LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069926.D
Acq On : 9 Dec 2021 21:26
Operator : JC/MD
Sample : M4970-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-18

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\82N120221W.M
Title : SW846 8260

Signal : TIC: VN069926.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.260	86	101	111	rBV3	120564	273013	3.09%	0.346%
2	2.448	159	171	190	rVB	545551	881348	9.97%	1.117%
3	3.145	414	431	456	rVB	803092	1824951	20.64%	2.313%
4	3.518	555	570	589	rBV3	136816	318883	3.61%	0.404%
5	4.264	824	848	859	rBV6	27620	100574	1.14%	0.127%
6	5.079	1129	1152	1166	rBV4	79418	283124	3.20%	0.359%
7	5.374	1233	1262	1296	rBV2	326909	1193232	13.50%	1.512%
8	5.621	1324	1354	1396	rBV2	1086379	3870017	43.78%	4.905%
9	6.501	1651	1682	1705	rBV3	183707	598730	6.77%	0.759%
10	7.150	1899	1924	1946	rBV3	225713	676563	7.65%	0.857%
11	7.847	2171	2184	2203	rVB4	37932	95177	1.08%	0.121%
12	8.024	2225	2250	2261	rBV	959151	2319437	26.24%	2.940%
13	8.088	2261	2274	2299	rVB	1729825	3998011	45.23%	5.067%
14	8.458	2384	2412	2427	rBV3	3172019	8840226	100.00%	11.204%
15	8.533	2427	2440	2493	rVB	3440557	8601808	97.30%	10.901%
16	8.968	2581	2602	2633	rBV	2742778	5786154	65.45%	7.333%
17	9.971	2961	2976	2990	rBV4	68195	134748	1.52%	0.171%
18	10.202	3043	3062	3068	rBV	493390	974020	11.02%	1.234%
19	10.440	3133	3151	3177	rBV	4439299	8337501	94.31%	10.566%
20	10.550	3178	3192	3217	rVB	846932	1696117	19.19%	2.150%
21	11.089	3379	3393	3401	rBV4	46679	90441	1.02%	0.115%
22	11.213	3421	3439	3467	rBV4	237537	541464	6.13%	0.686%
23	11.628	3570	3594	3614	rBV7	61666	174320	1.97%	0.221%
24	11.744	3618	3637	3662	rBV	4766505	8827355	99.85%	11.187%
25	11.846	3662	3675	3700	rVV	540328	1115018	12.61%	1.413%
26	11.956	3701	3716	3737	rVB	723560	1405033	15.89%	1.781%
27	12.087	3758	3765	3785	rVB7	48346	93079	1.05%	0.118%
28	12.280	3824	3837	3849	rVB	52352	90303	1.02%	0.114%
29	12.578	3939	3948	3962	rVB3	121154	218964	2.48%	0.278%
30	12.731	3987	4005	4034	rBV	3602297	6422232	72.65%	8.139%
31	12.921	4064	4076	4089	rBV	87226	145670	1.65%	0.185%
32	13.058	4119	4127	4145	rVB2	116156	211158	2.39%	0.268%
33	13.222	4169	4188	4203	rBV2	148110	264084	2.99%	0.335%
34	13.369	4223	4243	4263	rVB	295038	524279	5.93%	0.664%
35	13.675	4340	4357	4387	rBV	4013334	7035796	79.59%	8.917%
36	13.876	4422	4432	4453	rVB	272254	492290	5.57%	0.624%

LSC Area Percent Report

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ALS Vial : 24 Sample Multiplier: 1

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MSVOA_N
ClientSampleId :
MW-18

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_N\methods\82N120221W.M
Title : SW846 8260

37	14.329	4590	4601	4614	rVB	100986	171536	1.94%	0.217%
38	14.930	4807	4825	4839	rBV3	64831	128186	1.45%	0.162%
39	15.507	5025	5040	5059	rVB	75134	150403	1.70%	0.191%

