

Supporting information

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

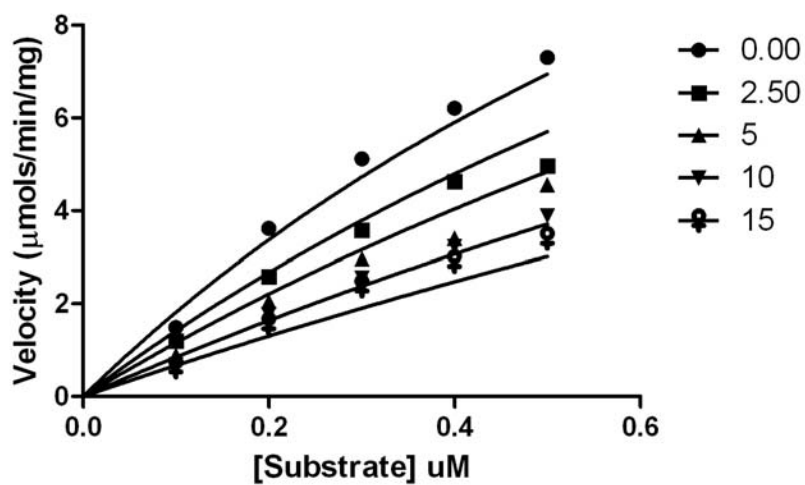
Igor Opsenica,[¶] James C. Burnett,^{§,*} Rick Gussio,[†] Dejan Opsenica,[‡] Nina Todorović,[‡] Charlotte A. Lanteri,[∇] Richard J. Sciotti,[∇] Montip Gettayacamin,[◇] Nicoletta Basilico,[∇] Donatella Taramelli,[∇] Jonathan E. Nuss,[#] Laura Wanner,[#] Rekha G. Panchal,[#] Bogdan A. Šolaja,^{¶,*} Sina Bavari^{#,*}

[¶]Faculty of Chemistry, University of Belgrade, Studentski trg 16, P.O. Box 51, 11158, Belgrade, Serbia; [§]Target Structure-Based Drug Discovery Group, SAIC-Frederick, Inc., National Cancer Institute at Frederick, P.O. Box B, Frederick, MD 21702, USA; [†]Developmental Therapeutics Program, National Cancer Institute at Frederick, P.O. Box B, F.V.C. 310, Frederick, MD 21702, USA; [‡]Institute of Chemistry, Technology, and Metallurgy, Belgrade, Serbia; [∇]Division of Experimental Therapeutics, Walter Reed Army Institute of Research, Silver Spring, MD 20910, USA; [◇]United States Army Medical Component, Armed Forces Research Institute of Medical Science, Department of Veterinary Medicine, Bangkok, Thailand; [∇]Dipartimento di Sanità Pubblica-Microbiologia-Virologia, Università di Milano, Via Pascal 36, 20133 Milano, Italy; [#]United States Army Medical Research Institute of Infectious Diseases, 1425 Porter Street, Frederick, MD 21702; USA

Table of contents

Figure S1	S2
Figure S2	S3
Table S1	S3
Table S2	S4
Combustion analyses	S4
HPLC purity chromatograms	S5 – S44

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



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

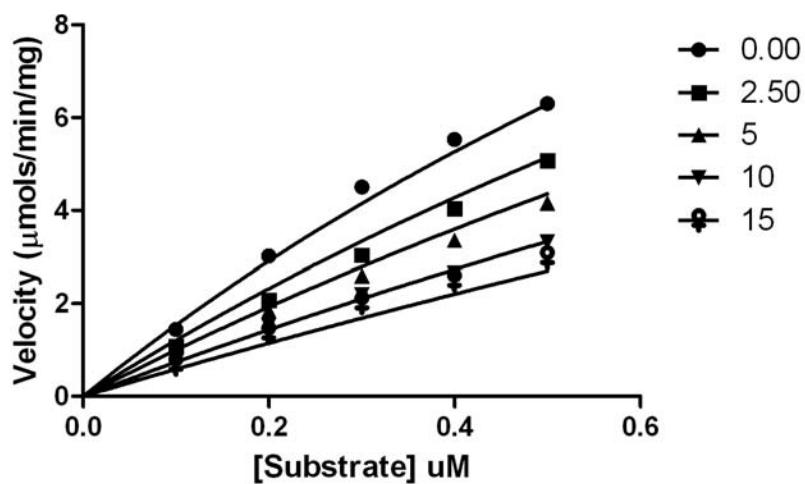


Figure S1: BoNT/A LC inhibition. Plots of the kinetics data from determination of the K_i values for **7** and **8** indicate that 1,7-DAAC-based SMNPIs are competitive inhibitors.

