LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061022\
Data File : VN072768.D
Acq On : 10 Jun 2022 16:34
Operator : JC\MD
Sample : N3293-18 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
52322-D

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_N\methods\82N060822W.M
Title : SW846 8260

Signal : TIC: VN072768.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	35	42	50	rBV4	10454	26692	1.05%	0.171%
2	2.405	66	71	80	rBV	28366	53833	2.11%	0.346%
3	2.581	94	101	112	rBV	92812	161809	6.35%	1.039%
4	4.287	381	391	402	rBV	70959	209018	8.21%	1.342%
5	7.057	849	862	873	rBV2	30079	88117	3.46%	0.566%
6	7.304	896	904	916	rBV2	18179	57633	2.26%	0.370%
7	7.563	941	948	957	rBV4	11671	30969	1.22%	0.199%
8	8.016	1015	1025	1031	rBV	365703	895647	35.17%	5.750%
9	8.081	1031	1036	1052	rVB	439811	991601	38.93%	6.367%
10	8.434	1083	1096	1109	rBV	426654	983834	38.63%	6.317%
11	8.963	1177	1186	1200	rBV	694317	1412997	55.48%	9.072%
12	9.151	1210	1218	1227	rBV	57285	130261	5.11%	0.836%
13	9.928	1344	1350	1358	rBV2	16659	31544	1.24%	0.203%
14	10.439	1426	1437	1454	rBV	1345847	2546893	100.00%	16.352%
15	10.651	1464	1473	1490	rBV2	79847	257728	10.12%	1.655%
16	11.145	1550	1557	1560	rBV	73104	145246	5.70%	0.933%
17	11.181	1560	1563	1578	rVB	106064	204933	8.05%	1.316%
18	11.739	1648	1658	1671	rBV	962191	1697684	66.66%	10.900%
19	11.863	1671	1679	1684	rBV	332753	551796	21.67%	3.543%
20	11.904	1684	1686	1691	rVB2	31906	40022	1.57%	0.257%
21	12.727	1813	1826	1838	rBV	1037213	1746064	68.56%	11.211%
22	13.163	1891	1900	1908	rBV2	375928	763274	29.97%	4.901%
23	13.227	1908	1911	1920	rVB3	55579	107212	4.21%	0.688%
24	13.422	1940	1944	1952	rVB3	23186	38230	1.50%	0.245%
25	13.527	1955	1962	1967	rBV2	42797	77144	3.03%	0.495%
26	13.574	1967	1970	1978	rVB5	24803	45185	1.77%	0.290%
27	13.669	1978	1986	1997	rBV	842185	1477463	58.01%	9.486%
28	13.769	1997	2003	2011	rVB	124524	204804	8.04%	1.315%
29	13.933	2025	2031	2038	rVB4	17179	33057	1.30%	0.212%
30	14.174	2062	2072	2084	rBV4	49817	108511	4.26%	0.697%
31	14.969	2202	2207	2213	rVB7	12193	25715	1.01%	0.165%
32	15.227	2241	2251	2258	rBV9	16147	51370	2.02%	0.330%
33	15.504	2294	2298	2312	rVB	63743	134402	5.28%	0.863%
34	15.763	2335	2342	2349	rBV3	64856	143278	5.63%	0.920%
35	16.615	2480	2487	2494	rBV2	46542	101235	3.97%	0.650%

LSC Area Percent Report

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ClientSampleId :
52322-D

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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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_N\methods\82N060822W.M
Title : SW846 8260

