Document Title

Document N – List of End Points of the Active Substance Flupyradifurone (BYI 02960)

Data Requirements

According to OECD format guidance for industry data submissions on plant protection products and their active substances Revision 2 May 2005 Document N

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OWNERSHIP STATEMENT

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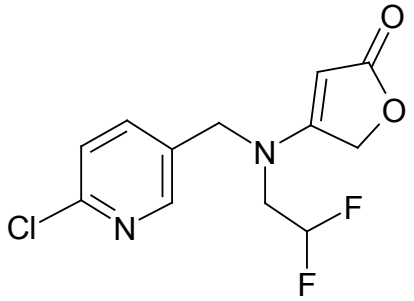
List of end points for the active substance BYI 02960 (Flupyradifurone) & its product Flupyradifurone SL 200

Chapter 1: Identity, physical and chemical properties, details of uses, further information, and proposed classification and labelling

Active substance (ISO Common Name)	Flupyradifurone
Function (*e.g.* fungicide)	Insecticide
Rapporteur Member State	Netherlands

Identity (OECD data point IIA 1)

Chemical name (IUPAC)	4-[(6-chloro-3-pyridylméthyl)(2,2-difluoroéthyl)amino]furan-2(5H)-one
Chemical name (CA)	2(5H)-furanone, 4-[[(6-chloro-3-pyridinyl)methyl](2,2-difluoroethyl)amino]-
CIPAC No	not available
CAS No	951659-40-8
EEC No (EINECS or ELINCS)	not available
FAO Specification (including year of publication)	not available
Minimum purity of the active substance as manufactured (g/kg)	960 g/kg
Identity of relevant impurities (of toxicological, environmental and/or other significance) in the active substance as manufactured (g/kg)	There are no relevant impurities
Molecular formula	$C_{12}H_{10}ClF_2N_2O_2$
Molecular mass	288.68 g/mol
Structural formula	

Physical-chemical properties (OECD data point IIA 2)

Melting point (state purity)	69.0 °C (purity 99.4%)
Boiling point (state purity)	No boiling point, test item decomposes at a temperature of 270°C (purity 99.4%)
Temperature of decomposition	Exothermal decomposition in the range 270 – 355°C (purity 99.4%)
Appearance (state purity)	White powder (purity 99.4%)
Relative density (state purity)	D=1.43 (purity 99.4%)
Surface tension	69.1 mN/m (20°C)
Vapour pressure (in Pa, state temperature)	1.7 x 10^{-6} Pa (25°C)
Henry's law constant (Pa m^3 mol^{-1})	8.2 x 10^{-8} Pa m^3 mol^{-1}
Solubility in water (g/l or mg/l, state temperature)	pH 4: 3.2 g/L at 20°C pH 7: 3.2 g/L at 20°C pH 9: 3.0 g/L at 20°C
Solubility in organic solvents (in g/l or mg/l, State temperature)	[g/L at 20 °C] methanol > 250 n-heptane 0.0005 toluene 3.7 dichloromethane > 250 acetone > 250 ethylacetate > 250 dimethyl sulfoxide > 250
Partition co-efficient (log P_{OW}) (state pH and temperature)	pH 4: log P_{OW} = 1.2 at 25°C pH 7: log P_{OW} = 1.2 at 25°C pH 9: log P_{OW} = 1.2 at 25°C
Hydrolytic stability (DT_{50}) (state pH and temperature)	pH 5: stable at 20°C
	pH 7: stable at 20°C
	pH 9: stable at 20°C
Dissociation constant	No dissociation occurs in aqueous solutions in the pH-range 1< pH <12
UV/VIS absorption (max.) (if absorption > 290 nm state ε at wavelength)	Peak maxima [nm] / molar absorptivity [1000 cm^2/mol] 213 / 9615.06 259 / 25800.49 No peak maxima above 290 nm, however, absorption extends at greater 290nm
Photostability (DT_{50}) (aqueous, sunlight, state pH)	SFO DT_{50} in sterile phosphate buffer (pH 7) = 13.8 experimental hrs. BYI 02960 should rapidly degrade by photolysis in top water layers exposed to sunlight, e. g. the DT50 under environmental conditions is calculated to be 1.75 days in Phoenix, AZ (latitude 33.3°N).
Quantum yield of direct phototransformation in water at λ > 290 nm	Φ = 0.000138 (mean, n = 2)
Flammability	Substance is not a highly flammable solid
Explosive properties	Not explosive

Safe GAPs (uses) in European Union

Crop and/ or situation (a)	Coun-try	Product Name	F G or I (b)	Pests or Group of pests controlled (c)	Formulation		Application				Application rate per treatment			PHI (days) (l)	Remarks: (m)
					Type (d-f)	Conc. of as (i)	method kind (f-h)	growth stage & season (j)	number min max (k)	interval between applications (min)	kg as/hL min max	water L/ha min max	kg as/ha min max		
Crop Protection Uses															
Hops	N-EU	Sivanto	F	aphids	SL	200	spray	31-75	1	n.a.	0.0045-0.0075	2000-3300	0.150	21	
Lettuce	N-EU (S-EU)	Sivanto	F	aphids	SL	200	spray	12-49	1	n.a.	0.0125-0.0250	500-1000	0.125	10	
Lettuce	n.a.	Sivanto	G	aphids	SL	200	spray	12-49	2	10	0.0125-0.0250	500-1000	0.125	3	
Environmental Science Uses (Home & Garden Uses) to be submitted in 2012															
Lettuce	N-EU S-EU	Sivanto	F	aphids	SL	050	spray	12-49	2	10	0.0125-0.0250	500-1000	0.125	3	Treatment of only a small area of the garden

Remarks:

- **(a)** For crops, the EU and Codex classifications (both) should be used; where relevant, the use situation should be described (*e.g.* fumigation of a structure)
- **(b)** Outdoor or field use (F), glasshouse application (G) or indoor application (I)
- **(c)** *e.g.* biting and suckling insects, soil born insects, foliar fungi, weeds
- **(d)** *e.g.* wettable powder (WP), emulsifiable concentrate (EC), granule (GR)
- **(e)** GCPF Codes - GIFAP Technical Monograph No 2, 1989
- **(f)** All abbreviations used must be explained
- **(g)** Method, *e.g.* high volume spraying, low volume spraying, spreading, dusting, drench
- **(h)** Kind, *e.g.* overall, broadcast, aerial spraying, row, individual plant, between the plants - type of equipment used must be indicated
- **(i)** g/kg or g/l
- **(j)** Growth stage at last treatment (BBCH Monograph, Growth Stages of Plants, 1997, Blackwell, ISBN 3-8263-3152-4), including where relevant, information on season at time of application
- **(k)** Indicate the minimum and maximum number of application possible under practical conditions of use must be provided
- **(l)** PHI - minimum pre-harvest interval
- **(m)** Remarks may include: Extent of use/economic importance/restrictions

Classification and proposed labelling (OECD data point IIA 10)

with respect to physical/chemical data

Classification:	none
Proposed label:	none
Symbol:	none
Indication of danger:	none
Risk phrases:	none
Safety phrases:	none

with respect to toxicological data

Classification:	Harmful
Proposed label:	See Doc. C
Symbol:	Xn
Indication of danger:	Harmful if swallowed
Risk phrases:	R 22
Safety phrases:	none

with respect to fate and behaviour data

Classification:	none
Proposed label:	none
Symbol:	none
Indication of danger:	none
Risk phrases:	none
Safety phrases:	none

with respect to ecotoxicological data

Classification:	Dangerous to the environment
Proposed label:	See Doc. C
Symbol:	N
Indication of danger:	Very toxic to aquatic organisms, may cause long-term adverse effect in the aquatic environment
Risk phrases:	R 50/53
Safety phrases:	S 60, S 61

Chapter 2: Methods of analysis

Analytical methods for the active substance (OECD data point IIA 4.2)

Technical as (principle of method)	HPLC-UV
Impurities in technical as (principle of method)	HPLC-DAD (diode array detector)
Plant protection product (principle of method)	HPLC-UV

Analytical methods for residues (OECD data points IIA 4.3 to IIA 4.8)

Food/feed of plant origin (principle of method and LOQ for methods for monitoring purposes)	HPLC-MS/MS: 0.01 mg/kg (BYI 02960) & 0.02 mg/kg (DFA); except for hops hops: 0.1 mg/kg (BYI 02960) & 0.2 mg/kg (DFA)
Food/feed of animal origin (principle of method and LOQ for methods for monitoring purposes)	HPLC-MS/MS: 0.01 mg/kg (BYI 02960) & 0.02 mg/kg (DFA)
Soil (principle of method and LOQ)	HPLC-MS/MS: 5 µg/kg
Water (principle of method and LOQ)	HPLC-MS/MS: 0.05 µg/L
Air (principle of method and LOQ)	HPLC-MS/MS: 7 µg/m
Body fluids and tissues (principle of method and LOQ)	not applicable

Chapter 3: Impact on human and animal health

Absorption, distribution, excretion and metabolism in mammals (OECD data point IIA 5.1)

Rate and extent of absorption	The gastrointestinal absorption of radioactivity was high and fast. It accounted for >80 % of the dose independent of the labelling position used.
Distribution	The maximum plasma concentration was reached in most cases within 1 or 2 hours after administration of low doses. Only after administration of the high dose the peak plasma concentration was observed between 2 an 4 hours after dosage. After reaching the peak concentration, the radioactivity levels in plasma declined steadily by several orders of magnitude in all studies independent of sex or labelling position of the test compound.
Potential for accumulation	There is no indication of any accumulation or significant retention of radioactivity in male and female rats. This observation is supported by the low Pow of 1.2. Concentrations of radioactivity detected in tissues and organs at sacrifice were either very low or below the limit of detection.
Rate and extent of excretion	Excretion was very fast, mainly renal and almost completed after 24 h. No radioactivity was detected in the expired air after dosing of the pyridinylmethyl- and ethyl-1-labelled compounds, proving the stability of these labelling positions in the molecule. Only after administration of [furanone-4-^{14}C]BYI 02960 between 1 and 3% of the administered radioactivity was exhaled. This demonstrated that for a small portion of the dose (higher in males than in females) the furanone ring of the molecule obviously was opened and underwent biotransformation to C-1 fragments.
Metabolism in animals	BYI 02960 was rather moderately metabolised in the rat. The parent compound represented the predominant part of the radioactivity in urine of male and female rats. The principal metabolic reactions of BYI 02960 in rats were: • hydroxylation followed by conjugation with glucuronic acid or sulfate, • cleavage of the difluoroethyl group forming BYI 02960-des-difluoroethyl, and difluoroacetic acid (DFA), • cleavage of the molecule at the pyridinylmethylene bridge forming 6-CNA, which was further conjugated with glycine to BYI 02960-hippuric acid and BYI 02960-difluoroethyl-amino-furanone. These main metabolic reactions were also observed in the livestock metabolism studies, however conjugation reactions and cleavage of the molecule (leading to metabolites of less toxicological concern) were more pronounced in livestock.
Toxicologically significant compounds (animals, plants and environment)	The main metabolic reactions observed in plants and livestock were also observed in the rat. Metabolites BYI 02960-difluoroethyl-aminofuranone, DFA, 6-

	CNA and BYI 02960-CHMP were additionally addressed by toxicological tests, which showed no concern. For plant and animal matrices, all metabolites were either covered by the toxicological endpoints derived for parent compound, or showed no consumer exposure or a consumer exposure below the threshold of toxicological concern (1.5 µg/kg bw). All metabolites present in the environment were minor and well below 5% of the applied radioactivity, except for DFA and 6-CNA. Both metabolites were covered by findings in the rat (< 10% of the dose administered) and by additional toxicological tests which showed no toxicological concern.

