CONCLUSION ON PESTICIDE PEER REVIEW

Conclusion regarding the peer review of the pesticide risk assessment of the active substances sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate

Issued on 30 September 2008

SUMMARY

Sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate are three of the 84 substances of the third stage Part B of the review programme covered by Commission Regulation (EC) No 1490/2002[1]. This Regulation requires the European Food Safety Authority (EFSA) to organise upon request of the EU-Commission a peer review of the initial evaluation, i.e. the draft assessment report (DAR), provided by the designated rapporteur Member State and to provide within six months a conclusion on the risk assessment to the EU-Commission.

Greece being the designated rapporteur Member State submitted the DAR on sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate in accordance with the provisions of Article 10(1) of the Regulation (EC) No 1490/2002, which was received by the EFSA on 27 September 2007. The peer review was initiated on 24 October 2007 by dispatching the DAR for consultation of the Member States and the sole applicant Arysta LifeScience SAS. Subsequently, the comments received on the DAR were examined and responded by the rapporteur Member State in the reporting table. This table was evaluated by the EFSA to identify the remaining issues. The identified issues as well as further information made available by the applicant upon request were evaluated in a series of scientific meetings with Member State experts in June – July 2008.

A final discussion of the outcome of the consultation of experts took place during a written procedure with the Member States in September 2008 leading to the conclusions as laid down in this report.

The conclusion was reached on the basis of the evaluation of the representative uses as plant growth stimulators in sugar beet, oilseed rape and tomato for qualitative and quantitative yield improvement as proposed by the notifier. Full details of the GAP can be found in the attached endpoints.

[1] OJ No L 224, 21.08.2002, p. 25, as amended by Regulation (EC) No 1095/2007 (OJ L 246, 21.9.2007, p. 19)

The representative formulated product for the evaluation was 'Atonik', a soluble concentrate (SL) containing 1 g/l sodium 5-nitroguaiacolate 2 g/l sodium *o*-nitrophenolate and 3 g/l sodium *p*-nitrophenolate.

The specifications for the technical materials currently should be regarded as provisional (September 2008).

Analytical methods as well as methods and data relating to physical, chemical and technical properties are available to ensure that quality control measurements of the plant protection product is possible; however a data gap was identified for additional validation data for determination of relevant impurities in the technical materials.

Adequate analytical methods are available to monitor all compounds given in the respective residue definitions in food/feed of plant origin and environmental matrices.

With regard to its toxicological properties, the mixture 'Atonik' was shown to be rapidly and extensively absorbed, widely distributed in the body without bioaccumulation and excreted mainly via urine. The proposed classification for the acute toxicity was **Xn**; **R22** "**Harmful if swallowed**" for the three active substances; **Xi**; **R36** "**Irritating to eyes**" for sodium *o*-nitrophenolate (Na *o*-NP) and sodium *p*-nitrophenolate (Na *p*-NP); and **Xi**; **R41** "**Risk of serious damage to eyes**" for sodium 5-nitroguaiacolate (Na 5-NG). In the short-term studies, the most sensitive species was the dog, with the lungs, liver and kidney as target organs at higher doses. However the NOAEL was based on clinical findings at lower doses (soft/mucous faeces and vomiting). Even though some positive results were observed during the *in vitro* genotoxicity studies, the negative results in the *in vivo* testing were supported by the absence of a carcinogenic potential in the long-term studies. With regard to reproductive toxicity testing, the fertility index was decreased in the presence of maternal toxicity at the high dose level, but no adverse effect was noted in the offspring. No teratogenic effect was observed in developmental studies with rats and rabbits. There were some indications of foetotoxicity in rabbits, but they were attributed to maternal toxicity. In the rabbit study, no maternal NOAEL could be derived since clinical signs were observed in dams at all dose levels.

For the derivation of the reference values, it was agreed to set values applicable separately to the three active substances. Additionally, it was decided to use the toxicological studies with the mixture 'Atonik' since they are providing lower NOAELs for the active substances (based on their ratio in the mixture) than the studies with the individual active substances. Consequently the agreed values were based on the lowest individual NOAEL value in the relevant study with the mixture, applicable to the three active substances as a conservative and pragmatic approach. Therefore the agreed **acceptable daily intake** (ADI) is **0.003 mg/kg bw/day** based on the 1-year dog study with the use of a safety factor of 100. Similarly, the agreed **acceptable operator exposure level** (AOEL) is **0.007 mg/kg**

bw/day based on the 90-day dog study and using a safety factor of 100. The agreed **acute reference dose** (ARfD) is **0.045 mg/kg bw** based on the developmental study with rabbit, and applying an increased safety factor of 300 due to the use of a LOAEL (maternal) instead of a NOAEL. In the absence of experimental results, the agreed dermal absorption value of 100% was adopted. The sum of the operator exposure estimates for the three active substances give a total exposure level below the AOEL when PPE is used during field application with tractor or greenhouse use, but the exposure is above the AOEL even with PPE in the case of hand-held application in field. The use of PPE is also required for workers re-entering treated fields, but the exposure level of bystander is below the AOEL.

Plant metabolism studies have been performed on sugar beet, tomato and rapeseed after foliar applications of ^{14}C-'Atonik', a mixture of the three active substances Na 5-NG, Na *o*-NP and Na *p*-NP, using exaggerated application rates up to 10 times the total normal dose rate. At harvest the TRR was low in beet roots, tomato fruits and rape seeds, in the range of 0.034 to 0.049 mg/kg and no parent active substances or unidentified metabolites were observed at levels higher than 0.013 mg/kg. However in beetroot leaves, it was considered that the two unknown metabolites M6 and M7 could be above 0.01 mg/kg when 'Atonik' is applied at a normal dose rate and additional information was requested on the possible structure of these two compounds. Three separate residue definitions were proposed in the DAR for each individual compound as "Na 5-NG", "Na *o*-NP" and "Na *p*-NP" respectively. Nevertheless, after the meeting and taking into account the conclusion of the PRAPeR 54 meeting on mammalian toxicology setting the same ADI and ARfD values for the three constituent active substances, the EFSA was of the opinion that it could be possible to propose a single residue definition for monitoring as "sum of 5-NG, *o*-NP and *p*-NP", this proposal having to be considered as not peer reviewed. No supervised residue trials were presented and the meeting of experts, considering low application rates and the metabolism study results, agreed that such trials are not necessary and confirmed the MRL values set at the LOQ. Processing studies and animal metabolism studies were not provided since significant residues of Na 5-NG, Na *o*-NP and Na *p*-NP are not expected in plant commodities. No rotational crop studies were submitted with regard to the low DT_{50} values. The MRLs of 0.01* mg/kg were initially proposed in the DAR for each of the individual active substances. Nevertheless and based on the single residue definition, the EFSA is of the opinion that MRLs of 0.03* mg/kg (sum of the LOQ achieved for each individual active substance) should be more appropriate. The chronic and acute consumer risk assessments showed that the TMDI and IESTI did not exceed the ADI and the ARfD respectively.

In soil under aerobic conditions Na 5-NG, Na *o*-NP and Na *p*-NP exhibit very low to low persistence forming the unknown major soil metabolite M5 (accounting for a maximum of 20.5% of applied radioactivity (AR)). Mineralisation to carbon dioxide was significant, accounting for 54.9-60.8% AR after 120 days. The formation of unextractable residues was a sink accounting for 32.1% to 41.1% of the applied radioactivity after 120 days. Na 5-NG exhibits medium to low mobility in soil, whereas

Na *o*-NP and Na *p*-NP exhibit high to low mobility in soil. There was no evidence of a correlation of adsorption with any soil parameter.

In dark natural sediment water systems, Na 5-NG, Na *o*-NP and Na *p*-NP degraded exhibiting fast disappearance from the water column and from the whole system. The terminal metabolite, carbon dioxide, accounted for 66.1-63.5% AR at 122 days (end of study). Unextracted sediment residues were a sink representing 30.7% - 34.6% AR at study end. Major metabolites were not found in this study, however in the aqueous photolysis study several unknown metabolites were observed. Risk assessment for these photolytic metabolites was required by the peer review. FOCUS surface water modelling was carried out up to step 2 for the individual active substances. These values form the basis for the risk assessment discussed in this conclusion.

The potential for groundwater exposure from the applied for intended uses of these active substances to exceed the parametric drinking water limit of 0.1 µg/L, was concluded to be low in geoclimatic situations that are represented by all 9 FOCUS groundwater scenarios. However, based on a worst case calculation for the unknown metabolite M5, in geoclimatic regions represented by the Jokionen FOCUS groundwater scenario, contamination of groundwater above the 0.1 µg/L limit cannot be excluded for application to sugar beet. Therefore the identification of this unknown metabolite M5 and ground water modelling with a second model were required by the peer review.

A low acute, short-term and long-term risk was assessed for terrestrial vertebrates in a first-tier assessment for the representative uses.

Na 5-NG, Na *o*-NP and Na *p*-NP were toxic to aquatic organisms (**N** "**Dangerous for the environment**", **R51/R53** "**Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment**"). Algae were the most sensitive organisms tested. As these active substances are "plant growth regulators" the meeting agreed to require further studies such as a second algae species and *Lemna* tests. On the basis of available data, a low first-tier risk was identified for aquatic organisms. According to the fate meeting conclusion, a data gap was identified to further address the risk to aquatic organisms from the photolytic metabolites.

The risk was assessed as low for bees, non-target arthropods, earthworms, soil macro and micro-organisms and other non-target organisms. No risk was expected to biological methods for sewage treatment, but the experts agreed that at member state level the effects should be addressed in case agricultural practices induce a possible concern to sewage treatment plants.

Key words: sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate, sodium *p*-nitrophenolate, peer review, risk assessment, pesticide, plant growth regulator

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BACKGROUND

Commission Regulation (EC) No 1490/2002 laying down the detailed rules for the implementation of the third stage of the work program referred to in Article 8(2) of Council Directive 91/414/EEC and amending Regulation (EC) No 451/2000 as amended by Commission Regulation (EC) No 1095/2007, regulates for the European Food Safety Authority (EFSA) the procedure of evaluation of the draft assessment reports provided by the designated rapporteur Member State. Sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate are three of the 84 substances of the third stage, part B, covered by the Regulation (EC) No 1490/2002 designating Greece as rapporteur Member State.

In accordance with the provisions of Article 10(1) of the Regulation (EC) No 1490/2002, Greece submitted the report of its initial evaluation of the dossier on sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate, hereafter referred to as the draft assessment report, received by the EFSA on 27 September 2007. Following an administrative evaluation, the draft assessment report was distributed for consultation in accordance with Article 11(2) of the Regulation (EC) No 1490/2002 on 24 October 2007 to the Member States and the main applicant Arysta LifeScience SAS as identified by the rapporteur Member State.

The comments received on the draft assessment report were evaluated and addressed by the rapporteur Member State. Based on this evaluation, the EFSA identified and agreed on lacking information to be addressed by the notifier as well as issues for further detailed discussion at expert level.

Taking into account the requested information received from the notifier, a scientific discussion took place in expert meetings in June – July 2008. The reports of these meetings have been made available to the Member States electronically.

A final discussion of the outcome of the consultation of experts took place during a written procedure with the Member States in September 2008 leading to the conclusions as laid down in this report.

During the peer review of the draft assessment report and the consultation of technical experts no critical issues were identified for consultation of the Scientific Panel on Plant Protection Products and their Residues (PPR).

In accordance with Article 11c(1) of the amended Regulation (EC) No 1490/2002, this conclusion summarises the results of the peer review on the active substance and the representative formulation evaluated as finalised at the end of the examination period provided for by the same Article. A list of the relevant endpoints for the active substance as well as the formulation is provided in appendix 1.

The documentation developed during the peer review was compiled as a **peer review report** comprising of the documents summarising and addressing the comments received on the initial evaluation provided in the rapporteur Member State's draft assessment report:

- the comments received,
- the resulting reporting table (revision 1-1; 6 May 2008),

as well as the documents summarising the follow-up of the issues identified as finalised at the end of the commenting period:

- the reports of the scientific expert consultation,
- the evaluation table (revision 2-1; 30 September 2008).

Given the importance of the draft assessment report including its addendum (compiled version of September 2008 containing all individually submitted addenda) and the peer review report with respect to the examination of the active substance, both documents are considered respectively as background documents A and B to this conclusion.

THE ACTIVE SUBSTANCE AND THE FORMULATED PRODUCT

Sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate are the common names for sodium 2-methoxy-5-nitrophenolate, sodium 2-nitrophenolate (or sodium *o*-nitrophenolate) and sodium 4-nitrophenolate (or sodium *p*-nitrophenolate) (IUPAC). No ISO common names exist for these compounds.

Sodium 5-nitroguaiacolate (Na 5-NG), sodium *o*-nitrophenolate (Na *o*-NP) and sodium *p*-nitrophenolate (Na *p*-NP) belong to the class of nitrophenolate plant growth regulators. They act as plant growth stimulators which increase nutrient uptake by the acceleration of cytoplasmic streaming and increase of assimilates uptake, by prolongation of auxin activity by inhibiting the IAA (indolylacetic acid) oxydases and inhibition of ABA (abscissic acid) effects and by increase of the nitrate reductase activity. They are translocated in plants systemically. Na 5-NG, Na *o*-NP and Na *p*-NP are used in agriculture in sugar beet, oilseed rape and tomato for qualitative and quantitative yield improvement.

The representative formulated product for the evaluation was 'Atonik', a soluble concentrate (SL) containing 1 g/l Na 5-NG, 2 g/l Na *o*-NP and 3 g/l Na *p*-NP, registered in EU member states under different trade names.

The representative uses evaluated comprise foliar spraying:

-on sugar beet, from growth stage of BBCH 12 up to growth stage of BBCH 49, in all EU countries, at maximum four applications at a maximum application rate per treatment of 1 g Na 5-NG, 2 g Na *o*-NP and 3 g Na *p*-NP/ha, with interval between applications of minimum 7-30 days;

-on oilseed rape, from growth stage of BBCH 31 up to growth stage of BBCH 69, in all EU countries, at maximum two applications at a maximum application rate per treatment of 1 g Na 5-NG, 2 g Na *o*-NP and 3 g Na *p*-NP/ha, with interval between applications of minimum 30-60 days;

-on tomato, at growth stages of BBCH 59, 69, 71, 79, 81, in all EU countries, at maximum five applications at a maximum application rate per treatment of 1 g Na 5-NG, 2 g Na *o*-NP and 3 g Na *p*-NP/ha, with interval between applications of minimum 14 days.

SPECIFIC CONCLUSIONS OF THE EVALUATION

1. Identity, physical/chemical/technical properties and methods of analysis

The minimum purity of the technical Na 5-NG could not be concluded on, as the experts at the PRAPeR Meeting 51 (June 2008) did not accept the technical specification for this active substance. The minimum purity of the technical Na *o*-NP is 980 g/kg and of the technical Na *p*-NP is 998 g/kg (values corresponding to the dihydrate form). No FAO specifications exist.

The experts at the PRAPeR Meeting 54 (July 2008) agreed that impurities phenol, 2,4-dinitrophenol and 2,6-dinitrophenol are toxicologically relevant and their upper level in the technical specification of the individual three active substances should be the LOQ. The LOQs for 2,4-dinitrophenol and 2,6-dinitrophenol in Na *o*-NP and Na *p*-NP are given in appendix 1. The LOQs for phenol are still open.

Besides the specifications, assessment of the data package revealed no issues that need to be included as critical areas of concern with respect to the identity, physical, chemical and technical properties of Na 5-NG, Na *o*-NP and Na *p*-NP or the respective formulation, however the following data gaps were identified:

-justification for the maximum level of 1 g/kg for impurity 1 of Na 5-NG technical material;

-to provide revised specification of technical Na 5-NG and to submit the amended report containing information about other two impurities;

-to provide revised specification of the impurities of technical Na *o*-NP and technical Na *p*-NP and to submit the amended report containing information about three impurities;

-confirmation of the identity of impurity 2 and based on the identity further data on the analytical method may be necessary;
-fully validated analytical method for the determination of the relevant impurities;
-to clarify if impurities in the technical materials contribute to the explosive properties of the active substance;
-information demonstrating that concentrations of the relevant impurities do not increase on storage.

As a consequence, the specifications for the technical materials currently should be regarded as provisional (September 2008).

The main data regarding the identity of Na 5-NG, Na *o*-NP and Na *p*-NP and their physical and chemical properties are given in appendix 1.

Adequate HPLC-UV methods are available for the determination of Na 5-NG, Na *o*-NP and Na *p*-NP in the technical materials and in the representative formulation and for the determination of the impurities in the technical materials, however a data gap was identified for additional validation data for the relevant impurities in the technical materials.

Sufficient test methods and data relating to physical, chemical and technical properties and analytical methods are available to ensure that quality control measurements of the plant protection product are possible.

Adequate methods are available to monitor all compounds given in the respective residue definitions in food/feed of plant origin and environmental matrices. The methods available determine the three compounds concurrently.

A HPLC-MS/MS method with column switching is available to monitor residues in food/feed of plant origin with LOQ 0.01 mg/kg (sugar beet, oil seed rape, tomatoes) for each individual compound.

Since residues in foodstuff of animal origin will not reach a level of significance, no analytical methods are required for the determination of Na 5-NG, Na *p*-NP and Na *o*-NP residues in matrices of animal origin.

Adequate HPLC-MS/MS methods with column switching are available to monitor residues of Na 5-NG, Na *o*-NP and Na *p*-NP in soil with LOQ of 0.01 mg/kg; in drinking, surface and ground water with a LOQ of 0.1µg/L and in air with a LOQ of 1.25µg/m^3 for each individual compound.

Analytical methods for the determination of residues in body fluids and tissues are not required as Na 5-NG, Na *o*-NP and Na *p*-NP are not classified as toxic or highly toxic.

2. Mammalian toxicology

The active substances were discussed by the experts in mammalian toxicology in July 2008 (PRAPeR meeting 54, round 11). The available toxicology and metabolism studies have been conducted with either the individual active substances (Na 5-NG, Na *o*-NP and Na *p*-NP) or different mixtures of these three active substances in a ratio 1:2:3 (dry formulation of 'Atonik' or 'Atonik' Manufacturing Use Product powder).

The information on the toxicological batches was provided in Volume 4 of the DAR, in addendum 1 to Volume 4 of the DAR, in Volume 3 (B.6) of the DAR, and summarised in a paper distributed during the meeting (see report of PRAPeR 54). The detailed composition was only available for three of the batches used in metabolism, acute and short-term studies with the individual active substances. Nevertheless, taking into account an unchanged manufacturing process and the low levels of impurities (often at the limit of quantification), it was agreed that they were sufficiently representative of the technical specifications. Additionally it was considered that the impurities phenol, 2,4-dinitrophenol and 2,6-dinitrophenol were relevant and should not exceed the limit of quantification in the technical specification of the three individual active substances.

2.1. Absorption, Distribution, Excretion and Metabolism (Toxicokinetics)

In the first study, the individual active substances (Na 5-NG, Na *o*-NP, Na *p*-NP) were investigated separately. Due to major limitations, the results were only considered as indicative of a rapid absorption.

In the second study, the mixture 'Atonik' was shown to be rapidly and extensively absorbed (max. blood concentration within 0.5h) with an increase of the ratio blood/plasma at 96 hours post dosing suggesting binding of radioactivity to blood cells. Widely distributed, with the highest concentrations in carcass, kidney, liver and the intestinal tract, the active substances did not show bioaccumulation and were mainly excreted via urine (82-95% within 96h). The major metabolic pathway (ca 60% of the administered dose) included glucurono- and sulfo- conjugations.

2.2. Acute toxicity

Based on studies with rats and rabbits, all three active substances of 'Atonik' mixture were considered to be of moderate acute oral toxicity (LD_{50} 716 mg/kg bw for Na 5-NG, 960 mg/kg bw for Na *o*-NP and 345 mg/kg bw for Na *p*-NP), and low acute dermal and inhalation toxicity (dermal LD_{50} >2000 mg/kg bw and LC_{50} greater than the maximum attainable concentration). Additionally, they are

not skin irritants or skin sensitizers (based on Buehler tests with limitations, but supported by medical data and a Magnusson & Kligman test with the formulation). However, all of them may cause irritation to the eyes of rabbits. Therefore, the proposed classification is **Xn**; **R22** "**Harmful if swallowed**" for the three active substances; **Xi**; **R36** "**Irritating to eyes**" for Na *o*-NP and Na *p*-NP; and **Xi**; **R41** "**Risk of serious damage to eyes**" for Na 5-NG based on irreversible effects in the eyes still present at the end of the test.

2.3. SHORT TERM TOXICITY

Oral short-term studies were performed with Na 5-NG (90-day dog), Na *o*-NP (90-day dog), Na *p*-NP (90-day dog) and the 'Atonik' mixture powder (28 and 90-day rat, 90-day and 1-year dog). The most sensitive species, based on the available data, was identified to be the dog.

In the 90-day rat study, the target organs were kidney and spleen. No NOAEL could be determined as pigmentation of spleen (and minimal pigmentation of the kidney) was observed at the lowest dose level, resulting in a LOAEL of 489 mg 'Atonik'/kg bw/day.

In the dog studies, the target organs at the high doses (≥12 mg/kg bw/day) were the lungs, liver and kidneys. However the meeting considered that clinical findings of soft/mucous faeces and vomiting at the mid dose were adverse effects determining the NOAEL in most of the studies. Consequently, the agreed relevant NOAEL for the 90-day studies was 6 mg 'Atonik'/kg bw/day and the agreed NOAEL for the 1-year study was 2.5 mg 'Atonik'/kg bw/day.

In the DAR, it was proposed to derive separate NOAELs for the three active substances based on the studies performed with 'Atonik' and using the ratio of the mixture (1:2:3 for Na 5-NG:Na *o*-NP:Na *p*-NP). Here is the proposal made during the meeting based on the agreed NOAELs for 'Atonik':

NOAELs (mg/kg bw/day)	'Atonik'	Na 5-NG	Na *o*-NP	Na *p*-NP
90-day dog	6	0.7	1.39	2.56
1-year dog	2.5	0.29	0.58	1.01

During the discussions it was agreed to consider the studies performed with the 'Atonik' mixture since the derived NOAELs for the three active substances were lower than those from the studies with the individual active substances. However, it was also noted that these derived NOAELs (from the NOAEL for the mixture) were only valid when the active substances are mixed in the same ratio since their individual contribution to the systemic toxicity of the mixture was not known.

2.4. GENOTOXICITY

The genotoxicity studies were performed separately with the three active substances. They were tested *in vitro* for gene mutation in an Ames test and in mouse lymphoma cells, for DNA damage in a Bacillus subtilis rec assay and for chromosome aberration in Chinese hamster ovary cells. Taking into account further details provided for some of these studies in addendum 1 to Volume 3 of the DAR (June 2008), the experts agreed that Na 5-NG was weakly positive for the induction of gene mutations in mouse lymphoma cells only in the presence of metabolic activation, and that Na *p*-NP was positive in the mouse lymphoma assay. The other results *in vitro* were all negative.

With regard to the *in vivo* testing, a micronucleus test in bone marrow cells of mice was performed for each compound with negative results, and the results after intraperitoneal administration for Na *o*-NP and Na *p*-NP were considered acceptable by the experts.

The need for further test to detect the gene mutation potential *in vivo* was discussed in the meeting. Even though the micronucleus test is not aimed at detecting gene mutation potential (but chromosome aberrations), the experts agreed that it was supported by the absence of carcinogenic potential in the long-term studies and that no further *in vivo* study was required.

2.5. LONG TERM TOXICITY

The long-term toxicity/carcinogenicity of the 'Atonik' mixture was investigated in rats (2-year study) and mice (18-month study).

Two rat studies were presented in the DAR, but the first one was of poor quality and considered to be unacceptable. For the second study, the additional results of gross and microscopic pathology examinations (provided in addendum 1 to of the DAR 3; June 2008) didn't reveal any carcinogenic potential. Due to an important food spillage during the study, the meeting agreed with the use of a conversion factor of 20 to estimate the achieved intakes. Therefore the systemic NOAEL was 500 mg 'Atonik'/kg bw/day based on clinical signs and decreased body weight gain at 1000 mg 'Atonik'/kg bw/day.

In the 18-month mouse study, no adverse effects (neither tumorigenic nor systemic effects) were observed up to the highest dose level, resulting in a NOAEL of 20000 ppm. Due to the food spillage, the proposed use of a conversion factor 7 was accepted for the derivation of the actual intake, resulting in a NOAEL of 2857 mg 'Atonik'/kg bw/day.

In the DAR, it was proposed to derive separate NOAELs for the three active substances based on the studies performed with 'Atonik' and using the ratio of the mixture (see further considerations in 2.3).

2.6. REPRODUCTIVE TOXICITY

The reproductive toxicity of 'Atonik' was assessed in two multigeneration studies with rats, and in two developmental studies, one with rats and the other with rabbits.

The first **multigeneration** study (Shouyang, 1990) had significant limitations and was considered unacceptable. In the second multigeneration study, the administration of 'Atonik' resulted in decreased fertility index in the presence of parental toxicity at the high dose level. Therefore the agreed parental and reproductive NOAEL was 300 mg 'Atonik'/kg bw/day, taking into account decreased body weight gain and histopathological alterations in several organs. No adverse effect was observed in the offspring up to a NOAEL of 600 mg 'Atonik'/kg bw/day.

