LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010522\
Data File : VN070486.D
Acq On : 5 Jan 2022 13:49
Operator : JC/MD
Sample : M5257-01
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021

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\82N122721W.M
Title : SW846 8260

Signal : TIC: VN070486.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.231	77	90	136	rVB4	133373	486390	1.22%	0.205%
2	8.016	2219	2247	2258	rBV	692518	1679190	4.22%	0.708%
3	8.078	2259	2270	2307	rVB	1220653	2858612	7.19%	1.205%
4	8.432	2380	2402	2432	rBV2	846557	1936571	4.87%	0.816%
5	8.963	2579	2600	2637	rBV	2166490	4586331	11.54%	1.933%
6	10.440	3131	3151	3169	rBV	3629731	6911046	17.39%	2.913%
7	11.451	3516	3528	3537	rBV4	295898	522857	1.32%	0.220%
8	11.521	3538	3554	3580	rVB6	1103053	3169844	7.97%	1.336%
9	11.626	3580	3593	3616	rVB	1548697	2653019	6.67%	1.118%
10	11.744	3618	3637	3655	rBV	3900093	7435114	18.70%	3.134%
11	11.843	3657	3674	3694	rBV	4481131	8507676	21.40%	3.586%
12	11.948	3695	3713	3737	rBV2	19265678	39750527	100.00%	16.756%
13	12.092	3756	3767	3769	rBV3	354247	485241	1.22%	0.205%
14	12.176	3786	3798	3809	rVB3	1867094	3420544	8.61%	1.442%
15	12.253	3810	3827	3852	rBV5	5181026	17776345	44.72%	7.493%
16	12.366	3859	3869	3880	rVB	6545208	10510701	26.44%	4.431%
17	12.452	3880	3901	3903	rBV6	3726053	7451001	18.74%	3.141%
18	12.733	3996	4006	4012	rBV2	4106061	6575389	16.54%	2.772%
19	12.766	4013	4018	4028	rVB	3673597	4708516	11.85%	1.985%
20	12.897	4059	4067	4081	rVB4	4243617	7897445	19.87%	3.329%
21	12.978	4082	4097	4106	rBV7	2796871	6346598	15.97%	2.675%
22	13.047	4110	4123	4137	rVV3	19439197	35678409	89.76%	15.040%
23	13.195	4170	4178	4187	rBV	3349991	5096446	12.82%	2.148%
24	13.246	4188	4197	4202	rVV4	3531815	5797940	14.59%	2.444%
25	13.281	4203	4210	4224	rVB	10023228	15858259	39.89%	6.685%
26	13.409	4252	4258	4267	rVB	2332886	3071426	7.73%	1.295%
27	13.602	4325	4330	4338	rVB	2668215	3002898	7.55%	1.266%
28	13.672	4349	4356	4375	rVB3	5387673	9569979	24.08%	4.034%
29	13.742	4376	4382	4396	rVB2	1776301	2558714	6.44%	1.079%
30	13.991	4464	4475	4487	rBV2	5171528	8500431	21.38%	3.583%
31	14.319	4588	4597	4609	rVV5	493497	826315	2.08%	0.348%
32	14.380	4613	4620	4635	rVB10	388808	696877	1.75%	0.294%
33	14.844	4784	4793	4808	rVB3	321398	500576	1.26%	0.211%
34	14.914	4810	4819	4832	rBV3	198682	399405	1.00%	0.168%

