LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN122718\
Data File : VN053206.D
Acq On : 27 Dec 2018 12:23
Operator : MD\SY
Sample : J6571-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 50082-50083

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\82N121818W.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	1.815	4	13	25	rBV2	169754	219967	1.22%	0.335%
2	2.317	157	169	191	rBV	1908491	3071081	17.08%	4.677%
3	3.265	445	464	496	rBV	664051	1565424	8.70%	2.384%
4	3.702	581	600	618	rBV	288146	722458	4.02%	1.100%
5	3.815	619	635	655	rBV	673926	1738230	9.67%	2.647%
6	4.056	694	710	739	rVB2	76018	218965	1.22%	0.333%
7	6.024	1307	1322	1354	rVB3	124161	398327	2.21%	0.607%
8	6.548	1461	1485	1507	rBV2	209890	643137	3.58%	0.980%
9	6.837	1546	1575	1595	rBV2	60087	190592	1.06%	0.290%
10	7.593	1790	1810	1821	rBV	602944	1511215	8.40%	2.302%
11	7.667	1821	1833	1856	rVB	1250941	2961113	16.47%	4.510%
12	8.027	1922	1945	1967	rBV	687374	1655185	9.20%	2.521%
13	8.586	2103	2119	2141	rBV	1968947	4094028	22.77%	6.235%
14	8.783	2165	2180	2193	rBV	277549	592917	3.30%	0.903%
15	9.168	2287	2300	2322	rVB	105472	217969	1.21%	0.332%
16	10.091	2569	2587	2600	rBV	2946366	5304984	29.50%	8.080%
17	10.799	2781	2807	2853	rBV	1240164	4015894	22.33%	6.116%
18	11.352	2968	2979	2985	rBV	179059	288474	1.60%	0.439%
19	11.406	2985	2996	3019	rVB	2543397	4446062	24.72%	6.772%
20	12.252	3251	3259	3274	rVB2	215977	380531	2.12%	0.580%
21	12.400	3292	3305	3321	rBV	2023303	3395285	18.88%	5.171%
22	12.827	3425	3438	3456	rBV	11619927	17983853	100.00%	27.391%
23	12.914	3456	3465	3485	rVB	271764	446557	2.48%	0.680%
24	13.075	3497	3515	3535	rBV	2202172	4020340	22.36%	6.123%
25	13.252	3561	3570	3586	rVB4	134768	246101	1.37%	0.375%
26	13.342	3586	3598	3612	rBV	2282876	3788642	21.07%	5.770%
27	13.448	3623	3631	3643	rVB	378970	580560	3.23%	0.884%
28	14.888	4069	4079	4092	rVB8	127355	254962	1.42%	0.388%
29	15.204	4163	4177	4190	rVB4	95676	220527	1.23%	0.336%
30	15.618	4293	4306	4327	rBV2	252385	483790	2.69%	0.737%

Sum of corrected areas: 65657170

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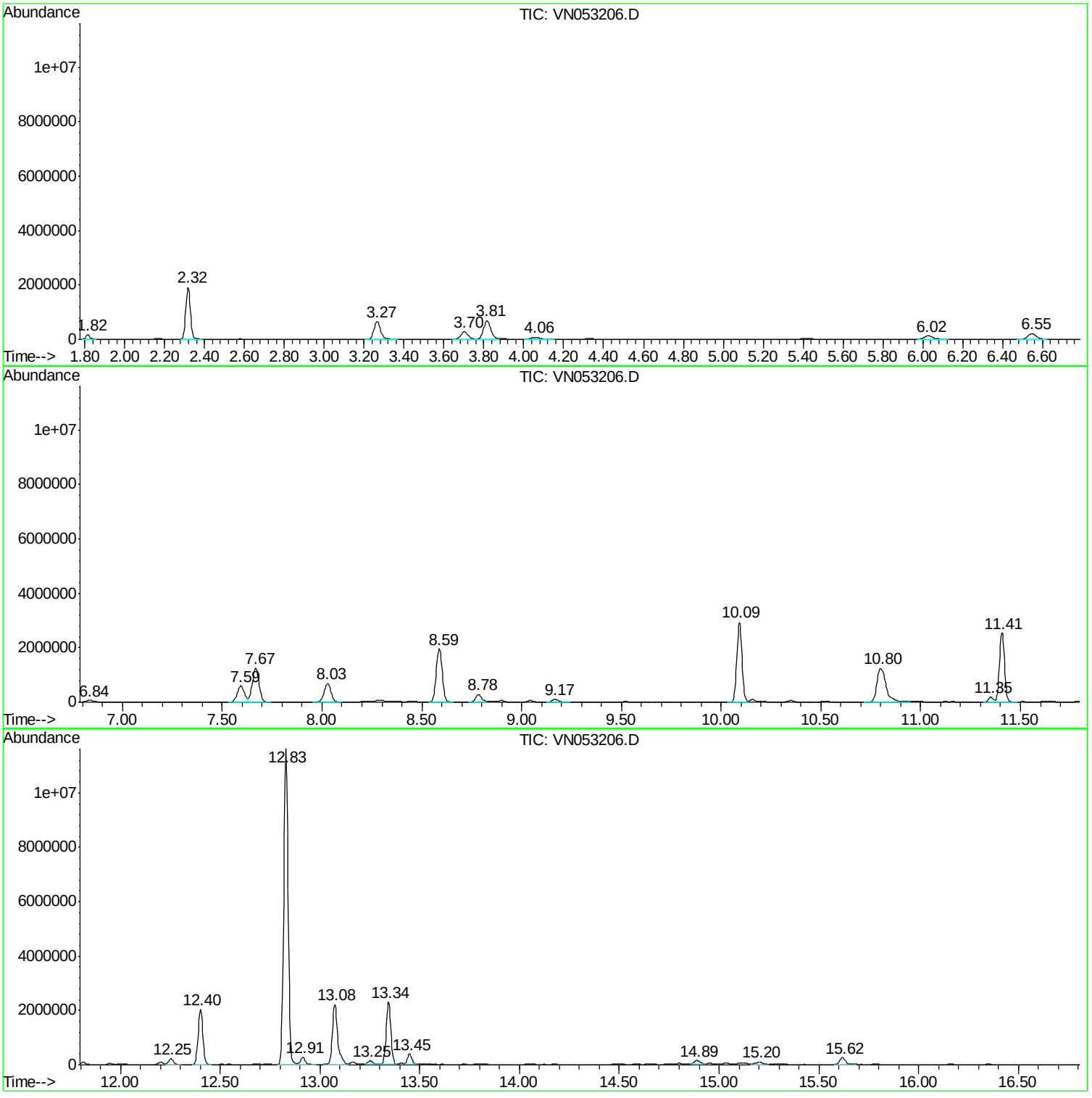
Data File : VN053206.D
Acq On : 27 Dec 2018 12:23
Operator : MD\SY
Sample : J6571-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
50082-50083

