LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052121\
Data File : VX022116.D
Acq On : 21 May 2021 15:33
Operator : JC/MD
Sample : M2473-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PILOT-PLANT-PROCESS-BLEED

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\82X051921W.M
Title : SW846 8260

Signal : TIC: VX022116.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	24	27	32	rBV	39876	38081	1.96%	0.668%
2	1.374	44	47	51	rBV	31172	29078	1.50%	0.510%
3	1.453	56	60	73	rBV	1802111	1939723	100.00%	34.039%
4	2.069	155	161	170	rBV	42939	67651	3.49%	1.187%
5	4.245	510	518	531	rBV2	9939	26801	1.38%	0.470%
6	4.690	580	591	606	rBV	187134	539325	27.80%	9.464%
7	5.025	637	646	656	rBV3	24557	75786	3.91%	1.330%
8	5.403	692	708	722	rVB	53489	154773	7.98%	2.716%
9	5.562	722	734	749	rBV	85419	236520	12.19%	4.151%
10	5.842	769	780	792	rBV	129668	350822	18.09%	6.156%
11	5.970	792	801	815	rVB	63195	167595	8.64%	2.941%
12	6.775	923	933	945	rBV	143862	344486	17.76%	6.045%
13	7.665	1073	1079	1093	rVB	19438	40517	2.09%	0.711%
14	8.653	1235	1241	1252	rBV	295632	483857	24.94%	8.491%
15	10.061	1466	1472	1480	rBV	289777	400141	20.63%	7.022%
16	10.945	1612	1617	1626	rVB	133730	175983	9.07%	3.088%
17	11.085	1634	1640	1649	rVB	225326	285936	14.74%	5.018%
18	12.024	1789	1794	1803	rVB	286312	341496	17.61%	5.993%

Sum of corrected areas: 5698571

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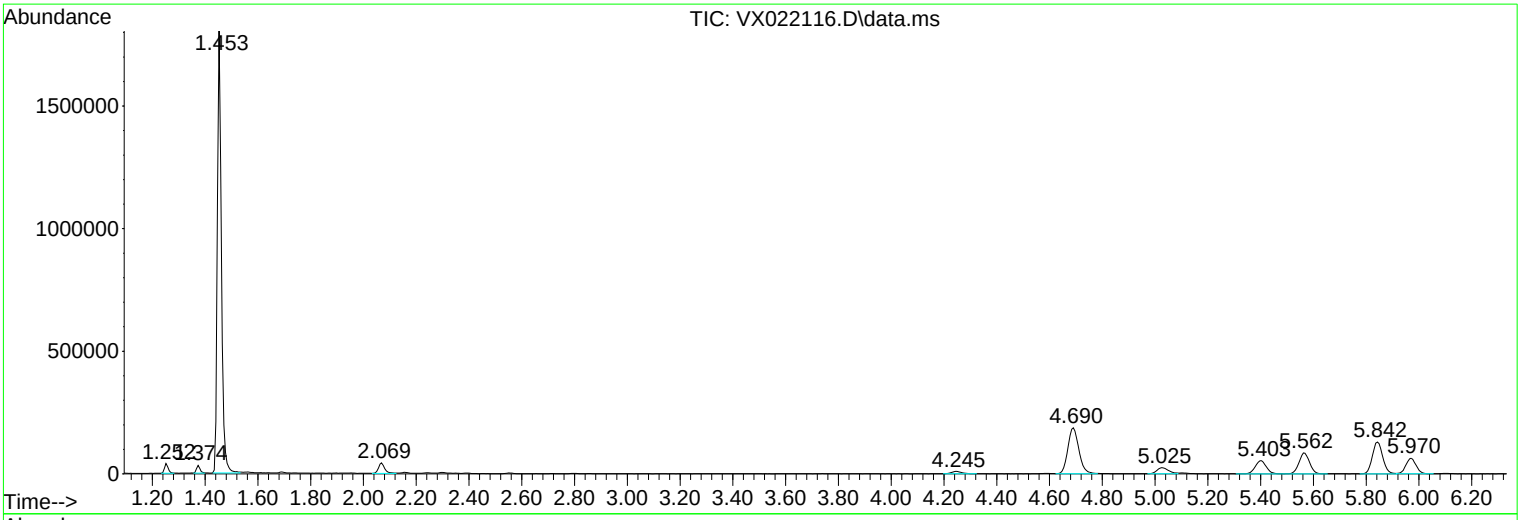
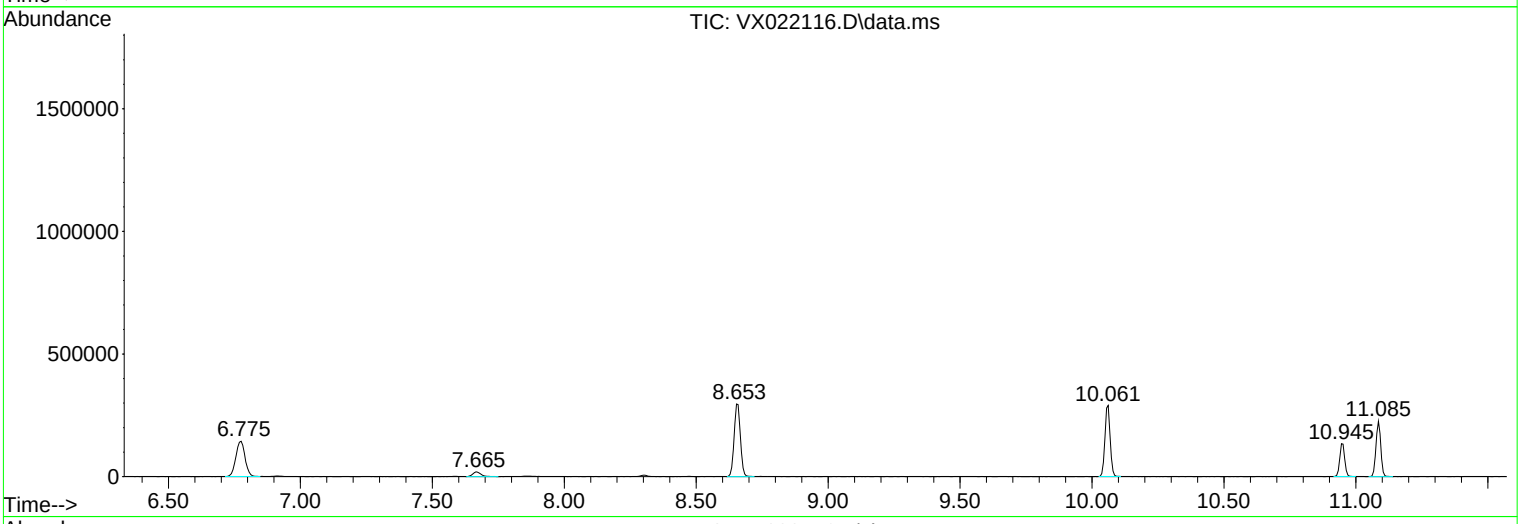
ALS Vial : 16 Sample Multiplier: 1

