LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069924.D
Acq On : 9 Dec 2021 20:35
Operator : JC/MD
Sample : M4969-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RW-1A

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: VN069924.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.445	163	170	183	rVB2	95354	142724	1.63%	0.207%
2	3.143	416	430	453	rVB	189009	429948	4.90%	0.624%
3	3.516	556	569	592	rVB5	55165	139995	1.59%	0.203%
4	4.293	821	859	879	rBV	62023	220491	2.51%	0.320%
5	4.586	949	968	991	rBV2	29184	90699	1.03%	0.132%
6	5.085	1130	1154	1166	rBV4	60741	212949	2.43%	0.309%
7	5.374	1234	1262	1305	rBV2	714681	2578828	29.37%	3.741%
8	5.621	1327	1354	1391	rVB2	502633	1776287	20.23%	2.577%
9	6.493	1651	1679	1703	rBV6	128441	491628	5.60%	0.713%
10	6.611	1703	1723	1739	rVB6	38231	111785	1.27%	0.162%
11	7.147	1902	1923	1940	rBV3	196478	575809	6.56%	0.835%
12	7.219	1943	1950	1976	rVB4	88616	217178	2.47%	0.315%
13	7.780	2144	2159	2171	rBV5	33757	88727	1.01%	0.129%
14	7.844	2174	2183	2203	rVB3	51686	122377	1.39%	0.178%
15	8.021	2226	2249	2261	rBV2	943504	2304641	26.25%	3.343%
16	8.086	2261	2273	2294	rVB	1670909	3869685	44.08%	5.613%
17	8.177	2299	2307	2329	rVB7	97045	245498	2.80%	0.356%
18	8.442	2385	2406	2426	rBV2	1202507	3251394	37.03%	4.716%
19	8.536	2427	2441	2455	rBV	500271	1104415	12.58%	1.602%
20	8.968	2582	2602	2629	rBV	2843925	6055726	68.97%	8.784%
21	9.199	2673	2688	2697	rBV2	98851	198769	2.26%	0.288%
22	9.424	2755	2772	2778	rBV6	81198	169045	1.93%	0.245%
23	9.797	2895	2911	2920	rBV6	138732	322470	3.67%	0.468%
24	9.880	2936	2942	2960	rVB4	61074	105043	1.20%	0.152%
25	9.974	2961	2977	2986	rBV3	201851	402480	4.58%	0.584%
26	10.199	3046	3061	3092	rBV2	404721	1077675	12.27%	1.563%
27	10.322	3094	3107	3120	rVB2	205577	371753	4.23%	0.539%
28	10.440	3133	3151	3168	rBV	4412620	8143210	92.75%	11.812%
29	10.550	3185	3192	3206	rVB3	96091	162307	1.85%	0.235%
30	10.636	3216	3224	3239	rVB4	58734	112776	1.28%	0.164%
31	10.856	3293	3306	3327	rVV3	132309	263282	3.00%	0.382%
32	10.945	3327	3339	3360	rVB2	121902	232727	2.65%	0.338%
33	11.089	3379	3393	3398	rBV2	222506	381974	4.35%	0.554%
34	11.127	3399	3407	3431	rVB	602596	1099014	12.52%	1.594%
35	11.457	3519	3530	3541	rBV4	76353	142845	1.63%	0.207%
36	11.588	3565	3579	3618	rVB3	264697	858887	9.78%	1.246%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069924.D
Acq On : 9 Dec 2021 20:35
Operator : JC/MD
Sample : M4969-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RW-1A

