

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
 Data File : VN055366.D
 Acq On : 2 May 2019 23:02
 Operator : JC/SP
 Sample : K2658-02 10X
 Misc : 6.06µ/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-SB-W2(17-20)

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	287643	722484	3.55%	0.354%
2	7.667	1821	1833	1857	rVB	469338	1136914	5.59%	0.557%
3	8.030	1927	1946	1973	rBV	322705	760858	3.74%	0.373%
4	8.587	2104	2119	2157	rBV	762737	1674407	8.23%	0.820%
5	10.091	2572	2587	2618	rBV	1319097	2831427	13.92%	1.387%
6	10.432	2684	2693	2708	rVB2	175857	336444	1.65%	0.165%
7	10.532	2711	2724	2732	rBV3	96426	205334	1.01%	0.101%
8	10.718	2771	2782	2794	rVB	376145	626243	3.08%	0.307%
9	10.821	2800	2814	2827	rBV	298934	624659	3.07%	0.306%
10	10.889	2827	2835	2843	rBV4	155816	282565	1.39%	0.138%
11	10.950	2846	2854	2862	rBV	414029	617301	3.04%	0.302%
12	11.004	2862	2871	2882	rVB	849425	1451804	7.14%	0.711%
13	11.059	2882	2888	2896	rVB	161742	228030	1.12%	0.112%
14	11.123	2896	2908	2916	rBV2	756046	1377475	6.77%	0.675%
15	11.207	2916	2934	2951	rVB6	968075	2945952	14.49%	1.443%
16	11.297	2951	2962	2983	rBV	972434	1927082	9.48%	0.944%
17	11.406	2984	2996	3014	rBV	1095868	2346389	11.54%	1.149%
18	11.490	3015	3022	3030	rBV5	153397	280615	1.38%	0.137%
19	11.541	3030	3038	3045	rBV	539217	826305	4.06%	0.405%
20	11.596	3045	3055	3062	rBV6	840230	1783122	8.77%	0.873%
21	11.654	3064	3073	3081	rBV2	2477093	4101849	20.17%	2.009%
22	11.699	3082	3087	3097	rVB2	1918495	2923744	14.38%	1.432%
23	11.757	3097	3105	3111	rBV3	457840	799665	3.93%	0.392%
24	11.812	3113	3122	3126	rBV3	279492	498438	2.45%	0.244%
25	11.850	3127	3134	3143	rVB3	1284874	1980841	9.74%	0.970%
26	11.924	3143	3157	3169	rBV7	4349354	10543567	51.85%	5.165%
27	12.043	3187	3194	3202	rVB	4971392	6746988	33.18%	3.305%
28	12.120	3210	3218	3223	rBV2	3286608	5278030	25.95%	2.585%
29	12.162	3224	3231	3250	rVB5	6663018	13155759	64.69%	6.444%
30	12.297	3265	3273	3280	rBV6	2122211	3800139	18.69%	1.861%
31	12.336	3280	3285	3295	rVB2	4250680	6584867	32.38%	3.226%
32	12.406	3296	3307	3316	rBV7	1953412	3931829	19.33%	1.926%
33	12.490	3317	3333	3339	rBV5	1382022	3856007	18.96%	1.889%
34	12.561	3348	3355	3371	rVB3	4899500	10672402	52.48%	5.228%

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35	12.644	3371	3381	3388	rBV5	2301773	4682865	23.03%	2.294%
36	12.728	3390	3407	3416	rVV6	6662632	19979643	98.25%	9.787%
37	12.779	3417	3423	3433	rVB3	3570353	5793238	28.49%	2.838%
38	12.866	3444	3450	3457	rBV5	1668411	2267995	11.15%	1.111%
39	12.927	3458	3469	3472	rBV3	1136334	2282410	11.22%	1.118%
40	12.963	3473	3480	3493	rVB3	5639980	9640448	47.41%	4.722%
41	13.040	3494	3504	3514	rBV	12299893	20335521	100.00%	9.961%
42	13.239	3552	3566	3574	rBV2	5016920	9833485	48.36%	4.817%
43	13.374	3602	3608	3624	rVB	2265387	3739701	18.39%	1.832%
44	13.593	3669	3676	3688	rBV2	1382787	2974658	14.63%	1.457%
45	13.660	3688	3697	3707	rVV3	4072027	7508601	36.92%	3.678%
46	13.712	3709	3713	3720	rVB2	828772	1007575	4.95%	0.494%
47	13.799	3736	3740	3745	rBV3	619827	788581	3.88%	0.386%
48	13.831	3746	3750	3760	rVV4	1467092	2130328	10.48%	1.044%
49	13.885	3761	3767	3777	rVB	1963564	3172931	15.60%	1.554%
50	13.991	3792	3800	3809	rVB5	1122340	1849360	9.09%	0.906%
51	14.175	3848	3857	3873	rVV7	1148602	3037083	14.93%	1.488%
52	14.246	3874	3879	3887	rVB	909390	1261499	6.20%	0.618%
53	14.294	3888	3894	3899	rBV3	311588	428400	2.11%	0.210%
54	14.329	3899	3905	3913	rVB2	623879	846193	4.16%	0.415%
55	14.522	3961	3965	3973	rVB3	272399	363447	1.79%	0.178%
56	14.580	3973	3983	3996	rVV2	1003339	1936823	9.52%	0.949%
57	14.644	3996	4003	4014	rVB2	251929	423621	2.08%	0.208%

