

Supplementary data for article:

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Supporting information

A chemotype that inhibits three unrelated pathogenic targets: the botulinum neurotoxin serotype A light chain, *P. falciparum* malaria, and the Ebola filovirus

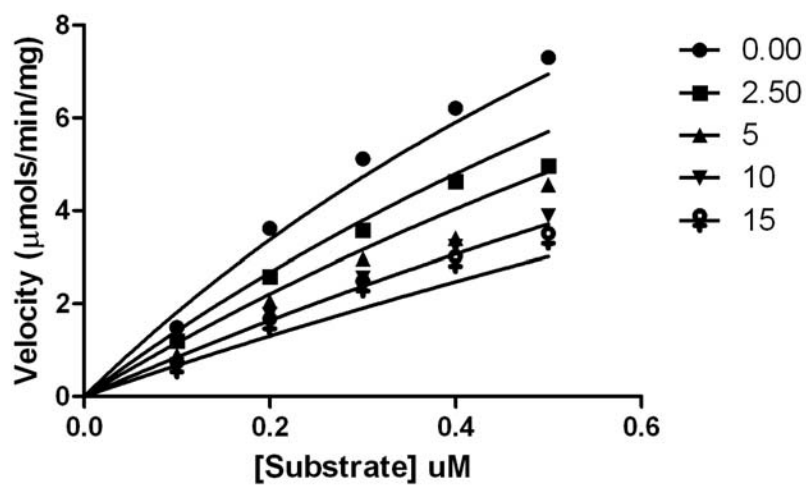
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Plot of the BoNT/A LC inhibition kinetics for **7**.



Plot of the BoNT/A LC inhibition kinetics for **8**.

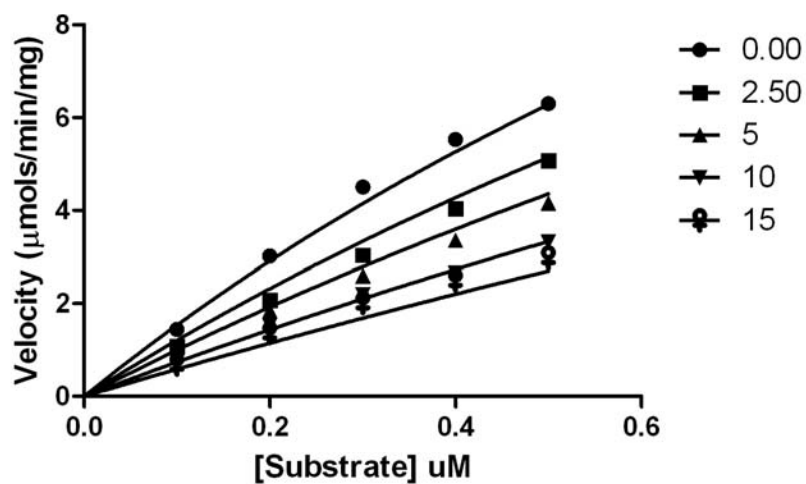


Figure S1: BoNT/A LC inhibition. Plots of the kinetics data from determination of the K_i values for **7** and **8** indicate that 1,7-DAAC-based SMNPIs are competitive inhibitors.

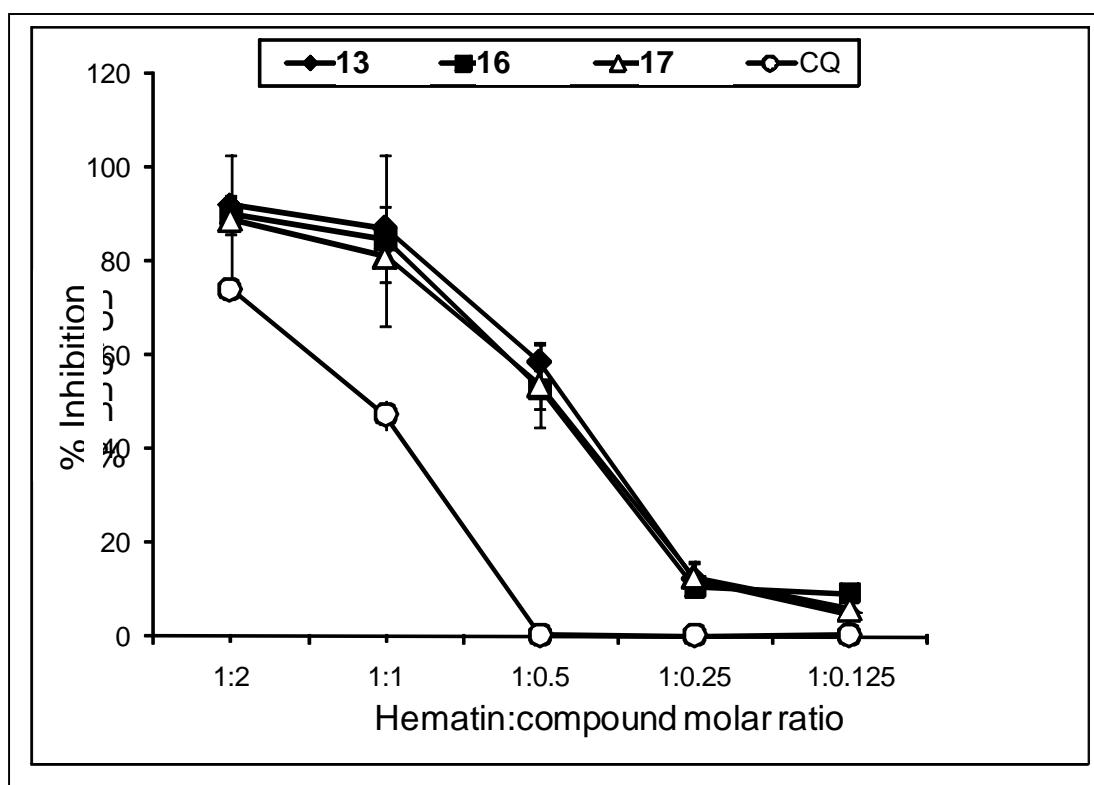


Figure S2: Plots of the dose-dependent inhibition of β -hematin formation by **13**, **16**, **17**, and **CQ**.

Table S1: The in vitro cytotoxicities of 1,7-DAAC SMNPIs versus the RAW 264.7 (mouse macrophage) cell line, and corresponding Selectivity Indices.

| Compound | In vitro cytotoxicity (nM) | | SI (IC ₅₀)* | | | SI (IC ₉₀)* | | |
|-----------|----------------------------|------------------|-------------------------|---------|----------|-------------------------|---------|----------|
| | IC ₅₀ | IC ₉₀ | D6 | W2 | TM91C235 | D6 | W2 | TM91C235 |
| 1 | 1155 | 1842 | 38.48 | 133.53 | 17.37 | 37.19 | 39.42 | 6.55 |
| 7 | 2148 | 2571 | 3.03 | 1.26 | 1.06 | 2.54 | 0.79 | 0.84 |
| 8 | 5260 | 9657 | 19.46 | 6.04 | 5.15 | 27.20 | 5.41 | 5.48 |
| 9 | 997 | 1892 | 9.64 | 2.83 | 18.19 | 9.00 | 2.67 | 2.71 |
| 10 | 2559 | 5348 | 163.93 | 278.46 | 167.58 | 256.87 | 171.25 | 205.53 |
| 11 | 9348 | 10717 | 1555.41 | 2686.21 | 2815.66 | 1189.46 | 1058.99 | 2827.70 |
| 12 | 444 | 444 | 29.92 | 57.29 | 12.95 | 11.27 | 17.52 | 4.66 |
| 13 | 4945 | 13645 | 295.05 | 609.74 | 190.93 | 422.71 | 487.32 | 338.75 |
| 14 | 1474 | 2109 | 159.18 | 211.18 | 59.34 | 120.00 | 93.73 | 51.16 |
| 15 | 1866 | 2108 | 212.29 | 339.27 | 176.87 | 159.58 | 137.15 | 141.19 |
| 16 | 7481 | 11029 | 1430.40 | 3740.50 | 929.32 | 1302.12 | 1728.68 | 635.31 |
| 17 | 10174 | 29917 | 1715.68 | 1662.42 | 1033.94 | 2374.36 | 2601.48 | 1815.35 |

* SI (Selectivity Index) = in vitro cytotoxicity (nM) / in vitro P.f. (nM)

Table S2. Antiviral inhibition provided by select 1,7-DAAC SMNPIs (primary screen data, % inhibition at 20 μ M conc. SMNPI)

| Compound | Ebola-GFP |
|-----------|-----------|
| 7 | 65 |
| 8 | 98 |
| 9 | 100 |
| 11 | 97 |
| 13 | 100 |
| 14 | 100 |
| 16 | 96 |
| 17 | 53 |

