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分担報告書

研究課題名：化学物質のヒト健康リスク評価における（定量的）構造活性相関および、
カテゴリーアプローチの実用化に関する研究

分担研究課題名：*In vivo* 遺伝毒性試験 QSAR の開発 -3 つの *in silico* モデルによる *in vitro*
染色体異常予測性の比較-

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研究要旨

Ames 試験の結果予測のための *in silico* モデルが多く開発されている一方で、*in vitro* 染色体異常試験（CA）の予測モデルは、さほど開発が進んでいない。しかし、Derek Nexus（Derek）、ADMEWORKS（AWorks）あるいは CASE Ultra（MCASE）は、Ames 変異原性と同様に *in vitro* CA も予測することができる。そこで、*in vitro* CA 予測モデルの現状を把握し、*in vivo* を含めた染色体損傷性を予測する QSAR の開発に資するために、拡張版 CGX データベースを用いてそれらの予測性を比較検証した。発がん性および非発がん性の 440 物質について *in vitro* CA 結果に対する各モデルの感受性と特異性は、Derek ではそれぞれ 56.0%および 86.9%、AWorks では 67.7%および 61.5%、MCASE では 91.0%および 64.9%で、MCASE の感受性は、他のモデルよりも高かった。化学物質クラスに対する *in silico* モデルの予測性に、モデル間の大きな違いは認められなかった。発がん物質に対する各モデルの感受性は、非発がん物質よりもわずかに高かった。これらの結果は、検討した *in silico* モデルはいずれも CGX データベース物質における CA 予測に有用であると考えられた。CA 予測の改善には、用いるデータの精緻化（例えば、高細胞毒性状況下の陽性知見の排除、相反知見の確定、質の高い GLP 試験データの利用等）や生体影響、特に *in vivo* における代謝への考慮が必要と考えられた。

A. 研究目的

Ames 試験の結果予測のための *in silico* モデルが多く開発されている一方で、*in vitro* 染色体異常試験（CA）の予測モデルは、さほど開発が進んでいない

ようである。しかし、市販の *in silico* モデルには、Ames 変異原性と同様に *in vitro* CA も予測することができるものがある。そこで、*in vitro* CA 予測モデルの現状を把握しその精度を向上させ、さら

に *in vivo* 染色体損傷性 (小核(MN)を含む) を高精度に予測する QSAR の開発に資するために、拡張版 CGX データベース(DB) を用いて 3 種の *in silico* モデル (Derek Nexus [Derek]、ADMEWORKS [AWorks]、CASE Ultra [MCase]) の *in vitro* CA 予測性を検証比較した。

B. 研究方法

構築した拡張版 CGX DB に対し、Derek、AWorks および MCase の 3 種の *in silico* モデルを適用し、*in vitro* CA に対する各モデルの予測性を検証比較した。また、一部の *in silico* モデルについては、*in vivo* MN に対する予測性を検証した。

B.1. 使用データベース

拡張版 CGX DB (Morita et al, 2016) を用いた。本 DB は CGX DB (発がん物質 756、非発がん物質 183 の計 939 物質を収載; Kirkland et al, 2005) の Ames および *in vitro* CA データを更新し、新規に *in vivo* MN 試験およびげっ歯類トランスジェニック遺伝子突然変異 (TGR) 試験データを追加したものである。

B.2. 解析対象からの除外

B.2.1 評価困難物質

In vitro CA データに対する複数の *in silico* モデルの予測性の比較を実施するにあたり、構造に基づく評価の困難性のため、拡張版 CGX DB より以下の物質を解析対象から除外した:

- 構造不特定物質および重合物質
- 一部の混合物 (異性体混合物を含む)
- 塩の有無・塩違いの物質 (フリー体と

塩類では原則的にはフリー体を評価、あるいは遺伝毒性データ数が少ない物質を除外するなどして同一構造の重複を除外)

- ケイ素化合物・フッ素化合物
- 金属化合物
- 一部の Technical grade 物質

これらの除外により、発がん物質 (C) 713、非発がん物質 (NC) 167 が解析対象となった。

B.2.2 *In vitro* CA/*in vivo* MN データ欠如物質

上記解析対象物質から *in vitro* CA あるいは *in vivo* MN データのないものを除外した。*In vitro* CA あるいは *in vivo* MN で陰性 (-) あるいは陽性 (+) のものを選択し、E (equivocal, 不明確) あるいは TC (Technical compromise, 試験内容に問題) のものは削除した。その結果、上述の解析対象の発がん物質 713、非発がん物質 167 は、最終的に発がん物質 394、非発がん物質 130 となった (合計 524 物質)。すなわち、これらは、少なくとも *in vitro* CA あるいは *in vivo* MN のいずれかについて陽性 (+) あるいは陰性 (-) のデータが存在する物質である。

B.3. 使用 *in silico* モデル

知識ベースとして Derek Nexus (ver. 5.0.2, KB2015) [Derek]、統計ベースとして ADMEWORKS (ver. 7.9.1.0) [AWorks] および CASE Ultra (ver. 1.6.0.3; CA-CHL, CA-CHO, MNT-mouse) [MCase] を用いた。*In vitro* CA の予測には Derek、AWorks、

MCase CA-CHL および MCase CA-CHO の4つを適用し、さらに MCase の CA-CHL と CA-CHO の結果は統合させ、MCase CA-CHL/CHO として評価した。また、*in vivo* MN の予測には MCase MNT-mouse を適用した。

B.4. 予測性評価

各 *in silico* モデルによる解析結果の表記 (アウトプット) はそれぞれ異なっている。そこで、各モデル間の比較を可能とするために、アウトプットを以下のようにまとめた (表 1) : 抽出した発がん物質 394、非発がん物質 130 に対する各 *in silico* モデルの予測結果を、+、-、E (Equivocal)、NA (Not applicable) に集約し、感受性 (Sensitivity)、特異性 (Specificity)、正確性 (Accuracy) あるいは適用性 (Applicability) を評価した。それぞれの算出方法を表 2 に示す。なお、MCase の CA-CHL (MCase CA-CHL) および CA-CHO (MCase CA-CHO) の結果の統合 (MCase CA-CHL/CHO) においては、両モデルで異なる予測 (+/- など) は陽性予測に重みを置き+にするとともに、NA/E と -/+ の不一致においては、確定的予測に重みを置いて-あるいは+とした (表 3)。

B.5. 化学物質のクラス分類

各 *in silico* モデルの化学物質グループ/クラスに対する特性を評価するために、解析対象の 524 物質 (394 の発がん物質 (C) および 130 の非発がん物質 (NC)) について主に構造に基づくクラス分類を行った。2007 年版 CGX DB (CGX 2007、JRC/EURL ECVAM) に記載された

「Chemical Grouping」をもとに、類似構造を集約した。また、CGX 2007 で「Miscellaneous」とされた物質、ならびに集約しても発がん物質と非発がん物質で 2 物質以下のグループは、すべて「Others」とした。

C. 研究結果

解析対象の発がん物質 394、非発がん物質 130 に対する *in vitro* CA および *in vivo* MN の試験結果 (+あるいは-)、ならびに各 *in silico* モデルの予測結果 (+、-、E (Equivocal)、NA (Not applicable)) を Appendix 1 (発がん物質) および Appendix 2 (非発がん物質) にまとめた。

C.1. 評価対象物質

In vitro CA ではデータ (+あるいは-のみを対象) の認められた 440 物質 (発がん物質 C、n=325、非発がん物質 NC、n=115) を抽出し、それらを対象に 3 種の *in silico* モデルの予測性を評価した。また、*in vivo* MN ではデータ (+あるいは-のみを対象) の認められた 337 物質 (C、n=266 および NC、n=71) を抽出し、それらを対象に *in silico* モデル (MCase: MNT-mouse) の予測性を評価した。

C.2. 各 *in silico* モデルの *in vitro* CA に対する予測性

In vitro CA について、各モデルの全物質 (発がん物質および非発がん物質、C+NC) および発がん物質 (C) あるいは非発がん物質 (NC) に対する感受性、特異性、正確性等を表 4 および表 5 ならびに図 1 に示した。全物質 (C+NC) に対する感受性および特異性は、Derek で

56.0%および86.9%、AWorksで67.7%および61.5%、MCase CA-CHLで87.4%および57.5%、MCase CA-CHOで76.2%および93.5%、統合したMCase CA-CHL/CHOで91.0%および64.9%であった。MCaseが比較的高い感受性を示した。正確性は、Derekで68.6%、AWorksで65.2%、MCase CA-CHLで76.3%、MCase CA-CHOで83.5%、統合したMCase CA-CHL/CHOで80.5%を示し、MCaseの正確性が高かった。適用性は、Derekで89.1%、AWorksで99.3%、MCase CA-CHLで77.7%、MCase CA-CHOで90.9%、統合したMCase CA-CHL/CHOで97.7%を示し、AWorksおよびMCaseが高かった。各 *in silico* モデルの発がん物質 (C) と非発がん物質 (NC) に対する比較では、顕著な特徴は認められなかったが、感受性については、いずれのモデルも非発がん物質よりも発がん物質に対するものがわずかに高かった。

C.3. MCase (MNT-mouse)の *in vivo* MN に対する予測性

MCase には、*in vivo* MN の予測に特化した *in silico* モデルの「MNT-mouse」がある。*In vivo* MN について、MNT-mouse の全物質 (C+NC) ならびに C あるいは NC 別に対する感受性、特異性、正確性等を表 6 および表 7 ならびに図 2 に示した。MNT-mouse の C+NC に対する感受性および特異性は 91.1%および57.0%で、極めて高い感受性を示したものの特異性は高いものではなかった。また、正確性および適用性は 72.4%および81.6%を示し、これらの値

は *in vitro* CA に対する各 *in silico* モデルの予測性 (正確性 65.2~83.5%、適用性 77.7~99.3%) と同程度であった。C と NA の比較では顕著な特徴は認められなかったが、NC で小核を誘発した 20 物質すべてを *in silico* でも陽性と予測していた。

C.4. 化学物質のクラス分類

最終的に 524 の解析対象物質を 36 クラスに分類した (表 8、Appendix 1 および 2)。表 8 に示したように各クラスの物質数は Others を含めて 3~69 であり、中には該当物質数が 5 個前後と少ない化学物質クラスもいくつか認められた。さらにその中で *in silico* 評価で-あるいは+となったもの、ならびに *in vitro* CA の実データは限られることから、クラス別解析には *in vitro* CA データを有する物質が 5 つ以上のクラスを対象とした。これにより、クラス別の解析は 22 クラスとなった (表 9)。*In silico* モデルの比較において、MCase は CHL と CHO を統合した CA-CHL/CHO を用いた。各クラスに対する *in silico* モデルの評価結果は、わずかな相違は存在するもののモデル間でほぼ一致した。わずかな相違は、Aromatic amines or amides、Aromatic nitro compounds および Azo compounds における Derek の陽性予測の少なさであった。*In silico* モデルの特徴として Alkylating agents、Aromatic amines or amides、Aromatic nitro compounds、Epoxides、Halides、N-nitro or N-nitroso compounds の多くは、いずれのモデルにおいても陽性予測がなされ、Alcohols、Alkenes、Azo compounds、Carboxylic

acids および Polyhalogenated aromatic compounds の多くについては陰性予測とされていた。残りの 11 の化学物質クラス (Amines/Amides/Imines、Carbamates、Halogenated compounds、Hydrazines、Ketones 、 Phenols 、 Phosphorous compounds、Ureas および Others) は、予測結果に明確な傾向は認められなかった (表 9)。

D. 考 察

In vitro CA 予測における各モデル (Derak、AWorks、MCase CA-CHL、MCase CA-CHO) の感受性は 56.0 ~ 87.4%、特異性は 57.5 ~ 93.5% および正確性は 65.2 ~ 83.5% であった。MCase の CA-CHL と CA-CHO を統合評価 (両モデル間での+と-の不一致は、+と評価) した MCase CA-CHL/CHO では感受性 91.0%、特異性 64.9% および正確性 80.5% であった。正確性に関するこれらの値は、Derak、AWorks、MCase の各 *in silico* モデルの CGX DB 物質に対する初期の Ames 予測における値 (正確性 65.6 ~ 92.7%; Hayashi et al, Mutation Res, 588, 129-135, 2005) と比較すると、若干低かった。また、各モデル間の感受性/特異性に関する比較では、Derek が低/高、AWorks が中/中、MCase CA-CHL が高/低、MCase CA-CHO が高/高の傾向を示し、MCase CA-CHL/CHO は高/中であった。これらの違いは、知識ベースと統計ベースによるアプローチの違いや、それらの構築に用いたデータベースの違いに起因するものと思われる。MCase CA-CHO の高い正確性 (83.5%) は、CGX DB の知見を CA-CHO モデルに適用しているためと

