

European Commission



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

FLUFENACET

Volume 3 – B.2 (AS)

Rapporteur Member State: Poland
Co-Rapporteur Member State: France

Version History

When	What
August 1997	Initial assessment. Draft Assessment Report for first inclusion to Annex I. RMS: FR
April 2016	Draft Renewal Assessment Report prepared according to the Commission; Regulation (EU) N° 1107/2009; RMS: PL; Co-RMS: FR
May 2017	Revision according to the CoRMS comments

Table of contents

B.2. PHYSICAL AND CHEMICAL PROPERTIES OF THE ACTIVE SUBSTANCE	4
B.2.1. MELTING POINT AND BOILING POINT	4
B.2.3. APPEARANCE (PHYSICAL STATE, COLOUR).....	6
B.2.4. SPECTRA (UV/VIS, IR, NMR, MS), MOLAR EXTINCTION AT RELEVANT WAVELENGTHS, OPTICAL PURITY	7
B.2.5. SOLUBILITY IN WATER.....	11
B.2.6. SOLUBILITY IN ORGANIC SOLVENTS	12
B.2.7. PARTITION COEFFICIENT N-OCTANOL/WATER.....	13
B.2.8. DISSOCIATION IN WATER.....	15
B.2.9. FLAMMABILITY AND SHELF-HEATING.....	15
B.2.10. FLASH POINT	16
B.2.11. EXPLOSIVE PROPERTIES	16
B.2.12. SURFACE TENSION	16
B.2.13. OXIDISING PROPERTIES.....	17
B.2.14. OTHER STUDIES	17
B.2.15. REFERENCES RELIED ON	22

B.2. PHYSICAL AND CHEMICAL PROPERTIES OF THE ACTIVE SUBSTANCE

In the tables below those studies which have not been evaluated previously are shown in black, while studies which have already been evaluated are greyed out.

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.1. MELTING POINT AND BOILING POINT						
Melting, freezing or solidification point B.2.1/01	EC A.1, OECD 102	Batch no.: 900124ELB01 purity 99.5 %	Two modifications of FOE 5043 can be observed with a melting point of 76 °C and 79 °C.	Acceptable	Y	Krohn, J.; 1992a M-004726-01-1
Boiling point B.2.1/02	EC A.2, OECD 103	Batch no.: 900124ELB01 purity 99.5 %	Not measurable, decomposition above 150 °C.	Acceptable	Y	Eberz, A., Berg, G.; 1993 M-004753-01-1
Decomposition Sublimation temperature B.2.1/03	/ OECD 113	Batch no.: 900124ELB01 purity 99.5 %	DTA: Exothermic reaction occurred above 160 °C. TGA: Weight loss under air and nitrogen atmosphere above 150 °C. On the basis of DTA/TGA-measurements FOE 5043 is thermally stable at room temperature.	Acceptable	Y	Eberz, A., Berg, G.; 1993 M-004753-01-1

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.2. VAPOUR PRESSURE, VOLATILITY						
Vapour pressure B.2.2/01	EC A.4, OECD 104	Batch no.: (pure active): 900124ELB01 purity 99.5 % Batch no.: (N-isomer): 910405ELB01 purity 98.5 %	Flufenacet- <i>N</i> -isomer: 9×10^{-5} Pa for 20 °C 2×10^{-4} Pa for 25 °C	Acceptable Flufenacet isomerizes by evaporation in a mixture containing Flufenacet- <i>N</i> -isomer as the main component and approx. 10 % of Flufenacet. Consequently only the vapour pressure of Flufenacet- <i>N</i> -isomer can be determined. Vapour pressures of Flufenacet- <i>N</i> -isomer determined at 50, 40, 30 and 25 °C were used to calculate by regression analysis the coefficients for the Clausius-Clapeyron equation which resulted in the vapour pressures for 20 and 25 °C.	Y	Krohn, J.; 1994a M-004730-01-1
Volatility (Henry's Law constant) B.2.2/02	Calculation	-	Henry's law constant at 20 °C 9×10^{-4} Pa x m ³ x mol ⁻¹ Henry's law constants at 20 °C at pH 4: 1.2×10^{-3} Pa x m ³ x mol ⁻¹ at pH 7: 1.3×10^{-3} Pa x m ³ x mol ⁻¹ at pH 9: 1.1×10^{-3} Pa x m ³ x mol ⁻¹	Acceptable Consequently, the Henry's Law Constant given is the one for the FOE 5043- <i>N</i> -Isomer calculated from its vapour pressure and water solubility. A new calculation has been performed since the necessary old water solubility study had applied an equilibration time of only 24 h. The new calculation is based on a new water solubility study of the FOE 5043- <i>N</i> -Isomer (M-461493-01-1).	N N	Krohn, J.; 1994b M-004737-01-1 Ziemer, F.; 2013 M-461497-01-1

B.2.3. APPEARANCE (PHYSICAL STATE, COLOUR)						
Physical state and colour B.2.3/01		Batch no.: 920902ELB01 purity 99.5 %	Active substance, pure: colourless, fine crystalline powder		N	Krohn, J.; 1995 M-004738-01-1
		Batch no.: 4-25-0009 purity 96.6 %	Active substance as manufactured: tan solid			Leibowitz, S. J.; 1994 M-004755-01-1
	OPPTS 830.630 2, OPPTS 830.6303	Batch no.: AE F133402-PU- 01 purity 98.65 % Batch no.: AE F133402-01- 01 purity 97.8 %	Active substance, pure: light beige powder Active substance as manufactured: beige powder	Acceptable A new study has been performed since the old study had not precisely described the testing procedure. A new study has been performed since the old study had not precisely described the testing procedure.	Y Y	Ziemer, F., Strunk, B.; 2012a M-438536-01-1 Ziemer, F., Strunk, B.; 2012b M-441058-01-1
Odour B.2.3/02		Batch no.: 920902ELB01 purity 99.5 %	Active substance, pure: faint, not characteristic		N	Krohn, J.; 1995 M-004738-01-1
		Batch no.: 4-25-0009 purity 96.6 %	Active substance as manufactured: pungent, like mercaptan		Y	Leibowitz, S. J.; 1994 M-004755-01-1
	OCSP 830.6304	Batch no.: AE F133402-PU- 01 purity 98.65 %	Active substance, pure: moderate, not characteristic	Acceptable A new study has been performed since the old study had not precisely described the testing procedure.	Y	Ziemer, F., Strunk, B.; 2012a M-438536-01-1
	OCSP 830.6304	Batch no.: AE F133402-01- 01	Active substance as manufactured: intensive, not characteristic	A new study has been performed since the old study had not precisely described the testing procedure.	Y	Ziemer, F., Strunk, B.; 2012b M-441058-01-1

		purity 97.8 %					
B.2.4. SPECTRA (UV/VIS, IR, NMR, MS), MOLAR EXTINCTION AT RELEVANT WAVELENGTHS, OPTICAL PURITY							
Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results		Comments (Acceptable / Non acceptable)	GLP	Reference
Ultraviolet/visible (UV/VIS) B.2.4/01	OPPTS 830.7050	Batch no.: 900124ELB01 purity 99.5 %	UV (acetonitrile)		-	Y	Etzel, W.; 1992 M-004722-01-1
		Batch no.: 900124ELB01 purity not available				N	Stupp, H.P.; 1993 M-004721-01-1
		Batch no.: K664072 Purity 97.8 %	UV Spectrum (Acetonitrile) pH: neutral		Acceptable A complete new set of spectral data has been prepared due to partly missing information, poor copies or non-GLP in the old studies.	Y	Ruengeler, W.; 2012 M-431269-01-1
			Wavelength	235 nm			
			Absorption [AU]	0.19433			
Spec. absorption [1000cm ² /g]	19.557						
Mol. absorption [1000cm ² /mol]	7106						
pH: 2							
Wavelength	201 nm	235 nm					
Absorption [AU]	0.44627	0.17985					
Spec. absorption [1000cm ² /g]	49.903	20.111					
Mol. absorption [1000cm ² /mol]	18131	7307					