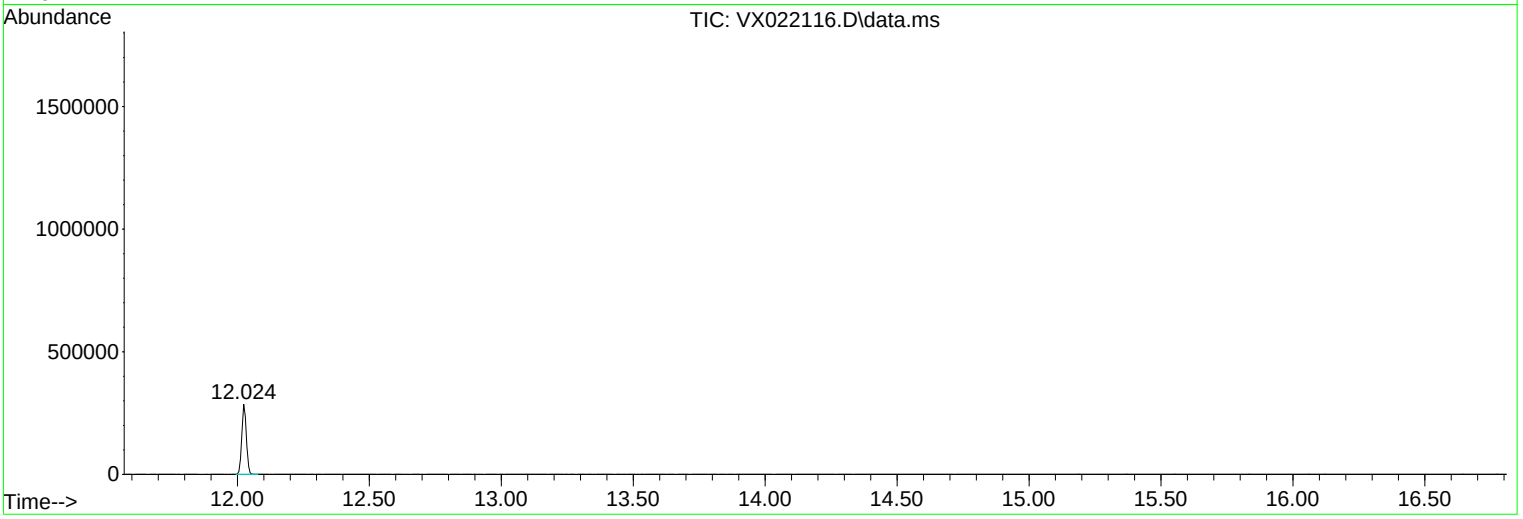
Instrument :
MSVOA_X
ClientSampleId :
PILOT-PLANT-PROCESS-BLEED

