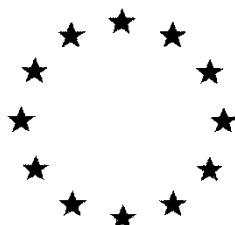


European Commission



**Draft Assessment Report prepared according to the Commission
Regulation (EU) N° 1107/2009**

XDE-729 Methyl (Halauxifen-methyl) Volume 3 – B.2

**Rapporteur Member State: United Kingdom
Co-Rapporteur Member State: France**

WARNING: This document forms part of an EC evaluation data package and should not be read in isolation. Registration must not be granted on the basis of this document.

Version History

When	What
2013-12-19	Initial DAR

WARNING: This document forms part of an EC evaluation data package and should not be read in isolation. Registration must not be granted on the basis of this document.

CONTENTS**Page****B.2 Physical and chemical properties****3**

B.2.1 Physical and chemical properties of the active substance

3

B.2.1a Physical properties of the degradation product X11449757

15

B.2.1b Physical properties of the degradation product X11393729 (XDE-729 acid)

23

B.2.1c Physical property of the degradation product X11406790

32

B.2.2 Physical, chemical and technical properties of the plant protection product

33

B.2.3 Summary of physical and chemical properties

49

B.2.4 References relied on

51

WARNING: This document forms part of an EC evaluation data package and should not be read in isolation. Registration must not be granted on the basis of this document.

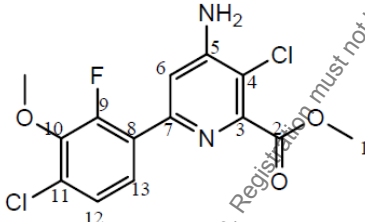
B.2 PHYSICAL AND CHEMICAL PROPERTIES**B.2.1 Physical and chemical properties of the active substance (XDE-729 methyl ester)****Table B.2.1** Summary of the physical and chemical properties of the active substance (studies were completed to an acceptable standard and results were considered to be valid unless specified otherwise)

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference
B.2.1.1 (IIA 2.1)	Melting point	Pure Active Ingredient - TSN031 117- 0005; 99.1%	EEC method A 1(Differential Scanning Calorimetry)	145.5°C	No comment/GLP-Yes	FAPC-G-10-84; Frank, A.
B.2.1.2 (IIA 2.1)	Boiling point	Pure Active Ingredient - TSN031 117- 0005; 99.1%	EEC method A 2	Decomposes before boiling	No comment/GLP-Yes	FAPC-G-10-84; Frank, A.
B.2.1.3 (IIA 2.1)	Temperature of decomposition or sublimation	Pure Active Ingredient - TSN031 117- 0005; 99.1%	EEC Method A1 (Differential Scanning Calorimetry)	221.06°C	No comment/GLP-Yes	FAPC-G-10-84; Frank, A.

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference
B.2.1.4 (IIA 2.2)	Relative density	Pure Active Ingredient - TSN031 117- 0005; 99.1%	EEC method A 3 (Pycnometer methods)	1.5057 g/cm ³ at 20.1 °C	Determined at 20.1°C GLP-Yes	NAFST-10-246; Elliott, T.
B.2.1.5 (IIA 2.3)	Vapour pressure	Pure Active Ingredient - TSN031 117- 0005; 99.1%	EEC method A 4 (Effusion method: Vapour pressure balance)	1.5 x 10 ⁻⁸ Pa at 25°C (1.1 x 10 ⁻¹⁰ mm Hg) and 5.9 x 10 ⁻⁹ Pa at 20°C (4.4 x 10 ⁻¹¹ mm Hg).	Determined at 25°C GLP-Yes Since vp is <0.0001Pa. Very slightly volatile	NAFST-10-92; Turner, B.
B.2.1.6 (IIA 2.3)	Volatility, Henry's law constant	Calculation	Not relevant	Unbuffered pH = 1.11 x 10 ⁻⁶ Pa m ³ /mol pH 5 = 1.23 x 10 ⁻⁶ Pa m ³ /mol pH 7 = 1.22 x 10 ⁻⁶ Pa m ³ /mol pH 9 = 1.20 x 10 ⁻⁶ Pa m ³ /mol (Calculated from water solubility and vp (units Pa m ³ mol ⁻¹))	GLP-Yes <1E-5 very slightly volatile	NAFST-11-115; Jones, J.
B.2.1.7 (IIA 2.4) And B.2.1.8 (IIA 2.4)	Appearance: physical state Appearance: colour	Pure Active Ingredient - TSN031 117- 0005; 99.1%	Ocular	Pure Active Ingredient - White powder at 24.2°C	No comment/GLP-Yes	FAPC-G-10-84; Frank, A.

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference
		Technical Grade Active Ingredient – TSN031 117-0006; 95.1%	Ocular	Technical Grade Active Ingredient – Off-white powder at 23.8°C	No comment/GLP-Yes	FAPC-G-10-83; Frank A.
B.2.1.9 (IIA 2.4)	Appearance: odour	Pure Active Ingredient - TSN031 117-0005; 99.1%	Olfactory	Mild	No comment/GLP-Yes	FAPC-G-10-84; Frank, A.
		Technical Grade Active Ingredient – TSN031 117-0006; 95.1%		Mild		FAPC-G-10-83; Frank, A.
B.2.1.10 (IIA 2.5)	Spectra: UV/VIS	Pure Active Ingredient - TSN031 117-0005; 99.1%	OPPTS 830.7050/OECD101	<u>λ max, nm</u> Neutral: 212, 249 Acidic: 215, 256 Basic: 212, 247 See molecular extinction (below) for coefficient at 290nm.	Determined at 25 ± 0.5°C GLP-Yes	NAFST-10-316; Habeeb, S.

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference																																																																														
B.2.1.10 (IIA 2.5)	Molecular extinction	Pure Active Ingredient - TSN031 117- 0005; 99.1%	OPPTS 830.7050/OECD101	<u>L mol⁻¹ cm⁻¹</u> Neutral:16,401-16,724 at 212 nm, 18,956-19,548 at 249 nm Acidic: 22,496-22,516 at 215 nm, 23,770-23,779 at 256 nm Basic: 19,023-19,099 at 212 nm, 21,979-22,061 at 247 nm The molar absorption coefficients at the solar cut-off wavelength at 290 nm are shown below: pH < 2 : 12,474 L mol⁻¹ cm⁻¹ pH 7 : 3,798 L mol⁻¹ cm⁻¹ pH > 10 : 4,337 L mol⁻¹ cm⁻¹	Determined at 25 ± 0.5°C Results are in corresponding order of λ max in section IIA 2.5. GLP-Yes At pH 2 ε > 10mol⁻¹cm⁻¹	NAFST-10-316; Habeeb, S.																																																																														
B.2.1.10 (IIA 2.5)	Spectra: IR	Pure Active Ingredient - TSN031 117- 0005; 99.1%	OPPTS 830.7050/OECD101	The IR was consistent with the structure of XDE-729 methyl <table><tr><th>Functional Group</th><th>Bond</th><th>Range (cm⁻¹)</th><th>Intensity</th><th>Mode</th><th>Absorption Bands in Spectrum</th></tr><tr><td>Amine (1°)</td><td>N-H</td><td>3400-3250</td><td>Medium</td><td>Stretch</td><td>3479.5, 3336.6</td></tr><tr><td>Aromatic</td><td>C-H</td><td>3100-3000</td><td>Strong</td><td>Stretch</td><td>3081.4</td></tr><tr><td>Alkane</td><td>C-H</td><td>3000-2850</td><td>Medium</td><td>Stretch</td><td>2944.3</td></tr><tr><td>Carbonyl (Ester)</td><td>C=O</td><td>1750-1735</td><td>Strong</td><td>Stretch</td><td>1731.3</td></tr><tr><td>Pyridine</td><td>C=N</td><td>1660-1560</td><td>Strong</td><td>Stretch</td><td>1610.3</td></tr><tr><td>Aromatic</td><td>C-C</td><td>1600-1585</td><td>Medium</td><td>Stretch</td><td>1582.9</td></tr><tr><td>Alkane</td><td>C-H</td><td>1470-1450</td><td>Medium</td><td>Bend</td><td>1450.1</td></tr><tr><td>Alkane</td><td>C-H</td><td>1370-1350</td><td>Medium</td><td>Rock</td><td>1365.7</td></tr><tr><td>Aromatic Amine</td><td>C-N</td><td>1335-1250</td><td>Strong</td><td>Stretch</td><td>1264.9</td></tr><tr><td>Ester, Ether</td><td>C-O</td><td>1320-1000</td><td>Strong</td><td>Stretch</td><td>1243.7</td></tr><tr><td>Aromatics</td><td>C-H</td><td>1290-1000</td><td>Weak</td><td>Asymmetric</td><td>1230.1</td></tr><tr><td>Aryl Halide</td><td>C-Cl</td><td>1100-900</td><td>Medium</td><td>Bend</td><td>1045.2</td></tr></table>	Functional Group	Bond	Range (cm ⁻¹)	Intensity	Mode	Absorption Bands in Spectrum	Amine (1°)	N-H	3400-3250	Medium	Stretch	3479.5, 3336.6	Aromatic	C-H	3100-3000	Strong	Stretch	3081.4	Alkane	C-H	3000-2850	Medium	Stretch	2944.3	Carbonyl (Ester)	C=O	1750-1735	Strong	Stretch	1731.3	Pyridine	C=N	1660-1560	Strong	Stretch	1610.3	Aromatic	C-C	1600-1585	Medium	Stretch	1582.9	Alkane	C-H	1470-1450	Medium	Bend	1450.1	Alkane	C-H	1370-1350	Medium	Rock	1365.7	Aromatic Amine	C-N	1335-1250	Strong	Stretch	1264.9	Ester, Ether	C-O	1320-1000	Strong	Stretch	1243.7	Aromatics	C-H	1290-1000	Weak	Asymmetric	1230.1	Aryl Halide	C-Cl	1100-900	Medium	Bend	1045.2		NAFST-10-316; Habeeb, S.
Functional Group	Bond	Range (cm ⁻¹)	Intensity	Mode	Absorption Bands in Spectrum																																																																															
Amine (1°)	N-H	3400-3250	Medium	Stretch	3479.5, 3336.6																																																																															
Aromatic	C-H	3100-3000	Strong	Stretch	3081.4																																																																															
Alkane	C-H	3000-2850	Medium	Stretch	2944.3																																																																															
Carbonyl (Ester)	C=O	1750-1735	Strong	Stretch	1731.3																																																																															
Pyridine	C=N	1660-1560	Strong	Stretch	1610.3																																																																															
Aromatic	C-C	1600-1585	Medium	Stretch	1582.9																																																																															
Alkane	C-H	1470-1450	Medium	Bend	1450.1																																																																															
Alkane	C-H	1370-1350	Medium	Rock	1365.7																																																																															
Aromatic Amine	C-N	1335-1250	Strong	Stretch	1264.9																																																																															
Ester, Ether	C-O	1320-1000	Strong	Stretch	1243.7																																																																															
Aromatics	C-H	1290-1000	Weak	Asymmetric	1230.1																																																																															
Aryl Halide	C-Cl	1100-900	Medium	Bend	1045.2																																																																															

