LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050719\
Data File : VN055438.D
Acq On : 7 May 2019 15:29
Operator : JC/SP
Sample : K2658-19 40X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-W5-6(13-17)

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\82N042919W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.593	1791	1810	1821	rBV2	297332	743751	10.72%	0.922%
2	7.667	1821	1833	1863	rVB	532362	1293183	18.63%	1.603%
3	8.027	1927	1945	1968	rBV	341404	799324	11.52%	0.991%
4	8.587	2104	2119	2161	rBV	788063	1726718	24.88%	2.141%
5	10.092	2571	2587	2620	rBV	1135688	2300660	33.15%	2.852%
6	10.432	2685	2693	2706	rVB4	42553	81062	1.17%	0.100%
7	10.718	2771	2782	2795	rVB	160134	269809	3.89%	0.334%
8	10.821	2800	2814	2827	rBV	91389	205088	2.95%	0.254%
9	10.889	2828	2835	2857	rVB6	48184	127430	1.84%	0.158%
10	11.005	2857	2871	2882	rBV2	337843	660013	9.51%	0.818%
11	11.124	2895	2908	2916	rBV3	245396	455196	6.56%	0.564%
12	11.194	2916	2930	2950	rVB5	381975	1142808	16.47%	1.417%
13	11.300	2950	2963	2982	rBV	672732	1215236	17.51%	1.507%
14	11.407	2984	2996	3015	rBV	984706	1896390	27.32%	2.351%
15	11.542	3030	3038	3044	rBV	169870	258902	3.73%	0.321%
16	11.596	3045	3055	3063	rVV6	277872	584741	8.42%	0.725%
17	11.654	3063	3073	3081	rVV2	710618	1373468	19.79%	1.703%
18	11.696	3082	3086	3096	rVB3	508252	755399	10.88%	0.936%
19	11.760	3096	3106	3111	rBV2	150339	262865	3.79%	0.326%
20	11.850	3126	3134	3142	rVB4	379473	577968	8.33%	0.717%
21	11.924	3143	3157	3168	rBV5	1223353	2882288	41.53%	3.573%
22	11.979	3170	3174	3179	rVV3	147606	163266	2.35%	0.202%
23	12.043	3186	3194	3203	rVB	2175021	3015997	43.45%	3.739%
24	12.120	3209	3218	3222	rBV3	1003995	1636851	23.58%	2.029%
25	12.156	3223	3229	3238	rVB3	1600463	2563597	36.94%	3.178%
26	12.294	3262	3272	3278	rBV5	1104292	2137808	30.80%	2.650%
27	12.336	3279	3285	3295	rVB	2368239	3581528	51.60%	4.440%
28	12.403	3295	3306	3316	rBV5	1059685	2031566	29.27%	2.519%
29	12.490	3317	3333	3339	rBV7	460317	1220995	17.59%	1.514%
30	12.561	3347	3355	3368	rVB2	1995599	3869059	55.74%	4.796%
31	12.644	3368	3381	3390	rBV6	948133	2289094	32.98%	2.838%
32	12.728	3392	3407	3416	rVV6	2458937	6940774	100.00%	8.604%
33	12.779	3418	3423	3433	rVB3	1407852	2181879	31.44%	2.705%
34	12.870	3443	3451	3458	rBV2	795265	1215165	17.51%	1.506%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050719\
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Sample : K2658-19 40X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-W5-6(13-17)

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\82N042919W.M
Title : SW846 8260

35	12.960	3472	3479	3493	rVB	3453967	5748448	82.82%	7.126%
36	13.037	3495	3503	3512	rBV5	669465	1171639	16.88%	1.452%
37	13.091	3514	3520	3528	rVB3	506325	748115	10.78%	0.927%
38	13.146	3530	3537	3540	rBV3	708020	966388	13.92%	1.198%
39	13.236	3552	3565	3574	rBV4	2598922	5081470	73.21%	6.299%
40	13.284	3575	3580	3587	rVB4	925859	1252452	18.04%	1.553%
41	13.590	3668	3675	3688	rBV3	661567	1251079	18.03%	1.551%
42	13.660	3689	3697	3707	rBV4	1388798	2454902	35.37%	3.043%
43	13.799	3736	3740	3744	rBV3	314291	392245	5.65%	0.486%
44	13.831	3746	3750	3760	rVV5	897165	1304295	18.79%	1.617%
45	13.886	3761	3767	3777	rVB	1036619	1635794	23.57%	2.028%
46	13.992	3791	3800	3810	rVB3	886972	1468889	21.16%	1.821%
47	14.050	3811	3818	3831	rVB10	228513	572965	8.26%	0.710%
48	14.127	3836	3842	3848	rBV2	223948	283335	4.08%	0.351%
49	14.178	3849	3858	3865	rBV6	414648	810140	11.67%	1.004%
50	14.246	3874	3879	3887	rVB	488772	682951	9.84%	0.847%
51	14.294	3888	3894	3899	rVV3	218407	278668	4.01%	0.345%
52	14.329	3900	3905	3913	rVB3	265911	361683	5.21%	0.448%
53	14.477	3945	3951	3959	rBV6	71207	141568	2.04%	0.176%
54	14.522	3960	3965	3973	rVB	151255	213181	3.07%	0.264%
55	14.580	3973	3983	3996	rVV2	536212	1001008	14.42%	1.241%
56	14.644	3997	4003	4015	rVB5	99675	172039	2.48%	0.213%
57	14.850	4061	4067	4073	rBV4	54049	72857	1.05%	0.090%
58	14.953	4091	4099	4111	rVB5	67410	138786	2.00%	0.172%

