LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN010719\
Data File : VN053299.D
Acq On : 7 Jan 2019 12:47
Operator : MD\SY
Sample : K1053-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : COMP-1-DRUM

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\82N010519W.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	3	13	33	rVB	701837	914760	2.47%	1.046%
2	2.310	153	167	221	rBV2	22582596	37076425	100.00%	42.386%
3	3.262	446	463	500	rBV	2654502	6175735	16.66%	7.060%
4	6.545	1460	1484	1505	rBV	313582	946381	2.55%	1.082%
5	7.185	1665	1683	1716	rBV	400422	1102623	2.97%	1.261%
6	7.593	1787	1810	1821	rBV	586012	1486978	4.01%	1.700%
7	7.667	1821	1833	1856	rVB	1185106	2808182	7.57%	3.210%
8	8.037	1924	1948	1972	rBV3	1203344	3217668	8.68%	3.678%
9	8.587	2103	2119	2144	rVB	1721595	3537605	9.54%	4.044%
10	8.783	2164	2180	2232	rBV	949408	2139567	5.77%	2.446%
11	10.091	2571	2587	2598	rBV	2738644	5042892	13.60%	5.765%
12	10.156	2598	2607	2631	rVB	1453869	2593695	7.00%	2.965%
13	11.406	2981	2996	3017	rBV	2405436	4197209	11.32%	4.798%
14	11.542	3032	3038	3049	rVV	657350	1101410	2.97%	1.259%
15	11.616	3050	3061	3084	rVB	658149	1220602	3.29%	1.395%
16	11.960	3153	3168	3190	rBV2	546530	1292830	3.49%	1.478%
17	12.400	3291	3305	3319	rBV	1989309	3311993	8.93%	3.786%
18	12.911	3450	3464	3479	rVB4	202688	413249	1.11%	0.472%
19	13.040	3482	3504	3513	rBV	315804	563512	1.52%	0.644%
20	13.342	3586	3598	3615	rBV	2209255	3879270	10.46%	4.435%
21	13.451	3625	3632	3644	rVB	295125	460695	1.24%	0.527%
22	13.725	3704	3717	3730	rBV	1146944	1906927	5.14%	2.180%
23	15.133	4136	4155	4169	rBV	1192475	2082251	5.62%	2.380%

Sum of corrected areas: 87472459

LSC Report - Integrated Chromatogram

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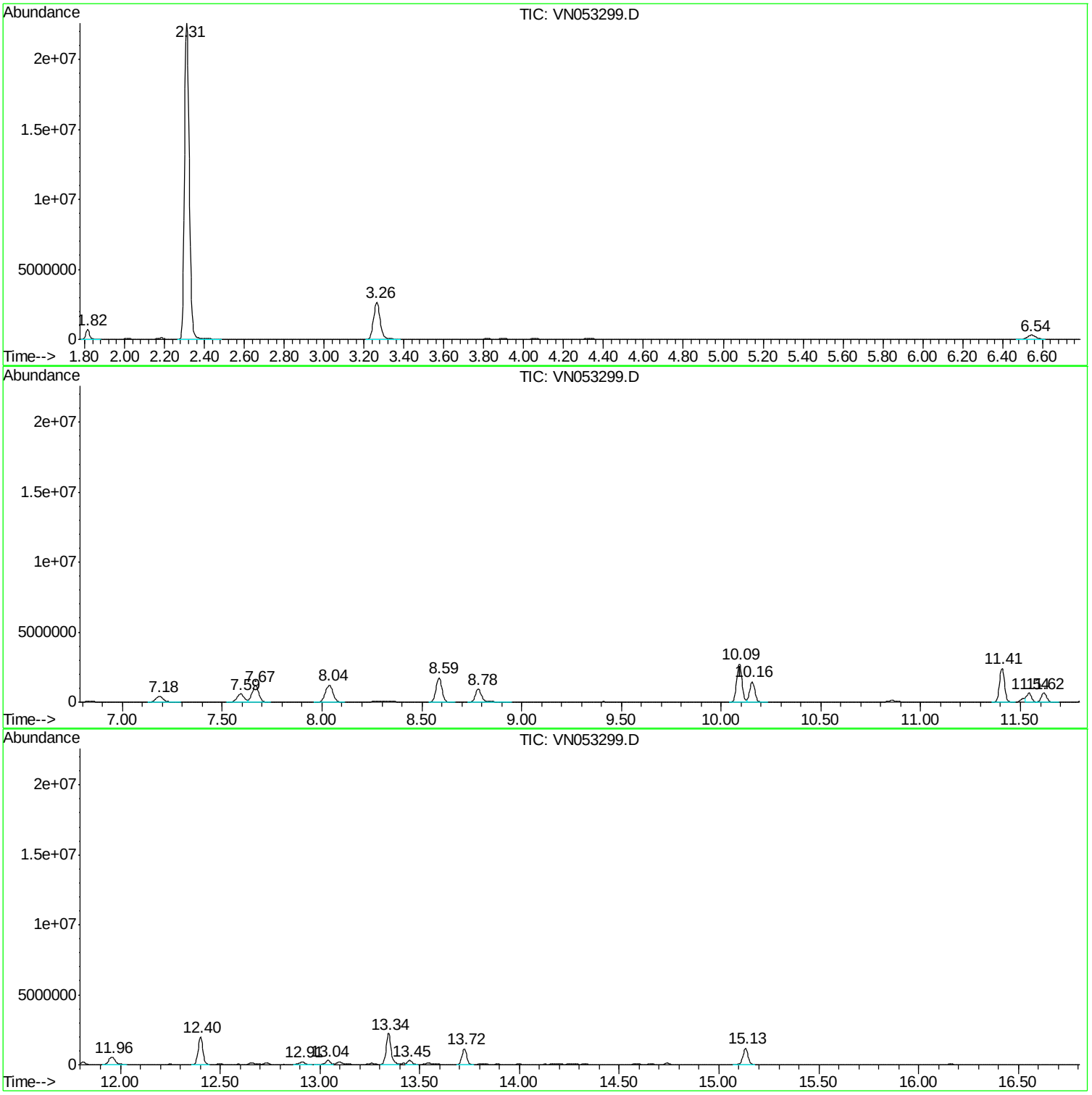
Data File : VN053299.D
Acq On : 7 Jan 2019 12:47
Operator : MD\SY
Sample : K1053-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : COMP-1-DRUM

