

Analytical methods for tiafenacil (DCC-3825) in sediment and tiafenacil and its metabolites M-01, M-12, M-13, M-36, and M-53 in sediment

Reports: ECM 1: EPA MRID No.: 50486868. Martin, K.H., K.S. Keller. 2017. Analytical method verification for the determination of DCC-3825 in sediment. Document No.: 548C-107. Unpublished study performed by EAG Laboratories, Easton, Maryland; sponsored by Ishihara Sangyo Kaisha, Ltd., Osaka, Japan, and FarmHannong Co., Ltd., Seoul, Korea; and submitted by ISK Biosciences Corporation, Concord, Ohio; 63 pages. Final report issued October 17, 2017.

ECM 2: EPA MRID No.: 50493809. Ogawa, K. 2017. Validation of an analytical method for the determination of DCC-3825 and its metabolites (M-01, M-12, M-13, M-36, M-53) in Sediment. Document No.: MFT03817E. Unpublished study performed by Safety Science Research Laboratories, Ishihara Sangyo Kaisha, Ltd., Shiga-ken, Japan; sponsored by Ishihara Sangyo Kaisha, Ltd., Osaka, Japan, and FarmHannong Co., Ltd., Seoul, Korea; and submitted by ISK Biosciences Corporation, Concord, Ohio; 102 pages. Final report issued February 8, 2017.

ILV: EPA MRID No. 50493810. Perez, R. 2017. Independent Laboratory Validation of Method MFT03817E: "Validation of an analytical method for the determination of DCC-3825 and its metabolites (M-01, M-12, M-13, M-36, M-53) in Sediment". ADPEN Study No. and Document No.: 17E1004. Report prepared by ADPEN Laboratories, Inc., Jacksonville, Florida; sponsored by Ishihara Sangyo Kaisha, Ltd., Osaka, Japan, and FarmHannong Co., Ltd., Seoul, Korea; and submitted by ISK Biosciences Corporation, Concord, Ohio; 254 pages. Final report issued October 13, 2017.

Document No.: MRIDs 50486868, 50493809 & 50493810

Guideline: 850.6100

Statements: ECM 1: The study was conducted in accordance with USEPA FIFRA GLP standards (40 CFR Part 160; pp. 1C, 3 of MRID 50486868). Signed and dated No Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 1B-1C, 3-4). An Authenticity statement was not included. ECM 2: The study did not contain a statement which stated that it was conducted in accordance with Good Laboratory Practice (GLP) standards (p. 1C of MRID 50493809). Signed and dated No Data Confidentiality, GLP, and Authenticity statements were provided (pp. 1B-1C, 2). A Quality Assurance statement was not included.

ILV: The study was conducted in accordance with USEPA FIFRA GLP standards (40 CFR Part 160; p. 3 of MRID 50493810). Signed and dated No Data Confidentiality, GLP, Quality Assurance, and Authenticity statements were provided (pp. 2-4).

Classification: This analytical method is classified as **supplemental**. MRID 50493809 and 5049310 are reliable environmental chemistry methods (ECM) with an

independent laboratory validation (ILV) to measure tiafenacil and the majority of degradates in sediment.

ECM 1: EPA MRID No.: 50486868: For EAG Laboratories Method 548C-107 (ECM 1): only one set of performance data was submitted, an ECM; no representative chromatograms of 10000×LOQ fortification were provided for review. An ILV was not provided.

ECM 2: MRID 50493809 and ILV MRID 50493810: the ECM did not report the method LOD.

PC Code: 012311

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This Data Evaluation Record may have been altered by the Environmental Fate and Effects Division subsequent to signing by CDM/CSS-Dynamac JV personnel. The CDM/CSS-Dynamac Joint Venture role does not include establishing Agency policies.

Executive Summary

Two Environmental Chemistry Methods (ECM) were submitted for quantitation of tiafenacil and its metabolites in sediment. The analytical method, **EAG Laboratories Method 548C-107 (ECM 1)**, is designed for the quantitative determination of tiafenacil (DCC-3825) in sediment at the LOQ of 0.01 mg/kg using LC/MS/MS. The analytical method, **ISK Biosciences Analytical Method MFT03817E (ECM 2)**, is designed for the quantitative determination of tiafenacil (DCC-3825) and its metabolites M-01, M-12, M-13, M-36, and M-53 in sediment at the LOQ of 0.01 mg/kg using LC/MS/MS. The LOQ cannot be compared to the lowest toxicological level of concern in sediment for tiafenacil because the submitted sediment toxicity data contained deficiencies.

The two methods use similar extraction and chromatographic procedures, but method MFT03817E (MRID 50493809) includes a solid phase extraction (SPE) step instead of centrifugation. Method MFT03817E methods were shown to be repeatable, reproducible, linear, and specific for the parent and metabolites and was the only method with an Independent Laboratory Validation.

MRID 50486868 contained the ECM for EAG Laboratories Method 548C-107 using characterized freshwater and saltwater sediments. For EAG Laboratories Method 548C-107, all submitted quantitation ion data pertaining to precision, repeatability, reproducibility, linearity, and specificity was acceptable. No representative chromatograms of 10000×LOQ fortification were provided for review. No ILV data was submitted for this method.

MRID 50493809 contained the ECM for ISK Biosciences Analytical Method MFT03817E using two characterized sediments. MRID 50493810 contained the ILV for ISK Biosciences Analytical Method MFT03817E using one characterized sediment and serves as the ILV for MRID 50493809.

For ISK Biosciences Analytical Method MFT03817E, The Limit of Detection (LOD) was not reported in the ECM. The ILV validated the method after the first trial with minor modifications of the analyzed ion transitions. All submitted data pertaining to precision, repeatability, reproducibility, linearity, and specificity was acceptable. The specificity of the method for all other analytes was supported by ECM and ILV representative chromatograms; however, persistent nearby contaminants were observed in all M-12 and M-53 chromatograms. Additionally, peak shouldering of the M-36 analyte peak was noted in all ILV chromatograms.

Table 1. Analytical Method Summary

| Analyte(s) by Pesticide | MRID | | EPA Review | Matrix | Method Date (dd/mm/yyyy) | Registrant | Analysis | Limit of Quantitation (LOQ) |
|-------------------------|--------------------------------|-----------------------------------|--------------|----------|--------------------------|-----------------------------|----------|-----------------------------|
| | Environmental Chemistry Method | Independent Laboratory Validation | | | | | | |
| Tiafenacil (DCC-3825) | 50486868 (ECM 1) ¹ | None submitted | Supplemental | Sediment | 17/10/2017 (ECM 1) | ISK Biosciences Corporation | LC/MS/MS | 0.01 mg/kg |
| Tiafenacil (DCC-3825) | 50493809 (ECM 2) ² | 50493810 ³ | | | 08/02/2017 (ECM 2) | | | |
| M-01 | | | | | | | | |
| M-12 | | | | | | | | |
| M-13 | | | | | | | | |
| M-36 | | | | | | | | |
| M-53 | | | | | | | | |

1 In ECM 1, the natural freshwater loamy sand sediment [80% sand, 20% silt, 0% clay; pH 5.6 (1:1 soil:water ratio), 1.8% organic carbon, 3.2% organic matter] obtained from West Bearskin Lake, Minnesota, and natural saltwater sand sediment [90% sand, 6% silt, 4% clay; pH 8.1 (1:1 soil:water ratio), 0.37% organic carbon, 0.64% organic matter] obtained from Wye River, Maryland, were used in the study (USDA soil texture classification; p. 12; Appendices 3-6, pp. 54-59 of MRID 50486868). Sediment classification was performed by Agvise Laboratories, Northwood, North Dakota.

