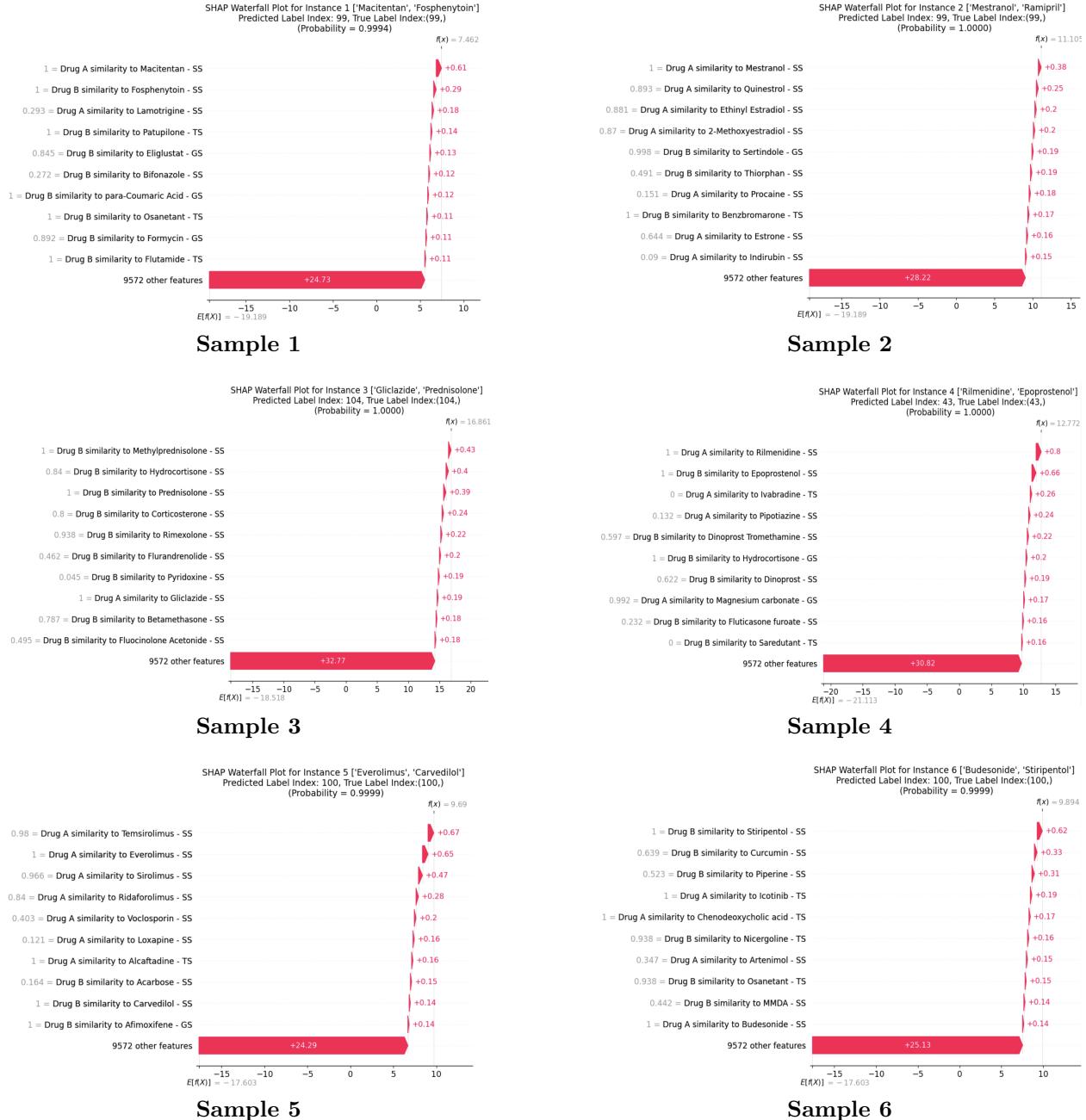
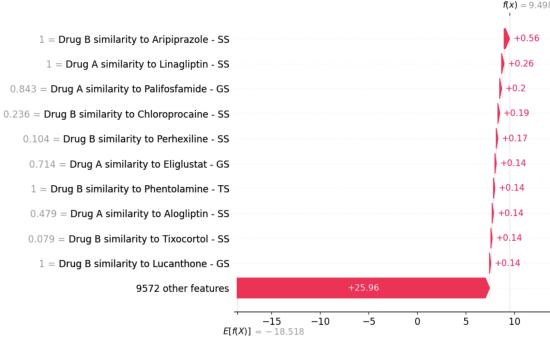


