

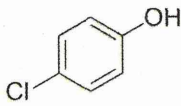
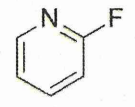
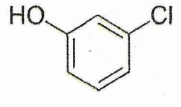
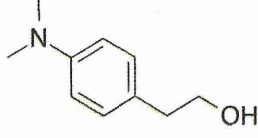
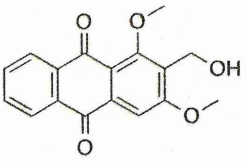
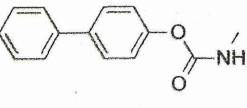
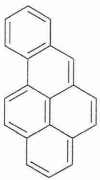
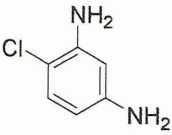
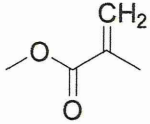
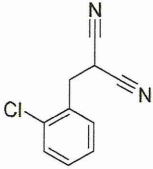
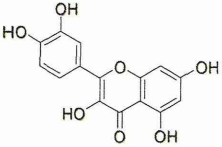
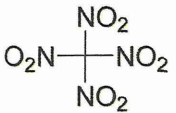
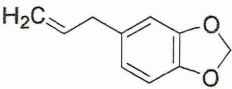
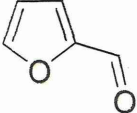
5		m0302	+	3340	1986	1354	0.68	58	-	+	-	-
6		m0465	+	2168	1243	925	0.74	55	-	-	+	+
7		m0536	+	3233	1933	1300	0.67	64	-	+	-	-
8		m0577	+	3270	1968	1302	0.66	56	-	+	-	-
9		m0663	-	2783	1538	1245	0.81	48	+	+	+	+
10		m0814	+	1800	971	829	0.85	46	-	+	-	-

表7 追加検証化合物 類似度 90%

	structure	ID	実測値	類似度 sim90%類似 学習母集団				予測値	最も類似し ている学習 母集団
				total	pos	neg	ratio		
1		c0001	+	1464	827	637	0.77	+	+
2		c0021	+	1458	882	576	0.65	+	+
3		c0043	-	135	42	93	0.45	-	-
4		c0047	-	572	272	300	0.91	+	+
5		c0054	+	1367	797	570	0.72	-	-
6		c0056	+	1	1	0	0.00	+	+
7		c0062	-	630	291	339	0.86	-	-
8		c0075	-	1226	647	579	0.89	-	-

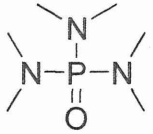
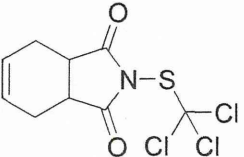
9		c0082	-	204	85	119	0.71	+	+
10		c0083	+	1	1	0	0.00	/	+

表 8 : 構造類似性に基づく毒性予測 (1)

	90%	TOP1	TOP3	TOP5
TN	95	123	121	120
TP	59	63	61	62
FN	13	10	12	11
FP	44	18	20	21
TOTAL	211	214	214	214
NG= FN+FP	57	28	32	32
未確定	3	0	0	0
カバー 率	0.986	1.000	1.000	1.000
予測率	0.730	0.869	0.850	0.850
感度	0.819	0.863	0.836	0.849
特異度	0.683	0.872	0.858	0.851

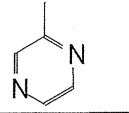
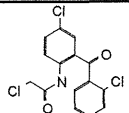
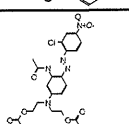
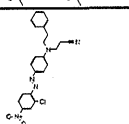
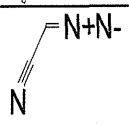
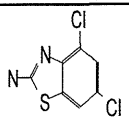
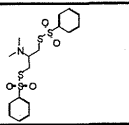
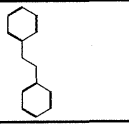
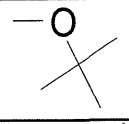

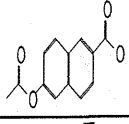
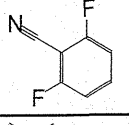
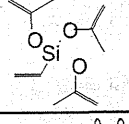
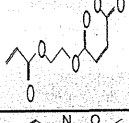
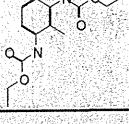
表 9 : 構造類似性に基づく毒性予測 (2)

