LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU070318\
Data File : VU025195.D
Acq On : 03 Jul 2018 17:37
Operator : MD/SY
Sample : J3783-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S10-0148

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.089	136	155	176	rBV	412816	503980	26.94%	3.109%
2	1.404	246	253	261	rBV	33747	34066	1.82%	0.210%
3	1.757	353	363	379	rBV	202013	268085	14.33%	1.654%
4	2.307	521	534	550	rVB2	11569	25943	1.39%	0.160%
5	2.709	643	659	678	rBV	136892	297620	15.91%	1.836%
6	2.998	732	749	766	rBV	31242	65857	3.52%	0.406%
7	3.998	1041	1060	1078	rBV4	52800	147472	7.88%	0.910%
8	4.098	1078	1091	1107	rVV3	10667	28853	1.54%	0.178%
9	4.230	1107	1132	1152	rVB5	16054	54042	2.89%	0.333%
10	4.886	1320	1336	1353	rBV	179714	404920	21.64%	2.498%
11	4.985	1353	1367	1384	rVV	273649	615499	32.90%	3.798%
12	5.085	1384	1398	1416	rVB2	76019	186549	9.97%	1.151%
13	5.262	1429	1453	1456	rBV7	14270	34995	1.87%	0.216%
14	5.313	1457	1469	1484	rVV	192911	410968	21.97%	2.536%
15	5.394	1484	1494	1506	rVV2	33409	72828	3.89%	0.449%
16	5.484	1506	1522	1527	rVV6	28376	70435	3.76%	0.435%
17	5.542	1527	1540	1558	rVV2	226257	571081	30.53%	3.523%
18	5.629	1558	1567	1583	rVB4	9650	22757	1.22%	0.140%
19	5.889	1631	1648	1671	rBV	359292	714672	38.20%	4.409%
20	6.416	1791	1812	1823	rBV6	36977	106327	5.68%	0.656%
21	6.481	1823	1832	1841	rVV3	14958	27135	1.45%	0.167%
22	6.542	1841	1851	1858	rVV3	16813	31804	1.70%	0.196%
23	6.593	1858	1867	1877	rVB2	19939	38680	2.07%	0.239%
24	6.741	1901	1913	1927	rVB6	15370	34165	1.83%	0.211%
25	6.825	1927	1939	1953	rBV3	11926	22847	1.22%	0.141%
26	6.931	1953	1972	1989	rBV	175446	384658	20.56%	2.373%
27	7.053	1994	2010	2023	rBV2	320763	652061	34.85%	4.023%
28	7.297	2059	2086	2104	rBV	293759	591092	31.59%	3.647%
29	7.567	2147	2170	2192	rBV	679049	1248965	66.76%	7.706%
30	7.715	2202	2216	2231	rBV2	33867	71254	3.81%	0.440%
31	7.921	2269	2280	2294	rVB2	62988	113500	6.07%	0.700%
32	8.050	2301	2320	2331	rBV3	21837	42763	2.29%	0.264%
33	8.165	2344	2356	2370	rBV2	44520	78837	4.21%	0.486%
34	8.317	2389	2403	2409	rBV	15558	28057	1.50%	0.173%

LSC Area Percent Report

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Sample : J3783-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S10-0148

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Title : SW846 8260

35	8.368	2409	2419	2425	rBV	133936	234107	12.51%	1.444%
36	8.493	2447	2458	2467	rBV4	15497	26406	1.41%	0.163%
37	8.609	2484	2494	2504	rBV2	19831	34544	1.85%	0.213%
38	8.783	2536	2548	2558	rBV2	10861	19829	1.06%	0.122%
39	8.950	2589	2600	2611	rBV	32143	55305	2.96%	0.341%
40	9.027	2611	2624	2634	rVV	123816	215252	11.51%	1.328%
41	9.095	2634	2645	2666	rVV	524005	877183	46.89%	5.412%
42	9.191	2667	2675	2682	rVV3	13277	23211	1.24%	0.143%
43	9.252	2682	2694	2721	rVV	1168381	1870844	100.00%	11.543%
44	9.381	2721	2734	2745	rVV	98694	172494	9.22%	1.064%
45	9.445	2746	2754	2765	rVB	23666	38136	2.04%	0.235%
46	9.953	2902	2912	2928	rVB5	9978	19613	1.05%	0.121%
47	10.169	2969	2979	2989	rBV	229229	360362	19.26%	2.223%
48	10.223	2989	2996	3011	rVB	61996	102037	5.45%	0.630%
49	10.310	3011	3023	3040	rBV	529383	863042	46.13%	5.325%
50	10.593	3100	3111	3131	rVB	208785	340083	18.18%	2.098%
51	10.712	3136	3148	3159	rVV2	48171	77043	4.12%	0.475%
52	10.776	3159	3168	3179	rVB	39889	63013	3.37%	0.389%
53	10.976	3221	3230	3247	rBV	50287	89753	4.80%	0.554%
54	11.152	3277	3285	3296	rVB2	15106	21328	1.14%	0.132%
55	11.329	3333	3340	3359	rVB2	38216	68416	3.66%	0.422%
56	11.432	3360	3372	3378	rVV2	34771	52829	2.82%	0.326%
57	11.487	3378	3389	3407	rVV	624153	992479	53.05%	6.123%
58	11.574	3407	3416	3426	rVB2	28617	42144	2.25%	0.260%
59	11.693	3443	3453	3462	rVB2	13619	20897	1.12%	0.129%
60	11.773	3462	3478	3487	rBV3	124435	238239	12.73%	1.470%
61	11.876	3499	3510	3528	rVB5	43811	99818	5.34%	0.616%
62	11.985	3535	3544	3552	rBV2	26206	37104	1.98%	0.229%
63	12.059	3554	3567	3581	rVB	62645	109478	5.85%	0.675%
64	12.149	3584	3595	3602	rBV	13220	20547	1.10%	0.127%
65	12.255	3613	3628	3634	rBV2	34648	58037	3.10%	0.358%
66	12.291	3634	3639	3651	rVV	30096	50683	2.71%	0.313%
67	12.358	3651	3660	3682	rVB3	62046	143910	7.69%	0.888%
68	12.654	3736	3752	3758	rBV	25196	46475	2.48%	0.287%
69	12.792	3780	3795	3803	rBV	9730	21522	1.15%	0.133%
70	13.123	3887	3898	3908	rBV3	136020	220556	11.79%	1.361%
71	13.294	3938	3951	3965	rVB	63928	101943	5.45%	0.629%

