

Anti-Modified Peptide Antibodies (AMPAs) in Rheumatoid Arthritis: Study of the Diagnostic Value of Citrullinated, Homocitrullinated, and Acetylated Fibrin/Filaggrin Chimeric Peptides

Isabel Haro ^{1,*}, Raul Castellanos-Moreira ², Raimon Sanmartí ² and María José Gómara ^{1,*}

¹ Unit of Synthesis and Biomedical Applications of Peptides, IQAC-CSIC, Jordi Girona 18–26, 08034 Barcelona, Spain

² Department of Rheumatology, Hospital Clínic of Barcelona, 08036 Barcelona, Spain; castellanos@clinic.cat (R.C.-M.); sanmarti@clinic.cat (R.S.)

* Correspondence: isabel.haro@iqac.csic.es (I.H.); mariajose.gomara@iqac.csic.es (M.J.G.)

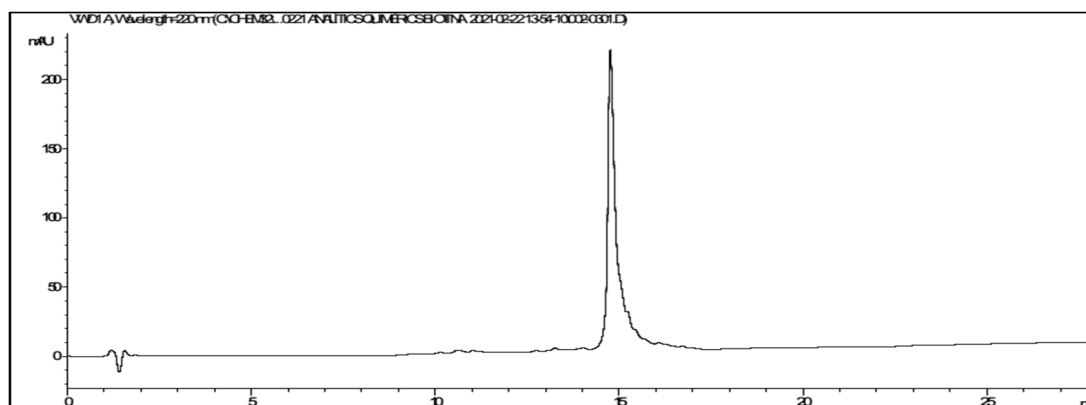
Supplementary Material:

Figure S1: Characterization of CFFCP by HPLC and ESI-MS

Figure S2: Characterization of CFFHP by HPLC and ESI-MS

Figure S3: Characterization of CFFAP by HPLC and ESI-MS

A)



B)

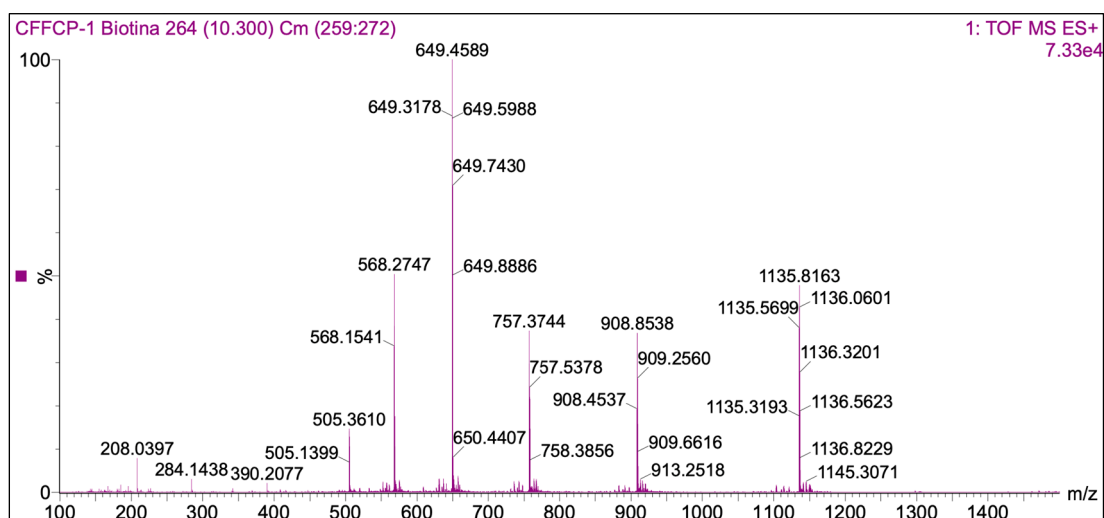
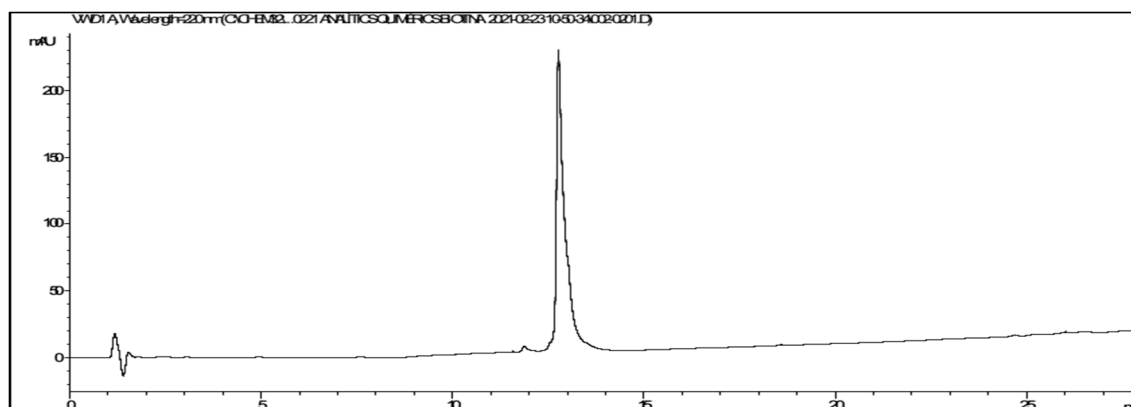


