LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050820\
Data File : VN061361.D
Acq On : 8 May 2020 14:59
Operator : JC/MD
Sample : L2544-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SS037MW266-200505

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

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	70	rBV	3965199	13214416	100.00%	65.120%
2	6.580	1532	1552	1577	rVB2	114796	356983	2.70%	1.759%
3	7.548	1835	1853	1861	rBV2	69343	167537	1.27%	0.826%
4	7.619	1862	1875	1892	rVV2	286092	765366	5.79%	3.772%
5	7.988	1975	1990	2012	rVV2	98950	236604	1.79%	1.166%
6	8.181	2040	2050	2065	rVV4	71152	225448	1.71%	1.111%
7	8.551	2148	2165	2194	rBV	215233	440183	3.33%	2.169%
8	9.046	2296	2319	2333	rBV	151612	365839	2.77%	1.803%
9	9.622	2484	2498	2513	rBV	71775	150604	1.14%	0.742%
10	10.059	2621	2634	2660	rBV	354420	663536	5.02%	3.270%
11	11.403	3031	3052	3067	rBV2	516666	1397284	10.57%	6.886%
12	12.377	3343	3355	3367	rBV	258707	427571	3.24%	2.107%
13	12.564	3398	3413	3424	rVB	71476	148931	1.13%	0.734%
14	13.319	3636	3648	3663	rVB	323323	558302	4.22%	2.751%
15	13.419	3663	3679	3691	rBV	97634	164751	1.25%	0.812%
16	13.866	3806	3818	3826	rBV	104134	163501	1.24%	0.806%
17	13.969	3841	3850	3860	rVV3	265831	456523	3.45%	2.250%
18	14.184	3901	3917	3935	rVB4	74177	182598	1.38%	0.900%
19	14.567	4023	4036	4049	rBV3	103682	206460	1.56%	1.017%

Sum of corrected areas: 20292437

LSC Report - Integrated Chromatogram

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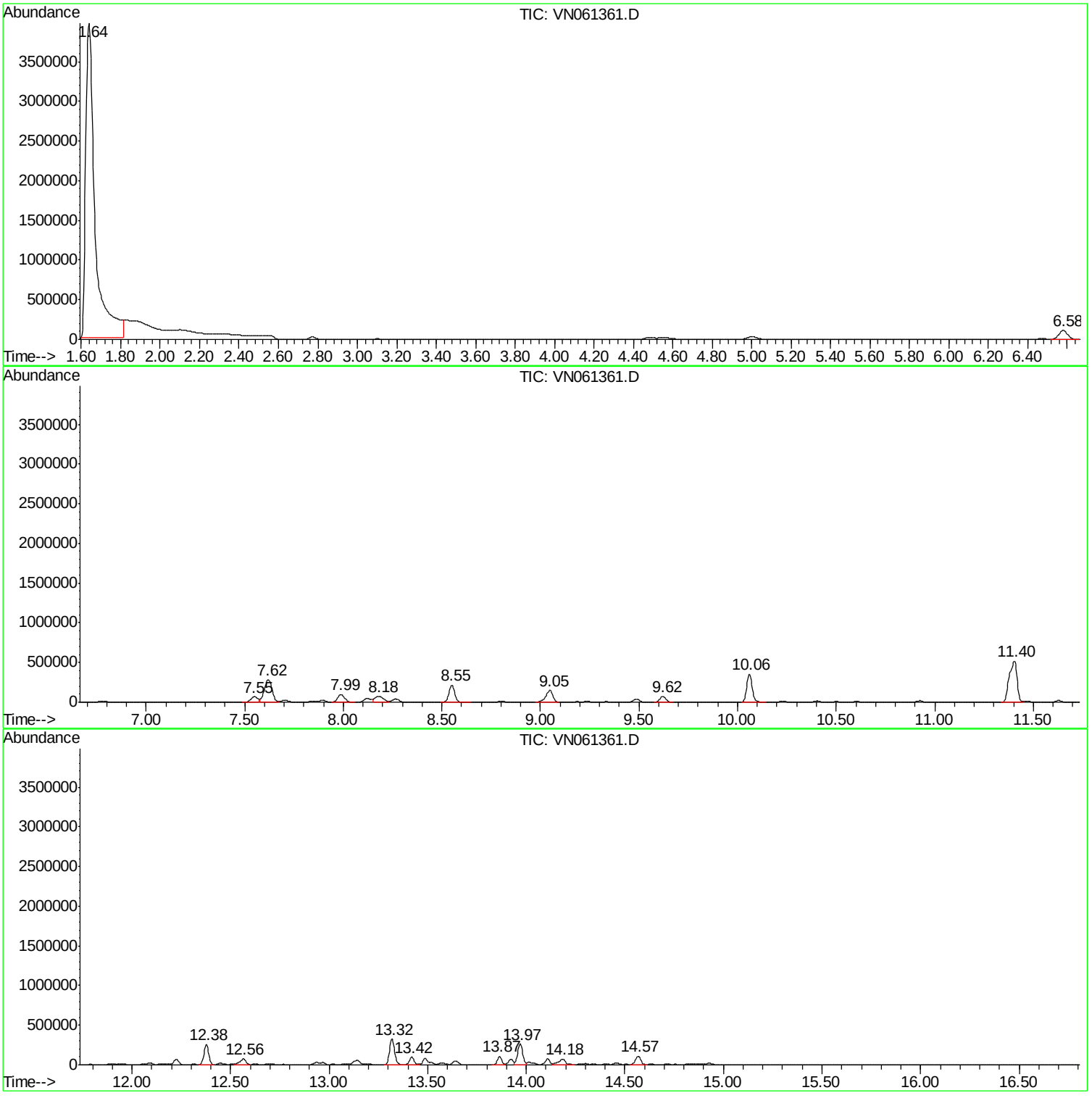
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SS037MW266-200505

