

-S9		+S9										* Classification after single data point		Classification after Triplicate analysis		Classification (final)		Comment
Code #	CAS #	Name	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI						
1	5341-61-7	Hydrazine dihydrochloride	4.44	1.443	2.312	0.00	1.30	4.44	1.715	1.579	0.58	0.00	neg	weak + Mix +S9	weak + Mix +S9			
1			14.04			2.08	0.00	14.04			1.17	0.63						
1			44.40			0.69	1.73	44.40			1.75	0.63						
1			140.41			0.00	0.00	140.41			0.58	1.27						
1			444.00			0.00	0.00	444.00			0.00	0.00						
1			1'404.00			0.00	0.00	1'404.00			0.00	0.00						
1			4'440.00			0.00	0.00	4'440.00			0.00	0.00						
3	50-00-0	Formaldehyde	4.44	2.13	7.475	2.35	0.94	4.44	1.775	5.365	4.51	0.37	pos Mix + -S9		pos Mix + -S9			
3			14.04			13.15	1.74	14.04			21.41	1.86						
3			44.40			1.41	0.27	44.40			14.08	0.19						
3			140.41			0.00	0.00	140.41			1.13	0.19						
3			444.00			0.00	0.00	444.00			0.00	0.00						
3			1'404.00			0.00	0.00	1'404.00			0.00	0.00						
3			4'440.00			0.00	0.00	4'440.00			0.00	0.00						
4	107-22-2	Glyoxal	4.44	2.13	7.475	0.47	0.54	4.44	1.775	5.365	2.82	0.37			pos Mix +- -S9; EQ 98 +S9			
4			14.04			5.16	0.80	14.04			6.20	0.93						
4			44.40			12.21	1.07	44.40			9.01	2.61						
4			140.41			2.35	0.94	140.41			5.63	0.93						
4			444.00			9.39	0.54	444.00			12.39	2.24						
4			1'404.00			0.00	0.00	1'404.00			0.56	0.00						
4			4'440.00			0.00	0.00	4'440.00			0.00	0.00						
5	111-30-8	Glutaraldehyde	5.00	3.797	2.953	0.00	1.02	4.44	2.993	3.959	1.34	0.51	neg		neg			
5			15.81			0.00	0.34	14.04			1.00	0.00						
5			50.00			0.00	0.68	44.40			1.00	0.76						
5			158.11			0.00	0.00	140.41			0.00	0.00						
5			500.00			0.00	0.00	444.00			0.00	0.00						
5			1'581.14			0.00	0.00	1'404.00			0.00	0.00						
5			5'000.00			0.00	0.00	4'440.00			ppt	ppt						
6	542-78-9	Propanedial	4.44	1.443	2.312	0.00	1.30	4.44	1.715	1.579	1.17	0.00	neg		neg			
6			14.04			1.39	0.43	14.04			0.58	0.00						
6			44.40			0.00	0.87	44.40			1.17	0.00						
6			140.41			0.69	0.00	140.41			0.00	0.63						
6			444.00			1.39	1.30	444.00			0.58	0.00						
6			1'404.00			0.69	0.00	1'404.00			0.00	0.63						
6			4'440.00			0.69	0.43	4'440.00			0.00	0.63						
7	7803-49-8	Hydroxylamine	4.44	2.13	7.475	0.00	0.80	4.44	1.775	5.365	0.56	0.56	neg		neg			
7			14.04			0.00	1.07	14.04			0.56	0.75						
7			44.40			0.00	0.40	44.40			1.13	0.00						
7			140.41			0.00	0.00	140.41			0.56	0.19						
7			444.00			0.00	0.00	444.00			0.00	0.00						
7			1'404.00			0.00	0.00	1'404.00			0.00	0.00						
7			4'440.00			0.00	0.00	4'440.00			0.00	0.00						
8	2610-05-1	Direct blue 1	1.28	1.443	2.312	0.00	1.30	1.28	1.715	1.579	1.17	0.00	neg	neg	neg			
8			4.05			0.00	0.00	4.05			0.58	0.00						
8			12.80			0.00	0.87	12.80			0.58	0.00						
8			40.48			0.69	0.00	40.48			2.33	0.00						
8			128.00			0.69	0.43	128.00			1.75	0.63						
8			404.77			0.00	0.43	404.77			ci	ci						
8			1'280.00			0.00	0.00	1'280.00			ci	ci						
9	119-90-4	o-Dianisidine	4.44	2.265	2.164	0.44	0.46	0.50	0.893	3.428	3.00	1.46	neg. Mix +S9; pos 98 +S9		neg. Mix +S9; pos 98 +S9	Mix neg., very low BL		
9			14.04			0.88	0.00	1.58			2.00	4.08						
9			44.40			0.44	2.77	5.00			1.00	8.17						
9			140.41			1.32	0.00	15.81			2.00	12.25						
9			444.00			0.00	0.46	50.00			3.00	14.00						
9			1'404.00			ppt	ppt	158.11			0.00	13.71						
9			4'440.00			ppt	ppt	500.00			0.00	7.88						
11	92-87-5	Benzidine	4.44	3.639	2.336	0.82	0.43	0.49	1.233	2.183	0.00	0.92	pos 98 +S9		pos 98 +S9			

