

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN080718\
 Data File : VN050429.D
 Acq On : 7 Aug 2018 14:12
 Operator : MD\SY
 Sample : J4297-04
 Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP-4

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	46	rBV	1289265	1951142	13.99%	1.911%
2	7.590	1839	1866	1877	rBV	489906	1230308	8.82%	1.205%
3	7.664	1878	1889	1911	rVB	724407	1694745	12.16%	1.660%
4	8.027	1984	2002	2026	rBV	504592	1182118	8.48%	1.158%
5	8.587	2160	2176	2207	rBV	1062008	2194726	15.74%	2.149%
6	10.091	2629	2644	2674	rVB	1980674	3664781	26.29%	3.589%
7	10.718	2829	2839	2851	rVB	128785	215252	1.54%	0.211%
8	10.821	2852	2871	2882	rBV	82243	185954	1.33%	0.182%
9	10.953	2904	2912	2919	rVV	117077	161824	1.16%	0.158%
10	11.008	2919	2929	2939	rVB2	368459	641441	4.60%	0.628%
11	11.123	2953	2965	2973	rBV5	162743	299860	2.15%	0.294%
12	11.210	2984	2992	3009	rVB3	241256	501011	3.59%	0.491%
13	11.297	3009	3019	3027	rBV2	107327	203721	1.46%	0.200%
14	11.410	3041	3054	3073	rBV	1483170	2645519	18.97%	2.591%
15	11.541	3088	3095	3102	rBV	141647	213443	1.53%	0.209%
16	11.599	3102	3113	3121	rBV6	271435	544717	3.91%	0.533%
17	11.657	3122	3131	3138	rBV2	445496	799191	5.73%	0.783%
18	11.760	3153	3163	3170	rBV4	127455	235018	1.69%	0.230%
19	11.853	3185	3192	3200	rBV4	138542	204534	1.47%	0.200%
20	11.924	3200	3214	3225	rBV6	742768	1851198	13.28%	1.813%
21	12.046	3244	3252	3259	rVB	1013777	1355506	9.72%	1.327%
22	12.120	3267	3275	3280	rBV2	601171	953990	6.84%	0.934%
23	12.159	3281	3287	3298	rVB3	885980	1618866	11.61%	1.585%
24	12.403	3354	3363	3372	rBV	1433846	2299635	16.49%	2.252%
25	12.448	3372	3377	3383	rVV3	224647	271746	1.95%	0.266%
26	12.564	3405	3413	3426	rVB3	1409006	2618393	18.78%	2.564%
27	12.648	3427	3439	3449	rBV8	581191	1531388	10.98%	1.500%
28	12.728	3451	3464	3473	rBV8	1250808	3254046	23.34%	3.187%
29	12.866	3495	3507	3515	rBV7	680385	1555916	11.16%	1.524%
30	12.924	3516	3525	3530	rVV4	1190483	2027997	14.55%	1.986%
31	12.963	3530	3537	3550	rVB	3166974	5167358	37.06%	5.061%
32	13.091	3571	3577	3587	rBV3	612626	1020125	7.32%	0.999%
33	13.143	3589	3593	3607	rVB5	626098	1219947	8.75%	1.195%
34	13.664	3746	3755	3765	rBV5	2785893	5445371	39.06%	5.333%

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Integration Parameters: RTEINT.P

Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : SW846 8260

35	13.934	3835	3839	3848	rVB2	1804676	2461861	17.66%	2.411%
36	14.175	3903	3914	3938	rVB10	4301435	13942173	100.00%	13.654%
37	14.336	3958	3964	3971	rVB4	2705700	3603581	25.85%	3.529%
38	14.644	4053	4060	4072	rVB2	8710484	13764752	98.73%	13.480%
39	15.120	4201	4208	4219	rVB	7507690	10796777	77.44%	10.574%
40	16.036	4487	4493	4507	rVB3	4204117	6581082	47.20%	6.445%

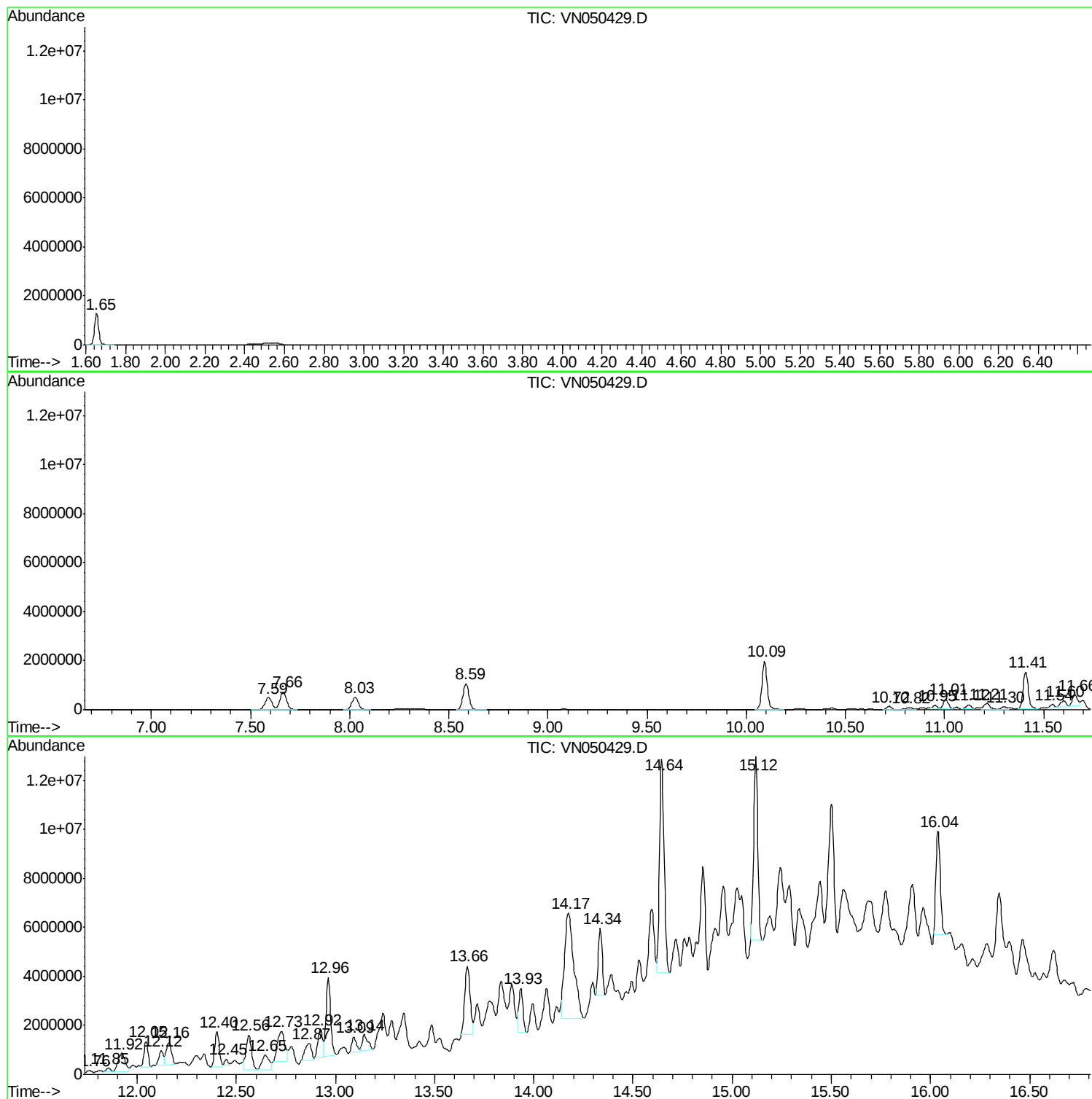
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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



