LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX041219\
Data File : VX008917.D
Acq On : 13 Apr 2019 03:59
Operator : JC/SP
Sample : K2371-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : OK-COMP

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_X\METHOD\82X040319W.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	1.642	65	80	96	rVB	818174	1270145	2.43%	1.225%
2	2.446	205	212	234	rBV	9101747	16471188	31.57%	15.881%
3	2.776	259	266	275	rBV	387156	683990	1.31%	0.659%
4	3.964	450	461	479	rBV	306092	799386	1.53%	0.771%
5	5.665	727	740	757	rVB	200125	573449	1.10%	0.553%
6	6.860	926	936	952	rBV	323692	779596	1.49%	0.752%
7	8.720	1235	1241	1246	rBV	602944	990668	1.90%	0.955%
8	8.799	1246	1254	1260	rBV	28304622	52179071	100.00%	50.309%
9	9.579	1374	1382	1387	rBV	1432138	1882241	3.61%	1.815%
10	9.634	1387	1391	1397	rVB	1799392	2400068	4.60%	2.314%
11	10.110	1464	1469	1478	rBV	581847	816324	1.56%	0.787%
12	10.250	1488	1492	1498	rVB	1318067	1673200	3.21%	1.613%
13	10.360	1502	1510	1516	rBV	5314443	6936857	13.29%	6.688%
14	10.701	1560	1566	1578	rVB	2218260	3112293	5.96%	3.001%
15	11.134	1632	1637	1642	rBV	484084	622300	1.19%	0.600%
16	11.433	1681	1686	1694	rVV	1428147	2409873	4.62%	2.323%
17	11.506	1694	1698	1707	rVB	766030	926812	1.78%	0.894%
18	11.664	1720	1724	1729	rVB	685742	896199	1.72%	0.864%
19	11.804	1740	1747	1752	rVB	1795324	2172313	4.16%	2.094%
20	12.079	1788	1792	1797	rVV	578001	741090	1.42%	0.715%
21	12.140	1797	1802	1807	rVB	1003734	1193343	2.29%	1.151%
22	12.268	1818	1823	1827	rBV	1938576	2416568	4.63%	2.330%
23	13.213	1970	1978	1989	rBV	1175101	1770775	3.39%	1.707%

Sum of corrected areas: 103717749

LSC Report - Integrated Chromatogram

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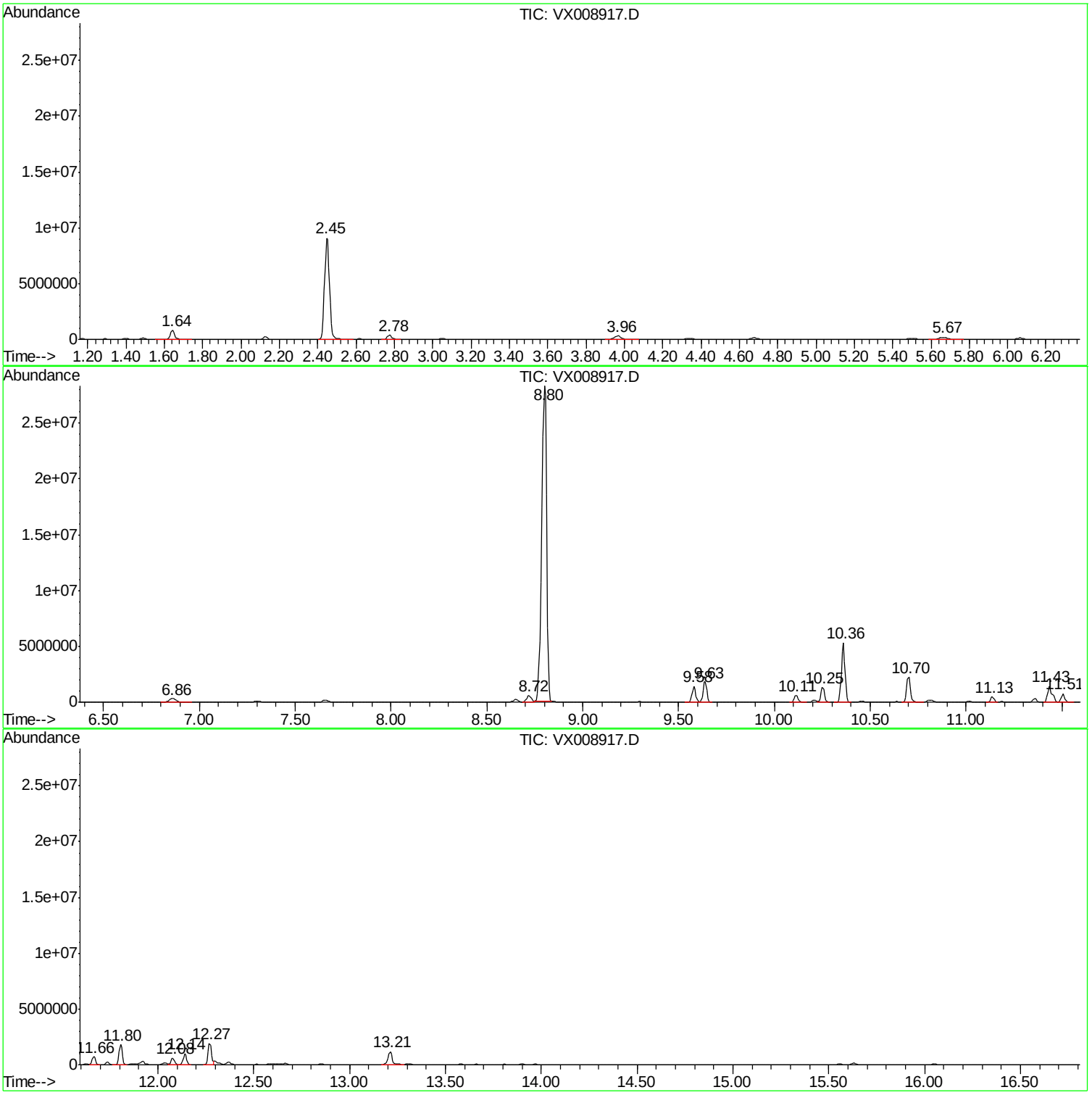
Operator : JC/SP
Sample : K2371-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
OK-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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