Sum of corrected areas: 78905245

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ClientSampleId :
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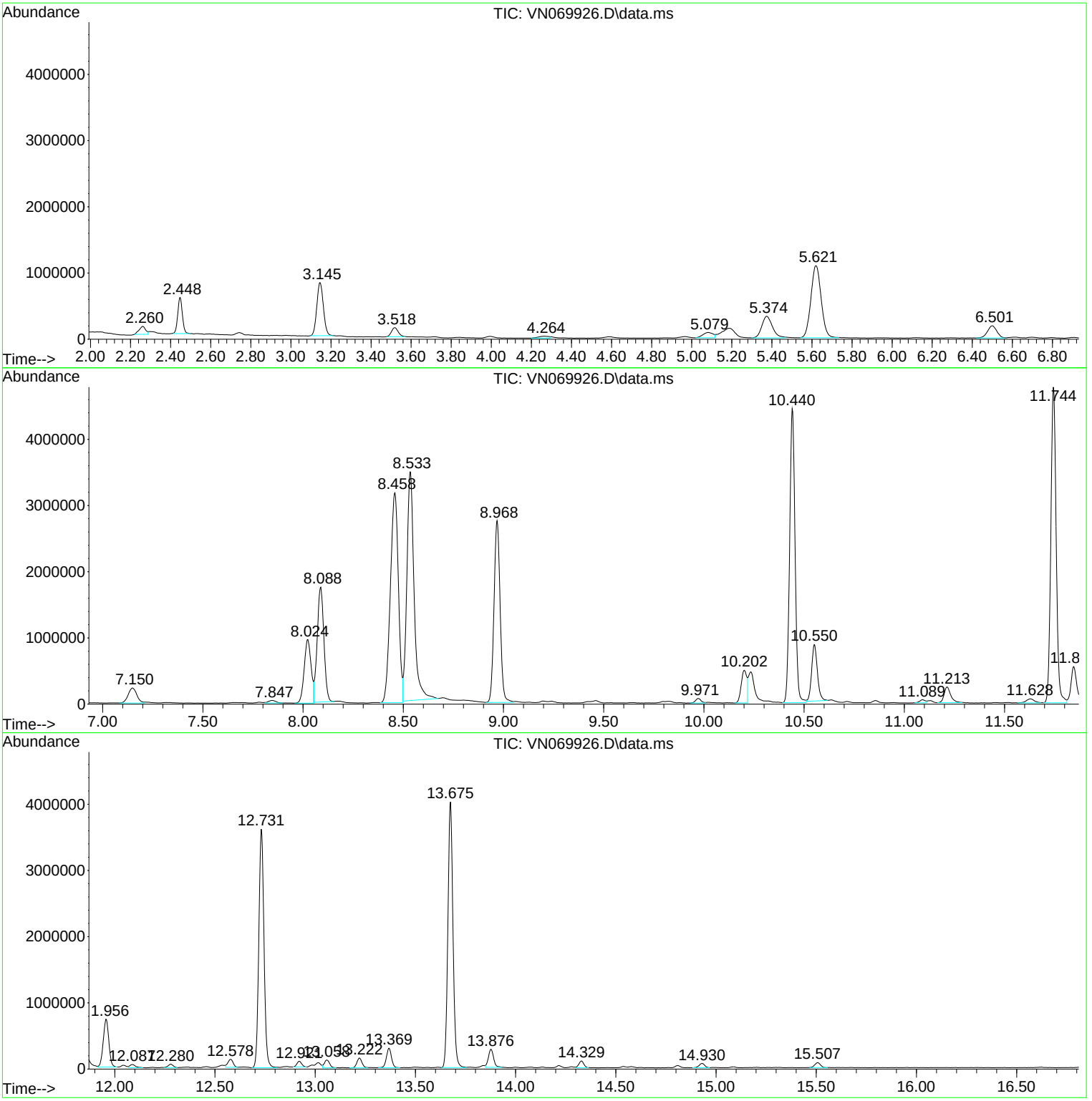
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