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Instrument : MSVOA_U
ClientSampleId : S10-0148

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Title : SW846 8260

72	13.612	4046	4050	4066	rVB6	10137	21255	1.14%	0.131%
73	13.747	4078	4092	4104	rBV	214704	355217	18.99%	2.192%

Sum of corrected areas: 16207901

LSC Report - Integrated Chromatogram

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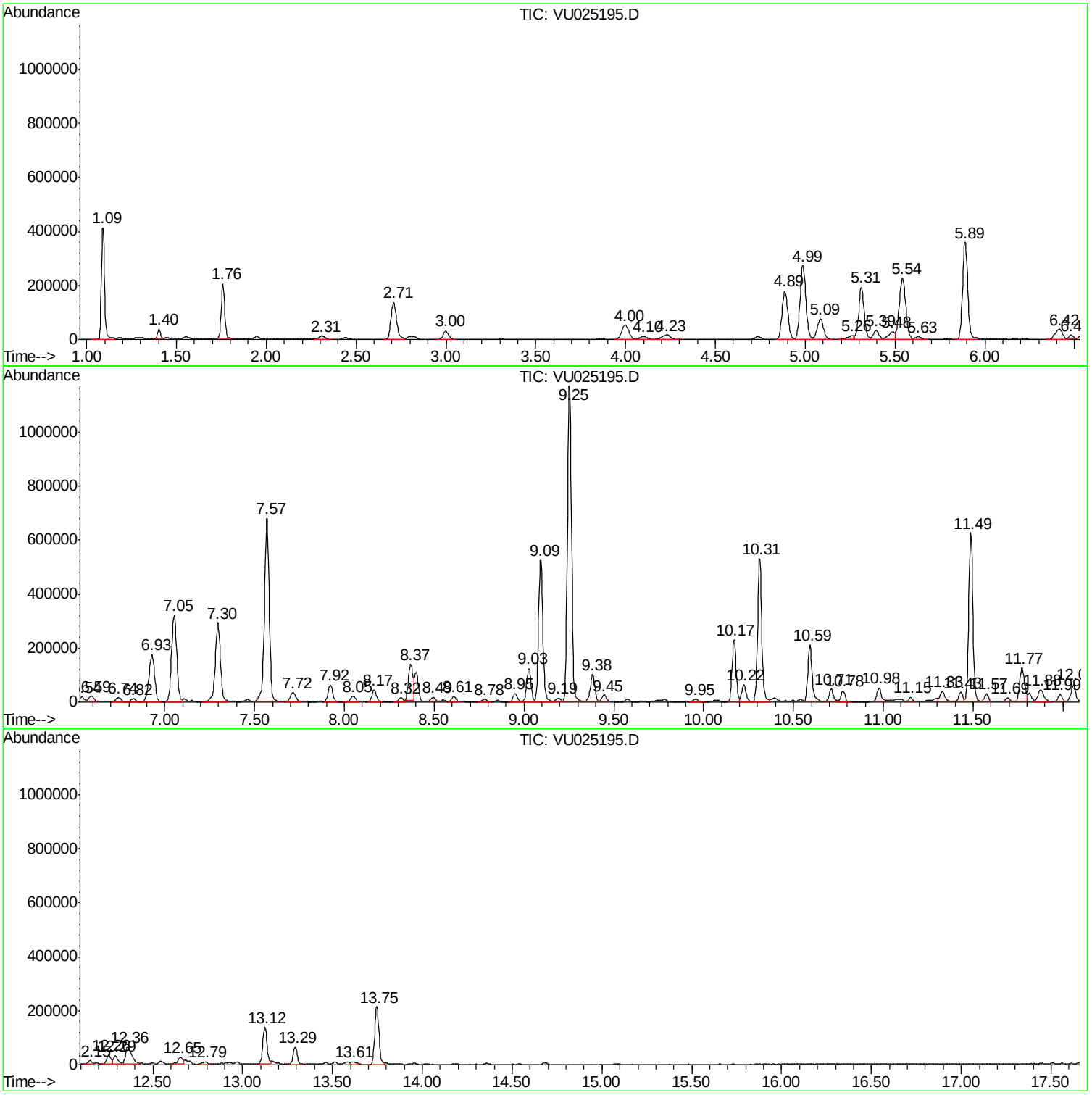
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S10-0148

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

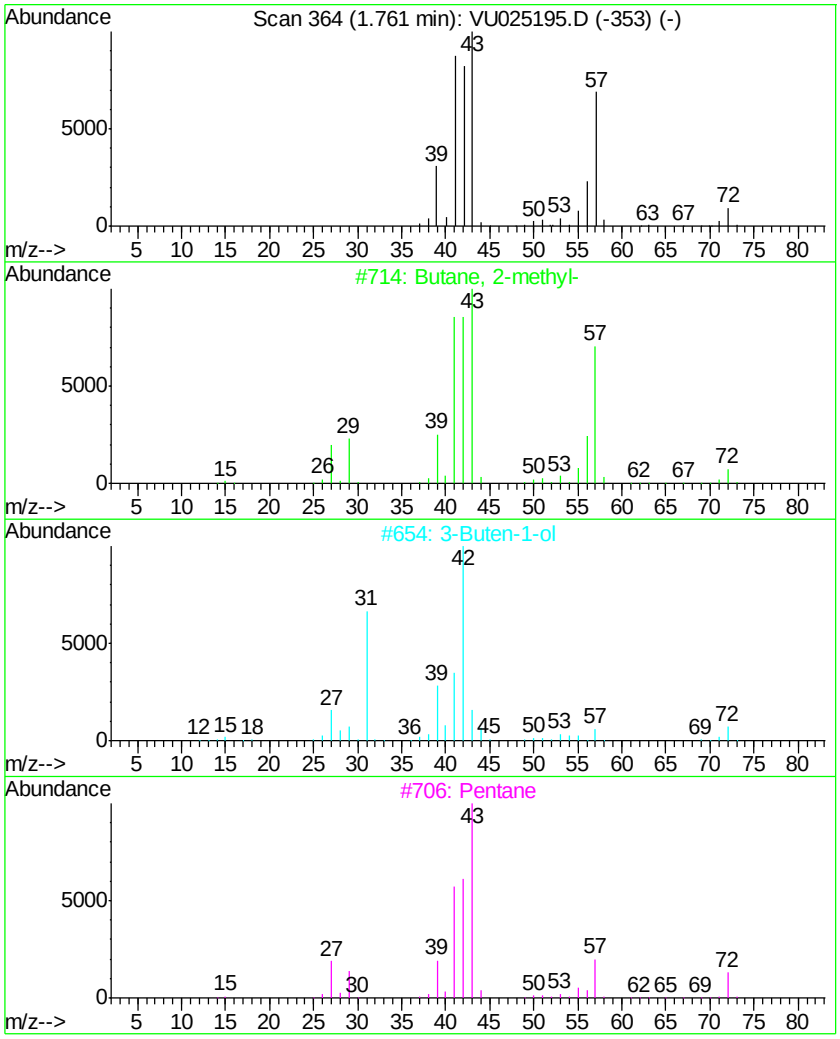
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

