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Potential anticancer peptides design from the cysteine rich plant defensins: An *in silico* approach

Mohd Shafique & Siddhartha P Sarma
NMR lab, Molecular Biophysics Unit, Indian Institute of Science, Bangalore-560 012, Karnataka, India

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Supplementary Data

Suppl. Table 1 — The dihedral angles χ_1, χ_2, χ_3, χ'_2, χ'_1 from representative conformations of defensins

BcDef1				first	
	$\chi1$	$\chi2$	$\chi3$	$\chi'2$	$\chi'1$
DB_1(3, 47)	73.8	-48.1	-99.2	-166.2	-57.0
DB_2(14, 34)	60.6	72.8	83.2	58.0	175.7
DB_3(20, 41)	-166.9	-161.3	-115.7	-157.0	-161.4
DB_4(24, 43)	-92.5	165.4	81.2	178.0	-54.8
BcDef1				second	
DB_1(3, 47)	84.7	-60.9	-83.7	-170.8	-53.0
DB_2(14, 34)	57.1	103.8	92.5	59.6	162.9
DB_3(20, 41)	-159.5	139.2	-99.7	-176.5	-177.3
DB_4(24, 43)	-125.9	-178.0	91.5	-162.7	-55.8
NaD1					
DB_1(3, 47)	-54.4	77.4	-91.2	175.7	-54.0
DB_2(14, 34)	-168.0	-65.7	-85.0	-28.1	-82.2
DB_3(20, 41)	172.5	47.3	103.8	49.7	-164.3
DB_4(24, 43)	-68.4	-36.5	-83.5	-49.5	-72.1
2lr3				first	
DB_1(3, 47)	-53.5	178.3	-86.6	-75.1	90.4
DB_2(14, 34)	38.4	61.6	108.9	160.6	-152.3
DB_3(20, 41)	179.3	-170.8	-96.4	-167.6	-175.2
DB_4(24, 43)	-81.3	172.4	87.1	175.5	-73.8
2lr3				second	
DB_1(3, 47)	75.9	-55.9	-74.1	-146.1	-63.0
DB_2(14, 34)	54.6	71.1	89.9	78.3	-169.5
DB_3(20, 41)	-158.8	-167.0	-112.0	168.8	173.8
DB_4(24, 43)	-66.5	175.7	103.5	170.9	-98.0
tpp3					
DB_1(4, 48)	-56.7	83.3	88.0	172.5	41.5
DB_2(16, 36)	-149.6	-67.5	-64.9	-55.2	-76.2
DB_3(22, 43)	177.0	35.5	93.8	52.9	165.3
DB_4(26, 45)	-62.6	-43.	-84.2	-59.3	-66.1
2n2r					
DB_1(4, 51)	57.6	-153.5	94.3	76.5	-75.4
DB_2(15, 36)	157.9	-178.1	-112.5	151.1	172.8
DB_3(21, 45)	167.5	173.2	-88.0	-128.7	-162.1
DB_4(25, 47)	-59.5	-66.2	-88.1	-49.8	-73.8

Disulphidetype	**Chi2**	**Chi3**	**Chi2'**
lefthandedspiral (LHS)	-	-	-
right-handedhook (RHH)	+	+	-
right-handedspiral (RHS)	+	+	+
shortright-handedhook(SRH)	-	+	-

Chi1	N-Cα-Cβ-S	Here,N belongstoresiduewithlower numberparticipatingin-S-S-bond
Chi2	Cα-Cβ-S-S′	
Chi 3	**Cβ-S-S′-C′β**	
Chi2′	S-S′-C′β-C′α	
Chi1′	S′-C′β-C′α-N	Here, N belongstoresiduewithhighernumber participating in-S-S-bond

Suppl. Table 2 —The percentage (%) of secondary structure elements present in most stable defensin conformations