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



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Data File : VN061361.D
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Operator : JC/MD
Sample : L2544-12
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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
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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

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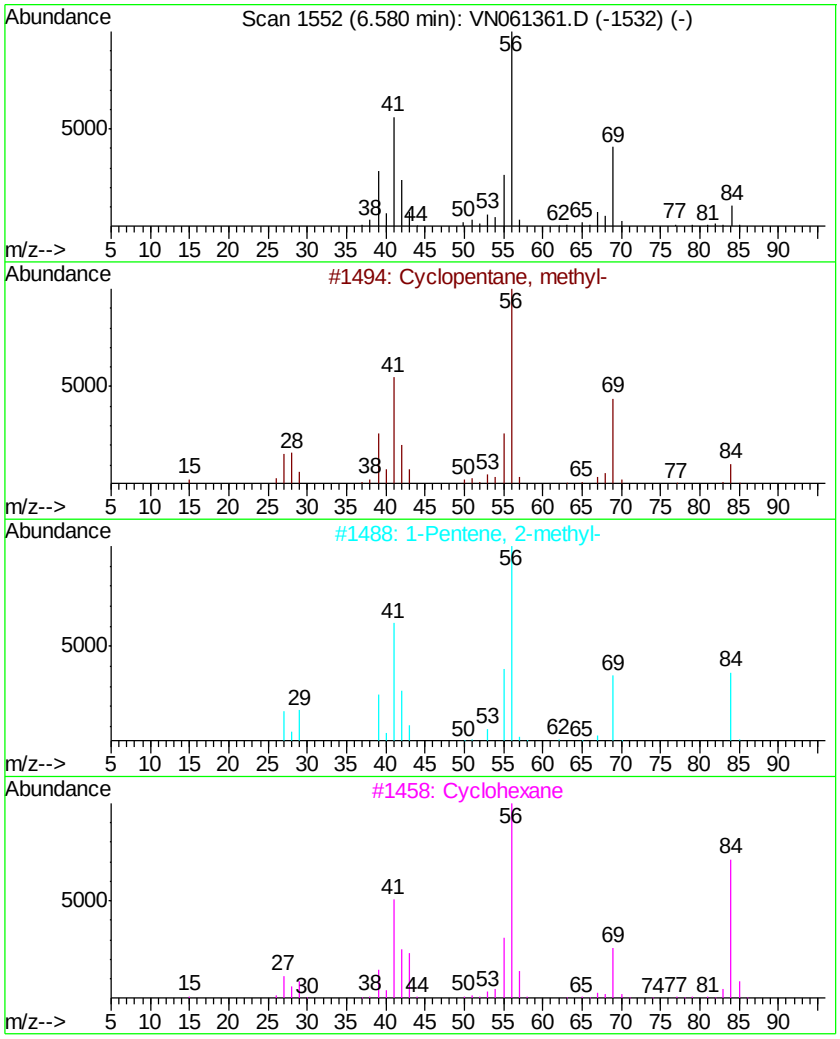
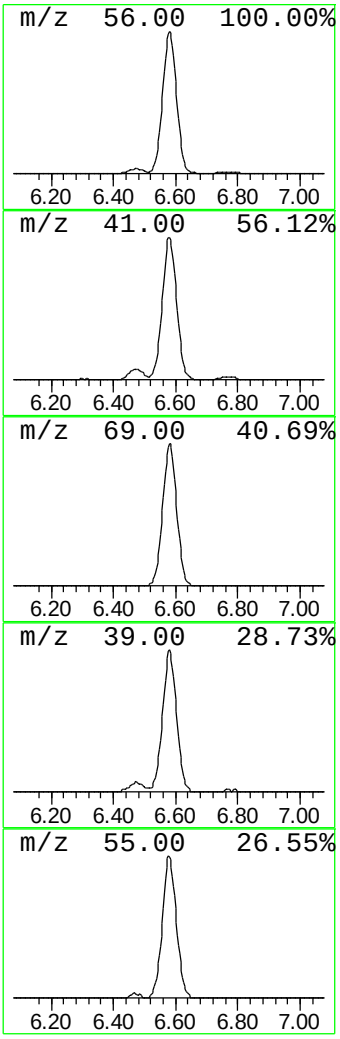
Peak Number 2 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	23.32 ug/l	356983	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	80
3	Cyclohexane	84	C6H12	000110-82-7	78
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	59