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference																																																
B.2.1.10 (IIA 2.5)	Spectra: NMR	Pure Active Ingredient - TSN031 117- 0005; 99.1%	OPPTS 830.7050/OECD101	The ¹H and ¹³C NMR spectra were consistent with the structure of XDE-729 methyl  <table><tr><th>Proton Label</th><th>PPM/Multiplicity</th><th>Integration</th></tr><tr><td>H1, H14</td><td>3.9 / doublet</td><td>592.8</td></tr><tr><td>H6</td><td>7.3 / doublet</td><td>100.5</td></tr><tr><td>H12</td><td>7.4 / doublet</td><td>100.0</td></tr><tr><td>H13</td><td>7.6 / triplet</td><td>100.4</td></tr><tr><td>NH₂ Protons</td><td>6.9 / singlet</td><td>195.66</td></tr></table> <table><tr><th>Carbon Label</th><th>PPM</th></tr><tr><td>C1</td><td>52.6</td></tr><tr><td>C2</td><td>165.6</td></tr><tr><td>C3, C5</td><td>110.8</td></tr><tr><td>C4</td><td>148.8</td></tr><tr><td>C5, C3</td><td>127.9</td></tr><tr><td>C6</td><td>151.9</td></tr><tr><td>C7</td><td>126.6</td></tr><tr><td>C8</td><td>110.5</td></tr><tr><td>C9</td><td>152.4, 154.9</td></tr><tr><td>C10</td><td>144.2</td></tr><tr><td>C11</td><td>149.0</td></tr><tr><td>C12</td><td>125.2</td></tr><tr><td>C13</td><td>125.2</td></tr><tr><td>C14</td><td>61.5</td></tr></table>	Proton Label	PPM/Multiplicity	Integration	H1, H14	3.9 / doublet	592.8	H6	7.3 / doublet	100.5	H12	7.4 / doublet	100.0	H13	7.6 / triplet	100.4	NH ₂ Protons	6.9 / singlet	195.66	Carbon Label	PPM	C1	52.6	C2	165.6	C3, C5	110.8	C4	148.8	C5, C3	127.9	C6	151.9	C7	126.6	C8	110.5	C9	152.4, 154.9	C10	144.2	C11	149.0	C12	125.2	C13	125.2	C14	61.5	Chemical shifts and integration for the protons conformed to expected results for XDE-729 methyl. Other recognized resonances were residual deuterated DMSO and water. No other extraneous resonances were observed. Elucidation of the splitting patterns from the spectra are possible from an expansion of the aliphatic region and aromatic region of the NMR spectra. Chemical shifts for the 14 carbons conformed to the expected results based on the structure of XDE-729 Methyl. Other recognized resonances were residual deuterated DMSO. No other extraneous resonances were observed.	NAFST-10-316 Habeeb, S
Proton Label	PPM/Multiplicity	Integration																																																				
H1, H14	3.9 / doublet	592.8																																																				
H6	7.3 / doublet	100.5																																																				
H12	7.4 / doublet	100.0																																																				
H13	7.6 / triplet	100.4																																																				
NH ₂ Protons	6.9 / singlet	195.66																																																				
Carbon Label	PPM																																																					
C1	52.6																																																					
C2	165.6																																																					
C3, C5	110.8																																																					
C4	148.8																																																					
C5, C3	127.9																																																					
C6	151.9																																																					
C7	126.6																																																					
C8	110.5																																																					
C9	152.4, 154.9																																																					
C10	144.2																																																					
C11	149.0																																																					
C12	125.2																																																					
C13	125.2																																																					
C14	61.5																																																					

section (Annex point)	study	purity	method	results		Comment/GLP (Y/N)	reference
B.2.1.10 (IIA 2.5)	Spectra: MS	Pure Active Ingredient - TSN031 117- 0005; 99.1%	OPPTS 830.7050/OECD101	<u>m/z</u> Positive mode (M+H) ⁺ : 345, 347, 349 Negative mode (M-H) ⁻ : 343, 345, 347 Ion scan shows peaks at molecular weights consistent with the expected fragmentation of XDE-729 methyl Parent ion showed a characteristic “plus two” isotope pattern, consistent with the presence of chlorine in the molecule.			NAFST-10-316; Habeeb, S.
B.2.1.11 (IIA 2.6)	Solubility in water	Pure Active Ingredient - TSN031 117- 0005; 99.1%	EEC method A 6	pH	mg/L	Determined at 20°C 0.1-10 slightly soluble GLP-Yes	NAFST-10-93; Turner, B.
				Purified	1.83		
				5	1.66		
				7	1.67		
				9	1.69		
B.2.1.12 (IIA 2.7)	Solubility in organic solvents (technical active substance)	Technic al Grade Active Ingredient – TSN031 117- 0006; 95.1%	EEC Method A6	Solvent	mg/L	Determined at 20°C GLP-Yes (<0.1 mg/l very slightly soluble 0.1-10 slightly soluble 10-1000 moderately soluble ≥1000 readily soluble)	NAFST-10-96; Turner, B.
				Methanol	38.1		
				Acetone	> 250		
				Xylene	9.13		
				1,2-dichloroethane	65.9		
				Ethyl Acetate	129		
				n-heptane	0.0361		
				n-octanol	9.83		

section (Annex point)	study	purity	method	results		Comment/GLP (Y/N)	reference
B.2.1.13 (IIA 2.8.1/01)	n-octanol/water partition co-efficient	See below	See below	pH to be investigated when pKa <12 (acids) or >2 (alkali), therefore see below for results.		Since the test substance is an ionisable compound, the partition coefficient of XDE-729 methyl was determined in buffer solutions at pH 5, 7 and 9. See below for results.	-
B.2.1.13 (IIA 2.8.2/01)	Effect of pH on n- octanol/water partition co-efficient	Pure Active Ingredie nt - TSN031 117-	EEC method A 8	pH	Log K _{ow}	Determined at 20°C GLP-Yes Given that the log K _{ow} > 3, the data suggests a potential	NAFST-10-95; Turner, B
				5	3.75		
				7	3.76		

section (Annex point)	study	purity	method	results		Comment/GLP (Y/N)	reference
		0005; 99.1%		9	3.92	to be fat soluble. It was noted that slightly lower and more variable results were obtained for the samples prepared in pH 9 buffer (at high fortification level 87% recovery, RSD=22% and at LOQ, 72% recovery and RSD=9%). However, the study report states that this may be due to the potential degradation of the ester to its acid form. Given the pH of the buffer, this is considered a reasonable explanation, and since the mean recoveries fall within the acceptable range, the data is considered fit for purpose.	
B.2.1.14 (IIA 2.9)	Stability in water			See section 2.1.15.			

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference
B.2.1.15 (IIA 2.9)	Hydrolysis rate	Radiolabeled test materials: INV031-089-0003 (97.4%), INV027-098-0002 (97.8%)	OECD guideline 111, USA EPA OPPTS 835.2120 (equiv. To EEC method C.7)	The hydrolytic stability of XDE-729 was investigated in sterile buffer solutions at pH 4 (10, 25, 50°C); pH 7 (10, 25, 50°C) and pH 9 (10, 25, 50°C). From Arrhenius analysis of the data, the half life of XDE-729 at 25°C was estimated: pH 4: DT₅₀ = 81 days. pH 7: DT₅₀ = 155 days. pH 9: DT₅₀ = 3 days. X11393729 was the only major transformation product observed in all three pH buffers and temperatures.	GLP – Yes Determined at 25 °C Radiolabelled material used in place of pure active substance, this is acceptable. As a radiolabelled balanced study, the identities of degradation products were determined by LC/MS and LC/MS/MS. Classification: pH 4: Slightly hydrolysing. pH 7: Slightly hydrolysing. pH 9: Readily hydrolysing.	090126, D. Liu, July 2011

XDE 729 Methyl (Halauxifen-methyl)

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference
B.2.1.16 (IIA 2.9)	Photochemical degradation	Radiola beled test material s: INV031 089- 0003 (97.4%), INV027 098- 0002 (97.8%)	OECD guideline 316, US EPA OPPTS 835.2240	ID of breakdown products: numerous photoproducts and CO ₂ Photochemical half-life: 0.129 hours (7.8 minutes) at 40° N latitude in summer sunlight Mass balance: 94 ± 3% of applied	Determined in sterile pH 7 buffer at 25 °C under xenon light GLP - yes <i>phototransformation in water DT50</i> <i>>30d slightly degradable</i> <i>10-30 moderately degradable</i> <i>4-10 fairly degradable</i> <i><10% photolysed at 20- 25 °C within 30d photolytically stable</i>	101793, B. Blakeslee, August 2011
B.2.1.17 (IIA 2.9)	Quantum yield	Radiola beled test material s: INV031 089- 0003 (97.4%), INV027 098- 0002 (97.8%)	OECD guideline 316, US EPA OPPTS 835.2240	Quantum yield: 5.63	GLP - yes	101793, B. Blakeslee, August 2011

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference
B.2.1.18 (IIA 2.9)	Dissociation constant (pKa)	Pure Active Ingredient - TSN031 117- 0005; 99.1%	OECD Test Guideline 112	2.84 ± 0.04 at 19.9°C	GLP – Yes Dissociation constant determined spectroscopically.	10-040-G; Cathie C.
B.2.1.19 (IIA 2.10)	Stability in air, photochemical oxidative degradation	N/A Calculated value	Atkinson calcn.	An atmospheric half-life of 2.155 days (25.866 hours) has been calculated.	GLP – No Assumes a hydroxyl radical concentration of 1.5x10 ⁶ radicals/cm ³ and a 12-hour day.	101450, B. Wendelburg, April 2011
B.2.1.20 (IIA 2.11)	Flammability and auto-flammability (technical active substance)	Technical Grade Active Ingredient – TSN031 117- 0006; 95.1%	Flammability: EEC method A 10 Auto-flammability: EEC method A 16	Flammability: Not highly flammable XDE-729 Methyl TGA1 burned (on melting) with a yellow flame, which extinguished immediately on removal of the burner flame. There was no propagation along the train. Auto flammability: No self-ignition temperature under the conditions of the test (up to a maximum temperature of 400°C).	GLP - Yes	NAFST-10-124; Turner, B.
B.2.1.21 (IIA 2.12)	Flash point (technical active substance)	-	EEC method A 9 (closed cup only)	Not required for a solid	-	

XDE 729 Methyl (Halauxifen-methyl)

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference
B.2.1.22 (IIA 2.13)	Explosive properties (technical active substance)	Technic al Grade Active Ingredie nt – TSN031 117- 0006; 95.1%	EEC method A 14	Not explosive according to EEC method A 14	Thermal, friction and shock test GLP - Yes	NAFST-10-124; Turner, B.
B.2.1.23 (IIA 2.15)	Oxidising properties (technical active substance)	Technic al Grade Active Ingredie nt – TSN031 117- 0006; 95.1%	EEC method A 17	Not oxidising according to EEC method A 17 (The mixtures of 2:1, 1:1 or 1:2 test substance/cellulose only burned slowly and did not burn to completion, Therefore, XDE- 729 Methyl TGAI was considered to be non- oxidising. By comparison, the reference mixture burned vigorously to completion in 25 seconds)	GLP - Yes	NAFST-10-124; Turner, B.
B.2.1.24 (IIA 2.14)	Surface tension	Technic al Grade Active Ingredie nt – TSN031 117- 0006; 95.1%	EEC method A 5, OECD Method 115 (Surface tension torsion balance using the OECD harmonised ring method).	The surface tension of a 90% saturated solution of XDE-729 Methyl TGAI was found to be 72.5 mN/m at 20°C . It is noted that the surface tension should have been determined using the pure active substance rather than TGAI; however, since the surface tension result indicates that the active substance is not surface active, this determination is considered fit for purpose. (For information, the notifier has informed the RMS that they intend to determine the surface tension using the pure active substance, the result of which should be available by the end of December 2013).	GLP - Yes	NAFST-10-124; Turner, B.

