LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050222\
Data File : VX028486.D
Acq On : 02 May 2022 20:18
Operator : JC/MD
Sample : N2642-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30988

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\82X041922W.M
Title : SW846 8260

Signal : TIC: VX028486.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.356	40	44	51	rBV	189511	175909	3.18%	0.622%
2	1.453	56	60	71	rBV	1338809	1660175	29.97%	5.867%
3	2.057	153	159	171	rBV	224494	347738	6.28%	1.229%
4	2.374	205	211	221	rBV	978694	1618835	29.23%	5.720%
5	2.532	230	237	253	rBV	654454	1176842	21.25%	4.159%
6	2.959	298	307	316	rVB2	26637	63973	1.16%	0.226%
7	4.233	505	516	530	rBV2	20039	61621	1.11%	0.218%
8	4.556	557	569	583	rBV	208509	586342	10.59%	2.072%
9	5.007	629	643	668	rBV	245207	795442	14.36%	2.811%
10	5.391	693	706	721	rBV2	296078	858620	15.50%	3.034%
11	5.556	721	733	748	rVB	392986	1118803	20.20%	3.954%
12	5.830	770	778	790	rBV	33442	94064	1.70%	0.332%
13	5.958	790	799	809	rBV	291856	773533	13.97%	2.733%
14	6.763	921	931	944	rBV	629209	1484913	26.81%	5.247%
15	7.214	997	1005	1018	rBV	99084	225421	4.07%	0.797%
16	8.574	1221	1228	1234	rBV	176440	286032	5.16%	1.011%
17	8.653	1234	1241	1247	rVV	1615997	2509657	45.31%	8.868%
18	8.720	1247	1252	1261	rVB	777795	1161649	20.97%	4.105%
19	10.055	1463	1471	1486	rBV	1440662	1954028	35.28%	6.905%
20	10.305	1507	1512	1519	rVB	81043	114933	2.08%	0.406%
21	10.647	1563	1568	1572	rBV	89033	134115	2.42%	0.474%
22	11.085	1634	1640	1651	rVB	1390682	1833456	33.10%	6.479%
23	11.573	1715	1720	1724	rBV	130771	169801	3.07%	0.600%
24	11.634	1724	1730	1739	rVB2	114121	173353	3.13%	0.613%
25	11.756	1745	1750	1756	rVB	79195	106041	1.91%	0.375%
26	12.024	1788	1794	1800	rBV	1700106	2003488	36.17%	7.080%
27	12.091	1800	1805	1810	rVB	57456	73808	1.33%	0.261%
28	12.219	1821	1826	1841	rBV	4619843	5538755	100.00%	19.572%
29	12.719	1902	1908	1913	rVB	196538	248516	4.49%	0.878%
30	12.805	1917	1922	1927	rVV	158661	210226	3.80%	0.743%
31	12.957	1942	1947	1954	rVB	420795	520845	9.40%	1.841%
32	13.780	2076	2082	2089	rVB	162645	217910	3.93%	0.770%

Sum of corrected areas: 28298844

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Acq On : 02 May 2022 20:18
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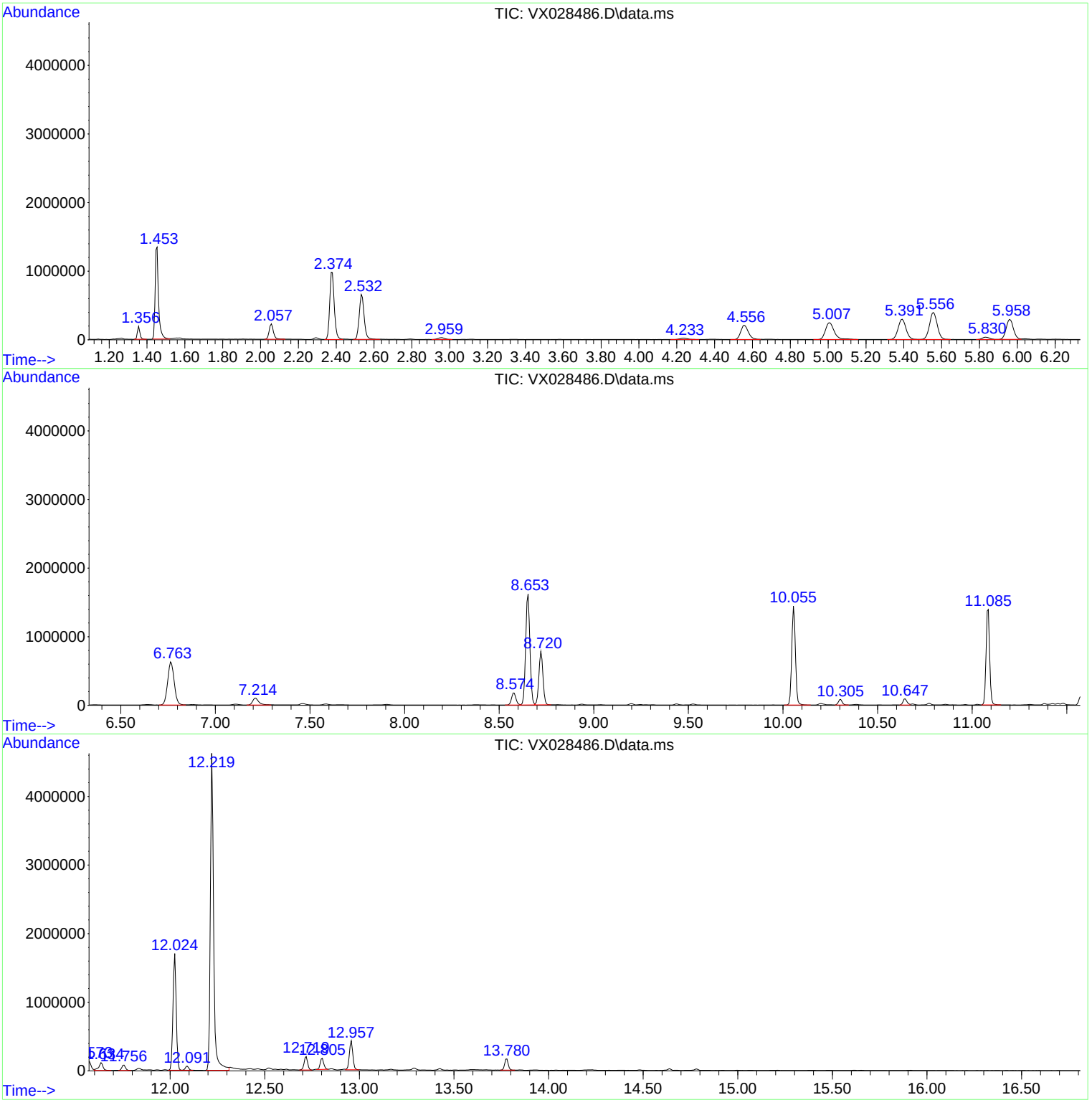
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30988

