LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068551.D
Acq On : 18 Sep 2021 5:38
Operator : JC/MD
Sample : M3798-04
Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : NAPL-07-(22-24)

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: VN068551.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.217	75	85	105	rVB3	11182	23962	1.00%	0.123%
2	2.716	256	271	272	rBV5	17996	26855	1.12%	0.137%
3	8.018	2226	2248	2259	rBV	329440	782752	32.68%	4.008%
4	8.083	2260	2272	2309	rVB	653546	1508220	62.97%	7.722%
5	8.434	2381	2403	2431	rBV	304519	699960	29.22%	3.584%
6	8.968	2580	2602	2635	rBV	801528	1698790	70.93%	8.698%
7	10.443	3132	3152	3190	rBV	1250389	2395135	100.00%	12.263%
8	10.977	3335	3351	3369	rVB4	37078	71331	2.98%	0.365%
9	11.349	3479	3490	3502	rVB4	17780	31727	1.32%	0.162%
10	11.459	3518	3531	3539	rBV3	20597	35692	1.49%	0.183%
11	11.521	3543	3554	3559	rBV4	14398	24093	1.01%	0.123%
12	11.628	3583	3594	3605	rBV2	24443	42614	1.78%	0.218%
13	11.749	3619	3639	3659	rBV	1243440	2257154	94.24%	11.556%
14	11.881	3679	3688	3697	rBV4	25234	41167	1.72%	0.211%
15	11.931	3698	3707	3717	rVV6	35911	75331	3.15%	0.386%
16	11.990	3718	3729	3738	rVV2	115496	226255	9.45%	1.158%
17	12.033	3740	3745	3758	rVB4	66141	102375	4.27%	0.524%
18	12.178	3786	3799	3811	rVB6	97053	177469	7.41%	0.909%
19	12.256	3812	3828	3841	rBV4	261517	582764	24.33%	2.984%
20	12.371	3861	3871	3882	rVB2	307471	492940	20.58%	2.524%
21	12.452	3882	3901	3905	rBV6	194623	411507	17.18%	2.107%
22	12.736	3993	4007	4022	rBV	1173138	2022799	84.45%	10.357%
23	12.900	4062	4068	4084	rVB7	196306	376062	15.70%	1.925%
24	12.980	4085	4098	4108	rBV7	104062	233962	9.77%	1.198%
25	13.061	4114	4128	4139	rBV7	267924	584503	24.40%	2.993%
26	13.112	4142	4147	4160	rVB4	159758	237203	9.90%	1.214%
27	13.200	4171	4180	4188	rBV4	164338	231308	9.66%	1.184%
28	13.248	4189	4198	4204	rVV4	162536	268840	11.22%	1.376%
29	13.286	4205	4212	4225	rVB2	375817	578690	24.16%	2.963%
30	13.412	4253	4259	4269	rVB3	112017	149288	6.23%	0.764%
31	13.570	4310	4318	4326	rVV4	151407	214098	8.94%	1.096%
32	13.608	4327	4332	4340	rVB4	91290	107296	4.48%	0.549%
33	13.677	4346	4358	4378	rVB	1328072	2323379	97.00%	11.896%
34	13.924	4442	4450	4452	rBV4	28265	30831	1.29%	0.158%
35	14.002	4468	4479	4489	rBV5	126757	220604	9.21%	1.129%
36	14.216	4553	4559	4570	rVB	63756	92755	3.87%	0.475%

LSC Area Percent Report

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Acq On : 18 Sep 2021 5:38
Operator : JC/MD
Sample : M3798-04
Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : NAPL-07-(22-24)

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	14.318	4589	4597	4611	rVB10	27151	53727	2.24%	0.275%
38	14.385	4612	4622	4636	rVV10	23285	42516	1.78%	0.218%
39	14.512	4663	4669	4676	rBV6	22540	31552	1.32%	0.162%
40	14.916	4809	4820	4829	rBV6	12459	24001	1.00%	0.123%