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N010519W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN010719\
Data File : VN053299.D
Acq On : 7 Jan 2019 12:47
Operator : MD\SY
Sample : K1053-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : COMP-1-DRUM

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N010519W.M
Quant Title : SW846 8260

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

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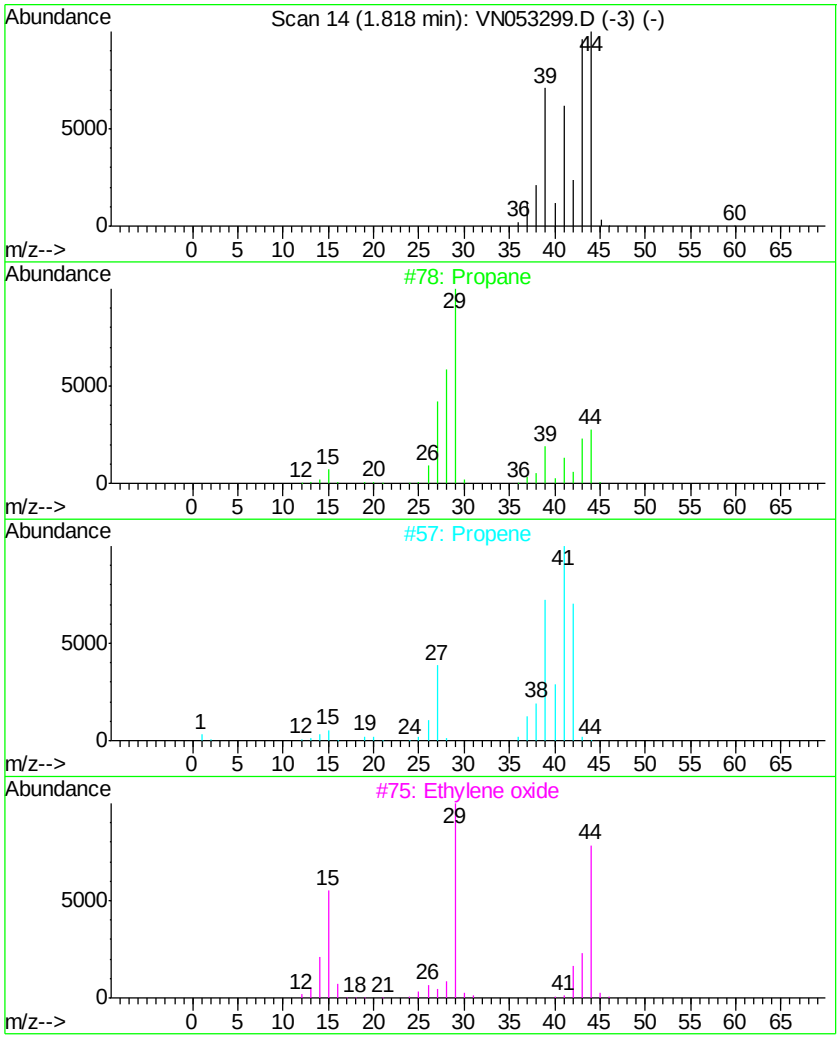
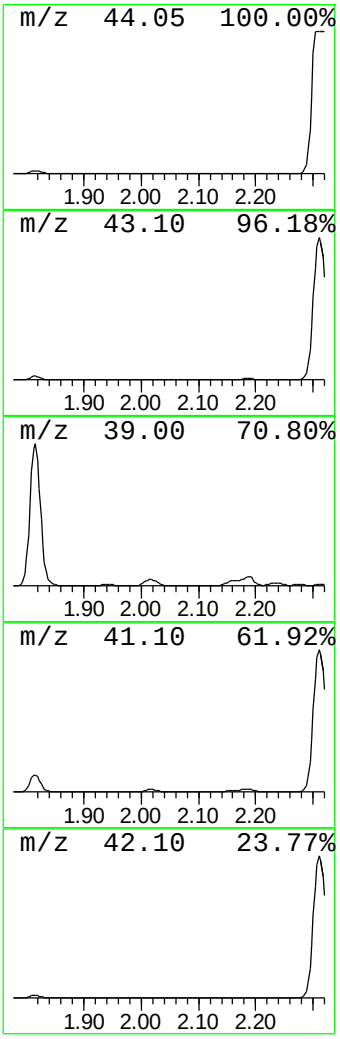
Peak Number 1 Propane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.82	16.29 ug/l	914760	Pentafluorobenzene	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	90
2	Propene	42	C3H6	000115-07-1	9
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Acetaldehyde	44	C2H4O	000075-07-0	3
5	Ethyne, fluoro-	44	C2HF	002713-09-9	3