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

37	11.744	3618	3637	3666	rBV	4775030	8779738	100.00%	12.735%
38	11.848	3667	3676	3699	rVB4	107115	282649	3.22%	0.410%
39	11.948	3702	3713	3727	rBV	123959	257724	2.94%	0.374%
40	12.090	3758	3766	3785	rVB10	45772	89171	1.02%	0.129%
41	12.358	3850	3866	3878	rBV5	61634	134895	1.54%	0.196%
42	12.578	3935	3948	3961	rBV	564751	932503	10.62%	1.353%
43	12.731	3988	4005	4030	rBV	3755346	6671317	75.99%	9.677%
44	12.849	4037	4049	4060	rBV8	44304	95689	1.09%	0.139%
45	12.919	4060	4075	4093	rVB	947666	1635690	18.63%	2.373%
46	13.058	4120	4127	4144	rVB7	67292	127903	1.46%	0.186%
47	13.219	4175	4187	4199	rBV2	88447	162229	1.85%	0.235%
48	13.358	4221	4239	4257	rVB2	66089	174608	1.99%	0.253%
49	13.675	4341	4357	4386	rBV	4005463	7155768	81.50%	10.380%
50	13.836	4406	4417	4423	rBV	329235	513028	5.84%	0.744%
51	13.876	4423	4432	4447	rVB	923754	1503209	17.12%	2.180%
52	14.217	4548	4559	4571	rVB	131525	208062	2.37%	0.302%
53	14.278	4572	4582	4588	rBV2	59813	95069	1.08%	0.138%
54	14.327	4589	4600	4620	rVB	551255	946814	10.78%	1.373%
55	14.538	4667	4679	4690	rBV2	80537	135063	1.54%	0.196%
56	14.809	4769	4780	4796	rVB2	142982	238537	2.72%	0.346%
57	14.930	4809	4825	4838	rBV3	176212	346770	3.95%	0.503%
58	15.306	4954	4965	4981	rVB5	44612	103835	1.18%	0.151%
59	15.504	5026	5039	5055	rVB	142147	273966	3.12%	0.397%

Sum of corrected areas: 68939278

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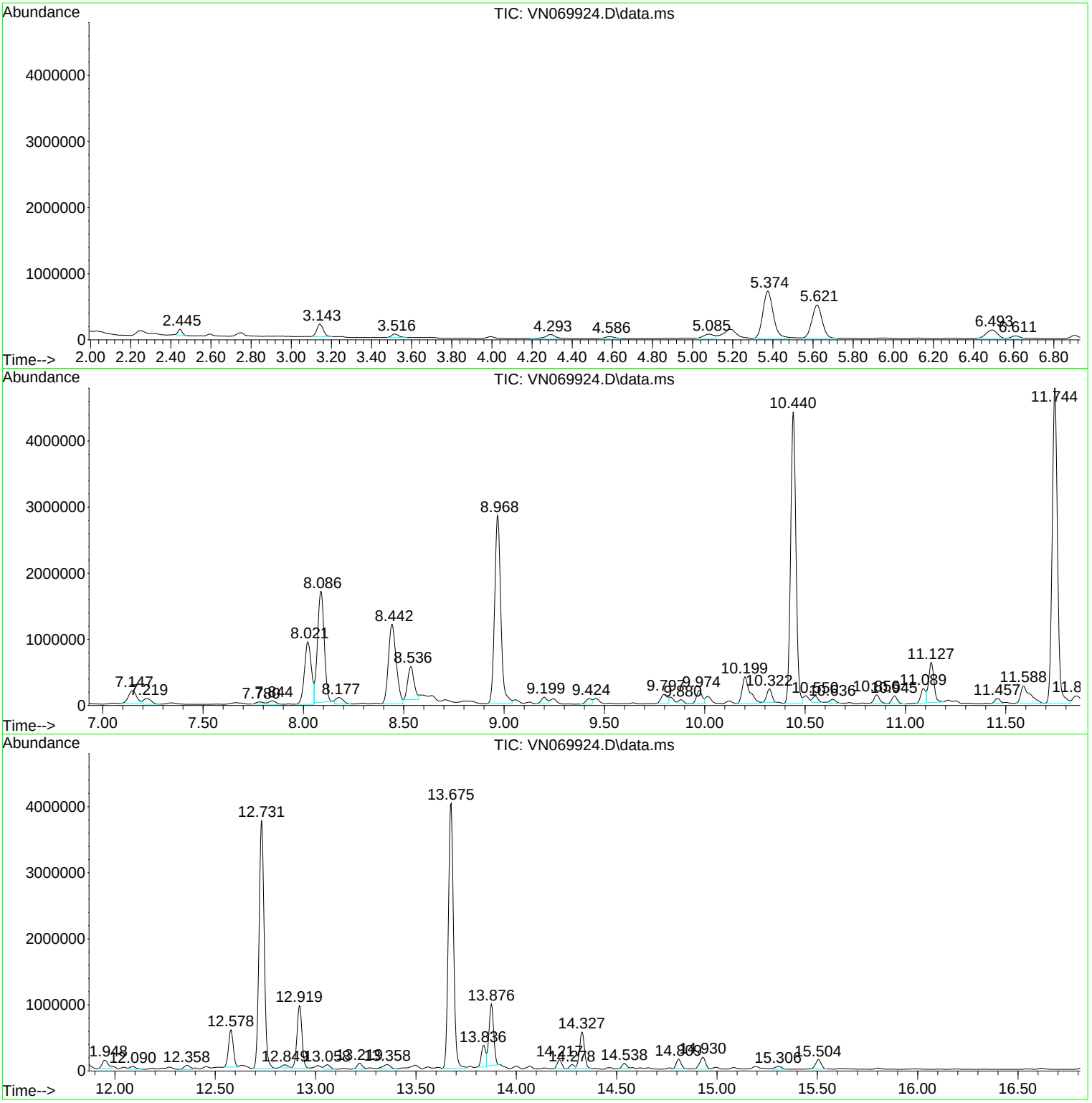
Operator : JC/MD
Sample : M4969-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RW-1A