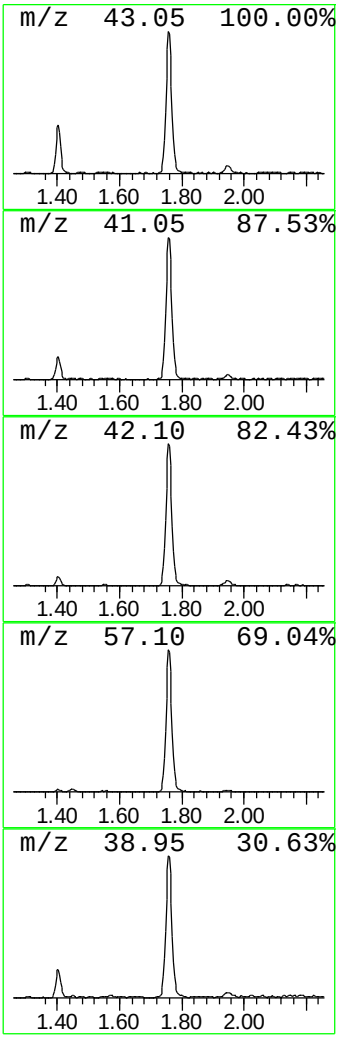
****

Peak Number 2 Butane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.76	21.78 ug/l	268085	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	38
3	Pentane	72	C5H12	000109-66-0	36
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	28





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Operator : MD/SY
Sample : J3783-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S10-0148

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

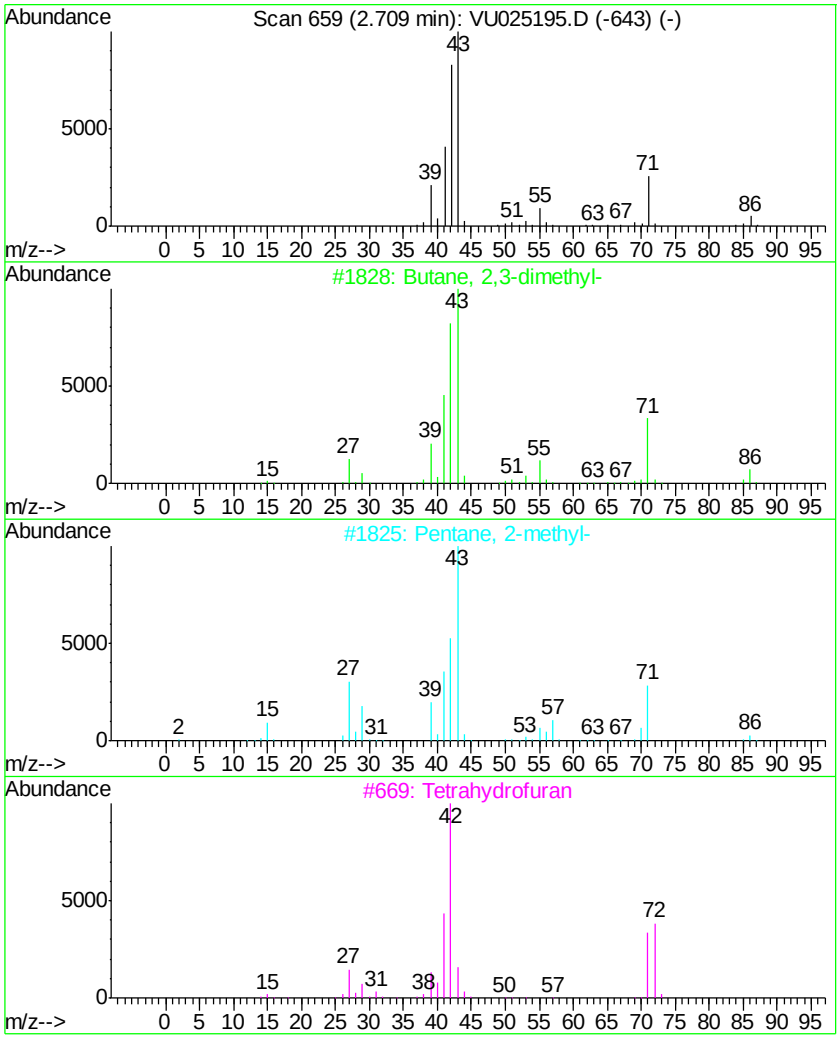
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

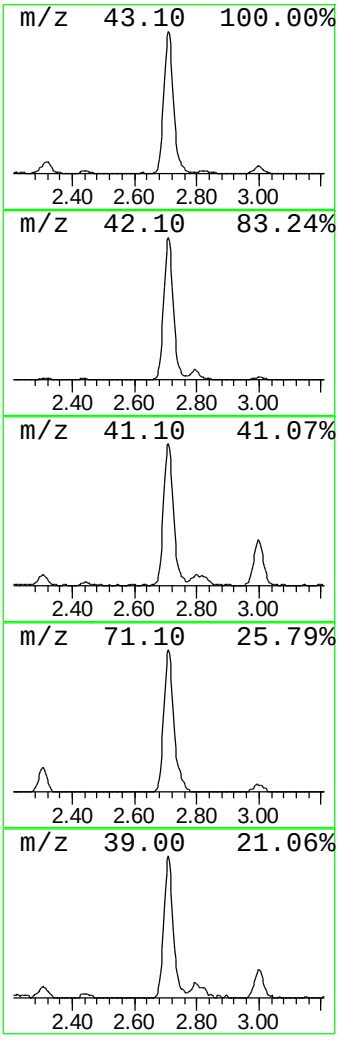
****

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.71	24.18 ug/l	297620	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	Tetrahydrofuran	72	C4H8O	000109-99-9	38
4	Butane, 2-methyl-	72	C5H12	000078-78-4	36
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	33