Acute toxicity (OECD data point IIA 5.2)

Rat LD_{50} oral	Category 4 (LD_{50} cut off = 2000 mg/kg)
Rat LD_{50} dermal	Category 5 / Unclassified LD_{50} > 2 000 mg/kg,
Rat LC_{50} inhalation	LC50 at 4 hours > 4671 mg/m3, Category 5 / Unclassified
Skin irritation	Non irritating, Category 5 / Unclassified
Eye irritation	Slight redness of the conjunctivae, reversed within 48 hours Category 5 / Unclassified
Skin sensitization (test method used and result)	Not sensitising, Category 5 / Unclassified

Short term toxicity (OECD data point IIA 5.3)

Target / critical effect	Liver effects in rodents and dogs, thyroid effects in rats, kidney effects in mice and dogs and degeneration of myofibers in skeletal muscles in dogs
Lowest relevant oral NOAEL / NOEL	12 mg/kg/day (90-day dog study)
Lowest relevant dermal NOAEL / NOEL	28-day dermal study ongoing for registration in Canada
Lowest relevant inhalation NOAEL / NOEL	Not required

Genotoxicity (OECD data point IIA 5.4)

Ames (*S. typh.*)	negative
HGPRT (CHO)	negative
CA (CHL)	negative
CA (human lymphocytes)	Not required
Mouse micronucleus	negative

Long term toxicity and carcinogenicity (OECD data point number IIA 5.5)

Target/critical effect	Liver in both species, thyroid and lung in rats and kidney in mice
Lowest relevant NOAEL / NOEL	15.8 mg/kg/day (2-year rat carcinogenicity)
Carcinogenicity	Not carcinogenic in both rats (> 80 mg/kg/day) and mice (>224 mg/kg/day)

Reproductive toxicity (OECD data point IIA 5.6)

Reproduction target / critical effect	Decreased cycle number, litter size and number of implants in F1 generation at the high dose; organ weight effects in P generation males, Decreased body weight or body weight gain in females at the intermediate and high doses, decreased body weight in F2 pups at the intermediate and high doses
Lowest relevant reproductive NOAEL / NOEL	7.8 mg/kg/day
Developmental target / critical effect	No teratogenicity in rats and rabbits. Decreased body weight or body weight gain in dams, decreased foetal weights and reduced ossification in a few skull bones in rat pups
Lowest relevant developmental NOAEL / NOEL	30 mg/kg/day (developmental toxicity in rats)

Neurotoxicity / delayed neurotoxicity (OECD data point IIA 5.7)

Acute neurotoxicity	Piloerection and dilated pupils -At high dose levels: lower muscle tone, rapid respiration, gait incoordination, tremors, reduced motor activity, impaired righting reflex, impaired flexor and tail pinch responses: NO(A)EL: 35 mg/kg, (m/f), LOAEL: 50 mg/kg (m/f)
Subchronic neurotoxicity	No adverse effects, NO(A)EL: 143/173 mg/kg (m/f), LOAEL: >143/173 mg/kg (m/f)

Other toxicological studies (OECD data points IIA 5.8 and IIA 5.10)

Toxicity on metabolites (IIA 5.8)	*In vitro* genotoxicity studies and subchronic studies performed on three metabolites: Difluoroacetic acid, BYI 02960-difluoroethylamino-furanone, BYI 02960-CHMP, showing no genotoxic potential and general toxicological profile less toxic than parent or similar to parent. An Ames test and an acute oral rat was also performed on BYI 02960-6CNA showing no toxicological issues.
Immunotoxicity (IIA 5.10)	No immunotoxicity in rats NOAEL immunotoxicity = 230 mg/kg/day NOAEL systemic toxicity = 50 mg/kg/day

Medical data (OECD data point IIA 5.9)

Limited as this is a new active ingredient

Summary (OECD data point IIA 5.11)

	Value	Study	Safety factor
ADI	0.078 mg kg/day	NOAEL of the rat 2-generation study	100
AOEL	0.12 mg	NOAEL of the 90-day dog study	100
Drinking water limit	0.234 mg/L	NOAEL of the rat 2-generation study	10% ADI
ARfD (acute reference dose)	0.35 mg/kg	NOAEL of the acute neurotox study	100

Dermal absorption (OECD data points IIA 5.9.9 and IIIA 7.6)

In vivo + in vitro dermal absorption studies	Human in vivo absorption values: 22% at 200 g/L 3% at 0.625 g/L 15% at 0.1 g/L

Acceptable exposure scenarios (including method of calculation)

Operator	<u>Field crop application (0.125 kg a.s./ha):</u> German Model: no PPE – 18% of the AOEL with PPE – <1% of the AOEL UK-POEM: no PPE – 65% of the AOEL with PPE – 6% of the AOEL <u>Broadcast air assisted application (0.150 kg a.s./ha):</u> German Model: no PPE – 13% of the AOEL with PPE – 4% of the AOEL UK-POEM: no PPE – 38% of the AOEL with PPE – 15% of the AOEL <u>Greenhouse application (0.125 kg a.s./ha):</u> Greenhouse Model (low crops) standard scenario: no PPE – 3% of the AOEL with PPE - <1% of the AOEL intensive scenario: no PPE – 77% of the AOEL with PPE – 3% of the AOEL
Workers	Exposure estimates for workers (considering worst case assumptions according to EUROPOEM) indicate that levels of exposure will be in maximum at 55% of the AOEL without PPE.
Bystanders	<u>Field crop application (German Model):</u> Bystanders <1% of AOEL (including children) Residents <1% of AOEL (including children) <u>Broadcast air assisted application (German Model):</u> Bystanders max. 3% of AOEL (including children) Residents <1% of AOEL (including children) <u>Greenhouse application:</u> No bystander/resident scenario for applications in greenhouses

Chapter 4: Residues

Metabolism in plants (OECD data point s IIA 6.2.1, IIA 6.7, IIIA 8.2 and IIIA 8.7)

Plant groups covered	Fruits: Pome fruit (apple), F Vegetables: Fruiting vegetables (tomato), F Vegetables: Root and tuber vegetables (potato), R Oilseeds: (cotton), P/O Rice/Cereals (rice), C
Rotational crops	Vegetables: Leaf vegetables (Swiss chard), L Vegetables: Root and tuber vegetables (turnips), R Cereals (spring wheat), C
Plant residue definition for monitoring	**Target and rotational crops:** BYI 02960, DFA
Plant residue definition for risk assessment	**Target and rotational crops:** BYI 02960 (parent), DFA, BYI 02960-difluoroethyl-aminofuranone
Conversion factor (monitoring to risk assessment)	1 (no conversion factor defined)

Metabolism in livestock (OECD data points IIA 6.2.2 to IIA 6.2.5, IIA 6.7, IIIA 8.4 and IIIA 8.7)

Animals covered	Poultry (laying hen) Ruminants (lactating goat)
Animal residue definition for monitoring	BYI 02960 (parent), DFA
Animal residue definition for risk assessment	BYI 02960 (parent), DFA
Conversion factor (monitoring to risk assessment)	1
Metabolism in rat and ruminant similar (yes/no)	Yes
Fat soluble residue: (yes/no)	No

Residues in succeeding crops (OECD data points IIA 6.6 and IIIA 8.6)

Confined rotation crop studies conducted with radiolabelled parent compound indicated that edible commodities of succeeding crops will show BYI 02960 residues above 0.01 mg/kg. In the field rotational crop studies, the highest residues were generally found in the first rotation, i.e. after the shortest plant-back interval of 25-30 days. Total BYI 02960 residues (sum of BYI 02960, DFA and DFEAF) were detected in marketable crops: - root crops (carrots and turnips): up to 0.14 mg/kg - turnip tops: up to 0.24 mg/kg - leafy crops (lettuce): up to 0.16 mg/kg - cereal grains (barley): up to 0.65 mg/kg - cereal straw (barley): up to 0.39 mg/kg - cereal forage (barley): up to 0.41 mg/kg Based on these results, MRLs for crops originating from crop rotation are proposed for leafy and root vegetables and cereals.

Stability of residues (OECD data points IIA 6.1 and IIIA 8.1)

During a storage period of 12 months under deep-freezer conditions, the components of the relevant residues of BYI 02960 (including parent compound, BYI 02960-difluoroethyl-aminofuranone, and DFA) were stable in orange fruit (high acid content), spinach leaves and tomato fruit (high water content), wheat grain (high starch content), bean seed (high protein content), coffee bean and soybean seed (high oil content), and sugar cane, representing a wide array of plant-based sample materials. The storage stability study will be continued until a storage period of 2 years has been covered.

Residues from livestock feeding studies (OECD data points IIA 6.4 and IIIA 8.4)

Intakes by livestock ≥ 0.1 mg/kg diet/day:	**Ruminant: yes** (4.8 mg/kg feed)	**Poultry: yes** (1.5 mg/kg feed)	**Pig: no**
Muscle	0.065 mg/kg[1] 0.045 mg/kg (1) <0.020 mg/kg (2)	0.093 mg/kg[1] <0.010 mg/kg (1) 0.083 mg/kg (2)	
Liver	0.174 mg/kg[1] 0.154 mg/kg (1) <0.020 mg/kg (2)	0.114 mg/kg[1] <0.01 mg/kg (1) 0.104 mg/kg (2)	
Kidney	0.179 mg/kg[1] 0.159 mg/kg (1) <0.020 mg/kg (2)		
Fat	0.042 mg/kg[1] 0.022 mg/kg (1) <0.020 mg/kg (2)	0.039 mg/kg[1] <0.010mg/kg (1) 0.029 mg/kg (2)	
Milk	0.045 mg/kg[1] 0.025 mg/kg (1) <0.020 mg/kg (2)		
Eggs		0.057 mg/kg[1] <0.010 mg/kg (1) 0.047 mg/kg (2	

[1] total residue of BYI 02960, consisting of BYI 02960 (1) and DFA (2)

Summary of critical residues data (OECD data points IIA 6.3 and IIIA 8.3)

Crop	Country and / or Region	Trials results relevant to the critical GAP (a)	Recommendation/comments	MRL	STMR (b)
Lettuce	greenhouse	0.80; 1.4; 1.8; 2.0; 2.2; 2.5; 2.7; 3.5; 6.0		9.0	2.2
Hops (dried cone)	EU-N	0.61; 0.73; 0.78; 1.1; 1.2; 1.6; 2.3; 2.4		4.0	1.2
Leafy vegetables (crop rotation)	EU	<0.04; 0.07; 0.09; 0.16		0.3	0.08
Root vegetables (crop rotation)	EU	0.06; 0.07; 0.08; 0.14		0.3	0.08
Cereals (crop rotation)	EU	0.11; 0.35; 0.65	In one trial, no grain samples could be taken due to damage by geese. Based on the data from straw, it is clear that the missing trial would have yielded residues well below the highest residues and probably below the current median.	1.5	0.23

(a) Numbers of trials in which particular residue levels were reported *e.g.* 3 x <0.01, 1 x 0.01, 6 x 0.02, 1 x 0.04, 1 x 0.08, 2 x 0.1, 2 x 0.15, 1 x 0.17
(b) Supervised Trials Median Residue *i.e.* the median residue level estimated on the basis of supervised trials relating to the critical GAP

Consumer risk assessment (OECD data points IIA 6.9 and IIIA 8.10)

ADI	0.078 mg/kg bw/day	
TMDI (European Diet) (% ADI)	**TMDI (% ADI)**	**Diet**
Top ten ADI usage results including top contributors	29.4	WHO Cluster diet B
	23.8	DK child
	20.3	IT children/toddlers
	18.8	NL child
	18.0	WHO cluster diet D
	16.9	ES child
	16.6	IE adult
	15.4	WHO cluster diet E
	15.4	DE child
	15.3	WHO cluster diet F
NEDI (% ADI) **Factors included in NEDI**	Not necessary since TMDI calculation for BYI 02960 shows that residues at the level of the proposed MRLs do not result in a chronic risk to the consumer.	
ARfD	0.35 mg/kg bw	
	IESTI 1 (%ARfD)	**Commoditiy**
	CHILDREN	
	53.8	lettuce
	7.5	broad-leaf endive (scarole)
	6.2	wheat
	6.2	rocket (rucola)
	5.6	lamb's lettuce
	ADULTS (GEN. POPULATION)	
	22.0	lettuce
	3.8	lamb's lettuce
	3.4	wheat
	3.2	rice
	3.1	barley
	IESTI 2 (%ARfD)	**Commoditiy**
	CHILDREN	
	32.3	lettuce
	7.5	broad-leaf endive (scarole)
	6.2	wheat
	6.2	rocket (rucola)
	5.6	lamb's lettuce
	ADULTS (GEN. POPULATION)	
	13.2	lettuce
	3.8	lamb's lettuce
	3.4	wheat
	3.2	rice
	3.1	barley

It should be noted that the use in lettuce does not include broad-leafed endive; use in "scarole" will not be registered in the EU and thus will not appear on any label. Its appearance in the list above is due to the proposed MRL for rotational leafy vegetables. Despite using the most conservative approach for the assessment of the acute risk (based on MRLs instead of HRs), it is evident that no acute risk for consumers will arise from the uses of BYI 02960 as presented in this dossier.