-S9						+S9						* Classification after	Classification after	Classification	Comment	
Code #	CAS #	Name	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	single data point	Triplicate analysis	(final)	
11			14.04			0.55	0.86	1.56			0.00	1.83				
11			44.40			0.55	0.86	4.92			0.00	5.04				
11			140.41			0.27	0.43	15.56			1.62	3.66				
11			444.00			0.00	0.43	49.20			0.00	5.96				
11			1'404.00			ppt	ppt	155.58			0.00	12.37				
11			4'440.00			ppt	ppt	492.00			0.00	12.37				
12	3761-53-3	Acid Red 26	1.92	2.265	2.164	0.44	2.77	1.92	0.74	2.65	0.00	1.51	neg	neg	neg	
12			6.07			0.44	1.39	6.07			0.00	0.38				
12			19.20			0.44	0.92	19.20			0.00	0.75				
12			60.72			ci	ci	60.72			0.00	0.75				
12			192.00			ci	ci	192.00			0.00	0.38				
12			607.16			ci	ci	607.16			0.00	0.38				
12			1'920.00			ci	ci	1'920.00			0.00	0.00				
13	107-06-2	1,2-Dichloroethane	4.44	2.13	7.475	0.47	0.94	4.44	1.775	5.365	1.69	0.75	weak + Mix -S9		weak + Mix -S9	
13			14.04			2.35	0.94	14.04			1.13	0.37				
13			44.40			2.35	1.07	44.40			2.82	0.56				
13			140.41			0.47	1.20	140.41			1.13	0.75				
13			444.00			1.88	0.27	444.00			0.56	0.37				
13			1'404.00			0.47	0.54	1'404.00			0.56	0.37				
13			4'440.00			0.47	0.13	4'440.00			0.00	0.00				
14	78-87-5	1,2-Dichloropropane	4.44	2.391	7.657	0.00	0.26	4.44	2.178	2.464	0.00	0.41	neg		neg	
14			14.04			0.42	0.52	14.04			0.00	0.00				
14			44.40			0.42	0.65	44.40			0.00	0.00				
14			140.41			0.84	0.65	140.41			0.46	1.62				
14			444.00			0.42	0.91	444.00			0.46	1.22				
14			1'404.00			1.25	0.78	1'404.00			0.92	0.00				
14			4'440.00			0.00	0.78	4'440.00			0.46	1.22				
17	78-94-4	Methyl vinyl ketone	4.44	2.13	7.475	0.47	0.54	4.44	1.775	5.365	0.00	0.37	neg		neg	
17			14.04			0.00	0.00	14.04			0.00	0.00				
17			44.40			0.00	0.00	44.40			0.00	0.00				
17			140.41			0.00	1.20	140.41			0.00	0.37				
17			444.00			0.00	0.00	444.00			0.00	0.00				
17			1'404.00			0.00	0.00	1'404.00			0.00	0.00				
17			4'440.00			0.00	0.00	4'440.00			0.00	0.00				
18	107-02-8	Acrolein	5.00	3.797	2.953	0.00	0.68	4.44	2.993	3.959	0.00	0.00	neg		neg	
18			15.81			0.00	0.34	14.04			0.00	0.00				
18			50.00			0.00	0.34	44.40			0.00	0.00				
18			158.11			0.00	1.02	140.41			0.00	0.00				
18			500.00			0.00	0.00	444.00			0.00	0.00				
18			1'581.14			0.00	0.00	1'404.00			0.00	0.00				
18			5'000.00			0.00	0.00	4'440.00			0.00	0.00				
20	107-18-6	2-Propen-1-ol	4.44	1.207	2.414	0.00	0.00	4.44	0.91	1.207	0.00	0.00	neg	neg	neg	
20			14.04			0.00	0.00	14.04			0.00	0.00				
20			44.40			0.00	0.00	44.40			0.00	0.00				
20			140.41			0.00	0.00	140.41			0.00	0.00				
20			444.00			0.00	0.00	444.00			0.00	0.00				
20			1'404.00			0.00	0.00	1'404.00			0.00	0.00				
20			4'440.00			0.00	0.00	4'440.00			0.00	0.00				
21	62-53-5	Aniline	4.44	2.13	7.475	0.00	0.94	4.44	1.775	5.365	0.00	0.75	neg		neg	
21			14.04			0.00	0.67	14.04			0.56	0.19				
21			44.40			0.94	0.94	44.40			1.13	0.93				
21			140.41			1.88	0.40	140.41			0.00	1.30				
21			444.00			0.47	1.07	444.00			0.56	0.56				
21			1'404.00			0.00	0.80	1'404.00			0.00	0.56				
21			4'440.00			0.00	0.13	4'440.00			0.00	0.56				
22	95-53-4	o-Toluidine	4.44	1	2.072	1.00	1.45	4.44	0.893	3.428	0.00	0.88	neg	weak + Mix +S9	weak + Mix +S9	
22			14.04			1.00	0.97	14.04			1.00	0.58				

