2.0 INTRODUCTION

The structure, CAS name, CAS registry number, and various physical properties of penthiopyrad and its metabolites are found in Appendix 1. This analytical method was validated on six soil types and is suitable for enforcement monitoring and data generation for regulatory studies.

In order to effectively extract incurred residues of penthiopyrad and its metabolites from soil, an extraction procedure was developed using 4:1 acetonitrile:water. Five-gram aliquots of soil were extracted twice with 4:1 acetonitrile:water by shaking at high speed followed by centrifugation. The extracts were combined and evaporated to remove the acetonitrile. The concentrated extract was transferred to a centrifuge tube and combined with ethyl acetate rinsates and 0.1% acetic acid. The extract was shaken and centrifuged before transferring the upper ethyl acetate layer into a new tube. Ethyl acetate was added to the aqueous phase, shaken, and centrifuged to ensure phase separation before combining the ethyl acetate extracts. Extract was adjusted to volume with ethyl acetate, capped, and mixed thoroughly. An aliquot of the ethyl acetate fraction was transferred to a centrifuge tube and evaporated to <0.5 mL under a flow of nitrogen in a water bath at 40 °C or lower. In order to remove any remaining ethyl acetate, additional methanol was added and evaporated again to <0.5 mL under a stream of nitrogen in a water bath at 40 °C or lower. Methanol was added, the tubes were capped, and mixed by hand before sonicating. Omni Solv water was added, the tubes were capped and mixed by hand before sonicating. Volume was adjusted with 50% methanol:water; samples were filtered into HPLC vials and diluted (if necessary) for LC/MS/MS analysis.

The validated LOQ was 5.0 ppb and the LOD was estimated to be 1.5 ppb. During method validation, acceptable recoveries for soil samples fortified at the LOQ, 10× the LOQ, and at the anticipated highest expected soil concentration (750 ppb) were demonstrated. A confirmation analysis using LC/MS/MS was also validated. Confirmation criteria and examples are discussed in this report.

3.0 MATERIALS

Equivalent equipment and materials may be substituted unless otherwise specified. Note any specification in the following descriptions before making substitutions. Substitutions should only be made *if equivalency/suitability has been verified with acceptable control and fortification recovery data*.

3.1 Equipment

Extractor

Reciprocal Shaker: Eberbach Corporation, Ann Arbor, MI; or equivalent wrist-action shaker.

Polypropylene Centrifuge Tubes: 30 x 115 mm, 50-mL BD Falcon Blue Max graduated tubes, Manufacturer #352070,

Fisher Cat. No. 14-432-22 (Fisher Scientific, Pittsburgh, PA)

17 x 120 mm, 15-mL BD Flcon blue Max Jr. graduated tubes, Manufacturer #352097, Fisher Cat. No. 14-959-70C (Fisher Scientific, Pittsburgh, PA)

Disposable Pipet: 5-mL Borosilicate glass, Fisherbrand, Cat. No. 13-678-25D

Pyrex Flat-Bottomed Flasks: 103 x 155 mm, 24/40 joint, Manufacturer No. 4100-500, Fisher Cat. No. 09-559 D (Fisher Scientific, Pittsburgh, PA)

Instrumentation

LC/MS/MS System: Sciex API 4000 (Applied Biosystems, Foster City, CA)

Balance: Mettler PM400 Analytical Balance (Mettler Instrument Corp., Hightstown, NJ)

Microman Pipettes: Capillary piston, 50-250 µL, Model M 250, Reference No. F148505 and 100-1000 µL, Model M1000, Reference No. F148506 (Gilson, Middleton, WI)

Evaporator: N-Evap® Model 111 Laboratory Sample Evaporator/Nitrogen Manifold fitted with Teflon®-coated Needles (Organomation Associates, South Berlin, MA) or equivalent apparatus attached to a dry, clean nitrogen source.

