

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN080718\
 Data File : VN050434.D
 Acq On : 7 Aug 2018 16:15
 Operator : MD\SY
 Sample : J4297-08
 Misc : 5.06µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-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\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	41	rBV	1419266	2143980	10.21%	1.486%
2	7.590	1847	1866	1877	rBV	572955	1433675	6.83%	0.993%
3	7.664	1877	1889	1914	rVB	933200	2222729	10.58%	1.540%
4	8.027	1985	2002	2021	rBV	582264	1349936	6.43%	0.935%
5	8.583	2161	2175	2192	rBV	1311290	2727579	12.99%	1.890%
6	10.091	2632	2644	2669	rVB	2561884	4982043	23.72%	3.452%
7	10.432	2745	2750	2765	rVB2	266169	441616	2.10%	0.306%
8	10.718	2831	2839	2850	rVB	502939	789105	3.76%	0.547%
9	10.821	2866	2871	2882	rVB	227034	329777	1.57%	0.228%
10	11.004	2919	2928	2939	rBV	1305316	2343559	11.16%	1.624%
11	11.213	2987	2993	3006	rVB2	743365	1259220	6.00%	0.872%
12	11.406	3044	3053	3072	rVB	1769646	3291314	15.67%	2.281%
13	11.545	3089	3096	3103	rBV	501974	795063	3.79%	0.551%
14	11.657	3124	3131	3139	rBV3	954281	1554058	7.40%	1.077%
15	11.921	3202	3213	3227	rBV7	2037586	5362813	25.53%	3.716%
16	12.046	3245	3252	3260	rVB	3255252	4672663	22.25%	3.238%
17	12.120	3269	3275	3280	rBV3	1417921	2122711	10.11%	1.471%
18	12.156	3282	3286	3297	rVB4	2301036	3708872	17.66%	2.570%
19	12.403	3354	3363	3373	rVB4	2180167	3804779	18.12%	2.636%
20	12.564	3406	3413	3427	rVB3	5504834	10988303	52.32%	7.614%
21	12.731	3452	3465	3475	rBV7	4176367	11107289	52.89%	7.696%
22	12.869	3503	3508	3516	rVB5	1483048	2032725	9.68%	1.408%
23	13.091	3571	3577	3587	rBV5	1500749	2513341	11.97%	1.741%
24	13.667	3746	3756	3765	rBV7	5457389	10690208	50.90%	7.407%
25	14.178	3905	3915	3939	rVB7	6186023	16355967	77.88%	11.333%
26	14.335	3958	3964	3971	rBV5	3840438	5102660	24.30%	3.536%
27	14.647	4054	4061	4072	rVB5	6890441	11894232	56.63%	8.241%
28	15.120	4200	4208	4218	rVB	14089045	21002237	100.00%	14.552%
29	16.036	4487	4493	4503	rBV	4921369	7301605	34.77%	5.059%

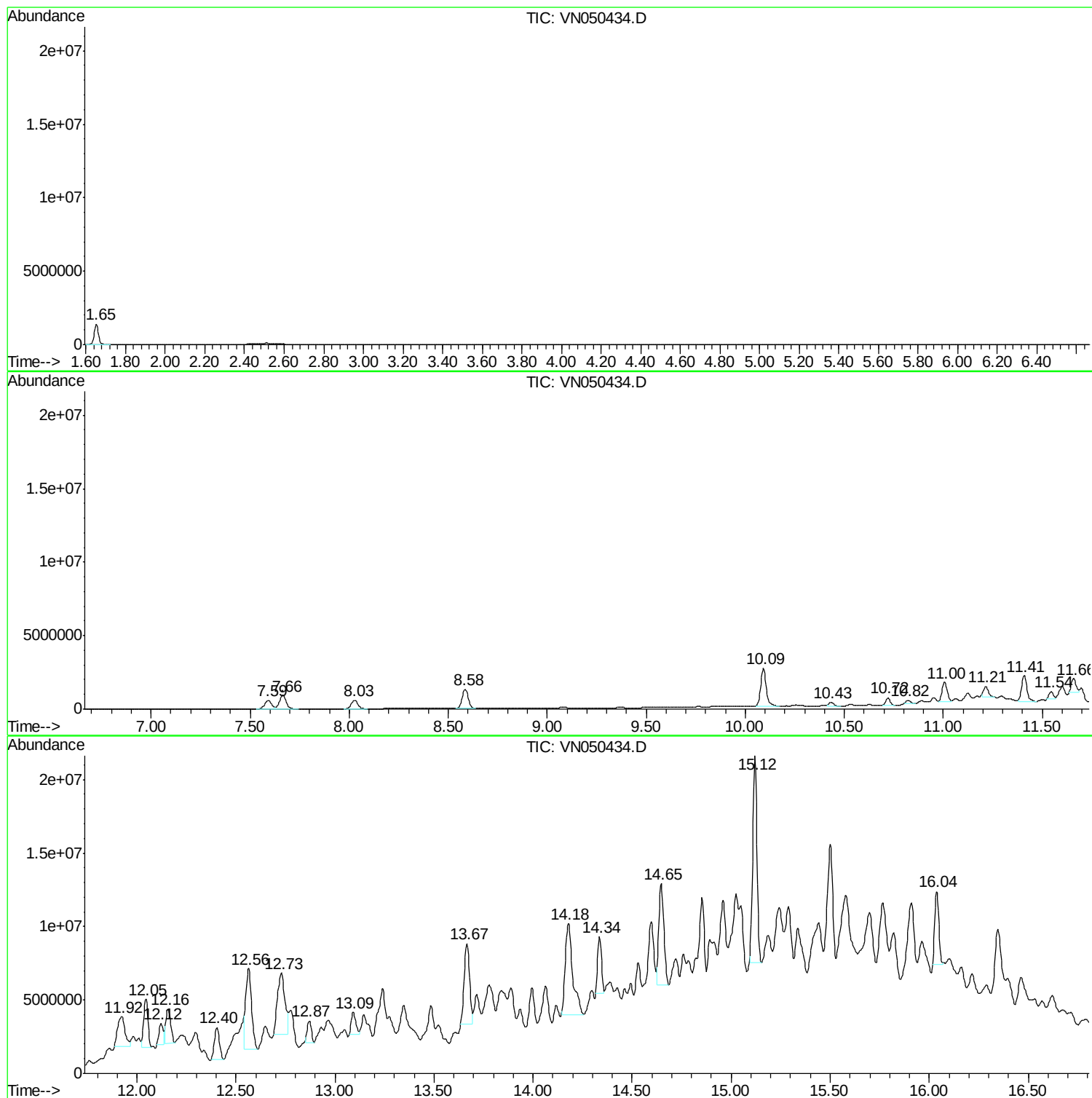
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Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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