-S9							+S9					* Classification after	Classification after	Classification	Comment	
Code #	CAS #	Name	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	single data point	Triplicate analysis	(final)	
22			44.40			1.00	0.00	44.40			0.00	0.00				
22			140.41			2.00	0.00	140.41			0.00	0.29				
22			444.00			1.00	0.48	444.00			1.00	0.29				
22			1'404.00			1.00	0.00	1'404.00			1.00	0.29				
22			4'440.00			0.00	0.00	4'440.00			2.00	0.00				
23	108-44-1	m-Toluidine	4.44	2.13	7.475	0.00	0.40	4.44	1.775	5.365	0.00	0.75	neg		neg	
23			14.04			1.41	0.67	14.04			0.00	0.75				
23			44.40			0.47	1.07	44.40			0.00	0.56				
23			140.41			0.94	0.94	140.41			0.00	0.00				
23			444.00			0.47	0.40	444.00			0.00	0.93				
23			1'404.00			0.00	0.54	1'404.00			1.13	0.00				
23			4'440.00			0.00	0.13	4'440.00			0.00	0.19				
24	106-49-0	p-Toluidine	4.44	0.948	0.948	1.00	1.00	4.44	1.233	2.183	0.81	0.46	+? Mix +S9		+? Mix +S9	
24			14.04			1.00	2.00	14.04			0.00	1.37				
24			44.40			2.00	1.00	44.40			0.81	1.37				
24			140.41			2.00	4.00	140.41			2.43	1.83				
24			444.00			1.00	2.00	444.00			0.81	1.83				
24			1'404.00			2.00	0.00	1'404.00			1.62	2.29				
24			4'440.00			0.00	0.00	4'440.00			4.06	0.00				
25	100-61-8	N-Methylaniline	4.44	1.207	2.414	0.00	0.83	4.44	0.91	1.207	1.00	0.83	EQ 98 +S9		EQ 98 +S9	
25			14.04			2.49	0.00	14.04			2.00	1.66				
25			44.40			0.83	0.83	44.40			0.00	3.31				
25			140.41			0.83	0.41	140.41			0.00	0.00				
25			444.00			0.00	0.83	444.00			0.00	3.31				
25			1'404.00			0.83	0.00	1'404.00			1.00	1.66				
25			4'440.00			0.00	0.00	4'440.00			0.00	0.00				
27	306-37-6	1,2-Dimethylhydrazine	5.00	2.315	2.953	1.73	0.68	5.00	3.033	0.713	0.33	1.00	pos Mix -S9		pos Mix -S9	
27			15.81			2.59	0.00	15.81			0.00	0.00				
27			50.00			4.75	0.00	50.00			0.33	1.00				
27			158.11			6.05	1.35	158.11			0.33	0.00				
27			500.00			18.14	0.34	500.00			0.33	2.00				
27			1'581.14			20.30	1.02	1'581.14			0.33	0.00				
27			5'000.00			1.73	1.69	5'000.00			0.00	1.00				
28	512-56-1	Trimethyl phosphate	5.00	3.797	2.953	2.63	0.34	4.44	2.993	3.959	1.00	0.25	weak + Mix +S9		weak + Mix +S9	
28			15.81			1.58	0.68	14.04			2.34	0.51				
28			50.00			1.32	1.02	44.40			3.68	0.25				
28			158.11			0.53	1.02	140.41			0.00	0.76				
28			500.00			1.32	0.68	444.00			2.34	0.25				
28			1'581.14			0.79	1.69	1'404.00			1.34	0.00				
28			5'000.00			1.58	1.02	4'440.00			1.67	0.76				
29	78-40-0	Triethyl phosphate	5.00	3.797	2.953	0.26	0.68	4.44	2.993	3.959	0.00	0.25	neg		neg	
29			15.81			0.00	0.00	14.04			0.33	0.25				
29			50.00			0.26	0.34	44.40			1.00	0.76				
29			158.11			1.05	0.34	140.41			0.33	1.01				
29			500.00			0.53	1.02	444.00			0.67	0.51				
29			1'581.14			0.26	0.34	1'404.00			0.33	0.51				
29			5'000.00			0.53	0.34	4'440.00			0.33	0.00				
30	115-96-8	Tris(2-chloroethyl) phosphate	5.00	2.315	2.953	0.86	0.34	5.00	3.033	0.713	0.00	1.00	neg	neg	neg	
30			15.81			0.00	1.02	15.81			0.00	1.00	+? 98 +S9			
30			50.00			1.30	0.68	50.00			0.66	0.00				
30			158.11			1.30	0.34	158.11			0.33	1.00				
30			500.00			0.43	0.68	500.00			0.33	1.00				
30			1'581.14			0.00	0.00	1'581.14			0.33	1.00				
30			5'000.00			0.00	0.00	5'000.00			0.33	42.00				
31	126-72-7	Tris(2,3-dibromopropyl) phos	5.00	2.315	2.953	0.86	0.68	5.00	3.033	0.713	0.66	0.00	pos Mix, 98 +S9		pos Mix, 98 +S9	
31			15.81			0.43	1.02	15.81			0.33	1.00				
31			50.00			0.86	0.34	50.00			1.98	2.00				