推察される。すなわち、CGX DB の *in vitro* CA 知見の多くは NTP の CHO 細胞を用いた染色体異常試験結果を引用しているためであろう。

拡張版 CGX DB では、*in vitro* CA において 10 mM を超える濃度でのみ陽性を示した物質は、陰性 (-) と評価している。このような物質は全部で 12 (発がん物質 7、非発がん物質 5) あり、それらの *in silico* 評価を表 10 にまとめた。*In silico* 評価における一般的な特徴は特段認められなかったが、CHL あるいは CHO 細胞を用いた試験に特化した MCase の *in silico* モデルにおいて、陽性評価が多い傾向がうかがわれた。当該物質の有する染色体異常誘発性は、直接的には処理濃度とは関連せず、また代謝などが関与した標的組織移行性 (曝露) のため *in vitro* と *in vivo* 知見の相違も認められる。さらに、*in vitro* CA の結果自体も、現行ガイドラインには適合しない高細胞毒性状況や長時間処理に起因した陽性知見が含まれていると推察される。このように、*in vitro* CA の知見自体が、用いる細胞や試験プロトコール (処理濃度、処理時間、細胞毒性基準、陽性判定基準 [以前の CHL を用いた試験による 10%法や統計処理] など) によって異なっているため、統一的結果を導き出すことが困難状況にある。さらに *in vivo* 知見を含め、生体にとって意味のある陽性を正しく陽性と予測するには、代謝の影響を考慮する必要がある、*in vitro* CA 知見も単に陽性陰性ではなく、代謝活性化系存在化下および非存在下における結果など詳細な知見を利用が不可欠と考えられる。補足的に実施した MCase MNT-mouse を用いた *in vivo* MN の *in silico* 予測では、良好な感

受性 (91.1%) が得られている。拡張版 CGX DB の *in vivo* MN 知見は骨髄あるいは末梢血を用いたいわゆる血液系小核試験の結果である。重要な発がん物質には *in vitro* CA において代謝活性化系存在化下で陽性を示しながら、*in vivo* 血液系小核試験では陰性を示すものが多く知られている。例えば、Aromatic amines or amides、N-nitro or N-nitroso compounds、Polycyclic aromatic hydrocarbons などであり、このような物質は肝臓を用いた小核試験では陽性知見を示す場合がある。CA の *in silico* 評価の開発は、代謝を考慮して進めていく必要がある。

発がん性物質の化学物質クラス毎の CA 誘発性に関する *in silico* 評価では、Amines/Amides/Imines、Carbamates、Halogenated compounds、Hydrazines、Ketones、Phenols、Phosphorous compounds および Ureas で、陰性陽性の予測がほぼ半分に分かれた。このようなクラスについては、使用データの精緻化が予測性の改善に効果があるかもしれない。

F. 結論

In vitro CA 予測に対する 3 つの *in silico* モデルの比較から、検討したモデルはいずれも CA 予測に有用であると考えられた。しかしながら、その予測性 (特に感受性) は、総体的に初期の Ames 予測よりも低いものであった。その改善には、用いるデータの精緻化 (例えば、高細胞毒性状況下の陽性知見の排除、相反知見の確定、質の高い GLP 試験データの利用等) や生体影響、特に *in vivo* における代謝への考慮が必要と考えられた。これらに対応することにより、さらなる予測精度の向上

が期待できる。

G. 研究発表

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H. 知的財産権の出願・登録状況
なし

表 1 解析対象除外物質一覧

In silico モデル ^⓪	結果のアウトプット ^⓪	最終表記 ^⓪
^⓪	Inactive ^⓪	- ^⓪
Derek ^⓪	Certain ^⓪	+ ^⓪
^⓪	Plausible ^⓪	+ ^⓪
^⓪	Equivocal ^⓪	E ^⓪
^⓪	- ^⓪	- ^⓪
AWorks ^⓪	+ ^⓪	+ ^⓪
^⓪	Not Applicable ^⓪	NA ^⓪
^⓪	Known negative ^⓪	- ^⓪
^⓪	Negative ^⓪	- ^⓪
^⓪	Known Positive ^⓪	+ ^⓪
MCase ^⓪	Positive ^⓪	+ ^⓪
^⓪	Known marginal ^⓪	+ ^⓪
^⓪	Inconclusive ^⓪	E ^⓪
^⓪	Out of Domain ^⓪	NA ^⓪

- , Negative; + , Positive; E, Equivocal; NA, Not Applicable^⓪

表 2 予測性の計算方法

+	In vitro or In vivo result			
	+	+	-	Total
In silico results	+	a	b	a+b
	-	c	d	c+d
	Total	a+c	b+d	a+b+c+d

No. of all chemicals evaluated (all) ↓

= (a+b+c+d) + E (equivocal result) + NA (Not applicable)

感受性 (Sensitivity, %) = a / (a+c)

特異性 (Specificity, %) = d / (b+d)

正確性 (Accuracy, %) = (a+d) / (a+b+c+d)

適用性 (Applicability, %) = (a+b+c+d) / all

表3 MCase の CA-CHL および CA-CHO 間の結果の統合

各結果	統合後
両者一致	一致結果
-と+での不一致	+
NA/E と -/+の不一致	該当する-/+のいずれか
E と NA の不一致	E

表4 各 in silico モデルの in vitro CA に対する予測性：全物質 (C+NC, n=440)

In silico model [No. of C/NC]	CA results	+	-	Total	E	NA	Sensitivity (%)	Specificity (%)	Accuracy (%)	Applica- bility (%)
Derek [287/105]	+	130	21	151						
	-	102	139	241	48	0	56.0	86.9	68.6	89.1
	Total	232	160	392						
AWorks [325/112]	+	178	67	245						
	-	85	107	192	0	3	67.7	61.5	65.2	99.3
	Total	263	174	437						
MCase (CA-CHL) [263/79]	+	188	54	242						
	-	27	73	100	64	34	87.4	57.5	76.3	77.7
	Total	215	127	342						
MCase (CA-CHO) [293/107]	+	176	11	187						
	-	55	158	213	23	17	76.2	93.5	83.5	90.9
	Total	231	169	400						
MCase (CA-CHL/CHO)* [318/112]	+	233	61	294						
	-	23	113	136	4	6	91.0	64.9	80.5	97.7
	Total	256	174	430						

C, Carcinogens; NC, Non-Carcinogens; E, Equivocal; NA, Not Applicable
 *: +/- or -/+ is considered as +, **: Accuracy (%) x Applicability (%)

表5 各 in silico モデルの in vitro CA に対する予測性：C (n=325)、NC (n=115)別

In silico model	CA results	+	-	Total	E	NA	Sensitivity (%)	Specificity (%)	Accuracy (%)	Applicability (%)
Carcinogens (n=325)										
Derek	+	107	16	123						
	-	77	87	164	38	0	58.2	84.5	67.6	88.3
	Total	184	103	287						
AWorks	+	145	43	188						
	-	68	69	137	0	0	68.1	61.6	65.8	100
	Total	213	112	325						
MCase (CA-CHL)	+	161	34	195						
	-	17	51	68	44	18	90.4	60.0	80.6	80.9
	Total	178	85	263						
MCase (CA-CHO)	+	145	7	152						
	-	39	102	141	19	13	78.8	93.6	98.8	90.2
	Total	184	109	293						
MCase (CA-CHL/CHO)*	+	194	39	233						
	-	13	72	85	3	4	93.7	64.9	83.7	97.8
	Total	207	111	318						
Non-Carcinogens (n=115)										
Derek	+	23	5	28						
	-	25	52	77	10	0	47.9	91.2	71.4	91.3
	Total	48	57	105						
AWorks	+	33	24	57						
	-	17	38	55	0	3	66.0	61.3	63.4	97.4
	Total	50	62	112						
MCase (CA-CHL)	+	27	20	47						
	-	10	22	32	20	16	73.0	52.4	62.0	68.7
	Total	37	42	79						
MCase (CA-CHO)	+	31	4	35						
	-	16	56	72	4	4	66.0	93.3	81.3	93.0
	Total	47	60	107						
MCase (CA-CHL/CHO)*	+	39	22	61						
	-	10	41	51	1	2	79.6	65.1	71.4	97.4
	Total	49	63	112						

*: +/- or -/+ is considered as +.

表6 MCase (MNT-mouse)の in vivo MN に対する予測性：全物質 (C+NC, n=337)

In silico model [No. of C/NC]	MN results	+	-	Total	E	NA	Sensitivity (%)	Specificity (%)	Accuracy (%)	Applicability (%)
MCase (MNT-mouse) [275/52]	+	113	65	178						
	-	11	86	97	39	23	91.1	57.0	72.4	81.6
	Total	124	151	275						

C, Carcinogens; NC, Non-Carcinogens; E, Equivocal; NA, Not Applicable

表7 MCase (MNT-mouse)の in vivo MN に対する予測性：C (n=266)、NC (n=71)別

In silico model	in vivo MN results	+	-	Total	E	NA	Sensitivity (%)	Specificity (%)	Accuracy (%)	Applicability (%)
Carcinogens (n=266)										
MCase (MNT-mouse)	+	93	52	145						
	-	11	67	78	27	16	89.4	56.3	71.7	83.8
	Total	104	119	223						
Non-Carcinogens (n=71)										
MCase (MNT-mouse)	+	20	13	33						
	-	0	19	19	12	7	100	59.4	75.0	73.2
	Total	20	32	52						

C, Carcinogens; NC, Non-Carcinogens; E, Equivocal; NA, Not Applicable

表 8 化学物質クラス一覧

#	Chemical Class	Carcinogens	Non-carcinogens	Total
1	Alcohols	5	2	7
2	Aldehydes	8	4	12
3	Alkalis, metal salts	0	3	3
4	Alkenes	8	2	10
5	Alkylating agents	20	6	26
6	Amines/Amides/Imines	15	10	25
7	Anthraquinones or quinones	3	0	3
8	Aromatic amines or amides	57	12	69
9	Aromatic nitro compounds	31	8	39
10	Azirines or aziridines	4	0	4
11	Azo compounds	21	5	26
12	Benzenes	13	2	15
13	Carbamates	7	7	14
14	Carboxylic acids	7	6	13
15	Catechols	4	2	6
16	Epoxides	11	2	13
17	Esters	2	1	3
18	Halides	18	3	21
19	Halogenated compounds	23	6	29
20	Hormones	4	0	4
21	Hydrazines	11	3	14
22	Isocyanates	3	0	3
23	Ketones	5	4	9
24	Nitriles	2	3	5
25	Nitro compounds or nitrites	4	0	4
26	N-nitro or N-nitroso compounds	24	0	24
27	Others	40	15	55
28	Phenyl compounds	3	0	3
29	Phenols	8	2	10
30	Phosphorous compounds	6	10	16
31	Phthalates	1	2	3
32	Polycyclic aromatic hydrocarbons	5	0	5
33	Polyhalogenated aromatic compounds	10	4	14
34	Quinolines	2	1	3
35	Resorcinols	1	3	4
36	Ureas	8	2	10
	Total	394	130	524

表 9 化学物質クラスとその in silico モデルによる予測性

Chemical class ^a	No. of chemicals	In vitro CA test	Positive prediction			Negative prediction			Tendency of in silico predictions
			+ / - / NTD	Derek	AWorks	MCase ^b	Derek	AWorks	
Alcohols	7	3 / 2 / 2	0	1	0	4	2	3	-
Aldehydes	12	7 / 5 / 0	5	4	3	3	2	5	ND
Alkenes	10	3 / 4 / 3	1	2	0	4	2	3	-
Alkylating agents	26	16 / 6 / 4	14	7	15	1	4	3	+
Amines/Amides/Imines	25	10 / 12 / 3	4	9	6	12	5	9	ND
Aromatic amines or amides	69	43 / 19 / 7	11	39	38	17	8	9	+
Aromatic nitro compounds	39	25 / 12 / 2	3	19	21	2	8	2	+
Azo compounds	26	7 / 12 / 7	1	5	4	12	8	2	-
Benzenes	15	6 / 7 / 2	2	4	3	6	5	6	ND
Carbamates	14	6 / 4 / 4	6	2	3	2	4	4	ND
Carboxylic acids	13	4 / 7 / 2	0	2	1	6	6	5	-
Epoxides	13	10 / 2 / 1	10	12	11	0	0	0	+
Halides	21	15 / 6 / 0	9	10	10	4	5	5	+
Halogenated compounds	29	12 / 12 / 5	7	8	5	9	7	11	ND
Hydrazines	14	4 / 4 / 6	2	2	2	2	3	2	ND
Ketones	9	6 / 3 / 0	0	2	1	3	3	3	ND
N-nitro or N-nitroso compounds	24	14 / 2 / 8	14	12	14	0	1	0	+
Phenols	10	7 / 3 / 0	3	1	3	3	3	3	ND
Phosphorous compounds	16	7 / 8 / 1	3	5	5	6	3	2	ND
Polyhalogenated aromatic compounds	14	5 / 7 / 2	1	1	1	6	2	6	-
Ureas	10	4 / 5 / 1	0	1	2	3	1	1	ND
Others	55	25 / 18 / 12	14	17	16	11	12	16	ND

+ : Positive; - : Negative; NTD, No test data; ND, Not determined;
a: Chemical classes with equal or more than 5 chemicals with in vitro CA test data
b: MCase CA-CHL/CHO

表 10 10 mM 以上で in vitro CA 陽性を示す物質の in silico 評価結果

ID	Chemical	In vitro CA	In vivo MN	In vitro CA Derek	In vitro CA Aworks	In vitro CA MCCase: CA-CHL	In vitro CA MCCase: CA-CHO	In vivo MN MCCase: MNT-mouse
C392	Hexanamide	-	-	-	-	-	+	E
C509	Nitrite, sodium	-	-	+	+	NA	+	+
C514	Nitrobenzene	-	-	-	-	+	-	-
C551	N-Nitrosodiethylamine	-	-	+	-	+	+	+
C664	Saccharin, sodium	-	-	-	+	-	-	E
C734	Trimethylphosphate	-	+	-	+	-	+	+
C744	Urethane	-	+	+	-	-	-	+
NC12	o-Anthranilic acid	-	-	-	-	+	E	-
NC20	Benzyl alcohol	-	-	-	-	-	+	-
NC124	4-Nitroanthranilic acid	-	-	E	+	+	+	-
NC144	1-Phenyl-2-thiourea	-	-	-	-	-	+	+
NC152	Resorcinol	-	+	-	-	+	+	+
No. of in silico-positive				3	4	5	8	6