'Atonik' was tested for **developmental** effects in rats and rabbits. In rats, the maternal NOAEL was 300 mg 'Atonik'/kg bw/day based on reduced body weight gain and mortality (one animal). In rabbits, no maternal NOAEL could be established since maternal toxicity (manifested by clinical signs including ptosis, lethargy and inanition) was observed at all doses tested. Therefore, a maternal LOAEL of 100 mg 'Atonik'/kg bw/day was agreed.

With regard to developmental effects in rats, the slight increases in post-implantation losses and early resorptions were not considered adverse, being within the historical background range. Thus the agreed developmental NOAEL was the highest dose tested of 600 mg 'Atonik'/kg bw/day.

For the rabbit study, additional results of the visceral and skeletal examination of the foetuses were provided in addendum 1 to Volume 3 of the DAR (June 2008). Based on these, the experts concluded that there was some foetotoxicity, possibly explained by maternal toxicity, but no concern about the teratogenic properties; and they agreed on a developmental NOAEL of 200 mg 'Atonik'/kg bw/day based on increased incidence of extra-ribs.

In the DAR, it was proposed to derive separate NOAELs for the three active substances based on the studies performed with 'Atonik' and using the ratio of the mixture (see further considerations in 2.3). The relevant proposals are summarised in the following table:

NOAELs (mg/kg bw/day)		'Atonik'	Na 5-NG	Na *o*-NP	Na *p*-NP
2-gen.: parental /reproductive		300	39.6	77.1	140.7
offspring		600	79.2	154.2	281.4
terato. rat:	maternal	300	45.0	90.3	167.7
	developmental	600	90.0	180.6	335.4
terato. rabbit:	maternal	<100	<13.6	<26.5	<50.2
	developmental*	200	27.2	51	100.4

* derivation of these individual NOAELs has been performed after the meeting since the NOAEL has been changed, based on the ratio of the three active substances in the tested mixture

2.7. NEUROTOXICITY

The available information on 'Atonik' and its individual active substances (Na 5-NG, Na *o*-NP and Na *p*-NP) does not give any indication of neurotoxicity. Furthermore these active substances do not belong to a chemical class which is suspected to cause delayed neurotoxic effects; such as organophosphates or carbamates.

2.8. FURTHER STUDIES

No data were presented in the DAR.

2.9. MEDICAL DATA

No illness related to 'Atonik' exposure has been recorded during the manufacturing process since 1952. There are no reports of clinical cases and poisoning incidents with 'Atonik', no available epidemiological data and no specific clinical tests for poisoning.

2.10. ACCEPTABLE DAILY INTAKE (ADI), ACCEPTABLE OPERATOR EXPOSURE LEVEL (AOEL) AND ACUTE REFERENCE DOSE (ARFD)

Acceptable daily intake (**ADI**)

Based on the available data, the dog appears to be the most sensitive species, and the 1-year dog study with the 'Atonik' mixture was considered the most appropriate for the setting of the ADI.

Considering that technical specifications have been considered separately for the three active substances, the experts agreed to derive individual ADIs for each active substance. In this aim, the separate NOAELs derived from the 1-year dog study were considered by the experts (see 2.3). As a very conservative and pragmatic approach, the meeting agreed finally on the lowest individual NOAEL value of 0.29 mg/kg bw/day (for Na 5-NG) resulting in an **ADI of 0.003 mg/kg bw/day** with the use of a safety factor 100, and applicable to the three active substances.

Acceptable operator exposure level (**AOEL**)

In the DAR, it was proposed to base the AOEL on the 90-day dog study with 'Atonik', and three values were derived based on the percentage of the individual active substances in the 'Atonik' mixture.

Using the same approach than for the ADI, and the lowest individual NOAEL (for Na 5-NG) derived from the 90-day dog study with 'Atonik', the agreed **AOEL was 0.007 mg/kg bw/day** with the use of a safety factor of 100, and applicable to the three active substances.

Acute reference dose (**ARfD**)

In accordance with the rapporteur Member State's proposal, it was agreed by the meeting to use the developmental rabbit study for the derivation of the acute reference dose (based on clinical signs observed in dams at the lowest dose level). Three separate ARfD were proposed in the DAR based on the ratio of the active substances in the 'Atonik' mixture.

Using the same approach than for the ADI and AOEL, the meeting agreed to use the lowest individual value (for Na 5-NG) derived from the maternal LOAEL for the mixture, and applicable to the three active substances. This resulted in an **ARfD of 0.045 mg/kg bw/day**, with the use of an increased safety factor of 300 for the use of a LOAEL instead of a NOAEL.

2.11. DERMAL ABSORPTION

No relevant studies have been submitted. A default dermal absorption value of 100% was used for all three active substances of 'Atonik' solution.

2.12. EXPOSURE TO OPERATORS, WORKERS AND BYSTANDERS

'Atonik' is a water-based soluble concentrate formulation containing 1, 2 and 3 g/L of Na 5-NG, Na *o*-NP and Na *p*-NP respectively. It is a plant growth stimulator intended for use on sugar beet, oilseed rape in the field and tomato both in the field (outdoor) and in greenhouse (indoor).

Operator exposure

The maximum application rate is 1L product/ha in a spray volume of 200-1000 L/ha, using tractor-mounted sprayer or hand-held knapsack sprayer (in field or greenhouse). The results of the exposure estimates were compared to the agreed AOEL in addendum 2 to Annex B of the DAR (September 2008) and are presented in the table below.

Estimated exposure presented as % of AOEL (0.007 mg/kg bw/day), according to calculations with the German[2], the UK POEM[3] and the Dutch greenhouse[4] models. The default for body weight of operator is 70 kg in the German model and 60 kg in the UK-POEM model. The worst case of 1L container size has been applied in the UK POEM.

Model	No PPE	With PPE[1]	With PPE[2]
Use in field: tractor boom sprayer			
German	Na 5-NG: 18 Na *o*-NP: 36 Na *p*-NP: 54	Na 5-NG: 7 Na *o*-NP: 14 Na *p*-NP: 21	n.a.
UK POEM	Na 5-NG: 169 Na *o*-NP: 337 Na *p*-NP: 506	Na 5-NG: 14 Na *o*-NP: 27 Na *p*-NP: 41	n.a.
Use in field: hand-held application			
German	n.a.	n.a.	n.a.
UK POEM	Na 5-NG: 125 Na *o*-NP: 250 Na *p*-NP: 375	Na 5-NG: 33 Na *o*-NP: 66 Na *p*-NP: 98	n.a.
Use in greenhouse: knapsack sprayer			
Dutch greenhouse	Na 5-NG: 41 Na *o*-NP: 82 Na *p*-NP: 123	n.a.	Na 5-NG: 4 Na *o*-NP: 9 Na *p*-NP: 13

PPE[1] (personal protective equipment): gloves during mixing/loading and application, PPE[2]: gloves and coverall, n.a. = not applicable.

Concerning the intended field application, the estimated operator exposure levels for each active substance are below the AOEL without the use of PPE according to the German model for the tractor application. During hand-held application, the exposure estimates with the UK POEM are below the AOEL only with the use of personal protective equipment. In the case of greenhouse use, estimates with the Dutch greenhouse model are below the AOEL when gloves and coverall are worn by the knapsack sprayer.

EFSA note (following a comment from the UK during the written procedure of the draft conclusion): The operator is exposed to the product 'Atonik'. Therefore the exposure assessment should consider the three active substances contained in 'Atonik' (Na 5-NG, Na *o*-NP and Na *p*-NP) and the exposure

[2] Lundehn J. R. *et al*.; Uniform Principles for Safeguarding the Health of Applicators of Plant Protection Products; Mitteilungen aus der Biologischen Bundesanstalt, Heft 277, Berlin 1992.
[3] Predictive operator exposure model (POEM; UK MAFF, 2003).
[4] Van Golstein Brouwers *et al*., 1996; Assessment of occupational exposure to pesticides in agriculture; TNO Report V 96.120.

estimates for the individual active substances should be added. This approach is supported by the EFSA.

In the case of tractor application in field, this would result in the need of PPE to have a total exposure below the AOEL (42%) with the German model. The exposure from greenhouse use would still need the same level of PPE to be below the AOEL (26%). In the case of hand-held application in field, this would lead to a total exposure greater than the AOEL (197%) even with the use of PPE (UK POEM).

Worker exposure

In the DAR, it was considered that workers did not need to enter treated areas shortly after application and therefore no estimation of exposure was provided. Numerical estimates were provided in column B of the evaluation table. However the meeting agreed that the values should be recalculated with the use of a higher transfer coefficient and the agreed AOEL. Final recalculations were provided in addendum 2 to Volume 3 of the DAR (September 2008) and showed an exposure level of 18% (Na 5-NG), 37% (Na *o*-NP) and 55% (Na *p*-NP) of the AOEL, without the use of personal protective equipment.

EFSA note (following a comment from the UK during the written procedure of the draft conclusion): The worker is exposed to the product 'Atonik'. Therefore the exposure assessment should consider the three active substances contained in 'Atonik' (Na 5-NG, Na *o*-NP and Na *p*-NP) and the exposure estimates for the individual active substances should be added. This approach is supported by the EFSA. Consequently, the total exposure level being above the AOEL (110%), the workers will need to use PPE (e.g. gloves) in order to have a re-entry exposure below the AOEL.

Bystander exposure

Numerical estimates of bystander exposure were not provided in the DAR. Considering that there is no agreed approach, the meeting suggested using the EUROPOEM model (which includes Lloyd and Bell data). Provided in addendum 2 to Volume 3 of the DAR (September 2008), the estimated exposure level during field use was 6% (Na 5-NG), 12% (Na *o*-NP) and 18% (Na *p*-NP) of the AOEL.

EFSA note (following a comment from the UK during the written procedure of the draft conclusion): The bystander is exposed to the product 'Atonik'. Therefore the exposure assessment should consider the three active substances contained in 'Atonik' (Na 5-NG, Na *o*-NP and Na *p*-NP) and the exposure estimates for the individual active substances should be added. This approach is supported by the EFSA. In any case, the resulting bystander exposure (36%) would not exceed the AOEL.

3. Residues

Na 5-NG, Na *o*-NP and Na *p*-NP were discussed at the PRAPeR experts' meeting for residues (PRAPeR 55, round 11) in July 2008.

3.1. NATURE AND MAGNITUDE OF RESIDUES IN PLANT

3.1.1 Primary crops

Metabolism studies have been performed on sugar beet, tomato and rapeseed using foliar applications of ^{14}C-'Atonik', a mixture of the three active substances Na 5-NG, Na *o*-NP and Na *p*-NP in the respective concentrations of 0.1%, 0.2% and 0.3%. Due to the low application rates defined in the critical GAP, these studies were performed using an exaggerated application rate corresponding to 5X, 6X and 10X total dose rate for sugar beet, tomato and rapeseed respectively. At harvest the total radioactivity was low in beet roots, tomato fruits and rape seeds, in the range of 0.034 mg/kg to 0.049 mg/kg, this TRR being expressed as the sum of the 3 constituent active substances. More than 80% of the TRR was extractable and characterised up to 11 individual radioactive fractions none being more than 0.013 mg/kg. Only fractions M1 and M2 were identified (as 5-nitroguaiacol and *p*-nitrophenol), the others being reported as "unknown" without any indication of their possible chemical structure. In beetroot leaves, the TRR observed at harvest 90 days after the second application was higher (0.399 mg/kg), the individual fractions M6 and M7 accounting for 0.105 mg/kg and 0.059 mg/kg (26% and 15% TRR). Considering the application rate, the experts were of the opinion that the metabolite M6 and eventually M7 could be above 0.01 mg/kg in beet leaves when 'Atonik' is applied at the normal dose rate. Therefore it was concluded that additional information should be requested on the possible structure of these two unknown metabolites.

Considering that the three active substances and the unknown metabolites were not observed in significant levels in the metabolism studies and taking into account that distinct ADI and ARfD have been initially set for each of the three constituent active substances, three separate residue definitions were proposed in the DAR for each individual compound as "Na 5-NG", "Na *o*-NP" and "Na *p*-NP" respectively. Nevertheless, after the meeting and considering the conclusion of the PRAPeR 54 on mammalian toxicology setting the same ADI and ARfD values for the three active substances (0.003 mg/kg/d and 0.045 mg/kg/d respectively), the EFSA was of the opinion that it could be possible to propose single residue definitions for the active substances as "sum of 5-NG, *o*-NP and *p*-NP" for monitoring and "sum of Na 5-NG, Na *o*-NP and Na *p*-NP" for risk assessment; these proposals having to be considered as not discussed and not peer reviewed. Moreover, since Na 5-NG, Na *o*-NP and Na *p*-NP denote similar toxic effects, it seems more appropriate to perform a single consumer risk assessment that takes into account the sum of the residues of these three active substances, rather to perform separate assessments for each individual compound.

No supervised residue trials were presented in the DAR. The meeting of experts, considering the low application rates (6 g/ha/application) and the results of the metabolism studies, agreed that such trials are not necessary since there are enough evidences to concluded that no significant residues are expected in edible plant commodities at harvest and the MRLs proposed at the LOQ were then confirmed. Nevertheless, residues trials were submitted by the applicant but they were not considered by the meeting in view of the restrictions concerning the acceptance of new (including newly submitted) studies after the submission of the DAR to EFSA, as laid down in Commission Regulation (EC) No. 1095/2007. These studies would be considered as confirmatory data only since no area of concern is foreseen. Storage stability studies relating to the residue trials were not provided since such trials were not presented in the DAR. However, in the metabolism studies and using an HPLC method, 'Atonik' was assumed to be stable before and after application, the samples being analysed immediately after sampling. No processing studies were provided since no significant residues of Na 5-NG, Na *o*-NP and Na *p*-NP are expected in plant commodities.

3.1.2 Succeeding and Rotational crops

No rotational crop studies have been provided, the highest DT_{50} being 2.2 days for Na *p*-NP.

3.2. NATURE AND MAGNITUDE OF RESIDUES IN LIVESTOCK

Since significant residues are not expected to result from the intended uses of the active substances in livestock feed, no metabolism or feeding studies were provided and no MRLs were proposed for products of animal origin.

3.3. CONSUMER RISK ASSESSMENT

According to the individual residue definitions initially proposed for each constituent active substance of 'Atonik' and taking into account the new ADI (0.003 mg/kg/d) and ARfD (0.045 mg/kg/d) proposed by the PRAPeR 54, separate risk assessments were performed for Na 5-NG, Na *o*-NP and Na *p*-NP. No chronic or acute concern was observed, the maximum TMDI and IESTI being less than 10% of the ADI and 2% of the ARfD. Considering the single residue definition proposed by the EFSA and using the EFSA model rev.2 and the proposed MRL of 0.03* mg/kg for tomatoes, rapeseeds and sugar beets, no chronic or acute concern are observed, the maximum TMDI being 24% of the ADI (UK toddler) and the maximum IESTI 4.3% of the ARfD (sugar beet), this consumer risk assessment being not peer reviewed

3.4. PROPOSED MRLS

Initially, MRLs of 0.01* mg/kg were set in the DAR for each individual constituent of 'Atonik', Na 5-NG, Na *o*-NP and Na *p*-NP. Based on the single residue definition for monitoring proposed by the EFSA as "sum of 5-NG, *o*-NP and *p*-NP", MRLs or 0.03* mg/kg are now proposed for the representative crops, as the sum of the LOQ of 0.01* mg/kg achieved for each individual active substance. This proposal has to be considered as it is not peer reviewed.

- Sugar beet 0.03* mg/kg
- Oil seed rape 0.03* mg/kg
- Tomato 0.03* mg/kg

4. Environmental fate and behaviour

Na 5-NG, Na *o*-NP and Na *p*-NP were discussed at the experts' meeting PRAPeR 52 for environmental fate and behaviour in June-July 2008 on basis of the Draft Assessment Report (September 2007) and addendum 1 (June 2008). After the meeting the rapporteur Member State submitted some information in addendum 2 (August 2008).

4.1. FATE AND BEHAVIOUR IN SOIL

4.1.1. ROUTE OF DEGRADATION IN SOIL

Soil experiments (4 different soils, OC% 1.0-1.8, pH 6.2-7.4) were carried out under aerobic conditions in the laboratory (20°C, 40% maximum water holding capacity (MWHC)) in the dark. The formations of residues not extracted by acetonitrile/water were a sink for the applied mixture ('Atonik') of ^{14}C-labelled Na 5-NG, Na *o*-NP and Na *p*-NP (in the range of 32.1% to 41.1% of the applied radioactivity (AR) after 120 days). Mineralisation to carbon dioxide was significant, accounted for 54.9-60.8% AR after 120 days. Significant amounts (4.5-10.3% AR) of volatile radioactivity, containing *o*-nitrophenolate, were trapped in ethylene glycol traps. The only extractable breakdown product for further consideration was the unknown metabolite M5 reaching a maximum of 20.5% AR after 7 days (assuming that this metabolite originated solely from Na 5-NG) (for details see addendum 1 to the DAR). A data gap was identified by the experts for identification and for further assessment of this unknown metabolite M5. In addition the route of degradation was investigated at 10°C in one of the above soils. Under these conditions mineralisation was 49.1% AR and the formation of non-extractable residues that accounted for 45.7% AR after 120 days of the study initiation. The only major (> 10% of AR) metabolite observed was the unknown metabolite M5.

Degradation of ^{14}C-labelled Na 5-NG, Na *o*-NP and Na *p*-NP was investigated under anaerobic conditions in one soil (loam, OC% 1.82, pH 7.34) at 20°C. The formation of non-extractable residues was a significant sink accounting for 74.8% AR at the end of the study (after 120 days), the maximum value was 77.25% AR at day 57 after the treatment. The mineralisation to carbon dioxide accounted for 9.4% AR at the end of the study. The unknown metabolite M7 accounted for up to 5.1% AR on the basis of the mixture of the three active substances, however this metabolite would exceed the trigger of 10% AR if it originates from only one of the individual active substances. Taking into account the ratio of the individual active substances in 'Atonik' is 1:2:3, the maximum proportion of M7 if originating solely from Na 5-NG, Na *o*-NP or Na *p*-NP would be 30.5%, 15.3% or 10.2% AR,

respectively. Therefore a data gap was identified by the experts at the meeting for identification of this unknown metabolite M7, however this data gap was considered as not essential to finalise the EU risk assessment. The EFSA identified the same case regarding the unknown metabolite M8 at a later stage of the peer review process, since metabolite M8 accounted for up to 3.3% AR on the basis of the mixture of Na 5-NG, Na *o*-NP and Na *p*-NP and would account for 19.7% AR if M8 evolved solely from Na 5-NG. This data gap for the identification of the unknown metabolite M8 (data gap identified by EFSA during the written procedure), however is also considered as not essential to finalise the EU risk assessment.

In a laboratory soil photolysis study, no photodegradation products were found and soil photolysis of the active substances was not regarded as a significant pathway of disappearance.

4.1.2. PERSISTENCE OF THE ACTIVE SUBSTANCE AND THEIR METABOLITES, DEGRADATION OR REACTION PRODUCTS

The rate of degradation of Na 5-NG, Na *o*-NP and Na *p*-NP was estimated from the results of the study using the four soils described in section 4.1.1 above. Single first-order (SFO) DT_{50} values (20 °C, 40% MWHC moisture content, 4 different soils) were calculated to be 0.1-0.6 day for Na 5-NG, 0.4-1.5 days for Na *o*-NP and 0.6-2.2 days for Na *p*-NP. In case of Na *o*-NP, some volatilisation was observed (see point 4.1.1 above) in the laboratory study and the experts at the meeting agreed that the disappearance of this compound is regarded as dissipation (degradation and volatilisation) and not only degradation. Therefore the DT_{50} values of 0.4-1.5 day should be read as dissipation values ($DisT_{50}$) for Na *o*-NP. For Na *o*-NP half-life in one soil had been presented in the DAR using Double First-Order in Parallel model (DFOP), which resulted a DT_{50} of 0.8 day (DT_{90} 18.4 days). The meeting of experts agreed that based on the statistics available in addendum 1 to the DAR, SFO kinetics (resulting DT_{50} of 1.45 day) could be accepted and used instead of the $DisT_{50}$ value from DFOP kinetics, however a graph for visual assessment would be needed to confirm the goodness of fit. As such an appropriate graph was not available for the peer review, this $DisT_{50}$ value of 1.45 day can not be confirmed. Therefore a data gap was identified for an appropriate graphical presentation of the dissipation kinetics of Na *o*-NP in that soil. As for PEC calculations a longer DT_{50} value (5.5 days, pseudo DT_{50} calculated from DT_{90} of 18.4 days) was used, this issue had no impact on the overall risk assessment. The DT_{50} values for Na 5-NG and Na *p*-NP used in the PEC calculations were also longer than the DT_{50} values referred to in this section.

At 10°C SFO DT_{50} values were calculated to be 0.3 day for Na 5-NG, 0.8 day for Na *o*-NP ($DisT_{50}$) and 3.3 days for Na *p*-NP (one soil, 40% MWHC moisture content).

The half-lives using first-order fitting of Na 5-NG, Na *o*-NP and Na *p*-NP under anaerobic conditions, were 3.3 days for both Na 5-NG and Na *o*-NP and 12.6 days for Na *p*-NP.

4.1.3. MOBILITY IN SOIL OF THE ACTIVE SUBSTANCE AND THEIR METABOLITES, DEGRADATION OR REACTION PRODUCTS

The adsorption / desorption of Na 5-NG, Na *o*-NP and Na *p*-NP was investigated in five soils, from which finally four were used (OC% 1.16-2.98, pH 5.7-7.5, clay content 7.5-34.2%) in a satisfactory batch adsorption experiment. Calculated adsorption K_foc values based on these four soils were: 166 to 1350 mL/g (mean 463.4 mL/g) (1/n 0.81 – 1.0) for Na 5-NG; 89 to 522 mL/g (mean 156.1 mL/g) (1/n 0.82 – 1.0) for Na *o*-NP; and 123 to 602 mL/g (mean 288.1 mL/g) (1/n 0.84 – 1.0) for Na *p*-NP. There was no evidence of a correlation of adsorption with any soil parameter.

4.2. FATE AND BEHAVIOUR IN WATER

4.2.1. SURFACE WATER AND SEDIMENT

Na 5-NG, Na *o*-NP and Na *p*-NP were essentially stable under sterile hydrolysis conditions at 50°C at pH 4, pH 7 and pH 9.

The aqueous photolysis of Na 5-NG, Na *o*-NP and Na *p*-NP was investigated under sterile conditions in the laboratory at pH 7. The rate of degradation (first-order DT_{50}) equated to summer sunlight at 30°N was determined as 2.8 days for Na 5-NG, 60.5 days for Na *o*-NP and 5.5 days for Na *p*-NP. Quantum yields of direct phototransformation were calculated to be $1.56x10^{-5}$ molecules/photon for Na 5-NG, $6.52x10^{-7}$ molecules/photon for Na *o*-NP and $3.77x10^{-6}$ molecules/photon for Na *p*-NP from the same study. It should be noted that in case of Na *o*-NP some volatilisation (*o*-nitrophenolate) was observed during the experiment (16.5% and 7.7% AR in the irradiated and the dark control samples by the study end). Products found above 10% of applied radioactivity were M3, M5, M8, M12 and M13 formed from Na 5-NG and M3, M5 and M6 formed from Na *p*-NP. As these metabolites were neither identified nor investigated further, a data gap was agreed by the experts in the PRAPeR 52 meeting for addressing the environmental risk assessment of these products.

A ready biodegradability test (OECD 301A) indicated that Na 5-NG, Na *o*-NP and Na *p*-NP are 'not readily biodegradable' using the criteria defined by the test.

In water-sediment studies (two systems studied at 20°C in the laboratory, sediment pH 7.17 and 7.47) Na 5-NG, Na *o*-NP and Na *p*-NP dissipated rapidly from the water partitioning to sediment in both systems. First-order half-life of the active substances were: 2.4 and 3.4 days for Na 5-NG; 1.9 and 2.2 days for Na *o*-Np and 2.7 and 2.8 days for Na *p*-NP. The observed degradations of the active substances in the whole system were also rapid, resulting in the following SFO DT_{50} values: 3.0 and 5.4 days for Na 5-NG, 2.0 and 2.2 days for Na *o*-Np and 3.0 and 3.6 days for Na *p*-NP.

Major metabolites were not found in this study. Mineralisation to carbon dioxide was a significant sink that accounted for 66.1-63.5% AR at 122 days. Residues not extracted from sediment by acetonitrile/water were a sink representing 30.7% and 34.6% AR at study end (122 days).

FOCUS surface water modelling was carried out up to step 2 for each of the individual active substances. The peer review agreed that PEC surface water and sediment, as presented in addendum 1 to the DAR were appropriate for use in the risk assessment. However calculations based on single applications and calculations with FOCUS step 3 were not available although required by the peer review (based on the SCP opinion[5]). Therefore a data gap was identified by the experts at the meeting for calculations based on single applications and FOCUS step 3 calculations. However the meeting of experts agreed that if step 3 calculations lead to higher values it would only be for a small number of scenarios, therefore this data gap was considered as not essential to finalise the EU risk assessment.

4.2.2. POTENTIAL FOR GROUND WATER CONTAMINATION OF THE ACTIVE SUBSTANCE THEIR METABOLITES, DEGRADATION OR REACTION PRODUCTS

The applied for representative uses of the three active substances (four applications to sugar beet, five applications to tomato and two applications to winter or spring oilseed rape) were simulated using FOCUS PELMO 3.3.2 and FOCUS PEARL 2.2.2 with the following input parameters: Na 5-NG single first-order DT_{50} 0.6 day, K_{foc} 463.4 mL/g, 1/n=1; Na *o*-NP single first-order DT_{50} 5.5 days, K_{foc} 156.1 mL/g, 1/n=1; Na *p*-NP single first-order DT_{50} 3.3 days, K_{foc} 288.1 mL/g, 1/n=1.

