

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012822\
 Data File : VX026666.D
 Acq On : 28 Jan 2022 20:59
 Operator : JC/MD
 Sample : N1319-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MH-2S

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\82X011122W.M
 Title : SW846 8260

Signal : TIC: VX026666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.392	206	214	223	rBV	10953	19262	1.11%	0.234%
2	5.391	694	706	722	rBV	78164	226553	13.10%	2.750%
3	5.556	722	733	746	rVV	135001	381242	22.04%	4.628%
4	5.964	789	800	813	rBV	88211	230872	13.34%	2.803%
5	6.342	851	862	874	rBV2	8483	22441	1.30%	0.272%
6	6.763	921	931	942	rBV	214729	531018	30.69%	6.446%
7	7.799	1093	1101	1117	rBV	732649	1245101	71.97%	15.114%
8	8.549	1218	1224	1234	rBV	123941	191422	11.06%	2.324%
9	8.653	1234	1241	1259	rVB	431004	685384	39.62%	8.320%
10	8.958	1286	1291	1299	rVB	13515	19453	1.12%	0.236%
11	9.250	1333	1339	1344	rBV	32404	48751	2.82%	0.592%
12	9.342	1350	1354	1359	rBV	78777	108211	6.25%	1.314%
13	9.482	1372	1377	1388	rBV	1285344	1730060	100.00%	21.001%
14	9.580	1388	1393	1412	rVB	146366	193912	11.21%	2.354%
15	9.915	1442	1448	1465	rBV	868576	1076948	62.25%	13.073%
16	10.055	1465	1471	1478	rBV	435813	575375	33.26%	6.985%
17	10.640	1561	1567	1581	rBV	30718	39745	2.30%	0.482%
18	11.085	1634	1640	1647	rBV	319020	414471	23.96%	5.031%
19	12.024	1788	1794	1802	rBV	398352	497593	28.76%	6.040%

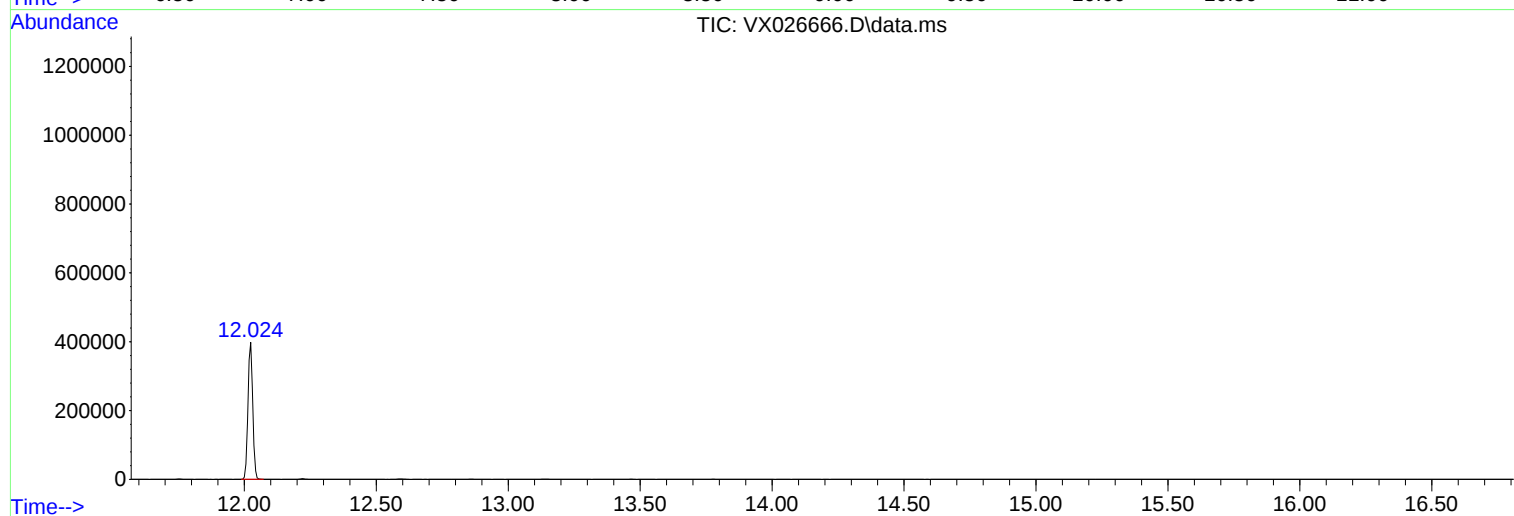
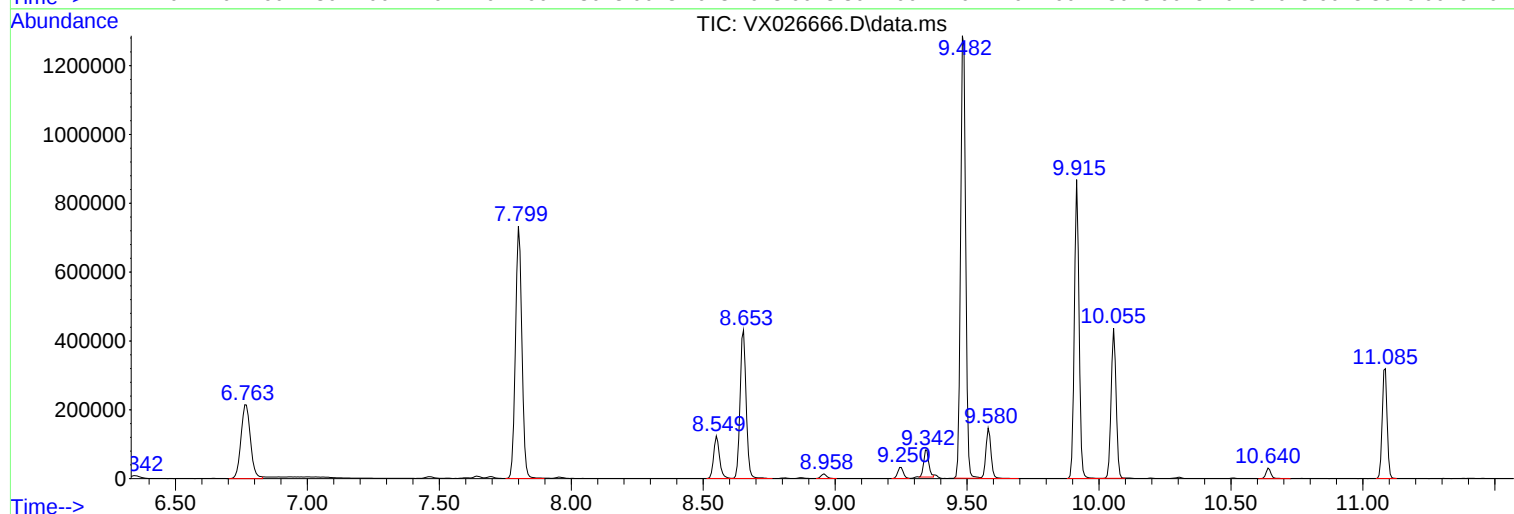
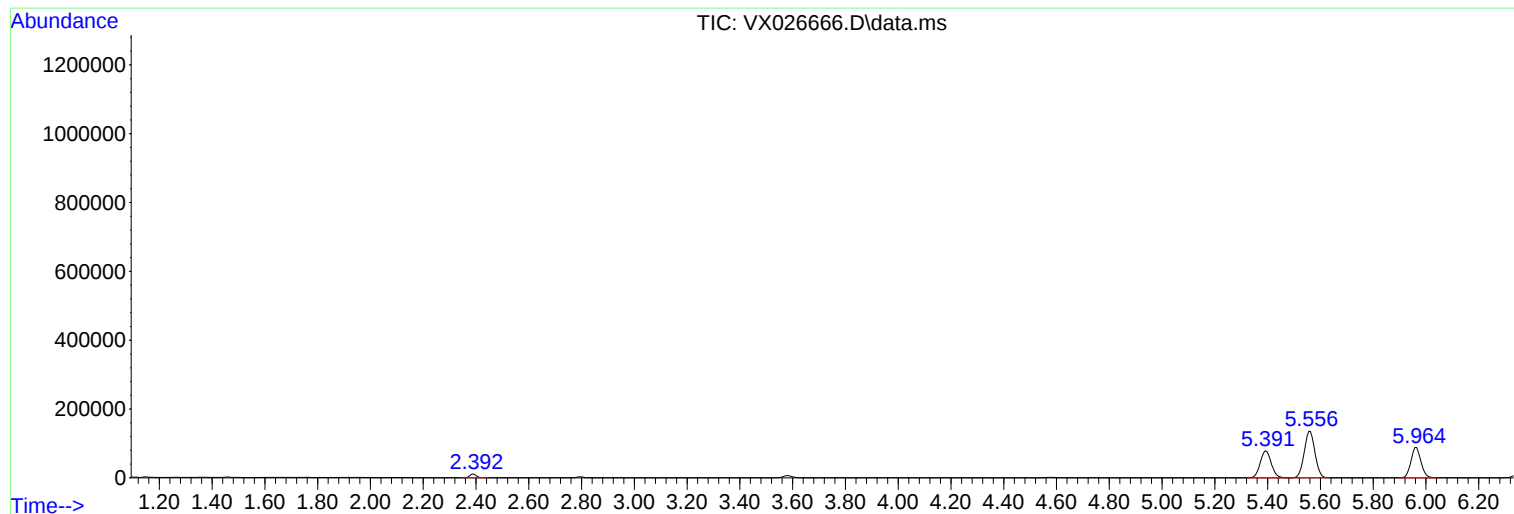
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Quant Title : SW846 8260