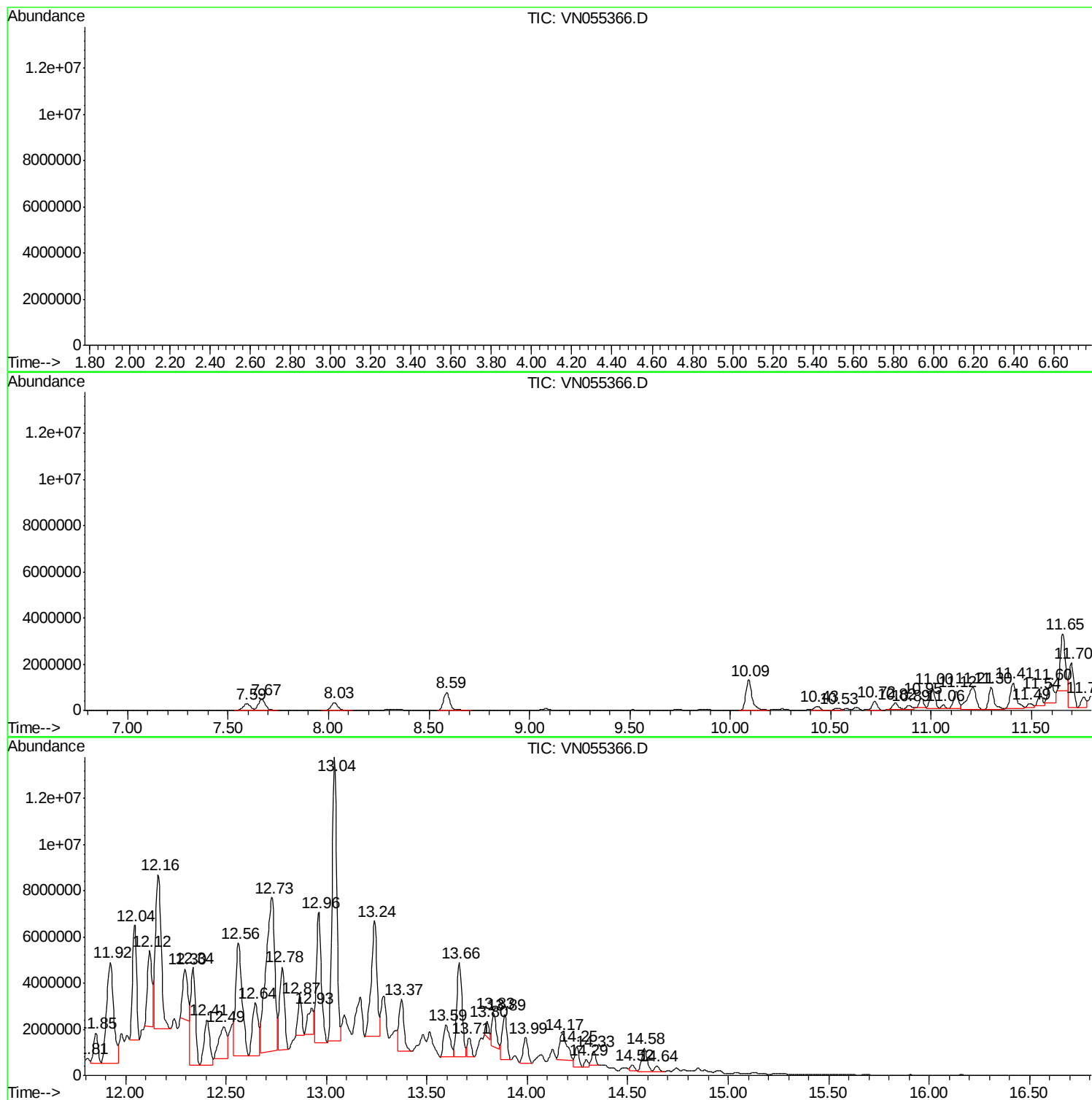
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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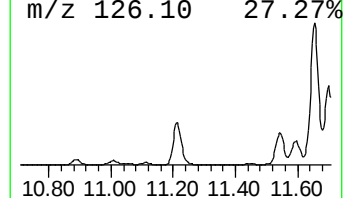
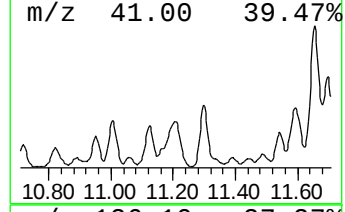
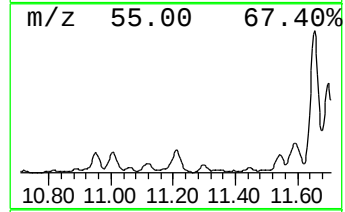
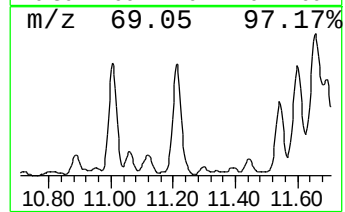
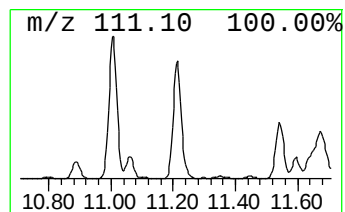
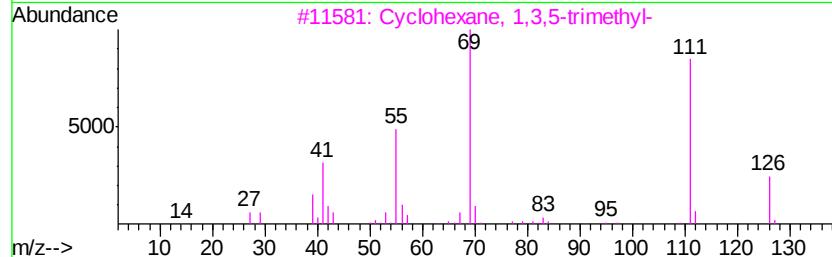
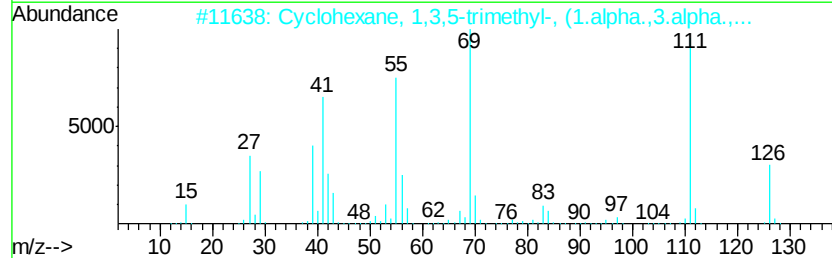
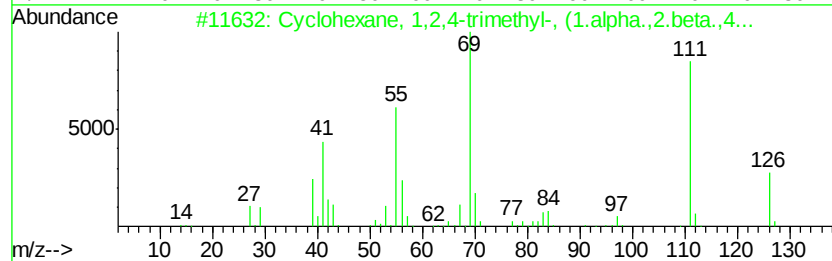
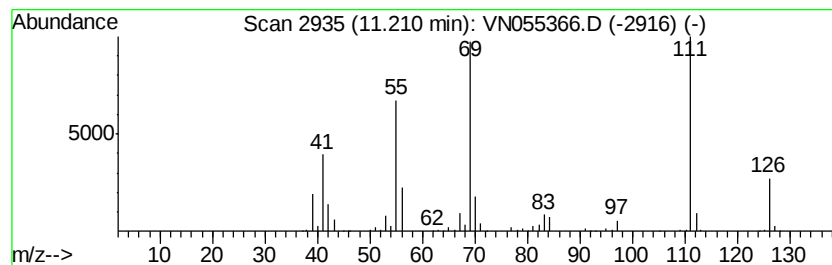
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1,2,4-trimethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.21	62.78 ug/l	2945950	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	97
2		Cvclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	87
3		Cvclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	83
4		Cvclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	81
5		Cvclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	80