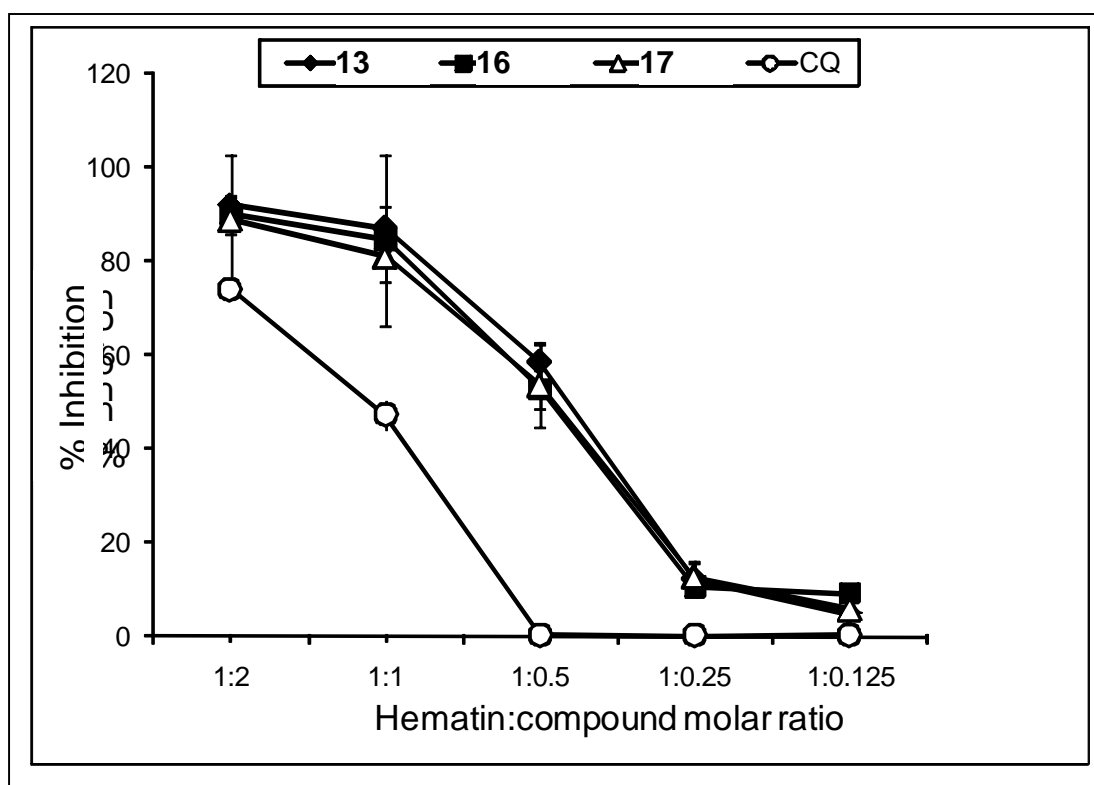


Figure S2: Plots of the dose-dependent inhibition of β -hematin formation by **13**, **16**, **17**, and **CQ**.

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.



