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Supporting information

**THEORETICAL STUDIES ON THE BIOACTIVE CONFORMATION OF
NERVE GROWTH FACTOR USING VBMC - A NOVEL VARIABLE BASIS MONTE CARLO
SIMULATED ANNEALING ALGORITHM FOR PEPTIDES**

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Table 1S. Equilibrium variable torsional angles (in degrees) of the amino and carboxyl termini of the most stable conformations of the NGF dimers and analogues.^a

		Active structures						Inactive structures					
No.		hNGF		mNGF		mNGFA3-9		hNGF-H4D		mNGFA1-8		BDNF	
<i>Amino terminus</i>													
11	ψ	E	82.9	E	85.9	E	89.2	E	80.9	E	63.7	E	68.2
	ϕ		55.7		56.3		57.8		57.2		47.9		56.3
	χ_1		-69.8		-72.0		-72.1		-75.0		-66.2		-76.9
	χ_2		72.7		71.7		66.0		72.6		71.2		70.1
	χ_3		-120.4		-111.7		-107.0		-104.8		-102.8		-97.7
10	ψ	G	-89.1	G	-95.1	G	-88.0	G	-129.5	G	-81.6	G	-134.1
	ϕ		-172.5		-178.6		-177.5		104.7		-80.8		155.0
9	ψ	R	-36.1	M	-21.1	S	146.5	R	-46.5	M	-66.6	R	71.4
	ϕ		-92.8		-91.4		-103.6		-80.9		157.5		-128.5
	χ_1		-77.2		-75.2		-66.7		-115.0		-142.4		-73.5
	χ_2		-173.9		-179.7		64.0		69.5		-69.7		-179.8
	χ_3		-175.5		179.9		-		-141.9		178.3		-71.4
	χ_4		134.3		-		-		98.1		-		-109.8
	ϕ		-116.5		-110.4		52.8		-53.7		-		-100.1
8	ψ	H	118.6	H	110.4	S	106.1	H	151.6		-	R	105.2
	ϕ		-116.5		-110.4		52.8		-53.7		-		-100.1

Table 1S, Cont'd 1.

	$\chi 1$	-89.7	-90.9	-45.9	-62.0	-	179.6
	$\chi 2$	-73.8	-71.5	-172.3	-72.5	-	-105.5
	$\chi 3$	-	-	-	-	-	162.1
	$\chi 4$	-	-	-	-	-	133.7
7	ψ F	135.7	F 129.4	-	F 142.3	-	A 161.6
	ϕ	-68.8	-89.0	-	-114.8	-	-166.6
	$\chi 1$	-171.6	-163.9	-	-170.7	-	-
	$\chi 2$	-96.3	-91.5	-	-100.2	-	-
6	ψ I	40.3	V 61.7	-	I 40.0	-	P 114.4
	ϕ	40.4	47.7	-	39.9	-	-
	$\chi 1$	-159.7	-177.3	-	-159.7	-	-
	$\chi 2$	87.1	-	-	88.6	-	-
5	ψ P	156.0	P 149.8	-	P 105.5	-	D 82.8
	ϕ	-	-	-	-	-	56.5
	$\chi 1$	-	-	-	-	-	-176.9
	$\chi 2$	-	-	-	-	-	-112.8
4	ψ H	121.4	H 122.1	-	D 117.9	-	S 136.2
	ϕ	-129.2	-129.8	-	-102.8	-	-53.4
	$\chi 1$	-162.5	-163.3	-	-66.4	-	-172.9
	$\chi 2$	-69.1	-69.2	-	-97.5	-	-178.3
3	ψ S	2.1	T -1.9	-	S -25.0	-	H 153.8
	ϕ	-91.9	-84.5	-	-68.2	-	48.2
	$\chi 1$	-171.8	-174.9	-	39.3	-	82.1
	$\chi 2$	-53.2	-51.2	-	-120.5	-	69.8
2	ψ S	138.5	S 139.4	-	S 38.5	-	-
	ϕ	-128.9	-114.1	-	50.8	-	-

Table 1S, Cont'd 2.

