LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059336.D
Acq On : 21 Nov 2019 15:28
Operator : JC/SP
Sample : K5957-07
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

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\82N112019W.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	7.567	1781	1802	1813	rBV	202953	517793	1.32%	0.154%
2	7.641	1813	1825	1845	rVB	423911	1013913	2.59%	0.302%
3	8.005	1921	1938	1963	rBV	243657	564988	1.44%	0.168%
4	8.567	2095	2113	2134	rBV	611110	1262599	3.22%	0.376%
5	10.082	2569	2584	2610	rBV	996834	1882570	4.80%	0.561%
6	10.712	2769	2780	2792	rVB	505717	852608	2.17%	0.254%
7	10.815	2798	2812	2825	rBV	322941	693741	1.77%	0.207%
8	11.001	2859	2870	2881	rBV2	924610	1667063	4.25%	0.497%
9	11.120	2894	2907	2914	rBV5	682310	1269921	3.24%	0.379%
10	11.204	2915	2933	2950	rVB6	1004202	3063661	7.81%	0.913%
11	11.297	2950	2962	2972	rBV	1161257	2105220	5.37%	0.628%
12	11.403	2984	2995	3004	rBV	843912	1562036	3.98%	0.466%
13	11.541	3029	3038	3044	rBV	606065	939865	2.40%	0.280%
14	11.596	3044	3055	3063	rVV5	1063092	2138197	5.45%	0.637%
15	11.654	3064	3073	3080	rVV	2130607	3956973	10.09%	1.180%
16	11.696	3081	3086	3096	rVB2	1828573	2883572	7.36%	0.860%
17	11.757	3096	3105	3112	rBV2	728741	1366617	3.49%	0.407%
18	11.853	3127	3135	3142	rBV4	1263849	1913332	4.88%	0.570%
19	11.924	3143	3157	3169	rBV6	4546783	11593737	29.57%	3.456%
20	11.982	3170	3175	3179	rBV3	826348	962210	2.45%	0.287%
21	12.046	3187	3195	3204	rVB	8322686	11926369	30.42%	3.555%
22	12.123	3210	3219	3222	rBV4	4170315	6559590	16.73%	1.956%
23	12.159	3224	3230	3240	rVB3	7425193	12748939	32.52%	3.801%
24	12.297	3263	3273	3282	rVB7	4561760	8219967	20.97%	2.450%
25	12.410	3295	3308	3317	rBV7	2577404	5825268	14.86%	1.737%
26	12.493	3317	3334	3339	rBV7	3081038	7646962	19.51%	2.280%
27	12.564	3349	3356	3369	rVB3	11546300	21721184	55.40%	6.475%
28	12.648	3370	3382	3392	rBV5	6076954	14888316	37.98%	4.438%
29	12.728	3394	3407	3417	rVV6	13316801	39204852	100.00%	11.687%
30	12.783	3419	3424	3434	rVB3	9001748	14389492	36.70%	4.290%
31	12.873	3445	3452	3458	rBV4	4481407	6206462	15.83%	1.850%
32	12.911	3459	3464	3467	rBV2	2105717	2495430	6.37%	0.744%
33	12.966	3476	3481	3495	rVB8	6225890	12257634	31.27%	3.654%
34	13.152	3533	3539	3542	rBV3	3454882	4700824	11.99%	1.401%

LSC Area Percent Report

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Sample : K5957-07
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

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\82N112019W.M
Title : SW846 8260

35	13.242	3553	3567	3589	rVB7	11664889	34739272	88.61%	10.356%
36	13.599	3673	3678	3686	rBV7	1630381	2575518	6.57%	0.768%
37	13.667	3689	3699	3709	rVV5	15283100	28969324	73.89%	8.636%
38	13.715	3710	3714	3722	rVB2	3543324	4555065	11.62%	1.358%
39	13.995	3793	3801	3812	rVB5	3244938	6436435	16.42%	1.919%
40	14.178	3848	3858	3886	rVB9	8277442	24556001	62.64%	7.320%
41	14.297	3887	3895	3900	rBV2	2376174	3597227	9.18%	1.072%
42	14.336	3901	3907	3914	rBV2	3393662	4413028	11.26%	1.316%
43	14.532	3962	3968	3976	rVB3	1170361	1583188	4.04%	0.472%
44	14.596	3980	3988	3998	rVV3	2131026	4064279	10.37%	1.212%
45	14.654	3998	4006	4016	rVB2	2132939	3581378	9.14%	1.068%
46	14.856	4063	4069	4075	rVB3	1055184	1360692	3.47%	0.406%
47	14.892	4075	4080	4091	rVV3	746833	1296287	3.31%	0.386%
48	14.959	4093	4101	4111	rVB4	1406318	2713140	6.92%	0.809%