Sum of corrected areas: 80664775

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050719\
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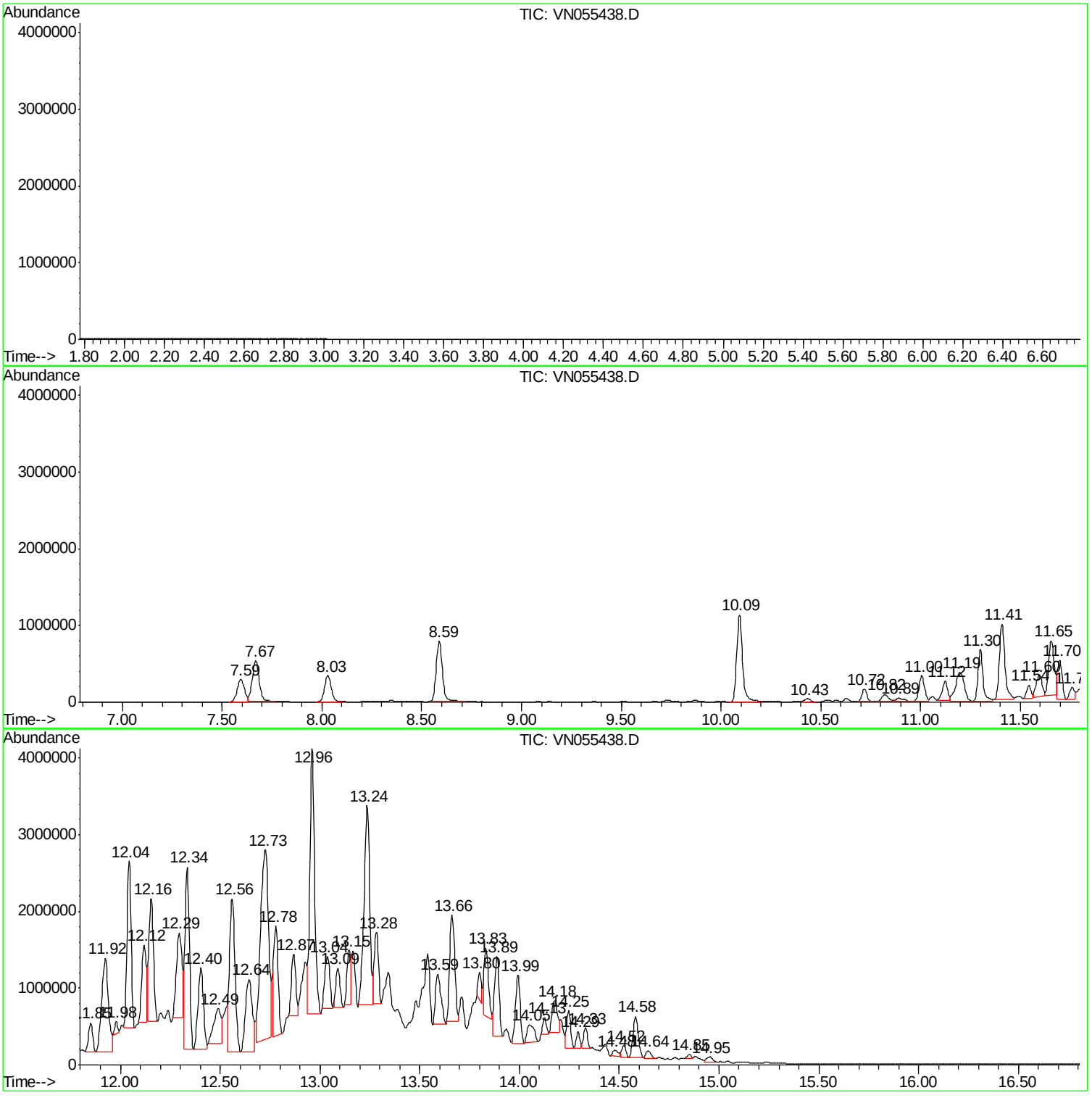
Operator : JC/SP
Sample : K2658-19 40X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-W5-6(13-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050719\
Data File : VN055438.D
Acq On : 7 May 2019 15:29
Operator : JC/SP
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Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-W5-6(13-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

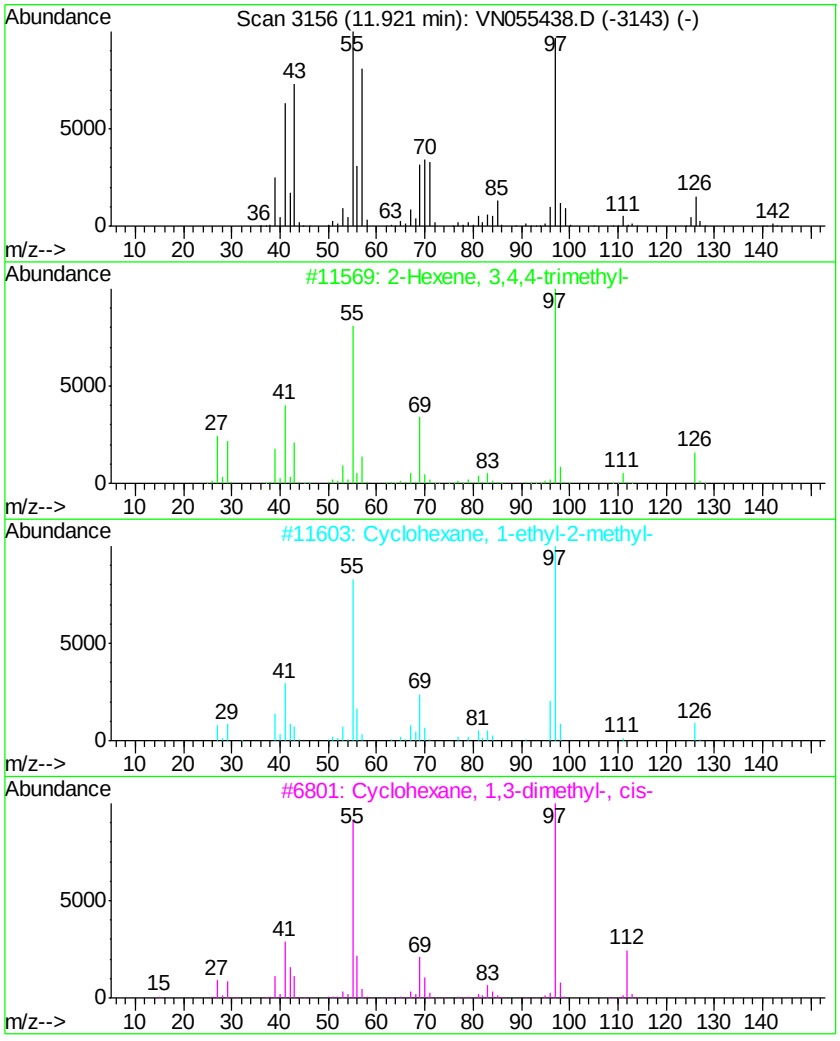
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