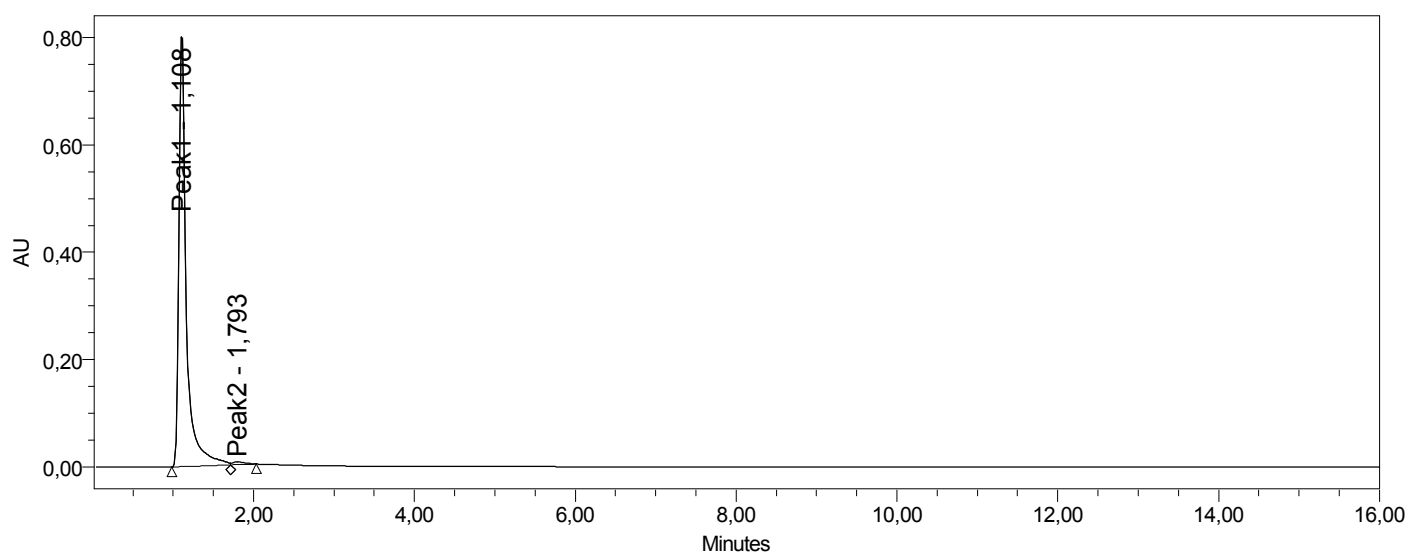
Multi Sample Summary

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



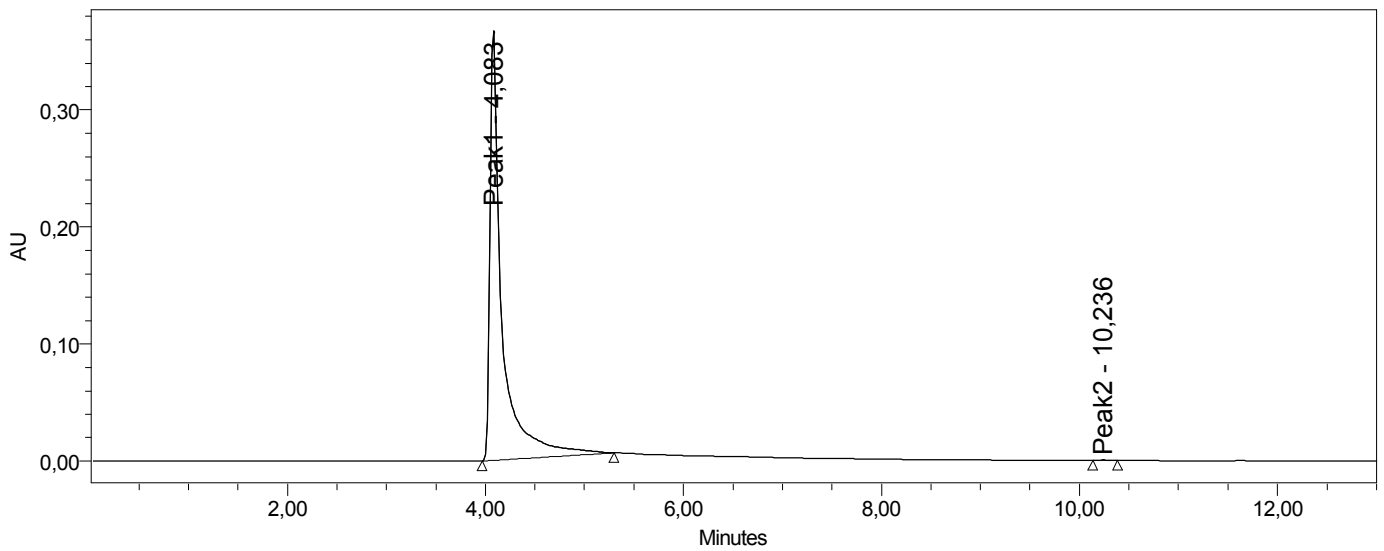
Multi Sample Summary

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



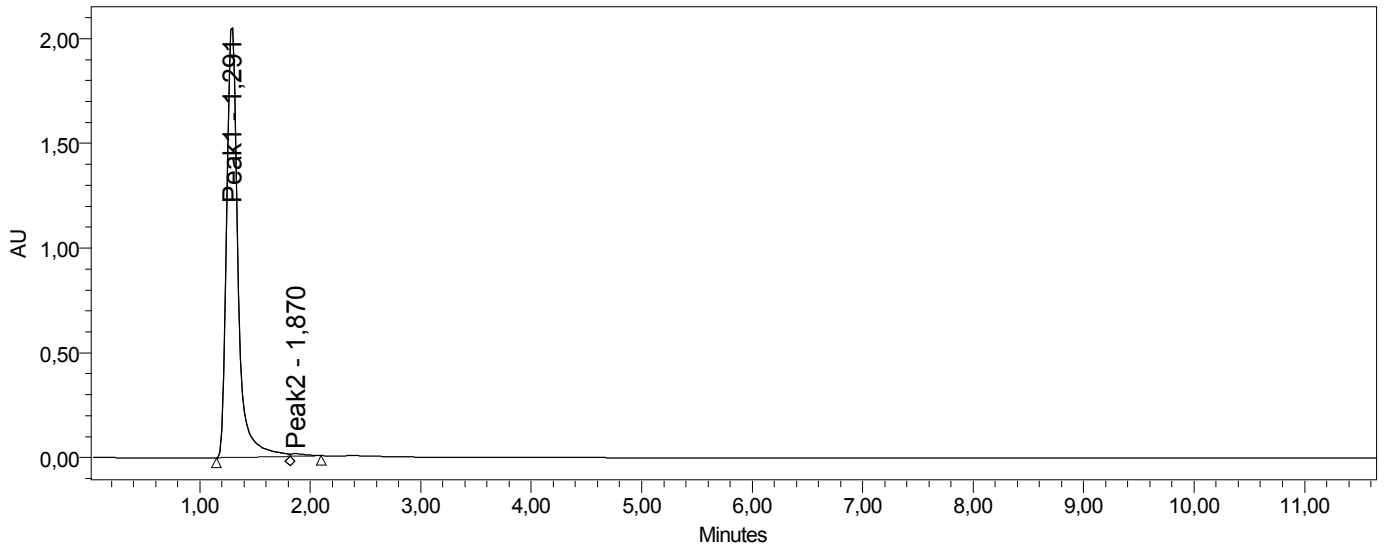