図 1 各 in silico モデルの in vitro CA に対する予測性

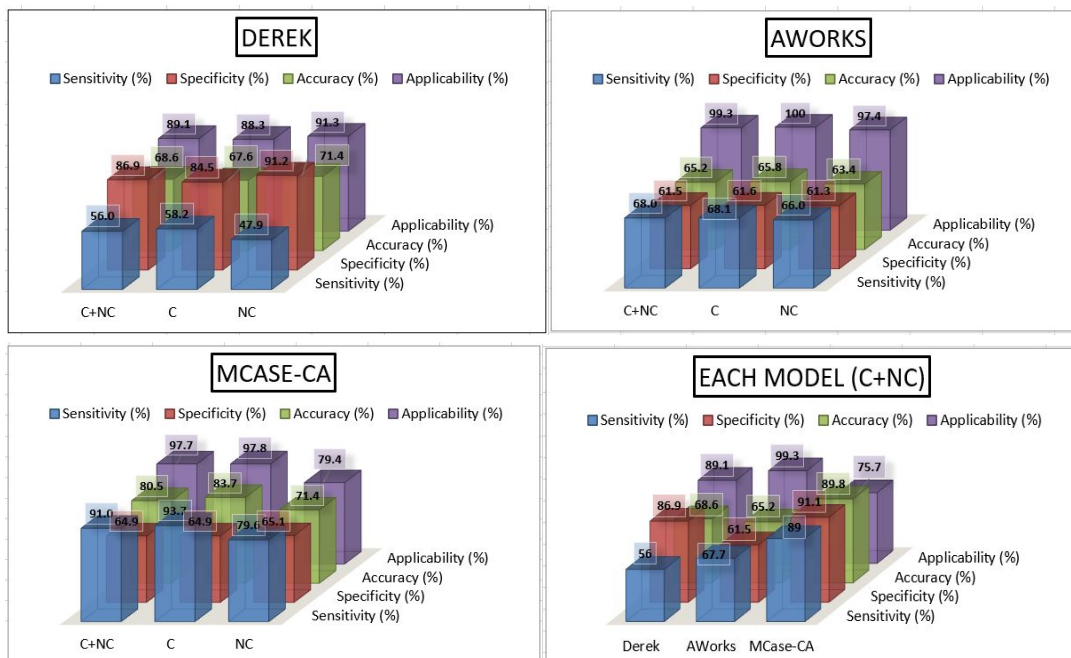
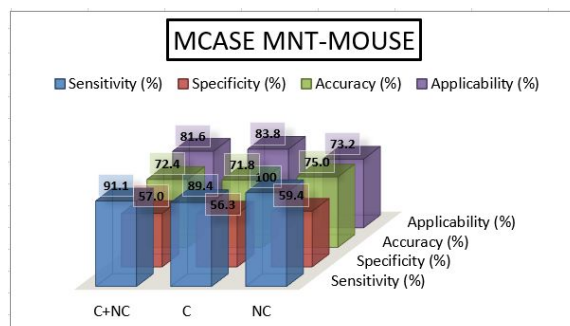


図2 MCCase (MNT-mouse)の in vivo MN に対する予測性



Appendix 1 Results of analysis from 3 in silico models for in vitro chromosomal aberrations (CA) to carcinogens

#	ID	Chemical	CAS No.	Chemical Grouping (GCG 2007)	Chemical Class	In vitro CA	In vitro E-MN*	In vitro CA Derak	In vitro CA Averta	In vitro CA MCass: CA-CHL	In vitro CA MCass: CA-CHO	In vitro MN MCass: MNT-mouse
1	C1	Acetaldehyde	75-07-0	Aldehyde or precursor	Aldehydes	+	+	-	+	+	+	+
2	C3	Acetamide	60-35-6	Aliphatic amide	Amines/Amides/imin es	-	-	-	-	-	NA	+
3	C4	Acetaminophen	103-90-2	Phenol or precursor	Phenols	+	-	-	+	+	+	-
4	C7	N-Acetyl-2-acetylaminofluorene	6096-44-8	Aromatic hydroxylamine or ester derivative	Aromatic amines or amides	+	+	+	E	+	+	E
5	C10	2-Acetylaminofluorene	53-96-3	Aromatic amine or amide	Aromatic amines or amides	+	+	-	+	+	+	+
6	C16	Acrylamide	79-06-1	Alpha-, beta-unsaturated amide or thioamide	Amines/Amides/imin es	+	+	+	+	+	+	+
7	C17	Acrylonitrile	107-13-1	Alpha-, beta-unsaturated nitrile	Nitriles	+	-	-	+	+	+	-
8	C18	Adchomycin D	50-76-0	Alpha-, beta-unsaturated imine	Amines/Amides/imin es	+	+	-	+	+	E	+
9	C20	Aflatoxin B1	1162-85-8	Bifuranoid mycotoxin or analogue	Others	+	+	-	-	+	NA	+
10	C22	Adm	309-00-2	Alkyl halide	Halides	+	-	-	+	-	-	-
11	C23	Allyl glycidyl ether	105-60-3	Glycidyl ether, amine, ester or derivative	Epoxydes	+	+	+	+	+	+	-
12	C24	Allyl isocyanate	57-06-7	Isocyanate or both isocyanate	Isocyanates	+	-	-	-	NA	+	NA
13	C25	Allyl isocyanate	2035-39-4	Alkene	Alkenes	+	+	-	-	+	+	-
14	C30	4-Aminobenzene	60-09-3	Aromatic amine compound	Azo compounds	+	+	-	+	+	+	+
15	C31	4-Aminobiphenyl	92-67-1	Aromatic amine or amide	Aromatic amines or amides	+	+	-	+	+	+	+
16	C33	1-Amino-2,4-dibromanthraquinone	81-49-2	Aromatic amine or amide	Aromatic amines or amides	-	-	-	+	+	-	+
17	C34	2-Amino-3,4-dimethylimidazo[4,5-f]quinoline (MeIQ)	77094-11-2	Quinoline	Quinolines	+	-	-	+	+	+	-
18	C35	2-Amino-3,8-dimethylimidazo[4,5-f]quinoline (MeIQx)	77500-04-0	Aromatic amine or amide	Aromatic amines or amides	+	+	-	+	+	+	E
19	C36	3-Amino-1,4-dimethyl-5H-pyrro[4,3-b]indole sulfate (Trp-P-1 sulfate)	68908-54-8	Aromatic amine or amide	Aromatic amines or amides	+	+	+	+	E	+	NA
20	C38	2-Aminopyrido[1,2-a:3'7'-d]imidazole (Glu-P-2)	67730-10-3	Aromatic amine or amide	Aromatic amines or amides	+	+	+	+	+	E	NA
21	C39	3-Amino-4-ethoxycarbonyl	17026-81-2	Aromatic amine or amide	Aromatic amines or amides	-	-	-	+	+	-	E
22	C40	3-Amino-9-ethylcarbazole HCl	6106-87-3	Aromatic amine or amide	Aromatic amines or amides	-	-	-	+	+	-	+
23	C43	2-Amino-6-methylpyrido[1,2-a:3'7'-d]imidazole (Glu-P-1)	67730-11-4	Aromatic amine or amide	Aromatic amines or amides	+	+	+	+	+	E	NA
24	C44	2-Amino-3-methylimidazo[4,5-f]quinoline (IQ)	76180-96-6	Quinoline	Quinolines	+	-	-	+	+	+	-
25	C46	2-Amino-1-methyl-6-phenylimidazo-[4,5-f]pyridine hydrochloride (PhIP HCl)	-	Aromatic amine or amide	Aromatic amines or amides	+	+	-	+	+	+	+
26	C47	3-Amino-1-methyl-5H-pyrro[4,3-b]indole sulfate (Trp-P-2 sulfate)	72264-88-1	Aromatic amine or amide	Aromatic amines or amides	+	+	+	+	+	-	NA
27	C52	2-Amino-4-nitrophenol	99-67-0	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	+	+	+	-
28	C53	2-Amino-5-nitrophenol	121-85-0	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	+	+	+	+
29	C54	4-Amino-2-nitrophenol	119-34-6	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	+	+	+	+
30	C56	2-Amino-6-nitrothiazole	121-66-4	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	+	+	+	+
31	C57	2-Amino-9H-pyrro[2,3-b]indole (A-alpha-C)	26148-88-8	Secondary amine	Amines/Amides/imin es	+	+	+	+	+	E	NA
32	C58	3-Amino-1,2,4-triazole (Amitrole)	61-42-6	Aromatic amine or amide	Aromatic amines or amides	-	-	-	+	+	NA	NA
33	C59	11-Aminoundecanoic acid	2432-99-7	Short chain aliphatic carboxylic acid	Carboxylic acids	-	-	-	-	-	-	-
34	C60	1-Amyl-1-nitrosourea	10589-74-9	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	+	+	+	+	+	+	+
35	C62	Aniline HCl	142-04-1	Aromatic amine or amide	Aromatic amines or amides	+	+	E	+	+	E	+
36	C63	o-Anilidine HCl	134-29-2	Aromatic amine or amide	Aromatic amines or amides	+	-	-	+	+	+	-
37	C65	Ancoline HCl	61-94-9	Alpha-, beta-unsaturated ester or thioester (class II or III)	Esters	+	+	+	+	-	+	+
38	C66	Anthracic acid	313-67-7	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	-	+	+	+
39	C70	Atrazine	1912-24-9	Potentially labile halogen	Halogenated compounds	+	+	-	-	-	-	NA
40	C71	Auramine O	2485-27-2	Aromatic amine or amide	Aromatic amines or amides	+	-	-	-	E	+	E
41	C72	5-Azacytidine	302-67-2	Nucleic acid derivative	Others	+	+	+	+	E	+	+
42	C73	Azaserine	115-02-6	Azo or azoxy compound	Azo compounds	+	+	-	-	E	E	NA
43	C74	Azathioprine	448-85-6	Aromatic nitro compound	Aromatic nitro compounds	+	+	+	+	E	+	+
44	C75	Azobenzene	103-33-3	Aromatic azo compound	Azo compounds	+	+	-	+	+	E	E
45	C79	Barbitol, sodium	144-02-6	(Thio)urea	Ureas	+	-	-	+	E	+	NA
46	C81	Benzal	17824-28-2	Benzothiazole	Others	+	+	-	+	+	E	+
47	C82	Benzaldehyde	100-52-7	Aldehyde or precursor	Aldehydes	+	+	-	+	+	-	+
48	C83	Benz[a]anthracene	56-85-3	Bay-region polycyclic aromatic hydrocarbon	Polycyclic aromatic hydrocarbons	+	+	+	+	+	-	+
49	C84	Benzene	71-43-2	Benzene	Benzenes	+	+	-	-	-	-	+
50	C85	Benzidine	92-67-6	Aromatic amine or amide	Aromatic amines or amides	+	+	-	+	+	+	+
51	C87	Benzo[<i>a</i>]uran	271-69-6	Benzene	Benzenes	-	-	-	+	+	-	+
52	C88	Benzo[<i>a</i>]pyrene	50-32-6	Bay-region polycyclic aromatic hydrocarbon	Polycyclic aromatic hydrocarbons	+	+	+	+	+	+	+
53	C89	1,4-Benzquinone	105-61-4	Quinone	Anthraquinones or quinones	+	+	+	+	-	-	-
54	C92	Benzyl acetate	142-11-4	Benzene	Benzenes	-	-	-	-	-	-	E
55	C93	Benzyl chloride	100-44-7	Alkylating agent	Alkylating agents	+	-	+	-	+	+	-
56	C94	o-Benzyl-p-chlorophenol	120-32-1	Phenol or precursor	Phenols	-	-	-	-	E	-	-
57	C96	2-Biphenylamine HCl	2185-82-4	Aromatic amine or amide	Aromatic amines or amides	+	-	-	-	+	+	-
58	C97	2,2-Dibromomethyl-1,3-propanediol, technical grade	3296-90-0	Halocalkane	Halogenated compounds	+	+	+	+	+	+	-
59	C98	Di(2-chloro-1-methyl)ether, technical grade	103-60-1	Alkylating agent	Alkylating agents	+	+	-	+	+	+	-
60	C103	Di(2,3-dibromopropyl)phosphate, magnesium salt	36711-31-6	vic-Dihalide	Halides	+	+	+	+	+	E	E
61	C107	Bromate, potassium	7756-01-2	Bromate	Others	+	+	+	+	NA	NA	NA

