Appendix F. EPI Suite v.4.1 Output File for Brodifacoum

```
CAS Number: 056073-10-0
SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM   : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
----------------------------- EPI SUMMARY (v4.10) -------------------------
 Physical Property Inputs:
    Log Kow (octanol-water):   8.50
    Boiling Point (deg C)  :   ------
    Melting Point (deg C)  :   230.00
    Vapor Pressure (mm Hg) :   ------
    Water Solubility (mg/L):   0.0038
    Henry LC (atm-m3/mole) :   ------

KOWWIN Program (v1.68) Results:
===============================

                  Log Kow(version 1.68 estimate): 8.51

Experimental Database Structure Match:
  Name     :  Brodifacoum
  CAS Num  :  056073-10-0
  Exp Log P:  8.50
  Exp Ref  :  TOMLIN,C (1997)

SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM   : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
-------+-----+-----------------------------------------+---------+--------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
-------+-----+-----------------------------------------+---------+--------
 Frag  |  2  |  -CH2-   [aliphatic carbon]             | 0.4911  |  0.9822
 Frag  |  2  |  -CH     [aliphatic carbon]             | 0.3614  |  0.7228
 Frag  |  2  |  =CH- or =C<  [olefinc carbon]          | 0.3836  |  0.7672
 Frag  | 24  |  Aromatic Carbon                        | 0.2940  |  7.0560
 Frag  |  1  |  -Br     [bromine, aromatic attach]     | 0.8900  |  0.8900
 Frag  |  1  |  -C(=O)O  [ester, aliphatic attach]     |-0.9505  | -0.9505
 Frag  |  1  |  -OH      [alcohol, olefinic attach]   |-0.8855  | -0.8855
 Factor|  1  |  Cyclic ester [olefinic type] correction|-0.2969  | -0.2969
 Const |     |  Equation Constant                      |         |  0.2290
-------+-----+-----------------------------------------+---------+--------
                                                     Log Kow   =   8.5143



MPBPVP (v1.43) Program Results:
===============================
Experimental Database Structure Match:
  Name     :  Brodifacoum
  CAS Num  :  056073-10-0
  Exp MP (deg C):  230
  Exp BP (deg C):  ---
  Exp VP (mm Hg):  ---

SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
```

CHEM   : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
---------- SUMMARY MPBVP v1.43 ----------

Boiling Point: 691.46 deg C (Adapted Stein and Brown Method)

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 290.08 deg C (Gold and Ogle Method)
Mean Melt Pt : 319.96 deg C (Joback; Gold,Ogle Methods)
  Selected MP: 302.03 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
  (Using BP: 691.46 deg C (estimated))
  (Using MP: 230.00 deg C (user entered))
    VP: 6.64E-027 mm Hg (Antoine Method)
      : 8.85E-025 Pa (Antoine Method)
    VP: 1.11E-018 mm Hg (Modified Grain Method)
      : 1.48E-016 Pa (Modified Grain Method)
    VP: 5.46E-015 mm Hg (Mackay Method)
      : 7.28E-013 Pa (Mackay Method)
  Selected VP: 1.11E-018 mm Hg (Modified Grain Method)
             : 1.48E-016 Pa (Modified Grain Method)
  Subcooled liquid VP: 1.77E-016 mm Hg (25 deg C, Mod-Grain method)
                     : 2.36E-014 Pa (25 deg C, Mod-Grain method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	2	-CH2- (ring)	26.44	52.88
Group	2	>CH- (ring)	21.66	43.32
Group	2	=C< (ring)	28.19	56.38
Group	1	-OH (alcohol)	106.27	106.27
Group	16	CH (aromatic)	28.53	456.48
Group	6	-C (aromatic)	30.76	184.56
Group	2	C (3a aromatic)	45.46	90.92
Group	1	-COO- (ring)	172.49	172.49
Group	1	-Br (to aromat)	61.85	61.85
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		1423.33
RESULT- corr		BOILING POINT in deg Kelvin		964.62
		BOILING POINT in deg C		691.46