Library Search Compound Report

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Data File : VX008917.D
Acq On : 13 Apr 2019 03:59
Operator : JC/SP
Sample : K2371-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : OK-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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

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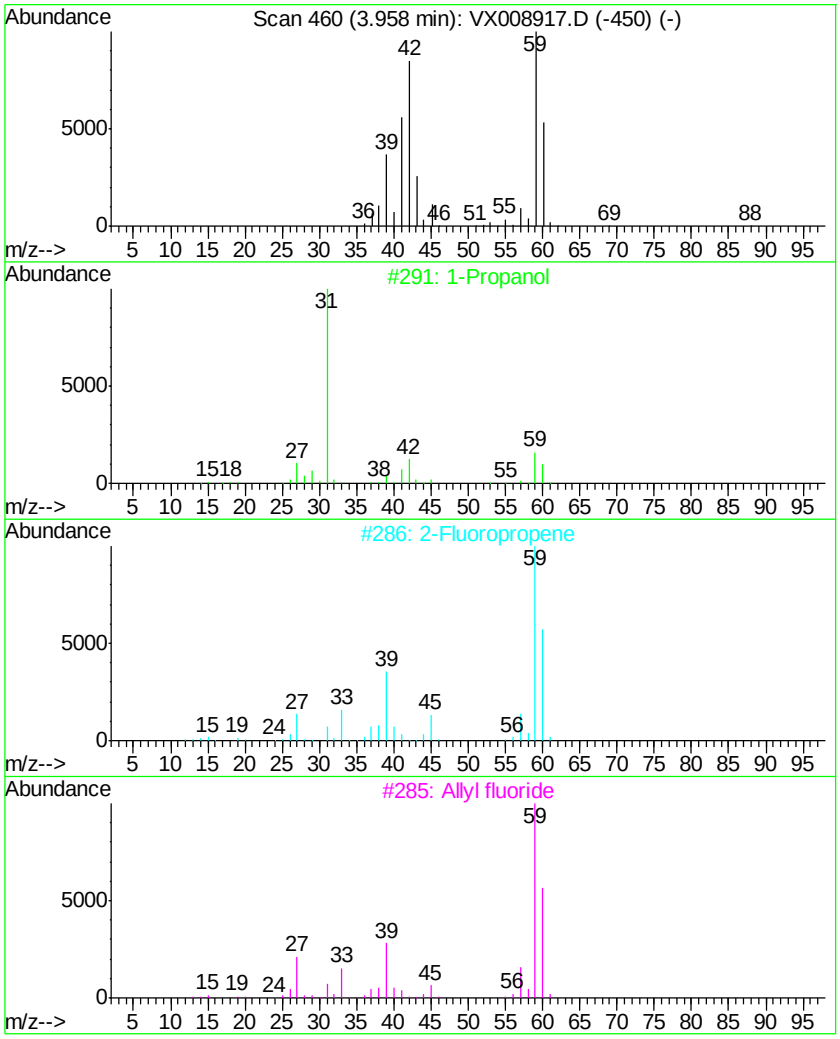
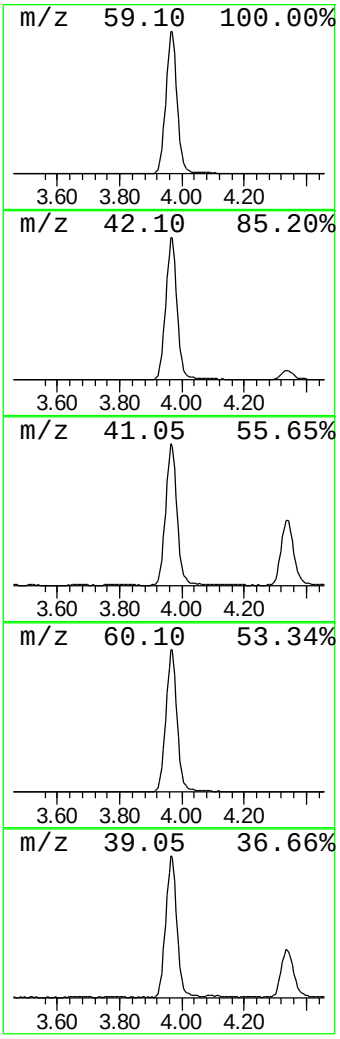
Peak Number 2 1-Propanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.96	69.70 ug/l	799386	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	2-Fluoropropene	60	C3H5F	001184-60-7	52
3	Allyl fluoride	60	C3H5F	000818-92-8	43
4	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	17
5	Cyclopropane	42	C3H6	000075-19-4	9





