LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068555.D
Acq On : 18 Sep 2021 7:19
Operator : JC/MD
Sample : M3798-08
Misc : 6.04g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : NAPL-06-(8-10)-END-POINT

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\82N090721W.M
Title : SW846 8260

Signal : TIC: VN068555.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	10.443	3134	3152	3187	rBV2	1957365	4218010	1.57%	0.259%
2	11.349	3479	3490	3502	rVB	1849233	3250787	1.21%	0.200%
3	11.457	3519	3530	3539	rBV2	1996231	3378171	1.26%	0.208%
4	11.526	3540	3556	3583	rVB5	4867691	15974827	5.95%	0.982%
5	11.631	3583	3595	3618	rVB	7119208	11736087	4.37%	0.721%
6	11.746	3619	3638	3656	rBV2	1669449	4460820	1.66%	0.274%
7	11.848	3657	3676	3680	rBV3	1281360	2744229	1.02%	0.169%
8	11.883	3681	3689	3697	rVB	2687539	3570559	1.33%	0.219%
9	11.961	3698	3718	3724	rBV4	21655973	44442806	16.55%	2.731%
10	12.036	3740	3746	3758	rVB2	8848028	13678031	5.09%	0.840%
11	12.181	3788	3800	3812	rVB4	9078711	16752392	6.24%	1.029%
12	12.259	3812	3829	3843	rBV4	34077191	76636141	28.54%	4.709%
13	12.374	3863	3872	3882	rVB	29522056	43970678	16.37%	2.702%
14	12.457	3882	3903	3907	rBV6	23736518	52260958	19.46%	3.211%
15	12.664	3976	3980	3999	rVB2	44728059	81543768	30.36%	5.011%
16	12.741	4000	4009	4015	rBV5	10718488	16941672	6.31%	1.041%
17	12.774	4016	4021	4030	rVB	13122355	16696131	6.22%	1.026%
18	12.905	4062	4070	4086	rVB4	31005261	66118076	24.62%	4.063%
19	12.988	4087	4101	4109	rBV6	59389121	108600539	40.44%	6.673%
20	13.061	4118	4128	4141	rVB8	137990626	268552979	100.00%	16.501%
21	13.117	4142	4149	4161	rVB4	28740167	45454270	16.93%	2.793%
22	13.205	4173	4182	4190	rBV3	20858637	32895342	12.25%	2.021%
23	13.291	4207	4214	4230	rVB2	40660145	61019861	22.72%	3.749%
24	13.374	4233	4245	4257	rBV3	99858466	181915781	67.74%	11.178%
25	13.567	4305	4317	4327	rBV4	50908819	92582492	34.47%	5.689%
26	13.613	4328	4334	4351	rVB3	21448821	36450349	13.57%	2.240%
27	13.710	4361	4370	4381	rVB2	49588670	77553596	28.88%	4.765%
28	13.871	4423	4430	4438	rBV3	20687925	27184650	10.12%	1.670%
29	13.913	4439	4446	4467	rVB5	31607920	62131938	23.14%	3.818%
30	13.999	4467	4478	4490	rBV4	32915516	55689929	20.74%	3.422%
31	14.133	4521	4528	4533	rBV	7774224	10534568	3.92%	0.647%
32	14.219	4551	4560	4572	rVB	14906626	22969050	8.55%	1.411%
33	14.324	4589	4599	4611	rVB5	11103536	18707065	6.97%	1.149%
34	14.383	4612	4621	4637	rVB7	4425189	9468458	3.53%	0.582%
35	14.463	4640	4651	4660	rBV3	4756153	7974092	2.97%	0.490%
36	14.512	4662	4669	4674	rBV3	3755253	5236693	1.95%	0.322%

LSC Area Percent Report

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ALS Vial : 49 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : NAPL-06-(8-10)-END-POINT

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\82N090721W.M
Title : SW846 8260

37	14.579	4689	4694	4703	rVB	5248352	6868995	2.56%	0.422%
38	14.624	4703	4711	4718	rBV2	3033377	3976794	1.48%	0.244%
39	14.852	4790	4796	4807	rVB2	2307093	3502322	1.30%	0.215%
40	14.914	4808	4819	4837	rBV4	4496750	9812593	3.65%	0.603%