Processing factors (OECD data points IIA 6.5 and IIIA 8.5)

Crop/processed crop	Number of studies	Transfer factor	% Transference
Lettuce	4		
Lettuce/outer leaves		1.8	
Lettuce/inner head parts		0.73	
Lettuce/inner leaves		0.76	
Lettuce/washed inner leaves		0.67	
Lettuce/washing water		0.07	
Hops	2		
Hops/hops draff		<0.1	
Hops/brewer´s yeast		<0.1	
Hops/beer		0.1	

Proposed MRLs (OECD data point IIA 6.7.2 and IIIA 8.7.2)

Plant commodities	Proposed MRLs
Lettuce	9.0
Hops	4.0
Leafy vegetables (crop rotation)	0.30
Root vegetables (crop rotation)	0.30
Cereals (crop rotation)	1.5
Animal matrices	
eggs	0.15
poultry meat (muscle)	0.20
poultry fat	0.07
poultry liver/offal	0.30
milk	0.07
bovine meat (muscle)	0.20
bovine fat	0.15
bovine liver	0.30
bovine kidney	0.40
other bovine offal	0.40

Chapter 5: Fate and behaviour in the environment

Route of degradation (aerobic) in soil (OECD data point IIA 7.1.1)

Mineralization after 100 days	PYM label 29.4 to 58.6% after 120 days FUR label 12.3 to 32% after 120 days ETH label 25.9 to 33.9% after 120 days PYR label 20.2 to 47.4 after 120 days By linear extrapolation between sampling point PYM label 26.2 to 51.6 %after 100 days FUR label 10.5 to 35.4% after 100 days ETH label 22.9 to 26.6% after 100 days PYR label 18.1 to 54.3% after 100 days
Non-extractable residues after 100 days	PYM label 12.5 to 16.8% after 120 days FUR label 16.4to 33.0% after 120 days ETH label 14.3 to 17.9% after 120 days PYR label 11.37 to 25.5 after 120 days By linear extrapolation between sampling point PYM label 12.3 to 15.9 %after 100 days FUR label 15.0 to 33.1% after 100 days ETH label 14.6 to 17.6% after 100 days PYR label 10.7 to 24.0% after 100 days
Relevant metabolites*) - name and/or code, % of applied (range and maximum)	DFA maximum 33.9% 6-CNA maximum 17.1%

*) An internationally agreed definition of the term *relevant metabolites* has not been elaborated. Pending the development of such a definition, applicants should consult the regulatory authority of the country to which application is to be made, for guidance concerning selection of the metabolites for which information must be reported

Route of degradation in soil (anaerobic & photolysis) (OECD data points IIA 7.1.2 & IIA 7.1.3)

Anaerobic degradation	Following an aerobic ageing period BYF 02960 showed moderate degradation under anaerobic conditions of the test. No major transformation products were detected for any of the three labels used. Mineralisation and formation of NER during the anaerobic phase was low (< 5%) and there were no major metabolites formed
Soil photolysis	Following exposure to artificial sunlight BYI 02960 was moderately degraded with low formation of CO_2 (0.1 to 2.2%) and NER (0.9 to 1.1%). There were no major metabolites formed .

Rate of degradation in soil (OECD data points IIA 7.2, IIA 7.3, IIIA 9.1 and IIIA 9.2)

	FOCUS Kinetic	EU trigger end-points
Method of Calculation **Laboratory studies** **(range or median, with n value, with r^2 value)**	DT_{50lab} (20°C, aerobic):	BYI 02960 (n=16, 6 soils) 33.0 to 242 days (SFO or DFOP) GeoMean 73 days 6-CNA (n=5) 2.9 to 36.6 days (SFO or DFOP) GeoMean 5.3 days DFA (n=3) 44.9-73.6 days (SFO) GeoMean 60.6 days
	DT_{90lab} (20°C, aerobic):	BYI 02960 (n=16, 6 soils) 209.3-> 1000 days (SFO or DFOP 6-CNA (n=5) 7.4 to 121 days (SFO/DFOP) DFA (n=3) 149-244.5 days (SFO) GeoMean 201 days
	DT_{50lab} (10°C, aerobic):	BYI 02960 (n=16, 6 soils) 85-624 days by calculation (Q_{10}= 2.58)
	DT_{50lab} (20°C, anaerobic):	Not calculable due to moderate degradation
	degradation in the saturated zone:	Not investigated
Field studies **(state location, range or median with n value)**	DT_{50f}:	Trigger values (non-normalised) DFOP Monheim, DEU 41.0 days Burscheid, DEU 42.8 days UK, 251 days Italy 8.3 days Spain 22.6 days Hanschedier Hof, DE 39.0 days
	DT_{90f}:	Trigger values (non-normalised) DFOP Monheim, DEU 749 days Burscheid, DEU 484 days UK, >1000 days Italy 279 days Spain 215 days Hanschedier Hof, DEU 579 days

Soil accumulation and plateau concentration	BYI 02960 Accumulation calculated for applications in successive years assuming a fast-phase half-life of 0.02 days and a slow-phase half-life of 462 days (worst-case DFOP kinetics of field study non-normalised) Hops 1 x 150g/ha plateau = 0.080 mg/kg (5cm depth) Lettuce 1 x 125g/ha plateau = 0.031 mg/kg (20cm depth)

Soil adsorption/desorption (OECD data points IIA 7.4.1 and IIA 7.4.2)

K_f /K_{oc}	$K_{F,oc}$ BYI 02960 $K_{F,OC}$ 6-CNA $K_{f\,oc}$ DFA	74.9-132.2 mean 98.3 (n=6) 70-129 (n=4) 1.7 – 9.5 (n=5)
K_d	$K_{d,\,oc}$ BYI 02960 Time dependant sorption	138-306 (n=6) Significant increase in sorption over time (2.6 to 4.4 fold over 120 days)
pH dependence (yes / no) **(if yes type of dependence)**	No	

Mobility in soil (OECD data points IIA 7.4.3 to IIA 7.4.8 and IIIA 9.3)

Column leaching	Not required Low to moderate mobility in Brazilian soils
Aged residues leaching	Not required
Lysimeter/ field leaching studies	Not required

PEC (soil) (OECD data point IIIA 9.4)

Method of calculation	DFOP kinetics of worst-case field study
Application rate	1 x 150g/ha (application on hops, 60% crop interception) 1 x 125 g/ha (application on lettuce, 25% crop interception)

Use in hops
BYI 02960

$PEC_{(s)}$ (mg/kg)		**Single application Actual 1 x 150g/ha [mg/kg]**	**Single application Time weighted average [mg/kg]**
Initial		0.080	
Short term	**24h**	0.058	0.069
	2d	0.058	0.066
	4d	0.058	0.063
Long term	**7d**	0.058	0.061
	14d	0.057	0.059
	21d	0.057	0.058
	28d	0.056	0.058
	50d	0.054	0.057
	100d	0.050	0.054

PECsoil considering accumulation plateau

	Residues distributed over … [cm]	**Seasonal $PEC_{s,\,max}$, max. soil residue in 1st year [mg/kg]**	**Long-term plateau C_{min} [mg/kg]**	**Background C_{min} + max. of 1 year in 5 cm [mg/kg]**
Hops 1 x 150 g/ha	**5**	0.080	0.080	0.160

Metabolite DFA

Method of calculation	Max. SFO from parent laboratory studies (DT_{50} 73.6 days)
Application rate	33.9% formed in soil

$PEC_{(s)}$ (mg/kg)	**Single application Actual 1 x 125g/ha [mg/kg]**	**Single application Time weighted average [mg/kg]**
Initial	0.009	

Metabolite 6-CNA

Method of calculation	Max. SFO from laboratory studies (DT_{50} 36.6 days)
Application rate	17.1% formed in soil

$PEC_{(s)}$ (mg/kg)	**Single application Actual 1 x 125g/ha [mg/kg]**	**Single application Time weighted average [mg/kg]**
Initial	0.007	--

Use in lettuce
BYI 02960

$PEC_{(s)}$ (mg/kg)		**Single application Actual 1 x 150g/ha [mg/kg]**	**Single application Time weighted average [mg/kg]**
Initial		0.125	
Short term	**24h**	0.091	0.108
	2d	0.091	0.102
	4d	0.091	0.098
Long term	**7d**	0.090	0.095
	14d	0.089	0.093
	21d	0.088	0.091
	28d	0.087	0.091
	50d	0.085	0.089
	100d	0.079	0.085

PECsoil considering accumulation plateau

	Residues distributed over … [cm]	**Seasonal $PEC_{s,\ max}$, max. soil residue in 1st year** [mg/kg]	**Long-term plateau / background conc. C_{min}** [mg/kg]	**Background C_{min} + max. of 1 year in 5 cm** [mg/kg]
Lettuce 1 x 125g/ha	**20**	0.031	0.031	**0.156**

Metabolite DFA

Method of calculation	Max. SFO from parent laboratory studies (DT_{50} 73.6 days)
Application rate	33.9% formed in soil

$PEC_{(s)}$ (mg/kg)	**Single application Actual 1 x 125g/ha [mg/kg]**	**Single application Time weighted average [mg/kg]**
Initial	0.014	

Metabolite 6-CNA

Method of calculation	Max. SFO from laboratory studies (DT_{50} 36.6 days)
Application rate	17.1% formed in soil

Use in lettuce

$PEC_{(s)}$ (mg/kg)	**Single application Actual 1 x 125g/ha [mg/kg]**	**Single application Time weighted average [mg/kg]**
Initial	0.012	--

Route and rate of degradation in water (OECD data points IIA 2.9 and IIA 7.5 to IIA 7.9)

Hydrolysis of active substance and relevant metabolites*) (DT_{50}) (state pH and temperature)	pH 4: stable at 50°C
	pH 7: stable at 50°C
	pH 9: stable at 50°C
Photolytic degradation of active substance and relevant metabolites	BYI 02960 rapid degradation DT_{50} 13.8 experimental hours (equivalent to 2.7 days, Athens, Greece) BYI 02960-succinamide (max. 39.6 %), BYI 02960-azabicyclosuccinamide (max. 25.9 %)
Readily biodegradable (yes/no)	NO
Degradation in water/sediment - DT_{50} water **- DT_{90} water** **- DT_{50} whole system** **- DT_{90} whole system**	Best-fit trigger 8.5- 34.5 days FOMC/DFOP (n=6) Best-fit trigger 174.6 - 345 days FOMC/DFOP (n=6) Best-fit trigger 193.1 - 285days SFO/DFOP (n=6) Best-fit trigger 641 – 947 days SFO (n=6) Modelling input parameters DT_{50} water 8.5-117.5 days DT_{50} whole system 193 – 285 days
Mineralization	PYR label 6.8 – 8.5%, after 119 days (n=2) FUR label 3.9 – 5.5% after 120 days (n=2) ETH label 0.9 - 1.5 % after 120 days (n=2)
Non-extractable residues	PYR label 13.6 - 25% after 119 days (n=2) FUR label 22.6 – 17.9% after 120 days (n=2) ETH label 15.2 - 26.6 % after 120 days (n=2)
Distribution in water / sediment systems (active substance)	Water 11.4 – 36.8 % after 119/120 days (n=6) Sediment 37.6 – 54.3 % after 119/120 days (n=6)
Distribution in water / sediment systems (metabolites)[2])	DFA Water 6.0% after 120 days Sediment 0.9% after 120 days