Sum of corrected areas: 237226632

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021

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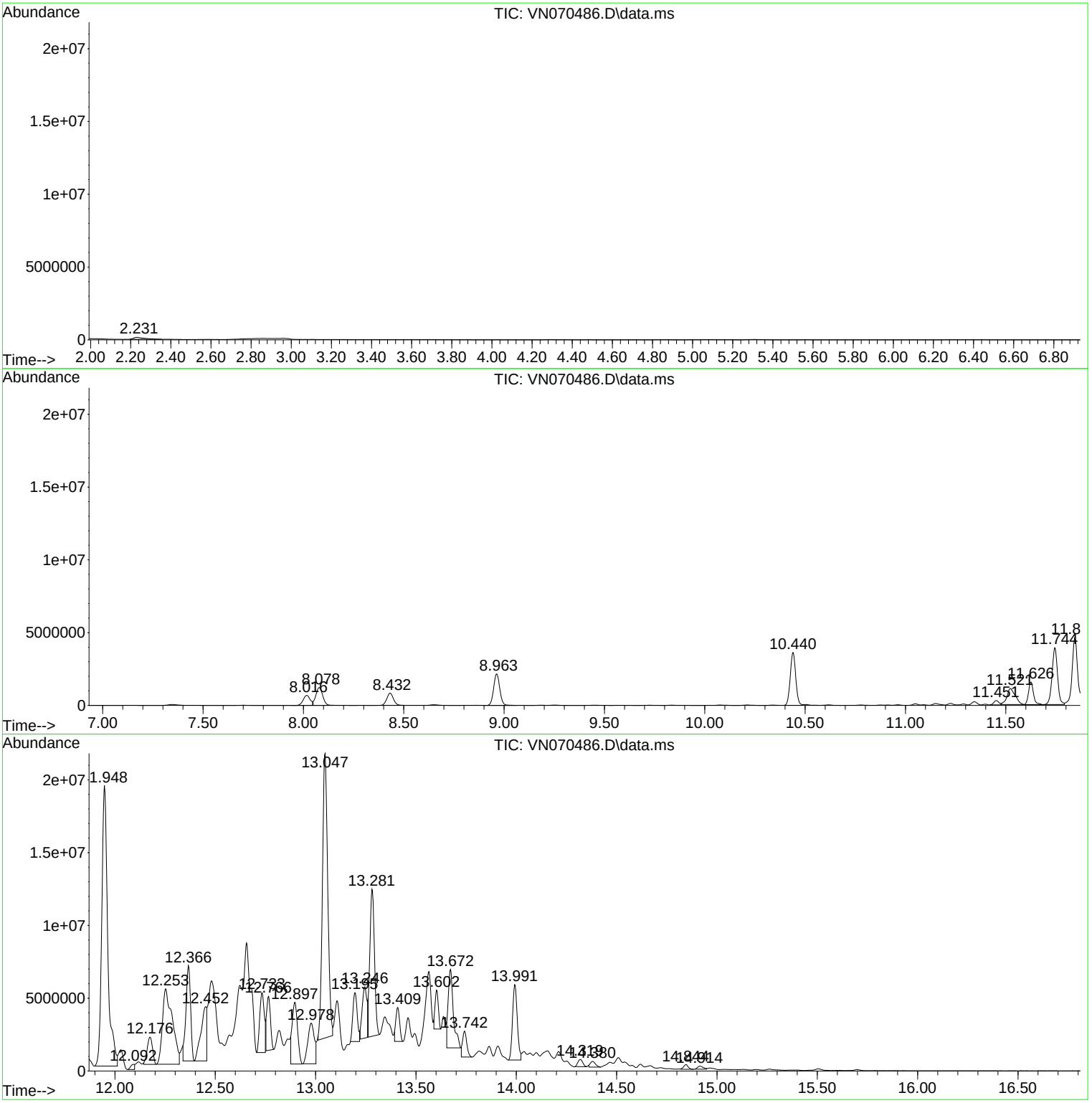
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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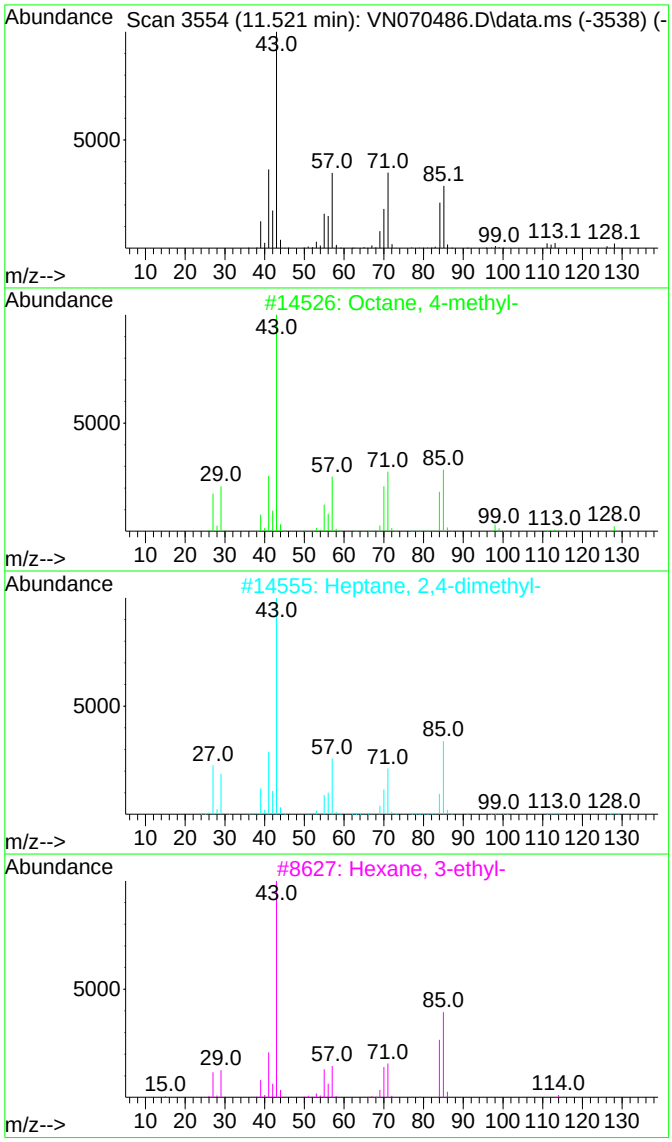
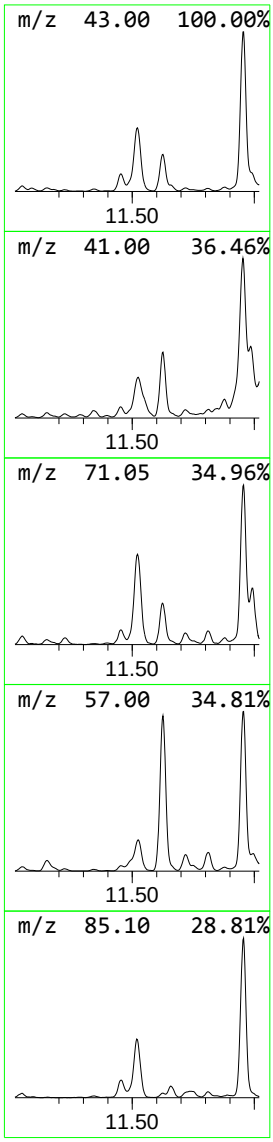
****
Peak Number 1 Octane, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.521	21.32 ug/l	3169840	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 4-methyl-	128	C9H20	002216-34-4	91
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
3	Hexane, 3-ethyl-	114	C8H18	000619-99-8	64
4	Heptane, 4-ethyl-	128	C9H20	002216-32-2	59
5	Octane	114	C8H18	000111-65-9	59





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Instrument :
MSVOA_N
ClientSampleId :
D3-12292021