Centrifuge: Beckman GS-6R and/or Beckman GP

Sonicator: Branson 5200

Chromatographic Supplies

HPLC Columns: Phenomenex Phenyl-Hexyl (3 µ x 4.6 mm x 150 mm); Serial No. 343415-11 or Phenomenex Luna C18(2) (3 µ x 4.6 mm x 150 mm); Serial #377814-53 (Phenomenex, Inc., Torrance, CA)

HPLC Vials: National Scientific 11 mm (PP) vial, crimp/snap, 250 µL, 100 PK, Part No. C4011-13 (Fisher Scientific, Pittsburgh, PA)

National Scientific, 12 x 32 mm (PP) vial, Target crimp/snap, Manufacturer No. C4011-14 (Fisher Scientific, Pittsburgh, PA)

Xypertek Syringe Filter: 13 mm, 0.2 µm PTFE, Manufacturer No. 9445601 (PJ Cobert, St. Louis, MO)

Disposable Syringes: BD Brand 3 mL Luer-Lok, Manufacturer No. 309585 (Fisher Scientific, Pittsburgh, PA)

3.2 Reagents and Standards

Equivalent reagents may be substituted for those listed below. To determine if impurities in substituted reagents interfere with analyses, appropriate amounts of the

solvents should be taken through the entire method using the chromatographic conditions specified in this report.

Acetonitrile (ACN): HPLC-grade acetonitrile, #A996-4 (Fisher Scientific, Pittsburgh, PA)

Methanol (MeOH): HPLC-grade, #065162 (Fisher Scientific, Pittsburgh, PA)

Ethyl Acetate: HPLC-grade, #CR484 (B & J, Muskegon, MI)

Formic Acid: Guaranteed Reagent 99% minimum, #FX0440-5, Code: 27048001 0 (Acros Organics, New Jersey)

Water: EM Omni Solv®, HPLC-grade water, #46306 (EM Science, Gibbstown, NJ)

LC/MS/MS Makeup Gas: 5% Methane/95% Argon, Part No. 2301-300 (MG Industries, Morrisville, PA)

MTF-753 (penthiopyrad,DPX-LEM17) reference material, obtained from Huntingdon Life Sciences, Eye, Suffolk, England, IP23 7PX

PAM, 753-A-OH, 753-F-DO, 753-T-DO, DM-753, PCA, and DM-PCA reference materials, obtained from Mitsui Chemicals Inc., Shiodome City Center 1-5-2, Higashi-Shimbashi, Minato-ku, Tokyo 105-7117 Japan

3.3 Safety and Health

No unusually hazardous materials are used in this method. All appropriate material safety data sheets should be read and followed, and proper personal protective equipment used. MSDS sheets for the analytes are available from DuPont Crop Protection, Global Technology Division, E. I. du Pont de Nemours and Company.

4.0 METHOD

4.1 Principle of the Analytical Method

In order to effectively extract incurred residues of penthiopyrad and its metabolites from soil, an extraction procedure was developed using 4:1 acetonitrile:water followed by shaking at high speed and centrifugation. The extracts were combined and evaporated at approximately 40 °C to remove the acetonitrile. The concentrated extracts were transferred to a centrifuge tube and combined with ethyl acetate rinsates and 0.1% acetic acid. The extracts were shaken and centrifuged before transferring the upper ethyl acetate layer into a new tube. Ethyl acetate was added to the aqueous phase, shaken, and centrifuged to combine the ethyl acetate extracts. Extract was adjusted to volume with ethyl acetate, capped, and mixed thoroughly. The ethyl acetate layers were transferred to centrifuge tubes and evaporated to dryness under a flow of nitrogen in a water bath at 40 °C or lower. The extracts were reconstituted in methanol and evaporated to <0.5 mL under a stream of nitrogen in a water bath at 40 °C or lower. Methanol was added, the tubes were capped, and mixed by hand before sonicating. Omni Solv water was added, the tubes were capped, and mixed by

hand, before sonicating. Volume was adjusted with 50% methanol:water, and samples were filtered into HPLC vials and diluted for LC/MS/MS analysis.

4.2 Analytical Procedure

4.2.1 Glassware and Equipment

Cleaning

Glassware should be scrubbed with a brush using a laboratory soap solution, rinsed two to five times with tap water, rinsed with distilled or deionized water, and finally rinsed with acetone or another suitable solvent and allowed to air dry prior to each use.

Due to the tendency of penthiopyrad and metabolites to adhere to surfaces when in water, it is extremely important not to wash analyte-contaminated glassware such as stock standard volumetric flasks in common wash areas. Contaminated glassware must be thoroughly rinsed with acetonitrile prior to following normal glassware cleaning procedures.

