

Table 13. Sci-Design

Methods	Molecule	Regex	RFP	ZINC
$\mathcal{D}(\text{best})$	2.26	2.78	3.75	4.01
End-to-End	2.68 ± 0.11	2.80 ± 0.00	3.79 ± 0.00	/
End-to-End + GradNorm	1.03 ± 0.03	2.80 ± 0.00	4.09 ± 0.24	/
End-to-End + PcGrad	1.59 ± 0.58	2.80 ± 0.00	3.84 ± 0.00	4.04 ± 0.04
Multi-Head	1.63 ± 0.51	2.80 ± 0.00	<u>4.06 ± 0.29</u>	<u>4.16 ± 0.00</u>
Multi-Head + GradNorm	1.24 ± 0.13	2.38 ± 0.00	3.75 ± 0.00	3.82 ± 0.00
Multi-Head + PcGrad	1.04 ± 0.02	2.80 ± 0.00	3.76 ± 0.01	3.90 ± 0.02
Multiple Models	2.39 ± 0.57	2.80 ± 0.00	3.86 ± 0.00	4.16 ± 0.00
Multiple Models + COMs	2.39 ± 0.00	2.55 ± 0.17	3.70 ± 0.01	3.97 ± 0.10
Multiple Models + RoMA	1.82 ± 0.00	/	/	3.95 ± 0.00
Multiple Models + IOM	/	/	/	/
Multiple Models + ICT	<u>2.66 ± 0.00</u>	/	/	4.05 ± 0.02
Multiple Models + Tri-Mentoring	2.03 ± 0.00	/	/	3.94 ± 0.00
MOBO	2.22 ± 0.08	5.12 ± 0.17	3.77 ± 0.00	4.26 ± 0.00
MOBO-ParEGO	2.16 ± 0.00	<u>3.83 ± 0.00</u>	/	4.05 ± 0.02
MOBO-JES	2.10 ± 1.04	N/A	N/A	N/A