#	ID	Chemical	CAS No.	Chemical Grouping (CGT 2007)	Chemical Class	In vitro CA	In vivo E-MN*	In vitro CA Derek	In vitro CA Auroto	In vitro CA MCase: CA-GHL	In vitro CA MCase: CA-CHO	In vivo MN MCase: MNT-mouse
62	C106	Bromocriptine mesylate	22260-81-1	Halogenated silone	Halogenated compounds	*	-	-	-	*	E	E
63	C109	Bromodichloromethane	75-27-4	Halogenated methane	Halogenated compounds	*	-	*	*	*	-	-
64	C110	Bromoethane	74-96-4	Alkylating agent	Alkylating agents	-	-	*	*	*	-	NA
65	C114	1,3-Substane	105-99-0	Alkene	Alkenes	-	*	-	-	-	-	*
66	C115	tert-Butyl alcohol	75-65-0	Alcohol	Alcohols	-	-	-	-	-	-	*
67	C116	Butylated hydroxytoluene	25013-16-5	4-Alkylphenol	Phenols	*	-	-	-	-	*	*
68	C117	Butylated hydroxytoluene	125-37-0	Benzene	Benzenes	-	-	-	-	-	-	*
69	C118	Butylparaldehyde	85-69-7	Phthalate	Phthalates	-	-	-	-	-	-	*
70	C122	N-o-Butyl-N-nitrosourea	869-01-2	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	*	-	*	*	*	*	*
71	C123	beta-Butyrolactone	3095-90-0	Beta-lactone	Others	-	*	-	-	NA	E	NA
72	C126	Caffeic acid	331-39-6	Catechol or precursor	Catechols	*	-	-	-	-	-	*
73	C130	Caprocin	404-05-1	Catechol or precursor	Catechols	-	-	-	-	-	-	*
74	C131	Captafol	2425-06-1	Potentially labile halogen	Halogenated compounds	*	-	*	*	*	E	E
75	C132	Capten	133-06-2	Potentially labile halogen	Halogenated compounds	*	*	*	*	*	*	*
76	C133	Carbamyl hydrazine HCl	563-41-7	Hydrazine or monoacyl- or monoalkylhydrazine	Hydrazines	-	-	*	-	E	NA	*
77	C136	Carbamyl	63-26-2	(Thio)acetamide	Carbamates	*	*	*	*	*	*	*
78	C137	Carbon tetrachloride	56-23-6	Halogenated methane	Halogenated compounds	-	-	E	-	-	-	*
79	C138	Carbonylmethylnitrosourea	60391-60-8	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	*	-	*	*	*	*	*
80	C140	Catechol	120-80-9	Catechol or precursor	Catechols	*	*	*	*	*	-	*
81	C141	Cetonal hydrate	302-17-0	Aldehyde or precursor	Aldehydes	*	*	-	-	NA	-	*
82	C142	Chloramben	133-90-4	Aromatic amine or amide	Aromatic amines or amides	*	-	*	*	*	*	*
83	C143	Chlorobutyl	305-03-3	Alkylating agent	Alkylating agents	*	*	*	-	*	*	*
84	C145	Chloride, analytical grade	57-74-9	Allyl halide	Halides	-	-	-	-	-	-	*
85	C146	Chloric acid	115-28-6	Allyl halide	Halides	*	-	-	-	-	-	*
86	C147	Chlorinated paraffin, C12	108171-26-2	Wax	Others	*	*	-	-	*	E	NA
87	C149	Chlorophazine	494-03-1	Alkylating agent	Alkylating agents	*	*	*	*	*	*	*
88	C152	p-Chloroaniline HCl	20265-96-7	Aromatic amine or amide	Aromatic amines or amides	-	*	-	*	*	*	*
89	C153	Chlorobenzene	108-90-7	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	*	-	-	-	-	-	*
90	C154	Chlorobenzofate	510-15-6	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	-	-	*	*	E	-	*
91	C155	Chlorobromomethane	124-45-1	Halogenated methane	Halogenated compounds	*	-	*	*	*	-	*
92	C157	Chloroethane	75-00-3	Alkylating agent	Alkylating agents	-	-	*	-	-	E	NA
93	C160	Chloroform	67-66-3	Halogenated methane	Halogenated compounds	-	-	E	-	E	-	*
94	C162	3-Chloro-2-methylpropene, technical grade	563-47-3	Allyl halide	Halides	*	-	*	*	*	*	*
95	C163	3-Chloromethylpyridine HCl	6959-66-4	Alkylating agent	Alkylating agents	*	*	*	*	*	*	*
96	C165	1-Chloro-4-nitrobenzene	100-00-6	Aromatic nitro compound	Aromatic nitro compounds	*	*	E	*	*	*	E
97	C166	3-(p-Chlorophenyl)-1,1-dimethylurea (AKA monuron)	150-65-6	(Thio)urea	Ureas	*	*	*	*	*	*	*
98	C167	4-Chloro-N-phenylethanediamine	5131-60-2	Aromatic amine or amide	Aromatic amines or amides	*	-	-	*	*	*	E
99	C168	4-Chloro-N-phenylethanediamine	95-63-0	Aromatic amine or amide	Aromatic amines or amides	*	*	-	*	*	*	*
100	C172	Chloroethanol	1097-65-6	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	*	-	-	-	-	*	*
101	C173	5-Chloro-o-toluidine	95-79-4	Aromatic amine or amide	Aromatic amines or amides	-	-	*	*	*	-	*
102	C179	Chlorpromazine hydrochloride	69-09-0	Aromatic amine or amide	Aromatic amines or amides	-	*	*	-	-	-	*
103	C180	Chrysozin	81-85-0	Hydroxylated anthraquinone or precursor	Anthraquinones or quinones	*	*	-	*	*	*	*
104	C181	C.I. Acid orange 3	6373-74-6	Aromatic nitro compound	Aromatic nitro compounds	*	-	E	-	*	*	E
105	C183	C.I. Acid red 114	6459-94-5	Aromatic azo compound	Azo compounds	-	-	-	-	*	*	*
106	C184	C.I. Basic red 9 (pararosaniline HCl)	569-61-9	Alpha-, beta-unsaturated imine	Amines/Amines/imines	-	-	-	*	*	*	*
107	C185	C.I. Direct black 38	1937-37-7	Aromatic azo compound	Azo compounds	-	*	-	-	*	*	*
108	C186	C.I. Direct blue 6	2602-66-2	Aromatic azo compound	Azo compounds	-	-	-	-	E	-	E
109	C187	C.I. Direct blue 14 (Thyran blue)	72-67-1	Aromatic azo compound	Azo compounds	-	-	-	-	-	-	E
110	C188	C.I. Direct blue 15	2429-74-5	Aromatic azo compound	Azo compounds	-	-	-	-	*	-	*
111	C189	C.I. Direct blue 216	26437-37-6	Aromatic azo compound	Azo compounds	-	-	-	-	*	-	*
112	C190	C.I. Direct brown 95	16071-86-6	Aromatic azo compound	Azo compounds	-	-	-	-	*	-	E
113	C191	C.I. Disperse blue 1	2475-65-8	Aromatic amine or amide	Aromatic amines or amides	*	-	-	*	*	*	E
114	C192	C.I. Disperse orange 2 (1-amino-3-methyl-anthraquinone)	62-28-0	Aromatic amine or amide	Aromatic amines or amides	*	-	*	*	*	*	E
115	C193	C.I. Disperse yellow 3	2832-60-8	Aromatic azo compound	Azo compounds	-	-	-	*	*	*	*
116	C194	Dimethyl anthranilate	67-29-6	Aromatic amine or amide	Aromatic amines or amides	-	-	-	-	-	-	*
117	C195	C.I. Pigment red 3	2425-85-6	Aromatic nitro compound	Aromatic nitro compounds	-	-	E	-	*	-	*
118	C196	Diprotionol	5214-04-3	Gem-dihalide	Halides	*	-	-	*	*	NA	NA
119	C197	C.I. Solvent yellow 3 (p-Aminocarbonylurea)	97-56-3	Aromatic azo compound	Azo compounds	-	*	-	*	*	*	*
120	C198	C.I. Solvent yellow 14	642-07-9	Aromatic azo compound	Azo compounds	-	*	-	*	*	*	*
121	C200	C.I. Vat yellow 4	128-65-6	(Di)aryl ketone	Ketones	-	-	-	-	E	-	*
122	C202	Disulfone	637-07-0	Fluorene	Others	*	-	-	*	*	*	E
123	C206	Coumarin	91-64-6	Coumarin	Others	*	-	-	*	*	*	E
124	C207	m-Cresidine	102-60-1	Aromatic amine or amide	Aromatic amines or amides	*	-	-	*	*	*	*
125	C208	p-Cresidine	120-71-6	Aromatic amine or amide	Aromatic amines or amides	-	-	-	*	*	-	*
126	C210	Cupferron	135-20-6	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	*	-	*	-	*	*	*
127	C214	Cyclophosphamide monophosphate	6055-19-2	Alkylating agent	Alkylating agents	*	*	*	*	*	*	*
128	C215	Cyfluthrin A	56895-13-3	Macrolactone	Others	-	-	-	-	E	-	*
129	C216	Cyfluthrin	21739-91-3	Halogenated silone	Halogenated compounds	*	-	E	-	NA	*	*
130	C217	D&G Red 9	5182-02-1	Aromatic azo compound	Azo compounds	-	*	-	*	*	-	*
131	C218	D&G Yellow 11 (AKA C.I. Solvent Yellow 33)	8003-22-3	Substituted vinyl ketone	Ketones	*	-	-	*	*	*	*
132	C220	p,p'-DDE	72-85-9	Halogenated silone	Halogenated compounds	*	-	-	-	-	-	*
133	C222	Dicarbazine	4342-03-4	Aryldialylhydrazine	Others	-	*	-	-	*	*	E
134	C223	Dibromide	1595-54-5	Mono- or di-alkylhydrazine	Hydrazines	-	-	*	-	-	-	*

