

No.	Class	Compound	CAS number
1	GenTox/Carcinogen	Etoposide	33419-42-0
2	GenTox/Carcinogen	Mitomycin C	50-07-7
3	GenTox/Carcinogen	Cisplatin	15663-27-1
4	GenTox/Carcinogen	1,2- Dimethylhydrazine	306-37-6
5	GenTox/Carcinogen	1,2-dibromoethane	106-93-4
6	GenTox/Carcinogen	Cyclophosphamide	6055-19-2
7	GenTox/Carcinogen	2-Acetylaminofluorene	53-96-3
8	GenTox/Carcinogen	Azidothymidine	30516-87-1
9	GenTox/Carcinogen	ENU	759-73-9
10	GenTox/Carcinogen	Acrylonitrile	107-13-1
11	GenTox/Carcinogen	Benzene	71-43-2
12	GenTox/Carcinogen	4,4' -Oxydianiline	101-80-4
13	GenTox/Carcinogen	Busulfan	55-98-1
14	GenTox/Carcinogen	Ethyl methanesulfonate	62-50-0
15	GenTox/Carcinogen	p-Chloroaniline	106-47-8
16	GenTox/Carcinogen	7,12-Dimethyl-benzanthracene	57-97-6
17	GenTox/Carcinogen	Benzo[a]pyrene	50-32-8
18	GenTox/Carcinogen	Cadmium Chloride	10108-64-2
19	GenTox/Carcinogen	Dimethylnitrosamine	62-75-9
20	GenTox/Carcinogen	2,4-Diaminotoluene	95-80-7
21	GenTox/Carcinogen	o-Anisidine	90-04-0
22	GenTox/Carcinogen	4-nitroquinoline-1-oxide	56-57-5
23	GenTox/Non-Carcinogen	6-Mercaptopurine	50-44-2
24	GenTox/Non-Carcinogen	Cytosine arabinose	147-94-4
25	GenTox/Non-Carcinogen	p-Phenylenediamine 2HCl	624-18-0
26	GenTox/Non-Carcinogen	8-Hydroxyquinoline	148-24-3
27	GenTox/Non-Carcinogen	9-Aminoacridine	90-45-9
28	GenTox/Non-Carcinogen	2,6-Diaminotoluene	823-40-5
29	GenTox/Non-Carcinogen	3-Nitropropionic acid	504-88-1
30	GenTox/Non-Carcinogen	p-Anisidine	104-94-9
31	GenTox/Non-Carcinogen	5-fluorouracil	51-21-8
32	GenTox/Non-Carcinogen	Phenol	108-95-2
33	Non-GT/Carc	Di(2-ethylhexyl)phthalate	117-81-7
34	Non-GT/Carc	Lead (ii) acetate	6080-56-4
35	Non-GT/Carc	2-Phenylphenol sodium salt	6152-33-6
36	Non-GT/Carc	Ropinirole hydrochloride	91374-20-8
37	Non-GT/Carc	Methyl carbamate	598-55-0
38	Non-GT/Carc	Cyclosporin A	59865-13-3
39	Non-GT/Carc	Sodium saccharin	128-44-9
40	Non-GT/Carc	Diethanolamine	111-42-2
41	Non-GT/Carc	Hexachloroethane	67-72-1
42	Non-GT/Carc	Melamine	108-78-1
43	Non-GT/Non-carc	Tunicamycin	11089-65-9
44	Non-GT/Non-carc	p-Nitrophenol	100-02-7
45	Non-GT/Non-carc	Phenanthrene	85-01-8
46	Non-GT/Non-carc	Tertiarybutylhydroquinone	1948-33-0
47	Non-GT/Non-carc	Benzyl alcohol	100-51-6
48	Non-GT/Non-carc	Vanillin	121-33-5
49	Non-GT/Non-carc	Erythromycin stearate	114-07-8
50	Non-GT/Non-carc	Sodium diclofenac	15307-79-6
51	Non-GT/Non-carc	o-anthranilic acid	118-92-3
52	Non-GT/Non-carc	Tolbutamide	64-77-7
53	Non-GT/Non-carc	2-ethyl-1,3-hexanediol	94-96-2
54	Non-GT/Non-carc	Chlorpheniramine maleate	113-92-8
55	Non-GT/Non-carc	Ampicillin trihydrate	7177-48-2
56	Non-GT/Non-carc	Sodium chloride	7647-14-5
57	Non-GT/Non-carc	D-mannitol	69-65-8
58	Non-GT/Non-carc	Allyl alcohol	107-18-6
59	Non-GT/Non-carc	(2-chloroethyl)trimethyl-NH3Cl	999-81-5
60	Non-GT/Non-carc	Sulfisoxazole	127-69-5
61	Non-GT/Non-carc	Sucrose	57-50-1
62	Non-GT/Non-carc	Cyclohexanone	108-94-1
63	Non-GT/Non-carc	1-Nitropropane	108-03-2
64	Non-GT/Non-carc	Phenformin HCl	834-28-6

