

			True Positive	True Negative	False Positive	False Negative	Coun t	Accu racy	Preci sion	F- meas recall	Sens itivity	Speci ficity	Bala nced Accu racy	Inform edness	LOR	MCC	Real Positive	
Endpoint	Algorithm	Descriptors																
Toxrefdb_CHR_Mouse_Kidney_1_AnyLesion:CHR_Mouse_Kidney_1_AnyLesion (discretized)	WEKA-RF	Spectrophores	29	108	79	17	233	0.59	0.27	0.63	0.38	0.63	0.58	0.6	98.792	6.56	0.17	46
Toxrefdb_CHR_Mouse_Liver_1_AnyLesion:CHR_Mouse_Liver_1_AnyLesion (discretized)	LibSVM	ALogPS_OEstimate	89	70	37	37	233	0.68	0.71	0.71	0.71	0.71	0.65	0.68	98.639	8.75	0.36	126
Toxrefdb_CHR_Mouse_Liver_2_PreneoplasticLesion:CHR_Mouse_Liver_2_PreneoplasticLesion (discretized)	ASNN	CDK	51	102	40	39	232	0.66	0.56	0.57	0.56	0.57	0.72	0.64	98.715	8.55	0.28	90
Toxrefdb_CHR_Mouse_Liver_3_NeoplasticLesion:CHR_Mouse_Liver_3_NeoplasticLesion (discretized)	ASNN	Spectrophores	41	119	45	28	233	0.69	0.48	0.59	0.53	0.59	0.73	0.66	98.68	8.04	0.3	69
Toxrefdb_CHR_Mouse_Spleen_1_AnyLesion:CHR_Mouse_Spleen_1_AnyLesion (discretized)	MLRA	Fragmentor	23	146	50	14	233	0.73	0.32	0.62	0.42	0.62	0.74	0.68	98.633	6.9	0.29	37
Toxrefdb_CHR_Rat_AdrenalGland_1_AnyLesion (discretized)	ASNN	GSFrag	21	158	50	14	243	0.74	0.3	0.6	0.4	0.6	0.76	0.68	98.64	6.89	0.28	35
Toxrefdb_CHR_Rat_Eye_1_AnyLesion:CHR_Rat_Eye_1_AnyLesion (discretized)	MLRA	ALogPS_OEstimate	25	139	66	13	243	0.67	0.27	0.66	0.39	0.66	0.68	0.67	98.664	6.58	0.25	38
Toxrefdb_CHR_Rat_Kidney_1_AnyLesion:CHR_Rat_Kidney_1_AnyLesion (discretized)	LibSVM	Fragmentor	43	128	29	43	243	0.7	0.6	0.5	0.54	0.5	0.82	0.66	98.685	9.02	0.33	86
Toxrefdb_CHR_Rat_Liver_1_AnyLesion:CHR_Rat_Liver_1_AnyLesion (discretized)	KNN	ALogPS_OEstimate	84	76	42	41	243	0.66	0.67	0.67	0.67	0.67	0.64	0.66	98.684	8.75	0.32	125
Toxrefdb_CHR_Rat_Liver_2_PreneoplasticLesion:CHR_Rat_Liver_2_PreneoplasticLesion (discretized)	PLS	Toxcast_assays, _Toxcast_Pathways	33	129	57	24	243	0.67	0.37	0.58	0.45	0.58	0.69	0.64	98.728	7.52	0.24	57
Toxrefdb_CHR_Rat_Lung_1_AnyLesion:CHR_Rat_Lung_1_AnyLesion (discretized)	FSMLR	Dragon6	19	136	71	17	243	0.64	0.21	0.53	0.3	0.53	0.66	0.59	98.815	6.48	0.14	36
Toxrefdb_CHR_Rat_Testes_1_AnyLesion:CHR_Rat_Testes_1_AnyLesion (discretized)	FSMLR	CDK,_Toxcast_assays,_Toxcast_Pathways	21	140	61	19	241	0.67	0.26	0.53	0.34	0.53	0.7	0.61	98.778	6.86	0.17	40
Toxrefdb_CHR_Rat_ThyroidGland_1_AnyLesion:CHR_Rat_ThyroidGland_1_AnyLesion (discretized)	MLRA	InductiveDescriptors	29	138	53	23	243	0.69	0.35	0.56	0.43	0.56	0.72	0.64	98.72	7.49	0.24	52
