Table S1. Comparison of improved UniSO-N with MLP and with in-context Transformer neural processes (TNP; Nguyen & Grover, 2022) on unconstrained tasks from Design-Bench and SOO-Bench, where the better one is **Bold**. $\mathcal{D}$(best) denotes the best score in the offline dataset. Note that offline BBO differs from online BBO as it evaluates solutions in a single batch rather than iteratively. Therefore, following Nguyen et al. (2024), we first maximize the UCB acquisition function on trained TNP through EA to obtain final candidates.

Task	$\mathcal{D}$(best)	UniSO-N + MLP	UniSO-N + TNP
Ant	165.326	**269.691 ± 77.425**	110.143 ± 229.571
D'Kitty	**199.363**	173.911 ± 46.662	-226.316 ± 317.276
Superconductor	**74.000**	67.333 ± 10.838	58.653 ± 20.171
TF Bind 8	0.439	**0.833 ± 0.005**	0.638 ± 0.000
TF Bind 10	0.005	**0.959 ± 0.115**	0.674 ± 0.000
GTOPX 2	-195.586	**-124.995 ± 56.170**	-183.413 ± 81.862
GTOPX 3	-151.190	**-62.622 ± 22.261**	-180.053 ± 93.678
GTOPX 4	-215.716	**-110.284 ± 17.559**	-130.988 ± 38.336
GTOPX 6	-112.599	**-57.435 ± 18.832**	-108.859 ± 25.493
Avg. Rank	/	**1.000 ± 0.000**	2.000 ± 0.000