

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111324\
 Data File : VN084838.D
 Acq On : 13 Nov 2024 19:59
 Operator : JC\MD
 Sample : P4732-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 PPE-Grab

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
 Title : SW846 8260

Signal : TIC: VN084838.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.283	49	56	75	rBV3	33042	94282	6.10%	0.792%
2	2.659	115	120	127	rVB	11940	22587	1.46%	0.190%
3	2.895	138	160	161	rBV10	21590	92271	5.97%	0.775%
4	4.436	412	422	430	rBV3	12018	35324	2.28%	0.297%
5	7.224	886	896	905	rBV6	11762	36785	2.38%	0.309%
6	8.159	1045	1055	1060	rBV	130185	317152	20.51%	2.665%
7	8.218	1060	1065	1076	rVB	245034	531450	34.38%	4.466%
8	8.571	1115	1125	1134	rBV	148675	330161	21.36%	2.774%
9	8.688	1134	1145	1152	rVV	90175	210910	13.64%	1.772%
10	8.765	1156	1158	1175	rVB5	12549	45175	2.92%	0.380%
11	9.094	1205	1214	1228	rBV	343886	715008	46.25%	6.008%
12	9.671	1302	1312	1317	rBV2	44964	105086	6.80%	0.883%
13	9.741	1317	1324	1333	rVB	860202	1545990	100.00%	12.990%
14	10.353	1421	1428	1438	rBV	158961	274163	17.73%	2.304%
15	10.565	1456	1464	1473	rBV	523304	977304	63.22%	8.212%
16	10.724	1485	1491	1499	rBV	202065	336949	21.80%	2.831%
17	10.982	1528	1535	1542	rBV	134800	231097	14.95%	1.942%
18	11.076	1545	1551	1559	rVV4	46320	88892	5.75%	0.747%
19	11.200	1559	1572	1580	rVV2	328731	661511	42.79%	5.558%
20	11.288	1580	1587	1598	rVB	239061	389090	25.17%	3.269%
21	11.600	1632	1640	1649	rBV	437660	688075	44.51%	5.782%
22	11.765	1663	1668	1675	rVB3	9248	17600	1.14%	0.148%
23	11.865	1675	1685	1695	rVV	487768	879005	56.86%	7.386%
24	11.959	1695	1701	1708	rVB2	9257	16961	1.10%	0.143%
25	12.206	1734	1743	1747	rBV3	10237	19368	1.25%	0.163%
26	12.300	1754	1759	1767	rVB	28731	46210	2.99%	0.388%
27	12.376	1767	1772	1777	rBV3	15366	26672	1.73%	0.224%
28	12.847	1841	1852	1860	rVB	427082	722993	46.77%	6.075%
29	13.329	1924	1934	1936	rBV7	14144	36564	2.37%	0.307%
30	13.482	1956	1960	1971	rVB7	7893	21084	1.36%	0.177%
31	13.688	1980	1995	2005	rBV7	25365	131885	8.53%	1.108%
32	13.788	2005	2012	2019	rVV	534570	905797	58.59%	7.611%
33	13.870	2022	2026	2034	rVB3	46499	83714	5.41%	0.703%
34	14.000	2040	2048	2060	rBV4	74701	253588	16.40%	2.131%
35	14.253	2083	2091	2101	rBV4	17469	72422	4.68%	0.609%
36	14.553	2137	2142	2152	rVB5	28690	74956	4.85%	0.630%

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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

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Title : SW846 8260

37	14.794	2176	2183	2185	rBV7	9099	17888	1.16%	0.150%
38	15.206	2247	2253	2260	rVB5	19360	35118	2.27%	0.295%
39	15.523	2295	2307	2319	rVB3	66075	246639	15.95%	2.072%
40	15.635	2319	2326	2335	rVB	190534	385250	24.92%	3.237%
41	15.806	2348	2355	2370	rVB5	32221	108236	7.00%	0.909%
42	16.782	2514	2521	2522	rBV2	36992	69908	4.52%	0.587%

