LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027966.D
Acq On : 04 Apr 2022 18:30
Operator : JC/MD
Sample : PB143824ZHE#03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#03

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82X032922W.M
Title : SW846 8260

Signal : TIC: VX027966.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	40	rBV	23894	33482	2.47%	0.534%
2	2.788	272	279	290	rBV	144621	269053	19.83%	4.289%
3	3.575	400	408	418	rBV3	6046	14339	1.06%	0.229%
4	5.391	693	706	722	rBV2	53954	159045	11.72%	2.535%
5	5.556	722	733	748	rVV2	99270	276348	20.37%	4.405%
6	5.958	787	799	813	rBV	59242	157025	11.57%	2.503%
7	6.348	853	863	873	rVB2	5796	15305	1.13%	0.244%
8	6.696	915	920	923	rBV3	8072	17658	1.30%	0.281%
9	6.763	923	931	941	rVB	146947	356306	26.26%	5.679%
10	7.799	1093	1101	1115	rBV	466363	795842	58.66%	12.685%
11	8.549	1217	1224	1234	rBV	89443	138895	10.24%	2.214%
12	8.653	1234	1241	1256	rVV	288924	462341	34.08%	7.369%
13	8.958	1285	1291	1298	rVB	9955	15036	1.11%	0.240%
14	9.244	1333	1338	1345	rBV	23688	34809	2.57%	0.555%
15	9.342	1350	1354	1359	rBV	62358	82609	6.09%	1.317%
16	9.482	1372	1377	1384	rBV	1002814	1356710	100.00%	21.625%
17	9.580	1388	1393	1403	rVB	120723	153556	11.32%	2.448%
18	9.915	1442	1448	1464	rBV	660940	810349	59.73%	12.916%
19	10.055	1464	1471	1478	rBV	306058	408418	30.10%	6.510%
20	10.640	1562	1567	1574	rBV	24667	29406	2.17%	0.469%
21	11.085	1634	1640	1648	rBV	262783	337549	24.88%	5.380%
22	12.024	1789	1794	1804	rVB	290463	349688	25.77%	5.574%