Sum of corrected areas: 1627456499

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068555.D
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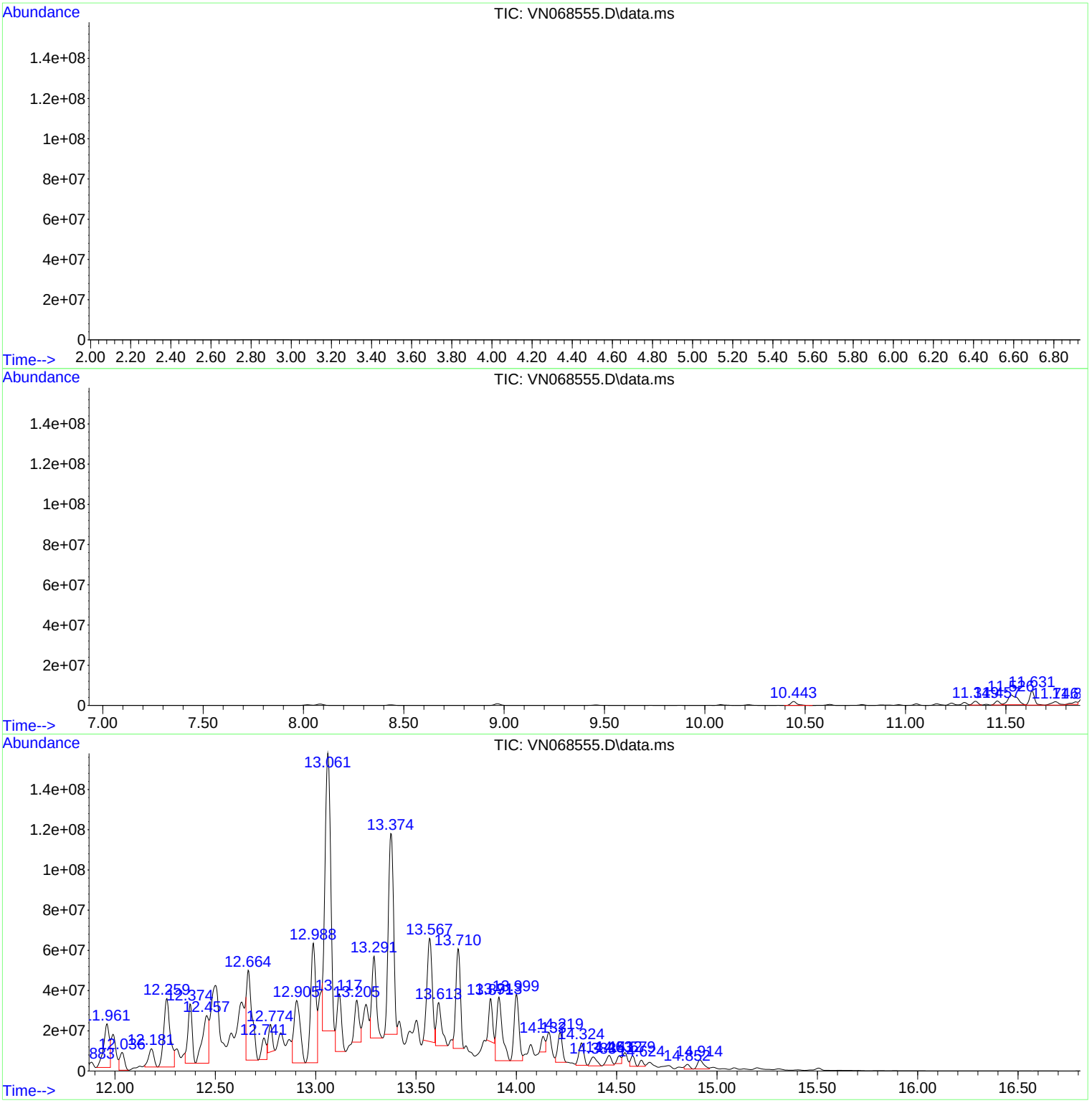
Operator : JC/MD
Sample : M3798-08
Misc : 6.04g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(8-10)-END-POINT

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068555.D
Acq On : 18 Sep 2021 7:19
Operator : JC/MD
Sample : M3798-08
Misc : 6.04g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(8-10)-END-POINT

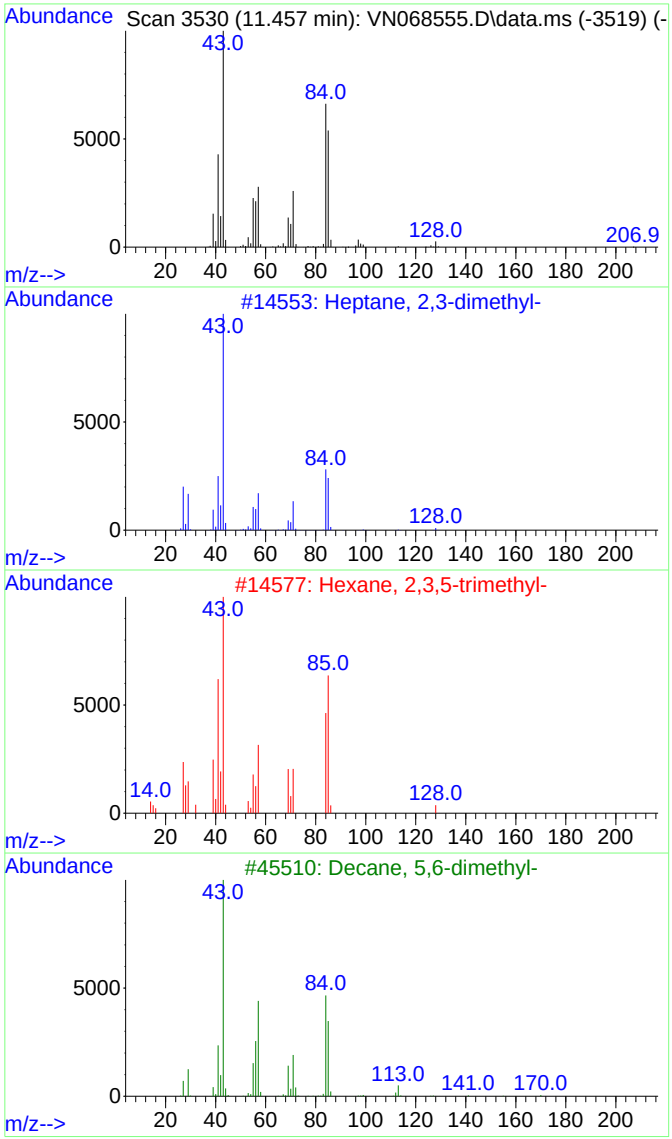
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

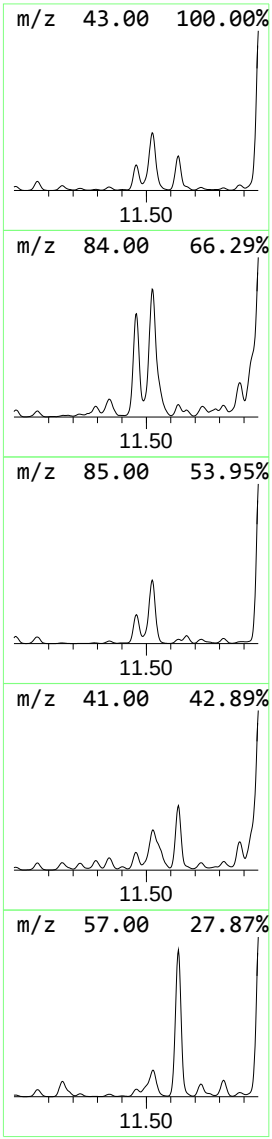
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Heptane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.457	37.86 ug/l	3378170	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	94
2	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	70
3	Decane, 5,6-dimethyl-	170	C12H26	001636-43-7	59
4	Hexane, 3-ethyl-	114	C8H18	000619-99-8	59
5	Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068555.D
Acq On : 18 Sep 2021 7:19
Operator : JC/MD
Sample : M3798-08
Misc : 6.04g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(8-10)-END-POINT

