# PERFORMANCE EVALUATION OF THE TENSOR TRAIN SAMPLER IN QUBO-BASED MACHINE LEARING ADMET CLASSIFICATION

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## ABSTRACT

Quantum Annealing (QA) on D-Wave's Advantage system and Tensor Train (TT) sampling are compared for QUBO-based ADMET classification. QA-based methods (QSVM, QBoost) leverage quantum effects to escape local minima, while TT sampling employs low-rank decompositions for efficient high-dimensional data handling. Benchmarks highlight TT sampling's potential for improved optimization in drug discovery.

## 1 INTRODUCTION

Quantum computing introduces novel methods for tackling combinatorial optimization via Quantum Annealing (QA), which reformulates problems as Quadratic Unconstrained Binary Optimization (QUBO) tasks Salloum et al. (2024c;b;a). Despite its promise, QA suffers from limited connectivity, as noted in previous work on QSVM and QBoost Salloum et al. (2025). In contrast, TT sampling, by decomposing high-dimensional tensors into sequentially combined core tensors Oseledets (2011), offers a scalable alternative for solving large QUBO problems Batsheva et al. (2023); Ryzhakov et al. (2024); Nikitin et al. (2022). We evaluate TT sampling for ADMET classification in drug discovery and compare its performance to QA-based and classical approaches.

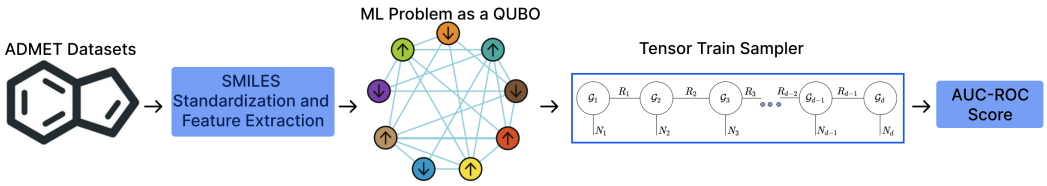


Figure 1: Quantum-Inspired Machine Learning Pipeline for ADMET Classification

Building on Salloum et al. (2025), this work introduces a Tensor Train (TT) decomposition-based approach, leveraging probabilistic tensor sampling to solve QUBO formulations. TT sampling efficiently handles high-dimensional data via structured decompositions, enabling scalable optimization. We evaluate this method on QUBO-based ML models for ADMET drug discovery datasets, benchmarking against D-Wave's QA models (e.g., QSVM, QBoost) and classical approaches like LightAutoML, comparing performance with prior reported results.

## 2 METHODOLOGY

TT decomposition represents a tensor $A \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ as:

$$A(i_1, i_2, \ldots, i_d) = \sum_{\alpha_1=1}^{r_1} \sum_{\alpha_2=1}^{r_2} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} G_1(i_1, \alpha_1) G_2(\alpha_1, i_2, \alpha_2) \cdots G_d(\alpha_{d-1}, i_d), \tag{1}$$

TT sampling efficiently approximates high-dimensional joint distributions $P(w)$ by sequentially sampling variables $w_1, w_2, \ldots, w_d$, conditioned on previously sampled values. This transforms high-dimensional sampling into a series of low-dimensional steps, avoiding the curse of dimensionality. The TT decomposition represents $P(w)$ using low-rank cores, enabling efficient computation of marginal and conditional probabilities. At each step, $w_k$ is sampled from:

$$P(w_k | w_1, \ldots, w_{k-1}) = \frac{P(w_1, \ldots, w_k)}{P(w_1, \ldots, w_{k-1})}, \tag{2}$$

computed via incremental core contractions, avoiding explicit high-dimensional tensor operations. TT sampling reduces complexity from $O(n^d)$ to $O(dnr^2)$, making it scalable. Figure 1 outlines the overall pipeline: starting from ADMET datasets (with molecular structures in SMILES format), the problem is formulated as a QUBO and then optimized using the TT sampler, with performance evaluated via the AUC-ROC metric.

