Endpoint	Algorithm	Descriptors	True	True	False	False	Count	Accurac	Precisio	recall	F-	Senseti	Specific	Balance	Informe	LOR	MCC	Real
Toxcast_ACEA_IC50:ACEA_IC50 (discretized)	WEKA-RF	Adriana	77	139	61	25	302	0.72	0.56	0.75	0.64	0.75	0.7	0.72	-98.6	8.41	0.43	102
Toxcast_ACEA_LOC2:ACEA_LOC2 (discretized)	PLS	ChemaxonDescriptors	61	144	69	30	304	0.67	0.47	0.67	0.55	0.67	0.68	0.67	-98.7	8.27	0.32	91
Toxcast_ACEA_LOCdec:ACEA_LOCdec (discretized)	MLRA	ChemaxonDescriptors	46	170	64	23	303	0.71	0.42	0.67	0.51	0.67	0.73	0.7	-98.6	7.97	0.34	69
Toxcast_ACEA_LOCinc:ACEA_LOCinc (discretized)	FSMLR	Mera,_Mersy	34	146	97	28	305	0.59	0.26	0.55	0.35	0.55	0.6	0.57	-98.9	7.3	0.12	62
Toxcast_Attagene Factorial cis AP-1:ATG_AP_1_CIS (discretized)	FSMLR	Adriana	32	166	82	21	301	0.66	0.28	0.6	0.38	0.6	0.67	0.64	-98.7	7.25	0.21	53
Toxcast_Attagene Factorial cis Ahr:ATG_Ahr_CIS (discretized)	WEKA-RF	Dragon6	34	158	90	20	302	0.64	0.27	0.63	0.38	0.63	0.64	0.63	-98.7	7.12	0.21	54
Toxcast_Attagene Factorial cis BRE:ATG_BRE_CIS (discretized)	WEKA-RF	ChemaxonDescriptors	68	128	81	25	302	0.65	0.46	0.73	0.56	0.73	0.61	0.67	-98.7	7.92	0.32	93
Toxcast_Attagene Factorial cis CMV:ATG_CMV_CIS (discretized)	PLS	Fragmentor	24	193	72	13	302	0.72	0.25	0.65	0.36	0.65	0.73	0.69	-98.6	6.78	0.27	37
Toxcast_Attagene Factorial cis CRE:ATG_CRE_CIS (discretized)	PLS	Dragon6	31	175	75	21	302	0.68	0.29	0.6	0.39	0.6	0.7	0.65	-98.7	7.36	0.23	52
Toxcast_Attagene Factorial cis EGR:ATG_EGR_CIS (discretized)	WEKA-RF	QNPR	25	189	73	15	302	0.71	0.26	0.63	0.36	0.63	0.72	0.67	-98.7	6.93	0.25	40
Toxcast_Attagene Factorial cis ERE:ATG_ERE_CIS (discretized)	KNN	GSFrag	26	179	86	12	303	0.68	0.23	0.68	0.35	0.68	0.68	0.68	-98.6	6.53	0.25	38
Toxcast_Attagene Factorial cis MRE:ATG_MRE_CIS (discretized)	WEKA-RF	Fragmentor	43	168	72	19	302	0.7	0.37	0.69	0.49	0.69	0.7	0.7	-98.6	7.59	0.33	62
Toxcast_Attagene Factorial cis NRF2/ARE:ATG_NRF2_ARE_CIS (discretized)	PLS	Fragmentor	110	107	37	50	304	0.71	0.75	0.69	0.72	0.69	0.74	0.72	-98.6	9.68	0.43	160
Toxcast_Attagene Factorial cis Oct-MLP:ATG_Oct_MLP_CIS (discretized)	WEKA-RF	ALogPS,_OEstate	65	142	73	22	302	0.69	0.47	0.75	0.58	0.75	0.66	0.7	-98.6	7.96	0.37	87
Toxcast_Attagene Factorial cis PPRE:ATG_PPRE_CIS (discretized)	LibSVM	Mera,_Mersy	67	138	44	54	303	0.68	0.6	0.55	0.58	0.55	0.76	0.66	-98.7	9.35	0.32	121
Toxcast_Attagene Factorial cis PXRE:ATG_PXRE_CIS (discretized)	WEKA-RF	ALogPS,_OEstate	181	51	29	43	304	0.76	0.86	0.81	0.83	0.81	0.64	0.72	-98.6	9.53	0.42	224
Toxcast_Attagene Factorial cis RORE:ATG_RORE_CIS (discretized)	WEKA-RF	ChemaxonDescriptors	26	180	87	10	303	0.68	0.23	0.72	0.35	0.72	0.67	0.7	-98.6	6.35	0.27	36
Toxcast_Attagene Factorial cis VDRE:ATG_VDRE_CIS (discretized)	FSMLR	Dragon6	98	128	43	33	302	0.75	0.7	0.75	0.72	0.75	0.75	0.75	-98.5	9.18	0.49	131
Toxcast_Attagene Factorial trans Era:ATG_ERa_TRANS (discretized)	ASNN	Dragon6	69	175	41	18	303	0.81	0.63	0.79	0.7	0.79	0.81	0.8	-98.4	8.6	0.57	87
