Optimising (Graph) Neural Networks Using Exact Solvers

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Mixed-integer optimisation of graph neural networks for computer-aided molecular design

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Highlights

- Mixed-integer linear programming formulation of graph neural networks.
- Formulations for Graph Convolutional Network and GraphSAGE.
- Showcase that such models can learn from non-euclidean data structures efficiently.
- Sample application to molecule discovery with optimal boiling points.

Training NN with MIP

Fischetti and Jo
2018

Grimstad and Andersson
2019

Anderson et al
2020

Thorbjarnarson and
Yorke-Smith, 2021

Maragno et al
2021

Schweidtmann et al
2022

Can we formulate Graph Convolutional Networks as Mixed Integer (Non-) Linear Problems?

1

MINLP formulation of GCN

MILP formulation of GraphSAGE

2

genetic algorithm approach to optimise GNNs

3

experiments on molecular boiling point optimisation

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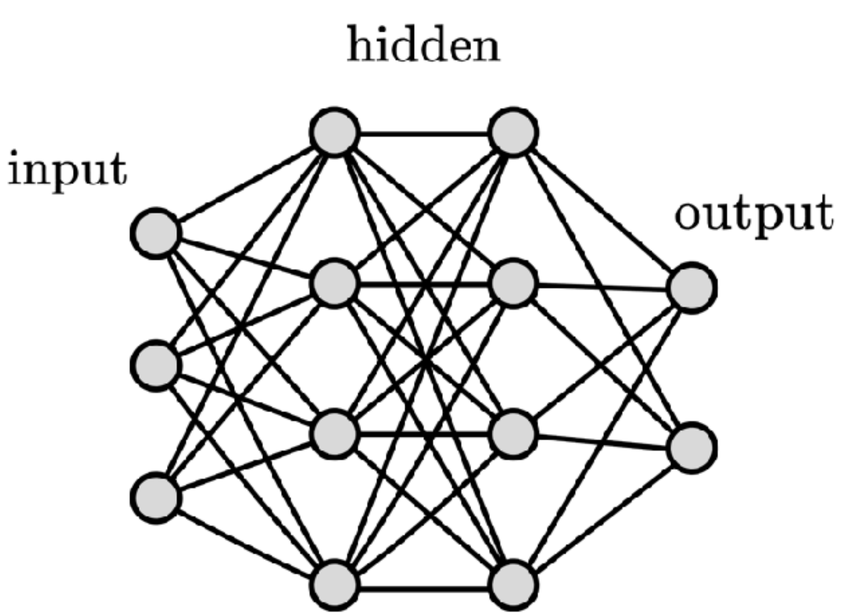