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Data File : VN069926.D
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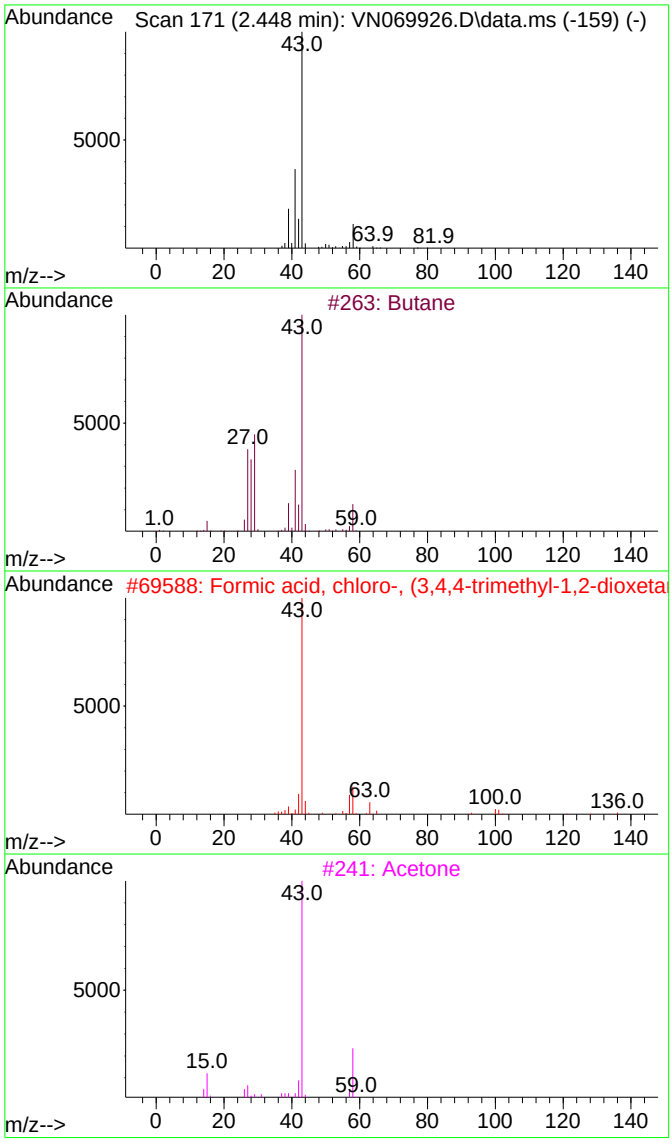
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

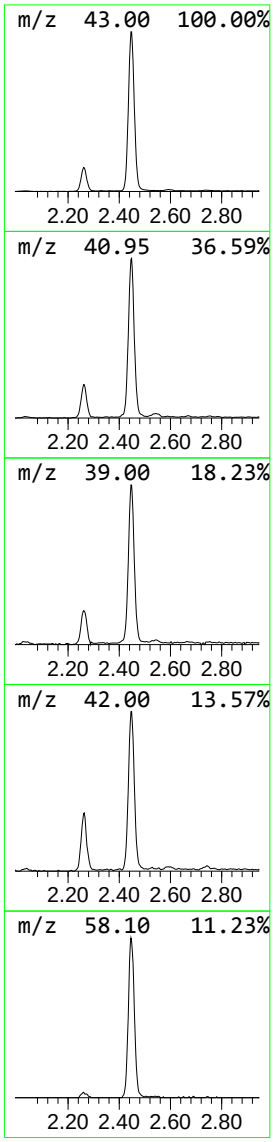
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.448	11.02 ug/l	881348	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	64
2	Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	9
3	Acetone	58	C3H6O	000067-64-1	4
4	Isobutane	58	C4H10	000075-28-5	4
5	Allyl acetate	100	C5H8O2	000591-87-7	4





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-18

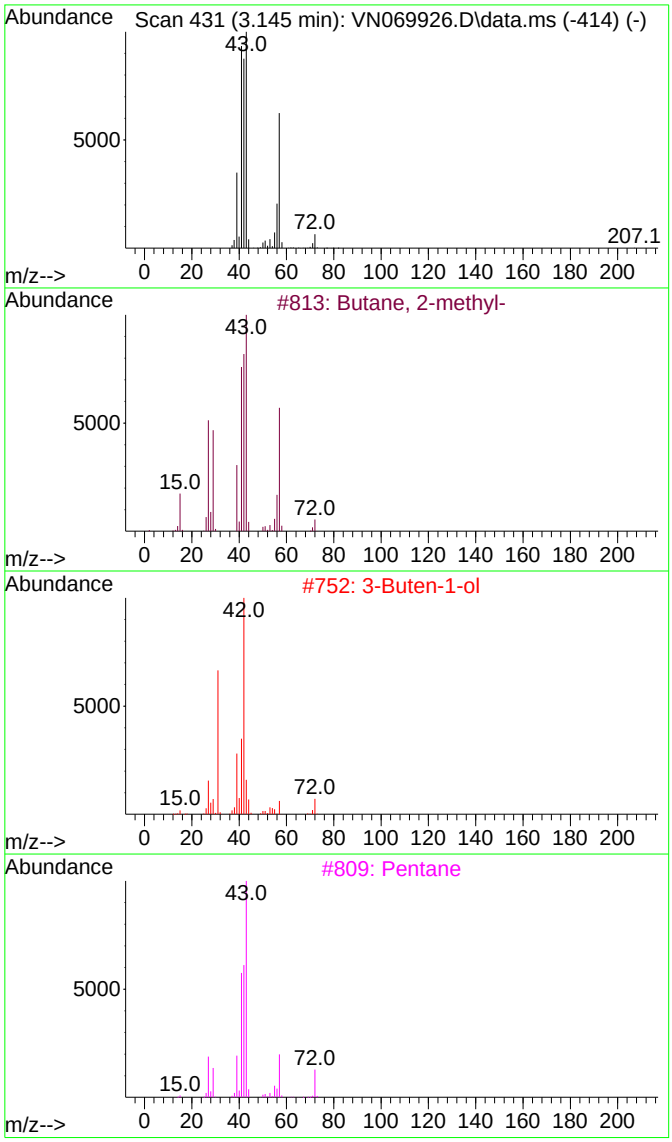
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