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069924.D
Acq On : 9 Dec 2021 20:35
Operator : JC/MD
Sample : M4969-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RW-1A

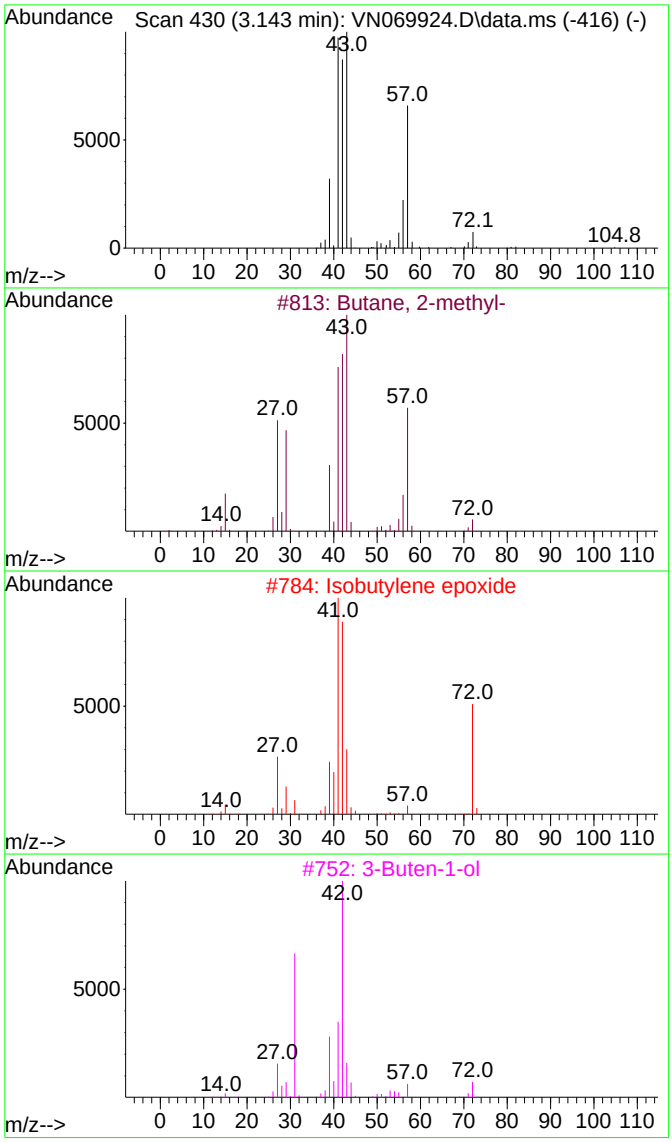
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

