LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059342.D
Acq On : 21 Nov 2019 17:40
Operator : JC/SP
Sample : K5957-10 10X
Misc : 5.69g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

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	1782	1803	1814	rBV	242623	605534	5.40%	0.461%
2	7.645	1814	1826	1846	rVB	494742	1166825	10.41%	0.887%
3	8.008	1921	1939	1960	rBV	284180	651925	5.82%	0.496%
4	8.571	2097	2114	2136	rBV	704528	1462756	13.06%	1.112%
5	9.718	2460	2471	2493	rVB3	55565	135553	1.21%	0.103%
6	9.860	2497	2515	2535	rBV2	48191	118357	1.06%	0.090%
7	10.082	2569	2584	2612	rBV	1182728	2229054	19.90%	1.695%
8	10.426	2683	2691	2707	rVB3	73259	138963	1.24%	0.106%
9	10.712	2769	2780	2792	rVB	257385	432680	3.86%	0.329%
10	10.815	2798	2812	2825	rBV	143828	310412	2.77%	0.236%
11	10.882	2825	2833	2841	rBV4	73234	123538	1.10%	0.094%
12	10.947	2844	2853	2860	rVV	252105	383289	3.42%	0.291%
13	11.001	2860	2870	2881	rVB2	485728	848966	7.58%	0.646%
14	11.120	2894	2907	2915	rBV3	359113	678583	6.06%	0.516%
15	11.191	2915	2929	2949	rVB5	625171	1752545	15.64%	1.333%
16	11.297	2949	2962	2982	rBV	1016388	1841936	16.44%	1.401%
17	11.403	2984	2995	3014	rBV	957454	1734196	15.48%	1.319%
18	11.509	3014	3028	3033	rBV2	270655	537354	4.80%	0.409%
19	11.599	3044	3056	3065	rBV6	463518	1381988	12.33%	1.051%
20	11.654	3066	3073	3080	rVV2	1046022	1901617	16.97%	1.446%
21	11.696	3081	3086	3096	rVB2	790626	1224248	10.93%	0.931%
22	11.757	3096	3105	3112	rBV2	216372	406125	3.62%	0.309%
23	11.850	3127	3134	3142	rVB3	504818	742754	6.63%	0.565%
24	11.924	3143	3157	3169	rBV5	1593820	3902702	34.83%	2.968%
25	11.979	3170	3174	3179	rBV2	223487	254836	2.27%	0.194%
26	12.046	3186	3195	3203	rBV	3095495	4262617	38.05%	3.242%
27	12.120	3209	3218	3223	rBV3	1477128	2478376	22.12%	1.885%
28	12.162	3223	3231	3249	rVB5	3102836	6152303	54.91%	4.679%
29	12.297	3265	3273	3279	rBV6	1197919	2307263	20.59%	1.755%
30	12.336	3280	3285	3296	rVB	3397245	5126156	45.75%	3.899%
31	12.406	3297	3307	3315	rBV5	1051702	1987428	17.74%	1.511%
32	12.451	3316	3321	3325	rBV3	271884	347613	3.10%	0.264%
33	12.561	3348	3355	3371	rVB3	2252188	5118014	45.68%	3.892%
34	12.654	3372	3384	3391	rBV4	2865387	5582897	49.83%	4.246%

LSC Area Percent Report

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Misc : 5.69g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

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	12.731	3403	3408	3418	rVB2	4409687	6710233	59.89%	5.103%
36	12.783	3419	3424	3434	rVB4	1843232	2783629	24.84%	2.117%
37	12.873	3445	3452	3459	rBV4	1071533	1693246	15.11%	1.288%
38	12.963	3473	3480	3493	rVB	5542833	9044988	80.73%	6.879%
39	13.040	3494	3504	3514	rBV	6660997	11204078	100.00%	8.521%
40	13.095	3515	3521	3530	rVB3	830916	1230557	10.98%	0.936%
41	13.149	3531	3538	3543	rBV3	1270479	2137678	19.08%	1.626%
42	13.239	3553	3566	3574	rBV4	3752773	7468604	66.66%	5.680%
43	13.287	3575	3581	3588	rVB3	1695827	2381910	21.26%	1.811%
44	13.377	3602	3609	3621	rVB	2768652	4604074	41.09%	3.502%
45	13.541	3655	3660	3667	rVB2	1432119	1917158	17.11%	1.458%
46	13.590	3668	3675	3689	rVB4	1677379	3268969	29.18%	2.486%
47	13.667	3690	3699	3708	rBV5	1821247	3328385	29.71%	2.531%
48	13.715	3709	3714	3718	rBV3	479912	607275	5.42%	0.462%
49	13.837	3747	3752	3761	rVB6	1316840	1914715	17.09%	1.456%
50	13.892	3763	3769	3777	rVB	1426515	2119264	18.92%	1.612%
51	13.937	3779	3783	3792	rVB3	453918	624895	5.58%	0.475%
52	13.998	3793	3802	3811	rVB3	1351117	2210703	19.73%	1.681%
53	14.066	3813	3823	3833	rVB8	363300	886964	7.92%	0.675%
54	14.181	3851	3859	3875	rVB7	817636	2047953	18.28%	1.558%
55	14.252	3876	3881	3889	rVB	664429	888493	7.93%	0.676%
56	14.300	3889	3896	3901	rBV3	371439	507480	4.53%	0.386%
57	14.336	3901	3907	3921	rVB3	537183	775521	6.92%	0.590%
58	14.529	3963	3967	3974	rVB3	242957	299526	2.67%	0.228%
59	14.586	3975	3985	3998	rVV2	826032	1722310	15.37%	1.310%
60	14.648	4000	4004	4016	rVB2	233635	360137	3.21%	0.274%
61	14.744	4028	4034	4044	rVB	278425	420438	3.75%	0.320%