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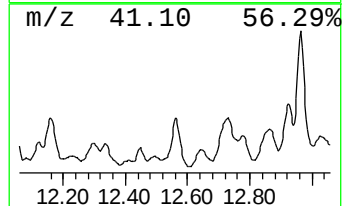
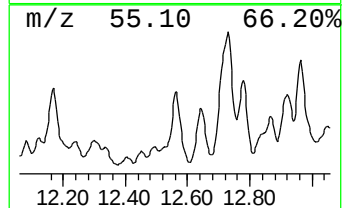
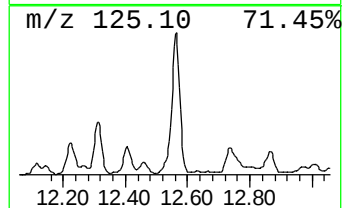
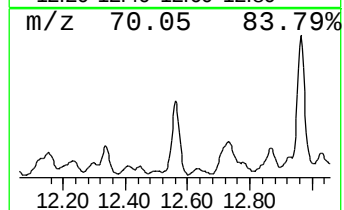
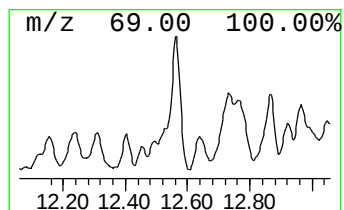
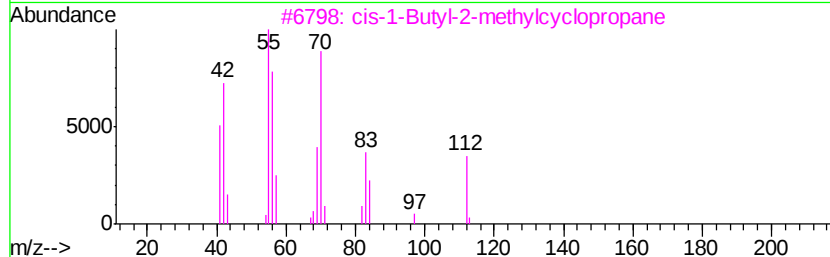
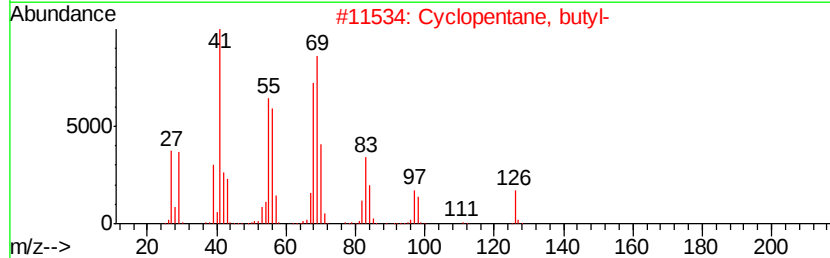
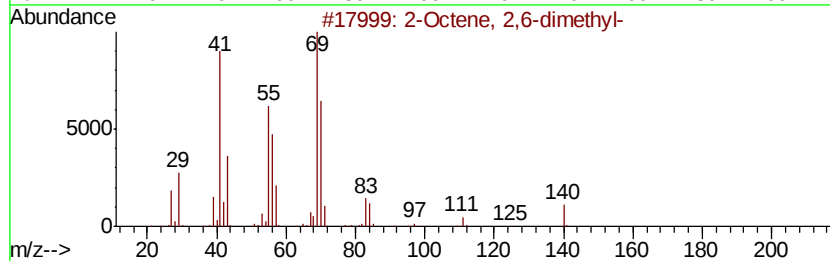
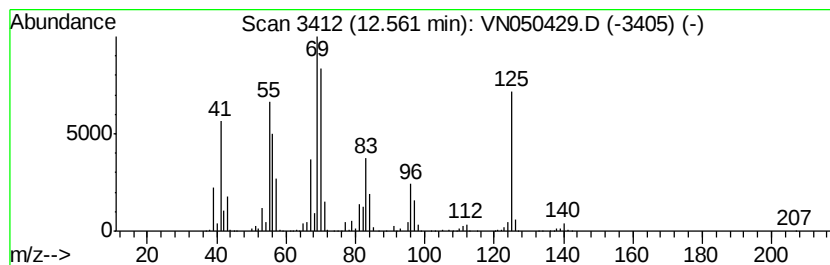
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N080618W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Octene, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	107.32 ug/l	2618390	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	64
2		Cyclopentane, butyl-	126	C9H18	002040-95-1	46
3		cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	46
4		Cyclopropane, 1,2-dimethyl-1-pen...	140	C10H20	062238-04-4	43
5		4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	062960-76-3	43