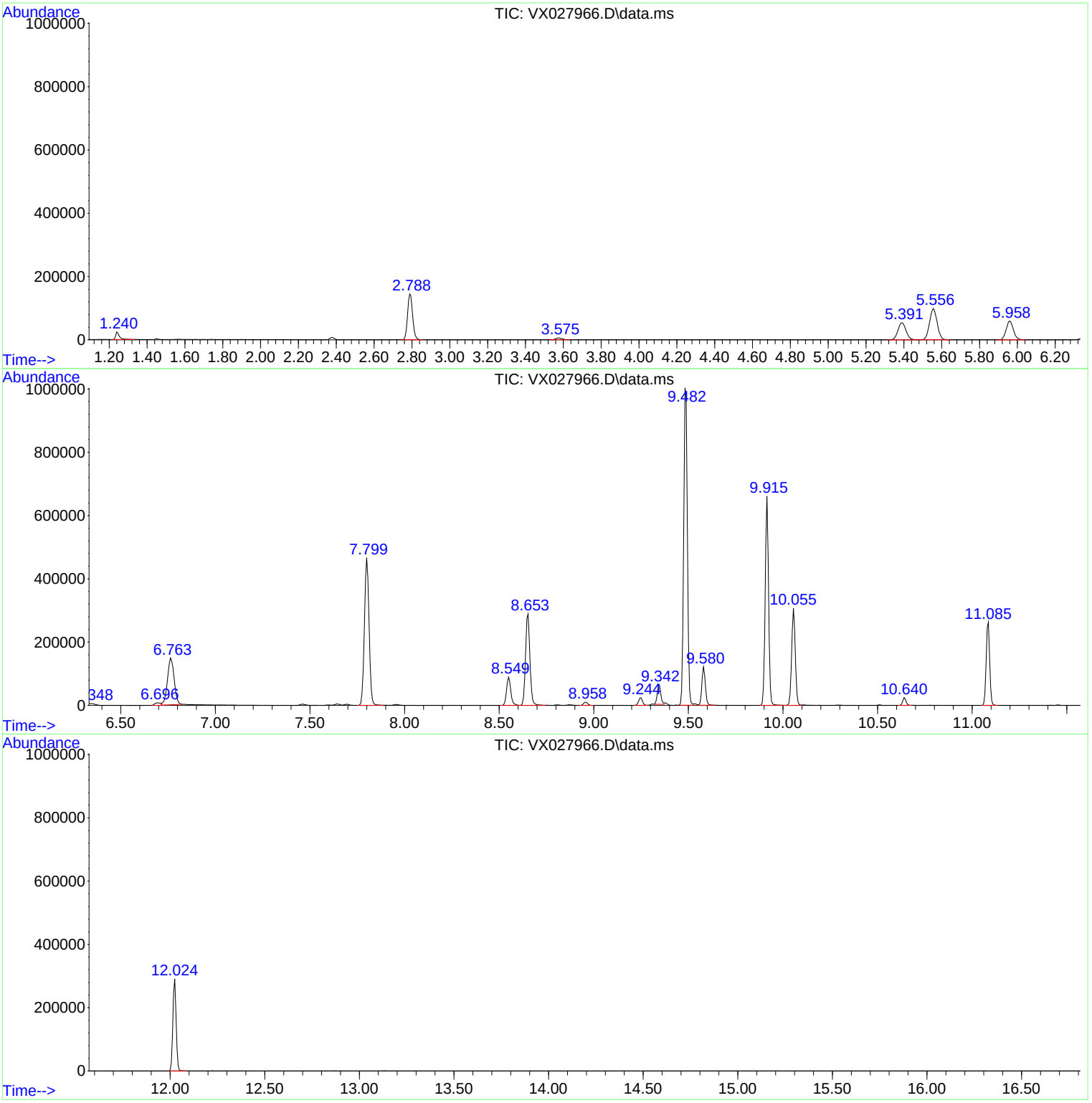
Sum of corrected areas: 6273769

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027966.D
Acq On : 04 Apr 2022 18:30
Operator : JC/MD
Sample : PB143824ZHE#03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027966.D
Acq On : 04 Apr 2022 18:30
Operator : JC/MD
Sample : PB143824ZHE#03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

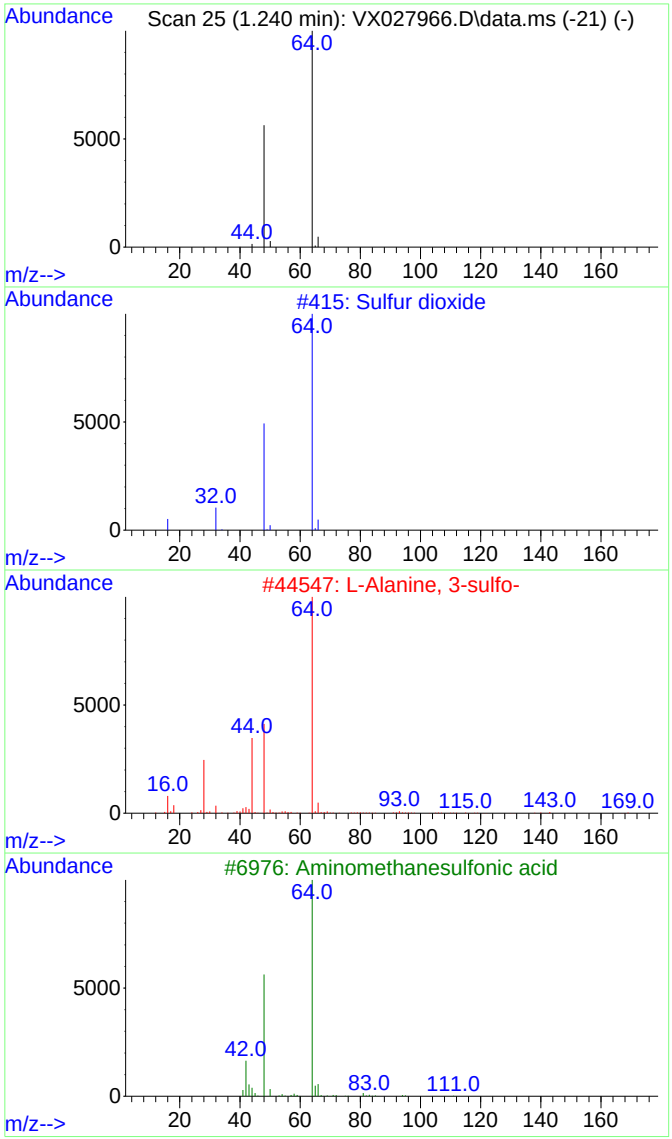
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

