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Supplementary Materials

Assessment of Potential Exposure to Research Chemicals in Academic Laboratories: Challenges and Opportunities for Scientists' Health Protection

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Table S1. P-scores assigned to the H-codes according to the most recent release of the MoVaRisCh document [28,29].

n	Cod	Phrase-ENG	P-Score	n	Cod	Phrase-ENG	P-Score
1	**H200**	Unstable explosives.	**1**	55	**H334**	May cause allergy or asthma symptoms or breathing difficulties if inhaled.	**9.0**
2	**H201**	Explosive; mass explosion hazard.	**1**	**56**	**H334**	May cause allergy or asthma symptoms or breathing difficulties if inhaled.	**8.0**
3	**H202**	Explosive, severe projection hazard.	**1**	**57**	**H334**	May cause allergy or asthma symptoms or breathing difficulties if inhaled.	**1**
4	**H203**	Explosive; fire, blast or projection hazard.	**1**	**58**	**H335**	May cause respiratory irritation.	**3.3**
5	**H204**	Fire or projection hazard.	**1**	**59**	**H336**	May cause drowsiness or dizziness.	**3.5**
6	**H205**	May mass explode in fire.	**1**	**60**	**H340**	May cause genetic defects []	**1**
7	**H220**	Extremely flammable gas.	**1**	**61**	**H341**	Suspected of causing genetic defects []	**8.0**
8	**H221**	Flammable gas.	**1**	**62**	**H350**	May cause cancer []	**1**
9	**H222**	Extremely flammable aerosol.	**1**	**63**	**H351**	Suspected of causing cancer []	**8.0**
10	**H223**	Flammable aerosol.	**1**	**64**	**H360**	May damage fertility or the unborn child []	**1**
11	**H224**	Extremely flammable liquid and vapour.	**1**	**65**	**H361**	Suspected of damaging fertility or the unborn child []	**8.0**
12	**H225**	Highly flammable liquid and vapour.	**1**	**66**	**H361d**	Suspected of damaging the unborn child	**7.5**
13	**H226**	Flammable liquid and vapour.	**1**	**67**	**H361f**	Suspected of damaging fertility	**7.5**
14	**H228**	Flammable solid.	**1**	**68**	**H361fd**	Suspected of damaging fertility. Suspected of damaging the unborn child	**8.0**
15	**H240**	Heating may cause an explosion.	**1**	**69**	**H362**	May cause harm to breast-fed children.	**6.0**
16	**H241**	Heating may cause a fire or explosion.	**1**	**70**	**H370**	Causes damage to organs []	**9.5**
17	**H242**	Heating may cause a fire.	**1**	**71**	**H371**	May cause damage to organs []	**8.0**
18	**H250**	Catches fire spontaneously if exposed to air.	**1**	**72**	**H372**	Causes damage to organs [] through prolonged or repeated exposure []	**8.0**
19	**H251**	Self-heating: may catch fire.	**1**	**73**	**H373**	May cause damage to organs [] through prolonged or repeated exposure []	**7.0**
20	**H252**	Self-heating in large quantities; may catch fire.	**1**	**74**	**H400**	Very toxic to aquatic life.	**1**
21	**H260**	In contact with water releases flammable gases which may ignite spontaneously.	**1**	**75**	**H410**	Very toxic to aquatic life with long lasting effects.	**1**
22	**H261**	In contact with water releases flammable gases.	**1**	**76**	**H411**	Toxic to aquatic life with long lasting effects.	**1**
23	**H270**	May cause or intensify fire; oxidiser.	**1**	**77**	**H412**	Harmful to aquatic life with long lasting effects.	**1**
24	**H271**	May cause fire or explosion; strong oxidiser.	**1**	**78**	**H413**	May cause long lasting harmful effects to aquatic life.	**1**
25	**H272**	May intensify fire; oxidiser.	**1**	**79**	**EUH001**	Explosive when dry.	**1**
26	**H280**	Contains gas under pressure; may explode if heated.	**1**	**80**	**EUH014**	Reacts violently with water.	**1**
27	**H281**	Contains refrigerated gas; may cause cryogenic burns or injury.	**1**	**81**	**EUH018**	In use may form flammable/explosive vapour-air mixture.	**1**
28	**H290**	May be corrosive to metals.	**1**	**82**	**EUH019**	May form explosive peroxides.	**1**
29	**H300_1**	Fatal if swallowed.	**3.0**	**83**	**EUH029**	Contact with water liberates toxic gas.	**3.0**
30	**H300_2**	Fatal if swallowed.	**2.5**	**84**	**EUH031**	Contact with acids liberates toxic gas.	**3.0**
31	**H300**	Fatal if swallowed.	**1**	**85**	**EUH032**	Contact with acids liberates very toxic gas.	**3.5**

