

Table 1. Test Chemical Information

Chemical	CAS No.	Source	Test Group ^a	Top Conc. (μM)	Other Genetox ^b	Mammalian Cell Genetox Expectation ^c (-S9)	References and Miscellaneous Notes
1-Decyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	433337-23-6	IoLiTec Ionic Liquids Technologies Inc. via NTP	A	8.93	No NTP data, no publications	Insufficient data	NA
1-Methyl-3-tetradecylimidazolium bis(trifluoromethylsulfonyl)imide	404001-49-6	IoLiTec Ionic Liquids Technologies Inc. via NTP	A	4	No NTP data, no publications	Insufficient data	NA
1, 1, 3-Trichloropropanone	921-03-9	TCI America via NTP	A	6.31	Ames pos. (± S9), <i>in vitro</i> CA pos. (± S9, stronger without S9), <i>in vivo</i> mouse MN neg., <i>in vivo</i> MN pos. (newt larvae), not tested by NTP	Positive	Leadscope (http://www.leadscope.com), Blazak et al. (1988), and Le Curieux et al. (1994)
1, 2-Benzenediamine, N-phenyl-(a.k.a. N-Phenyl-o-phenylenediamine)	534-85-0	Sigma-Aldrich	A	50.25	No NTP data, no publications	Insufficient data	NA
1, 2-Phenylenediamine HCl2	615-28-1	Acros Organics via NTP	A	102	Ames pos., <i>in vitro</i> MLA, CA pos., <i>in vivo</i> MN pos.	Positive	EURL ECVAM Genotoxicity and Carcinogenicity Consolidated Database of Ames Positive Chemicals
2-Methoxy-3, 4-dihydro-2H-pyran	5/1/54	Acros Organics	A	25	<i>in vitro</i> Hprt pos. (-S9)	Positive	BG RCI Toxicological Evaluations, no. 266
2, 2', 5, 5'-Tetrachlorobenzidine	15721-02-5	TCI America via NTP	A	6.25	Ames pos. (+S9), not tested by NTP	Insufficient data	IARC Monograph no. 27 (1982)
2, 3-Dibromopropionic acid	600-05-5	Sigma-Aldrich via NTP	A	203	Ames pos., no NTP data	Insufficient data	Søderlund et al. (1979)
2, 4-Bis(1-methyl-1-phenylethyl)phenol	2772-45-4	Sigma-Aldrich via NTP	A	49.7	No NTP data, no publications	Insufficient data	NA
2, 4-Di-tert-butylphenol	96-76-4	Sigma-Aldrich via NTP	A	99.5	No NTP data, no publications	Insufficient data	NA
2, 4-Diaminotoluene	95-80-7	Sigma-Aldrich via NTP	A	196	Ames pos. (+S9), <i>in vitro</i> CA and SCE pos., <i>in vivo</i> MN pos.	Positive	NTP (https://doi.org/10.22427/NTP-DATA-1); Leadscope
2, 6-Toluenediamine	823-40-5	Sigma-Aldrich via NTP	A	204	<i>in vitro</i> CA pos., <i>in vivo</i> MN pos.; NTP tested the dihydrochloride salt: <i>in vitro</i> CA pos., <i>in vivo</i> MN pos.	Positive	Leadscope; NTP
3-Butyl-1-nitro-3-nitrosoguanidine	13010-08-7	Sigma-Aldrich via NTP	A	72.1	Ames pos., not tested by NTP	Insufficient data	Leadscope

Table 1. (continued)