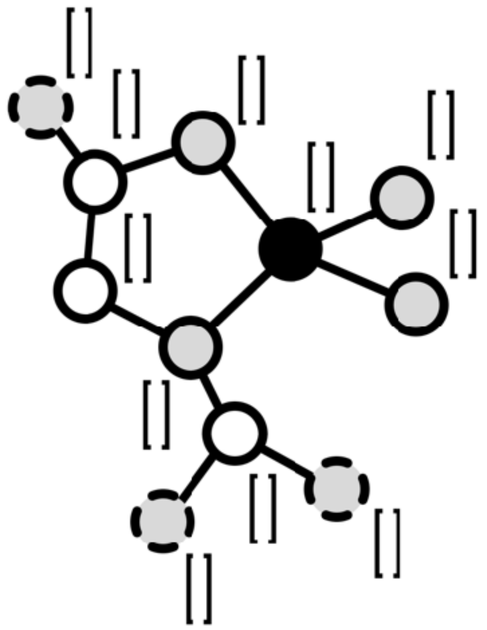

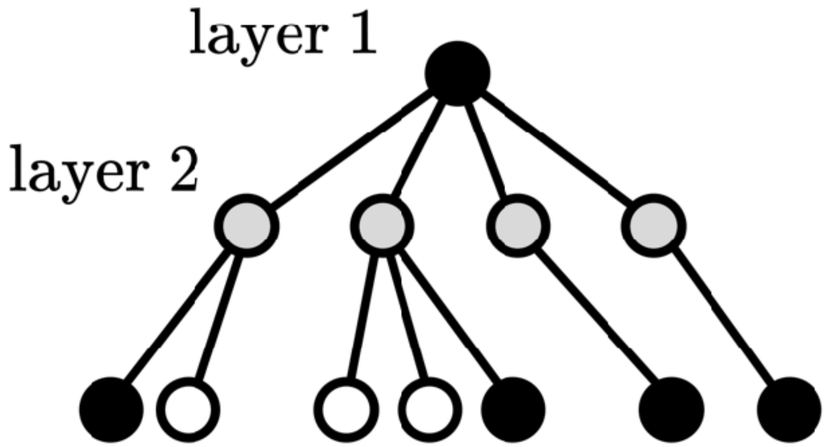

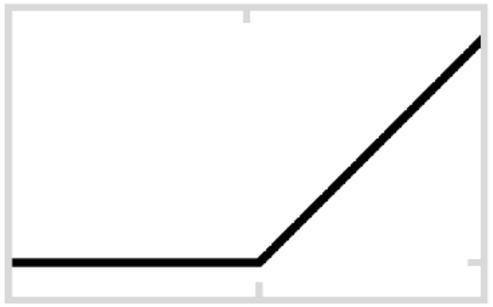

$$
\begin{aligned}
\text{maximise} \quad & x_1^K \\
\text{subject to} \quad & \boldsymbol{W}^K \boldsymbol{x}^{K-1} + b^K = x_1^K \\
& \boldsymbol{W}_j^k \boldsymbol{x}^{k-1} + b_j^k = x_j^k - s_j^k && \forall k \in \{1, \ldots, K-1\}, \forall j \in \{1, \ldots, n_k\} \\
& x_j^k \leq u_j^k z_j^k && \forall k \in \{1, \ldots, K-1\}, \forall j \in \{1, \ldots, n_k\} \\
& s_j^k \leq -l_j^k (1 - z_j^k) && \forall k \in \{1, \ldots, K-1\}, \forall j \in \{1, \ldots, n_k\} \\
& x_j^k, s_j^k \geq 0 && \forall k \in \{1, \ldots, K-1\}, \forall j \in \{1, \ldots, n_k\} \\
& z_j^k \in \{0, 1\} && \forall k \in \{1, \ldots, K-1\}, \forall j \in \{1, \ldots, n_k\} \\
& x^0 \in \Omega
\end{aligned}
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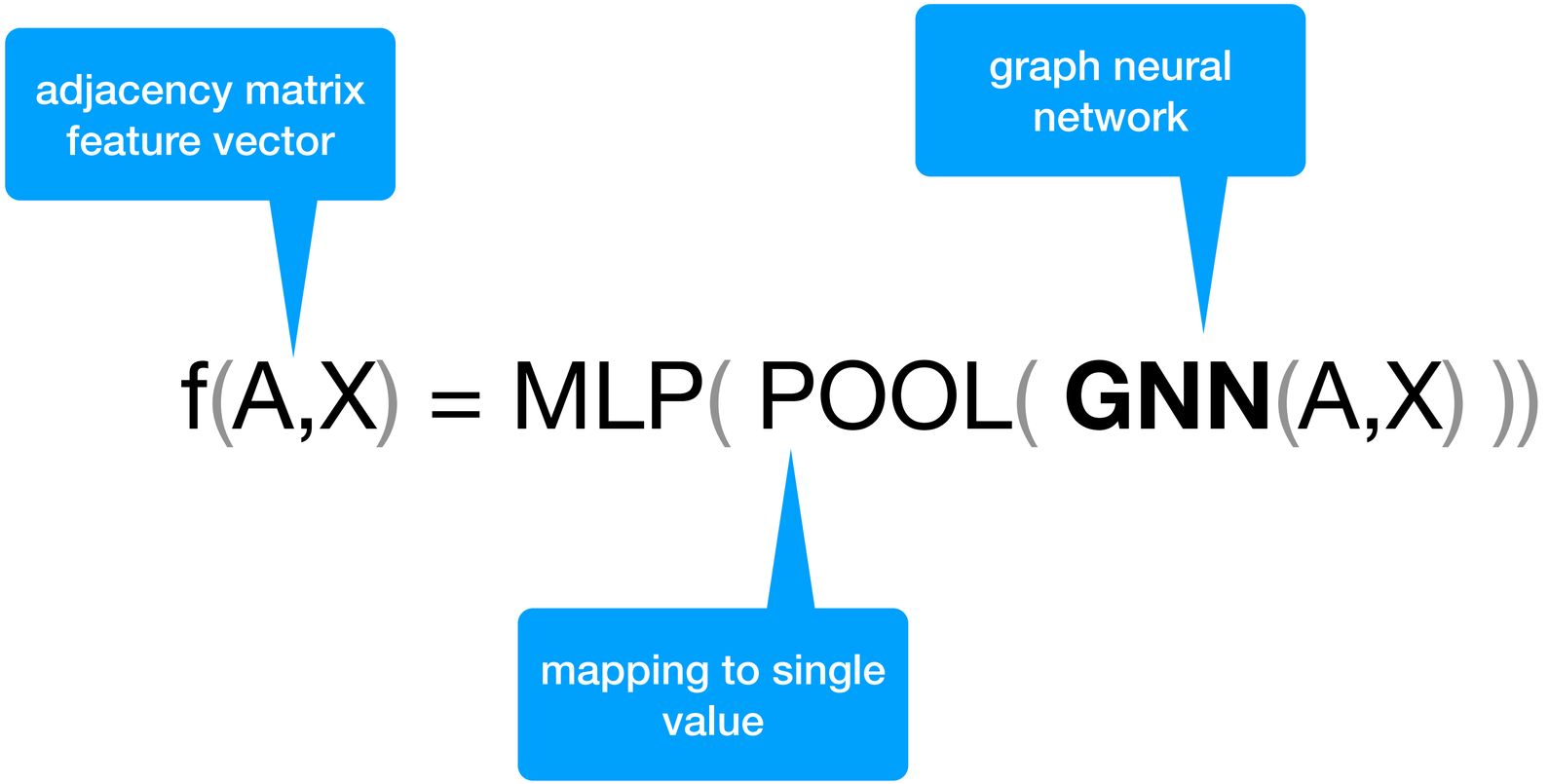
Matteo Fischetti and Jason Jo: Deep neural networks and mixed integer linear optimization. Constraints, 23(3):296–309, 2018



$$H^{(k+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(k)}W^{(k)}\right)$$

GCN structure

$$\sum_{l|\tilde{A}_{il}=1} \frac{1}{\sqrt{d_i^+ d_l^+}} \boldsymbol{W}_j^{k^T} \boldsymbol{H}_l^{(k-1)} = H_{ij}^k - S_{ij}^k$$

$$H_{ij}^k \leq U_{ij}^k Z_{ij}^k$$

$$S_{ij}^k \leq -L_{ij}^k (1 - Z_{ij}^k)$$

$$0 \leq H_{ij}^k, S_{ij}^k \in \mathbb{R}$$

$$Z_{ij}^k \in \{0, 1\}$$

$$A, H^0 \in \Omega$$

MINLP model

$$x_j^0 = \sum_{i=1}^{N} H_{ij}^K \quad \forall j \in \{1, \ldots, n_K\}$$

pooling

Unknown graph structure

$$\sum_{l|\tilde{A}_{il}=1} \frac{1}{\sqrt{d_i^+ d_l^+}} \boldsymbol{W}_j^{k\,T} \boldsymbol{H}_l^{(k-1)} = H_{ij}^k - S_{ij}^k$$

can make bilinear

add a boolean var

GUROBI OPTIMIZATION

$$H_{ij}^{(k)} = \sigma\left(\hat{\boldsymbol{W}}_j^{kT}\boldsymbol{H}_i^{(k-1)} + \bar{\boldsymbol{W}}_j^{kT}\sum_{l|A_{il}=1}\boldsymbol{H}_l^{(k-1)}\right)$$

GraphSAGE structure

$$(\hat{\boldsymbol{W}}_j^k)^T\boldsymbol{H}_i^{(k-1)} + (\bar{\boldsymbol{W}}_j^k)^T\sum_l \boldsymbol{b}_{il}^{(k-1)} = H_{ij}^k - S_{ij}^k$$

$$H_{ij}^k \leq U_{ij}^k Z_{ij}^k$$

$$S_{ij}^k \leq -L_{ij}^k(1 - Z_{ij}^k)$$

$$\boldsymbol{H}_l^k - \boldsymbol{M}(1 - A_{il}) \leq \boldsymbol{b}_{il}^k$$

$$\boldsymbol{b}_{il}^k \leq \boldsymbol{H}_l^k + \boldsymbol{M}(1 - A_{il})$$

$$-\boldsymbol{M}(A_{il}) \leq \boldsymbol{b}_{il}^k \leq \boldsymbol{M}(A_{il})$$

$$\boldsymbol{H}_i^0 = \boldsymbol{x}_i$$

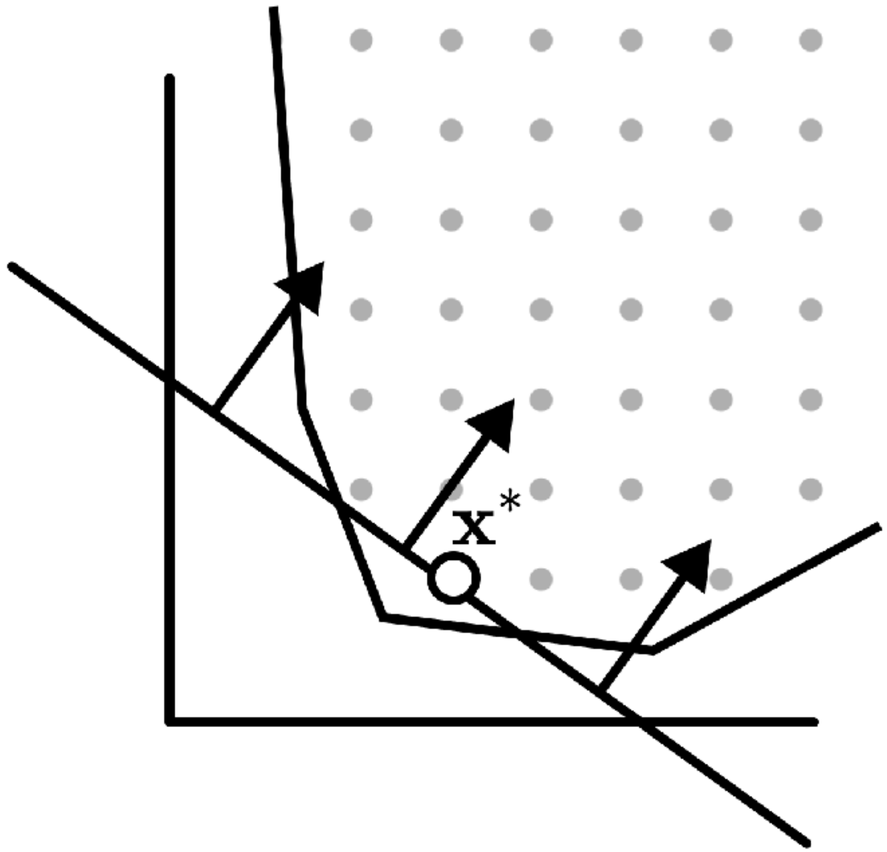
$$H_j^{*K} = \sum_i H_{ij}^K$$

$$0 \leq H_{ij}^k, S_{ij}^k \in \mathbb{R}$$

$$Z_{ij}^k \in \{0, 1\}$$

details in the paper :)