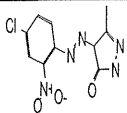
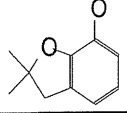
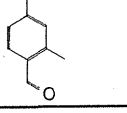
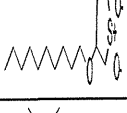
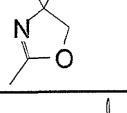
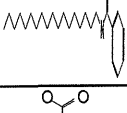
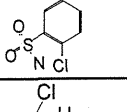
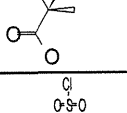
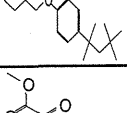
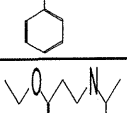
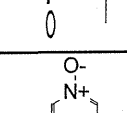
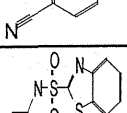
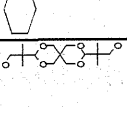
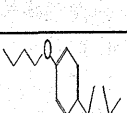
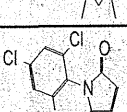
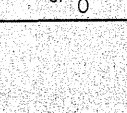
	4	3	QSAR	4+QSAR	3+QSAR
TN	77	115	42	118	123
TP	48	59	14	62	64
FN	2	6	7	9	9
FP	4	11	13	17	17
TOTAL	131	191	76	206	213
NG= FN+FP	6	17	20	26	26
未確定	83	23	8	8	1
カバー 率	0.612	0.893	0.905	0.963	0.995
予測率	0.954	0.911	0.737	0.874	0.878
感度	0.960	0.908	0.667	0.873	0.877
特異度	0.951	0.913	0.764	0.874	0.879

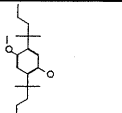
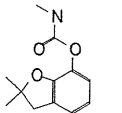
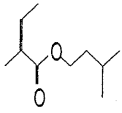
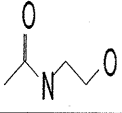
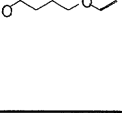
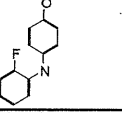
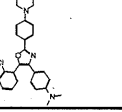
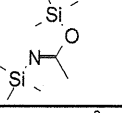
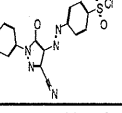
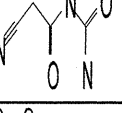
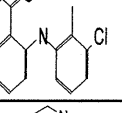
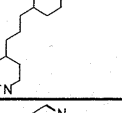
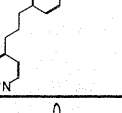
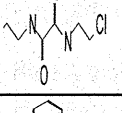
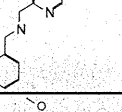
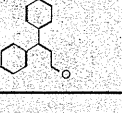
表 10

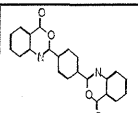
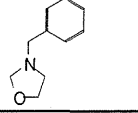
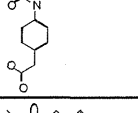
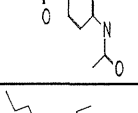
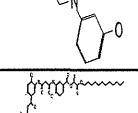
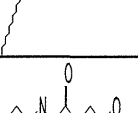
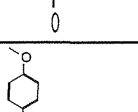
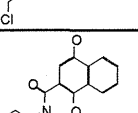
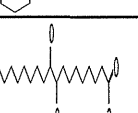
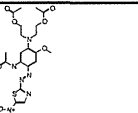
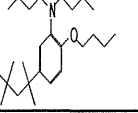
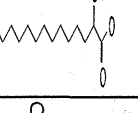
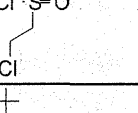
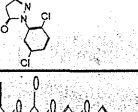
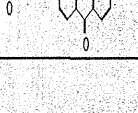

予測手法	AMES	TOP1	TOP3	TOP5	ALL3
TN	874	635	633	655	563
FP	0	239	241	219	157
TP	126	62	55	49	40
FN	0	64	71	77	54
ALL	1000	1000	1000	1000	814
COVERAGE	1	1	1	1	0.814
CONCORDANCE	1	0.697	0.688	0.704	0.741
SPECIFICITY	1	0.727	0.724	0.749	0.782
SENSITIVITY	1	0.492	0.437	0.389	0.426

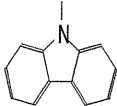
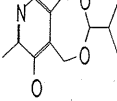
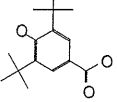
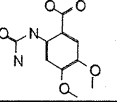
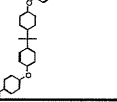
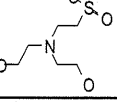
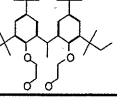
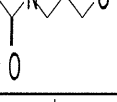
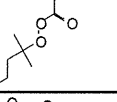
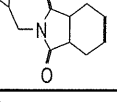
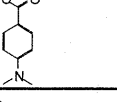
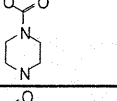
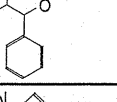
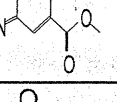
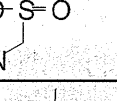
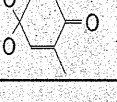
表11