2 In ECM 2, Swiss Lake sand sediment [95% sand, 3% silt, 2% clay; pH 6.1 (water), 0.6% organic carbon by wet oxidation] and Calwich Abbey sandy silt loam sediment [39% sand, 49% silt, 13% clay; pH 7.9 (water), 4.9% organic carbon by wet oxidation] obtained from Calwich Abbey Lake were used in the study (USDA Soil texture classification not specified; p. 14; Table 1, p. 22 of MRID 50493809; see Reviewer Comment #7). Both sediments were supplied by Envigo CRS Ltd. in June 2016.

3 In the ILV, the clay loam sediment [Lab Code # 170110002-018 0-2³; 40% sand, 20% silt, 40% clay; pH 7.4 (1:1 soil:water ratio), 1.5% organic matter] obtained from California was used in the study (USDA soil texture classification; p. 12; Appendix B, pp. 115-119 of MRID 50493810). Sediment classification was performed by Agvise Laboratories, Northwood, North Dakota. The source of the sediment was not further specified.

I. Principle of the Method

EAG Laboratories Method 548C-107 (ECM 1)

Sediment samples (1.00 g) were fortified (tiafenacil acetonitrile fortification solutions), as necessary, and mixed via vortex for *ca.* 30 seconds (pp. 12-13; Figure 2, pp. 26-27 of MRID 50486868). The samples were extracted twice with 0.2% formic acid in acetonitrile via mixing (vortex for *ca.* 15 minutes). After centrifugation (1962 RCF for 1 minute), the extract was decanted into a 50-mL polypropylene centrifuge tube. The combined extracts were brought to 50 mL using 0.2% formic acid in acetonitrile. The samples were diluted with acetonitrile:HPLC-grade water:formic acid (50:50:0.1, v:v:v), and further diluted using combined matrix-matched acetonitrile:HPLC-grade water:formic acid (50:50:0.1, v:v:v), as necessary. Samples were prepared in autosampler vials for LC/MS/MS analysis. The procedure was also outlined for the separating overlying water, pore water, and freshwater and saltwater sediment (Figure 1, p. 25).

Tiafenacil was identified and quantified by LC/MS/MS using an Applied Biosystems/MDS Sciex API 3000 LC/MS/MS coupled with an Agilent 1200 Series Infinity HPLC System (p. 13; Table 1, p. 20 of MRID 50486868). The following conditions were employed: Thermo Betasil C-18 analytical column (50 mm x 2.1 mm, 5 μ m particle size; column temperature 40°C) and a Thermo Betasil C-18 guard column (10 mm x 2.1 mm) eluted with a gradient mobile phase of (A) 0.1% formic acid in HPLC-grade water and (B) 0.1% formic acid in acetonitrile [time, percent A:B; time 0.00-0.50 min. 80.0:20.0, 2.50-4.00 min. 20.0:80.0, 4.10-8.00 min. 80.0:20.0] injection volume of 50.0 μ L; and positive ESI ionization MRM scan mode at 500.00°C heater gas temperature. Tiafenacil was identified using two ion transitions (quantitation and confirmation, respectively): m/z 512.128 \rightarrow 479.900 and m/z 512.150 \rightarrow 380.900 for tiafenacil (DCC-3825). Expected retention time was *ca.* 5.2 minutes for tiafenacil (DCC-3825).

ISK Biosciences Analytical Method MFT03817E (ECM 2)

Sediment samples (20 g) were fortified (0.2 mL of 1.0 or 10.0 μ g/mL mixed fortification solutions), as necessary (pp. 15-16 of MRID 50493809). The samples were extracted twice with 90 mL of acetonitrile:water (80:20, v:v) and 0.9 mL of formic acid via shaking for 30 minutes. After centrifugation (3000 rpm for 5 minutes), the extract was decanted into a clean flask. The combined extracts were brought to 200 mL using acetonitrile:water (80:20, v:v). An Oasis HLB VAC RC (60 mg) solid phase extraction (SPE) column was pre-conditioned with 5 mL each of methanol then water:acetic acid (100:1, v:v). The sample was applied to and passed through the column. After the column was washed with 5 mL of water, the analytes were eluted with 9.5 mL of methanol:water (70:30, v:v). The volume of the eluate was adjusted to 10 mL with methanol:water (70:30, v:v).

Analytes were identified and quantified by LC/MS/MS using a Waters Acquity UPLC system coupled to an AB Sciex API 5000 mass spectrometer (pp. 16-17 of MRID 50486868, 50493809). The following conditions were employed for all analytes: Kinetex Biphenyl column (2.1 \times 150 mm, 2.6 μ m; column temperature 40°C) eluted with an isocratic mobile phase of 0.1% formic acid in water:0.1% formic acid in methanol (25:75, v:v); injection volume of 4 μ L; and positive ESI ionization MRM scan mode at 600°C heater gas temperature. Analytes were identified using

two ion transitions (quantitation and confirmation, respectively): m/z 512.2→381.0 and m/z 512.2→152.2 for tiafenacil (DCC-3825), m/z 498.1→381.0 and m/z 498.1→359.1 for M-01, m/z 427.2→380.7 and m/z 427.2→152.0 for M-12, m/z 426.1→380.9 and m/z 426.1→152.0 for M-13, m/z 443.1→218.1 and m/z 443.1→353.0 for M-36, and m/z 445.1→371.0 and m/z 445.1→355.0 for M-53. Expected retention times were 1.74, 1.34, 1.63, 1.33, 1.43, and 1.11 minutes for tiafenacil (DCC-3825), M-01, M-12, M-13, M-36, and M-53, respectively.

ILV

The ILV was performed as an independent validation of ECM 2 (pp. 6, 14 of MRID 50493810). ECM 1 was not performed in the ILV.