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



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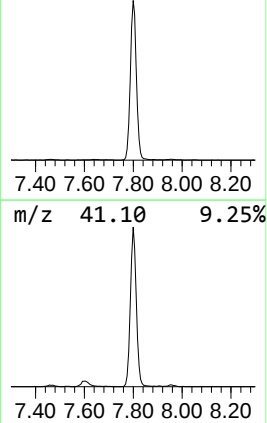
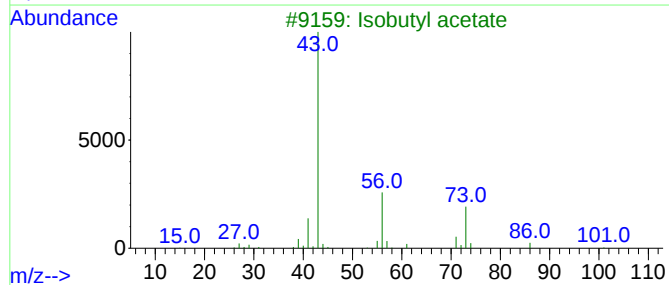
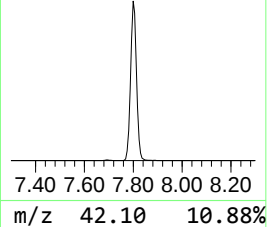
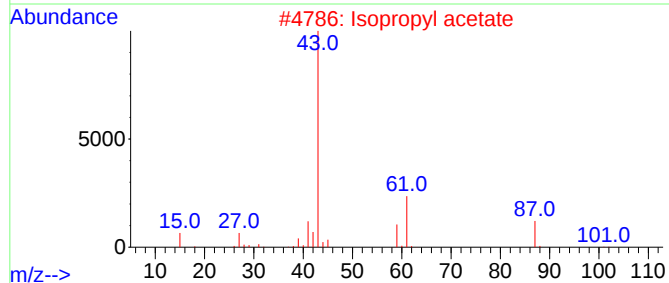
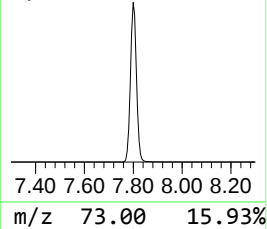
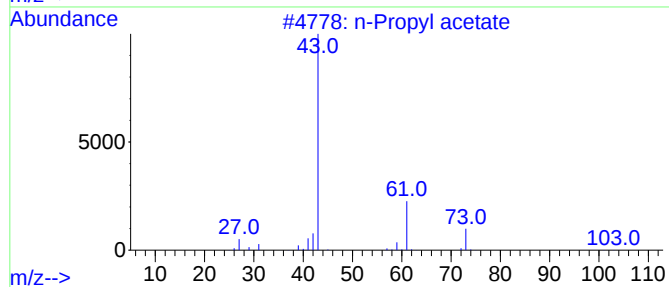
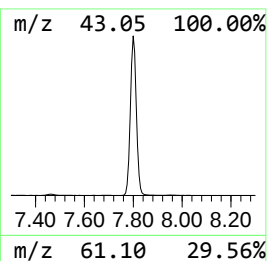
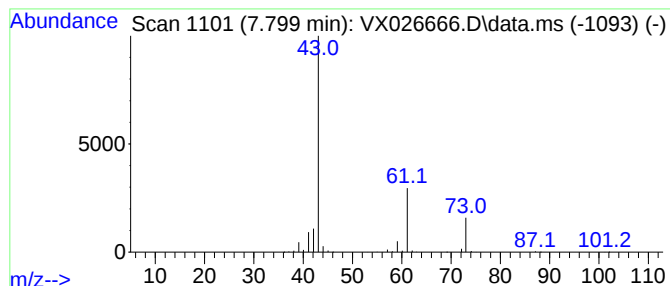
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	117.24 ug/l	1245100	1,4-Difluorobenzene	6.769

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



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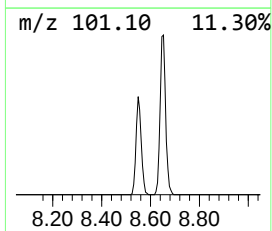
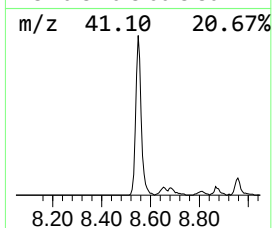
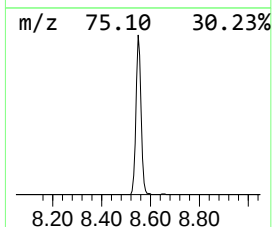
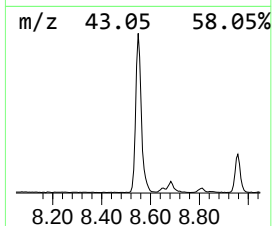
