

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN050820\
 Data File : VN061362.D
 Acq On : 8 May 2020 15:22
 Operator : JC/MD
 Sample : L2544-13
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 ST008MW038-200505

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\82N042720W.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	1.638	3	15	128	rBV	3892961	14736836	100.00%	54.620%
2	2.770	350	367	395	rBV	393577	802459	5.45%	2.974%
3	4.481	873	899	935	rBV	364102	1280476	8.69%	4.746%
4	6.474	1495	1519	1545	rBV2	217789	702770	4.77%	2.605%
5	7.548	1835	1853	1864	rBV2	70624	176225	1.20%	0.653%
6	7.625	1864	1877	1887	rVV	143497	339278	2.30%	1.257%
7	7.706	1887	1902	1928	rVB	468596	1213928	8.24%	4.499%
8	7.989	1976	1990	2014	rVB	94940	222416	1.51%	0.824%
9	8.172	2014	2047	2068	rBV	734170	1998666	13.56%	7.408%
10	8.551	2149	2165	2184	rBV	227524	464021	3.15%	1.720%
11	9.490	2441	2457	2475	rBV	437684	876643	5.95%	3.249%
12	9.622	2481	2498	2527	rVB	631405	1335689	9.06%	4.951%
13	9.992	2597	2613	2623	rBV	83862	156587	1.06%	0.580%
14	10.059	2623	2634	2663	rVB	367883	686097	4.66%	2.543%
15	11.381	3032	3045	3065	rBV2	343288	771057	5.23%	2.858%
16	12.377	3341	3355	3369	rBV	262936	436753	2.96%	1.619%
17	13.320	3636	3648	3664	rVB	326534	553789	3.76%	2.053%
18	13.969	3841	3850	3861	rVB3	139543	227157	1.54%	0.842%

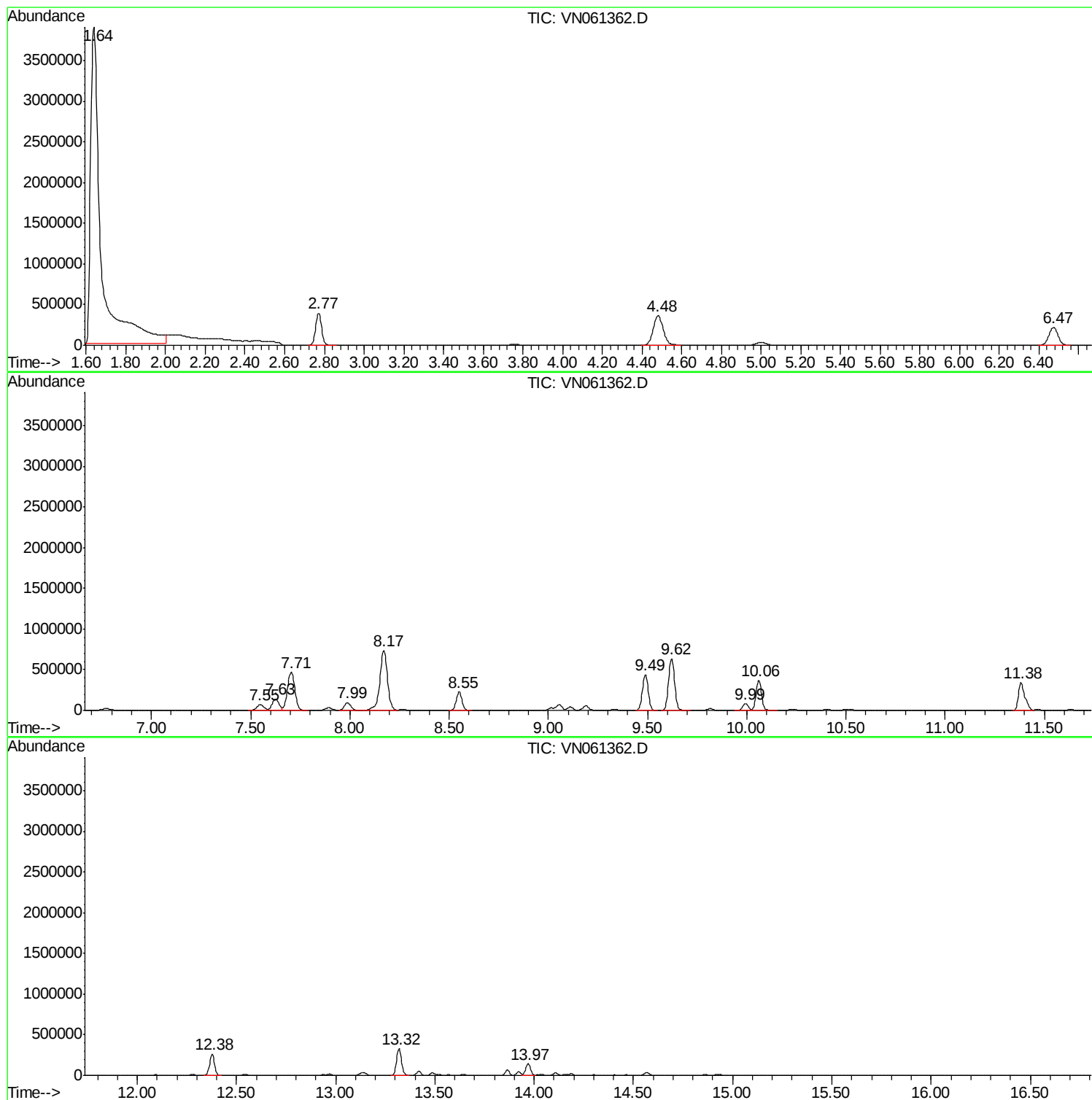
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ClientSampleId :
ST008MW038-200505

