LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN061920\
Data File : VN061964.D
Acq On : 19 Jun 2020 20:00
Operator : JC/MD
Sample : L3033-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : KY032MW006-200616

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	2.156	99	119	138	rBV	9327913	16251432	20.25%	6.552%
2	2.670	262	279	309	rBV	1309548	2724897	3.40%	1.099%
3	3.773	608	622	635	rVV	1260238	3187501	3.97%	1.285%
4	3.850	636	646	681	rVV	621555	1755982	2.19%	0.708%
5	6.606	1481	1503	1529	rBV2	334621	976357	1.22%	0.394%
6	6.799	1532	1563	1616	rBV2	19117427	65523783	81.66%	26.416%
7	7.159	1651	1675	1719	rBV	4199778	11351007	14.15%	4.576%
8	9.005	2232	2249	2280	rBV	821730	1639860	2.04%	0.661%
9	9.165	2280	2299	2335	rVB	1114272	2238307	2.79%	0.902%
10	9.860	2496	2515	2530	rBV	1961463	3680496	4.59%	1.484%
11	9.959	2530	2546	2567	rVV	12547234	24964292	31.11%	10.064%
12	10.066	2567	2579	2585	rVV	604093	1130405	1.41%	0.456%
13	10.133	2585	2600	2637	rVB2	34807213	80244522	100.00%	32.351%
14	10.326	2648	2660	2688	rVB	1844931	3231482	4.03%	1.303%
15	11.252	2932	2948	2959	rBV	707224	1249526	1.56%	0.504%
16	11.381	2978	2988	3008	rVB2	632332	1824030	2.27%	0.735%
17	11.484	3008	3020	3039	rBV	717530	1326073	1.65%	0.535%
18	11.590	3040	3053	3064	rBV	1404408	2585986	3.22%	1.043%
19	11.921	3144	3156	3169	rBV	835612	1443355	1.80%	0.582%
20	13.143	3520	3536	3548	rVB2	1178096	1977517	2.46%	0.797%
21	13.336	3582	3596	3605	rVV2	1410277	3069699	3.83%	1.238%
22	13.628	3672	3687	3707	rVB	6117094	10209058	12.72%	4.116%
23	14.197	3851	3864	3881	rVB	1262112	2187781	2.73%	0.882%
24	14.821	4047	4058	4069	rBV	1210952	2001674	2.49%	0.807%
25	15.104	4133	4146	4167	rVB	731930	1269663	1.58%	0.512%