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

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







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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PILOT-PLANT-PROCESS-BLEED

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

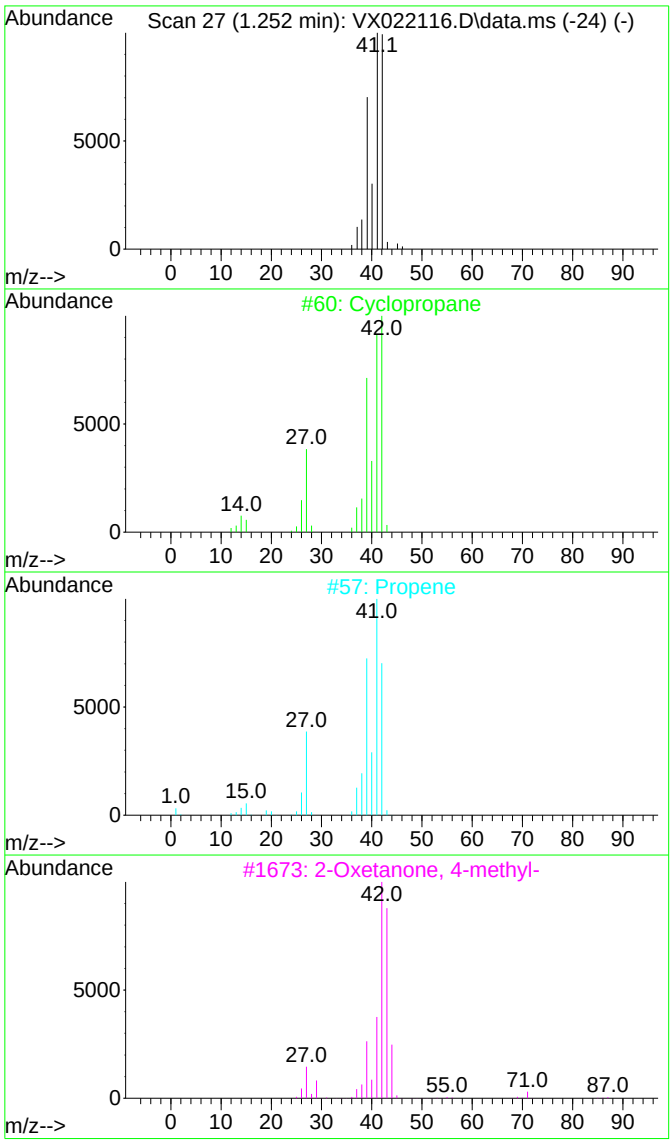
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

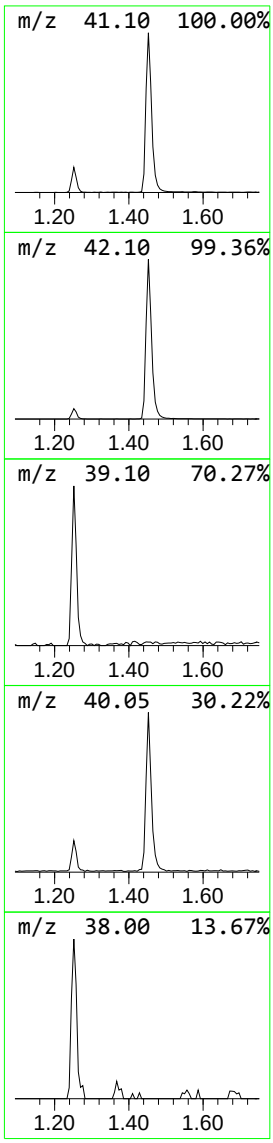
****

Peak Number 1 Cyclopropane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	8.05 ug/l	38081	Pentafluorobenzene	5.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane	42	C3H6	000075-19-4	90
2	Propene	42	C3H6	000115-07-1	83
3	2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	4
4	Methyl isocyanide	41	C2H3N	000593-75-9	3
5	Acetonitrile	41	C2H3N	000075-05-8	3





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Data File : VX022116.D
Acq On : 21 May 2021 15:33
Operator : JC/MD
Sample : M2473-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PILOT-PLANT-PROCESS-BLEED