#	ID	Chemical	CAS No.	Chemical Grouping (DGX 2007)	Chemical Class	In vitro CA	In vivo E-AM*	In vitro CA Deriv.	In vitro CA Aestria	In vitro CA MCase: CA-CHL	In vitro CA MCase: CA-CHO	In vitro MN MCase: MNT-mouse
135	C234	Danthron	117-10-2	Hydroxylated anthraquinone or precursor	Anthraquinones or quinones	+	-	+	-	E	+	-
136	C235	Deabromodiphenyl oxide	1163-19-8	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	-	+	-	+	-	-	-
137	C236	2,4-Diaminotoluene sulphate	39156-41-7	Aromatic amine or amide	Aromatic amines or amides	+	-	-	+	+	+	E
138	C237	2,4-Diaminophenol 2HCl	137-09-7	Aromatic amine or amide	Aromatic amines or amides	-	-	-	+	+	+	E
139	C238	2,4-Diaminotoluene	96-60-7	Aromatic amine or amide	Aromatic amines or amides	+	-	-	+	+	+	-
140	C240	Dacapan	439-148	Aromatic amine or amide	Aromatic amines or amides	-	+	-	-	E	-	+
141	C242	DBenz(a)anthracene	53-70-3	Bay-region polycyclic aromatic hydrocarbon	Polycyclic aromatic hydrocarbons	-	+	+	+	+	-	+
142	C244	1,2-Dibromo-3-chlorobenzene	96-12-8	vic-Dihalide	Halides	+	+	+	+	+	+	-
143	C246	1,2-Dibromobenzene	106-93-4	vic-Dihalide	Halides	+	-	+	+	+	+	+
144	C247	Dibromomethyl	469-41-8	Alkylating agent	Alkylating agents	+	+	+	-	+	+	+
145	C250	1,3-Dibutyl-N-nitrosourea	56954-82-8	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	+	-	+	+	+	+	+
146	C251	Dichloroacetic acid	79-43-6	Gem-Dhalide	Halides	+	-	-	-	-	-	-
147	C253	1,4-Dichlorobenzene	106-46-7	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	-	-	-	-	-	-	-
148	C257	1,2-Dichloroethane	107-06-2	vic-Dihalide	Halides	+	-	-	-	+	+	-
149	C258	Dichloromethane	75-09-2	Halogenated methane	Halogenated compounds	+	-	E	+	+	+	-
150	C259	2,6-Dichloro-p-phenylenediamine	609-20-1	Aromatic amine or amide	Aromatic amines or amides	+	-	-	+	+	+	E
151	C260	1,2-Dichlorobenzene	78-47-6	vic-Dihalide	Halides	+	-	+	-	+	+	NA
152	C261	1,3-Dichloropropene (AKA Telone II)	542-75-6	Allyl halide	Halides	-	-	+	+	+	+	+
153	C262	Dichlorvos	62-73-7	Allyl ester of phosphoric or phosphonic acid	Phosphorus compounds	+	-	+	+	+	+	-
154	C263	Dieldrin	115-32-2	Di- to poly-halogenated alkane or cycloalkane	Halogenated compounds	-	-	-	-	-	-	-
155	C264	Dieldrin	60-87-1	Epoxyde	Epoxydes	+	+	-	+	-	-	+
156	C265	Delphinolamine	111-40-2	Secondary amine	Amines/Amides/imin es	-	-	-	-	-	-	-
157	C266	Di(2-ethylhexyl)adipate	103-23-1	2-Alkylalkane carboxylic acid or precursor	Carboxylic acids	-	-	-	-	-	-	-
158	C269	Di(2-ethylhexyl)phthalate	117-61-7	2-Alkylalkane carboxylic acid or precursor	Carboxylic acids	-	-	-	-	-	-	+
159	C271	Diethylstilbestrol	56-63-1	4,4'-Dihydroxydiphenyl- ethane or -ethene	Phenyl compounds	+	-	-	-	+	+	+
160	C272	Diethylstilbestrol diacetate	132-82-3	Phenyl ester	Phenyl compounds	-	-	-	-	E	-	E
161	C273	N,N-Diethyl-2-thiourea	105-85-6	(Thio)urea	Ureas	-	-	-	-	-	-	+
162	C275	Diglycidyl neocotrol ether, technical grade	101-95-6	Glycidyl ether, amine, ester or acide	Epoxydes	+	-	-	-	-	-	+
163	C277	3,4-Dihydrocoumarin	119-64-6	Phenyl ester	Phenyl compounds	-	+	-	-	E	-	-
164	C281	1,2-Dihydro-2,2,4,4-tetrahydroquinoline	147-47-7	Secondary amine	Amines/Amides/imin es	-	-	-	+	NA	-	NA
165	C282	Dimethoxane	825-00-2	Aldehyde or precursor	Aldehydes	+	-	+	-	-	-	E
166	C284	3,7-Dimethoxyberzidine-4,4-diacetate	91-40-0	Isocyanate or isothiocyanate	Isocyanates	+	-	+	+	+	+	+
167	C285	3,7-Dimethoxyberzidine 2HCl	20325-40-0	Aromatic amine or amide	Aromatic amines or amides	-	-	-	+	+	E	+
168	C287	N,N-Dimethyl-4-aminoazobenzene	60-11-7	Aromatic azo compound	Azo compounds	+	-	-	+	E	+	+
169	C291	N,N-Dimethylcitra	121-69-7	Aromatic amine or amide	Aromatic amines or amides	+	-	-	+	+	+	+
170	C292	7,12-Dimethylberzylanthracene	57-97-6	Bay-region polycyclic aromatic hydrocarbon	Polycyclic aromatic hydrocarbons	+	+	+	-	+	+	+
171	C293	3,7-Dimethylberzidine	119-93-7	Aromatic amine or amide	Aromatic amines or amides	+	-	-	+	+	+	E
172	C295	Dimethylacetamid chloride	79-44-7	Carbonylic acid halide	Carboxylic acids	+	-	-	+	E	+	+
173	C296	1,1-Dimethylhydrazine	57-14-7	Mono- or di-alkylhydrazine	Hydrazines	+	+	-	+	+	+	NA
174	C297	1,2-Dimethylhydrazine 2HCl	308-37-6	Mono- or di-alkylhydrazine	Hydrazines	+	+	-	+	+	+	NA
175	C299	Dimethyl hydrogen phosphite	869-85-9	Phosphorus compound	Phosphorus compounds	+	+	-	+	NA	+	+
176	C305	Dimethylvinyl chloride	513-37-1	Halogenated alkene	Halogenated compounds	-	+	-	+	-	-	+
177	C309	2,4-Dinitrotoluene	121-14-2	Aromatic nitro compound	Aromatic nitro compounds	-	-	E	-	+	-	-
178	C310	2,6-Dinitrotoluene	805-20-2	Aromatic nitro compound	Aromatic nitro compounds	-	-	E	-	E	-	-
179	C312	1,4-Dioxane	123-91-1	Dioxane	Others	-	-	-	+	-	-	+
180	C314	5,5-Dibenzothiazolone	57-41-0	Macellinaceous	Others	-	-	-	+	-	-	E
181	C316	Doyleine succinate	562-10-7	Short chain aliphatic carboxylic acid	Carboxylic acids	-	-	-	+	E	-	-
182	C319	Enchlorbutin	105-89-0	Epoxyde	Epoxydes	+	-	+	+	+	+	+
183	C320	1,2-Epoxybutane	105-85-7	Epoxyde	Epoxydes	+	-	-	+	+	+	+
184	C321	17-B-Estradiol	50-28-2	Hormones	Hormones	-	-	-	-	-	-	+
185	C323	Estrogole	140-67-0	Allylbenzene, propargyl- benzene or 1'-hydroxy derivatives	Benzenes	-	-	-	+	-	E	-
186	C324	Ethinyl estradiol	57-43-6	Ethinyl or analogue	Hormones	-	-	-	-	-	-	-
187	C325	Ethinamate	535-33-4	Thioamide	Amines/Amides/imin es	+	-	+	+	+	+	+
188	C327	DL-Ethionine	67-21-0	Amino acid or derivative	Others	-	-	-	-	NA	-	+
189	C328	o-Ethoxybenzamide	935-73-0	Aromatic amine or amide	Aromatic amines or amides	+	-	-	+	+	-	+
190	C329	Ethyl acrylate	140-85-6	Alpha-, beta-unsaturated ester or thioester (class I or II)	Esters	+	-	+	+	+	+	+
191	C330	Ethyl alcohol	64-17-6	Alcohol	Alcohols	-	-	-	-	NA	NA	NA
192	C333	Ethylbenzene	100-61-4	Benzene	Benzenes	-	-	-	-	-	-	-
193	C334	Ethylene glycol monobutyl ether	111-15-2	Alcohol	Alcohols	-	-	-	-	-	-	-
194	C336	Ethylene oxide	75-21-8	Epoxyde	Epoxydes	-	+	+	+	+	+	E
195	C337	N,N-Ethylmethiourea	96-46-7	(Thio)urea	Ureas	-	-	-	-	+	+	+
196	C340	Ethyl methane sulphate	62-80-0	Alkylating agent	Alkylating agents	+	+	+	+	+	+	+
197	C341	N-Ethyl-N-nitro-N-nitrosourea	63985-23-4	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	+	-	+	+	+	+	+
198	C345	1-Ethyl-N-nitrosourea	759-73-9	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	+	+	+	+	+	+	+
199	C349	FD&C Red 1 (Pontauk 3R)	3954-29-8	Aromatic azo compound	Azo compounds	-	-	-	-	+	-	E
200	C359	5-Fluorouracil	51-21-6	Substituted pyrimidine or purine nucleoside	Others	+	+	+	+	+	+	+
201	C360	Fluvestin	93267-64-1	Alkene	Alkenes	-	-	-	-	+	E	E
202	C361	Formaldehyde	50-00-0	Aldehyde or precursor	Aldehydes	+	-	-	+	+	+	+
203	C366	Fumonisin B1	116395-83-0	Short chain aliphatic carboxylic acid	Carboxylic acids	+	+	-	-	-	-	+
204	C367	Furin	110-05-9	Furin	Others	+	+	+	+	NA	+	-
205	C368	Furfural	98-01-1	Aldehyde or precursor	Aldehydes	+	+	+	+	+	+	-

#	ID	Chemical	CAS No.	Chemical Grouping (CIGX 2007)	Chemical Class	In vitro CA	In vitro E-ANN*	In vitro CA Derek	In vitro CA Avertis	In vitro CA MCase: CA-CHL	In vitro CA MCase: CA-CHO	In vitro MN MCase: MNT-mouse
206	C369	Furfuryl Alcohol	96-00-0	Alcohol	Alcohols	+	-	+	+	+	+	NA
207	C370	Furosemide	54-31-9	Aryl sulfonamide	Amines/Amides/Amides	+	-	-	+	+	+	NA
208	C371	Furylfuramide (AF-2)	3690-53-7	Aromatic nitro compound	Aromatic nitro compounds	+	+	E	+	+	+	+
209	C373	Gentian violet (AKA Hexamethyl-p-rosaniline chloride)	548-63-9	Aromatic amine or amide	Aromatic amines or amides	-	-	+	-	E	-	E
210	C378	Glycidol	585-53-5	Epoxyde	Epoxydes	+	+	+	+	+	+	+
211	C377	Glyoxal	128-07-0	Substituted vinyl ketone	Ketones	+	-	E	+	+	-	+
212	C378	Haloperidol	52-06-0	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	+	+	-	-	E	-	+
213	C379	HC Blue 1 (Impure and purified)	2794-94-3	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	+	+	+	NA
214	C382	Heptachlor	76-44-8	Alkyl halide	Halides	+	-	+	+	+	NA	+
215	C384	Hexachlorobutadiene	87-66-3	Halogenated alkene	Halogenated compounds	-	-	-	-	-	-	-
216	C388	gamma-1,2,3,4,5,6-Hexachlorocyclohexane (AKA Lindane)	50-09-9	Alkylating agent	Alkylating agents	-	-	-	-	-	-	-
217	C389	Hexachlorobutene	87-72-1	Di- to poly-halogenated alkene or cycloalkene	Halogenated compounds	-	-	-	-	-	-	-
218	C392	Hexanamide	628-02-4	Aliphatic amide	Amines/Amides/Amides	-	-	-	-	-	+	E
219	C396	Hydrazine sulphate	10034-93-2	Hydrazine or monoacyl- or monoalkylphosphoryl-hydrazine	Hydrazines	+	+	+	+	+	-	-
220	C400	Hydroquinone	123-65-7	Hydrazine or precursor	Hydrazines	+	-	-	-	NA	+	NA
221	C401	Hydrogen Peroxide	7722-84-1	Hydroperoxide	Others	+	-	-	-	-	-	-
222	C402	Hydroquinone	123-31-9	Phenol or precursor	Phenols	+	+	+	-	+	+	+
223	C403	N-Hydroxy-2-acetylaminofluorene	53-95-2	Aromatic hydroxylamine or ester derivative	Aromatic amines or amides	+	+	+	+	E	+	NA
224	C416	ICRF 159	21416-67-5	Piperazine	Others	-	+	-	-	E	-	+
225	C418	Isobutyl alcohol	5034-32-9	Aliphatic alcohol	Aliphatic alcohols	-	-	-	-	NA	NA	E
226	C419	Isobutyl nitrite	542-66-3	Alkyl nitrite, nitrous acid or nitrite salt	Nitro compounds or nitrites	+	+	-	-	NA	+	+
227	C421	Isonic acid	54-85-3	Hydrazine or monoacyl- or monoalkylphosphoryl-hydrazine	Hydrazines	+	+	+	+	E	E	+
228	C423	Isoflurone	76-69-1	Substituted vinyl ketone	Ketones	+	-	E	-	-	-	E
229	C426	Isonone	76-72-6	Alkene	Alkenes	-	+	-	-	E	-	+
230	C428	Isonone (AKA Chlorozone)	143-50-0	Gem-dihalide	Halides	-	-	+	-	NA	-	NA
231	C427	Isocaripine	303-34-4	Pyroline ester, pyrroline N-oxide ester, pyrrole ester or pyrrole alcohol	Others	+	+	+	-	E	+	+
232	C431	O-Isonone	5989-27-5	Alkene	Alkenes	-	-	-	-	E	-	E
233	C433	Malonaldihyde sodium salt	24362-04-5	Alpha-, beta-unsaturated aldehyde	Aldehydes	-	-	+	+	-	-	-
234	C434	Manganese ethylenebis(carbamate)	12427-38-2	Thiourea disulphide or thiocarbamate	Carbamates	+	+	-	-	NA	NA	+
235	C436	Melanine	105-75-1	Aromatic amine or amide	Aromatic amines or amides	-	-	-	-	+	-	-
236	C437	Melphalan	146-02-3	Aliphatic amide	Aliphatic amides	+	+	+	+	+	+	+
237	C438	2-Mercaptobenzothiazole	146-30-4	Aromatic azo compound	Azo compounds	+	-	-	-	+	+	-
238	C441	Melipex	57-39-6	Adizine or aziridine	Adizines or aziridines	-	+	+	+	NA	NA	+
239	C442	Methapyline hydrochloride	135-23-9	Aromatic amine or amide	Aromatic amines or amides	+	-	-	-	E	+	-
240	C443	Methadathion	990-37-8	Alkyl ester of phosphoric or phosphonic acid	Phosphorous compounds	-	-	-	+	+	+	+
241	C444	Methicillin	60-56-0	(Thio)lactam	Lactams	+	-	-	+	E	NA	+
242	C448	4-Methylphenol (AKA Hydroquinone monomethyl ether)	150-76-6	Phenol or precursor	Phenols	+	+	-	-	E	-	-
243	C449	2-Methylsuccinonitrile	295-61-7	Picoline	Others	+	+	+	+	+	+	+
244	C451	Methylazobenzene	592-62-1	Azo or azoxy compound	Azo compounds	+	-	-	-	+	NA	E
245	C452	alpha-Methylbenzyl alcohol	96-05-1	Alcohol	Alcohols	+	-	-	-	-	+	-
246	C454	Methyl tert-butyl ether	1634-04-1	Ether	Others	-	-	-	-	-	-	-
247	C455	Methyl carbamate	593-85-0	(Thio)carbamate	Carbamates	-	-	-	-	+	-	-
248	C456	4-Methylcatechol	482-85-6	Catechol or precursor	Catechols	+	+	+	+	+	-	+
249	C457	3-Methylcholanthrene	56-49-5	Bay-region polycyclic aromatic hydrocarbon	Polycyclic aromatic hydrocarbons	+	+	+	-	+	-	+
250	C458	Methyl clenafate	21340-68-1	Fibrate	Others	-	-	-	-	+	-	E
251	C460	3-Methyl-4-dimethylaminobenzene	66-20-1	Aromatic amine or amide	Azo compounds	+	-	-	-	+	E	+
252	C462	4,4-Methylenebis(2-chloroaniline)	101-14-4	Aromatic amine or amide	Aromatic amines or amides	+	-	-	+	+	+	+
253	C464	4,4-Methylenebis(N,N-dimethylaniline)	101-61-1	Aromatic amine or amide	Aromatic amines or amides	-	-	+	+	E	-	-
254	C466	4,4-Methylene dianiline 2HCl	13562-44-8	Aromatic amine or amide	Aromatic amines or amides	+	+	E	+	+	+	+
255	C467	Methylugenol	93-15-2	Alkylbenzene, propargyl-, benzene or 1'-hydroxy derivatives	Benzenes	-	-	E	+	E	-	E
256	C472	Methyl methanesulphonate	66-27-3	Aliphatic amide	Aliphatic amides	+	+	+	+	+	+	NA
257	C474	2-Methyl-1-nitroanthraquinone	129-15-7	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	+	+	+	E
258	C476	N-Methyl-N'-nitro-N-nitrosoguanidine	70-25-7	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	+	+	+	+	+	+	+
259	C478	4-(Methylnitrosamino)-1-(3-pyridyl)-1-pyrazole (MNNO)	64061-91-4	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	+	-	-	-	+	+	+
260	C484	Methylnitrosocyanamide	33968-17-6	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	+	+	+	+	+	+	+
261	C487	N-Methylglycyamide	924-62-5	N-methylol derivative	Others	+	-	-	-	+	+	+
262	C488	Methylphenolate HCl	295-59-9	Secondary amine	Amines/Amides/Amides	+	-	-	+	+	+	-
263	C489	Metronidazole	443-45-1	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	+	E	NA	+
264	C492	Mitomycin C	50-07-7	Adizine or aziridine	Adizines or aziridines	+	+	+	+	+	+	+
265	C494	Monoacetyl hydrazine	1056-57-1	Hydrazine or monoacyl- or monoalkylphosphoryl-hydrazine	Hydrazines	+	+	+	-	E	NA	+
266	C496	Monocrobaline	315-22-0	Pyroline ester, pyrroline N-oxide ester, pyrrole ester or pyrrole alcohol	Others	+	+	E	+	E	+	+
267	C496	Nalafenol	3771-19-5	Benzene	Benzenes	-	-	-	-	+	E	-
268	C499	Nalidixic acid	309-05-2	Quinolone-3-carboxylic acid or naphthyridine analogue	Carboxylic acids	+	-	-	-	+	-	-
269	C500	Naphthalene	91-20-3	Benzene	Benzenes	+	-	-	+	+	+	+
270	C501	1,5-Naphthalenediamine	2243-82-1	Aromatic amine or amide	Aromatic amines or amides	+	-	-	+	+	+	-
271	C502	2-Naphthylamine	91-69-8	Aromatic amine or amide	Aromatic amines or amides	+	-	-	-	+	+	+