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042720W.M
Quant Title : SW846 8260

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



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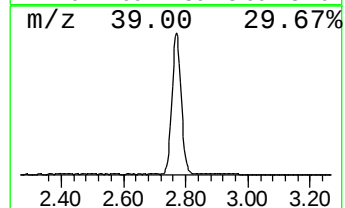
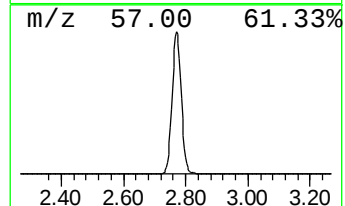
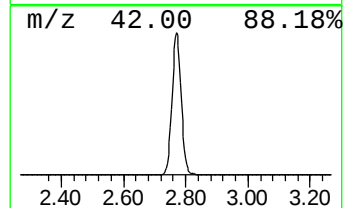
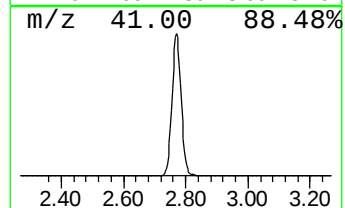
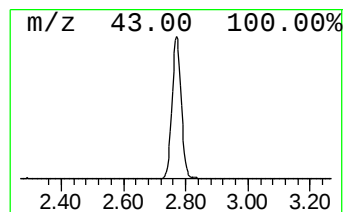
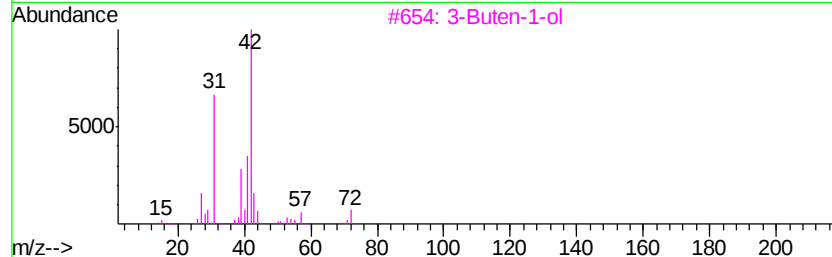
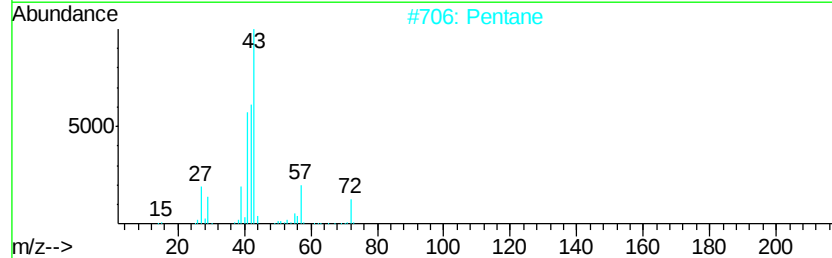
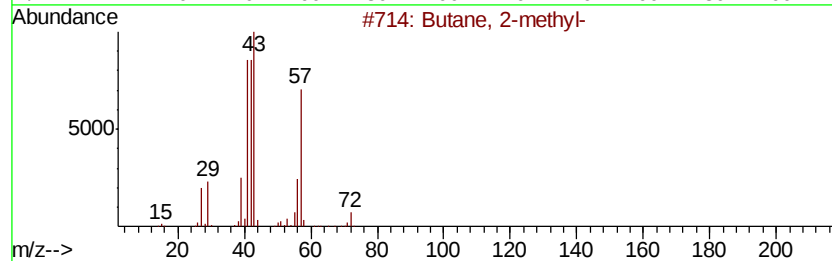
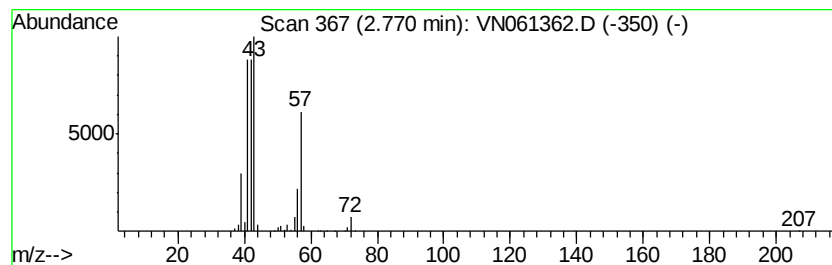
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042720W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.77	118.26 ug/l	802459	Pentafluorobenzene	7.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94	
2	Pentane	72	C5H12	000109-66-0	33	
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28	
4	2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	25	
5	1-Butene	56	C4H8	000106-98-9	9	