Flufenacet

Volume 3 – B.2 (AS)

			<table><tr><td colspan="2">pH: 10</td></tr><tr><td>Wavelength</td><td>235 nm</td></tr><tr><td>Absorption [AU]</td><td>0.19565</td></tr><tr><td>Spec. absorption [1000cm²/g]</td><td>19.710</td></tr><tr><td>Mol. absorption [1000cm²/mol]</td><td>7161</td></tr></table>	pH: 10		Wavelength	235 nm	Absorption [AU]	0.19565	Spec. absorption [1000cm ² /g]	19.710	Mol. absorption [1000cm ² /mol]	7161														
pH: 10																											
Wavelength	235 nm																										
Absorption [AU]	0.19565																										
Spec. absorption [1000cm ² /g]	19.710																										
Mol. absorption [1000cm ² /mol]	7161																										
Infrared (IR) B.2.4/02		Batch no.: 900124ELB01 purity 99.5 %	IR (KBr-plate)	-	Y	Etzel, W.; 1992 M-004722-01-1																					
		Batch no.: 900124ELB01 purity not available	IR (KBr-plate)		N	Grohs, R.; 1993 M-004723-01-1																					
	OCSPP 830.7050	Batch no.: K664072 Purity 97.8 % Batch no.: K664072 Purity 97.8 %	<table><tr><td colspan="2">Diamond ATR Unit</td></tr><tr><td>Wavenumber</td><td>Functional Group</td></tr><tr><td>742/1222</td><td>R-F R-F</td></tr><tr><td>848</td><td>CH o.o.p.</td></tr><tr><td>1033</td><td>R-O-R</td></tr><tr><td>1150</td><td>R-C=N-R</td></tr><tr><td>1176</td><td>CH i.p.</td></tr><tr><td>1253</td><td>R-N-N-R</td></tr><tr><td>1327/1370</td><td>R-CH (CH₃)₂</td></tr><tr><td>1484</td><td>Ring</td></tr><tr><td>1653</td><td>R-CO-NR₂</td></tr></table> The results confirmed the structure.	Diamond ATR Unit		Wavenumber	Functional Group	742/1222	R-F R-F	848	CH o.o.p.	1033	R-O-R	1150	R-C=N-R	1176	CH i.p.	1253	R-N-N-R	1327/1370	R-CH (CH ₃) ₂	1484	Ring	1653	R-CO-NR ₂	Acceptable A complete new set of spectral data has been prepared due to partly missing information, poor copies or non-GLP in the old studies.	Y
Diamond ATR Unit																											
Wavenumber	Functional Group																										
742/1222	R-F R-F																										
848	CH o.o.p.																										
1033	R-O-R																										
1150	R-C=N-R																										
1176	CH i.p.																										
1253	R-N-N-R																										
1327/1370	R-CH (CH ₃) ₂																										
1484	Ring																										
1653	R-CO-NR ₂																										

Nuclear magnetic resonance (NMR) B.2.4/03		Batch no.: 900124ELB01 purity 99.5 %	¹ H-NMR (300.133 MHz, CDCl ₃)		Y	Etzel, W.; 1992 M-004722-01-1					
		Batch no.: 900124ELB01 purity not available	¹³ C-NMR (75.48 MHz, CDCl ₃)		N	Etzel, W.; 1993 M-004724-01-1					
	OCSP 830.7050	Batch no.: K664072 Purity 97.8%	¹ H-NMR (601.60 MHz, CDCl ₃) ¹³ C-NMR (151.27 MHz, CDCl ₃) The spectra confirmed the structure	Acceptable A complete new set of spectral data has been prepared due to partly missing information, poor copies or non-GLP in the old studies	Y	Ruengeler, W.; 2012 M-431269-01-1					
Mass spectra (MS) B.2.4/04		Batch no.: 900124ELB01 purity 99.5 %	Mass spectra (Electron Impact Ionisation)		Y	Etzel, W.; 1992 M-004722-01-1					
		Batch no.: 900124ELB01 purity not available	Mass spectra (Electron Impact Ionisation)		N	Thielking, G.; 1993 M-004725-01-1					
	OCSP 830.7050	Batch no.: K664072 Purity 97.8 %	Mass spectrum (LC-MS/ESI ⁺ -spectrum) The spectrum confirmed the structure <table><tr><td>m/z value</td><td>Assgnment</td></tr><tr><td>364.1</td><td>[M+H]⁺</td></tr><tr><td>727.1</td><td>[2M+H]⁺</td></tr></table>	m/z value	Assgnment	364.1	[M+H] ⁺	727.1	[2M+H] ⁺	Acceptable A complete new set of spectral data has been prepared due to partly missing information, poor copies or non-GLP in the old studies	Y
m/z value	Assgnment										
364.1	[M+H] ⁺										
727.1	[2M+H] ⁺										

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
Spectra for impurities B.2.4/05	-	-	-	None of the impurities present in the active substance as manufactured is of toxicological or environmental significance.	-	-
Spectra for purified active substance Optical purity B.2.4/06	-	-	-	Not relevant as the active substance is not a resolved optical isomer.	-	-

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.5. SOLUBILITY IN WATER						
Solubility in water B.2.5/01	EC A.6 OECD 105	Batch no.: 900124ELB01 purity 99.5 %	pH 4 56 mg/L at 20°C pH 7 56 mg/L at 20°C pH 9 53 mg/L at 20°C	-	Y	Krohn, J.; 1992b M-004742-01-1
	EC A.6 OECD 105	Batch no.: AE F133402-PU-01 purity 98.65 %	pH 6.9 51 mg/L at 20°C	Acceptable A new study has been performed since the old study had applied an equilibration time of only 24 h. The partition coefficient of Flufenacet (pure substance) was found to be not pH dependent in the range of pH 4 – pH 9. (refer to M-438516-01-1) Furthermore, no dissociation constant pKa was found in aqueous solution of Flufenacet in the pH range of 1 < pH < 12. (refer to M-438182-01-1) Consequently the water solubility is also pH independent in this pH range. Therefore the water solubility was determined in distilled water only.	Y	Ziemer, F., Peschke, C.; 2012 M-438187-01-1