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Data File : VX008917.D
Acq On : 13 Apr 2019 03:59
Operator : JC/SP
Sample : K2371-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : OK-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

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

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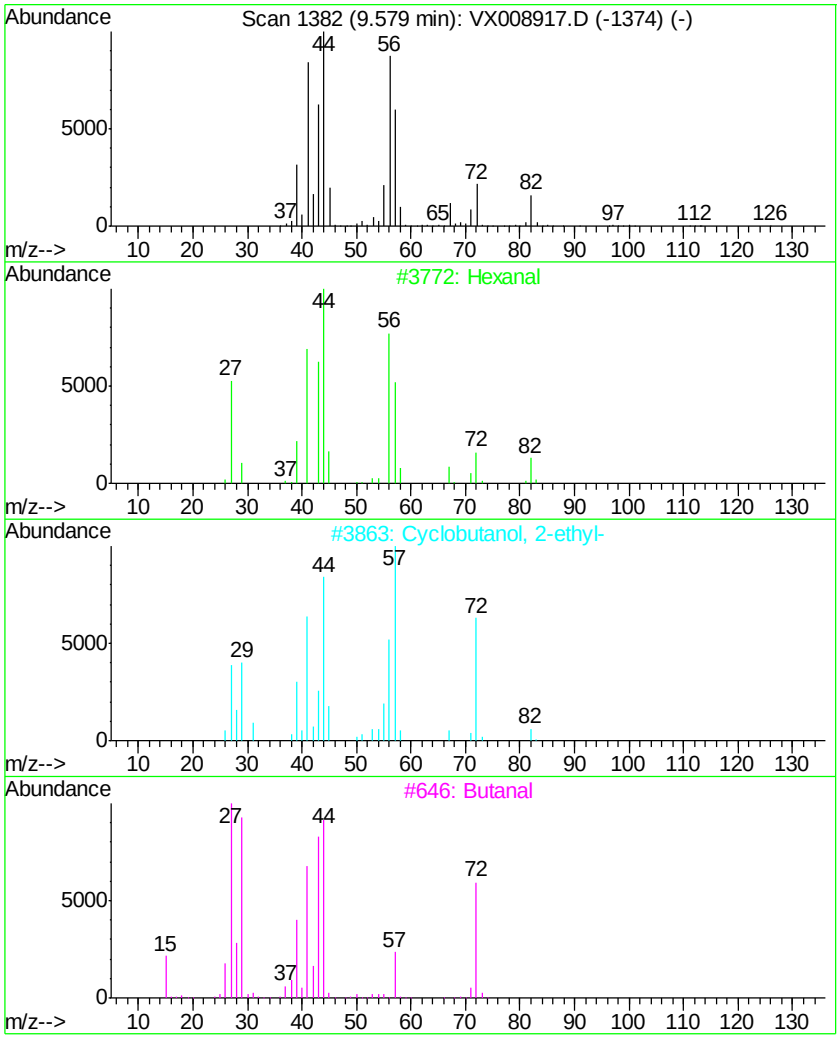
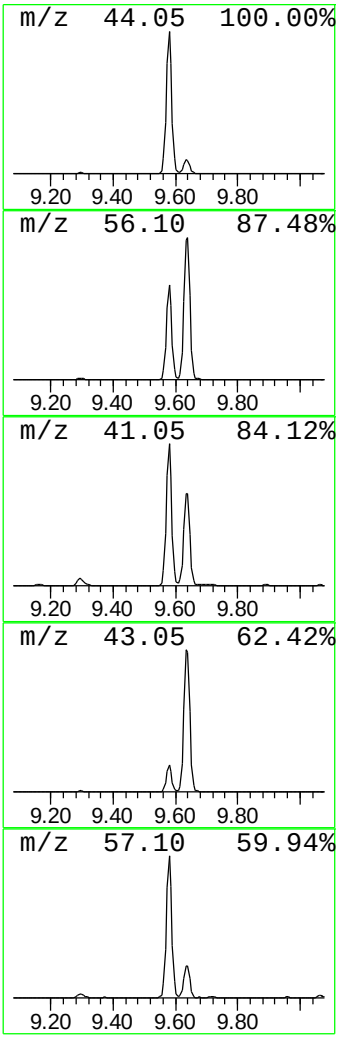
Peak Number 3 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.58	115.29 ug/l	1882240	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	90
2	Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	36
3	Butanal	72	C4H8O	000123-72-8	35
4	Butanal, 3-methyl-	86	C5H10O	000590-86-3	32
5	1,5-Pentanediol	104	C5H12O2	000111-29-5	28





Library Search Compound Report

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Data File : VX008917.D
Acq On : 13 Apr 2019 03:59
Operator : JC/SP
Sample : K2371-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : OK-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

