

IARA Results

1. Overview

Initial query compounds	1
Compounds successfully predicted	1
Compounds excluded due to lack of targets	0

2. Query Compound Profiling

Compound Name	Chemical Structure	ChEMBL ID	Presence in Training Set	Target Proteins	Morgan Fingerprint
QUERY_COMP_X	-	-	-	3	NO (Zero-Padded)

3. Compound-Target Protein Mapping

Compound Name	ChEMBL ID	Target Uniprot ID	Uniprot Name	Organism	PCHEMBL Value	Linked to PPI?
QUERY_COMP_X	-	P03372	Estrogen receptor	Homo sapiens	7.0	YES
QUERY_COMP_X	-	P10275	Androgen receptor	Homo sapiens	6.0	YES
QUERY_COMP_X	-	Q14994	Nuclear receptor subfamily 1 g...	Homo sapiens	7.0	YES

4. Organ-specific Predictions

AD: Applicability Domain

ChEMBL ID	Compound Name	HEART Youden Threshold: 0.64	LIVER Youden Threshold: 0.34	NERVOUS SYSTEM Youden Threshold: 0.57	KIDNEY Youden Threshold: 0.59
-	QUERY_COMP_X	Hazard (0.87) In AD	Hazard (0.77) Out AD	Hazard (0.89) In AD	No Hazard (0.31) In AD

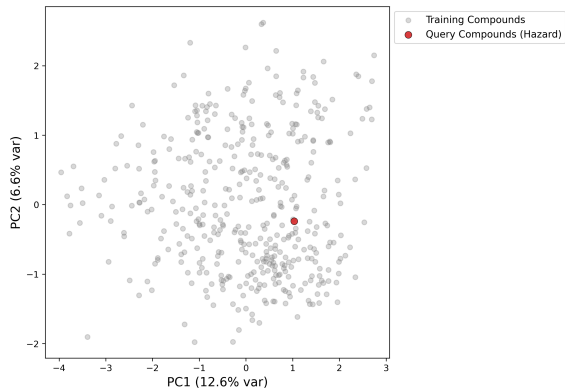
5. Applicability Domain

The Applicability Domain (AD) evaluates whether a query compound is similar enough to the model's training data to ensure a reliable prediction. If a compound lies beyond the dataset's coverage, the model's prediction carries higher uncertainty. To evaluate this, two plots are shown below:

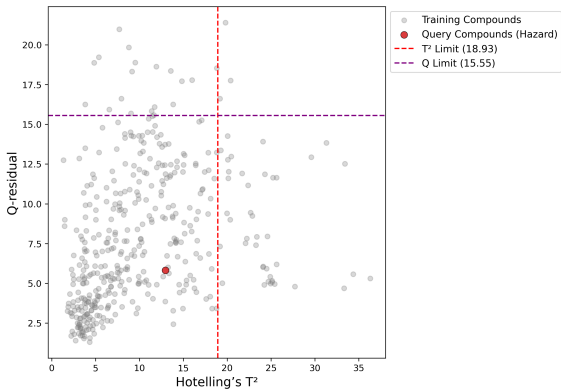
- PCA Projection Maps:** Compare the features of query compounds against the training distribution to highlight whether they fall within the model's feature space or lie outside it.
- Limits Boundary Plots:** Display Hotelling's T² and Q-residual thresholds to determine whether each compound sits within the model's statistical reliability boundary.

HEART

PCA PROJECTION MAP
Heart Latent Space



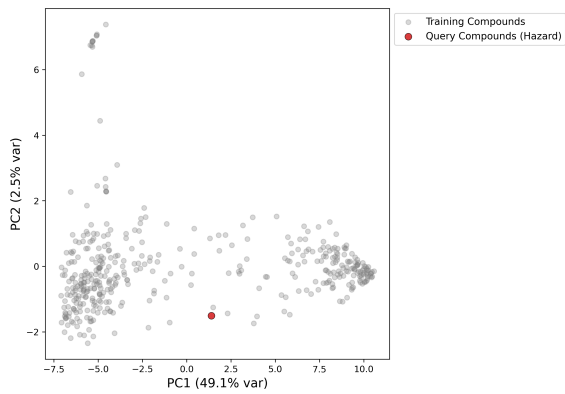
LIMITS BOUNDARY DISTRIBUTION
Heart T² vs Q-Residual Space