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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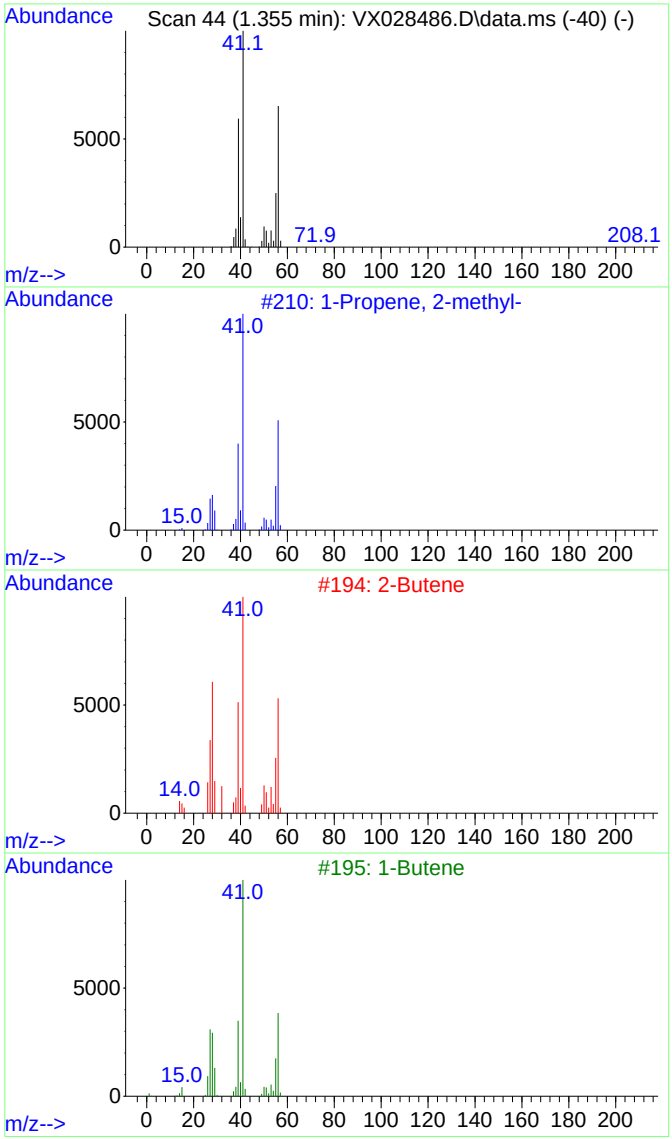
Quant Title : SW846 8260

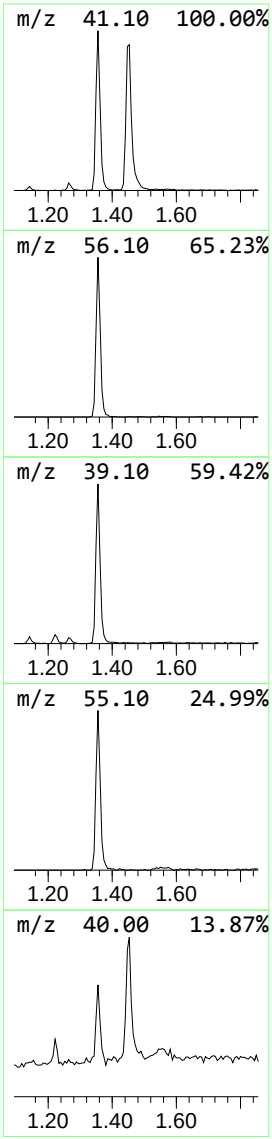
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Propene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.355	7.86 ug/l	175909	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	87
2	2-Butene	56	C4H8	000107-01-7	72
3	1-Butene	56	C4H8	000106-98-9	58
4	Cyclobutane	56	C4H8	000287-23-0	49
5	2-Butene, (Z)-	56	C4H8	000590-18-1	49





