

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN110819\
 Data File : VN059136.D
 Acq On : 8 Nov 2019 16:15
 Operator : JC/SP
 Sample : K5742-07 10X
 Misc : 9.20g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SB-35-(6-8)

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\82N110619W.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	7.564	1781	1801	1812	rBV	287821	717585	29.52%	2.842%
2	7.641	1813	1825	1844	rVB	568590	1344354	55.31%	5.324%
3	8.001	1917	1937	1964	rBV	338573	790936	32.54%	3.132%
4	8.564	2095	2112	2137	rBV	810887	1697023	69.82%	6.721%
5	9.062	2245	2267	2279	rBV7	11823	32659	1.34%	0.129%
6	10.078	2567	2583	2611	rBV	1280344	2430552	100.00%	9.626%
7	10.275	2627	2644	2663	rBV3	32015	114130	4.70%	0.452%
8	10.422	2682	2690	2702	rVB3	24992	46340	1.91%	0.184%
9	10.522	2709	2721	2729	rBV6	17128	35468	1.46%	0.140%
10	10.712	2772	2780	2789	rVB2	17030	26454	1.09%	0.105%
11	10.943	2845	2852	2860	rVB2	26258	38420	1.58%	0.152%
12	10.998	2860	2869	2879	rVB3	40495	69776	2.87%	0.276%
13	11.117	2896	2906	2913	rBV6	15163	26545	1.09%	0.105%
14	11.204	2925	2933	2949	rVB3	40327	83345	3.43%	0.330%
15	11.291	2949	2960	2968	rBV3	18002	34408	1.42%	0.136%
16	11.400	2981	2994	3015	rBV	1112653	1975111	81.26%	7.822%
17	11.538	3029	3037	3044	rBV3	17922	27438	1.13%	0.109%
18	11.596	3045	3055	3060	rBV6	18766	38838	1.60%	0.154%
19	11.651	3062	3072	3080	rBV2	63608	113332	4.66%	0.449%
20	11.802	3110	3119	3126	rBV8	14141	27855	1.15%	0.110%
21	11.847	3127	3133	3142	rVB4	24335	34494	1.42%	0.137%
22	11.921	3142	3156	3167	rBV7	86322	222549	9.16%	0.881%
23	12.043	3187	3194	3201	rVB	66035	90617	3.73%	0.359%
24	12.114	3202	3216	3222	rBV5	67042	135450	5.57%	0.536%
25	12.162	3223	3231	3241	rVB3	98794	174109	7.16%	0.690%
26	12.294	3262	3272	3279	rBV7	76628	150083	6.17%	0.594%
27	12.332	3281	3284	3293	rVB4	72950	90957	3.74%	0.360%
28	12.400	3293	3305	3318	rBV	909557	1556345	64.03%	6.163%
29	12.561	3350	3355	3368	rVB5	108881	184874	7.61%	0.732%
30	12.644	3370	3381	3392	rBV5	67140	176143	7.25%	0.698%
31	12.728	3395	3407	3416	rVV4	223941	502746	20.68%	1.991%
32	12.779	3417	3423	3433	rVB4	132671	222415	9.15%	0.881%
33	12.869	3444	3451	3458	rBV6	83872	134561	5.54%	0.533%
34	12.959	3474	3479	3492	rVB4	180462	298187	12.27%	1.181%

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SB-35-(6-8)

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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35	13.037	3494	3503	3511	rVB3	116208	205856	8.47%	0.815%
36	13.091	3512	3520	3529	rBV	111113	184675	7.60%	0.731%
37	13.149	3531	3538	3551	rVB9	95177	225118	9.26%	0.892%
38	13.239	3551	3566	3573	rBV2	379959	766401	31.53%	3.035%
39	13.342	3588	3598	3610	rBV	980499	1635080	67.27%	6.475%
40	13.663	3689	3698	3707	rBV5	444978	828856	34.10%	3.282%
41	13.712	3708	3713	3721	rVB	207439	284271	11.70%	1.126%
42	13.995	3795	3801	3809	rVB4	181392	270452	11.13%	1.071%
43	14.059	3811	3821	3832	rVV5	282915	630341	25.93%	2.496%
44	14.181	3847	3859	3873	rBV6	705172	1695866	69.77%	6.716%
45	14.252	3874	3881	3889	rVB	551105	774422	31.86%	3.067%
46	14.335	3901	3907	3915	rVB3	464189	590497	24.29%	2.339%
47	14.528	3962	3967	3974	rVB	249905	317613	13.07%	1.258%
48	14.586	3976	3985	3996	rBV2	727598	1587453	65.31%	6.287%
49	14.647	3997	4004	4014	rVB4	621497	1033435	42.52%	4.093%
50	14.856	4064	4069	4075	rBV5	219708	262356	10.79%	1.039%
51	15.110	4143	4148	4154	rBV2	232093	314287	12.93%	1.245%

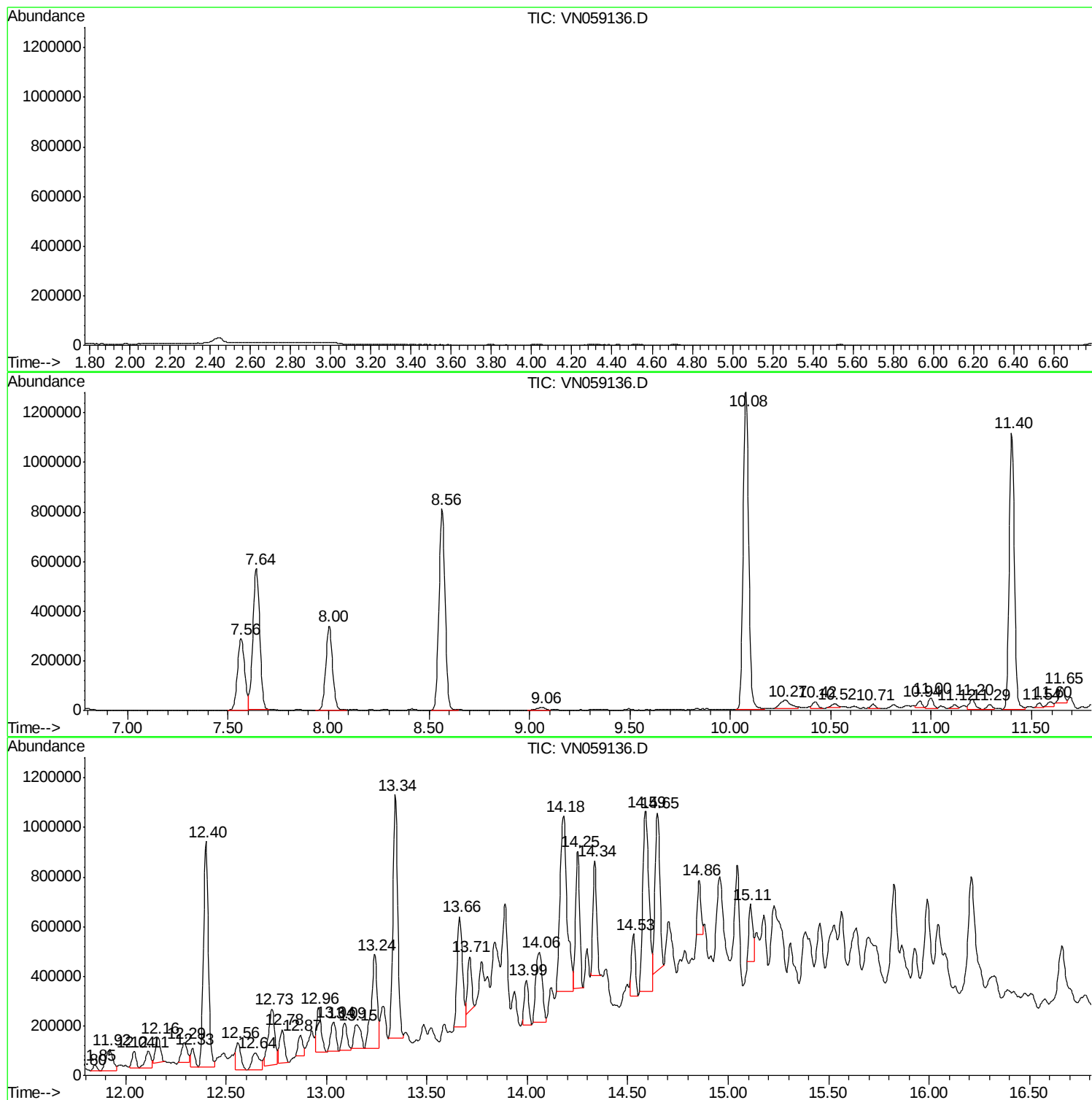
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Quant Title : SW846 8260