Helping the solver



Helping the solver

$$(\hat{\boldsymbol{W}}_j^k)^T \boldsymbol{H}_i^{(k-1)} + (\bar{\boldsymbol{W}}_j^k)^T \sum_l \boldsymbol{b}_{il}^{(k-1)} = H_{ij}^k - S_{ij}^k$$

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feasibility-based bounds tightening

domain-specific side constraints

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MILP formulation of GraphSAGE

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genetic algorithm approach to optimise GNNs

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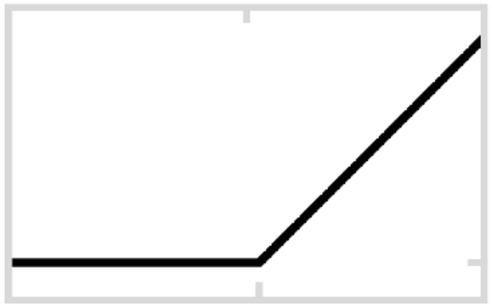

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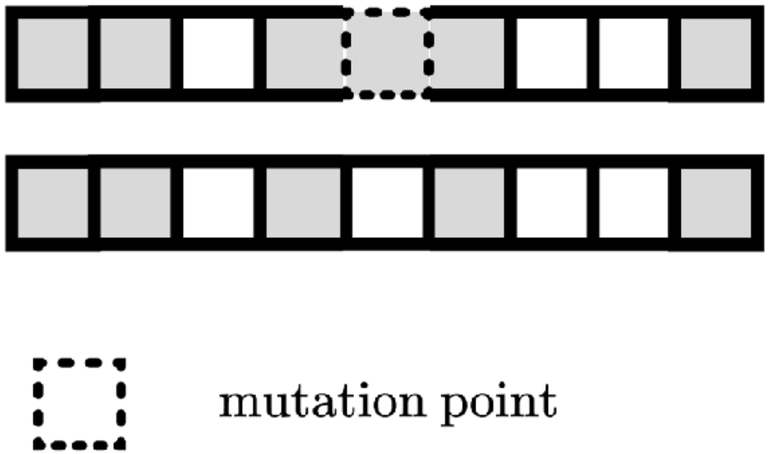
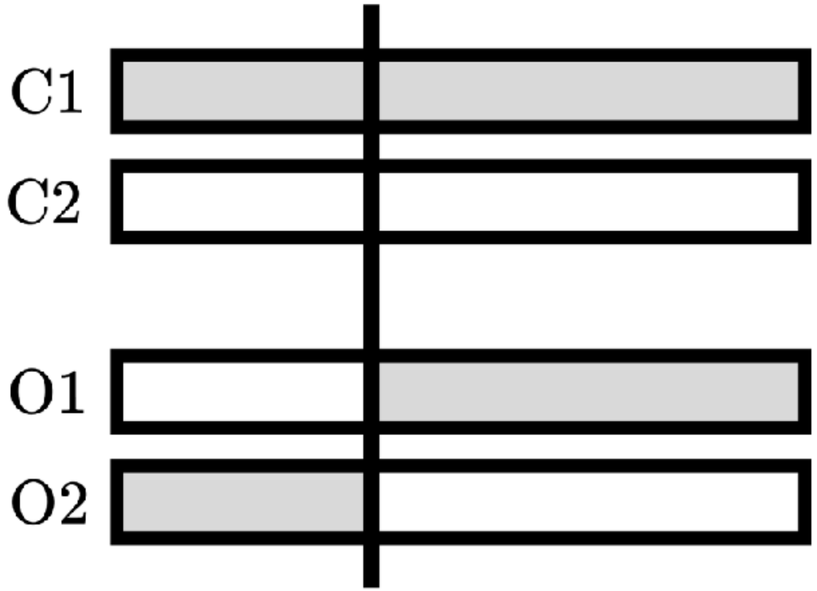
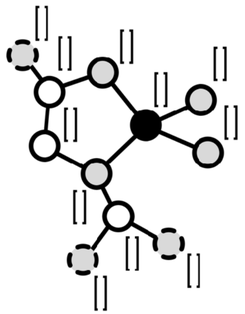
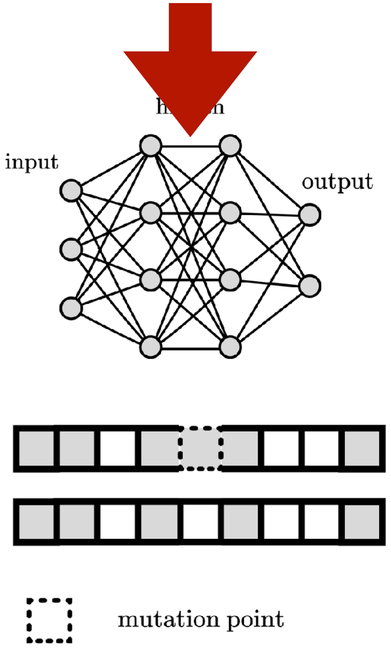
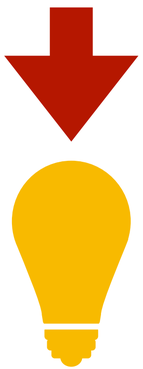