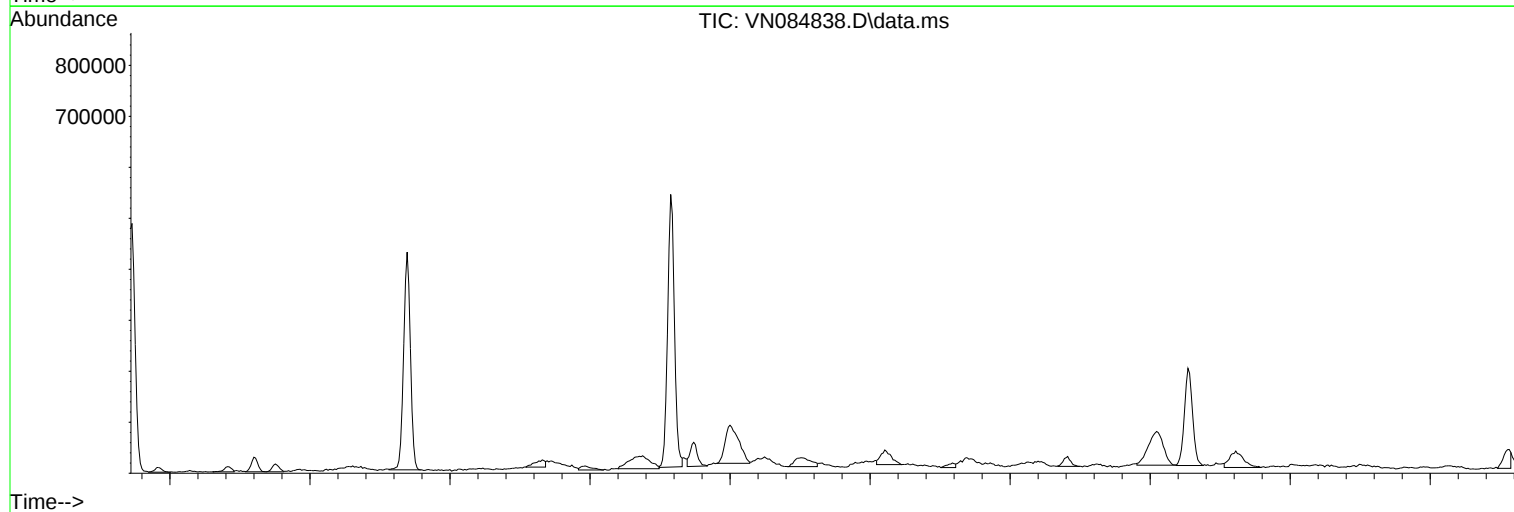
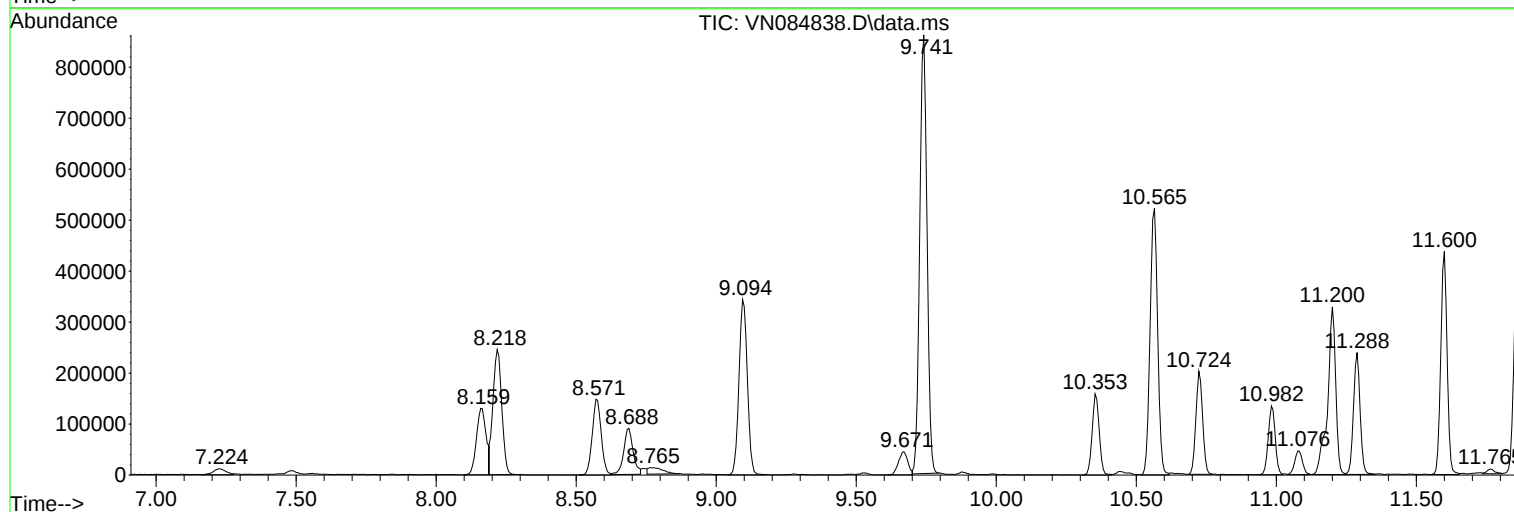
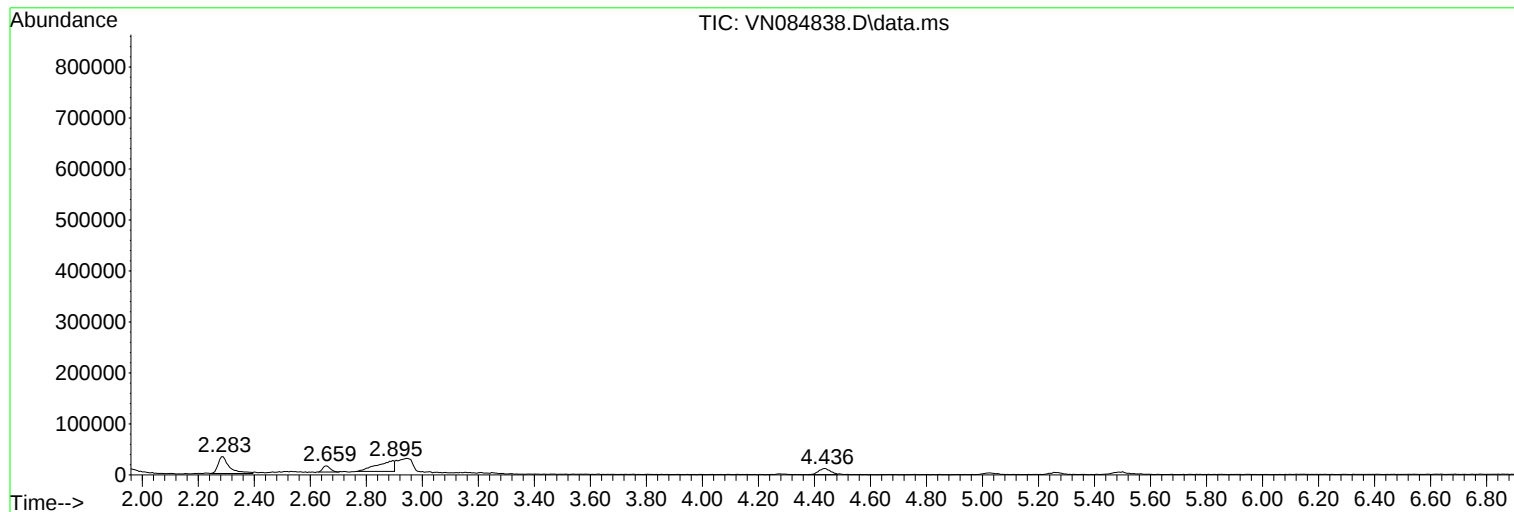
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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