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Data File : VX028486.D
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Operator : JC/MD
Sample : N2642-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30988

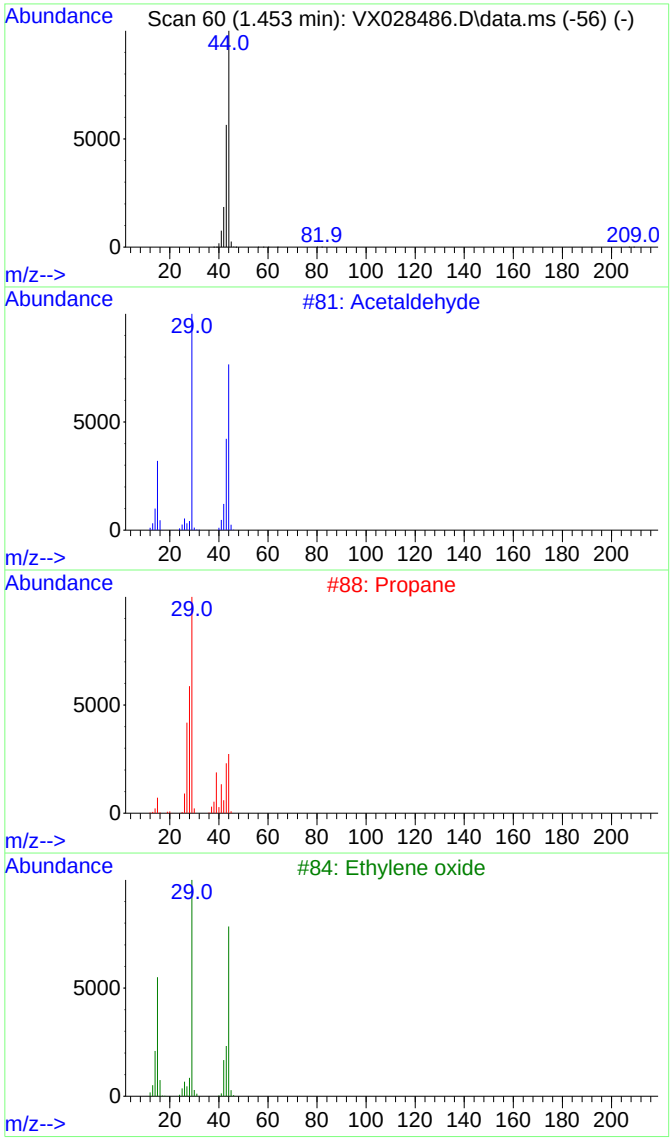
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

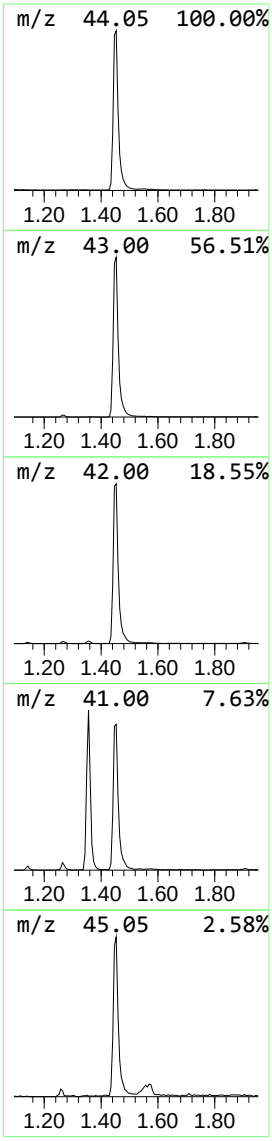
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	74.19 ug/l	1660180	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	64
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Hydrogen isocyanate	43	CHNO	000075-13-8	3