Sum of corrected areas: 15575201

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Acq On : 10 Jun 2022 16:34
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Instrument :
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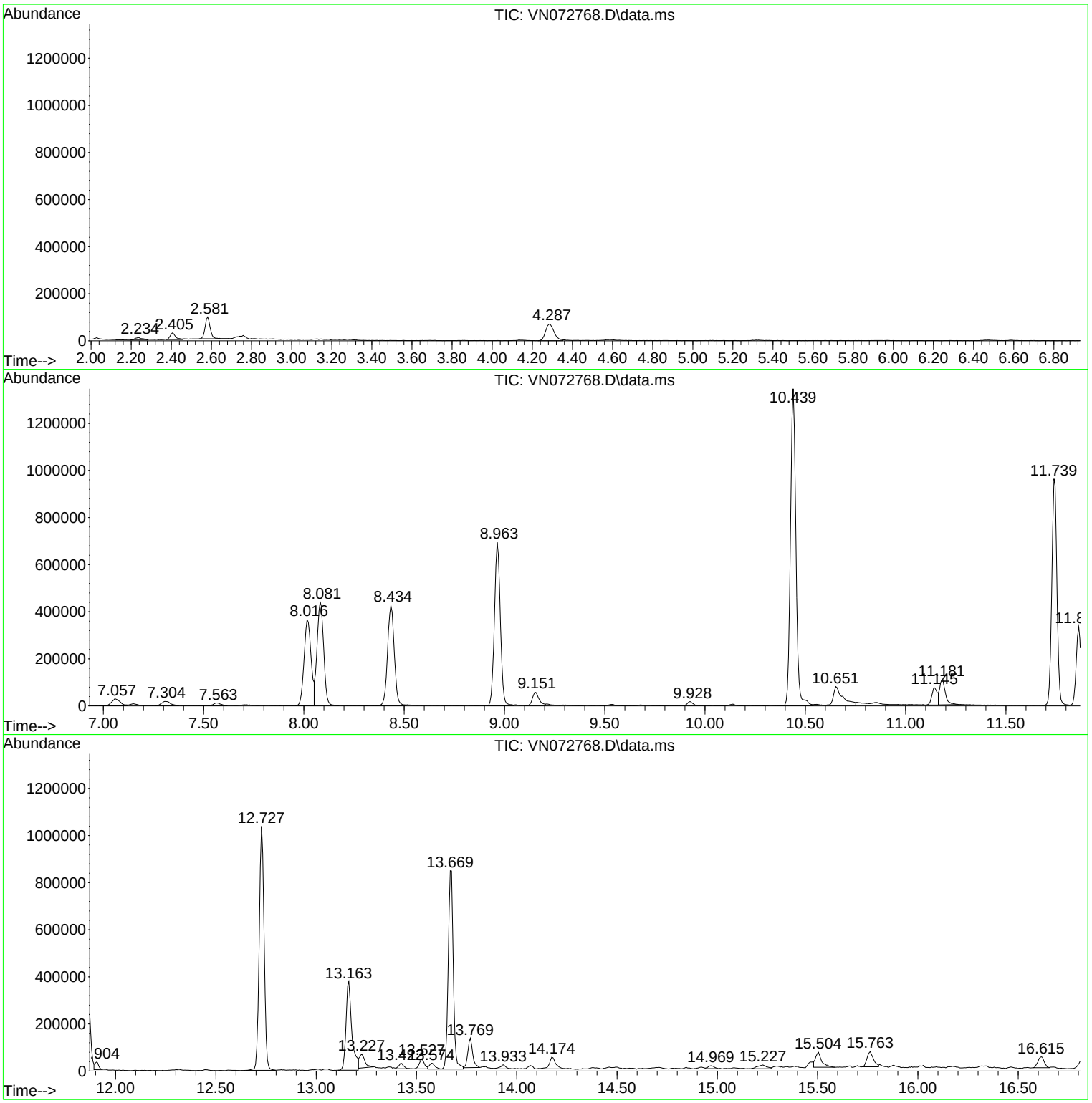
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Data File : VN072768.D
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