B.2.6. SOLUBILITY IN ORGANIC SOLVENTS

Solubility inorganic solvents B.2.6/01	OECD 105	Batch no.: 900124ELB01 purity 99.5 %	Solvent	Solubility [g/L] at 20 °C	-	Y	Krohn J.; 1992c M-004744-01-1
			Acetone	>20 0			
			Acetonitrile	>200			
			Toluene	>200			
			Dichloromethane	>200			
			Hexane	8.7			
			propanol	170			
			n-octanol	88			
			Dimethyl formamide	>200			
			Dimethyl sulfoxide	>200			
			Propylene glycol	74			
	EC A.6 OECD 105	Batch no.: AE F133401-01- 01 Purity 97.8 %	Solvent	Solubility [g/L] at 20 °C	Acceptable A new study has been performed since the old study is missing a complete method validation and a solubility testing in an ester (e.g. ethyl acetate).	Y	Eyrich, U., Ziemer, F.; 2012 M-429219-01-1
			Methanol	> 280			
			n-heptane	6.4			
			Xylene	> 280			
			1,2-dichloroethane	> 280			
			Acetone	> 280			
			Ethyl acetate	> 280			
			Dimethyl sulfoxide	> 280			

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.7. PARTITION COEFFICIENT N-OCTANOL/WATER						
Partition coefficient n-octanol/water B.2.7/01	EC A.8 OECD 117 (shake flask method)	Batch no.: 900124ELB01 purity 99.5 %	Determination of the partition coefficient of Flufenacet in 1-octanol / water (24 °C) Pow 1600 log Pow 3.2	The effect of pH (4-10) was not investigated because there is no influence of pH on the water solubility.	Y	Krohn, J.; 1992d M-004745-01-1
	EC A.8, OECD 117 (HPLC-method)	Batch no.: AE F133402 00 1B99 0001 purity 99.6 %	Determination of the partition coefficient of Flufenacet in 1-octanol / water (25 °C) pH 7 Pow 3200 log Pow 3.5	Acceptable A new study has been performed since the pH-value of the mobile phase was not defined in the old study.	Y	Ziemer, F., Charter, G.E.; 2012 M-438516-01-1
n-Octanol/water partition coefficient of metabolites FOE oxalate, M01	EC A.8 OECD 117 (shake flask method)	Batch no.: BCS-AB16305-01-02 (free acid) purity 99.1 %	Determination of the partition coefficient of FOE oxalate, M01 in 1-octanol / water (23 °C) pH 5 Pow 0.010 log Pow 2.0 pH 7 0.007 2.2 pH 9 0.004 2.4	Acceptable	Y	Ziemer, F., Peschke, C.; 2012c M-436227-01-1
n-Octanol/water partition coefficient of metabolites FOE sulfonic acid, M02	EC A.8, OECD 117 (shake flask method)	Batch no.: M00096 (sodium salt) purity 74 %	Determination of the partition coefficient of FOE sulfonic acid, M02 in 1-octanol / water (20 °C) Pow 0.0019 log Pow - 2.72	Acceptable The measured value does not depend on the pH value between 4 and 9 as the test substance is the sodium salt of a strong acid.	Y	Krohn, J.; 1998a M-005351-01-1
n-Octanol/water partition coefficient of metabolites FOE methylsulfide, M05	EC A.8, OECD 117 (HPLC-method)	Batch no.: BCS-CP38571-01-01 purity 98.0 %	Determination of the partition coefficient of FOE methylsulfide, M05 in 1-octanol / water (25 °C) pH 5 Pow 398 log Pow 2.6 pH 7 398 2.6 pH 9 398 2.6	Acceptable	Y	Bogdoll, B.; Peschke, C.; 2011a M-420022-01-1

n-Octanol/water partition coefficient of metabolites FOE methylsulfone, M07	EC A.8, OECD 117 (HPLC-method)	Batch no.: BCS-C062475-01-01 Purity 97.2 %	Determination of the partition coefficient of FOE methylsulfone, M07 in 1-octanol / water (25 °C) Pow log Pow pH 5 50 1.7 pH 7 50 1.7 pH 9 50 1.7	Acceptable	Y	Bogdoll, B.; Strunk, B.; 2011b M-420210-01-1
n-Octanol/water partition coefficient of metabolites FOE thiadone, M09	EC A.8, OECD 107 (shake flask method)	Batch no.: M00385 purity 99 %	Determination of the partition coefficient of FOE thiadone, M09 in 1-octanol / water (20 °C) Pow log Pow pH 4.3 83 1.92 pH 7 4.2 0.62 pH 9.4 0.13 - 0.90	Acceptable	Y	Krohn, J.; 1998b M-004764-01-1
n-Octanol/water partition coefficient of metabolites trifluoroethansulfonic acid, M44	EC A.8, OECD 107 (shake flask method)	Batch no.: BCS-CU62474-01-01 (sodium salt) purity 99.4 %	Determination of the partition coefficient of FOE 5043-trifluoroethansulfonic acid, M44 in 1-octanol / water (23 °C) Pow log Pow pH 5 0.00101 - 3.00 pH 7 0.00113 - 2.95 pH 9 0.00069 - 3.16	Acceptable	Y	Ziemer, F., Peschke, C.; 2012b M-432717-01-1
n-Octanol/water partition coefficient of metabolites Trifluoroacetic acid, M45	EC A.8, OECD 107 (shake flask method)	Batch no.: AE C502988-01-01 (free acid) purity 99.5 %	Determination of the partition coefficient of Trifluoroacetic acid, M45 in 1-octanol / water (20 °C) Pow log Pow pH 5 3.544*10 ⁻³ - 2.5 pH 7 2.554*10 ⁻³ - 2.6 pH 9 1.486*10 ⁻³ - 2.8	Acceptable The partition coefficients of Trifluoroacetic acid were determined in a pH range of 5 – 9. Therefore, the partition coefficient of the Trifluoroacetate is likewise covered by this study.	Y	Schneider, S.; 2011 M-420136-01-1
Effect of pH (4 to 10) on the n-octanol/water partition coefficient	EC A.8, OECD 117 (HPLC-method)	Batch no.: AE F133402 00 1B99 0001 purity 99.6 %	The partition coefficient (1-octanol / water) of Flufenacet at different pH-values (25 °C) Pow log Pow pH 4 3200 3.5 pH 7 3200 3.5 pH 9 3200 3.5	Acceptable	Y	Ziemer, F., Charter, G.E.; 2012 M-438516-01-1