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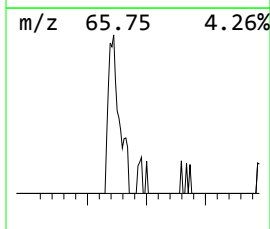
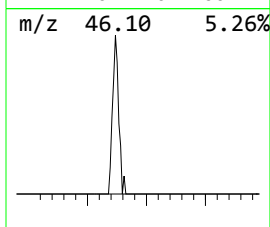
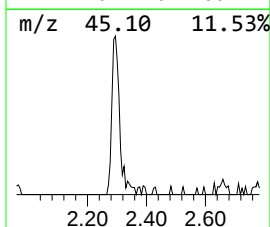
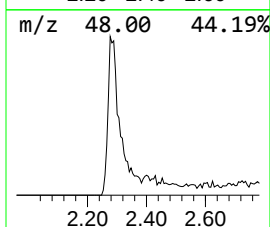
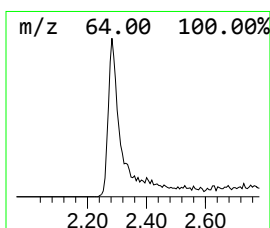
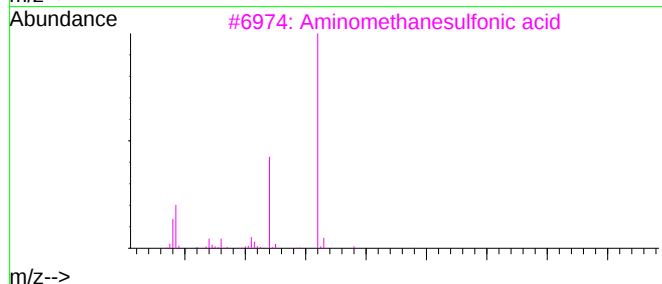
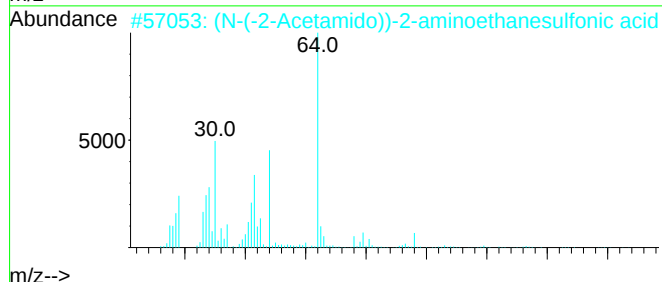
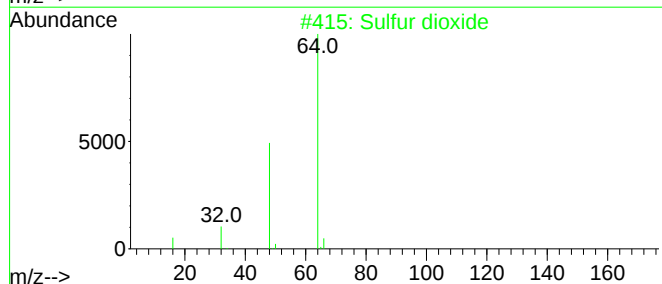
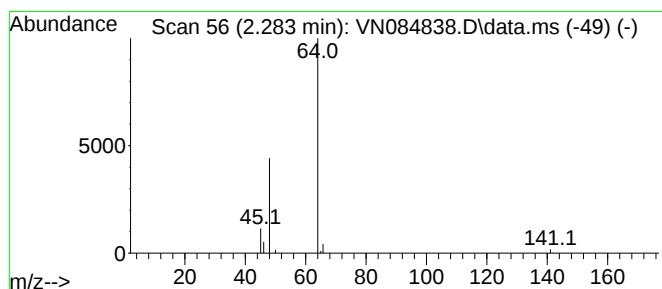
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.283	8.87 ug/l	94282	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	64
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	9
5	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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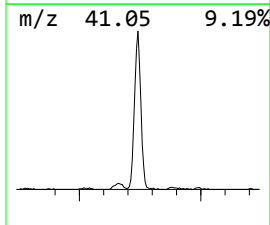
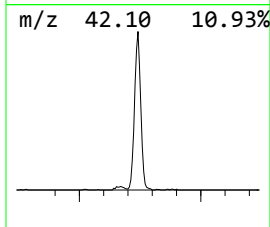
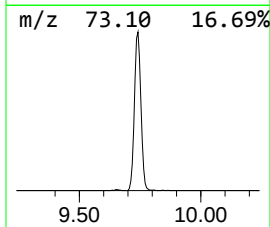
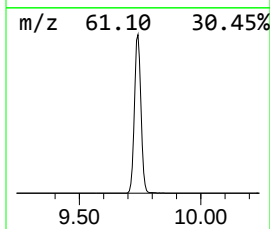
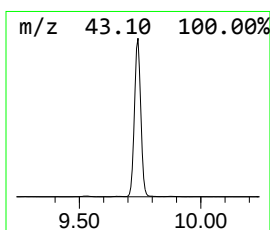
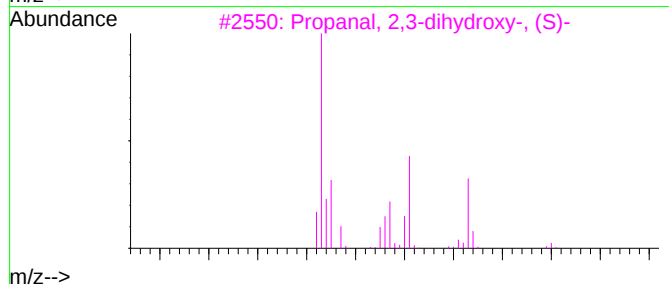
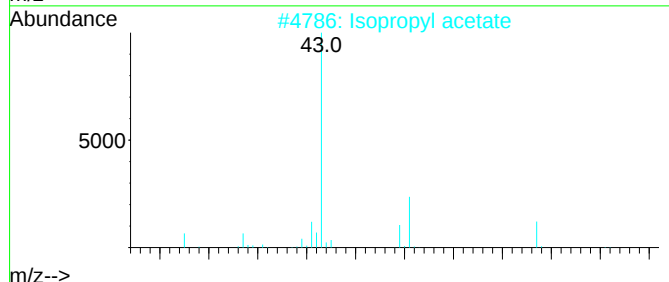
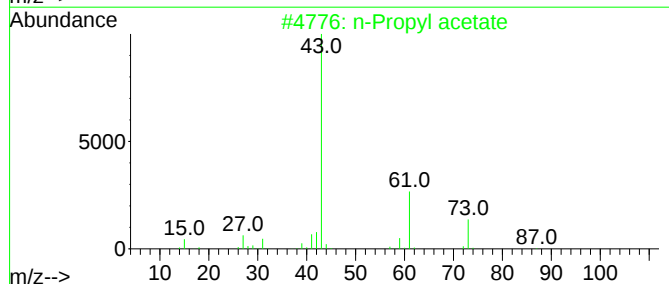
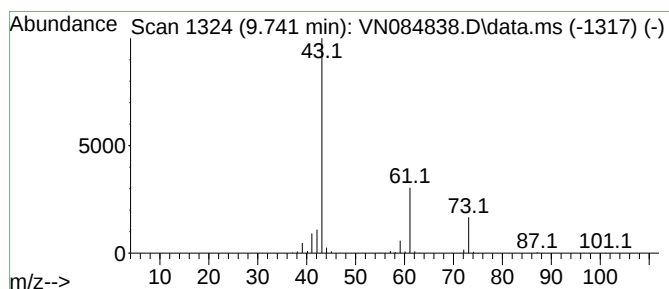
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.741	108.11 ug/l	1545990	1,4-Difluorobenzene	9.094

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	38
3	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	4