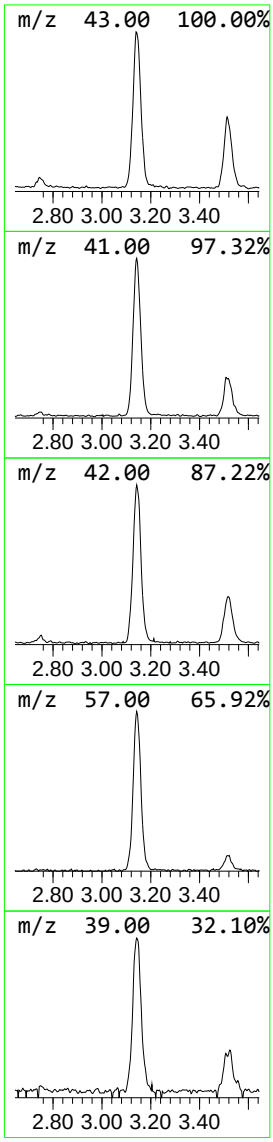
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.143	5.56 ug/l	429948	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Isobutylene epoxide	72	C4H8O	000558-30-5	53
3	3-Buten-1-ol	72	C4H8O	000627-27-0	47
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	42
5	Pentane	72	C5H12	000109-66-0	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069924.D
Acq On : 9 Dec 2021 20:35
Operator : JC/MD
Sample : M4969-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RW-1A

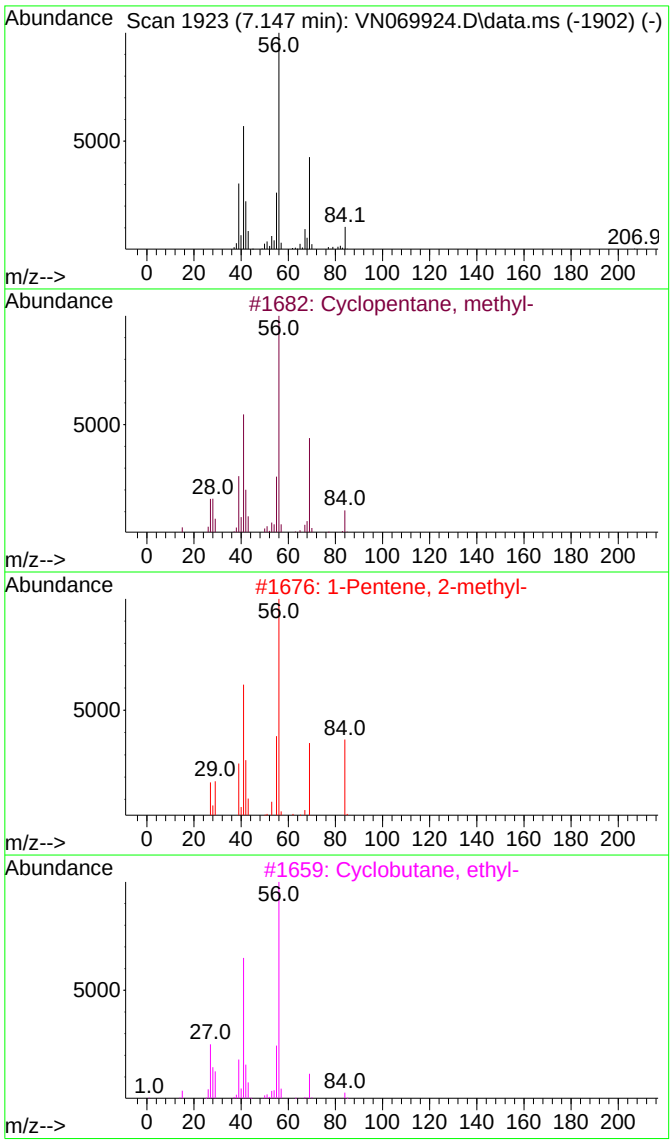
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

