

Distribution of available data, promised data, QSAR/read across, waiving and resulting test needs

Annex V-VIII No.	Information	Annex	Annex V (1 - 10 tpa)					Annex VI (10 - 100 tpa)					Annex VII (100 - 1000 tpa)					Annex VIII (> 1000 tpa)				
			Data	Promised	QSAR/r.a.	Waiving	Test	Data	Promised	QSAR/r.a.	Waiving	Test	Data	Promised	QSAR/r.a.	Waiving	Test	Data	Promised	QSAR/r.a.	Waiving	Test
5.1	State	V	100%				0%	100%				0%	100%				0%	100%				0%
5.2	Melting/freezing	V	100%				0%	100%				0%	100%				0%	100%				0%
5.3	Boiling	V	100%				0%	100%				0%	100%				0%	100%				0%
5.4	Density	V	100%				0%	100%				0%	100%				0%	100%				0%
5.5	Vapour pressure	V	100%				0%	100%				0%	100%				0%	100%				0%
5.6	Surface tension	V	100%				0%	100%				0%	100%				0%	100%				0%
5.7	Water solubility	V	100%				0%	100%				0%	100%				0%	100%				0%
5.8	Water extractivity	V	100%				0%	100%				0%	100%				0%	100%				0%
5.9	Log Pow	V	56%	8%	36%		0%	56%	8%	36%		0%	56%	8%	36%		0%	56%	8%	36%		0%
5.10	Flash-point	V	100%				0%	100%				0%	100%				0%	100%				0%
5.11	Flammability	V	100%				0%	100%				0%	100%				0%	100%				0%
5.12	Explosive properties	V	100%				0%	100%				0%	100%				0%	100%				0%
5.13	Self-ignition temp.	V	100%				0%	100%				0%	100%				0%	100%				0%
5.14	Oxidising properties	V	100%				0%	100%				0%	100%				0%	100%				0%
5.15	Granulometry	V	100%				0%	100%				0%	100%				0%	100%				0%
5.16	Light stability	VI						100%					100%					100%				0%
5.17	Long-term extractivity	VI						100%					100%					100%				0%
5.18	Stability organic solvent	VII											100%					100%				0%
5.19	Dissociation constant	VII											100%					100%				0%
5.20	Viscosity	VII											100%					100%				0%
5.21	Reactivity	VII											100%					100%				0%
6.1	Skin irritation/corrosion	V	17%	33%	30%	4%	16%															
6.1.1	In vivo skin irritation	VI						17%	48%	21%	3%	11%	22%	45%	20%	3%	11%	73%	20%	4%	1%	2%
6.2	Eye irritation	V	17%	33%	15%	7%	28%															
6.2.1	In vivo eye irritation	VI						17%	48%	11%	5%	20%	22%	45%	10%	5%	19%	73%	20%	2%	1%	4%
6.3	Skin sensitisation	V	17%		37%	9%	37%	17%		37%	9%	37%	22%		35%	9%	34%	48%		23%	6%	23%
6.4.1	Gene mutation bacteria	V	17%	33%	35%	3%	12%	17%	48%	25%	2%	9%	22%	45%	23%	2%	8%	60%	4%	36%	0%	0%
6.4.2	Cytogenicity mam. cells	V	17%	33%	35%	3%	12%	17%	48%	25%	2%	9%	22%	45%	23%	2%	8%	60%	4%	36%	0%	0%
6.4.3	Gene mutation mam. cells	VI						17%	48%	25%	5%	6%	22%	45%	23%	9%	1%	60%	4%	36%	0%	0%
6.4.4	Further mutagenicity	VIII	3%			74%	23%	3%			74%	23%	7%			71%	22%	38%	4%	36%	0%	47%
6.5.1	Acute oral tox	VI						17%	48%	25%	2%	9%	22%	45%	23%	2%	8%	75%	2%	23%	0%	0%
6.5.2	Acute inhalation tox	VI						17%	58%	5%	5%	20%	22%	55%	5%	19%	75%	2%	23%	0%	0%	
6.5.3	Acute dermal tox	VI						17%	58%	5%	5%	20%	22%	55%	5%	19%	75%	2%	23%	0%	0%	
6.6.1	Short-term repeated dose	VI						20%	56%	7%	17%	29%	50%	9%	13%	60%	3%	37%	0%	0%	0%	
6.6.2	Sub-chronic tox	VII						3%	68%	23%	6%	7%	28%	52%	13%	14%	48%	26%	48%	12%	12%	
6.6.3	Long-term repeated tox	VIII															5%	29%	61%	5%	5%	
6.7.1	Developm. tox screening	VI						17%		58%	7%	18%	22%		55%	7%	17%	48%	7%	45%	0%	0%
