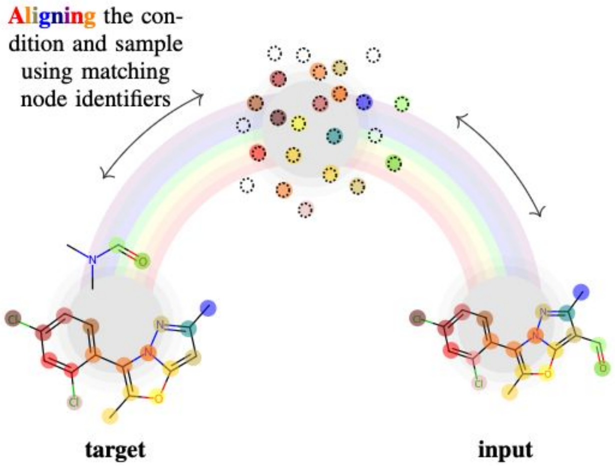
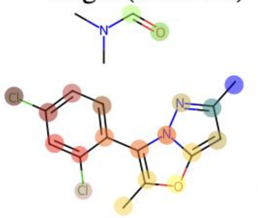
Equivariant Denoisers Cannot Copy Graphs: Align Your Graph Diffusion Models!

Najwa Laabid*, Severi Rissanen*, Markus Heinonen, Arno Solin, Vikas Garg.



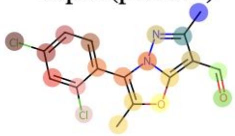
Problem: Graph Translation using Graph diffusion

Target (reactants)



$\mathbf{x}_0$

Input (product)



$\mathbf{Y}$

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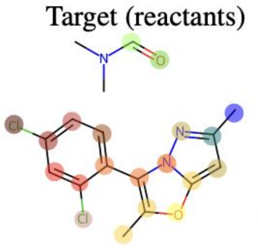

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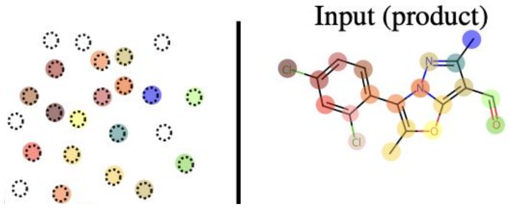

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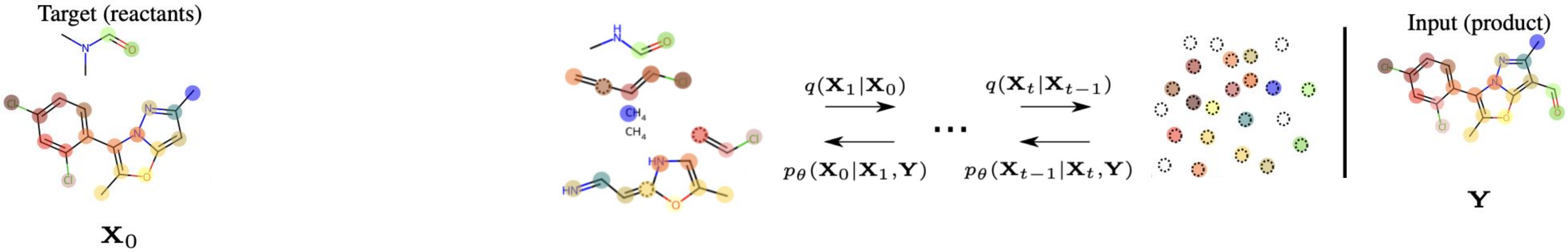

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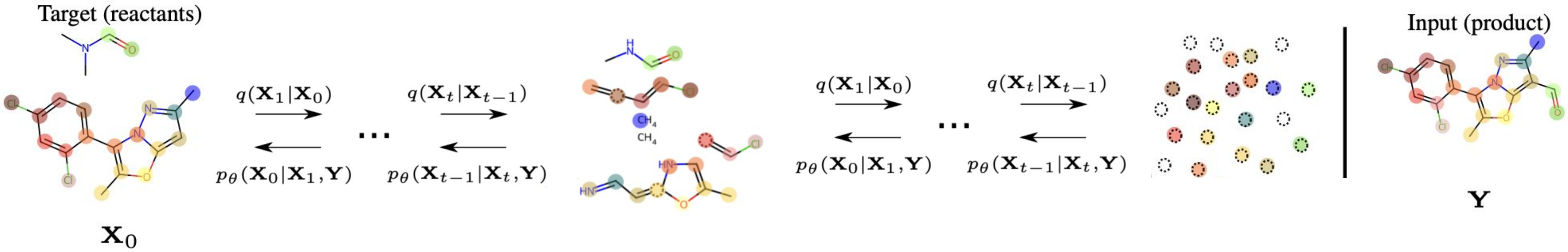

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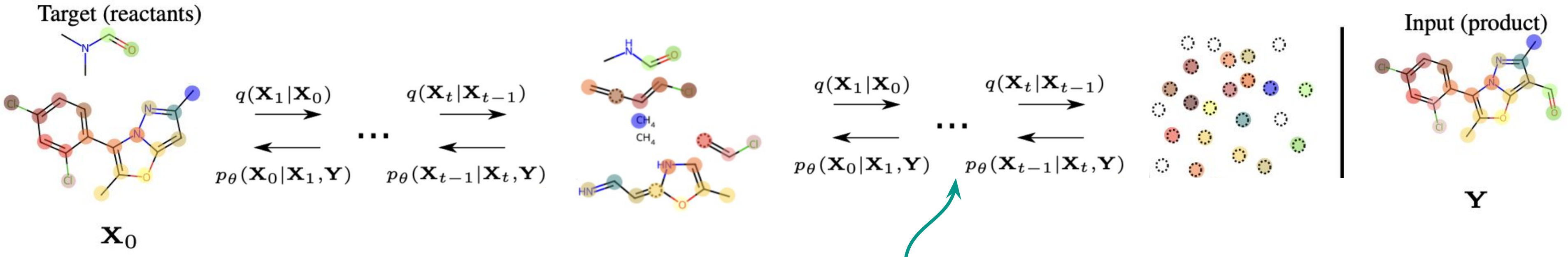

$$= \sum_{\mathbf{X}_0} q(\mathbf{X}_0|\mathbf{X}_T,\mathbf{X}_0)\, p_\theta(\mathbf{X}_0|\mathbf{X}_T,\mathbf{Y},\mathbf{P}^{\mathbf{Y}\to\mathbf{X}})$$

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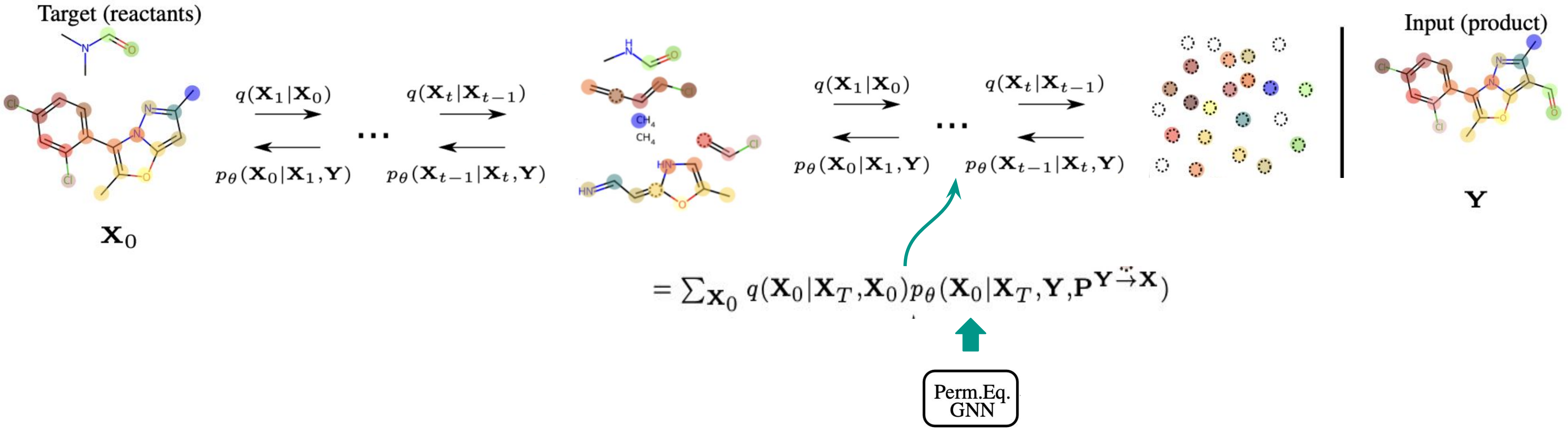