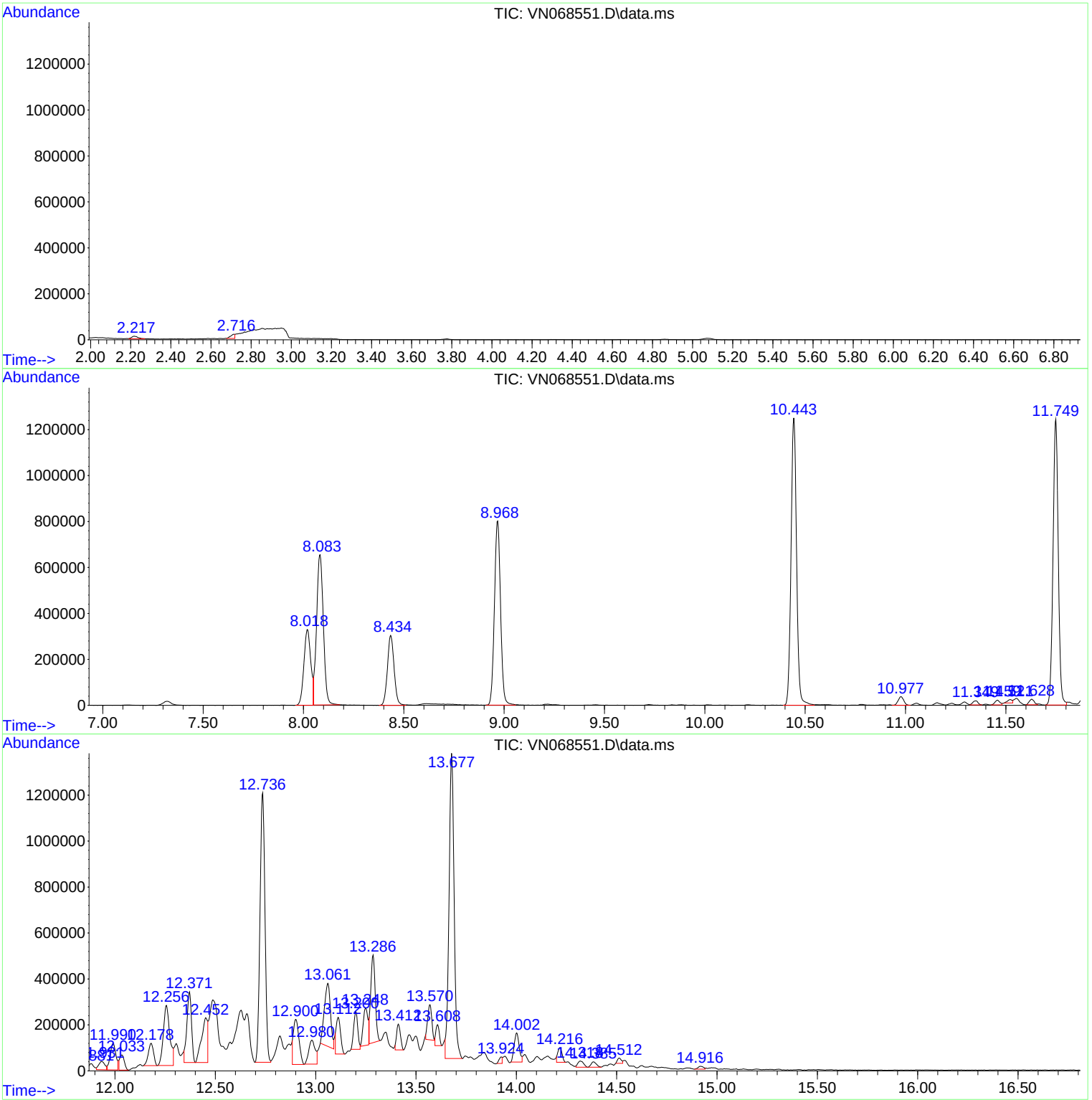
Sum of corrected areas: 19531507

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068551.D
Acq On : 18 Sep 2021 5:38
Operator : JC/MD
Sample : M3798-04
Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(22-24)

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 : VN068551.D
Acq On : 18 Sep 2021 5:38
Operator : JC/MD
Sample : M3798-04
Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(22-24)

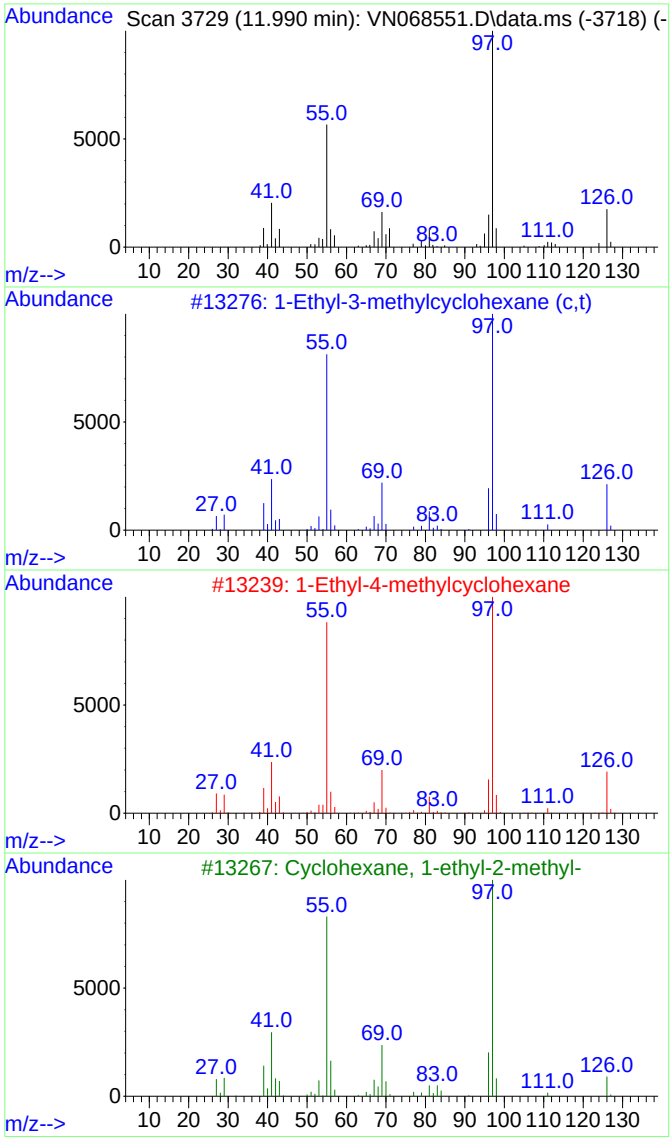
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

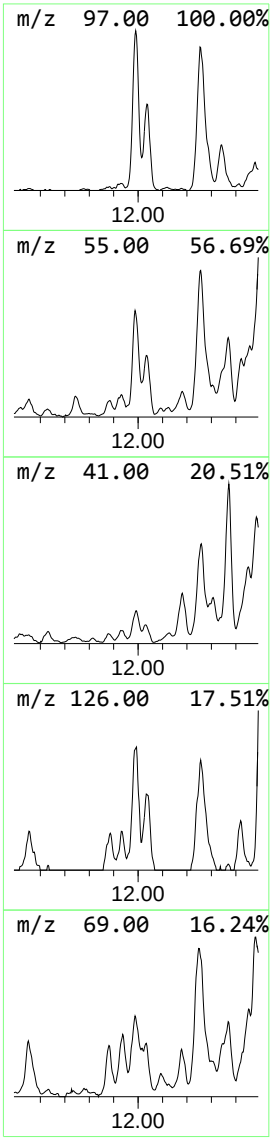
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Ethyl-3-methylcyclohexane... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.991	5.01 ug/l	226255	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	93
2	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	91
3	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	90
4	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	87
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068551.D
Acq On : 18 Sep 2021 5:38
Operator : JC/MD
Sample : M3798-04
Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(22-24)

