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Table 7. Mean (time averaged*) (ϕ, ψ) values observed for the dendrotoxins.

Res No.	DtX		DpI		DpK	
	ϕ	ψ	ϕ	ψ	ϕ	ψ
	69	143	-71	123		
	68	61	49	-56		
1	64	104	-132	-50	107	-109
2	68	-99	-62	-73	88	-128
3	-72	-106	-67	-39	-120	-70
4	-39	-13	-76	-26	-155	46
5	-70	-41	-76	-24	-71	-28
6	-104	-10	-125	-57	-54	74
7	121	116	-166	114	-68	126
8	67	14	-121	-131	-61	158
9	-103	58	-83	72	35	56
10	-75	124	-64	117	-137	128
11	-97	156	98	-44	-168	55
12	133	-113	-98	177	-79	96
13	-109	22	-69	-5	-78	-40
14	-67	139	-94	154	-117	168
15	-92	-28	-112	37	107	174
16	-90	134	-95	137	-73	126
17	-136	130	-110	90	-140	102
18	-46	138	-64	127	-66	125
19	-147	138	-141	134	-141	147
20	-126	126	-102	152	-126	161
21	-127	140	-150	160	-110	111
22	-85	157	-82	157	-78	165
23	-83	126	-79	120	-74	109
24	-65	111	-75	113	-81	148
25	-80	-29	-68	-33	-83	-55
26	-84	-58	-75	-56	-169	54
27	121	-29	65	-17	-52	144

Table 7. (continued).

Res No.	DtX		DpI		DpK	
	ϕ	ψ	ϕ	ψ	ϕ	ψ
28	-106	-30	-163	58	-160	-23
29	-89	157	-88	169	-46	-176
30	-92	102	-117	121	-145	138
31	-83	154	-132	-167	-75	164
32	-131	130	-164	175	-95	122
33	-78	163	-92	166	-89	162
34	-102	90	-91	117	-69	108
35	10	51	-98	151	-72	140
36	75	64	103	-12	75	52
37	-169	-78	-110	-54	-165	-70
38	134	178	155	124	62	144
39	167	-16	-59	92	-94	38
40	-108	-36	-151	108	-168	-71
41	-59	139	-67	108	-62	156
42	-59	-24	-87	-26	-50	-37
43	-131	43	-95	25	-109	73
44	-119	120	-123	123	46	-84
45	-96	145	-87	144	-83	64
46	-140	-16	-108	-41	-151	84
47	-62	147	-64	147	-61	138
48	-62	-42	-63	-29	-59	-39
49	-59	-40	-75	-46	-63	-29
50	-54	-51	-54	-28	-74	-51
51	-62	-47	-73	-51	-65	-19
52	-74	-50	-80	-24	-91	-52
53	-85	-34	-85	-41	-102	-44
54	-75	-39	-128	-30	-34	-45
55	-79	-40	-80	64	81	-78
56	-162	99	-19	127	-175	-153
57			-175	-69		

* Averaging was computed using trajectories over 100ps using the MDANAL module of AMBER [28].

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Table 8. Non-bonded contacts between the dendrotoxins® and kallikrein at the anti-protease site.

