Attachment #13 Environmental Assessment

1. **Date:** August 20, 2018
2. **Submitter:** Enviro Tech Chemical Services, Inc.
3. **Address:** 500 Winmoore Way, Modesto, CA. 95358
4. **Description of Proposed Action:**

    a. **Description of the Requested Action:** The action requested in the submission is for dipicolinic acid (DPA) to be used in peroxyacetic acid solutions authorized in effective Food Contact Notifications with the following limitations in use-level for:

        1. meat carcasses, parts, trim and organs at a maximum use level of 1.64 ppm
        2. poultry carcasses, parts, trim and organs at a maximum use level of 2.73 ppm
        3. processed and preformed meat and poultry at a maximum use level of 0.44 ppm
        4. fruits and vegetables in food processing facilities at a maximum use level of 0.68 ppm
        5. fish and seafood at a maximum use level of 0.38 ppm
        6. brines, sauces and marinades at a maximum use level of 0.10 ppm, and
        7. The commercial sterilization of aseptic filling systems, glass and plastic food packaging and their enclosures prior to filling at a maximum use level of 9.0 ppm.

    The Enviro Tech peroxyacetic acid formulations impacted by this notification are as follows:

        iii. Formulations manufactured by Enviro Tech for use in accordance with 21 CFR 173.370.

        iv. Formulations manufactured by Enviro Tech for use in accordance with 21 CFR 173.315.

v. Formulations notified in Enviro Tech FCN No. 699, 887, 908, 1132, 1419, 1654, 1738, 1806 and 1851.

b. **The Need for the Action:** The FCS (DPA) improves stability of concentrated peroxyacetic acid formulations during storage until they are diluted with water.

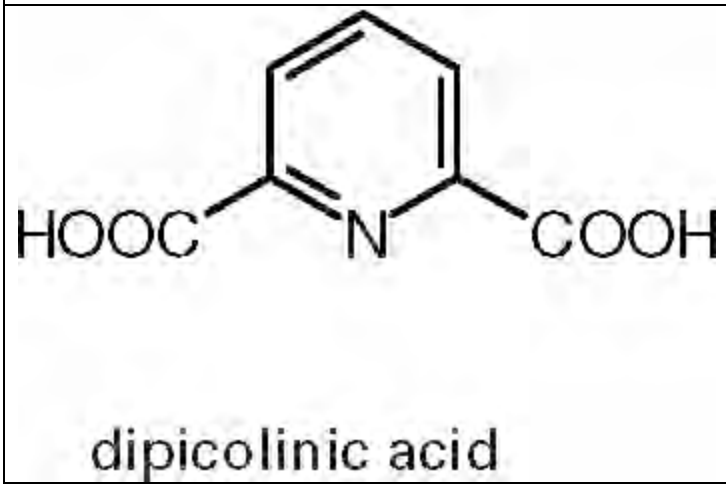
c. **Brief Discussion of the Use and Disposal of the FCS:** The FCS (DPA) is intended to be added to peroxyacetic acid (PAA) formulations used in food processing facilities and applied to meat, pre-formed meat, poultry, fish, seafood, fruits and vegetables, and food-contact surfaces of glass and plastic containers in accordance with each respective FCN. The FCS solution lost during use is typically diluted with other liquid waste products at the processing plant. The diluted FCS solution will then be disposed of with processing plant wastewater according to National Pollutant Discharge Elimination System (NPDES) regulations. For processing plants that hold a NPDES permit (i.e., direct dischargers), the FCS solution in the wastewater will be treated on-site before direct discharge to surface waters. For processing plants without such NPDES permits (i.e., indirect dischargers), the FCS solution in the wastewater would travel through the sanitary sewer system into Publicly Owned Treatment Works (POTWs) for standard wastewater treatment processes before movement into aquatic environments.

The potential use and disposal of FCS solution is discussed below and describes worst case scenarios and associated potential risks along with the Environmental Introduction Concentration (EIC) and Expected Environmental Concentration (EEC) calculations.