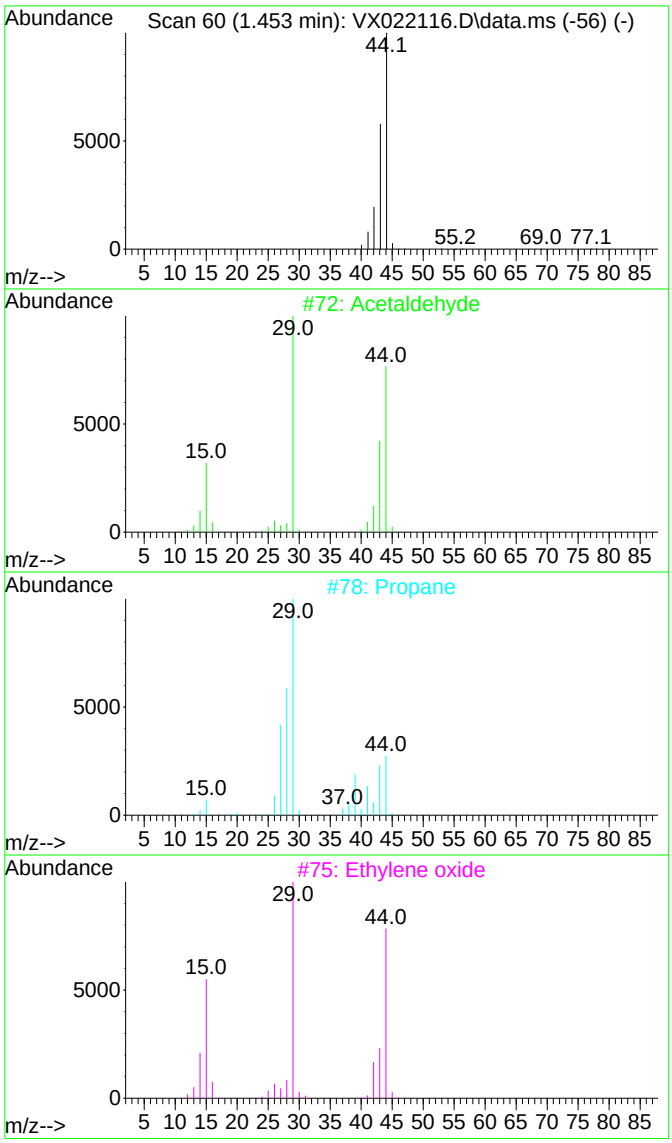
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

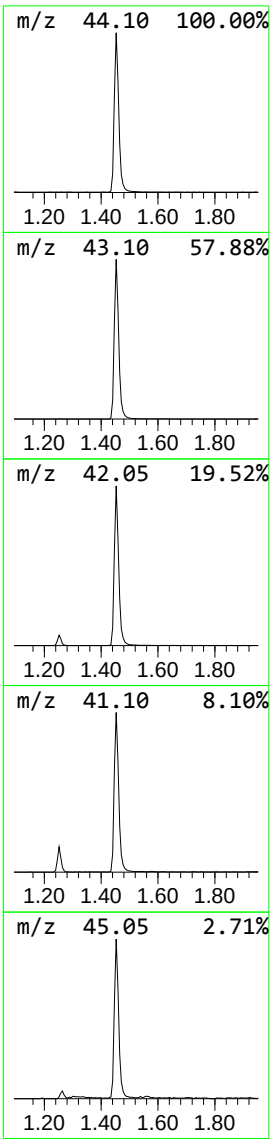
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	410.06 ug/l	1939720	Pentafluorobenzene	5.568

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	Ethyne, fluoro-	44	C2HF	002713-09-9	3
5	Methane, diazo-	42	CH2N2	000334-88-3	3





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Data File : VX022116.D
Acq On : 21 May 2021 15:33
Operator : JC/MD
Sample : M2473-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PILOT-PLANT-PROCESS-BLEED