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30988

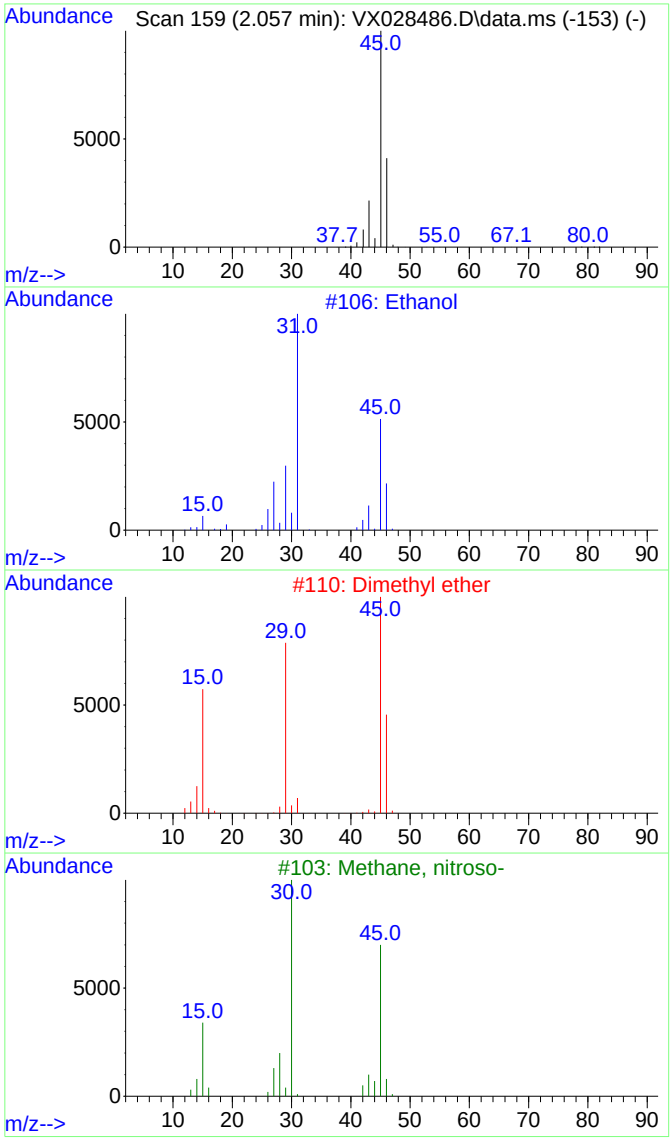
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

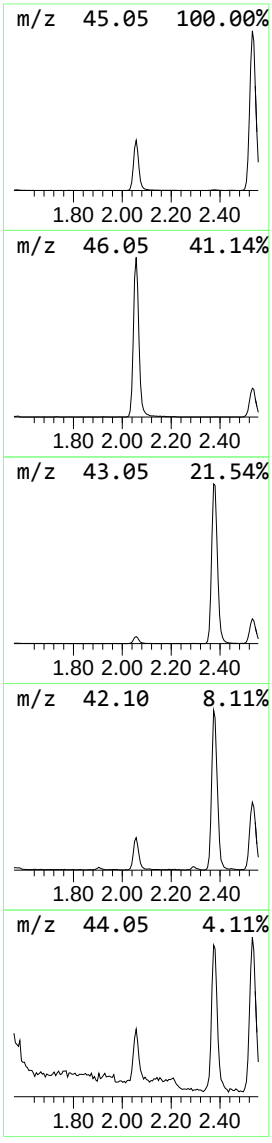
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.057	15.54 ug/l	347738	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
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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Data File : VX028486.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30988

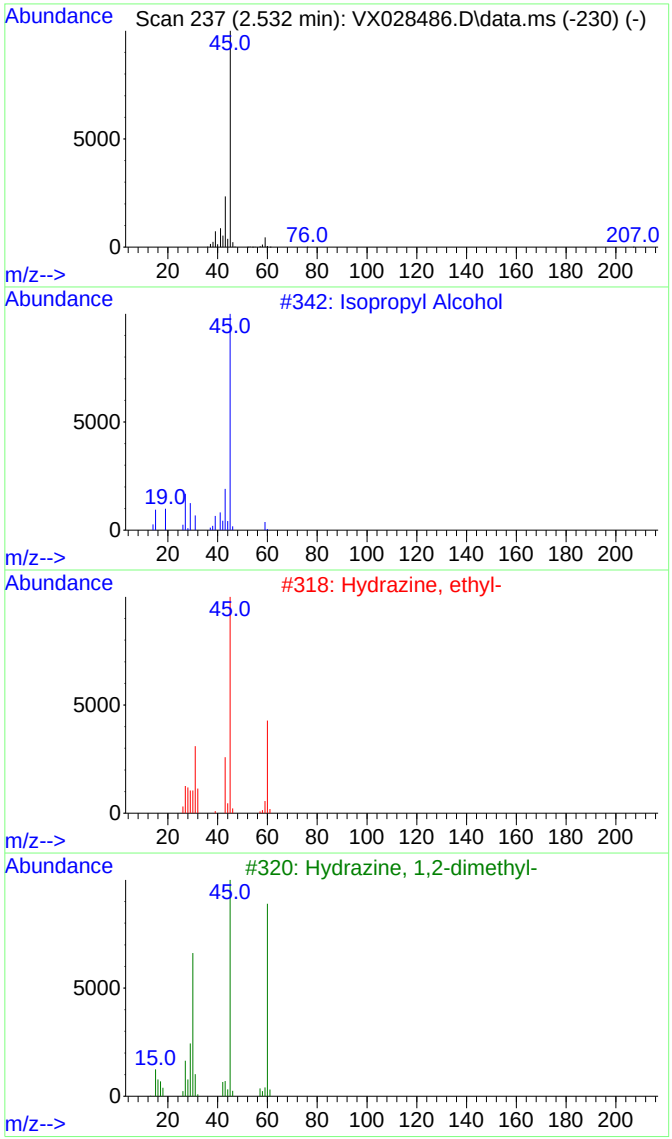
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

