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The Effect of Oxidative Stress on Bursopentin Peptide Structure: A Theoretical Study

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Supplementary Results

Table S1. The percentage value of zero represents no secondary structure. The value obtained in the parentheses shows the amount of turn in 2000 structures. CKRVY has not RMSD value because this is the reference structure.

Peptide RMSD / Å Radius of Gyration / Å	Residue	Secondary Structure Element 3-10 helix	Parallel β-Sheet	Antiparallel β-Sheet	Turn
	Cys[1]	0.00	0.00	0.00	0.00
CKRVY	Lys[2]	0.05 (1)	0.00	0.00	0.95 (19)
-	Arg[3]	0.05 (1)	0.00	0.00	1.50 (30)
5.800 ± 0.397	Val[4]	0.05 (1)	0.00	0.00	0.55 (11)
	Tyr[5]	0.00	0.00	0.00	0.00
	Cys[1]	0.00	0.00	0.00	0.00
cKRVY	Lys[2]	0.10 (2)	0.00	0.00	1.15 (23)
5.58 ± 0.11	Arg[3]	0.10 (2)	0.00	0.00	1.40 (28)
5.858 ± 0.397	Val[4]	0.10 (2)	0.00	0.00	0.25 (5)
	Tyr[5]	0.00	0.00	0.00	0.00
	Cys[1]	0.00	0.00	0.00	0.00
CkRVY	Lys[2]	0.00	0.00	0.00	4.70 (94)
6.28 ± 0.20	Arg[3]	0.00	0.00	0.00	4.95 (99)
5.886 ± 0.393	Val[4]	0.00	0.00	0.00	0.25 (5)
	Tyr[5]	0.00	0.00	0.00	0.00
	Cys[1]	0.00	0.00	0.00	0.00
CKrVY	Lys[2]	0.15 (3)	0.05 (1)	0.65 (13)	11.50 (230)
5.74 ± 0.42	Arg[3]	0.15 (3)	0.00	0.00	13.85 (277)
5.740 ± 0.417	Val[4]	0.15 (3)	0.00	0.00	2.65 (53)
	Tyr[5]	0.00	0.05 (1)	0.65 (13)	0.00
CKRvY	Cys[1]	0.00	0.00	0.00	0.00
5.85 ± 0.35	Lys[2]	0.10 (2)	0.00	0.10	0.55 (11)
5.854 ± 0.350	Arg[3]	0.10 (2)	0.00	0.00	1.30 (26)
	Val[4]	0.10 (2)	0.00	0.00	0.75 (15)
	Tyr[5]	0.00	0.00	0.10	0.00

Peptide RMSD / Å Radius of Gyration / Å	Residue	Secondary Structure Element 3-10 helix	Parallel β-Sheet	Antiparallel β-Sheet	Turn
	Cys[1]	0.00	0.00	0.00	0.00
CKRVy	Lys[2]	0.05 (1)	0.00	0.00	0.60 (12)
5.96 ± 0.35	Arg[3]	0.05 (1)	0.00	0.00	0.75 (15)
5.960 ± 0.352	Val[4]	0.05 (1)	0.00	0.00	0.25 (5)
	Tyr[5]	0.00	0.00	0	0.00

Table S2. Bond lengths and dihedral angles within residue 3 of *bursopentin* with the C_α of each residue in the L configuration, in the extended conformation ($LLLLL_{EXT}$) and minimum energy conformation ($LLLLL_{MIN}$). The bond lengths within each respective residue containing a C_α-centered radical (R) and the C_α in the D configuration (D) are also shown. Each parameter is also shown for the respective residue containing a C_α-centered radical (R) and the C_α in the D configuration (D). Each structure was optimized at the B3LYP/6-31G(d) level of theory using the SMD solvent model. (*) represents the position of the residue that is undergoing analysis.

