



Environment
Agency



Toxicological advice on air pollutants

Hazard Ranking of Substances for Development of EALs for Substance Emissions to Air from Carbon Capture Technologies

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Author(s):

Dr Sarah Bull & Dr Jo Wilding

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Research contractor:

Cambridge Environmental Assessments, part of RSK ADAS Ltd. Battlegate Road,
Boxworth, Cambridgeshire, CB23 4NN.

Environment Agency's Project Manager:

David Howard

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Executive summary

The objective of this task was to undertake the prioritisation of a list for the development of Environmental Assessment Levels (EALs) for air relating to substances proposed for use in amine-based carbon capture technologies including their primary breakdown products. The prioritisation was based on an existing prioritisation methodology, developed for published EALs in 2021/22, which was based on 1) a screening assessment of their relative hazard to human health, and 2) the availability of updated authoritative opinions.

Hazard classifications were collated for all substances. Hazards were scored according to severity and route of exposure, focussing on classifications that have been agreed in Europe and are legally binding (i.e. harmonised classifications) or those proposed by industry (notified classifications) relating to inhalation exposure or exposure via air (e.g. eye irritation). Sixteen of the 40 substances had a harmonised hazard classification, 14 had a notified classification, and ten have no data.

For many substances, only notified classifications or no data were available. Therefore, an additional screening assessment was undertaken for these substances to try and fill the data gaps and improve confidence in the hazard ranking. Substances assigned to Cramer class II or III were assessed for structural alerts for carcinogenicity, mutagenicity, and skin sensitisation (as a proxy for respiratory sensitisation). Chemicals were also scored according to their review by authoritative bodies.

Three of the 14 notified substances were assigned a Cramer class III, as were all ten of the substances with no data. Therefore, 13 were assessed for structural alerts for mutagenicity, carcinogenicity, and skin sensitisation.

The highest-ranking chemicals based on harmonised classifications (Group 1), notified classifications and structural alerts (Group 2), and structural alerts (Group 3) were identified.

Introduction

The Environment Agency regulates chemical emissions from industrial and waste management activities under the Environmental Permitting Regulations 2016 (as amended). Horizontal Guidance document H1 is the principal guidance on environmental risk assessment for new permit applications. Applicants use H1 to identify and manage significant emissions that could impact public health and the environment.

In assessing risks to health, H1 recommends that predicted emissions are screened against EALs for the chemicals of concern. EALs are defined as air concentrations indicative of non-appreciable or minimal concern to health from short- or long-term inhalation exposure. They cover about 90 substances including industrial chemicals and classical air pollutants.

The Environment Agency published its current methodology for the derivation of EALs in 2012 with a greater emphasis on a robust review of the scientific evidence on adverse health effects (EA, 2012). Working in partnership with the UK Health Security Agency (formerly Public Health England) and industry, the Environment Agency seeks to update EALs in line with the latest scientific evidence.

Post combustion carbon capture (PCC) technologies using amine-based systems are an emerging approach to reducing carbon dioxide emissions from fossil fuel energy production. New or retrofitted PCC installations are an important part of the UK strategy to achieve Net Zero by 2050. Installations will be permitted under the Environmental Permitting Regulations (England and Wales) 2016, as amended, to identify and mitigate risks to human health and the wider environment.

Amine-based systems used in PCC release small quantities of spent solvent and their transformation products to air and water under normal operating conditions. These chemical emissions are an important consideration in the application for an environmental permit, and the EA relies on EALs to identify and mitigate potential operational risks through the permitting process. Operators are required to review of the scientific evidence on adverse health effects of their potential emissions and to identify suitable EALs.

The main objective of the current project was to prioritise the substances proposed for use by amine-based carbon capture technologies including their main breakdown products, in order to inform future development of EALs for air. The substances reviewed are set out in Table 1.

Methodology

The methodology by which a prioritised list of substances was determined is outlined below.

Step 1. Collating the original list of chemicals

A list of substances, abbreviations and CAS Numbers was provided by the Environment Agency (see Table 1).

