Table 2: Large molecule generation performance. Only iterative denoising-based methods are reported here. Respective full versions in Tab. 10 (Guacamol) and Tab. 9 (MOSES), Appendix G.3.

	Guacamol					MOSES						
Model	Val. ↑	V.U. ↑	V.U.N.↑	KL div ↑	FCD ↑	Val. ↑	Unique. ↑	Novelty ↑	Filters ↑	FCD ↓	SNN ↑	Scaf ↑
Training set	100.0	100.0	0.0	99.9	92.8	100.0	100.0	0.0	100.0	0.01	0.64	99.1
DiGress (Vignac et al., 2022)	85.2	85.2	85.1	92.9	68.0	85.7	**100.0**	95.0	97.1	**1.19**	0.52	14.8
DisCo (Xu et al., 2024)	86.6	86.6	86.5	92.6	59.7	88.3	**100.0**	**97.7**	95.6	1.44	0.50	15.1
Cometh (Siraudin et al., 2024)	98.9	98.9	97.6	96.7	72.7	90.5	99.9	92.6	**99.1**	1.27	0.54	16.0
DeFoG (10% steps)	91.7	91.7	91.2	92.3	57.9	83.9	99.9	96.9	96.5	1.87	0.50	**23.5**
DeFoG	**99.0**	**99.0**	**97.9**	**97.7**	**73.8**	**92.8**	99.9	92.1	98.9	1.95	**0.55**	14.4