6.7.2	Developm. tox study	VI						3%	15%	73%	10%	7%	14%	22%	57%	32%		10%	21%	37%	37%	
6.7.3	Two-generation reprotox	VII						3%	0%	85%	12%	7%	7%	0%	82%	11%	26%	0%	27%	47%	47%	
6.8.1	Toxicokinetics	VI						17%				83%	7%			93%					100%	
6.9	Carcinogenicity	VIII															44%			52%	4%	
7.1.1	Short-term daphnia	V	17%	17%	46%	4%	16%	17%	24%	41%	4%	14%	22%	22%	39%	3%	13%	62%	6%	32%	0%	0%
7.1.2	Growth inhibition algae	V	17%		58%	5%	20%	17%		58%	5%	20%	22%		55%	5%	19%	51%	7%	42%	0%	0%
7.1.3	Short-term fish	VI						17%	24%	41%	4%	14%	22%	22%	39%	3%	13%	62%	5%	33%	0%	0%
7.1.4	Active sludge resp.	VI						17%			30%	53%	22%		28%	50%	57%			15%	28%	
7.1.5	Long-term daphnia tox	VII (V)			30%	67%	3%	3%		29%	65%	3%	7%		28%	60%	5%	18%		25%	53%	5%
7.1.6	Long-term fish tox	VII						3%		29%	65%	3%	7%		28%	60%	5%	14%		26%	55%	5%
7.2.1.1	Ready biodeg	V	17%	33%	35%	4%	11%	17%	48%	25%	3%	8%	22%	45%	23%	3%	7%	62%	7%	31%	0%	0%
7.2.1.2	Simulation surface water	VII										92%	8%			92%	8%	92%		8%	92%	8%
7.2.1.3	Simulation soil	VII										92%	8%			92%	8%	92%		8%	92%	8%
7.2.1.4	Simulation sediment	VII										92%	8%			92%	8%	92%		8%	92%	8%
7.2.1.5	Confirmatory biodeg rates	VIII																		99%	1%	
7.2.2.1	Hydrolysis	VI						17%		25%	21%	37%	22%		23%	20%	35%	41%		18%	15%	26%
7.2.3	Deg. products	VII															1%				1%	1%
7.3.1	Adsorption/desorption	VI						17%		50%	23%	11%	22%		47%	21%	10%			60%	27%	13%
7.3.2	Accumulation	VII											7%		18%	63%	12%	30%		13%	48%	9%
7.3.3	Further a/d studies	VII															1%					1%
7.3.4	Further fate & behaviour	VIII																				1%
7.4.1	Short-term earthworm	VII											7%		84%	9%	30%			63%	7%	
7.4.2	Soil micro-organisms	VII											7%		84%	9%	30%			63%	7%	
7.4.3	Short-term plants	VII											7%		84%	9%	32%			61%	7%	
7.4.4	Long-term earthworm	VIII																		96%	4%	
7.4.5	Long-term invertebrates	VIII																		96%	4%	
7.4.6	Long-term plant	VIII																		96%	4%	
7.5	Long-term sediment	VIII																		92%	8%	
7.6	Long-term bird	VIII																		99%	1%	
8	Other relevant information	V					100%	0%				100%	0%			100%	22%				100%	
9	Analytical methods	VII											22%		70%	8%	22%			70%	8%	

Assumptions

		Remarks/source		
Number of substances	Annex V	19200	17500 WP	
	Annex VI	4977	IUCLID	
	Annex VII	2461	IUCLID	
	Annex VIII	2704	IUCLID	
		Total	29342	
		1700 Type 3 (isolated and transported) intermediates > 1000 tpa		
VCI initiative	Annex V	40%	Guestimate on substances produced in Germany	
	Annex VI + VII	57%	4258 substances produced in Germany (IUCLID)	
	Annex VIII	74%	1997 substances produced in Germany (IUCLID)	
Data availability	Base set	Level 1	Level 2	
	Data Annex V	17%	3%	2% RPA & Statistics Sweden (2002)
	Data Annex VI	17%	3%	2% RPA & Statistics Sweden (2002)
	Data Annex VII	22%	7%	5% RPA & Statistics Sweden (2002)
QSAR/read-across	EU acceptance after US-EPA endpoints	70%	Assumed 15% lower for aquatic tox, 15-20% lower for health endpoints than US-EPA (US HPV Challenge Program)	
	Good =	60%	Guestimate, assignment to endpoints after Niemela, Danish EPA (pers. comm.)	