-S9							+S9					* Classification after	Classification after	Classification	Comment	
Code #	CAS #	Name	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	single data point	Triplicate analysis	(final)	
31			158.11			0.00	0.68	158.11			15.83	28.00				
31			500.00			0.43	0.68	500.00			15.83	25.00				
31			1'581.14			0.86	0.34	1'581.14			15.83	21.00				
31			5'000.00			0.43	0.34	5'000.00			15.83	23.00				
34	60-35-5	Acetamide	4.44	1.443	2.312	0.69	0.43	4.44	1.715	1.579	1.17	0.00	neg		neg	
34			14.04			1.39	0.87	14.04			0.58	0.00				
34			44.40			0.00	1.30	44.40			1.75	0.63				
34			140.41			0.69	1.73	140.41			1.17	0.00				
34			444.00			0.69	0.00	444.00			0.58	0.00				
34			1'404.00			0.69	0.43	1'404.00			1.17	0.00				
34			4'440.00			0.00	0.00	4'440.00			0.58	0.63				
36	54827-17-7	3,3',5,5'-Tetramethylbenzidin	4.44	2.265	2.164	0.00	0.00	4.44	0.74	2.65	0.00	0.38	neg		neg	
36			14.04			0.00	0.92	14.04			0.00	0.38				
36			44.40			0.00	0.92	44.40			0.00	0.75				
36			140.41			0.88	0.92	140.41			0.00	0.38				
36			444.00			ppt	ppt	444.00		ppt	ppt					
36			1'404.00			ppt	ppt	1'404.00		ppt	ppt					
36			4'440.00			ppt	ppt	4'440.00		ppt	ppt					
39	107-20-0	Chloroacetaldehyde	4.44	2.13	7.475	3.29	0.80	4.44	1.775	5.365	0.56	0.37	EQ Mix -S9		EQ Mix -S9	
39			14.04			1.41	1.20	14.04			0.56	0.75				
39			44.40			2.82	0.94	44.40			1.69	0.19				
39			140.41			1.88	0.67	140.41			1.13	0.93				
39			444.00			0.00	0.00	444.00			6.20	0.00				
39			1'404.00			0.00	0.00	1'404.00			0.00	0.00				
39			4'440.00			0.00	0.00	4'440.00			0.00	0.00				
41	548-62-9	Crystal violet	0.96	1.443	2.312	0.69	0.43	0.96	1.715	1.579	0.00	0.00	neg		neg	
41			3.04			1.39	0.00	3.04			1.17	0.00				
41			9.60			0.00	0.00	9.60			3.50	0.00				
41			30.36			0.00	0.00	30.36			1.17	0.00				
41			96.00			0.00	0.00	96.00		ci	ci					
41			303.58			2.08	0.00	303.58		ci	ci					
41			960.00			0.00	0.00	960.00		ci	ci					
58	117-79-3	2-Aminoanthraquinone	1.92	2.265	2.164	0.88	2.31	1.92	0.74	2.65	0.00	11.32	pos 98 + S9		pos 98 + S9	
58			6.07			1.32	1.39	6.07			0.00	17.74				
58			19.20			ppt	ppt	19.20			0.00	17.74				
58			60.72			ppt	ppt	60.72			0.00	18.11				
58			192.00			ppt	ppt	192.00			1.00	18.11				
58			607.16			ppt	ppt	607.16		ppt	ppt					
58			1'920.00			ppt	ppt	1'920.00		ppt	ppt					
62	117-10-2	Danthron	0.49	2.265	2.164	0.88	0.46	0.49	0.74	2.65	0.00	0.38	neg		neg	
62			1.56			0.44	0.00	1.56			0.00	0.75				
62			4.92			1.32	0.46	4.92			1.00	0.75				
62			15.56			0.00	0.92	15.56			0.00	1.51				
62			49.20			ppt	ppt	49.20			1.00	0.00				
62			155.58			ppt	ppt	155.58			0.00	0.00				
62			492.00			ppt	ppt	492.00			0.00	0.00				
63	90-94-8	Michler's ketone	0.97	2.46	2.649	1.22	0.76	0.97	1.776	1.975	1.69	0.51	pos Mix +S9		pos Mix +S9	
63			3.07			0.81	0.00	3.07			2.25	0.00				
63			9.72			0.81	0.76	9.72			2.25	2.53				
63			30.74			0.81	0.76	30.74			6.19	1.01				
63			97.20			1.63	0.38	97.20			5.07	0.51				
63			307.37			ppt	ppt	307.37		ppt	ppt					
63			972.00			ppt	ppt	972.00		ppt	ppt					
65	108-95-2	Phenol	4.44	2.391	7.657	0.00	1.70	4.44	2.178	2.464	0.92	1.62	weak + 98 +S9		weak + 98 +S9	
65			14.04			1.25	1.04	14.04			0.00	0.41				
65			44.40			0.00	1.04	44.40			1.38	0.00				
65			140.41			0.42	1.31	140.41			0.00	2.03				