	$\chi 1$	173.3		169.7	-	-173.2	-	-
	$\chi 2$	-141.9		-139.8	-	-120.6	-	-
1	ψ S	133.0	S	127.9	-	S 131.9	-	-
	ϕ	48.6		49.4	-	-133.8	-	-
	$\chi 1$	-43.2		-44.1	-	-43.5	-	-
	$\chi 2$	-171.5		-172.4	-	-173.6	-	-

Carboxyl terminus

112'	ϕ L	-113.3	L	-113.0	L	-112.4	L	-112.0	L	-111.5	L	-110.6
	ψ	98.8		98.7		99.2		97.7		89.9		100.1
	$\chi 1$	-72.3		-71.6		-71.6		-71.7		-71.8		-72.1
	$\chi 2$	163.7		163.0		162.6		162.2		161.9		161.1
113'	ϕ S	-83.4	S	-77.2	S	-77.4	S	-76.8	S	-91.9	T	-89.5
	ψ	136.1		146.0		143.5		141.7		149.4		134.0
	$\chi 1$	177.0		179.4		176.3		175.6		169.6		57.4
	$\chi 2$	65.2		60.6		59.0		57.5		73.2		-179.7
114'	ϕ R	-66.7	R	-71.5	R	-78.0	R	-75.1	R	-117.0	I	-57.9
	ψ	-47.0		-53.7		-59.3		-57.1		-31.9		-32.2
	$\chi 1$	-99.1		-145.6		-93.4		177.5		-168.1		-162.1
	$\chi 2$	-173.1		-179.8		-171.5		-159.7		86.5		87.9
	$\chi 3$	170.4		-173.6		-172.9		58.1		-73.8		-
	$\chi 4$	138.4		140.3		141.5		124.7		173.4		-
115'	ϕ K	-163.2	K	-162.1	K	-167.1	K	-163.0	K	-133.4	K	-167.7
	ψ	110.6		132.0		153.3		157.6		141.7		126.1
	$\chi 1$	-139.8		-143.3		-140.1		-137.8		-164.0		-142.2
	$\chi 2$	78.7		81.7		85.0		79.3		172.4		83.5

Table 1S, Cont'd 3.

χ_3	-96.4	-97.9	-95.8	-97.4	133.9	-100.4
χ_4	129.5	120.9	131.0	133.6	-73.6	109.2
χ_5	-39.1	-35.6	-47.7	-44.1	9.6	-9.5
116' ϕ A	-60.5	A -69.6	A -58.2	A -63.9	A -51.6	R -61.4
ψ	-47.5	-40.7	-47.5	-42.4	-45.3	-39.3
χ_1	-	-	-	-	-	-80.9
χ_2	-	-	-	-	-	-173.4
χ_3	-	-	-	-	-	174.3
χ_4	-	-	-	-	-	129.6
117' ϕ V	-71.8	T -85.5	T -64.6	V -41.0	T -114.6	G -73.3
ψ	112.0	116.4	108.2	130.2	168.4	77.3
χ_1	-74.3	53.4	50.9	-66.2	57.2	-
χ_2	-	60.5	58.0	-	-170.5	-
118' ϕ R	-93.8	R -118.2	R -58.5	R -125.2	R -51.5	R -49.0
ψ	-57.9	-48.4	-37.6	141.3	-56.3	-40.3
χ_1	-104.3	-80.9	-109.5	-126.2	-153.8	-125.9
χ_2	79.1	109.1	73.3	106.7	88.0	98.0
χ_3	147.7	116.1	-76.3	-78.8	-74.9	-76.6
χ_4	147.0	116.1	-87.2	-98.5	-125.9	-111.5

^aTorsional angles are designated according to the IUPAC rules (IUPAC-IUB Commission on Biochemical Nomenclature. *Biochemistry* 1970, 9, 3471-3479).