Toxcast_Attagene Factorial trans PPARg:ATG_PPARg_TRANS (discretized)	WEKA-RF	Mera,_Mersy	112	106	55	28	301	0.72	0.67	0.8	0.73	0.8	0.66	0.73	-98.5	8.72	0.46	140
Toxcast_Attagene Factorial trans PXR:ATG_PXR_TRANS (discretized)	WEKA-RF	Fragmentor	79	145	57	21	302	0.74	0.58	0.79	0.67	0.79	0.72	0.75	-98.5	8.37	0.48	100
Toxcast_Attagene Factorial trans RARa:ATG_RARa_TRANS (discretized)	WEKA-RF	QNPR	35	192	62	13	302	0.75	0.36	0.73	0.48	0.73	0.76	0.74	-98.5	7.3	0.38	48
Toxcast_BrEPI_IL_1b_TNF_a_IFN_g_24_CD87_uPAR_up:BSK_BE3C_uPAR_up (discretized)	KNN	Mera,_Mersy	45	137	32	89	303	0.6	0.58	0.34	0.43	0.34	0.81	0.57	-98.9	9.75	0.17	134
Toxcast_BrEPI_IL_1b_TNF_a_IFN_g_24_CXCL10_IP_10_down:BSK_BE3C_IP10_down (discretized)	PLS	Adriana	66	145	60	32	303	0.7	0.52	0.67	0.59	0.67	0.71	0.69	-98.6	8.56	0.36	98
Toxcast_BrEPI_IL_1b_TNF_a_IFN_g_24_HLA_DR_down:BSK_BE3C_hLADR_down (discretized)	WEKA-RF	Adriana	64	141	73	23	301	0.68	0.47	0.74	0.57	0.74	0.66	0.7	-98.6	7.98	0.36	87
Toxcast_BrEPI_IL_1b_TNF_a_IFN_g_24_IL_1alpha_up:BSK_BE3C_IL1a_up (discretized)	LibSVM	Adriana	28	182	62	30	302	0.7	0.31	0.48	0.38	0.48	0.75	0.61	-98.8	7.84	0.2	58
Toxcast_BrEPI_IL_1b_TNF_a_IFN_g_24_MMP_1_up:BSK_BE3C_MMP1_up (discretized)	ASNN	Dragon6	25	216	50	13	304	0.79	0.33	0.66	0.44	0.66	0.81	0.73	-98.5	7.3	0.36	38
Toxcast_BrEPI_IL_1b_TNF_a_IFN_g_24_PAI_I_down:BSK_BE3C_PAI1_down (discretized)	FSMLR	Dragon6	42	161	79	22	304	0.67	0.35	0.66	0.45	0.66	0.67	0.66	-98.7	7.57	0.27	64
Toxcast_BrEPI_IL_1b_TNF_a_IFN_g_24_TGF_beta1_down:BSK_BE3C_TGFb1_down (discretized)	WEKA-J48	Mera,_Mersy	17	211	47	30	305	0.75	0.27	0.36	0.31	0.36	0.82	0.59	-98.8	7.77	0.16	47
Toxcast_BrEPI_IL_1b_TNF_a_IFN_g_24_uPA_down:BSK_BE3C_uPA_down (discretized)	WEKA-J48	Adriana	33	159	62	50	304	0.63	0.35	0.4	0.37	0.4	0.72	0.56	-98.9	8.37	0.11	83
Toxcast_Cellumen Cell Number:CLM_CellLoss_24hr (discretized)	PLS	Dragon6	38	194	44	26	302	0.77	0.46	0.59	0.52	0.59	0.82	0.7	-98.6	8.4	0.38	64
Toxcast_Cellumen Cell Number:CLM_CellLoss_72hr (discretized)	PLS	Dragon6	134	106	32	31	303	0.79	0.81	0.81	0.81	0.81	0.77	0.79	-98.4	9.54	0.58	165
Toxcast_Cellumen Mito Mass:CLM_MitoMass_24hr (discretized)	ASNN	Fragmentor	42	170	63	29	304	0.7	0.4	0.59	0.48	0.59	0.73	0.66	-98.7	8.12	0.29	71
Toxcast_Cellumen Mito Mass:CLM_MitoMass_72hr (discretized)	WEKA-J48	Dragon6	35	173	67	28	303	0.69	0.34	0.56	0.42	0.56	0.72	0.64	-98.7	7.86	0.24	63
Toxcast_Cellumen Mito Mem Potential:CLM_MitoMembPot_1hr (discretized)	ASNN	Fragmentor	48	168	59	28	303	0.71	0.45	0.63	0.52	0.63	0.74	0.69	-98.6	8.27	0.34	76
Toxcast_Cellumen Mito Mem Potential:CLM_MitoMembPot_1hr (discretized)	FSMLR	Dragon6	48	168	59	28	303	0.71	0.45	0.63	0.52	0.63	0.74	0.69	-98.6	8.27	0.34	76
Toxcast_Cellumen Mito Mem Potential:CLM_MitoMembPot_24hr (discretized)	WEKA-RF	ALogPS,_OEstate	31	194	68	12	305	0.74	0.31	0.72	0.44	0.72	0.74	0.73	-98.5	7.02	0.34	43