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	2	-CH2- (ring)	7.75	15.50
Group	2	>CH- (ring)	19.88	39.76
Group	2	=C< (ring)	37.02	74.04
Group	1	-OH (alcohol)	44.45	44.45
Group	16	CH (aromatic)	8.13	130.08
Group	6	-C (aromatic)	37.02	222.12
Group	2	C (3a aromatic)	37.02	74.04
Group	1	-COO- (ring)	53.60	53.60
Group	1	-Br (to aromat)	43.43	43.43
*		Equation Constant		122.50

```
   RESULT    |  MELTING POINT in deg Kelvin  |  819.52
 RESULT-limit|  MELTING POINT in deg Kelvin  |  623.00
             |  MELTING POINT in deg C       |  349.84
-------------------------------------------------------
```

```
Water Sol from Kow (WSKOW v1.42) Results:
=========================================

          Water Sol: 5.276e-006 mg/L

Experimental Water Solubility Database Match:
  Name     :  Brodifacoum
  CAS Num  :  056073-10-0
  Exp WSol :  0.0038 mg/L (20 deg C)
  Exp Ref  :  TOMLIN,C (1997); pH 5.2

SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM   : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
---------------------------------- WSKOW v1.42 Results ------------------------
Log Kow  (estimated)  :  8.51
Log Kow (experimental):  8.50
    Cas No: 056073-10-0
    Name  : Brodifacoum
    Refer : TOMLIN,C (1997)
Log Kow used by Water solubility estimates:  8.50 (user entered)

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction

      Melting Pt (Tm) = 230.00 deg C (Use Tm = 25 for all liquids)

      Correction(s):         Value
      --------------------   -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -10.997
   Water Solubility at 25 deg C (mg/L):  5.276e-006



WATERNT Program (v1.01) Results:
================================

                  Water Sol (v1.01 est): 6.8599e-007 mg/L

Experimental Water Solubility Database Match:
  Name     :  Brodifacoum
  CAS Num  :  056073-10-0
  Exp WSol :  0.0038 mg/L (20 deg C)
  Exp Ref  :  TOMLIN,C (1997); pH 5.2

SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM   : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
-------+-----+---------------------------------------------+----------+---------
```

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH [aliphatic carbon]	-0.5285	-1.0570
Frag	2	=CH- or =C< [olefinc carbon]	-0.3646	-0.7292
Frag	16	Aromatic Carbon (C-H type)	-0.3359	-5.3738
Frag	1	-Br [bromine, aromatic attach]	-0.5661	-0.5661
Frag	1	-C(=O)O [ester, aliphatic attach]	0.5757	0.5757
Frag	8	Aromatic Carbon (C-substituent type)	-0.5400	-4.3196
Frag	2	-CH2- [aliphatic carbon, cyclic]	-0.3308	-0.6617
Frag	1	-OH [alcohol, olefinic attach]	0.0000	0.0000
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -11.8825
Water Solubility (mg/L) at 25 dec C =6.8599e-007

ECOSAR Program (v1.00) Results:
==========

SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM : Brodifacoum
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
Log Kow: 8.51 (KowWin estimate)
Melt Pt: 230.00 deg C
Wat Sol: 0.0038 mg/L (measured)

