

Appendix 1:

DPR31 Table 11, Table12, and Table13 記載のデータに基づく一致率、感度、ならびに特異度について  
 DRP31 Table 11, Table12, and Table13 に掲載データから、SHE CTA のデータが記載されている化合物（有機化合物および無機化合物）を抽出し、まとめ直した結果を記載する。

有機化合物

		Carcinogenicity		
		Carcinogen	Non carcinogen	
SHE CTA	Positive	107	16	123
	Negative	20	47	67
		127	63	190

Concordance	81.1
Sensitivity	84.3
Specificity	74.6

無機化合物

		Carcinogenicity		
		Carcinogen	Non-carcinogen	
SHE CTA	Positive	47	5	52
	Negative	1	2	3
		48	7	55

Concordance	89.1
Sensitivity	97.9
Specificity	28.6

有機化合物+無機化合物

		Carcinogenicity		
		Carcinogen	non carcinogen	
SHE CTA	Positive	154	21	175
	Negative	21	49	70
		175	70	245

Concordance	82.9
Sensitivity	88.0
Specificity	70.0

## Appendix 1-1

SHE CTAの結果とげっ歯類がん原物質ならびに非がん原物質との相関について

げっ歯類がん原物質での結果(有機化合物)

物質名	pH別結果		SHE CTAの結果	
	pH6.7	pH $\geq$ 7.0	陽性	陰性
Acetamide		+	+	
2AAF		+	+	
Acrylamide	+	+	+	
Acrylonitrile	+	+	+	
ActinomycinD		+	+	
Aflatoxin B1		+	+	
2-Amino-5-azotoluene		+	+	
4-Amino-1,1'-biphenyl (4-Aminobiphenyl)		+	+	
2-Aminoanthracene		+	+	
p-Aminoazobenzene		+	+	
Amitrole [3-Aminotriazole]		+	+	
Aniline		-		-
o-Anisidine		+	+	
Anthraquinone	-			-
Aroclor 1254		-		-
Aroclor 1260		+	+	
5-Azacytidine		+	+	
Benomyl	-			-
Benz(a)anthracene		+	+	
Benzene		+	+	
Benzidine		+	+	
Benzo(a)pyrene	+	+	+	
Benzoyl peroxide		+	+	
Benzyl chloride		+	+	
HC Blue 1		+	+	
5-Bromo-2'-deoxyuridine		+	+	
Butylated hydroxytoluene (BHT)		+	+	
Butylbenzylphthalate	+		+	
Catechol		+	+	
Chloral hydrate	+		+	
Chlordane Analytical		+	+	

物質名	pH別結果		SHE CTAの結果	
	pH6.7	pH $\geq$ 7.0	陽性	陰性
p-Chloroaniline		+	+	
Chlorothalonil		+	+	
Chrysene Benzophenanthrene		+	+	
Cinnamyl anthranilate	+	+	+	
Clofibrate	+	+	+	
Cyclophosphamide		+	+	
Decabromo diphenyloxide	-			-
2,4-Diaminotoluene	+	+	+	
Dibenz(a,h)anthracene		+	+	
Dichlorodiphenyl trichloroethane(DDT)		-		-
2,6-Dichloro-p-phenylenediamine		+	+	
Dichlorvos		+	+	
Diepoxybutane, 1,2 :3,4		+	+	
Diethanolamine	+		+	
di (2-Ethylhexyl) phthalate(DEHP)	+	+	+	
Diethylstilbestrol (DES)	-	+	+	
N,N'-Diethylthiourea	+		+	
N,N'-Dimethyl-4-aminoazobenzene [4-Dimethylamino-azobenzene]		+	+	
7,12-Dimethyl benzanthracene		+	+	
1,2-Dimethylhydrazine		+	+	
2,4-Dinitrotoluene	+	-	+	
2,6-Dinitrotoluene	+		+	
Diphenylhydantoin		+	+	
Epichlorhydrin	+		+	
1,2-Epoxybutane		+	+	
Estradiol		+	+	
Ethinylestradiol		-		-
l-Ethionine		+	+	
Ethyl alcohol [Ethanol]	-	-		-
Ethyl benzene	+		+	
Ethyl methanesulfonate		+	+	
Formaldehyde	+		+	
Furfuryl alcohol	-			-
Furylfuramide (AF-2)		+	+	