1 Supplementary material - Waterfall plots for all the 48 samples in the test dataset.

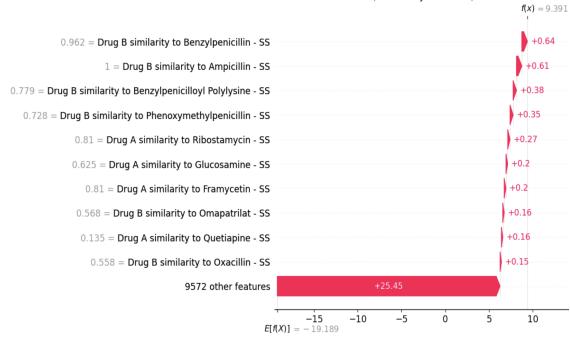


SHAP Waterfall Plot for Instance 7 ['Linagliptin', 'Aripiprazole']
Predicted Label Index: 104, True Label Index:(104.)
(Probability = 0.9999)



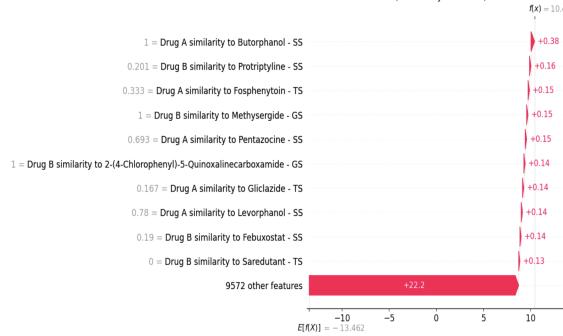
Sample 7

SHAP Waterfall Plot for Instance 8 ['Gentamicin', 'Ampicillin']
Predicted Label Index: 99, True Label Index:(99.)
(Probability = 0.9999)



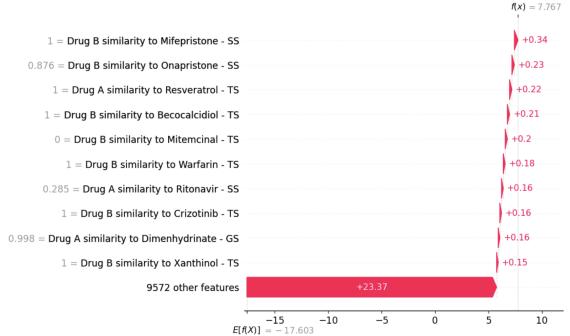
Sample 8

SHAP Waterfall Plot for Instance 9 ['Butorphanol', 'Sulpiride']
Predicted Label Index: 73, True Label Index:(73.)
(Probability = 1.0000)



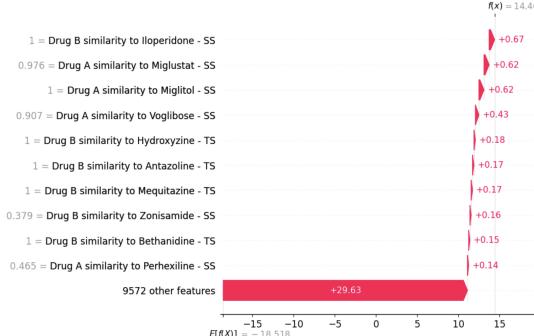
Sample 9

SHAP Waterfall Plot for Instance 10 ['Dabrafenib', 'Mifepristone']
Predicted Label Index: 100, True Label Index:(100.)
(Probability = 0.9996)



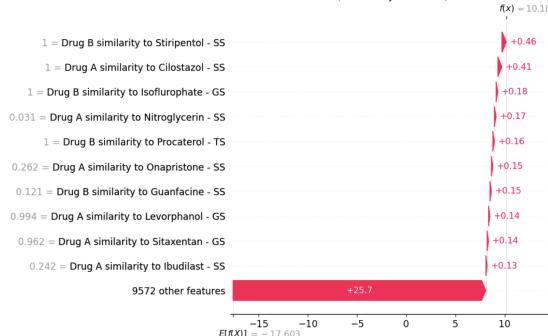
Sample 10

SHAP Waterfall Plot for Instance 11 ['Miglitol', 'Iloperidone']
Predicted Label Index: 104, True Label Index:(104.)
(Probability = 1.0000)