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.8. DISSOCIATION IN WATER						
Dissociation constant B.2.8/01	OECD 112	Batch no.: 900124ELB01 purity 99.5 %	The substance does not show basic or acidic properties in water. It is not possible to specify a pK value of the substance in aqueous systems.	-	Y	Stupp, H.P.; 1992 M-004739-01-1
	OECD 112	Batch no.: AE F133402-PU-01 purity 98.65%	No dissociation constant pKa was found in aqueous solution of Flufenacet pure substance in the pH-range of 1 < pH < 12.	Acceptable A new study has been performed since the old study has used the titration method which is not suitable for compounds with low water solubility.	Y	Wiche, A., Ziemer, F.; 2012 M-438182-01-1
B.2.9. FLAMMABILITY AND SHELF-HEATING						
Flammability B.2.9/01	EC A.10	Batch no.: A-25-0010 purity 94.5 %	Flufenacet is not highly flammable in the sense of EC Guideline A.10. The test substance melted when approached by the ignition flame.	Acceptable It can be concluded from the negative test according to A10 that the active substance should not be classified as flammable solid according to CLP.	Y	Mix, K.H.; 1995 M-004754-01-1
Self heating B.2.9/02	EC A.16	Batch no.: A-25-0010 purity 94.5 %	Flufenacet does not undergo spontaneous combustion up to 420 °C.	Acceptable	Y	Mix, K.H.; 1995 M-004754-01-1
	BCC-Test	Batch no.: A-25-0010 purity 94.5 %	Flufenacet does not undergo spontaneous combustion in 1 liter Bowes-Cameron-Cage-Test in the sense of RID-, ADR- and UN-Recommendations on the transport of dangerous goods.	Acceptable	Y	Mix, K.H.; 1995 M-004754-01-1

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.10. FLASH POINT						
Flash point B.2.10/01	-	-	Not applicable. The active substance is a solid; its melting point is > 40 °C	-	-	-
B.2.11. EXPLOSIVE PROPERTIES						
Explosive properties B.2.11/01	EC A.14	Batch no.: A-25-0010 purity 94.5 %	Flufenacet is not explosive in the sense of EC guideline A.14.	Acceptable It can be concluded from the negative test according to A14 that active substance should not be classified as explosive solid according to CLP.	Y	Mix, K.H.; 1995 M-004754-01-1
B.2.12. SURFACE TENSION						
Surface tension B.2.12/01	EC A.5 OECD 115	Batch no.: 920902ELB01 purity 99.5 %	$\sigma = 60 \text{ mN/m}$ at 20 °C	According EU Guideline A.5 substances giving solutions with a surface tension below 60 mN/m must be classified as surface-active Consequently FOE 5043 should be regarded as weakly surface-active.	Y	Krohn, J.; 1995a M-004741-01-1
		Batch no.: AE F133402-01-01 purity 97.8%	$\sigma = 59.4 \text{ mN/m}$ at 20 °C The determination concentration is: 47 mg/L	Acceptable A new study has been performed since purified active substance was used in the old study and the test concentration was not correctly adjusted.	Y	Eyrich, U., Ziemer, F.; 2012 M-439214-01-1

Test or Study Annex Point	Guideline and method	Test material purity and specification	Used methods / Results	Comments (Acceptable / Non acceptable)	GLP	Reference
B.2.13. OXIDISING PROPERTIES						
Oxidizing properties B.2.13/01	EC A.17	Batch no.: AEF133402-01- 17 purity 97.49 %	Flufenacet has no oxidizing properties in the sense of EC guideline A.17.	Acceptable It can be concluded from the negative test according to A17 that active substance should not be classified as oxidising solid according to CLP.	Y	Smeykal, H.; 2012a M-434552-01-1
B.2.14. OTHER STUDIES						
Relative density of purified active substance	EC A.3, OECD 109	Batch no.: 920902ELB01 purity 99.5 %	D = 1.45 g/mL at 20 °C	Acceptable	Y	Krohn, J.; 1995b M-004727-01-1
PC data of metabolites FOE oxalate, M01	water solubility: EC A.6, OECD 105, OPPTS 830.7840	Batch no.: BCS-AB16305- 01-02 (free acid) purity 99.1 %	Water solubility FOE oxalate, M01: pH 5: > 120 g/L pH 7: > 120 g/L pH 9: > 120 g/L all at 20 °C	Acceptable	Y	Zierner, F.; Klößner, C.; 2012 M-433165-01-1
	dissociation constant: OECD 112	Batch no.: BCS-AB16305- 01-02 (free acid) purity 99.1 %	Dissociation constant FOE oxalate, M01: pKa = 1.6	Acceptable	Y	Wiche, A., Zierner, F.; 2012 M-436674-01-1
	vapour pressure: EC A.4, OECD 104	Batch no.: BCS-AB16305- 01-02 (free acid) purity 99.1 %	Vapour pressure FOE oxalate, M01: 4.5 x 10 ⁻⁷ Pa for 20 °C 1.7 x 10 ⁻⁶ Pa for 25 °C 7.9 x 10 ⁻⁴ Pa for 50 °C	Acceptable	Y	Smeykal, H.; 2012b M-429179-01-1
	Henry's law constant	Batch no.: BCS-AB16305- 01-02 (free acid) purity 99.1 %	Henry's law constant FOE oxalate, M01: at pH 5: < 8.4 x 10 ⁻¹⁰ Pa x m ³ x mol ⁻¹ at pH 7: < 6.8 x 10 ⁻¹⁰ Pa x m ³ x mol ⁻¹ at pH 9: < 6.8 x 10 ⁻¹⁰ Pa x m ³ x mol ⁻¹	Acceptable	Y	Zierner, F.; 2012b M-433622-01-1

Flufenacet
Volume 3 – B.2 (AS)

PC data of metabolites FOE sulfonic acid, M02	water solubility: EC A.6, OECD 105, OPPTS 830.7840	Batch no.: M00096 (sodium salt) purity 74 %	Water solubility FOE sulfonic acid, M02: unbuffered: 55 g/L at 20 °C	Acceptable	Y	Krohn, J.; 1998a M-005351-01-1
	dissociation constant: OECD 112	Statement	Dissociation constant FOE sulfonic acid, M02: Sulfonic acids are strong acids with pKa-values comparable to those of strong mineral acids. It requires special measurement techniques to determine experimentally pKa-values of strong acids. However, it is well known that sulfonic acids have pKa- values < 1 or dissociation constants > 10.	Acceptable The test substance is the sodium salt of a strong acid and the solubility does not depend on the pH-value (range 4 – 9).	N	Krohn, J.; 1998a M-005351-01-1
PC data of metabolites FOE methylsulfide, M05	water solubility: EC A.6, OECD 105, OPPTS 830.7840	Batch no.: BCS-CP38571-01-01 purity 98.0 %	Water solubility FOE methylsulfide, M05: pH 6.1: 2.0 g/L at 20 °C	Acceptable Since the partition coefficient of M05 was found to be not pH dependent (range 5 – 9) consequently the water solubility is also pH independent in this pH range.	Y	Wiche, A.; Bogdoll, B.; 2011a M-420027-01-1
	dissociation constant:	Statement	Dissociation constant FOE methylsulfide, M05: M05 has no dissociation constant.	Acceptable	N	Ziemer, F.; 2012a M-423244-01-1

Flufenacet
Volume 3 – B.2 (AS)

