

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
 Data File : VX027964.D
 Acq On : 04 Apr 2022 17:44
 Operator : JC/MD
 Sample : PB143824ZHE#01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PB143824ZHE#01

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: VX027964.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	22	25	37	rBV	27308	36201	2.88%	0.625%
2	5.391	692	706	720	rBV2	50134	148501	11.82%	2.565%
3	5.556	722	733	750	rVB	93648	266579	21.22%	4.605%
4	5.958	790	799	812	rBV	47229	126415	10.06%	2.184%
5	6.696	914	920	923	rBV	6903	13703	1.09%	0.237%
6	6.763	923	931	942	rVB	143685	349862	27.84%	6.043%
7	7.799	1093	1101	1116	rBV	515354	884150	70.36%	15.272%
8	8.549	1217	1224	1234	rBV	85445	129949	10.34%	2.245%
9	8.653	1234	1241	1249	rBV	290730	458473	36.49%	7.919%
10	8.958	1285	1291	1299	rBV	9384	13713	1.09%	0.237%
11	9.250	1333	1339	1345	rBV	23267	33887	2.70%	0.585%
12	9.348	1350	1355	1359	rBV	55139	74369	5.92%	1.285%
13	9.482	1372	1377	1388	rBV	954970	1256536	100.00%	21.704%
14	9.580	1388	1393	1403	rVB	107779	137890	10.97%	2.382%
15	9.915	1442	1448	1461	rBV	624801	769229	61.22%	13.287%
16	10.055	1465	1471	1478	rBV	300801	398383	31.70%	6.881%
17	10.640	1560	1567	1571	rBV	23821	28454	2.26%	0.491%
18	11.085	1634	1640	1648	rBV	254446	327550	26.07%	5.658%
19	12.024	1789	1794	1804	rVB	278702	335533	26.70%	5.796%

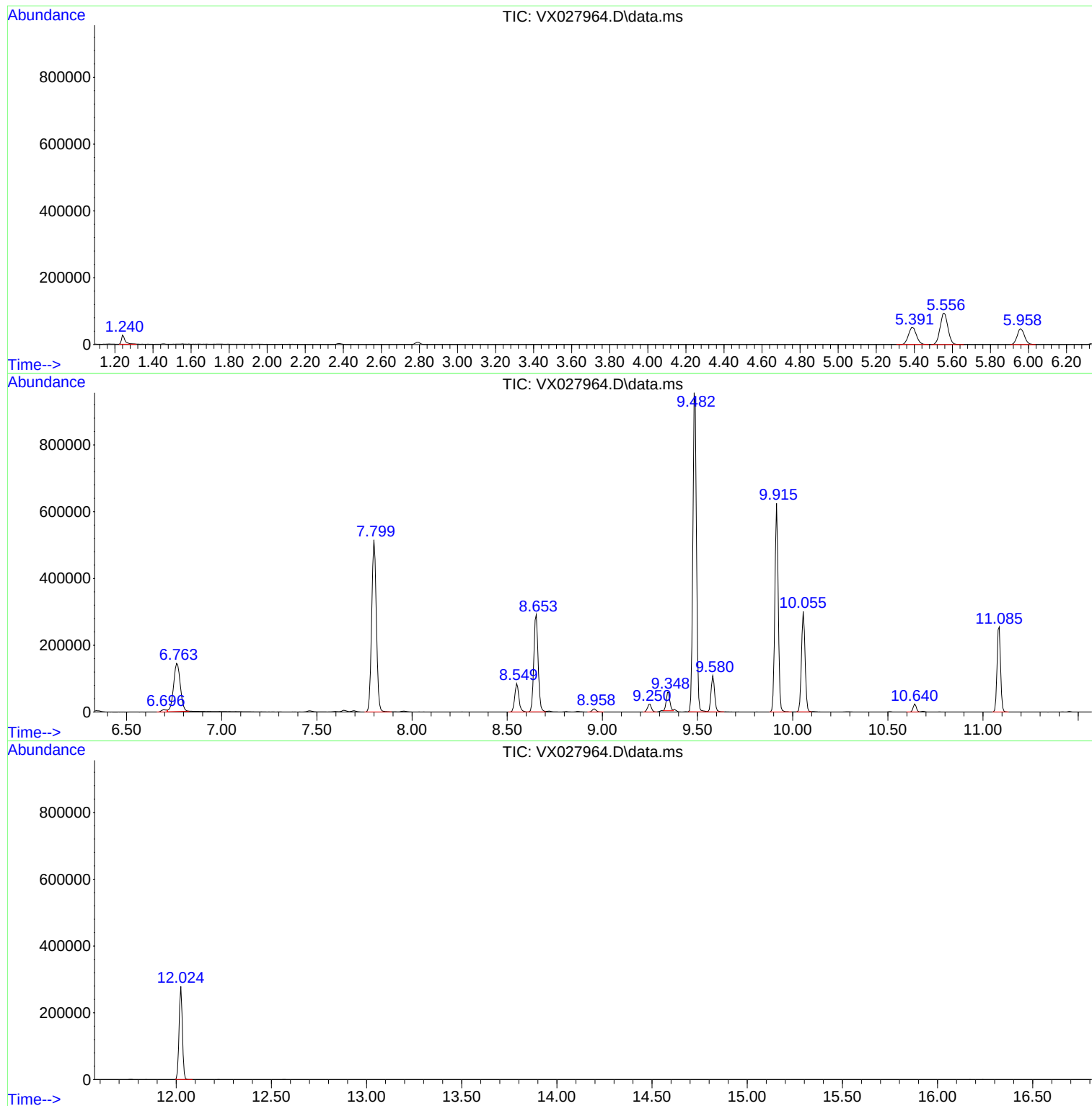
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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



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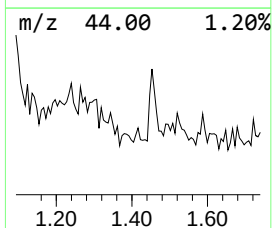
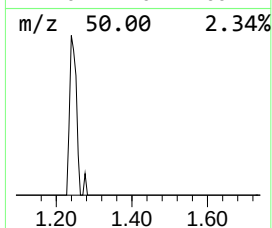
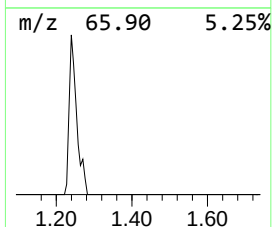
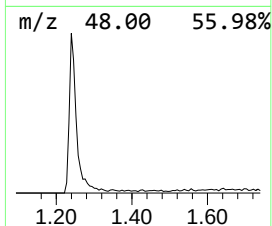
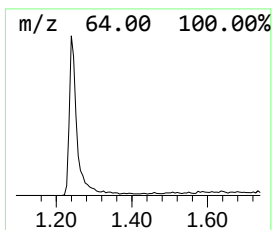