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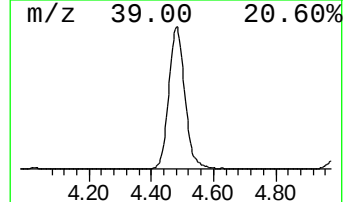
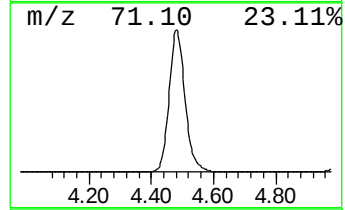
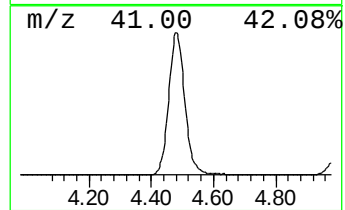
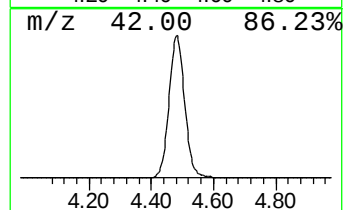
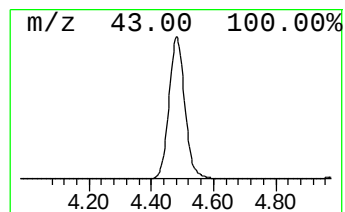
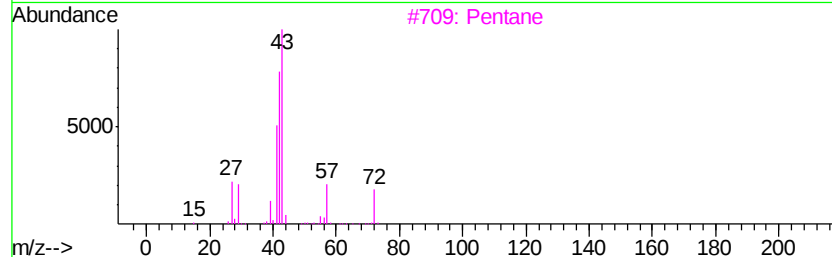
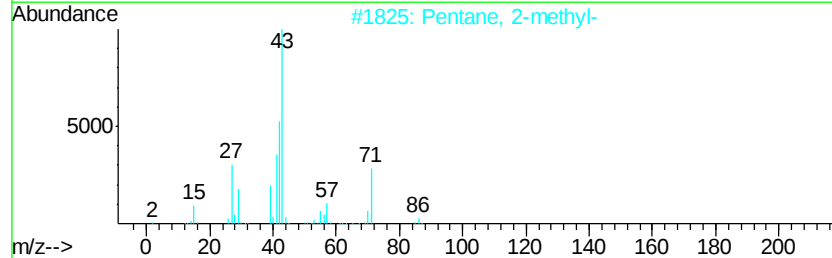
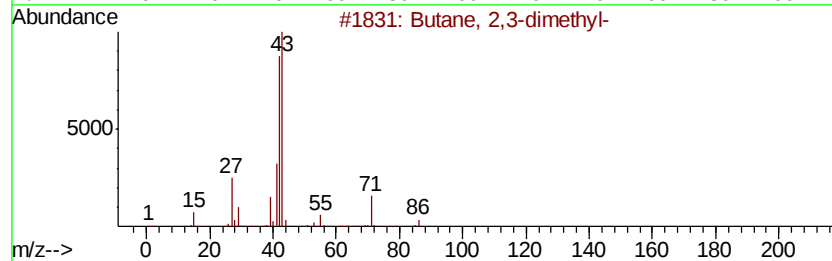
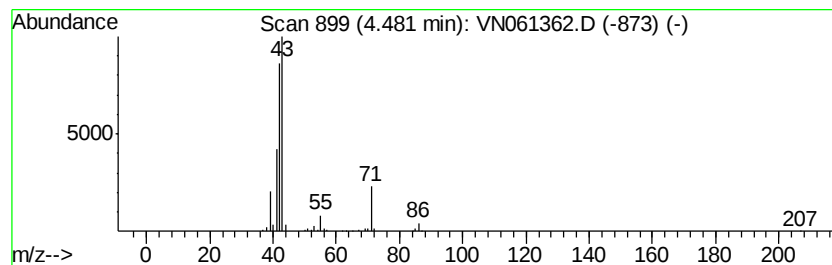
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042720W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	188.71 ug/l	1280480	Pentafluorobenzene	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3		Pentane	72	C5H12	000109-66-0	38
4		Butane, 2-methyl-	72	C5H12	000078-78-4	36
5		Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12