Figure S1. Characterization of CFFCP by HPLC and ESI-MS. (A) HPLC was performed on an Eclipse Plus C18 column (Agilent, 3.5 μ m, 4.6 \times 100 mm) with a linear gradient (5%-95%) of 0.05% TFA in ACN (solvent B) into 0.05% TFA in water (solvent A) over 30 min at 1 mL/min flow rate. (B) The mass spectrum was recorded in positive ion mode in the m/z 100-1500 range. LRMS: calculated m/z for $C_{181}H_{305}N_{75}O_{57}S_3$: 1136.01 [M+4H]⁴⁺, 909.01 [M+5H]⁵⁺, 757.68 [M+6H]⁶⁺, 649.58 [M+7H]⁷⁺, 568.51 [M+8H]⁸⁺, 505.45 [M+9H]⁹⁺; found by MS (ESI): 1135.82 [M+4H]⁴⁺, 908.85 [M+5H]⁵⁺, 757.37 [M+6H]⁶⁺, 649.46 [M+7H]⁷⁺, 568.27 [M+8H]⁸⁺, 505.36 [M+9H]⁹⁺.

A)



B)

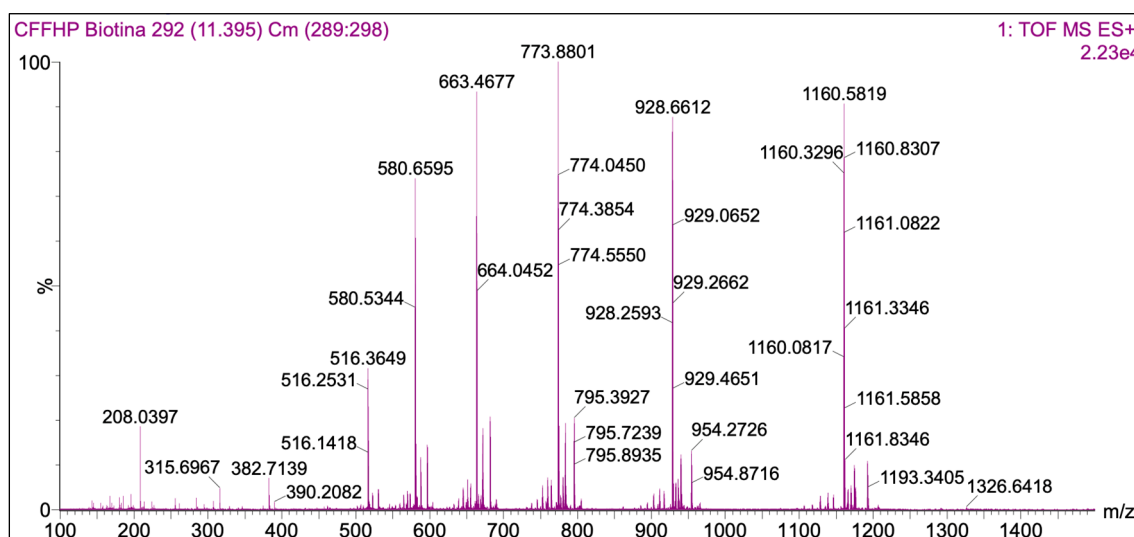
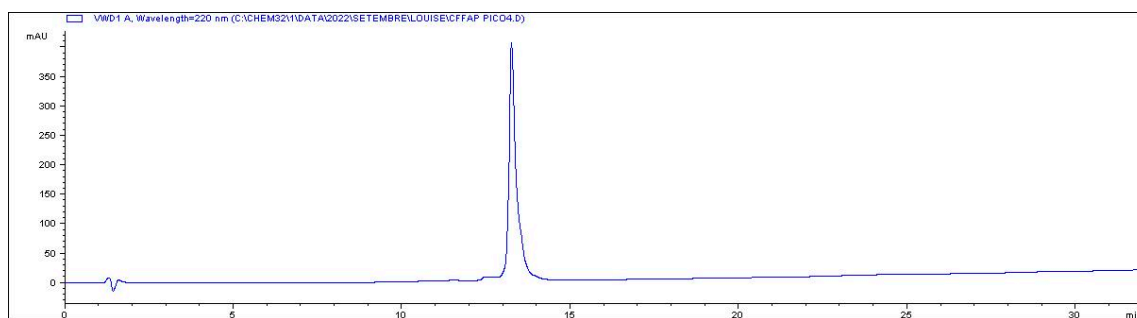