-S9						+S9													
Code #	CAS #	Name	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	* Classification after single data point	Classification after Triplicate analysis	Classification (final)	Comment			
65			444.00			0.84	0.65	444.00			0.00	2.44							
65			1'404.00			0.00	0.78	1'404.00			0.00	0.81							
65			4'440.00			0.00	0.00	4'440.00			0.00	1.22							
66	123-31-9	Hydroquinone	1.92	1.443	2.312	0.00	0.43	1.92	1.715	1.579	0.00	1.90	neg		neg				
66			6.07			0.00	0.43	6.07			0.00	0.00							
66			19.20			0.00	0.43	19.20			0.58	0.63							
66			60.72			0.00	0.00	60.72			0.00	1.27							
66			192.00			0.69	0.00	192.00			0.58	1.27							
66			607.16			0.69	0.43	607.16			0.00	0.63							
66			1'920.00			0.00	0.87	1'920.00			1.17	ci							
67	120-80-9	Catechol	4.44	1.443	2.312	0.00	0.00	4.44	1.715	1.579	0.58	0.63	neg		neg				
67			14.04			0.69	0.87	14.04			0.00	0.00							
67			44.40			0.00	0.87	44.40			0.00	0.63							
67			140.41			0.69	0.43	140.41			0.00	1.90							
67			444.00			0.00	0.00	444.00			1.75	0.00							
67			1'404.00			0.00	0.00	1'404.00			1.75	0.63							
67			4'440.00			0.00	0.00	4'440.00		ci		ci							
68	71-43-2	Benzene	4.44	2.391	7.657	0.84	0.39	4.44	2.178	2.464	0.46	0.41	neg		neg				
68			14.04			0.42	0.65	14.04			0.46	0.81							
68			44.40			0.42	1.18	44.40			0.00	0.81							
68			140.41			0.00	0.91	140.41			0.46	1.22							
68			444.00			0.00	0.78	444.00			0.00	0.00							
68			1'404.00			0.00	0.39	1'404.00			0.00	0.41							
68			4'440.00			0.00	0.00	4'440.00			0.00	0.00							
69	85-44-9	Phthalic anhydride	4.44	2.51	1.897	0.40	2.11	4.44	1.513	1.448	0.66	0.00	neg	neg	neg				
69			14.04			0.80	1.58	14.04			0.66	1.38							
69			44.40			0.80	0.00	44.40			0.00	0.00							
69			140.41			0.00	0.00	140.41			0.66	1.38							
69			444.00			0.00	0.00	444.00			0.66	0.00							
69			1'404.00			0.00	0.00	1'404.00			0.00	1.38							
69			4'440.00			0.00	0.00	4'440.00			0.66	0.00							
71	88-99-3	Phthalic acid	4.44	0.948	0.948	2.00	1.00	4.44	1.233	2.183	0.00	0.00	EQ 98 -S9		EQ 98 -S9				
71			14.04			0.00	2.00	14.04			0.00	0.92							
71			44.40			2.00	2.00	44.40			0.00	0.92							
71			140.41			2.00	3.00	140.41			1.62	0.00							
71			444.00			0.00	2.00	444.00			0.00	2.29							
71			1'404.00			2.00	0.00	1'404.00			0.81	0.92							
71			4'440.00			1.00	4.00	4'440.00			0.00	1.37							
72	101-61-1	N,N,N',N'-Tetramethyl-4,4'-m	1.92	2.265	2.164	0.00	0.00	1.92	0.74	2.65	1.00	0.75	neg		neg				
72			6.07			0.88	0.46	6.07			3.00	1.51							
72			19.20			1.32	0.46	19.20			0.00	0.75							
72			60.72			0.00	0.00	60.72			1.00	0.00							
72			192.00			0.00	no data	192.00			0.00	0.38							
72			607.16			0.00	no data	607.16			2.00	0.00							
72			1'920.00			ppt	ppt	1'920.00			ppt	ppt							
73	101-14-4	4,4'-Methylene-bis(1-chlorani	4.44	2	2.227	1.50	0.90	0.15	1.445	2	0.69	1.50	pos Mix, 98 +S9		pos Mix, 98 +S9				
73			14.04			0.00	0.90	0.48			0.69	0.50							
73			44.40			0.50	2.25	1.51			0.69	1.00							
73			140.41			0.00	0.90	4.78			2.08	2.50							
73			444.00			ppt	ppt	15.12			4.15	2.50							
73			1'404.00			ppt	ppt	47.81			8.30	5.50							
73			4'440.00			ppt	ppt	151.20			20.76	3.00							
74	139-65-1	4,4'-Thiodianiline	5.00	2.46	2.649	3.25	1.13	5.00	1.776	1.975	19.14	14.18	pos Mix, 98 +S9; pos Mix -S9		pos Mix, 98 +S9; pos Mix -S9				
74			15.81			4.47	1.13	15.81			27.03	22.78							
74			50.00			2.85	0.76	50.00			27.03	24.30							
74			158.11			3.25	1.89	158.11			27.03	24.30							
74			500.00			0.81	0.00	500.00			11.82	0.00							

-S9								+S9				* Classification after single data point		Classification after Triplicate analysis		Classification (final)		Comment
Code #	CAS #	Name	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI						
74			1'581.14			ppt	ppt	1'581.14			ppt	ppt						
74			5'000.00			ppt	ppt	5'000.00			ppt	ppt						
75	101-80-4	Diaminodiphenyl ether	4.44	2	2.227	0.50	0.90	0.49	1.445	2	1.38	1.00	pos Mix, 98 +S9; EQ Mix -S9			pos Mix, 98 +S9; EQ Mix -S9		
75			14.04			2.00	1.35	1.56			3.46	0.50						
75			44.40			2.50	1.80	4.92			10.38	5.00						
75			140.41			0.00	1.80	15.56			31.14	7.00						
75			444.00			2.50	1.80	49.20			33.22	14.00						
75			1'404.00			ppt	ppt	155.58			33.22	21.50						
75			4'440.00			ppt	ppt	492.00			33.22	22.50						
77	101-77-9	4,4'-Methylenedianiline	4.44	2	2.227	0.00	1.35	1.52	1.445	2	0.69	2.00	pos Mix, 98 +S9			pos Mix, 98 +S9		
77			14.04			1.00	1.35	4.81			5.54	1.50						
77			44.40			0.50	0.45	15.20			8.30	1.50						
77			140.41			1.00	0.00	48.07			15.22	2.00						
77			444.00			ppt	ppt	152.00			13.15	3.00						
77			1'404.00			ppt	ppt	480.00			9.69	3.50						
77			4'440.00			ppt	ppt	1'520.00			0.00	15.00						
89	79-06-1	Acrylamide	4.44	1.443	2.312	0.69	0.43	4.44	1.715	1.579	0.00	0.00	neg			neg		
89			14.04			0.69	0.43	14.04			0.00	0.63						
89			44.40			0.69	0.43	44.40			0.58	0.00						
89			140.41			0.00	0.00	140.41			0.58	1.90						
89			444.00			0.00	0.43	444.00			0.58	1.27						
89			1'404.00			0.00	0.00	1'404.00			1.17	0.63						
89			4'440.00			0.00	0.87	4'440.00			0.00	0.00						
90	121-14-2	2,4-Dinitrotoluene	4.44	3.639	2.336	0.55	1.71	0.15	1.233	2.183	0.00	0.46	pos 98 -S9			pos 98 -S9		
90			14.04			0.00	5.99	0.48			0.00	0.00						
90			44.40			1.37	11.13	1.52			0.00	1.37						
90			140.41			1.65	15.41	4.79			0.81	0.00						
90			444.00			ppt	ppt	15.16			0.81	1.37						
90			1'404.00			ppt	ppt	47.94			0.00	1.37						
90			4'440.00			ppt	ppt	151.60			0.00	3.21						
91	606-20-2	2,6-Dinitrotoluene	4.44	3.639	2.336	0.55	0.43	0.49	1.233	2.183	0.00	0.00	neg	weak + Mix +S9; pos 98 +-S9		weak + Mix +S9; pos 98 +-S9		
91			14.04			0.55	0.86	1.56			0.00	0.00						
91			44.40			0.82	0.43	4.92			0.81	0.46						
91			140.41			0.82	0.86	15.56			0.00	0.46						
91			444.00			0.82	2.57	49.20			0.81	0.92						
91			1'404.00			ppt	ppt	155.58			1.62	0.46						
91			4'440.00			ppt	ppt	492.00			1.62	0.46						
92	95-80-7	2,4-Diaminotoluene	4.44	2.51	1.897	0.80	1.05	4.44	1.513	1.448	0.66	2.07	pos Mix, 98 +S9; EQ 98 -S9			pos Mix, 98 +S9; EQ 98 -S9		
92			14.04			0.40	1.58	14.04			2.64	2.07						
92			44.40			0.80	0.00	44.40			3.97	3.45						
92			140.41			0.80	2.11	140.41			1.98	9.67						
92			444.00			0.00	1.05	444.00			0.66	24.17						
92			1'404.00			1.20	2.11	1'404.00			4.63	33.15						
92			4'440.00			0.80	1.58	4'440.00			7.93	33.15						
93	823-40-5	2,6-Diaminotoluene	4.44	2.391	7.657	0.84	0.65	1.52	2.178	2.464	0.00	0.41	weak + Mix +S9; pos 98 +S9			weak + Mix +S9; pos 98 +S9		
93			14.04			1.67	1.57	4.79			0.46	0.00						
93			44.40			0.42	0.78	15.16			1.38	0.41						
93			140.41			0.84	0.39	47.94			0.00	0.00						
93			444.00			0.84	1.96	151.60			0.00	2.03						
93			1'404.00			0.42	1.18	479.40			2.30	5.68						
93			4'440.00			ppt	ppt	1'516.00			3.21	19.07						
94	598-55-0	Methyl carbamate	4.44	2.391	7.657	0.00	0.65	4.44	2.178	2.464	0.00	0.41	neg			neg		
94			14.04			0.42	1.31	14.04			0.92	0.41						
94			44.40			0.00	1.44	44.40			0.46	0.00						
94			140.41			1.25	0.65	140.41			0.00	0.81						
94			444.00			0.00	0.78	444.00			0.00	0.81						
94			1'404.00			0.00	0.78	1'404.00			0.00	0.41						

