

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN100618\
 Data File : VN051717.D
 Acq On : 6 Oct 2018 4:10
 Operator : MD\SY
 Sample : J5165-06 40X
 Misc : 5.89g/5.00mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 47 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 EP1-MW-H-092718(7-10)

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\82N100418W.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	2.101	83	102	103	rBV4	16728	38728	1.07%	0.130%
2	7.593	1790	1810	1821	rBV	499489	1247175	34.55%	4.182%
3	7.667	1821	1833	1859	rVB	781992	1864860	51.66%	6.253%
4	8.030	1927	1946	1971	rBV	476863	1131437	31.34%	3.794%
5	8.587	2099	2119	2147	rBV	1042096	2197915	60.89%	7.369%
6	10.091	2568	2587	2619	rBV	1911398	3609940	100.00%	12.104%
7	11.008	2862	2872	2883	rVB2	38610	65950	1.83%	0.221%
8	11.124	2896	2908	2916	rBV5	20094	39205	1.09%	0.131%
9	11.214	2927	2936	2949	rVB5	31531	65125	1.80%	0.218%
10	11.297	2951	2962	2971	rBV2	21871	40920	1.13%	0.137%
11	11.406	2981	2996	3017	rBV	1433147	2582199	71.53%	8.658%
12	11.542	3030	3038	3045	rBV6	24495	37732	1.05%	0.127%
13	11.596	3045	3055	3063	rBV8	35095	68494	1.90%	0.230%
14	11.654	3063	3073	3081	rBV3	90444	163941	4.54%	0.550%
15	11.757	3097	3105	3111	rBV6	20382	36929	1.02%	0.124%
16	11.853	3127	3135	3142	rVB4	45704	69869	1.94%	0.234%
17	11.924	3143	3157	3169	rBV7	169619	418349	11.59%	1.403%
18	12.043	3186	3194	3203	rBV	266727	378451	10.48%	1.269%
19	12.120	3209	3218	3223	rBV4	163790	279179	7.73%	0.936%
20	12.159	3224	3230	3240	rVB5	245655	440888	12.21%	1.478%
21	12.294	3266	3272	3279	rBV6	82108	126986	3.52%	0.426%
22	12.336	3280	3285	3294	rVB2	236340	341475	9.46%	1.145%
23	12.403	3294	3306	3318	rBV	1298992	2268338	62.84%	7.606%
24	12.487	3319	3332	3340	rBV10	83403	227329	6.30%	0.762%
25	12.561	3347	3355	3371	rVB4	321542	684960	18.97%	2.297%
26	12.644	3371	3381	3388	rBV8	126958	272281	7.54%	0.913%
27	12.728	3389	3407	3417	rBV9	344456	957467	26.52%	3.210%
28	12.869	3444	3451	3458	rBV6	138565	199449	5.52%	0.669%
29	12.963	3472	3480	3493	rVB2	742420	1201424	33.28%	4.028%
30	13.040	3493	3504	3513	rBV	983444	1600604	44.34%	5.367%
31	13.088	3514	3519	3529	rVB4	116963	176530	4.89%	0.592%
32	13.146	3530	3537	3541	rBV3	159463	235456	6.52%	0.789%
33	13.239	3561	3566	3573	rVB2	213378	270277	7.49%	0.906%
34	13.284	3575	3580	3588	rVV3	210658	299369	8.29%	1.004%

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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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35	13.345	3588	3599	3624	rVB2	1255992	2976438	82.45%	9.980%
36	13.590	3667	3675	3688	rBV5	176838	357817	9.91%	1.200%
37	13.660	3689	3697	3707	rBV5	290245	528291	14.63%	1.771%
38	13.802	3736	3741	3745	rBV2	94512	132657	3.67%	0.445%
39	13.831	3746	3750	3760	rVV4	227944	337745	9.36%	1.132%
40	13.889	3761	3768	3776	rVB	260199	397533	11.01%	1.333%
41	13.995	3792	3801	3810	rVB4	179825	306980	8.50%	1.029%
42	14.127	3834	3842	3849	rBV3	82084	141138	3.91%	0.473%
43	14.178	3850	3858	3865	rBV10	88243	177970	4.93%	0.597%
44	14.249	3874	3880	3887	rVB	133645	189133	5.24%	0.634%
45	14.294	3888	3894	3900	rBV4	60736	82536	2.29%	0.277%
46	14.332	3901	3906	3913	rVB4	63676	77172	2.14%	0.259%
47	14.525	3960	3966	3973	rVB	42469	57159	1.58%	0.192%
48	14.583	3974	3984	3996	rVV2	139808	269105	7.45%	0.902%
49	14.644	3997	4003	4015	rVB4	34086	60181	1.67%	0.202%
50	14.741	4026	4033	4042	rVB2	37832	55549	1.54%	0.186%
51	14.953	4094	4099	4112	rVB5	21608	38166	1.06%	0.128%