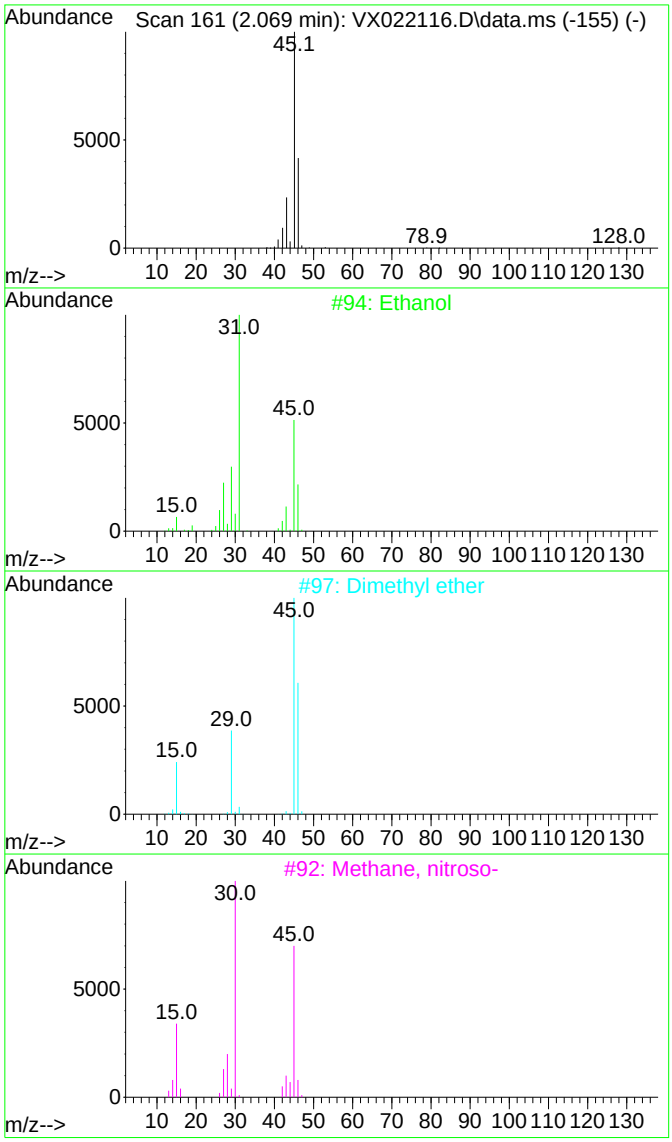
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

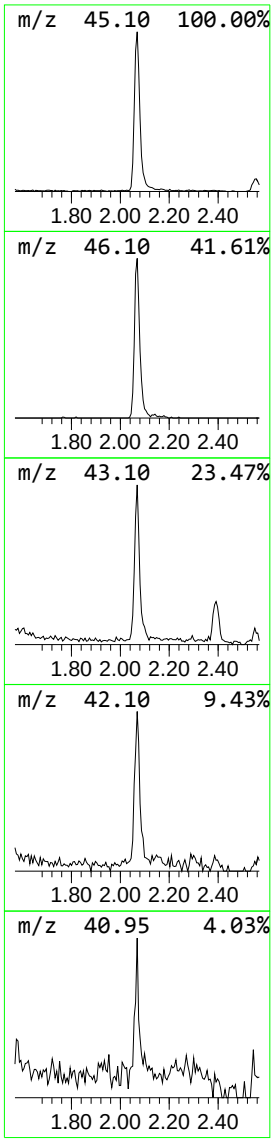
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	14.30 ug/l	67651	Pentafluorobenzene	5.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	56
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	4-Penten-2-ol	86	C5H10O	000625-31-0	4





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Operator : JC/MD
Sample : M2473-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PILOT-PLANT-PROCESS-BLEED

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

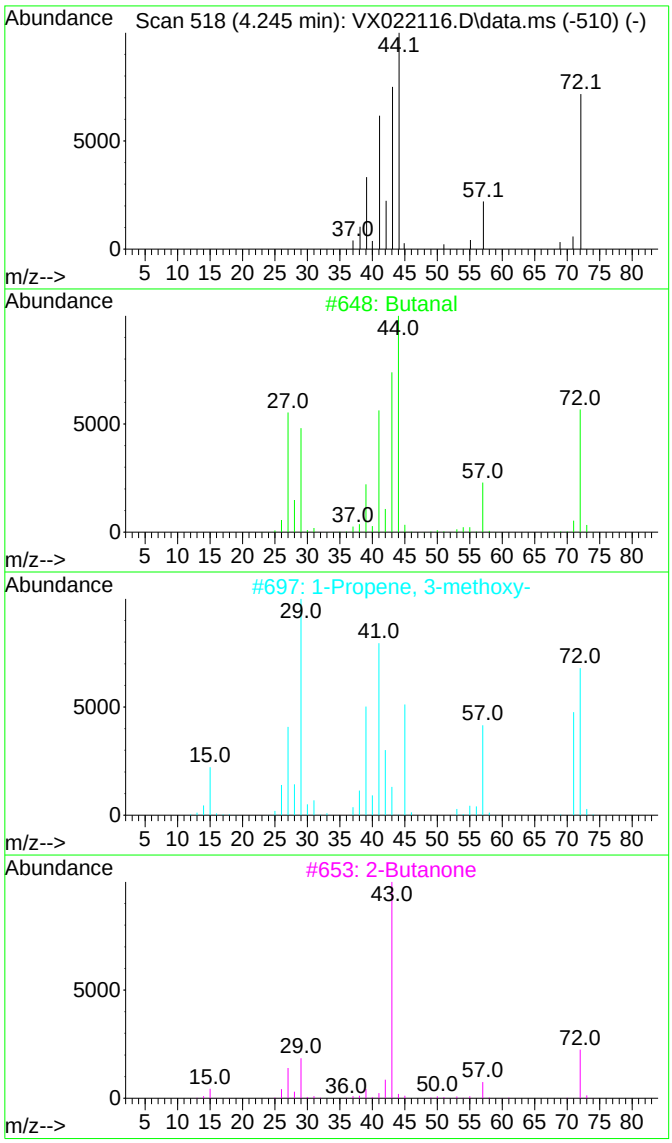
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