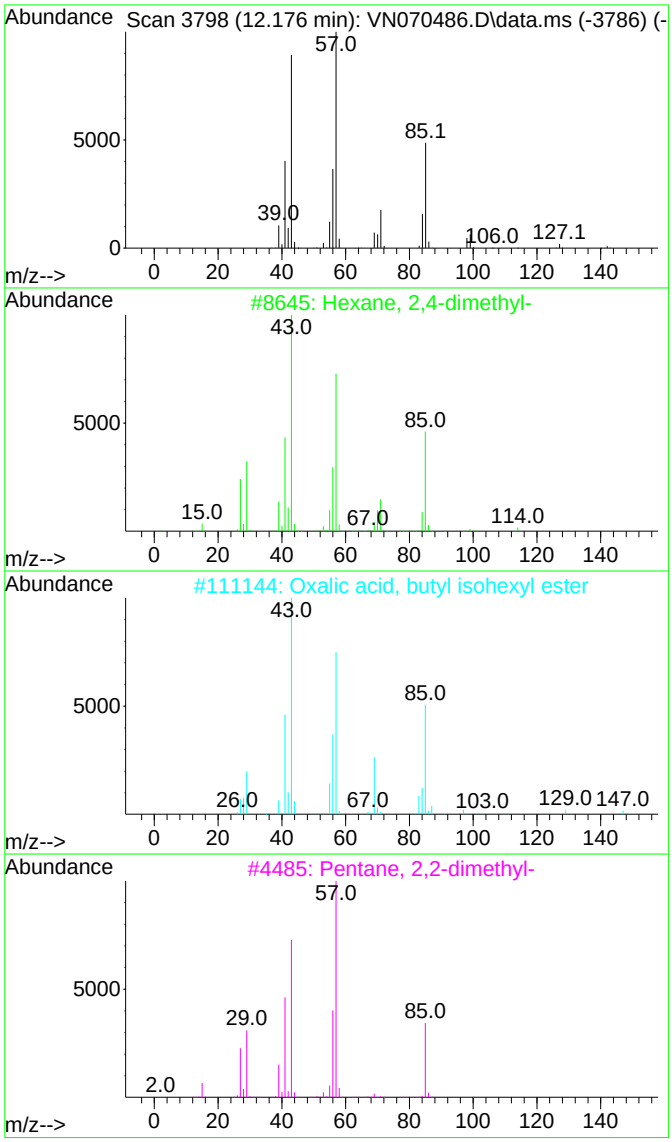
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

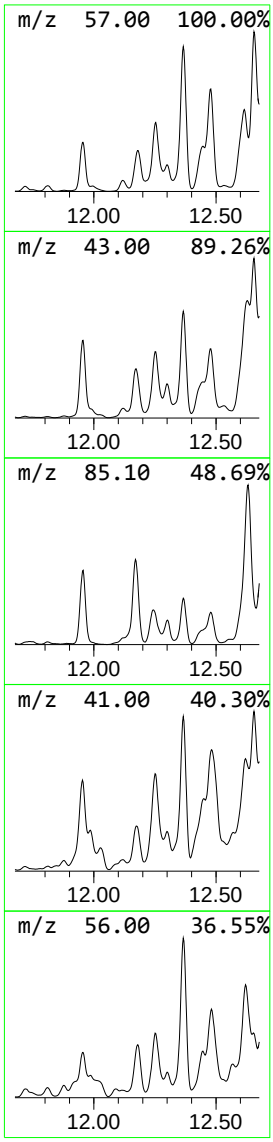
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexane, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.176	23.00 ug/l	3420540	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	78
2	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	59
3	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50
4	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	50
5	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	47





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Operator : JC/MD
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Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021

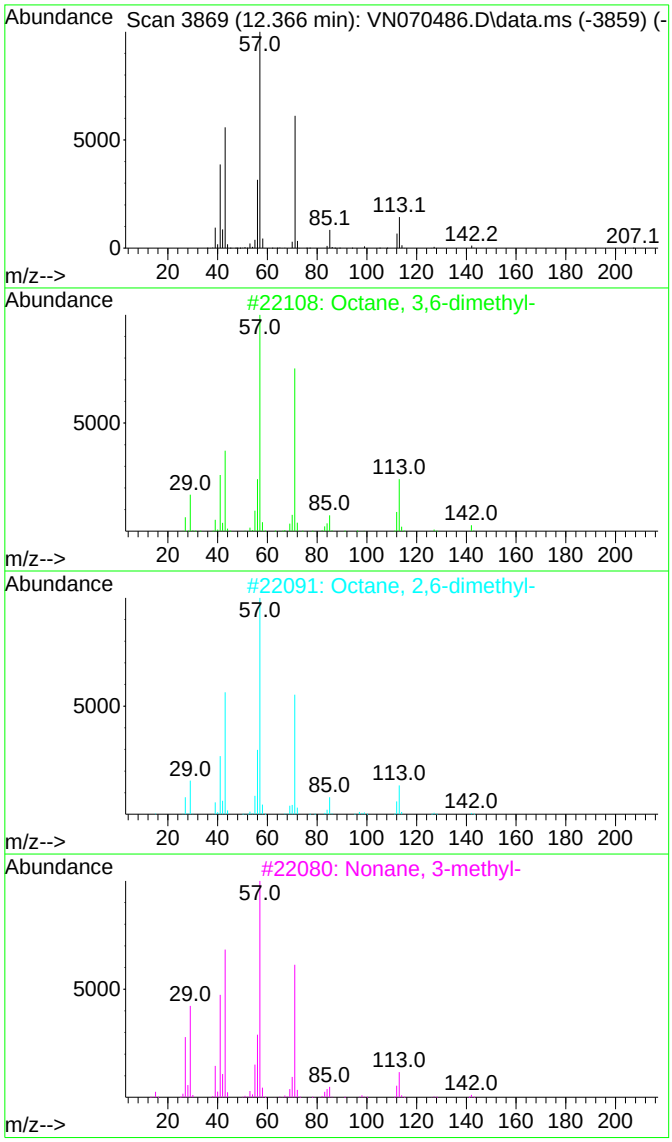
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