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

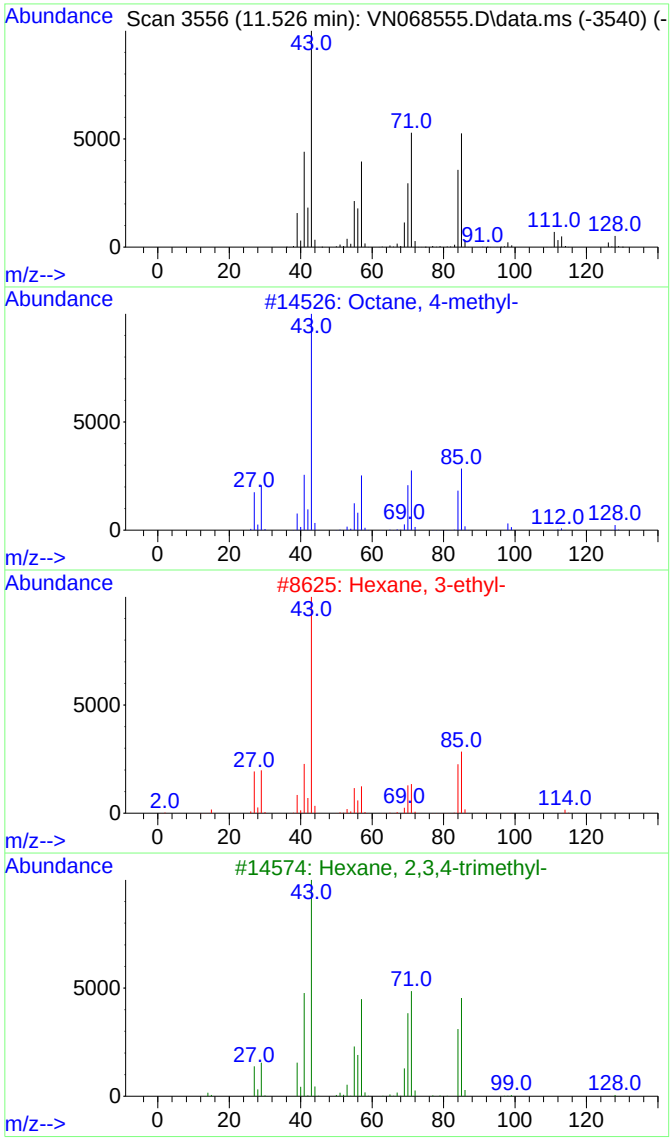
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

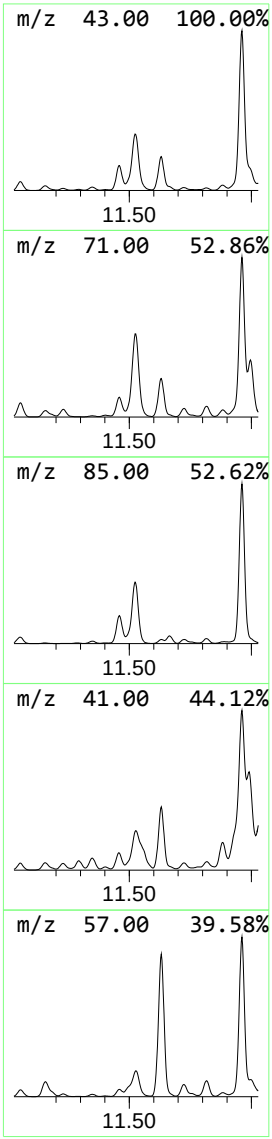
****

Peak Number 2 Octane, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.527	179.06 ug/l	15974800	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 4-methyl-	128	C9H20	002216-34-4	87
2	Hexane, 3-ethyl-	114	C8H18	000619-99-8	68
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
4	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068555.D
Acq On : 18 Sep 2021 7:19
Operator : JC/MD
Sample : M3798-08
Misc : 6.04g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(8-10)-END-POINT

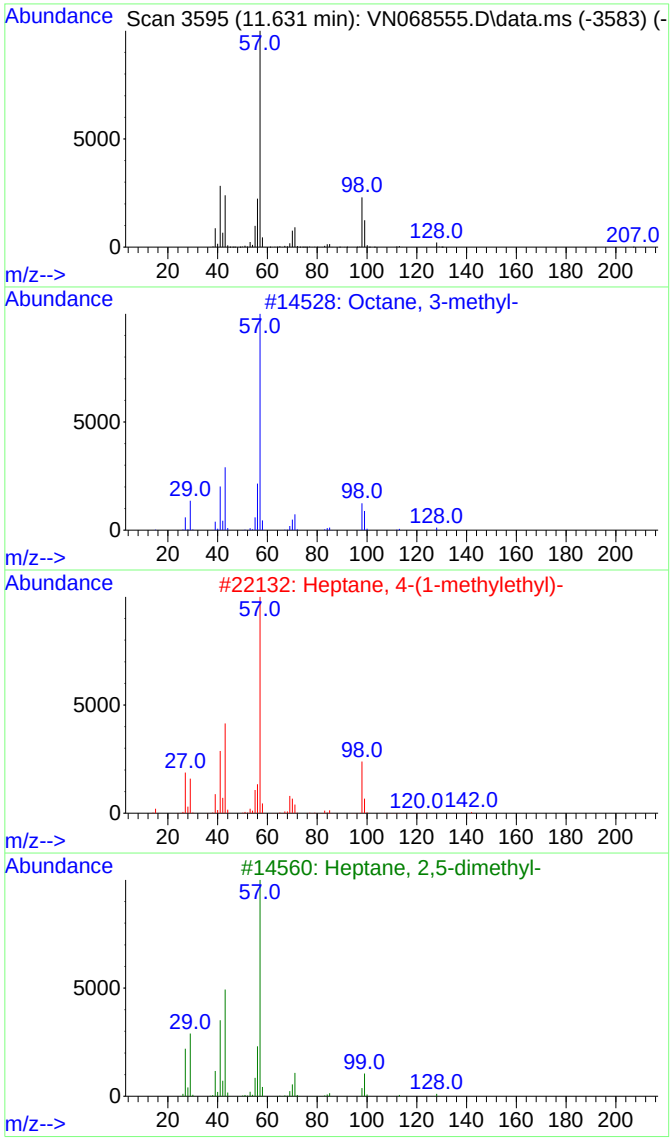
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