Table 1. List of substances (shaded chemicals are breakdown products)

Substance	Cas Nos	Abbreviation	Chemical group
Ethanolnitramine	74386-82-6	MEA-NO ₂	Nitramine
Dimethylamine	124-40-3	DMA	Secondary amine
Dimethylnitramine	4164-28-7	DMA-NO ₂	Nitramine
Piperazine	110-85-0	PZ	Secondary amine
Mononitropiperazine (1-nitropiperazine)	42499-41-2	MNPZ	Nitramine
Nitrosopiperazine	5632-47-3	NPZ	Nitrosamine
2-amino-2-methyl-propanol	124-68-5	AMP	Primary amine
2-methyl-2-(nitroamino)-1-propanol	1239666-60-4	AMP-NO ₂	Nitramine
Diethanolamine	111-42-2	DEA	Secondary amine
N-nitroso-diethanolamine	1116-54-7	NDELA	Nitrosamine
Nitrodiethanolamine	4185-47-1	DEA-NO ₂	Nitramine
Diethylamine/ethylethanamine	109-89-7 / 61193-06-4	DiEA	Secondary amine

N-nitrosodiethylamine	55-18-5	NDEA	Nitrosamine
Diethylnitramine	7119-92-8	DiEA-NO2	Nitramine
Ethylamine	75-04-7	EA	Primary amine
Trimethylamine	75-50-3	TMA	Tertiary amine
Methylamine	74-89-5	MMA/MA	Primary amine
N-nitromethanamine	598-57-2	MA-NO2	Nitramine
N-(2-hydroxyethyl) ethylenediamine (dihydrochloride)	20267-35-0	HEEDA	Primary amine/ Secondary amine
Morpholine	110-91-8	MOR	Secondary amine
N-nitrosomorpholine	59-89-2	NMOR	Nitrosamine
N-nitromorpholine	4164-32-3	MOR-NO2	Nitramine
Ethylenediamine	107-15-3	EDA	Primary amine
Methyldiethanolamine	42977-89-9	MDEA	Tertiary amine
N-Methyldiethanolamine	105-59-9	MDEA	Tertiary amine
2-(diethylamino)ethanol	100-37-8	DEELA	Tertiary amine
N-ethyl-diethanolamine	139-87-7	EDELA	Tertiary amine
Glycine	56-40-6	GLY	Primary amine
N-(2-hydroxyethyl) glycine	5835-28-9	HEGLY	Secondary amine
Methylethanolamine/mono methylethanolamine	109-85-3/ 6909-61-1	MMEA	Secondary amine / Primary amine
N-nitroso-(2-hydroxyethyl)glycine	80556-89-4	NHEGLY	Nitrosamine
N-nitrosopiperidine	100-75-4	NPIP	Nitrosamine

Triethylamine	121-44-8	TEA	Tertiary amine
Triethanolamine	102-71-6	TELA	Tertiary amine
Tris(hydroxymethyl)amino methane	77-86-1	TRIS	Primary amine
Monoethanolamine**	141-43-5	MEA	Primary amine
N-nitrosodimethylamine**	62-75-9	NDMA	Nitrosamine
1. 2-(Ethylamine) ethanol	110-73-6	EAE	Secondary amine
N-Ethyl-N(2Hydroxyethyl) nitrosamine	13147-25-6	EHEN	Nitrosamine
3-Aminopropanol	156-87-6	-	Primary amine

Step 2. Collating hazard data

Harmonised hazard classifications¹ were collated from the European Chemicals Agency (ECHA) database (<https://echa.europa.eu/>). If not available, notified² hazard classifications were collated.

Only hazards that could occur following exposure to a chemical via inhalation exposure were noted, including acute toxicity, eye irritation, mutagenicity, carcinogenicity, reproductive toxicity, specific target organ toxicity following a single exposure (STOT SE) and specific target organ toxicity following repeated exposure (STOT RE). Data were collected in terms of the hazard statement code (e.g. H331) and the health hazard statement (e.g. toxic if inhaled).

For endpoints such as reproductive toxicity, STOT SE, STOT RE and carcinogenicity, if the supporting data in the REACH dossier (if available) clearly identified the route of exposure to be other than inhalation (e.g. via oral or dermal exposure) the hazard statement codes were excluded. Where the route of exposure was not definitively known, the hazard classifications were included in the dataset as a precautionary approach.