Sum of corrected areas: 248044685

LSC Report - Integrated Chromatogram

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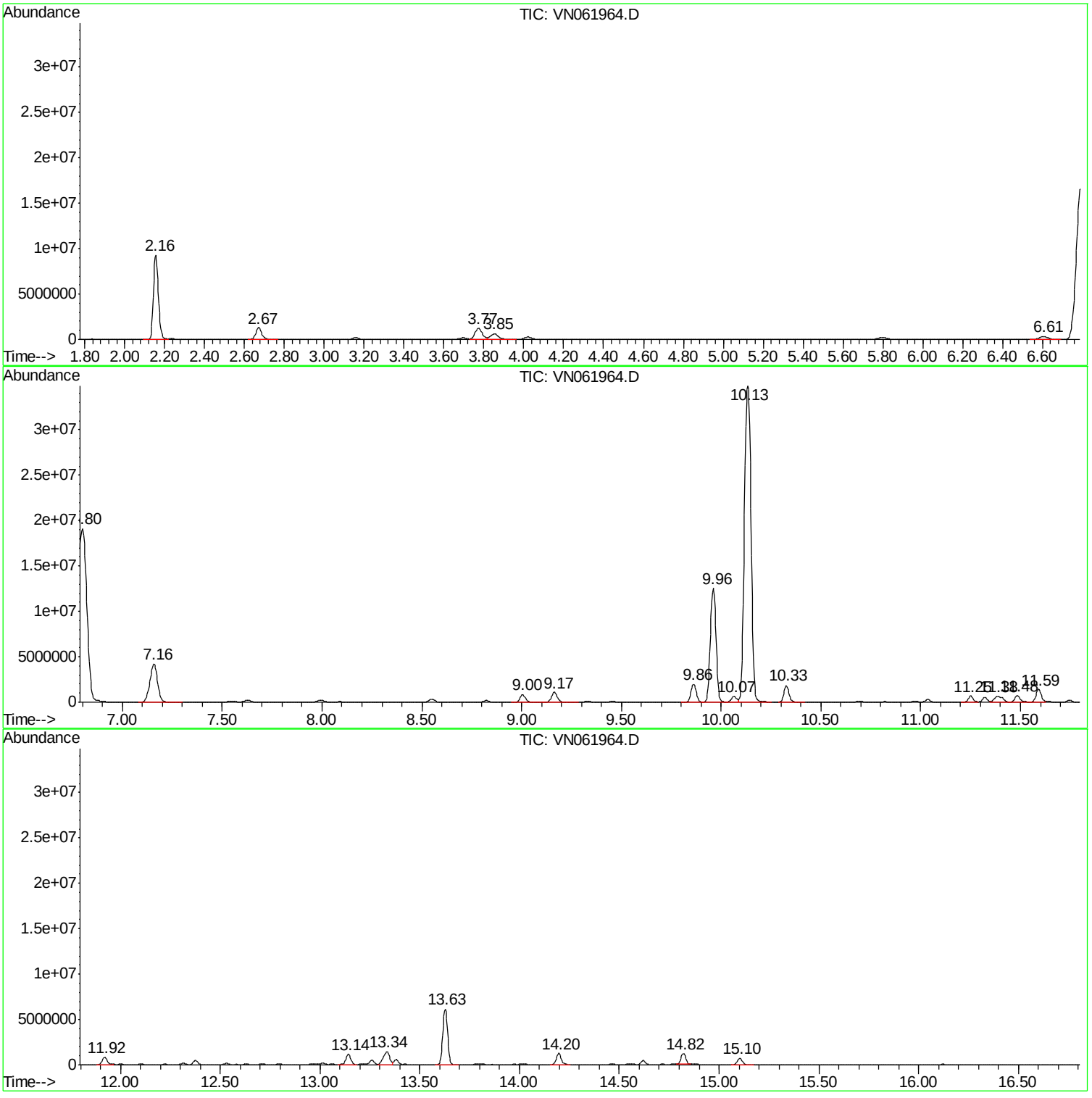
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : KY032MW006-200616

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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Instrument : MSVOA_N
ClientSampleId : KY032MW006-200616

