Section A3 Physical and Chemical Properties of Active Substance

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	OECD 102 (1995), capillary/liquid bath method	99.4 % Batch No. AC12140-35 (pure active ingredient, PAI)	Melting range = 166.1–168.2°C	Two experiments conducted under air and nitrogen atmosphere, respectively, gave identical results.	Y	1	**A3.1.1/01:** Dxxxx Axxxx (2001) Determination of the melting point, the appearance, the thermal stability and the stability in air of BAS 322 I (PAI) (Flocoumafen, Reg. No. 4060804 identical with CL 183540). BxxxxAxxxx, Lxxxx, Gxxxx, Report No. PCP06480, November 29, 2001(unpublished). (BASF-Ref.: 2001/1017610)	
	OECD 102 (1995), capillary/liquid bath method	98.6 % Batch No. M02 (technical grade active ingredient, TGAI)	Melting range = 166.1–168.3 °C	Two experiments conducted under air and nitrogen atmosphere, respectively, gave identical results.	Y	1	**A3.1.1/02:** Dxxxx Axxxx (2002) Determination of the melting point and the appearance of Flocoumafen (TGAI) (BAS 322 I, Reg. No. 40608004 identical with CL 183540). Bxxxx Axxxx, Lxxxx, Gxxxx, Report No. PCP06579, January 25, 2002 (unpublished). (BASF-Ref.: 2002/1004164)	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)		Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
		Guideline: not stated a) Kofler melting point apparatus b) Differential thermal analyis (DTA)	Cis-isomer: > 99 % Trans-isomer: c. 95 %	Melting ranges: a) Kofler method: Cis-isomer: 185–188 °C Trans-isomer: 158–163 °C b) DTA: Cis-isomer: T_m = 188 °C Trans-isomer: T_m = 158 °C	Study is considered of limited relevance as the two isomers of the a.s. were examined separately. The study further suffers from unclear method descriptions.	N	3	**A3.1.1/03:** Wxxxx Rxxxx, Cxxxx Pxxxx (1985) Determination of the melting point and differential thermal analysis of the cis and trans isomers of the rodenticide WL108366. Sxxxx Rxxxx Lxxxx, Sxxxx, Uxxxx, Report No. SBRN.85.283, October 1985 (unpublished). (BASF-Ref.: FL-303-001)	
3.1.2	Boiling point	Guideline: not stated Differential scanning calorimetry (DSC)	99.4 % Batch No. AC12140-35 (pure active substance, PAI)	No boiling point was observed in two DSC runs at atmospheric pressure, but decomposition started at c. 280 °C.	Result is adopted from the study on the melting point and thermal stability (A3.1.1, A3.10). Therefore, guideline compliance is not stated. However, as DSC is a valid method for determining the boiling point, compliance to OECD guideline 103 and EC method A.2 can be assumed.	Y	1	Cross-reference: **A3.1.1/01**	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)		Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
		Guideline: not stated Differential scanning calorimetry (DSC)	98.6 % Batch No. M02 (technical grade active substance, TGAI)	No boiling point was observed in two DSC runs at atmospheric pressure, but decomposition started at c. 280 °C.	Result is adopted from the study on the melting point and thermal stability (A3.1.1, A3.10). Therefore, guideline compliance is not stated. However, as DSC is a valid method for determining the boiling point, compliance to OECD guideline 103 and EC method A.2 can be assumed.	Y	1	Cross-reference: **A3.1.1/02**	
3.1.3	Bulk density/ relative density	EC method A.3; OECD 109 Gay-Lussac pycnometer according to ISO 1183, method B.	99.4 % Batch No. AC12140-35 (pure active substance, PAI)	D_4^{20} = 1.40		Y	1	**A3.1.3/01:** Wxxxx Hxxxx (2001) Determination of the density of Flocoumafen (Reg. No. 4060804, CL# 183540, BAS 322 I) according to EC Council Directive 92/69/EEC, A.3 and OECD Guideline No. 109. Bxxxx Gxxxx, Kxxxx, Gxxxx, Report No. 01 50 40 229, December 19, 2001 (unpublished). (BASF-Ref.: 2001/1019645)	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.2 Vapour pressure (IIA3.2)	EC method A.4; OECD 104 Vapour pressure balance (effusion method)	99.4 % Batch No. AC12140-35 (pure active substance, PAI)	p (20 °C) < 1 × 10^{-3} Pa p (25 °C) < 1 × 10^{-3} Pa p (50 °C) < 1 × 10^{-3} Pa		Y	1	**A3.2/01:** Fxxxx Jxxxx (2001) Flocoumafen (Reg. No. 4060804, CL# 183540, BAS 322 I) – Vapour pressure. Sxxxx Axxxx, Fxxxx, Gxxxx, Report No. 20011316.01, December 17, 2001 (unpublished). (BASF-Ref.: 2001/1019644)	
3.2.1 Henry's Law Constant (IIA3.2)	Calculation based on vapour pressure and water solubility H = p × MW / c	Not applicable	H < 3.871 Pa × m^3/mol		n.a.	1	**A3.2/02:** Oxxxx Uxxxx (2002): Henry's law constant for flocoumafen. Bxxxx Axxxx, Report, February 14, 2002 (unpublished). (BASF-Ref.: 2002/1004465)	
	QSAR model calculation by bond contributions using program HENRYWIN (U.S. EPA)	Not applicable (model calculation)	H = 7.43 × 10^{-8} Pa × m^3/mol		n.a.	1	**A3.2/03:** Sxxxx Txxxx (2003) Model calculation of Henry's law constant of Flocoumafen. Exxxx Cxxxx Gxxxx, Hannover, Germany, Report no. BAS-030801-01, August 1, 2003 (unpublished)	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.3 Appearance (IIA3.3)								
3.3.1 Physical state	Not applicable	99.4 % Batch No. AC12140-35 (pure active substance, PAI)	Substance is a fine crystalline solid.		Y	1	Cross-reference: **A3.1.1/01**	X
3.3.2 Colour	Not applicable	99.4 % Batch No. AC12140-35 (pure active substance, PAI)	White		Y	1	Cross-reference: **A3.1.1/01**	X
3.3.3 Odour	Not applicable	99.4 % Batch No. AC12140-35 (pure active substance, PAI)	Odourless		Y	1	Cross-reference: **A3.1.1/01**	X

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.4 Absorption spectra (IIA3.4)								
UV/VIS (1)	OECD 101	99.4 % Batch No. AC12140-35 (pure active substance, PAI)	UV spectra were recorded in water at pH 6.8 and 12.8 (acidic pH not possible) and in methanol at pH 5.0 and 0.7 (as a substitute for acidic conditions in water). Above 290 nm, absorption maxima were recorded at approx. 310 nm (slightly variable depending on solvent and pH). Graphical representations are given in Figure A3- 1 to Figure A3- 3. Molar absorption coefficients at maxima above 290 nm were determined and are presented in detail in Table A3- 1.		Y	1	**A3.4/01:** Dxxxx Axxxx (2003) UV spectra of BAS 322I (Reg.No. 4060804, identical with CL 183540). Report No. 174136_1, Bxxxx Axxxx Cxxxx Lxxxx, Lxxxx, Gxxxx, September 29, 2003 (unpublished). (BASF-Ref.: 2003/1013886)	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
UV/VIS (2)	Standard spectroscopic method (UV/VIS)	Batch No.: AC 11303-85 Purity: 99.4 %	UV spectra in acetonitrile for the purified active substance (mixture of isomers), the cis- and the trans-isomer, respectively, are presented in Figure A3- 5 - Figure A3- 7. UV/VIS Spectra in aqueous solution for the purified active substance (mixture of isomers), are included in the original report but are omitted from this summary due to availability of more adequate data (see above, reference A3.4/01)		Y	1	**A3.4/02:** Yxxxx Zxxxx (2001): A spectral database for purified active ingredients CL 183540, CL 153080, and CL 153081. Bxxxx Axxxx Rxxxx, Pxxxx, Uxxxx, Report No. APBR 1187, August 28, 2001 (unpublished). (BASF-Ref.: FL-360-002)	X
IR	Standard spectroscopic method (IR)	Batch No.: AC 11303-85 Purity: 99.4 %	IR spectra for the purified active substance (mixture of isomers), the cis- and the trans-isomer, respectively, are presented in Figure A3- 8 - Figure A3- 10.		Y	1	**A3.4/02**	
NMR	Standard spectroscopic methods (NMR)	Batch No.: AC 11303-85 Purity: 99.4 %	NMR spectra for the purified active substance (mixture of isomers), the cis- and the trans-isomer, respectively, are presented in Figure A3- 11 - Figure A3- 16.		Y	1	**A3.4/02**	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
MS	Standard spectroscopic methods (MS)	Batch No.: AC 11303-85 Purity: 99.4 %	Mass spectra for the purified active substance (mixture of isomers), the cis- and the trans-isomer, respectively, are presented in Figure A3- 17 - Figure A3- 19.		Y	1	**A3.4/02**	
3.5 Solubility in water (IIA3.5)	EC method A.6; OECD 105 Column elution method with levelling vessel Support material: Chromosorb W/AW 60-80 mesh (Merck) Analysis by HPLC; l = 210 nm; mobile phase: CH_3CN : H_2O : HCOOH = 700: 300: 1;	99.4 % Batch No. AC12140-35 (pure active substance, PAI)	Temperature: 20 °C Solubility (mg/l ± SD) pH 4 0.0024 ± 0.00003 pH 7 0.114 ± 0.005 pH 9 14.0 ± 0.39 The solubility in deionised water was determined to be 0.14 ± 0.045 mg/l	The effect of temperature was not studied. However, in view of the molecular structure and the extremely low solubility at 20° C only negligible effects of temperature on water solubility are expected. Therefore, abandonment of investigating the effect of temperature seems justified.	Y	1	**A3.5/01:** Dxxxx Axxxx (2002) Determination of the solubility in water at 20 °C of Flocoumafen (PAI) (BAS 322 I, Reg. No. 4060804 identical with CL# 183540). Bxxxx Axxxx, Lxxxx, Gxxxx, Report No. PCP06477, February 1, 2002 (unpublished). (BASF-Ref.: 2002/1004203)	X