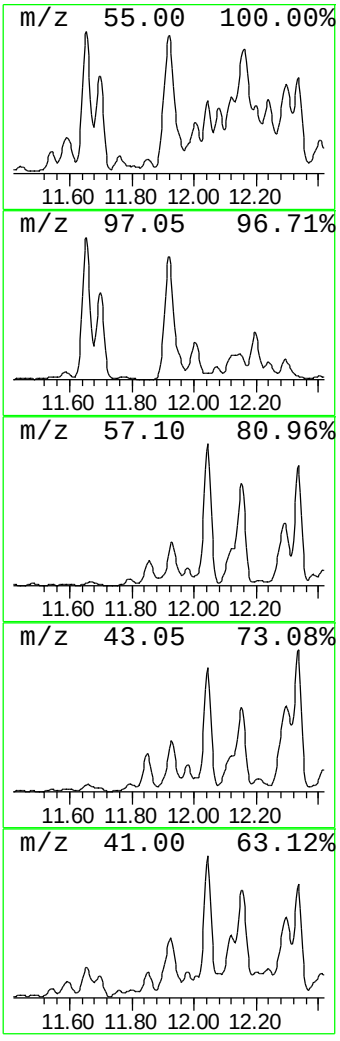
****

Peak Number 1 unknown11.92 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	75.99 ug/l	2882290	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	45
2	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	45
3	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	43
4	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	43
5	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050719\
Data File : VN055438.D
Acq On : 7 May 2019 15:29
Operator : JC/SP
Sample : K2658-19 40X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-W5-6(13-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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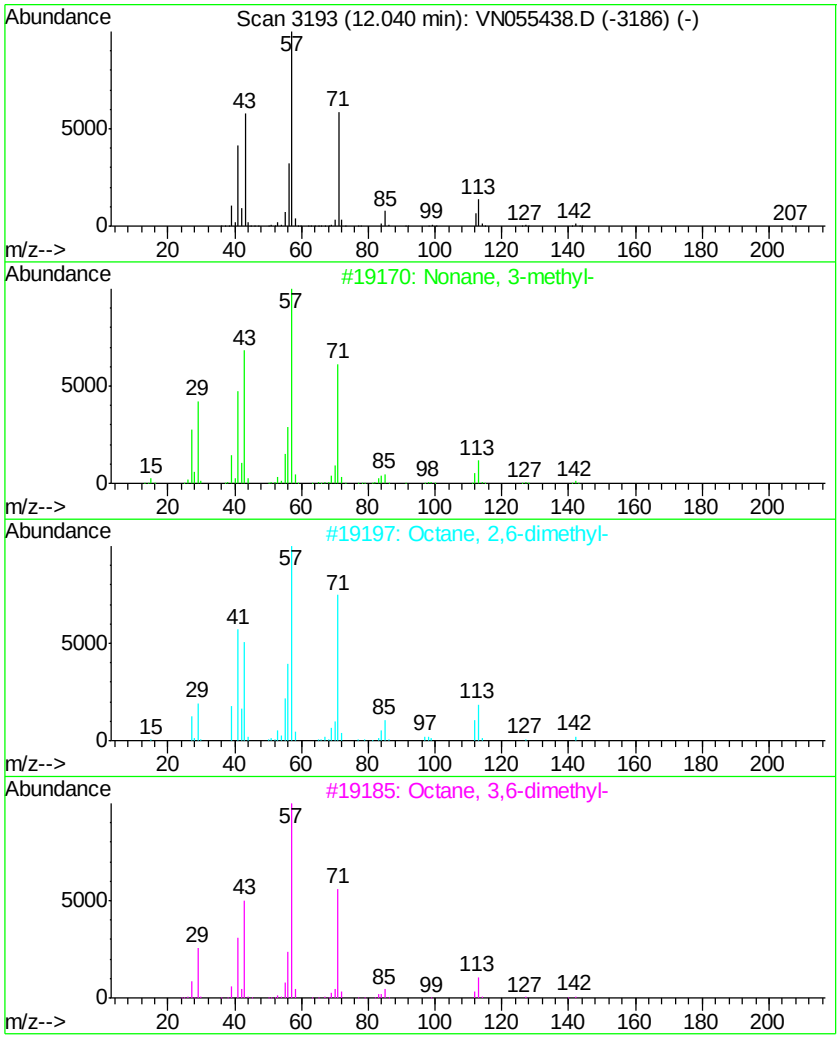
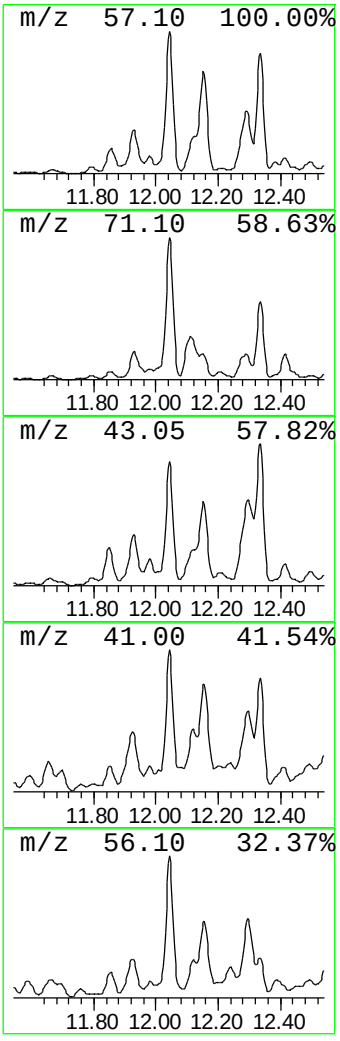
Peak Number 2 Nonane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	79.52 ug/l	3016000	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	91
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	87
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	86
4	Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	59
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050719\
Data File : VN055438.D
Acq On : 7 May 2019 15:29
Operator : JC/SP
Sample : K2658-19 40X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-W5-6(13-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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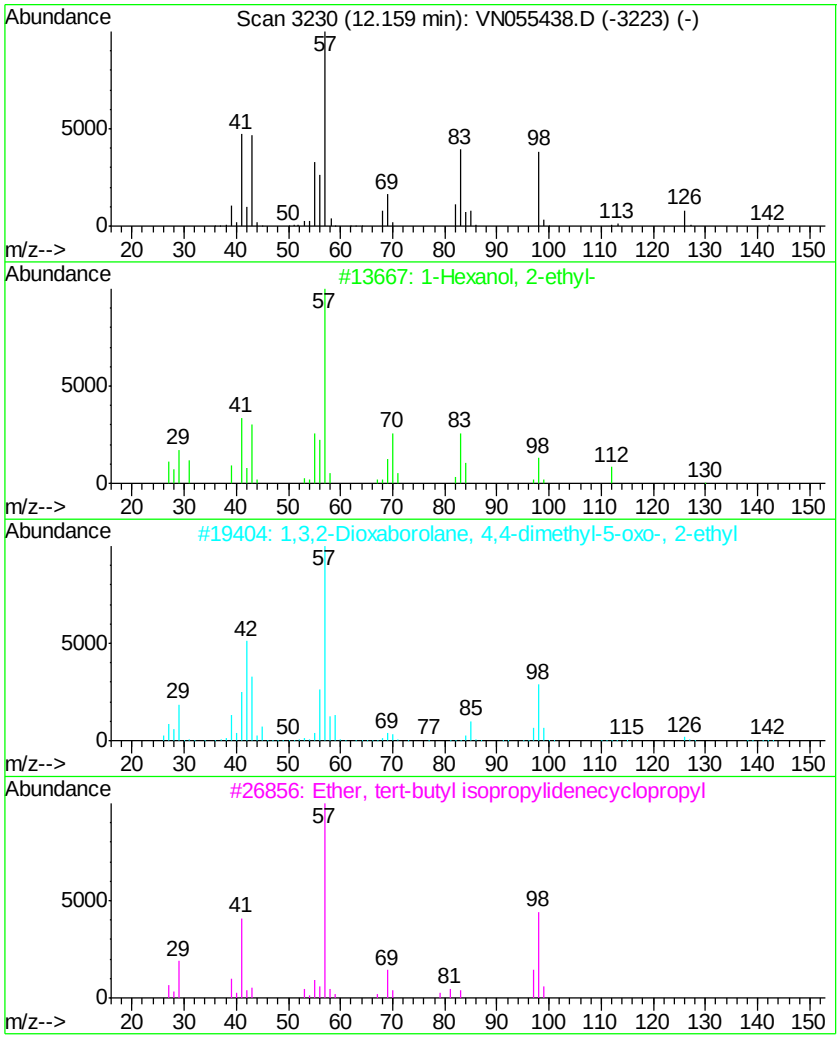
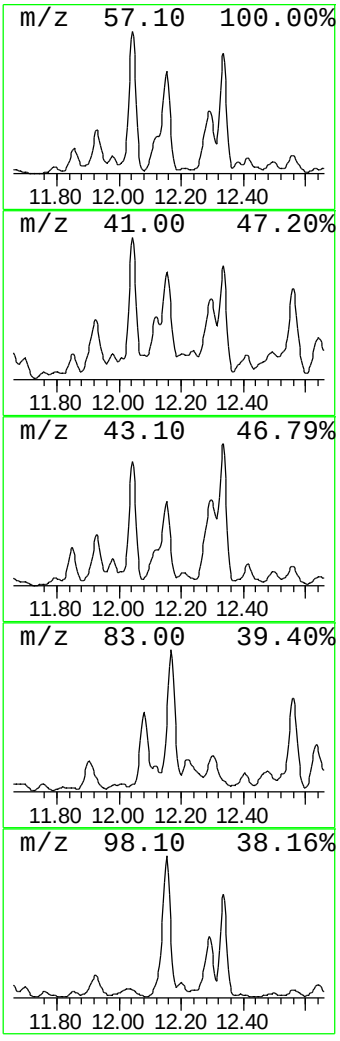
Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	67.59 ug/l	2563600	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
2	1,3,2-Dioxaborolane, 4,4-dimethy...	142	C6H11BO3	1000063-89-2	47
3	Ether, tert-butyl isopropylidene...	154	C10H18O	024524-56-9	43
4	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	40
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050719\
Data File : VN055438.D
Acq On : 7 May 2019 15:29
Operator : JC/SP
Sample : K2658-19 40X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-W5-6(13-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

