

Supplementary data for article:

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Supporting information

4-Amino-7-chloroquinolines: probing ligand efficiency provides botulinum neurotoxin serotype A light chain inhibitors with significant antiprotozoal activity

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HPLC analyses for purity.

HPLC analysis was performed in two diverse systems:

1. Octadecylsilica was used as the stationary phase (Symmetry C18 analytical column, 4.6 mm \times 150 mm, 5 μ m, series no. 021336278136 37). Compounds were dissolved in methanol (final concentrations were 0.1-0.5 mg/ml and injection volume was 10 μ l). Eluent was made from the following solvents: 0.2% formic acid in water (A) and methanol (B). The analyses were performed at the UV max of the compounds (at 254 nm for compounds **6**, **7**, **8**, **9**, **10**, **12**, **16**, **18**, **19**, **20**, **21**, **22**, and **23**, and at 330 nm for compounds **11**, **13** and **17**) - to maximize selectivity.

For data processing, Empower software was used.

Compounds **8**, **9**, **10**, **11**, **12**, **13**, **14**, **15**, and **16** were eluted using the following gradient protocol: 0-3 min 10% A, 3-6 min 10% A \rightarrow 90 % A, 6-9 min 90% A, 9-12 min 90% A \rightarrow 10 % A, 12-13 min 10% A. Compounds **6**, **7**, **17**, **18**, **19**, **20**, **21**, **22**, and **23** were eluted using the following gradient protocol: 0-3 min 6% A, 3-6 min 6% A \rightarrow 90 % A, 6-9 min 94% A, 9-12 min 94% A \rightarrow 6 % A, 12-13 min 6% A.

Compound	RT	Area (%)
6	1.936	97.93
7	1.794	96.02
8	1.880	96.72
9	2.044	96.68

10	2.044	98.52
11	1.802	97.70
12	2.005	98.67
13	1.853	99.41
14	1.928	99.90
15	2.062	99.53
16	2.179	98.53
17	2.162	98.03
18	1.901	97.82
19	1.978	95.14
20	2.208	98.27
21	2.044	98.01
22	1.968	97.36
23	1.791	95.41

2. Octadecylsilica was used as the stationary phase (Nucleosil C18 analytical column, 4 mm _ 150 mm, 5 μ m). Compounds were dissolved in methanol (final concentrations were 0.1-0.5 mg/ml and injection volume was 10 μ l). Eluent was made from the following solvents: 0.2% formic acid in water (A) and methanol (B). The analyses were performed at the UV max of the compounds (at 254 nm for compounds **6, 7, 8, 9, 10, 12, 16, 18, 19, 20, 21, 22**, and **23**, and at 330 nm for compounds **11, 13**, and **17**) to maximize selectivity.

For data processing, Empower software was used.

Compounds **8, 9, 10, 11, 12, 13, 14, 15**, and **16** were eluted using the following gradient protocol: 0-3 min 10% A, 3-6 min 10% A \rightarrow 90 % A, 6-9 min 90% A, 9-12 min 90% A \rightarrow 10 % A, 12-13 min 10% A. Compounds **6, 7, 17, 18, 19, 20, 21, 22**, and **23** were eluted

using gradient protocol: 0-3 min 6% A, 3-6 min 6% A → 90 % A, 6-9 min 94% A, 9-12 min 94% A → 6 % A, 12-13 min 6% A.

Compound	RT	Area (%)
6	2.058	97.11
7	1.842	96.31
8	1.979	96.84
9	2.192	96.72
10	1.878	98.02
11	1.801	99.84
12	2.042	98.53
13	1.874	99.78
14	1.948	99.67
15	1.804	99.79
16	2.095	97.72
17	2.123	99.93
18	1.856	96.79
19	1.978	96.32
20	2.373	99.38
21	1.891	97.72
22	1.893	97.51
23	1.782	95.59



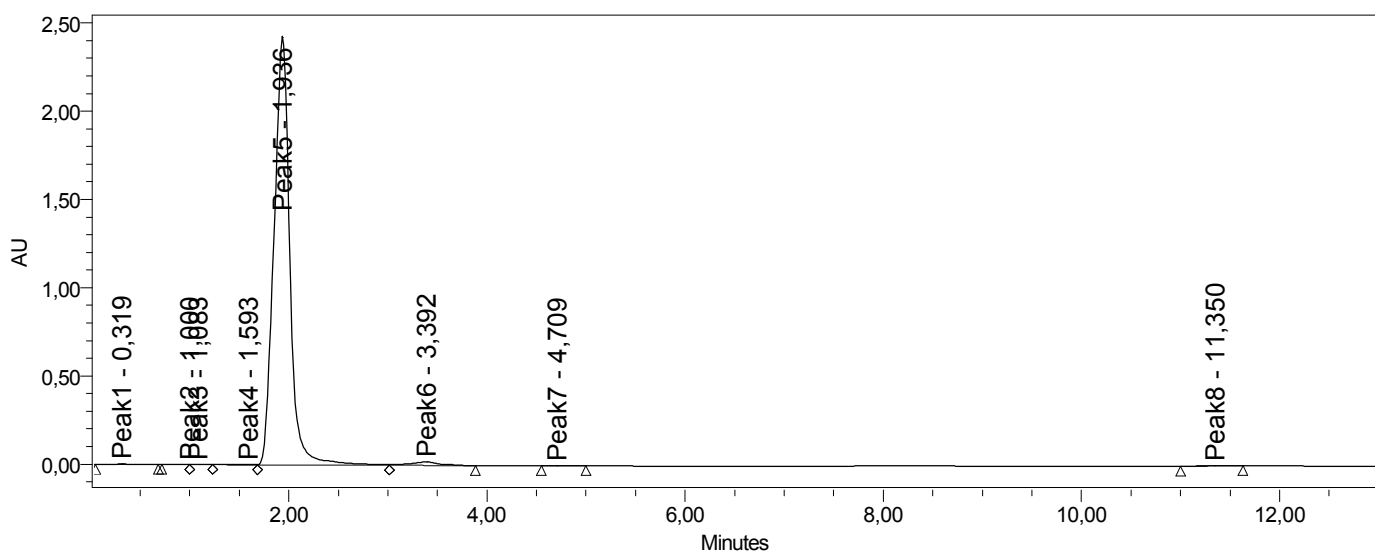
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO95 Compound 6	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2.8.2012 11:25:50
Vial:	6	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	2.8.2012 12:11:47
Injection Volume:	10,00 ul	Processing Method:	IO95
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,319	33591	0,12	2203
2	Peak2	1,000	10212	0,04	1221
3	Peak3	1,083	20806	0,08	1804
4	Peak4	1,593	57690	0,21	3887
5	Peak5	1,936	26981879	97,93	2426344
6	Peak6	3,392	404378	1,47	20429
7	Peak7	4,709	7942	0,03	586
8	Peak8	11,350	35491	0,13	1781



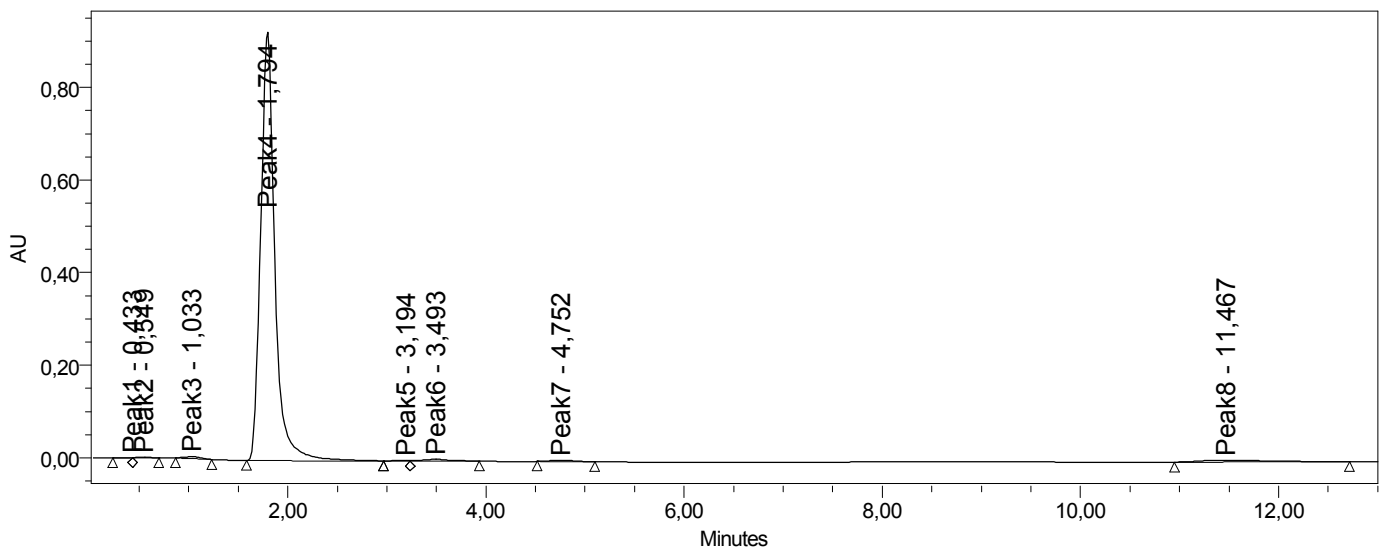
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Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO96 Compound 7	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2.8.2012 11:40:15
Vial:	7	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	2.8.2012 12:13:48
Injection Volume:	10,00 ul	Processing Method:	IO96
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,433	4249	0,04	537
2	Peak2	0,549	11701	0,12	1254
3	Peak3	1,033	46190	0,48	4108
4	Peak4	1,794	9228142	96,02	927391
5	Peak5	3,194	22106	0,23	2113
6	Peak6	3,493	88491	0,92	4159
7	Peak7	4,752	42330	0,44	2843
8	Peak8	11,467	167674	1,74	3432



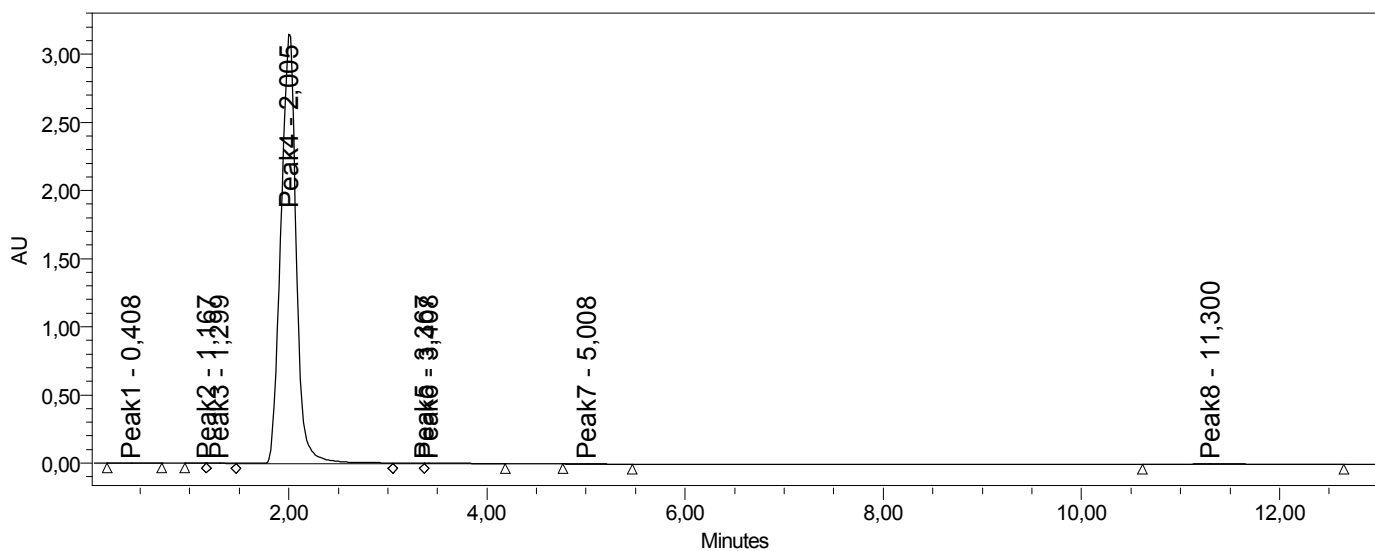
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Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO10 Compound 12	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1.8.2012 14:17:23
Vial:	12	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 14:32:48
Injection Volume:	10,00 ul	Processing Method:	IO10
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,408	12625	0,04	599
2	Peak2	1,167	6534	0,02	963
3	Peak3	1,299	25450	0,07	1872
4	Peak4	2,005	34098473	98,67	3154123
5	Peak5	3,367	83369	0,24	5497
6	Peak6	3,408	157057	0,45	5689
7	Peak7	5,008	31093	0,09	1846
8	Peak8	11,300	142471	0,41	2633