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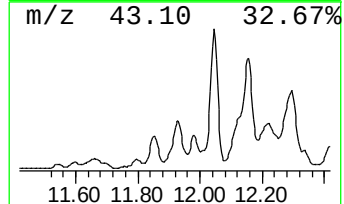
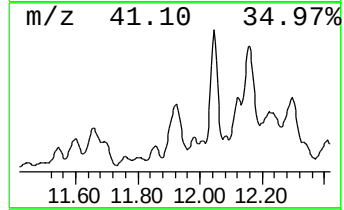
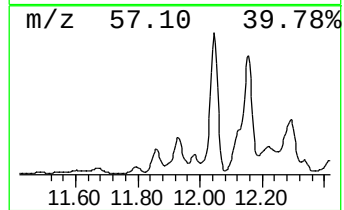
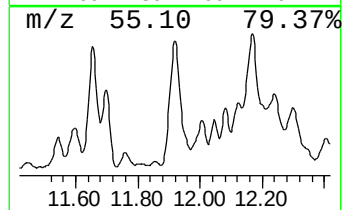
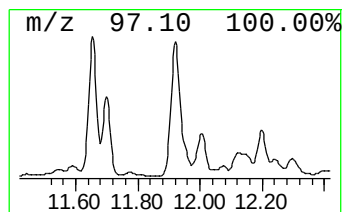
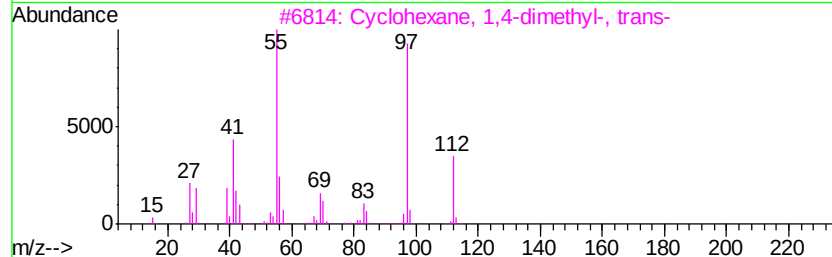
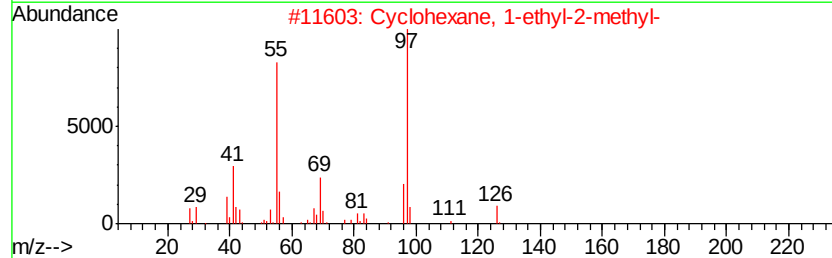
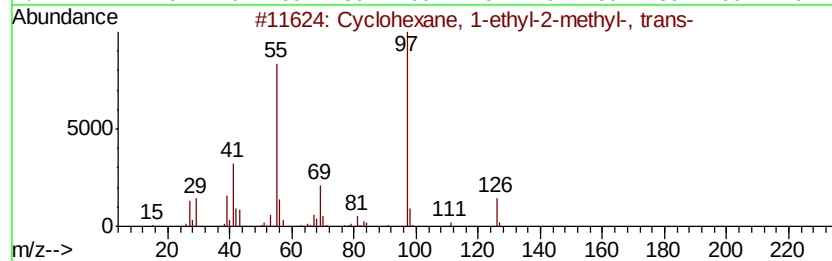
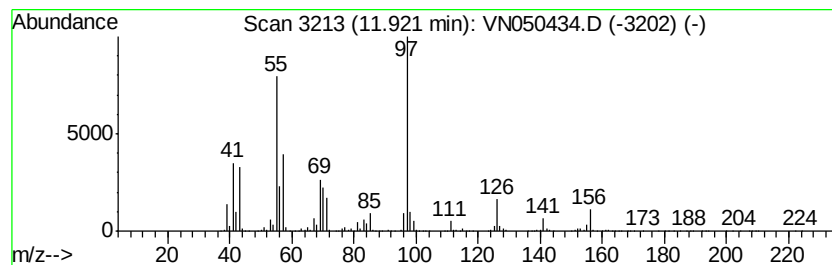
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Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1-ethyl-2-meth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	81.47 ug/l	5362810	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, 1-ethyl-2-methyl-, ...	126 C9H18	004923-78-8 70
2		Cyclohexane, 1-ethyl-2-methyl-	126 C9H18	003728-54-9 64
3		Cyclohexane, 1,4-dimethyl-, trans-	112 C8H16	002207-04-7 59
4		3,5-Dimethyl-3-heptene	126 C9H18	059643-68-4 52
5		2-Hexene, 3,4,4-trimethyl-	126 C9H18	053941-19-8 52