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN010719\
Data File : VN053299.D
Acq On : 7 Jan 2019 12:47
Operator : MD\SY
Sample : K1053-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : COMP-1-DRUM

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N010519W.M
Quant Title : SW846 8260

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

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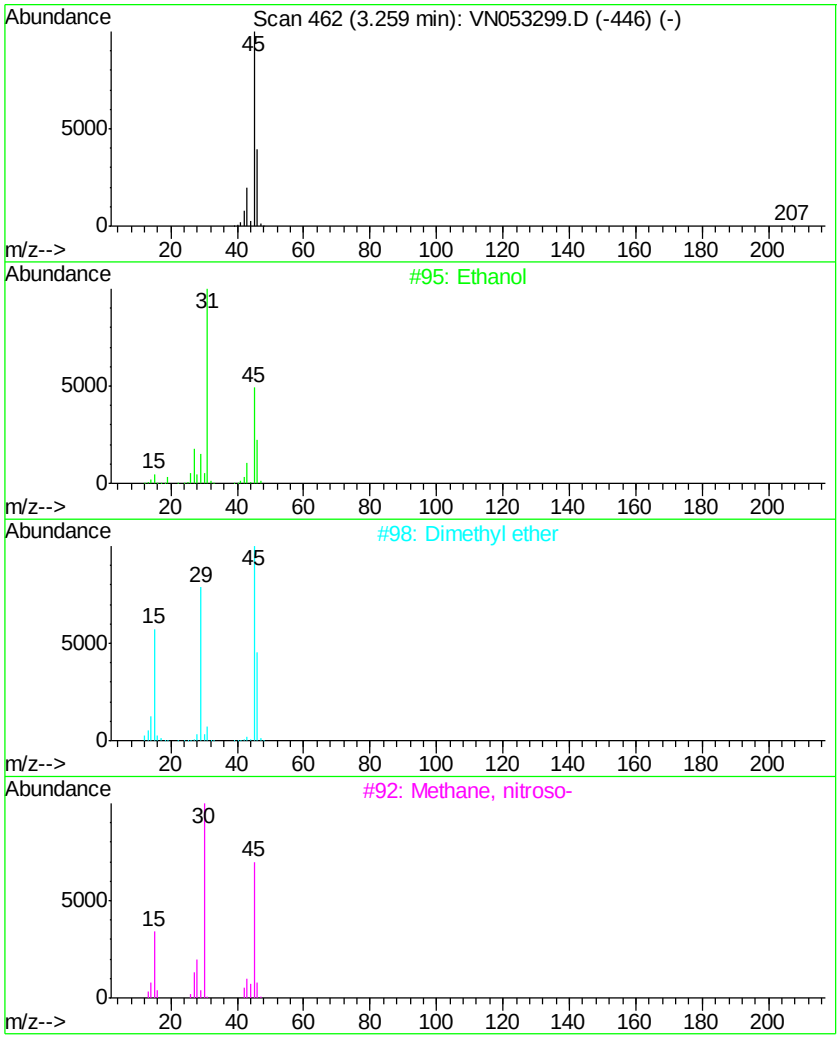
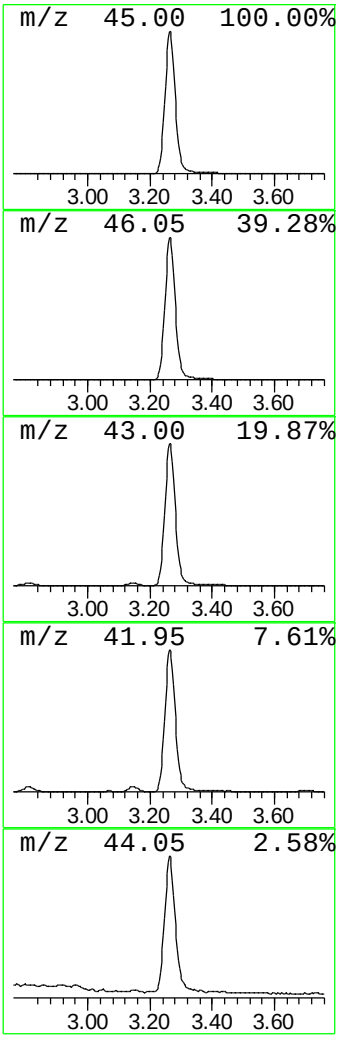
Peak Number 3 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.26	109.96 ug/l	6175740	Pentafluorobenzene	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	83
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





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN010719\
Data File : VN053299.D
Acq On : 7 Jan 2019 12:47
Operator : MD\SY
Sample : K1053-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : COMP-1-DRUM

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N010519W.M
Quant Title : SW846 8260