ECOSAR v1.00 Class(es) Found

Acrylates
Vinyl/Allyl Alcohols

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Acrylates	Fish	96-hr	LC50	0.196 *
Acrylates	Daphnid	48-hr	LC50	0.158 *
Acrylates	Green Algae	96-hr	EC50	0.821 *
Acrylates	Fish	30-day	ChV	0.000247
Acrylates	Daphnid		ChV	0.000599 !
Acrylates	Green Algae		ChV	0.062 *
Acrylates	Fish (SW)	96-hr	LC50	0.217 *
Acrylates	Mysid Shrimp (SW)	96-hr	LC50	0.006 *
Acrylates	Fish (SW)		ChV	0.007 *!
Acrylates	Mysid Shrimp (SW)		ChV	1.51e-007 !
Vinyl/Allyl Alcohols	Fish	96-hr	LC50	1.735 *
Vinyl/Allyl Alcohols	Daphnid	48-hr	LC50	0.527 *
Vinyl/Allyl Alcohols	Green Algae	96-hr	EC50	0.035 *
Vinyl/Allyl Alcohols	Fish		ChV	0.000159 !
Vinyl/Allyl Alcohols	Daphnid		ChV	0.000755 !
Vinyl/Allyl Alcohols	Green Algae		ChV	0.022 *
Neutral Organic SAR (Baseline Toxicity)	Fish	96-hr	LC50	0.00124
	Daphnid	48-hr	LC50	0.00157
	Green Algae	96-hr	EC50	0.010 *

: Fish	ChV	0.000102	
: Daphnid	ChV	0.000459	
: Green Algae	ChV	0.012	*

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Note: ! = exclamation designates: The toxicity value was determined from a predicted SAR using established acute-to-chronic ratios and ECOSAR regression techniques which are documented in the supporting Technical Reference Manual. When possible, this toxicity value should be considered in a weight of evidence approach.

Acrylates:

For Fish, Daphnid and Mysid Shrimp Acute Toxicity Values: If the log Kow of the chemical is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000

Vinyl/Allyl Alcohols:

For Fish and Daphnid Acute Toxicity Values: If the log Kow of the chemical is greater than 5.0, or if the compound is solid and the LC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For Green Algae Acute Toxicity Values: If the log Kow of the chemical is greater than 6.4, or if the compound is solid and the EC50 exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

For All Chronic Toxicity Values: If the log Kow of the chemical is greater than 8.0, or if the compound is solid and the ChV exceeds the water solubility by 10X, no effects at saturation are predicted for these endpoints.

ECOSAR v1.00 SAR Limitations:

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)

Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
Maximum Mol Wt: 1000

HENRYWIN (v3.20) Program Results:
==========

Bond Est : 5.40E-013 atm-m3/mole (5.47E-008 Pa-m3/mole)
Group Est: Incomplete

SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43

HENRYWIN v3.20 Results

CLASS		BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	6	Hydrogen to Carbon (aliphatic) Bonds		-0.7181
HYDROGEN	16	Hydrogen to Carbon (aromatic) Bonds		-2.4687
HYDROGEN	1	Hydrogen to Oxygen Bonds		3.2318
FRAGMENT	3	C-C		0.3489
FRAGMENT	3	C-Car		0.4858
FRAGMENT	1	C-Cd		0.0635
FRAGMENT	24	Car-Car		6.3314
FRAGMENT	1	Car-Br		0.2454
FRAGMENT	1	Cd-CO		1.9260
FRAGMENT	1	CO-O		0.0714
FRAGMENT	1	Car-Car Ring-to-Ring (biphenyl-type)		0.1490
FRAGMENT	1	Cd-O		0.2051
FRAGMENT	1	Car-Cd		0.4371
FRAGMENT	1	Car-O		0.3473
FRAGMENT	1	Cd=Cd		0.0000
RESULT		BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	10.656

HENRYs LAW CONSTANT at 25 deg C = 5.40E-013 atm-m3/mole
= 2.21E-011 unitless
= 5.47E-008 Pa-m3/mole