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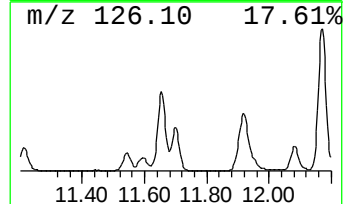
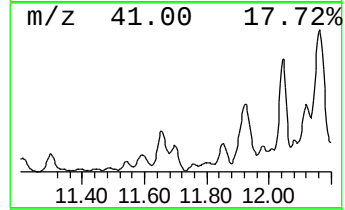
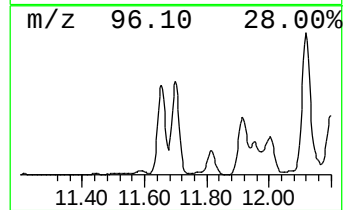
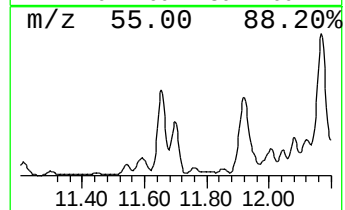
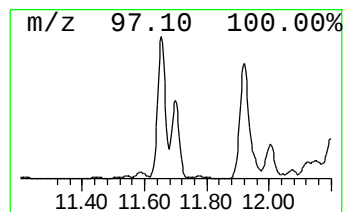
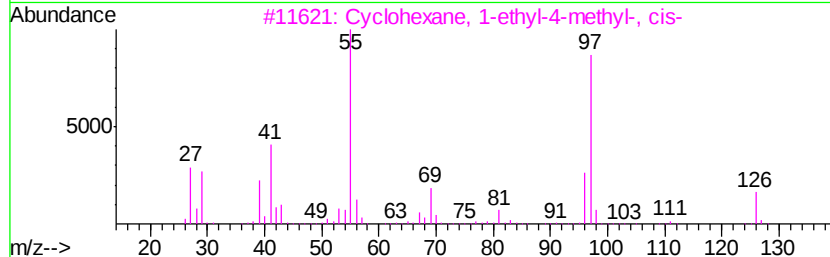
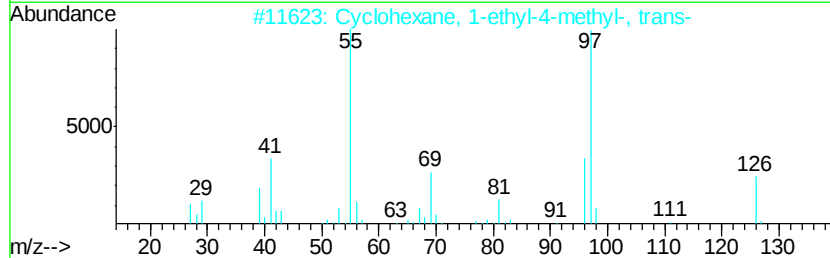
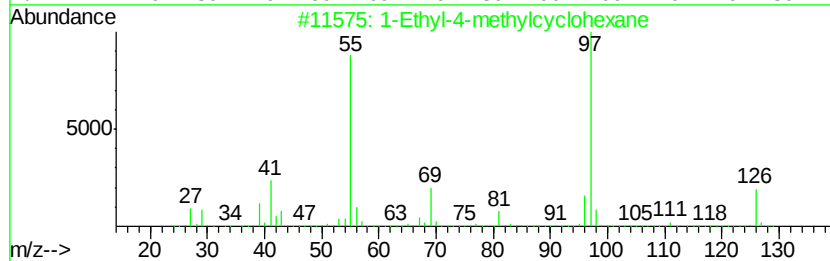
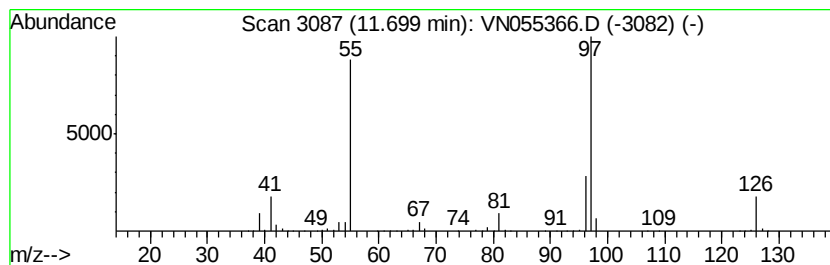
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Ethyl-4-methylcyclohexane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.70	62.30 ug/l	2923740	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	87
2		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	86
3		Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	86
4		3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	64
5		Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	64



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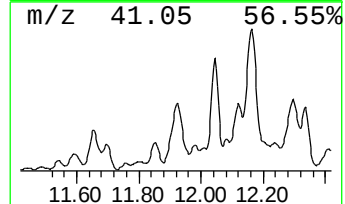
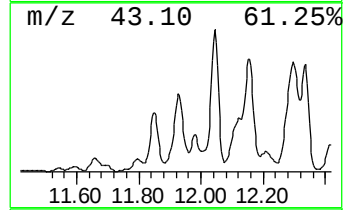
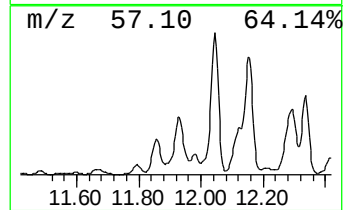
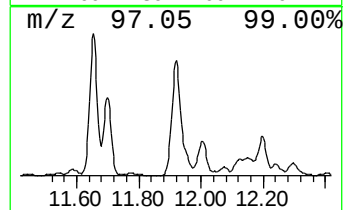
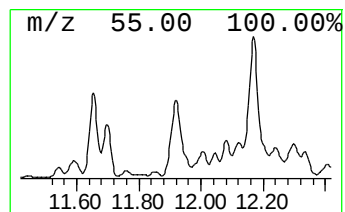
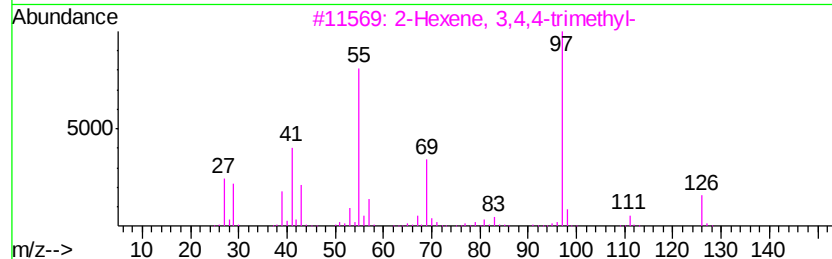
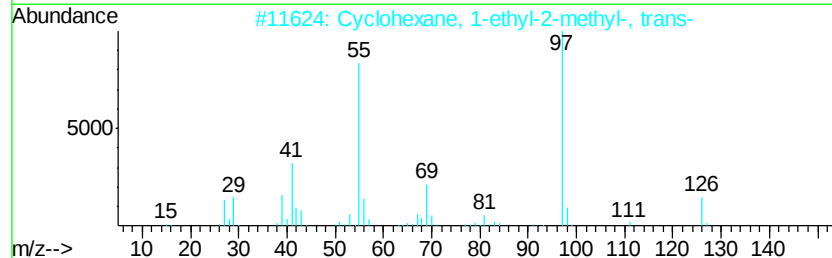
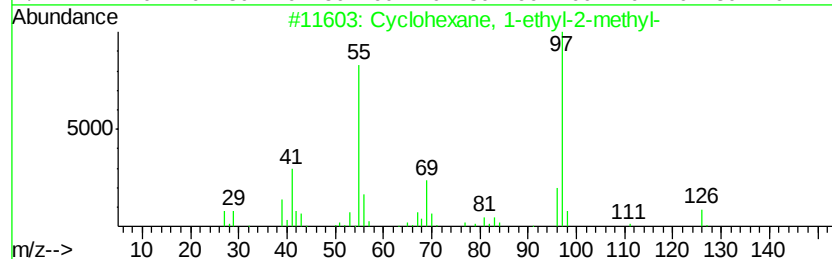
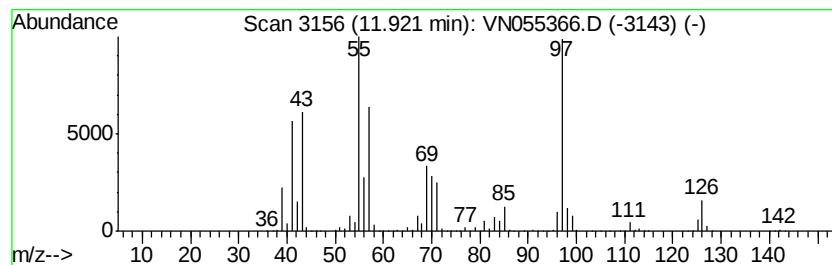
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.92	224.68 ug/l	10543600	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	60
2		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	49
3		2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	49
4		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	47
5		Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	47