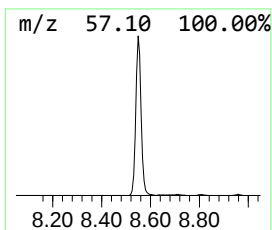
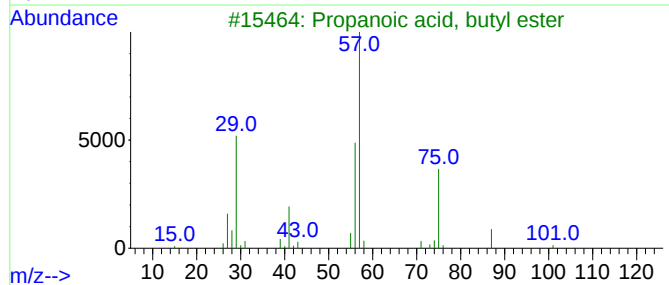
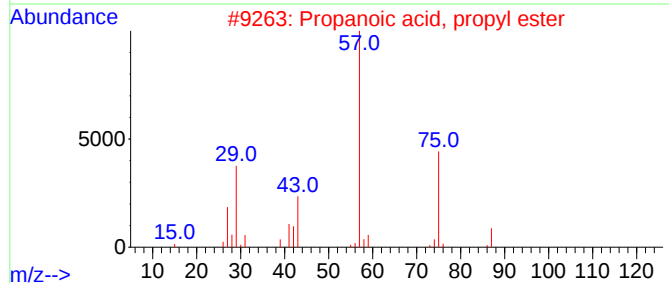
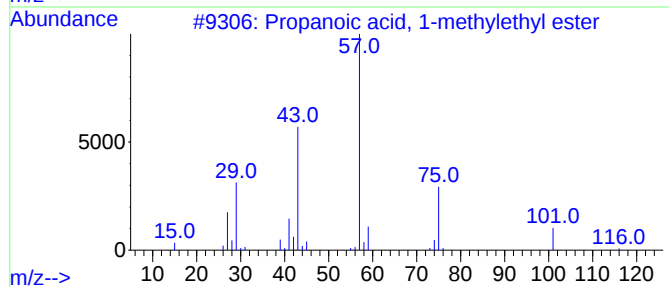
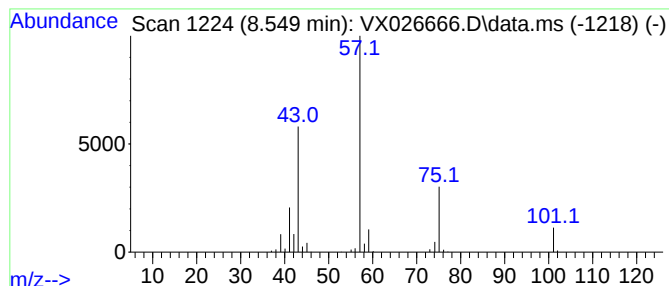
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	16.63 ug/l	191422	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
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			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10



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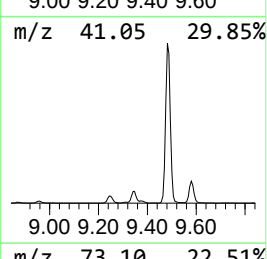
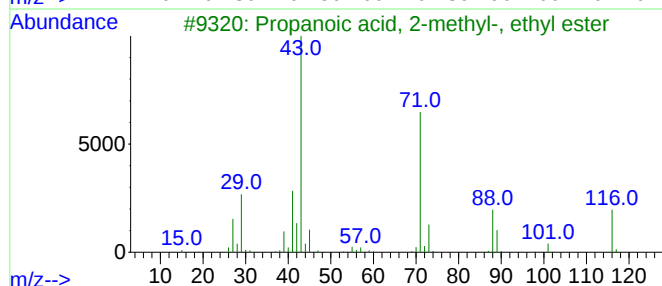
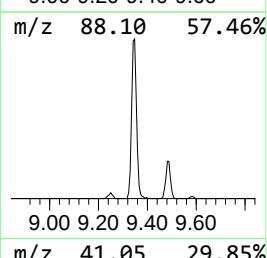
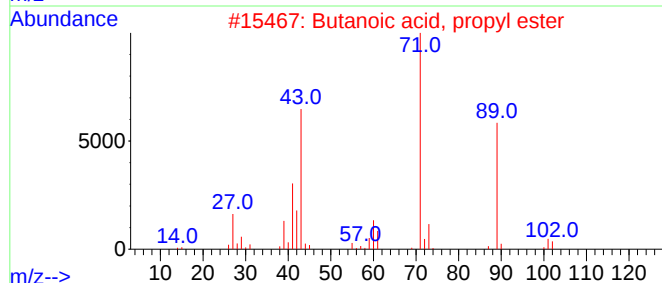
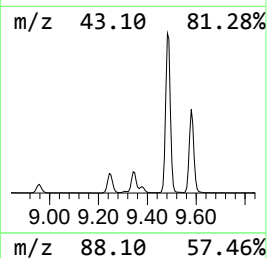
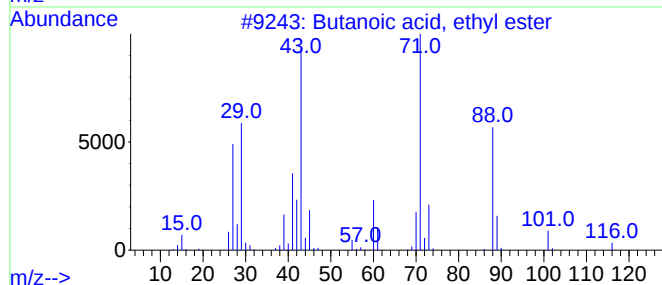
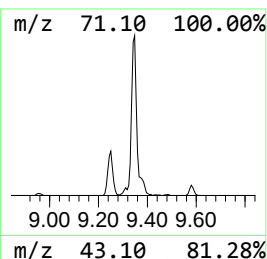
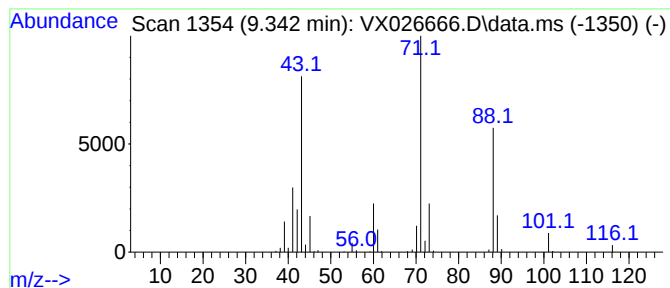