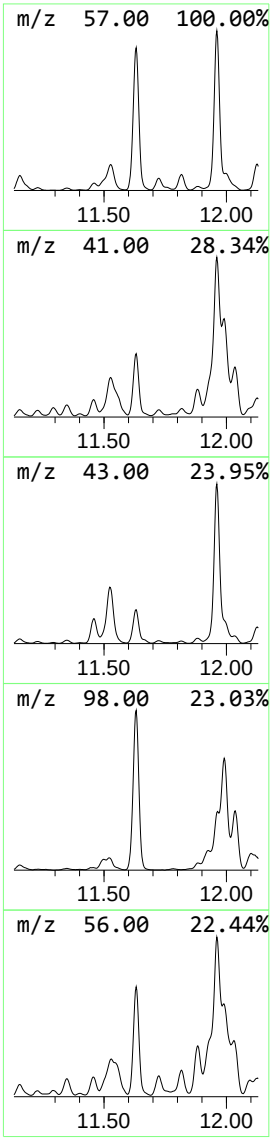
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Octane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.631	131.55 ug/l	11736100	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-	128	C9H20	002216-33-3	87
2	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	72
3	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	58
4	Heptane, 4-propyl-	142	C10H22	003178-29-8	53
5	Undecane, 6-methyl-	170	C12H26	017302-33-9	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068555.D
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Operator : JC/MD
Sample : M3798-08
Misc : 6.04g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(8-10)-END-POINT

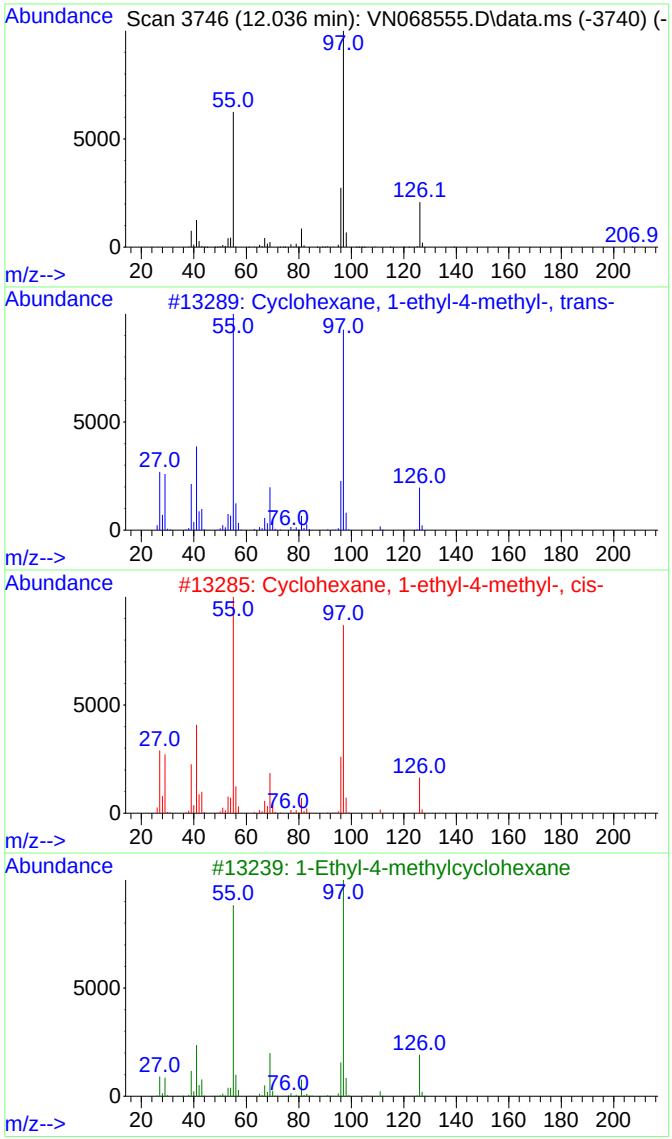
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

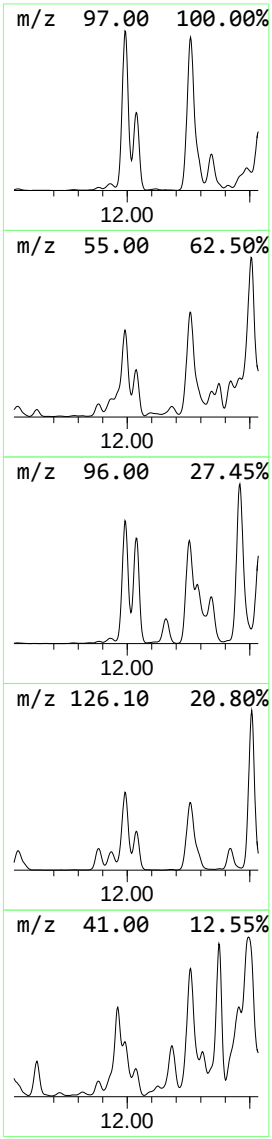
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.036	153.31 ug/l	13678000	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	90
2	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	83
3	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	78
4	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	72
5	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068555.D
Acq On : 18 Sep 2021 7:19
Operator : JC/MD
Sample : M3798-08
Misc : 6.04g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(8-10)-END-POINT