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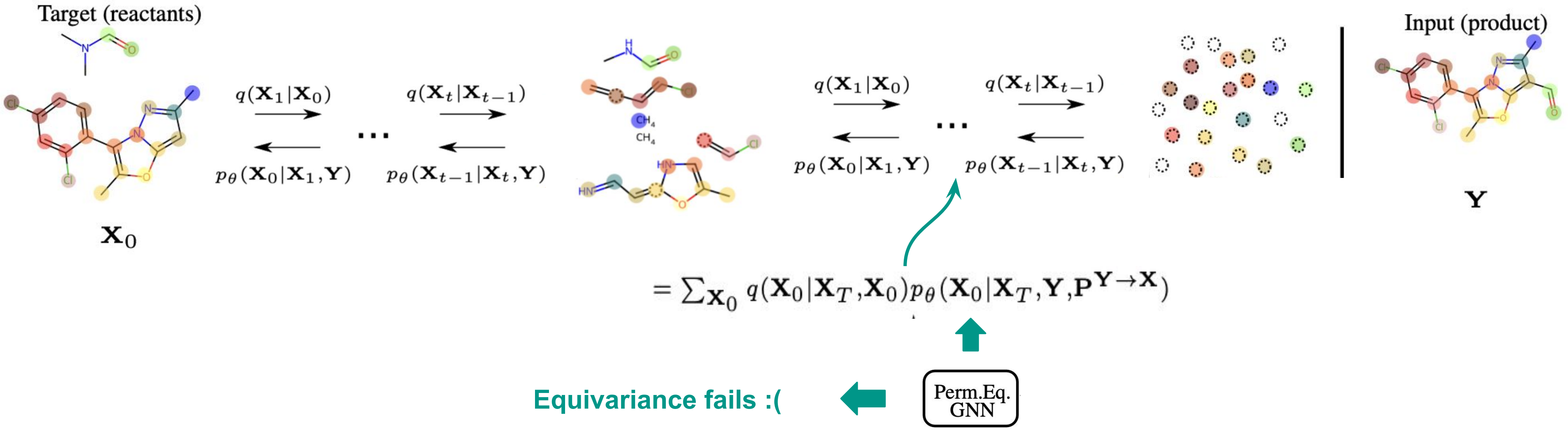
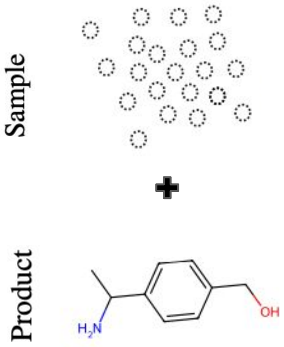


Why does the Equivariant Denoiser Fail?



● = blank ◌ = absorbing

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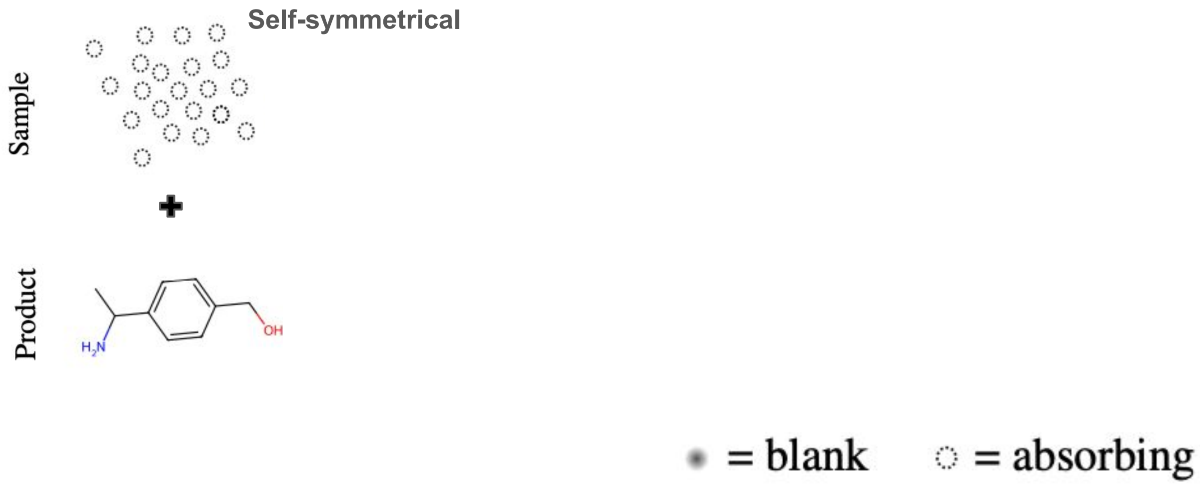

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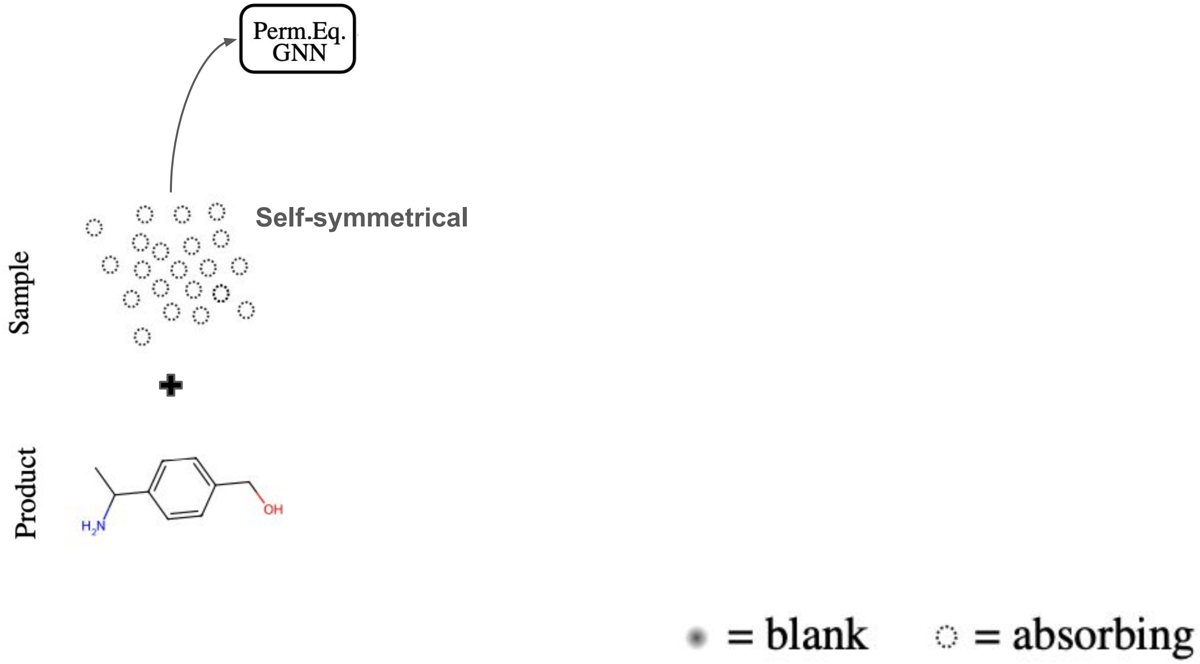

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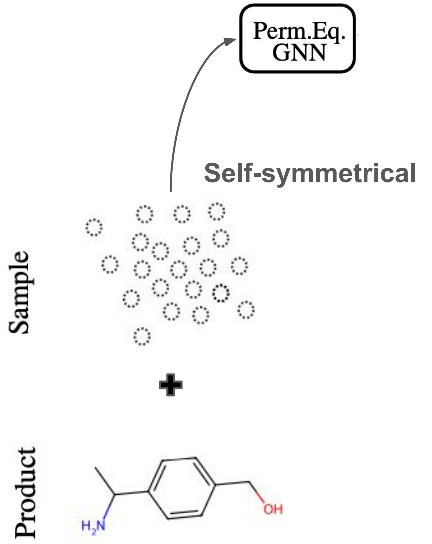
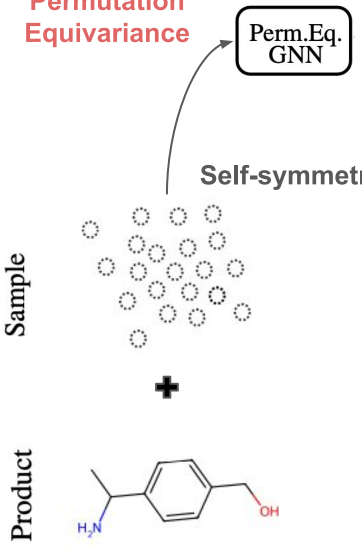
Assign different labels



Why does the Equivariant Denoiser Fail?