Combustion analyses

| Compound | Calculated | Found |
|---|--------------------------|--------------------------|
| 7 (C ₂₄ H ₃₀ N ₆ × 4HCl × 4H ₂ O (620.44)) | C 46.46; H 6.82; N 13.55 | C 45.99; H 6.70; N 13.54 |
| 8 (C ₂₂ H ₂₆ N ₆ × 4HCl × 2H ₂ O (556.36)) | C 47.49; H 6.16; N 15.11 | C 47.46; H 5.76; N 15.02 |
| 9 (C ₂₈ H ₃₈ N ₆ × 4HCl × 6H ₂ O (712.58)) | C 47.19; H 7.64; N 11.79 | C 47.12; H 8.07; N 12.02 |
| 10 (C ₂₆ H ₃₄ N ₆ × 4HCl × 4H ₂ O (648.49)) | C 48.15; H 7.15; N 12.96 | C 48.08; H 6.68; N 12.67 |
| 11 (C ₃₂ H ₄₆ N ₆ × 4HCl × 2H ₂ O (696.62)) | C 55.17; H 7.81; N 12.06 | C 54.78; H 7.44; N 11.70 |
| 11 (C ₃₀ H ₄₂ N ₆ × 4HCl × 4H ₂ O (704.60)) | C 51.14; H 7.72; N 11.93 | C 51.62; H 7.15; N 11.81 |
| 12 (C ₃₂ H ₄₂ N ₆ × 4HCl × 7H ₂ O (782.67)) | C 49.11; H 7.73; N 10.74 | C 48.86; H 7.46; N 10.78 |
| 13 (C ₃₀ H ₃₈ N ₆ × 4HCl × 11H ₂ O (826.68)) | C 43.59; H 7.80; N 10.17 | C 44.02; H 7.57; N 10.26 |
| 14 (C ₃₄ H ₄₆ N ₆ × 4HCl × 4H ₂ O (756.67)) | C 53.97; H 7.73; N 11.11 | C 53.47; H 8.07; N 11.09 |
| 15 (C ₃₂ H ₄₂ N ₆ × 4HCl × 3H ₂ O (710.61)) | C 54.09; H 7.38; N 11.83 | C 53.45; H 7.79; N 11.79 |
| 16 (C ₃₂ H ₄₂ N ₆ O ₂ × 4HCl × 6H ₂ O (796.65)) | C 48.24; H 7.34; N 10.55 | C 48.43; H 7.26; N 10.60 |
| 17 (C ₃₀ H ₃₈ N ₆ O ₂ × 4HCl × 4H ₂ O (732.57)) | C 49.19; H 6.88; N 11.47 | C 49.54; H 6.08; N 11.52 |

HPLC analyses for purity.

Compounds were analyzed for purity (HPLC) using a Waters 1525 HPLC dual pump system equipped with an Alltech, SelectTM degasser system and dual λ 2487 UV-VIS detector.

Octadecylsilica was used as the stationary phase (Symmetry C18 analytical column, 4.6 \times 150 mm, 5 μ m, Ser. No. 021336278136 37). Eluent was made from solvents 0.2 % formic acid in water (A) and methanol (B).

Compound **1** was eluted using gradient protocol 0-1.5 min 75% A, 3-9 min 75% \rightarrow 25% A, 9-11 min 25% A, 11-12 min 25% \rightarrow 75% A, flow 1.00 mL/min, wavelength 385 nm.

Compounds **6, 7, 8, 12, 14, 16**, were eluted using gradient protocol 0-1.5 min 60% A, 1.5-12 min 60% \rightarrow 40% A, 12-15 min 40 % A, 15-16 min 40% \rightarrow 60% A, flow 1.00 mL/min, wavelength 385 nm.

Compound **9** was eluted using gradient protocol 0-1.5 min 90% A, 1.5-12 min 90% \rightarrow 10% A, 12-15 min 10 % A, 15-16 min 10% \rightarrow 90% A, flow 1.00 mL/min, wavelength 363 nm.

Compound **10** was eluted using gradient protocol 0-1.5 min 80% A, 1.5-12 min 80% \rightarrow 20% A, 12-15 min 20 % A, 15-16 min 20% \rightarrow 80% A, flow 1.00 mL/min, wavelength 385 nm.

Compound **11** was eluted using gradient protocol 0-3 min 90% A, 3-9 min 90% \rightarrow 10% A, 9-11 min 10 % A, 11-12 min 10% \rightarrow 90% A, flow 1.00 mL/min, wavelength 385 nm.

Compound **13** was eluted using gradient protocol 0-1.5 min 55% A, 1.5-12 min 55% \rightarrow 45% A, 12-15 min 45 % A, 15-16 min 45% \rightarrow 55% A, flow 1.00 mL/min, wavelength 385 nm.

Compound **15** was eluted using gradient protocol 0-3 min 85% A, 3-9 min 85% \rightarrow 15% A, 9-11 min 15 % A, 11-12 min 15% \rightarrow 85% A, flow 1.00 mL/min, wavelength 360 nm.

Compound **17** was eluted using gradient protocol 0-1.5 min 95% A, 1.5-12 min 95% \rightarrow 5% A, 12-15 min 5 % A, 15-16 min 5% \rightarrow 95% A, flow 1.00 mL/min, wavelength 385nm.

For data processing, Empower software was used. All compounds were > 95% pure.



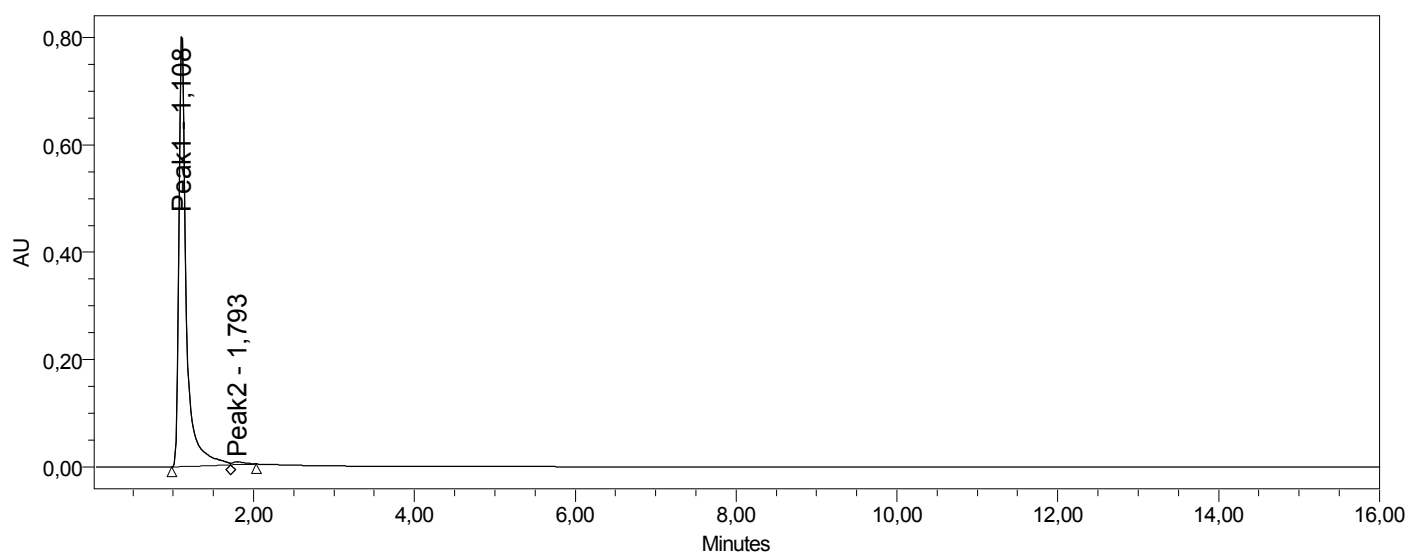
Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | | | |
|-------------------|------------------------------|---------------------|---------------------|
| Sample Name: | 80 20 385 Compound 16 | Acquired By: | System |
| Sample Type: | Unknown | Date Acquired: | 17.11.2010 10:49:33 |
| Vial: | 2 | Acq. Method Set: | 60 40 385 BDI 17_MS |
| Injection #: | 1 | Date Processed: | 17.11.2010 15:43:32 |
| Injection Volume: | 10,00 ul | Processing Method: | 16 |
| Run Time: | 16,0 Minutes | Channel Name: | 2487Channel 1 |
| Sample Set Name: | | Proc. Chnl. Descr.: | |



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|-------|---------|--------|--------|
| 1 | Peak1 | 1,108 | 5300067 | 98,93 | 804835 |
| 2 | Peak2 | 1,793 | 57090 | 1,07 | 5681 |



Reported by User: System

Project Name: Hrizeni

Instrument Method: 60 40 385 BDI 17_IM

Stored: 16.11.2010 14:47:14

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 385
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|---------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,60 | Solvent A | 2%HCOOH |
| Flow B | 0,40 | Solvent B | MeOH |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|------|-----|-------|
| 1 | | 1,00 | 60,0 | 40,0 | 0,0 | |
| 2 | 1,50 | 1,00 | 60,0 | 40,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 3 | 12,00 | 1,00 | 40,0 | 60,0 | 0,0 | 6 |
| 4 | 15,00 | 1,00 | 40,0 | 60,0 | 0,0 | 6 |



Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 5 | 16,00 | 1,00 | 60,0 | 40,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|---------------------|------------|----------|---------------------|---------------|--------|-----------|
| 1 | 60 40 385 BDI 17_IM | Instrument | | 16.11.2010 14:47:14 | System | No | 1293 |

Method Version Summaries

| | Method Version |
|---|----------------|
| 1 | 1 |



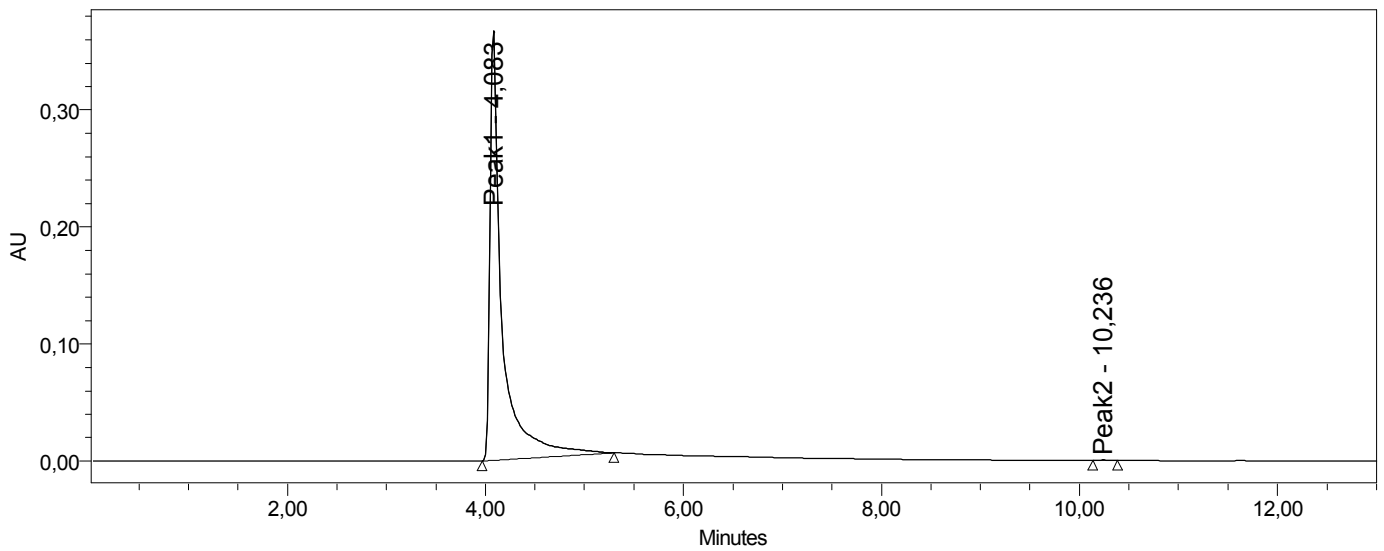
Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | | | |
|-------------------|-----------------------------|---------------------|---------------------|
| Sample Name: | 95 5 385 Compound 17 | Acquired By: | System |
| Sample Type: | Unknown | Date Acquired: | 16.11.2010 12:36:01 |
| Vial: | 7 | Acq. Method Set: | 95 5 385 BG11_MS |
| Injection #: | 1 | Date Processed: | 17.11.2010 15:38:52 |
| Injection Volume: | 10,00 ul | Processing Method: | 17 |
| Run Time: | 13,0 Minutes | Channel Name: | 2487Channel 1 |
| Sample Set Name: | | Proc. Chnl. Descr.: | |



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|--------|---------|--------|--------|
| 1 | Peak1 | 4,083 | 3129992 | 99,90 | 363680 |
| 2 | Peak2 | 10,236 | 3235 | 0,10 | 680 |



Reported by User: System

Project Name: Hrizeni

Instrument Method: 95 5 385 BG11_IM

Stored: 10.11.2010 11:57:49

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 385
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|---------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,95 | Solvent A | 2%HCOOH |
| Flow B | 0,05 | Solvent B | MeOH |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|-----|-----|-------|
| 1 | | 1,00 | 95,0 | 5,0 | 0,0 | |
| 2 | 1,50 | 1,00 | 95,0 | 5,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|-----|------|-----|-------|
| 3 | 12,00 | 1,00 | 5,0 | 95,0 | 0,0 | 6 |
| 4 | 15,00 | 1,00 | 5,0 | 95,0 | 0,0 | 6 |



Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|-----|-----|-------|
| 5 | 16,00 | 1,00 | 95,0 | 5,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|------------------|------------|----------|---------------------|---------------|--------|-----------|
| 1 | 95 5 385 BG11_IM | Instrument | | 10.11.2010 11:57:49 | System | No | 1107 |

Method Version Summaries

| | Method Version |
|---|----------------|
| 1 | 1 |



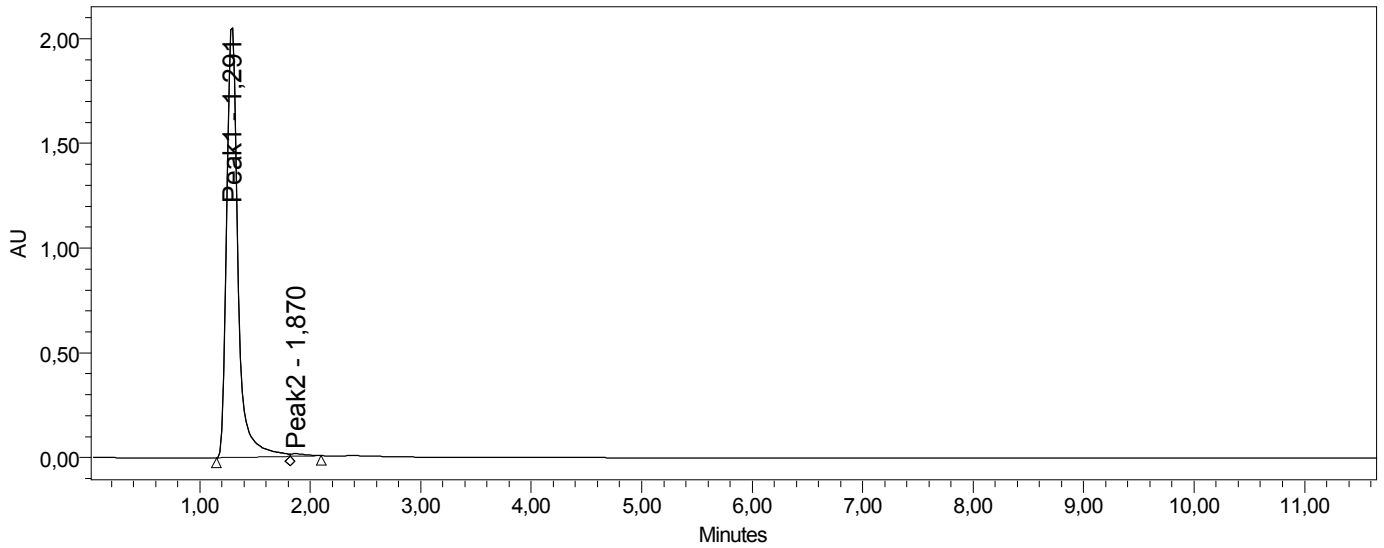
Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | | | |
|-------------------|------------------------------|---------------------|---------------------|
| Sample Name: | 55 45 385 Compound 13 | Acquired By: | System |
| Sample Type: | Unknown | Date Acquired: | 16.11.2010 15:33:42 |
| Vial: | 14 | Acq. Method Set: | 55 45 385 BDI 17_MS |
| Injection #: | 1 | Date Processed: | 17.11.2010 15:40:53 |
| Injection Volume: | 10,00 ul | Processing Method: | 13 |
| Run Time: | 15,0 Minutes | Channel Name: | 2487Channel 1 |
| Sample Set Name: | | Proc. Chnl. Descr.: | |



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|-------|----------|--------|---------|
| 1 | Peak1 | 1,291 | 14857040 | 99,26 | 2079380 |
| 2 | Peak2 | 1,870 | 111135 | 0,74 | 12538 |



Reported by User: System

Project Name: Hrizeni

Instrument Method: 55 45 385 BDI 17_IM

Stored: 16.11.2010 15:14:58

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 385
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|---------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,55 | Solvent A | 2%HCOOH |
| Flow B | 0,45 | Solvent B | MeOH |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|------|-----|-------|
| 1 | | 1,00 | 55,0 | 45,0 | 0,0 | |
| 2 | 1,50 | 1,00 | 55,0 | 45,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 3 | 12,00 | 1,00 | 45,0 | 55,0 | 0,0 | 6 |
| 4 | 15,00 | 1,00 | 45,0 | 55,0 | 0,0 | 6 |



Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 5 | 16,00 | 1,00 | 55,0 | 45,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|---------------------|------------|----------|---------------------|---------------|--------|-----------|
| 1 | 55 45 385 BDI 17_IM | Instrument | | 16.11.2010 15:14:58 | System | No | 1300 |