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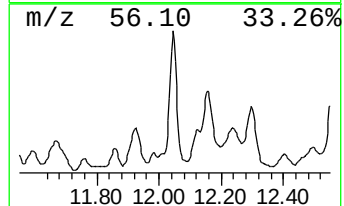
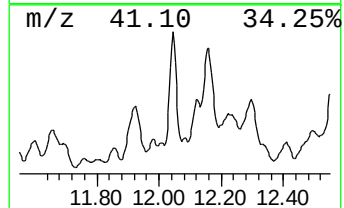
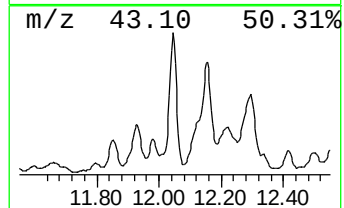
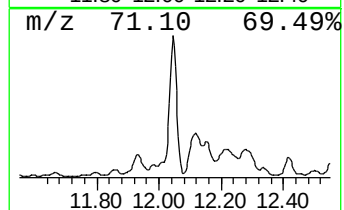
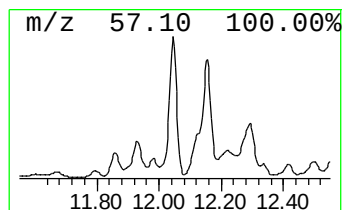
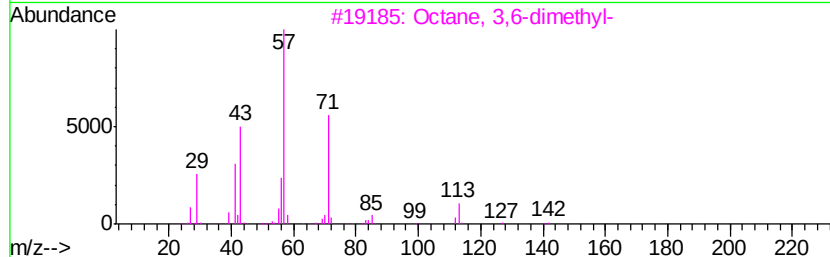
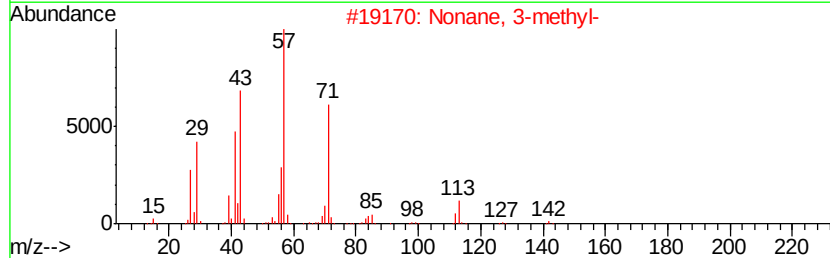
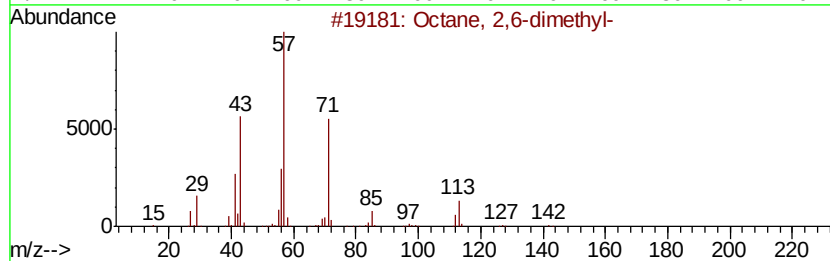
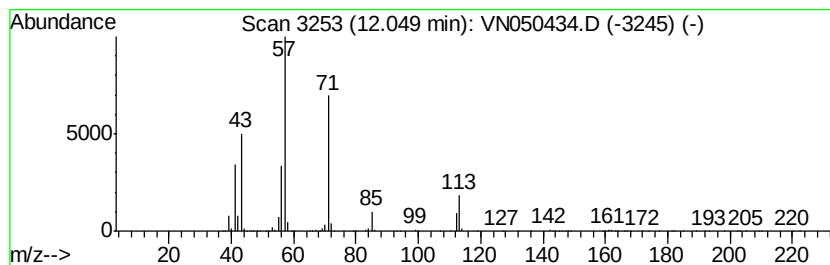
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Quant Title : SW846 8260

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

Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	70.98 ug/l	4672660	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	91
2		Nonane, 3-methyl-	142	C10H22	005911-04-6	86
3		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	80
4		Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	72
5		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	59



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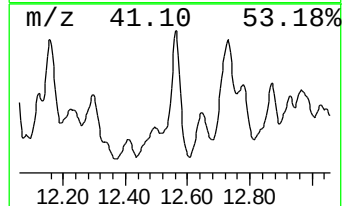
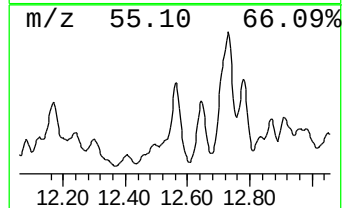
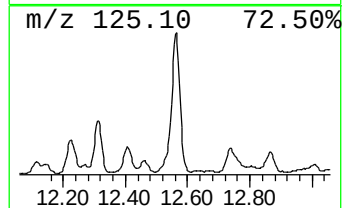
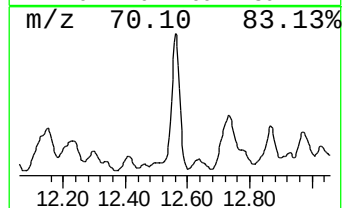
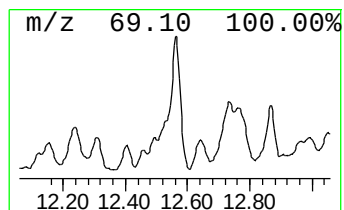
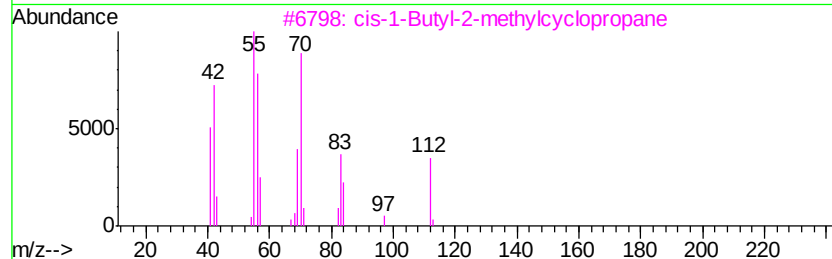
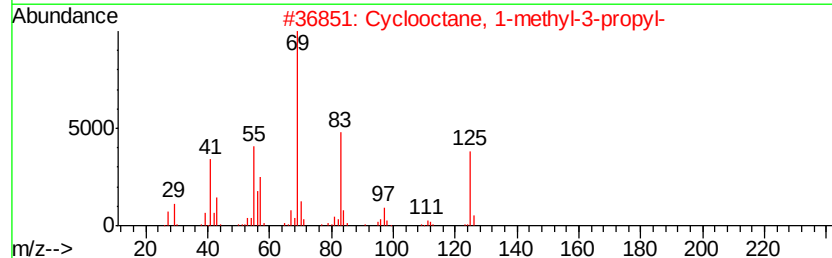
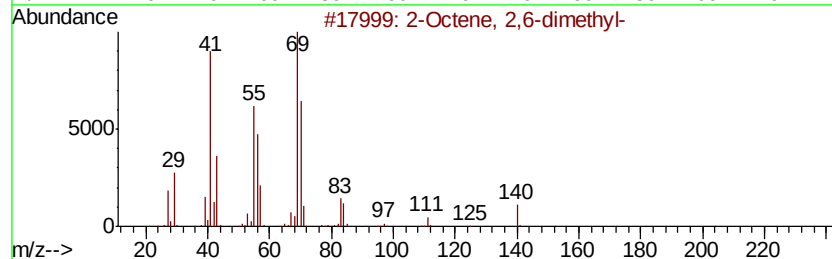
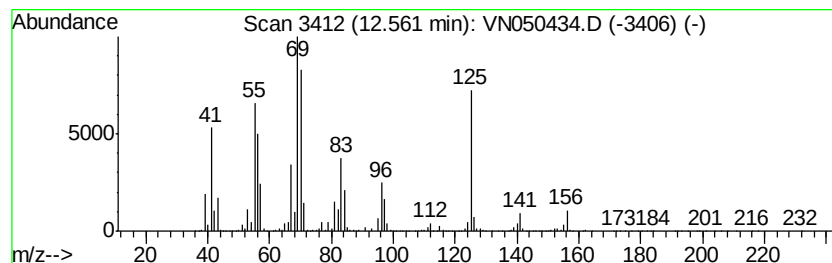
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Octene, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	218.60 ug/l	10988300	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Octene, 2,6-dimethyl-	140 C10H20	004057-42-5	60
2	Cyclooctane, 1-methyl-3-propyl-	168 C12H24	255885-37-1	47
3	cis-1-Butyl-2-methylcyclopropane	112 C8H16	038851-69-3	46
4	Ketone, vinyl-pyrrolidinyl-	125 C7H11NO	042104-70-1	46
5	Cyclohexane, 2,4-diethyl-1-methyl-	154 C11H22	061142-70-9	43