Chemical	CAS No.	Source	Test Group ^a	Top Conc. (μM)	Other Genetox ^b	Mammalian Cell Genetox Expectation ^c (-S9)	References and Miscellaneous Notes
3-Iodo-2-propynyl-N-butylcarbamate	55406-53-6	Sigma-Aldrich	A	6.21	No NTP data, no publications	Insufficient data	NA
3-Methoxycatechol	934-00-9	Sigma-Aldrich via NTP	A	74.8	No NTP data; genotoxic upon nitrosation	Insufficient data	Ohshima et al. (1989)
3-Phenylprop-2-enal (trans-Cinnamaldehyde)	14371-10-9	Sigma-Aldrich via NTP	A	101	Ames pos. (weak), in vitro SCE pos., in vitro CA pos. (although NTP study was neg.)	Positive	Leadscope; NTP
4-(Benzyloxy)phenol	103-16-2	Sigma-Aldrich via NTP	A	49.25	No NTP data, no publications	Insufficient data	NA
4-Methylcatechol	452-86-8	Sigma-Aldrich via NTP	A	24.4	Ames neg., in vitro CA pos., in vivo MN neg.	Positive	NTP; Leadscope; Stich et al. (1981)
4, 4'-Diaminoazobenzene	538-41-0	Acros Organics via NTP	A	102	Ames pos. (+S9), no NTP data	Insufficient data	Shahin (1989)
4, 4'-Thiodiphenol	2664-63-3	Sigma-Aldrich via NTP	A	189	No NTP data, no publications	Insufficient data	NA
6-Azacytidine	3131-60-0	RTI International via NTP	A	100	in vitro MN pos. (K-)	Positive	Stopper et al. (1995); nucleoside analog
6-Thioguanine	154-42-7	Sigma-Aldrich via NTP	A	3.09	Ames pos., in vitro CA pos., in vivo MN pos.	Positive	NTP; nucleoside analog
8-Hydroxyquinoline	148-24-3	Sigma-Aldrich via NTP	A	8.88	Ames pos., in vitro CA and MLA pos.	Positive	NTP
Adriamycin HCl (a.k.a. Doxorubicin HCl)	25316-40-9	Toronto Research Chemicals Inc. via NTP	A	0.2	Ames pos., in vitro CA pos., in vivo MN pos.	Positive	Leadscope; NTP; topoisomerase 2 inhibitor
Ampicillin trihydrate	7177-48-2	Sigma-Aldrich	A	1000	Ames neg., in vitro CA neg. (pos. at conc. higher than therapeutic plasma conc., in vivo MN neg.	Negative	Kirkland et al. (2016)
Anisomycin		Sigma-Aldrich	A	10	in vitro MN neg. with high levels of apoptosis	Negative	Maik Schuler, Richard Spellman, Maria Engel (personal communication); protein biosynthesis inhibitor
Apigenin	520-36-5	Sigma-Aldrich via NTP	A	49.7	Ames neg.	Insufficient data	NTP
AZD2858	486424-20-8	Selleckchem	A	49.98	in vitro CA and MN pos.	Positive	Personal communication, Ann Doherty; Glycogen Synthase Kinase-3 inhibitor

Table 1. (continued)

Chemical	CAS No.	Source	Test Group ^a	Top Conc. (μM)	Other Genetox ^b	Mammalian Cell Genetox Expectation ^c (-S9)	References and Miscellaneous Notes
Beta-Lapachone	4707-32-8	Selleckchem	A	100	<i>in vitro</i> CA and comet pos.	Positive	Degrassi et al. (1993) , Vanni et al. (1998) ; Topoisomerase I inhibitor
Bis(1-piperidinylthioxomethyl) hexasulfide	971-15-3	Pfaltz & Bauer, Inc. via NTP	A	12.75	No NTP data, no publications	Insufficient data	NA
Bis[4-(glycidyloxy)phenyl]methane	3/6/95	Sigma-Aldrich via NTP	A	50.25	No NTP data, no publications	Insufficient data	NA
Bisphenol AF	1478-61-1	3B Scientific Corporation via NTP	A	70.7	Ames neg., <i>in vivo</i> MN neg	Insufficient data	NTP
Cadmium acetate dihydrate	4/4/43	ICN Biomedicals, Inc. via NTP	A	4.44	other Cd salts: <i>in vitro</i> MN, CA, and <i>Hprt</i> pos., <i>in vivo</i> CA and MN pos.	Positive	Kirkland et al. (2016)
Cadmium Cl	10108-64-2	Sigma-Aldrich via NTP	A	3.15	<i>in vitro</i> MN, CA, and <i>Hprt</i> pos., <i>in vivo</i> CA and MN pos.	Positive	Kirkland et al. (2016)
Chlorocholine chloride	999-81-5	Sigma-Aldrich	A	1000	Ames neg., <i>in vitro</i> CA neg, <i>in vivo</i> CA neg.	Negative	Kirkland et al. (2016)
Copper dimethyldithiocarbamate	137-29-1	TCI America via NTP	A	0.354	No NTP data; other soluble Cu compounds: <i>in vitro</i> SCE and <i>Hprt</i> pos.	Positive	Sideris et al. (1988)
Dasatinib	302962-49-8	Selleckchem	A	25	Ames neg., clastogenic when tested in CHO cells (±S9), <i>in vivo</i> MN neg.	Positive	Sprycel package insert (2010); tyrosine kinase inhibitor, especially Ber-Abl, Scr, c-Kit
Digitonin	11024-24-1	Sigma-Aldrich via NTP	A	6.34	Ames neg.	Insufficient data	NTP
Dodecyl gallate (lauryl gallate)	1166-52-5	Sigma-Aldrich via NTP	A	6.84	<i>in vitro</i> comet pos. (although aspects of this study not performed to current standards), no NTP data	Insufficient data	Savia et al. (2005)
Ethanamine, 2-chloro-N, N-diethyl-, HCl	869-24-9	Sigma-Aldrich via NTP	A	101	No NTP data, no publications	Insufficient data	NA
Gefitinib	184475-35-2	Sigma-Aldrich	A	25	<i>in vitro</i> and <i>in vivo</i> genetic toxicity neg.	Negative	Iressa package insert (2003); EGFR tyrosine kinase inhibitor
Genistein	446-72-0	Sigma-Aldrich via NTP	A	197	Ames pos. (+S9), <i>in vitro</i> CA pos.	Positive	NTP; Leadscope; topoisomerase 2 inhibitor