Sum of corrected areas: 335442739

LSC Report - Integrated Chromatogram

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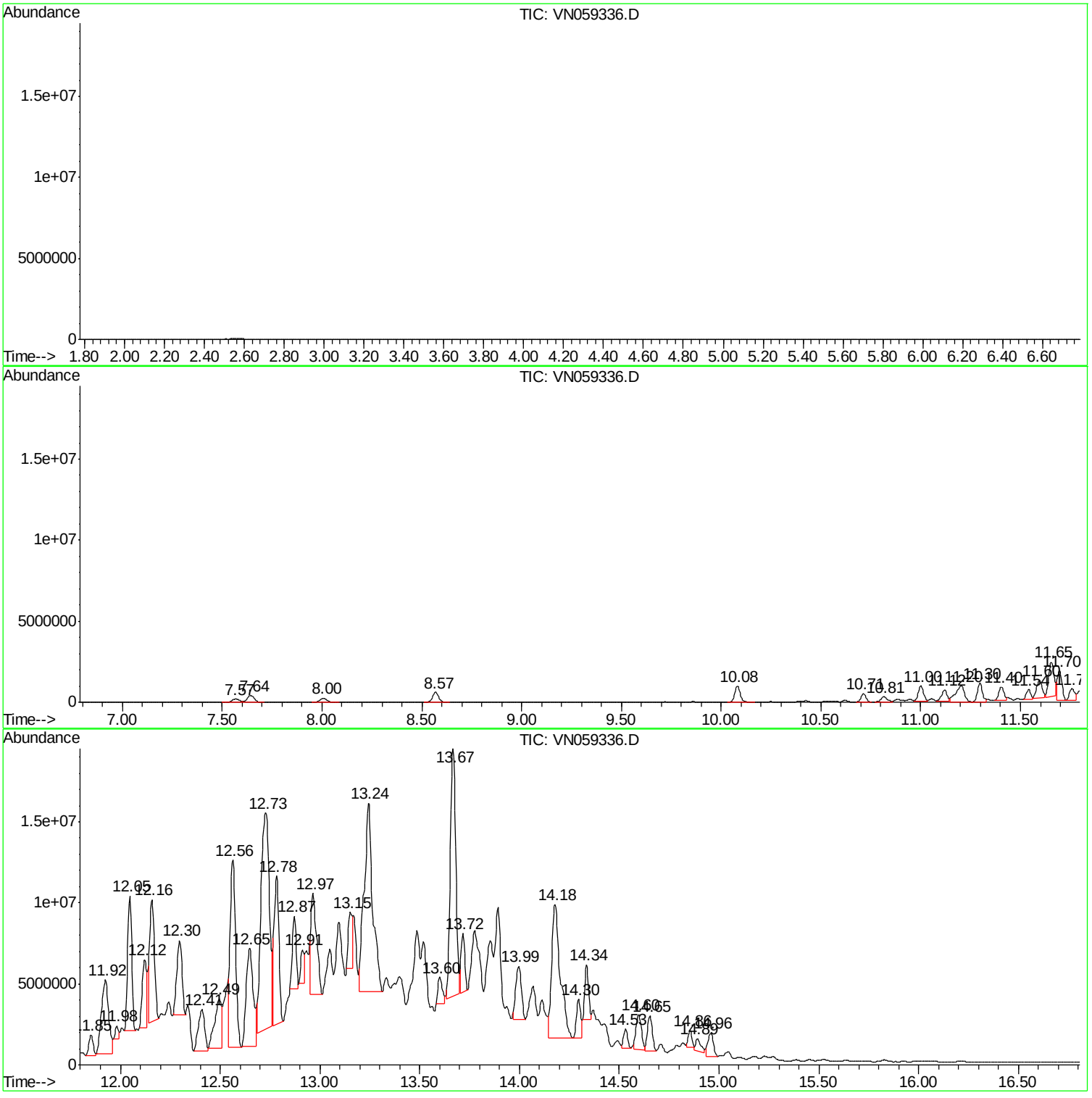
Data File : VN059336.D
Acq On : 21 Nov 2019 15:28
Operator : JC/SP
Sample : K5957-07
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059336.D
Acq On : 21 Nov 2019 15:28
Operator : JC/SP
Sample : K5957-07
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

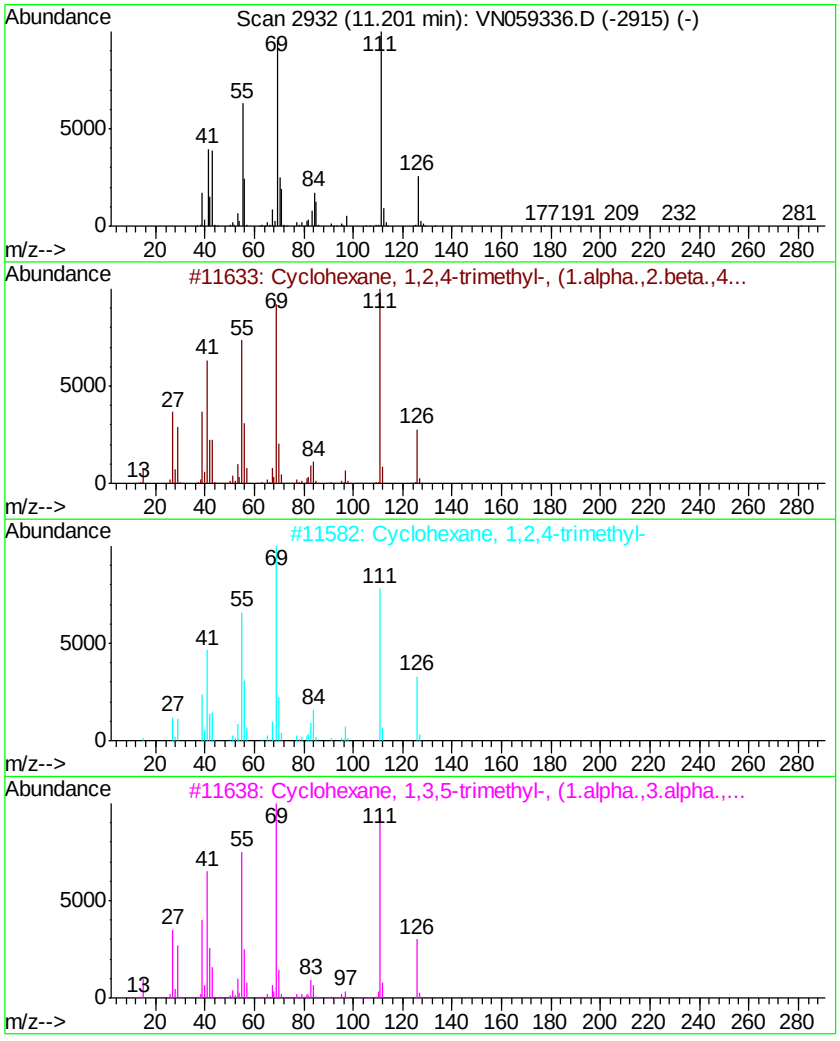
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

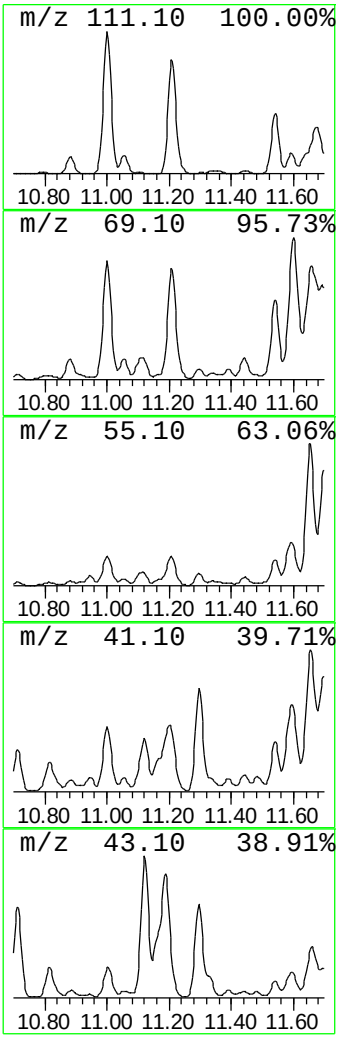
****

Peak Number 1 Cyclohexane, 1,2,4-trimethy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	98.07 ug/l	3063660	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	94
2	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	93
3	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	87
4	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	74
5	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	74