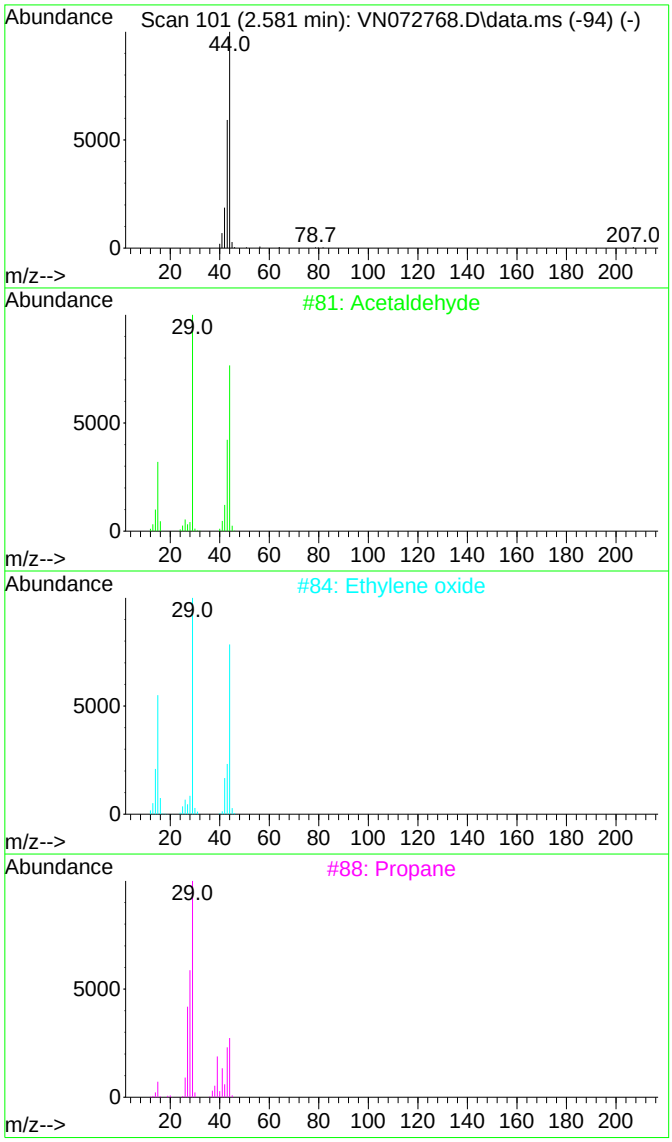
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

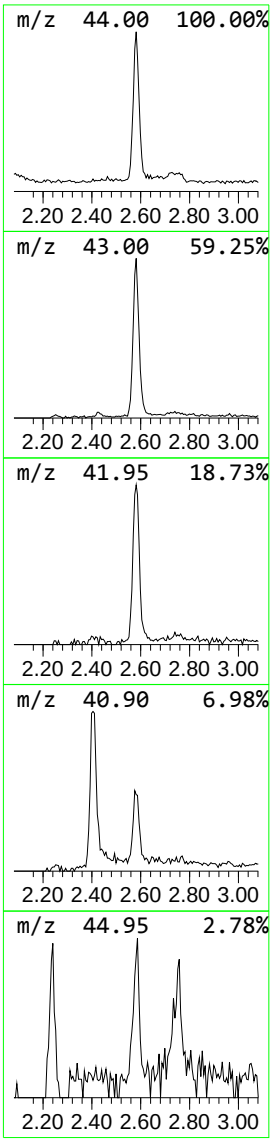
****

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.581	8.16 ug/l	161809	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	64
2	Ethylene oxide	44	C2H4O	000075-21-8	9
3	Propane	44	C3H8	000074-98-6	5
4	1,2-Propanediamine	74	C3H10N2	000078-90-0	4
5	O-Methylisourea	74	C2H6N2O	002440-60-0	4





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Instrument :
MSVOA_N
ClientSampleId :
52322-D