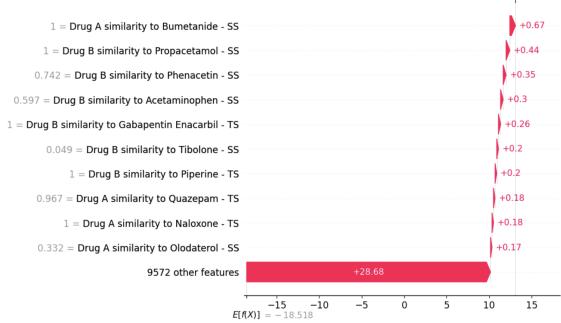
Sample 11

SHAP Waterfall Plot for Instance 12 ['Cilostazol', 'Stiripentol']
Predicted Label Index: 100, True Label Index:(100.)
(Probability = 1.0000)



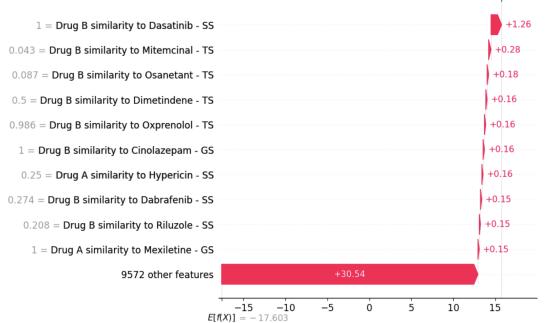
Sample 12

SHAP Waterfall Plot for Instance 13 ['Bumetanide', 'Propacetamol']
Predicted Label Index: 104, True Label Index:(104.)
(Probability = 1.0000)



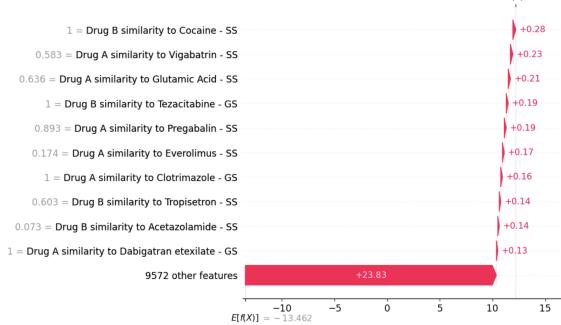
Sample 13

SHAP Waterfall Plot for Instance 14 ['Levomephentanyl Acetate', 'Dasatinib']
Predicted Label Index: 100, True Label Index:(100.)
(Probability = 1.0000)



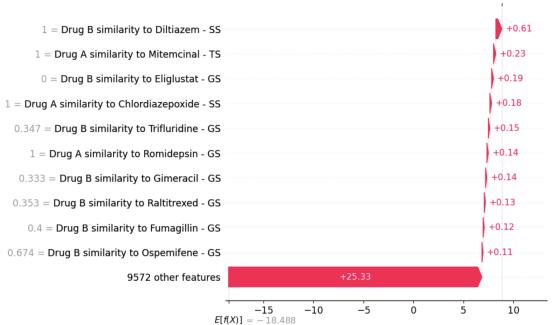
Sample 14

SHAP Waterfall Plot for Instance 15 ['Gabapentin', 'Cocaine']
Predicted Label Index: 73, True Label Index:(73.)
(Probability = 1.0000)



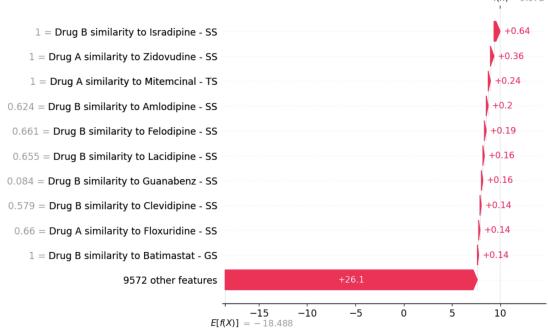
Sample 15

SHAP Waterfall Plot for Instance 16 ['Chlordiazepoxide', 'Diltiazem']
Predicted Label Index: 68, True Label Index:(68.)
(Probability = 0.9999)



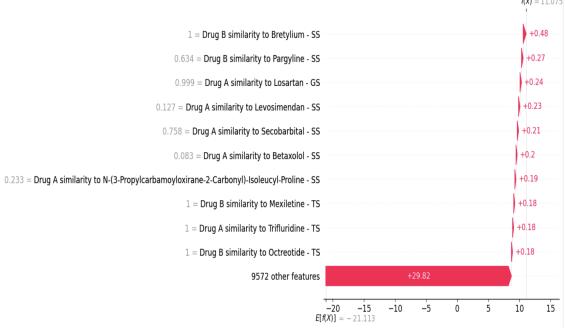
Sample 16

SHAP Waterfall Plot for Instance 17 ['Zidovudine', 'Isradipine']
Predicted Label Index: 68, True Label Index:(68.)
(Probability = 1.0000)