Multi Sample Summary

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



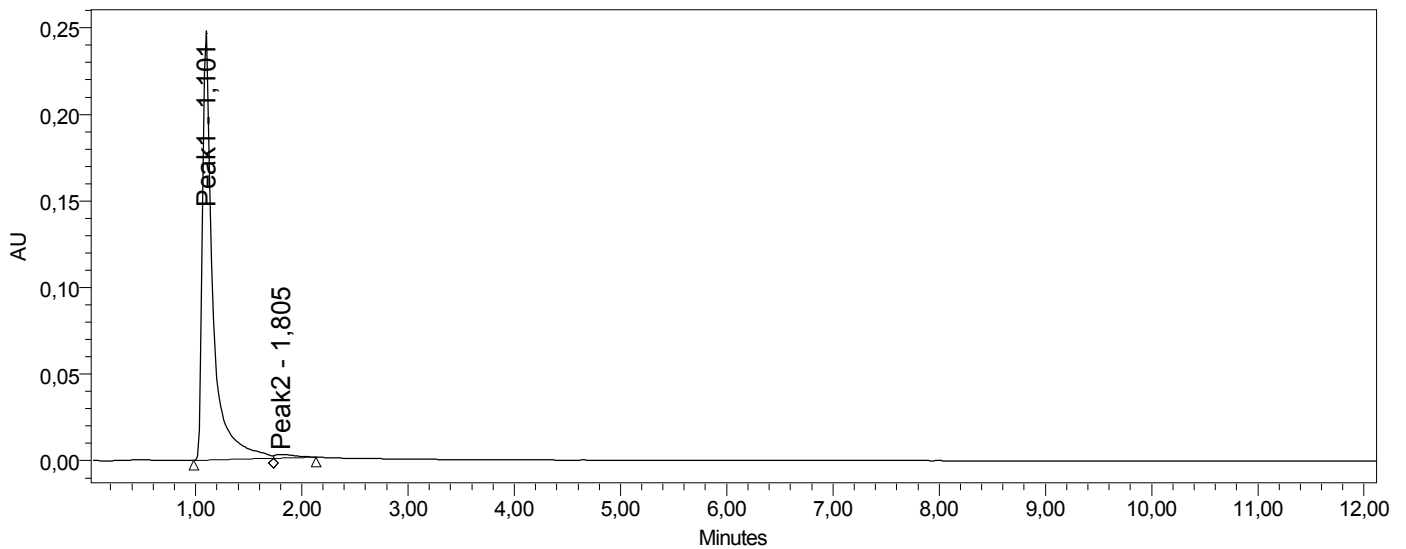
Multi Sample Summary

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

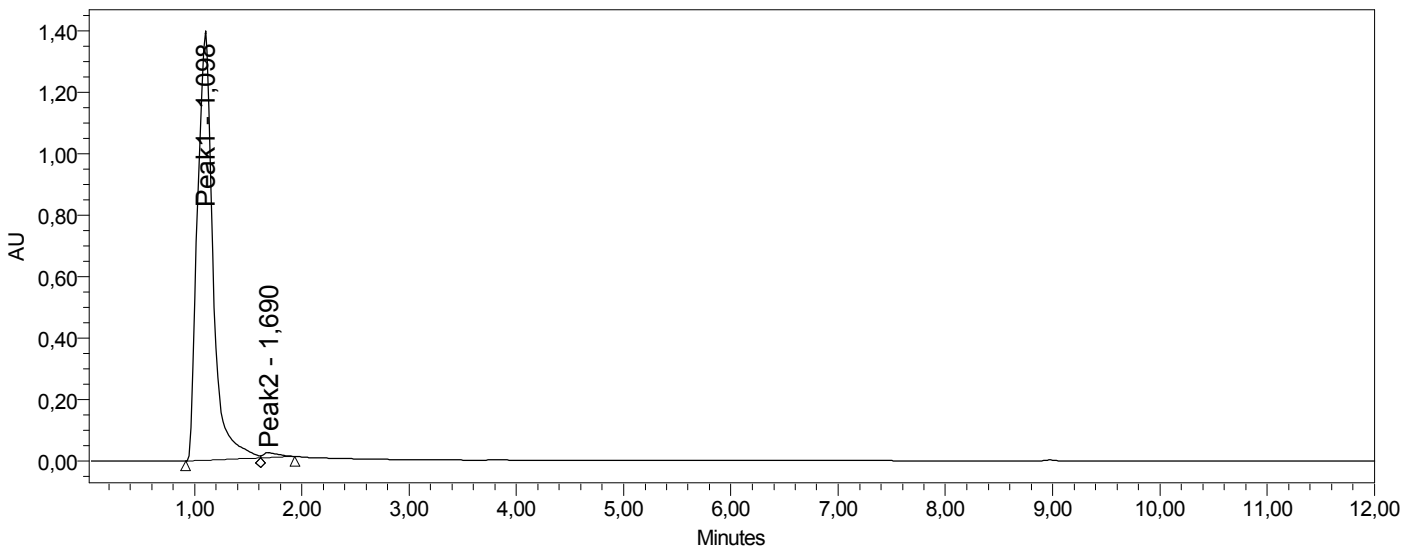
	Method Version
1	1

Reported by User: System

