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family representative structures of [Glu<sup>5</sup>,L/D-Ala<sup>6,7</sup>,Lys<sup>8</sup>]Ac-Ala<sub>13</sub>-NH<sub>2</sub> with energies ≤ 10.0 Kcal/mol above the lowest observed energy structure.

$\phi^3$	$\psi^3$	$\phi^4$	$\psi^4$	$\phi^5$	$\psi^5$	$\phi^6$	$\psi^6$	$\phi^7$	$\psi^7$	$\phi^8$	$\psi^8$	$\phi^9$	$\psi^9$	$\phi^{10}$	$\psi^{10}$	$\phi^{11}$	$\psi^{11}$	$\phi^{12}$	$\psi^{12}$
Model "LL" [Glu <sup>5</sup> ,Lys <sup>8</sup> ]Ac-Ala <sub>13</sub> -NH <sub>2</sub>																			
-64.6	-45.4	-60.5	-41.9	-71.0	-37.1	-56.3	-41.2	-62.0	-45.4	-63.2	-42.9	-62.3	-44.6	-61.9	-43.0	-62.3	-40.6	-68.0	-39.8
-75.6	-49.1	-68.7	-52.9	-92.8	95.3	-40.7	102.0	66.9	34.2	-79.6	79.3	-61.0	-40.2	-60.2	-37.3	-67.8	-34.5	-68.7	-40.9
-83.4	-41.6	-76.3	-36.4	-84.9	72.2	-80.7	144.5	-80.3	-39.5	-55.9	-45.9	-76.7	-47.7	-59.6	-40.1	-65.3	-38.9	-67.5	-39.7
-67.6	-42.5	-71.6	-3.7	-60.7	-22.5	-54.4	-43.2	-88.0	83.5	-56.2	-40.9	-61.7	-38.0	-65.7	-41.4	-59.3	-43.6	-67.1	-39.8
-78.6	150.8	-138.0	-7.0	-101.3	151.6	-89.0	-45.6	-78.7	90.3	-52.9	-43.8	-65.9	-47.2	-71.2	-46.4	-67.0	-34.6	-67.6	-39.6
-75.7	138.2	-160.1	138.7	-86.3	124.5	-86.5	-31.6	-80.3	102.1	-76.6	85.8	-85.9	-35.5	-69.0	-37.8	-135.6	102.3	-94.2	134.7
-73.6	-52.9	-108.7	91.6	-142.1	-40.7	-79.8	108.4	-134.0	139.8	-59.9	-21.7	-55.9	-40.6	-70.1	-21.9	-73.4	-45.6	-66.6	-54.2
-64.9	-46.4	-60.8	-43.0	-69.9	-29.5	-68.5	-41.8	-73.9	-20.5	-65.6	132.5	-55.1	-35.5	-62.7	-40.9	-74.0	-43.9	-64.7	-41.7
125.8	78.1	-139.3	-58.7	-90.5	76.8	-77.1	-48.5	-63.9	-54.0	-69.0	-29.1	-64.6	-46.6	-61.4	-43.9	-62.6	-39.3	-69.3	-38.9
Model "LD" [Glu <sup>5</sup> ,DAla <sup>7</sup> ,Lys <sup>8</sup> ]Ac-Ala <sub>13</sub> -NH <sub>2</sub>																			
-80.9	-49.8	-65.3	-52.1	-91.2	101.7	-63.2	112.7	84.9	17.7	-84.4	79.1	-63.4	-41.8	-61.3	-38.4	-68.7	-34.6	-70.0	-40.5
-71.1	-44.3	-66.5	-48.4	-135.6	104.3	-75.2	96.3	127.7	-76.9	-62.0	-64.7	-71.1	-27.9	-54.5	-50.0	-72.2	-42.6	-73.1	-43.8
106.6	-49.1	-97.4	-27.3	-86.9	119.3	-57.3	140.3	93.8	-73.6	-61.8	-44.0	-64.9	-37.7	-68.5	-31.9	-67.8	-41.7	-69.4	-57.7
-84.9	-54.2	-71.7	-49.3	-90.7	81.9	-74.6	123.6	144.3	-73.1	-74.7	129.0	-56.8	-56.0	-65.7	-29.9	-69.5	-43.1	-67.8	-41.2
158.6	-57.5	-64.6	-54.4	-92.3	67.8	-156.1	98.9	125.3	-73.1	-92.6	105.6	-72.6	-68.7	-75.7	-10.6	-76.5	-43.2	-69.1	-54.4
-81.2	162.5	-121.2	-10.9	-120.8	86.0	-151.6	94.8	132.9	-70.6	-74.0	-53.8	-67.9	-23.6	-60.6	-61.5	-86.3	-26.9	-71.3	-39.2
-72.9	-45.3	-70.3	-54.5	-88.7	78.9	-94.7	89.8	113.9	-92.1	-85.9	115.0	-67.4	-48.7	-66.2	-19.9	-75.3	-46.3	-66.1	-53.5
-66.4	146.7	-70.4	-42.0	-88.6	69.5	-88.6	74.7	72.1	46.0	-82.8	85.0	-45.9	-39.7	-70.1	-44.9	-77.4	-52.3	-109.6	91.8
-73.9	155.5	-116.3	-37.8	-134.3	100.7	-79.7	96.5	143.6	54.2	-132.1	55.0	43.3	-101.7	-77.3	-38.9	-66.8	-48.6	-123.3	87.8
-84.9	-53.6	-66.4	-50.5	-85.3	88.9	-63.9	118.9	86.2	-77.6	65.7	-80.8	-65.8	-52.8	-69.4	-27.6	-65.9	-43.4	-73.1	-48.8