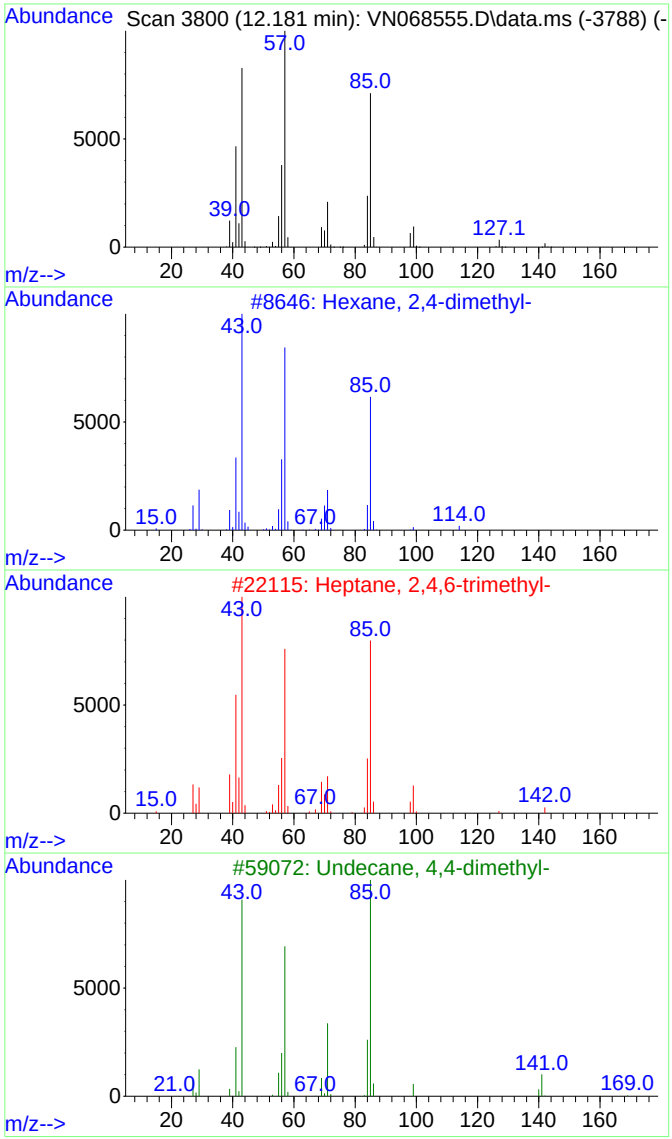
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

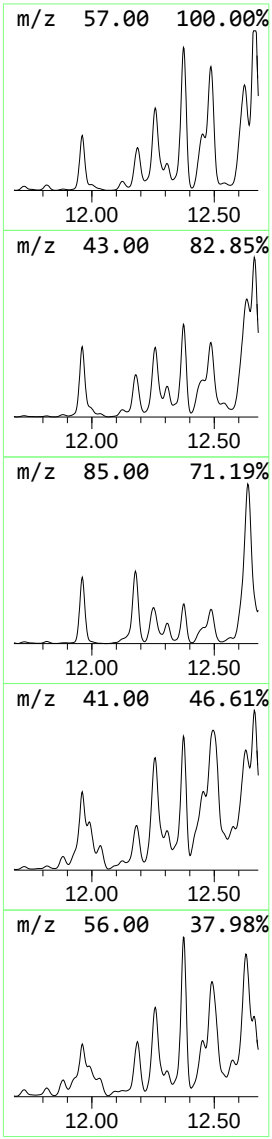
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexane, 2,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.181	187.77 ug/l	16752400	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
2	Heptane, 2,4,6-trimethyl-	142	C10H22	002613-61-8	68
3	Undecane, 4,4-dimethyl-	184	C13H28	017312-68-4	64
4	Sulfurous acid, butyl hexyl ester	222	C10H22O3S	1000309-17-3	53
5	Sulfurous acid, butyl isohexyl e...	222	C10H22O3S	1000309-17-2	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
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Operator : JC/MD
Sample : M3798-08
Misc : 6.04g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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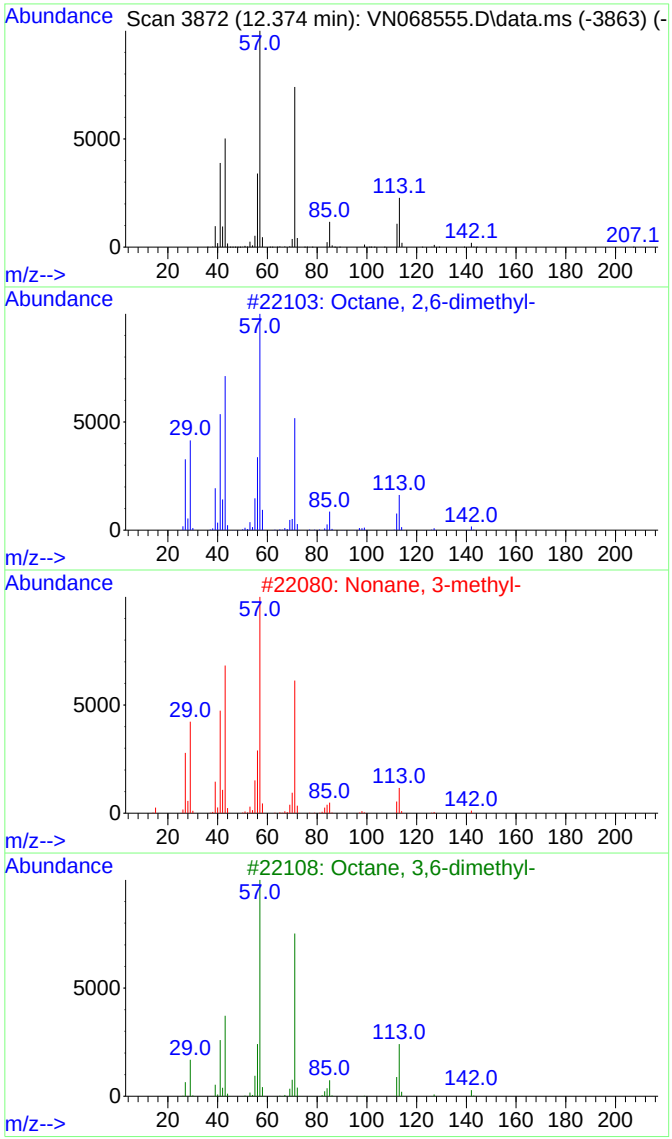
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

