Appendix A
Experimental Results on 250K ZINC Dataset

We conducted experiments on the ZINC dataset, which has a larger data size compared to the QM9 dataset. In order to reduce training time, we modified the batch size to 128 during training.

A. *Effect of noise sampling methods on performance.*

TABLE A.1
Effect of noise sampling methods on performance.

Sampling method	Sampling size	Validity ↑	Uniqueness ↑	Novelty ↑	Diversity ↑
Normal	100	**85 (85.00%)**	**80 (94.11%)**	**36 (45.00%)**	0.93
	300	251 (83.60%)	216 (86.05%)	**98 (45.00%)**	0.93
	500	412 (82.40%)	335 (81.31%)	142 (42.39%)	0.93
	700	546 (78.00%)	416 (76.19%)	183 (43.99%)	0.93
	900	703 (78.33%)	501 (71.26%)	218 (43.51%)	0.93
	1000	779 (77.90%)	524 (67.26%)	226 (43.12%)	0.93
Uniform	100	68 (68.00%)	**62 (91.17%)**	**27 (43.54%)**	0.91
	300	**209 (69.67%)**	176 (84.21%)	74 (42.04%)	0.91
	500	343 (68.60%)	251 (73.17%)	101 (40.23%)	0.91
	700	441 (63.00%)	283 (64.17%)	113 (39.92%)	0.91
	900	564 (62.67%)	349 (61.87%)	136 (38.96%)	0.91
	1000	619 (61.90%)	366 (59.12%)	142 (28.79%)	0.91

Table A.1 shows the experimental results using different sampling methods on the ZINC dataset. The batch size for the experiment is 128, and the number of epochs is set to 150. Overall, the results indicate that the use of random sampling methods outperforms uniform sampling. Both validity and uniqueness metrics gradually decrease as the number of samples increases. In terms of novelty, the results of the random sampling method show a less significant decrease with an increasing number of samples, while the results of uniform sampling exhibit a substantial decline. This is consistent with our experimental findings on the QM9 dataset.

B. *Effect of training epochs on performance.*

TABLE A.2
Effect of training epochs on performance.

Epochs	Sampling size	Validity ↑	Uniqueness ↑	Novelty ↑	Diversity ↑
100	100	**79 (79.00%)**	**74 (93.6%)**	26 (35.13%)	0.89
	500	385 (77.00%)	301 (73.95%)	108 (35.88%)	0.89
	1000	723 (72.30%)	446 (61.69%)	**161 (36.10%)**	0.89
150	100	**85 (85.00%)**	**80 (94.11%)**	**36 (45.00%)**	0.93
	500	412 (82.40%)	335 (81.31%)	142 (42.39%)	0.93
	1000	779 (77.90%)	524 (67.26%)	226 (43.12%)	0.93
200	100	**83 (83.00%)**	**76 (91.57%)**	31(40.79%)	0.93
	500	403 (80.60%)	341 (84.62%)	139 (40.76%)	0.93
	1000	753 (75.30%)	552 (73.31%)	**231 (41.85%)**	0.93

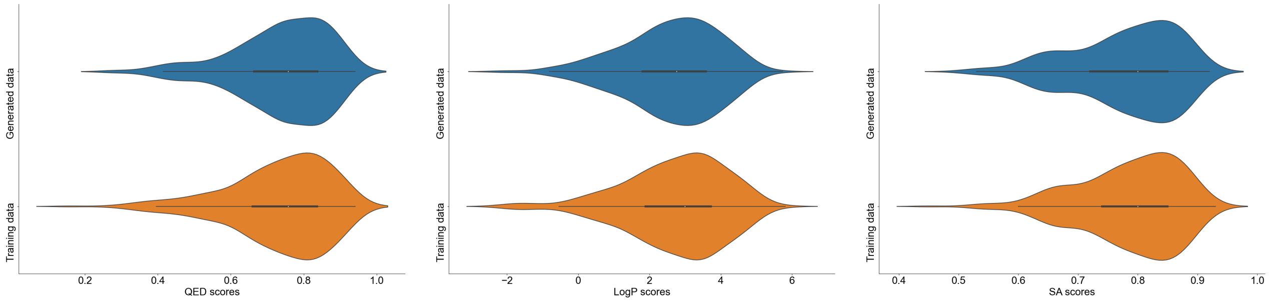
We conducted experiments on the ZINC dataset using epochs sizes of 100, 150, and 200 respectively. The experimental results are presented in Table A.2. All three metrics achieved the best results when the number of epochs was set to 150. Although the dataset is larger compared to QM9, the batch size has also increased. Therefore, the optimal results did not occur at larger epoch sizes.

