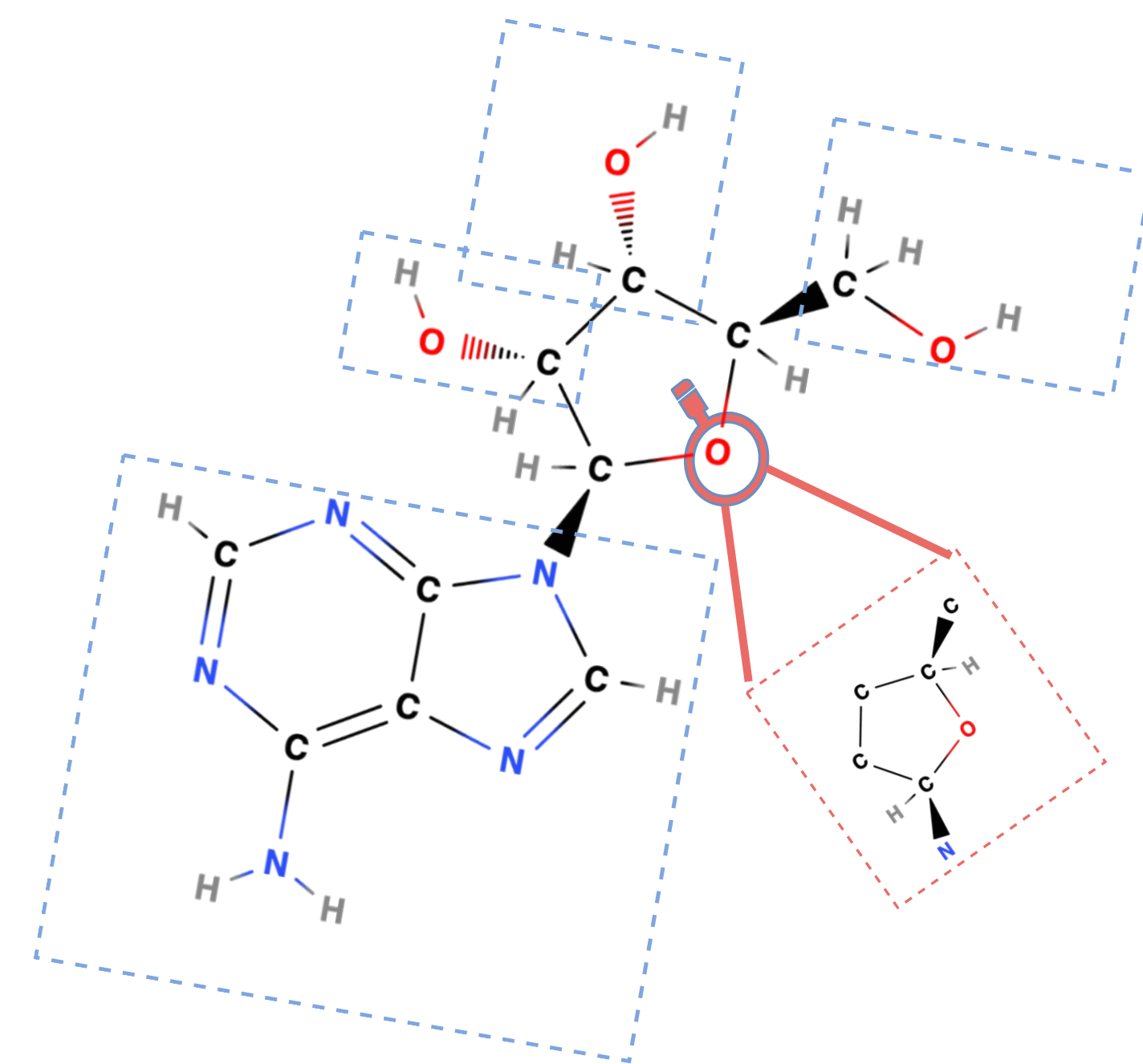