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

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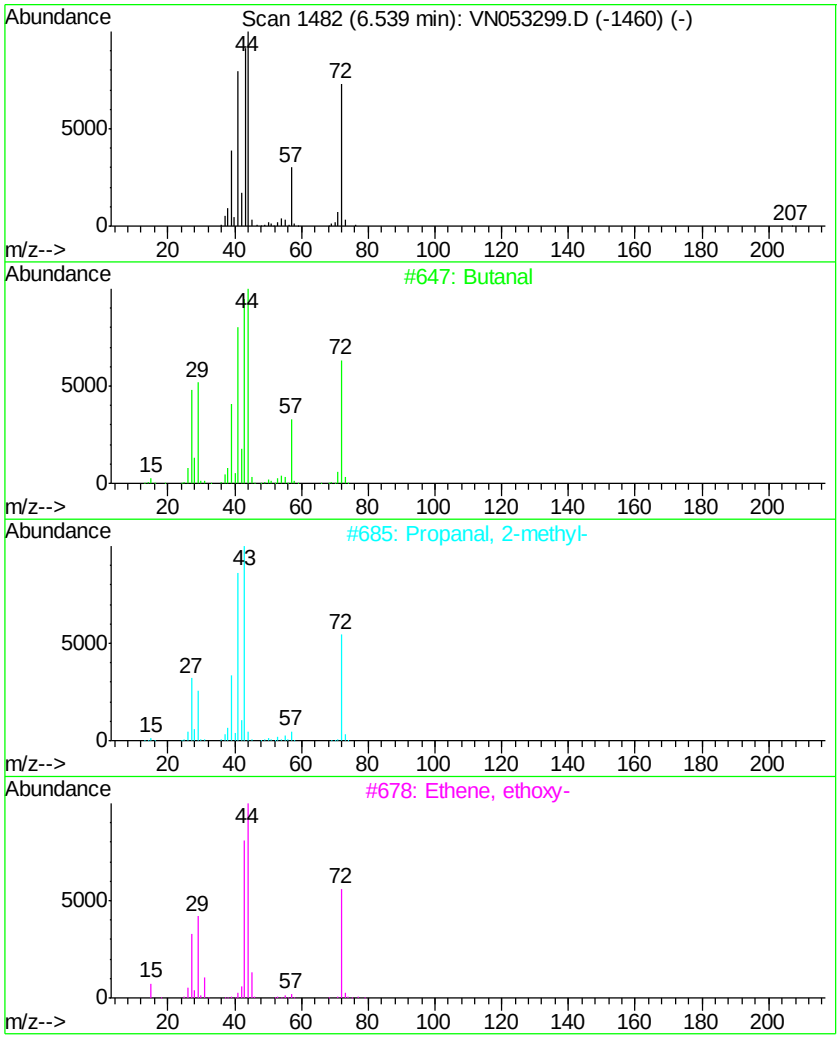
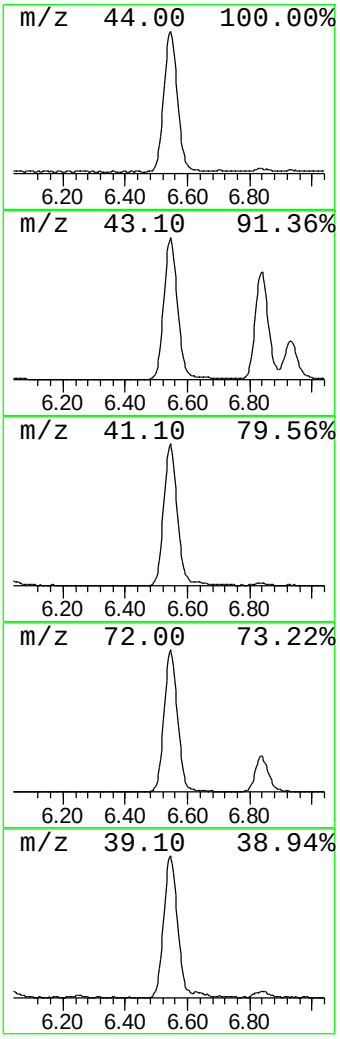
Peak Number 4 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	16.85 ug/l	946381	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	58
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	58
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
5	Isobutylene epoxide	72	C4H8O	000558-30-5	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN010719\
Data File : VN053299.D
Acq On : 7 Jan 2019 12:47
Operator : MD\SY
Sample : K1053-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : COMP-1-DRUM

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N010519W.M
Quant Title : SW846 8260

