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## Development of novel small-size peptides as putative therapeutic drugs

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# APPENDIX A

## SUPPLEMENTARY MATERIAL

### CHAPTER 2

Supplementary materials associated with this chapter can be found, in the online version, at doi:10.1016/j.bmc.2006.07.007.

### CHAPTER 3

Supplementary materials associated with this chapter can be found, in the online version, at doi:10.1016/j.bmc.2008.02.072.

### CHAPTER 4

Supplementary materials associated with this article can be found in the online version, at doi:10.1016/j.ejmech.2008.02.019.

### CHAPTER 5

Supplementary materials associated with this article can be found in the online version, at doi:10.1021/jp901057w

### CHAPTER 7

**TABLE 7.1S:** conformational search and clustering results for PN20 and PN22 optimized at the EDMC/SRFOPT/EC-CEP/3 level of theory. Total ( $E_{\text{tot}}$ , kcal.mol<sup>-1</sup>) and relative ( $\Delta E$ , kcal.mol<sup>-1</sup>) energies are also shown. All conformational families shown here have relative population (%PF) higher than 0.5%.

PN20		Elect.	Rand.	Ther.	Tot.
Generated <sup>a</sup>	4566	65514	156	70236	
Accepted <sup>b</sup>	459	4419	122	5000	

  

Family	NF <sup>c</sup>	%PF <sup>d</sup>	E <sub>tot</sub>	ΔE
1	1210	24.2	-36.89	0.00
2	276	5.52	-34.33	2.55
3	188	3.76	-35.22	1.66
4	185	3.7	-33.26	3.62
5	134	2.68	-33.21	3.68
6	121	2.42	-34.08	2.81
7	113	2.26	-31.40	5.48
8	99	1.98	-34.03	2.85
9	97	1.94	-33.93	2.95
10	83	1.66	-33.33	3.56
11	74	1.48	-29.38	7.50
12	70	1.4	-34.31	2.58
13	69	1.38	-33.70	3.19
14	68	1.36	-33.60	3.29
15	55	1.1	-32.82	4.07
16	48	0.96	-32.67	4.22
17	45	0.9	-33.51	3.38
18	43	0.86	-33.24	3.64
19	41	0.82	-31.20	5.69
20	36	0.72	-32.54	4.34
21	34	0.68	-34.15	2.73
22	33	0.66	-32.60	4.29
23	32	0.64	-32.87	4.02
24	32	0.64	-32.51	4.38
25	31	0.62	-32.32	4.57
26	30	0.6	-31.76	5.13
27	30	0.6	-29.97	6.92
28	28	0.56	-33.70	3.19
29	26	0.52	-32.77	4.12
30	26	0.52	-32.06	4.82

  

PN22		Elect.	Rand.	Ther.	Tot.
Generated <sup>a</sup>	5185	73574	318	79077	
Accepted <sup>b</sup>	542	4332	126	5000	

  

Family	NF <sup>c</sup>	%PF <sup>d</sup>	E <sub>tot</sub>	ΔE
1	3119	62.38	-6.76	0.00
2	425	8.5	-6.19	0.57
3	260	5.2	-6.15	0.61
4	107	2.14	-4.39	2.37
5	93	1.86	-3.97	2.79
6	69	1.38	-2.18	4.58
7	43	0.86	-4.42	2.34
8	40	0.8	-3.41	3.36
9	35	0.7	-4.28	2.49
10	33	0.66	-3.12	3.64
11	31	0.62	-1.20	5.56

<sup>a</sup>Number of conformations generated electrostatically, randomly and thermally during the conformational search.  
<sup>b</sup>Number of conformations accepted from those generated electrostatically, randomly and thermally during the conformational search.  
<sup>c</sup>NF represents the total number of conformational families as result of the clustering run.  
<sup>d</sup>%PF represents the percent relative population based on a total of 5000 accepted conformations.