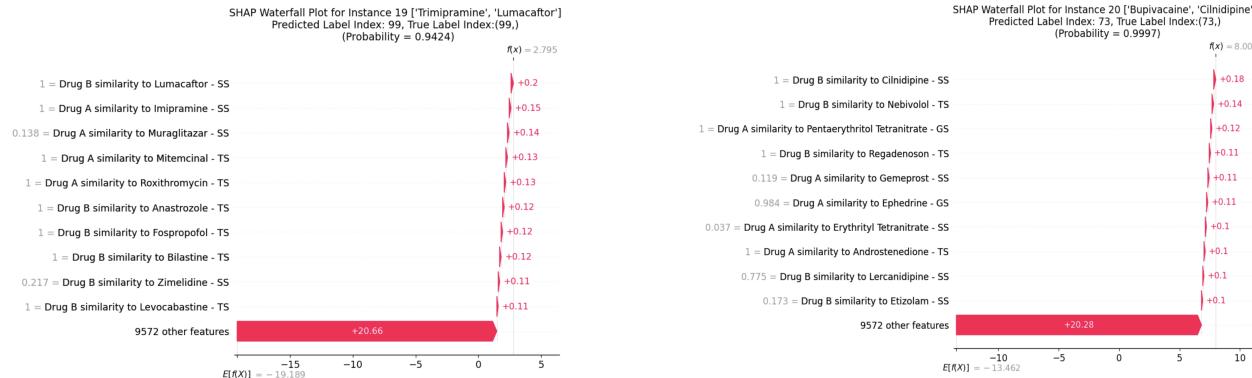


Sample 17

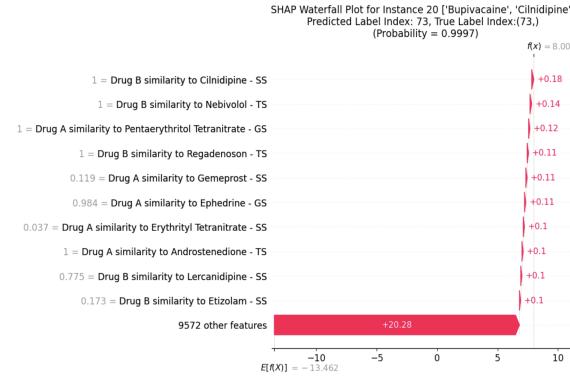
SHAP Waterfall Plot for Instance 18 ['Thiamylal', 'Bretlyium']
Predicted Label Index: 43, True Label Index:(43.)
(Probability = 1.0000)



