Supplementary Materials

Switching the N-Capping Region from all-L to all-D Amino Acids in a VEGF Mimetic Helical Peptide

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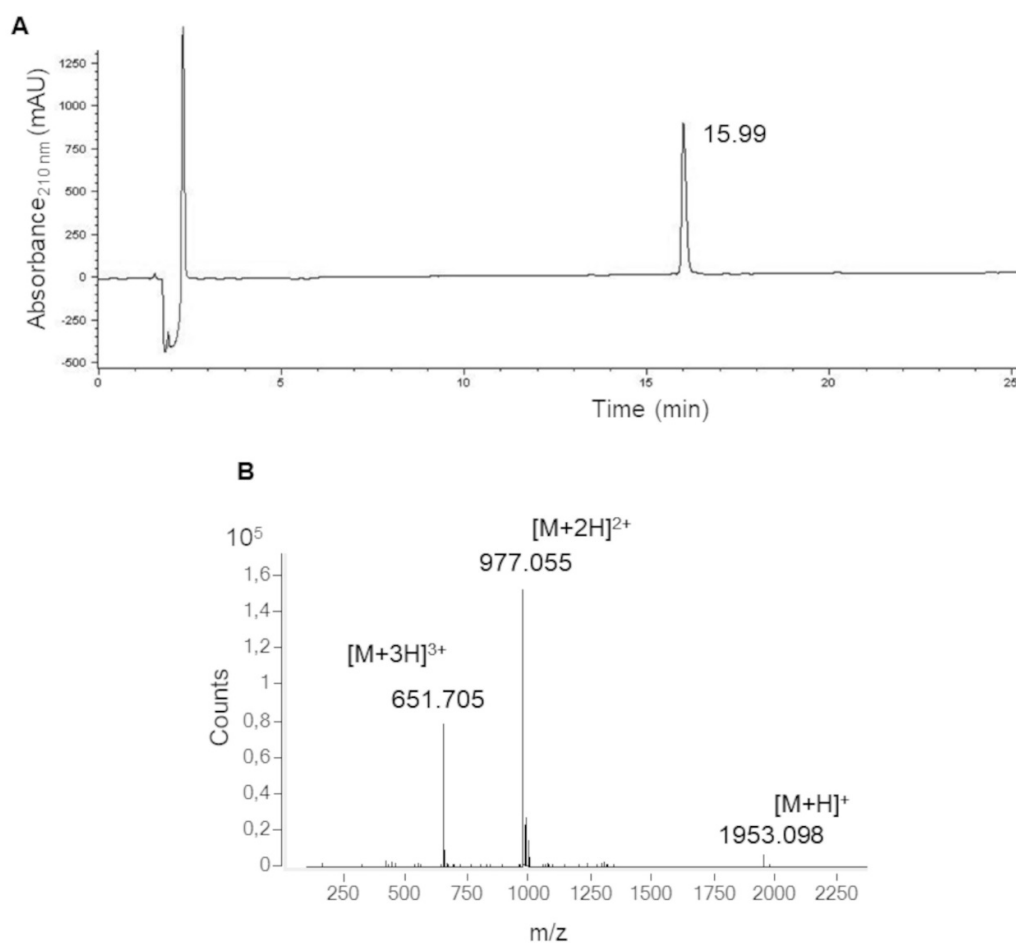
Figure S1. (**A**) RP-HPLC chromatographic profile revealed at 210 nm of pure D-QK. (**B**) ESI-mass spectrum of the species eluted at 15.99 min.

Table S1. Chemical shifts of D-QK protons in water and in water/TFE 70/30 v/v.