LIVER

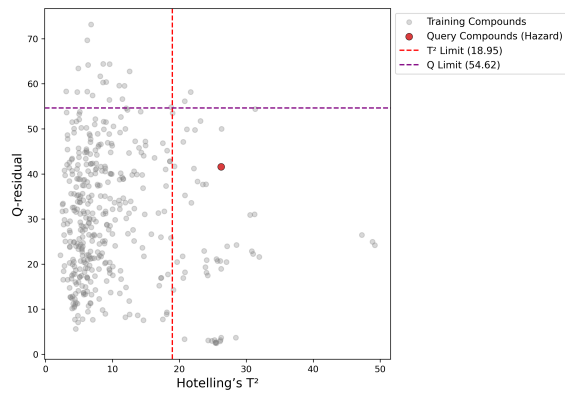
PCA PROJECTION MAP

Liver Latent Space



LIMITS BOUNDARY DISTRIBUTION

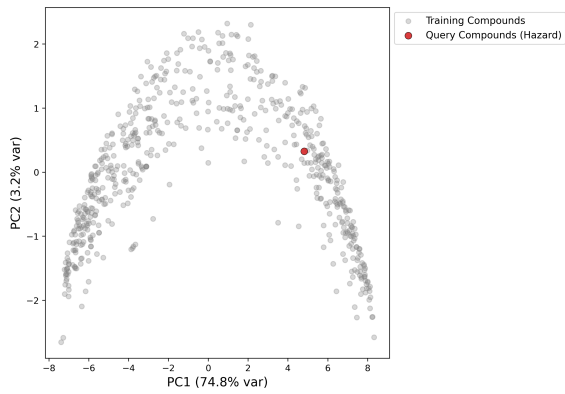
Liver T² vs Q-Residual Space



NERVOUS SYSTEM

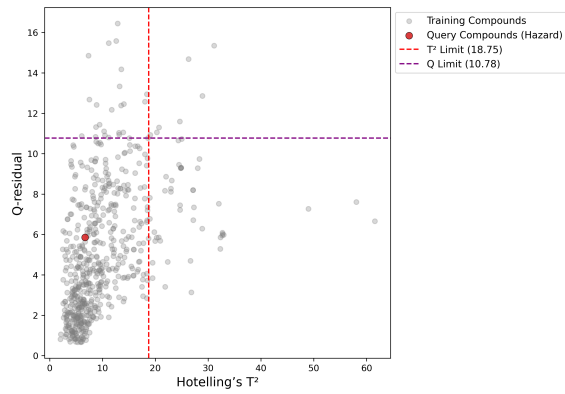
PCA PROJECTION MAP

Nervous System Latent Space



LIMITS BOUNDARY DISTRIBUTION

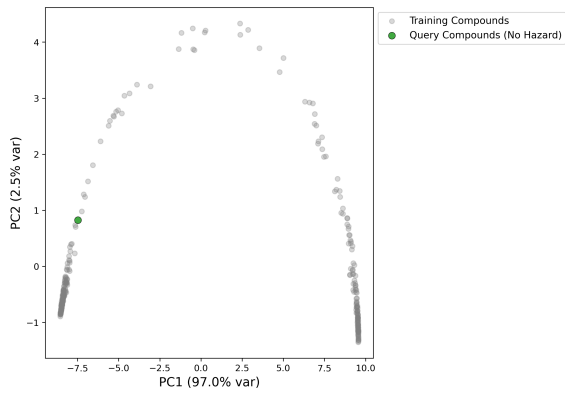
Nervous System T² vs Q-Residual Space



KIDNEY

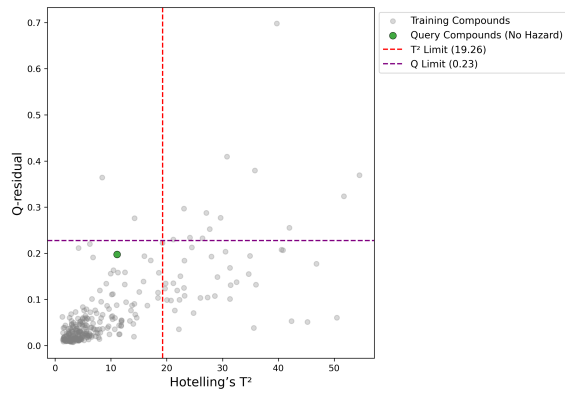
PCA PROJECTION MAP

Kidney Latent Space



LIMITS BOUNDARY DISTRIBUTION

Kidney T² vs Q-Residual Space



6. Excluded Query Compounds

No compounds were excluded. All query compounds have at least one protein target.