LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN061920\
Data File : VN061962.D
Acq On : 19 Jun 2020 19:11
Operator : JC/MD
Sample : L3033-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : LF001MW001-200615

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\82N061620W.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	2.140	103	114	115	rBV	17595562	26162594	45.55%	9.900%
2	3.770	605	621	634	rBV	1199732	3035789	5.29%	1.149%
3	3.850	634	646	682	rVV	1225028	3400759	5.92%	1.287%
4	6.779	1528	1557	1636	rBV2	17959000	57440296	100.00%	21.736%
5	7.622	1807	1819	1839	rVB2	243998	603634	1.05%	0.228%
6	7.998	1915	1936	1955	rBV3	382273	992547	1.73%	0.376%
7	8.551	2097	2108	2128	rVB	340157	723727	1.26%	0.274%
8	9.863	2495	2516	2530	rBV	292004	643313	1.12%	0.243%
9	9.963	2530	2547	2567	rVV	22354520	45711047	79.58%	17.298%
10	10.066	2567	2579	2586	rVV	648750	1276332	2.22%	0.483%
11	10.130	2586	2599	2647	rVB	25268259	50551323	88.01%	19.129%
12	10.326	2647	2660	2686	rBV	540146	948482	1.65%	0.359%
13	11.406	2974	2996	3008	rBV2	4391114	8417910	14.66%	3.185%
14	11.483	3008	3020	3033	rVV	3481702	5720170	9.96%	2.165%
15	11.593	3040	3054	3085	rVB	6691236	12948402	22.54%	4.900%
16	11.921	3138	3156	3172	rBV	4535894	7456175	12.98%	2.821%
17	12.377	3285	3298	3311	rBV	450918	753991	1.31%	0.285%
18	12.631	3366	3377	3383	rBV	1074425	1753249	3.05%	0.663%
19	12.709	3393	3401	3420	rVB	1309982	2061665	3.59%	0.780%
20	12.866	3438	3450	3465	rVB	687895	1105814	1.93%	0.418%
21	13.014	3485	3496	3509	rVB	3584636	5671224	9.87%	2.146%
22	13.258	3563	3572	3581	rVV2	602390	957876	1.67%	0.362%
23	13.345	3581	3599	3614	rVB3	2969317	6203486	10.80%	2.347%
24	13.519	3633	3653	3660	rBV	416180	794792	1.38%	0.301%
25	13.628	3674	3687	3704	rVB	9854302	16396986	28.55%	6.205%
26	15.104	4127	4146	4171	rBV	1480026	2531497	4.41%	0.958%