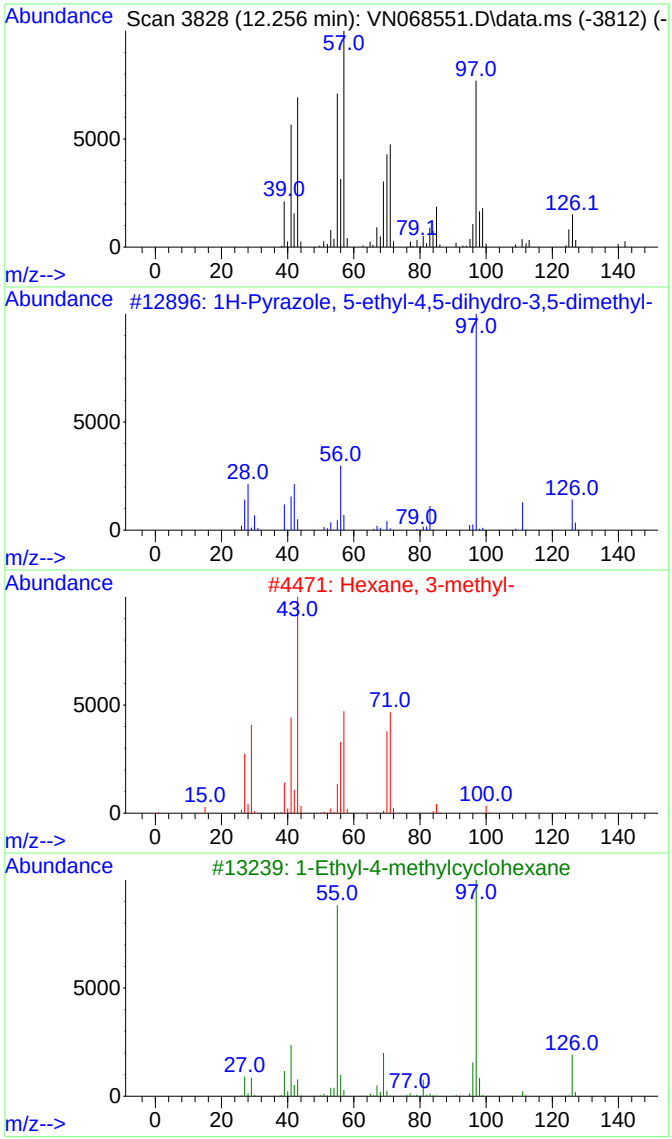
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

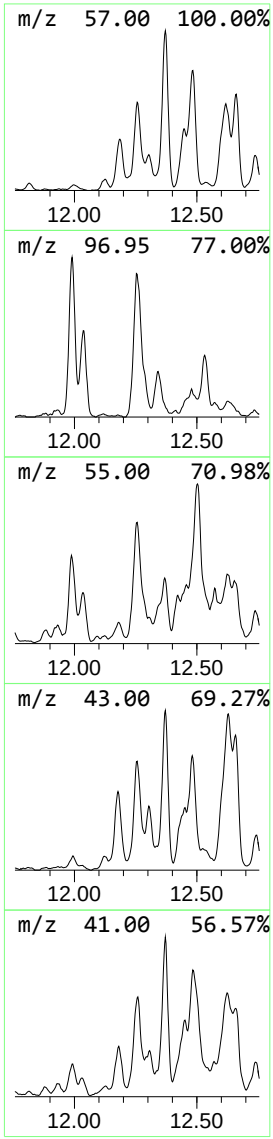
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown12.256 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.256	12.91 ug/l	582764	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole, 5-ethyl-4,5-dihydro...	126	C7H14N2	021981-22-6	38
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	35
3	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	30
4	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	30
5	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	30





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068551.D
Acq On : 18 Sep 2021 5:38
Operator : JC/MD
Sample : M3798-04
Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(22-24)

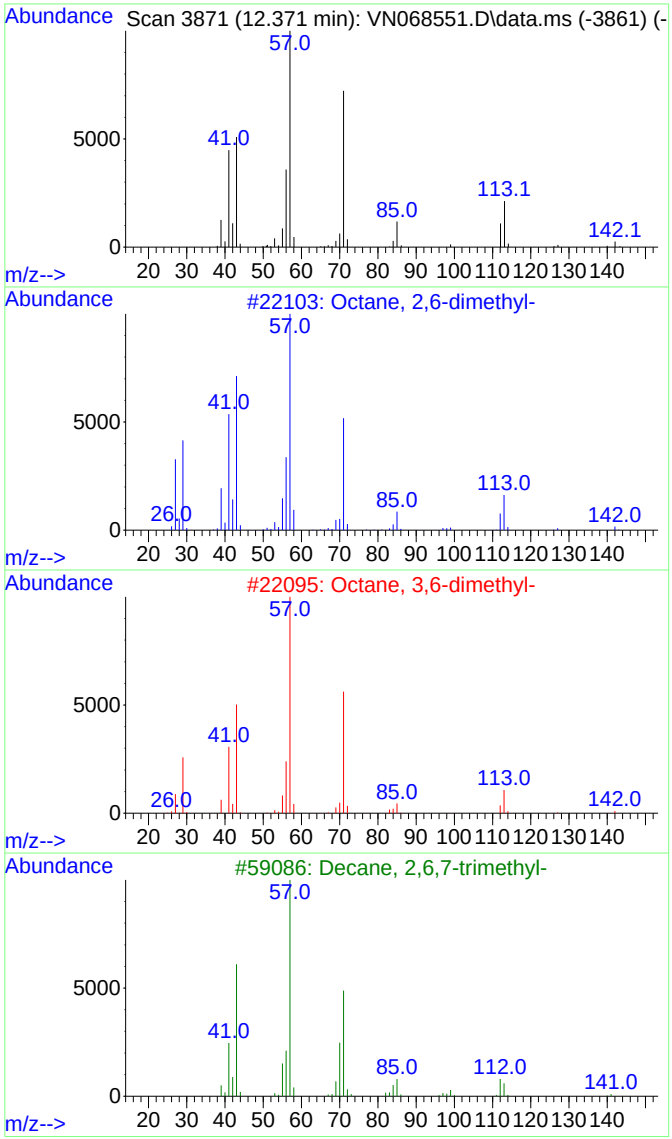
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

