LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU101118\
Data File : VU027608.D
Acq On : 11 Oct 2018 18:50
Operator : MD/SY
Sample : J5456-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MS-FRAC-TANK

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\82U101118W.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	1.476	86	94	103	rBV	21699	24921	1.73%	0.230%
2	2.247	325	334	345	rVB	24085	35817	2.49%	0.331%
3	2.328	347	359	387	rBV	313946	512889	35.60%	4.735%
4	2.456	388	399	421	rVB	52225	100937	7.01%	0.932%
5	2.836	503	517	537	rBV2	29014	62476	4.34%	0.577%
6	3.186	612	626	649	rVB3	16411	36337	2.52%	0.335%
7	3.993	861	877	903	rBV	76117	198553	13.78%	1.833%
8	4.267	949	962	990	rBV	107126	264579	18.37%	2.443%
9	4.887	1139	1155	1171	rBV3	102949	229806	15.95%	2.122%
10	4.987	1172	1186	1207	rVV	165566	362822	25.19%	3.350%
11	5.312	1269	1287	1299	rBV	126104	264633	18.37%	2.443%
12	5.392	1299	1312	1328	rVB	342889	720981	50.05%	6.656%
13	5.787	1419	1435	1453	rBV	246605	522263	36.25%	4.821%
14	5.887	1454	1466	1500	rVV	265646	560969	38.94%	5.179%
15	6.032	1500	1511	1537	rVB	34481	81812	5.68%	0.755%
16	6.176	1546	1556	1584	rBV	35377	80172	5.57%	0.740%
17	6.421	1618	1632	1660	rBV	214134	420253	29.17%	3.880%
18	6.582	1676	1682	1699	rVB	8957	16038	1.11%	0.148%
19	6.787	1731	1746	1748	rBV2	29573	43916	3.05%	0.405%
20	6.826	1749	1758	1784	rVB	117807	245766	17.06%	2.269%
21	6.958	1789	1799	1817	rVV	12113	22709	1.58%	0.210%
22	7.369	1916	1927	1944	rBV	16270	30188	2.10%	0.279%
23	7.463	1944	1956	1977	rBV	287613	564952	39.22%	5.216%
24	7.566	1977	1988	2006	rVV	400768	727870	50.53%	6.720%
25	7.704	2020	2031	2063	rVB	101863	204795	14.22%	1.891%
26	7.906	2082	2094	2137	rBV	773862	1440546	100.00%	13.299%
27	8.167	2162	2175	2188	rBV	71193	133675	9.28%	1.234%
28	8.231	2189	2195	2212	rVB2	15916	28252	1.96%	0.261%
29	8.369	2227	2238	2256	rBV2	68941	127863	8.88%	1.180%
30	8.485	2263	2274	2295	rVB9	8664	27030	1.88%	0.250%
31	8.588	2296	2306	2313	rVV6	10266	20884	1.45%	0.193%
32	8.636	2314	2321	2328	rVV	21974	38922	2.70%	0.359%
33	8.681	2329	2335	2355	rVB2	24100	44272	3.07%	0.409%
34	8.784	2356	2367	2390	rBV2	16873	36545	2.54%	0.337%

LSC Area Percent Report

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Operator : MD/SY
Sample : J5456-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MS-FRAC-TANK

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\82U101118W.M
Title : SW846 8260

35	8.951	2408	2419	2435	rBV	45427	86064	5.97%	0.795%
36	9.051	2436	2450	2452	rVV6	12674	25260	1.75%	0.233%
37	9.090	2452	2462	2484	rVB	337980	588468	40.85%	5.433%
38	9.218	2494	2502	2506	rBV	12034	16729	1.16%	0.154%
39	9.260	2507	2515	2535	rVB2	72088	155182	10.77%	1.433%
40	9.376	2544	2551	2564	rVB3	12949	22754	1.58%	0.210%
41	9.459	2564	2577	2588	rBV3	13393	30919	2.15%	0.285%
42	9.781	2668	2677	2684	rBV3	11862	19695	1.37%	0.182%
43	9.922	2715	2721	2734	rVB2	10529	17422	1.21%	0.161%
44	10.051	2747	2761	2764	rBV4	18147	30847	2.14%	0.285%
45	10.196	2796	2806	2830	rVV	137194	270617	18.79%	2.498%
46	10.308	2830	2841	2865	rVB2	267364	498539	34.61%	4.602%
47	10.421	2866	2876	2889	rBV4	19855	38082	2.64%	0.352%
48	10.572	2907	2923	2933	rBV8	7508	19978	1.39%	0.184%
49	11.102	3073	3088	3095	rBV2	40936	67368	4.68%	0.622%
50	11.144	3095	3101	3114	rVB5	16145	29545	2.05%	0.273%
51	11.421	3178	3187	3196	rBV	61704	95282	6.61%	0.880%
52	11.485	3196	3207	3219	rVV	305185	478612	33.22%	4.418%
53	12.041	3372	3380	3386	rBV2	11111	18203	1.26%	0.168%
54	12.363	3473	3480	3495	rVB4	17131	29947	2.08%	0.276%
55	12.485	3510	3518	3534	rBV7	9689	20958	1.45%	0.193%
56	14.202	4045	4052	4062	rVB2	25433	37132	2.58%	0.343%