4.2.2 Preparation of Solutions

The following solutions should be prepared weekly and stored at room temperature unless stated otherwise:

4:1 Acetonitrile:Deionized Water Extraction Solvent - Separately measure 800 mL acetonitrile and 200 mL deionized water and mix in a 1000-mL glass bottle.

0.1% Acetic Acid - Dilute 0.1 mL glacial acetic acid to 100 mL with deionized water.

1 M Ammonium Acetate - Dissolve 7.7 g ammonium acetate in deionized water and adjust the volume to 100 mL. This solution is used in the preparation of Mobile Phase A.

50:50 Methanol:Deionized Water - Separately measure 500 mL methanol and 500 mL deionized water and mix in a 1000 mL glass bottle.

Mobile Phase A: 10mM Ammonium Acetate in Deionized Water - Dilute 10 mL of 1 M ammonium acetate to 1000 mL final volume with deionized water.

Mobile Phase B: Methanol

4.2.3 Preparation and Stability of Standards

The preparation of these standard solutions may be achieved by the use of alternative dilutions if necessary. Solutions of reference items should be stored at 4 °C and have a maximum expiration date of 3 months from preparation.

Use Class A volumetric flasks when preparing standard solutions.

1000-μg/mL Stock Standard Solutions - Weigh accurately 10 mg (adjusted for purity) of each standard into separate 10-mL volumetric flasks. Dissolve and make up to volume with methanol.

10-μg/mL Mixed Standard - Pipette 1.0 mL of each stock standard into a 100-mL volumetric flask and make to volume with methanol.

1-μg/mL Mixed Standard - Pipette 5 mL of the 10-μg/mL mixed standard into a 50-mL volumetric flask and make to volume with methanol.

0.1-μg/mL Mixed Standard - Pipette 1.0 mL of the 10-μg/mL mixed standard into a 100-mL volumetric flask and make to volume with methanol.

The following standard solutions will be used in the preparation of calibration standards:

400-ng/mL Mixed Standard - Pipette 2.0 mL of the 10-μg/mL mixed standard into a 50-mL volumetric flask. Adjust to volume with methanol.

200-ng/mL Mixed Standard - Pipette 2.0 mL of the 10-μg/mL mixed standard into a 100-mL volumetric flask. Adjust to volume with methanol.

100-ng/mL Mixed Standard - Pipette 0.5 mL of the 10-μg/mL mixed standard into a 50-mL volumetric flask. Adjust to volume with methanol.

40.0-ng/mL Mixed Standard - Pipette 0.2 mL of the 10-μg/mL mixed standard into a 50-mL volumetric flask. Adjust to volume with methanol.

20.0-ng/mL Mixed Standard - Pipette 0.1 mL of the 10-μg/mL mixed standard into a 50-mL volumetric flask. Adjust to volume with methanol.

10.0-ng/mL Mixed Standard - Pipette 5.0 mL of the 100-ng/mL mixed standard into a 50-mL volumetric flask. Adjust to volume with methanol.

2.00-ng/mL Mixed Standard - Pipette 1.0 mL of the 100-ng/mL mixed standard into a 50-mL volumetric flask. Adjust to volume with methanol.

Calibration standards are prepared at a maximum interval of every three calendar days.

CALIBRATION CURVE PREPARATION			
INITIAL STD NG/ML	INITIAL STD VOL (ML)	FINAL VOL. (ML)	FINAL STD CONC. (NG/ML)
400	0.100	2.00	20
200	0.100	2.00	10
100	0.100	2.00	5
40.0	0.100	2.00	2
20.0	0.100	2.00	1
10.0	0.100	2.00	0.5
2.00	0.100	2.00	0.1

4.2.4 *Source of Samples*

All soil control samples used for method validation were obtained from DuPont studies. Soil characterization results are summarized in the following table.

