

Supplementary material

From:

Pilot screening of potential matrikines resulting from collagen breakages through ionizing radiation

J. Montanari¹, L. Schwob², A. Marie-Brasset¹, C. Vinatier³, C. Lepleux¹, R. Antoine⁴, J. Guicheux³, J.C. Pouilly^{1*} and F. Chevalier^{1*}

¹ UMR6252 CIMAP, CEA - CNRS - ENSICAEN - Université de Caen Normandie, 14000 Caen, France

² Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany

³ Nantes Université, Oniris, CHU Nantes, INSERM, Regenerative Medicine and Skeleton, RMeS, UMR 1229, F-44000 Nantes, France.

⁴ Institut Lumière Matière, University of Lyon, Université Claude Bernard Lyon 1, CNRS, Lyon F-69622, France

* Corresponding authors:

Dr. Jean-Christophe Pouilly and Dr. François Chevalier

Emails: pouilly@ganil.fr ; chevalier@ganil.fr

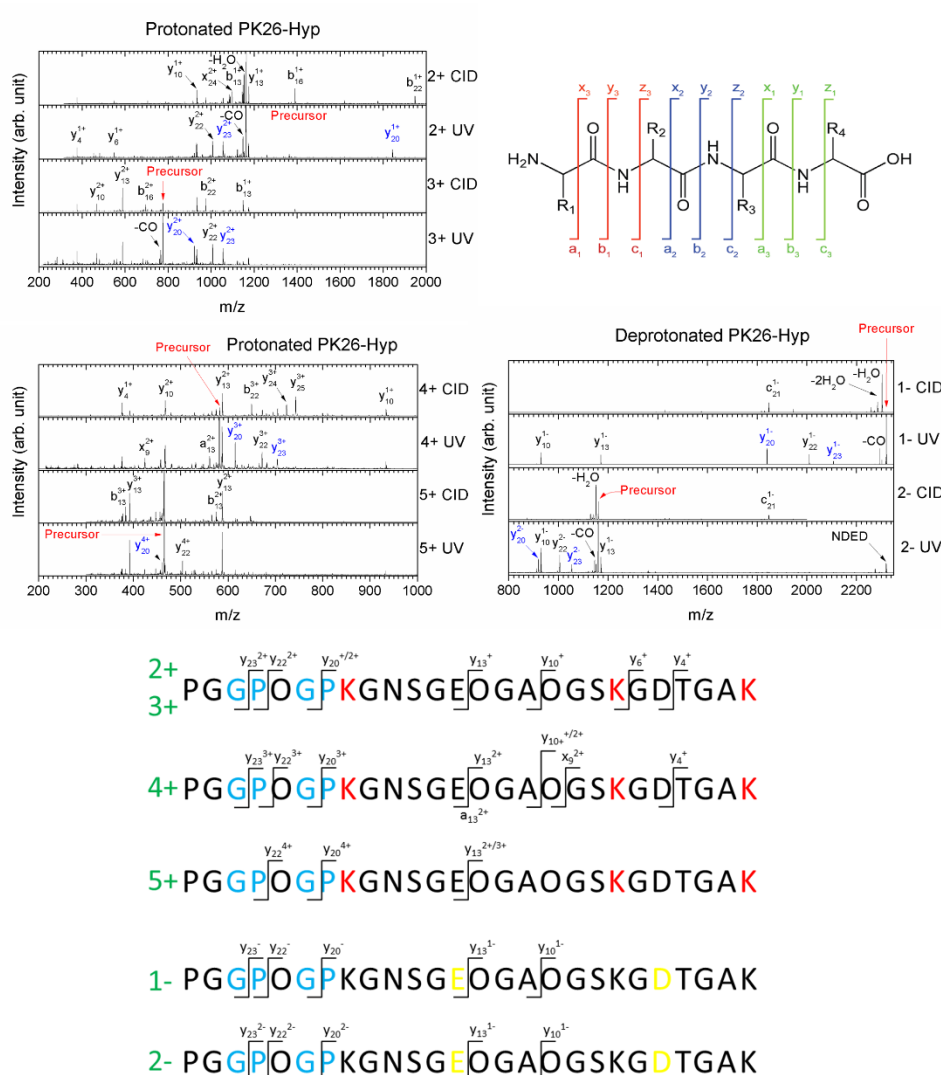
Table S1

List of selected peptide according to the Gly - Pro bond breakage within the collagen II sequence with size between 10 and 15 AA (P02458 - CO2A1_HUMAN ; UniProtKB reviewed, Swiss-Prot)

