

Document Title

**Tier 2 Summary of the Physical and Chemical Properties
of the Active Substance
Flupyradifurone (BYI 2960)**

Data Requirements

**Regulation (EC) No 1107/2009
Regulatory Directive 2003-01/Canada/PMRA
OPPTS guidelines/US/EPA**

**Annex IIA
Section 1, Point 2
Document M**

**According to OECD format guidance for industry data submissions
on plant protection products and their active substances**

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**IIA 2 Physical and chemical properties of the active substance**

Test or Study & Annex point	Guideline and method	Test material purity and specification	Findings	Comments	GLP Y/N	Reference
IIA 2.1 Melting point and boiling point						
IIA 2.1.1 Melting point, freezing point or solidification point, purified a.s.	EC A.1, OECD 102 OPPTS 830.7200	BYI 02960, pure NLL 7780-47-4 purity 99.4 % w/w	The melting point of Flupyradifurone, pure at atmospheric pressure is 69.0 °C.		Y	Smeykal, H.; 2010; M-367370-01-1
		BYI 02960, technical PFV107N004 purity 97.6 % w/w	The melting point of Flupyradifurone, technical at atmospheric pressure is 67.1 °C.			Smeykal, H.; 2011; M-414242-01-1
IIA 2.1.2 Boiling point of purified active substance	EC A.2, OECD 103 OPPTS 830.7220	BYI 02960, pure NLL 7780-47-4 purity 99.4 % w/w	The test item had no boiling point at atmospheric conditions; the test item decomposed first at a temperature of 270 °C		Y	Smeykal, H.; 2010; M-367370-01-1
		BYI 02960, technical PFV107N004 purity 97.6 % w/w	The test item had no boiling point; the test item decomposes first starting at a temperature of 245 °C.			Smeykal, H.; 2011; M-414242-01-1

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Test or Study & Annex point	Guideline and method	Test material purity and specification	Findings	Comments	GLP Y/N	Reference
IIA 2.3.1 Vapour pressure of purified active substance	EC A.4, OECD 104 OPPTS 830.7950	BYI 02960, pure NLL 7780-21-1 purity 99.9 % w/w	Extrapolated: 9.1 x 10 ⁻⁷ Pa for 20 °C 1.7 x 10 ⁻⁶ Pa for 25 °C 2.6 x 10 ⁻⁵ Pa for 50 °C		Y	Smeykal, H.; 2008; M-309853-01-1
IIA 2.3.2 Henry's law constant	Directive 94/37/EEC	Calculation	Henry's law constant at 20 °C in distilled water (pH: 7.0) 8.2 x 10 ⁻⁸ Pa x m ³ x mol ⁻¹ Henry's law constants at 20 °C at different pH values: at pH 4: 8.2 x 10 ⁻⁸ Pa x m ³ x mol ⁻¹ at pH 9: 8.2 x 10 ⁻⁸ Pa x m ³ x mol ⁻¹		N	Bogdoll, B.; Eyrich, U.; 2011; M-414341-01-1
IIA 2.4 Appearance						
IIA 2.4.1 Description of the physical state and colour, pure and techn. a.s.	OPPTS 830.6302, OPPTS 830.6303	BYI 02960, pure NLL 7780-47-4 purity 99.4 % w/w BYI 02960, technical PFV107N004 purity 97.6 % w/w	Active substance, pure (at 21°C): white powder Active substance, technical (at 23°C): beige powder		Y	Bogdoll, B.; Strunk, B.; 2011; M-412655-01-1 Eyrich, U., Bogdoll, B.; 2011; M-414072-01-1



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Test or Study & Annex point	Guideline and method	Test material purity and specification	Findings	Comments	GLP Y/N	Reference
IIA 2.4.2 Description of the odour - purified and technical active substance	OPPTS 830.6304	BYI 02960, pure NLL 7780-47-4 purity 99.4 % w/w BYI 02960, technical PFV107N004 purity 97.6 % w/w	active substance, pure (at 21°C): weak, not characteristic Active substance, technical (at 23°C): distinct, solvent-like odour		Y	Bogdoll, B.; Strunk, B.; 2011; M-412655-01-1 Eyrich, U., Bogdoll, B.; 2011; M-414072-01-1
IIA 2.5 Spectra and molecular extinction at relevant wavelengths						
IIA 2.5.1 Spectra for purified active substance						
IIA 2.5.1.1 UV/VIS	OECD 101 OPPTS 830.7050	BYI 02960, pure AZ 15413 purity 99.4 % w/w	UV (methanol) Recorded range of wavelengths: 200 – 800 nm		Y	Peters, S.; 2009; M-345761-01-1
IIA 2.5.1.2 IR	OECD 101 OPPTS 830.7050	BYI 02960, pure AZ 15413 purity 99.4 % w/w	FT-IR Assignment of wave number to functional groups, s. report		Y	Peters, S.; 2009; M-345761-01-1
IIA 2.5.1.3 NMR	OECD 101 OPPTS 830.7050	BYI 02960, pure AZ 15413 purity 99.4 % w/w	¹ H-NMR (600.13 MHz, d3- acetonitrile) ¹³ C-NMR (150.90 MHz, d3- acetonitrile) Results, s. report		Y	Peters, S.; 2009; M-345761-01-1