Table 1. (continued)

Chemical	CAS No.	Source	Test Group ^a	Top Conc. (μ M)	Other Genetox ^b	Mammalian Cell Genetox Expectation ^c (-S9)	References and Miscellaneous Notes
Glutaraldehyde	111-30-8	Sigma-Aldrich via NTP	A	18	Ames pos., <i>in vitro</i> CA and MLA pos., <i>in vivo</i> MN neg. and equivocal	Positive	NTP
Hesperadin	422513-13-1	Selleckchem	A	0.25	<i>in vitro</i> MN pos., aberrant metaphases	Positive	Hauf et al. (2003) and Kurihara et al. (2006); Aurora B kinase inhibitor
Hydroquinone	123-31-9	Sigma-Aldrich via NTP	A	49.75	Ames pos. (although NTP study was neg.), <i>in vitro</i> CA pos. (although NTP study was only pos. +S9), <i>in vitro</i> MLA pos (\pm S9), <i>in vivo</i> MN pos.	Positive	Leadscope, NTP
Irinotecan	57852-57-0	Selleckchem	A	5	Ames neg., <i>in vitro</i> cytogenetics pos., <i>in vivo</i> MN pos.	Positive	Camptosar packet insert (2014); topoisomerase 1 inhibitor
Malachite green oxalate	2437-29-8	TCI America via NTP	A	0.25	Generally Ames neg. in absence of S9, <i>in vitro</i> CA neg., <i>in vivo</i> MN and <i>Hprt</i> neg.	Negative	NTP Toxicity Report Series No. 71 (2004), Au and Hsu (1979), and Mittelstaedt et al. (2004)
Menthol	89-78-1	Sigma-Aldrich	A	499.8	Ames neg., <i>in vitro</i> CA neg. and pos. reports, <i>in vitro</i> MN neg. in p53 competent human cells	Negative	Kirkland et al. (2016)
Mercuric chloride	7487-94-7	Sigma-Aldrich via NTP	A	6.22	Ames neg., <i>in vitro</i> CA pos., MLA pos.	Positive	NTP
Monocrotaline	315-22-0	Sigma-Aldrich via NTP	A	201	<i>in vitro</i> MN pos.; <i>in vivo</i> MN pos.	Positive	MacGregor et al. (1990) and Müller et al. (1992)
N-Phenyl-1, 4-benzenediamine HCl (a.k.a. p-anilinoaniline)	2198-59-6	Acros Organics via NTP	A	49.5	<i>in vitro</i> comet pos., no NTP data	Positive	Elliott and Reiners (2008)
Osimertinib	1421373-65-0	Selleckchem	A	7.8	<i>in vitro</i> and <i>in vivo</i> genetic toxicity neg.	Negative	Tagrisso, package insert (2012); EGFR kinase inhibitor
Oxiranemethanamine, N-[4-(oxiranylmethoxy)phenyl]-N-(oxiranylmethyl)-	5026-74-4	Sigma-Aldrich via NTP	A	12.5	No NTP data, no publications	Insufficient data	NA