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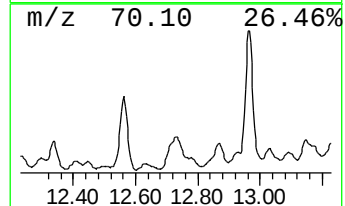
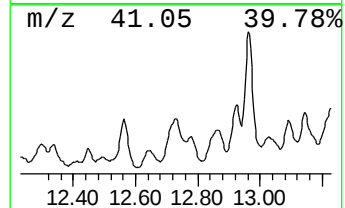
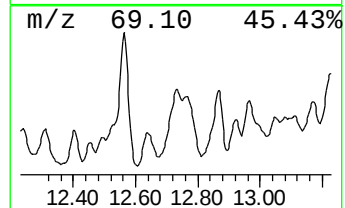
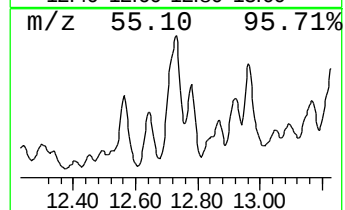
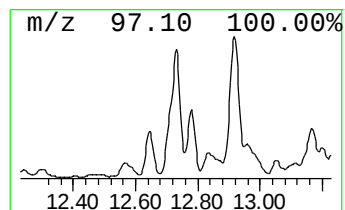
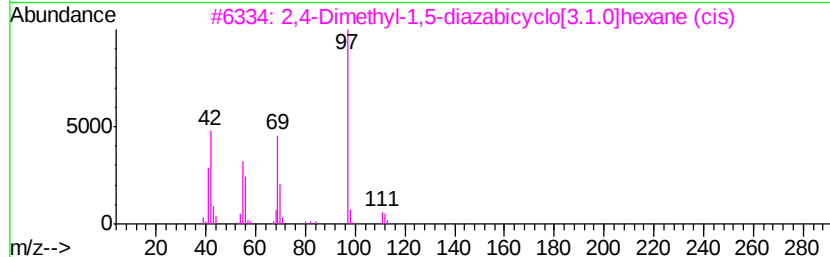
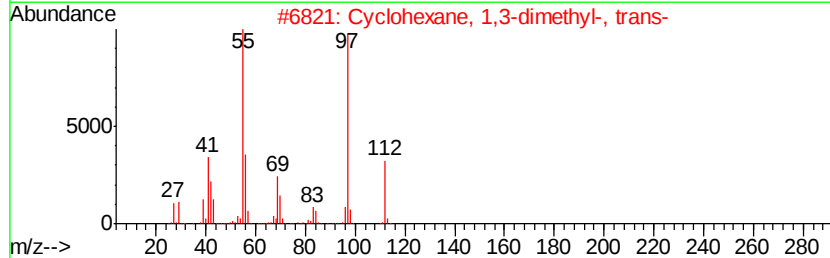
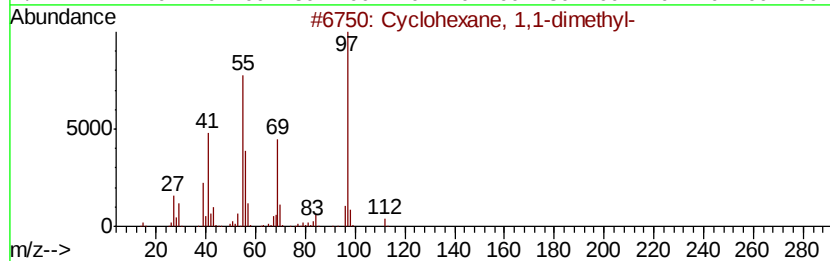
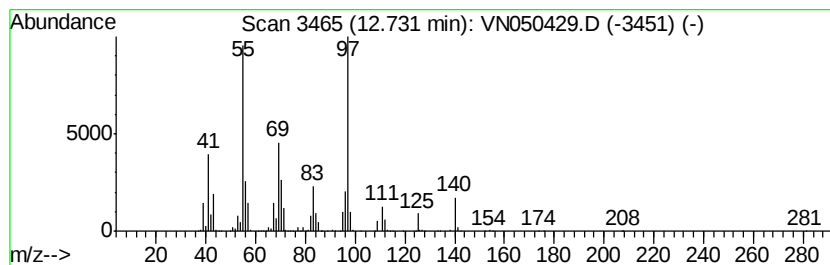
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexane, 1,1-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	133.37 ug/l	3254050	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	55
2		Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	52
3		2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	100463-01-2	52
4		Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	49
5		2,4-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	1000283-20-9	46



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Misc : 6.24uL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

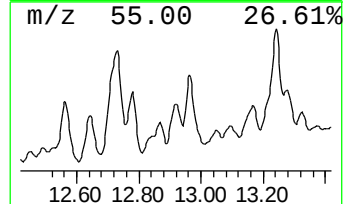
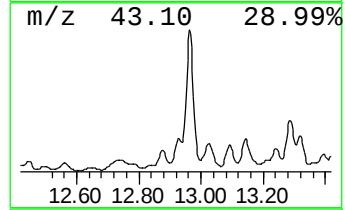
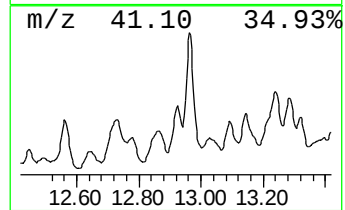
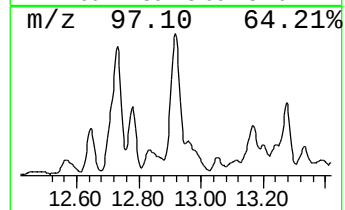
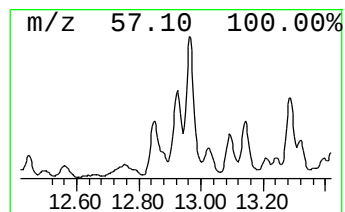
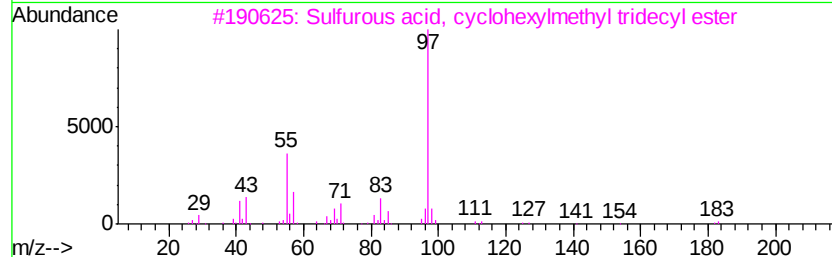
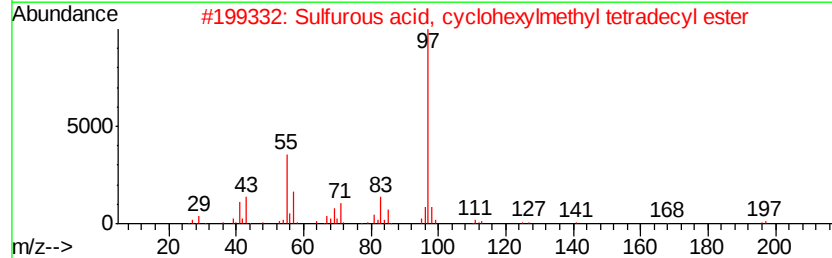
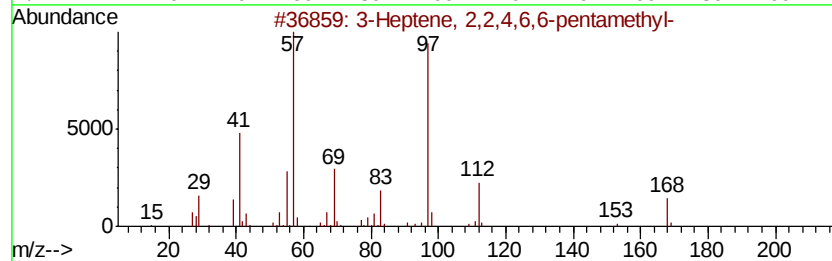
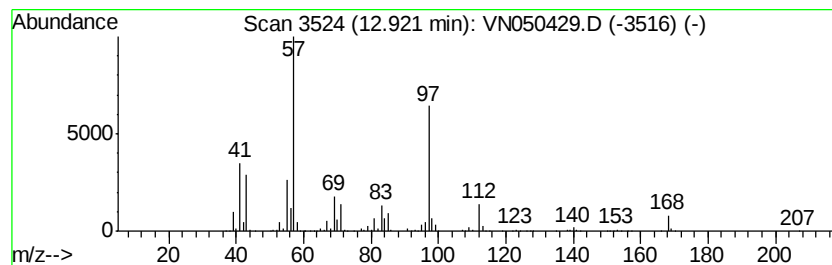
Instrument :
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Quant Title : SW846 8260

