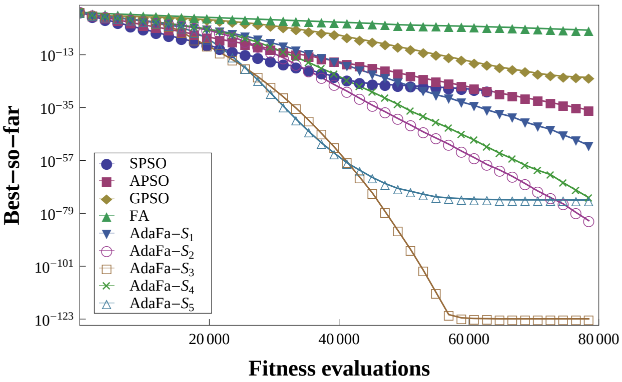
Supplementary Materials
Adaptive Firefly Algorithm: Parameter Analysis and its Application

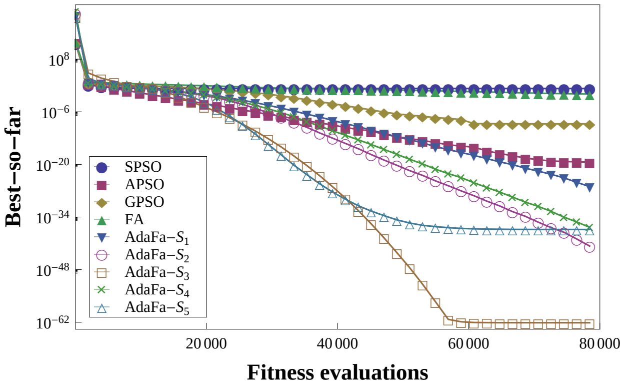
1 Numerical experiments

Table S1: Benchmark Functions

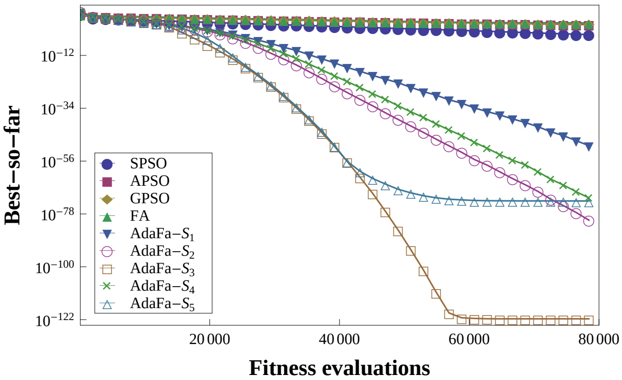
	Test function	Search range	f_{min}
Unimodal	$F_1(X)=\sum_{i=1}^{D} x_i^2$	[-100,100]^D	0
	$F_2(X)=\sum_{i=1}^{D}\lvert x_i\rvert+\prod_{i=1}^{D}\lvert x_i\rvert$	[-10,10]^D	0
	$F_3(X)=\sum_{i=1}^{D}\left(\sum_{j=1}^{i} x_j\right)^2$	[-100,100]^D	0
	$F_4(X)=\sum_{i=1}^{D-1}\left[100(x_i^2-x_{i+1})^2+(x_i-1)^2\right]$	[-10,10]^D	0
	$F_5(X)=\sum_{i=1}^{D}\lfloor x_i+0.5\rfloor^2$	[-100,100]^D	0
	$F_6(X)=\sum_{i=1}^{D} ix_i^4+random[0,1)$	[-1.28,1.28]^D	0
Multimodal	$F_7(X)=\sum_{i=1}^{D}\left(-x_i\sin(\sqrt{\lvert x_i\rvert})\right)$	[-500,500]^D	-418.9829×D
	$F_8(X)=\sum_{i=1}^{D}\left(x_i^2-10\cos(2\pi x_i)+10\right)$	[-5.12,5.12]^D	0
	$F_9(X)=\sum_{i=1}^{D}\left(y_i^2-10\cos(2\pi y_i)+10\right)$ where $y_i=\begin{cases} x_i & \lvert x_i\rvert<0.5 \\ \dfrac{round(2x_i)}{2} & \lvert x_i\rvert\geqslant 0.5\end{cases}$	[-5.12,5.12]^D	0
	$F_{10}(X)= -20exp\left(-0.2\sqrt{\frac{1}{D}\sum_{i=1}^{D} x_i^2}\right) -exp\left(\frac{1}{D}\sum_{i=1}^{D}\cos(2\pi x_i)\right)+20+e$	[-32,32]^D	0
	$F_{11}(X)=\frac{1}{4000}\sum_{i=1}^{D} x_i^2-\prod_{i=1}^{D}\cos(\frac{x_i}{\sqrt{i}})+1$	[-600,600]^D	0
	$F_{12}(X)= \dfrac{\pi}{D}\left\{10\sin^2(\pi y_i)+\sum_{i=1}^{D-1}(y_i-1)^2[1+10\sin^2(\pi y_{i+1})] +(y_D-1)^2\right\}+\sum_{i=1}^{D} u(x_i,10,100,4)$ where $y_i=0.25(x_i+1)+1$, $u(x_i,a,k,m)=\begin{cases} k(x_i-a)^m & x_i\geqslant a \\ 0 & -a<x_i<a \\ k(-x_i-a)^m & x_i<-a\end{cases}$	[-50,50]^D	0



