

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN080718\
 Data File : VN050431.D
 Acq On : 7 Aug 2018 15:01
 Operator : MD\SY
 Sample : J4297-06
 Misc : 5.10µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-6

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\82N080618W.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	1.651	3	19	43	rBV	1397025	2105094	19.53%	2.697%
2	7.590	1844	1866	1877	rBV	550463	1374626	12.75%	1.761%
3	7.664	1877	1889	1914	rVB	842962	2017207	18.72%	2.585%
4	8.027	1983	2002	2025	rBV	566263	1316821	12.22%	1.687%
5	8.587	2161	2176	2200	rBV	1224639	2569586	23.84%	3.292%
6	10.091	2632	2644	2674	rVB	2301861	4359377	40.45%	5.586%
7	10.718	2832	2839	2849	rVB	180338	282498	2.62%	0.362%
8	11.005	2920	2928	2939	rVB	515790	889416	8.25%	1.140%
9	11.214	2986	2993	3008	rVB	313393	564530	5.24%	0.723%
10	11.410	3043	3054	3071	rBV	1694360	3055655	28.35%	3.915%
11	11.654	3125	3130	3139	rVB2	423539	606387	5.63%	0.777%
12	11.921	3200	3213	3225	rBV7	1042217	2695308	25.01%	3.453%
13	12.046	3245	3252	3259	rVB	1657523	2216067	20.56%	2.839%
14	12.120	3268	3275	3280	rBV3	881391	1461238	13.56%	1.872%
15	12.403	3353	3363	3374	rBV2	1975057	3401792	31.56%	4.359%
16	12.561	3405	3412	3426	rVB3	3013001	5539093	51.40%	7.097%
17	12.648	3428	3439	3450	rBV7	1190504	3109877	28.86%	3.985%
18	12.728	3452	3464	3472	rBV6	2072510	5096168	47.29%	6.530%
19	13.664	3746	3755	3765	rBV5	2915649	5177149	48.04%	6.633%
20	14.175	3905	3914	3938	rVB9	3023247	9159310	84.99%	11.736%
21	14.336	3958	3964	3971	rVB4	2544540	3414931	31.69%	4.376%
22	15.117	4201	4207	4217	rVB	7554957	10777200	100.00%	13.809%
23	16.037	4488	4493	4506	rVB2	4458371	6856953	63.62%	8.786%