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

Peak Number 3 3-Heptene, 2,2,4,6,6-pentam... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	83.12 ug/l	2028000	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	3-Heptene, 2,2,4,6,6-pentamethyl-	168 C12H24	000123-48-8	58
2	Sulfurous acid, cyclohexylmethyl...	374 C21H42O3S	1000309-22-2	50
3	Sulfurous acid, cyclohexylmethyl...	360 C20H40O3S	1000309-22-1	50
4	Cyclohexane, 1,3-dimethyl-, trans-	112 C8H16	002207-03-6	47
5	Sulfurous acid, cyclohexylmethyl...	346 C19H38O3S	1000309-22-0	47



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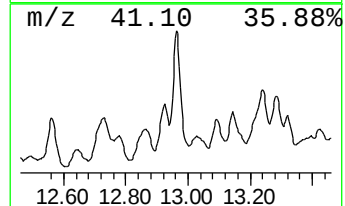
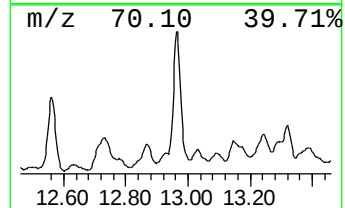
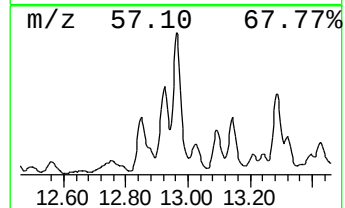
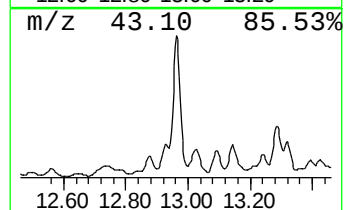
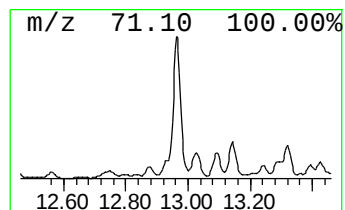
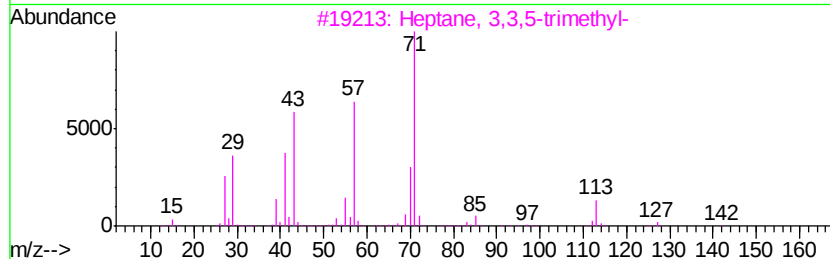
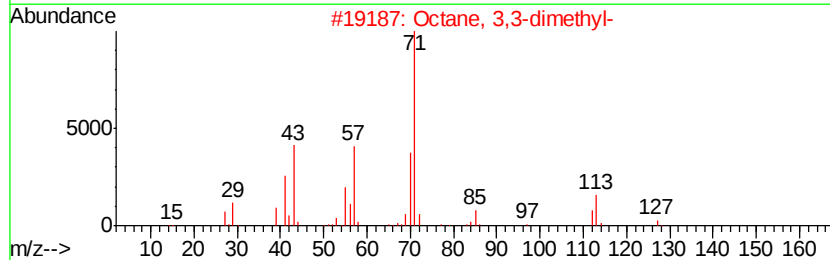
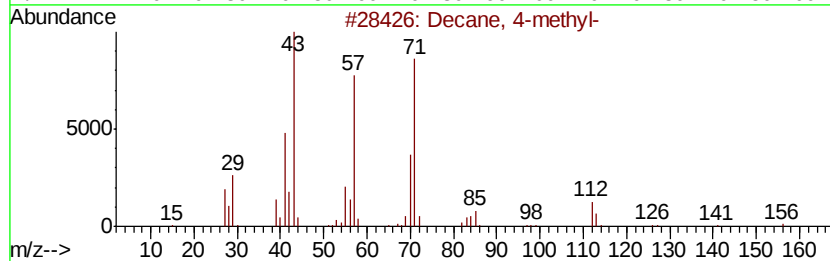
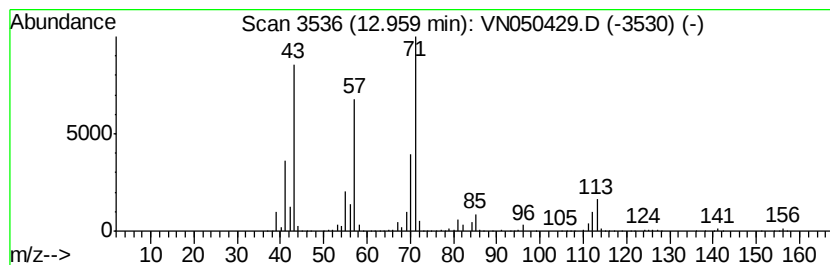
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Decane, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	211.79 ug/l	5167360	1,4-Dichlorobenzene-d4	13.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 4-methyl-	156	C11H24	002847-72-5	83	
2	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	78	
3	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	72	
4	4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	72	
5	Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	59	