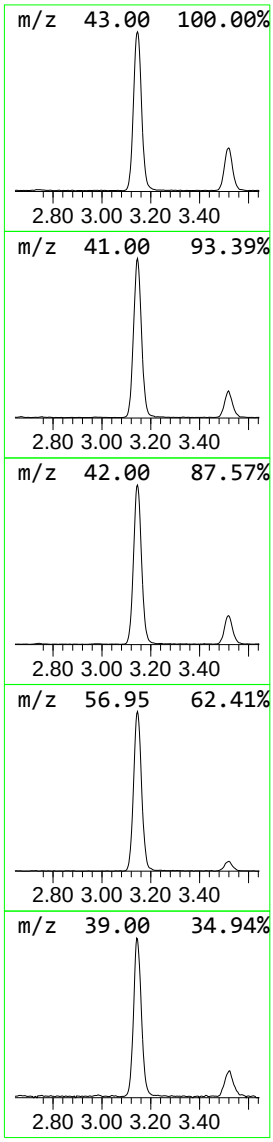
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.145	22.82 ug/l	1824950	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	23
5	Azetidine	57	C3H7N	000503-29-7	9





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Data File : VN069926.D
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Operator : JC/MD
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-18

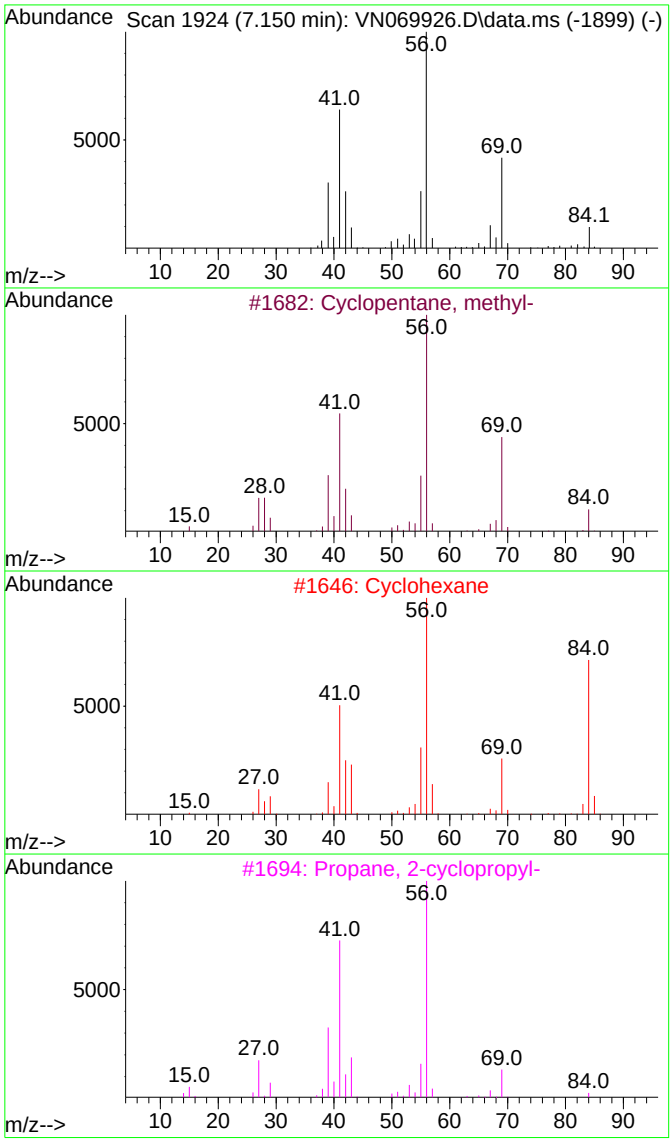
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