Sum of corrected areas: 264263080

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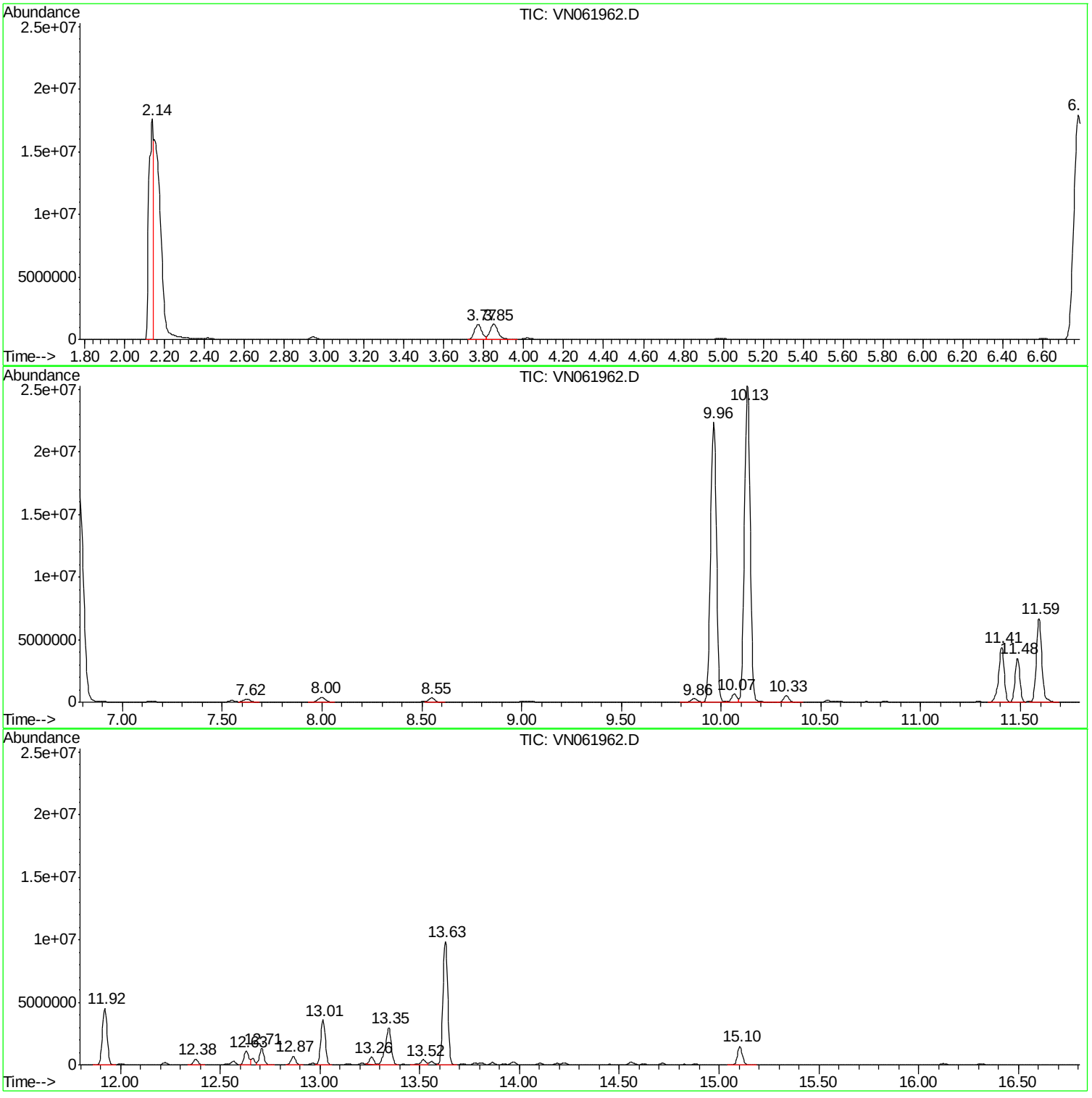
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : LF001MW001-200615

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061620W.M
Quant Title : SW846 8260

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



Library Search Compound Report

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Quant Title : SW846 8260

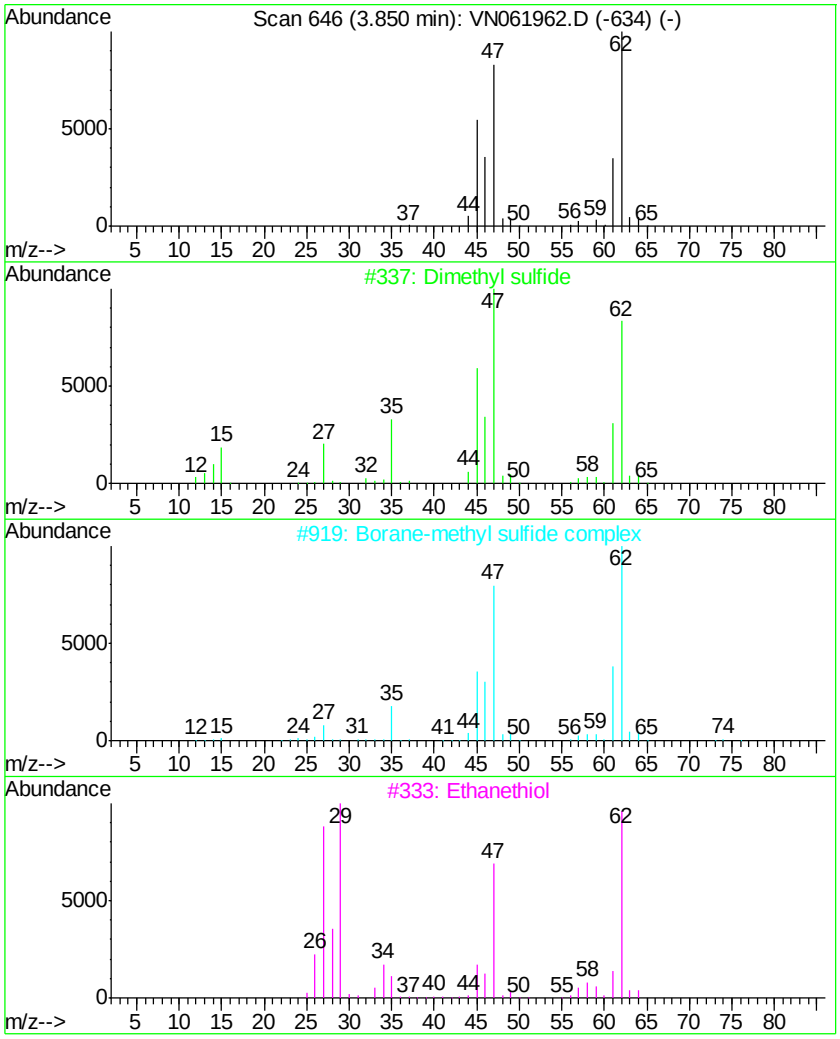
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