Sum of corrected areas: 131488586

LSC Report - Integrated Chromatogram

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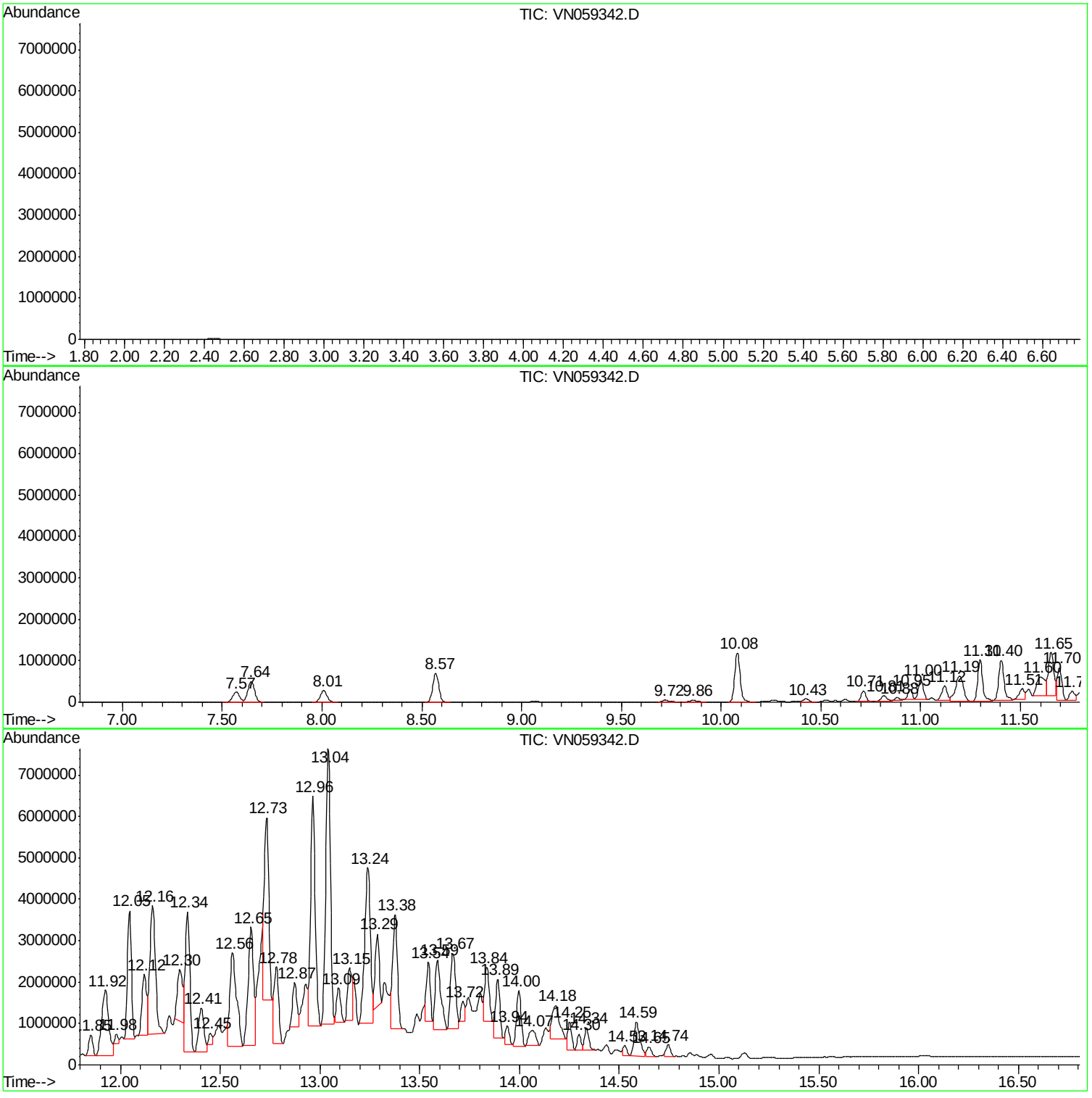
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-4-(16-18)

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

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ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

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

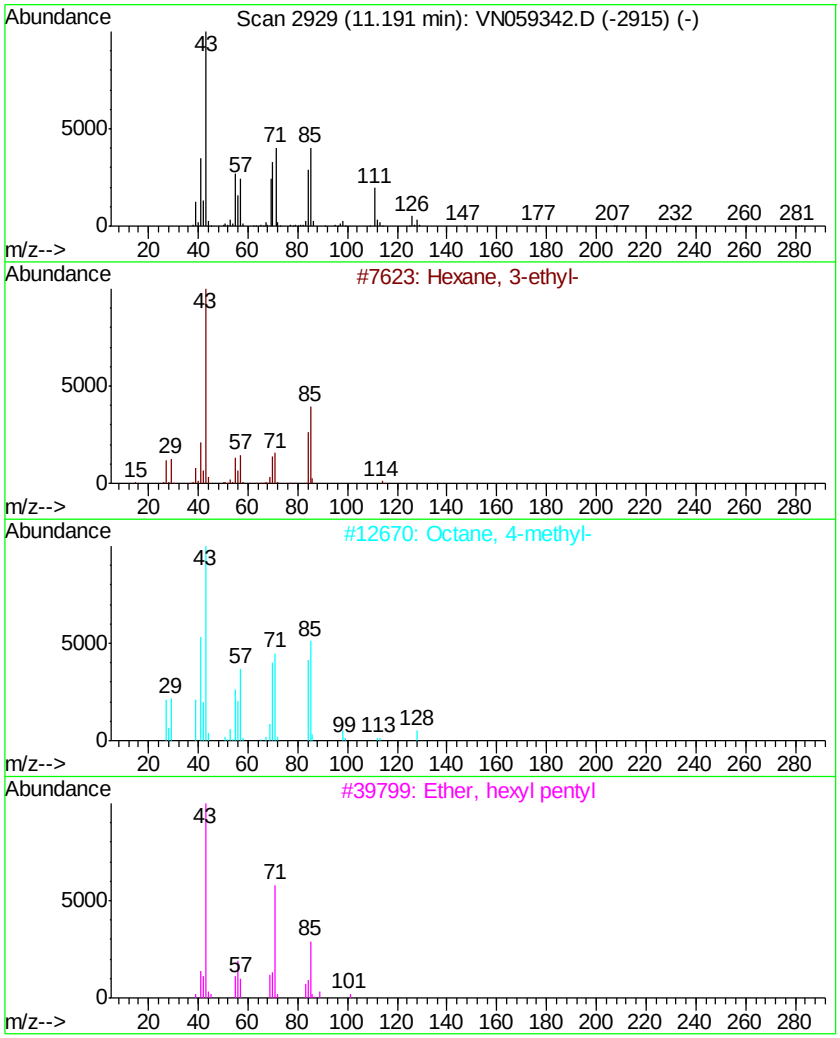
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