Sum of corrected areas: 10832046

LSC Report - Integrated Chromatogram

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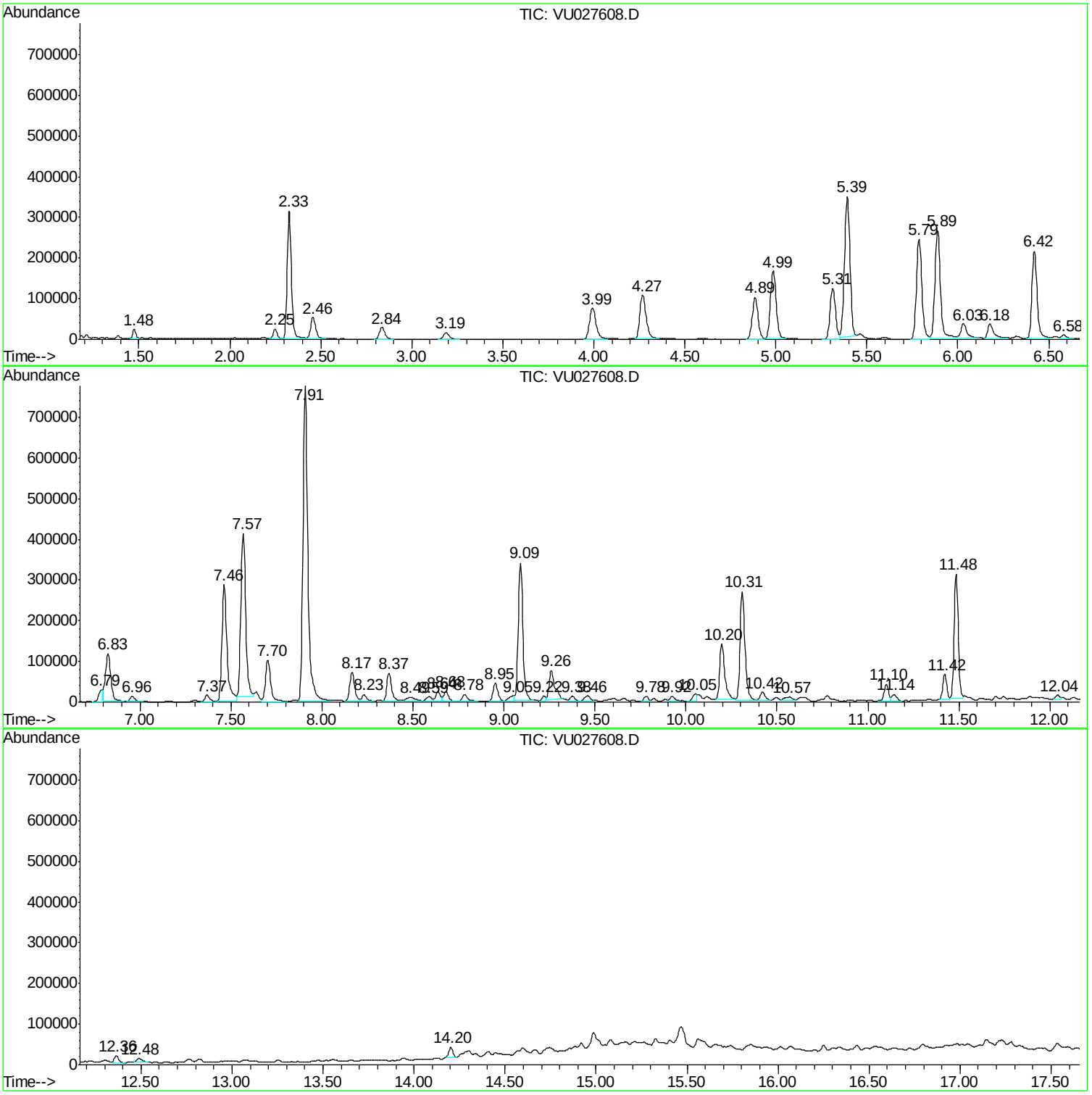
Data File : VU027608.D
Acq On : 11 Oct 2018 18:50
Operator : MD/SY
Sample : J5456-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MS-FRAC-TANK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U101118W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU101118\
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Acq On : 11 Oct 2018 18:50
Operator : MD/SY
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ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MS-FRAC-TANK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U101118W.M
Quant Title : SW846 8260

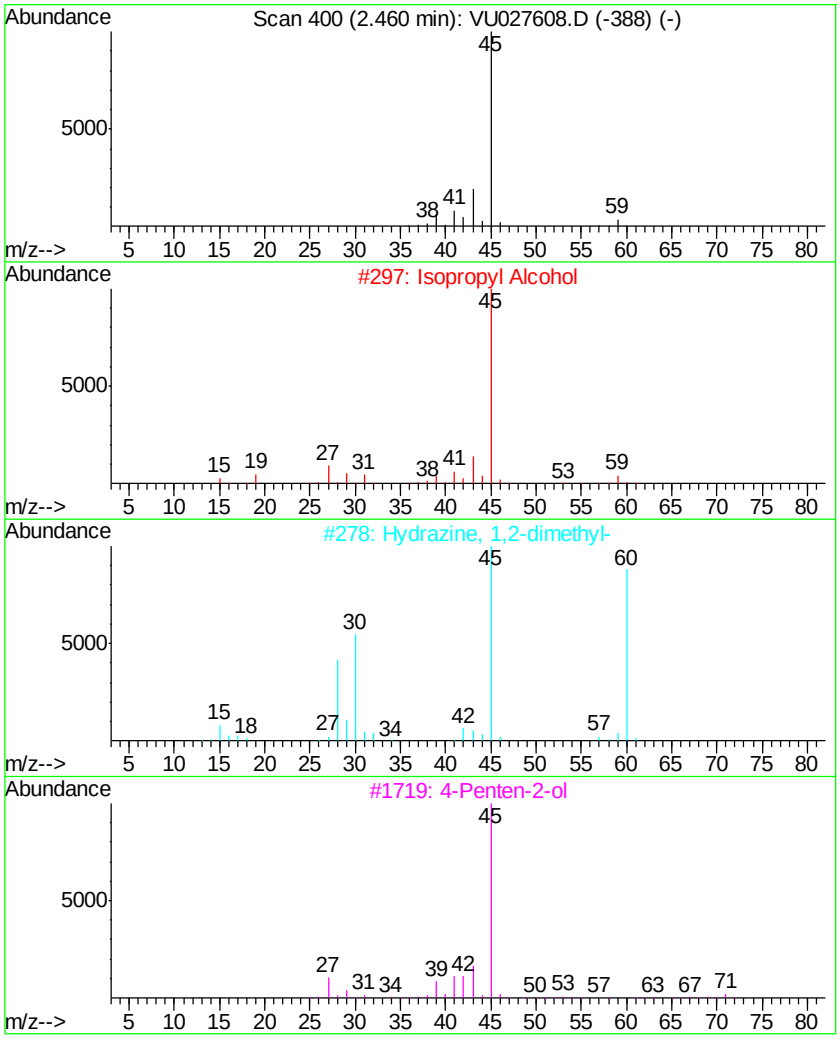
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

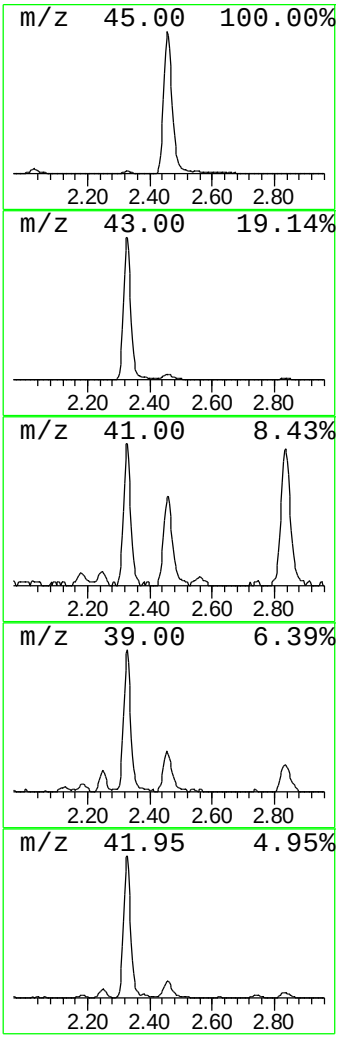
****

Peak Number 1 Isopropyl Alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.46	13.91 ug/l	100937	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3	4-Penten-2-ol	86	C5H10O	000625-31-0	9
4	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
5	Formamide	45	CH3NO	000075-12-7	5





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Data File : VU027608.D
Acq On : 11 Oct 2018 18:50
Operator : MD/SY
Sample : J5456-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MS-FRAC-TANK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U101118W.M
Quant Title : SW846 8260