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



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Instrument :
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ClientSampled :
SB-35-(6-8)

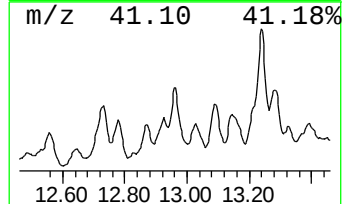
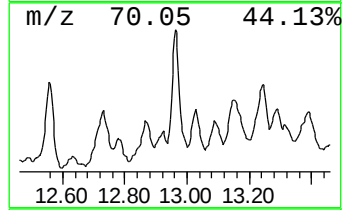
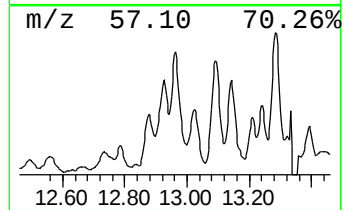
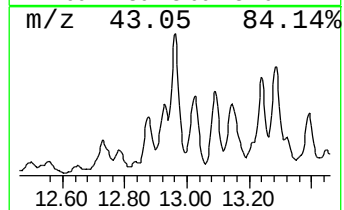
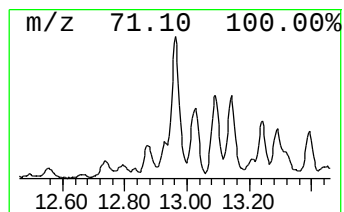
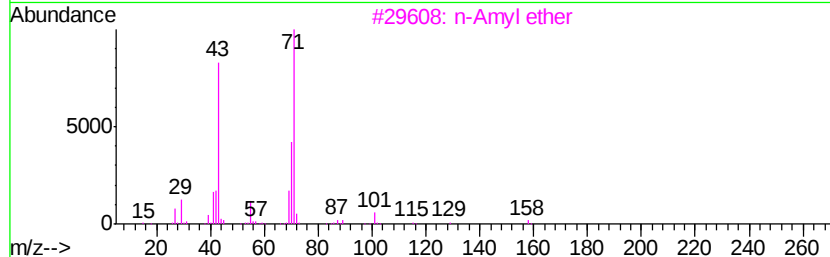
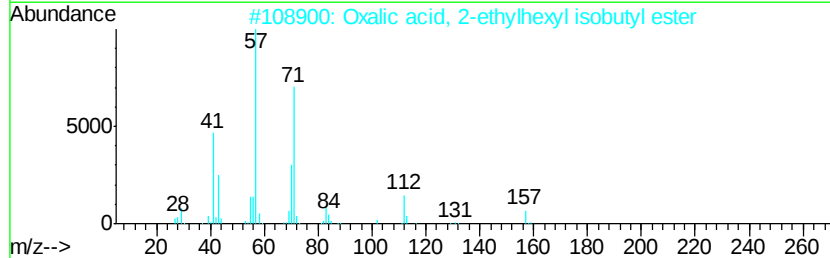
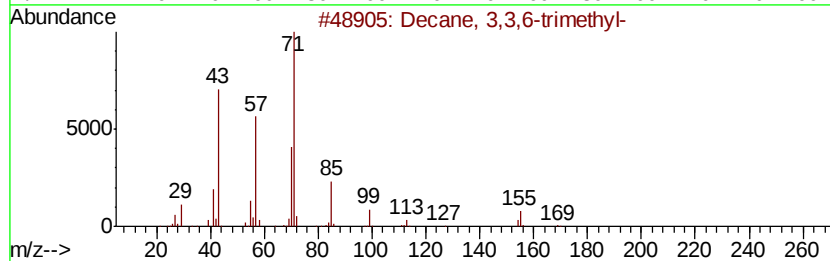
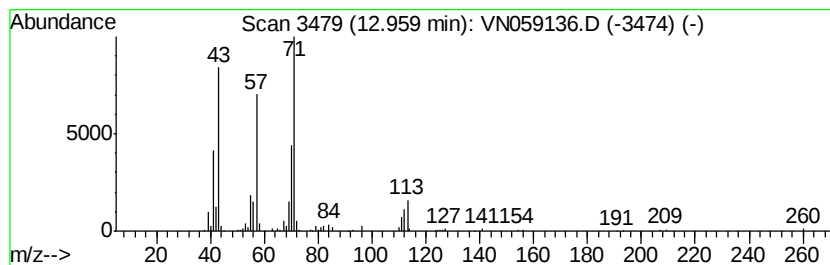
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N110619W.M
Quant Title : SW846 8260

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

Peak Number 1 Decane, 3,3,6-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	9.12 ug/l	298187	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 3,3,6-trimethyl-	184	C13H28	062338-14-1	64
2		Oxalic acid, 2-ethylhexyl isobut...	258	C14H26O4	1000309-38-5	64
3		n-Amyl ether	158	C10H22O	000693-65-2	64
4		Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	64
5		Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	64