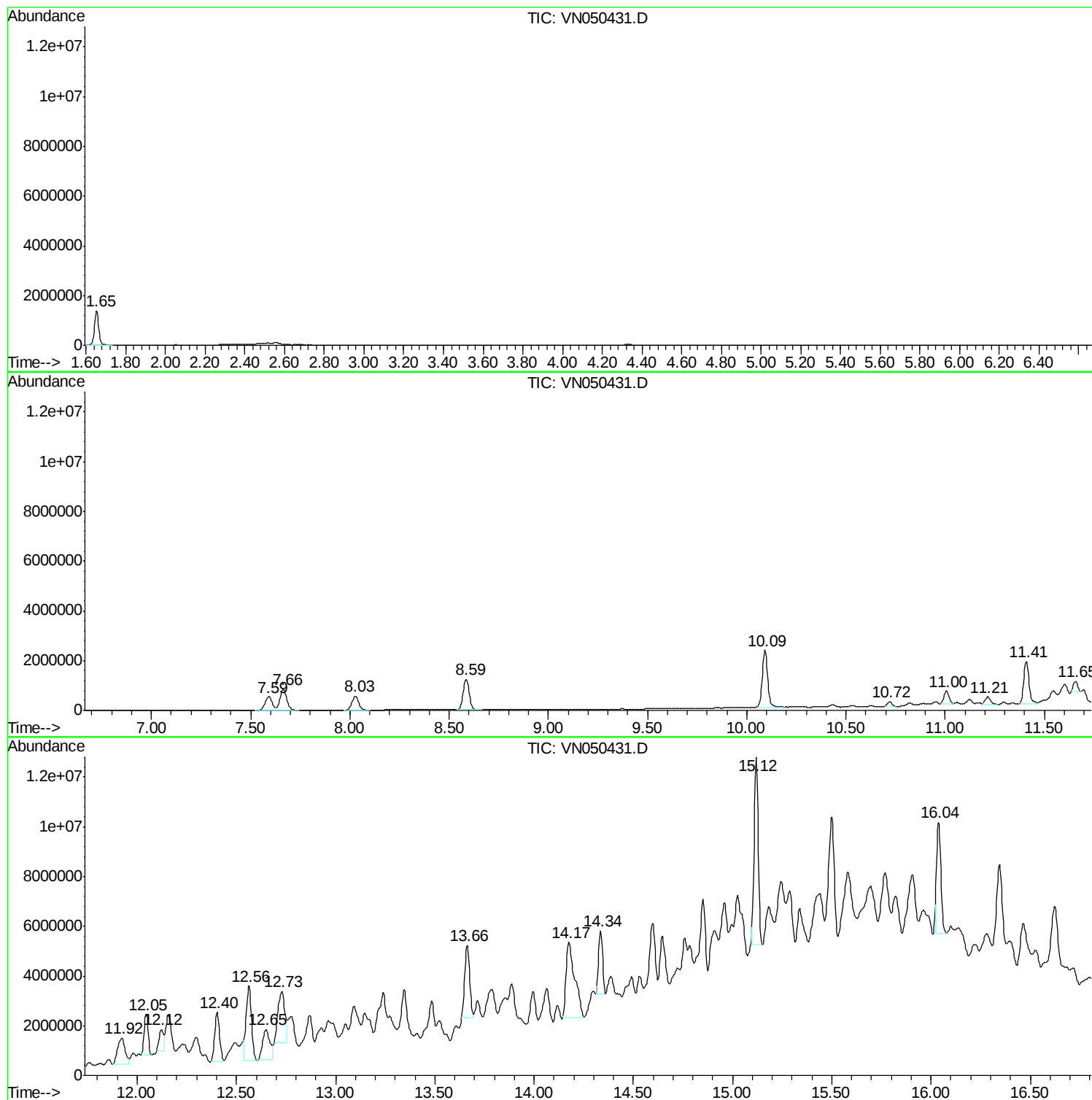
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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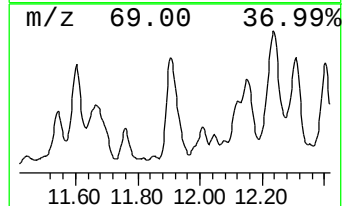
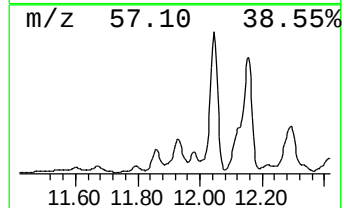
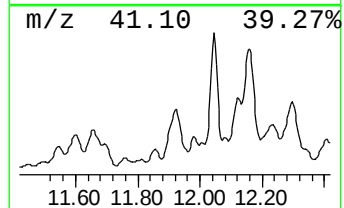
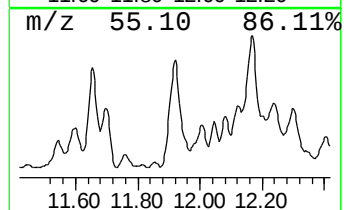
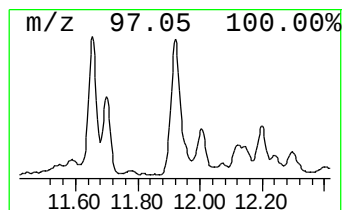
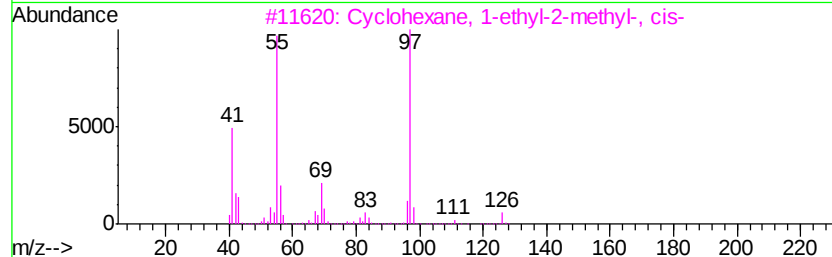
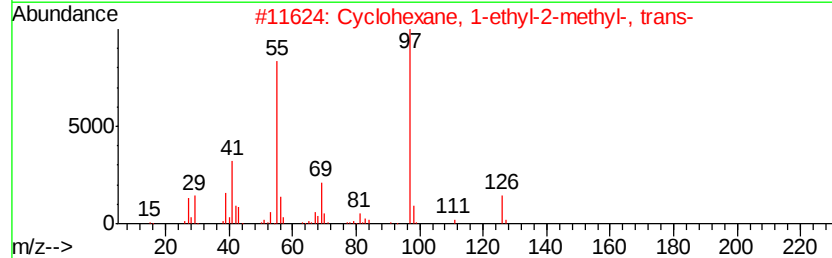
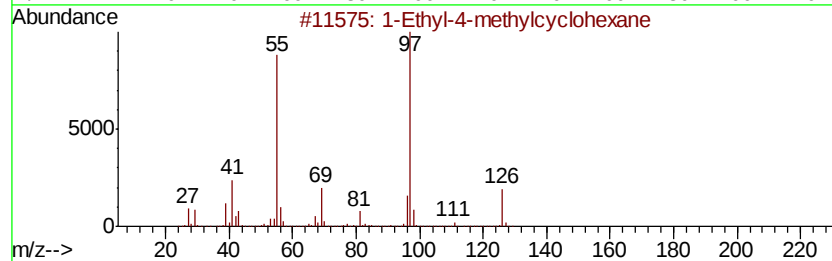
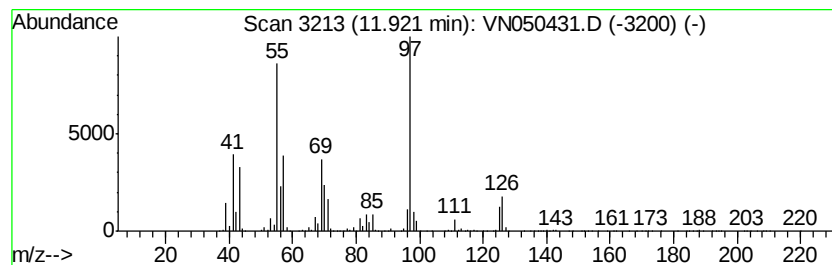
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Ethyl-4-methylcyclohexane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	44.10 ug/l	2695310	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	70
2		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	62
3		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	59
4		3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	58
5		2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	58