*) An internationally agreed definition of the term *relevant metabolites* has not been elaborated. Pending the development of such a definition, applicants should consult the regulatory authority of the country to which application is to be made, for guidance concerning selection of the metabolites for which information must be reported

PEC (surface water) (OECD data points IIIA 9.7)

Application to Hops
BYI 02960

Method of calculation	**BYI 02960** FOCUS Surface Water Steps 1, 2, 3, 4 K_{oc}, 98.4 mL/g, (arithmetic mean) Freundlich Exponent, , 0.866 (arithmetic mean) Degradation, , Soil DT_{50}, 94.8 days, (GeoMean lab. Studies at 20°C and field capacity) Water/Sediment Total , DT_{50} 228 days, DT_{50} Water 228 days Sediment 1000 days(default)
Application rate	**1 x 150g/ha spray application to hops**
Main routes of entry	Spray drift

FOCUS Step 2

$PEC_{(sw)}$	**Single application Actual Maximum (S. Europe) µg/L**	**Single application Time weighted average µg/L**
Initial	17.36	
1	16.9727	17.1682
2	16.9212	17.0576
4	16.8186	16.9637
7	16.6659	16.8688
14	16.3150	16.6793
21	15.9715	16.5004
28	15.6352	16.3260
42	14.9837	15.9864
50	14.6237	15.7970
100	12.5615	14.6817

FOCUS Step 3

$PEC_{(sw)}$	**Single application Maximum µg/L**
R1, pond	0.394
R1, stream	5.531

FOCUS Step 4

$PEC_{(sw)}$	**Buffer zone m**	**PECsw [µg/L] Drift reduction**			
		25%	**50%**	**75%**	**90%**
R1, pond	0	0.296	0.197	0.099	0.039
R1, stream	0	4.149	2.766	1.383	0.553
R1, pond	5m (drift)	0.445	0.223	0.111	0.045
R1, stream	5m (drift)	4.515	2.258	1.129	0.452
R1, pond	10m (drift)	0.253	0.126	0.063	0.025
R1, stream	10m (drift)	2.354	1.177	0.589	0.235
R1, pond	15m (drift)	0.141	0.071	0.035	0.014
R1, stream	15m (drift)	1.554	0.777	0.388	0.155
R1, pond	20m (drift)	0.078	0.039	0.02	0.008
R1, stream	20m (drift)	0.708	0.354	0.177	0.071

Metabolite DFA

Method of calculation	**Metabolite DFA** FOCUS Surface Water Steps 1,2 K_{oc}, 6.8 mL/g, (arithmetic mean) Degradation, , Soil DT_{50} 44.7 days, (GeoMean lab. Studies at 20°C and field capacity) Water/Sediment Total system , DT_{50} 249 days, Water DT_{50} 249 days (Sedciment default 1000 days) Maximum occurance Water/sediment 6.9% Soil 33.9%
Application rate	1 x 150g/ha spray application to hops
Main routes of entry	Run-off/Drainage

FOCUS Step 2

$PEC_{(sw)}$	**Single application Maximum (S. Europe) µg/L**
Initial	1.268

Metabolite 6-CNA

Method of calculation	**Metabolite 6-CNA** FOCUS Surface Water Steps 1,2 K_{oc}, 88 mL/g, (arithmetic mean) Degradation, , Soil DT_{50} 4.7 days, (GeoMean lab. Studies) Water/Sediment Total system , DT_{50} 1000 days (default), Water DT_{50} 1000 days (default) Sediment DT_{50} 100 days (default) Maximum occurance Water/sediment 0% Soil 17.1%
Application rate	1 x 150g/ha spray application to hops

FOCUS Step 2

$PEC_{(sw)}$	**Single application Maximum (S. Europe) µg/L**
Initial	0.463

Metabolite BYI 02960-succinamide

Method of calculation	**Metabolite BYI 02960-succinamide** FOCUS Surface Water Steps 1,2 K_{oc}, 0 mL/g, Degradation, , Soil DT_{50} 0.1 days, (model STEP2 does not accept 0 days) Water/Sediment Total system , DT_{50} 1000 days (default), Water DT_{50} 1000 days (default) Sediment DT_{50} 1000 days (default) Maximum occurance Water/sediment 39.6% Soil 0%
Application rate	1 x 150g/ha spray application to hops
Main routes of entry	Formed from BYI 02960 in water

FOCUS Step 2

$PEC_{(sw)}$	**Single application Maximum (S. Europe) µg/L**
Initial	4.065

Metabolite BYI 02960-azabicyclosuccinamide

Method of calculation	**Metabolite BYI 02960-azabicyclosuccinamide** FOCUS Surface Water Steps 1,2 K_{oc}, 0 mL/g, Degradation, , Soil DT_{50} 0.1 days, (model STEP2 does not accept 0 days) Water/Sediment Total system , DT_{50} 1000 days (default), Water DT_{50} 1000 days (default) Sediment DT_{50} 1000 days (defualt) Maximum occurance Water/sediment 25.9% Soil 0%
Application rate	1 x 150g/ha spray application to hops
Main routes of entry	Formed from BYI 02960 in water

FOCUS Step 2

$PEC_{(sw)}$	**Single application Maximum (S. Europe) µg/L**
Initial	2.499

Application to Lettuce
BYI 02960

Method of calculation	**BYI 02960** FOCUS Surface Water Steps 1, 2, 3,4 K_{oc}, 98.4 mL/g, (arithmetic mean) Freundlich Exponent, , 0.866 (arithmetic mean) Degradation, , Soil DT_{50}, 94.8 days, (GeoMean lab. Studies at 20°C and field capacity) Water/Sediment Total , DT_{50} 228 days DT_{50} Water 228 days Sediment 1000 days(default)
Application rate	**1 x 125g/ha spray application to lettuce**
Main routes of entry	Spray drift/Run-off/ Drainage

FOCUS Step 2

$PEC_{(sw)}$	**Single application Maximum (S. Europe) µg/L**	**Single application Time weighted average µg/L**
Initial	11.78	-
1	11.7001	11.7381
2	11.6645	11.7102
4	11.5938	11.6697
7	11.4886	11.6146
14	11.2467	11.4909
21	11.0099	11.3699
28	10.7780	11.2508
42	10.3289	11.0178
50	10.0807	10.8877
100	8.6592	10.1198

FOCUS Step 3

$PEC_{(sw)}$	**Major entry route S = spray drift, R=run-off, D= drainflow**	**Single application Actual Maximum µg/L**
D3 (ditch, 1st)	S	0.830
D3 (ditch, 2nd)	S	0.840
D4 (pond, 1st)	D	1.035
D4 (stream, 1st)	S	0.794
D6 (ditch, 1st)	D	1.268
R1 (pond, 1st)	R	0.060
R1 (stream, 1st)	R	0.858
R1 (pond, 2nd)	R	0.097
R1 (stream, 2nd)	R	1.186
R2 (stream, 1st)	R	1.586
R2 (stream, 2nd)	R	0.940
R3 (stream, 1st)	R	2.226
R3 (stream, 2nd)	R	3.570
R4 (stream, 1st)	S	0.522
R4 (stream, 2nd)	R	4.808

FOCUS Step 4

FOCUS Scenario	Buffer zone	PECsw [µg/L] Drift reduction			
		25%	50%	75%	90%
D3 (ditch, 1st)	0m	0.632	0.434	0.235	0.117
D3 (ditch, 2nd)		0.643	0.446	0.249	0.130
D4 (pond, 1st)		1.034	1.034	1.033	1.033
D4 (stream, 1st)		0.721	0.721	0.721	0.721
D6 (ditch, 1st)		1.268	1.268	1.268	1.268
R1 (pond, 1st)		0.055	0.050	0.045	0.043
R1 (stream, 1st)		0.858	0.858	0.858	0.858
R1 (pond, 2nd)		0.092	0.087	0.082	0.079
R1 (stream, 2nd)		1.186	1.186	1.186	1.186
R2 (stream, 1st)		1.586	1.586	1.586	1.586
R2 (stream, 2nd)		0.940	0.940	0.940	0.940
R3 (stream, 1st)		2.226	2.226	2.226	2.226
R3 (stream, 2nd)		3.570	3.570	3.570	3.570
R4 (stream, 1st)		0.392	0.261	0.131	0.074
R4 (stream, 2nd		4.808	4.808	4.808	4.808

FOCUS Scenario	Buffer zone	PECsw [µg/L] Drift reduction			
		25%	50%	75%	90%
D3 (ditch, 1st)	5m (drift)	0.252	0.145	0.091	0.059
D3 (ditch, 2nd)		0.265	0.158	0.105	0.073
D4 (pond, 1st)		1.035	1.034	1.033	1.033
D4 (stream, 1st)		0.721	0.721	0.721	0.721
D6 (ditch, 1st)		1.268	1.268	1.268	1.268
R1 (pond, 1st)		0.057	0.049	0.045	0.042
R1 (stream, 1st)		0.858	0.858	0.858	0.858
R1 (pond, 2nd)		0.094	0.086	0.082	0.079
R1 (stream, 2nd)		1.186	1.186	1.186	1.186
R2 (stream, 1st)		1.586	1.586	1.586	1.586
R2 (stream, 2nd)		0.940	0.940	0.940	0.940
R3 (stream, 1st)		2.226	2.226	2.226	2.226
R3 (stream, 2nd)		3.570	3.570	3.570	3.570
R4 (stream, 1st)		0.191	0.095	0.074	0.074
R4 (stream, 2nd)		4.808	4.808	4.808	4.808

FOCUS Scenario	Buffer zone	PECsw [µg/L] Drift reduction			
		25%	50%	75%	90%
D3 (ditch, 1st)	10m (drift)	0.151	0.094	0.066	0.049
D3 (ditch, 2nd)	10m (drift)	0.165	0.108	0.080	0.063
D4 (pond, 1st)	10m (drift)	1.034	1.033	1.033	1.033
D4 (stream, 1st)	10m (drift)	0.721	0.721	0.721	0.721
D6 (ditch, 1st)	10m (drift)	1.268	1.268	1.268	1.268
R1 (pond, 1st)	10m (drift)	0.029	0.022	0.019	0.018
R1 (stream, 1st)	10m (run-off)	0.389	0.389	0.389	0.389
R1 (pond, 2nd)	10m (drift)	0.043	0.037	0.034	0.032
R1 (stream, 2nd)	10m (run-off)	0.540	0.540	0.540	0.540
R2 (stream, 1st)	10m (run-off)	0.716	0.716	0.716	0.716
R2 (stream, 2nd)	10m (run-off)	0.422	0.422	0.422	0.422
R3 (stream, 1st)	10m (run-off)	1.009	1.009	1.009	1.009
R3 (stream, 2nd)	10m (run-off)	1.630	1.630	1.630	1.630
R4 (stream, 1st)	10m (drift)	0.101	0.051	0.034	0.034
R4 (stream, 2nd)	10m (run-off)	2.184	2.184	2.184	2.184