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.6 Dissociation constant (-)	OECD guideline 112 Furthermore: determination by solubility as cited in the guideline (Albert & Sergeant 1962).	99.4 % Batch No. AC12140-35 (pure active substance, PAI)	Due to the low solubility, none of the experimental methods was practicable for obtaining plausible results. Therefore, pK_a was estimated based on the solubility data determined in section A3.5 (see above) and on the intrinsic solubility of the neutral molecule (at pH = 2), S_i = 0.0012 mg/l. $pK_a = 4.5 \pm 0.4$		Y	1	**A3.6/01:** Dxxxx Axxxx (2002): Determination of the dissociation constant of Flocoumafen (PAI) BAS 322I (Reg. No. 4060804 identical with CL# 183540). Bxxxx Axxxx, Lxxxx, Gxxxx, Report No. PCP06478, February 21, 2002 (unpublished) (BASF-Ref.: 2002/1004543)	
	Calculation method based on the molecular structure: Program ACD/pK_a DB, version 4.06, Advanced Chemistry Development Inc.	Not applicable	$pK_a = 4.5 \pm 1.0$		n. a.	2	**A3.6/02:** Mxxxx Cxxxx (2001): Flocoumafen (BAS 322 I): Calculation of the dissociation constant, pK_a. Bxxxx Axxxx Rxxxx, Pxxxx, Uxxxx, Report No. ENV 01-022, March 30, 2001 (unpublished). (BASF-Ref.: FL-390-010)	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.7 Solubility in organic solvents, including the effect of temperature on solubility (IIIA3.1)	Adopted from OECD guideline 105 (water solubility) Shake flask method Analysis by HPLC; l = 210 nm; mobile phase: CH_3CN : H_2O : HCOOH = 700: 300: 1	98.6 % Batch No.: M02	No temperature effects were investigated The solubilities in eight solvents of different polarity are presented in Table A3- 2.		Y	1	**A3.7/01:** Dxxxx Axxxx (2002): Determination of the solubility in organic solvents at 20 °C of Flocoumafen (TGAI) (BAS 322 I Reg. No. 4060804 identical with CL# 183540). Bxxxx Axxxx, Lxxxx, Gxxxx, Report No. PCP06479, February 11, 2002 (unpublished). (BASF-Ref.: 2002/1004232)	X
3.8 Stability in organic solvents used in b.p. and identity of relevant breakdown products (IIIA3.2)				Not relevant, since organic solvents are not contained in a.s. or b.p.				

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.9 Partition coefficient n-octanol/water (IIA3.6)	EC method A.8; OECD guideline 107 Shake flask method	99.4 % Batch No. AC12140-35 (pure active substance, PAI)	Temperature: 20 °C pH 7: log P_{ow} = 6.12 pH 9: log P_{ow} = 5.11	log P_{ow} at pH 4 was not determined experimentally, as it can be assumed to be higher than 6.12, which lies beyond the ranges of applicability of the method.	Y	1	**A3.9/01:** Dxxxx Axxxx (2002): Determination of the octanol/water partition coefficient at 20 °C of Flocoumafen (PAI) (BAS 322 I Reg. No. 4060804 identical with CL 183540). Bxxxx Axxxx, Lxxxx, Gxxxx, Report No. PCP06597, February 1, 2002 (unpublished). (BASF-Ref.: 2002/1004233)	X
3.10 Thermal stability, identity of relevant breakdown products (IIA3.7)	OECD guideline 113 Differential scanning calorimetry	99.4 % Batch No. AC12140-35 (pure active substance, PAI)	Flocoumafen is stable under air and nitrogen up to 250 °C.		Y	1	Cross-reference: **A3.1.1/01**	X
3.11 Flammability, including auto-flammability and identity of combustion products (IIA3.8)	EC method A.10	99.9 % Batch No.: Floc 01	The substance could not be ignited. Therefore, burning time cannot be reported. Flocoumafen is not “highly flammable” according to the criteria of EC method A.10.		Y	1	**A3.11/01:** Kxxxx Hxxxx (1996): Determination of the flammability of Flocoumafen, TM. Nxxxx Bxxxx, Sxxxx, Nxxxx, Report No. 165959, January 9, 1996 (unpublished). (BASF-Ref.: FL-330-002)	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
	EC method A.16	99.9 % Batch No.: Floc 01	No self-ignition of the test substance was observed.		Y	1	**A3.11/02:** Kxxxx Hxxxx (1996) Determination of the self-ignition temperature of Flocoumafen, TM. Nxxxx Bxxxx, Sxxxx, Nxxxx, Report No. 165961, January 9, 1996 (unpublished). (BASF-Ref.: FL-330-001)	X
3.12 Flash-point (IIA3.9)				Not relevant Data are only required for liquids with ignitable vapours.				
3.13 Surface tension (IIA3.10)				EC method A.5 expressly states that the surface tension of a compound need not to be determined if the water solubility is lower than 1 mg/l. In view of the results reported under 3.5 above, experimental determination of the surface tension is not considered to be required.				

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.14 Viscosity (-)				Not applicable The substance is solid, which is why viscosity cannot be determined.				
3.15 Explosive properties (IIA3.11)	Model calculation (program CHETAH 7.2)	Not applicable (model calculation)	Maximum heat of decomposition = –508 cal/g Difference between Heat of Combustion and Heat of Decomposition = –6351 cal/g Oxygen balance = –215 % In conclusion, structural aspects and estimated thermodynamic properties indicate that Flocoumafen need not be considered to have explosive properties.	In EC method A.14, it is expressly mentioned that an experimental determination of the explosivity of a compound is not required, if available thermodynamic data (reaction enthalpies) and/or the absence of certain reactive groups in the structural formula indicate that the substance will not decompose violently under formation of gases or release of energy (and thus does not pose a risk for explosivity). Thus, the conduct of further experimental verification is not considered to be required.	n. a.	1	**A3.15/01:** Bxxxx Rxxxx (2004) Explosivity of flocoumafen technical. Exxxx Cxxxx Gxxxx, Hxxxx, Gxxxx, Report No. BASF-040112-01, January 13, 2004 (unpublished).	

Section A3 Physical and Chemical Properties of Active Substance

Subsection (Annex Point)	Method	Purity/ Specification	Results	Remarks/ Justification	GLP (Y/N)	Reliability	Reference	Official use only
3.16 Oxidizing properties (IIA3.12)	Model calculation (program CHETAH 7.2)	Not applicable (model calculation)	Maximum heat of decomposition = –508 cal/g Difference between Heat of Combustion and Heat of Decomposition = –6351 cal/g Oxygen balance = –215 % In conclusion, structural aspects and estimated thermodynamic properties indicate that Flocoumafen need not be considered to have oxidising properties.	In EEC method A.17, it is expressly mentioned that an experimental determination of the oxidising properties of a compound is not required if available thermodynamic data and the absence of certain reactive groups in the structural formula indicate that the substance will not react exothermally with combustible material. Thus, the conduct of further experimental verification is not considered to be required.	n. a.	1	**A3.16/01:** Bxxxx Rxxxx (2004) Oxidising properties of flocoumafen technical. Exxxx Cxxxx Gxxxx, Hxxxx, Gxxxx, Report No. BASF-040112-02, January 13, 2004 (unpublished).	
3.17 Reactivity towards container material (IIA3.13)	Not applicable	Typical for technical grade material	Lupolen is used as packaging material. To date, corrosiveness towards packaging material, containers, and apparatus has not been observed.		n. a.	1	**A3.17/01:** Kxxxx (2001): Corrosiveness of Flocoumafen. Bxxxx Axxxx, Lxxxx, Gxxxx, Report No. 2001/1017474, August 23, 2001 (unpublished). (BASF-Ref.: 2001/1017474)	

Evaluation by Competent Authorities	
Use separate "evaluation boxes" to provide transparency as to the comments and views submitted	
	EVALUATION BY RAPPORTEUR MEMBER STATE (*)
Date	22 April 2005
Materials and Methods	(3.3.1) Data for the TGAI (Batch No. M02) are given in reference A.3.1.1/02 (3.3.2) Data for the TGAI (Batch No. M02) are given in reference A.3.1.1/02 (3.3.3) Data for the TGAI (Batch No. M02) are given in reference A.3.1.1/02 (3.4) The batch no. and purity of trans and cis references in A3.4/02 were AC9771-103B, purity 96.4% and AC9771-103A, purity 99.6%, respectively. (3.5) The BASF reference for A3.5/01 should read 2002/1004206 (3.7) The study was performed with the TGAI and not with PAI. This is considered acceptable because the purity of the TGAI was > 98%. The solubilities were determined at 20°C. The following major guideline deviations were observed: (1) the initial concentration did not exceed sufficiently the saturated concentration for the solvents EtAc, DCM, ACN and acetone, and (2) steady state was not reached for the solvent n-heptane. (3.11) The BASF reference for A3.11/02 should read FL-332-001. The following was added by the RMS: The cis/trans ratio of batch Floc01 is 53/47.
Results and discussion	(3.3.1) Physiscal state for the TGAI (Batch No. M02): fine crystalline solid (3.3.2) Colour for the TGAI (Batch No. M02): white (3.3.3) Odour for the TGAI (Batch No. M02): odourless (3.10) The following was added by the RMS: "Flocoumafen is ….. up to 250°C, *when decomposition started*" (3.11) The following was added by the RMS: "No self-ignition …. was observed, *up to 400°C*"
Conclusion	-
Reliability	2
Acceptability	Acceptable, with the exception of (3.7) for the solvents EtAc, DCM, ACN, acetone and n-heptane.