SOIL ID	SOIL TYPE	PH	%CLAY	% SAND	% SILT	% ORGANIC MATERIAL
California	Sandy Loam	7.81	7.6	62.8	29.6	0.9
Washington	Sandy Loam	7.44	8.8	71.6	19.6	1.1
Missouri	Silt Loam	6.20	24.0	16.0	60.0	2.3
Georgia	Loamy Sand	6.78	8.0	84.0	8.0	0.7
Ontario	Loam	6.68	11.6	48.0	40.4	1.9
Saskatchewan	Clay Loam	7.53	28.8	21.2	50.0	3.5

4.2.5 *Storage and Preparation of Samples*

Before extraction, soil is allowed to thaw and a 5-g representative soil sample is removed from the homogeneously mixed sample.

4.2.6 *Sample Fortification Procedures*

Two appropriately fortified control samples should be analyzed with each set of samples to assess the analytical efficiency of the method. One of these will normally be fortified at the LOQ and the other at 10 times the LOQ (or at a level higher than anticipated in the treated samples).

All fortifications were made directly to the soil in the centrifuge bottles after weighing the sample. Five-gram samples were fortified with the mixed fortification standard solutions.

FORTIFICATION LEVEL (PPB)	VOLUME OF 0.100 µG/ML MIXED STANDARD REQUIRED (ML)	VOLUME OF 1.00 µG/ML MIXED STANDARD REQUIRED (ML)	VOLUME OF 10.0 µG/ML MIXED STANDARD REQUIRED (ML)
5	0.250	-	-
50	-	0.250	-
750	-	-	0.375

After fortification, all samples were allowed to air dry for 10 minutes to allow the fortification solvent to evaporate.

4.2.7 Sample Extraction

Use the procedures described below to extract residues of penthiopyrad and metabolites from soil samples.

1. Weigh 5.0 ± 0.1 grams of soil into a 50-mL centrifuge tube. Fortify samples as appropriate.
2. Add 40 mL of the 4:1 acetonitrile:water to the centrifuge tube. Tightly cap the tube and shake at high speed for 30 minutes. Centrifuge the sample at approximately 2500 RPM for 5 minutes. A firm pellet will form at the bottom of the centrifuge tube. Decant the supernatant into a 500-mL flask.
3. Repeat Step 2, combining extracts into the 500-mL flask.
4. Rotary evaporate the extract to remove the acetonitrile at approximately 40 °C or lower leaving approximately 10 ml of aqueous phase.
5. Transfer concentrated extract to a 50-mL centrifuge tube. Rinse the flask with 10- and 15-mL aliquots of ethyl acetate adding each rinsate to the 50-mL centrifuge tube, then add 5 mL of 0.1% acetic acid.
6. Cap and shake sample at low speed for 5 minutes; centrifuge the sample at approximately 1500 RPM for 3 minutes.
7. Transfer the upper ethyl acetate layer into a new 50-mL tube, add 20 mL of ethyl acetate to the aqueous phase and repeat Step 6 combining the ethyl acetate extracts. Adjust extract volume to 50 mL with ethyl acetate, cap, and mix thoroughly.
8. Pipette a 5-mL aliquot into a 15-mL polypropylene tube. Evaporate to less than 0.5 mL under a stream of nitrogen in a water bath at approximately 40 °C or lower. Avoid going to dryness.
9. Add 4 mL of methanol and evaporate to less than 0.5 mL under a stream of nitrogen in a water bath at approximately 40 °C or lower. Repeat this step, if necessary, to achieve solvent exchange.
10. Add 1.0 mL of methanol and cap the tubes. Mix the sample by swirling at least 20 seconds using a vortex mixer or by hand, and sonicate for 2 minutes.

11. Add 1.0 mL of Omni Solv Water and cap the tubes. Mix the sample by swirling at least 20 seconds using a vortex mixer or by hand and sonicate for 2 minutes. Adjust volume with 50% methanol:water to make the final volume 2.5 mL.
12. Filter samples with a 3-mL syringe and 0.2-µm PTFE filter into an HPLC vial. Dilute as necessary.

Extracts will be stable for approximately 72 hours if stored at 4°C.