C. *Effect of training data volumes on performance.*

Similar to the QM9 dataset, we randomly selected 10% of the data from the ZINC dataset as a subset to examine the impact of dataset size on experimental metrics. The results of the experiment are shown in Table A.3. It can be observed that as

TABLE A.3
Effect of training data volumes on performance.

Training data	Sampling size	Validity ↑	Uniqueness ↑	Novelty ↑	Diversity ↑
ZINC_25k	100	**79 (79.00%)**	**69 (87.34%)**	**67 (97.10%)**	0.94
	300	233 (77.66%)	193 (82.83%)	185 (95.85%)	0.94
	500	386 (77.20%)	294 (76.16%)	276 (93.88%)	0.94
	700	536 (76.57%)	387 (72.20%)	365 (94.32%)	0.94
	900	658 (73.11%)	425 (64.58%)	394 (92.71%)	0.94
	1000	723 (72.30%)	453 (62.65%)	412 (90.95%)	0.94
ZINC_250k	100	**85 (85.00%)**	80 (94.11%)	**36 (45.00%)**	0.93
	300	251 (83.60%)	**216 (86.05%)**	**98 (45.00%)**	0.93
	500	412 (82.40%)	335 (81.31%)	142 (42.39%)	0.93
	700	546 (78.00%)	416 (76.19%)	183 (43.99%)	0.93
	900	703 (78.33%)	501 (71.26%)	218 (43.51%)	0.93
	1000	779 (77.90%)	524 (67.26%)	226 (43.12%)	0.93



(a) Drug-likeness (QED) (b) Solubility (LogP) (c) Synthesizability (SA)

Fig. A.1. Distribution plots of QED, LogP, and SA scores on ZINC and generated data.

the training data size increases, the effectiveness and uniqueness metrics improve. However, unlike the previous experiments, novelty decreases with an increase in data size, which is consistent with the earlier findings.

Figure A.1 shows the distribution of QED scores, LogP scores, and SA scores for real molecules and generated molecules. The training data is sourced from ZINC, while the generated data is obtained by sampling under a condition of 1000 samples.

Appendix B
Experimental Results on 5K ZINC Subset

We also conducted experiments on the 5k ZINC dataset, which is a subset of the ZINC dataset consisting of 5,000 molecules. As the latter dataset has a smaller data volume compared to ZINC, we focused on testing the sampling methods and the training epochs.

A. Effect of noise sampling methods on performance.

We reported the experimental results using different sampling methods on the 5k ZINC subset in Table B.1. From the experimental results, it can be observed that due to insufficient training data, the effectiveness and uniqueness of the generated molecules by the model are lower compared to the complete dataset, especially with a significant decrease in uniqueness. Although the percentage of novelty is higher than that of ZINC, this is influenced directly by the volume of training data and the number of generated molecules.

B. Effect of training epochs on performance.

Due to the small size of the dataset itself, we conducted experiments using 15, 30, and 50 epochs respectively. The results of the experiments are shown in Table B.2.When the training data size is reduced, the uniqueness of the generated molecules is lower. This means that the generator has limited knowledge of the original data distribution and can only generate some repetitive data to deceive the discriminator's inspection.