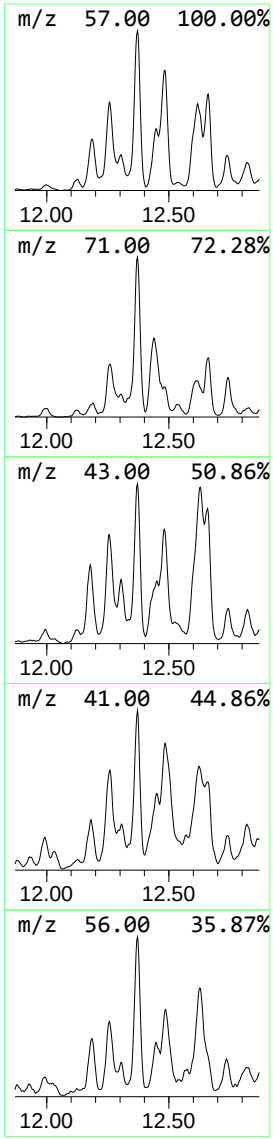
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Octane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.371	10.92 ug/l	492940	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	90
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	87
3	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	72
4	Heptane, 5-ethyl-2-methyl-	142	C10H22	013475-78-0	53
5	3-Bromooctane	192	C8H17Br	000999-64-4	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068551.D
Acq On : 18 Sep 2021 5:38
Operator : JC/MD
Sample : M3798-04
Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(22-24)

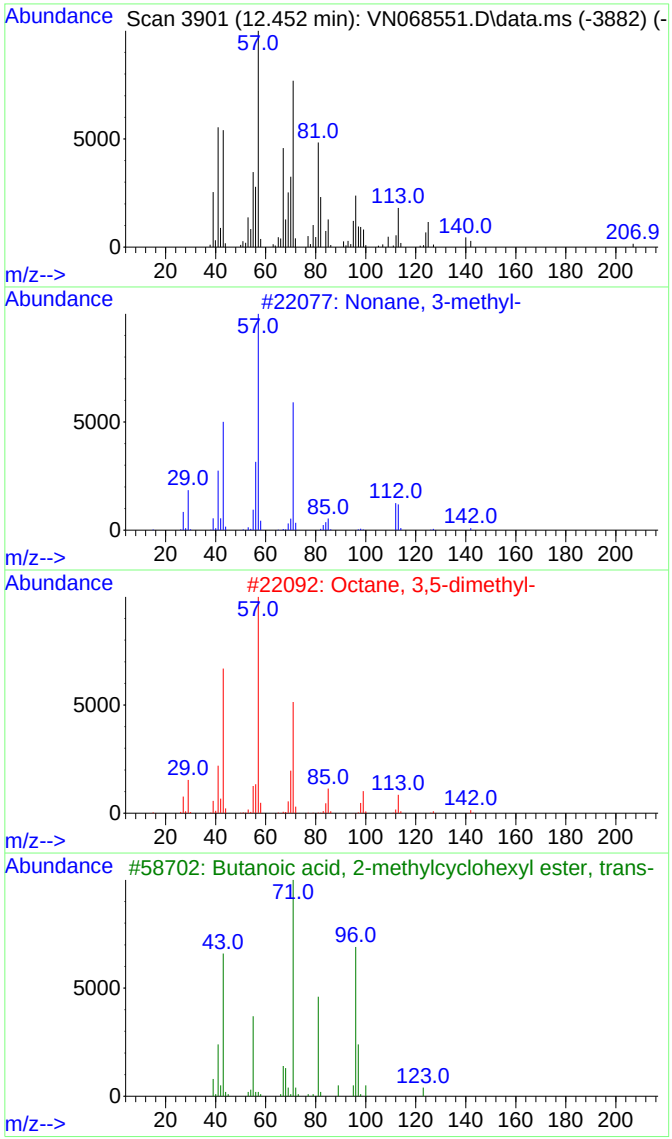
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

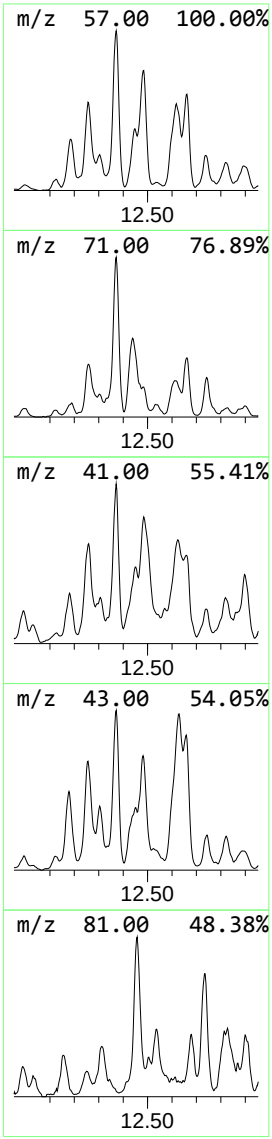
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown12.452 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.452	9.12 ug/l	411507	Chlorobenzene-d5	11.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	46
2	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	43
3	Butanoic acid, 2-methylcyclohexy...	184	C11H20O2	015287-80-6	38
4	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	35
5	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068551.D
Acq On : 18 Sep 2021 5:38
Operator : JC/MD
Sample : M3798-04
Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(22-24)