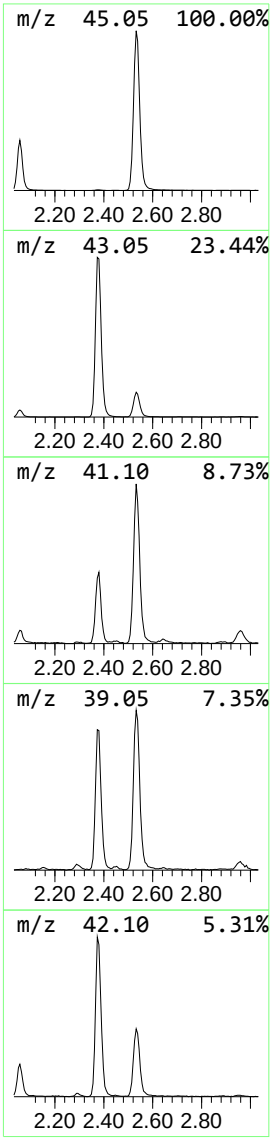
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.532	52.59 ug/l	1176840	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4
5	2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4





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Sample : N2642-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30988

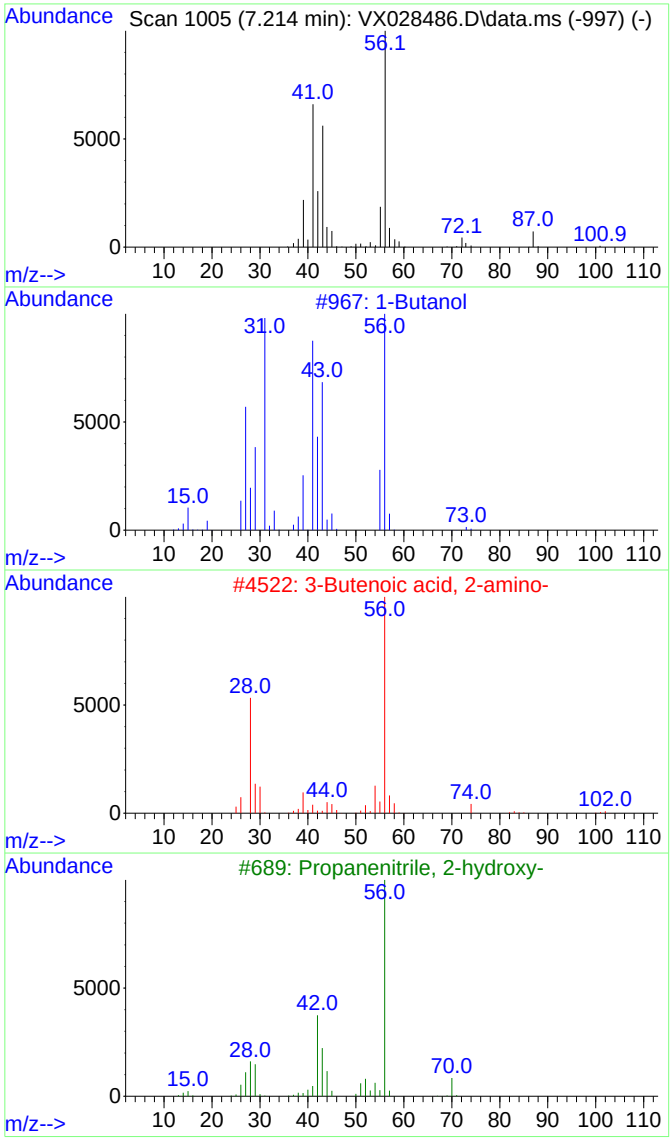
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

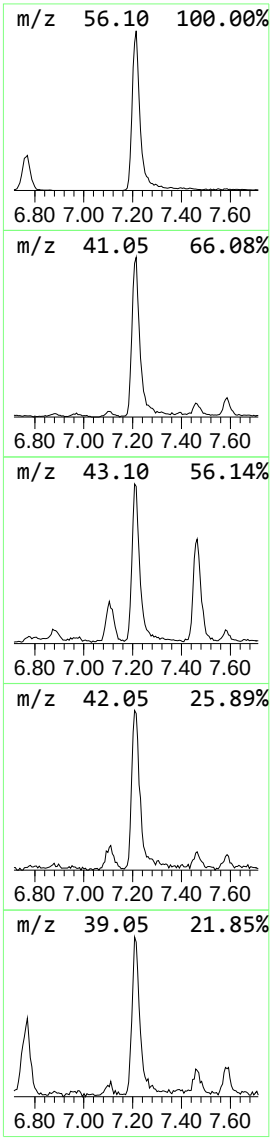
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	7.59 ug/l	225421	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	72
2	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	53
3	Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	50
4	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	39
5	1-Butanamine, N-ethylidene-	99	C6H13N	006898-74-4	39