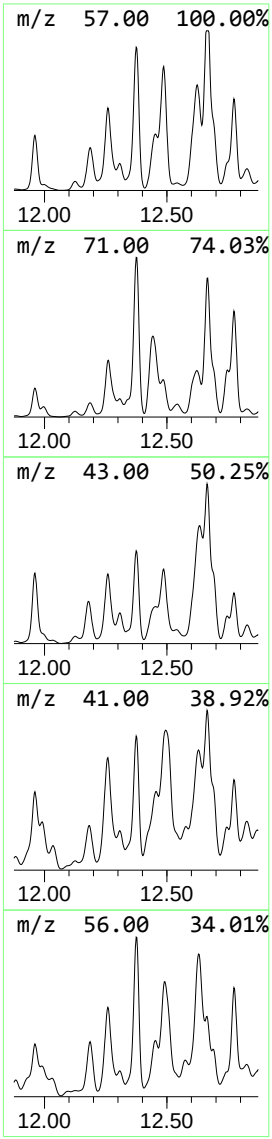
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.374	492.85 ug/l	43970700	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	90
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	90
4	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	72
5	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	59





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ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(8-10)-END-POINT

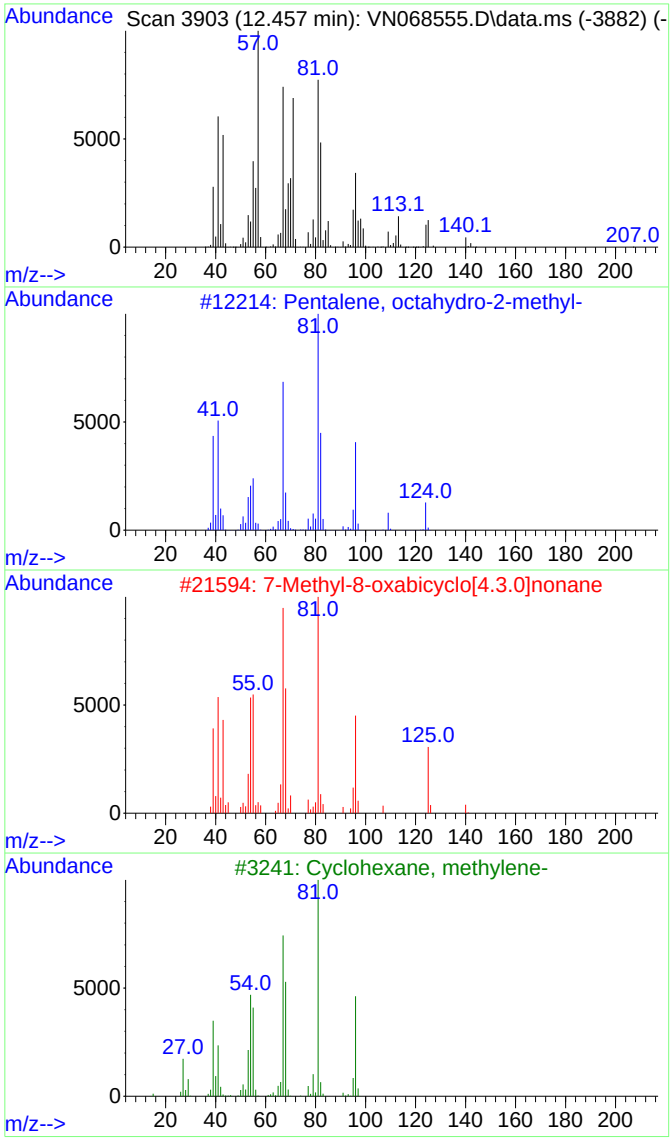
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

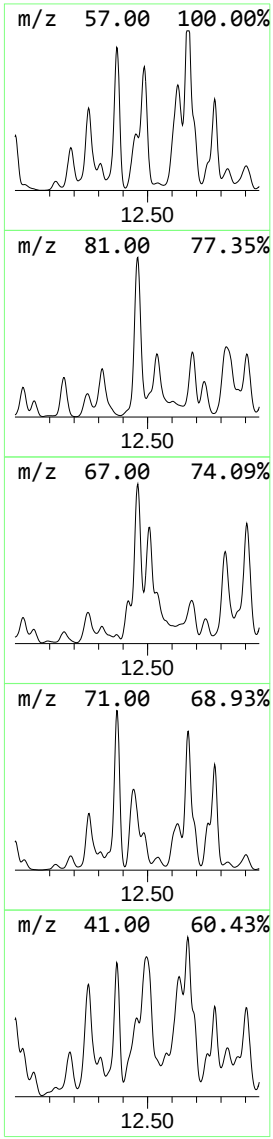
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentalene, octahydro-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	585.78 ug/l	52261000	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	55
2	7-Methyl-8-oxabicyclo[4.3.0]nonane	140	C9H16O	1000216-87-6	49
3	Cyclohexane, methylene-	96	C7H12	001192-37-6	49
4	3-Hepten-2-ol, (E)-	114	C7H14O	067077-39-8	46
5	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068555.D
Acq On : 18 Sep 2021 7:19
Operator : JC/MD
Sample : M3798-08
Misc : 6.04g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(8-10)-END-POINT