5. Identification of Substance:

Chemical Name: Dipicolinic Acid
Common or Trade Name: DPA
CAS Registry Number: 499-83-2
CAS Registry Name: Pyridine-2,6-dicarboxylic Acid

The structure and molecular weight for DPA are:

Structure	Molecular Weight (g/mol)
 dipicolinic acid	167.12

Appearance	White crystalline powder
Density	No data available
Solubility	0.2gm in 10 mL of 95% ethanol
Melting point	242-246 degrees C
Water content	0.20%w/w max
Sulphated ash	0.20% w/w max
Chloride	200 ppm max
Iron	25 ppm max
pH	2.0 (5g/L H_2O, 20 degrees C)
Storage	Store at room temperature
Assay	≥99.00%

6. Introduction of Substance into the Environment:

a. Introduction of substances into the environment as a result of manufacture:

The FCS solution will be manufactured in EPA approved facilities at the addresses listed below and no unusual or factual threat to the environment exist. Enviro Tech does not manufacture DPA, but rather will purchase it from a supplier and use it in select peroxyacetic acid formulations as

outlined above. Enviro Tech's addition of DPA is not expected to appreciably increase the environmental load of DPA beyond some small quantity in effluent water from food processing facilities.

Establishment Number	**Establishment Name**	**Establishment Site Address**
63838-CA-01	Enviro Tech Chemical Services, Inc.	500 Winmoore Way, Modesto CA
63838-AR-01	Enviro Tech Chemical Services – Plant 6	724 Phillips County Road 411, Helena, AR 72342

Attached are the Facility Registry Service (FRS) website pages that document the EPA Establishment Numbers at the addresses listed above. Below are the website links: http://iaspub.epa.gov/enviro/fii_query_detail.disp_program_facility?p_registry_id=110024498890 and https://iaspub.epa.gov/enviro/fii_query_detail.disp_program_facility?p_registry_id=110063867383. No extraordinary environmental circumstances would apply to the continued on-going manufacture of the FCS solution.

b. Introduction of substances into the environment as a result of use/disposal:

For discussion of the environmental impacts of the other components of the PAA formulations (PAA, H_20_2, HEDP, etc.), we incorporate by reference the EAs for FCNs 699, 887, 908, 1132, 1419, 1654, 1738, 1806, and 1851 (available through https://www.accessdata.fda.gov/scripts/fdcc/?set=ENV-FCN). Please see Limitations/Specifications table below:

	Limitations/Specifications			
FCN	PAA Conc. (ppm)	H_2O_2 Conc. (ppm)	HEDP Conc. (ppm)	Dipic Conc (ppm)
699[1]	190	75	10	0.38
887[1]	220	85	11	0.44
908[1]	220	85	11	0.44
1132 (Poultry)[1]	1000	385	50	2.00
1132 (Meat)[1]	400	155	20	0.80
1419[2]	2000	770	100	2.73
1654[1]	50	18	6	0.10
1738 (Meat)[2]	1200	275	33	1.64
1738 (Produce)[2]	500	115	14	0.68
1806[2]	2000	770	100	2.73
1851[3]	4500	6600	180	9.00

[1] based on 15% PAA, 1.1079 g/mL

[2] based on 22% PAA, 1.1127 g/mL

[3] based on 15% PAA, 1.1355 g/mL

The FCS (DPA) solution is provided as a concentrate that is diluted on site. Following use, the FCS solution will be discharged into the wastewater generated by the food processing facilities. The FCS is water soluble and expected to remain in the wastewater stream. The diluted FCS solution will be disposed of with processing plant wastewater according to National Pollutant Discharge Elimination System (NPDES) regulations. For processing plants that hold a NPDES permit (i.e., direct dischargers), the FCS solution in wastewater will be treated on-site before direct discharge to surface waters. For processing plants without such NPDES permits (i.e., indirect dischargers), the FCS solution in the wastewater would travel through the sanitary sewer system into Publicly Owned Treatment Works (POTWs) for standard wastewater treatment processes before movement into aquatic environments.

To determine the EIC for the FCS, we will assume, in a worst-case scenario, that all the water used in a processing plant is treated with the FCS solution. The EIC may then be calculated by multiplying the concentration of the FCS by the estimated percentage of degradation associated with use of the

FCS. The maximum concentration of the FCS will be used to calculate the EIC. To be conservative, we will assume no adsorption of the FCS to wastewater sludge in sewage treatment plants for the below Estimated Environmental Concentration (EEC) calculations.