4.3 Instrumentation for the Method

4.3.1 LC/MS/MS Analysis of Penthiopyrad and Metabolites

PE Sciex API 4000-LC/MS/MS System with Analyst Software

Typical HPLC Conditions:

System:	Agilent HP1100 HPLC
Column:	4.6 mm i.d. × 150 mm, Phenomenex Phenyl-Hexyl analytical column with 3-µm diameter packing
Column Temperature:	40 °C
Injection Volume:	25 µL
Autosampler Temperature:	20 °C
Flow Rate:	0.90 mL/min (split, 0.45 mL/min into source)
Conditions:	Time %A %B Flow 0.0 80 20 0.90 0.01 80 20 0.90 3.0 25 75 0.90 4.0 20 80 0.90 6.0 10 90 0.90 6.1 1 99 0.90 9.0 1 99 0.90 9.1 80 20 0.90 9.6 80 20 0.90 13.5 80 20 0.90 A: 0.01 M aq. Formic Acid (F.A.) B: Methanol Flow in mL/min
Approximate Retention Times	(Minutes)
Penthiopyrad	8.16
753-A-OH	7.39
753-F-DO	7.22
753-T-DO	7.85
PAM	4.92
Total Run Time:	13.5 minutes

The valve switching times are given in the following table.

TIME (MINUTES)	COLUMN ELUATE FLOW
0.0-4.00	Waste
4.00-9.60	MS source
9.60-end	Waste

System:	Agilent HP1100 HPLC
Column:	4.6 mm i.d. × 150 mm, Phenomenex Luna, C-18(2) analytical column with 3-μm diameter packing
Column Temperature:	40 °C
Injection Volume:	75 µL
Autosampler Temperature:	20 °C
Flow Rate:	0.90 mL/min (split, 0.45 mL/min into source)
Conditions:	Time %A %B Flow 0.0 80 20 0.90 0.01 80 20 0.90 0.5 80 20 0.90 3.0 20 80 0.90 3.8 1 99 0.90 5.8 1 99 0.90 7.25 1 99 0.90 7.5 80 20 0.90 12.0 80 20 0.90 A: 0.01 M aq. Formic Acid (F.A.) B: Methanol Flow in mL/min
Approximate Retention Times	(Minutes)
PCA	5.65
DM-PCA	5.35
Total Run Time:	12.0 minutes

The valve switching times are given in the following table.

TIME (MINUTES)	COLUMN ELUATE FLOW
0.0-3.80	Waste
3.80-7.25	MS source
7.25-end	Waste

APCI-LC/MS/MS Conditions:

ANALYTES MONITORED	ION MODE	IONS MONITORED FOR QUANTIFICATION	ACQUISITION TIMING (MIN.)
Penthiopyrad	MRM	360.1 → 276.0 AMU	7.99 – 8.78
		IONS MONITORED FOR CONFIRMATION	
		360.1 → 177.0 AMU	
Polarity	Positive		
Probe Temp	450 °C		
Nebulizing Gas (GS1)	45.00		
Nebulizing Gas (GS2)	50.00		
Curtain Gas Setting	15.00		
CAD Gas Setting	5.00		
Declustering Potential	50.00		
Entrance Potential	10.00		
Collision Cell Exit Potential	19.00		
Collision Energy	22.00		

ANALYTES MONITORED	ION MODE	IONS MONITORED FOR QUANTIFICATION	ACQUISITION TIMING (MIN.)
753-A-OH	MRM	376.1 → 152.1 AMU	7.26 – 7.90
		IONS MONITORED FOR CONFIRMATION	
		376.1 → 177.0 AMU	
Polarity	Positive		
Probe Temp	450 °C		
Nebulizing Gas (GS1)	45.00		
Nebulizing Gas (GS2)	50.00		
Curtain Gas Setting	15.00		
CAD Gas Setting	5.00		
Declustering Potential	40.00		
Entrance Potential	10.00		
Collision Cell Exit Potential	13.00		
Collision Energy	32.00		

Analytes Monitored	Ion Mode	Ions Monitored for Quantification	Acquisition Timing (Min.)
753-F-DO	MRM	376.1 → 182.1 AMU	7.09 – 7.83
		Ions Monitored for Confirmation	
		376.1 → 177.0 AMU	
Polarity	Positive		
Probe Temp	450 °C		
Nebulizing Gas (GS1)	45.00		
Nebulizing Gas (GS2)	50.00		
Curtain Gas Setting	15.00		
CAD Gas Setting	5.00		
Declustering Potential	45.00		
Entrance Potential	10.00		
Collision Cell Exit Potential	16.00		
Collision Energy	16.00		