In the ILV, ECM 2 was performed as written, except for minor LC/MS/MS instrument (AB Sciex 6500 MS) and parameter modifications (MS ion transitions; pp. 11, 14, 22; Table 14, p. 39 of MRID 50493810). The LC/MS/MS conditions were the same as the ECM 2. Analytes were identified using two ion transitions (quantitation and confirmation, respectively): m/z 512→381 and m/z 512→152 for tiafenacil (DCC-3825), m/z 498→381 and m/z 498→59 for M-01, m/z 427→381 and m/z 427→152 for M-12, m/z 426→381 and m/z 426→152 for M-13, m/z 443→218 and m/z 443→353 for M-36, and m/z 445→371 and m/z 445→355 for M-53. These MS transitions were similar to those of ECM 2, except for the M-01 confirmation transition. Expected retention times were *ca.* 2.15, 1.63, 2.01, 1.61, 1.69, and 1.70 minutes for tiafenacil (DCC-3825), M-01, M-12, M-13, M-36, and M-53, respectively.

LOQ/LOD

For EAG Laboratories Method 548C-107, the Limit of Quantification (LOQ) for tiafenacil in sediment was 0.01 mg/kg in ECM 1 (p. 15 of MRID 50486868). The Limit of Detection (LOD) for tiafenacil in sediment was reported as 0.00000883 mg/kg and 0.00000834 mg/kg using matrix-matched standards and solvent-based standards, respectively, for freshwater and 0.00000329 mg/kg and 0.00000565 mg/kg using matrix-matched standards and solvent-based standards, respectively, for freshwater in ECM 1.

For ISK Biosciences Analytical Method MFT03817E, the LOQ for tiafenacil and its metabolites (M-01, M-12, M-13, M-36, and M-53) in sediment was 0.01 mg/kg in ECM 2 and ILV (pp. 9, 19 of MRID 50493809; pp. 6, 21-22 of MRID 50493810). The LOD was not specifically reported in the ECM 2, but <30% of the LOQ was reported as “no apparent response”. The “no apparent response” threshold for all analytes in sediment was reported as 0.003 mg/kg (30% of the LOQ) in the ILV.

II. Recovery Findings

ECM 1 (MRID 50486868): For EAG Laboratories Method 548C-107, mean recoveries and relative standard deviations (RSDs) were within guideline requirements (mean 70-120%; RSD \leq 20%) for analysis of tiafenacil (DCC-3825) at fortification levels of 0.01 mg/kg (LOQ) and 100 mg/kg (10000 \times LOQ) in two sediment matrices using both solvent-based and matrix-matched standards (Tables 2-5, pp. 21-24). No samples were prepared at 10 \times LOQ. Two ion transitions were used to identify tiafenacil, but results were only provided for the quantitation ion transition. A confirmation method is not usually required when LC/MS or GC/MS is used as the primary method to generate study data because the ion ratios are used to confirm the identity of the compound. The natural freshwater loamy sand sediment [80% sand, 20% silt, 0% clay; pH 5.6 (1:1 soil:water ratio), 1.8% organic carbon, 3.2% organic matter] obtained from West Bearskin Lake, Minnesota, and natural saltwater sand sediment [90% sand, 6% silt, 4% clay; pH 8.1 (1:1 soil:water ratio), 0.37% organic carbon, 0.64% organic matter] obtained from Wye River, Maryland, were used in the study (USDA soil texture classification; p. 12; Appendices 3-6, pp. 54-59). Sediment classification was performed by Agvise Laboratories, Northwood, North Dakota.

ECM 2 (MRID 50493809): For ISK Biosciences Analytical Method MFT03817E, mean recoveries and RSDs were within guideline requirements for analysis of tiafenacil (DCC-3825), M-01, M-12, M-13, M-36, and M-53 at fortification levels of 0.01 mg/kg (LOQ) and 0.1 mg/kg (10 \times LOQ) in two sediment matrices (Tables 2-25, pp. 22-33; DER Attachment 2). All analytes were identified using two ion transitions; performance data (recovery results) for the quantitation and confirmation ion analyses were comparable. Swiss Lake sand sediment [95% sand, 3% silt, 2% clay; pH 6.1 (water), 0.6% organic carbon by wet oxidation] and Calwich Abbey sandy silt loam sediment [39% sand, 49% silt, 13% clay; pH 7.9 (water), 4.9% organic carbon by wet oxidation] obtained from Calwich Abbey Lake were used in the study (USDA Soil texture classification not specified; p. 14; Table 1, p. 22 of MRID 50493809; see Reviewer Comment #7). Both sediments were supplied by Envigo CRS Ltd. in June 2016.

ILV (MRID 50493810): For ISK Biosciences Analytical Method MFT03817E, mean recoveries and RSDs were within guideline requirements for analysis of tiafenacil (DCC-3825), M-01, M-12, M-13, M-36, and M-53 at fortification levels of 0.01 mg/kg (LOQ) and 0.1 mg/kg (10 \times LOQ) in one sediment matrix (Tables 1-12, pp. 25-36). All analytes were identified using two ion transitions; performance data (recovery results) for the quantitation and confirmation ion analyses were comparable, except for the LOQ analysis of M-53. The clay loam sediment [Lab Code # 170110002-018 0-2"; 40% sand, 20% silt, 40% clay; pH 7.4 (1:1 soil:water ratio), 1.5% organic matter] obtained from California was used in the study (USDA soil texture classification; p. 12; Appendix B, pp. 115-119 of MRID 50493810). Sediment classification was performed by Agvise Laboratories, Northwood, North Dakota. The source of the sediment was not further specified. For all analytes, the method was validated after the first trial with insignificant modifications of the analytical parameters (pp. 11, 14, 22). EAG Laboratories Method 548C-107 was not performed.

Table 2. Initial Validation Method Recoveries for Tiafenacil (DCC-3825) and its Metabolites M-01, M-12, M-13, M-36, and M-53 in Sediment