Method Version Summaries

| | Method Version |
|---|----------------|
| 1 | 1 |



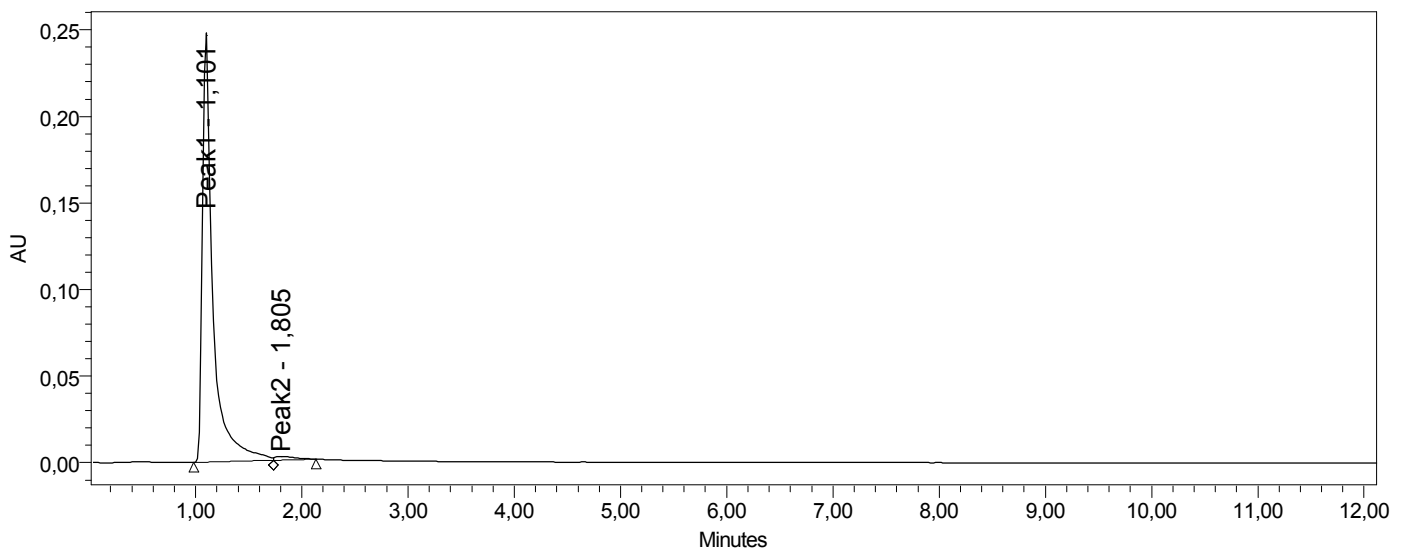
Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | | | |
|-------------------|-----------------------------|---------------------|---------------------|
| Sample Name: | 60 40 385 Compound 6 | Acquired By: | System |
| Sample Type: | Unknown | Date Acquired: | 17.11.2010 13:35:45 |
| Vial: | 8 | Acq. Method Set: | 60 40 385 BDI 17_MS |
| Injection #: | 1 | Date Processed: | 17.11.2010 15:48:08 |
| Injection Volume: | 10,00 ul | Processing Method: | 6 |
| Run Time: | 14,0 Minutes | Channel Name: | 2487Channel 1 |
| Sample Set Name: | | Proc. Chnl. Descr.: | |



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|-------|---------|--------|--------|
| 1 | Peak1 | 1,101 | 1703103 | 98,43 | 244353 |
| 2 | Peak2 | 1,805 | 27203 | 1,57 | 2213 |



Reported by User: System

Project Name: Hrizeni

Instrument Method: 60 40 385 BDI 17_IM

Stored: 16.11.2010 14:47:14

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 385
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|---------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,60 | Solvent A | 2%HCOOH |
| Flow B | 0,40 | Solvent B | MeOH |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|------|-----|-------|
| 1 | | 1,00 | 60,0 | 40,0 | 0,0 | |
| 2 | 1,50 | 1,00 | 60,0 | 40,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 3 | 12,00 | 1,00 | 40,0 | 60,0 | 0,0 | 6 |
| 4 | 15,00 | 1,00 | 40,0 | 60,0 | 0,0 | 6 |



Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 5 | 16,00 | 1,00 | 60,0 | 40,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|---------------------|------------|----------|---------------------|---------------|--------|-----------|
| 1 | 60 40 385 BDI 17_IM | Instrument | | 16.11.2010 14:47:14 | System | No | 1293 |

Method Version Summaries

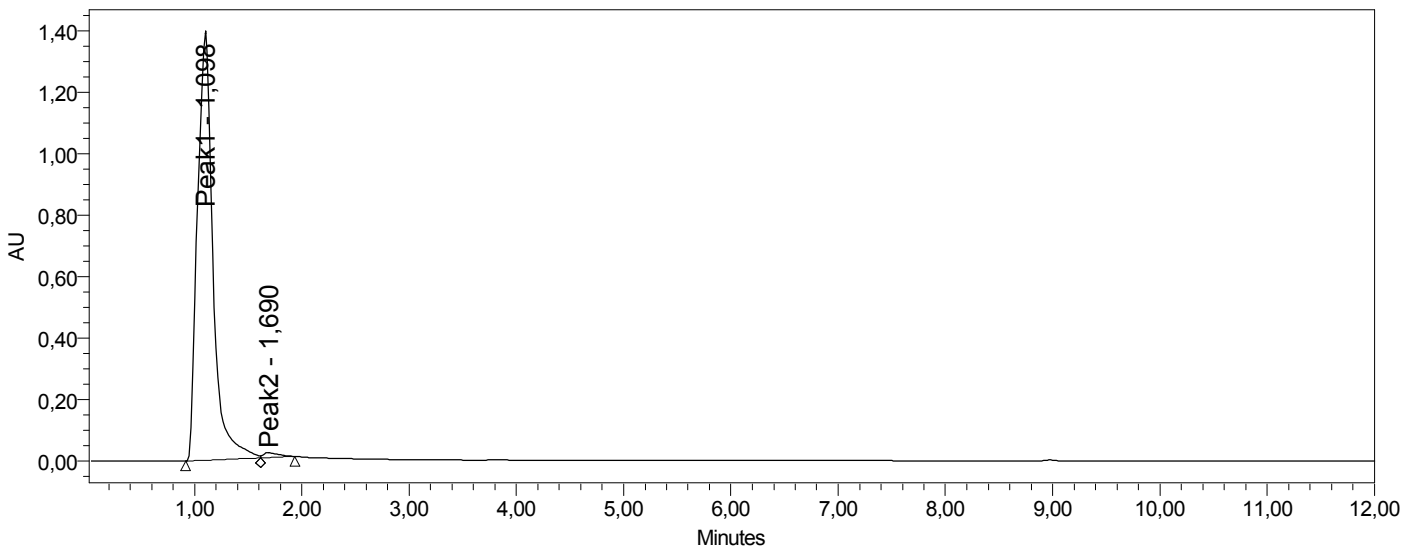
| | Method Version |
|---|----------------|
| 1 | 1 |

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | |
|--|---|
| <p>Sample Name: 75 25 385 Compound 1 Sample Type: Unknown Vial: 6 Injection #: 1 Injection Volume: 10,00 ul Run Time: 12,0 Minutes Sample Set Name:</p> | <p>Acquired By: System Date Acquired: 11.11.2010 14:10:45 Acq. Method Set: 75 25 385 BG11_MS Date Processed: 17.11.2010 15:14:15 Processing Method: 1 Channel Name: 2487Channel 1 Proc. Chnl. Descr.:</p> |
|--|---|



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|-------|----------|--------|---------|
| 1 | Peak1 | 1,098 | 13999309 | 98,88 | 1393080 |
| 2 | Peak2 | 1,690 | 158155 | 1,12 | 16023 |



Reported by User: System

Project Name: Hrizeni

Instrument Method: 75 25 385 BG11_IM

Stored: 11.11.2010 13:50:09

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 385
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|---------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,75 | Solvent A | 2%HCOOH |
| Flow B | 0,25 | Solvent B | MeOH |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|------|-----|-------|
| 1 | | 1,00 | 75,0 | 25,0 | 0,0 | |
| 2 | 3,00 | 1,00 | 75,0 | 25,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 3 | 9,00 | 1,00 | 25,0 | 75,0 | 0,0 | 6 |
| 4 | 11,00 | 1,00 | 25,0 | 75,0 | 0,0 | 6 |

Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 5 | 12,00 | 1,00 | 75,0 | 25,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|-------------------|------------|----------|---------------------|---------------|--------|-----------|
| 1 | 75 25 385 BG11_IM | Instrument | | 11.11.2010 13:50:09 | System | No | 1155 |