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Instrument : MSVOA_N
ClientSampleId : SS037MW266-200505

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

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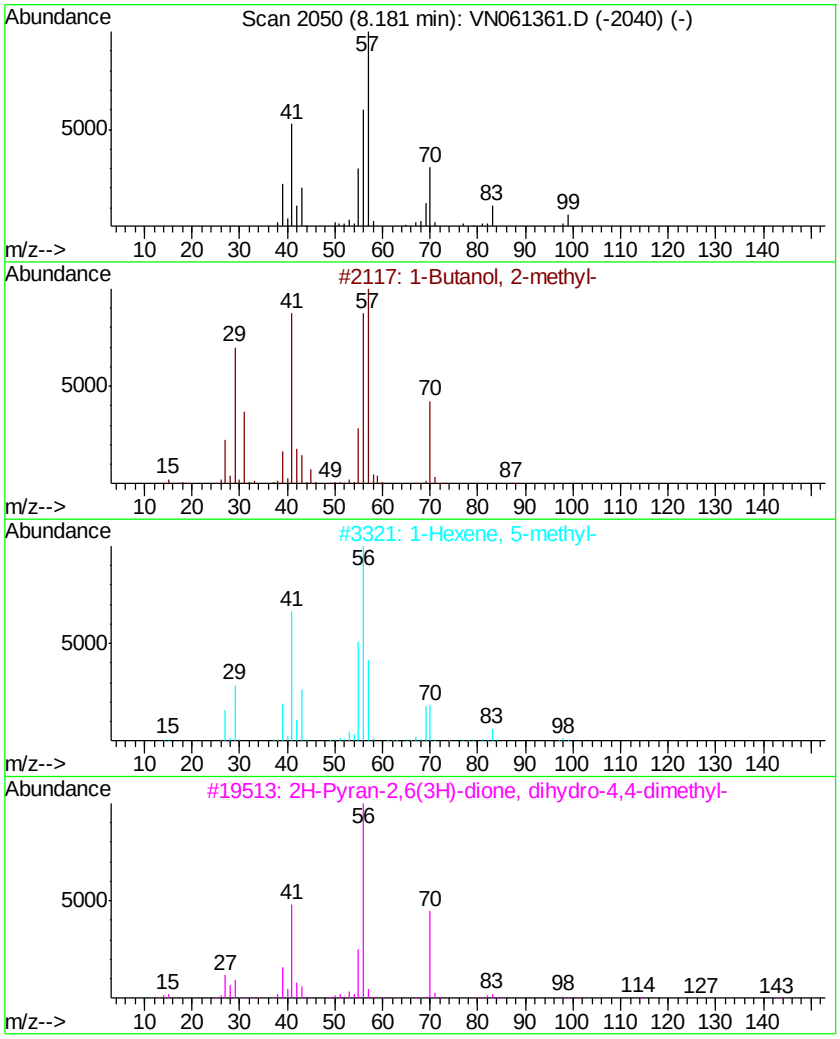
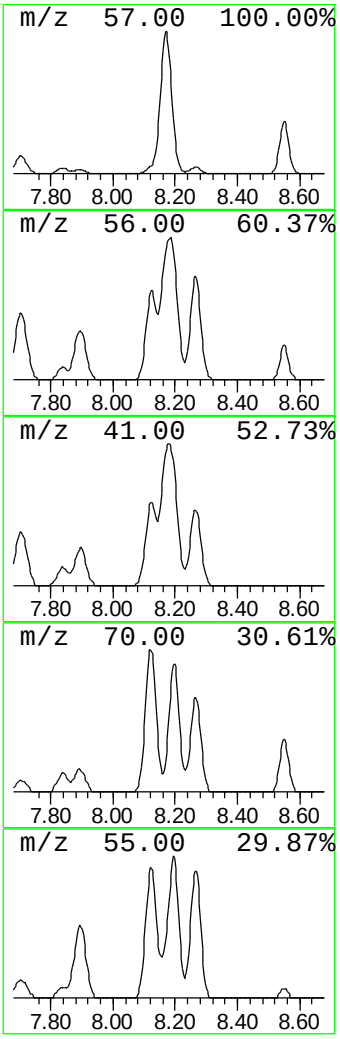
Peak Number 3 1-Butanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	25.61 ug/l	225448	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	59
2	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	53
3	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	50
4	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	45
5	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	40