Toxcast_Cellumen Phospho-H2AX:CLM_OxidativeStress_72hr (discretized)	KNN	ChemaxonDescriptors	51	146	89	19	305	0.65	0.36	0.73	0.49	0.73	0.62	0.67	-98.7	7.4	0.3	70
Toxcast_Cellumen Phospho-H3:CLM_MitoticArrest_24hr (discretized)	WEKA-RF	ALogPS,_OEstate	35	182	66	20	303	0.72	0.35	0.64	0.45	0.64	0.73	0.69	-98.6	7.6	0.3	55
Toxcast_Cellumen Phospho-H3:CLM_MitoticArrest_72hr (discretized)	LibSVM	CDK	80	137	46	41	304	0.71	0.63	0.66	0.65	0.66	0.75	0.7	-98.6	9.2	0.41	121
Toxcast_Cellumen Phospho-c-jun:CLM_StressKinase_1hr (discretized)	PLS	Dragon6	37	196	54	16	303	0.77	0.41	0.7	0.51	0.7	0.78	0.74	-98.5	7.71	0.4	53
Toxcast_Cellumen Phospho-c-jun:CLM_StressKinase_24hr (discretized)	WEKA-J48	ALogPS,_OEstate	16	228	41	18	303	0.81	0.28	0.47	0.35	0.47	0.85	0.66	-98.7	7.43	0.26	34

Toxcast_Cellumen Phospho-c-jun:CLM_StressKinase_72hr (discretized)	KNN	Fragmentor	33	152	107	11	303	0.61	0.24	0.75	0.36	0.75	0.59	0.67	-98.7	6.3	0.24	44
Toxcast_Cellumen a-tubulin:CLM_MicrotubuleCSK_24hr (discretized)	PLS	Dragon6	53	168	65	18	304	0.73	0.45	0.75	0.56	0.75	0.72	0.73	-98.5	7.84	0.41	71
Toxcast_Cellumen a-tubulin:CLM_MicrotubuleCSK_72hr (discretized)	PLS	QNPR	50	175	54	26	305	0.74	0.48	0.66	0.56	0.66	0.76	0.71	-98.6	8.37	0.39	76
Toxcast_Cellumen_Hepat_Apoptosis:CLM_Hepat_Apoptosis_1hr (discretized)	ASNN	Spectrophores	26	179	85	14	304	0.67	0.23	0.65	0.34	0.65	0.68	0.66	-98.7	6.69	0.23	40
Toxcast_Cellumen_Hepat_CellLoss:CLM_Hepat_CellLoss_24hr (discretized)	MLRA	ChemaxonDescriptors	39	177	70	16	302	0.72	0.36	0.71	0.48	0.71	0.72	0.71	-98.6	7.4	0.34	55
Toxcast_Cellumen_Hepat_CellLoss:CLM_Hepat_CellLoss_48hr (discretized)	FSMLR	Mera,_Mersy	41	178	64	20	303	0.72	0.39	0.67	0.49	0.67	0.74	0.7	-98.6	7.76	0.34	61
Toxcast_Cellumen_Hepat_DNADamage:CLM_Hepat_DNADamage_1hr (discretized)	PLS	GSFrag	23	185	82	15	305	0.68	0.22	0.61	0.32	0.61	0.69	0.65	-98.7	6.71	0.21	38
Toxcast_Cellumen_Hepat_DNADamage:CLM_Hepat_DNADamage_48hr (discretized)	KNN	Fragmentor	40	184	71	7	302	0.74	0.36	0.85	0.51	0.85	0.72	0.79	-98.4	6.66	0.43	47
Toxcast_Cellumen_Hepat_DNATexture:CLM_Hepat_DNATexture_48hr (discretized)	PLS	Fragmentor	18	218	55	14	305	0.77	0.25	0.56	0.34	0.56	0.8	0.68	-98.6	6.96	0.26	32
Toxcast_Cellumen_Hepat_NuclearSize:CLM_Hepat_NuclearSize_48hr (discretized)	FSMLR	QNPR	23	205	67	8	303	0.75	0.26	0.74	0.38	0.74	0.75	0.75	-98.5	6.41	0.33	31
Toxcast_Cellumen_Hepat_Steatosis:CLM_Hepat_Steatosis_24hr (discretized)	FSMLR	QNPR	27	179	75	21	302	0.68	0.26	0.56	0.36	0.56	0.7	0.63	-98.7	7.25	0.21	48
Toxcast_Cellumen_Hepat_Steatosis:CLM_Hepat_Steatosis_48hr (discretized)	KNN	ALogPS,_OEstate	39	156	94	15	304	0.64	0.29	0.72	0.42	0.72	0.62	0.67	-98.7	6.92	0.27	54
Toxcast_CellzDirect CYP1A1:CLZD_CYP1A1_24 (discretized)	LibSVM	Dragon6	67	178	31	27	303	0.81	0.68	0.71	0.7	0.71	0.85	0.78	-98.4	9.26	0.56	94
Toxcast_CellzDirect CYP1A1:CLZD_CYP1A1_48 (discretized)	WEKA-J48	ALogPS,_OEstate	73	161	39	29	302	0.77	0.65	0.72	0.68	0.72	0.81	0.76	-98.5	9.09	0.51	102