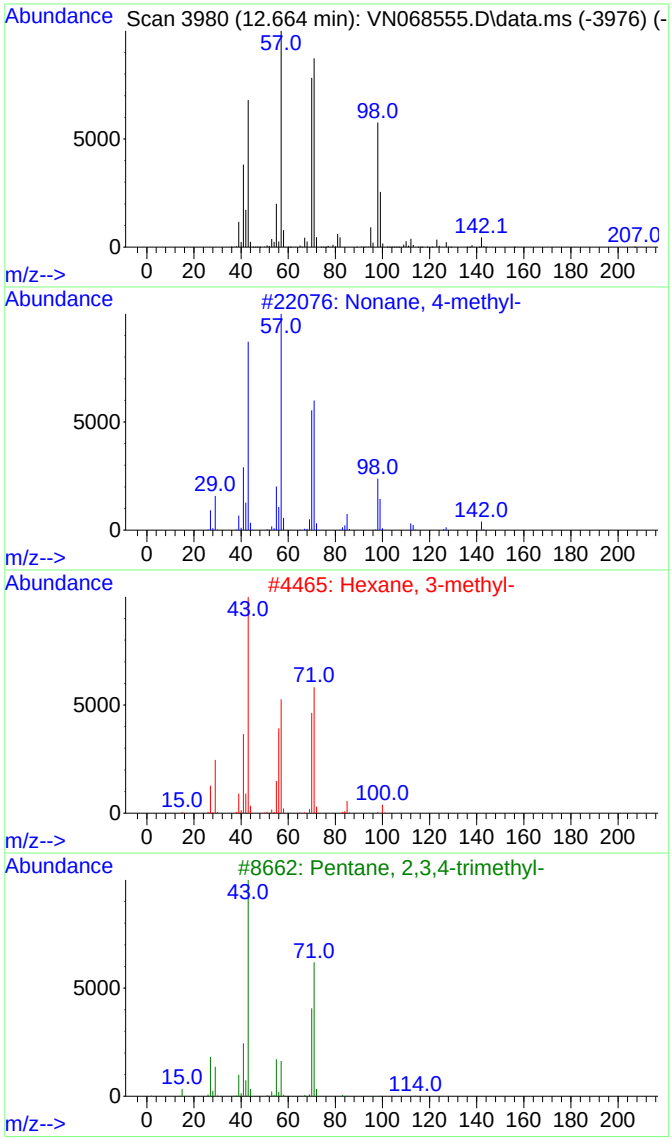
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

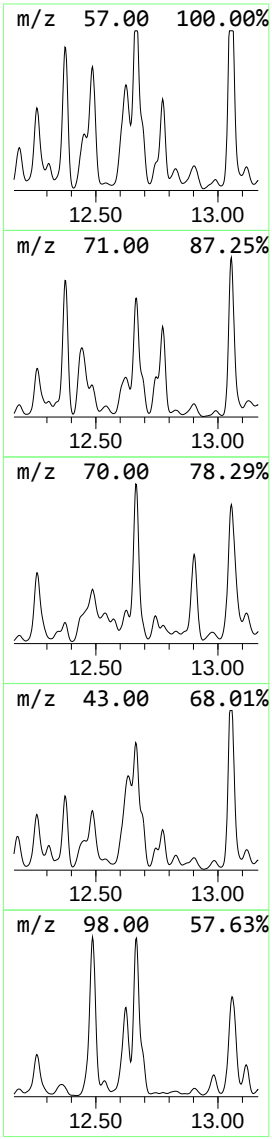
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Nonane, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.664	914.00 ug/l	81543800	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	64
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	50
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	50
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068555.D
Acq On : 18 Sep 2021 7:19
Operator : JC/MD
Sample : M3798-08
Misc : 6.04g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(8-10)-END-POINT

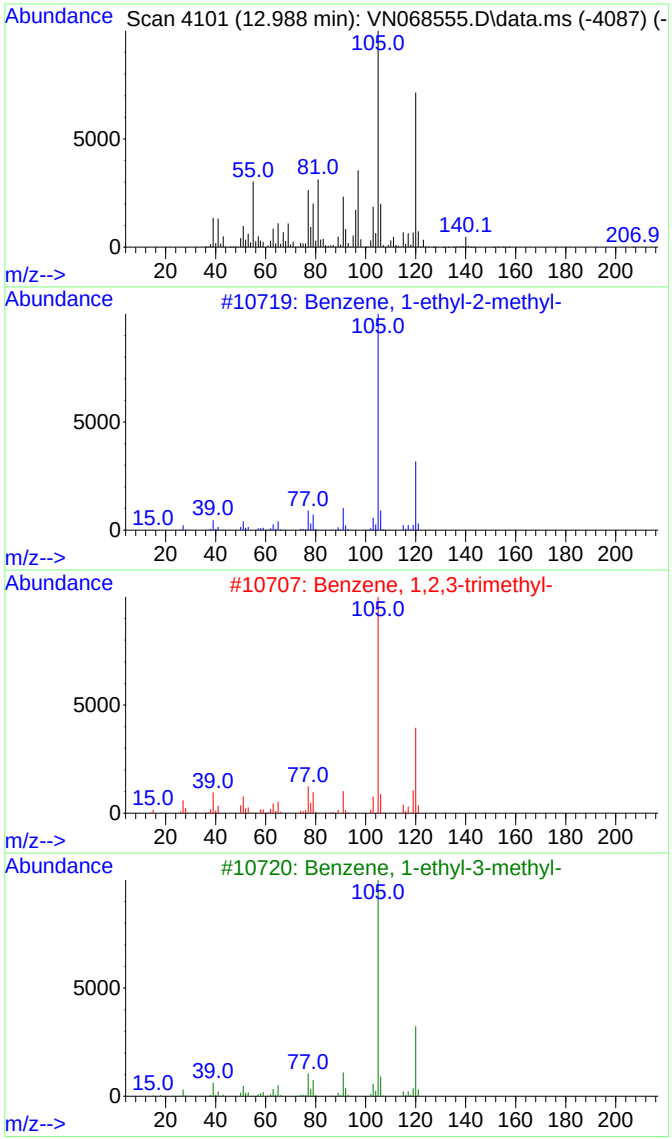
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