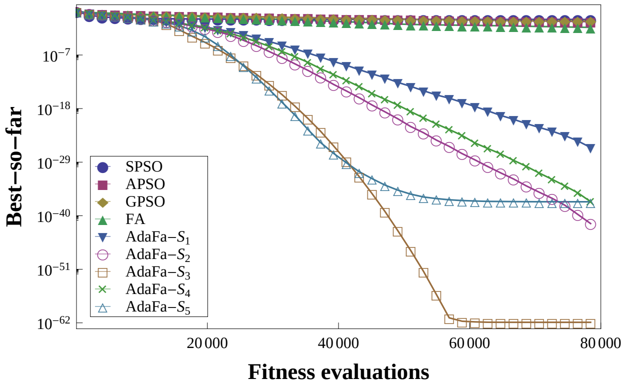
(a) F_1



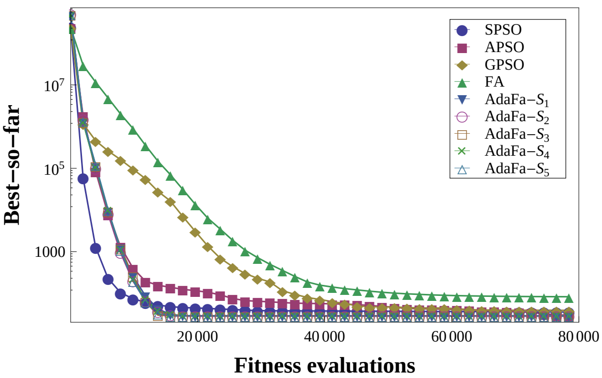
(b) F_2



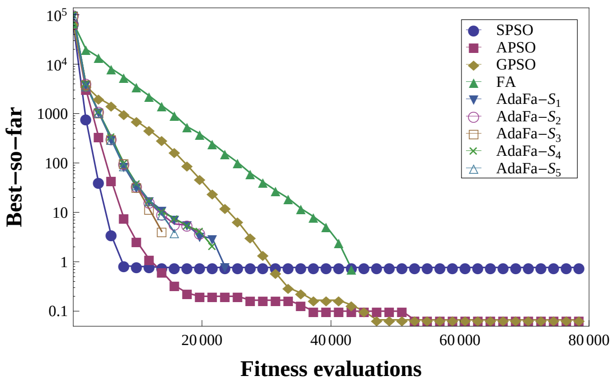
(c) F_3



(d) F_4



(e) F_5



(f) F_6

Fig. S1: The mean value over the benchmark functions with 30-dimensions.