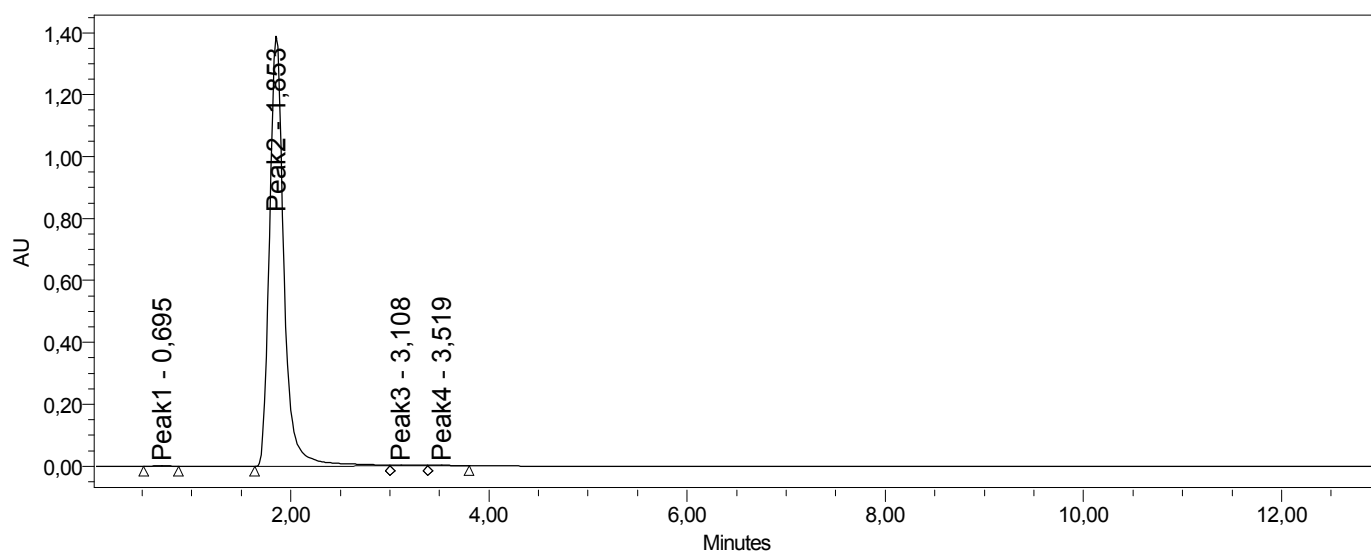
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Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO11 Compound 13	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1.8.2012 14:03:40
Vial:	11	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 14:18:55
Injection Volume:	10,00 ul	Processing Method:	IO11
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,695	4928	0,03	462
2	Peak2	1,853	14127146	99,41	1387510
3	Peak3	3,108	51094	0,36	2665
4	Peak4	3,519	28263	0,20	2068



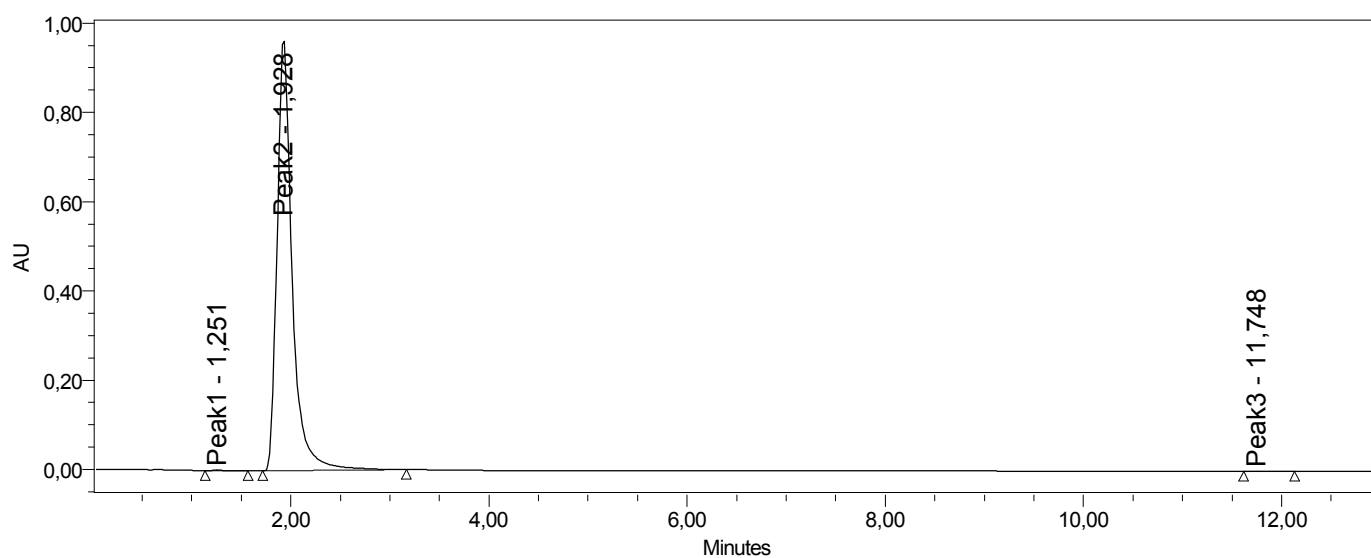
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO97 Compound 14	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	3.8.2012 14:34:41
Vial:	20	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	3.8.2012 14:49:43
Injection Volume:	10,00 ul	Processing Method:	IO97
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,251	6236	0,06	454
2	Peak2	1,928	10226964	99,90	963588
3	Peak3	11,748	4453	0,04	350



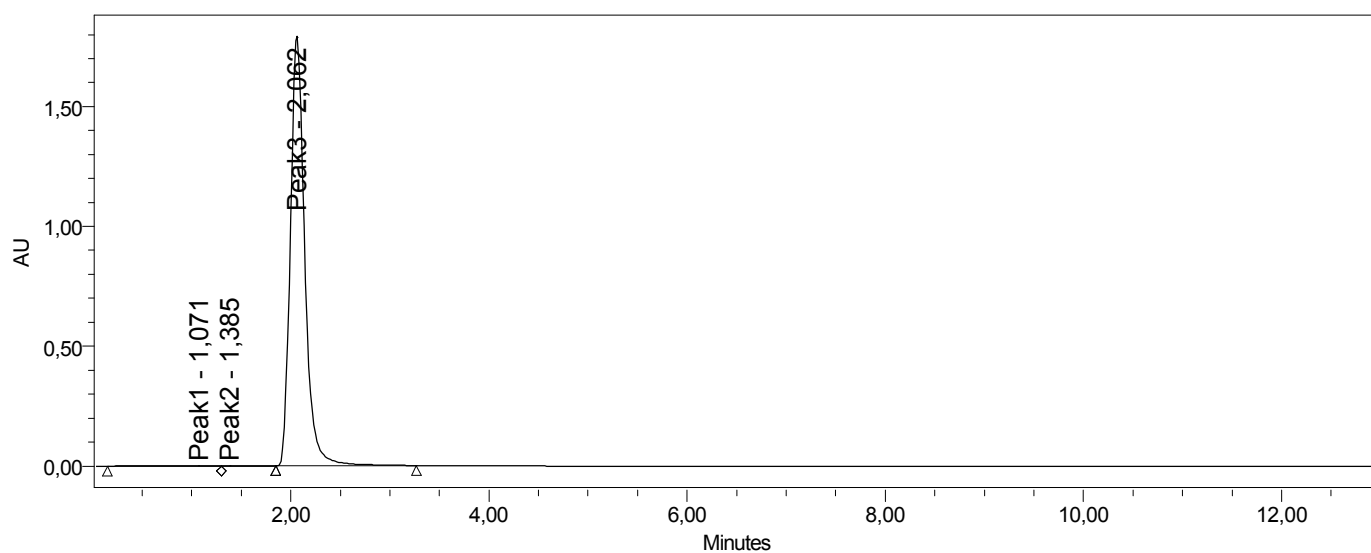
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO98 Compound 15	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	3.8.2012 14:48:23
Vial:	21	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	3.8.2012 15:03:41
Injection Volume:	10,00 ul	Processing Method:	IO98
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,071	64033	0,35	1233
2	Peak2	1,385	21690	0,12	1223
3	Peak3	2,062	18093432	99,53	1792933



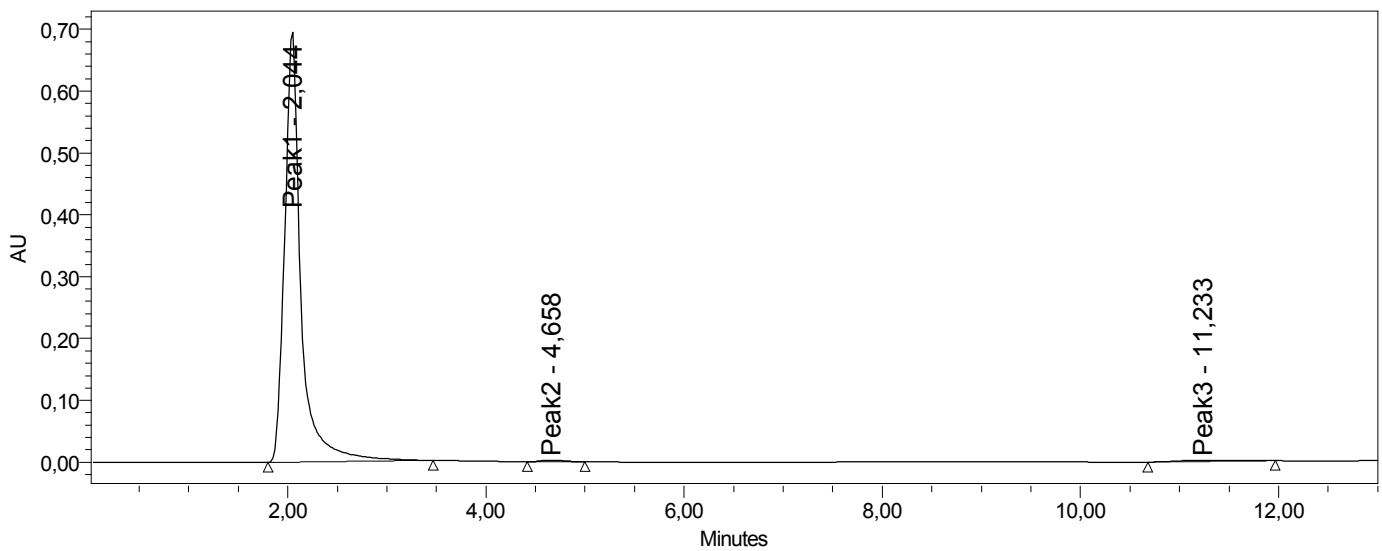
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Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	SD8 Compound 10	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2.8.2012 9:57:53
Vial:	1	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	2.8.2012 10:13:47
Injection Volume:	10,00 ul	Processing Method:	SD8
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,044	7938949	98,52	695658
2	Peak2	4,658	33582	0,42	2508
3	Peak3	11,233	86061	1,07	2120



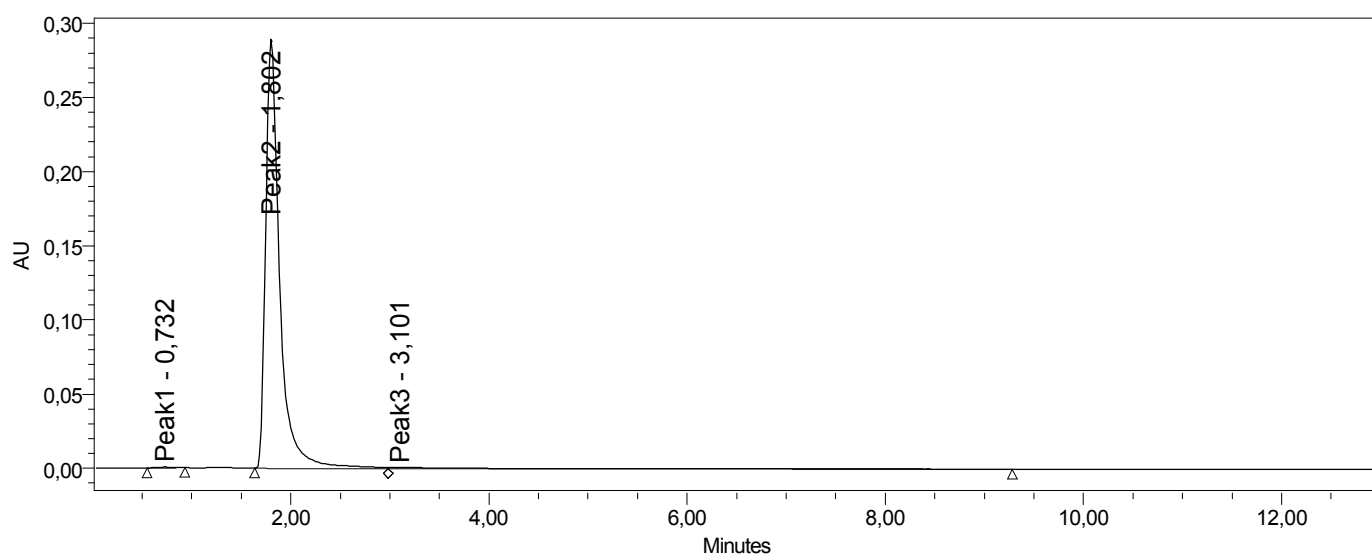
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Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	SD9 Compound 11	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2.8.2012 10:12:06
Vial:	2	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	2.8.2012 10:28:34
Injection Volume:	10,00 ul	Processing Method:	SD9
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,732	5932	0,20	554
2	Peak2	1,802	2867781	97,70	288756
3	Peak3	3,101	61641	2,10	843