Remarks	The cis/trans ratio of batch AC12140-35 (PAI) is 59/41 (ratio's of this batch were reported as part of the study regarding degradation in soil; reference A7.2.1/02) The cis/trans ratio of batch AC 11303-85 is 58.96%/40.97%. A separate certificate of analysis was provided. For batch M02 (TGAI) the cis/trans ratio was not reported. This is considered acceptable because, as emphasised by the notifier, the batch was produced according to the same manufacturing process as all other batches tested which all comply with the specification of the active substance flocoumafen. The comment by the notifier seems to be supported by the results of the melting point determination for which two studies are available; one based on batch M02 and one based on batch AC12140-35 (cis/trans 59/41).
	COMMENTS FROM ...
Date	
Materials and Methods	
Results and discussion	
Conclusion	
Reliability	
Acceptability	
Remarks	

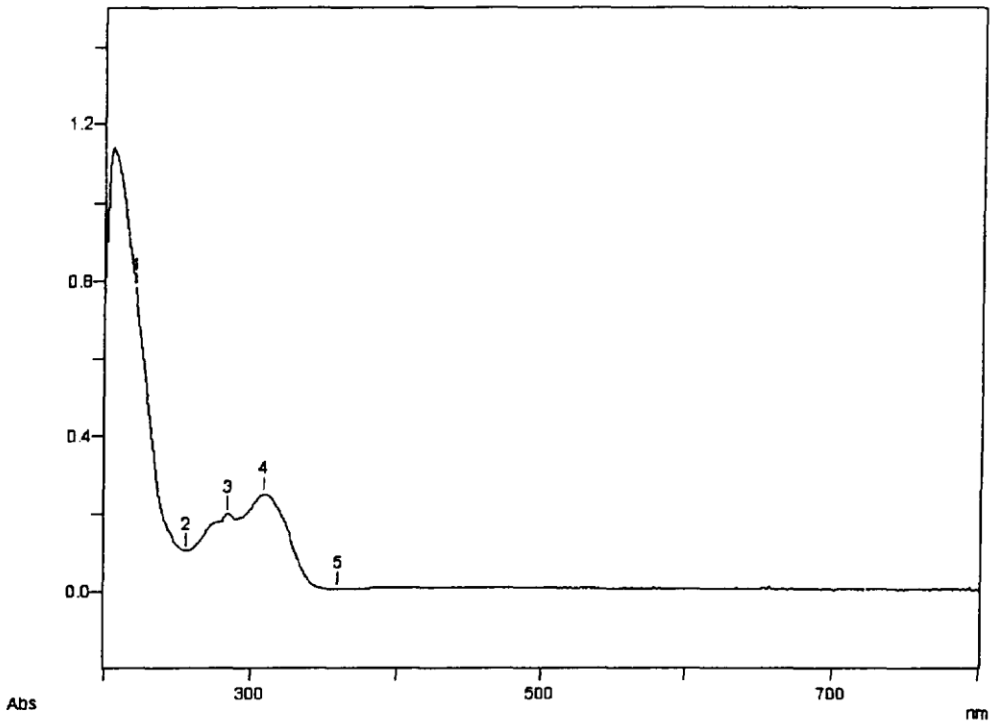

Figure A3- 1: UV/VIS spectrum of Flocoumafen in Methanol (pH = 5.0).

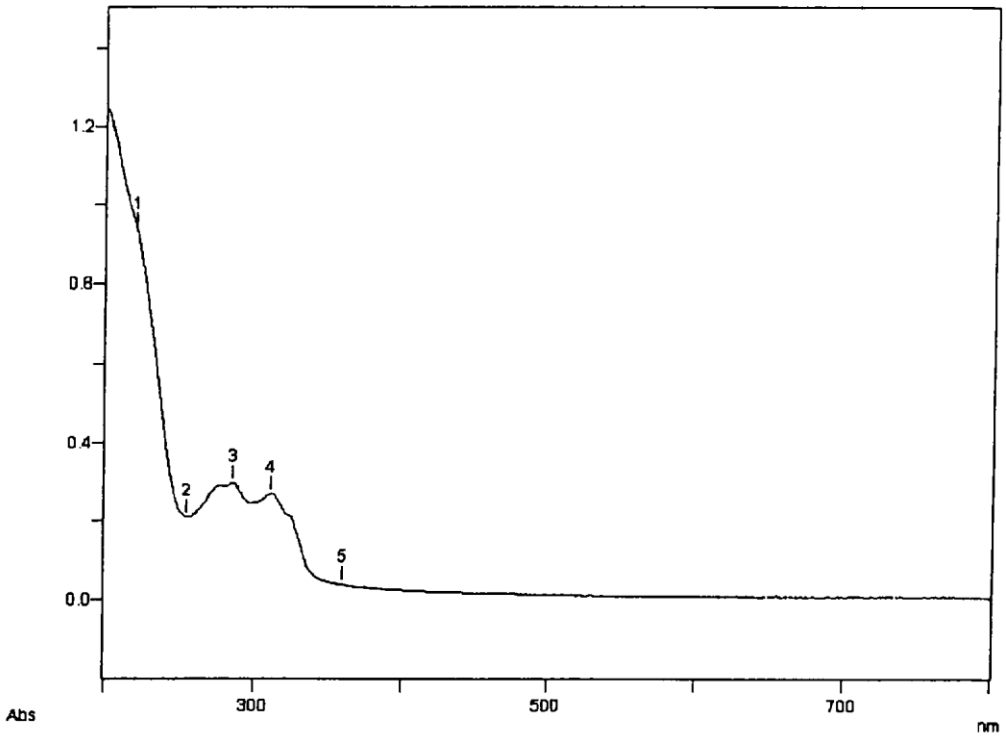

Figure A3- 2: UV/VIS spectrum of Flocoumafen in aqueous solution (pH = 6.8).

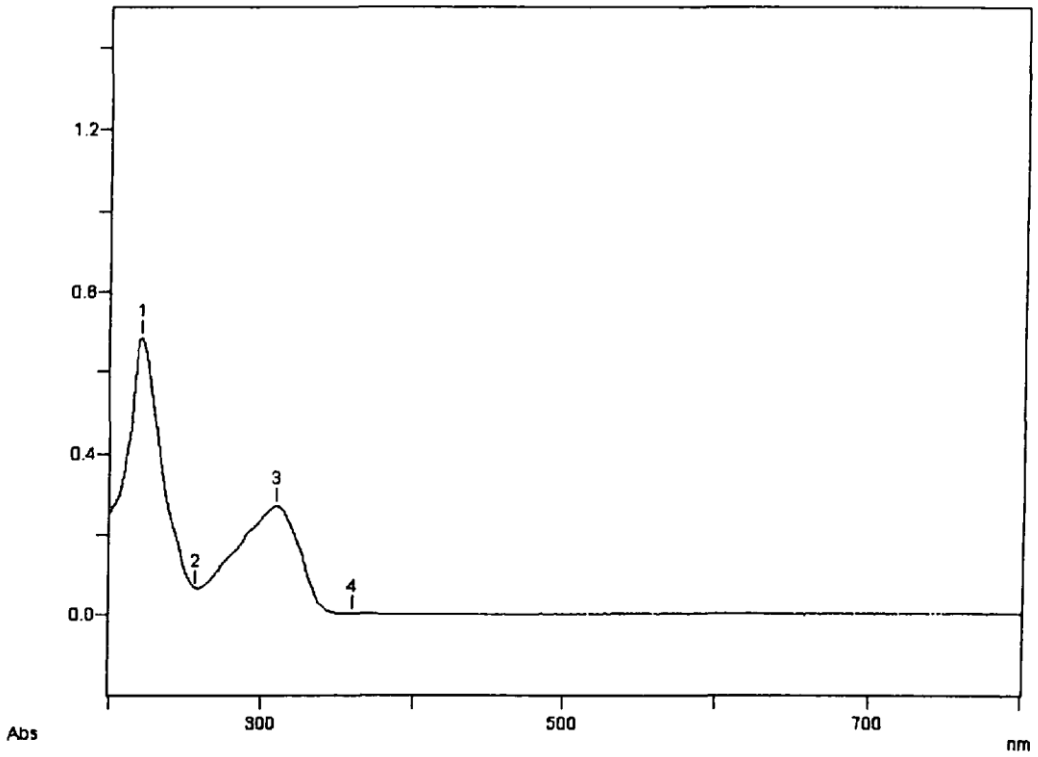

Figure A3- 3: UV/VIS spectrum of Flocoumafen in aqueous solution (pH = 12.8).