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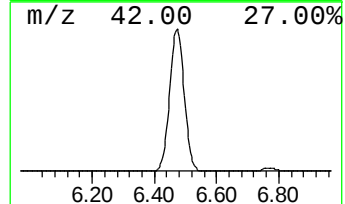
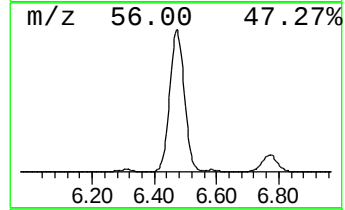
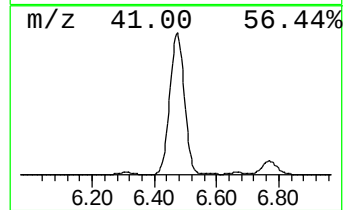
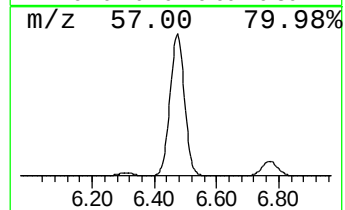
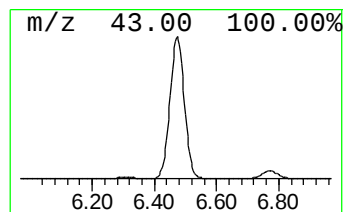
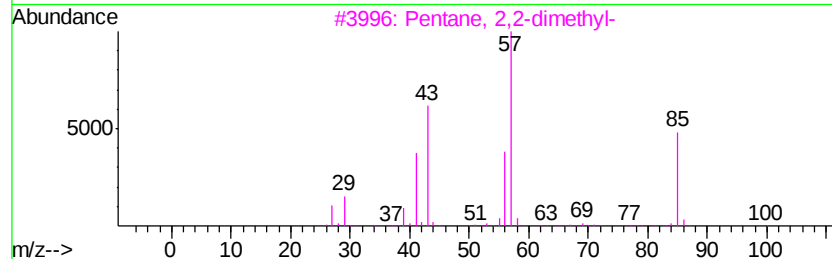
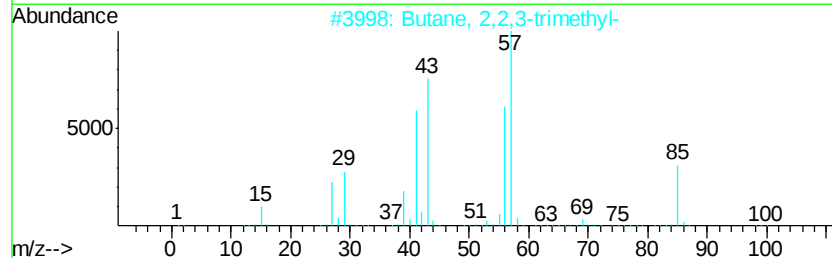
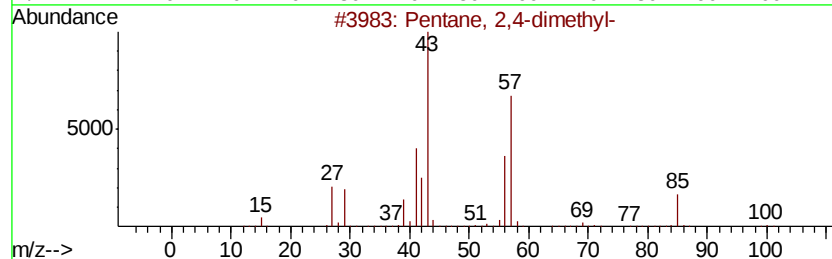
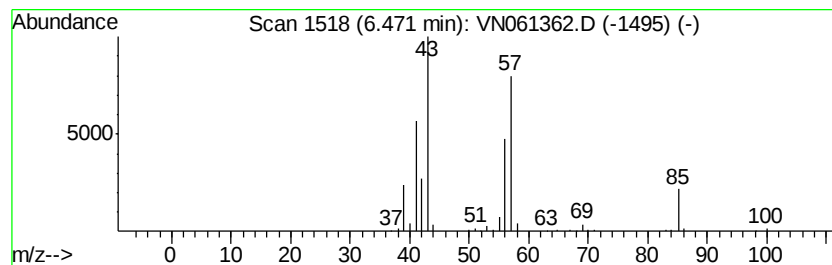
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentane, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	103.57 ug/l	702770	Pentafluorobenzene	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
3		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50
4		Heptane, 3-methyl-	114	C8H18	000589-81-1	50
5		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	50



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Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ST008MW038-200505

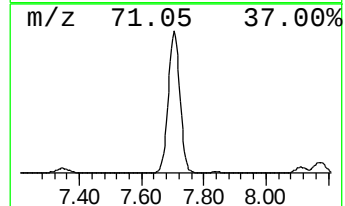
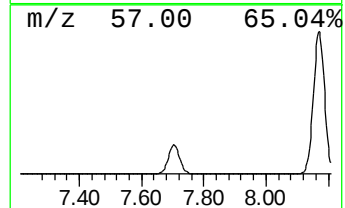
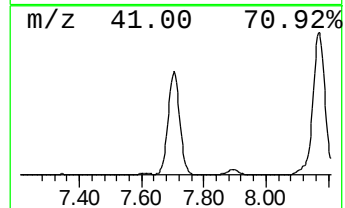
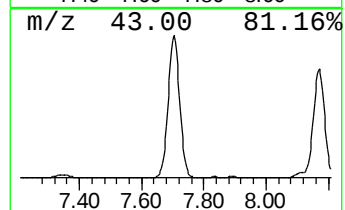
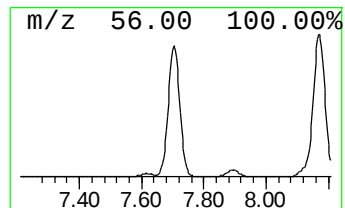
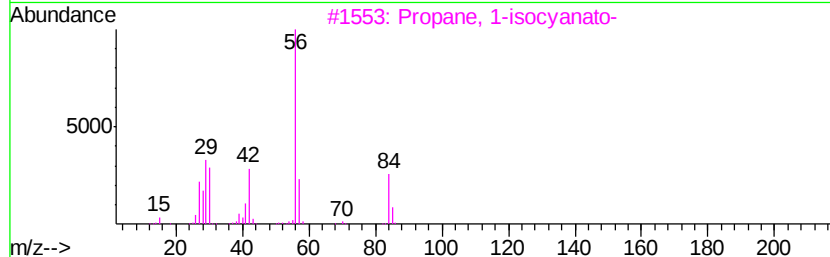
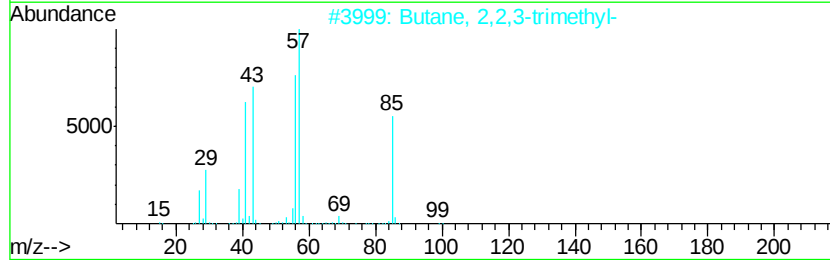
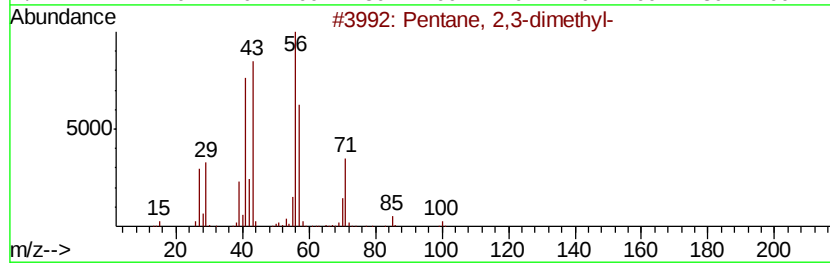
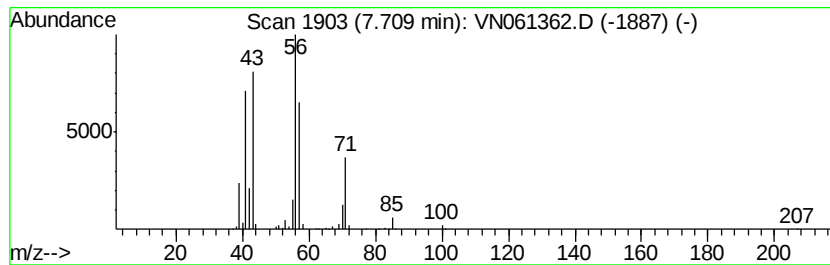
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.71	178.90 ug/l	1213930	Pentafluorobenzene	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	95
2		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	40
3		Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	40
4		Aziridine, 2-methyl-	57	C3H7N	000075-55-8	38
5		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	37