#	Peptide sequence	Formula	M.W.	Lenght
35	PAGAAAGARGNDGQPG	C ₅₁ H ₈₂ N ₂₀ O ₂₀	1295.32	PG-15
36	PSGAPGEDGRPG	C ₄₄ H ₆₉ N ₁₅ O ₁₈	1096.11	PG-12
37	PQGARGQPGVMGFPG	C ₆₃ H ₉₈ N ₂₀ O ₁₈ S ₁	1455.64	PG-15
38	PRGLPGTPGTDG	C ₄₇ H ₇₇ N ₁₅ O ₁₇	1124.20	PG-12
39	PPGRAGEPGLQG	C ₄₈ H ₇₈ N ₁₆ O ₁₆	1135.23	PG-12
40	PGIDMSAFAGLG	C ₅₀ H ₇₈ N ₁₂ O ₁₆ S ₁	1135.29	PG-12
41	PRGPPGPQGATG	C ₄₆ H ₇₄ N ₁₆ O ₁₅	1091.18	PG-12
42	PKGEPPAGPQGA PG	C ₅₇ H ₈₉ N ₁₇ O ₁₉	1316.42	PG-15
43	PMGPRGLPGERGRTG	C ₆₃ H ₁₀₈ N ₂₄ O ₁₉ S ₁	1537.75	PG-15
44	PPGPSGDQGASGPAG	C ₅₁ H ₇₈ N ₁₆ O ₂₁	1251.26	PG-15
45	PKGASGPAGPPGAQG	C ₅₃ H ₈₅ N ₁₇ O ₁₈	1248.35	PG-15
46	PPGPAGANGEKGEVG	C ₅₆ H ₈₉ N ₁₇ O ₂₁	1336.41	PG-15
47	PPGPVGPGLTG	C ₄₈ H ₇₆ N ₁₂ O ₁₄	1045.19	PG-12
48	PPGPRGRSGETG	C ₄₇ H ₇₈ N ₁₈ O ₁₇	1167.23	PG-12
49	PAGPPGNPPGPG	C ₄₅ H ₆₇ N ₁₃ O ₁₄	1014.09	PG-12
50	PRGDRGDKGEKGAPG	C ₆₀ H ₁₀₁ N ₂₃ O ₂₂	1496.58	PG-15
51	PAGPSGPRGPPG	C ₄₅ H ₇₁ N ₁₅ O ₁₄	1046.14	PG-12
52	PKGDRGDVGEKG	C ₄₉ H ₈₃ N ₁₇ O ₁₉	1214.29	PG-12
53	PSGDQGASGPAGPSG	C ₄₉ H ₇₆ N ₁₆ O ₂₂	1241.22	PG-15
54	PPGEKGEPPGDDG	C ₄₇ H ₇₁ N ₁₃ O ₂₁	1154.14	PG-12
55	PVGPSGKDGANGIPG	C ₅₆ H ₉₁ N ₁₇ O ₂₀	1322.42	PG-15
56	PEQEFVGDIG	C ₄₈ H ₇₁ N ₁₁ O ₁₈	1090.14	PG-10
57	DQGASGPAGPSG	C ₃₉ H ₆₁ N ₁₃ O ₁₈	999.98	DG-12