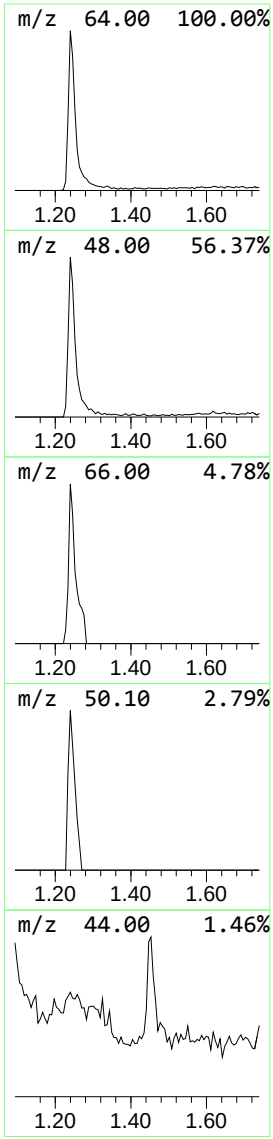
****

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	6.06 ug/l	33482	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027966.D
Acq On : 04 Apr 2022 18:30
Operator : JC/MD
Sample : PB143824ZHE#03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#03

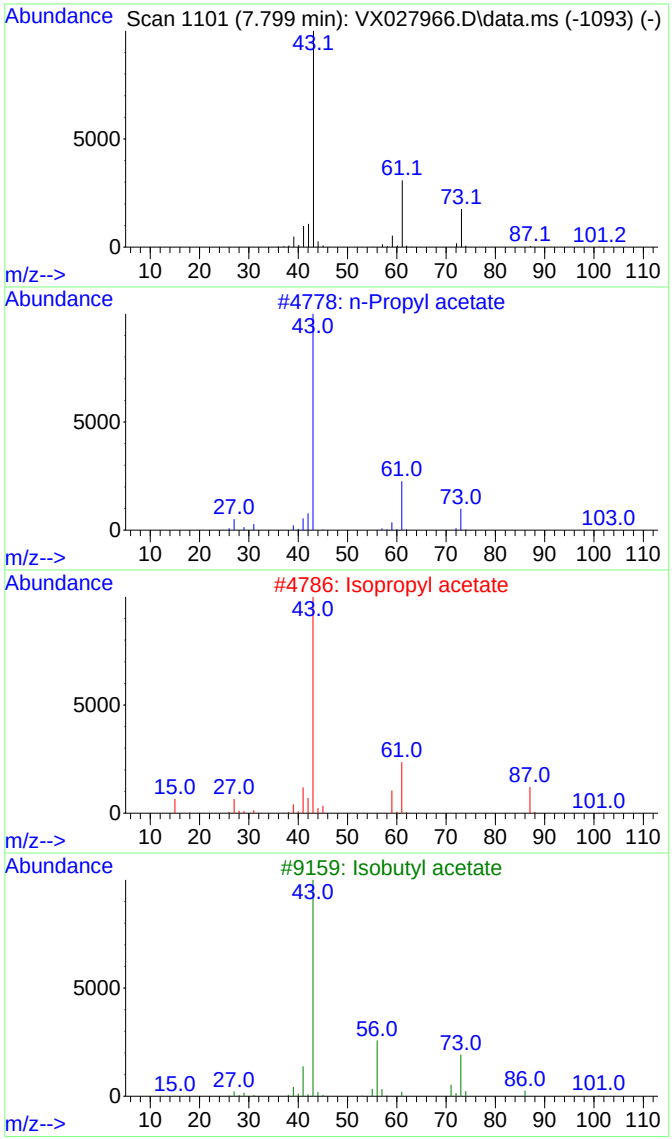
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