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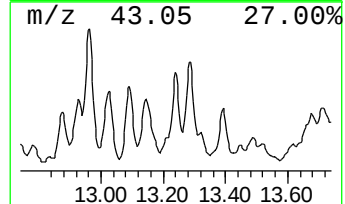
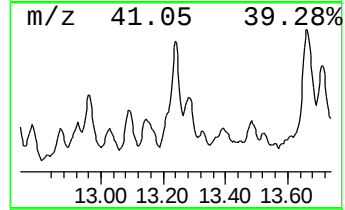
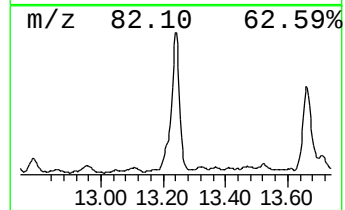
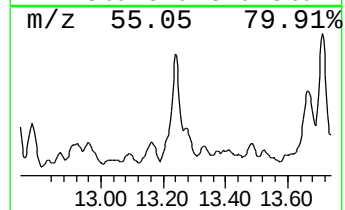
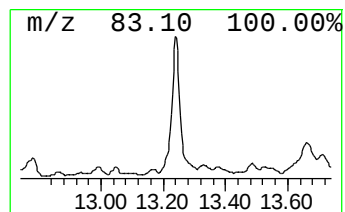
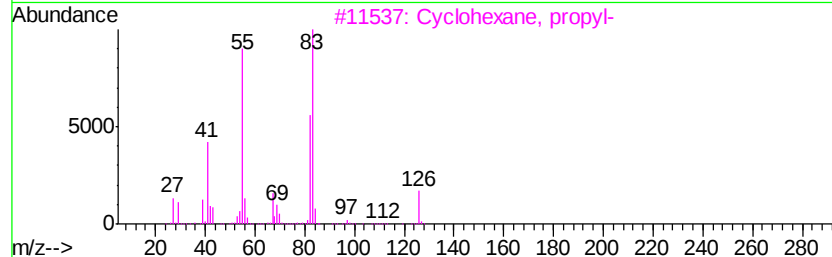
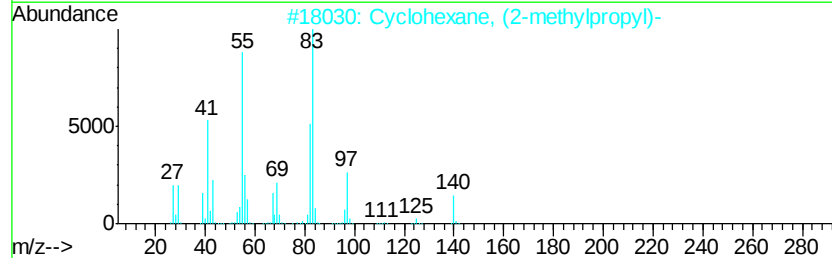
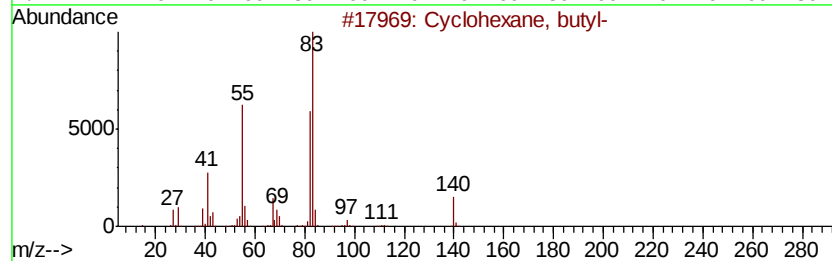
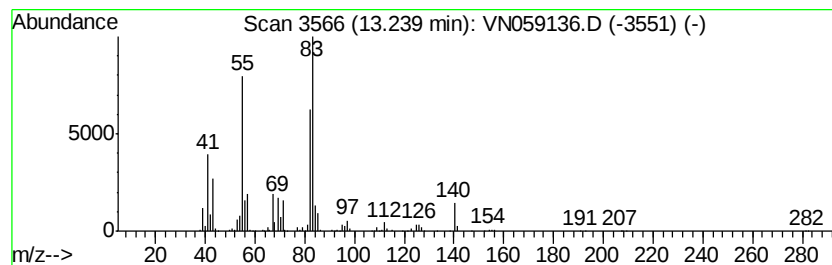
Instrument :
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ClientSampled :
SB-35-(6-8)

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

Peak Number 2 Cyclohexane, butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.24	23.44 ug/l	766401	1,4-Dichlorobenzene-d4	13.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cvclohexane, butyl-	140	C10H20	001678-93-9	93
2	Cvclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	86
3	Cvclohexane, propyl-	126	C9H18	001678-92-8	83
4	Cvclohexane, pentyl-	154	C11H22	004292-92-6	74
5	Cvclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	74



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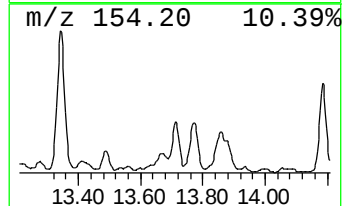
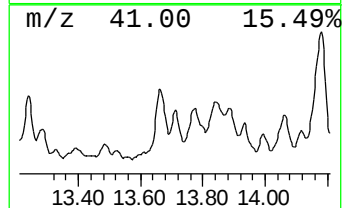
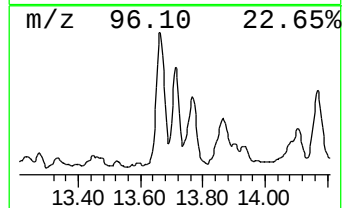
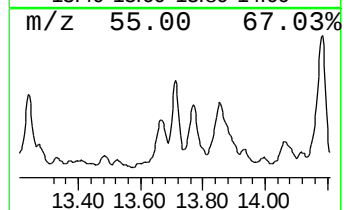
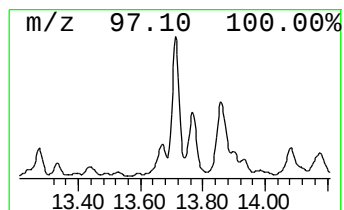
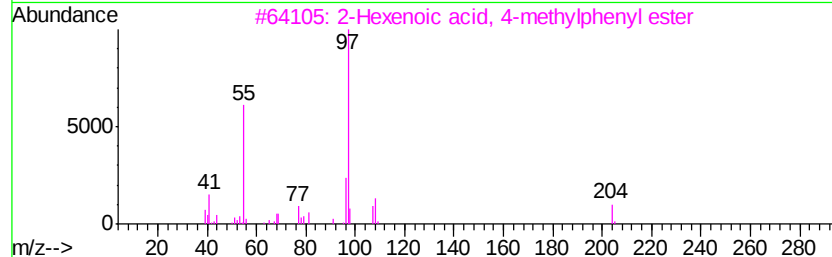
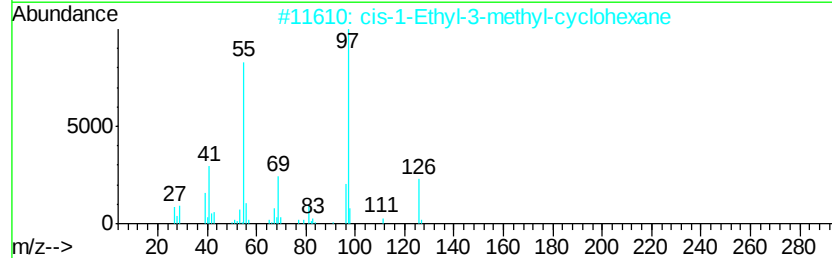
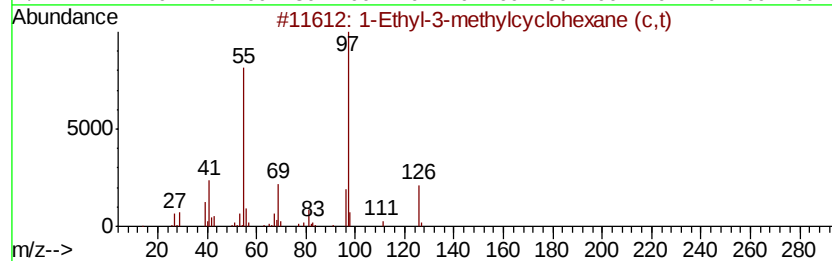
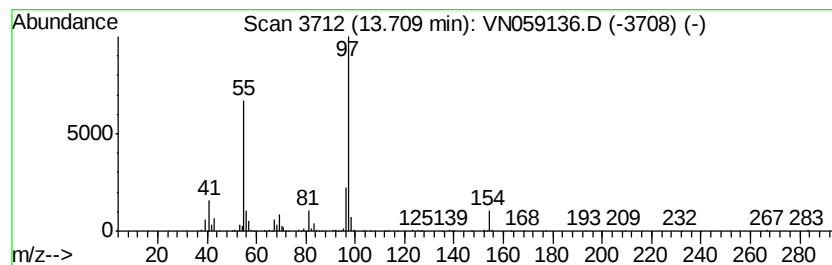
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Ethyl-3-methylcyclohexane... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.71	8.69 ug/l	284271	1,4-Dichlorobenzene-d4	13.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	72
2	cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	72
3	2-Hexenoic acid, 4-methylphenyl ...	204	C13H16O2	069687-91-8	72
4	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	64
5	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	59