¹ A harmonised classification is a legally binding minimum classification for a substance.

² Substances must be notified to the Classification and Labelling (C&L) Inventory regarding their substance identity, classification and identity. Hence notified hazard classifications are those submitted to the C&L inventory.

Step 3. Scoring chemicals according to hazard classifications

Step 3a. Scoring based on hazard classifications

Hazard classifications were assigned a score of 1-3 according to the severity of the classification as shown in Table 2.

Table 2. Scores for endpoints based on hazard classifications

Score	Acute inhalation	Eye irritation	Mutagenicity	Carcinogenicity	Reproductive toxicity	STOT SE	STOR RE	Respiratory sensitisation	Skin sensitisation
Score 1	H332 Harmful if inhaled					H336 May cause respiratory irritation			
Score 2	H331 Toxic if inhaled	H319 Causes serious eye irritation	H341 Suspected of causing genetic defects	H351 Suspected of causing cancer	H361 ³ Suspected of damaging fertility or the unborn child	H335 May cause drowsiness or dizziness	H373 May cause damage to organs through prolonged or repeated exposure	H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.	H317 May cause an allergic skin reaction
Score 3	H330 Fatal if inhaled	H318 Causes serious eye damage	H340 May cause genetic defects	H350 ⁴ May cause cancer	H360 ⁵ May damage fertility or the unborn child	H370 Causes damage to organs	H372 Causes damage to organs through prolonged or repeated exposure		

STOT SE; specific non-lethal effects on organs or organ systems following a single exposure to a chemical.

STOT RE; specific toxicity on organs or organ systems arising from repeated exposure to a chemical. This is an example of a chronic effect.

The sum of the scores was calculated.

³ Includes H361d – Suspected of damaging the unborn child; H361f - Suspected of damaging fertility; H361fd - Suspected of damaging fertility. Suspected of damaging the unborn child.

⁴ Includes H350i - May cause cancer by inhalation.

⁵ Includes H360D - May damage the unborn child; H360FD - May damage fertility. May damage the unborn child; H350Fd - May damage fertility. Suspected of damaging the unborn child; H360Df - May damage the unborn child. Suspected of damaging fertility.

For example, dimethylamine (CAS No. 124-40-3) has a harmonised classification for H332 (harmful if inhaled; score = 1), H318 (causes serious eye damage; score = 3) and H335 (may cause respiratory irritation; score = 2). The sum of the scores is six.

Step 3b. Identification of Cramer class

For substances with notified classifications or those for which there are no data, Toxtree v3.10⁶ was used to determine the Cramer class to estimate the relative hazard.

The Cramer Decision Tree classifies organic chemicals into one of three classes, namely I (low), II (intermediate) and III (high), which reflects the probability of low, moderate, or high toxicity (Roberts et al., 2015). More specifically,

- Class I represents substances with simple chemical structures and for which efficient modes of metabolism exist, suggesting a low order of oral toxicity. This class would include normal constituents of the body (excluding hormones); simply-branched, acyclic aliphatic hydrocarbons; common carbohydrates; common terpenes; substances that are sulfonate or sulfamate salts, without any free primary amines.
- Class II represents substances which possess structures that are less innocuous than Class I substances, but do not contain structural features suggestive of toxicity like those substances in Class III. This class would include common components of food; substances containing no functional groups other than alcohol, aldehyde, side-chain ketone, acid, ester, or sodium, potassium, or calcium sulfonate or sulfamate, or acyclic acetal or ketal and are either a monocycloalkanone or a bicyclic substance with or without a ring ketone.
- Class III are substances with chemical structures that permit no strong initial presumption of safety or may even suggest significant toxicity or have reactive functional groups. This class would include structures that contain elements other than carbon, hydrogen, oxygen, nitrogen or divalent sulphur; certain benzene derivatives; certain heterocyclic substances; aliphatic substances containing more than three types of functional groups (EFSA, 2019).

The chemical structure of each chemical was translated into Simplified Molecular Input Line Entry System (SMILES) notation, based on information collated from PubChem, peer reviewed literature or using an online convertor. The SMILES notation for each chemical was entered into the Revised Cramer Decision Tree in Toxtree v3.10 to identify the probable Cramer class.