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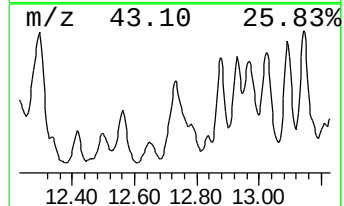
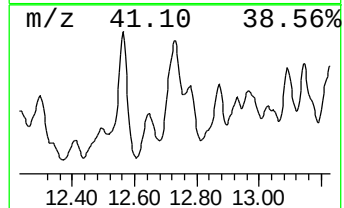
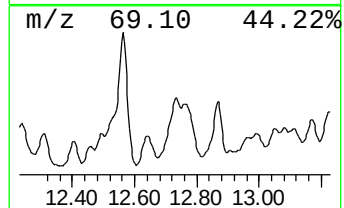
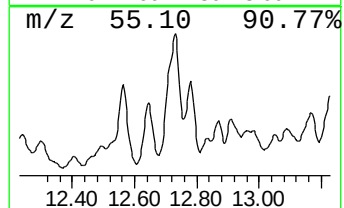
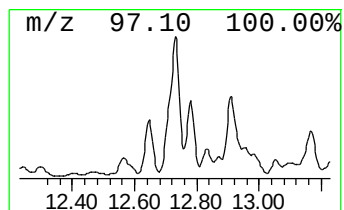
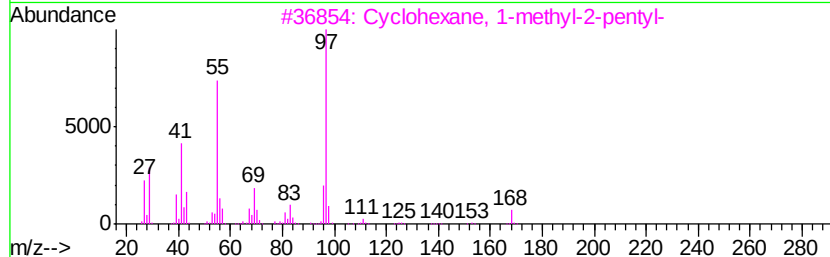
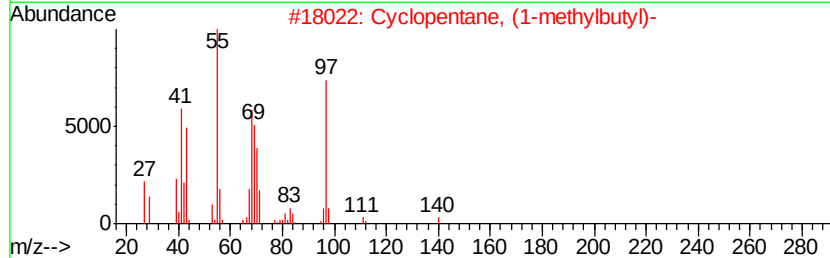
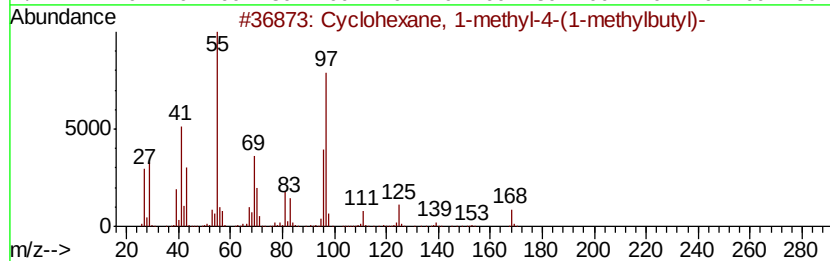
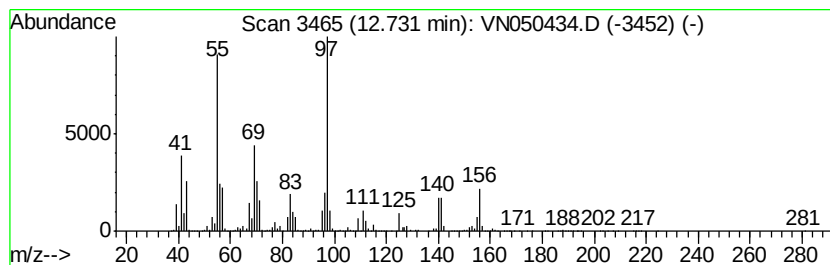
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Peak Number 4 Cyclohexane, 1-methyl-4-(1-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	220.97 ug/l	11107300	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-methyl-4-(1-methyl-4-(1-methylbutyl)-	168	C12H24	054411-00-6	49
2		Cyclopentane, (1-methylbutyl)-	140	C10H20	004737-43-3	49
3		Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	49
4		4-Hepten-3-one, 2,6-dimethyl-	140	C9H16O	056259-14-4	46
5		Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	46