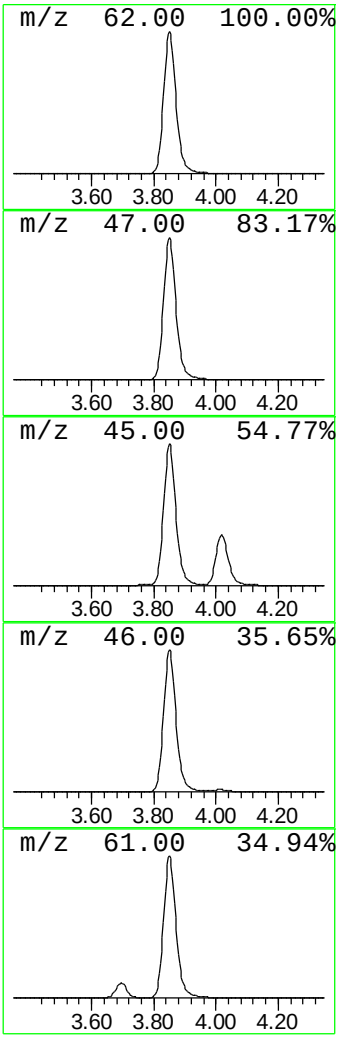
****

Peak Number 1 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.85	281.69 ug/l	3400760	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl sulfide	62	C2H6S	000075-18-3	94
2	Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90
3	Ethanethiol	62	C2H6S	000075-08-1	78
4	Ethene, chloro-	62	C2H3Cl	000075-01-4	9
5	Boric acid	62	BH3O3	010043-35-3	5





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Operator : JC/MD
Sample : L3033-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : LF001MW001-200615

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061620W.M
Quant Title : SW846 8260