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ClientSampleId :
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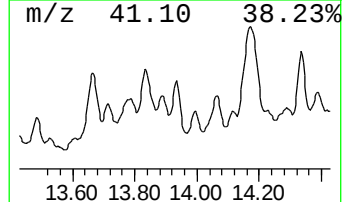
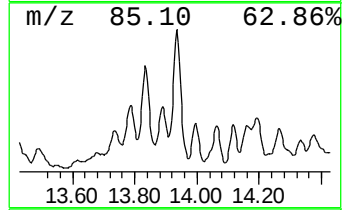
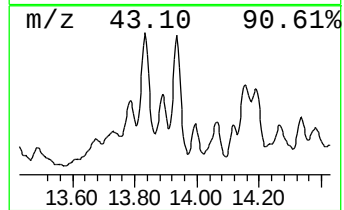
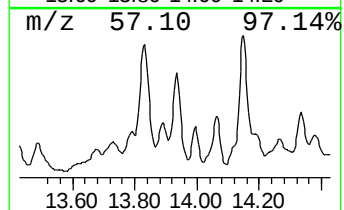
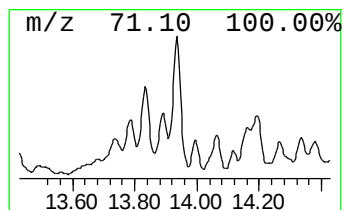
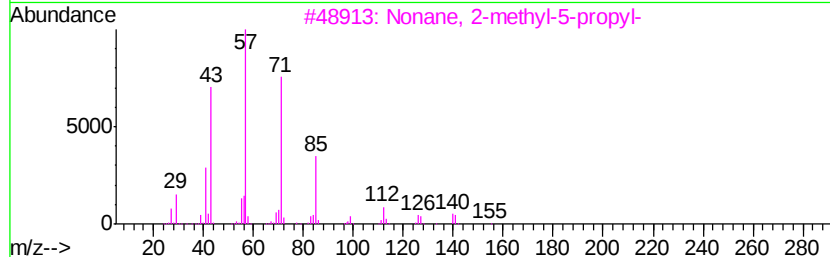
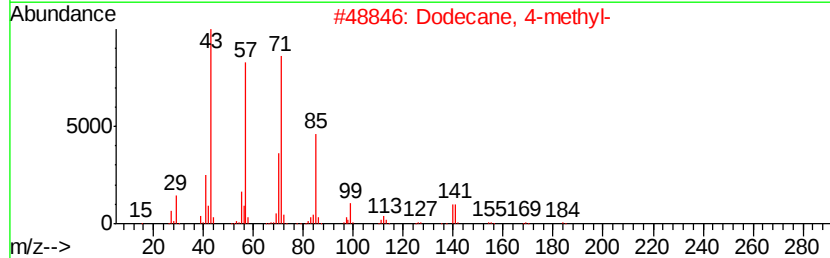
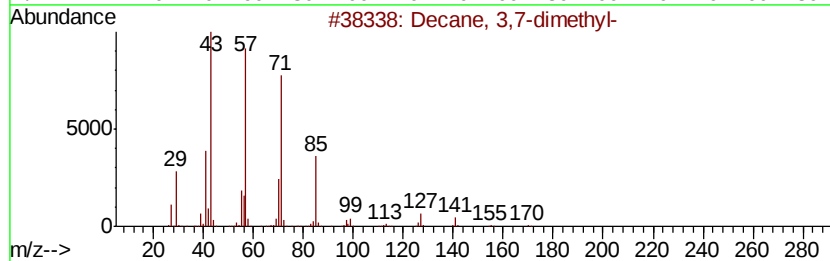
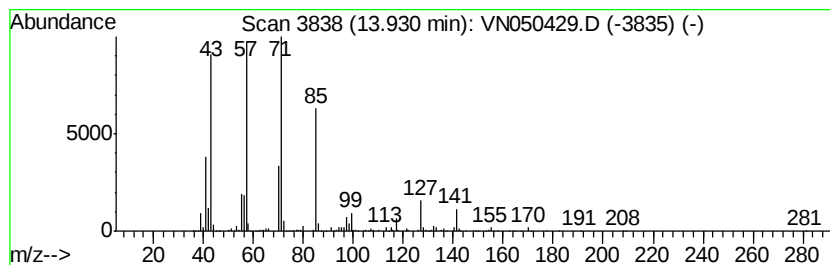
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Quant Title : SW846 8260

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

Peak Number 5 Decane, 3,7-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	100.90 ug/l	2461860	1,4-Dichlorobenzene-d4	13.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	72	
2	Dodecane, 4-methyl-	184	C13H28	006117-97-1	72	
3	Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	59	
4	Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	53	
5	Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	53	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN080718\
Data File : VN050429.D
Acq On : 7 Aug 2018 14:12
Operator : MD\SY
Sample : J4297-04
Misc : 6.24u/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
TP-4

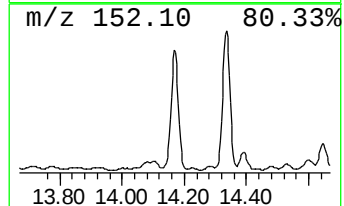
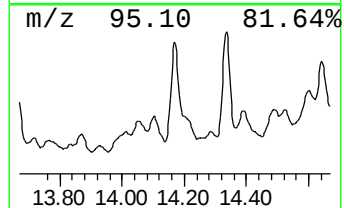
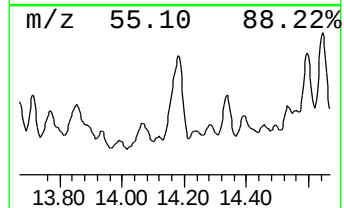
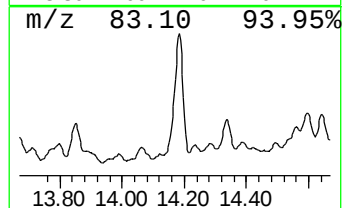
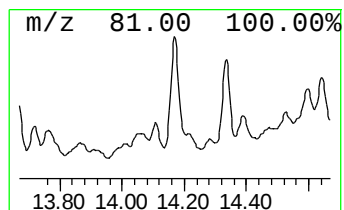
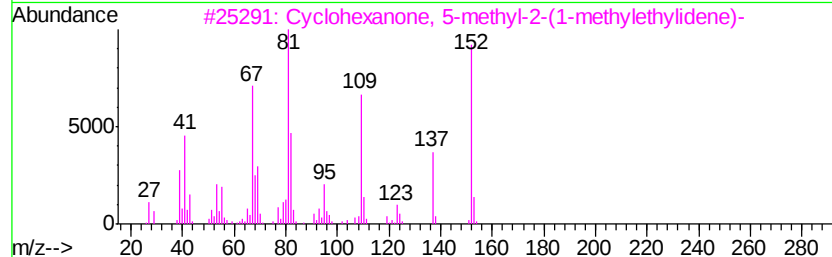
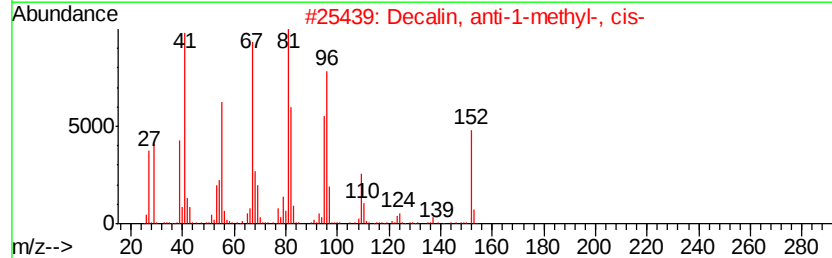
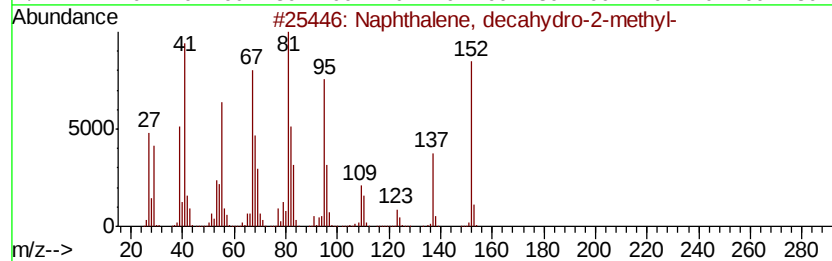
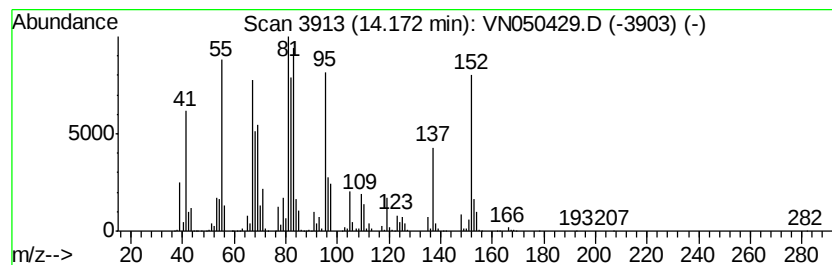
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, decahydro-2-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	571.43 ug/l	13942200	1,4-Dichlorobenzene-d4	13.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	96
2		Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	49
3		Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	46
4		Bicyclo[3.3.2]decan-9-one	152	C10H16O	028054-91-3	46
5		Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	006876-13-7	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN080718\
Data File : VN050429.D
Acq On : 7 Aug 2018 14:12
Operator : MD\SY
Sample : J4297-04
Misc : 6.24u/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