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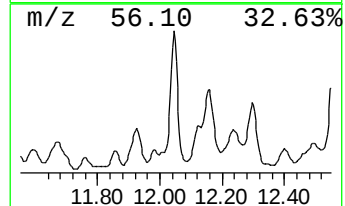
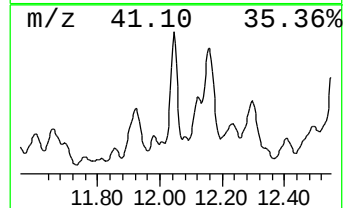
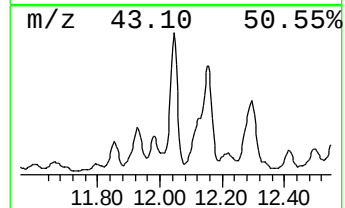
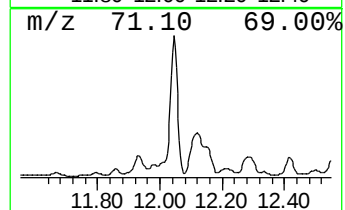
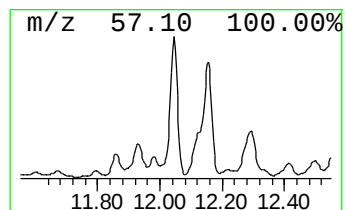
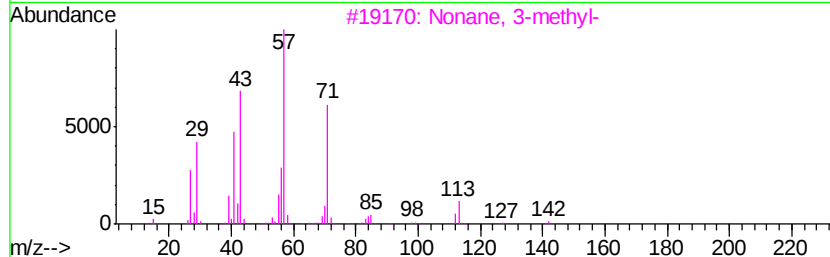
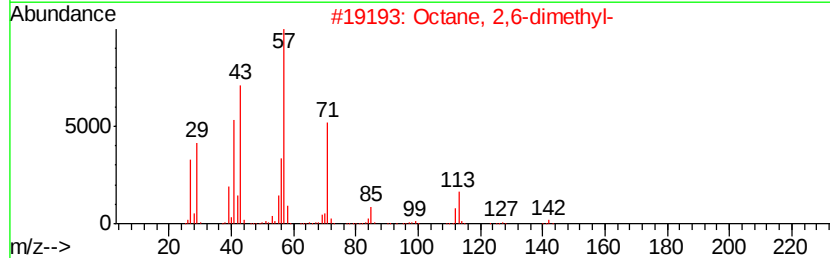
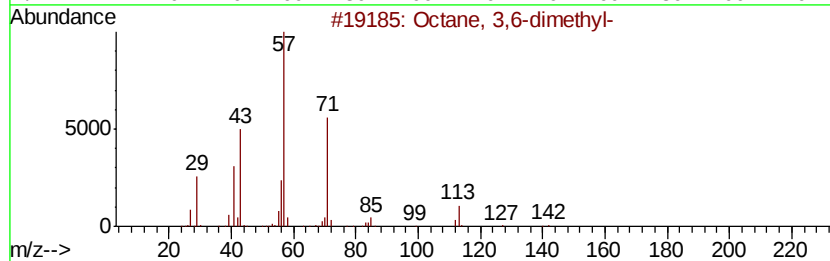
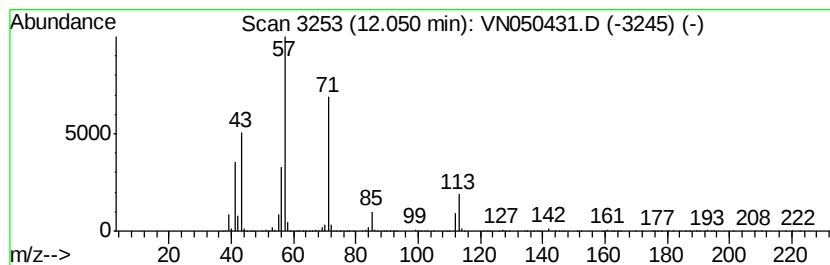
Instrument :
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ClientSampleId :
TP-6

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Quant Title : SW846 8260

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Peak Number 3 Octane, 3,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.05	36.26 ug/l	2216070	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	91	
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91	
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	90	
4	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	59	
5	Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	53	



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Misc : 5.10µL/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
TP-6

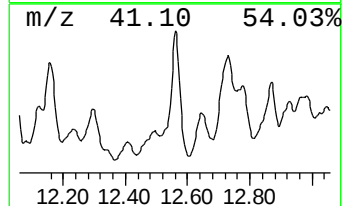
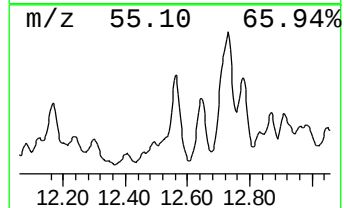
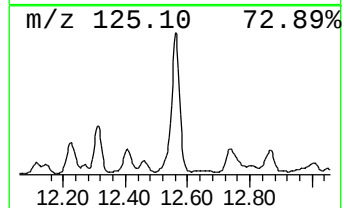
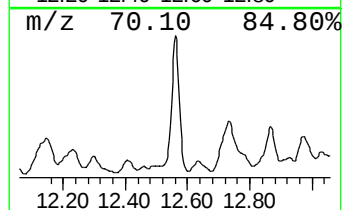
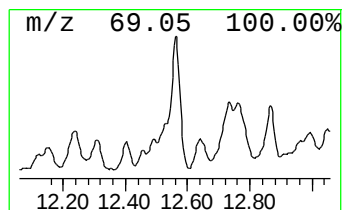
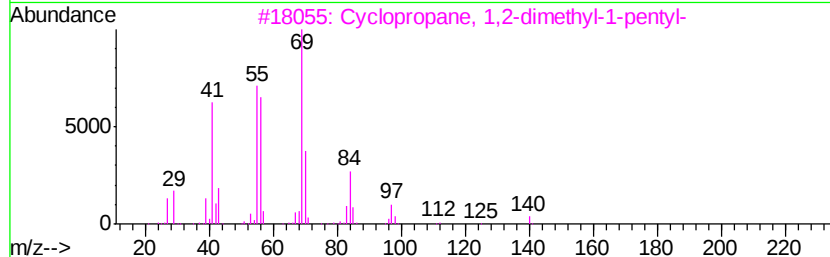
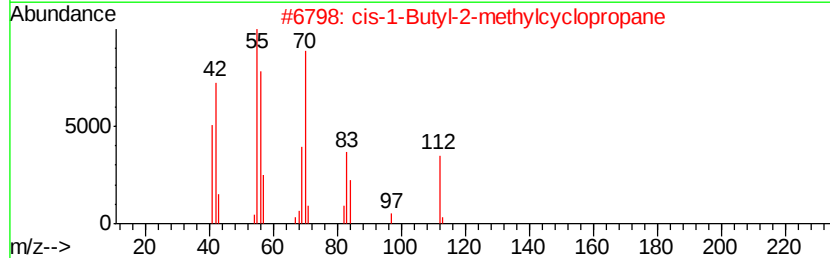
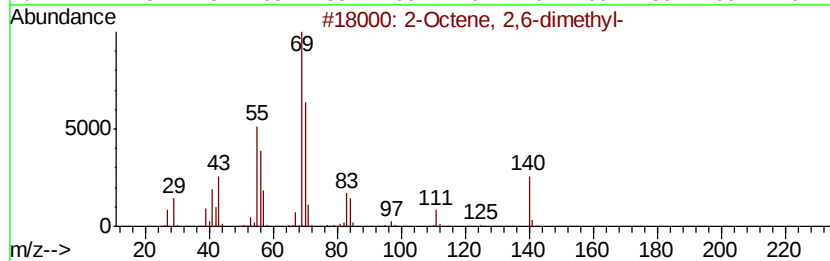
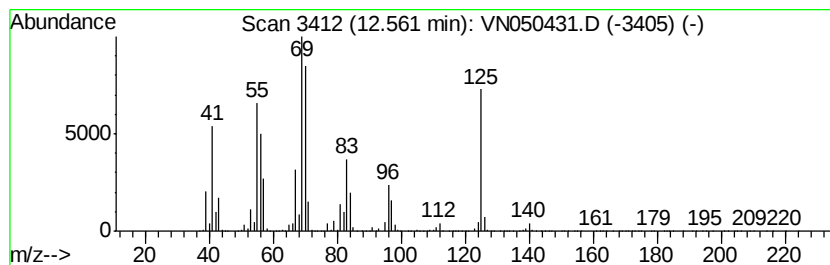
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Octene, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	53.50 ug/l	5539090	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	58
2		cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	50
3		Cyclopropane, 1,2-dimethyl-1-pen...	140	C10H20	062238-04-4	49
4		trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	45
5		Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	38



