Ecotox Report for Case # P-21-0095

General

[redacted]		**Report Status:**	Complete
Status Date:	03/30/2021	**Chemistry Date:**	03/25/2021
Hazard Date:	04/01/2021	**Hazard Chair:**	
Consolidated PMN:	N	**Consolidated Set:**	
Ecotox Related Cases:	Analogue: [redacted]		
Health Related Cases:			
Submitter:			
CAS Number:			
Chemical Name:			
Use:			
Trade Name:			
PV-max(kg/yr):		**Ecotox Assessor:**	Nelson, Megan

Fate Summary Statement

Fate Summary Statement:	

Physical Chemical Information

Molecular Weight:			
Wt% < 500:		**Wt% < 1000:**	
Physical State - Neat:			
Melting Point:		**Melting Point (est):**	
MP (EPI):			
Vapor Pressure:		**Vapor Pressure (est):**	
VP (EPI):			
Water Solubility:		**Water Solubility (est):**	
Water Solubility (EPI):			
Henry's Law::			

Log Koc:		**Log Koc (EPI):**	
Log Kow:		**Log Kow (EPI):**	
Log Kow Comment:			

SAT Concern Level

Ecotox Rating (1):	1
Ecotox Rating Comment (1):	
Ecotox Rating (2):	
Ecotox Rating Comment (2):	
Ecotox Route of Exposure:	No releases to water

Ecotox Comments

Exposure Based Review (Eco):	
Ecotox Comments:	
Exposure Based Testing:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments

Eco Toxicity Comment:

Fate Ratings

Removal in WWT/POTW (Overall):						
Condition	**Rating Values**	**1**	**2**	**3**	**4**	**Comment**
Fish BCF:						
Log Fish BCF:						

Removal in WWT/POTW (Overall):						
Condition	**Rating Values**	**Rating Description**				**Comment**
		1	**2**	**3**	**4**	
WWT/POTW Sorption:		Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:		Extensive	Moderate	Low	Negligible	
Biodegradation Removal:		Unknown	High	Moderate	Negligible	
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:		<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		Days	Weeks	Months	Months	
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months	
Hydrolysis (t1/2 at pH 7,25C) B:		Minutes	Hours	Days	Months	
Sorption to Soils/Sediments:		V. Strong	Strong	Moderate	Low	
Migration to Ground Water:		Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	
Bio Comments:						
Fate Comments:						

Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	96-h	LC50	*		Predictions are based on analogue test data ([redacted] * = no effects at saturation
Daphnid	48-h	LC50	*		Predictions are based on analogue test data [redacted] * = no effects at saturation
Green Algae	96-h	EC50	*		Predictions are based on analogue test data [redacted] * = no effects at saturation
Fish	-	Chronic Value	*		Predictions are based on the negligible water solubility of the new chemical substance; * = no effects at saturation
Daphnid	-	Chronic Value	*		Predictions are based on the negligible water solubility of the new chemical substance; * = no effects at saturation
Green Algae	-	Chronic Value	*		Predictions are based on analogue test data [redacted] * = no effects at saturation

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Sediment Inv.	10-day	LC50	>10,000 mg/kg dry sediment		Predictions are based on analogue test data [redacted]

Ecotox Value Comments: Predictions are based on analogue data [redacted] and the negligible water solubility of the new chemical substance; MW [redacted]; Log Kow = 14.02 (P, top left), 20.82 (P, top right); liquid with a MP = -45C (M); S = 1.42E-9 mg/L (P, left), 1.51E-16 mg/L (P, top right); effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO3; and TOC <2.0 mg/L.

All of the following studies were previously submitted and reviewed under [redacted] All analogues and tests were acceptable for [redacted]

Acute Fish Ecotoxicity Test:
Testing laboratory conducted a 96-hour acute toxicity limit test in zebrafish (Brachydanio rerio) with Durasyn 162 (analog; purity: >99%) under static conditions. The number of dead fish was recorded after incubation times of 24, 48, 72, and 96 hours. This study followed OECD test guideline No. 203 (1992). Following a screening test, single replicates of seven B. rerio each were exposed to a dilution water control (drinking water) or the test substance prepared as a water accommodated fraction (WAF) at a nominal loading level of 10,000 mg/L. Recovery of the test item was 84.3% at the end of the study, as determined by IR analysis. To prepare the WAF, 10 g of test item was introduced into 1 L of dilution water whilst shaking. The shaking continued for 24 hours at room temperature. Thereafter, the suspension was filtered through a filter paper which was previously rinsed thoroughly with ultrapure water. Over the course of the study, temperature was 25±1°C, pH ranged from 7.9-8.8 and dissolved oxygen ranged from 8.4-8.7 mg/L. A loading rate of 2.3 fish/L was calculated. The fish were exposed to a light-dark cycle of 16 and 8 hours, respectively. No mortalities occurred in any of the control or test replicates. Based on nominal loading level, the 96-hour LL50 was >10,000 mg/L (WAF). This is an acceptable test.
96-hour LL50 >10,000 mg/L (WAF)