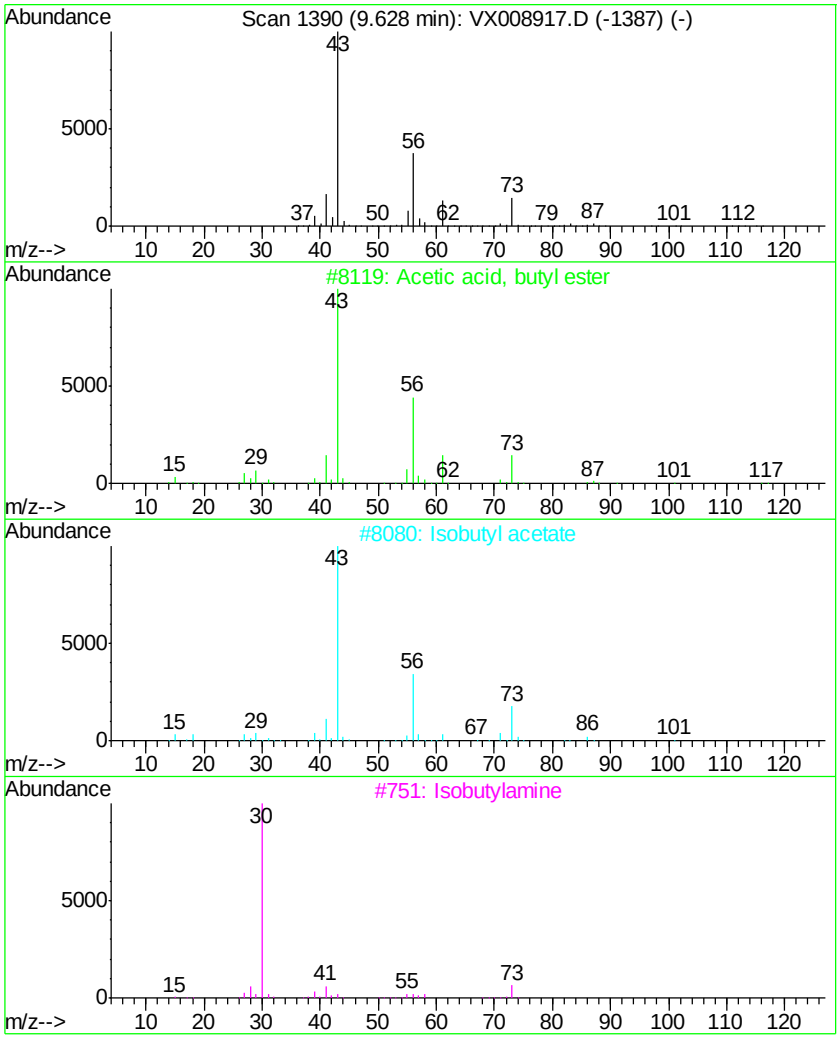
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

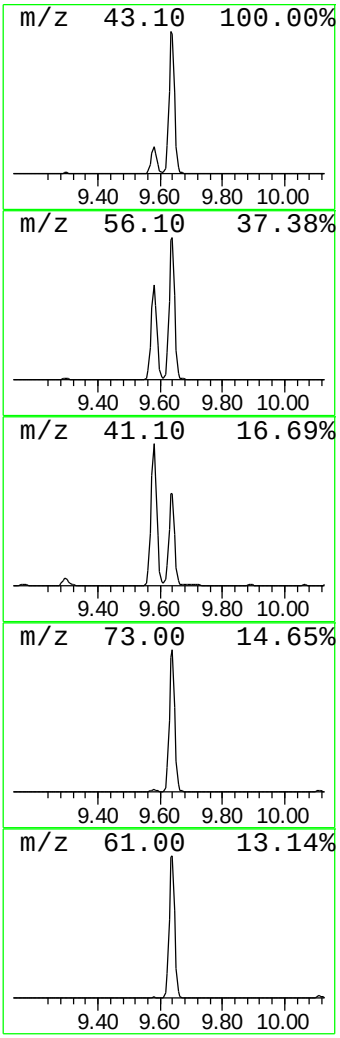
****

Peak Number 4 Acetic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.63	147.01 ug/l	2400070	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Isobutyl acetate	116	C6H12O2	000110-19-0	40
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	9





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Data File : VX008917.D
Acq On : 13 Apr 2019 03:59
Operator : JC/SP
Sample : K2371-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : OK-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