Project Name: Hrizeni

SAMPLE INFORMATION

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



	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

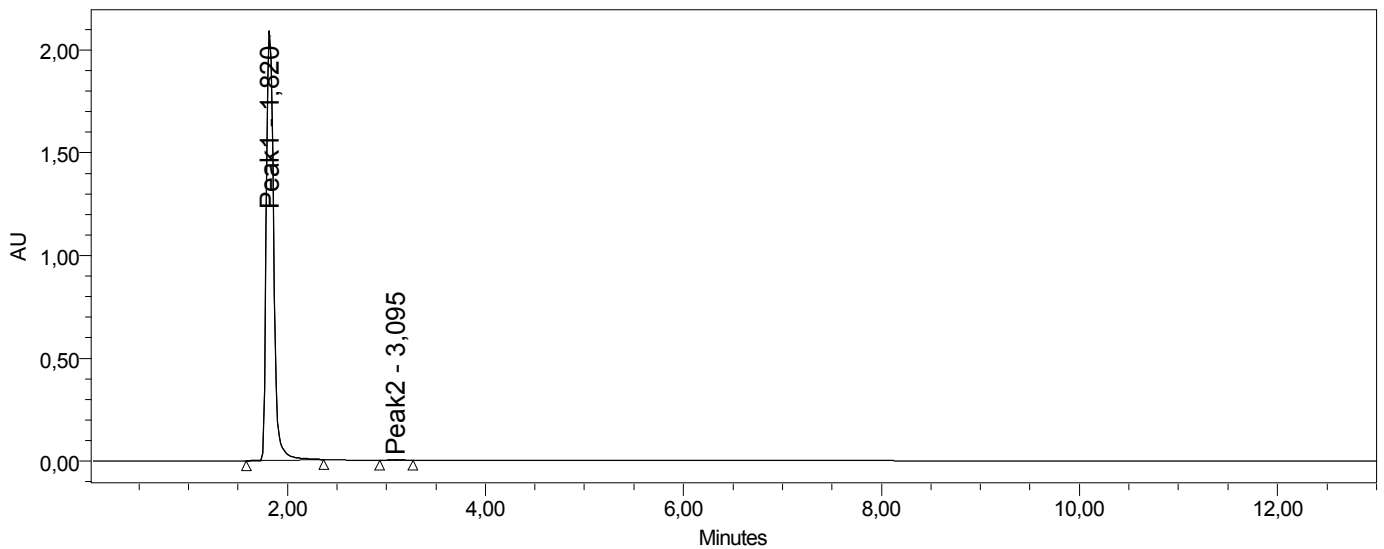
	Method Version
1	1

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