#	ID	Chemical	CAS No.	Chemical Grouping (DQX 2007)	Chemical Class	In vitro CA	In vivo E-MN*	In vitro CA Derek	In vitro CA Aroclor	In vitro CA MCase: CA-CHL	In vitro CA MCase: CA-CHO	In vitro MN MCase: MNT-mouse
272	C505	Nitrazide	139-94-6	Aromatic nitro compound	Aromatic nitro compounds	-	-	E	+	E	-	+
273	C506	Nitroacetic acid	139-13-9	Nitrite	Nitrite	-	-	-	-	-	-	-
274	C509	Nitric acidum	7632-00-0	Alkyl nitrite, nitrous acid or nitrite salt	Nitro compounds or nitrite	-	-	+	+	NA	+	+
275	C510	5-Nitroacenaphthene	602-67-9	Aromatic nitro compound	Aromatic nitro compounds	-	-	E	-	+	E	-
276	C512	5-Nitro- <i>o</i> -enolidine	99-89-2	Aromatic nitro compound	Aromatic nitro compounds	-	-	E	+	+	-	-
277	C513	<i>o</i> -Nitroanisole	91-23-6	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	-	+	-	-
278	C514	Nitrobenzene	98-96-3	Aromatic nitro compound	Aromatic nitro compounds	-	-	-	-	+	-	-
279	C515	6-Nitrobenzimidazole	94-82-0	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	+	+	+	-
280	C516	<i>p</i> -Nitrobenzoic acid	62-23-7	Aromatic nitro compound	Aromatic nitro compounds	+	-	+	+	+	+	E
281	C518	Nitrofen	1836-75-5	Aromatic nitro compound	Aromatic nitro compounds	-	-	E	-	+	-	E
282	C519	5-Nitro-2-furandehyde semicarbazone (AKA Nitrofurazone)	59-87-0	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	+	+	+	+
283	C520	1-(5-Nitrofururylidene)amino]hydantoin (AKA Nitrofurantoin)	67-30-9	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	+	+	+	+
284	C530	Nitrogen mustard	51-75-2	Alkylating agent	Alkylating agents	+	+	-	-	+	+	+
285	C533	Nitromethane	75-52-6	Aliphatic nitro	Nitro compounds or nitrite	+	-	-	-	E	-	-
286	C534	2-Nitro- <i>p</i> -phenylenediamine	5307-14-2	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	+	+	+	E
287	C535	1-Nitropyrene	5522-43-0	Aromatic nitro compound	Aromatic nitro compounds	+	+	+	+	+	-	+
288	C537	4-Nitroquinoline-N-oxide	56-87-6	Aromatic N-oxide or N-hydroxy butomer	Others	+	+	E	+	+	+	+
289	C549	Nitroacetylbutylamine	924-16-3	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	-	-	-	-	+	+	+
290	C550	N-Nitrosodiphenylamine	1116-54-7	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	-	-	+	-	+	+	+
291	C551	N-Nitrosodiphenylamine (diethylnitrosamine)	55-18-6	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	-	-	+	-	+	+	+
292	C556	N-Nitrosodimethylamine (dimethylnitrosamine)	62-75-9	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	+	+	-	-	+	+	+
293	C558	N-Nitrosodiphenylamine	86-30-6	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	-	-	+	+	+	+	+
294	C559	<i>p</i> -Nitrosodiphenylamine	156-10-6	Aromatic nitro compound	Aromatic nitro compounds	+	-	+	E	+	+	+
295	C560	N-Nitrosodipropylamine	621-64-7	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	-	-	+	+	+	+	+
296	C563	Nitrosodimethylamine	10596-96-6	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	-	-	+	+	+	+	+
297	C567	N-Nitroso-N-methylurea	66493-5	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	+	+	+	+	+	+	+
298	C568	N-Nitrosomorpholine	59-89-2	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	-	-	+	+	+	+	+
299	C563	N-Nitrosopiperidine	105-75-4	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	-	-	+	-	+	+	+
300	C594	N-Nitrosopyrrolidine	905-65-2	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	-	-	+	-	+	+	+
301	C602	5-Nitro- <i>o</i> -toluidine	99-85-8	Aromatic nitro compound	Aromatic nitro compounds	+	-	E	+	+	+	-
302	C604	Oxazolin A	303-47-9	Macrolactone	Others	-	-	-	-	-	-	-
303	C605	Oxazepam	604-75-1	Aromatic amine or amide	Aromatic amines or amides	-	-	-	-	NA	-	-
304	C606	4,4'-Oxydianiline	101-80-4	Aromatic amine or amide	Aromatic amines or amides	+	+	-	+	+	+	+
305	C609	N-Oxydethylene bis(carbamyl-N-oxydethylene sulphamide)	13752-61-7	Thiol or thiol exchange agent	Others	+	-	+	+	NA	+	+
306	C610	Oxymethole	434-07-1	Alpha-, beta-unsaturated aldehyde	Aldehydes	-	-	+	-	NA	-	NA
307	C611	Ozone	10028-15-6	Macrolactone	Others	+	-	-	+	NA	NA	NA
308	C612	Pentachloroantone	1825-21-4	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	-	-	-	+	-	-	-
309	C613	Pentachloroethane	78-01-7	Gem-dihalide	Halides	+	-	-	-	+	-	-
310	C614	Pentachloronitrobenzene	62-46-6	Aromatic nitro compound	Aromatic nitro compounds	-	-	E	+	E	-	-
311	C617	Pentaerlene	60102-37-6	Epoxide	Epoxides	+	-	E	+	+	+	+
312	C618	Phenacetin	62-44-2	Aromatic amine or amide	Aromatic amines or amides	+	+	-	+	+	-	+
313	C620	Phenazopyridine HCl	136-40-3	Aromatic azo compound	Azo compounds	+	+	-	-	+	+	+
314	C622	Phenobarbital	50-06-6	(Thio)urea	Ureas	+	+	-	-	+	+	+
315	C624	Phenolphthalein	77-49-6	Phenol or precursor	Phenols	+	+	-	-	+	+	+
316	C625	Phenocycbenzamine HCl	63-60-3	Alkylating agent	Alkylating agents	+	-	-	+	+	+	-
317	C626	Phenylbutazone	50-33-9	Hydrazine or precursor	Hydrazines	+	-	-	+	+	+	+
318	C627	1-Phenyl-3,3-dimethylbutane	7227-91-0	Antidiabetic agent	Others	+	+	-	-	+	+	+
319	C630	Phenylglycidyl ether	122-60-1	Glycidyl ether, amine, ester or amide	Epoxides	-	+	+	+	+	-	+
320	C631	Phenylhydrazine HCl	59-86-1	Arylhydrazine or N-oxide heterocycle	Hydrazines	+	+	+	+	+	NA	+
321	C633	<i>o</i> -Phenyphenol	90-43-7	Phenol or precursor	Phenols	+	-	-	-	+	-	+
322	C635	Piperonal butoxide	91-20-9	Benzodioxole	Others	-	-	-	-	E	-	+
323	C636	Piperonyl butoxide	120-60-7	Benzodioxole	Others	-	-	-	-	E	-	E
324	C638	Polybrominated biphenyl mixture	67774-32-7	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	-	-	-	+	E	-	E
325	C642	Pitracicline (primidone)	125-33-7	Formaldehyde donor	Others	-	-	-	+	E	-	-
326	C643	Probenecid	57-96-9	Benzene	Benzenes	-	-	-	-	-	-	E
327	C646	Progesterone HCl (Nabufen)	365-10-1	Mono- or di-alkylhydroxide	Hydroxides	-	+	+	-	NA	NA	+
328	C646	Progesterone	87-63-0	Hormone	Hormones	-	-	-	-	-	-	-
329	C647	Propene sulfone	1120-71-4	Alkylating agent	Alkylating agents	+	+	-	+	+	+	NA
330	C648	beta-Proiolactone	87-57-8	Beta-lactone	Others	+	-	-	-	+	+	+
331	C649	1,2-Propylene oxide	75-66-9	Epoxide	Epoxides	+	+	+	+	+	+	+
332	C652	N-Propyl-N-nitro-N-nitrosoguanidine	13010-07-6	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	-	-	-	-	-	-	-
333	C653	N-Propyl-N-nitrosourea	816-67-9	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	+	+	+	+	+	+	+
334	C655	Pertidine	110-95-1	Pertidine	Others	-	-	-	-	-	-	-
335	C656	Pyrimine maleate	59-33-6	Aromatic amine or amide	Aromatic amines or amides	-	-	-	-	E	-	-
336	C657	Pyrimethamine	58-14-0	Aromatic amine or amide	Aromatic amines or amides	+	+	+	+	+	+	E

