Supporting Information

Data-driven derivation of molecular substructures that enhance drug activity in Gram-negative bacteria

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Synthetic Data Generation

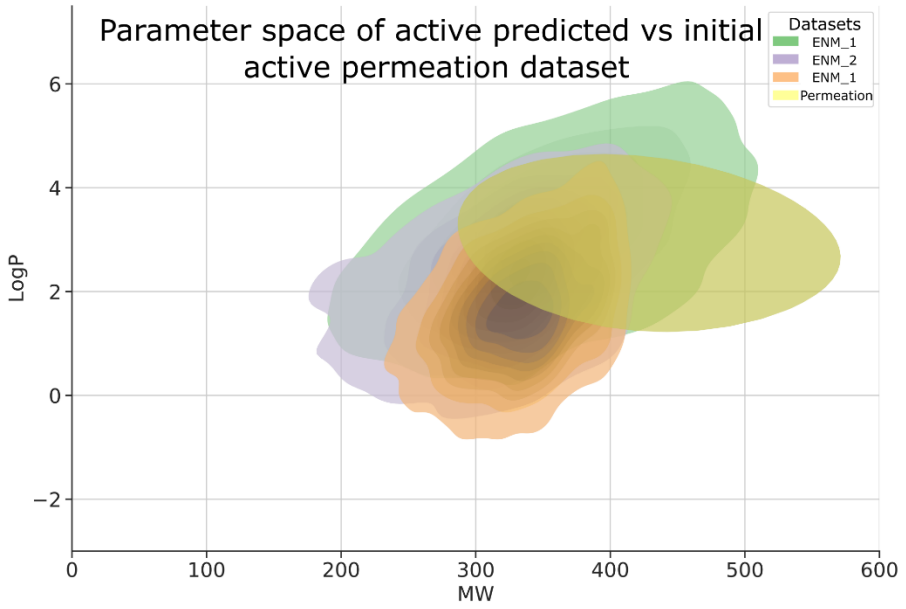

Fig. S1: Chemical space, represented by LogP and MW parameters, for three datasets: ENM_1--ENM_3 used to predict permeation compared to the initial permeation dataset (GN-actives only).

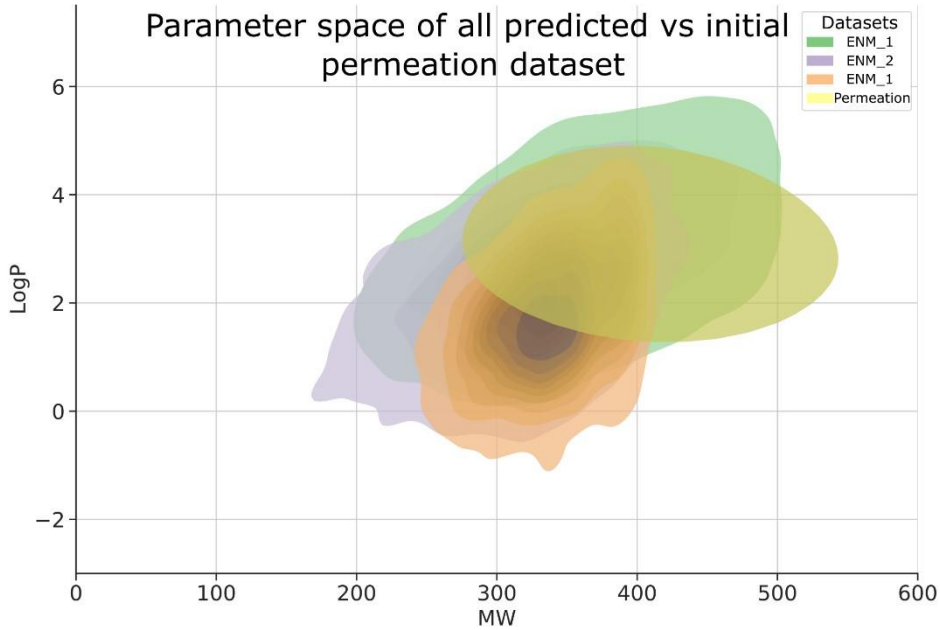

Fig. S2: Chemical space, represented by LogP and MW parameters, for three datasets: ENM_1--ENM_3 used to predict permeation compared to the initial permeation dataset (all data).