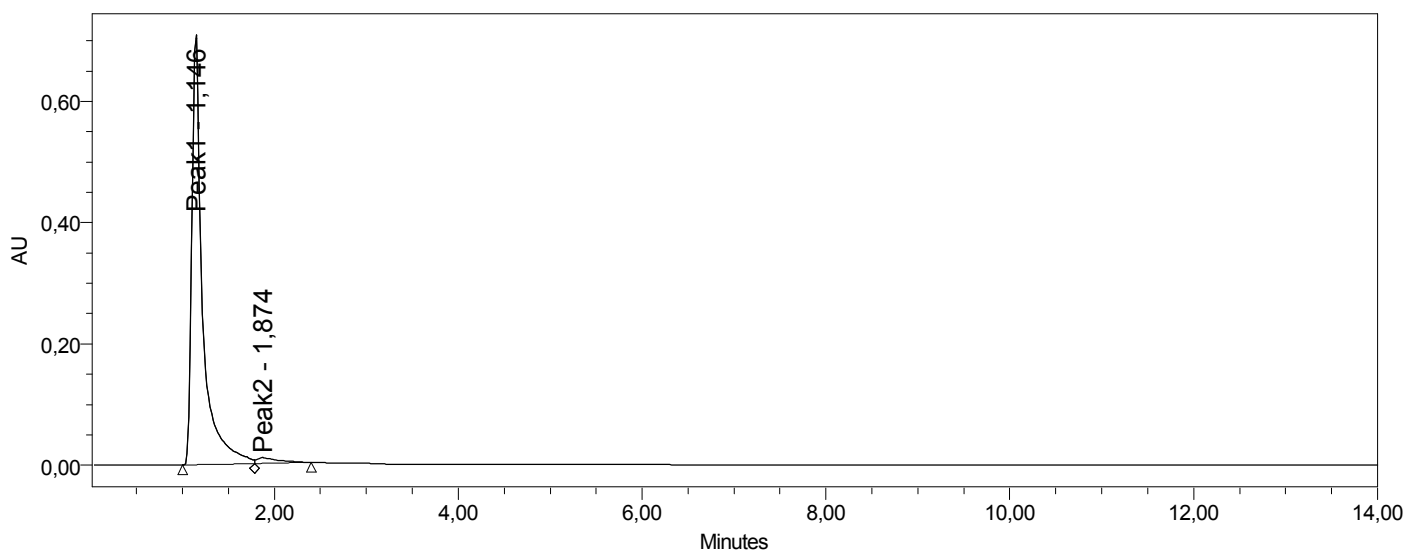
Multi Sample Summary

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

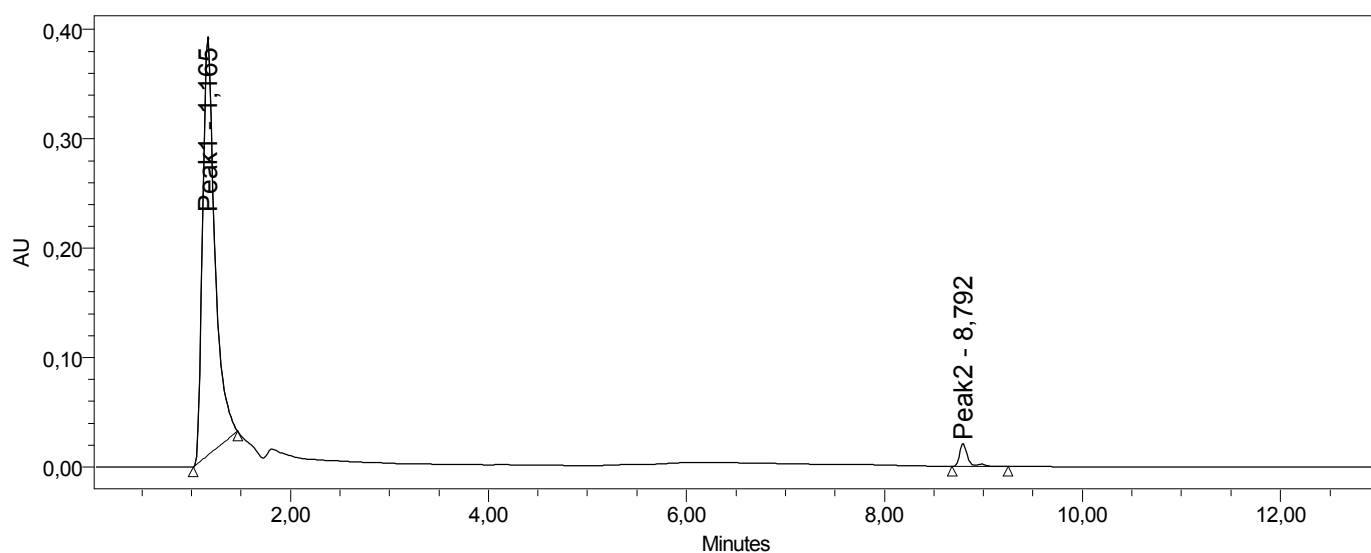
	Method Version
1	1

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



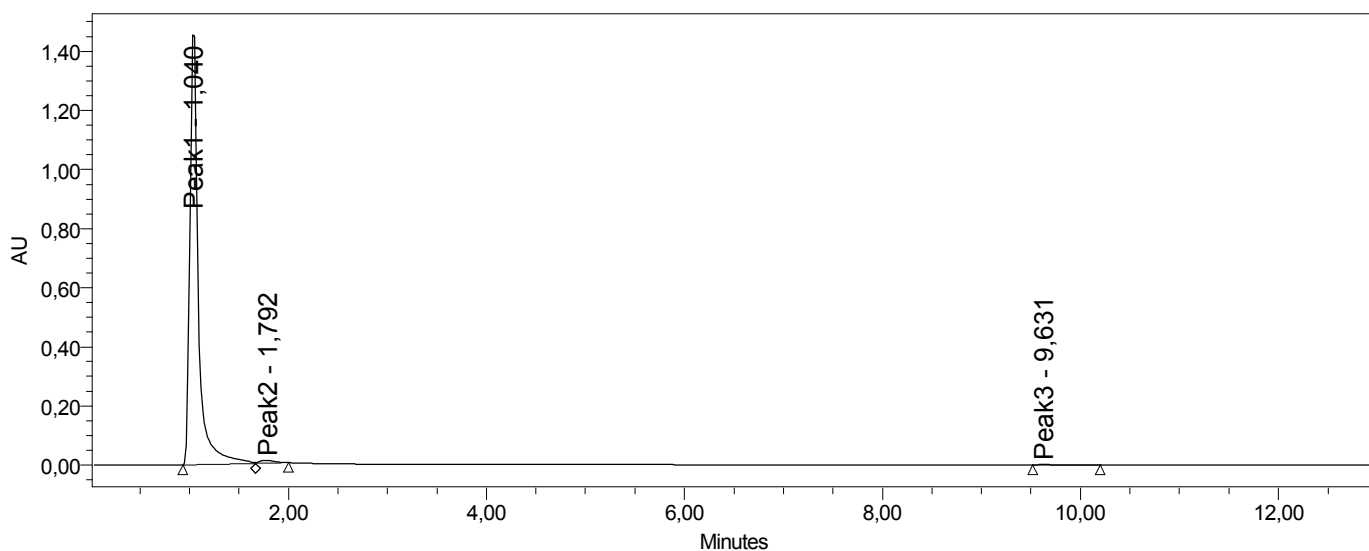