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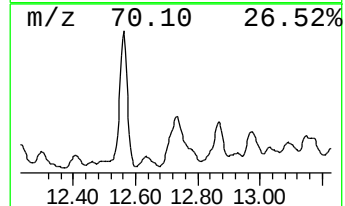
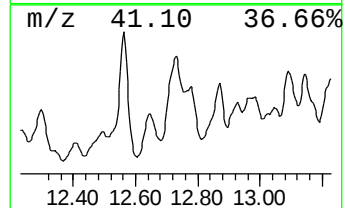
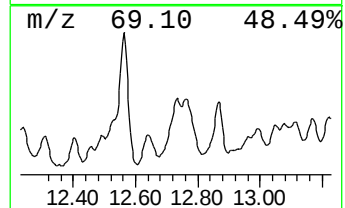
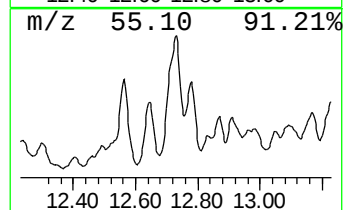
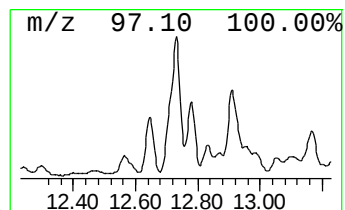
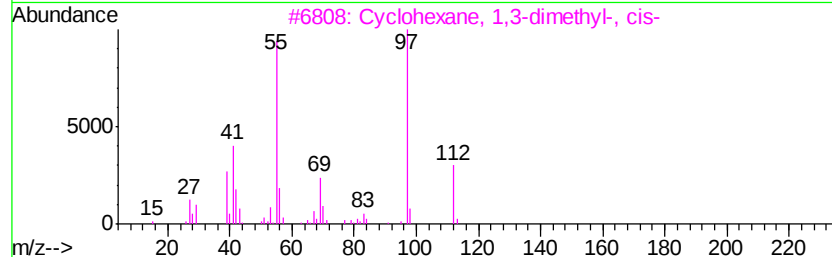
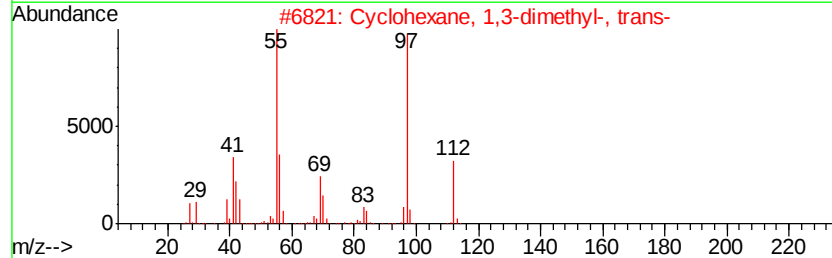
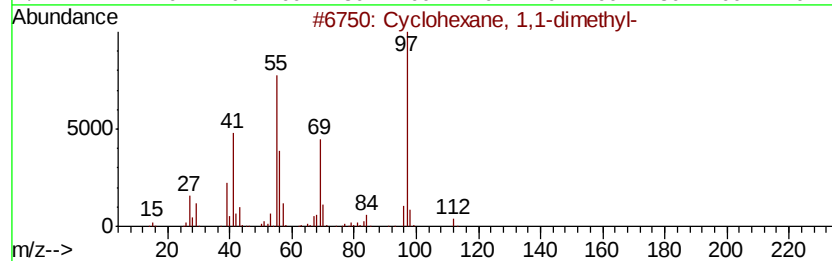
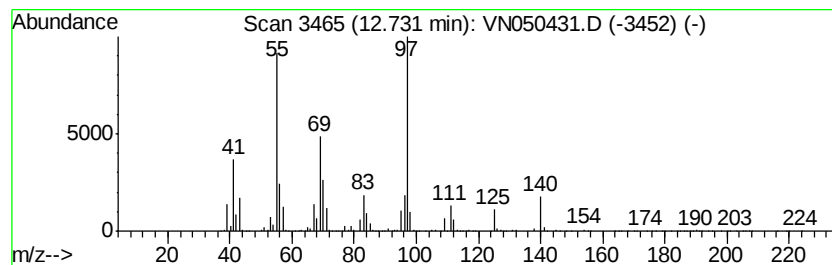
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexane, 1,1-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	49.22 ug/l	5096170	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	60
2		Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	49
3		Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	49
4		4-Propyl-2-hydroxycyclopent-2-en...	140	C8H12O2	082147-26-0	43
5		2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	1000283-20-9	43