Table S1. *Cont*.

n	Cod	Phrase-ENG	P-Score	n	Cod	Phrase-ENG	P-Score
32	**H301**	Toxic if swallowed.	**2.3**	**86**	**EUH044**	Risk of explosion if heated under confinement.	**1**
33	**H302**	Harmful if swallowed.	**2.0**	**87**	**EUH066**	Repeated exposure may cause skin dryness or cracking.	**2.5**
34	**H304**	May be fatal if swallowed and enters airways.	**5.0**	**88**	**EUH070**	Toxic by eye contact	**6.0**
35	**H310_1**	Fatal in contact with skin.	**6.5**	**89**	**EUH071**	Corrosive to the respiratory tract.	**6.5**
36	**H310_2**	Fatal in contact with skin.	**5.5**	**90**	**EUH201A**	Warning! Contains lead.	**1**
37	**H310**	Fatal in contact with skin.	**1**	**91**	**EUH201**	Contains lead. Should not be used on surfaces liable to be chewed or sucked by children.	**6.0**
38	**H311**	Toxic in contact with skin.	**4.5**	**92**	**EUH202**	Cyanoacrylate. Danger. Bonds skin and eyes in seconds. Keep out of the reach of children.	**4.5**
39	**H312**	Harmful in contact with skin.	**3.0**	**93**	**EUH203**	Contains chromium (VI). May produce an allergic reaction.	**4.5**
40	**H314_1A**	Causes severe skin burns and eye damage.	**6.3**	**94**	**EUH204**	Contains isocyanates. May produce an allergic reaction.	**7.0**
41	**H314_1B**	Causes severe skin burns and eye damage.	**5.8**	**95**	**EUH205**	Contains epoxy constituents. May produce an allergic reaction.	**4.5**
42	**H314_1C**	Causes severe skin burns and eye damage.	**5.5**	**96**	**EUH206**	Warning! Do not use together with other products. May release dangerous gases (chlorine).	**3.0**
43	**H314**	Causes severe skin burns and eye damage.	**1**	**97**	**EUH207**	Warning! Contains cadmium. Dangerous fumes are formed during use. See information supplied by the manufacturer. Comply with the safety instructions.	**8.0**
44	**H315**	Causes skin irritation.	**2.5**	**98**	**EUH208**	Contains (name of sensitising substance). May produce an allergic reaction.	**4.0**
45	**H317_1A**	May cause an allergic skin reaction.	**6.0**	**99**	**EUH209A**	Can become flammable in use.	**1**
46	**H317_1B**	May cause an allergic skin reaction.	**4.5**	**100**	**EUH209**	Can become highly flammable in use.	**1**
47	**H317**	May cause an allergic skin reaction.	**1**	**101**	**EUH210**	Safety data sheet available on request.	**1**
48	**H318**	Causes serious eye damage.	**4.5**	**102**	**EUH211**	Warning! Hazardous respirable droplets may be formed when sprayed. Do not breathe spray or mist.	**5.5**
49	**H319**	Causes serious eye irritation.	**3.0**	**103**	**EUH212**	Warning! Hazardous respirable dust may be formed when used. Do not breathe dust.	**5.5**
50	**H330**	Fatal if inhaled.	**8.5**	**104**	**EUH380**	May cause endocrine disruption in humans	**10.0**
51	**H330**	Fatal if inhaled.	**7.5**	**105**	**EUH381**	Suspected of causing endocrine disruption in humans	**8.0**
52	**H330**	Fatal if inhaled.	**1**	**106**	**EUH401**	To avoid risks to human health and the environment, comply with the instructions for use.	**1**
53	**H331**	Toxic if inhaled.	**6.0**				
54	**H332**	Harmful if inhaled.	**4.5**				

Note. When no P-score is assigned, a default value of 1 is reported.

Table S2. List and main toxicological and regulatory properties of the 60 substances involved in the preparation of the 54 products described in ref [22], for which documentation is available.