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

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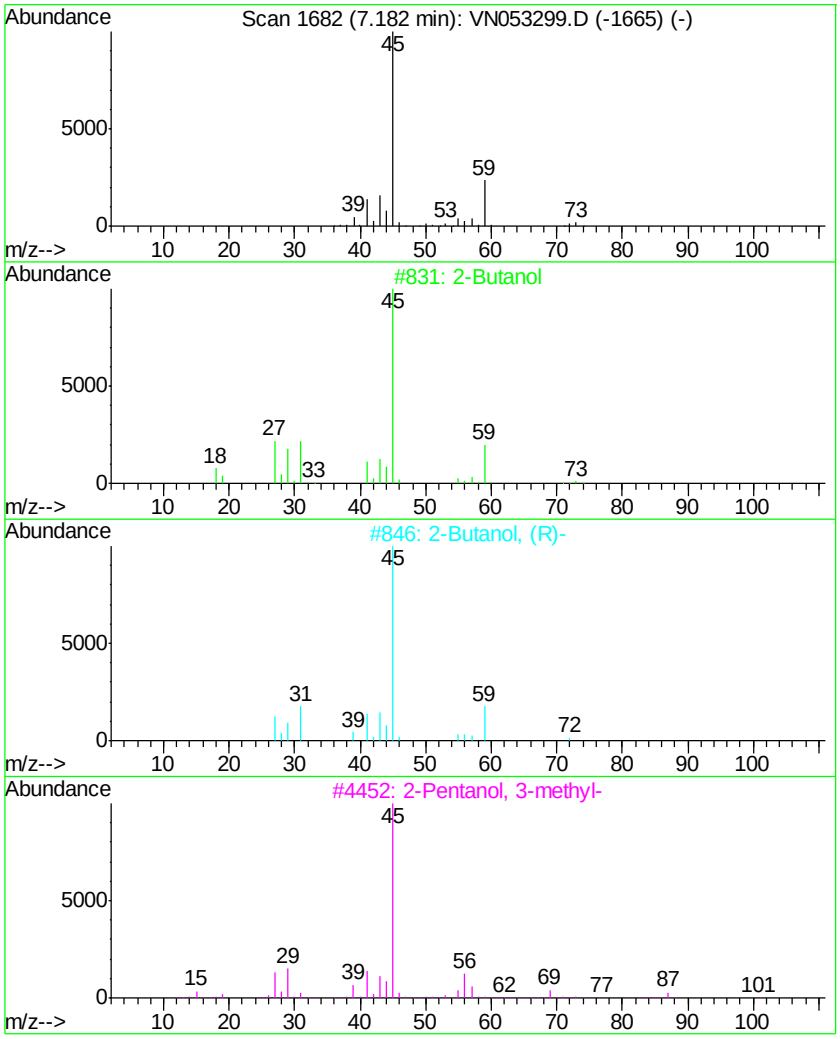
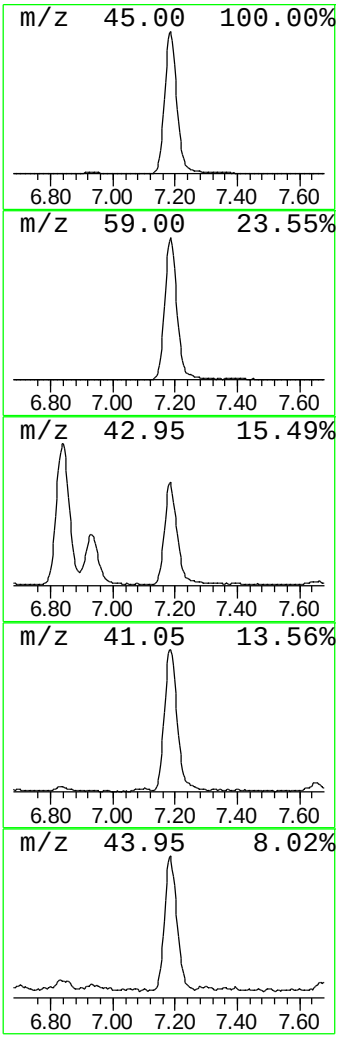
Peak Number 5 2-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.18	19.63 ug/l	1102620	Pentafluorobenzene	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol	74	C4H10O	000078-92-2	83
2	2-Butanol, (R)-	74	C4H10O	014898-79-4	78
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	59
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	42
5	Isoamyl lactate	160	C8H16O3	019329-89-6	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN010719\
Data File : VN053299.D
Acq On : 7 Jan 2019 12:47
Operator : MD\SY
Sample : K1053-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 8 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : COMP-1-DRUM

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N010519W.M
Quant Title : SW846 8260