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Operator : JC/MD
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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SS037MW266-200505

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

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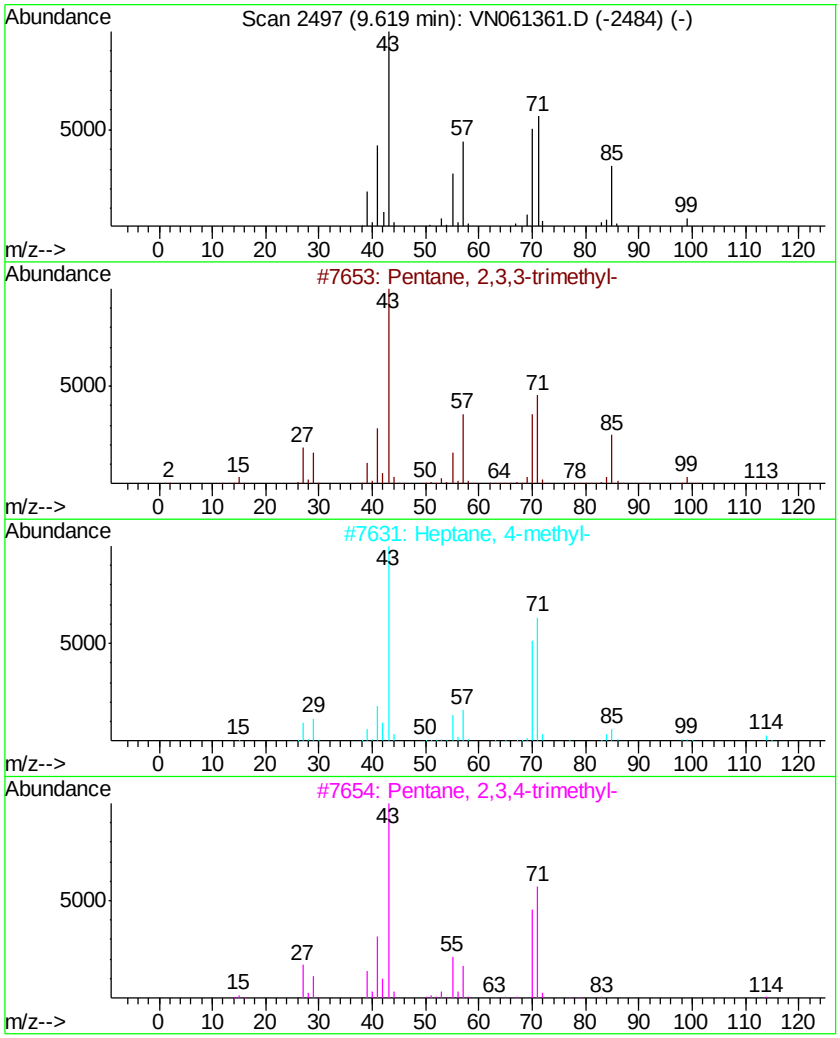
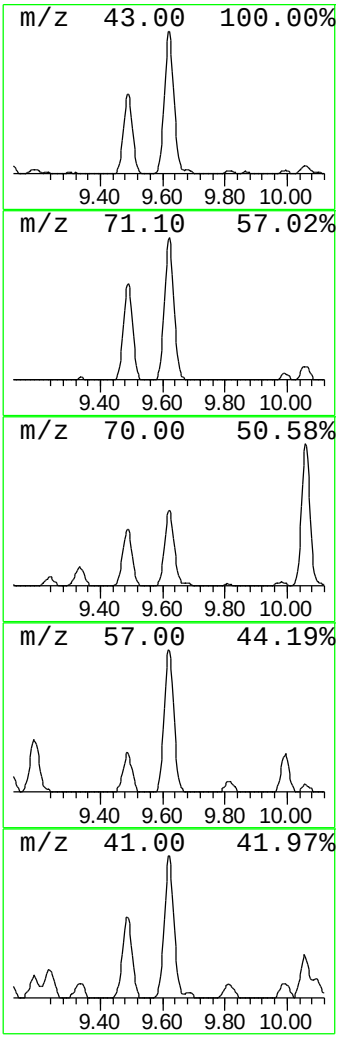
Peak Number 4 Pentane, 2,3,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	17.11 ug/l	150604	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53