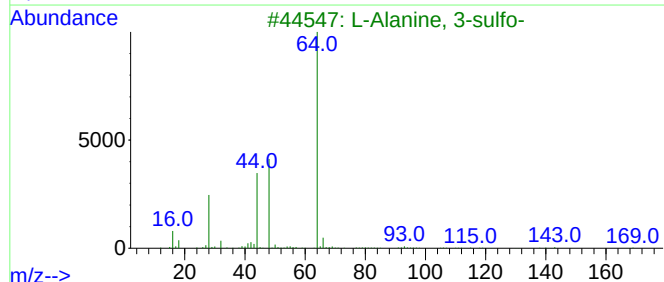
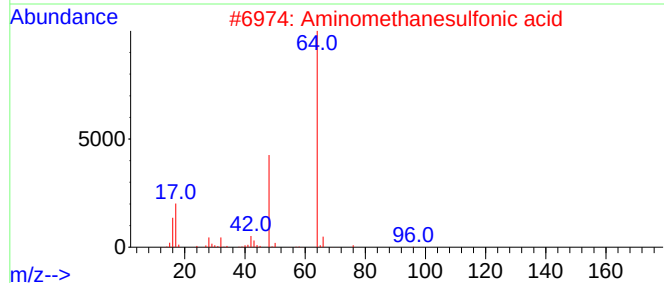
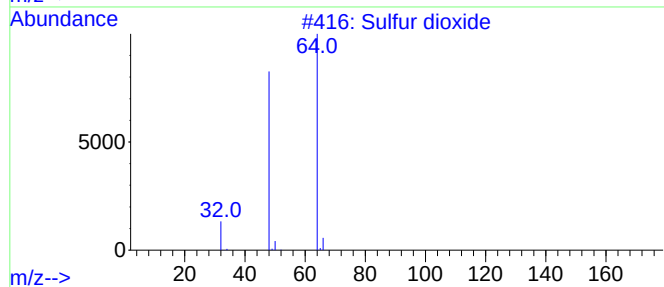
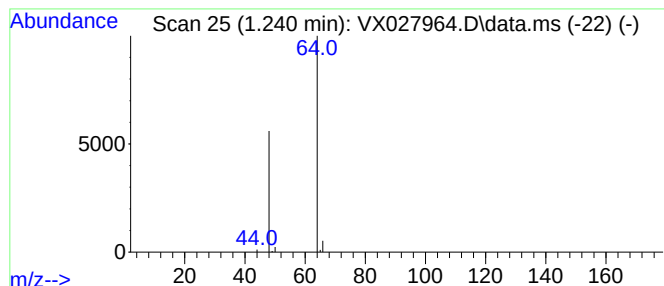
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	6.79 ug/l	36201	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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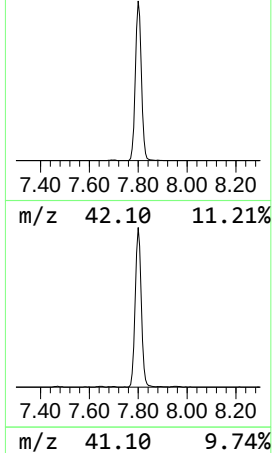
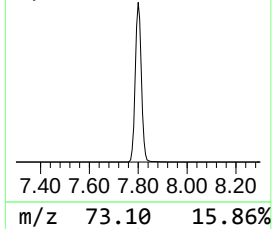
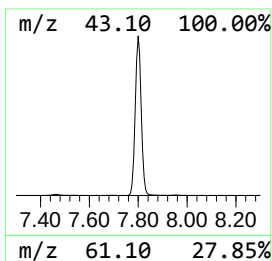
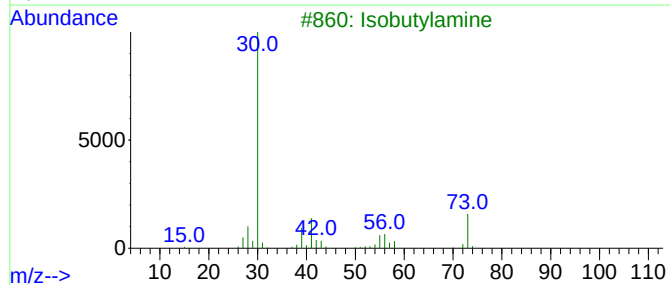
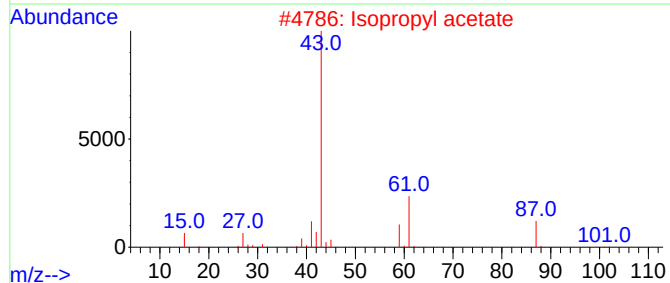
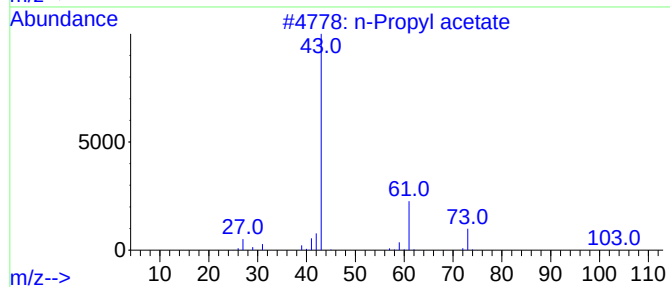
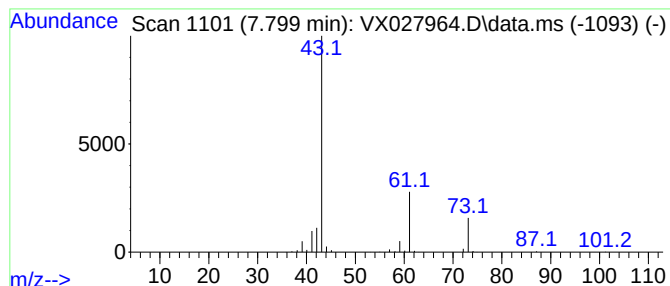
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Peak Number 2 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	126.36 ug/l	884150	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			Isobutylamine	73	C4H11N	000078-81-9	9