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	1 Cd (C)(CO)	ESTIMATE	0.10
	1 CH2 (C)(C)		-0.15
	1 CH2 (C)(Car)		-0.19
	1 CH (C)(C)(Car)		0.29
	16 Car-H (Car)(Car)		1.76
	3 Car (C)(Car)(Car)		2.10
	2 Car (Car)(Car)(Car) external	ESTIMATE	0.66
	1 Car (Car)(Car)(Br)		0.49
	1 Car (Car)(Car)(O)		-0.43
	1 CO (Cd)(O)	ESTIMATE	4.00
	1 Car (Car)(Car)(Cd)	ESTIMATE	0.75
	MISSING Value for: CH (C)(Cd)(Car)		
	MISSING Value for: Cd (O)(Car)		

```
        |              MISSING Value for:  O-H (Cd)
        |              MISSING Value for:  O (CO)(Car)
--------+-----------------------------------------------+------------+--------
 RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  | INCOMPLETE |  9.38
--------+-----------------------------------------------+------------+--------


For Henry LC Comparison Purposes:
  Exper Database:  none available
  User-Entered Henry LC:  not entered
  Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
     HLC:  2.012E-016 atm-m3/mole  (2.038E-011 Pa-m3/mole)
     VP:   1.11E-018 mm Hg (source: MPBPVP)
     WS:   0.0038 mg/L (source: User-Entered)



Log Octanol-Air (KOAWIN v1.10) Results:
=======================================

          Log Koa: 19.156

SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM   : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
--------------------------- KOAWIN v1.10 Results --------------------------

Log Koa (octanol/air) estimate:  19.156
    Koa (octanol/air) estimate:  1.432e+019
 Using:
   Log Kow:  8.50  (user entered)
   HenryLC:  5.4e-013  atm-m3/mole (HenryWin est)
   Log Kaw:  -10.656  (air/water part.coef.)

 LogKow  : 8.50 (exp database)
 LogKow  : 8.51 (KowWin estimate)
 Henry LC: --- atm-m3/mole(exp database)
 Henry LC: 5.4e-013 atm-m3/mole (HenryWin bond estimate)

 Log Koa (octanol/air) estimate:  19.166 (from KowWin/HenryWin)



BIOWIN (v4.10) Program Results:
==============================
SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM   : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
--------------------------- BIOWIN v4.10 Results ---------------------------

   Biowin1 (Linear Model Prediction)    :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Months
   Biowin4 (Primary  Biodegradation Timeframe):  Weeks
   Biowin5 (MITI Linear Model Prediction)    :  Does Not Biodegrade Fast
   Biowin6 (MITI Non-Linear Model Prediction):  Does Not Biodegrade Fast
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  NO
```

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	0.1587	0.1587
Frag	1	Ester [-C(=O)-O-C]	0.1742	0.1742
Frag	1	Aromatic bromide [-Br]	-0.1103	-0.1103
Frag	3	Alkyl substituent on aromatic ring	0.0547	0.1640
MolWt	*	Molecular Weight Parameter		-0.2492
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		0.8849

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	1.1178	1.1178
Frag	1	Ester [-C(=O)-O-C]	4.0795	4.0795
Frag	1	Aromatic bromide [-Br]	-1.6779	-1.6779
Frag	3	Alkyl substituent on aromatic ring	0.5771	1.7313
MolWt	*	Molecular Weight Parameter		-7.4327
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.6957

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	0.1600	0.1600
Frag	1	Ester [-C(=O)-O-C]	0.1402	0.1402
Frag	1	Aromatic bromide [-Br]	-0.1360	-0.1360
Frag	3	Alkyl substituent on aromatic ring	-0.0749	-0.2246
MolWt	*	Molecular Weight Parameter		-1.1567
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		1.9821

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	0.1294	0.1294
Frag	1	Ester [-C(=O)-O-C]	0.2290	0.2290
Frag	1	Aromatic bromide [-Br]	-0.1535	-0.1535
Frag	3	Alkyl substituent on aromatic ring	-0.0685	-0.2056
MolWt	*	Molecular Weight Parameter		-0.7552
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.0919

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	0.1611	0.1611
Frag	1	Ester [-C(=O)-O-C]	0.3437	0.3437
Frag	1	Aromatic bromide [-Br]	0.1668	0.1668
Frag	1	Aromatic-CH2	-0.0557	-0.0557
Frag	2	Aromatic-CH	-0.0098	-0.0195
Frag	16	Aromatic-H	0.0082	0.1315
Frag	1	-CH2- [cyclic]	0.0197	0.0197
MolWt	*	Molecular Weight Parameter		-1.5572
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		-0.0974