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Operator : MD/SY
Sample : J3783-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S10-0148

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

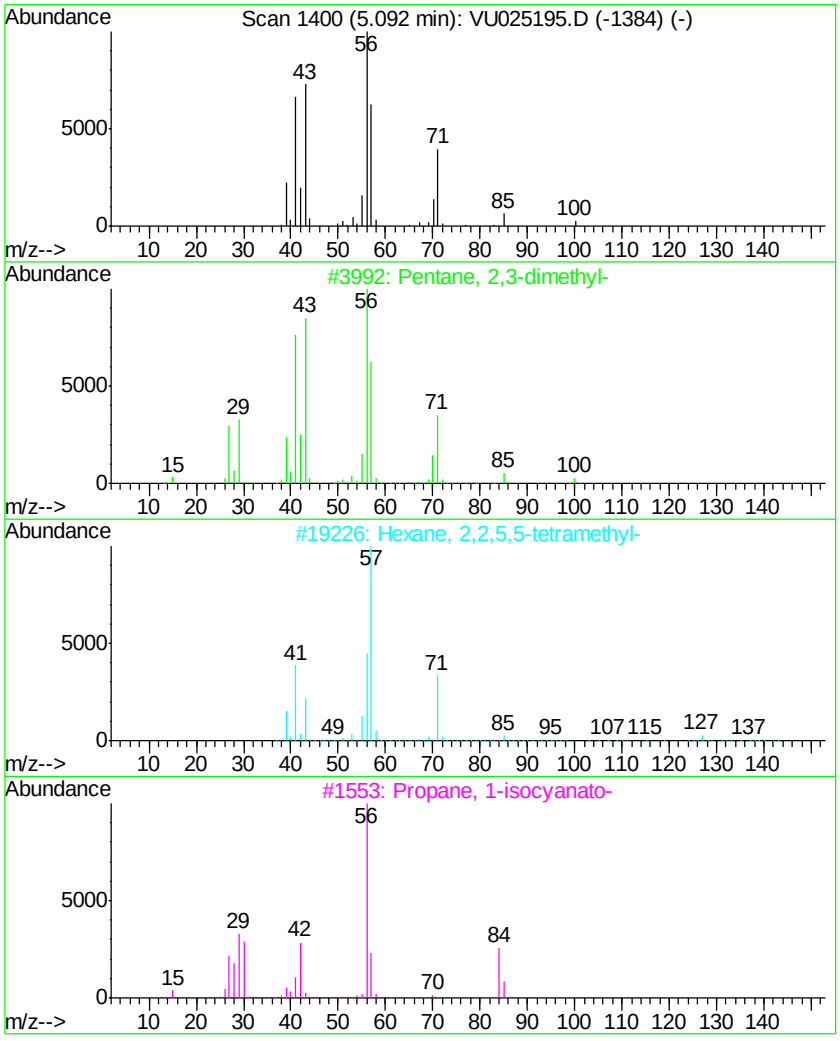
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

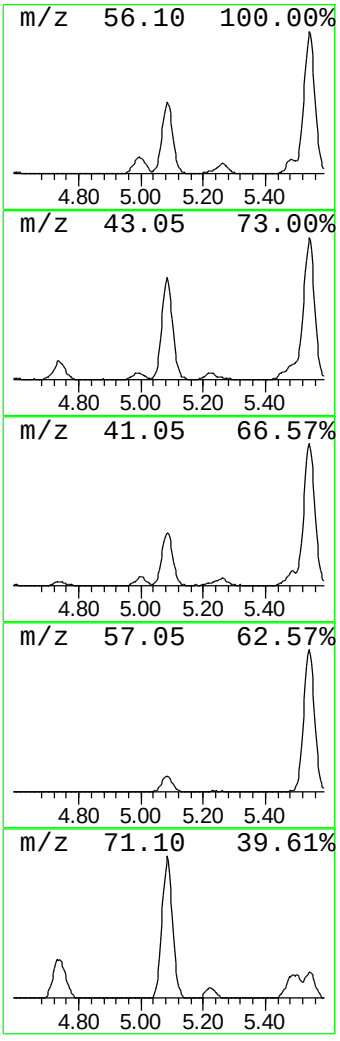
****

Peak Number 4 Pentane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	15.15 ug/l	186549	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	95
2	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	64
3	Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	47
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	46
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

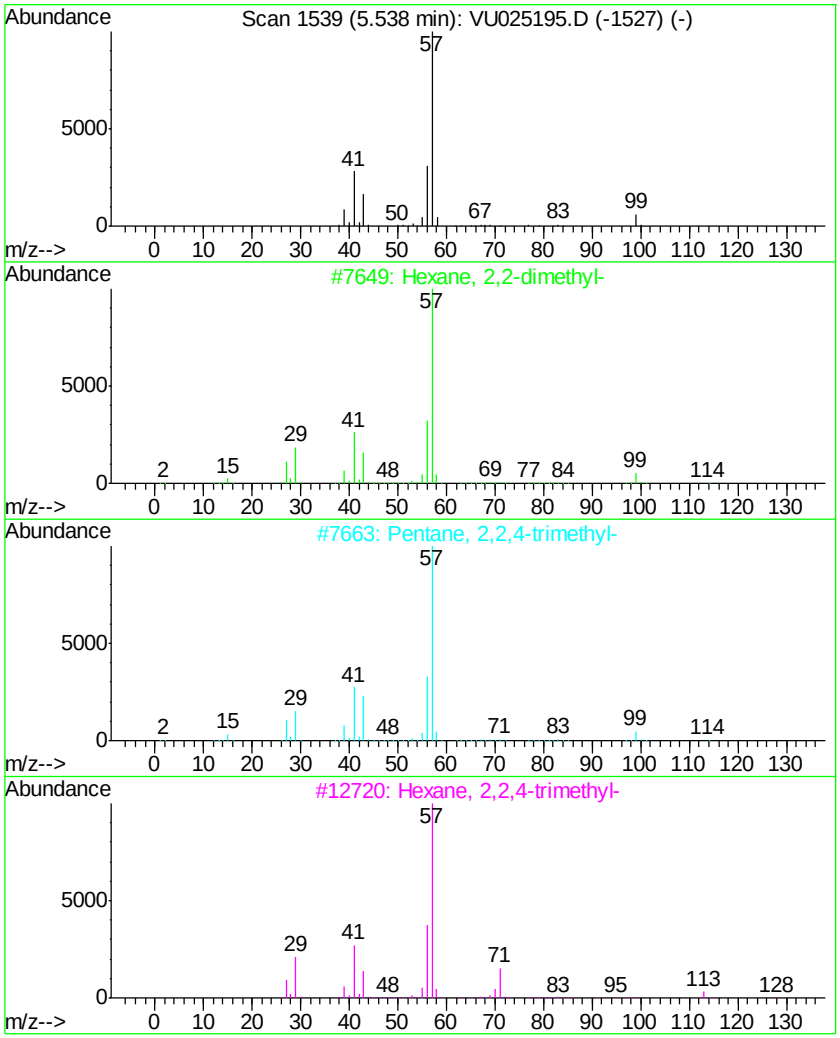
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