Assign different labels
+
Maintain Permutation Equivariance

Self-symmetrical



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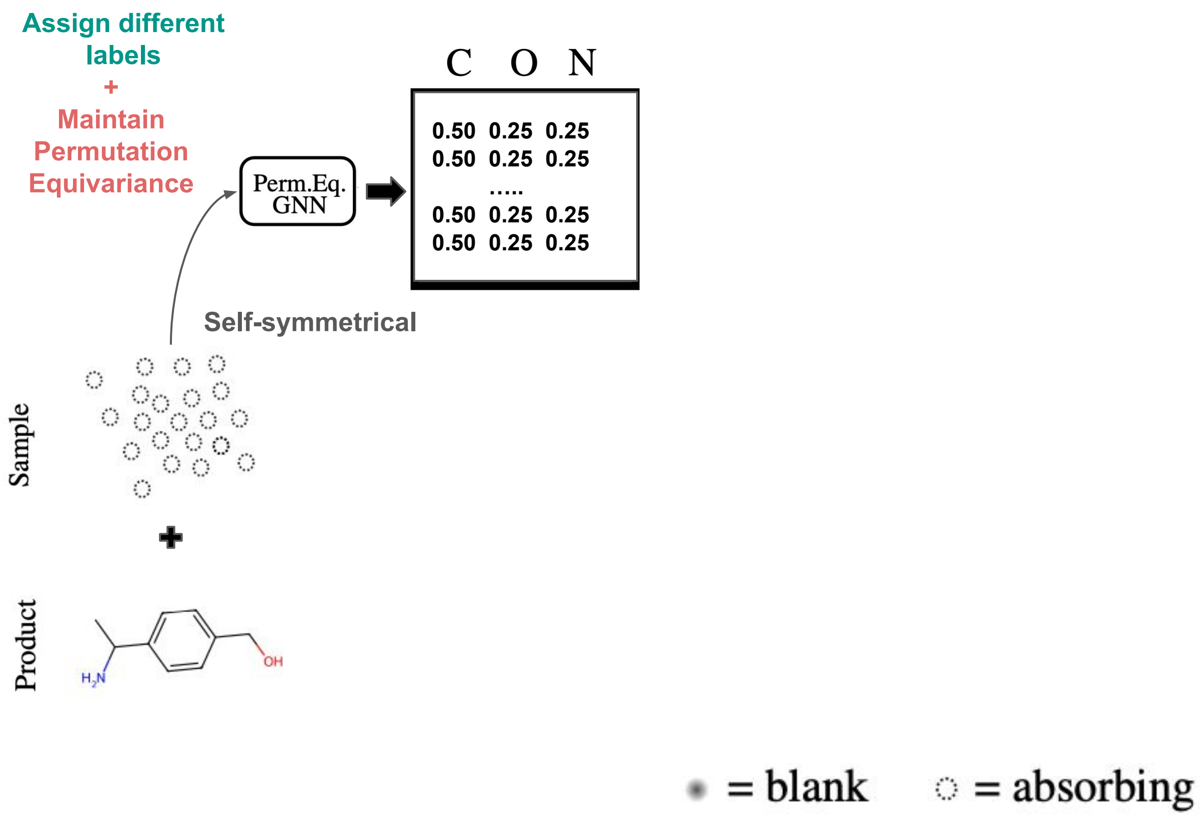

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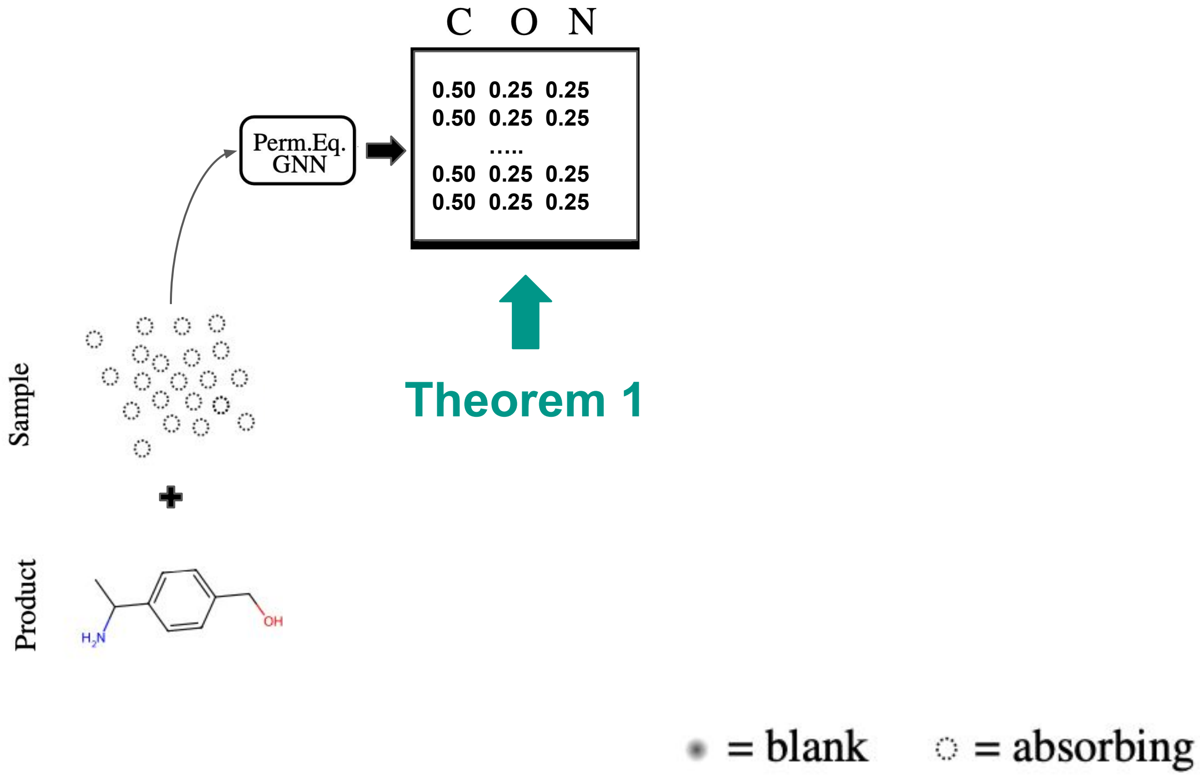

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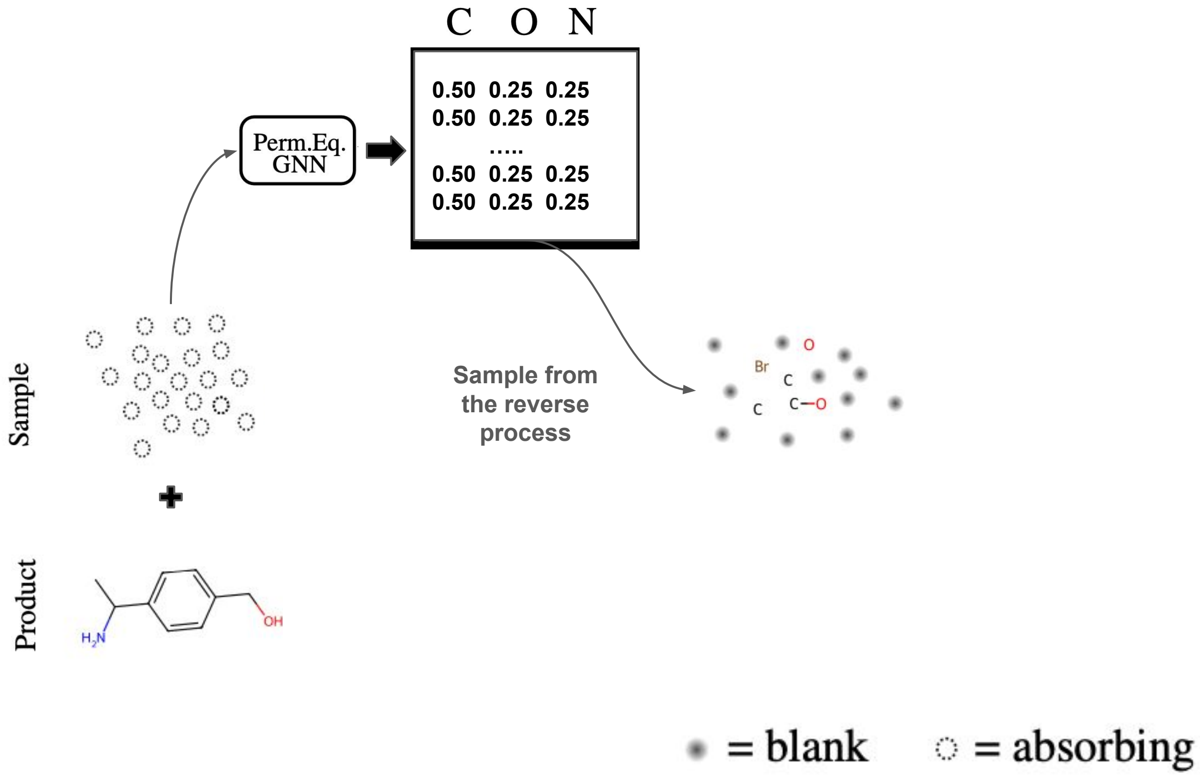