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

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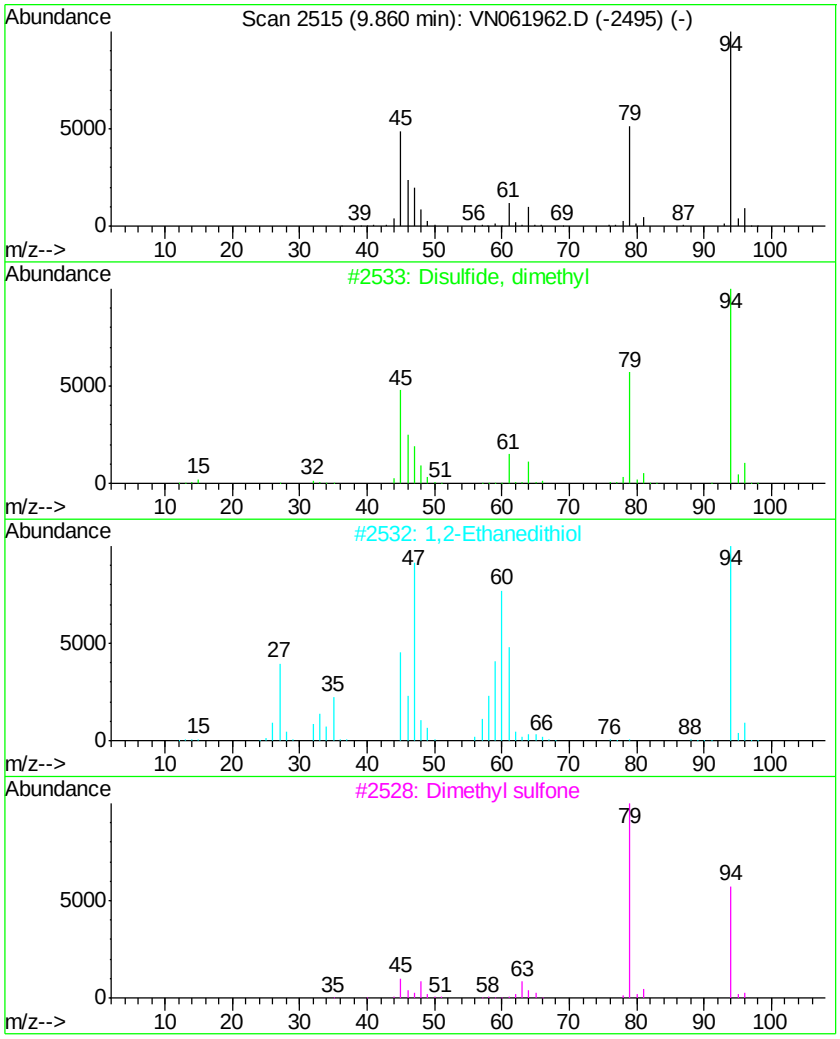
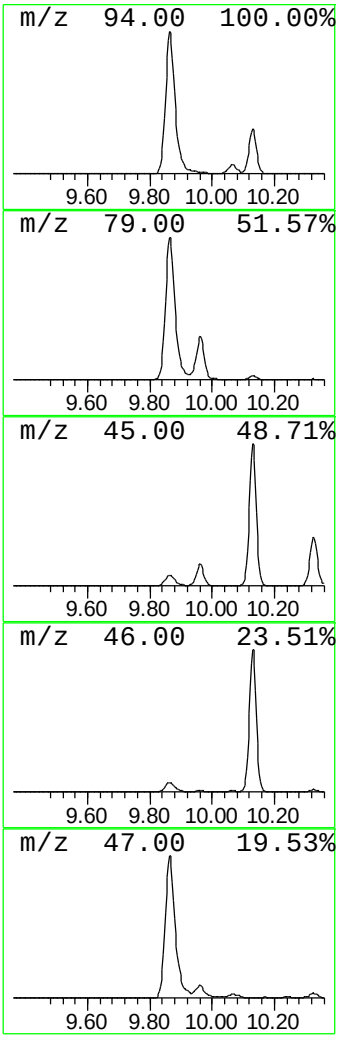
Peak Number 2 Disulfide, dimethyl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	44.44 ug/l	643313	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
2	1,2-Ethanedithiol	94	C2H6S2	000540-63-6	52
3	Dimethyl sulfone	94	C2H6O2S	000067-71-0	50
4	Methanesulfonyl chloride	114	CH3ClO2S	000124-63-0	7
5	(Trifluoromethyl)acetylene	94	C3HF3	000661-54-1	5





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Operator : JC/MD
Sample : L3033-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : LF001MW001-200615

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061620W.M
Quant Title : SW846 8260