Table 1. (continued)

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Palbociclib	827022-33-3	Sigma-Aldrich	A	12.49	Ames neg., <i>in vitro</i> and <i>in vivo</i> MN pos., <i>in vitro</i> MN shown to arise from aneugenic MoA, <i>in vitro</i> ChromAb neg.	Positive	Ibrance package insert (2015), Wu et al. (2015, personal communication), Zhanna Sobol; cyclin-dependent kinase inhibitor
Pentabromoethane	75-95-6	Supelco via NTP	A	142	Ames neg., no publications	Insufficient data	NTP
Pyrimethamine	58-14-0	Sigma-Aldrich via NTP	A	6.34	Ames neg., <i>in vitro</i> SCE and CA pos.	Positive	NTP
Resveratrol	501-36-0	ChromaDex, Inc. via NTP	A	202	<i>in vitro</i> clastogenesis	Positive	Basso et al. (2013), Fox et al. (2012), and Leone et al. (2012); topoisomerase 2 inhibitor
sec-Butylparaben	17696-61-6	TCI America via NTP	A	201	No NTP data, no publications	Insufficient data	NA
Selenious acid	7783-00-8	Sigma-Aldrich via NTP	A	100	<i>in vitro</i> comet pos., <i>in vitro</i> CA pos.	Positive	Cemeli et al. (2003) and Nakamuro et al. (1976)
Selenium dioxide	8/4/46	Sigma-Aldrich via NTP	A	102	<i>in vitro</i> SCE pos. (human lymphocytes)	Positive	Ray and Altenberg (1980)
Sesamol	533-31-3	Sigma-Aldrich via NTP	A	199	Ames neg., pro-oxidant at high conc.	Insufficient data	NTP; Khamphio et al. (2016)
Strobane	8001-50-1	Chem Service, Inc. via NTP	A	49.2	No NTP data, no publications	Insufficient data	NA
Tannic acid	1401-55-4	Santa Cruz Biotechnology, Inc. via NTP	A	72.3	<i>in vitro</i> CA and MN pos.	Positive	EFSA Journal (2014)
Tetraphenylethane glycidyl ether	7328-97-4	Sigma-Aldrich via NTP	A	31.25	<i>in vitro</i> MN pos.	Positive	Nishihara et al. (2016)
Topiramate	97240-79-4	Sigma-Aldrich	A	1000	Ames neg., <i>in vitro</i> CA and MLA neg., <i>in vivo</i> CA neg.	Negative	Kirkland et al. (2016)
Tozasertib (a.k.a. VX-680)	639089-54-6	Selleckchem	A	1	<i>in vitro</i> MN pos. (primarily K+, also polyploidy)	Positive	Gollapudi et al. (2014); pan-Aurora kinase inhibitor, especially Aurora A
Tribromoacetaldehyde	115-17-3	Sigma-Aldrich via NTP	A	2.64	<i>in vitro</i> comet pos., <i>in vitro</i> MN neg.	Positive (owing to clear TK6 comet positive results with high levels of oxidized bases)	Jeong et al. (2015) and Liviack et al. (2010)

Table 1. (continued)