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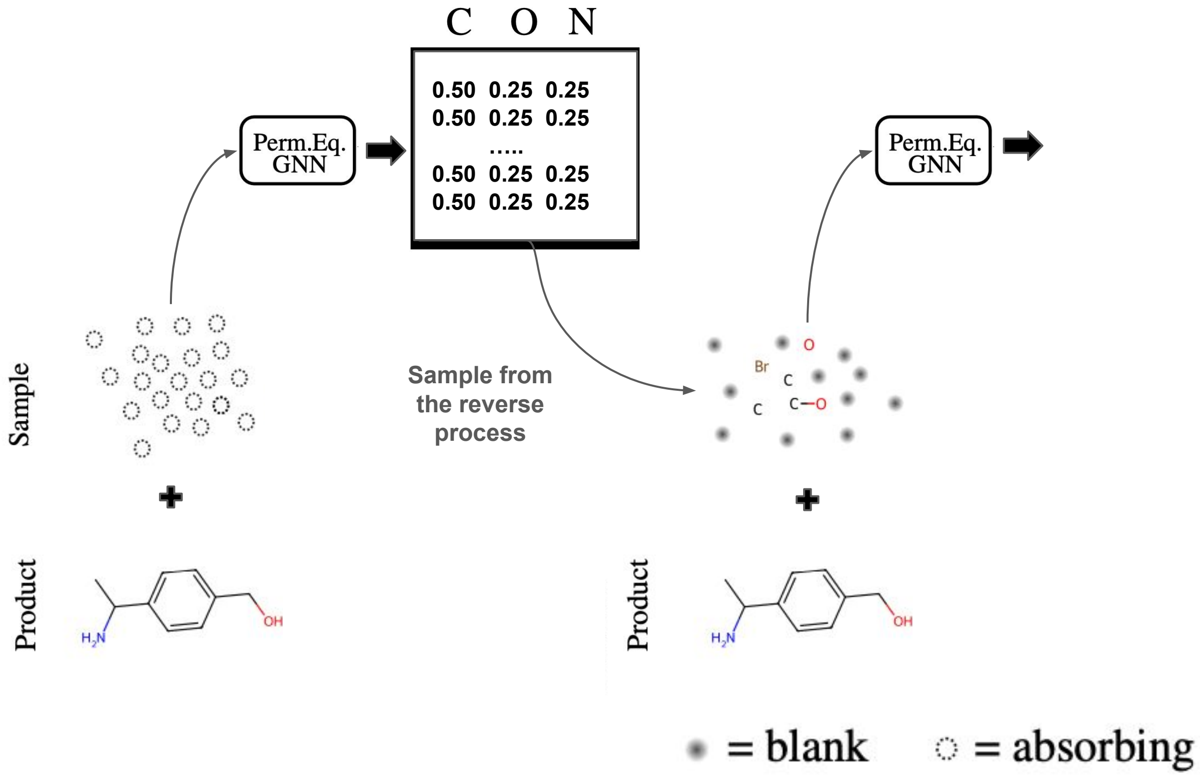

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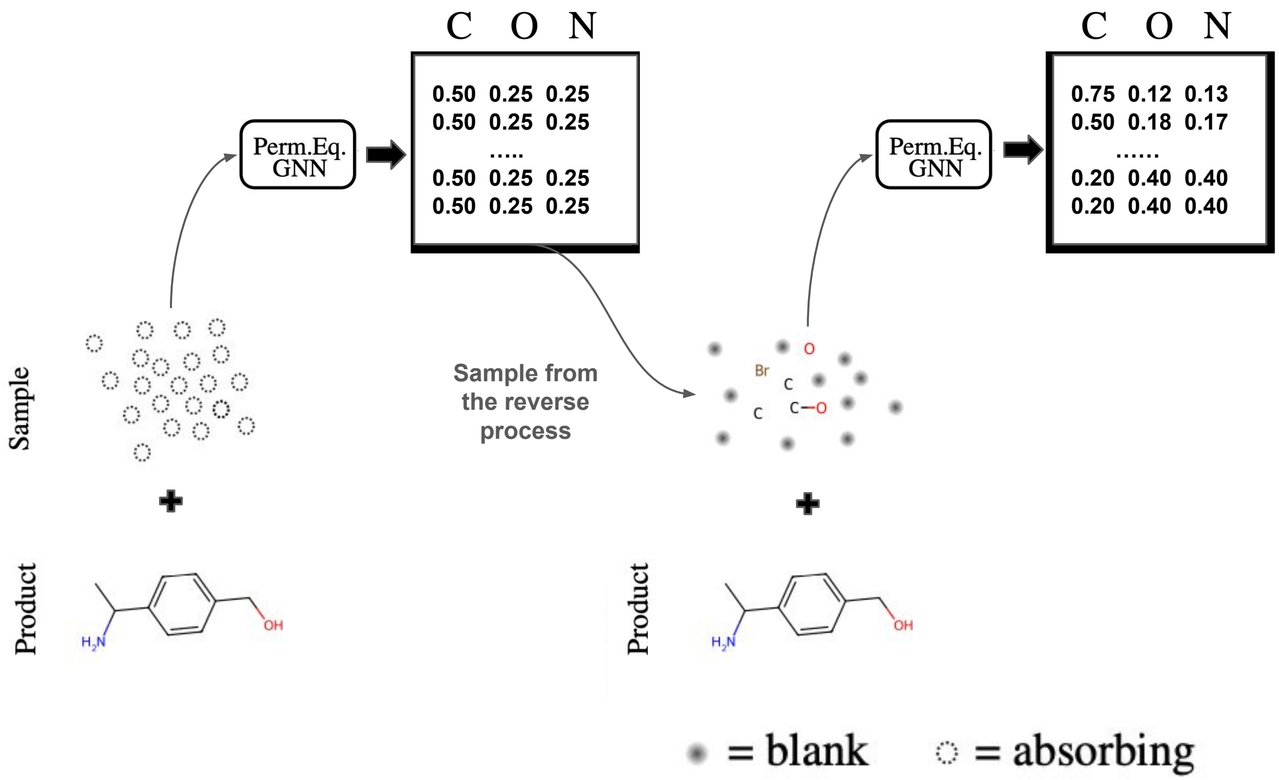