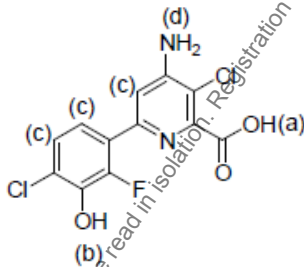
Table B.2.1a Physical properties of the degradation product X11449757 are shown below (this impurity is regarded as ecotoxicologically relevant in soil and water compartments):

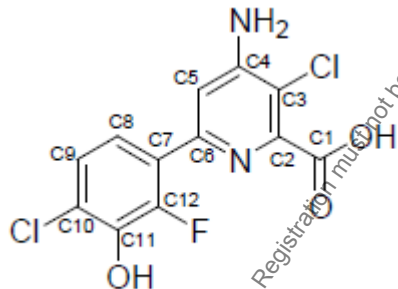
section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference
B.2.1.5a (IIA 2.3)	Vapour pressure	X11449 757; TSN031 413- 0003; 99%	EEC method A 4 (Effusion method: Vapour pressure balance)	8×10^{-5} Pa at 25°C and 5×10^{-5} Pa at 20°C	GLP-Yes Since vp is <0.0001Pa. Very slightly volatile	NAFST-10-322; Comb, A.
B.2.1.10a (IIA 2.5)	Spectra: UV/VIS	X11449 757; TSN031 413- 0003; 99%	OPPTS 830.7050/OECD101	<u>λ max, nm</u> Neutral: 211, 246 Acidic: 217, 259 Basic: 239 Study report states that no absorption maxima were observed above 290 nm, indicating that the test substance has little or no potential to undergo photolytic degradation in the environment. However, at pH 2 $\epsilon > 10 \text{ mol}^{-1} \text{ cm}^{-1}$ (see molar extinction below)	Determined at $25 \pm 0.5^\circ\text{C}$ GLP-Yes	NAFST-11-114; Elliott, T.
B.2.1.10a (IIA 2.5)	Molecular extinction	X11449 757; TSN031 413- 0003; 99%	OPPTS 830.7050/OECD101	<u>$L \text{ M}^{-1} \text{ cm}^{-1}$</u> Neutral: 23,923 at 211nm, 29,318 at 246 nm, 5,535 at 290 nm Acidic: 18,099 at 217nm, 20,016 at 259nm, 13,140 at 290nm Basic: 36,707 at 239 nm, 4,526 at 290 nm (solar cut off limit)	Determined at $25 \pm 0.5^\circ\text{C}$ GLP-Yes At pH 2 $\epsilon > 10 \text{ mol}^{-1} \text{ cm}^{-1}$ Results are in corresponding order of λ max in section IIA 2.5.	NAFST-11-114; Elliott, T.

XDE 729 Methyl (Halauxifen-methyl)

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference																																																												
B.2.1.10a (IIA 2.5)	Spectra: IR	X11449 757; TSN031 413- 0003; 99%	OPPTS 830.7050/OECD101	Infrared spectra of X11449757 show absorption bands consistent with the structure. Absorption Bands of Functional Groups in the IR Spectrum of X11449757: <table><tr><th rowspan="2">Functional Group</th><th colspan="4">Absorption Band Type</th><th rowspan="2">Absorption Bands in Spectrum</th></tr><tr><th>Bond</th><th>Range (cm⁻¹)</th><th>Intensity</th><th>Mode</th></tr><tr><td rowspan="2">Aromatic</td><td>C-H</td><td>3100-3000</td><td>Medium</td><td>Stretch</td><td>3094</td></tr><tr><td>C-C</td><td>1600-1400</td><td>Medium-Weak</td><td>Stretch</td><td>1517</td></tr><tr><td rowspan="2">Amine</td><td>N-H</td><td>3250-3400</td><td>Strong</td><td>Stretch</td><td>3429</td></tr><tr><td>C-N</td><td>1000-1250</td><td>Medium</td><td>Stretch</td><td>1139</td></tr><tr><td rowspan="2">Carboxylic acid</td><td>C=O</td><td>1705-1720</td><td>Strong</td><td>Stretch</td><td>1655</td></tr><tr><td>O-H</td><td>2500-3300</td><td>Broad</td><td>Stretch</td><td>2800-3200</td></tr><tr><td>Phenol</td><td>O-H</td><td>3200-3500</td><td>Strong</td><td>Stretch</td><td>3261</td></tr><tr><td rowspan="2">Aryl Halide</td><td>C-F</td><td>1010-1350</td><td>Strong</td><td>Stretch</td><td>1275</td></tr><tr><td>C-Cl</td><td>780-680</td><td>Strong</td><td>Stretch</td><td>789</td></tr></table>	Functional Group	Absorption Band Type				Absorption Bands in Spectrum	Bond	Range (cm ⁻¹)	Intensity	Mode	Aromatic	C-H	3100-3000	Medium	Stretch	3094	C-C	1600-1400	Medium-Weak	Stretch	1517	Amine	N-H	3250-3400	Strong	Stretch	3429	C-N	1000-1250	Medium	Stretch	1139	Carboxylic acid	C=O	1705-1720	Strong	Stretch	1655	O-H	2500-3300	Broad	Stretch	2800-3200	Phenol	O-H	3200-3500	Strong	Stretch	3261	Aryl Halide	C-F	1010-1350	Strong	Stretch	1275	C-Cl	780-680	Strong	Stretch	789	GLP - Yes	NAFST-11-114; Elliott, T.
Functional Group	Absorption Band Type					Absorption Bands in Spectrum																																																												
	Bond	Range (cm ⁻¹)	Intensity	Mode																																																														
Aromatic	C-H	3100-3000	Medium	Stretch	3094																																																													
	C-C	1600-1400	Medium-Weak	Stretch	1517																																																													
Amine	N-H	3250-3400	Strong	Stretch	3429																																																													
	C-N	1000-1250	Medium	Stretch	1139																																																													
Carboxylic acid	C=O	1705-1720	Strong	Stretch	1655																																																													
	O-H	2500-3300	Broad	Stretch	2800-3200																																																													
Phenol	O-H	3200-3500	Strong	Stretch	3261																																																													
Aryl Halide	C-F	1010-1350	Strong	Stretch	1275																																																													
	C-Cl	780-680	Strong	Stretch	789																																																													

XDE 729 Methyl (Halauxifen-methyl)

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference																		
B.2.1.10a (IIA 2.5)	Spectra: NMR	X11449 757; TSN031 413- 0003; 99%	OPPTS 830.7050/OECD101	The ¹³C NMR and ¹H spectra for X11449757 support the given structure of X11449757. Resonance assignments, as numbered in the figure below, are summarized in the following table:  <table><thead><tr><th>Proton Label</th><th>PPM/Multiplicity</th><th>Integration (protons)</th></tr></thead><tbody><tr><td>(a)</td><td>12-14.5 / broad singlet</td><td>1</td></tr><tr><td>(b)</td><td>10.517 / singlet</td><td>1</td></tr><tr><td>(c)</td><td>2.271-7.329 / multiplet</td><td>2</td></tr><tr><td>(c)</td><td>7.200 / doublet</td><td>1</td></tr><tr><td>(d)</td><td>6.830 / singlet</td><td>2</td></tr></tbody></table> <td> Chemical shifts and integration for the protons conformed to expected results for X11449757. No extraneous resonances were observed. The expanded aromatic region demonstrated that the aromatic protons are present as a single proton at 7.20, and a multiplet at 7.30, the integration of which corresponds to a further two aromatic protons. Due to complicated splitting, it is not possible to further elucidate the splitting pattern. However, the spectra is in line with what would be expected from the molecular structure. The applicant states that the spectrum is too complex for specific assignments of each resonance. However, consideration of the spectrum demonstrates that it is consistent with the molecular structure in terms of the number of carbon peaks (taking account fluorine splitting carbons). </td> <td>NAFST-11-114; Elliott, T.</td>	Proton Label	PPM/Multiplicity	Integration (protons)	(a)	12-14.5 / broad singlet	1	(b)	10.517 / singlet	1	(c)	2.271-7.329 / multiplet	2	(c)	7.200 / doublet	1	(d)	6.830 / singlet	2	Chemical shifts and integration for the protons conformed to expected results for X11449757. No extraneous resonances were observed. The expanded aromatic region demonstrated that the aromatic protons are present as a single proton at 7.20, and a multiplet at 7.30, the integration of which corresponds to a further two aromatic protons. Due to complicated splitting, it is not possible to further elucidate the splitting pattern. However, the spectra is in line with what would be expected from the molecular structure. The applicant states that the spectrum is too complex for specific assignments of each resonance. However, consideration of the spectrum demonstrates that it is consistent with the molecular structure in terms of the number of carbon peaks (taking account fluorine splitting carbons).	NAFST-11-114; Elliott, T.
Proton Label	PPM/Multiplicity	Integration (protons)																						
(a)	12-14.5 / broad singlet	1																						
(b)	10.517 / singlet	1																						
(c)	2.271-7.329 / multiplet	2																						
(c)	7.200 / doublet	1																						
(d)	6.830 / singlet	2																						

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference						
				 <table><tr><th>Carbon Label</th><th>PPM</th></tr><tr><td>C1</td><td>166.614</td></tr><tr><td>C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12</td><td>151.847, 151.118, 150.328, 149.026, 148.670, 141.953, 125.674, 124.806, 122.481, 120.173, 109.969</td></tr></table>	Carbon Label	PPM	C1	166.614	C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12	151.847, 151.118, 150.328, 149.026, 148.670, 141.953, 125.674, 124.806, 122.481, 120.173, 109.969	This is acceptable.	
Carbon Label	PPM											
C1	166.614											
C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12	151.847, 151.118, 150.328, 149.026, 148.670, 141.953, 125.674, 124.806, 122.481, 120.173, 109.969											

section (Annex point)	study	purity	method	results		Comment/GLP (Y/N)	reference													
B.2.1.10a (IIA 2.5)	Spectra: MS	X11449 757; TSN031 413- 0003; 99%	OPPTS 830.7050/OECD101	<table><thead><tr><th>M/Z</th><th>PEAK ASSIGNMENT</th></tr></thead><tbody><tr><td>317, 319, 321 (positive mode)</td><td>C₁₂H₇Cl₂FN₂O₃ [H⁺]</td></tr><tr><td>299, 301, 303 (positive mode)</td><td>C₁₂H₆Cl₂FN₂O₂</td></tr><tr><td>271, 273, 275 (positive mode)</td><td>C₁₁H₆Cl₂FN₂O</td></tr></tbody></table> The Q1 scan also shows a fragment at 236/238 m/z. <table><thead><tr><th>M/Z</th><th>PEAK ASSIGNMENT</th></tr></thead><tbody><tr><td>236, 238 (positive mode)</td><td>C₁₁H₆ClFN₂O</td></tr></tbody></table> All consistent with the expected fragmentation of X11449757		M/Z	PEAK ASSIGNMENT	317, 319, 321 (positive mode)	C ₁₂ H ₇ Cl ₂ FN ₂ O ₃ [H ⁺]	299, 301, 303 (positive mode)	C ₁₂ H ₆ Cl ₂ FN ₂ O ₂	271, 273, 275 (positive mode)	C ₁₁ H ₆ Cl ₂ FN ₂ O	M/Z	PEAK ASSIGNMENT	236, 238 (positive mode)	C ₁₁ H ₆ ClFN ₂ O		NAFST-11-114; Elliott, T.	
M/Z	PEAK ASSIGNMENT																			
317, 319, 321 (positive mode)	C ₁₂ H ₇ Cl ₂ FN ₂ O ₃ [H ⁺]																			
299, 301, 303 (positive mode)	C ₁₂ H ₆ Cl ₂ FN ₂ O ₂																			
271, 273, 275 (positive mode)	C ₁₁ H ₆ Cl ₂ FN ₂ O																			
M/Z	PEAK ASSIGNMENT																			
236, 238 (positive mode)	C ₁₁ H ₆ ClFN ₂ O																			
B.2.1.11a (IIA 2.6)	Solubility in water	X11449 757; TSN031 413- 0003; 99%	EEC method A 6	<table><thead><tr><th>pH</th><th>mg/L</th></tr></thead><tbody><tr><td>Purified</td><td>9.8</td></tr><tr><td>5</td><td>2.12</td></tr><tr><td>7</td><td>265</td></tr><tr><td>9</td><td>> 250 g/L</td></tr></tbody></table>	pH	mg/L	Purified	9.8	5	2.12	7	265	9	> 250 g/L	Determined at 20°C Purified: slightly soluble pH 5: slightly soluble pH 7: moderately soluble pH 9: moderately-readily soluble GLP-Yes	NAFST-10-321; Comb, A.				
pH	mg/L																			
Purified	9.8																			
5	2.12																			
7	265																			
9	> 250 g/L																			
B.2.1.12a (IIA 2.7)	Solubility in organic solvents (technical active substance)	X11449 757; TSN031 413- 0003; 99%	EEC Method A6	<table><thead><tr><th>Solvent</th><th>mg/L</th></tr></thead><tbody><tr><td>Methanol</td><td>120</td></tr><tr><td>Acetone</td><td>7.0</td></tr><tr><td>Xylene</td><td><0.1</td></tr><tr><td>1,2-dichloroethane</td><td><0.1</td></tr><tr><td>Ethyl Acetate</td><td>0.3</td></tr><tr><td>n-heptane</td><td><0.1</td></tr></tbody></table>	Solvent	mg/L	Methanol	120	Acetone	7.0	Xylene	<0.1	1,2-dichloroethane	<0.1	Ethyl Acetate	0.3	n-heptane	<0.1	Determined at 20°C GLP-Yes It is noted in the study report that the recovery results from the test in ethyl acetate were higher and more variable than expected. Therefore the	NAFST-10-324; Comb, A.
Solvent	mg/L																			
Methanol	120																			
Acetone	7.0																			
Xylene	<0.1																			
1,2-dichloroethane	<0.1																			
Ethyl Acetate	0.3																			
n-heptane	<0.1																			

section (Annex point)	study	purity	method	results		Comment/GLP (Y/N)	reference
				n-octanol	2.6	solubility was only reported to the nearest one significant figure. (<0.1 mg/l very slightly soluble 0.1-10 slightly soluble 10-1000 moderately soluble ≥1000 readily soluble)	