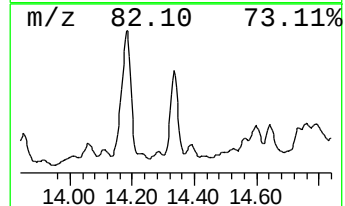
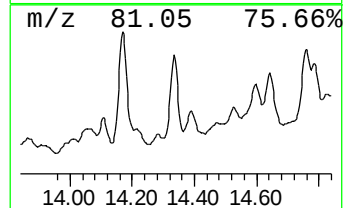
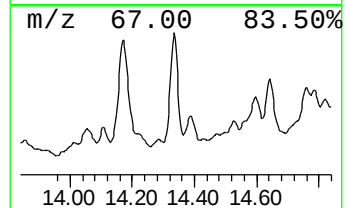
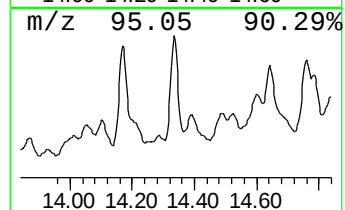
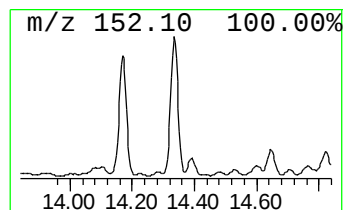
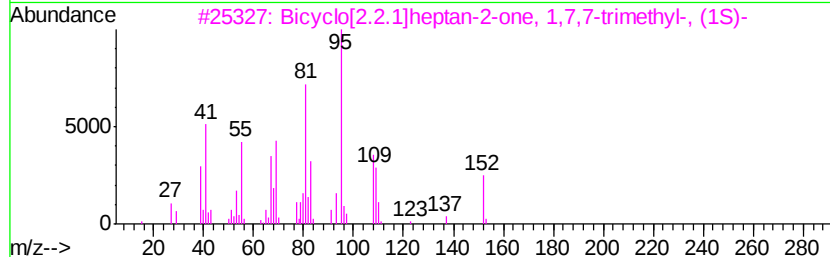
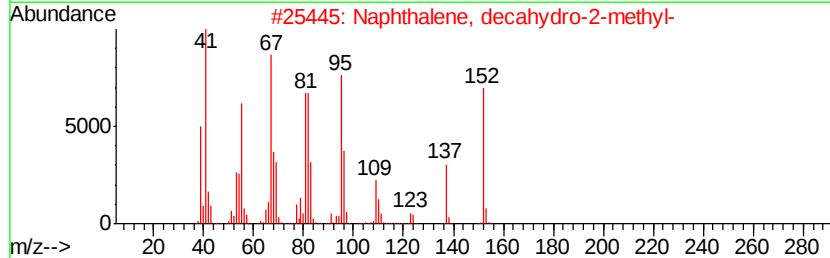
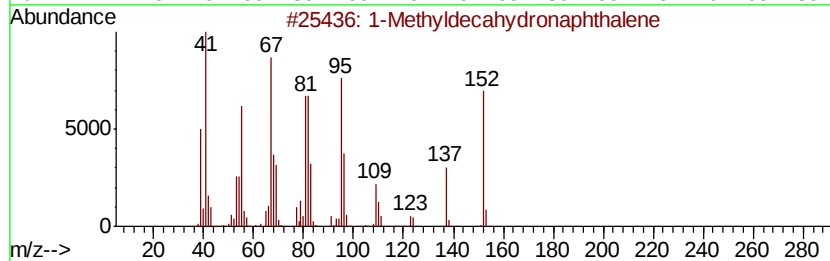
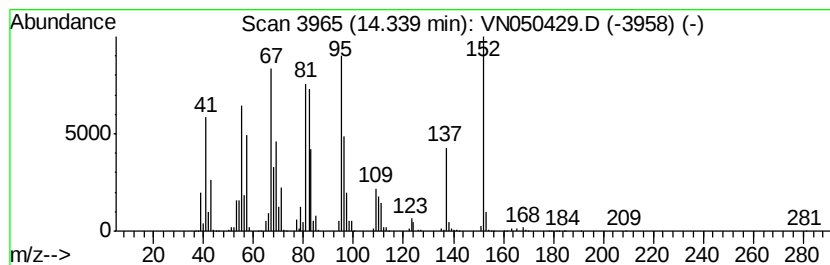
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ClientSampleId :
TP-4

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 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	147.69 ug/l	3603580	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		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152 C10H16O	000464-48-2 70
4		trans-Decalin, 2-methyl-	152 C11H20	1000152-47-3 64
5		8-Dodecen-1-ol, (Z)-	184 C12H24O	040642-40-8 53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN080718\
Data File : VN050429.D
Acq On : 7 Aug 2018 14:12
Operator : MD\SY
Sample : J4297-04
Misc : 6.24u/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
TP-4