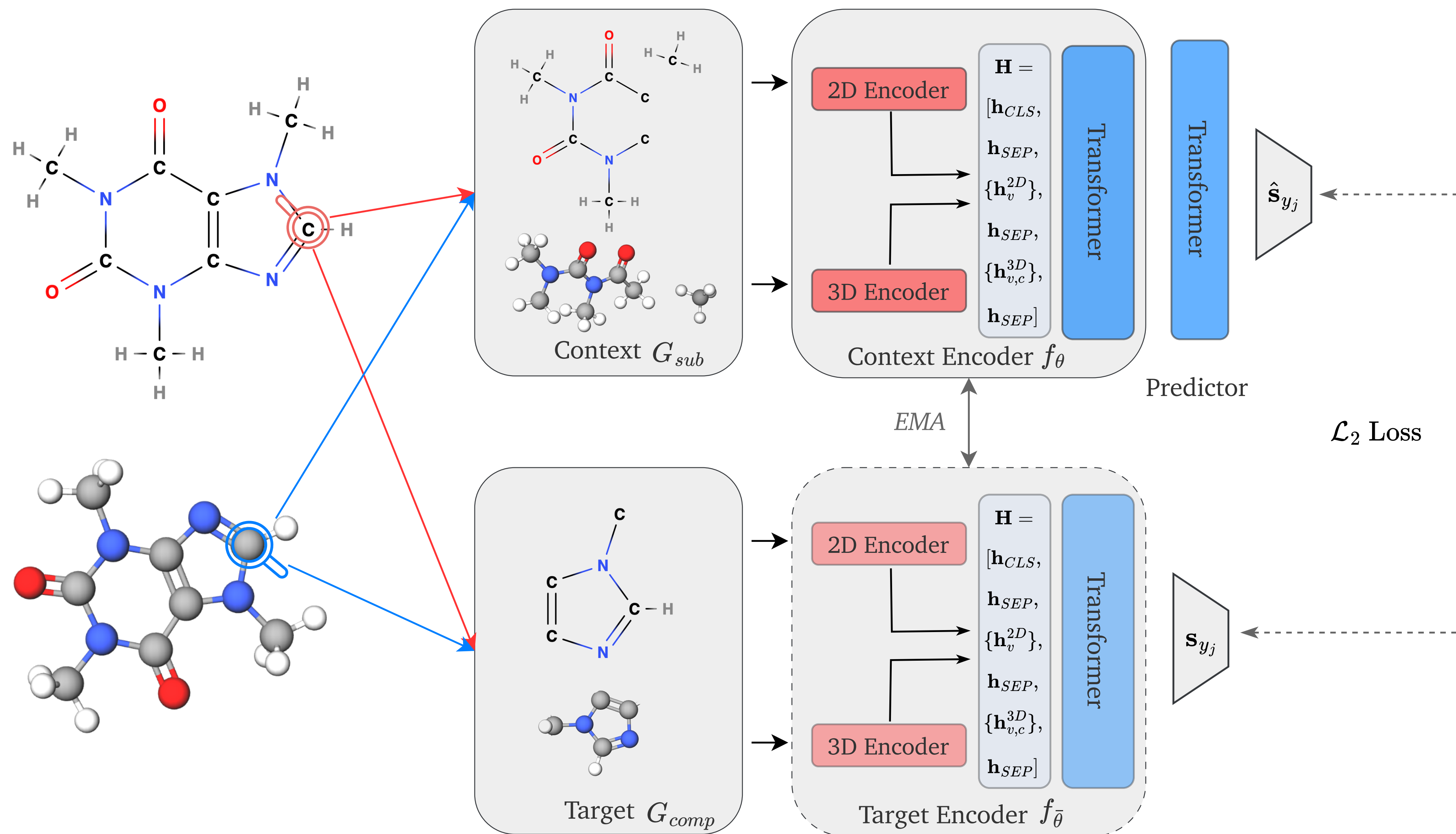