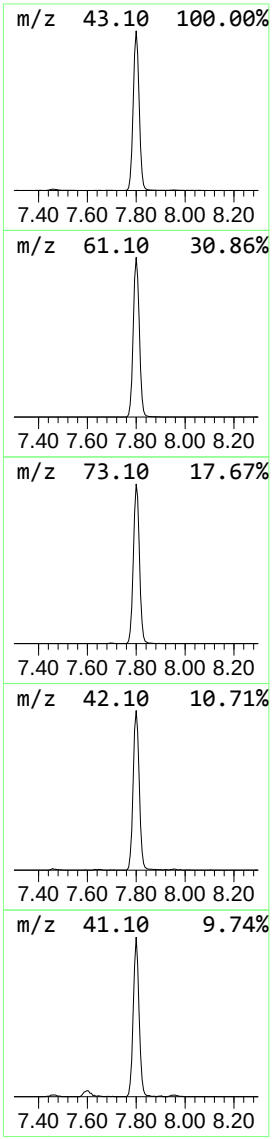
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	111.68 ug/l	795842	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Isopropyl acetate	102	C5H10O2	000108-21-4	36
3	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027966.D
Acq On : 04 Apr 2022 18:30
Operator : JC/MD
Sample : PB143824ZHE#03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#03

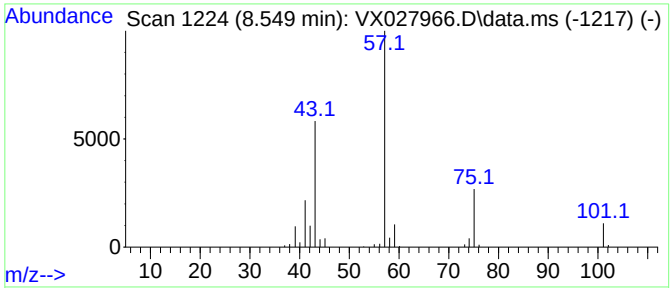
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

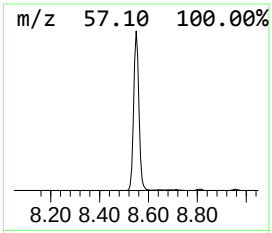
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

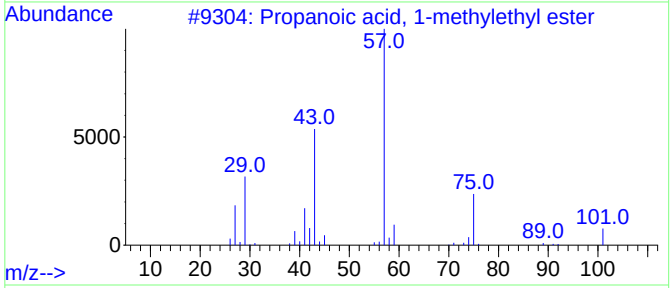
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

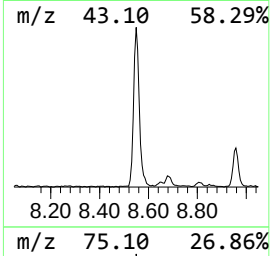
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	17.00 ug/l	138895	Chlorobenzene-d5	10.055

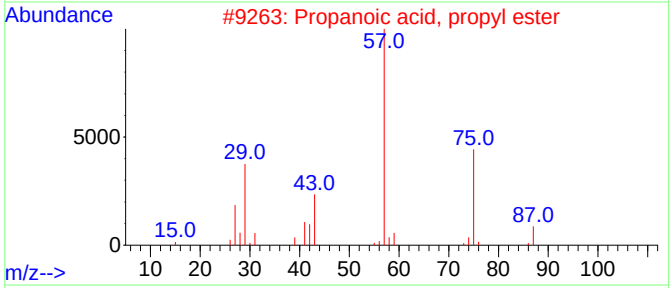
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	90
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5	Azetidine	57	C3H7N	000503-29-7	12