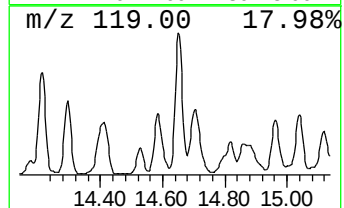
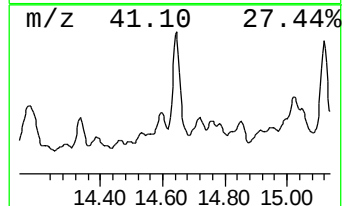
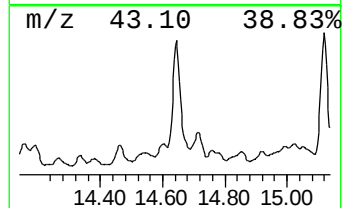
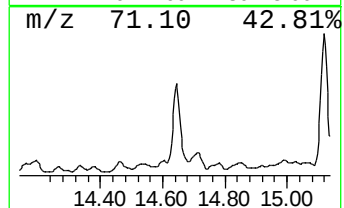
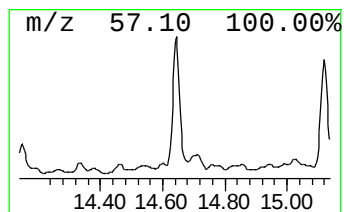
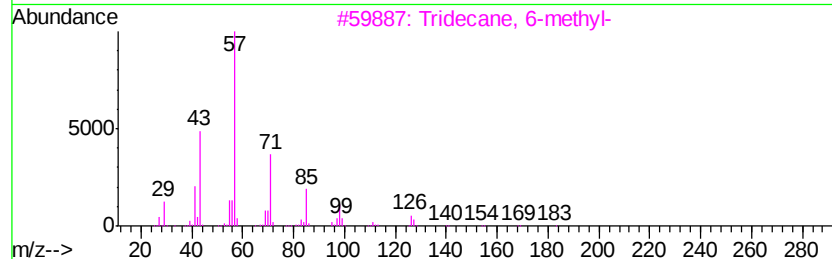
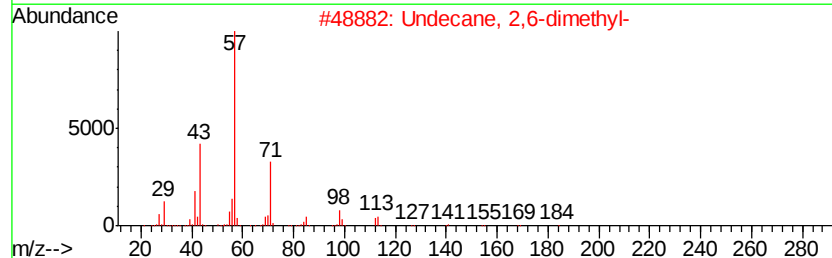
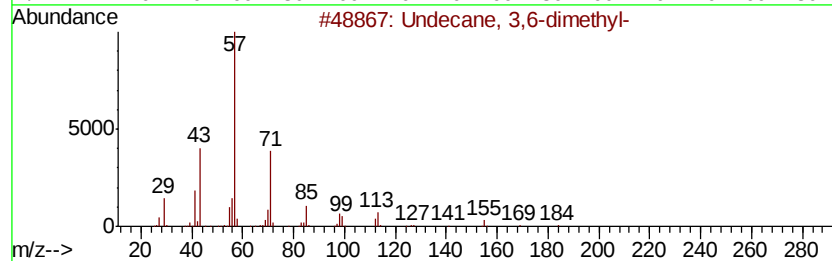
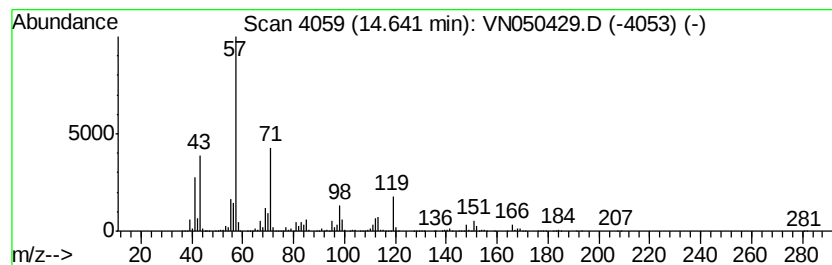
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Quant Title : SW846 8260

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

Peak Number 8 Undecane, 3,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	564.15 ug/l	13764800	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	70
2	Undecane, 2,6-dimethyl-		184	C13H28	017301-23-4	55
3	Tridecane, 6-methyl-		198	C14H30	013287-21-3	50
4	Dodecane, 6-methyl-		184	C13H28	006044-71-9	50
5	Decane, 2,6,8-trimethyl-		184	C13H28	062108-26-3	49



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN080718\
Data File : VN050429.D
Acq On : 7 Aug 2018 14:12
Operator : MD\SY
Sample : J4297-04
Misc : 6.24µ/5mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-4

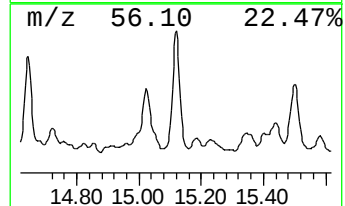
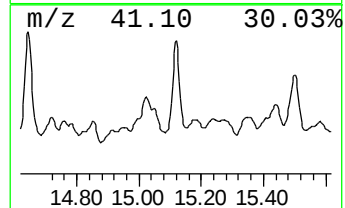
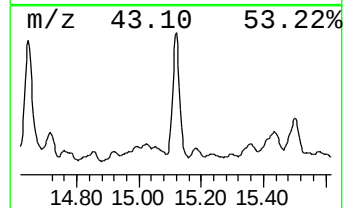
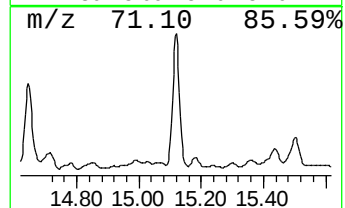
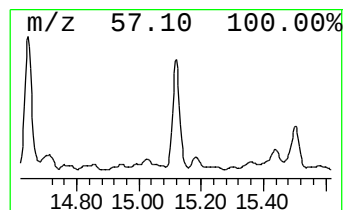
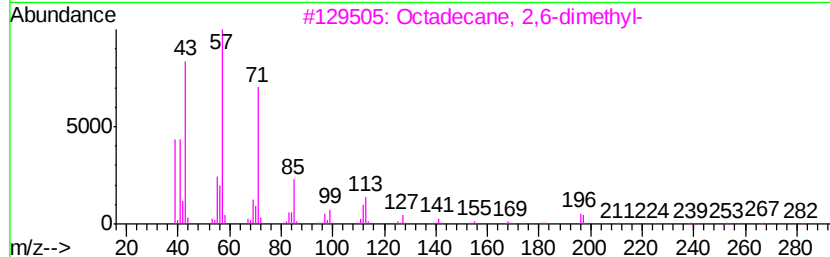
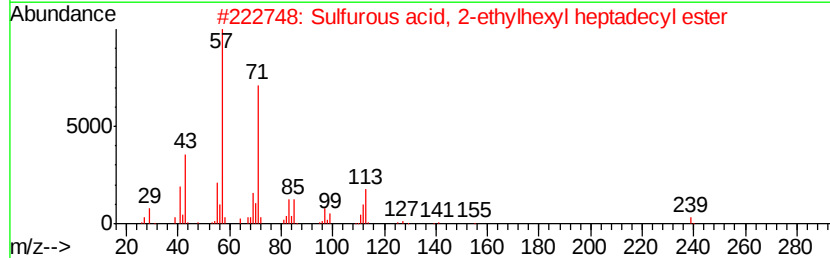
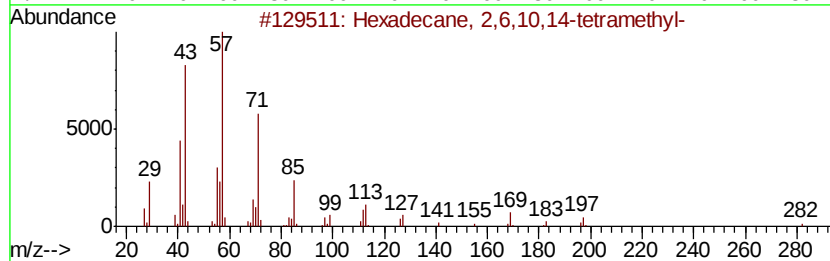
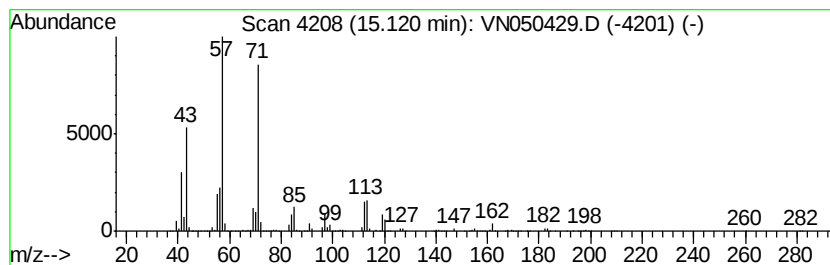
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Quant Title : SW846 8260

