

# 1 Molecule Design

Method	$N_r^* = 1$	$N_r^* = 5$	$\text{LogP}^* = -2$	$\text{LogP}^* = 10$
No Guidance	$0.118 \pm 0.019$	$0.118 \pm 0.019$	$0.118 \pm 0.019$	$0.118 \pm 0.019$
DG	$0.142 \pm 0.025$	$0.131 \pm 0.016$	$0.111 \pm 0.015$	$0.144 \pm 0.038$
<b>SPS-SC</b>	$0.140 \pm 0.024$	$0.125 \pm 0.018$	$0.121 \pm 0.018$	$0.165 \pm 0.052$
<b>SPS-SD</b>	$0.125 \pm 0.020$	$0.110 \pm 0.017$	$0.107 \pm 0.016$	$0.158 \pm 0.045$

Table 1: **Diversity ( $\downarrow$ ) of Molecular Design.** The diversity is measured by average Tanimoto Similarity ( $\downarrow$ ) of their Morgan fingerprint (using RDKit). SPS-SC and SPS-SD show comparable diversity to the baseline guidance methods.

$A \backslash K$	1	2	4	8	16
1	$0.118 \pm 0.019$	$0.140 \pm 0.024$	$0.138 \pm 0.023$	$0.136 \pm 0.023$	$0.134 \pm 0.022$
2	$0.122 \pm 0.019$	$0.137 \pm 0.024$	$0.136 \pm 0.022$	$0.135 \pm 0.024$	—
4	$0.123 \pm 0.020$	$0.134 \pm 0.023$	$0.135 \pm 0.023$	—	—
8	$0.128 \pm 0.019$	$0.134 \pm 0.022$	—	—	—
16	$0.132 \pm 0.025$	—	—	—	—

Table 2: **Diversity ( $\downarrow$ ) of SPS-SC Across Different Active Size  $A$  and Branch-Out Size  $K$  in Molecular Design** ( $N_r^* = 1$ ).

# 2 DNA Enhancer Design

Method	Class 1	Class 2	Class 3
No Guidance	373	373	373
DG	343	335	331
<b>SPS-G</b>	321	335	358

Table 3: **Diversity ( $\uparrow$ ) of DNA Enhancer Design.** Diversity is measured by the average pairwise Hamming distance ( $\uparrow$ ) of the sampled sequences. SPS-G achieves comparable diversity to the baseline.

$A \backslash K$	1	2	4	8
1	335	333	333	334
2	340	336	337	339
4	330	337	339	339
8	331	335	338	340

Table 4: **Diversity ( $\uparrow$ ) of SPS-G Across Different Active Size  $A$  and Branch-Out Size  $K$  in DNA Enhancer Design.** It’s measured by average pairwise Hamming distance ( $\uparrow$ ). Increasing the active or branch-out size maintains diversity. Results are for Class 2.