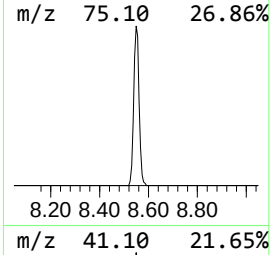


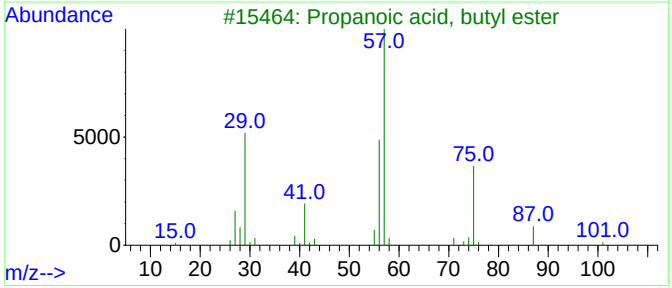


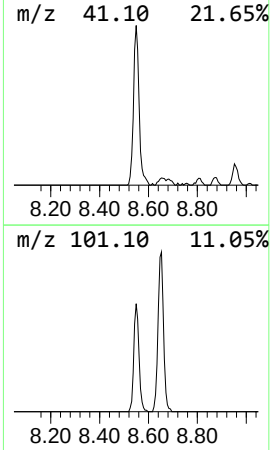












Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027966.D
Acq On : 04 Apr 2022 18:30
Operator : JC/MD
Sample : PB143824ZHE#03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#03

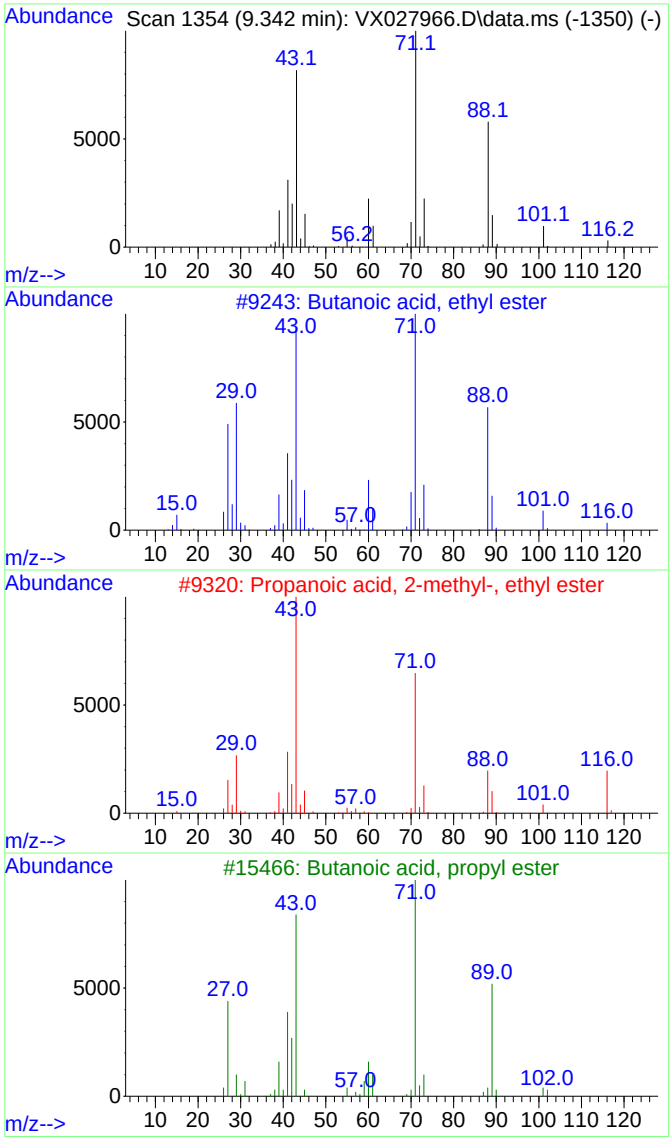
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

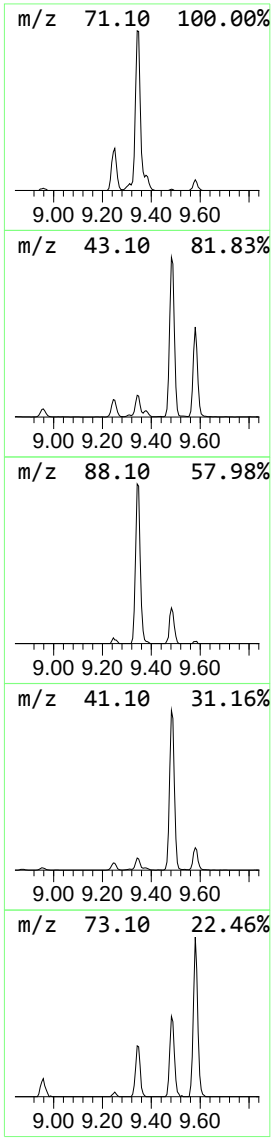
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	10.11 ug/l	82609	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
4	Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	43
5	3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027966.D
Acq On : 04 Apr 2022 18:30
Operator : JC/MD
Sample : PB143824ZHE#03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#03