物質名	pH別結果		SHE CTAの結果	
	pH6.7	pH $\geq$ 7.0	陽性	陰性
Genistein	-			-
Glycidaldehyde		+	+	
Griseofulvin	-			-
Hexachloro-1,3-butadiene		+	+	
Hexamethyl phosphoramidate		+	+	
Hydroquinone		+	+	
N-Hydroxy-2-acetylaminofluorene		+	+	
d-Limonene	-	-		-
Melphalan [Sarkolysin ][Phenyl alanine mustard]		+	+	
Metaproterenol hemisulfate	-			-
Methapyrilene HCl	+	+	+	
3-Methoxy-4-aminoazobenzene		+	+	
Methyl eugenol	+		+	
Methyl iodide		+	+	
Methyl methane sulfonate (MMS)		+	+	
Methylazoxymethanol acetate		+	+	
Methylcarbamate (Methyl urethane)	-	-		-
3-Methylcholanthrene (MCA)	+	+	+	
Methylclofenapate		+	+	
[Bis(pdimethylamino)diphenylmethane		+	+	
Mezerein		+	+	
Mitomycin C		+	+	
Monuron		+	+	
2-Naphthylamine	+	+	+	
Nitrilotriacetic Acid	-	-		-
N-(4-(5-Nitro-furanyl)-2-thiazolyl)formamide		+	+	
2-Nitro-p-phenylenediamine [2-Nitro-1,4-phenylenediamine]		+	+	
5-Nitro-o-toluidine [2-Amino-4-nitrotoluene]		-		-
2-Nitropropane		+	+	
4-Nitroquinoline-1-oxide [4-Nitroquinoline-N-oxide]		+	+	
N-Nitroso-N-ethylaniline		+	+	
[N-Ethyl-N-nitrosourea (ENU)] [1-Ethyl-1-nitrosourea]		+	+	
nitrosoguanidinen(MNNG)]	+	+	+	
N-Nitrosodiethylamine [Diethyl nitrosamine]		+	+	

物質名	pH別結果		SHE CTAの結果	
	pH6.7	pH $\geq$ 7.0	陽性	陰性
N-Nitrosodiphenylamine [Diphenyl nitrosamine]		+	+	
Okadaic acid		+	+	
4,4'-Oxydianiline		+	+	
Oxymetholone	+		+	
Phenacetin	-			-
Phenobarbital sodium Phenobarbital	+	+	+	
Phenolphthalein		+	+	
Phorbol 12,13-didecanoate (PDD)		+	+	
Polybrominated biphenyls	+		+	
Procarbazine HCl		+	+	
$\beta$ -Propionolactone		+	+	
Propylene oxide	+		+	
1,2-Propyleneimine (Propyleneimine)		+	+	
Pyridine	-			-
Reserpine	+	+	+	
p-Rosaniline (CI Basic Red 9) [Magenta]		+	+	
Safrole		+	+	
Testosterone		+	+	
12-O- Tetradecanoyl phobol-13-acetate (TPA)	+	+	+	
Tetrahydrofuran	-			-
Thioacetamide		+	+	
Thiourea		+	+	
o-Toluidine		+	+	
o-Toluidine HCl	+		+	
2,4,6-Trichlorophenol		+	+	
Tris(2-ethylhexyl)phosphate (TEHP)	-			-
Urethane [Ethyl carbamate]	+	+	+	
Wyeth-14,643	+	+	+	

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げっ菌類非がん原物質での結果 (有機化合物)

物質名	pH別結果		SHE CTAの結果	
	pH6.7	pH $\geq$ 7.0	陽性	陰性
Acetone		-		-
4-Acetylaminofluorene	-	-		-

物質名	pH別結果		SHE CTAの結果	
	pH6.7	pH $\geq$ 7.0	陽性	陰性
Acid red 14 (IC)	-			-
Acrylic Acid		-		-
Ampicillin	-			-
Anilazine	-			-
p-Anisidine	+		+	
Anthracene	-	-		-
l-Ascorbic acid	-	-		-
Benzo(e)pyrene		-		-
Benzoin		-		-
Bisphenol A	-			-
HC Blue 2	-	-		-
n-Butyl acrylate		-		-
2-tert-Butyl-1,4-hydroquinone	-			-
Caffeine		-		-
Caprolactam	-	+	+	
Chloramphenicol		-		-
o-Chloroaniline		-		-
Colcemid (IC)	+	+	+	
Dexamethasone		-		-
2,6-Diaminotoluene	-			-
Diazepam	-			-
2,4-Dichlorophenol		+	+	
2,4-Dichlorophenoxyacetic acid		-		-
2,4-Dimethoxyaniline HCl	-			-
Dimethylformamide		-		-
EDTA, trisodium salt trihydrate	-	-		-
Eugenol	-	+	+	
Geranyl acetate		+	+	
8-Hydroxyquinoline		-		-
Isobutyraldehyde	-			-
Lithocholic acid		+	+	
d-Mannitol	-			-
6-Mercaptopurine		-		-
Methotrexate		-		-