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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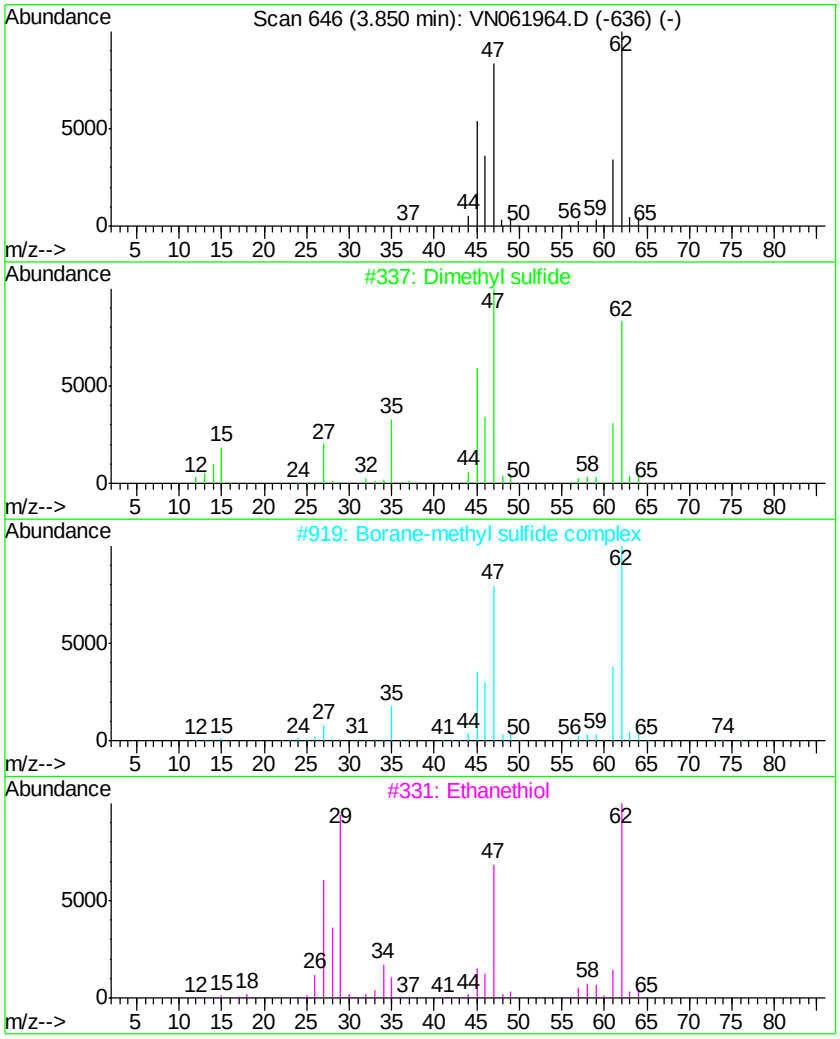
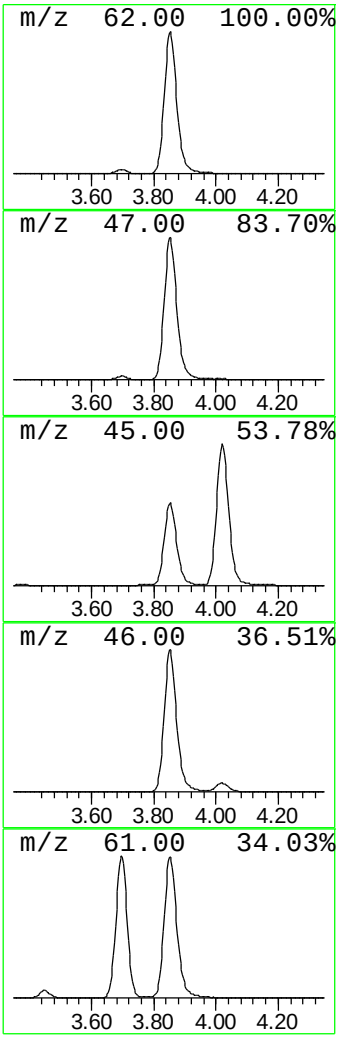
Peak Number 1 Dimethyl sulfide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.85	7.73 ug/l	1755980	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 : L3033-06
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ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : KY032MW006-200616

