Table 1: Hyperparameter Ablation

Methods	Vina Score(↓)	Vina Min(↓)	QED(↑)	SA(↑)
	Avg.	Avg.	Avg.	Avg.
BFM(ζ=0)	-5.77	-6.76	0.47	0.54
PFM(ζ=0.5)	-6.68	-7.48	0.48	0.48
PFM(ζ=1)	-6.78	-7.25	0.48	0.52
PFM(ζ=1.5)	-7.12	-7.58	0.49	0.51

Table 2: Additional Evaluation

Methods	ClashRatio(↓)		RMSD(↑)	SE(↓)			Similarity(↓)	Validity(↑)	Uniqueness(↑)	#Atoms/mol.
	CCA	CM	%<2A	25%	50%	75%	Avg.	Avg.	Avg.	Avg.
Ref	-	-	34.0	34	107	196	-	100%	-	22.8
LiGAN	**0.0096**	**0.0718**	**43.8**	212	619	1855	0.22	-	87.28%	19.7
GraphBP	0.8634	0.9974	-	**46**	**105**	464	**0.15**	-	100%	23.1
Pocket2Mol	0.0576	0.4499	30.8	102	189	**374**	0.26	**98.31%**	100%	17.7
TargetDiff	0.0483	0.4920	29.4	369	1243	13871	0.30	90.35%	99.63%	24.2
DecompDiff	0.0462	0.5248	23.9	379	983	4133	0.34	71.96%	99.99%	20.9
IPDiff	0.0313	0.3463	-	600	2720	6299	0.18	88.16%	100%	24.5
PFM	0.0145	0.2040	36.7	229	783	1708	0.20	95.12%	100%	22.6

Table 3:Distribution of different ring sizes

Methods	3-Ring	4-Ring	5-Ring	6-Ring	7-Ring	8-Ring
Ref	0.0130	0.0020	0.2855	0.6894	0.0098	0.0003
LiGAN	0.2238	0.0698	0.2599	0.4049	0.0171	0.0096
GraphBP	0.0000	0.2429	0.1922	0.1765	0.1533	0.1113
Pocket2Mol	0.0000	0.1585	0.1822	0.4373	0.1410	0.0478
TargetDiff	0.0000	0.0188	0.2856	0.4918	0.1209	0.0298
DecompDiff	0.0302	0.0378	0.3407	0.4386	0.1137	0.0196
IPDiff	0.0000	0.0206	0.2573	0.4327	0.1794	0.0509
PFM	0.0000	0.1291	0.2567	0.5010	0.0748	0.0307

Table 4: Performance Before and After Perturbation

Methods	**Vina Score(↓)**	**Vina Min(↓)**	**QED(↑)**	**SA(↑)**
	Avg.	Avg.	Avg.	Avg.
BFM(FM LOSS)	-4.27	-6.04	0.46	0.50
BFM(TOTAL LOSS)	-5.77	-6.76	0.47	0.54
PFM(FM LOSS)	-6.48	-6.79	0.43	0.57
PFM(TOTAL LOSS)	-7.12	-7.58	0.49	0.51