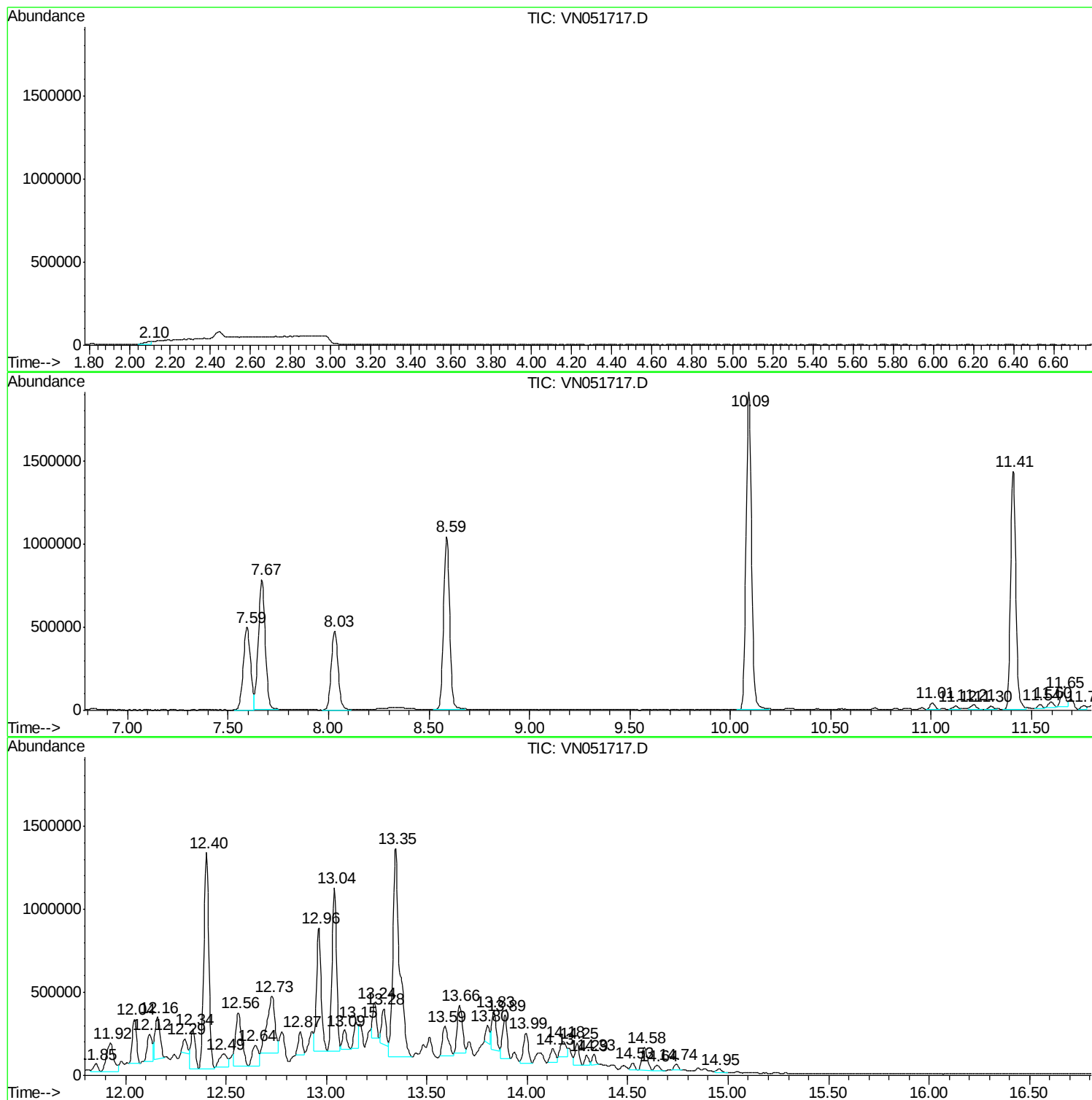
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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



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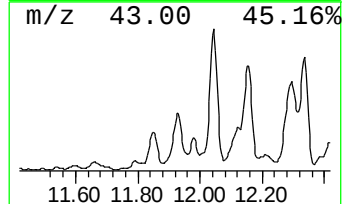
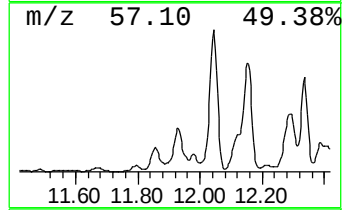
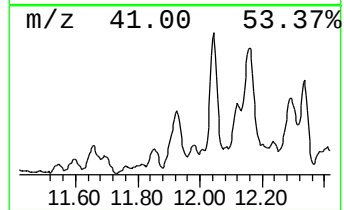
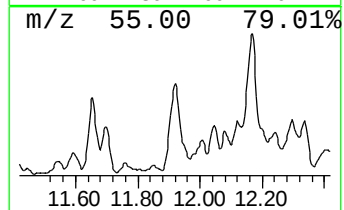
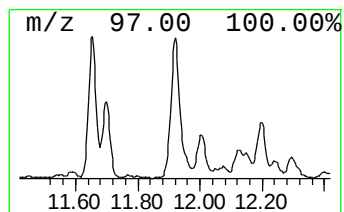
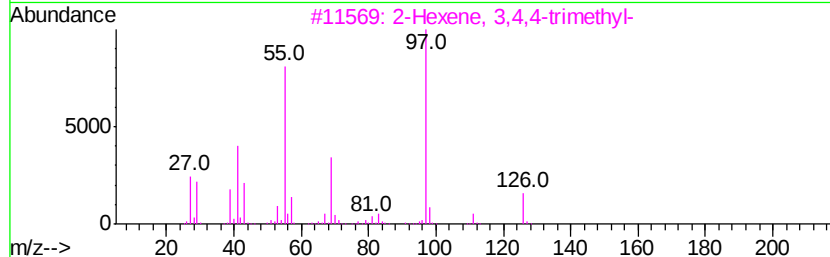
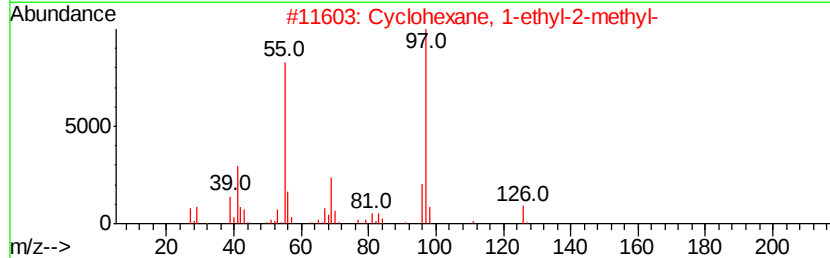
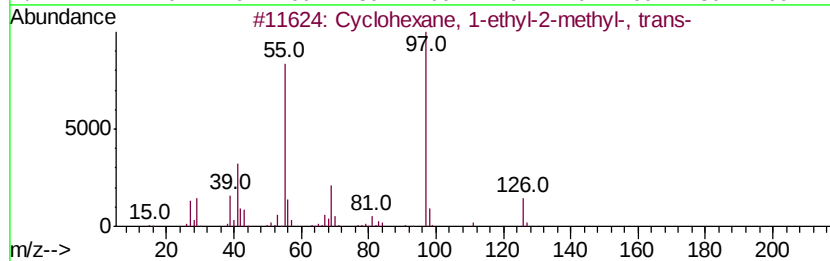
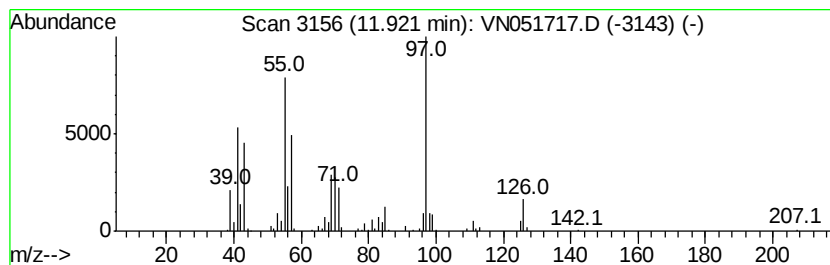
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.92	8.10 ug/l	418349	Chlorobenzene-d5	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	64
2	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	64
3	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	60
4	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	52
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	52



