indpoint oxcast_ACEA_IC50:ACEA_IC50	Algorithm	Descriptors Tru	e Tru	ue Fal	se Fal	se Co	ount A	ccurac P	ecisio re	call F-	- S	enseti S _l	ecific B	alance Ir	forme L	OR M	CC Re	al
	WEKA-RF	Adriana ChemaxonDesc	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
discretized)	PLS	riptors	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
oxcast_ACEA_LOCdec:ACEA_LOCdec (discretized)	MLRA	ChemaxonDesc riptors	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
	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
oxcast_Attagene Factorial cis AP-	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
oxcast_Attagene Factorial cis																		
oxcast_Attagene Factorial cis	WEKA-RF	Dragon6 ChemaxonDesc	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
BRE:ATG_BRE_CIS (discretized) oxcast_Attagene Factorial cis	WEKA-RF	riptors	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
	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
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
oxcast_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
oxcast_Attagene Factorial cis	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
oxcast_Attagene Factorial cis																		
MRE:ATG_MRE_CIS (discretized) oxcast_Attagene Factorial cis	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
IRF2/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
•	. 20							0.7 1	0.70	0.00	0.72	0.00	0	0.12	00.0	0.00	0.10	
oxcast_Attagene Factorial cis Oct- MLP:ATG_Oct_MLP_CIS (discretized)	WEKA-RF	ALogPS,_OEsta te	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
oxcast_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
oxcast_Attagene Factorial cis PXRE:ATG_PXRE_CIS (discretized)		ALogPS,_OEsta																
oxcast_Attagene Factorial cis		te ChemaxonDesc	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
RORE:ATG_RORE_CIS (discretized) oxcast Attagene Factorial cis	WEKA-RF	riptors	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
/DRE: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
	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
oxcast_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
oxcast_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
oxcast_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
oxcast_BrEPI_IL_1b_TNF_a_IFN_g_ 4_CD87_uPAR_up:BSK_BE3C_uPA																		
R_up (discretized) oxcast_BrEPI_IL_1b_TNF_a_IFN_g	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
4_CXCL10_IP_10_down:BSK_BE3C																		
IP10_down (discretized) oxcast_BrEPI_IL_1b_TNF_a_IFN_g_	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
4_HLA_DR_down:BSK_BE3C_hLAD	WEKA-RF	Adriana	64	444	70	23	301	0.68	0.47	0.74	0.57	0.74	0.66	0.7	-98.6	7.98	0.36	07
oxcast_BrEPI_IL_1b_TNF_a_IFN_g_	WENA-RE	Adriana	64	141	73		301	0.00	0.47	0.74	0.57	0.74	0.00	0.7	-90.0	7.90	0.30	87
4_IL_1alpha_up:BSK_BE3C_IL1a_u (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
oxcast_BrEPI_IL_1b_TNF_a_IFN_g_ 4_MMP_1_up:BSK_BE3C_MMP1_u																		
(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
oxcast_BrEPI_IL_1b_TNF_a_IFN_g_ 4_PAI_I_down:BSK_BE3C_PAI1_do																		
	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
4_TGF_betal_down:BSK_BE3C_TG																		
b1_down (discretized) oxcast_BrEPI_IL_1b_TNF_a_IFN_g_	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
4_uPA_down:BSK_BE3C_uPA_dow	MEKA 140	Adriana	22	150	60	E0	204	0.00	0.25	0.4	0.27	0.4	0.70	0.50	00.0	0.07	0.44	00
oxcast_Cellumen Cell	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
Number:CLM_CellLoss_24hr	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
oxcast_Cellumen Cell		90	50				302	51	20	3.00	J.UL	2.00	5.04	0.1	50.0	5.7	2.00	
lumber: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
oxcast_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
oxcast_Cellumen Mito Mass:CLM_MitoMass_72hr																		
	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
Potential:CLM_MitoMembPot_1hr	40111	F	40	405		0.5	000		0 :-	0.00	0	0.00			00.5	0.0-	0.5:	
oxcast_Cellumen Mito Mem	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
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
oxcast_Cellumen Mito Mem	1 JIVILR	•	+0	100	JB	20	303	U./ I	U.40	0.03	0.02	0.03	0.74	0.09	-30.0	0.21	U.34	/6
otential:CLM_MitoMembPot_24hr	WEKA-RF	ALogPS,_OEsta te	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
		ChemaxonDesc																
	KNN	riptors	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
I2AX:CLM_OxidativeStress_72hr discretized)																		
I2AX:CLM_OxidativeStress_72hr discretized) oxcast_Cellumen Phospho-		ALogPS: OFsta			66	20	303	0.72	0.35	0.64	0.45	0.64	0.73	0.69	-98.6	7.6	0.3	55
oxcast_Cellumen Phospho- d:CLM_MitoticArrest_24hr discretized)	WEKA-RF	ALogPS,_OEsta te	35	182	00													
#2AX:CI_M_OxidativeStress_72hr discretized) Toxcast_Cellumen Phospho- ## discretized Toxcast_Cellumen Phospho- ## discretized Toxcast_Cellumen Phospho- ## discretized Toxcast_Cellumen Phospho- ## discretized Toxcast_Cellumen Phospho-	WEKA-RF	te																