Figure S2. Characterization of CFFHP by HPLC and ESI-MS. (A) HPLC was performed on an Eclipse Plus C18 column (Agilent, 3.5 μ m, 4.6 \times 100 mm) with a linear gradient (5%-95%) of 0.05% TFA in ACN (solvent B) into 0.05% TFA in water (solvent A) over 30 min at 1 mL/min flow rate. (B) The mass spectrum was recorded in positive ion mode in the m/z 100-1500 range. LRMS: calculated m/z for $C_{184}H_{310}N_{78}O_{58}S_3$: 1160.79 [M+4H]⁴⁺, 928.83 [M+5H]⁵⁺, 774.19 [M+6H]⁶⁺, 663.74 [M+7H]⁷⁺, 580.90 [M+8H]⁸⁺, 516.46 [M+9H]⁹⁺; found by MS (ESI): 1160.58 [M+4H]⁴⁺, 928.66 [M+5H]⁵⁺, 773.88 [M+6H]⁶⁺, 663.46 [M+7H]⁷⁺, 580.66 [M+8H]⁸⁺, 516.36 [M+9H]⁹⁺.

A)



B)

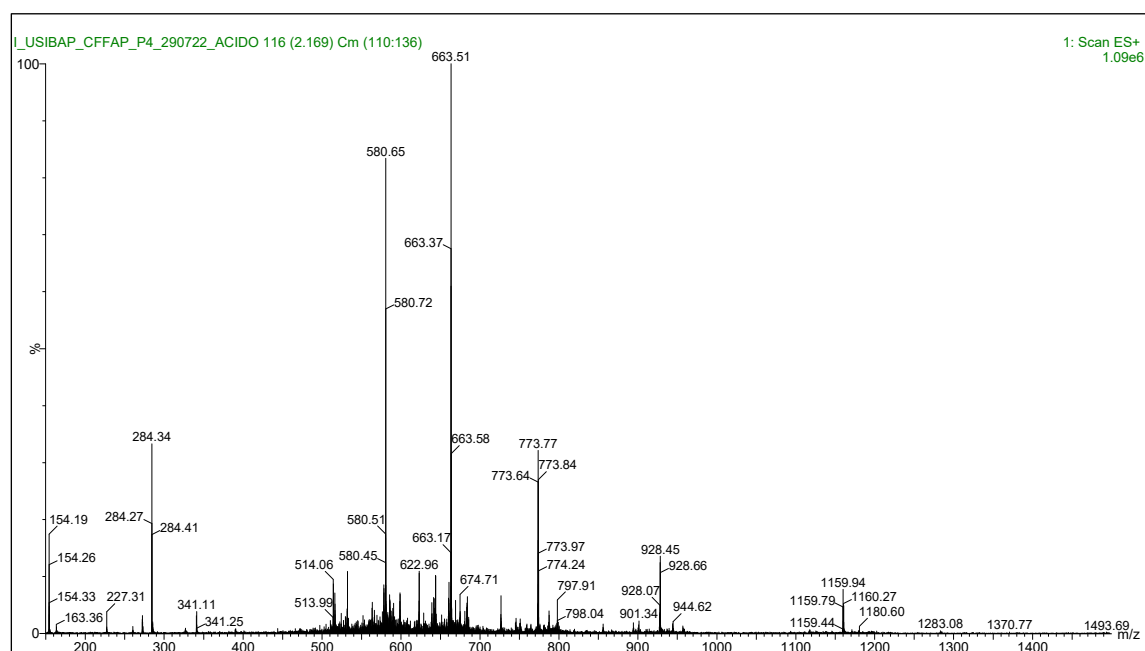


Figure S3. Characterization of CFFAP by HPLC and ESI-MS. (A) HPLC was performed on an Eclipse Plus C18 column (Agilent, 3.5 μ m, 4.6 \times 100 mm) with a linear gradient (5%-95%) of 0.05% TFA in ACN (solvent B) into 0.05% TFA in water (solvent A) over 30 min at 1 mL/min flow rate. (B) The mass spectrum was recorded in positive ion mode in the m/z 100-1500 range. LRMS: calculated m/z for $C_{187}H_{313}N_{75}O_{58}S_3$: 1160.04 [M+4H]⁴⁺, 928.34 [M+5H]⁵⁺, 773.70 [M+6H]⁶⁺, 663.31 [M+7H]⁷⁺, 580.53 [M+8H]⁸⁺; found by MS (ESI): 1159.94 [M+4H]⁴⁺, 928.45 [M+5H]⁵⁺, 773.77 [M+6H]⁶⁺, 663.51 [M+7H]⁷⁺, 580.65 [M+8H]⁸⁺.