A worst case calculation regarding the unidentified metabolite M5 was submitted during the peer review (addendum 1 to the DAR) using the following input parameters: dose 0.186 g/ha (6g x maximum occurrence of 3.1% AR in soil degradation study, pseudo application); half-life in soil 120 days (considering that, for all soils in the soil degradation study, M5 was not detected in the last sample at day 120); Koc 1 mL/g (considering really high mobility as no adsorption data are available), 1/n=1.These simulations regarding the metabolite M5 were conducted using only FOCUS PELMO 3.3.2.

Na 5-NG, Na *o*-NP and Na *p*-NP were calculated to be present in leachate leaving the top 1m soil layer at 80th percentile annual average concentrations of <0.001µg/L.

For the unknown metabolite M5 this range was 0.004-0.024 µg/L for tomato and oil seed rape applications. For simulations for applications to sugar beet this range was 0.015-0.123 µg/L, with the 0.1 µg/L parametric drinking water limit being exceeded at the Jokionen scenario (0.123µg/L) (see

[5] 5 SCP/GUIDE-FOC-SW/002-Final Opinion of the Scientific Committee on Plants regarding the evaluation of a document concerning FOCUS surface scenarios in the context of Council Directive 91/414/EEC

addendum 1 to the DAR). A data gap was therefore agreed by the Member State experts for simulation with a second model for the unknown metabolite M5.

4.3. FATE AND BEHAVIOUR IN AIR

The vapour pressure of the active substances (<$1.3x10^{-5}$ Pa for Na 5-NG and Na *p*-NP, $7.75x10^{-5}$ Pa for Na *o*-NP at 25°C) means that Na 5-NG, Na *o*-NP and Na *p*-NP would be classified under the national scheme of The Netherlands as very slightly volatile, indicating significant losses due to volatilisation would not be expected. It should be noted that under acidic conditions some volatilisation of the phenolic form of Na *o*-NP may occur. Calculations using the method of Atkinson (using the software APOWIN) for indirect photo-oxidation in the atmosphere through reaction with hydroxyl radicals resulted in an atmospheric half-life estimated at about 2.2 days for both Na 5-NG and 2.3 days for Na *o*-NP and Na *p*-NP (assuming an atmospheric hydroxyl radical concentration of $1.5x10^{6}$ radicals cm^{-3}, 12 hours a day) indicating some potential for long range aerial transport of these active substances.

5. Ecotoxicology

Sodium 5-nitroguaicolate (Na 5-NG), sodium *ortho*-nitrophenolate (NA *o*-NP) and sodium *para*-nitrophenolate (Na *p*-NP), were discussed at the PRAPeR experts' meeting for ecotoxicology (PRAPeR 53, subgroup 1) in July 2008 on the basis of DAR and addendum 1 from June 2008.

The representative use evaluated was as a plant growth stimulator on sugar beet, oilseed rape and tomato. The formulated product was 'Atonik SL' containing 1 g/l of 5-NG, 2 g/l of *o*-NP and 3 g/l of *p*-NP.

The risk assessment was conducted according to the following guidance documents: Risk Assessment for Birds and Mammals. SANCO/4145/2000 September 2002; Aquatic Ecotoxicology, SANCO/3268/2001 rev.4 final, October 2002; Terrestrial Ecotoxicology, SANCO/10329/2002 rev.2 final, October 2002; Risk Assessment for non-target arthropods, ESCORT 2, SETAC, March 2000.

Information on the amount of impurity was missing for some test material used in the ecotoxicological studies. Even though the experts of Member States considered these impurities not relevant, a data gap was proposed for the applicant to provide an analysis of the "batches" not covered by the technical specification used in the ecotoxicological studies.

5.1. RISK TO TERRESTRIAL VERTEBRATES

The submitted studies with Na 5-NG, NA *o*-NP and Na *p*-NP indicated a low acute and short-term toxicity to birds. The lowest LD_{50} of 1046 mg a.s./kg bw/d and the lowest LC_{50} of 1412 mg a.s./kg

bw/d were observed in studies on *Colinus virginianus* exposed to sodium Na *o*-NP and Na *p*-NP, respectively (the daily dose LC_{50} value was recalculated by the EFSA after the meeting on the basis of an average feed consumption of 6.89 g/d and an average body weight of 22.89 g and it takes into account the correction for purity of 83.5%). A chronic study was conducted with the product 'Atonik' in a higher concentrated form than the representative formulation. The experts of the Member States discussed the consequences of the lower measured concentrations of the Na *o*-NP compared to the nominal (about 50% of the nominal) concentration and they agreed that, as the tested preparation was 100 times more concentrated, it represented a worst-case exposure. No treatment-related effects were observed at the highest nominal test concentration (NOEC = 1000 mg product/kg feed, corresponding to 95.6 mg product/kg bw/d).

On the basis of mammalian toxicity data (rat), the lowest acute toxicity value was observed for Na *p*-NP (LD_{50} = 345.5 mg a.s./kg bw). A NOAEL of 300 mg product/kg bw/d was observed in a 2-generation reproduction study.

TERs were calculated for medium herbivorous birds, insectivorous birds and medium herbivorous mammals. A potential combined acute risk was assessed for herbivorous and insectivorous birds on the basis of a LD_{50} (mix) of 238.536 g/kg bw, calculated according to the Finney's formula (revised guidance document birds and mammals). The uptake by drinking water was also taken into account. All the TER values in the first-tier risk assessment were above the Annex VI trigger values, indicating a low risk to terrestrial vertebrates.

5.2. RISK TO AQUATIC ORGANISMS

Studies with the three active substances and the formulated product were provided and peer reviewed (see the DAR and addendum 1). Among the studies with the active substance, Na *p*-NP was slightly more toxic (acutely) than the others. Algae were the most sensitive organisms tested (the lowest 72-h E_bC_{50} =2.5 mg a.s./L, *Scenedesmus subspicatus*). Since the active substances are "plant growth regulators", two data gaps were confirmed at the meeting to provide studies on the effects on a second algae species and on aquatic plants. The experts discussed if the second algae species should be tested with the formulation or with each active substance separately. The outcome of the discussion during the meeting was to check which endpoints are more toxic (from the a.s. or the formulated product). On the basis of the value for the formulation (EC_{50} >100 mg Product/L, *S.subspicatus*) expressed as active substances (>0.1 mg Na 5-NG/L, >0.2 mg Na *o*-NP/L, > 0.3 mg Na *p*-NP/L), the product appears slightly more toxic than each substance tested individually. However, while drafting the conclusion EFSA noted that such a comparison is not feasible: the formulation study is a limit test with "a greater than" value as endpoint. As algae were the most sensitive organisms, the EFSA conclusion is that the study on the second algae species should be conducted for each active substance

separately. As for aquatic plant no studies were available, the experts agreed that the effects on *Lemna* should be assessed for each active substance separately.

As for fish and invertebrates the lowest endpoints observed were 96-h LC_{50} = 25 mg Na *p*-NP/L (*Oncorhynchus mykiss*), 48-h EC_{50} = 27.7 mg Na *p*-NP/L (*Daphnia magna*). The acute endpoints from studies with a solution of 'Atonik' indicated a similar toxicity of each substance when formulated (96-h LC_{50} = 6800 mg product/L equivalent to 20.64 mg Na 5-NG/L, 41.28 mg Na *o*-NP/L and 61.92 mg Na *p*-NP/L (*Cyprinus carpio)*; 48-h EC_{50} = 2000 mg product/L equivalent to 6 mg Na 5-NG/L, 12 mg Na *o*-NP/L, 18 mg Na *p*-NP/L, (*Daphnia magna*)). The chronic toxicity for fish and invertebrates was tested only with the formulated product: 21-d NOEC = 10 mg product/L (*Oncorhynchus mykiss*) and 21-d NOEC = 1.0 mg product/L (*Daphnia magna*).

The proposed classification for the active substances was N "Dangerous for the environment", R51/R53 "Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment" on the basis of the algae endpoints. No classification was proposed for the product.

TERs were calculated on the basis of initial concentrations of Step 1&2 of the $FOCUS_{sw}$. The TERlt for fish and invertebrates was calculated on the basis of the formulation endpoints converted to active substances. The sum of each a.s. endpoint was then compared to the sum of the PEC values. All the TER values were well above the Annex VI triggers, indicating a low risk from the active substances following the recommended uses.

The relevance of the photolytic metabolites of nitrophenolic compounds was discussed at the experts' meeting. Since the experts of the fate meeting recognised M3, M5, M6, M8, M12 (metabolites of Na 5-NG) and M3, M5, M6 (metabolites of Na *p*-NP) relevant to be assessed in aquatic environment, a data gap was identified to further address the risk of these photolytic metabolites. The experts agreed that in a conservative approach the risk assessment could be conducted by considering the metabolites 10 times more toxic than the parents, therefore new studies should not be generated.

5.3. RISK TO BEES

Acute oral and contact toxicity studies were conducted with each active substance and with the formulated product ('Atonik'). As for oral exposure, Na *p*-NP (LD_{50} 61.2 µg a.s./bee) was more toxic than the Na 5-NG and Na *o*-NP but the lowest endpoint was observed with the formulation product (LD_{50} 57.12 µg product/bee). The contact toxicity of the active substances and the product was low (LD_{50} >100 µg a.s./bee). The HQ values were below the Annex VI trigger of 50 indicating a low risk to bees from the representative uses evaluated.

5.4. RISK TO OTHER ARTHROPOD SPECIES

No standard laboratory tests were conducted with the indicator species *Aphidius rhopalosiphi* and *Typhlodromus pyri*. However studies were provided on *Amblyseius californicus*, *Aphidius colemani*, *Poecilus cupreus*, *Coccinella septenpunctata.* No significant effects were observed on mortality and reproduction performance. The Rapporteur Member State calculated the HQs values on the basis of the higher tested rate (LR_{50} >2 l/ha). Since the trigger 2 is only validated for *T.pyri* and *A.rhopalosiphi*, it was agreed that it would be more appropriate to compare the percentage of effect with the trigger of 50%.

Overall, it was concluded that the risk to non-target arthropods was low.

5.5. RISK TO EARTHWORMS

The acute and chronic toxicity to earthworms was tested with a mixed powder of 3 technical grade active substances of 'Atonik'. Due to some ambiguous results in the acute study, the LC_{50} was set at the lower tested concentration (14-d LC_{50} > 101.8 mg product/kg soil). Chronic testing gave an 8-week NOEC of 37 mg product/kg soil. According to the TER calculations the risk to earthworms was assessed as low.

5.6. RISK TO OTHER SOIL NON-TARGET MACRO-ORGANISMS

No studies required since the field DT_{90} in soil was <100 d.

5.7. RISK TO SOIL NON-TARGET MICRO-ORGANISMS

No effects > 25 % on soil respiration and nitrification were observed in tests with formulated product 'Atonik' up to a concentration of 4.0 mg a.s./kg soil dw indicating a low risk to soil non-target micro-organisms for the representative uses evaluated.

5.8. RISK TO OTHER NON-TARGET-ORGANISMS (FLORA AND FAUNA)

Herbicidal effects of the formulation 'Atonik' on vegetative vigour and emergence were investigated in tests with the following plant species: *Allium cepa, Avena sativa, Lolium perenne, Triticum aestivum, Brassica oleracea, Daucus carota, Fagopyrum* sp. *Lactuga sativa, Pisum sativum and Solanum esculentum*. No effects were observed at the highest tested concentration for all tested species (ER_{50} > 5 L product/ha). The TERs were >81 based on the estimated exposure rate of 0.1 L/ha from spray drift at 1m distance, indicating a low risk.

5.9. RISK TO BIOLOGICAL METHODS OF SEWAGE TREATMENT

No data were provided on the effects on biological methods of sewage treatment. The applicant argued that under the recommended uses it is unlikely that sewage treatment plants are affected, due to the fast degradation of the product in the environment. Even if the experts agreed that this is not an

area of concern, a data gap was identified to further address the effects at Member State level in case the agricultural practices induce a possible concern to sewage treatment plants.

6. Residue definitions

Soil

Definition for risk assessment: Na 5-NG, Na *o*-NP, Na *p*-NP, unknown metabolite M5, unknown metabolite M7 (anaerobic metabolite), unknown metabolite M8 (anaerobic metabolite)

Definition for monitoring: 5-nitroguaiacole, *o*-nitrophenol and *p*-nitrophenol

Water

Ground water

Definition for exposure assessment: Na 5-NG, Na *o*-NP, Na *p*-NP, unknown metabolite M5, unknown metabolite M7 (anaerobic metabolite), unknown metabolite M8 (anaerobic metabolite)

Definition for monitoring: 5-nitroguaiacole, *o*-nitrophenol and *p*-nitrophenol (pending identification and further assessment of the potential for contamination of groundwater by soil metabolite, M5)

Surface water

Definition for risk assessment: Na 5-NG, Na *o*-NP, Na *p*-NP, M3 (from photolysis, from Na 5-NG), M3 (from photolysis, from Na *p*-NP), M5 (from soil), M5 (from photolysis, from Na 5-NG), M5 (from photolysis, from Na *p*-NP), M6 (from photolysis, from Na *p*-NP), M8 (from photolysis, from Na 5-NG), M12 (from photolysis, from Na 5-NG), M13 (from photolysis, from Na 5-NG)

Definition for monitoring: 5-nitroguaiacole, *o*-nitrophenol and *p*-nitrophenol (pending the assessment of the potential impact to aquatic organisms of the major photodegradation products M3, M5, M8, M12 and M13 formed from Na 5-NG and M3, M5 and M6 formed from Na *p*-NP)

Air

Definition for risk assessment: Na 5-NG, Na *o*-NP, Na *p*-NP

Definitions for monitoring: 5-nitroguaiacole, *o*-nitrophenol and *p*-nitrophenol

Food of plant origin

Definition for risk assessment:	sum of Na 5-NG, Na *o*-NP and Na *p*-NP
Definition for monitoring:	sum of 5-nitroguaiacole, *o*-nitrophenol and *p*-nitrophenol

Food of animal origin

Definition for risk assessment:	not necessary
Definition for monitoring:	not necessary

Overview of the risk assessment of compounds listed in residue definitions for the environmental compartments

Soil

Compound (name and/or code)	**Persistence**	**Ecotoxicology**
Na 5-NG	Very low persistence SFO DT_{50} 0.1-0.6 day (20 °C, 40% MWHC)	Not relevant
Na *o*-NP	Very low to low persistence SFO DT_{50} 0.4-1.5 day (20 °C, 40% MWHC)	Not relevant
Na *p*-NP	Very low to low persistence SFO DT_{50} 0.6-2.2 day (20 °C, 40% MWHC)	Not relevant
unknown metabolite M5	No information	No information
unknown metabolite M7 (anaerobic metabolite)	No information	No information
unknown metabolite M8 (anaerobic metabolite)	No information	No information

Ground water

Compound (name and/or code)	Mobility in soil	> 0.1 µg / L 1m depth for the representative uses (at least one FOCUS scenario or relevant lysimeter)	Pesticidal activity	Toxicological relevance	Ecotoxicological activity
Na 5-NG	Medium to low mobility Kfoc 166 to 1350 mL/g	No		Yes	Yes
Na *o*-NP	High to low mobility Kfoc 89 to 522 mL/g	No		Yes	Yes
Na *p*-NP	High to low mobility Kfoc 123 to 602 mL/g	No		Yes	Yes
unknown metabolite M5	No information	Yes, one scenario (Jokionen, 0.123 µg/L) from the 9 scenarios for sugar beet Data gap for a second modelling		No information available. Assessment required pending on the identification.	No information Assessment required pending on the identification.

Compound (name and/or code)	Mobility in soil	> 0.1 µg / L 1m depth for the representative uses (at least one FOCUS scenario or relevant lysimeter)	Pesticidal activity	Toxicological relevance	Ecotoxicological activity
unknown metabolite M7 (anaerobic metabolite)	No information	No information		No information available.	No information
unknown metabolite M8 (anaerobic metabolite)	No information	No information		No information available.	No information

Surface water and sediment

Compound (name and/or code)	Ecotoxicology
Na 5-NG	Toxic to aquatic organisms. The risk was assessed as low
Na *o*-NP	Toxic to aquatic organisms. The risk was assessed as low
Na *p*-NP	Toxic to aquatic organisms. The risk was assessed as low
M3 (from photolysis, from Na 5-NG)	Data gap
M3 (from photolysis, from Na *p*-NP)	Data gap

M5 (from soil)	Data gap
M5 (from photolysis, from Na 5-NG)	Data gap
M5 (from photolysis, from Na *p*-NP)	Data gap
M6 (from photolysis, from Na *p*-NP)	Data gap
M8 (from photolysis, from Na 5-NG)	Data gap
M12 (from photolysis, from Na 5-NG)	Data gap
M13 (from photolysis, from Na 5-NG)	Data gap

Air

Compound (name and/or code)	**Toxicology**
Na 5-NG	low acute toxicity by inhalation (rat LC_{50} >2.38 mg/L air)
Na *o*-NP	low acute toxicity by inhalation (rat LC_{50} >1.24 mg/L air)
Na *p*-NP	low acute toxicity by inhalation (rat LC_{50} >1.20 mg/L air)

LIST OF STUDIES TO BE GENERATED, STILL ONGOING OR AVAILABLE BUT NOT PEER REVIEWED

- Revised specification of technical Na 5-NG and the amended report containing information about other two impurities (relevant for all representative uses evaluated, date of submission unknown, data gap identified by the rapporteur Member State and confirmed by the experts of PRAPeR 51 meeting, June 2008; refer to chapter 1).
- Revised specification of the impurities of technical Na *o*-NP and technical Na *p*-NP and the amended report containing information about three impurities (relevant for all representative uses evaluated, date of submission unknown, data gap identified by the experts of PRAPeR 51 meeting, June 2008; refer to chapter 1).
- Justification for the maximum level of 1 g/kg for impurity 1 of Na 5-NG technical material (relevant for all representative uses evaluated, date of submission unknown, data gap identified by the rapporteur Member State and confirmed by the experts of PRAPeR 51 meeting, June 2008; refer to chapter 1).
- Confirmation of the identity of impurity 2 and based on the identity, further data on the analytical method may be necessary (relevant for all representative uses evaluated, date of submission unknown, data gap identified by the rapporteur Member State and confirmed by the experts of PRAPeR 51 meeting, June 2008; refer to chapter 1).
- Fully validated analytical method for determination of the relevant impurities (relevant for all representative uses evaluated, date of submission unknown, data gap identified by the EFSA after of PRAPeR expert meeting 54, July 2008; refer to chapter 1 and 2).
- To clarify if the impurities in the technical materials contribute to the explosive properties of the active substance (relevant for all representative uses evaluated, date of submission unknown, data gap identified by the experts of PRAPeR 51 meeting, June 2008; refer to chapter 1).
- Information demonstrating that the relevant impurities are not increasing on storage (relevant for all representative uses evaluated, date of submission unknown, data gap identified by the EFSA after the of PRAPeR expert meetings, June 2008; refer to chapter 1 and 2).
- To provide information on the possible chemical structure of the radioactive fractions identified as M6 and M7 in leaves in the sugar beet metabolism study (relevant for all representative uses evaluated, date of submission unknown, data gap identified by the experts of PRAPeR 55 meeting, July 2008; refer to section 3.1.1).
- Identification of the unknown soil metabolite M5 and assessment of the potential contamination of groundwater with a second model, and if necessary a groundwater relevance assessment for this metabolite (relevant for all uses evaluated, data gap identified by PRAPeR meeting of experts July 2008, date of submission unknown, refer to chapter 4.1.1 and 4.2.2).
- Identification of the unknown anaerobic soil metabolite M7 (relevant for uses where anaerobic conditions of the soil cannot be excluded, not essential to finalise the EU risk assessment, data

gap identified by PRAPeR meeting of experts July 2008, date of submission unknown; refer to chapter 4.1.1).

- Identification of unknown anaerobic soil metabolite M8 (relevant for uses where anaerobic conditions of the soil cannot be excluded, not essential to finalise the EU risk assessment, data gap identified by EFSA, date of submission unknown; refer to chapter 4.1.1).
- Appropriate graphical presentation of the dissipation kinetic of Na *o*-NP in soil II (relevant for all uses evaluated, data gap identified by PRAPeR meeting of experts July 2008, date of submission unknown; refer to chapter 4.1.2).
- Assessment of the potential impact to the environment of the major photodegradation products M3, M5, M8, M12 and M13 formed from Na 5-NG and M3, M5 and M6 formed from Na *p*-NP (relevant for all uses evaluated, data gap identified by PRAPeR meeting of experts July 2008, date of submission unknown; refer to chapter 4.2.1).
- Calculations of PEC_{SW} and PEC_{sed} values based on single applications as well as using FOCUS step 3 tools (relevant for all uses evaluated, not essential to finalise the EU risk assessment, data gap identified by PRAPeR meeting of experts July 2008, date of submission unknown; refer to chapter 4.2.1).
- Analysis of the "batches" not covered by the technical specification used in the ecotoxicological studies (relevant for all representative uses evaluated, date of submission unknown, data gap identified by the experts of PRAPeR 53 meeting, July 2008; refer to section 5).
- Studies on a second algae species and *Lemna* with each active substance (relevant for all representative uses evaluated, date of submission unknown, data gap identified by the experts of PRAPeR 53 meeting, July 2008; refer to section 5.2).
- To address the risk to aquatic organisms from photolytic metabolites (relevant for all representative uses evaluated, date of submission unknown, data gap identified by the experts of PRAPeR 53 meeting, July 2008; refer to section 5.2).
- To further address the effects at Member State level in case the agricultural practices induce a possible concern to sewage treatment plants (relevant for all representative uses evaluated, date of submission unknown, data gap identified by the experts of PRAPeR 53 meeting, July 2008; refer to section 5.9)

CONCLUSIONS AND RECOMMENDATIONS

Overall conclusions

The conclusion was reached on the basis of the evaluation of the representative uses as proposed by the applicants which comprise foliar spraying:

-on sugar beet, from growth stage of BBCH 12 up to growth stage of BBCH 49, in all EU countries, at maximum four applications at a maximum application rate per treatment of 1 g Na

5-NG, 2 g Na *o*-NP and 3 g Na *p*-NP/ha, with interval between applications of minimum 7-30 days;

-on oilseed rape, from growth stage of BBCH 31 up to growth stage of BBCH 69, in all EU countries, at maximum two applications at a maximum application rate per treatment of 1 g Na 5-NG, 2 g Na *o*-NP and 3 g Na *p*-NP/ha, with interval between applications of minimum 30-60 days;

-on tomato, at growth stages of BBCH 59, 69, 71, 79, 81, in all EU countries, at maximum five applications at a maximum application rate per treatment of 1 g Na 5-NG, 2 g Na *o*-NP and 3 g Na *p*-NP/ha, with interval between applications of minimum 14 days.

The representative formulated product for the evaluation was 'Atonik', a soluble concentrate (SL) containing 1 g/l Na 5-NG 2 g/l Na *o*-NP and 3 g/l Na *p*-NP.

The specifications for the technical materials currently should be regarded as provisional (September 2008).

Analytical methods as well as methods and data relating to physical, chemical and technical properties are available to ensure that quality control measurements of the plant protection products are possible, however a data gap was identified for additional validation data for the determination of relevant impurities in the technical materials.

Adequate analytical methods are available to monitor all compounds given in the respective residue definitions in food/feed of plant origin and environmental matrices.

With regard to its toxicological properties, the mixture 'Atonik' was shown to be rapidly and extensively absorbed, widely distributed in the body without bioaccumulation and excreted mainly via urine. The proposed classification for the acute toxicity was **Xn**; **R22** "**Harmful if swallowed"** for the three active substances; **Xi**; **R36** "**Irritating to eyes**" for Na *o*-NP and Na *p*-NP; and **Xi**; **R41** "**Risk of serious damage to eyes**" for Na 5-NG. In the short-term studies, the most sensitive species was the dog, with the lungs, liver and kidney as target organs at higher doses. However the NOAEL was based on clinical findings at lower doses. Even though some positive results were observed during the *in vitro* genotoxicity studies, the negative results in the *in vivo* testing were supported by the absence of a carcinogenic potential in the long-term studies. With regard to the reproductive toxicity testing, a decreased fertility index was noted in the presence of maternal toxicity at the high dose level, but no adverse effect in the offspring. No teratogenic effect was observed in the developmental studies with rats and rabbits, and some findings of foetotoxicity were attributed to

maternal toxicity. In addition, no maternal NOAEL could be derived for the rabbit since clinical signs were observed in dams at all dose levels.

For the derivation of the reference values, it was agreed to set values applicable separately to the three active substances. Additionally, it was decided to use the toxicological studies with the mixture 'Atonik' since they are providing lower NOAELs for the active substances (based on their ratio in the mixture) than the studies with the individual active substances. Consequently the agreed values were based on the lowest individual NOAEL value in the relevant study with the mixture, applicable to the three active substances as a conservative and pragmatic approach. Therefore the agreed **acceptable daily intake** (ADI) is **0.003 mg/kg bw/day** based on the 1-year dog study with the use of a safety factor of 100. Similarly, the agreed **acceptable operator exposure level** (AOEL) is **0.007 mg/kg bw/day** based on the 90-day dog study and using a safety factor of 100. And finally the agreed **acute reference dose** (ARfD) is **0.045 mg/kg bw** based on the developmental study with rabbit, and applying an increased safety factor of 300 due to the use of a LOAEL (maternal) instead of a NOAEL. In the absence of experimental results, the agreed dermal absorption value of 100% was adopted. The sum of the operator exposure estimates for the three active substances give a total exposure level below the AOEL when PPE is used during field application with tractor or greenhouse use, but the exposure is above the AOEL even with PPE in the case of hand-held application in field. The use of PPE is also required for workers re-entering treated fields, but the exposure level of bystander is below the AOEL.