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Test or Study & Annex point	Guideline and method	Test material purity and specification	Findings	Comments	GLP Y/N	Reference
IIA 2.5.2.1 UV/VIS				None of the impurities present in the active substance as manufactured is of toxicological or environmental significance	Y	
IIA 2.5.2.2 IR				Please refer to the statement above, under annex point IIA 2.5.2.1		
IIA 2.5.2.3 NMR				Please refer to the statement above, under annex point IIA 2.5.2.1		
IIA 2.5.2.4 MS				Please refer to the statement above, under annex point IIA 2.5.2.1		
IIA 2.6 Solubility of purified active substance in water (pH 4-10)						
IIA 2.6 Solubility of purified active substance in water (pH 4-10)	EC A.6, OECD 105 OPPTS 830.7840	BYI 02960, pure NLL 7780-47-4 purity 99.4 % w/w	pH 4 (buffer) 3.2 g/L at 20°C pH 9 (buffer) 3.0 g/L at 20°C In distilled water: pH 7 3.2 g/L at 20°C	Flask method	Y	Wiche, A., Bogdoll, B.; 2011; M-409513-01-1
IIA 2.7 Solubility in organic solvents at 15 to 25°C						
IIA 2.7 Solubility in organic solvents at 15 to 25°C	EC A.6, OECD 105 OPPTS 830.7840	BYI 02960, pure NLL 7780-47-4 purity 99.4 % w/w	[g/L at 20 °C] methanol > 250 n-heptane 0.0005 toluene 3.7 dichloromethane > 250 acetone > 250 ethylacetate > 250 dimethyl sulfoxide > 250		Y	Eyrich, U., Bogdoll, B.; 2011; M-414064-01-1



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Test or Study & Annex point	Guideline and method	Test material purity and specification	Findings	Comments	GLP Y/N	Reference
IIA 2.8 Partition coefficient						
IIA 2.8.1 n-Octanol/water partition coefficient	EC A.8, OECD 117 OPPTS 830.7570 (HPLC-method)	BYI 02960, pure NLL 7780-47-4 purity 99.4 % w/w	Determination of the partition coefficient of Flupyradifurone in 1-octanol / water (25 °C) Pow log Pow pH 7 16 1.2		Y	Bogdoll, B.; Stunk, B.; 2011; M-414485-01-1
IIA 2.8.2 Effect of pH (4 to 10) on the n-octanol/ water partition coefficient		BYI 02960, pure NLL 7780-47-4 purity 99.4 % w/w	The partition coefficient (1-octanol / water) of Flupyradifurone at different pH-values and at 25 °C was: Pow log Pow pH 4 16 1.2 pH 7 16 1.2 pH 9 16 1.2		Y	Bogdoll, B.; Stunk, B.; 2011; M-414485-01-1
IIA 2.9 Hydrolysis and photolysis						
IIA 2.9.1 Hydrolysis rate at pH 4, 7 and 9 under sterile and dark conditions	US EPA Subdiv N, Sec. 161-1 CAN PMRA, DACO 8.2.3.2 OECD 111	[Furanone-4- ¹⁴ C] BYI 02960, pure Vial No. C-1116 Radiochemical purity 99%	BYI 02960 is hydrolytically stable at ambient temperature in the range of pH 4 to pH9.	3 minor components were observed during 5 days at 50°C which accounted for a total of 4.9%, none were more than 2.7% of the applied activity in any of the pH	Y	Mislankar, S.; Woodard, D., 2011 M-398952-01-1