WARNING: This document forms part of an EC evaluation data package and should not be read in isolation. Registration must not be granted on the basis of this document.

section (Annex point)	study	purity	method	results		Comment/GLP (Y/N)	reference
B.2.1.13a (IIA 2.8.1/01)	n-octanol/water partition co-efficient	See below	See below	pH to be investigated when pKa <12 (acids) or >2 (alkali), therefore see below for results.		Since the test substance is an ionisable compound, the partition coefficient of X11449757 was determined in buffer solutions at pH 5, 7 and 9. See below for results.	-
B.2.1.13a (IIA 2.8.2/01)	Effect of pH on n- octanol/water partition co-efficient	X11449 757; TSN031 413- 0003; 99%	OECD 117	pH	Log K _{ow}	Determined at 25°C GLP-Yes X11449757 is hydrophilic. The data suggest a low propensity for bioaccumulation.	NAFST-10-320; Comb, A.
				5	<0.3		
				7	<0.3		
				9	<0.3		

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference
B.2.1.18a (IIA 2.9)	Dissociation constant (pKa)	X11449 757; TSN031 413- 0003; 99%	OECD Test Guideline 112	5.6 for the carboxylic acid and 7.1 for the phenolic functional group	GLP – Yes It was noted that there were only two calculated pKa values in the range of environmental pH values. The carboxylic acid group was estimated to have a pKa value of 3.3 and the phenol group had an estimated pKa value of 6.8. Meanwhile, the amine group had a predicted dissociation which was significantly out of the environmental range and this lead to the conclusion that the lone pair on the nitrogen atom was delocalised around the conjugated molecule and would therefore not contribute to ionisation in the environmental pH range. Determination was by spectrophotometric method.	NAFST-10-323; Comb, A.

Table B.2.1b Physical properties of the degradation product X11393729 (XDE-729 acid) are shown below:

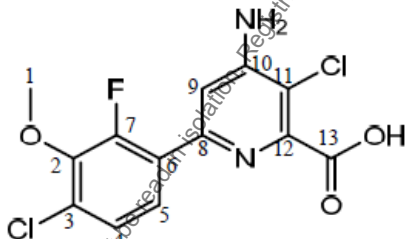
section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference
B.2.1.5b (IIA 2.3)	Vapour pressure	X11393 729; TSN030 751- 0004; 99%	EEC method A 4	3×10^{-5} Pa at 25°C and 2×10^{-5} Pa at 20°C	GLP-Yes Since vp is <0.0001Pa. Very slightly volatile	NAFST-11-18; Comb, A.
B.2.1.10b (IIA 2.5)	Spectra: UV/VIS	X11393 729; TSN030 751- 0004; 99%	OPPTS 830.7050/OECD101	<u>λ max, nm</u> Neutral: 212, 244- 245 Acidic: 210-213; 253 Basic: 212, 244 The molar absorption coefficients at the solar cut-off wavelength at 290 nm were calculated as 15,681, 4,301, and 4,238 L mol⁻¹ cm⁻¹ for XDE-729 at pH <2, pH7, and pH>10, respectively	Determined at 25 ± 0.5°C GLP-Yes Note-in applicants M III summary the range of λ max under neutral conditions is incorrectly stated as 212, 244-253 nm.	NAFST-10-317; Habeeb, S.

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference
B.2.1.10b (IIA 2.5)	Molecular extinction	X11393 729; TSN030 751- 0004; 99%	OPPTS 830.7050/OECD101	$\text{L M}^{-1} \text{ cm}^{-1}$ Neutral: 29,748 to 30,330 at 212nm, 36,098 to 36,617 at 244 to 245 nm, Acidic: 23,960 to 26,089 at 210-213nm, 30,018 to 34,170 at 253nm Basic: 30,540 to 31,567 at 212 nm, 36,953 to 37,647 at 244 nm The molar absorption coefficients at the solar cut-off wavelength at 290 nm were calculated as 15,681, 4,301, and 4,238 L mol⁻¹ cm⁻¹ for XDE-729 at pH <2, pH7, and pH>10, respectively	Determined at 25 ± 0.5°C GLP-Yes Results are in corresponding order of λ max in section IIA 2.5. At pH 2 $\epsilon > 10 \text{ mol}^{-1} \text{ cm}^{-1}$ Note-in applicants M III summary the extinction coefficient under basic conditions at 244 nm is incorrectly stated as 36,953 to 97,647.	NAFST-10-317; Habeeb, S.

XDE 729 Methyl (Halauxifen-methyl)

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference																																																																																										
B.2.1.10b (IIA 2.5)	Spectra: IR	X11393 729; TSN030 751- 0004; 99%	OPPTS 830.7050/OECD101	Infrared spectra of X11393729 show absorption bands consistent with the structure. Absorption Bands of Functional Groups in the IR Spectrum of X11393729: <table><thead><tr><th>Functional Group</th><th>Bond</th><th>Range (cm⁻¹)</th><th>Intensity</th><th>Mode</th><th>Absorption Bands in Spectrum</th></tr></thead><tbody><tr><td>Amine (1°)</td><td>N-H</td><td>3400-3250</td><td>Medium</td><td>Stretch</td><td>3444.9, 3333.1</td></tr><tr><td>Aromatic</td><td>C-H</td><td>3100-3000</td><td>Strong</td><td>Stretch</td><td>3193.4</td></tr><tr><td>Carboxylic Acid</td><td>O-H</td><td>3300-2500</td><td>Medium</td><td>Stretch</td><td>3030.7</td></tr><tr><td>Alkane</td><td>C-H</td><td>3000-2850</td><td>Medium</td><td>Stretch</td><td>2947.4</td></tr><tr><td>Carbonyl (Ester)</td><td>C=O</td><td>1760-1680</td><td>Strong</td><td>Stretch</td><td>1761.3</td></tr><tr><td>Pyridine</td><td>C=N</td><td>1600-1560</td><td>Strong</td><td>Stretch</td><td>1646.5</td></tr><tr><td>Aromatic</td><td>C-C</td><td>1600-1585</td><td>Medium</td><td>Stretch</td><td>1562.4</td></tr><tr><td>Alkane</td><td>C-H</td><td>1470-1450</td><td>Medium</td><td>Bend</td><td>1475.0</td></tr><tr><td>Carboxylic Acid</td><td>O-H</td><td>1440-1395</td><td>Medium</td><td>Bend</td><td>1421.7</td></tr><tr><td>Carboxylic Acid</td><td>C=O</td><td>1320-1000</td><td>Strong</td><td>Stretch</td><td>1240.6</td></tr><tr><td>Aromatic Amine</td><td>C-N</td><td>1335-1250</td><td>Strong</td><td>Stretch</td><td>1322.0</td></tr><tr><td>Aromatics</td><td>C-H</td><td>1290-1000</td><td>Weak</td><td>Asymmetric</td><td>1214.9</td></tr><tr><td>Aryl Halide</td><td>C-Cl</td><td>1100-900</td><td>Medium</td><td>Bend</td><td>1059.2</td></tr><tr><td>Carboxylic Acid</td><td>O-H</td><td>950-910</td><td>Medium</td><td>Bend</td><td>924.3</td></tr></tbody></table>	Functional Group	Bond	Range (cm ⁻¹)	Intensity	Mode	Absorption Bands in Spectrum	Amine (1°)	N-H	3400-3250	Medium	Stretch	3444.9, 3333.1	Aromatic	C-H	3100-3000	Strong	Stretch	3193.4	Carboxylic Acid	O-H	3300-2500	Medium	Stretch	3030.7	Alkane	C-H	3000-2850	Medium	Stretch	2947.4	Carbonyl (Ester)	C=O	1760-1680	Strong	Stretch	1761.3	Pyridine	C=N	1600-1560	Strong	Stretch	1646.5	Aromatic	C-C	1600-1585	Medium	Stretch	1562.4	Alkane	C-H	1470-1450	Medium	Bend	1475.0	Carboxylic Acid	O-H	1440-1395	Medium	Bend	1421.7	Carboxylic Acid	C=O	1320-1000	Strong	Stretch	1240.6	Aromatic Amine	C-N	1335-1250	Strong	Stretch	1322.0	Aromatics	C-H	1290-1000	Weak	Asymmetric	1214.9	Aryl Halide	C-Cl	1100-900	Medium	Bend	1059.2	Carboxylic Acid	O-H	950-910	Medium	Bend	924.3	GLP - Yes	NAFST-10-317; Habeeb, S.
Functional Group	Bond	Range (cm ⁻¹)	Intensity	Mode	Absorption Bands in Spectrum																																																																																											
Amine (1°)	N-H	3400-3250	Medium	Stretch	3444.9, 3333.1																																																																																											
Aromatic	C-H	3100-3000	Strong	Stretch	3193.4																																																																																											
Carboxylic Acid	O-H	3300-2500	Medium	Stretch	3030.7																																																																																											
Alkane	C-H	3000-2850	Medium	Stretch	2947.4																																																																																											
Carbonyl (Ester)	C=O	1760-1680	Strong	Stretch	1761.3																																																																																											
Pyridine	C=N	1600-1560	Strong	Stretch	1646.5																																																																																											
Aromatic	C-C	1600-1585	Medium	Stretch	1562.4																																																																																											
Alkane	C-H	1470-1450	Medium	Bend	1475.0																																																																																											
Carboxylic Acid	O-H	1440-1395	Medium	Bend	1421.7																																																																																											
Carboxylic Acid	C=O	1320-1000	Strong	Stretch	1240.6																																																																																											
Aromatic Amine	C-N	1335-1250	Strong	Stretch	1322.0																																																																																											
Aromatics	C-H	1290-1000	Weak	Asymmetric	1214.9																																																																																											
Aryl Halide	C-Cl	1100-900	Medium	Bend	1059.2																																																																																											
Carboxylic Acid	O-H	950-910	Medium	Bend	924.3																																																																																											

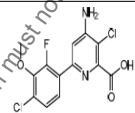
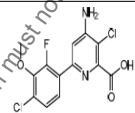
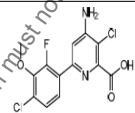
XDE 729 Methyl (Halauxifen-methyl)