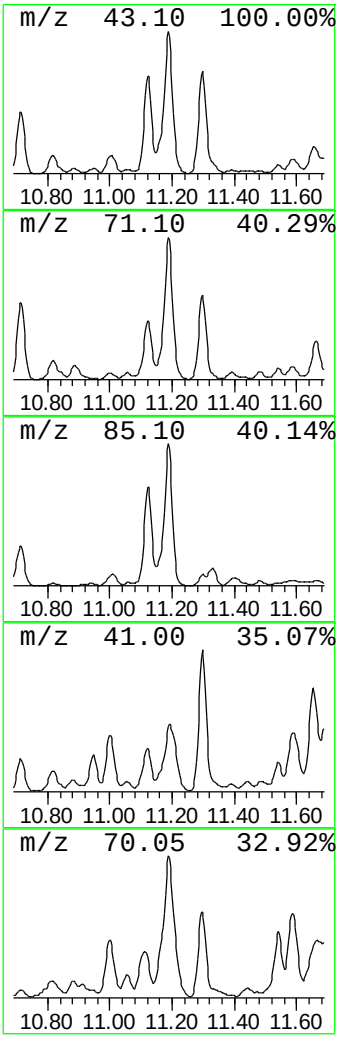
****

Peak Number 1 Hexane, 3-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	50.53 ug/l	1752550	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-ethyl-	114	C8H18	000619-99-8	72
2	Octane, 4-methyl-	128	C9H20	002216-34-4	72
3	Ether, hexyl pentyl	172	C11H24O	032357-83-8	53
4	Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	53
5	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	49





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059342.D
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Operator : JC/SP
Sample : K5957-10 10X
Misc : 5.69g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

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

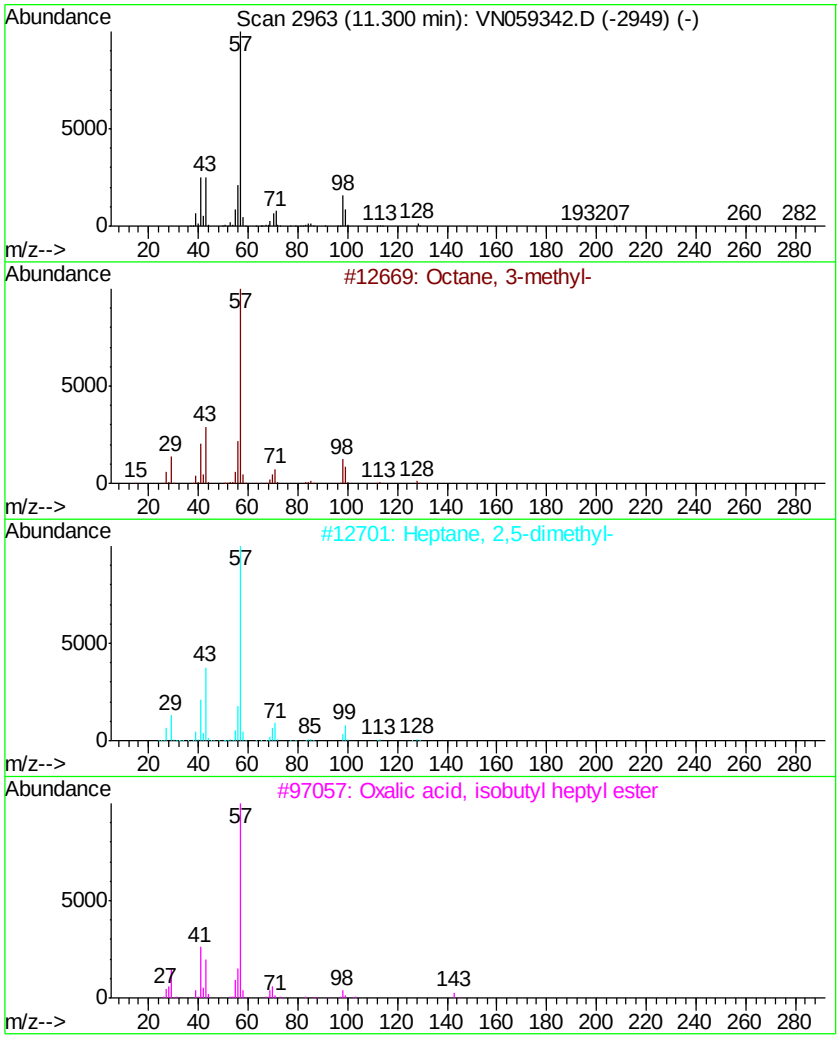
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

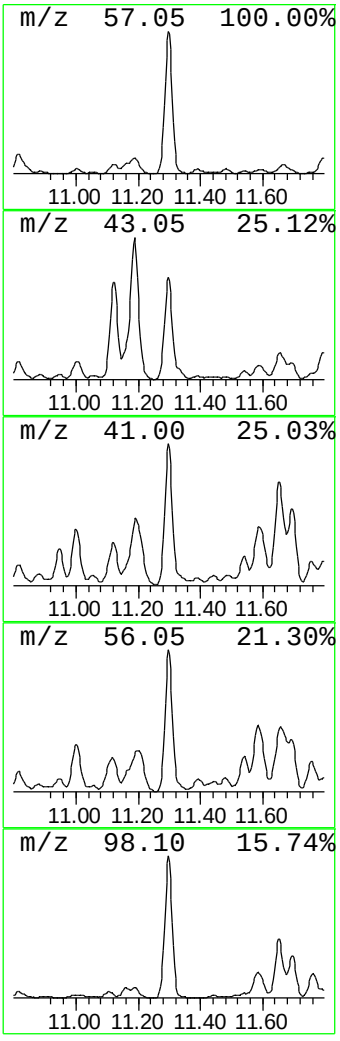
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	53.11 ug/l	1841940	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	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	59
4	Undecane, 6-methyl-	170	C12H26	017302-33-9	53
5	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	50





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Data File : VN059342.D
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Operator : JC/SP
Sample : K5957-10 10X
Misc : 5.69g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

