MHG-GNN: Combination of Molecular Hypergraph Grammar with Graph Neural Network (Supplementary Material)

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A Supplementary Material

A.1 Detailed Performance

Table 1: Performance on various downstream tasks (test datasets, R^2 score)

Method		Polymer			Photoresist		Chromophore
		Density	Bulk modulus	Refractive index	HOMO	LUMO	λ_{max} on NIR
MHG-GNN$_3$	(1024)	0.578	0.523	0.863	0.884	0.835	0.793
MHG-GNN$_5$	(1536)	0.503	**0.528**	0.863	0.890	0.838	0.828
MHG-GNN$_6$	(1792)	**0.588**	0.516	0.863	0.885	0.845	0.832
MHG-GNN$_7$	(2048)	0.577	0.522	**0.866**	**0.896**	**0.848**	**0.845**
MHG-GNN$_8$	(2304)	0.566	0.520	0.865	0.885	0.841	0.813
MHG-GNN	(selected)	0.578	0.516	0.865	0.896	0.845	0.845
ECFP6	(1024)	0.523	0.482	0.823	0.791	0.782	0.708
Mordred	(1613)	0.567	0.505	0.859	0.894	0.830	0.842

Table 1 comprehensively shows R^2 scores calculated with the test datasets. The size of the latent space is denoted next to each model name. The numbers showing the best performance are marked in bold. The performance of MHG-GNN selected is also shown.

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