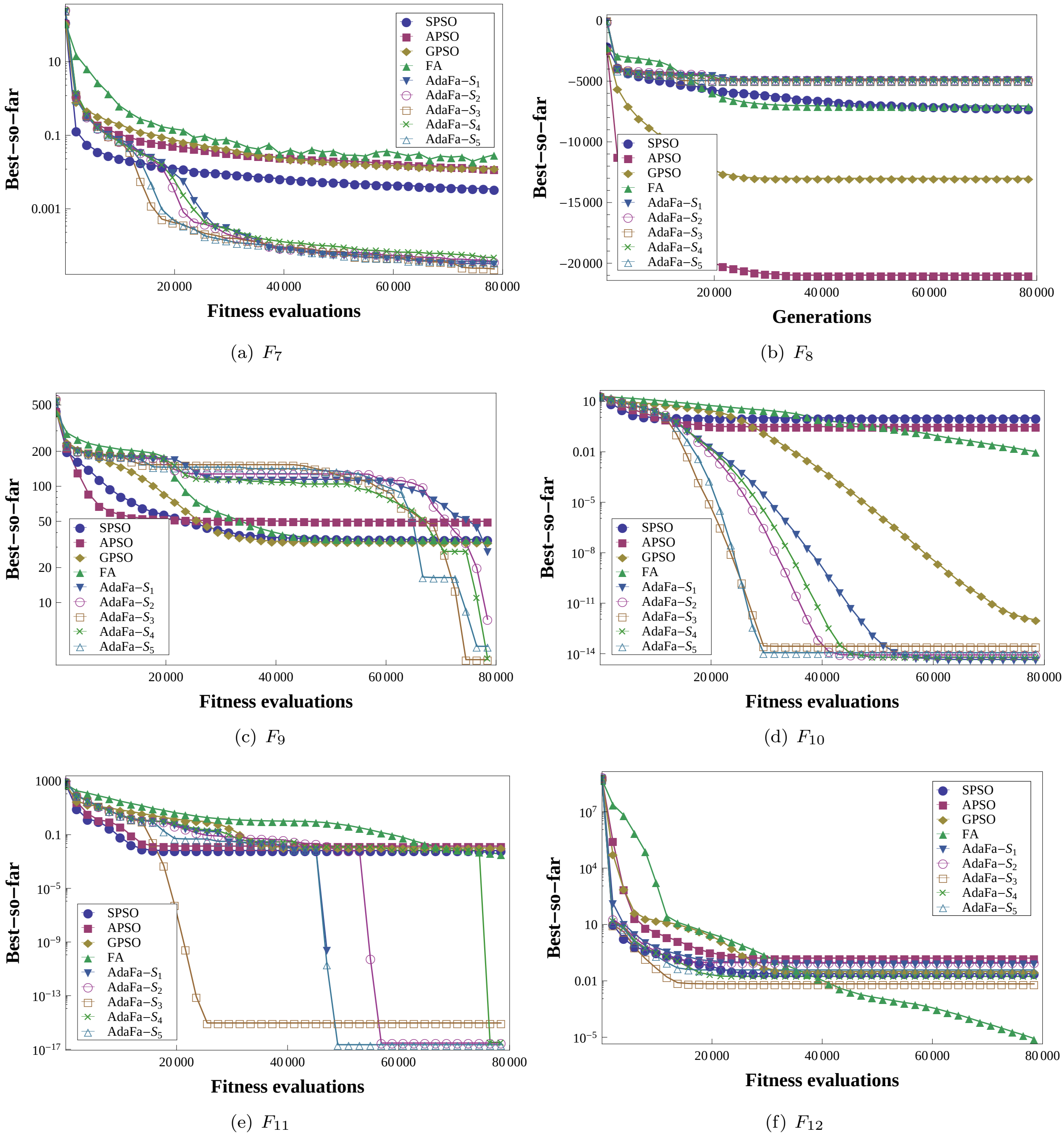


Fig. S1: (*Continue.*) The mean values over the benchmark functions with 30-dimensions.