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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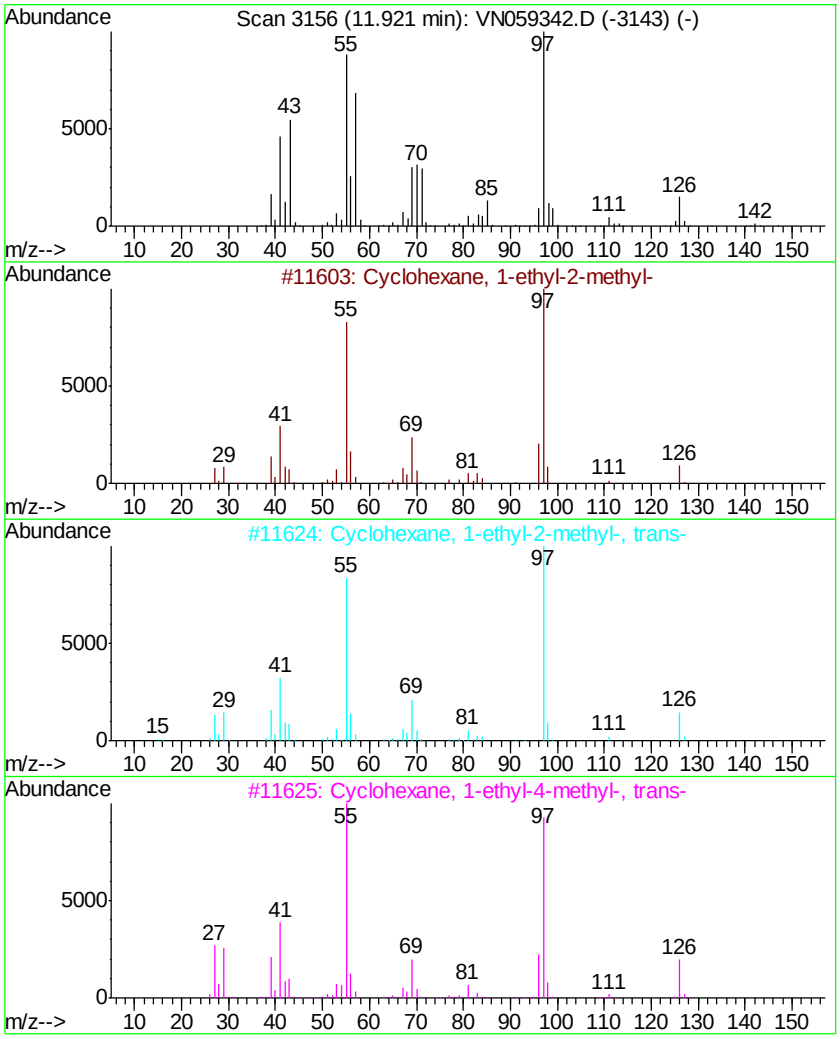
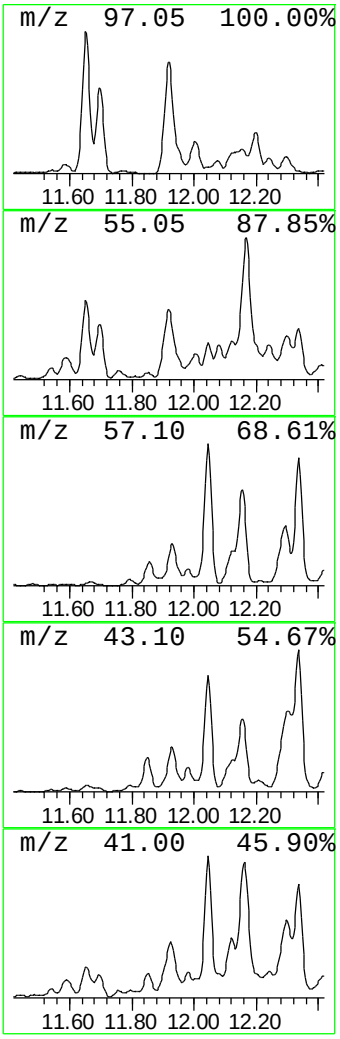
Peak Number 3 unknown11.92 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	112.52 ug/l	3902700	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	45
2	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	43
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	43
4	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	43
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	43





Library Search Compound Report

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Misc : 5.69g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
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TIC Library : C:\DATABASE\NIST11.L
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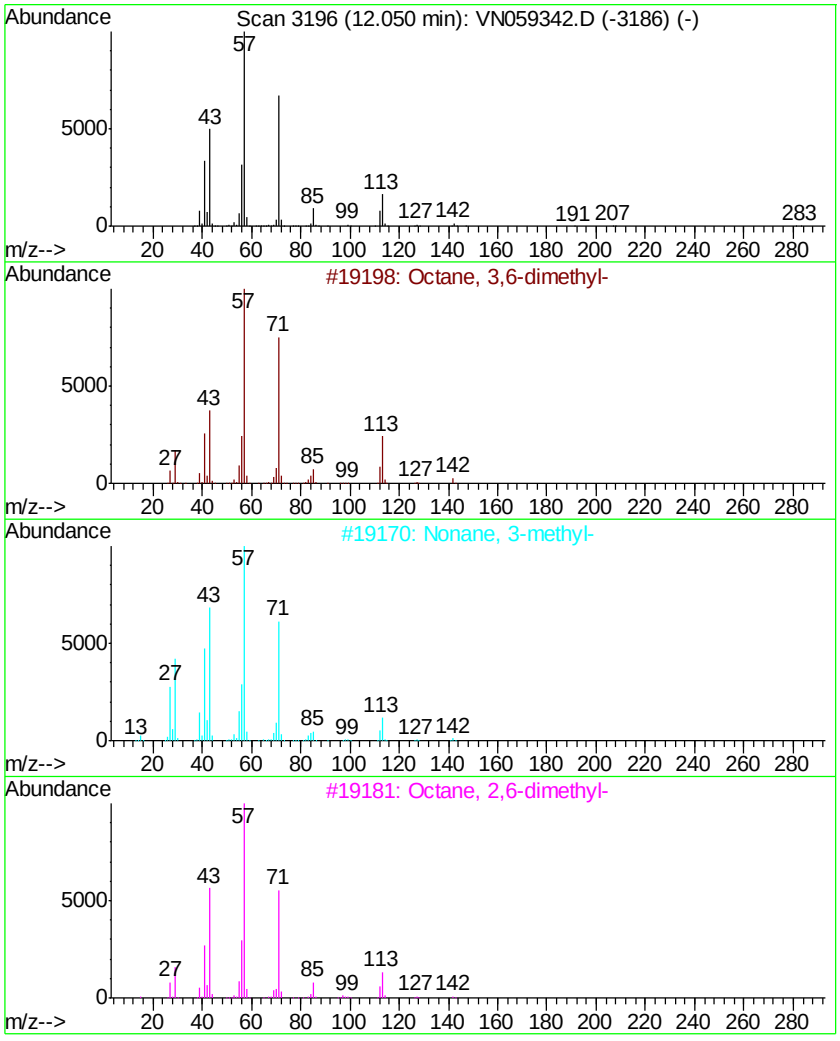
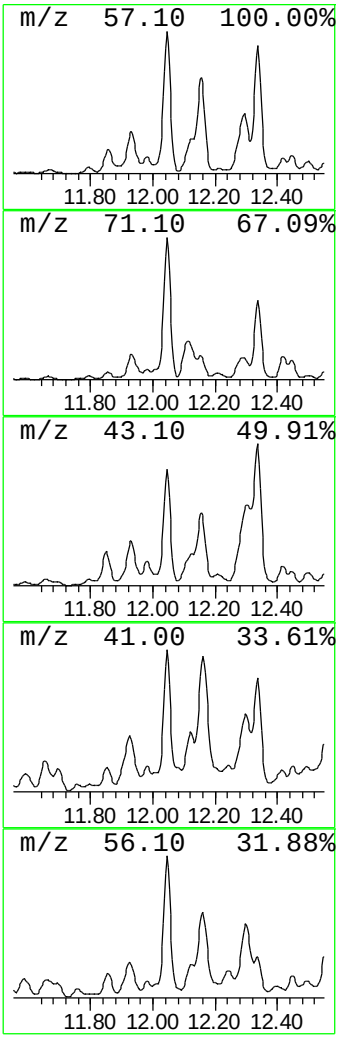
Peak Number 4 Octane, 3,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	122.90 ug/l	4262620	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	91
3	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
4	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	72
5	Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	59





