

ID to discriminate every tested sequence		Which method used to select: BO: Bayesian Optimization, GMM: Gaussian Mixture Model	The length of a profile HMM model	The maximum probable pattern generated from profile HMM model. The asterisk indicates insertion.	The maximum probable sequence derived from "max_model"	The log probability of a sequence generated from the profile HMM	Normalized binding affinity of the proposed sequence	The x position where the profile HMM model was taken	The y position where the profile hmm model was taken	The length of the derived sequence	Base pairing probability matrix (upper-right); Secondary structure (lower-left)	Secondary structure calculated by CentroidFold[^1]	Structural profiles calculated by CapR[^2], where the horizontal axis show positions of sequence [^1]: https://doi.org/10.1093/bioinformatics/btn601 [^2]: https://doi.org/10.1186/sb-2014-15-1-r16	Secondary structure calculated by RNAfold[^3]
ID	data	method	target_len	max_model	max_seq	log_proba	normalized	pos_x	pos_y	seq_len	base_paring_probabilities	secondary_structure	CapR	secondary_structure(RNAfold)
A-PC	A				GCGGAGAUUCUGAGGGUUCUCCUGUCCAG		100							
A-BO-3	A	BO	30	GUAGAGAUUCUGAGGGUUCUCCUGUU*CUA	GUAGAGAUUCUGAGGGUUCUCCUGUUGCUA	-14.35	100.6	1.26	-0.43	30				
A-BO-1	A	BO	30	GUUGAGAUUCUGAGGGUUCUCCUGUU*CCC	GUUGAGAUUCUGAGGGUUCUCCUGUUGCCC	-14.42	101.2	1.69	-0.55	30				
A-BO-4	A	BO	30	GUAGAGAUUCUGAGGGUUCUCCUGUU*ACC	GUAGAGAUUCUGAGGGUUCUCCUGUUGACC	-14.42	102.5	1.55	-0.20	30				
A-BO2-8	A	BO	30	GGUAGAGAUUCUGAGGGUUCUCCUGUUACUA	GGUAGAGAUUCUGAGGGUUCUCCUGUUACUA	-16.12	105.8	0.90	-0.44	30				
A-GMM-1	A	GMM	30	GUAGAGAUUCUGAGGGUUCUCCUGCUAUA	GUAGAGAUUCUGAGGGUUCUCCUGCUAUA	-13.33	107.1	1.36	0.22	29				
A-BO2-7	A	BO	30	GUAGAGAUUCUGAGGGUUCUCCUGUUCCA	GUAGAGAUUCUGAGGGUUCUCCUGUUGCCA	-14.43	116.2	1.51	-0.63	30				
A-BO2-2	A	BO	30	GUAGAGAUUCUGAGGGUUCUCCGUUACA	GUAGAGAUUCUGAGGGUUCUCCGUUACA	-13.88	119.8	1.29	-0.08	29				

ID to discriminate every tested sequence		Which method used to select; A: Dataset A, B: Dataset B	The length of a profile HMM model	The maximum probable pattern generated from profile HMM model. The asterisk indicates insertion.	The maximum probable sequence derived from "max_model"	The log probability of a sequence generated from the profile HMM	Normalized binding affinity of the proposed sequence	The x position where the profile HMM model was taken	The y position where the profile HMM model was taken	The length of the derived sequence	Base pairing probability matrix (upper-right); Secondary structure (lower-left)	Secondary structure calculated by CentroidFold["1"]	Structural profiles calculated by CapR["2"], where the horizontal axis show positions of sequence ["2": https://doi.org/10.1186/bio-2014-15-1-r16]	Secondary structure calculated by RNAfold["3"]
ID	data	method	target_len	max_model	max_seq	log_proba	normalized	pos_x	pos_y	seq_len	base_paring_probabilities	secondary_structure	CapR	secondary_structure(RNAfold)
B-PC	B				GCUGUGUCUACGUCCGAUUGGGACCUGCACGGCCAUG		100							
B-BO-8	B	BO	40	U*C*C*CCC*CGCGCACAUUACGCAACACUCCCCCUGCC	UGCGCGCCCGCGCACAUUACGCAACACUCCCCCUGCC	-24.20	134.9	1.55	-0.53	40				
B-BO-9	B	BO	40	U*C*C*CCCAGCGCACAUUACGUAAAACCCCCCUACC	UGCGCGCCCAGCGCACAUUACGUAAAACCCCCCUACC	-23.65	151.6	0.99	-1.17	38				
B-GMM-9	B	GMM	40	U*C*C*CCC*AGCGCACAUUACGAAAAUCCCCCUGCC	UGCGCGCCCGAGCGCACAUUACGCAAAUCCCCCUGCC	-24.47	190.7	1.24	0.07	39				
B-GMM-4	B	GMM	40	U*C*C*CCCAGCGCACAUUACGUAAAACUCCCCCUACC	UGCGCGCCCAGCGCACAUUACGUAAAACUCCCCCUACC	-23.33	229.1	1.10	-0.99	39				
B-BO-4	B	BO	40	U*C*C*CCCAGCGCACAUUACGCAACACUCCCCCUGCC	UGCGCGCCCGAGCGCACAUUACGCAACACUCCCCCUGCC	-23.80	231.0	1.53	-0.81	39				
B-BO-5	B	BO	40	U*C*C*CCC*AGCGCACAUUACGUAAAACUCCCCCUACC	UGCGCGCCCAGCGCACAUUACGUAAAACUCCCCCUACC	-25.79	245.2	1.23	-0.68	40				