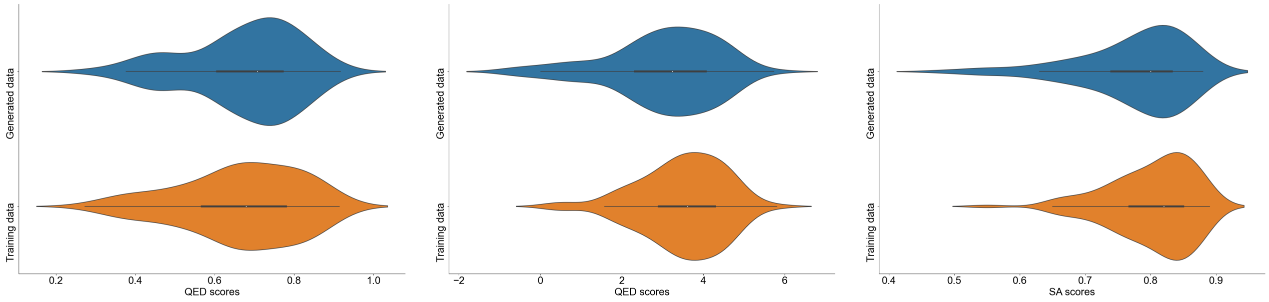
TABLE B.1
EFFECT OF NOISE SAMPLING METHODS ON PERFORMANCE.

Sampling method	Sampling size	Validity ↑	Uniqueness ↑	Novelty ↑	Diversity ↑
Normal	100	62 (62.00%)	30 (48.38%)	**30 (100.00%)**	0.85
	300	198 (66.00%)	89 (44.94%)	**89 (100.00%)**	0.85
	500	**350 (70.00%)**	164 (46.85%)	160 (97.56%)	0.85
	700	446 (63.71%)	**221 (49.55%)**	215 (97.28%)	0.85
	900	606 (67.30%)	276 (45.54%)	253 (91.33%)	0.85
	1000	693 (69.30%)	313 (45.16%)	284 (90.73%)	0.85
Uniform	100	55 (55.00%)	25 (45.46%)	24 (96.00%)	0.83
	300	**183 (67.30%)**	81 (44.26%)	**89 (97.53%)**	0.83
	500	321 (64.20%)	**146 (45.48%)**	138 (94.52%)	0.83
	700	422 (60.28%)	191 (45.26%)	183 (95.81%)	0.83
	900	580 (64.44%)	241 (40.91%)	233 (96.68%)	0.83
	1000	669 (66.90%)	282 (42.15%)	270 (95.74%)	0.83

TABLE B.2
EFFECT OF TRAINING EPOCHS ON PERFORMANCE.

Epochs	Sampling size	Validity ↑	Uniqueness ↑	Novelty ↑	Diversity ↑
15	100	62 (62.00%)	**30 (48.38%)**	**30 (100.00%)**	0.85
	500	**350 (70.00%)**	164 (46.85%)	160 (97.56%)	0.85
	1000	693 (69.30%)	313 (45.16%)	284 (90.73%)	0.85
30	100	65 (65.00%)	32 (49.23%)	**32 (98.46%)**	0.84
	500	331 (66.20%)	**214 (56.91%)**	205 (95.79%)	0.84
	1000	**667 (66.70%)**	346 (47.07%)	329 (95.09%)	0.84
50	100	58 (58.00%)	**30 (51.85%)**	**30 (100.00%)**	0.84
	500	334 (66.80%)	159 (47.60%)	156 (98.11%)	0.83
	1000	**675 (67.50%)**	302 (44.74%)	284 (93.11%)	0.84

Figure B.1 shows the distribution of QED scores, LogP scores, and SA scores for real molecules and generated molecules. The training data is sourced from 5K ZINC, while the generated data is obtained by sampling under a condition of 1000 samples.



(a) Drug-likeness (QED)

(b) Solubility (LogP)

(c) Synthesizability (SA)

Fig. B.1. Distribution plots of QED, LogP, and SA scores on 5K ZINC and generated data.