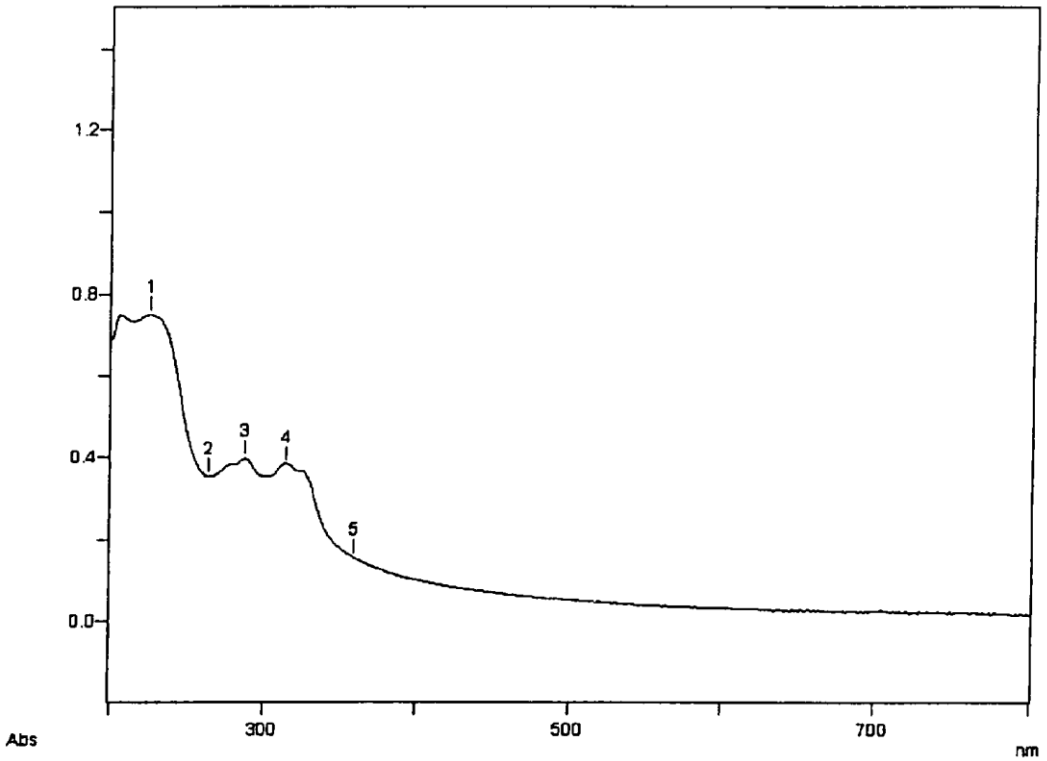

Figure A3- 4: UV/VIS spectrum of Flocoumafen in Methanol (pH = 0.7).

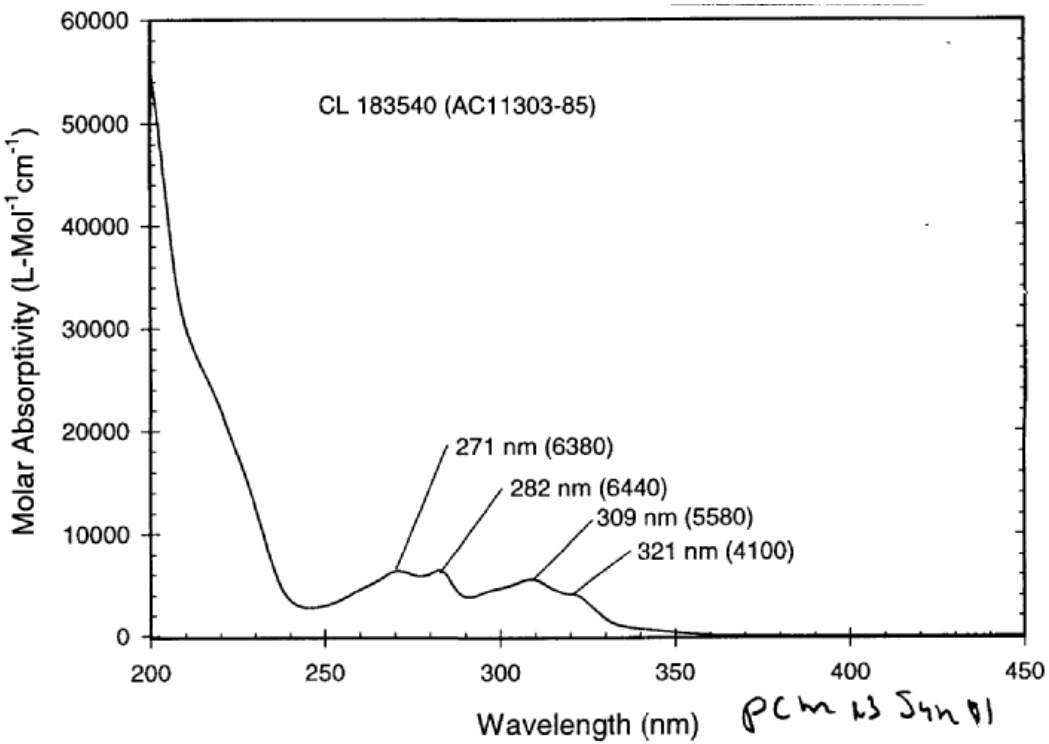

Figure A3- 5: UV spectrum of flocoumafen (mixture of cis- and trans-isomers) in acetonitrile.

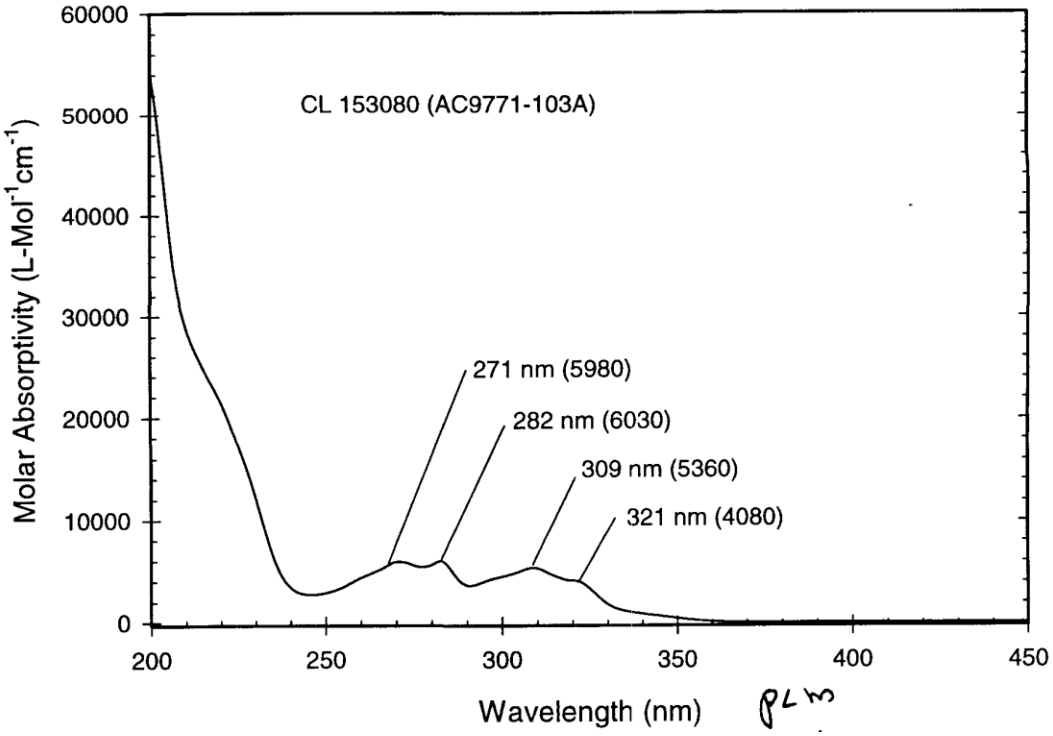

Figure A3- 6: UV spectrum of flocoumafen (cis-isomer) in acetonitrile.