FOCUS Scenario	Buffer zone	PECsw [µg/L] Drift reduction			
		25%	50%	75%	90%
D3 (ditch, 1st)	15m (drift)	0.115	0.076	0.057	0.045
D3 (ditch, 2nd)	15m (drift)	0.129	0.090	0.071	0.059
D4 (pond, 1st)	15m (drift)	1.034	1.033	1.033	1.033
D4 (stream, 1st)	15m (drift)	0.721	0.721	0.721	0.721
D6 (ditch, 1st)	15m (drift)	1.268	1.268	1.268	1.268
R1 (pond, 1st)	15m (drift)	0.018	0.013	0.011	0.009
R1 (stream, 1st)	15m (run-off)	0.204	0.204	0.204	0.204
R1 (pond, 2nd)	15m (drift)	0.025	0.021	0.018	0.017
R1 (stream, 2nd)	15m (run-off)	0.283	0.283	0.283	0.283
R2 (stream, 1st)	15m (run-off)	0.375	0.375	0.375	0.375
R2 (stream, 2nd)	15m (run-off)	0.220	0.220	0.220	0.220
R3 (stream, 1st)	15m (run-off)	0.528	0.528	0.528	0.528
R3 (stream, 2nd)	15m (run-off)	0.856	0.856	0.856	0.856
R4 (stream, 1st)	15m (drift)	0.069	0.035	0.018	0.018
R4 (stream, 2nd)	15m (run-off)	1.144	1.144	1.144	1.144

FOCUS Scenario	Buffer zone	PECsw [µg/L] Drift reduction			
		25%	50%	75%	90%
D3 (ditch, 1st)	20m (drift)	0.097	0.067	0.052	0.045
D3 (ditch, 2nd)	20m (drift)	0.110	0.081	0.066	0.057
D4 (pond, 1st)	20m (drift)	1.033	1.033	1.033	1.033
D4 (stream, 1st)	20m (drift)	0.721	0.721	0.721	0.721
D6 (ditch, 1st)	20m (drift)	1.268	1.268	1.268	1.268
R1 (pond, 1st)	20m (drift)	0.016	0.012	0.010	0.009
R1 (stream, 1st)	20m (run-off)	0.204	0.204	0.204	0.204
R1 (pond, 2nd)	20m (drift)	0.024	0.020	0.018	0.016
R1 (stream, 2nd)	20m (run-off)	0.283	0.283	0.283	0.283
R2 (stream, 1st)	20m (run-off)	0.375	0.375	0.375	0.375
R2 (stream, 2nd)	20m (run-off)	0.220	0.220	0.220	0.220
R3 (stream, 1st)	20m (run-off)	0.528	0.528	0.528	0.528
R3 (stream, 2nd)	20m (run-off)	0.856	0.856	0.856	0.856
R4 (stream, 1st)	20m (drift)	0.053	0.026	0.018	0.018
R4 (stream, 2nd)	20m (run-off)	1.144	1.144	1.144	1.144

Metabolite DFA

Method of calculation	**Metabolite DFA** FOCUS Surface Water Steps 1,2 K_{oc}, 6.8 mL/g, (arithmetic mean) Degradation, , Soil DT_{50} 44.7 days, (GeoMean lab. Studies at 20°C and field capacity) Water/Sediment Total system , DT_{50} 249 days, Water DT_{50} 249 days (Sediment default 1000 days) Maximum occurance Water/sediment 6.9% Soil 33.9%
Application rate	**1 x 125g/ha spray application to lettuce**
Main routes of entry	Run-off/Drainage

FOCUS Step 2

$PEC_{(sw)}$	**Single application Maximum (S. Europe) µg/L**
Initial	1.1339

Metabolite 6-CNA

Method of calculation	**Metabolite 6-CNA** FOCUS Surface Water Steps 1,2 K_{oc}, 88 mL/g, (arithmetic mean) Degradation, , Soil DT_{50} 4.7 days, (GeoMean lab. Studies) Water/Sediment Total system , DT_{50} 1000 days (default), Water DT_{50} 1000 days (default) Sediment DT_{50} 1000 days (default) Maximum occurance Water/sediment 0% Soil 17.1%
Application rate	**1 x 125g/ha spray application to lettuce**

FOCUS Step 2

$PEC_{(sw)}$	**Single application Maximum (S. Europe) µg/L**
Initial	0.579

Metabolite BYI 02960-succinamide

Method of calculation	**Metabolite BYI 02960-succinamide** FOCUS Surface Water Steps 1,2 K_{oc}, 0 mL/g, Degradation, , Soil DT_{50} 0.1 days, (model STEP2 does not accept 0 days) Water/Sediment Total system , DT_{50} 1000 days (default), Water DT_{50} 1000 days (default) Sediment DT_{50} 1000 days (defualt) Maximum occurance Water/sediment 39.6% Soil 0%
Application rate	**1 x 125g/ha spray application to lettuce**
Main routes of entry	Formed from BYI 02960 in water

FOCUS Step 2

$PEC_{(sw)}$	**Single application Maximum (S. Europe) µg/L**
Initial	0.48/4

Metabolite BYI 02960-azabicyclosuccinamide

Method of calculation	**Metabolite BYI 02960-azabicyclosuccinamide** FOCUS Surface Water Steps 1,2 K_{oc}, 0 mL/g, Degradation, , Soil DT_{50} 0.1 days, (model STEP2 does not accept 0 days) Water/Sediment Total system , DT_{50} 1000 days (default), Water DT_{50} 1000 days (default) Sediment DT_{50} 1000 days (defualt) Maximum occurance Water/sediment 25.9% Soil 0%
Application rate	**1 x 125g/ha spray application to lettuce**
Main routes of entry	Formed from BYI 02960 in water

FOCUS Step 2

$PEC_{(sw)}$	**Single Application Maximum (S. Europe) µg/L**
Initial	0.297

PEC (sediment)

Application to Hops
BYI 02960

Method of calculation	**BYI 02960** FOCUS Surface Water Steps 1, 2, 3, 4 K_{oc}, 98.4 mL/g, (arithmetic mean) Freundlich Exponent, , 0.866 (arithmetic mean) Degradation, , Soil DT_{50}, 94.8 days, (GeoMean lab. Studies at 20°C and field capacity) Water/Sediment Total , DT_{50} 228 days, DT_{50} Water 228 days Sediment 1000 days(default)
Application rate	**1 x 150g/ha spray application to hops**
Main routes of entry	Spray drift

FOCUS Step 2

$PEC_{(sed)}$	**Single application Actual Maximum (S. Europe) µg/kg**	**Single application Time weighted average µg/kg**
Initial	16.70	-
1	16.6504	16.6758
2	16.5999	16.6505
4	16.4993	16.6000
7	16.3495	16.5247
14	16.0052	16.3507
21	15.6682	16.1792
28	15.3383	16.0101
42	14.6992	15.6789
50	14.3460	15.4938
100	12.3230	14.4013

FOCUS Step 3

$PEC_{(sed)}$	**Single Application Maximum µg/kg**
R1, pond	0.795
R1, stream	0.362

FOCUS Step 4

	Buffer zone m	**PECsed [µg/kg] Drift reduction**			
		25%	**50%**	**75%**	**90%**
R1, pond	0	0.607	0.415	0.218	0.094
R1, stream	0	0.273	0.184	0.093	0.072
R1, pond	5m (drift)	0.891	0.465	0.244	0.105
R1, stream	5m (drift)	0.297	0.151	0.076	0.071
R1, pond	10m (drift)	0.522	0.273	0.142	0.061
R1, stream	10m (drift)	0.157	0.080	0.04	0.031
R1, pond	15m (drift)	0.302	0.158	0.083	0.036
R1, stream	15m (drift)	0.104	0.053	0.032	0.03
R1, pond	20m (drift)	0.174	0.091	0.048	0.021
R1, stream	20m (drift)	0.048	0.025	0.017	0.016

Metabolite DFA

Method of calculation	**Metabolite DFA** FOCUS Surface Water Steps 1,2 K_{oc}, 6.8 mL/g, (arithmetic mean) Degradation, , Soil DT_{50} 44.7 days, (GeoMean lab. Studies at 20°C and field capacity) Water/Sediment Total system , DT_{50} 249 days, Water DT_{50} 249 days (Sedciment default 1000 days) Maximum occurance Water/sediment 6.9% Soil 33.9%
Application rate	1 x 150g/ha spray application to hops
Main routes of entry	Run-off/Drainage

FOCUS Step 2

$PEC_{(sed)}$	**Single Application Maximum (S. Europe) µg/kg**
Initial	0.086

Metabolite 6-CNA

Method of calculation	**Metabolite 6-CNA** FOCUS Surface Water Steps 1,2 K_{oc}, 88 mL/g, (arithmetic mean) Degradation, , Soil DT_{50} 4.7 days, (GeoMean lab. Studies) Water/Sediment Total system , DT_{50} 1000 days (default), Water DT_{50} 1000 days (default) Sediment DT_{50} 100 days (default) Maximum occurance Water/sediment 0% Soil 17.1%
Application rate	1 x 150g/ha spray application to hops

FOCUS Step 2

$PEC_{(sed)}$	**Single application Maximum (S. Europe) µg/kg**
Initial	0.408

Metabolite BYI 02960-succinamide

Method of calculation	**Metabolite BYI 02960-succinamide** FOCUS Surface Water Steps 1,2 K_{oc}, 0 mL/g, Degradation, , Soil DT_{50} 0.1 days, (model STEP2 does not accept 0 days) Water/Sediment Total system , DT_{50} 1000 days (default), Water DT_{50} 1000 days (default) Sediment DT_{50} 1000 days (default) Maximum occurance Water/sediment 39.6% Soil 0%
Application rate	1 x 150g/ha spray application to hops
Main routes of entry	Formed from BYI 02960 in water

FOCUS Step 2

$PEC_{(sed)}$	**Single application Maximum (S. Europe) µg/kg**
Initial	< 0.001

Metabolite BYI 02960-azabicyclosuccinamide

Method of calculation	**Metabolite BYI 02960-azabicyclosuccinamide** FOCUS Surface Water Steps 1,2 K_{oc}, 0 mL/g, Degradation, , Soil DT_{50} 0.1 days, (model STEP2 does not accept 0 days) Water/Sediment Total system , DT_{50} 1000 days (default), Water DT_{50} 1000 days (default) Sediment DT_{50} 1000 days (defualt) Maximum occurance Water/sediment 25.9% Soil 0%
Application rate	1 x 150g/ha spray application to hops
Main routes of entry	Formed from BYI 02960 in water

FOCUS Step 2

$PEC_{(sed)}$	**Single application Maximum (S. Europe) µg/kg**
Initial	< 0.001

Application to Lettuce
BYI 02960

Method of calculation	**BYI 02960** FOCUS Surface Water Steps 1, 2, 3,4 K_{oc}, 98.4 mL/g, (arithmetic mean) Freundlich Exponent, , 0.866 (arithmetic mean) Degradation, , Soil DT_{50}, 94.8 days, (GeoMean lab. Studies at 20°C and field capacity) Water/Sediment Total , DT_{50} 228 days DT_{50} Water 228 days Sediment 1000 days(default)
Application rate	**1 x 125g/ha spray application to lettuce**
Main routes of entry	Spray drift/Run-off/ Drainage

FOCUS Step 2

PEC(sed)	**Single application Actual Maximum (S. Europe) µg/kg**	**Single application Time weighted average µg/kg**
Initial	11.51	-
1	11.4779	11.4954
2	11.4431	11.4779
4	11.3737	11.4431
7	11.2704	11.3912
14	11.0331	11.2713
21	10.8008	11.1531
28	10.5734	11.0365
42	10.1328	10.8082
50	9.8893	10.6806
100	8.4948	9.9275

FOCUS Step 3

PEC(sed)	**Major entry route S = spray drift, R=run-off, D= drainflow**	**Single application Actual Maximum µg/kg**
D3 (ditch, 1st)	S	0.380
D3 (ditch, 2nd)	S	0.460
D4 (pond, 1st)	D	4.545
D4 (stream, 1st)	S	1.772
D6 (ditch, 1st)	D	1.766
R1 (pond, 1st)	R	0.162
R1 (stream, 1st)	R	0.211
R1 (pond, 2nd)	R	0.254
R1 (stream, 2nd)	R	0.334
R2 (stream, 1st)	R	0.521
R2 (stream, 2nd)	R	0.342
R3 (stream, 1st)	R	0.469
R3 (stream, 2nd)	R	1.011
R4 (stream, 1st)	S	0.054
R4 (stream, 2nd)	R	1.255