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

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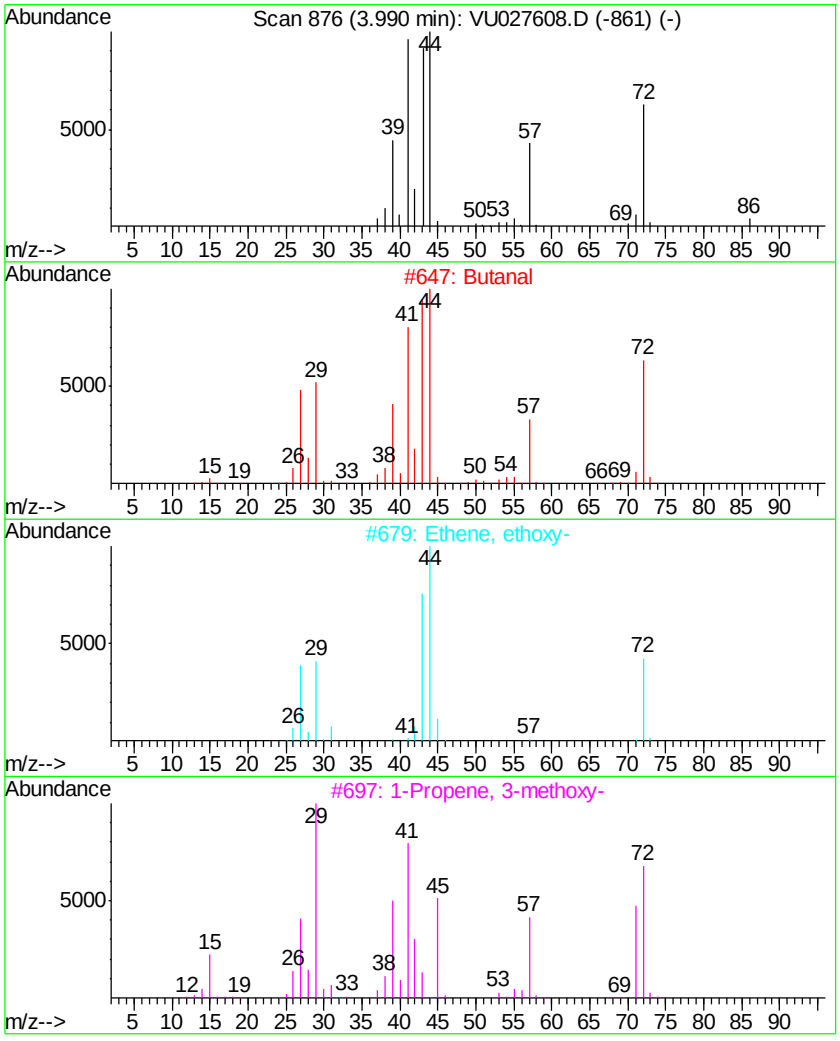
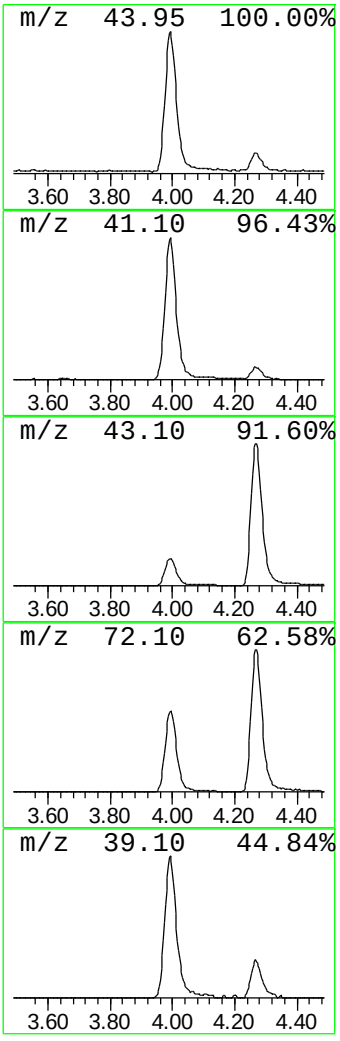
Peak Number 2 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	27.36 ug/l	198553	Pentafluorobenzene	4.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	47
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5	O-Methylisourea	74	C2H6N2O	002440-60-0	33





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU101118\
Data File : VU027608.D
Acq On : 11 Oct 2018 18:50
Operator : MD/SY
Sample : J5456-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MS-FRAC-TANK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U101118W.M
Quant Title : SW846 8260

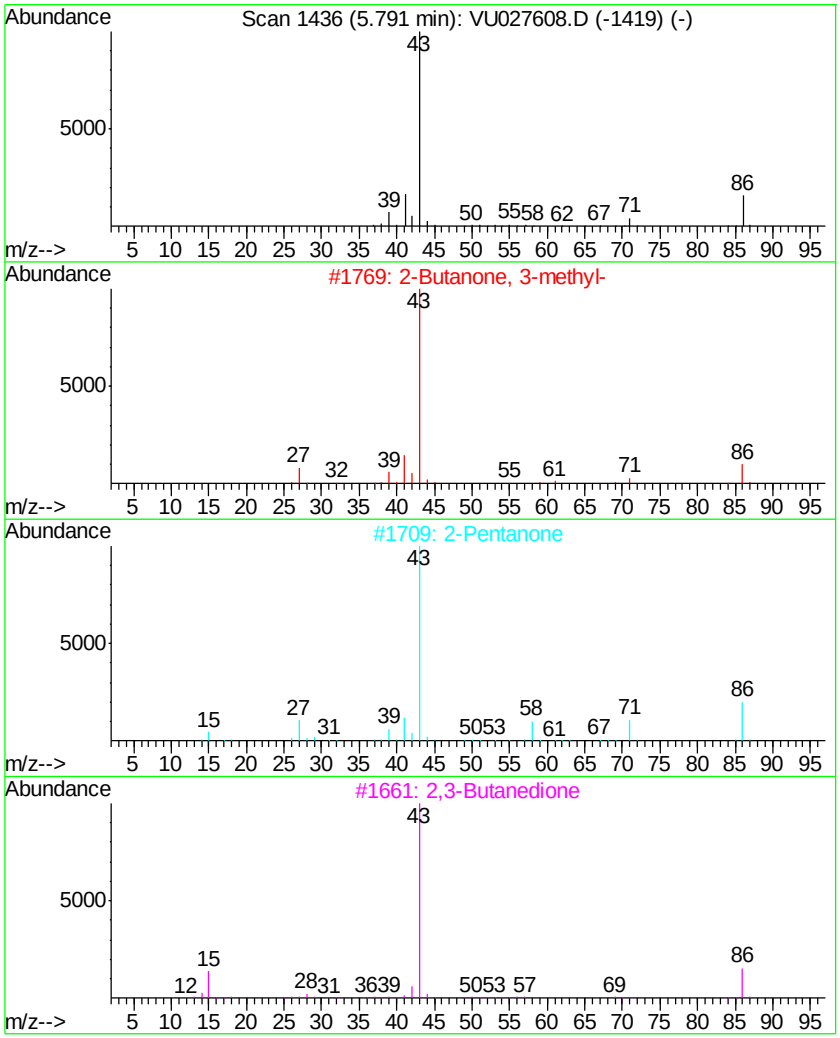
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