#	ID	Chemical	CAS No.	Chemical Grouping (CGX 2007)	Chemical Class	In vitro CA	In vivo E-MN*	In vitro CA Derek	In vitro CA Aroclor	In vitro CA MCase: CA-CHL	In vitro CA MCase: CA-CHO	In vitro MN MCase: MN1-mouse
337	C856	Quercetin	117-39-6	Flavonol	Others	+	-	+	+	+	+	-
338	C859	p-Gulonic dioxime	105-11-3	Oxime	Others	+	-	-	+	+	+	-
339	C860	Resorcinol	90-98-6	Phenol or precursor	Phenols	-	+	-	-	-	-	+
340	C861	Resorcinol acetate	127-67-9	Resorcinol or precursor	Others	+	-	-	-	-	E	+
341	C864	Saccharin, sodium	128-44-9	Aryl sulfonamide	Amines/Amides/Imine	-	-	-	+	-	-	E
342	C865	Safrole	94-69-7	Alylbenzene, propargyl- benzene or 1'-hydroxy derivatives	Benzenes	+	-	+	+	+	-	E
343	C874	Drepanolololol	18803-86-4	N-nitro or N-nitroso compound	N-nitro or N-nitroso compounds	-	+	+	+	+	+	+
344	C876	Styrene	100-42-6	Alkene	Alkenes	+	+	-	+	+	-	+
345	C877	Styrene oxide	96-09-3	Epoxyde	Epoxydes	+	-	+	+	+	+	+
346	C878	Succinic anhydride	108-30-6	Carboxylic acid anhydride	Others	-	-	-	-	-	-	-
347	C880	Sulfamerazine	57-66-1	Aromatic amine or amide	Aromatic amines or amides	-	-	-	+	+	-	+
348	C893	6X Purple	2611-60-7	Aromatic am compound	Azo compounds	-	-	-	-	-	-	+
349	C895	Tamoxifen citrate	54965-34-1	Macrolactone	Others	-	+	-	-	-	-	E
350	C897	Testosterone	58-22-0	Hormones	Hormones	-	-	-	-	-	E	-
351	C899	2,3,7,8-Tetrachlorodibenzo-p-dioxin	1746-01-6	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	-	-	-	-	+	-	+
352	C890	1,1,1,2-Tetrachloroethane	630-30-6	Alkylating agent	Alkylating agents	+	+	-	-	-	-	+
353	C891	1,1,2,2-Tetrachloroethane	79-34-6	Gas-diluent	Halides	-	+	-	-	E	-	+
354	C892	Tetrachloroethylene	127-18-4	Halogenated alkene	Halogenated compounds	-	-	-	-	-	-	-
355	C893	Tetrachlorovinphos	961-11-6	Alkyl ester of phosphoric or phosphonic acid	Phosphorus compounds	-	-	-	+	+	-	+
356	C894	12-O-Tetradecanoylphorbol 13-acetate	16561-36-6	Substituted vinyl ketone	Ketones	+	-	-	-	-	E	+
357	C896	Tetrahydrofuran	108-99-9	Furan	Others	-	-	-	+	-	-	-
358	C896	Tetrahydrofuran	509-14-0	Aliphatic nitro	Nitro compounds or nitriles	+	-	-	-	E	+	NA
359	C899	Thioacetamide	62-55-6	Thioamide	Amines/Amides/Imine	-	+	-	-	-	NA	+
360	C700	4,4-Thiodianiline	134-65-1	Aromatic amine or amide	Aromatic amines or amides	+	-	-	+	+	+	+
361	C702	Thio-tpa	52-24-4	Adrine or azidine	Adrines or azidines	+	+	+	+	+	+	+
362	C704	Thiourea	62-56-6	(Thiourea)	Ureas	-	-	-	-	-	-	+
363	C706	Toluene	108-88-3	Benzene	Benzenes	-	+	-	-	-	-	-
364	C707	2,4-Toluene diisocyanate	50-40-0	Isocyanate or isothiocyanate	Isocyanates	-	-	-	-	-	-	E
365	C709	o-Toluenesulfonamide	80-19-7	Aryl sulfonamide	Amines/Amides/Imine	-	-	-	-	-	-	-
366	C711	o-Toluidine	95-63-4	Aromatic amine or amide	Aromatic amines or amides	+	+	E	+	+	-	-
367	C716	Trenimon	60-76-6	Adrine or azidine	Adrines or azidines	+	+	+	+	E	+	+
368	C718	Triacetene	395-01-0	Aromatic amine or amide	Aromatic amines or amides	+	-	+	+	+	-	E
369	C719	Tribromomethane	75-25-2	Halogenated methane	Halogenated compounds	+	-	+	+	+	-	-
370	C720	Trichloroacetic acid	76-03-9	Di- to poly-halogenated alkane or cycloalkane	Halogenated compounds	-	-	-	-	-	-	-
371	C722	1,1,2-Trichloroethane	79-00-6	Alkylating agent	Alkylating agents	+	-	-	-	+	+	NA
372	C723	Trichloroethylene (with and without epichlorohydrin)	79-01-6	Halogenated alkene	Halogenated compounds	-	-	-	-	-	-	E
373	C724	N-Trichloromethylphthalimide	133-07-3	Potentially labile halogen	Halogenated compounds	+	+	+	+	E	-	E
374	C725	2,4,6-Trichlorophenol	88-06-2	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	-	+	+	+	-	-	E
375	C726	1,2,3-Trichloropropane	96-18-4	vic-Dihalide	Halides	+	+	-	-	+	+	NA
376	C727	Triethanolamine	102-71-6	Ethanolamine	Amines/Amides/Imine	-	-	-	-	-	-	-
377	C729	Trifluorin, technical grade	1562-09-8	Aromatic nitro compound	Aromatic nitro compounds	-	-	E	-	-	-	-
378	C730	2,4,5-Trimethyleniline	137-17-7	Aromatic amine or amide	Aromatic amines or amides	+	-	E	+	+	+	-
379	C733	1,2,4-Trimethylbenzene	95-63-6	Benzene	Benzenes	-	-	-	-	-	-	+
380	C734	Trimethylphosphate	513-56-1	Alkyl ester of phosphoric or phosphonic acid	Phosphorus compounds	-	+	-	+	-	+	+
381	C736	Trimethylthiourea	2489-77-2	(Thiourea)	Ureas	-	-	-	+	E	-	+
382	C738	TriO-chloromethylphosphate	115-96-6	Alkylating agent	Alkylating agents	-	+	+	+	+	-	E
383	C740	TriO,3-dimercaptosulfonophosphate	126-73-7	vic-Dihalide	Halides	+	+	+	+	+	+	+
384	C741	TriO-ethylhexylphosphate	76-40-2	Alkyl ester of phosphoric or phosphonic acid	Phosphorus compounds	-	-	-	-	-	-	-
385	C744	Urethane	51-79-6	Alkyl carbamate	Carbamates	-	+	+	-	-	-	+
386	C746	Vinyl acetate	108-05-4	Enol ether	Others	-	-	-	+	NA	NA	+
387	C747	Vinyl bromide	593-60-2	Halogenated alkene	Halogenated compounds	-	-	-	+	NA	NA	NA
388	C748	Vinyl carbamate	15905-73-9	Vinyl carbamate	Carbamates	-	+	+	-	NA	NA	+
389	C749	Vinyl chloride	75-01-4	Halogenated alkene	Halogenated compounds	-	+	-	+	NA	+	+
390	C750	4-Vinylcyclohexane	100-45-3	Alkene	Alkenes	-	-	-	+	-	-	-
391	C751	Vinylidene chloride (1,1-Dichloroethylene)	75-35-4	Alkene	Alkenes	-	-	-	+	+	-	-
392	C754	Zearalenone	17904-92-4	Beactinol or precursor	Beactinols	+	+	-	-	E	+	+
393	C755	Zinc dimethyldithiocarbamate (Zinc)	137-30-4	(Thio)carbamate	Carbamates	+	+	+	-	E	+	+
394	C756	Zinc ethylenedithiocarbamate (Zinc)	12122-67-7	Thium disulfide or dithiocarbamate	Carbamates	-	+	-	-	NA	NA	+

*: Erythrocyte MN test with bone marrow or peripheral blood

Appendix 2 Results of analysis from 3 in silico models for in vitro chromosomal aberrations (CA) to non-carcinogens

#A	ID	Chemical	CAS No.	Chemical Grouping (CGX 2007)	Chemical Class	In vitro CA	In vitro E-MN*	In vitro CA Deriv	In vitro CA Azo/ox	In vitro CA MCas: CA-CHL	In vitro CA MCas: CA-CHO	In vitro MN MCas: MNT-mouse
1	NC1	Acetohexamide	968-81-0	Aryl sulphonamide	Amines/Amides/Amides	+	-	-	+	-	-	E
2	NC2	Acetonitrile [AKA ethyl nitrile]	75-05-8	Nitrile	Nitriles	-	+	-	-	NA	-	+
3	NC3	Acrolein	107-02-8	Alpha, beta-unsaturated aldehyde	Aldehydes	-	-	-	+	E	-	NA
4	NC8	Aldicarb	116-06-3	(Thio)carbamate	Carbamates	-	-	-	-	NA	-	NA
5	NC8	d-Amphetamine sulfate	60-13-0	Amine	Amines/Amides/Amides	-	+	-	-	-	-	+
6	NC9	Anipollin trihydrate	7177-48-2	Ring-strained amide, ester thioamide or thioester	Amines/Amides/Amides	-	-	-	+	NA	-	-
7	NC10	Anisole	101-05-3	Potentially labile halogen	Halogenated compounds	-	-	-	+	E	-	-
8	NC12	o-Arthralic acid	118-62-3	Aromatic amine or amide	Aromatic amines or amides	-	-	-	-	+	E	-
9	NC13	Ascorbic acid	50-81-7	Carboxylic acid	Carboxylic acids	-	+	-	-	-	-	+
10	NC17	Benzoate, sodium	532-32-1	Benzene	Benzenes	+	-	-	-	-	E	+
11	NC18	Benzoin	119-52-9	(Diary) ketone	Ketones	-	-	-	+	+	-	E
12	NC19	1H-Benzothiazole	65-14-7	Benzene	Benzenes	+	-	-	+	+	-	+
13	NC20	Benzyl alcohol	100-51-6	Alcohol	Alcohols	-	+	-	-	-	-	+
14	NC23	Bromomethane	74-83-9	Alylating agent	Alylating agents	-	+	+	+	-	-	+
15	NC24	n-Butyl chloride	109-69-3	Alylating agent	Alylating agents	-	+	+	+	-	-	+
16	NC26	gamma-Butyrolactone	96-48-0	Miscellaneous	Others	-	-	-	-	-	+	-
17	NC27	Caffeine	58-08-2	Substituted pyrimidine or purine	Others	+	+	+	+	+	-	-
18	NC28	Carbolactam	105-60-2	Lactam	Others	-	-	-	-	-	-	-
19	NC29	Carbonyl	77-85-8	Halobalene	Halogenated compounds	+	-	-	+	+	E	+
20	NC31	4-(Chloroacetyl)-acetamide	140-49-8	Alylating agent	Alylating agents	+	+	+	+	+	+	E
21	NC32	p-Chloroaniline	106-47-8	Aromatic amine or amide	Aromatic amines or amides	+	-	-	+	+	+	+
22	NC33	o-Chlorobenzaldehyde [AKA malonitrile, o-chlorobenzylidene]	2696-41-1	Alpha, beta-unsaturated nitrile	Nitriles	+	-	+	-	E	+	NA
23	NC35	(2-Chloroethyl)trimethylammonium chloride	299-81-5	Alylating agent	Alylating agents	-	+	-	-	+	-	-
24	NC36	2-(Chloromethyl)pyridine HCl	6290-47-3	Alylating agent	Alylating agents	-	+	-	-	+	-	-
25	NC38	Chlorpheniramine maleate	113-22-8	Pyridine	Others	+	-	-	-	E	+	E
26	NC39	Chlorpropamide	94-20-2	Aryl sulphonamide	Amines/Amides/Amides	-	-	-	-	-	-	+
27	NC40	C.I. acid orange 10	1936-15-8	Aromatic azo compound	Azo compounds	+	-	-	-	E	-	+
28	NC41	C.I. food red 3 [AKA Acid red 14]	3567-80-9	Aromatic azo compound	Azo compounds	-	-	-	-	+	-	E
29	NC42	C.I. pigment red 23 [AKA pigment red 23]	6471-40-4	Aromatic nitro compound	Aromatic nitro compounds	-	-	-	E	-	-	+
30	NC43	C.I. pigment yellow 12	6398-85-6	Azo or azoxy compound	Azo compounds	-	-	-	-	E	-	+
31	NC44	Codaine	76-67-3	Miscellaneous	Others	-	-	-	-	-	-	E
32	NC45	Coumaphos	56-72-4	Alkyl ester of phosphoric or phosphonic acid	Phosphorous compounds	-	-	-	+	+	+	+
33	NC46	Cyanamide, calcium	156-62-7	Cyanate, cyanamide or cyanogen halide	Others	-	-	-	+	NA	-	NA
34	NC47	Cyclohexanone	108-94-1	(Diary) ketone	Ketones	-	-	-	-	-	-	-
35	NC49	Deltamethrin	52919-83-5	Halogenated alkene	Halogenated compounds	-	+	-	-	NA	-	+
36	NC50	Diallyl phthalate	131-17-9	Phthalate	Phthalates	+	-	-	-	-	-	-
37	NC52	2,6-Diaminotoluene 2HCl	15481-70-6	Aromatic amine or amide	Aromatic amines or amides	-	-	-	+	+	+	+
38	NC53	2,5-Diaminotoluene sulfate	6380-80-1	Aromatic amine or amide	Aromatic amines or amides	+	-	+	+	+	+	E
39	NC54	Diazinon	333-41-5	Alkyl ester of phosphoric or phosphonic acid	Phosphorous compounds	+	+	-	-	+	-	+
40	NC56	1,2-Dichlorobenzene	95-60-1	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	-	-	-	-	E	-	-
41	NC59	1,1-Dichloroethane	75-34-3	Gem-dihalide	Halides	-	+	-	-	-	-	+
42	NC60	2,4-Dichlorophenol	120-83-2	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	+	-	+	-	+	-	E
43	NC61	N,N-Dicyclohexylthiourea	1212-28-9	Thiol or thiol exchange agent	Others	-	-	-	-	-	-	+
44	NC62	Dialdin, photo-	13366-73-0	Epoxide	Epoxides	-	-	-	+	E	-	-
45	NC63	Dimethoate	60-61-8	Alkyl ester of phosphoric or phosphonic acid	Phosphorous compounds	+	+	+	+	+	+	+
46	NC64	Dimethoate, commercial grade [AKA acetic acid ester with 2,5-dimethyl-n-dioxan-4-ol]	625-00-2	Aldehyde or precursor	Aldehydes	+	+	-	-	-	+	E
47	NC65	2,4-Dimethoxyaniline HCl	54150-89-5	Aromatic amine or amide	Aromatic amines or amides	+	-	-	+	+	+	-
48	NC67	Dimethylformamide	68-12-2	Aldehyde or precursor	Aldehydes	-	-	-	+	NA	-	-
49	NC68	Dimethyl sebacate	120-51-6	Phthalate	Phthalates	-	-	-	-	-	-	E
50	NC69	Dioxathion [AKA phosphorothioic acid, 5,5-p-dioxane-2,3-diylo-0,0',0'-trisethyl ester]	78-34-2	Alkyl ester of phosphoric or phosphonic acid	Phosphorous compounds	-	-	-	-	+	-	-
51	NC70	Diphenhydramine HCl	147-24-0	Miscellaneous	Others	+	+	+	-	-	-	-
52	NC71	Diphenyl-p-phenylenediamine	74-31-7	Secondary amine	Amines/Amides/Amides	-	-	-	+	+	+	+
53	NC72	2,5-Dithioburea	142-46-1	Hydrazine or precursor	Hydrazines	-	-	-	-	NA	-	+
54	NC73	EDTA, sodium salt trihydrate	446-34-9 69501-25-0	Carboxylic acid	Carboxylic acids	-	-	-	-	-	-	-
55	NC74	Endrin	72-20-8	Epoxide	Epoxides	-	-	-	-	-	-	-
56	NC75	Ephedrine sulphate	134-72-5	Secondary amine	Amines/Amides/Amides	-	-	-	-	-	-	-
57	NC77	Erythromycin stearate	643-22-1	Aldehyde or precursor	Aldehydes	-	+	-	-	-	-	E
58	NC79	p,p'-Ethyl-DDD [AKA pethane]	72-66-0	Gem-dihalide	Halides	-	-	-	-	E	-	-
59	NC80	Ethyl telluride	20941-85-5	Thiazum disulphide or dithiocarbamate	Carbamates	+	+	+	NA	NA	E	+
60	NC81	Etholeic	41340-28-4	Carboxylic acid	Carboxylic acids	-	-	-	-	+	E	-
61	NC82	Eugenol	97-83-0	Catechol or precursor	Catechols	+	-	+	+	+	+	-