4			Isobutyl acetate	116	C6H12O2	000110-19-0	9
5			1-Butanamine	73	C4H11N	000109-73-9	5



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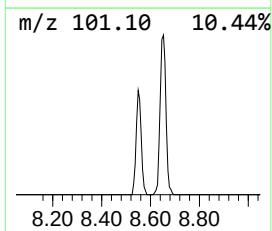
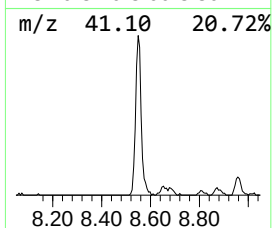
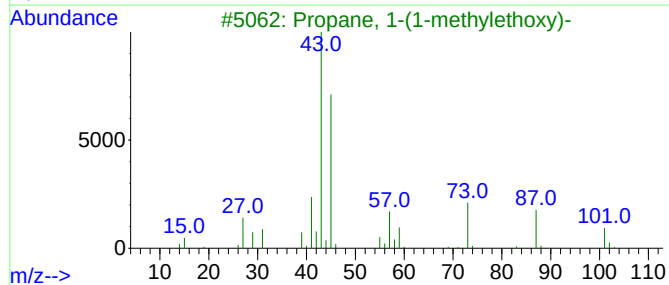
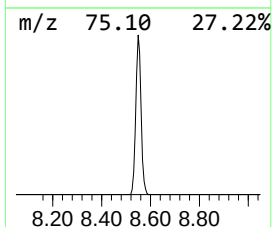
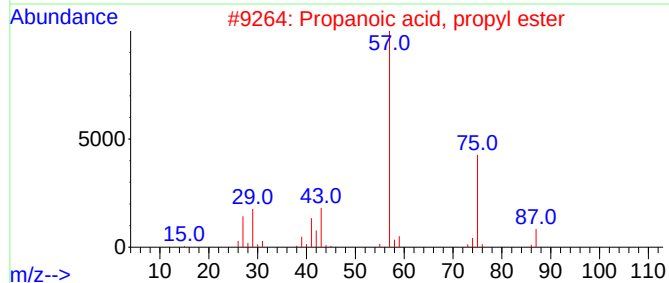
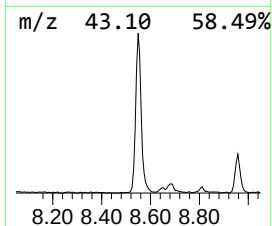
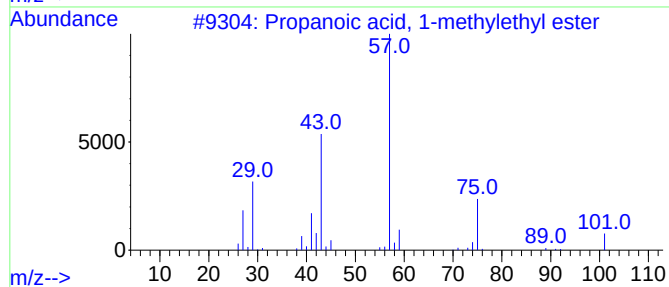
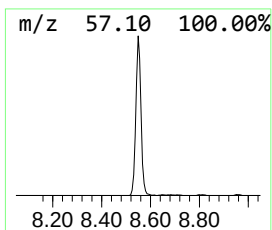
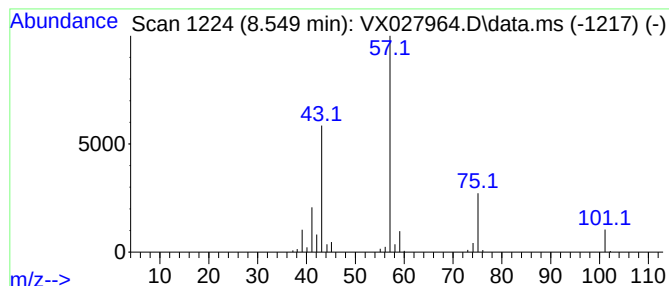
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Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	16.31 ug/l	129949	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	40
3			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4			o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	16
5			Isobutane	58	C4H10	000075-28-5	9