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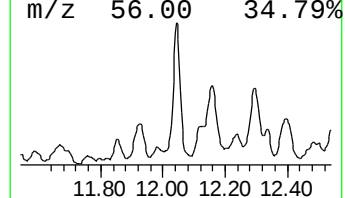
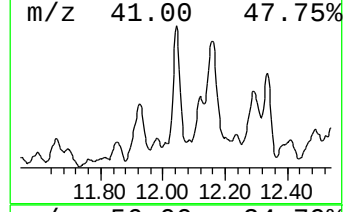
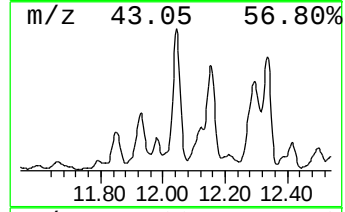
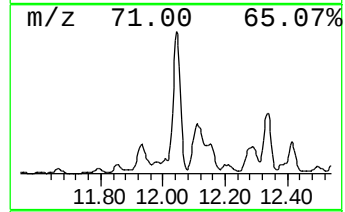
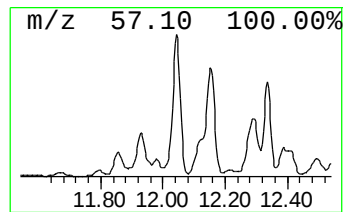
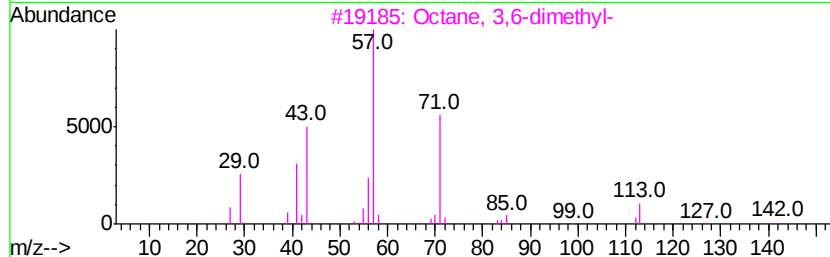
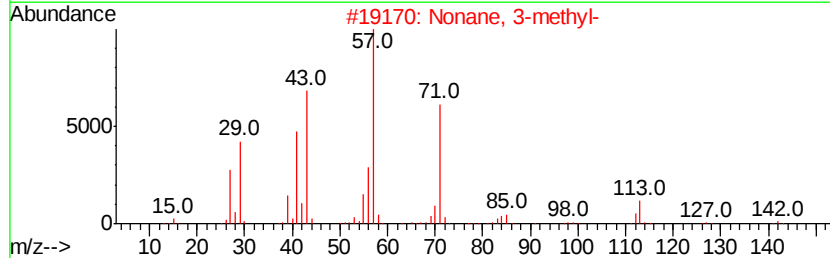
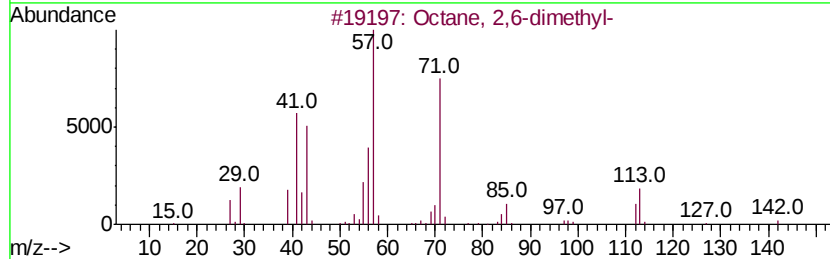
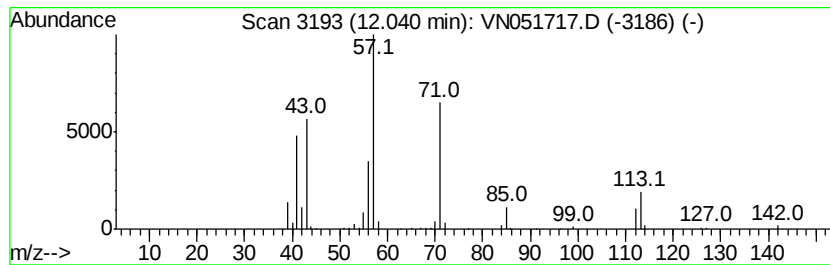
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	7.33 ug/l	378451	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octane, 2,6-dimethyl-	142 C10H22	002051-30-1	87
2	Nonane, 3-methyl-	142 C10H22	005911-04-6	72
3	Octane, 3,6-dimethyl-	142 C10H22	015869-94-0	64
4	Undecane, 6,6-dimethyl-	184 C13H28	017312-76-4	59
5	Nonane, 4-methyl-5-propyl-	184 C13H28	062185-55-1	53