Analytes Monitored	Ion Mode	Ions Monitored for Quantification	Acquisition Timing (Min.)
753-T-DO	MRM	392.1 → 177.0 AMU	7.70 – 8.49
		Ions Monitored for Confirmation	
		392.1 → 177.0 AMU	
Polarity	Positive		
Probe Temp	450 °C		
Nebulizing Gas (GS1)	45.00		
Nebulizing Gas (GS2)	50.00		
Curtain Gas Setting	15.00		
CAD Gas Setting	5.00		
Declustering Potential	45.00		
Entrance Potential	10.00		
Collision Cell Exit Potential	14.00		
Collision Energy	40.00		

Analytes Monitored	Ion Mode	Ions Monitored for Quantification	Acquisition Timing (Min.)
PAM	MRM	194.1 → 174.0 AMU	4.85 - 5.27
		Ions Monitored for Confirmation	
		194.1 → 134.0 AMU	
Polarity	Positive		
Probe Temp	450 °C		
Nebulizing Gas (GS1)	45.00		
Nebulizing Gas (GS2)	50.00		
Curtain Gas Setting	15.00		
CAD Gas Setting	5.00		
Declustering Potential	40.00		
Entrance Potential	10.00		
Collision Cell Exit Potential	16.00		
Collision Energy	15.00		

Analytes Monitored	Ion Mode	Ions Monitored for Quantification	Acquisition Timing (Min.)
PCA	MRM	193.1 → 109.0 AMU	5.53 – 5.92
		Ions Monitored for Confirmation	
		193.1 → 149.0 AMU	
Polarity	Negative		
Probe Temp	450 °C		
Nebulizing Gas (GS1)	45.00		
Nebulizing Gas (GS2)	50.00		
Curtain Gas Setting	15.00		
CAD Gas Setting	5.00		
Declustering Potential	-43.00		
Collision Cell Exit Potential	-16.00		
Collision Energy	-32.00		

ANALYTES MONITORED	ION MODE	IONS MONITORED FOR QUANTIFICATION	ACQUISITION TIMING (MIN.)
DM-PCA	MRM	178.9 → 159.0 AMU	5.25 – 5.70
		IONS MONITORED FOR CONFIRMATION	
		178.9 → 111.0 AMU	
Polarity	Negative		
Probe Temp	450 °C		
Nebulizing Gas (GS1)	45.00		
Nebulizing Gas (GS2)	50.00		
Curtain Gas Setting	15.00		
CAD Gas Setting	5.00		
Declustering Potential	-40.00		
Collision Cell Exit Potential	-10.00		
Collision Energy	-17.00		

4.3.2 *Calibration Procedure and Sample Analysis*

A 1.0-ng/mL chromatographic standard should be analyzed prior to the start of analyses to establish that the instrument is working properly. If a signal-to-noise ratio of at least 3 to 1 is not attained, the instrument must be tuned or cleaned prior to sample analysis. Signal-to-noise ratio of approximately 5 to 10 is preferred. Operating parameters must be tailored to the particular instrument used, especially if it is to be an alternate vendor's instrument, and should be checked daily. Each run should begin and end with a standard injection. All sample injections should be bracketed by a standard with no more than four samples between standards.

4.4 Calculations

Recovery data was calculated using an average response factor for bracketing standard approach. The standards are dispersed approximately every third injection during an injection sequence.

4.4.1 *Method*

$$\text{ppb Found} = \frac{(\text{Peak Area}) \times (\text{RF}_{\text{Ave}}) \times (\text{Final Volume}) \times (\text{Aliquot Factor}) \times (\text{Dilution Factor})}{(\text{Sample Weight})}$$

The percent recovery found was calculated as follows:

$$\%\ \text{Recovery} = \frac{(\text{ppb Found})}{(\text{Fortification Level})} \times 100$$

4.4.2 *Example*

For a California soil sample fortified with penthiopyrad at 5.0 ppb (10 March 2007, Sample CA Control + 5.0 ppb), the concentration found was calculated as follows:

RF_{Ave} = 7.8487E-06

ppb found was calculated as follows:

$$\text{ppb Found} = \frac{(118227) \times (7.8487e - 6) \times (2.5\,\text{mL}) \times (10) \times (1)}{(5\,\text{g})}$$