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

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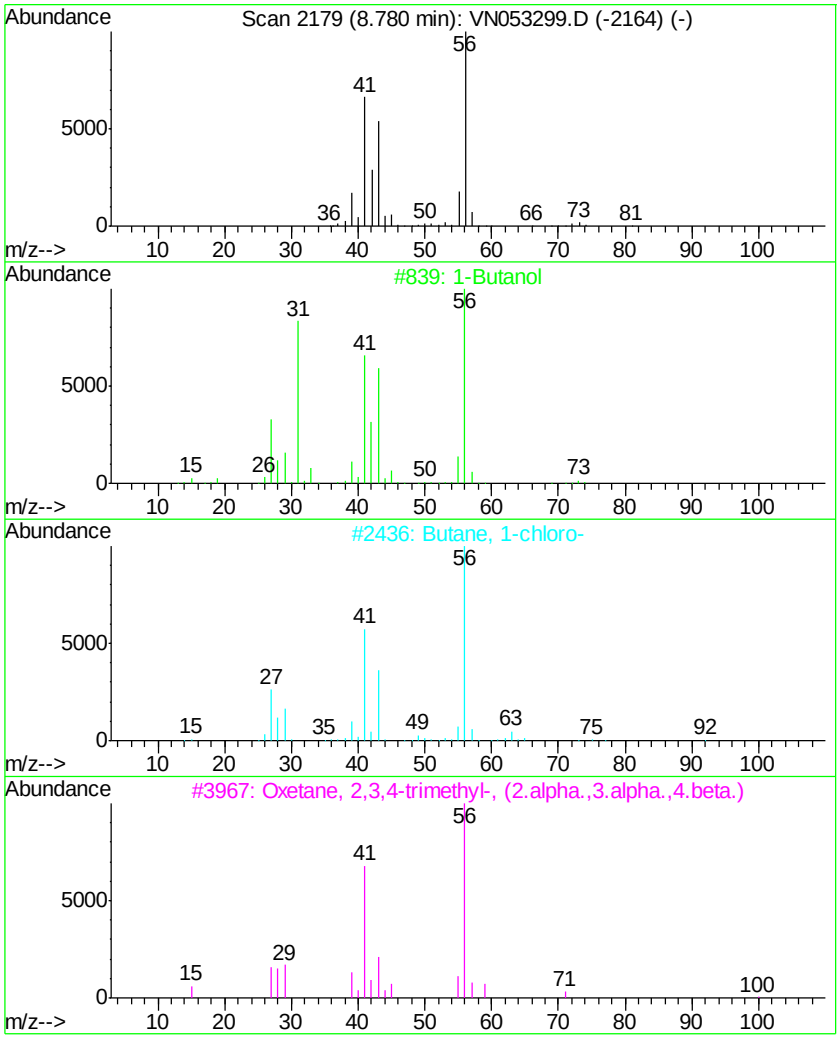
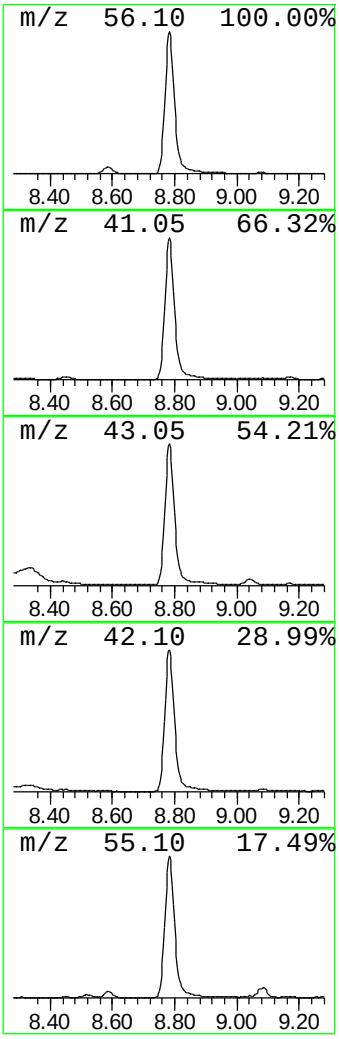
Peak Number 6 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.78	30.24 ug/l	2139570	1,4-Difluorobenzene	8.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	45
3	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	38
4	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	33
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9





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Operator : MD\SY
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ALS Vial : 8 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : COMP-1-DRUM

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N010519W.M
Quant Title : SW846 8260

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

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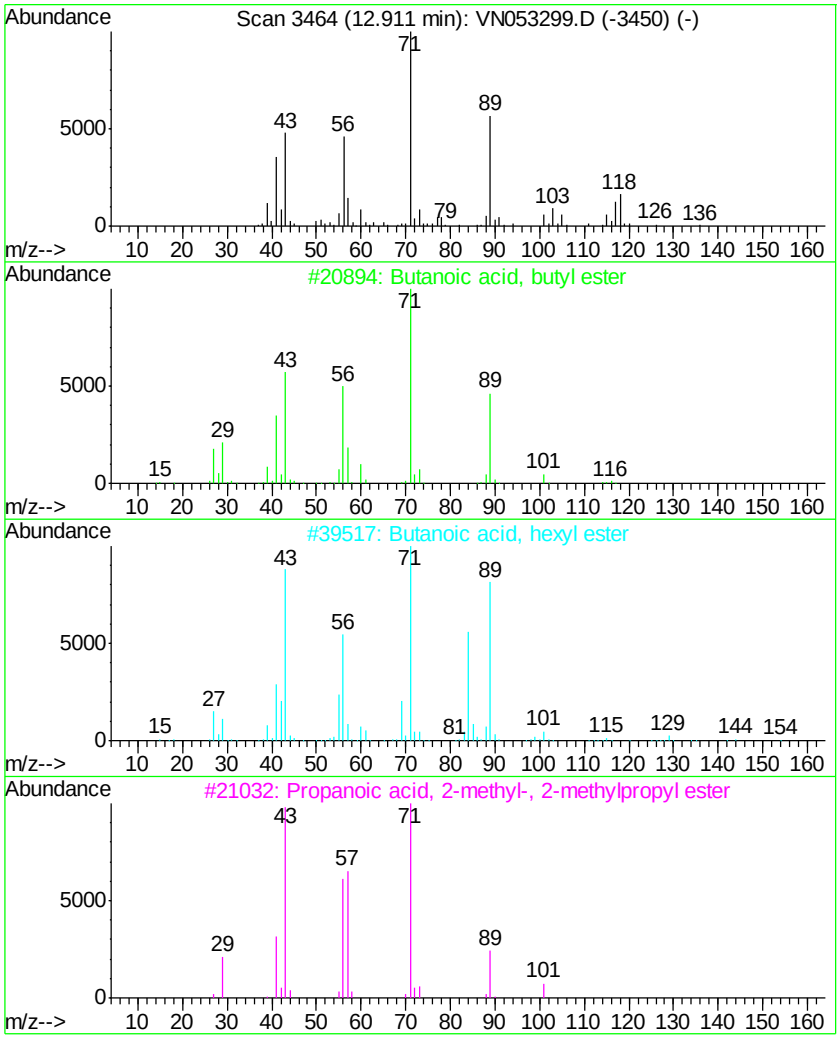
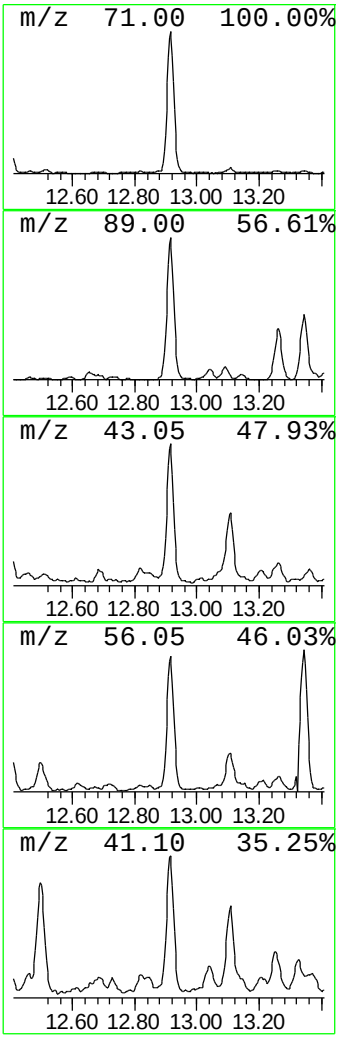
Peak Number 7 Butanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	5.33 ug/l	413249	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
2	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	59
3	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
4	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	47
5	3,4-dimethyl-5-phenyloxazolidine	177	C11H15NO	1000378-93-9	40