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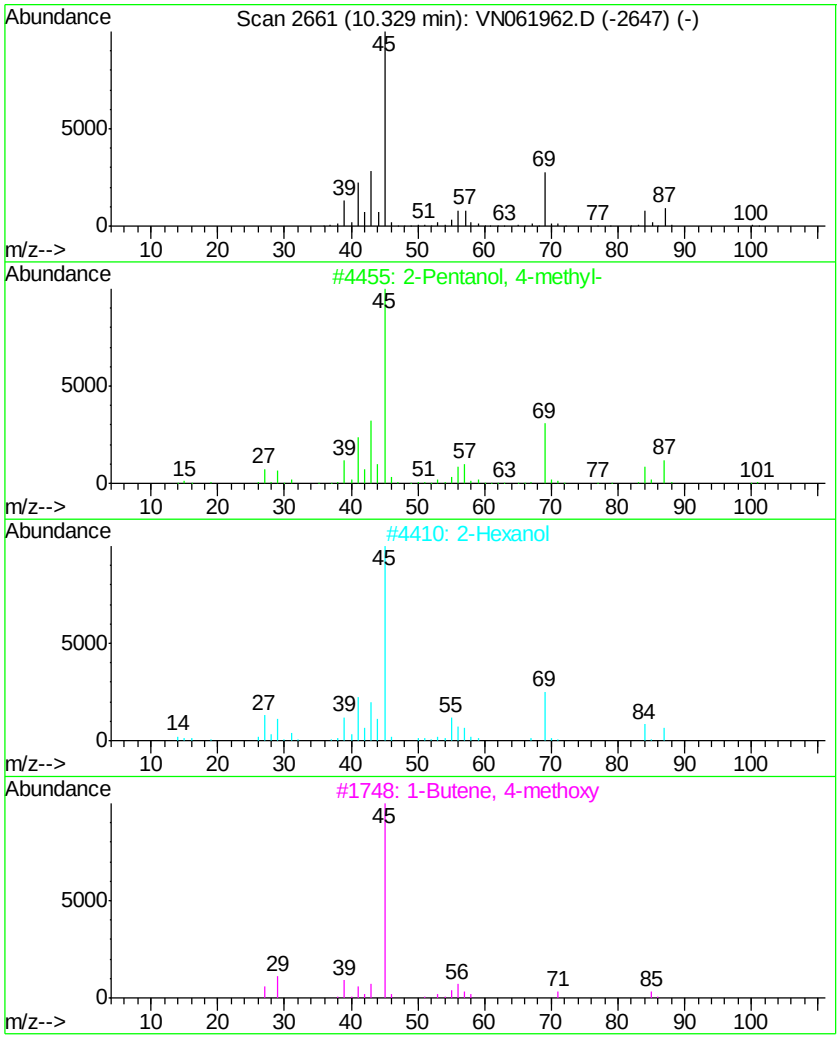
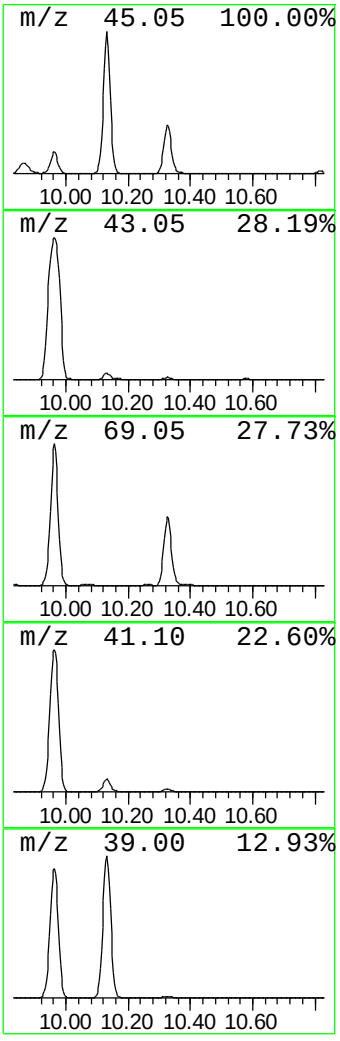
Peak Number 3 2-Pentanol, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	5.63 ug/l	948482	Chlorobenzene-d5	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	90
2	2-Hexanol	102	C6H14O	000626-93-7	78
3	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	59
4	2-Heptanol	116	C7H16O	000543-49-7	59
5	2-Octanol	130	C8H18O	000123-96-6	56





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ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : LF001MW001-200615