Learning the Neighborhood: Contrast-Free Multimodal Self- Supervised Molecular Graph Pretraining



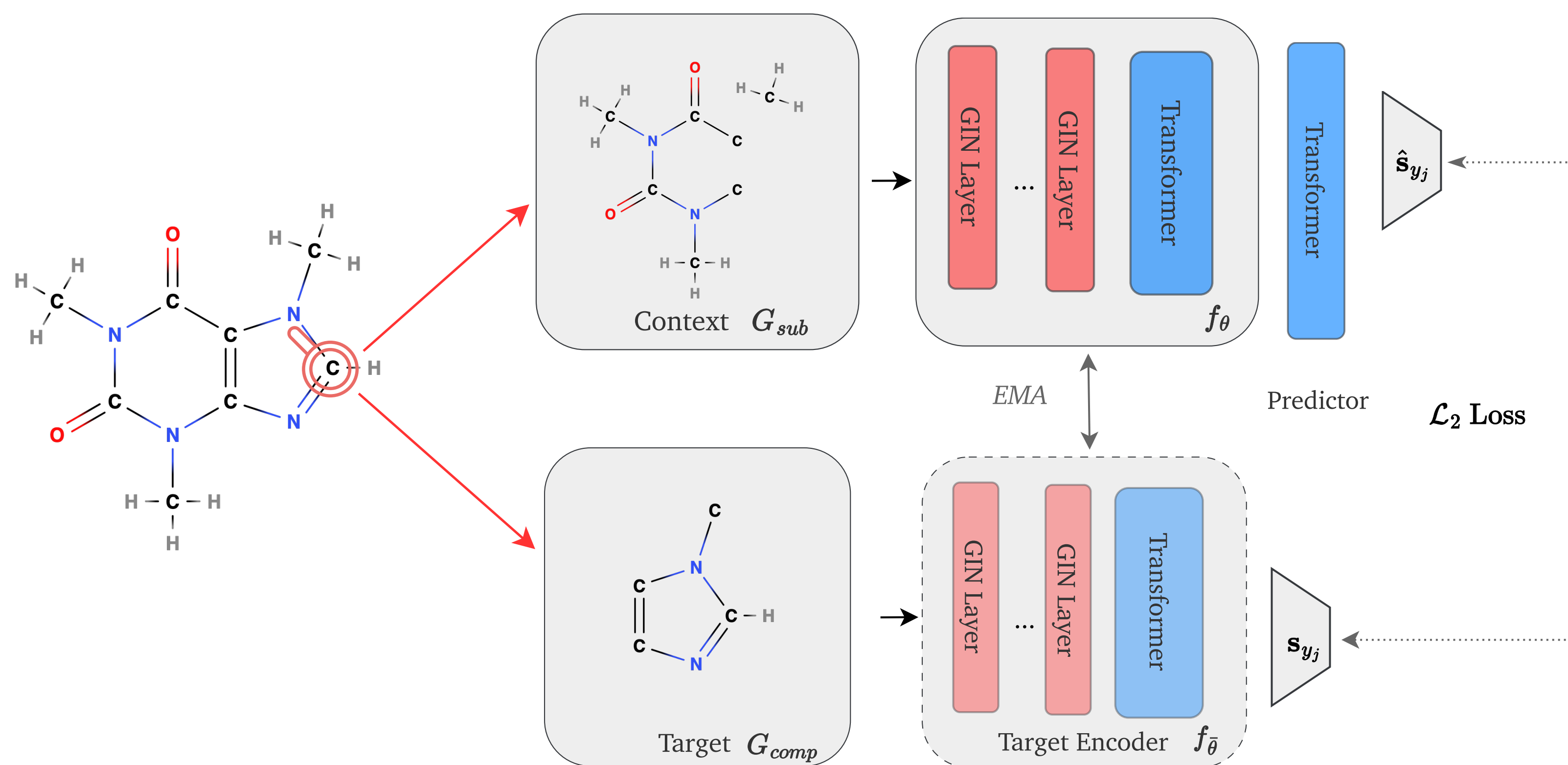
Boshra Ariguib, Mathias Niepert, Andrei Manolache

Contrast-Free Multimodal Self-Supervised Pre-training (C-FREE)



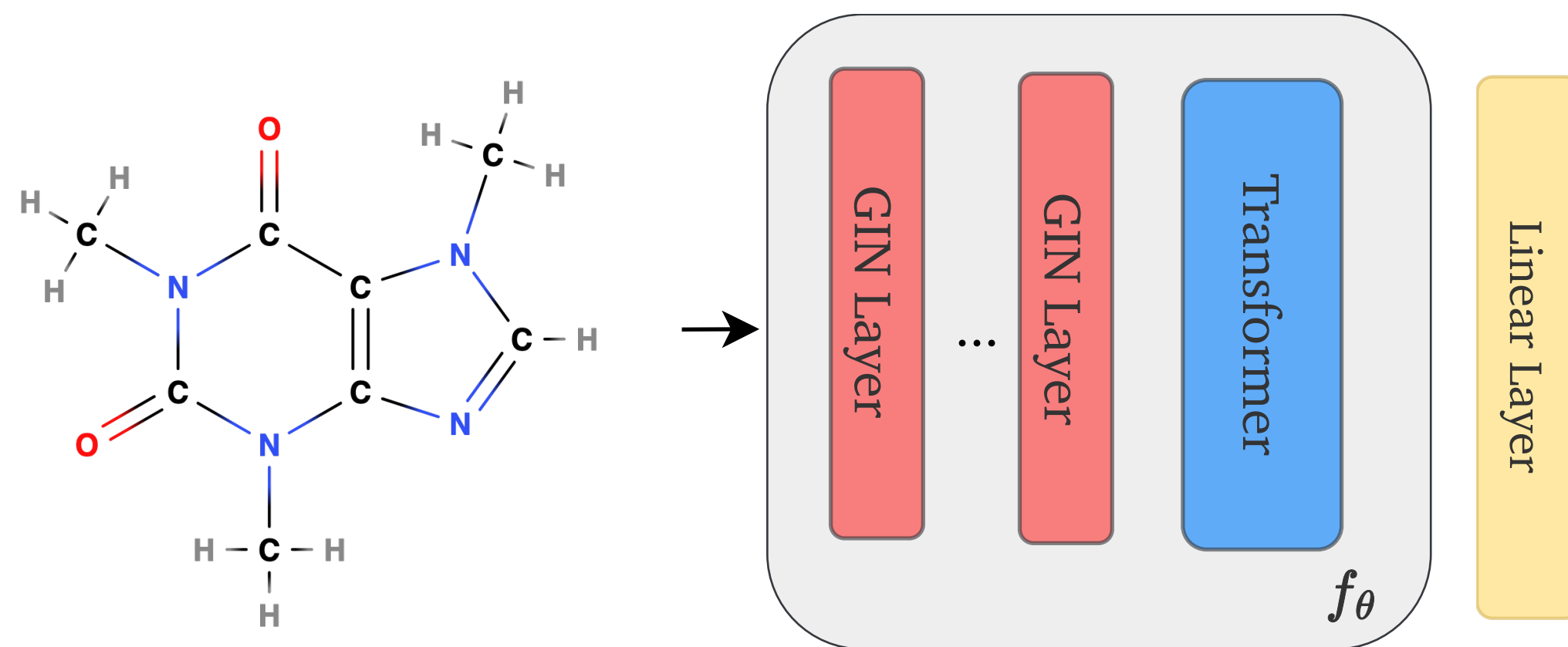
Contrast-Free Self-Supervised Pre-training