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30988

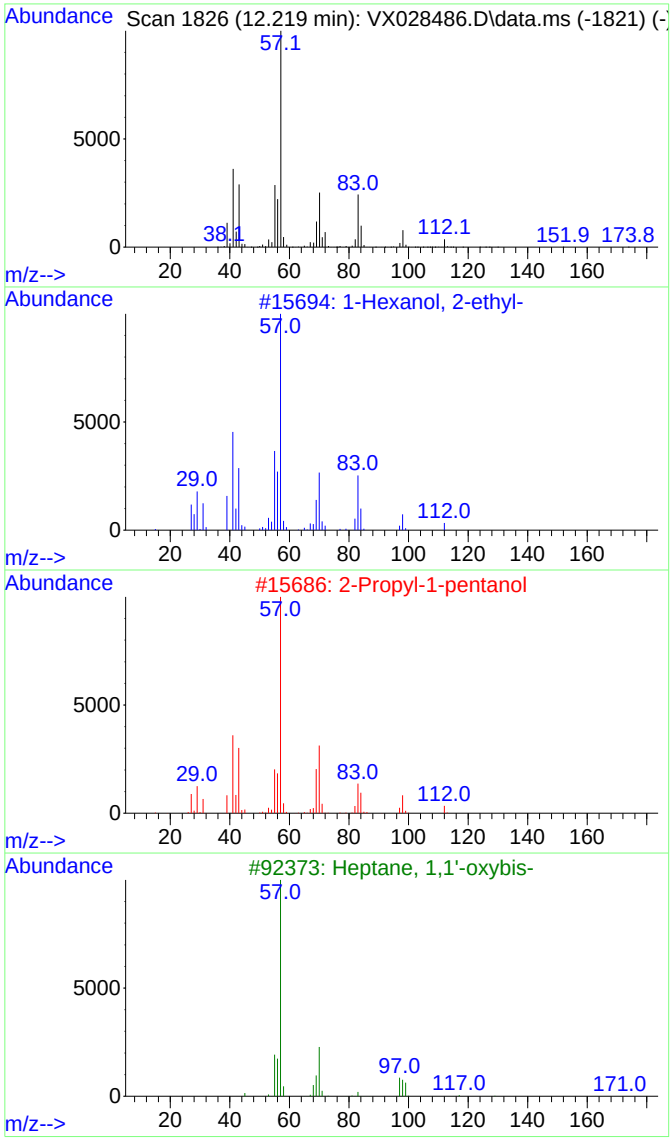
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

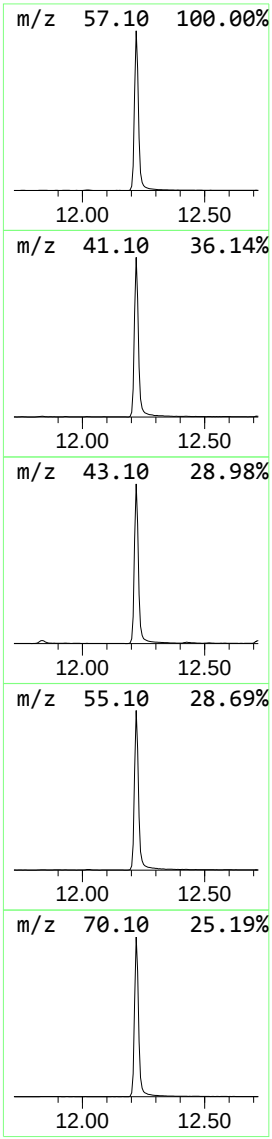
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	138.23 ug/l	5538760	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45
5	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	43





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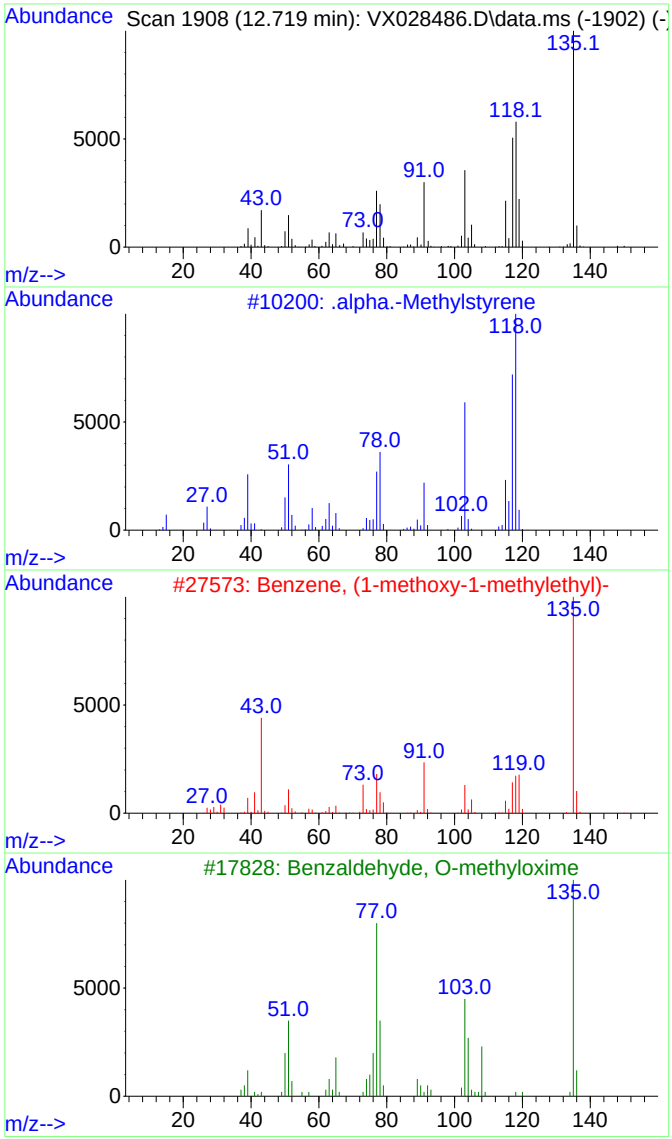
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