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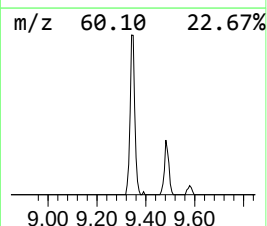
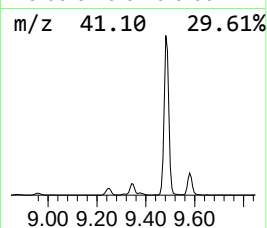
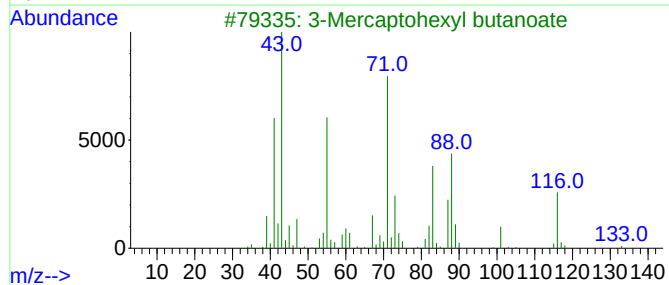
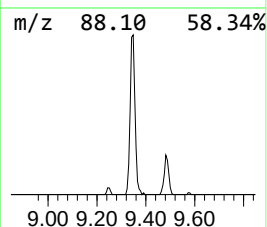
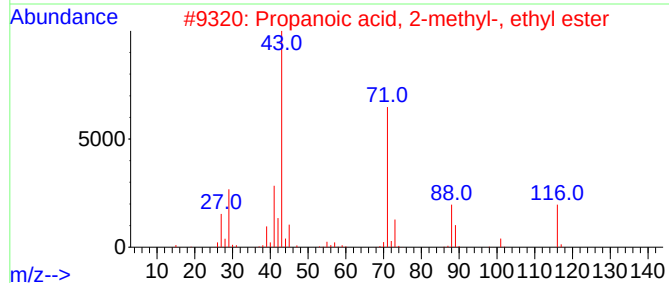
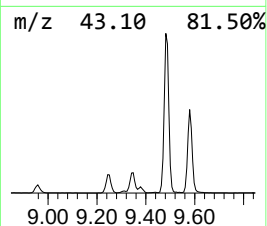
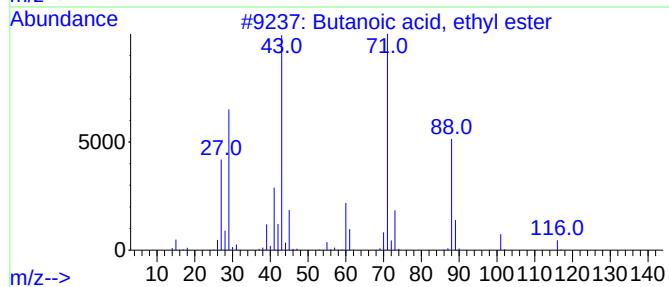
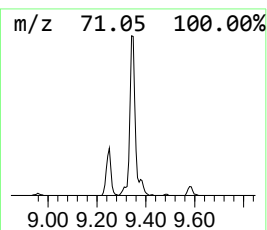
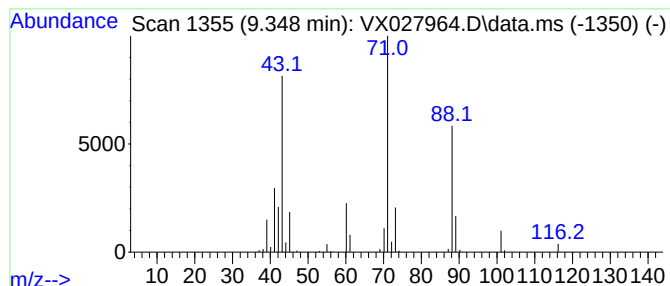
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Peak Number 4 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.348	9.33 ug/l	74369	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	59
3			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	53
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
5			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	47



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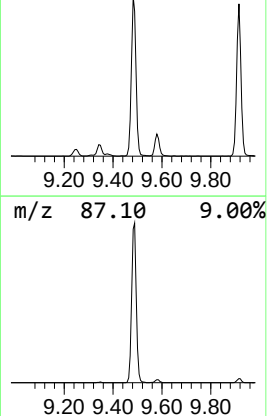