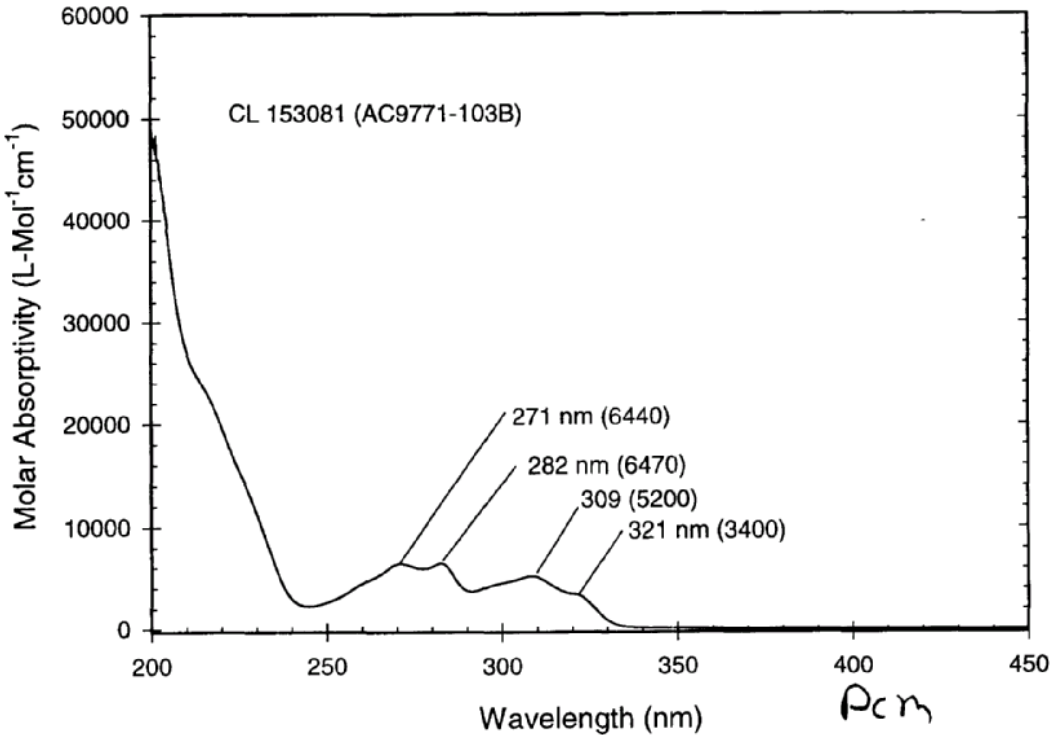

Figure A3- 7: UV spectrum of flocoumafen (trans-isomer) in acetonitrile.

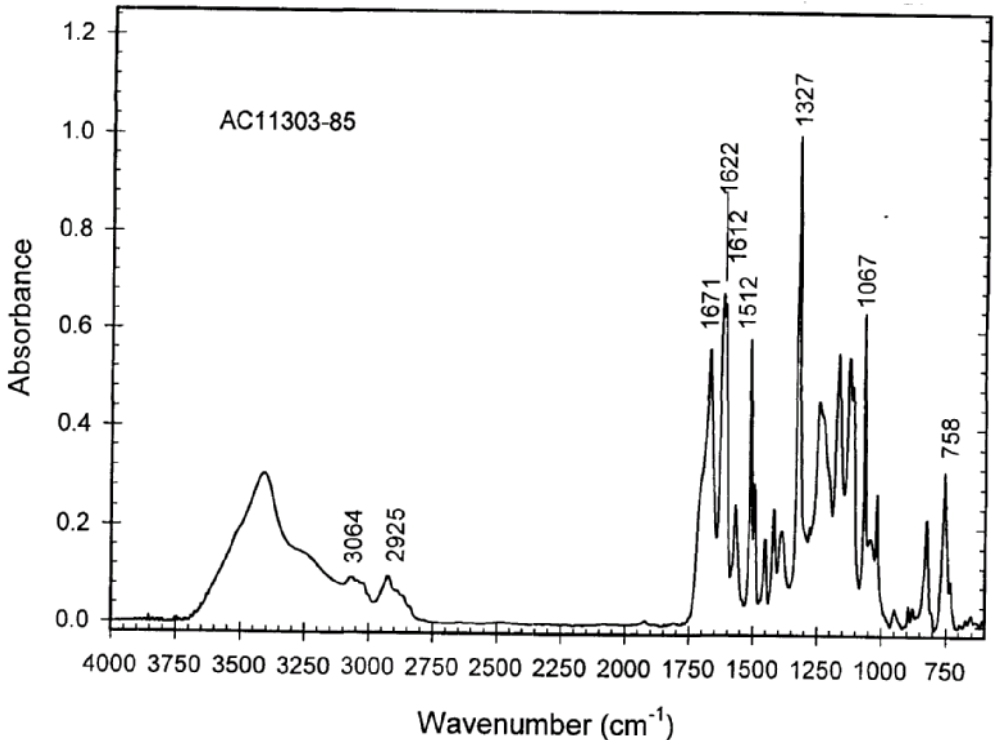

Figure A3- 8: Fourier transform infrared spectrum of flocoumafen (mixture of cis- and trans-isomer).

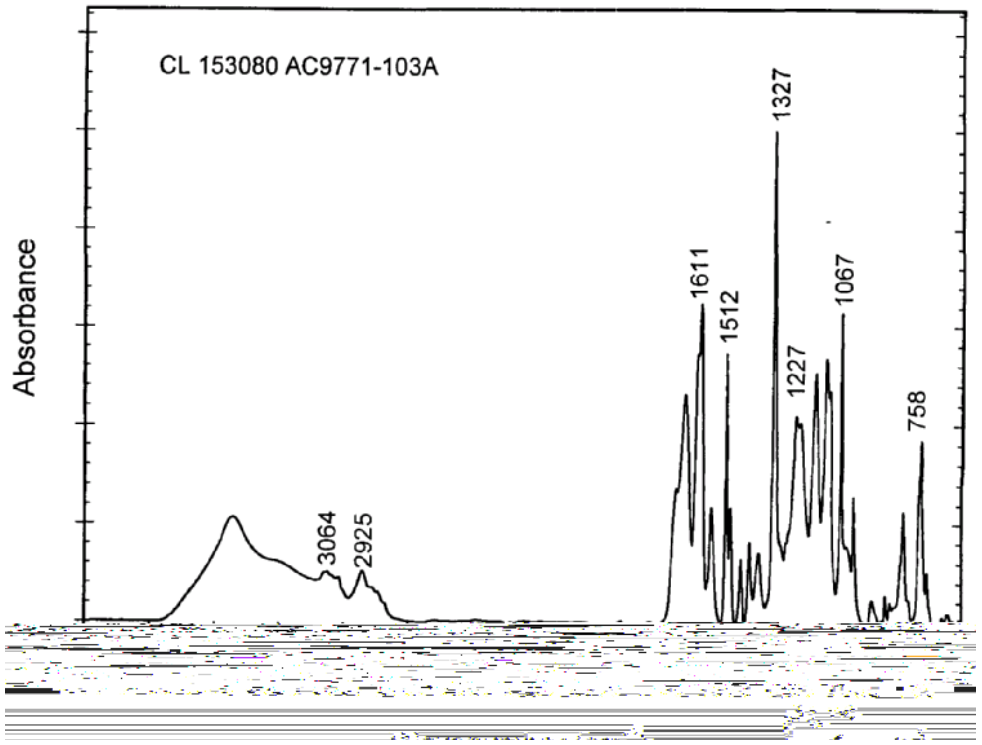

Figure A3- 9: Fourier transform infrared spectrum of flocoumafen (cis-isomer).

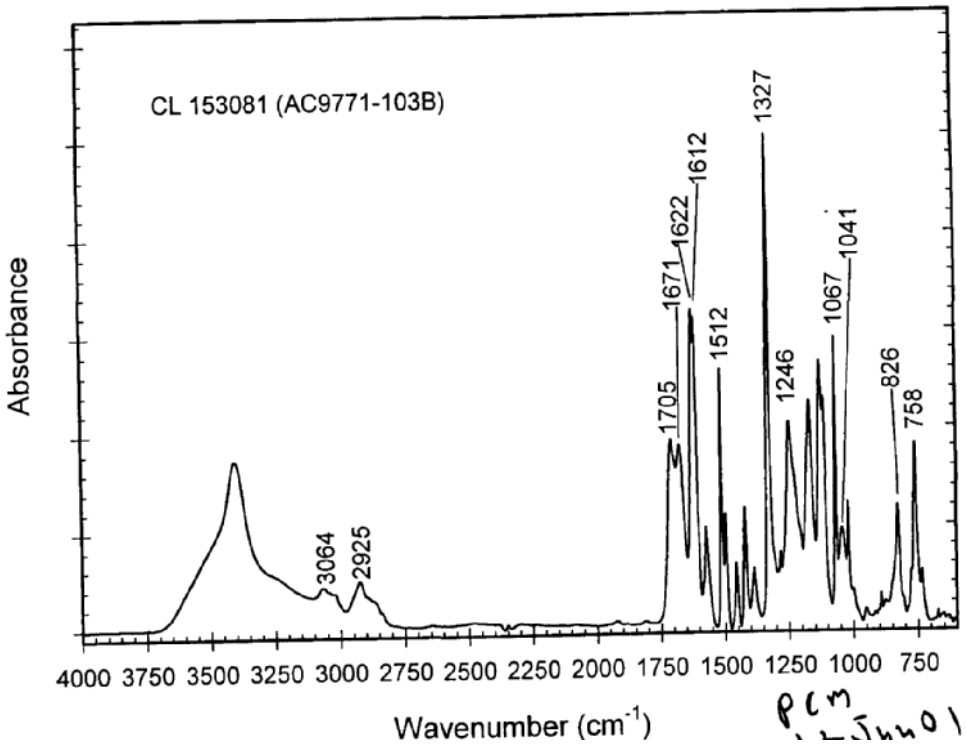

Figure A3- 10: Fourier transform infrared spectrum of flocoumafen (trans-isomer).