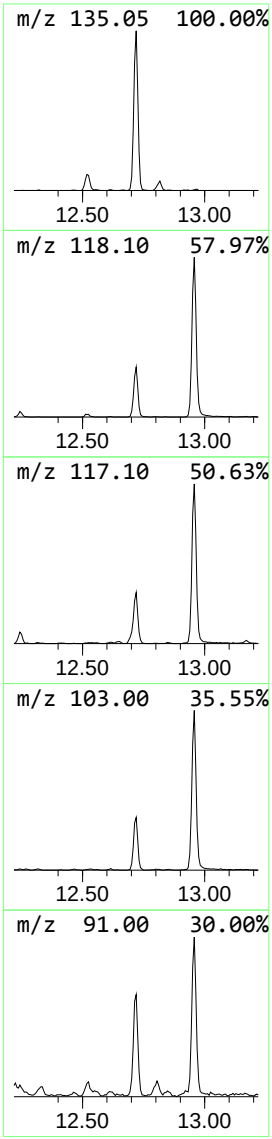
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 .alpha.-Methylstyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.719	6.20 ug/l	248516	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Methylstyrene	118	C9H10	000098-83-9	50
2	Benzene, (1-methoxy-1-methylethyl)-	150	C10H14O	000935-67-1	43
3	Benzaldehyde, O-methyloxime	135	C8H9NO	003376-32-7	38
4	(Z) Phenylpropyl cinnamate	266	C18H18O2	1000414-29-1	27
5	1-Methyl-1-phenylcyclobutane	146	C11H14	007306-05-0	27





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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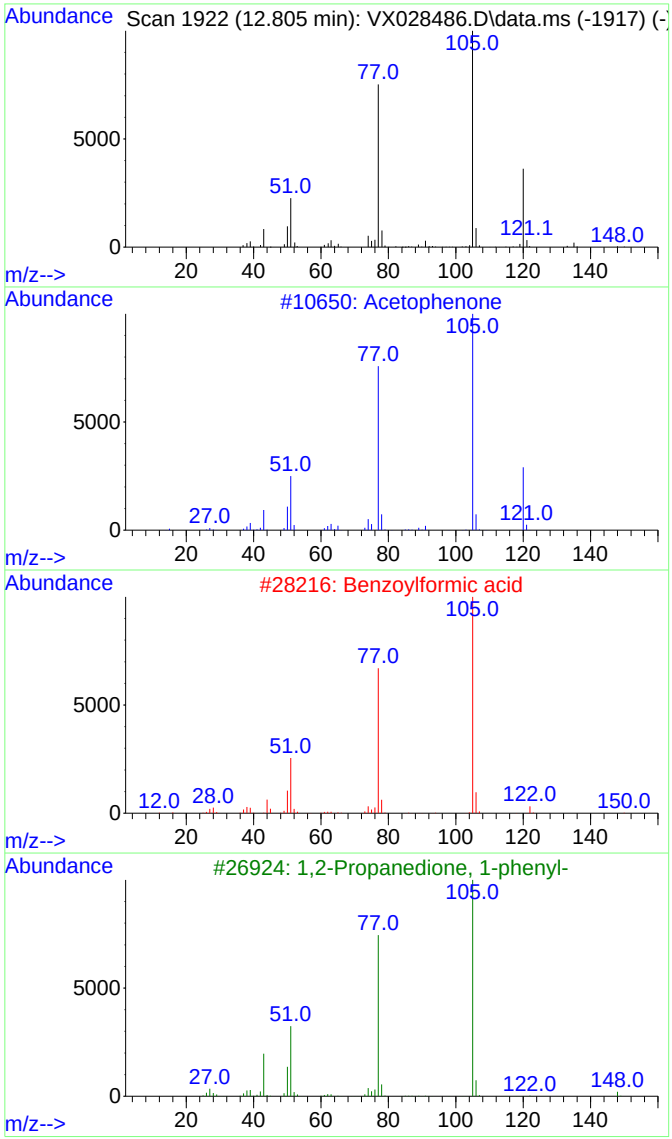
Quant Title : SW846 8260

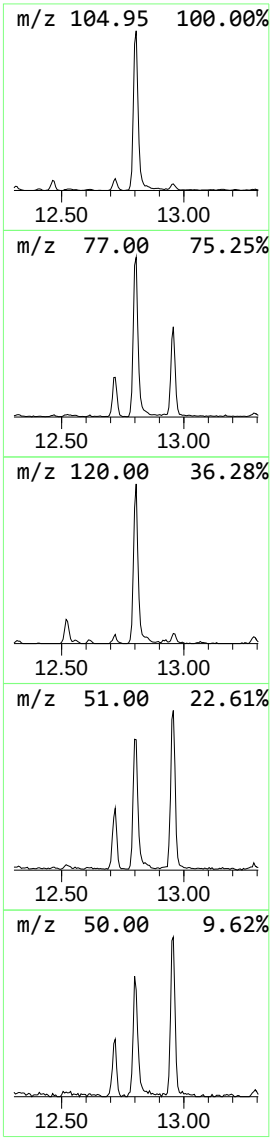
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Acetophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.805	5.25 ug/l	210226	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetophenone	120	C8H8O	000098-86-2	95
2	Benzoylformic acid	150	C8H6O3	000611-73-4	81
3	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	74
4	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	72
5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	64