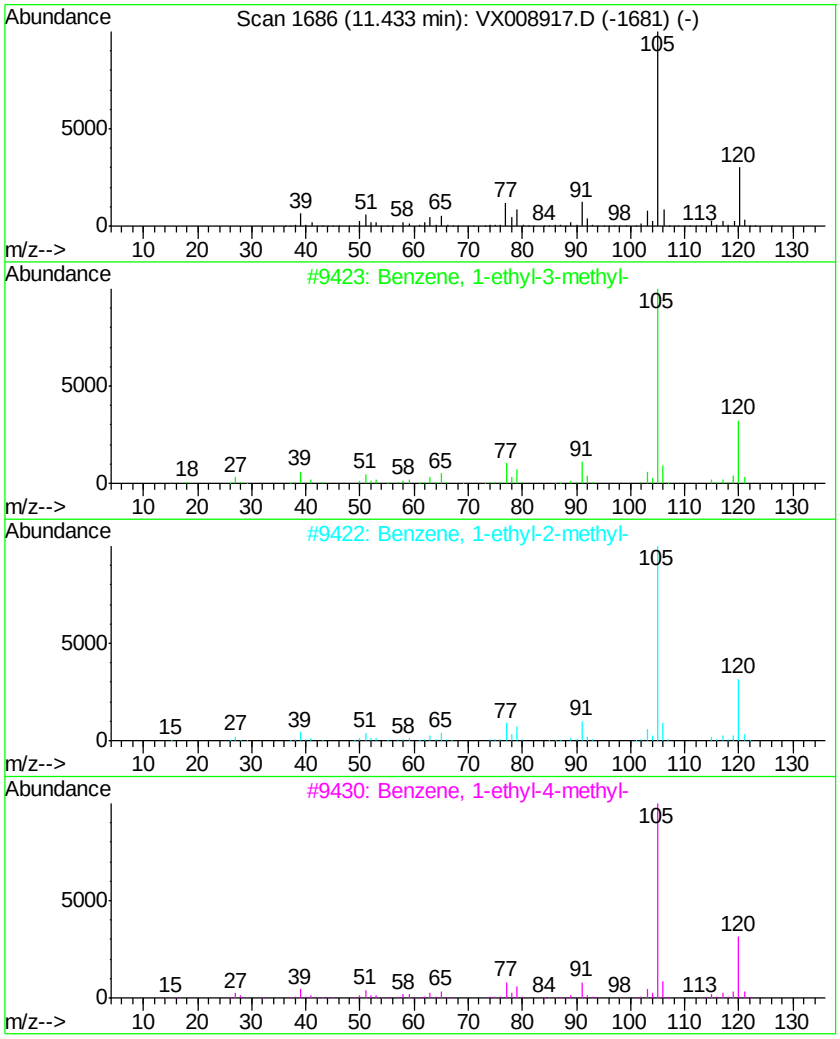
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

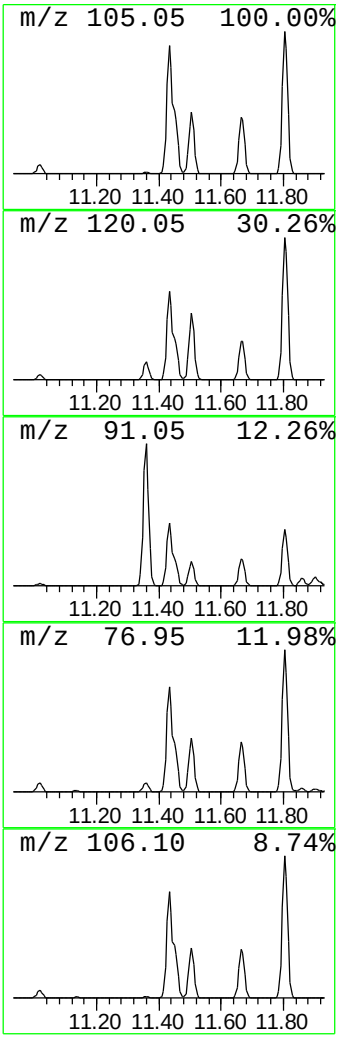
****

Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	162.59 ug/l	2409870	1,4-Dichlorobenzene-d4	12.08

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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Acq On : 13 Apr 2019 03:59
Operator : JC/SP
Sample : K2371-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : OK-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

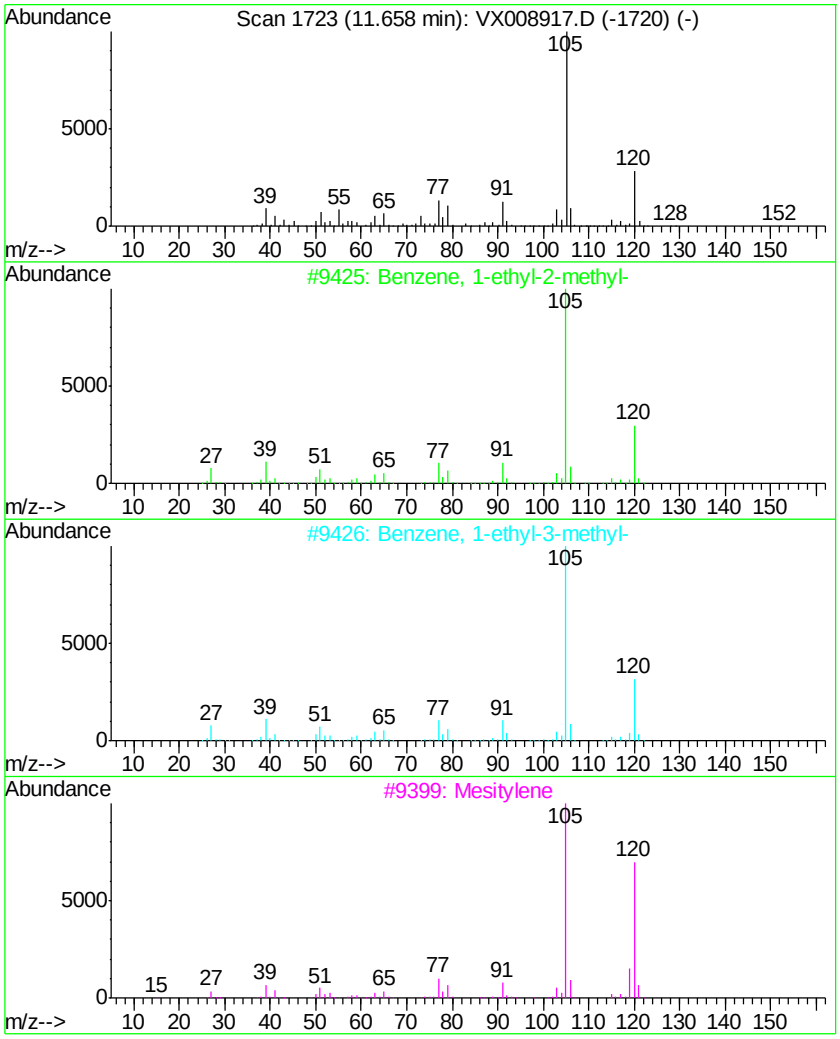
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