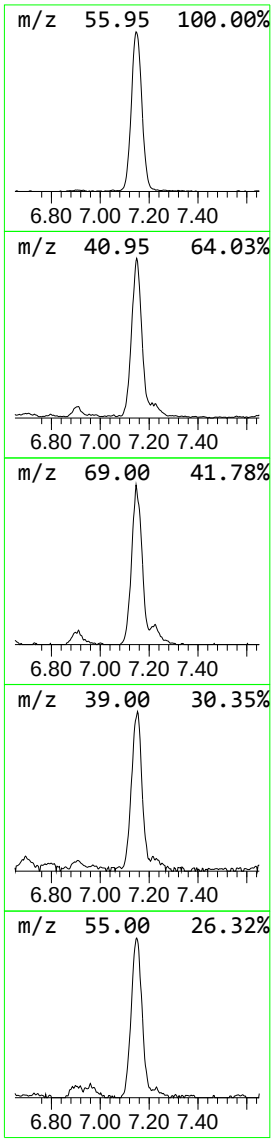
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.150	8.46 ug/l	676563	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclohexane	84	C6H12	000110-82-7	72
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64





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Sample : M4970-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-18

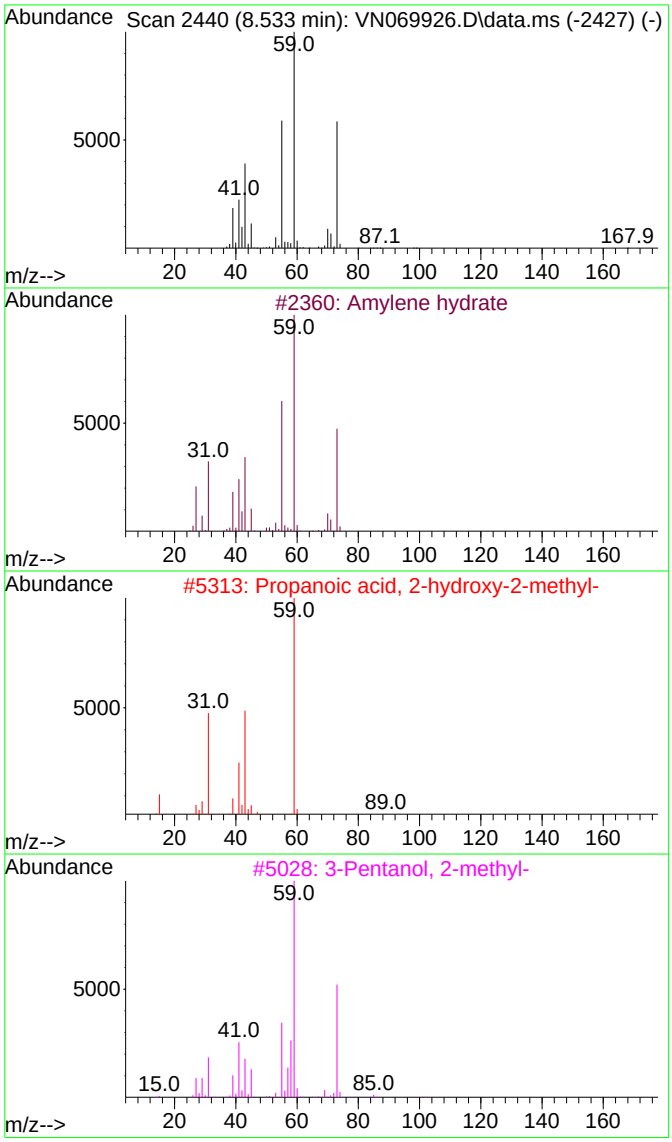
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