Toxcast_CellzDirect CYP1A1:CLZD_CYP1A1_6 (discretized)	ASNN	Dragon6	42	188	50	25	305	0.75	0.46	0.63	0.53	0.63	0.79	0.71	-98.6	8.31	0.38	67
Toxcast_CellzDirect CYP1A2:CLZD_CYP1A2_24 (discretized)	PLS	Dragon6	66	171	40	26	303	0.78	0.62	0.72	0.67	0.72	0.81	0.76	-98.5	8.92	0.51	92
Toxcast_CellzDirect CYP1A2:CLZD_CYP1A2_48 (discretized)	LibSVM	CDK	94	146	28	32	300	0.8	0.77	0.75	0.76	0.75	0.84	0.79	-98.4	9.67	0.59	126
Toxcast_CellzDirect CYP1A2:CLZD_CYP1A2_6 (discretized)	PLS	Dragon6	44	166	75	21	306	0.69	0.37	0.68	0.48	0.68	0.69	0.68	-98.6	7.65	0.31	65
Toxcast_CellzDirect CYP2B6:CLZD_CYP2B6_24 (discretized)	WEKA-J48	ALogPS,_OEstate	154	95	27	28	304	0.82	0.85	0.85	0.85	0.85	0.78	0.81	-98.4	9.64	0.62	182
Toxcast_CellzDirect CYP2B6:CLZD_CYP2B6_48 (discretized)	PLS	CDK	147	79	30	44	300	0.75	0.83	0.77	0.8	0.77	0.72	0.75	-98.5	9.75	0.48	191
Toxcast_CellzDirect CYP2B6:CLZD_CYP2B6_6 (discretized)	ASNN	Fragmentor	140	98	24	42	304	0.78	0.85	0.77	0.81	0.77	0.8	0.79	-98.4	10.1	0.56	182
Toxcast_CellzDirect CYP2C9:CLZD_CYP2C9_48 (discretized)	PLS	ALogPS,_OEstate	29	182	74	18	303	0.7	0.28	0.62	0.39	0.62	0.71	0.66	-98.7	7.2	0.25	47
Toxcast_CellzDirect CYP2C9:CLZD_CYP2C9_6 (discretized)	WEKA-RF	GSFrag	25	171	91	17	304	0.64	0.22	0.6	0.32	0.6	0.65	0.62	-98.8	6.73	0.18	42
Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_24 (discretized)	LibSVM	CDK	91	136	38	36	301	0.75	0.71	0.72	0.71	0.72	0.78	0.75	-98.5	9.38	0.5	127
Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_48 (discretized)	WEKA-J48	CDK	137	102	33	31	303	0.79	0.81	0.82	0.81	0.82	0.76	0.79	-98.4	9.49	0.57	168
Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_6 (discretized)	WEKA-RF	Fragmentor	59	150	65	31	305	0.69	0.48	0.66	0.55	0.66	0.7	0.68	-98.6	8.37	0.33	90
Toxcast_CellzDirect GSTA2:CLZD_GSTA2_48 (discretized)	FSMLR	Mera,_Mersy	31	178	84	8	301	0.69	0.27	0.79	0.4	0.79	0.68	0.74	-98.5	6.34	0.33	39
Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_24 (discretized)	WEKA-RF	Fragmentor	27	192	68	15	302	0.73	0.28	0.64	0.39	0.64	0.74	0.69	-98.6	7.09	0.28	42
Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_48 (discretized)	PLS	Fragmentor	53	150	75	26	304	0.67	0.41	0.67	0.51	0.67	0.67	0.67	-98.7	7.95	0.3	79
Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_6 (discretized)	KNN	ChemaxonDescriptors	35	144	112	12	303	0.59	0.24	0.74	0.36	0.74	0.56	0.65	-98.7	6.35	0.22	47
Toxcast_CellzDirect UGT1A1:CLZD_UGT1A1_24 (discretized)	WEKA-RF	ChemaxonDescriptors	55	140	90	17	302	0.65	0.38	0.76	0.51	0.76	0.61	0.69	-98.6	7.32	0.32	72
Toxcast_CellzDirect UGT1A1:CLZD_UGT1A1_48 (discretized)	LibSVM	ALogPS,_OEstate	58	179	42	24	303	0.78	0.58	0.71	0.64	0.71	0.81	0.76	-98.5	8.71	0.49	82
Toxcast_HDFn_IL_1b_TNF_a_IFN_g_EGF_FGF_PDGFbb_24_CD106_VCAM_1_down:BSK_hDFCGF_VCAM1_down (discretized)	WEKA-J48	CDK	57	142	50	55	304	0.65	0.53	0.51	0.52	0.51	0.74	0.62	-98.8	9.11	0.25	112
Toxcast_HDFn_IL_1b_TNF_a_IFN_g_EGF_FGF_PDGFbb_24_CXCL10_IP_10_down:BSK_hDFCGF_IP10_down (discretized)	MLRA	ChemaxonDescriptors	70	136	56	44	306	0.67	0.56	0.61	0.58	0.61	0.71	0.66	-98.7	8.93	0.32	114