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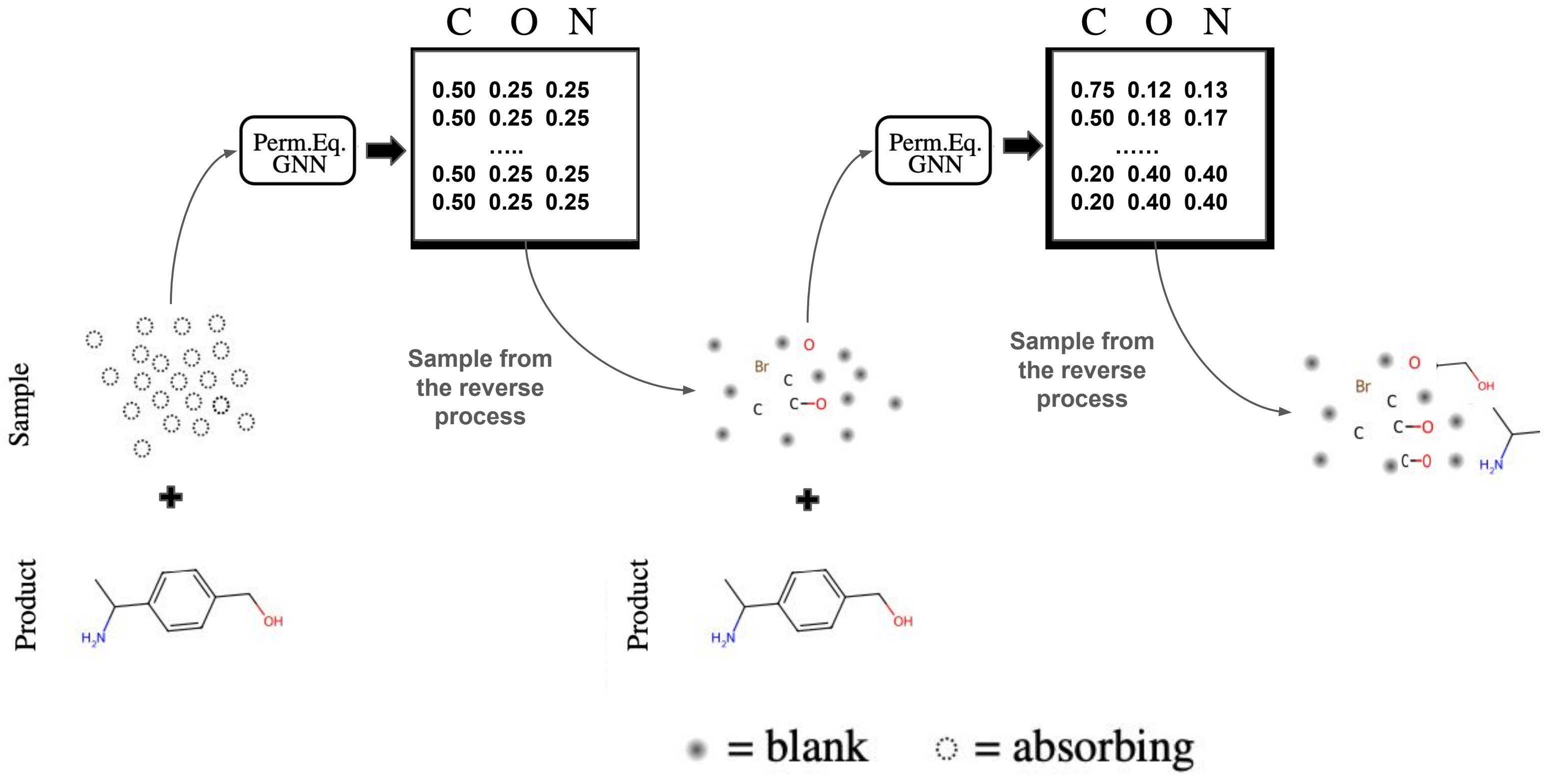

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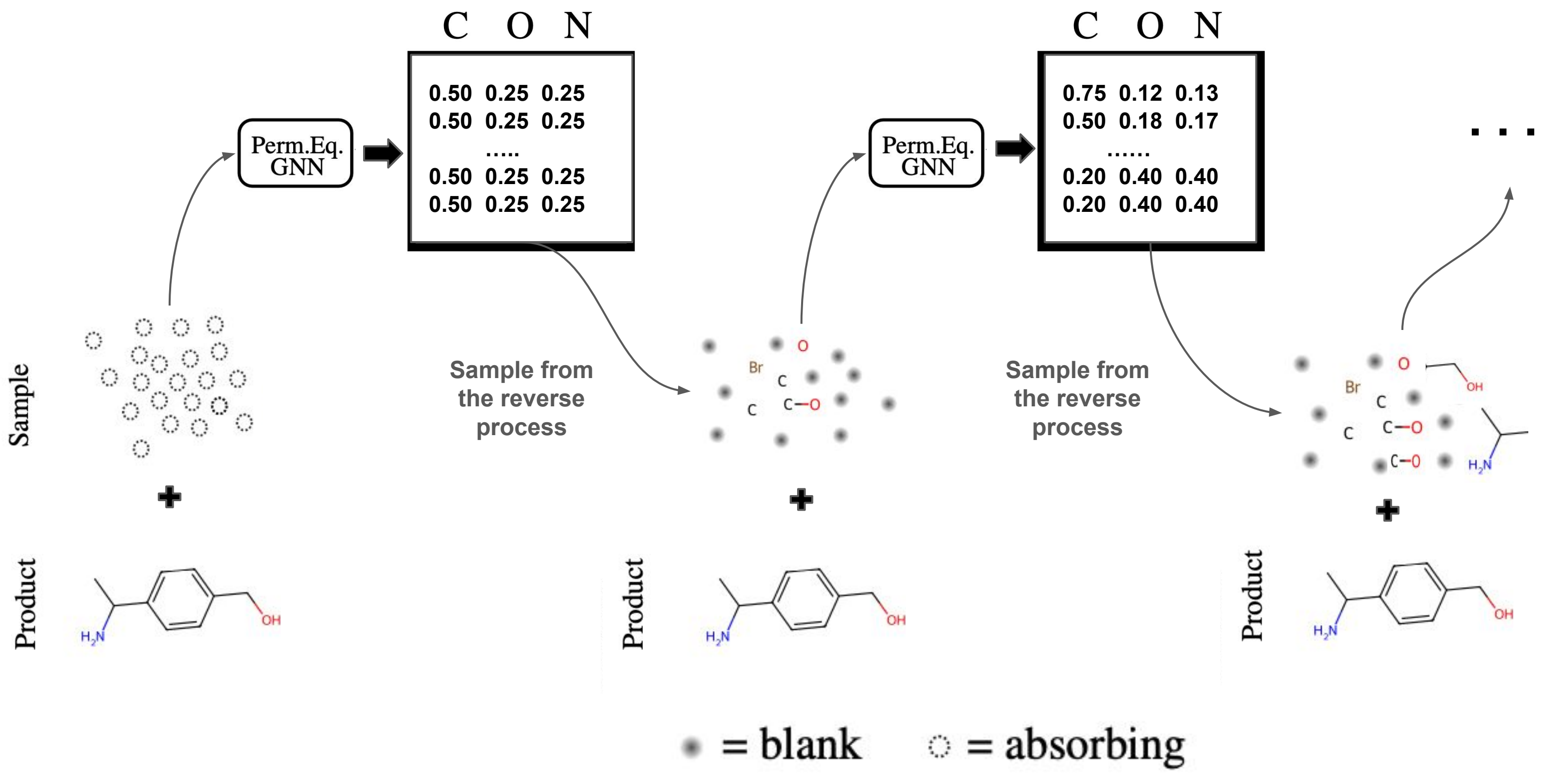