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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



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Instrument : MSVOA_N
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

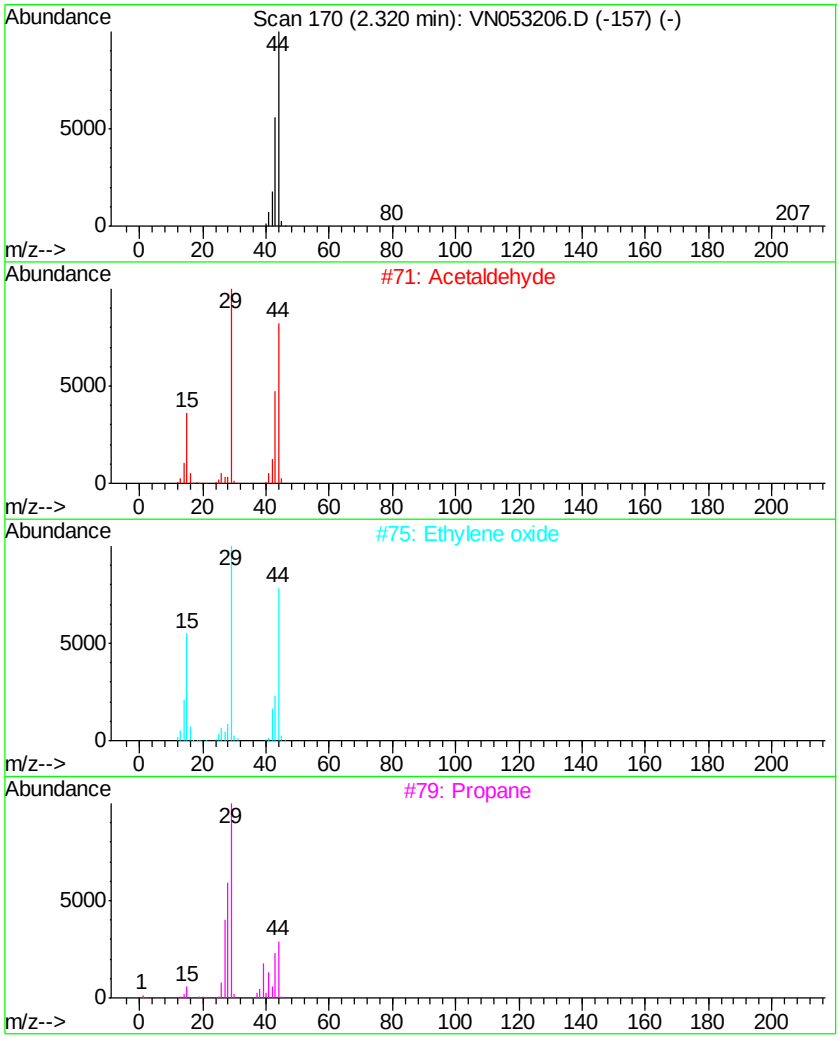
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

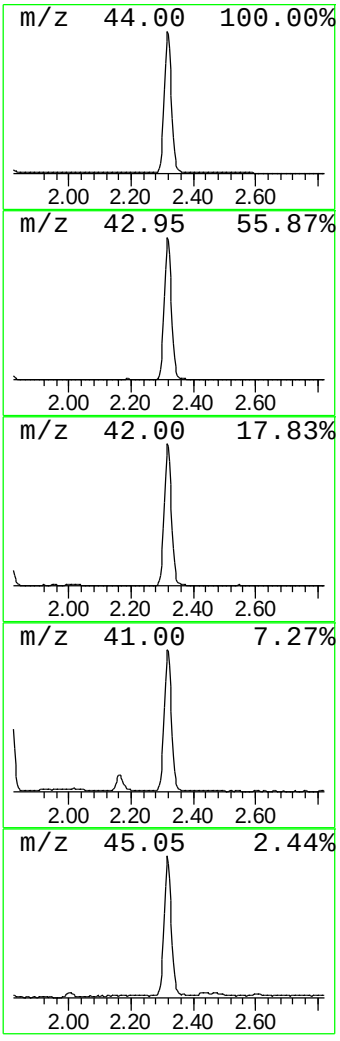
****

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	51.86 ug/l	3071080	Pentafluorobenzene	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	64
2	Ethylene oxide	44	C2H4O	000075-21-8	5
3	Propane	44	C3H8	000074-98-6	4
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Carbon dioxide	44	CO2	000124-38-9	3





Library Search Compound Report

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ALS Vial : 9 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 50082-50083

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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