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Instrument :
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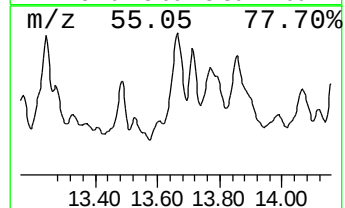
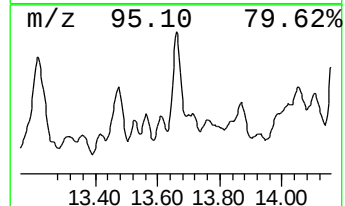
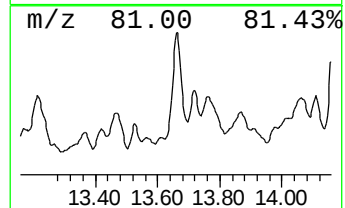
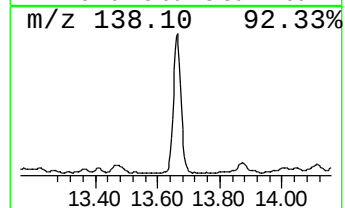
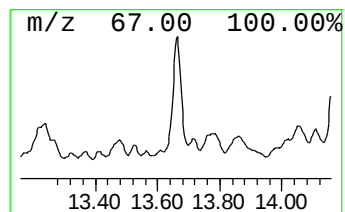
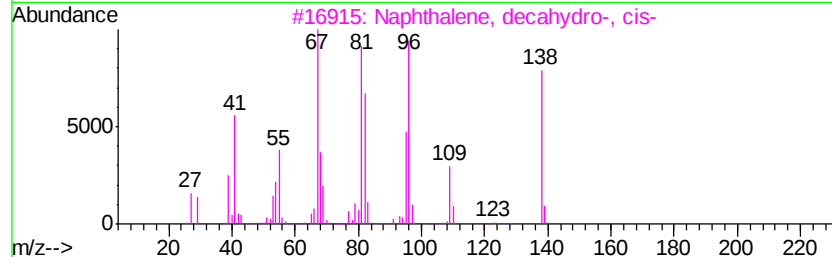
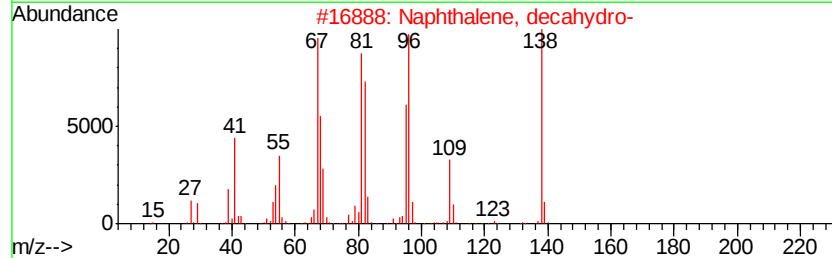
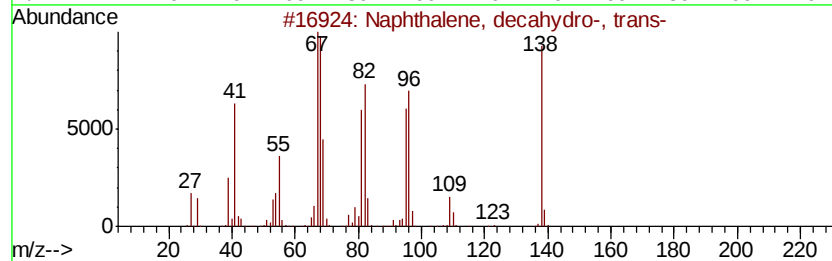
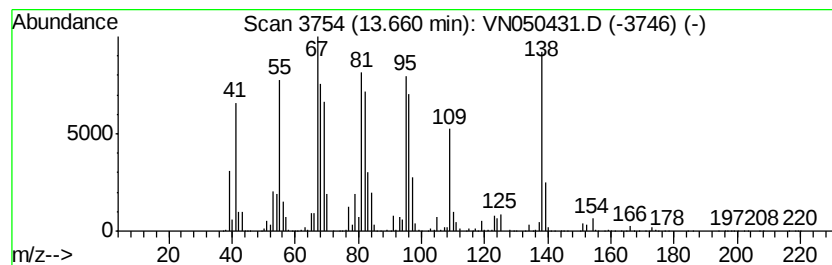
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, decahydro-, tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	50.00 ug/l	5177150	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	93
2		Naphthalene, decahydro-	138	C10H18	000091-17-8	91
3		Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	70
4		2,6-Dimethylbicyclo[3.2.1]octane	138	C10H18	1000215-28-2	70
5		Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	70