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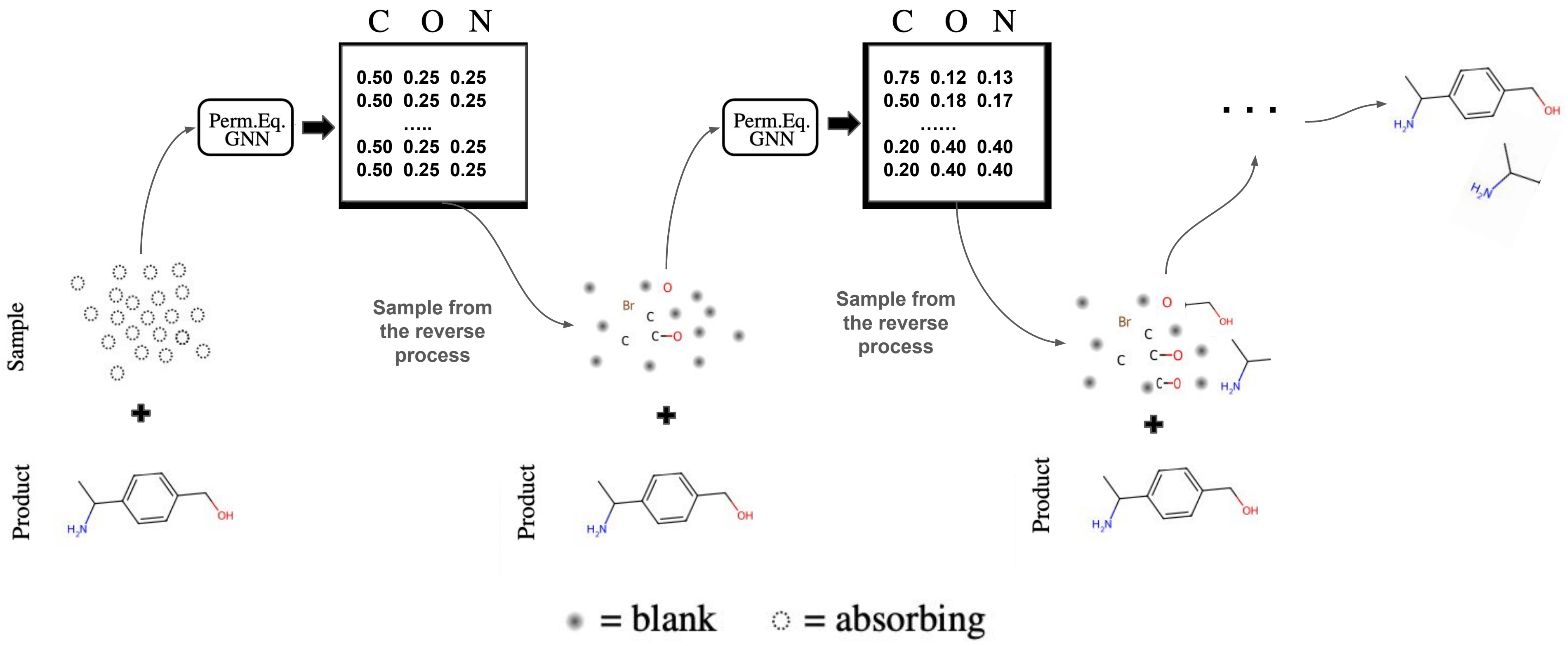
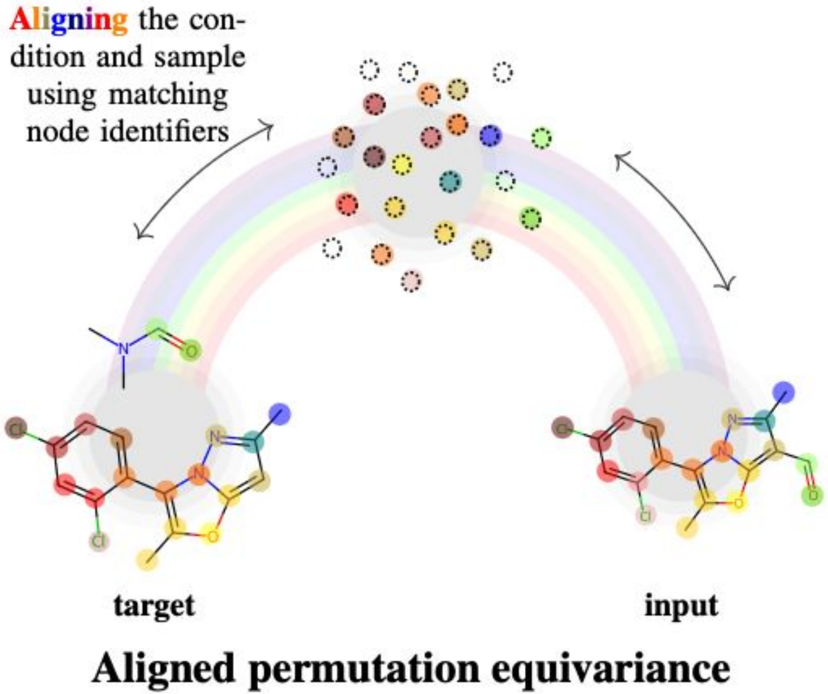


Aligned Equivariance



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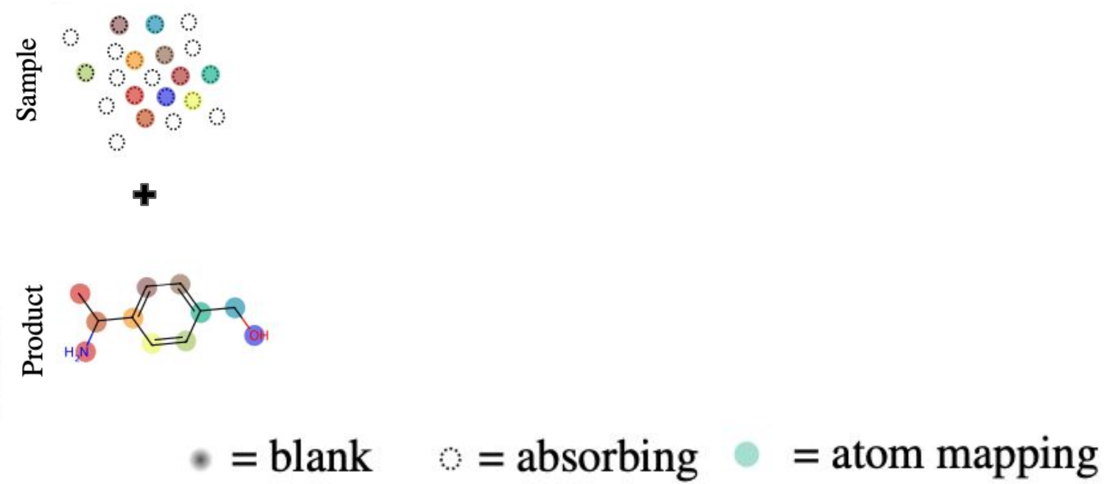

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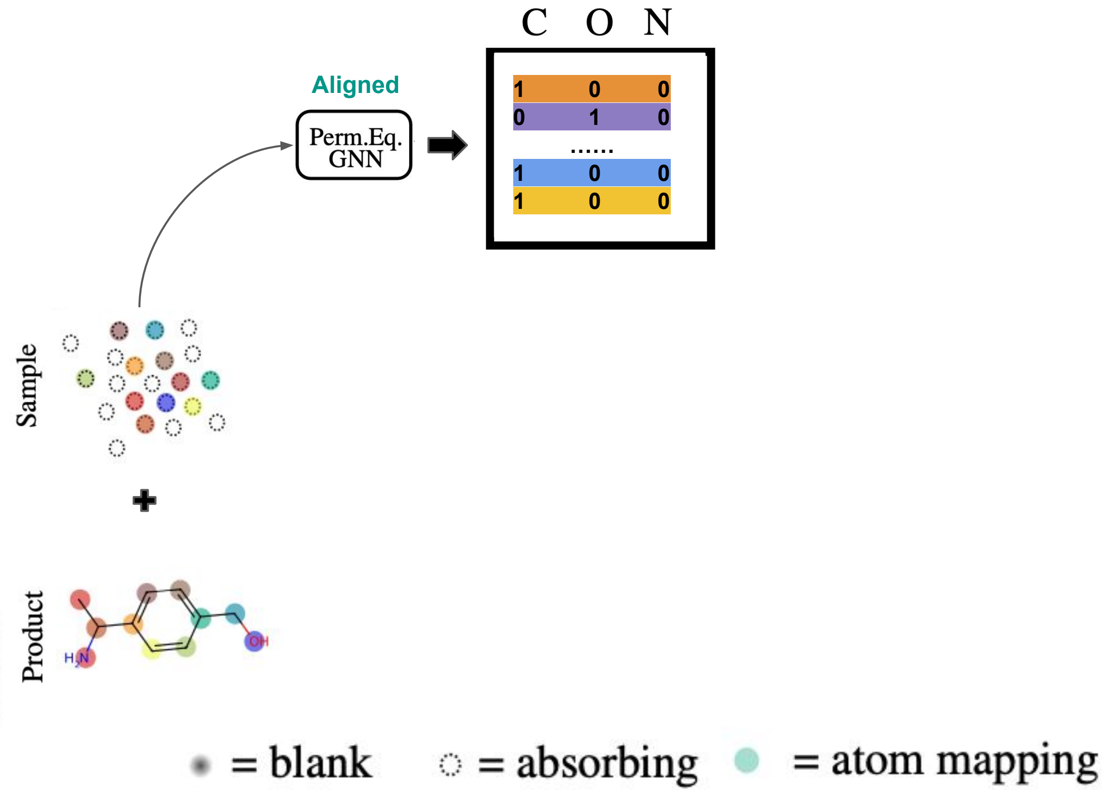