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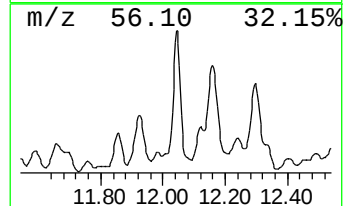
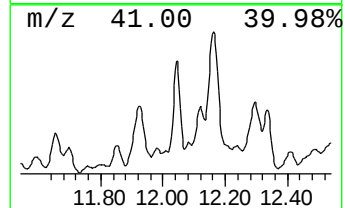
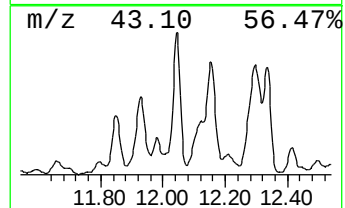
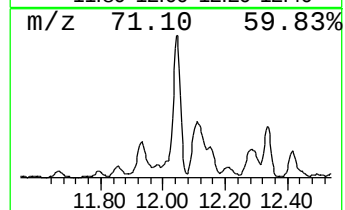
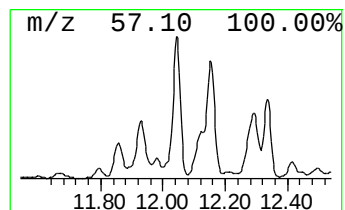
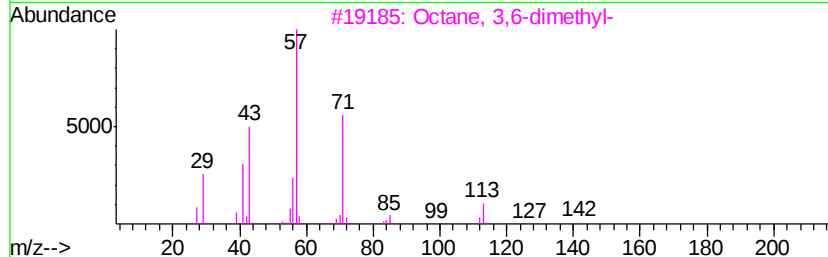
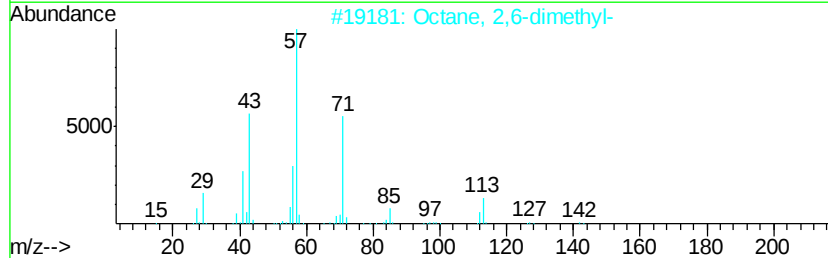
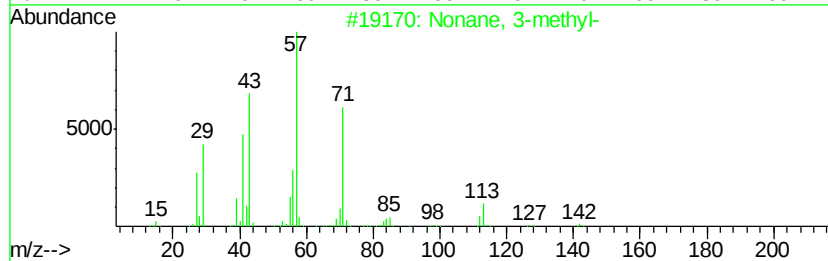
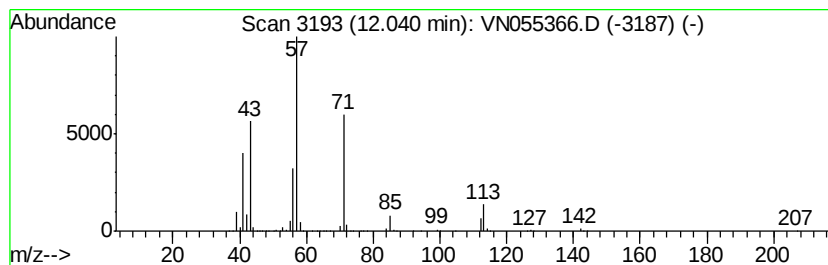
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Nonane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	143.77 ug/l	6746990	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonane, 3-methyl-	142	C10H22	005911-04-6	91
2		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
3		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91
4		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	59
5		Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	56



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Operator : JC/SP
Sample : K2658-02 10X
Misc : 6.06g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-W2(17-20)

