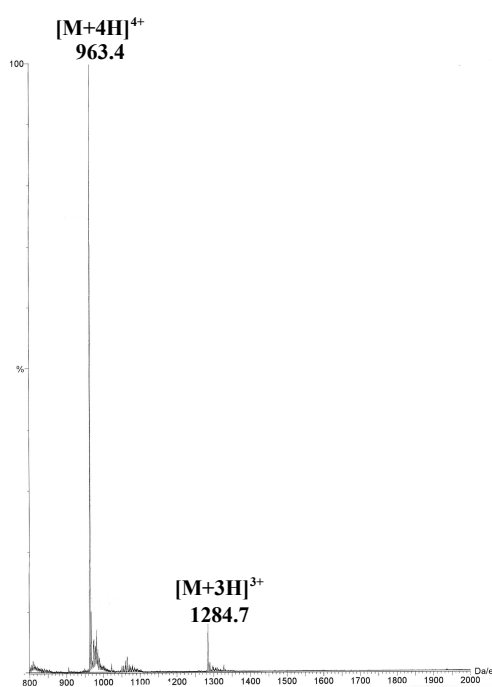


RAFT(c[-RGDfK-])₂,(c[-RβADfK-])₂ : **3**.

RP-HPLC: Conditions B, 214 nm: **RT = 14.2 min**

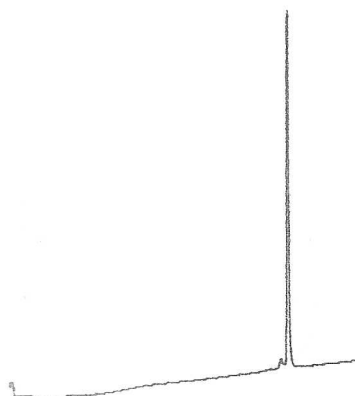


ESI-MS: calcd 3850.2, **found 3849.9**

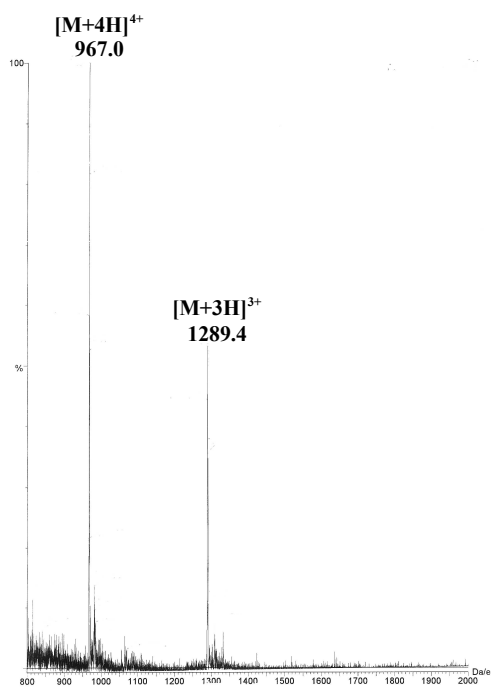


RAFT(c[-RGDfK-]),(c[-RβADfK-])₃: **4**.

RP-HPLC: Conditions B, 214 nm: **RT = 14.4 min**

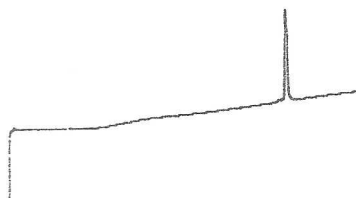


ESI-MS: calcd 3864.3, **found 3865.2**

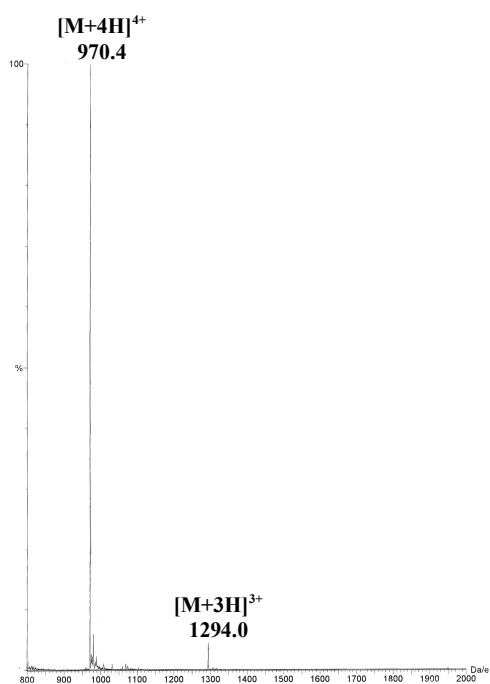


RAFT(c[-R β ADfK-])₄: **5**.

RP-HPLC : Conditions B, 214 nm: **RT = 14.4 min**

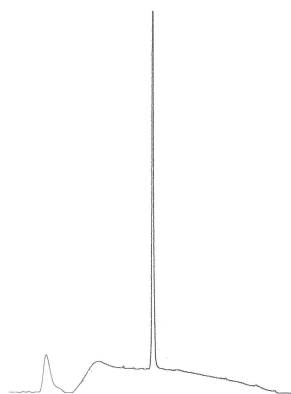


ESI-MS: calcd 3878.3, **found 3878.3**



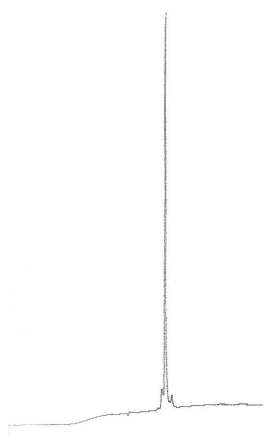
RAFT(c[-RGDfK-])₁₆: **6**.

RP-HPLC: Conditions C, 214 nm: **RT = 18.4 min**



RAFT(c[-RGDfK-])₄: **7**.

RP-HPLC: Conditions D, 214 nm: **RT = 11.1 min**



ESI-MS: calcd 3822.2, **found 3822.6**