-S9							+S9					* Classification after	Classification after	Classification	Comment	
Code #	CAS #	Name	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	single data point	Triplicate analysis	(final)	
94			4'440.00			0.00	1.04	4'440.00			0.00	0.41				
95	51-79-6	Urethane	4.44	1.443	2.312	0.00	0.43	4.44	1.715	1.579	0.58	0.63	neg	neg	neg	
95			14.04			1.39	0.87	14.04			0.00	1.90				
95			44.40			0.00	0.43	44.40			0.00	0.00				
95			140.41			0.00	0.43	140.41			0.00	0.63				
95			444.00			0.00	0.87	444.00			0.00	0.00				
95			1'404.00			2.08	0.43	1'404.00			0.58	1.27				
95			4'440.00			1.39	0.43	4'440.00			0.58	0.63				
97	53-96-3	2-Acetylaminofluorene	4.44	2.51	1.897	0.00	0.00	0.49	1.513	1.448	0.00	3.45	pos Mix, 98 +S9		pos Mix, 98 +S9	
97			14.04			0.40	1.05	1.56			3.30	13.81				
97			44.40			0.40	0.53	4.92			7.93	31.77				
97			140.41			0.00	0.00	15.56			14.54	33.15				
97			444.00			0.00	0.53	49.20			31.06	33.15				
97			1'404.00		ppt	ppt		155.58			31.06	33.15				
97			4'440.00		ppt	ppt		492.00			29.74	33.15				
100	56-49-5	3-Methylcholanthrene	0.10	3.212	2.072	0.62	0.00	0.10	0.893	3.428	1.00	1.17	pos Mix, 98 +S9		pos Mix, 98 +S9	
100			0.32			0.31	0.00	0.32			0.00	2.33				
100			1.00			0.31	0.00	1.00			15.00	2.04				
100			3.16			1.25	0.48	3.16			25.00	6.42				
100			10.00			0.93	0.48	10.00			31.00	12.84				
100			31.62			1.25	1.45	31.62			28.00	12.54				
100			100.00			2.18	1.45	100.00			33.00	14.00				
101	62-50-0	Ethyl methanesulfonate	4.44	2.13	7.475	0.00	1.20	4.44	1.775	5.365	0.00	0.37	pos Mix +- S9		pos Mix +- S9	
101			14.04			0.47	1.74	14.04			0.00	0.56				
101			44.40			1.41	1.34	44.40			0.00	0.19				
101			140.41			0.00	1.07	140.41			1.13	0.93				
101			444.00			1.41	0.94	444.00			0.56	0.56				
101			1'404.00			10.80	0.94	1'404.00			11.83	0.93				
101			4'440.00			22.54	0.67	4'440.00			27.04	2.24				
102	134-32-7	1-Naphthylamine	4.44	2.265	2.164	0.44	1.85	4.44	0.74	2.65	0.00	0.75	neg	pos Mix +S9	pos Mix +S9	
102			14.04			0.00	0.00	14.04			0.00	1.13				
102			44.40			0.44	0.00	44.40			0.00	1.13				
102			140.41			0.00	0.92	140.41			0.00	3.77				
102			444.00			1.32	0.46	444.00			0.00	1.13				
102			1'404.00			0.00	0.00	1'404.00			0.00	0.00				
102			4'440.00			ppt	ppt	4'440.00			0.00	0.00				
103	91-59-8	2-Naphthylamine	4.44	2.265	2.164	0.00	1.39	4.44	0.74	2.65	2.00	4.91	pos Mix, 98 +S9		pos Mix, 98 +S9	
103			14.04			0.00	0.00	14.04			3.00	9.06				
103			44.40			1.32	1.39	44.40			18.00	15.09				
103			140.41			0.44	0.92	140.41			41.00	16.23				
103			444.00			0.44	0.00	444.00			11.00	7.17				
103			1'404.00			ppt	ppt	1'404.00			ppt	ppt				
103			4'440.00			ppt	ppt	4'440.00			ppt	ppt				
104	60-11-7	p-Dimethylaminoazobenzene	1.92	2.51	1.897	0.00	cont	0.20	1.513	1.448	0.00	1.38	pos Mix, 98 +S9		pos Mix, 98 +S9	
104			6.07			0.40	cont	0.63			0.00	0.69				
104			19.20			0.40	0.53	2.00			3.30	0.69				
104			60.72			0.40	1.05	6.33			3.30	4.14				
104			192.00			0.00	0.00	20.00			1.98	6.91				
104			607.16			ppt	ppt	63.25			4.63	5.52				
104			1'920.00			ppt	ppt	200.00			31.73	4.14				
107	92-67-1	4-Aminobiphenyl	4.44	2.265	2.164	0.00	0.00	4.44	0.74	2.65	22.00	16.60	pos Mix, 98 +S9		pos Mix, 98 +S9	
107			14.04			0.44	0.00	14.04			32.00	18.11				
107			44.40			0.00	1.85	44.40			26.00	18.11				
107			140.41			0.88	0.00	140.41			24.00	18.11				
107			444.00			0.00	0.00	444.00			0.00	0.00				
107			1'404.00			ppt	ppt	1'404.00			0.00	0.00				
107			4'440.00			ppt	ppt	4'440.00			ppt	ppt				