The environmental introduction concentration (EIC) of the FCS is based on use and disposal of the FCS solution at the end of a work day into the food processor's on-site pre-treatment facility assuming no degradation of the FCS solution. The subsequent EECs including EEC_{sludge} and EEC_{water} are calculated below assuming no partition to sludge. With respect to the EEC_{water} calculation, a 10-fold dilution factor is recommended for use when estimating surface water concentrations[(1)]. Below are the worst-case EIC and EEC_{sludge} and EEC_{water} calculations for the FCS:

FCS EIC = 9 ppm FCS x 100% remaining = 9 ppm
EEC_{sludge} = 9 ppm FCS x 0% partition to sludge = 0 ppm
FCS EEC_{water} = (9 ppm FCS x 100% partition to water) / 10 fold dilution factor = 0.9 ppm FCS

7. Fate of the Substance in the Environment:

It has been shown that the FCS (DPA), a poly-substituted pyridine derivative readily biodegrades under both aerobic and anaerobic conditions[(2)(3)(4)]. In presenting a review on the microbial metabolism of pyridines, including DPA, Kaiser, et al. describe aerobic metabolism of DPA to carbon dioxide, ammonium, and water, and anaerobic metabolism to dihydroxypyridine which is then rapidly photodegraded to organic acids (i.e., propionic acid, acetic acid), carbon dioxide, and ammonium.

As indicated above, the highest amount of FCS that may be released into the environment would be a maximum of 0.9 ppm.
Extrapolation of the data trend discussed in the study referenced

above (which showed complete degradation of 20 ppm levels in 8 days) results in anticipated degradation in approximately one hour (20 ppm/192 hours = 0.1 ppm/hr).

8. Environmental Effects of Released Substances:

There is little available ecotoxicity data for the FCS (DPA). The Safety Data Sheet (SDS) from one supplier states that the freshwater fish 96 hour LC_{50} is 322 mg/L for the fathead minnow.[5] The Ecological Structure Activity Relationships (ECOSAR) Class Program is a computerized predictive system maintained and developed by the U.S. EPA that estimates aquatic toxicity. The program estimates a chemical's acute (short-term) toxicity and chronic (long-term or delayed) toxicity to aquatic organisms, such as fish, aquatic invertebrates, and aquatic plants, by using computerized Structure Activity Relationships (SARs)[6]. This program is a sub-routine of the Estimation Program Interface (EPI) Suite – a structure-function predictive modeling suite also developed and maintained by the U.S. EPA[7]. The ECOSAR results for DPA predict the following acute and chronic toxicity endpoints tabulated below[8]. The complete ECOSAR report for this analysis is attached to this EA (see Attachment B).

ECOSAR Class	Organism	Endpoint	mg/L
Pyridine-alpha-acid	Fish	96 hr LC_{50}	324
	Fish	ChV	29[31]
Neutral Organic SAR	Fish	96 hr LC_{50}	2657
	Daphnid	48 hr LC_{50}	1322
	Green Algae	96 hr EC_{50}	570
	Fish	ChV	222
	Daphnid	ChV	89
	Green Algae	ChV	111

These values are all much higher than the "worst-case" scenario of an EEC_{water} of 0.9 ppm, which is over 32 times lower than the lowest chronic toxicity endpoint for the most sensitive species. Thus, the use of DPA at such a minimal level is not expected to result in any adverse environmental effects.

9. Use of Resources and Energy:

The proposed use of the FCS would not pose any significant additional burden on existing resources or energy in the manufacture, transport, use or disposal of the FCS above and beyond those already existing, and the proposed use will not create any significant additional burden on resources or energy. The FCS (DPA) is used to enhance the stability of existing products already on the market. Enviro Tech will not be producing DPA, it will be purchased from a supplier and combined with existing peroxyacetic acid formulations. The disposal of the FCS would not significantly increase any wastewater usage or processing costs any more than a similar volume of a product. We do not expect any significant effect on the use of energy and resources with approval of this notification.