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Test or Study & Annex point	Guideline and method	Test material purity and specification	Findings	Comments	GLP Y/N	Reference
IIA 2.9.2 Direct phototransformation in sterile water using artificial light	OPPTS 835.2240 CAN PMRA, DACO 8.3.3.2 EU Com. Dir. 94/37/EC EU Com.Dir. 95/36/EC	[Furanone-4- ¹⁴ C] BYI 02960, pure Vial No. C-1116A Radiochemical purity 99.3%	1 st order half-life for photolytic degradation of BYI 02960 in sterile phosphate buffer (pH 7) was 13.8 experimental hrs.	Based on this experimental half-life, the half-life of BYI 02960 under environmental conditions is calculated to be 1.75 days in Phoenix, AZ (latitude 33.3°N). Therefore, based on the results of this study, BYI 02960 should rapidly degrade by aqueous photolysis in the environment.	Y	Hall, L.R., 2011 M-418426-01-1
IIA 2.9.3 Quantum yield of direct phototransformation	Test Method: ECETOC (Polychromatic Light Source); EU: 91/414/EEC Amended by 94/37/EC and 95/36/EC	BYI 02960, pure NLL 7780-47-4 purity 99.4 % w/w	A mean quantum yield of $\Phi = 0.000138$ was calculated on the basis of UV absorption data and the degradation kinetics determined from 2 degradation experiments.	Environmental half-lives of sunlight exposed top surface water layers containing BYI 02960 can be estimated using respective models (GC SOLAR or Klopffer Model) dependent on season and location of exposure.	Y	Heinemann, O. 2011 M-414756-01-2
IIA 2.9.4 Lifetime in the top layer of aqueous systems (calculated and real)	ECETOC, OPPTS 835.2240 DACO 8.2.3.3.2 GC SOLAR or Klopffer Model	[Furanone-4- ¹⁴ C] BYI 02960, pure Vial No. C-1116A Radiochemical purity 99.3% BYI 02960, pure NLL 7780-47-4 purity 99.4 % w/w	This point is covered by point IIA 2.9.2/3 and in more detail by point IIA 7.6.		Y -	Hall, L.R., 2011 M-418426-01-2 Heinemann, O. 2011 M-414756-01-1
IIA 2.9.5 Dissociation in water of purified active substance	OECD 112 OPPTS 830.7370	BYI 02960, pure NLL 7780-47-4 purity 99.4 % w/w	No dissociation occurs in aqueous solutions in the pH-range 1 < pH < 12		Y	Wiche, A., Bogdoll, B.; 2011; M-414102-01-1



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Test or Study & Annex point	Guideline and method	Test material purity and specification	Findings	Comments	GLP Y/N	Reference
IIA 2.10 Estimated photochemical oxidative degradation						
IIA 2.10 Estimated photochemical oxidative degradation	Calculation according to Atkinson by AOPWIN™, version 1.92a (U.S. EPA, 2008)		The half-life time ($t_{1/2}$) was estimated within a range of 4.4 hours (short-term scenario) to 13.1 hours (long-term scenario), depending on the mean concentration of hydroxyl radicals present in the troposphere. In addition, BYI 02960 is susceptible to reactions with ozone, however, that attack and its resulting chemical half-life is considered to be more slowly by a factor of 2 to 10. As a consequence of the short half-life in air, no long-range transport of BYI 02960 in the atmosphere is likely to occur nor an accumulation of BYI02960 in the environmental compartment air.		-	Hellpointner, E.; 2010 M-398741-01-2
IIA 2.11 Flammability including auto-flammability						
IIA 2.11.1 Flammability of the active substance as manufactured	EC A.10	BYI 02960, technical PFV107N004 purity 97.6 % w/w	Technical substance is not a highly flammable solid in the sense of the EC guideline (EC) No. 440/2008, Method A.10		Y	Smeykal, H.;2011; M-414249-01-1



Test or Study & Annex point	Guideline and method	Test material purity and specification	Findings	Comments	GLP Y/N	Reference
IIA 2.11.2 Auto-flammability of the active substance as manufactured	EC A.16	BYI 02960, technical PFV107N004 purity 97.6 % w/w	No self-ignition temperature was observed up to the maximum test temperature of 401 °C.		Y	Smeykal, H.; 2011; M-414252-01-1
	BCC-Test (UN-Test N.4)		Flupyradifurone has not to be classified as a self-heating substance in Division 4.2 according to the UN transport regulations.		Y	Smeykal, H.; 2011; M-414257-01-1
IIA 2.12 Flash point of the active substance as manufactured						
IIA 2.12 Flash point of the active substance as manufactured				Not applicable. The active substance as manufactured is a solid; its melting point is > 40 °C.		
IIA 2.13 Explosive properties of the active substance as manufactured						
IIA 2.13 Explosive properties of the active substance as manufactured	EC A.14 OECD 113 OPPTS 830.6316	BYI 02960, technical PFV107N004 purity 97.6 % w/w	Not explosive in the sense of EC guideline A.14 and in the sense of the EPA Product Properties Test Guideline OPPTS 830.6316.		Y	Smeykal, H.; 2011; M-414250-01-1
IIA 2.14 Surface tension of the active substance as manufactured						