2 Applications of AdaFa variants

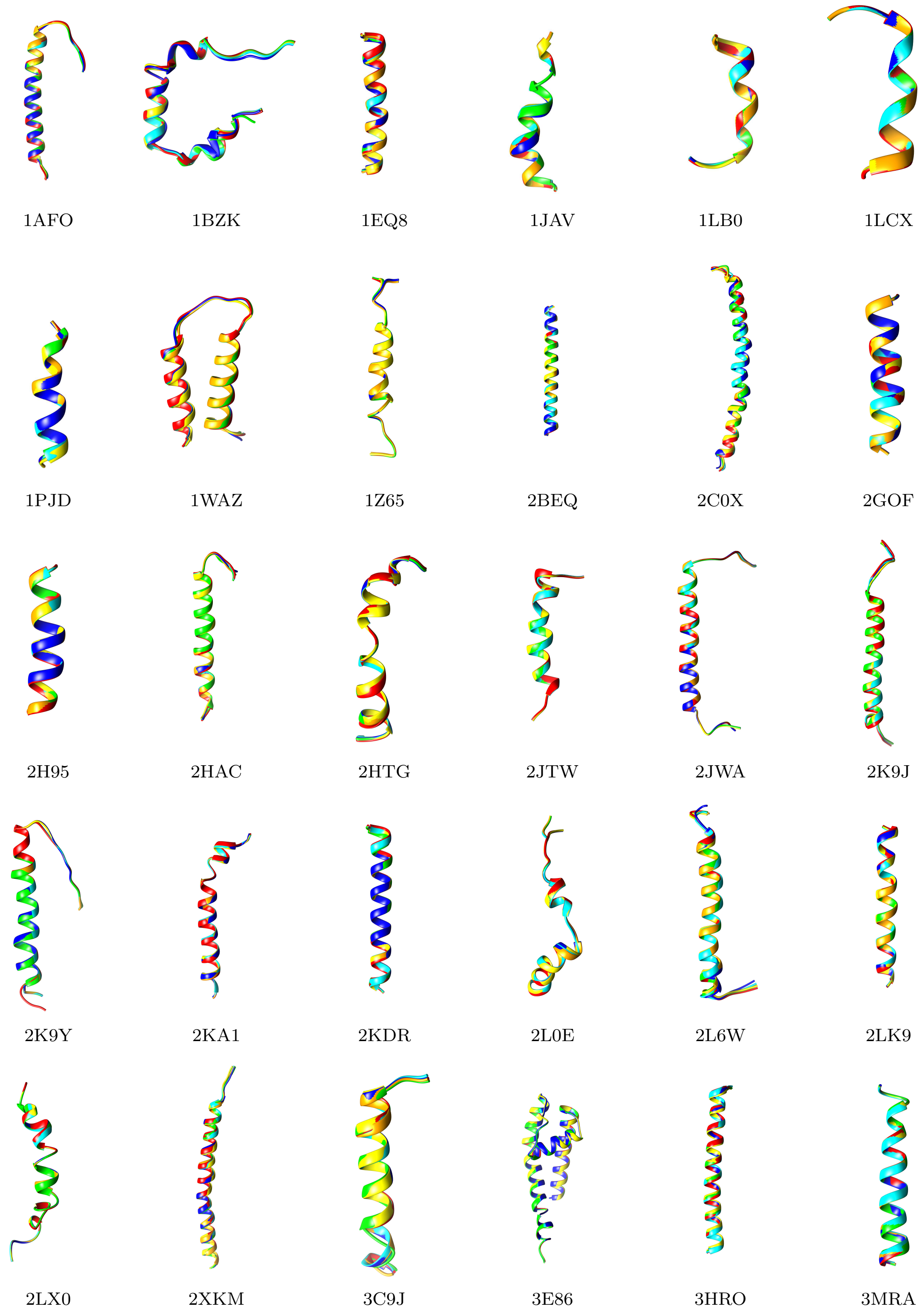


Fig. S2: The similarity between native protein structure (red) and the reconstructed structures (AdaFa-S_1: blue, AdaFa-S_2: green, AdaFa-S_3: yellow, AdaFa-S_4: cyan, AdaFa-S_5: orange).