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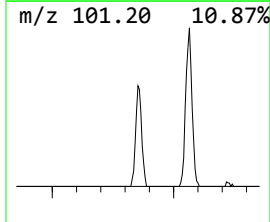
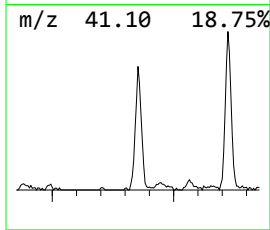
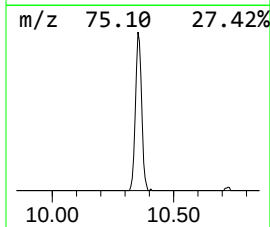
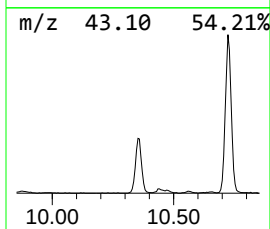
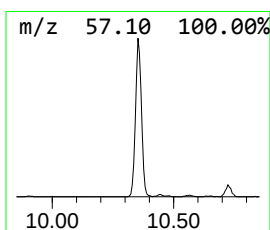
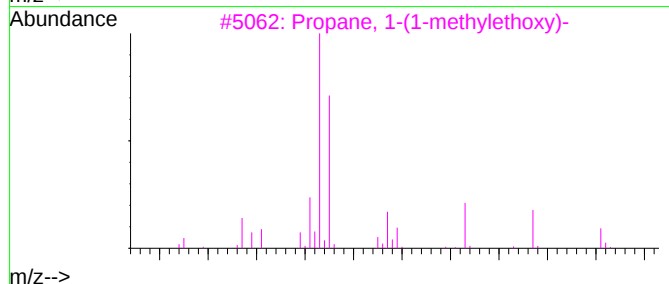
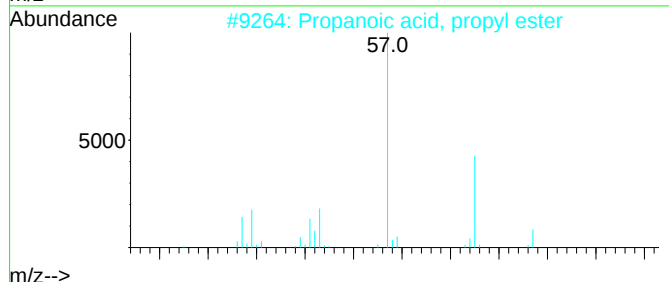
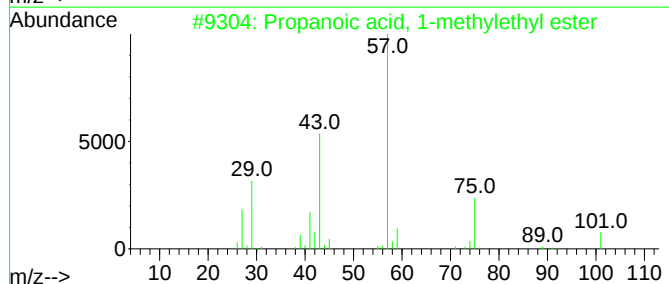
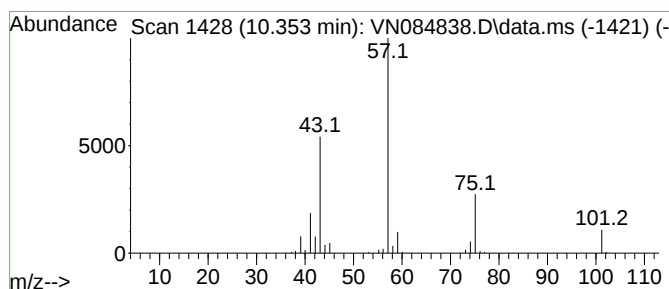
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TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.353	19.17 ug/l	274163	1,4-Difluorobenzene	9.094	
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	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
5	o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	16



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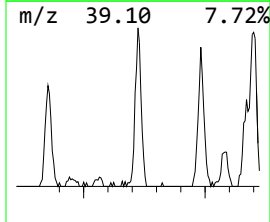
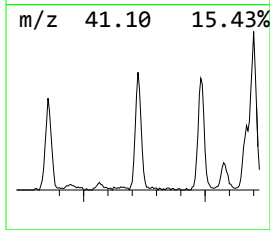
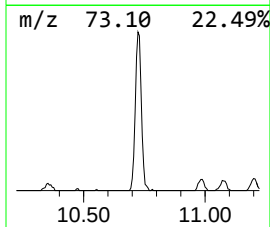
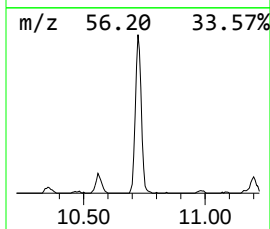
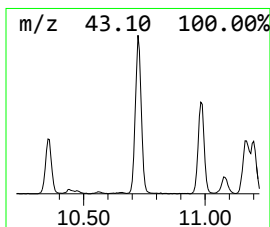
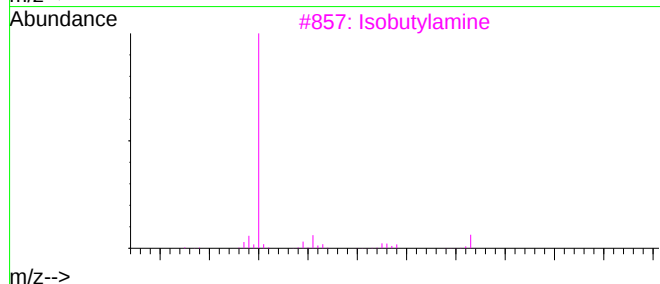
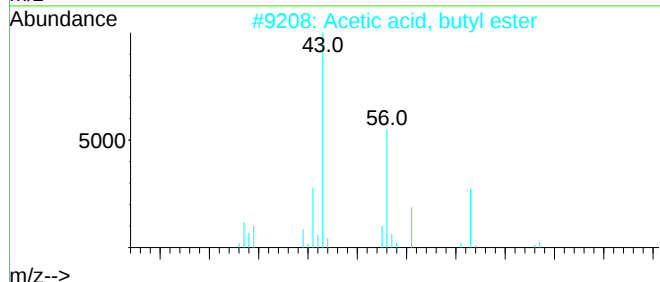
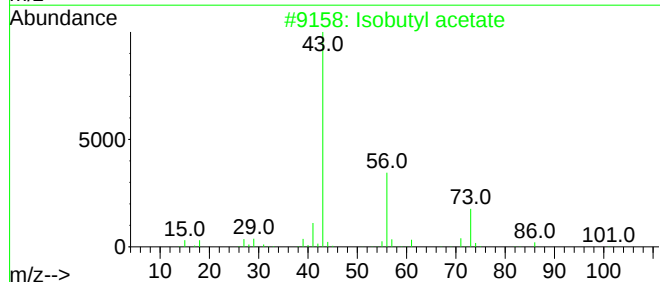
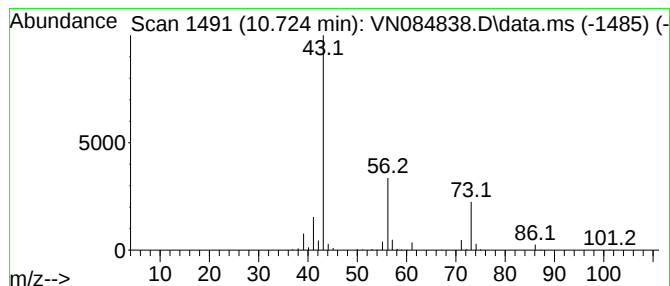
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.724	19.17 ug/l	336949	Chlorobenzene-d5	11.865	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	83
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	36
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
5	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	9