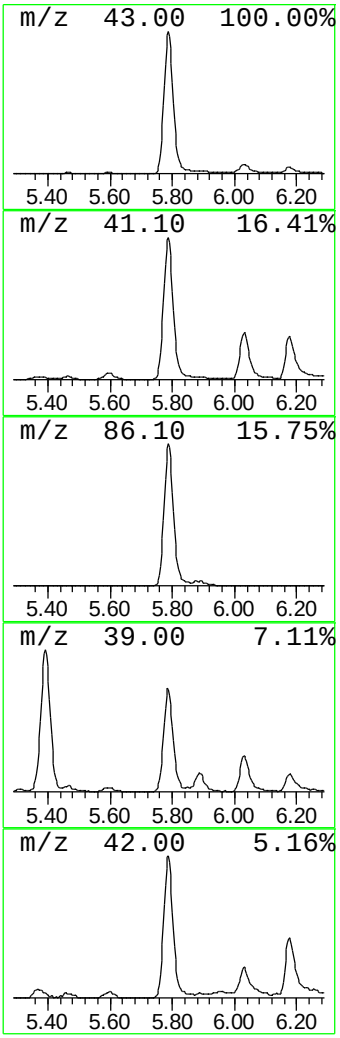
****

Peak Number 3 2-Butanone, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.79	46.55 ug/l	522263	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	72
2	2-Pentanone	86	C5H10O	000107-87-9	64
3	2,3-Butanedione	86	C4H6O2	000431-03-8	50
4	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9
5	1-Propen-2-ol, formate	86	C4H6O2	032978-00-0	7





Library Search Compound Report

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Data File : VU027608.D
Acq On : 11 Oct 2018 18:50
Operator : MD/SY
Sample : J5456-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MS-FRAC-TANK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U101118W.M
Quant Title : SW846 8260

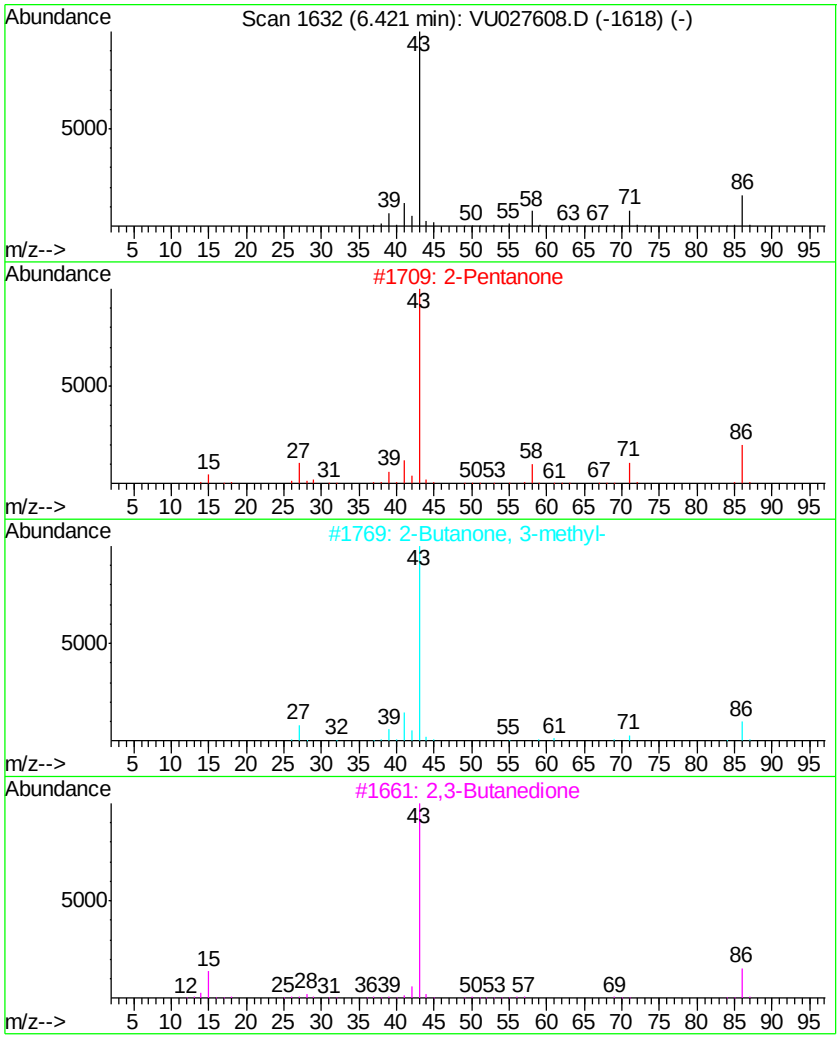
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

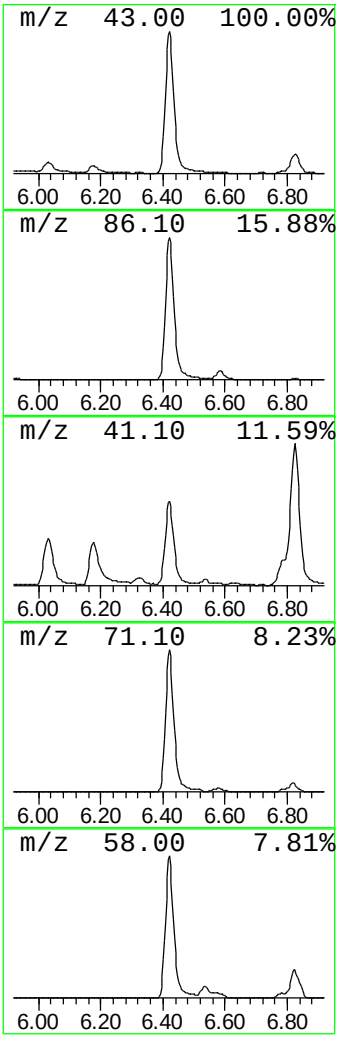
****

Peak Number 4 2-Pentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	37.46 ug/l	420253	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	91
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53
3	2,3-Butanedione	86	C4H6O2	000431-03-8	50
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9





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ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MS-FRAC-TANK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U101118W.M
Quant Title : SW846 8260