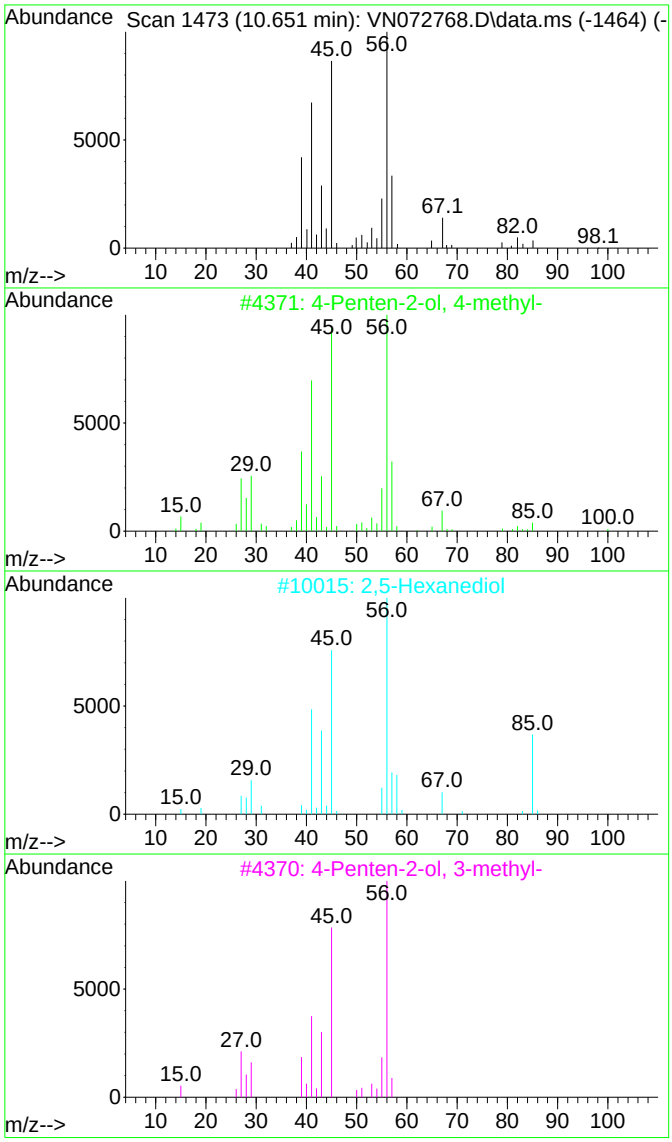
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

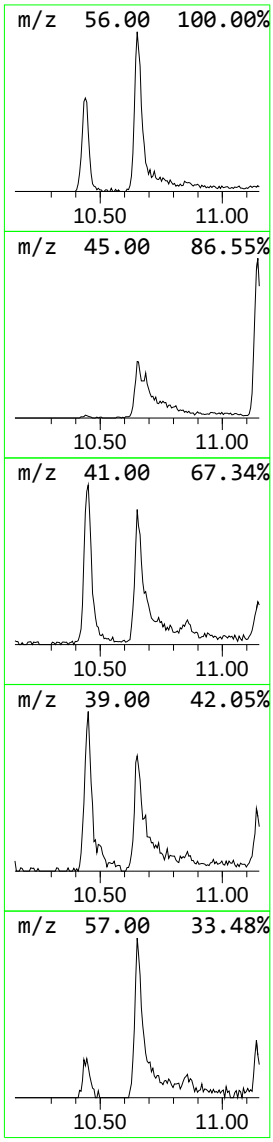
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 4-Penten-2-ol, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	7.59 ug/l	257728	Chlorobenzene-d5	11.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-ol, 4-methyl-	100	C6H12O	002004-67-3	64
2	2,5-Hexanediol	118	C6H14O2	002935-44-6	59
3	4-Penten-2-ol, 3-methyl-	100	C6H12O	001569-59-1	53
4	Oxetane, 2,3,4-trimethyl-	100	C6H12O	053778-61-3	53
5	2-Butene	56	C4H8	000107-01-7	35





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Data File : VN072768.D
Acq On : 10 Jun 2022 16:34
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
52322-D