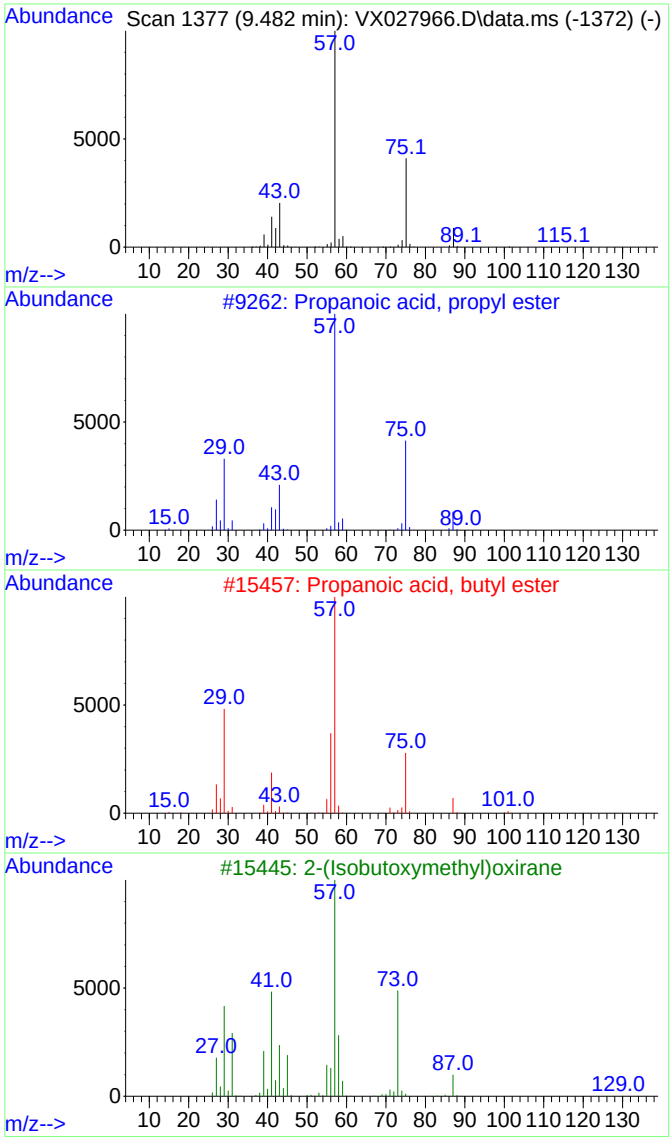
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

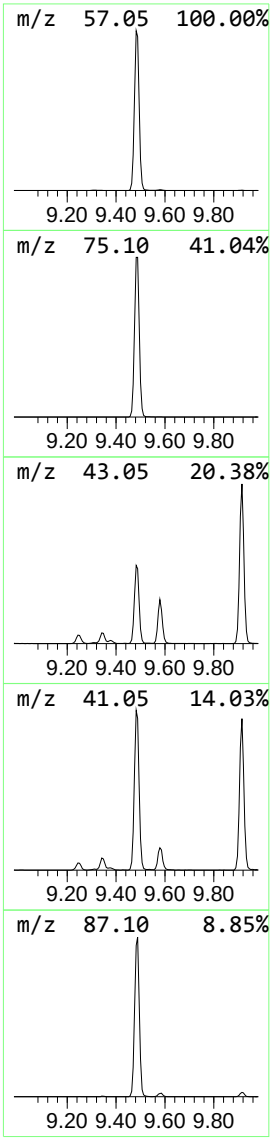
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	166.09 ug/l	1356710	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	39
3	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7
5	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027966.D
Acq On : 04 Apr 2022 18:30
Operator : JC/MD
Sample : PB143824ZHE#03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