Chemical	CAS No.	Source	Test Group ^a	Top Conc. (μM)	Other Genetox ^b	Mammalian Cell Genetox Expectation ^c (-S9)	References and Miscellaneous Notes
Tributyltetradecylphosphonium Cl	81741-28-8	Cytec Industries Inc. via NTP	A	1	No NTP data, no publications	Insufficient data	NA
Tributyltetradecylphosphonium dodecylbenzenesulfonate	NOCAS_49391	IoLiTec Ionic Liquids Technologies Inc. via NTP	A	1	No NTP data, no publications	Insufficient data	NA
Tris (2-ethylhexyl) phosphate	78-42-2	Sigma-Aldrich	A	1000	Ames neg., in vitro CA neg., in vivo CA and MN neg.	Negative	Kirkland et al. (2016)
Zafirlukast	107753-78-6	Sigma-Aldrich	A	124.9	Ames neg., in vitro MLA, CA and Hprt neg.	Negative	Kirkland et al. (2016)
Zinc dibutylidithiocarbamate	136-23-2	TCI America via NTP	A	8.83	Ames neg., in vitro CA pos., in vitro MLA neg.	Positive	Matsuoka et al. (2005) and Tinklera et al. (1998)
Ziram	137-30-4	Sigma-Aldrich via NTP	A	0.177	Ames pos., in vitro CA pos.	Positive	NTP
ZM-447439	331771-20-1	Selleckchem	A	25	in vitro MN pos. (primarily K+, also polyploidy)	Positive	Gollapudi et al. (2014) ; Aurora kinase A/B inhibitor
1-Amino-2-methylantraquinone	82-28-0	Sigma-Aldrich via NTP	S	99	Ames pos. (+S9); in vitro CA pos. (+S9, CHO cells), in vitro SCE pos. (± S9, CHO)	Insufficient data	NTP
2-Amino-5-azotoluene	97-56-3	Sigma-Aldrich via NTP	S	70.7	Ames pos. (+S9)	Insufficient data	NTP
2-Hydroxyanthraquinone	605-32-3	TCI America via NTP	S	70.7	Ames pos. (+S9, weak)	Insufficient data	REACH Monitor (2012)
3'-Methyl-4-dimethylaminoazobenzene	55-80-1	TCI America via NTP	S	21.7	Ames pos. (-S9, weak)	Insufficient data	Lefevre and Ashby (1981)
4-(Dimethylamino)azobenzene	60-11-7	Sigma-Aldrich via NTP	S	70.7	Ames pos. (+S9), in vitro MLA pos. (+S9), in vivo MN pos.	Negative	NTP; Leadscope
4-Azoxyanisole	1562-94-3	Sigma-Aldrich via NTP	S	17.49	Ames pos. (+S9)	Insufficient data	NTP
Biochanin A	491-80-5	Sigma-Aldrich via NTP	S	201	DNA adducts and aneuploidy in SHE cells without S9	Positive	Tsutsui et al. (2003)
Cyproterone acetate	427-51-0	Sigma-Aldrich via NTP	S	122.8	in vitro CA with metabolically competent cells, in vivo MN pos.	Insufficient data	Leadscope; Kasper et al. (2001)
D&C Yellow 11	8003-22-3	Sigma-Aldrich via NTP	S	35.7	Ames, in vitro CA pos.	Positive	NTP
N-Phenyl-1-naphthylamine	90-30-2	Sigma-Aldrich via NTP	S	101	Ames, in vitro CA neg.	Negative	NTP

Table 1. (continued)