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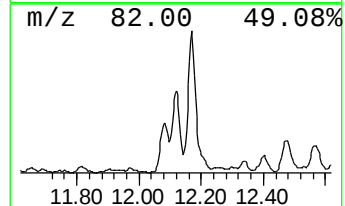
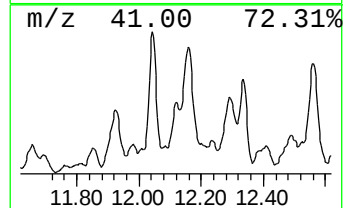
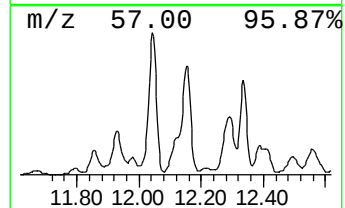
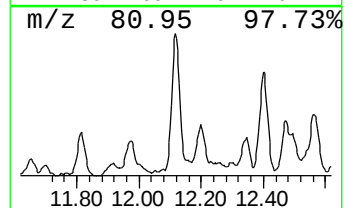
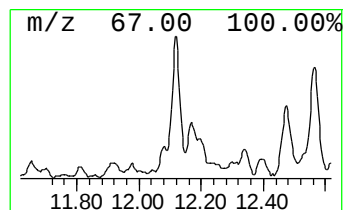
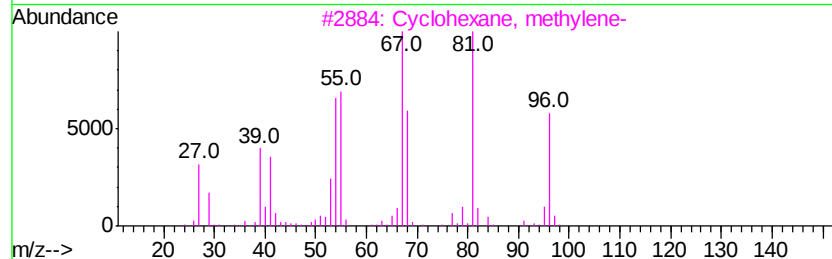
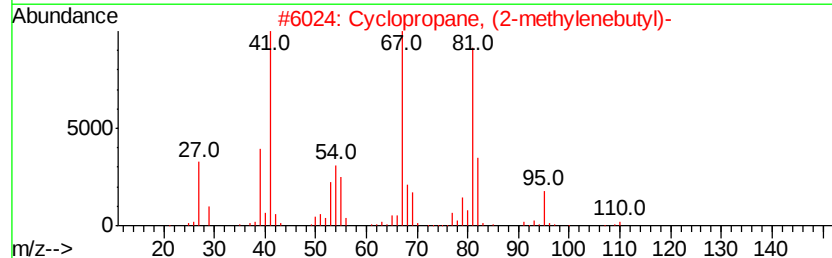
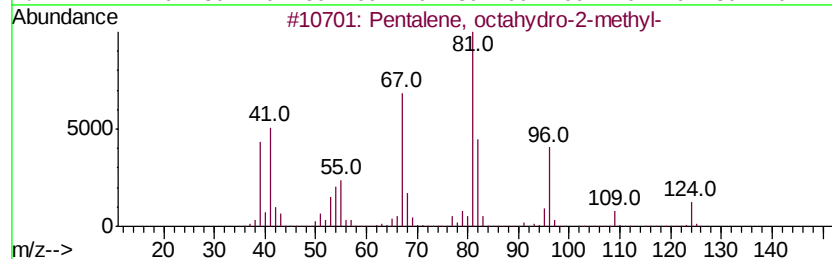
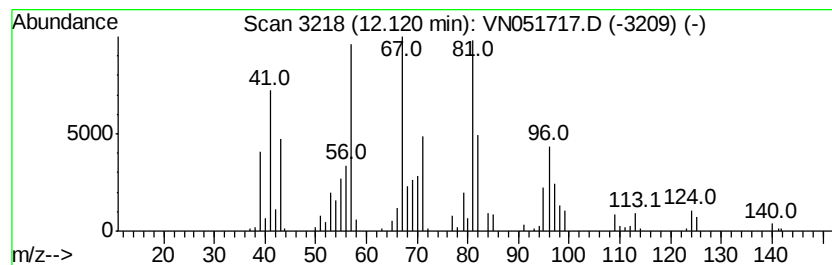
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentalene, octahydro-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	5.41 ug/l	279179	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pentalene, octahydro-2-methyl-	124 C9H16	003868-64-2 60
2		Cyclopropane, (2-methylenebutyl)-	110 C8H14	074685-56-6 53
3		Cyclohexane, methylene-	96 C7H12	001192-37-6 49
4		7-Methyl-8-oxabicyclo[4.3.0]nonane	140 C9H16O	1000216-87-6 49
5		Cyclohexene,3-propyl-	124 C9H16	003983-06-0 43



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ALS Vial : 47 Sample Multiplier: 28