**Method
Version
Summaries**

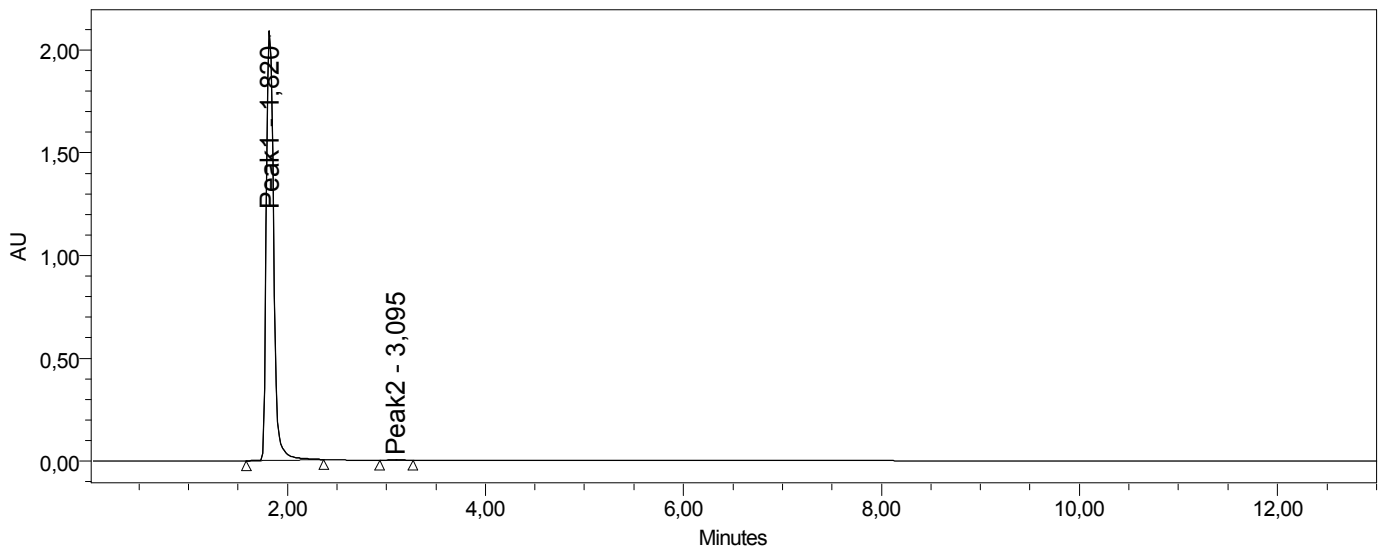
| | Method Version |
|---|----------------|
| 1 | 1 |

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | | | |
|-------------------|------------------------------|---------------------|---------------------|
| Sample Name: | 85 15 360 Compound 15 | Acquired By: | System |
| Sample Type: | Unknown | Date Acquired: | 12.11.2010 14:37:44 |
| Vial: | 5 | Acq. Method Set: | 85 15 360 BG15_MS |
| Injection #: | 1 | Date Processed: | 17.11.2010 15:30:13 |
| Injection Volume: | 10,00 ul | Processing Method: | 15 |
| Run Time: | 13,0 Minutes | Channel Name: | 2487Channel 1 |
| Sample Set Name: | | Proc. Chnl. Descr.: | |



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|-------|----------|--------|---------|
| 1 | Peak1 | 1,820 | 10798053 | 99,75 | 2107835 |
| 2 | Peak2 | 3,095 | 26682 | 0,25 | 2605 |

Reported by User: System

Project Name: Hrizeni

Instrument Method: 85 15 360 BG15_IM

Stored: 12.11.2010 14:03:54

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 360
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|---------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,85 | Solvent A | 2%HCOOH |
| Flow B | 0,15 | Solvent B | MeOH |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|------|-----|-------|
| 1 | | 1,00 | 85,0 | 15,0 | 0,0 | |
| 2 | 3,00 | 1,00 | 85,0 | 15,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 3 | 9,00 | 1,00 | 15,0 | 85,0 | 0,0 | 6 |
| 4 | 12,00 | 1,00 | 15,0 | 85,0 | 0,0 | 6 |



Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 5 | 13,00 | 1,00 | 85,0 | 15,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|-------------------|------------|----------|---------------------|---------------|--------|-----------|
| 1 | 85 15 360 BG15_IM | Instrument | | 12.11.2010 14:03:54 | System | No | 1213 |

**Method
Version
Summaries**

| | Method Version |
|---|----------------|
| 1 | 1 |



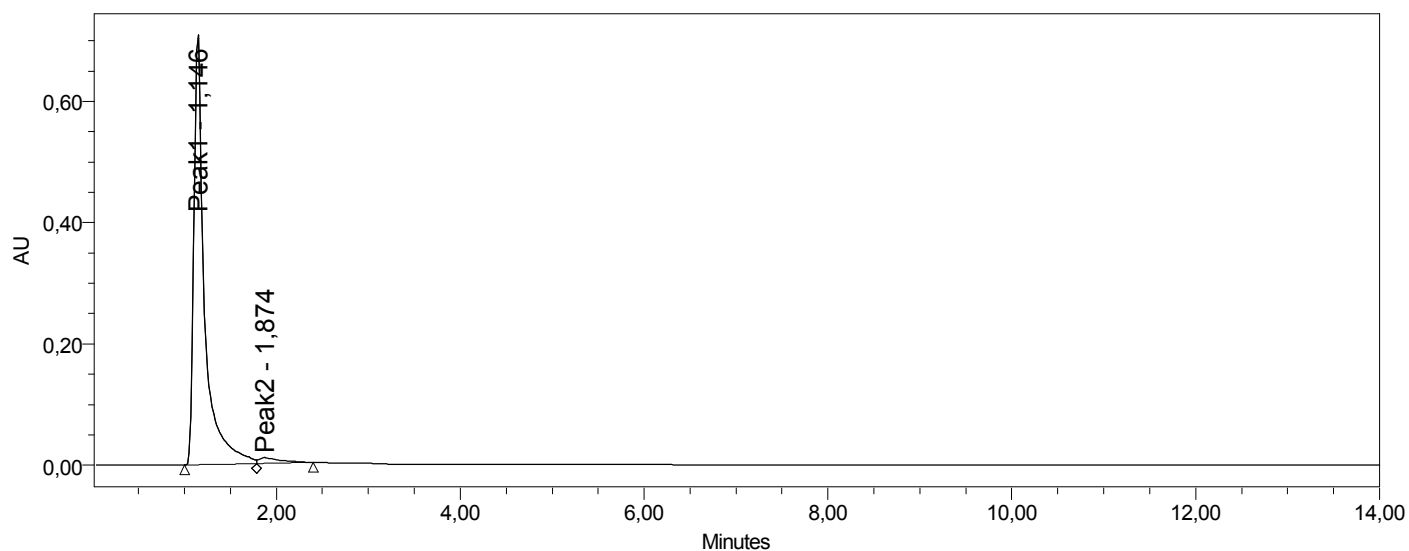
Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | | | |
|-------------------|------------------------------|---------------------|---------------------|
| Sample Name: | 60 40 385 Compound 14 | Acquired By: | System |
| Sample Type: | Unknown | Date Acquired: | 17.11.2010 13:50:36 |
| Vial: | 9 | Acq. Method Set: | 60 40 385 BDI 17_MS |
| Injection #: | 1 | Date Processed: | 17.11.2010 15:49:43 |
| Injection Volume: | 10,00 ul | Processing Method: | 14 |
| Run Time: | 14,0 Minutes | Channel Name: | 2487Channel 1 |
| Sample Set Name: | | Proc. Chnl. Descr.: | |



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|-------|---------|--------|--------|
| 1 | Peak1 | 1,146 | 5760099 | 97,40 | 703490 |
| 2 | Peak2 | 1,874 | 153713 | 2,60 | 9566 |



Reported by User: System

Project Name: Hrizeni

Instrument Method: 60 40 385 BDI 17_IM

Stored: 16.11.2010 14:47:14

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 385
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|---------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,60 | Solvent A | 2%HCOOH |
| Flow B | 0,40 | Solvent B | MeOH |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|------|-----|-------|
| 1 | | 1,00 | 60,0 | 40,0 | 0,0 | |
| 2 | 1,50 | 1,00 | 60,0 | 40,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 3 | 12,00 | 1,00 | 40,0 | 60,0 | 0,0 | 6 |
| 4 | 15,00 | 1,00 | 40,0 | 60,0 | 0,0 | 6 |



Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 5 | 16,00 | 1,00 | 60,0 | 40,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|---------------------|------------|----------|---------------------|---------------|--------|-----------|
| 1 | 60 40 385 BDI 17_IM | Instrument | | 16.11.2010 14:47:14 | System | No | 1293 |