FOCUS Step 4

FOCUS Scenario	Buffer zone	PECsed [µg/kg] Drift reduction			
		25%	50%	75%	90%
D3 (ditch, 1st)	0m	0.335	0.334	0.333	0.332
D3 (ditch, 2nd)		0.419	0.399	0.398	0.397
D4 (pond, 1st)		4.538	4.531	4.524	4.520
D4 (stream, 1st)		1.771	1.771	1.771	1.771
D6 (ditch, 1st)		1.766	1.765	1.765	1.764
R1 (pond, 1st)		0.148	0.134	0.119	0.111
R1 (stream, 1st)		0.210	0.208	0.207	0.206
R1 (pond, 2nd)		0.240	0.225	0.210	0.201
R1 (stream, 2nd)		0.333	0.332	0.330	0.330
R2 (stream, 1st)		0.520	0.520	0.519	0.518
R2 (stream, 2nd)		0.342	0.341	0.341	0.340
R3 (stream, 1st)		0.466	0.462	0.459	0.456
R3 (stream, 2nd)		1.006	1.000	0.995	0.991
R4 (stream, 1st)		0.041	0.027	0.025	0.024
R4 (stream, 2nd		1.253	1.251	1.249	1.248

FOCUS Scenario	Buffer zone	PECsed [µg/kg] Drift reduction			
		25%	50%	75%	90%
D3 (ditch, 1st)	5m (drift)	0.333	0.332	0.332	0.332
D3 (ditch, 2nd)		0.398	0.397	0.397	0.396
D4 (pond, 1st)		4.541	4.529	4.523	4.520
D4 (stream, 1st)		1.771	1.771	1.771	1.771
D6 (ditch, 1st)		1.765	1.764	1.764	1.764
R1 (pond, 1st)		0.154	0.130	0.117	0.11
R1 (stream, 1st)		0.208	0.207	0.206	0.206
R1 (pond, 2nd)		0.247	0.221	0.208	0.201
R1 (stream, 2nd)		0.331	0.330	0.33	0.329
R2 (stream, 1st)		0.519	0.518	0.518	0.518
R2 (stream, 2nd)		0.341	0.341	0.34	0.34
R3 (stream, 1st)		0.460	0.458	0.456	0.455
R3 (stream, 2nd)		0.997	0.993	0.991	0.99
R4 (stream, 1st)		0.025	0.025	0.024	0.024
R4 (stream, 2nd)		1.250	1.248	1.247	1.247

FOCUS Scenario	Buffer zone	PECsed [µg/kg] Drift reduction			
		25%	50%	75%	90%
D3 (ditch, 1st)	10m (drift)	0.332	0.332	0.332	0.332
D3 (ditch, 2nd)	10m (drift)	0.397	0.397	0.396	0.396
D4 (pond, 1st)	10m (drift)	4.534	4.526	4.522	4.519
D4 (stream, 1st)	10m (drift)	1.771	1.771	1.771	1.771
D6 (ditch, 1st)	10m (drift)	1.764	1.764	1.764	1.764
R1 (pond, 1st)	10m (drift)	0.083	0.064	0.055	0.049
R1 (stream, 1st)	10m (run-off)	0.097	0.097	0.097	0.096
R1 (pond, 2nd)	10m (drift)	0.122	0.103	0.094	0.088
R1 (stream, 2nd)	10m (run-off)	0.157	0.157	0.157	0.156
R2 (stream, 1st)	10m (run-off)	0.228	0.228	0.228	0.228
R2 (stream, 2nd)	10m (run-off)	0.151	0.151	0.151	0.151
R3 (stream, 1st)	10m (run-off)	0.219	0.217	0.216	0.216
R3 (stream, 2nd)	10m (run-off)	0.452	0.450	0.449	0.448
R4 (stream, 1st)	10m (drift)	0.012	0.012	0.012	0.011
R4 (stream, 2nd)	10m (run-off)	0.585	0.584	0.584	0.584

FOCUS Scenario	Buffer zone	PECsed [µg/kg] Drift reduction			
		25%	50%	75%	90%
D3 (ditch, 1st)	15m (drift)	0.332	0.332	0.332	0.332
D3 (ditch, 2nd)	15m (drift)	0.397	0.396	0.396	0.396
D4 (pond, 1st)	15m (drift)	4.531	4.524	4.521	4.519
D4 (stream, 1st)	15m (drift)	1.771	1.771	1.771	1.771
D6 (ditch, 1st)	15m (drift)	1.764	1.764	1.764	1.764
R1 (pond, 1st)	15m (drift)	0.055	0.039	0.032	0.027
R1 (stream, 1st)	15m (run-off)	0.053	0.052	0.052	0.052
R1 (pond, 2nd)	15m (drift)	0.076	0.060	0.052	0.047
R1 (stream, 2nd)	15m (run-off)	0.086	0.085	0.085	0.085
R2 (stream, 1st)	15m (run-off)	0.122	0.122	0.122	0.122
R2 (stream, 2nd)	15m (run-off)	0.081	0.081	0.081	0.081
R3 (stream, 1st)	15m (run-off)	0.119	0.118	0.117	0.117
R3 (stream, 2nd)	15m (run-off)	0.245	0.243	0.242	0.242
R4 (stream, 1st)	15m (drift)	0.008	0.006	0.006	0.006
R4 (stream, 2nd)	15m (run-off)	0.318	0.317	0.317	0.316

FOCUS Scenario	Buffer zone	PECsed [µg/kg] Drift reduction			
		25%	50%	75%	90%
D3 (ditch, 1st)	20m (drift)	0.332	0.332	0.332	0.332
D3 (ditch, 2nd)	20m (drift)	0.397	0.396	0.396	0.396
D4 (pond, 1st)	20m (drift)	4.529	4.523	4.520	4.518
D4 (stream, 1st)	20m (drift)	1.771	1.771	1.771	1.771
D6 (ditch, 1st)	20m (drift)	1.764	1.764	1.764	1.764
R1 (pond, 1st)	20m (drift)	0.050	0.037	0.03	0.026
R1 (stream, 1st)	20m (run-off)	0.052	0.052	0.052	0.052
R1 (pond, 2nd)	20m (drift)	0.071	0.057	0.05	0.046
R1 (stream, 2nd)	20m (run-off)	0.086	0.085	0.085	0.085
R2 (stream, 1st)	20m (run-off)	0.122	0.122	0.122	0.122
R2 (stream, 2nd)	20m (run-off)	0.081	0.081	0.081	0.081
R3 (stream, 1st)	20m (run-off)	0.118	0.117	0.117	0.117
R3 (stream, 2nd)	20m (run-off)	0.244	0.243	0.242	0.242
R4 (stream, 1st)	20m (drift)	0.007	0.006	0.006	0.006
R4 (stream, 2nd)	20m (run-off)	0.317	0.317	0.317	0.316

Metabolite DFA

Method of calculation	**Metabolite DFA** FOCUS Surface Water Steps 1,2 K_{oc}, 6.8 mL/g, (arithmetic mean) Degradation, , Soil DT_{50} 44.7 days, (GeoMean lab. Studies at 20°C and field capacity) Water/Sediment Total system , DT_{50} 249 days, Water DT_{50} 249 days (Sediment default 1000 days) Maximum occurance Water/sediment 6.9% Soil 33.9%
Application rate	**1 x 125g/ha spray application to lettuce**
Main routes of entry	Run-off/Drainage

FOCUS Step 2

$PEC_{(sed)}$	**Single application Maximum (S. Europe) µg/kg**
Initial	0.091

Metabolite 6-CNA

Method of calculation	**Metabolite 6-CNA** FOCUS Surface Water Steps 1,2 K_{oc}, 88 mL/g, (arithmetic mean) Degradation, , Soil DT_{50} 4.7 days, (GeoMean lab. Studies) Water/Sediment Total system , DT_{50} 1000 days (default), Water DT_{50} 1000 days (default) Sediment DT_{50} 1000 days (default) Maximum occurance Water/sediment 0% Soil 17.1%
Application rate	**1 x 125g/ha spray application to lettuce**

FOCUS Step 2

$PEC_{(sed)}$	**Single application Maximum (S. Europe) µg/kg**
Initial	0.509

Metabolite BYI 02960-succinamide

Method of calculation	**Metabolite BYI 02960-succinamide** FOCUS Surface Water Steps 1,2 K_{oc}, 0 mL/g, Degradation, , Soil DT_{50} 0.1 days, (model STEP2 does not accept 0 days) Water/Sediment Total system , DT_{50} 1000 days (default), Water DT_{50} 1000 days (default) Sediment DT_{50} 1000 days (defualt) Maximum occurance Water/sediment 39.6% Soil 0%
Application rate	**1 x 125g/ha spray application to lettuce**
Main routes of entry	Formed from BYI 02960 in water

FOCUS Step 2

$PEC_{(sed)}$	**Single application Maximum (S. Europe) µgkg**
Initial	<0.001

Metabolite BYI 02960-azabicyclosuccinamide

Method of calculation	**Metabolite BYI 02960-azabicyclosuccinamide** FOCUS Surface Water Steps 1,2 K_{oc}, 0 mL/g, Degradation, , Soil DT_{50} 0.1 days, (model STEP2 does not accept 0 days) Water/Sediment Total system , DT_{50} 1000 days (default), Water DT_{50} 1000 days (default) Sediment DT_{50} 1000 days (defualt) Maximum occurance Water/sediment 25.9% Soil 0%
Application rate	**1 x 125g/ha spray application to lettuce**
Main routes of entry	Formed from BYI 02960 in water

FOCUS Step 2

$PEC_{(sed)}$	**Single Application Maximum (S. Europe) µg/kg**
Initial	<0.001

PEC (ground water) (OECD data point IIIA 9.6)

Method of calculation and type of study (*e.g.* modelling, monitoring, lysimeter)	FOCUS Groundwater 2009 Tiered approach Tier 1 Laboratory DT_{50} SFO at 20°C and filed capacity Tier 2a Laboratory DT_{50} DFOP approach (FOCUS 2009) Tier 2a Laboratory TDS approach
Application rate	1 x 150g/ha in Hops 1 x 125 g/ha in Lettuce

$PEC_{(gw)}$	
Maximum concentration	See below
Average annual concentration *(Results quoted for modelling with FOCUS gw scenarios, according to FOCUS guidance)*	See below

Tier 1

Scenario	BYI 02960			
	Hops (every year), 1 x 150 g/ha		Hops (every 2nd year), 1 x 150 g/ha	
	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]
Châteaudun	0.453	0.415	0.193	0.168
Hamburg	0.579	0.634	0.283	0.249
Kremsmuenster	0.430	0.481	0.172	0.196
Piacenza	0.359	0.442	0.154	0.211
Porto	0.220	0.286	0.093	0.122
Sevilla	0.223	0.063	0.091	0.022
Thiva	0.183	0.155	0.073	0.059

Tier 2a (DFOP)

Scenario	BYI 02960			
	Hops (every year), 1 x 150 g/ha		Hops (every 2nd year), 1 x 150 g/ha	
	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]
Châteaudun	0.272	0.251	0.116	0.102
Hamburg	0.346	0.380	0.172	0.151
Kremsmuenster	0.257	0.287	0.103	0.118
Piacenza	0.213	0.263	0.093	0.127
Porto	0.133	0.171	0.056	0.073
Sevilla	0.137	0.039	0.056	0.015
Thiva	0.111	0.095	0.045	0.037

Tier 2a(TDS)