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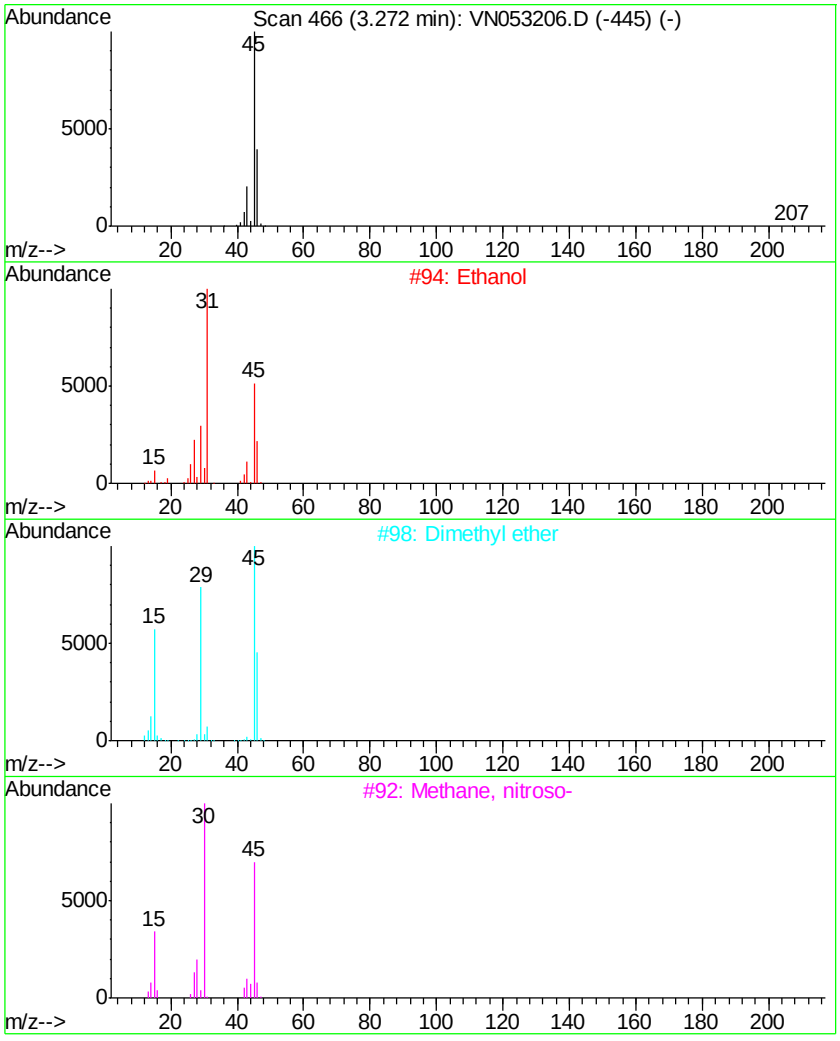
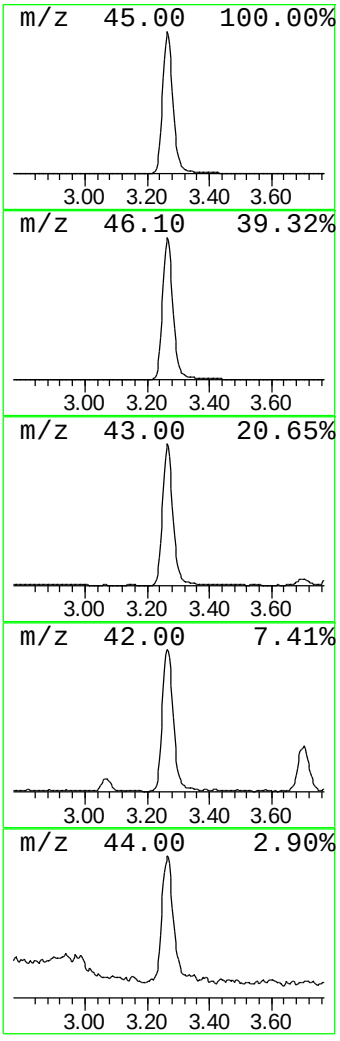
Peak Number 2 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.27	26.43 ug/l	1565420	Pentafluorobenzene	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	74
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4





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Operator : MD\SY
Sample : J6571-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 50082-50083

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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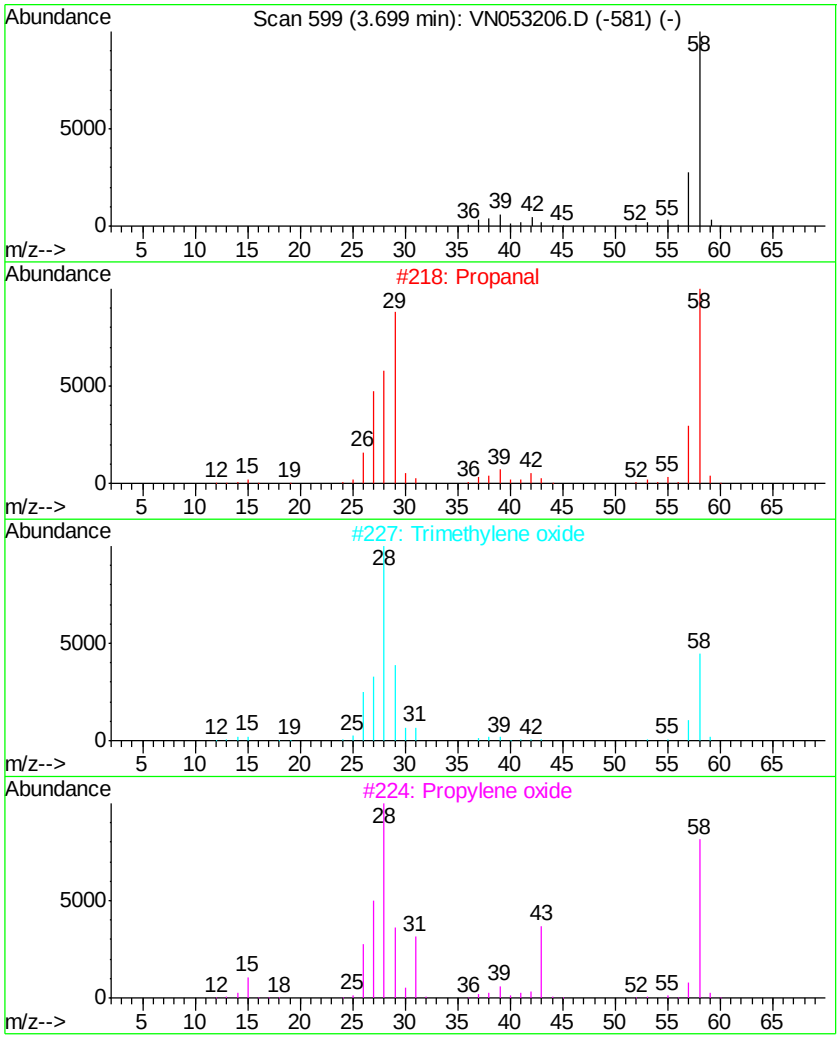
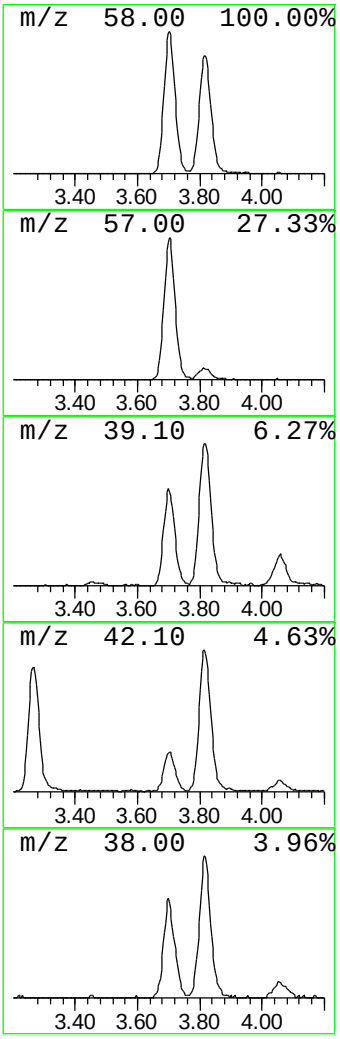
Peak Number 3 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.70	12.20 ug/l	722458	Pentafluorobenzene	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	Propylene oxide	58	C3H6O	000075-56-9	5
4	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	4
5	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	4