Toxrefdb_CHR_Rat_ThyroidGland_2_PreneoplasticLesion:CHR_Rat_ThyroidGland_2_PreneoplasticLesion (discretized)	WEKA-RF	GSFrag	27	126	77	13	243	0.63	0.26	0.68	0.38	0.68	0.62	0.65	98.704	6.41	0.22	40
Toxrefdb_Chronic Mouse Endpoint for All effect related to apoptosis and necrosis:CHR_Mouse_LiverNecrosis (discretized)	ASNN	ALogPS_OEstimate	26	149	45	13	233	0.75	0.37	0.67	0.47	0.67	0.77	0.72	98.565	7.07	0.35	39
Toxrefdb_Chronic Mouse Endpoint for All neoplastic and non-neoplastic proliferative liver lesions:CHR_Mouse_LiverProliferativeLesions (discretized)	ASNN	Fragmentor	47	109	36	41	233	0.67	0.57	0.53	0.55	0.53	0.75	0.64	98.714	8.69	0.29	88
Toxrefdb_Chronic Mouse Endpoint for All neoplastic lesions (any target):CHR_Mouse_Tumorigen (discretized)	ASNN	CDK	55	94	48	35	232	0.64	0.53	0.61	0.57	0.61	0.66	0.64	98.727	8.25	0.27	90
Toxrefdb_Chronic Mouse Endpoint for All neoplastic liver lesions:CHR_Mouse_LiverTumors (discretized)	ASNN	Spectrophores	41	119	45	28	233	0.69	0.48	0.59	0.53	0.59	0.73	0.66	98.68	8.04	0.3	69
Toxrefdb_Chronic Mouse Endpoint for All non-neoplastic and neoplastic kidney pathology:CHR_Mouse_KidneyPathology (discretized)	WEKA-RF	Spectrophores	29	108	79	17	233	0.59	0.27	0.63	0.38	0.63	0.58	0.6	98.792	6.56	0.17	46
Toxrefdb_Chronic Mouse Endpoint for Liver hypertrophy (individual effect):CHR_Mouse_LiverHypertrophy (discretized)	WEKA-RF	Fragmentor	37	121	51	24	233	0.68	0.42	0.61	0.5	0.61	0.7	0.66	98.69	7.68	0.28	61

Toxrefdb_Chronic Rat Endpoint for All neoplastic and non- neoplastic proliferative liver lesions:CHR_Rat_LiverProliferativ eLesions (discretized)	WEKA-J48	Toxcast_assays, _Toxcast_Pathw ays	30	137	46	30	243	0.69	0.39	0.5	0.44	0.5	0.75	0.62	98.751	7.92	0.23	60
Toxrefdb_Chronic Rat Endpoint for All neoplastic and non- neoplastic proliferative thyroid lesions:CHR_Rat_ThyroidProlifer ativeLesions (discretized)	WEKA-RF	GSFrag	27	126	77	13	243	0.63	0.26	0.68	0.38	0.68	0.62	0.65	98.704	6.41	0.22	40
Toxrefdb_Chronic Rat Endpoint for All neoplastic lesions (any target):CHR_Rat_Tumorigen (discretized)	FSMLR	Mera_, Mersy	51	90	57	44	242	0.58	0.47	0.54	0.5	0.54	0.61	0.57	98.851	8.19	0.15	95
Toxrefdb_Chronic Rat Endpoint for Any cholinesterase inhibition measurement (e.g., brain and erythrocyte):CHR_Rat_Cholineste raseInhibition (discretized)	ASNN	Fragmentor	39	191	10	3	243	0.95	0.8	0.93	0.86	0.93	0.95	0.94	98.121	7.83	0.83	42
