LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059341.D
Acq On : 21 Nov 2019 17:17
Operator : JC/SP
Sample : K5957-06 10X
Misc : 5.45g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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	7.571	1780	1803	1814	rBV	237580	603159	2.93%	0.223%
2	7.644	1814	1826	1847	rVB	497787	1181621	5.75%	0.437%
3	8.008	1917	1939	1959	rBV	280299	646299	3.14%	0.239%
4	8.570	2097	2114	2133	rBV	713873	1480214	7.20%	0.547%
5	9.069	2246	2269	2281	rBV2	132163	315237	1.53%	0.117%
6	9.860	2495	2515	2538	rBV3	101823	287860	1.40%	0.106%
7	10.082	2569	2584	2611	rVB2	1454300	3044101	14.80%	1.126%
8	10.249	2628	2636	2660	rVB6	99754	277610	1.35%	0.103%
9	10.426	2682	2691	2705	rVB	310399	578711	2.81%	0.214%
10	10.525	2709	2722	2730	rBV3	161923	335926	1.63%	0.124%
11	10.622	2744	2752	2761	rVB	175791	274678	1.34%	0.102%
12	10.715	2770	2781	2793	rVB	545888	932477	4.53%	0.345%
13	10.815	2798	2812	2825	rBV	441793	920996	4.48%	0.341%
14	10.882	2825	2833	2841	rVV3	234361	419980	2.04%	0.155%
15	10.947	2844	2853	2861	rVV	851219	1400026	6.81%	0.518%
16	11.001	2861	2870	2880	rVV2	1239889	2153962	10.47%	0.797%
17	11.056	2881	2887	2895	rVB	228689	318597	1.55%	0.118%
18	11.120	2895	2907	2915	rBV2	1021353	1844996	8.97%	0.682%
19	11.201	2915	2932	2950	rVB5	1520571	4580792	22.28%	1.694%
20	11.297	2950	2962	2982	rBV	1974563	3693006	17.96%	1.366%
21	11.403	2983	2995	3005	rBV2	1015104	1990113	9.68%	0.736%
22	11.490	3014	3022	3030	rBV4	263383	583936	2.84%	0.216%
23	11.541	3030	3038	3044	rVV	632763	877312	4.27%	0.324%
24	11.596	3044	3055	3063	rBV8	1149587	2657341	12.92%	0.983%
25	11.654	3064	3073	3080	rVV2	3678485	6279582	30.54%	2.322%
26	11.696	3081	3086	3096	rVB2	2631352	4212919	20.49%	1.558%
27	11.760	3096	3106	3111	rBV3	561051	999511	4.86%	0.370%
28	11.808	3112	3121	3127	rBV3	464883	925823	4.50%	0.342%
29	11.853	3127	3135	3143	rBV3	1699546	2604739	12.67%	0.963%
30	11.924	3143	3157	3169	rBV5	5511285	13680166	66.52%	5.060%
31	12.046	3187	3195	3203	rBV	6611240	9242782	44.95%	3.418%
32	12.120	3210	3218	3223	rBV4	4316281	7034656	34.21%	2.602%
33	12.165	3224	3232	3251	rVB5	8924718	17649019	85.82%	6.527%
34	12.297	3264	3273	3280	rBV7	3601353	7320841	35.60%	2.708%

LSC Area Percent Report

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Misc : 5.45g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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

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Peak separation: 5

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

35	12.339	3281	3286	3296	rVB2	7690702	11274387	54.83%	4.170%
36	12.410	3296	3308	3316	rBV9	2165983	4538560	22.07%	1.679%
37	12.493	3317	3334	3340	rBV8	1725181	5044647	24.53%	1.866%
38	12.564	3349	3356	3371	rVB4	6185441	12956834	63.01%	4.792%
39	12.654	3371	3384	3391	rBV6	5142145	11111983	54.04%	4.110%
40	12.734	3403	3409	3418	rVB3	10674390	16867737	82.03%	6.238%
41	12.783	3419	3424	3434	rVB3	4692946	7107173	34.56%	2.629%
42	12.873	3445	3452	3458	rBV6	2313746	3360100	16.34%	1.243%
43	12.966	3474	3481	3494	rVB3	8233468	14053639	68.34%	5.198%
44	13.043	3494	3505	3514	rBV	11594000	20564064	100.00%	7.606%
45	13.168	3534	3544	3552	rVB5	2273808	5064278	24.63%	1.873%
46	13.242	3553	3567	3575	rBV3	6825754	13539530	65.84%	5.008%
47	13.377	3602	3609	3626	rVB	5024421	8352062	40.61%	3.089%
48	13.593	3669	3676	3689	rBV4	1843732	3887372	18.90%	1.438%
49	13.667	3690	3699	3709	rVV4	5176560	9360197	45.52%	3.462%
50	13.715	3710	3714	3722	rVB2	1196732	1461357	7.11%	0.540%
51	13.837	3748	3752	3761	rVV5	1406684	2005196	9.75%	0.742%
52	13.892	3763	3769	3778	rVB	2637881	4152089	20.19%	1.536%
53	13.995	3793	3801	3811	rVB5	1352466	2298978	11.18%	0.850%
54	14.181	3850	3859	3875	rVB6	1797776	4624430	22.49%	1.710%
55	14.252	3876	3881	3889	rVB	1140642	1542498	7.50%	0.570%
56	14.300	3889	3896	3901	rBV3	531905	760752	3.70%	0.281%
57	14.336	3901	3907	3915	rVB2	912116	1198332	5.83%	0.443%
58	14.528	3963	3967	3975	rVB3	342389	436223	2.12%	0.161%
59	14.586	3976	3985	3997	rVV3	1330559	2600386	12.65%	0.962%
60	14.651	3998	4005	4016	rVB3	510971	870906	4.24%	0.322%