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Operator : JC/SP
Sample : K5957-10 10X
Misc : 5.69g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

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

TIC Library : C:\DATABASE\NIST11.L
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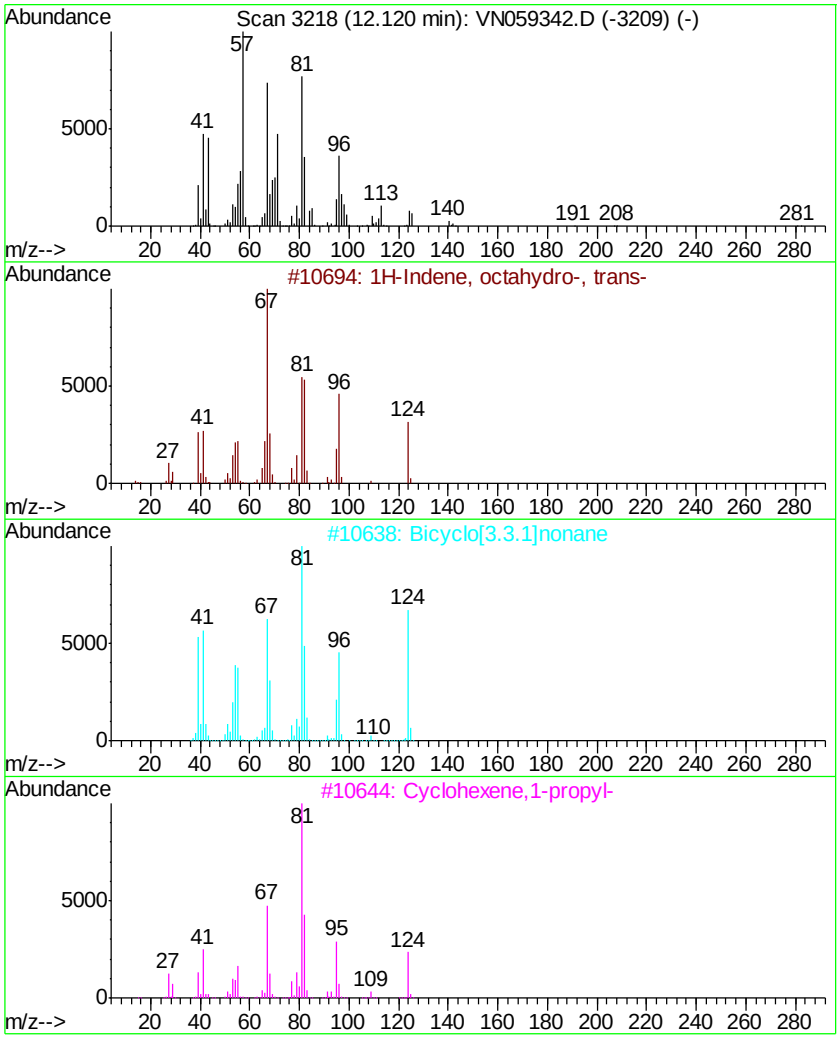
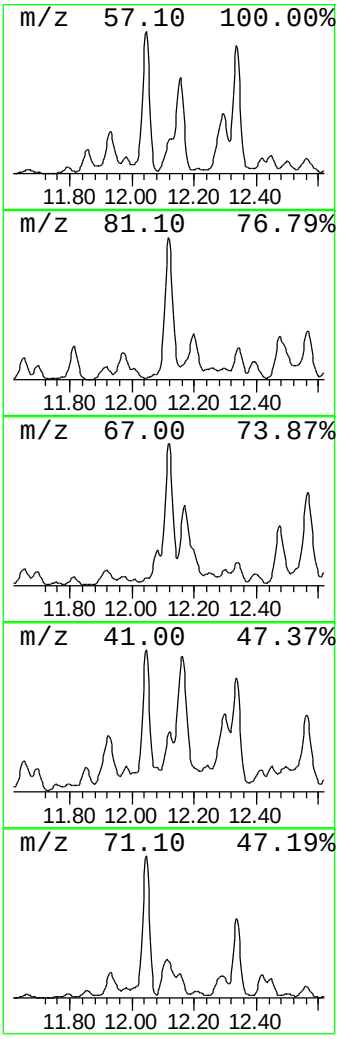
****

Peak Number 5 unknown12.12 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	71.46 ug/l	2478380	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	41
2	Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	38
3	Cyclohexene,1-propyl-	124	C9H16	002539-75-5	35
4	Cyclohexene,3-propyl-	124	C9H16	003983-06-0	30
5	Cycloheptene	96	C7H12	000628-92-2	30





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Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