	Fair =	30%	Guestimate, assignment to endpoints after Niemela, Danish EPA (pers. comm.)	
	Poor =	0%	Guestimate, assignment to endpoints after Niemela, Danish EPA (pers. comm.)	
6.5 Acute tox - distribution of tests	6.5.1 Oral	90%	Guestimate	
	6.5.2 Inhalation	50%	Guestimate	
	6.5.3 Dermal	40%	Guestimate	
6.6 Repeated dose tox - distribution of tests	6.6.1 Short-term repeated dose (28d)	85%	Guestimate	
	6.6.2 Sub-chronic tox (90d)	20%	Guestimate	
	6.6.3 Long-term repeated dose (>12m)	5%	Guestimate	
6.7 Development tox - distribution of tests	Annex VI	Annex VII	Annex VIII	
	6.7.1 Screening study	95%	0%	0% Guestimate
	6.7.2 Development tox. study	15%	100%	100% Guestimate
	6.7.3 Two-generation repro-tox. study	5%	5%	100% Guestimate
7.2 Simulation tests - distribution of tests	7.2.1.2 Simulation surface water	80%	Guestimate	
	7.2.1.3 Simulation soil	15%	Guestimate	
	7.2.1.4 Simulation sediment	15%	Guestimate	
7.4 Terrestrial ecotox - distribution of tests	7.4.1 Earthworms	45%	Guestimate	
	7.4.2 Micro-organisms	20%	Guestimate	
	7.4.3 Plants	45%	Guestimate	
Not testable		20%	Estimate based on Allanou et al. (1999)	
6.4.4 Further mutagenicity tests required		30%	Positive results in in vitro tests (Andrew Smith, UK HSE, pers. comm.)	
6.6.1 Exposure based waiving (Annex VI)		10%		
6.6.1 Requirement at Annex VII		75%		
6.6.2 Requirement at Annex VI, VII + VIII		25%		
6.6.3 Requirement at Annex VIII		10%		
6.7.1 Exposure based waiving (Annex VI)		10%		
6.7.2 Positive in 6.7.1		15%		
6.7.2 Requirement at Annex VII		90%		
6.7.3 Requirement at Annex VI + VII due to positive 6.6		15%		
6.7.3 Requirement at Annex VII + VIII		80%		
6.9 Waiving of missing data		90%		
7.1.4 Readily biodegradable substances		20%		
7.1.5+6 RA based needs at low tonnages (<100 tpa)		5%		
7.1.5+6 RA based needs at higher tonnages (>100 tpa)		10%		
7.2.1.1 Inorganics		10%	5% of 80000 EINECS entries having a molecular formula are inorganics, but probably many more among 20000 entries without molecular formula (Niemela, Danish EPA, pers. comm.)	