The 2D Pipeline



Contrast-Free Self-Supervised Pre-training

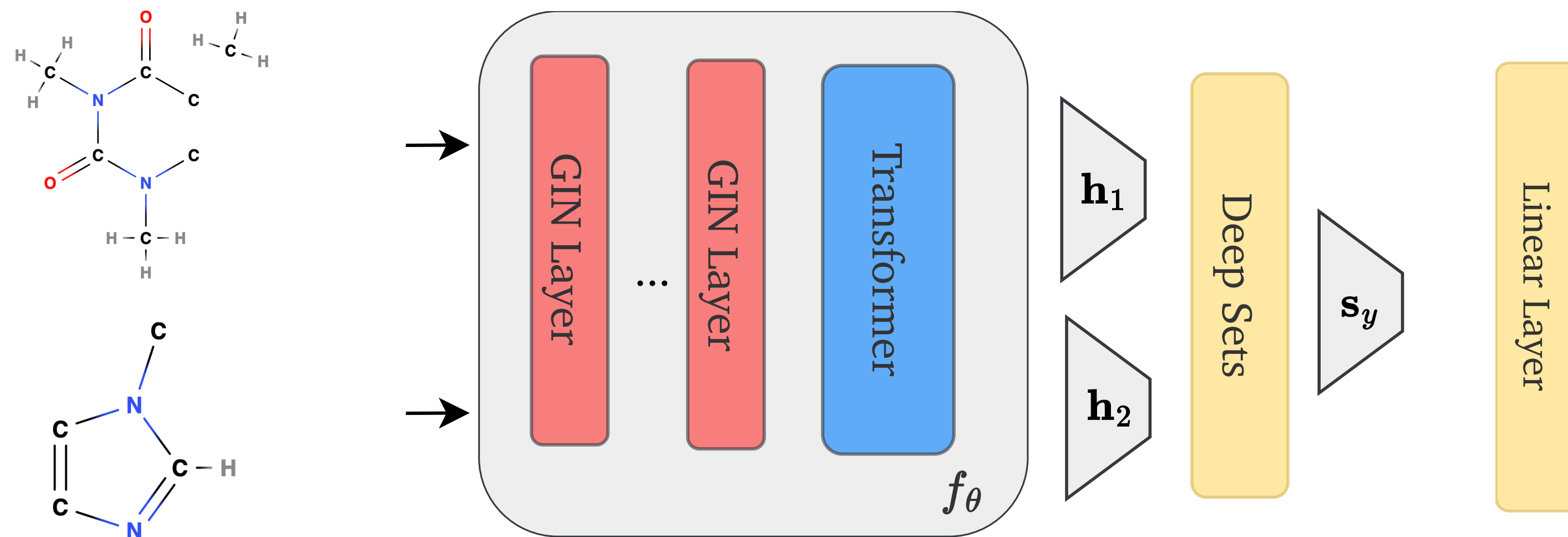
Downstream Task: Linear Head



Full Molecule Evaluation

Contrast-Free Self-Supervised Pre-training

Downstream Task: Deep Sets



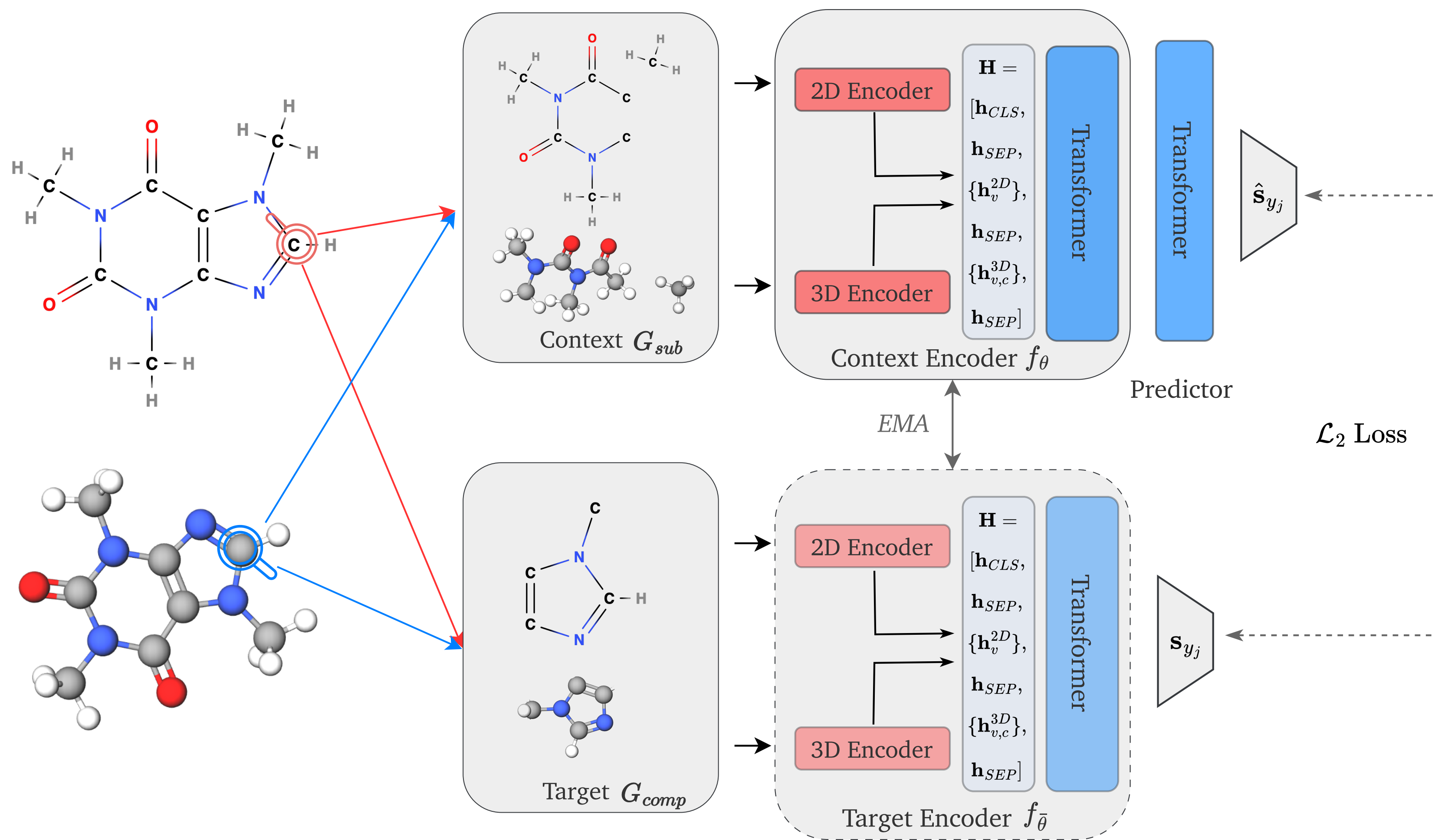
Contrast-Free Self-Supervised Pre-training