Toxcast_HDFn_IL_1b_TNF_a_IFN_g_EGF_FGF_PDGFbb_24_CXCL9_MIG_down:BSK_hDFCGF_MIG_down (discretized)	PLS	Dragon6	29	186	61	27	303	0.71	0.32	0.52	0.4	0.52	0.75	0.64	-98.7	7.81	0.23	56

Toxcast_HDFn_IL_1b_TNF_a_IFN_g_EGF_FGF_PDGFbb_24_Collagen_III_down:BSK_hDFCGF_CollagenIII_down (discretized)	FSMLR	ChemaxonDescriptors	74	133	78	20	305	0.68	0.49	0.79	0.6	0.79	0.63	0.71	-98.6	7.86	0.39	94
Toxcast_HDFn_IL_1b_TNF_a_IFN_g_EGF_FGF_PDGFbb_24_EGFR_up:BSK_hDFCGF_EGFR_up (discretized)	PLS	ChemaxonDescriptors	31	155	96	20	302	0.62	0.24	0.61	0.35	0.61	0.62	0.61	-98.8	6.95	0.17	51
Toxcast_HDFn_IL_1b_TNF_a_IFN_g_EGF_FGF_PDGFbb_24_MMP_1_up:BSK_hDFCGF_MMP1_up (discretized)	ASNN	GSFrag	62	142	56	44	304	0.67	0.53	0.58	0.55	0.58	0.72	0.65	-98.7	8.86	0.3	106
Toxcast_HDFn_IL_1b_TNF_a_IFN_g_EGF_FGF_PDGFbb_24_M_CSF_down:BSK_hDFCGF_MCSF_down (discretized)	WEKA-J48	ALogPS,_OEstate	59	158	45	43	305	0.71	0.57	0.58	0.57	0.58	0.78	0.68	-98.6	9.11	0.36	102
Toxcast_HDFn_IL_1b_TNF_a_IFN_g_EGF_FGF_PDGFbb_24_PAI_I_down:BSK_hDFCGF_PAI1_down (discretized)	PLS	InductiveDescriptors	66	143	70	25	304	0.69	0.49	0.73	0.58	0.73	0.67	0.7	-98.6	8.15	0.37	91
Toxcast_HDFn_IL_1b_TNF_a_IFN_g_EGF_FGF_PDGFbb_24_Proliferation_72hr_down:BSK_hDFCGF_Proliferation_down (discretized)	LibSVM	Adriana	108	128	37	29	302	0.78	0.74	0.79	0.77	0.79	0.78	0.78	-98.4	9.3	0.56	137
Toxcast_HDFn_IL_1b_TNF_a_IFN_g_EGF_FGF_PDGFbb_24_SRB_down:BSK_hDFCGF_SRB_down (discretized)	MLRA	ChemaxonDescriptors	28	198	67	10	303	0.75	0.29	0.74	0.42	0.74	0.75	0.74	-98.5	6.78	0.35	38
Toxcast_HEK_HDFn_IL_1b_TNF_a_IFN_g_TGF_b_24_CCL2_MCP_1_down:BSK_KF3CT_MCP1_down (discretized)	PLS	Mera,_Mersy	21	195	74	13	303	0.71	0.22	0.62	0.33	0.62	0.72	0.67	-98.7	6.64	0.23	34
Toxcast_HEK_HDFn_IL_1b_TNF_a_IFN_g_TGF_b_24_CXCL10_IP_10_down:BSK_KF3CT_IP10_down (discretized)	LibSVM	InductiveDescriptors	49	151	54	52	306	0.65	0.48	0.49	0.48	0.49	0.74	0.61	-98.8	8.89	0.22	101
Toxcast_HEK_HDFn_IL_1b_TNF_a_IFN_g_TGF_b_24_IL_1alpha_down:BSK_KF3CT_IL1a_down (discretized)	FSMLR	ChemaxonDescriptors	29	179	76	19	303	0.69	0.28	0.6	0.38	0.6	0.7	0.65	-98.7	7.21	0.23	48
Toxcast_HEK_HDFn_IL_1b_TNF_a_IFN_g_TGF_b_24_MMP_9_down:BSK_KF3CT_MMP9_down (discretized)	FSMLR	Dragon6	70	152	59	24	305	0.73	0.54	0.74	0.63	0.74	0.72	0.73	-98.5	8.4	0.43	94
Toxcast_HEK_HDFn_IL_1b_TNF_a_IFN_g_TGF_b_24_TIMP_2_down:BSK_KF3CT_TIMP2_down (discretized)	ASNN	Dragon6	22	211	55	18	306	0.76	0.29	0.55	0.38	0.55	0.79	0.67	-98.7	7.37	0.27	40
Toxcast_HEK_HDFn_IL_1b_TNF_a_IFN_g_TGF_b_24_uPA_down:BSK_KF3CT_uPA_down (discretized)	FSMLR	Mera,_Mersy	19	189	79	18	305	0.68	0.19	0.51	0.28	0.51	0.71	0.61	-98.8	6.76	0.15	37
Toxcast_HUVEC_IL_1b_TNF_a_IFN_g_24_CCL2_MCP_1_down:BSK_3C_MCP1_down (discretized)	FSMLR	Dragon6	37	186	58	23	304	0.73	0.39	0.62	0.48	0.62	0.76	0.69	-98.6	7.94	0.33	60