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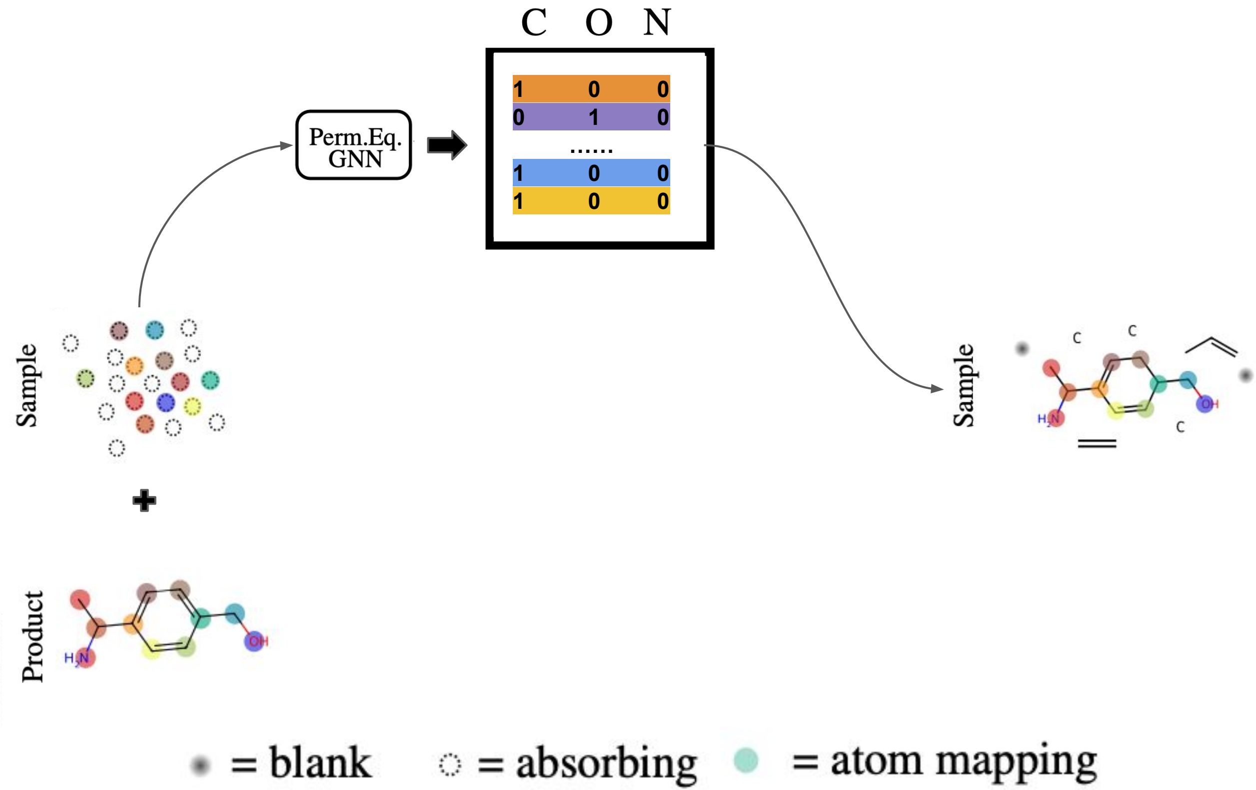
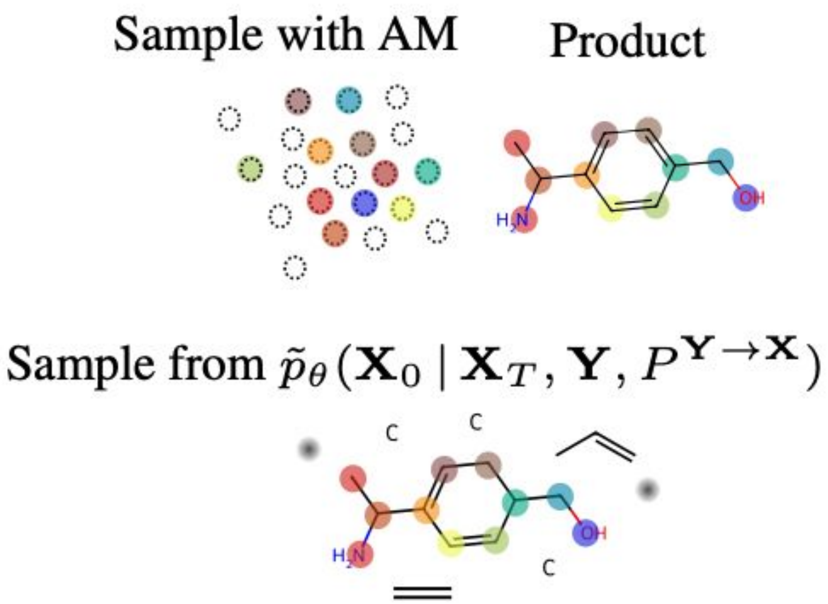
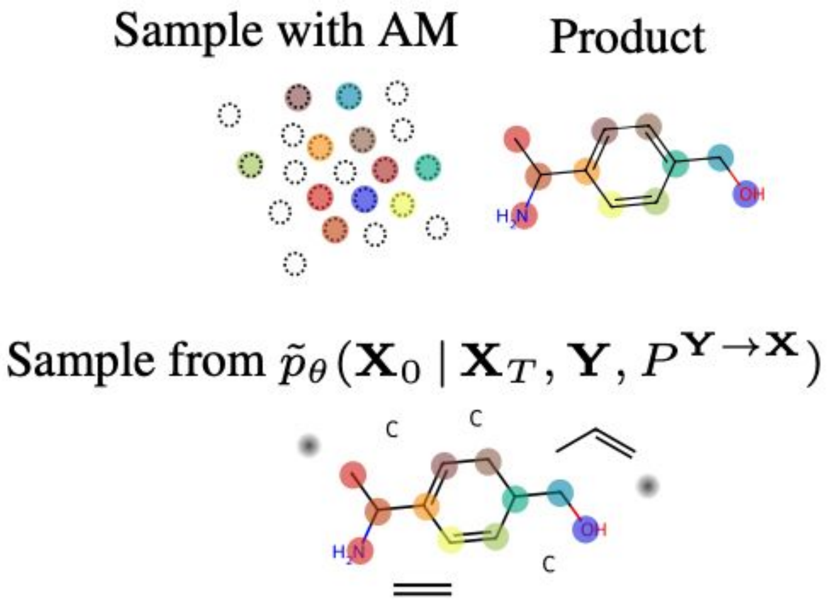


Alignment Methods



★ **Input-Alignment**

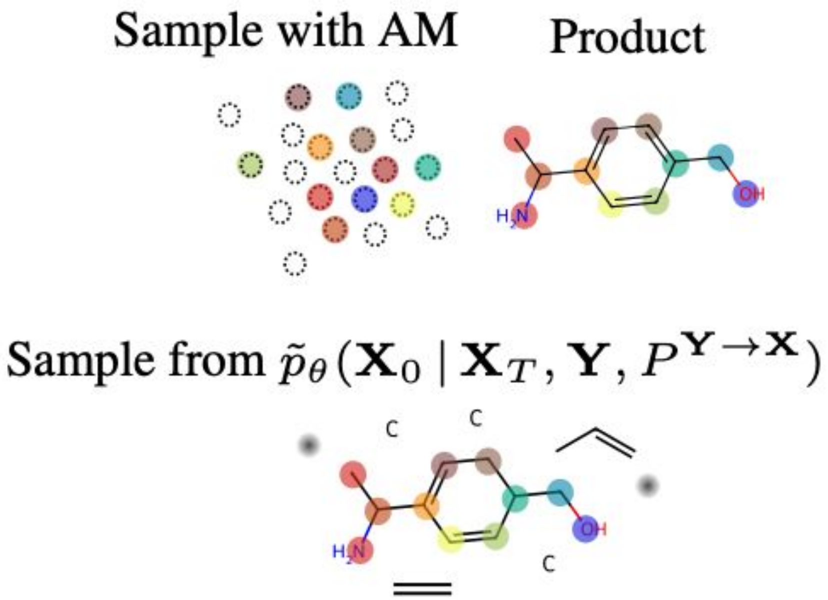
Alignment Methods



Input-Alignment

Skip Connection

Alignment Methods



★ Input-Alignment

★ Skip Connection

★ Laplacian Positional Encodings

Results

Topk accuracy on USPTO-50k

Method	$\mathbf{k=1}\uparrow$	$\mathbf{k=3}\uparrow$	$\mathbf{k=5}\uparrow$	$\mathbf{k=10}\uparrow$	$\widehat{\mathbf{MRR}}\uparrow$
Unaligned	4.1	6.5	7.8	9.8	0.056
DiffAlign-input	44.1	65.9	72.2	78.7	0.554
DiffAlign-PE	49.0	70.7	76.6	**81.8**	0.601
DiffAlign-PE+skip	**54.7**	**73.3**	**77.8**	81.1	**0.639**