Toxrefdb_Chronic Rat Endpoint for Kidney nephropathy (individual effect):CHR_Rat_KidneyNephrop athy (discretized)	FSMLR	Dragon6	16	154	53	20	243	0.7	0.23	0.44	0.3	0.44	0.74	0.59	98.812	6.88	0.15	36
Toxrefdb_Chronic Rat Endpoint for Liver hypertrophy (individual effect):CHR_Rat_LiverHypertroph y (discretized)	PLS	Spectrophores	51	106	74	12	243	0.65	0.41	0.81	0.54	0.81	0.59	0.7	98.602	6.82	0.35	63
Toxrefdb_DEV_rabbit_Developme ntal (dLEL_rabbit):DEV_rabbit_Develo pmental (discretized)	FSMLR	Dragon6	63	84	43	41	231	0.64	0.59	0.61	0.6	0.61	0.66	0.63	98.733	8.54	0.27	104
Toxrefdb_DEV_rabbit_Maternal (mLEL_rabbit):DEV_rabbit_Mater nal (discretized)	FSMLR	CDK_, Toxcast_ assays_, Toxcast _Pathways	151	10	10	59	230	0.7	0.94	0.72	0.81	0.72	0.5	0.61	98.781	9.11	0.13	210
Toxrefdb_DEV_rat_Developmenta l (dLEL_rat):DEV_rat_Developmen tal (discretized)	FSMLR	GSFrag	88	72	32	55	247	0.65	0.73	0.62	0.67	0.62	0.69	0.65	98.692	9.3	0.3	143
Toxrefdb_DEV_rat_Maternal (mLEL_rat):DEV_rat_Maternal (discretized)	WEKA-J48	CDK_, Toxcast_ Pathways	165	22	9	50	246	0.76	0.95	0.77	0.85	0.77	0.71	0.74	98.523	9.89	0.35	215
Toxrefdb_Developmental Rabbit General FetalWeightReduction:DEV_rabbi t_Developmental_GeneralFetal_F etalWeightReduction (discretized)	WEKA-RF	GSFrag	31	115	72	13	231	0.63	0.3	0.7	0.42	0.7	0.61	0.66	98.68	6.52	0.25	44
Toxrefdb_Developmental Rabbit Maternal Systemic:DEV_rabbit_Maternal_ GeneralMaternal_Systemic (discretized)	MLRA	Adriana	99	20	10	101	230	0.52	0.91	0.5	0.64	0.5	0.67	0.58	98.838	9.89	0.11	200
Toxrefdb_Developmental Rabbit PregnancyRelated MaternalPregLoss:DEV_rabbit_M aternal_PregnancyRelated_Mater nalPregLoss (discretized)	FSMLR	ALogPS_, OESta te	95	52	45	39	231	0.64	0.68	0.71	0.69	0.71	0.54	0.62	98.755	8.38	0.25	134
Toxrefdb_Developmental Rabbit Skeletal Axial:DEV_rabbit_Developmental _Skeletal_Axial (discretized)	PLS	CDK	28	126	52	24	230	0.67	0.35	0.54	0.42	0.54	0.71	0.62	98.754	7.43	0.22	52
Toxrefdb_Developmental Rat General FetalWeightReduction:DEV_rat_D evelopmental_GeneralFetal_Fetal WeightReduction (discretized)	WEKA-RF	Fragmentor	57	97	66	27	247	0.62	0.46	0.68	0.55	0.68	0.6	0.64	98.726	7.75	0.26	84
Toxrefdb_Developmental Rat General GeneralFetalPathology:DEV_rat_ Developmental_GeneralFetal_Ge neralFetalPathology (discretized)	FSMLR	Toxcast_assays	18	152	61	16	247	0.69	0.23	0.53	0.32	0.53	0.71	0.62	98.757	6.63	0.18	34