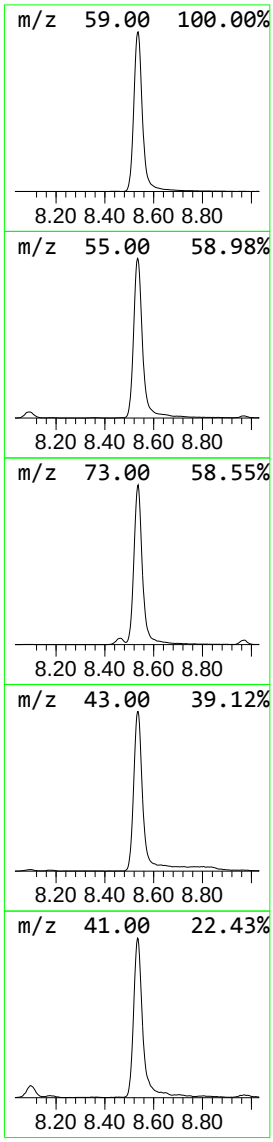
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.533	74.33 ug/l	8601810	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	83
2	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	42
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	38
4	HEX-5-EN-3-OL	100	C6H12O	000688-99-3	17
5	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	9





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-18

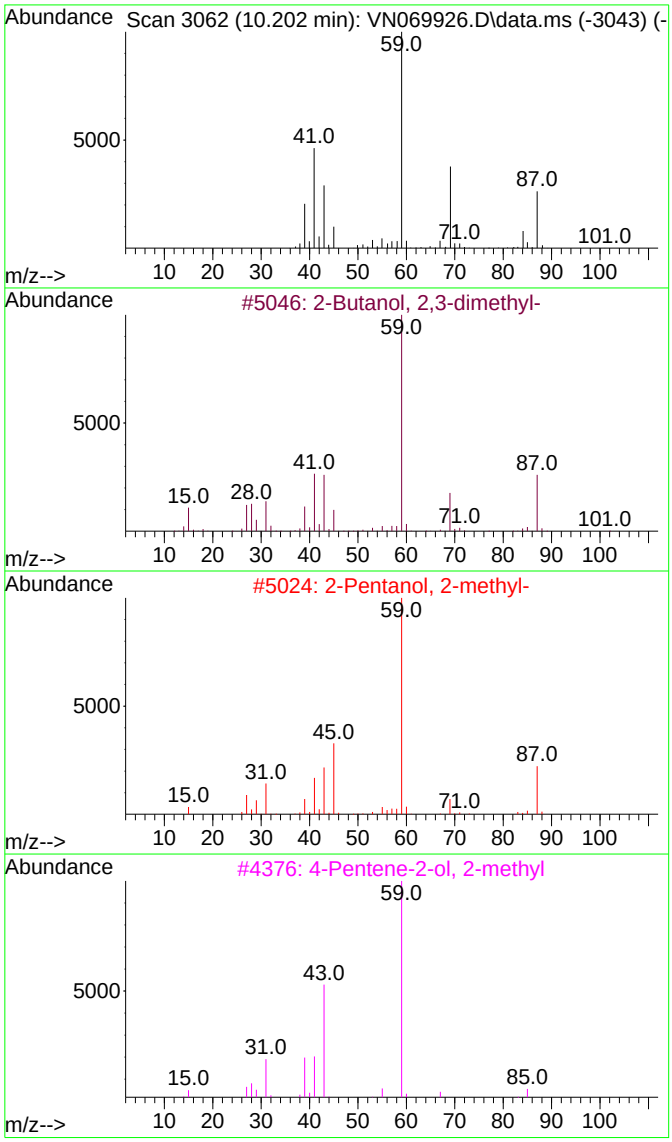
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

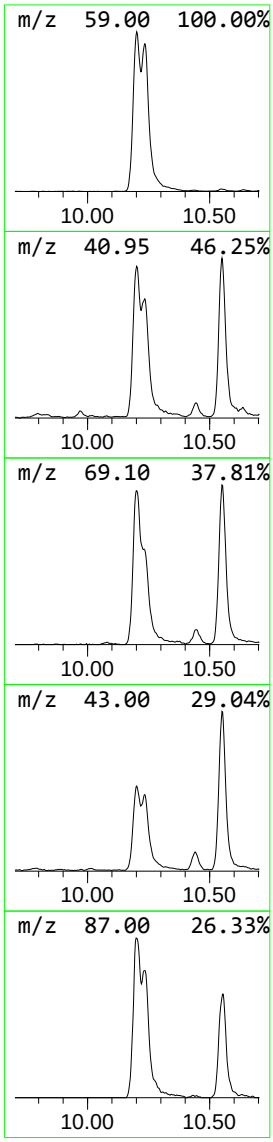
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Butanol, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.202	8.42 ug/l	974020	1,4-Difluorobenzene	8.968