Atom 1	Site	Molecule	Atom 2	Molecule	Dist. (Å)
N^{ε} (Arg 13)	p3	DtX	N (Gly216)	kallikrein	3.61
N^{ε} (Arg 13)	p3	DtX	O (Gly216)	kallikrein	2.90
N^{ε} (Arg 13)	p3	DtX	N (His 217)	kallikrein	3.92
$N^{\eta 2}$ (Arg 13)	p3	DtX	O^{γ} (Tyr 99)	kallikrein	3.23
C (Tyr 15)	p1	DtX	O^{γ} (Ser 195)	kallikrein	3.12
O (Tyr 15)	p1	DtX	O^{γ} (Ser 195)	kallikrein	3.15
N (Tyr 15)	p1	DtX	O^{γ} (Ser 195)	kallikrein	3.35
N (Tyr 15)	p1	DtX	$N^{\varepsilon 2}$ (His 57)	kallikrein	3.77
N (Tyr 15)	p1	DtX	O (Ser 214)	kallikrein	3.70
O^{γ} (Tyr 15)	p1	DtX	O (Trp 215)	kallikrein	2.90
O^{γ} (Tyr 15)	p1	DtX	O^{γ} (Thr 190)	kallikrein	3.06
O^{γ} (Tyr 15)	p1	DtX	N (Trp 215)	kallikrein	3.34
O^{γ} (Tyr 15)	p1	DtX	N (Ser 214)	kallikrein	3.87
O^{γ} (Tyr 15)	p1	DtX	O (Ile 227)	kallikrein	3.72
O^{γ} (Tyr 15)	p1	DtX	O^{γ} (Ser 226)	kallikrein	3.60
$O^{\delta 1}$ (Asp 16)	p1'	DtX	O (Gln 41)	kallikrein	3.31
$O^{\delta 1}$ (Asp 16)	p1'	DtX	N (Cys 42)	kallikrein	3.23
$O^{\delta 1}$ (Asp 16)	p1'	DtX	O (Gly 193)	kallikrein	3.89
N (Asp 16)	p1'	DtX	O^{γ} (Ser 195)	kallikrein	3.76
N (Asp 16)	p1'	DtX	O (Ser 195)	kallikrein	2.63
$O^{\delta 2}$ (Asp 16)	p1'	DtX	N (Gln 41)	kallikrein	3.84
$O^{\delta 2}$ (Asp 16)	p1'	DtX	O (Gln 41)	kallikrein	2.67
$O^{\delta 2}$ (Asp 16)	p1'	DtX	N (Gln 42)	kallikrein	3.48
N (Lys 17)	p2'	DtX	N (Gly 193)	kallikrein	3.74
O (Lys 17)	p2'	DtX	O (Phe 40)	kallikrein	3.42
N^{ζ} (Lys 17)	p2'	DtX	N (Cys 42)	kallikrein	3.47
N^{ζ} (Lys 17)	p2'	DtX	O (Cys 42)	kallikrein	3.77
N^{ζ} (Lys 17)	p2'	DtX	O (Gly 193)	kallikrein	3.06
O (Gly 41)		DtX	O^{γ} (Tyr 99)	kallikrein	3.95
$N^{\eta 2}$ (Arg 13)	p3	DpI	O^{γ} (Tyr 99)	kallikrein	3.57
N^{ε} (Arg 13)	p3	DpI	O (Gly 216)	kallikrein	2.92
C (Tyr 15)	p1	DpI	O^{γ} (Ser 195)	kallikrein	3.40
C^{α} (Tyr 15)	p1	DpI	O^{γ} (Ser 195)	kallikrein	3.06
N (Tyr 15)	p1	DpI	O (Ser 214)	kallikrein	2.99
N (Tyr 15)	p1	DpI	$N^{\varepsilon 2}$ (His 57)	kallikrein	3.93
N (Tyr 15)	p1	DpI	O^{γ} (Ser 195)	kallikrein	3.25
O (Tyr 15)	p1	DpI	$N^{\varepsilon 2}$ (His 57)	kallikrien	3.81

