Sustainable Futures

Summary Assessment

Using

P2 Framework Models

This document was developed to help compile estimation results from U.S. EPA OPPT's P2 Framework Models www.epa.gov/oppt/p2framework/ and is used by OPPT during Sustainable Futures (SF) training described at www.epa.gov/opptintr/newchems/sustainablefutures.htm. Participants in the voluntary SF Pilot Project are asked to submit the information contained in this assessment along with their SF PMNs in their choice of format.
Use of this specific format is not mandatory.

Chemical Assessed (Sample Chemical 3):
1,3,5-triazine-2,4-diamine, 6-nonyl

CAS Registry Number:
5921-65-3

Participant Name:
SF Trainers

Date of Assessment:

Use the following document to create a **Sustainable Future Summary Assessment** for Sample Chemical 3. The boxes that are shaded dark gray will need to be filled in with the appropriate data during the hand-on sessions corresponding to each of the sections.

Within some shaded cells there will be references such as (EPI), (ECOSAR), (E-FAST), (exp), or (calculated). These refer to how the values were derived and it is important that these references are always included with the data for the SF Chemical.

In this example document there are also additional notations within some cells that refer to the **Interpretive Guidance Document** which look like ***"IGD, page X"***. This notation is provided to assist in completing each section during the hands-on sessions and is specific to those cells (endpoints) where they are located. The Interpretive Guidance Document is useful when determining values or interpreting data.

The first page of the SF document is shown on the right and contains: 

- Information on the chemicals structure, identity, use, and manufacturing.

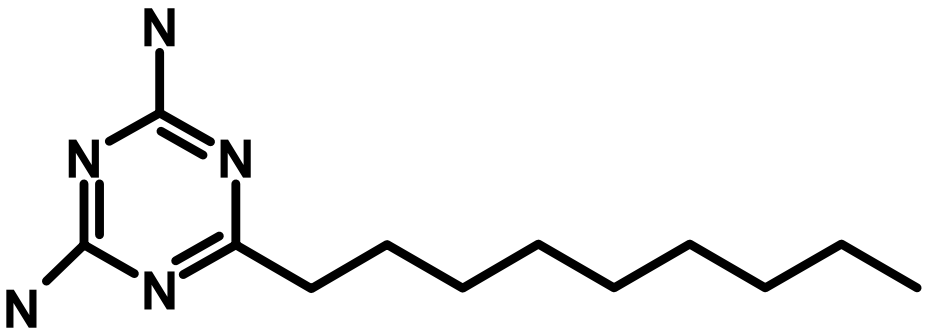
- A summary of all the findings from the SF Assessment for environmental transport and fate, aquatic toxicity, human health effects hazards, PBT Profiler screen, and the risk assessment that should be completed *AT THE END* of the training seminar (shaded boxes on the bottom).

At the end of the training session, after all hands-on session have been completed, return to this page and complete the summary section.

Step-by-Step instructions for the all of the Hands-On Sessions can be found in Appendix A of this document.

Please turn to the next page to begin filling out the SF Summary Assessment for:

Sample Chemical 3

Record ID: Training Session Sample Chemical 3	CAS No. 5921-65-3
	**MW:** 237.35
	MF: $C_{12}H_{23}N_5$
	Physical Form: Solid
	Submitter: SF Trainers, Inc.
	Trade Name: STICKTIGHT
	Use: An activator used in soldering flux for circuit boards
	Production Volume: 10,000 kg/yr

SMILES: n1c(nc(nc1N)CCCCCCCCC)N

Name: 1,3,5-triazine-2,4-diamine, 6-nonyl-

Synonyms:

SUSTAINABLE FUTURES SUMMARY:

Concern Level	HIGH	MODERATE	LOW
Persistence			
Bioconcentration			
Cancer Health Hazard			
Non-Cancer Health Hazard			
Aquatic Toxicity Hazard			
Is the chemical predicted to be a PBT by PBT Profiler?			
Overall Hazard Concern	Human Health: Aquatic:		
Overall Risk	Human Health: Aquatic:		