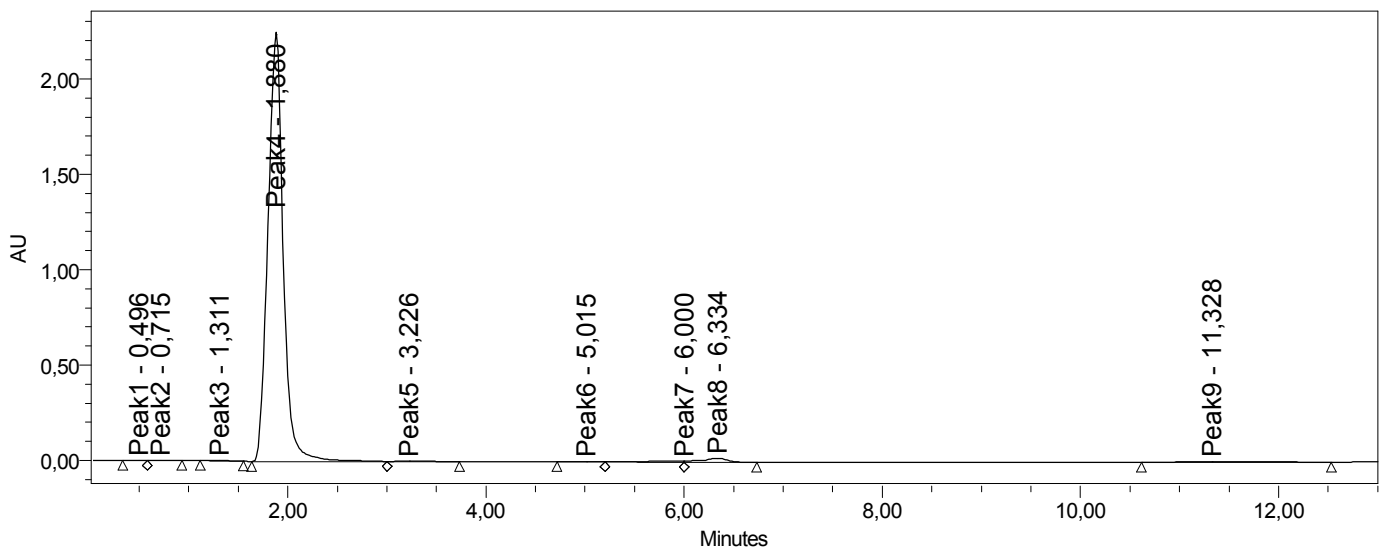
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO05 Compound 8	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1.8.2012 14:45:37
Vial:	14	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 14:59:56
Injection Volume:	10,00 ul	Processing Method:	IO05
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,496	6774	0,03	764
2	Peak2	0,715	13509	0,05	1361
3	Peak3	1,311	43388	0,17	3523
4	Peak4	1,880	24138482	96,72	2247882
5	Peak5	3,226	62244	0,25	2378
6	Peak6	5,015	32436	0,13	1764
7	Peak7	6,000	166522	0,67	6402
8	Peak8	6,334	346517	1,39	19958
9	Peak9	11,328	147376	0,59	2472



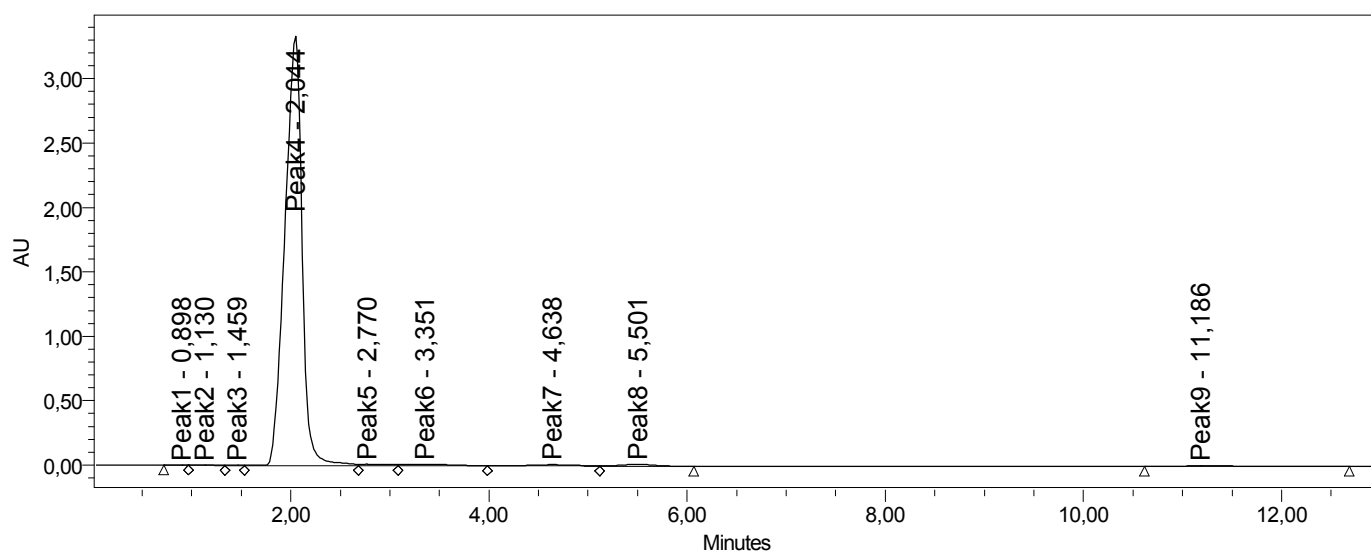
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Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO6 Compound 9	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1.8.2012 14:31:23
Vial:	13	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 14:46:54
Injection Volume:	10,00 ul	Processing Method:	IO06
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,898	6785	0,02	736
2	Peak2	1,130	25169	0,06	1701
3	Peak3	1,459	9828	0,02	977
4	Peak4	2,044	40220570	96,68	3340405
5	Peak5	2,770	236496	0,57	12275
6	Peak6	3,351	347572	0,84	10475
7	Peak7	4,638	308974	0,74	8835
8	Peak8	5,501	287432	0,69	12988
9	Peak9	11,186	158602	0,38	2777



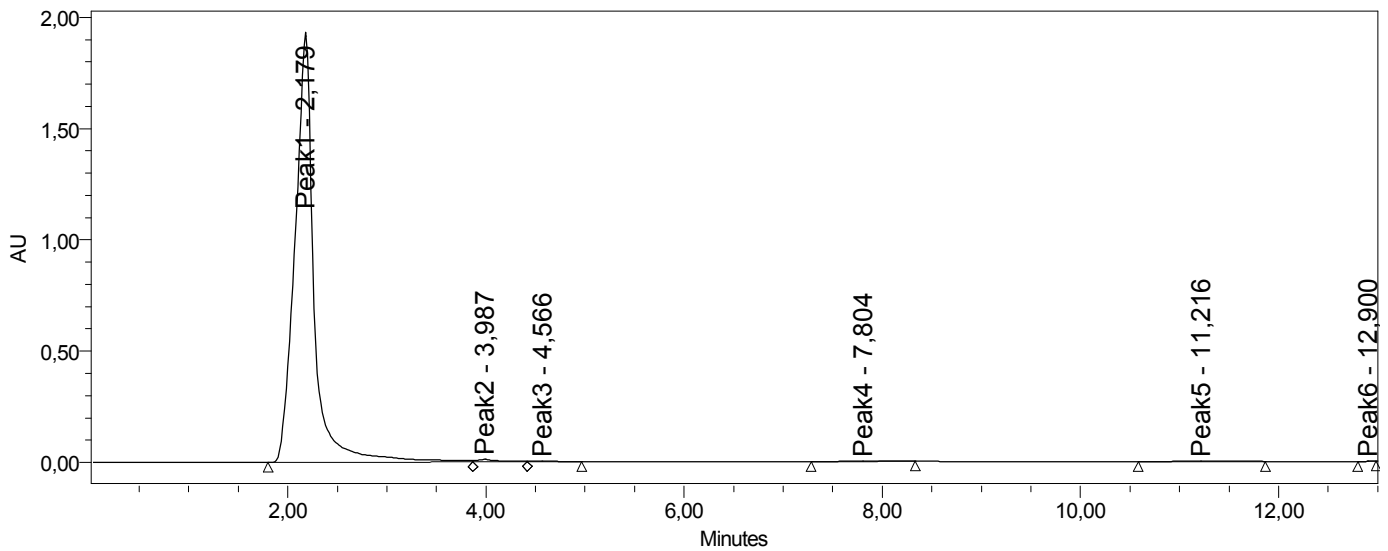
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Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO78 Compound 16	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1.8.2012 13:49:24
Vial:	10	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 14:05:19
Injection Volume:	10,00 ul	Processing Method:	IO78
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,179	25988498	98,53	1931763
2	Peak2	3,987	166730	0,63	10958
3	Peak3	4,566	47066	0,18	2580
4	Peak4	7,804	45351	0,17	1532
5	Peak5	11,216	128686	0,49	3415
6	Peak6	12,900	203	0,00	30



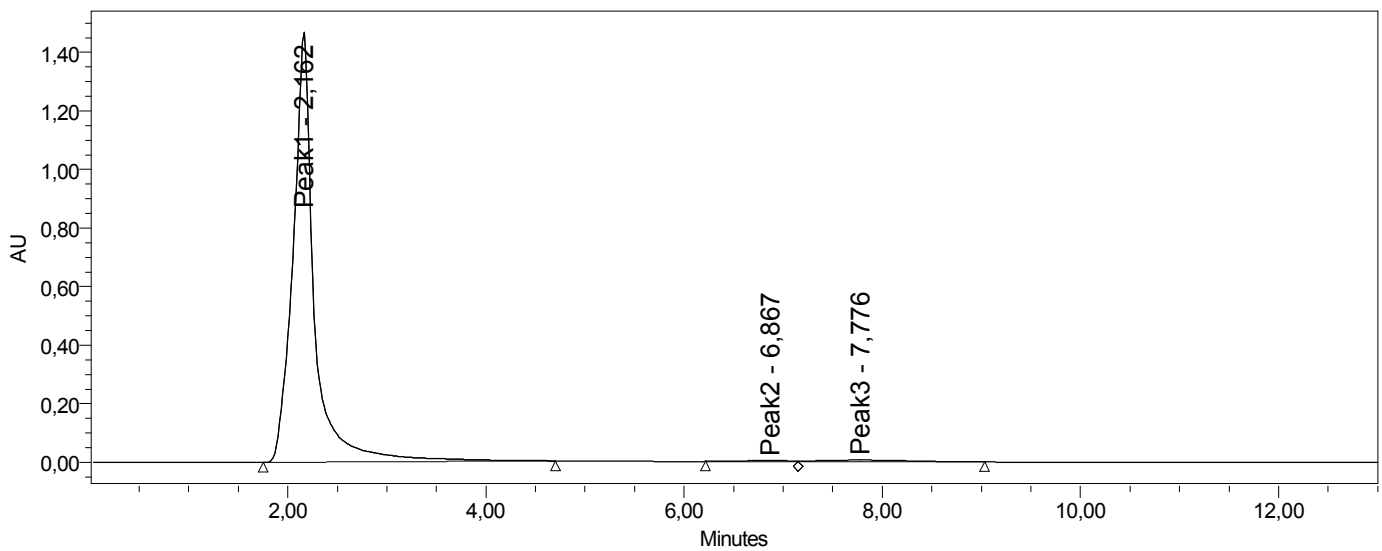
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Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO79 Compound 17	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2.8.2012 10:37:10
Vial:	3	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	2.8.2012 10:54:00
Injection Volume:	10,00 ul	Processing Method:	IO79
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,162	22083477	98,03	1466942
2	Peak2	6,867	102950	0,46	2644
3	Peak3	7,776	339705	1,51	5898



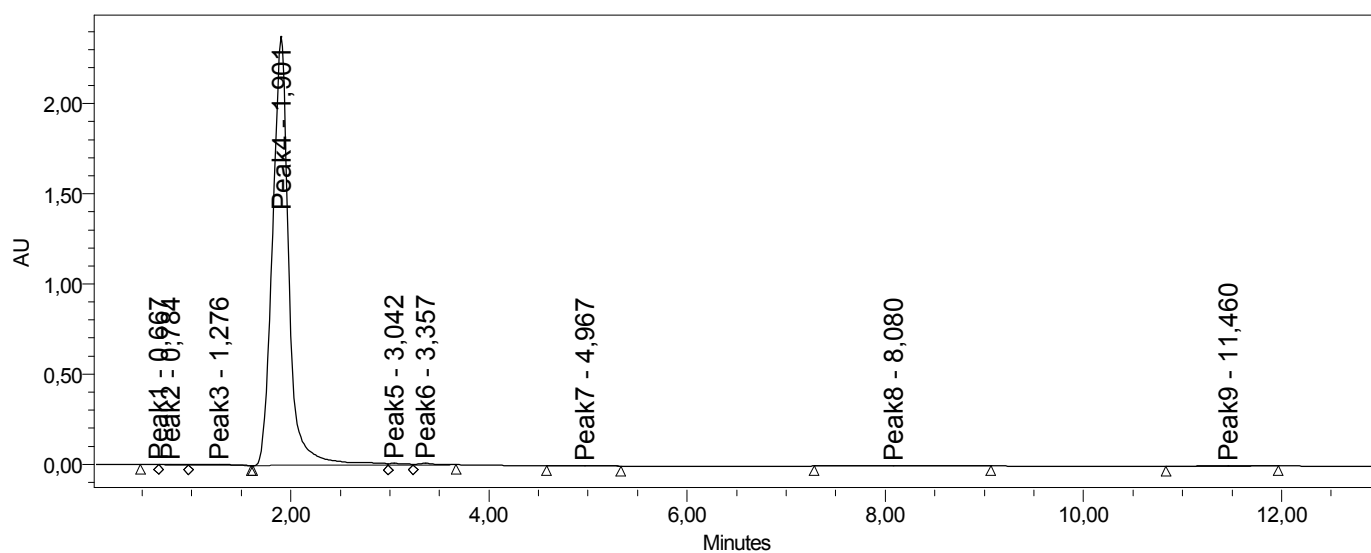
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	TM01 Compound 18	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2.8.2012 12:24:37
Vial:	10	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	2.8.2012 12:40:33
Injection Volume:	10,00 ul	Processing Method:	TM01
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,667	6009	0,02	1057
2	Peak2	0,784	34561	0,12	2238
3	Peak3	1,276	102381	0,37	5597
4	Peak4	1,901	27408851	97,82	2376025
5	Peak5	3,042	107075	0,38	8549
6	Peak6	3,357	95816	0,34	8663
7	Peak7	4,967	32104	0,11	1314
8	Peak8	8,080	139406	0,50	2254
9	Peak9	11,460	94167	0,34	2851