Plant metabolism studies have been performed on sugar beet, tomato and rapeseed after foliar applications of ^{14}C-'Atonik', a mixture of the three active substances Na 5-NG, Na *o*-NP and Na *p*-NP, using exaggerated application rates up to 10 times the total normal dose rate. At harvest the TRR was low in beet roots, tomato fruits and rape seeds, in the range of 0.034 to 0.049 mg/kg and no parent active substances or unidentified metabolites were observed at levels higher than 0.013 mg/kg. However in beetroot leaves, it was considered that the two unknown metabolites M6 and M7 could be above 0.01 mg/kg when 'Atonik' is applied at a normal dose rate and additional information was requested on the possible structure of these two compounds. Three separate residue definitions were proposed in the DAR for each individual compound as "Na 5-NG", "Na *o*-NP" and "Na *p*-NP" respectively. Nevertheless, after the meeting and taking into account the conclusion of the PRAPeR 54 meeting on mammalian toxicology setting the ADI and ARfD values for the three constituent active substances, the EFSA was of the opinion that it could be possible to propose a single residue definition for monitoring as "sum of 5-NG, *o*-NP and *p*-NP", this proposal having to be considered as not peer reviewed. No supervised residue trials were presented and the meeting of experts, considering low application rates and the metabolism study results, agreed that such trials are not necessary and confirmed the MRL values set at the LOQ. No processing studies and animal metabolism studies were provided since any significant residues of Na 5-NG, Na *o*-NP and Na *p*-NP are expected in plant commodities. No rotational crop studies were submitted with regard to the low

DT_{50} values. The MRLs of 0.01* mg/kg were initially proposed in the DAR for each of the individual active substances. Nevertheless and based on the single residue definition, the EFSA is of the opinion that MRLs of 0.03* mg/kg (sum of the LOQ achieved for each individual active substance) should be more appropriate. The chronic and acute consumer risk assessments showed that the TMDI and IESTI did not exceed the ADI and the ARfD respectively.

The information available on the fate and behaviour in the environment is not sufficient to carry out an appropriate environmental exposure assessment for the active substances at the EU level. Identification of unknown aerobic soil metabolite M5 and unknown anaerobic soil metabolites M7 and M8 is required. Appropriate graphical presentation would be necessary for a proper evaluation of the dissipation kinetic and the determination of the DT_{50} value of Na *o*-NP in soil II. An assessment of the potential impact to the environment of the major photodegradation products is necessary. FOCUS step 3 calculations for PEC_{SW} and PEC_{sed} values would be needed on the basis of the SCP opinion[6]. For the applied for intended uses, the potential for groundwater contamination by Na 5-NG, Na *o*-NP and Na *p*-NP above the parametric drinking water limit of 0.1 µg/L is low. However for the unknown metabolite M5, in geoclimatic regions represented by the Jokionen FOCUS groundwater scenario, contamination of groundwater above the 0.1 µg/L limit cannot be excluded therefore simulations with a second model are needed.

A low acute, short-term and long-term risk was assessed for terrestrial vertebrates in a first-tier assessment for the representative uses.

Na 5-NG, Na *o*-NP and Na *p*-NP were toxic to aquatic organisms (**N** "**Dangerous for the environment**", **R51/R53** "**Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment**"). Algae were the most sensitive organisms tested. As these active substances are "plant growth regulators" the meeting agreed to require further studies such as a second algae species and *Lemna* tests. On the basis of available data, a low first-tier risk was identified for aquatic organisms. According to the fate meeting conclusion, a data gap was identified to further address the risk to aquatic organisms from the photolytic metabolites.

The risk was assessed as low for bees, non-target arthropods, earthworms, soil macro and micro-organisms and other non-target organisms. No risk was expected to biological methods for sewage treatment, but the experts agreed that at member state level the effects should be addressed in case agricultural practices induce a possible concern to sewage treatment plants.

6 SCP/GUIDE-FOC-SW/002-Final Opinion of the Scientific Committee on Plants regarding the evaluation of a document concerning FOCUS surface scenarios in the context of Council Directive 91/414/EEC

Particular conditions proposed to be taken into account to manage the risk(s) identified

- Use of personal protective equipment by the operator is needed during field application with tractor or greenhouse use in order to have an estimated total exposure below the AOEL (refer to 2.12).
- Use of personal protective equipment by the worker is needed during re-entry in order to have an estimated total exposure below the AOEL (refer to 2.12).

Critical areas of concern

- Specifications not finalized.
- The assessment of the potential groundwater contamination by the unknown soil metabolite M5 can not be finalised.

Appendix 1 – list of endpoints

APPENDIX 1 – LIST OF ENDPOINTS FOR THE ACTIVE SUBSTANCE AND THE REPRESENTATIVE FORMULATION

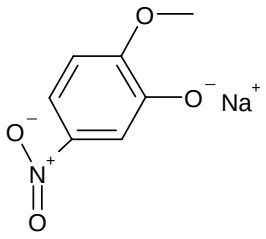
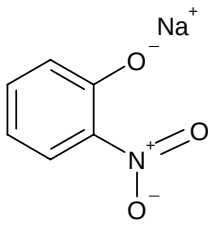
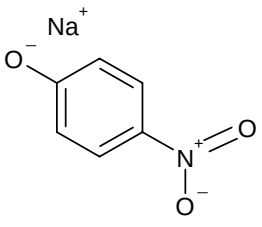
(Abbreviations used in this list are explained in appendix 2)

Identity, Physical and Chemical Properties, Details of Uses, Further Information

Active substance (ISO Common Name) ‡	**Sodium 5-nitroguaiacolate** (No ISO common name is allocated)	**Sodium *o*-nitrophenolate** (No ISO common name is allocated)	**Sodium *p*-nitrophenolate** (No ISO common name is allocated)
Function (*e.g.* fungicide)	Plant growth stimulator	Plant growth stimulator	Plant growth stimulator
Rapporteur Member State	Greece	Greece	Greece
Co-rapporteur Member State	-	-	-

Appendix 1 – list of endpoints

Identity (Annex IIA, point 1)

Chemical name (IUPAC) ‡	Sodium 2-methoxy-5-nitrophenolate	Sodium 2-nitrophenolate; sodium *o*-nitrophenolate	Sodium 4-nitrophenolate; sodium *p*-nitrophenolate
Chemical name (CA) ‡	3-hydroxy-4-methoxynitrobenzene sodium salt	Sodium o-nitrophenolate	Sodium *p*-nitrophenolate
CIPAC No ‡	Not allocated	Not allocated	Not allocated
CAS No ‡	67233-85-6	824-39-5	824-78-2
EC No (EINECS or ELINCS) ‡	Not allocated	Not allocated	Not allocated
FAO Specification (including year of publication) ‡	None	None	None
Minimum purity of the active substance as manufactured ‡	Open	980 g/kg	998 g/kg (corresponds to dihydrate form)
Identity of relevant impurities (of toxicological, ecotoxicological and/or environmental concern) in the active substance as manufactured	None	*Phenol* *Max content: open* *2,4 dinitrophenol* *max content: 0.14 g/kg* *2,6 dinitrophenol* *max content: 0.32 g/kg*	*Phenol* *max content: open* *2,4 dinitrophenol* *max content: 0.07 g/kg* *2,6 dinitrophenol* *max content:0.09 g/kg*
Molecular formula ‡	$C_7H_6NNaO_4$	$C_6H_4NNaO_3$	$C_6H_4NNaO_3$
Molecular mass ‡	191.1 g/mol	161.1 g/mol	161.1 g/mol
Structural formula ‡			

Appendix 1 – list of endpoints

Physical and chemical properties (Annex IIA, point 2)

	Sodium 5-nitroguaiacolate	**Sodium *o*-nitrophenolate**	**Sodium *p*-nitrophenolate**
Melting point (state purity) ‡	No melting point before decomposition (99.2%)	No melting point before decomposition (100.3%)	No melting point before decomposition (99.3 %)
Boiling point (state purity) ‡	Decomposition before boiling	Decomposition before boiling	Decomposition before boiling
Temperature of decomposition (state purity)	Decomposition occurred between 145°C and 360°C (99.2%)	Decomposition occurred between 280°C and 354°C (100.3%)	Decomposition occurred above 175°C (99.3%)
Appearance (state purity) ‡	Red crystalline powder (99.2%)	Red crystalline powder (100.3%)	Bright yellow fine granular powder (99.3%)
Vapour pressure (state temperature, state purity) ‡	< 1.00 x 10^{-7} mm Hg at 25°C (<1.33 x 10^{-5} Pa) (99.7%)	5.81 x 10^{-7} mmHg at 25°C (7.75 x 10^{-5} Pa) (99.3%)	< 1.00 x 10^{-7} mm Hg at 25°C (<1.33 x 10^{-5} Pa) (99.8%)
Henry's law constant ‡	Calculated values at 25°C: 4.51 x 10^{-4} Pa m^3/mol	Calculated values at 25°C: 5.55 x 10^{-4} Pa m^3/mol	Calculated values at 25°C: 5.55 x 10^{-4} Pa m^3/mol
Solubility in water (state temperature, state purity and pH) ‡	at 20°C: pH 4: 1.29 g/L pH 7: 1.83 g/L pH 10: 86.8 g/L (99.2%)	Pure a.s. at 20°C: pH 4: 0.78 g/L pH 7: 2.76 g/L pH 10: 181.6 g/L (100.3%)	Pure a.s. at 20°C: pH 4: 14.7 g/L pH 7: 13.9 g/L pH 10: 57.4 g/L (99.3%)
Solubility in organic solvents ‡ (state temperature, state purity)	Solubility in g/l at 20°C: n-heptane 2.8 x 10^{-3} o-xylene 2.9 x 10^{-2} 1,2-dichloroethane 3.9 x 10^{-2} Acetone 1.7 x 10^{-1} Methanol 53 Ethyl acetate 0.05 (99.2%)	Solubility in g/l at 20 °C: n-heptane < 2.0 x 10^{-4} o-xylene < 2.8 x 10^{-4} 1,2-dichloroethane < 5 x 10^{-4} Acetone 1.2 Methanol 47 Ethyl acetate 0.18 (100.3%)	Solubility in g/l at 20 °C: n-heptane 9.4 x 10^{-5} o-xylene 1.0 x 10^{-3} 1,2-dichloroethane 2.5 x 10^{-3} Acetone 2.4 Methanol 181 Ethyl acetate 0.18 (99.3%)
Surface tension ‡ (state concentration and temperature, state purity)	At 20°C: 73.06 mN/m (1g/L aqueous solution) (99.2%)	At 20°C: 73.62 mN/m (1g/L aqueous solution) (100.3%)	At 20°C: 73.31 mN/m (1g/L aqueous solution) (99.3%)
Partition co-efficient ‡ (state temperature, pH and purity)	At 20°C: at pH 4, log P_{ow} = 1.491 at pH 7, log P_{ow} = 1.62 at pH 10, log P_{ow} = -0.25 (99.2%)	At 20°C: at pH 4, log P_{ow} = 1.70 at pH 7, log P_{ow} = 1.12 at pH 10, log P_{ow} = -1.03 (100.3%)	At 20°C: at pH 4, log P_{ow} = 1.82 at pH 7, log P_{ow} = 1.28 at pH 10, log P_{ow} = -0.93 (99.3%)

Appendix 1 – list of endpoints

	pK_a = 8.21. at 22° C (99.2%)	pK_a = 7.16. at 22°C (100.3%)	pK_a = 7.16. at 22°C (99.3%)
Dissociation constant (state purity) ‡			
UV/VIS absorption (max.) incl. ε ‡ (state purity, pH)	***UV/Vis*** (99.2%) : *Neutral media* Concentration of Na 5NG: 1.36 x 10^{-4} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 210 / 1.24721 / 9194 241 / 0.91285 / 6729 342 / 0.77181 / 5689 *Alkaline media* Concentration of Na 5NG: 5.46 x 10^{-5} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 227 / 0.54549 / 9996 Concentration of Na 5NG: 1.36 x 10^{-4} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 263 / 1.7044 / 12564 322 / 0.69922 / 5154 418 / 0.51765 / 3816 *Acidic media* Concentration of Na 5NG: 5.46 x 10^{-5} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 210 / 0.55229 / 10120 Concentration of Na 5NG: 1.36 x 10^{-4} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 241 / 1.04414 / 7697 343 / 0.88823 / 6547	***UV/Vis*** (100.3%) : *Neutral media* Concentration of Na oNP: 6.43 x 10^{-5} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 213 / 0.72011 / 11198 Concentration of Na oNP: 1.56 x 10^{-4} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 278 / 0.83359 / 5338 359 / 0.37076 / 2374 *Alkaline media* Concentration of Na oNP: 6.43 x 10^{-5} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 227 / 0.93634 / 14560 Concentration of Na oNP: 1.56 x 10^{-4} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 282 / 0.64996 / 4162 417 / 0.72265 / 4627 *Acidic media* Concentration of Na oNP: 6.43 x 10^{-5} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 209 / 0.81460 / 12667 Concentration of Na oNP: 1.56 x 10^{-4} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 277 / 0.94242 / 6035 349 / 0.46271 / 2963	***UV/Vis*** (99.3%) : *Neutral media* Concentration of Na pNP: 1.28 x 10^{-4} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 226 / 0.84037 / 6551 320 / 0.85736 / 6683 399 / 0.92717 / 7227 *Alkaline media* Concentration of Na pNP: 5.14 x 10^{-5} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 229 / 0.28630 / 5568 Concentration of Na pNP: 3.2 x 10^{-5} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 401 / 0.59869 / 18666 *Acidic media* Concentration of Na pNP: 5.14 x 10^{-5} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 207 / 0.26595 / 5173 Concentration of Na pNP: 1.28 x 10^{-4} mol/l λ (nm) / Absorbance / ε [l/(cm*mol] 226 / 0.90121 / 7025 316 / 1.29344 / 10082

Appendix 1 – list of endpoints

Flammability ‡ (state purity)	Highly flammable (99.2%)	Highly flammable (100.3%)	Highly flammable (99.3%)
Explosive properties ‡ (state purity)	Explosive properties (99.3%)	Explosive properties (100.3%)	Explosive properties (99.3%)
Oxidising properties ‡ (state purity)	Not determined since Na 5 NG has explosive properties.	Not determined since Na o-NP has explosive properties.	Not determined since Na p-NP has explosive properties.

Appendix 1 – list of endpoints

Summary of representative uses evaluated (*sodium 5-nitroguaiacolate, sodium ortho-nitrophenolate and sodium para-nitrophenolate*)

Crop and/ or situation (a)	Member State or Country	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 a.s. (i)	method kind (f-h)	growth stage & season (j)	number min max (k)	interval between applications (min)	g a.s./hL min max	water L/ha min max	g as/ha min max		
Sugar beet	N	ATONIK	F	Plant growth stimulator	SL	Na 5NG 1 g/l Na oNP 2 g/l Na pNP 3 g/l	Spraying	From BBCH 12 To BBCH 49	4	7 - 30	Na 5-NG 0.25 - 0.5 Na oNP 0.5 - 1 Na pNP 0.5 – 0.75	200 - 400	Na 5NG 1 Na oNP 2 Na pNP 3	15	
Sugar beet	S	ATONIK	F	Plant growth stimulator	SL	Na 5NG 1 g/l Na oNP 2 g/l Na pNP 3 g/l	Spraying	From BBCH 12 To BBCH 49	4	7 -30	Na 5-NG 0.25 - 0.5 Na oNP 0.5 - 1 Na pNP 0.5 – 0.75	200 - 400	Na 5NG 1 Na oNP 2 Na pNP 3	15	
Oilseed rape	N	ATONIK	F	Plant growth stimulator	SL	Na 5NG 1 g/l Na oNP 2 g/l Na pNP 3 g/l	Spraying	From BBCH 31 to BBCH 69	2	30 - 60	Na 5-NG 0.25 – 0.5 Na oNP 0.5 - 1 Na pNP 0.5 – 0.75	200 - 400	Na 5NG 1 Na oNP 2 Na pNP 3	30	

Appendix 1 – list of endpoints

Crop and/ or situation (a)	Member State or Country	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 a.s. (i)	method kind (f-h)	growth stage & season (j)	number min max (k)	interval between applications (min)	g a.s./hL min max	water L/ha min max	g as/ha min max		
Oilseed rape	S	ATONIK	F	Plant growth stimulator	SL	Na 5NG 1 g/l Na oNP 2 g/l Na pNP 3 g/l	Spraying	From BBCH 31 to BBCH 69	2	30 - 60	Na 5-NG 0.25 – 0.5 Na oNP 0.5 - 1 Na pNP 0.5 – 0.75	200 - 400	Na 5NG 1 Na oNP 2 Na pNP 3	30	
Tomato	N	ATONIK	F or G	Plant growth stimulator	SL	Na 5NG 1 g/l Na oNP 2 g/l Na pNP 3 g/l	Spraying	BBCH 59 BBCH 69 BBCH 71 BBCH 79 BBCH 81	5	14	Na 5-NG 0.1 - 0.25 Na oNP 0.2 - 0.5 Na pNP 0.3 – 0.75	400 - 1000	Na 5NG 1 Na oNP 2 Na pNP 3	3	
Tomato	S	ATONIK	F or G	Plant growth stimulator	SL	Na 5NG 1 g/l Na oNP 2 g/l Na pNP 3 g/l	spraying	BBCH 59 BBCH 69 BBCH 71 BBCH 79 BBCH 81	5	14	Na 5-NG 0.1 - 0.25 Na oNP 0.2 - 0.5 Na pNP 0.3 – 0.75	400 - 1000	Na 5NG 1 Na oNP 2 Na pNP 3	3	

(a) In case of group of crops the Codex classification should be used
(b) Outdoor or field use (F), or glasshouse application (G)
(c) e.g. biting and sucking insects, soil born insects, foliar fungi
(d) e.g. wettable powder (WP), emulsifiable concentrate (EC), granule (GR)
(e) GCPF codes - GIFAP Technical monograph N°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
(i) g/kg or g/l
(j) Growth stage at last treatment
(k) Indicate the minimum and maximum number of application possible under practical conditions of use
(l) PHI = minimum Pre-Harvest Interval
(m) Remarks may include: extent of use/economic importance/restrictions (e.g. feeding, grazing)/minimal intervals between applications

Appendix 1 – list of endpoints

Methods of Analysis

Analytical methods for the active substance (Annex IIA, point 4.1)

Active substance (ISO Common Name)	**Sodium 5-nitroguaiacolate**	**Sodium *o*-nitrophenolate**	**Sodium *p*-nitrophenolate**
Technical as (analytical technique)	**- HPLC/UV**	**- HPLC/UV**	**- HPLC/UV**
Impurities in technical as (analytical technique)	**- HPLC-UV**	**- HPLC-UV**	**- HPLC-UV**
Plant protection product (analytical technique)	**- HPLC-UV**	**- HPLC-UV**	**- HPLC-UV**

Analytical methods for residues (Annex IIA, point 4.2)

Residue definitions for monitoring purposes

Active substance (ISO Common Name)		**Sodium 5-nitroguaiacolate**	**Sodium *o*-nitrophenolate**	**Sodium *p*-nitrophenolate**
Food of plant origin		5-nitroguaiacole	*o*-nitrophenol	*p*-nitrophenol
Food of animal origin		Not necessary because no MRL needs to be set for products of animal origin.	Not necessary because no MRL needs to be set for products of animal origin.	Not necessary because no MRL needs to be set for products of animal origin.
Soil		5-nitroguaiacole	*o*-nitrophenol	*p*-nitrophenol
Water	surface	5-nitroguaiacole	*o*-nitrophenol	*p*-nitrophenol
	drinking/ground	5-nitroguaiacole	*o*-nitrophenol	*p*-nitrophenol
Air		5-nitroguaiacole	*o*-nitrophenol	*p*-nitrophenol

Appendix 1 – list of endpoints

Analytical methods for residues (Annex IIA, point 4.2)

Food/feed of plant origin (analytical technique and LOQ for methods for monitoring purposes)	Substrates: sugar beet, oil seed rape, tomatoes, Analysis: HPLC/MS/MS Determined analyte: 5-nitroguaiacole, *o*-nitrophenol, *p*-nitrophenol LOQ: 0.01 mg/kg for each compound Substrates: oil seed rape Analysis: HPLC/ MS/MS Determined analyte: 5-nitroguaiacole, *o*-nitrophenol, *p*-nitrophenol LOQ: 0.01 mg/kg for each compound Substrates: tomatoes Analysis: HPLC/MS/MS Determined analyte: 5-nitroguaiacole, *o*-nitrophenol, *p*-nitrophenol LOQ: 0.01 mg/kg for each compound
Food/feed of animal origin (principle of method and LOQ for methods for monitoring purposes)	Since residues in animal tissues will not reach a level of significance, no analytical methods are required for the determination of Na-5-nitroguaiacolate, Na *p*-nitrophenolate and Na *o*-nitrophenolate residues in matrices of animal origin.
Soil (principle of method and LOQ)	Substrates: soil Analysis: HPLC/MS/MS Determined analyte: 5-nitroguaiacole, *o*-nitrophenol, *p*-nitrophenol LOQ: 0.01 mg/kg for each compound
Water (principle of method and LOQ)	Substrates: drinking water, ground water, surface water Analysis: HPLC/MS/MS Determined analyte: 5-nitroguaiacole, *o*-nitrophenol, *p*-nitrophenol LOQ: 0.1 µg/L for each compound
Air (principle of method and LOQ)	Substrates: air Analysis: HPLC/MS/MS Determined analyte: 5-nitroguaiacole, *o*-nitrophenol, *p*-nitrophenol LOQ: 1.25 µg/m^3 for each compound
Body fluids and tissues (principle of method and LOQ)	Not required because sodium 5-nitroguaiacolate, sodium *o*-nitrophenolate and sodium *p*-nitrophenolate are not classified as toxic or highly toxic.

Appendix 1 – list of endpoints

Classification and proposed labelling with regard to physical and chemical data (Annex IIA, point 10)

Active substance	**Sodium 5-nitroguaiacolate**	**Sodium *o*-nitrophenolate**	**Sodium *p*-nitrophenolate**
	RMS/peer review proposal:		
	Hazard Symbol: "F, E" Indication of Danger: "Highly Flammable" "Explosive" Risk Phrases: "R2: Risk of explosion by shock, friction, fire or other sources of ignition" "R11: Highly Flammable" Safety Phrase: "S16: Keep away from sources of ignition – No smoking"	Hazard Symbol: "F, E" Indication of Danger: "Highly Flammable" "Explosive" Risk Phrases: "R2: Risk of explosion by shock, friction, fire or other sources of ignition" "R11: Highly Flammable" Safety Phrase: "S16: Keep away from sources of ignition – No smoking"	Hazard Symbol: "F, E" Indication of Danger: "Highly Flammable" "Explosive" Risk Phrases: "R2: Risk of explosion by shock, friction, fire or other sources of ignition" "R11: Highly Flammable" Safety Phrase: "S16: Keep away from sources of ignition – No smoking"

Appendix 1 – list of endpoints

Impact on Human and Animal Health

Absorption, distribution, excretion and metabolism (toxicokinetics) (Annex IIA, point 5.1)

Rate and extent of absorption ‡	Rapid and extensive (>80% based on urinary excretion)
Distribution ‡	Widely distributed
Potential for accumulation ‡	No evidence of accumulation
Rate and extent of excretion ‡	Mainly excreted *via* urine (up to 95% within 96 hours)
Metabolism in animals ‡	Extensively metabolized. Main metabolites in urine: glucuro and sulfo conjugates
Toxicologically relevant compounds ‡ (animals and plants)	None
Toxicologically relevant compounds ‡ (environment)	Impurities: phenol, 2,4-dinitrophenol, 2,6-dinitrophenol

Acute toxicity (Annex IIA, point 5.2)

Rat LD_{50} oral ‡	Na 5-NG: 716.0 mg/kg bw Na *o*-NP: 960.1 mg/kg bw Na *p*-NP: 345.5 mg/kg bw	**R22**
Rabbit, rat LD_{50} dermal ‡	Na 5-NG: > 2000 mg/kg bw Na *o*-NP: > 2000 mg/kg bw Na *p*-NP: > 2000 mg/kg bw	
Rat LC_{50} inhalation ‡	Na 5-NG: > 2.38 mg/L air (MAC) Na *o*-NP: > 1.24 mg/L air (MAC) Na *p*-NP: > 1.20 mg/L air (MAC)	
Skin irritation ‡	Na 5-NG: Non skin irritant Na *o*-NP: Non skin irritant Na *p*-NP: Non skin irritant	
Eye irritation ‡	Na 5-NG: Severe eye irritant	**R41**
	Na *o*-NP: Eye irritant	**R36**
	Na *p*-NP: Eye irritant	**R36**
Skin sensitisation ‡	Na 5-NG: Non skin sensitizer (Buehler test) Na *o*-NP: Non skin sensitizer (Buehler test) Na *p*-NP: Non skin sensitizer (Buehler test)	-

Appendix 1 – list of endpoints

Short term toxicity (Annex IIA, point 5.3)

Target / critical effect ‡	Target organs: gastro-intestinal tract (dog), kidney (rat, dog), spleen (rat), liver and lungs (dog). Effects: repeated vomiting, thin and/or mucous faeces (dog), kidney and splenic pigmentation (rat), increased tubulonephrosis and waxy cast and/or lymphocytic infiltrate of the kidneys (dog), increased focal proliferation of MPS-cells of liver (dog)	
Relevant oral NOAEL ‡	90-day rat: LOAEL 489 mg **Atonik* MUP** powder*** (AMP)**/kg bw/day 90-day dog: Na 5-NG: 0.7 mg/kg bw/day Na *o*-NP: 1.39 mg/kg bw/day Na *p*-NP: 2.56 mg/kg bw/day 1-yr dog: Na 5-NG: 0.29 mg/kg bw/day Na *o*-NP: 0.58 mg/kg bw/day Na *p*-NP: 1.0 mg/kg bw/day	
Relevant dermal NOAEL ‡	No data - not required	
Relevant inhalation NOAEL ‡	No data - not required	

Genotoxicity ‡ (Annex IIA, point 5.4)

Na 5-NG: Not a genotoxic agent Na *o*-NP: Not a genotoxic agent Na *p*-NP: *In vitro* mutagen. Unlikely to be genotoxic *in vivo*.	

Long term toxicity and carcinogenicity (Annex IIA, point 5.5)

Target/critical effect ‡	Decreased body weight gain (♂ rat).	
Relevant NOAEL ‡	rat: 500 mg AMP/kg bw/day (2-yr) mouse: 2857 mg AMP/kg bw/day (18-mo)	
Carcinogenicity ‡	No evidence of carcinogenic potential	

Appendix 1 – list of endpoints

Reproductive toxicity (Annex IIA, point 5.6)

Reproduction toxicity

Reproduction target / critical effect ‡	Decreased fertility index in the presence of parental systemic toxicity (decreased body weight gain). No adverse effect in the offspring.
Relevant parental NOAEL ‡	300 mg AMP/kg bw/day
Relevant reproductive NOAEL ‡	300 mg AMP/kg bw/day
Relevant offspring NOAEL ‡	600 mg AMP/kg bw/day

Developmental toxicity

Developmental target / critical effect ‡	No developmental effects at maternally toxic doses (rats) Increased incidence of extra-ribs at maternally toxic doses (rabbits)
Relevant maternal NOAEL ‡	Rat: 300 mg AMP/kg bw/day Rabbit: <100 mg AMP/kg bw/day equivalent to Na 5-NG< 13.6 mg/kg bw/day Na *o*-NP< 26.5 mg/kg bw/day Na *p*-NP< 50.2 mg/kg bw/day
Relevant developmental NOAEL ‡	Rat: 600 mg AMP/kg bw/day Rabbit: 200 mg AMP/kg bw/day

Neurotoxicity (Annex IIA, point 5.7)

Acute neurotoxicity ‡	No data available - not required
Repeated neurotoxicity ‡	No data available - not required
Delayed neurotoxicity ‡	No data available - not required

Other toxicological studies (Annex IIA, point 5.8)

Mechanism studies ‡	No data available
Studies performed on metabolites or impurities‡	No data available

Medical data‡ (Annex IIA, point 5.9)

No record of illness related to Atonik exposure during the manufacturing process since 1952. No reports of clinical cases and poisoning incidents with Atonik.

Appendix 1 – list of endpoints

Summary (Annex IIA, point 5.10)	Value (mg/kg bw/d)	Study	Safety factor
ADI ‡	Na 5-NG: 0.003 Na *o*-NP: 0.003 Na *p*-NP: 0.003	1-year oral dog	100
AOEL ‡	Na 5-NG: 0.007 Na *o*-NP: 0.007 Na *p*-NP: 0.007	90-day oral dog	100 (100% oral absorption)
ARfD ‡	Na 5-NG: 0.045 Na *o*-NP: 0.045 Na *p*-NP: 0.045	Developmental rabbit	300*

* additional safety factor of 3 due to the use of a LOAEL

Dermal absorption‡ (Annex IIIA, point 7.3)
100% (default value)

Appendix 1 – list of endpoints

Exposure scenarios (Annex IIIA, point 7.2)

Operator	Intended application of Atonik on suger beet, oilseed rape & tomatoes at a maximum application rate of 1 L product/ha (1, 2 & 3g a.i./ha for Na 5-NG, Na *o*-NP & Na *p*-NP, respectively). **Field application** Tractor-mounted application[1] **No PPE** — **Gloves** **Na 5-NG:** German: 18 — 7 % of AOEL UK POEM: 169 — 14% of AOEL **Na *o*-NP:** German: 36 — 14% of AOEL UK POEM: 337 — 27% of AOEL **Na *p*-NP:** German: 54 — 21% of AOEL UK POEM: 506 — 41% of AOEL Handheld application (UKPOEM)[2] Na 5-NG: 125 — 33 % of AOEL Na *o*-NP: 250 — 66% of AOEL Na *p*-NP: 375 — 98% of AOEL **Greenhouse application (Dutch model)[3]** Na 5-NG: 41 — 4 % of AOEL Na *o*-NP: 82 — 9% of AOEL Na *p*-NP: 123 — 13% of AOEL
Workers	Estimated exposure according to EUROPOEM II[4] Na 5-NG: 18 % of AOEL Na *o*-NP: 37 % of AOEL Na *p*-NP: 55 % of AOEL
Bystanders	Estimated exposure according to EUROPOEM II[5] Na 5-NG: 6 % of AOEL Na *o*-NP: 12 % of AOEL Na *p*-NP: 18 % of AOEL

EFSA note[1] : total exposure to the 3 a.s. is below the AOEL only when PPE is used (42 and 82%).
EFSA note[2] : total exposure to the 3 a.s. is above the AOEL even with the use of PPE (197%).
EFSA note[3] : total exposure to the 3 a.s. is below the AOEL only when PPE is used (26%).
EFSA note[4] : total exposure to the 3 a.s. is above the AOEL when no PPE is used (110%).
EFSA note[5] : total exposure to the 3 a.s. is below the AOEL (36%).

Classification and proposed labelling with regard to toxicological data (Annex IIA, point 10)

	RMS/peer review proposal
(a) Sodium 5-Nitroguaiacolate	R22, R41
(b) Sodium *o*-Nitrophenolate	R22, R36
(c) Sodium *p*-Nitrophenolate	R22, R36

Appendix 1 – list of endpoints

Metabolism in plants (Annex IIA, point 6.1 and 6.7, Annex IIIA, point 8.1 and 8.6)

Plant groups covered	Fruit crops (Tomato), Root/Tuber crops (sugar beet) and Pulses/Oilseed crops (rape seed)
Rotational crops	Not Required
Metabolism in rotational crops similar to metabolism in primary crops?	Not relevant
Processed commodities	Not Required
Residue pattern in processed commodities similar to residue pattern in raw commodities?	Not Required
Plant residue definition for monitoring	Sum 5-nitroguaiacolate + *o*-nitrophenolate + *p*-nitrophenolate Proposed by EFSA after the meeting but not peer reviewed
Plant residue definition for risk assessment	Sum Sodium 5-nitroguaiacolate + Sodium *o*-nitrophenolate + Sodium *p*-nitrophenolate Proposed by EFSA after the meeting but not peer reviewed
	None

Metabolism in livestock (Annex IIA, point 6.2 and 6.7, Annex IIIA, point 8.1 and 8.6)

Animals covered	Not Relevant
Time needed to reach a plateau concentration in milk and eggs	Not Relevant
Animal residue definition for monitoring	Not Relevant
Animal residue definition for risk assessment	Not Relevant
Conversion factor (monitoring to risk assessment)	Not Relevant
Metabolism in rat and ruminant similar (yes/no)	Not Relevant
Fat soluble residue: (yes/no)	

Residues in succeeding crops (Annex IIA, point 6.6, Annex IIIA, point 8.5)

	Not required, as there is very fast degradation of the parent and its metabolites in soil (DT_{50lab} << 30 days, aerobic 10°C/20°C)

Appendix 1 – list of endpoints

Stability of residues (Annex IIA, point 6 introduction, Annex IIIA, point 8 Introduction)

No specific studies were conducted to address this point

Residues from livestock feeding studies (Annex IIA, point 6.4, Annex IIIA, point 8.3)

	Ruminant:	Poultry:	Pig:
	Conditions of requirement of feeding studies		
Expected intakes by livestock ≥ 0.1 mg/kg diet (dry weight basis) (yes/no - If yes, specify the level)	No	No	No
Metabolism studies indicate potential level of residues ≥ 0.01 mg/kg in edible tissues (yes/no)	Not Required	Not Required	Not Required
	Feeding studies (Specify the feeding rate in cattle and poultry studies considered as relevant) Residue levels in matrices : Mean (max) mg/kg		
Muscle			
Liver			
Kidney			
Fat			
Milk			
Eggs			

Appendix 1 – list of endpoints

Summary of residues data according to the representative uses on raw agricultural commodities and feedingstuffs (Annex IIA, point 6.3, Annex IIIA, point 8.2)

Crop	Northern or Mediterranean Region, field or glasshouse, and any other useful information	Trials results relevant to the representative uses (a)	Recommendation/comments	MRL estimated from trials according to the representative use	HR (c)	STMR (b)
Tomatoes		Not required				
Oilseed Rape		Not required				
Sugar Beet		Not required				

(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 representative use
(c) Highest residue

Appendix 1 – list of endpoints

Consumer risk assessment (Annex IIA, point 6.9, Annex IIIA, point 8.8)

ADI	Na 5-NG: 0.003 mg/kg b.w./day Na *o*-NP: 0.003 mg/kg b.w./day Na *p*-NP: 0.003 mg/kg b.w./day
TMDI (% ADI) according to EFSA Model rev2 (using the MRLs of 0.03* mg/kg proposed by EFSA)	maximum TMDI 23.5% ADI (UK Toddler)
TMDI (% ADI) according to national (to be specified) diets	-
IEDI (WHO European Diet) (% ADI)	-
NEDI (specify diet) (% ADI)	-
Factors included in IEDI and NEDI	-
ARfD	Na 5-NG: 0.045 mg/kg b.w./day Na *o*-NP: 0.045 mg/kg b.w./day Na *p*-NP: 0.045 mg/kg b.w./day
IESTI (% ARfD) EFSA model rev.2 (using the MRLs of 0.03* mg/kg proposed by EFSA)	4.3% Sugar bee (root), 3.9% Tomatoes and 0.1% Rape seed
NESTI (% ARfD) according to national (to be specified) large portion consumption data	Not Applicable
Factors included in IESTI and NESTI	Not Applicable

Processing factors (Annex IIA, point 6.5, Annex IIIA, point 8.4)

Crop/ process/ processed product	Number of studies	Processing factors		Amount transferred (%) (Optional)
		Transfer factor	Yield factor	

Appendix 1 – list of endpoints

Proposed MRLs (Annex IIA, point 6.7, Annex IIIA, point 8.6)

Sugar beet	0.03* mg/kg (proposed by EFSA after the meeting and not peer reviewed)
Oil seed rape	0.03* mg/kg (proposed by EFSA after the meeting and not peer reviewed)
Tomato	0.03* mg/kg (proposed by EFSA after the meeting and not peer reviewed)
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.....	

When the MRL is proposed at the LOQ, this should be annotated by an asterisk after the figure.

Appendix 1 – list of endpoints

A. <u>Sodium 5-nitroguaiacolate</u>

Route of degradation (aerobic) in soil (Annex IIA, point 7.1.1.1.1)

Mineralization after 100 days ‡	54.9% - 60.8% after 120 d, [^{14}C-Atonik]-label (n^7=*4*) at 20°C 49.1% after 120 d, [^{14}C-Atonik]-label (n=1) at 10°C
Non-extractable residues after 100 days ‡	32.1% - 41.1% after 120 d, [^{14}C-Atonik]-label (n=4) at 20°C 45.7% after 120 d, [^{14}C-Atonik]-label (n=1) at 10°C
Metabolites requiring further consideration ‡ - name and/or code, % of applied (range and maximum)	Unidentified M5, maximum 20.5% AR with respect to Na 5-NG, the compound with the smallest ratio in the mix of the three compounds (n= *4*) (day 7, 20°C)

Route of degradation in soil - Supplemental studies (Annex IIA, point 7.1.1.1.2)

Anaerobic degradation ‡

Mineralization after 100 days	9.4% after 120 d, [^{14}C-Atonik]-label (n=1) at 20°C
Non-extractable residues after 100 days	74.8% after 120 d, [^{14}C-Atonik]-label (n=1) at 20°C
Metabolites that may require further consideration for risk assessment - name and/or code, % of applied (range and maximum)	Unidentified M7, > 10% AR assuming formation from one of the individual compounds Unidentified M8, > 10% AR assuming formation only from Na 5-NG

Soil photolysis ‡

Metabolites that may require further consideration for risk assessment - name and/or code, % of applied (range and maximum)	None

[7] n corresponds to the number of soils.

Appendix 1 – list of endpoints

Rate of degradation in soil (Annex IIA, point 7.1.1.2, Annex IIIA, point 9.1.1)

Laboratory studies ‡

5-NG	Aerobic conditions						
Soil type	X[8]	pH	t. °C / % MWHC	DT_{50} /DT_{90} (d)	DT_{50} (d) 20°C pF2/10kPa	St. (r^2)	Method of calculation
Silt loam		7.2	20 °C / 40 %	0.1 / 0.4	0.1	0.9871	SFO
Sandy loam		6.3	20 °C / 40 %	0.2 / 0.7	0.2	0.9906	SFO
Clay loam		6.2	20 °C / 40 %	0.1 / 0.4	0.1	0.9732	SFO
Loam		7.4	20 °C / 40 %	0.6 / 2.1	0.6	0.9624	SFO
Silt loam		7.2	10 °C / 40 %	0.3 / 0.9	-	0.9746	SFO
Geometric mean/median							

Field studies ‡

5-NG	Aerobic conditions
As ^{14}C-5NG degraded very rapidly in soil with DT_{50lab} << 60 days whatever the conditions considered, field studies are not required.	

pH dependence ‡ (yes / no) (if yes type of dependence)	No
Soil accumulation and plateau concentration ‡	not relevant

[8] X This column is reserved for any other property that is considered to have a particular impact on the degradation rate.

Appendix 1 – list of endpoints

Laboratory studies ‡

Parent	Anaerobic conditions						
Soil type	X[9]	pH	t. °C / % MWHC	DT_{50} /DT_{90} (d)	DT_{50} (d) 20°C pF2/10kPa	St. (r^2)	Method of calculation
Loam		7.34	20 °C	3.3 / 11	3.3	0.9993	SFO

Soil adsorption/desorption (Annex IIA, point 7.1.2)

5-NG							
Soil Type	OC %	Soil pH	Kd (mL/g)	Koc (mL/g)	Kf (mL/g)	Kfoc (mL/g)	1/n
Loamy sand	2.17	5.7			3.604	166	0.98
Silty clay loam	1.16	6.6			15.654	1350	1.00
Clay loam	2.98	7.5			19.156	643	0.84
Loam	1.22	7.3			3.905	320	0.85
Arithmetic mean/median						463.4/482	
pH dependence, Yes or No			No				

Mobility in soil (Annex IIA, point 7.1.3, Annex IIIA, point 9.1.2)

Column leaching ‡	No study was conducted in addition as the soil adsorption/desorption with the active substance was conducted using batch equilibrium technique.
Aged residues leaching ‡	No study was conducted.

[9] X This column is reserved for any other property that is considered to have a particular impact on the degradation rate.

Appendix 1 – list of endpoints

Lysimeter/ field leaching studies ‡	In the light of the results obtained in adsorption/desorption study in relation to its fast degradation, no lysimeter study was conducted to estimate the leaching potential of the parent and its metabolites.

PEC (soil) (Annex IIIA, point 9.1.3)

5-NG Method of calculation	DT_{50} (d): 0.6 days Kinetics: SFO Worst case from lab studies.
Application data	Depth of soil layer: 5 cm Soil bulk density: 1.5 g/cm^3 Application rate(s): 1 g as/ha Sugar beet: 4 applications per year from BBCH 12 to BBCH 49 with a 7 days interval. LIF (Leaf interception factor): 20% for the first application, 70% for the second and third application and 90% for the last application.

$PEC_{(s)}$ (mg/kg)	Single application Actual	Single application Time weighted average	Multiple application Actual	Multiple application Time weighted average
Initial			1.335E-04	
Short term				
24h			4.204E-05	7.913E-05
2d			1.324E-05	5.203E-05
4d			1.314E-06	2.860E-05
Long term				
7d			4.105E-08	1.650E-05
28d			1.195E-18	4.126E-06
50d			1.095E-29	2.310E-06
100d			8.988E-55	1.155E-06
Plateau concentration				

Appendix 1 – list of endpoints

5-NG Method of calculation	DT_{50} (d): 0.6 days Kinetics: SFO Worst case from lab studies.
Application data	Depth of soil layer: 5 cm Soil bulk density: 1.5 g/cm^3 Application rate(s): 1 g as/ha Tomatoes: 5 applications per year at BBCH 59, BBCH 69, BBCH 71, BBCH 79 and BBCH 81 with a 14 days interval. LIF (Leaf interception factor): 80%.

$PEC_{(s)}$ (mg/kg)	Single application Actual	Single application Time weighted average	Multiple application Actual	Multiple application Time weighted average
Initial			2.667E-04	
Short term				
24h			8.399E-05	1.581E-04
2d			2.646E-05	1.040E-04
4d			2.625E-06	5.714E-05
Long term				
7d			8.203E-08	3.297E-05
28d			2.387E-18	8.244E-06
50d			2.188E-29	4.617E-06
100d			1.796E-54	2.308E-06
Plateau concentration				

5-NG Method of calculation	DT_{50} (d): 0.6 days Kinetics: SFO Worst case from lab studies.
Application data	Depth of soil layer: 5 cm Soil bulk density: 1.5 g/cm^3 Application rate(s): 1 g as/ha Oilseed rape: 2 applications per year from BBCH 31 to BBCH 69 with a 30 days interval. LIF (Leaf interception factor): 80%.

Appendix 1 – list of endpoints

PEC$_{(s)}$ (mg/kg)	Single application Actual	Single application Time weighted average	Multiple application Actual	Multiple application Time weighted average
Initial			2.667E-04	
Short term				
24h			8.399E-05	1.581E-04
2d			2.646E-05	1.040E-04
4d			2.625E-06	5.714E-05
Long term				
7d			8.203E-08	3.297E-05
28d			2.387E-18	8.244E-06
50d			2.188E-29	4.617E-06
100d			1.796E-54	2.308E-06
Plateau concentration				

Route and rate of degradation in water (Annex IIA, point 7.2.1)

Hydrolytic degradation of the active substance and metabolites > 10 % ‡	[^{14}C]-5NG was found to be hydrolytically stable at pH 4, 7 and 9 at a temperature of 50°C in the dark. No degradation of the test item was observed during 5 days of incubation at 50°C.
Photolytic degradation of active substance and metabolites above 10 % ‡	The test item 5NG was steadily photodegraded under simulated sunlight in sterile buffer solution at pH 7. Its experimental photolytic half life (DT50) was determined using first-order reaction kinetics to be 2 days of continuous irradiation under "Suntest" conditions. Its corresponding half life (DT50) at latitude 30°N was calculated to be about 3 summer days. Unidentified major metabolites: M3, M5, M8, M12, M13
Quantum yield of direct phototransformation in water at Σ > 290 nm	1.56 . 10^{-5} molecules degraded photon^{-1}
Readily biodegradable ‡ (yes/no)	No

Appendix 1 – list of endpoints

Degradation in water / sediment

Parent	Distribution: max in water 14.3-17.4% AR at day 0, max in sediment 2.6-4.6% AR at day 3 equivalent to 18.2-26.4% of the amount initially applied Na 5-NG									
Water / sediment system	pH water phase	pH sed	t. °C	DT_{50}-DT_{90} whole sys.	St. (r^2)	DT_{50}-DT_{90} water	St. (r^2)	DT_{50}-DT_{90} sed	St. (r^2)	Method of calculation
river system	-	7.47	20	5.4-18.1	0.9906	3.4-11.2	0.9953	-	-	-
pond system	-	7.17	20	3.0-10.0	0.9660	2.4-7.9	0.9667	-	-	-
Geometric mean/median				3.2-14.1		2.9-9.6		-		

Mineralization and non extractable residues					
Water / sediment system	pH water phase	pH sed	Mineralization x % after n d. (end of the study).	Non-extractable residues in sed. Max x % after n d	Non-extractable residues in sed. Max x % after n d (end of the study)
river system	-	7.47	66.1% after 122 d	41.9% max at 61d	30.7% at 122d
pond system	-	7.17	63.5% after 122 d	49.3% max at 15d	34.6% at 122d

PEC (surface water) and PEC sediment (Annex IIIA, point 9.2.3)

5-NG Parameters used in FOCUSsw step 1 and 2	Molecular weight (g/mol): - Water solubility (mg/L): 1830 K_{OC}/K_{OM} (L/kg): 463.4 DT_{50} soil (d): 0.6 days (Lab, In accordance with FOCUS SFO) DT_{50} water/sediment system (d): 5.4 (representative worst case from sediment water studies) DT_{50} water (d): 5.4 DT_{50} sediment (d): 5.4
Parameters used in FOCUSsw step 3 (if performed)	Version control no.'s of FOCUS software: Vapour pressure: Kom/Koc: 1/n: (Freundlich exponent general or for soil ,susp. solids or sediment respectively)

Appendix 1 – list of endpoints

Application rate	1 g a.i./ha Sugarbeet: 4 applications per year with a 7 days interval. LIF (Leaf interception factor) : 70%. Tomatoes: 5 applications per year with a 14 days interval. LIF (Leaf interception factor): 80%. Oilseed rape: 2 applications per year with a 30 days interval. LIF (Leaf interception factor): 80%.

SUGAR BEET – minimal crop cover

5NG

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.861		3.819	
1	0.745	0.803	3.452	3.635
2	0.655	0.751	3.036	3.437
4	0.507	0.664	2.349	3.057
7	0.345	0.560	1.598	2.582
14	0.140	0.394	0.651	1.818
21	0.057	0.293	0.265	1.355
28	0.023	0.229	0.108	1.060
42	0.004	0.157	0.018	0.724
50	0.001	0.132	0.006	0.610
100	0.000	0.066	0.000	0.305

Appendix 1 – list of endpoints

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.009	---	0.018	---
1	0.007	0.008	0.017	0.018
2	0.006	0.007	0.015	0.017
4	0.005	0.006	0.017	0.016
7	0.003	0.005	0.012	0.016
14	0.001	0.003	0.005	0.012
21	0.001	0.003	0.002	0.009
28	0.000	0.002	0.001	0.007
42	0.000	0.001	0.000	0.005
50	0.000	0.001	0.000	0.004
100	0.000	0.001	0.000	0.002

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0090	---	0.0181	---
1	0.0065	0.0078	0.0171	0.0176
2	0.0056	0.0069	0.0151	0.0168
4	0.0046	0.0060	0.0167	0.0161
7	0.0028	0.0049	0.0113	0.0151
14	0.0011	0.0034	0.0046	0.0113
21	0.0005	0.0025	0.0019	0.0086
28	0.0002	0.0020	0.0008	0.0067
42	0.0000	0.0013	0.0001	0.0046
50	0.0000	0.0011	0.0000	0.0039
100	0.0000	0.0006	0.0000	0.0019

Appendix 1 – list of endpoints

SUGAR BEET – average crop cover

5NG

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.8609		3.8190	
1	0.7449	0.8029	3.4516	3.6353
2	0.6551	0.7510	3.0358	3.4373
4	0.5068	0.6644	2.3485	3.0574
7	0.3448	0.5599	1.5979	2.5824
14	0.1404	0.3937	0.6506	1.8183
21	0.0572	0.2933	0.2649	1.3553
28	0.0233	0.2294	0.1079	1.0602
42	0.0039	0.1566	0.0179	0.7235
50	0.0014	0.1319	0.0064	0.6095
100	0.0000	0.0661	0.0000	0.3053

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0090	---	0.0181	---
1	0.0065	0.0078	0.0171	0.0176
2	0.0056	0.0069	0.0151	0.0168
4	0.0045	0.0060	0.0161	0.0159
7	0.0027	0.0048	0.0110	0.0148
14	0.0011	0.0033	0.0045	0.0110
21	0.0004	0.0024	0.0018	0.0083
28	0.0002	0.0019	0.0007	0.0065
42	0.0000	0.0013	0.0001	0.0045
50	0.0000	0.0011	0.0000	0.0038
100	0.0000	0.0005	0.0000	0.0019

Appendix 1 – list of endpoints

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0090	---	0.0181	---
1	0.0065	0.0078	0.0171	0.0176
2	0.0056	0.0069	0.0151	0.0168
4	0.0044	0.0059	0.0158	0.0158
7	0.0026	0.0048	0.0108	0.0147
14	0.0011	0.0033	0.0044	0.0109
21	0.0004	0.0024	0.0018	0.0082
28	0.0002	0.0019	0.0007	0.0065
42	0.0000	0.0013	0.0001	0.0044
50	0.0000	0.0011	0.0000	0.0037
100	0.0000	0.0005	0.0000	0.0019

Tomatoes
5NG

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	1.0761		4.7738	
1	0.9311	1.0036	4.3146	4.5442
2	0.8189	0.9387	3.7948	4.2966
4	0.6335	0.8305	2.9356	3.8217
7	0.4310	0.6999	1.9974	3.2280
14	0.1755	0.4921	0.8133	2.2729
21	0.0715	0.3667	0.3311	1.6942
28	0.0291	0.2868	0.1348	1.3252
42	0.0048	0.1957	0.0224	0.9044
50	0.0017	0.1649	0.0080	0.7619
100	0.0000	0.0826	0.0000	0.3816

Appendix 1 – list of endpoints

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0068	---	0.0123	---
1	0.0047	0.0057	0.0120	0.0121
2	0.0039	0.0050	0.0107	0.0117
4	0.0032	0.0043	0.0115	0.0112
7	0.0019	0.0035	0.0079	0.0105
14	0.0008	0.0024	0.0032	0.0079
21	0.0003	0.0018	0.0013	0.0059
28	0.0001	0.0014	0.0005	0.0047
42	0.0000	0.0009	0.0001	0.0032
50	0.0000	0.0008	0.0000	0.0027
100	0.0000	0.0004	0.0000	0.0013

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0068	---	0.0123	---
1	0.0047	0.0057	0.0120	0.0121
2	0.0039	0.0050	0.0107	0.0117
4	0.0032	0.0043	0.0113	0.0111
7	0.0019	0.0035	0.0077	0.0104
14	0.0008	0.0023	0.0031	0.0077
21	0.0003	0.0017	0.0013	0.0058
28	0.0001	0.0014	0.0005	0.0046
42	0.0000	0.0009	0.0001	0.0031
50	0.0000	0.0008	0.0000	0.0026
100	0.0000	0.0004	0.0000	0.0013

Appendix 1 – list of endpoints

Winter Oil seed rape

5NG

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.4305		1.9095	
1	0.3724	0.4014	1.7258	1.8177
2	0.3276	0.3755	1.5179	1.7187
4	0.2534	0.3322	1.1742	1.5287
7	0.1724	0.2800	0.7989	1.2912
14	0.0702	0.1969	0.3253	0.9092
21	0.0286	0.1467	0.1325	0.6777
28	0.0116	0.1147	0.0539	0.5301
42	0.0019	0.0783	0.0089	0.3617
50	0.0007	0.0659	0.0032	0.3048
100	0.0000	0.0330	0.0000	0.1526

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0091	---	0.0162	---
1	0.0062	0.0076	0.0158	0.0160
2	0.0052	0.0067	0.0141	0.0155
4	0.0042	0.0057	0.0151	0.0147
7	0.0025	0.0046	0.0103	0.0138
14	0.0010	0.0031	0.0042	0.0103
21	0.0004	0.0023	0.0017	0.0078
28	0.0002	0.0018	0.0007	0.0061
42	0.0000	0.0012	0.0001	0.0042
50	0.0000	0.0010	0.0000	0.0035
100	0.0000	0.0005	0.0000	0.0018

Appendix 1 – list of endpoints

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0091	---	0.0162	---
1	0.0062	0.0076	0.0158	0.0160
2	0.0052	0.0067	0.0141	0.0155
4	0.0041	0.0056	0.0147	0.0146
7	0.0025	0.0045	0.0100	0.0136
14	0.0010	0.0031	0.0041	0.0101
21	0.0004	0.0023	0.0017	0.0076
28	0.0002	0.0018	0.0007	0.0060
42	0.0000	0.0012	0.0001	0.0041
50	0.0000	0.0010	0.0000	0.0035
100	0.0000	0.0005	0.0000	0.0017

Summer Oil seed rape

5NG

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.4305		1.9095	
1	0.3724	0.4014	1.7258	1.8177
2	0.3276	0.3755	1.5179	1.7187
4	0.2534	0.3322	1.1742	1.5287
7	0.1724	0.2800	0.7989	1.2912
14	0.0702	0.1969	0.3253	0.9092
21	0.0286	0.1467	0.1325	0.6777
28	0.0116	0.1147	0.0539	0.5301
42	0.0019	0.0783	0.0089	0.3617
50	0.0007	0.0659	0.0032	0.3048
100	0.0000	0.0330	0.0000	0.1526

Appendix 1 – list of endpoints

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0091	---	0.0162	---
1	0.0062	0.0076	0.0158	0.0160
2	0.0052	0.0067	0.0141	0.0155
4	0.0042	0.0057	0.0151	0.0147
7	0.0025	0.0046	0.0103	0.0138
14	0.0010	0.0031	0.0042	0.0103
21	0.0004	0.0023	0.0017	0.0078
28	0.0002	0.0018	0.0007	0.0061
42	0.0000	0.0012	0.0001	0.0042
50	0.0000	0.0010	0.0000	0.0035
100	0.0000	0.0005	0.0000	0.0018

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0091	---	0.0162	---
1	0.0062	0.0076	0.0158	0.0160
2	0.0052	0.0067	0.0141	0.0155
4	0.0041	0.0056	0.0147	0.0146
7	0.0025	0.0045	0.0100	0.0136
14	0.0010	0.0031	0.0041	0.0101
21	0.0004	0.0023	0.0017	0.0076
28	0.0002	0.0018	0.0007	0.0060
42	0.0000	0.0012	0.0001	0.0041
50	0.0000	0.0010	0.0000	0.0035
100	0.0000	0.0005	0.0000	0.0017

Appendix 1 – list of endpoints

PEC (ground water) (Annex IIIA, point 9.2.1)

Method of calculation and type of study (*e.g.* modelling, field leaching, lysimeter)	**5-NG** FOCUS working group recommendations. Standard FOCUS groundwater scenarios • FOCUS PELMO 3.3.2 • PEARL 2.2.2 Worst case DT_{50} 0.6 d (no normalisation to 10kPa or pF2, 20 °C with Q10 of 2.2 was conducted). Kf_{OC}: median 463.4 ml/g, $^1/_n$= 1. **Metabolite M5** FOCUS working group recommendations. Standard FOCUS groundwater scenarios • FOCUS PELMO 3.3.2 Considering that for all soils, M5 was not detected in the last sample, day120, the DT50 is lower than 120 days. This value was used as worst case for risk assessment No adsorption data is available, a high mobility was considered (Koc = 1)
Application rate	**5-NG:** 1 g a.i./ha with PELMO and PEARL 2.2.2 Sugarbeet: 4 applications at 1 L/ha every 7 days until 15 days before harvest. First application 20% foliar crop interception, second and third application 70%, fourth application 90% foliar crop interception. Tomatoes: 5 applications at 1 L/ha with 14 days between each application and 3 days before harvest. 80% foliar crop interception. Oilseed rape: 2 applications at 1 L/ha with 30 days between each one with a PHI of 30 days. 80% foliar crop interception. **Metabolite M5** Considering the soil degradation study conducted with atonik, it is showing a maximum of metabolite M5 at 3.1% of total applied radioactivity, therefore an equivalent dose of 6*3.1%=0.186 g/ha was found at maximum.

Appendix 1 – list of endpoints

PEC(gw) - FOCUS modelling results (80th percentile annual average concentration at 1m)

5-NG	Same results with PELMO 3.3.2 and PEARL 2.2.2
Average annual concentration, all scenarios, all crops	< 0.001 µg/L

M5	**PELMO 3.3.2**
Average annual concentrations, µg/L	

Scenario	SUGARBEET	TOMATOES	WINTER OSR	SUMMER OSR
Chateaudun	0.047	0.029	0.010	-
Hamburg	0.087	-	0.013	-
Jokionen	0.123	--	-	0.024
Kremsmunster	0.060	-	0.011	-
Okehampton	0.065	-	0.008	0.011
Piacenza	0.037	0.023	0.005	-
Porto	0.035	0.024	0.005	0.009
Sevilla	0.015	0.004	-	-
Thiva	0.045	0.021	-	-

Fate and behaviour in air (Annex IIA, point 7.2.2, Annex III, point 9.3)

Direct photolysis in air ‡	Not available, not required
Quantum yield of direct phototransformation	The quantum yield of 5-NG was determined as Φ(5NG) = 1.56 . 10-5 molecules degraded photon-1 in water
Photochemical oxidative degradation in air ‡	Photochemical oxidative degradation in air : Model calculation according to Atkinson using the computer program AOPWIN. The half-life of sodium 5-nitroguaiacolate was calculated as 2.2 days when considering a day comprising 12 hours of sunlight and 1.1 days when considering a day comprising 24 hours of sunlight.
Volatilisation ‡	No information submitted
Metabolites	-

Appendix 1 – list of endpoints

PEC (air)

Method of calculation	Expert judgement, based on vapour pressure, dimensionless Henry's Law Constant

$PEC_{(a)}$

Maximum concentration	Not calculated – not required

Residues requiring further assessment

Environmental occurring metabolite requiring further assessment by other disciplines (toxicology and ecotoxicology).	Soil: Na 5-NG, M5, M7 (anaerobic), M8 (anaerobic) Groundwater: 5-NG, M5, M7 (anaerobic), M8 (anaerobic) Surface water: 5-NG, M5 (from soil), from aqueous photolysis study: M3, M5, M8, M12, M13. Note that the M5 from soil may be different to the M5 from aqueous photolysis. Sediment: 5-NG Air: 5-NG

Monitoring data, if available (Annex IIA, point 7.4)

Soil (indicate location and type of study)	No data provided - none requested
Surface water (indicate location and type of study)	No data provided - none requested
Ground water (indicate location and type of study)	No data provided - none requested
Air (indicate location and type of study)	No data provided - none requested

Appendix 1 – list of endpoints

Points pertinent to the classification and proposed labelling with regard to fate and behaviour data

Not readily biodegradable

B. Sodium ortho-nitrophenolate

Route of degradation (aerobic) in soil (Annex IIA, point 7.1.1.1.1)

Mineralization after 100 days ‡	54.9% - 60.8% after 120 d, [^{14}C-Atonik]-label (n^{10}=*4*) at 20°C 49.1% after 120 d, [^{14}C-Atonik]-label (n=1) at 10°C
Non-extractable residues after 100 days ‡	32.1% - 41.1% after 120 d, [^{14}C-Atonik]-label (n=4) at 20°C 45.7% after 120 d, [^{14}C-Atonik]-label (n=1) at 10°C
Metabolites requiring further consideration ‡ - name and/or code, % of applied (range and maximum)	Unidentified M5, maximum 20.5% AR with respect to Na 5-NG, the compound with the smallest ratio in the mix of the three compounds (n= *4*) (day 7, 20°C)

Route of degradation in soil - Supplemental studies (Annex IIA, point 7.1.1.1.2)

Anaerobic degradation ‡

Mineralization after 100 days	9.4% after 120 d, [^{14}C-Atonik]-label (n=1) at 20°C
Non-extractable residues after 100 days	74.8% after 120 d, [^{14}C-Atonik]-label (n=1) at 20°C
Metabolites that may require further consideration for risk assessment - name and/or code, % of applied (range and maximum)	Unidentified M7, > 10% AR assuming formation from one of the individual compounds Unidentified M8, > 10% AR assuming formation only from Na 5-NG

Soil photolysis ‡

Metabolites that may require further consideration for risk assessment - name and/or code, % of applied (range and maximum)	None

[10] n corresponds to the number of soils.

Appendix 1 – list of endpoints

Rate of degradation in soil (Annex IIA, point 7.1.1.2, Annex IIIA, point 9.1.1)

Laboratory studies ‡

o-NP	Aerobic conditions						
Soil type	X[1]	pH	t. °C / % MWHC	$DisT_{50}$ /DT_{90} (d)	$DisT_{50}$ (d) 20°C pF2/10kPa	St. (r^2)	Method of calculation
Silt loam		7.2	20 °C / 40 %	0.4 / 1.3	0.4	0.9924	SFO
Sandy loam		6.3	20 °C / 40 %	1.45 / 4.82*	1.45	0.9999	SFO
Clay loam		6.2	20 °C / 40 %	0.6 / 1.9	0.6	0.9858	SFO
Loam		7.4	20 °C / 40 %	1.5 / 5.0	1.5	0.9478	SFO
Silt loam		7.2	10 °C / 40 %	0.8 / 2.6	-	0.9045	SFO
Geometric mean/median							

Remark: dissipation includes volatilisation observed in the study
* validity of the values were not confirmed by the peer review

Field studies ‡

o-NP	Aerobic conditions
As ^{14}C-oNP degraded very rapidly in soil with DT_{50lab} << 60 days whatever the conditions considered, field studies are not required.	

pH dependence ‡ (yes / no) (if yes type of dependence)	No
Soil accumulation and plateau concentration ‡	Not relevant

[1] X This column is reserved for any other property that is considered to have a particular impact on the degradation rate.

Appendix 1 – list of endpoints

Laboratory studies ‡

Parent	Anaerobic conditions						
Soil type	X[1]	pH	t. °C / % MWHC	DT_{50} /DT_{90} (d)	DT_{50} (d) 20°C pF2/10kPa	St. (r^2)	Method of calculation
Loam		7.34	20 °C	3.3 / 10.8	3.3	0.9998	SFO

Soil adsorption/desorption (Annex IIA, point 7.1.2)

o-NP							
Soil Type	OC %	Soil pH	Kd (mL/g)	Koc (mL/g)	Kf (mL/g)	Kfoc (mL/g)	1/n
Loamy sand	2.17	5.7			1.937	89	0.98
Silty clay loam	1.16	6.6			6.053	522	1.00
Clay loam	2.98	7.5			2.812	94	0.82
Loam	1.22	7.3			1.657	136	0.82
Arithmetic mean/median						156.1/115	
pH dependence, Yes or No			No				

Mobility in soil (Annex IIA, point 7.1.3, Annex IIIA, point 9.1.2)

Column leaching ‡	No study was conducted in addition as the soil adsorption/desorption with the active substance was conducted using batch equilibrium technique.
Aged residues leaching ‡	No study was conducted.

[1] X This column is reserved for any other property that is considered to have a particular impact on the degradation rate.

Appendix 1 – list of endpoints

Lysimeter/ field leaching studies ‡	In the light of the results obtained in adsorption/desorption study in relation to its fast degradation, no lysimeter study was conducted to estimate the leaching potential of the parent and its metabolites.

PEC (soil) (Annex IIIA, point 9.1.3)

o-NP Method of calculation	DT_{50} (d): 1.5 days Kinetics: SFO Worst case from lab. studies
Application data	Depth of soil layer: 5 cm Soil bulk density: 1.5 g/cm^3 Application rate(s): 2 g as/ha Sugar beet: 4 applications per year from BBCH 12 to BBCH 49 with a 7 days interval. LIF (Leaf interception factor): 20% for the first application, 70% for the second and third application and 90% for the last application.

$PEC_{(s)}$ (mg/kg)	Single application Actual	Single application Time weighted average	Multiple application Actual	Multiple application Time weighted average
Initial			2.995E-04	
Short term				
24h			1.887E-04	2.399E-04
2d			1.189E-04	1.955E-04
4d			4.717E-05	1.365E-04
Long term				
7d			1.179E-05	8.896E-05
28d			7.198E-10	2.315E-05
50d			2.768E-14	1.296E-05
100d			2.557E-24	6.482E-06
Plateau concentration				

Appendix 1 – list of endpoints

o-NP Method of calculation	DT_{50} (d): 1.5 days Kinetics: SFO Worst case from lab. studies
Application data	Depth of soil layer: 5 cm Soil bulk density: 1.5 g/cm^3 Application rate(s): 2 g as/ha Tomatoes: 5 applications per year at BBCH 59, BBCH 69, BBCH 71, BBCH 79 and BBCH 81 with a 14 days interval. LIF (Leaf interception factor): 80%.

$PEC_{(s)}$ (mg/kg)	Single application Actual	Single application Time weighted average	Multiple application Actual	Multiple application Time weighted average
Initial			5.342E-04	
Short term				
24h			3.365E-04	4.277E-04
2d			2.120E-04	3.486E-04
4d			8.413E-05	2.435E-04
Long term				
7d			2.103E-05	1.586E-04
28d			1.284E-09	4.128E-05
50d			4.936E-14	2.312E-05
100d			4.560E-24	1.156E-05
Plateau concentration				

o-NP Method of calculation	DT_{50} (d): 1.5 days Kinetics: SFO Worst case from lab studies
Application data	Depth of soil layer: 5 cm Soil bulk density: 1.5 g/cm^3 Application rate(s): 2 g as/ha Oilseed rape: 2 applications per year from BBCH 31 to BBCH 69 with a 30 days interval. LIF (Leaf interception factor): 80%.

Appendix 1 – list of endpoints

PEC$_{(s)}$ (mg/kg)	Single application Actual	Single application Time weighted average	Multiple application Actual	Multiple application Time weighted average
Initial			5.333E-04	
Short term				
24h			3.360E-04	4.271E-04
2d			2.117E-04	3.481E-04
4d			8.399E-05	2.431E-04
Long term				
7d			2.100E-05	1.584E-04
28d			1.282E-09	4.122E-05
50d			4.928E-14	2.308E-05
100d			4.553E-24	1.154E-05
Plateau concentration				

Route and rate of degradation in water (Annex IIA, point 7.2.1)

Hydrolytic degradation of the active substance and metabolites > 10 % ‡	[^{14}C]-oNP was found to be hydrolytically stable at pH 4, 7 and 9 at a temperature of 50°C in the dark. No degradation of the test item was observed during 5 days of incubation at 50°C.
Photolytic degradation of active substance and metabolites above 10 % ‡	The test item oNP was steadily photodegraded under simulated sunlight in sterile buffer solution at pH 7. Its experimental photolytic half life (DT50) was determined using first-order reaction kinetics to be 37 days of continuous irradiation under "Suntest" conditions. Its corresponding half life (DT50) at latitude 30°N was calculated to be about 60 summer days. Note: some volatilisation was observed during the experiment Theoretical photolytic half life (latitude 30°N, summer) using quantum yield was determined to be 88 days.
Quantum yield of direct phototransformation in water at Σ > 290 nm	6.52 x 10^{-7} molecules degraded photon^{-1}
Readily biodegradable ‡ (yes/no)	No

Appendix 1 – list of endpoints

Degradation in water / sediment

Parent	Distribution: max in water 32.3-33.9% AR at day 0, max in sediment 0.5-0.8% AR at day 3 equivalent to 1.5-2.4% of the amount initially applied Na o-NP									
Water / sediment system	pH water phase	pH sed	t. °C	DT_{50}-DT_{90} whole sys.	St. (r^2)	DT_{50}-DT_{90} water	St. (r^2)	DT_{50}-DT_{90} sed	St. (r^2)	Method of calculation
river system	-	7.47	20	2.0-6.8	0.9930	1.9-6.4	0.9924	-	-	-
pond system	-	7.17	20	2.2-7.5	0.9828	2.2-7.3	0.9838	-	-	-
Geometric mean/median				2.1-7.2		2.1-6.8		-		

Mineralization and non extractable residues					
Water / sediment system	pH water phase	pH sed	Mineralization x % after n d. (end of the study).	Non-extractable residues in sed. Max x % after n d	Non-extractable residues in sed. Max x % after n d (end of the study)
river system	-	7.47	66.1% after 122 d	41.9% max at 61d	30.7% at 122d
pond system	-	7.17	63.5% after 122 d	49.3% max at 15d	34.6% at 122d

PEC (surface water) and PEC sediment (Annex IIIA, point 9.2.3)

o-NP Parameters used in FOCUSsw step 1 and 2	Molecular weight (g/mol): - Water solubility (mg/L): 2760 K_{OC}/K_{OM} (L/kg): 156.1 DT_{50} soil (d): 5.5 days DT_{50} water/sediment system (d): 2.2 (representative worst case from sediment water studies) DT_{50} water (d): 2.2 DT_{50} sediment (d): 2.2
Parameters used in FOCUSsw step 3 (if performed)	Version control no.'s of FOCUS software: Vapour pressure: Kom/Koc: 1/n: (Freundlich exponent general or for soil ,susp. solids or sediment respectively)

Appendix 1 – list of endpoints

Application rate	2 g a.i./ha Sugarbeet: 4 applications per year with a 7 days interval. LIF (Leaf interception factor) : 70%. Tomatoes: 5 applications per year with a 14 days interval. LIF (Leaf interception factor): 80%. Oilseed rape: 2 applications per year with a 30 days interval. LIF (Leaf interception factor): 80%.

SUGAR BEET – minimal crop cover

oNP

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.5702		0.8614	
1	0.4138	0.4920	0.6459	0.7537
2	0.3020	0.4235	0.4714	0.6539
4	0.1608	0.3237	0.2510	0.5018
7	0.0625	0.2296	0.0975	0.3563
14	0.0069	0.1274	0.0107	0.1978
21	0.0008	0.0859	0.0012	0.1333
28	0.0001	0.0645	0.0001	0.1001
42	0.0000	0.0430	0.0000	0.0668
50	0.0000	0.0361	0.0000	0.0561
100	0.0000	0.0181	0.0000	0.0280

Appendix 1 – list of endpoints

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.1360	---	0.2104	---
1	0.0991	0.1175	0.1546	0.1825
2	0.0723	0.1016	0.1128	0.1581
4	0.0385	0.0778	0.0601	0.1213
7	0.0150	0.0552	0.0234	0.0861
14	0.0016	0.0307	0.0026	0.0478
21	0.0002	0.0207	0.0003	0.0322
28	0.0000	0.0155	0.0000	0.0242
42	0.0000	0.0103	0.0000	0.0161
50	0.0000	0.0087	0.0000	0.0135
100	0.0000	0.0043	0.0000	0.0068

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0918	---	0.1415	---
1	0.0668	0.0793	0.1043	0.1229
2	0.0488	0.0686	0.0761	0.1066
4	0.0260	0.0525	0.0405	0.0818
7	0.0101	0.0373	0.0158	0.0581
14	0.0011	0.0207	0.0017	0.0322
21	0.0001	0.0139	0.0002	0.0217
28	0.0000	0.0105	0.0000	0.0163
42	0.0000	0.0070	0.0000	0.0109
50	0.0000	0.0059	0.0000	0.0091
100	0.0000	0.0029	0.0000	0.0046

Appendix 1 – list of endpoints

SUGAR BEET – average crop cover

oNP
Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.5702		0.8614	
1	0.4138	0.4920	0.6459	0.7537
2	0.3020	0.4235	0.4714	0.6539
4	0.1608	0.3237	0.2510	0.5018
7	0.0625	0.2296	0.0975	0.3563
14	0.0069	0.1274	0.0107	0.1978
21	0.0008	0.0859	0.0012	0.1333
28	0.0001	0.0645	0.0001	0.1001
42	0.0000	0.0430	0.0000	0.0668
50	0.0000	0.0361	0.0000	0.0561
100	0.0000	0.0181	0.0000	0.0280

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0532	---	0.0812	---
1	0.0386	0.0459	0.0603	0.0707
2	0.0282	0.0397	0.0440	0.0615
4	0.0150	0.0304	0.0234	0.0472
7	0.0058	0.0216	0.0091	0.0335
14	0.0006	0.0120	0.0010	0.0186
21	0.0001	0.0081	0.0001	0.0125
28	0.0000	0.0061	0.0000	0.0094
42	0.0000	0.0040	0.0000	0.0063
50	0.0000	0.0034	0.0000	0.0053
100	0.0000	0.0017	0.0000	0.0026

Appendix 1 – list of endpoints

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0366	---	0.0553	---
1	0.0266	0.0316	0.0415	0.0484
2	0.0194	0.0273	0.0303	0.0421
4	0.0103	0.0209	0.0161	0.0324
7	0.0040	0.0148	0.0063	0.0230
14	0.0004	0.0082	0.0007	0.0128
21	0.0000	0.0055	0.0001	0.0086
28	0.0000	0.0042	0.0000	0.0065
42	0.0000	0.0028	0.0000	0.0043
50	0.0000	0.0023	0.0000	0.0036
100	0.0000	0.0012	0.0000	0.0018

Tomatoes

o-NP

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.5702		0.8614	
1	0.4138	0.4920	0.6459	0.7537
2	0.3020	0.4235	0.4714	0.6539
4	0.1608	0.3237	0.2510	0.5018
7	0.0625	0.2296	0.0975	0.3563
14	0.0069	0.1274	0.0107	0.1978
21	0.0008	0.0859	0.0012	0.1333
28	0.0001	0.0645	0.0001	0.1001
42	0.0000	0.0430	0.0000	0.0668
50	0.0000	0.0361	0.0000	0.0561
100	0.0000	0.0181	0.0000	0.0280

Appendix 1 – list of endpoints

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0392	---	0.0596	---
1	0.0285	0.0338	0.0445	0.0521
2	0.0208	0.0292	0.0324	0.0453
4	0.0111	0.0224	0.0173	0.0348
7	0.0043	0.0159	0.0067	0.0247
14	0.0005	0.0088	0.0007	0.0137
21	0.0001	0.0059	0.0001	0.0092
28	0.0000	0.0045	0.0000	0.0069
42	0.0000	0.0030	0.0000	0.0046
50	0.0000	0.0025	0.0000	0.0039
100	0.0000	0.0013	0.0000	0.0019

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0271	---	0.0408	---
1	0.0197	0.0234	0.0307	0.0358
2	0.0144	0.0202	0.0224	0.0312
4	0.0076	0.0155	0.0119	0.0240
7	0.0030	0.0110	0.0046	0.0170
14	0.0003	0.0061	0.0005	0.0095
21	0.0000	0.0041	0.0001	0.0064
28	0.0000	0.0031	0.0000	0.0048
42	0.0000	0.0021	0.0000	0.0032
50	0.0000	0.0017	0.0000	0.0027
100	0.0000	0.0009	0.0000	0.0013

Appendix 1 – list of endpoints

Winter Oil seed rape

oNP

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.5702		0.8614	
1	0.4138	0.4920	0.6459	0.7537
2	0.3020	0.4235	0.4714	0.6539
4	0.1608	0.3237	0.2510	0.5018
7	0.0625	0.2296	0.0975	0.3563
14	0.0069	0.1274	0.0107	0.1978
21	0.0008	0.0859	0.0012	0.1333
28	0.0001	0.0645	0.0001	0.1001
42	0.0000	0.0430	0.0000	0.0668
50	0.0000	0.0361	0.0000	0.0561
100	0.0000	0.0181	0.0000	0.0280

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0431	---	0.0652	---
1	0.0313	0.0372	0.0489	0.0570
2	0.0228	0.0322	0.0357	0.0497
4	0.0122	0.0246	0.0190	0.0382
7	0.0047	0.0175	0.0074	0.0271
14	0.0005	0.0097	0.0008	0.0151
21	0.0001	0.0065	0.0001	0.0101
28	0.0000	0.0049	0.0000	0.0076
42	0.0000	0.0033	0.0000	0.0051
50	0.0000	0.0027	0.0000	0.0043
100	0.0000	0.0014	0.0000	0.0021

Appendix 1 – list of endpoints

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0236	---	0.0347	---
1	0.0171	0.0203	0.0266	0.0307
2	0.0125	0.0175	0.0194	0.0269
4	0.0066	0.0134	0.0104	0.0207
7	0.0026	0.0095	0.0040	0.0147
14	0.0003	0.0053	0.0004	0.0082
21	0.0000	0.0036	0.0000	0.0055
28	0.0000	0.0027	0.0000	0.0041
42	0.0000	0.0018	0.0000	0.0028
50	0.0000	0.0015	0.0000	0.0023
100	0.0000	0.0007	0.0000	0.0012

Summer Oil seed rape

oNP

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.5702		0.8614	
1	0.4138	0.4920	0.6459	0.7537
2	0.3020	0.4235	0.4714	0.6539
4	0.1608	0.3237	0.2510	0.5018
7	0.0625	0.2296	0.0975	0.3563
14	0.0069	0.1274	0.0107	0.1978
21	0.0008	0.0859	0.0012	0.1333
28	0.0001	0.0645	0.0001	0.1001
42	0.0000	0.0430	0.0000	0.0668
50	0.0000	0.0361	0.0000	0.0561
100	0.0000	0.0181	0.0000	0.0280

Appendix 1 – list of endpoints

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0431	---	0.0652	---
1	0.0313	0.0372	0.0489	0.0570
2	0.0228	0.0322	0.0357	0.0497
4	0.0122	0.0246	0.0190	0.0382
7	0.0047	0.0175	0.0074	0.0271
14	0.0005	0.0097	0.0008	0.0151
21	0.0001	0.0065	0.0001	0.0101
28	0.0000	0.0049	0.0000	0.0076
42	0.0000	0.0033	0.0000	0.0051
50	0.0000	0.0027	0.0000	0.0043
100	0.0000	0.0014	0.0000	0.0021

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0236	---	0.0347	---
1	0.0171	0.0203	0.0266	0.0307
2	0.0125	0.0175	0.0194	0.0269
4	0.0066	0.0134	0.0104	0.0207
7	0.0026	0.0095	0.0040	0.0147
14	0.0003	0.0053	0.0004	0.0082
21	0.0000	0.0036	0.0000	0.0055
28	0.0000	0.0027	0.0000	0.0041
42	0.0000	0.0018	0.0000	0.0028
50	0.0000	0.0015	0.0000	0.0023
100	0.0000	0.0007	0.0000	0.0012

PEC (ground water) (Annex IIIA, point 9.2.1)

Method of calculation and type of study (*e.g.* modelling, field leaching, lysimeter)	**o-NP** FOCUS working group recommendations. Standard FOCUS groundwater scenarios • FOCUS PELMO 3.3.2 • PEARL 2.2.2 Worst case DT_{50} 5.5 d (no normalisation to 10kPa or pF2, 20 °C with Q10 of 2.2 was conducted). (Note: the longest lab DT_{50} is 1.5 days) Kf_{OC}: median 156.1, $^{1}/_{n}$= 1

Appendix 1 – list of endpoints

Application rate	**o-NP: 2** g a.i./ha with PELMO and PEARL 2.2.2 Sugarbeet: 4 applications at 1 L/ha every 7 days until 15 days before harvest. First application 20% foliar crop interception, second and third application 70%, fourth application 90% foliar crop interception. Tomatoes: 5 applications at 1 L/ha with 14 days between each application and 3 days before harvest. 80% foliar crop interception. Oilseed rape: 2 applications at 1 L/ha with 30 days between each one with a PHI of 30 days. 80% foliar crop interception.

PEC(gw) - FOCUS modelling results (80th percentile annual average concentration at 1m)

o-NP	Same results with PELMO 3.3.2 and PEARL 2.2.2
Average annual concentration, all scenarios, all crops	< 0.001 µg/L

Fate and behaviour in air (Annex IIA, point 7.2.2, Annex III, point 9.3)

Direct photolysis in air ‡	Not available, not required
Quantum yield of direct phototransformation	The quantum yield of o-NP was determined as Φ(oNP) = 6.52 x 10-7 molecules degraded photon-1 in water
Photochemical oxidative degradation in air ‡	Photochemical oxidative degradation in air: Model calculation according to Atkinson using the computer program AOPWIN. The half-life of Sodium ortho-nitrophenolate was calculated as 2.3 days when considering a day comprising 12 hours of sunlight and 1.2 days when considering a day comprising 24 hours of sunlight.
Volatilisation ‡	No information submitted
Metabolites	-

Appendix 1 – list of endpoints

PEC (air)

Method of calculation	Expert judgement, based on vapour pressure, dimensionless Henry's Law Constant

$PEC_{(a)}$

Maximum concentration	Not calculated – not required

Residues requiring further assessment

Environmental occurring metabolite requiring further assessment by other disciplines (toxicology and ecotoxicology).	Soil: Na o-NP, M5, M7 (anaerobic), M8 (anaerobic) Groundwater: o-NP,M5, M7 (anaerobic) , M8 (anaerobic) Surface water: o-NP, M5 (from soil). Note that the M5 from soil may be different to the M5 from aqueous photolysis. Sediment: o-NP Air: o-NP

Monitoring data, if available (Annex IIA, point 7.4)

Soil (indicate location and type of study)	No data provided - none requested
Surface water (indicate location and type of study)	No data provided - none requested
Ground water (indicate location and type of study)	No data provided - none requested
Air (indicate location and type of study)	No data provided - none requested

Points pertinent to the classification and proposed labelling with regard to fate and behaviour data

Not readily biodegradable

Appendix 1 – list of endpoints

C. Sodium para-nitrophenolate

Route of degradation (aerobic) in soil (Annex IIA, point 7.1.1.1.1)

Mineralization after 100 days ‡	54.9% - 60.8% after 120 d, [^{14}C-Atonik]-label (n[13]=4) at 20°C 49.1% after 120 d, [^{14}C-Atonik]-label (n=1) at 10°C
Non-extractable residues after 100 days ‡	32.1% - 41.1% after 120 d, [^{14}C-Atonik]-label (n=4) at 20°C 45.7% after 120 d, [^{14}C-Atonik]-label (n=1) at 10°C
Metabolites requiring further consideration ‡ - name and/or code, % of applied (range and maximum)	Unidentified M5, maximum 20.5% AR with respect to Na 5-NG, the compound with the smallest ratio in the mix of the three compounds (n= *4*) (day 7, 20°C)

Route of degradation in soil - Supplemental studies (Annex IIA, point 7.1.1.1.2)

Anaerobic degradation ‡

Mineralization after 100 days	9.4% after 120 d, [^{14}C-Atonik]-label (n=1) at 20°C
Non-extractable residues after 100 days	74.8% after 120 d, [^{14}C-Atonik]-label (n=1) at 20°C
Metabolites that may require further consideration for risk assessment - name and/or code, % of applied (range and maximum)	Unidentified M7, > 10% AR assuming formation from one of the individual compounds Unidentified M8, > 10% AR assuming formation only from Na 5-NG

Soil photolysis ‡

Metabolites that may require further consideration for risk assessment - name and/or code, % of applied (range and maximum)	None

[13] n corresponds to the number of soils.

Appendix 1 – list of endpoints

Rate of degradation in soil (Annex IIA, point 7.1.1.2, Annex IIIA, point 9.1.1)

Laboratory studies ‡

p-NP	Aerobic conditions						
Soil type	X[1]	pH	t. °C / % MWHC	DT_{50} /DT_{90} (d)	DT_{50} (d) 20°C pF2/10kPa	St. (r^2)	Method of calculation
Silt loam		7.2	20 °C / 40 %	1.3 / 4.4	1.3	0.9318	SFO
Sandy loam		6.3	20 °C / 40 %	2.2 / 7.5	2.2	0.9931	SFO
Clay loam		6.2	20 °C / 40 %	0.6 / 1.9	0.6	0.9648	SFO
Loam		7.4	20 °C / 40 %	0.8 / 2.7	0.8	0.9672	SFO
Silt loam		7.2	10 °C / 40 %	3.3 / 11	-	0.9845	SFO
Geometric mean/median							

Field studies ‡

p-NP	Aerobic conditions
As ^{14}C-pNP degraded very rapidly in soil with DT_{50lab} << 60 days whatever the conditions considered, field studies are not required.	

pH dependence ‡ (yes / no) (if yes type of dependence)	No
Soil accumulation and plateau concentration ‡	Not relevant

[1] X This column is reserved for any other property that is considered to have a particular impact on the degradation rate.

Appendix 1 – list of endpoints

Laboratory studies ‡

p-NP	Anaerobic conditions						
Soil type	X[1]	pH	t. °C / % MWHC	DT_{50} /DT_{90} (d)	DT_{50} (d) 20°C pF2/10kPa	St. (r^2)	Method of calculation
Loam		7.34	20 °C	12.6 / 41.8	12.6	0.9607	SFO

Soil adsorption/desorption (Annex IIA, point 7.1.2)

p-NP							
Soil Type	OC %	Soil pH	Kd (mL/g)	Koc (mL/g)	Kf (mL/g)	Kfoc (mL/g)	1/n
Loamy sand	2.17	5.7			2.676	123	0.98
Silty clay loam	1.16	6.6			6.979	602	1.00
Clay loam	2.98	7.5			8.031	269	0.84
Loam	1.22	7.3			4.224	346	0.85
Arithmetic mean/median						288.1/308	
pH dependence, Yes or No			No				

Mobility in soil (Annex IIA, point 7.1.3, Annex IIIA, point 9.1.2)

Column leaching ‡	No study was conducted in addition as the soil adsorption/desorption with the active substance was conducted using batch equilibrium technique.
Aged residues leaching ‡	No study was conducted.

[1] X This column is reserved for any other property that is considered to have a particular impact on the degradation rate.

Appendix 1 – list of endpoints

Lysimeter/ field leaching studies ‡	In the light of the results obtained in adsorption/desorption study in relation to its fast degradation, no lysimeter study was conducted to estimate the leaching potential of the parent and its metabolites.

PEC (soil) (Annex IIIA, point 9.1.3)

p-NP Method of calculation	DT_{50} (d): 2.2 days Kinetics: SFO Worst case from lab. studies
Application data	Depth of soil layer: 5 cm Soil bulk density: 1.5 g/cm^3 Application rate(s): 3 g as/ha Sugar beet: 4 applications per year from BBCH 12 to BBCH 49 with a 7 days interval. LIF (Leaf interception factor): 20% for the first application, 70% for the second and third application and 90% for the last application.

PEC(s) (mg/kg soil)		Multiple application Actual	Multiple application Time weighted average
Initial		5.511E-04	
Short term	24h	4.022E-04	4.727E-04
	2d	2.935E-04	4.088E-04
	4d	1.563E-04	3.133E-04
Long term	7d	6.073E-05	2.223E-04
	28d	8.127E-08	6.246E-05
	50d	7.937E-11	3.498E-05
	100d	1.143E-17	1.749E-05

Plateau concentration	

p-NP Method of calculation	DT_{50} (d): 2.2 days Kinetics: SFO Worst case from lab. studies

Appendix 1 – list of endpoints

Application data	Depth of soil layer: 5 cm Soil bulk density: 1.5 g/cm^3 Application rate(s): 3 g as/ha Tomatoes: 5 applications per year at BBCH 59, BBCH 69, BBCH 71, BBCH 79 and BBCH 81 with a 14 days interval. LIF (Leaf interception factor): 80%.

PEC(s) (mg/kg soil)		Multiple application Actual	Multiple application Time weighted average
Initial		8.098E-04	
Short term	24h	5.910E-04	6.947E-04
	2d	4.313E-04	6.008E-04
	4d	2.297E-04	4.604E-04
Long term	7d	8.924E-05	3.267E-04
	28d	1.194E-07	9.178E-05
	50d	1.166E-10	5.141E-05
	100d	1.680E-17	2.570E-05
Plateau concentration			

p-NP Method of calculation	DT_{50} (d): 2.2 days Kinetics: SFO Worst case from lab. studies
Application data	Depth of soil layer: 5 cm Soil bulk density: 1.5 g/cm^3 Application rate(s): 3 g as/ha Oilseed rape: 2 applications per year from BBCH 31 to BBCH 69 with a 30 days interval. LIF (Leaf interception factor): 80%.

Appendix 1 – list of endpoints

PEC(s) (mg/kg soil)		Multiple application Actual	Multiple application Time weighted average
Initial		8.001E-04	
Short term	24h	5.838E-04	6.863E-04
	2d	4.260E-04	5.935E-04
	4d	2.269E-04	4.548E-04
Long term	7d	8.817E-05	3.228E-04
	28d	1.180E-07	9.068E-05
	50d	1.152E-10	5.079E-05
	100d	1.659E-17	2.539E-05
Plateau concentration			

Route and rate of degradation in water (Annex IIA, point 7.2.1)

Hydrolytic degradation of the active substance and metabolites > 10 % ‡	[^{14}C]-pNP was found to be hydrolytically stable at pH 4, 7 and 9 at a temperature of 50°C in the dark. No degradation of the test item was observed during 5 days of incubation at 50°C.
Photolytic degradation of active substance and metabolites above 10 % ‡	The test item pNP was steadily photodegraded under simulated sunlight in sterile buffer solution at pH 7. Its experimental photolytic half life (DT50) was determined using first-order reaction kinetics to be 3 days of continuous irradiation under "Suntest" conditions. Its corresponding half life (DT50) at latitude 30°N was calculated to be about 6 summer days. Unidentified major metabolites: M3, M5, M6
Quantum yield of direct phototransformation in water at Σ > 290 nm	For p-NP the quantum yield was determined to be : Φ (pNP) = 3.77 x 10^{-6} molecules degraded photon^{-1}
Readily biodegradable ‡ (yes/no)	No

Degradation in water / sediment

Parent	Distribution: max in water 50.2-50.9% AR at day 0, max in sediment 2.9-11.8% AR at day 3 equivalent to 5.8-26.2% of the amount initially applied Na p-NP									
Water / sediment system	pH water phase	pH sed	t. °C	DT_{50}-DT_{90} whole sys.	St. (r^2)	DT_{50}-DT_{90} water	St. (r^2)	DT_{50}-DT_{90} sed	St. (r^2)	Method of calculation
river system	-	7.47	20	3.6-11.9	0.9328	2.7-9.1	0.9711	-	-	-
pond system	-	7.17	20	3.0-10.1	0.9736	2.8-9.4	0.9815	-	-	-
Geometric mean/median				3.3-11		2.8-9.2		-		

Appendix 1 – list of endpoints

Mineralization and non extractable residues					
Water / sediment system	pH water phase	pH sed	Mineralization x % after n d. (end of the study).	Non-extractable residues in sed. Max x % after n d	Non-extractable residues in sed. Max x % after n d (end of the study)
river system	-	7.47	66.1% after 122 d	41.9% max at 61d	30.7% at 122d
pond system	-	7.17	63.5% after 122 d	49.3% max at 15d	34.6% at 122d

PEC (surface water) and PEC sediment (Annex IIIA, point 9.2.3)

p-NP Parameters used in FOCUSsw step 1 and 2	Molecular weight (g/mol): - Water solubility (mg/L): 13900 K_{OC}/K_{OM} (L/kg): 288.1 DT_{50} soil (d): 3.3 days (Lab, In accordance with FOCUS SFO) DT_{50} water/sediment system (d): 3.6 (representative worst case from sediment water studies) DT_{50} water (d): 3.6 DT_{50} sediment (d): 3.6
Parameters used in FOCUSsw step 3 (if performed)	Version control no.'s of FOCUS software: Vapour pressure: Kom/Koc: 1/n: (Freundlich exponent general or for soil ,susp. solids or sediment respectively)
Application rate	3 g a.i./ha Sugarbeet: 4 applications per year with a 7 days interval. LIF (Leaf interception factor) : 70%. Tomatoes: 5 applications per year with a 14 days interval. LIF (Leaf interception factor): 80%. Oilseed rape: 2 applications per year with a 30 days interval. LIF (Leaf interception factor): 80%.

Appendix 1 – list of endpoints

SUGAR BEET – minimal crop cover

pNP

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	3.0003		8.3258	
1	2.4495	2.7249	7.0571	7.6914
2	2.0205	2.4765	5.8211	7.0554
4	1.3748	2.0767	3.9607	5.9433
7	0.7716	1.6343	2.2228	4.6856
14	0.2005	1.0290	0.5775	2.9532
21	0.0521	0.7227	0.1501	2.0745
28	0.0135	0.5492	0.0390	1.5765
42	0.0009	0.3677	0.0026	1.0555
50	0.0002	0.3089	0.0006	0.8868
100	0.0000	0.1545	0.0000	0.4434

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.1061	---	0.2969	---
1	0.0868	0.0965	0.2502	0.2736
2	0.0716	0.0879	0.2064	0.2509
4	0.0487	0.0738	0.1404	0.2114
7	0.0274	0.0581	0.0788	0.1666
14	0.0071	0.0366	0.0205	0.1050
21	0.0018	0.0257	0.0053	0.0738
28	0.0005	0.0195	0.0014	0.0561
42	0.0000	0.0131	0.0001	0.0375
50	0.0000	0.0110	0.0000	0.0315
100	0.0000	0.0055	0.0000	0.0158

Appendix 1 – list of endpoints

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0738	---	0.2039	---
1	0.0602	0.0670	0.1734	0.1886
2	0.0497	0.0610	0.1431	0.1734
4	0.0338	0.0512	0.0973	0.1463
7	0.0190	0.0403	0.0546	0.1154
14	0.0049	0.0254	0.0142	0.0727
21	0.0013	0.0178	0.0037	0.0511
28	0.0003	0.0135	0.0010	0.0388
42	0.0000	0.0091	0.0001	0.0260
50	0.0000	0.0076	0.0000	0.0218
100	0.0000	0.0038	0.0000	0.0109

SUGAR BEET – average crop cover

pNP

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	3.0003		8.3258	
1	2.4495	2.7249	7.0571	7.6914
2	2.0205	2.4765	5.8211	7.0554
4	1.3748	2.0767	3.9607	5.9433
7	0.7716	1.6343	2.2228	4.6856
14	0.2005	1.0290	0.5775	2.9532
21	0.0521	0.7227	0.1501	2.0745
28	0.0135	0.5492	0.0390	1.5765
42	0.0009	0.3677	0.0026	1.0555
50	0.0002	0.3089	0.0006	0.8868
100	0.0000	0.1545	0.0000	0.4434

Appendix 1 – list of endpoints

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0456	---	0.1224	---
1	0.0369	0.0412	0.1063	0.1143
2	0.0304	0.0374	0.0877	0.1057
4	0.0207	0.0314	0.0596	0.0893
7	0.0116	0.0247	0.0335	0.0705
14	0.0030	0.0155	0.0087	0.0445
21	0.0008	0.0109	0.0023	0.0312
28	0.0002	0.0083	0.0006	0.0237
42	0.0000	0.0056	0.0000	0.0159
50	0.0000	0.0047	0.0000	0.0134
100	0.0000	0.0023	0.0000	0.0067

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0335	---	0.0875	---
1	0.0269	0.0302	0.0775	0.0825
2	0.0222	0.0274	0.0639	0.0766
4	0.0151	0.0229	0.0435	0.0649
7	0.0085	0.0180	0.0244	0.0513
14	0.0022	0.0113	0.0063	0.0324
21	0.0006	0.0080	0.0016	0.0227
28	0.0001	0.0061	0.0004	0.0173
42	0.0000	0.0041	0.0000	0.0116
50	0.0000	0.0034	0.0000	0.0097
100	0.0000	0.0017	0.0000	0.0049

Appendix 1 – list of endpoints

Tomatoes

pNP

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.7501		2.0814	
1	0.6124	0.6812	1.7643	1.9229
2	0.5051	0.6191	1.4553	1.7638
4	0.3437	0.5192	0.9902	1.4858
7	0.1929	0.4086	0.5557	1.1714
14	0.0501	0.2572	0.1444	0.7383
21	0.0130	0.1807	0.0375	0.5186
28	0.0034	0.1373	0.0097	0.3941
42	0.0002	0.0919	0.0007	0.2639
50	0.0000	0.0772	0.0001	0.2217
100	0.0000	0.0386	0.0000	0.1109

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0367	---	0.0990	---
1	0.0297	0.0332	0.0857	0.0923
2	0.0245	0.0302	0.0707	0.0853
4	0.0167	0.0253	0.0481	0.0721
7	0.0094	0.0199	0.0270	0.0569
14	0.0024	0.0125	0.0070	0.0359
21	0.0006	0.0088	0.0018	0.0252
28	0.0002	0.0067	0.0005	0.0192
42	0.0000	0.0045	0.0000	0.0128
50	0.0000	0.0038	0.0000	0.0108
100	0.0000	0.0019	0.0000	0.0054

Appendix 1 – list of endpoints

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0268	---	0.0705	---
1	0.0216	0.0242	0.0622	0.0664
2	0.0178	0.0220	0.0513	0.0616
4	0.0121	0.0184	0.0349	0.0522
7	0.0068	0.0145	0.0196	0.0412
14	0.0018	0.0091	0.0051	0.0260
21	0.0005	0.0064	0.0013	0.0183
28	0.0001	0.0049	0.0003	0.0139
42	0.0000	0.0033	0.0000	0.0093
50	0.0000	0.0027	0.0000	0.0078
100	0.0000	0.0014	0.0000	0.0039

Winter Oil seed rape

pNP

Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.7501		2.0814	
1	0.6124	0.6812	1.7643	1.9229
2	0.5051	0.6191	1.4553	1.7638
4	0.3437	0.5192	0.9902	1.4858
7	0.1929	0.4086	0.5557	1.1714
14	0.0501	0.2572	0.1444	0.7383
21	0.0130	0.1807	0.0375	0.5186
28	0.0034	0.1373	0.0097	0.3941
42	0.0002	0.0919	0.0007	0.2639
50	0.0000	0.0772	0.0001	0.2217
100	0.0000	0.0386	0.0000	0.1109

Appendix 1 – list of endpoints

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0424	---	0.1130	---
1	0.0343	0.0383	0.0987	0.1059
2	0.0283	0.0348	0.0814	0.0980
4	0.0192	0.0292	0.0554	0.0829
7	0.0108	0.0229	0.0311	0.0654
14	0.0028	0.0144	0.0081	0.0413
21	0.0007	0.0101	0.0021	0.0290
28	0.0002	0.0077	0.0005	0.0220
42	0.0000	0.0052	0.0000	0.0148
50	0.0000	0.0043	0.0000	0.0124
100	0.0000	0.0022	0.0000	0.0062

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0260	---	0.0657	---
1	0.0207	0.0234	0.0597	0.0627
2	0.0171	0.0211	0.0492	0.0586
4	0.0116	0.0177	0.0335	0.0498
7	0.0065	0.0139	0.0188	0.0394
14	0.0017	0.0087	0.0049	0.0249
21	0.0004	0.0061	0.0013	0.0175
28	0.0001	0.0047	0.0003	0.0133
42	0.0000	0.0031	0.0000	0.0089
50	0.0000	0.0026	0.0000	0.0075
100	0.0000	0.0013	0.0000	0.0037

Appendix 1 – list of endpoints

Summer Oil seed rape

pNP
Step 1

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.7501		2.0814	
1	0.6124	0.6812	1.7643	1.9229
2	0.5051	0.6191	1.4553	1.7638
4	0.3437	0.5192	0.9902	1.4858
7	0.1929	0.4086	0.5557	1.1714
14	0.0501	0.2572	0.1444	0.7383
21	0.0130	0.1807	0.0375	0.5186
28	0.0034	0.1373	0.0097	0.3941
42	0.0002	0.0919	0.0007	0.2639
50	0.0000	0.0772	0.0001	0.2217
100	0.0000	0.0386	0.0000	0.1109

Step 2 - S

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0424	---	0.1130	---
1	0.0343	0.0383	0.0987	0.1059
2	0.0283	0.0348	0.0814	0.0980
4	0.0192	0.0292	0.0554	0.0829
7	0.0108	0.0229	0.0311	0.0654
14	0.0028	0.0144	0.0081	0.0413
21	0.0007	0.0101	0.0021	0.0290
28	0.0002	0.0077	0.0005	0.0220
42	0.0000	0.0052	0.0000	0.0148
50	0.0000	0.0043	0.0000	0.0124
100	0.0000	0.0022	0.0000	0.0062

Appendix 1 – list of endpoints

Step 2 - N

Time after max peak(d)	PECsw (µg/L)		PECsed (µg/kg dry sediment)	
	Actual	TWA	Actual	TWA
0	0.0260	---	0.0657	---
1	0.0207	0.0234	0.0597	0.0627
2	0.0171	0.0211	0.0492	0.0586
4	0.0116	0.0177	0.0335	0.0498
7	0.0065	0.0139	0.0188	0.0394
14	0.0017	0.0087	0.0049	0.0249
21	0.0004	0.0061	0.0013	0.0175
28	0.0001	0.0047	0.0003	0.0133
42	0.0000	0.0031	0.0000	0.0089
50	0.0000	0.0026	0.0000	0.0075
100	0.0000	0.0013	0.0000	0.0037

PEC (ground water) (Annex IIIA, point 9.2.1)

Method of calculation and type of study (*e.g.* modelling, field leaching, lysimeter)	**p-NP** FOCUS working group recommendations. Standard FOCUS groundwater scenarios • FOCUS PELMO 3.3.2 • PEARL 2.2.2 Worst case DT_{50} 3.3 d (no normalisation to 10kPa or pF2, 20 °C with Q10 of 2.2 was conducted). (Note: the longest lab DT_{50} is 2.2 days) Kf_{OC}: median 288.1, $^{1}/_{n}$= 1.
Application rate	**p-NP: 3** g a.i./ha with PELMO and PEARL 2.2.2 Sugarbeet: 4 applications at 1 L/ha every 7 days until 15 days before harvest. First application 20% foliar crop interception, second and third application 70%, fourth application 90% foliar crop interception. Tomatoes: 5 applications at 1 L/ha with 14 days between each application and 3 days before harvest. 80% foliar crop interception. Oilseed rape: 2 applications at 1 L/ha with 30 days between each one with a PHI of 30 days. 80% foliar crop interception.