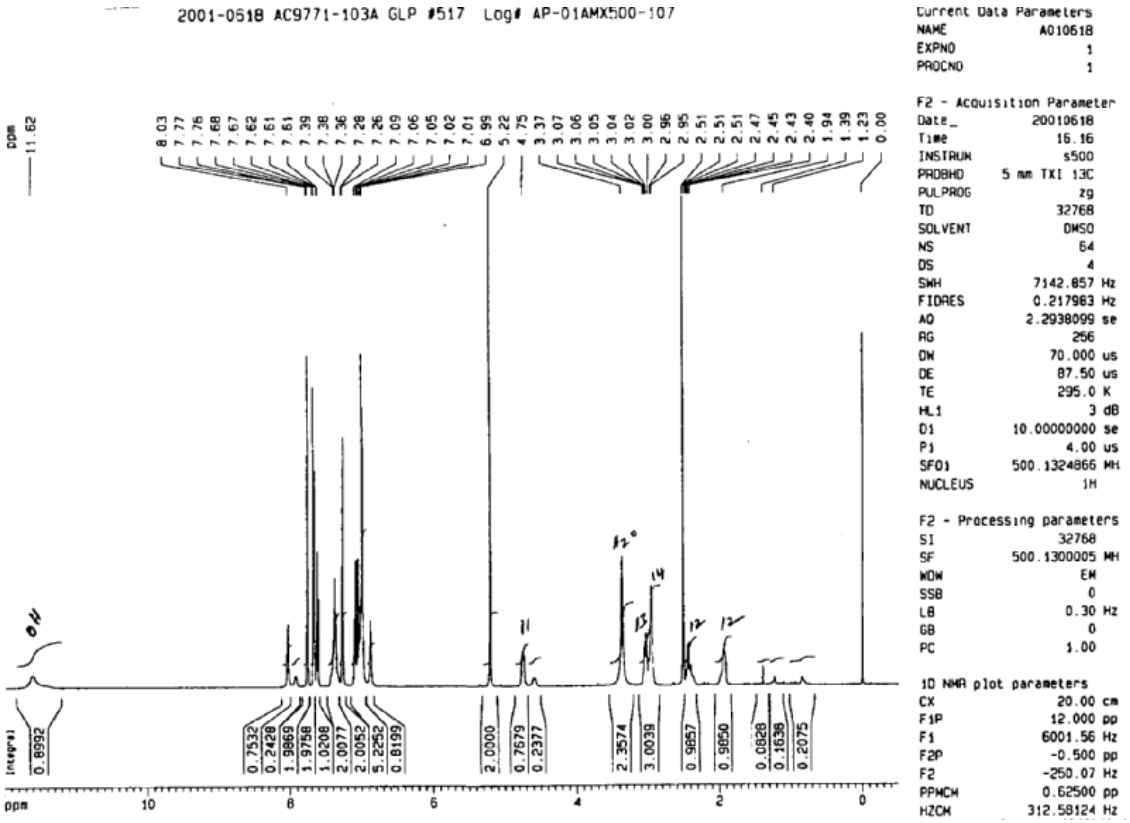

Figure A3- 11: Proton-NMR spectrum of flocoumafen (mixture of cis- and trans-isomer) in d_6-DMSO.

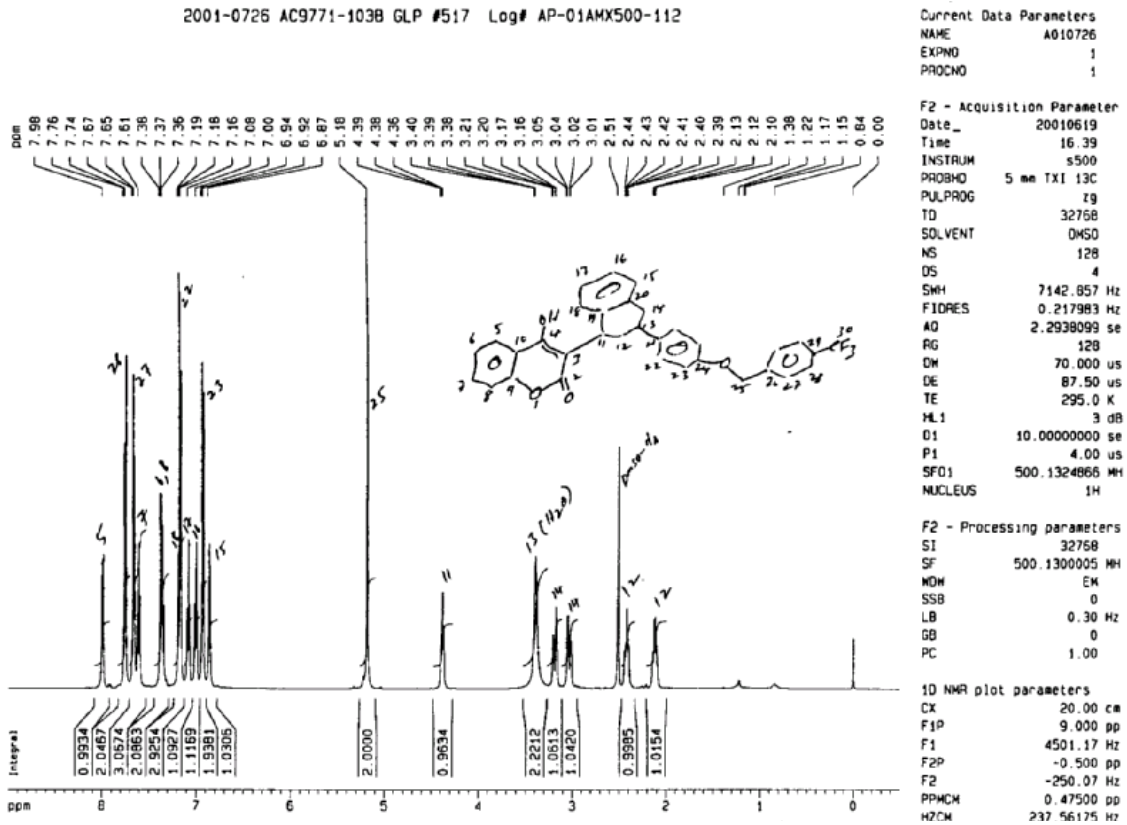

Figure A3- 12: Proton-NMR spectrum of flocoumafen (cis-isomer) in d_6-DMSO.

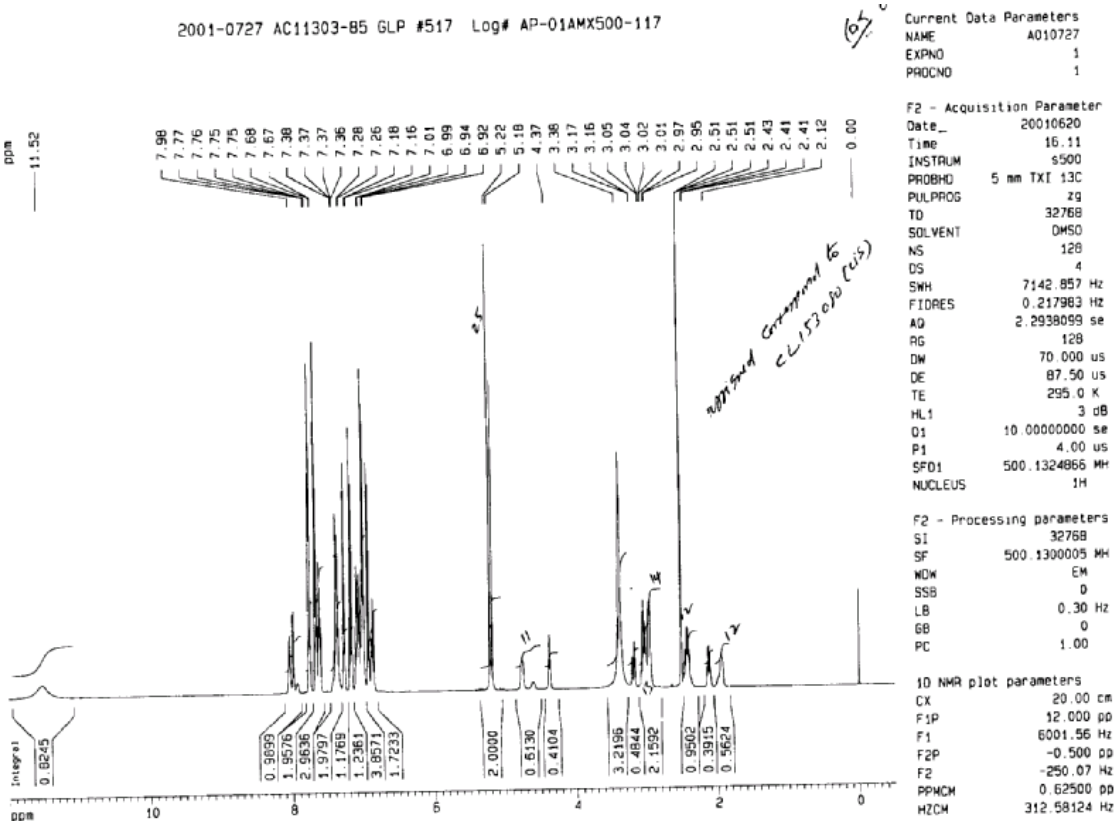

Figure A3- 13: Proton-NMR spectrum of flocoumafen (trans-isomer) in d_6-DMSO.