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	1.0041	1.0041
Frag	1	Ester [-C(=O)-O-C]	2.4462	2.4462
Frag	1	Aromatic bromide [-Br]	1.5021	1.5021
Frag	1	Aromatic-CH2	-0.1246	-0.1246
Frag	2	Aromatic-CH	0.2624	0.5248
Frag	16	Aromatic-H	0.1201	1.9223
Frag	1	-CH2- [cyclic]	0.2365	0.2365
MolWt	*	Molecular Weight Parameter		-15.1108
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0062

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	0.1328	0.1328
Frag	1	Ester [-C(=O)-O-C]	0.1719	0.1719
Frag	1	Aromatic bromide [-Br]	0.0000	0.0000
Frag	3	Alkyl substituent on aromatic ring	-0.1145	-0.3434
Frag	1	Aromatic-CH2	-0.0073	-0.0073
Frag	2	Aromatic-CH	0.0331	0.0662
Frag	16	Aromatic-H	-0.0954	-1.5269
Frag	1	-CH2- [cyclic]	-0.1200	-0.1200
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-0.7907

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data

(see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

```
BioHCwin (v1.01) Program Results:
================================
SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM   : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
-------------------------- BioHCwin v1.01 Results --------------------------

  NO Estimate Possible ... Structure NOT a Hydrocarbon
    (Contains atoms other than C, H or S (-S-))



AEROWIN Program (v1.00) Results:
================================
 Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
  Vapor pressure (liquid/subcooled):  2.36E-014 Pa (1.77E-016 mm Hg)
  Log Koa (Koawin est  ): 19.156
   Kp (particle/gas partition coef. (m3/ug)):
       Mackay model           :  1.27E+008
       Octanol/air (Koa) model:  3.52E+006
   Fraction sorbed to airborne particulates (phi):
       Junge-Pankow model     :  1
       Mackay model           :  1
       Octanol/air (Koa) model:  1


AOP Program (v1.92) Results:
============================
SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM   : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
------------------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction       =   7.8831 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
**Addition to Olefinic Bonds =  38.5000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings =  11.6952 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  58.2183 E-12 cm3/molecule-sec
   HALF-LIFE =     0.184 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     2.205 Hrs
.......................  ** Designates Estimation(s) Using ASSUMED Value(s)
------------------- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) -----------
   OVERALL OZONE Rate Constant =    13.650000 E-17 cm3/molecule-sec
   HALF-LIFE =      0.084 Days (at 7E11 mol/cm3)
   HALF-LIFE =      2.015 Hrs

Experimental Database:  NO Structure Matches
Fraction sorbed to airborne particulates (phi):
  1 (Junge-Pankow, Mackay avg)
```

```
  1 (Koa method)
     Note: the sorbed fraction may be resistant to atmospheric oxidation



KOCWIN Program (v2.00) Results:
==============================
SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM   : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
---------------------------  KOCWIN v2.00 Results  ---------------------------

  Koc Estimate from MCI:
  ----------------------
         First Order Molecular Connectivity Index  ........... : 17.081
         Non-Corrected Log Koc (0.5213 MCI + 0.60)  ..........  :  9.5039
         Fragment Correction(s):
                  1   Aliphatic Alcohol  (-C-OH)  ...........  : -1.3179
                  1   Ester  (-C-CO-O-C-) or (HCO-O-C) ......  : -1.2970
         Corrected Log Koc  ................................. :  6.8890

                          Estimated Koc:  7.745e+006  L/kg   <===========

  Koc Estimate from Log Kow:
  --------------------------
         Log Kow  (User entered   )  ........................ :  8.50
         Non-Corrected Log Koc (0.55313 logKow + 0.9251)  .... :  5.6267
         Fragment Correction(s):
                  1   Aliphatic Alcohol  (-C-OH)  ...........  : -0.4114