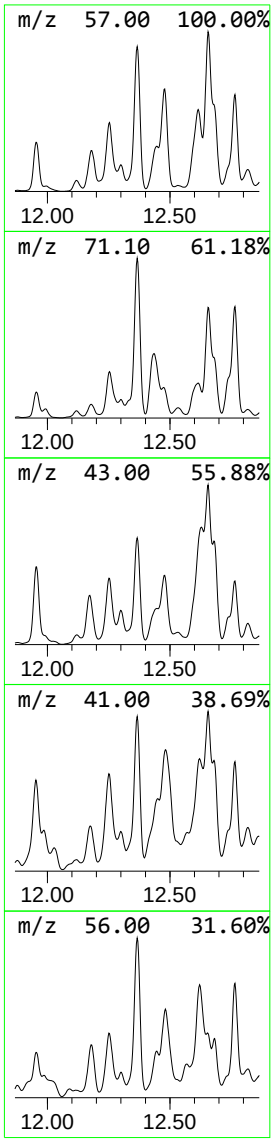
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Octane, 3,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.366	70.68 ug/l	10510700	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	91
4	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	59
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010522\
Data File : VN070486.D
Acq On : 5 Jan 2022 13:49
Operator : JC/MD
Sample : M5257-01
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021

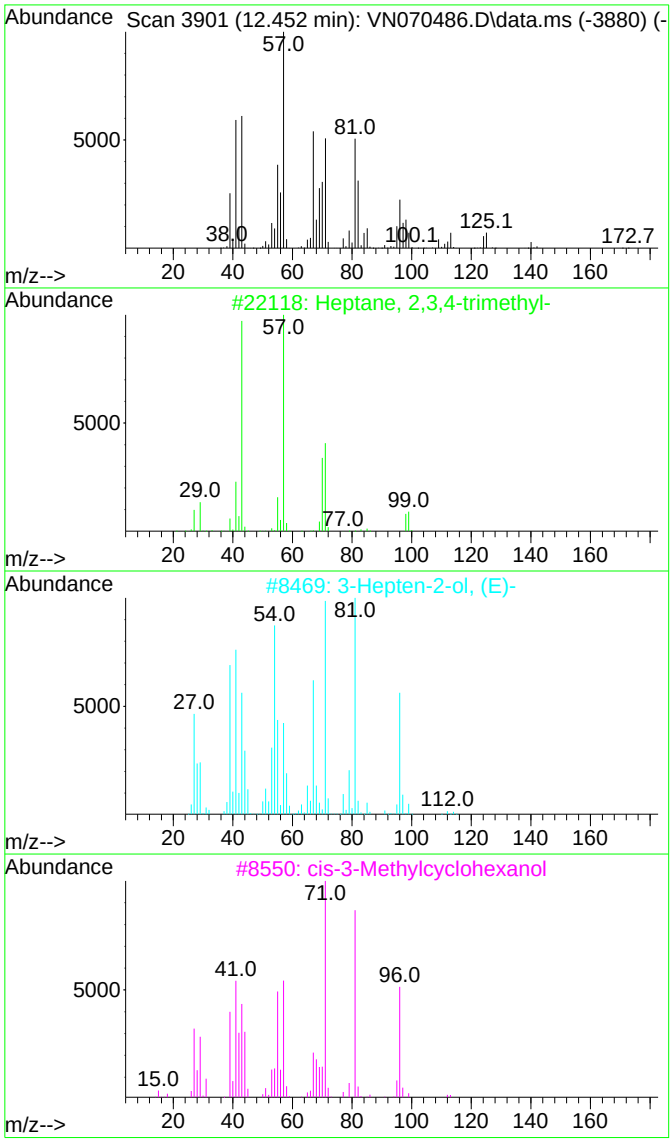
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

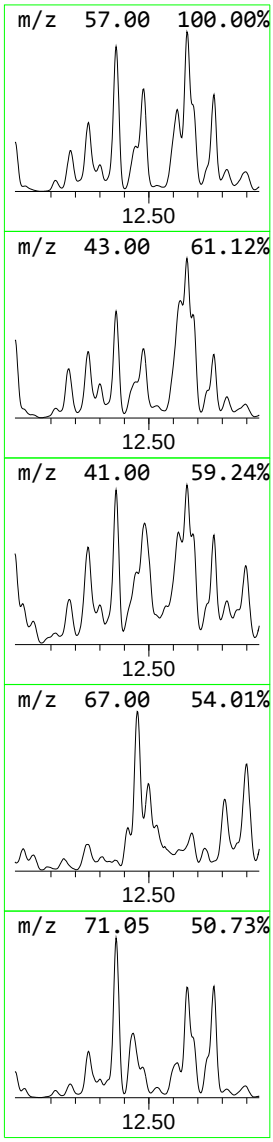
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown12.452 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.452	50.11 ug/l	7451000	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	35
2	3-Hepten-2-ol, (E)-	114	C7H14O	067077-39-8	30
3	cis-3-Methylcyclohexanol	114	C7H14O	005454-79-5	27
4	Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	27
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	27





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Operator : JC/MD
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Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021