Distributions of pMIC caused by transforms from Tab. 5

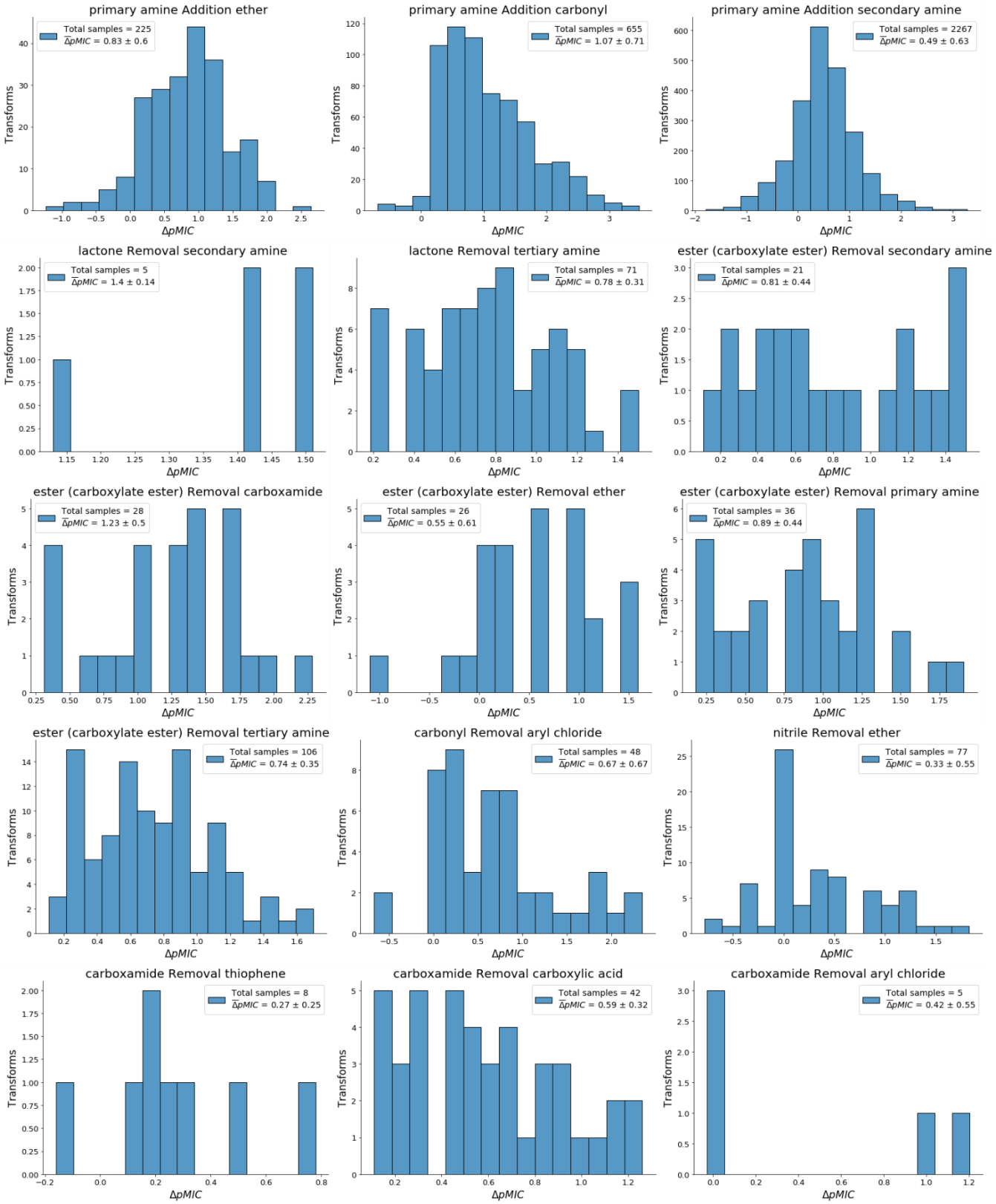

Fig. S3: Distributions of change in pMIC caused by every transform from Tab. 5. Histogram titles correspond to first three columns of Tab. 5: 'Main Moiety', '±', 'Exchange Moiety' for every transform. (part 1)