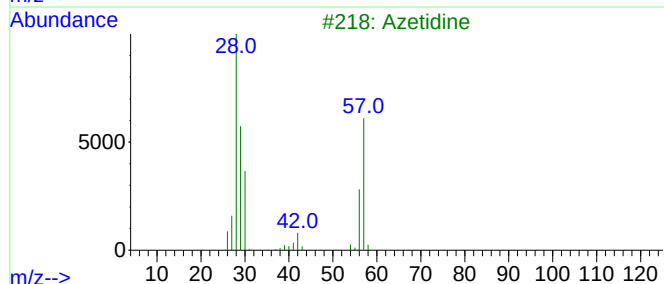
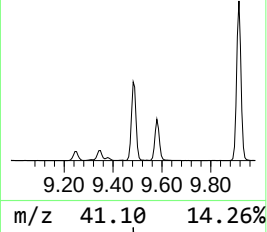
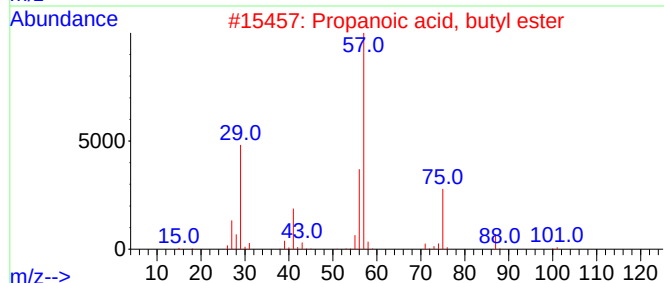
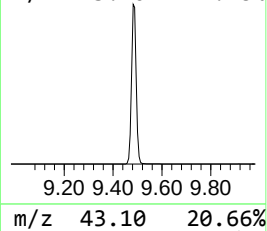
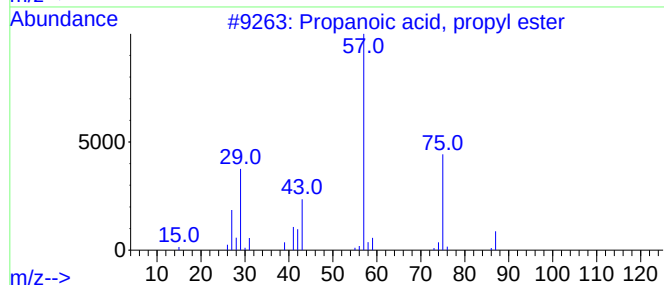
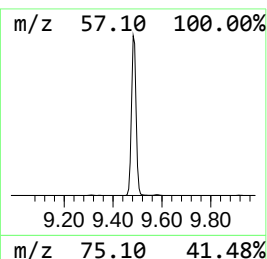
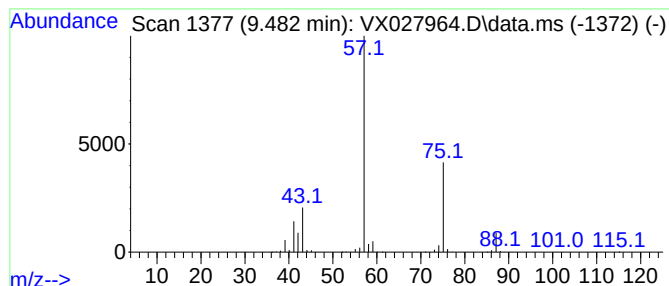
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Peak Number 5 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	157.71 ug/l	1256540	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			Azetidine	57	C3H7N	000503-29-7	9
4			Isobutyl ether	130	C8H18O	000628-55-7	9
5			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9



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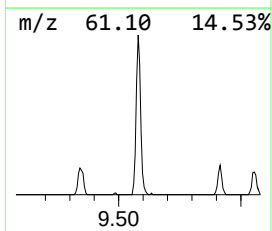
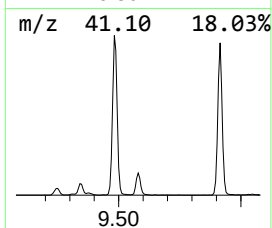
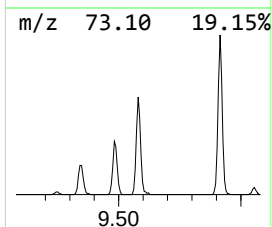
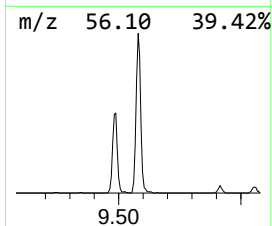
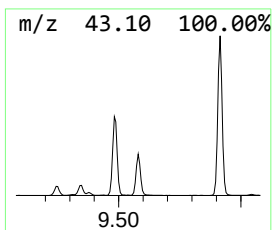