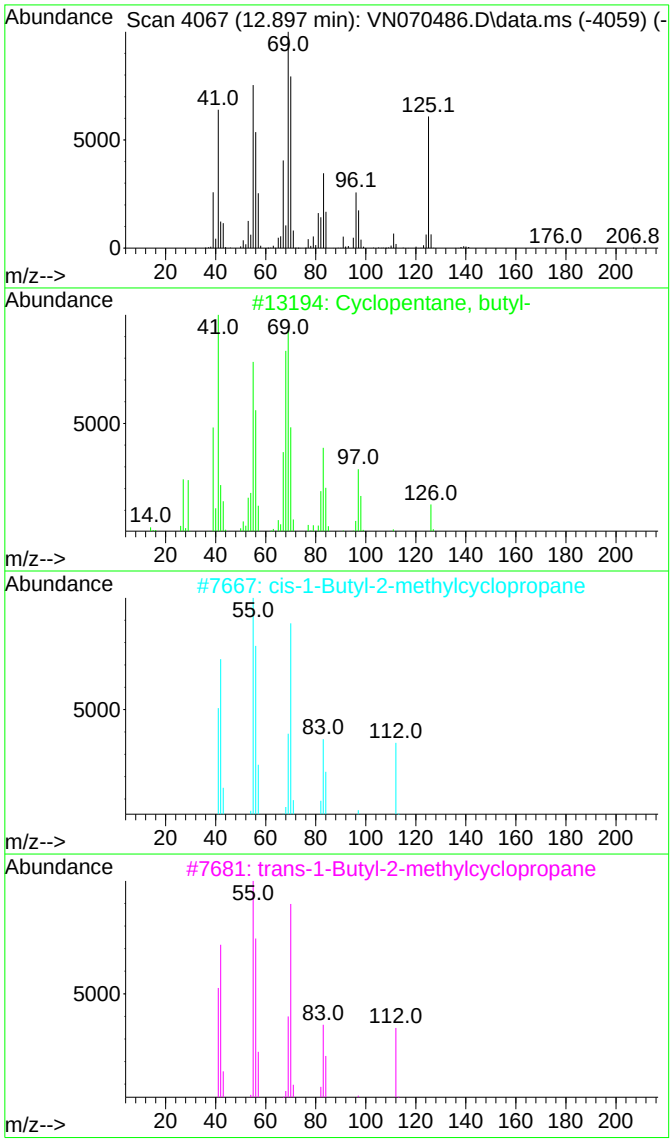
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

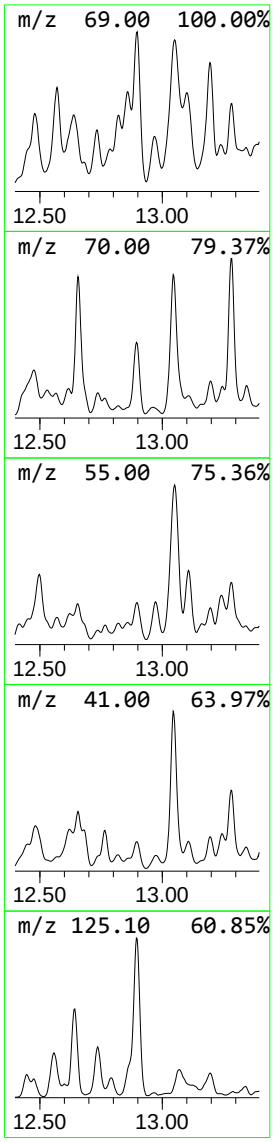
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.897	41.26 ug/l	7897450	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, butyl-	126	C9H18	002040-95-1	50
2	cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	50
3	trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	43
4	4-Nonene, 5-methyl-	140	C10H20	015918-07-7	43
5	Cycloheptanone, 3-methyl-, (R)-	126	C8H14O	013609-58-0	38





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Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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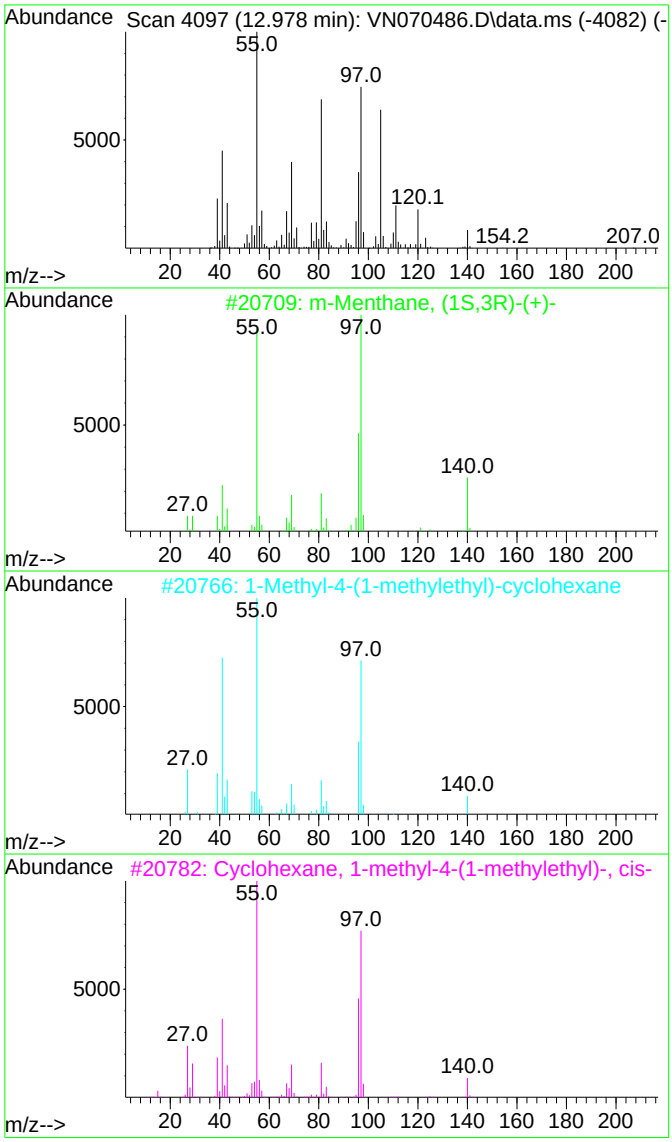
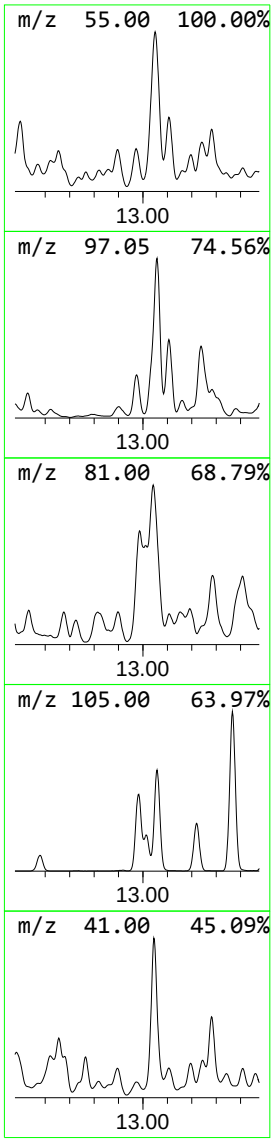
****
Peak Number 6 m-Menthane, (1S,3R)-(+)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.977	33.16 ug/l	6346600	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Menthane, (1S,3R)-(+)-	140	C10H20	013837-66-6	64
2	1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	62
3	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	62
4	m-Menthane, (1S,3S)-(+)-	140	C10H20	013837-67-7	58
5	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	58





