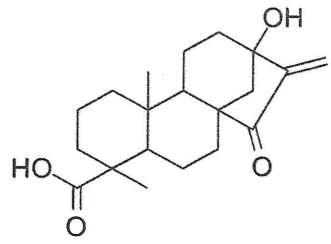
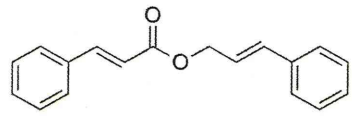
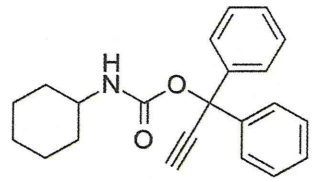
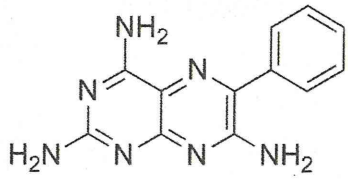
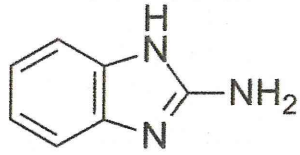
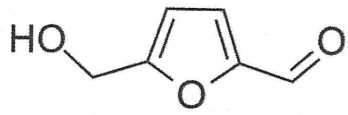
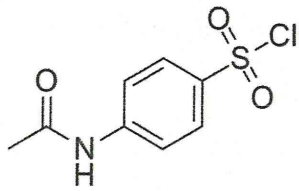
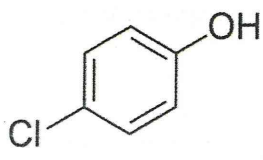
60		m0896	15-oxosteviol	+
61		m0930	cinnamylcinnamate	+
62		m0959	1,1-diphenyl-2-propynyl-N-cyclohexylcarbamate	+

表２　　検証化合物１０化合物

1		m0078	triamterene	-
2		m0081	2-aminobenzimidazole	-
3		m0121	5-hydroxymethylfurfural	-
4		m0283	4-(acetylamino)benzenesulfonyl chloride	-
5		m0302	4-chlorophenol	+

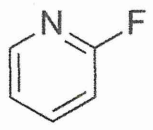
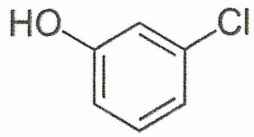
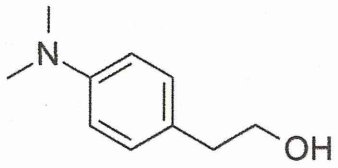
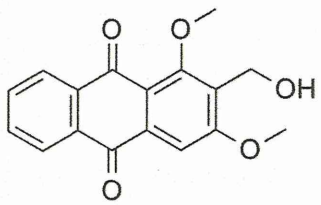
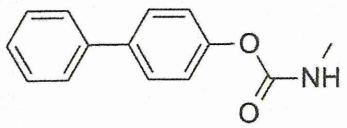
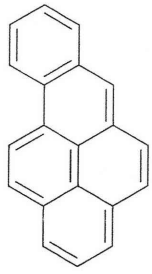
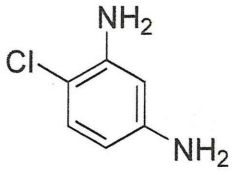
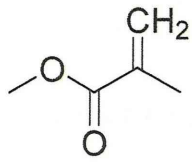
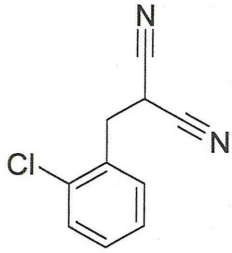
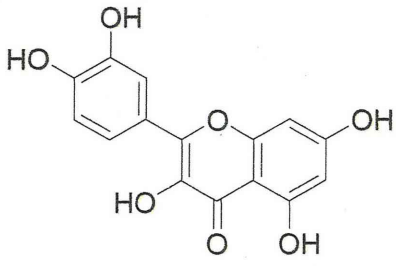
6		m0465	2-fluoropyridine	+
7		m0536	3-chlorophenol	+
8		m0577	4-(dimethylamino)benzeneethanol	+
9		m0663	2-(hydroxymethyl)-1,3-dimethoxyanthraquinone	-
10		m0814	p-biphenylyl n-methylcarbamate	+

表３　　追加検証化合物１０化合物

	Structure	ID	Name	AMES
1		c0001	benzo[a]pyrene	+
2		c0021	4-chloro-m-phenylenediamine	+
3		c0043	methyl methacrylate	-
4		c0047	o-chlorobenzalmalononitrile	-
5		c0054	quercetin	+

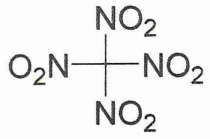
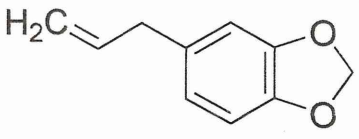
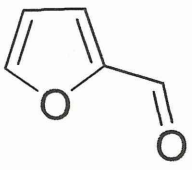
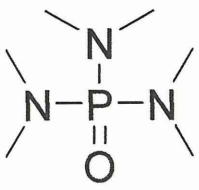
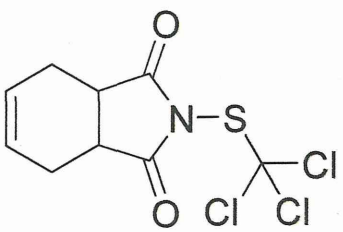
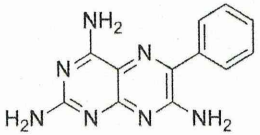
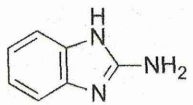
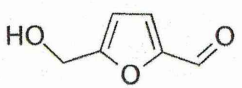
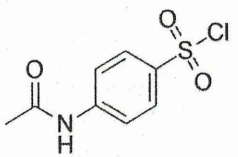
6		c0056	tetranitromethane	+
7		c0062	safrole	-
8		c0075	furfural	-
9		c0082	hexamethylphosphoramide	-
10		c0083	captan	+