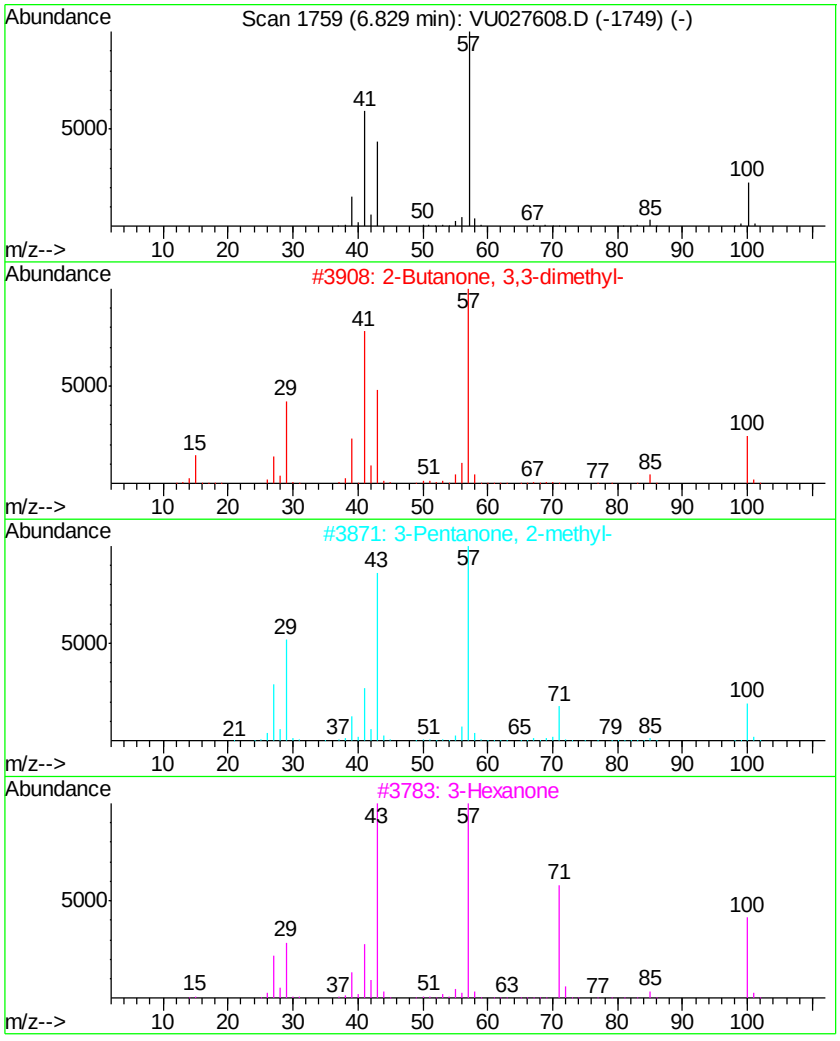
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

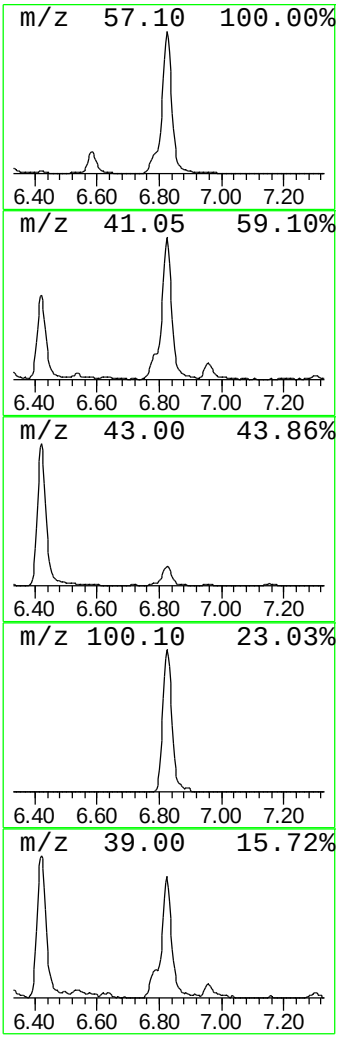
****

Peak Number 5 2-Butanone, 3,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.83	21.91 ug/l	245766	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	72
2	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
3	3-Hexanone	100	C6H12O	000589-38-8	53
4	Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	47
5	Propane, 1-(ethenyloxy)-2-methyl-	100	C6H12O	000109-53-5	45





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Instrument : MSVOA_U
ClientSampleId : MS-FRAC-TANK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U101118W.M
Quant Title : SW846 8260

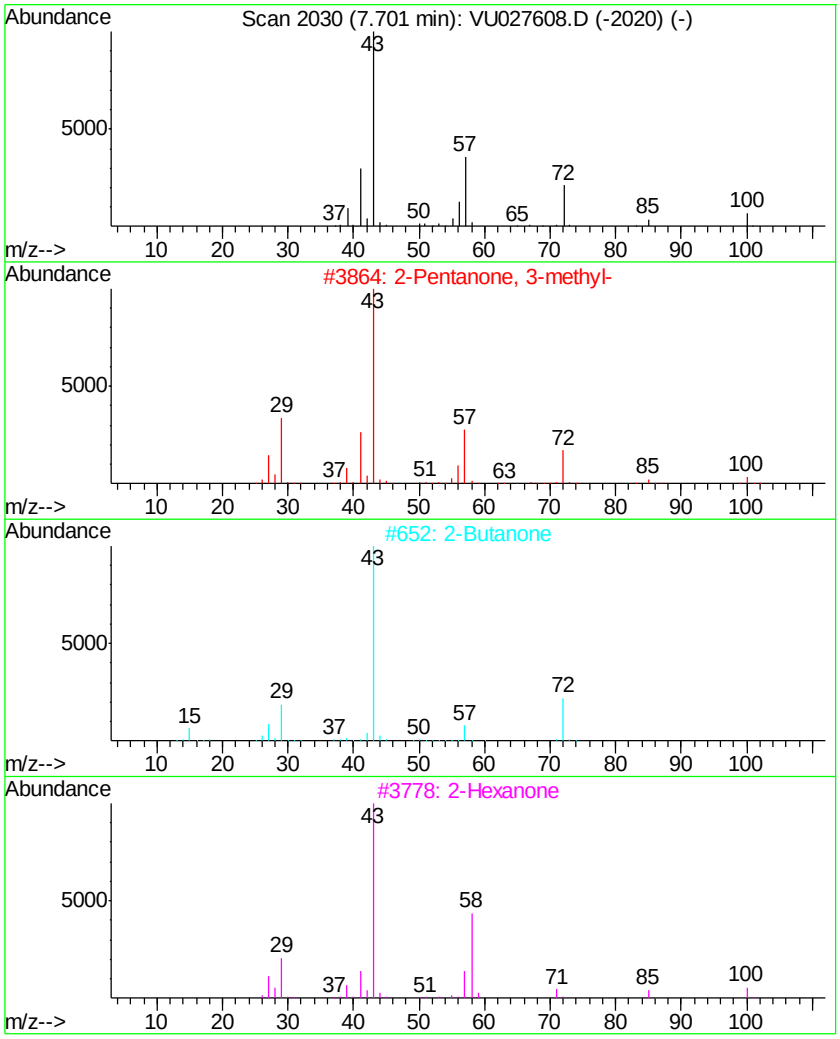
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