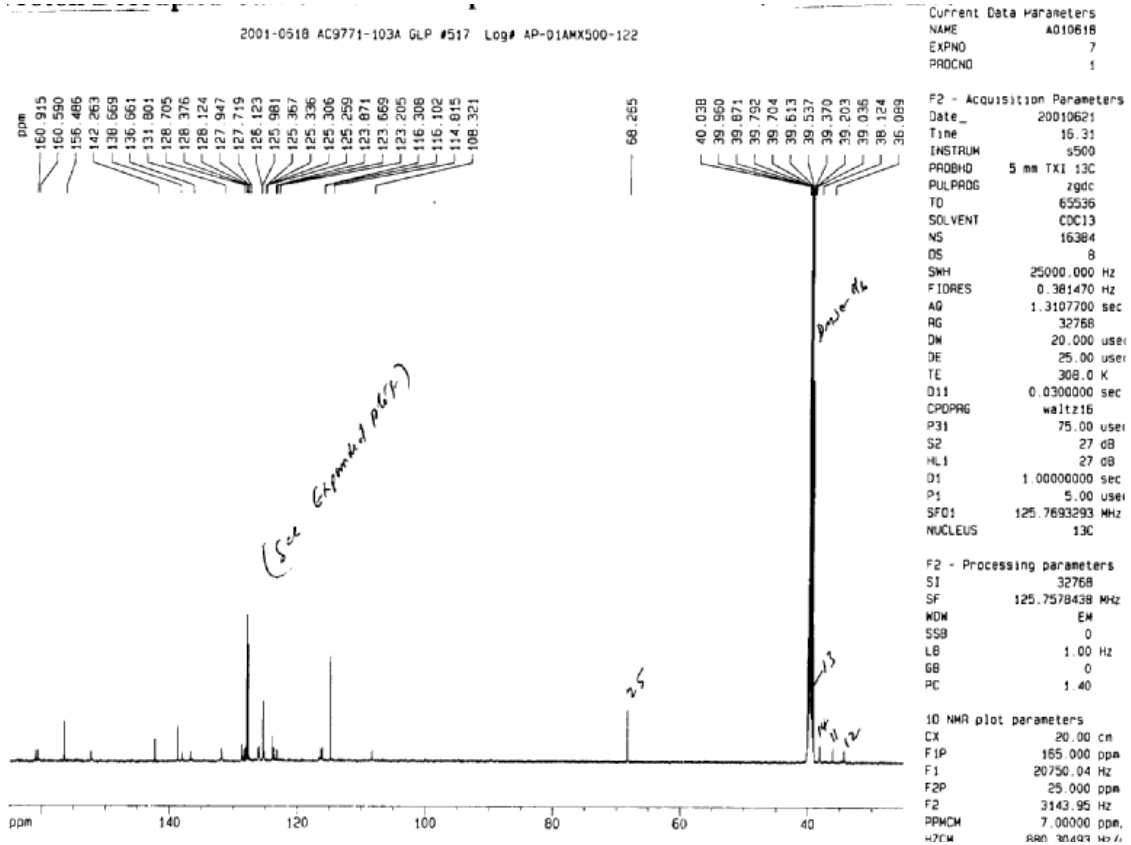

Figure A3- 14: Proton-decoupled ^{13}C-NMR spectrum of flocoumafen (mixture of cis- and trans-isomers) in $CDCl_3$.

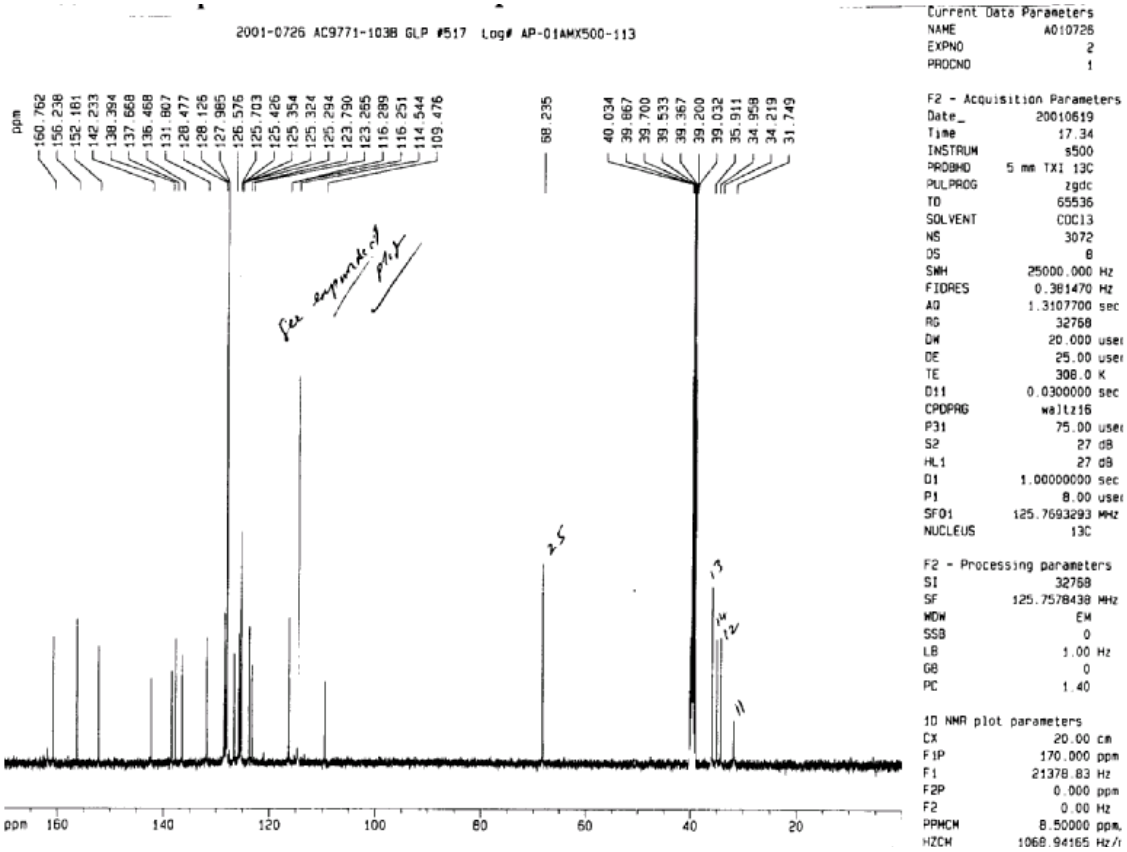

Figure A3- 15: Proton-decoupled ^{13}C-NMR spectrum of flocoumafen (cis-isomer) in $CDCl_3$.

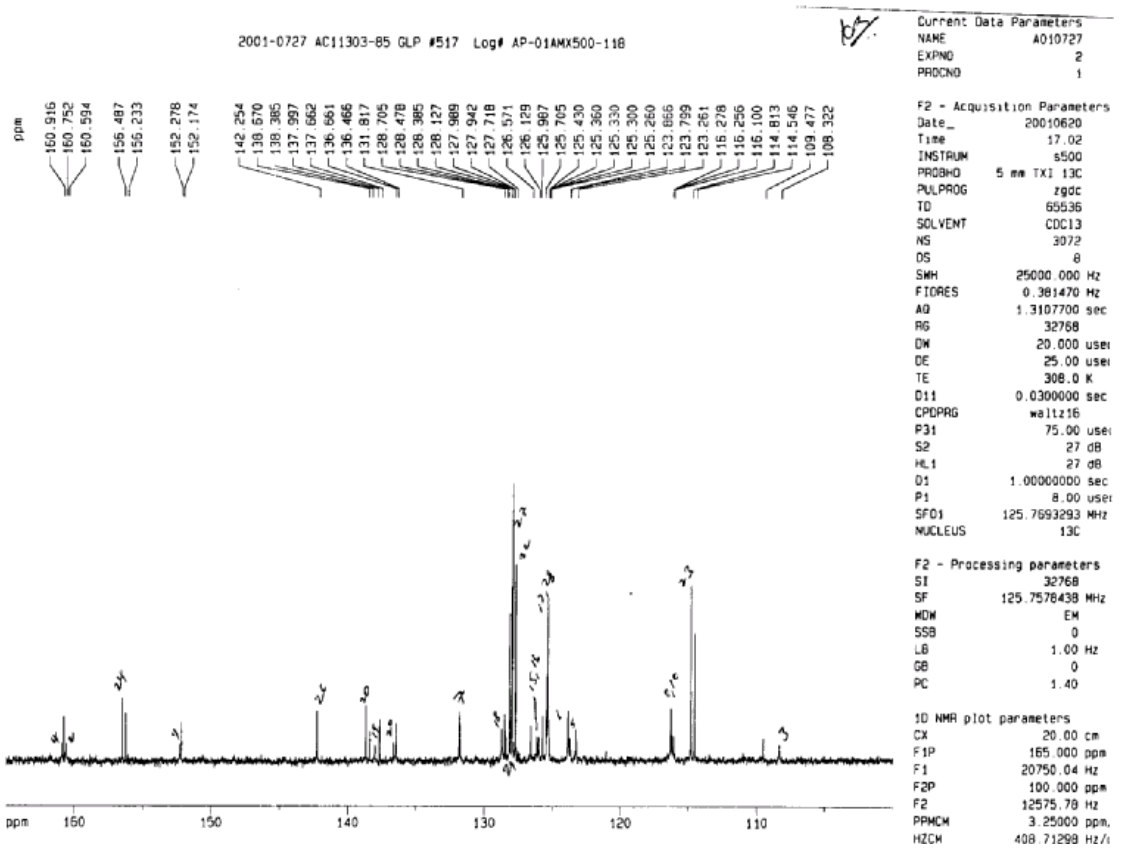

Figure A3- 16: Proton-decoupled ^{13}C-NMR spectrum of flocoumafen (trans-isomer) in $CDCl_3$.