Acute Invertebrate Ecotoxicity Test:
Testing laboratory conducted a 48-hour acute toxicity limit test in the water flea (Daphnia magna) with Alkane 5 (analog; purity not stated) under static conditions. This study followed OECD test guideline No. 202 (1984), "Daphnia sp., Acute Immobilisation Test and Reproduction Test referenced as Method C.2 of Commission Directive 92/69/EEC and US EPA Code of Federal Regulations Title 40, Part 797, Section 1300. Following a range-finding test, four replicates of ten D. magna each were exposed to the test substance prepared as a water accommodated fraction (WAF) at a nominal loading level of 1000 mg/L for 48 hours under static test conditions. An additional two replicates of D. magna were exposed to a dilution water control

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
					(reconstituted freshwater). The stability of the test substance could not be confirmed by TOC analysis; GC-MS analysis showed the concentration of the test material in the WAF to be no higher than background levels of hydrocarbon exhibited in control samples, thereby indicating chemical analysis by this method was not appropriate. The test solution was prepared approximately 24 hours prior to the start of the study by dispensing 2.0 g of test substance onto the surface of 2 L of dilution water and stirring for 20 hours at a rate of 600-670 rpm. The depth of the vortex was approximately 20-25% of depth of the mixing vessel. After 20 hours, stirring was stopped and the mixture was allowed to stand for 4 hours prior to removal of the aqueous phase or WAF for testing. This WAF was dispersed into the four replicate test vessels each containing 200 mL of test culture. The test vessels were covered to reduce evaporation. At the start of mixing, the test substance was observed to be contained within the vortex and present as clear, oily globules on the water surface. However, after the stirring and standing periods, the test substance was observed at the water surface only. During testing, the WAF was observed to be a clear, colorless solution. Over the course of the study, temperature was maintained at 21.0°C, pH ranged from 7.7-7.8 and dissolved oxygen ranged from 7.9-8.4 mg/L. The theoretical hardness of the dilution water hardness was 270 mg/L as CaCO3; TOC was ≤1.48 mg/L. A loading rate of 50 daphnids/L was calculated. No immobilization was observed in any of the control or test replicates. Based on nominal loading levels, the 48-hour EL50 was >1000 mg/L (WAF). This is an acceptable test. 48-hour EL50 >1000 mg/L (WAF) Chronic Invertebrate Ecotoxicity Test: 1) [redacted] conducted a 21-day full life-cycle toxicity limit test in the water flea (Daphnia magna) with Durasyn 162 (analog; purity: >99%) under static-renewal conditions with daily renewal at a photoperiod of 16 hours light: 8 hours darkness. This study followed OECD test guideline No. 211 (1997), and OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures (2000). Ten replicates of Daphnia magna (< 24 hours old) cultures each were exposed to a dilution water control (fortified well water) or the test substance prepared as a water accommodated fraction (WAF) at a nominal loading level of 125 mg/L. To prepare the WAFs, 0.544 mL of the test substance was directly added to 3.5 L of fortified well water in a 4.0-L glass jar containing a 2.5-inch Teflon-coated stir bar. The mass of the test substance to be added (0.4373 g) was based on the experimentally-determined specific gravity of 0.8039 g/mL. The glass jar was placed on a magnetic stir plate and stirred with no vortex for 48 ± 1 hour. The WAF was then allowed to settle for 1 hour prior to use. The WAF was removed from an outlet port, located 2 cm from the bottom of the glass jar. The WAF was drawn off directly into each replicate exposure vessel. WAFs were freshly prepared at each renewal. Throughout the exposure period, no observations of undissolved test substance were noted in any of the test solutions prepared from the WAF in this study. Over the course of the study, temperature ranged from 19-24ºC in