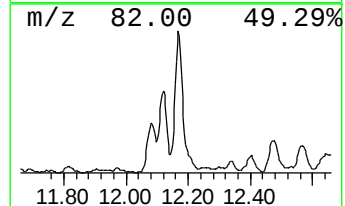
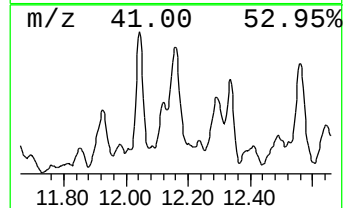
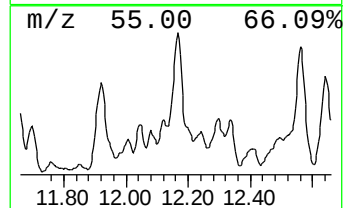
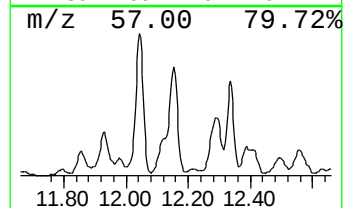
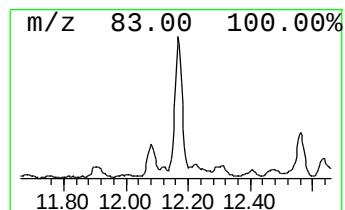
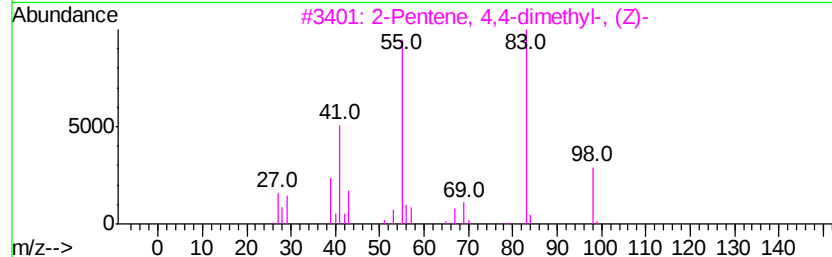
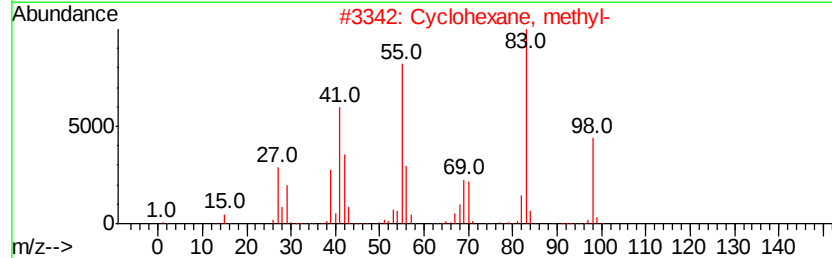
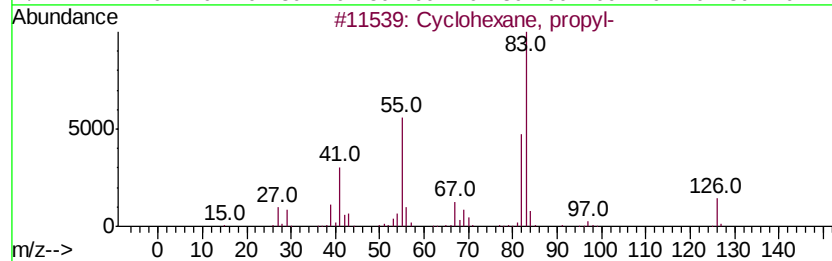
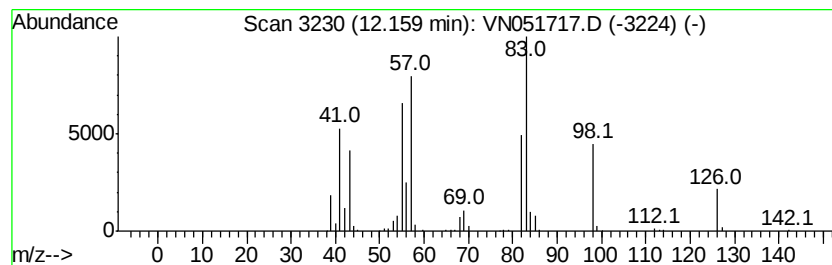
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclohexane, propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.16	8.54 ug/l	440888	Chlorobenzene-d5	11.41		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclohexane, propyl-	126	C9H18	001678-92-8	53
2		Cvclohexane, methyl-	98	C7H14	000108-87-2	52
3		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	49
4		Cvclohexane, ethyl-	112	C8H16	001678-91-7	47
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	47