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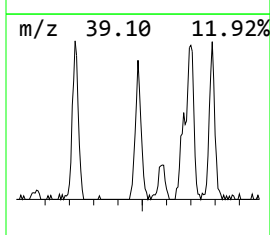
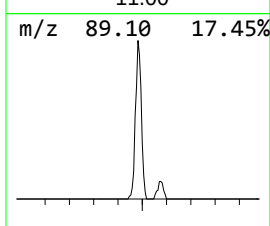
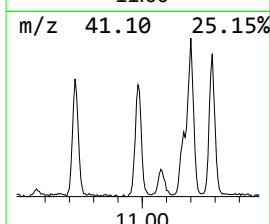
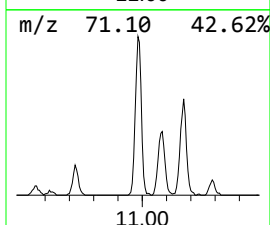
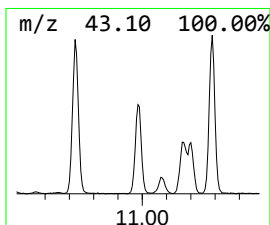
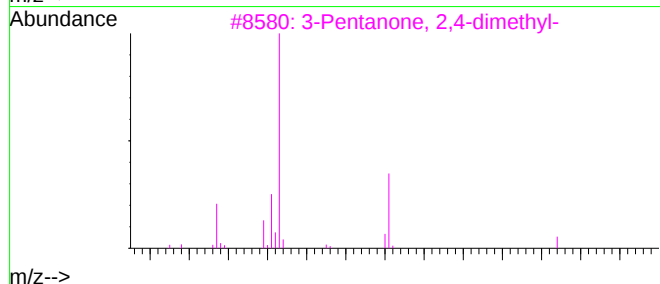
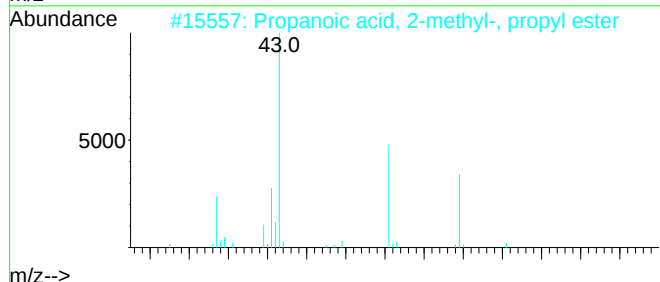
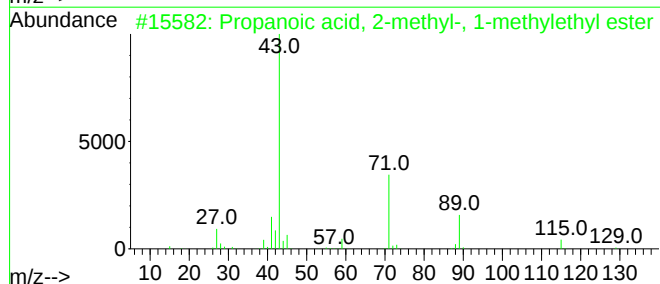
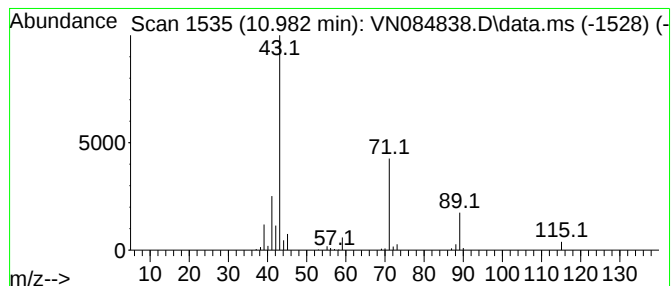
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.982	13.15 ug/l	231097	Chlorobenzene-d5	11.865	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	53
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	45
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111324\
Data File : VN084838.D
Acq On : 13 Nov 2024 19:59
Operator : JC\MD
Sample : P4732-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-Grab