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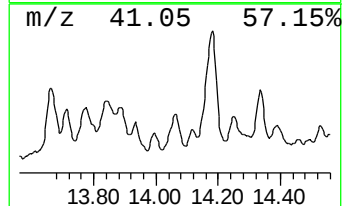
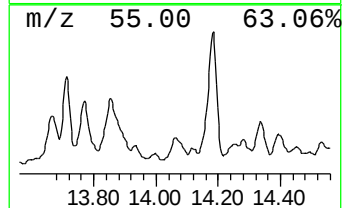
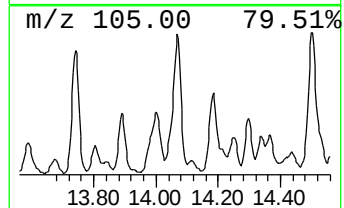
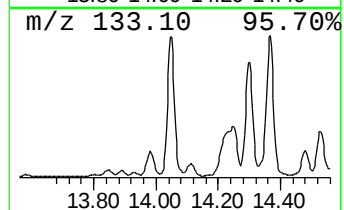
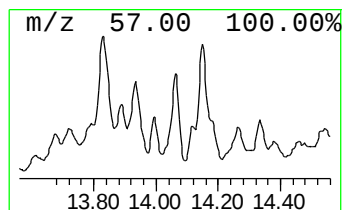
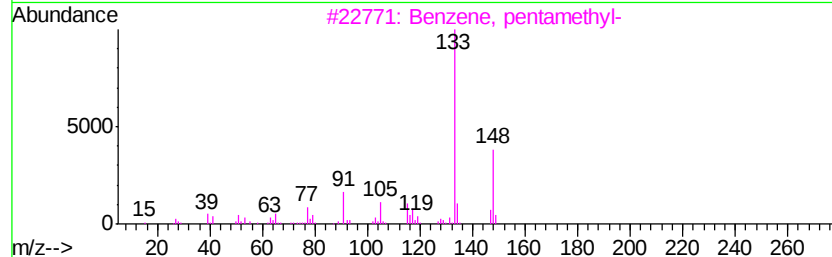
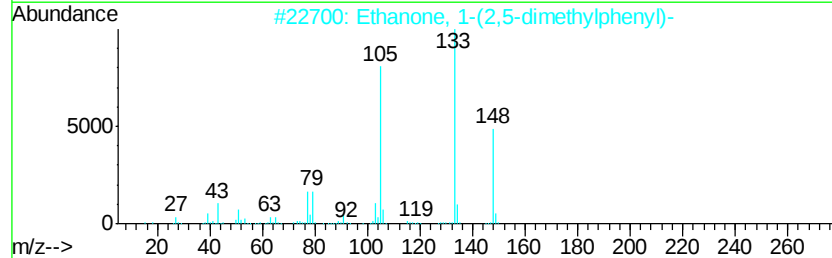
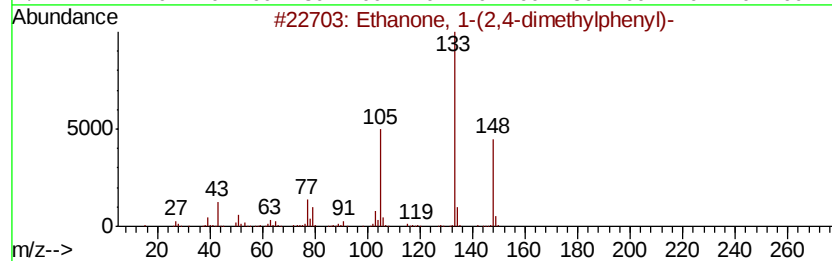
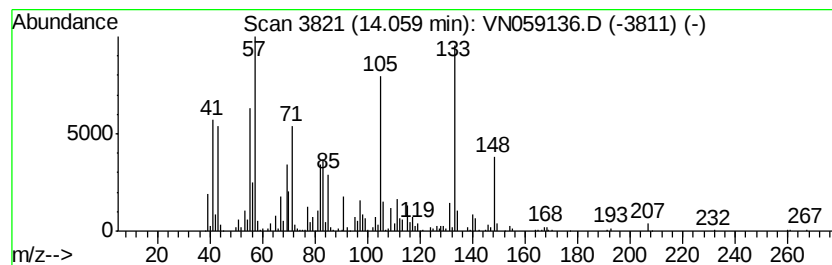
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanone, 1-(2,4-dimethylph... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.06	19.28 ug/l	630341	1,4-Dichlorobenzene-d4	13.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Ethanone, 1-(2,4-dimethylphenyl)-	148 C10H12O	000089-74-7	90
2	Ethanone, 1-(2,5-dimethylphenyl)-	148 C10H12O	002142-73-6	78
3	Benzene, pentamethyl-	148 C11H16	000700-12-9	55
4	Benzene, 1-ethyl-4-(1-methylethyl)-	148 C11H16	004218-48-8	55
5	Benzene, 1,4-diethyl-2-methyl-	148 C11H16	013632-94-5	53