Multi Sample Summary

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



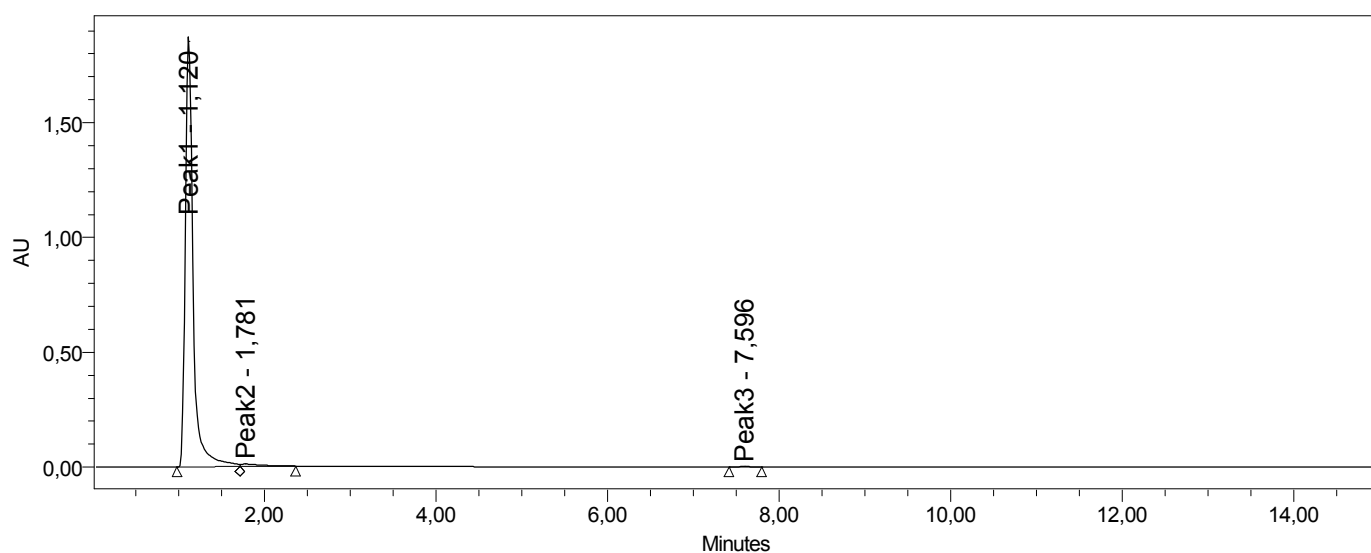
Multi Sample Summary

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



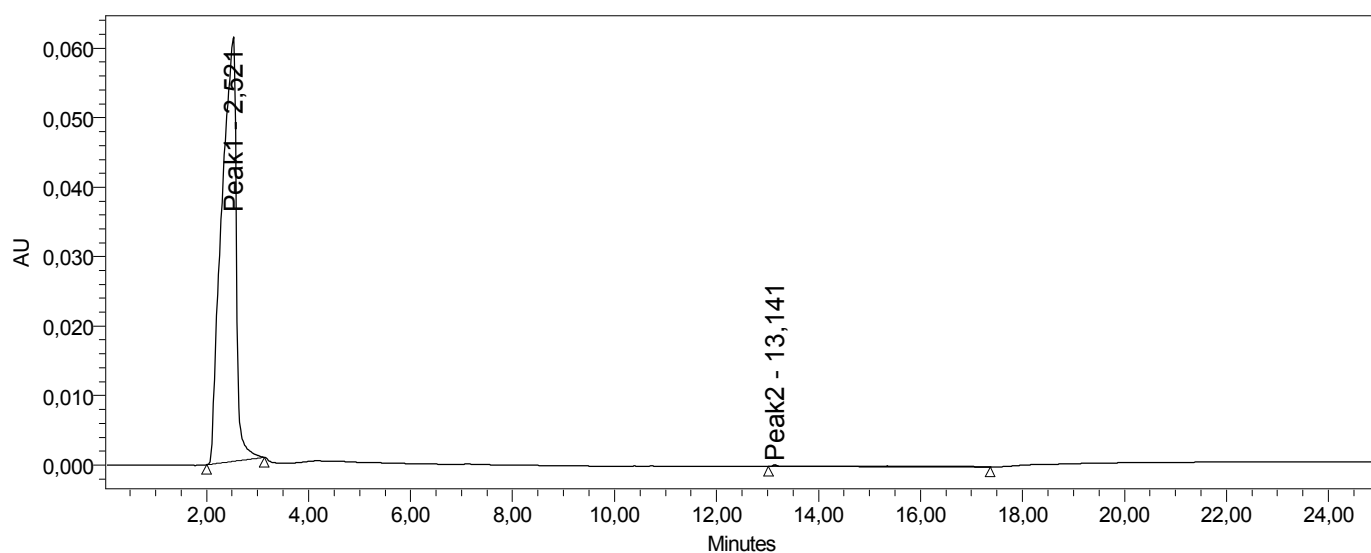
Multi Sample Summary