Library Search Compound Report

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ALS Vial : 9 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 50082-50083

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

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

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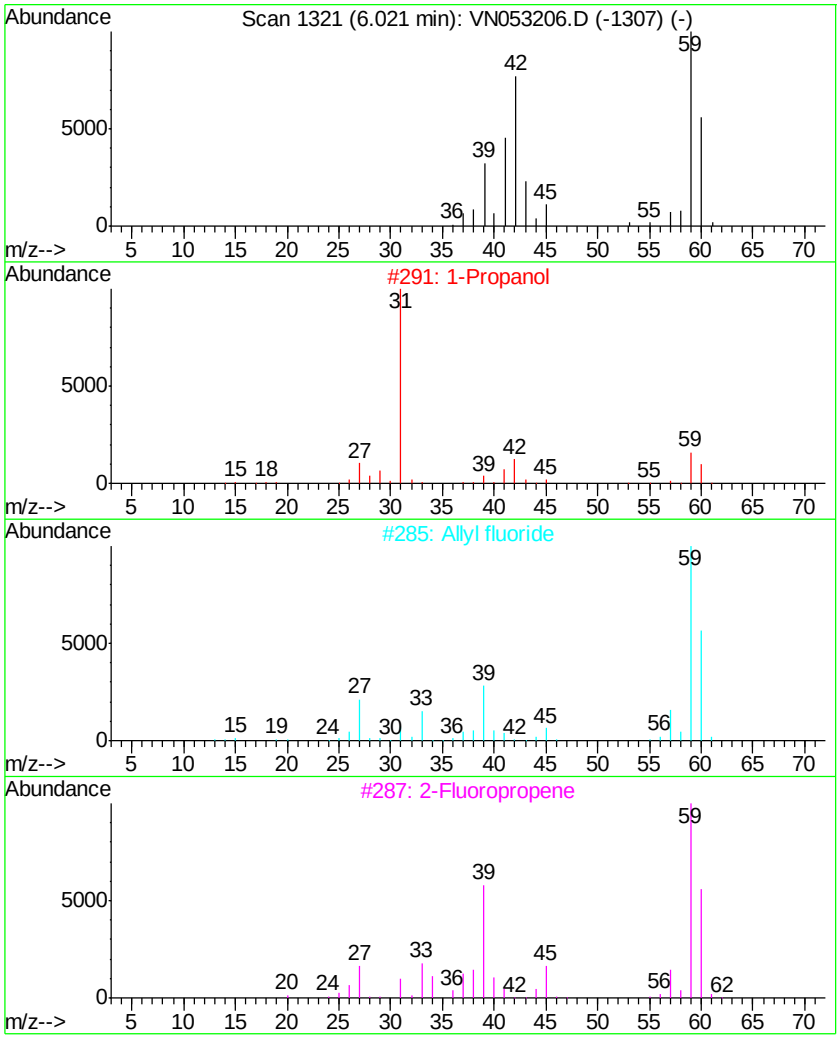
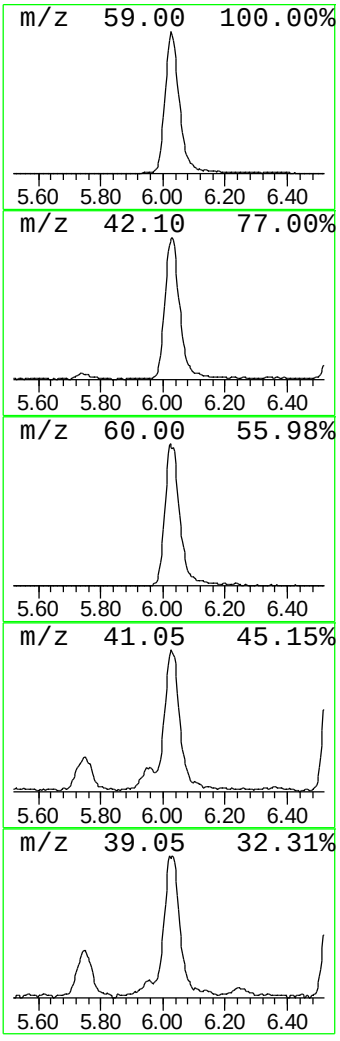
Peak Number 4 1-Propanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.02	6.73 ug/l	398327	Pentafluorobenzene	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	Allyl fluoride	60	C3H5F	000818-92-8	47
3	2-Fluoropropene	60	C3H5F	001184-60-7	43
4	Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9
5	Acetaldoxime	59	C2H5NO	000107-29-9	7





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Sample : J6571-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 50082-50083