| Analyte | Fortification Level (mg/kg) | Number of Tests | Recovery Range (%) | Mean Recovery (%) | Standard Deviation (%) ¹ | Relative Standard Deviation (%) |
|--|-----------------------------|-----------------|--------------------|-------------------|-------------------------------------|---------------------------------|
| ECM 1 - EAG Laboratories Method 548C-107^{2,3,4} | | | | | | |
| Freshwater Loamy Sand Sediment | | | | | | |
| Solvent-based Standards | | | | | | |
| Tiafenacil (DCC-3825) | 0.01 (LOQ) | 5 | 79.7-90.7 | 83.5 | 4.36 | 5.21 |
| | 100 | 5 | 82.9-91.5 | 85.9 | 3.52 | 4.09 |
| Matrix-matched Standards | | | | | | |
| Tiafenacil (DCC-3825) | 0.01 (LOQ) | 5 | 90.6-101 | 94.1 | 4.11 | 4.37 |
| | 100 | 5 | 93.2-104 | 96.8 | 4.32 | 4.46 |
| Saltwater Sand Sediment | | | | | | |
| Solvent-based Standards | | | | | | |
| Tiafenacil (DCC-3825) | 0.01 (LOQ) | 5 | 84.0-88.3 | 86.4 | 1.58 | 1.82 |
| | 100 | 5 | 83.9-88.6 | 86.2 | 1.68 | 1.95 |
| Matrix-matched Standards | | | | | | |
| Tiafenacil (DCC-3825) | 0.01 (LOQ) | 5 | 84.5-86.8 | 86.2 | 0.988 | 1.15 |
| | 100 | 5 | 81.4-88.7 | 85.6 | 2.84 | 3.31 |
| ECM 2 - ISK Biosciences Analytical Method MFT03817E^{5,6} | | | | | | |
| Swiss Lake Sand Sediment | | | | | | |
| Quantitation Ion Transition | | | | | | |
| Tiafenacil (DCC-3825) | 0.01 (LOQ) | 5 | 97.6-104.0 | 101.9 | 2.6 | 2.6 |
| | 0.1 | 5 | 96.2-101.0 | 99.8 | 2.0 | 2.1 |
| M-01 | 0.01 (LOQ) | 5 | 92.5-96.1 | 94.7 | 1.3 | 1.4 |
| | 0.1 | 5 | 93.0-94.9 | 94.2 | 0.8 | 0.8 |
| M-12 | 0.01 (LOQ) | 5 | 94.2-99.3 | 96.8 | 1.9 | 1.9 |
| | 0.1 | 5 | 98.2-100.3 | 99.2 | 0.8 | 0.8 |
| M-13 | 0.01 (LOQ) | 5 | 91.6-100.5 | 97.2 | 3.3 | 3.4 |
| | 0.1 | 5 | 93.6-97.1 | 95.7 | 1.3 | 1.4 |
| M-36 | 0.01 (LOQ) | 5 | 98.4-105.2 | 101.6 | 2.7 | 2.6 |
| | 0.1 | 5 | 100.3-101.9 | 101.2 | 0.7 | 0.7 |
| M-53 | 0.01 (LOQ) | 5 | 100.4-103.6 | 101.8 | 1.5 | 1.5 |
| | 0.1 | 5 | 98.2-101.4 | 100.0 | 1.2 | 1.1 |
| Confirmation Ion Transition | | | | | | |
| Tiafenacil (DCC-3825) | 0.01 (LOQ) | 5 | 96.3-103.0 | 100.8 | 2.6 | 2.6 |
| | 0.1 | 5 | 96.7-99.1 | 97.8 | 1.0 | 1.0 |
| M-01 | 0.01 (LOQ) | 5 | 92.2-98.5 | 95.0 | 2.5 | 2.6 |
| | 0.1 | 5 | 93.5-95.7 | 94.8 | 0.8 | 0.9 |
| M-12 | 0.01 (LOQ) | 5 | 92.4-104.6 | 101.3 | 5.1 | 5.0 |
| | 0.1 | 5 | 94.6-99.9 | 97.9 | 2.2 | 2.3 |
| M-13 | 0.01 (LOQ) | 5 | 97.6-99.7 | 98.5 | 0.8 | 0.8 |
| | 0.1 | 5 | 93.5-96.8 | 95.8 | 1.3 | 1.4 |
| M-36 | 0.01 (LOQ) | 5 | 98.6-104.7 | 101.9 | 2.4 | 2.4 |
| | 0.1 | 5 | 98.1-102.8 | 100.5 | 2.0 | 2.0 |
| M-53 | 0.01 (LOQ) | 5 | 91.3-103.3 | 97.9 | 5.3 | 5.4 |
| | 0.1 | 5 | 97.3-100.1 | 98.5 | 1.0 | 1.1 |

| Analyte | Fortification Level (mg/kg) | Number of Tests | Recovery Range (%) | Mean Recovery (%) | Standard Deviation (%) ¹ | Relative Standard Deviation (%) |
|---|-----------------------------|-----------------|--------------------|-------------------|-------------------------------------|---------------------------------|
| Calwich Abbey Sandy Silt Loam Sediment | | | | | | |
| Quantitation Ion Transition | | | | | | |
| Tiafenacil (DCC-3825) | 0.01 (LOQ) | 5 | 100.0-103.8 | 101.9 | 1.5 | 1.5 |
| | 0.1 | 5 | 97.6-101.5 | 99.6 | 1.6 | 1.6 |
| M-01 | 0.01 (LOQ) | 5 | 91.2-94.2 | 92.4 | 1.1 | 1.2 |
| | 0.1 | 5 | 89.8-92.8 | 91.5 | 1.1 | 1.2 |
| M-12 | 0.01 (LOQ) | 5 | 95.5-102.0 | 98.3 | 2.4 | 2.4 |
| | 0.1 | 5 | 94.0-96.9 | 95.5 | 1.1 | 1.1 |
| M-13 | 0.01 (LOQ) | 5 | 89.9-95.0 | 93.3 | 2.1 | 2.2 |
| | 0.1 | 5 | 90.3-94.8 | 92.4 | 1.7 | 1.8 |
| M-36 | 0.01 (LOQ) | 5 | 93.6-100.2 | 97.0 | 2.8 | 2.9 |
| | 0.1 | 5 | 90.3-94.6 | 93.4 | 1.8 | 1.9 |
| M-53 | 0.01 (LOQ) | 5 | 93.1-104.7 | 96.0 | 4.9 | 5.1 |
| | 0.1 | 5 | 91.1-92.4 | 91.8 | 0.6 | 0.6 |
| Confirmation Ion Transition | | | | | | |
| Tiafenacil (DCC-3825) | 0.01 (LOQ) | 5 | 97.0-101.3 | 99.2 | 1.6 | 1.6 |
| | 0.1 | 5 | 95.5-98.2 | 97.2 | 1.1 | 1.1 |
| M-01 | 0.01 (LOQ) | 5 | 81.9-95.6 | 89.0 | 5.1 | 5.7 |
| | 0.1 | 5 | 89.2-93.2 | 90.9 | 1.6 | 1.8 |
| M-12 | 0.01 (LOQ) | 5 | 96.7-101.0 | 99.3 | 2.1 | 2.2 |
| | 0.1 | 5 | 94.3-97.3 | 96.1 | 1.2 | 1.2 |
| M-13 | 0.01 (LOQ) | 5 | 90.1-96.1 | 94.0 | 2.5 | 2.6 |
| | 0.1 | 5 | 90.6-94.4 | 92.7 | 1.4 | 1.5 |
| M-36 | 0.01 (LOQ) | 5 | 95.6-109.8 | 101.6 | 5.7 | 5.6 |
| | 0.1 | 5 | 89.8-94.6 | 92.5 | 2.1 | 2.3 |
| M-53 | 0.01 (LOQ) | 5 | 88.0-97.7 | 93.4 | 3.7 | 4.0 |
| | 0.1 | 5 | 87.9-91.5 | 90.0 | 1.3 | 1.5 |

Data (uncorrected recovery results, p. 17 of MRID 50486868; p. 18 of MRID 50493809) were obtained from Tables 2-5, pp. 21-24 of MRID 50486868; Tables 2-25, pp. 22-33 of 50493809 and DER Attachment 2.