EPI Suite Hands-On Session:
Predictions for the *"Physical/Chemical Properties"* Section
and the
***"Environmental Transport and Fate"* Section**

Run the EPI Suite Model and fill in only the shaded cells for the **Physical/Chemical Properties and Environmental Transport and Fate** Sections shown on the page to the right. ➡

Input: Enter the CAS Registry number into EPI Suite as the identifier for Sample Chemical 3. Experimental data on the SF chemical should also be entered into the data entry screen for EPI Suite.

Enter into EPI Suite data entry screen:
CAS Registry Number: 5921-65-3 (Enter CAS Number and the structure and name will automatically be retrieved from the internal database)
Melting Point: 120 deg C (took the average of the experimental range, 115-125 deg C)

Output: Predictions from EPI Suite for the physical/chemical properties and environmental transport and fate endpoints should be entered into the table. Transfer the value for each endpoint from the EPI results screen to the appropriate boxes in each section. Note: The reference (EPI) has already been entered.

Byproducts should only be assessed when there is sufficient experimental data to indicate that the degradation products or metabolites are the active species contributing to the toxicity of the chemical.

Physical/Chemical Properties give the assessor an indication of how the chemical may behave in the environment as well as potential routes of exposure. For example, chemicals with low water solubility will have low concentrations in aqueous media and are less likely to reach concentrations that may cause harm to aquatic species.

Environmental Fate and Transport Properties will give the assessor an indication of what the potential risks may be to the environment. For example, knowing the approximate time for a chemical to biodegrade will help the assessor determine chemical concentrations at downstream locations or help the assessor to determine the chemical's persistence in the environment.

See the Interpretive Guidance Document, page 1, for criteria for each endpoint listed under the Physical/Chemical Properties and Environmental Transport and Fate Sections.

CAS No. 5921-65-3	**Submitter:** SF Trainers, Inc.
PHISICAL/CHEMICAL PROPERTIES:	
Melting Point (deg C)	115-125 (exp, evaluated using 120 deg C as input for EPI)
Boiling Point (deg C)	(EPI)
Boiling Point Pressure (mm Hg)	(EPI)
Vapor Pressure (mm Hg)	(EPI)
Water Solubility	mg/l (EPI)
Log K_{ow}	(EPI)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	atm-m^3/mole (EPI)
Soil Adsorption Coefficient – K_{oc}	(EPI)
Bioconcentration Factor – BCF	(EPI)
Persistence	
Experimental Biodeg Tests	
Ultimate Biodeg Model	(EPI)
Primary Biodeg Model	(EPI)
BOD or COD	
Atmospheric Half-life	(EPI)
Hydrolysis Half-life	
Volatilization Half-life for Model River	(EPI)
Volatilization Half-life for Model Lake	(EPI)
Removal in Sewage Treatment Plant	(EPI)
Ready Biodegradability	(EPI)
Byproducts	
Degradation Products	Not Assessed
Metabolites	Not Assessed

ECOSAR Hands-On Session:
Predictions for the *"Aquatic Toxicity"* Section

Run ECOSAR and fill in only the shaded cells for the **Aquatic Toxicity** section on the right. ➡

Input: Enter the chemical structure into ECOSAR using SMILES notation. Experimental data on the SF chemical should also be entered into the data entry screen for ECOSAR.

Output: Please enter a complete profile of 3 acute values and 3 chronic values into the Aquatic Toxicity section on the right. These values for Sample Chemical 2 can be found in the ECOSAR output. Please refer to the Interpretive Guidance Document page 5, and using the criteria, assign an ***"Overall Level of Concern for Aquatic Toxicity"*** based on the predicted data from the toxicity profile.