	Chemical Substance	Role	CAS	H-codes	MW	Cat	GcHIx	Exposure Limits
1	water	A	7732-18-5	considered as wastewater	18.02	C	0.0	
2	1 N HCl	A	7647-01-0	H290 H314 H318 H335	36.50	B	15.0	
3	NaOH 1N	A	1310-73-2	H290 H314 H318	40.00	B	11.8	
4	LiOH (monohydrate)	A	1310-66-3	H302 H314 H318	41.96	B	12.8	
5	NH4Cl	A	12125-02-9	H302 H319	53.49	B	5.0	
6	NaCl (brine)	A	7647-14-5	not hazardous	58.44	B	0.0	
7	SiO_2 silica gel for chromatography	A	7631-86-9	not hazardous	60.08	B	0.0	
8	Sodium acetate	A	127-09-3	not hazardous	82.03	B	0.0	
9	$NaHCO_3$	A	497-19-8	H319	84.00	B	3.0	
10	Na_2CO_3	A	497-19-8	H319	105.99	B	3.0	
11	$NaHSO_4$ 1 M	A	681-38-1	H318	120.10	B	4.5	
12	K_2CO_3	A	584-08-7	H315 H319 H335	138.21	B	8.8	
13	Na_2SO_4	A	7757-82-6	not hazardous	142.04	B	0.0	
14	NaH	R	7646-69-7	H228 H260 H290 H314 H318	24.00	B	13.8	
15	Iron powder	R	7439-89-6	H228	56.00	B	1.0	
16	Allyl alcohol	R	107-18-6	H301 H331 H310 H315 H319 H361fd H335 H400 H410 H412	58.08	A	34.0	
17	hydroxylamine water sol NH_2OH 50% W	R	7803-49-8	H290 H302 H312 H315 H317 H319 H351 H373 H410 H411	69.49	B	34.5	
18	Triethylamine	R	121-44-8	H225 H331 H311 H314 H318 H335 H301	101.19	A	27.8	
19	hydroxylamine-OTMS NH_2OTMS	R	22737-36-6	H225 H314	105.21	B	7.3	
20	L-proline	R	147-85-3	not hazardous	115.13	B	0.0	
21	N,N-dimethylaniline	R	121-69-7	H301 + H311 + H331 H351 H411	121.18	A	21.5	
22	dimethylaminopyridine DMAP	R	1122-58-3	H301+H331 H310 H315 H318 H370 H411	122.17	B	22.8	
23	2,4-diamino-6-hydroxypyrimidine	R	56-06-4	H315 H319	126.12	B	5.5	
24	5-methylindole	R	614-96-0	H315 H319 H335	131.17	B	8.8	
25	1-Hydroxybenzotriazole HOBt	R	2592-95-2	H203 H319 H412	135.12	B	5.0	
26	Phosphorus oxychloride $POCl_5$	R	10025-87-3	H302 H314 H330 H372 EUH014 EUH029	153.33	A	28.8	
27	Azobis-isobutyronitrile AIBN	R	78-67-1	H242 H302+H332 H412	164.21	B	8.5	
28	4-chloro-7H-pyrrolo[2,3-d]pyrimidin-2-amine	R	84955-31-7	H319	168.59	B	3.0	
29	6-chloro-9H-purin-2-amine	R	10310-21-1	H315 H319 H335	169.57	B	8.8	