I2AX.CI.M. OxidativeStress_72hr discretized) oxcast_Cellumen Phospho- 13:CLM. MitoticArrest_24hr discretized) oxcast_Cellumen Phospho- 13:CLM. MitoticArrest_72hr discretized)			35 80	182	46	41	304	0.71	0.63	0.66	0.65	0.66	0.75	0.7	-98.6	9.2	0.41	121
I2AX.C.I.M. OxidativeStress_72hr discretized) oxcast_Cellumen Phospho- 13:C.I.M. MitoticArrest_24hr discretized) oxcast_Cellumen Phospho- 13:C.I.M. MitoticArrest_72hr discretized) oxcast_Cellumen Phospho- oxcast_Cellumen	WEKA-RF LibSVM	CDK	80	137	46													121
I2AX.C.I.M. OxidativeStress_72hr discretized) oxcast_Cellumen Phospho- 13:C.I.M. MitoticArrest_24hr discretized) oxcast_Cellumen Phospho- 13:C.I.M. MitoticArrest_72hr discretized) oxcast_Cellumen Phospho- oxcast_Cellumen	WEKA-RF	te				41	304	0.71	0.63	0.66	0.65	0.66	0.75	0.74	-98.6 -98.5	9.2 7.71	0.41	121 53

Toxcast_Cellumen Phospho-c- jun:CLM_StressKinase_72hr																		
(discretized) Toxcast Cellumen a-	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
tubulin:CLM_MicrotubuleCSK_24hr	DI O	D	50	400	05	40	004	0.70	0.45	0.75	0.50	0.75	0.70	0.70	00.5	7.04		-,
(discretized) Toxcast_Cellumen a-	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
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:	T LO	QNER	30	175	34	20	303	0.74	0.40	0.00	0.50	0.00	0.70	0.71	-90.0	0.57	0.55	70
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:C																		
LM_Hepat_CellLoss_24hr (discretized)	MLRA	ChemaxonDesc riptors	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:C LM_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_DNADama ge:CLM_Hepat_DNADamage_1hr																		
(discretized) Toxcast_Cellumen_Hepat_DNADama	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
ge:CLM_Hepat_DNADamage_48hr																		
(discretized) Toxcast_Cellumen_Hepat_DNATextur	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
e:CLM_Hepat_DNATexture_48hr																		
(discretized) Toxcast_Cellumen_Hepat_NuclearSiz	PLS	Fragmentor	18	218	55	14	305	0.77	0.25	0.56	0.34	0.56	8.0	0.68	-98.6	6.96	0.26	32
e: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:C	TOWLIN	QNEN	25	203	01		303	0.75	0.20	0.74	0.50	0.74	0.73	0.73	-90.5	0.41	0.55	- 51
LM_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:C LM Hepat Steatosis 48hr				-		-												
(discretized)	KNN	ALogPS,_OEsta te	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		ALogPS,_OEsta																
(discretized) Toxcast_CellzDirect	WEKA-J48	te	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
CYP1A1:CLZD_CYP1A1_6		_																
(discretized) Toxcast CellzDirect	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
CYP1A2:CLZD_CYP1A2_24	DI O	D	00	474	40	00	000	0.70	0.00	0.70	0.07	0.70	0.04	0.70	00.5	0.00	0.54	
(discretized) Toxcast_CellzDirect	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
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	2.00 4 IAI	SSIC	J**	170	20	02	550	0.0	0.77	0.70	0.70	0.70	0.04	0.10	-50.4	5.01	0.00	120
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		ALogPS,_OEsta									-							
(discretized)	WEKA-J48	te	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	<u> </u>																	1
(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																		
					24	40	304	0.70	0.85	0.77	0.81	0.77	0.8				0.56	182
(discretized) Toxcast CellzDirect	ASNN	Fragmentor	140	98		42		0.78		0.77				0.79	-98.4	10.1		
Toxcast_CellzDirect CYP2C9:CLZD_CYP2C9_48		ALogPS,_OEsta																
Toxcast_CellzDirect CYP2C9:CLZD_CYP2C9_48 (discretized)	ASNN PLS		29	98	74	18	303	0.78	0.28	0.62	0.39	0.62	0.71	0.79	-98.4 -98.7	7.2	0.25	47
Toxcast_CellzDirect CYP2C9:CLZD_CYP2C9_48 (discretized) Toxcast_CellzDirect CYP2C9:CLZD_CYP2C9_6	PLS	ALogPS,_OEsta te	29	182	74	18	303	0.7	0.28	0.62				0.66	-98.7	7.2		
Toxcast_CellzDirect CYP2C9:CL.ZD_CYP2C9_48 (discretized) Toxcast_CellzDirect CYP2C9:CL.ZD_CYP2C9_6 (discretized) Toxcast_CellzDirect		ALogPS,_OEsta									0.39	0.62	0.71				0.25	47
Toxcast_CellzDirect CYP2C9:CLZD_CYP2C9_48 (discretized) Toxcast_CellzDirect CYP2C9:CLZD_CYP2C9_6 (discretized) Toxcast_CellzDirect CYP3A9:CLZD_CYP3A4_24	PLS WEKA-RF	ALogPS,_OEsta te GSFrag	29 25	182	74 91	18	303 304	0.7	0.28	0.62	0.32	0.6	0.65	0.66	-98.7 -98.8	7.2 6.73	0.18	42
Toxcast_CelizDirect CYP2C9:CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2C9:CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3C9-CEIZDIrect CYP3C9-CEIZDI	PLS	ALogPS,_OEsta te	29	182	74	18	303	0.7	0.28	0.62				0.66	-98.7	7.2		
Toxcast_CelizDirect CYP2C9:CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2C9:CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3C4:CLZD_CYP3C4_24 (discretized) (discretized)	PLS WEKA-RF	ALogPS,_OEsta te GSFrag	29 25	182	74 91	18	303 304	0.7	0.28	0.62	0.32	0.6	0.65	0.66	-98.7 -98.8	7.2 6.73	0.18	42
Toxcast_CelizDirect CYP2C9:CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2C9:CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect Toxcast_CelizDirect	PLS WEKA-RF LibSVM	ALogPS,_OEsta te GSFrag	29 25 91	182 171 136	74 91 38	18 17 36	303 304 301	0.7 0.64 0.75	0.28 0.22 0.71	0.62 0.6 0.72	0.32	0.6	0.65	0.66 0.62 0.75	-98.7 -98.8 -98.5	7.2 6.73 9.38	0.18	42 127