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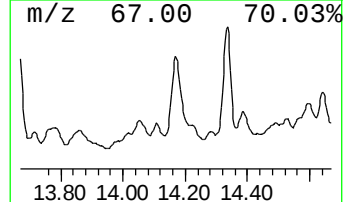
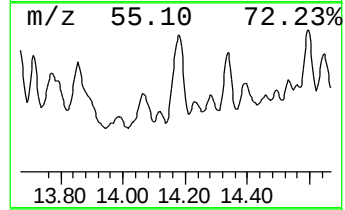
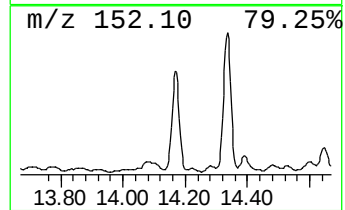
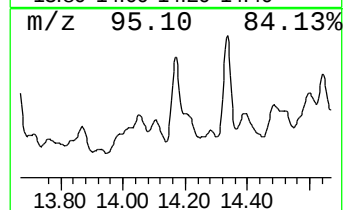
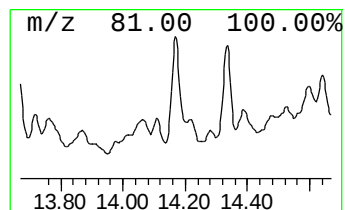
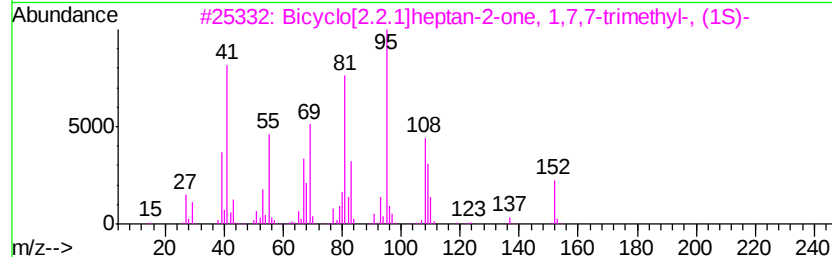
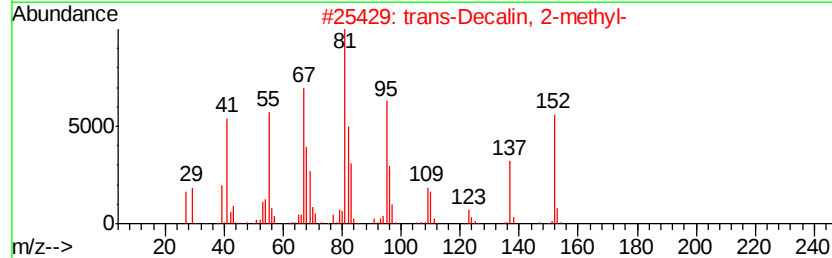
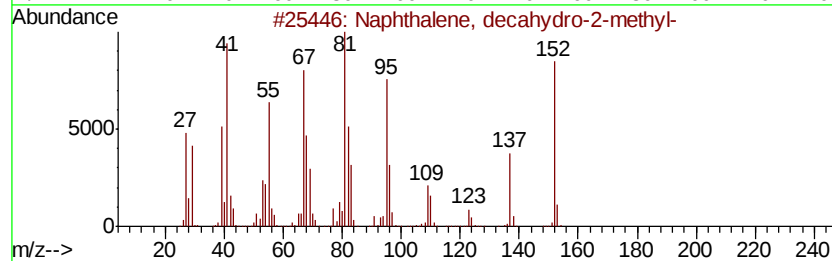
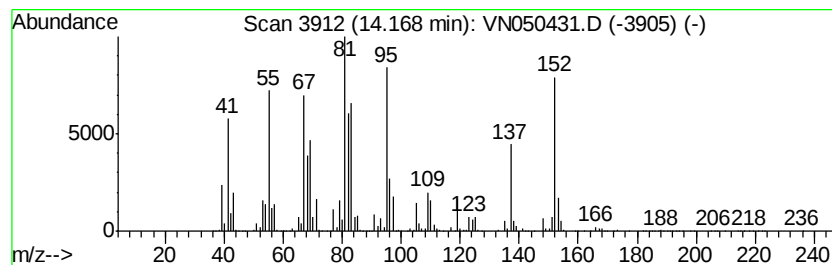
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, decahydro-2-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	88.46 ug/l	9159310	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	90
2		trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	58
3		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	49
4		1-Hexadecyne	222	C16H30	000629-74-3	49
5		8-Hexadecyne	222	C16H30	019781-86-3	46



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN080718\
Data File : VN050431.D
Acq On : 7 Aug 2018 15:01
Operator : MD\SY
Sample : J4297-06
Misc : 5.10µL/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

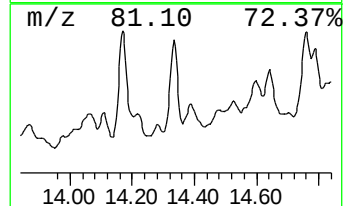
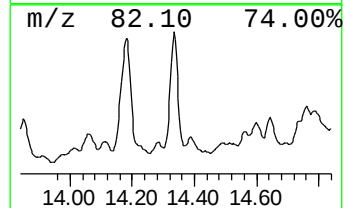
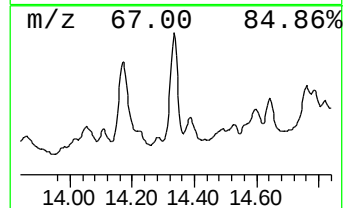
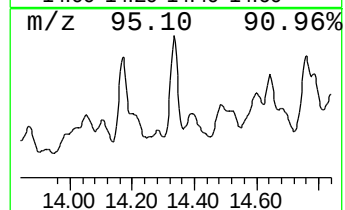
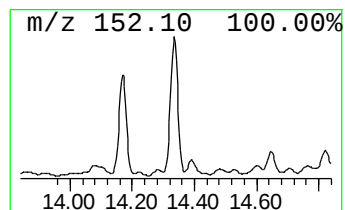
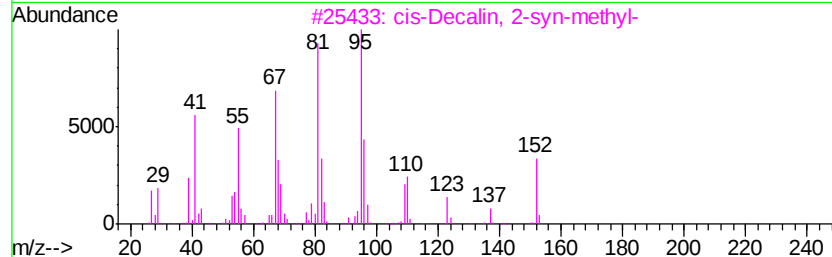
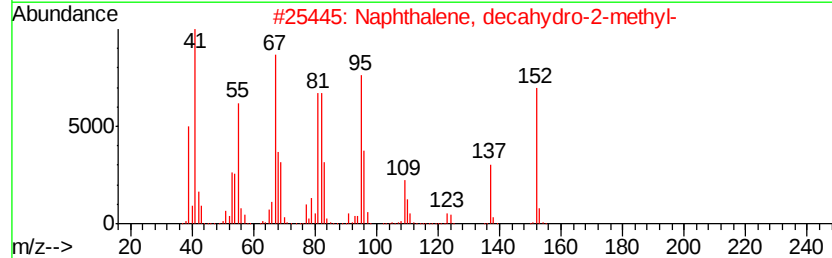
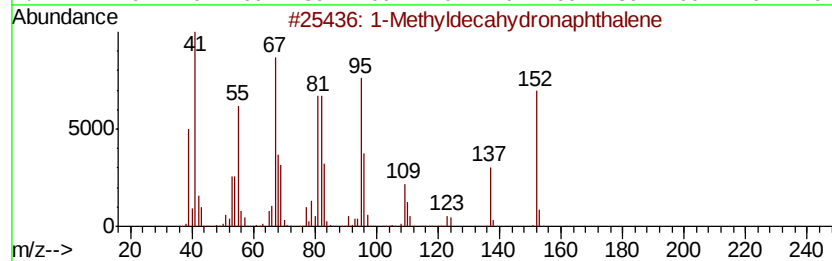
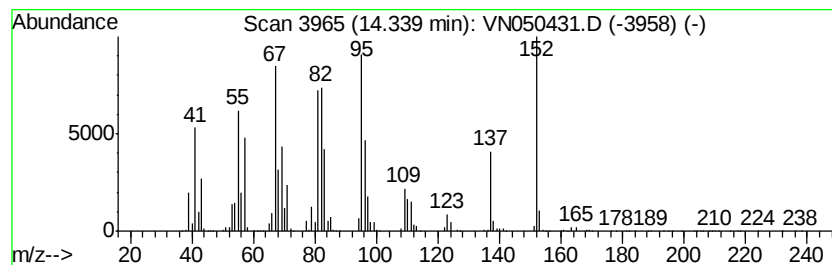
Instrument :
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ClientSampleId :
TP-6