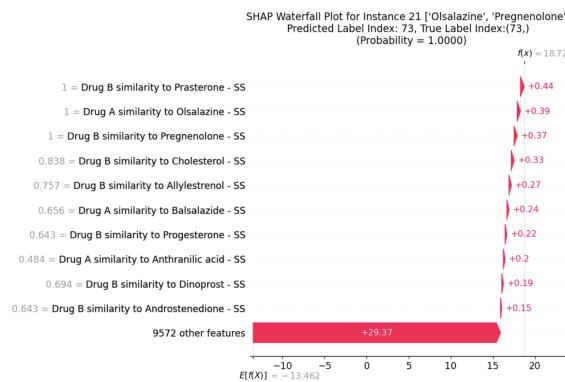
Sample 18



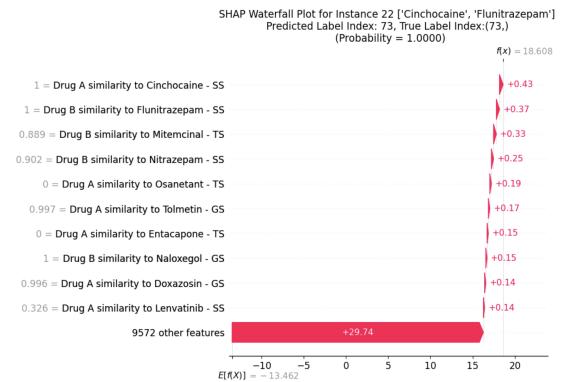
Sample 19



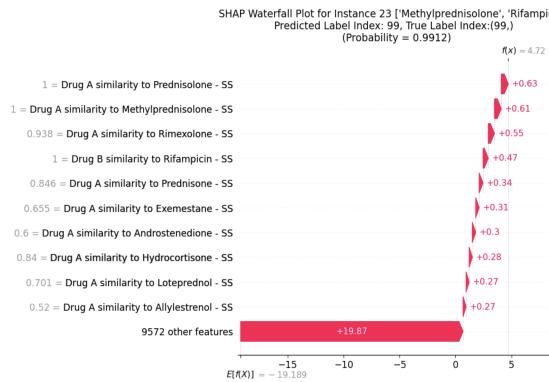
Sample 20



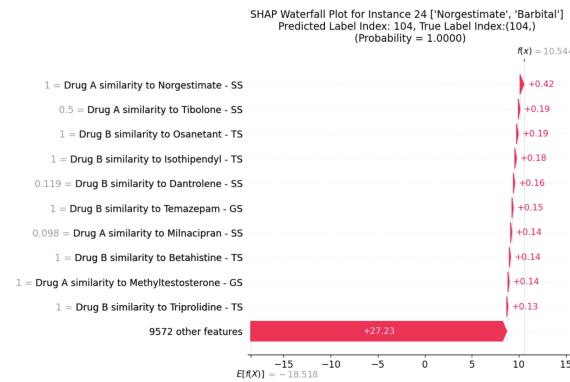
Sample 21



Sample 22

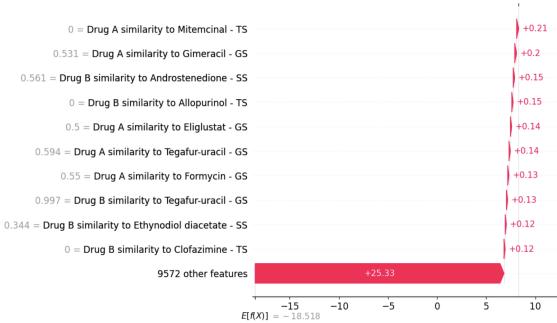


Sample 23



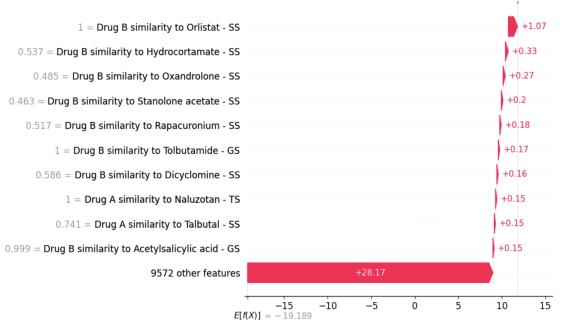
Sample 24

SHAP Waterfall Plot for Instance 25 ['Empagliflozin', 'Dienogest']
Predicted Label Index: 104, True Label Index(104.)
(Probability = 0.9998)



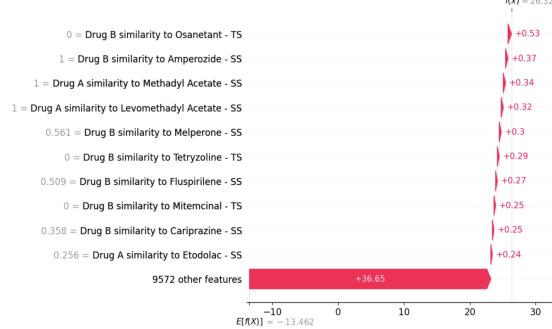
Sample 25

SHAP Waterfall Plot for Instance 26 ['Methibarbil', 'Orlistat']
Predicted Label Index: 99, True Label Index(99.)
(Probability = 1.0000)



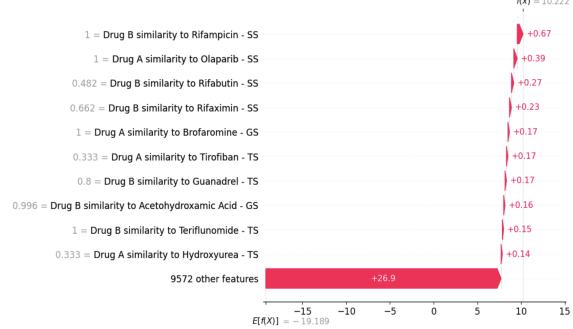
Sample 26

SHAP Waterfall Plot for Instance 27 ['Methadyl Acetate', 'Amperozide']
Predicted Label Index: 73, True Label Index(73.)
(Probability = 1.0000)



Sample 27

SHAP Waterfall Plot for Instance 28 ['Olaparib', 'Rifampicin']
Predicted Label Index: 99, True Label Index(99.)
(Probability = 1.0000)