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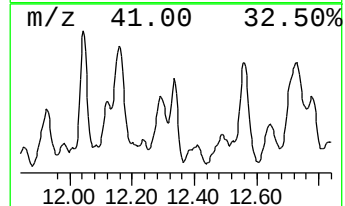
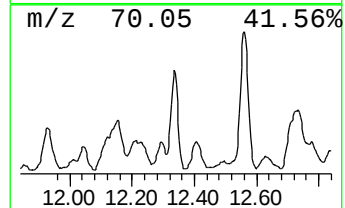
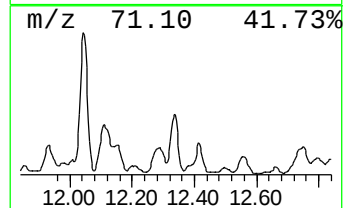
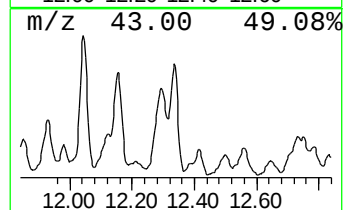
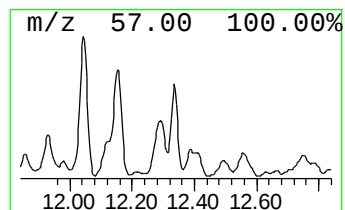
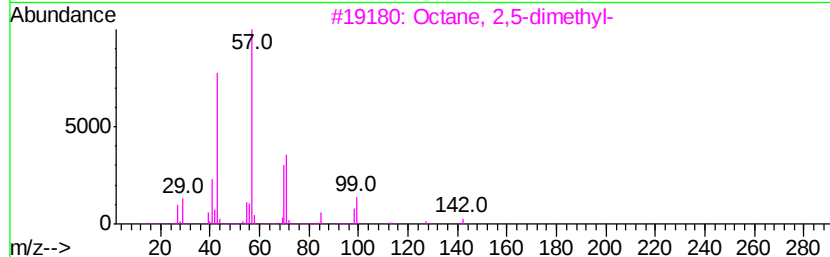
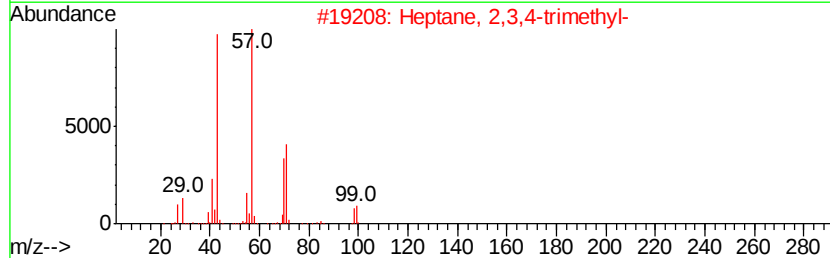
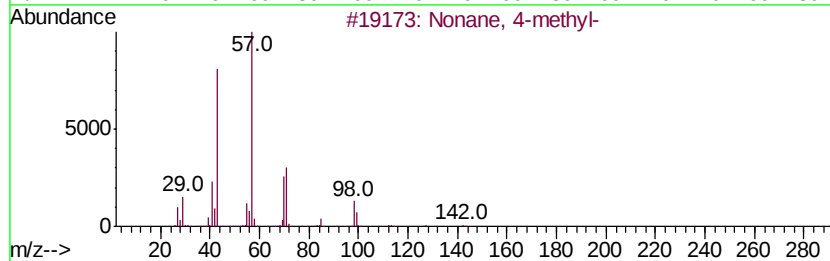
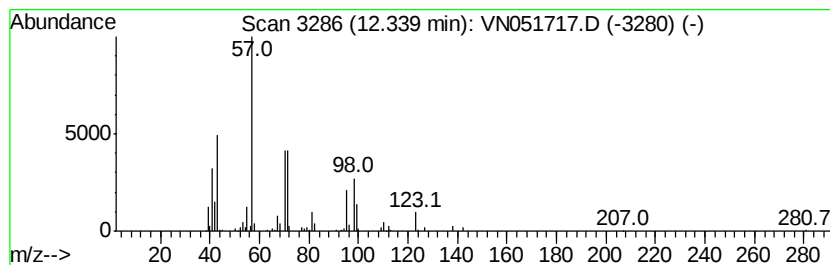
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	6.61 ug/l	341475	Chlorobenzene-d5	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	72	
2	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	53	
3	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	53	
4	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	53	
5	Heptane, 4-propyl-	142	C10H22	003178-29-8	38	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN100618\
Data File : VN051717.D
Acq On : 6 Oct 2018 4:10
Operator : MD\SY
Sample : J5165-06 40X
Misc : 5.89µ/5.00mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 28

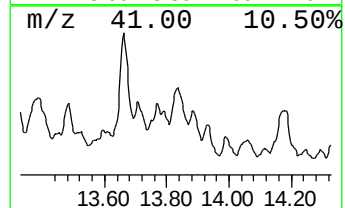
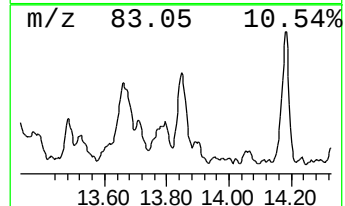
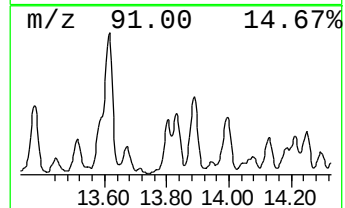
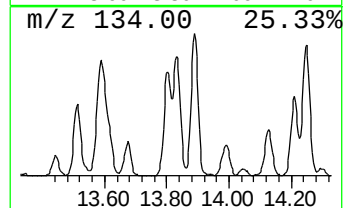
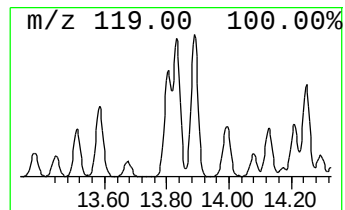
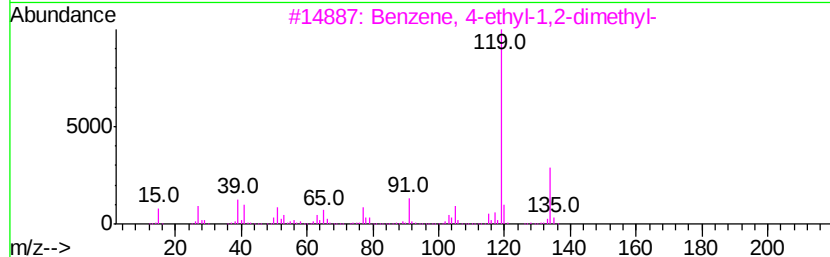
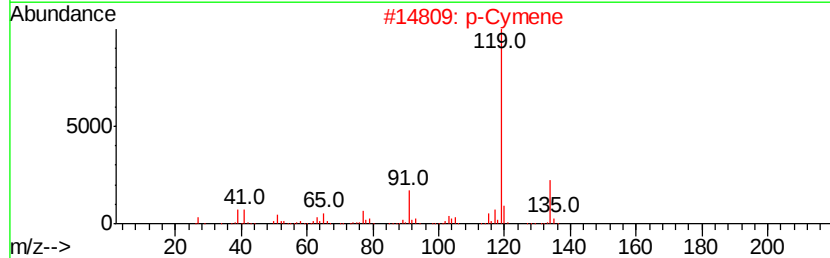
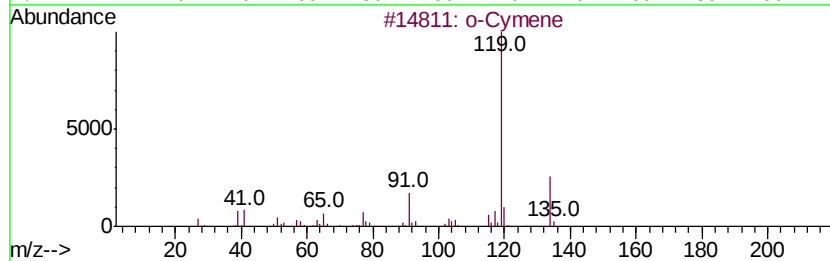
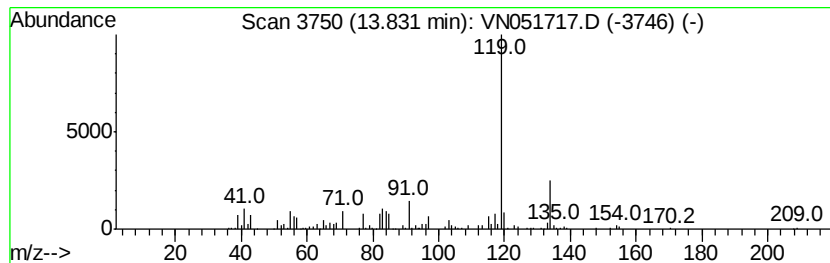
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-H-092718(7-10)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 6 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	5.67 ug/l	337745	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		o-Cymene	134 C10H14	000527-84-4 94
2		p-Cymene	134 C10H14	000099-87-6 93
3		Benzene, 4-ethyl-1,2-dimethyl-	134 C10H14	000934-80-5 81
4		Benzene, 1-methyl-3-(1-methyleth...	134 C10H14	000535-77-3 81
5		Benzene, 1-ethyl-2,4-dimethyl-	134 C10H14	000874-41-9 81