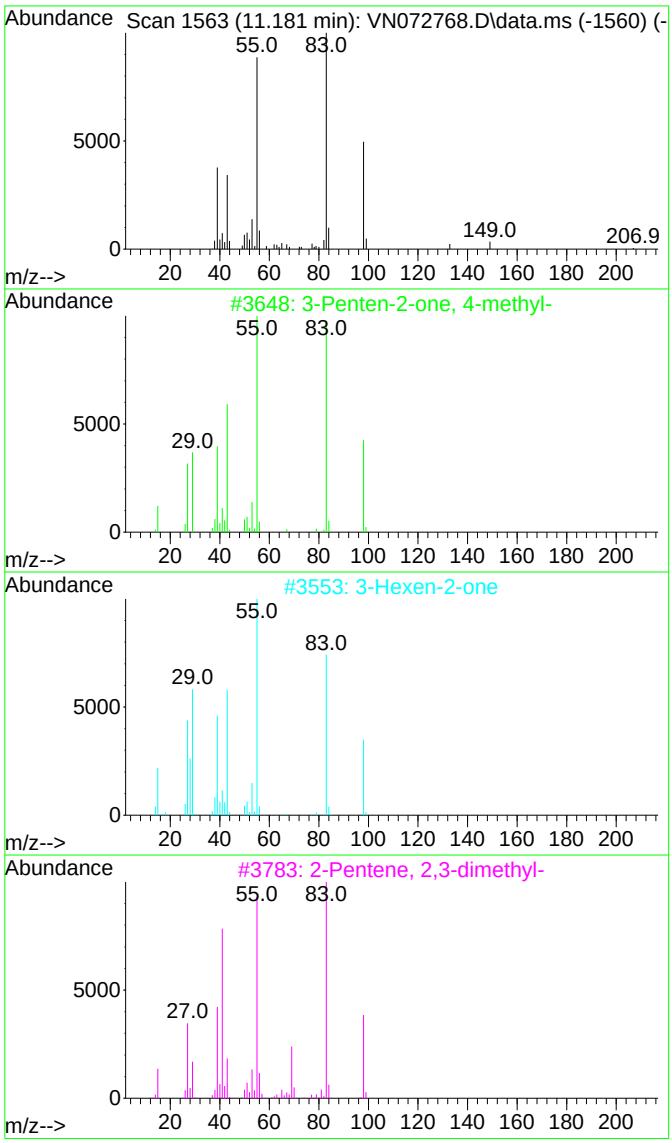
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

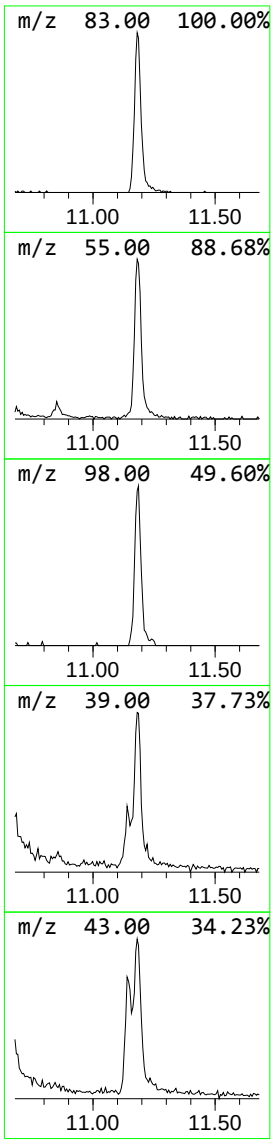
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.181	6.04 ug/l	204933	Chlorobenzene-d5	11.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	86
4	Cyclohexane, methyl-	98	C7H14	000108-87-2	80
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78