#A	ID	Chemical	CAS No.	Chemical Grouping (COX 2007)	Chemical Class	In vitro CA	In vivo E-MN*	In vitro CA Derek	In vitro CA Aowora	In vitro CA MCase: CA-CHL	In vitro CA MCase: CA-CHO	In vitro MN MNT-mouse
62	NC84	FD & C red no. 3 [AKA fluorescein, 2, 4, 5, 7-tetraiodo, disodium salt]	16423-88-0	Polyhalogenated aromatic	Polyhalogenated aromatic compounds	+	-	-	+	+	NA	E
63	NC85	FD & C yellow no. 5 [AKA tartrazine]	1934-21-0	Azo or azoxy compound	Azo compounds	+	-	-	+	+	-	+
64	NC86	FD & C yellow no. 6 [AKA Food yellow 3]	2783-94-0	Aromatic azo compound	Azo compounds	-	-	-	+	+	-	+
65	NC87	Paraminoudf. formulated [AKA p-dimethylaminobenzenediazo sulphonic acid, sodium salt]	140-66-7	Aromatic amine or amide	Aromatic amines or amides	-	-	-	+	E	-	E
66	NC88	Parthion	55-38-9	Alkyl ester of phosphoric or phosphonic acid	Phosphorous compounds	+	-	-	+	+	-	+
67	NC89	Fenvalerate [AKA cyano-3-phenoxyphenylmethyl-4-chloro-alpha-1-methoxyhydrobenzoin acetate]	51630-58-1	Nitrile	Nitriles	+	+	-	-	NA	+	+
68	NC90	Fluometuron [AKA urea, 1,1-dimethyl-3-(alpha, alpha, alpha-trifluoro-methyl)-]	2164-17-2	(Thio)urea	Ureas	-	-	-	+	E	-	E
69	NC95	HC blue no. 2 [AKA ethanol, 2,2'-(4-(2-hydroxyethylamino)-3-nitrophenylimino)di-]	33229-34-4	Aromatic nitro compound	Aromatic nitro compound	-	-	E	-	+	-	-
70	NC96	HC yellow 4	58920-43-8	Aromatic nitro compound	Aromatic nitro compound	-	-	E	-	+	-	E
71	NC97	Hexachlorocyclopentadiene	77-47-4	Gem-dihalide	Halides	+	-	-	+	+	+	+
72	NC100	4-Hexylresorcinol	136-77-6	Resorcinol or precursor	Resorcinols	-	-	-	-	+	-	-
73	NC101	Hydrochlorothalide	58-93-6	Aryl sulphamide	Amines/Amides/Amines	-	-	-	+	+	-	NA
74	NC102	B-hydroxyquinoline [AKA B-quinolone]	146-24-3	Quinoline	Quinolines	+	-	-	+	+	+	+
75	NC103	Iodoform [AKA methane, triiodo-]	75-47-8	Halogenated methane	Halogenated compounds	-	-	E	+	NA	-	NA
76	NC104	Isopropyl-N-(3-chlorophenyl)carbamate	101-21-3	Alkyl carbamate	Carbamates	-	-	+	-	-	-	E
77	NC106	4,4'-isopropylidenediphenol	80-06-7	Biphenol or precursor	Others	+	-	-	-	E	-	-
78	NC106	Lead dimethylthiocarbamate	19010-66-3	(Thio)carbamate	Carbamates	+	-	+	+	E	+	+
79	NC108	Lithocholic acid	434-13-9	Short chain aliphatic carboxylic acid	Carboxylic acids	+	-	-	-	+	-	-
80	NC111	Malathion	7121-75-5	Alkyl ester of phosphoric or phosphonic acid	Phosphorous compounds	+	+	+	+	+	+	+
81	NC112	Malic hydrazide	123-33-1	Hydrazine or precursor	Hydrazines	-	-	-	+	NA	+	NA
82	NC114	3-Mercapto	8048-6	Miscellaneous	Others	-	-	-	-	-	-	E
83	NC115	Methoxycarbonyl	59-08-2	Aromatic amine or amide	Aromatic amines or amides	+	+	+	-	-	+	+
84	NC116	Methoxychlor	72-43-6	Di- to poly-halogenated alkane or cycloalkane	Halogenated compounds	-	-	-	-	-	-	-
85	NC118	Methyl methacrylate	80-02-6	Alpha-, beta-unsaturated ester or thioester (class II or III)	Esters	+	-	+	+	E	+	-
86	NC119	Methyl parathion [AKA phosphorothioic acid, O, O-dimethyl o-(p-nitrophenyl)water]	298-00-0	Alkyl ester of phosphoric or phosphonic acid	Phosphorous compounds	-	+	E	+	+	-	E
87	NC120	Monochloroacetic acid	79-11-6	Alkylating agent	Alkylating agents	-	+	+	-	-	-	+
88	NC121	N-(1-Naphthyl)ethylenediamine 2HCl [AKA PL-80776]	1485-25-4	Secondary amine	Amines/Amides/Amines	+	-	-	+	+	+	+
89	NC123	p-Nitroaniline	100-01-6	Aromatic nitro compound	Aromatic nitro compound	+	-	E	+	+	+	+
90	NC124	4-Nitrobenzoic acid	619-17-0	Aromatic nitro compound	Aromatic nitro compound	-	-	E	+	+	+	-
91	NC125	3-Nitro-4-hydroxyphenylacetic acid (AKA roxarsone)	121-19-7	Aromatic nitro compound	Aromatic nitro compound	-	-	-	NA	+	NA	NA
92	NC126	1-Nitronaphthalene	86-67-7	Aromatic nitro compound	Aromatic nitro compound	+	-	E	+	+	+	+
93	NC127	4-Nitro-o-phenylenediamine	99-56-9	Aromatic nitro compound	Aromatic nitro compound	+	-	E	+	+	-	+
94	NC133	Cyclotriazine HCl	2096-86-0	Substituted vinyl ketone	ketones	-	+	-	-	E	-	-
95	NC134	Parathion	56-38-2	Alkyl ester of phosphoric or phosphonic acid	Phosphorous compounds	-	-	E	+	+	-	E
96	NC135	Penicillin VK	132-98-9	6-aminocaprylic acid or precursor	Carboxylic acids	+	-	-	+	NA	-	-
97	NC136	Pentawortol inbenzate with 80% d-lactose monohydrate	78-11-6	Alcohol	Alcohols	-	-	-	+	E	-	NA
98	NC137	Phenformin HCl	834-25-6	Miscellaneous	Others	-	-	-	-	E	-	+
99	NC138	Phenol	108-95-2	Phenol or precursor	Phenols	+	+	-	-	-	+	+
100	NC139	p-Phenylenediamine 2HCl	624-18-0	Aromatic amine or amide	Aromatic amines or amides	+	-	+	+	+	+	+
101	NC140	Phenylephrine HCl	61-78-7	Secondary amine	Amines/Amides/Amines	-	-	-	+	NA	-	+
102	NC141	1-Phenyl-3-methyl-5-pyrazolone	89-25-6	Hydrazine or precursor	Hydrazines	-	-	-	+	+	-	E
103	NC144	1-Phenyl-2-thiourea	103-85-5	Aromatic azo compound	Azo compounds	-	-	-	-	-	+	+
104	NC145	Phthalimide	88-06-0	Aromatic amine or amide	Aromatic amines or amides	-	-	-	+	-	-	+
106	NC146	Phthalic anhydride	88-44-9	Cyclic acid anhydride	Others	+	-	-	-	E	-	E
108	NC149	Promethazine HCl	58-33-3	Aromatic amine or amide	Aromatic amines or amides	-	-	-	-	-	-	-
107	NC150	Propylene [AKA propene]	115-07-1	Alkene	Alkenes	-	-	-	+	-	-	-
108	NC151	Propyl galate	121-79-9	Catechol or precursor	Catechols	+	+	+	+	+	+	+
109	NC152	Resorcinol	108-46-3	Resorcinol or precursor	Resorcinols	-	-	-	-	+	+	+
110	NC153	Rhodamine 6G [AKA basic red 1]	989-38-8	Aromatic amine or amide	Aromatic amines or amides	-	-	-	-	+	+	+
111	NC154	Selenone	83-78-4	Coumarin	Others	-	-	-	-	+	-	+
112	NC155	Sodium chloride	7782-18-2	Alkali, alkali earth, metal salt	Alkali, metal salts	+	+	+	+	NA	NA	NA
113	NC156	Sodium diethyldithiocarbamate trihydrate [AKA carbamic acid, diethylthio, sodium salt]	146-35-5 20924-25-3	(Thio)carbamate	Carbamates	-	-	+	-	NA	-	+
114	NC157	Sodium hypochlorite	7681-52-9	Alkali, alkali earth, metal salt	Alkali, metal salts	-	-	+	-	-	-	-
115	NC158	Sorbic acid	110-44-1	Carboxylic acid	Carboxylic acids	-	-	-	+	-	-	+
116	NC160	Sulfisoxazole	127-69-5	Aromatic amine or amide	Aromatic amines or amides	-	-	-	+	-	-	-
117	NC161	3-Subtlene	77-79-2	Miscellaneous	Others	-	-	-	+	NA	-	-
118	NC164	Tetracycline HCl	54-75-8	Substituted vinyl ketone	ketones	+	-	-	-	E	-	+
119	NC165	Tetraethylthiuram disulfide [AKA disulfide, bis(dialkylthiocarbonyl)]	97-77-8	Thiuram disulfide or dithiocarbamate	Carbamates	+	+	+	-	-	+	+

[注] NC144 の 1-Phenyl-2-thiourea は、Azo compd とクラス分類しているが、Urea に変更

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#A	ID	Chemical	CAS No.	Chemical Grouping (CGX 2007)	Chemical Class	In vitro CA	In vivo E-MN*	In vitro CA Derek	In vitro CA Aroclor	In vitro CA MCas: CA-CHL	In vitro CA MCas: CA-CHO	In vivo MN MCas: MNT-mouse
120	NC166	1- <i>trans</i> - <i>cis</i> -8- <i>β</i> -Tetrahydrocannabinol	1972-08-3	Reacrolin or precursor	Reacrolin		+	-	-	+	-	+
121	NC167	Tetraakis(hydroxymethyl)phosphonium chloride	124-84-1	Phosphorus compound	Phosphorous compounds	+	-	-	-	NA	+	NA
122	NC169	Tetramethylthiuram disulfide	137-26-8	Thiuram disulphide or dithiocarbamate	Carbamates		+	+	+	+	+	+
123	NC170	4,4-Thiobis(5-tert-butyl-m-cresol) [AKA santrozol]	95-69-5	Phenol or precursor	Phenols	-		-	-	-	-	-
124	NC173	Tolbutamide	64-77-7	Aryl sulphonamide	Amides/Amides/Amides	-	+	-	-	-	-	+
125	NC174	1,1,1-Trichloroethane, technical grade	71-68-6	Di- to poly-halogenated alkane or cycloalkane	Halogenated compounds		-	-	-	-	+	-
126	NC176	2,4,5-Trichlorophenoxyacetic acid	93-76-5	Polyhalogenated aromatic	Polyhalogenated aromatic compounds		-	-	-	+	+	+
127	NC177	Tricetyl phosphate	1330-78-5	Phosphoric acid ester	Phosphorous compounds	-		-	-	-	-	E
128	NC178	Triphenyltin hydroxide	76-87-0	Alkali, alkali earth, metal salt	Alkali, metal salts	-	+	-	NA	NA	NA	NA
129	NC180	L-Tryptophan	73-22-3	Amino acid or derivative	Others	-		-	-	-	-	-
130	NC183	Vinyl toluene (65-71% m- and 32-35% p-) [AKA benzene, ethenyl(methyl)-]	25013-15-4	Alkene	Alkenes	+	+	-	+	-	-	+

*: Erythrocyte MN test with bone marrow or peripheral blood