30	5-(chloromethyl)benzo[d][1,3]dioxole	R	20850-43-5	H315 H319 H335 H351 H272	170.59	B	16.8	
31	N-Bromosuccinimmide NBS	R	128-08-5	H290 H315 H317 H319 H341 H400	177.98	B	22.5	
32	N-(3-dimetilaminopropil)-N′-etilcarbodiimide EDCI	R	25952-53-8	H302 H311 H315 H319 H317 H373 H400 H410	191.70	B	27.0	
33	1-(bromomethyl)-4-nitrobenzene	R	586-78-7	H302	202.01	B	2.0	
34	di-t-butylcarbonate Boc_2O	R	24424-99-5	H301+H331 H310 H315 H318 H370 H411	218.25	B	32.3	
35	Methyl 2-(bromomethyl)oxazole-4-carboxylate	R	175551-77-6	H302 H315 H319 H335	220.02	B	10.8	
36	2-(4-(bromomethyl)-2-chlorophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane	R	166330-03-6	H302 H312 H315 H319 H332 H335	220.90	B	18.3	
37	2-(chloromethyl)-4-methoxy-3,5-dimethylpyridine	R	86604-75-3	H315 H319 H317 H335 H413	222.11	B	15.8	
38	Pd(OAc)2	R	3375-31-3	H318 H317 H400 H410	224.51	B	12.5	
39	N-Iodosuccinimide NIS	R	516-12-1	H315 H319 H317 H341 H400 H410	224.98	B	21.5	
40	Benzyltriethylammonium chloride	R	56-37-1	H315 H319 H335	227.77	B	8.8	
41	Methyl 4-(bromomethyl)benzoate	R	2417-72-3	H290 H314 H318	229.07	B	11.8	
42	Methyl 5-(bromomethyl)thiophene-2-carboxylate	R	108499-32-7	H302 H314 H318_1	235.10	B	12.8	
43	Ethyl 4-iodobenzoate	R	51934-41-9	no-haz	276.07	B	0.0	
44	5-bromo-6-(bromomethyl)benzo[d][1,3]dioxole	R	5434-47-9	not assigned	293.94	B	0.0	
45	2-(4-(bromomethyl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane	R	138500-85-3	H315 H319	297.00	B	5.5	
46	Cs_2CO_3	R	534-17-8	H318 H361f H373	325.80	B	19.5	
47	$Pd(PPh_3)_4$	R	14221-01-3	H302	1155.56	B	2.0	
48	Methyl alcohol (chromatography)	S	67-56-1	H225 H301 H331 H311 H370	32.10	A	23.3	8h; 260 mg/m^3; STEL15: N.ass. TLV-C: N.ass. Skin
49	Acetonitrile (dry)	S	75-05-8	H225 H302 H332 H312 H319	41.05	A	13.5	8h: 35 mg/m^3 STEL15: N.ass. TLV-C: N.ass. Skin
50	ethyl alcohol	S	64-17-5	H225 H319	46.07	A	4.0	
51	Dichloromethane DCM (dry)	S	75-09-2	H315 H319 H351 H336	50.10	A	17.0	8h; 175 mg/m^3 STEL15; 353 mg/m^3; TLV-C: N.ass. Skin

Table S2. *Cont*.

	Chemical Substance	Role	CAS	H-codes	MW	Cat	GcHIx	Exposure Limits
52	tetrahydrofuran THF	S	109-99-9	H225 H302 H319 H351 H335 H336 EUH019	72.11	A	21.8	8h; 150 mg/m^3; STEL15; 300 mg/m^3; TLV-C: N.ass. Skin
53	Dimethylformamide DMF (dry)	S	68-12-2	H226 H312+H332 H319 H360D	73.09	A	19.5	not in Italy
54	diethyl-ether Et_2O	S	60-29-7	H224 H302 H336 EUH019 EUH066	74.12	A	10.0	not in Italy
55	n-hexane	S	110-54-3	H225 H315 H361f H336 H372 H304 H411	86.18	A	21.0	8h; 72 mg/m^3; STEL15: N.ass TLV-C: N.ass. Skin: N.ass
56	ethyl acetate	S	141-78-6	H225 H319 H336	88.10	A	7.5	8h; 734 mg/m^3; STEL15; 1468 mg/m^3; TLV-C: N.ass. Skin: N.ass
57	1,4-dioxane	S	123-91-1	H225 H319 H335 H350 EUH019 EUH066	88.11	A	11.8	8h; 73 mg/m^3; STEL15; N.ass. TLV-C: N.ass. Skin
58	toluene	S	108-88-3	H225 H315 H361d H336 H373 H304 H412	92.14	A	27.5	8h; 192 mg/m^3; STEL15; 384 mg/m^3; TLV-C: N.ass. Skin
59	2,2,2-Trifluoroethanol TFE	S	75-89-8	H226 H301+H331 H318 H360F H373	100.00	A	28.3	not in Italy
60	Carbon tetrachloride CCl4	S	56-23-5	H301 H331 H311 H317 H351 H372 H412 H420	153.82	A	35.8	8h; 6.4 mg/m^3; STEL15; 32 mg/m^3; TLV-C: N.ass. Skin

Notes. [a]: Chemical substances are listed in the following order: S (solvent, n); R (reagent, n); A (auxiliary, n); P (reaction product, n); next in the order of their classification according to available information [c]: next by increasing molecular mass [b]: preparation as described in the article; [c]: substance classification (A: substance with exposure limits); B (substance with SDS but no exposure limits; C (substance without SDS); [d]: H phrases in the SDS; [e]: Exposure limits (TLVs in Italy, from All. XXXVIII and XLIII of Decree 81/08); [f]: Hazard Index calculated for Health (toxic) effects according to the gravity factors of the Inforisk RA tool [24]; [g]: Hazard Index for non-health effects (fire and explosion) expressed as the number of Hazard codes reported in the SDS; [h]: Exempt from. REACH registration.