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061620W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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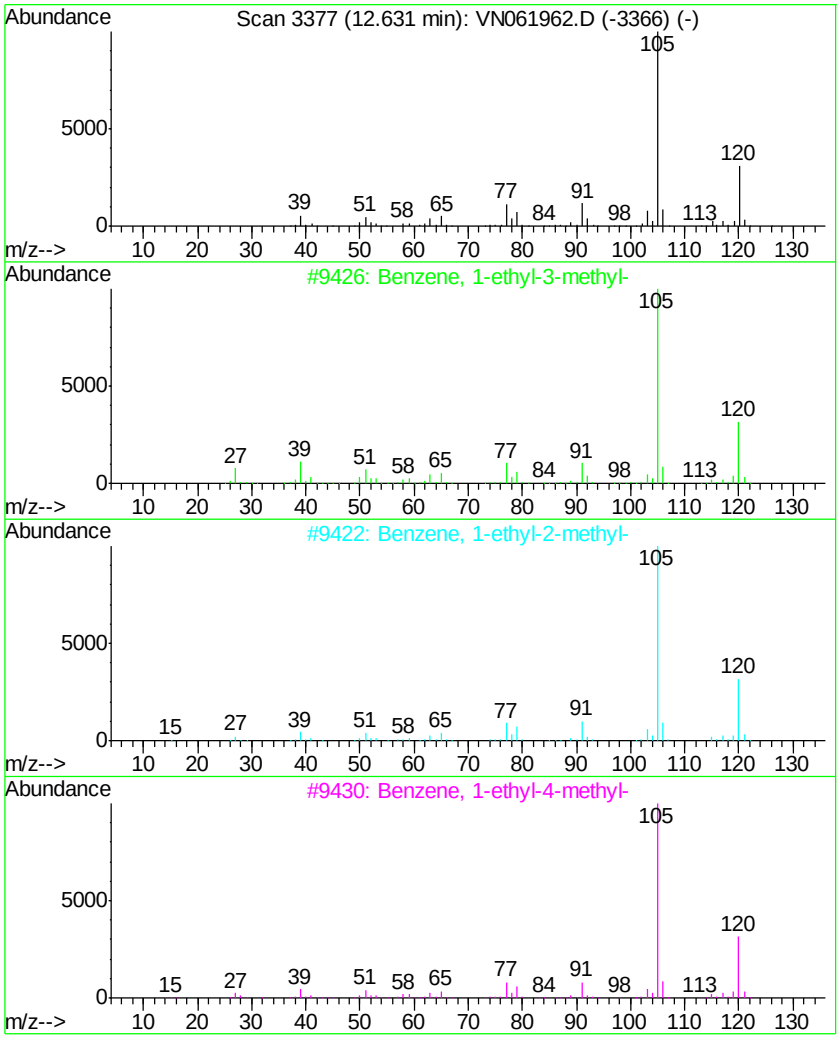
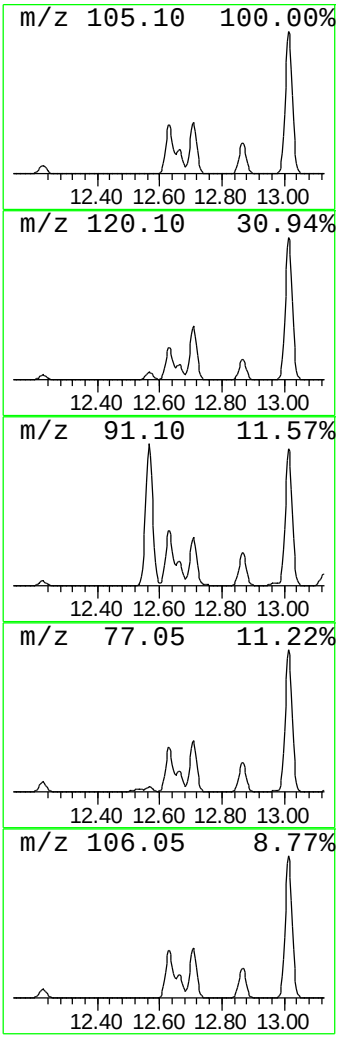
Peak Number 4 Benzene, 1-ethyl-3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	14.13 ug/l	1753250	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Mesitylene	120	C9H12	000108-67-8	91





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ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : LF001MW001-200615

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N061620W.M
Quant Title : SW846 8260