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059336.D
Acq On : 21 Nov 2019 15:28
Operator : JC/SP
Sample : K5957-07
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

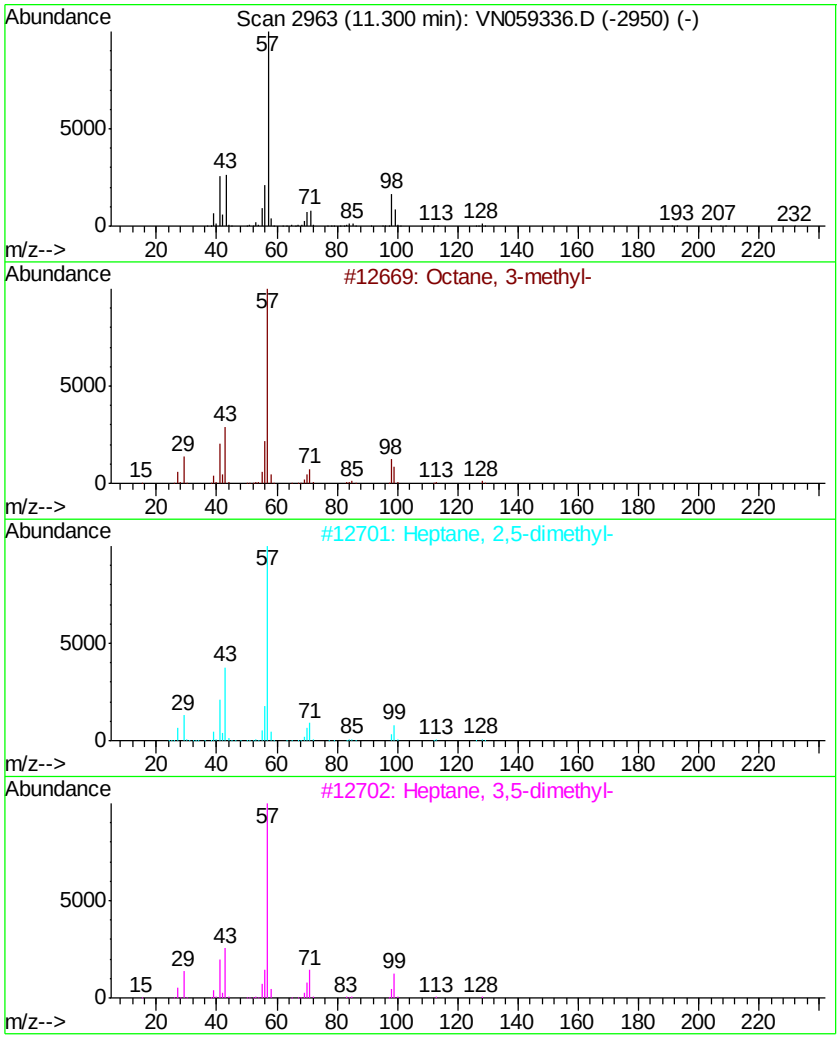
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

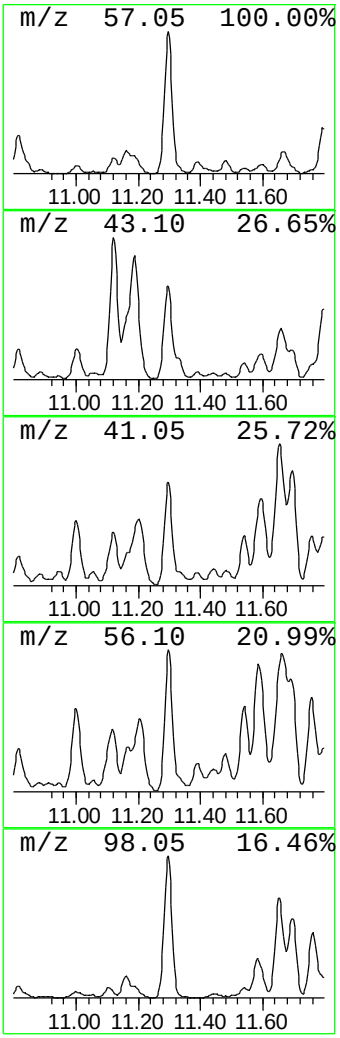
****

Peak Number 2 Octane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	67.39 ug/l	2105220	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-	128	C9H20	002216-33-3	91
2	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	72
3	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	64
4	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	64
5	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059336.D
Acq On : 21 Nov 2019 15:28
Operator : JC/SP
Sample : K5957-07
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

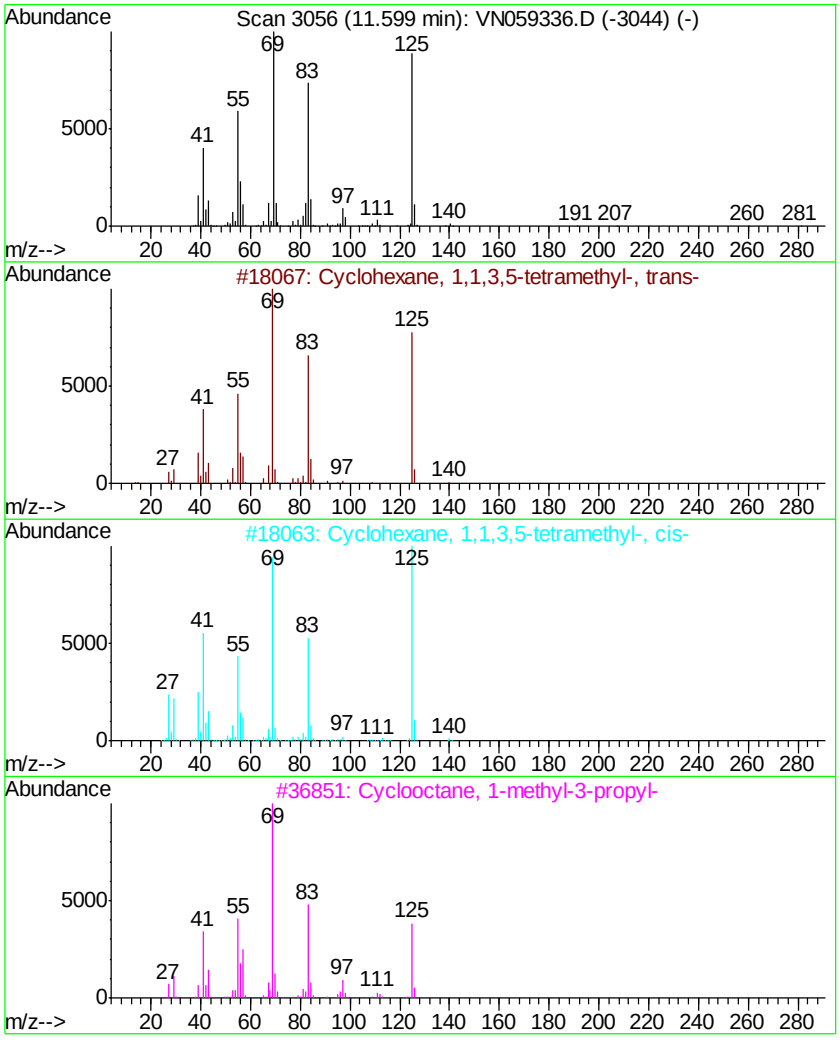
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