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN010719\
Data File : VN053299.D
Acq On : 7 Jan 2019 12:47
Operator : MD\SY
Sample : K1053-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : COMP-1-DRUM

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N010519W.M
Quant Title : SW846 8260

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

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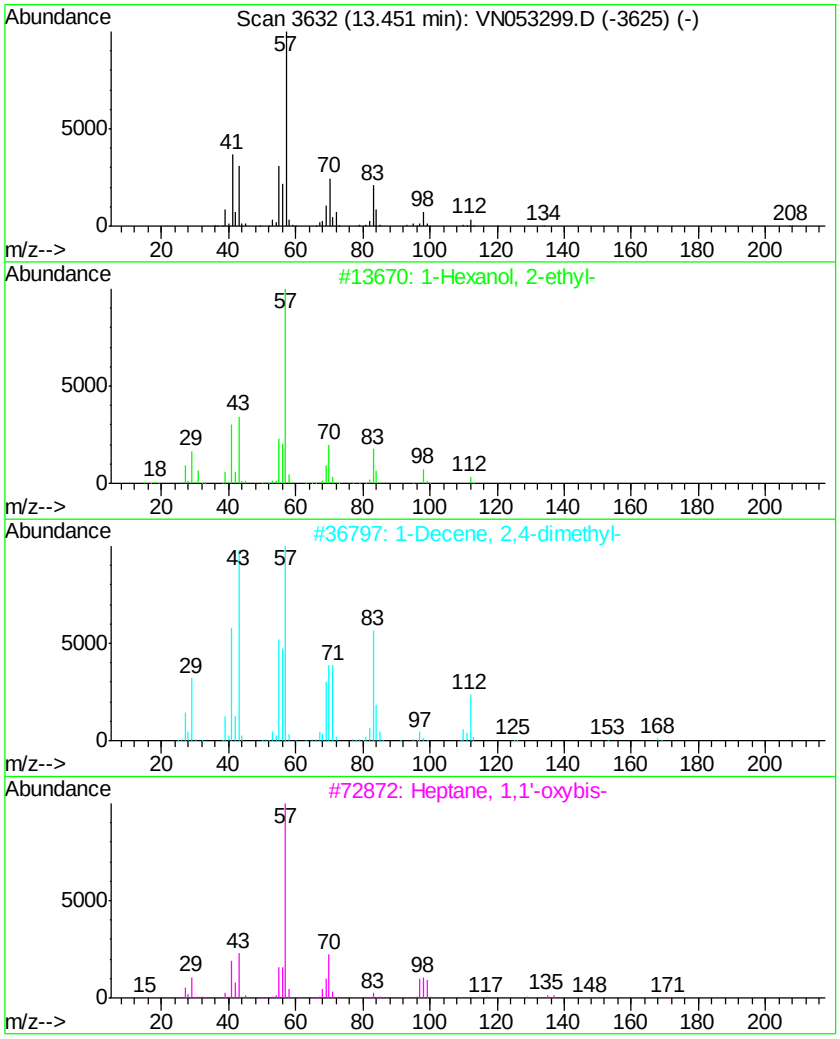
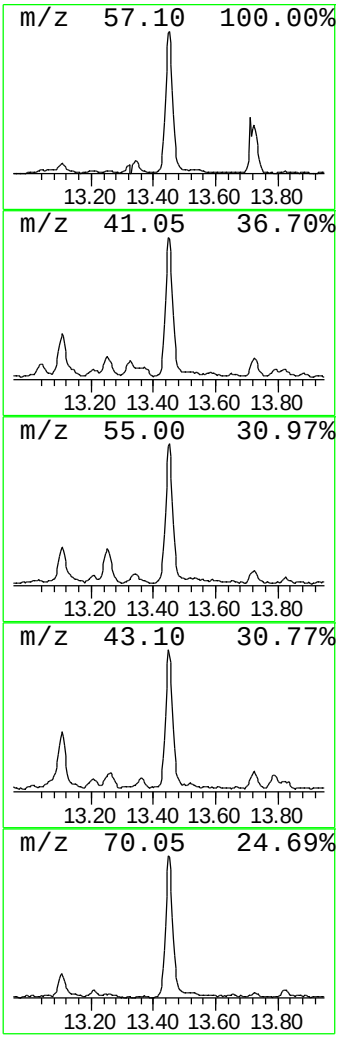
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	5.94 ug/l	460695	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	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47
4	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	40
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	40