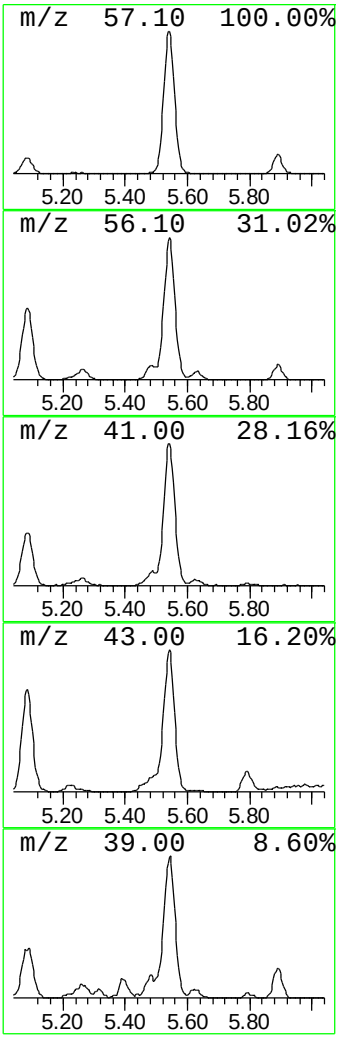
****

Peak Number 5 Hexane, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.54	39.95 ug/l	571081	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
3	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	78
4	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	72





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

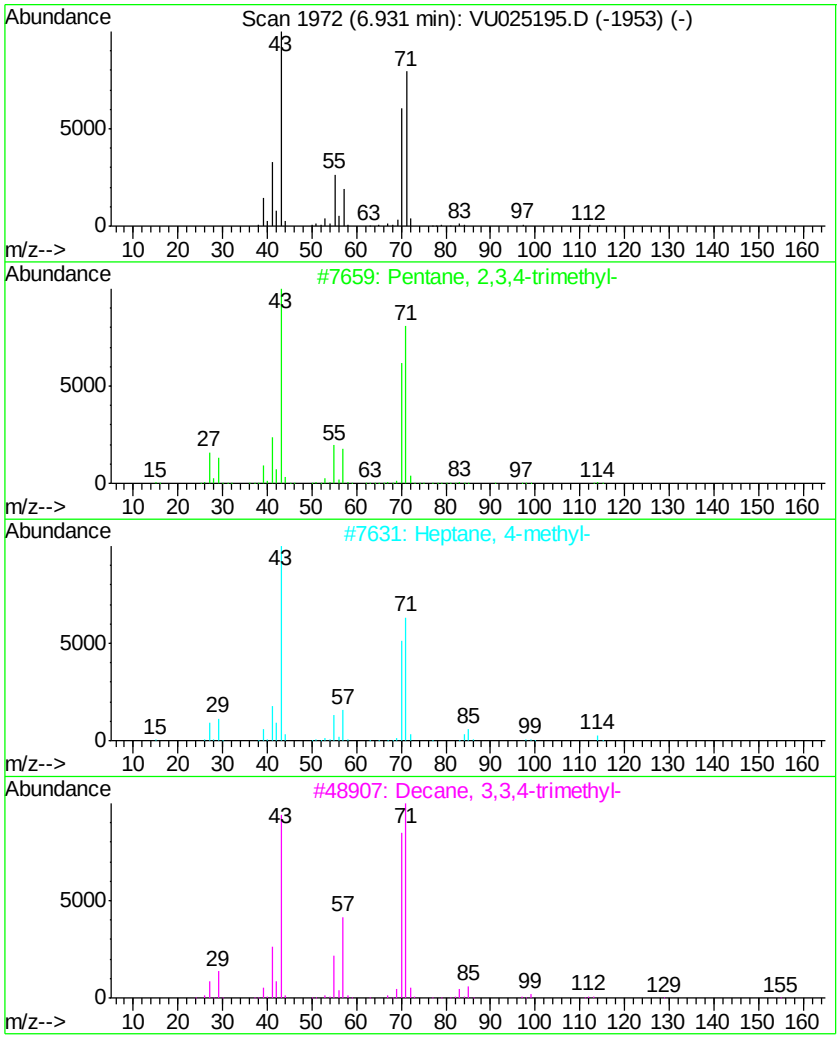
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

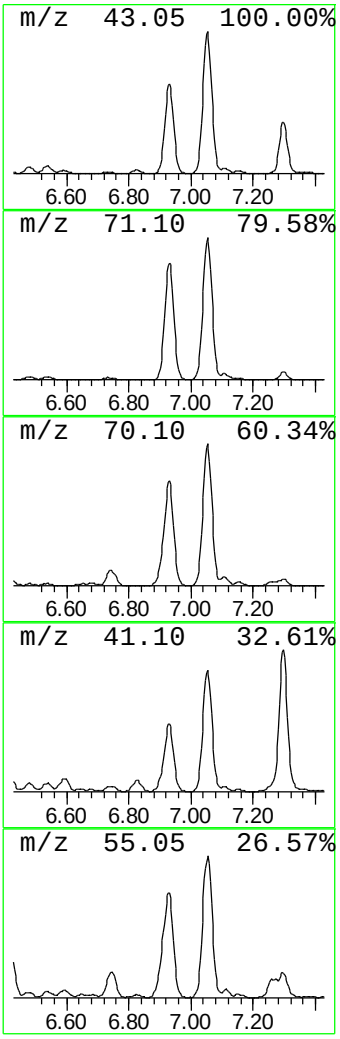
****

Peak Number 6 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.93	26.91 ug/l	384658	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	78
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