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference																		
B.2.1.10b (IIA 2.5)	Spectra: NMR	X11393 729; TSN030 751- 0004; 99%	OPPTS 830.7050/OECD101	The ¹³C NMR and ¹H spectra for X11393729 support the given structure of X11393729. Resonance assignments, as numbered in the figure below, are summarized in the following table:  <table><thead><tr><th>Proton Label</th><th>PPM/Multiplicity</th><th>Integration</th></tr></thead><tbody><tr><td>H1</td><td>3.9 / doublet</td><td>299.2</td></tr><tr><td>H9</td><td>7.2 / doublet</td><td>100.98</td></tr><tr><td>H4, H5</td><td>7.4 / doublet, 7.6 / doublet</td><td>100.45, 100.0</td></tr><tr><td>NH₂ Protons</td><td>6.8 / singlet</td><td>196.1</td></tr><tr><td>OH Proton</td><td>13.6 / singlet</td><td>86.68</td></tr></tbody></table> <td> Chemical shifts and integration for the protons conformed to expected results for XDE-729 (acid). No extraneous resonances were observed. An expansion of the aliphatic region and aromatic region of the NMR spectra demonstrates that splitting patterns are complicated, possibly by the presence of fluorine; however, the spectra confirm the expected structure. Chemical shifts for the 13 carbons conformed to the expected results based on the structure of XDE-729(acid). Other recognized resonances were residual deuterated DMSO. No other extraneous resonances were </td> <td>NAFST-10-317; Habeeb, S.</td>	Proton Label	PPM/Multiplicity	Integration	H1	3.9 / doublet	299.2	H9	7.2 / doublet	100.98	H4, H5	7.4 / doublet, 7.6 / doublet	100.45, 100.0	NH ₂ Protons	6.8 / singlet	196.1	OH Proton	13.6 / singlet	86.68	Chemical shifts and integration for the protons conformed to expected results for XDE-729 (acid). No extraneous resonances were observed. An expansion of the aliphatic region and aromatic region of the NMR spectra demonstrates that splitting patterns are complicated, possibly by the presence of fluorine; however, the spectra confirm the expected structure. Chemical shifts for the 13 carbons conformed to the expected results based on the structure of XDE-729(acid). Other recognized resonances were residual deuterated DMSO. No other extraneous resonances were	NAFST-10-317; Habeeb, S.
Proton Label	PPM/Multiplicity	Integration																						
H1	3.9 / doublet	299.2																						
H9	7.2 / doublet	100.98																						
H4, H5	7.4 / doublet, 7.6 / doublet	100.45, 100.0																						
NH ₂ Protons	6.8 / singlet	196.1																						
OH Proton	13.6 / singlet	86.68																						

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference																												
				<table><tr><th>Carbon Label</th><th>PPM</th></tr><tr><td>C1</td><td>61.551</td></tr><tr><td>C2</td><td>144.252, 144.112</td></tr><tr><td>C3</td><td>148.497</td></tr><tr><td>C4</td><td>125.254</td></tr><tr><td>C5</td><td>125.254</td></tr><tr><td>C6</td><td>110.238</td></tr><tr><td>C7</td><td>152.433, 154.944</td></tr><tr><td>C8</td><td>126.679, 126.772</td></tr><tr><td>C9</td><td>151.829</td></tr><tr><td>C10</td><td>110.238, 110.130</td></tr><tr><td>C11</td><td>150.434</td></tr><tr><td>C12</td><td>127.795</td></tr><tr><td>C13</td><td>166.596</td></tr></table>	Carbon Label	PPM	C1	61.551	C2	144.252, 144.112	C3	148.497	C4	125.254	C5	125.254	C6	110.238	C7	152.433, 154.944	C8	126.679, 126.772	C9	151.829	C10	110.238, 110.130	C11	150.434	C12	127.795	C13	166.596	observed. GLP - Yes.	
Carbon Label	PPM																																	
C1	61.551																																	
C2	144.252, 144.112																																	
C3	148.497																																	
C4	125.254																																	
C5	125.254																																	
C6	110.238																																	
C7	152.433, 154.944																																	
C8	126.679, 126.772																																	
C9	151.829																																	
C10	110.238, 110.130																																	
C11	150.434																																	
C12	127.795																																	
C13	166.596																																	

WARNING: This document forms part of an EC evaluation data package and should not be read in isolation. Pre-approval must be granted on the basis of this document.

XDE 729 Methyl (Halauxifen-methyl)

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference						
B.2.1.10b (IIA 2.5)	Spectra: MS	X11393 729; TSN030 751- 0004; 99%	OPPTS 830.7050/OECD101	The mass spectrum supports the given structure of XDE-729 (acid). <table><tr><th>m/z</th><th>PEAK ASSIGNMENT</th><th>STRUCTURE</th></tr><tr><td>331, 333, 335 (positive mode) 329, 331, 333 (negative mode)</td><td>C₁₇H₉Cl₂FN₂O₃</td><td></td></tr></table> The Q1 scan also shows peaks at 313/315/317 m/z, 285/287/289 m/z, 250/252 m/z, 235/237 m/z in the positive mode and 285/287/289 m/z and 270/272/274 m/z in the negative modes were due to isotopic distribution of the molecule.	m/z	PEAK ASSIGNMENT	STRUCTURE	331, 333, 335 (positive mode) 329, 331, 333 (negative mode)	C ₁₇ H ₉ Cl ₂ FN ₂ O ₃		GLP – Yes.	NAFST-10-317; Habeeb, S.
m/z	PEAK ASSIGNMENT	STRUCTURE										
331, 333, 335 (positive mode) 329, 331, 333 (negative mode)	C ₁₇ H ₉ Cl ₂ FN ₂ O ₃											

XDE 729 Methyl (Halauxifen-methyl)

section (Annex point)	study	purity	method	results	Comment/GLP (Y/N)	reference																					
				<table><tr><th>M/Z</th><th>PEAK ASSIGNMENT</th><th>STRUCTURE</th></tr><tr><td>313/315/317 (Positive Mode)</td><td>C₁₃H₉Cl₂FN₂O₂⁺</td><td></td></tr><tr><td>285/287/289 (Positive Mode)</td><td>C₁₂H₈Cl₂FN₂O⁺</td><td></td></tr><tr><td>250/252 (Positive Mode)</td><td>C₁₂H₈ClFN₂O⁺</td><td> or or </td></tr><tr><td>235/237 (Positive Mode)</td><td>C₁₂H₇ClFNO⁺</td><td> or </td></tr><tr><td>285/287/289 (Negative Mode)</td><td>C₁₂H₈Cl₂FN₂O⁻</td><td> or </td></tr><tr><td>270/272/274 (Negative Mode)</td><td>C₁₂H₇Cl₂FNO⁻</td><td> or </td></tr></table> The fragmentation pattern is consistent with the structure of XDE-729 (acid).	M/Z	PEAK ASSIGNMENT	STRUCTURE	313/315/317 (Positive Mode)	C ₁₃ H ₉ Cl ₂ FN ₂ O ₂ ⁺		285/287/289 (Positive Mode)	C ₁₂ H ₈ Cl ₂ FN ₂ O ⁺		250/252 (Positive Mode)	C ₁₂ H ₈ ClFN ₂ O ⁺	 or or 	235/237 (Positive Mode)	C ₁₂ H ₇ ClFNO ⁺	 or 	285/287/289 (Negative Mode)	C ₁₂ H ₈ Cl ₂ FN ₂ O ⁻	 or 	270/272/274 (Negative Mode)	C ₁₂ H ₇ Cl ₂ FNO ⁻	 or 		
M/Z	PEAK ASSIGNMENT	STRUCTURE																									
313/315/317 (Positive Mode)	C ₁₃ H ₉ Cl ₂ FN ₂ O ₂ ⁺																										
285/287/289 (Positive Mode)	C ₁₂ H ₈ Cl ₂ FN ₂ O ⁺																										
250/252 (Positive Mode)	C ₁₂ H ₈ ClFN ₂ O ⁺	 or or 																									
235/237 (Positive Mode)	C ₁₂ H ₇ ClFNO ⁺	 or 																									
285/287/289 (Negative Mode)	C ₁₂ H ₈ Cl ₂ FN ₂ O ⁻	 or 																									
270/272/274 (Negative Mode)	C ₁₂ H ₇ Cl ₂ FNO ⁻	 or 																									

section (Annex point)	study	purity	method	results		Comment/GLP (Y/N)	reference
B.2.1.11b (IIA 2.6)	Solubility in water	X11393 729; TSN030 751- 0004; 99%	EEC method A 6	pH	mg/L	Determined at 20°C Purified: moderately soluble pH 5: moderately soluble pH 7: readily soluble pH 9: readily soluble GLP-Yes	NAFST-11-17; Comb, A.
				Purified	84.0		
				5	102		
				7	3.07 g/L		
				9	46.1 g/L		
B.2.1.12b (IIA 2.7)	Solubility in organic solvents (technical active substance)	X11393 729; TSN030 751- 0004; 99%	EEC Method A6	Solvent	Solubility	Determined at 20°C GLP-Yes <u>Classification of solubility</u> (<0.1 mg/l very slightly soluble 0.1-10 slightly soluble 10-1000 moderately soluble ≥1000 readily soluble)	NAFST-11-19; Comb, A.
				Methanol	4.2 g/L		
				Acetone	4.4 g/L		
				Xylene	8.5 mg/L		
				1,2-dichloroethane	130 mg/L		
				Ethyl Acetate	1.2 g/L		
				n-heptane	<0.2 mg/L		
				n-octanol	430 mg/L		

section (Annex point)	study	purity	method	results		Comment/GLP (Y/N)	reference
B.2.1.13b (IIA 2.8.1/01)	n-octanol/water partition co-efficient	See below	See below	pH to be investigated when pKa <12 (acids) or >2 (alkali), therefore see below for results.		Since the test substance is an ionisable compound, the partition coefficient of X11449757 was determined in buffer solutions at pH 5, 7 and 9. See below for results.	-
B.2.1.13b (IIA 2.8.2/01)	Effect of pH on n- octanol/water partition co-efficient	X11393 729; TSN030 751- 0004; 99%	EEC Method A8	pH	Log K _{ow}	Determined at 20°C GLP-Yes XDE-729 (acid) is slightly hydrophobic at low pH and hydrophilic at neutral or alkaline pH. The data suggest a low propensity for bioaccumulation.	NAFST-11-16; Comb, A.
				5	0.42		
				7	-0.83		
				9	-1.01		
B.2.1.18b (IIA 2.9)	Dissociation constant (pKa)	X11393 729; TSN030 751- 0004; 99%	OECD Test Guideline 112	5.11 ± 0.01 at 21.9°C		GLP – Yes Determination was by spectrophotometric method.	10-039-G; Cathie, C.

Table B.2.1c Physical property of the degradation product X11406790 is shown below:

section (Annex point)	study	purity	method	results			Comment/GLP (Y/N)	reference
B.2.1.5c (IIA 2.3)	Effect of pH on n-octanol/water partition co-efficient	X11406790; TSN302182; 95%	EEC method A8	pH	Log Kow		GLP-Yes	NAFST-12-45; Comb, A.
				5	0.96			
				7	< 0.3			
				9	< 0.3			

WARNING: This document forms part of an EC evaluation data package and should not be read in isolation. Registration must not be granted on the basis of this document.