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

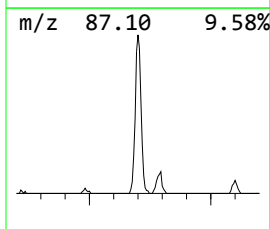
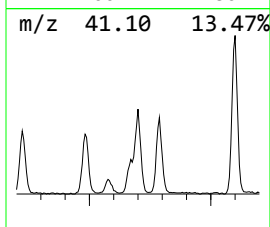
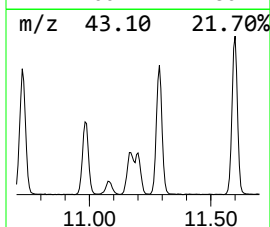
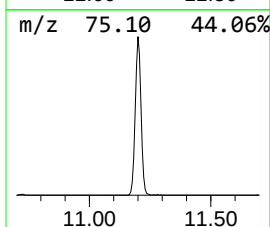
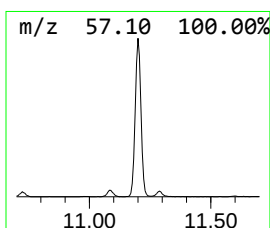
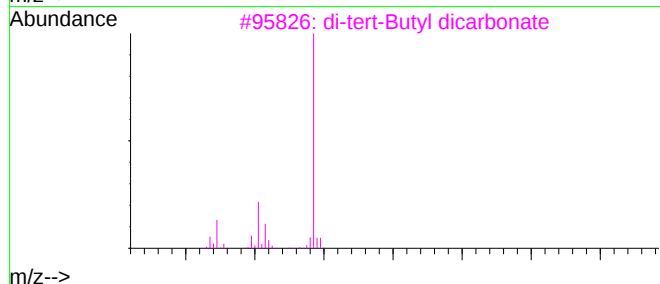
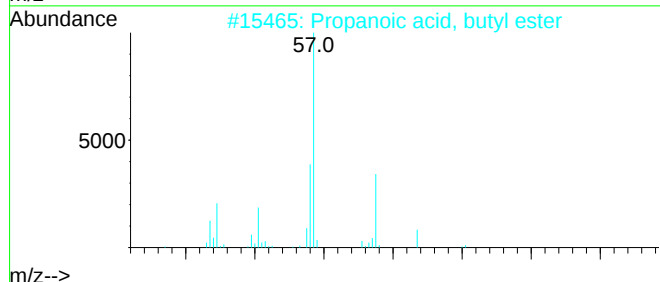
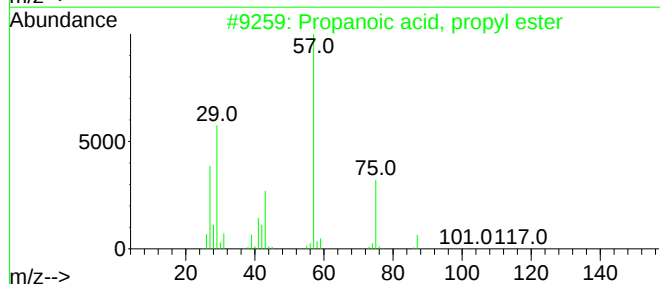
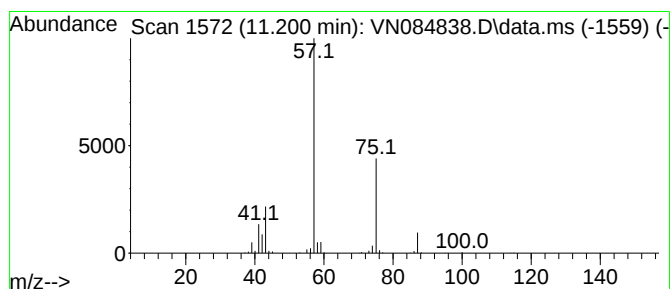
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.200	37.63 ug/l	661511	Chlorobenzene-d5	11.865

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	36
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4	Isobutyl ether	130	C8H18O	000628-55-7	9
5	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111324\
Data File : VN084838.D
Acq On : 13 Nov 2024 19:59
Operator : JC\MD
Sample : P4732-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-Grab

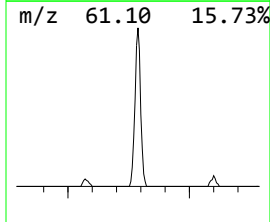
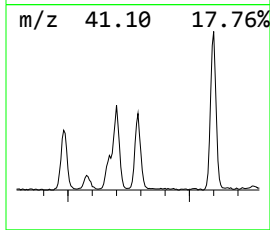
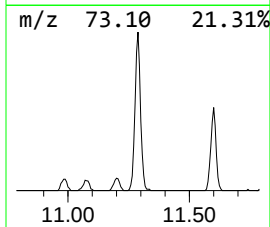
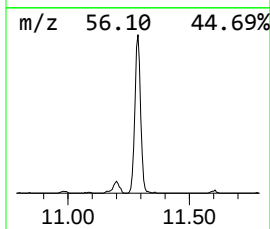
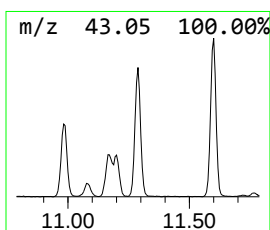
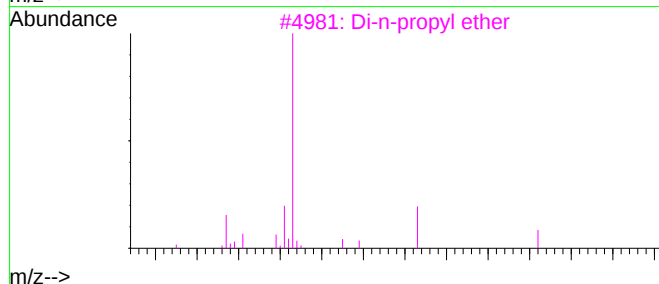
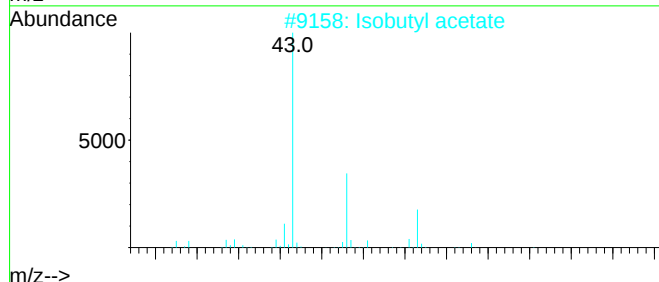
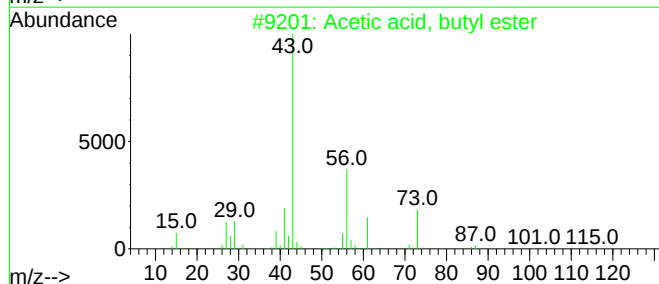