Toxcast_HUVEC_IL_1b_TNF_a_IFN_g_24_CD141_Thrombomodulin_up:BSK_3C_Thrombomodulin_up (discretized)	LibSVM	InductiveDescriptors	27	200	56	19	302	0.75	0.33	0.59	0.42	0.59	0.78	0.68	-98.6	7.55	0.3	46
Toxcast_HUVEC_IL_1b_TNF_a_IFN_g_24_CD62E_E_Selectin_down:BSK_3C_Eselectin_down (discretized)	ASNN	Fragmentor	24	193	66	21	304	0.71	0.27	0.53	0.36	0.53	0.75	0.64	-98.7	7.33	0.22	45
Toxcast_HUVEC_IL_1b_TNF_a_IFN_g_24_CD87_uPAR_down:BSK_3C_uPAR_down (discretized)	KNN	GSFrag	47	171	52	34	304	0.72	0.47	0.58	0.52	0.58	0.77	0.67	-98.7	8.59	0.33	81
Toxcast_HUVEC_IL_1b_TNF_a_IFN_g_24_CXCL8_IL_8_down:BSK_3C_IL8_down (discretized)	WEKA-RF	ALogPS,_OEstate	23	189	77	14	303	0.7	0.23	0.62	0.34	0.62	0.71	0.67	-98.7	6.73	0.23	37
Toxcast_HUVEC_IL_1b_TNF_a_IFN_g_24_HLA_DR_down:BSK_3C_hLADR_down (discretized)	WEKA-RF	Dragon6	78	120	79	27	304	0.65	0.5	0.74	0.6	0.74	0.6	0.67	-98.7	8.09	0.33	105
Toxcast_HUVEC_IL_1b_TNF_a_IFN_g_24_Proliferation_down:BSK_3C_Proliferation_down (discretized)	ASNN	Dragon6	96	145	40	25	306	0.79	0.71	0.79	0.75	0.79	0.78	0.79	-98.4	9.09	0.57	121
Toxcast_HUVEC_IL_1b_TNF_a_IFN_g_24_SRB_down:BSK_3C_SRB_down (discretized)	WEKA-RF	Dragon6	42	180	68	12	302	0.74	0.38	0.78	0.51	0.78	0.73	0.75	-98.5	7.24	0.4	54
Toxcast_HUVEC_IL_1b_TNF_a_IFN_g_24_Visual_down:BSK_3C_Vis_down (discretized)	MLRA	ALogPS,_OEstate	70	146	56	32	304	0.71	0.56	0.69	0.61	0.69	0.72	0.7	-98.6	8.69	0.39	102
Toxcast_HUVEC_IL_4_Histamine_24_CCL26_Eotaxin_3_down:BSK_4H_Eotaxin3_down (discretized)	MLRA	ALogPS,_OEstate	31	180	73	19	303	0.7	0.3	0.62	0.4	0.62	0.71	0.67	-98.7	7.32	0.26	50
Toxcast_HUVEC_IL_4_Histamine_24_CCL2_MCP_1_down:BSK_4H_MCP1_down (discretized)	WEKA-RF	ALogPS,_OEstate	79	151	59	16	305	0.75	0.57	0.83	0.68	0.83	0.72	0.78	-98.4	8.11	0.51	95
Toxcast_HUVEC_IL_4_Histamine_24_CD106_VCAM_1_down:BSK_4H_VCAM1_down (discretized)	ASNN	Dragon6	52	177	47	27	303	0.76	0.53	0.66	0.58	0.66	0.79	0.72	-98.6	8.59	0.42	79
Toxcast_HUVEC_IL_4_Histamine_24_CD62P_P_selectin_down:BSK_4H_P selectin_down (discretized)	LibSVM	ALogPS,_OEstate	43	177	60	22	302	0.73	0.42	0.66	0.51	0.66	0.75	0.7	-98.6	7.96	0.35	65
Toxcast_HUVEC_IL_4_Histamine_24_SRB_down:BSK_4H_SRB_down (discretized)	PLS	GSFrag	20	215	54	13	302	0.78	0.27	0.61	0.37	0.61	0.8	0.7	-98.6	7.	0.29	33
Toxcast_HUVEC_PBMC_LPS_24_CCL2_MCP_1_down:BSK_LPS_MPC1_down (discretized)	FSMLR	Mera,_Mersy	38	177	69	20	304	0.71	0.36	0.66	0.46	0.66	0.72	0.69	-98.6	7.61	0.31	58
Toxcast_HUVEC_PBMC_LPS_24_CD106_VCAM_1_down:BSK_LPS_VCAM1_down (discretized)	WEKA-RF	Mera,_Mersy	80	145	57	19	301	0.75	0.58	0.81	0.68	0.81	0.72	0.76	-98.5	8.29	0.5	99
Toxcast_HUVEC_PBMC_LPS_24_CD40_down:BSK_LPS_CD40_down (discretized)	FSMLR	Dragon6	65	147	72	20	304	0.7	0.47	0.76	0.59	0.76	0.67	0.72	-98.6	7.91	0.39	85
Toxcast_HUVEC_PBMC_LPS_24_CD62E_E_Selectin_down:BSK_LPS_Eselectin_down (discretized)	ASNN	Adriana	41	169	71	20	301	0.7	0.37	0.67	0.47	0.67	0.7	0.69	-98.6	7.61	0.31	61
Toxcast_HUVEC_PBMC_LPS_24_CXCL8_IL_8_down:BSK_LPS_IL8_down (discretized)	FSMLR	Adriana	51	168	63	19	301	0.73	0.45	0.73	0.55	0.73	0.73	0.73	-98.5	7.89	0.4	70