10. Mitigation Measures:

The proposed use of the FCS is not reasonably expected to result in any significant adverse environmental impacts that would require mitigation measures of any kind.

11. Alternatives to Proposed Action:

There are no potential adverse environmental effects that would necessitate alternative actions to that proposed in this FCN. The alternative of not approving the action proposed herein would simply result in the continued use of existing antimicrobial agents and such action would have no significant environmental impact.

12. List of Preparers:

a. Michael Harvey, President & CEO, Enviro Tech Chemical Services, Inc.
   Education: B.S. Cal. State University, Chico (Chemistry)
   Experience: 31 years of experience conducting ecological risk assessments and preparing regulatory submissions that have been submitted to the EPA and FDA
b. Brent Bankosky, COO, Enviro Tech Chemical Services, Inc.
   Education: BS., MBA, Pennsylvania State University, MS, Lehigh University
   Experience: 13 years of experience preparing EPA and FDA regulatory submissions
c. Jonathan N. Howarth, Sr. Vice President, Technology, Enviro Tech Chemical Services, Inc.
   Education: Ph.D., Physical Chemistry, Univ. of Southampton, England; BS (Honors), Applied Chemistry, Leicester Polytechnic, England
   Experience: 26 years of experience preparing EPA and FDA regulatory submissions
d. Joseph Donabed, R&D Manager, Enviro Tech Chemical Services, Inc.
   Education: BS, Cal. State University Stanislaus
   Experience: 7 years of experience preparing EPA and FDA regulatory submissions
e. Tina Rodrigues, Director, Regulatory Affairs, Enviro Tech Chemical Services, Inc.
   Education: BS, Cal. State University Stanislaus
   Experience: 10 years of experience preparing EPA and FDA regulatory submissions

13. Certification:

The undersigned official certifies that the information presented is true, accurate, and complete to the best of the knowledge of Enviro Tech Chemical Services, Inc.

Date: August 20, 2018
Signature:

Name and Title: Michael S. Harvey, President & CEO

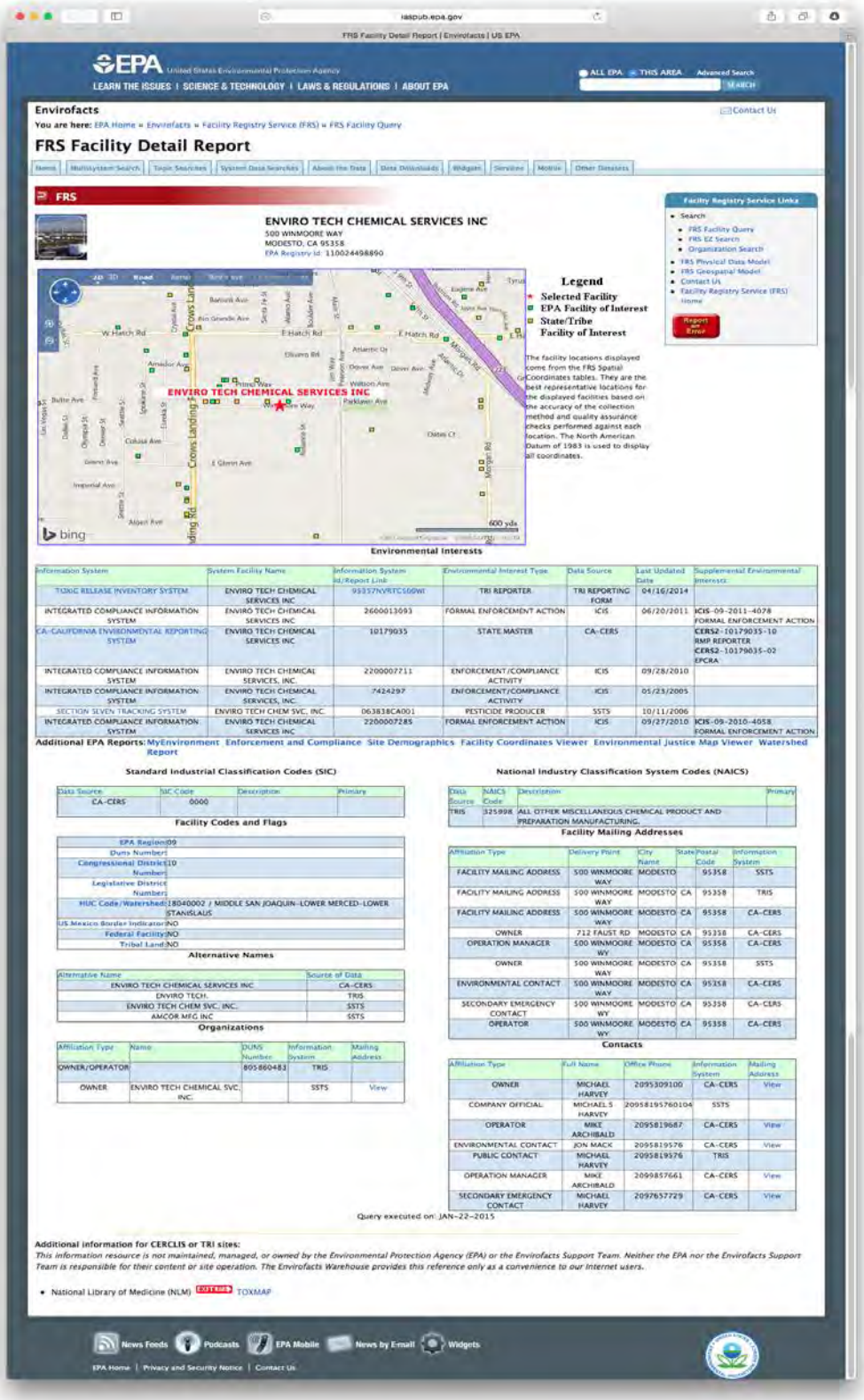
14. BIBLIOGRAPHY and LITERATURE CITATIONS