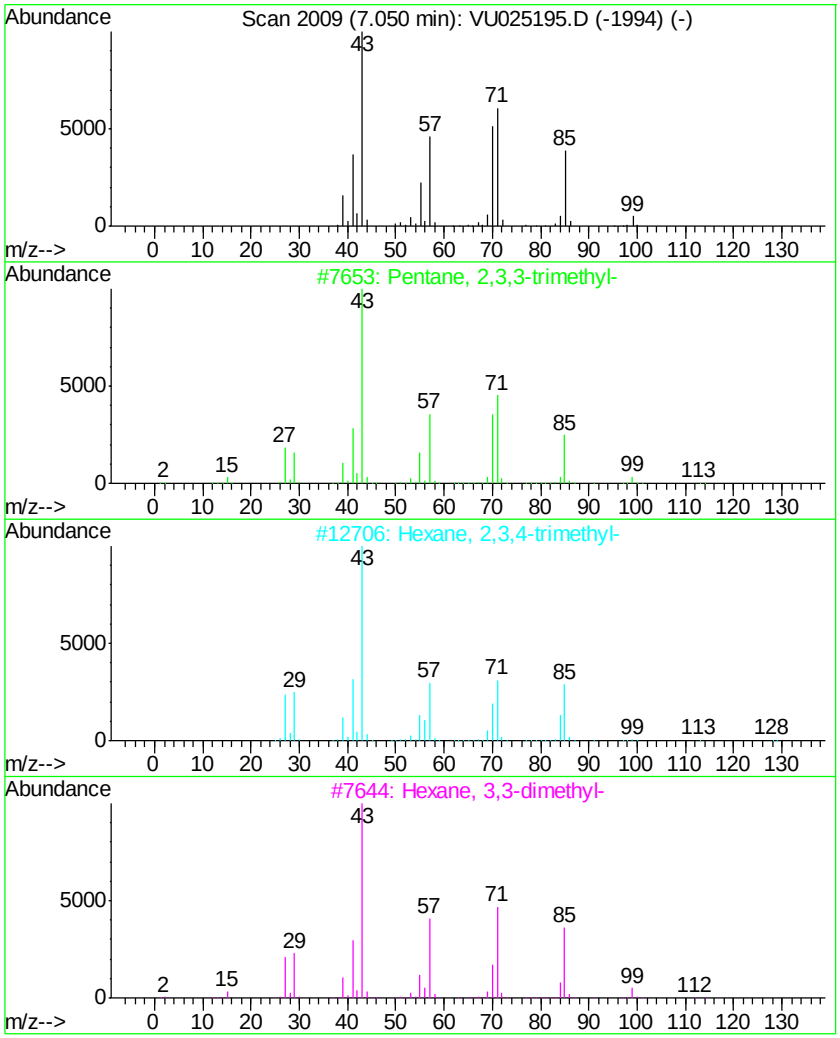
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

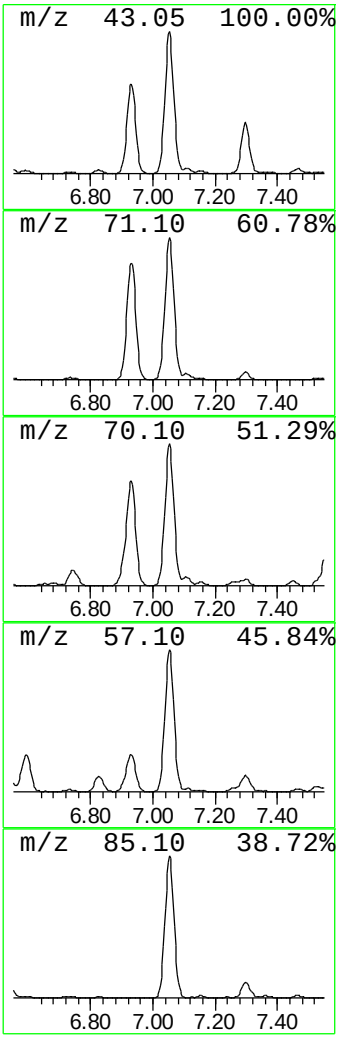
****

Peak Number 7 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	45.62 ug/l	652061	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
3	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	50