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

Peak Number 8 1-Methyldecahydronaphthalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	32.98 ug/l	3414930	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Methyldecahydronaphthalene	152 C11H20	002958-75-0	96
2	Naphthalene, decahydro-2-methyl-	152 C11H20	002958-76-1	96
3	cis-Decalin, 2-syn-methyl-	152 C11H20	1000155-85-6	89
4	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152 C10H16O	000464-48-2	70
5	trans-Decalin, 2-methyl-	152 C11H20	1000152-47-3	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN080718\
Data File : VN050431.D
Acq On : 7 Aug 2018 15:01
Operator : MD\SY
Sample : J4297-06
Misc : 5.10µL/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
TP-6

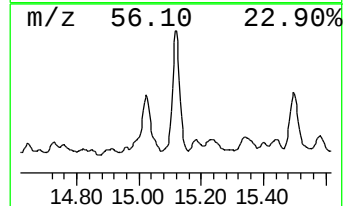
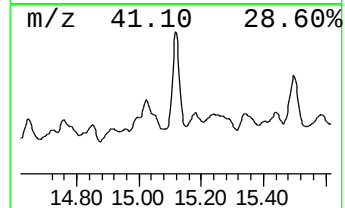
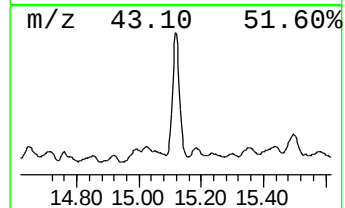
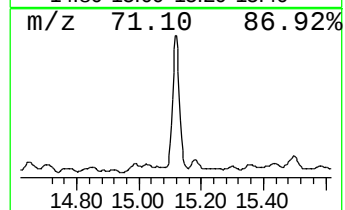
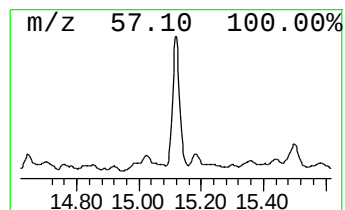
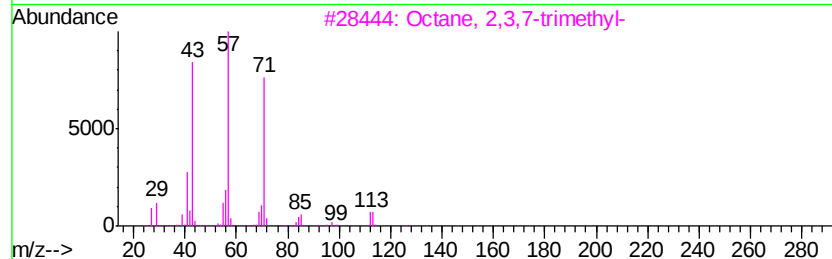
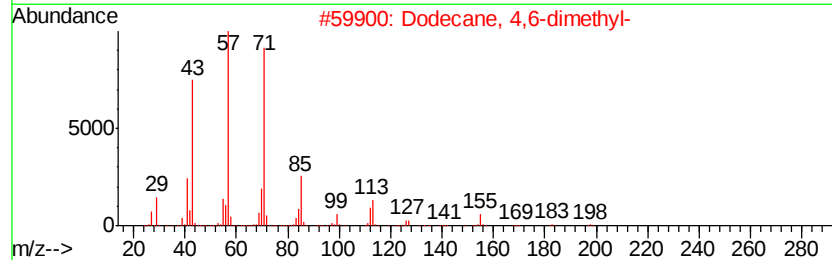
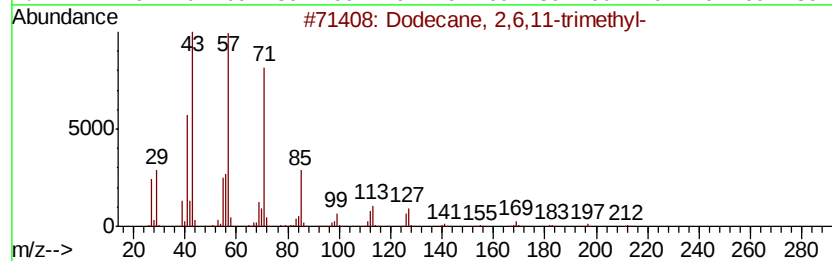
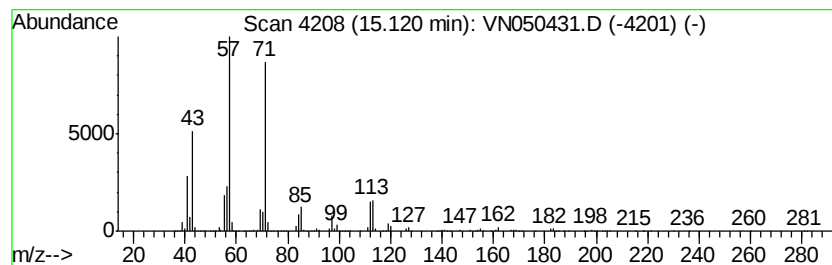
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Quant Title : SW846 8260