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

TIC Library : C:\Database\NIST20.L
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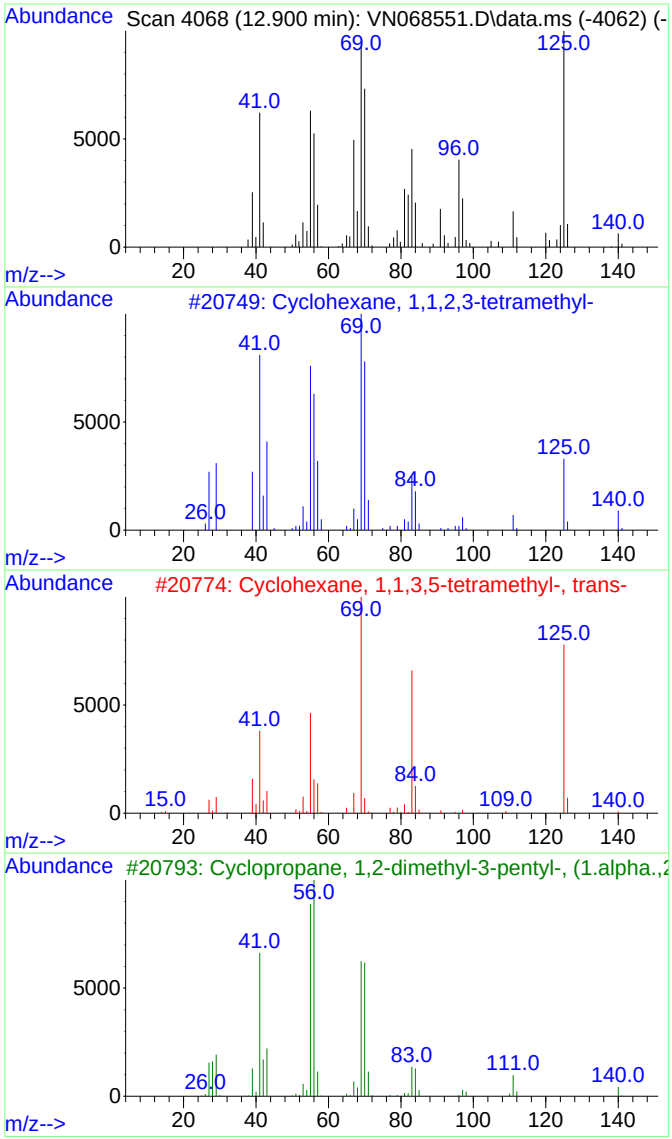
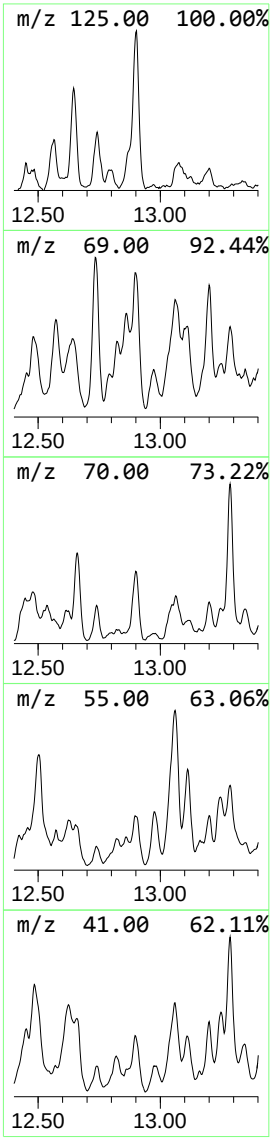
****
Peak Number 5 unknown12.900 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.900	8.09 ug/l	376062	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	46
2	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	43
3	Cyclopropane, 1,2-dimethyl-3-pen...	140	C10H20	062238-10-2	30
4	1-Decene	140	C10H20	000872-05-9	30
5	1,3,5-Trimethyl-1H-pyrazol-4-amine	125	C6H11N3	028466-21-9	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
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Operator : JC/MD
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Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(22-24)

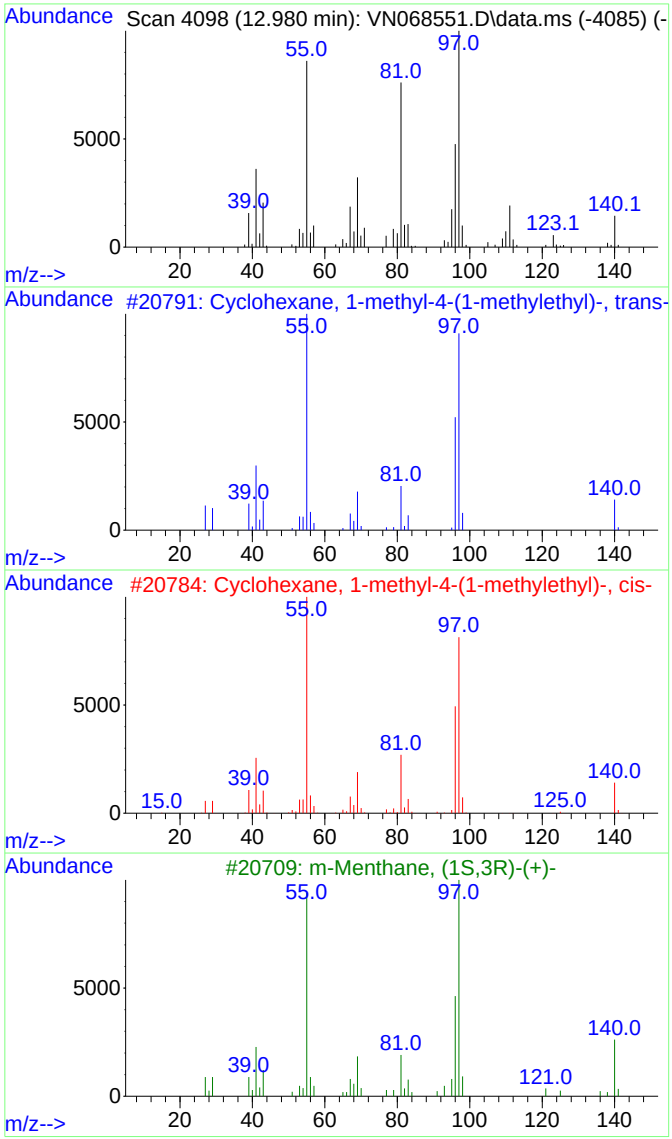
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