(1) Rapaport, Robert A., 1988. Prediction of consumer product chemical concentrations as a function of publically owned treatment works treatment type and riverine dilution.
Environmental Toxicology and Chemistry 7(2), 107-115. Found online at:
http://onlinelibrary.wiley.com/doi/10.1002/etc.5620070204/abstract.

(2) J.A. Amador and B.P. Tatlor, “Coupled metabolic and photolytic pathway for degradation of pyridinecarboxylic acids, especially dipicolinic acid” Applied and Environmental Microbiology 1990, 56(5), 1352-1356.
(3) B. Seyfried and B. Schnink, “Fermentive degradation of dipicolinic acid (Pyridine-2,6- dicarboxylic acid) by a defined coculture of strictly anaerobic bacteria,” Biodegradation, 1990, 1(1), 1-7.
(4) J.P. Kaiser, Y. Feng, and J.M. Bollag, “Microbial metabolism of pyridine, quinolone, acridine, and their derivatives under aerobic and anaerobic conditions,” Microbiological Reviews, 1996, 60(3), 483-498.
(5) See representative SDS for DPA available at: https://www.sigmaaldrich.com/MSDS/MSDS/DisplayMSDSPage.do?country=US&language=en&productNumber=P63808&brand=ALDRICH&PageToGoToURL=https%3A%2F%2Fwww.sigmaaldrich.com%2Fcatalog%2Fsearch%3Fterm%3Ddipicolinic%2Bacid%26interface%3DAll%26N%3D0%26mode%3Dpartialmax%26lang%3Den%26region%3DUS%26focus%3Dproduct.
(6) Information on ECOSAR can be found at https://www.epa.gov/tsca-screening-tools/ecological- structure-activity-relationships-ecosar-predictive-model.
(7) EPISuite predicts various physical-chemical properties and environmental fate endpoints and also include models for environmental transport. Running the tool will give the user an indication of the transport and persistence of a chemical. Information on EPI Suite is available at https://www.epa.gov/tsca-screening- tools/epi-suitetm-estimation-program-interface.
(8) See EPI Suite – ECOSAR Program Results for CAS 499-83-2; Attachment B

Attachment A

EPA FRS Facility Detail Report Exhibit



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FRS Facility Detail Report | Envirofacts | US EPA