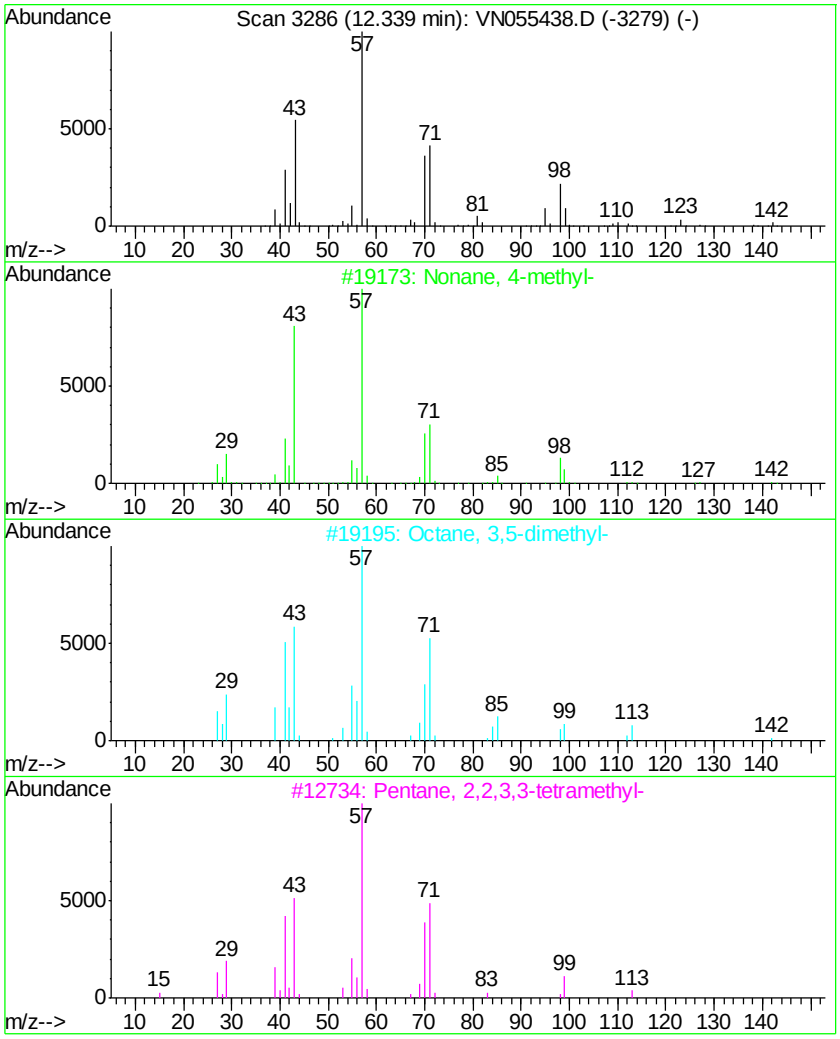
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

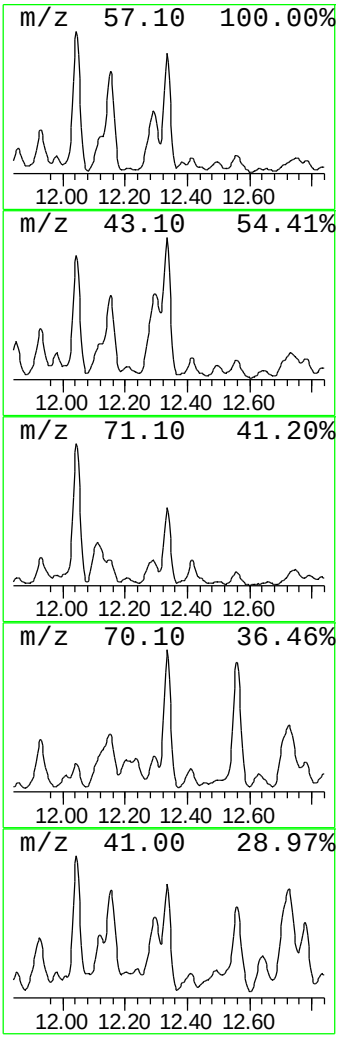
****

Peak Number 4 Nonane, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	94.43 ug/l	3581530	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	80
2	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	64
3	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	53
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	47
5	Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050719\
Data File : VN055438.D
Acq On : 7 May 2019 15:29
Operator : JC/SP
Sample : K2658-19 40X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-W5-6(13-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