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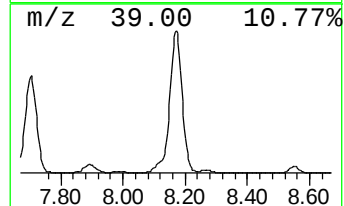
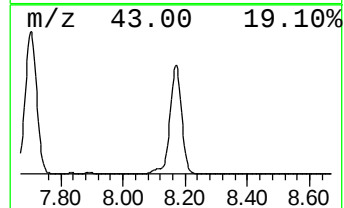
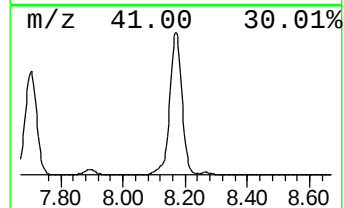
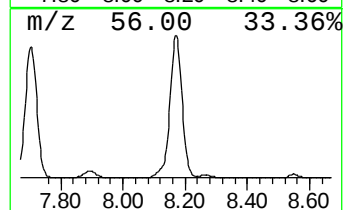
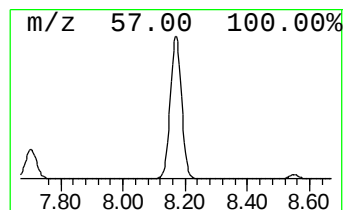
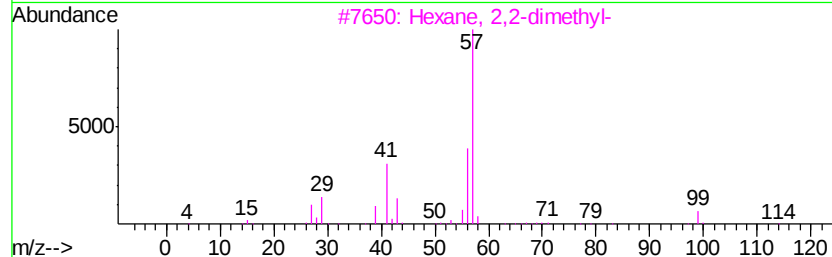
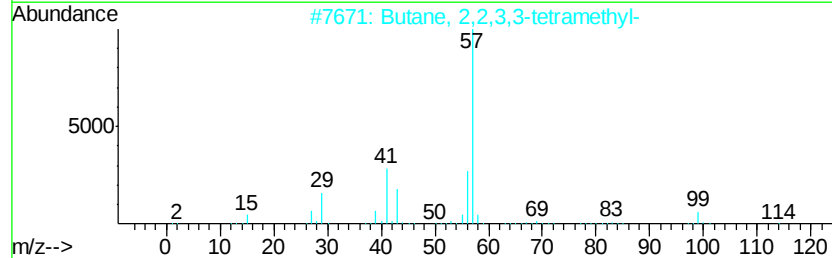
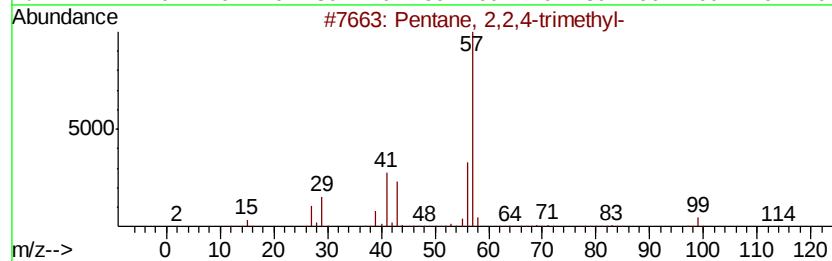
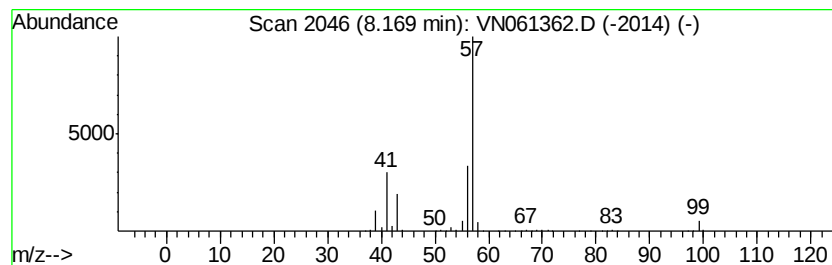
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,2,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	215.36 ug/l	1998670	1,4-Difluorobenzene	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
3		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
4		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	78
5		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64