EPA United States Environmental Protection Agency

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FRS Facility Detail Report

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FRS

ENVIRO TECH CHEMICAL SERVICES INC
500 WINMOORE WAY
MODESTO, CA 95358
EPA Registry Id: 110024498890

Facility Registry Service Links
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- FRS EZ Search
- Organization Search
- FRS Physical Data Model
- FRS Geospatial Model
- Contact Us
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- EPA Facility of Interest
- State/Tribe Facility of Interest

The facility locations displayed come from the FRS Spatial Coordinates tables. They are the best representative locations for the displayed facilities based on the accuracy of the collection method and quality assurance checks performed against each location. The North American Datum of 1983 is used to display all coordinates.

Environmental Interests

Information System	System Facility Name	Information System Id/Report Link	Environmental Interest Type	Data Source	Last Updated Date	Supplemental Environmental Interests
TOXIC RELEASE INVENTORY SYSTEM	ENVIRO TECH CHEMICAL SERVICES INC	95357NVRTCS00WI	TRI REPORTER	TRI REPORTING FORM	04/16/2014	
INTEGRATED COMPLIANCE INFORMATION SYSTEM	ENVIRO TECH CHEMICAL SERVICES INC	2600013093	FORMAL ENFORCEMENT ACTION	ICIS	06/20/2011	ICIS-09-2011-4078 FORMAL ENFORCEMENT ACTION
CA-CALIFORNIA ENVIRONMENTAL REPORTING SYSTEM	ENVIRO TECH CHEMICAL SERVICES INC	10179035	STATE MASTER	CA-CERS		CERS2-10179035-10 RMP REPORTER CERS2-10179035-02 EPCRA
INTEGRATED COMPLIANCE INFORMATION SYSTEM	ENVIRO TECH CHEMICAL SERVICES, INC.	2200007711	ENFORCEMENT/COMPLIANCE ACTIVITY	ICIS	09/28/2010	
INTEGRATED COMPLIANCE INFORMATION SYSTEM	ENVIRO TECH CHEMICAL SERVICES, INC.	7424297	ENFORCEMENT/COMPLIANCE ACTIVITY	ICIS	05/23/2005	
SECTION SEVEN TRACKING SYSTEM	ENVIRO TECH CHEM SVC, INC.	063838CA001	PESTICIDE PRODUCER	SSTS	10/11/2006	
INTEGRATED COMPLIANCE INFORMATION SYSTEM	ENVIRO TECH CHEMICAL SERVICES INC	2200007285	FORMAL ENFORCEMENT ACTION	ICIS	09/27/2010	ICIS-09-2010-4058 FORMAL ENFORCEMENT ACTION

Additional EPA Reports: MyEnvironment Report | Enforcement and Compliance | Site Demographics | Facility Coordinates Viewer | Environmental Justice Map Viewer | Watershed

Standard Industrial Classification Codes (SIC)

Data Source	SIC Code	Description	Primary
CA-CERS	0000		

National Industry Classification System Codes (NAICS)

Data Source	NAICS Code	Description	Primary
TRIS	325998	ALL OTHER MISCELLANEOUS CHEMICAL PRODUCT AND PREPARATION MANUFACTURING.	

Facility Codes and Flags

EPA Region	09
Dun's Number	
Congressional District Number	10
Legislative District Number	
HUC Code/Watershed	18040002 / MIDDLE SAN JOAQUIN--LOWER MERCED--LOWER STANISLAUS
US Mexico Border Indicator	NO
Federal Facility	NO
Tribal Land	NO

Facility Mailing Addresses

Affiliation Type	Delivery Point	City Name	State	Postal Code	Information System
FACILITY MAILING ADDRESS	500 WINMOORE WAY	MODESTO		95358	SSTS
FACILITY MAILING ADDRESS	500 WINMOORE WAY	MODESTO	CA	95358	TRIS
FACILITY MAILING ADDRESS	500 WINMOORE WAY	MODESTO	CA	95358	CA-CERS
OWNER	712 FAUST RD	MODESTO	CA	95358	CA-CERS
OPERATION MANAGER	500 WINMOORE WY	MODESTO	CA	95358	CA-CERS
OWNER	500 WINMOORE WAY	MODESTO	CA	95358	SSTS
ENVIRONMENTAL CONTACT	500 WINMOORE WAY	MODESTO	CA	95358	CA-CERS
SECONDARY EMERGENCY CONTACT	500 WINMOORE WY	MODESTO	CA	95358	CA-CERS
OPERATOR	500 WINMOORE WY	MODESTO	CA	95358	CA-CERS