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

Peak Number 9 Dodecane, 2,6,11-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	104.08 ug/l	10777200	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	81
2		Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	72
3		Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	72
4		Tridecane, 7-methyl-	198	C14H30	026730-14-3	72
5		Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN080718\
Data File : VN050431.D
Acq On : 7 Aug 2018 15:01
Operator : MD\SY
Sample : J4297-06
Misc : 5.10µL/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-6

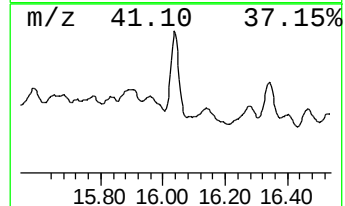
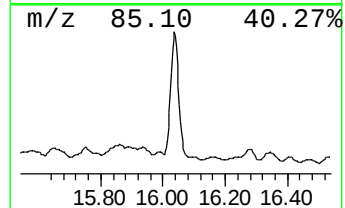
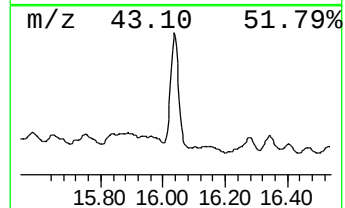
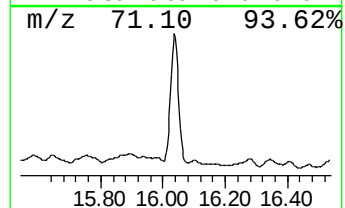
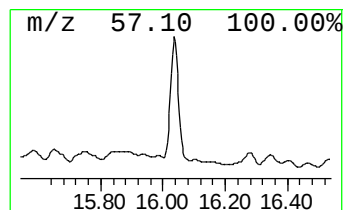
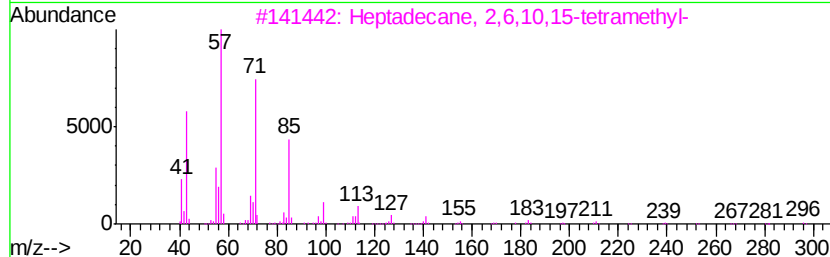
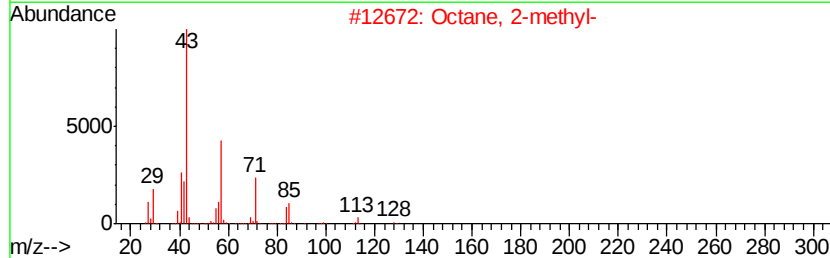
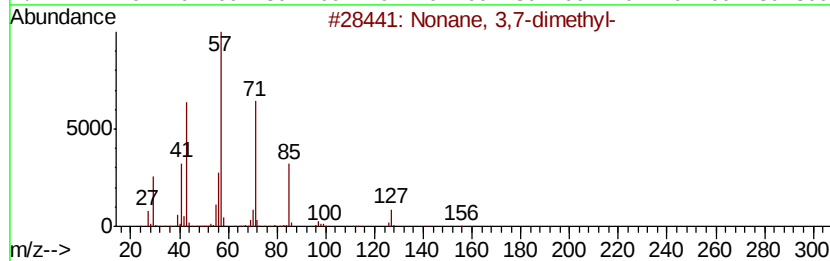
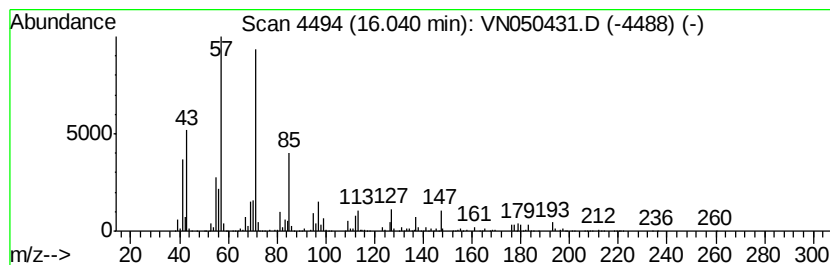
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

Peak Number 10 Nonane, 3,7-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	66.22 ug/l	6856950	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	87
2		Octane, 2-methyl-	128	C9H20	003221-61-2	81
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
4		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	74
5		Octane, 5-ethyl-2-methyl-	156	C11H24	062016-18-6	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN080718\
Data File : VN050431.D
Acq On : 7 Aug 2018 15:01
Operator : MD\SY
Sample : J4297-06
Misc : 5.10g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.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
1-Ethyl-4-methylc...	11.92	44.1	ug/l	2695310	3	11.41	3055660	50.0
Octane, 3,6-dimet...	12.05	36.3	ug/l	2216070	3	11.41	3055660	50.0
2-Octene, 2,6-dim...	12.56	53.5	ug/l	5539090	4	13.35	5177150	50.0
Cyclohexane, 1,1-...	12.73	49.2	ug/l	5096170	4	13.35	5177150	50.0
Naphthalene, deca...	13.66	50.0	ug/l	5177150	4	13.35	5177150	50.0
Naphthalene, deca...	14.17	88.5	ug/l	9159310	4	13.35	5177150	50.0
1-Methyldecahydro...	14.34	33.0	ug/l	3414930	4	13.35	5177150	50.0
Dodecane, 2,6,11-...	15.12	104.1	ug/l	10777200	4	13.35	5177150	50.0
Nonane, 3,7-dimet...	16.04	66.2	ug/l	6856950	4	13.35	5177150	50.0