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O (Tyr 15)	p1	DpI	Oγ (Ser 195)	kallikrein	3.60
Oγ (Tyr 15)	p1	DpI	O (Trp 215)	kallikrein	3.59
Oγ (Tyr 15)	p1	DpI	Oγ (Thr 190)	kallikrein	3.81
Oγ (Tyr 15)	p1	DpI	N (Gly 216)	kallikrein	3.29
Oγ (Tyr 15)	p1	DpI	Oγ (Ser 226)	kallikrein	2.76
Oγ (Tyr 15)	p1	DpI	O (Thr 190)	kallikrein	3.99
N (Gln 16)	p1'	DpI	N (Gly 193)	kallikrein	2.89
N (Gln 16)	p1'	DpI	N (Asp 194)	kallikrein	3.40
N (Gln 16)	p1'	DpI	N (Ser 195)	kallikrein	3.37
O (Gln 16)	p1'	DpI	N (Gly 193)	kallikrein	3.81
Oε1 (Gln 16)	p1'	DpI	N (Cys 42)	kallikrein	3.75
Oε1 (Gln 16)	p1'	DpI	O (Gln 41)	kallikrein	2.61
Oε1 (Gln 16)	p1'	DpI	N (Gly 193)	kallikrein	3.82
Oε1 (Gln 16)	p1'	DpI	O (Gly 193)	kallikrein	3.15
Oε1 (Gln 16)	p1'	DpI	N (Asp 194)	kallikrein	3.79
Nε2 (Gln 16)	p1'	DpI	O (Cys 42)	kallikrein	3.30
Nε2 (Gln 16)	p1'	DpI	N (Gly 43)	kallikrein	3.00
Nε2 (Gln 16)	p1'	DpI	O (Gly 193)	kallikrein	2.90
Nε2 (Gln 16)	p1'	DpI	N (Asp 194)	kallikrein	3.70
Nε2 (Gln 16)	p1'	DpI	N (Ser 195)	kallikrein	3.82
Nε2 (Gln 16)	p1'	DpI	O (Ser 195)	kallikrein	3.37
N (Lys 17)	p2'	DpI	O (Gln 41)	kallikrein	3.12
N (Lys 17)	p2'	DpI	N (Gly 193)	kallikrein	3.36
O (Lys 17)	p2'	DpI	O (Phe 40)	kallikrein	3.58
O (Lys 17)	p2'	DpI	O (Gln 41)	kallikrein	3.77
Nζ (Lys 17)	p2'	DpI	N (Phe 40)	kallikrein	3.94
Nζ (Lys 17)	p2'	DpI	N (Gln 41)	kallikrein	3.95
Nζ (Lys 17)	p2'	DpI	O (Phe 40)	kallikrein	2.78
N (Lys 15)	p1	DpK	Oγ (Ser 195)	kallikrein	3.27
N (Lys 15)	p1	DpK	O (Ser 214)	kallikrein	3.33
N (Lys 15)	p1	DpK	Nε2 (His57)	kallikrein	3.19
O (Lys 15)	p1	DpK	Nε2 (His57)	kallikrein	3.63
O (Lys 15)	p1	DpK	Oγ (Ser 195)	kallikrein	3.43
Nζ (Lys 15)	p1	DpK	N (Trp 216)	kallikrein	2.92
Nζ (Lys 15)	p1	DpK	O (Trp 215)	kallikrein	3.97
N (Arg 16)	p1'	DpK	N (Gly 193)	kallikrein	2.66
N (Arg 16)	p1'	DpK	N (Ser 195)	kallikrein	3.09
N (Arg 16)	p1'	DpK	N (Asp 194)	kallikrein	2.97
N (Arg 16)	p1'	DpK	O (Cys 191)	kallikrein	3.90
O (Arg 16)	p1'	DpK	O (Gln 41)	kallikrein	3.59
O (Arg 16)	p1'	DpK	N (Gly 193)	kallikrein	3.81
Nε (Arg 16)	p1'	DpK	O (Cys 42)	kallikrein	3.33

