Characterization of the Interactions between Calmodulin and Death Receptor 5 in Triple-Negative and Estrogen Receptor Positive Breast Cancer Cells: An Integrated Experimental and Computational Study*

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*Running Title: Calmodulin and death receptor 5 interactions in breast cancer cells

Supporting Materials

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DR5CR 5'	CTCGAGTTAGGACATGGCAGAGTCTGC
DR5CR 3'	CTCGAGTTAGGACATGGCAGAGTCTGC
DR5DD 5'	CACCGGATCCCCAGCAAATGAAGGTGATCCC
DR5DD 3'	CTCGAGTTACAACAAGTGGTCCTCAATCTT
DR5DDdel 5'	AGCTCTGGAAAGTTCATGTAT
DR5DDdel 3'	AACCAGCAGCCTCCTCCTCTG
DR5BSD 5'	ATGGACAATGAGATAAAGGTG
DR5BSD 3'	GGAGTCAAAGGGCACCAAGTC
DR5E355K 5'	AAGCCGCTCATGAGGAAGTTG
DR5E355K 3'	CCAGGAGTCAAAGGGCACC
DR5R359A 5'	GCCAAGTTGGGCCTCATGGAC
DR5R359A 3'	CATGAGCGGCTCCCAGGAGTC

Table S2. Sterochemical quality scores of the DR5 DD models.

	PROCHECK[a]				ERRAT[b]		WHATCHECK[c]		Verify_3D[d]
Template	*Favored residues*	*allowed residues*	*generously allowed residues*	*disallowed residues*		*Packing quality*	*Ramachandram appearance*	*X1/X2 rotamer normality*	
1ICH+1DDF	98.7%	1.3%	0.0%	0.0%	90.8	-2.281	2.918	-1.666	77.7%

a. PROCHECK evaluates the residual φ/ψ angles in the Ramachandran plots. The good model should not have no disallowed residues shown by PEOCHECK.
b. ERRAT analyzes patterns of non-bonded interactions and gives an overall quality score for the entire model and good models generally produce scores above 80.
c. WHATCHECK does extensive checking of many sterochemical parameters of the residues in the model. While a positive score means better than average, a negative score of -4.0 or lower indicates a serious problem with the structure.
d. Verify_3D: analyzing the compatibility of an atomic model (3D) with its own amino acid sequence (1D). The good model should have the more than 75% score for Verify_3D.