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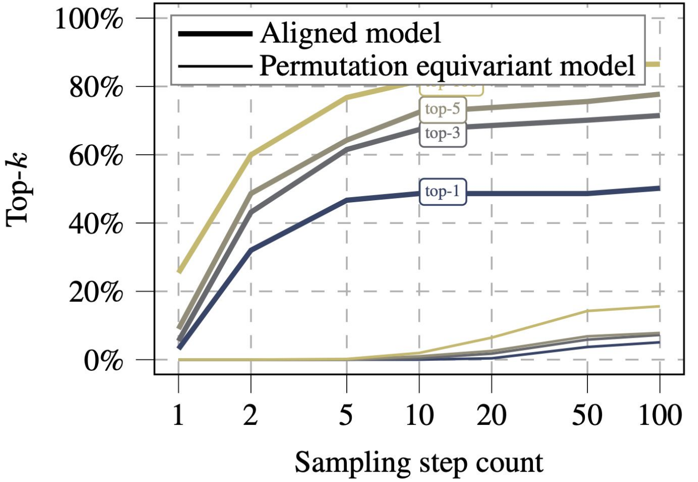

Results

Topk accuracy on USPTO-50k

	Method	$\mathbf{k}=\mathbf{1}\uparrow$	$\mathbf{k}=\mathbf{3}\uparrow$	$\mathbf{k}=\mathbf{5}\uparrow$	$\mathbf{k}=\mathbf{10}\uparrow$	$\widehat{\mathbf{MRR}}\uparrow$
Pre-trained	RSMILES (Zhong et al., 2022)	56.3	**79.2**	**86.2**	**91.0**	0.680
	PMSR (Jiang et al., 2023)	**62.0**	78.4	82.9	86.8	**0.704**
Temp.	Retrosym (Coley et al., 2017b)	37.3	54.7	63.3	74.1	0.480
	GLN (Dai et al., 2019)	52.5	74.7	81.2	87.9	0.641
	LocalRetro (Chen & Jung, 2021)	**52.6**	**76.0**	**84.4**	**90.6**	**0.650**
Synthon	GraphRetro (Somnath et al., 2021)	**53.7**	68.3	72.2	75.5	0.611
	RetroDiff (Wang et al., 2023)	52.6	**71.2**	**81.0**	83.3	**0.629**
	MEGAN (Sacha et al., 2021)	48.0	70.9	78.1	**85.4**	0.601
	G2G (Shi et al., 2020a)	48.9	67.6	72.5	75.5	0.582
Template-free	SCROP (Zheng et al., 2019)	43.7	60.0	65.2	68.7	0.521
	Tied Transformer (Kim et al., 2021)	47.1	67.1	73.1	76.3	0.572
	Aug. Transformer (Tetko et al., 2020)	48.3	-	73.4	77.4	0.569
	Retrobridge (*) (Igashov et al., 2024)	50.3	**74.0**	**80.3**	**85.1**	0.622
	GTA_aug (Seo et al., 2021)	51.1	67.6	74.8	81.6	0.605
	Graph2SMILES (Tu & Coley, 2022)	52.9	66.5	70.0	72.9	0.597
	Retroformer (Wan et al., 2022)	53.2	71.1	76.6	82.1	0.626
	DualTF_aug (Sun et al., 2021)	53.6	70.7	74.6	77.0	0.619
Ours	Unaligned	4.1	6.5	7.8	9.8	0.056
	DiffAlign-input	44.1	65.9	72.2	78.7	0.554
	DiffAlign-PE	49.0	70.7	76.6	81.8	0.601
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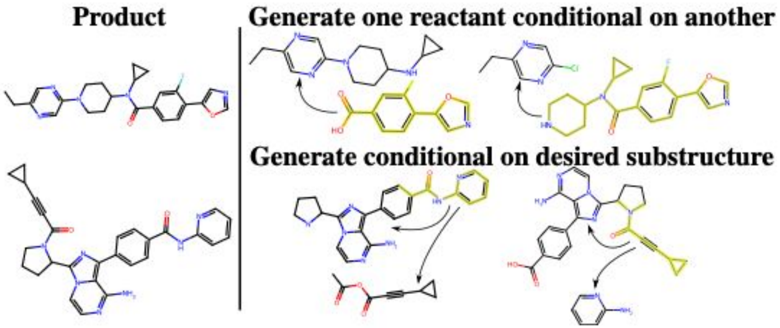
Results

Inpainting



Results

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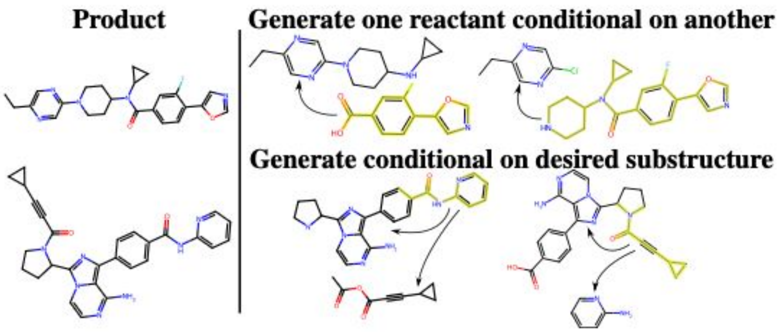
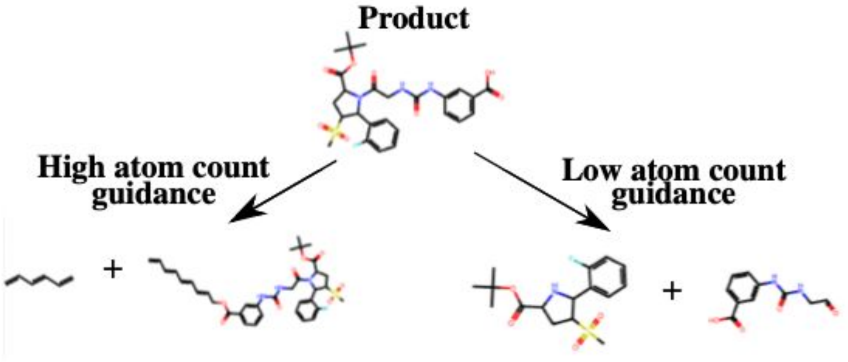


Inference Guidance



Conclusion

Graph Diffusion

+

Equivariant Denoiser

=

$$
\begin{array}{ccc}
C & O & N \\
\hline
0.5 & 0.25 & 0.25 \\
0.5 & 0.25 & 0.25 \\
0.5 & 0.25 & 0.25 \\
0.5 & 0.25 & 0.25
\end{array}
$$

Conclusion

Graph Diffusion

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Equivariant Denoiser

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$$\begin{array}{ccc} C & O & N \\ \hline 0.5 & 0.25 & 0.25 \\ 0.5 & 0.25 & 0.25 \\ 0.5 & 0.25 & 0.25 \\ 0.5 & 0.25 & 0.25 \end{array}$$

Graph Diffusion

+

Aligned Equivariance

=

$$\begin{array}{ccc} C & O & N \\ \hline 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{array}$$

Conclusion

Graph Diffusion

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Equivariant Denoiser

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$$\begin{array}{ccc} C & O & N \\ \hline 0.5 & 0.25 & 0.25 \\ 0.5 & 0.25 & 0.25 \\ 0.5 & 0.25 & 0.25 \\ 0.5 & 0.25 & 0.25 \end{array}$$

Graph Diffusion

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★A key issue with equivariant denoisers

Conclusion

Graph Diffusion

+

Equivariant Denoiser

=

C	O	N
0.5	**0.25**	**0.25**
0.5	**0.25**	**0.25**
0.5	**0.25**	**0.25**
0.5	**0.25**	**0.25**

Graph Diffusion

+

Aligned Equivariance

=

C	O	N
1	0	0
0	**1**	0
1	0	0
0	0	**1**

★**A key issue with equivariant denoisers**

★**It works:** SOTA-matching in retrosynthesis

Conclusion

Graph Diffusion

+

Equivariant Denoiser

=

$$\begin{array}{ccc} C & O & N \\ \end{array}$$
$$\begin{bmatrix} 0.5 & 0.25 & 0.25 \\ 0.5 & 0.25 & 0.25 \\ 0.5 & 0.25 & 0.25 \\ 0.5 & 0.25 & 0.25 \end{bmatrix}$$

Graph Diffusion

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Aligned Equivariance

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- ★ **A key issue with equivariant denoisers**
- ★ **It works:** SOTA-matching in retrosynthesis
- ★ **Inpainting and inference-time Guidance**