Library Search Compound Report

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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SS037MW266-200505

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

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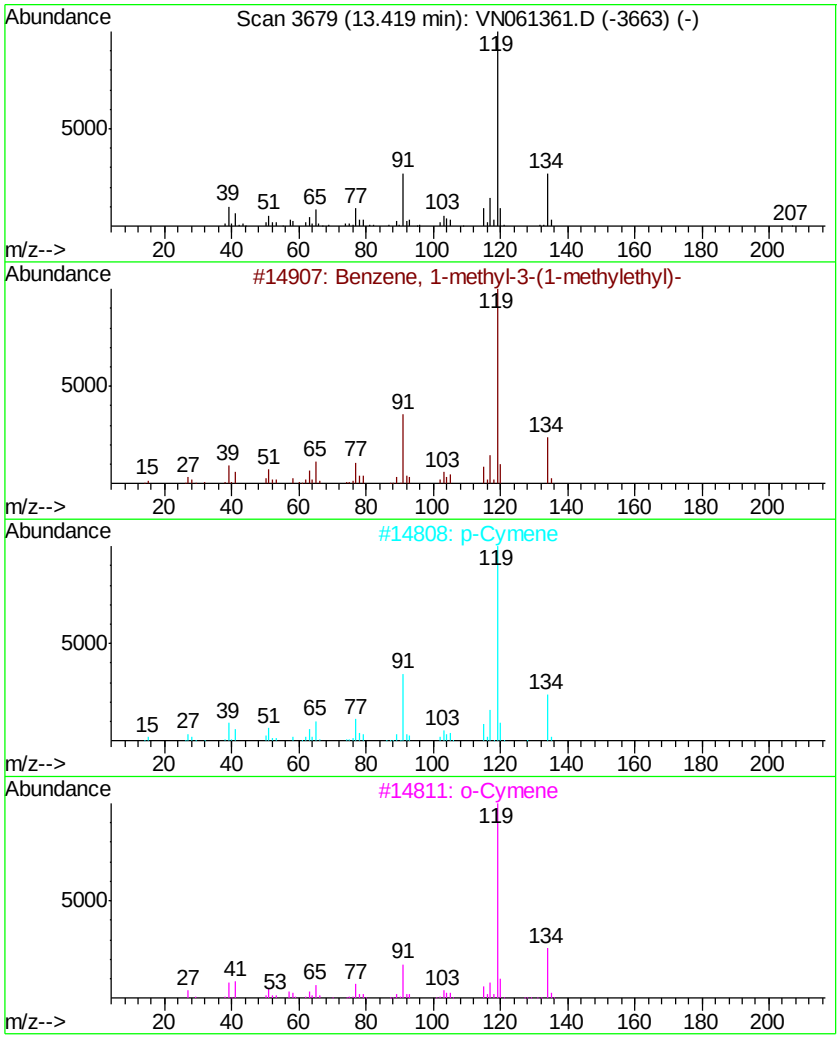
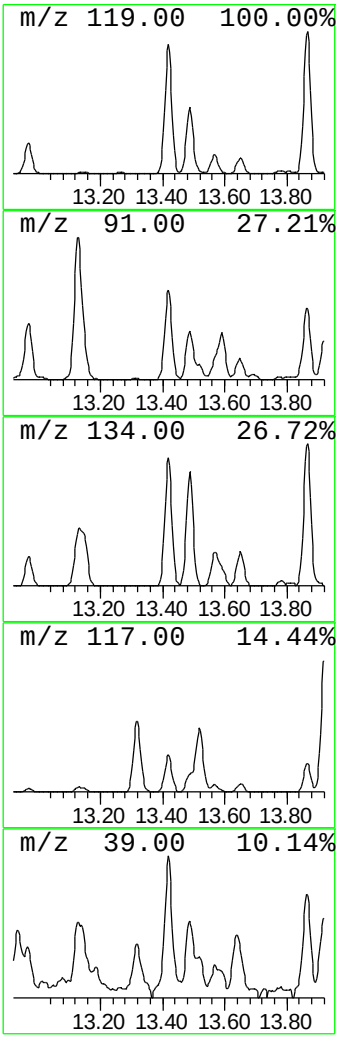
Peak Number 5 Benzene, 1-methyl-3-(1-meth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	14.75 ug/l	164751	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
2	p-Cymene	134	C10H14	000099-87-6	95
3	o-Cymene	134	C10H14	000527-84-4	94
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91