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Test or Study & Annex point	Guideline and method	Test material purity and specification	Findings	Comments	GLP Y/N	Reference
IIA 2.17.1 Storage stability	OPPTS 830.6317	BYI 02960, technical 2009-000239 purity 96.6% PFV087N002 purity 98.7% PFV087N007 purity 98.6%	The results from 24 months stability study at ambient temperature (22.1°C) and 30°C showed Flupyradifurone to be stable in polypropylene and polyethylene containers. Even at elevated temperature no decomposition of the test substance and the storage vessels could be established.	Not required by Regulation 1107/2009	Y	Wagner, S.; 2011; M-411305-01-1
IIA 2.17.2 Stability (temperature, metals)	OPPTS 830.6313 and OPPTS 830.6320		The results from a two weeks 54°C stability study showed Flupyradifurone (BYI 02960) to be stable in presence of the metals and metal ions. After completion of the accelerated storage test no decomposition of the test substance could be established. In the presence of metals (iron and aluminum) changes in color during the test period could not be observed. In the 2 weeks/54°C accelerated corrosion characteristics study to plastic containers, Flupyradifurone (BYI 02960) did not cause corrosion to the container materials polypropylene and polyethylene.	Not required by Regulation 1107/2009.	Y	Wagner, S.; 2011; M-413798-01-1
IIA 2.18	Other/special studies					



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Test or Study & Annex point	Guideline and method	Test material purity and specification	Findings	Comments	GLP Y/N	Reference
IIA 2.18 Other/special studies						
Oxidation or reduction properties	OPPTS 830.6314	BYI 02960, technical PFV107N004 purity 97.6 % w/w	Technical Flupyradifurone (BYI 02960) was found to be non-reactive at room temperature with ammonium dihydrogen phosphate, metallic iron or aqueous solution of 0.1 N potassium permanganate in terms of significant temperature increase or evolution of gas. No significant temperature increase was observed for all applied test mixtures, i.e. the temperature increase was clearly below 5°C in the course of the experiments. No evolution of gas was observed for all applied test mixtures.		Y	Eyrich, U., Bogdoll, B.; 2011; M-414080-01-1
Complex Formation Ability in Water	OECD 108	BYI 02960, technical PFV107N004 purity 97.6 % w/w	Flupyradifurone had a weak complex forming ability for cobalt compared to EDTA and no measurable complex forming ability for cadmium, copper, chromium, lead and zinc ions.		Y	Petrovic, P.; 2011; M-414563-01-1
Particle size, fiber length and diameter distribution	OPPTS 830.7520 OECD 110 CIPAC MT 187 ISO13320-1	BYI 02960, technical PFV107N004 purity 97.6 % w/w	Median particle size 24.7 µm L ₁₀ = 5.1 µm L ₉₀ = 170.3 µm		Y	Smeykal, H.; 2011; M-414246-01-1



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Test or Study & Annex point	Guideline and method	Test material purity and specification	Findings	Comments	GLP Y/N	Reference
IIA 2.18 Other/special studies (continued) Viscosity	OPPTS 830.7100	Statement	The experimental test of the viscosity is not applicable because - the test of the viscosity is applicable to fluids only. - the technical grade active substance of Flupyradifurone is a powder.		N	Ziemer, F.; 2011; M-417799-01-1
Miscibility	OPPTS 830.6319	Statement	The experimental test of the miscibility is not applicable for the following reasons: - the test of the miscibility is applicable to emulsifiable fluids only. - The technical grade active substance of Flupyradifurone is a powder at room temperature.		N	Ziemer, F.; 2011; M-417793-01-1
Dielectric breakdown voltage	OPPTS 830.6321	Statement	The experimental test of the dielectric breakdown voltage is not applicable because - the test of the dielectric breakdown voltage is applicable to liquids only. - the technical grade active substance of Flupyradifurone is a powder at room temperature.		N	Ziemer, F.; 2011; M-417802-01-1
Metallic impurities		BYI 02960, technical PFV107N003 purity 98.9 % w/w	Metallic impurities Cd, Pb, Hg were determined with <0.05 mg/kg. The content of Cr is 0.21 mg/kg, the content of As is 0.15 mg/kg		Y	Schloesser, G.; Mans, H. C.; 2011; M-412025-01-1

**IIA 2.19 Summary and evaluation of points 2.1 to 2.18**

Flupyradifurone is an insecticide. Its vapour pressure and volatility are very low. The solubility in water is about 3.2 g/L at a range of pH between 4 and 9. With a log Pow of 1.2 it has no bioaccumulative potential in lipophilic matrices. Flupyradifurone is hydrolytically stable under acidic, neutral and under alkaline conditions at ambient temperature. The hydrolytic degradation is negligible under acidic, neutral and alkaline conditions. Flupyradifurone is rather susceptible for reactions with hydroxyl radicals with photochemical degradation process to contribute significantly to the overall degradation of the substance in case of its occurrence in the atmosphere.

Its flammability, explosive and oxidizing properties are not critical