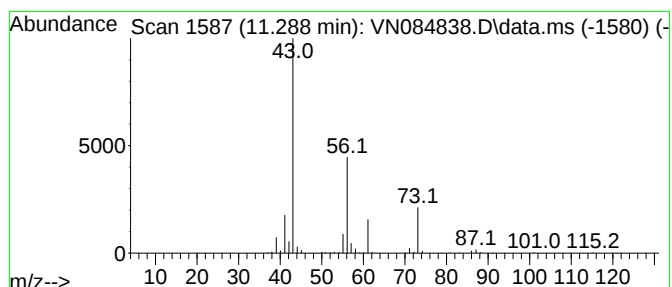
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.288	22.13 ug/l	389090	Chlorobenzene-d5	11.865	
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	Di-n-propyl ether	102	C6H14O	000111-43-3	25
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_N\Data\VN111324\
Data File : VN084838.D
Acq On : 13 Nov 2024 19:59
Operator : JC\MD
Sample : P4732-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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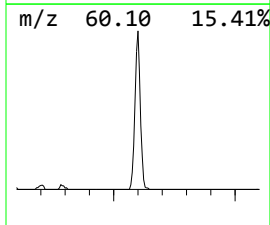
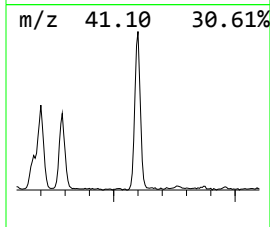
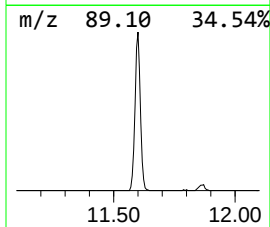
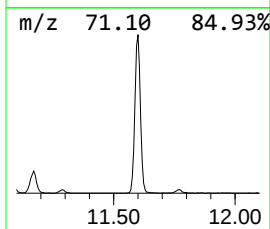
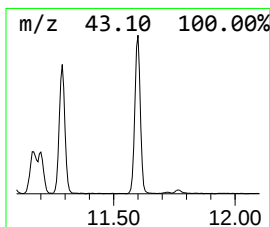
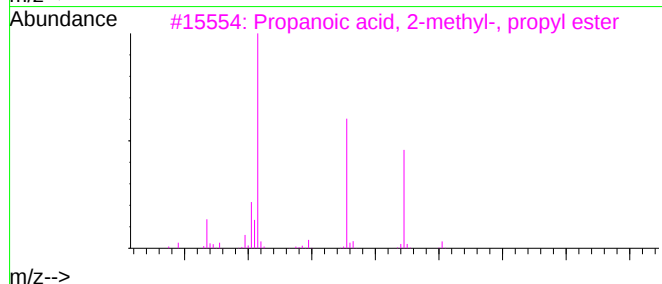
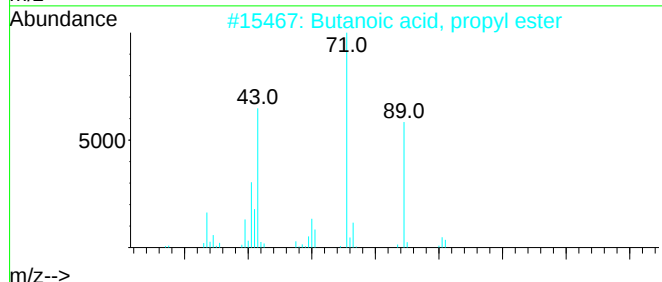
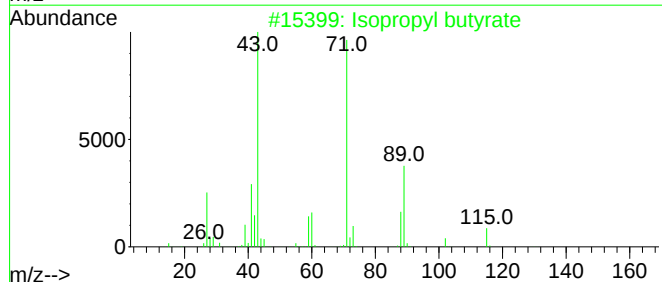
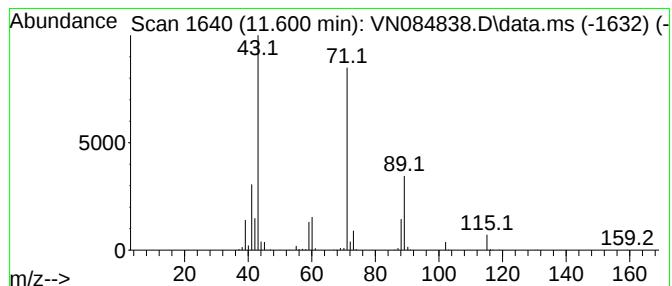
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.600	39.14 ug/l	688075	Chlorobenzene-d5	11.865	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
5	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111324\
Data File : VN084838.D
Acq On : 13 Nov 2024 19:59
Operator : JC\MD
Sample : P4732-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-Grab