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021

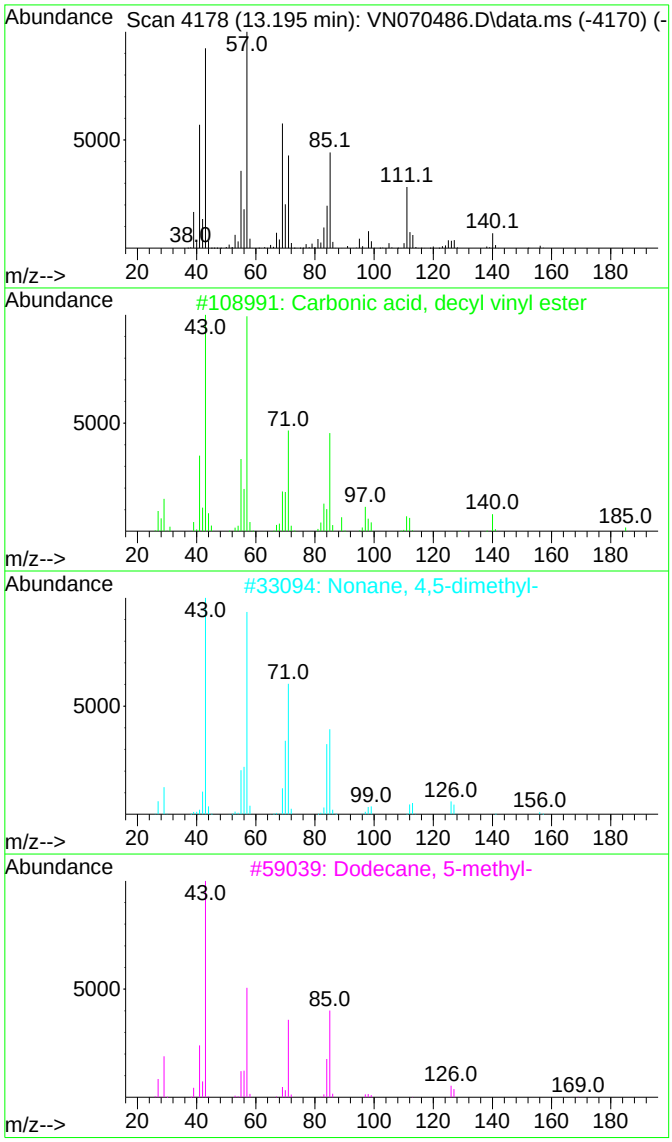
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

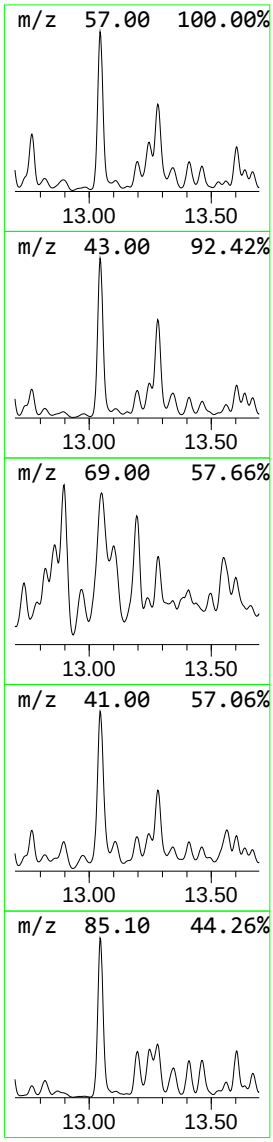
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Carbonic acid, decyl vinyl ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.195	26.63 ug/l	5096450	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, decyl vinyl ester	228	C13H24O3	1000383-25-7	64
2	Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	58
3	Dodecane, 5-methyl-	184	C13H28	017453-93-9	50
4	Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	50
5	Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	47