-S9							+S9						* Classification after	Classification after	Classification	Comment
Code #	CAS #	Name	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	single data point	Triplicate analysis	(final)	
108	90-04-0	o-Anisidine	5.00	3.797	2.953	0.26	1.35	4.44	2.993	3.959	1.00	0.51	neg		neg	
108			15.81			1.05	0.34	14.04			0.67	0.76				
108			50.00			1.58	1.02	44.40			1.00	1.26				
108			158.11			0.79	0.68	140.41			0.67	1.01				
108			500.00			0.79	1.02	444.00			0.33	0.25				
108			1'581.14			1.32	0.68	1'404.00			0.67	0.00				
108			5'000.00			0.53	0.00	4'440.00			1.67	0.25				
109	680-31-9	Hexamethylphosphoramide	5.00	3.797	2.953	0.26	0.34	4.44	2.993	3.959	0.33	0.25	+? Mix +S9		+? Mix +S9	
109			15.81			0.79	1.35	14.04			0.33	1.01				
109			50.00			1.05	0.00	44.40			0.33	0.00				
109			158.11			0.53	2.03	140.41			0.00	1.01				
109			500.00			0.79	0.34	444.00			0.00	0.76				
109			1'581.14			0.53	1.35	1'404.00			1.00	1.52				
109			5'000.00			2.63	1.02	4'440.00			11.03	3.54				
110	107-13-1	Acrylonitrile	4.44	2.391	7.657	0.00	1.04	4.44	2.178	2.464	0.00	1.22	weak + 98 +S9		weak + 98 +S9	
110			14.04			0.42	1.04	14.04			0.46	0.41				
110			44.40			0.84	0.52	44.40			0.46	1.22				
110			140.41			0.42	0.78	140.41			0.92	0.81				
110			444.00			0.00	0.91	444.00			0.92	1.22				
110			1'404.00			1.25	1.18	1'404.00			0.00	2.03				
110			4'440.00			0.84	1.04	4'440.00			0.92	2.03				
111	26628-22-8	Sodium azide	4.44	1.443	2.312	0.69	0.00	4.44	1.715	1.579	1.17	0.63	neg		neg	
111			14.04			0.00	0.43	14.04			0.00	0.63				
111			44.40			0.00	0.00	44.40			0.58	0.00				
111			140.41			0.00	0.00	140.41			0.00	0.00				
111			444.00			0.00	0.00	444.00			0.00	0.00				
111			1'404.00			0.00	0.00	1'404.00			0.00	0.00				
111			4'440.00			0.00	0.00	4'440.00			0.00	0.00				
112	79-44-7	Dimethylcarbamoyl chloride	4.44	2.391	7.657	0.84	1.70	4.44	2.178	2.464	0.92	2.44	pos Mix +- S9; pos 98 +S9		pos Mix +- S9; pos 98 +S9	
112			14.04			0.00	0.78	14.04			0.00	0.81				
112			44.40			1.25	0.91	44.40			1.38	1.62				
112			140.41			1.25	1.44	140.41			2.75	1.22				
112			444.00			2.51	1.31	444.00			4.13	1.62				
112			1'404.00			9.62	1.31	1'404.00			9.64	3.25				
112			4'440.00			15.89	3.40	4'440.00			13.31	9.74				
114	431-03-8	2,3-Butanedione	5.00	3.797	2.953	0.26	0.34	4.44	2.993	3.959	0.00	1.52	neg		neg	
114			15.81			1.05	1.35	14.04			0.00	1.01				
114			50.00			1.05	0.68	44.40			0.00	0.51				
114			158.11			1.58	1.02	140.41			0.00	1.52				
114			500.00			0.79	0.34	444.00			0.00	0.76				
114			1'581.14			0.53	0.00	1'404.00			0.33	0.51				
114			5'000.00			0.00	0.00	4'440.00			0.00	0.00				
115	92-36-4	2-(4-Aminophenyl)-6-methylb	4.44	3.639	2.336	0.55	0.43	0.05	1.233	2.183	0.00	0.92	pos Mix, 98 +S9		pos Mix, 98 +S9	
115			14.04			0.00	0.86	0.16			0.00	5.04				
115			44.40			0.27	0.00	0.49			0.00	14.66				
115			140.41			ppt	ppt	1.56			1.62	21.99				
115			444.00			ppt	ppt	4.92			6.49	21.99				
115			1'404.00			ppt	ppt	15.56			6.49	21.99				
115			4'440.00			ppt	ppt	49.20			11.35	21.99				
118	120-12-7	Anthracene	1.20	3.749	1.822	0.27	0.00	1.20	0.91	2.771	0.00	0.72	pos 98 +S9		pos 98 +S9	
118			3.80			0.00	0.00	3.80			1.00	4.69				
118			12.00			0.27	0.55	12.00			2.00	7.58				
118			37.95			0.00	1.65	37.95			2.00	5.41				
118			120.00			0.53	1.65	120.00			0.00	3.61				
118			379.47			ppt	ppt	379.47			ppt	ppt				
118			1'200.00			ppt	ppt	1'200.00			ppt	ppt				