1 Standard deviations were reviewer-calculated for ECM 2 since these values were not reported in the study report (MRID 50493809). Rules of significant figures were followed.

2 The natural freshwater loamy sand sediment [80% sand, 20% silt, 0% clay; pH 5.6 (1:1 soil:water ratio), 1.8% organic carbon, 3.2% organic matter] obtained from West Bearskin Lake, Minnesota, and natural saltwater sand sediment [90% sand, 6% silt, 4% clay; pH 8.1 (1:1 soil:water ratio), 0.37% organic carbon, 0.64% organic matter] obtained from Wye River, Maryland, were used in the study (USDA soil texture classification; p. 12; Appendices 3-6, pp. 54-59 of MRID 50486868). Sediment classification was performed by Agvise Laboratories, Northwood, North Dakota.

3 Tiafenacil was identified using two ion transitions (quantitation and confirmation, respectively): m/z 512.128→479.900 and m/z 512.150→380.900 for tiafenacil (DCC-3825).

4 Only results for the quantitation ion transition were reported.

5 The Swiss Lake sand sediment [95% sand, 3% silt, 2% clay; pH 6.1 (water), 0.6% organic carbon by wet oxidation] and Calwich Abbey sandy silt loam sediment [39% sand, 49% silt, 13% clay; pH 7.9 (water), 4.9% organic carbon by wet oxidation] obtained from Calwich Abbey Lake were used in the study (USDA Soil texture classification not specified; p. 14; Table 1, p. 22 of MRID 50493809; see Reviewer Comment #7). Both sediments were supplied by Envigo CRS Ltd. in June 2016.

6 Analytes were identified using two ion transitions (quantitation and confirmation, respectively): m/z 512.2→381.0 and m/z 512.2→152.2 for tiafenacil (DCC-3825), m/z 498.1→381.0 and m/z 498.1→359.1 for M-01, m/z

427.2→380.7 and m/z 427.2→152.0 for M-12, m/z 426.1→380.9 and m/z 426.1→152.0 for M-13, m/z 443.1→218.1 and m/z 443.1→353.0 for M-36, and m/z 445.1→371.0 and m/z 445.1→355.0 for M-53.

Table 3. Independent Validation Method Recoveries for Tiafenacil (DCC-3825) and its Metabolites M-01, M-12, M-13, M-36, and M-53 in Sediment

| Analyte | Fortification Level (mg/kg) | Number of Tests | Recovery Range (%) | Mean Recovery (%) | Standard Deviation (%) | Relative Standard Deviation (%) |
|--|-----------------------------|-----------------|--------------------|-------------------|------------------------|---------------------------------|
| ECM 1 - EAG Laboratories Method 548C-107 | | | | | | |
| Not performed | | | | | | |
| ECM 2 - ISK Biosciences Analytical Method MFT03817E⁵ | | | | | | |
| Clay Loam Sediment | | | | | | |
| Quantitation Ion Transition | | | | | | |
| Tiafenacil (DCC-3825) | 0.01 (LOQ) | 5 | 106.9-112.1 | 110 | 1.9 | 1.7 |
| | 0.1 | 5 | 93.3-96.0 | 95 | 1.1 | 1.2 |
| M-01 | 0.01 (LOQ) | 5 | 113.3-115.7 | 114 | 1.0 | 0.9 |
| | 0.1 | 5 | 97.5-99.9 | 99 | 0.9 | 0.9 |
| M-12 | 0.01 (LOQ) | 5 | 104.7-124.7 | 112 | 8.3 | 7.4 |
| | 0.1 | 5 | 88.9-104.5 | 100 | 6.5 | 6.5 |
| M-13 | 0.01 (LOQ) | 5 | 113.1-116.3 | 114 | 1.3 | 1.1 |
| | 0.1 | 5 | 98.2-101.0 | 100 | 1.2 | 1.2 |
| M-36 | 0.01 (LOQ) | 5 | 102.8-109.6 | 106 | 2.6 | 2.5 |
| | 0.1 | 5 | 94.8-97.8 | 97 | 1.3 | 1.3 |
| M-53 | 0.01 (LOQ) | 5 | 108.2-114.9 | 111 | 2.8 | 2.5 |
| | 0.1 | 5 | 96.2-100.1 | 99 | 1.6 | 1.6 |
| Confirmation Ion Transition | | | | | | |
| Tiafenacil (DCC-3825) | 0.01 (LOQ) | 5 | 104.2-110.7 | 108 | 2.6 | 2.4 |
| | 0.1 | 5 | 94.5-96.7 | 96 | 0.9 | 1.0 |
| M-01 | 0.01 (LOQ) | 5 | 108.2-115.8 | 111 | 2.9 | 2.6 |
| | 0.1 | 5 | 96.5-99.9 | 99 | 1.4 | 1.4 |
| M-12 | 0.01 (LOQ) | 5 | 103.5-117.1 | 111 | 5.5 | 4.9 |
| | 0.1 | 5 | 93.8-111.5 | 102 | 8.0 | 7.8 |
| M-13 | 0.01 (LOQ) | 5 | 111.8-117.2 | 114 | 2.2 | 1.9 |
| | 0.1 | 5 | 99.4-101.9 | 101 | 1.0 | 0.9 |
| M-36 | 0.01 (LOQ) | 5 | 101.8-104.6 | 103 | 1.3 | 1.3 |
| | 0.1 | 5 | 96.0-98.6 | 97 | 1.0 | 1.0 |
| M-53 | 0.01 (LOQ) | 5 | 92.8-118.2 | 99 | 11.0 | 11.2 |
| | 0.1 | 5 | 94.4-101.8 | 98 | 2.8 | 2.8 |

Data (uncorrected recovery results,) were obtained from Tables 1-12, pp. 25-36 of MRID 50493810.

1 The clay loam sediment [Lab Code # 170110002-018 0-2"; 40% sand, 20% silt, 40% clay; pH 7.4 (1:1 soil:water ratio), 1.5% organic matter] obtained from California was used in the study (USDA soil texture classification; p. 12; Appendix B, pp. 115-119). Sediment classification was performed by Agvise Laboratories, Northwood, North Dakota. The source of the sediment was not further described.

2 Analytes were identified using two ion transitions (quantitation and confirmation, respectively): m/z 512→381 and m/z 512→152 for tiafenacil (DCC-3825), m/z 498→381 and m/z 498→59 for M-01, m/z 427→381 and m/z 427→152 for M-12, m/z 426→381 and m/z 426→152 for M-13, m/z 443→218 and m/z 443→353 for M-36, and m/z 445→371 and m/z 445→355 for M-53. These MS transitions were similar to those of the ECM, except for the M-01 confirmation transition.