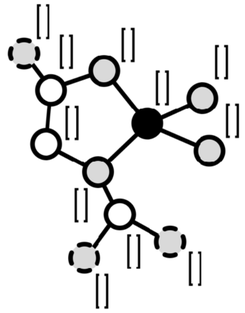


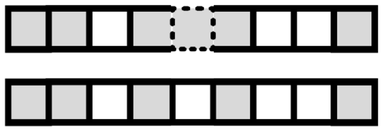


mutation point

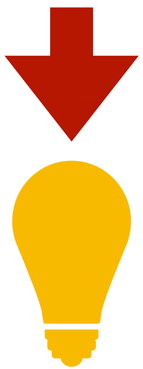


Directly optimise Graph Neural Networks with a (simple) genetic algorithm





mutation point



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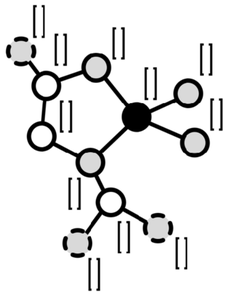
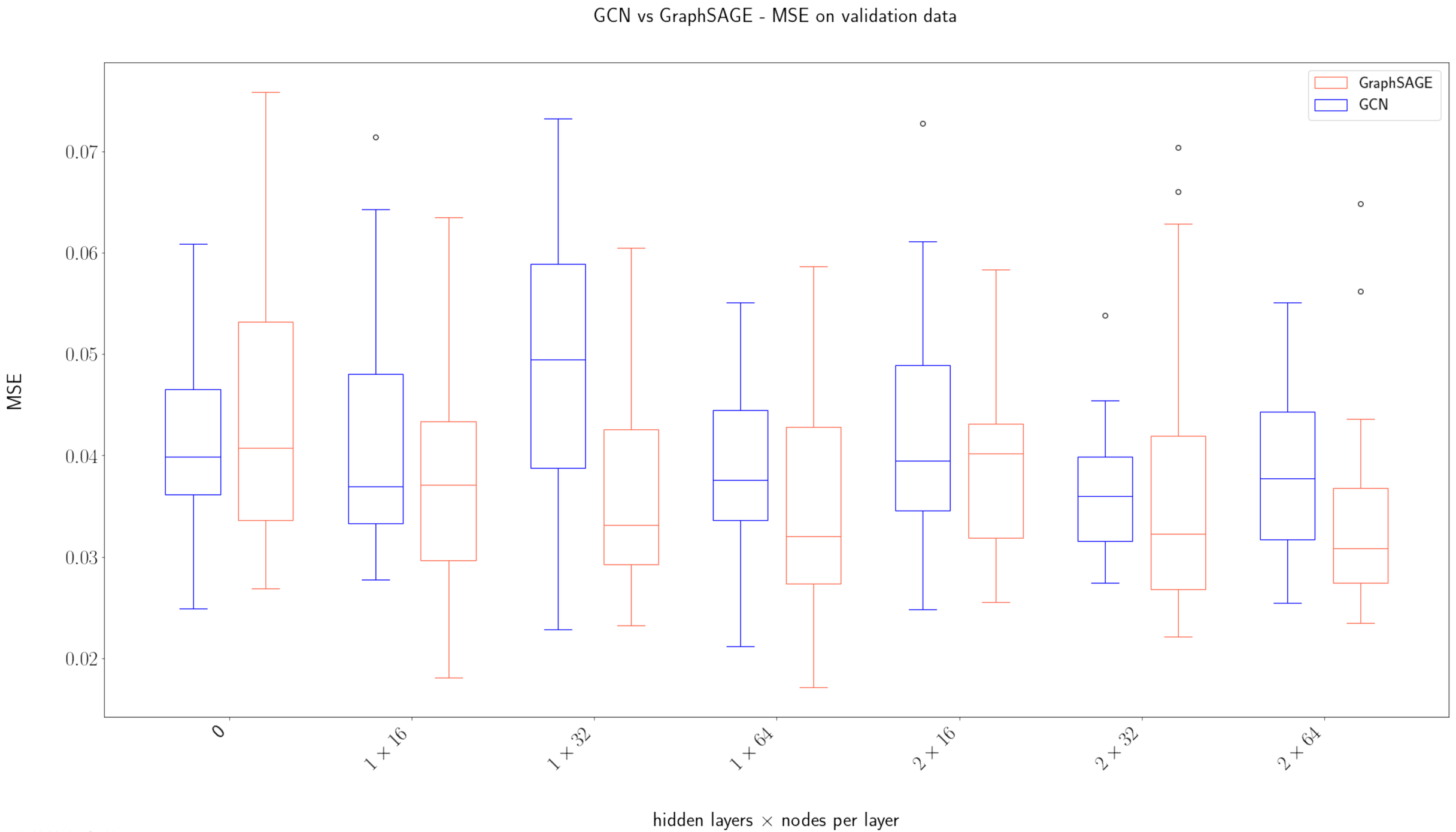


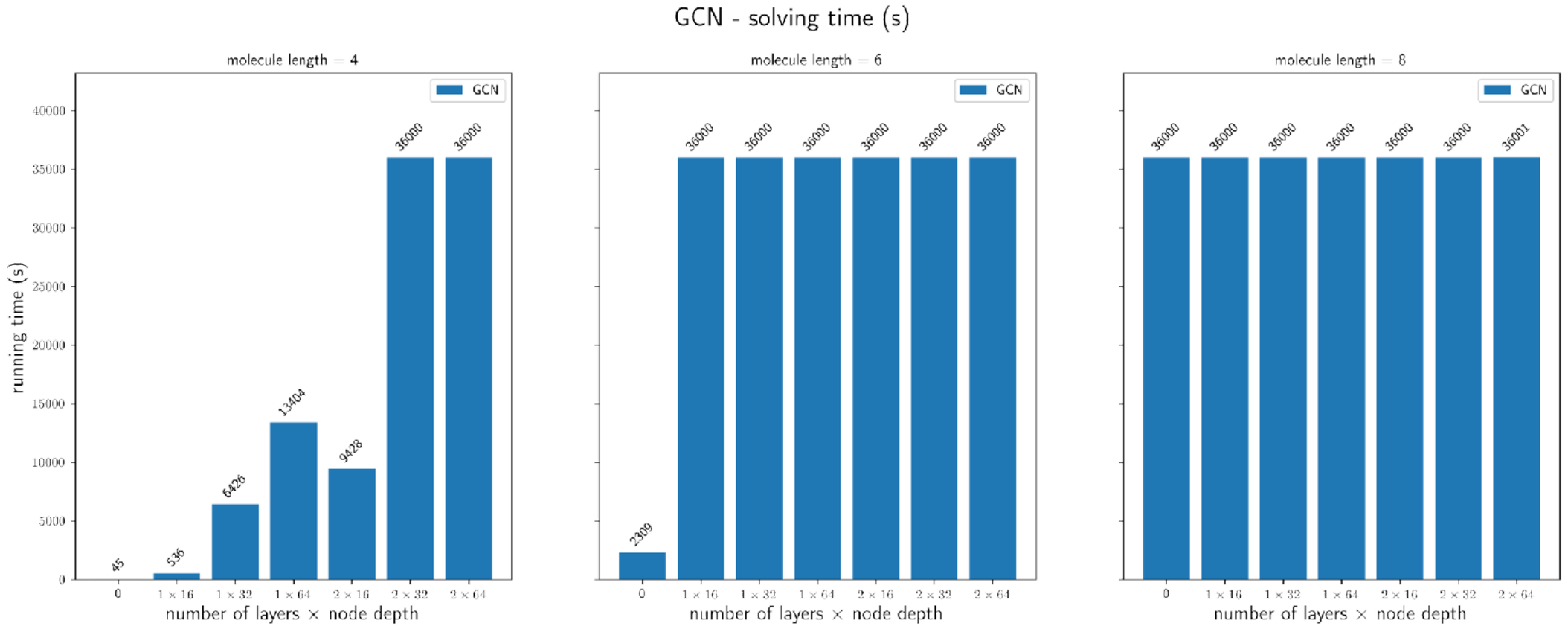
train GNN (using standard training mechanism)