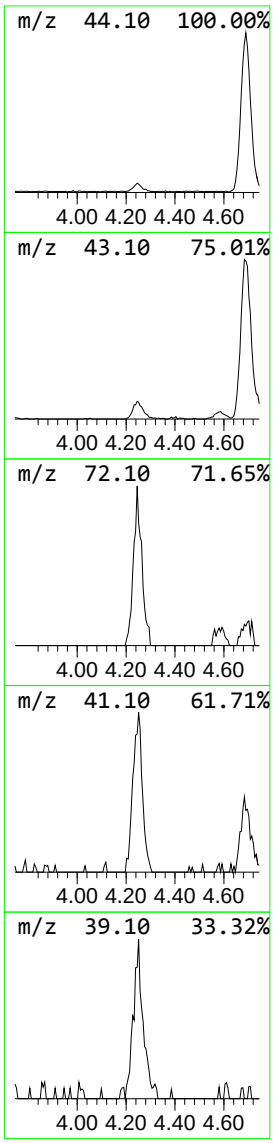
****

Peak Number 4 Butanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.245	5.67 ug/l	26801	Pentafluorobenzene	5.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	86
2	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	16
3	2-Butanone	72	C4H8O	000078-93-3	9
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	9
5	Isobutylene epoxide	72	C4H8O	000558-30-5	9





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Data File : VX022116.D
Acq On : 21 May 2021 15:33
Operator : JC/MD
Sample : M2473-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PILOT-PLANT-PROCESS-BLEED

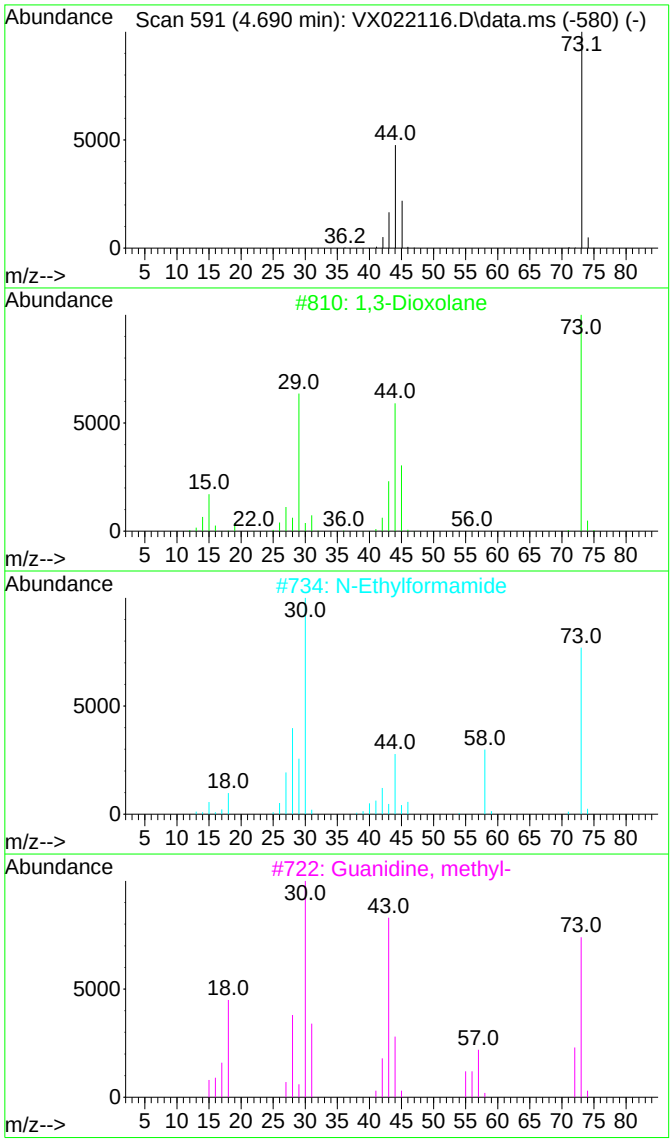
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