Method Version Summaries

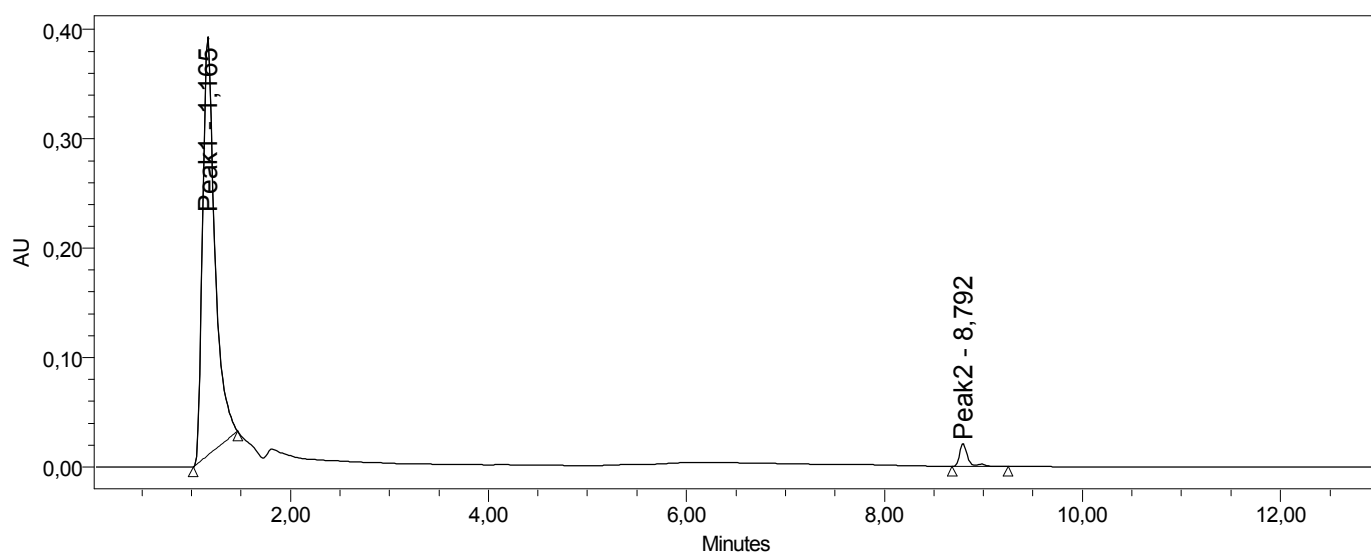
| | Method Version |
|---|----------------|
| 1 | 1 |

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | |
|---|-------------------------------------|
| Sample Name: 90 10 385 Compound 11 | Acquired By: System |
| Sample Type: Unknown | Date Acquired: 15.11.2010 13:56:35 |
| Vial: 5 | Acq. Method Set: 90 10 385 BG17_MS |
| Injection #: 1 | Date Processed: 17.11.2010 15:32:34 |
| Injection Volume: 10,00 ul | Processing Method: 11 |
| Run Time: 13,0 Minutes | Channel Name: 2487Channel 1 |
| Sample Set Name: | Proc. Chnl. Descr.: |



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|-------|---------|--------|--------|
| 1 | Peak1 | 1,165 | 3311131 | 96,50 | 380532 |
| 2 | Peak2 | 8,792 | 120028 | 3,50 | 20674 |



Reported by User: System

Project Name: Hrizeni

Instrument Method: 90 10 385 BG17_IM

Stored: 15.11.2010 13:26:34

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 385
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|---------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,90 | Solvent A | 2%HCOOH |
| Flow B | 0,10 | Solvent B | MeOH |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|------|-----|-------|
| 1 | | 1,00 | 90,0 | 10,0 | 0,0 | |
| 2 | 3,00 | 1,00 | 90,0 | 10,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 3 | 9,00 | 1,00 | 10,0 | 90,0 | 0,0 | 6 |
| 4 | 11,00 | 1,00 | 10,0 | 90,0 | 0,0 | 6 |



Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 5 | 12,00 | 1,00 | 90,0 | 10,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|-------------------|------------|----------|---------------------|---------------|--------|-----------|
| 1 | 90 10 385 BG17_IM | Instrument | | 15.11.2010 13:26:34 | System | No | 1236 |

Method Version Summaries

| | Method Version |
|---|----------------|
| 1 | 1 |



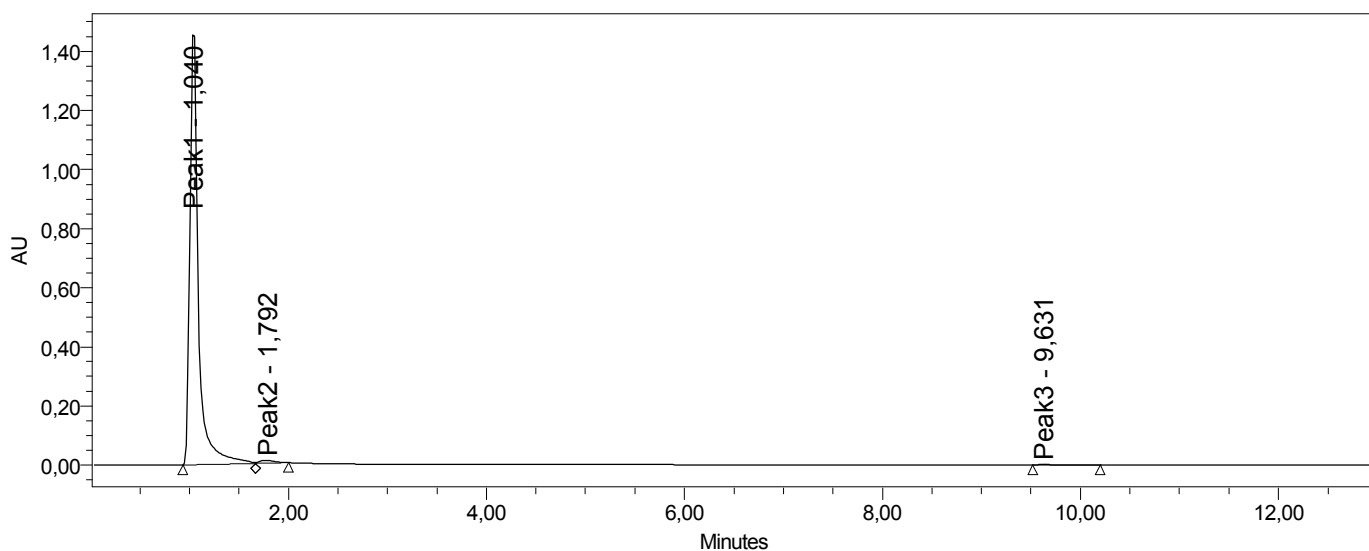
Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | | | |
|-------------------|------------------------------|---------------------|---------------------|
| Sample Name: | 80 20 385 Compound 10 | Acquired By: | System |
| Sample Type: | Unknown | Date Acquired: | 16.11.2010 10:27:11 |
| Vial: | 1 | Acq. Method Set: | 80 20 385 BG11_MS |
| Injection #: | 1 | Date Processed: | 17.11.2010 15:36:54 |
| Injection Volume: | 10,00 ul | Processing Method: | 10 |
| Run Time: | 13,0 Minutes | Channel Name: | 2487Channel 1 |
| Sample Set Name: | | Proc. Chnl. Descr.: | |



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|-------|---------|--------|---------|
| 1 | Peak1 | 1,040 | 8831324 | 98,66 | 1462575 |
| 2 | Peak2 | 1,792 | 99387 | 1,11 | 8790 |
| 3 | Peak3 | 9,631 | 20324 | 0,23 | 2867 |



Reported by User: System

Project Name: Hrizeni

Instrument Method: 80 20 385 BG11_IM

Stored: 11.11.2010 11:21:36

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 385
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|---------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,80 | Solvent A | 2%HCOOH |
| Flow B | 0,20 | Solvent B | MeOH |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|------|-----|-------|
| 1 | | 1,00 | 80,0 | 20,0 | 0,0 | |
| 2 | 1,50 | 1,00 | 80,0 | 20,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 3 | 12,00 | 1,00 | 20,0 | 80,0 | 0,0 | 6 |
| 4 | 15,00 | 1,00 | 20,0 | 80,0 | 0,0 | 6 |



Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 5 | 16,00 | 1,00 | 80,0 | 20,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|-------------------|------------|----------|---------------------|---------------|--------|-----------|
| 1 | 80 20 385 BG11_IM | Instrument | | 11.11.2010 11:21:36 | System | No | 1145 |