Sum of corrected areas: 270382698

LSC Report - Integrated Chromatogram

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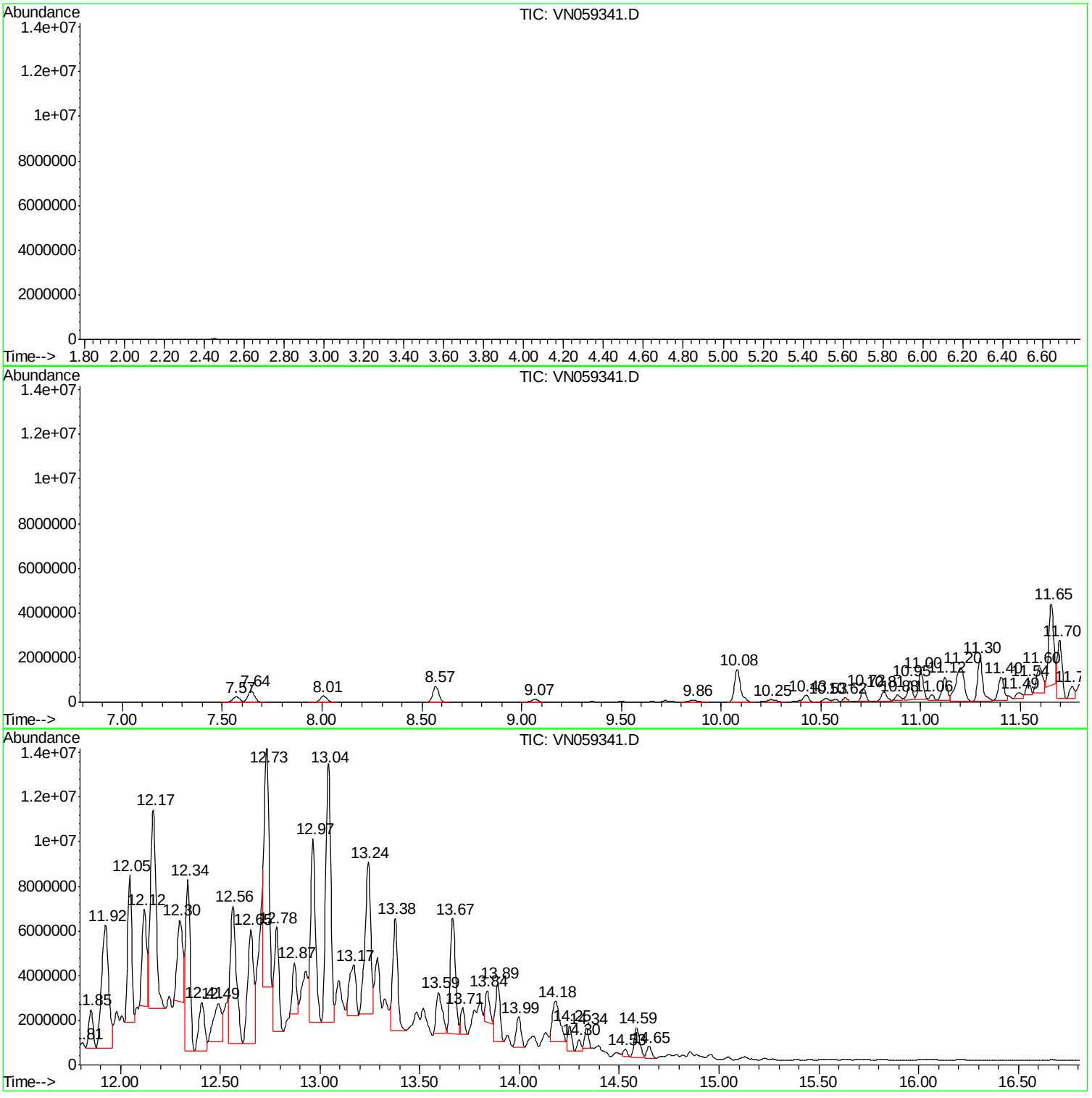
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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

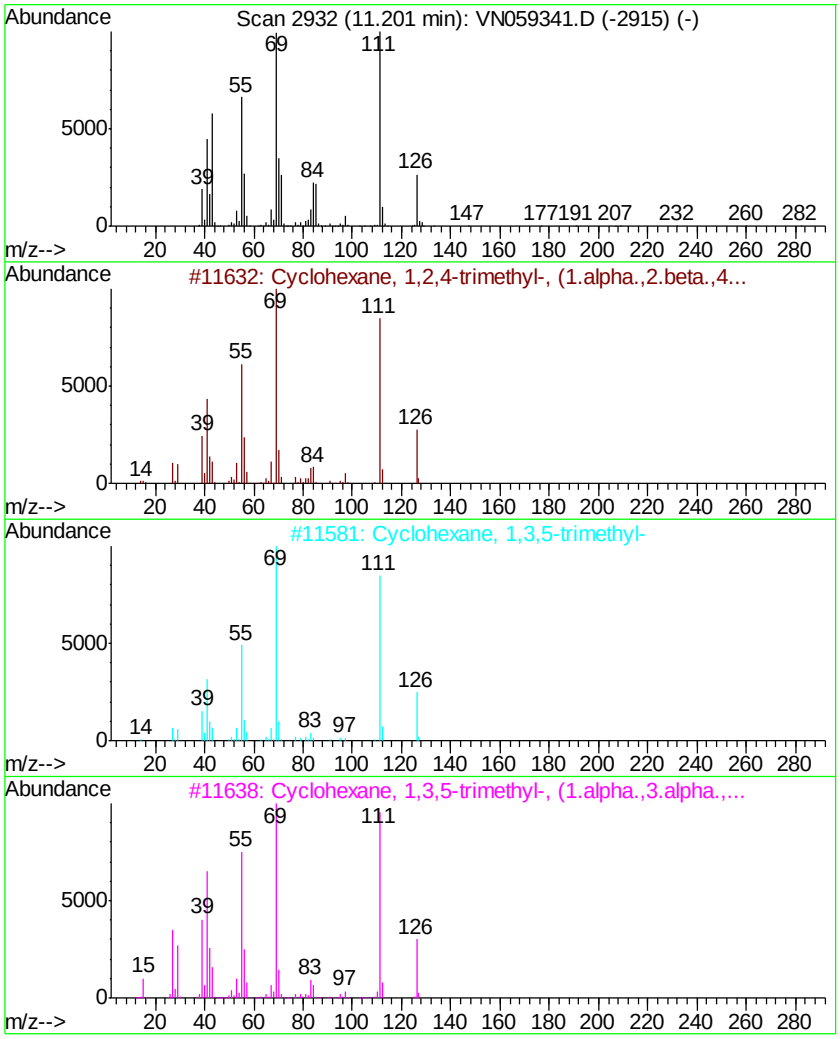
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

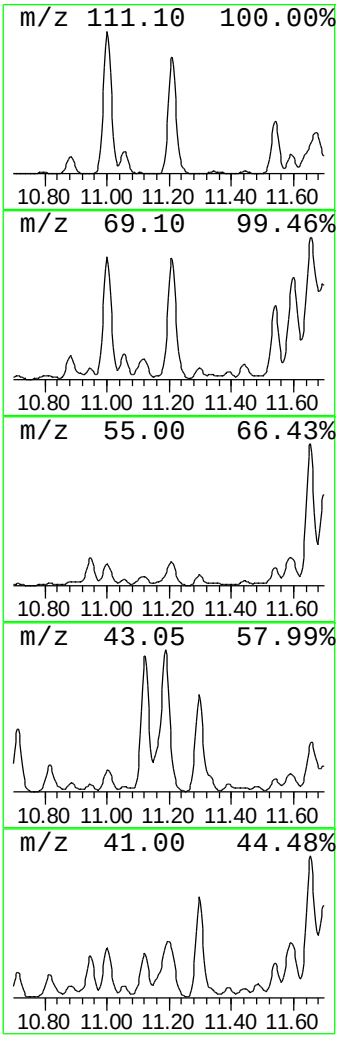
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	115.09 ug/l	4580790	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	76
2	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	70
3	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	68
4	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	62
5	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	62