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

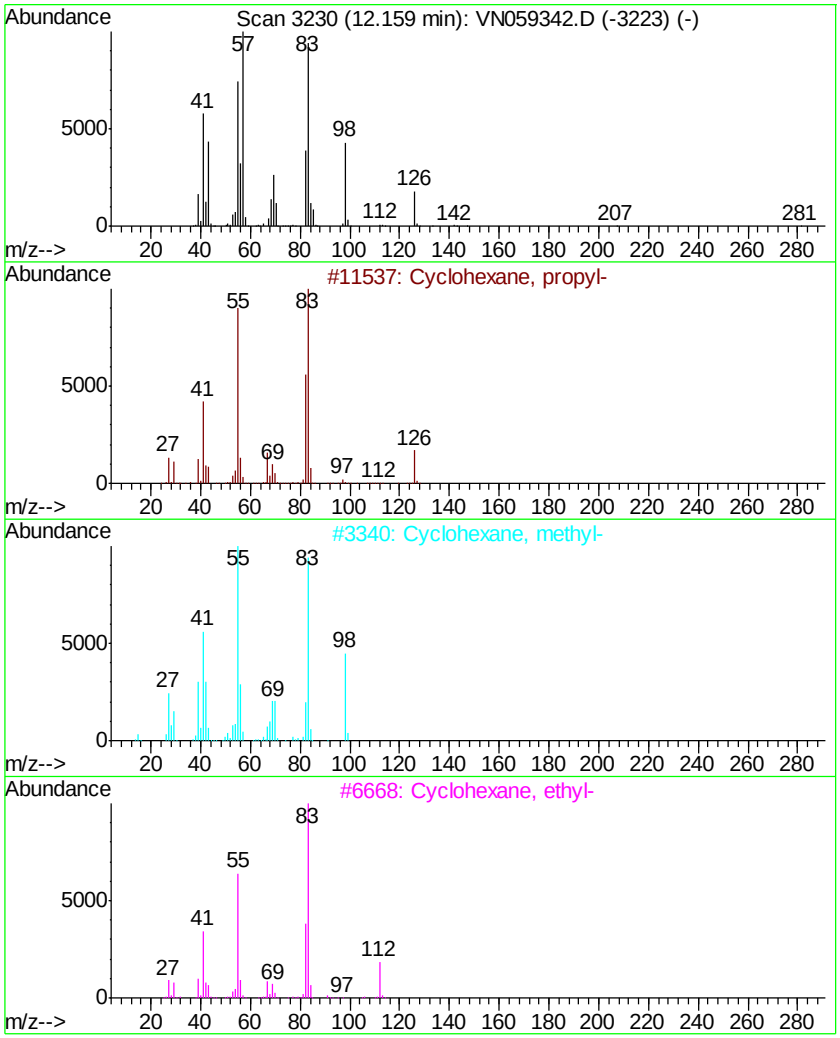
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

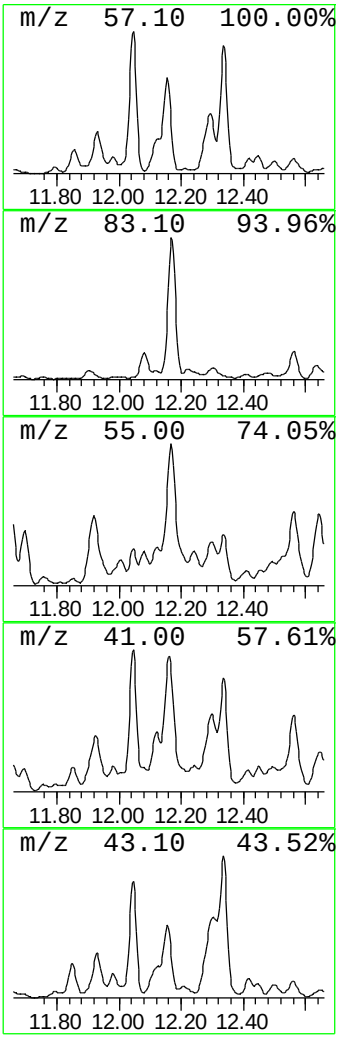
****

Peak Number 6 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	177.38 ug/l	6152300	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	68
2	Cyclohexane, methyl-	98	C7H14	000108-87-2	58
3	Cyclohexane, ethyl-	112	C8H16	001678-91-7	50
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	49
5	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	47





Library Search Compound Report

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ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

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

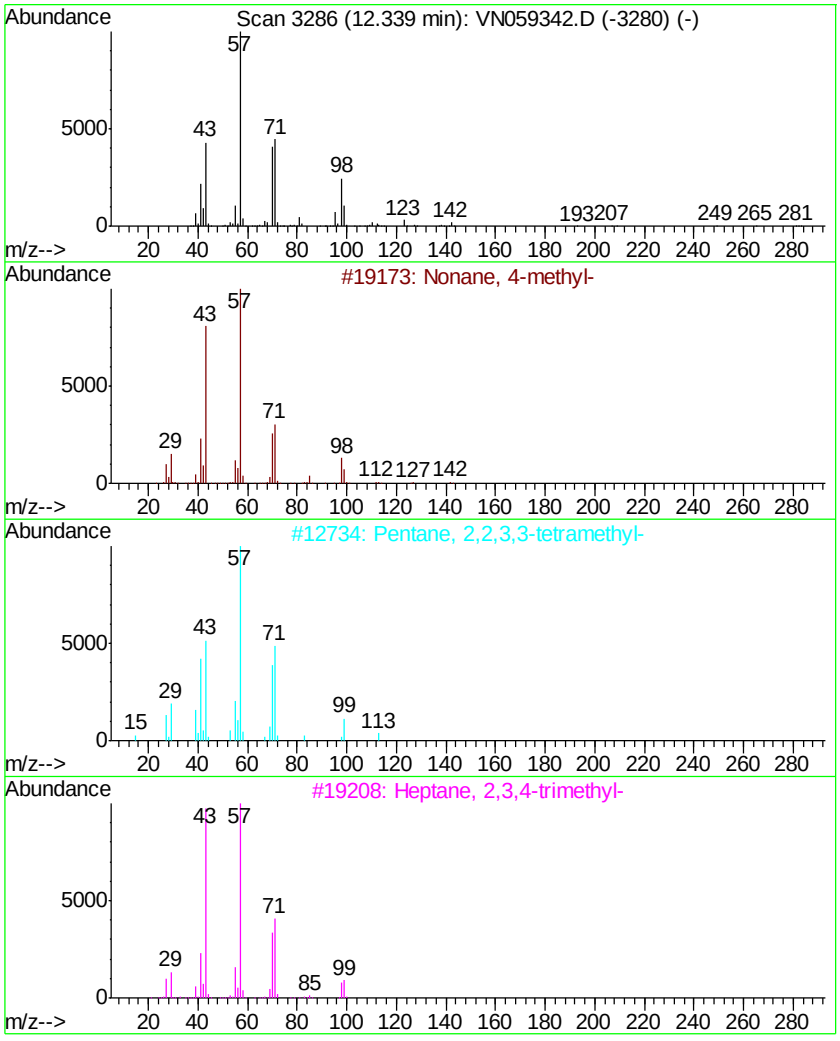
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