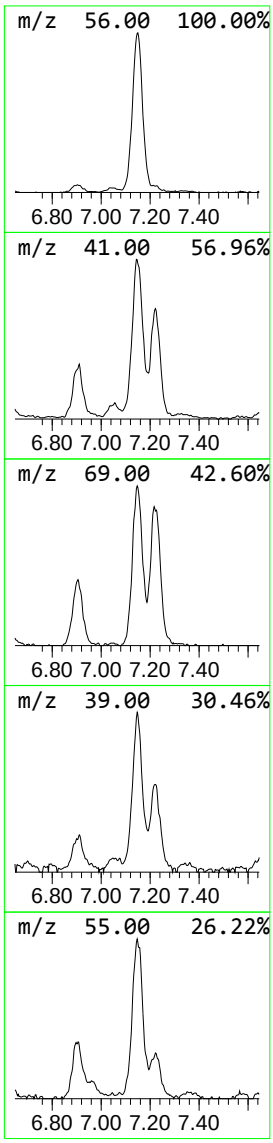
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.147	7.44 ug/l	575809	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	Cyclohexane	84	C6H12	000110-82-7	56
5	Cyclobutane	56	C4H8	000287-23-0	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069924.D
Acq On : 9 Dec 2021 20:35
Operator : JC/MD
Sample : M4969-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RW-1A

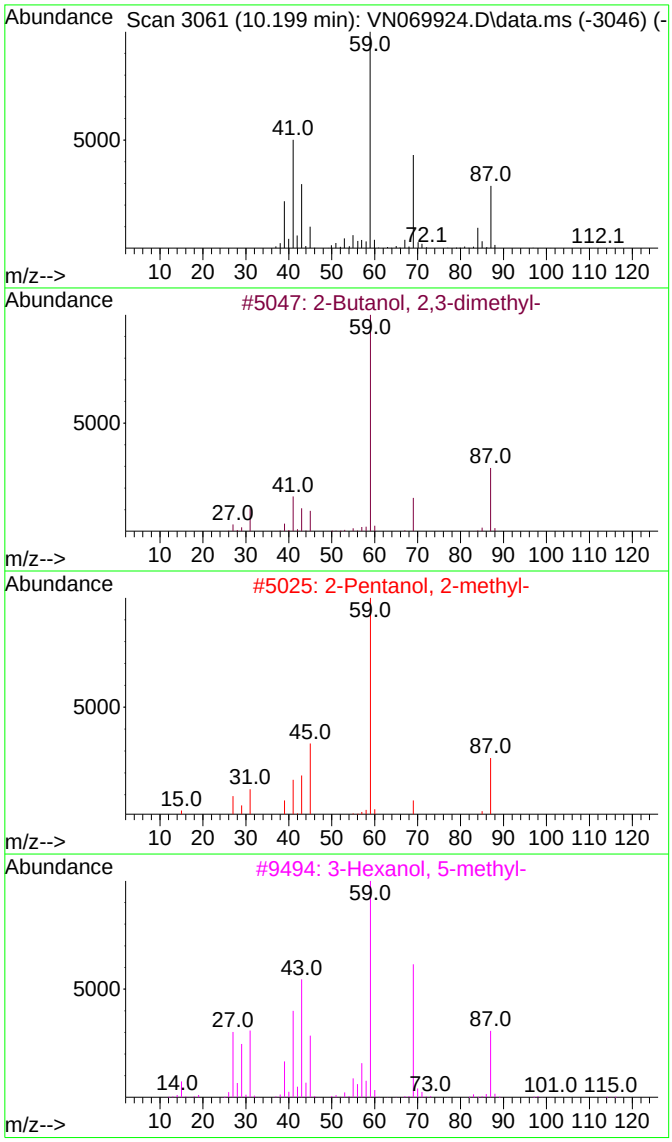
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

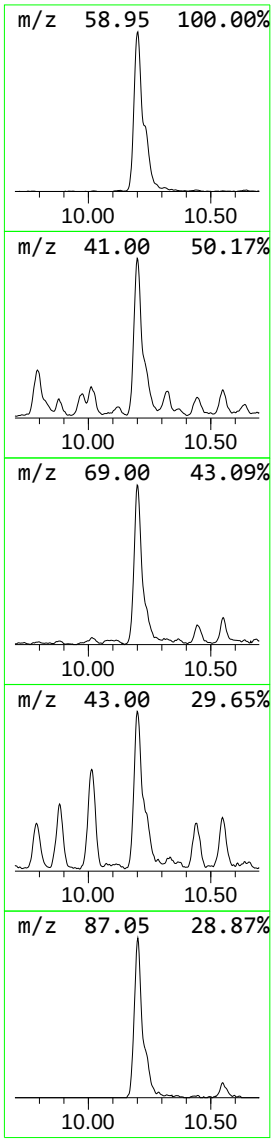
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.199	8.90 ug/l	1077680	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	78
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	50
3	3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	45
4	DL-Lactamide, N,O-dimethyl-	117	C5H11NO2	1000452-56-3	45
5	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069924.D
Acq On : 9 Dec 2021 20:35
Operator : JC/MD
Sample : M4969-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RW-1A