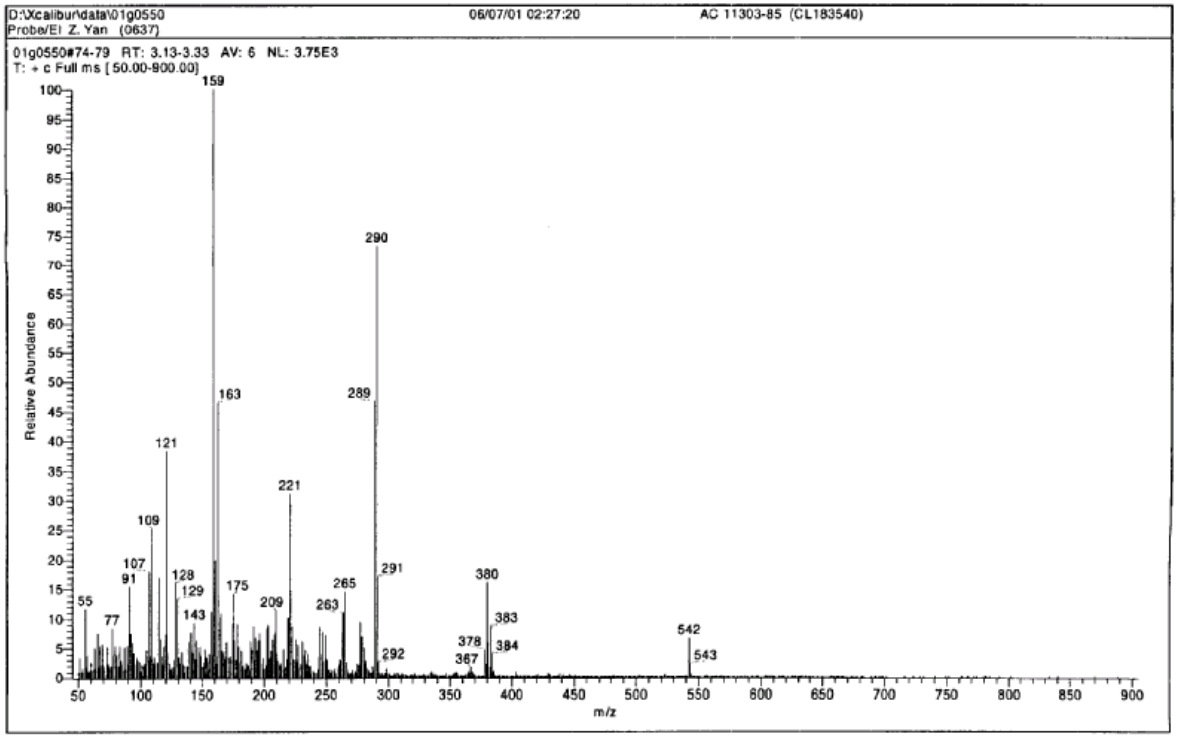

Figure A3- 17: Electron ionisation mass spectrum for flocoumafen, mixture of cis- and trans-isomers as used in the technical material.

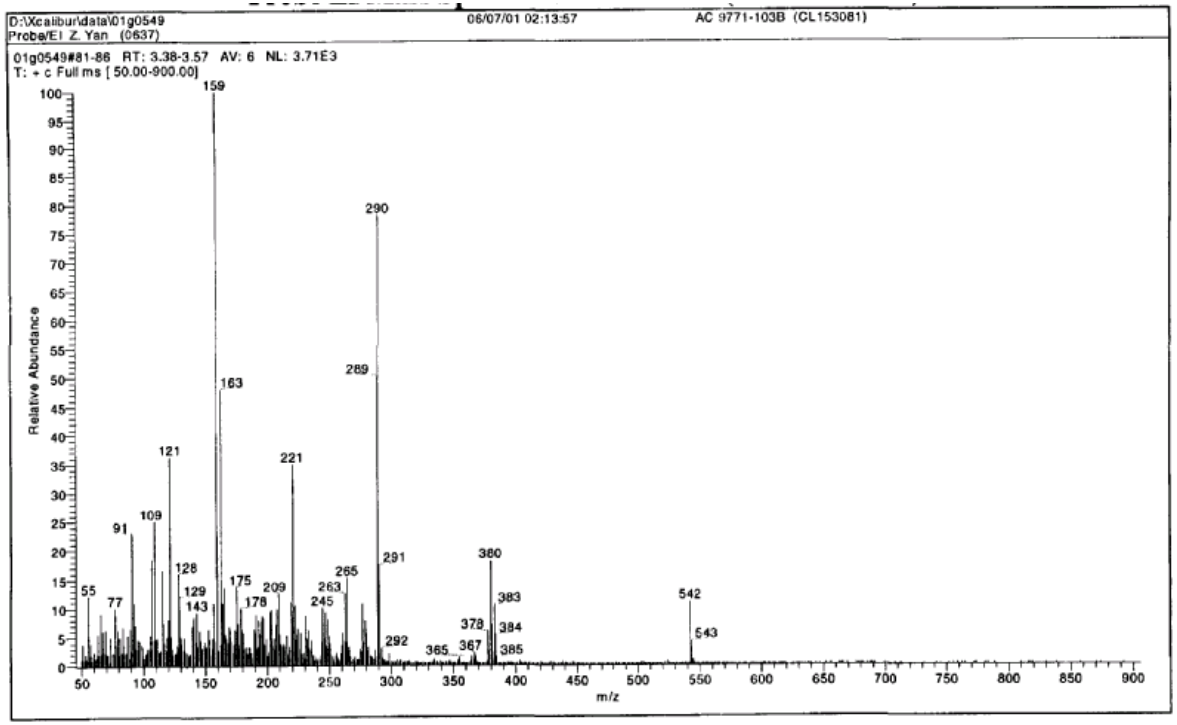

Figure A3- 18: Electron ionisation mass spectrum for flocoumafen, cis-isomer.

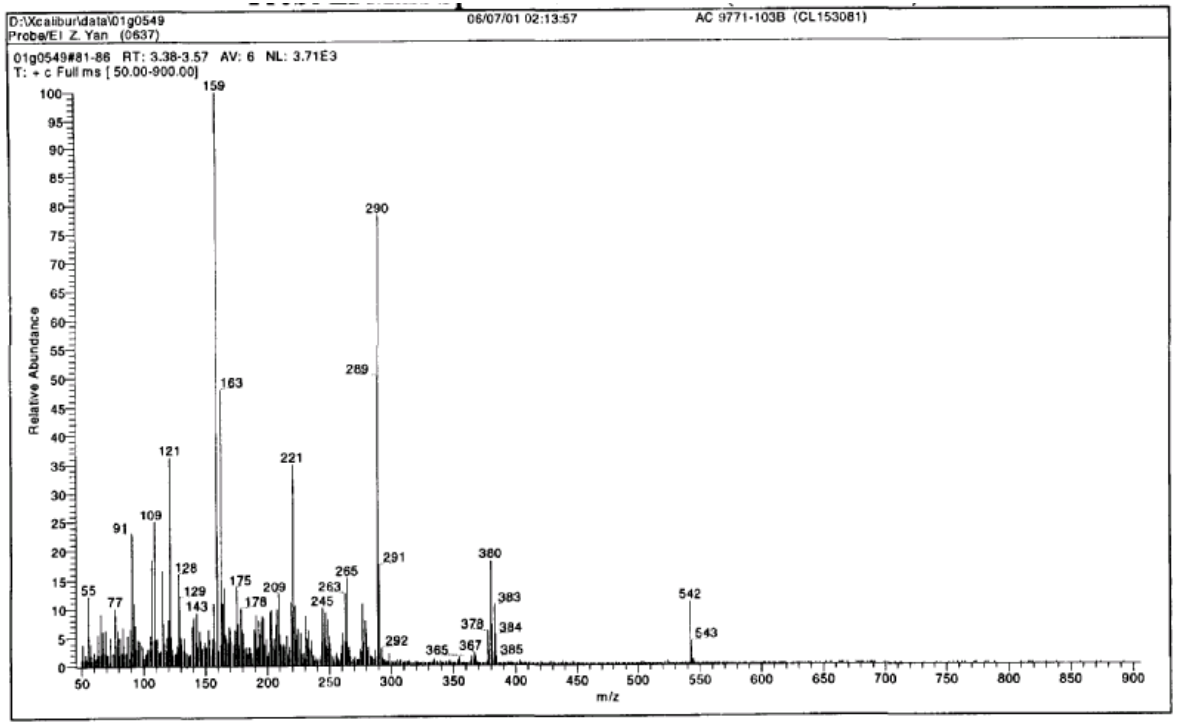

Figure A3- 19: Electron ionisation mass spectrum for flocoumafen, trans-isomer.

Table A3- 1: Molar extinction coefficients (ε) of flocoumafen at various pH conditions.

pH	Solvent	λ [nm]	ε [l × mol^{-1} × cm^{-1}]
5.0	Methanol	308.7	13173
0.7	Methanol	314.6	20291
6.8	Water	311.2	14162
12.8	Water	309.5	14326

Table A3- 2: Solubility of flocoumafen in eight organic solvents of different polarity. Concentrations refer to volume of pure solvent.

Solvent	Solubility (g/100 ml)
Methanol	1.41
Toluene	3.13
n-Octanol	1.74
n-Heptane	0.032
Ethyl-acetate	5.98
Dichloromethane	14.6
Acetonitrile	1.37
Acetone	35.0