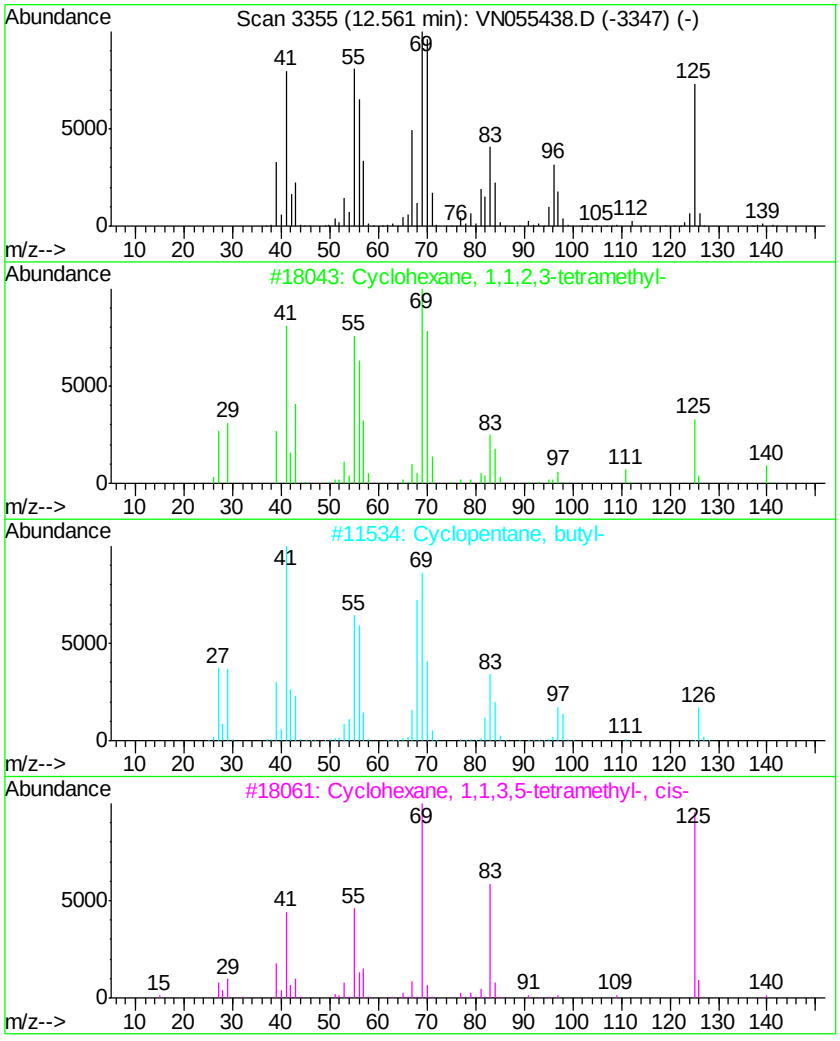
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

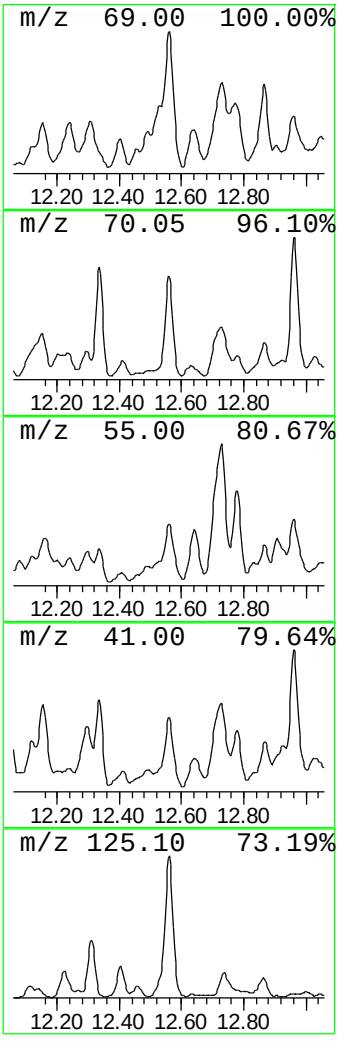
****

Peak Number 5 Cyclohexane, 1,1,2,3-tetram... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	154.46 ug/l	3869060	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	50
2	Cyclopentane, butyl-	126	C9H18	002040-95-1	45
3	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	43
4	cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	41
5	trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	41





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ClientSampleId : EP1-SB-W5-6(13-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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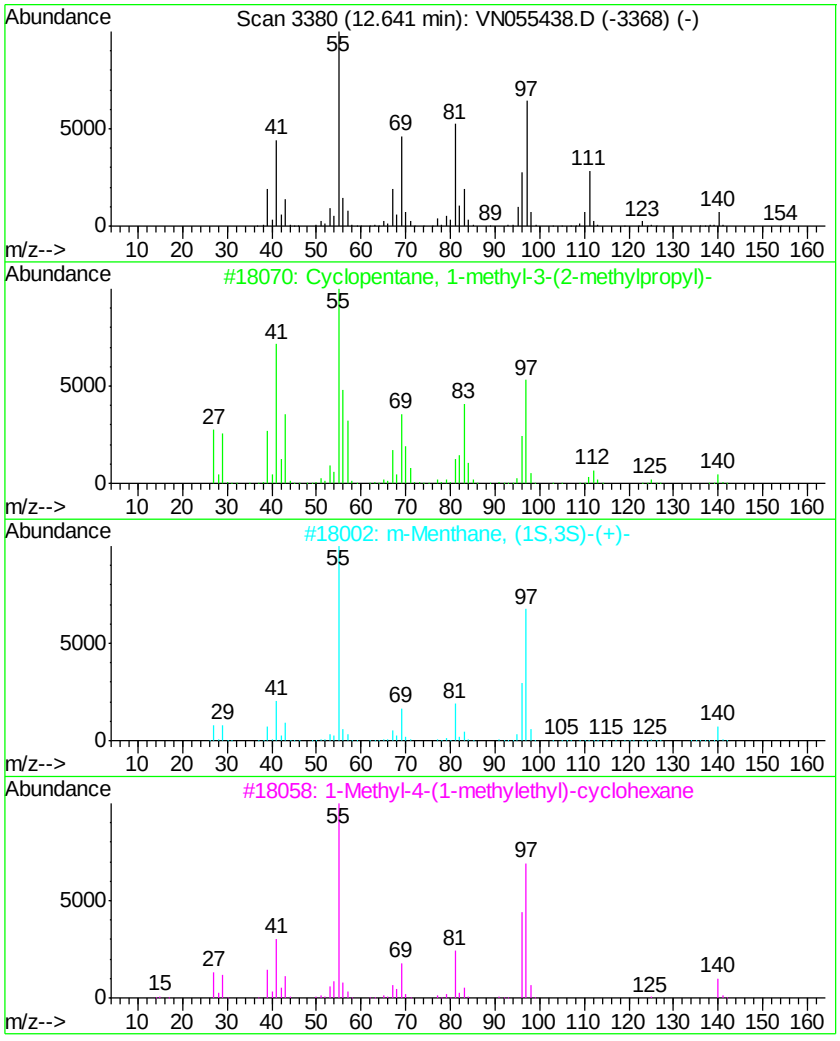
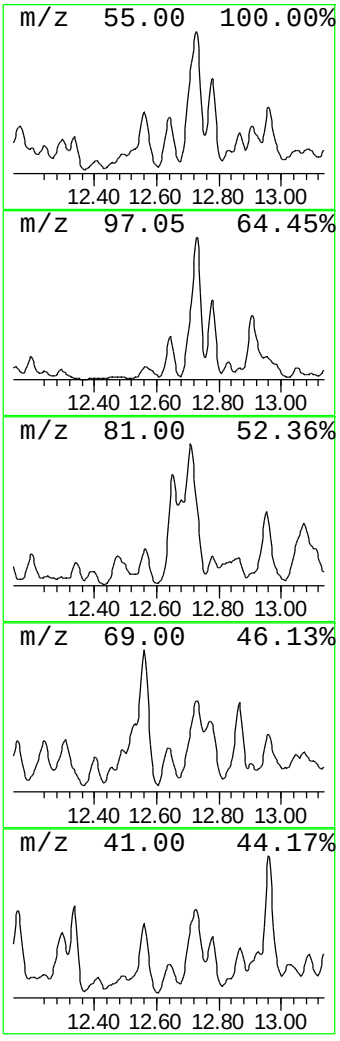
Peak Number 6 Cyclopentane, 1-methyl-3-(2... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	91.38 ug/l	2289090	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1-methyl-3-(2-meth...	140	C10H20	029053-04-1	58
2	m-Menthane, (1S,3S)-(+)-	140	C10H20	013837-67-7	50
3	1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	49
4	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	47
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	47