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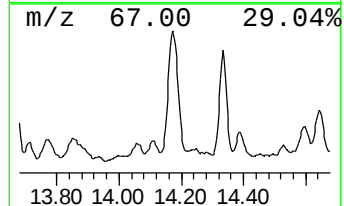
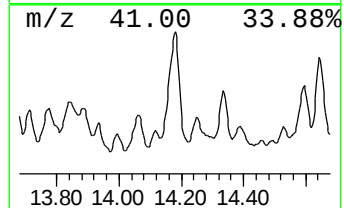
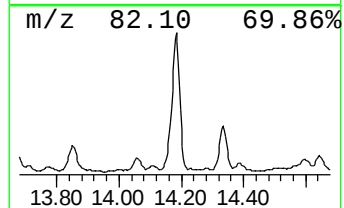
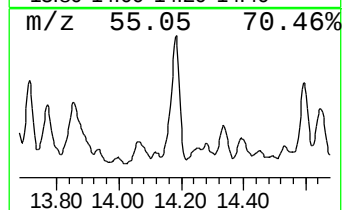
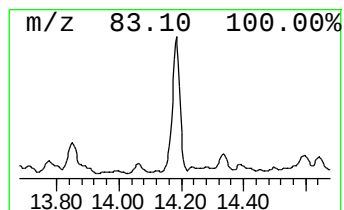
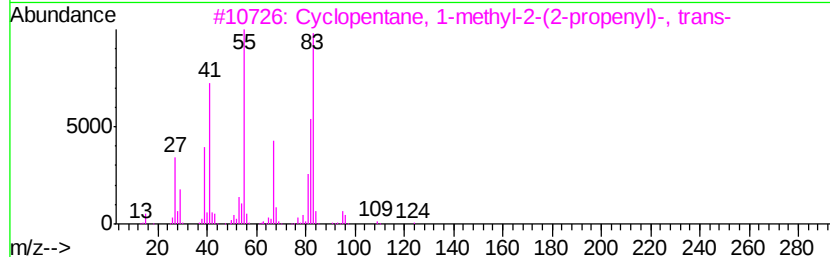
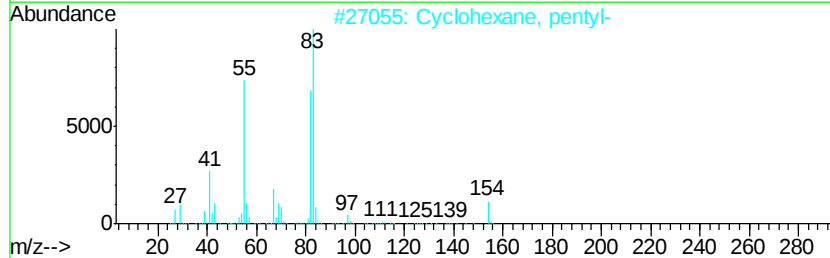
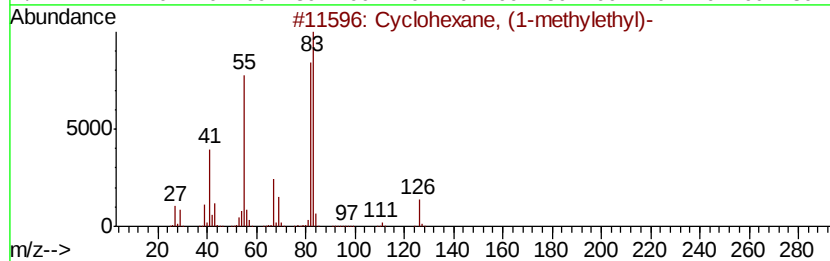
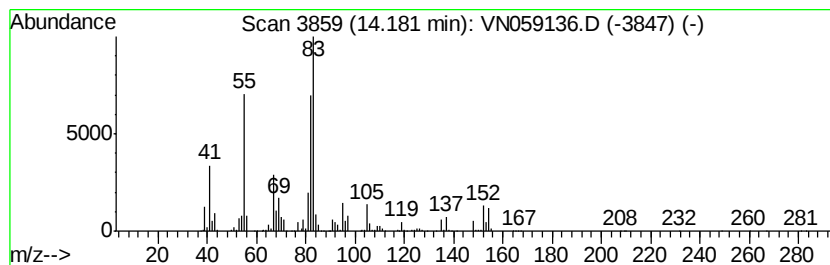
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, (1-methylethyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	51.86 ug/l	1695870	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	70
2		Cyclohexane, pentyl-	154	C11H22	004292-92-6	70
3		Cyclopentane, 1-methyl-2-(2-propenyl)-	124	C9H16	050746-53-7	64
4		Cyclohexane, 1,1'-(1,2-ethanediv...)	194	C14H26	003321-50-4	53
5		Cyclohexane, butyl-	140	C10H20	001678-93-9	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN110819\
Data File : VN059136.D
Acq On : 8 Nov 2019 16:15
Operator : JC/SP
Sample : K5742-07 10X
Misc : 9.20g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-35-(6-8)

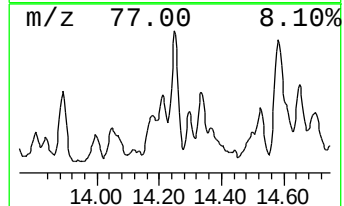
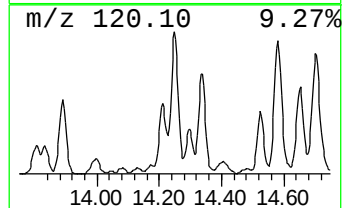
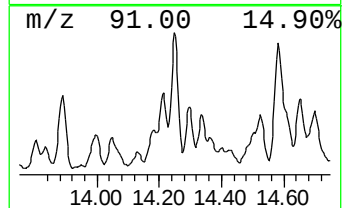
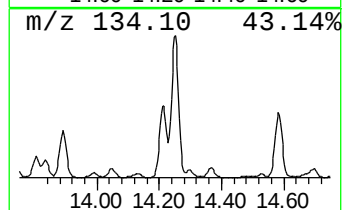
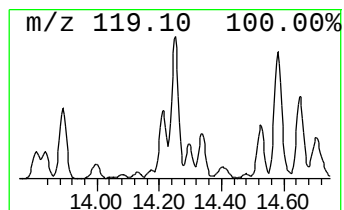
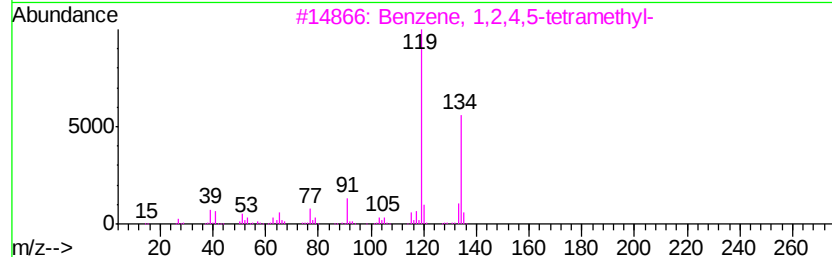
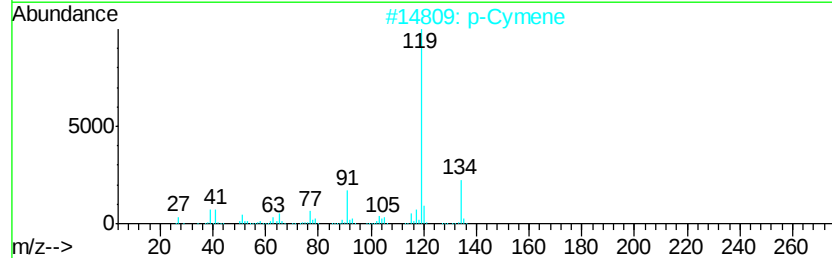
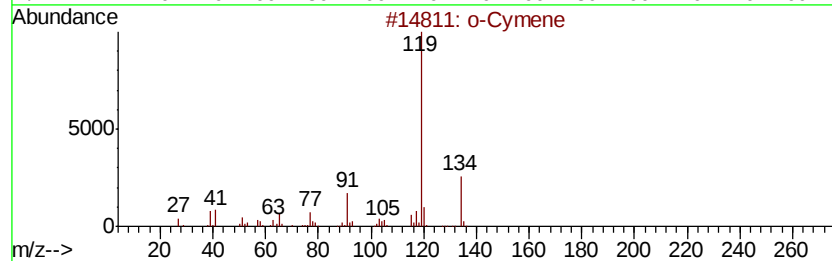
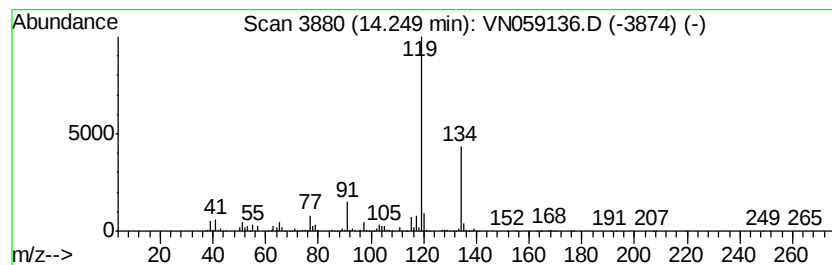
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Quant Title : SW846 8260