Toxcast_CellzDirect CYP2C9-CLZD_CYP2C9_48 (discretized) Toxcast_CellzDirect CYP2C9-CLZD_CYP2C9_6 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_6 (discretized)	PLS WEKA-RF LibSVM	ALogPS,_OEsta te GSFrag	29 25 91	182 171 136	74 91 38	18 17 36	303 304 301	0.7 0.64 0.75	0.28 0.22 0.71	0.62 0.6 0.72	0.32	0.6	0.65	0.66 0.62 0.75	-98.7 -98.8 -98.5	7.2 6.73 9.38	0.18	42 127
Toxcast_CelizDirect CYP2C9_CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2C9_CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6	PLS WEKA-RF LibSVM WEKA-J48	ALogPS_OEsta te GSFrag CDK	29 25 91 137	182 171 136 102	74 91 38 33	18 17 36 31	303 304 301 303	0.7 0.64 0.75 0.79	0.28 0.22 0.71	0.62 0.6 0.72 0.82	0.32 0.71 0.81	0.6 0.72 0.82	0.65 0.78 0.76	0.66 0.62 0.75 0.79	-98.7 -98.8 -98.5 -98.4	7.2 6.73 9.38 9.49	0.18 0.5 0.57	127 168
Toxcast_CellzDirect CYP2C9:CLZD_CYP2C9_48 (discretized) Toxcast_CellzDirect CYP2C9:CLZD_CYP2C9_6 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CellzDirect GSTA2:CLZD_GSTA2_48 (discretized)	PLS WEKA-RF LibSVM WEKA-J48	ALogPS_OEsta te GSFrag CDK	29 25 91 137	182 171 136 102	74 91 38 33	18 17 36 31	303 304 301 303	0.7 0.64 0.75 0.79	0.28 0.22 0.71	0.62 0.6 0.72 0.82	0.32 0.71 0.81	0.6 0.72 0.82	0.65 0.78 0.76	0.66 0.62 0.75 0.79	-98.7 -98.8 -98.5 -98.4	7.2 6.73 9.38 9.49	0.18 0.5 0.57	127 168
Toxcast_CellzDirect CYP2C9:CLZD_CYP2C9_48 (discretized) Toxcast_CellzDirect CYP2C9:CLZD_CYP2C9_6 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_GSTA2_48 (discretized) Toxcast_CellzDirect SYTA2:CLZD_GSTA2_48 (discretized) Toxcast_CellzDirect	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR	ALogPS,_OEsta te GSFrag CDK CDK Fragmentor Mera,_Mersy	29 25 91 137 59	182 171 136 102 150	74 91 38 33 65	18 17 36 31	303 304 301 303 305 301	0.7 0.64 0.75 0.79 0.69	0.28 0.22 0.71 0.81 0.48 0.27	0.62 0.6 0.72 0.82 0.66 0.79	0.32 0.71 0.81 0.55	0.6 0.72 0.82 0.66	0.65 0.78 0.76 0.7	0.66 0.62 0.75 0.79 0.68	-98.7 -98.8 -98.5 -98.4 -98.6	7.2 6.73 9.38 9.49 8.37	0.18 0.5 0.57 0.33	127 168 90
Toxcast_CelizDirect CYP2C9-CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2C9-CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect GSTA2:CLZD_GSTA2_48 (discretized) Toxcast_CelizDirect SSTA2:CLZD_GSTA2_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_24 (discretized)	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF	ALogPS,_OEsta te GSFrag CDK CDK Fragmentor	29 25 91 137 59	182 171 136 102	74 91 38 33	18 17 36 31	303 304 301 303 305	0.7 0.64 0.75 0.79	0.28 0.22 0.71 0.81	0.62 0.6 0.72 0.82 0.66	0.32 0.71 0.81 0.55	0.6 0.72 0.82 0.66	0.65 0.78 0.76	0.66 0.62 0.75 0.79	-98.7 -98.8 -98.5 -98.4	7.2 6.73 9.38 9.49 8.37	0.18 0.5 0.57	127 168 90
Toxcast_CelizDirect CYP2C9-CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2C9-CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect CSTA2_CLZD_GSTA2_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_24 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_24 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR WEKA-RF	ALogPS_OEsta te GSFrag CDK CDK Fragmentor Mera_Mersy Fragmentor	29 25 91 137 59 31	182 171 136 102 150 178	74 91 38 33 65 84	18 17 36 31 31 8	303 304 301 303 305 301 302	0.7 0.64 0.75 0.79 0.69 0.69	0.28 0.22 0.71 0.81 0.48 0.27	0.62 0.6 0.72 0.82 0.66 0.79	0.32 0.71 0.81 0.55 0.4	0.6 0.72 0.82 0.66 0.79	0.65 0.78 0.76 0.7 0.68	0.66 0.62 0.75 0.79 0.68 0.74	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5	7.2 6.73 9.38 9.49 8.37 6.34	0.18 0.5 0.57 0.33 0.33	127 168 90 39
Toxcast_CelizDirect CYP2G9-CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2C9-CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_24 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized)	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR	ALogPS,_OEsta te GSFrag CDK CDK Fragmentor Mera,_Mersy	29 25 91 137 59	182 171 136 102 150	74 91 38 33 65	18 17 36 31 31	303 304 301 303 305 301	0.7 0.64 0.75 0.79 0.69	0.28 0.22 0.71 0.81 0.48 0.27	0.62 0.6 0.72 0.82 0.66 0.79	0.32 0.71 0.81 0.55	0.6 0.72 0.82 0.66	0.65 0.78 0.76 0.7	0.66 0.62 0.75 0.79 0.68	-98.7 -98.8 -98.5 -98.4 -98.6	7.2 6.73 9.38 9.49 8.37 6.34	0.18 0.5 0.57 0.33	127 168 90
Toxcast_CelizDirect CYP2G9.CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2G9.CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect CSTA2:CLZD_GSTA2_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_24 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR WEKA-RF	ALogPS_OEsta te GSFrag CDK CDK Fragmentor Mera_Mersy Fragmentor Fragmentor ChemaxonDesc	29 25 91 137 59 31 27 53	182 171 136 102 150 178 192	74 91 38 33 65 84 68	18 17 36 31 31 8 15	303 304 301 303 305 301 302	0.7 0.64 0.75 0.79 0.69 0.69 0.73	0.28 0.22 0.71 0.81 0.48 0.27 0.28	0.62 0.6 0.72 0.82 0.66 0.79 0.64	0.32 0.71 0.81 0.55 0.4 0.39	0.6 0.72 0.82 0.66 0.79 0.64	0.65 0.78 0.76 0.7 0.68 0.74 0.67	0.66 0.62 0.75 0.79 0.68 0.74 0.69	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5	7.2 6.73 9.38 9.49 8.37 6.34 7.09	0.18 0.5 0.57 0.33 0.33 0.28	127 168 90 39 42