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Instrument :
MSVOA_X
ClientSampleId :
30988

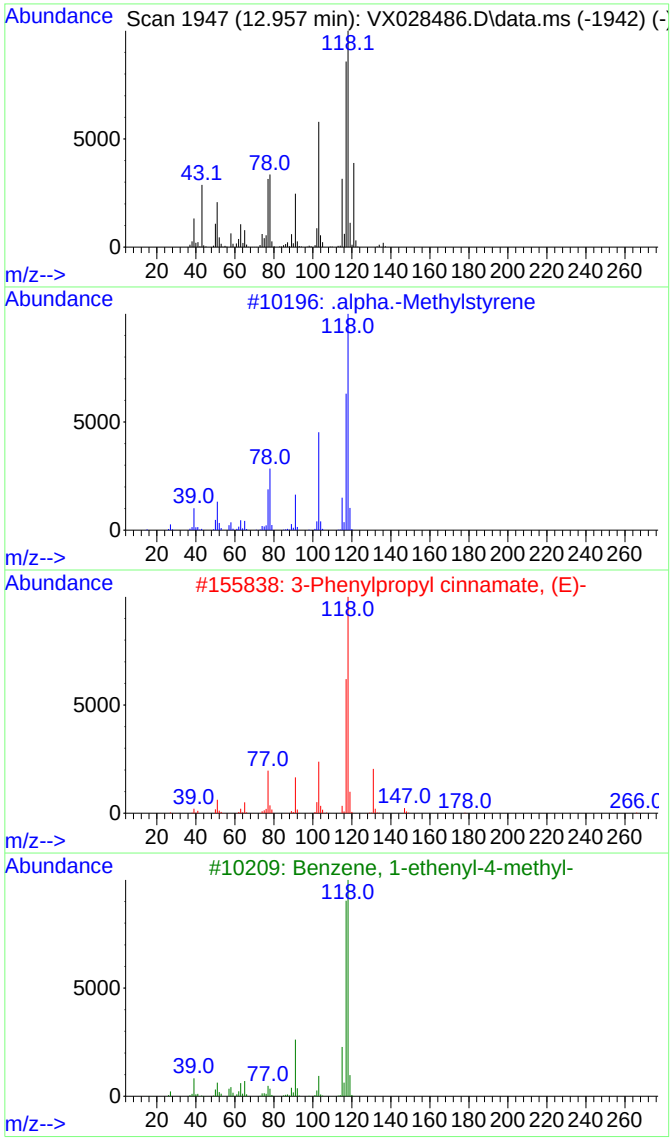
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

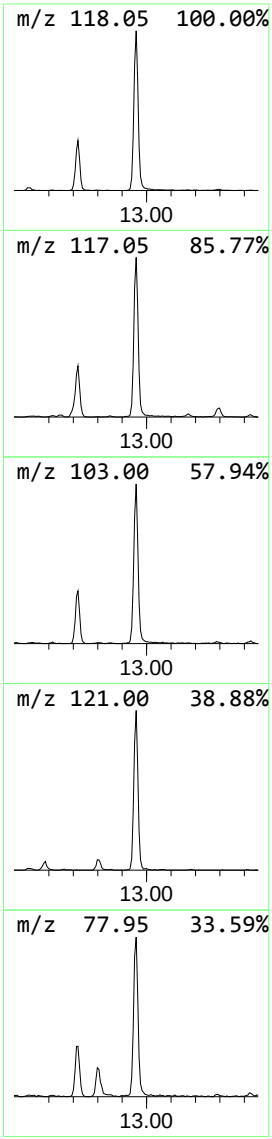
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 3-Phenylpropyl cinnamate, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.957	13.00 ug/l	520845	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Methylstyrene	118	C9H10	000098-83-9	95
2	3-Phenylpropyl cinnamate, (E)-	266	C18H18O2	290311-72-7	53
3	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	53
4	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	49
5	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX050222\
Data File : VX028486.D
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Instrument :
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ClientSampleId :
30988

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041922W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Propene, 2-me...	1.355	7.9	ug/l	175909	1	5.556	1118800	50.0
Acetaldehyde	1.453	74.2	ug/l	1660180	1	5.556	1118800	50.0
Ethanol	2.057	15.5	ug/l	347738	1	5.556	1118800	50.0
Isopropyl Alcohol	2.532	52.6	ug/l	1176840	1	5.556	1118800	50.0
1-Butanol	7.214	7.6	ug/l	225421	2	6.763	1484910	50.0
1-Hexanol, 2-et...	12.219	138.2	ug/l	5538760	4	12.024	2003490	50.0
.alpha.-Methyls...	12.719	6.2	ug/l	248516	4	12.024	2003490	50.0
Acetophenone	12.805	5.3	ug/l	210226	4	12.024	2003490	50.0
3-Phenylpropyl ...	12.957	13.0	ug/l	520845	4	12.024	2003490	50.0