58	PSGAPGEDGRPPPG	C ₅₆ H ₈₆ N ₁₈ O ₂₁	1347.39	PG-15
59	PPGPSGDQGASG	C ₄₁ H ₆₃ N ₁₃ O ₁₈	1026.02	PG-12
60	PTGVTGPKGARGAQQ	C ₅₆ H ₉₆ N ₂₀ O ₁₉	1353.48	PG-15
61	PPGPPGPSGKDG	C ₄₆ H ₇₁ N ₁₃ O ₁₆	1062.13	PG-12
62	PAGPPGEKGEPPGDDG	C ₅₇ H ₈₆ N ₁₆ O ₂₄	1379.39	PG-15
63	PSGKDGPKGARGDSG	C ₅₅ H ₉₂ N ₂₀ O ₂₂	1385.44	PG-15
64	PIGPPGPRGRSGETG	C ₆₀ H ₉₉ N ₂₁ O ₂₀	1434.56	PG-15
65	PAGPPGNPPGPPPG	C ₅₇ H ₈₄ N ₁₆ O ₁₇	1265.37	PG-15
66	PRGRDGEPTPGNPG	C ₅₉ H ₉₄ N ₂₂ O ₂₂	1463.51	PG-15
67	PRGLPGERGRTG	C ₅₁ H ₈₉ N ₂₁ O ₁₆	1252.38	PG-12
68	PGFPGAPGAKGEAG	C ₅₄ H ₈₁ N ₁₅ O ₁₇	1212.31	PG-14
69	PEGAPGKDGGRGLTG	C ₅₆ H ₉₃ N ₁₉ O ₂₁	1368.45	PG-15
70	PAGANGEKGEVG	C ₄₄ H ₇₂ N ₁₄ O ₁₈	1085.13	PG-12
71	PPGATGFPGAAGR VG	C ₅₈ H ₉₀ N ₁₈ O ₁₇	1311.45	PG-15
72	PAGEPGREGSPGADG	C ₅₄ H ₈₄ N ₁₈ O ₂₃	1353.35	PG-15
73	PAGARGIQGPQG	C ₄₆ H ₇₇ N ₁₇ O ₁₅	1108.21	PG-12
74	PMGPMGPRGPPG	C ₄₉ H ₇₉ N ₁₅ O ₁₃ S ₂	1150.37	PG-12
75	PAGPPGPVGPAGG	C ₄₆ H ₇₁ N ₁₃ O ₁₄	1030.13	PG-13
76	PQGPSGAPGPQG	C ₄₄ H ₆₈ N ₁₄ O ₁₆	1049.09	PG-12
77	PPGSNGNPPGPPG	C ₄₄ H ₆₆ N ₁₄ O ₁₆	1047.08	PG-12
78	PPGSNGNPPGPPPG	C ₅₆ H ₈₃ N ₁₇ O ₁₉	1298.36	PG-15
79	SNGNPPGPPPG	C ₄₄ H ₆₆ N ₁₄ O ₁₆	1047.08	SG-12
80	PPGPIDMSAFAGLG	C ₆₂ H ₉₅ N ₁₅ O ₁₉ S ₁	1386.57	PG-15