Toxcast_CelizDirect CYP2G9.CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2C9.CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_68 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect GSTA2:CLZD_GSTA2_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_24 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR WEKA-RF	ALogPS_OEsta te GSFrag CDK CDK Fragmentor Mera_Mersy Fragmentor Fragmentor ChemaxonDesc riptors	29 25 91 137 59 31	182 171 136 102 150 178	74 91 38 33 65 84	18 17 36 31 31 8	303 304 301 303 305 301 302	0.7 0.64 0.75 0.79 0.69 0.69	0.28 0.22 0.71 0.81 0.48 0.27	0.62 0.6 0.72 0.82 0.66 0.79	0.32 0.71 0.81 0.55 0.4	0.6 0.72 0.82 0.66 0.79	0.65 0.78 0.76 0.7 0.68	0.66 0.62 0.75 0.79 0.68 0.74	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5	7.2 6.73 9.38 9.49 8.37 6.34	0.18 0.5 0.57 0.33 0.33	127 168 90 39
Toxcast_CelizDirect CYP2C9-CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2C9-CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4-CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4-CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4-CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4-CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect GSTA2-CLZD_GSTA2_48 (discretized) Toxcast_CelizDirect SULT2A1-CLZD_SULT2A1_24 (discretized) Toxcast_CelizDirect SULT2A1-CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1-CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1-CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect SULT2A1-CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect SULT2A1-CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect UCST4A1-CLZD_GSULT2A1_6 (discretized) Toxcast_CelizDirect UCST4A1-CLZD_UCST1A1_24	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR WEKA-RF PLS KNN	ALogPS_OEsta te GSFrag CDK CDK Fragmentor Mera_Mersy Fragmentor Fragmentor ChemaxonDesc riptors ChemaxonDesc	29 25 91 137 59 31 27 53 35	182 171 136 102 150 178 192 150	74 91 38 33 65 84 68 75	18 17 36 31 31 8 15 26	303 304 301 303 305 301 302 304 303	0.7 0.64 0.75 0.79 0.69 0.69 0.73 0.67	0.28 0.22 0.71 0.81 0.48 0.27 0.28 0.41	0.62 0.6 0.72 0.82 0.66 0.79 0.64 0.67	0.32 0.71 0.81 0.55 0.4 0.39 0.51	0.6 0.72 0.82 0.66 0.79 0.64 0.67	0.65 0.78 0.76 0.7 0.68 0.74 0.67	0.66 0.62 0.75 0.79 0.68 0.74 0.69 0.67	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5 -98.7	7.2 6.73 9.38 9.49 8.37 6.34 7.09 7.95	0.18 0.5 0.57 0.33 0.33 0.28 0.3	127 168 90 39 42 79
Toxcast_CelizDirect CYP2G9-CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2C9-CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_STA2_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_24 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_CelizDirect	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR WEKA-RF	ALogPS_OEsta te GSFrag CDK CDK Fragmentor MeraMersy Fragmentor Fragmentor ChemaxonDesc riptors ChemaxonDesc riptors	29 25 91 137 59 31 27 53	182 171 136 102 150 178 192	74 91 38 33 65 84 68	18 17 36 31 31 8 15	303 304 301 303 305 301 302	0.7 0.64 0.75 0.79 0.69 0.69 0.73	0.28 0.22 0.71 0.81 0.48 0.27 0.28	0.62 0.6 0.72 0.82 0.66 0.79 0.64	0.32 0.71 0.81 0.55 0.4 0.39	0.6 0.72 0.82 0.66 0.79 0.64	0.65 0.78 0.76 0.7 0.68 0.74 0.67	0.66 0.62 0.75 0.79 0.68 0.74 0.69	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5	7.2 6.73 9.38 9.49 8.37 6.34 7.09	0.18 0.5 0.57 0.33 0.33 0.28	127 168 90 39 42
Toxcast_CellzDirect CYP2C9-CLZD_CYP2C9_48 (discretized) Toxcast_CellzDirect CYP2C9-CLZD_CYP2C9_6 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CellzDirect CSTA2-CLZD_CSTA2_48 (discretized) Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_24 (discretized) Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_46 (discretized) Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CellzDirect	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR WEKA-RF PLS KNN	ALogPS_OEsta te GSFrag CDK CDK Fragmentor Mera_Mersy Fragmentor Fragmentor ChemaxonDesc riptors ChemaxonDesc	29 25 91 137 59 31 27 53 35	182 171 136 102 150 178 192 150	74 91 38 33 65 84 68 75	18 17 36 31 31 8 15 26	303 304 301 303 305 301 302 304 303	0.7 0.64 0.75 0.79 0.69 0.69 0.73 0.67	0.28 0.22 0.71 0.81 0.48 0.27 0.28 0.41	0.62 0.6 0.72 0.82 0.66 0.79 0.64 0.67	0.32 0.71 0.81 0.55 0.4 0.39 0.51	0.6 0.72 0.82 0.66 0.79 0.64 0.67	0.65 0.78 0.76 0.7 0.68 0.74 0.67	0.66 0.62 0.75 0.79 0.68 0.74 0.69 0.67	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5 -98.7	7.2 6.73 9.38 9.49 8.37 6.34 7.09 7.95	0.18 0.5 0.57 0.33 0.33 0.28 0.3	127 168 90 39 42 79 47