B.2.2 Physical, chemical and technical properties of the plant protection product

Product name: 'GF-2573' (an Emulsion Concentrate (EC) containing 7.817 g active substance XDE-729 methyl/L)

Table B.2.2 Summary of the physical and chemical properties of the plant protection product

section (Annex point)	study	method	results	comment	reference
B.2.2.1 (IIIA 2.1)	Appearance: physical state	Visual inspection	Liquid (25.5°C)	GLP-Yes	NAFST-11- 26; Rozniak, M
B.2.2.2 (IIIA 2.1)	Appearance: colour	Visual inspection	Yellow	GLP-Yes	NAFST-11- 26; Rozniak, M
B.2.2.3 (IIIA 2.1)	Appearance: odour	Olfactory Inspection	Solvent Odour	GLP-Yes	NAFST-11- 26; Rozniak, M
B.2.2.4 (IIIA 2.2)	Explosive properties	EEC method A 14	Not explosive according to EEC method A14	GLP-Yes	NAFST-11- 36; Turner, B.

section (Annex point)	study	method	results	comment	reference
B.2.2.5 (IIIA 2.2)	Oxidising properties	EEC A21	Non-oxidising according to EEC method A21 The mean pressure rise time for the reference mixture (1:1 w/w mixture of 65% w/w aqueous nitric acid and cellulose) was 7.0 seconds. Pressure rise times were not obtained for the test substance mixtures (1:1 w/w mixture of the test substance and cellulose) since the pressure failed to reach the upper limit value of the range under test. Since the test substance mixture failed to reach 2070 kPa within the 60 seconds allowed for the test, the test substance was considered to be a non-oxidiser.	GLP-Yes	NAFST-11-36; Turner, B.
B.2.2.6 (IIIA 2.3)	Flammability	EEC method A 10, A 11 or A 12	Not relevant	-	-
B.2.2.7 (IIIA 2.3)	Auto-flammability	EEC method A 15	Auto-ignition temperature = 234°C.	GLP-Yes	NAFST-11-36; Turner, B.

section (Annex point)	study	method	results	comment	reference
B.2.2.8 (IIIA 2.3)	Flash point	EEC A9	>100°C	GLP-Yes	FAPC-G-12-1; Frank, A.
B.2.2.9 (IIIA 2.4)	Acidity/alkalinity	Not Relevant	Not relevant for an EC formulation.		-
B.2.2.10 (IIIA 2.4)	pH	ASTM E 70-77	5.271 at 21.0°C (1% solution)	GLP-Yes	NAFST-11-26; Rozniak, M.
B.2.2.11 (IIIA 2.5)	Surface tension	EEC method A 5	0.27% v/v dilution at 20°C: 33.0 mN/m 1.25% v/v dilution at 20°C: 29.5 mN/m	GLP-Yes A written statement was provided stating that the hydrocarbon content does not exceed 10%. This statement is confirmed by reference to the formulation details in document J. The product does NOT require further consideration as an aspiration hazard.	NAFST-11-36; Turner, B.
B.2.2.12 (IIIA 2.5)	Viscosity	OECD Test Guideline 114	Newtonian; 6.87 mPa·s at 19.9°C and 4.22 mPa·s at 40.0°C	GLP-Yes 4.22 mPa·s is equivalent to $4.663 \times 10^{-6} \text{ m}^2/\text{s}$.	NAFST-11-26; Rozniak, M.
B.2.2.13 (IIIA 2.6)	Relative density	EEC Method A 3	0.905	GLP-Yes	NAFST-11-26; Rozniak, M.
B.2.2.14 (IIIA 2.6)	Bulk (tap) density	Not Relevant	Not required for EC formulations	-	-
B.2.2.14	Storage stability	CIPAC	<u>Storage at 54°C for 18 days in</u>		FOR-10-37

section (Annex point)	study	method	results	comment	reference
(IIIA 2.7)		Method MT 46	<u>glass container.</u> <u>Active ingredient content</u> Before storage: 0.842 Wt% (wt/wt) Following storage: 0.834 Wt% (wt/wt) i.e 99.0% retained. <u>Cloquintocet-mexyl</u> Before storage: 0.795 Wt% (wt/wt) Following storage: 0.795 Wt% (wt/wt) i.e 100.0% retained. <u>Appearance</u> Study report states that throughout the study the test substance was observed to be a yellow clear homogeneous liquid.	Stability of active substance and safener acceptable over accelerated storage.	
		CIPAC MT 75.3	<u>pH (1% dilution)</u> Before storage: 5.30 Following storage: 5.37	pH stable over accelerated storage.	
		CIPAC MT 47.2	<u>Persistent Foam</u> At 1.4 %v/v concentration Before storage: 41 mL after 1 min Following Storage: 43 mL after 1 min.	No significant changes in persistent foam over storage. All foam measurements within acceptable limits (≤ 60 mL after 1 min). Levels of foam at 1.4% v/v are acceptable. Since the maximum recommended in use concentration is 1% v/v, this	
		CIPAC MT			

section (Annex point)	study	method	results	comment	reference
		36.3	<u>Emulsion Characteristics</u> The minimum and maximum concentrations were tested at 0.04% v/v and 1.5 %v/v respectively; this encompasses the proposed use rate. No significant changes in emulsion stability were observed during storage. For each time point, the emulsion stability was within acceptable limits (< 2 mL cream after 30 minutes, trace oil). All samples remained emulsified throughout the entire test. <u>Cold Storage (7 days at 0° C in glass container)</u> <u>pH (1% dilution)</u> Before storage: 5.30 Following storage: 5.53 <u>Emulsion Characteristics</u> The minimum and maximum concentrations were tested at 0.04% v/v and 1.5 %v/v respectively; this encompasses the proposed use rate.	result confirms levels of foam at the proposed use rate are expected to be acceptable. Acceptable emulsion characteristics before and after storage. Acceptable retention of properties during accelerated storage. Properties within acceptable limits. Acceptable retention of properties during low temperature storage. Properties within acceptable limits.	FOR-10-38

section (Annex point)	study	method	results	comment	reference
			No significant changes in emulsion stability were observed during storage. For each time point, the emulsion stability was within acceptable limits (< 2 mL cream after 30 minutes, trace oil). All samples remained emulsified throughout the entire test. <u>Storage at 40°C for 8 weeks in PET and F-HDPE.</u> <u>Active ingredient content</u> <u>PET container</u> Before storage: 0.842 Wt% (wt/wt) Following storage: 0.847 Wt% (wt/wt) i.e 100.6% retained. <u>Active ingredient content</u> <u>F-HDPE container</u> Before storage: 0.842 Wt% (wt/wt) Following storage: 0.839 Wt% (wt/wt) i.e 99.6% retained. <u>Cloquintocet-mexyl</u> <u>PET container</u> Before storage: 0.795 Wt% (wt/wt) Following storage: 0.799 Wt% (wt/wt) i.e 100.5% retained.	Stability of active substance and safener acceptable over storage.	

section (Annex point)	study	method	results	comment	reference
			<u>Cloquintocet-mexyl</u> <u>F-HDPE container</u> Before storage: 0.795 Wt% (wt/wt) Following storage: 0.795 Wt% (wt/wt) i.e 100.0% retained. <u>Appearance</u> Study report states that throughout the entire study the test substance was observed to be a clear yellow to light yellow liquid. <u>Packaging observations</u> Both bottle types remained in good condition throughout the entire study and showed no evidence of corrosion or other effects that would interfere with the safe handling of the product. Each filled test container was weighed at the eight week sampling point. Results of the weighing showed no significant weight change from the initial weights for both bottle types. <u>pH (1% dilution)</u>	pH stable over storage. No significant changes in persistent foam over storage. All foam measurements within acceptable limits (≤ 60 mL after 1 min). Levels	
		CIPAC MT 75.3			
		CIPAC MT 47.2			

section (Annex point)	study	method	results	comment	reference
		CIPAC MT 36.3	Before storage: 5.30 Following storage (PET): 5.13 Following storage (F-HDPE): 5.22 <u>Persistent Foam</u> At 1.5 %v/v concentration Before storage: 41 mL after 1 min Following Storage (PET): 40 mL after 1 min. Following Storage (F-HDPE): 42 mL after 1 min. <u>Emulsion Characteristics</u> The minimum and maximum concentrations were tested at 0.04% v/v and 1.5 %v/v respectively; this encompasses the proposed use rate. No significant changes in emulsion stability were observed during storage. For each time point, the emulsion stability was within acceptable limits (< 2 mL cream after 30 minutes, trace oil). All samples remained emulsified throughout the entire test.	of foam at 1.5% v/v encompasses the proposed use rate, therefore levels of foam are expected to be acceptable according to the maximum use rate given on the proposed label/according to the GAP. Acceptable emulsion characteristics before and after storage. Acceptable retention of properties during accelerated storage for 8 weeks at 40°C. Properties within acceptable limits.	

section (Annex point)	study	method	results	comment	reference
B.2.2.15 (IIIA 2.7)	Shelf life	CIPAC MT46 In-house HPLC method according to Study ID: DAS-AM-G- 10-34	<u>12 months at ambient temperature.</u> <u>XDE-729 methyl content</u> <u>PET container</u> Before storage: 0.842 Wt% (wt/wt) Following storage: 0.838 Wt% (wt/wt) i.e 99.5% retained. <u>XDE-729 methyl content</u> <u>F-HDPE container</u> Before storage: 0.842 Wt% (wt/wt) Following storage: 0.831 Wt% (wt/wt) i.e 98.7% retained. <u>Cloquintocet-mexyl content</u> <u>PET container</u> Before storage: 0.795 Wt% (wt/wt) Following storage: 0.798 Wt% (wt/wt) i.e 100.4% retained. <u>Cloquintocet-mexyl content</u> <u>F-HDPE container</u> Before storage: 0.795 Wt% (wt/wt)	Interim report that is part of an on-going 2 years storage study	FOR-10-40.01; Stock, M.

section (Annex point)	study	method	results	comment	reference
			Following storage: 0.803 Wt% (wt/wt) i.e 101.0% retained. <u>pH (1% w/v dilution)</u> Before storage: 5.74 Following storage (PET): 5.20 (-0.54) Following storage (F-HDPE): 5.62 (-0.12) <u>Persistent Foam</u> At 1.5 %v/v concentration. Before storage: 41 mL after 1 min Following Storage (PET): 33 mL after 1 min. Following Storage (F-HDPE): 31 mL after 1 min. <u>Emulsion Characteristics</u> The minimum and maximum concentrations were tested at 0.04% v/v and 1.5 %v/v respectively; this encompasses the proposed use rate. No changes in emulsion stability were observed during storage. For each time point, the emulsion	No significant changes in persistent foam over storage. All foam measurements within acceptable limits (≤ 60 mL after 1 min). As above, 1.5% v/v encompasses the proposed maximum use rate. Acceptable emulsion characteristics before and after storage.	

section (Annex point)	study	method	results	comment	reference
		Visual	stability was 0ml and therefore within acceptable limits (< 2 mL cream after 30 minutes, trace oil). All samples remained emulsified throughout the entire test. <u>Appearance</u> Study report states that throughout the entire study the test substance was observed to be a clear yellow to light yellow liquid. <u>Packaging observations</u> Both bottle types remained in good condition throughout the entire study and showed no evidence of corrosion or other effects that would interfere with the safe handling of the product. Each filled test container was weighed and observed to determine if the package condition changed from the time of study initiation.. Results of the weighing showed no significant weight	Acceptable retention of properties during 12 months storage at ambient temperature. Properties within acceptable limits.	

section (Annex point)	study	method	results	comment	reference
			change from the initial weights for both bottle types. Both bottle types remained in good condition throughout the entire study and showed no evidence of corrosion or other effects that would interfere with the safe handling of the product.		

WARNING: This document forms part of an EC evaluation data package and should not be read in isolation. Registration must not be granted on the basis of this document.