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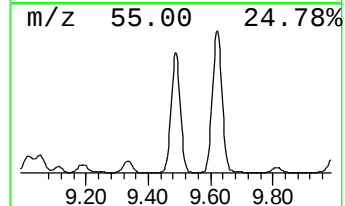
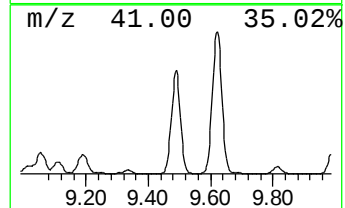
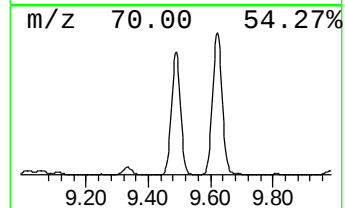
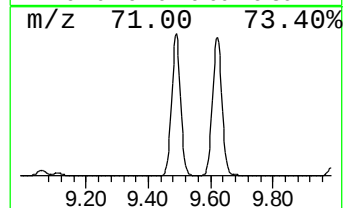
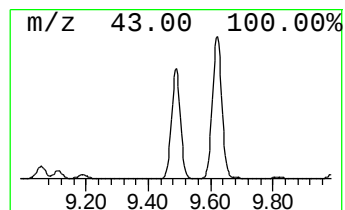
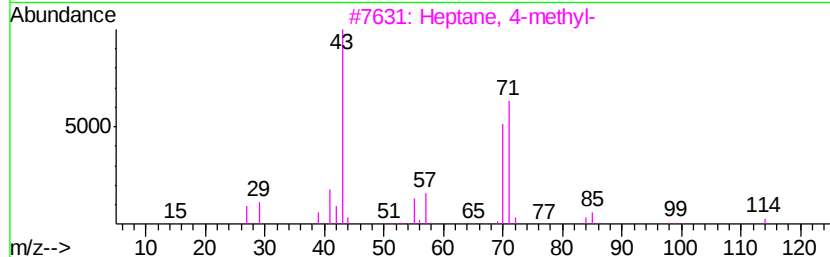
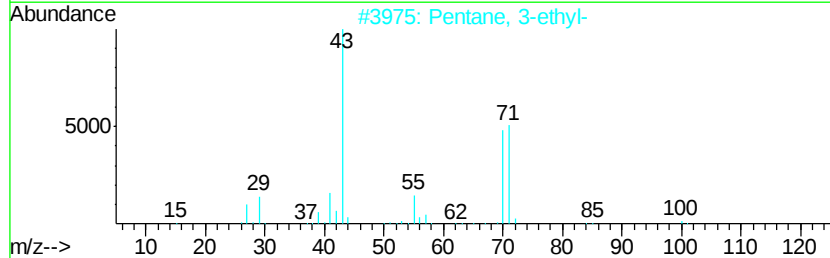
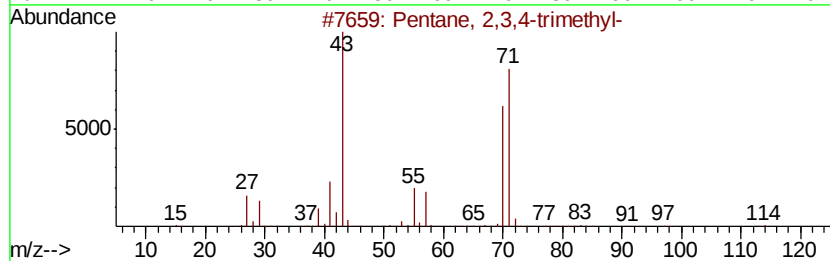
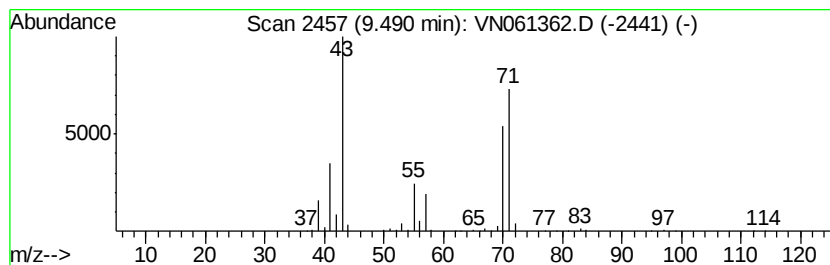
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.49	94.46 ug/l	876643	1,4-Difluorobenzene	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2		Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4		2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
5		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN050820\
Data File : VN061362.D
Acq On : 8 May 2020 15:22
Operator : JC/MD
Sample : L2544-13
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ST008MW038-200505