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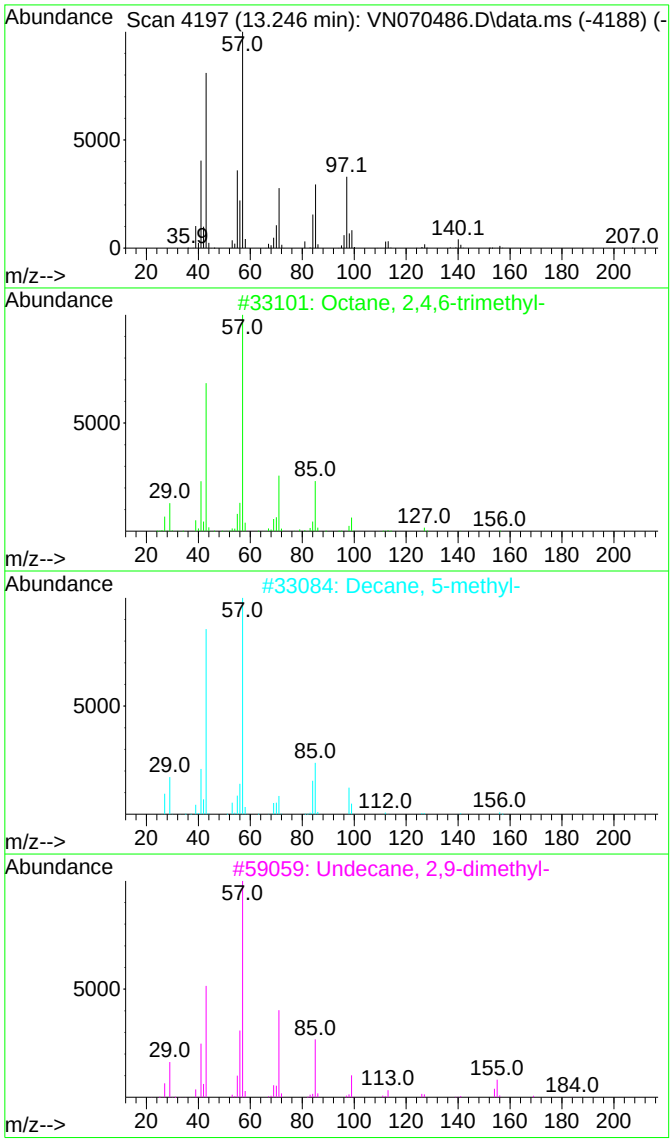
Quant Title : SW846 8260

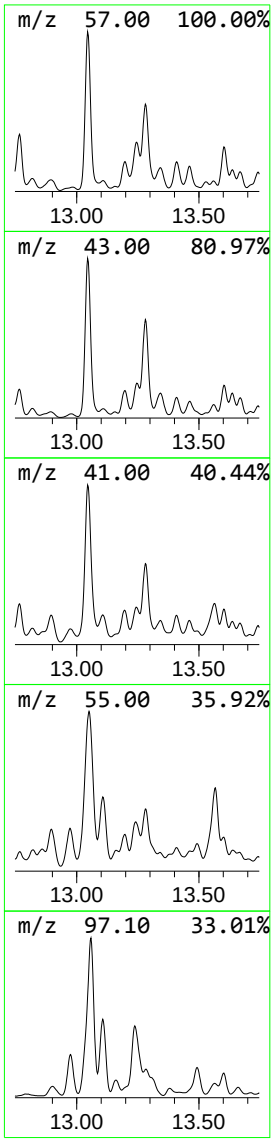
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Octane, 2,4,6-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.246	30.29 ug/l	5797940	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	50
2	Decane, 5-methyl-	156	C11H24	013151-35-4	49
3	Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	47
4	Propyl triacontyl ether	481	C33H68O	1000406-28-6	47
5	Tetradecane, 5-methyl-	212	C15H32	025117-32-2	47





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Data File : VN070486.D
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Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

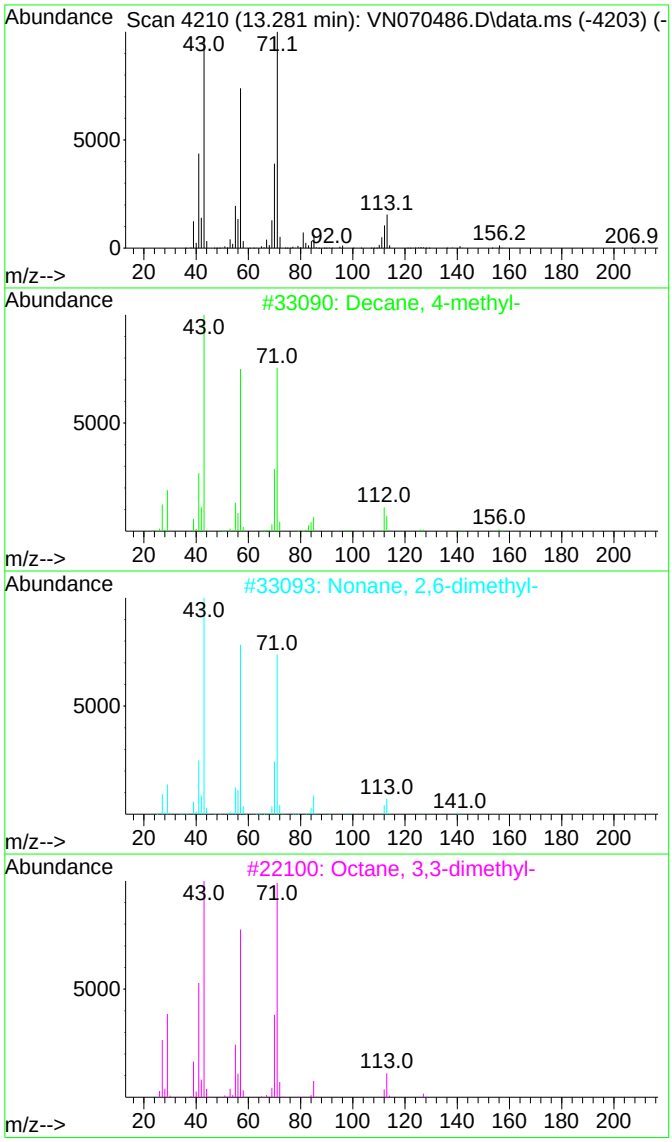
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

