

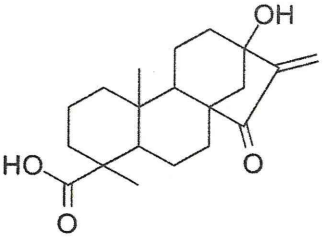
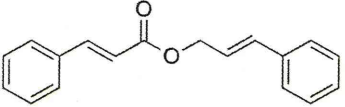
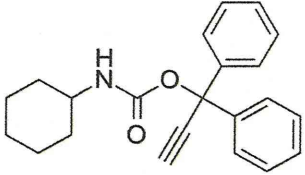
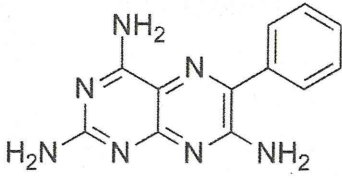
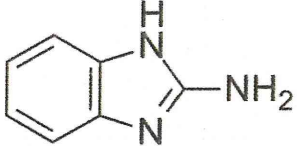
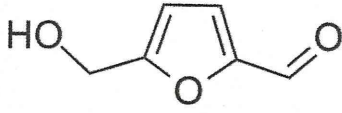
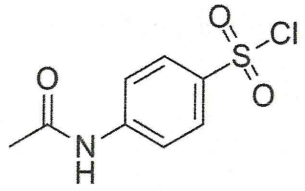
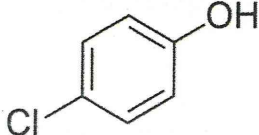
60	 <p>The structure shows a complex polycyclic steroid-like molecule with a carboxylic acid group (HO-C=O) on the left, a ketone group (C=O) on the right, and a hydroxyl group (OH) at the top right. It features several fused and bridged rings.</p>	m0896	15-oxosteviol	+
61	 <p>The structure consists of two cinnamyl groups (a phenyl ring attached to a propene chain) linked together via an ester bond (-COO-).</p>	m0930	cinnamylcinnamate	+
62	 <p>The structure features a cyclohexane ring attached to a carbonyl group (C=O), which is further bonded to an oxygen atom. This oxygen atom is part of a carbamate group that is also bonded to a propargyl group (a propene chain with a terminal triple bond) and two phenyl rings.</p>	m0959	1,1-diphenyl-2-propynyl- N-cyclohexylcarbamate	+

表 2

検証化合物 1 O 化合物

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

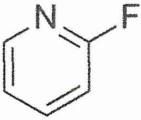
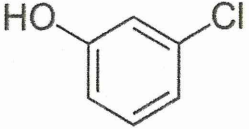
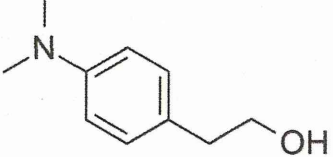
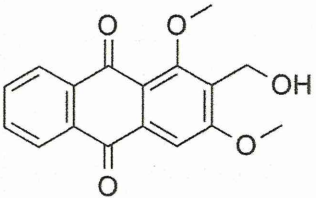
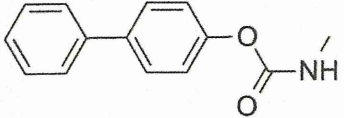
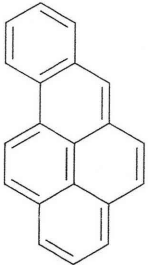
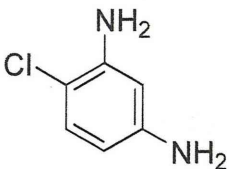
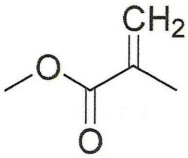
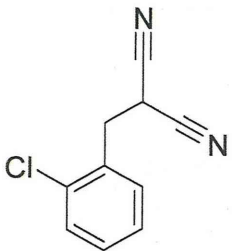
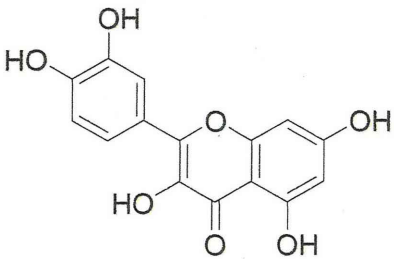
6		m0465	2-fluoropyridine	+
7		m0536	3-chlorophenol	+
8		m0577	4-(dimethylamino)benzyl alcohol	+
9		m0663	2-(hydroxymethyl)-1,3-dimethoxyanthraquinone	-
10		m0814	p-biphenyl n-methylcarbamate	+