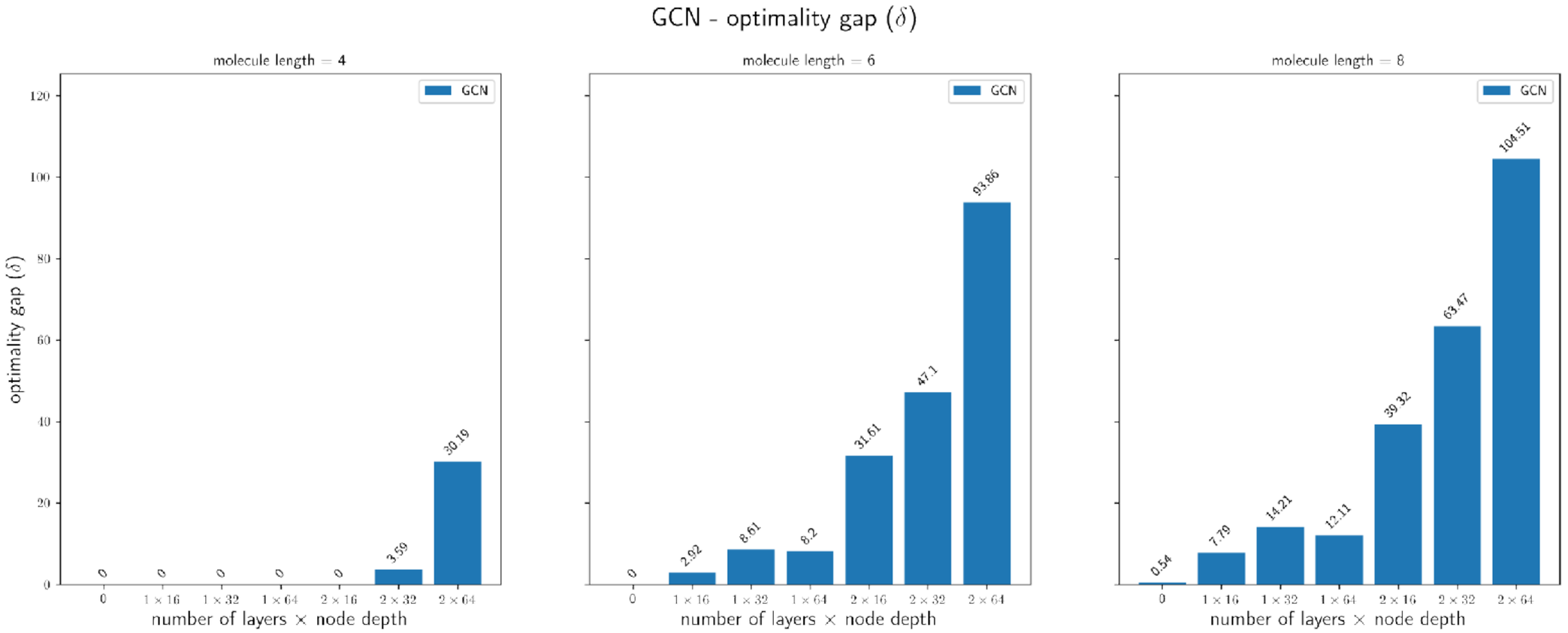
find molecular structures such that boiling point is optimised

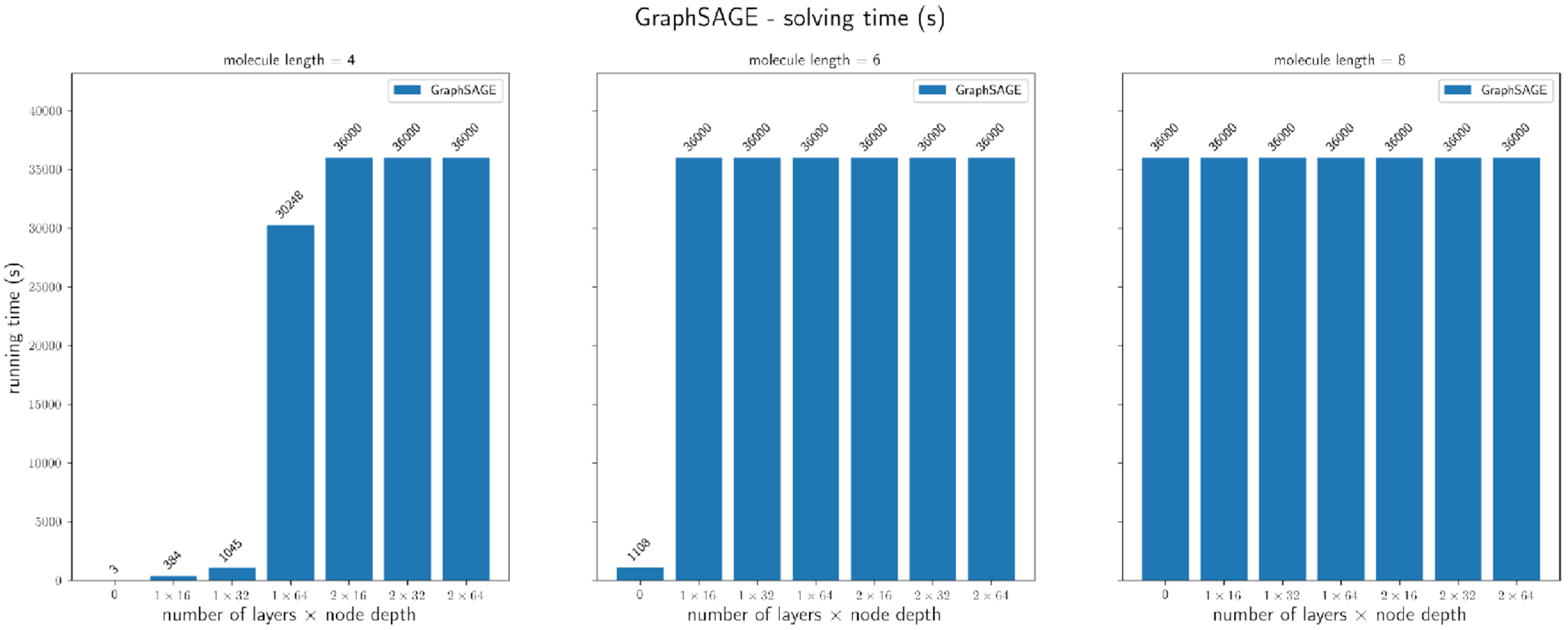
(using Gurobi solver with embedded trained GNN)

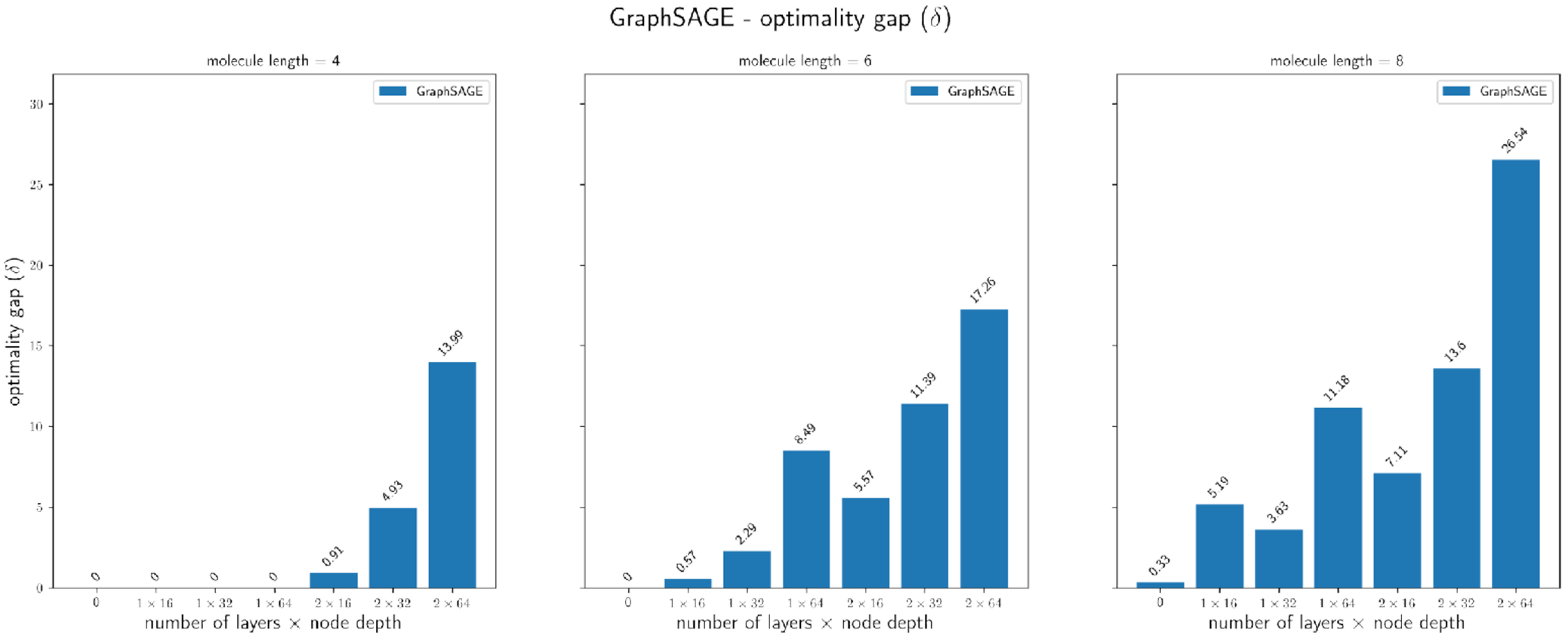
examine output molecules by human expert scientist