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N^{ε} (Arg 16)	p1'	DpK	N (Gly 43)	kallikrein	2.62
N^{ε} (Arg 16)	p1'	DpK	O (Gly 193)	kallikrein	3.13
N^{ε} (Arg 16)	p1'	DpK	O (Ser 195)	kallikrein	3.53
$N^{\eta 1}$ (Arg16)	p1'	DpK	$O^{\varepsilon 1}$ (Gln 30)	kallikrein	3.64
$N^{\eta 1}$ (Arg16)	p1'	DpK	N (Trp 141)	kallikrein	3.26
$N^{\eta 2}$ (Arg 16)	p1'	DpK	O (Asp 194)	kallikrein	3.59
$N^{\eta 2}$ (Arg 16)	p1'	DpK	O (Gly 193)	kallikrein	2.60
$N^{\eta 2}$ (Arg 16)	p1'	DpK	N (Asp 194)	kallikrein	3.56
$N^{\eta 2}$ (Arg 16)	p1'	DpK	N (Trp 141)	kallikrein	3.22
$N^{\eta 2}$ (Arg 16)	p1'	DpK	N (Gly 142)	kallikrein	3.78
$N^{\eta 2}$ (Arg 16)	p1'	DpK	$O^{\delta 2}$ (Asp 194)	kallikrein	2.83
N (Lys 17)	p2'	DpK	O (Gln 41)	kallikrein	2.72
N (Lys 17)	p2'	DpK	N (Gly 193)	kallikrein	3.31
O (Lys 17)	p2'	DpK	N (Gln 41)	kallikrein	3.78
O (Lys 17)	p2'	DpK	O (Phe 40)	kallikrein	3.18
No(Lys 17)	p2'	DpK	O (Gln 41)	kallikrein	3.17
N^{ζ} (Lys 17)	p2'	DpK	N (Gln 41)	kallikrein	2.90
N^{ζ} (Lys 17)	p2'	DpK	O (Phe 40)	kallikrein	2.81
N^{ζ} (Lys 17)	p2'	DpK	O (Gln 41)	kallikrein	3.55

® Atom names of the amino acids are based on IUPAC nomenclature[58]. The sequence numbering is based on BPTI structure

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Table 9. Non-bonded contacts between the dendrotoxins® and trypsin at the anti-protease site.

Atom1	site	Mol. 1	Atom2	Mol2.	Dist. (Å)
N^{ε} (Arg 13)	p3	DtX	O (Gly 216)	trypsin	3.60
N^{ε} (Arg 13)	p3	DtX	N (Gly 216)	trypsin	3.56
O (Cys 14)	p2	DtX	$N^{\varepsilon 2}$ (Gln 192)	trypsin	2.79
N (Tyr 15)	p1	DtX	O^{γ} (Ser 195)	trypsin	2.78
N (Tyr 15)	p1	DtX	O (Ser 214)	trypsin	3.70
O (Tyr 15)	p1	DtX	O^{γ} (Ser 195)	trypsin	3.27
O^{γ} (Tyr 15)	p1	DtX	N (Ser 214)	trypsin	3.50
O^{γ} (Tyr 15)	p1	DtX	O (Val 227)	trypsin	3.29
O^{γ} (Tyr 15)	p1	DtX	N (Trp 215)	trypsin	3.21
O^{γ} (Tyr 15)	p1	DtX	O^{γ} (Ser 190)	trypsin	3.11
O^{γ} (Tyr 15)	p1	DtX	O (Trp 215)	trypsin	3.14
N (Asp 16)	p1'	DtX	N (Gly 193)	trypsin	2.69
$O^{\delta 1}$ (Asp 16)	p1'	DtX	$N^{\varepsilon 2}$ (His 40)	trypsin	3.14
$O^{\delta 1}$ (Asp 16)	p1'	DtX	N (Phe 41)	trypsin	3.80
$O^{\delta 1}$ (Asp 16)	p1'	DtX	N (Cys 42)	trypsin	3.01
$O^{\delta 1}$ (Asp 16)	p1'	DtX	O (Phe 41)	trypsin	3.55
$O^{\delta 1}$ (Asp 16)	p1'	DtX	O (Gly 193)	trypsin	2.94
$O^{\delta 1}$ (Asp 16)	p1'	DtX	N (Gly 193)	trypsin	3.87
$O^{\delta 2}$ (Asp 16)	p1'	DtX	N (Phe 41)	trypsin	3.83
$O^{\delta 2}$ (Asp 16)	p1'	DtX	N (Cys 42)	trypsin	3.52
$O^{\delta 2}$ (Asp 16)	p1'	DtX	O (Phe 41)	trypsin	2.60
N (Lys 17)	p2'	DtX	N (Gly 193)	trypsin	3.78
N^{ζ} (Lys 17)	p2'	DtX	N (His 40)	trypsin	3.72
N^{ε} (Arg 13)	p3	DpI	O (Gly 216)	trypsin	3.24
N (Cys 14)	p2	DpI	$N^{\varepsilon 2}$ (Gln 192)	trypsin	3.79
O (Cys 14)	p2	DpI	$N^{\varepsilon 2}$ (Gln 192)	trypsin	2.80
N (Tyr 15)	p1	DpI	O^{γ} (Ser 195)	trypsin	3.21
N (Tyr 15)	p1	DpI	O (Ser 214)	trypsin	3.13
O (Tyr 15)	p1	DpI	$N^{\varepsilon 2}$ (His 57)	trypsin	3.89
O (Tyr 15)	p1	DpI	O^{γ} (Ser 195)	trypsin	3.53
O^{γ} (Tyr 15)	p1	DpI	O (Ser 190)	trypsin	3.88
O^{γ} (Tyr 15)	p1	DpI	O (Gly 219)	trypsin	3.26
O^{γ} (Tyr 15)	p1	DpI	O (Trp 215)	trypsin	3.41
O^{γ} (Tyr 15)	p1	DpI	N (Gly 216)	trypsin	3.44
N (Gln 16)	p1'	DpI	N (Asp 194)	trypsin	3.17
N (Gln 16)	p1'	DpI	N (Ser 195)	trypsin	3.12
N (Gln 16)	p1'	DpI	N (Gly 193)	trypsin	2.91
N (Gln 16)	p1'	DpI	O (Cys 191)	trypsin	3.82
O (Gln 16)	p1'	DpI	N (Gly 193)	trypsin	3.54