Toxrefdb_Developmental Rat Maternal Systemic:DEV_rat_Maternal_Gen eralMaternal_Systemic (discretized)	FSMLR	CDK	159	23	10	54	246	0.74	0.94	0.75	0.83	0.75	0.7	0.72	98.557	9.88	0.33	213
Toxrefdb_Developmental Rat PregnancyRelated MaternalPregLoss:DEV_rat_Mate rnal_PregnancyRelated_Maternal PregLoss (discretized)	WEKA-RF	ChemaxonDesc riptsors	48	96	68	35	247	0.58	0.41	0.58	0.48	0.58	0.59	0.58	98.836	7.79	0.15	83

Toxrefdb_Developmental Rat Skeletal Appendicular:DEV_rat_Developmental_Skeletal_Appendicular (discretized)	ASNN	Toxcast_assays, _Toxcast_Pathways	22	156	43	26	247	0.72	0.34	0.46	0.39	0.46	0.78	0.62	98.758	7.67	0.22	48
Toxrefdb_Developmental Rat Skeletal Axial:DEV_rat_Developmental_Skeletal_Axial (discretized)	KNN	QNPR	67	97	40	43	247	0.66	0.63	0.61	0.62	0.61	0.71	0.66	98.683	8.86	0.32	110
Toxrefdb_Developmental Rat Skeletal Cranial:DEV_rat_Developmental_Skeletal_Cranial (discretized)	PLS	Fragmentor	19	155	53	20	247	0.7	0.26	0.49	0.34	0.49	0.75	0.62	98.768	7.06	0.19	39
Toxrefdb_Developmental rabbit Developmental GeneralFetal:DEV_rabbit_Developmental_GeneralFetal (discretized)	ASNN	QNPR	36	125	51	19	231	0.7	0.41	0.65	0.51	0.65	0.71	0.68	98.635	7.46	0.32	55
Toxrefdb_Developmental rabbit Developmental Skeletal:DEV_rabbit_Developmental_Skeletal (discretized)	FSMLR	CDK,_Toxcast_assays	38	115	50	27	230	0.67	0.43	0.58	0.5	0.58	0.7	0.64	98.718	7.79	0.26	65
Toxrefdb_Developmental rabbit Maternal GeneralMaternal:DEV_rabbit_Maternal_GeneralMaternal (discretized)	MLRA	Adriana	99	20	10	101	230	0.52	0.91	0.5	0.64	0.5	0.67	0.58	98.838	9.89	0.11	200
Toxrefdb_Developmental rabbit Maternal PregnancyRelated:DEV_rabbit_Maternal_PregnancyRelated (discretized)	FSMLR	ALogPS,_OEState	95	52	45	39	231	0.64	0.68	0.71	0.69	0.71	0.54	0.62	98.755	8.38	0.25	134
Toxrefdb_Developmental rat Developmental GeneralFetal:DEV_rat_Developmental_GeneralFetal (discretized)	LibSVM	Adriana	52	109	45	40	246	0.65	0.54	0.57	0.55	0.57	0.71	0.64	98.727	8.54	0.27	92
Toxrefdb_Developmental rat Developmental Skeletal:DEV_rat_Developmental_Skeletal (discretized)	FSMLR	Dragon6	75	88	40	44	247	0.66	0.65	0.63	0.64	0.63	0.69	0.66	98.682	8.9	0.32	119
Toxrefdb_Developmental rat Maternal GeneralMaternal:DEV_rat_Maternal_GeneralMaternal (discretized)	FSMLR	CDK	159	23	10	54	246	0.74	0.94	0.75	0.83	0.75	0.7	0.72	98.557	9.88	0.33	213
Toxrefdb_Developmental rat Maternal PregnancyRelated:DEV_rat_Maternal_PregnancyRelated (discretized)	WEKA-RF	ChemaxonDescriptors	48	96	68	35	247	0.58	0.41	0.58	0.48	0.58	0.59	0.58	98.836	7.79	0.15	83