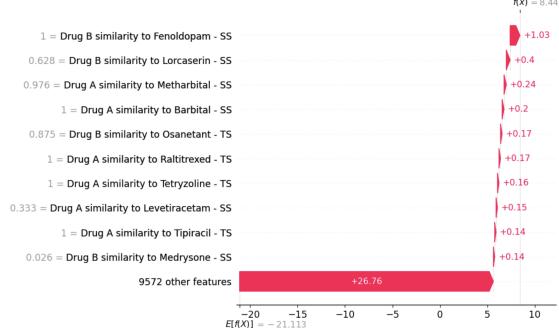
Sample 28

SHAP Waterfall Plot for Instance 29 ['Alfentanil', 'Methocarbamol']
Predicted Label Index: 73, True Label Index(73.)
(Probability = 1.0000)



Sample 29

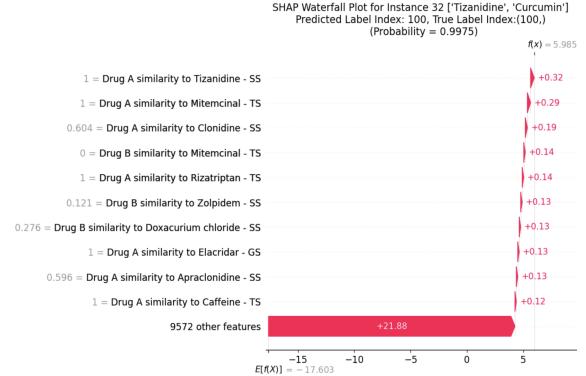
SHAP Waterfall Plot for Instance 30 ['Barbital', 'Fenoldopam']
Predicted Label Index: 43, True Label Index(43.)
(Probability = 0.9998)