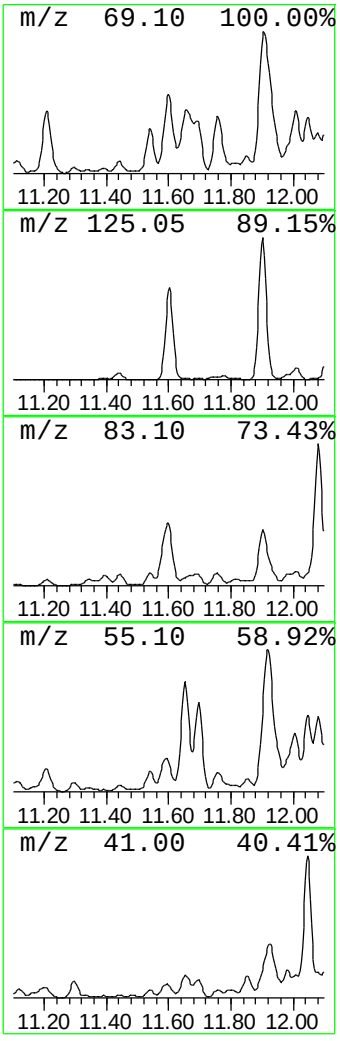
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, 1,1,3,5-tetram... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	68.44 ug/l	2138200	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	87
2	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	72
3	Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	64
4	2,2-Dimethyl-3-heptene trans	126	C9H18	019550-75-5	45
5	Cyclohexane, propyl-	126	C9H18	001678-92-8	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059336.D
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Operator : JC/SP
Sample : K5957-07
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

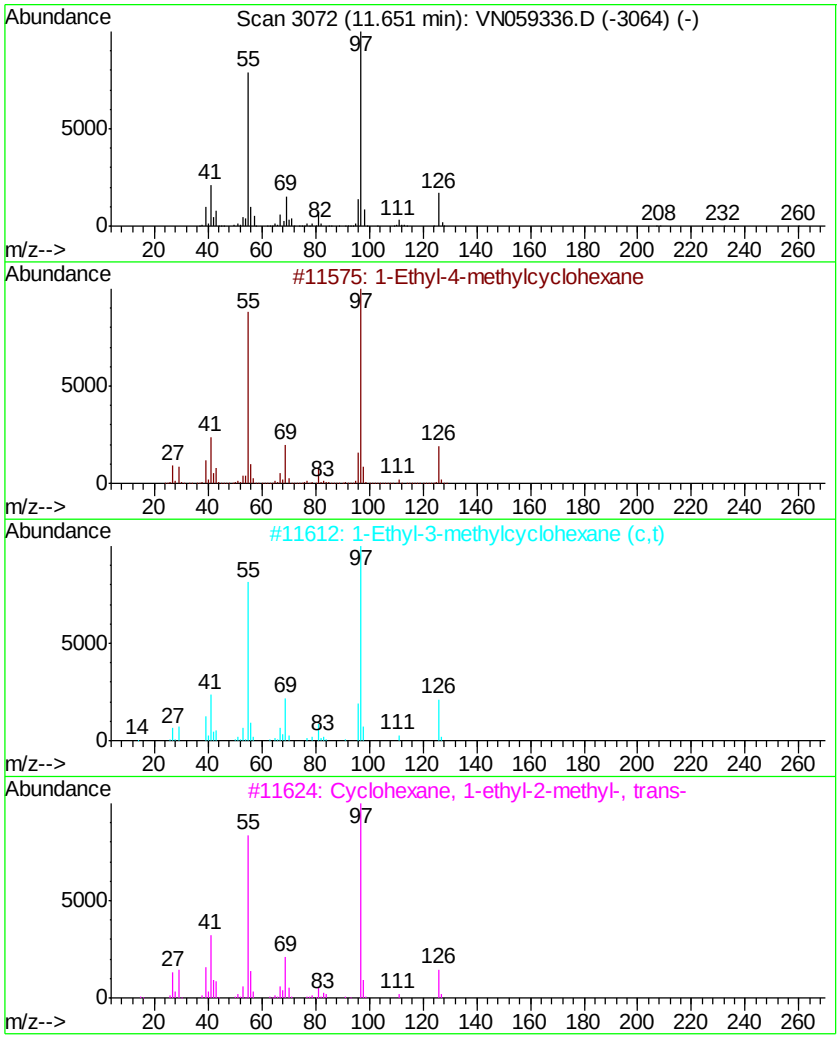
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