Method Version Summaries

| | Method Version |
|---|----------------|
| 1 | 1 |



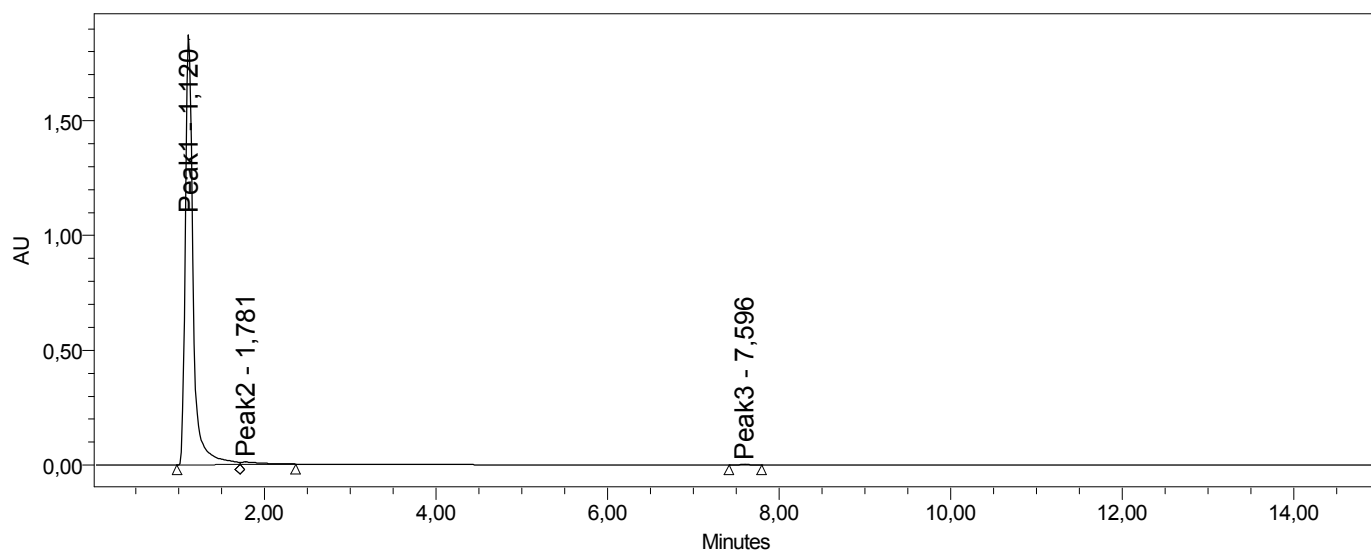
Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | | | |
|-------------------|-----------------------------|---------------------|---------------------|
| Sample Name: | 60 40 385 Compound 8 | Acquired By: | System |
| Sample Type: | Unknown | Date Acquired: | 17.11.2010 12:56:22 |
| Vial: | 6 | Acq. Method Set: | 60 40 385 BDI 17_MS |
| Injection #: | 1 | Date Processed: | 17.11.2010 15:45:02 |
| Injection Volume: | 10,00 ul | Processing Method: | 8 |
| Run Time: | 15,0 Minutes | Channel Name: | 2487Channel 1 |
| Sample Set Name: | | Proc. Chnl. Descr.: | |



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|-------|----------|--------|---------|
| 1 | Peak1 | 1,120 | 12039151 | 98,39 | 1868506 |
| 2 | Peak2 | 1,781 | 180104 | 1,47 | 11421 |
| 3 | Peak3 | 7,596 | 16947 | 0,14 | 1788 |



Reported by User: System

Project Name: Hrizeni

Instrument Method: 60 40 385 BDI 17_IM

Stored: 16.11.2010 14:47:14

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 385
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|---------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,60 | Solvent A | 2%HCOOH |
| Flow B | 0,40 | Solvent B | MeOH |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|------|-----|-------|
| 1 | | 1,00 | 60,0 | 40,0 | 0,0 | |
| 2 | 1,50 | 1,00 | 60,0 | 40,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 3 | 12,00 | 1,00 | 40,0 | 60,0 | 0,0 | 6 |
| 4 | 15,00 | 1,00 | 40,0 | 60,0 | 0,0 | 6 |



Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 5 | 16,00 | 1,00 | 60,0 | 40,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|---------------------|------------|----------|---------------------|---------------|--------|-----------|
| 1 | 60 40 385 BDI 17_IM | Instrument | | 16.11.2010 14:47:14 | System | No | 1293 |

Method Version Summaries

| | Method Version |
|---|----------------|
| 1 | 1 |



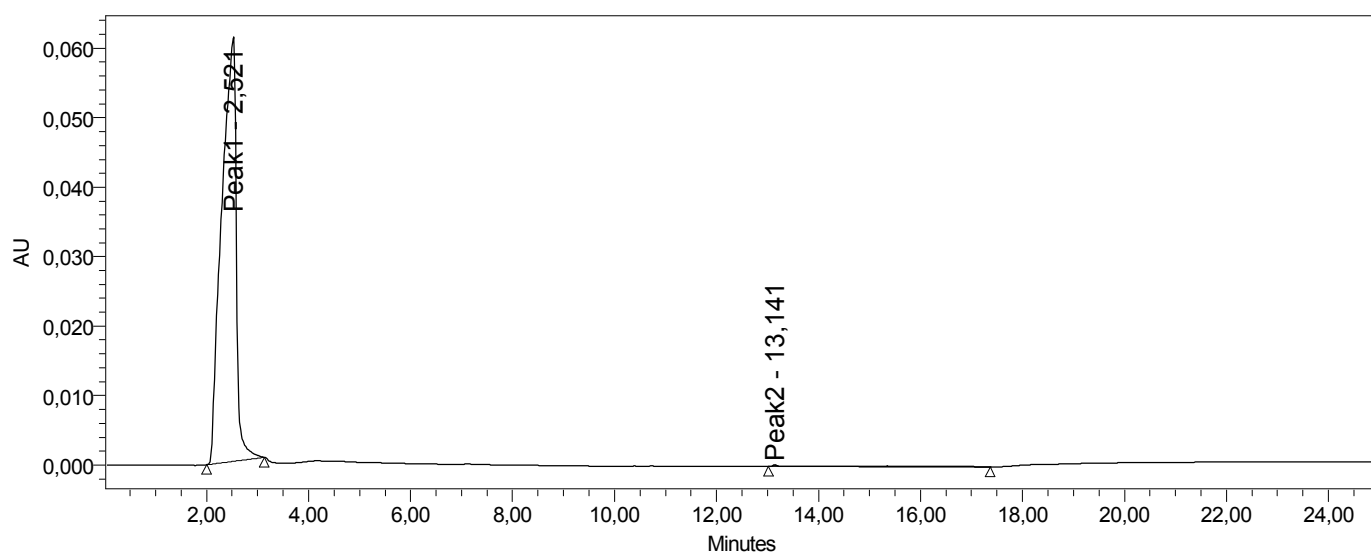
Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | | | |
|-------------------|--------------------------|---------------------|-------------------------|
| Sample Name: | 363 nm Compound 9 | Acquired By: | System |
| Sample Type: | Unknown | Date Acquired: | 9.11.2010 13:50:13 |
| Vial: | 1 | Acq. Method Set: | cistoca hrizeni90 10_MS |
| Injection #: | 1 | Date Processed: | 17.11.2010 15:11:12 |
| Injection Volume: | 10,00 ul | Processing Method: | 9 |
| Run Time: | 25,0 Minutes | Channel Name: | 2487Channel 1 |
| Sample Set Name: | | Proc. Chnl. Descr.: | |



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|--------|---------|--------|--------|
| 1 | Peak1 | 2,521 | 1217818 | 98,68 | 62038 |
| 2 | Peak2 | 13,141 | 16280 | 1,32 | 199 |



Reported by User: System

Project Name: Hrizeni

Instrument Method: cistoca hrizeni90 10_IM

Stored: 9.11.2010 13:17:11

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 360
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|-----------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,90 | Solvent A | 0.2%HCOOH |
| Flow B | 0,10 | Solvent B | Metanol |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|------|-----|-------|
| 1 | | 1,00 | 90,0 | 10,0 | 0,0 | |
| 2 | 1,50 | 1,00 | 90,0 | 10,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 3 | 12,00 | 1,00 | 10,0 | 90,0 | 0,0 | 6 |
| 4 | 15,00 | 1,00 | 10,0 | 90,0 | 0,0 | 6 |

Multi Sample Summary



Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 5 | 16,00 | 1,00 | 90,0 | 10,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|-------------------------|------------|----------|--------------------|---------------|--------|-----------|
| 1 | cistoca hrizeni90 10_IM | Instrument | | 9.11.2010 13:17:11 | System | No | 1073 |

