Genetic algorithm optimization of tree-based models to predict cargo- and

carrier-related factors affecting drug release from liposomes

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Fig. S1 Scatter plots based on XGBoost-genetic algorithm predictions. T20%: time required for releasing 20% of drug molecules; T50%: time required for releasing 50% of drug molecules



Fig. S2 Scatter plots based on random forest-genetic algorithm predictions. T20%: time required for releasing 20% of drug molecules; T50%: time required for releasing 50% of drug molecules



Fig. S3 SHAP summary plots of compounds with a log P > 1. MW: molecular weight; T20%: time required for releasing 20% of drug molecules; T50%: time required for releasing 50% of drug molecules; Tm: phase transition temperature



Fig. S4 SHAP summary plots of compounds with a log P < 1. MW: molecular weight; T20%: time required for releasing 20% of drug molecules; T50%: time required for releasing 50% of drug molecules; Tm: phase transition temperature



Fig. S5 SHAP summary plots of all compounds included in the dataset. MW: molecular weight; T20%: time required for releasing 20% of drug molecules; T50%: time required for releasing 50% of drug molecules; Tm: phase transition temperature