PC data of metabolites FOE methylsulfone, M07	water solubility: EC A.6, OECD 105, OPPTS 830.7840	Batch no.: BCS-C062475-01-01 purity 97.2 %	Water solubility FOE methylsulfone, M07: pH 7: 4.1 g/L at 20 °C	Acceptable Since the partition coefficient of M07 was found to be not pH dependent (range 5 – 9) consequently the water solubility is also pH independent in this pH range.	Y	Wiche, A., Bogdoll, B.; 2011b M-420028-01-1
	dissociation constant: OECD 112	Batch no.: BCS-C062475-01-01 purity 97.2 %	Dissociation constant FOE methylsulfone M07: No dissociation constant (pKa) was found in aqueous solution of the test item in the pH range of 1.1 < pH < 12.0.	Acceptable	Y	Schmidt, M.; 2011 M-414377-01-1
	vapour pressure: EC A.4, OECD 104	Batch no.: BCS-C062475-01-01 purity 97.2 %	Vapour pressure FOE methylsulfone, M07: 8.6 x 10 ⁻⁴ Pa for 20 °C 1.6 x 10 ⁻³ Pa for 25 °C 2.8 x 10 ⁻² Pa for 50 °C	Acceptable	Y	Smeykal, H.; 2011a M-411303-01-1
	Henry's law constant	Calculation	Henry's law constant FOE methylsulfone, M07: at pH 7: 5.7 x 10 ⁻⁵ Pa x m ³ x mol ⁻¹	Acceptable	N	Ziemer, F., Eyrich, U.; 2011 M-420714-01-1
PC data of metabolites FOE thiadone, M09	water solubility: EC A.6, OECD 105, OPPTS 830.7840	Batch no.: M00385 purity 99 %	Water solubility FOE thiadone, M09: pH 3 – 3.3: 30.2 g/L pH 5.77: 95.5 g/L pH 7 - 9: > 100 g/L all at 20 °C		Y	Krohn, J.; 1998b M-004764-01-1
	dissociation constant: OECD 112	Batch no.: M00385 purity 99 %	Dissociation constant FOE thiadone, M09: pKa = 5.73		Y	Krohn, J.; 1998b M-004764-01-1
	vapour pressure: EC A.4, OECD 104	Batch no.: M00385 purity 99 %	Vapour pressure FOE thiadone, M09: 2.05 Pa for 20 °C 3.37 Pa for 25 °C		Y	Krohn, J.; 1998b M-004764-01-1
	Henry's law	Calculation	Henry's law constant FOE thiadone, M09:		N	Krohn, J.; 1998b

Flufenacet
Volume 3 – B.2 (AS)

	constant		at pH < 5: $0.012 \text{ Pa} \times \text{m}^3 \times \text{mol}^{-1}$			M-004764-01-1
PC data of metabolites FOE 5043-trifluoroethansulfonic acid, M44	water solubility: EC A.6, OECD 105, OPPTS 830.7840	Batch no.: BCS-CU62474-01-01 (sodium salt) purity 99.4 %	Water solubility FOE 5043-trifluoroethansulfonic acid, M44: pH 5: > 160 g/L pH 7: > 160 g/L pH 9: > 160 g/L all at 20 °C	Acceptable	Y	Ziemer, F.; Peschke, C.; 2012b M-432716-01-1
	dissociation constant: OECD 112	Batch no.: BCS-CU62474-01-01 (sodium salt) purity 99.4 %	Dissociation constant FOE 5043-trifluoroethansulfonic acid, M44: No dissociation constant (pKa) was found in aqueous solution of the test item in the pH range of $2.0 < \text{pH} < 12.0$.		Y	Schmidt, M.; 2012 M-434048-01-1
	vapour pressure: EC A.4, OECD 104	Batch no.: BCS-CU62474-01-01 (sodium salt) purity 99.4 %	Vapour pressure FOE 5043-trifluoroethansulfonic acid, M44: < $1 \times 10^{-8} \text{ Pa}$ for 20 °C < $1 \times 10^{-7} \text{ Pa}$ for 25 °C < $1 \times 10^{-6} \text{ Pa}$ for 50 °C		Y	Smeykal, H.; 2012c M-429683-01-1
	Henry's law constant	Calculation (sodium salt)	Henry's law constant FOE 5043-trifluoroethansulfonic acid, M44: at pH 5: < $1.2 \times 10^{-11} \text{ Pa} \times \text{m}^3 \times \text{mol}^{-1}$ at pH 7: < $1.2 \times 10^{-11} \text{ Pa} \times \text{m}^3 \times \text{mol}^{-1}$ at pH 9: < $1.2 \times 10^{-11} \text{ Pa} \times \text{m}^3 \times \text{mol}^{-1}$		N	Ziemer, F.; 2012c M-433635-01-1

Flufenacet
Volume 3 – B.2 (AS)

PC data of metabolites Trifluoroacetic acid, M45	water solubility: EC A.6, OECD 105, OPPTS 830.7840	Batch no.: AE C502988-01-01 (free acid) purity 99.5 %	Water solubility Trifluoroacetic acid, M45: pH 0.4 – 12.6: > 500 g/L at approx. 20 °C	Acceptable The water solubility of Trifluoroacetic acid was determined in a pH range of 0.4 – 12.6. Therefore, the water solubility of the Trifluoroacetate is likewise covered by this study.	Y	Schneider, S.; 2011 M-420129-01-1
	dissociation constant: OECD 112	Batch no.: AE C502988-01-01 (free acid) purity 99.5 %	Dissociation constant Trifluoroacetic acid, M45: pKa = 1.3	Acceptable The Trifluoroacetic acid has been used for the determination of the dissociation constant to ensure the experimental feasibility by titration with sodium hydroxide solution. The pKb value can be calculated by using the formula $pKb = 14 - pKa$.	Y	Winkler, S.; 2011 M-418628-01-1
	vapour pressure: EC A.4, OECD 104	Batch no.: AE 1046319-PU-01 (sodium salt) purity 99.5 %	Vapour pressure Trifluoroacetic acid, M45: < 1.0×10^{-6} Pa for 20 °C < 1.0×10^{-6} Pa for 25 °C < 1.0×10^{-6} Pa for 50 °C	Acceptable	Y	Smeykal, H.; 2011b M-420190-01-1
	Henry's law constant	Calculation (sodium salt)	Henry's law constant Trifluoroacetic acid, M45: at 20 °C: < 2.7×10^{-10} Pa x m ³ x mol ⁻¹	Acceptable	N	Ziemer, F.; 2011 M-420526-01-1

Flufenacet is an oxyacetamide herbicide. It is weakly soluble in water. Its vapour pressure is not determinable, because of isomerization to Flufenacet-*N*-isomer. The vapour pressure and volatility of Flufenacet-*N*-isomer are very low. Its log Pow of 3.5 requires particular consideration with respect to bioconcentration in aquatic organisms. Its flammability, explosive and oxidizing properties are not critical.

B.2.15. REFERENCES RELIED ON

No scientific publications relevant for the section physical and chemical properties were selected by the applicant.