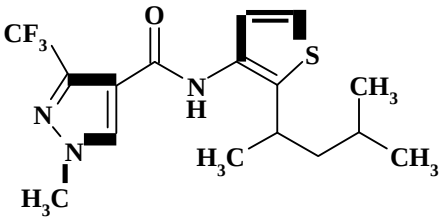
ppb Found = 4.640

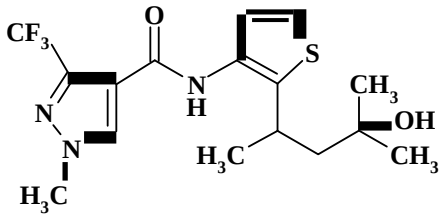
The percent recovery found was calculated as follows:

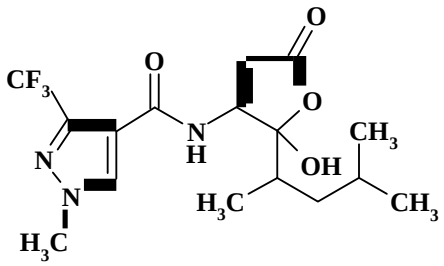
$$\%\,\text{Recovery} = \frac{(4.640\,\text{ppb})}{(5.0\,\text{ppb})}\ \text{x}\ 100$$

% Recovery = 93%

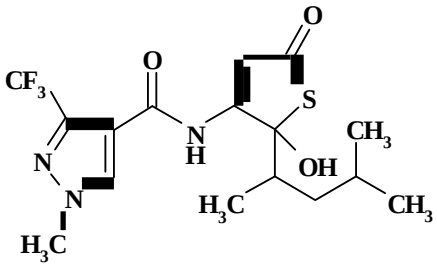
APPENDIX 1 STRUCTURE AND PROPERTIES OF PENTHIOPYRAD AND METABOLITES

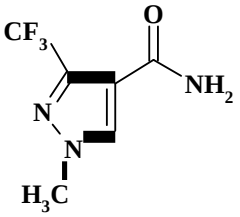
Common Name	Penthiopyrad (MTF-753)
Structure	
DPX Number	DPX-LEM17
CAS Chemical Name	N-[2-(1,3-Dimethylbutyl)-3-thienyl]-1-methyl-3-(trifluoromethyl)-1H-Pyrazole-4-carboxamide
CAS Number	183675-82-3
Formula	$C_{16}H_{20}F_3N_3OS$
Molecular Weight	359.414

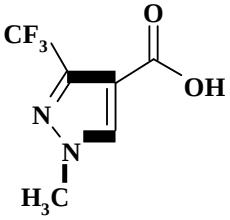
Common Name	753-A-OH
Structure	
DPX Number	IN-PGH53
Formula	$C_{16}H_{20}F_3N_3O_2S$
Molecular Weight	375.413

Common Name	753-F-DO
Structure	
DPX Number	IN-PGH59
Formula	$C_{16}H_{20}F_3N_3O_4$
Molecular Weight	375.35

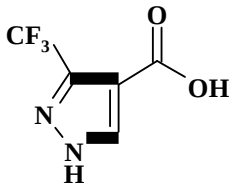
APPENDIX 1 STRUCTURE AND PROPERTIES OF PENTHIOPYRAD AND METABOLITES (CONTINUED)

Common Name	753-T-DO
Structure	
DPX Number	IN-PGH58
Formula	$C_{16}H_{20}F_3N_3O_3S$
Molecular Weight	391.42

Common Name	PAM
Structure	
DPX Number	IN-PGH45
Formula	$C_6H_6F_3N_3O$
Molecular Weight	193.127

Common Name	PCA
Structure	
DPX Number	IN-MR507
Formula	$C_6H_5F_3N_2O_2$
Molecular Weight	194.112

APPENDIX 1 STRUCTURE AND PROPERTIES OF PENTHIOPYRAD AND METABOLITES (CONTINUED)

Common Name	DM-PCA
Structure	
DPX Number	IN-DRJ75
Formula	$C_5H_3F_3N_2O_2$
Molecular Weight	180.085