Figure S1

Top: mass spectra of the ionic products of collision-induced dissociation (CID) and UV photoabsorption at 220 nm for the doubly- and triply-protonated PK26-Hyp peptide. The usual nomenclature for peptide backbone fragmentation is used and presented on the right for a tetrapeptide with side-chains noted R1 to R4: a, b and c (x, y and z) fragment ions have the charge located on the N-terminal (C-terminal) side after cleavage of the bond crossed by the corresponding line. Fragments from Gly–Pro peptide bond cleavage are depicted in blue and loss of neutral molecules is indicated by a minus sign. Bottom: main backbone fragment ions of the protonated PK26-Hyp peptide created after UV photoabsorption, as a function of peptide charge state. O stands for hydroxyproline, Gly–Pro sub-sequences are highlighted in blue, lysine residues in red, acidic residues in yellow.



Figures S2

Location of **group A peptides** within the collagen sequence P02458 - CO2A1_HUMAN

MIRLGAPQTLVLLTLLVA AVLRCQGQDVQEAGSCVQDGQRYNDKDVWKPEPCRICVCDTGTVL CDDIICEDVKDCLSPEIPFGE
CCPICPTDLATASGQPGPKGQKGEPGDIKDIVGPKGPPGPQGPAGEQQPRGDRGDKGEKGAPG **PRGRDGEPTGPNPG** PPG
PPGPPGPPGLGGNFAAQMAGGFDEKAGGAQLGVMQGMGPMGPRGPPGAPAGPQGFQGNPGEPGEPGVSGPMGP
RGPPGPPGKPGDDGEAGKPGKAGERGPPGPQARGFPGTPLPGVKGHRGYPGLDGAKGEAGAPGVKGESGSPGENGSPG
PMGPRGLPGERGRTGPAGAAGARGNDGQPG PAGPPGPVGPAGGPGFPGAPGAKGEAGPTGARGPEGAQGP RGEPTGPGS
PGPAGASGNPGTDGIPGAKGSAGAPGIAGAPGFPG **PRGPPGPQGATG** PLGPKGQTGEPIAGFKGEQGPKEGPGAPGQGA
PGPAGEEGKRGARGEPPGVGPIPPGERGAPGNRGFPQQDGLAGPKGAPGERGPSGLAGPKGANGDPGRPGEPGLPGARG
LTGRPGDAGPQGVKG **PSGAPGEDGRPG** PPG **PQGARGQPGVMGFPG** PKGANGEPGKAGEKGLPGAPGLRGLPGKDGETGA
AGPPGPAGPAGERGEQGAPGPSGFQGLPGPPGPPGEGGKPGDQGVPEAGAPGLVGPRGER **GFPGER** GSPGAQGLQGP **PR**
GLPGTPGTDGPKGASGPAGPPGAQG PPG LQGMPPERGAAGIAG **PKGDRGDVGEKG** PEGAPGKDGG RGLTGPIG **PPGPAGA**
NKEKGEVG PPGPAGSAGARGAPGERGETGPPGPAGFAGPPGADGQPGAKGEQGEAGQKGDAGAPGPQGPSGAPGPQGPT
GVTGPKGARGAQPPGATGFPGAAGRVGPPGSNGNPGPPGPPGPSGKDGPKGARGDSG **PPGRAGEPGLQG** PAGPPGEKG
EPGDDGPSGAEGPPGPQGLAGQRGIVGLPGQRGERGFPLGPSGEPGKQGAPGASGDRGPPGPVGPPLTG PAGEPGREG
SPGADGPPGRDGAAGVKGDRGETGAVGAPGAPGPPGSPGAPPTGKQDGRGEAGA QGPMGPSG **PAGARGIQGPQG** PRG
DKGEAGEPGERGLKGHRGFTGLQGLPG **PPGPSGDQGASGPAGPSGPRGPPG** PVGPSGKD GANGIPGPIG **PPGPRGRSGETG**
PAGPPGNPGPPGPPGPPGIDMSAFAGLG PREKGPDP LQYMRADQAAGGLRQHDAEVDATL KSLNNQIESIRSPEGSRKNP
ARTCRDLKLCHPEWKS G DYWIDPNQGCTLDAMKVFCNMETGETCVYPNPANVPKKNWSSKSKEKKHIWFGETINGGFHFS
YGDDNLAPNTANVQMTFLRLSTEGSQNITYHCKNSIAYLDEAAGNLKKALLIQGSNDVEIRAEGNSRFTYTALKDGCTKHTGK
WGKTVIEYRSQKTSRLPIIDIAPMDIGGPEQFVGVDIGPVCFL

46	PPGPAGANGEKGEVG
80	PPGPGIDMSAFAGLG
40	PGIDMSAFAGLG
39	PPGRAGEPGLQG
41	PRGPPGPQGATG
49	PAGPPGNPGPPG
38	PRGLPGTPGTDG
52	PKGDRGDVGEKG
48	PPGPRGRSGETG
51	PAGPSGPRGPPG
73	PAGARGIQGPQG
53	PSGDQGASGPAGPSG
66	PRGRDGEPTGPNPG
35	PAGAAGARGNDGQPG
36	PSGAPGEDGRPG
37	PQGARGQPGVMGFPG
65	PAGPPGNPGPPGPPG
43	PMGPRGLPGERGRTG
45	PKGASGPAGPPGAQG
59	PPGPSGDQGASG