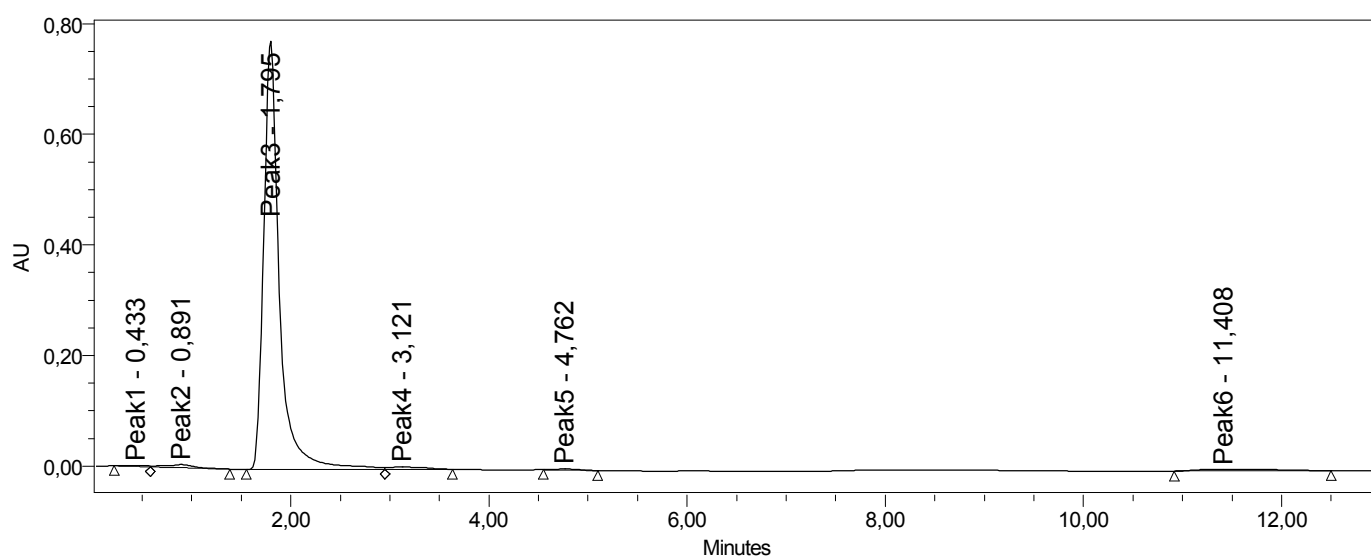
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	TM02 Compound 19	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2.8.2012 12:39:09
Vial:	11	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	2.8.2012 12:54:33
Injection Volume:	10,00 ul	Processing Method:	TM02
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,433	30818	0,34	2030
2	Peak2	0,891	107269	1,19	5630
3	Peak3	1,795	8576294	95,14	775278
4	Peak4	3,121	106966	1,19	4512
5	Peak5	4,762	32782	0,36	2258
6	Peak6	11,408	160043	1,78	3287



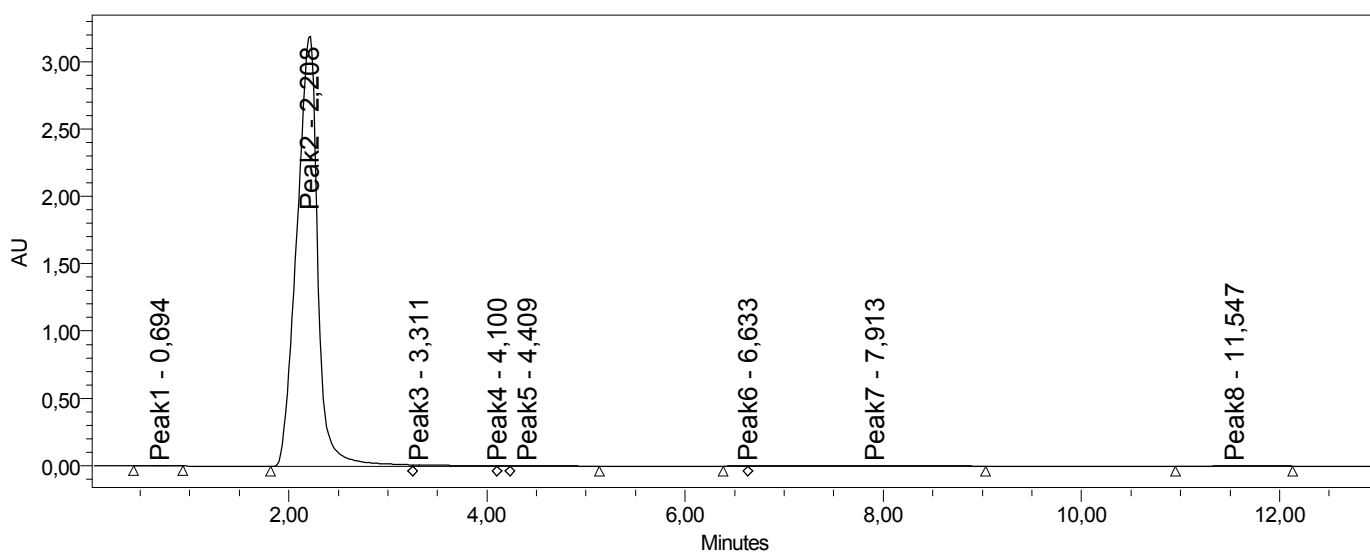
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO93 Compound 20	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2.8.2012 11:11:58
Vial:	5	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	2.8.2012 11:27:20
Injection Volume:	10,00 ul	Processing Method:	IO93
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,694	42980	0,09	3401
2	Peak2	2,208	47129864	98,27	3207740
3	Peak3	3,311	304256	0,63	9869
4	Peak4	4,100	24307	0,05	3185
5	Peak5	4,409	107756	0,22	4370
6	Peak6	6,633	5795	0,01	735
7	Peak7	7,913	234440	0,49	3236
8	Peak8	11,547	108902	0,23	3428



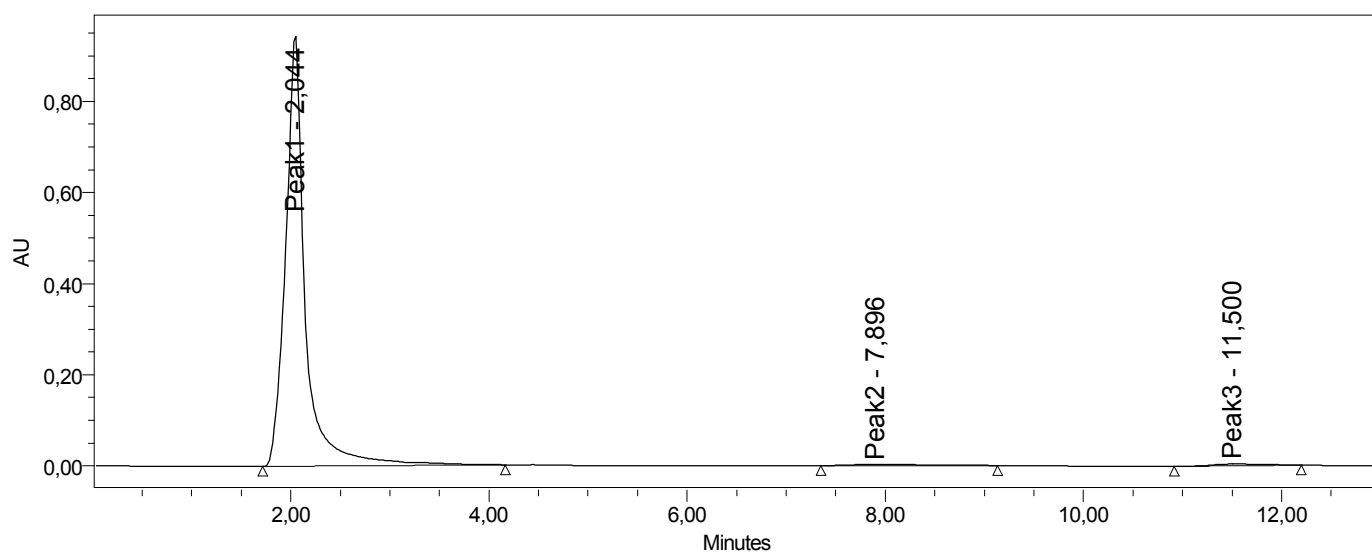
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Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO92 Compound 21	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2.8.2012 10:56:16
Vial:	4	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	2.8.2012 11:21:24
Injection Volume:	10,00 ul	Processing Method:	IO92
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,044	13100468	98,01	945182
2	Peak2	7,896	129378	0,97	2264
3	Peak3	11,500	136215	1,02	3960



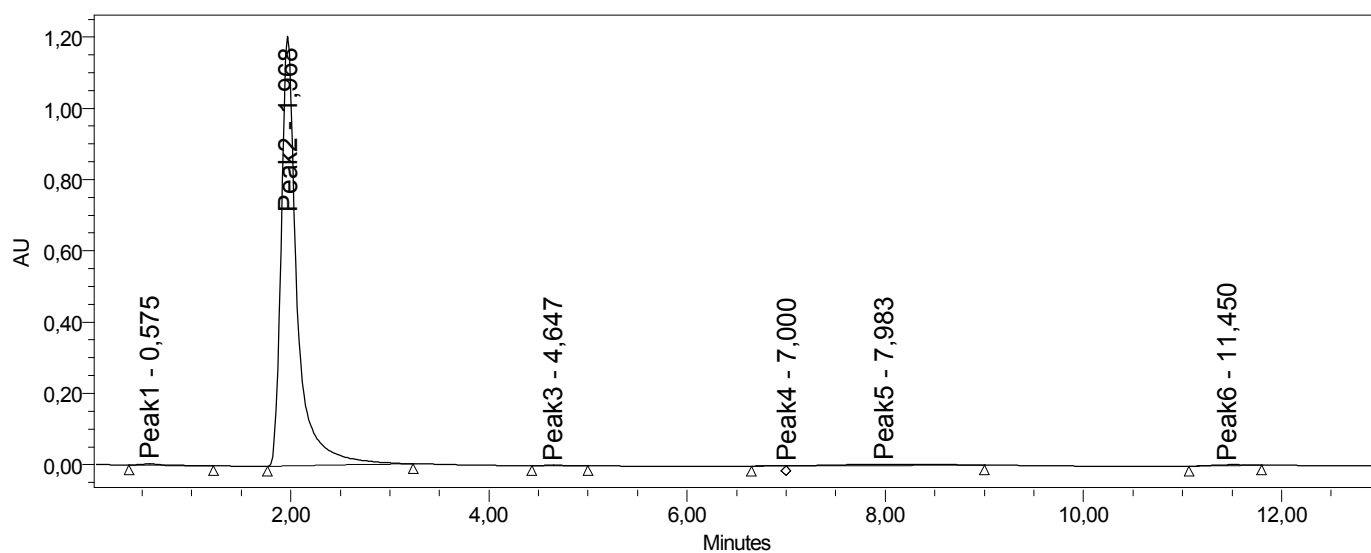
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Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO100 Compound 22	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2.8.2012 11:55:57
Vial:	8	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	2.8.2012 12:15:15
Injection Volume:	10,00 ul	Processing Method:	IO100
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,575	57142	0,41	3911
2	Peak2	1,968	13479586	97,36	1203157
3	Peak3	4,647	18150	0,13	1195
4	Peak4	7,000	7303	0,05	673
5	Peak5	7,983	236567	1,71	3446
6	Peak6	11,450	46841	0,34	2128



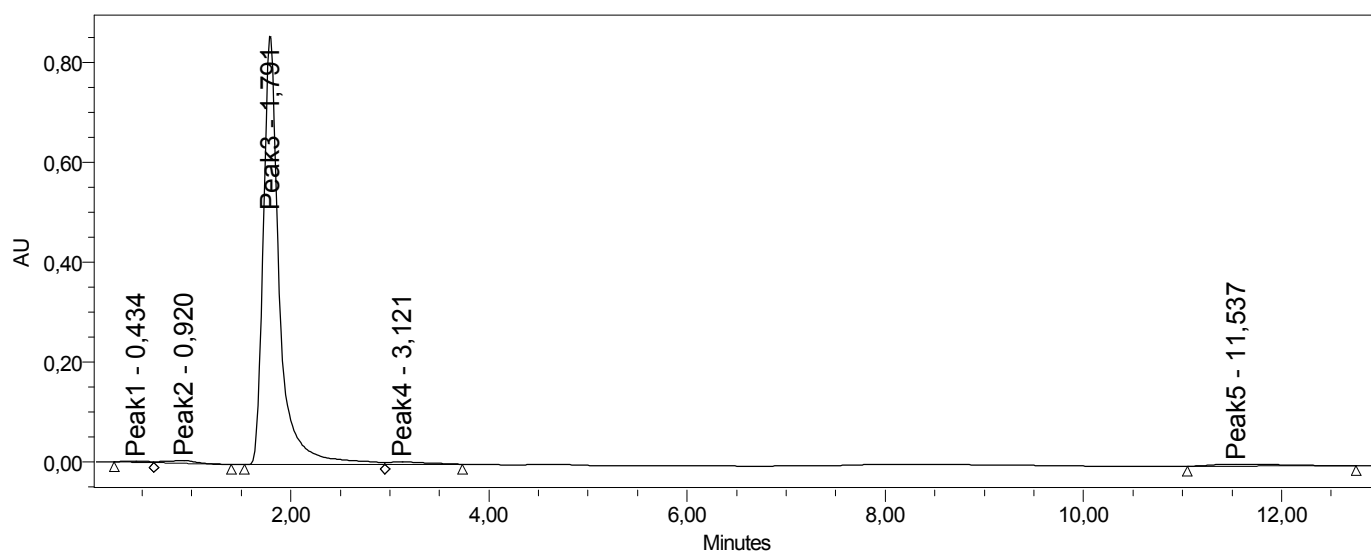
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO101 Compound 23	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	2.8.2012 12:10:27
Vial:	9	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	2.8.2012 12:26:22
Injection Volume:	10,00 ul	Processing Method:	IO101
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,434	37968	0,37	2193
2	Peak2	0,920	117750	1,15	5877
3	Peak3	1,791	9786913	95,41	862554
4	Peak4	3,121	134982	1,32	5478
5	Peak5	11,537	179917	1,75	3637