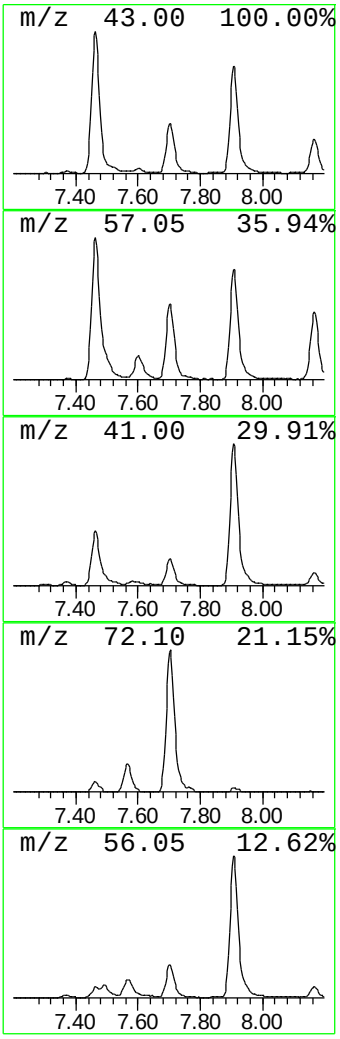
****

Peak Number 6 2-Pentanone, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	17.40 ug/l	204795	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	90
2	2-Butanone	72	C4H8O	000078-93-3	53
3	2-Hexanone	100	C6H12O	000591-78-6	47
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	47
5	5,9-Dodecadien-2-one, 6,10-dimet...	208	C14H24O	1000132-10-9	28





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ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MS-FRAC-TANK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U101118W.M
Quant Title : SW846 8260

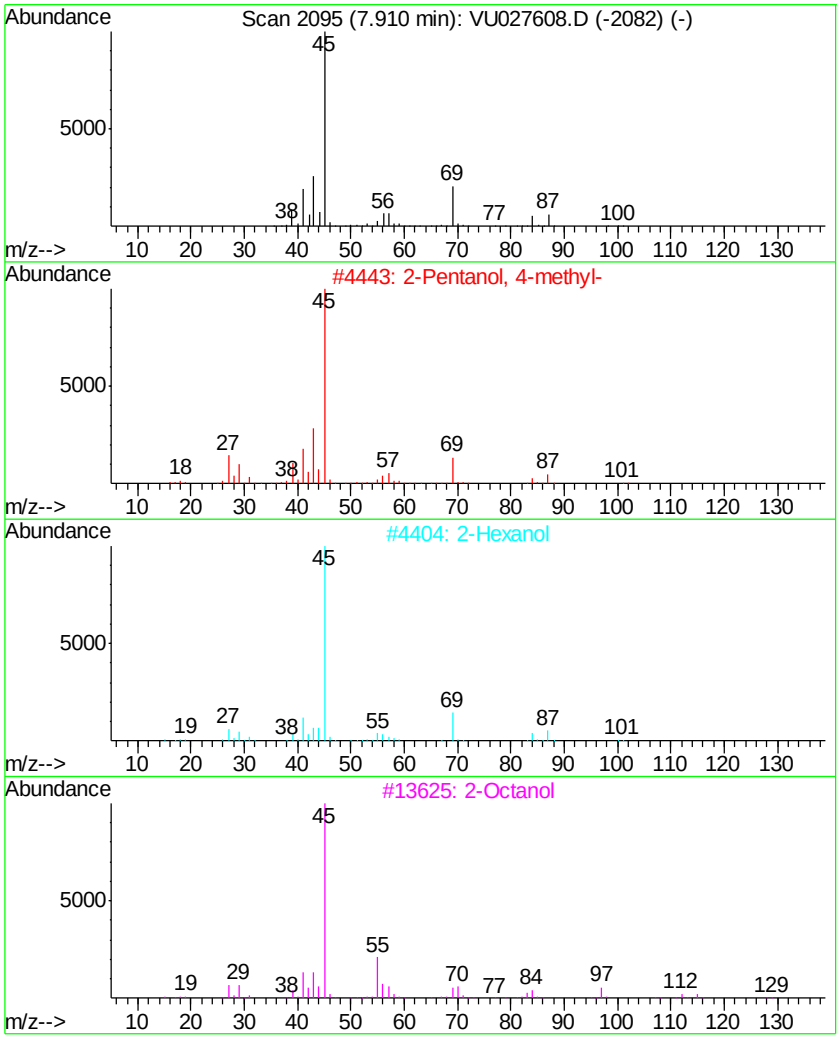
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

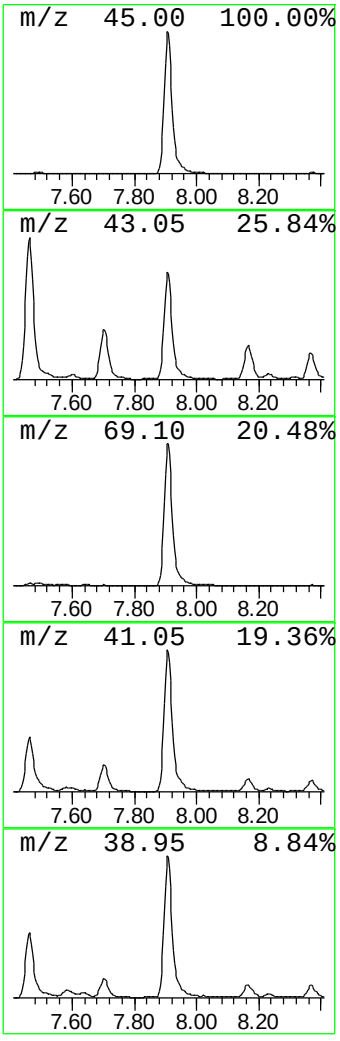
****

Peak Number 7 2-Pentanol, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.91	122.40 ug/l	1440550	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	83
2	2-Hexanol	102	C6H14O	000626-93-7	78
3	2-Octanol	130	C8H18O	000123-96-6	64
4	2-Octanol, (S)-	130	C8H18O	006169-06-8	64
5	2-Octanol, (R)-	130	C8H18O	005978-70-1	64





Library Search Compound Report

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Operator : MD/SY
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ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U101118W.M
Quant Title : SW846 8260