⁶ <http://toxtree.sourceforge.net/>

Step 3c. Scoring based on structural alerts

Due to the lack of robust data for substances with notified classifications (Group 2) or lack of data (Group 3) for some substances, structural alerts for a number of endpoints were identified for substances classified as Cramer class II (intermediate toxicity) or III (high toxicity) in Step 3b. Due to time constraints, and their likely impact on prioritisation, the identification of structural alerts was not carried out for substances classified as Cramer class I (low toxicity). Where a substance already had a notified hazard classification for an endpoint, structural alerts for that endpoint were not investigated.

Structural alerts were derived from Toxtree v3.10, based on SMILES codes, for carcinogenicity, mutagenicity and skin sensitisation⁷ using the following decision trees:

- carcinogenicity and mutagenicity
 - genotoxicity and non-genotoxicity rulebase by ISS
 - DNA binding alerts
- mutagenicity
 - *in vitro* mutagenicity (Ames test) alerts by ISS
 - structure alerts for the *in vivo* micronucleus assay in rodents)
- skin sensitisation as a proxy for respiratory sensitisation
 - reactivity domains
 - protein binding alerts

If a structural alert was identified for any endpoint, the substance was considered to be positive and allocated the following classifications:

- H341 – suspected of causing genetic defects
- H351 – suspected of causing cancer
- H317 – may cause an allergic skin reaction

These hazard classifications were then scored according to Table 2. Due to classifications being based on modelled data, score 3 i.e. H340 (may cause genetic damage) and H350 (may cause cancer) was not allocated due to the uncertainty in the modelled data.

⁷ The potential of a substance to elicit respiratory sensitisation is not a hazard endpoint that can be predicted in Toxtree using structural alerts. Therefore, skin sensitisation was used as a proxy for respiratory sensitisation.

The sum of the scores for the hazard classifications (notified substances) and scores for modelled data was calculated.

Step 4. Scoring chemicals according to toxicological reviews

Toxicological reviews collated are presented in Table 3.

Table 3. Authoritative body toxicological reviews

Authoritative body	Dataset
Agency for Toxic Substances and Disease Registry (ATSDR)	Toxicological profiles
World Health Organisation (WHO)	International Programme on Chemical Safety (IPCS) WHO International Agency for Research on Cancer (IARC)
US Environmental Protection Agency (US EPA)	Integrated Risk Information System (IRIS) Acute Exposure Guideline Levels for Airborne Chemicals (AEGs)
Organisation for Economic Co-operation and Development (OECD) Chemicals Database	Screening Information Dataset (SIDS) Chemicals identified as a High Production Volume (HPV) chemical
European Chemicals Agency (ECHA)	Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) dossiers Harmonised Classification and Labelling (CLH) dossiers Substances of Very High Concern (SVHC) dossiers
Australian Industrial Chemicals Introduction Scheme (AICIS)	Tier II assessments (human health)
Health Canada	Screening Assessment Priority Substance List Assessment

Any toxicological review was given a score of 1. The scores were summed.

For example, n-nitrosodimethylamine (CAS No. 62-75-9) had five toxicological reviews (ATSDR, WHO IPCS, WHO IARC, US EPA IRIS, Health Canada), so was assigned a score of 5. Piperazine (CAS No. 110-85-0) had two toxicological reviews (REACH dossier, AICIS2) so was assigned a score of 2.

Step 5. Overall prioritisation

Prioritisation was based on the total hazard score determined in Step 3. Because of the additional uncertainty in the reporting of harmonised and notified substances, the prioritisation was reported separately for each group: (i) substances with harmonised classifications (Group 1), substances with notified classifications (Group 2) or substances with no data (Group 3). The score for the availability of relevant toxicological reviews by authoritative bodies is reported for each substance, but it was not used to prioritise substances in each table.

Results

Step 1. Collating the original list of chemicals

The substance list comprised 40 substances (Table 1).

Step 2. Collating hazard data

Sixteen of the 40 substances had a harmonised hazard classification, 14 of 40 had a notified classification, and ten of 40 did not have data due to not having been assessed by ECHA.