Residue	Proton	Chemical Shift, ppm (H_2O)	Chemical Shift, ppm (H_2O/TFE 70/30 v/v)
D-Lys1	HN	8.08	7.86
	Hα	4.31	4.49
	Hβ2-Hβ3	-	1.78
D-Leu2	HN	8.30	8.21
	Hα	4.13	4.24
	Hβ2-Hβ3	1.49	1.65
	Hγ	1.35	1.51
D-Thr3	HN	7.96	8.19
	Hα	4.47	4.36
	Hβ	4.58	4.48
	Hγ21-Hγ22-Hγ23	1.37	1.16
Trp4	HN	8.07	7.84
	Hα	4.60	4.46
	Hβ2-Hβ3	3.21	3.33
	Hδ1	7.21	7.29
	Hε1	10.1	9.98
	Hζ3	7.15	7.10
	Hζ2	7.46	7.44
	Hη2	7.25	7.14
Gln5	HN	8.23	8.56
	Hα	4.05	3.85
	Hβ2-Hβ3	2.00	1.89
	Hγ2-Hγ3	2.11	2.18
	Hε21	6.82	6.78
	Hε22	7.40	7.35
Glu6	HN	8.11	7.81
	Hα	4.21	4.09
	Hβ2-Hβ3	1.93/1.84	2.07/1.95
	Hγ2-Hγ3	2.27	2.36
Leu7	HN	8.09	7.72
	Hα	4.21	3.95
	Hβ2-Hβ3	1.67/1.38	1.82/1.70
	Hγ	1.51	1.52
	Hδ11- Hδ12- Hδ13	0.90	0.99
	Hδ21- Hδ22- Hδ23	0.80	0.89
Tyr8	HN	7.96	8.40
	Hα	4.39	4.17
	Hβ2-Hβ3	3.00/2.85	3.11/3.05
	Hδ1- Hδ2	7.08	7.15
	Hε1– Hε2	6.81	6.79
Gln9	HN	8.02	7.92
	Hα	4.17	4.09
	Hβ2-Hβ3	1.99/1.92	2.24/2.19
	Hγ2-Hγ3	2.24	2.56/2.47
	Hε21	6.70	6.74
	Hε22	7.33	7.30
Leu10	HN	8.98	7.69
	Hα	4.16	4.15
	Hβ2-Hβ3	1.58/1.48	1.88/1.80
	Hγ	1.20	1.61
	Hδ11- Hδ12- Hδ13	0.85	0.89

	Hδ21- Hδ22- Hδ23	0.77	-
Lys11	HN	7.99	8.14
	Hα	4.19	4.17
	Hβ2-Hβ3	1.10	1.18/1.15
	Hγ2-Hγ3	1.53	1.58
Tyr12	HN	8.06	8.04
	Hα	4.48	4.43
	Hβ2-Hβ3	2.97/2.83	3.08/2.76
	Hδ1- Hδ2	7.06	7.08
	Hε1– Hε2	6.77	6.80
Lys13	HN	8.23	7.90
	Hα	4.28	4.23
	Hβ2-Hβ3	1.87	1.96
	Hγ2-Hγ3	1.78	1.71
Gly14	HN	7.84	7.99
	Hα	3.94	3.96
Ile15	HN	7.91	8.07
	Hα	4.11	4.06
	Hβ	1.76	1.70
	Hγ	0.95	1.00
	Hγ12– Hγ13	1.45	1.22

The proton chemical shifts of D-QK are relative to water protons (4.75 ppm).

Table S2. Coupling constants of D-QK protons in water and in water/TFE 70/30 v/v.

Residue	Coupling Constants, Hz (H_2O)	Coupling Constants, Hz (H_2O /TFE 70/30 v/v)
Lys1	-	-
Leu2	-	7.5
Thr3	7.0	6.5
Trp4	6.8	6.5
Gln5	6.1	6.0
Glu6	6.0	6.1
Leu7	-	6.2
Tyr8	7.0	6.0
Gln9	6.5	6.2
Leu10	6.5	6.0
Lys11	-	-
Tyr12	7.0	6.5
Lys13	7.0	7.0
Gly14	-	-
Ile15	8.0	7.8

Table S3. NMR structural statistics of the D-QK peptide in H_2O.

PARAMETER	VALUE
NOE upper distance limit	90
Intra-residue	57
Short distance	23
Medium/long distance	10
Number of dihedral angle constraints	41
Residual target function, Å	0.43 ± 0.05

Residual NOE violations	
Number >0.1	±1
Maximum, Å	0.18 ± 0.03

Residual angle violations	
Number >2.0	0 ± 0
Maximum, Å	0

R.M.S.D.[a] to the mean coordinates, Å	
N–Cα–C′ (5–12)	0.37 ± 0.05
All heavy atoms (5–12)	1.17 ± 0.11

Ramachandran plot residues[b] (%)	
In most favored regions	60.0
In additional allowed regions	33.9
In generously allowed regions	6.1
In disallowed regions	0.0

a Calculated by MOLMOL. b Calculated by CYANA 2.1.

Table S4. NMR structural statistics of the D-QK peptide in H_2O/TFE 70/30.

PARAMETER	VALUE
NOE upper distance limit	135
Intra-residue	71
Short distance	30
Medium/long distance	34
Number of dihedral angle constraints	61
Residual target function, Å	0.38 ± 0.05
Residual NOE violations	
Number >0.1	±1
Maximum, Å	0.15 ± 0.02
Residual angle violations	
Number >2.0	0 ± 0
Maximum, Å	0
R.M.S.D.[a] to the mean coordinates, Å	
N–Cα–C′ (5–12)	0.13 ± 0.05
All heavy atoms (5–12)	0.99 ± 0.06
Ramachandran plot residues[b] (%)	
In most favored regions	88.3

In additional allowed regions	11.7
In generously allowed regions	0.0
In disallowed regions	0.0

a Calculated by MOLMOL. b Calculated by CYANA 2.1.