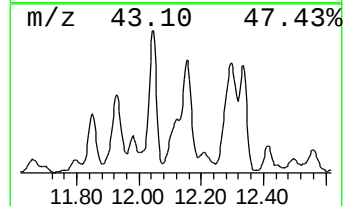
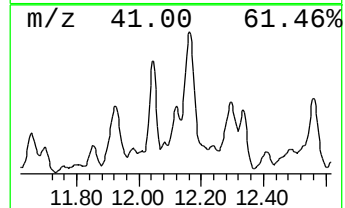
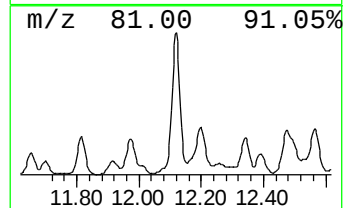
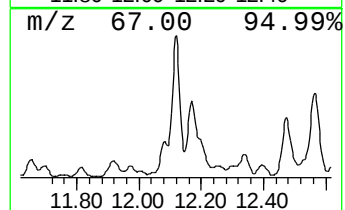
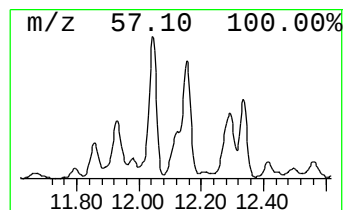
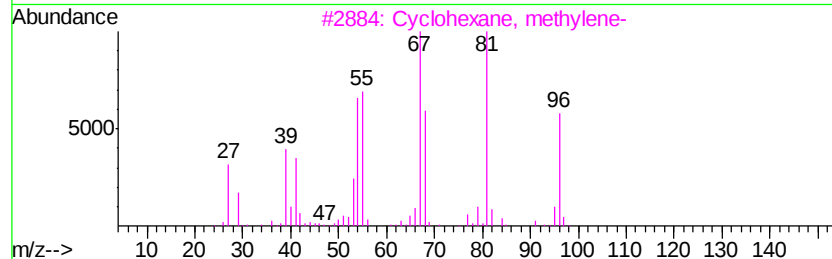
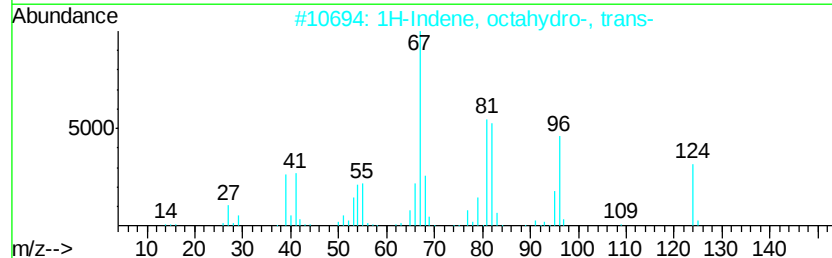
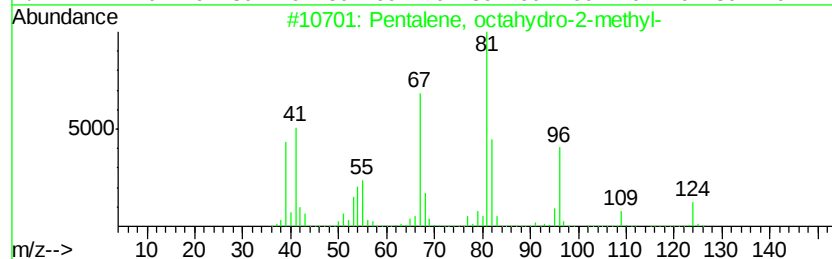
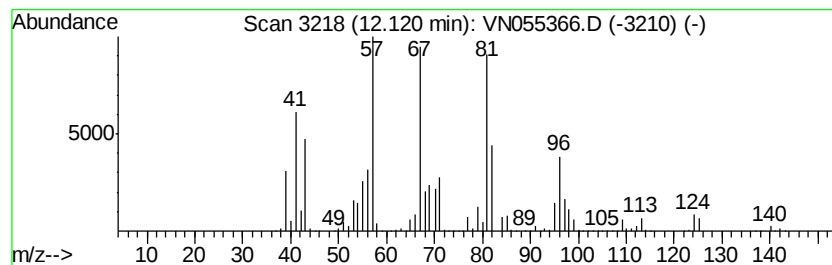
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Quant Title : SW846 8260

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

Peak Number 5 Pentalene, octahydro-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	112.47 ug/l	5278030	Chlorobenzene-d5	11.41

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	64
2	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	53
3	Cyclohexane, methylene-	96	C7H12	001192-37-6	49
4	7-Methyl-8-oxabicyclo[4.3.0]nonane	140	C9H16O	1000216-87-6	43
5	Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055366.D
Acq On : 2 May 2019 23:02
Operator : JC/SP
Sample : K2658-02 10X
Misc : 6.06g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 35 Sample Multiplier: 1

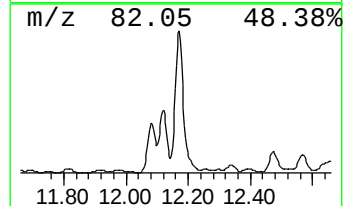
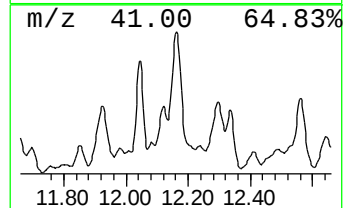
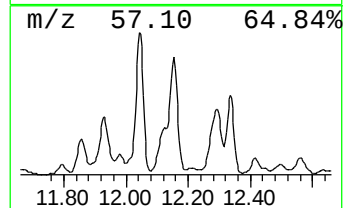
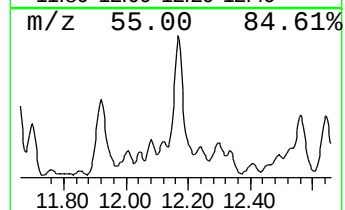
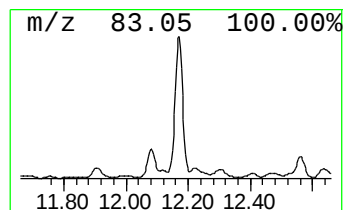
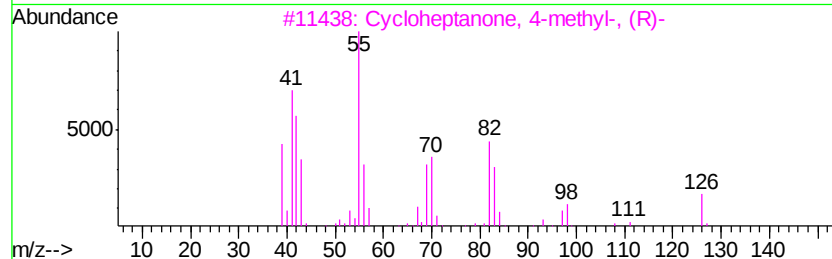
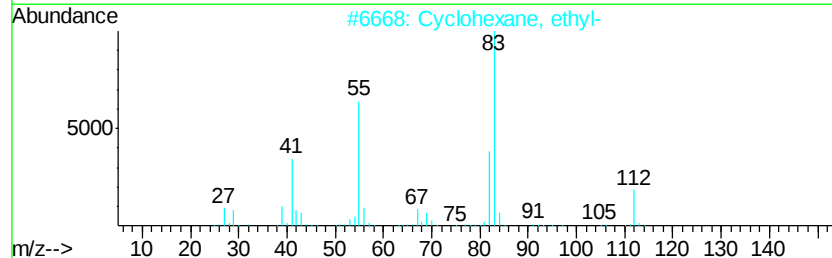
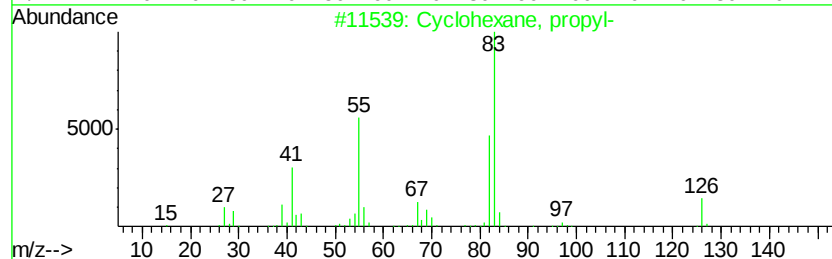
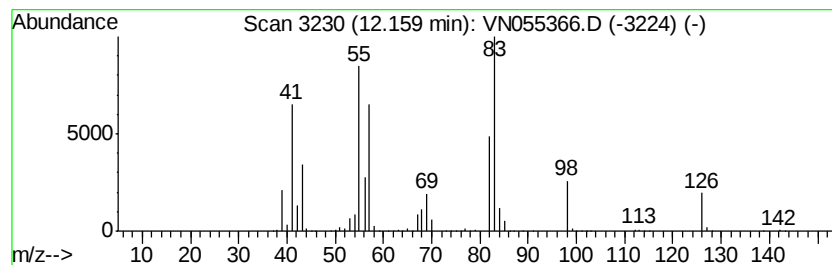
Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-W2(17-20)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.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	280.34 ug/l	13155800	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexane, propyl-	126	C9H18	001678-92-8	83
2		Cvclohexane, ethyl-	112	C8H16	001678-91-7	64
3		Cvcloheptanone, 4-methyl-, (R)-	126	C8H14O	013609-59-1	52
4		Cvclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	52
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055366.D
Acq On : 2 May 2019 23:02
Operator : JC/SP
Sample : K2658-02 10X
Misc : 6.06g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 35 Sample Multiplier: 1