Model "DL" [Glu <sup>5</sup> ,DAIa <sup>6</sup> ,Lys <sup>8</sup> ]Ac-Ala <sub>13</sub> -NH <sub>2</sub>																			
19.2	19.7	-76.7	-34.3	-133.0	64.6	83.2	-138.5	-56.9	-45.0	-63.8	-39.3	-61.7	-47.2	-61.3	-40.5	-65.2	-40.3	-73.5	-50.0
27.1	53.0	-91.0	-49.4	-145.7	146.1	90.6	-83.5	-84.8	77.5	-83.9	108.1	-60.8	-40.5	-61.3	-38.8	-70.4	-40.7	-65.7	-40.9
68.1	-41.5	-65.3	-50.6	-137.4	133.4	131.7	-70.9	-72.5	-57.0	-109.2	75.2	-62.5	-44.6	-74.3	-26.5	-76.1	-44.6	-66.2	-52.6
71.0	-54.5	-96.2	64.3	-60.7	152.0	95.0	-66.3	-63.9	-54.5	60.0	-88.2	-65.1	-43.6	-63.8	-30.4	-67.4	-30.6	-72.7	-54.5
31.9	70.0	-108.0	-48.7	-81.6	-40.2	93.3	-65.4	-55.9	-52.5	-67.5	-30.9	-65.9	-46.4	-61.0	-44.1	-62.2	-39.4	-68.6	-38.4
68.6	-41.8	-64.6	-38.7	-64.3	-48.9	86.9	-77.1	-80.0	76.0	-72.0	-32.4	-60.9	-43.9	-70.2	-33.9	-66.9	-42.5	-72.4	-54.8
64.8	-42.7	-62.4	-35.3	-71.2	-53.3	72.2	-127.2	-145.7	80.5	-134.1	113.9	-65.9	-41.7	-63.5	-35.6	-67.0	-41.7	-65.9	-41.1
26.7	78.8	-134.3	-54.7	68.9	-75.7	144.2	-91.2	-93.2	125.0	-136.6	52.4	-75.9	-43.1	-65.1	-45.5	-65.9	-35.3	-66.6	-40.6
19.9	21.1	-75.4	-39.5	-118.9	81.4	85.0	-119.9	-82.4	88.2	-66.4	-38.9	-61.8	-39.9	-67.0	-45.8	-61.4	-39.9	-69.2	-37.8
-61.6	-25.8	-87.6	-36.2	-83.9	74.1	81.0	-113.5	-67.6	-46.0	-79.7	5.7	-58.0	-53.6	-62.6	-38.4	-65.8	-45.4	-71.5	-26.3
-65.5	149.1	-96.6	-48.6	-70.2	0.6	102.3	-71.7	-84.2	69.7	-140.3	98.6	-56.5	-31.0	-68.3	-39.2	-80.0	-49.7	-110.0	91.2
Model "DD" [Glu <sup>5</sup> ,DAIa <sup>6,7</sup> ,Lys <sup>8</sup> ]Ac-Ala <sub>13</sub> -NH <sub>2</sub>																			
-86.6	-49.9	-76.8	-39.6	-83.0	-47.6	133.5	68.1	119.9	-77.6	-75.3	-18.9	-54.4	-26.9	-72.7	-53.1	-70.8	-47.5	-114.3	89.2
106.0	96.6	-152.4	98.6	-83.3	68.4	60.4	31.5	69.3	24.4	-93.0	62.8	-72.3	-34.9	-70.0	-47.3	-74.2	-45.0	-112.9	88.6
-60.8	-43.4	-58.7	-44.1	-83.4	40.0	72.0	42.1	83.4	-87.0	53.2	-99.6	-70.4	-28.8	-74.7	-33.1	-68.9	-54.9	-113.2	92.8
-68.4	-43.5	-65.1	-48.1	-131.5	123.1	153.2	-68.8	111.4	-126.0	71.1	-75.3	-68.9	-17.3	-67.1	-45.2	-71.4	-47.0	-115.2	86.5
-72.1	143.0	-158.4	103.4	-81.0	98.8	-51.6	97.9	137.5	-60.7	-79.5	103.3	-55.1	-43.3	-64.8	-40.3	-66.7	-42.2	-54.5	-42.5
-70.3	-47.3	-67.2	-40.1	-78.1	-37.1	110.8	68.9	124.4	-83.2	-83.3	122.1	-58.9	-44.0	-62.7	-39.1	-68.8	-41.0	-67.0	-40.5
-72.1	-47.8	-58.1	-42.4	-137.6	135.4	115.4	-79.7	-44.5	-52.6	-49.7	-50.5	-64.5	-43.6	-63.0	-42.8	-62.7	-40.7	-69.0	-40.1
106.5	96.2	-154.0	121.2	-77.8	94.1	123.4	75.1	127.4	-84.3	-58.4	-61.0	-62.9	-19.7	-75.1	-45.9	-65.5	-50.8	-116.0	90.5
108.8	116.3	-80.3	-33.6	54.6	47.3	76.4	-110.7	126.5	-75.0	-102.2	-69.5	-69.9	-44.0	-65.7	-23.3	-74.3	-47.7	-65.6	-52.6
-63.9	-37.9	-67.4	-56.1	-141.5	145.3	150.6	-80.7	95.4	-120.4	66.0	88.5	-58.4	-40.1	-63.1	-39.2	-72.3	-44.2	-67.3	-41.0
-74.8	-41.3	-66.8	-47.6	69.6	-68.3	68.6	62.4	84.9	-83.4	-146.2	-65.8	-81.1	-16.3	-63.5	-59.0	-84.1	-21.3	-70.6	-47.0