Location of **group C peptides** within the collagen sequence P02458 - CO2A1_HUMAN

MIRLGAPQTLVLLTLLVAAVLRCQGQDVQEAGSCVQDQRYNDKDVWKPEPCRICVCDTGTVLCDIIICEDVKDCLSPEIPFGE
CCPICPTDLATASGQPGPKGQKGEPGDIKDIVGPKGPPGPQGPAGEQQPRGDRGDKGEKGAPGPRGRDGEPTGPNPGPPG
PPGPPGPPGLGGNFAAQMAAGGFDEKAGGAQLGVMQGPMPGMPGPRGPPGPAGAPGPQGFQGNPGEPGEPGVSGPMGP
RGPPGPPGKPGDDGEAGKPGKAGERGPPGPQGARGFPGTPGLPGVKGHRGYPGLDGAKGEAGAPGVKGESGSPGENGSPG
PMG**PRGLPGERGRTG**PAGAAGARGNDGQGPAGPPGPVGPAGG**PGFPGAPGAKGEAG**PTGARGPEGAQGPREGPTPGS
PGPAGASGNPGTDGIPGAKGSAGAPGIAGAPGFPGPRGPPGPQGATGPLGPKGQTGEPIAGFKGEQGPKEGPGPAGPQGA
PGPAGEEGKRGARGEPGGVGPIGPPGERGAPGNRGFPQDGLAGPKGAPGERGPSGLAGPKGANGDPGRPGEPGLPGARG
LTGRPGDAGPQKVGPSGAPGEDGRPGPPGPQGARGQPGVMGFPGPKGANGEPGKAGEKGLPGAPGLRGLPGKDGETGA
AGPPGPAGPAGERGEQGAPGPSGFQGLPGPPGPPGEGGKPGDQGVPEAGAPGLVGPRGER**GFPGER**GSPGAQGLQGPR
GLPGTPGTDGPKGASGPAGPPGAQGPGLQGMPPERGAAGIAGPKGDRGDVGEKG**PEGAPGKDGGGRGLTG**PIGPPGPAGA
NGEKGEVGPSPAGSAGARGAPGERGETGPPGPAGFAGPPGADGQPGAKGEQGEAGQKGDAGAPGPQGPSGAPGPQGPT
GVTGPKGARGAQPPGATGFPGAAGRVGPPGSNGNPGPPGPPGPSGKDGPKGARGDSGPPGRAGEPGLQGPAGPPGEKG
EPGDDGPSGAEGPPGPQGLAGQRGIVGLPGQRGERGFPLGPSGEPGKQGAPGASGDRGPPGPVGPPLTGPAGEPGREG
SPGADGPPGRDGAAGVKGDRGETGAVGAPGAPGPPGSPGAGPTGKQGDREAGAQQGPMGPSGPAGARGIQGPQGPRG
DKGEAGEPGERGLKGRGFTGLQGLPG**PPGPSGDQGASGPAG**PSGPRGPPGPVGPSGKDANGIPG**PIGPPGPRGRSGETG**
PAGPPGNPGPPGPPGPPGIDMSAFAGLGPREGPDPLQYMRADQAAGGLRQHDAEVDATLKSNNQIESIRSPEGSRKNP
ARTCRDLKLCHPEWKS GDYWIDPNQGCTLDAMKVFCNMETGETCVYPNPANVPKNWWSSKSKEKKHIWFGETINGGFHFS
YGDDNLAPNTANVQMTFLRLSTEGSQNITYHCKNSIAYLDEAAGNLKKALLIQGSNDVEIRAEGNSRFTYTALKDGCTKHTGK
WGKTVIEYRSQKTSRLPIIDIAPMDIGGPEQEFVGDIGPVCFL