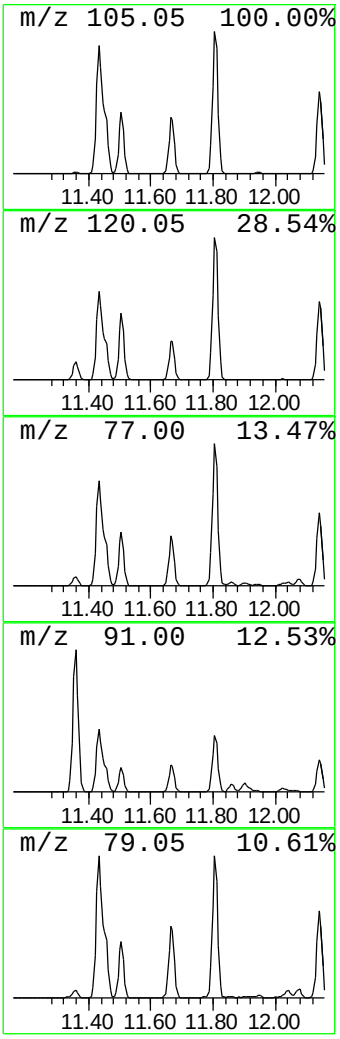
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	60.46 ug/l	896199	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Library Search Compound Report

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Sample : K2371-01
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ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : OK-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

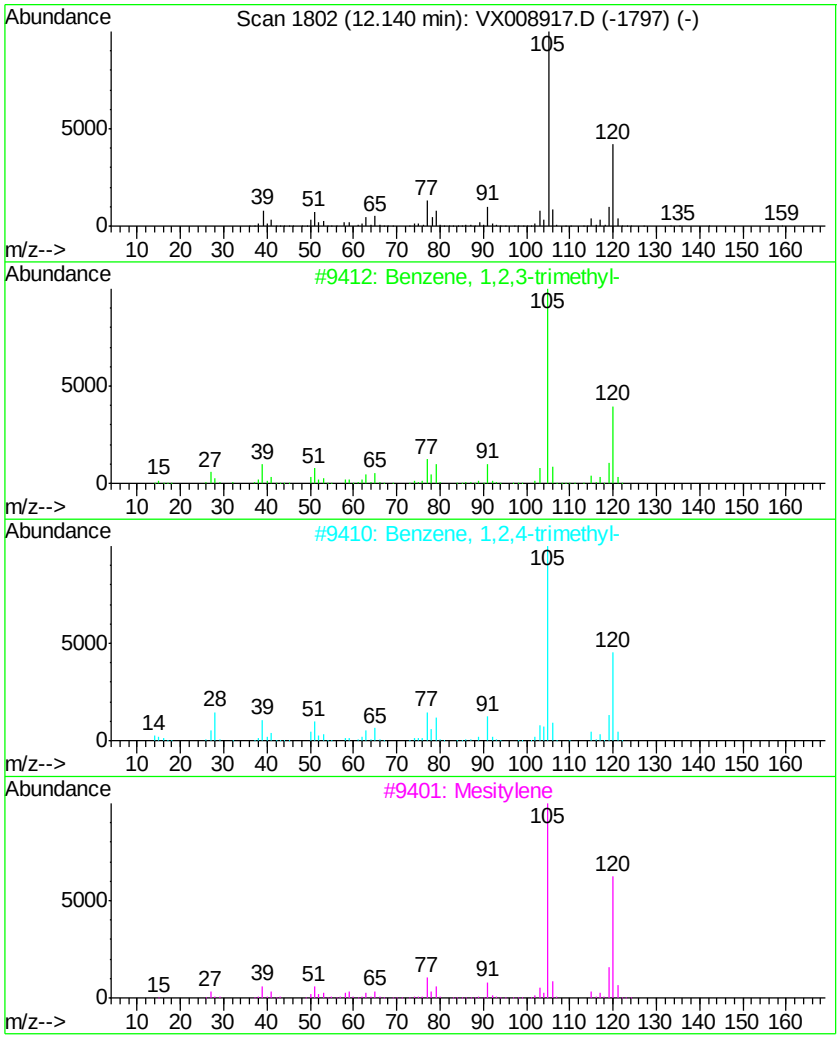
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