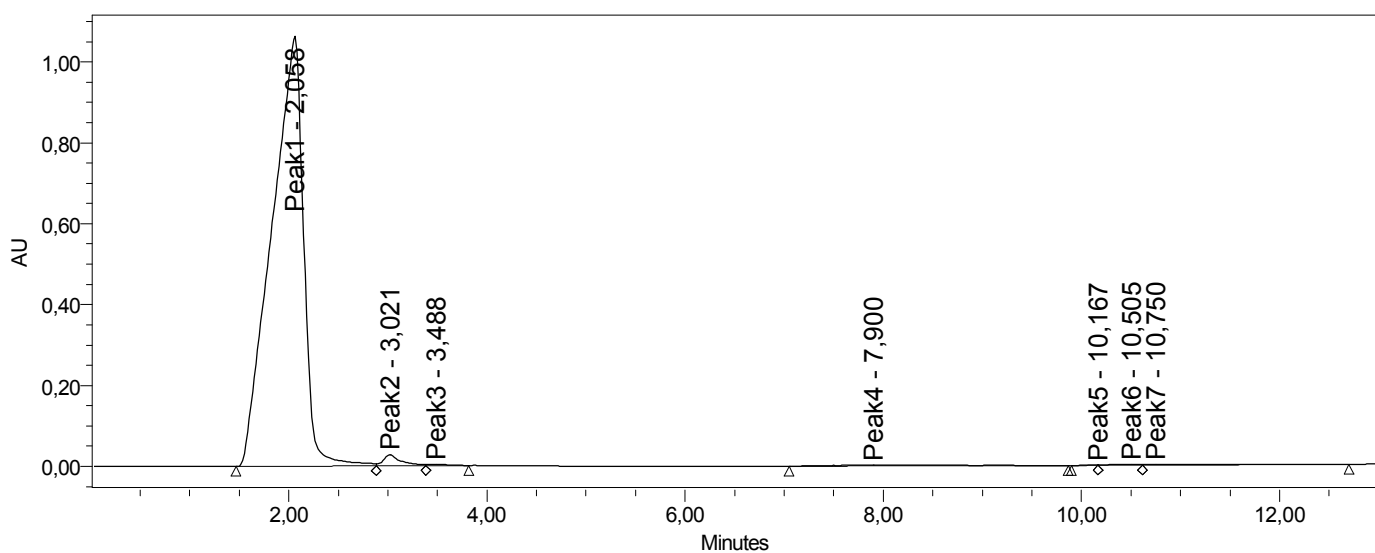
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO95 Compound 6	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	31.7.2012 14:49:29
Vial:	14	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	31.7.2012 15:07:27
Injection Volume:	10,00 ul	Processing Method:	IO95
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,058	23724510	97,11	1067892
2	Peak2	3,021	336967	1,38	27618
3	Peak3	3,488	39803	0,16	2894
4	Peak4	7,900	152380	0,62	1710
5	Peak5	10,167	3800	0,02	436
6	Peak6	10,505	41773	0,17	1997
7	Peak7	10,750	130128	0,53	2037



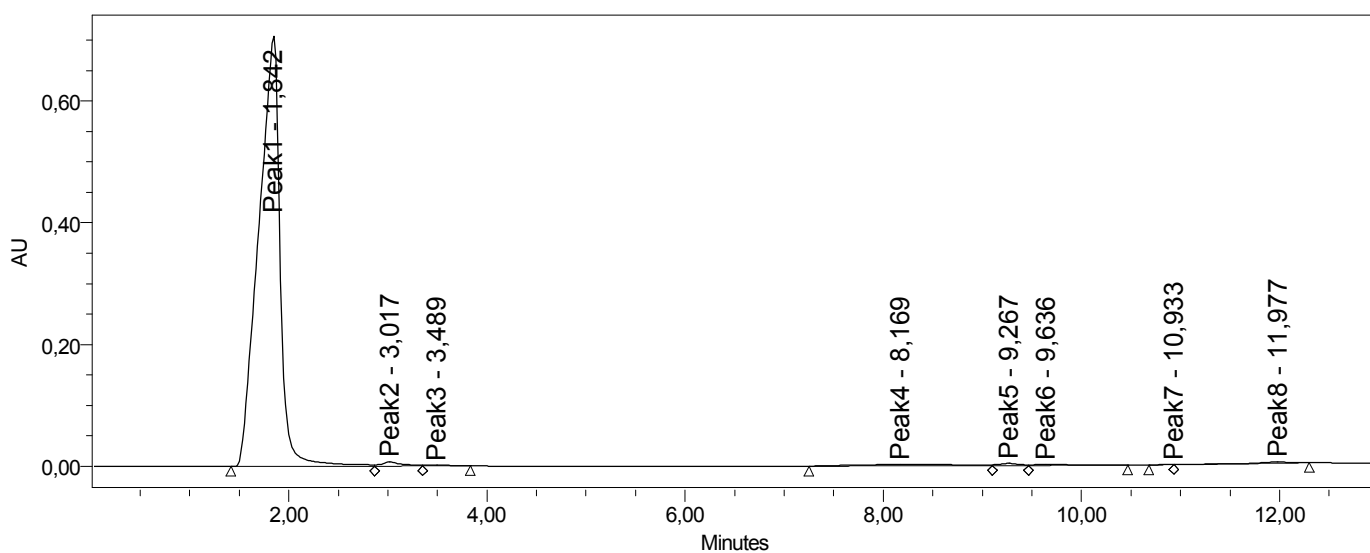
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO96 Compound 7	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	31.7.2012 15:11:22
Vial:	15	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	31.7.2012 15:26:20
Injection Volume:	10,00 ul	Processing Method:	IO96
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,842	10600174	96,31	710139
2	Peak2	3,017	94399	0,86	6989
3	Peak3	3,489	25080	0,23	1747
4	Peak4	8,169	152781	1,39	1926
5	Peak5	9,267	45694	0,42	3446
6	Peak6	9,636	35845	0,33	1183
7	Peak7	10,933	1568	0,01	173
8	Peak8	11,977	50958	0,46	2240



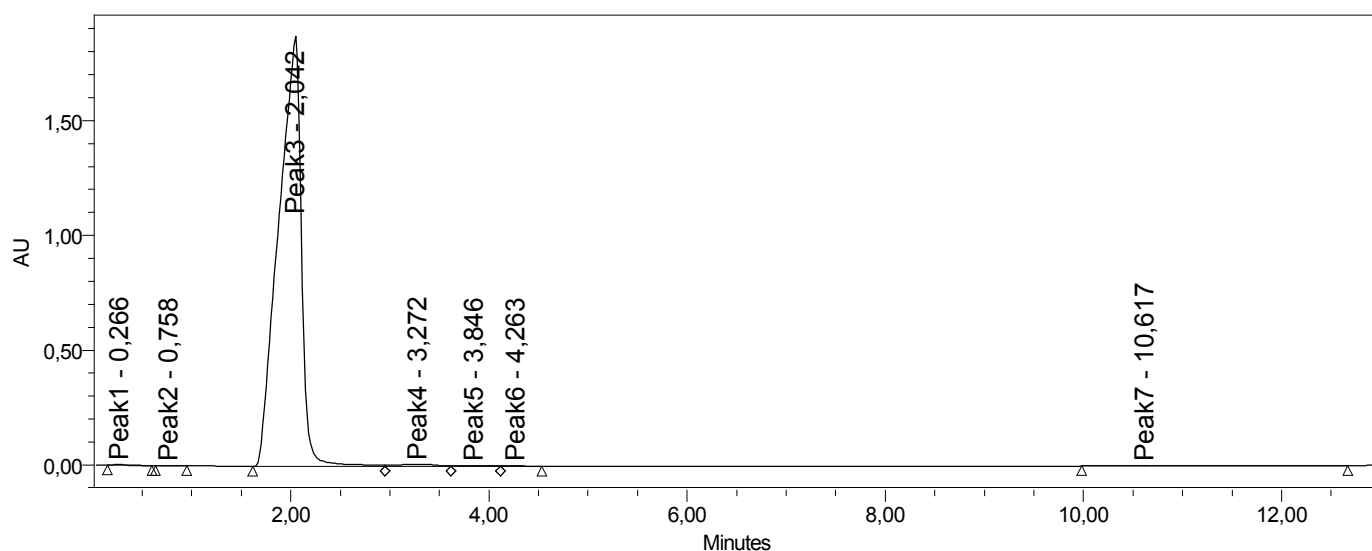
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO10 Compound 12	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1.8.2012 10:53:15
Vial:	4	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 12:24:52
Injection Volume:	10,00 ul	Processing Method:	IO10k2
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,266	31154	0,10	4079
2	Peak2	0,758	4411	0,01	529
3	Peak3	2,042	29698579	98,53	1880232
4	Peak4	3,272	207850	0,69	7943
5	Peak5	3,846	54953	0,18	2348
6	Peak6	4,263	21233	0,07	1723
7	Peak7	10,617	123276	0,41	1455



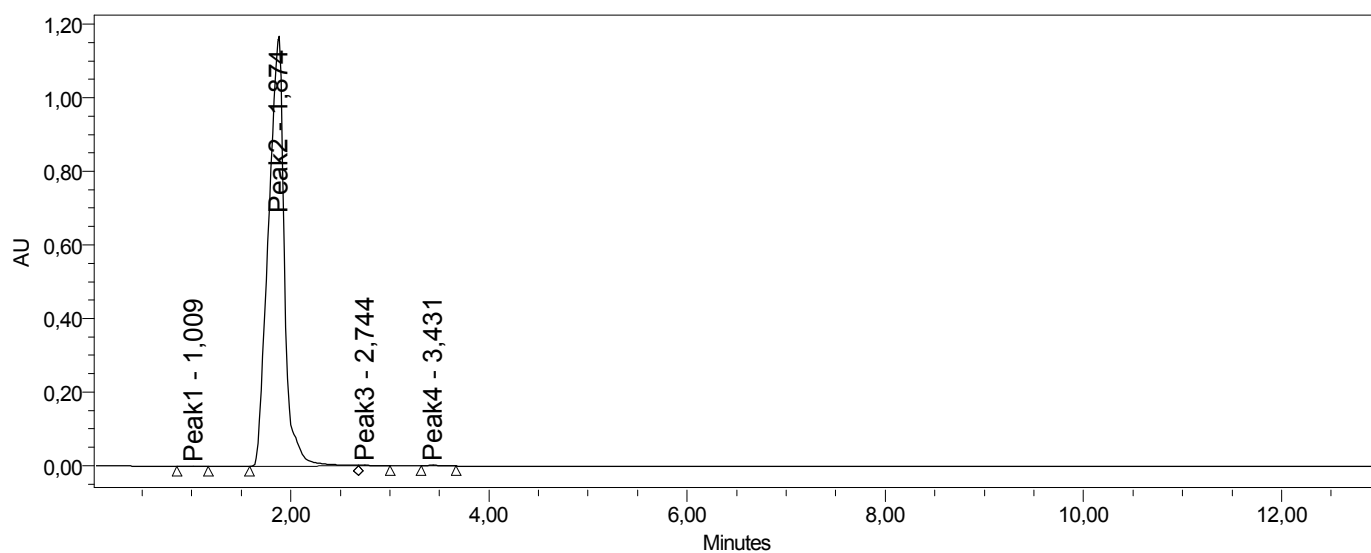
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO11 Compound 13	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1.8.2012 11:08:15
Vial:	5	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 14:09:50
Injection Volume:	10,00 ul	Processing Method:	IO11
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,009	3201	0,02	350
2	Peak2	1,874	13062944	99,78	1178924
3	Peak3	2,744	13062	0,10	1356
4	Peak4	3,431	12515	0,10	1708