Peptide Structure	Bond Length (Å)						Dihedral Angle			Backbone Length / Å
	"n – 1" amide	N–H	N-C_α	C_α-C_β	Cα-C	C=O	"n + 1" amide	ϕ / degrees	ψ / degrees	
CKRVY$_{EXT}$	----	1.010	1.488	1.525	1.523	1.229	1.335	----	137.7	16.40
C˙KRVY$_{EXT}$	----	1.037	1.459	1.472	1.473	1.251	1.346	----	178.8	15.81
cKRVY$_{EXT}$	----	1.023	1.505	1.532	1.538	1.239	1.338	----	-132.3	16.09
C**K**RVY$_{EXT}$	1.336	1.016	1.462	1.548	1.534	1.243	1.342	-151.0	146.4	16.40
CK˙RVY$_{EXT}$	1.361	1.022	1.380	1.495	1.470	1.256	1.354	-177.8	175.7	16.19
CkRVY$_{EXT}$	1.338	1.016	1.462	1.546	1.533	1.242	1.344	153.1	-141.8	15.05
CK**R**VY$_{EXT}$	1.342	1.015	1.459	1.550	1.533	1.242	1.344	-153.0	149.9	16.40
CKR˙VY$_{EXT}$	1.366	1.021	1.380	1.499	1.468	1.255	1.363	176.6	179.6	14.46
CKrVY$_{EXT}$	1.343	1.015	1.462	1.546	1.533	1.244	1.341	162.1	-139.9	14.50
CKR**V**Y$_{EXT}$	1.344	1.015	1.460	1.560	1.536	1.247	1.336	-136.3	152.6	16.40
CKRV˙Y$_{EXT}$	1.365	1.022	1.387	1.512	1.473	1.262	1.348	-156.9	176.5	16.53
CKRvY$_{EXT}$	1.342	1.015	1.461	1.561	1.534	1.247	1.338	155.8	-146.9	14.97
CKRV**Y**$_{EXT}$	1.336	1.018	1.460	1.564	1.555	1.265	-----	-159.5	-----	16.40
CKRVY˙$_{EXT}$	1.365	1.022	1.387	1.512	1.492	1.273	-----	-177.5	-----	15.02
CKRVy$_{EXT}$	1.339	1.016	1.460	1.557	1.550	1.263	-----	161.1	-----	16.15
CKRVY$_{MIN}$	----	1.027	1.497	1.536	1.537	1.238	1.339	0.0	152.32	14.01
C˙KRVY$_{MIN}$	----	1.037	1.460	1.473	1.471	1.250	1.348	0.0	178.88	15.81
cKRVY$_{MIN}$	----	1.030	1.499	1.534	1.536	1.238	1.339	0.0	-143.51	16.10
C**K**RVY$_{MIN}$	1.339	1.014	1.462	1.540	1.542	1.240	1.345	-151.0	146.45	14.01
CK˙RVY$_{MIN}$	1.360	1.023	1.380	1.500	1.469	1.256	1.353	-177.8	175.76	17.23

CkRVY$_{MIN}$	1.338	1.016	1.463	1.546	1.532	1.243	1.342	153.6	-140.7	15.04
CK<u>R</u>VY$_{MIN}$	1.345	1.015	1.456	1.550	1.533	1.241	1.346	-153.0	150.0	14.01
CKR˙VY$_{MIN}$	1.368	1.024	1.404	1.501	1.473	1.248	1.367	138.9	-31.0	3.37
CKrVY$_{MIN}$	1.345	1.015	1.467	1.536	1.541	1.237	1.352	131.3	-80.2	3.42
CKR<u>V</u>Y$_{MIN}$	1.346	1.013	1.456	1.556	1.542	1.247	1.338	-136.3	152.7	14.01
CKRV˙Y$_{MIN}$	1.369	1.017	1.393	1.509	1.481	1.251	1.355	45.0	-150.8	12.83
CKRvY$_{MIN}$	1.346	1.013	1.459	1.553	1.543	1.243	1.345	62.7	-144.3	12.58
CKRV<u>Y</u>$_{MIN}$	1.338	1.019	1.459	1.562	1.557	1.260	----	-159.4	0.0	14.01
CKRVY˙$_{MIN}$	1.369	1.018	1.398	1.501	1.487	1.274	----	45.9	0.0	11.93
CKRVy$_{MIN}$	1.346	1.013	1.462	1.544	1.552	1.267	----	76.6	0.0	12.00
<u>C</u>KRVY$_{RMSD}$	----	1.008	1.486	1.548	1.536	1.235	1.342	0.0	157.4	15.02
C˙KRVY$_{RMSD}$	----	1.009	1.487	1.548	1.540	1.235	1.342	0.0	-179.7	14.07
cKRVY$_{RMSD}$	----	1.028	1.504	1.532	1.537	1.239	1.339	0.0	-156.6	15.08
C<u>K</u>RVY$_{RMSD}$	1.342	1.012	1.478	1.542	1.539	1.236	1.338	-69.4	144.6	15.02
CK˙RVY$_{RMSD}$	1.334	1.013	1.483	1.542	1.538	1.233	1.340	27.2	4.4	12.73
CkRVY$_{RMSD}$	1.344	1.015	1.461	1.540	1.537	1.240	1.347	79.4	14.2	15.67
CK<u>R</u>VY$_{RMSD}$	1.338	1.011	1.478	1.544	1.537	1.232	1.334	-144.9	166.2	15.02
CKR˙VY$_{RMSD}$	1.350	1.014	1.460	1.537	1.542	1.247	1.338	-133.7	61.4	13.88
CKrVY$_{RMSD}$	1.377	1.017	1.391	1.499	1.465	1.253	1.336	-164.0	48.9	12.29
CKR<u>V</u>Y$_{RMSD}$	1.334	1.009	1.478	1.544	1.536	1.236	1.337	39.5	159.1	15.02
CKRV˙Y$_{RMSD}$	1.371	1.017	1.391	1.514	1.486	1.253	1.353	42.4	-148.7	13.05
CKRvY$_{RMSD}$	1.351	1.014	1.457	1.557	1.548	1.245	1.346	73.1	-153.2	13.35
CKRV<u>Y</u>$_{RMSD}$	1.337	1.015	1.474	1.537	1.541	1.251	-----	-137.2	-----	15.02
CKRVY˙$_{RMSD}$	1.370	1.017	1.400	1.502	1.483	1.273	-----	45.4	----	11.8
CKRVy$_{RMSD}$	1.345	1.014	1.466	1.542	1.553	1.266	-----	57.4	0.0	12.01