	Structure	MolW	NIHS	AMES_CL	Item	TOP1	TOP3	TOP5
1.		88.0669	C	-	JP.109-08-0	-	-	-
2		332.525	C	-	JP.14405-03-9	+	+	+
3		481.7178	A	+	JP.1533-78-4	+	+	+
4		413.7314	A	+	JP.19649-68-4	+	+	+
5		66.0415	B	+	JP.13138-21-1	+	-	-
6		215.0593	C	-	JP.16582-59-5	-	-	+
7		410.4462	B	+	JP.17606-31-4	-	-	-
8		168.1498	C	-	JP.103-29-7	-	-	-
9		76.0529	C	-	JP.1634-04-4	-	-	-
10		1.29E+03	C	-	JP.104267-74-5	-	-	-
11		220.1367	C	-	JP.17295-26-0	-	-	-
12		136.0784	C	-	JP.1897-52-5	-	-	-
13		208.2014	C	-	JP.15332-99-7	-	-	-
14		204.0927	C	-	JP.19201-36-6	-	-	-
15		248.1501	C	-	JP.16648-51-4	-	-	-

16		273.5917	B	+	JP.14730-30-4	-	-	-
17		152.1058	C	-	JP.1563-38-8	-	-	-
18		124.0957	C	-	JP.15764-16-6	-	-	-
19		248.213	C	-	JP.18760-44-6	-	-	-
20		102.0703	C	-	JP.1772-43-6	-	-	-
21		330.2736	C	-	JP.19083-52-4	-	-	+
22		229.5972	C	-	JP.1205-30-7	-	-	-
23		116.5025	A	+	JP.16674-04-7	-	-	-
24		331.7087	C	-	JP.113576-52-6	+	+	+
25		156.0945	C	-	JP.15206-55-0	-	-	-
26		142.0911	C	-	JP.16217-22-4	+	+	+
27		116.077	C	-	JP.14906-64-0	-	+	-
28		280.2813	C	-	JP.16170-33-5	-	-	-
29		276.1569	C	-	JP.1455-42-1	+	+	+
30		232.192	C	-	JP.111753-22-1	-	-	-
31		272.4715	C	-	JP.13167-25-4	-	-	-

32		260.2021	B	+	JP.109870-95-3	-	-	-
33		206.1333	C	-	JP.1563-66-2	+	+	+
34		152.1058	C	-	JP.10482-55-0	-	-	-
35		94.0483	A	+	JP.142-26-7	-	-	-
36		104.063	C	-	JP.17832-28-9	-	-	-
37		205.1436	C	-	JP.1741-78-2	+	+	+
38		441.7829	C	-	JP.10004-39-4	-	-	-
39		182.2627	C	-	JP.10416-59-8	-	-	-
40		377.721	B	+	JP.118938-30-0	-	-	-
41		122.0617	C	-	JP.1448-98-2	+	-	+
42		249.6083	C	-	JP.13710-19-5	+	+	-
43		184.1525	C	-	JP.16898-52-5	-	-	-
44		184.1525	C	-	JP.17252-51-6	+	+	+
45		202.9824	C	-	JP.16813-43-7	-	+	+
46		186.1485	B	+	JP.1539-42-0	+	+	+
47		252.1801	C	-	JP.19618-37-2	-	-	-

48		356.2464	C	-	JP.18600-59-4	+	+	+
49		150.1131	B	+	JP.13657-16-4	+	+	+
50		182.1119	C	-	JP.18699-02-0	-	-	-
51		206.1333	C	-	JP.13475-17-7	-	-	-
52		198.1559	C	-	JP.100010-02-4	+	+	+
53		823.4161	C	-	JP.123660-04-8	-	-	-
54		164.0752	C	-	JP.1871-89-2	-	+	+
55		159.5487	A	+	JP.18217-00-0	-	-	-
56		266.1868	C	-	JP.100362-51-4	-	-	-
57		280.1902	C	-	JP.120-87-6	-	-	-
58		484.3144	B	+	JP.134764-36-6	+	+	+
59		342.2843	C	-	JP.108780-97-8	-	+	+
60		232.2136	C	-	JP.126660-84-2	-	-	-
61		158.9912	B	+	JP.1622-32-8	-	-	-
62		313.0747	C	-	JP.111672-81-2	-	-	-
63		336.2104	C	-	JP.1823-18-3	+	+	+

64		170.1458	A	+	JP.1484-12-4	+	+	+
65		206.1333	C	-	JP.1622-67-9	-	-	-
66		228.1587	C	-	JP.1421-49-4	-	-	-
67		240.1281	C	-	JP.128254-00-2	+	+	+
68		384.3012	C	-	JP.13080-86-9	+	-	-
69		198.1329	C	-	JP.10191-18-1	-	-	-
70		520.4044	C	-	JP.103556-61-2	-	-	-
71		106.059	C	-	JP.10601-73-7	-	-	-
72		180.1159	C	-	JP.118364-97-9	-	+	+
73		194.1226	A	+	JP.17620-38-1	+	-	-
74		178.1232	C	-	JP.10287-53-3	-	-	-
75		144.0871	C	-	JP.120-43-4	+	+	-
76		170.1012	C	-	JP.1078-17-7	-	-	-
77		170.1045	C	-	JP.113053-50-2	-	-	-
78		106.0806	C	-	JP.13881-91-9	-	-	-
79		180.1159	C	-	JP.14203-64-6	-	-	-