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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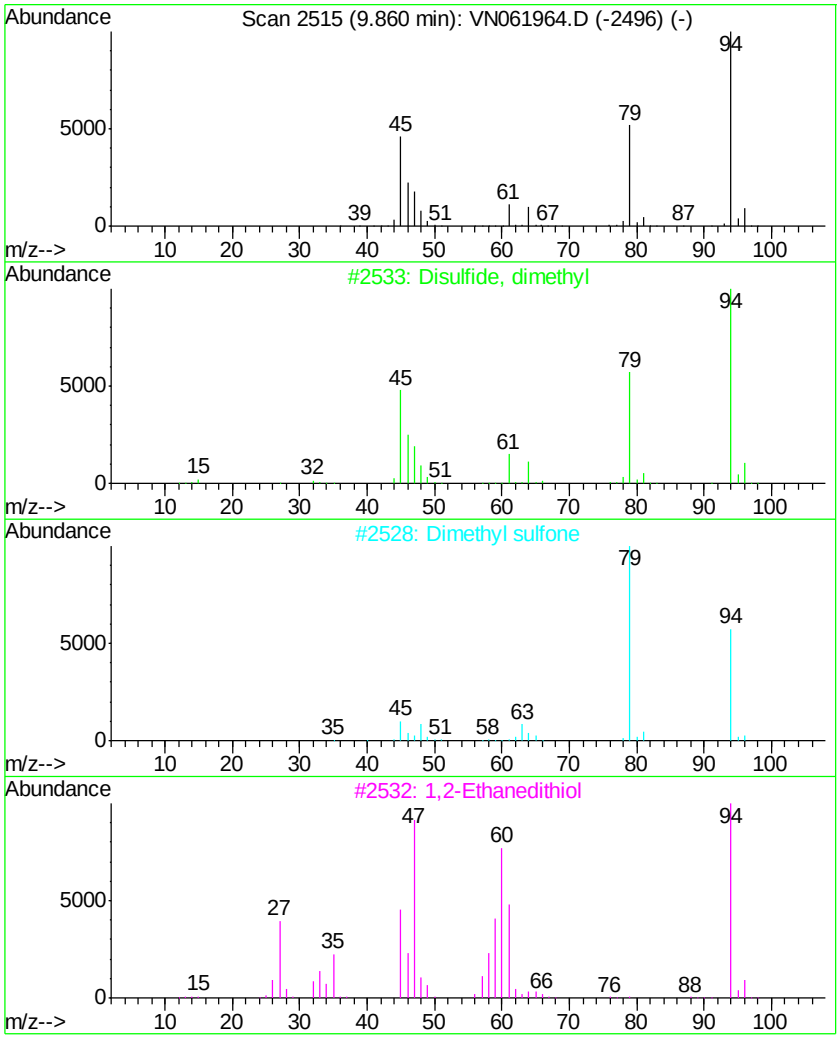
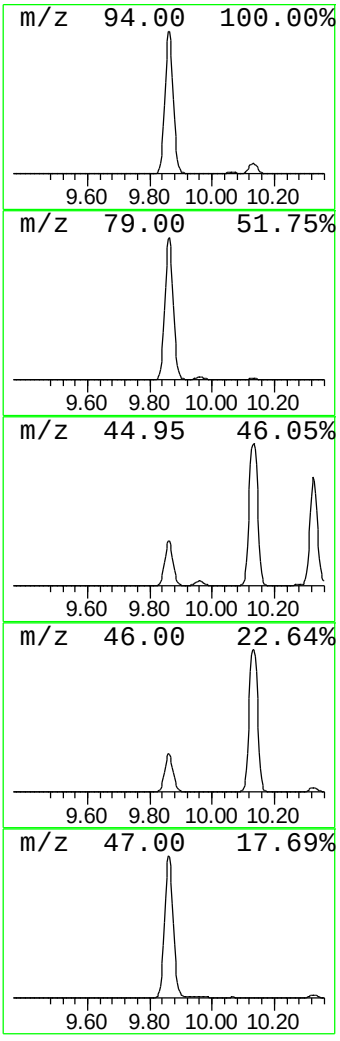
Peak Number 2 Disulfide, dimethyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	112.22 ug/l	3680500	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
2	Dimethyl sulfone	94	C2H6O2S	000067-71-0	56
3	1,2-Ethanedithiol	94	C2H6S2	000540-63-6	52
4	Methanesulfonyl chloride	114	CH3ClO2S	000124-63-0	7
5	Methane, bromo-	94	CH3Br	000074-83-9	5





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Instrument : MSVOA_N
ClientSampleId : KY032MW006-200616