Toxcast_CelizDirect CYP2C9-CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2C9-CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect GSTA2:CLZD_GSTA2_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_24 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect UGST41:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_48 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_48 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_48 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_48 (discretized) Toxcast_DelizDirect UGT1A1:CLZD_UGT1A1_48	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR WEKA-RF PLS KNN WEKA-RF	ALogPS_OEsta te GSFrag CDK CDK Fragmentor Mera_Mersy Fragmentor Fragmentor ChemaxonDesc riptors ALogPS_OEsta	29 25 91 137 59 31 27 53 35	182 171 136 102 150 178 192 150 144 140	74 91 38 33 65 84 68 75 112	18 17 36 31 31 8 15 26 12	303 304 301 303 305 301 302 304 303 303	0.7 0.64 0.75 0.79 0.69 0.69 0.73 0.67 0.59	0.28 0.22 0.71 0.81 0.48 0.27 0.28 0.41 0.24 0.38	0.62 0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74	0.32 0.71 0.81 0.55 0.4 0.39 0.51 0.36	0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74	0.65 0.78 0.76 0.7 0.68 0.74 0.67 0.56	0.66 0.62 0.75 0.79 0.68 0.74 0.69 0.67	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5 -98.6 -98.7 -98.7	7.2 6.73 9.38 9.49 8.37 6.34 7.09 7.95 6.35	0.18 0.5 0.57 0.33 0.33 0.28 0.3 0.22	127 168 90 39 42 79
Toxcast_CelizDirect CYP2G9.CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2G9.CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect CSTA2:CLZD_CSTA2_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_24 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_48 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_48 (discretized)	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR WEKA-RF PLS KNN WEKA-RF LibSVM	ALogPS_OEsta te GSFrag CDK CDK Fragmentor Mera_Mersy Fragmentor ChemaxonDescriptors ChemaxonDescriptors ALogPS_OEsta te	29 25 91 137 59 31 27 53 35	182 171 136 102 150 178 192 150 144 140	74 91 38 33 65 84 68 75 112	18 17 36 31 31 8 15 26 12	303 304 301 303 305 301 302 304 303 303	0.7 0.64 0.75 0.79 0.69 0.69 0.73 0.67 0.59	0.28 0.22 0.71 0.81 0.48 0.27 0.28 0.41 0.24 0.38	0.62 0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74	0.32 0.71 0.81 0.55 0.4 0.39 0.51 0.36	0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74	0.65 0.78 0.76 0.7 0.68 0.74 0.67 0.56	0.66 0.62 0.75 0.79 0.68 0.74 0.69 0.67	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5 -98.6 -98.7 -98.7	7.2 6.73 9.38 9.49 8.37 6.34 7.09 7.95 6.35	0.18 0.5 0.57 0.33 0.33 0.28 0.3 0.22	127 168 90 39 42 79 47
Toxcast_Celizbirect CYP2C9-CLZD_CYP2C9_48 (discretized) Toxcast_Celizbirect CYP2C9-CLZD_CYP2C9_6 (discretized) Toxcast_Celizbirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_Celizbirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_Celizbirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_Celizbirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_Celizbirect STA2_CLZD_GSTA2_48 (discretized) Toxcast_Celizbirect SULT2A1:CLZD_SULT2A1_24 (discretized) Toxcast_Celizbirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_Celizbirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_Celizbirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_Celizbirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_Celizbirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_Celizbirect UGT1A1:CLZD_UGT1A1_48 (discretized) Toxcast_Celizbirect UGT1A1:CLZD_UGT1A1_48 (discretized) Toxcast_HDFn_IL_1b_TNF_a_IFN_g_ EGF_FGF_PDGFbb_24_CD106_VCA M_1_down:BSK_hDFCGF_VCAM1_d	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR WEKA-RF PLS KNN WEKA-RF LibSVM	ALogPS_OEsta te GSFrag CDK CDK Fragmentor Mera_Mersy Fragmentor Fragmentor ChemaxonDesc riptors ALogPS_OEsta	29 25 91 137 59 31 27 53 35	182 171 136 102 150 178 192 150 144 140	74 91 38 33 65 84 68 75 112	18 17 36 31 31 8 15 26 12	303 304 301 303 305 301 302 304 303 303	0.7 0.64 0.75 0.79 0.69 0.69 0.73 0.67 0.59	0.28 0.22 0.71 0.81 0.48 0.27 0.28 0.41 0.24 0.38	0.62 0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74	0.32 0.71 0.81 0.55 0.4 0.39 0.51 0.36	0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74	0.65 0.78 0.76 0.7 0.68 0.74 0.67 0.56	0.66 0.62 0.75 0.79 0.68 0.74 0.69 0.67	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5 -98.6 -98.7 -98.7	7.2 6.73 9.38 9.49 8.37 6.34 7.09 7.95 6.35	0.18 0.5 0.57 0.33 0.33 0.28 0.3 0.22	127 168 90 39 42 79 47
Toxcast_CelizDirect CYP2C9-CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2C9-CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_68 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect GSTA2_CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_24 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_CelizDirect Toxcast_DelizDirect Toxcast_DelizDirec	PLS WEKA-RF LibSVM WEKA-J48 WEKA-FF FSMLR WEKA-RF PLS KNN WEKA-RF LibSVM	ALogPS_OEsta te GSFrag CDK CDK Fragmentor Mera_Mersy Fragmentor Fragmentor ChemaxonDescriptors ChemaxonDescriptors ALogPS_OEsta te	29 25 91 137 59 31 27 53 35 55	182 171 136 102 150 178 192 150 144 140 179	74 91 38 33 65 84 68 75 112 90 42	18 17 36 31 31 8 15 26 12 17	303 304 301 303 305 301 302 304 303 302 303	0.7 0.64 0.75 0.79 0.69 0.69 0.73 0.67 0.59 0.65	0.28 0.22 0.71 0.81 0.48 0.27 0.28 0.41 0.24 0.38	0.62 0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74 0.76	0.32 0.71 0.81 0.55 0.4 0.39 0.51 0.36	0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74	0.65 0.78 0.76 0.7 0.68 0.74 0.67 0.56	0.66 0.62 0.75 0.79 0.68 0.74 0.69 0.65 0.69	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5 -98.6 -98.7 -98.7 -98.6	7.2 6.73 9.38 9.49 8.37 6.34 7.09 7.95 6.35 7.32	0.18 0.5 0.57 0.33 0.33 0.28 0.3 0.22 0.32	127 168 90 39 42 79 47 72 82