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Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	9.40 ug/l	108211	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	95
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53
3			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
4			Butanoic acid, 3-methylbutyl ester	158	C9H18O2	000106-27-4	43
5			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	42



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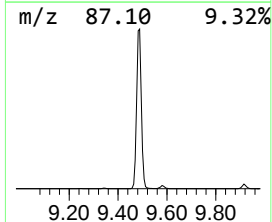
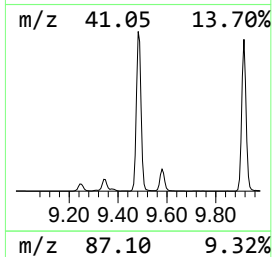
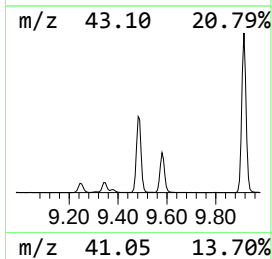
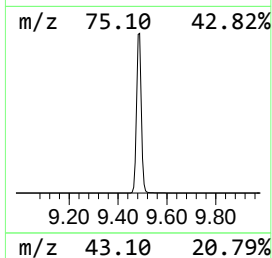
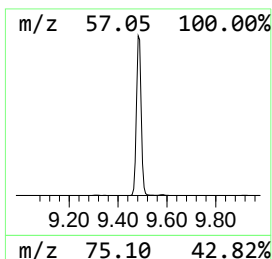
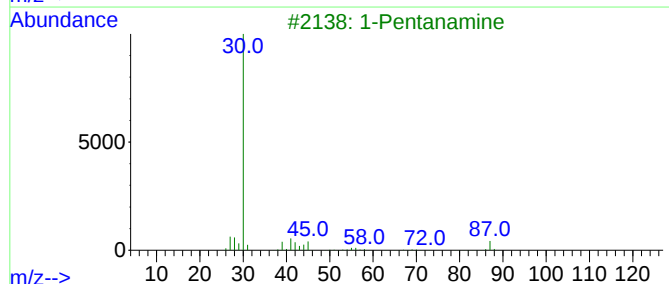
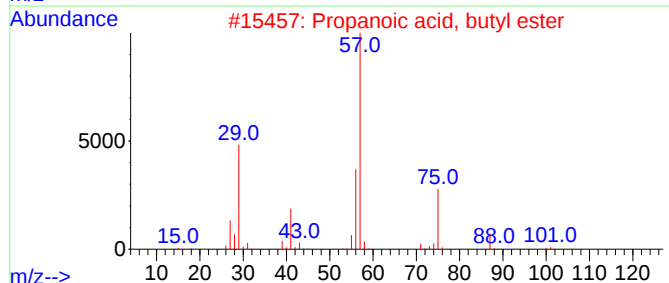
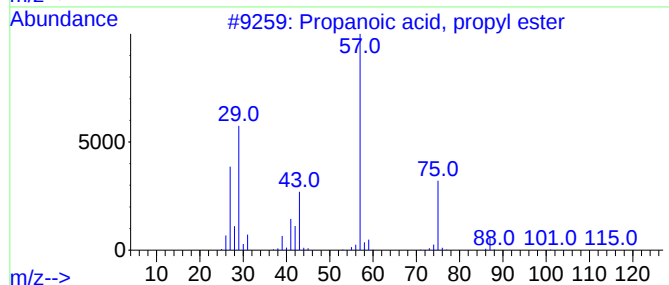
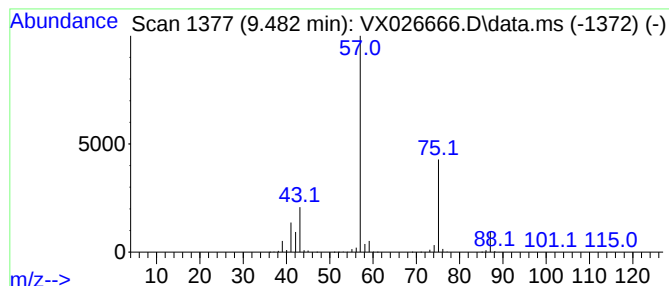
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Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	150.34 ug/l	1730060	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	28
3			1-Pentanamine	87	C5H13N	000110-58-7	10
4			Azetidine	57	C3H7N	000503-29-7	9
5			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9



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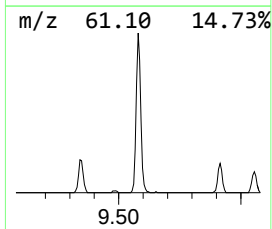
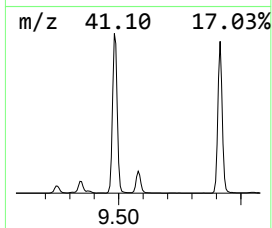
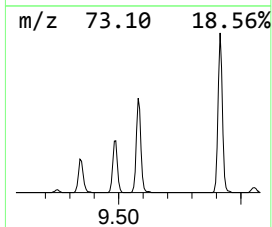
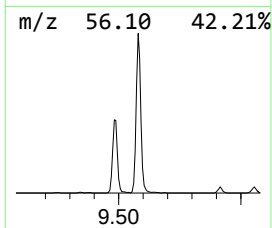
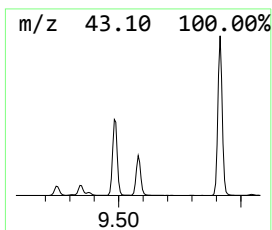
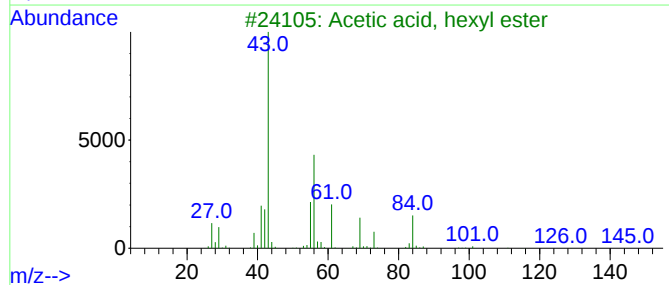
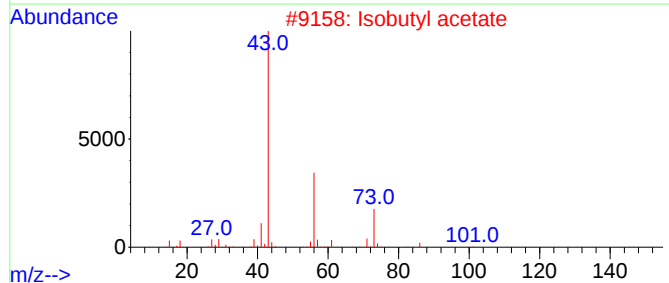
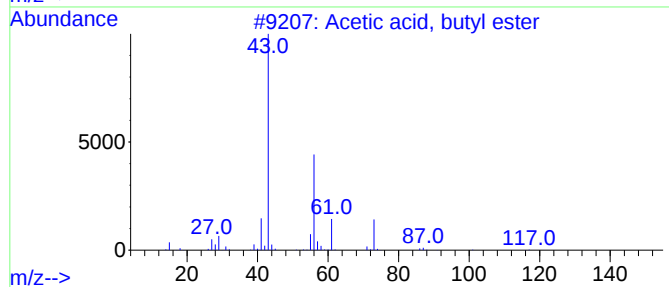
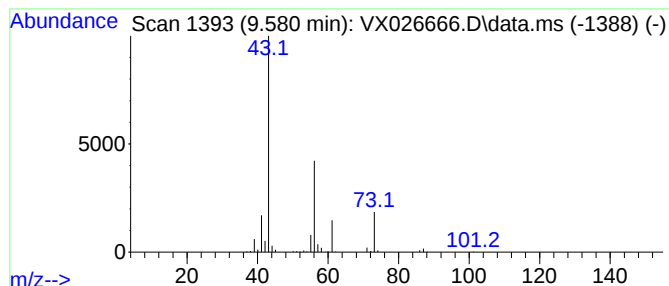
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Peak Number 5 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	16.85 ug/l	193912	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	38
4			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17
5			Isobutylamine	73	C4H11N	000078-81-9	9



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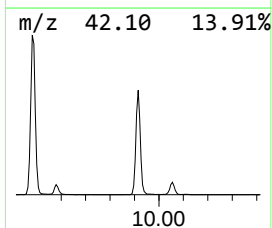
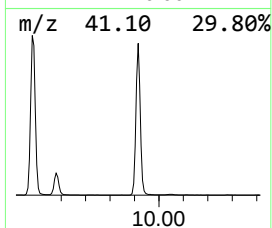
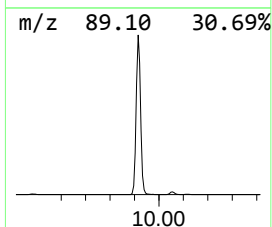
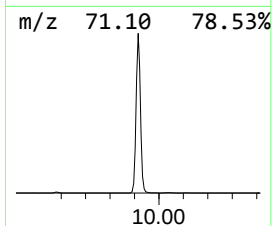
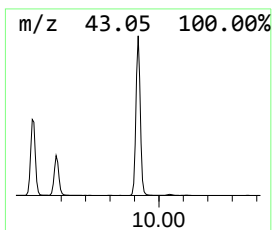
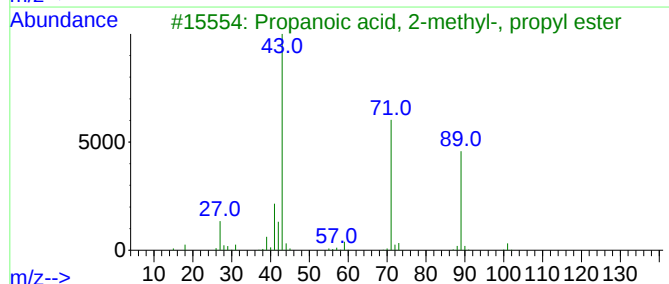
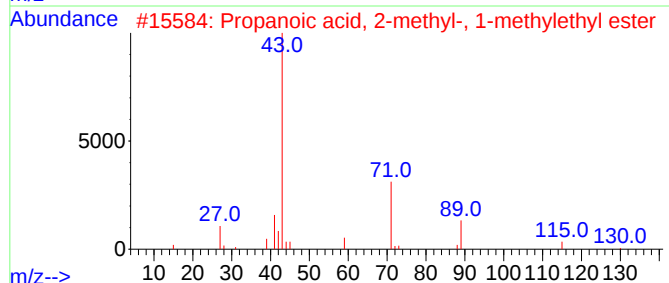
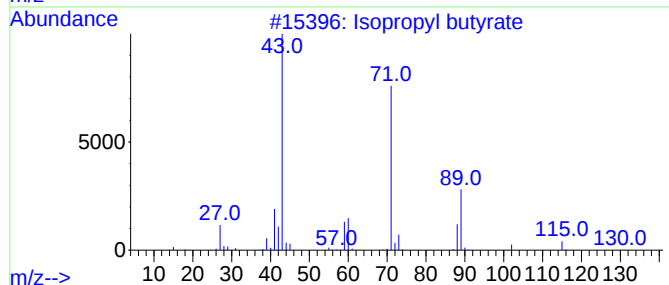
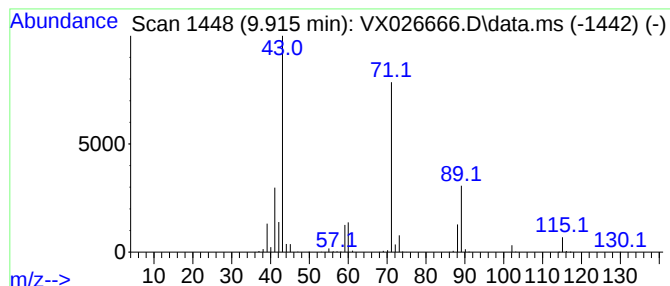
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	93.59 ug/l	1076950	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-, 1-met...	130	C7H14O2	000617-50-5	78
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	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\VX012822\
Data File : VX026666.D
Acq On : 28 Jan 2022 20:59
Operator : JC/MD
Sample : N1319-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MH-2S

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.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
n-Propyl acetate	7.799	117.2	ug/l	1245100	2	6.769	531018	50.0
Propanoic acid,...	8.549	16.6	ug/l	191422	3	10.055	575375	50.0
Butanoic acid, ...	9.342	9.4	ug/l	108211	3	10.055	575375	50.0
Propanoic acid,...	9.482	150.3	ug/l	1730060	3	10.055	575375	50.0
Acetic acid, bu...	9.580	16.9	ug/l	193912	3	10.055	575375	50.0
Isopropyl butyrate	9.915	93.6	ug/l	1076950	3	10.055	575375	50.0