OncoLogic Hands-On Session:
Predictions for the *"Cancer Health Effects"* Section

Run OncoLogic and fill in only the shaded cells for the **Cancer Health Effects** section on the right. ➡

Input: Complete a ***SAR Analysis*** in OncoLogic for Chemical 3. The appropriate chemical class for this structure is the ***"aromatic amines".*** *Please Note: The best way to determine the appropriate class is to compare the chemical structure and the functional groups it contains to the classes listed in the OncoLogic User's Manual.*

Output: A "Justification Report" will be generated at the end of this session that will give the predicted concern level from OncoLogic. This prediction will be entered into the ***"OncoLogic Results"*** cell in the Cancer Health Effects section. Experimental data for the chemical or appropriate analog should also be entered if available. For this chemical, the experimental data have already been entered into the table.Refer to the Interpretive Guidance Document, page 7, to assign the **"Overall Level of Concern for Carcinogenicity"** based on the predicted and experimental data.

Non-Cancer Health Effects Hands-On Session:
Data for the *"Non-Cancer Health Effects"* Section

There are currently no computerized tools to assist in the **Non-Cancer Health Effects** evaluation process. This portion of the SF Assessment relies on experimental data for the SF chemical or appropriate analog. The experimental data identified for Sample Chemical 3 have already been entered into the appropriate shaded cells in the Non-Cancer Health Effects section to the right. ➡

If a Moderate or High level of concern is determined based on the data for any endpoint, then a **NOAEL or LOAEL** value (or both) must be identified for that endpoint. For these examples, the values have already been provided in the sheet. These values will be used later for calculations to determine potential risks to human health.

Please determine the concern level for each of the endpoints with experimental data using the criteria on page 8 of the Interpretive Guidance Document and then assign an "**Overall Level of Concern for Non-Cancer Health Effects"** based on the most sensitive endpoint (highest individual concern level and lowest NOAEL or LOAEL value).

CAS No. 5921-65-3	**Submitter:** SF Trainers, Inc.
AQUATIC TOXICITY:	
ECOSAR CLASS	(2 ECOSAR classes)
Acute Effects	
Fish LC_{50}	(ECOSAR, triazines)
Daphnid LC_{50}	(ECOSAR, anilines)
Green Algae EC_{50}	(ECOSAR, anilines)
Chronic Effects	
Fish ChV	(ECOSAR, triazines)
Daphnid ChV	(ECOSAR, anilines)
Green Algae ChV	(96hr aniline EC50/4)
Overall Level of Concern For Aquatic Toxicity	(IGD Page 5)
CANCER HEALTH EFFECTS:	
Experimental Data	Melamine has been shown to induce tumors via stone formation (1)
OncoLogic Result	(IGD Page 6) concern predicted based on the aromatic amines category
Overall Hazard Concern Level for Carcinogenicity	(IGD Page 7)

NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Oral LD_{50} values for the submitted substance range from ≈3000 to 7000 mg/kg (2).
Irritation	The structural analog melamine produced very slight irritation in laboratory animals and no irritation in a human patch test (3).
Skin Sensitization	The structural analog melamine did not induce skin sensitization in humans (3).
Reproductive Effects	No reproductive toxicity tests were located; however, the structural analog melamine did not affect reproductive tissues in oral subchronic and chronic tests in rats and mice (1).
Immune System Effects	No immune toxicity tests were identified; however, the structural analog melamine did not affect immune system tissues in oral subchronic and chronic tests in rats and mice (1)
Genotoxicity	The structural analog melamine tested negative in an unscheduled DNA synthesis test (4)
Mutagenicity	The structural analog melamine tested negative in an Ames test (+/- S9) and a sex-linked recessive lethal mutation test in Drosophila (4).
Developmental Toxicity	The structural analog melamine did not cause developmental toxicity in rats administered via i.p. injection at up to 70 mg/kg-day (5).
Neurotoxicity	No relevant studies were located
Systemic Effects	(IGD Page 8) based on analogy to melamine, which has been shown to affect the urinary bladder in rats and mice in subchronic and chronic studies. Effects have included ulceration, stone formation, and tumor formation. Tumor formation, however, has been shown to be a secondary effect caused by test-substance crystallization and stone formation in the urinary bladder. LOAEL ≈112.5 mg/kg-day, NOAEL ≈50 mg/kg-day (1).
Overall Hazard Concern Level for Non-Cancer Health Effects	