Annex point / reference number	Author(s)	Year	Title Source (<i>where different from company</i>) Company name, Report No., Date, GLP status (<i>where relevant</i>), published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner
KCA 2.1 /01	Krohn, J.	1992	Melting point of FOE 5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC167, Edition Number: M-004726-01-1 Date: 1992-07-31 GLP/GEP: yes, unpublished	N	N	-	Bayer CropScience
KCA 2.1 /02	Eberz, A.; Berg, G.	1993	Thermal stability of the active ingredient FOE 5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC176, Edition Number: M-004753-01-1 Date: 1993-09-01 GLP/GEP: yes, unpublished	N	N	-	Bayer CropScience
KCA 2.2 /01	Krohn, J.	1994	Vapour pressure curve of FOE 5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC170, Edition Number: M-004730-01-1 Date: 1994-01-25 GLP/GEP: yes, unpublished	N	N	-	Bayer CropScience
KCA 2.2 /02	Krohn, J.	1994	Calculation of the Henry Law Constant of FOE 5043/FOE 5043-N-isomer Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC185, Edition Number: M-004737-01-1 Date: 1994-03-02 GLP/GEP: no, unpublished	N	N	-	Bayer CropScience
KCA 2.2 /03	Ziemer, F.	2013	AE 1218900 (FOE5043-N-isomer): Calculation of the Henry's Law constants Bayer CropScience, Report No.: AF13/019, Edition Number: M-461497-01-1 Date: 2013-08-13 GLP/GEP: no, unpublished	N	Y	A new calculation has been performed since the necessary old water solubility study had applied an equilibration time of only 24 h. The new calculation is based on a new water solubility study of the FOE 5043-N-Isomer	Bayer CropScience

Annex point / reference number	Author(s)	Year	Title Source (<i>where different from company</i>) Company name, Report No., Date, GLP status (<i>where relevant</i>), published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner
KCA 2.3 /01	Leibowitz, S. J.	1994	The physical properties of BAY FOE 5043 technical Miles Inc., Agriculture Division, Kansas City, MO, USA Bayer CropScience, Report No.: 106605, Edition Number: M-004755-01-1 Date: 1994-07-14 GLP/GEP: yes, unpublished	N	N	-	Bayer CropScience
KCA 2.3 /02	Krohn, J.	1995	Appearance and odour of FOE 5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC1071, Edition Number: M-004738-01-1 Date: 1995-11-07 GLP/GEP: no, unpublished	N	N	-	Bayer CropScience
KCA 2.3 /03	Ziemer, F.; Strunk, B.	2012	Flufenacet (FOE 5043, AE F133402), pure substance: Physical characteristics colour, physical state and odour Bayer CropScience, Report No.: PA12/078, Edition Number: M-438536-01-1 Date: 2012-09-06 GLP/GEP: yes, unpublished	N	Y	A new study has been performed since the old study had not precisely described the testing procedure.	Bayer CropScience
KCA 2.3 /04	Ziemer, F.; Strunk, B.	2012	Flufenacet (FOE 5043, AE F133402), technical substance: Physical characteristics colour, physical state and odour Bayer CropScience, Report No.: PA12/087, Edition Number: M-441058-01-1 Date: 2012-10-31 GLP/GEP: yes, unpublished	N	Y	A new study has been performed since the old study had not precisely described the testing procedure.	Bayer CropScience
KCA 2.4 /01	Stupp, H. P.	1993	Spectra of FOE 5043 - UV spectrum Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC162, Edition Number: M-004721-01-1 Date: 1993-10-12 GLP/GEP: no, unpublished	N	N	-	Bayer CropScience
KCA 2.4 /02	Etzel, W.	1992	Spectroscopic identification of FOE 5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC163, Edition Number: M-004722-01-1 Date: 1992-12-02 GLP/GEP: yes, unpublished	N	N	-	Bayer CropScience

Annex point / reference number	Author(s)	Year	Title Source (<i>where different from company</i>) Company name, Report No., Date, GLP status (<i>where relevant</i>), published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner
KCA 2.4 /03	Grohs, R.	1993	Spectra of FOE 5043 - infrared spectrum Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC164, Edition Number: M-004723-01-1 Date: 1993-08-31 GLP/GEP: no, unpublished	N	N	-	Bayer CropScience
KCA 2.4 /04	Etzel, W.	1993	Spectra of FOE 5043 - NMR spectrum Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC165, Edition Number: M-004724-01-1 Date: 1993-11-05 GLP/GEP: no, unpublished	N	N	-	Bayer CropScience
KCA 2.4 /05	Thielking, G.	1993	Spectra of FOE 5043 - mass spectrum Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC166, Edition Number: M-004725-01-1 Date: 1993-08-30 GLP/GEP: no, unpublished	N	N	-	Bayer CropScience
KCA 2.4 /06	Ruengeler, W.	2012	Spectral data set of flufenacet a.i. - Reference material Bayer CropScience, Report No.: 15-600-2566, Edition Number: M-431269-01-1 Date: 2012-05-16 GLP/GEP: yes, unpublished	N	Y	A complete new set of spectral data has been prepared due to partly missing information, poor copies or non-GLP in the old studies	Bayer CropScience
KCA 2.5 /01	Krohn, J.	1992	Water solubility of FOE 5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC173, Edition Number: M-004742-01-1 Date: 1992-07-28 GLP/GEP: yes, unpublished	N	N	-	Bayer CropScience
KCA 2.5 /02	Krohn, J.	1994	Water solubility of FOE 5043-N-Isomer Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC186, Edition Number: M-004756-01-1 Date: 1994-02-22 GLP/GEP: yes, unpublished	N	N	-	Bayer CropScience

Annex point / reference number	Author(s)	Year	Title Source (<i>where different from company</i>) Company name, Report No., Date, GLP status (<i>where relevant</i>), published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner
KCA 2.5 /03	Krohn, J.	1998	Water solubility, partition coefficient in octanol-water and pKa-value of sulfonic acid - FOE5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: 141200953, Edition Number: M-005351-01-1 Date: 1998-08-24 GLP/GEP: yes, unpublished ...also filed: KCA 2.7 /02 ...also filed: KCA 2.8 /02	N	N	-	Bayer CropScience
KCA 2.5 /04	Peschke, C.; Ziemer, F.	2012	Flufenacet (FOE 5043, AE F133402), pure substance: Solubility in distilled water (flask method) Bayer CropScience, Report No.: PA12/059, Edition Number: M-438187-01-1 Date: 2012-09-13 GLP/GEP: yes, unpublished	N	Y	A new study has been performed since the old study had applied an equilibration time of only 24 h.	Bayer CropScience
KCA 2.5 /05	Ziemer, F.; Peschke, C.	2013	AE 1218900 (FOE5043-N-isomer): Water solubility at pH 4, pH 7 and pH 9 (flask method) Bayer CropScience, Report No.: PA13/088, Edition Number: M-461493-01-1 Date: 2013-08-13 GLP/GEP: yes, unpublished	N	Y	A new study has been performed since the old had not precisely described the testing procedure	Bayer CropScience
KCA 2.6 /01	Krohn, J.	1992	Solubility of FOE 5043 in representative polar and unpolar solvents Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC174, Edition Number: M-004744-01-1 Date: 1992-07-27 GLP/GEP: yes, unpublished	N	N	-	Bayer CropScience
KCA 2.6 /02	Eyrich, U.; Ziemer, F.	2012	Flufenacet (FOE 5043, AE F133402), technical substance: Solubility in organic solvents Bayer CropScience, Report No.: PA12/025, Edition Number: M-429219-01-1 Date: 2012-04-19 GLP/GEP: yes, unpublished	N	Y	A new study has been performed since the old study is missing a complete method validation and a solubility testing in an ester (e.g. ethyl acetate)	Bayer CropScience