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-chlorobenzal malononitrile	-
5		c0054	quercetin	+

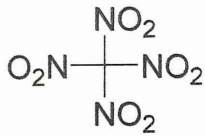
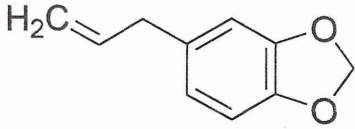
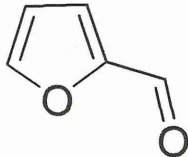
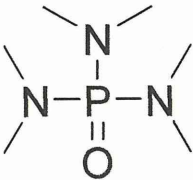
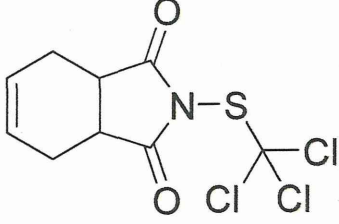
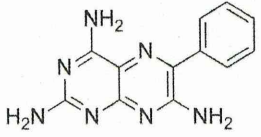
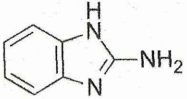
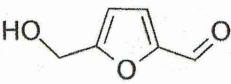
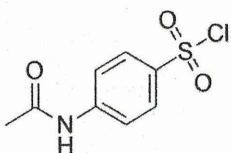
6		c0056	tetranitromethane	+
7		c0062	safrole	-
8		c0075	furfural	-
9		c0082	hexamethylphosphoramide	-
10		c0083	captan	+

表 4 類似度 90%

	structure	ID	実測値	T1(5067件) 類似度 sim90%				モデルの descriptor 件数 (iMLR)	予測値	予測値	予測値	予測値
				*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)					(iMLR, sim90) NN	(iMLR, sim90) TILSQ	(iMLR, sim90) SVM	(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	-	-	+	-

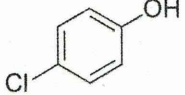
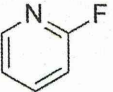
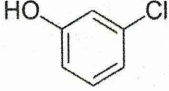
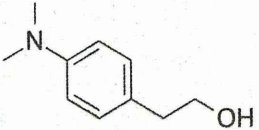
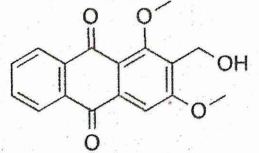
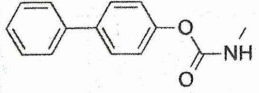
5		m0302	+	1584	917	667	0.73	53	-	-	+	-
6		m0465	+	771	478	293	0.61	38	-	+	-	+
7		m0536	+	1488	862	626	0.73	44	-	-	-	-
8		m0577	+	902	467	435	0.93	29	+	-	-	-
9		m0663	-	576	263	313	0.84	20	+	+	+	+
10		m0814	+	163	85	78	0.92	17	+	+	+	+

表5 類似度 95%

	structure	ID	実測値	T1(5067件) 類似度 sim95%				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
				*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)	total	pos	neg					
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					

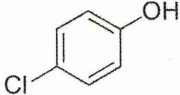
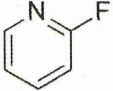
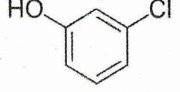
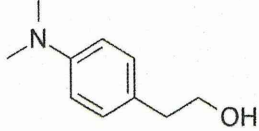
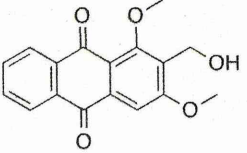

5		m0302	+	193	70	123	0.57	20	-	+	+	-
6		m0465	+	48	24	24	1.00	12	-	+	-	+
7		m0536	+	159	52	107	0.49	17	-	-	-	-
8		m0577	+	11	8	3	0.38					
9		m0663	-	30	24	6	0.25					
10		m0814	+	8	6	2	0.33					

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	予測値	予測値	予測値
				(iMLR, Sim85)	(iMLR, Sim85)	(iMLR, Sim85)	(iMLR, Sim85)		NN	TILSQ	SVM	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	+	+	+	+