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

TIC Library : C:\DATABASE\NIST11.L
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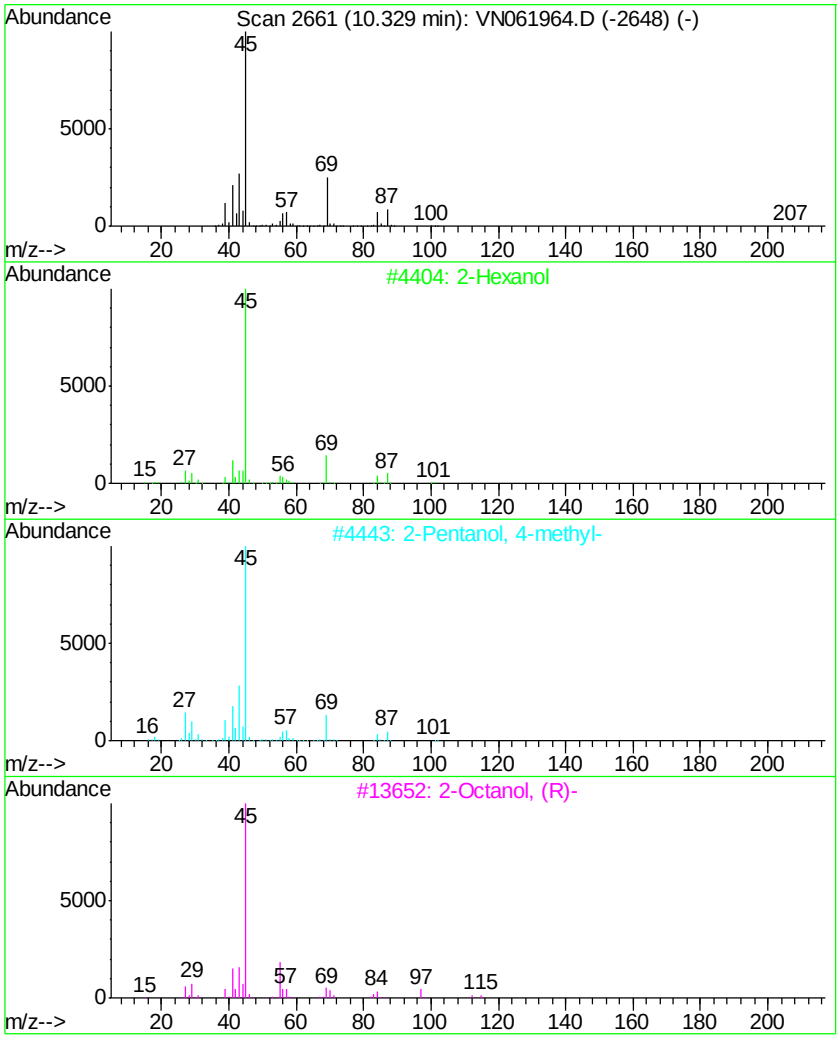
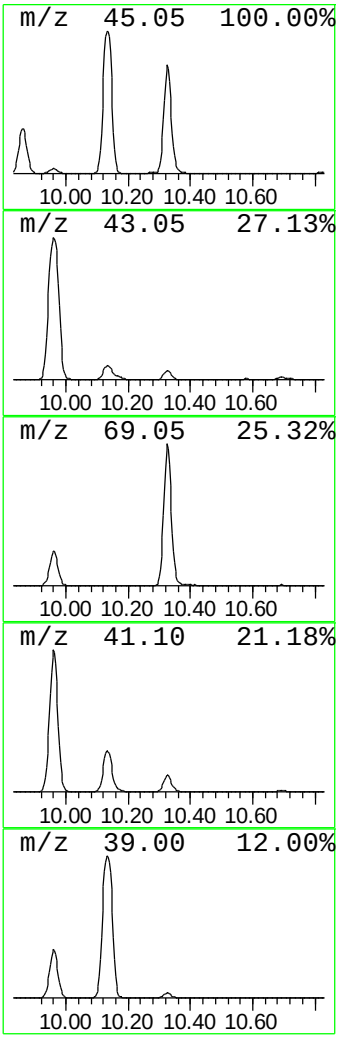
Peak Number 3 2-Hexanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	88.58 ug/l	3231480	Chlorobenzene-d5	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol	102	C6H14O	000626-93-7	83
2	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	83
3	2-Octanol, (R)-	130	C8H18O	005978-70-1	78
4	2-Octanol	130	C8H18O	000123-96-6	64
5	2-Octanol, (S)-	130	C8H18O	006169-06-8	64





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ClientSampleId : KY032MW006-200616