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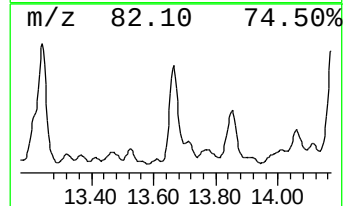
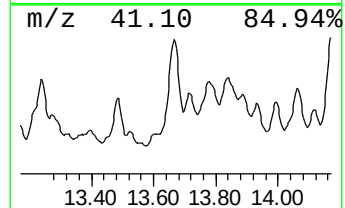
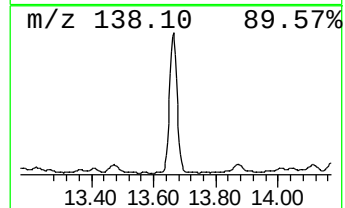
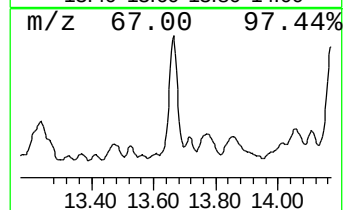
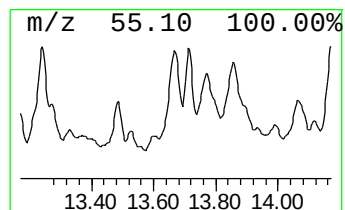
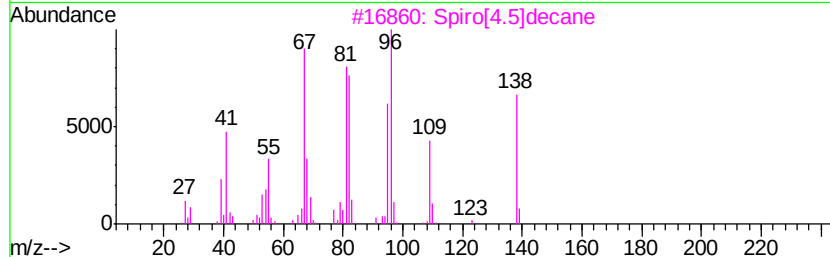
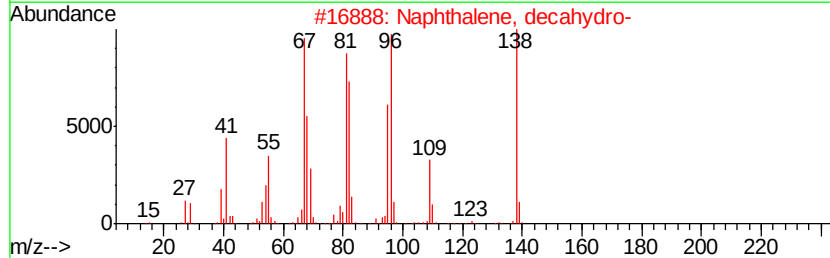
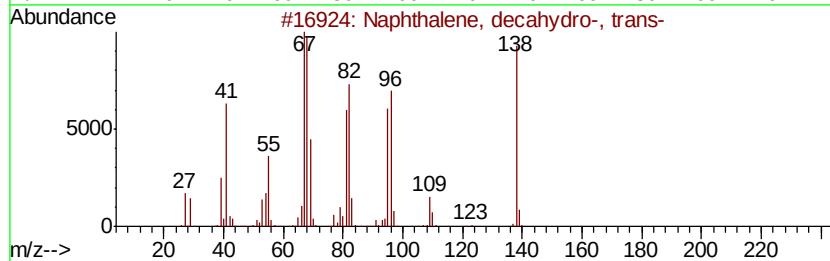
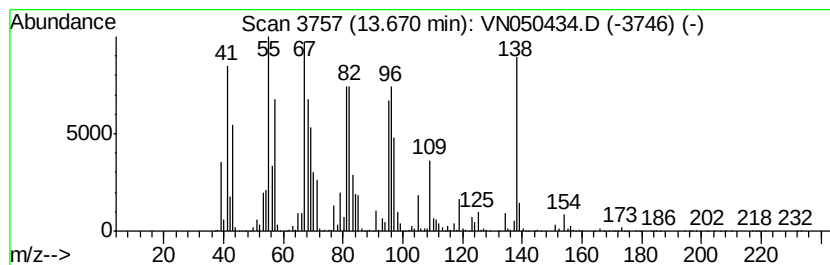
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Naphthalene, decahydro-, tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	212.67 ug/l	10690200	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, decahydro-, trans-	138 C10H18	000493-02-7 93
2		Naphthalene, decahydro-	138 C10H18	000091-17-8 90
3		Spiro[4.5]decane	138 C10H18	000176-63-6 90
4		Cyclodecanol	156 C10H20O	001502-05-2 87
5		Naphthalene, decahydro-, cis-	138 C10H18	000493-01-6 81