B.2.2.16 (IIIA 2.8)	Wettability	Not Relevant	Not required for EC formulations	-	-
B.2.2.17 (IIIA 2.8)	Persistent foaming	CIPAC Method MT 47	All foam measurements were within acceptable limits (≤ 60 mL foam) in Standard water D.	No significant changes in persistent foam over storage. All foam measurements within acceptable limits (≤ 60 mL after 1 min). Levels of foam at 1.4% v/v are acceptable. Since the maximum recommended in use concentration is 1% v/v, this result confirms levels of foam at the proposed use rate are expected to be acceptable. GLP - No	FOR-10-37; Stock, M.
B.2.2.18 (IIIA 2.8)	Suspensibility	CIPAC Method MT 15, MT 161 or MT 168	Not required for EC formulations		
B.2.2.19 (IIIA 2.8)	Suspension stability	CIPAC Method MT 160 or MT 174	Not required for EC formulations		
B.2.2.20 (IIIA 2.8)	Dilution stability	CIPAC Method MT 41	Not required for EC formulations		
B.2.2.21 (IIIA 2.8)	Dry sieve test	CIPAC Method MT 59.1	Not required for EC formulations		

B.2.2.22 (IIIA 2.8)	Wet sieve test	CIPAC Method MT 59.3 or MT 167	Not required for EC formulations		
B.2.2.23 (IIIA 2.8)	Particle size distribution	OECD Method 110 CIPAC MT 58.3 or MT 170	Not required for EC formulations		
B.2.2.24 (IIIA 2.8)	Content of dust/fines	CIPAC Method MT 171 or OECD Method 110	Not required for EC formulations		
B.2.2.25 (IIIA 2.8)	Attrition and friability	CIPAC Method MT 178 Or CIPAC Method MT 178.2	Not required for EC formulations		

B.2.2.26 (IIIA 2.8)	Emulsifiability, re-emulsifiability and emulsion stability	CIPAC Methods MT 36.3	Emulsion stability was within acceptable limits (< 2 mL cream after 30 minutes, trace oil) for all time points (initial, following 30 minutes, 2 hours, 24 hours. Re-emulsification (30 secs after inversion) and final emulsion stability (30 minutes) were also acceptable). All samples remained emulsified throughout the entire test. The test was carried out using Standard water A and D. The low and high use rates tested were 0.04% and 1.5% respectively, this range encompasses the proposed use rate.	GLP - Yes Acceptable emulsion characteristics	FOR-10-37; Stock, M.
B.2.2.27 (IIIA 2.8)	Stability of dilute emulsion	CIPAC Methods MT 20 or MT 173	Addressed above.		
B.2.2.28 (IIIA 2.8)	Flowability	CIPAC Method MT 172	Not required for EC formulations		
B.2.2.29 (IIIA 2.8)	Pourability (rinsibility)	CIPAC Method MT 148	Not required for EC formulations		
B.2.2.30 (IIIA 2.8)	Dustability	CIPAC Method MT 34	Not required for EC formulations		
B.2.2.31 (IIIA 2.8)	Adherence and distribution to seeds	CIPAC Method MT 175	Not required for EC formulations		

compatibility			No information on physical and chemical compatibility has been submitted; this is acceptable however, since the dossier does not make any positive recommendations for tank mixing.		
---------------	--	--	---	--	--

WARNING: This document forms part of an EC evaluation data package and should not be read in isolation. Registration must not be granted on the basis of this document.

B.2.2.32 Summary of physical and chemical compatibility with other products (IIIA 2.9)**B.2.3 Summary of physical and chemical properties****B.2.3.1 Active substance**

XDE-729 is a white solid with a mild odour. It has a relative density D_4^{20} of 1.5057. The melting point is 145.5°C, with decomposition before boiling. The temperature of decomposition or sublimation is 221.06°C. ^1H NMR, ^{13}C NMR, TSI+/TSI- MS and IR spectra support the structure of XDE-729. XDE-729 is not explosive, flammable, auto-flammable or oxidising. XDE-729 is very slightly volatile with a vapour pressure of 1.5×10^{-8} Pa at 25°C. Aqueous solubility is not pH dependent with XDE-729 being slightly soluble at pH 5 (1.66 mg/L), pH 7 (1.67 mg/L) and at pH 9 (1.69 mg/L). XDE-729 is very slightly volatile in solution at pH 5, pH 7 and pH 9 (Henry's law constant at 25°C is $1.23 \times 10^{-6} \text{ Pa}\cdot\text{m}^3\cdot\text{mol}^{-1}$, $1.22 \times 10^{-6} \text{ Pa}\cdot\text{m}^3\cdot\text{mol}^{-1}$, $1.20 \times 10^{-6} \text{ Pa}\cdot\text{m}^3\cdot\text{mol}^{-1}$). The pKa is 2.84 ± 0.04 at 20°C. Thus volatilisation is not expected to contribute significantly to the dissipation of XDE-729 in the environment. The hydrolysis half-life of XDE-729 is 81 days in solution at pH 4 at 25°C, 155 days at pH 7 (25°C) and 3 days at pH 9 (25°C). Therefore XDE-729 is classified as slightly hydrolysing at pH 4 and 7 and readily hydrolysing at pH 9. There is significant absorbance >290 nm in the UV-Vis spectrum for XDE-729 when in solution at pH < 2, therefore at low pH XDE-729 is photolytically labile. At pH 7 and pH > 10, there is no significant absorbance >290 nm in the UV-vis spectrum, therefore at higher pH XDE-729 is photolytically stable. The estimated atmospheric half-life for XDE-729 is estimated to be 25.87 hours. XDE-729 is very slightly soluble in n-heptane (0.0361 mg/L), slightly soluble in n-octanol and xylene (9.83 mg/L, 9.13 mg/L) and moderately soluble in ethyl acetate, 1,2-dichloromethaneacetone, acetone and methanol (129 mg/L, 65.9 mg/L, >250 mg/L and 38.1 mg/L). The n-octanol/water partition coefficient is not pH dependent ($\text{Log}_{10}\text{P}_{\text{OW}} = 3.75$ at pH 5, $\text{Log}_{10}\text{P}_{\text{OW}} = 3.76$ at pH 7 and $\text{Log}_{10}\text{P}_{\text{OW}} = 3.92$ at pH 9). The data suggest a potential to be fat soluble. The surface tension of a 90% aqueous solution of XDE-729 at 20°C is 72.5 mN.m⁻¹.

Degradation Product X11449757

^1H NMR, ^{13}C NMR, MS and IR spectra support the structure of X11449757. X11449757 is very slightly volatile with a vapour pressure of 8.0×10^{-5} Pa at 25°C. Aqueous solubility is pH dependent with X11449757 being slightly soluble at pH 5 (2.12 mg/L), moderately soluble at pH 7 (265 mg/L) and moderately-readily soluble at pH 9 (> 250 g/L). The pKa is 5.6 for the carboxylic acid and 7.1 for the phenolic functional group. There is significant absorbance >290 nm in the UV-Vis spectrum for X11449757 when in solution at pH < 2, therefore at low pH X11449757 is photolytically labile. At pH 7 and pH > 10, there is no significant absorbance >290 nm in the UV-vis spectrum, therefore at higher pH X11449757 is photolytically stable. X11449757 is very slightly soluble in n-heptane, 1,2-dichloroethane and xylene (<0.1 mg/L), slightly soluble in ethyl acetate, acetone and n-octanol (0.3 mg/L, 7.0 mg/L, 2.6 mg/L) and moderately soluble in methanol (120 mg/L). The n-octanol/water partition coefficient is not pH dependent ($\text{Log}_{10}\text{P}_{\text{OW}} < 0.3$ at pH 5, pH 7 and pH 9). The data suggest a low propensity for bioaccumulation.

Degradation Product X11393729 (XDE-729 acid)

¹H NMR, ¹³C NMR, MS and IR spectra support the structure of X11393729 (XDE-729 acid). X11393729 (XDE-729 acid) is very slightly volatile with a vapour pressure of 3.0×10^{-5} Pa at 25°C. Aqueous solubility is pH dependent with X11393729 (XDE-729 acid) being moderately soluble at pH 5 (102 mg/L), and readily soluble at pH 7 and pH 9 (3.07g/L, 46.1g/L). The pKa is 5.11 ± 0.01 at 21.9°C. There is significant absorbance >290 nm in the UV-Vis spectrum for X11393729 (XDE-729 acid) when in solution at pH < 2, therefore at low pH X11393729 (XDE-729 acid) is photolytically labile. At pH 7 and pH >10, there is no significant absorbance >290nm in the UV-vis spectrum, therefore at higher pH X11393729 (XDE-729 acid) is photolytically stable. X11393729 (XDE-729 acid) is very slightly soluble in n-heptane (<0.2 mg/L), slightly soluble in xylene, (8.5 mg/L) and moderately soluble in n-octanol and 1,2-dichloromethane (430 mg/L and 130 mg/L) and readily soluble in ethyl acetate, acetone and methanol (1.2 g/L, 4.4 g/L and 4.2 g/L). The n-octanol/water partition coefficient is slightly pH dependent ($\text{Log}_{10}P_{\text{OW}} = 0.42$ at pH 5, $\text{Log}_{10}P_{\text{OW}} = -0.83$ at pH 7 and $\text{Log}_{10}P_{\text{OW}} = -1.01$ pH 9). The data suggest a low propensity for bioaccumulation.

Degradation Product X11406790

The n-octanol/water partition coefficient is slightly pH dependent ($\text{Log}_{10}P_{\text{OW}} = 0.96$ at pH 5, $\text{Log}_{10}P_{\text{OW}} = <0.3$ at pH 7 and $\text{Log}_{10}P_{\text{OW}} = <0.3$ pH 9). The data suggest a low propensity for bioaccumulation.

B.2.3.2 Plant protection product

The representative plant protection product for XDE-729 is 'GF-2573'. 'GF-2573' is an Emulsion Concentrate (EC) formulation containing 7.817g active substance XDE-729 methyl/L and 7.5 g cloquintocet-mexyl/L. 'GF-2573' is a yellow liquid (25.5°C) with a solvent odour, it is not classified for physico-chemical properties. When analysed by HPLC, the active substance content in the formulation was within specification. The pH of a 1% dispersion in water is pH 5.3. 'GF-2573' has a relative density of 0.905. Surface tension for a 0.27% v/v dilution at 20°C was 33.0 mN/m and for a 1.25% v/v dilution at 20°C was 29.5 mN/m. Viscosity at 40°C was 4.22 mPa.s. A written statement was provided stating that the hydrocarbon content does not exceed 10%. This statement is confirmed by reference to the formulation details in document J. The product does not require further consideration as an aspiration hazard. Levels of persistent foam and emulsion characteristics are within acceptable limits. The active substance content and all physicochemical properties were acceptably retained after accelerated storage (18 days at 54°C) and 12 months storage at ambient temperature; a 2-year shelf life study is ongoing, acceptable retention of properties were demonstrated following cold temperature storage.

Two studies were submitted to address effectiveness of tank cleaning procedures as part of the submission. These studies have not been evaluated as part of the consideration for authorisation of XDE-729 methyl, they are for consideration by efficacy experts during evaluation of the product at member state level. It is noted however, that the notifier concludes that there is potential for low levels of crop injury to subsequent crops, and therefore as a precautionary approach, the following label text has been suggested for GF-2573 by the notifier:

TANK CLEANING

XDE-729 methyl (GF-2573) is active to a range of broad-leaved crop species. To avoid subsequent injury to crops other than cereals (wheat, durum wheat, spelt, barley, rye, triticale), all spraying equipment must be thoroughly cleaned both inside and out.

The use of a proprietary cleaner such All Clear Extra at 0.5 % v/v or bleach containing 5 % hypochlorite is advised where sensitive crops are likely to be sprayed following use of XDE-729 methyl containing products.