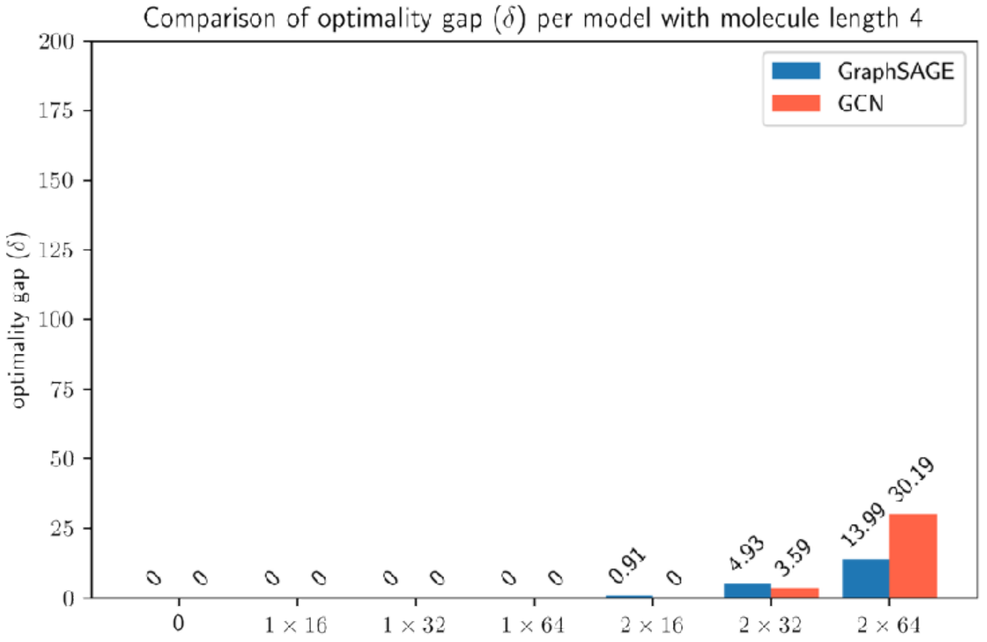


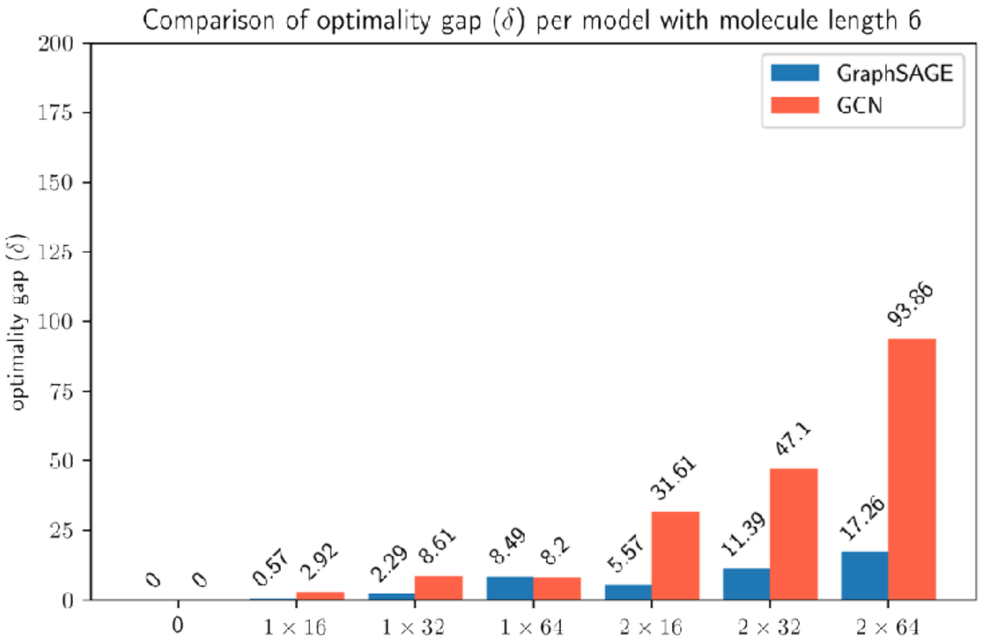


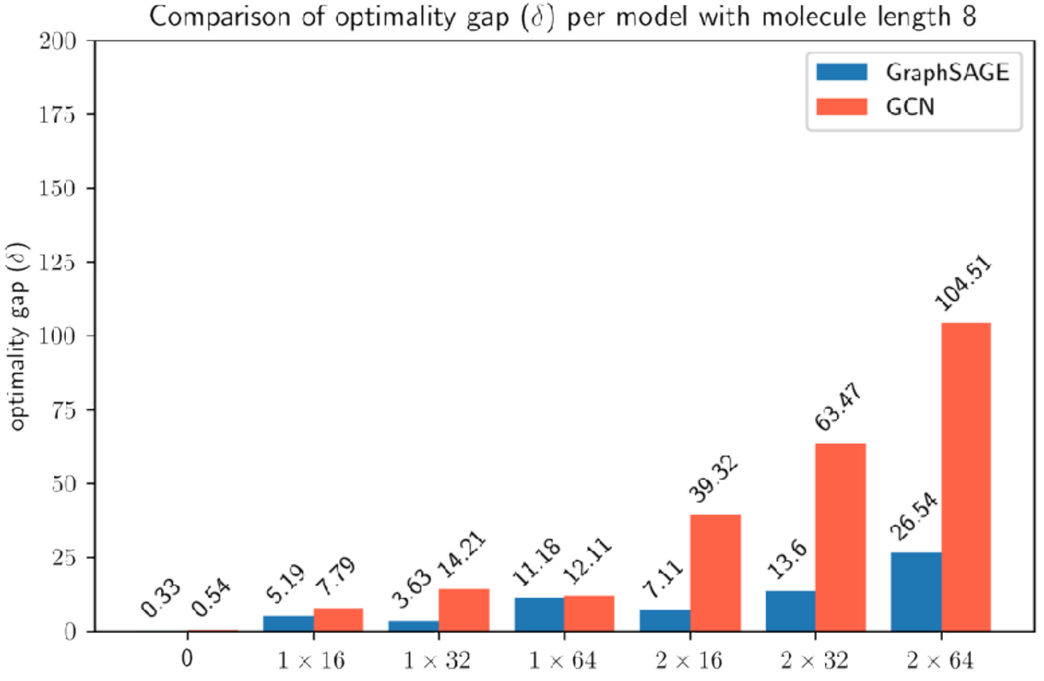


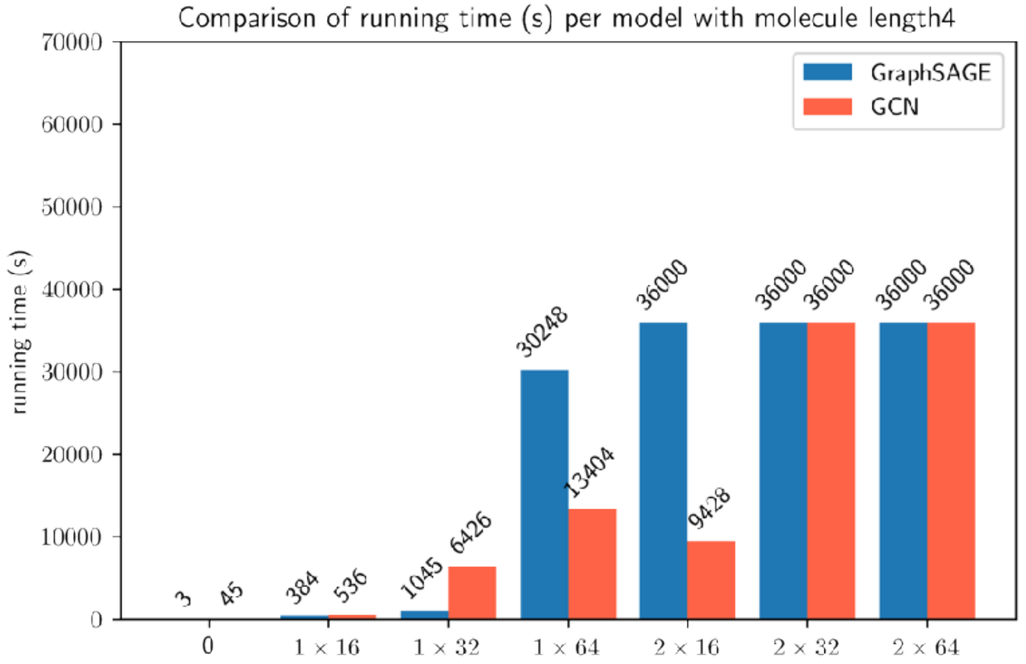