Scenario	BYI 02960			
	Hops (every year), 1 x 150 g/ha		Hops (every 2nd year), 1 x 150 g/ha	
	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]
Châteaudun	0.116	0.100	0.044	0.035
Hamburg	0.175	0.175	0.069	0.065
Kremsmuenster	0.135	0.157	0.049	0.056
Piacenza	0.118	0.157	0.041	0.065
Porto	0.056	0.087	0.020	0.030
Sevilla	0.042	0.007	0.014	0.002
Thiva	0.030	0.023	0.010	0.006

Tier 1

Scenario	BYI 02960 (field use)							
	Lettuce, 1st cropping, every year, 1 x 125 g/ha		Lettuce, 2nd cropping, every year, 1 x 125 g/ha		Lettuce, 2nd cropping, every year, 1 x 125 g/ha		Lettuce, 2nd cropping, every 2nd year, 1 x 125 g/ha	
	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]
Châteaudun	0.413	0.298	0.556	0.396	0.154	0.111	0.207	0.142
Hamburg	0.809	0.724	1.081	0.983	0.379	0.298	0.443	0.401
Jokioinen	0.325	0.269	-	-	0.109	0.088	-	-
Kremsmuenster	0.595	0.517	0.698	0.637	0.242	0.210	0.291	0.255
Porto	0.327	0.413	0.643	0.713	0.137	0.177	0.253	0.305
Sevilla	0.018	0.005	0.025	0.006	0.006	0.002	0.009	0.002
Thiva	0.313	0.221	-	-	0.109	0.069	-	-

Tier 2a (DFOP)

Scenario	BYI 02960 (field use)							
	Lettuce, 1st cropping, every year, 1 x 125 g/ha		Lettuce, 2nd cropping, every year, 1 x 125 g/ha		Lettuce, 2nd cropping, every year, 1 x 125 g/ha		Lettuce, 2nd cropping, every 2nd year, 1 x 125 g/ha	
	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]
Châteaudun	0.269	0.194	0.355	0.257	0.095	0.068	0.126	0.087
Hamburg	0.630	0.462	0.751	0.708	0.230	0.179	0.270	0.244
Jokioinen	0.213	0.175	-	-	0.068	0.055	-	-
Kremsmuenster	0.382	0.347	0.451	0.417	0.146	0.128	0.177	0.155
Porto	0.216	0.255	0.431	0.461	0.082	0.105	0.153	0.182
Sevilla	0.016	0.005	0.025	0.006	0.004	0.001	0.006	0.002
Thiva	0.224	0.149	-	-	0.067	0.043	-	-

Tier 2a (TDS)

Scenario	BYI 02960 (field use)							
	Lettuce, 1st cropping, every year, 1 x 125 g/ha		Lettuce, 2nd cropping, every year, 1 x 125 g/ha		Lettuce, 2nd cropping, every year, 1 x 125 g/ha		Lettuce, 2nd cropping, every 2nd year, 1 x 125 g/ha	
	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]	PEARL PEC_{gw} [µg/L]	PELMO PEC_{gw} [µg/L]
Châteaudun	0.085	0.053	0.111	0.070	0.025	0.015	0.034	0.020
Hamburg	0.263	0.194	0.329	0.272	0.099	0.075	0.132	0.107
Jokioinen	0.055	0.046	-	-	0.014	0.011	-	-
Kremsmuenster	0.181	0.157	0.216	0.198	0.064	0.052	0.075	0.067
Porto	0.090	0.133	0.176	0.247	0.032	0.052	0.061	0.086
Sevilla	0.001	<0.001	0.001	<0.001	<0.001	<0.001	<0.001	<0.001
Thiva	0.047	0.036	-	-	0.014	0.009	-	-

Fate and behaviour in air (OECD data points IIA 7.10 and IIIA 9.9)

Direct photolysis in air	Not required due to low volatility
Quantum yield of direct phototransformation *at $\lambda > 290$ nm*	Quantum yield $\Phi = 0.000138$ was determined according to ECETOC method in aqueous solution
Photochemical oxidative degradation in air	Latitude: ..... Season: ..... DT_{50}: …..... A half-life time (T1/2) of 4.4 hours was calculated for a 'short term' atmospheric hydroxyl radical concentration of 1.5 x 10^6 OH radicals / cm3 being accepted as typical average over 12 daylight hours per day for the temperate zone
Volatilization	from plant surfaces: Not required due to low vapour pressure (9.1 x 10^{-7} Pa)
	from soil: Not required due to low vapour pressure (9.1 x 10^{-7} Pa)

PEC (air)

Method of calculation	Not required due to low volatility

$PEC_{(a)}$

Maximum concentration	Not required due to low volatility

Definition of the Residue (OECD data point IIA 7.11)

Relevant to the environment	Definition for further evaluation Metabolites found in soil or aquatic degradation tests are not necessarily relevant by default but are defined for assessments of environmental exposure in soil and water. Soil: BYI 02960, DFA, 6-CNA Groundwater: BYI 02960, DFA, 6-CNA Surface water and sediment: BYI 02960, DFA, 6-CNA, BYI 02960-succinamide, BYI 02960-azabicyclosuccinamide

Monitoring data, if available (OECD data point IIA 7.12)

Soil (indicate location and type of study)	Not available (new active substance)
Surface water (indicate location and type of study)	Not available (new active substance)
Ground water (indicate location and type of study)	Not available (new active substance)
Air (indicate location and type of study)	Not available (new active substance)

Chapter 6: Effects on non-target species

Effects on terrestrial vertebrates (OECD data points IIA 8.1, IIIA 10.1 and IIIA 10.3)

Acute toxicity to mammals	LD50 1607 mg a.i./kg bw
Reproductive toxicity to mammals	Tier 1 7.8mg/kg bw/day Tier 2 (refined) 39.2 mg/kg bw/d
Acute toxicity to birds	LD50 active substance Colinus virginanus 232 mg a.i./kg LD50 BYI 02960 SL200 431 mg a.i./kg bw
Dietary toxicity to birds	LC50 Colinus virginanus > 4876 mg a.i./ kg diet (> 470 mg a.i./kg bw)
Reproductive toxicity to birds	NOAEL Colinus virginanus 302 mg a.i./kg bw (40 mg a.i./kg bw) End –point for Tier 1 reproductive risk assessment 23.2 mg a.i./kg bw/day (Lowest acute LD50 divided by 10)

Toxicity/exposure ratios for terrestrial vertebrates (OECD data points IIIA 10.1 and IIIA 10.3)

Application rate (kg as/ha)	Crop	Category (*e.g.* insectivorous bird)	Time-scale	TER	TER risk assesment trigger*
1 x 150g/ha	Hop	Small insectivorous bird "finch" (Chaffinch)	Acute	61	10
1 x 150g/ha	Hop	Small granivorous bird "finch"(Goldfinch)	Acute	126	10
1 x 150g/ha	Hop	Small insectivorous bird "finch" (Chaffinch)	Long-term	28	5
1 x 150g/ha	Hop	Small granivorous bird "finch"(Goldfinch)	Long-term	51	5
1 x 150g/ha	Hop	Small insectivorous mammal “shrew” Common shrew	Acute	1984	10
1 x 150g/ha	Hop	Small herbivorous mammal "vole" Common vole	Acute	262	10
1 x 150g/ha	Hop	Small omnivorous mammal “mouse” Wood mouse	Acute	1246	10
1 x 150g/ha	Hop	Small insectivorous mammal “shrew” Common shrew	Long-term	52	5
1 x 150g/ha	Hop	Small herbivorous mammal "vole" Common vole	Long-term	4.5 (tier 1)	5
				12.6 to 22.8 (refined)	5
1 x 150g/ha	Hop	Small omnivorous mammal “mouse” Wood mouse	Long-term	25	5
1 x 125g/ha	Lettuce	Medium herbivorous /granivorous bird "pigeon" (Wood pigeon)	Acute	20	10
1 x 125g/ha	Lettuce	Small granivorous bird "finch" (Serin)	Acute	68	10
1 x 125g/ha	Lettuce	Small omnivorous bird “lark” (Woodlark)	Acute	77	10
1 x 125g/ha	Lettuce	Small insectivorous bird “wagtail” (Yellow wagtail)	Acute	69	10
1 x 125g/ha	Lettuce	Medium herbivorous /granivorous bird "pigeon" (Wood pigeon)	Long-term	9	5

1 x 125g/ha	Lettuce	Small granivorous bird "finch" (Serin)	Long-term	28	5
1 x 125g/ha	Lettuce	Small omnivorous bird “lark” (Woodlark)	Long-term	32	5
1 x 125g/ha	Lettuce	Small insectivorous bird “wagtail” (Yellow wagtail)	Long-term	31	5
1 x 125g/ha	Lettuce	Small insectivorous mammal “shrew” Common shrew	Acute	2381	10
1 x 125g/ha	Lettuce	Small herbivorous mammal "vole" Common vole	Acute	94	10
1 x 125g/ha	Lettuce	Large herbivorous mammal “lagomorph” Rabbit	Acute	366	10
1 x 125g/ha	Lettuce	Small omnivorous mammal “mouse” Wood mouse	Acute	747	10
1 x 125g/ha	Lettuce	Small insectivorous mammal “shrew” Common shrew	Long-term	62	5
1 x 125g/ha	Lettuce	Small herbivorous mammal "vole" Common vole	Long-term	1.6 (Tier 1)	5
				4.5-22.8 (refined	5
1 x 125g/ha	Lettuce	Large herbivorous mammal “lagomorph” Rabbit	Long-term	8	5
1 x 125g/ha	Lettuce	Small omnivorous mammal “mouse” Wood mouse	Long-term	15	5

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Toxicity data for aquatic species (most sensitive species of each group)
(OECD data points IIA 8.2 and IIIA 10.2)

Group	Test substance	Time-scale	Endpoint	Toxicity (mg/l)
Laboratory tests				
Fish species				
Pimephales promelas	BYI 02960	acute	LC50	> 70.5
Pimephales promelas	BYI 02960	chronic	NOEC	4.41
Oncorhynchus mykiss	BYI 02960 SL200	acute	LC50	> 105
Oncorhynchus mykiss	BYI 02960 – succinamide	acute	LC50	> 100
Oncorhynchus mykiss	DFA	acute	LC50	> 10
Invertebrate				
Chironomus riparius	BYI 02960	acute	EC50	0.062
Chironomus riparius	BYI 02960	chronic	NOEC	0.0105
Chironomus riparius	BYI 02960 SL200	chronic	NOEC	0.012
Chironomus riparius	BYI 02960 – succinamide	acute	EC50	> 100
Daphnia magna	BYI 02960 – succinamide	chronic	NOEC	43.3
Chironomus riparius	BYI 02960 – azabicyclosuccinamide	acute	EC50	> 100
Daphnia magna	DFA	acute	EC50	> 10
Chironomus riparius	DFA	chronic	NOEC	> 100
Chironomus tenants	6-CNA	acute	LC50	1
Chironomus riparius	6-CNA	chronic	NOEC	> 100
Algal species				
Pseudokirchneriella subcapitata	BYI 02960	chronic	E_rC_{50}	> 80

Pseudokirchneriella subcapitata	BYI 02960 SL200	chronic	E_rC_{50}	> 42.5
Pseudokirchneriella subcapitata	BYI 02960 – succinamide	chronic	E_rC_{50}	> 10
Pseudokirchneriella subcapitata	DFA	chronic	E_rC_{50}	> 10
Pseudokirchneriella subcapitata	6-CNA	chronic	E_rC_{50}	> 100
Aquatic plants				
Lemna gibba	BYI 02960	Chronic	E_bC_{50}	> 67.7
Microcosm or mesocosm tests:				
Not applicable				

Toxicity/exposure ratios for the most sensitive aquatic organisms (OECD data point IIIA 10.2.1)