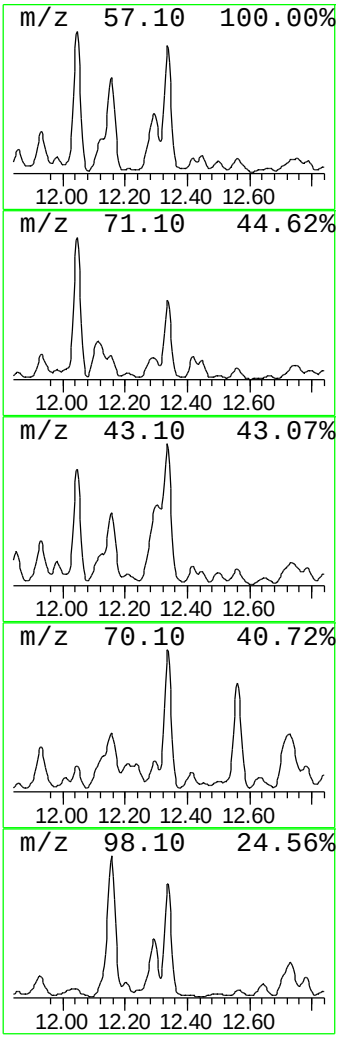
****

Peak Number 7 Nonane, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	147.80 ug/l	5126160	Chlorobenzene-d5	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	78
2	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	59
3	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	50
4	Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	43
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059342.D
Acq On : 21 Nov 2019 17:40
Operator : JC/SP
Sample : K5957-10 10X
Misc : 5.69g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

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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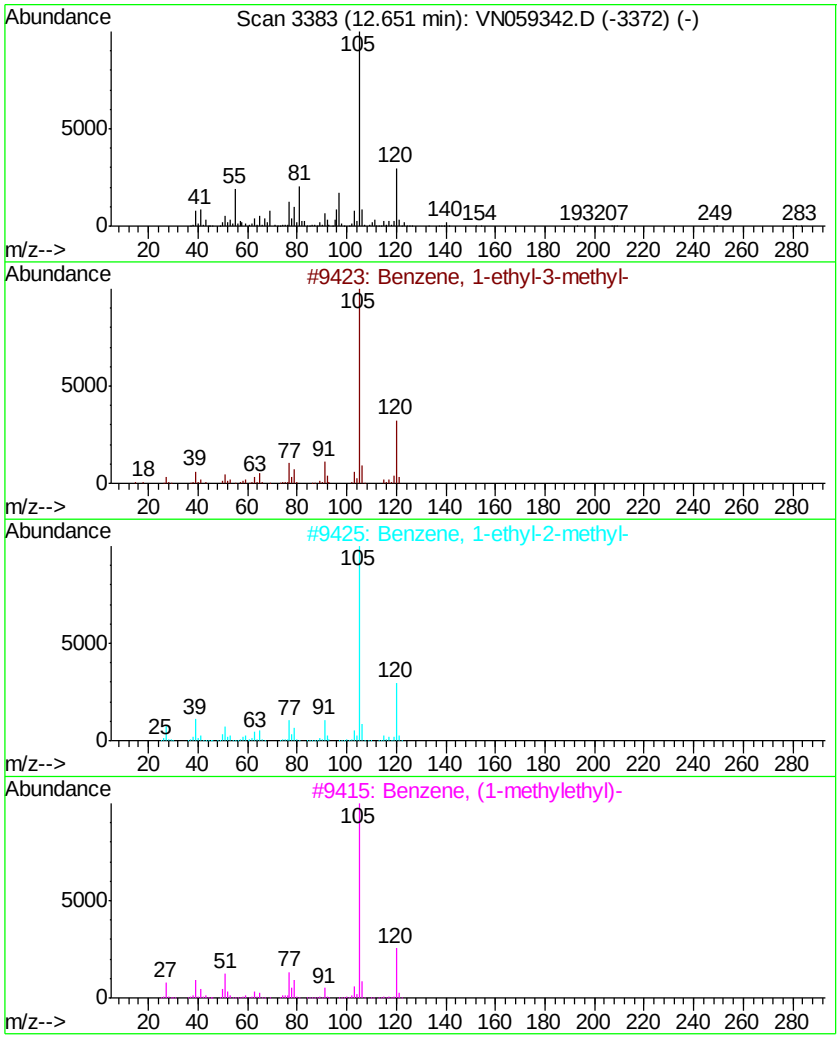
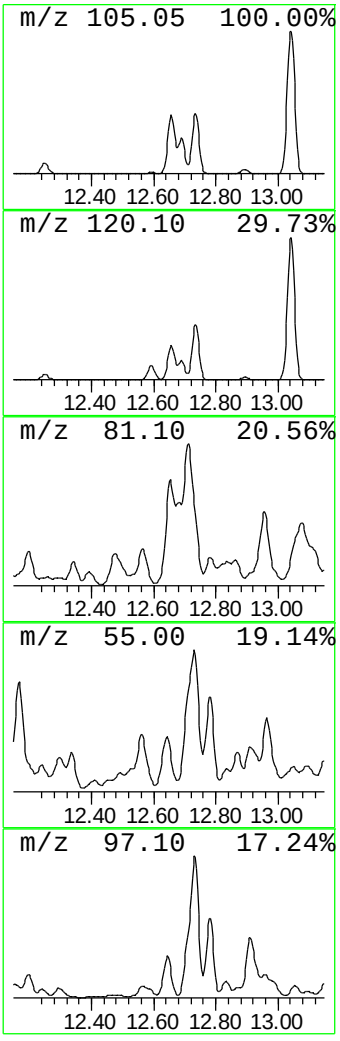
Peak Number 8 Benzene, 1-ethyl-3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	60.63 ug/l	5582900	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	86
3	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	70
4	Mesitylene	120	C9H12	000108-67-8	70
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	70





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Data File : VN059342.D
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Operator : JC/SP
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ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