BcDef1 Method	DSSP	DSSP_CONT	STRIDE	Average
Helix	25.5	25.5	23.4	24.8
Sheet	27.7	27.7	31.9	29.1
Other	46.8	46.8	44.7	46.1
NaD1				
Helix	21.7	21.7	23.9	22.43
Sheet	32.6	32.6	32.6	32.6
Other	45.7	45.7	43.5	44.97
2l3r				
Helix	17.0	17.0	17.0	17
Sheet	8.5	8.5	51.1	22.7
Other	74.5	74.5	31.9	60.3
tpp3				
Helix	20.8	20.8	22.9	21.5
Sheet	25	25	31.3	27.1
Other	54.2	54.2	45.8	51.4
2n2r				
Helix	19.6	19.6	17.6	18.93
Sheet	27.5	27.5	31.4	28.8
Other	52.9	52.9	51.0	52.27

Suppl. Table 3 — SVM-data for defensins

BcDef						
FKGTCLSEKN	1.52	Anticp	0.64	0.86	0.90	8.54
CRGLRRRCFC	1.51	Anticp	0.65	0.98	1.60	10.45
CASVCETEGF	1.36	Anticp	0.63	0.25	0.40	3.80
RRRCFCTRPC	1.33	Anticp	0.62	0.98	1.70	10.45
KGTCLSEKNC	1.24	Anticp	0.63	0.86	0.90	8.36
2lr3						
CRGFRRRCFC	1.45	Anticp	0.67	0.98	1.60	10.45
RRRCFCTTHC	1.38	Anticp	0.57	0.88	1.50	9.35
CASVCQTERF	1.29	Anticp	0.63	0.50	0.90	6.30
RGFRRRCFCT	1.27	Anticp	0.66	0.98	1.70	11.53
DHNCASVCQT	1.17	Anticp	0.57	0.27	0.80	5.09
2N2R						
LEKARHGSCN	1.47	Anticp	0.57	0.88	1.10	8.57
KNQCIRLEKA	1.35	Anticp	0.65	1.23	1.30	9.36
AHKCICYFPC	1.11	Anticp	0.55	0.51	0.40	8.25
VCGNNNACKN	1.08	Anticp	0.69	0.37	1.00	8.38
CKNQCIRLEK	1.02	Anticp	0.66	1.23	1.30	8.98
TPP3DSSCRKYCIK						
	1.56	Anticp	0.65	0.98	1.20	8.94
RKYCIKEKFT	1.37	Anticp	0.66	1.47	1.30	9.65
CSKLQRKCLC	1.30	Anticp	0.62	1.10	1.10	9.20
CRKYCIKEKF	1.24	Anticp	0.67	1.47	1.20	9.33
SKLQRKCLCT	1.24	Anticp	0.61	1.10	1.20	9.53
NaD1						

KPPCRKACIS	1.52	Anticp	0.58	0.98	0.90	9.53
SKILRRCLCT	1.40	Anticp	0.61	0.86	1.20	9.72
CRKACISEKF	1.38	Anticp	0.64	1.11	1.00	8.98
TKPPCRKACI	1.34	Anticp	0.57	0.98	0.90	9.53
RKACISEKFT	1.32	Anticp	0.63	1.11	1.10	9.36

Suppl. Table 4 — Peptides designed with SVM

Defensin	Sequence	Method	Result	Score
BcDef1		SVM	NEGATIVE	-0.833
TPP3	DSSCREYCIK	SVM	POSITIVE	0.444
2N2R	LEKCRHGSCN	SVM	POSITIVE	0.453
	LEKARHGSCK	SVM	POSITIVE	0.462
	CRGFRRRCFC	SVM	POSITIVE	0.461
2L2R	RRRCFCTEHC	SVM	POSITIVE	0.459
	KPPCRKACIC	SVM	POSITIVE	0.454
NaD1	KPPCRKACIK	SVM	POSITIVE	0.457
	FEKARHGSCN	SVM	POSITIVE	0.451