

Fig. 4. Comparison of our method against the MiDi for the VesSAP and Circle of Willis (CoW) datasets. We show the results for learning coordinates (x, y, z) , edge angles $(\mathcal{E} \angle)$, edge orientation (θ, ϕ, ψ) and edge length $(l_{\mathcal{E}})$. We also compare the statistics for node degree $(deg(\mathcal{V}))$, number of edges $(|\mathcal{E}|)$, and the Betti values $(\beta_0 \beta_1)$. The ground truth distribution is in purple, the distribution learned by MiDi is in orange, and our method is in green. As observed, our method emulates the statistics of the ground truth graphs more faithfully than MiDi. The degree of distribution of MiDi vs. our method on the VesSAP dataset is especially interesting. While the VesSAP graphs contain no degree 2 nodes, MiDi generates graphs with a large number of degree 2 nodes. Our method overcomes this shortcoming and generates minimal degree 2 nodes.

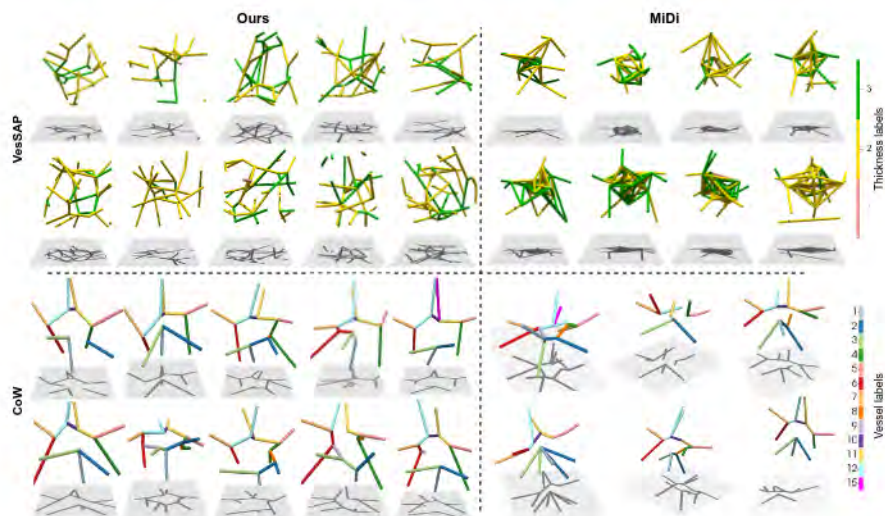


Fig. 5. VesSAP and CoW graphs generated by our model and MiDi, respectively. Note that, in the case of VesSAP, MiDi failed to capture the node coordinate distribution, which is the driving property for correct edge distribution, and hence produces an over-connected graph, resulting in a high Betti number error. However, MiDi fares relatively well in the CoW configuration, which resembles a molecular layout. In contrast, our model is able to generate diverse and valid novel graphs for both datasets.

Table 3. Details of the hyper-parameters used by the baselines (Congress and MiDi) and our method. We report the number of transformer blocks used by the models, the number of attention heads in each transformer block, the number of denoising steps, and the node and edge projection dimensions. We report the parameters of our edge denoising and coordinate diffusion modules in separate columns for clarity. We have tried to use a similar number of trainable parameters for all three methods for a fair comparison.

Model Specification	Congress[24]	Ours	
	MiDi[25]	Edge Network	Node Network
Model Type	Transformer	Transformer	MLPs+MSA
# blocks	8	8	2
# attention heads	8	8	4
# node features	128	128	256
# edge features	64	64	-
# denoising steps	1000	1000	1000