Chemical	CAS No.	Source	Test Group ^a	Top Conc. (μM)	Other Genetox ^b	Mammalian Cell Genetox Expectation ^c (-S9)	References and Miscellaneous Notes
N, N'-Diphenyl-p-phenylenediamine	74-31-7	Sigma-Aldrich via NTP	S	35.3	Ames pos. (+S9), <i>in vitro</i> SCE pos. (±S9), <i>in vitro</i> CA pos. (although NTP study was neg.)	Positive	NTP; Leadscope
Phenethyl anthranilate	133-18-6	Sigma-Aldrich via NTP	S	201	Ames neg.	Insufficient data	NTP
Rosuvastatin calcium	147098-20-2	Sigma-Aldrich via NTP	S	707	Ames neg., <i>in vitro</i> MLA and CA neg.	Negative	Kirkland et al. (2016)
Saquinavir mesylate	149845-06-7	Roche Research Center via NTP	S	52.7	Ames, <i>in vitro</i> CA, <i>in vivo</i> MN neg.	Negative	Invirase package insert (2012); HIV protease inhibitor
1, 3-Dichlorobenzene	541-73-1	Sigma-Aldrich via NTP	I	199	<i>Escherichia coli</i> and <i>in vivo</i> MN pos., NTP Ames neg.	Positive	EPA, toxicological review of dichlorobenzenes (2006); NTP
2-Amino-6-methoxybenzothiazole	1747-60-0	Sigma-Aldrich via NTP	I	71	Ames pos. (+S9), <i>in vitro</i> CA pos. (much stronger with S9), <i>in vitro</i> MLA pos. (+S9), <i>in vivo</i> MN pos. in female mice, <i>in vivo</i> MN neg. in male mice	Negative	NTP
2-Butoxyethanol	111-76-2	Sigma-Aldrich via NTP	I	200	Ames neg., <i>in vitro</i> SCE and CA neg.; <i>in vivo</i> MN neg.	Negative	NTP
2-Methoxy-5-methylaniline (a.k.a. p-Cresidine)	120-71-8	Sigma-Aldrich via NTP	I	194	Ames pos. (+S9), <i>in vitro</i> CA pos. (+S9, weak), <i>in vivo</i> MN pos.; NTP study was neg.	Negative	Leadscope; NTP
9, 10-Dihydrobenzo[a]pyrene-7(8H)-one	3331-46-2	Sigma-Aldrich via NTP	I	191	No NTP data, no publications	Insufficient data	NA
Acetic acid, mercapto-, monoammonium salt	5421-46-5	TCI America via NTP	I	201	No NTP data, no publications	Insufficient data	NA
Black cohosh extract	84776-26-1	Frutarom Switzerland Ltd. via NTP	I	25	<i>in vitro</i> MN pos., <i>in vivo</i> MN pos.	Positive	NTP; Mercado-Feliciano et al. (2012)
C.I. Basic Orange 2	532-82-1	Sigma-Aldrich via NTP	I	197	Ames pos. (+S9)	Insufficient data	NTP
Daidzein	486-66-8	Sigma-Aldrich via NTP	I	198	Ames neg., <i>in vitro</i> CA neg.	Negative	NTP; Leadscope
Dimethylsulfoxide	67-68-5	Gaylord Chemical Company, LLC via NTP	I	1% v/v	Ames neg., <i>in vitro</i> CA neg.	Negative	Common solvent, not expected to cause <i>in vitro</i> genotoxicity at conc. tested

Table 1. (continued)

Chemical	CAS No.	Source	Test Group ^a	Top Conc. (μM)	Other Genetox ^b	Mammalian Cell Genetox Expectation ^c (-S9)	References and Miscellaneous Notes
Metronidazole	443-48-1	Sigma-Aldrich via NTP	I	205	Ames pos. (± S9), <i>in vitro</i> CA pos., <i>in vivo</i> MN pos.	Positive	NTP; Leadscope
Resorcinol	108-46-3	Sigma-Aldrich via NTP	I	195	Some pos. findings such as <i>in vitro</i> CA pos. (CHO), but generally neg. in p53-competent cell lines	Negative (in p53 competent cells)	Kirkland et al. (2016) and Stich et al. (1981)
Sorbic acid	110-44-1	Sigma-Aldrich via NTP	I	199	Ames neg.; <i>in vitro</i> CA, <i>in vivo</i> MN pos.	Positive	Leadscope; NTP
Thiocarbazide	2231-57-4	Alfa Aesar via NTP	I	205	Ames neg.	Insufficient data	Leadscope
Vinpocetine	42971-09-5	Maypro Industries, LLC via NTP	I	100	Ames neg., <i>in vivo</i> MN neg., <i>in vivo</i> comet stomach neg., blood neg., liver equivocal	Insufficient data	NTP

^aTest Group A: adequately tested, either positive by at least 1 analysis method, or if negative tested to limit conc. or approached/achieved cytotoxicity limit, n = 74; Group S: top concentration limited by solubility (in DMSO), n = 14. Group I: inadequately tested, negative result and did not approach or achieve cytotoxicity limit, and did not reach limit conc. or solubility limit, n = 15.

^bUnless otherwise stated Ames and *in vitro* mammalian cell results refer to test conditions in the absence of exogenous metabolic activation.

^cInsufficient means an expected *in vitro* mammalian cell genotoxicity call cannot be made at this time for lack of sufficient conventional genotoxicity data.