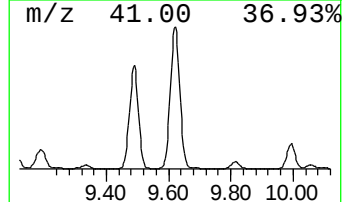
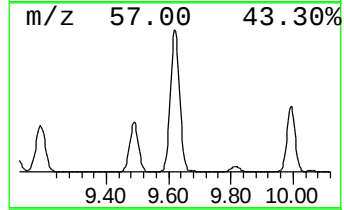
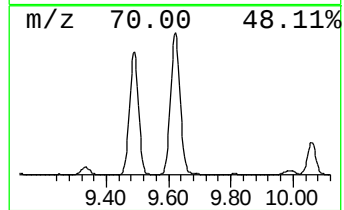
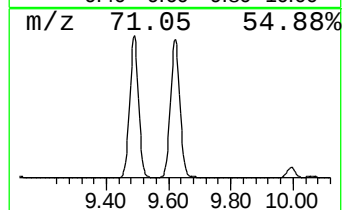
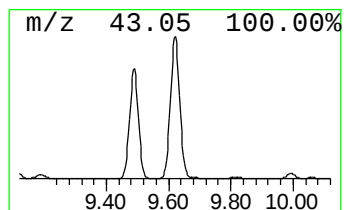
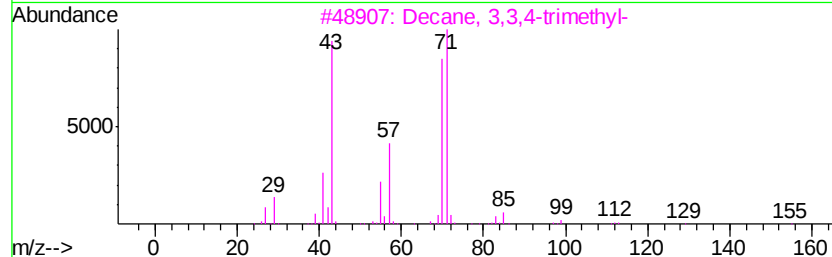
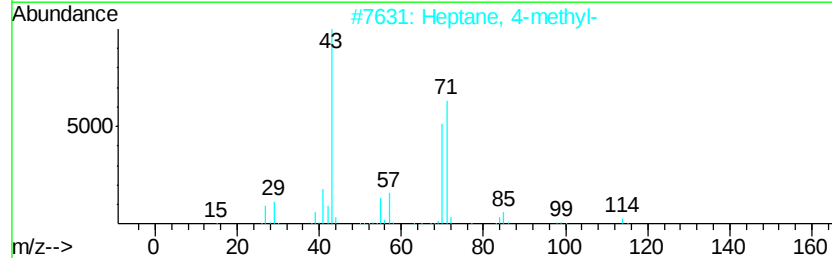
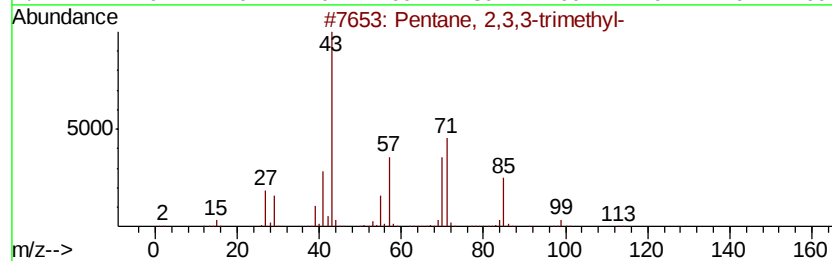
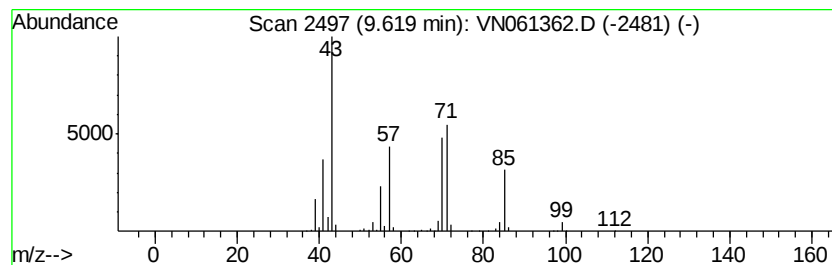
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Quant Title : SW846 8260

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

Peak Number 8 Pentane, 2,3,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	143.93 ug/l	1335690	1,4-Difluorobenzene	8.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
4		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	59



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN050820\
Data File : VN061362.D
Acq On : 8 May 2020 15:22
Operator : JC/MD
Sample : L2544-13
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 14 Sample Multiplier: 1