Results: Linear Evaluation

		MOLECULENET DATASETS							
		BBBP (↑)	Tox21 (↑)	ToxCast (↑)	SIDER (↑)	CLINTOX (↑)	HIV (↑)	BACE (↑)	AVG (↑)
RANDOM INIT.		50.7 $\pm$ 2.5	64.9 $\pm$ 0.5	53.2 $\pm$ 0.3	53.2 $\pm$ 1.1	63.1 $\pm$ 2.3	66.1 $\pm$ 0.7	63.4 $\pm$ 1.8	59.2
CL	INFOGRAPH	65.9 $\pm$ 0.6	65.8 $\pm$ 0.7	54.6 $\pm$ 0.1	57.2 $\pm$ 1.0	61.4 $\pm$ 4.8	71.4 $\pm$ 0.6	67.4 $\pm$ 4.9	63.4
	GROVER	67.0 $\pm$ 0.3	63.9 $\pm$ 0.3	53.6 $\pm$ 0.4	59.9 $\pm$ 1.7	65.0 $\pm$ 6.4	67.8 $\pm$ 1.0	69.0 $\pm$ 4.7	63.7
	GRAPHCL	64.7 $\pm$ 1.7	69.1 $\pm$ 0.5	56.2 $\pm$ 0.2	59.5 $\pm$ 0.9	60.8 $\pm$ 3.0	72.5 $\pm$ 1.4	77.0 $\pm$ 1.7	65.7
	JOAO	66.1 $\pm$ 0.8	68.1 $\pm$ 0.2	55.1 $\pm$ 0.4	58.3 $\pm$ 0.3	65.3 $\pm$ 6.1	73.8 $\pm$ 1.2	71.1 $\pm$ 0.8	65.4
	GRAPHMVP	69.2 $\pm$ 1.8	63.8 $\pm$ 0.3	55.5 $\pm$ 0.3	58.6 $\pm$ 0.4	58.7 $\pm$ 1.9	68.6 $\pm$ 1.0	73.3 $\pm$ 4.7	64.0
NON-CL	EDGE PRED	54.2 $\pm$ 1.0	66.2 $\pm$ 0.2	54.4 $\pm$ 0.1	56.1 $\pm$ 0.1	65.4 $\pm$ 5.0	73.6 $\pm$ 0.4	71.4 $\pm$ 1.2	63.0
	ATTR MASK	62.7 $\pm$ 2.7	65.7 $\pm$ 0.8	56.1 $\pm$ 0.2	58.3 $\pm$ 1.5	61.9 $\pm$ 6.4	65.5 $\pm$ 1.4	64.8 $\pm$ 2.6	62.1
	GPT-GNN	62.0 $\pm$ 0.9	64.9 $\pm$ 0.7	55.4 $\pm$ 0.2	55.3 $\pm$ 0.8	55.0 $\pm$ 5.1	71.2 $\pm$ 1.5	61.0 $\pm$ 1.2	60.7
	CONT. PRED	55.5 $\pm$ 2.0	67.9 $\pm$ 0.7	54.0 $\pm$ 0.3	57.1 $\pm$ 0.5	67.4 $\pm$ 4.3	66.2 $\pm$ 1.5	54.4 $\pm$ 3.2	60.4
	C-FREE _{LIN}	60.5 $\pm$ 1.7	76.1 $\pm$ 0.2	62.7 $\pm$ 0.4	59.0 $\pm$ 0.6	62.7 $\pm$ 1.0	68.7 $\pm$ 0.4	75.8 $\pm$ 0.9	66.6
	C-FREE _{DS}	64.2 $\pm$ 3.8	76.7 $\pm$ 0.6	63.9 $\pm$ 0.3	58.0 $\pm$ 0.7	71.4 $\pm$ 3.7	65.5 $\pm$ 0.6	73.9 $\pm$ 0.7	67.7