Step 3. Scoring chemicals according to hazard

Step 3a. Scoring based on harmonised or notified classifications

Hazard classifications were assigned a score of one to three according to the severity of the endpoint, as shown in Table 2.

Table and Table show the number of substances that were assigned scores for each hazard endpoint based on harmonised classifications (Group 1) and notified classifications (Group 2), respectively.

Table 4. Number of substances with harmonised classifications per endpoint (Group 1)

Score	Acute inhalation	Eye irritation	Mutagenicity	Carcinogenicity	Reproductive toxicity	STOT SE	STOR RE	Respiratory sensitisation
1	8							
2		3				4		2
3	1	4		2				
Total number of substances	9	7	0	2	0	4	0	2

Table 5. Number of substances with notified classifications per endpoint (Group 2)

Score	Acute inhalation	Eye irritation	Mutagenicity	Carcinogenicity	Reproductive toxicity	STOT SE	STOR RE	Respiratory sensitisation	Skin sensitisation
1									
2		3	1	3		3		1	1
3		2		2					
Total number of substances	0	5	1	5	0	3	0	1	1

For chemicals with harmonised classifications, the highest total scores based on hazard was 6. The highest scoring substances based on harmonised classifications are shown in Table 6.

Table 6. Substances with the highest score based on harmonised classifications (Group 1)

Substance	CAS No.	Abbreviation	Score
Dimethylamine	124-40-3	DMA	6
Trimethylamine	75-50-3	TMA	6
Methylamine	74-89-5	MMA/MA	6
N-nitrosodimethylamine**	62-75-9	NDMA	6

Step 3b. Cramer class and scoring based on structural alerts

As per the methodology, all substances with notified classifications (Group 2) and those with no data (Group 3) were assigned a Cramer class (Table and Table , respectively).

Table 7. Cramer classes for substances with notified classifications (Group 2)

Substance	CAS No.	Abbreviation	Cramer class
Nitrosopiperazine	5632-47-3	NPZ	3
Nitrodiethanolamine	4185-47-1	DEA-NO2	3
N-nitrosodiethylamine	55-18-5	NDEA	3
N-nitrosomorpholine	59-89-2	NMOR	3
N-ethyl-diethanolamine	139-87-7	EDELA	3
Glycine	56-40-6	GLY	1
N-(2-hydroxyethyl) glycine	5835-28-9	HEGLY	3
Methylethanolamine/monomethylethanolamine	109-85-3/ 6909-61-1	MMEA	1
N-nitrosopiperidine	100-75-4	NPIP	3
Triethanolamine	102-71-6	TELA	3
Tris(hydroxymethyl)aminomethane	77-86-1	TRIS	3
1. 2-(Ethylamine) ethanol	110-73-6	EAE	3
N-Ethyl-N(2Hydroxyethyl) nitrosamine	13147-25-6	EHEN	3
3-Aminopropanol	156-87-6	-	1

Table 8. Cramer classes for substances with no data (Group 3)

Substance	CAS No.	Abbreviation	Cramer class
Ethanolnitramine	74386-82-6	MEA-NO2	3
Dimethylnitramine	4164-28-7	DMA-NO2	3
Mononitropiperazine (1-nitropiperazine)	42499-41-2	MNPZ	3
2-methyl-2-(nitroamino)-1-propanol	1239666-60-4	AMP-NO2	3
Diethylnitramine	7119-92-8	DiEA-NO2	3
N-nitromethanamine	598-57-2	MA-NO2	3
N-(2-hydroxyethyl) ethylenediamine (dihydrochloride)	20267-35-0	HEEDA	3
N-nitromorpholine	4164-32-3	MOR-NO2	3
Methyldiethanolamine	42977-89-9	MDEA	3
N-nitroso-(2-hydroxyethyl)glycine	80556-89-4	NHEGLY	3

Step 3c. Scoring based on structural alerts

For substances classified as Cramer class II or III, structural alerts for mutagenicity, carcinogenicity and skin sensitisation were assessed in ToxTree.

Table shows the number of substances assigned scores for each endpoint based on notified hazard classifications and structural alerts (Group 2) and Table shows the number of substances assigned scores for each endpoint based on structural alerts using Toxtree (Group 3).