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN100618\
Data File : VN051717.D
Acq On : 6 Oct 2018 4:10
Operator : MD\SY
Sample : J5165-06 40X
Misc : 5.89g/5.00mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-H-092718(7-10)

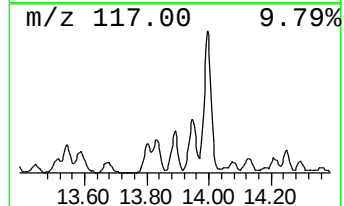
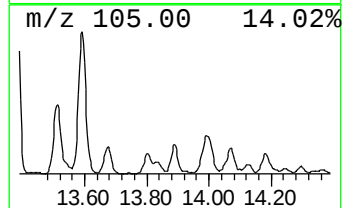
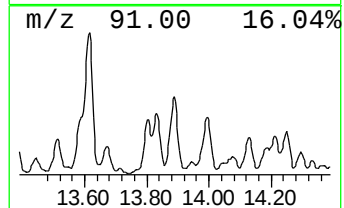
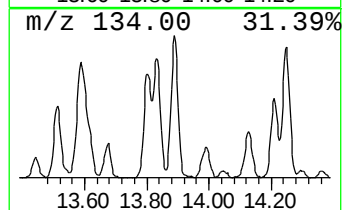
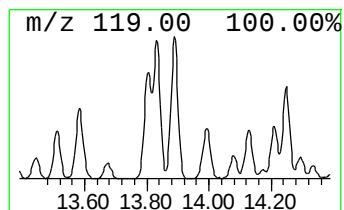
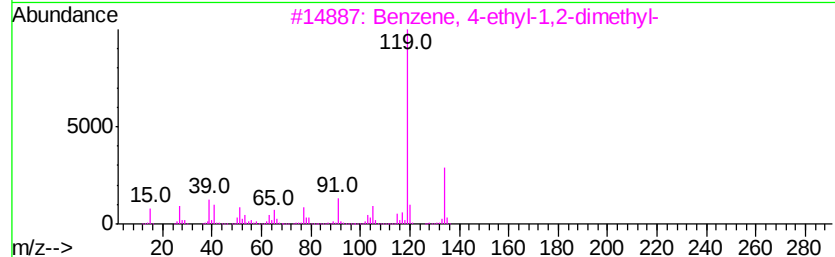
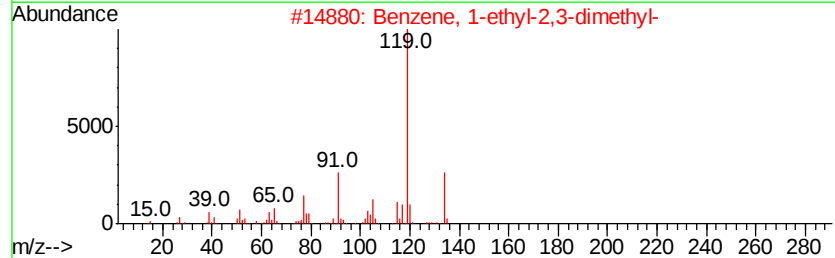
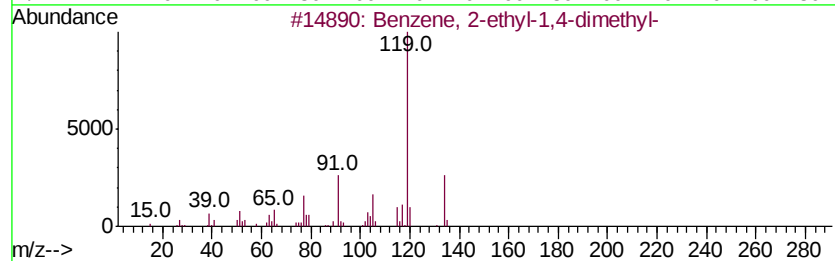
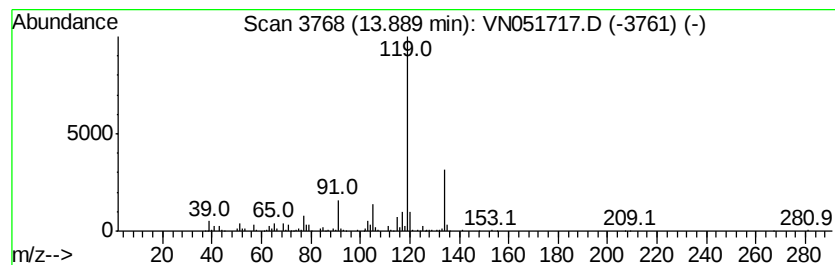
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	6.68 ug/l	397533	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
3		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
4		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
5		o-Cymene	134	C10H14	000527-84-4	94