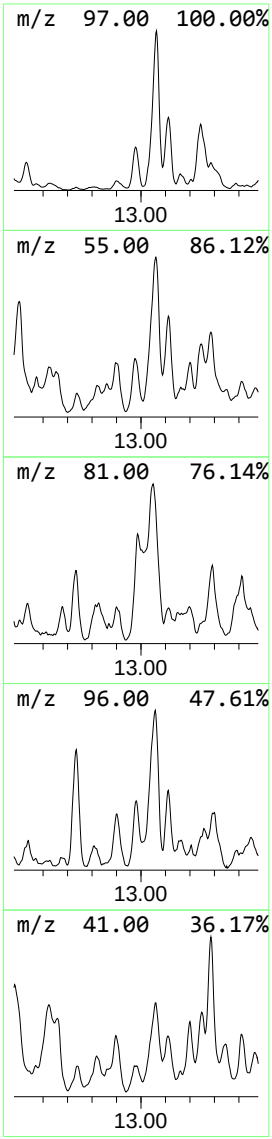
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclohexane, 1-methyl-4-(1-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	5.03 ug/l	233962	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	60
2	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	49
3	m-Menthane, (1S,3R)-(+)-	140	C10H20	013837-66-6	47
4	m-Menthane, (1S,3S)-(+)-	140	C10H20	013837-67-7	43
5	Oxalic acid, butyl cyclohexylmet...	242	C13H22O4	1000309-68-2	43





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Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(22-24)

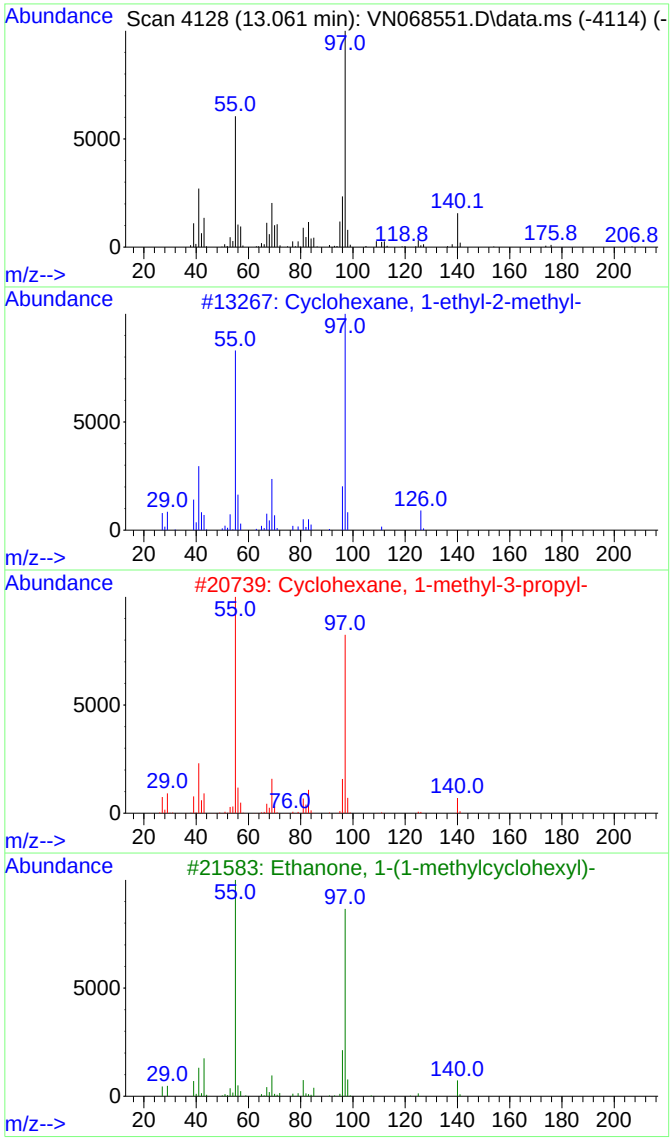
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

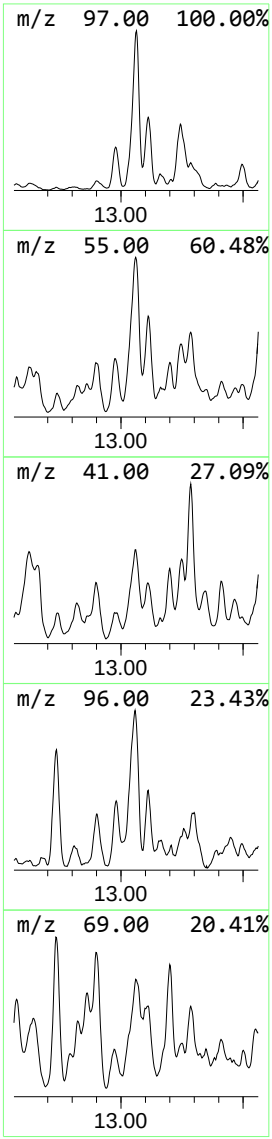
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.061	12.58 ug/l	584503	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	76
2	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	68
3	Ethanone, 1-(1-methylcyclohexyl)-	140	C9H16O	002890-62-2	64
4	m-Menthane, (1S,3R)-(+)-	140	C10H20	013837-66-6	53
5	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068551.D
Acq On : 18 Sep 2021 5:38
Operator : JC/MD
Sample : M3798-04
Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(22-24)