Toxrefdb_MGR_rat_FemaleReproductiveTract:MGR_rat_FemaleReproductiveTract (discretized)	FSMLR	QNPR	31	111	85	13	240	0.59	0.27	0.7	0.39	0.7	0.57	0.64	98.729	6.32	0.21	44
Toxrefdb_MGR_rat_MaleReproductiveTract:MGR_rat_MaleReproductiveTract (discretized)	KNN	CDK	31	118	72	18	239	0.62	0.3	0.63	0.41	0.63	0.62	0.63	98.746	6.86	0.21	49
Toxrefdb_MGR_rat_OffspringSurvival:MGR_rat_OffspringSurvival (discretized)	ASNN	Fragmentor	56	103	51	30	240	0.66	0.52	0.65	0.58	0.65	0.67	0.66	98.68	8.15	0.31	86
Toxrefdb_MGR_rat_ReproductiveOutcome:MGR_rat_ReproductiveOutcome (discretized)	WEKA-RF	InductiveDescriptors	40	113	62	25	240	0.64	0.39	0.62	0.48	0.62	0.65	0.63	98.739	7.54	0.23	65
Toxrefdb_MGR_rat_ReproductivePerformance:MGR_rat_ReproductivePerformance (discretized)	PLS	CDK,_Toxcast_Pathways	30	140	49	20	239	0.71	0.38	0.6	0.47	0.6	0.74	0.67	98.659	7.48	0.29	50
Toxrefdb_Multigeneration Rat Endpoint for Decreased Litter Size:MGR_Rat_LitterSize (discretized)	WEKA-RF	Fragmentor	26	122	74	18	240	0.62	0.26	0.59	0.36	0.59	0.62	0.61	98.787	6.69	0.17	44
Toxrefdb_Multigeneration Rat Endpoint for Kidney microscopic and gross pathologies and weight changes:MGR_Rat_Kidney (discretized)	PLS	CDK	49	119	50	21	239	0.7	0.49	0.7	0.58	0.7	0.7	0.7	98.596	7.83	0.37	70
Toxrefdb_Multigeneration Rat Endpoint for Lactation Index= (# of pups alive on day 21/ total # of pups born alive)x100:MGR_Rat_LactationPND21 (discretized)	WEKA-J48	InductiveDescriptors	25	146	52	17	240	0.71	0.32	0.6	0.42	0.6	0.74	0.67	98.667	7.13	0.27	42

Toxrefdb_Multigeneration Rat Endpoint for Liver microscopic and gross pathologies and weight changes:MGR_Rat_Liver (discretized)	PLS	Mera_Mersy	72	93	44	31	240	0.69	0.62	0.7	0.66	0.7	0.68	0.69	98.622	8.48	0.37	103
Toxrefdb_Multigeneration Rat Endpoint for Ovary microscopic and gross pathologies and weight changes:MGR_Rat_Ovary (discretized)	FSMLR	GSFrag	24	110	95	11	240	0.56	0.2	0.69	0.31	0.69	0.54	0.61	98.778	5.79	0.16	35
Toxrefdb_Multigeneration Rat Endpoint for Testicular microscopic and gross pathologies and weight changes:MGR_Rat_Testis (discretized)	ASNN	Dragon6	21	141	60	18	240	0.68	0.26	0.54	0.35	0.54	0.7	0.62	98.76	6.84	0.19	39
Toxrefdb_Multigeneration Rat Endpoint for Viability Index= (# of pups alive on day 4/ total # of pups born alive)x100:MGR_Rat_ViabilityPN D4 (discretized)	ASNN	Toxcast_Pathways	39	119	54	28	240	0.66	0.42	0.58	0.49	0.58	0.69	0.63	98.73	7.81	0.25	67