Toxcast_CelizDirect CYP2G9.CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2G9.CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect SUT2A1:CLZD_SUT2A1_24 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_48 (discretized) Toxcast_DelizDirect UGT1A1:CLZD_UGT1A1_48 (discretized) Toxcast_HDFn_IL_1b_TNF_a_IFN_g EGF_FGF_PGFbb_24_CXCL10_IP Toxcast_HDFn_IL_1b_TNF_a_IFN_g EGF_FGF_PGFbb_24_CXCL10_IP	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR WEKA-RF PLS KNN WEKA-RF LibSVM	ALogPS_OEsta te GSFrag CDK CDK Fragmentor Mera_Mersy Fragmentor ChemaxonDesc riptors ALogPS_OEsta te CDK CDK CDK ChemaxonDesc riptors ChemaxonDesc riptors	29 25 91 137 59 31 27 53 35 55 58	182 171 136 102 150 178 192 150 144 140 179	74 91 38 33 65 84 68 75 112 90 42	18 17 36 31 31 8 15 26 12 17 24	303 304 301 303 305 301 302 304 303 303 304	0.7 0.64 0.75 0.79 0.69 0.69 0.73 0.67 0.59 0.85	0.28 0.22 0.71 0.81 0.48 0.27 0.28 0.41 0.24 0.38 0.58	0.62 0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74 0.76 0.71	0.32 0.71 0.81 0.55 0.4 0.39 0.51 0.64 0.52	0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74 0.76 0.71	0.65 0.78 0.76 0.7 0.68 0.74 0.67 0.56 0.61 0.81	0.66 0.62 0.75 0.79 0.68 0.74 0.69 0.65 0.69 0.76	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5 -98.6 -98.7 -98.6 -98.7 -98.8	7.2 6.73 9.38 9.49 8.37 6.34 7.09 7.95 6.35 7.32 8.71	0.18 0.5 0.57 0.33 0.33 0.28 0.3 0.22 0.32 0.49	127 168 90 39 42 79 47 72 82
Toxcast_CelizDirect CYP2G9.CLZD_CYP2C9_48 (discretized) Toxcast_CelizDirect CYP2AG.CLZD_CYP2C9_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CelizDirect GSTA2:CLZD_GSTA2_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_24 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CelizDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_CelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_DelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_DelizDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_HDFn_IL_1b_TNF_a_IFN_g_ EGF_FG_PDGFbb_24_CD10_IP-10_down.BSK_hDFCGF_IP10_down.BSK_hDFCGF_IP10_down.BSK_hDFCGF_IP10_down.BSK_hDFCGF_IP10_down.BSK_hDFCGF_IP10_down.BSK_hDFCGF_IP10_down.BSK_hDFCGF_IP10_down.BSK_hDFCGF_IP10_ID_IP10_IDXCast_HDFn_IL_1b_TNF_a_IFN_g_ INVALIDATIONAL TOXAL T	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR WEKA-RF PLS KNN WEKA-RF LibSVM	ALogPS_OEsta te GSFrag CDK CDK Fragmentor Mera_Mersy Fragmentor Fragmentor ChemaxonDescriptors ChemaxonDescriptors ALogPS_OEsta te	29 25 91 137 59 31 27 53 35 55	182 171 136 102 150 178 192 150 144 140 179	74 91 38 33 65 84 68 75 112 90 42	18 17 36 31 31 8 15 26 12 17	303 304 301 303 305 301 302 304 303 302 303	0.7 0.64 0.75 0.79 0.69 0.69 0.73 0.67 0.59 0.65	0.28 0.22 0.71 0.81 0.48 0.27 0.28 0.41 0.24 0.38	0.62 0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74 0.76	0.32 0.71 0.81 0.55 0.4 0.39 0.51 0.36	0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74	0.65 0.78 0.76 0.7 0.68 0.74 0.67 0.56	0.66 0.62 0.75 0.79 0.68 0.74 0.69 0.65 0.69	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5 -98.6 -98.7 -98.7 -98.6	7.2 6.73 9.38 9.49 8.37 6.34 7.09 7.95 6.35 7.32	0.18 0.5 0.57 0.33 0.33 0.28 0.3 0.22 0.32	127 168 90 39 42 79 47 72 82
Toxcast_CellzDirect CYP2C9-CLZD_CYP2C9_48 (discretized) Toxcast_CellzDirect CYP2C9-CLZD_CYP2C9_6 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_24 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_48 (discretized) Toxcast_CellzDirect CYP3A4:CLZD_CYP3A4_6 (discretized) Toxcast_CellzDirect CSTA2:CLZD_GYP3A4_6 (discretized) Toxcast_CellzDirect GSTA2:CLZD_GSTA2_48 (discretized) Toxcast_CellzDirect GSTA2:CLZD_SULT2A1_24 (discretized) Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_48 (discretized) Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CellzDirect SULT2A1:CLZD_SULT2A1_6 (discretized) Toxcast_CellzDirect UGT1A1:CLZD_UGT1A1_24 (discretized) Toxcast_CellzDirect UGT1A1:CLZD_UGT1A1_48 (discretized) Toxcast_DellzDirect UGT1A1:CLZD_UGT1A1_48 (discretized)	PLS WEKA-RF LibSVM WEKA-J48 WEKA-RF FSMLR WEKA-RF PLS KNN WEKA-RF LibSVM	ALogPS_OEsta te GSFrag CDK CDK Fragmentor Mera_Mersy Fragmentor ChemaxonDesc riptors ALogPS_OEsta te CDK CDK CDK ChemaxonDesc riptors ChemaxonDesc riptors	29 25 91 137 59 31 27 53 35 55 58	182 171 136 102 150 178 192 150 144 140 179	74 91 38 33 65 84 68 75 112 90 42	18 17 36 31 31 8 15 26 12 17 24	303 304 301 303 305 301 302 304 303 303 304	0.7 0.64 0.75 0.79 0.69 0.69 0.73 0.67 0.59 0.85	0.28 0.22 0.71 0.81 0.48 0.27 0.28 0.41 0.24 0.38 0.58	0.62 0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74 0.76 0.71	0.32 0.71 0.81 0.55 0.4 0.39 0.51 0.64 0.52	0.6 0.72 0.82 0.66 0.79 0.64 0.67 0.74 0.76 0.71	0.65 0.78 0.76 0.7 0.68 0.74 0.67 0.56 0.61 0.81	0.66 0.62 0.75 0.79 0.68 0.74 0.69 0.65 0.69 0.76	-98.7 -98.8 -98.5 -98.4 -98.6 -98.5 -98.6 -98.7 -98.6 -98.7 -98.8	7.2 6.73 9.38 9.49 8.37 6.34 7.09 7.95 6.35 7.32 8.71	0.18 0.5 0.57 0.33 0.33 0.28 0.3 0.22 0.32 0.49	127 168 90 39 42 79 47 72 82