7.2.1.2-4 RA based needs		10%		
7.2.1.5 RA based needs for confirmatory tests		1%		
7.2.3, 7.3.3+4 Requirement due to RA results		1%		
7.3.1+2 Waiving due to log Pow < 3		60%	Based on ~40% of organics with log Pow > 3 (Niemela, Danish EPA, pers. comm.)	
7.4.1-3 Likelihood of soil exposure		25%	Based on ~25% of organics with log Pow > 4 (Niemela, Danish EPA, pers. comm.)	
7.4.1-3 Exposure based waiving		50%		
7.4.4-6 Waiving		95%		
7.5 Waiving of missing data		90%		
7.6 Likelihood of bird exposure		1%		
9. Request of analytical methods		10%		

Test needs in addition to already available, required, promised, etc.

Annex V-VIII I	Information	Annex	Annex V	Annex VI	Annex VII	Annex VIII	Total tests	
5.1	State	V	0	0	0	0	0	0
5.2	Melting/freezing	V	0	0	0	0	0	0
5.3	Boiling	V	0	0	0	0	0	0
5.4	Density	V	0	0	0	0	0	0
5.5	Vapour pressure	V	0	0	0	0	0	0
5.6	Surface tension	V	0	0	0	0	0	0
5.7	Water solubility	V	0	0	0	0	0	0
5.8	Water extractivity	V	0	0	0	0	0	0
5.9	Log Pow	V	0	0	0	0	0	0
5.10	Flash-point	V	0	0	0	0	0	0
5.11	Flammability	V	0	0	0	0	0	0
5.12	Explosive properties	V	0	0	0	0	0	0
5.13	Self-ignition temp.	V	0	0	0	0	0	0
5.14	Oxidising properties	V	0	0	0	0	0	0
5.15	Granulometry	V	0	0	0	0	0	0
5.16	Light stability	VI	0	0	0	0	0	0
5.17	Long-term extractivity	VI	0	0	0	0	0	0
5.18	Stability organic solvent	VII	0	0	0	0	0	0
5.19	Dissociation constant	VII	0	0	0	0	0	0
5.20	Viscosity	VII	0	0	0	0	0	0
5.21	Reactivity	VII	0	0	0	0	0	0
6.1	Skin irritation/corrosion	V	3060	0	0	0	3060	10.4%
6.1.1	In vivo skin irritation	VI	0	565	263	61	889	3.0%
6.2	Eye irritation	V	5354	0	0	0	5354	18.2%
6.2.1	In vivo eye irritation	VI	0	989	460	107	1556	5.3%
6.3	Skin sensitisation	V	7012	1818	845	619	10293	35.1%
6.4.1	Gene mutation bacteria	V	2295	424	197	0	2916	9.9%
6.4.2	Cytogenicity mam. cells	V	2295	424	197	0	2916	9.9%
6.4.3	Gene mutation mam. cells	VI	0	275	25	0	299	1.0%
6.4.4	Further mutagenicity	VIII	4470	1159	549	402	6580	22.4%
6.5.1	Acute oral tox	VI	0	381	177	0	559	1.9%
6.5.2	Acute inhalation tox	VI	0	496	230	0	726	2.5%
6.5.3	Acute dermal tox	VI	0	397	184	0	581	2.0%
6.6.1	Short-term repeated dose	VI	0	860	315	0	1175	4.0%
6.6.2	Sub-chronic tox	VII	0	290	320	325	935	3.2%
6.6.3	Long-term repeated tox	VIII	0	0	0	144	144	0.5%
6.7.1	Developm. tox screening	VI	0	892	415	0	1307	4.5%
6.7.2	Developm. tox study	VI	0	492	1401	1000	2893	9.9%
6.7.3	Two-generation reprotox	VII	0	579	275	1281	2135	7.3%
6.8.1	Toxicokinetics	VI	0	4131	2289	2704	9124	31.1%
6.9	Carcinogenicity	VIII	0	0	0	121	121	0.4%
7.1.1	Short-term daphnia	V	3060	708	329	0	4096	14.0%
7.1.2	Growth inhibition algae	V	3825	991	461	0	5277	18.0%
7.1.3	Short-term fish	VI	0	708	329	0	1036	3.5%
7.1.4	Active sludge resp.	VI	0	2644	1229	744	4616	15.7%
7.1.5	Long-term daphnia tox	VII	538	135	128	124	925	3.2%
7.1.6	Long-term fish tox	VII	0	135	128	130	394	1.3%
7.2.1.1	Ready biodeg	V	2065	381	177	0	2624	8.9%
7.2.1.2	Simulation surface water	VII	0	319	158	173	649	2.2%