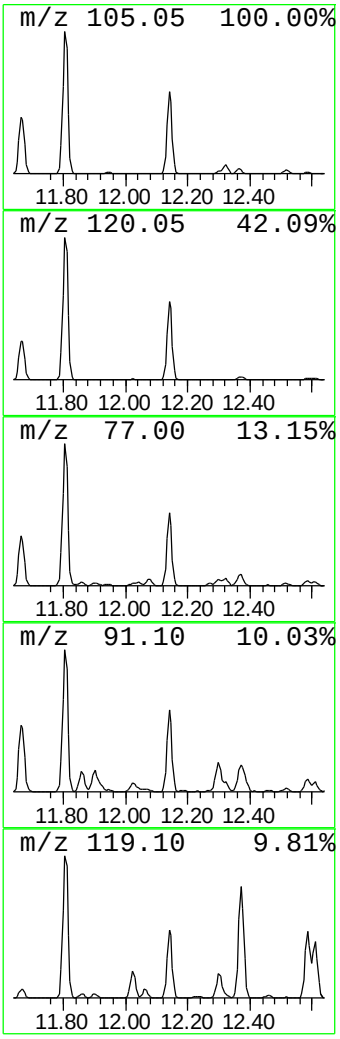
****

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	80.51 ug/l	1193340	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87





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ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : OK-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X040319W.M
Quant Title : SW846 8260

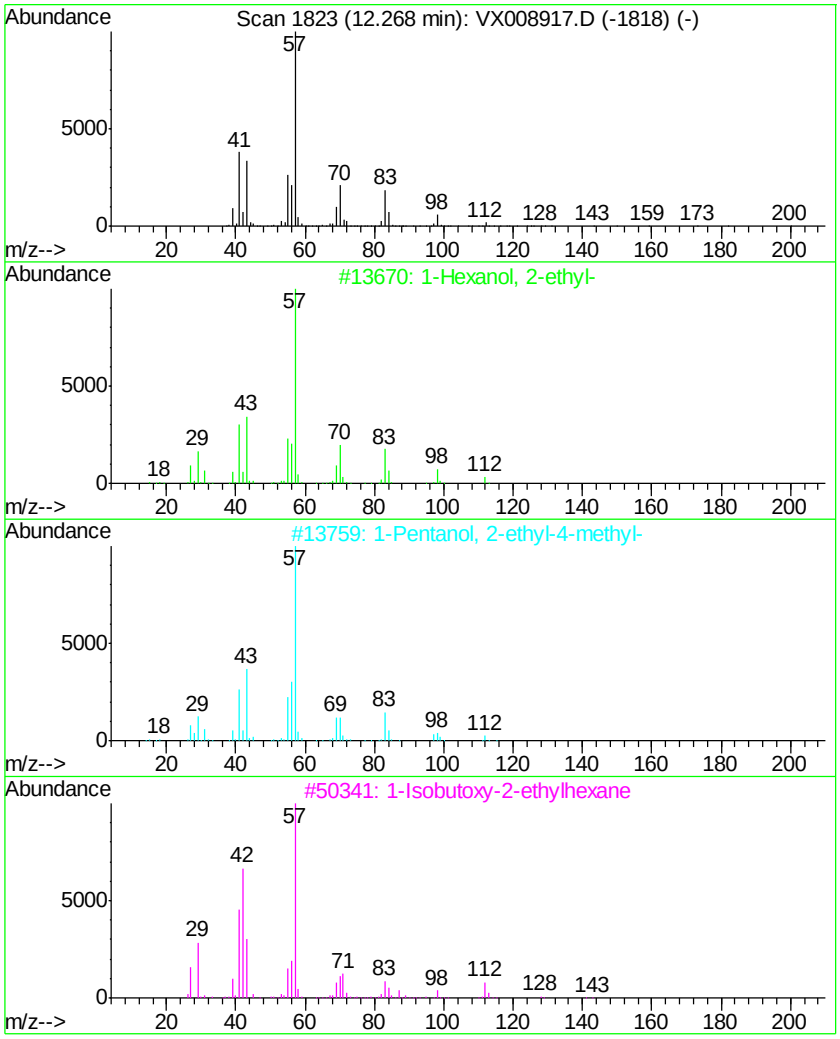
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

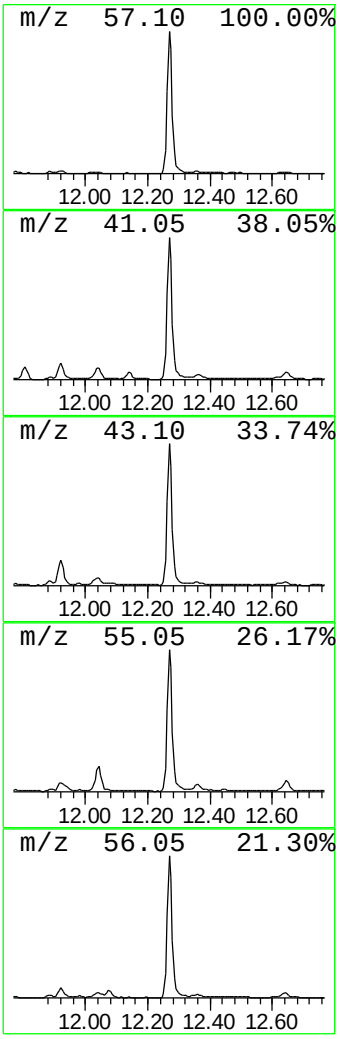
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	163.04 ug/l	2416570	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	53
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50