67	PRGLPGERGRTG
69	PEGAPGKDGGGRGLTG
44	PPGPSGDQGASGPAG
64	PIGPPGPRGRSGETG
68	PGFPGAPGAKGEAG

Domains of Collagen alpha-1(II) chain (UNIPROT P02458 - CO2A1_HUMAN)

MIRLGAPQTLVLLTLLVAAVLRCQGQDVQEAGSCVQDGQRYNDKDVWKPEPCRICVCDTGTVLCDIIICEDVKDCLSPFGE
CCPICPTDLATASGQPGPKGQKGEPGDIKDIVGPKGPPGPQGPAGEQGPRGDRGDKGEKGAPGPRGRDGEPTGPNPGPPG
PPGPPGPPGLGNNFAAQMAGGFDEKAGGAQLGVMQGPMGPMGPRGPPGPAGAPGPQGFQGNPGEPGEPVSGPMGP
RGPPGPPGKPGDDGEAGKPGKAGERGPPGPQGARGFPPTPLGPKGVKHRGYPGLDGAKEAGAPGVKGESGSPGENGSPG
PMGPRGLPGERGRTGPAGAAGARGNDGQGPAGPPGPVGPAGGPGFPGAPGAKGEAGPTGARGPEGAQGPARGPTPGS
PGPAGASGNPGTDGIPGAKGSAGAPGIAGAPGFPGRGPPGPQGATGPLGPKGQTGEPGIAGFKGEQGPKEGPGAPGQGA
PGPAGEEGKRARGEPGGVGPVGPGERGAPGNRGFPQDGLAGPKGAPGERGPSGLAGPKGANGDPGRPGEPGLPGARG
LTGRPGDAGPQGVGSPGAPGEDGRPGPPGPQARGQPGVMGFPKPGANGEPGKAGEKGLPGAPGLRGLPGKDGETGA
AGPPGPAGPAGERGEQAPGPSGFQGLPGPPGPPGEGGKPGDQGVPEAGAPGLVGRGERGFPGERGSPGAQGLQGPR
GLPGTPGTDGPKGASGPAGPPGAQGPGLQGMPPERGAAGIAGPKGDRGDVGEKGPEGAPGKDGGRLTGPIGPPGPAGA
NGEKGEVGPMPGASAGARGAPERGETGPPGPAGFAGPPGADGQPGAKGEQGEAGQKGDAGAPGPQGPSGAPGPQGPT
GVTGPKGARGAQPPGATGFPGAAGRVPGPSNGNPGPPGPPGSGKDGPKGARGDSGPPGRAGEPGLQGAPPPGEKG
EPGDDGPSGAEGPPGPQGLAGQRGIVGLPGQRGERGFPGLGPSGEPGKQGAPGASGDRGPPGPVGPGLTGPAEPGREG
SPGADGPPGRDGAAGVKGDRGETGAVGAPGAPPPGSPGAPPTGKQGDREAGAQQPMGPPSGPAGARGIQGPQGPGRG
DKGEAGEPGERGLKHRGFTGLQGLPGPPGPSGDQASGPAGPSGPRGPPGPVGPSKDGANGIPGPIGPPGPRGRSGETG
PAGPPGNPGPPGPPGPPGPGIDMSAFAGLGPREGPDPLQYMRADQAAGGLRQHD AEVDATLKS LNNQIESIRSPEGSRKNP
ARTCRDLKLCHPEWKS GDY WIDPNQGCTLDAMKVFCNMETGETCVYPNPANVPKKNWWSSKSKEKKHIWFGETINGGFHFS
YGDDNLAPNTANVQMTFLRLSTEGSQNITYHCKNSIAYLDEAAGNLKALLIQGSNDVEIRAEGNSRFTYTALKDGCTKHTGK
WGKTVIEYRSQKTSRLPIIDIAPMDIGGPEQEFQVDPVCF

Fibrillar collagen NC1

Triple-helical region

GFPGER (GFOGER after proline hydroxylation) : Collagen-binding A-domains of Integrins alpha1 beta 1 and alpha 2 beta1