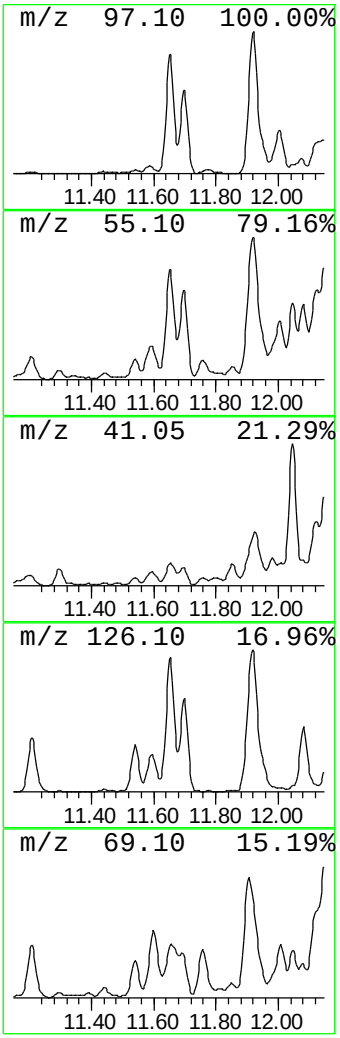
****

Peak Number 4 1-Ethyl-4-methylcyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	126.66 ug/l	3956970	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	95
2	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	94
3	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	87
4	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	87
5	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	81





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Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

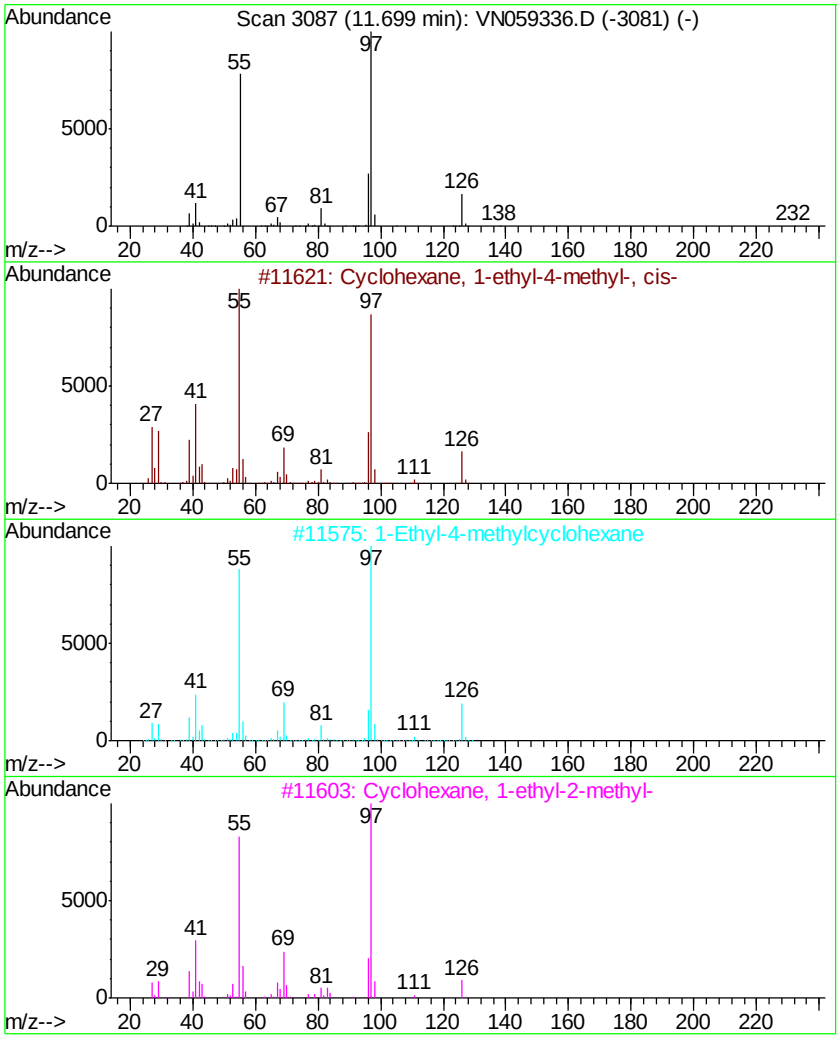
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

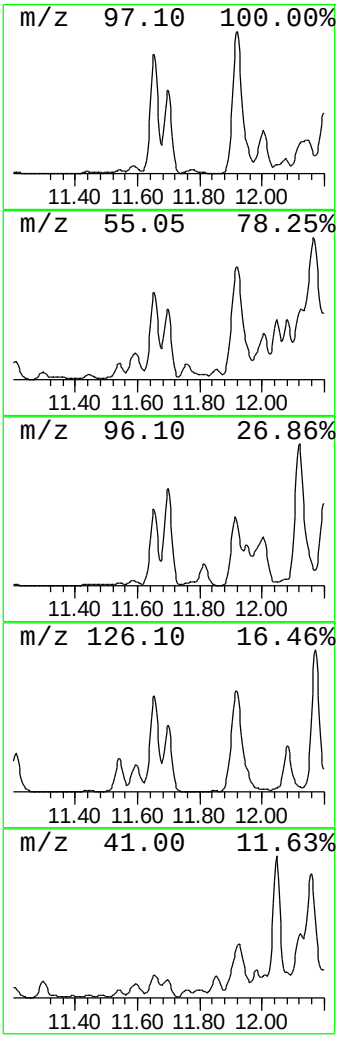
****

Peak Number 5 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	92.30 ug/l	2883570	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	90
2	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	87
3	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	72
4	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	59
5	4-Octen-3-one	126	C8H14O	014129-48-7	59





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Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