ChemSTEER Hands-On Session:
Predictions for the *"Industrial Release and Exposure Values"* Section

ChemSTEER will not be run for these Sample chemicals. The predicted values from ChemSTEER have already been entered into the appropriate shaded cells for the **Occupational Exposure Values and Environmental Release Values** sections on the right. ➡

The occupational exposure values for dermal contact and inhalation will later be used to determine the potential risk from occupational exposure. The environmental release data will be used as input into E-FAST for determination of general population exposure values.

E-FAST Hands-On Session:
Predictions for the *"General Population Exposure Values "* Section

Run E-FAST and fill in only the shaded cells for the **General Population Exposure Values** Section on the page to the right. ➡

Refer to the Interpretive Guidance Document, page 9, for a brief description of the acute, chronic, and cancer exposure values.

Input: Run the General Population Exposure from Industrial Release Module in E-FAST
Use: Chemical Intermediate
SIC Code: Organic Chemicals Manufacture
High End PDM Analysis (This is the more conservative model)

Output: "SIC Code" tab will have the results for the **PEC, Drinking Water Exposures**, and **Fish Ingestion "7q10" Exposures** which should be entered into the table. The "PDM SIC" tab in E-FAST will have results for the **number of days the PEC exceeds the COC**.

Risk Assessment Hands-On Session:
Determination of risk for the *"Risk Assessment"* Section

Please fill in all of the shaded cells for the **Risk Assessment** Section on the page to the right to determine potential risk. ➡

For ***Occupational Exposure,*** an MOE for each Non-Cancer endpoint with a moderate or high hazard concern will need to be calculated based on either an inhalation or dermal occupational exposure value from ChemSTEER, depending on which route of exposure is the most sensitive (i.e. has the lowest exposure concentration).

For ***General Population Exposure*** an acute MOE (if applicable) should be calculated based on an acute value (LD_{50}) and E-FAST acute exposure values to identify potential acute risk. *An acute MOE is not applicable for Sample Chemical 3*. A chronic MOE for each non-cancer endpoint with a moderate or high hazard concern should also be calculated based on E-FAST exposure values for the general population. An MOE should be calculated for each of the endpoints with NOAEL and LOAEL values, and the lowest MOE value identified will be used to determine overall potential chronic risk. That value should be entered into the SF assessment for "MOE – Chronic General Population Exposure".

For ***Aquatic Toxicity*** the assessor must calculate an acute and chronic "***Concentration of Concern (COC)",*** the concentration at which potential acute or chronic aquatic toxicity may be of concern for aquatic species. Refer to the Interpretive Guidance Document, page 10, for the calculation of acute and chronic COC's. A comparison of the acute COC to the predicted environmental concentration (PEC) determined in E-FAST will be done to determine acute risk. If the Acute COC exceeds the PEC, then the potential for risk exists. For chronic risk, determine how many days per year the PEC exceeds the COC (E-Fast results). If the PEC is exceeded for more than 20 days per year, then the potential for chronic aquatic risk exists.