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059341.D
Acq On : 21 Nov 2019 17:17
Operator : JC/SP
Sample : K5957-06 10X
Misc : 5.45g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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

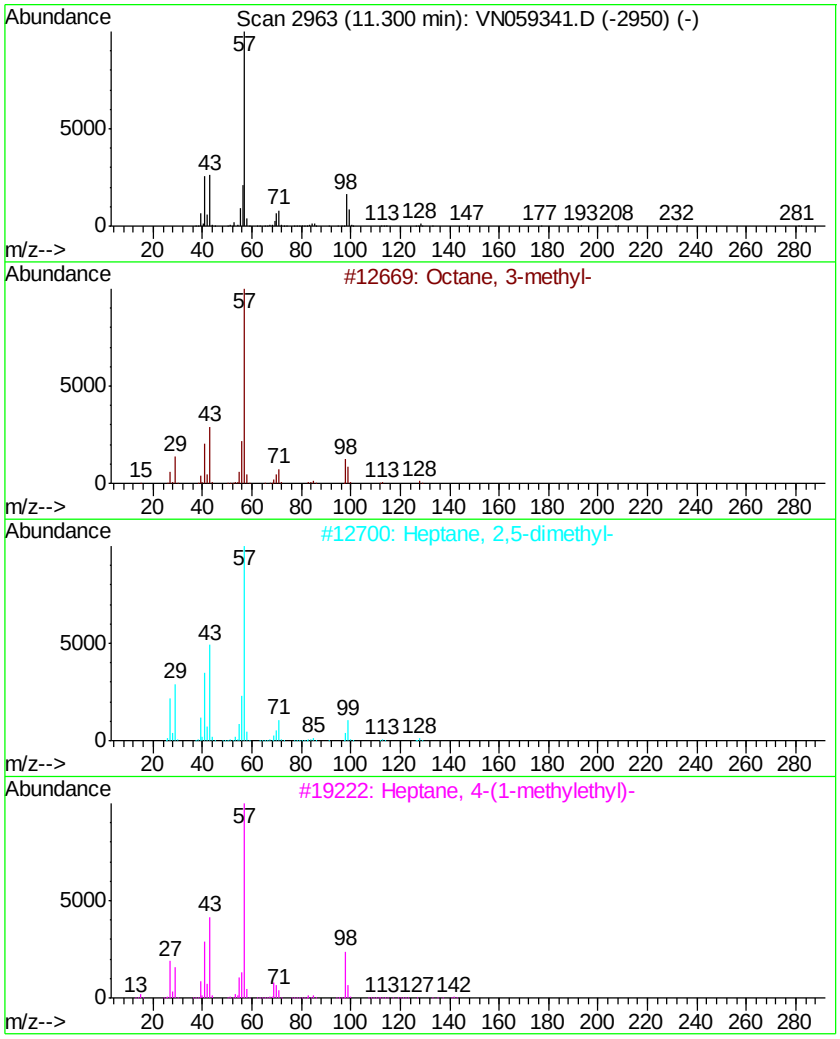
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

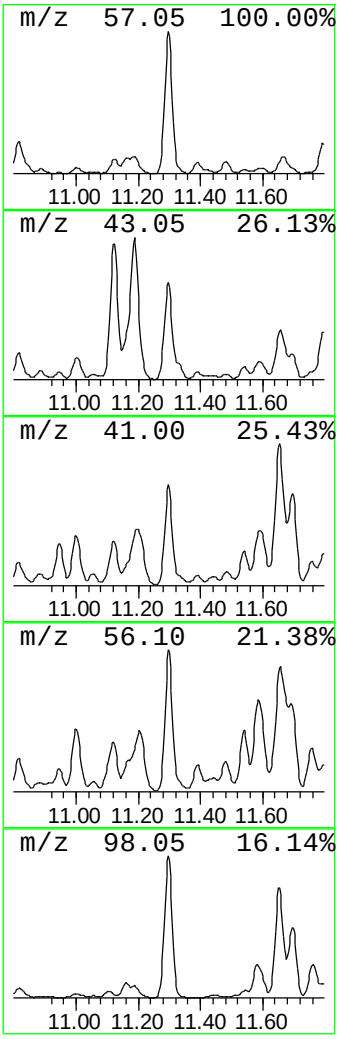
****

Peak Number 2 Octane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	92.78 ug/l	3693010	Chlorobenzene-d5	11.40

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, 4-(1-methylethyl)-	142	C10H22	052896-87-4	64
4	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	59
5	Undecane, 6-methyl-	170	C12H26	017302-33-9	53





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Operator : JC/SP
Sample : K5957-06 10X
Misc : 5.45g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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

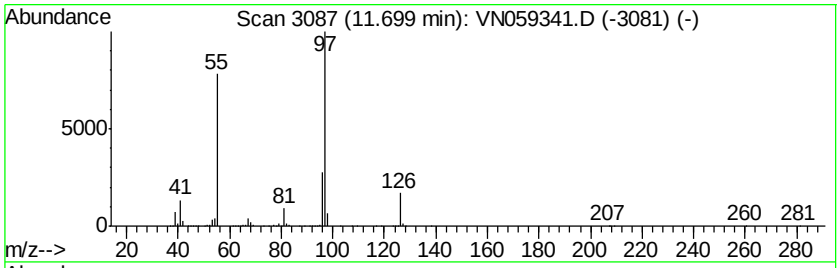
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

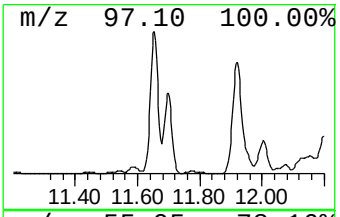
****

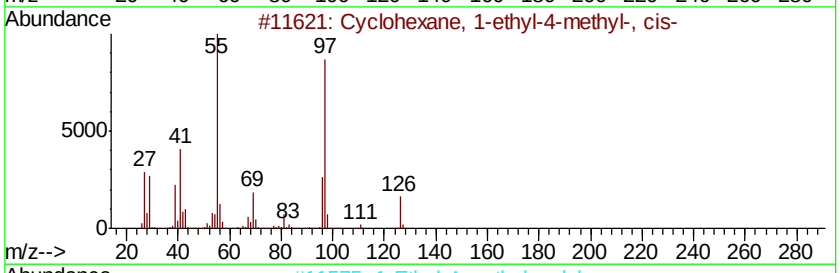
Peak Number 3 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 7

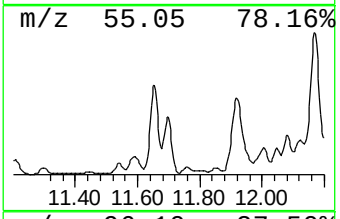
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	105.85 ug/l	4212920	Chlorobenzene-d5	11.40