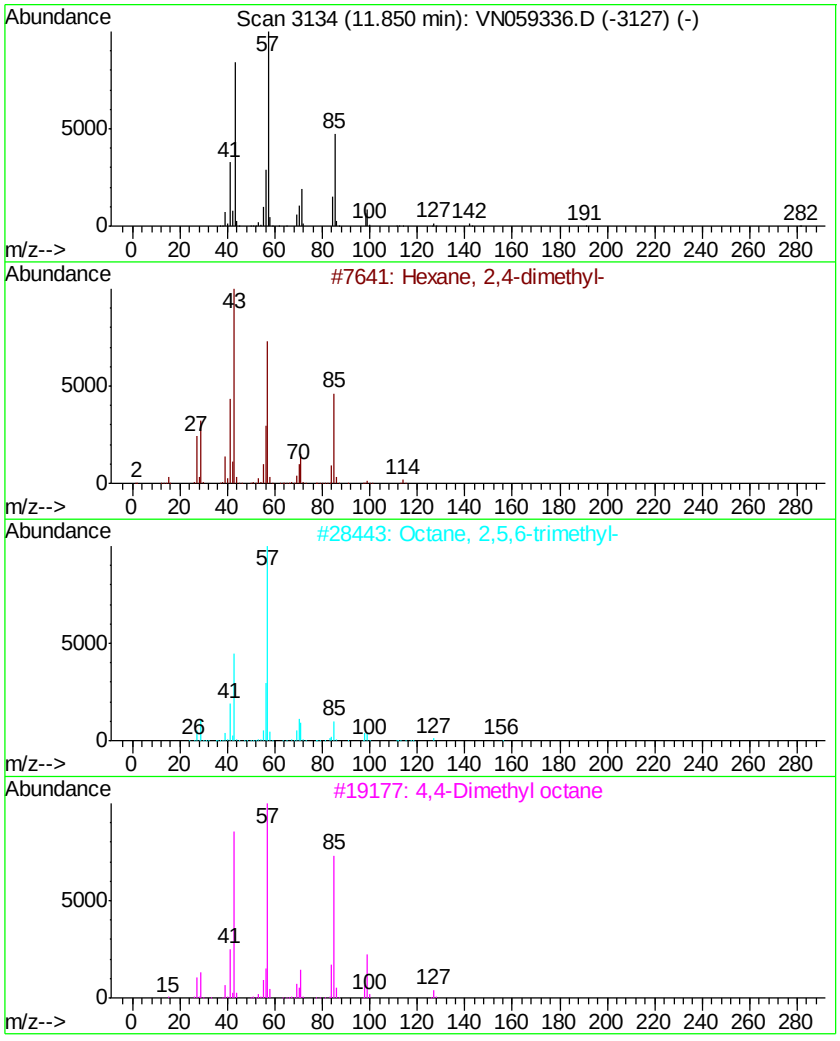
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

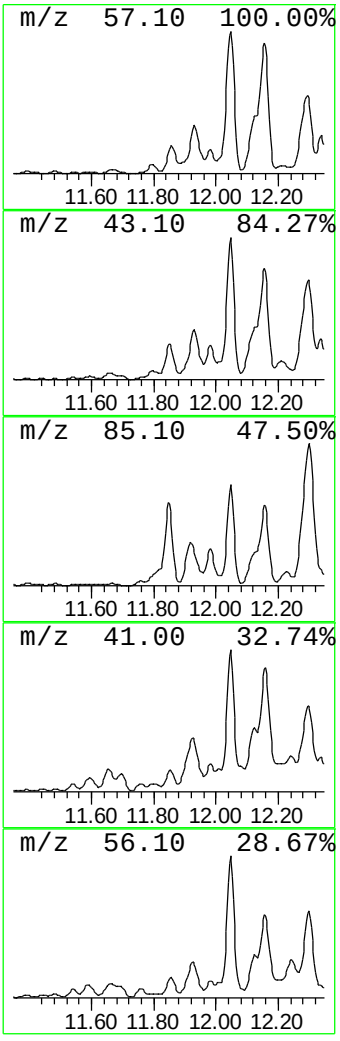
****

Peak Number 6 Hexane, 2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	61.24 ug/l	1913330	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
2	Octane, 2,5,6-trimethyl-	156	C11H24	062016-14-2	64
3	4,4-Dimethyl octane	142	C10H22	015869-95-1	59
4	Heptane, 2,2,3,3,5,6,6-heptamethyl-	198	C14H30	007225-67-4	53
5	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059336.D
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Operator : JC/SP
Sample : K5957-07
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

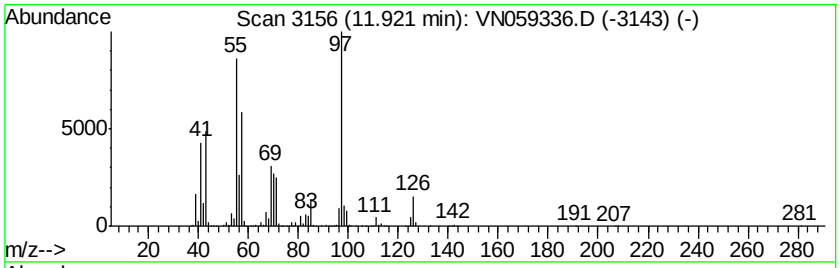
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

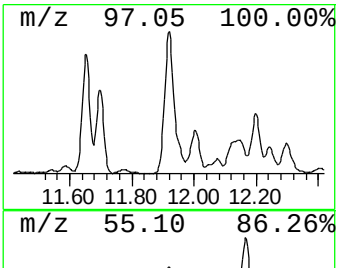
****

Peak Number 7 2-Hexene, 3,4,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	371.11 ug/l	11593700	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	53
2	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	53
3	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	49
4	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	49
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	49





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059336.D
Acq On : 21 Nov 2019 15:28
Operator : JC/SP
Sample : K5957-07
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

