*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 |