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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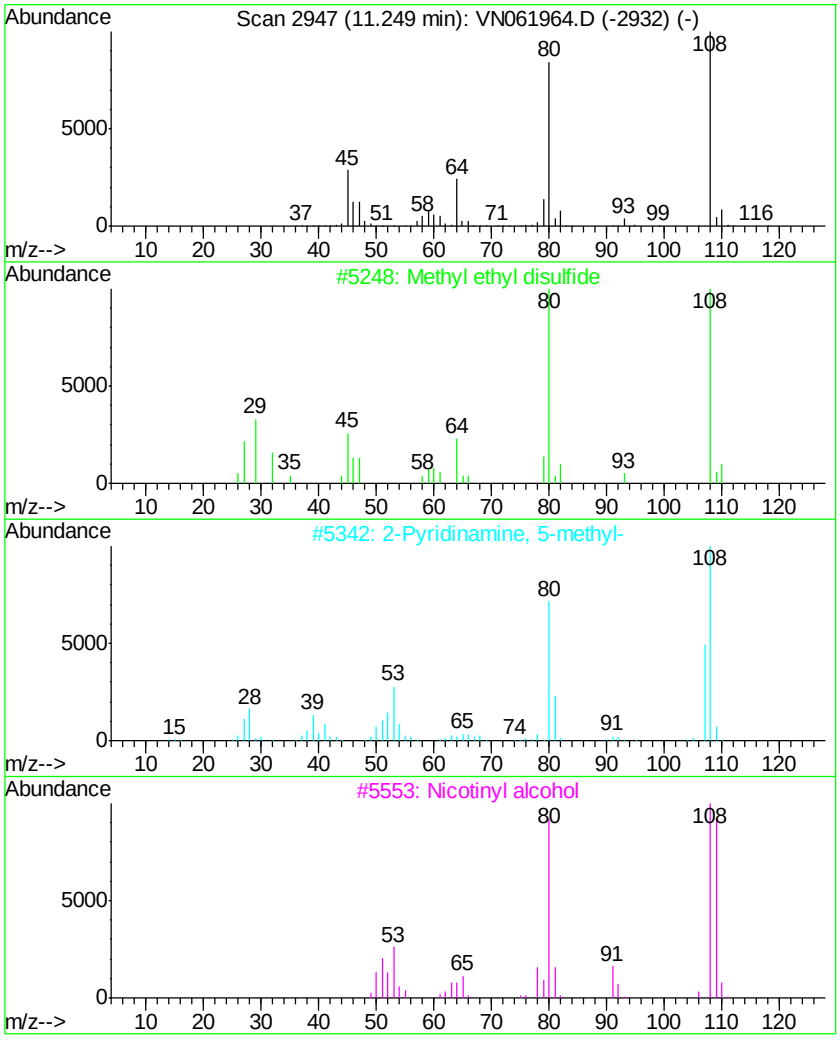
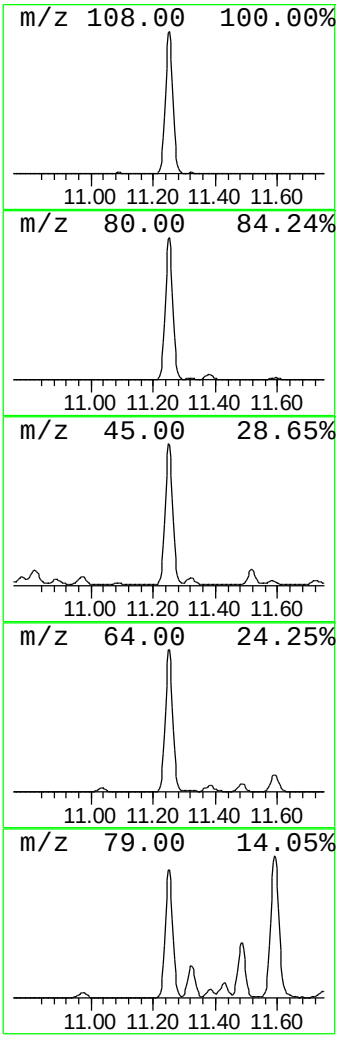
Peak Number 4 Methyl ethyl disulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.25	34.25 ug/l	1249530	Chlorobenzene-d5	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl ethyl disulfide	108	C3H8S2	020333-39-5	91
2	2-Pyridinamine, 5-methyl-	108	C6H8N2	001603-41-4	72
3	Nicotinyl alcohol	109	C6H7NO	000100-55-0	64
4	Methanesulfonic acid, methyl ester	110	C2H6O3S	000066-27-3	59
5	Dimethyl phosphite	110	C2H7O3P	000868-85-9	42