BYI 02960

Application rate (kg as/ha)	Crop	Organism	Time-scale	Distance (m)	Scenario	TER	TER risk assesment trigger*
1 x 0.150	Hop	*Chironomus riparius*	acute	Step 3	R1 pond	157	100
			acute	Step 3	R1 stream	11	100
			acute	Step 4 0m + 90% drift reduction	R1 stream	112	100
			chronic	Step 3	R1 pond	30	10
			chronic	Step 3	R1 stream	2	10
			chronic	Step 4 0m + 90% drift reduction	R1 stream	22	10
1 x 0.125	Lettuce	*Chironomus riparius*	acute	Step 3	D3 ditch, 1	75	100
			acute		D3 ditch, 2	74	100
			acute		D4 pond	60	100
			acute		D4 stream	78	100
			acute		D6 ditch,	49	100
			acute		R1 pond, 1	1033	100
			acute		R1 stream,1	72	100
			acute		R1 pond, 2	639	100
			acute		R1 stream, 2	52	100
			acute		R2 stream, 1	39	100
			acute		R2 stream, 2	66	100
			acute		R3 stream, 1	28	100
			acute		R3 stream, 2	17	100
			acute		R4 stream, 1	119	100
			acute		R4 stream, 2	13	100
			acute	Step 4	D3 ditch, 1	143	100

				0m + 50% drift reduction			
			acute	Step 4 0m + 50% drift reduction	D3 ditch, 2	139	100
			acute	Step 4 10m	R1 stream, 1	159	100
			acute		R1 stream, 2	115	100
			acute		R2 stream, 2	147	100
			acute	Step 4 20m	D4 pond, 1	60	100
			acute		D4 stream, 1	86	100
			acute		D6 ditch, 1	49	100
			acute		R2 stream, 1	165	100
			acute		R3 stream, 1	117	100
			acute		R3 stream, 2	72	100
			acute		R4 stream, 2	54	100
			chronic	Step 3	D3 ditch, 1	14	10
			chronic		D3 ditch, 2	14	
			chronic		D4 pond, 1	12	
			chronic		D4 stream, 1	15	
			chronic		D6 ditch, 1	9	
			chronic		R1 pond, 1	200	
			chronic		R1 stream, 1	14	
			chronic		R1 pond, 2	124	
			chronic		R1 stream, 2	10	
			chronic		R2 stream, 1	8	
			chronic		R2 stream, 2	13	
			chronic		R3 stream, 1	5	
			chronic		R3 stream, 2	3	
			chronic		R4 stream, 1	23	
			chronic		R4 stream, 2	2	
			chronic	Step 4 10m	D6 ditch, 1	9.5	
			chronic		R2 stream, 1	17	
			chronic		R3 stream, 1	12	
			chronic		R3 stream, 2	7	
			chronic		R4 stream, 2	5	

			chronic	Step 4 20m	D6 ditch, 1	9.5	
			chronic		R3 stream, 2	14	
			chronic		R4 stream, 2	10.5	

BYI 02960 metabolites

Application rate (kg as/ha)	Crop	Organism	Time-scale	Distance (m)	TER	TER risk assesment trigger*
BYI 02960 succinamide						
1 x 0.150	Hop	*C. riparius*	acute	Step 2	> 24 600	100
1 x 0.125	Lettuce	*C. riparius*	acute	Step 2	> 206 612	100
BYI 02960 -azabicyclosuccinamide						
1 x 0.150	Hop	*C. riparius*	acute	Step 2	> 40 016	100
1 x 0.125	Lettuce	*C. riparius*	acute	Step 2	> 336 700	100
6-CNA						
1 x 0.150	Hop	*C. tentans*	acute	Step 2	2 160	100
1 x 0.150	Hop	*C. riparius*	chronic	Step 2	≥ 215 983	10
1 x 0.125	Lettuce	*C. tentans*	acute	Step 2	1 727	100
1 x 0.150	Hop	*C. riparius*	chronic	Step 2	≥ 172 712	10
DFA						
1 x 0.150	Hop	*C. riparius*	chronic	Step 2	≥ 70 274	10
1 x 0.125	Lettuce	*C. riparius*	chronic	Step 2	≥ 41 982	100

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Bioconcentration

	No fish bioconcentration study presented or required Log Pow < 3
Bioconcentration factor (BCF)	
Risk assessment trigger (practical conditions of use) for the bioconcentration factor	
Clearance time (CT_{50}) (CT_{90})	
Level of residues (%) in organisms after the 14 day depuration phase	

Effects on honeybees (OECD data points IIA 8.7 and IIIA 10.4)

Acute oral toxicity	BYI 02960	LD_{50} 1.2 µg/bee
	BYI 02960 SL200	LD_{50} 3.2 µg/bee
	BYI 02960-DFEAF	LD_{50} > 82.5 µg/bee
	BYI 02960-OH	LD_{50} > 105.3 µg/bee
	DFA	LD_{50} > 107/9 µg/bee
	6-CNA	LD_{50} > 107.1 µg/bee
	BYI 02960 –CHMP	LD_{50} > 106.7 µg/bee
Acute contact toxicity	BYI 02960	LD_{50} 122.8 µg/bee
	BYI 02960 SL200	LD_{50} 15.7 µg a.i /bee
	BYI 02960-DFEAF	LD_{50} > 100 µg/bee
	BYI 02960-OH	LD_{50} > 100 µg/bee
	DFA	LD_{50} > 100 µg/bee
	6-CNA	LD_{50} > 100 µg/bee
	BYI 02960 -CHMP	LD_{50} > 100 µg/bee

Hazard quotients for honey bees (OECD data point number IIIA 10.4.1)

Application rate (kg as/ha)	Crop	Route	Hazard quotient	Hazard quotient risk assessment trigger *
Laboratory tests				
1 x 0.150	Hops	Oral Oral Contact Contact	125 (a.i.) 47 (SL 200) 1.2 (a.i.) 9.6 (SL 200)	50 50 50 50
1 x 0.125	Lettuce	Oral Oral Contact Contact	104 (a.i.) 39 (SL200) 1.0 (a.i.) 8.0 (SL200)	50 50 50 50
Field or semi-field tests				
Six independent semi-field (gauze tunnel) studies, where BYI 02960 formulations were applied to the highly bee attractive surrogate crop Phacelia tanacetifolia with honey bees actively foraging on the crop (i.e. during bee flight). In one pilot research semi-field study, BYI 02960 was applied during bee flight at a rate of 75 and 150 g a.i./ha, respectively, and in a 2nd pilot research semi-field study, BYI 02960 was applied during bee flight at a rate of 150 g a.i./ha. In four further independent (GLP-compliant) semi-field studies, conducted in Germany, Denmark and Italy, BYI 02960 was always applied at a rate corresponding to 200 g a.i./ha during full flowering of Phacelia tanacetifolia with honey bees actively foraging on the crop (i.e. during bee flight). In all of these four GLP-compliant semi-field studies, the Phacelia-crop received, in addition to the full-flowering treatment, a pre-flowering application, just before onset of flowering, also at a rate corresponding to 200 g a.i./ha. In two of these four GLP-compliant semi-field studies, there was in addition to the two sequential foliar applications also a soil treatment at a rate corresponding to 300 g a.i./ha at the day of sowing of the Phacelia-seeds. In one of these four GLP-compliant semi-field studies, additionally a detailed, quantitative digital brood assessment of individually marked cells has been conducted. The results of all of the six semi-field (tunnel) studies under forced and as such worst-case exposure conditions consistently did not show any adverse effects on mortality, foraging activity, behaviour, brood-, food- and population development or on overall colony vitality.				

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Effects on other arthropod species (OECD data points IIA 8.8.1, IIA 8.8.2 and IIIA 10.5)

Species	Stage	Test Substance	Dose (g as/ha)	Endpoint	Effect	Annex VI Trigger*
Laboratory tests						
Tier 1 glass plates						
Aphidius rhopalosiphi	Adult	BYI 02960 SL 200	LR_{50} < 0.5	Mortality	100%	50%-
Typhlodromus pyri	Adult	BYI 02960 SL 200	LR_{50} 17.3	Mortality	< 50%	50%
Extended laboratory						
Aphidius rhopalosiphi	Adult	BYI 02960 SL 200	LR_{50} 2.02	Mortality	100%	50%
Typhlodromus pyri	Adult	BYI 02960 SL 200	LR_{50} 177	Mortality	< 50%	50%
Coccinella septempunctata	Adult	BYI 02960 SL 200	LR_{50} 273.9	Mortality	< 50%	50%
Aleochara bilineata	Adult	BYI 02960 SL 200	ER_{50} > 300	Reproduction	13%	50%

Aged residue laboratory						
Aphidius rhopalosiphi	Adult	BYI 02960 SL 200	2 x 250 at 10 day interval;	Mortality Reproduction	< 50% after 42 d < 50% after 49d	50%
Orius laevigatus	adult	BYI 02960 SL 200	2 x 250 at 10 day interval;	Mortality	< 50% after 28 days	50%
Field or semi-field tests						
BYI 02960 SL 200 (g/L) Netherlands: NTA full fauna off-crop field study. Spray application rates: 0.51, 1.7, 5.1, 21 g a.i./ha Community level NOER = 21 g a.i./ha Population level NOER = 5.1 g a.i./ha Population level NOEAER = 21 g a.i./ha SW France: NTA full fauna off-crop field study. Spray application rates: 0.51, 1.7, 5.1, 21 g a.i./ha Community level NOER = 21 g a.i./ha Population level NOER = 1.7 g a.i./ha Population level NOEAER = 21 g a.i./ha NOER: No Observed Effect Rate NOEAER: No Observed Ecologically Adverse Effect Rate						

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Effects on earthworms (OECD data points IIA 8.9 and IIIA 10.6)

Acute toxicity	BYI 02960	LC50 192.9 mg/kg dws
	BYI 02960 SL200	LC50 709 mg product/kg dws
	DFA	LC50 > 1000 mg/kg dws
	6-CNA	LC50 > 1000 mg/kg dws
Reproductive toxicity	BYI 02960 SL200	NOEC 8.9 mg prod/kg soil
	DFA	NOEC 62 mg/kg dws
	6-CNA	NOEC 95 mg/kg dws
Field Study Eartworm fauna	Reduction of abundance (-33%) and biomass (-38%) at 1500 g a.i./ha and biomass at 600 g a.i./ha (-36%) after 1 month; full recovery of earthworm population after 11 months	

Toxicity/exposure ratios for earthworms (OECD data point IIIA 10.6.1)

Application rate (kg as/ha)	Crop	Substance	Time-scale	TER	Risk assessment trigger *
1 x 0.150g	Hop	BYI 02960 SL200	acute	1509	10
		BYI 02960	acute	1206	10
		DFA	acute	> 111 111	10
		6-CNA	acute	≥ 142 857	10
		BYI 02960 SL200	chronic	19	5
		DFA	chronic	6889	5
		6-CNA	chronic	13 571	5
1 x 0.125	Lettuce	BYI 02960 SL200	acute	1035	10
		BYI 02960	acute	1237	10
		DFA	acute	> 71 429	10
		6-CNA	acute	> 83 333	10
		BYI 02960 SL200	chronic	13	5
		DFA	chronic	4429	5
		6-CNA	chronic	7917	5

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Toxicity/exposure ratios for other soil non-target macro-organisms (OECD data point IIIA 10.6.6)

Application rate (kg as/ha)	Crop	Substance	Time-scale	TER	Risk assessment trigger *
Folsomia candida **1 x 150g/ha**	Hop	BYI 02960 SL200	Chronic	12	5
		DFA	Chronic	≥ 7143	5
		6-CNA	Chronic	7500	5
1 x 125g/ha	Lettuce	BYI 02960 SL200	Chronic	≥ 1460	5
		DFA	Chronic	≥ 71 429	5
		6-CNA	Chronic	≥ 8333	5

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Effects on soil micro-organisms (OECD data points IIA 8.10 and IIIA 10.7)

Nitrogen mineralization	< 25% effect after 28 days 12.44 L product/ha
Carbon mineralization	< 25% effect after 28 days 12.45 L product/ha