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$O^{\varepsilon 1}$ (Gln 16)	p1'	DpI	$N^{\varepsilon 2}$ (His 40)	trypsin	3.05
$O^{\varepsilon 1}$ (Gln 16)	p1'	DpI	N (Cys 42)	trypsin	3.16
$O^{\varepsilon 1}$ (Gln 16)	p1'	DpI	O (Phe 41)	trypsin	3.02
$O^{\varepsilon 1}$ (Gln 16)	p1'	DpI	O (Gly 193)	trypsin	3.60
$O^{\varepsilon 1}$ (Gln 16)	p1'	DpI	N (Gly 194)	trypsin	3.64
$O^{\varepsilon 1}$ (Gln 16)	p1'	DpI	N (Gly 193)	trypsin	3.83
$N^{\varepsilon 2}$ (Gln 16)	p1'	DpI	$N^{\varepsilon 2}$ (His 40)	trypsin	2.86
$N^{\varepsilon 2}$ (Gln 16)	p1'	DpI	O (Cys 42)	trypsin	3,56
$N^{\varepsilon 2}$ (Gln 16)	p1'	DpI	N (Gly 43)	trypsin	3.11
$N^{\varepsilon 2}$ (Gln 16)	p1'	DpI	O (Ser 195)	trypsin	3.56
$N^{\varepsilon 2}$ (Gln 16)	p1'	DpI	O (Gly 193)	trypsin	2.94
$N^{\varepsilon 2}$ (Gln 16)	p1'	DpI	N (Asp 194)	trypsin	3.20
$N^{\varepsilon 2}$ (Gln 16)	p1'	DpI	O (Asp 194)	trypsin	3.99
$N^{\varepsilon 2}$ (Gln 16)	p1'	DpI	N (Ser 195)	trypsin	3.89
N (Lys 17)	p2'	DpI	O (Phe 41)	trypsin	3.25
N (Lys 17)	p2'	DpI	N (Gly 193)	trypsin	3.13
O (Lys 17)	p2'	DpI	O (His 40)	trypsin	3.77
O (Lys 17)	p2'	DpI	O (Phe 41)	trypsin	3.92
N^{ζ} (Lys 17)	p2'	DpI	N (His 40)	trypsin	3.65
N^{ζ} (Lys 17)	p2'	DpI	O (His 40)	trypsin	2.70
N (Ile 18)	p3'	DpI	O (Phe 41)	trypsin	3.95
N (Cys 14)	p2	DpK	$N^{\varepsilon 2}$ (Gln 192)	trypsin	3.97
O (Cys 14)	p2	DpK	$N^{\varepsilon 2}$ (Gln 192)	trypsin	3.13
N (Lys 15)	p1	DpK	$N^{\varepsilon 2}$ (His 57)	trypsin	3.47
N (Lys 15)	p1	DpK	O^{γ} (Ser 1995)	trypsin	3.04
N (Lys 15)	p1	DpK	O (Ser 214)	trypsin	3.61
O (Lys 15)	p1	DpK	N (Ser 195)	trypsin	3.88
O (Lys 15)	p1	DpK	$N^{\varepsilon 2}$ (His 57)	trypsin	3.81
O (Lys 15)	p1	DpK	O^{γ} (Ser 1995)	trypsin	3.53
N^{ζ} (Lys 15)	p1	DpK	O (Trp 215)	trypsin	3.86
N^{ζ} (Lys 15)	p1	DpK	N (Gly 216)	trypsin	3.17
N (Arg 16)	p1'	DpK	N (Asp 194)	trypsin	2.72
N (Arg 16)	p1'	DpK	N (Ser 195)	trypsin	2.80
N (Arg 16)	p1'	DpK	N (Gly 193)	trypsin	2.69
N (Arg 16)	p1'	DpK	O (Cys 191)	trypsin	3.93
O (Arg 16)	p1'	DpK	O (Phe 41)	trypsin	3.46
O (Arg 16)	p1'	DpK	N (Gly 193)	trypsin	3.55
N^{ε} (Arg 16)	p1'	DpK	O (Cys 42)	trypsin	3.60
N^{ε} (Arg 16)	p1'	DpK	N (Gly 43)	trypsin	2.93
N^{ε} (Arg 16)	p1'	DpK	O (Ser 195)	trypsin	3.77
N^{ε} (Arg 16)	p1'	DpK	$N^{\varepsilon 2}$ (His 40)	trypsin	3.01
N^{ε} (Arg 16)	p1'	DpK	O (Gly 193)	trypsin	3.15