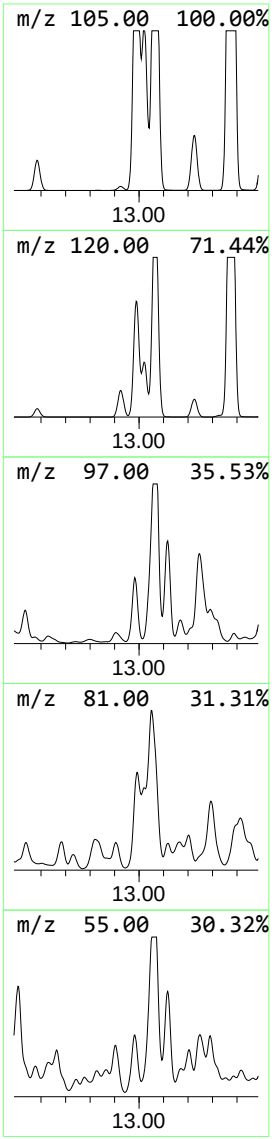
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.988	70.02 ug/l	108601000	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	83
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	64
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	64
4	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	52
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068555.D
Acq On : 18 Sep 2021 7:19
Operator : JC/MD
Sample : M3798-08
Misc : 6.04g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-06-(8-10)-END-POINT

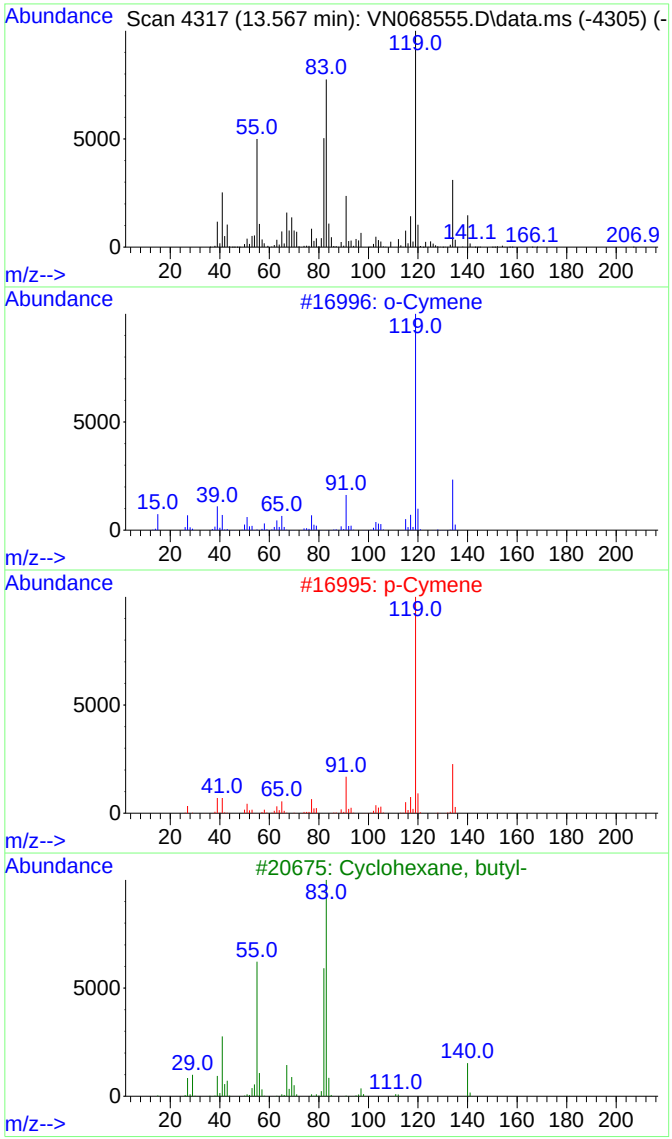
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

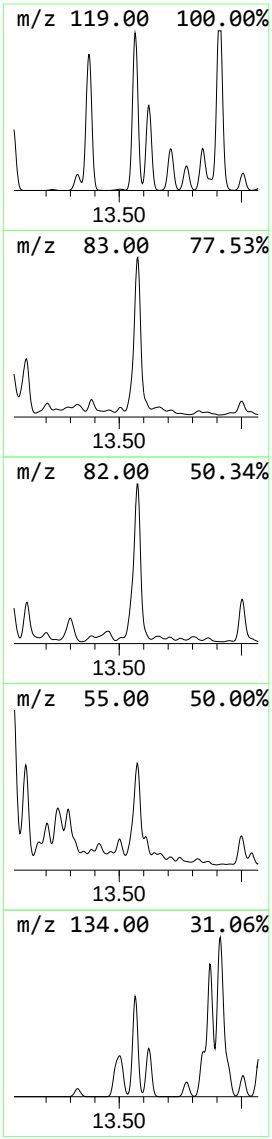
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.568	59.69 ug/l	92582500	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	89
2	p-Cymene	134	C10H14	000099-87-6	89
3	Cyclohexane, butyl-	140	C10H20	001678-93-9	86
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	86
5	Cyclohexane, propyl-	126	C9H18	001678-92-8	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068555.D
Acq On : 18 Sep 2021 7:19
Operator : JC/MD
Sample : M3798-08
Misc : 6.04g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 49 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : NAPL-06-(8-10)-END-POINT

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.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
Heptane, 2,3-di...	11.457	37.9	ug/l	3378170	3	11.749	4460820	50.0
Octane, 4-methyl-	11.527	179.1	ug/l	15974800	3	11.749	4460820	50.0
Octane, 3-methyl-	11.631	131.6	ug/l	11736100	3	11.749	4460820	50.0
Cyclohexane, 1-...	12.036	153.3	ug/l	13678000	3	11.749	4460820	50.0
Hexane, 2,4-dim...	12.181	187.8	ug/l	16752400	3	11.749	4460820	50.0
Octane, 2,6-dim...	12.374	492.9	ug/l	43970700	3	11.749	4460820	50.0
Pentalene, octa...	12.457	585.8	ug/l	52261000	3	11.749	4460820	50.0
Nonane, 4-methyl-	12.664	914.0	ug/l	81543800	3	11.749	4460820	50.0
Benzene, 1-ethy...	12.988	70.0	ug/l	108601000	4	13.677	77553600	50.0
o-Cymene	13.568	59.7	ug/l	92582500	4	13.677	77553600	50.0