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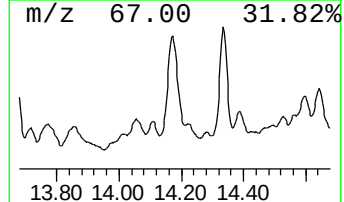
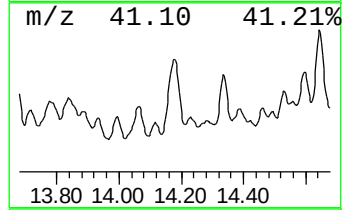
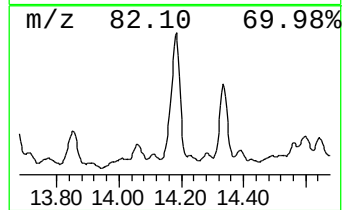
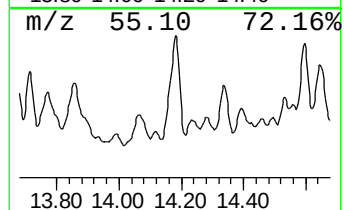
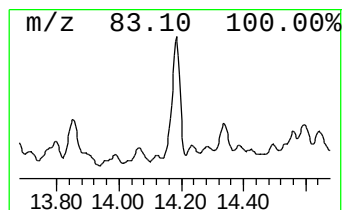
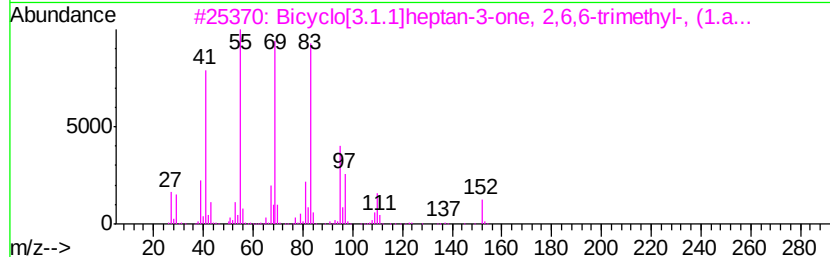
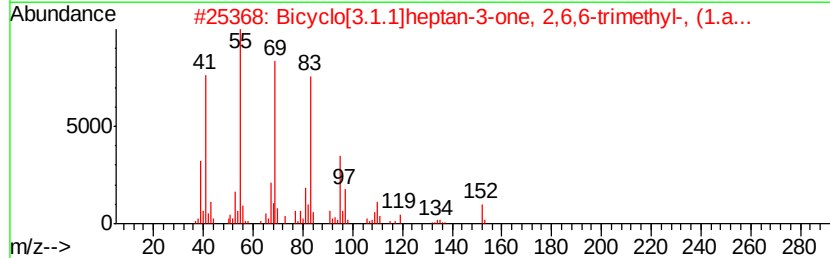
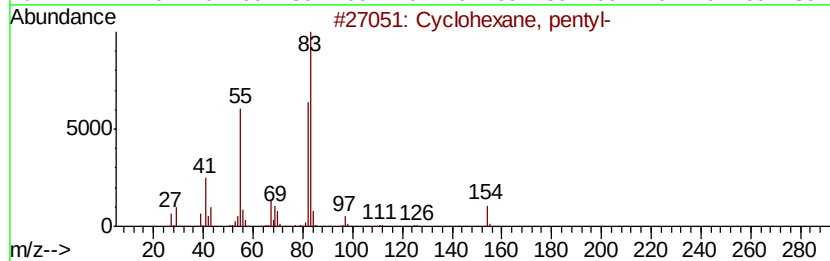
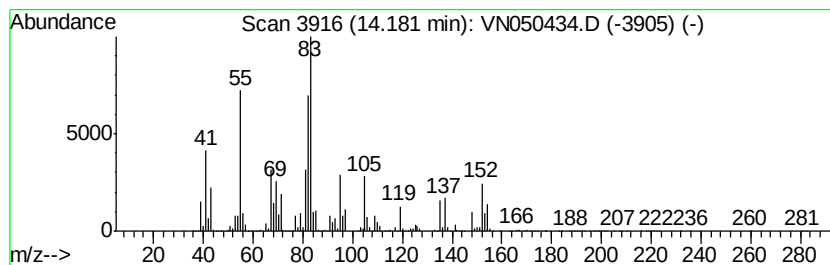
Instrument :
MSVOA_N
ClientSampleId :
TP-8

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 6 Cyclohexane, pentyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	325.38 ug/l	16356000	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, pentyl-	154 C11H22	004292-92-6 50
2		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152 C10H16O	015358-88-0 46
3		Bicyclo[3.1.1]heptan-3-one, 2,6,...	152 C10H16O	000547-60-4 43
4		Cyclopentane, 1-methyl-2-(2-prop...	124 C9H16	050746-53-7 43
5		Cyclohexane, (1-methylbutyl)-	154 C11H22	061208-94-4 38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN080718\
Data File : VN050434.D
Acq On : 7 Aug 2018 16:15
Operator : MD\SY
Sample : J4297-08
Misc : 5.06µ/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-8

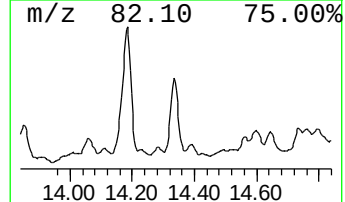
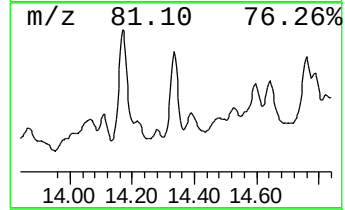
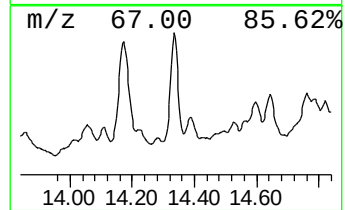
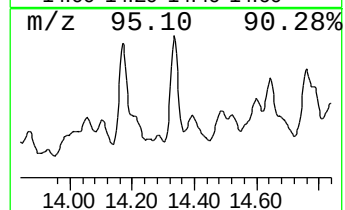
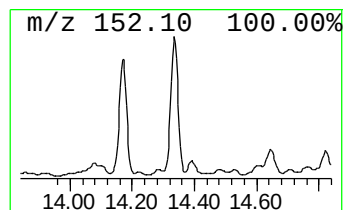
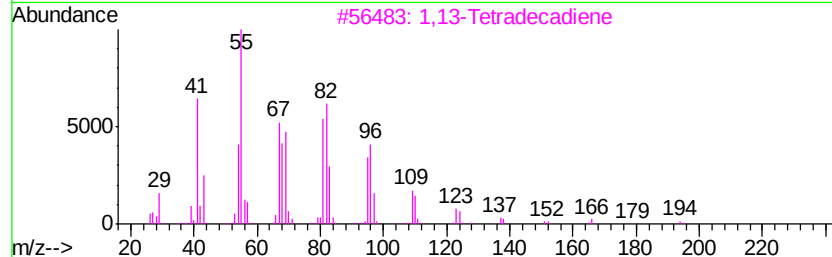
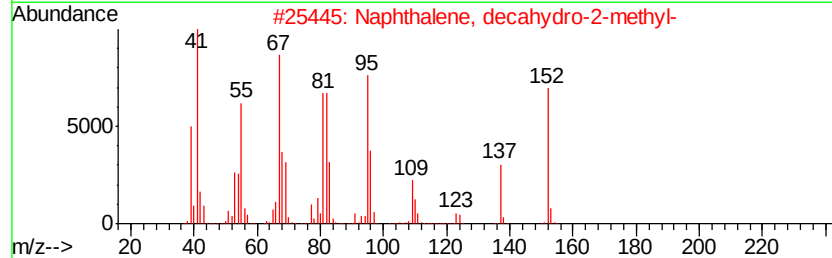
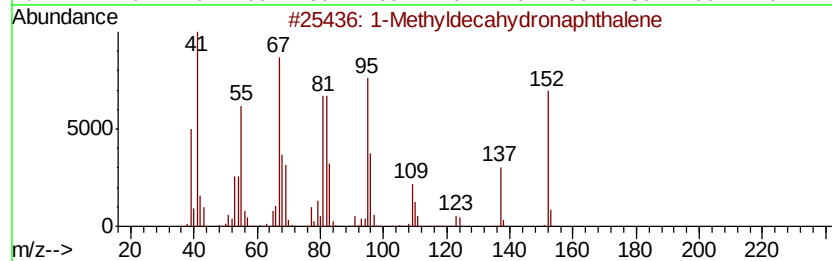
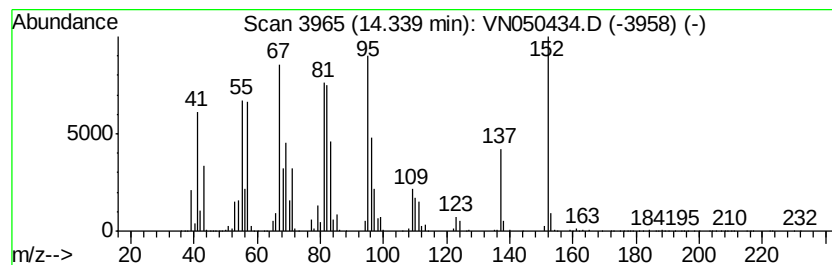
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