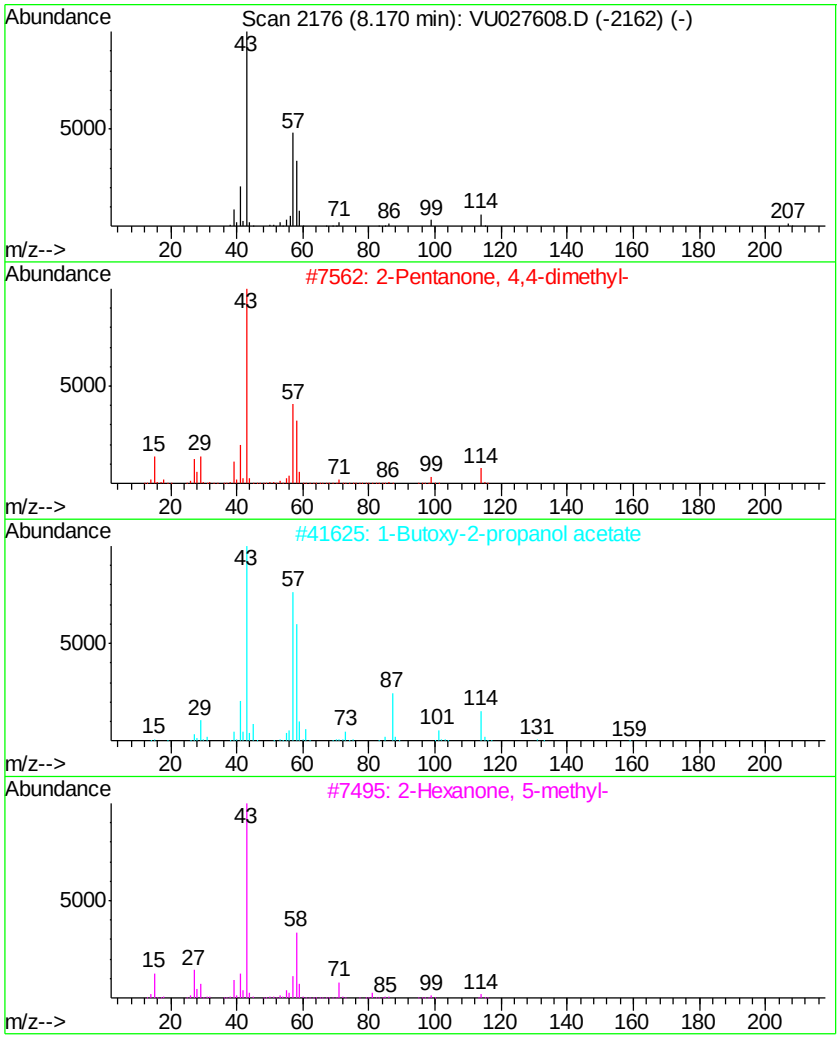
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

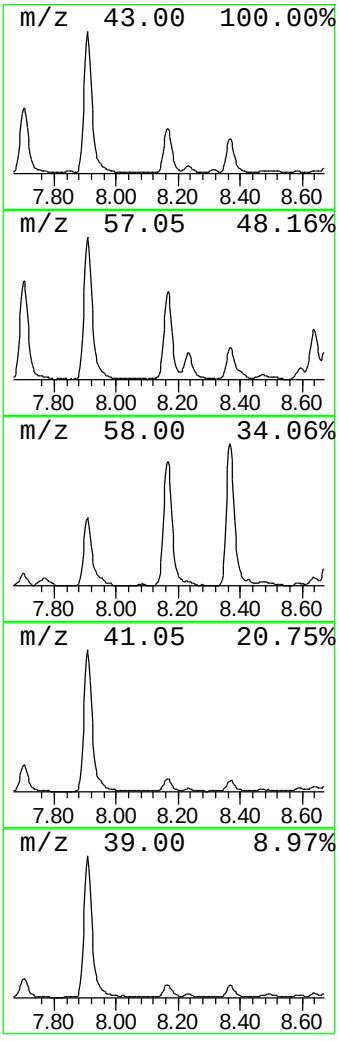
****

Peak Number 8 2-Pentanone, 4,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	11.36 ug/l	133675	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	90
2	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	64
3	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	59
4	2-Heptanone	114	C7H14O	000110-43-0	25
5	Butanal, 2-methyl-	86	C5H10O	000096-17-3	17





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU101118\
Data File : VU027608.D
Acq On : 11 Oct 2018 18:50
Operator : MD/SY
Sample : J5456-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MS-FRAC-TANK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U101118W.M
Quant Title : SW846 8260

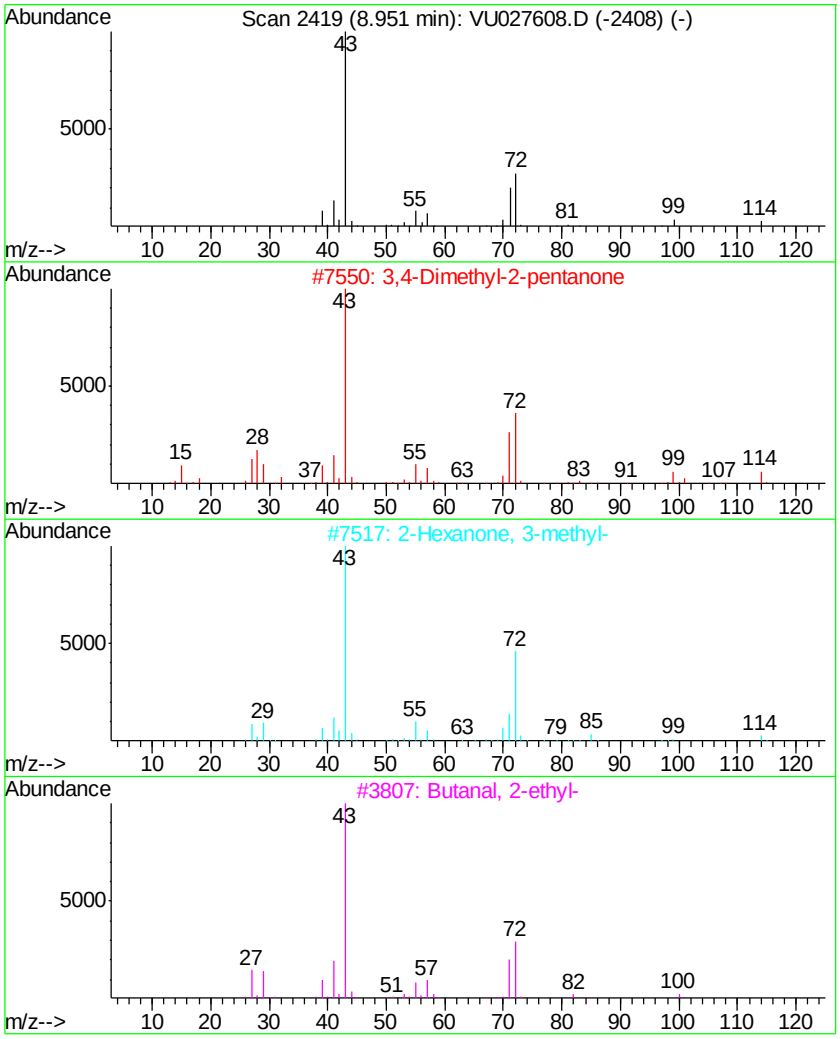
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