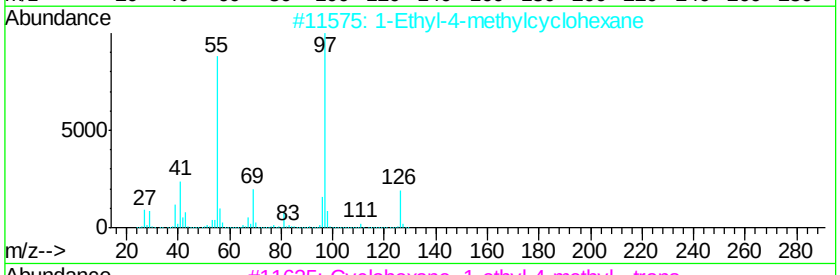
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	86
2	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	72
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	72
4	Cyclopentane, 1-hydroxymethyl-1,...	128	C8H16O	1000156-73-8	64
5	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	59

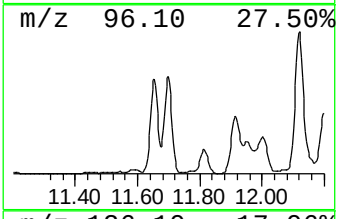


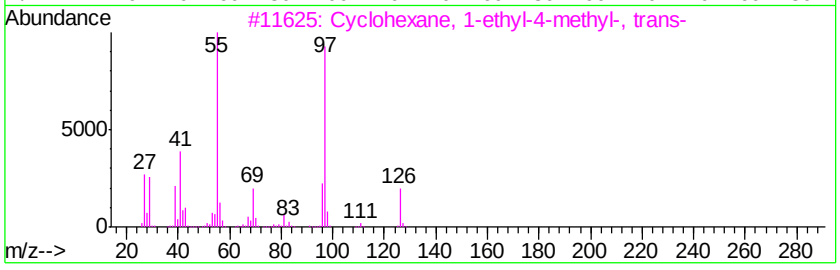


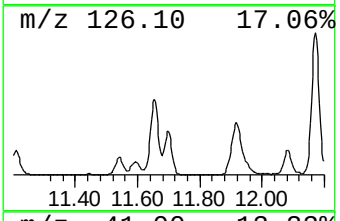


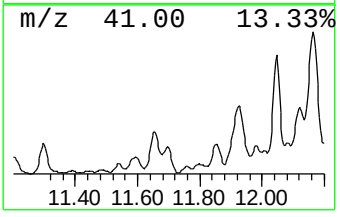












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Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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

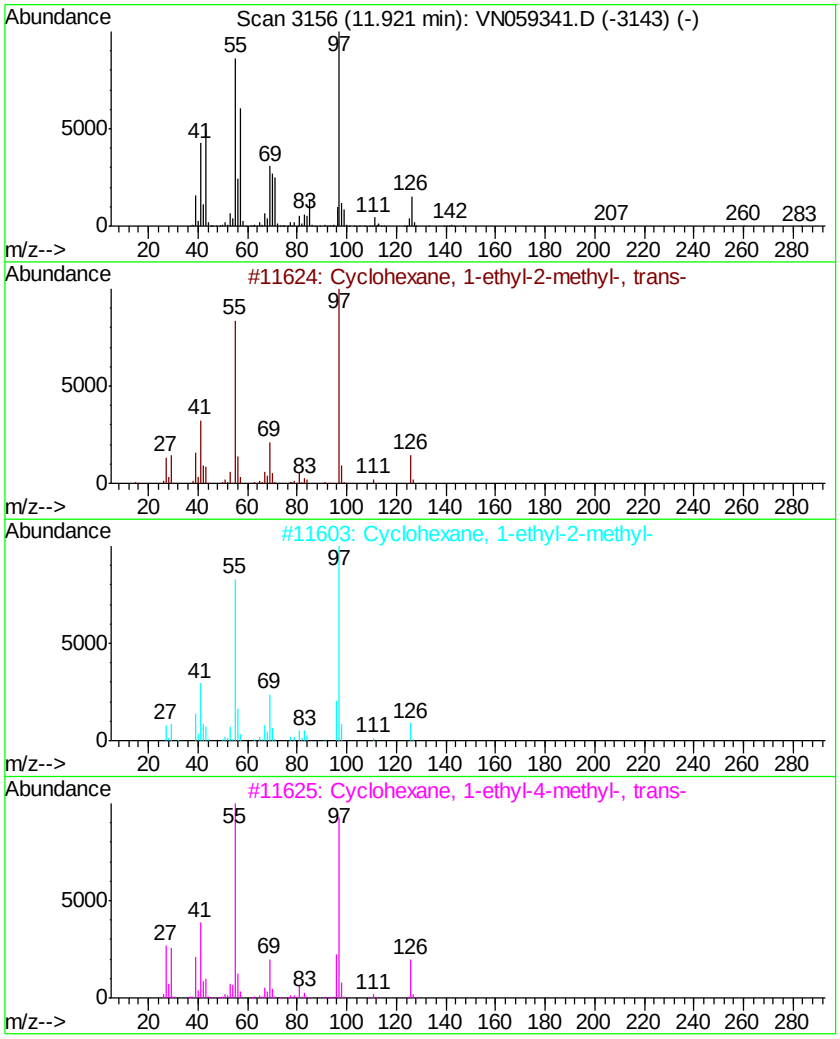
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

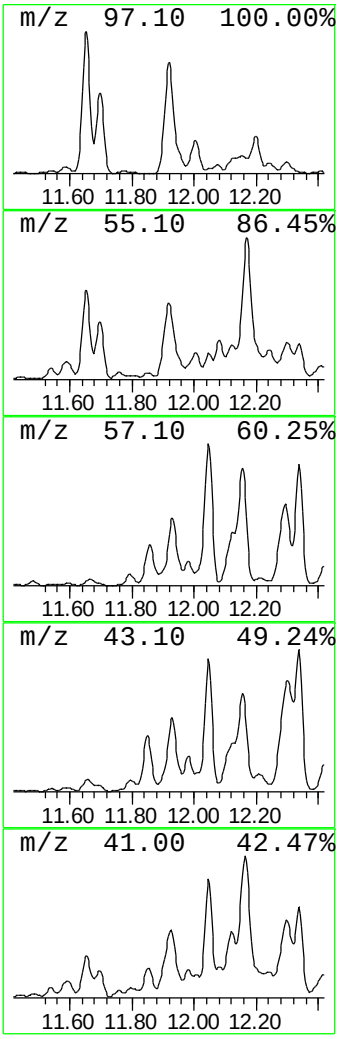
****

Peak Number 4 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	343.70 ug/l	13680200	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	60
2	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	53
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	49
4	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	49
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	49





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Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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

