

Supporting information

“Can peptide folding simulations provide predictive information for aggregation propensity?”

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Studied hexapeptide sequences that are non-fibril-forming

DLLKNG	KVEHSD	STAIIE	STVIDE	STVQIE
ERIEKV	LKNGER	STDIIE	STVIEE	STVSIE
EVDLLK	LSQPKI	STGIIE	STVIGE	STVVIE
FFYTPK	NLGPVL	STIIIE	STVIIP	STYIIE
FTPTEK	PKIQVY	STMIIE	STVINE	SWVIIE
GERGFF	PTVIIE	STPIIE	STVIPE	VKWDRD
HLVEAL	QPKIVK	STTIIE	STVIQE	WSFYLL
IQRTPK	RVNHVT	STVAIE	STVITE	YQLENY
KTVIIE	SGFHPS	STVDIE	STVIWE	YVSGFH
KTVIVE	SHLVEA	STVGIE	STVMIE	
KTVLIE	SPVIIE	STVIAE	STVPIE	

Studied hexapeptide sequences that are fibril-forming

ATVIIE	MTVIIE	SQVIIE	STVIIF	STVTIE
DTVIIE	NFGAIL	SSVIIE	STVIII	STVWIE
ETVIIE	NHVTLS	STEIIE	STVIIL	STVYIE
FLVHSS	NTVIIE	STFIIE	STVIIM	SVVIIE
FTVIIE	QTVIIE	STLIIE	STVIIN	SYVIIE
FYLLYY	SAVIIE	STNIIE	STVIIQ	TTVIIE
GTVIIE	SDVIIE	STQIIE	STVIIS	VEALYL
ITVIIE	SEVIIE	STSIIE	STVIIT	VQIVYK
KDWSFY	SFVIIE	STVEIE	STVIIV	VTVIIE
KIVKWD	SGVIIE	STVFIE	STVIIW	WTVIIE
LLYYTE	SIVIIE	STVIFE	STVIIY	YTVIIE
LTVIIE	SLVIIE	STVIAA	STVIYE	
LVEALY	SMVIIE	STVIID	STVLIE	
LYQLEN	SNVIIE	STVIIE	STVNIE	

Studied decapeptide sequences that are non-fibril forming:

CNDGKTPGAV	HSQWNKPSKP	NHVTLSQPKI	TQYERESQAY
DVRQYVQGCG	KVEHSDLSFS	RTLKRLGMDG	TTTKGENFTE
GIRAWVAWRN	LNCYVSGFHP	RYPNQVYYRP	

Studied decapeptide sequences that are fibril forming:

DLSFSKDWSF	KDWSFYLLYY	SMVLFSSPPV	VHDCVNITIK
ISFLIFLIVG	LANWMCLAKW	SSPPVILLIS	YLLYYTEFTP
ILLISFLIFL	RCELARTLKR	TEFTPTEKDE	