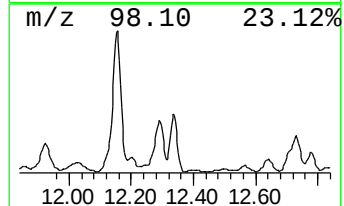
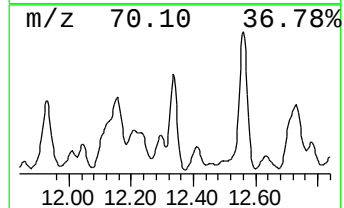
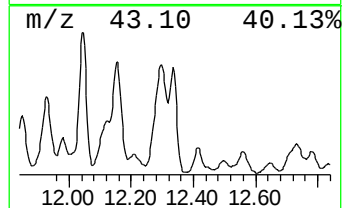
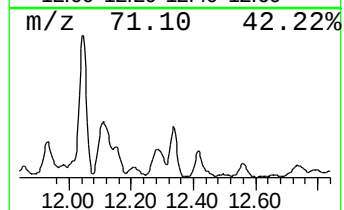
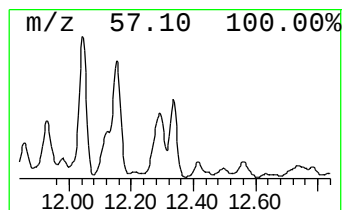
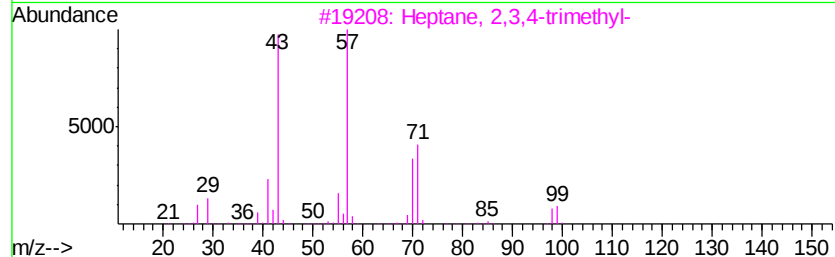
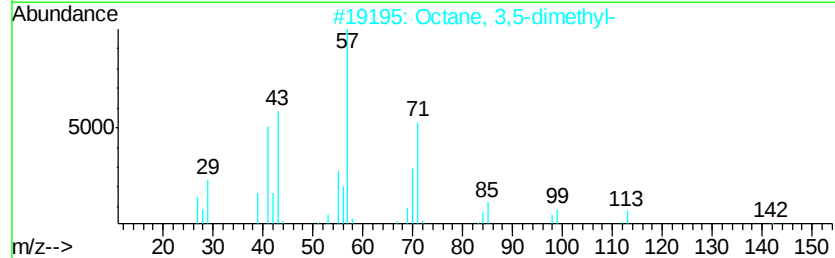
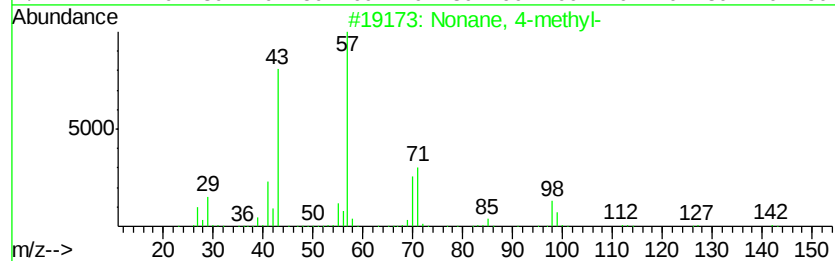
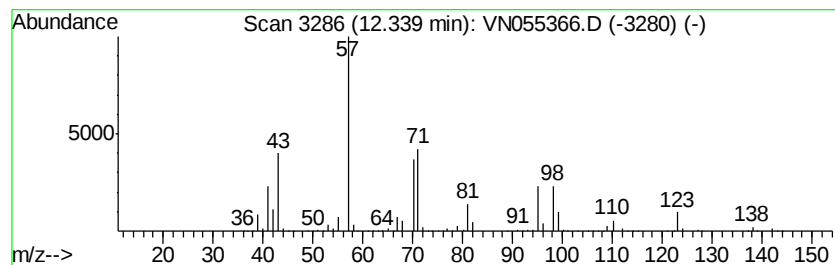
Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-W2(17-20)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 7 Nonane, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.34	140.32 ug/l	6584870	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonane, 4-methyl-	142	C10H22	017301-94-9	64
2		Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53
3		Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	50
4		Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	47
5		Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN050219\
Data File : VN055366.D
Acq On : 2 May 2019 23:02
Operator : JC/SP
Sample : K2658-02 10X
Misc : 6.06µ/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 35 Sample Multiplier: 1