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN100618\
Data File : VN051717.D
Acq On : 6 Oct 2018 4:10
Operator : MD\SY
Sample : J5165-06 40X
Misc : 5.89µ/5.00mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 28

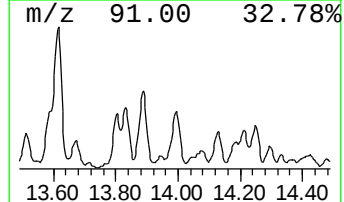
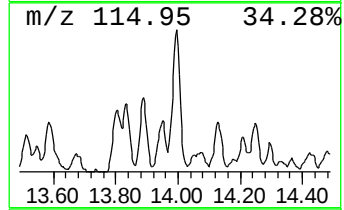
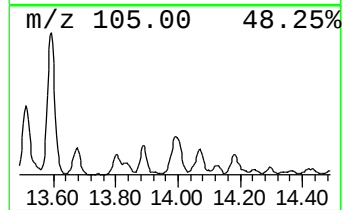
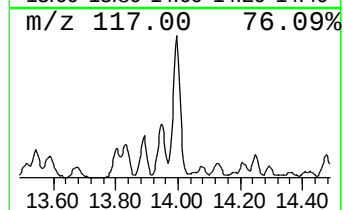
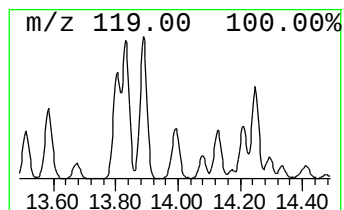
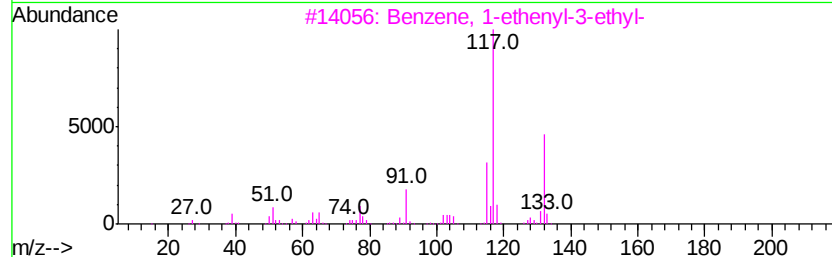
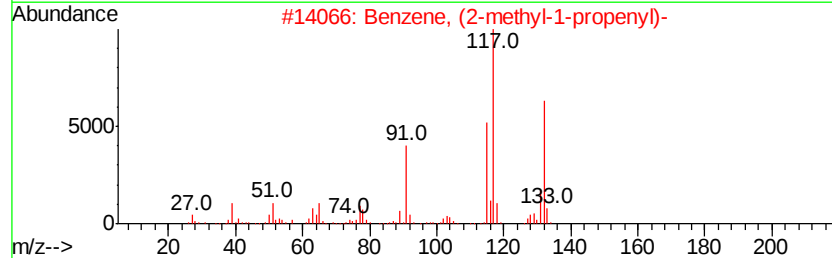
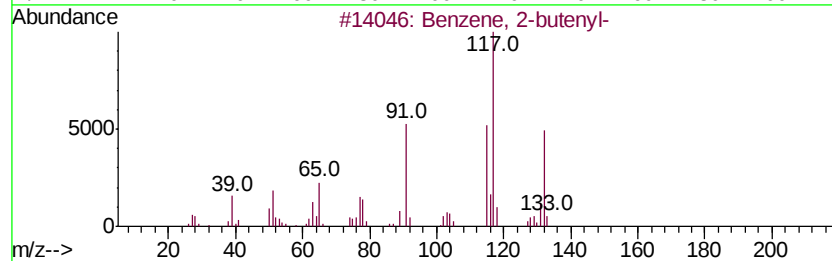
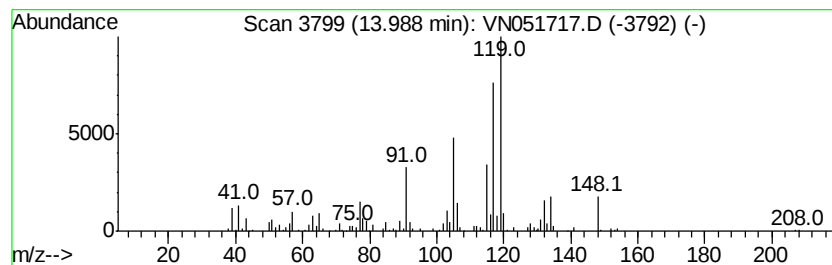
Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-H-092718(7-10)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-butenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	5.16 ug/l	306980	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 2-butenyl-	132 C10H12	001560-06-1 80
2		Benzene, (2-methyl-1-propenyl)-	132 C10H12	000768-49-0 55
3		Benzene, 1-ethenyl-3-ethyl-	132 C10H12	007525-62-4 55
4		Benzene, (2-methylcyclopropyl)-	132 C10H12	1000327-39-0 50
5		1-Phenyl-1-butene	132 C10H12	000824-90-8 50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN100618\
Data File : VN051717.D
Acq On : 6 Oct 2018 4:10
Operator : MD\SY
Sample : J5165-06 40X
Misc : 5.89g/5.00mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 47 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
EP1-MW-H-092718(7-10)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.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	8.1	ug/l	418349	3	11.41	2582200	50.0
Octane, 2,6-dimet...	12.04	7.3	ug/l	378451	3	11.41	2582200	50.0
Pentalene, octahy...	12.12	5.4	ug/l	279179	3	11.41	2582200	50.0
Cyclohexane, propyl-	12.16	8.5	ug/l	440888	3	11.41	2582200	50.0
Nonane, 4-methyl-	12.34	6.6	ug/l	341475	3	11.41	2582200	50.0
o-Cymene	13.83	5.7	ug/l	337745	4	13.35	2976440	50.0
Benzene, 2-ethyl-...	13.89	6.7	ug/l	397533	4	13.35	2976440	50.0
Benzene, 2-butenyl-	13.99	5.2	ug/l	306980	4	13.35	2976440	50.0