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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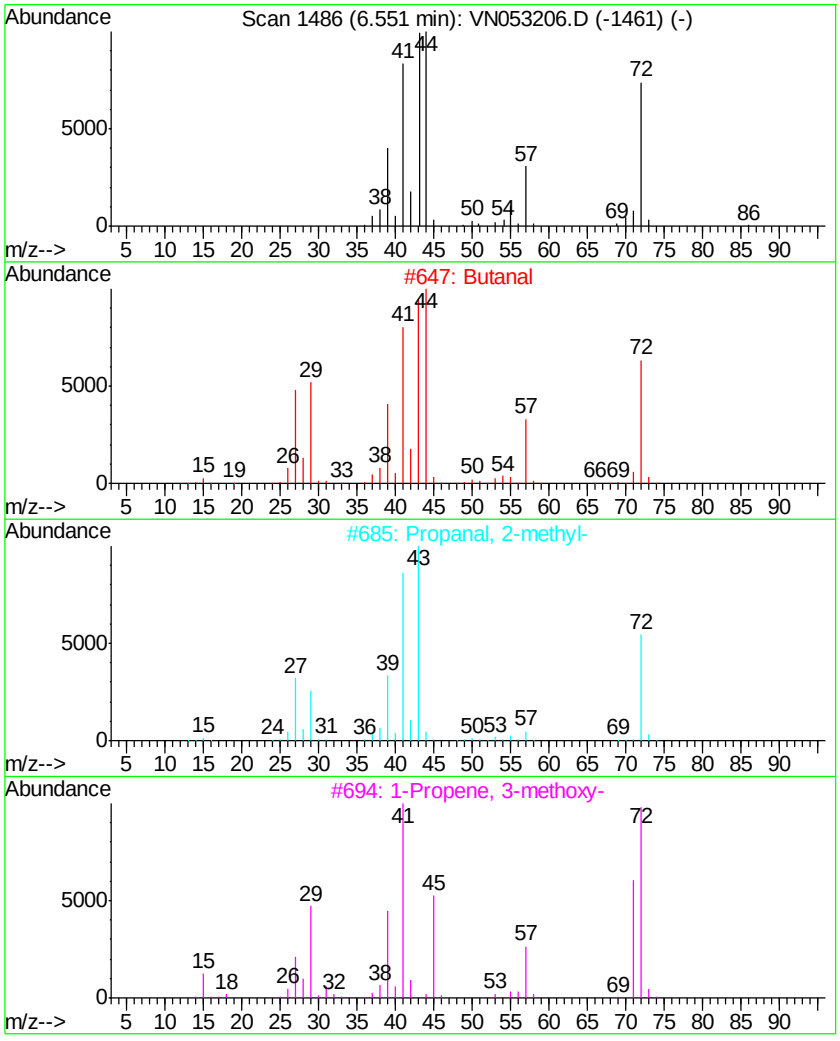
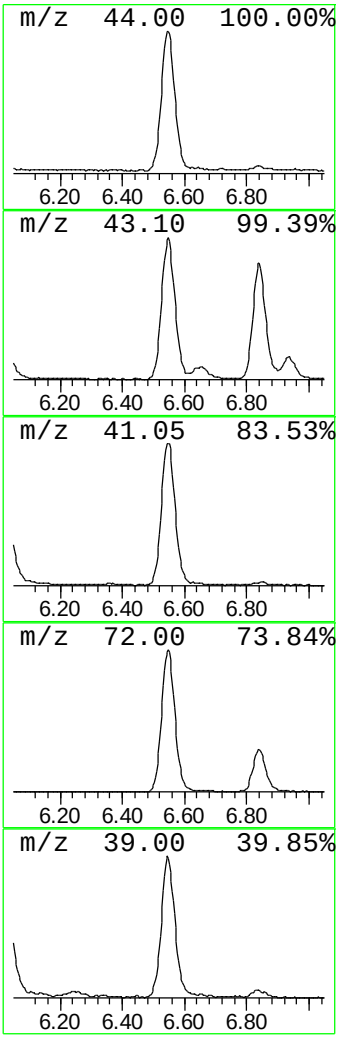
Peak Number 5 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	10.86 ug/l	643137	Pentafluorobenzene	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4	Ethene, ethoxy-	72	C4H8O	000109-92-2	42
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





Library Search Compound Report

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ALS Vial : 9 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 50082-50083

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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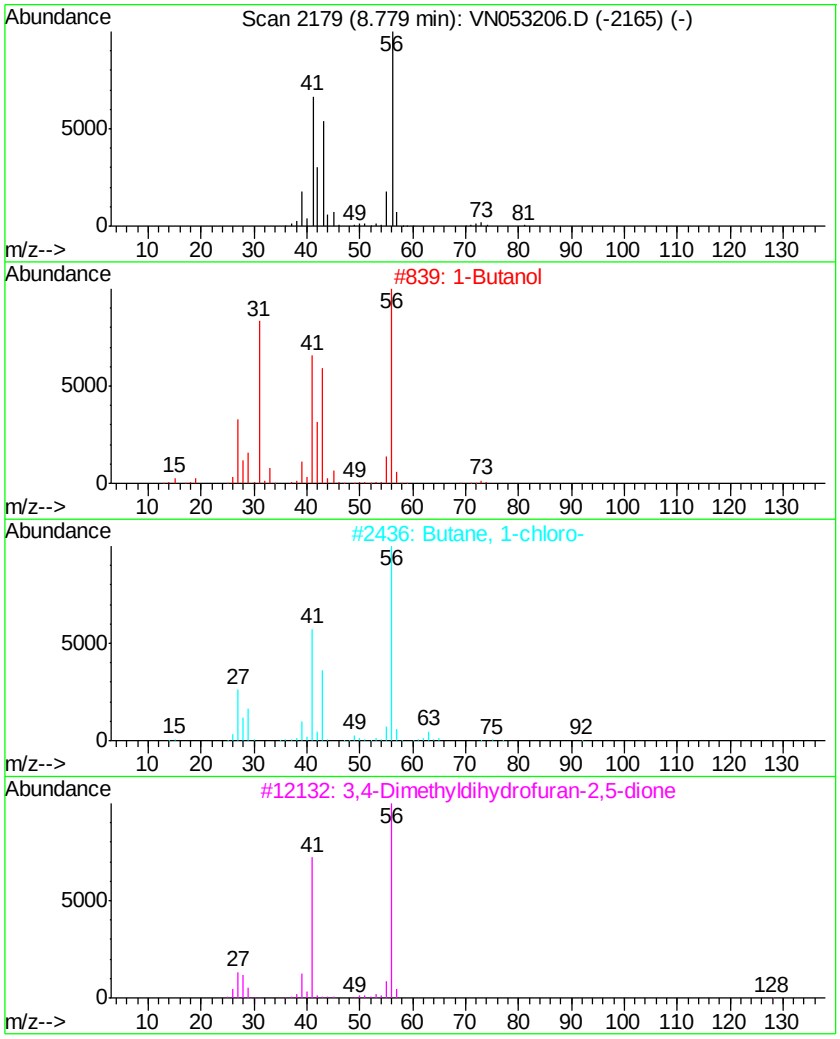
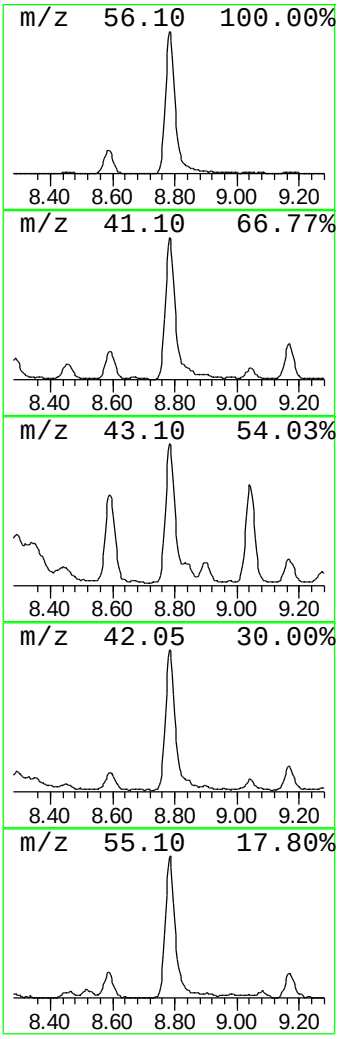
Peak Number 6 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.78	7.24 ug/l	592917	1,4-Difluorobenzene	8.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	45
3	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	38
4	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	9