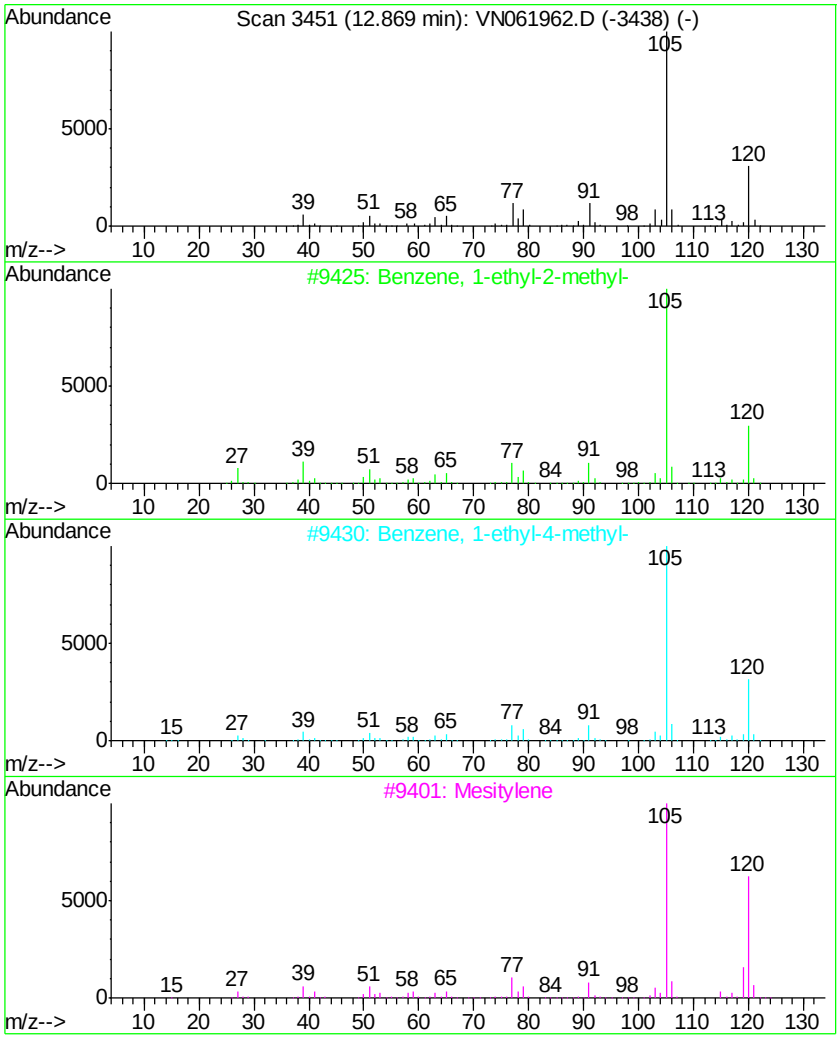
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

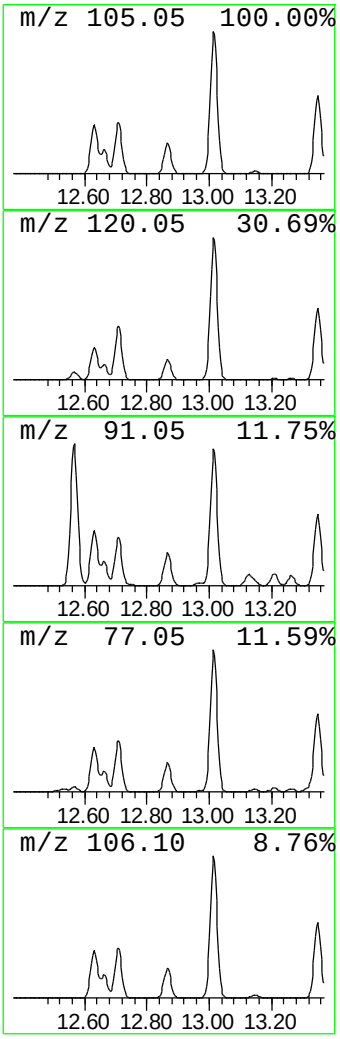
****

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	8.91 ug/l	1105810	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