Table 9. Number of substances with notified classifications and structural alerts per endpoint (Group 2)

Score	Acute inhalation	Eye irritation	Mutagenicity	Carcinogenicity	Reproductive toxicity	STOT SE	STOR RE	Respiratory sensitisation	Skin sensitisation
1									
2		3	1 (10)	3 (5)		3		1	1 (8)
3		2		2					
Total number of substances	0	5	1 (10)	5 (5)	0	3	0	1	1 (8)

Data in () indicate modelled data

Table 10. Number of substances with structural alerts per endpoint (Group 3)

Score	Acute inhalation	Eye irritation	Mutagenicity	Carcinogenicity	Reproductive toxicity	STOT SE	STOR RE	Respiratory sensitisation	Skin sensitisation
1									
2			(10)	(10)					(4)
3									
Total number of substances	0	0	(10)	(10)	0	0	0	0	(4)

Data in () indicate modelled data

The highest total scores based on hazard were:

- 10 for substances with notified classifications and modelled data (Group 2)
- 5 for substances with no data, based on modelled data only (Group 3)

The highest scoring substances based on notified classifications and structural alerts (Group 2), and those based on structural alerts alone (Group 3) are shown in Table and Table , respectively.

Table 11. Substances with the highest score based on notified classifications and structural alerts (Group 2)

Substance	CAS No.	Abbreviation	Score
N-ethyl-diethanolamine	139-87-7	EDELA	10
N-(2-hydroxyethyl) glycine	5835-28-9	HEGLY	9
Nitrosopiperazine	5632-47-3	NPZ	8
1. 2-(Ethylamine) ethanol	110-73-6	EAE	8
Triethanolamine	102-71-6	TELA	7
N-nitrosodiethylamine	55-18-5	NDEA	6
Tris(hydroxymethyl)aminomethane	77-86-1	TRIS	6
N-Ethyl-N(2Hydroxyethyl) nitrosamine	13147-25-6	EHEN	6
N-nitrosomorpholine	59-89-2	NMOR	5
N-nitrosopiperidine	100-75-4	NPIP	5

Table 12. Substances with the highest score based on structural alerts (Group 3)

Substance	CAS No.	Abbreviation	Score
Ethanolnitramine	74386-82-6	MEA-NO ₂	5
Methyldiethanolamine	42977-89-9	MDEA	5
N-nitroso-(2-hydroxyethyl)glycine	80556-89-4	NHEGLY	5

Step 4. Scoring chemicals according to toxicological reviews

To take account of recent authoritative opinions, chemicals were scored according to the total number of toxicological reviews carried out by authoritative bodies listed in Table 3.

Overall, 20 substances had no toxicological review so were assigned a score of zero, eight substances only had been assessed by one or two authoritative bodies, so were assigned a score of one or two. Ten substances had three or four authoritative reviews and two substances had five reviews. Table 13 lists the chemicals with a review score \geq two. Almost all substances in the table had a harmonised hazard classification.

Table 13. List of substances with a review score above zero (i.e., there is at least one authoritative reviews published for this substance)

Substance	Group	Review score
Morpholine	1 (Harmonised classification)	6
Ethylenediamine	1 (Harmonised classification)	5
Triethylamine	1 (Harmonised classification)	5
N-nitrosodimethylamine**	1 (Harmonised classification)	5
Dimethylamine	1 (Harmonised classification)	4
Diethanolamine	1 (Harmonised classification)	3

Ethylamine	1 (Harmonised classification)	3
Methylamine	1 (Harmonised classification)	3
N-Methyldiethanolamine	1 (Harmonised classification)	3
2-(diethylamino)ethanol	1 (Harmonised classification)	3
Monoethanolamine**	1 (Harmonised classification)	3
Triethanolamine	2 (Notified classification)	3
Piperazine	1 (Harmonised classification)	2
Diethylamine/ethylethanamine	1 (Harmonised classification)	2
Trimethylamine	1 (Harmonised classification)	2

Step 5. Overall ranking

An overall prioritisation list and well as prioritisation lists for the three groups of substances – those with harmonised classifications (Group 1), those with notified classifications (Group 2), or substances with no data (Group 3) have been developed.