Alternative Names

Alternative Name	Source of Data
ENVIRO TECH CHEMICAL SERVICES INC	CA-CERS
ENVIRO TECH	TRIS
ENVIRO TECH CHEM SVC, INC.	SSTS
AMCOR MFG INC	SSTS

Organizations

Affiliation Type	Name	DUNS Number	Information System	Mailing Address
OWNER/OPERATOR		805860483	TRIS	
OWNER	ENVIRO TECH CHEMICAL SVC, INC.		SSTS	View

Contacts

Affiliation Type	Full Name	Office Phone	Information System	Mailing Address
OWNER	MICHAEL HARVEY	2095309100	CA-CERS	View
COMPANY OFFICIAL	MICHAEL S HARVEY	20958195760104	SSTS	
OPERATOR	MIKE ARCHIBALD	2095819687	CA-CERS	View
ENVIRONMENTAL CONTACT	JON MACK	2095819576	CA-CERS	View
PUBLIC CONTACT	MICHAEL HARVEY	2095819576	TRIS	
OPERATION MANAGER	MIKE ARCHIBALD	2095857661	CA-CERS	View
SECONDARY EMERGENCY CONTACT	MICHAEL HARVEY	2097657729	CA-CERS	View

Query executed on: JAN-22-2015

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FRS Facility Detail Report

ENVIRO TECH CHEMICAL SERVICES-PLANT 6
EPA Registry Id: 110063867383
724 PHILLIPS COUNTY ROAD 411
HELENA, AR 72342

Facility Registry Service Links:

- Facility Registry Service (FRS) Overview
- FRS Facility Query
- FRS Organization Query
- EZ Query
- FRS Physical Data Model
- FRS Geospatial Model

Legend

- Selected Facility
- EPA Facility of Interest
- State/Tribe Facility of Interest

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Environmental Interests

Information System	System Facility Name	Information System Id/Report Link	Environmental Interest Type	Data Source	Last Updated Date	Supplemental Environmental Interests
NATIONAL POLLUTANT DISCHARGE ELIMINATION SYSTEM (ICIS-NPDES)	ENVIRO TECH CHEMICAL SERVICES - PLANT 6	AFR004410	ICIS-NPDES NON-MAJOR	ICIS		ICIS-ENFORCEMENT/COMPLIANCE ACTIVITY
NATIONAL POLLUTANT DISCHARGE ELIMINATION SYSTEM (ICIS-NPDES)	ENVIRO TECH CHEMICAL SERVICES - PLANT 6	AFR001410	STORM WATER INDUSTRIAL	ICIS		ICIS-ENFORCEMENT/COMPLIANCE ACTIVITY
TOXIC RELEASE INVENTORY SYSTEM	ENVIRO TECH CHEMICAL SERVICES-PLANT 6	72AHWNETC724PH	TRI REPORTER	TRIS	06/13/2016	

Additional EPA Reports: MyEnvironment Enforcement and Compliance Site Demographics Facility Coordinates Viewer Environmental Justice Map Viewer Watershed Report

Standard Industrial Classification Codes (SIC)

Data Source	SIC Code	Description	Primary
NPDES	2869	INDUSTRIAL ORGANIC CHEMICALS, NOT ELSEWHERE CLASSIFIED	
NPDES	2819	INDUSTRIAL INORGANIC CHEMICALS, NOT ELSEWHERE CLASSIFIED	

Facility Codes and Flags

EPA Region:	06
Duns Number:	
Congressional District Number:	01
Legislative District Number:	
HUC Code/Watershed:	08020203 / LOWER WHITE
US Mexico Border Indicator:	
Federal Facility:	NO
Tribal Land:	NO

Alternative Names

No Alternative Names returned.