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

Peak Number 6 o-Cymene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	23.68 ug/l	774422	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	o-Cymene	134	C10H14	000527-84-4	94
2		p-Cymene	134	C10H14	000099-87-6	94
3		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
4		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	93
5		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	93



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN110819\
Data File : VN059136.D
Acq On : 8 Nov 2019 16:15
Operator : JC/SP
Sample : K5742-07 10X
Misc : 9.20g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-35-(6-8)

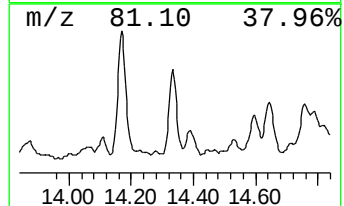
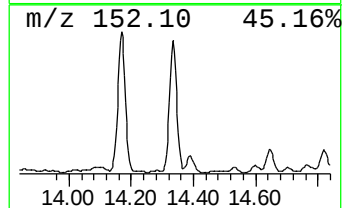
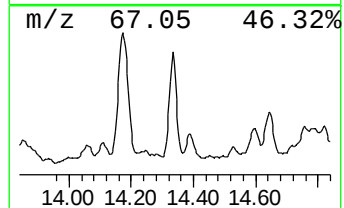
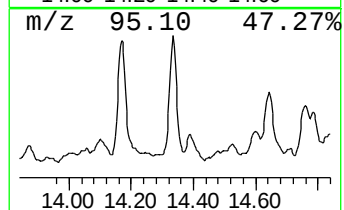
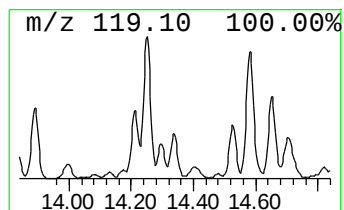
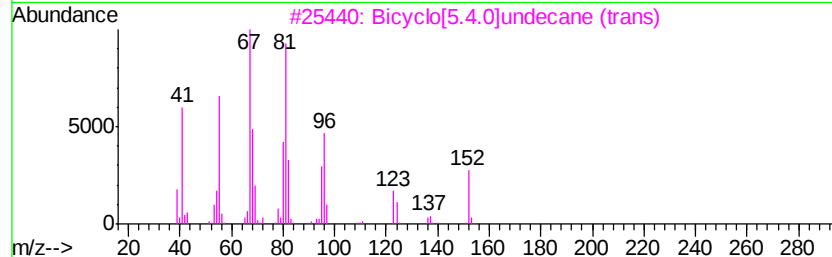
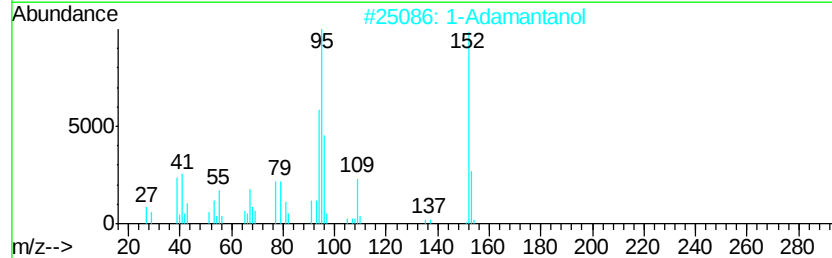
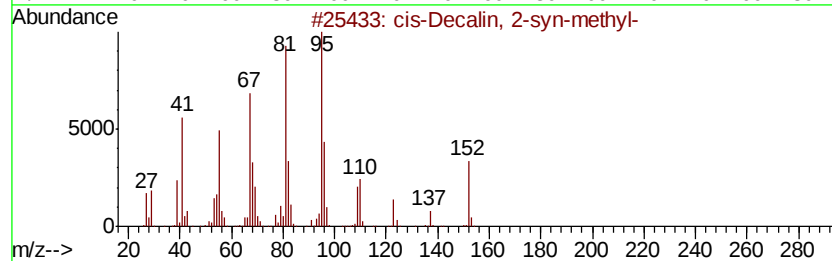
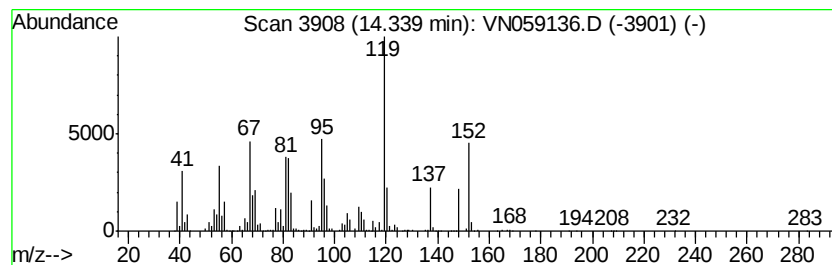
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.34 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	18.06 ug/l	590497	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	46
2		1-Adamantanol	152	C10H16O	000768-95-6	25
3		Bicyclo[5.4.0]undecane (trans)	152	C11H20	021394-30-9	22
4		Methanimidamide, N,N-dimethyl-N'...	152	C7H12N4	1000327-41-1	18
5		4-Methyl-1,3-heptadiene	110	C8H14	017603-57-5	15



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN110819\
Data File : VN059136.D
Acq On : 8 Nov 2019 16:15
Operator : JC/SP
Sample : K5742-07 10X
Misc : 9.20g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
SB-35-(6-8)