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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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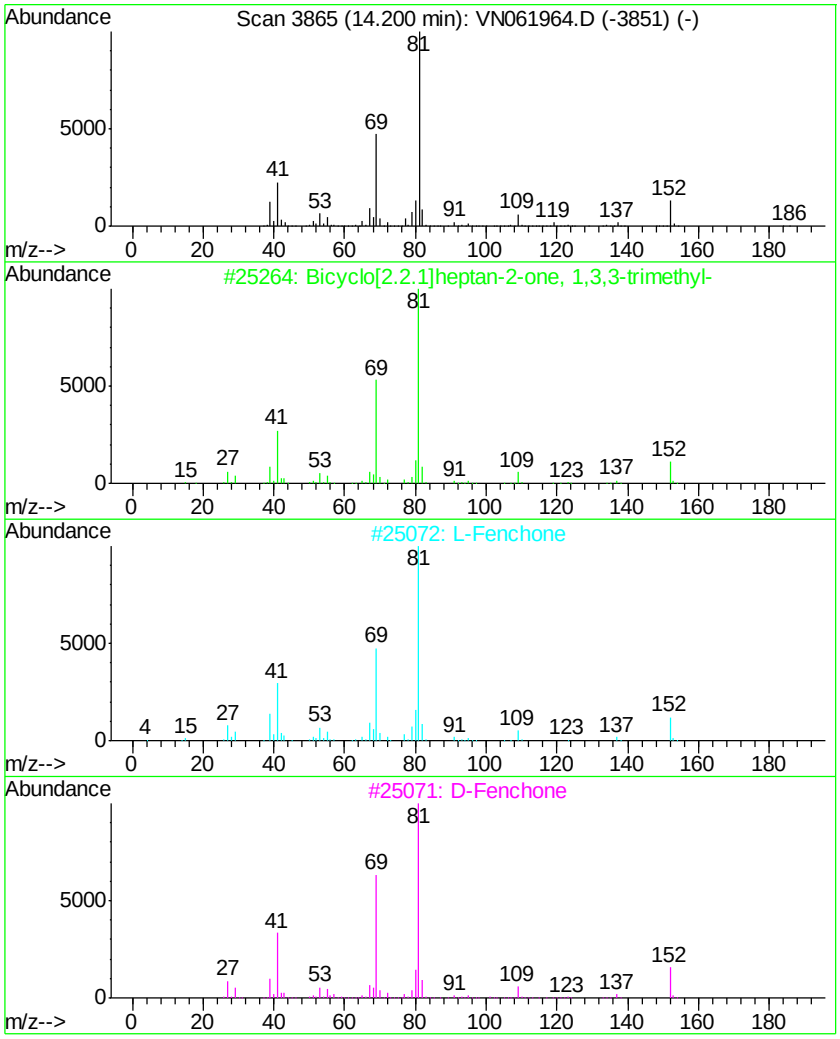
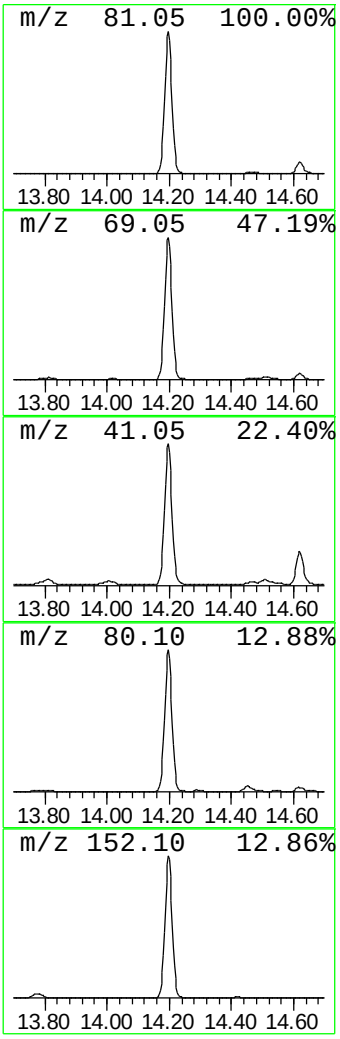
Peak Number 5 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	35.64 ug/l	2187780	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	95
2	L-Fenchone	152	C10H16O	007787-20-4	95
3	D-Fenchone	152	C10H16O	004695-62-9	94
4	Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	42
5	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	40