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Data File : VN053206.D
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ALS Vial : 9 Sample Multiplier: 28

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
Quant Title : SW846 8260

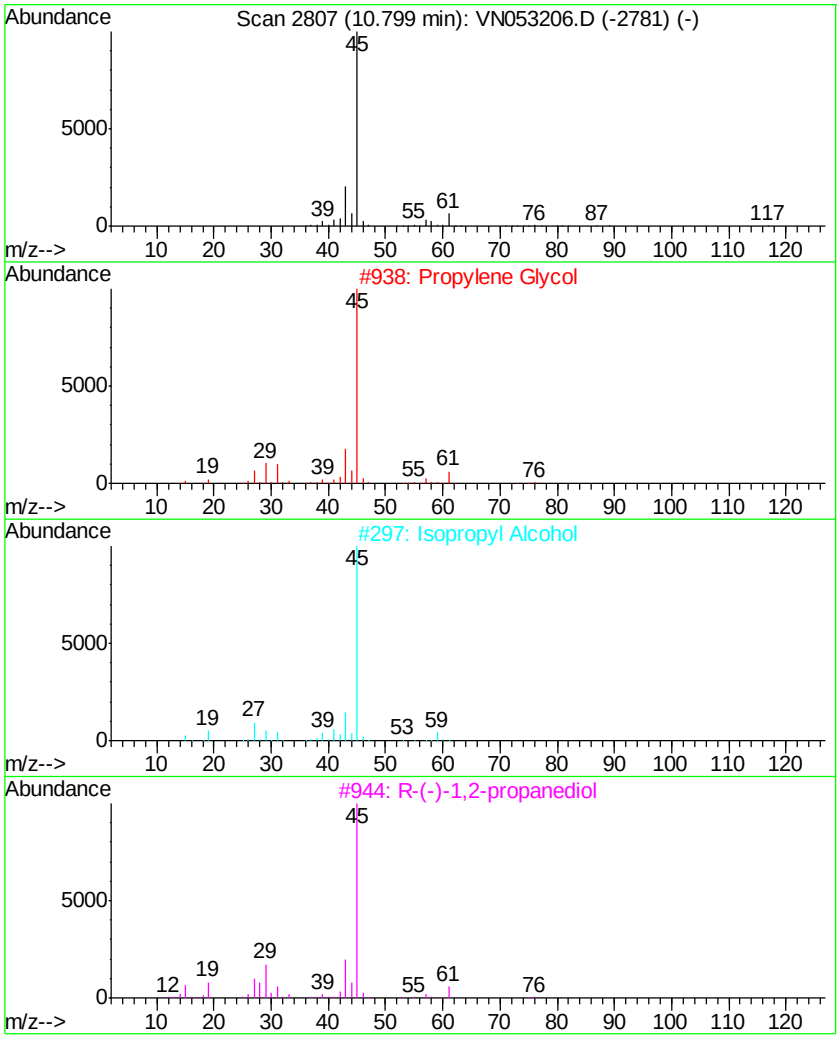
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

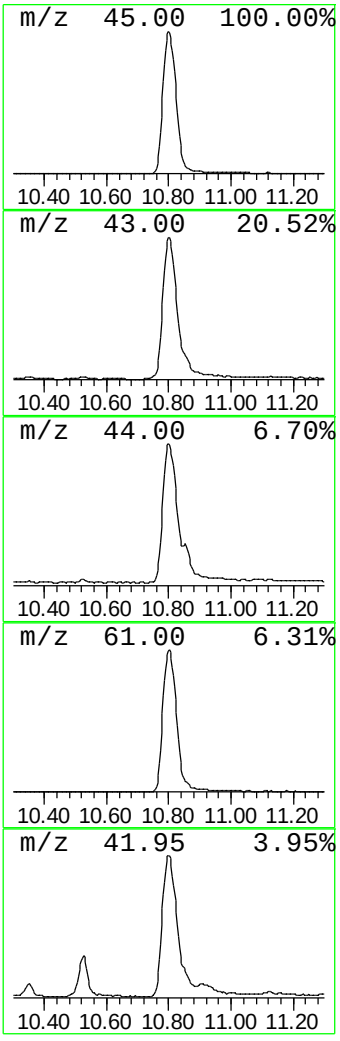
****

Peak Number 7 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	45.16 ug/l	4015890	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	80
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5	(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	9