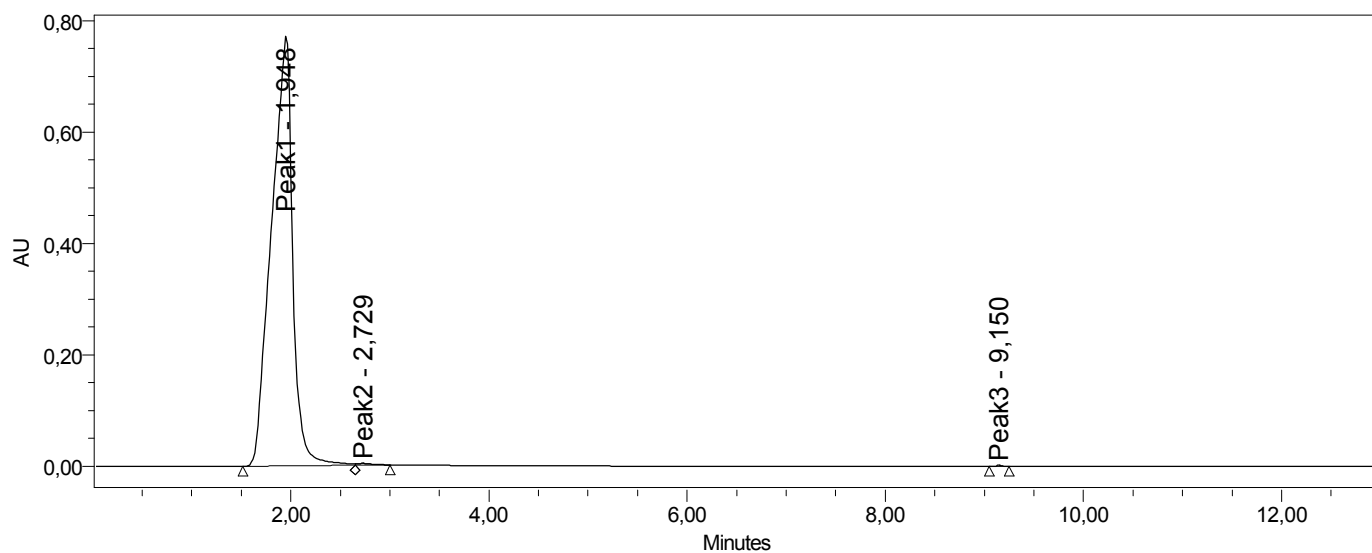
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO97 Compound 14	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7.8.2012 9:51:22
Vial:	1	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	7.8.2012 10:11:02
Injection Volume:	10,00 ul	Processing Method:	IO97
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,948	11450697	99,67	771715
2	Peak2	2,729	30275	0,26	3089
3	Peak3	9,150	7119	0,06	2112



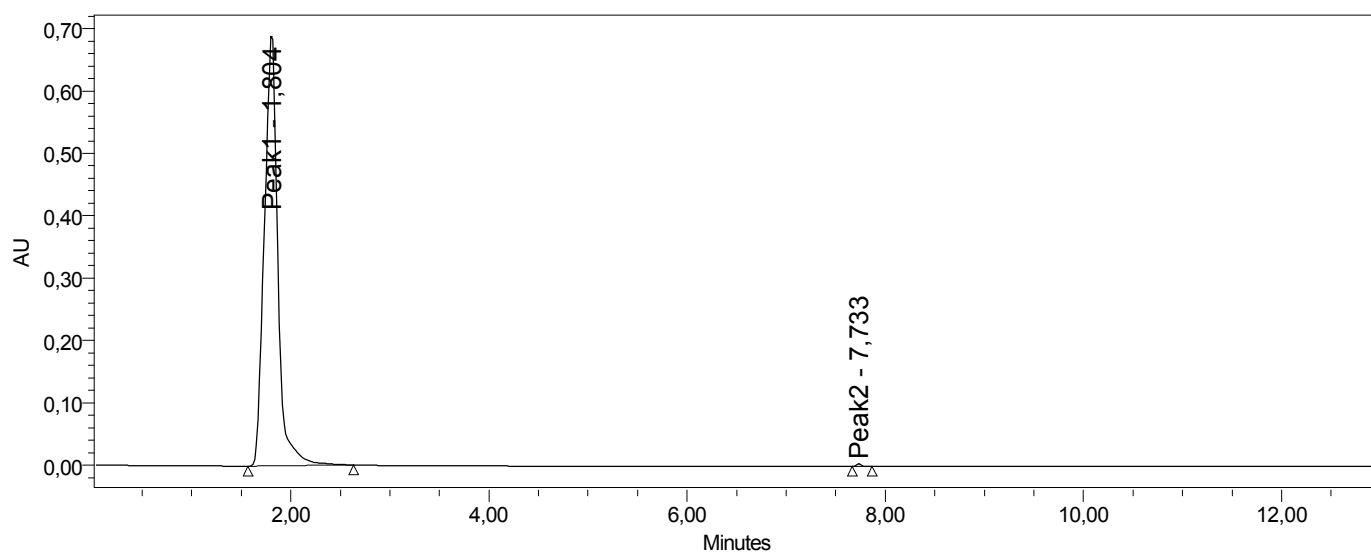
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO98	Compound 15	Acquired By:	System
Sample Type:	Unknown		Date Acquired:	7.8.2012 10:06:01
Vial:	2		Acq. Method Set:	10902543300513m_MS
Injection #:	1		Date Processed:	7.8.2012 10:29:13
Injection Volume:	10,00 ul		Processing Method:	IO98
Run Time:	13,0 Minutes		Channel Name:	2487Channel 2
Sample Set Name:			Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,804	6545868	99,79	688585
2	Peak2	7,733	13825	0,21	4082



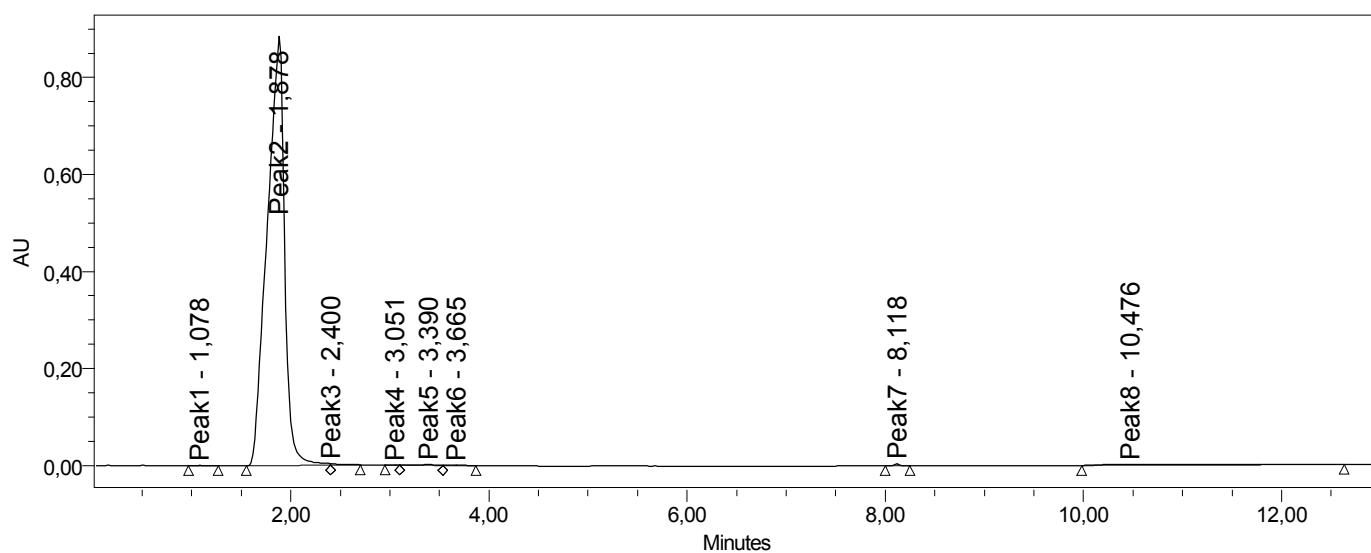
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	SD8 Compound 10	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	31.7.2012 11:43:51
Vial:	2	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	31.7.2012 12:48:53
Injection Volume:	10,00 ul	Processing Method:	SD8
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,078	5467	0,05	760
2	Peak2	1,878	10811776	98,02	886249
3	Peak3	2,400	22373	0,20	3030
4	Peak4	3,051	3036	0,03	660
5	Peak5	3,390	21871	0,20	1489
6	Peak6	3,665	9909	0,09	939
7	Peak7	8,118	13327	0,12	3841
8	Peak8	10,476	142908	1,30	1675



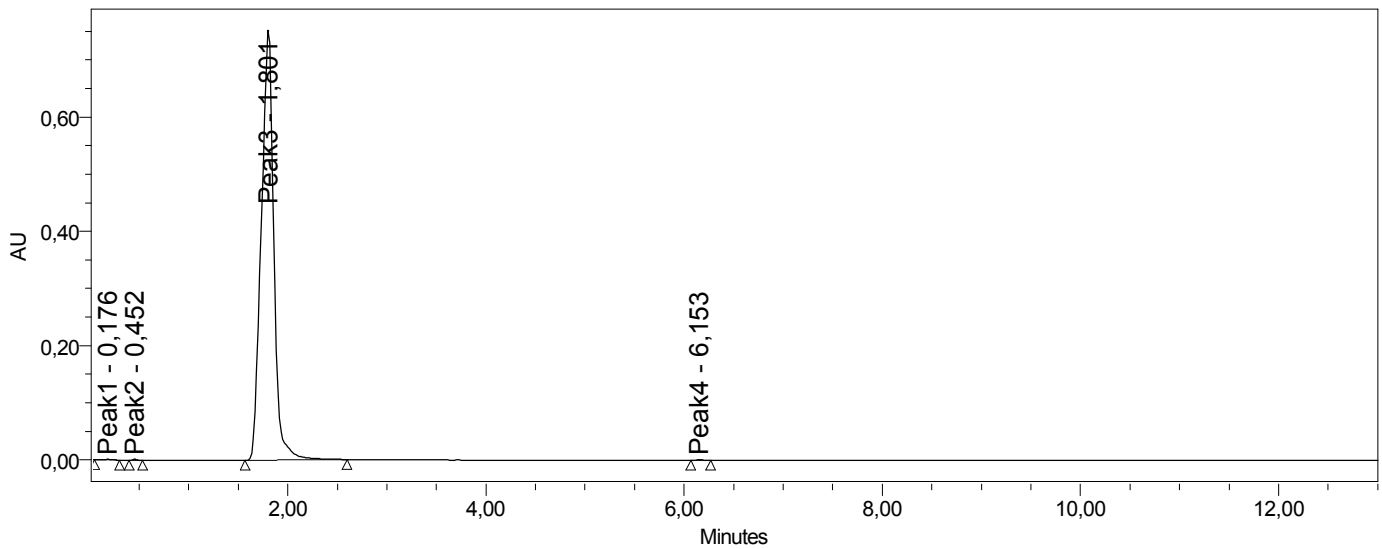
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	SD9 Compound 11	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	31.7.2012 11:59:40
Vial:	3	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 10:45:27
Injection Volume:	10,00 ul	Processing Method:	SD9
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,176	3995	0,06	947
2	Peak2	0,452	3336	0,05	1166
3	Peak3	1,801	6621154	99,84	749451
4	Peak4	6,153	3151	0,05	1017



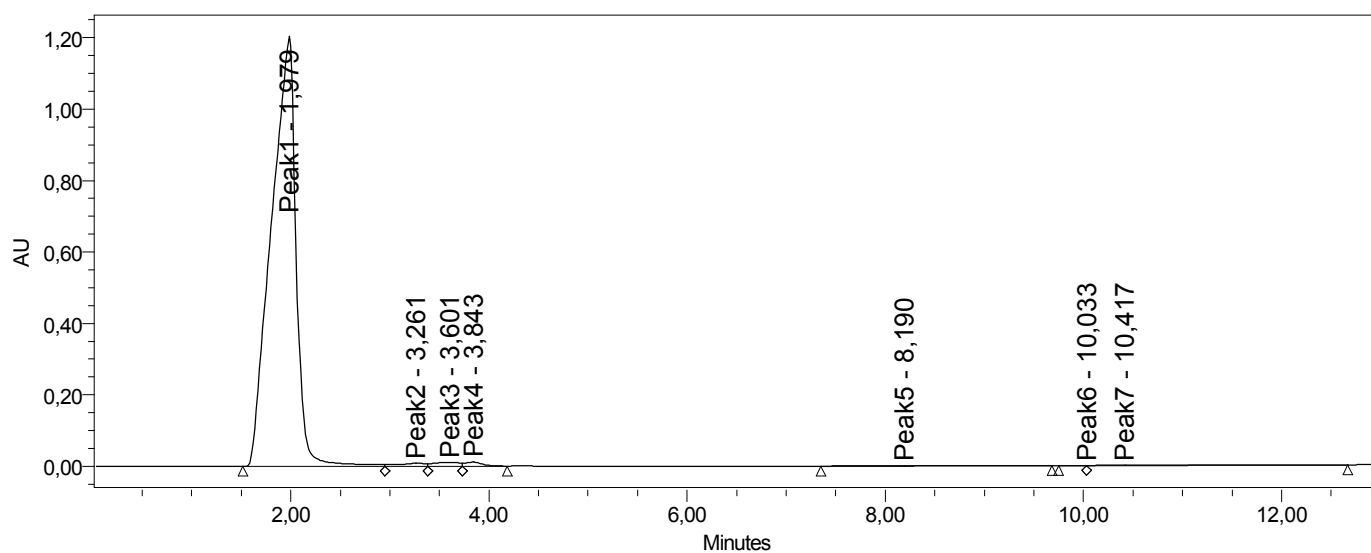
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO05 Compound 8	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1.8.2012 10:16:10
Vial:	2	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 11:01:55
Injection Volume:	10,00 ul	Processing Method:	IO05
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,979	20808363	96,84	1206445
2	Peak2	3,261	162461	0,76	7697
3	Peak3	3,601	191257	0,89	10783
4	Peak4	3,843	132608	0,62	11469
5	Peak5	8,190	46606	0,22	632
6	Peak6	10,033	3027	0,01	371
7	Peak7	10,417	142269	0,66	1634