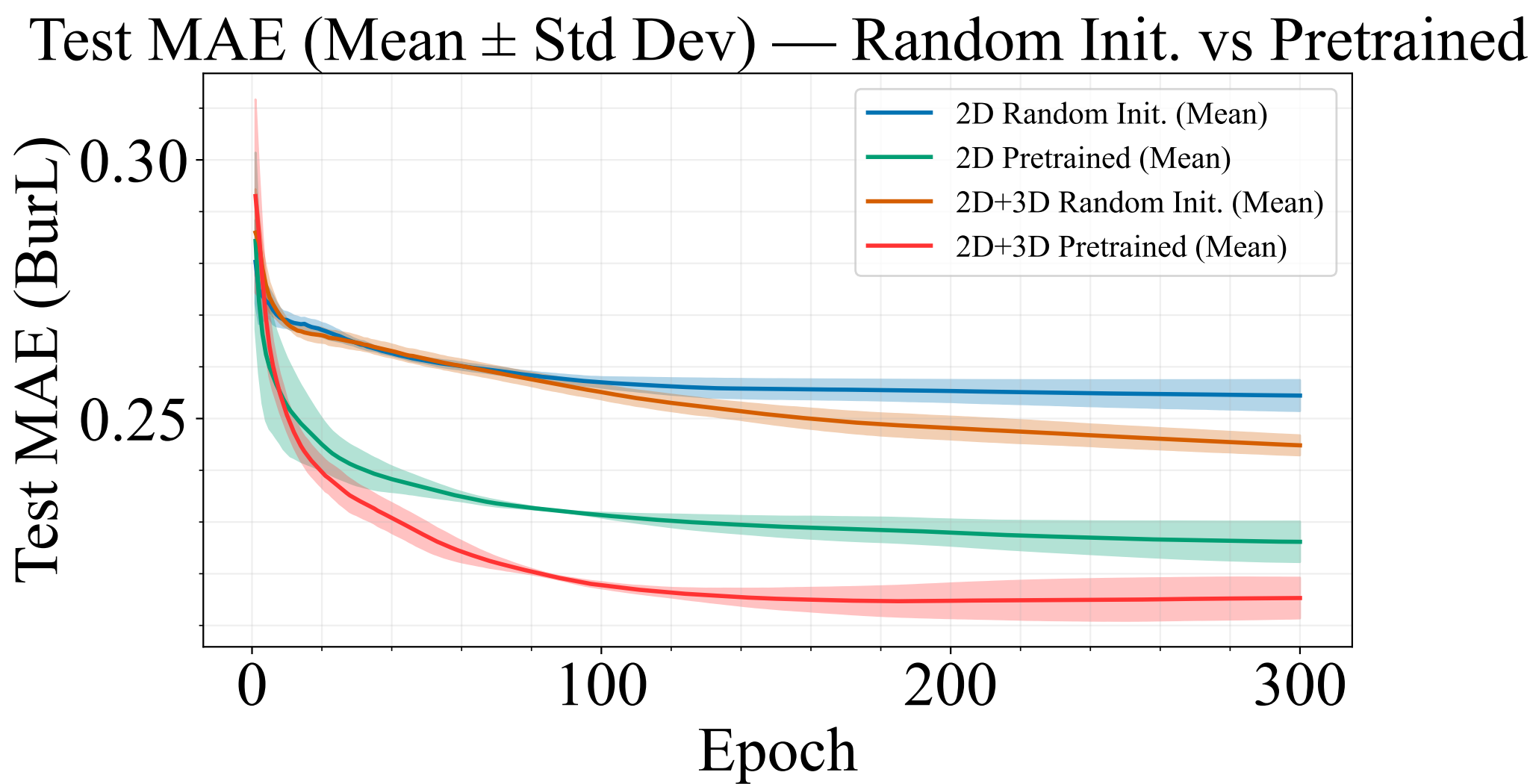
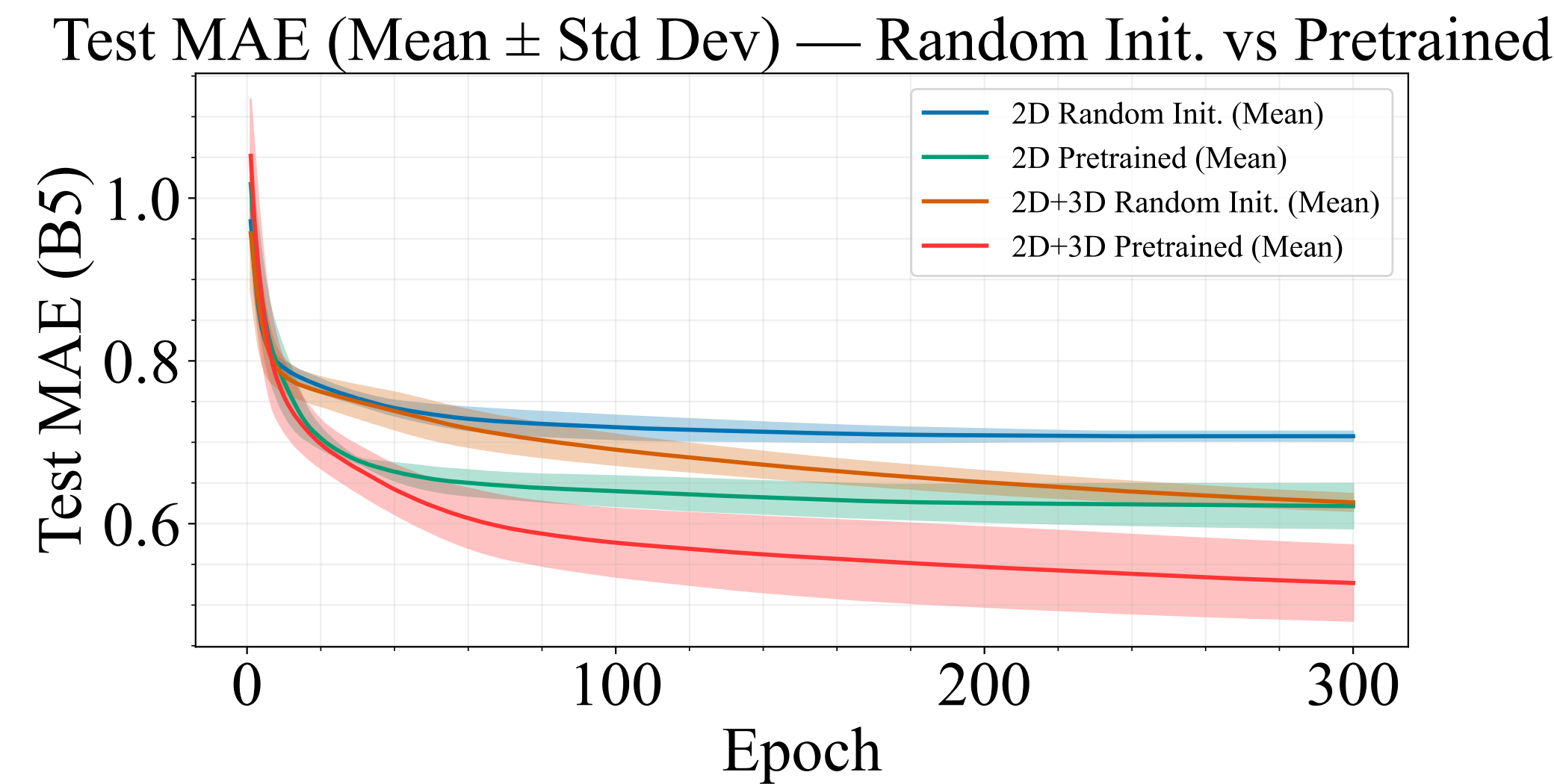
Contrast-Free **Multimodal** Self-Supervised Pre-training