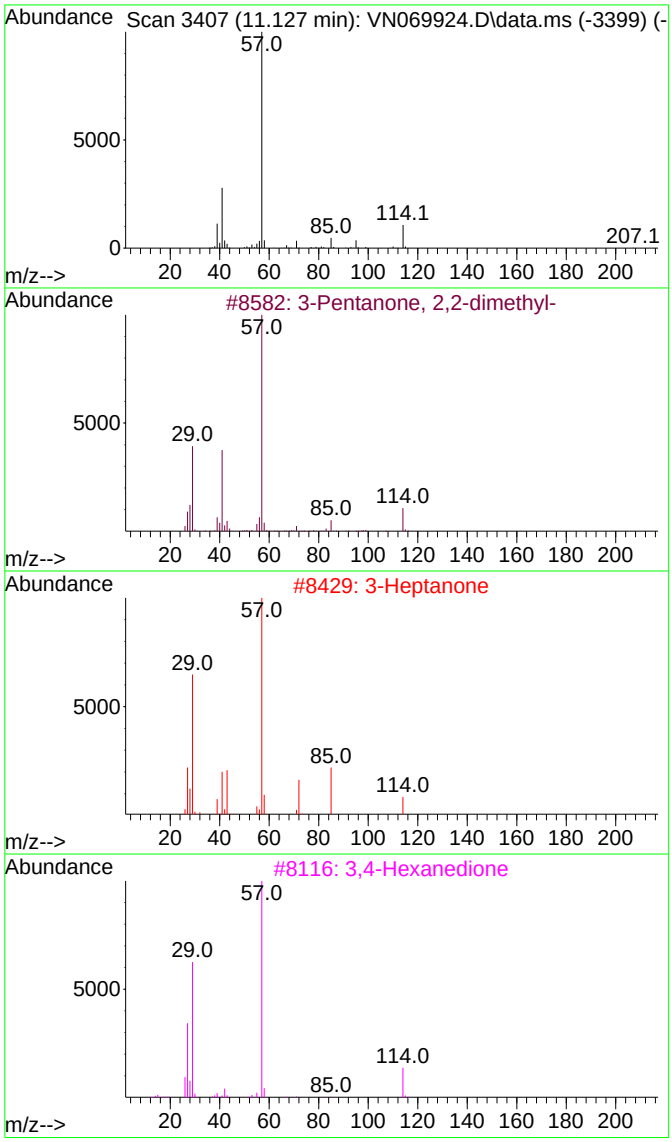
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

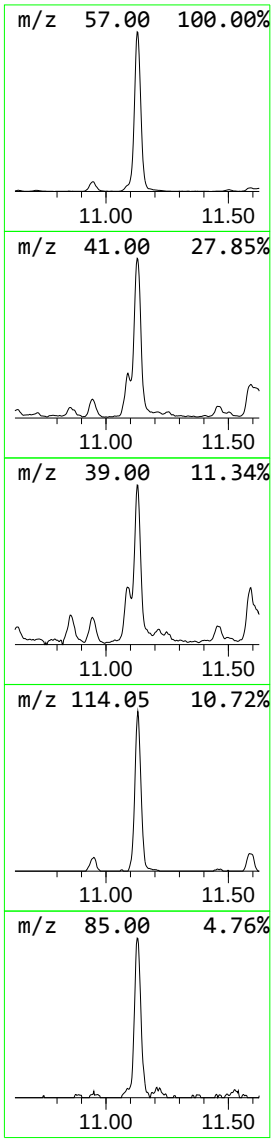
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Pentanone, 2,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.127	6.26 ug/l	1099010	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	64
2	3-Heptanone	114	C7H14O	000106-35-4	47
3	3,4-Hexanedione	114	C6H10O2	004437-51-8	47
4	3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	43
5	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	37