7.2.1.3	Simulation soil	VII	0	60	30	32	122	0.4%
7.2.1.4	Simulation sediment	VII	0	60	30	32	122	0.4%
7.2.1.5	Confirmatory biodeg rates	VIII	0	0	0	22	22	0.1%
7.2.2.1	Hydrolysis	VI	0	1851	860	715	3425	11.7%
7.2.3	Deg. products	VII	0	0	25	27	52	0.2%
7.3.1	Adsorption/desorption	VI	0	529	246	346	1121	3.8%
7.3.2	Accumulation	VII	0	0	293	242	535	1.8%
7.3.3	Further a/d studies	VII	0	0	25	27	52	0.2%
7.3.4	Further fate & behaviour	VIII	0	0	0	27	27	0.1%
7.4.1	Short-term earthworm	VII	0	0	103	85	188	0.6%
7.4.2	Soil micro-organisms	VII	0	0	46	38	84	0.3%
7.4.3	Short-term plants	VII	0	0	103	83	186	0.6%
7.4.4	Long-term earthworm	VIII	0	0	0	108	108	0.4%
7.4.5	Long-term invertebrates	VIII	0	0	0	108	108	0.4%
7.4.6	Long-term plant	VIII	0	0	0	108	108	0.4%
7.5	Long-term sediment	VIII	0	0	0	216	216	0.7%
7.6	Long-term bird	VIII	0	0	0	22	22	0.1%
8	Other relevant information	V	19200	4977	2461	2704	29342	100.0%
9	Analytical methods	VII	0	0	192	211	403	1.4%
								Check
			53173	27668	15490	13089	109420	109420

Cost estimate of test needs

Annex V-VIII	Information	Annex	Cost/test (EURO)	Annex V (KEURO)	Annex VI (KEURO)	Annex VII (KEURO)	Annex VIII (KEURO)	Total cost (KEURO)	Remarks on test costs
5.1	State	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.2	Melting/freezing	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.3	Boiling	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.4	Density	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.5	Vapour pressure	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.6	Surface tension	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.7	Water solubility	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.8	Water extractivity	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.9	Log Pow	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.10	Flash-point	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.11	Flammability	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.12	Explosive properties	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.13	Self-ignition temp.	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.14	Oxidising properties	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.15	Granulometry	V	0	0	0	0	0	0	0 Assumed to be available, no costs
5.16	Light stability	VI	0	0	0	0	0	0	0 Assumed to be available, no costs
5.17	Long-term extractivity	VI	0	0	0	0	0	0	0 Assumed to be available, no costs
5.18	Stability organic solvent	VII	0	0	0	0	0	0	0 Assumed to be available, no costs
5.19	Dissociation constant	VII	0	0	0	0	0	0	0 Assumed to be available, no costs
5.20	Viscosity	VII	0	0	0	0	0	0	0 Assumed to be available, no costs
5.21	Reactivity	VII	0	0	0	0	0	0	0 Assumed to be available, no costs
6.1	Skin irritation/corrosion	V	885	2708	0	0	0	2708	
6.1.1	In vivo skin irritation	VI	885	0	500	232	54	787	
6.2	Eye irritation	V	948	5076	0	0	0	5076	
6.2.1	In vivo eye irritation	VI	948	0	938	436	101	1475	