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Instrument :
MSVOA_N
ClientSampleId :
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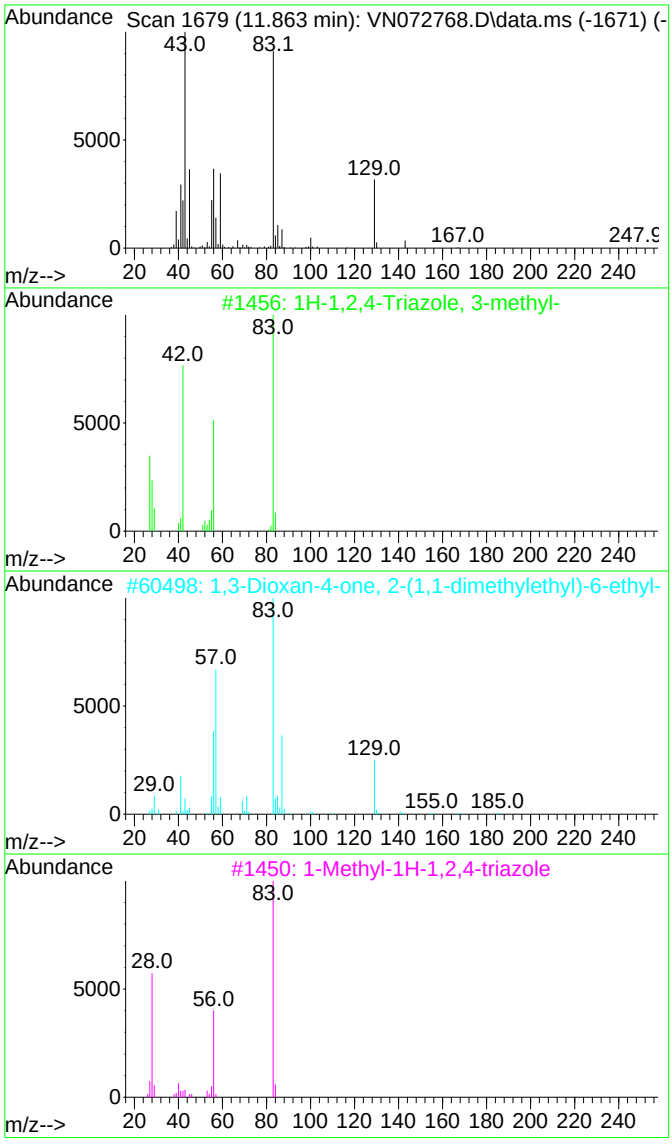
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

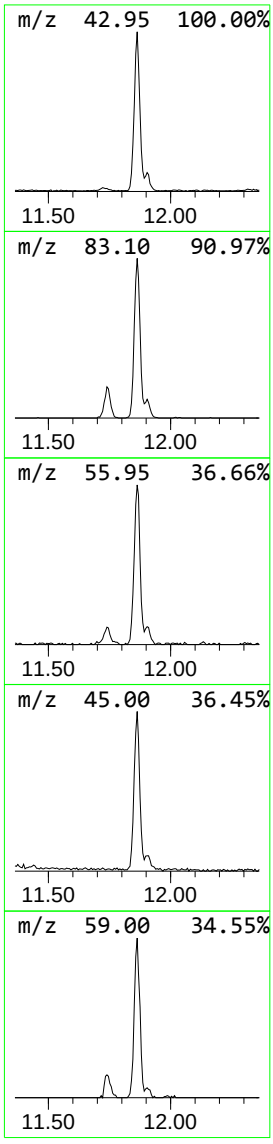
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown11.863 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	16.25 ug/l	551796	Chlorobenzene-d5	11.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	43
2	1,3-Dioxan-4-one, 2-(1,1-dimethy...	186	C10H18O3	113505-80-9	33
3	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	32
4	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	22
5	3-Methylbut-2-enoic acid, 4-nitr...	221	C11H11NO4	1000307-59-8	12





