

# 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/](http://www.epa.gov/oppt/p2framework/) and is used by OPPT during Sustainable Futures (SF) training described at [www.epa.gov/opptintr/newchems/sustainablefutures.htm](http://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 1):**  
*1,2-Dichloro-4-nitro-5-pentylbenzene*

**CAS Registry Number:**  
Not Located

**Participant Name:**  
SF Trainers

**Date of Assessment:**

Use the following document to create a **Sustainable Future Summary Assessment** for Sample Chemical 1. 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 is also additional notation 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: 

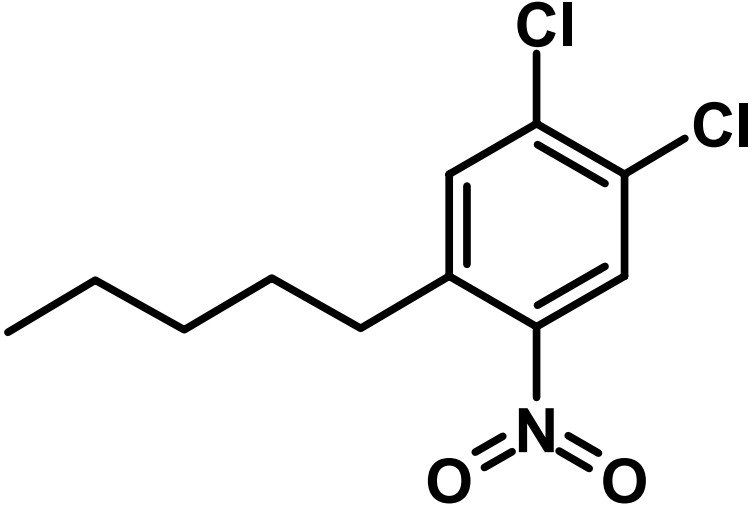
- Information on the chemicals structure, identity, use, and manufacturing.
- A summary of all the findings from the SF Assessment for environmental transport and fate, aquatic toxicity, human health effects hazards, PBT Profiler screen, and the risk assessments that should be completed *AT THE END* 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 1**

<b>Record ID: Training Session Sample Chemical 1</b>	<b>CAS No.</b>
	<b>MW:</b> 262.14
	<b>MF:</b> C <sub>11</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>1</sub> O <sub>2</sub>
	<b>Physical Form:</b> Solid
	<b>Submitter:</b> SF Trainers, Inc.
	<b>Trade Name:</b> INTERSYN
	<b>Use:</b> Synthetic Intermediate
	<b>Production Volume:</b> 50,000 kg/yr

**SMILES:** c1(cc(c(cc1Cl)CCCCC)(N(=O)=O))Cl


**Name:** 1,2-dichloro-4-nitro-5-pentylbenzene

**Synonyms:** Pentyl, dichloro, nitrobenzene

**SUSTAINABLE FUTURES SUMMARY:**

Concern Level	HIGH	MODERATE	LOW
Persistence	<input type="text"/>		
Bioconcentration	<input type="text"/>		
Cancer Health Hazard	<input type="text"/>		
Non-Cancer Health Hazard	<input type="text"/>		
Aquatic Toxicity Hazard	<input type="text"/>		
Is the chemical predicted to be a PBT by PBT Profiler?	<input type="text"/>		
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 chemical structure into EPI Suite’s data entry screen using SMILES notation. The SMILES notation for Sample Chemical 1 is in a file called **exsmiles.txt** on the desktop. 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:**

SMILES: c1(cc(c(cc1Cl)CCCC)(N(=O)=O))Cl  
No experimental data located for this chemical

**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.	Submitter: SF Trainers, Inc.
<b>PHYSICAL/CHEMICAL PROPERTIES</b>	
Melting Point (deg C)	(EPI)
Boiling Point (deg C)	(EPI)
Boiling Point Pressure (mm Hg)	(EPI)
Vapor Pressure (mm Hg)	(EPI)
Water Solubility	mg/L (EPI)
Log K <sub>ow</sub>	(EPI)
<b>ENVIRONMENTAL TRANSPORT AND FATE:</b>	
<b>Transport</b>	
Henry's Law Constant – HLC	atm/m <sup>3</sup> -mole (EPI)
Soil Adsorption Coefficient – K <sub>oc</sub>	(EPI)
Bioconcentration Factor – BCF	(EPI)
<b>Persistence</b>	
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)
<b>Byproducts</b>	
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, although no data was located for this chemical.

**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 1. The appropriate chemical class for this structure is the **“halogenated nitroaromatics”**. *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 and assign an **“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 1 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).