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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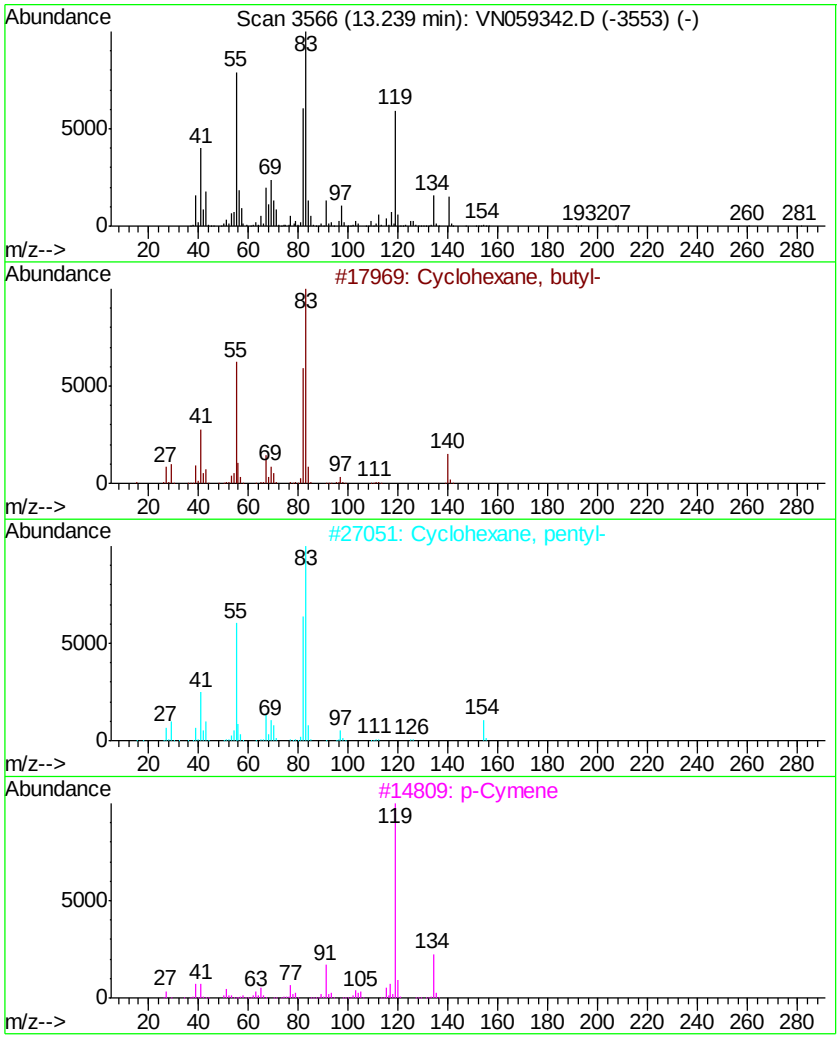
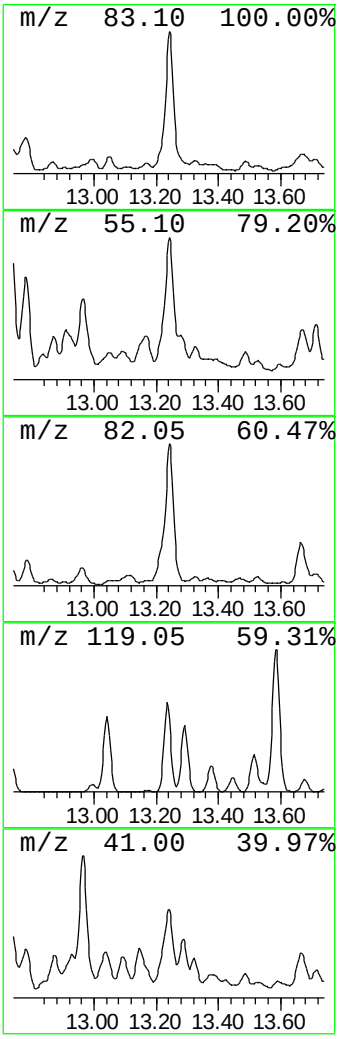
Peak Number 9 Cyclohexane, butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	81.11 ug/l	7468600	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, butyl-	140	C10H20	001678-93-9	76
2	Cyclohexane, pentyl-	154	C11H22	004292-92-6	62
3	p-Cymene	134	C10H14	000099-87-6	59
4	o-Cymene	134	C10H14	000527-84-4	59
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	56





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Data File : VN059342.D
Acq On : 21 Nov 2019 17:40
Operator : JC/SP
Sample : K5957-10 10X
Misc : 5.69g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

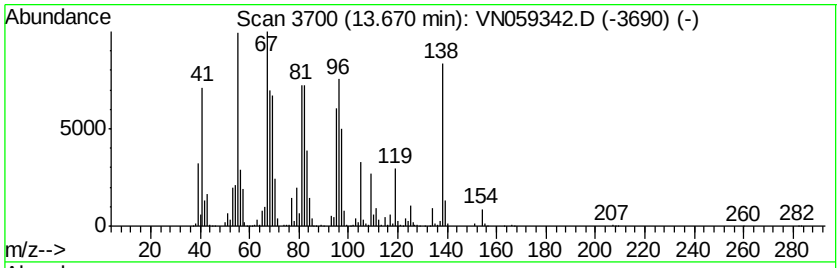
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112019W.M
Quant Title : SW846 8260

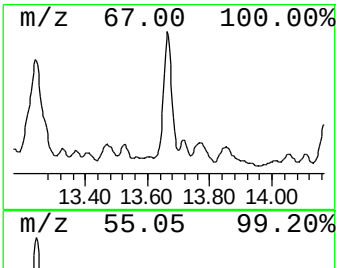
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, decahydro-, tr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	36.15 ug/l	3328390	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	95
2	Naphthalene, decahydro-	138	C10H18	000091-17-8	93
3	9-Borabicyclo[3.3.1]nonane, 9-hy...	138	C8H15BO	063366-65-4	87
4	Cyclodecene	138	C10H18	003618-12-0	87
5	Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112119\
Data File : VN059342.D
Acq On : 21 Nov 2019 17:40
Operator : JC/SP
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Instrument : MSVOA_N
ClientSampleId : MW-4-(16-18)

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
Hexane, 3-ethyl-	11.19	50.5	ug/l	1752550	3	11.40	1734200	50.0
Octane, 3-methyl-	11.30	53.1	ug/l	1841940	3	11.40	1734200	50.0
unknown11.92	11.92	112.5	ug/l	3902700	3	11.40	1734200	50.0
Octane, 3,6-dimet...	12.05	122.9	ug/l	4262620	3	11.40	1734200	50.0
unknown12.12	12.12	71.5	ug/l	2478380	3	11.40	1734200	50.0
Cyclohexane, propyl-	12.16	177.4	ug/l	6152300	3	11.40	1734200	50.0
Nonane, 4-methyl-	12.34	147.8	ug/l	5126160	3	11.40	1734200	50.0
Benzene, 1-ethyl-...	12.65	60.6	ug/l	5582900	4	13.35	4604070	50.0
Cyclohexane, butyl-	13.24	81.1	ug/l	7468600	4	13.35	4604070	50.0
Naphthalene, deca...	13.67	36.1	ug/l	3328390	4	13.35	4604070	50.0