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



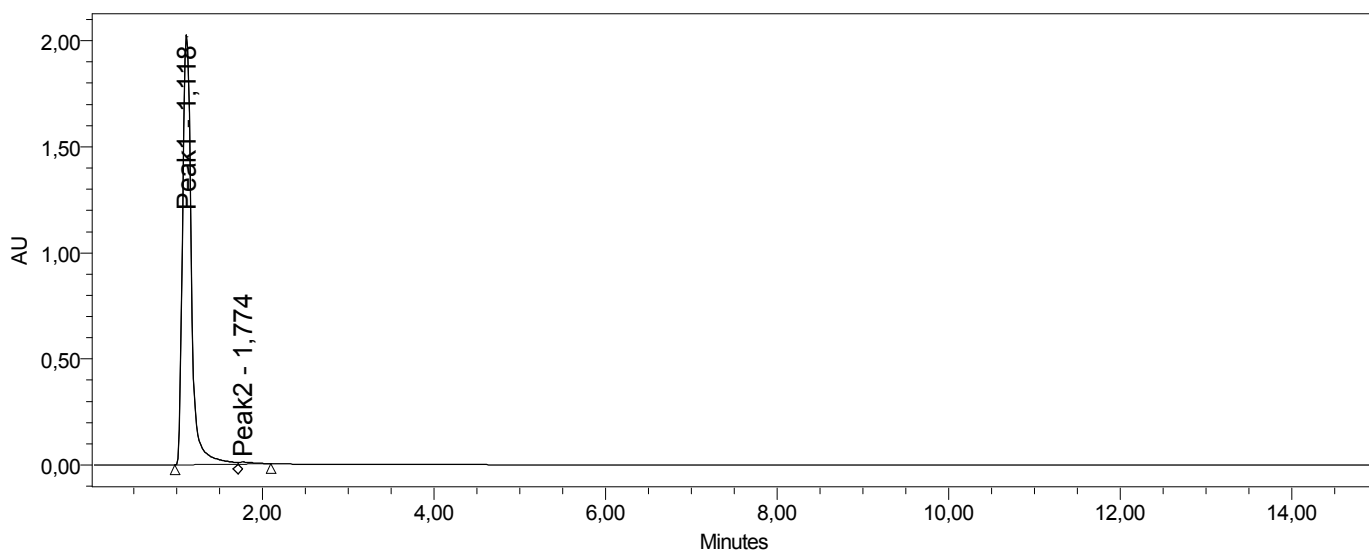
Multi Sample Summary

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



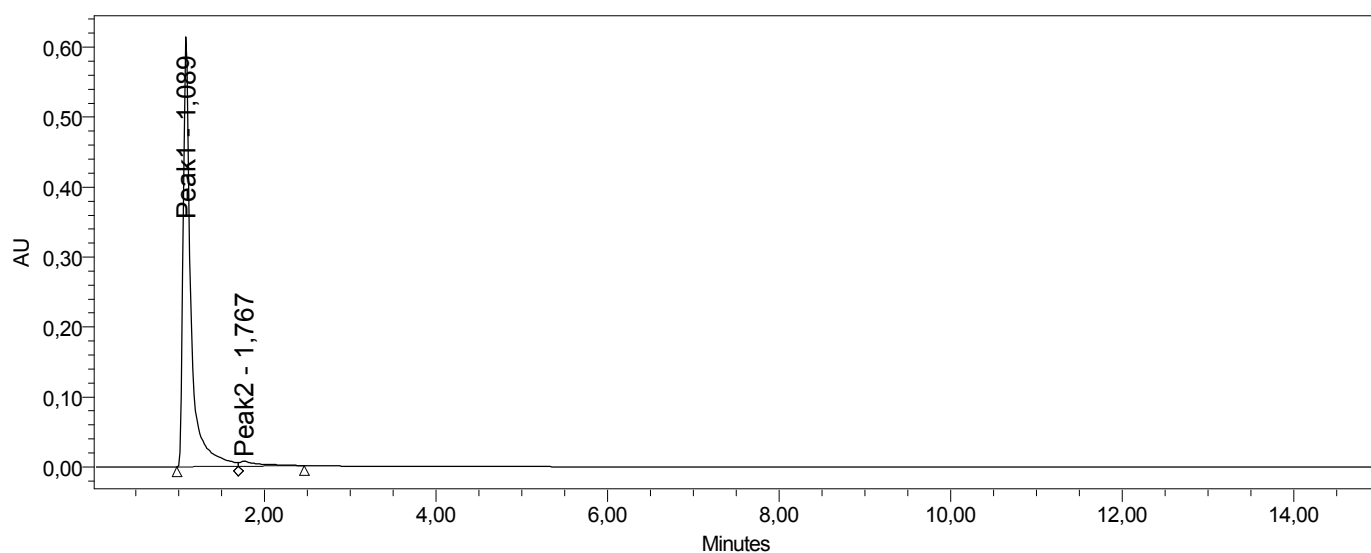
Multi Sample Summary

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