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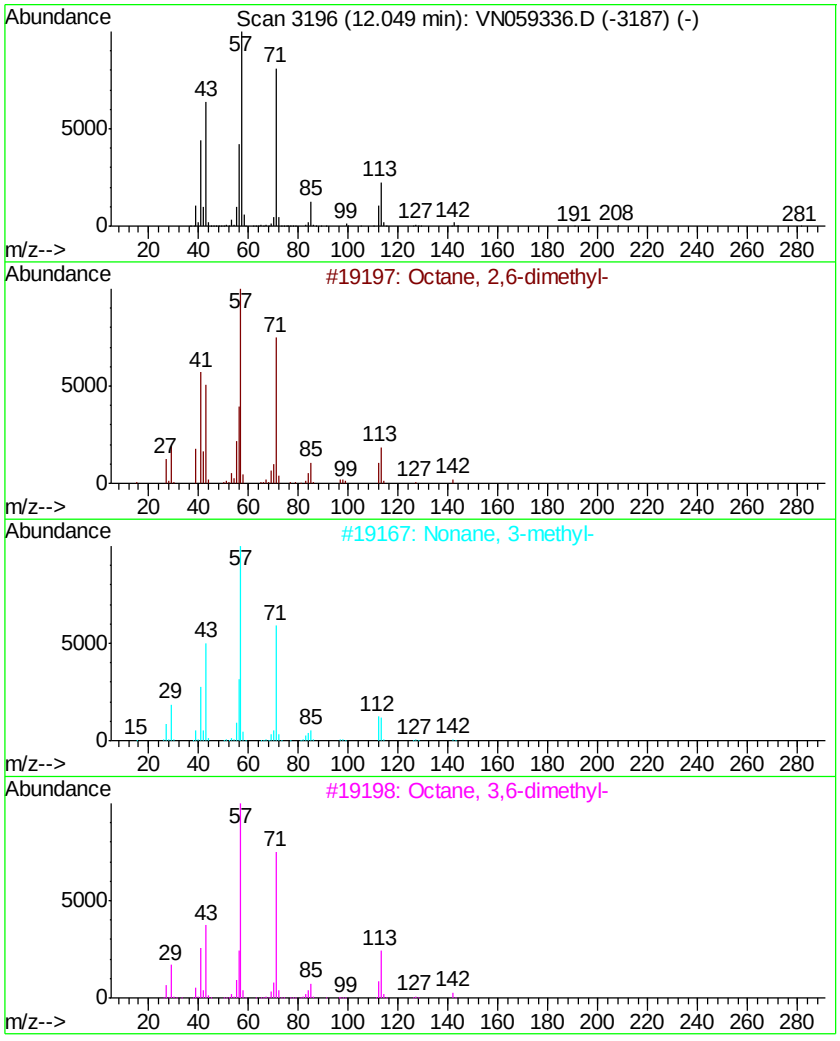
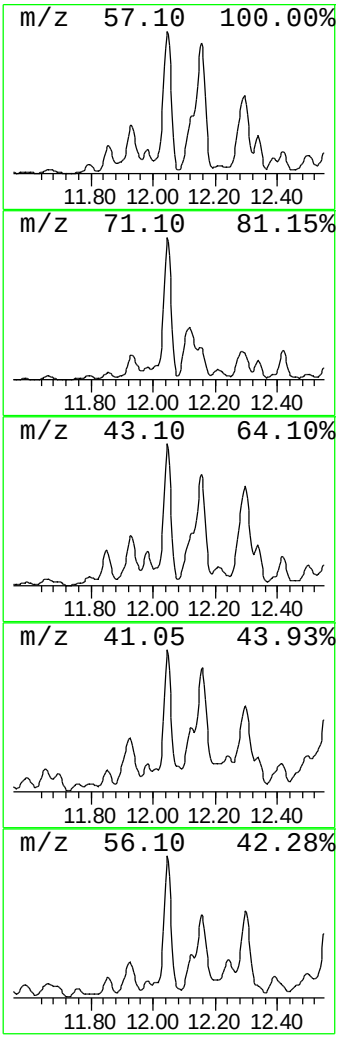
Peak Number 8 Octane, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	381.76 ug/l	11926400	Chlorobenzene-d5	11.41

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	83
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	80
4	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	59
5	Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059336.D
Acq On : 21 Nov 2019 15:28
Operator : JC/SP
Sample : K5957-07
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

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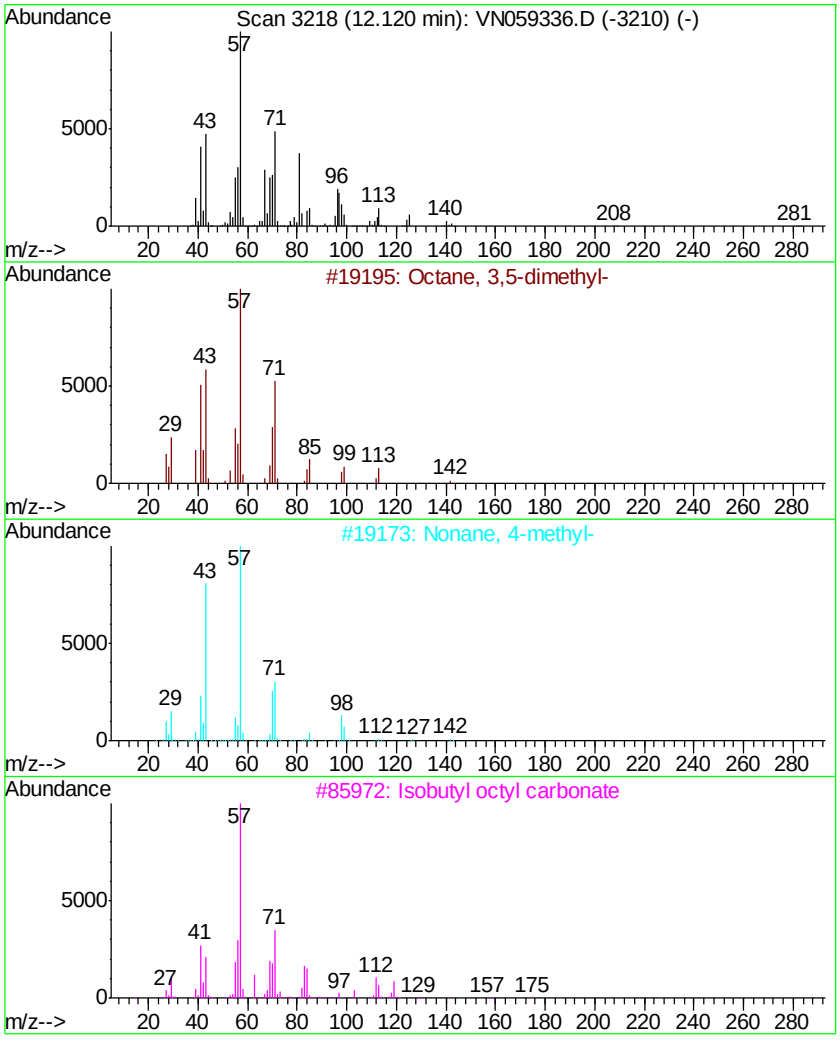
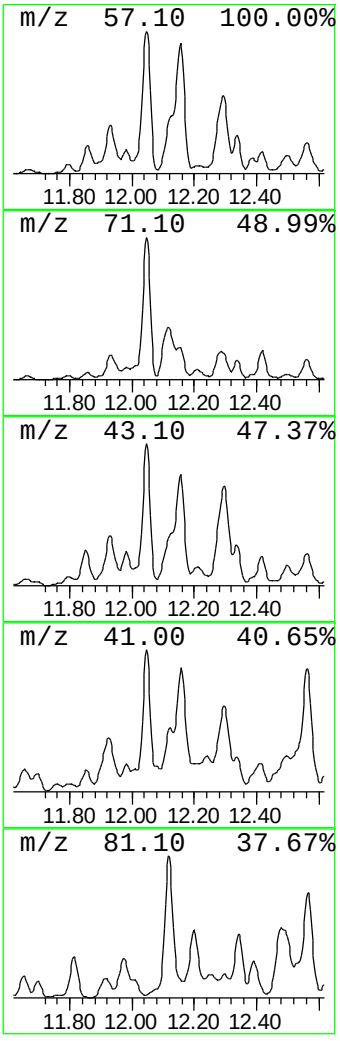
Peak Number 9 Octane, 3,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	209.97 ug/l	6559590	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53
2	Nonane, 4-methyl-	142	C10H22	017301-94-9	49
3	Isobutyl octyl carbonate	230	C13H26O3	1000372-74-6	47
4	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	43
5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059336.D
Acq On : 21 Nov 2019 15:28
Operator : JC/SP
Sample : K5957-07
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