Assessment "calls" for a single experiment:

GFP induction factor	Viability	Dose-response	Call for expt.
≥2.0 at 1 or more concentrations	≥0.25	Yes	+
≥2.0 at 1 or more concentrations	≥0.25	No	+
>1.5 but <2.0	≥0.25	Yes	(+)
≥2.0 only at 1 or more toxic concentrations	<0.25	No	-
<1.5 at all concentrations	≥0.25 but approaches 0.25 or limited by precipitation	No	-
<1.5 at all concentrations	≥0.25 but with limited toxicity and not limited by precipitation	No	(-)
<1.5 at all concentrations	≥0.25 but limited by ppt	No	-
≥2.0 only at a single low or intermediate concentration but clearly <2.0 at higher concentrations	≥0.25	No	I

Assessment calls across 3 experiments:

Calls in 3 experiments (in any order)	Overall call for reporter with – or +S9 condition
+++	+
++I	+
+II	I
III	I
++-	+
++(-)	+
++(+)	+
+(+)(+)	+
(+)(+)(+)	E
+(+)I	E
+(+)-	E
+(+)(-)	E
(+)(+)-	-
(+)(+)(-)	(-)*
(+)I-	-
+I-	E
+--	-
+(-)	(-)*
(+)--	-
(+)(-)	(-)*
---	-
--(-)	-

* negative with restrictions. Compounds could be tested at higher doses

LAB 1	LAB 2	LAB 3	LAB 4	LAB 5	LAB 6	LAB 7
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DNA damage

Compounds	30	Compounds	24	Compounds	25	Compounds	26	Compounds	24	Compounds	30	Compounds	27
Acceptable	29	Acceptable	22	Acceptable	23	Acceptable	19	Acceptable	20	Acceptable	24	Acceptable	22
Not acceptable	1	Not acceptable	2	Not acceptable	2	Not acceptable	7	Not acceptable	4	Not acceptable	6	Not acceptable	5
WLR	96,7	WLR	91,7	WLR	92,0	WLR	73,1	WLR	83,3	WLR	80,0	WLR	81,5

Oxidative stress

Compounds	30	Compounds	24	Compounds	30	Compounds	27	Compounds	24	Compounds	30	Compounds	27
Acceptable	30	Acceptable	18	Acceptable	22	Acceptable	21	Acceptable	22	Acceptable	21	Acceptable	22
Not acceptable	0	Not acceptable	6	Not acceptable	8	Not acceptable	6	Not acceptable	2	Not acceptable	9	Not acceptable	5
WLR	100,0	WLR	75,0	WLR	73,3	WLR	77,8	WLR	91,7	WLR	70,0	WLR	81,5

Protein damage

Compounds	30	Compounds	24	Compounds	24	Compounds	27	Compounds	24	Compounds	30	Compounds	24
Acceptable	29	Acceptable	22	Acceptable	21	Acceptable	20	Acceptable	24	Acceptable	26	Acceptable	18
Not acceptable	1	Not acceptable	2	Not acceptable	3	Not acceptable	7	Not acceptable	0	Not acceptable	4	Not acceptable	6
WLR	96,7	WLR	91,7	WLR	87,5	WLR	74,1	WLR	100,0	WLR	86,7	WLR	75,0

p53 activation

Compounds	30	Compounds	24	Compounds	23	Compounds	27	Compounds	24	Compounds	30	Compounds	27
Acceptable	29	Acceptable	17	Acceptable	19	Acceptable	16	Acceptable	21	Acceptable	25	Acceptable	22
Not acceptable	1	Not acceptable	7	Not acceptable	4	Not acceptable	11	Not acceptable	3	Not acceptable	5	Not acceptable	5
WLR	96,7	WLR	70,8	WLR	82,6	WLR	59,3	WLR	87,5	WLR	83,3	WLR	81,5