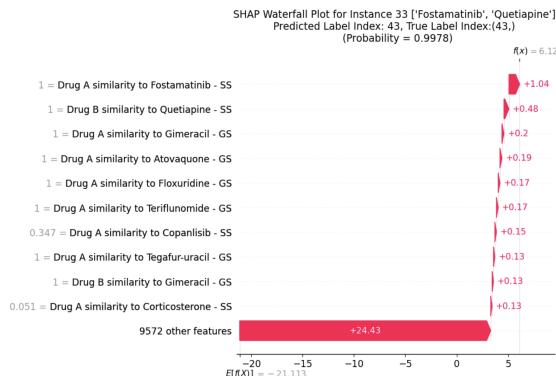
Sample 30



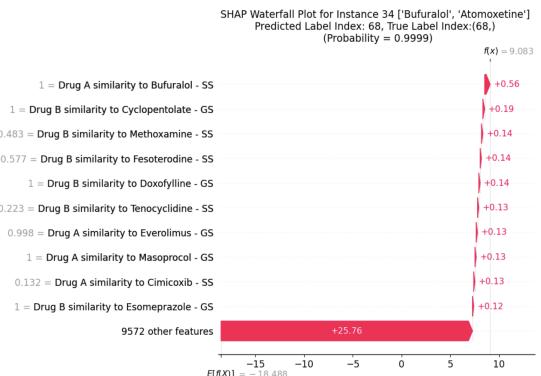
Sample 31



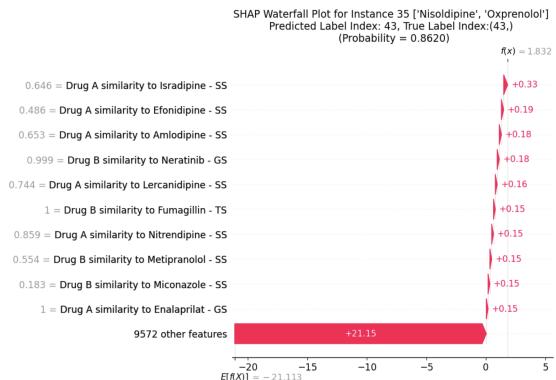
Sample 32



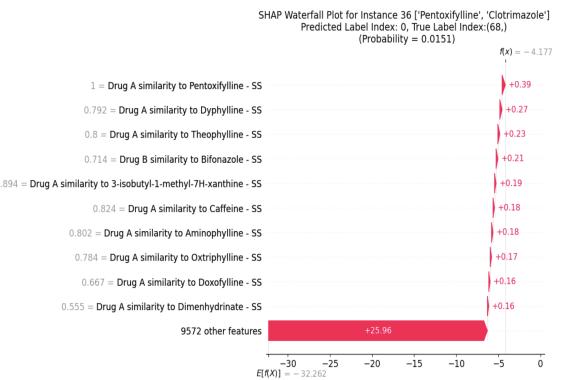
Sample 33



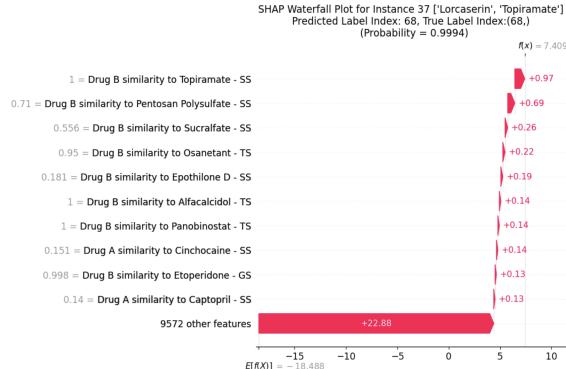
Sample 34



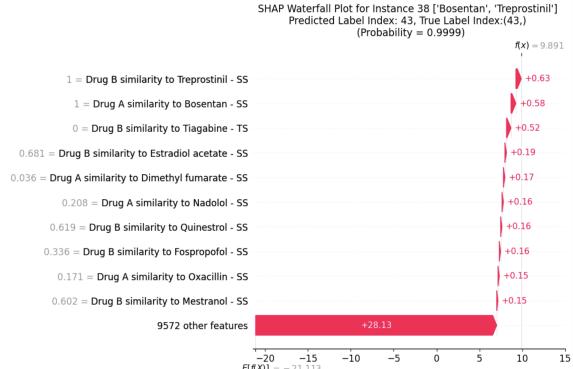
Sample 35



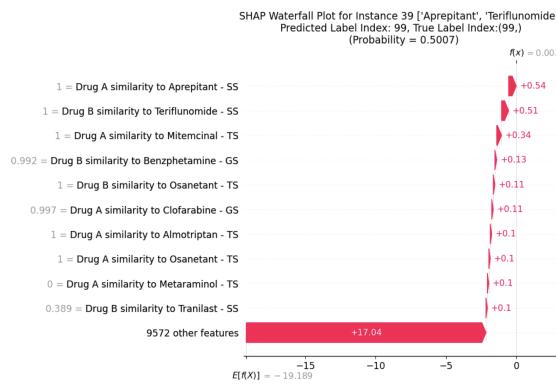
Sample 36



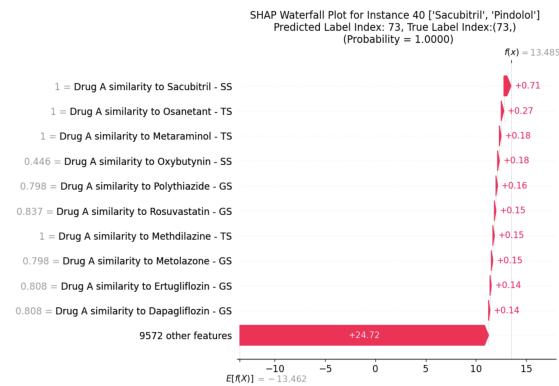
Sample 37



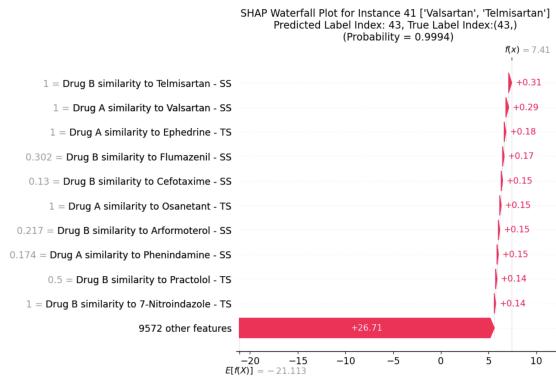
Sample 38



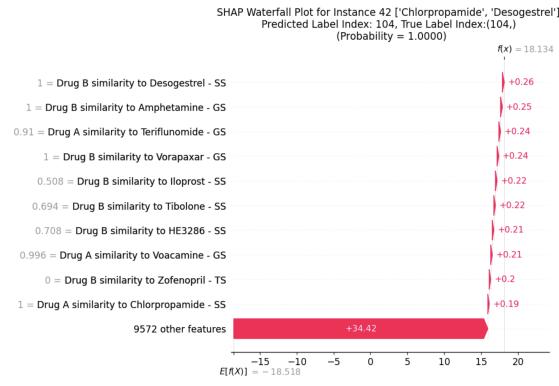
Sample 39



Sample 40

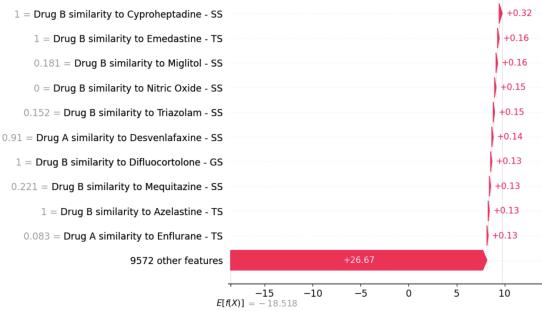


Sample 41



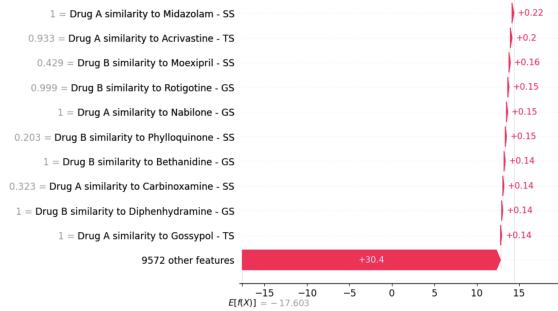
Sample 42

SHAP Waterfall Plot for Instance 43 ['Venlafaxine', 'Cyproheptadine']
Predicted Label Index: 104, True Label Index:(104.)
(Probability = 0.9999)
 $f(x) = 9.738$



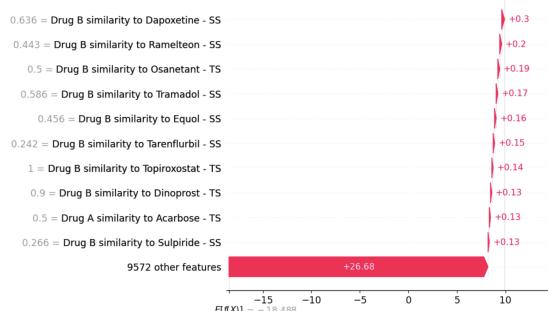
Sample 43

SHAP Waterfall Plot for Instance 44 ['Midazolam', 'Candoxatril']