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
					test vessels and 21-24°C in the water bath containing test vessels. The pH ranged from 7 6 8 1, and dissolved oxygen ranged from 7 5 9 4 mg/L Dilution water hardness ranged from 150-180 mg/L as CaCO3; TOC ranged from 0.51-1 6 mg/L A loading rate of 12 5 daphnids/L was calculated The percent immobility in the control and test group was 0% and 20%, respectively. Mean number of offspring released per female, mean total body length and mean dry weight of the treated group were not statistically different when compared to control group measurements Based on nominal loading level, the 21 day NOEL and LOEL for survival, reproduction and growth were 125 mg/L (WAF) and 125 mg/L (WAF), respectively Survival of daphnids and production of offspring were manually observed using an Olympus SZ40 dissecting scope in combination with a calibrated Olympus objective micrometer. This is an acceptable test. 21 day NOEL (survival, reproduction and growth) 125 mg/L (WAF) 21-day LOEL (survival, reproduction and growth) >125 mg/L (WAF) GMATC ChV 125 mg/L (WAF) 2) Testing laboratory conducted a 21 day full life cycle toxicity limit test in the water flea (Daphnia magna) with Durasyn 166 (analog; purity: >99%) under semi static conditions with daily renewal This study followed OECD test guideline No. 211 (1997) and OECD Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures (2000) Ten replicates of a single daphnid each were exposed to a dilution water control (fortified well water) or the test substance prepared as a water accommodated fraction (WAF) at a nominal loading level of 125 mg/L. To prepare WAFs, 0.539 mL of test substance was directly added into 3 5 L of fortified well water in a 4 0 L screw-capped glass jar containing a 2.5-inch Teflon-coated stir bar. The mass of test substance to be added (0 4372 g) was based on the experimentally determined specific gravity of 0.8112 g/mL. The screw-capped glass jar was placed on a magnetic stir plate and stirred with no vortex for 48 hours The WAF was then allowed to settle for 1 hour prior to use. The WAF was removed from an outlet port, located 2 cm from the bottom of the screw capped glass jar and drawn off directly into each replicate exposure vessel. After settling, the exposure solutions were observed to be clear and colorless with no visible undissolved test substance. WAFs were freshly prepared at each renewal. Throughout the exposure period, no observations of undissolved test substance were noted in any of the test solutions prepared from the WAF in this study. Over the course of the study, temperature ranged from 19 21ºC in the test vessels and 21-24°C in the water bath containing the test vessels. The pH ranged from 7 6 8 1, and dissolved oxygen ranged from 7 4 9 5 mg/L dilution water hardness was 148-172 mg/L as CaCO3; TOC ranged from 0.51-1.6 mg/L prior to testing A loading rate of 12 5 daphnids/L was calculated The percent immobility in the control and test group was 0% and 20%, respectively Mean number of offspring released per female, mean total body length and mean dry weight of the treated group were not statistically different when compared to control group measurements Based on nominal loading

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
					level, the 21-day NOEL and LOEL for survival, growth and reproduction were 125 mg/L (WAF) and >125 mg/L (WAF), respectively. This is an acceptable test. 21-day NOEL (survival, reproduction and growth) = 125 mg/L (WAF) 21-day LOEL (survival, reproduction and growth) >125 mg/L (WAF) GMATC = ChV > 125 mg/L (WAF) Chronic Bacterial Ecotoxicity Test: Testing laboratory conducted a 16-hour chronic toxicity test in the bacteria Pseudomonas putida with Durasyn 162 (analog; purity: >99%). This study followed DIN 38412, Part 8 (1991). Three replicates of P. putida (10 mL of inoculums each) were exposed to a dilution water control (deionized water) or the test item at a nominal concentration of 100, 1000 or 10,000 mg/L for 16 +/- 1 hour. To prepare the test solutions, 80 mL of dilution water was added to test vessels containing the test substance. Thereafter, 2.5 mL of mineral solutions I and II and 5 mL of mineral solution III were added. The compositions of the mineral solutions were as follows: (I) 20 g NaNO3, 4.8 g K2HPO4 and 2.4 g KH2PO4 in 1 L of dilution water; (II) 88 g glucose-monohydrate in 1 L of dilution water; (III) 4 g MgSO4 x 7H2O and 0.01 g iron citrate in 1 L of dilution water. The test solutions were then incubated on a shaking machine. Compared to the control, the percent inhibition at 100, 1000 and 10,000 g/L was 3.7%, -3.8% and 4.4%, respectively. Based on nominal concentrations, the 16-hour NOEC and LOEC were 10,000 mg/L and >10,000 mg/L, respectively. This is an acceptable test. 16-hour NOEC = 10,000 mg/L 16-hour LOEC >10,000 mg/L Algal Ecotoxicity Test: Testing laboratory conducted a 96-hour inhibition test in green algae (Selenastrum capricornutum) with Alkane 5 (analog; purity not stated) under static conditions. This study followed OECD test guideline No. 201 (1984), “Alga, Growth Inhibition Test” referenced as Method C.3 of Commission Directive 92/69/EEC and US EPA Code of Federal Regulations, Title 40, Part 797, Section 1050. Following a range-finding test, six replicates of S. capricornutum (~104 cells/mL) were exposed to the test substance prepared as a water accommodated fraction (WAF) at a nominal loading level of 1000 mg/L. An additional three replicates of S. capricornutum were exposed to a dilution water control (culture medium). The stability of the test item could not be confirmed by TOC analysis; GC-MS analysis showed the concentration of the test material in the WAF to be no higher than background levels of hydrocarbon exhibited in control samples, thereby indicating chemical analysis by this method was not appropriate. The algal cultures were illuminated with a light intensity of about 7000 lux with constant shaking. Approximately 24 hours prior to the start of the study, a 2000 mg/L loading level was prepared by adding 4000 mg of the test substance to the surface of 2 L of culture medium and stirring for 20 hours at rate of 615 rpm (control) or 580 rpm (test WAF).