                  1   Ester  (-C-CO-O-C-) or (HCO-O-C) ......  : -0.0656
         Corrected Log Koc  ................................. :  5.1497

                          Estimated Koc:  1.411e+005  L/kg   <===========



HYDROWIN Program (v2.00) Results:
=================================
SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM   : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
--------------------------- HYDROWIN v2.00 Results ---------------------------
 Hydrolyzable Function detected:  Cyclic Ester

  -C-C(=O)-O-C...
   |____________|

     QSARs are not currently available to estimate hydrolysis rates for
     cyclic carboxlic acid esters.  Rates may be similar to non-cyclic
     esters; however, steric hindrance and ring strain effects may be
     important.
         Butyrolactone (a 5-member ring) hydrolyzes very slowly in neutral
     water with the hydrolysis rate increasing in alkaline conditions (Kirk-
     Othmer, 4th ed, 1:212, 1991).  In contrast, Propiolactone (a 4-member
     ring) has a reported neutral rate constant of 0.0000568/sec at 25 deg
     (Gold & Butler, 1962) which corresponds to a half-life of 3.39 days.
```

```
BCFBAF Program (v3.01) Results:
==============================
SMILES : c1cc(Br)ccc1c(cc2)ccc2C3Cc4ccccc4C(C5=C(O)c6ccccc6OC5(=O))C3
CHEM   : Brodifacoum
MOL FOR: C31 H23 Br1 O3
MOL WT : 523.43
--------------------------------- BCFBAF v3.01 --------------------------------
Summary Results:
  Log BCF (regression-based estimate):  3.39  (BCF = 2.45e+003 L/kg wet-wt)
  Biotransformation Half-Life (days) :  351  (normalized to 10 g fish)
  Log BAF (Arnot-Gobas upper trophic):  6.53  (BAF = 3.38e+006 L/kg wet-wt)

Log Kow (experimental):  8.50
Log Kow used by BCF estimates:  8.50 (user entered)

Equation Used to Make BCF estimate:
   Log BCF = -0.49 log Kow + 7.554 + Correction

      Correction(s):                    Value
       No Applicable Correction Factors

   Estimated Log BCF =  3.389  (BCF = 2449 L/kg wet-wt)

============================================================
Whole Body Primary Biotransformation Rate Estimate for Fish:
============================================================
------+-----+-----------------------------------------+---------+---------
 TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]                | -0.0616 | -0.0616
 Frag |  1  |  Ester   [-C(=O)-O-C]                    | -0.7605 | -0.7605
 Frag |  1  |  Aromatic bromide   [-Br]                |  0.3964 |  0.3964
 Frag |  3  |  Alkyl substituent on aromatic ring      |  0.1781 |  0.5342
 Frag |  1  |  Aromatic-CH2                            | -0.3365 | -0.3365
 Frag |  2  |  Aromatic-CH                             | -0.4629 | -0.9259
 Frag | 16  |  Aromatic-H                              |  0.2664 |  4.2620
 Frag |  1  |  -CH2-  [cyclic]                         |  0.0963 |  0.0963
 Frag |  2  |  Number of fused acyclic rings           |  0.6477 |  1.2953
 Frag |  2  |  Number of fused 6-carbon aromatic rings | -0.5779 | -1.1557
 Frag |  1  |  Biphenyl                                | -0.5319 | -0.5319
 Frag |  1  |  Tetralin                                |  0.0000 |  0.0000
 L Kow|  *  |  Log Kow =   8.50 (user-entered   )      |  0.3073 |  2.6124
 MolWt|  *  |  Molecular Weight Parameter              |         | -1.3422
 Const|  *  |  Equation Constant                       |         | -1.5058
============+=========================================+=========+=========
   RESULT   |        LOG Bio Half-Life (days)          |         |  2.5451
   RESULT   |            Bio Half-Life (days)          |         |   350.9
   NOTE     |  Bio Half-Life Normalized to 10 g fish at 15 deg C  |
============+=========================================+=========+=========

Biotransformation Rate Constant:
 kM (Rate Constant):  0.001976 /day (10 gram fish)
 kM (Rate Constant):  0.001111 /day (100 gram fish)
 kM (Rate Constant):  0.0006247 /day (1 kg fish)
 kM (Rate Constant):  0.0003513 /day (10 kg fish)
```