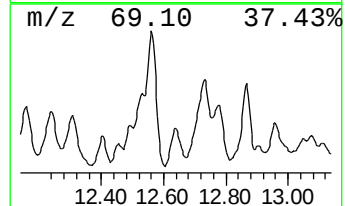
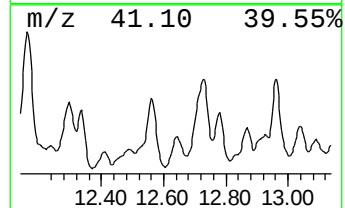
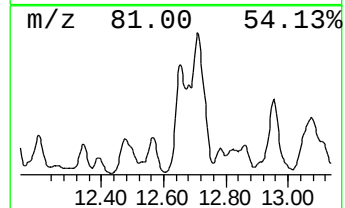
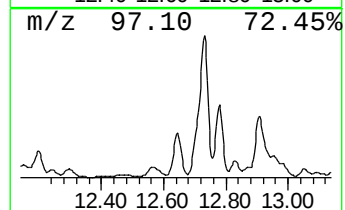
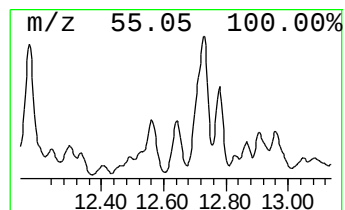
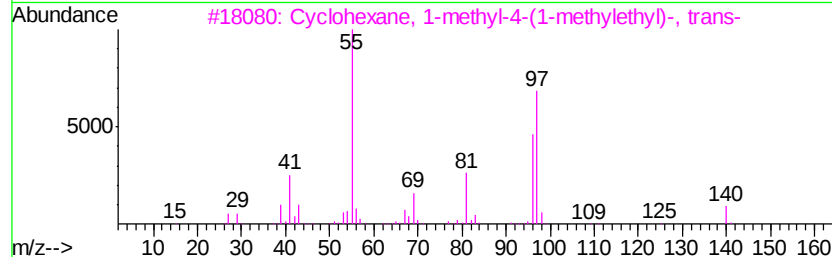
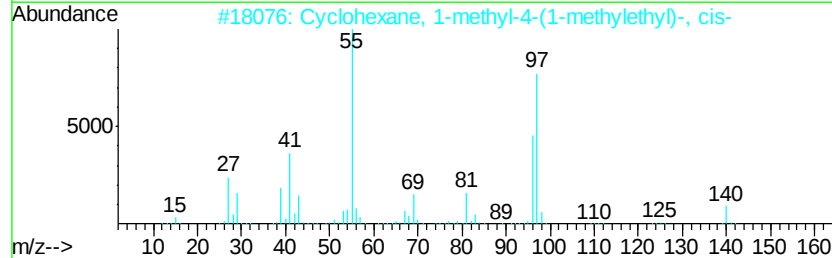
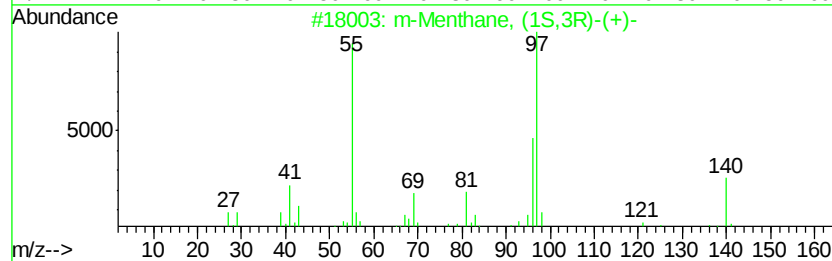
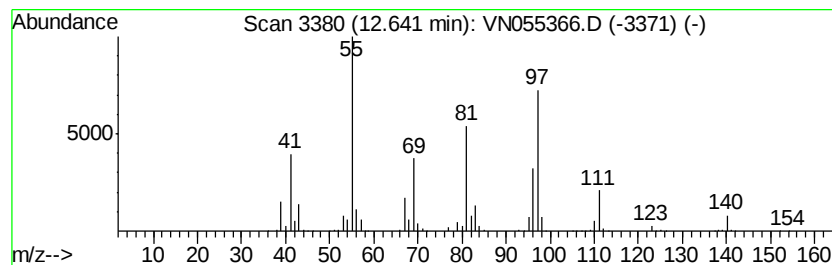
Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-W2(17-20)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 8 m-Menthane, (1S,3R)-(+)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	62.61 ug/l	4682870	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	m-Menthane, (1S,3R)-(+)-	140 C10H20	013837-66-6	80
2	Cyclohexane, 1-methyl-4-(1-methyl-...	140 C10H20	006069-98-3	74
3	Cyclohexane, 1-methyl-4-(1-methyl-...	140 C10H20	001678-82-6	74
4	m-Menthane, (1S,3S)-(+)-	140 C10H20	013837-67-7	72
5	1-Methyl-4-(1-methylethyl)-cyclo...	140 C10H20	000099-82-1	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055366.D
Acq On : 2 May 2019 23:02
Operator : JC/SP
Sample : K2658-02 10X
Misc : 6.06g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-W2(17-20)

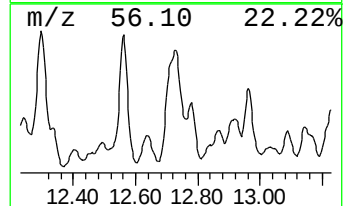
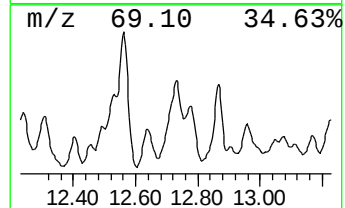
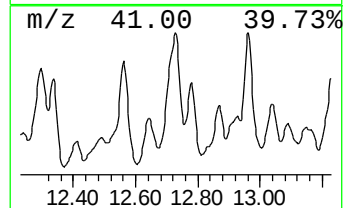
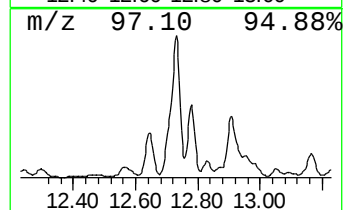
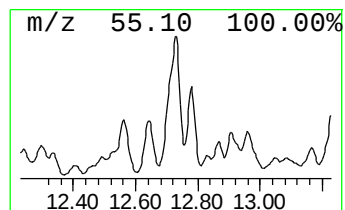
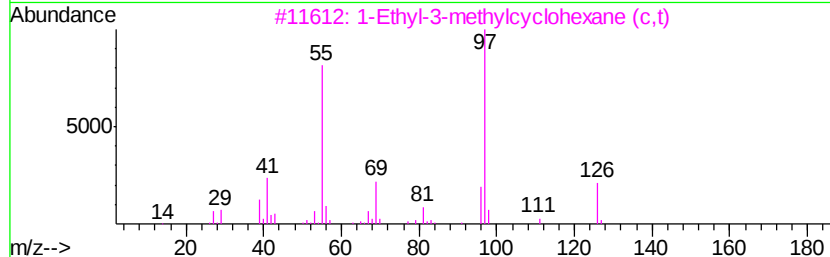
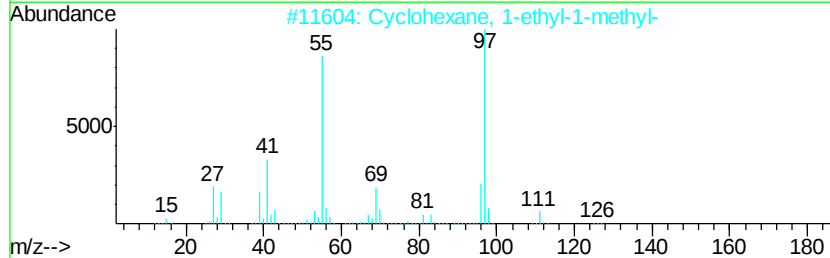
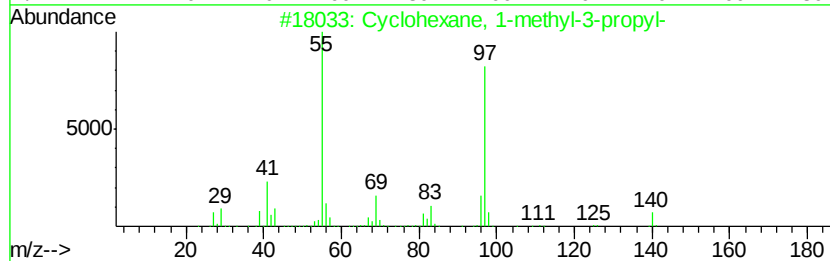
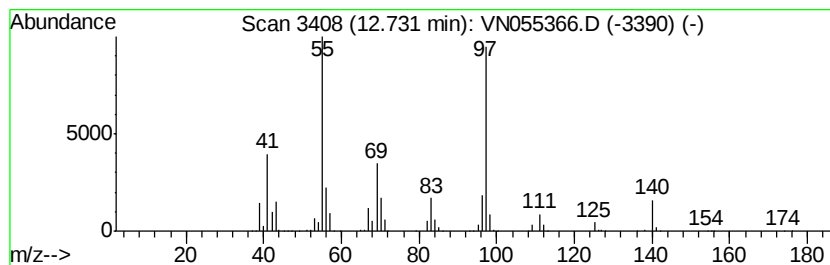
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 9 Cyclohexane, 1-methyl-3-pro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	267.13 ug/l	19979600	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	72
2		Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	64
3		1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	59
4		1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	59
5		Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	58