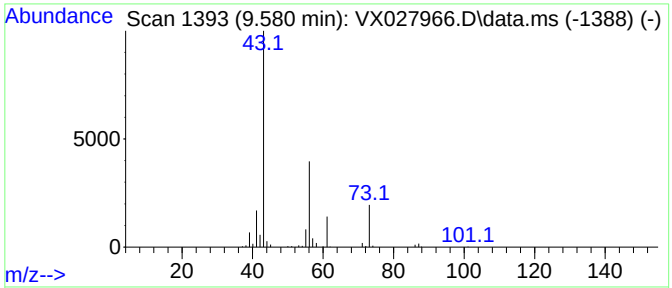
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

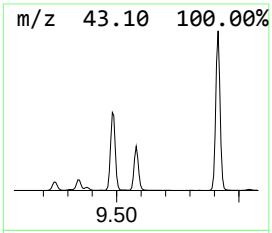
****

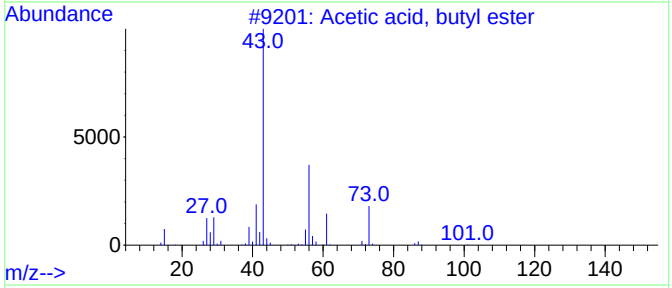
Peak Number 6 Acetic acid, butyl ester Concentration Rank 4

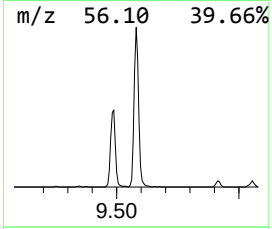
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	18.80 ug/l	153556	Chlorobenzene-d5	10.055

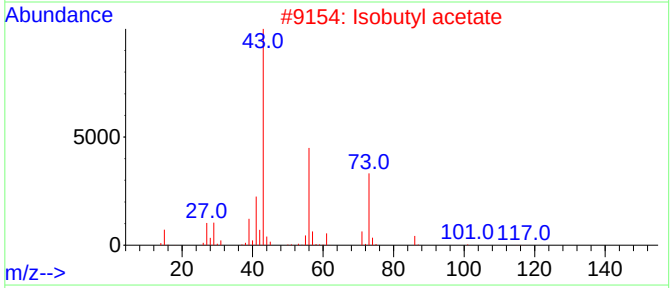
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Isobutyl acetate	116	C6H12O2	000110-19-0	45
3	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	33
4	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
5	Isobutylamine	73	C4H11N	000078-81-9	9

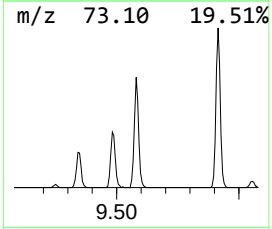


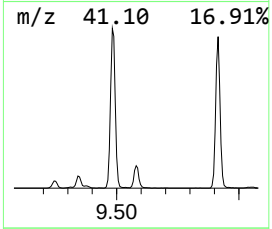


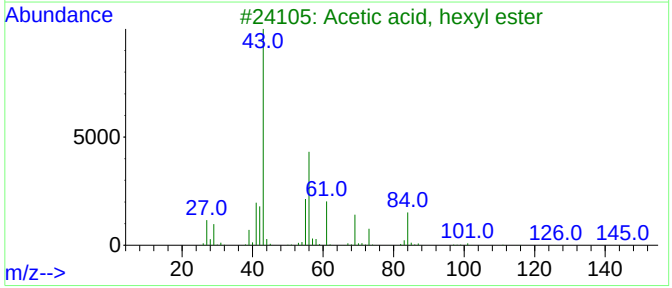


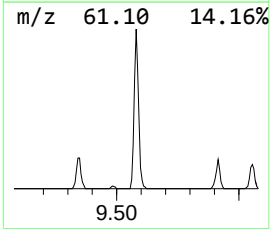












Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027966.D
Acq On : 04 Apr 2022 18:30
Operator : JC/MD
Sample : PB143824ZHE#03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