Peak Number 7 1-Methyldecahydronaphthalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	101.51 ug/l	5102660	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		1,13-Tetradecadiene	194	C14H26	021964-49-8	81
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	70



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN080718\
Data File : VN050434.D
Acq On : 7 Aug 2018 16:15
Operator : MD\SY
Sample : J4297-08
Misc : 5.06µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

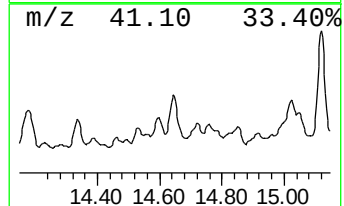
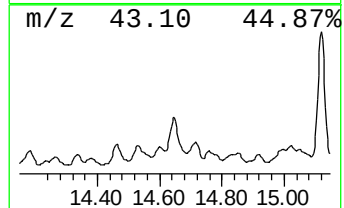
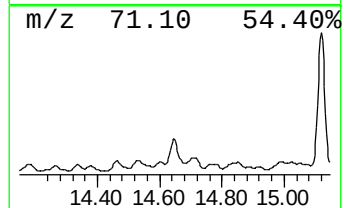
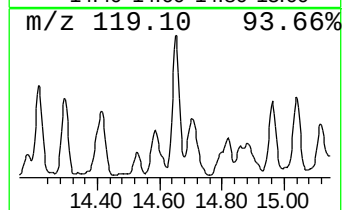
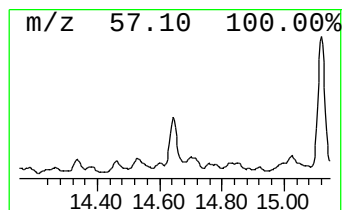
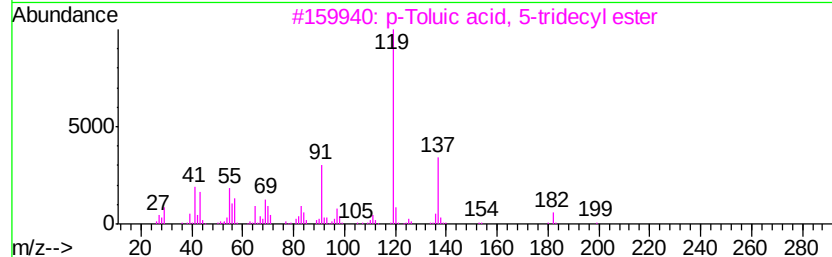
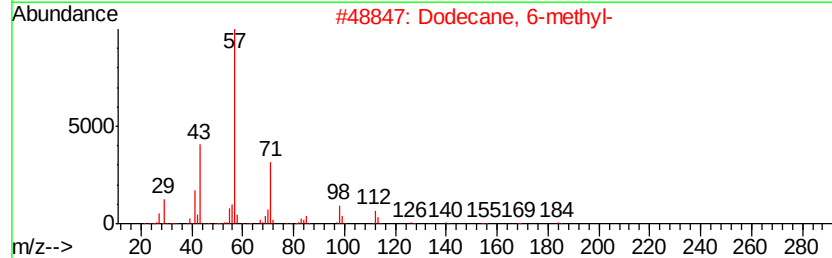
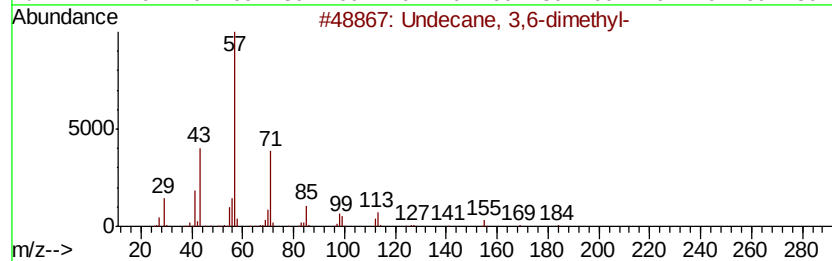
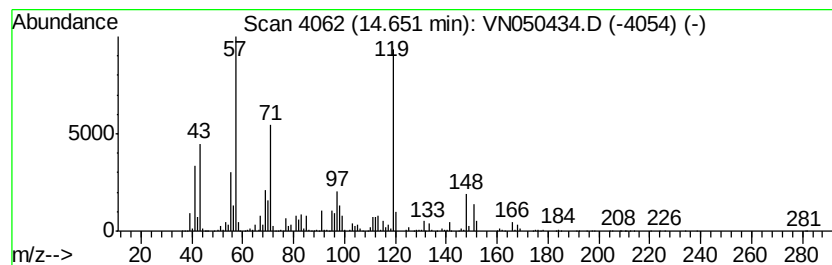
Instrument :
MSVOA_N
ClientSampleId :
TP-8