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Quant Title : SW846 8260

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

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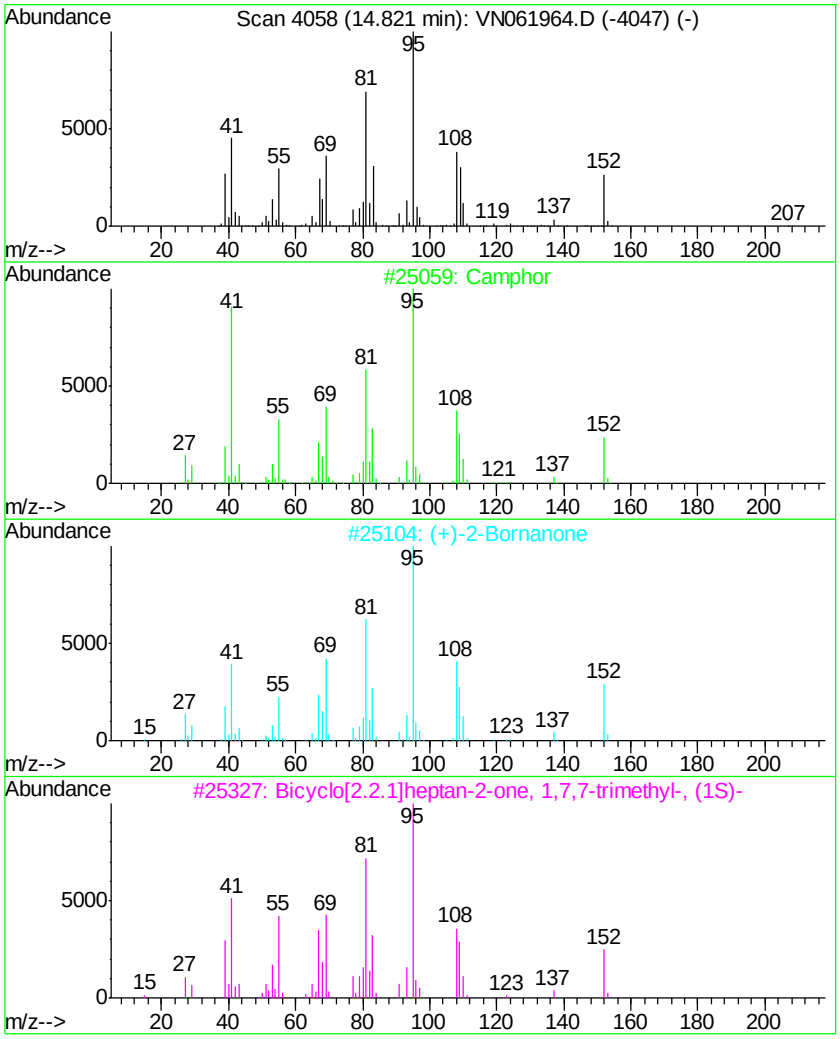
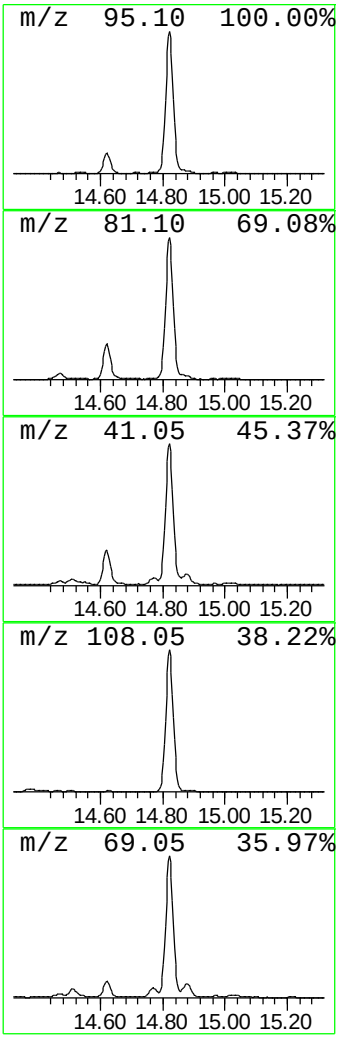
Peak Number 6 Camphor Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	32.60 ug/l	2001670	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Camphor	152	C10H16O	000076-22-2	98
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	96
4	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46
5	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	38





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	7.7	ug/l	1755980	1	7.63	11351000	50.0
Disulfide, dimethyl	9.86	112.2	ug/l	3680500	2	8.55	1639860	50.0
2-Hexanol	10.33	88.6	ug/l	3231480	3	11.38	1824030	50.0
Methyl ethyl disu...	11.25	34.3	ug/l	1249530	3	11.38	1824030	50.0
Bicyclo[2.2.1]hep...	14.20	35.6	ug/l	2187780	4	13.32	3069700	50.0
Camphor	14.82	32.6	ug/l	2001670	4	13.32	3069700	50.0