表４　　類似度 90%

	structure	ID	実測値	T1(5067 件)　類似度 sim90% ＊実測値が矛盾した化合物(22)を除く ＊検証化合物自身を学習母集団から除外する（重複なし）				モデルの descriptor 件数 (iMLR)	予測値 (iMLR, sim90) NN	予測値 (iMLR, sim90) TILSQ	予測値 (iMLR, sim90) SVM	予測値 (iMLR, sim90) ADA
				total	pos	neg	ratio		予測値	予測値	予測値	予測値
1		m0078	-	799	544	255	0.47	24	+	+	+	+
2		m0081	-	921	607	314	0.52	39	+	+	+	+
3		m0121	-	992	466	526	0.89	30	+	+	-	+
4		m0283	-	107	50	57	0.88	43	-	-	+	-

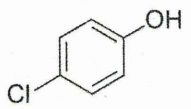
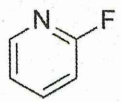
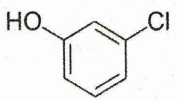
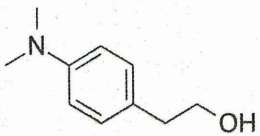
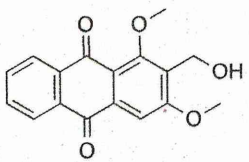
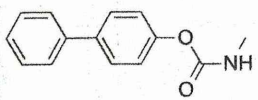
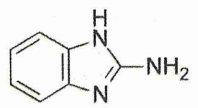
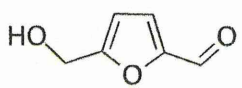
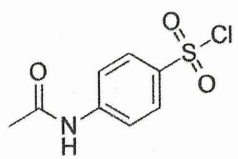
5		m0302	+	1584	917	667	0.73	53	-	-	+	-
6		m0465	+	771	478	293	0.61	38	-	+	-	+
7		m0536	+	1488	862	626	0.73	44	-	-	-	-
8		m0577	+	902	467	435	0.93	29	+	-	-	-
9		m0663	-	576	263	313	0.84	20	+	+	+	+
10		m0814	+	163	85	78	0.92	17	+	+	+	+

表５　　類似度 95%

	structure	ID	実測値	T1(5067 件)　類似度 sim95% ＊実測値が矛盾した化合物(22)を除く ＊検証化合物自身を学習母集団から除外する（重複なし）				モデルの descriptor 件数(iMLR)	予測値 (iMLR, sim95) NN	予測値 (iMLR, sim95) TILSQ	予測値 (iMLR, sim95) SVM	予測値 (iMLR, sim95) ADA
				total	pos	neg	ratio		予測値	予測値	予測値	予測値
1		m0078	-	24	23	1	0.04					
2		m0081	-	43	34	9	0.26					
3		m0121	-	12	4	8	0.50					
4		m0283	-	5	1	4	0.25					

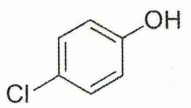
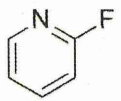
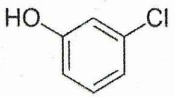
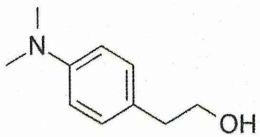
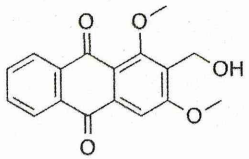
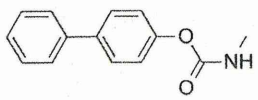
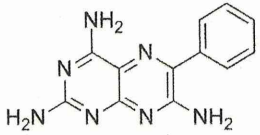
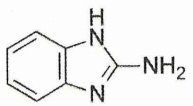
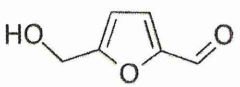
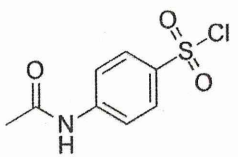
5		m0302	+	193	70	123	0.57	20	-	+	+	-
6		m0465	+	48	24	24	1.00	12	-	+	-	+
7		m0536	+	159	52	107	0.49	17	-	-	-	-
8		m0577	+	11	8	3	0.38					
9		m0663	-	30	24	6	0.25					
10		m0814	+	8	6	2	0.33					

表６　　類似度 85%

	structure	ID	実測値	T1(5067 件)　類似度 sim85% ＊実測値が矛盾した化合物(22)を除く ＊検証化合物自身を学習母集団から除外する（重複なし）				モデルの descriptor 件数(iMLR)	予測値 (iMLR, Sim85) NN	予測値 (iMLR, Sim85) TILSQ	予測値 (iMLR, Sim85) SVM	予測値 (iMLR, Sim85) ADA
				total	pos	neg	ratio		予測値	予測値	予測値	予測値
1		m0078	-	2369	1468	901	0.61	52	+	+	+	+
2		m0081	-	2495	1495	1000	0.67	63	-	+	+	+
3		m0121	-	3218	1864	1354	0.73	57	+	+	+	+
4		m0283	-	823	395	428	0.92	32	+	+	+	+