III. Method Characteristics

For EAG Laboratories Method 548C-107, the LOQ for tiafenacil in sediment was 0.01 mg/kg in ECM 1 (p. 15 of MRID 50486868). In the ECM 1, the LOQ was defined as the lowest fortification level tested which the methodology was validated, yielding acceptable results (mean recovery 70-110%, RSD <20%) and blanks not exceeding 30%. No calculations were reported to support the LOQ. The LOD for tiafenacil in sediment was reported as 0.00000883 mg/kg and 0.00000834 mg/kg using matrix-matched standards and solvent-based standards, respectively, for freshwater and 0.00000329 mg/kg and 0.00000565 mg/kg using matrix-matched standards and solvent-based standards, respectively, for freshwater in ECM 1. The LOD was calculated for each system as the lowest analytical standard concentration (0.000250 mg/kg) divided by the signal to noise ratio and that result times three times the dilution factor of the matrix blank samples (20.0).

For ISK Biosciences Analytical Method MFT03817E, the LOQ for tiafenacil and its metabolites (M-01, M-12, M-13, M-36, and M-53) in sediment was 0.01 mg/kg in ECM 2 and ILV (pp. 9, 19 of MRID 50493809; pp. 6, 21-22 of MRID 50493810). In the ECM 2, the LOQ was defined as the lowest fortification level tested which yielded a mean recovery ranging from 70% to 110% at a relative standard deviation of <20% and blanks not exceeding 30%. The LOQ was reported in the ILV from the ECM without justification. No calculations were reported to support the LOQ. The LOD was not specifically reported in the ECM 2, but <30% of the LOQ was reported as “no apparent response”. The “no apparent response” threshold all analytes in sediment was reported as 0.003 mg/kg (30% of the LOQ) in the ILV; In the ILV, the LOD was defined as the absolute amount of analyte injected into the LC/MS/MS using the lowest calibration standard (0.1 ng/mL). The ILV also reported that acceptable signal-to-noise ratios (S/N >3:1) were demonstrated for all analytes at the LOD; no calculations for the LOD were provided in the ILV.

Table 4a. Method Characteristics - EAG Laboratories Method 548C-107 (ECM 1)

| Analyte | | Tiafenacil (DCC-3825) | | |
|--|--|---|-------------------------|------------------|
| Calibration Standards | | Solvent-based | Matrix-matched | |
| Limit of Quantitation (LOQ) | ECM | 0.01 mg/kg | | |
| | ILV | Not performed¹ | | |
| Limit of Detection (LOD) | ECM | Freshwater | 0.00000834 mg/kg | 0.00000883 mg/kg |
| | | Saltwater | 0.00000565 mg/kg | 0.00000329 mg/kg |
| | ILV | Not performed | | |
| Linearity (calibration curve r^2 and concentration range) ² | ECM | Freshwater | $r^2 = 0.9982$ | $r^2 = 0.9987$ |
| | | Saltwater | $r^2 = \mathbf{0.9860}$ | $r^2 = 0.9973$ |
| | ILV | Not performed | | |
| Concentration range | | 0.000250-0.00250 mg/mL | | |
| Repeatable | ECM ³ | Yes at LOQ and 10000×LOQ (two characterized sediments). No samples prepared at 10×LOQ. | | |
| | ILV | Not performed | | |
| Reproducible | No at LOQ; only one set of performance data provided. No at 10×LOQ; no performance data provided. | | | |
| Specificity | ECM | Yes, no matrix interferences were observed. No representative chromatograms of 10000×LOQ fortification. | | |
| | ILV | Not performed | | |

Data were obtained from p. 15 (LOQ/LOD); Tables 2-5, pp. 21-24 (recovery data); Figures 3-26, pp. 28-51 (calibration curves & chromatograms) of MRID 50486868 (ECM 1); DER Attachment 2.

¹ EAG Laboratories Method 548C-107 (MRID 50486868) did not have an ILV.

² Reported correlation coefficients were reviewer-calculated from r values reported in the study report (Figures 3, 9, 15, and 21, pp. 28, 34, 40, and 46, respectively, of MRID 50486868; DER Attachment 2). Significant figures of r^2 were limited to four.

³ In ECM 1, the natural freshwater loamy sand sediment [80% sand, 20% silt, 0% clay; pH 5.6 (1:1 soil:water ratio), 1.8% organic carbon, 3.2% organic matter] obtained from West Bearskin Lake, Minnesota, and natural saltwater sand sediment [90% sand, 6% silt, 4% clay; pH 8.1 (1:1 soil:water ratio), 0.37% organic carbon, 0.64% organic matter] obtained from Wye River, Maryland, were used in the study (USDA soil texture classification; p. 12; Appendices 3-6, pp. 54-59 of MRID 50486868). Sediment classification was performed by Agvise Laboratories, Northwood, North Dakota.

⁶ See Figures 49-66, pp. 59-67; Figures 103-120, pp. 86-94 of MRID 50486868, 50493809; and Figures 23-24, pp. 109-110; Figures 35-36, pp. 121-122; Figures 44-45, pp. 130-131; Figures 52-53, pp. 138-139 of MRID 50493810.

⁷ Based on Figure 35, p. 121 and Figure 53, p. 139 of MRID 50493810.

Linearity is satisfactory when $r^2 \geq 0.995$.

Table 4b. Method Characteristics - ISK Biosciences Analytical Method MFT03817E (ECM 2)

| Analyte | | Tiafenacil (DCC-3825) | M-01 | M-12 | M-13 | M-36 | M-53 |
|--|--------------------|---|---|--|---|---|--|
| Limit of Quantitation (LOQ) | | 0.01 mg/kg | | | | | |
| Limit of Detection (LOD) | ECM | Not reported | | | | | |
| | ILV | 0.003 mg/kg | | | | | |
| Linearity (calibration curve r^2 and concentration range) ¹ | ECM | $r^2 = 0.9998$ (Q & C) | $r^2 = 0.1000$ (Q) $r^2 = 0.9998$ (C) | $r^2 = 0.9996$ (Q) $r^2 = 0.9994$ (C) | $r^2 = 0.9996$ (Q) $r^2 = 0.9998$ (C) | $r^2 = 0.9998$ (Q) $r^2 = 0.9996$ (C) | $r^2 = 0.9998$ (Q) $r^2 = 0.9994$ (C) |
| | | 0.010-10 ng/mL | | | | | |
| | ILV | $r^2 = 0.9992$ (Q) $r^2 = 0.9994$ (C) | $r^2 = 0.9996$ (Q) $r^2 = 0.9998$ (C) | $r^2 = 0.9992$ (Q) $r^2 = 0.9974$ (C) | $r^2 = 1.0000$ (Q & C) | $r^2 = 0.9942$ (Q) $r^2 = 0.9940$ (C) | $r^2 = 0.9998$ (Q) $r^2 = 0.9990$ (C) |
| | | 0.004-0.4 ng | | | | | |
| Repeatable | ECM ² | Yes at LOQ and 10×LOQ (two characterized sediments). | | | | | |
| | ILV ^{3,4} | Yes at LOQ and 10×LOQ (one characterized sediment). | | | | | |
| Reproducible | | Yes at LOQ and 10×LOQ. | | | | | |
| Specificity | ECM | Yes, matrix interferences were <1% of the LOQ (based on peak area). | Yes, matrix interferences were <1% of the LOQ (based on peak area). | Yes, no matrix interferences were observed. Persistent contaminants at RT - 0.3 min of analyte were observed in all chromatograms. | Yes, matrix interferences were <1% of the LOQ (based on peak area). | Yes, matrix interferences were <1% of the LOQ (based on peak area). Peak fronting was noted. | Yes, no matrix interferences were observed. Persistent contaminants at RT + 0.3 min of analyte were observed in all chromatograms. |
| | ILV | Yes, no matrix interferences were observed. | Yes, no matrix interferences were observed. | Yes, no matrix interferences were observed. Some baseline noise was noted around the analyte peak at LOQ. Persistent contaminants at RT - 0.4 min of analyte were observed in all chromatograms. | Yes, no matrix interferences were observed. | Yes, no matrix interferences were observed; however, peak shouldering was noted. ⁵ | Yes, no matrix interferences were observed. Persistent contaminants at RT ± 0.3 min of analyte were observed in all chromatograms. |