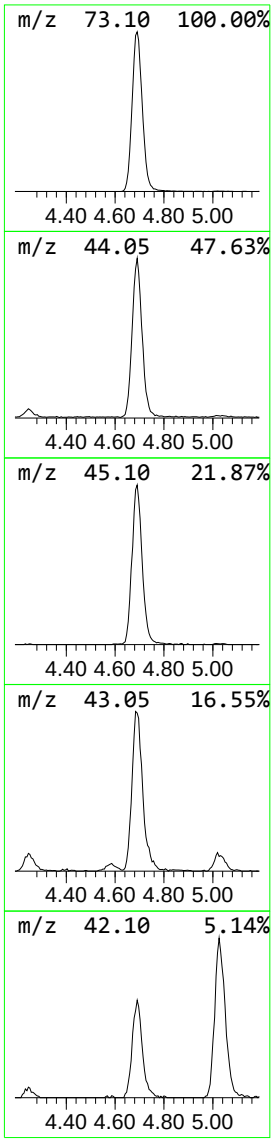
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,3-Dioxolane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.690	114.01 ug/l	539325	Pentafluorobenzene	5.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane	74	C3H6O2	000646-06-0	86
2	N-Ethylformamide	73	C3H7NO	000627-45-2	5
3	Guanidine, methyl-	73	C2H7N3	000471-29-4	5
4	Ethylene oxide	44	C2H4O	000075-21-8	5
5	Formamide, N,N-dimethyl-	73	C3H7NO	000068-12-2	4





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PILOT-PLANT-PROCESS-BLEED

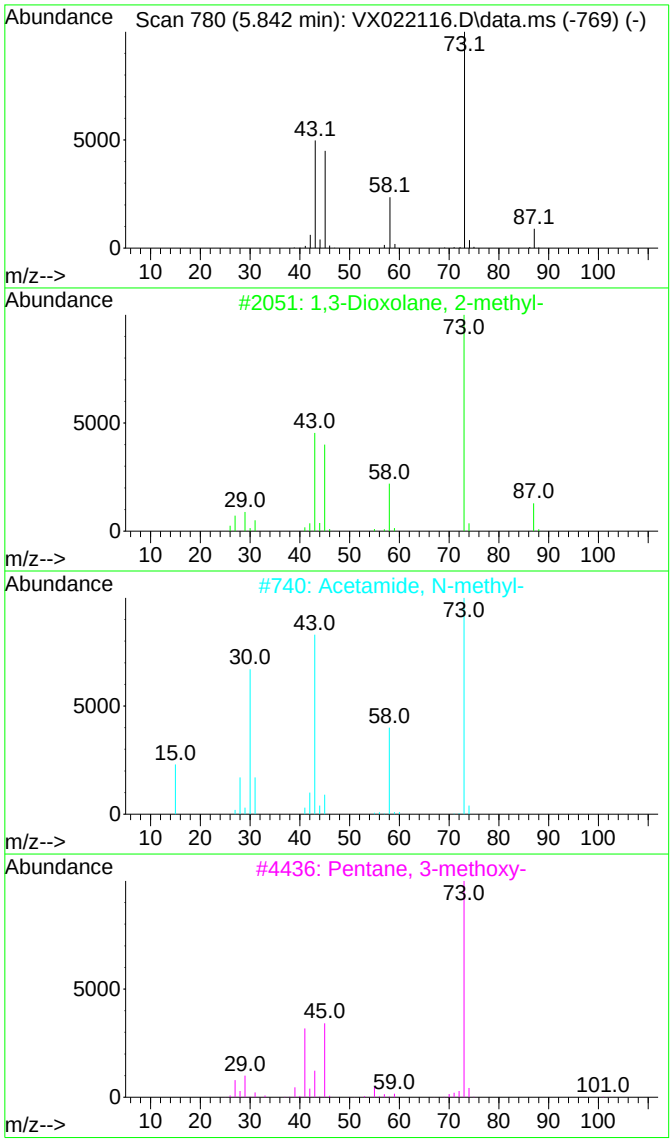
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