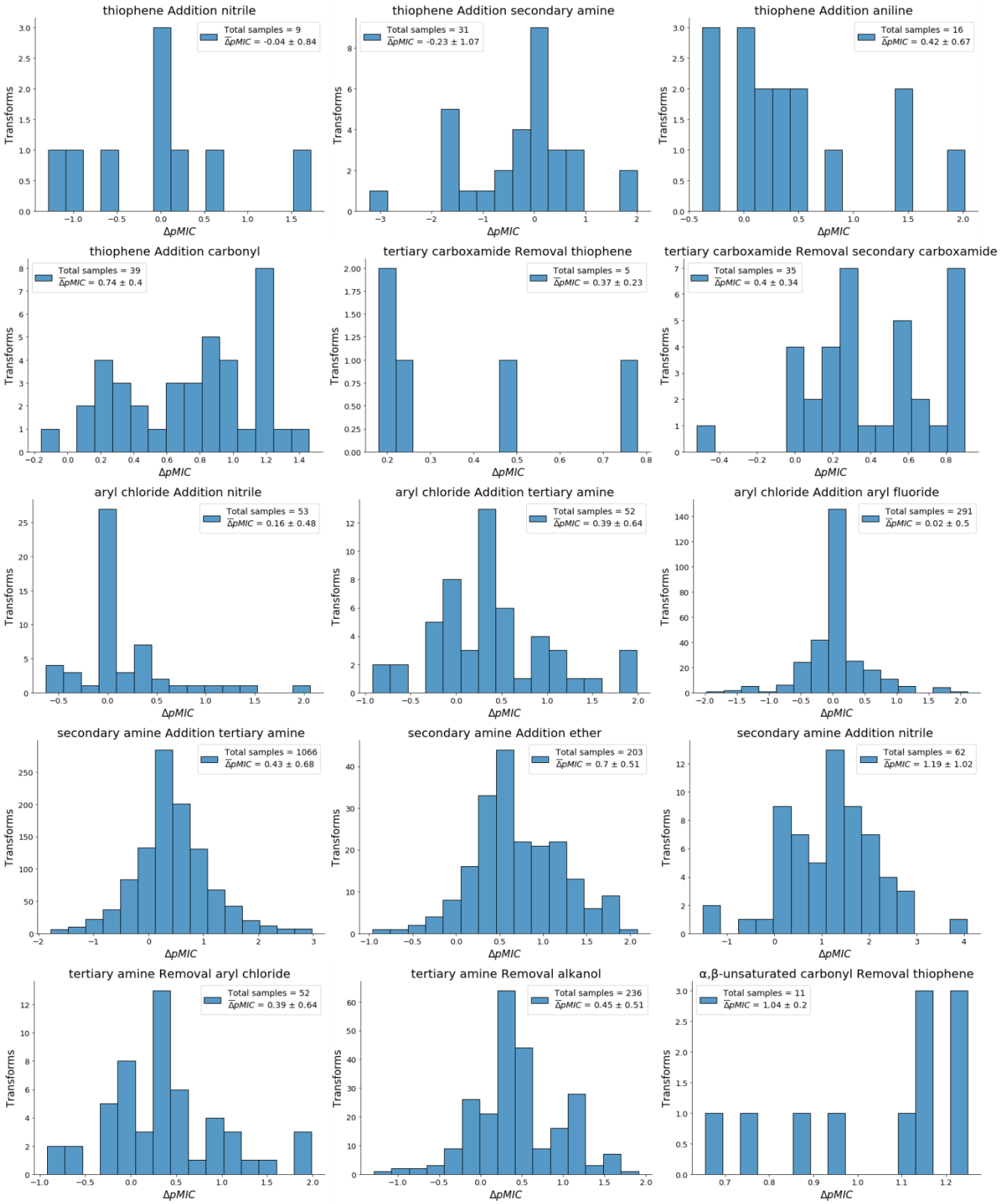

Fig. S3: Distributions of change in pMIC caused by every transform from Tab. 5. Histogram titles correspond to first three columns of Tab. 5 : 'Main Moiety', '±', 'Exchange Moiety' for every transform. (part 2)