Toxcast_HUVEC_PBMC_LPS_24_M_CSF_down:BSK_LPS_MCSF_down (discretized)	WEKA-RF	ALogPS,_OEstate	48	156	82	16	302	0.68	0.37	0.75	0.49	0.75	0.66	0.7	-98.6	7.33	0.33	64

Toxcast_HUVEC_PBMC_LPS_24_PGE2_down:BSK_LPS_PGE2_down (discretized)	PLS	GSFrag	48	181	61	12	302	0.76	0.44	0.8	0.57	0.8	0.75	0.77	-98.5	7.49	0.46	60
Toxcast_HUVEC_PBMC_LPS_24_PGE2_up:BSK_LPS_PGE2_up (discretized)	WEKA-RF	Fragmentor	48	210	27	20	305	0.85	0.64	0.71	0.67	0.71	0.89	0.8	-98.4	8.94	0.57	68
Toxcast_HUVEC_PBMC_LPS_24_SRB_down:BSK_LPS_SRB_down (discretized)	WEKA-J48	GSFrag	21	225	43	13	302	0.81	0.33	0.62	0.43	0.62	0.84	0.73	-98.5	7.32	0.35	34
Toxcast_HUVEC_PBMC_LPS_24_TNF_alpha_down:BSK_LPS_TNFa_down (discretized)	LibSVM	Dragon6	36	221	24	21	302	0.85	0.6	0.63	0.62	0.63	0.9	0.77	-98.5	8.87	0.52	57
Toxcast_HUVEC_PBMC_SEB_TSST_24_CCL2_MCP_1_down:BSK_SAg_MCP1_down (discretized)	FSMLR	Adriana	65	145	71	21	302	0.7	0.48	0.76	0.59	0.76	0.67	0.71	-98.6	7.96	0.39	86
Toxcast_HUVEC_PBMC_SEB_TSST_24_CD38_down:BSK_SAg_CD38_down (discretized)	LibSVM	Mera,_Mersy	77	140	47	38	302	0.72	0.62	0.67	0.64	0.67	0.75	0.71	-98.6	9.09	0.41	115
Toxcast_HUVEC_PBMC_SEB_TSST_24_CD38_up:BSK_SAg_CD38_up (discretized)	WEKA-J48	Spectrophores	23	192	63	25	303	0.71	0.27	0.48	0.34	0.48	0.75	0.62	-98.8	7.5	0.19	48
Toxcast_HUVEC_PBMC_SEB_TSST_24_CD40_down:BSK_SAg_CD40_down (discretized)	WEKA-RF	ALogPS,_OEstate	74	132	64	34	304	0.68	0.54	0.69	0.6	0.69	0.67	0.68	-98.6	8.57	0.34	108
Toxcast_HUVEC_PBMC_SEB_TSST_24_CD62E_E_Selectin_down:BSK_SAg_Eselectin_down (discretized)	WEKA-RF	ALogPS,_OEstate	93	122	58	31	304	0.71	0.62	0.75	0.68	0.75	0.68	0.71	-98.6	8.73	0.42	124
Toxcast_HUVEC_PBMC_SEB_TSST_24_CD69_down:BSK_SAg_CD69_down (discretized)	FSMLR	Dragon6	86	139	43	36	304	0.74	0.67	0.7	0.69	0.7	0.76	0.73	-98.5	9.22	0.46	122
Toxcast_HUVEC_PBMC_SEB_TSST_24_CXCL8_IL_8_down:BSK_SAg_IL8_down (discretized)	ASNN	Dragon6	69	154	50	30	303	0.74	0.58	0.7	0.63	0.7	0.75	0.73	-98.5	8.78	0.43	99
Toxcast_HUVEC_PBMC_SEB_TSST_24_PBMC_Cytotoxicity_down:BSK_SAg_PBMCCytotoxicity_down (discretized)	WEKA-RF	QNPR	33	209	46	15	303	0.8	0.42	0.69	0.52	0.69	0.82	0.75	-98.5	7.76	0.42	48
Toxcast_HUVEC_PBMC_SEB_TSST_24_PBMC_Cytotoxicity_up:BSK_SAg_PBMCCytotoxicity_up (discretized)	WEKA-RF	Adriana	69	120	82	32	303	0.62	0.46	0.68	0.55	0.68	0.59	0.64	-98.7	8.1	0.26	101
Toxcast_HUVEC_PBMC_SEB_TSST_24_Proliferation_down:BSK_SAg_Proliferation_down (discretized)	ASNN	Dragon6	107	127	37	33	304	0.77	0.74	0.76	0.75	0.76	0.77	0.77	-98.5	9.41	0.54	140
Toxcast_NCGC Reporter Gene Assay PXR Agonist (Human):NCGC_PXR_Agonist_human (discretized)	FSMLR	Dragon6	47	189	48	18	302	0.78	0.49	0.72	0.59	0.72	0.8	0.76	-98.5	8.14	0.46	65
Toxcast_Novascreen Human CYP1A2 :NVS_ADME_hCYP1A2 (discretized)	ASNN	Adriana	32	206	51	11	300	0.79	0.39	0.74	0.51	0.74	0.8	0.77	-98.5	7.31	0.43	43