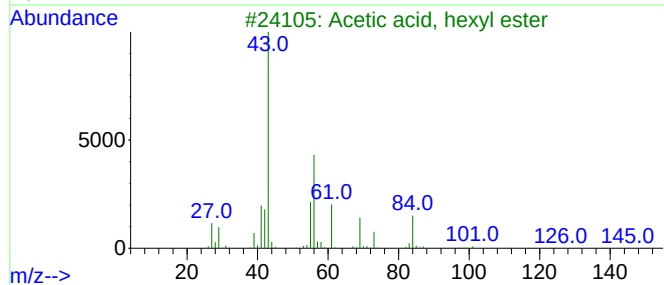
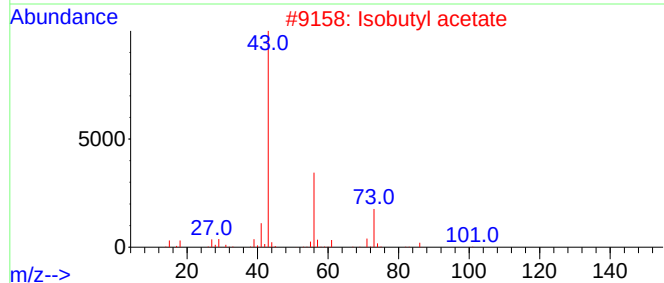
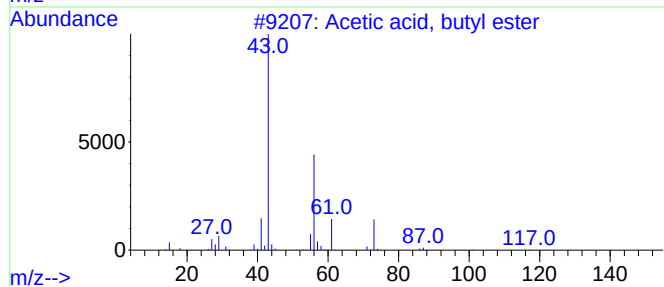
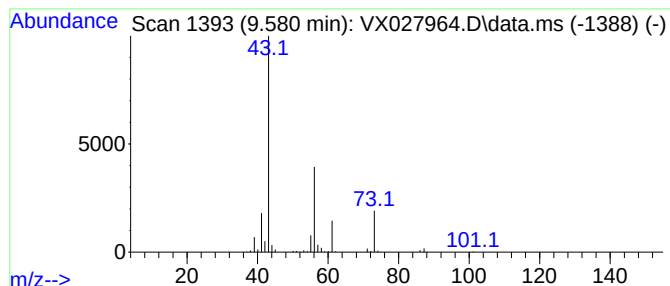
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	17.31 ug/l	137890	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	40
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 : VX027964.D
Acq On : 04 Apr 2022 17:44
Operator : JC/MD
Sample : PB143824ZHE#01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#01

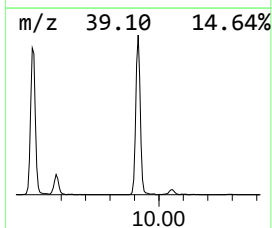
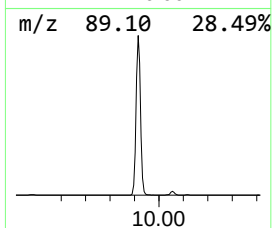
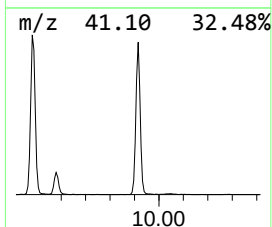
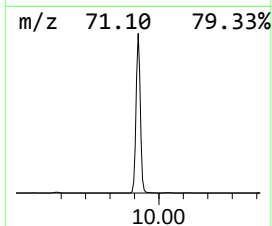
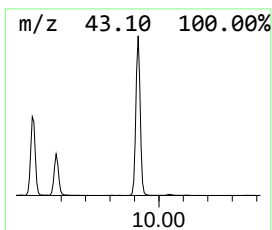
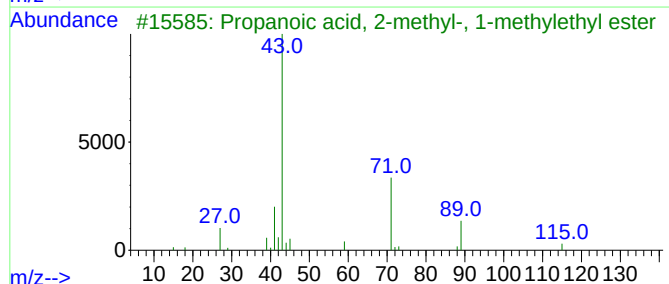
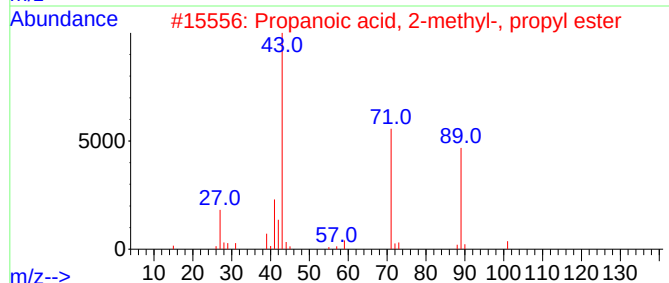
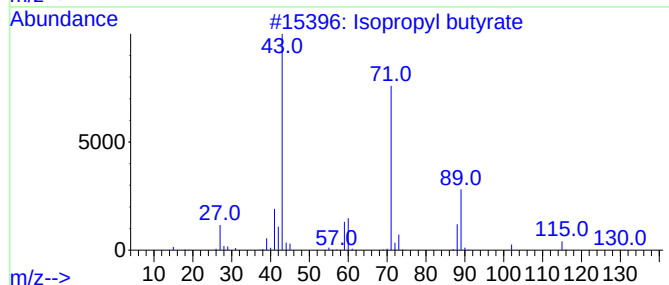
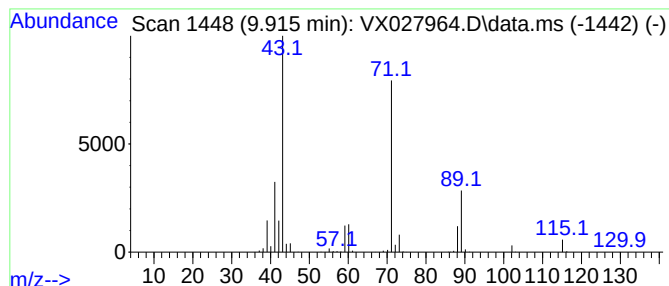
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Quant Title : SW846 8260

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	96.54 ug/l	769229	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	94
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027964.D
Acq On : 04 Apr 2022 17:44
Operator : JC/MD
Sample : PB143824ZHE#01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PB143824ZHE#01

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	6.8	ug/l	36201	1	5.556	266579	50.0
n-Propyl acetate	7.799	126.4	ug/l	884150	2	6.763	349862	50.0
Propanoic acid,...	8.549	16.3	ug/l	129949	3	10.055	398383	50.0
Butanoic acid, ...	9.348	9.3	ug/l	74369	3	10.055	398383	50.0
Propanoic acid,...	9.482	157.7	ug/l	1256540	3	10.055	398383	50.0
Acetic acid, bu...	9.580	17.3	ug/l	137890	3	10.055	398383	50.0
Isopropyl butyrate	9.915	96.5	ug/l	769229	3	10.055	398383	50.0