6.3	Skin sensitisation	V	3925	27521	7134	3315	2428	40399	
6.4.1	Gene mutation bacteria	V	2300	5278	975	453	0	6706	Test prices from Safepharm
6.4.2	Cytogenicity mam. cells	V	18000	41306	7630	3545	0	52481	Test prices from Safepharm
6.4.3	Gene mutation mam. cells	VI	12000	0	3295	296	0	3591	Test prices from Safepharm
6.4.4	Further mutagenicity	VIII	19584	87536	22691	10757	7880	128864	
6.5.1	Acute oral tox	VI	1785	0	681	316	0	997	
6.5.2	Acute inhalation tox	VI	12725	0	6308	2931	0	9239	
6.5.3	Acute dermal tox	VI	2196	0	871	405	0	1276	
6.6.1	Short-term repeated dose	VI	41527	0	35714	13061	0	48775	
6.6.2	Sub-chronic tox	VII	118506	0	34327	37972	38528	110827	
6.6.3	Long-term repeated tox	VIII	359769	0	0	0	51754	51754	Including 6.9
6.7.1	Developm. tox screening	VI	19612	0	17499	8132	0	25631	
6.7.2	Developm. tox study	VI	164614	0	81060	230575	164657	476293	Two species
6.7.3	Two-generation reprotox	VII	176170	0	102059	48385	225606	376050	
6.8.1	Toxicokinetics	VI	0	0	0	0	0	0	0 Information derived from available int
6.9	Carcinogenicity	VIII	0	0	0	0	0	0	0 Included in 6.6.3
7.1.1	Short-term daphnia	V	3755	11489	2657	1235	0	15381	
7.1.2	Growth inhibition algae	V	4973	19020	4930	2291	0	26241	
7.1.3	Short-term fish	VI	5059	0	3580	1664	0	5244	
7.1.4	Active sludge resp.	VI	1931	0	5105	2372	1437	8914	
7.1.5	Long-term daphnia tox	VII	13990	7521	1891	1793	1737	12942	
7.1.6	Long-term fish tox	VII	18354	0	2481	2352	2390	7224	
7.2.1.1	Ready biodeg	V	12304	25412	4694	2181	0	32286	
7.2.1.2	Simulation surface water	VII	9694	0	3088	1527	1678	6292	
7.2.1.3	Simulation soil	VII	9694	0	579	286	315	1180	
7.2.1.4	Simulaton sediment	VII	9694	0	579	286	315	1180	
7.2.1.5	Confirmatory biodeg rates	VIII	9694	0	0	0	210	210	
7.2.2.1	Hydrolysis	VI	6091	0	11272	5238	4353	20864	
7.2.3	Deg. products	VII	20000	0	0	492	541	1033	Test cost is a guess
7.3.1	Adsorption/desorption	VI	2585	0	1367	635	895	2897	
7.3.2	Accumulation	VII	52692	0	0	15437	12766	28203	
7.3.3	Further a/d studies	VII	4266	0	0	105	115	220	
7.3.4	Further fate & behaviour	VIII	36000	0	0	0	973	973	
7.4.1	Short-term earthworm	VII	5467	0	0	563	466	1029	
7.4.2	Soil micro-organisms	VII	3000	0	0	138	114	251	
7.4.3	Short-term plants	VII	8115	0	0	836	671	1507	
7.4.4	Long-term earthworm	VIII	76000	0	0	0	8220	8220	
7.4.5	Long-term invertebrates	VIII	76000	0	0	0	8220	8220	
7.4.6	Long-term plant	VIII	76000	0	0	0	8220	8220	
7.5	Long-term sediment	VIII	76000	0	0	0	16440	16440	
7.6	Long-term bird	VIII	76000	0	0	0	1644	1644	
8	Other relevant information	V	0	0	0	0	0	0	0 Information derived from available int
9	Analytical methods	VII	4000	0	0	768	844	1611	Average of European contract institut
			Sum	232867	363904	401011	563572	1561355	1561355 Check
				14.9%	23.3%	25.7%	36.1%		
			Cost/subst. (KEURO)	12.1	73.1	162.9	208.4		
			Cost/tonne (EURO)	4043	2437	543	69		
			Cost/tonne 10 years (E	404	244	54	7		

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