<b>CAS No.</b>	<b>Submitter:</b> SF Trainers, Inc.
<b>AQUATIC TOXICITY:</b>	
<b>ECOSAR Class</b>	
<b>Acute Toxicity</b>	
<b>Fish LC<sub>50</sub></b>	(ECOSAR) (Note: K <sub>ow</sub> is above the cutoff for this effect, IGD Page 5)
<b>Daphnid LC<sub>50</sub></b>	(ECOSAR) (Note: K <sub>ow</sub> is above the cutoff for this effect, IGD Page 5)
<b>Green Algae EC<sub>50</sub></b>	(ECOSAR)
<b>Chronic Toxicity</b>	
<b>Fish ChV</b>	(ECOSAR)
<b>Daphnid ChV</b>	(ECOSAR)
<b>Green Algae ChV</b>	(ECOSAR)
<b>Overall Hazard Concern Level for Aquatic Toxicity</b>	(IGD page 5)
<b>CANCER HEALTH EFFECTS:</b>	
<b>Experimental data</b>	None identified
<b>OncoLogic Results</b>	(IGD page 7)
<b>Overall Hazard Concern Level for Carcinogenicity</b>	(IGD Page 7)
<b>NON-CANCER HEALTH EFFECTS:</b>	
<b>Acute Toxicity</b>	
<b>Irritation</b>	
<b>Skin Sensitizer</b>	
<b>Reproductive Effects</b>	
<b>Developmental Effects</b>	(IGD, page 8), based on analogy to 1,2-dichloro-4-nitrobenzene, which induced developmental effects in rats dosed via oral gavage. NOAEL = 10 mg/kg-day; LOAEL = 30 mg/kg-day (1).
<b>Immune System Effects</b>	
<b>Genotoxicity</b>	
<b>Mutagenicity</b>	
<b>Systemic Effects</b>	
<b>Overall Hazard Concern Level for Non-Cancer Health Effects</b>	

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

ChemSTEER will not be run for these example 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 the 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<sub>50</sub>) and E-FAST acute exposure values to identify potential acute risk. *An acute MOE is not applicable for Sample Chemical 1.* 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 COCs. 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.

**Refer to the Interpretive Guidance Document, page 10, for a more complete description of the Risk Assessment Process and MOE calculations and criteria.**



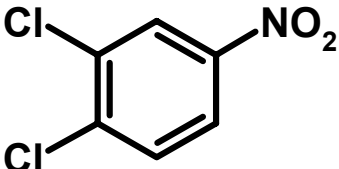
CAS No. 5921-65-3		Submitter: SF Trainers, Inc.	
<b>EXPOSURE MODELS:</b>			
<b>INDUSTRIAL RELEASE AND EXPOSURE VALUES: CHEMSTEER</b>			
Process	Organic Chemicals Manufacture	Number of Release Days	12
SIC Code / NPDES #		Number of Facilities	1
<b>Occupational Exposure Values</b>			
	<b>Cancer LADD</b>	<b>Chronic ADD</b>	<b>Acute APDR</b>
Dermal	1.6 x 10 <sup>-3</sup> mg/kg-day	3.0 x 10 <sup>-3</sup> mg/kg-day	0.510 mg/kg-day
Inhalation	2.2 x 10 <sup>-2</sup> mg/kg-day	6.0 x 10 <sup>-1</sup> mg/kg-day	0.599 mg/kg-day
<b>Environmental Release Values</b>			
Release to Water	48 kg/year		
Release to Air (Fugitive)	N/A		
Release to Landfill	N/A		
Release from Incineration	N/A		
Other Release Activities	N/A		
<b>GENERAL POPULATION EXPOSURE VALUES: E-FAST</b>			
<b>Aquatic Exposure:</b>			
Predicted Environmental Concentration (PEC)			
PEC Exceeds COC (days / year)			
<b>Human Exposure:</b>			
	<b>Cancer LADDpot</b>	<b>Chronic ADDpot</b>	<b>Acute ADRpot</b>
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
<b>RISK ASSESMENT:</b>			
MOE – Occupational Exposure			
MOE – Acute General Population Exposure	N/A (IGD Page 12)		
MOE – Chronic General Population Exposure			
Acute COC – Aquatic Exposure			
Chronic COC - Aquatic Exposure			
<b>CONCLUSIONS:</b>			
<b>Risk from Occupational Exposure:</b> <b>Acute Risk to General Population: N/A</b> <b>Chronic Risk to General Population:</b> <b>Acute Risk to Aquatic Environment:</b> <b>Chronic Risk to Aquatic Environment:</b>			

### **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 1 is shown on the right. 


**Table I - Selected Analogs**

<b>Analog</b>	<b>Structure</b>	<b>Concern Identified</b>	<b>Basis of Concern</b>
<b>1,2-dichloro-4-nitrobenzene</b>		<b>Developmental Toxicity</b>	Induced malformations in fetuses of orally treated rats at $\geq 30$ mg/kg-day

**References**

1. Monsanto Company; USEPA Status Report: Nitrated Orthene (1990), EPA Document No. 8EHQ-0590-0972, Fiche No. OTS0524331-1. (Cited in HSDB, 2003).
2. HSDB (Hazardous Substances Data Bank). 2003. 3,4-DICHLORONITROBENZENE CASRN: 99-54-7. 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: