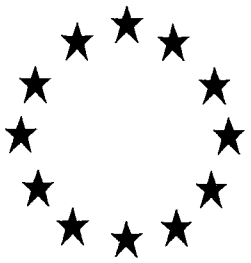
Competent Authority Report
According to Directive 98/8/EC



Bromadiolone (PT14)

The Bromadiolone Task Force

DOCUMENT III-A

Section 1-3: Applicant, Identity and Physical and Chemical Properties

Rapporteur Member State: Sweden

Final CAR April 2011

KEMI
Kemikalieinspektionen
Swedish Chemicals Agency

Table of Contents; DOC III-A1-A3

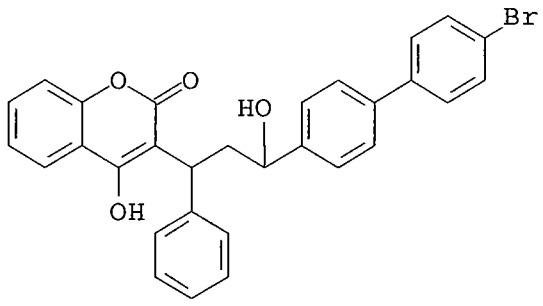
Section A1 Applicant

Annex Points IIA, I.1.1 to 1.2

1.1	**Applicant**	Name:	Bromadiolone Task Force
		1. Name: Address: Telephone: Fax: E-mail address:	**Activa / Tezza S.R.L.** V. le Lombardia, 22, 20131 Milano, Italy +39 (-02) -7063-7301 /03/04 +39- (02) -7063-7228 activa@activa.it
		2. Name: Address: Telephone: Fax: E-mail address:	**Babolna Bioenvironmetnal Centre Ltd,** H-1107 Budapest, Szallas u.6, Hungary +36-1-4320-400 +31-1-4320-401 info@babolna-bio.hu
		3. Name: Address: Telephone: Fax number: E-mail address:	**Laboratorios Agrochem S.L.** Tres Rieres, 10, 08292 Esparreguera, Spain 0034 93 777 4853 0034 93 777 5059 atencion@agrochem.es
		4. Name: Address: Telephone: Fax: E-mail address:	**PelGar International Ltd.** Unit 13 Newman Lane, Alton, Hampshire, United Kingdom [redacted] [redacted] [redacted]@pelgar.co.uk
		Secretariat:	**Bromadiolone Task Force** c/o Babolna Bio Ltd 1107 Budapest, Szallas u.6. – Hungary Contact name: [redacted] Direct phone number: [redacted] Fax number: [redacted] E-mail address: [redacted]@babolna-bio.com
1.2	**Manufacturer of Active Substance (if different)**	Name: Address:	**XXXXX** XXXXX
1.3	**Manufacturer of Product(s) (if different)** **1) Product 1**	Name: Address: Contact name: Direct phone number: Fax number: E-mail address:	**Bromadiolone Task Force** c/o Babolna Bio Ltd 1107 Budapest, Szallas u.6. – Hungary [redacted] [redacted] [redacted] [redacted]@babolna-bio.com

Section A2 Identity of Active Substance

Annex Points IIA, II.2.1 to 2.9

Subsection			Official use only
2.1	**Common name (IIA2.1)**	Bromadiolone	
2.2	**Chemical name (IIA2.2)**	IUPAC NAME: 3-[3-(4'-bromobiphenyl-4-yl)-3-hydroxy-1-phenylpropyl]-4-hydroxycoumarin C.A. NAME: 3-[3-(4'-bromo[1,1'-biphenyl]-4-yl-)-3-hydroxy-1-phenylpropyl]-4-hydrox-2H-1-benzopyran-2-one	X1
2.3	**Manufacturer's development code number(s) (IIA2.3)**	None	
2.4	**CAS No and EC numbers (IIA2.4)**		
2.4.1	**CAS-No**	28772-56-7	
2.4.2	**EC-No**	249-205-9	
2.4.3	**Other**	CIPAC NUMBER: 371 RTECS: GN493470	
2.5	**Molecular and structural formula, molecular mass (IIA2.5)**		
2.5.1	**Molecular formula**	$C_{30}H_{23}BrO_4$	
2.5.2	**Structural formula**		
2.5.3	**Molecular mass**	527.4	
2.6	**Method of manufacture of the active substance (IIA2.1)**	This information is regarded as commercially sensitive. Please refer to Appendix XIA 'Information claimed as confidential' to review this information.	X2

Section A2 Identity of Active Substance

Annex Points IIA, II.2.1 to 2.9

2.7	**Specification of the purity of the active substance, as appropriate (IIA2.7)**	This information is regarded as commercially sensitive. Please refer to Appendix XIA 'Information claimed as confidential' to review this information.	X3
2.8	**Identity of impurities and additives, as appropriate (IIA2.8)**	This information is regarded as commercially sensitive. Please refer to Appendix XIA 'Information claimed as confidential' to review this information.	X2
2.8.1	**Isomeric composition**	90:10 – 70:30	X4
2.9	**The origin of the natural active substance or the precursor(s) of the active substance (IIA2.9)**	Synthesis.	

Evaluation by Competent Authorities

EVALUATION BY RAPPORTEUR MEMBER STATE

Date	December 2004
Materials and methods	The applicant's version is adopted.
Conclusion	The applicant's version is adopted.
Reliability	**Subsection 2.8.1- Isomeric composition** Reliability indicator 1 **All other subsections under section A1 and section A2** Reliability indicator 0: Not applicable since no studies were performed for these subsections.
Acceptability	All points under section A1 and section A2 have been addressed and the information provided is sufficient and acceptable.
Remarks	X1: The IUPAC name should be given according to the published name for the ISO-common name bromadiolone: 3-[(1*RS*,3*RS*;1*RS*,3*SR*)-3-(4'-bromobiphenyl-4-yl)-3-hydroxy-1-phenylpropyl]-4-hydroxycoumarin which indicates the stereochemistry The European Food Safety Agency (EFSA) has concluded that this name covers all possible ratios for the two diastereomers and it is thus considered appropriate for the substance evaluated in this CAR. X2: Please refer to the Annex Confidential Data and Information to the CAR. X3: It should be noted that the purity of the active substance as manufactured cannot be treated as confidential information: The minimum purity is 98% and it is supported by batch analysis (Annex Confidential Data and Information)

Section A2 Identity of Active Substance

Annex Points IIA, II.2.1 to 2.9

	X4: The range refers to the diastereomeric ratio of the technical bromadiolone (see further the Annex Confidential Data and Information).

A2.10 Exposure data

Annex Point IIA, II.2.10

This is addressed in the Annex Confidential Data and Information

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.1 Melting point, boiling point, relative density (IIA3.1)								
3.1.1 Melting point								
Melting pt. 1	OPPTS Series 830 Section 7200	96% bromadiolone	**result:** 196°C - 210°C **pressure:** Atmospheric	Range was from wet point to no solid particles remaining	Y	1	Anderson W, (1999) Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98	X1
Melting pt. 2	Method A1 of 92/69/EEC (which constitutes annex V of 67/548/EEC)	98.8%	***result:*** 172.36 to 201.66°C **pressure**: atmospheric	Bromadiolone is a mixture of isomers therefore broad range is expected.	Y	1	Mullee and O'Connor, 2006, Determination of general physico-chemical properties SafePharm, report number 2073/0002	X2
3.1.2 Boiling point								

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
Boiling pt. 1			**result:** **pressure:**	Not determined as solid at room temperature	Y	1	Anderson W, (1999) Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98	X3
Boiling pt. 2	Method A2 of 92/69/EEC which constitutes Annex V of 67/548/EEC	98.8%	**Result:** test material decomposed at 260 to 360°C	Bpt not determined as the material decomposed.			Mullee and O'Connor, 2006, Determination of general physico-chemical properties SafePharm, report number 2073/0002	X4
3.1.3 Bulk density/ relative density								
Relative density 1	OPPTS Series 830 Section 7200. OECD 109	96% bromadiolone	Relative Density = 0.680 g/ml		Y	1	Anderson W, (1999) Product Chemistry: Technical	X5

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
Relative density 2	Method A3 of 92/69/EEC which constitutes Annex V of 67/548/EEC	98.8%	Relative density = 1.45 Temperature = 20.5°±C		Y	1	Grade Product Stillmeadow Incorporated report 4745-98 Mullee and O'Connor, 2006, Determination of general physico-chemical properties SafePharm, report number 2073/0002	X6
3.2 Vapour pressure (IIA3.2)								
Vapour pressure 1	OECD 104	99.9% bromadiolone	**temperature:** 45°C **result:** <0.05 mPa		Y	1	Fabbrini Dr R, (1997) BROMADIOLONE Determination of the Vapour Pressure. ChemService	X7

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
Vapour pressure 2	OPPTS Series 830, section 7950		< 10^{-7} torr at 25°C		N	3	report CH-14/96-C-BDL Anderson W, (1999) Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98	X8
3.2.1 Henry's Law Constant (IIA3.2)	US EPA Epiwin v3.12, Henry v3.10 Three methods of calculating the Henry's Law Constant have been employed. 1) A bond estimation method. 2) Calculation based on EPIWINs experimental database values. 3) Calculation based on experimental values obtained by Activa/PelGar	Not applicable	**1) Calculated using bond estimation method:** 4.01 x 10^{-9} Pa.m^3/mol (4.06 x 10^{-14} atm.m^3/mol) **2) Calculated on experimental database values:** 5.48 x 10^{-10} atm.m^3/mol @ 20°C **3) Calculated on experimental values:** 8.675 x 10^{-9} atm.m^3/mol @ 25°C.	**2)** The input parameter for this are 19 mg/L for water solubility (Tomlin, C 1997) and 1.5 x 10^{-08} mm Hg for vapour pressure (Hartley, D & Kidd, H 1983). **3)** The input parameters for this are 1.2 mg/L for water solubility and 1.5 x 10^{-08} mm Hg for vapour	N/A	4 Calculation method, therefore guideline not applicable.	US EPA, EPIWIN v3.12, EPI Suite Software, 2004	X9

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
	Taskforce.			pressure				
3.3 Appearance (IIA3.3)							Anderson W, (1999) Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98	X10
3.3.1 Physical state			Solid; fine powder					
3.3.2 Colour			White to off-white					
3.3.3 Odour			No odour					
3.4 Absorption spectra (IIA3.4)								
UV/VIS	OPPTS Series 830 Section 7050. OECD 101	96% bromadiolone		None	Y	1	Anderson W, (1999) Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98	X11

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
UV/VIS 2	OECD 101	Bromadiolone technical 98%	In methanol (2 x 10^{-5} M) Maxima: 263 nm (ε = 32325 L.mol^{-1}.cm^{-1}) 310 nm (ε = 11095 L.mol^{-1}.cm^{-1})		Y	1	Drake R.M. (2005), Determination of the Direct Photolysis Rate in Water by Sunlight of Bromadiolone, Chemex Environmental International Limited, Cambridge, UK	X12
IR	KBr pellet	Not stated	Maxima: 3400-3200 (OH), 1670 (CO), 1630, 1610, 1565, 1500, 1460, 1400, 1200, 1110, 820, 760 cm^{-1}		N	1	Novak L, (2005), IR, MS, ^{1}H- and ^{13}C-NMR Spectra of Bromadiolone, Budapest University of Technology and Economics, Institute for	X13

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
NMR	H (DMSO-d_6 solution, TMS internal std.)	Not stated	Chemical shifts (intensity, assignment): Anti-stereoisomer: 2.54 (1 H, 2'CH_2), 2.66 (1, 2'CH_2), 4.48 (1, 3'CH), 4.67 (1, 1'CH), 7.13 (1, aroma. H), 7.23 (3, aroma. H and 8 CH), 7.26 (1, 6 CH), 7.37 (2, 3'' & 5''CH), 7.48 (2, aroma.H), 7.50 (1, 7CH), 7.54 (4, 2'', 6'', 2''', 6'''CH), 7.61 (2, 3''' & 6'''CH), 8.02 (1, 5CH), 11.6 (1, 4C-OH) Syn-isomer: 2.17 (1, 2'CH_2), 2.90 (1, 2'CH_2), 4.46 (1, 3'CH), 4.80 (1, 1'CH), 5.3 (1, 3'C-OH), 7.14 (1, aroma. H), 7.24 (2, aroma. H), 7.32 (1, aroma. H), 7.34 (1, 6CH), 7.37 (2, 3'' %5''CH), 7.40 (2, aroma. H), 7.54 (2, 2''' & 6'''CH), 7.55 (2, 2'' & 6''CH), 7.57 (1, 7CH), 7.61 (2, 3''' & 6'''CH), 8.02 (1, 5CH), 11.5 (1, 4C-OH)		N	1	Organic Chemistry Novak L, (2005), IR, MS, ^{1}H- and ^{13}C-NMR Spectra of Bromadiolone, Budapest University of Technology and Economics, Institute for Organic Chemistry	X13

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
	C-13 (DMSO-d_6 solution, TMS internal std.)	Not stated	Chemical shifts (assignment): Anti-stereoisomer: 36.71 (C-1'), 41.53 (C-2'), 70.77 (C-3'), 107.68 (C-3), 115.85 (C-8), 117.20 (C-4a), 120.50 (C-4'''), 123.21 (C-6), 123.40 (C-5), 125.57 (C-4''''), 126.04 (C-2'' & C-''), 126.32 (C-3'' & C-5''), 127.75 (C-2'''' & C-6''''), 128.02 (C-2'''' & C-6''''), 128.50 (C-2''' & C-6'''), 131.15 (C-7), 131.57 (C-3''' & C-5'''), 137.21 (C-4''), 139.17 (C-1'''), 143.84 (C-1''''), 146.10 (C-1''), 152.08 (C-8a), 161.67 (C-4), 161.91 (C-2) Syn-isomer: 36.97 (C-1'), 41.12 (C-2'), 70.99 (C-3'), 106.69 (C-3), 115.99 (C-8), 116.31 (C-4a), 120.51 (C-4'''), 123.27 (C-6), 123.40 (C-5), 125.66 (C-4''''), 126.07 (C-2'' & C-6''), 126.23 (C-3'' & C-5''), 127.59 (C-2'''' & C-6''''), 127.83 (C-2'''' & C-6''''),		N	1		X13

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
MS	-	Not stated	128.52 (C-2''' & C-6'''), 131.57 (C-3''' & C-5'''), 137.08 (C-4''), 139.15 (C-1'''), 143.87 (C-1''''), 146.19 (C-1''), 152.02 (C-8a), 161.18 (C-4), 161.56 (C-2) m/z | Intensity relative to base peak | Proposed fragments 551 | 1.4% | M+Na, (^{81}Br) 549 | 1.3% | M+Na, (^{79}Br) 511 | 1.8% | M+H-H_2O, (^{81}Br) 509 | 1.8% | M+H-H_2O, (^{79}Br) 251 | 11% | M-BrC_6H_4 C_6H_4CHOH		N	1	Novak L, (2005), IR, MS, ^{1}H- and ^{13}C-NMR Spectra of Bromadiolone, Budapest University of Technology and Economics, Institute for Organic Chemistry	X14
3.5 Solubility in water (IIA3.5)								
Water solubility 1	OPPTS Series 830 Section 7840. OECD 105	98% bromadiolone	**result:** 1.21 ppm **temperature:** 25°C **pH:** 7	Very low water solubility	Y	1	Anderson W, (1999) Product Chemistry: Technical	X15

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
							Grade Product Stillmeadow Incorporated report 4745-98	
Water solubility 2	Method A6 of 92/69/EEC which constitutes Annex V of 67/548/EEC	98.8%	**Result :** 1.14E-04g/l at pH 5 (20°C) 5.63 E-04g/l at pH 6.9 (10°C) 2.48E-03g/l at pH 6.8 (20°C) 2.66 E-03g/l at pH 6.8 (30°C) 0.180 g/l at pH 9 (20°C)	Between 10-30°C there is little effect on solubility at pH6.8-6.9, when compared to the effect of pH over the range 5-9. The increased solubility with increasing pH is believed to be due to the dissociation of the phenol group on the 4-hydroxycoumarin , resulting in greater polarity and hence increased solubility	Y	1	Mullee and O'Connor, 2006, Determination of general physico-chemical properties,Safe Pharm, report number 2073/0002	X16
3.6 Dissociation constant (-)	Calculation by ACD/pKa		<u>Enolic form</u> $pKa_1 = 13.94 \pm 0.20$	ACD-generated pKa has been given instead of	N	2	ACD/I-Lab Web service (ACD/pKa	X17

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
			$pKa_2 = 4.50 \pm 0.20$ Keto form $pKa_1 = 14.16 \pm 0.20$ $pKa_2 = 9.06 \pm 0.20$	experimental data because of its low water solubility. It would be especially difficult to test a substance that is likely to have a high pKa			8.03)	
3.7 **Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)**	Flask method, Method A6	98.8% bromadiolone	**result:** Dimethylformamide 730 g/l at 20°C Ethanol 8.2g/l @20°C Ethyl acetate 25g/l @20°C Soluble in acetone; slightly soluble in chloroform; practically insoluble in diethyl ether and hexane. **Results:** **n-heptane:** 3.10×10^{-3} g/l at 15.0 ± 0.5°C 3.43×10^{-3} g/l at 25 ± 0.5°C **methanol:**		n/a	2	The Pesticide Manual, 11th edition, British crop protection council O'Connor. BJ and Mullee. DM (2005) Determination of solubility in organic solvents and surface	X18

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
			13.8 g/l at 15.0 ± 0.5°C 15.0 g/l at 25 ± 0.5°C				tension. SafePharm Laboratories. Project numbrt 2073/001	
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)	-			Only if additional data are required (see BPD, TNsG)			See justification	
3.9 Partition coefficient n-octanol/water (IIA3.6)	*including effects of pH (5-9)*							
log Pow 1	OPPTS Series 830 Section 7570. OECD 117	96% bromadiolone	**result:** LogP = 7.0 **temperature:** 23°C **pH:**		Y	1	Anderson W, (1999) Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98	X19
log Pow 2	Shake-flask method,	98.8%	**Result:** log P>5.00 at pH 4.9	The decreasing log P is expected as	Y	1	Mullee and O'Connor,	X20

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
	A8 and OECD 107		Log P =3.8 at pH 7.1 Log P =2.47 at pH 9.1	the pH rises due to dissociation of the hydrogen on the phenol group giving the molecule a greater polarity and hence a lower solubility in octanol relative to water.			2006, Determination of general physico-chemical properties SafePharm Ltd, report number 2073/0003	
3.10 **Thermal stability, identity of relevant breakdown products (IIA3.7)**	CIPAC MT 46. OPPTS Series 830 Section 6313	96% bromadiolone	Instability unlikely Insignificant weight loss only		Y	1	Anderson W, (1999) Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98	X21
Thermal stability 2	OECD 113	98.8%	Result: Thermally stable and stable in air up to a temperature of at least 150°C (423K)		Y	1	Mullee and O'Connor, 2006, Determination of general physico-chemical properties	X22

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
							SafePharm Ltd, report number 2073/0003	
3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)			Non-flammable					X23
3.12 Flash-point (IIA3.9) Flash-point 1 Flash point 2			Not relevant					X24
3.13 Surface tension (IIA3.10)								

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
Surface tension 1 Surface tension 2	Ring based method on ISO 304, Method A5	98.8% bromadiolone	**result:** 72.1 mN/m **concentration:** 1.47 x 10^{-3} g/l aqueous solution **temperature:** 21.0 ± 0.5 °C		Y	1	O'Connor B J, Mullee D M (2005) Bromadiolone Technical: Determination of solubility in organic solvents and surface tension SPL project Number: 2073/001	X25
3.14 Viscosity (-)	-		**result:** **temperature:**	Only if additional data are required (see BPD, TNsG)				X26
3.15 Explosive properties (IIA3.11)	-			Not relevant				X27
3.16 Oxidising properties (IIA3.12)	-			Not relevant				X28

Section A3 Physical and Chemical Properties of Active Substance

Annex Points IIA, III.3.1.1 to 3.13, Annex Points IIIA, III.1 to 2 and TnsG Chapter 3, Part A, Point 3.6 and Point 3.14

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.17 Reactivity towards container material (IIA3.13)	Not reactive							X29

Evaluation by Competent Authorities

EVALUATION BY RAPPORTEUR MEMBER STATE

Date

April 2007

Evaluation of data submitted under section A3

3.1.1 Melting point

Materials and Method

X1: Study No. 1-The test material is described as LX 125-01 and no further information is given on the identity. The test was performed with technical material instead of purified material.

Study No. 2-The melting point was determined using DSC. The Lot No of the test material was 02474 and it appears to be technical material instead of purified material. However, the purity is considered sufficiently high.

Results

X1: Study No. 1:-The result is based on three trials. The substance was reported to possibly decompose upon melting since it changed colour and did not resolidify upon cooling.

X2: Study No. 2- The reported result is from the last of the two performed tests. The mean result is:
171.95-202.08°C.

Two non separated peaks are shown in the DSC-thermogram which is characteristic of the melting of the two diastereomers of bromadiolone. The endotherm corresponding to the minor diastereomer reaches its minimum at approximately 182°C and the endotherm corresponding to the major diastereomer reaches its minimum at approximately 198°C. The test material was reported to decompose upon melting.

Reliability

X1: Study No. 1- The study report does not confirm that the tested material is bromadiolone representative of the material under evaluation. The reliability is thus set to:

Reliability indicator 3

Study No. 2-Reliability indicator 1

Acceptability

The first study is not considered acceptable due to insufficient reporting and the result thereof will therefore not be presented in document II-A. The second study and the result thereof are acceptable.

3.1.2 Boiling point

Materials and Method

X3: Study No. 1-As given in X1 above the identity of the tested material is not clear. No test was performed in this reference.

X4: Study No. 2-The boiling point was assessed using DSC. The Lot No of the test material was 02474 and it appears to be technical material instead of purified material. However, the purity is considered sufficiently high.

Results

X3: Study No. 1-The applicant's version is adopted.

X4: The reported temperature of decomposition is in the report described as the start of the broad shallow endotherm indicative of possible loss of volatile decomposition products. The melting point study indicates that the substance

decomposes already upon melting. It will thus be reported that it decomposes upon melting starting at 260°C

Reliability
X4: Study No. 1-Since no experimental testing was performed the reliability is set to:

Reliability indicator 0: Not applicable since no experimental study was performed.

Study No. 2-Reliability indicator 1

Acceptability
No determination was performed in the first study and the reference is therefore not relevant for this parameter and will not be presented in Document II-A.

The second study and the results thereof are acceptable.

3.1.3 Bulk density/relative density

Materials and Method
X5: Study No. 1- As given in X1 above the identity of the tested material is not clear. Further the study was performed using a Le Châtelier density bottle, which taken the reported result into account, seems to determine the bulk density rather than the density or relative density.

X6: The relative density was determined using a gas comparison pycnometer. The Lot No of the test material was 02474 and it appears to be technical material instead of purified material. However, the purity is considered sufficiently high.

Results
X5: Study No. 1-The result should probably be seen as the bulk density and not the density.

X6: Study no. 2-The density was determined at 20.5°C ± 0.5°C and the result is hereby best expressed as:

density: 1.45 g/cm^3 at 20.5°C ± 0.5°C

Reliability
X5: Study No. 1- The used method does not determine the relative density and the identity of the tested material is not clear. The reliability is thus set:

Reliability indicator 3

Study No. 2- Reliability indicator 1

Acceptability
The first study is not considered acceptable due to insufficient reporting and methodological deficiencies. The result thereof will therefore not be presented in document II-A. The second study and the result thereof is acceptable.

3.2 Vapour pressure

Materials and Method
X7: Study No. 1-The test was performed using the gas saturation method of OECD 104, by direct measurement at 45 °C. Since the obtained result was below the recommended range defined by the method no further study at higher temperature was performed.

X8: Study No. 2- As given in X1 above the identity of the tested material is not clear.

No test was performed in this study, since literature values indicated that the vapour pressure of the test substance is below 10^{-7} torr at 25 °C (~1.33×10^{-5} Pa).

Results
X7: Study No. 1-The result is for 45 °C and no estimation of the vapour pressure at 20 °C or 25 °C is reported. A more accurate result should probably been

obtained by measurements at higher temperature followed by extrapolation to room temperature. However, since the obtained result is <0.05 mPa at 45 °C, the vapour pressure of bromadiolone should not be of health nor environmental concern.

Moreover, literature values (see 3.2.1) indicates that the vapour pressure of bromadiolone is less than 10^{-5} Pa at 20°C.

X8: Study No. 2-The result reported in this study is only a literature value since no measurement was performed.

Reliability
Study 1-Reliability indicator 1

X8: Study 2-Reliability indicator 0: Not applicable since no experimental measurement was performed in this study and the result reported is taken from literature and no reference is given.

Acceptability
The first study and the result thereof are considered acceptable. The result given from the second study is not considered acceptable and will not be presented in Document II-A.

3.2.1 Henry's Law Constant

Materials and Method
X9: The two first results are based on literature values or calculations.

The third result is based on the calculation using the experimentally determined water solubility at uncontrolled pH (see 3.5) and the vapour pressure taken from literature (Hartley, D & Kidd, H 1983).

However, since the water solubility study (Anderson, W. 1999) at uncontrolled pH is not considered acceptable the Henry's law constant should be calculated using the water solubility determined in the acceptable study (Mullee and O'Connor, 2006).

Results
X9: Results 2 and 3 should be given as:

2) 5.553×10^{-5} Pa.m^3/mol at 20°C

3) Using the water solubility from Mullee and O'Connor at pH 6.8 and 20°C (2.48 mg/l) and the vapour pressure form Hartley, D & Kidd, H 1983 (2.0×10^{-6} Pa) the following is obtained:

H=4.252×10^{-4} Pa.m^3/mol

Reliability
X9: Since none of the reported values are based only on experimentally determined results the reliability is set to:

Reliability indicator 0: Not applicable since the results are not based only on experimentally determined figures.

Acceptability
The approach of calculating the Henry's law constant based on the experimentally determined water solubility and the literature value for vapour pressure is considered acceptable. The vapour pressure is indicated to be sufficiently low not to require an experimental value (i.e. less than 10^{-5} Pa).

The other two results will not be reported in Document II-A since the reliability of these values cannot be judged.

3.3 Appearance

X10: The test material is described as LX 125-01 and no further information is given on the identity. It is thus concluded that this study cannot be relied on for the appearance.

However, for colour and physical state it is considered acceptable to rely on the phtolysis study (Drake, 2005; see A3.4/02 below), where the material is described as a white powder.

It is considered acceptable to waive a study on odour of bromadiolone as it is classified as toxic by inhalation.

3.4 Absorption spectra

Materials and Method

UV/VIS

X11: Study 1- The test material is described as LX 125-01 and no further information is given on the identity. The test was performed with technical material instead of purified material.

UV-VIS spectra were determined in neutral media (90% methanol in water), acidified media (90% methanol in water + 1 M HCl) and alkaline media (90% methanol in water + 1 M NaOH).

X12: Study 2- The UV-VIS spectrum was generated on technical material instead of purified material.

IR, NMR and MS

X13: The study was not performed in accordance with GLP. Moreover, the purity of the tested material is not stated. However, according to the spectral analysis the purity was high.

NMR

The applicant's version is adopted.

MS

X14: The MS-spectra was generated using FAB (Fast Atom Bombardment) techniques with argon as ionization source.

Results

UV/VIS

X12: Study 1-The following absorption maxima and corresponding molar absorption coefficients were obtained for respective media:

Neutral:	λ_{max} [nm]	Molar extinction coefficient [l x mol^{-1} x cm^{-1}]
	263	36400
	310	13700

Acidic:	λ_{max} [nm]	Molar extinction coefficient [l x mol^{-1} x cm^{-1}]
	265	36850
	311	13100

Alkaline:	λ_{max} [nm]	Molar extinction coefficient [l x mol^{-1} x cm^{-1}]
	260	33000
	312	15450

Study 2-The applicant's version is adopted

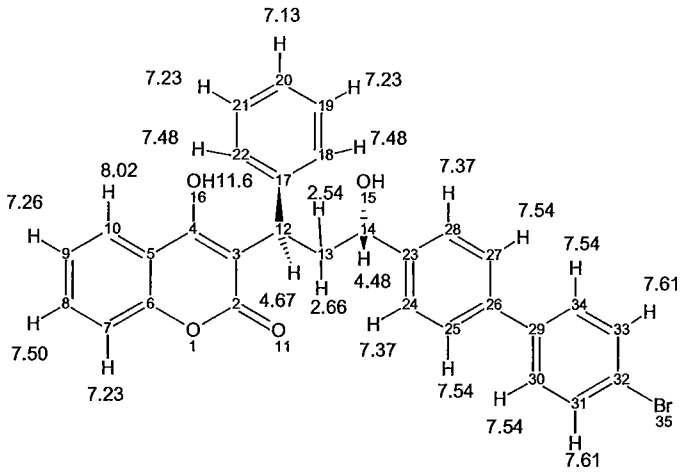
IR

The applicant's version is adopted.

NMR

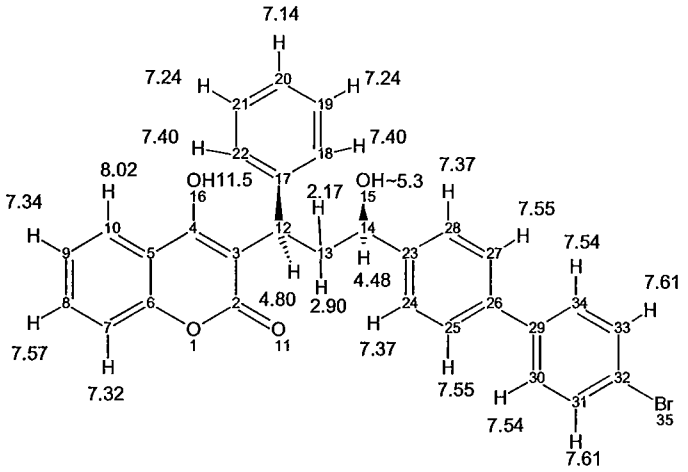
X13: ^{1}H- and ^{13}C-spectra were determined for the separate diasteromers (*syn* and *anti*). Bromadiolone is a mixture of the two diasteromers which means that the NMR-spectra of technical bromadiolone are an overlay of the signals shown below for the separate diastereomers.

^{1}H-Anti isomer



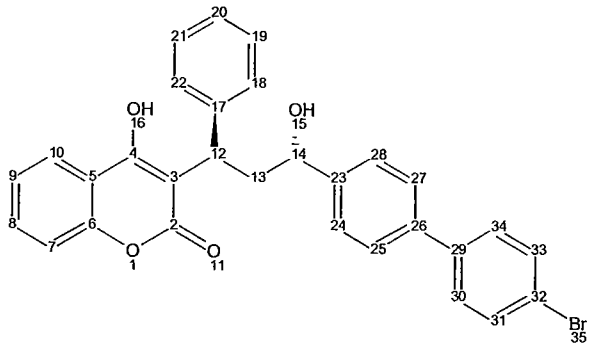
Chemical shift δ (ppm)	Intensity	Assignment
2.54 (m)	1 H	C13 CH_2
2.66 (m)	1 H	C13 CH_2
4.48 (dd, *J*=7.1 and 5.1 Hz)	1 H	C14 CH
4.67 (m-t, *J*=7.4 Hz)	1 H	C12-H
7.13 (t, *J*=7 Hz)	1 H	C20 aromat. H
7.23 (m)	3 H	C7, C19 and C21 aromat. H
7.26 (m)	1 H	C9 aromat. H
7.37 (d, *J*=8 Hz)	2 H	C24 and C28 aromat. H
7.50 (m)	1 H	C8 aromat. H
7.54 (d, *J*=8.1 Hz)	4 H	C25, C27, C30 and C34 aromat. H
7.61 (d, *J*=8.4 Hz)	2 H	C31 and C33 aromat. H
8.02 (d, *J*=7.9 Hz)	1 H	C10 aromat. H
11.6 (br. s)	1 H	O16 H

^{1}H-Syn isomer



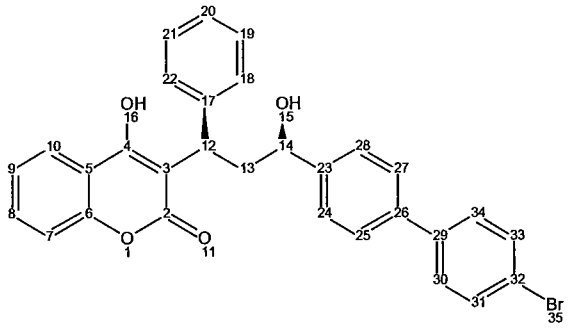
Chemical shift δ (ppm)	Intensity	Assignment
2.17 (m)	1 H	C13 CH_2
2.90 (m)	1 H	C13 CH_2
4.46 (dd, *J*=9.2 and 3.4 Hz)	1 H	C14 CH
4.80 (dd, *J*=11 and 4.4 Hz)	1 H	C12-H
5.3 (br. s)	1 H	O15 H
7.14 (t, *J*=7.2 Hz)	1 H	C20 aromat. H
7.24 (t, *J*=7.5 Hz)	2 H	C19 and C21 aromat. H
7.32 (d, *J*=7.8 Hz)	1 H	C7 aromat. H
7.34 (t, *J*=8 Hz)	1 H	C9 aromat. H
7.37 (d, *J*=8 Hz)	2 H	C24 and C28 aromat. H
7.40 (d, *J*=7.7 Hz)	2 H	C18 and C22 aromat. H
7.54 (d, *J*=8 Hz)	2 H	C30 and C34 aromat. H
7.55 (d, *J*=8 Hz)	2 H	C25 and C27 aromat. H
7.57 (t, *J*=7.8 Hz)	1 H	C8 aromat. H
7.61 (d, *J*=8.4 Hz)	2 H	C31 and C33 aromat. H
8.02 (d, *J*=7.9 Hz)	1 H	C10 aromat. H
11.5 (br. s)	1 H	O16 H

^{13}C-Anti isomer



Chemical shift δ (ppm)	Assignment
36.71	C12
41.53	C13
70.77	C14
107.68	C3
115.85	C7
117.20	C5
120.50	C32
123.21	C9
123.40	C10
125.57	C20
126.04	C24 and C27
126.32	C25 and C28
127.75	C19 and C21
128.02	C18 and C22
128.50	C31 and C34
131.15	C8
131.57	C31 and C33
137.21	C26
139.17	C29
143.84	C17
146.10	C23
152.08	C6
161.67	C4
161.91	C2

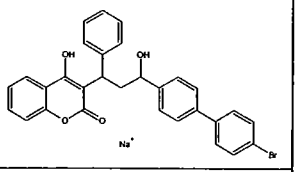
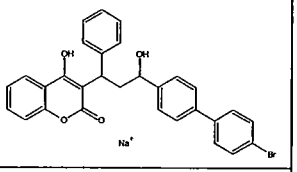
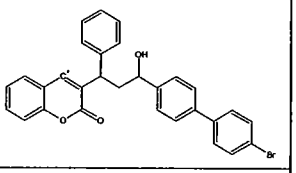
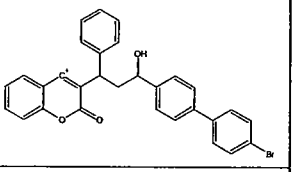
^{13}C-Syn isomer



Chemical shift δ (ppm)	Assignment
36.97	C12
41.12	C13
70.99	C14
106.69	C3
115.99	C7
116.31	C5
120.51	C32
123.27	C10
123.55	C9
125.66	C20
126.07	C25 and C27
126.23	C24 and C28
127.59	C18 and C22
127.83	C19 and C21
128.52	C30 and C34
131.57	C8, C31 and C33
137.08	C26
139.15	C29
143.87	C17
146.19	C23
152.02	C6
161.18	C4
161.56	C2

MS

X14: The structures for the proposed fragments in MS are as follows:

Mass (m/z)	Relative intensities (in % of base peak)	Proposed fragments	Structure of fragment
551	1.4	M + Na (according to ^{81}Br isotope)	
549	1.3	M + Na (according to ^{79}Br isotope)	
511	1.8	M +H-H_2O (^{81}Br)	
509	1.8	M + H-H_2O (^{79}Br)	
251	11	M-$BrC_6H_4C_6H_4CHOH$	

Reliability

UV-VIS

X11: Study 1-The study report does not confirm that the tested material is bromadiolone representative of the material under evaluation. The reliability is thus set to:

Reliability indicator 3

Study 2- Reliability indicator 1

IR, NMR and MS-spectroscopy

X13 and X14: Since the study was not performed in accordance with GLP and the purity of the tested material is not stated the reliability is lowered to:

Reliability indicator 2

Acceptability

For UV/VIS the first study is not accepted as the test material is not confirmed to be bromadiolone. The results of the second study indicate that the first study is for bromadiolone but it still considered that only the second study can be relied on for this parameter.

For the other spectral data the methods and the obtained results are acceptable. All the spectra are consistent with the structure of bromadiolone.

3.5 Solubility in water

Materials and Method

X15: Study 1-As given previously the identity of the tested material is not clear.

Moreover, the flask method was used, which is only applicable for solubilities $>10^{-2}$ g/l.

Further, the solubility was determined in HPLC-water without pH control and the pH of the solutions is not stated.

X16: Study No. 2- The Lot No of the test material was 02474 and it appears to be technical material instead of purified material. However, the purity is considered sufficiently high. The temperature dependency of the solubility was assessed using the flask-method procedure. The substance was shaken with double-distilled water at 30°C for 24 h. Three samples were then equilibrated at 30°C, 20°C and 10°C. It should be noted that this is a preliminary test and due to the low solubility a definite test at pH 7 using the column method should have been performed.

The solubility at pH 5 was determined using the column method whereas the solubility at pH 9 was determined using the flask-method. Buffers were used at both pH.

All quantifications were determined by HPLC.

Results

X15: Study No. 1-The result should be given as 1.2 mg/l.

X16: Study No. 2-The peak profile of the chromatograms differed between the standards and the sample solutions indicating that the minor diastereomer has a somewhat higher solubility in water than the major diastereomer.

Reliability

X15: Study No. 1- Since the identity of the tested material is not clear and the flask-method was used instead of the column method, the reliability is lowered to:

Reliability indicator 3

X16: Study No. 2-Since no definite test was performed at pH 7 the reliability is lowered to:

Reliability indicator 2

Acceptability

The first study is not considered acceptable since the test material is not confirmed to be bromadiolone and the result thereof will not be presented in Document II-A. The second study is considered acceptable despite that no definite test at pH 7 was performed since three results were determined at that pH.

3.6 Dissociation constant

Materials and Method

X17: The low solubility of bromadiolone makes it technically not feasible to perform an experimental study on the dissociation constant. It is therefore considered acceptable to present the ACD-generated pKa for information.

Results

X17: When structurally analysing bromadiolone it is reasonably to think that it should have a maximum of four pKa's (i.e. two pKa for the enolic form and two for the keto-form). The presented ACD generated pKa's supports this theoretic reflection.

Moreover in the Merk's index, 12th edition, an experimentally obtained pKa value for bromadiolone of 4.05 (ref: Budvaris et al. 1989) is given which is in line with the ACD-generated pKa for the enolic form.

Further, the test on the solubility in water (see 3.5 above) shows that a significant increase in solubility is obtained at pH 9 compared to pH 7, which supports the ACD-generated pKa of 9.06 for the keto-form.

Reliability

X17: Since no experimental testing was performed the reliability is set to:

Reliability indicator 0: Not applicable since no experimental testing was performed.

Acceptability

It is considered acceptable to present the computer generated pKa since it is not technically feasible to perform any experimental testing for this parameter.

3.7 Solubility in organic solvents, including the effect of temperature on solubility

Materials and Method

X18: The Lot No of the test material was 02474 and it appears to be technical material.

Results

X18: The results are based on the total solubility of bromadiolone in the different media. However it was shown that the diastereomeric ratios of the solvates were significantly different from the technical material, which indicated a much higher solubility of the less occurring isomer in bromadiolone.

Reliability

X18: Since the study was performed in accordance with GLP and in accordance with relevant guidelines the reliability is increased to :

Reliability indicator 1

Acceptability

The used method and the obtained results are acceptable. The results taken from the Pesticide Manual will not be listed in Document II-A.

3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products

See the justification below the evaluation box.

3.9 Partition coefficient n-octanol/water

Materials and Method

X19: Study No. 1- As given in X1 above the identity of the tested material is not clear. Moreover, the pH effect was not assessed and the actual pH used is not stated.

X20: Study No. 2- The Lot No of the test material was 02474 and it appears to be technical material instead of purified material. However, the purity is considered sufficiently high. Buffered solutions were used for all tests. Quantification in both phases was done by means HPLC-UV

Results

Study No. 1-The applicant's version is adopted.

X20: Study No. 2-The results are for 25 ± 1°C. The content of bromadiolone in the aqueous phase in the test at pH 5 was too low to be determined by the analytical method.

LOQ is set to 0.01 mg/l and using that figure and the content found in the organic phase a log Pow of >5 is obtained.

Reliability

X19: Study No. 1-The identity of the test material is not clear. Further the test on solubility in water indicates that a pH dependency of the log P_{ow} is anticipated. The reliability is thus lowered to:

Reliability indicator 3:

Study No. 2- Reliability indicator 1

Acceptability

The first study is not considered acceptable since the pH dependency was not assessed and as the test material is not confirmed to be bromadiolone. Further the log P_{ow} determined in the first study might be representative for the undissociated substance. However since the pH is not stated this cannot be concluded on. Hereby, the result form this study will not be listed in Document II-A.

The second study and the result thereof are acceptable.

3.10 Thermal stability, identity of relevant breakdown products

Materials and Method

X21: Study No. 1- As given in X1 above the identity of the tested material is not clear. Moreover, an accelerated storage stability test at 54°C for 14 days was performed instead of testing the thermal stability to the point of melting, sublimation or decomposition as required for this parameter. In addition to this the stability in light and towards metal/metal ions was assessed in this study.

X22: Study No. 2- The Lot No of the test material was 02474. The study was performed using DSC in accordance with OECD 113 (in N_2 and air atmosphere).

Results

X21: Study No. 1-The substance was shown to be stable at 54°C for 14 days.

Furthermore it was shown to be stable for at least 72 days when exposed to 12 h simulated sun light each day.

Moreover, it was shown to be stable for at least 14 days at 20°C and 37°C when exposed to aluminium metal, aluminium ions, iron metal and ferric ions.

X22: Study No. 2-In addition to the reported results for this parameter, the melting point and boiling point was assessed in the same study. Those results (see 3.1.1 and 3.1.2) will also be reported in Document II-A for this parameter.

Reliability

X21: Study No. 1-The study itself is considered reliable (i.e. reliability indicator 1). However, the reliability of the study to address this parameter is:

Reliability indicator 3

Study No. 2- Reliability indicator 1

Acceptability

The first study is not considered acceptable to address this parameter as the test material is not confirmed to be bromadiolone. The second study is acceptable and the results thereof will be presented in Document II-A alongside the results presented in A3.1.1 and A3.1.2.

3.11 Flammability of gases, flammability in contact with water and pyrophoric properties

X23: See the justification below the evaluation box.

3.12 Flash-point

X24: See the justification below the evaluation box.

3.13 Surface tension

Materials and Method

X25: The Lot No of the test material was 02474 and it appears to be technical material. The surface tension was tested for a 90% saturated solution.

Results

The applicant's version is adopted

Reliability

Reliability indicator 1

Acceptability

The used method and the obtained results are acceptable

3.14 Viscosity

X26: See the justification below the evaluation box.

3.15 Explosive properties

X27: See the justification below the evaluation box.

3.16 Oxidising properties

X28: See the justification below the evaluation box.

	3.17 Reactivity towards container material X29: See the justification below the evaluation box.
Remarks	There are no further remarks

Justifications for non-submission of data under section A3

Section A3.8 Annex Point IIIA, III.2	Stability in organic solvents used in biocidal products and identity of relevant break down products	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	Official use only
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ] Scientifically unjustified [x]** **Other justification [ ]**	
Detailed justification:	The study is scientifically unnecessary as the active substance is not used in organic solvents.	
	Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	April 2007	
Evaluation of applicant's justification	Neither technical bromadiolone as manufactured nor the representative product Protect wax blocks contain any organic solvents. This data requirement is therefore not relevant.	
Conclusion	The applicant's justification is acceptable.	
Remarks	There are no further remarks.	

Section A3.11 Annex Point IIA, III.3.8	Flammability including auto-flammability and identity of combustion products	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ]	**Technically not feasible [ ] Scientifically unjustified [x]**	
Limited exposure [ ]	**Other justification [ ]**	
Detailed justification:	No evidence of flammability in use and consideration of chemical structure suggests no flammable properties.	
	Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	April 2007	
Evaluation of applicant's justification	As data on flammability is available from the other applicant for Annex I-inclusion it could be concluded that bromadiolone is not highly flammable. The justification is thus accepted at this stage. However, as the TNsG on Data Requirements does not leave room for theoretical considerations with respect to flammability, in contrast to explosive and oxidizing properties, data might be needed for product authorisation at member state level.	
Conclusion	Justification accepted for Annex I-inclusion, but data will be needed for product authorisation.	
Remarks	No remarks.	

Section A3.12 Annex Point IIA, III.3.9	Flash-point	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ] Scientifically unjustified [x]** **Other justification [ ]**	
Detailed justification:	No evidence of flammability in use and consideration of chemical structure suggests no flammable properties.	
Evaluation by Competent Authorities		
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	April 2007	
Evaluation of applicant's justification	The flash-point is only needed to be determined for liquids and this parameter is therefore not applicable to bromadiolone	
Conclusion	The applicant's justification is acceptable	
Remarks	There are no further remarks	

Section A3.14 TnsG Chapter 3, Part A, Point 3.14	Viscosity	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ]	**Technically not feasible [ ] Scientifically unjustified [x]**	
Limited exposure [ ]	**Other justification [ ]**	
Detailed justification:	The study to determine the viscosity of the active substance is not applicable to bromadiolone, as the physical nature is not in liquid state.	
	Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	April 2007	
Evaluation of applicant's justification	The applicant's justification is acceptable	
Conclusion	The applicant's justification is acceptable	
Remarks	There are no further remarks	

Section A3.15 Annex Point IIA, III.3.11	Explosive properties	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ]	**Technically not feasible [ ] Scientifically unjustified [x]**	
Limited exposure [ ]	**Other justification [ ]**	
Detailed justification:	Consideration of structure and physico-chemical properties does not suggest any explosive potential. Widespread experimental and commercial use over many years has not shown any exothermic or explosive activity	
Evaluation by Competent Authorities		
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	April 2007	
Evaluation of applicant's justification	There are no groups in the structure of bromadiolone that would imply explosive properties. The applicant's justification is therefore acceptable	
Conclusion	The applicant's justification is acceptable	
Remarks	There are no further remarks	

Section A3.16 Annex Point IIA, III.3.12	Oxidizing properties	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ] Scientifically unjustified [x]** **Other justification [ ]**	
Detailed justification:	Consideration of structure and physico-chemical properties does not suggest any oxidising potential. Widespread experimental and commercial use over many years has not shown any signs of oxidising activity	X
	Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	April 2007	
Evaluation of applicant's justification	There are no groups in the structure of bromadiolone that would imply oxidizing properties. The applicant's justification is therefore acceptable	
Conclusion	The applicant's justification is acceptable	
Remarks	There are no further remarks.	

Section A3.17 Annex Point IIA, III.3.13	Reactivity towards container material	
	JUSTIFICATION FOR NON-SUBMISSION OF DATA	**Official use only**
Other existing data [ ] **Limited exposure [ ]**	**Technically not feasible [ ] Scientifically unjustified [x]** **Other justification [ ]**	
Detailed justification:	Consideration of chemical structure and physico-chemical properties show the compound is stable and largely unreactive. Widespread experimental and commercial use over many years has not shown any signs of reaction with container materials	X
	Evaluation by Competent Authorities	
	EVALUATION BY RAPPORTEUR MEMBER STATE	
Date	April 2007	
Evaluation of applicant's justification	There are no groups in the structure of bromadione that indicate the substance to be reactive toward any container materials used. .	
Conclusion	The applicant's justification is acceptable.	
Remarks	There are no further remarks.	

Reference list of studies submitted (by Section No.)

Section No / Reference No	Author(s)	Year	Title. Source (where different from company) Company, Report No. GLP (where relevant) / (Un)Unpublished	Data Protection Claimed (Yes/No)	Owner
A2.8.1	Garofani, S	2004	Bromadiolone technical analysis of five batch samples, Chem Service S.r.l., CH-039/2004, GLP, (Un)	Y	Task Force
A3.1	Anderson W	1999	Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98GLP, Unpublished	Y	Task Force
A3.2	Fabbrini Dr R	1997	BROMADIOLONE Determination of the Vapour Pressure. ChemService report CH-14/96-C-BDL GLP, Unpublished	Y	Task Force
A3.2.1	SafePharm Laboratories	2004	US EPA, EPIWIN v3.12, EPI Suite Software, 2004	Y	Task Force
A3.3	Anderson W	1999	Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98 GLP, Unpublished	Y	Task Force
A3.4	Anderson W	1999	Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98GLP, Unpublished	Y	Task Force
A3.4	Novak L	2005	IR, MS, ^{1}H- and ^{13}C-NMR Spectra of Bromadiolone, Budapest University of Technology and Economics, Institute for Organic Chemistry	Y	Task Force
A3.5	Anderson W	1999	Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98GLP, Unpublished	Y	Task Force
A3.7	O'Connor B J, Mullee D M	2005	Bromadiolone Technical: Determination of solubility in organic solvents and surface tension SPL project Number: 2073/001 GLP, Unpublished	Y	Task Force
A3.9	Anderson W	1999	Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98GLP, Unpublished	Y	Task Force
A3.10	Anderson W	1999	Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98GLP, Unpublished	Y	Task Force
A3.13	O'Connor B J, Mullee D M	2005	Bromadiolone Technical: Determination of solubility in organic solvents and surface tension SPL project Number: 2073/001	Y	Task Force

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			GLP, Unpublished		

Reference list of studies submitted (by Author)

Author(s)	Section No / Reference No	Year	Title. Source (where different from company) Company, Report No. GLP (where relevant) / (Un)Unpublished	Data Protection Claimed (Yes/No)	Owner
Anderson W	A3.1	1999	Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98GLP, Unpublished	Y	Task Force
Anderson W	A3.3	1999	Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98 GLP, Unpublished	Y	Task Force
Anderson W	A3.4	1999	Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98GLP, Unpublished	Y	Task Force
Anderson W	A3.5	1999	Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98GLP, Unpublished	Y	Task Force
Anderson W	A3.9	1999	Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98GLP, Unpublished	Y	Task Force
Anderson W	A3.10	1999	Product Chemistry: Technical Grade Product Stillmeadow Incorporated report 4745-98GLP, Unpublished	Y	Task Force
O'Connor B J, Mullee D M	A3.7	2005	Bromadiolone Technical: Determination of solubility in organic solvents and surface tension SPL project Number: 2073/001 GLP, Unpublished	Y	Task Force
O'Connor B J, Mullee D M	A3.13	2005	Bromadiolone Technical: Determination of solubility in organic solvents and surface tension SPL project Number: 2073/001 GLP, Unpublished	Y	Task Force
Fabbrini Dr R	A3.2	1997	BROMADIOLONE Determination of the Vapour Pressure. ChemService report CH-14/96-C-BDL GLP, Unpublished	Y	Task Force
Garofani, S	A2.8.1	2004	Draft Report: Bromadiolone technical analysis of five batch samples, Chem Service S.r.l., CH-039/2004, GLP, (Un)	Y	Task Force
Novak L	A3.4	2005	IR, MS, ^{1}H- and ^{13}C-NMR Spectra of Bromadiolone, Budapest University of Technology and Economics, Institute for Organic Chemistry	Y	Task Force

Author(s)	Section No / Reference No	Year	Title. Source (where different from company) Company, Report No. GLP (where relevant) / (Un)Unpublished	Data Protection Claimed (Yes/No)	Owner
SafePharm Laboratories	A3.2.1	2004	US EPA, EPIWIN v3.12, EPI Suite Software, 2004	Y	Task Force