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050719\
Data File : VN055438.D
Acq On : 7 May 2019 15:29
Operator : JC/SP
Sample : K2658-19 40X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-W5-6(13-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

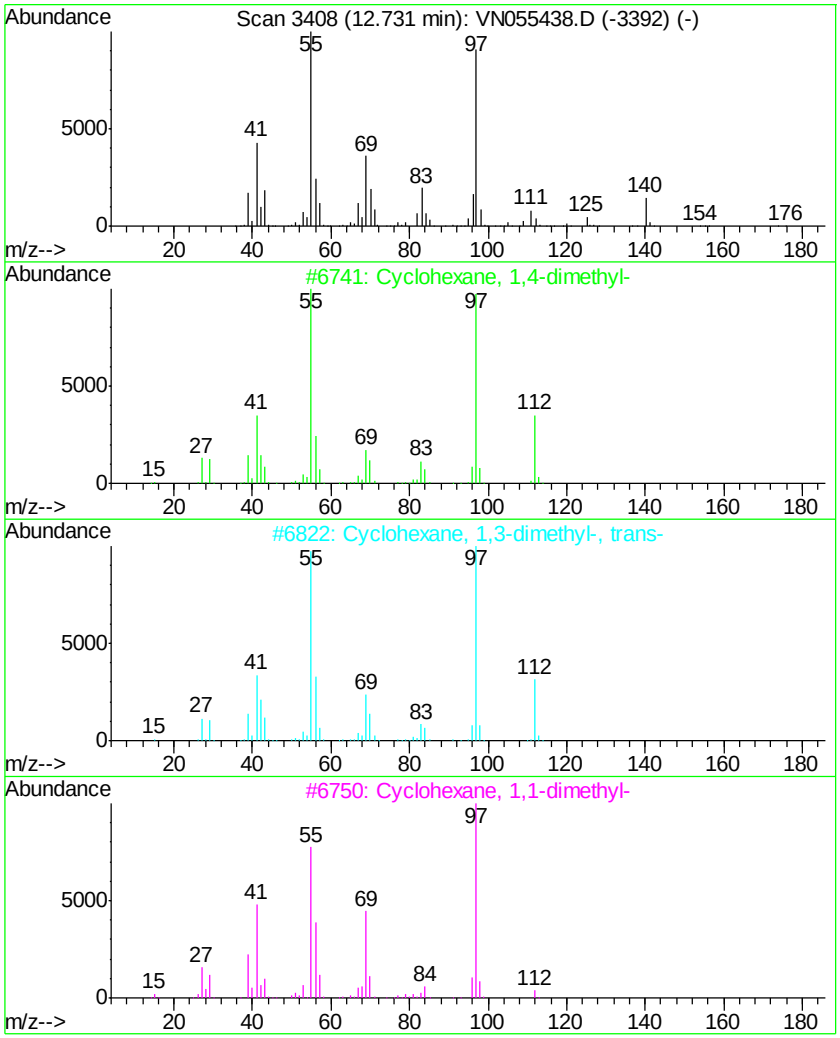
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

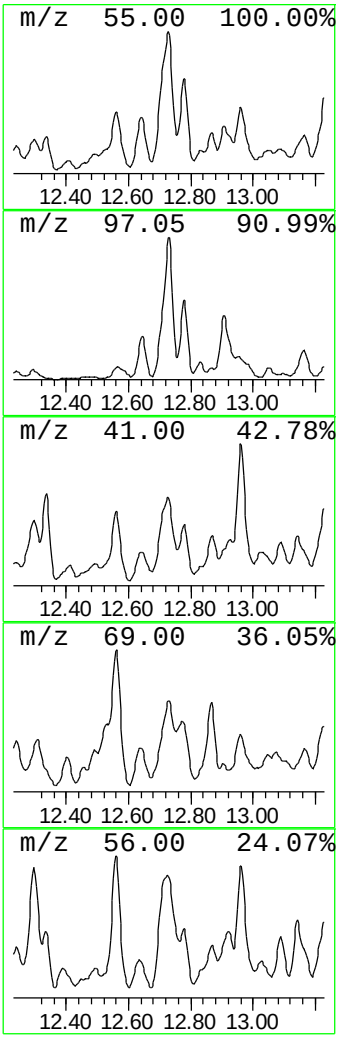
****

Peak Number 7 Cyclohexane, 1,4-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	277.09 ug/l	6940770	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	64
2	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	64
3	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	58
4	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	58
5	2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	100463-01-2	58