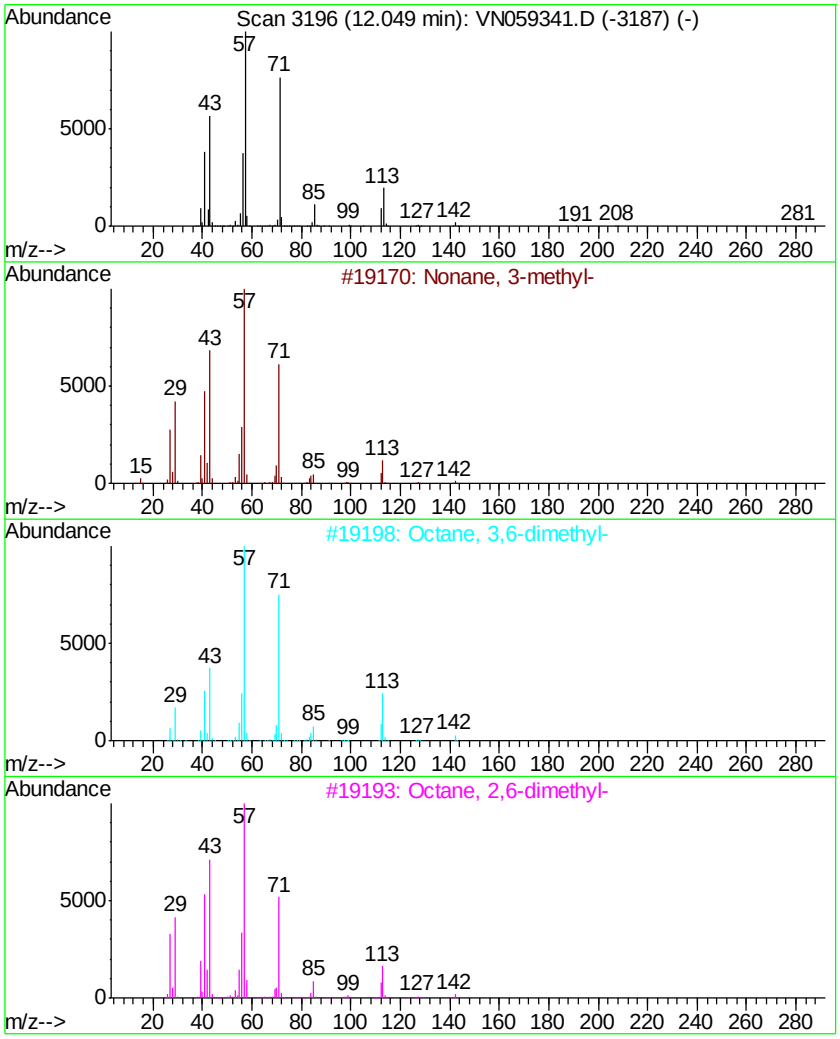
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

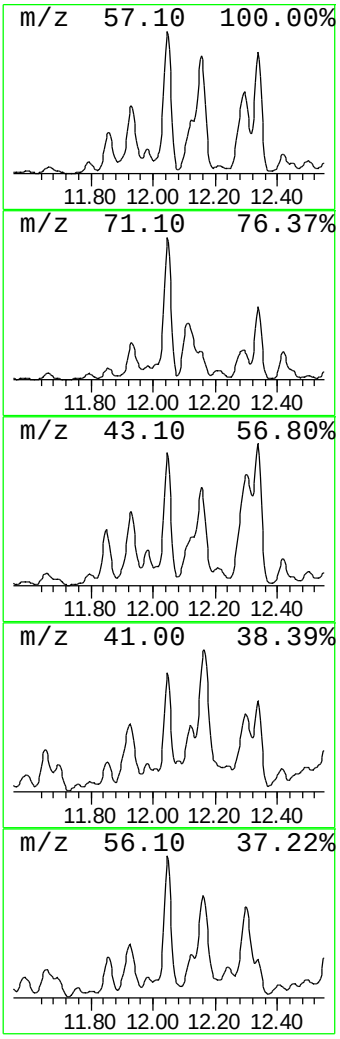
****

Peak Number 5 Nonane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	232.22 ug/l	9242780	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	91
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	90
3	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	83
4	Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	78
5	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	72





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

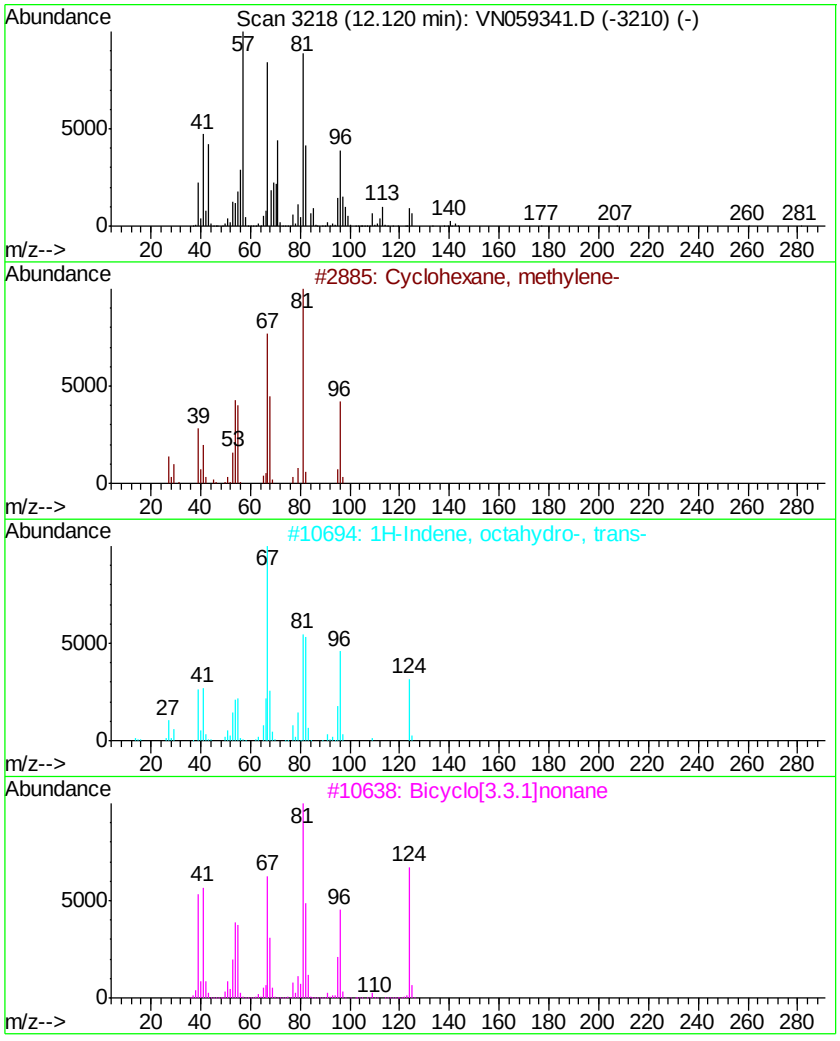
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