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
Data File : VN055366.D
Acq On : 2 May 2019 23:02
Operator : JC/SP
Sample : K2658-02 10X
Misc : 6.06µ/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EP1-SB-W2(17-20)

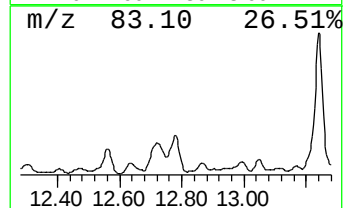
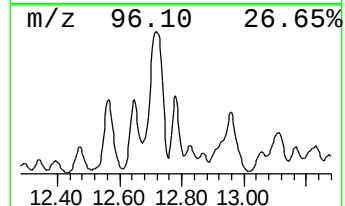
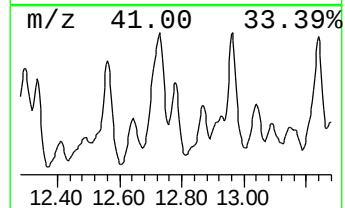
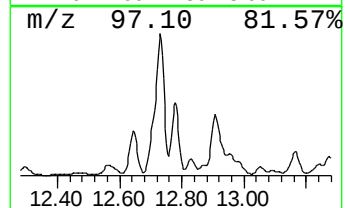
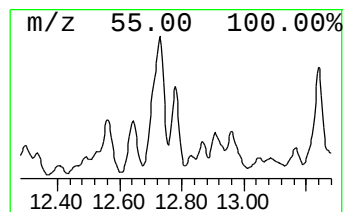
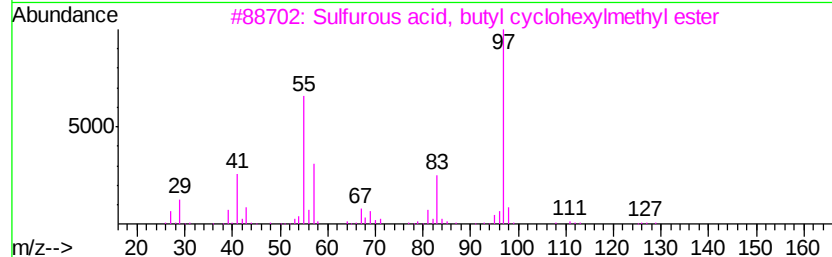
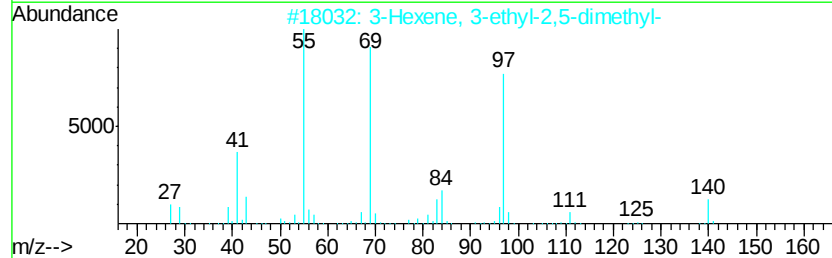
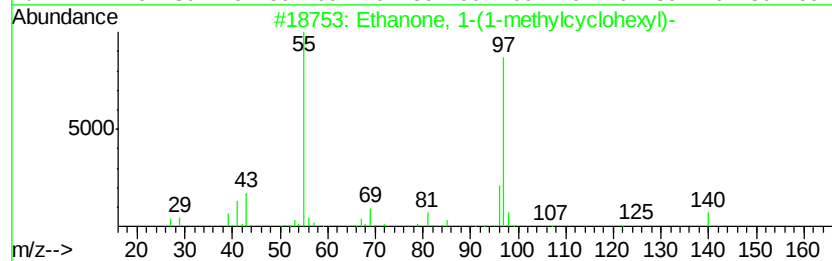
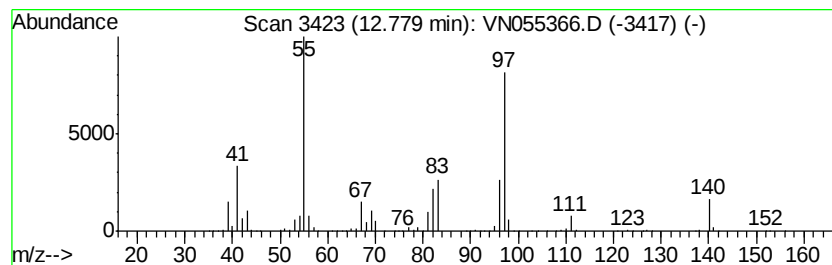
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042919W.M
Quant Title : SW846 8260

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

Peak Number 10 Ethanone, 1-(1-methylcyclohexyl) Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	77.46 ug/l	5793240	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 1-(1-methylcyclohexyl)-	140	C9H16O	002890-62-2	59
2		3-Hexene, 3-ethyl-2,5-dimethyl-	140	C10H20	062338-08-3	58
3		Sulfurous acid, butyl cyclohexyl...	234	C11H22O3S	1000309-21-4	53
4		Oxalic acid, cyclohexylmethyl et...	214	C11H18O4	1000309-68-0	53
5		Oxalic acid, butyl cyclohexylmet...	242	C13H22O4	1000309-68-2	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050219\
 Data File : VN055366.D
 Acq On : 2 May 2019 23:02
 Operator : JC/SP
 Sample : K2658-02 10X
 Misc : 6.06g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-SB-W2(17-20)

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane, 1,2,...	11.21	62.8	ug/l	2945950	3	11.41	2346390	50.0
1-Ethyl-4-methylc...	11.70	62.3	ug/l	2923740	3	11.41	2346390	50.0
Cyclohexane, 1-et...	11.92	224.7	ug/l	10543600	3	11.41	2346390	50.0
Nonane, 3-methyl-	12.04	143.8	ug/l	6746990	3	11.41	2346390	50.0
Pentalene, octahy...	12.12	112.5	ug/l	5278030	3	11.41	2346390	50.0
Cyclohexane, propyl-	12.16	280.3	ug/l	13155800	3	11.41	2346390	50.0
Nonane, 4-methyl-	12.34	140.3	ug/l	6584870	3	11.41	2346390	50.0
m-Menthane, (1S,3...	12.64	62.6	ug/l	4682870	4	13.35	3739700	50.0
Cyclohexane, 1-me...	12.73	267.1	ug/l	19979600	4	13.35	3739700	50.0
Ethanone, 1-(1-me...	12.78	77.5	ug/l	5793240	4	13.35	3739700	50.0