B.2.4 References relied on

Annex Point/ Reference Number	Author(s)	Year	Title Source (where different from the Company), Company, Report Number, GLP or GEP status (where relevant), Published or not	Data Protection claimed (Y/N)	Owner
B.2.1.1	Frank, A.	2011	Determination of Color, Physical State, Odor, Melting Point and Decomposition Temperatures of XDE-729 Methyl Pure Active Ingredient. Dow AgroSciences LLC DAS Report No.: FAPC-G-10-84 (Accession Number) 2007676 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.2	Frank, A.	2011	Determination of Color, Physical State, Odor, Melting Point and Decomposition Temperatures of XDE-729 Methyl Pure Active Ingredient. Dow AgroSciences LLC DAS Report No.: FAPC-G-10-84 (Accession Number) 2007676 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.3	Frank, A.	2011	Determination of Color, Physical State, Odor, Melting Point and Decomposition Temperatures of XDE-729 Methyl Pure Active Ingredient. Dow AgroSciences LLC DAS Report No.: FAPC-G-10-84 (Accession Number) 2007676 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.4	Elliott, T	2010	XDE-729 methyl PAI: Determination of Density for Solids. (EU) ABC Laboratories, Inc. DAS Report No.: NAFST-10-246 (Accession Number) 2007536 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.5	Turner, B.	2011	Determination of Vapour Pressure for XDE-729 methyl Huntingdon Life Sciences Ltd DAS Report No.: NAFST-10-92 (Accession Number) 2008310 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS

Annex Point/ Reference Number	Author(s)	Year	Title Source (where different from the Company), Company, Report Number, GLP or GEP status (where relevant), Published or not	Data Protection claimed (Y/N)	Owner
B.2.1.6	Jones, J.	2011	Calculation of the Henry's Law Constants for XDE-729 methyl from Unbuffered and pH 5, 7, and 9 Buffered Water Dow AgroSciences LLC DAS Report No.: NAFST-11-115 (Accession Number) 2008393 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.7 B.2.1.8 B.2.1.9	Frank, A.	2011	Determination of Color, Physical state, Odor, Melting Point and Decomposition Temperature of XDE-729 Methyl Pure Active Ingredient. Dow AgroSciences LLC DAS Report No.: FAPC-G-10-84 (Accession Number) 2007676 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.7 B.2.1.8 B.2.1.9	Frank, A.	2011	Determination of Color, Odor, Physical State, Oxidizing and Reducing Action, Explodability, pH and Bulk Density of XDE-729 Methyl Technical Grade Active Ingredient. Dow AgroSciences LLC DAS Report No.: FAPC-G-10-83 (Accession Number) 2007675 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.10	Habeeb, S.	2011	X11393728: XDE-729 Methyl: Determination of Spectral Characteristics (UV/Visible Absorption and Molar Absorptivity, Mass Spectrum, Infrared Spectrum, and NMR) ABC Laboratories, Inc; Spectral Data Services, Inc DAS Report No.: NAFST-10-316 (Accession Number) 2008011 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.11	Turner, B.	2011	Determination of Water Solubility for XDE-729 Methyl Huntingdon Life Sciences Ltd DAS Report No.: NAFST-10-93 (Accession Number) 2008311 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS

Annex Point/ Reference Number	Author(s)	Year	Title Source (where different from the Company), Company, Report Number, GLP or GEP status (where relevant), Published or not	Data Protection claimed (Y/N)	Owner
B.2.1.12	Turner, B.	2011	Determination of Organic Solvent Solubility for XDE-729 Methyl TGA Huntingdon Life Sciences Ltd DAS Report No.: NAFST-10-96 (Accession Number) 2008658 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.13	Turner, B.	2011	Determination of Octanol/Water Partition Coefficient for XDE-729 Methyl by Shake Flask Method Huntingdon Life Sciences Ltd DAS Report No.: NAFST-10-95 (Accession Number) 2008312 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.14 B.2.1.15	Liu, D.; Smiht, K.P.; Adelfinskaya, Y.	2011	Hydrolysis of XDE-729 ME at pH 4, 7 and 9 Dow AgroSciences LLC DAS Report No.: 090126 (Accession Number) 2009565 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.16 B.2.1.17	Blakeslee, B.A.; Balcer, J.L.; Laughlin, L.A.	2011	Aqueous Photolysis of XDE-729 ME in pH 7 Buffer and Natural Water Under Xenon Light Dow AgroSciences LLC DAS Report No.: 101793 (Accession Number) 2009567 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.18	Cathie, C.	2011	Determination of Dissociation Constant of XDE- 729 methyl Using UV-Visible Spectrophotometry Dow AgroSciences (NZ) Ltd DAS Report No.: 10-040-G (Accession Number) 2008365 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.19	Wendleburg, B.M.; Boulton, J.P.	2011	Estimation of the Photochemical Oxidation Rate of XDE-729 Dow AgroSciences LLC DAS Report No.: 101450 (Accession Number) 2008281 GLP/GEP (Y/N): N Published (Y/N): N	Y	DAS
B.2.1.20	Turner, B.	2011	Determination of surface Tension, Flammability (solids), Explosive Properties, Relative Self- Ignition Temperature for Solids and Oxidising Properties for XDE-729 Methyl TGA Huntingdon Life Sciences, Ltd DAS Report No.: NAFST-10-124 (Accession Number) 2008721 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS

Annex Point/ Reference Number	Author(s)	Year	Title Source (where different from the Company), Company, Report Number, GLP or GEP status (where relevant), Published or not	Data Protection claimed (Y/N)	Owner
B.2.1.22	Turner, B.	2011	Determination of surface Tension, Flammability (solids), Explosive Properties, Relative Self-Ignition Temperature for Solids and Oxidising Properties for XDE-729 Methyl TGAI Huntingdon Life Sciences, Ltd DAS Report No.: NAFST-10-124 (Accession Number) 2008721 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.23	Turner, B.	2011	Determination of surface Tension, Flammability (solids), Explosive Properties, Relative Self-Ignition Temperature for Solids and Oxidising Properties for XDE-729 Methyl TGAI Huntingdon Life Sciences, Ltd DAS Report No.: NAFST-10-124 (Accession Number) 2008721 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.24	Turner, B.	2011	Determination of surface Tension, Flammability (solids), Explosive Properties, Relative Self-Ignition Temperature for Solids and Oxidising Properties for XDE-729 Methyl TGAI Huntingdon Life Sciences, Ltd DAS Report No.: NAFST-10-124 (Accession Number) 2008721 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
Annex Point/ Reference Number	Author(s)	Year	Title Source (where different from the Company), Company, Report Number, GLP or GEP status (where relevant), Published or not	Data Protection claimed (Y/N)	Owner
B.2.1.5	Comb, A.L.	2011	Determination of Vapour Pressure for X11449757 Huntingdon Life Sciences Ltd DAS Report No.: NAFST-10-322 (Accession Number) 2009378 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.10	Elliot, T.	2011	X11449757: Determination of Spectral Characteristics (UV/Visible Absorption and Molar Absorptivity, Mass Spectrum, Infrared Spectrum, and NMR) ABC Laboratories, Inc DAS Report No.: NAFST-11-114 (Accession Number) 2009156 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.11	Comb, A.L.	2011	Determination of Water Solubility for X11449757 Huntingdon Life Sciences Ltd DAS Report No.: NAFST-10-321 (Accession Number) 2009569 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS

Annex Point/ Reference Number	Author(s)	Year	Title Source (where different from the Company), Company, Report Number, GLP or GEP status (where relevant), Published or not	Data Protection claimed (Y/N)	Owner
B.2.1.12	Comb, A.L.	2011	Determination of Organic Solvent Solubility for X11449757 Huntingdon Life Sciences Ltd DAS Report No.: NAFST-10-324 (Accession Number) 2009536 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.13	Comb, A.L.	2011	Determination of Octanol/Water Partition Coefficient for X11449757 by HPLC Method Huntingdon Life Sciences Ltd DAS Report No.: NAFST-10-320 (Accession Number) 2009377 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.18	Comb, A.L.	2011	Determination of Dissociation Constant for X11449757 Huntingdon Life Sciences Ltd DAS Report No.: NAFST-10-323 (Accession Number) 2009564 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.5	Comb, A.L.	2011	Determination of Vapour Pressure for XDE-729 acid (X11393729) Huntingdon Life Sciences Ltd DAS Report No.: NAFST-11-18 (Accession Number) 2009380 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.10	Habeeb, S.	2011	X11393729: XDE-729 Methyl: Determination of Spectral Characteristics (UV/Visible Absorption and Molar Absorptivity, Mass Spectrum, Infrared Spectrum, and NMR) ABC Laboratories, Inc; Spectral Data Services, Inc. DAS Report No.: NAFST-10-317 (Accession Number) 2008012 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.11	Comb, A.L.	2011	Determination of Water Solubility for XDE-729 acid (X11393729) Huntingdon Life Sciences Ltd DAS Report No.: NAFST-11-17 (Accession Number) 2009379 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.12	Comb, A.L.	2011	Determination of Organic Solvent Solubility for XDE-729 acid (X11393729) Huntingdon Life Sciences Ltd DAS Report No.: NAFST-11-19 (Accession Number) 2009537 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS

Annex Point/ Reference Number	Author(s)	Year	Title Source (where different from the Company), Company, Report Number, GLP or GEP status (where relevant), Published or not	Data Protection claimed (Y/N)	Owner
B.2.1.13	Comb, A.L.	2011	Determination of Octanol/Water Partition Coefficient for XDE-729 acid (X11393729) by Shake Flask Method Huntingdon Life Sciences Ltd DAS Report No.: NAFST-11-16 (Accession Number) 2009395 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.18	Cathie, C.	2011	Determination of Dissociation Constant of XDE-729 Using UV-Visible Spectrophotometry Dow AgroSciences (NZ) Ltd DAS Report No.: 10-039-G (Accession Number) 2007519 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.1.5	Comb, A.L.	2012	Determination of Octanol/Water Partition Coefficient HPLC method Huntingdon Life Sciences Ltd. DAS Report No: NAFST-12-45 (Accession Number): 2012655 GLP/GEP (Y/N): N Published (Y/N): N	Y	DAS

Plant Protection product GF-2573

Annex Point/ Reference Number	Author(s)	Year	Title Source (where different from the Company), Company, Report Number, GLP or GEP status (where relevant), Published or not	Data Protection claimed (Y/N)	Owner
B.2.2.1 B.2.2.2 B.2.2.3	Rozniak, M.	2011	Determination of Color, Odor, Physical state, Oxidizing and Reducing Action, Flashpoint, pH, Viscosity and Density of GF-2573, an End Use Product Containing XDE-729 Methyl and Cloquintocet-mexyl under GLP Impact Analytical, USA DAS Report No.: NAFST-11-26 (Accession Number) 2007895 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.2.4 B.2.2.5 B.2.2.7	Turner, B.	2011	Determination of Surface Tension, Explosive Properties, Auto-Ignition (liquids and gases) and Oxidising Properities (liquids) for GF-2573 Huntingdon Life Sciences Ltd DAS Report No.: NAFST-11-36 (Accession Number) 2008487 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS

Annex Point/ Reference Number	Author(s)	Year	Title Source (where different from the Company), Company, Report Number, GLP or GEP status (where relevant), Published or not	Data Protection claimed (Y/N)	Owner
B.2.2.8	Frank, A	2012	Determination of Flammability of GF-2573 an End Use Product Containing XDE-729 methyl and Cloquintocet-mexyl Dow AgroSciences LLC Study ID: FAPC-G-12-1 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.2.8	Frank, A	2012	Determination of Flammability of GF-2573 an End Use Product Containing XDE-729 methyl and Cloquintocet-mexyl Dow AgroSciences LLC DAS Report No.: FAPC-G-12-1 (Accession Number) 2011128 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.2.10	Rozniak, M.	2011	Determination of Color, Odor, Physical state, Oxidizing and Reducing Action, Flashpoint, pH, Viscosity and Density of GF-2573, an End Use Product Containing XDE-729 Methyl and Cloquintocet-mexyl under GLP Impact Analytical, USA DAS Report No.: NAFST-11-26 (Accession Number) 2007895 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.2.11	Turner, B.	2011	Determination of Surface Tension, Explosive Properties, Auto-Ignition (liquids and gases) and Oxidising Properites (liquids) for GF-2573 Huntingdon Life Sciences Ltd DAS Report No.: NAFST-11-36 (Accession Number) 2008487 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.2.12 B.2.2.13	Rozniak, M.	2011	Determination of Color, Odor, Physical state, Oxidizing and Reducing Action, Flashpoint, pH, Viscosity and Density of GF-2573, an End Use Product Containing XDE-729 Methyl and Cloquintocet-mexyl under GLP Impact Analytical, USA DAS Report No.: NAFST-11-26 (Accession Number) 2007895 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS

Annex Point/ Reference Number	Author(s)	Year	Title Source (where different from the Company), Company, Report Number, GLP or GEP status (where relevant), Published or not	Data Protection claimed (Y/N)	Owner
B.2.2.14	Tebbe, C.	2011a	Accelerated Storage Stability of GF-2573 in Glass Dow AgroSciences LLC DAS Report No.: FOR-10-37 (Accession Number) 2008963 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.2.14	Tebbe, C.	2011b	Eight Week Accelerated Storage Stability of GF-2573 in PET and F-HDPE Dow AgroSciences LLC DAS Report No.: FOR-10-38 (Accession Number) 2008264 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS
B.2.2.15	Tebbe, C.	2012	Storage Stability and Package Corrosion Characteristics of GF-2573 in PET and F-HDPE; Two year Ambient Study Dow AgroSciences LLC DAS Report No.: FOR-10-40 (Accession Number) 2012622 GLP/GEP (Y/N): Y Published (Y/N): N	Y	DAS