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

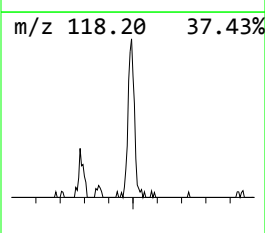
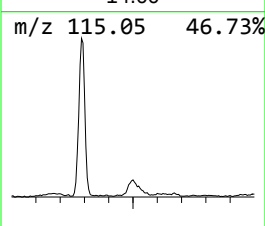
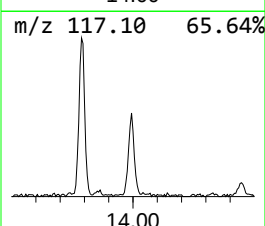
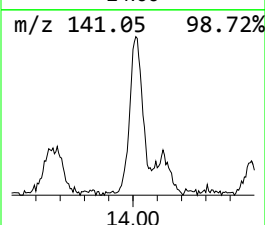
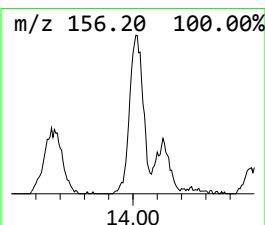
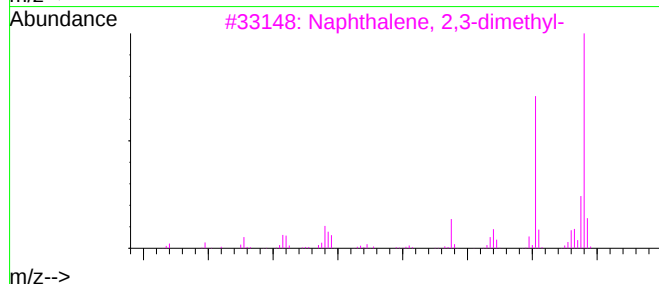
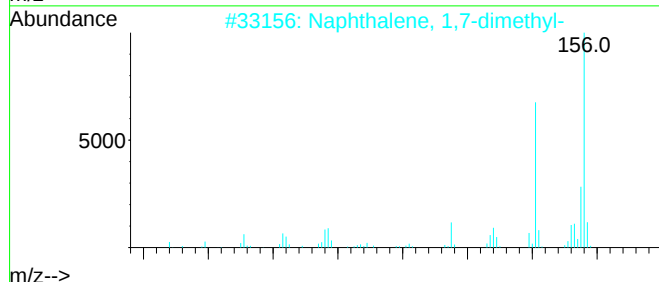
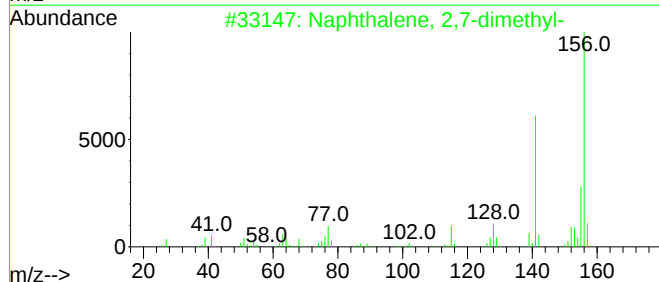
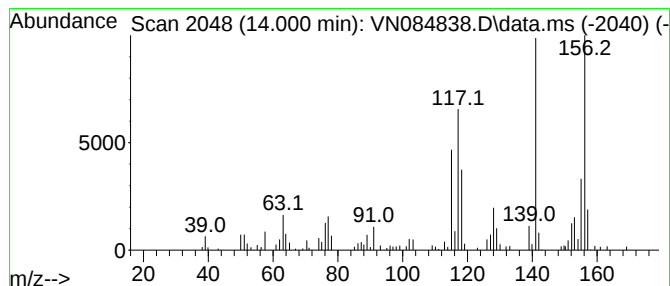
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 9 Naphthalene, 2,7-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.000	14.00 ug/l	253588	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	94
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	92
3	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	91
4	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	91
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111324\
Data File : VN084838.D
Acq On : 13 Nov 2024 19:59
Operator : JC\MD
Sample : P4732-05
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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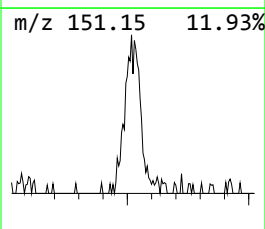
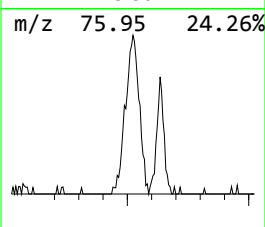
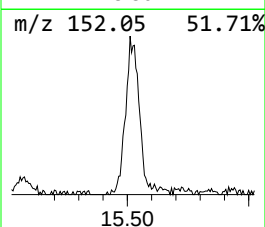
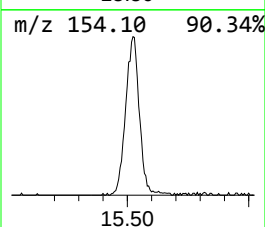
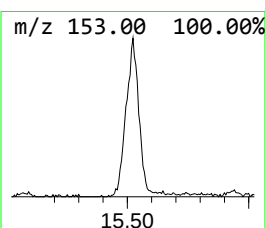
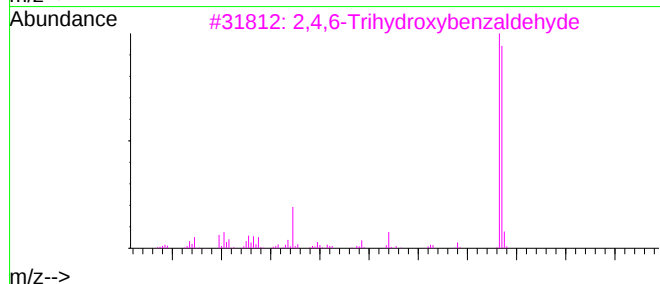
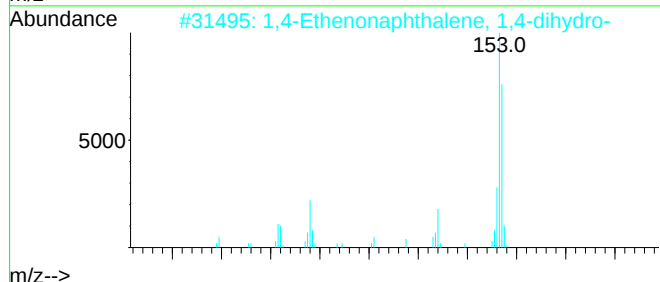
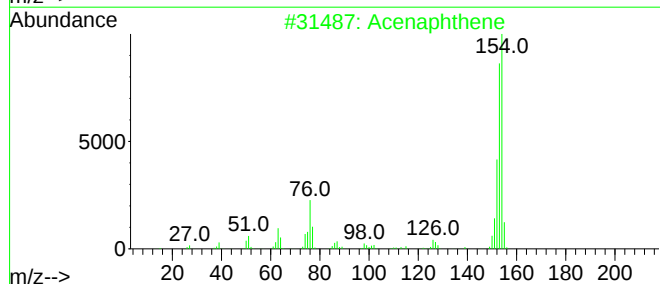
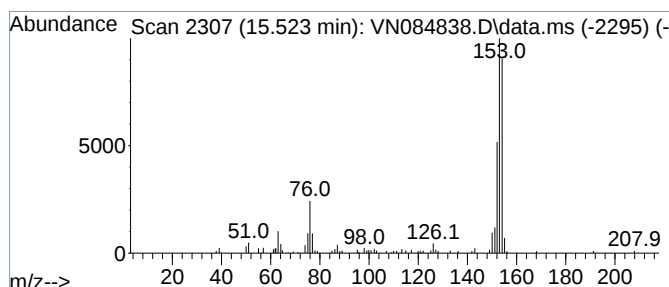
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Quant Title : SW846 8260

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

Peak Number 10 Acenaphthene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.523	13.61 ug/l	246639	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	90
2	1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	59
3	2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	50
4	3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5	.beta.-(1-Naphthyl)acrylic acid	198	C13H10O2	013026-12-5	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111324\
Data File : VN084838.D
Acq On : 13 Nov 2024 19:59
Operator : JC\MD
Sample : P4732-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PPE-Grab

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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

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					#	RT	Resp	Conc
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n-Propyl acetate	9.741	108.1	ug/l	1545990	2	9.094	715008	50.0
Propanoic acid,...	10.353	19.2	ug/l	274163	2	9.094	715008	50.0
Isobutyl acetate	10.724	19.2	ug/l	336949	3	11.865	879005	50.0
Propanoic acid,...	10.982	13.2	ug/l	231097	3	11.865	879005	50.0
Propanoic acid,...	11.200	37.6	ug/l	661511	3	11.865	879005	50.0
Acetic acid, bu...	11.288	22.1	ug/l	389090	3	11.865	879005	50.0
Isopropyl butyrate	11.600	39.1	ug/l	688075	3	11.865	879005	50.0
Naphthalene, 2,...	14.000	14.0	ug/l	253588	4	13.788	905797	50.0
Acenaphthene	15.523	13.6	ug/l	246639	4	13.788	905797	50.0