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
   Estimated Log BCF (upper trophic) = 2.986 (BCF = 967.3 L/kg wet-wt)
   Estimated Log BAF (upper trophic) = 6.529 (BAF = 3.38e+006 L/kg wet-wt)
   Estimated Log BCF (mid trophic)   = 3.155 (BCF = 1430 L/kg wet-wt)
   Estimated Log BAF (mid trophic)   = 6.200 (BAF = 1.586e+006 L/kg wet-wt)
   Estimated Log BCF (lower trophic) = 3.207 (BCF = 1609 L/kg wet-wt)
   Estimated Log BAF (lower trophic) = 5.952 (BAF = 8.956e+005 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
   Estimated Log BCF (upper trophic) = 3.240 (BCF = 1739 L/kg wet-wt)
   Estimated Log BAF (upper trophic) = 6.895 (BAF = 7.844e+006 L/kg wet-wt)

Volatilization From Water

Chemical Name: Brodifacoum

Molecular Weight   : 523.43 g/mole
Water Solubility   : 0.0038 ppm
Vapor Pressure   : -----
Henry's Law Constant: 5.4E-013 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	2.481E+009	2.706E+010
HALF-LIFE (days) :	1.034E+008	1.128E+009
HALF-LIFE (years) :	2.83E+005	3.087E+006

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
(using Biowin/EPA draft method)
PROPERTIES OF: Brodifacoum

Molecular weight (g/mol)	523.43
Aqueous solubility (mg/l)	0.0038
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	5.4E-013
Air-water partition coefficient	2.20844E-011
Octanol-water partition coefficient (Kow)	3.16228E+008
Log Kow	8.5
Biomass to water partition coefficient	6.32456E+007
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	999.99	1000.00
-Aeration tank	0.01	100.00	100.00
-Settling tank	0.01	100.00	100.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	1.9E-002	100.00
Primary sludge	5.90E+000	1.1E-002	58.96
Waste sludge	1.31E+000	2.5E-003	13.14
Primary volatilization	2.29E-014	4.4E-017	0.00
Settling volatilization	2.02E-014	3.9E-017	0.00
Aeration off gas	5.00E-014	9.5E-017	0.00
Primary biodegradation	1.73E-001	3.3E-004	1.73
Settling biodegradation	1.68E-001	3.2E-004	1.68
Aeration biodegradation	2.21E+000	4.2E-003	22.14
Final water effluent	2.35E-001	4.5E-004	2.35
Total removal	9.76E+000	1.9E-002	97.65
Total biodegradation	2.55E+000	4.9E-003	25.55

(** Total removal recommended maximum is 95 percent)

Level III Fugacity Model (Full-Output):

Chem Name : Brodifacoum
Molecular Wt: 523.43
Henry's LC : 5.4e-013 atm-m3/mole (Henrywin program)
Vapor Press : 1.11e-018 mm Hg (Mpbpwin program)
Liquid VP : 1.18e-016 mm Hg (super-cooled)
Melting Pt : 230 deg C (user-entered)
Log Kow : 8.5 (user-entered)
Soil Koc : 7.75e+006 (KOCWIN MCI method)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0156	1.38	1000
Water	2.76	1.44e+003	1000
Soil	36.9	2.88e+003	1000
Sediment	60.3	1.3e+004	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.13e-022	926	18.5	30.9	0.616
Water	5.91e-020	157	326	5.23	10.9
Soil	1.34e-021	1.05e+003	0	35	0
Sediment	9.88e-020	381	142	12.7	4.75

Persistence Time: 3.94e+003 hr
Reaction Time: 4.7e+003 hr
Advection Time: 2.43e+004 hr
Percent Reacted: 83.8
Percent Advected: 16.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 1.383
Water: 1440
Soil: 2880
Sediment: 1.296e+004
Biowin estimate: 1.982 (months)

```
Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```