For substances with harmonised classifications (Group 1), the hazard scoring was only based on the harmonised classifications data. As such classifications are derived from experimental data, it was deemed unnecessary to identify structural alerts for such chemicals.

For substances with notified classifications (Group 2), hazard scoring was based both on the notified classifications as well as structural alerts. The data on which notified classifications are based are not available and such classifications are not peer reviewed, hence are considered to be less robust. Moreover, full data packages may not be available for such substances so data for some endpoints may indeed not be available. Therefore, as a precautionary approach, structural alerts were also used to score these substances.

For substances with no data (Group 3), the hazard scoring was based solely on structural alerts identified in ToxTree.

Table 14 shows the ranked order of all chemicals and Table 15, Table 16, and Table 17, show the substances in ranked order, based on harmonised classifications (Group 1), notified classifications and structural alerts (Group 2), and structural alerts (Group 3), respectively. The score for toxicological review is shown for information purposes only and has not been used in the prioritisation.

Table 14. Rank order of all substances (shaded rows are breakdown products)

Substance	CAS No.	Abbreviation	Group	Hazard score	Tox review score
N-ethyl-diethanolamine	139-87-7	EDELA	2	10	0
N-(2-hydroxyethyl) glycine	5835-28-9	HEGLY	2	9	0
Nitrosopiperazine	5632-47-3	NPZ	2	8	0
1. 2-(Ethylamine) ethanol	110-73-6	EAE	2	8	1
Triethanolamine	102-71-6	TELA	2	7	3
3-Aminopropanol	156-87-6		2	7	1
Dimethylamine	124-40-3	DMA	1	6	4
N-nitrosodiethylamine	55-18-5	NDEA	2	6	0
Trimethylamine	75-50-3	TMA	1	6	2
Methylamine	74-89-5	MMA/MA	1	6	3
Tris(hydroxymethyl)aminomethane	77-86-1	TRIS	2	6	1
N-nitrosodimethylamine**	62-75-9	NDMA	1	6	5
N-Ethyl-N(2-Hydroxyethyl) nitrosamine	13147-25-6	EHEN	2	6	0
Ethanolnitramine	74386-82-6	MEA-NO ₂	3	5	0
N-(2-hydroxyethyl) ethylenediamine (dihydrochloride)	20267-35-0	HEEDA	3	5	0
N-nitrosomorpholine	59-89-2	NMOR	2	5	1
Methyldiethanolamine	42977-89-9	MDEA	3	5	0
Methylethanolamine/monomethylethanolamine	109-85-3/ 6909-61-1	MMEA	2	5	0
N-nitroso-(2-hydroxyethyl)glycine	80556-89-4	NHEGLY	3	5	0
N-nitrosopiperidine	100-75-4	NPIP	2	5	0
Dimethylnitramine	4164-28-7	DMA-NO ₂	3	4	0
Mononitropiperazine (1-nitropiperazine)	42499-41-2	MNPZ	3	4	0
2-methyl-2-(nitroamino)-1-propanol	1239666-60-4	AMP-NO ₂	3	4	0
Nitrodiethanolamine	4185-47-1	DEA-NO ₂	2	4	0
Diethylnitramine	7119-92-8	DiEA-NO ₂	3	4	0
Ethylamine	75-04-7	EA	1	4	3
N-nitromethanamine	598-57-2	MA-NO ₂	3	4	0
N-nitromorpholine	4164-32-3	MOR-NO ₂	3	4	0
Diethanolamine	111-42-2	DEA	1	3	3

N-nitroso-diethanolamine	1116-54-7	NDELA	1	3	0
Glycine	56-40-6	GLY	2	3	0
Piperazine	110-85-0	PZ	1	2	2
2-amino-2-methyl-propanol	124-68-5	AMP	1	2	1
Ethylenediamine	107-15-3	EDA	1	2	3
N-Methyldiethanolamine	105-59-9	MDEA	1	2	3
Diethylamine/ethylethanamine	109-89-7 / 61193-06-4	DiEA	1	1	2
Morpholine	110-91-8	MOR	1	1	4
2-(diethylamino)ethanol	100-37-8	DEELA	1	1	3
Triethylamine	121-44-8	TEA	1	1	5
Monoethanolamine**	141-43-5	MEA	1	1	3