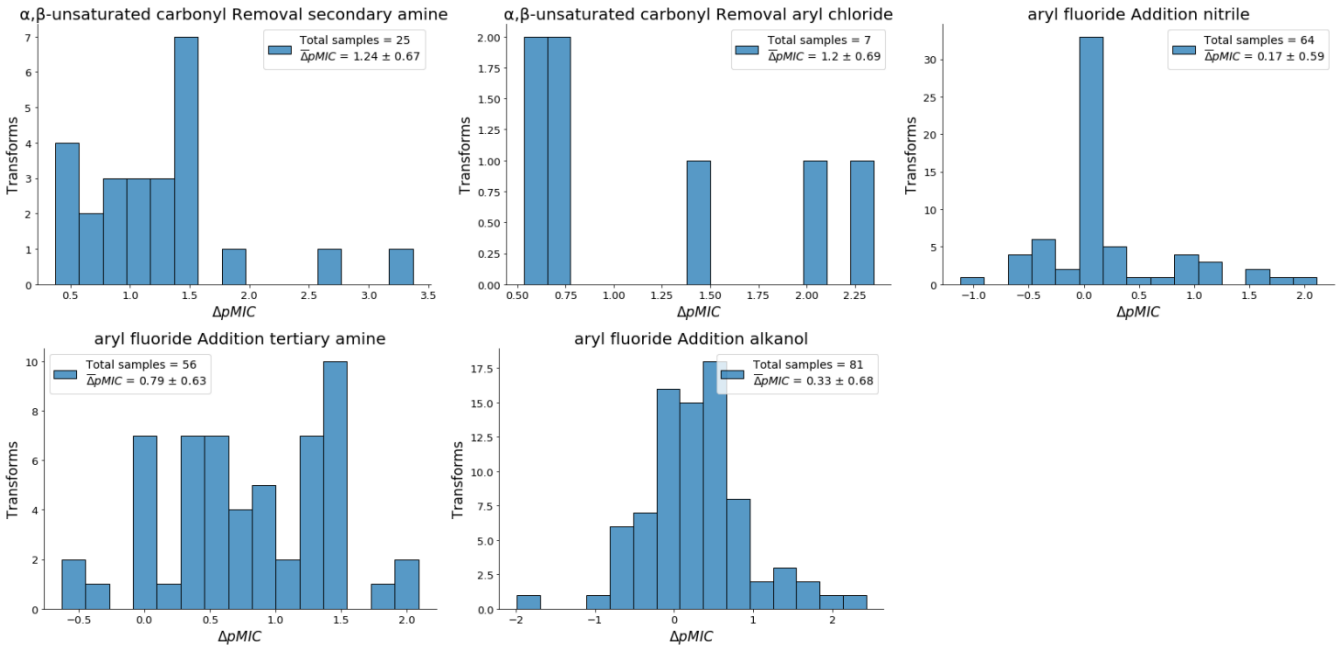

Fig. S3: Distributions of change in pMIC caused by every transform from Tab. 5. Histogram titles correspond to first three columns of Tab. 5 : 'Main Moiety', '±', 'Exchange Moiety' for every transform. (part 3)