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RW-1A

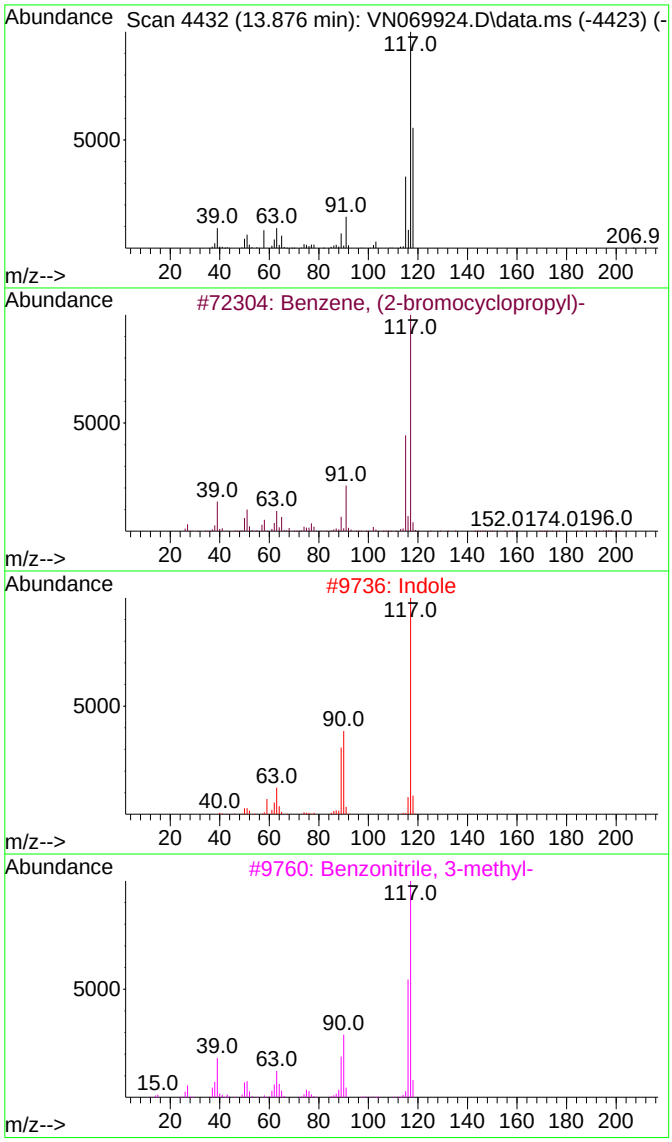
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

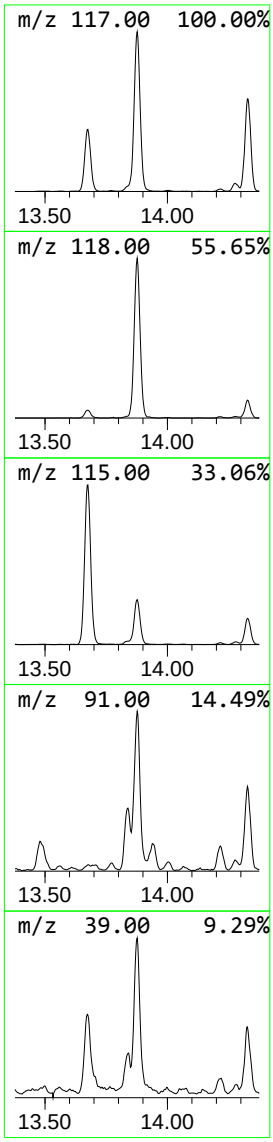
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, (2-bromocyclopropyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	10.50 ug/l	1503210	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	59
2	Indole	117	C8H7N	000120-72-9	50
3	Benzonitrile, 3-methyl-	117	C8H7N	000620-22-4	49
4	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	42
5	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	42