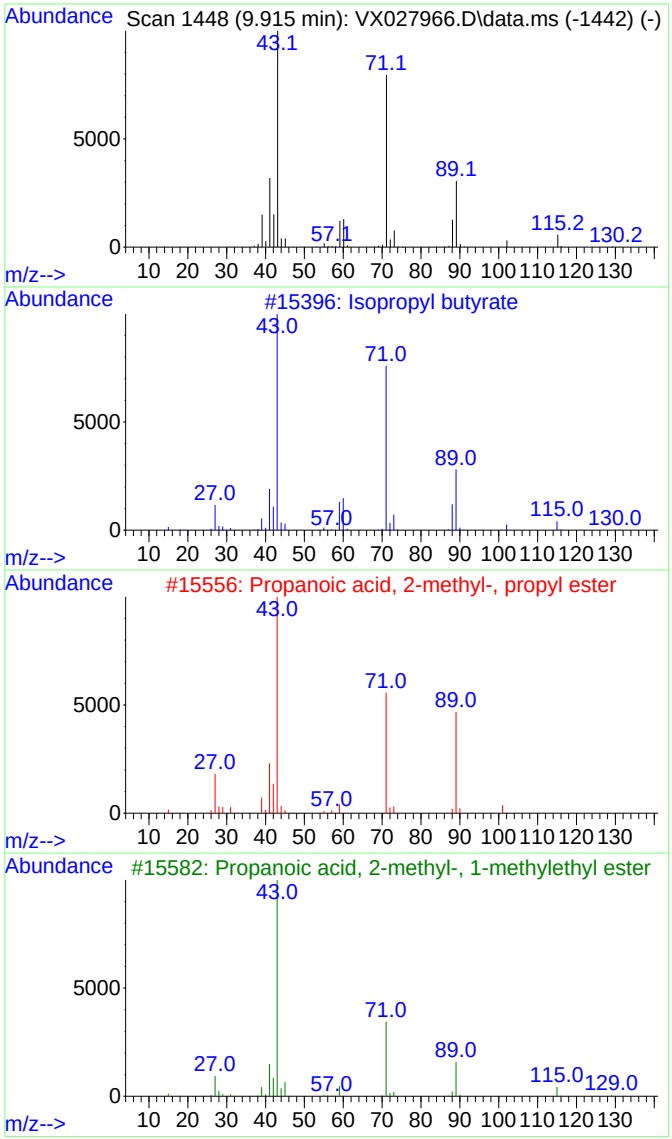
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

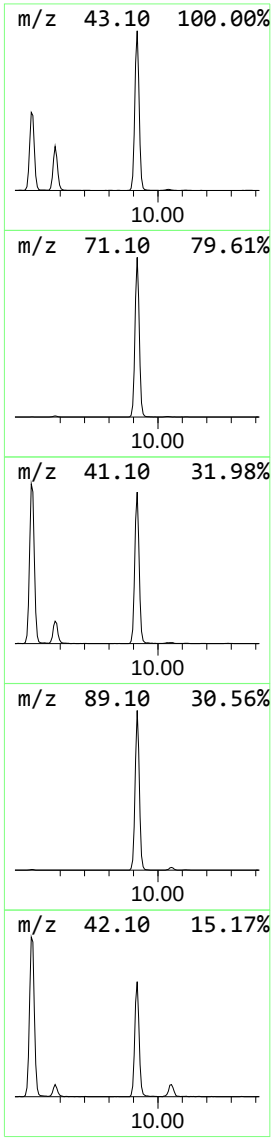
****

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	99.21 ug/l	810349	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	95
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
4	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027966.D
Acq On : 04 Apr 2022 18:30
Operator : JC/MD
Sample : PB143824ZHE#03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.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
Sulfur dioxide	1.240	6.1	ug/l	33482	1	5.556	276348	50.0
n-Propyl acetate	7.799	111.7	ug/l	795842	2	6.763	356306	50.0
Propanoic acid,...	8.549	17.0	ug/l	138895	3	10.055	408418	50.0
Butanoic acid, ...	9.342	10.1	ug/l	82609	3	10.055	408418	50.0
Propanoic acid,...	9.482	166.1	ug/l	1356710	3	10.055	408418	50.0
Acetic acid, bu...	9.580	18.8	ug/l	153556	3	10.055	408418	50.0
Isopropyl butyrate	9.915	99.2	ug/l	810349	3	10.055	408418	50.0