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Sample : L2544-12
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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : SS037MW266-200505

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

TIC Library : C:\DATABASE\NIST11.L
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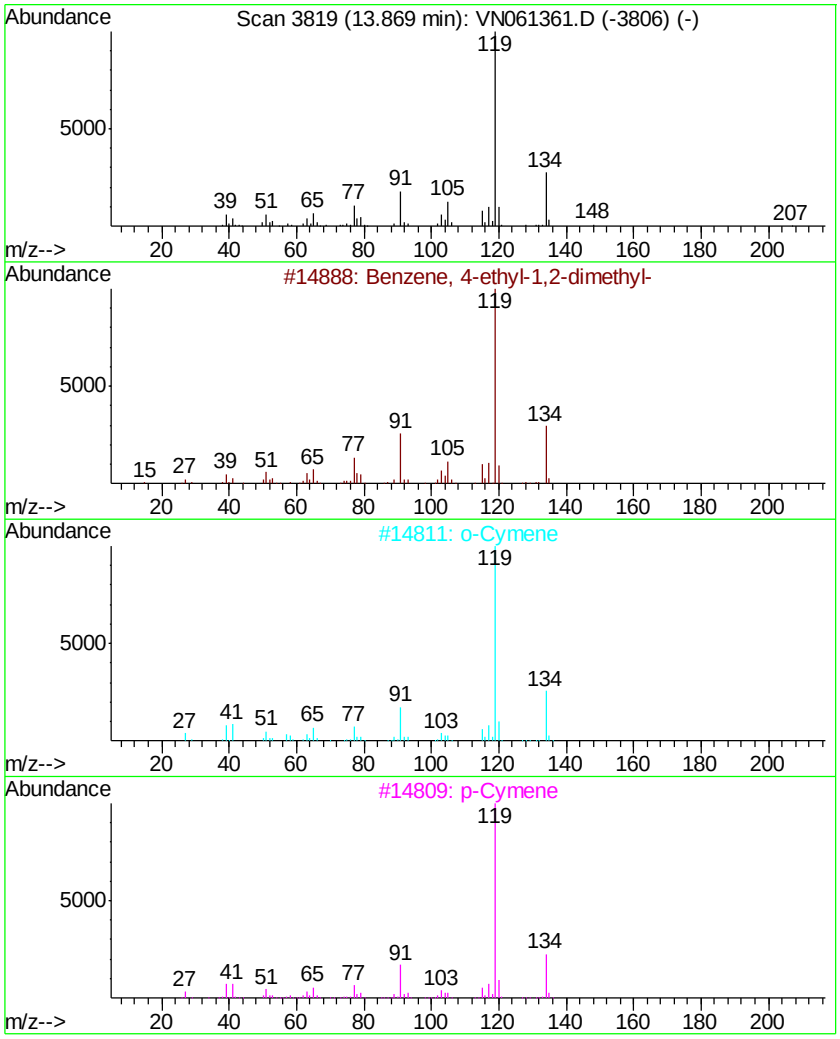
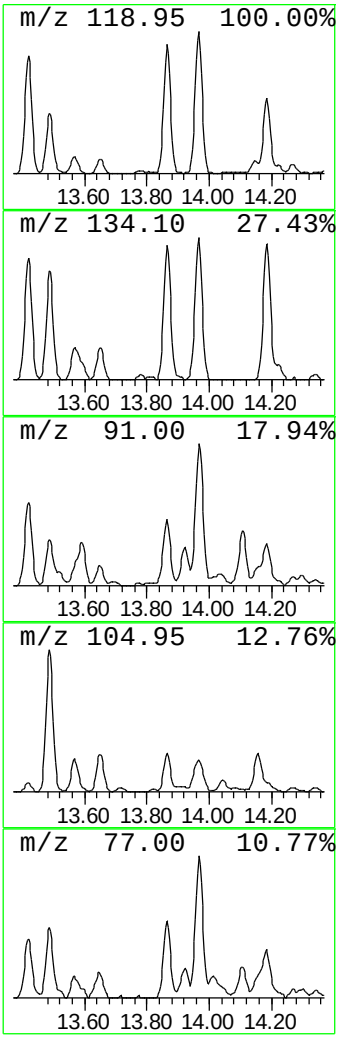
****

Peak Number 6 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	14.64 ug/l	163501	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2	o-Cymene	134	C10H14	000527-84-4	95
3	p-Cymene	134	C10H14	000099-87-6	95
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94





Library Search Compound Report

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Instrument : MSVOA_N
ClientSampleId : SS037MW266-200505