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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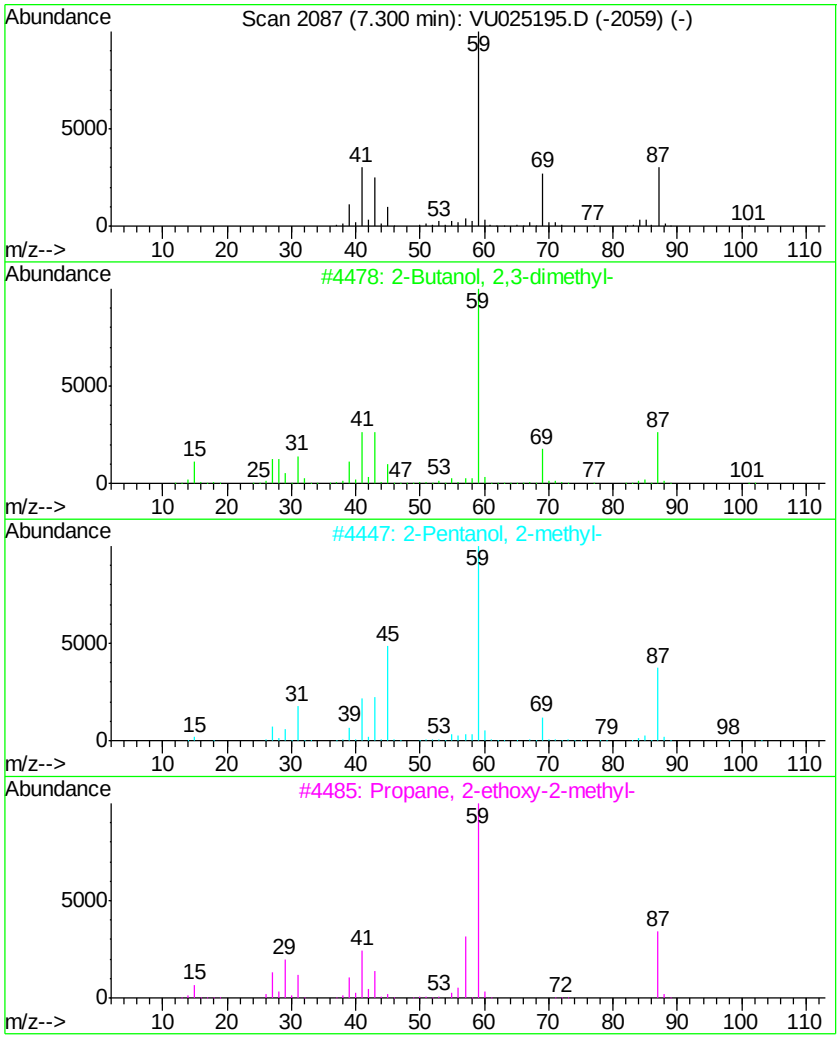
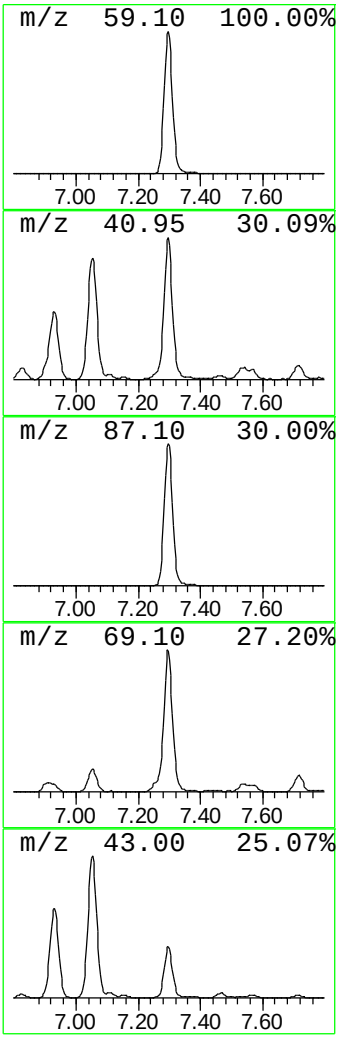
Peak Number 8 2-Butanol, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	41.35 ug/l	591092	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	56
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
4	3-Heptanol	116	C7H16O	000589-82-2	40
5	Propanoic acid, 2-hydroxy-2-meth...	118	C5H10O3	002110-78-3	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU070318\
Data File : VU025195.D
Acq On : 03 Jul 2018 17:37
Operator : MD/SY
Sample : J3783-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S10-0148

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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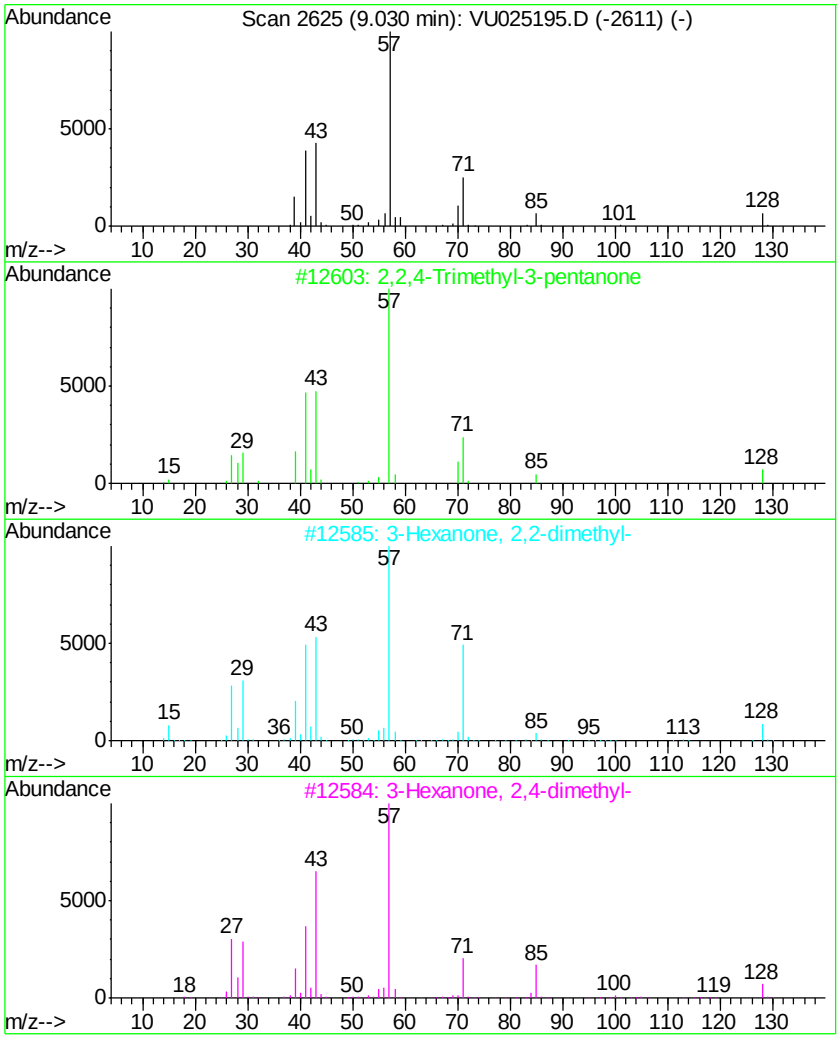
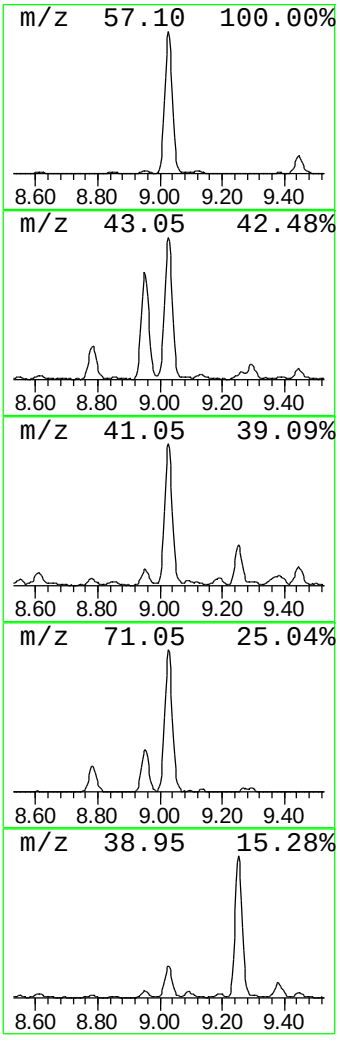
Peak Number 9 2,2,4-Trimethyl-3-pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.03	12.27 ug/l	215252	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-3-pentanone	128	C8H16O	005857-36-3	87
2	3-Hexanone, 2,2-dimethyl-	128	C8H16O	005405-79-8	47
3	3-Hexanone, 2,4-dimethyl-	128	C8H16O	018641-70-8	43
4	3-Hexanone, 2,5-dimethyl-	128	C8H16O	001888-57-9	40
5	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU070318\
Data File : VU025195.D
Acq On : 03 Jul 2018 17:37
Operator : MD/SY
Sample : J3783-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S10-0148