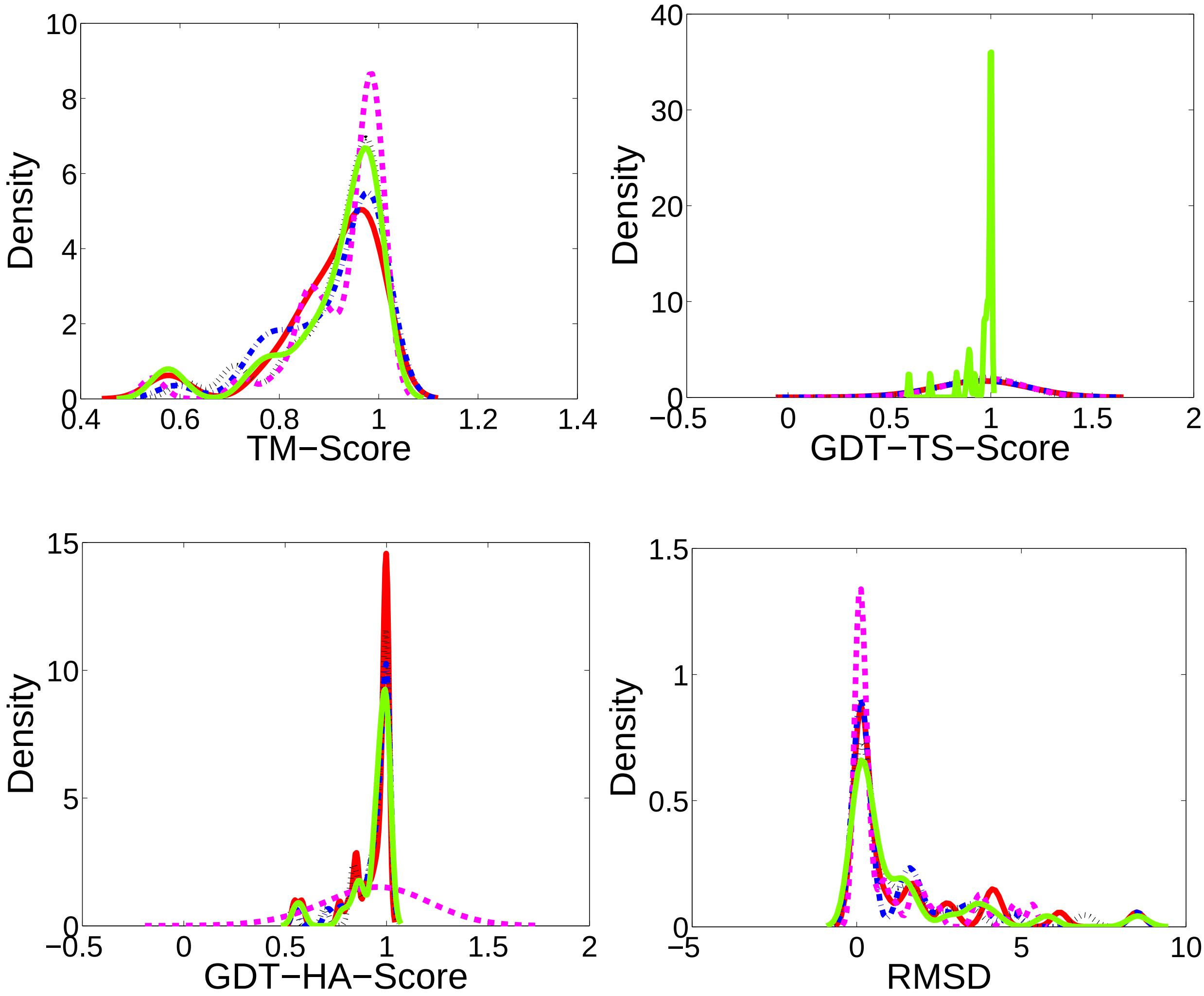


Fig. S3: The kernel smoothing density estimates of (a) TM-Score, (b) GDT-TS-Score, (c) GDT-HA-Score, and (d) RMSD achieved over the constrains with 10% Gaussian white noise. AdaFa-S_1–AdaFa-S_5 were represented by red solid line, black dotted line, blue dotted dashed line, magenta dashed line, and green solid line, respectively