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

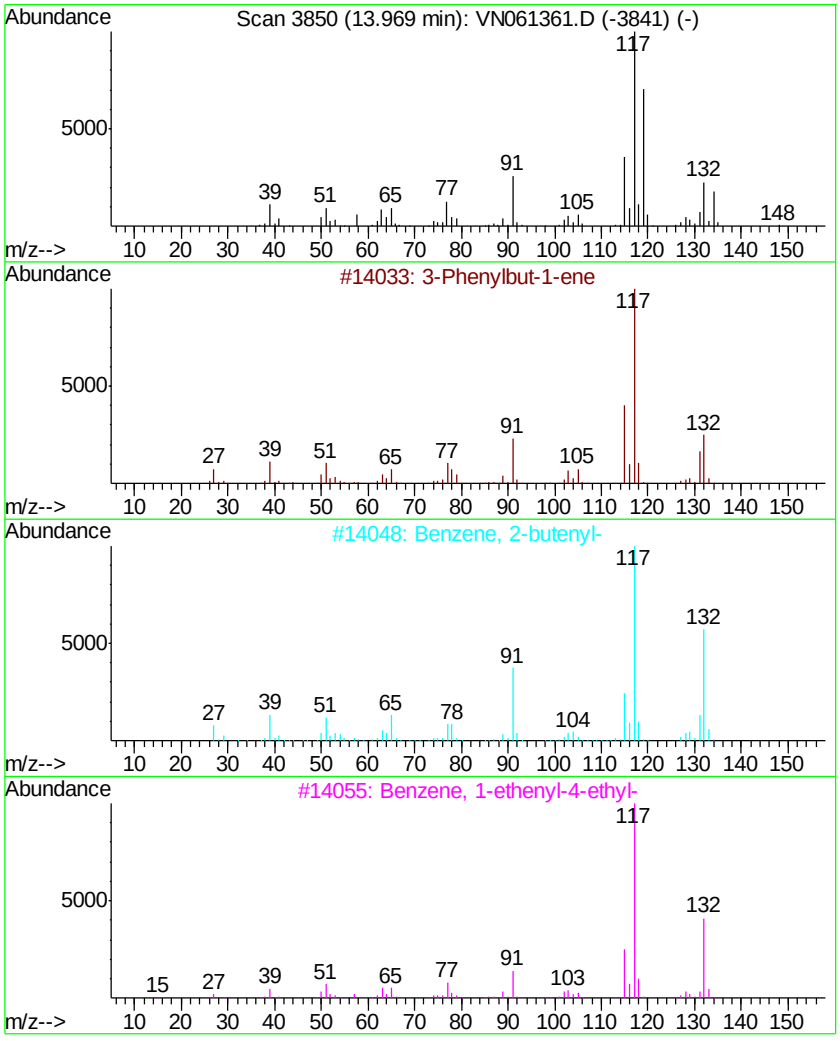
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

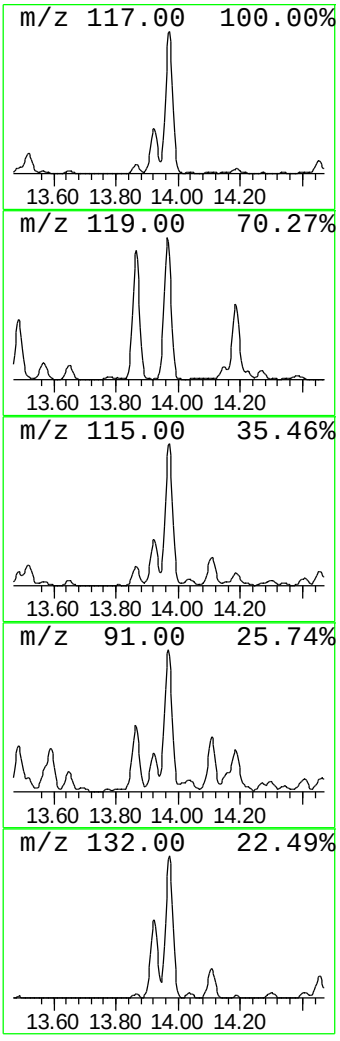
****

Peak Number 7 3-Phenylbut-1-ene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	40.89 ug/l	456523	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylbut-1-ene	132	C10H12	000934-10-1	86
2	Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	70
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	70