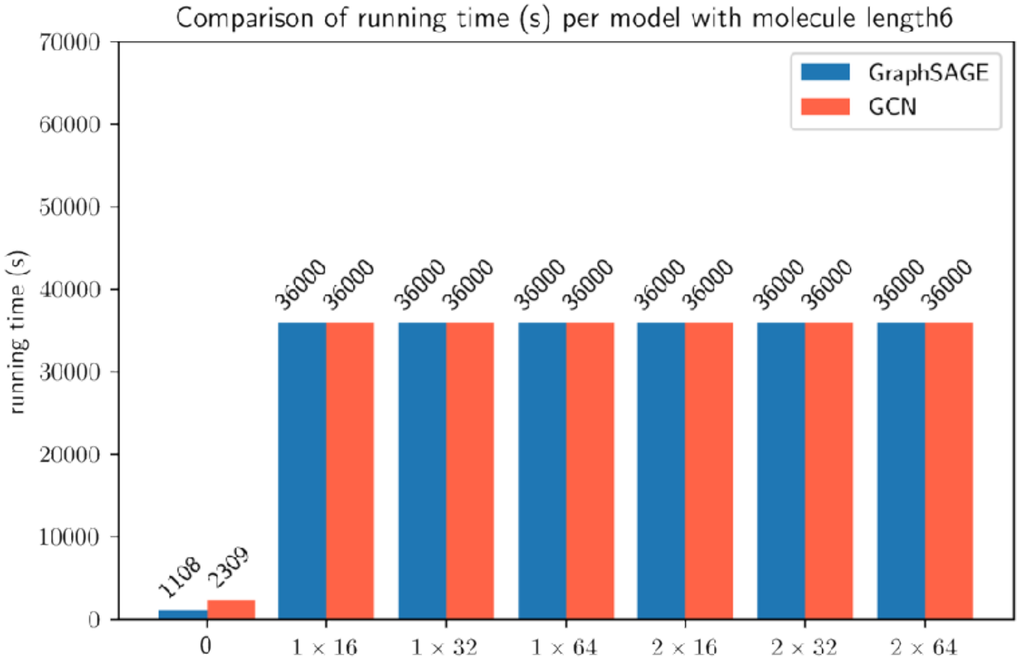


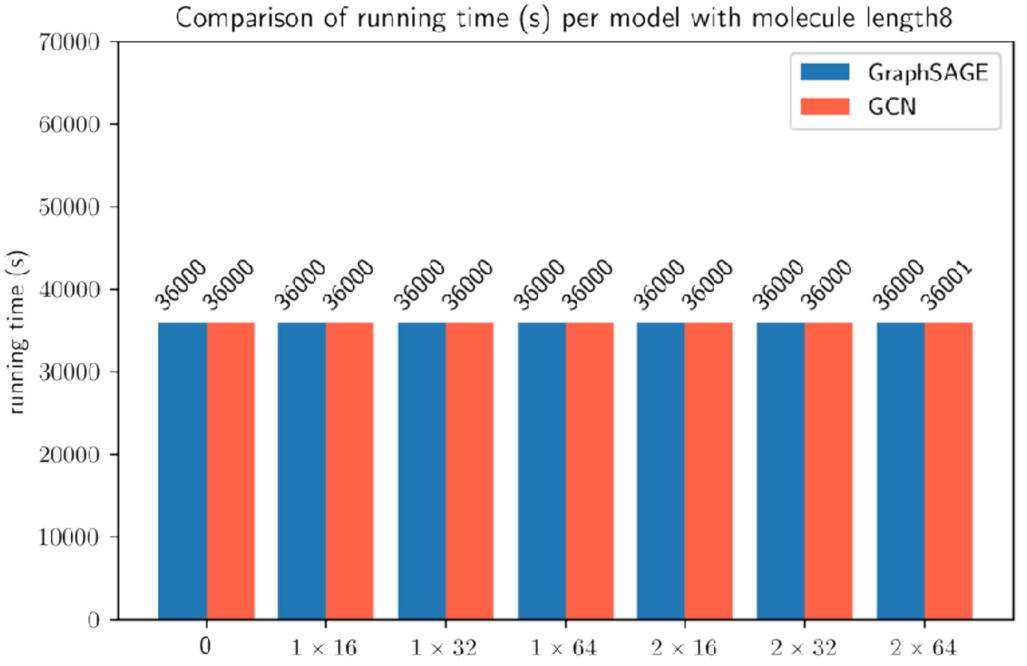


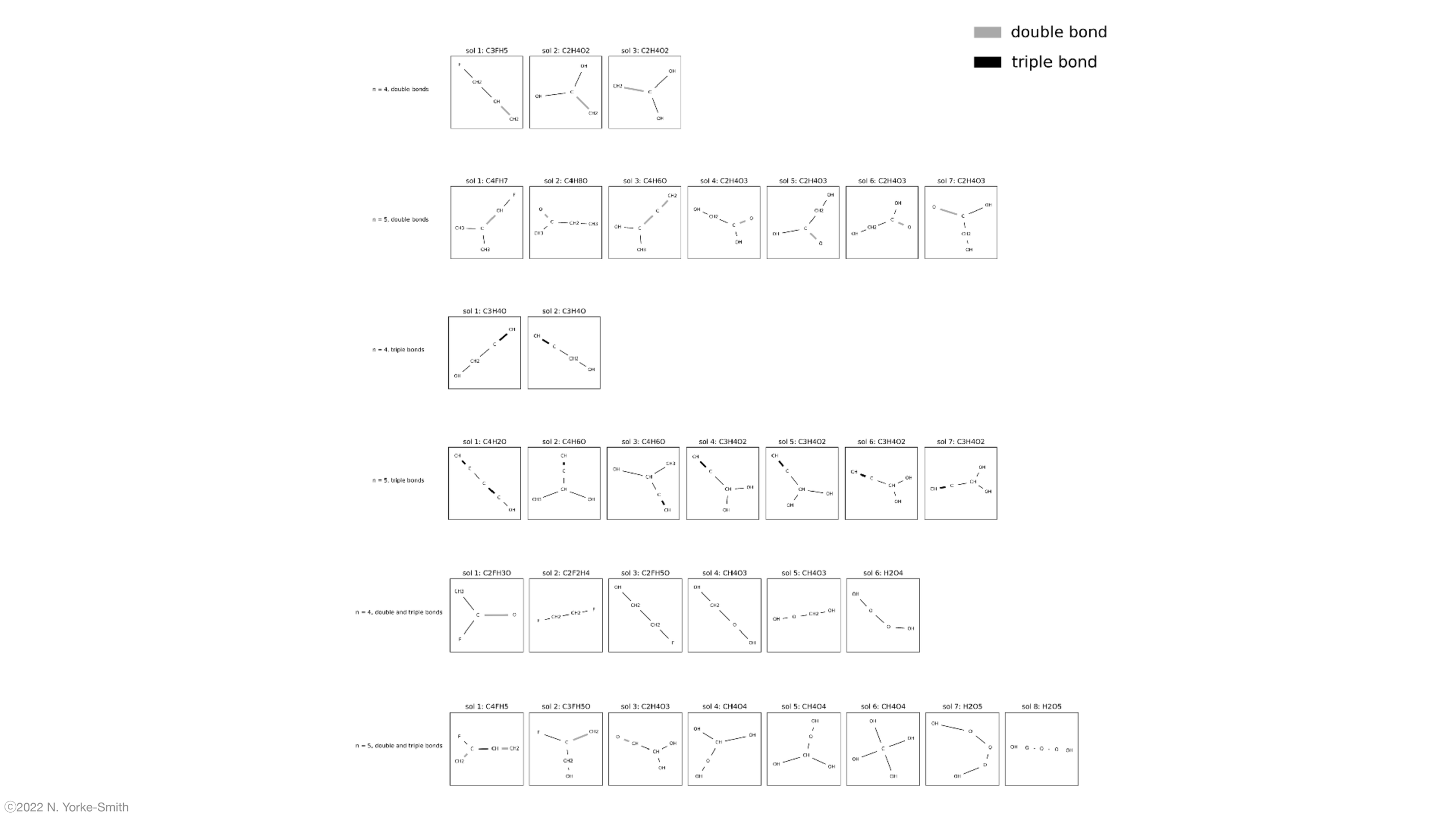