Toxcast_Novascreen Human CYP2B6 :NVS_ADME_hCYP2B6 (discretized)	ASNN	ALogPS,_OEstate	29	241	25	7	302	0.89	0.54	0.81	0.64	0.81	0.91	0.86	-98.3	7.65	0.6	36
Toxcast_Novascreen Human CYP2C18 :NVS_ADME_hCYP2C18 (discretized)	LibSVM	ALogPS,_OEstate	29	244	19	10	302	0.9	0.6	0.74	0.67	0.74	0.93	0.84	-98.3	8.26	0.62	39
Toxcast_Novascreen Human CYP2C19:NVS_ADME_hCYP2C19 (discretized)	WEKA-J48	ChemaxonDescriptors	78	150	49	28	305	0.75	0.61	0.74	0.67	0.74	0.75	0.74	-98.5	8.82	0.47	106
Toxcast_Novascreen Human CYP2C9 :NVS_ADME_hCYP2C9 (discretized)	PLS	ALogPS,_OEstate	34	222	33	13	302	0.85	0.51	0.72	0.6	0.72	0.87	0.8	-98.4	8.04	0.52	47
Toxcast_Novascreen Human CYP3A5:NVS_ADME_hCYP3A5 (discretized)	LibSVM	Dragon6	38	222	33	9	302	0.86	0.54	0.81	0.64	0.81	0.87	0.84	-98.3	7.8	0.58	47
Toxcast_Novascreen Human PXR:NVS_NR_hPXR (discretized)	PLS	Dragon6	55	164	54	29	302	0.73	0.5	0.65	0.57	0.65	0.75	0.7	-98.6	8.51	0.38	84
Toxcast_Novascreen Human peripheral-type benzodiazepine receptor (PBR):NVS_MP_hPBR (discretized)	PLS	CDK	31	182	76	11	300	0.71	0.29	0.74	0.42	0.74	0.71	0.72	-98.6	6.76	0.32	42
Toxcast_Novascreen Rat CYP2C11 :NVS_ADME_rCYP2C11 (discretized)	FSMLR	Dragon6	41	223	35	3	302	0.87	0.54	0.93	0.68	0.93	0.86	0.9	-98.2	6.82	0.65	44
Toxcast_Novascreen Rat CYP2C6 :NVS_ADME_rCYP2C6 (discretized)	WEKA-RF	ALogPS,_OEstate	35	211	49	7	302	0.81	0.42	0.83	0.56	0.83	0.81	0.82	-98.4	7.04	0.5	42
Toxcast_Novascreen Rat CYP3A1 :NVS_ADME_rCYP3A1 (discretized)	LibSVM	Dragon6	31	227	29	15	302	0.85	0.52	0.67	0.58	0.67	0.89	0.78	-98.4	8.23	0.5	46
Toxcast_Novascreen Rat CYP3A2 :NVS_ADME_rCYP3A2 (discretized)	LibSVM	ALogPS,_OEstate	39	211	38	14	302	0.83	0.51	0.74	0.6	0.74	0.85	0.79	-98.4	8.05	0.51	53
Toxcast_Novascreen Rat peripheral-type benzodiazepine receptor (PBR):NVS_MP_rPBR (discretized)	LibSVM	CDK	61	179	42	18	300	0.8	0.59	0.77	0.67	0.77	0.81	0.79	-98.4	8.48	0.54	79
Toxcast_SMC_IL_1b_TNF_a_IFN_g_24_CCL2_MCP_1_down:BSK_SM3C_MCP1_down (discretized)	WEKA-J48	Mera,_Mersy	29	180	46	49	304	0.69	0.39	0.37	0.38	0.37	0.8	0.58	-98.8	8.64	0.17	78
Toxcast_SMC_IL_1b_TNF_a_IFN_g_24_CD106_VCAM_1_down:BSK_SM3C_VCAM_1_down (discretized)	WEKA-RF	Mera,_Mersy	28	190	73	10	301	0.72	0.28	0.74	0.4	0.74	0.72	0.73	-98.5	6.65	0.32	38
Toxcast_SMC_IL_1b_TNF_a_IFN_g_24_Proliferation_down:BSK_SM3C_Proliferation_down (discretized)	ASNN	Dragon6	87	142	40	35	304	0.75	0.69	0.71	0.7	0.71	0.78	0.75	-98.5	9.3	0.49	122
Toxcast_Solidus (All Enzymes):Solidus_AllEnzyme (discretized)	KNN	Fragmentor	37	210	30	25	302	0.82	0.55	0.6	0.57	0.6	0.88	0.74	-98.5	8.79	0.46	62
Toxcast_Solidus (No Enzymes):Solidus_NoEnzyme (discretized)	WEKA-RF	ALogPS,_OEstate	39	187	53	23	302	0.75	0.42	0.63	0.51	0.63	0.78	0.7	-98.6	8.09	0.36	62
Toxcast_Solidus (P450):Solidus_P450 (discretized)	KNN	ALogPS,_OEstate	48	186	37	32	303	0.77	0.56	0.6	0.58	0.6	0.83	0.72	-98.6	8.97	0.43	80
Toxcast_Solidus (Phase II):Solidus_PhaseII (discretized)	WEKA-RF	ChemaxonDescriptors	39	181	66	16	302	0.73	0.37	0.71	0.49	0.71	0.73	0.72	-98.6	7.48	0.36	55