Predicted Label Index: 100, True Label Index:(100.)
(Probability = 1.0000)
 $f(x) = 14.376$



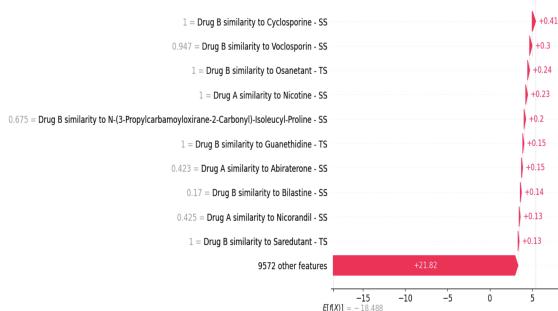
Sample 44

SHAP Waterfall Plot for Instance 45 ['Ondansetron', 'Atomoxetine']
Predicted Label Index: 68, True Label Index:(68.)
(Probability = 0.9999)
 $f(x) = 9.901$



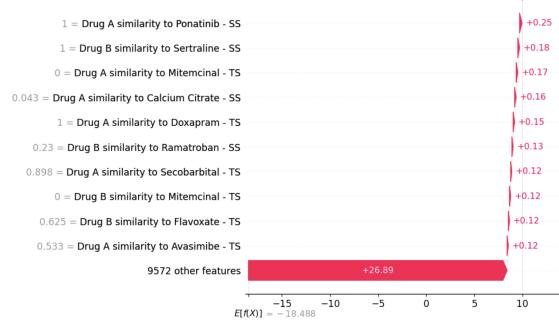
Sample 45

SHAP Waterfall Plot for instance 46 ['Cyclosporine']
Predicted Label Index: 68, True Label Index:(68.)
(Probability = 0.9955)
 $f(x) = 5.41$



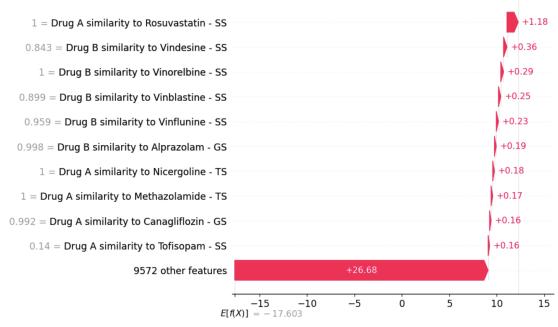
Sample 46

SHAP Waterfall Plot for Instance 47 ['Ponatinib', 'Sertraline']
Predicted Label Index: 68, True Label Index:(68.)
(Probability = 1.0000)
 $f(x) = 9.95$



Sample 47

SHAP Waterfall Plot for Instance 48 ['Rosuvastatin', 'Vinorelbine']
Predicted Label Index: 100, True Label Index:(100.)
(Probability = 1.0000)
 $f(x) = 12.25$



Sample 48