oxcast_HDFn_IL_1b_TNF_a_IFN_g GF_FGF_PDGFbb_24_Collagen_III																		
own:BSK_hDFCGF_CollagenIII_dow (discretized)		ChemaxonDesc riptors	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
oxcast_HDFn_IL_1b_TNF_a_IFN_g																		
GF_FGF_PDGFbb_24_EGFR_up:B K_hDFCGF_EGFR_up (discretized)	PLS	ChemaxonDesc riptors	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
Foxcast_HDFn_IL_1b_TNF_a_IFN_g FGF_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_dow		M																
n:BSK_hDFCGF_MCSF_down discretized)	WEKA-J48	ALogPS,_OEsta te	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
oxcast_HDFn_IL_1b_TNF_a_IFN_g GF_FGF_PDGFbb_24_PAI_I_down:		to the fire December																
BSK_hDFCGF_PAI1_down discretized)	PLS	InductiveDescrip tors	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
oxcast_HDFn_IL_1b_TNF_a_IFN_g GF_FGF_PDGFbb_24_Proliferation																		
2hr_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
oxcast_HDFn_IL_1b_TNF_a_IFN_g GF_FGF_PDGFbb_24_SRB_down:		01																
SK_hDFCGF_SRB_down discretized)	MLRA	ChemaxonDesc riptors	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
oxcast_HEK_HDFn_IL_1b_TNF_a_I N_g_TGF_b_24_CCL2_MCP_1_do																		
rn: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
oxcast_HEK_HDFn_IL_1b_TNF_a_I N_g_TGF_b_24_CXCL10_IP_10_dc	1																	
rn:BSK_KF3CT_IP10_down	LibSVM	InductiveDescrip tors	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
oxcast_HEK_HDFn_IL_1b_TNF_a_I N_g_TGF_b_24_IL_1alpha_down:B	EOM: D	ChemaxonDesc	~~	470	70	40	000	0.00	0.00	• •	0.00	2.5	<u> </u>	0.0-	00 -	70:	0.00	
SK_KF3CT_IL1a_down (discretized) oxcast_HEK_HDFn_IL_1b_TNF_a_I		riptors	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
N_g_TGF_b_24_MMP_9_down:BSk KF3CT_MMP9_down (discretized) oxcast HEK_HDFn_IL_1b_TNF_a_I	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
N_g_TGF_b_24_TIMP_2_down:BSk		D	00	044		40	000	0.70	0.00	0.55	0.00	0.55	0.70	0.07	00.7	7.07	0.07	40
KF3CT_TIMP2_down (discretized) oxcast_HEK_HDFn_IL_1b_TNF_a_I	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
N_g_TGF_b_24_uPA_down:BSK_K 3CT_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
oxcast_HUVEC_IL_1b_TNF_a_IFN_ _24_CCL2_MCP_1_down:BSK_3C_	ECMI D	DC	27	100	50	22	204	0.70	0.20	0.00	0.40	0.00	0.70	0.00	00.0	7.04	0.22	
MCP1_down (discretized) oxcast_HUVEC_IL_1b_TNF_a_IFN_	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
_24_CD141_Thrombomodulin_up:B :K_3C_Thrombomodulin_up	Libova	InductiveDescrip	07	200	50	10	202	0.75	0.22	0.50	0.40	0.50	0.70	0.00	00.0	7.55	0.0	40
discretized) oxcast_HUVEC_IL_1b_TNF_a_IFN_	LibSVM	tors	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
_24_CD62E_E_Selectin_down:BSK_ C_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
oxcast_HUVEC_IL_1b_TNF_a_IFN_ j_24_CD87_uPAR_down:BSK_3C_u		005	47	474	50	0.4	004	0.70	0.47	0.50	0.50	0.50	0.77	0.07	00.7	0.50	0.00	0.4
PAR_down (discretized) Oxcast_HUVEC_IL_1b_TNF_a_IFN_	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
j_24_CXCL8_IL_8_down:BSK_3C_IL s_down (discretized)	WEKA-RF	ALogPS,_OEsta te	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
oxcast_HUVEC_IL_1b_TNF_a_IFN_ j_24_HLA_DR_down:BSK_3C_hLAD		DC	70	100	70	07	204	0.05	0.5	0.74	0.0	0.74	0.0	0.67	00.7	0.00	0.22	405
R_down (discretized) oxcast_HUVEC_IL_1b_TNF_a_IFN_ 24 Proliferation down:BSK 3C Pr	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
24_Proliferation_down.BSK_3C_Proliferation_down (discretized) oxcast_HUVEC_IL_1b_TNF_a_IFN_	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
_24_SRB_down:BSK_3C_SRB_dow (discretized)		DC	42	100	60	40	202	0.74	0.20	0.70	0.54	0.70	0.70	0.75	00.5	7.04	0.4	
oxcast_HUVEC_IL_1b_TNF_a_IFN_ 24 Visual down:BSK 3C Vis dow	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
(discretized)	MLRA	ALogPS,_OEsta te	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
oxcast_HUVEC_IL_4_Histamine_24 CL26_Eotaxin_3_down:BSK_4H_Eo		ALogPS,_OEsta	24	100	70	10	202	0.7	0.3	0.62	0.4	0.62	0.74	0.67	00.7	7.00	0.00	
axin3_down (discretized) oxcast_HUVEC_IL_4_Histamine_24 CCL2_MCP_1_down:BSK_4H_MCP1		te ALogPS,_OEsta	31	180	73	19	303	0.7	0.3	0.02	0.4	0.62	0.71	0.67	-98.7	7.32	0.26	50
down (discretized) oxcast_HUVEC_IL_4_Histamine_24	WEKA-RF	te	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
D106_VCAM_1_down:BSK_4H_VC .M1_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
oxcast_HUVEC_IL_4_Histamine_24 D62P_P_selectin_down:BSK_4H_P		ALogPS,_OEsta	32	177	41	21	303	0.70	0.55	0.00	0.50	0.00	0.73	0.72	-90.0	0.55	0.42	15
electin_down (discretized) oxcast_HUVEC_IL_4_Histamine_24	LibSVM	te	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
iRB_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
oxcast_HUVEC_PBMC_LPS_24_CC	;	GSFIAG	20	210	34	13	302	0.76	0.21	0.01	0.37	0.01	0.0	0.7	-90.0	7.	0.29	33
2_MCP_1_down:BSK_LPS_MPC1_c wn (discretized) bxcast_HUVEC_PBMC_LPS_24_CD	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