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 8 Undecane, 3,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	236.62 ug/l	11894200	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Undecane, 3,6-dimethyl-	184 C13H28	017301-28-9	38
2	Dodecane, 6-methyl-	184 C13H28	006044-71-9	35
3	p-Toluic acid, 5-tridecyl ester	318 C21H34O2	1000299-80-5	27
4	Undecane, 2,6-dimethyl-	184 C13H28	017301-23-4	25
5	Undecane, 2,5-dimethyl-	184 C13H28	017301-22-3	25



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN080718\
Data File : VN050434.D
Acq On : 7 Aug 2018 16:15
Operator : MD\SY
Sample : J4297-08
Misc : 5.06µL/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
TP-8

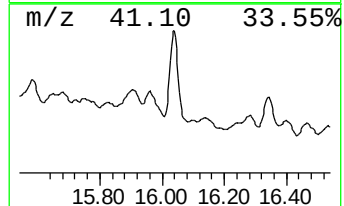
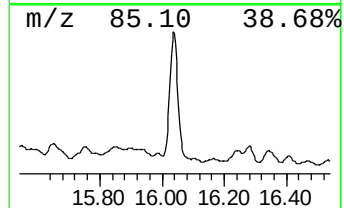
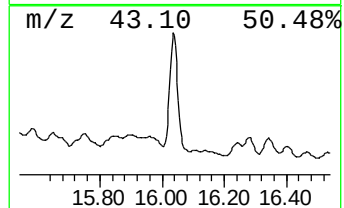
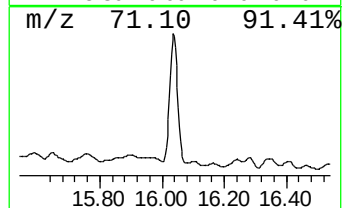
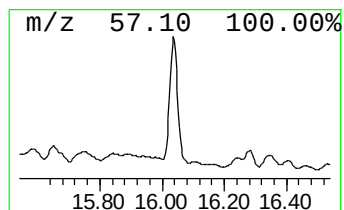
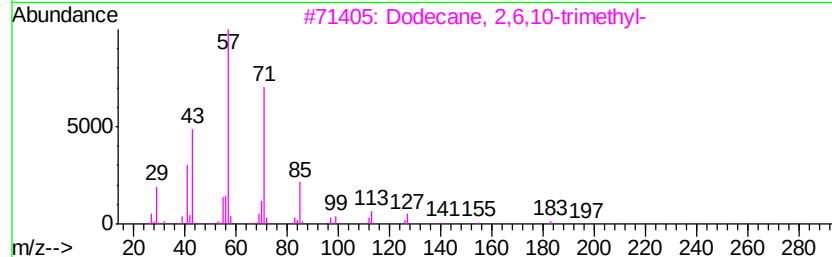
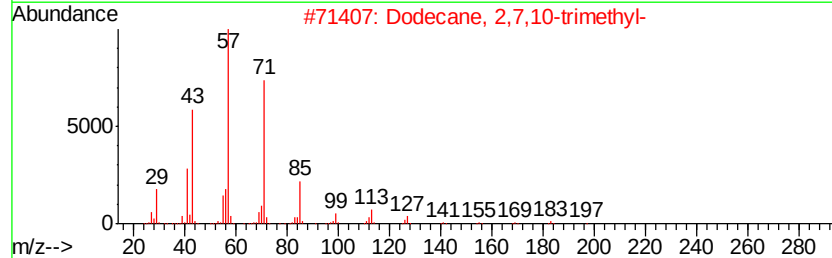
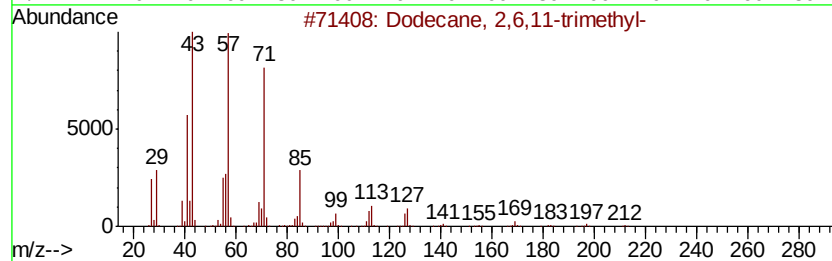
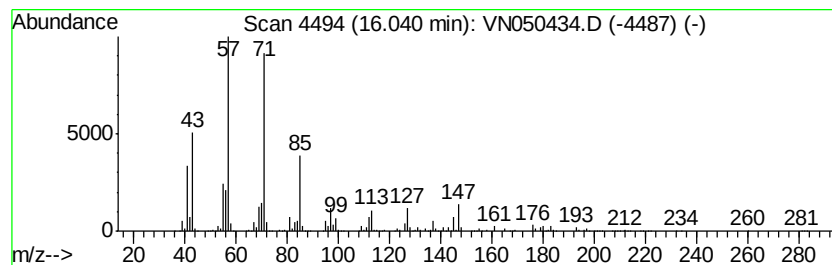
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

Peak Number 10 Dodecane, 2,6,11-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	145.26 ug/l	7301610	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	90
2		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
3		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64
4		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	59
5		Decane, 5-propyl-	184	C13H28	017312-62-8	58



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN080718\
Data File : VN050434.D
Acq On : 7 Aug 2018 16:15
Operator : MD\SY
Sample : J4297-08
Misc : 5.06g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-8

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
Cyclohexane, 1-et...	11.92	81.5	ug/l	5362810	3	11.41	3291310	50.0
Octane, 2,6-dimet...	12.05	71.0	ug/l	4672660	3	11.41	3291310	50.0
2-Octene, 2,6-dim...	12.56	218.6	ug/l	10988300	4	13.35	2513340	50.0
Cyclohexane, 1-me...	12.73	221.0	ug/l	11107300	4	13.35	2513340	50.0
Naphthalene, deca...	13.67	212.7	ug/l	10690200	4	13.35	2513340	50.0
Cyclohexane, pentyl-	14.18	325.4	ug/l	16356000	4	13.35	2513340	50.0
1-Methyldecahydro...	14.34	101.5	ug/l	5102660	4	13.35	2513340	50.0
Undecane, 3,6-dim...	14.65	236.6	ug/l	11894200	4	13.35	2513340	50.0
Dodecane, 2,6,11-...	16.04	145.3	ug/l	7301610	4	13.35	2513340	50.0