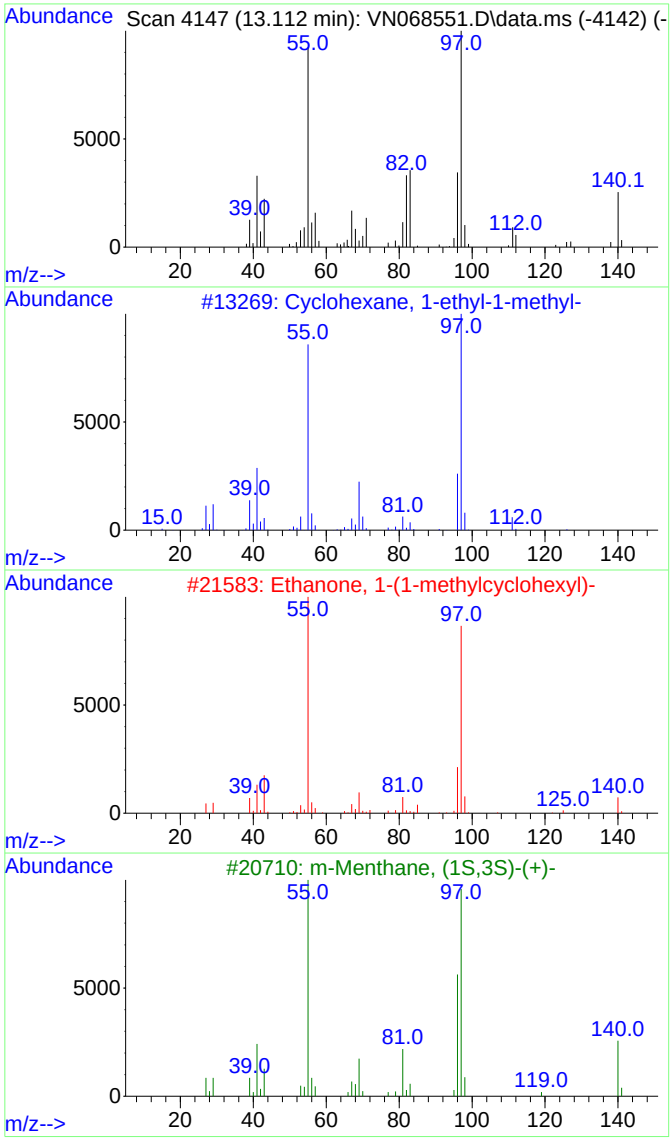
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

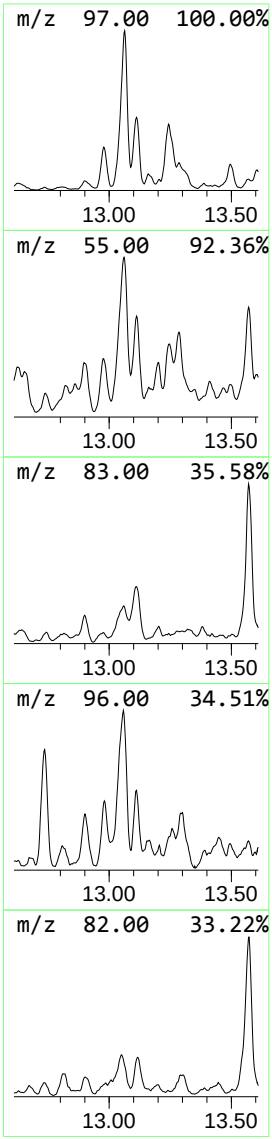
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclohexane, 1-ethyl-1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.111	5.10 ug/l	237203	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	53
2	Ethanone, 1-(1-methylcyclohexyl)-	140	C9H16O	002890-62-2	53
3	m-Menthane, (1S,3S)-(+)-	140	C10H20	013837-67-7	52
4	Oxalic acid, cyclohexylmethyl pr...	228	C12H20O4	1010309-68-1	50
5	Oxalic acid, cyclohexylmethyl is...	270	C15H26O4	1000309-68-3	50





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Data File : VN068551.D
Acq On : 18 Sep 2021 5:38
Operator : JC/MD
Sample : M3798-04
Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(22-24)

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

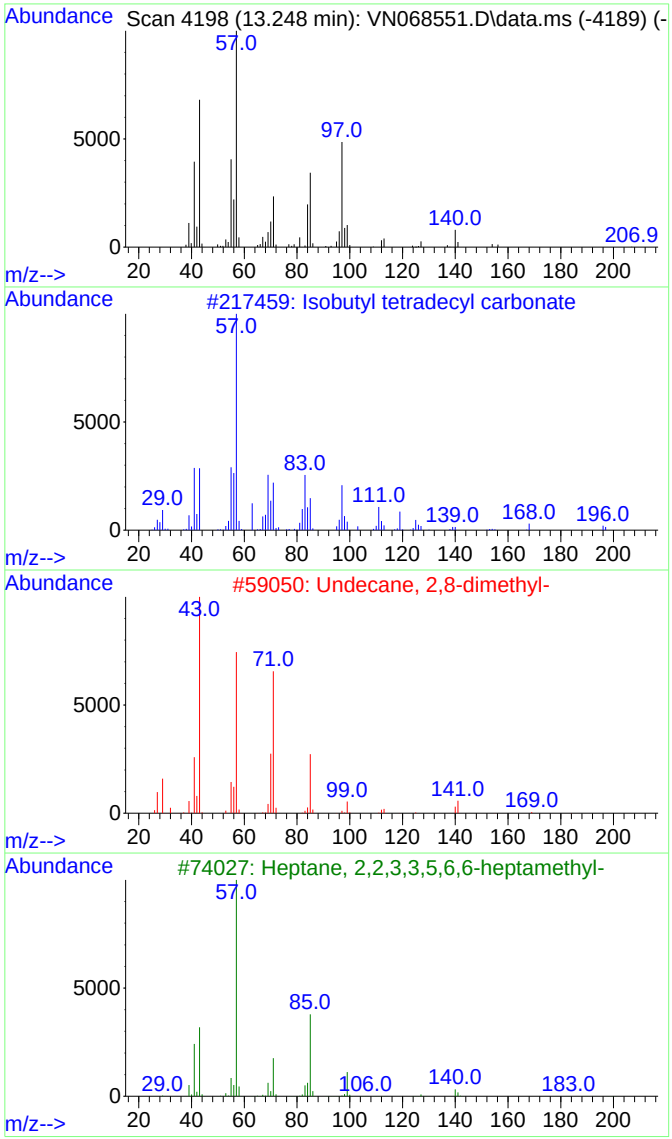
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