Final Pipeline



Contrast-Free **Multimodal** Self-Supervised Pre-training

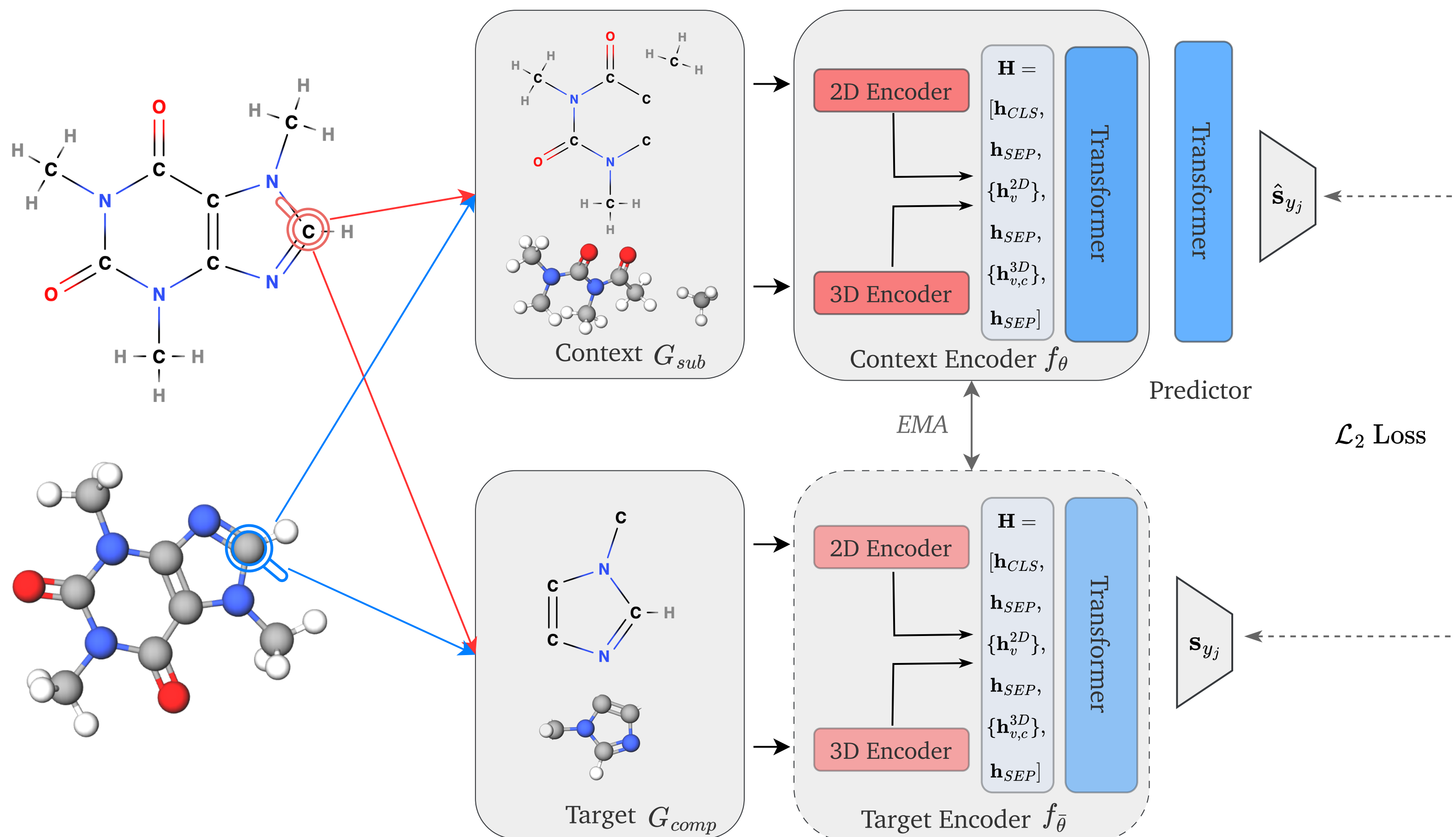
Results: Full Fine-Tuning



Contrast-Free Multimodal Molecular Self-Supervised Graph Pre-training

Efficient
Downstream
Performance

Transferrable
Representations



No Negatives

No Reconstruction



See you in South Korea!