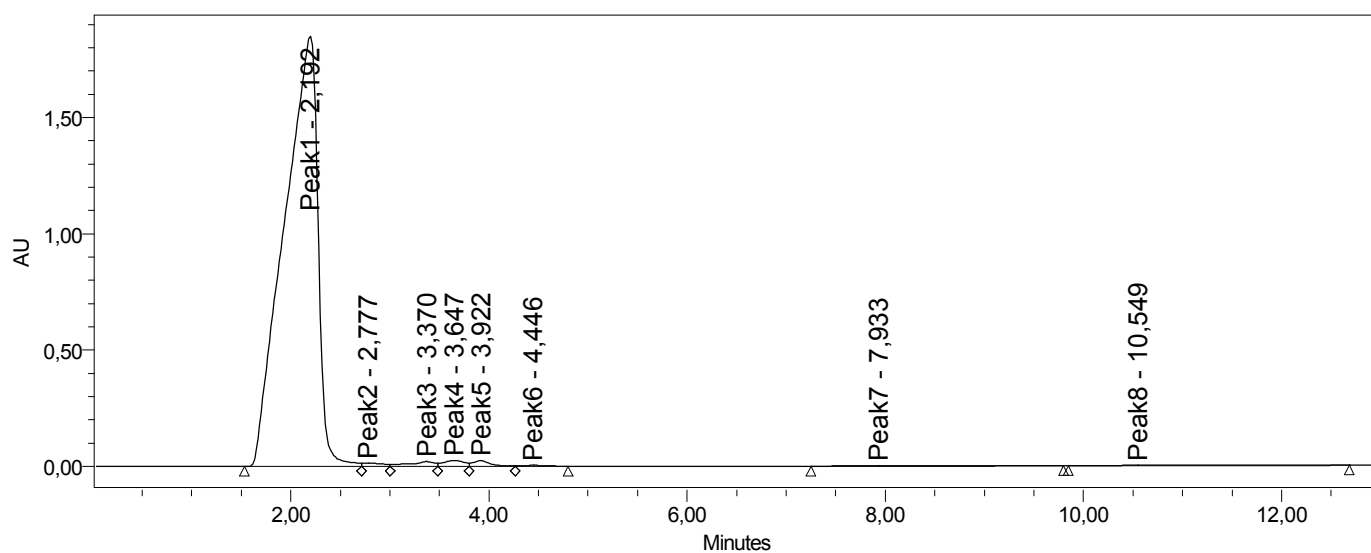
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO06 Compound 9	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1.8.2012 10:38:04
Vial:	3	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 11:04:15
Injection Volume:	10,00 ul	Processing Method:	IO06
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,192	43577656	96,72	1853498
2	Peak2	2,777	194874	0,43	13758
3	Peak3	3,370	361256	0,80	19954
4	Peak4	3,647	355535	0,79	24292
5	Peak5	3,922	282089	0,63	23496
6	Peak6	4,446	46249	0,10	3408
7	Peak7	7,933	73873	0,16	909
8	Peak8	10,549	163980	0,36	1847



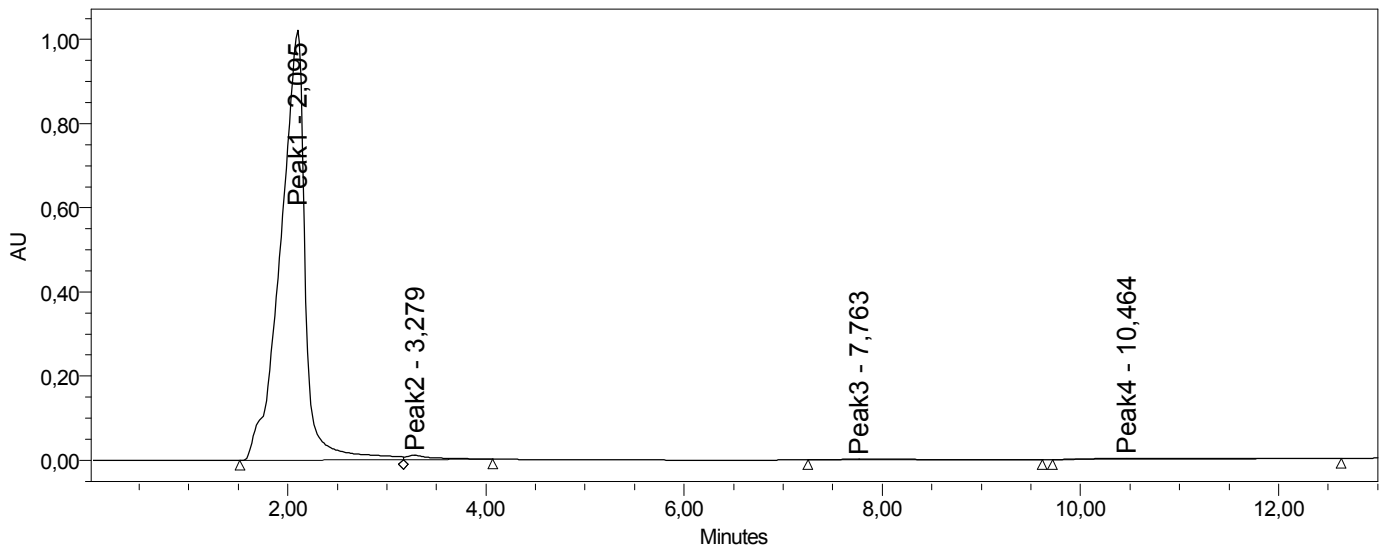
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO78 Compound 16	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	31.7.2012 13:11:40
Vial:	7	Acq. Method Set:	10902543300513m_MS
Injection #:	1	Date Processed:	31.7.2012 13:35:01
Injection Volume:	10,00 ul	Processing Method:	IO78
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,095	17612029	97,72	1022315
2	Peak2	3,279	195727	1,09	10420
3	Peak3	7,763	61748	0,34	830
4	Peak4	10,464	153354	0,85	1781



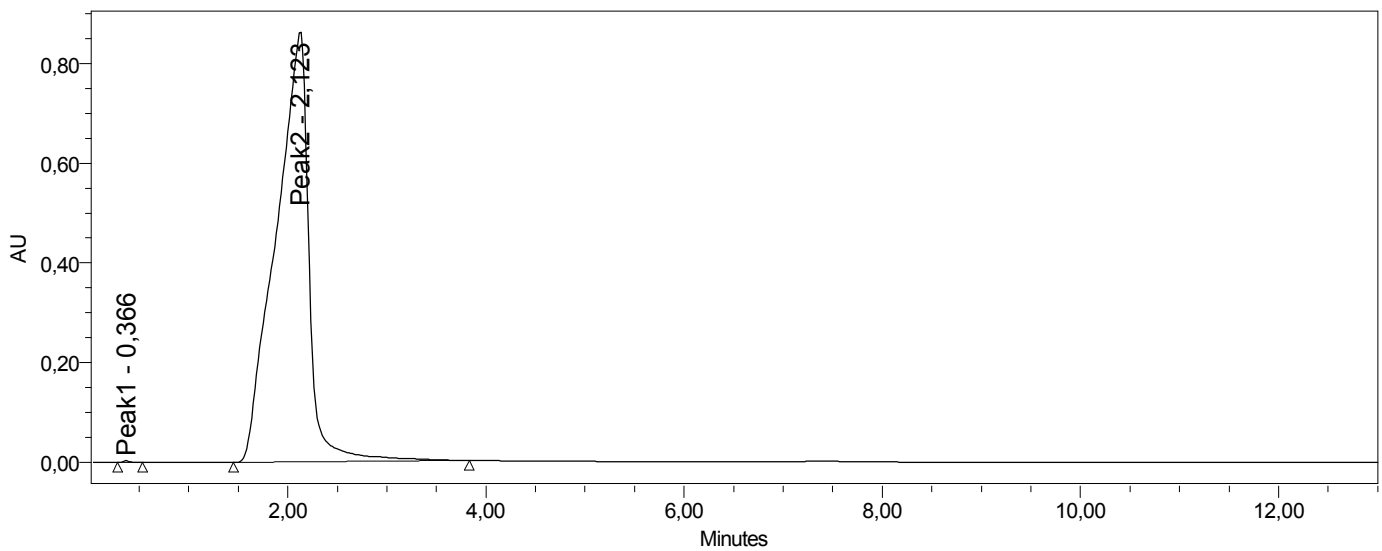
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO79 Compound 17	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	31.7.2012 13:48:38
Vial:	10	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 10:48:57
Injection Volume:	10,00 ul	Processing Method:	IO79
Run Time:	13,0 Minutes	Channel Name:	2487Channel 2
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,366	14192	0,07	3192
2	Peak2	2,123	19994440	99,93	867416



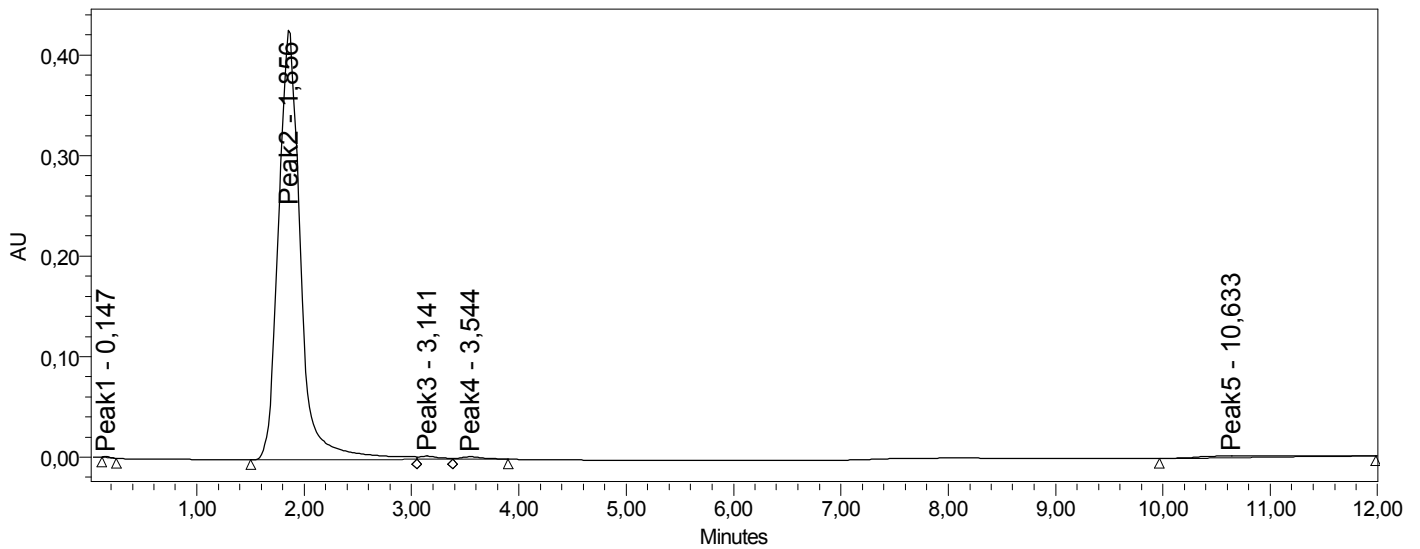
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	TM01 Compound 18	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1.8.2012 12:15:55
Vial:	9	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 12:31:03
Injection Volume:	10,00 ul	Processing Method:	TM01
Run Time:	12,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,147	2803	0,04	720
2	Peak2	1,856	6088874	96,79	426777
3	Peak3	3,141	43284	0,69	3375
4	Peak4	3,544	37749	0,60	2476
5	Peak5	10,633	117973	1,88	2024



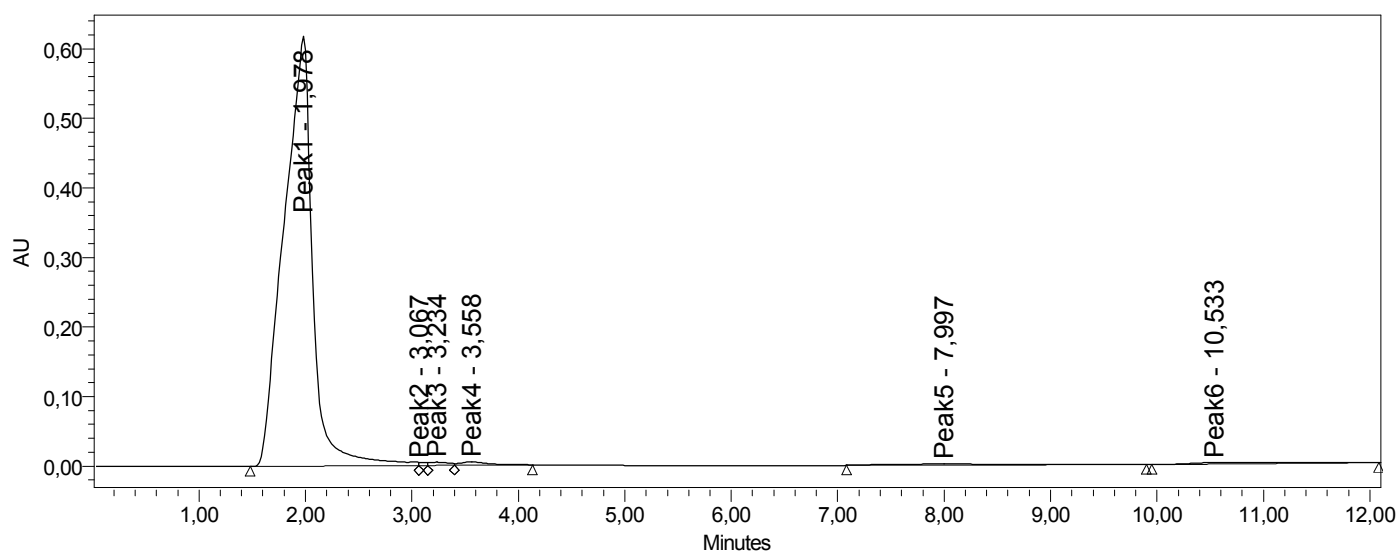
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	TM02 Compound 19	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1.8.2012 11:59:28
Vial:	8	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	1.8.2012 12:12:39
Injection Volume:	10,00 ul	Processing Method:	TM02
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,978	11563786	96,32	618552
2	Peak2	3,067	21994	0,18	4809
3	Peak3	3,234	58029	0,48	4749
4	Peak4	3,558	92306	0,77	4937
5	Peak5	7,997	146090	1,22	1645
6	Peak6	10,533	123491	1,03	1970