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050719\
Data File : VN055438.D
Acq On : 7 May 2019 15:29
Operator : JC/SP
Sample : K2658-19 40X
Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-W5-6(13-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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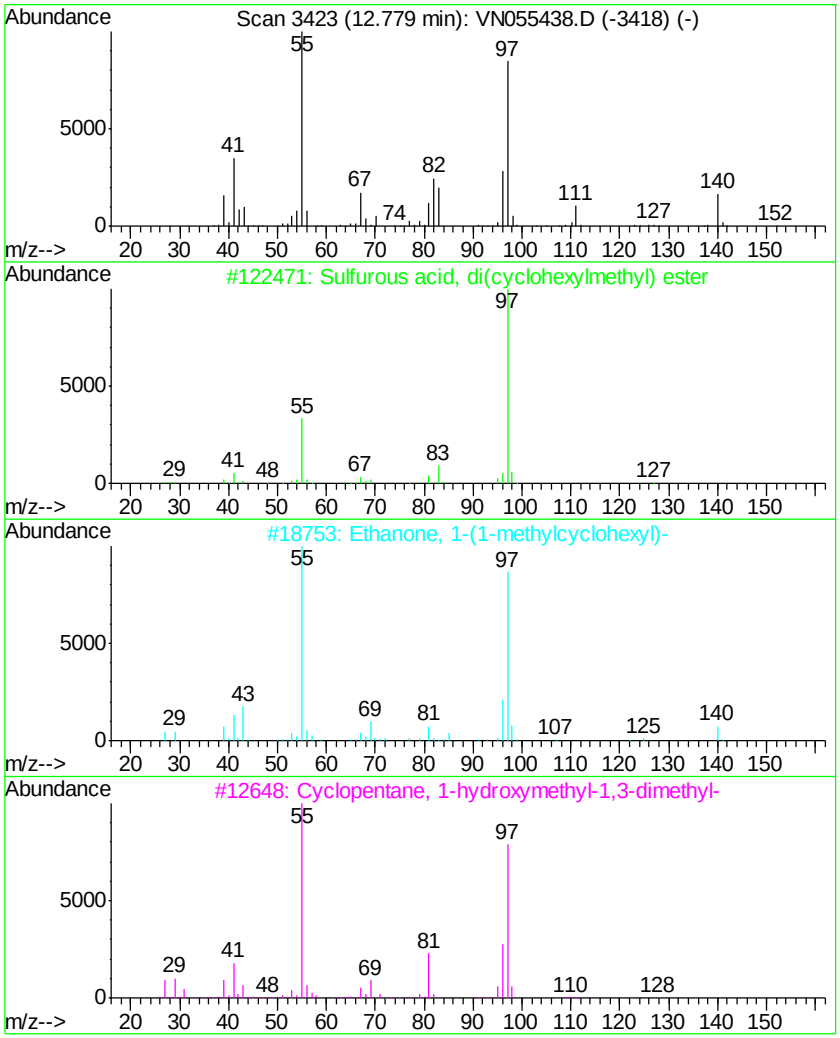
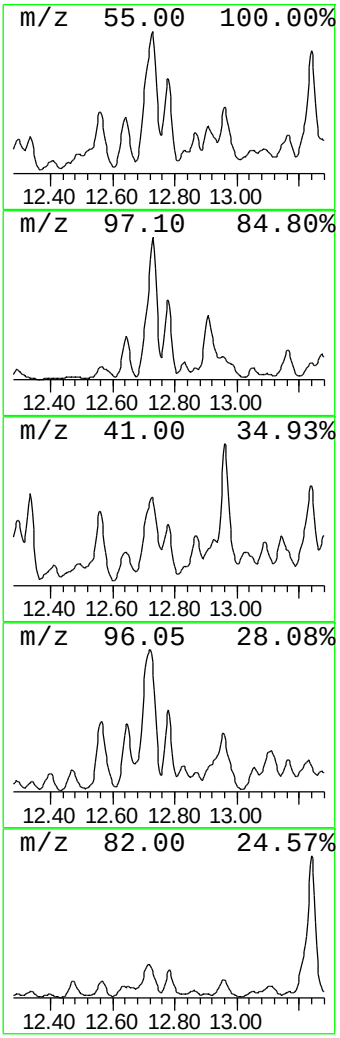
Peak Number 8 Sulfurous acid, di(cyclohex... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	87.10 ug/l	2181880	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1000309-22-7	64
2	Ethanone, 1-(1-methylcyclohexyl)-	140	C9H16O	002890-62-2	53
3	Cyclopentane, 1-hydroxymethyl-1,...	128	C8H16O	1000156-73-8	50
4	3-Hexene, 3-ethyl-2,5-dimethyl-	140	C10H20	062338-08-3	50
5	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	46





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050719\
Data File : VN055438.D
Acq On : 7 May 2019 15:29
Operator : JC/SP
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Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-W5-6(13-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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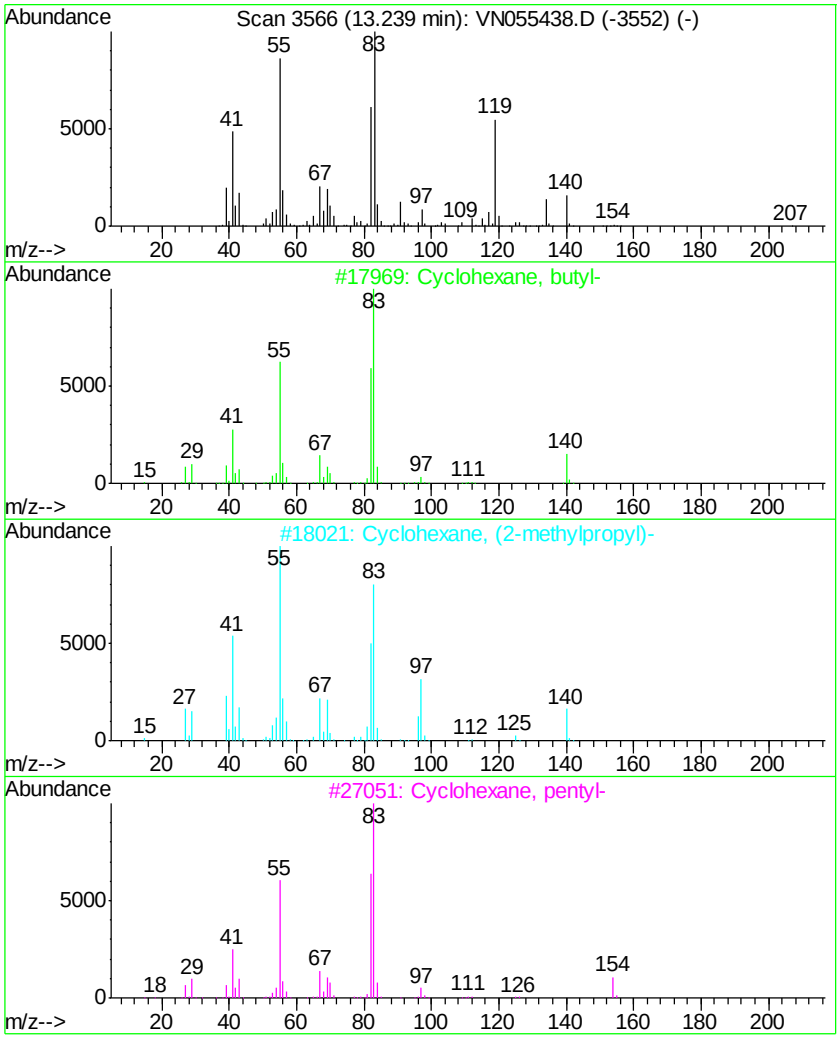
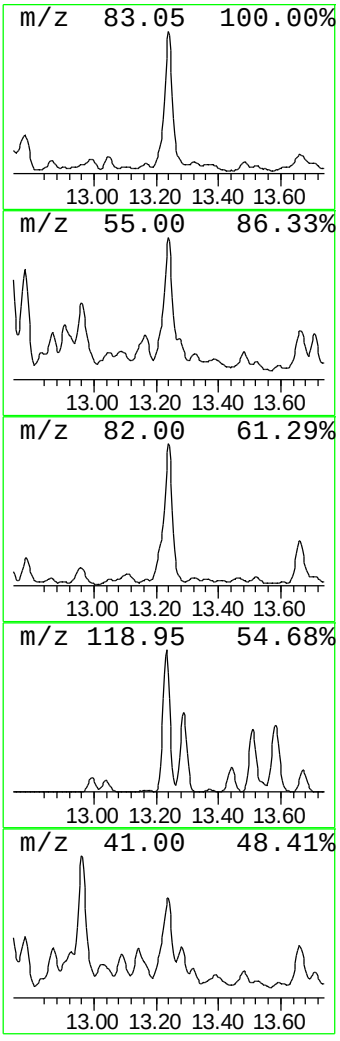
Peak Number 9 Cyclohexane, butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	202.86 ug/l	5081470	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, butyl-	140	C10H20	001678-93-9	76
2	Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	62
3	Cyclohexane, pentyl-	154	C11H22	004292-92-6	62
4	p-Cymene	134	C10H14	000099-87-6	56
5	o-Cymene	134	C10H14	000527-84-4	53