Data were obtained from pp. 9, 19 (LOQ/LOD); Tables 2-25, pp. 22-33 (recovery data); Figures 1-12, pp. 34-39 (calibration curve); Figures 13-120, pp. 40-93 (chromatograms) of MRID 50493809; pp. 6, 21-22 (LOQ/LOD); Tables 1-12, pp. 25-36 (recovery data); Figures 1-6, pp. 41-46 (calibration curves); Figures 7-

36, pp. 47-106 (chromatograms); Appendix D, pp. 223-234 (calibration data) of MRID 50493810; DER Attachment 2. Q = Quantitation ion transition; C = Confirmatory ion transition.

- 1 Reported correlation coefficients were reviewer-calculated from r values reported in the study report (Figures 1-12, pp. 34-39 of 50493809; Appendix D, pp. 223-234 of MRID 50493810; DER Attachment 2). Significant figures of r^2 were limited to four.
- 2 In ECM 2, Swiss Lake sand sediment [95% sand, 3% silt, 2% clay; pH 6.1 (water), 0.6% organic carbon by wet oxidation] and Calwich Abbey sandy silt loam sediment [39% sand, 49% silt, 13% clay; pH 7.9 (water), 4.9% organic carbon by wet oxidation] obtained from Calwich Abbey Lake were used in the study (USDA Soil texture classification not specified; p. 14; Table 1, p. 22 of MRID 50493809; see Reviewer Comment #7). Both sediments were supplied by Envigo CRS Ltd. in June 2016.
- 3 In the ILV, the clay loam sediment [Lab Code # 170110002-018 0-2"; 40% sand, 20% silt, 40% clay; pH 7.4 (1:1 soil:water ratio), 1.5% organic matter] obtained from California was used in the study (USDA soil texture classification; p. 12; Appendix B, pp. 115-119 of MRID 50493810). Sediment classification was performed by Agvise Laboratories, Northwood, North Dakota. The source of the sediment was not further specified.
- 4 For all analytes, the method was validated after the first trial with insignificant modifications of the analytical parameters (pp. 11, 14, 22 of MRID 50493810).
- 5 See Figures 31-32, pp. 101-102 of MRID 50493810. This peak shouldering was also seen in the ILV calibration standards (Figure 11, pp. 71-76). Linearity is satisfactory when $r^2 \geq 0.995$.

IV. Method Deficiencies and Reviewer's Comments

1. For EAG Laboratories Method 548C-107, only one set of performance data was submitted, an ECM in MRID 50486868. No ILV of the EAG Laboratories Method 548C-107 was submitted.
2. The following additional deficiencies were noted for EAG Laboratories Method 548C-107 in MRID 50486868:

No samples were prepared at the 10×LOQ fortification level. OCSPP guidelines state that a minimally complete sample set includes a reagent blank, two matrix blanks, five samples spiked at the LOQ, and five samples spiked at 10× LOQ for each matrix. While spikes at 10x the LOQ were not specifically analyzed. Samples were examined at 100 mg/kg-sediment.

No representative chromatograms of 10000×LOQ fortification were provided for review.

3. For ISK Biosciences Analytical Method MFT03817E, following deficiencies were noted:

The LOD was not specifically reported in the ECM, but <30% of the LOQ was reported as “no apparent response” (pp. 9, 19 of MRID 50493809).

4. Matrix effects were studied in the ILV and determined to be insignificant for all analytes, except M-36; however, solvent-based calibrations were used for analysis of all analytes (p. 17 of MRID 50493810).
5. Peak shouldering of the M-36 analyte peak was noted in all ILV chromatograms (Figure 11, pp. 71-76; Figures 31-32, pp. 101-102 of MRID 50493810). The reviewer noted that that the chemical purity of M-36 was 99.2% in the ILV (p. 14 of MRID 50493810).
6. Persistent contaminants at RT – 0.3 to 0.4 min. of M-12 and ± 0.3 min of M-53 were observed in all M-12 and M-53 chromatograms of the ECM and ILV (Figures 13-120, pp. 40-93 of MRID 50493809; and Figures 7-36, pp. 47-106 of MRID 50493810). The study author did not address these contaminants. The reviewer noted that that the chemical purities of M-12 and M-53 were 97.4-98.6% and 93.9-94.7%, respectively, in the ECM and ILV (pp. 13-14 of MRID 50493809; pp. 13-14 of MRID 50493810).
7. The ILV sediment [clay loam sediment; Lab Code # 170110002-018 0-2”; 40% sand, 20% silt, 40% clay; pH 7.4 (1:1 soil:water ratio), 1.5% organic matter] can be compared to the ILV soil used in the submitted soil method validation [mainly sandy loam (characterized as such in five of six depths) with one depth characterized as sandy clay loam; Agvise Sample IDs 15-1291 to 15-1296; 63-65% sand, 16-22% silt, 15-21% clay; pH 6.4-8.4; 0.22-1.7% organic carbon] since that ILV soil was collected from the tiafenacil terrestrial field dissipation study (Trial ID PSM-15-06-03, GPL Study # 150614) located in Northwood, North Dakota (p. 12; Appendix B, pp. 115-119 of MRID

50493810; p. 31 of MRID 50493806). USDA soil texture classification used for both sediment matrices.