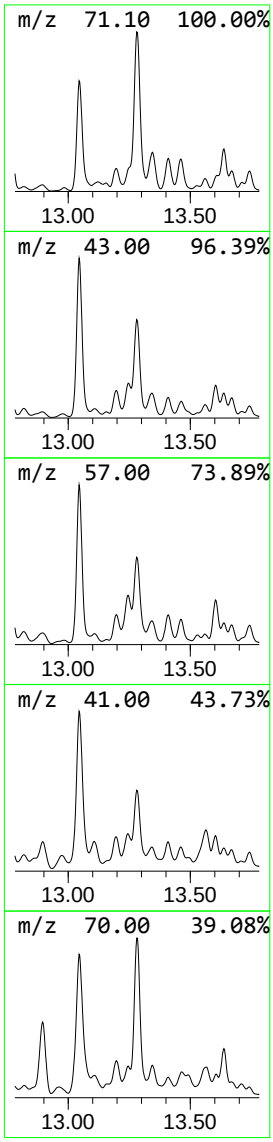
****

Peak Number 9 unknown13.281 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.281	82.85 ug/l	15858300	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 4-methyl-	156	C11H24	002847-72-5	90
2	Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	87
3	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	72
4	4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	64
5	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010522\
Data File : VN070486.D
Acq On : 5 Jan 2022 13:49
Operator : JC/MD
Sample : M5257-01
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

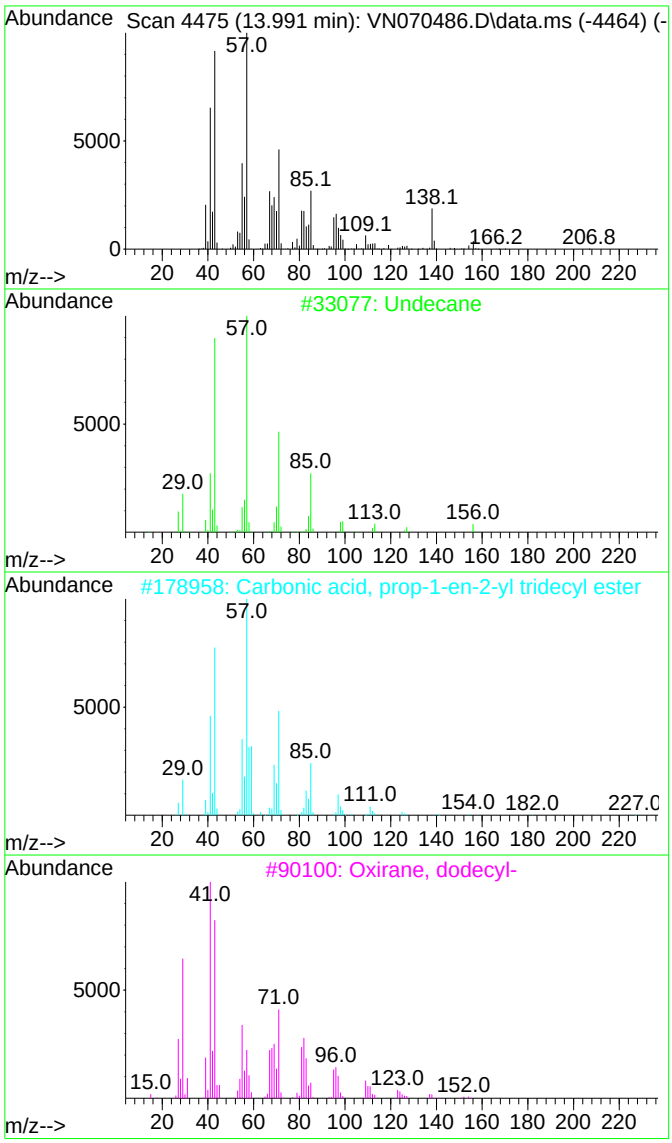
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

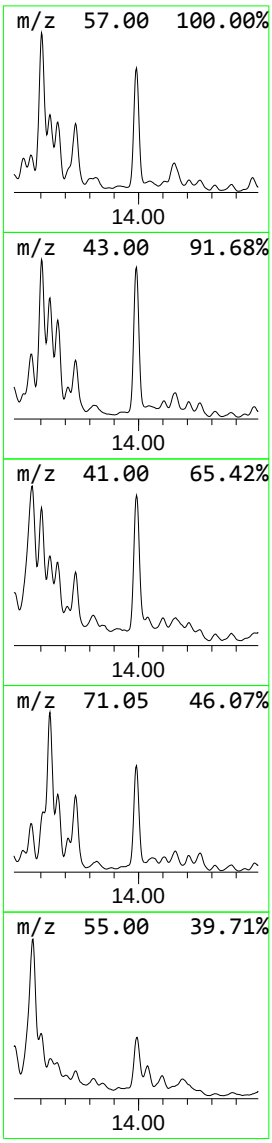
****

Peak Number 10 unknown13.991 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.991	44.41 ug/l	8500430	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	46
2	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	45
3	Oxirane, dodecyl-	212	C14H28O	003234-28-4	43
4	Cyclononanone, 2-hydroxy-	156	C9H16O2	000496-83-3	43
5	Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010522\
Data File : VN070486.D
Acq On : 5 Jan 2022 13:49
Operator : JC/MD
Sample : M5257-01
Misc : 4.99g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
D3-12292021

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.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
Octane, 4-methyl-	11.521	21.3	ug/l	3169840	3	11.744	7435110	50.0
Hexane, 2,4-dim...	12.176	23.0	ug/l	3420540	3	11.744	7435110	50.0
Octane, 3,6-dim...	12.366	70.7	ug/l	10510700	3	11.744	7435110	50.0
unknown12.452	12.452	50.1	ug/l	7451000	3	11.744	7435110	50.0
Cyclopentane, b...	12.897	41.3	ug/l	7897450	4	13.672	9569980	50.0
m-Menthane, (1S...	12.977	33.2	ug/l	6346600	4	13.672	9569980	50.0
Carbonic acid, ...	13.195	26.6	ug/l	5096450	4	13.672	9569980	50.0
Octane, 2,4,6-t...	13.246	30.3	ug/l	5797940	4	13.672	9569980	50.0
unknown13.281	13.281	82.8	ug/l	15858300	4	13.672	9569980	50.0
unknown13.991	13.991	44.4	ug/l	8500430	4	13.672	9569980	50.0