## 3 RESULTS AND NOTABLE EXCEPTIONS

Table 1 shows that while LightAutoML outperforms other models on 9 of 10 ADMET datasets, tensor-based TT-Sampler models (TT-Boost, TT-SVM) consistently deliver strong performance—especially on datasets like #5 (BBB_Martins) and #8 (hERG) where feature interactions are critical. The key observations include:

- **Dataset #10 (Carcinogens_Lagunin):** TT-SVM scores 0.8876 versus LightAutoML's 0.8258, demonstrating the efficacy of tensor methods for complex toxicity endpoints.
- **Dataset #3 (Pgp_Broccatelli):** QSVM records 0.6102 compared to TT-SVM's 0.8203, highlighting the challenges QA models face with non-linear decision boundaries.

Figures 2 and 3 illustrate these performance differences.

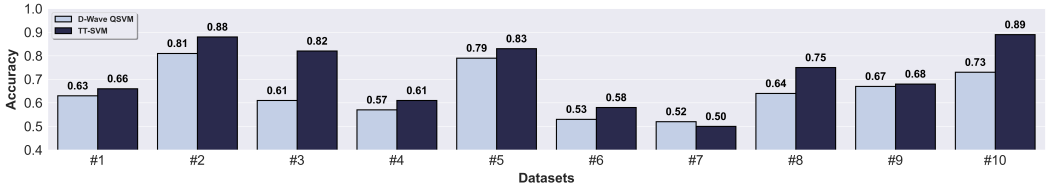


Figure 2: QSVM vs. TT-SVM

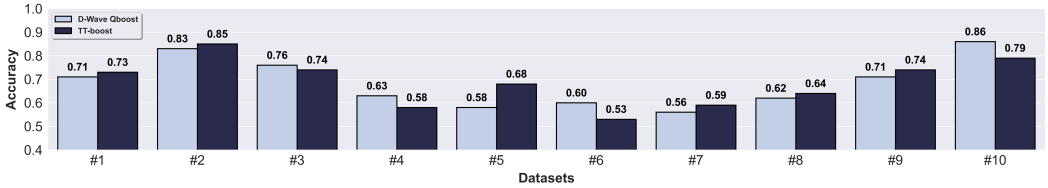


Figure 3: QBoost vs. TT-Boost

## 4 CONCLUSION

Although LightAutoML remains a strong baseline, tensor-based methods—especially those leveraging the TT-Sampler—offer a robust and practical approach for ADMET prediction. Notably, the TT-Sampler proves to be an excellent tool for solving QUBO problems, efficiently capturing complex feature interactions. In contrast, QA models still require significant refinement to address scalability and stability challenges. Future work should explore hybrid models that integrate tensor decomposition with QA to further enhance predictive performance.

### ACKNOWLEDGMENTS

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## A SUPPLEMENTARY MODEL EVALUATION RESULTS

Table 1: AUC-ROC Scores for ADMET Classification Models

| Dataset | LightAutoML | QBoost | QSVM | TT-Boost | TT-SVM |
|---|---|---|---|---|---|
| PAMPA_NCATS (#1) | **0.8463** | 0.7102 | 0.6316 | 0.7312 | 0.6563 |
| HIA_Hou (#2) | **0.9962** | 0.8323 | 0.8123 | 0.8489 | 0.8779 |
| Pgp_Broccatelli (#3) | **0.9446** | 0.7638 | 0.6102 | 0.7434 | 0.8203 |
| Bioavailability_Ma (#4) | **0.7599** | 0.6254 | 0.5713 | 0.5829 | 0.6129 |
| BBB_Martins (#5) | **0.9310** | 0.5826 | 0.7939 | 0.6812 | 0.8336 |
| CYP2C9_Substrate (#6) | **0.6975** | 0.6048 | 0.5347 | 0.5310 | 0.5753 |
| CYP3A4_Substrate (#7) | **0.6442** | 0.5554 | 0.5204 | 0.5910 | 0.4937 |
| hERG (#8) | **0.8185** | 0.6155 | 0.6382 | 0.6440 | 0.7519 |
| DILI (#9) | **0.9113** | 0.7103 | 0.6689 | 0.7374 | 0.6769 |
| Carcinogens_Lagunin (#10) | 0.8258 | 0.8614 | 0.7306 | 0.7897 | **0.8876** |

*Note*: Bold values indicate the highest score per dataset.
AUC-ROC scores closer to 1.0 represent better performance. TT methods show competitive results, particularly for datasets #2, #5, and #10, while LightAutoML dominates most benchmarks.