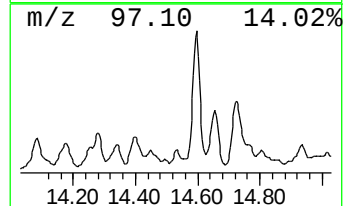
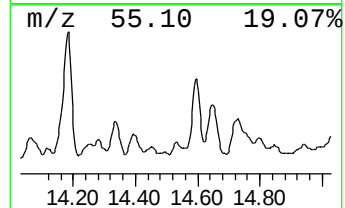
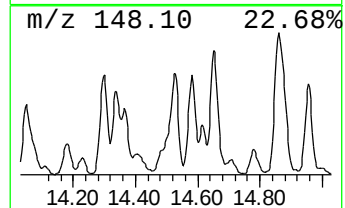
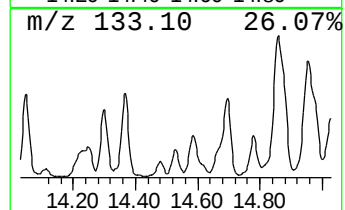
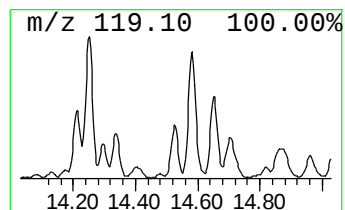
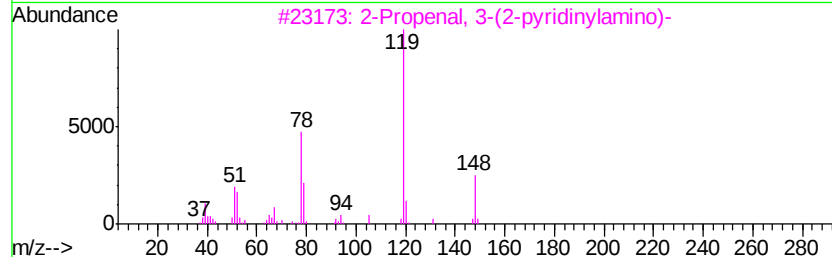
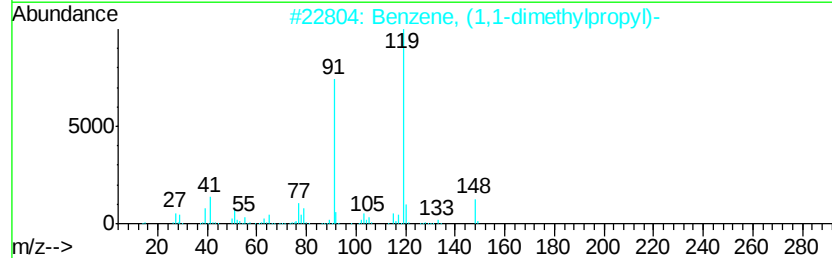
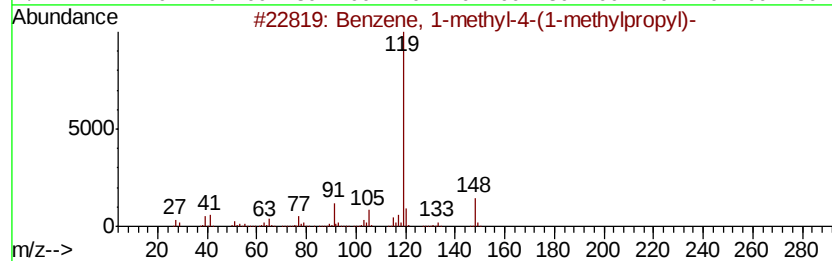
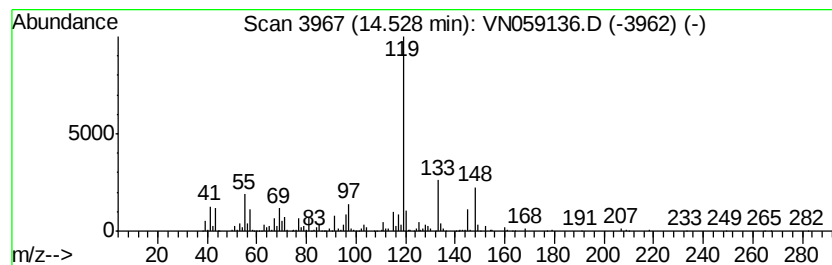
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-methyl-4-(1-meth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	9.71 ug/l	317613	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	58
2		Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	50
3		2-Propenal, 3-(2-pyridinylamino)-	148	C8H8N2O	068970-82-1	50
4		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	49
5		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN110819\
Data File : VN059136.D
Acq On : 8 Nov 2019 16:15
Operator : JC/SP
Sample : K5742-07 10X
Misc : 9.20µ/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
SB-35-(6-8)

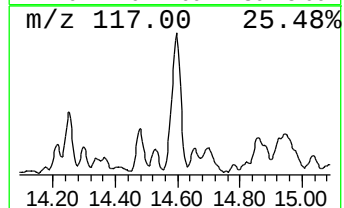
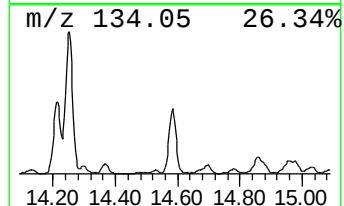
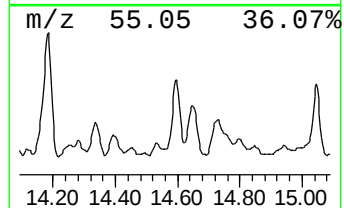
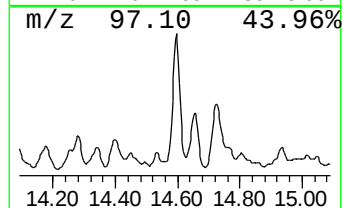
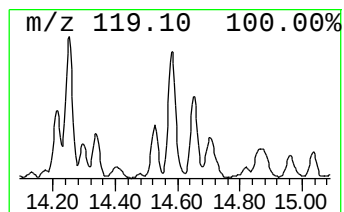
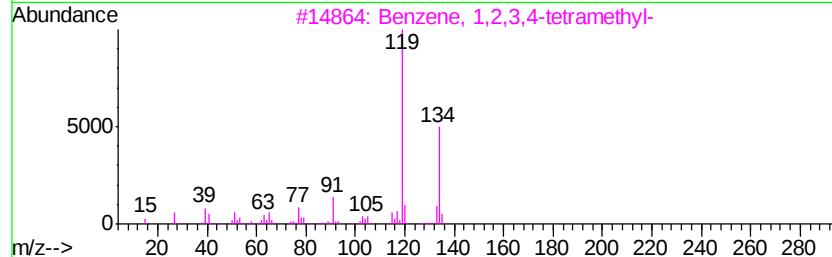
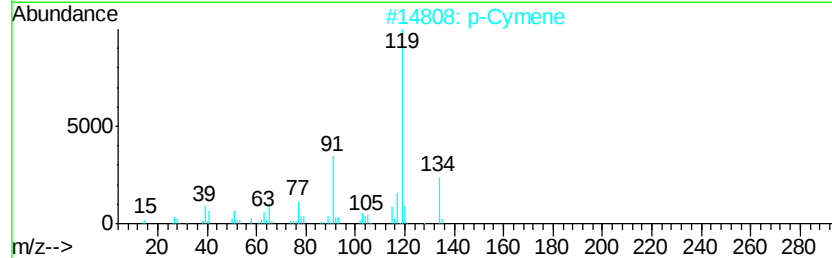
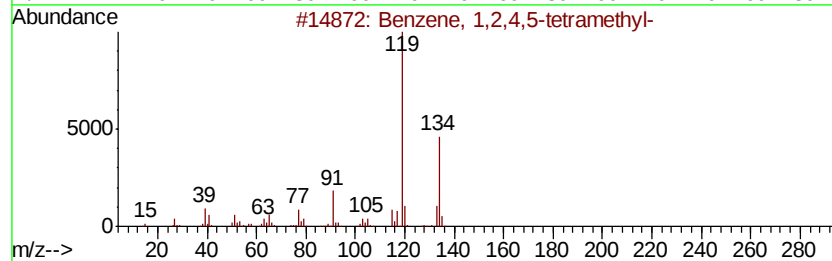
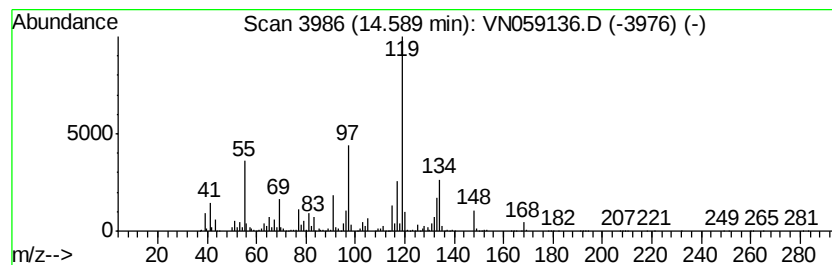
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N110619W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	48.54 ug/l	1587450	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	76
2		p-Cymene	134	C10H14	000099-87-6	76
3		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	76
4		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	70
5		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	70