Table 15. Rank order of substances based on harmonised classifications (Group 1)

Substance	CAS No.	Abbreviation	Hazard score
Dimethylamine	124-40-3	DMA	6
Trimethylamine	75-50-3	TMA	6
Methylamine	74-89-5	MMA/MA	6
N-nitrosodimethylamine**	62-75-9	NDMA	6
Ethylamine	75-04-7	EA	4
Diethanolamine	111-42-2	DEA	3
N-nitroso-diethanolamine	1116-54-7	NDELA	3
Piperazine	110-85-0	PZ	2
2-amino-2-methyl-propanol	124-68-5	AMP	2
Ethylenediamine	107-15-3	EDA	2
N-Methyldiethanolamine	105-59-9	MDEA	2
Diethylamine/ethylethanamine	109-89-7 / 61193-06-4	DiEA	1
Morpholine	110-91-8	MOR	1
2-(diethylamino)ethanol	100-37-8	DEELA	1
Triethylamine	121-44-8	TEA	1
Monoethanolamine**	141-43-5	MEA	1

Table 16. Rank order of substances based on notified classifications and structural alerts (Group 2)

Substance	CAS No.	Abbreviation	Hazard score
N-ethyl-diethanolamine	139-87-7	EDELA	10
N-(2-hydroxyethyl) glycine	5835-28-9	HEGLY	9
Nitrosopiperazine	5632-47-3	NPZ	8
1, 2-(Ethylamine) ethanol	110-73-6	EAE	8
Triethanolamine	102-71-6	TELA	7
3-Aminopropanol	156-87-6		7
N-nitrosodiethylamine	55-18-5	NDEA	6
Tris(hydroxymethyl)aminomethane	77-86-1	TRIS	6
N-Ethyl-N(2Hydroxyethyl) nitrosamine	13147-25-6	EHEN	6
N-nitrosomorpholine	59-89-2	NMOR	5
Methylethanolamine/monomethylethanolamine	109-85-3/ 6909-61-1	MMEA	5
N-nitrosopiperidine	100-75-4	NPIP	5
Nitrodiethanolamine	4185-47-1	DEA-NO2	4
Glycine	56-40-6	GLY	3

* The rank for hazard is based on notified classifications only. The substance was assigned Cramer class I and therefore endpoints were not modelled.

Table 17. Rank order of substances based on structural alerts (Group 3)

Substance	CAS No.	Abbreviation	Hazard score
Ethanolnitramine	74386-82-6	MEA-NO2	5
N-(2-hydroxyethyl) ethylenediamine (dihydrochloride)	20267-35-0	HEEDA	5
Methyldiethanolamine	42977-89-9	MDEA	5
N-nitroso-(2-hydroxyethyl)glycine	80556-89-4	NHEGLY	5
Dimethylnitramine	4164-28-7	DMA-NO2	4
Mononitropiperazine (1-nitropiperazine)	42499-41-2	MNPZ	4
2-methyl-2-(nitroamino)-1-propanol	1239666-60-4	AMP-NO2	4
Diethylnitramine	7119-92-8	DiEA-NO2	4
N-nitromethanamine	598-57-2	MA-NO2	4
N-nitromorpholine	4164-32-3	MOR-NO2	4

List of abbreviations

AEGLs	Acute Exposure Guideline Levels for Airborne Chemicals (AEGLs)
AICIS	Australian Industrial Chemicals Introduction Scheme
ATSDR	Agency for Toxic Substances and Disease Registry
CLH	Harmonised classification and labelling
EAL	Environmental Assessment Levels
ECHA	European Chemicals Agency
HPV	High Production Volume
IARC	International Agency for Research on Cancer
IPCS	International Programme on Chemical Safety
OECD	Organisation for Economic Co-operation and Development
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SIDS	Screening Information Dataset
SVHC	Substances of Very High Concern
TTC	Threshold of toxicological concern
US EPA	US Environmental Protection Agency
UK HSA	UK Health Security Agency
WHO	World Health Organisation

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Appendix

Appendix to include Excel spreadsheets