物質名	pH別結果		SHE CTAの結果	
	pH6.7	pH $\geq$ 7.0	陽性	陰性
Methoxychlor	+	-	+	
1-Naphthylamine	-	-		-
Naphthyl isothiocyanate		-		-
4-Nitro-o-phenylenediamine (4-Nitro-1,2-benzenediamine)	-	+	+	
6-Nitrobenzo[a]pyrene		+	+	
3-Nitropropionic acid	-			-
Pentoxifylline	-			-
Phenanthrene		-		-
Phenol		+	+	
p-Phenylenediamine 2HCl(4-Aminoaniline dihydrochloride)	-			-
Phthalic anhydride	-	-		-
Pyrene		-		-
HC Red 3		-		-
Resorcinol	-	+	+	
Rotenone	+		+	
Saccharin (acid form)		-		-
Sodium xylenesulfonate	-			-
Sorbic acid		-		-
Succinic anhydride		+	+	
Sulfisoxazole	-			-
Tetracycline hydrochloride		-		-
Tetraethylthiuramdisulfide (Disulfiram)	+		+	
Thiabendazole	-			-
2,4,5-Trichlorophenoxyacetic acid		-		-
Triphenyltin hydroxide	-			-
Vincristine sulfate (IC)		+	+	
FD and C Yellow n°6		-		-

## Appendix I-2

SHE CTAの結果とげっ歯類がん原物質ならびに非がん原物質との相関について  
げっ歯類がん原物質での結果(無機化合物)

物質名	pHの条件		SHE CTAの結果	
	pH6.7	pH $\geq$ 7.0	陽性	陰性
Amosite		+	+	
Anthophyllite		+	+	
Barium chromate		+	+	
Basic lead silicochromate		+	+	
Beryllium sulfate		+	+	
Beryllium sulfate tetrahydrate		+	+	
Biotite		+	+	
Cadmium acetate		+	+	
Cadmium chloride	+	+	+	
Calcium chromate		+	+	
Chromium trioxide		+	+	
Chrysotile	+	+	+	
cis-Platinum diammine dichloride		+	+	
Cobalt sulfate heptahydrate		+	+	
Cristobalite		+	+	
Glass fibre 100		+	+	
Glass fibre 110				
Hydrogen peroxide	+	+	+	
Lead acetate	+	+	+	
Lead chromate		+	+	
Lead molybdenum chromates		+	+	
Lead sulphate chromates		+	+	
Magnetite		+	+	
Nemalite Brucite		+	+	
Nickel (metallic)		+	+	
Nickel chloride		+	+	
Nickel monoxide		+	+	
Nickel subsulfide		+	+	



物質名	pHの条件		SHE CTAの結果	
	pH6.7	pH $\geq$ 7.0	陽性	陰性
Nickel sulfate		+	+	
Nickel sulfate heptahydrate	+		+	
Nickel sulfate hexahydrate		+	+	
Nickel sulfide(crystalline)		+	+	
Potassium chromate		+	+	
Potassium dichromate		+	+	
Quartz Min-U-Sil5 Silica Quartz		+	+	
Refractory ceramic fibre-1,2,3,4		+	+	
Sodium arsenate		+	+	
Sodium arsenite		+	+	
Sodium chromate tetrahydrate		+	+	
Sodium dichromate		+	+	
Sodium nitrite		+	+	
Strontium chromate		+	+	
Titanium dioxide	-	-		-
Tremolite		+	+	
Vanadium (V) pentoxide	+	+	+	
Zinc chloride	+		+	
Zinc chromate		+	+	
Zinc oxide		+	+	
Zinc potassium chromatesd		+	+	

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## げっ歯類非がん原物質での結果(無機化合物)

物質名	pHの条件		SHE CTAの結果	
	pH6.7	pH $\geq$ 7.0	陽性	陰性
Chromium (III) chloride		-		-
Chromium (III) oxide		+	+	
Chromium (metallic)		+	+	
Diatomaceous earths		+	+	
Ferric oxide		-		-
Sodium fluoride	-	+	+	

物質名	pHの条件		SHE CTAの結果	
	pH6.7	pH $\geq$ 7.0	陽性	陰性
Titanocene dichloride		+	+	
			5	2

## Appendix II

SHE CTAとIARCクラス分類によるヒトがん原物質との相関について解析結果  
有機化合物(げっ歯類がん原物質)