-S9						+S9						* Classification after single data point	Classification after Triplicate analysis	Classification (final)	Comment	
Code #	CAS #	Name	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI	Dose (µg/ml)	TAMix BL	TA98 BL	TAMix FI	TA98 FI				
126	62-56-6	Thiourea	5.00	2.315	2.953	1.73	1.02	4.44	3.033	0.713	0.66	2.00	neg		neg	
126			15.81			1.30	1.02	14.04			0.33	2.00				
126			50.00			2.59	1.69	44.40			1.32	2.00				
126			158.11			0.86	1.02	140.41			2.64	2.00				
126			500.00			1.30	0.00	444.00			0.33	1.00				
126			1'581.14			0.86	1.02	1'404.00			0.00	2.00				
126			5'000.00			1.73	0.68	4'440.00			0.33	1.00				
127	3068-88-0	beta-Butyrolactone	5.00	3.797	2.953	0.00	0.34	4.44	2.993	3.959	0.67	1.01	pos Mix, 98 +- S9		pos Mix, 98 +- S9	
127			15.81			2.63	1.02	14.04			1.34	1.77				
127			50.00			4.21	2.37	44.40			3.34	1.52				
127			158.11			6.58	2.03	140.41			5.68	1.52				
127			500.00			12.11	7.79	444.00			13.70	3.79				
127			1'581.14			12.64	12.53	1'404.00			16.04	9.09				
127			5'000.00			8.95	7.79	4'440.00			16.04	10.86				
128	96-48-0	gamma-Butyrolactone	4.44	2.13	7.475	1.88	0.80	4.44	1.775	5.365	2.25	0.56	neg	neg	neg	
128			14.04			0.00	1.34	14.04			0.56	0.56				
128			44.40			0.47	0.94	44.40			0.56	0.56				
128			140.41			0.47	1.87	140.41			0.56	0.56				
128			444.00			0.00	1.74	444.00			1.13	1.12				
128			1'404.00			0.47	0.94	1'404.00			0.00	0.75				
128			4'440.00			0.00	0.13	4'440.00			1.13	0.56				
129	75-52-5	Nitromethane	5.00	3.797	2.953	0.26	0.34	4.44	2.993	3.959	0.33	0.00	neg		neg	
129			15.81			0.79	0.34	14.04			0.33	1.26				
129			50.00			0.53	0.34	44.40			1.34	1.01				
129			158.11			0.79	1.02	140.41			0.33	0.51				
129			500.00			0.26	0.34	444.00			0.67	0.25				
129			1'581.14			0.00	0.00	1'404.00			0.00	0.76				
129			5'000.00			0.53	0.00	4'440.00			1.00	0.76				
130	79-46-9	2-Nitropropane	5.00	2.315	2.953	0.43	0.00	4.44	3.033	0.713	0.66	0.00	pos Mix +S9; weak + 98 +S9; EQ Mix -S9		pos Mix +S9; weak + 98 +S9; EQ Mix -S9	
130			15.81			0.86	0.68	14.04			2.31	2.00				
130			50.00			2.59	0.68	44.40			1.98	0.00				
130			158.11			0.86	1.02	140.41			4.29	2.00				
130			500.00			0.43	0.00	444.00			2.97	0.00				
130			1'581.14			0.86	1.02	1'404.00			4.29	3.00				
130			5'000.00			2.16	2.37	4'440.00			2.64	3.00				
135	151-21-3	Sodium lauryl sulfate	4.44	1.443	2.312	0.00	0.87	0.44	1.715	1.579	0.00	1.90	neg		neg	
135			14.04			0.00	0.43	1.40			0.58	1.90				
135			44.40			0.00	0.00	4.44			0.58	0.63				
135			140.41			0.00	0.43	14.04			0.58	0.00				
135			444.00			0.00	0.00	44.40			0.58	0.00				
135			1'404.00			0.00	0.00	140.40			0.00	1.27				
135			4'440.00			0.00	0.00	444.00			0.00	0.00				

* Evaluation criteria are described in Table II in the paper

Baseline (BL) = Mean spont. rate + STD, but at least 1.0

FI = Fold Induction

Fold induction over baseline between 2 and 4

Fold induction over baseline >4

Baseline set to 1 for FI calculation

ppt Precipitate

ci Color interference

cont contaminated