Compound		Lab 1	Lab 2	Lab 3	Lab 4	Lab 5	Lab 6	Lab 7	Overall	Weighted calculation	
										Pos	Neg
1	Etoposide	P	P	P					P	1.00	
2	Mitomycin C	P		P	P				P	1.00	
3	Cisplatin	P		P				P	P	1.00	
4	1,2-Dimethylhydrazine	P	P					N	P	0.67	0.33
5	1,2-dibromoethane				I	P	P		P	1.00	
6	Cyclophosphamide	P		P					P	1.00	
7	2-Acetylaminofluorene				P	P		P	P	1.00	
8	Azidothymidine				I	P			P	1.00	
9	ENU		P				P	P	P	1.00	
10	Acrylonitrile				N	N		N	N		1.00
11	Benzene		I	I					N		1.00
12	4,4'-Oxydianiline		P				P	P	P	1.00	
13	Busulfan	P			P				P	1.00	
14	Ethyl methanesulfonate	P		I	P				P	1.00	
15	p-Chloroaniline				I	P	P		P	1.00	
16	7,12-Dimethyl-benzanthracene		P	P		I			P	1.00	
17	Benzo[a]pyrene		P	P		N			P	0.67	0.33
18	Cadmium Chloride		N				N	N	N	1.00	
19	Dimethylnitrosamine		N		I			N	N	1.00	
20	2,4-Diaminotoluene				I	P	P		P	1.00	
21	o-Arsidine	P		I				P	P	1.00	
22	4-nitroquinoline-1-oxide			P				P	P	1.00	
23	6-Mercaptopurine	P		I	I				P	1.00	
24	Cytosine arabinoside		P				P	P	P	1.00	
25	p-Phenylenediamine 2HCl	P				P	P		P	1.00	
26	8-Hydroxyquinoline			P	P			P	P	1.00	
27	9-Aminoacridine	P	P					P	P	1.00	
28	2,6-Diaminotoluene				N	P			P	0.67	0.33
29	3-Nitropropionic acid	P		P					P	1.00	
30	p-Arsidine		P	I					P	1.00	
31	5-fluorouracil	P	P		P				P	1.00	
32	Phenol	P				P	P		P	1.00	
33	Di(2-ethylhexyl)phthalate				I	N		N	N		1.00
34	Lead (II) acetate	P	N			I			E	0.50	0.50
35	2-Phenylphenol sodium salt		N	I					N	1.00	
36	Ropinrole hydrochloride		I				N	N	N	1.00	
37	Methyl carbamate		N				N	N	N	1.00	
38	Cyclosporin A		N		I	I			N	1.00	
39	Sodium saccharin		N	N			N		N	1.00	
40	Diethanolamine		N	N			N	N	N	1.00	
41	Hexachloroethane			N				N	N	1.00	
42	Melamine	P			I			N	E	0.50	0.50
43	Tunicamycin		N					N	N	1.00	
44	p-Nitrophenol		N				P	N	N	0.33	0.67
45	Phenanthrene		N	N	N				N	1.00	
46	Tertiarybutylhydroquinone	P			N			N	N	0.33	0.67
47	Benzyl alcohol		N	I			N		N	1.00	
48	Vanillin	P		N					N	0.33	0.67
49	Erythromycin stearate		N				N	P	N	0.33	0.67
50	Sodium diclofenac				I			P	N	0.50	0.50
51	o-anthranic acid		N	N					N	1.00	
52	Tolbutamide		N		N	I			N	1.00	
53	2-ethyl-1,3-hexanediol		N	N	I				N	1.00	
54	Chlorpheniramine maleate		N	N				N	N	1.00	
55	Ampicillin trihydrate				I	N	N		N	1.00	
56	Sodium chloride				N	N			N	1.00	
57	D-mannitol		N		I	I			N	1.00	
58	Allyl alcohol				I	I	N	N	N	1.00	
59	(2-chloroethyl)trimethyl-NH3Cl				I	N	N		N	1.00	
60	Sulfisoxazole				I	N	N		N	1.00	
61	Sucrose				I	N			N	1.00	
62	Cyclohexanone		N	N	I				N	1.00	
63	1-Nitropropane		N	N					N	1.00	
64	Phenformin HCl		N				N	N	N	1.00	