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Quant Title : SW846 8260

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

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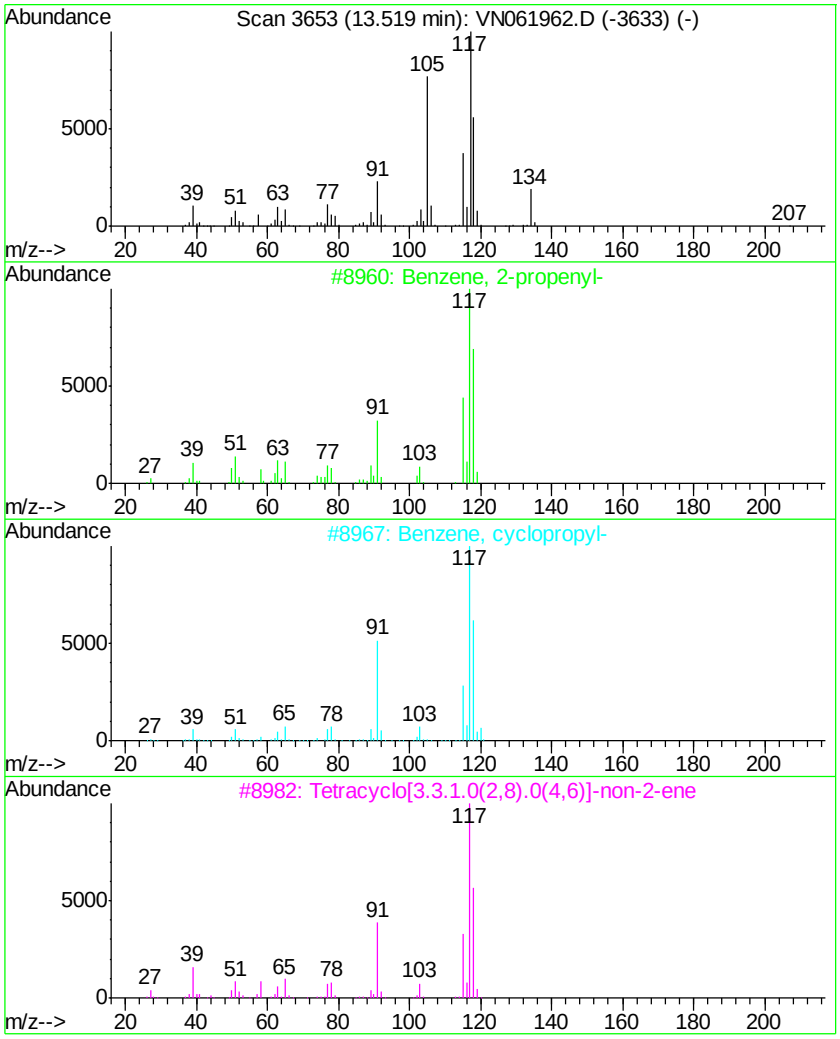
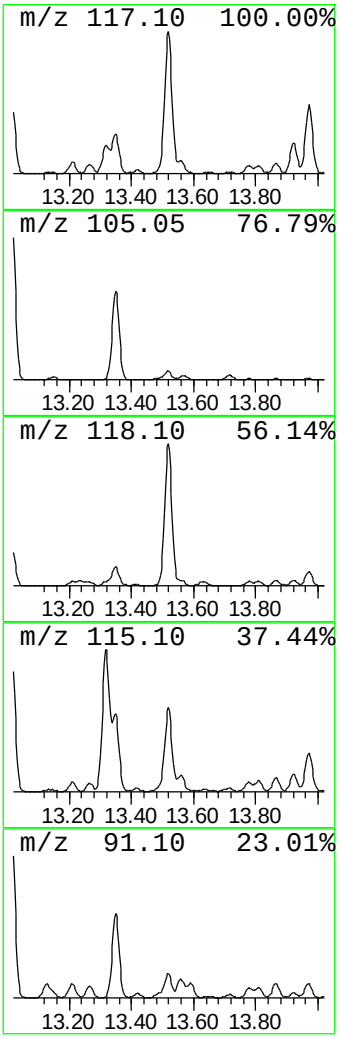
Peak Number 6 Benzene, 2-propenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	6.41 ug/l	794792	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	70
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	70
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	70





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Dimethyl sulfide	3.85	281.7	ug/l	3400760	1	7.63	603634	50.0
Disulfide, dimethyl	9.86	44.4	ug/l	643313	2	8.55	723727	50.0
2-Pentanol, 4-met...	10.33	5.6	ug/l	948482	3	11.38	8417910	50.0
Benzene, 1-ethyl-...	12.63	14.1	ug/l	1753250	4	13.32	6203490	50.0
Benzene, 1-ethyl-...	12.87	8.9	ug/l	1105810	4	13.32	6203490	50.0
Benzene, 2-propenyl-	13.52	6.4	ug/l	794792	4	13.32	6203490	50.0