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	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	53
4	Propane, 1-ethoxy-	88	C5H12O	000628-32-0	53
5	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	39





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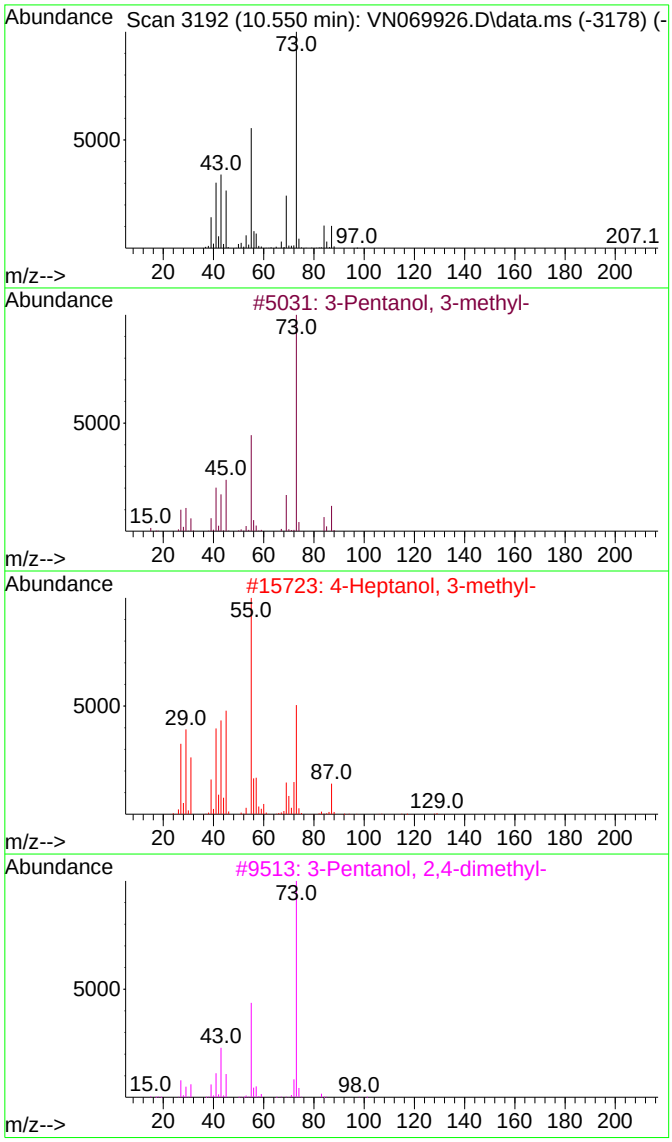
Quant Title : SW846 8260

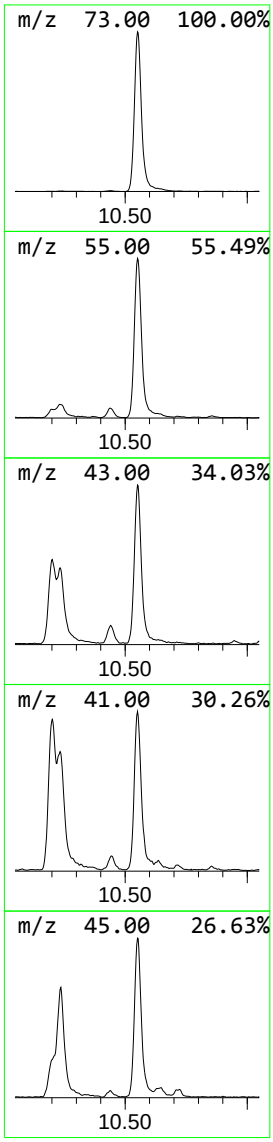
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Pentanol, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.550	9.61 ug/l	1696120	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	78
2	4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	59
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
4	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	37
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	35





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
Butane	2.448	11.0	ug/l	881348	1	8.086	3998010	50.0
Butane, 2-methyl-	3.145	22.8	ug/l	1824950	1	8.086	3998010	50.0
Cyclopentane, m...	7.150	8.5	ug/l	676563	1	8.086	3998010	50.0
Amylene hydrate	8.533	74.3	ug/l	8601810	2	8.968	5786150	50.0
2-Butanol, 2,3-...	10.202	8.4	ug/l	974020	2	8.968	5786150	50.0
3-Pentanol, 3-m...	10.550	9.6	ug/l	1696120	3	11.744	8827360	50.0