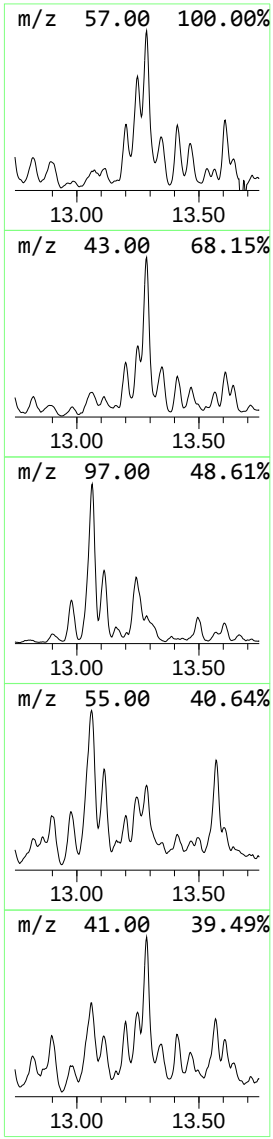
****

Peak Number 9 unknown13.248 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.248	5.79 ug/l	268840	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	43
2	Undecane, 2,8-dimethyl-	184	C13H28	017301-25-6	38
3	Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	007225-67-4	38
4	Nonane	128	C9H20	000111-84-2	38
5	Decane, 2,6,6-trimethyl-	184	C13H28	062108-24-1	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068551.D
Acq On : 18 Sep 2021 5:38
Operator : JC/MD
Sample : M3798-04
Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
NAPL-07-(22-24)

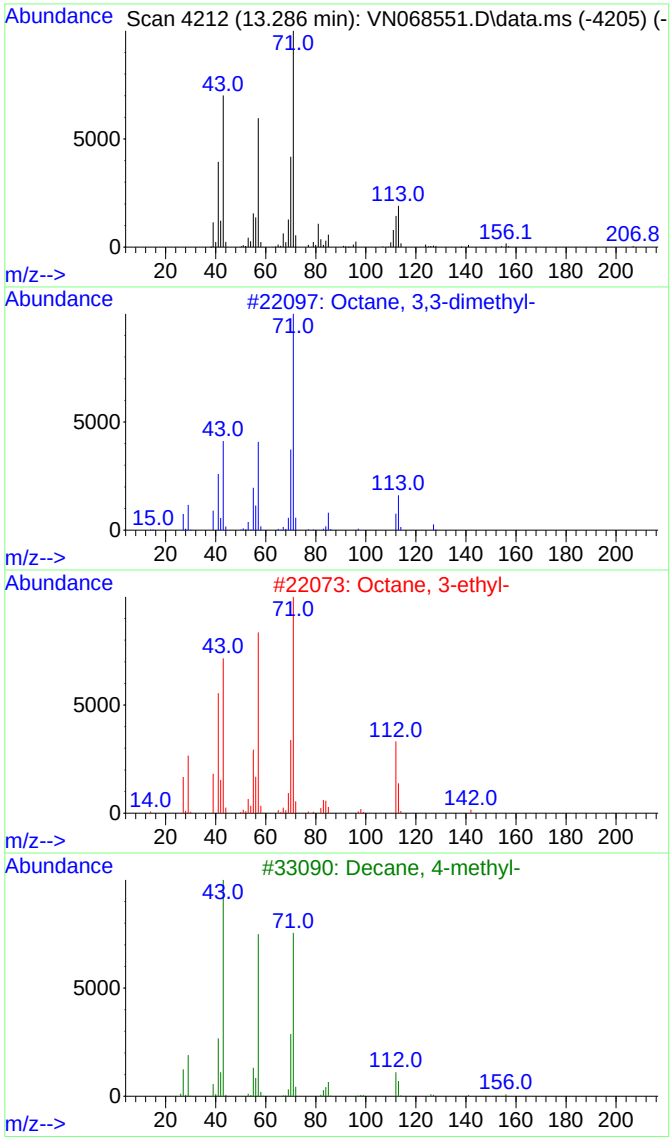
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

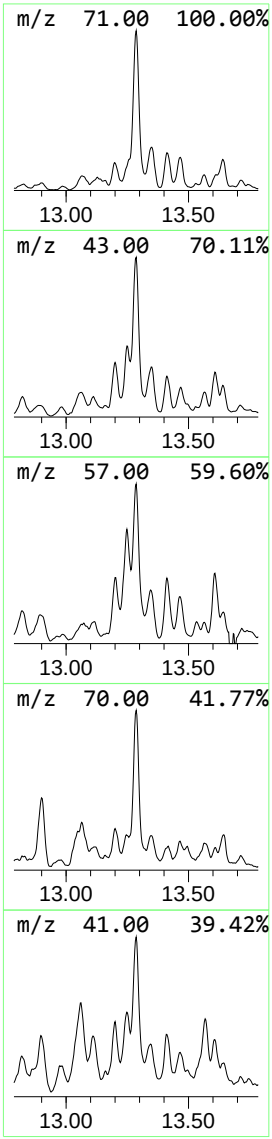
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Octane, 3,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	12.45 ug/l	578690	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	72
2	Octane, 3-ethyl-	142	C10H22	005881-17-4	64
3	Decane, 4-methyl-	156	C11H24	002847-72-5	64
4	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	59
5	n-Amyl ether	158	C10H22O	000693-65-2	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091721\
Data File : VN068551.D
Acq On : 18 Sep 2021 5:38
Operator : JC/MD
Sample : M3798-04
Misc : 6.92g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : NAPL-07-(22-24)

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
1-Ethyl-3-methy...	11.991	5.0	ug/l	226255	3	11.749	2257150	50.0
unknown12.256	12.256	12.9	ug/l	582764	3	11.749	2257150	50.0
Octane, 2,6-dim...	12.371	10.9	ug/l	492940	3	11.749	2257150	50.0
unknown12.452	12.452	9.1	ug/l	411507	3	11.749	2257150	50.0
unknown12.900	12.900	8.1	ug/l	376062	4	13.677	2323380	50.0
Cyclohexane, 1-...	12.980	5.0	ug/l	233962	4	13.677	2323380	50.0
Cyclohexane, 1-...	13.061	12.6	ug/l	584503	4	13.677	2323380	50.0
Cyclohexane, 1-...	13.111	5.1	ug/l	237203	4	13.677	2323380	50.0
unknown13.248	13.248	5.8	ug/l	268840	4	13.677	2323380	50.0
Octane, 3,3-dim...	13.286	12.4	ug/l	578690	4	13.677	2323380	50.0