CAS No. 5921-65-3		Submitter: SF Trainers, Inc.	
EXPOSURE MODELS:			
INDUSTRIAL RELEASE AND EXPOSURE VALUES: CHEMSTEER			
Process	Organic Chemicals Manufacture	**Number of Release Days**	25
SIC Code / NPDES #		**Number of Facilities**	1
Occupational Exposure Values			
	Cancer LADD	**Chronic ADD**	**Acute APDR**
Dermal	1.8×10^{-3} mg/kg-day	2.1×10^{-3} mg/kg-day	6.8×10^{-2} mg/kg-day
Inhalation	4.1×10^{-4} mg/kg-day	6.2×10^{-4} mg/kg-day	7.2×10^{-3} mg/kg-day
Environmental Release Values			
Release to Water		50 kg/year	
Release to Air (Fugitive)		N/A	
Release to Landfill		N/A	
Release from Incineration		N/A	
Other Release Activities		N/A	
GENERAL POPULATION EXPOSURE VALUES: E-FAST			
Aquatic Exposure:			
Predicted Environmental Concentration (PEC)			
PEC Exceeds COC (days / year)			
Human Exposure:			
	Cancer LADDpot	**Chronic ADDpot**	**Acute ADRpot**
Drinking Water			
Fish Ingestion			
Fugitive Emissions	N/A	N/A	N/A
Incineration Emissions	N/A	N/A	N/A
Landfill Leaching	N/A	N/A	N/A
Dermal – Consumer Use	N/A	N/A	N/A
Inhalation – Consumer Use	N/A	N/A	N/A
RISK ASSESMENT:			
MOE – Occupational Exposure			
MOE – Acute General Population Exposure			
MOE – Chronic General Population Exposure			
Acute COC – Aquatic Exposure			
Chronic COC - Aquatic Exposure			

CONCLUSIONS:

Risk from Occupational Exposure:

Acute Risk to General Population:

Chronic Risk to General Population:

Acute Risk to Aquatic Environment:

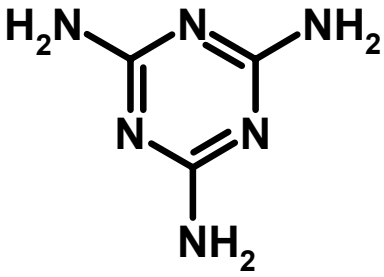
Chronic Risk to Aquatic Environment:

Analog Table:

In order to identify toxicity studies that were used either for the aquatic toxicity, human health cancer, or human health non-cancer sections an analog table should be included with chemical name (either for the SF chemical or appropriate analog), chemical structure, endpoint, and a brief summary of the test data used to support conclusions reached in the SF Assessment. Also supply a list of references so that the studies can easily be retrieved.

The analog table for Sample Chemical 3 is shown on the right. 

Table I - Selected Analogs

Analog	Structure	Concern Identified	Basis of Concern
Melamine		**Systemic toxicity**	Urinary bladder effects in rats and mice exposed in the diet in subchronic and chronic tests. LOAEL ≈112.5 mg/kg-day; NOAEL ≈ 50 mg/kg-day.

References

1. **NTP (National Toxicology Program). 1983. Toxicology and Carcinogenesis Studies of Melamine (CAS No. 108-78-1) in F344/N Rats and B6C3F1 Mice (Feed Study). Technical Report Series No. 245. U.S. Department of Health and Human Services. National Institutes of Health.**

2. **NTP. 2003. Health and Safety report for melamine. Available on-line at http://ntp-server.niehs.nih.gov**

3. **Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982. 2772 (Cited in HSDB).**

4. **IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work).p. V39 341. (Cited in HSDB, 2003)**

5. **IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-PRESENT. (Multivolume work).p. V39 340 (1986).**

6. **HSDB (Hazardous Substances Data Bank). 2003. Melamine. Available on-line at http://toxnet.nlm.nih.gov.**

Summary Section

This section should be used to verbally summarize findings from the Hazard, Exposure, and Risk Sections. It is important that you draw conclusions about your chemical using the analytical data that you obtained during the assessment for each of the individual sections shown on the right.

SUMMARY SECTION:

Physical/Chemical Properties:

Environmental Fate:

Aquatic Toxicity:

Human Health, Cancer:

Human Health, Non-Cancer:

Occupational Exposure:

Population and Environmental Exposure:

Environmental Risk assessment:

Human Risk Assessment: