

Table S1: Correlation coefficients for the PHF6, IB12 and AS51 FMA models of the decameric phase.

Decamer	PHF6		IB12		AS51	
	Train	Test	Train	Test	Train	Test
PHF6	0.49	0.40		0.43		0.76
IB12		0.44	0.69	0.65		0.71
AS51		0.47		0.34	0.76	0.75

Row-wise: Sampling density of the peptide system used for FMA model building. Column-wise: Sampling density of the peptide system used for FMA model validation.