Organizations

No Organizations returned.

National Industry Classification System Codes (NAICS)

Data Source	NAICS Code	Description	Primary
TRIS	325998	ALL OTHER MISCELLANEOUS CHEMICAL PRODUCT AND PREPARATION MANUFACTURING.	
NPDES	325180	OTHER BASIC INORGANIC CHEMICAL MANUFACTURING	

Facility Mailing Addresses

Affiliation Type	Delivery Point	City Name	State	Postal Code	Information Systems
MAILING ADDRESS	500 WINMOORE WAY	MODESTO	CA	95358	NPDES
MAILING ADDRESS	500 WINMOORE WAY	MODESTO	CA	95358	TRIS
OPERATOR	500 WINMOORE WAY	MODESTO	CA	95358	NPDES

Contacts

Affiliation Type	Full Name	Office Phone	Information System	Mailing Address
OPERATOR	PHILLIP HARVEY	8005632254	NPDES	View

Query executed on: NOV-11-2016

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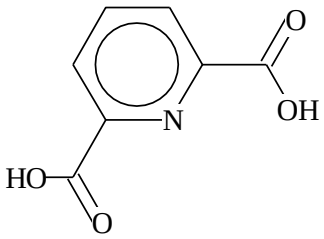
Attachment B:

EPI Suite – ECOSAR Program Results for DPA, Date of Analysis: 04-15-2016

The Ecological Structure Activity Relationships (ECOSAR) Class Program is a computerized predictive system maintained and developed by the U.S. EPA that estimates aquatic toxicity. The program estimates a chemical's acute (short-term) toxicity and chronic (long-term or delayed) toxicity to aquatic organisms, such as fish, aquatic invertebrates, and aquatic plants, by using computerized Structure Activity Relationships (SARs). Information on ECOSAR can be found at: https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model.

EPI Suite – ECOSAR Program Results For CAS 499-83-2



SMILES : O=C(O)c(nc(cc1)C(=O)O)c1
CHEM : 2,6-Pyridinedicarboxylic acid
MOL FOR: C7 H5 N1 O4
MOL WT : 167.12
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------

ECOSAR Program (v1.11) Results:

==========

ECOSAR Version 1.11 Results Page

SMILES :	O=C(O)c(nc(cc1)C(=O)O)c1	
CHEM :	2,6-Pyridinedicarboxylic acid	
CAS Num:		
ChemID1:		
MOL FOR:	C7 H5 N1 O4	
MOL WT :	167.12	
Log Kow:	0.567	(EPISuite Kowwin v1.68 Estimate)
Log Kow:		(User Entered)
Log Kow:		(PhysProp DB exp value - for comparison only)
Melt Pt:		(User Entered for Wat Sol estimate)
Melt Pt:	249.00	(deg C, PhysProp DB exp value for Wat Sol est, 249 dec)
Wat Sol:	4829	(mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol:		(User Entered)
Wat Sol:	5000	(mg/L, PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: 0.567 (EPISuite Kowwin v1.68 Estimate)

Wat Sol: 5000 (mg/L, PhysProp DB exp value)

ECOSAR v1.11 Class-specific Estimations

Pyridine-alpha-Acid

Predicted

ECOSAR Class	Organism	Duration	End Pt	mg/L (ppm)
Pyridine-alpha-Acid:	Fish	96-hr	LC50	323.608
Pyridine-alpha-Acid:	Fish		ChV	29.342 !
Neutral Organic SAR:	Fish	96-hr	LC50	2656.694
(Baseline Toxicity):	Daphnid	48-hr	LC50	1321.570
:	Green Algae	96-hr	EC50	569.703
:	Fish		ChV	222.165
:	Daphnid		ChV	89.187
:	Green Algae		ChV	111.124

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

NOTE: ! = exclamation designates: The toxicity value was estimated through application of acute-to-chronic ratios per methods outlined in the ECOSAR Methodology Document provided in the ECOSAR Help Menu.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Pyridine-alpha-Acid :

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (EC50)
Maximum LogKow: 8.0 (ChV)

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)