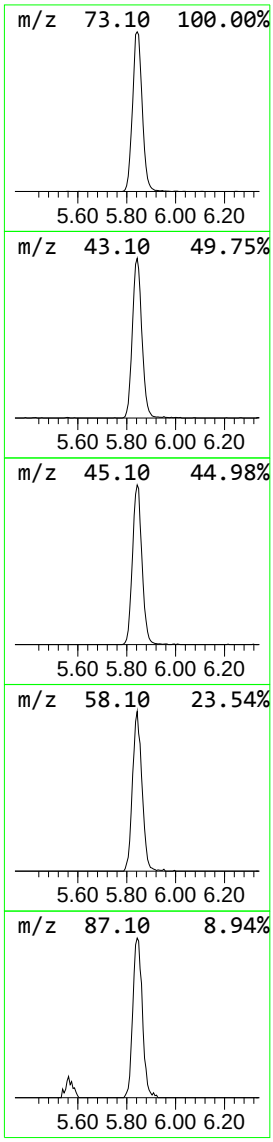
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3-Dioxolane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.842	74.16 ug/l	350822	Pentafluorobenzene	5.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	37
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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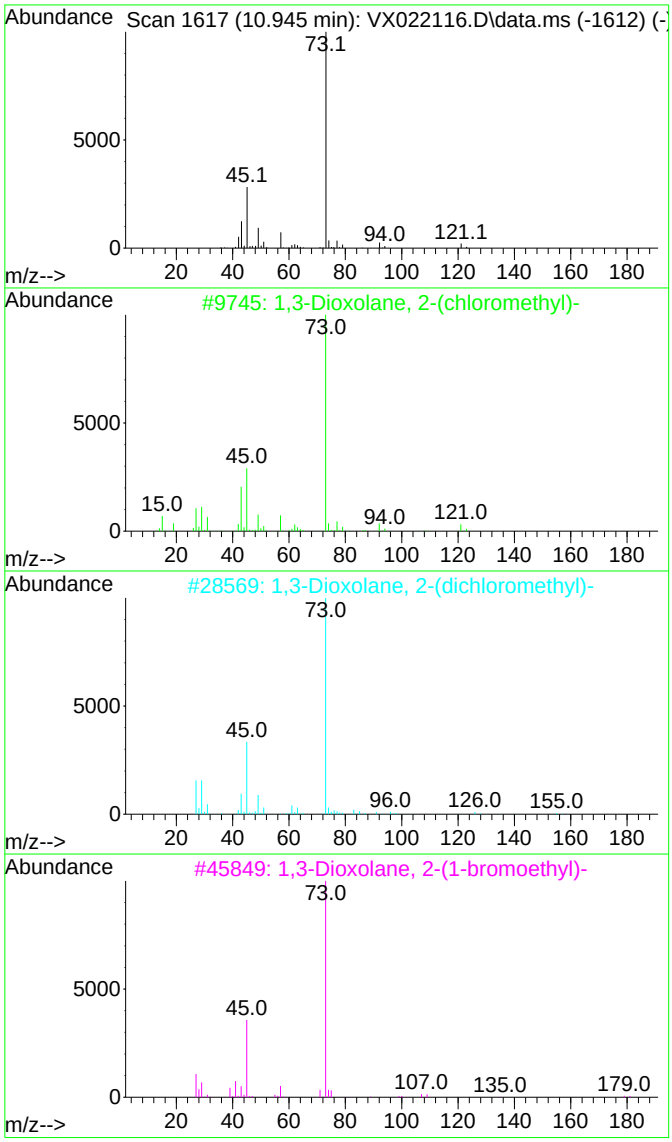
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

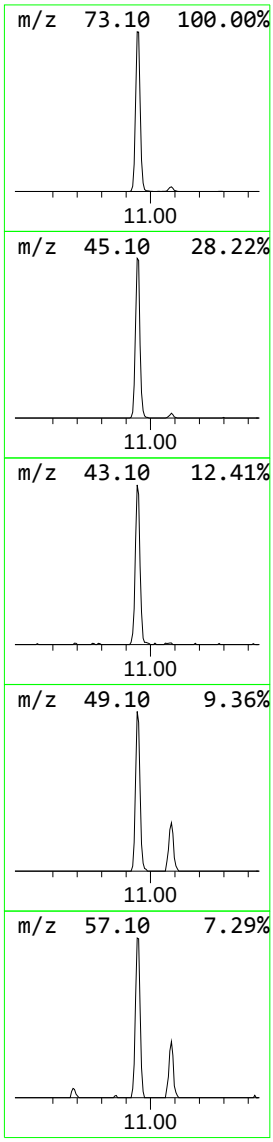
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,3-Dioxolane, 2-(chloromet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.945	21.99 ug/l	175983	Chlorobenzene-d5	10.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	50
2	1,3-Dioxolane, 2-(dichloromethyl)-	156	C4H6Cl2O2	002612-35-3	45
3	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	33
4	1,3-Dioxolane, 2-(phenylmethyl)-	164	C10H12O2	000101-49-5	33
5	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	28





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
Cyclopropane	1.252	8.1	ug/l	38081	1	5.568	236520	50.0
Acetaldehyde	1.453	410.1	ug/l	1939720	1	5.568	236520	50.0
Ethanol	2.069	14.3	ug/l	67651	1	5.568	236520	50.0
Butanal	4.245	5.7	ug/l	26801	1	5.568	236520	50.0
1,3-Dioxolane	4.690	114.0	ug/l	539325	1	5.568	236520	50.0
1,3-Dioxolane, ...	5.842	74.2	ug/l	350822	1	5.568	236520	50.0
1,3-Dioxolane, ...	10.945	22.0	ug/l	175983	3	10.061	400141	50.0