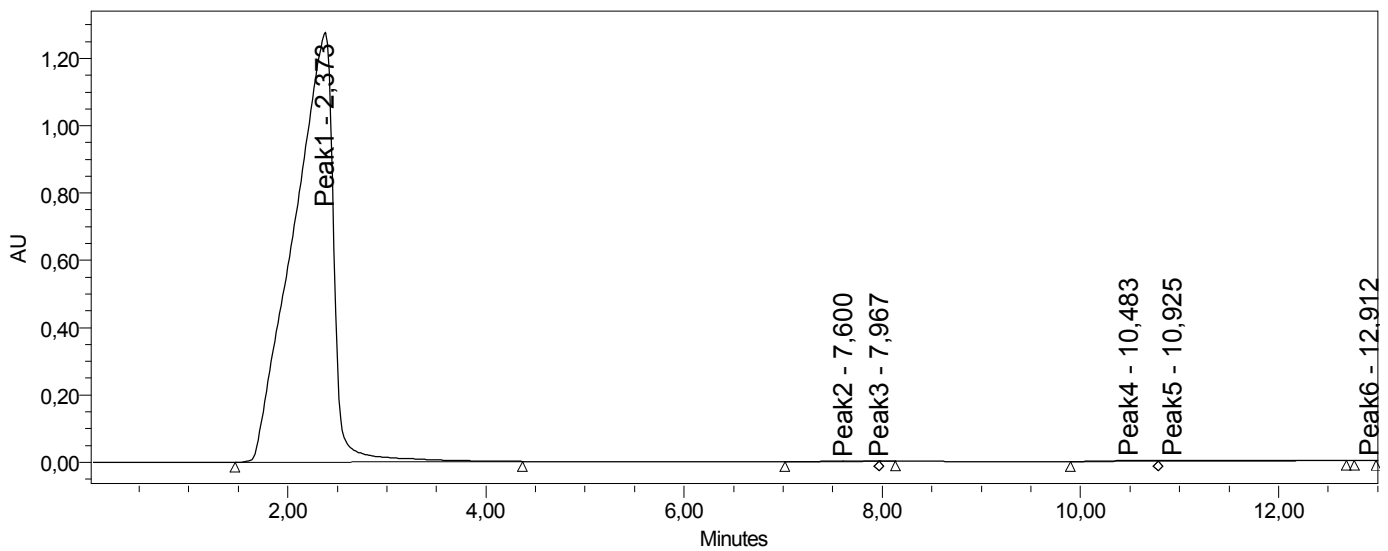
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO93 Compound 20	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	31.7.2012 14:28:19
Vial:	13	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	31.7.2012 15:09:26
Injection Volume:	10,00 ul	Processing Method:	IO93
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	2,373	35670434	99,38	1282628
2	Peak2	7,600	38339	0,11	1029
3	Peak3	7,967	3066	0,01	649
4	Peak4	10,483	69094	0,19	2132
5	Peak5	10,925	108022	0,30	1823
6	Peak6	12,912	2798	0,01	437



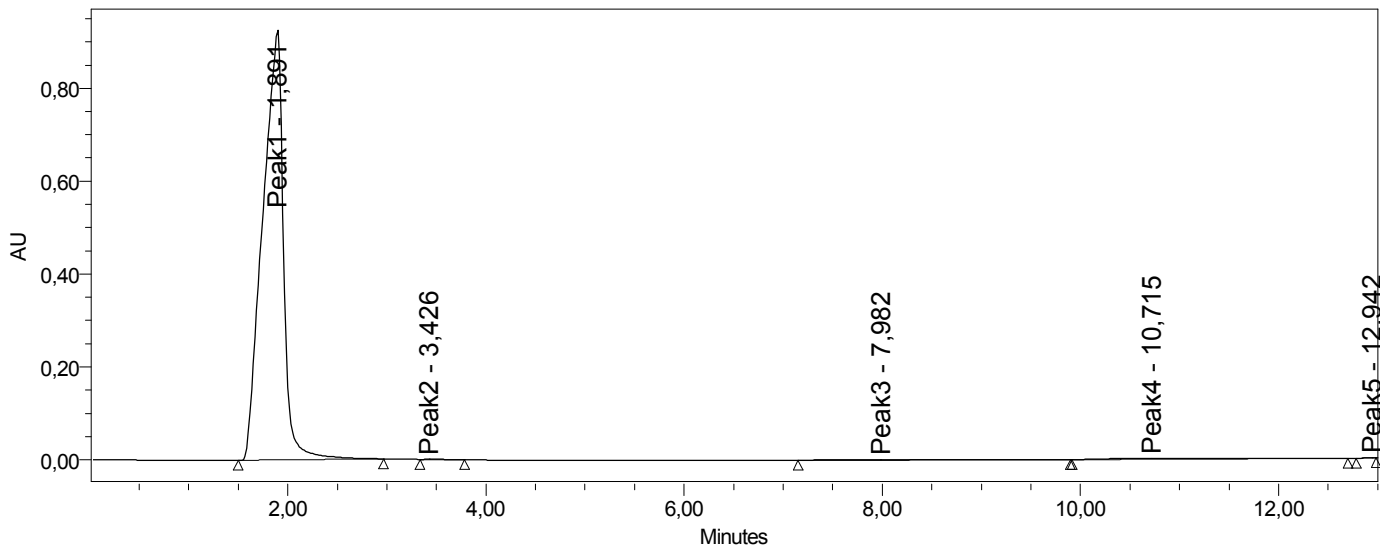
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO92 Compound 21	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	31.7.2012 14:05:24
Vial:	11	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	31.7.2012 14:21:33
Injection Volume:	10,00 ul	Processing Method:	IO92
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	1,891	13505939	97,72	931597
2	Peak2	3,426	10866	0,08	884
3	Peak3	7,982	118632	0,86	1368
4	Peak4	10,715	182802	1,32	2213
5	Peak5	12,942	2558	0,02	413



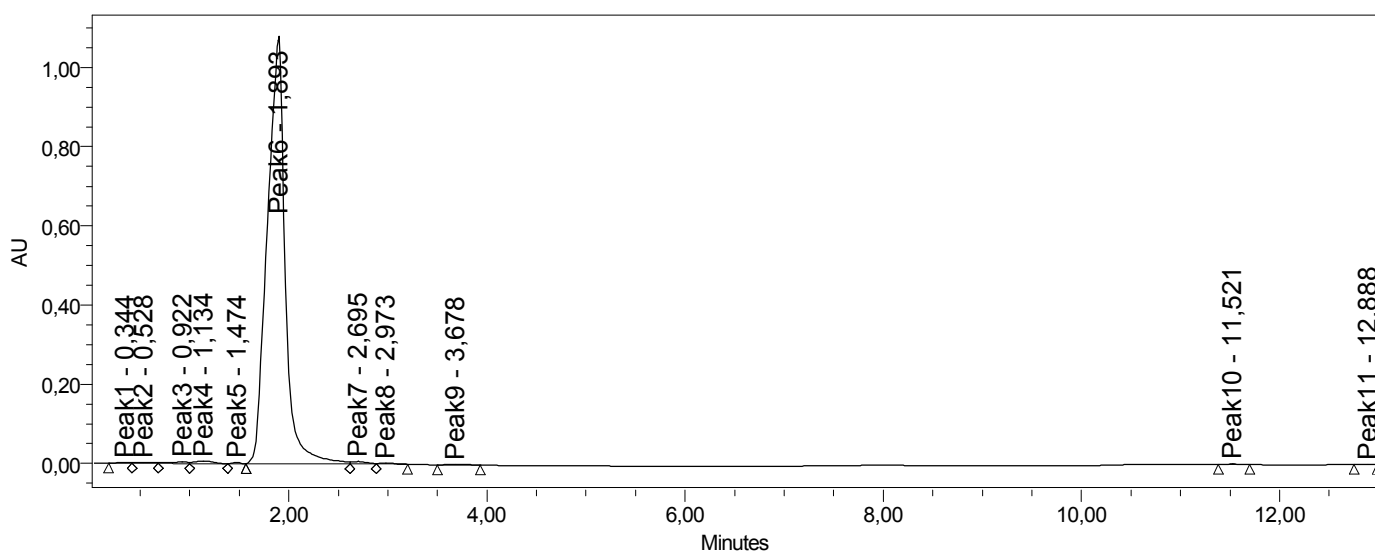
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO100 Compound 22	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	31.7.2012 15:25:10
Vial:	16	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	31.7.2012 15:41:09
Injection Volume:	10,00 ul	Processing Method:	IO100
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,344	14432	0,10	1568
2	Peak2	0,528	35142	0,25	2685
3	Peak3	0,922	58178	0,42	4396
4	Peak4	1,134	82098	0,59	5740
5	Peak5	1,474	18120	0,13	3516
6	Peak6	1,893	13518635	97,51	1082989
7	Peak7	2,695	66686	0,48	6232
8	Peak8	2,973	22548	0,16	1992
9	Peak9	3,678	28013	0,20	2264
10	Peak10	11,521	15656	0,11	2157
11	Peak11	12,888	3871	0,03	599



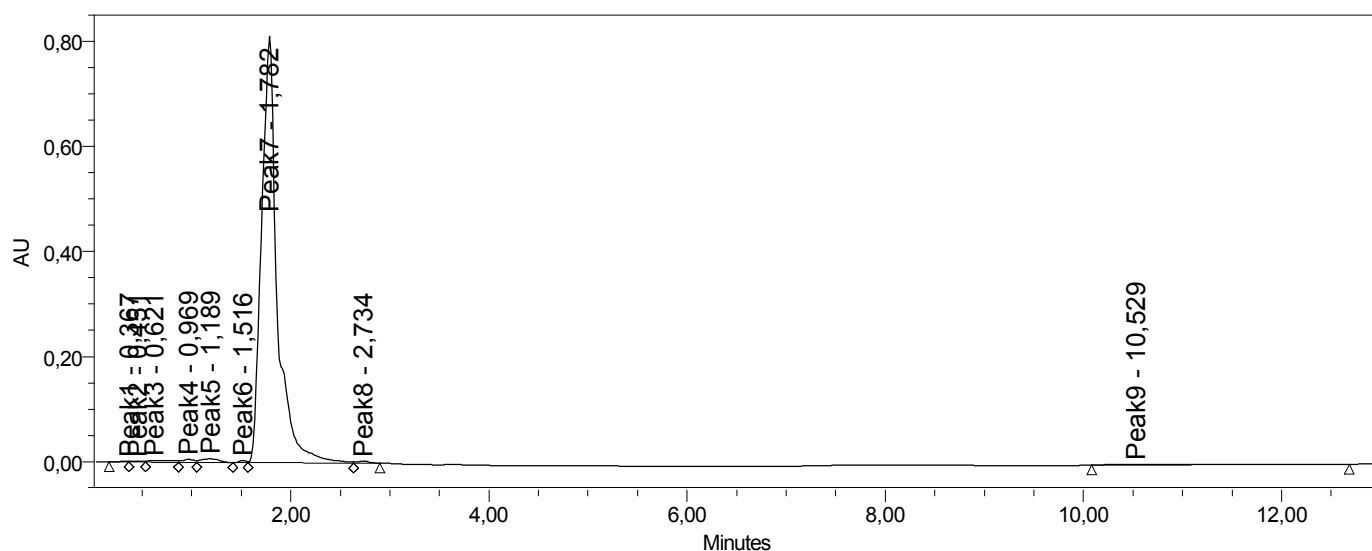
Multi Sample Summary

Reported by User: System

Project Name: Organskajedinjenja

SAMPLE INFORMATION

Sample Name:	IO101 Compound 23	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	31.7.2012 15:38:54
Vial:	17	Acq. Method Set:	6942543300513m_MS
Injection #:	1	Date Processed:	31.7.2012 15:57:20
Injection Volume:	10,00 ul	Processing Method:	IO101
Run Time:	13,0 Minutes	Channel Name:	2487Channel 1
Sample Set Name:		Proc. Chnl. Descr.:	



	Peak Name	RT	Area	% Area	Height
1	Peak1	0,367	7617	0,08	1135
2	Peak2	0,451	16901	0,18	1914
3	Peak3	0,621	57719	0,62	3255
4	Peak4	0,969	46713	0,50	5434
5	Peak5	1,189	87787	0,94	6506
6	Peak6	1,516	18558	0,20	3804
7	Peak7	1,782	8955714	95,59	808799
8	Peak8	2,734	32320	0,34	3749
9	Peak9	10,529	145260	1,55	1754