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

Peak Number 9 Hexadecane, 2,6,10,14-tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	442.51 ug/l	10796800	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80
2		Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	80
3		Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	72
4		Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
5		Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN080718\
Data File : VN050429.D
Acq On : 7 Aug 2018 14:12
Operator : MD\SY
Sample : J4297-04
Misc : 6.24uL/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-4

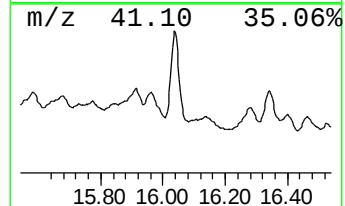
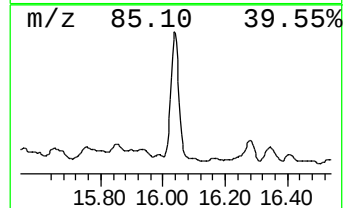
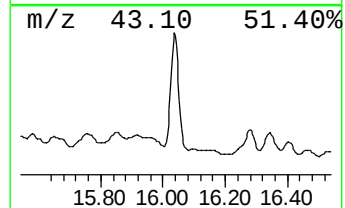
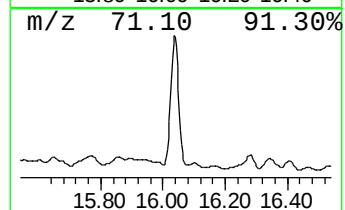
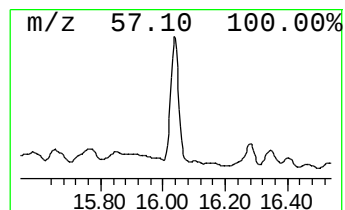
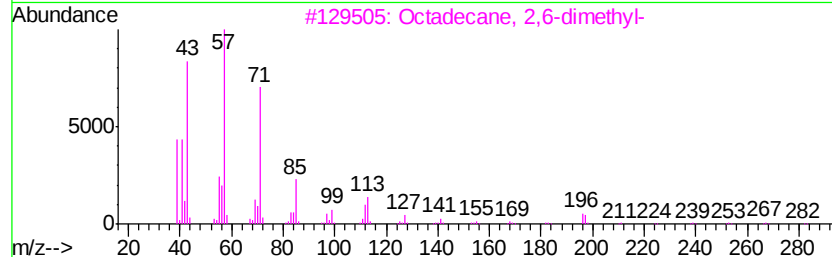
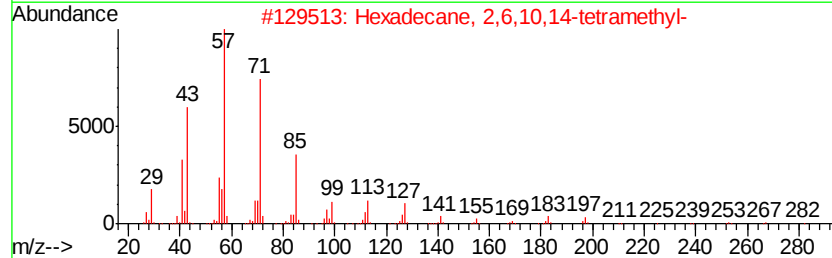
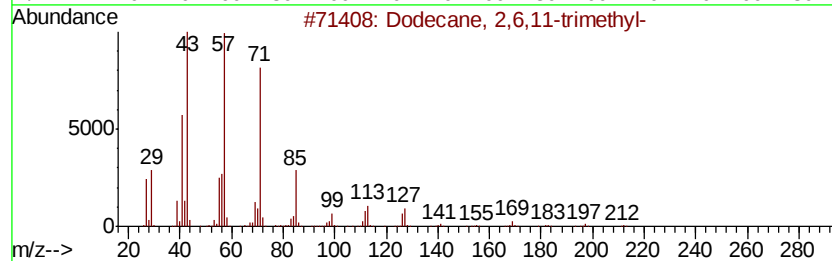
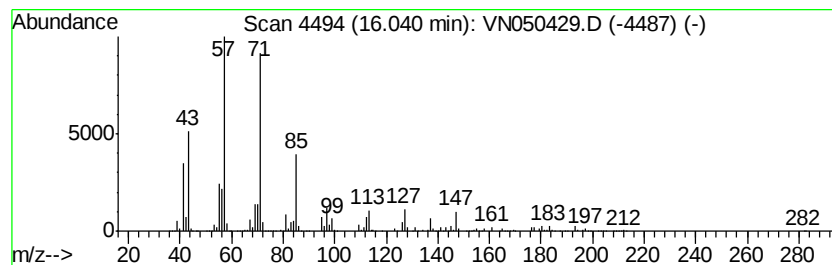
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Quant Title : SW846 8260

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

Peak Number 10 Dodecane, 2,6,11-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	269.73 ug/l	6581080	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	89
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	87
3		Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	80
4		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64
5		Decane, 5-propyl-	184	C13H28	017312-62-8	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN080718\
Data File : VN050429.D
Acq On : 7 Aug 2018 14:12
Operator : MD\SY
Sample : J4297-04
Misc : 6.24g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-4

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
2-Octene, 2,6-dim...	12.56	107.3	ug/l	2618390	4	13.35	1219950	50.0
Cyclohexane, 1,1-...	12.73	133.4	ug/l	3254050	4	13.35	1219950	50.0
3-Heptene, 2,2,4,...	12.92	83.1	ug/l	2028000	4	13.35	1219950	50.0
Decane, 4-methyl-	12.96	211.8	ug/l	5167360	4	13.35	1219950	50.0
Decane, 3,7-dimet...	13.93	100.9	ug/l	2461860	4	13.35	1219950	50.0
Naphthalene, deca...	14.17	571.4	ug/l	13942200	4	13.35	1219950	50.0
1-Methyldecahydro...	14.34	147.7	ug/l	3603580	4	13.35	1219950	50.0
Undecane, 3,6-dim...	14.64	564.1	ug/l	13764800	4	13.35	1219950	50.0
Hexadecane, 2,6,1...	15.12	442.5	ug/l	10796800	4	13.35	1219950	50.0
Dodecane, 2,6,11-...	16.04	269.7	ug/l	6581080	4	13.35	1219950	50.0