In ECM 2, the Calwich Abbey sediment matrix was classified as sandy silt loam sediment, but USDA Soil texture classification not specified (p. 14; Table 1, p. 22 of MRID 50493809). The reviewer noted that the particle distribution based on USDA soil classification was 39% sand, 49% silt, 13% clay; however, these values summed to 99%, not 100%. Using the soil texture calculator based on USDA soil texture particle distributions, the reviewer determined that the sediment was loam.

8. The estimation of LOQ and LOD in ECM 1, ECM 2, and ILV was not based on scientifically acceptable procedures as defined in 40 CFR Part 136 (p. 15 of MRID 50486868; pp. 9, 19 of MRID 50493809; pp. 6, 21-22 of MRID 50493810). In the ECM 1 and 2, the LOQ was defined as the lowest fortification level tested which yielded acceptable results (mean recovery 70-110%, RSD <20%) and blanks not exceeding 30% of the LOQ. The LOQ was reported in the ILV from the ECM 2 without justification. No calculations were reported to support the LOQ. In ECM 1, the LOD was calculated for each system as the lowest analytical standard concentration (0.000250 mg/kg) divided by the signal to noise ratio and that result times three times the dilution factor of the matrix blank samples (20.0). In the ILV, the LOD was defined as the absolute amount of analyte injected into the LC/MS/MS using the lowest calibration standard (0.01 ng/mL). The ILV also reported that acceptable signal-to-noise ratios (S/N >3:1) were demonstrated for all analytes at the LOD; no calculations for the LOD were provided in the ILV. Detection limits should not be based on arbitrary values.
9. The ILV reported that no communication between the ILV Study Director and Study Monitor occurred, and the sponsors did not visit the testing facility during the study (p. 22 of MRID 50493810).
10. Storage stability was studied in the ILV, and it was determined that all analytes were stable for up to 7 days of storage (storage conditions not reported; p. 18 of MRID 50493810).
11. In the ILV, the time required to complete the extraction of one set of 13 samples required *ca.* 24 hours of work, including calculation of results (p. 21 of MRID 50493810).

V. References

U.S. Environmental Protection Agency. 2012. Ecological Effects Test Guidelines, OCSPP 850.6100, Environmental Chemistry Methods and Associated Independent Laboratory Validation. Office of Chemical Safety and Pollution Prevention, Washington, DC. EPA 712-C-001.

40 CFR Part 136. Appendix B. Definition and Procedure for the Determination of the Method Detection Limit-Revision 1.11, pp. 317-319.

Attachment 1: Chemical Names and Structures

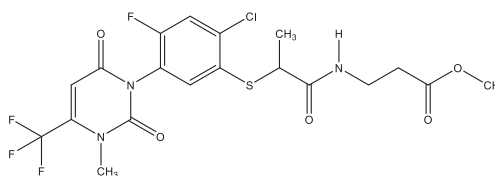
Tiafenacil (DCC-3825)

IUPAC Name: Methyl 3-[(2RS)-2-{2-chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1(6H)-yl]phenylthio}propionamido]propionate

CAS Name: Methyl N-[2-[[2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluorophenyl]thio]-1-oxopropyl]-β-alaninate

CAS Number: 1220411-29-9

SMILES String: O=C(C=C(C(F)(F)F)N1C)N(C2=C(F)C=C(Cl)C(SC(C)C(N([H])CCC(O)C)=O)=O)=C2)C1=O



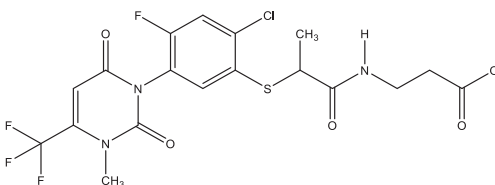
M-01 (DCC-3825-M-01)

IUPAC Name: 3-(2-((2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydropyrimidin-1(2H)-yl)phenyl)thio)propanamido)propanoic acid

CAS Name: Not reported

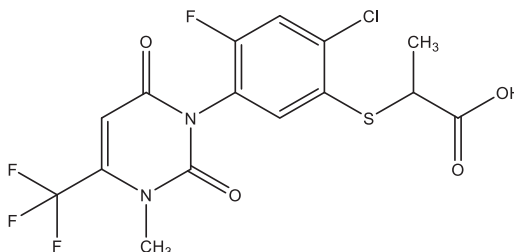
CAS Number: Not reported

SMILES String: O=C(C=C(C(F)(F)F)N1C)N(C2=C(F)C=C(Cl)C(SC(C)C(N([H])CCC(O)=O)=O)=O)=C2)C1=O

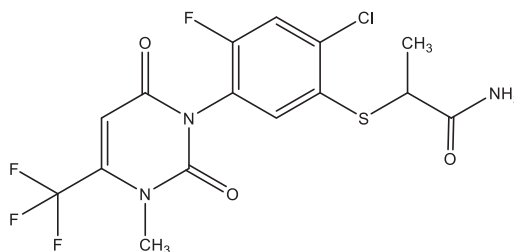


M-12 (DCC-3825-M-12)

IUPAC Name: 2-((2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydropyrimidin-1(2H)-yl)phenyl)thio)propanoic acid
CAS Name: Not reported
CAS Number: Not reported
SMILES String: O=C(C=C(C(F)(F)F)N1C)N(C2=C(F)C=C(Cl)C(SC(C)C(O)=O)=C2)C1=O

**M-13 (DCC-3825-M-13)**

IUPAC Name: 2-((2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydropyrimidin-1(2H)-yl)phenyl)thio)propanamide
CAS Name: Not reported
CAS Number: Not reported
SMILES String: O=C(C=C(C(F)(F)F)N1C)N(C2=C(F)C=C(Cl)C(SC(C)C(N)=O)=C2)C1=O



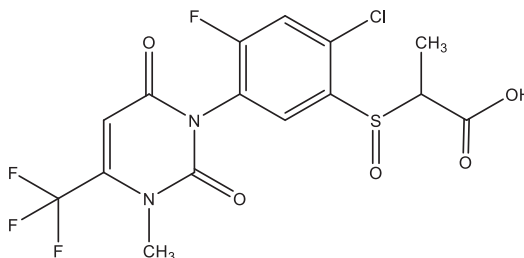
M-36 (DCC-3825-M-36)

IUPAC Name: 2-((2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydropyrimidin-1(2H)-yl)phenyl)sulfinyl)propanoic acid

CAS Name: Not reported

CAS Number: Not reported

SMILES String: CN(C(N1C2=C(F)C=C(Cl)C(S(C(C)C(O)=O)=O)=C2)=O)C(C(F)(F)F)=CC1=O

**M-53 (DCC-3825-M-53)**

IUPAC Name: 2-((2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)tetrahydropyrimidin-1(2H)-yl)phenyl)sulfinyl)propanoic acid

CAS Name: Not reported

CAS Number: Not reported

SMILES String: CN(C(N1C2=C(F)C=C(Cl)C(S(C(C)C(O)=O)=O)=C2)=O)C(C(F)(F)F)C1=O