Annex point / reference number	Author(s)	Year	Title Source (<i>where different from company</i>) Company name, Report No., Date, GLP status (<i>where relevant</i>), published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner
KCA 2.7 /01	Krohn, J.	1992	Partition coefficient of FOE 5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC175, Edition Number: M-004745-01-1 Date: 1992-07-20 GLP/GEP: yes, unpublished ...also filed: KCA 8.2.2.3 /02	N	N	-	Bayer CropScience
KCA 2.7 /02	Krohn, J.	1998	Water solubility, partition coefficient in octanol-water and pKa-value of sulfonic acid - FOE5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: 141200953, Edition Number: M-005351-01-1 Date: 1998-08-24 GLP/GEP: yes, unpublished ...also filed: KCA 2.5 /03 ...also filed: KCA 2.8 /02	N	N	-	Bayer CropScience
KCA 2.7 /03	Krohn, J.	1998	Physical and chemical properties of FOE 5043 - Thiadone Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: 141200948, Edition Number: M-004764-01-1 Date: 1998-06-23 GLP/GEP: yes, unpublished	N	N	-	Bayer CropScience
KCA 2.7 /04	Bogdoll, B.; Peschke, C.	2011	BCS-CP38571 (Flufenacet-methylsulfide): Partition coefficients 1-octanol / water at pH 5, pH 7 and pH 9 (HPLC method) Bayer CropScience, Report No.: PA11/068, Edition Number: M-420022-01-1 Date: 2011-12-12 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.7 /05	Schneider, S.	2011	Trifluoroacetic acid (AE C502988): Partition coefficients 1-octanol / water at pH 5, pH 7 and pH 9 (shake flask method) Allessa Chemie GmbH, Frankfurt am Main, Germany Bayer CropScience, Report No.: B 027/2010, Edition Number: M-420136-01-1 Date: 2011-12-14 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.7 /06	Bogdoll, B.; Strunk, B.	2011	BCS-CO62475 (flufenacet-methylsulfone): Partition coefficients 1-octanol / water at pH 5, pH 7 and pH 9 (HPLC method) Bayer CropScience, Report No.: PA11/070, Edition Number: M-420210-01-1 Date: 2011-12-12 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience

Annex point / reference number	Author(s)	Year	Title Source (<i>where different from company</i>) Company name, Report No., Date, GLP status (<i>where relevant</i>), published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner
KCA 2.7 /07	Ziemer, F.; Peschke, C.	2012	Sodium 2,2,2-trifluoroethanesulfonate (BCS-CU62474): Partition coefficients 1-octanol / water at pH 5, pH 7 and pH 9 (shake flask method) Bayer CropScience, Report No.: PA12/028, Edition Number: M-432717-01-1 Date: 2012-06-15 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.7 /08	Ziemer, F.; Peschke, C.	2012	BCS-AB16305 (FOE 5043-oxalate): Partition coefficients 1-octanol / water at pH 5, pH 7 and pH 9 (shake flask method) Bayer CropScience, Report No.: PA12/007, Edition Number: M-436227-01-1 Date: 2012-08-01 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.7 /09	Ziemer, F.; Charter, G. E.	2012	Flufenacet (FOE 5043, AE F133402), pure substance: Partition coefficients 1-octanol / water at pH 4, pH 7 and pH 9 (HPLC method) Bayer CropScience, Report No.: PA12/040, Edition Number: M-438516-01-1 Date: 2012-09-06 GLP/GEP: yes, unpublished	N	Y	A new study has been performed since the pH-value of the mobile phase was not defined in the old study.	Bayer CropScience
KCA 2.8 /01	Stupp, H. P.	1992	Dissociation constant and pH value of FOE 5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC172, Edition Number: M-004739-01-1 Date: 1992-12-03 GLP/GEP: yes, unpublished	N	N	-	Bayer CropScience
KCA 2.8 /02	Krohn, J.	1998	Water solubility, partition coefficient in octanol-water and pKa-value of sulfonic acid - FOE5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: 141200953, Edition Number: M-005351-01-1 Date: 1998-08-24 GLP/GEP: yes, unpublished ...also filed: KCA 2.5 /03 ...also filed: KCA 2.7 /02	N	N	-	Bayer CropScience
KCA 2.8 /03	Zeng, Z.; Wood, S.	1992	Stability of FOE 5043 in sterile aqueous buffer solution Miles Inc., Agriculture Division, Stilwell, KS, USA Bayer CropScience, Report No.: MR102623, Edition Number: M-002203-01-1 Date: 1992-03-12 GLP/GEP: yes, unpublished ...also filed: KCA 7.2.1.1 /01	N	N	-	Bayer CropScience

Annex point / reference number	Author(s)	Year	Title Source (<i>where different from company</i>) Company name, Report No., Date, GLP status (<i>where relevant</i>), published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner
KCA 2.8 /04	Wiche, A.; Ziemer, F.	2012	Flufenacet (FOE 5043, AE F133402), pure substance: Dissociation constant in water Bayer CropScience, Report No.: PA12/080, Edition Number: M-438182-01-1 Date: 2012-09-13 GLP/GEP: yes, unpublished	N	Y	A new study has been performed since the old study has used the titration method which is not suitable for compounds with low water solubility.	Bayer CropScience
KCA 2.9 /01	Mix, K. H.	1995	Determination of safety-relevant parameters of FOE 5043 T Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC859, Edition Number: M-004754-01-1 Date: 1995-06-06 GLP/GEP: yes, unpublished ...also filed: KCA 2.10 /01 ...also filed: KCA 2.11 /01	N	N	-	Bayer CropScience
KCA 2.10 /01	Mix, K. H.	1995	Determination of safety-relevant parameters of FOE 5043 T Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC859, Edition Number: M-004754-01-1 Date: 1995-06-06 GLP/GEP: yes, unpublished ...also filed: KCA 2.11 /01 ...also filed: KCA 2.9 /01	N	N	-	Bayer CropScience
KCA 2.11 /01	Mix, K. H.	1995	Determination of safety-relevant parameters of FOE 5043 T Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC859, Edition Number: M-004754-01-1 Date: 1995-06-06 GLP/GEP: yes, unpublished ...also filed: KCA 2.10 /01 ...also filed: KCA 2.9 /01	N	N	-	Bayer CropScience
KCA 2.12 /01	Krohn, J.	1995	Surface tension of FOE 5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC894, Edition Number: M-004741-01-1 Date: 1995-04-25 GLP/GEP: yes, unpublished	N	N	-	Bayer CropScience