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Operator : MD\SY
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ALS Vial : 8 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : COMP-1-DRUM

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N010519W.M
Quant Title : SW846 8260

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

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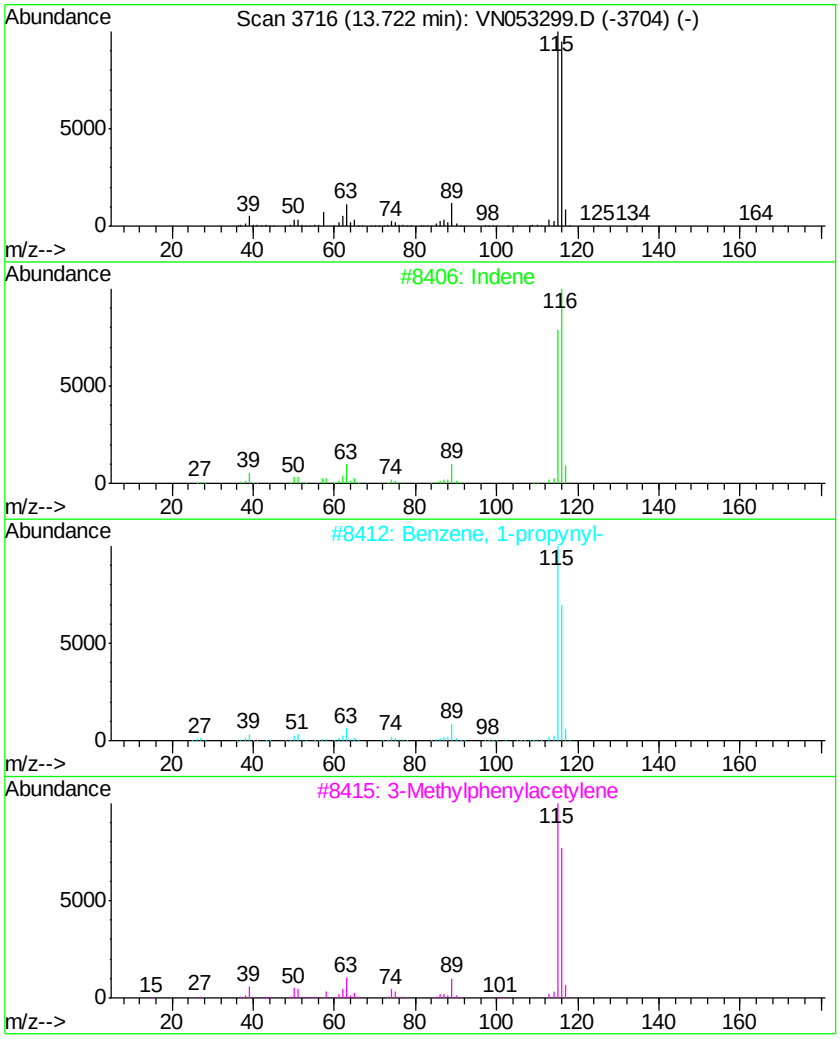
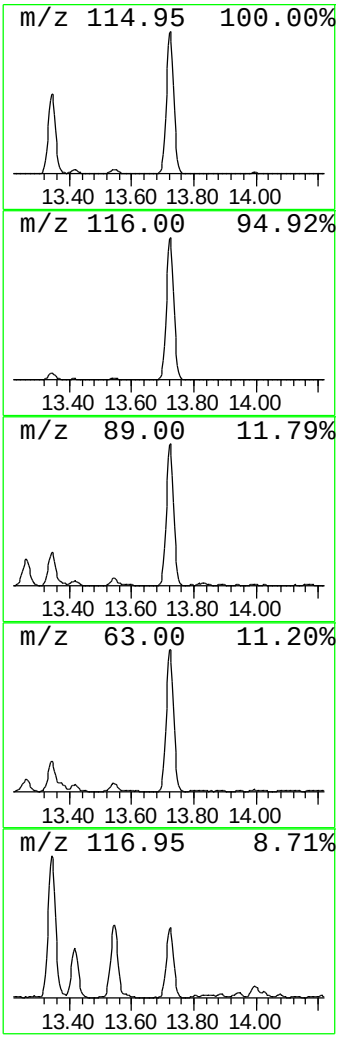
Peak Number 9 Indene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	24.58 ug/l	1906930	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5	2-Methylphenylacetylene	116	C9H8	000766-47-2	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN010719\
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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
Propane	1.82	16.3	ug/l	914760	1	7.67	2808180	50.0
Ethanol	3.26	110.0	ug/l	6175740	1	7.67	2808180	50.0
Butanal	6.54	16.9	ug/l	946381	1	7.67	2808180	50.0
2-Butanol	7.18	19.6	ug/l	1102620	1	7.67	2808180	50.0
1-Butanol	8.78	30.2	ug/l	2139570	2	8.59	3537610	50.0
Butanoic acid, bu...	12.91	5.3	ug/l	413249	4	13.35	3879270	50.0
1-Hexanol, 2-ethyl-	13.45	5.9	ug/l	460695	4	13.35	3879270	50.0
Indene	13.72	24.6	ug/l	1906930	4	13.35	3879270	50.0