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Quant Title : SW846 8260

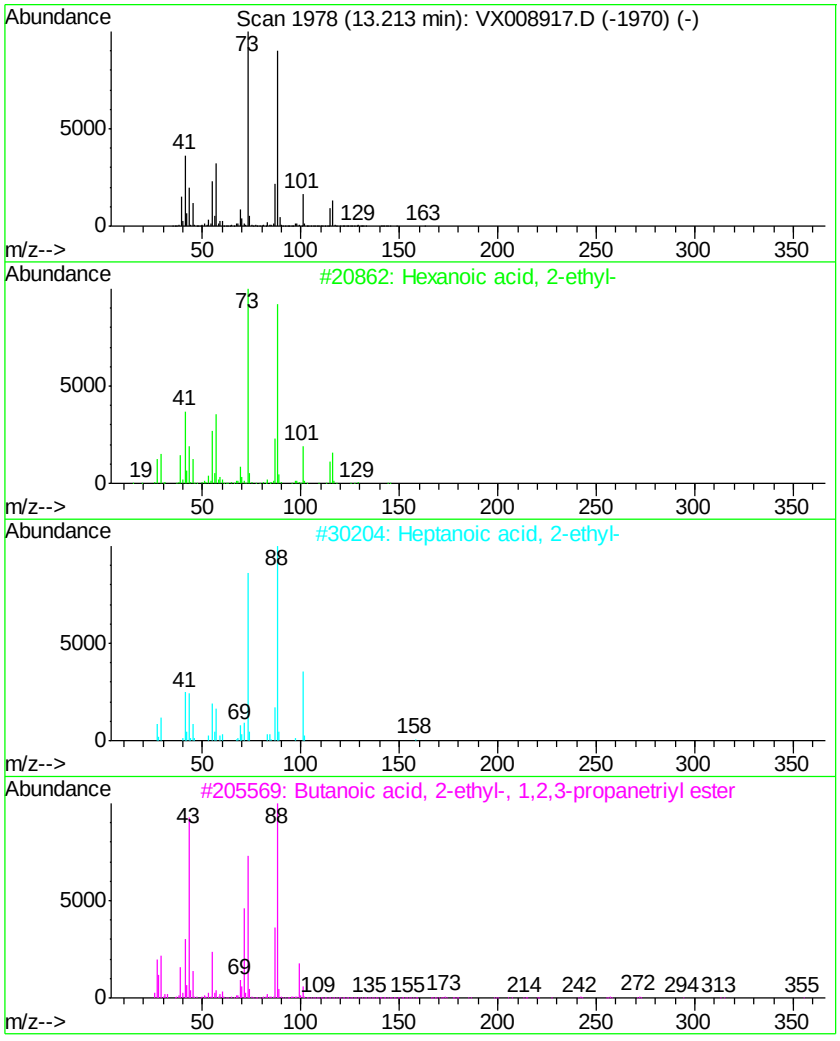
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

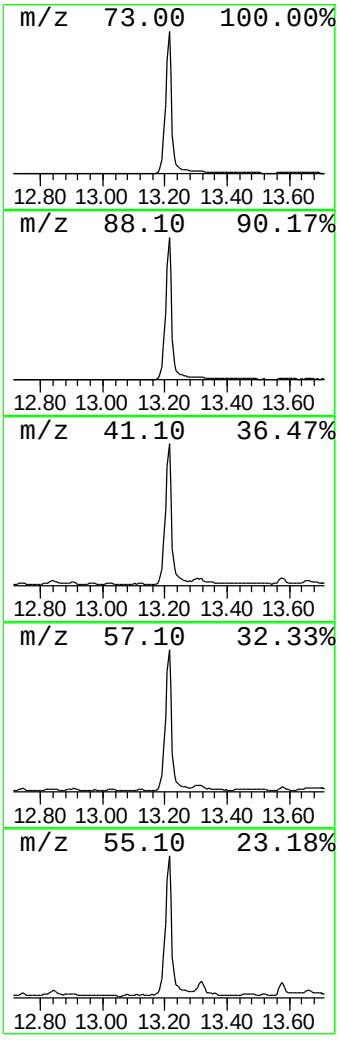
****

Peak Number 9 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	119.47 ug/l	1770780	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	91
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	45
4	Heptanoic acid, 2,6-dimethyl-, m...	172	C10H20O2	033315-72-9	40
5	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40





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
1-Propanol	3.96	69.7	ug/l	799386	1	5.67	573449	50.0
Hexanal	9.58	115.3	ug/l	1882240	3	10.12	816324	50.0
Acetic acid, buty...	9.63	147.0	ug/l	2400070	3	10.12	816324	50.0
Benzene, 1-ethyl-...	11.43	162.6	ug/l	2409870	4	12.08	741090	50.0
Benzene, 1-ethyl-...	11.66	60.5	ug/l	896199	4	12.08	741090	50.0
Benzene, 1,2,3-tr...	12.14	80.5	ug/l	1193340	4	12.08	741090	50.0
1-Hexanol, 2-ethyl-	12.27	163.0	ug/l	2416570	4	12.08	741090	50.0
Hexanoic acid, 2-...	13.21	119.5	ug/l	1770780	4	12.08	741090	50.0