Annex point / reference number	Author(s)	Year	Title Source (<i>where different from company</i>) Company name, Report No., Date, GLP status (<i>where relevant</i>), published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner
KCA 2.12 /02	Eyrich, U.; Ziemer, F.	2012	Flufenacet (FOE 5043, AE F133402), technical substance: Determination of the surface tension Bayer CropScience, Report No.: PA12/055, Edition Number: M-439214-01-1 Date: 2012-09-26 GLP/GEP: yes, unpublished	N	Y	A new study has been performed since purified active substance was used in the old study and the test concentration was not correctly adjusted.	Bayer CropScience
KCA 2.13 /01	Smeykal, H.	2012	Flufenacet (FOE 5043, AE F133402), technical substance: oxidizing properties Siemens AG, Frankfurt am Main, Germany Bayer CropScience, Report No.: 20120116.02, Edition Number: M-434552-01-1 Date: 2012-07-12 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /01	Krohn, J.	1995	Density of FOE 5043 Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: PC1037, Edition Number: M-004727-01-1 Date: 1995-09-29 GLP/GEP: yes, unpublished	N	N	-	Bayer CropScience
KCA 2.14 /02	Hellpointner, E.	1995	Assessment of the Henry's law constant of thiadone, 3-trifluoromethyl-1,3,4-thiadiazol-2(3H)one, by the Sar program Henrywin Bayer AG, Leverkusen, Germany Bayer CropScience, Report No.: 107282, Edition Number: M-103764-01-1 Date: 1995-10-23 GLP/GEP: no, unpublished	N	N	-	Bayer CropScience
KCA 2.14 /03	Schmidt, M.	2011	BCS-CO62475 (Flufenacet-methylsulfone): Determination of the dissociation constant in water Bayer CropScience, Report No.: 15-630-2538, Edition Number: M-414377-01-1 Date: 2011-09-13 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience

Annex point / reference number	Author(s)	Year	Title Source (<i>where different from company</i>) Company name, Report No., Date, GLP status (<i>where relevant</i>), published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner
KCA 2.14 /04	Smeykal, H.	2011	BCS-CO62475 (Flufenacet-methylsulfone): Vapour pressure Siemens AG, Frankfurt am Main, Germany Bayer CropScience, Report No.: 20110244.01, Edition Number: M-411303-01-1 Date: 2011-07-19 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /05	Winkler, S.	2011	Trifluoro acetic acid (AE C502988): Determination of the dissociation constant in water Siemens AG, Frankfurt am Main, Germany Bayer CropScience, Report No.: 20100672.02, Edition Number: M-418628-01-1 Date: 2011-11-18 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /06	Wiche, A.; Bogdoll, B.	2011	BCS-CP38571 (Flufenacet-methylsulfide): Solubility in distilled water (flask method) Bayer CropScience, Report No.: PA11/067, Edition Number: M-420027-01-1 Date: 2011-12-12 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /07	Wiche, A.; Bogdoll, B.	2011	BCS-CO62475 (Flufenacet-methylsulfone): Water solubility at pH 7 (flask method) Bayer CropScience, Report No.: PA11/069, Edition Number: M-420028-01-1 Date: 2011-12-12 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /08	Schneider, S.	2011	Trifluoroacetic acid (AE C502988): Miscibility with distilled water and solubility in water in a pH range of 0.4 to 12.6 Allessa Chemie GmbH, Frankfurt am Main, Germany Bayer CropScience, Report No.: B 026/2010, Edition Number: M-420129-01-1 Date: 2011-12-14 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /09	Smeykal, H.	2011	Sodium trifluoroacetate (AE 1046319): Vapour pressure Siemens AG, Frankfurt am Main, Germany Bayer CropScience, Report No.: 20100681.01, Edition Number: M-420190-01-1 Date: 2011-12-07 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience

Annex point / reference number	Author(s)	Year	Title Source (<i>where different from company</i>) Company name, Report No., Date, GLP status (<i>where relevant</i>), published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner
KCA 2.14 /10	Ziemer, F.; Eyrich, U.	2011	BCS-CO62475 (Flufenacet-methylsulfone): Calculation of the Henry's law constant Bayer CropScience, Report No.: AF11/020, Edition Number: M-420714-01-1 Date: 2011-12-15 GLP/GEP: no, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /11	Ziemer, F.	2012	BCS-CP38571 (flufenacet-methylsulfide): Statement on the dissociation constant Bayer CropScience, Report No.: AF12/003, Edition Number: M-423244-01-1 Date: 2012-01-20 GLP/GEP: n.a., unpublished	N	N	-	Bayer CropScience
KCA 2.14 /12	Smeykal, H.	2012	BCS-AB16305 (FOE 5043-oxalate): Vapour pressure Siemens AG, Frankfurt am Main, Germany Bayer CropScience, Report No.: 20120034.01, Edition Number: M-429179-01-1 Date: 2012-04-16 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /13	Smeykal, H.	2012	Sodium 2,2,2-trifluoroethanesulfonate (BCS-CU62474): Vapour pressure Siemens AG, Frankfurt am Main, Germany Bayer CropScience, Report No.: 20120063.01, Edition Number: M-429683-01-1 Date: 2012-04-18 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /14	Ziemer, F.; Peschke, C.	2012	Sodium 2,2,2-trifluoroethanesulfonate (BCS-CU62474): Water solubility at pH 5, pH 7 and pH 9 Bayer CropScience, Report No.: PA12/027, Edition Number: M-432716-01-1 Date: 2012-06-15 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /15	Ziemer, F.; Kloeckner, C.	2012	BCS-AB16305 (FOE 5043-oxalate): Water solubility at pH 5, pH 7 and pH 9 Bayer CropScience, Report No.: PA12/008, Edition Number: M-433165-01-1 Date: 2012-06-21 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience

Annex point / reference number	Author(s)	Year	Title Source (<i>where different from company</i>) Company name, Report No., Date, GLP status (<i>where relevant</i>), published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner
KCA 2.14 /16	Ziemer, F.	2012	BCS-AB16305 (FOE 5043-oxalate): Calculation of the Henry's law constants Bayer CropScience, Report No.: AF12/020, Edition Number: M-433622-01-1 Date: 2012-07-02 GLP/GEP: no, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /17	Ziemer, F.	2012	Sodium 2,2,2-trifluoroethanesulfonate (BCS-CU62474): Calculation of the Henry's law constants Bayer CropScience, Report No.: AF12/025, Edition Number: M-433635-01-1 Date: 2012-07-02 GLP/GEP: no, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /18	Schmidt, M.	2012	Sodium 2,2,2-trifluoroethanesulfonate (BCS-CU62474) - Determination of the dissociation constant in water Bayer CropScience, Report No.: 15-630-2572, Edition Number: M-434048-01-1 Date: 2012-07-04 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /19	Wiche, A.; Ziemer, F.	2012	BCS-AB16305 (FOE 5043-oxalate): Dissociation constant in water Bayer CropScience, Report No.: PA12/042, Edition Number: M-436674-01-1 Date: 2012-08-17 GLP/GEP: yes, unpublished	N	Y	Guideline requirement	Bayer CropScience
KCA 2.14 /20	Ziemer, F.	2011	Sodium trifluoroacetate (AE 1046319): Calculation of the Henry's Law constant Bayer CropScience, Report No.: AF11/032, Edition Number: M-420526-01-1 Date: 2011-12-22 GLP/GEP: no, unpublished	N	Y	Guideline requirement	Bayer CropScience