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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		mNGFΔ3-9		hNGF-H4D		mNGFΔ1-8		BDNF	
Amino terminus													
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
	χ1		-69.8		-72.0		-72.1		-75.0		-66.2		-76.9
	χ2		72.7		71.7		66.0		72.6		71.2		70.1
	χ3		-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
	χ1		-77.2		-75.2		-66.7		-115.0		-142.4		-73.5
	χ2		-173.9		-179.7		64.0		69.5		-69.7		-179.8
	χ3		-175.5		179.9		-		-141.9		178.3		-71.4
	χ4		134.3		-		-		98.1		-		-109.8
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.

	$\chi 3$		-96.4		-97.9		-95.8		-97.4		133.9	-100.4
	$\chi 4$		129.5		120.9		131.0		133.6		-73.6	109.2
	$\chi 5$		-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
	$\chi 1$		-		-		-		-		-	-80.9
	$\chi 2$		-		-		-		-		-	-173.4
	$\chi 3$		-		-		-		-		-	174.3
	$\chi 4$		-		-		-		-		-	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
	$\chi 1$		-74.3		53.4		50.9		-66.2		57.2	-
	$\chi 2$		-		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
	$\chi 1$		-104.3		-80.9		-109.5		-126.2		-153.8	-125.9
	$\chi 2$		79.1		109.1		73.3		106.7		88.0	98.0
	$\chi 3$		147.7		116.1		-76.3		-78.8		-74.9	-76.6
	$\chi 4$		147.0		116.1		-87.2		-98.5		-125.9	-111.5

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