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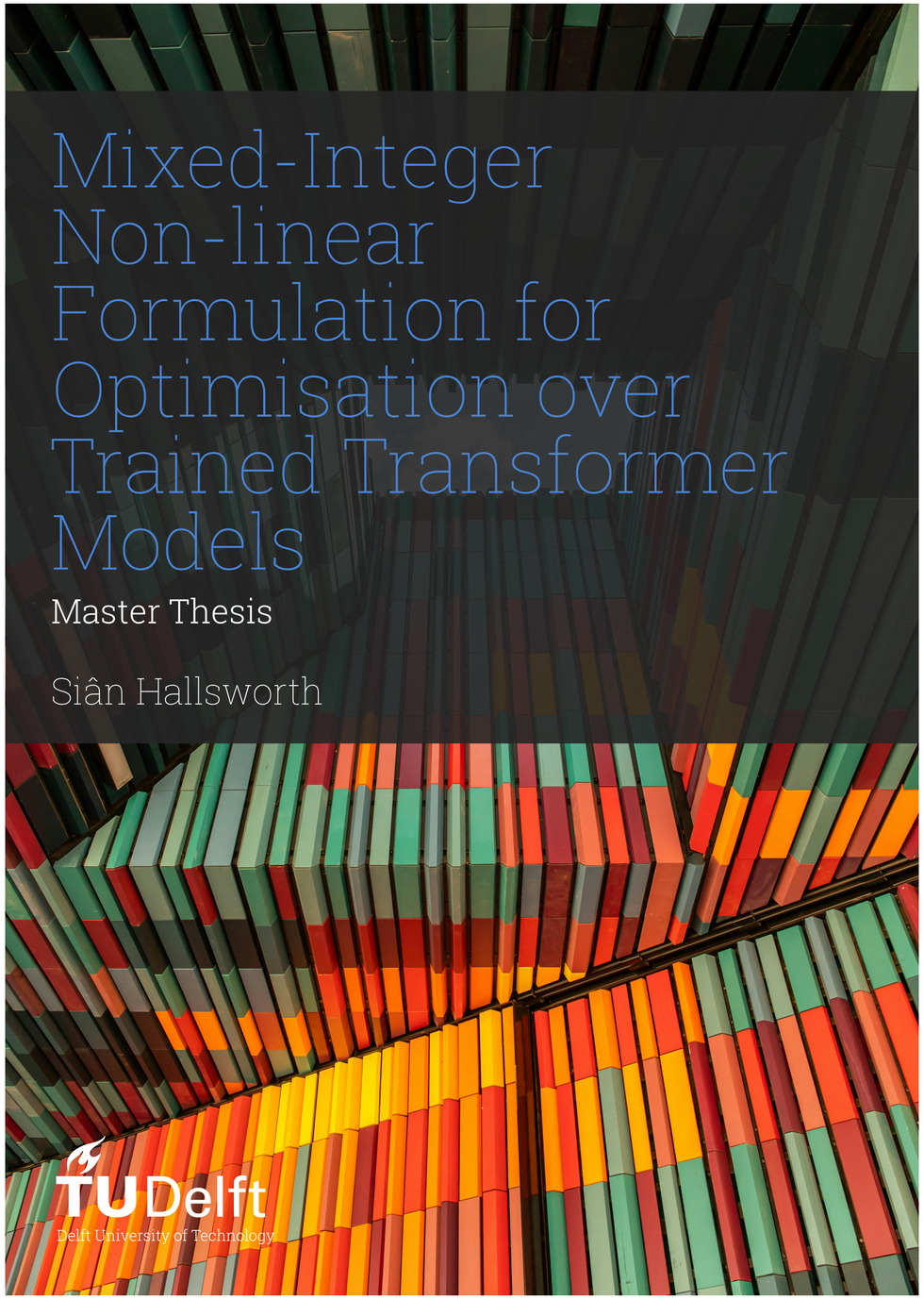

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