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

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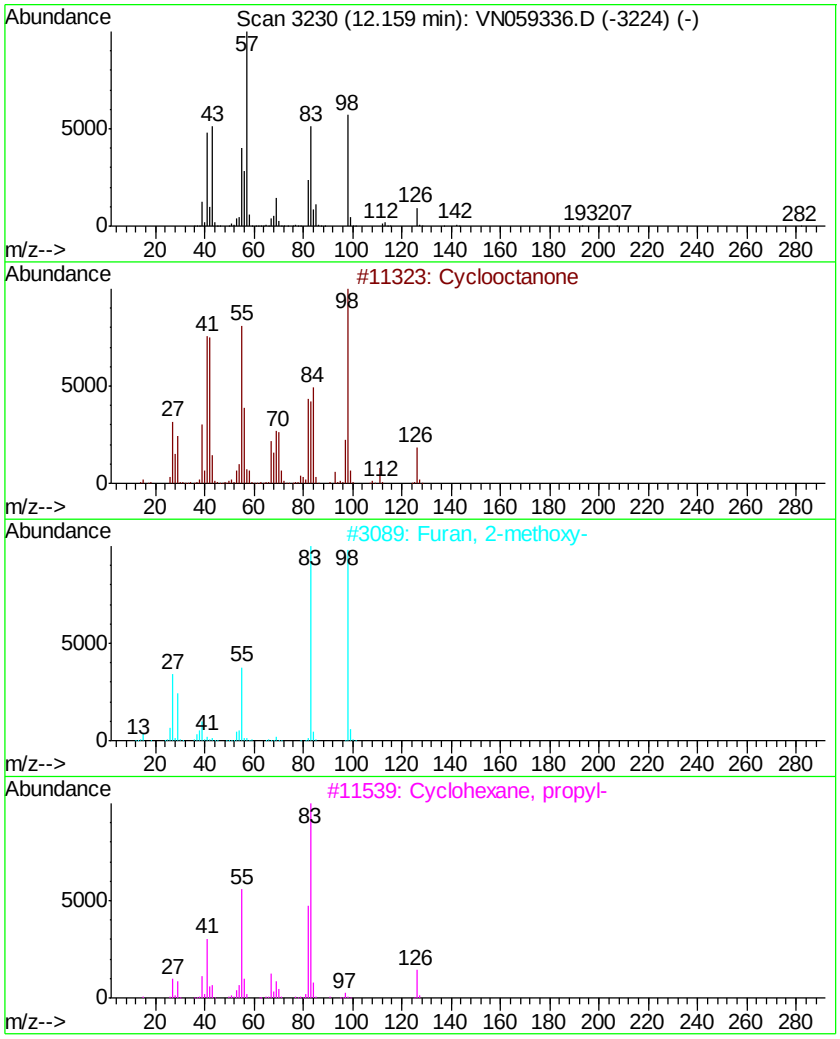
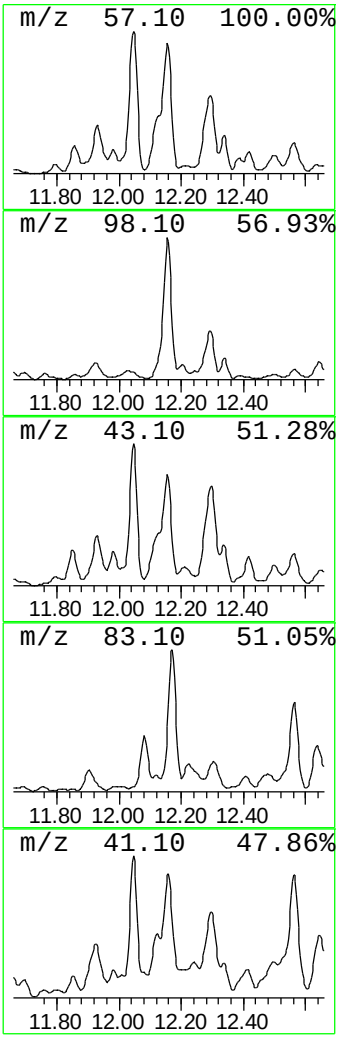
Peak Number 10 unknown12.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	408.09 ug/l	12748900	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctanone	126	C8H14O	000502-49-8	43
2	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	38
3	Cyclohexane, propyl-	126	C9H18	001678-92-8	38
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	38
5	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059336.D
Acq On : 21 Nov 2019 15:28
Operator : JC/SP
Sample : K5957-07
Misc : 3.31g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(12-14)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
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
Cyclohexane, 1,2,...	11.20	98.1	ug/l	3063660	3	11.41	1562040	50.0
Octane, 3-methyl-	11.30	67.4	ug/l	2105220	3	11.41	1562040	50.0
Cyclohexane, 1,1,...	11.60	68.4	ug/l	2138200	3	11.41	1562040	50.0
1-Ethyl-4-methylc...	11.65	126.7	ug/l	3956970	3	11.41	1562040	50.0
Cyclohexane, 1-et...	11.70	92.3	ug/l	2883570	3	11.41	1562040	50.0
Hexane, 2,4-dimet...	11.85	61.2	ug/l	1913330	3	11.41	1562040	50.0
2-Hexene, 3,4,4-t...	11.92	371.1	ug/l	11593700	3	11.41	1562040	50.0
Octane, 2,6-dimet...	12.05	381.8	ug/l	11926400	3	11.41	1562040	50.0
Octane, 3,5-dimet...	12.12	210.0	ug/l	6559590	3	11.41	1562040	50.0
unknown12.16	12.16	408.1	ug/l	12748900	3	11.41	1562040	50.0