Appendix 1 – list of endpoints

PEC(gw) - FOCUS modelling results (80th percentile annual average concentration at 1m)

p-NP	Same results with PELMO 3.3.2 and PEARL 2.2.2
Average annual concentration, all scenarios, all crops	< 0.001 µg/L

Fate and behaviour in air (Annex IIA, point 7.2.2, Annex III, point 9.3)

Direct photolysis in air ‡	Not available, not required
Quantum yield of direct phototransformation	For p-NP the quantum yield was determined to be : Φ (pNP) = 3.77 x 10-6 molecules degraded photon-1 in water
Photochemical oxidative degradation in air ‡	Photochemical oxidative degradation in air: Model calculation according to Atkinson using the computer program AOPWIN. The half-life of Sodium para-nitrophenolate dihydrate was calculated as 2.3 days when considering a day comprising 12 hours of sunlight and 1.2 days when considering a day comprising 24 hours of sunlight.
Volatilisation ‡	No information submitted
Metabolites	-

PEC (air)

Method of calculation	Expert judgement, based on vapour pressure, dimensionless Henry's Law Constant

$PEC_{(a)}$

Maximum concentration	Not calculated – not required

Appendix 1 – list of endpoints

Residues requiring further assessment

Environmental occurring metabolite requiring further assessment by other disciplines (toxicology and ecotoxicology).	Soil: Na p-NP, M5, M7 (anaerobic), M8 (anaerobic) Groundwater: p-NP, M5, M7 (anaerobic), M8 (anaerobic) Surface water: p-NP, M5 (from soil), from aqueous photolysis study: M3, M5, M6. Note that the M5 from soil may be different to the M5 from aqueous photolysis. Sediment: p-NP Air: p-NP

Monitoring data, if available (Annex IIA, point 7.4)

Soil (indicate location and type of study)	No data provided - none requested
Surface water (indicate location and type of study)	No data provided - none requested
Ground water (indicate location and type of study)	No data provided - none requested
Air (indicate location and type of study)	No data provided - none requested

Points pertinent to the classification and proposed labelling with regard to fate and behaviour data

Not readily biodegradable

Appendix 1 – list of endpoints

Chapter 6: Effects on Non-target Species

Na 5-NG: sodium 5-nitroguaiacolate

Na *o*-NP: sodium *ortho*-nitrophenolate

Na *p*-NP: sodium *para*-nitrophenolate

Effects on terrestrial vertebrates (Annex IIA, point 8.1, Annex IIIA, points 10.1 and 10.3)

Species	Test substance	Time scale	Endpoint (mg/kg bw/day)	Endpoint (mg/kg feed)
Birds ‡				
Colinus virginianus	a.s. Na 5-NG	Acute	LD_{50} = 2067	
Colinus virginianus	a.s. Na *o*-NP	Acute	LD_{50} = 1046	
Colinus virginianus	a.s. Na *p*-NP	Acute	LD_{50} > 1670	
	Mixture	Acute **Finney formula**	LD_{50} (MIX) = 238536	
Colinus virginianus	a.s. Na 5-NG	Short-term	LC_{50} = 1830	
Colinus virginianus	a.s. Na *o*-NP	Short-term	LC_{50} > 2698	
Mallard duck	a.s. Na *o*-NP		LC_{50} > 2539	
Colinus virginianus	a.s. Na *p*-NP	Short-term	LC_{50} > 1412	
Colinus virginianus	Product[1)]	Long-term	95 mg product/kg bw/d	1000 ppm

Appendix 1 – list of endpoints

Mammals ‡				
rat	a.s. Na 5-NG	Acute	LD_{50} = 716 mg a.s./kg b.w.	
rat	a.s. Na *o*-NP	Acute	LD_{50} = 960.1 mg a.s./kg b.w. (rat)	
rat	a.s. Na *p*-NP	Acute	LD_{50} = 345.5 mg a.s./kg b.w. (rat	
rat	Preparation	Acute	LD_{50} > 5000 mg ATONIK/kg b.w	
rat	Preparation	Long-term 2-generation study	$NOAEL_{parental}$ = 300 mg MUP of ATONIK /kg bw/day	
Additional higher tier studies ‡				

[1)] Measured concentration 50% of the nominal, but the tested preparation is 100 times more concentrate than the representative

Toxicity/exposure ratios for terrestrial vertebrates (Annex IIIA, points 10.1 and 10.3)

Sugar beet (4 applications), oilseed rape (2 applications), and tomato (5 applications).
Application rate: 1 g Na 5-NG/ha, 2 g Na oNP /ha, 3 g Na pNP /ha

Indicator species/Category	Time scale	ETE	TER	Annex VI Trigger
Tier 1 (Birds)				
Medium herbivorous bird	Acute Na 5-NG	0.13	15914	10
Medium herbivorous bird	Acute Na *o*-NP	0.26	4026	10
Medium herbivorous bird	Acute Na *p*-NP	0.39	>4295	10
Medium herbivorous bird (**Finney formula**)	Acute (mixture)	129.88	1840	10
Insectivorous birds	Acute Na 5-NG	0.05	38221	10

Appendix 1 – list of endpoints

Indicator species/Category	Time scale	ETE	TER	Annex VI Trigger
Insectivorous birds	Acute Na *o*-NP	0.11	9671	10
Insectivorous birds	Acute Na *p*-NP	0.16	>10293	10
Insectivorous birds (**Finney formula**)	Acute (mixture)	106	2250	10
Medium herbivorous bird	Short-term Na 5-NG	0.07	26143	10
Medium herbivorous bird	Short-term Na *o*-NP	0.14	>18136	10
Medium herbivorous bird	Short-term Na *p*-NP	0.20	>7060	10
Insectivorous birds	Short-term Na 5-NG	0.03	61000	10
Insectivorous birds	Short-term Na *o*-NP	0.06	>42317	10
Insectivorous birds	Short-term Na *p*-NP	0.09	>15689	10
Medium herbivorous bird	Long-term	0.36	266	5
Insectivorous birds	Long-term	0.3	317	5
Drinking water (na 5-NP) - acute		0.27	7665	10
Drinking water (oNP) - acute		0.54	1439	10
Drinking water (pNP) - acute		0.81	2064	10

Appendix 1 – list of endpoints

Indicator species/Category	Time scale	ETE	TER	Annex VI Trigger
Higher tier refinement (Birds): not required				
Tier 1 (Mammals)				
Medium herbivorous mammal	Acute Na 5-NG	0.05	14320	10
Medium herbivorous mammal	Acute Na *o*-NP	0.09	10948	10
Medium herbivorous mammal	Acute Na *p*-NP	0.14	2467	10
Medium herbivorous mammal	Long-term	0.13	2307	5
Drinking water (Na 5-NP) - acute		0.16	4563	10
Drinking water (oNP) - acute		0.31	3060	10
Drinking water (oNP) - acute		0.47	734	10
Higher tier refinement (Mammals): not required				

Toxicity data for aquatic species (most sensitive species of each group) (OECD data point numbers IIA 8.2 – IIA 8.6 and IIIA 10.2.2 – IIIA 10.2.7)

Group	**Test substance**	**Time-scale**	**Endpoint**	**Toxicity (mg/L)**
Laboratory tests				
Fish (Rainbow trout)	Na 5-NG	Acute, 96 hours, flow through	LC_{50} NOEC	37.4 10.9
Fish (Rainbow trout)	Na *o*-NP	Acute, 96 hours, flow through	LC_{50} NOEC	69 26
Fish (Rainbow trout)	Na *p*-NP	Acute, 96 hours, flow through	LC_{50} NOEC	25.0 12.5
Fish (*Cyprinus carpio*)	ATONIK solution*	Acute, 96 hours, semi-static	LC_{50} NOEL	6800 1800
Fish (Zebra fish)	MUP of ATONIK	Chronic, 21 days, semi-static	NOEC	10 7.74**
Invertebrate (*Daphnia Magna)*	Na 5-NG	Acute, 48 hours, flow through	LC_{50}	71.1
Invertebrate (*Daphnia Magna)*	Na *o*-NP	Acute, 48 hours, flow through	LC_{50}	>68.8
Invertebrate (*Daphnia Magna)*	Na *p*-NP	Acute, 48 hours, flow through	LC_{50}	27.7
Invertebrate (*Daphnia Magna)*	ATONIK solution*	Acute, 48 hours, static	LC_{50} NOEC	2000 560

Appendix 1 – list of endpoints

Group	Test substance	Time-scale	Endpoint	Toxicity (mg/L)
Invertebrate (*Daphnia Magna)*	MUP of ATONIK	Chronic, 21 days, semi-static	NOEC	1.0 0.0774**
Algae (*Scenedesmus subspicatus)*	Na 5-NG	72 hours, static	EbC_{50} Er C_{50}	6.2 >21
Algae (*Scenedesmus subspicatus)*	Na *o*-NP	72 hours, static	EbC_{50} Er C_{50}	4.8 >10
Algae (*Scenedesmus subspicatus)*	Na *p*-NP	72 hours, static	EbC_{50} Er C_{50}	2.5 >4.6
Algae (*Scenedesmus subspicatus)*	ATONIK	72 hours, static	EC_{50} NOEC	> 100 100 (equal to 0.1 Na 5-NG, 0.2 Na *o*-NP, 0.3 Na *p*-NP

*Atonik solution containing 0.3% of sodium 5-nitroguaiacolate, 0.6% sodium ortho-nitrophenolate, 0.9% sodium para-nitrophenolate
**based on the sum of purity of active substances

Appendix 1 – list of endpoints

Toxicity/exposure ratios for the most sensitive aquatic organisms (Annex IIIA, point 10.2)

FOCUS Step1
Sugar beet (4 applications), oilseed rape (2 applications), and tomato (5 applications).
Application rate: 1 g Na 5-NG/ha, 2 g Na oNP /ha, 3 g Na pNP /ha

Sugar beet

Test substance	Organism	Toxicity endpoint (mg/L)	Time scale	PEC_i (mg/L)	PEC_{twa}	TER	Annex VI Trigger
Na *p*-NP	Fish	25	Acute	0.003		8333	100
ATONIK	Fish	7.74	Chronic	0.0043*		1747	10
Na *p*-NP	Aquatic invertebrates	27.7	Acute	0.003		9233	100
ATONIK	Aquatic invertebrates	0.0774	Chronic	0.0043*		17	10
Na *p*-NP	Algae	2.5	Chronic	0.003		833	10
a.s.	Higher plants		Chronic				10
a.s.	Sediment-dwelling organisms		Chronic				10
Metabolites	Relevant organisms						
Product	Relevant organisms						

Appendix 1 – list of endpoints

Tomato

Test substance	Organism	Toxicity endpoint (mg/L)	Time scale	PEC_i (mg/L)	PEC_{twa}	TER	Annex VI Trigger
Na *p*-NP	Fish	25	Acute	0.00075		33333	100
ATONIK	Fish	7.74	Chronic	0.0024*		3230	10
Na *p*-NP	Aquatic invertebrates	27.7	Acute	0.00075		36933	100
ATONIK	Aquatic invertebrates	0.0774	Chronic	0.0024*		32	10
Na *p*-NP	Algae	2.5	Chronic	0.00075		3333	10
a.s.	Higher plants		Chronic				10
a.s.	Sediment-dwelling organisms		Chronic				10
Metabolites	Relevant organisms						
Product	Relevant organisms						

Appendix 1 – list of endpoints

Oilseed rape

Test substance	Organism	Toxicity endpoint (mg/L)	Time scale	PEC_i (mg/L)	PEC_{twa}	TER	Annex VI Trigger
Na *p*-NP	Fish	25	Acute	0.00075		33333	100
ATONIK	Fish	7.74	Chronic	0.00175*		4421	10
Na *p*-NP	Aquatic invertebrates	27.7	Acute	0.00075		36933	100
ATONIK	Aquatic invertebrates	0.0774	Chronic	0.00175*		44	10
Na *p*-NP	Algae	2.5	Chronic	0.00075		3333	10
a.s.	Higher plants		Chronic				10
a.s.	Sediment-dwelling organisms		Chronic				10
Metabolites	Relevant organisms						
Product	Relevant organisms						

* PEC calculated as sum of the PEC of each active substance

Bioconcentration				
	Active substance	Metab. 1	Metab. 2	Metab. 3
$logP_{O/W}$	Not relevant			
Bioconcentration factor (BCF) ‡	Not relevant			
Annex VI Trigger for the bioconcentration factor	Not relevant			
Clearance time (days) (CT_{50})	Not relevant			
(CT_{90})	Not relevant			
Level and nature of residues (%) in organisms after the 14 day depuration phase	Not relevant			

Appendix 1 – list of endpoints

Effects on honeybees (Annex IIA, point 8.3.1, Annex IIIA, point 10.4)

Test substance	Acute oral toxicity (LD_{50} µg/bee)	Acute contact toxicity (LD_{50} µg/bee)
Na 5-NG	131.6	> 100
Na *o*-NP	123.5	> 100
Na *p*-NP	61.2	= 111
Preparation	57.12 µg product/bee	> 100 µg product/bee
Field or semi-field tests: not relevant		

Hazard quotients for honey bees (Annex IIIA, point 10.4)

Sugar beet (4 applications), oilseed rape (2 applications), and tomato (5 applications).
Application rate: 1 g Na 5-NG/ha, 2 g Na oNP /ha, 3 g Na pNP /ha

Test substance	Route	Hazard quotient	Annex VI Trigger
Na 5-NG	Contact	< 0.01	50
Na 5-NG	oral	0.008	50
Na *o*-NP	Contact	< 0.02	50
Na *o*-NP	oral	0.02	50
Na *p*-NP	Contact	0.03	50
Na *p*-NP	oral	0.05	50
Preparation	Contact	< 10	50
	oral	17.5	50

Effects on other arthropod species (Annex IIA, point 8.3.2, Annex IIIA, point 10.5)

Laboratory tests with standard sensitive species

Species	Test Substance	Endpoint	Effect (LR_{50} g/ha)
Typhlodromus pyri ‡		Mortality	
Aphidius rhopalosiphi ‡		Mortality	

Appendix 1 – list of endpoints

Crop and application rate

Test substance	Species	Effect (LR_{50} g/ha)	HQ in-field	HQ off-field	Trigger
	Typhlodromus pyri				2
	Aphidius rhopalosiphi				2

Further laboratory and extended laboratory studies ‡

Species	Life stage	Test substance, substrate and duration	Dose (g/ha)	Endpoint	% effect	Trigger value
Amblyseius californicus		laboratory	1 and 2 L ATONIK/ha	Mortality Reproductive performance	1.2, and 10.3% No effect	50 %
Aphidius colemani		aboratory	1 and 2 L ATONIK/ha	Mortality Reproductive performance	No effect No effect	50 %
Poecilus cupreus		Extended laboratory		Mortality Feeding dynamics	No effect No effect	50 %
Coccinella sept		aboratory		Mortality larvae Reproductive performance Corrected mortality Reproductive performance	No effect No effect 39% No effect	50 %
Coccinella sept.		Extended laboratory	1 L ATONIK/ha 2 L ATONIK/ha 4 L ATONIK/ha	Corrected mortality	4.8% 14.3% 9.5%	

Field or semi-field tests

Appendix 1 – list of endpoints

Effects on earthworms, other soil macro-organisms and soil micro-organisms (Annex IIA points 8.4 and 8.5. Annex IIIA, points, 10.6 and 10.7)

Test organism	Test substance	Time scale	Endpoint
Earthworms			
	a.s. ‡	Acute 14 days	none
	a.s. ‡	Chronic 8 weeks	none
Eisenia fetida	Preparation	Acute	LC_{50}: >101.8 mg MUP of Atonik /kg soil (= 11.8 Na 5-NG, 23.6 Na oNP, 43.4 Na pNP mg/kg soil)
Eisenia fetida	Preparation	Chronic	NOEC = 37.0 mg MUP of Atonik /kg soil (= 4.3 Na 5-NG, 8.6 Na oNP, 15.8 Na pNP mg/kg soil)
	Metabolite 1	Acute	none
	Metabolite 1	Chronic	none
Other soil macro-organisms: not relevant			
Soil micro-organisms			
Nitrogen mineralisation	Preparation		No effect (< 25%) at 0.8 and 4.0 mg ATONIK /kg soil after 28 days
Carbon mineralisation	Preparation		No effect (< 25%) at 0.8 and 4.0 mg ATONIK /kg soil after 28 days
Field studies: not relevant			

Appendix 1 – list of endpoints

Toxicity/exposure ratios for soil organisms

Sugar beet

Test organism	Test substance	Time scale	Soil PEC	TER	Trigger
Earthworms					
Eisenia fetida	Na 5-NG	Acute	0.000133	88722	10
Eisenia fetida	Na 5-NG	Chronic	0.000133	32331	5
Eisenia fetida	Na *o*-NP	Acute	0.0003	39333	10
Eisenia fetida	Na *o*-NP	Chronic	0.0003	14333	5
Eisenia fetida	Na *p*-NP	Acute	0.0005511	21412	10
Eisenia fetida	Na *p*-NP	Chronic	0.0005511	7803	5

Tomato

Test organism	Test substance	Time scale	Soil PEC	TER	Trigger
Earthworms					
Eisenia fetida	Na 5-NG	Acute	0.000267	88390	10
Eisenia fetida	Na 5-NG	Chronic	0.000267	32210	5
Eisenia fetida	Na *o*-NP	Acute	0.000534	44195	10
Eisenia fetida	Na *o*-NP	Chronic	0.000534	16105	5
Eisenia fetida	Na *p*-NP	Acute	0.00081	29136	10
Eisenia fetida	Na *p*-NP	Chronic	0.00081	10617	5

Oilseed rape

Test organism	Test substance	Time scale	Soil PEC	TER	Trigger
Earthworms					
Eisenia fetida	Na 5-NG	Acute	0.000267	162547	10
Eisenia fetida	Na 5-NG	Chronic	0.000267	59176	5
Eisenia fetida	Na *o*-NP	Acute	0.000533	81426	10
Eisenia fetida	Na *o*-NP	Chronic	0.000533	29644	5
Eisenia fetida	Na *p*-NP	Acute	0.0008	54250	10
Eisenia fetida	Na *p*-NP	Chronic	0.0008	19750	5

Appendix 1 – list of endpoints

Effects on non target plants (Annex IIA, point 8.6, Annex IIIA, point 10.8)

Preliminary screening data

Not required for herbicides as ER_{50} tests should be provided.

Laboratory dose response tests

Most sensitive species	Test substance	ER_{50} (g/ha)[2] vegetative vigour	ER_{50} (g/ha)[2] emergence	Exposure[1] (g/ha)[2]	TER	Trigger
All tested species	ATONIK	EC_{25} > 5 L Atonik/ha	EC_{25} > 5 L Atonik/ha	PEC 0.1L[3] 1 m buffer	81	≥ 5

[1] Exposure has been based on Ganzelmeier drift data
[2] for preparations indicate whether dose is expressed in units of as or preparation
[3] Worst case for sugar beet (4 applications every 7 days, MAF=2.23)

Additional studies (e.g. semi-field or field studies)

Not relevant

Effects on biological methods for sewage treatment (Annex IIA 8.7)

Test type/organism	Endpoint
Activated sludge	
Pseudomonas sp	

Ecotoxicologically relevant compounds (consider parent and all relevant metabolites requiring further assessment from the fate section)

Compartment	
soil	-
water	Photolytic metabolites
sediment	-
groundwater	-

Appendix 1 – list of endpoints

Classification and proposed labelling with regard to ecotoxicological data (Annex IIA, point 10 and Annex IIIA, point 12.3)

	RMS/peer review proposal
Active substance	Sodium 5-nitroguaiacolate: N, R51/R53 Sodium *ortho*-nitrophenolate: N, R51/R53* Sodium *para*-nitrophenolate: N, R51/R53**

	RMS/peer review proposal
Preparation	ATONIK: -

* based on EC_b50
** based on EC_r50

Appendix 1 – list of endpoints

Code/Trivial name	Chemical name	Structural formula
M1	5-nitroguaiacol (5NG)	
M2	para-nitrophenol (pNP)	
M3	Unkown fraction	
M4	Unkown fraction	
M5	Unkown fraction	
M6	Unkown fraction	
M7	Unkown fraction	
M8	Unkown fraction	
M9	Unkown fraction	
M10	Unkown fraction	
M11	Unkown fraction	
M12	Unkown fraction	
M13	Unkown fraction	

Appendix 2 – abbreviations

APPENDIX 2 – ABBREVIATIONS

ADI	acceptable daily intake
AOEL	acceptable operator exposure level
AR	ppplied radioactivity
ARfD	acute reference dose
a.s.	active substance
bw	body weight
CA	Chemical Abstract
CAS	Chemical Abstract Service
CIPAC	Collaborative International Pesticide Analytical Council Limited
d	day
DAR	draft assessment report
DFOP	Double First Order in Parallel mode
DM	dry matter
DT_{50}	period required for 50 percent dissipation (define method of estimation)
DT_{90}	period required for 90 percent dissipation (define method of estimation)
ε	decadic molar extinction coefficient
EC_{50}	effective concentration
EEC	European Economic Community
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINKS	European List of New Chemical Substances
EMDI	estimated maximum daily intake
ER50	emergence rate, median
EU	European Union
FAO	Food and Agriculture Organisation of the United Nations
FOCUS	Forum for the Co-ordination of Pesticide Fate Models and their Use
GAP	good agricultural practice
GCPF	Global Crop Protection Federation (formerly known as GIFAP)
GS	growth stage
h	hour(s)
ha	hectare
hL	hectolitre
HPLC	high pressure liquid chromatography or high performance liquid chromatography
HQ	hazard quotient
ISO	International Organisation for Standardisation
IUPAC	International Union of Pure and Applied Chemistry

Appendix 2 – abbreviations

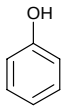
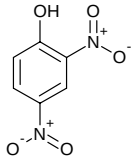
K_{oc}	organic carbon adsorption coefficient
L	litre
LC	liquid chromatography
LC-MS	liquid chromatography-mass spectrometry
LC-MS-MS	liquid chromatography with tandem mass spectrometry
LC_{50}	lethal concentration, median
LD_{50}	lethal dose, median; dosis letalis media
LOAEL	lowest observable adverse effect level
LOD	limit of detection
LOQ	limit of quantification (determination)
mo	month
MAC	maximum achievable concentration
µg	microgram
mN	milli-Newton
MRL	maximum residue limit or level
MS	mass spectrometry
MWHC	maximum waterholding capacity
NESTI	national estimated short term intake
NIR	near-infrared-(spectroscopy)
nm	nanometer
NOAEL	no observed adverse effect level
NOEC	no observed effect concentration
NOEL	no observed effect level
OC	organic carbon content
PEC	predicted environmental concentration
PEC_A	predicted environmental concentration in air
PEC_S	predicted environmental concentration in soil
PEC_{SW}	predicted environmental concentration in surface water
PEC_{GW}	predicted environmental concentration in ground water
PHI	pre-harvest interval
pK_a	negative logarithm (to the base 10) of the dissociation constant
PPE	personal protective equipment
ppm	parts per million (10^{-6})
ppp	plant protection product
r^2	coefficient of determination
RPE	respiratory protective equipment
SFO	single first order
SL	soluble concentrate

Appendix 2 – abbreviations

STMR	supervised trials median residue
TER	toxicity exposure ratio
TMDI	theoretical maximum daily intake
UV	ultraviolet
WHO	World Health Organisation
WG	water dispersible granule
yr	year

Appendix 3 – used compound code(s)

APPENDIX 3 – USED COMPOUND CODE(S)

Code/Trivial name	Chemical name	Structural formula
phenol	phenol	
2,4-dinitrophenol	2,4-dinitrophenol	
2,6-dinitrophenol	2,6-dinitrophenol