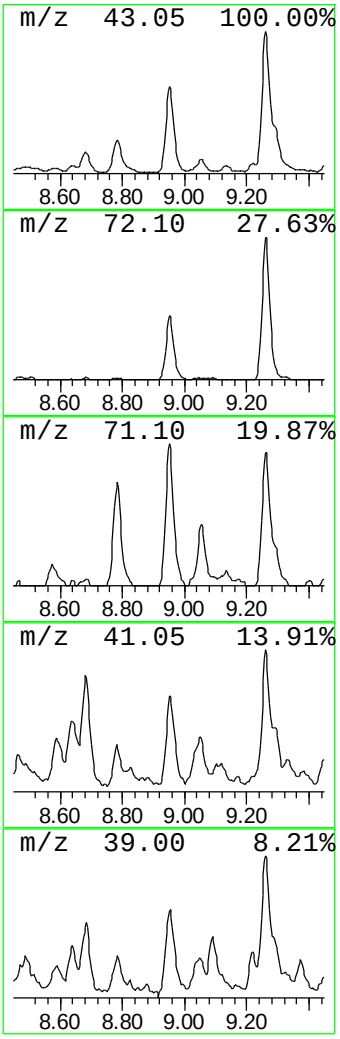
****

Peak Number 9 3,4-Dimethyl-2-pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.95	7.31 ug/l	86064	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	72
2	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	53
3	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	45
4	2-Butanone	72	C4H8O	000078-93-3	43
5	2-Buten-1-ol, acetate	114	C6H10O2	000628-08-0	42





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU101118\
Data File : VU027608.D
Acq On : 11 Oct 2018 18:50
Operator : MD/SY
Sample : J5456-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MS-FRAC-TANK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U101118W.M
Quant Title : SW846 8260

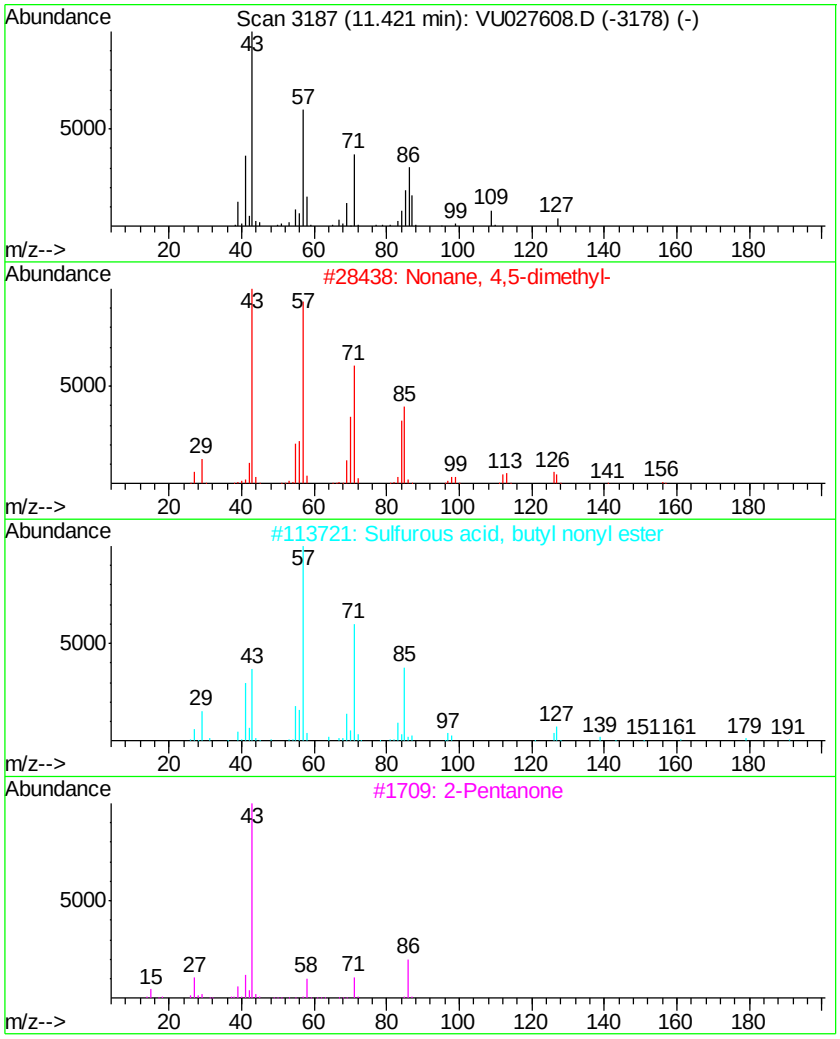
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

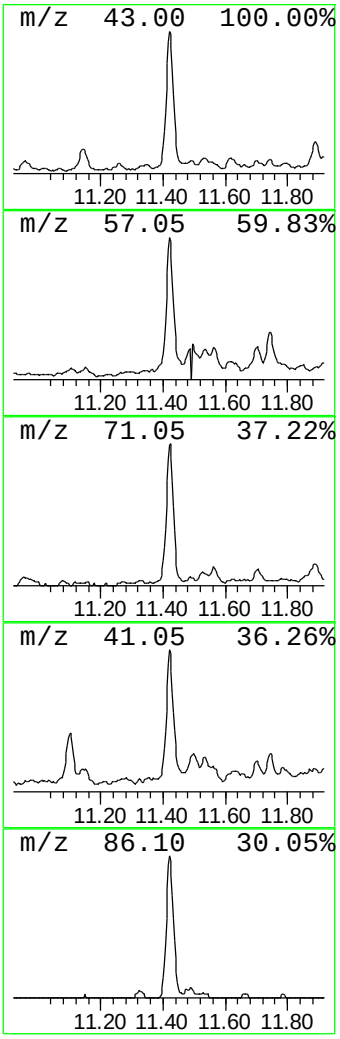
****

Peak Number 10 unknown11.42 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	9.95 ug/l	95282	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	32
2	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	28
3	2-Pentanone	86	C5H10O	000107-87-9	27
4	Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	25
5	Eicosane	282	C20H42	000112-95-8	23





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU101118\
Data File : VU027608.D
Acq On : 11 Oct 2018 18:50
Operator : MD/SY
Sample : J5456-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : MS-FRAC-TANK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U101118W.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
Isopropyl Alcohol	2.46	13.9	ug/l	100937	1	4.99	362822	50.0
Butanal	3.99	27.4	ug/l	198553	1	4.99	362822	50.0
2-Butanone, 3-met...	5.79	46.5	ug/l	522263	2	5.89	560969	50.0
2-Pentanone	6.42	37.5	ug/l	420253	2	5.89	560969	50.0
2-Butanone, 3,3-d...	6.83	21.9	ug/l	245766	2	5.89	560969	50.0
2-Pentanone, 3-me...	7.70	17.4	ug/l	204795	3	9.09	588468	50.0
2-Pentanol, 4-met...	7.91	122.4	ug/l	1440550	3	9.09	588468	50.0
2-Pentanone, 4,4-...	8.17	11.4	ug/l	133675	3	9.09	588468	50.0
3,4-Dimethyl-2-pe...	8.95	7.3	ug/l	86064	3	9.09	588468	50.0
unknown11.42	11.42	9.9	ug/l	95282	4	11.48	478612	50.0