	化学物質名	ヒトがん原物質IARC分類グループ					SHECTA結果	
		1	2A	2B	3	4	陽性	陰性
1	Acetamide			○			○	
3	Acrylamide		○				○	
4	Acrylonitrile			○			○	
5	ActinomycinD				○		○	
6	Aflatoxin B1	○					○	
7	2-Amino-5-azotoluene			○			○	
8	4-Amino-1,1'-biphenyl (4-Aminobiphenyl)	○					○	
10	p-Aminoazobenzene			○			○	
11	Amitrole [3-Aminotriazole]				○		○	
12	Aniline				○			○
13	o-Anisidine			○			○	
17	5-Azacytidine		○				○	
19	Benz(a)anthracene		○				○	
20	Benzene	○					○	
21	Benzidine	○					○	
22	Benzo(a)pyrene	○					○	
24	Benzyl chloride		○				○	
25	HC Blue 1			○			○	
27	Butylated hydroxytoluene (BHT)				○		○	
28	Butylbenzylphthalate				○		○	
29	Catechol			○			○	
30	Chloral hydrate				○		○	
31	Chlordane Analytical			○			○	
32	p-Chloroaniline			○			○	
33	Chlorothalonil			○			○	
34	Chrysene Benzophenanthrene				○		○	
35	Cinnamyl anthranilate				○		○	
36	Clofibrate				○		○	
37	Cyclophosphamide	○					○	
39	2,4-Diaminotoluene			○			○	
40	Dibenz(a,h)anthracene		○				○	

	化学物質名	ヒトがん原物質IARC分類グループ					SHECTA結果	
		1	2A	2B	3	4	陽性	陰性
41	Dichlorodiphenyl trichloroethane(DDT)			○				○
42	2,6-Dichloro-p-phenylenediamine				○		○	
43	Dichlorvos			○			○	
44	Diepoxybutane, 1,2 :3,4			○			○	
45	Diethanolamine				○		○	
46	di (2-Ethylhexyl) phthalate(DEHP)				○		○	
47	Diethylstilbestrol (DES)	○					○	
48	N,N'-Diethylthiourea				○		○	
49	N,N'-Dimethyl-4-aminoazobenzene [4-Dimethylamino-azobenzene]			○			○	
51	1,2-Dimethylhydrazine		○				○	
52	2,4-Dinitrotoluene			○			○	
53	2,6-Dinitrotoluene			○			○	
54	Diphenylhydantoin			○			○	
55	Epichlorhydrin		○				○	
56	1,2-Epoxybutane			○			○	
57	Estradiol	○					○	
58	Ethinylestradiol	○						○
60	Ethyl alcohol [Ethanol]	○						○
61	Ethyl benzene			○			○	
62	Ethyl methanesulfonate			○			○	
63	Formaldehyde		○				○	
65	Furylfuramide (AF-2)			○			○	
67	Glycidaldehyde			○			○	
68	Griseofulvin			○				○
69	Hexachloro-1,3-butadiene				○		○	
70	Hexamethyl phosphoramidate			○			○	
71	Hydroquinone				○		○	
73	d-Limonene				○			○
74	Melphalan [Sarkolysin ][Phenyl alanine mustard]	○					○	
80	Methyl methane sulfonate (MMS)		○				○	
81	Methylazoxymethanol acetate			○			○	
82	Methylcarbamate (Methyl urethane)				○			○
85	4,4'-Methylene bis-(N,N'-dimethylaniline) [Bis(pdimethylamino)diphenylmethane]				○		○	

化学物質名	ヒトがん原物質IARC分類グループ					SHECTA結果	
	1	2A	2B	3	4	陽性	陰性
87 Mitomycin C			○			○	
88 Monuron				○		○	
89 2-Naphthylamine	○					○	
90 Nitrotriacetic Acid			○				○
92 2-Nitro-p-phenylenediamine [2-Nitro-1,4-phenylenediamine]				○		○	
93 5-Nitro-o-toluidine [2-Amino-4-nitrotoluene]				○			○
94 2-Nitropropane			○			○	
97 N-Nitroso-N-ethylurea [N-Ethyl-N-nitrosourea (ENU)] [1-Ethyl-1-nitrosourea]		○				○	
98 N-Nitroso-N-methylnitroguanidine [N-Methyl-N'-nitro-N-nitrosoguanidinen(MNNG)]		○				○	
99 N-Nitrosodiethylamine [Diethyl nitrosamine]		○				○	
102 4,4'-Oxydianiline			○			○	
104 Phenacetin		○					○
105 Phenobarbital sodium Phenobarbital			○			○	
106 Phenolphthalein			○			○	
110 β -Propionolactone			○			○	
111 Propylene oxide			○			○	
112 1,2-Propyleneimine (Propyleneimine)			○			○	
113 Pyridine				○			○
114 Reserpine				○		○	
115 p-Rosaniline (CI Basic Red 9) [Magenta]			○			○	
116 Safrole			○			○	
117 Testosterone		○				○	
120 Thioacetamide			○			○	
121 Thiourea				○		○	
122 o-Toluidine	○					○	
124 2,4,6-Trichlorophenol			○			○	
126 Urethane [Ethyl carbamate]		○				○	
物質数	13	15	39	24		80	11