The following outcome was omitted from the analysis (corresponds with NA in column B to H)

- only 1 out of 3 with a valid prediction was available
- inconclusive result for two runs (as such only 1 prediction available)
- equivocal

N of chemicals	BLR (%)	Sensitivity % (n/N)	Specificity % (n/N)
59	83,1	86.7% (26/30)	90.2% (28.17/29)

No	DNA	Oxidative stress	Protein damage	Cell stress
	Bcl2 / Rtkn	Srxn1 / Blvrb	Ddit3	Btg2
1	PPP	PPP	NNN	PPP
2	PP	PPP	NNN	PP
3	PPP	PPP	NNN	PPP
4	NPP	NPP	NNN	(N)*PP
5	PP	PPP	NNN	NP
6	PP	PPP	INN	PPN
7	PPP	PPP	NNN	NN
8	PP	PPP	PNN	PP
9	PPP	PPP	NNN	PPP
10	NNN	NNP	NNN	N(N)*N
11	N	NNN	NNN	NN
12	PPP	PPP	NNN	PPP
13	PPP	NPP	NNN	PPP
14	PP	PPP	NNN	PP
15	PP	PPP	NNN	NPN
16	PP	NNP	ENP	NP
17	P(N)*P	P(N)*P	P(N)*P	(N)*P
18	N(N)*N	PPP	PNP	N(N)*P
19	NN	NNN	NNN	NN
20	PP	NPP	NPE	P
21	PP	PPP	NPN	PP
22	PPP	PNP	NNN	PPP
23	P	PPP	INN	P
24	PPP	EEP	NNN	PP
25	PPP	PPP	NNN	PPP
26	PPP	PPP	PPP	PPP
27	PPP	NPP	NNN	PPP
28	PPN	PPN	PPN	PN
29	PPP	PPP	NEN	PPP
30	PP	PPP	IIP	PP
31	PPP	PPP	NNN	PPP
32	PPP	PPP	NNN	PPP
33	NN	NNN	PPP	NN
34	PN	PPP	NNN	PPN
35	N	PPP	IPP	NP
36	N(N)*	N(N)*I	N(N)*N	N(N)*N
37	N(N)*N	N(N)*N	N(N)*N	N(N)*N
38	N	PPP	PPP	N
39	NNN	PPP	NNN	NNN
40	N(N)*N	N(N)*N	N(N)*N	N(N)*N
41	NNN	NNP	NNN	NNN
42	(N)*P	PNN	NNN	N(N)*(N)*
43	NNN	INP	IPP	NNN
44	NPN	NPN	PNP	NNN
45	NNN	PPP	NPP	NNN
46	NPN	PPP	PPP	PPN
47	NN	PNN	NNN	NN
48	N(N)*P	PNP	NNN	P(N)*N
49	P(N)*N	PNP	IPP	N(N)*N
50	NP	PPP	PIN	PP
51	N(N)*N	N(N)*N	NNN	N(N)*N
52	NN	PPP	PPN	PN
53	NN	PPP	ENN	NNN
54	NNN	PPP	NNN	NNN
55	NN	NNN	NNN	NN
56	NN(N)*	NNN	NN(N)*	NNN
57	N	NNN	INN	N
58	(N)*N	(N)*PP	(N)*NN	(N)*N
59	(N)*N	(N)*NN	(N)*NN	(N)*NN
60	NN	NPE	NNN	NN
61	NN	NNN	NNN	NN
62	NN	NNN	NNN	NN
63	NNN	NNN	NNN	NNN
64	NNN	EPE	PPP	NNN

BLR	DNA	Oxidative stress	Protein damage	Cell stress
	Bcl2 / Rtkn	Srxn1 / Blvrb	Ddit3	Btg2
	83,1	71,0	82,5	78,3