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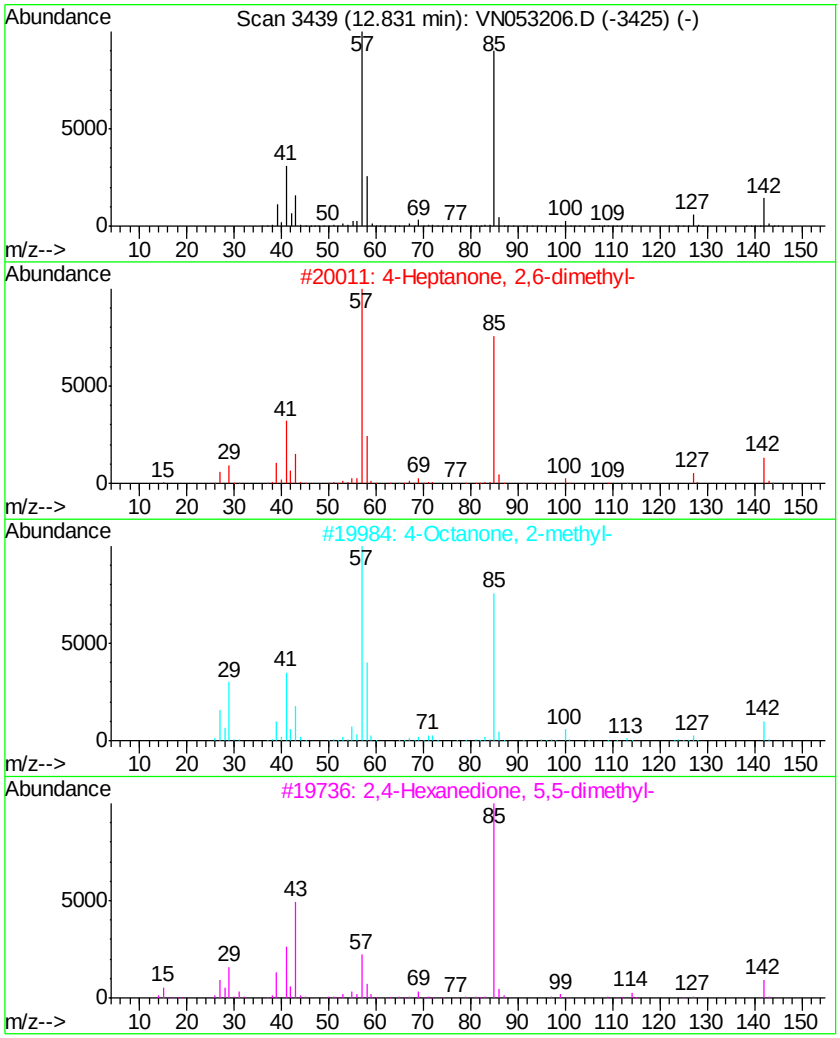
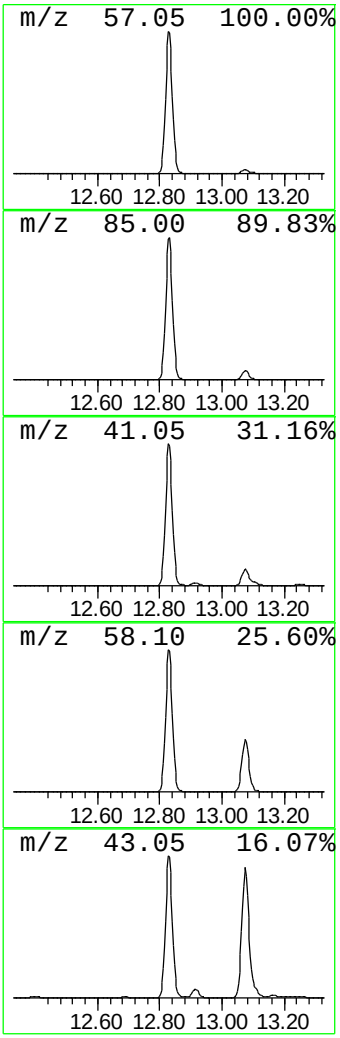
Peak Number 8 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	237.34 ug/l	17983900	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	64
3	2,4-Hexanedione, 5,5-dimethyl-	142	C8H14O2	007307-04-2	59
4	5-Nonanone	142	C9H18O	000502-56-7	59
5	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	50





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Quant Title : SW846 8260

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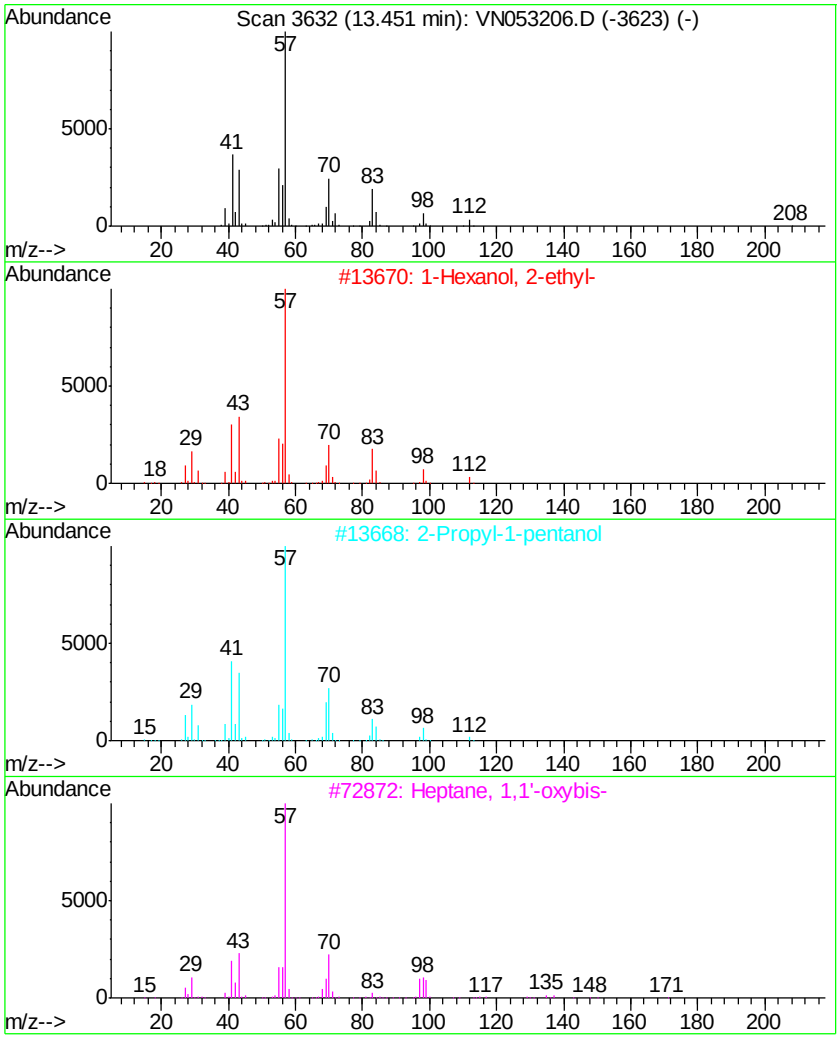
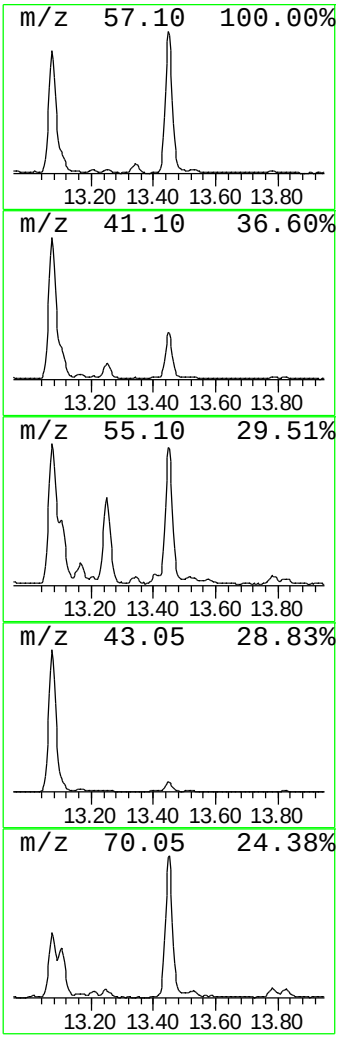
****