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Data File : VN055438.D
Acq On : 7 May 2019 15:29
Operator : JC/SP
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Misc : 5.85g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : EP1-SB-W5-6(13-17)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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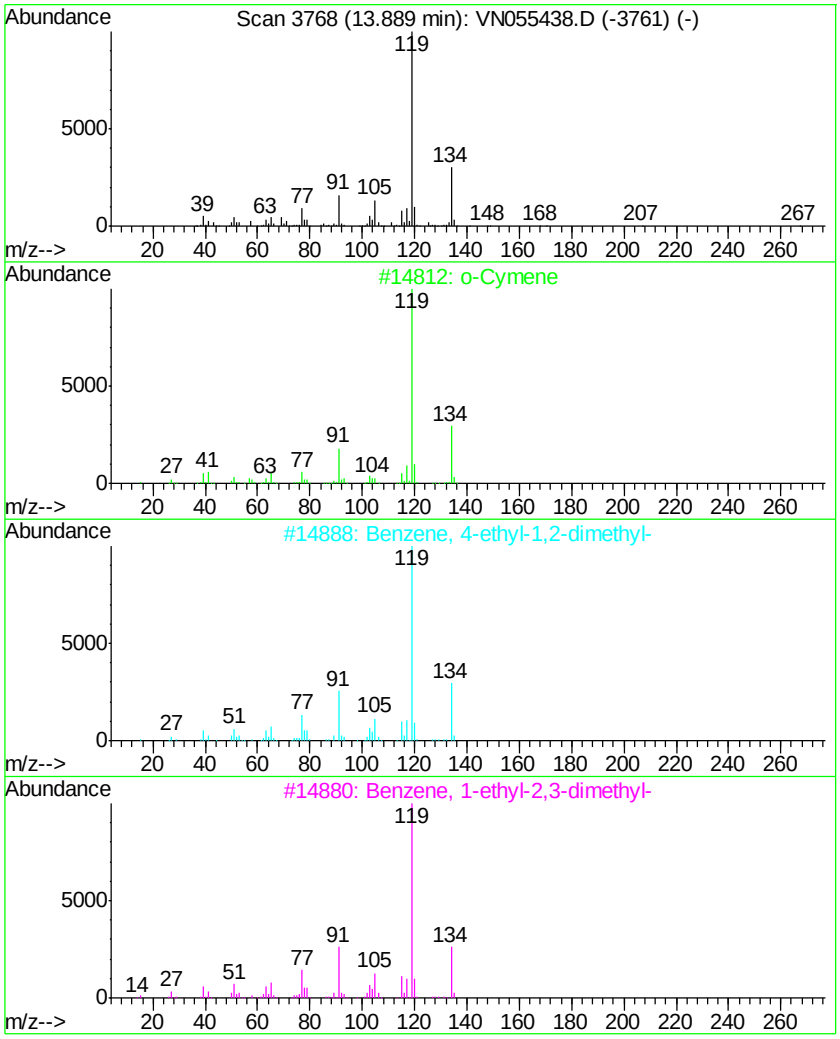
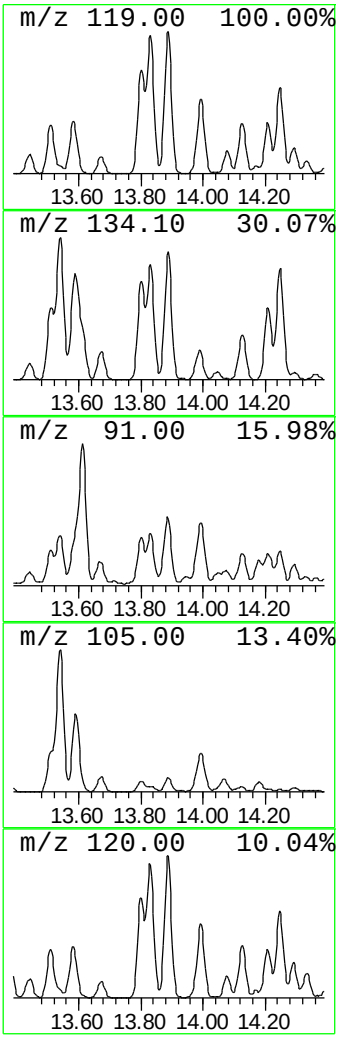
Peak Number 10 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	65.30 ug/l	1635790	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	95
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
5	p-Cymene	134	C10H14	000099-87-6	94





Tentatively Identified Compound (LSC) summary

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Data File : VN055438.D
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ClientSampleId : EP1-SB-W5-6(13-17)

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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown11.92	11.92	76.0	ug/l	2882290	3	11.41	1896390	50.0
Nonane, 3-methyl-	12.04	79.5	ug/l	3016000	3	11.41	1896390	50.0
1-Hexanol, 2-ethyl-	12.16	67.6	ug/l	2563600	3	11.41	1896390	50.0
Nonane, 4-methyl-	12.34	94.4	ug/l	3581530	3	11.41	1896390	50.0
Cyclohexane, 1,1,...	12.56	154.5	ug/l	3869060	4	13.34	1252450	50.0
Cyclopentane, 1-m...	12.64	91.4	ug/l	2289090	4	13.34	1252450	50.0
Cyclohexane, 1,4-...	12.73	277.1	ug/l	6940770	4	13.34	1252450	50.0
Sulfurous acid, d...	12.78	87.1	ug/l	2181880	4	13.34	1252450	50.0
Cyclohexane, butyl-	13.24	202.9	ug/l	5081470	4	13.34	1252450	50.0
o-Cymene	13.89	65.3	ug/l	1635790	4	13.34	1252450	50.0