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RW-1A

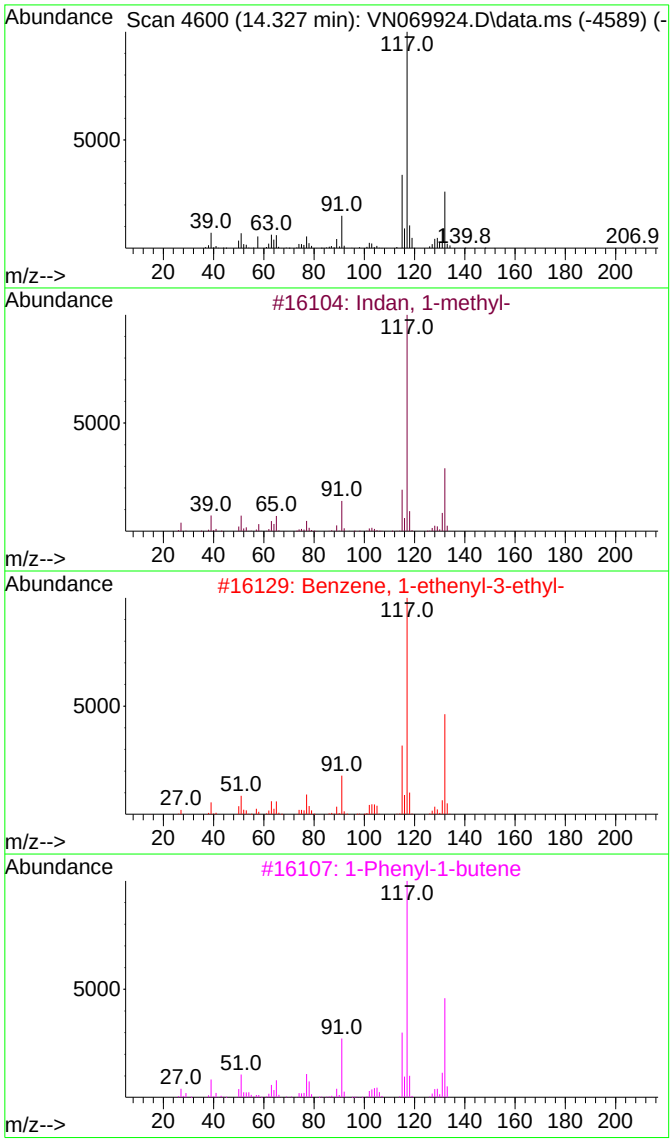
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

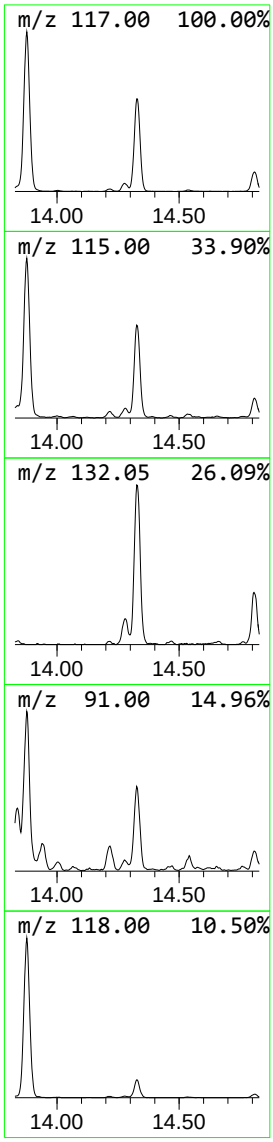
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indan, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	6.62 ug/l	946814	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	87
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	80
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	80
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069924.D
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Operator : JC/MD
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RW-1A

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methyl-	3.143	5.6	ug/l	429948	1	8.088	3869690	50.0
Cyclopentane, m...	7.147	7.4	ug/l	575809	1	8.088	3869690	50.0
2-Butanol, 2,3-...	10.199	8.9	ug/l	1077680	2	8.968	6055730	50.0
3-Pentanone, 2,...	11.127	6.3	ug/l	1099010	3	11.744	8779740	50.0
Benzene, (2-bro...	13.876	10.5	ug/l	1503210	4	13.675	7155770	50.0
Indan, 1-methyl-	14.327	6.6	ug/l	946814	4	13.675	7155770	50.0