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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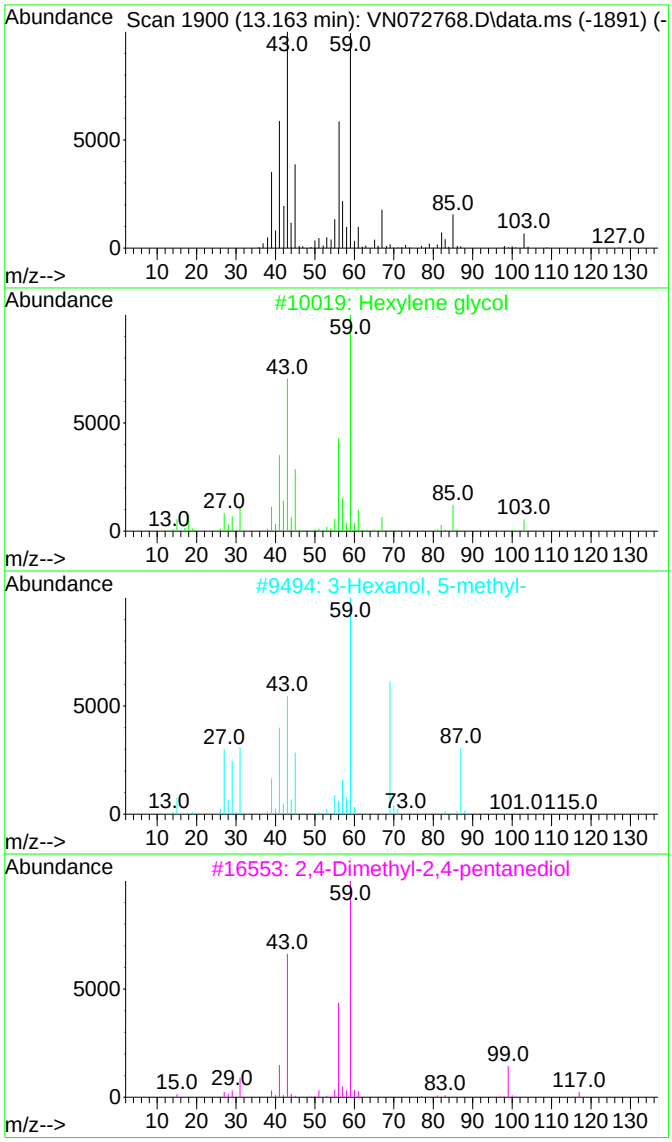
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060822W.M
Quant Title : SW846 8260

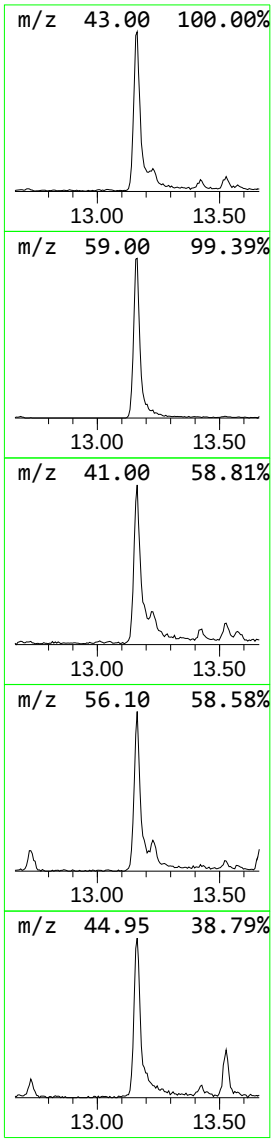
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexylene glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	25.83 ug/l	763274	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene glycol	118	C6H14O2	000107-41-5	78
2	3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	47
3	2,4-Dimethyl-2,4-pentanediol	132	C7H16O2	024892-49-7	37
4	1,3-Dioxane, 2,2-dimethyl-5-hydr...	132	C6H12O3	1000381-75-6	35
5	Guanidine	59	CH5N3	000113-00-8	35