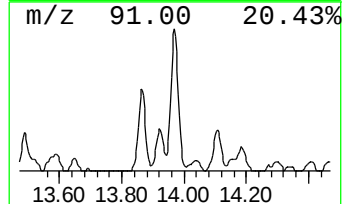
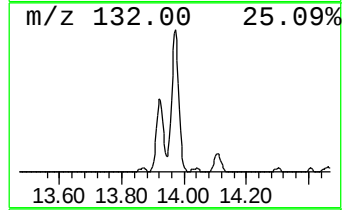
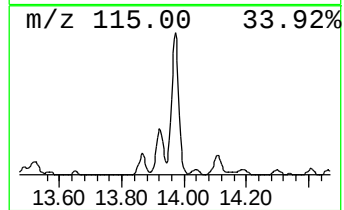
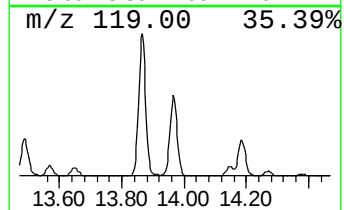
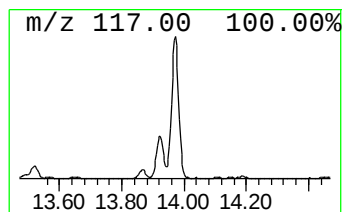
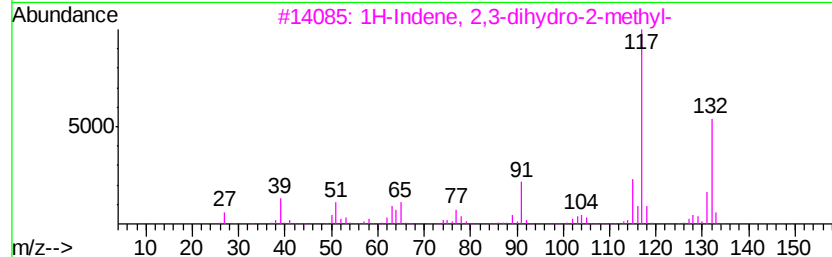
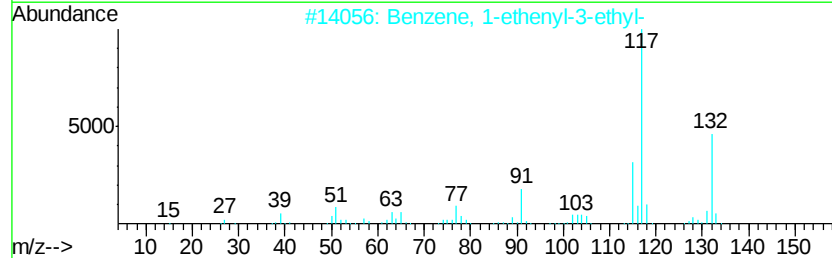
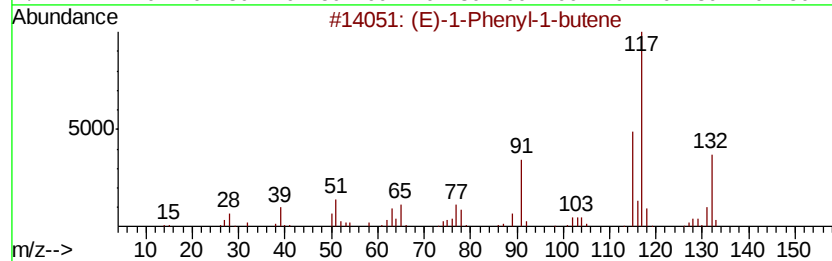
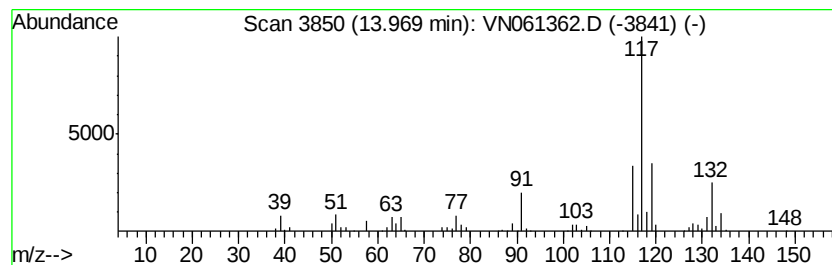
Instrument :
MSVOA_N
ClientSampleId :
ST008MW038-200505

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042720W.M
Quant Title : SW846 8260

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

Peak Number 9 (E)-1-Phenyl-1-butene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.97	20.51 ug/l	227157	1,4-Dichlorobenzene-d4	13.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	90
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	76
3	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	76
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	74
5	Benzene, (1-methyl-1-propenyl)-, ...	132	C10H12	000768-00-3	74



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050820\
Data File : VN061362.D
Acq On : 8 May 2020 15:22
Operator : JC/MD
Sample : L2544-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ST008MW038-200505

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042720W.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
Butane, 2-methyl-	2.77	118.3	ug/l	802459	1	7.63	339278	50.0
Butane, 2,3-dimet...	4.48	188.7	ug/l	1280480	1	7.63	339278	50.0
Pentane, 2,4-dime...	6.47	103.6	ug/l	702770	1	7.63	339278	50.0
Pentane, 2,3-dime...	7.71	178.9	ug/l	1213930	1	7.63	339278	50.0
Pentane, 2,2,4-tr...	8.17	215.4	ug/l	1998670	2	8.55	464021	50.0
Pentane, 2,3,4-tr...	9.49	94.5	ug/l	876643	2	8.55	464021	50.0
Pentane, 2,3,3-tr...	9.62	143.9	ug/l	1335690	2	8.55	464021	50.0
(E)-1-Phenyl-1-bu...	13.97	20.5	ug/l	227157	4	13.32	553789	50.0