DXCast_HUVEC_PBMC_LPS_24_CL 06_VCAM_1_down:BSK_LPS_VCA 11_down (discretized)	WEKA-RF	Mera Morey	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
oxcast_HUVEC_PBMC_LPS_24_CD		Mera,_Mersy	oU	145	υl	19	301	0.75	0.00	U.01	0.00	0.01	0.72	0.76	-90.0	0.29	0.5	99
0_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
oxcast_HUVEC_PBMC_LPS_24_CD 2E_E_Selectin_down:BSK_LPS_Ese	•	Adriana	44	160	74	20	204	0.7	0.27	0.67	0.47	0.67	0.7	0.60	00.0	764	0.24	~-
ectin_down (discretized) oxcast_HUVEC_PBMC_LPS_24_CX	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
CL8_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		ALogPS,_OEsta																
discretized)	WEKA-RF	te	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

T																		
Toxcast_HUVEC_PBMC_LPS_24_PG E2_down:BSK_LPS_PGE2_down	•																	
(discretized)	PLS	GSFrag	48	181	61	12	302	0.76	0.44	8.0	0.57	8.0	0.75	0.77	-98.5	7.49	0.46	60
Toxcast_HUVEC_PBMC_LPS_24_PG E2_up:BSK_LPS_PGE2_up	•																	
(discretized) Toxcast HUVEC PBMC LPS 24 SR	WEKA-RF	Fragmentor	48	210	27	20	305	0.85	0.64	0.71	0.67	0.71	0.89	8.0	-98.4	8.94	0.57	68
B down:BSK LPS SRB down	i.																	
(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_TN F_alpha_down:BSK_LPS_TNFa_dow	ı																	
n (discretized) Toxcast_HUVEC_PBMC_SEB_TSST_	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
24_CCL2_MCP_1_down:BSK_SAg_N	Ā																	
CP1_down (discretized) Toxcast_HUVEC_PBMC_SEB_TSST_	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
24_CD38_down:BSK_SAg_CD38_do	-																	
wn (discretized) Toxcast HUVEC PBMC SEB TSST	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
24_CD38_up:BSK_SAg_CD38_up	-																	
(discretized) Toxcast_HUVEC_PBMC_SEB_TSST_	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
24_CD40_down:BSK_SAg_CD40_do	=	ALogPS,_OEsta																
wn (discretized) Toxcast_HUVEC_PBMC_SEB_TSST_	WEKA-RF	te	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
24_CD62E_E_Selectin_down:BSK_S	-	ALogPS,_OEsta																
Ag_Eselectin_down (discretized) Toxcast_HUVEC_PBMC_SEB_TSST_	WEKA-RF	te	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
24_CD69_down:BSK_SAg_CD69_do																		
wn (discretized) Toxcast_HUVEC_PBMC_SEB_TSST_	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
24_CXCL8_IL_8_down:BSK_SAg_IL8		D	0.5	45.	50	00	000	0 = :	0.50		0.00	c -		0 ==	00 -	0	0.10	
_down (discretized) Toxcast_HUVEC_PBMC_SEB_TSST_	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
24_PBMC_Cytotoxicity_down:BSK_S																		
Ag_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_Pro	ī																	
iferation_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_huma																		
n (discretized)	FSMLR	Dragon6	47	189	48	18	302	0.78	0.49	0.72	0.59	0.72	8.0	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	8.0	0.77	-98.5	7.31	0.43	43
Toxcast_Novascreen Human CYP2B6		ALogPS,_OEsta																
:NVS_ADME_hCYP2B6 (discretized) Toxcast_Novascreen Human	ASNN	te	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
CYP2C18:NVS_ADME_hCYP2C18	Libovaa	ALogPS,_OEsta	20	244	10	40	202	0.0	0.0	0.74	0.07	0.74	0.00	0.04	00.0	0.00	0.00	20
(discretized) Toxcast_Novascreen Human	LibSVM	te	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
CYP2C19:NVS_ADME_hCYP2C19 (discretized)	WEKA-J48	ChemaxonDesc riptors	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
(discretized)	WEIGHO	приого	70	130	40	20	303	0.73	0.01	0.74	0.07	0.74	0.73	0.74	-90.5	0.02	0.47	100
Toxcast_Novascreen Human CYP2C9 :NVS_ADME_hCYP2C9 (discretized)		ALogPS,_OEsta te	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	1 20	ic .	04	222	- 00	10	002	0.00	0.01	0.12	0.0	0.72	0.07	0.0	-50.4	0.04	0.02	
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) Toxcast_Novascreen Human	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
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) Toxcast_Novascreen Rat CYP2C6		Dragon6 ALogPS,_OEsta	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
:NVS_ADME_rCYP2C6 (discretized) Toxcast Novascreen Rat CYP3A1	WEKA-RF	te	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
: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,_OEsta te	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-								50			2.0		2.00					- 55
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_SM	· · ·																	
3C_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_P	r																	
oliferation_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		ALogPS,_OEsta																
						22	202	0.75	0.42	0.63	0.51	0.63	0.78	0.7	-98.6	8.09	0.36	62
(discretized)	WEKA-RF	te	39	187	53	23	302	0.75	0.42	0.00	0.01	0.00		•				
(discretized) Toxcast_Solidus (P450):Solidus_P450 (discretized)			39 48	187	37	32	303	0.75	0.42	0.6	0.58	0.6	0.83	0.72	-98.6	8.97	0.43	80
(discretized) Toxcast_Solidus (P450):Solidus_P450 (discretized) Toxcast_Solidus (Phase	KNN	te ALogPS,_OEsta te ChemaxonDesc	48	186	37	32	303	0.77	0.56	0.6	0.58	0.6	0.83	0.72	-98.6	8.97		
(discretized) Toxcast_Solidus (P450):Solidus_P450 (discretized))	te ALogPS,_OEsta te															0.43	80 55