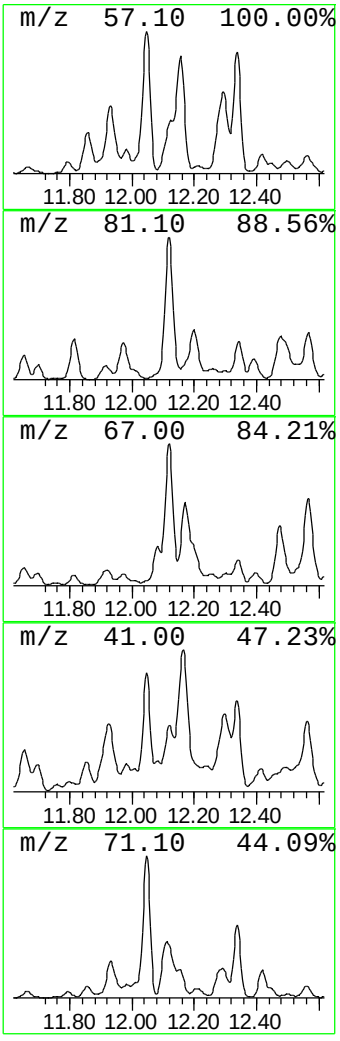
****

Peak Number 6 Cyclohexane, methylene- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	176.74 ug/l	7034660	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, methylene-	96	C7H12	001192-37-6	52
2	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	49
3	Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	46
4	1H-Indene, octahydro-, cis-	124	C9H16	004551-51-3	30
5	2-Butenenitrile, 2-amino-3-methyl-	96	C5H8N2	1000196-28-0	30





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059341.D
Acq On : 21 Nov 2019 17:17
Operator : JC/SP
Sample : K5957-06 10X
Misc : 5.45g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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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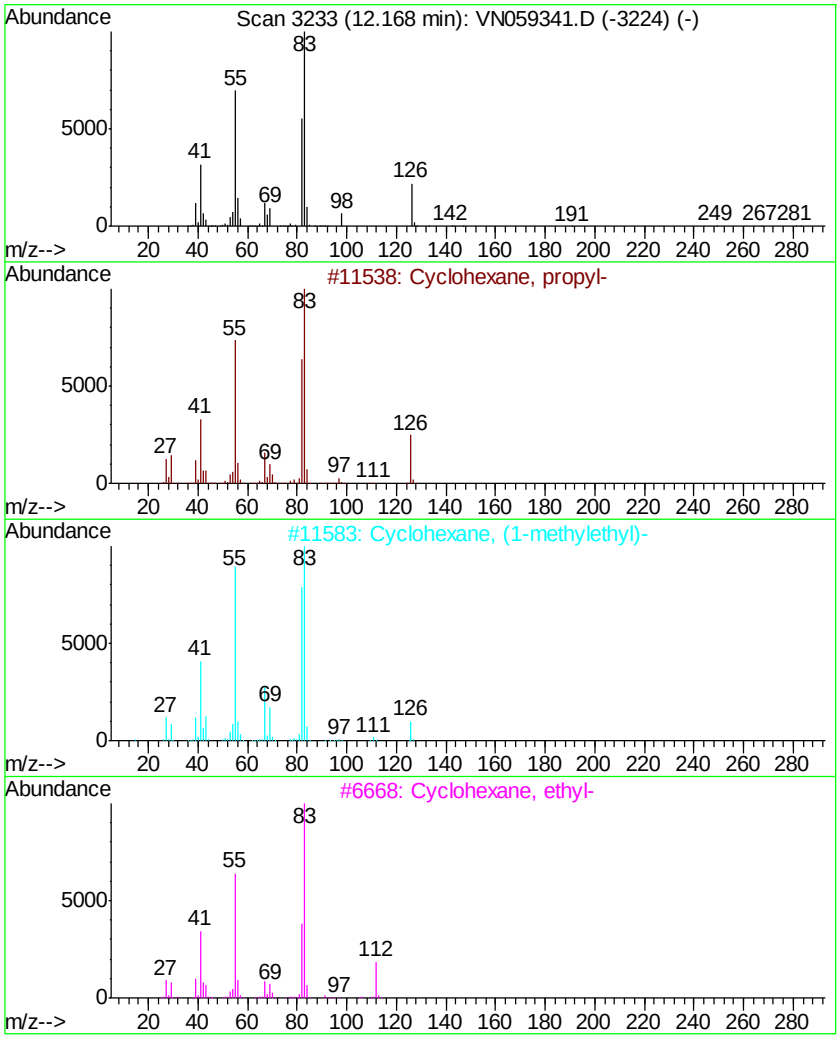
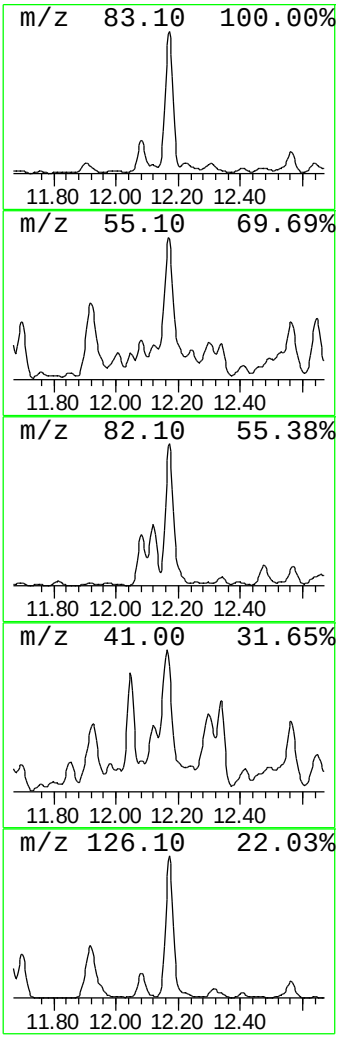
Peak Number 7 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	443.42 ug/l	17649000	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	90
2	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	64
3	Cyclohexane, ethyl-	112	C8H16	001678-91-7	64
4	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	53
5	Oxalic acid, cyclohexyl dodecyl ...	340	C20H36O4	1000309-31-4	50