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
					The depth of the vortex was approximately 20-25% of the depth of the mixing vessel. After 20 hours, stirring was stopped and the mixture was allowed to stand for 4 hours prior to removal of the aqueous phase or WAF for testing. An aliquot (150 mL) of this WAF was diluted 50:50 with algal suspension to give a final loading level of 1000 mg/L (WAF). The test flasks were covered with aluminum foil. At the start of the mixing period, the test substance was observed to be contained within the vortex and floating on the surface of the test medium. Samples were taken at 0, 24, 48, 72, and 96 hours and the absorbance measured at 665 nm using a Jenway 6100 Spectrophotometer. The cell densities if the control cultures at 0, 24, 48, 72, and 96 hours were determined by direct counting with the aid of a haemocytometer to confirm that the absorbance values were sufficiently well correlated with cell densities to be used to monitor the growth of the test cultures. However, after the stirring and standing periods, the test material was observed to be floating on the surface of the test medium only. During testing, the WAF was observed to be a clear, colorless solution. Over the course of the study, temperature ranged from 24 ± 1°C and pH ranged from 7.5-9.9. The mean cell density of control cultures increased by a factor of 124 within 96 hours. No microscopic abnormalities were detected in any of the control or test replicates. Based on the nominal loading level, the 96-hour EL50 for biomass was >1000 mg/L (WAF). The 48-hour EL50 for growth rate was >1000 mg/L (WAF). The 96-hour NOEL and LOEL for biomass were 1000 mg/L (WAF) and >1000 mg/L (WAF), respectively. This is an acceptable test. 48-hour EL50 (growth rate) >1000 mg/L (WAF) 96-hour EL50 (biomass) >1000 mg/L (WAF) 96-hour NOEL (biomass) = 1000 mg/L (WAF) 96-hour LOEL (biomass) >1000 mg/L (WAF) GMATC = ChV > 1000 mg/L (WAF) Acute Sediment Invertebrate Ecotoxicity Test: Testing laboratory conducted a 10-day sediment re-worker test in amphipods (Corophium volutator) with Durasyn 156 (analog; purity: 100%) under static conditions. This study followed PARCOM Protocol 1995 Part A “Protocols on Methods for the Testing of Chemicals used in the Offshore Oil Industry.” Four replicates of twenty C. volutator each were exposed to natural sediment spiked with the test substance at nominal concentrations of 0 (control), 480, 1000, 2200, 4800 and 10,000 mg/kg dry sediment. Each treatment concentration was mixed for 10 minutes with a hand-held mixer. Each replicate contained ~200 mL of natural sediment (water content: 64.5%) and 800 mL of overlying synthetic seawater. All treatments were prepared and dispensed 12-24 hours prior to initiating the test. Over the course of testing, temperature ranged from 20.1-20.7°C, pH ranged from 7.0-8.0, dissolved oxygen ranged from 7.8-81 mg/L, and salinity ranged from 17.3-18.5 ppt. The percent mortality at 0 (control), 480, 1000, 2200, 4800 and 10,000 mg/kg dry sediment was 11.25%, 2.5%, 12.5%, 12.5%, 11.25% and 7.5%, respectively. Concurrent 10-day control mortality was 11%. Based on nominal concentrations, the 10-day LC50

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
		was >10,000 mg/kg dry sediment. This is an acceptable test.			
		10-day LC50 >10,000 mg/kg dry sediment			

Ecotox Factors

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic(ppb):	*			Acute and chronic COCs were not calculated because acute and chronic toxicity values are no effects at saturation. * = no effects at saturation
Chronic Aquatic(ppb):	*			Acute and chronic COCs were not calculated because acute and chronic toxicity values are no effects at saturation. * = no effects at saturation

Factors	Values	Comments
SARs:		
SAR Class:		
TSCA NCC Category?	Neutral Organics	

Recommended Testing:

Ecotox Factors Comments: Environmental Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using hazard data for an analogous chemical and the negligible water solubility of the new chemical substance. This substance falls within the TSCA New Chemicals Category of Neutral Organics. Acute and chronic toxicity values estimated for fish, aquatic invertebrates, and algae are all no effects at saturation. These toxicity values indicate that the new chemical substance is expected to have low environmental hazard. Because hazards are not expected up to the water solubility limit, acute and chronic concentrations of concern are not identified.

Environmental Risk: Risks from acute and chronic exposures to the environment are not expected at any concentration of the new chemical substance soluble in the water (i.e., no effects at saturation).

Comments/Telephone Log

Artifact	Update/Upload Time
[redacted]	[redacted]