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$N^{\eta 1}$ (Arg 16)	p1'	DpK	$O^{\varepsilon 1}$ (Gln 30)	trypsin	3.37
$N^{\eta 1}$ (Arg 16)	p1'	DpK	N (Trp 141)	trypsin	2.78
$N^{\eta 1}$ (Arg 16)	p1'	DpK	$N^{\varepsilon 2}$ (His 40)	trypsin	3.46
$N^{\eta 1}$ (Arg 16)	p1'	DpK	O (Gly 193)	trypsin	3.99
$N^{\eta 2}$ (Arg 16)	p1'	DpK	N (Trp 141)	trypsin	3.04
$N^{\eta 2}$ (Arg 16)	p1'	DpK	N (Gly 142)	trypsin	3.74
$N^{\eta 2}$ (Arg 16)	p1'	DpK	O (Gly 193)	trypsin	2.56
$N^{\eta 2}$ (Arg 16)	p1'	DpK	N (Asp 194)	trypsin	3.48
$N^{\eta 2}$ (Arg 16)	p1'	DpK	$O^{\delta 2}$ (Asp 194)	trypsin	2.64
$N^{\eta 2}$ (Arg 16)	p1'	DpK	O (Asp 194)	trypsin	3.50
N (Lys 17)	p2'	DpK	O (His 40)	trypsin	3.77
N (Lys 17)	p2'	DpK	O (Phe 41)	trypsin	2.84
N (Lys 17)	p2'	DpK	N (Gly 193)	trypsin	3.28
O (Lys 17)	p2'	DpK	O (His 40)	trypsin	3.39
O (Lys 17)	p2'	DpK	N (Phe 41)	trypsin	3.68
O (Lys 17)	p2'	DpK	O (Phe 41)	trypsin	3.58
N^{ζ} (Lys 17)	p2'	DpK	N (His 40)	trypsin	3.33
N (Ile 18)	p3'	DpK	O (Phe 41)	trypsin	3.95

® Atom names of the amino acids are based on IUPAC nomenclature[58]. The sequence numbering is based on BPTI structure