Library Search Compound Report

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Data File : VN059341.D
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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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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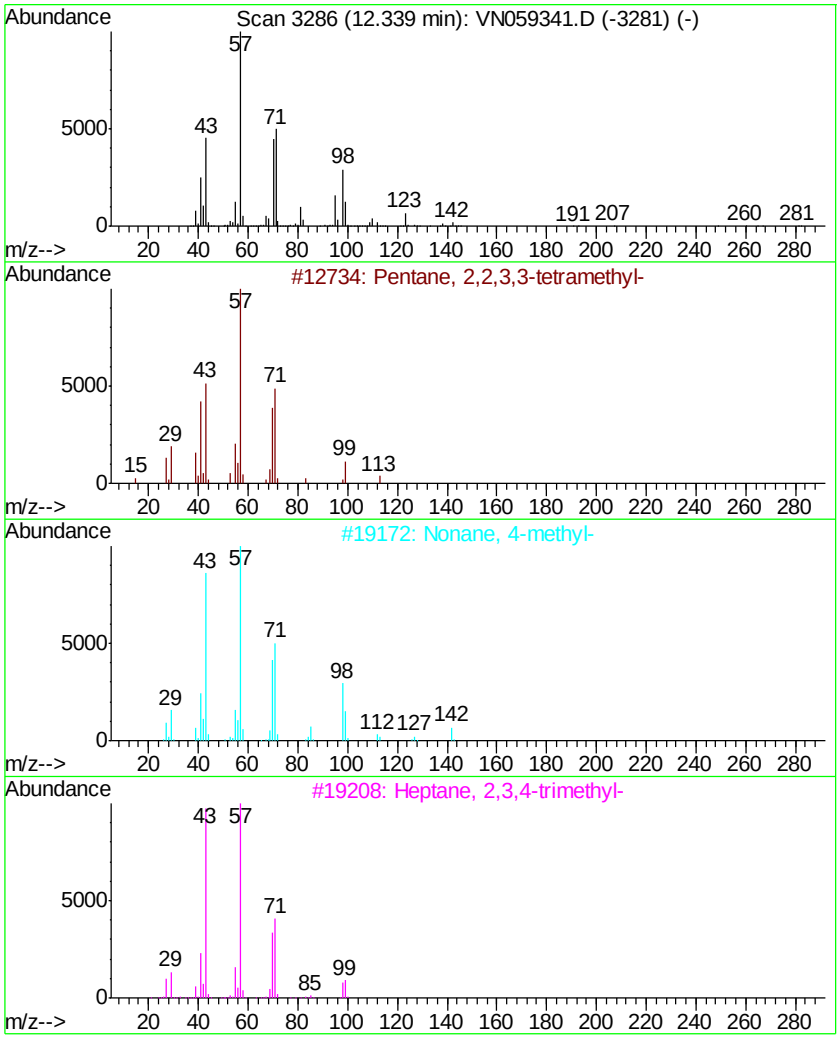
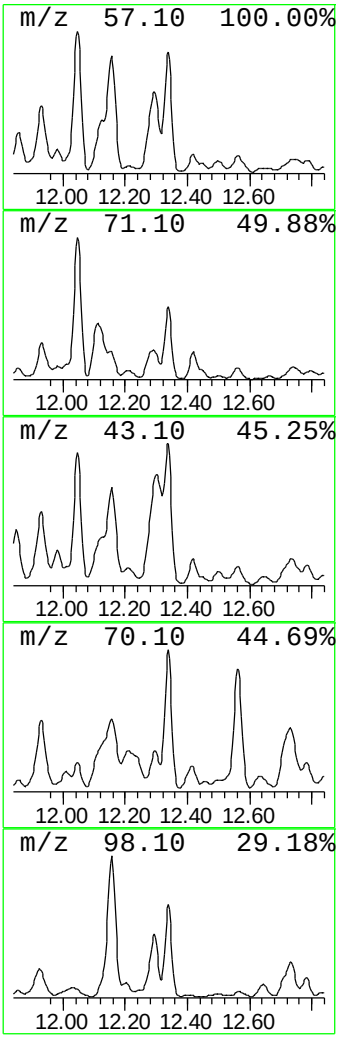
Peak Number 8 Pentane, 2,2,3,3-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	283.26 ug/l	11274400	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	53
2	Nonane, 4-methyl-	142	C10H22	017301-94-9	42
3	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	40
4	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	38
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	32





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Data File : VN059341.D
Acq On : 21 Nov 2019 17:17
Operator : JC/SP
Sample : K5957-06 10X
Misc : 5.45g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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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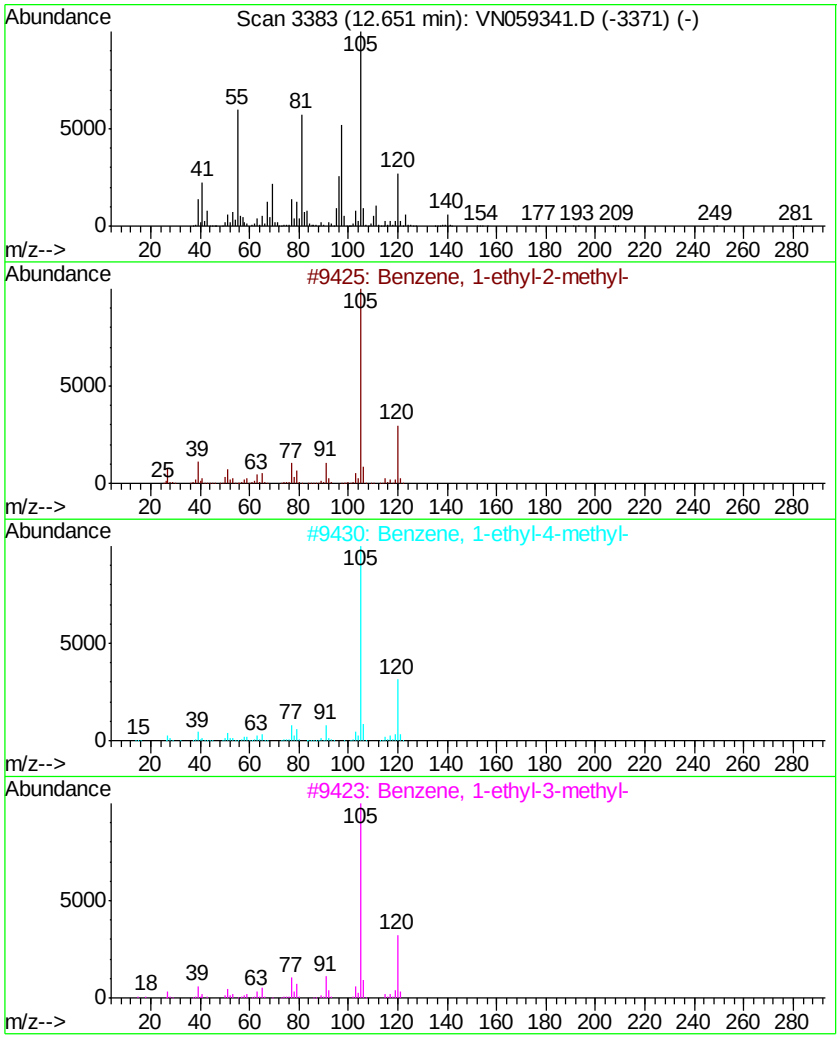
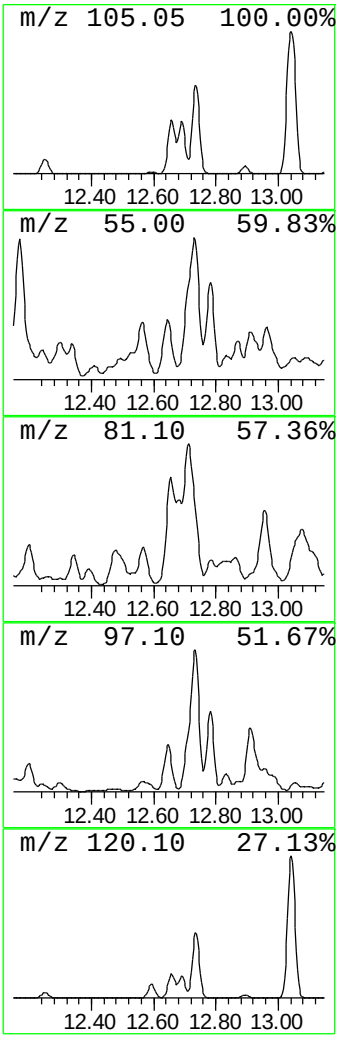
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	66.52 ug/l	11112000	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	60
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	35
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	25
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	20
5	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	20