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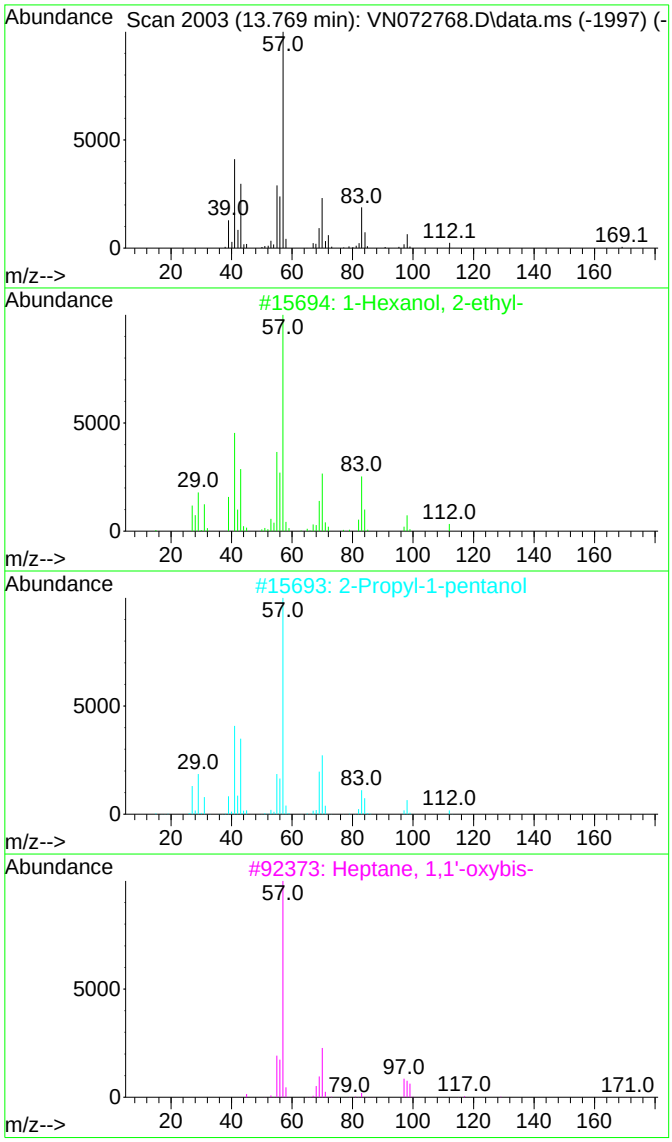
Quant Title : SW846 8260

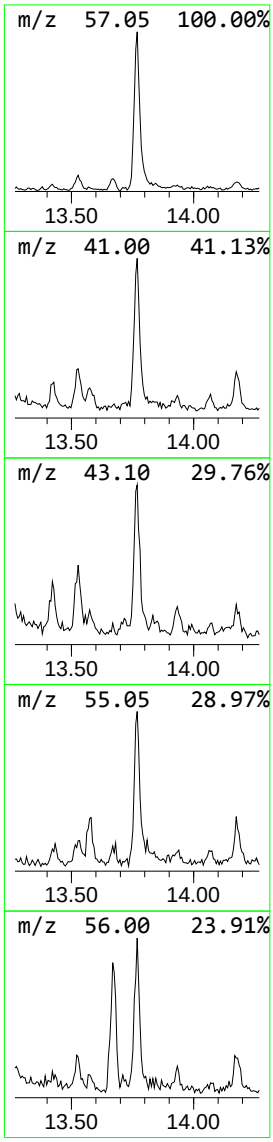
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.769	6.93 ug/l	204804	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
4	Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	47
5	1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	47





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetaldehyde	2.581	8.2	ug/l	161809	1	8.081	991601	50.0
4-Penten-2-ol, ...	10.651	7.6	ug/l	257728	3	11.739	1697680	50.0
3-Penten-2-one,...	11.181	6.0	ug/l	204933	3	11.739	1697680	50.0
unknown11.863	11.863	16.3	ug/l	551796	3	11.739	1697680	50.0
Hexylene glycol	13.163	25.8	ug/l	763274	4	13.675	1477460	50.0
1-Hexanol, 2-et...	13.769	6.9	ug/l	204804	4	13.675	1477460	50.0