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	7.66 ug/l	580560	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	42
4	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	40
5	Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	39





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Quant Title : SW846 8260

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

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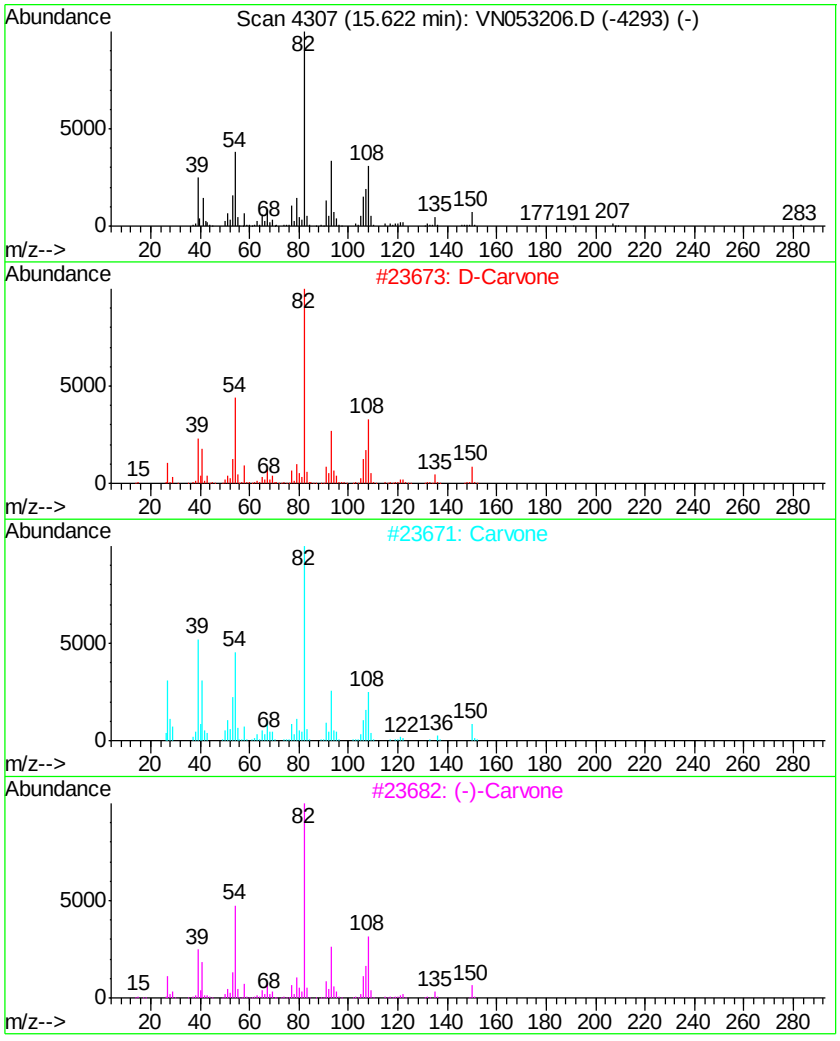
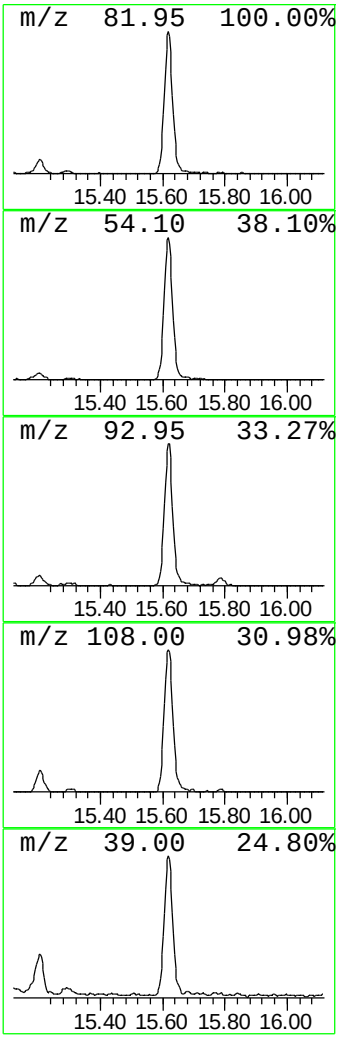
Peak Number 10 D-Carvone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	6.38 ug/l	483790	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Carvone	150	C10H14O	002244-16-8	95
2	Carvone	150	C10H14O	000099-49-0	95
3	(-)-Carvone	150	C10H14O	006485-40-1	94
4	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	47
5	1H-Imidazole, 2-methyl-	82	C4H6N2	000693-98-1	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN122718\
Data File : VN053206.D
Acq On : 27 Dec 2018 12:23
Operator : MD\SY
Sample : J6571-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 50082-50083

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121818W.M
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
Acetaldehyde	2.32	51.9	ug/l	3071080	1	7.67	2961110	50.0
Ethanol	3.27	26.4	ug/l	1565420	1	7.67	2961110	50.0
Propanal	3.70	12.2	ug/l	722458	1	7.67	2961110	50.0
1-Propanol	6.02	6.7	ug/l	398327	1	7.67	2961110	50.0
Butanal	6.55	10.9	ug/l	643137	1	7.67	2961110	50.0
1-Butanol	8.78	7.2	ug/l	592917	2	8.59	4094030	50.0
Propylene Glycol	10.80	45.2	ug/l	4015890	3	11.41	4446060	50.0
4-Heptanone, 2,6-...	12.83	237.3	ug/l	17983900	4	13.35	3788640	50.0
1-Hexanol, 2-ethyl-	13.45	7.7	ug/l	580560	4	13.35	3788640	50.0
D-Carvone	15.62	6.4	ug/l	483790	4	13.35	3788640	50.0