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN110819\
Data File : VN059136.D
Acq On : 8 Nov 2019 16:15
Operator : JC/SP
Sample : K5742-07 10X
Misc : 9.20µ/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-35-(6-8)

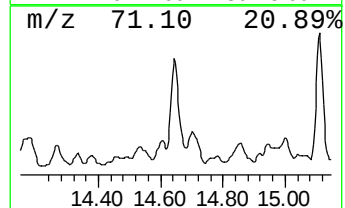
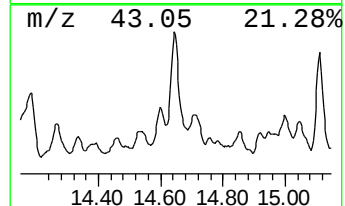
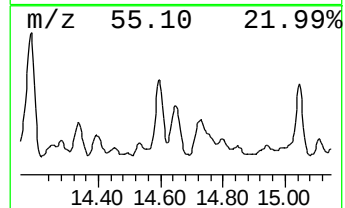
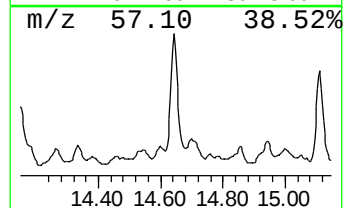
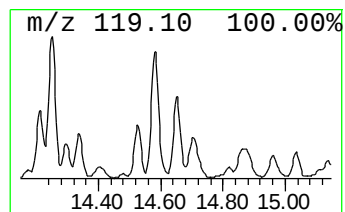
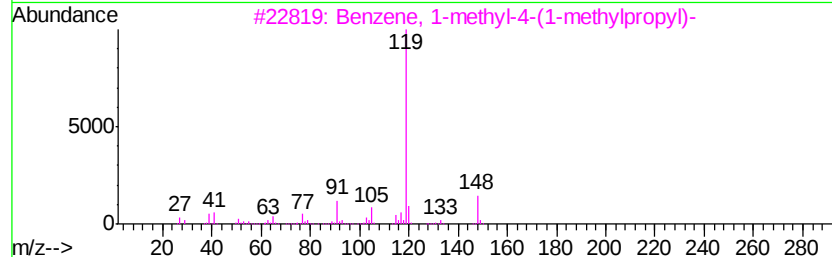
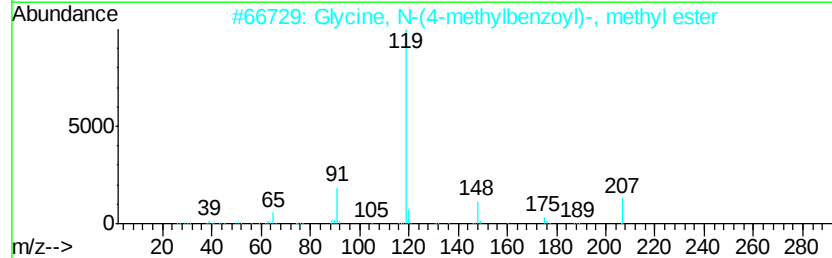
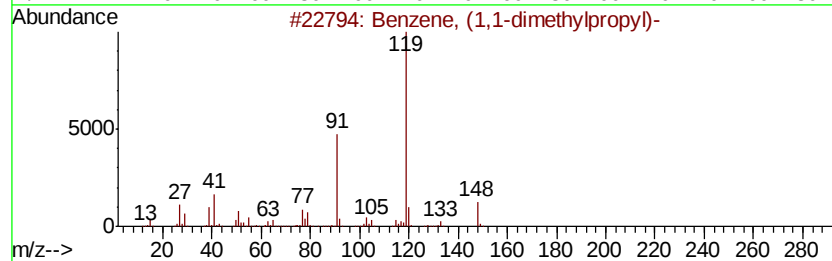
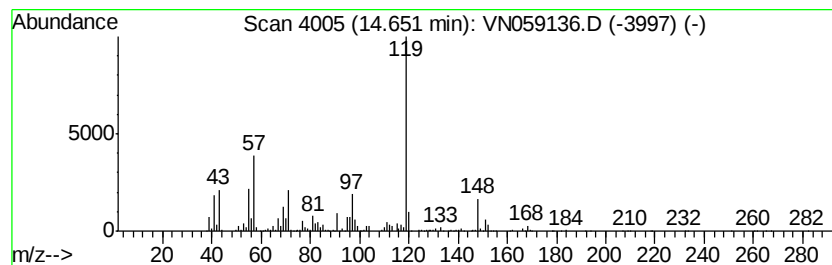
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N110619W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown14.65 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	31.60 ug/l	1033440	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	49
2		Glycine, N-(4-methylbenzoyl)-, m...	207	C11H13NO3	001208-23-7	47
3		Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	47
4		Benzoic acid, 2-methyl-, (2-isop...	268	C18H20O2	032276-66-7	43
5		Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	43



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN110819\
Data File : VN059136.D
Acq On : 8 Nov 2019 16:15
Operator : JC/SP
Sample : K5742-07 10X
Misc : 9.20g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SB-35-(6-8)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N110619W.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
Decane, 3,3,6-tri...	12.96	9.1	ug/l	298187	4	13.34	1635080	50.0
Cyclohexane, butyl-	13.24	23.4	ug/l	766401	4	13.34	1635080	50.0
1-Ethyl-3-methylc...	13.71	8.7	ug/l	284271	4	13.34	1635080	50.0
Ethanone, 1-(2,4-...	14.06	19.3	ug/l	630341	4	13.34	1635080	50.0
Cyclohexane, (1-m...	14.18	51.9	ug/l	1695870	4	13.34	1635080	50.0
o-Cymene	14.25	23.7	ug/l	774422	4	13.34	1635080	50.0
unknown14.34	14.34	18.1	ug/l	590497	4	13.34	1635080	50.0
Benzene, 1-methyl...	14.53	9.7	ug/l	317613	4	13.34	1635080	50.0
Benzene, 1,2,4,5-...	14.59	48.5	ug/l	1587450	4	13.34	1635080	50.0
unknown14.65	14.65	31.6	ug/l	1033440	4	13.34	1635080	50.0