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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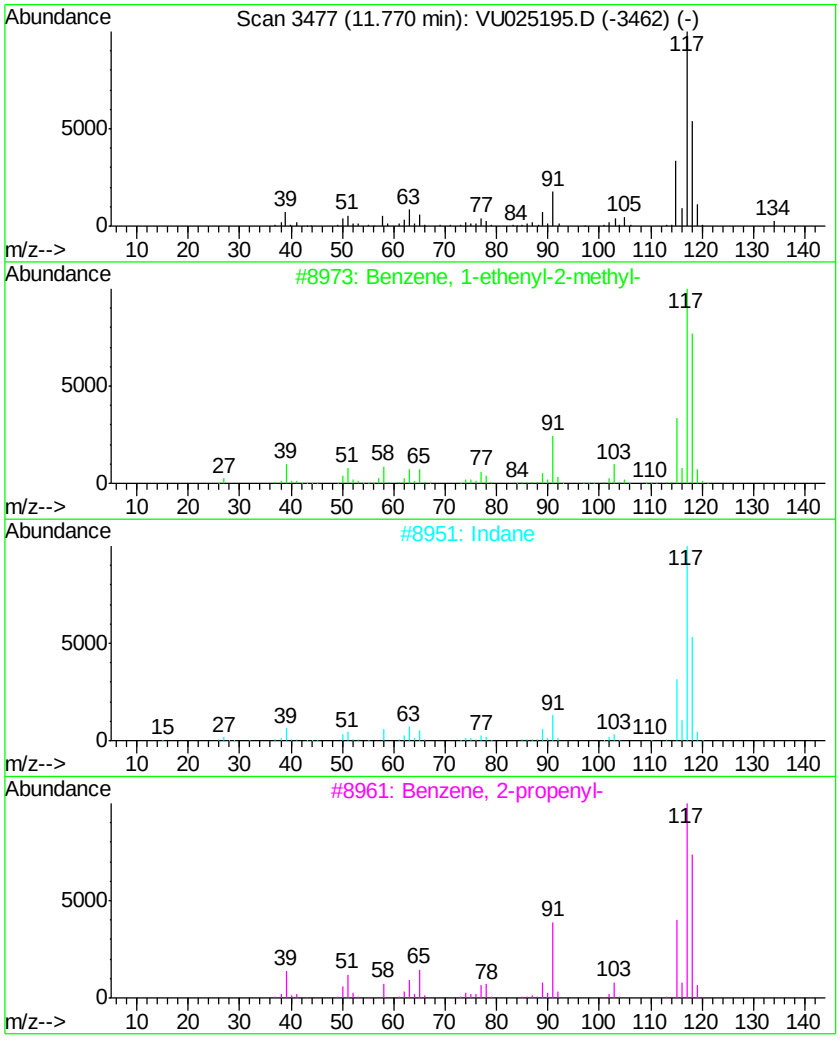
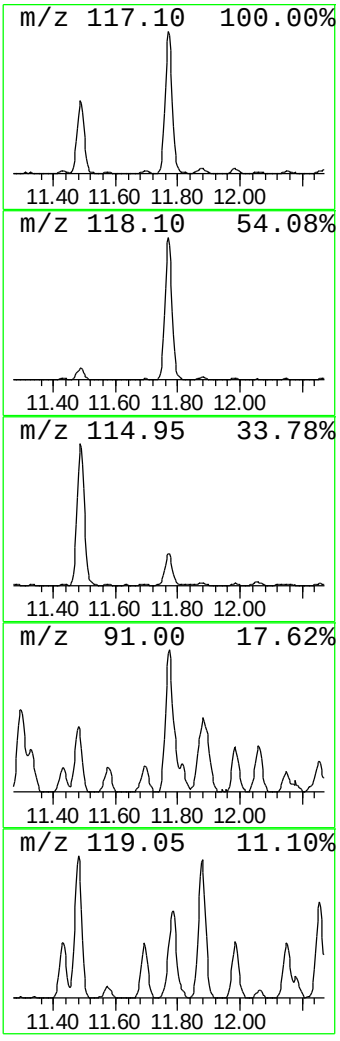
Peak Number 10 Benzene, 1-ethenyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	12.00 ug/l	238239	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
2	Indane	118	C9H10	000496-11-7	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
4	Deltacyclene	118	C9H10	007785-10-6	68
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU070318\
Data File : VU025195.D
Acq On : 03 Jul 2018 17:37
Operator : MD/SY
Sample : J3783-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : S10-0148

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U061318W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methyl-	1.76	21.8	ug/l	268085	1	4.99	615499	50.0
Butane, 2,3-dimet...	2.71	24.2	ug/l	297620	1	4.99	615499	50.0
Pentane, 2,3-dime...	5.09	15.2	ug/l	186549	1	4.99	615499	50.0
Hexane, 2,2-dimet...	5.54	40.0	ug/l	571081	2	5.89	714672	50.0
Pentane, 2,3,4-tr...	6.93	26.9	ug/l	384658	2	5.89	714672	50.0
Pentane, 2,3,3-tr...	7.05	45.6	ug/l	652061	2	5.89	714672	50.0
2-Butanol, 2,3-di...	7.30	41.4	ug/l	591092	2	5.89	714672	50.0
2,2,4-Trimethyl-3...	9.03	12.3	ug/l	215252	3	9.09	877183	50.0
Benzene, 1-etheny...	11.77	12.0	ug/l	238239	4	11.49	992479	50.0