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Quant Title : SW846 8260

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

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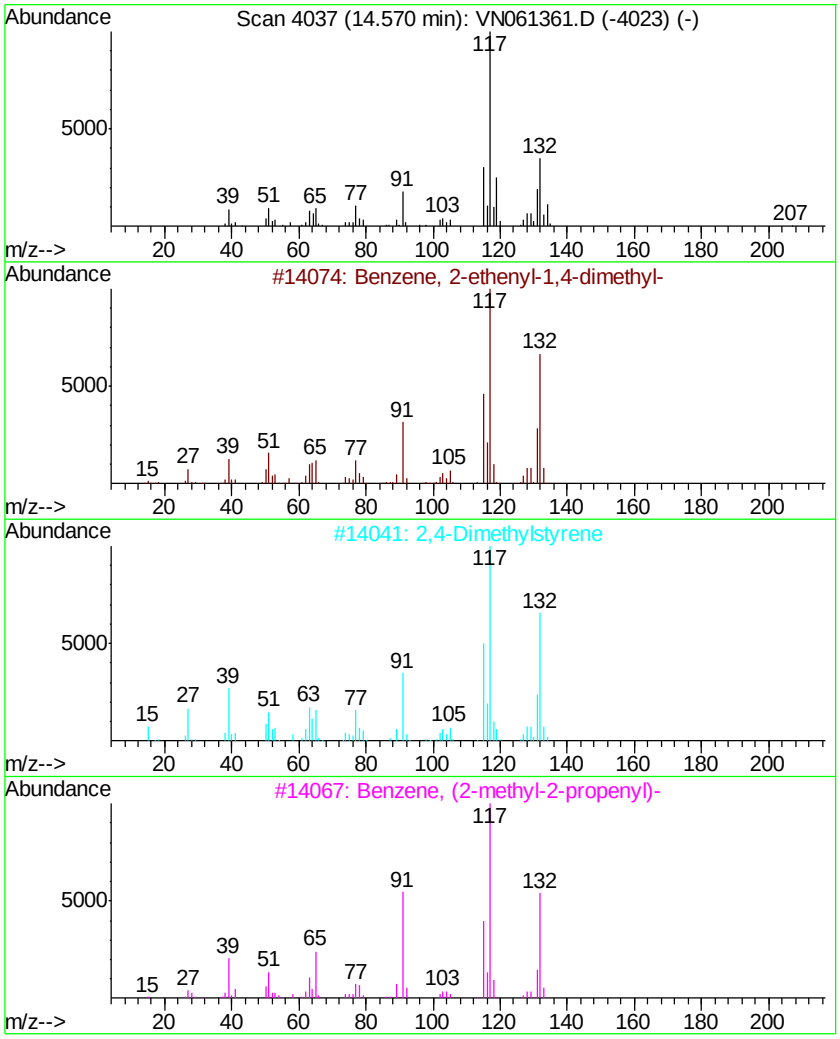
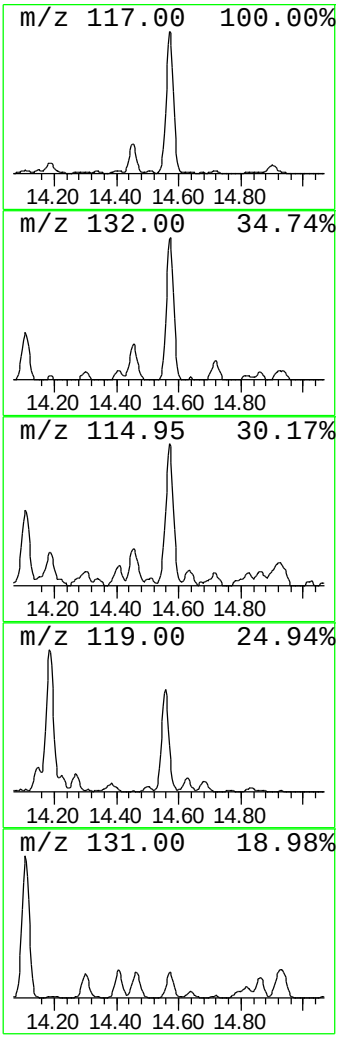
Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	18.49 ug/l	206460	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	2,4-Dimethylstyrene	132	C10H12	002234-20-0	95
3	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	76
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	70





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentane, met...	6.58	23.3	ug/l	356983	1	7.63	765366	50.0
1-Butanol, 2-methyl-	8.18	25.6	ug/l	225448	2	8.55	440183	50.0
Pentane, 2,3,3-tr...	9.62	17.1	ug/l	150604	2	8.55	440183	50.0
Benzene, 1-methyl...	13.42	14.8	ug/l	164751	4	13.32	558302	50.0
Benzene, 4-ethyl-...	13.87	14.6	ug/l	163501	4	13.32	558302	50.0
3-Phenylbut-1-ene	13.97	40.9	ug/l	456523	4	13.32	558302	50.0
Benzene, 2-etheny...	14.57	18.5	ug/l	206460	4	13.32	558302	50.0