**Method
Version
Summaries**

| | Method Version |
|---|----------------|
| 1 | 1 |



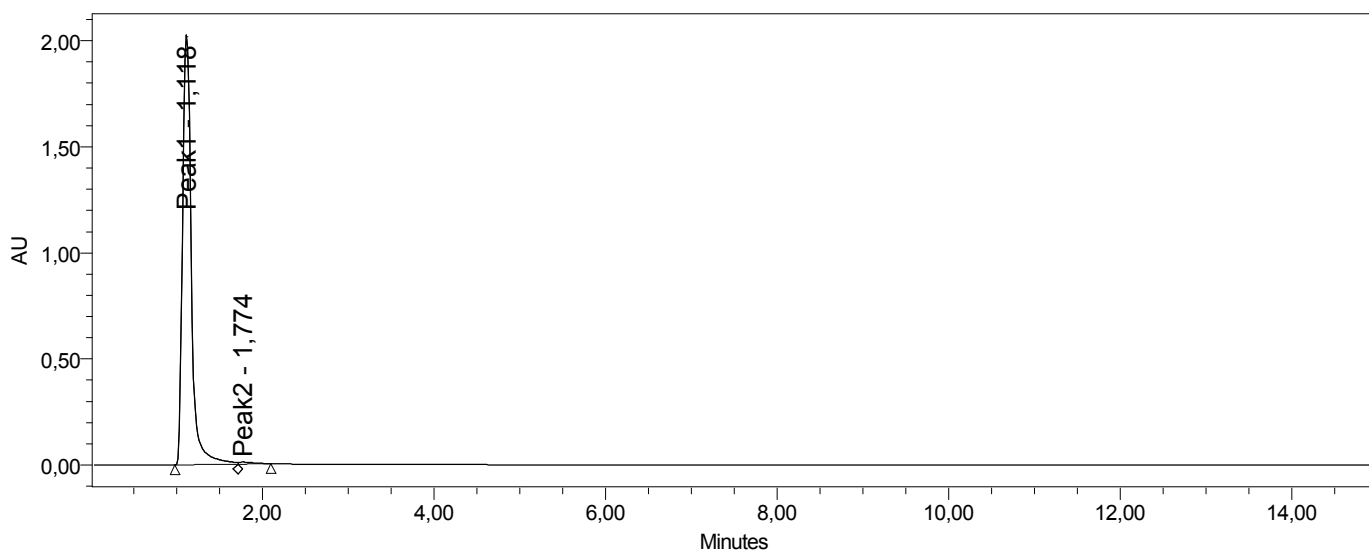
Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | | | |
|-------------------|-----------------------------|---------------------|---------------------|
| Sample Name: | 60 40 385 Compound 7 | Acquired By: | System |
| Sample Type: | Unknown | Date Acquired: | 18.11.2010 13:23:19 |
| Vial: | 4 | Acq. Method Set: | 60 40 385 BDI 17_MS |
| Injection #: | 1 | Date Processed: | 18.11.2010 13:39:53 |
| Injection Volume: | 10,00 ul | Processing Method: | 7 |
| Run Time: | 15,0 Minutes | Channel Name: | 2487Channel 1 |
| Sample Set Name: | | Proc. Chnl. Descr.: | |



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|-------|----------|--------|---------|
| 1 | Peak1 | 1,118 | 14643983 | 99,28 | 2035861 |
| 2 | Peak2 | 1,774 | 105772 | 0,72 | 9450 |



Reported by User: System

Project Name: Hrizeni

Instrument Method: 60 40 385 BDI 17_IM

Stored: 16.11.2010 14:47:14

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 385
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|---------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,60 | Solvent A | 2%HCOOH |
| Flow B | 0,40 | Solvent B | MeOH |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|------|-----|-------|
| 1 | | 1,00 | 60,0 | 40,0 | 0,0 | |
| 2 | 1,50 | 1,00 | 60,0 | 40,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 3 | 12,00 | 1,00 | 40,0 | 60,0 | 0,0 | 6 |
| 4 | 15,00 | 1,00 | 40,0 | 60,0 | 0,0 | 6 |



Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 5 | 16,00 | 1,00 | 60,0 | 40,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|---------------------|------------|----------|---------------------|---------------|--------|-----------|
| 1 | 60 40 385 BDI 17_IM | Instrument | | 16.11.2010 14:47:14 | System | No | 1293 |

Method Version Summaries

| | Method Version |
|---|----------------|
| 1 | 1 |



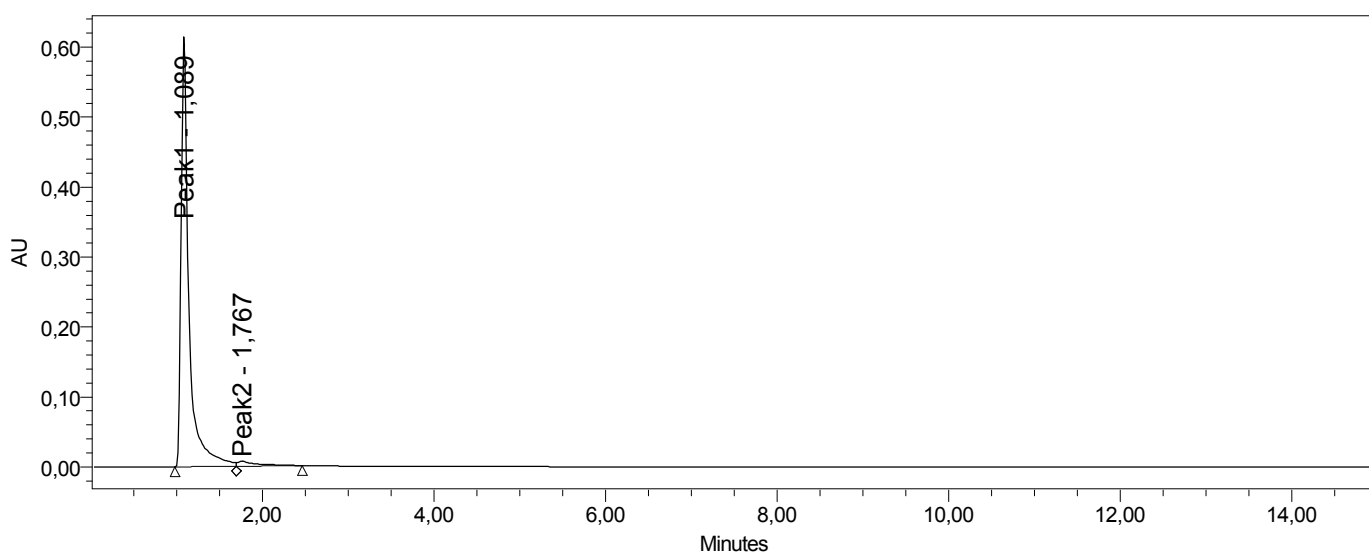
Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

| | | | |
|-------------------|------------------------------|---------------------|---------------------|
| Sample Name: | 60 40 385 Compound 12 | Acquired By: | System |
| Sample Type: | Unknown | Date Acquired: | 19.11.2010 10:48:41 |
| Vial: | 2 | Acq. Method Set: | 60 40 385 BDI 17_MS |
| Injection #: | 1 | Date Processed: | 19.11.2010 11:05:21 |
| Injection Volume: | 10,00 ul | Processing Method: | 12 |
| Run Time: | 15,0 Minutes | Channel Name: | 2487Channel 1 |
| Sample Set Name: | | Proc. Chnl. Descr.: | |



| | Peak Name | RT | Area | % Area | Height |
|---|-----------|-------|---------|--------|--------|
| 1 | Peak1 | 1,089 | 3934623 | 97,26 | 609111 |
| 2 | Peak2 | 1,767 | 111043 | 2,74 | 7129 |



Reported by User: System

Project Name: Hrizeni

Instrument Method: 60 40 385 BDI 17_IM

Stored: 16.11.2010 14:47:14

W2487 Instrument Setup

Type W2487
 Instrument Status On
 Dual Wavelength False
 Pulse Period Seconds 1,0
 Pulse Repeat Period Seconds 1,0

W2487 Channel Information

Channel Name 2487Channel 1
 Description
 Use Channels On
 Wavelength 385
 Output Mode Absorbance A (Ch1)
 Data Mode Absorbance A (Ch1)
 Sampling Rate 1
 Filter Type Hamming
 Aups 2,0000
 Time Constant 1,0
 AU Offset 0,000
 Voltage Offset 0
 Polarity +
 AutoZero Wavelength True
 AutoZero Keypad True
 AutoZeroEvent Input True
 AutoZero Inject True
 Chart Mark Enable True
 Ratio AuMinimum 0,1000
 Minimum Ratio 0,00
 Maximum Ratio 2,00

PCM/15xx Instrument Setup

| | | | |
|-------------------|----------|------------|---------|
| Type | PCM/15xx | Low Limit | 0,0 |
| Instrument Status | On | Total Flow | 1,00 |
| Pump Mode | Gradient | Use Events | On |
| Flow A | 0,60 | Solvent A | 2%HCOOH |
| Flow B | 0,40 | Solvent B | MeOH |
| Flow C | 0,00 | Solvent C | |
| High Limit | 4000,0 | | |

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|------|------|------|------|-----|-------|
| 1 | | 1,00 | 60,0 | 40,0 | 0,0 | |
| 2 | 1,50 | 1,00 | 60,0 | 40,0 | 0,0 | 6 |

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 3 | 12,00 | 1,00 | 40,0 | 60,0 | 0,0 | 6 |
| 4 | 15,00 | 1,00 | 40,0 | 60,0 | 0,0 | 6 |



Multi Sample Summary

Reported by User: System

Project Name: Hrizeni

PCM/15xx Gradient Table

| | Time | Flow | %A | %B | %C | Curve |
|---|-------|------|------|------|-----|-------|
| 5 | 16,00 | 1,00 | 60,0 | 40,0 | 0,0 | 6 |

Revision History

This method contains 1 items in the revision history.

Method Version Summaries

| | Name | Type | Comments | Date | Modified User | Locked | Method Id |
|---|---------------------|------------|----------|---------------------|---------------|--------|-----------|
| 1 | 60 40 385 BDI 17_IM | Instrument | | 16.11.2010 14:47:14 | System | No | 1293 |

Method Version Summaries

| | Method Version |
|---|----------------|
| 1 | 1 |