Library Search Compound Report

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Sample : K5957-06 10X
Misc : 5.45g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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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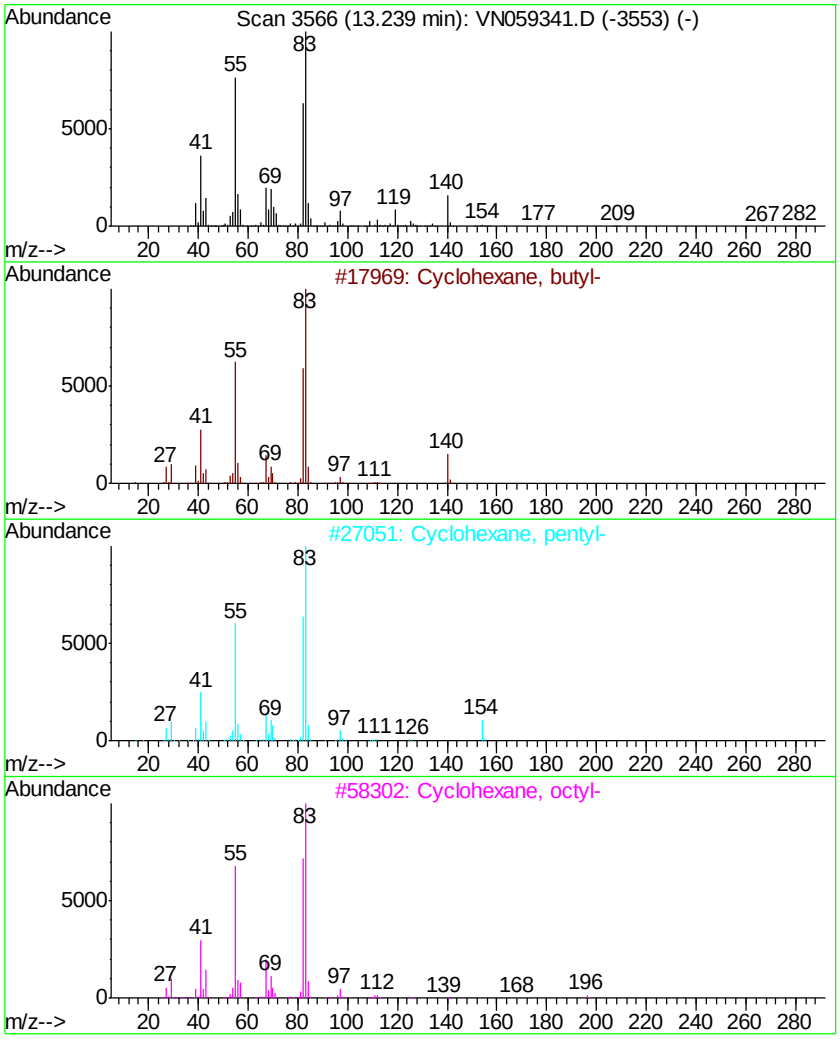
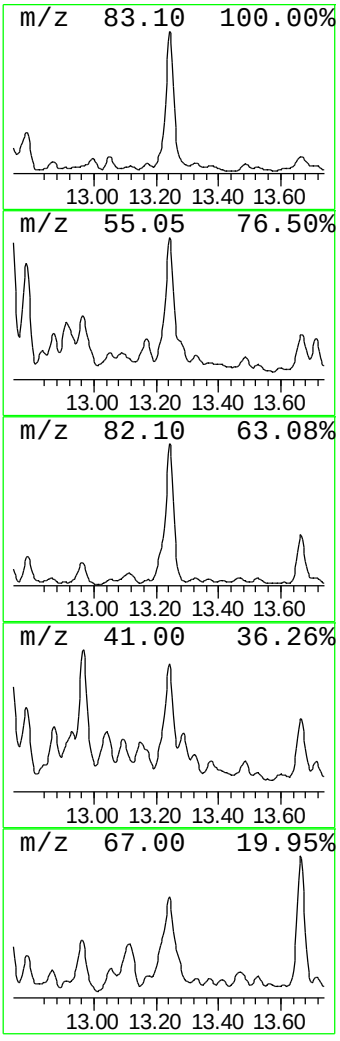
Peak Number 10 Cyclohexane, butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	81.06 ug/l	13539500	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, butyl-	140	C10H20	001678-93-9	95
2	Cyclohexane, pentyl-	154	C11H22	004292-92-6	94
3	Cyclohexane, octyl-	196	C14H28	001795-15-9	86
4	Cyclohexane, propyl-	126	C9H18	001678-92-8	83
5	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059341.D
Acq On : 21 Nov 2019 17:17
Operator : JC/SP
Sample : K5957-06 10X
Misc : 5.45g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-3-(17-20)

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	115.1	ug/l	4580790	3	11.40	1990110	50.0
Octane, 3-methyl-	11.30	92.8	ug/l	3693010	3	11.40	1990110	50.0
Cyclohexane, 1-et...	11.70	105.8	ug/l	4212920	3	11.40	1990110	50.0
Cyclohexane, 1-et...	11.92	343.7	ug/l	13680200	3	11.40	1990110	50.0
Nonane, 3-methyl-	12.05	232.2	ug/l	9242780	3	11.40	1990110	50.0
Cyclohexane, meth...	12.12	176.7	ug/l	7034660	3	11.40	1990110	50.0
Cyclohexane, propyl-	12.17	443.4	ug/l	17649000	3	11.40	1990110	50.0
Pentane, 2,2,3,3-...	12.34	283.3	ug/l	11274400	3	11.40	1990110	50.0
Benzene, 1-ethyl-...	12.65	66.5	ug/l	11112000	4	13.35	8352060	50.0
Cyclohexane, butyl-	13.24	81.1	ug/l	13539500	4	13.35	8352060	50.0