

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032025\
 Data File : VN086032.D
 Acq On : 20 Mar 2025 18:21
 Operator : JC\MD
 Sample : Q1606-11
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 N48965

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_N\methods\82N031825W.M

Title : SW846 8260

Signal : TIC: VN086032.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.789	303	312	326	rBV	50606	138057	8.81%	1.898%
2	7.553	940	952	966	rBV	640167	1566687	100.00%	21.537%
3	8.165	1046	1056	1060	rBV	136896	318716	20.34%	4.381%
4	8.224	1060	1066	1076	rVB	213970	484213	30.91%	6.656%
5	8.577	1113	1126	1135	rBV	136900	308934	19.72%	4.247%
6	9.100	1206	1215	1225	rBV	302021	613450	39.16%	8.433%
7	9.265	1235	1243	1250	rBV2	30710	70000	4.47%	0.962%
8	10.565	1455	1464	1474	rBV	460736	843394	53.83%	11.594%
9	11.288	1579	1587	1597	rBV	153259	251517	16.05%	3.458%
10	11.865	1675	1685	1698	rBV	416223	754969	48.19%	10.378%
11	12.017	1704	1711	1718	rBV	218186	356309	22.74%	4.898%
12	12.394	1769	1775	1781	rVB2	15685	27308	1.74%	0.375%
13	12.606	1802	1811	1819	rBV5	6342	16336	1.04%	0.225%
14	12.847	1845	1852	1858	rBV	343316	580982	37.08%	7.987%
15	13.788	2006	2012	2020	rVV	398879	665165	42.46%	9.144%
16	13.870	2020	2026	2033	rVB2	69561	119062	7.60%	1.637%
17	14.006	2042	2049	2057	rVB7	17486	39716	2.54%	0.546%
18	14.476	2125	2129	2133	rBV4	9151	15691	1.00%	0.216%
19	14.864	2192	2195	2201	rVB5	11006	18819	1.20%	0.259%
20	14.941	2201	2208	2216	rBV9	9050	22271	1.42%	0.306%
21	15.388	2277	2284	2290	rVV7	12203	26165	1.67%	0.360%
22	15.776	2343	2350	2358	rBV8	6910	20677	1.32%	0.284%
23	16.188	2415	2420	2426	rVB7	7453	15950	1.02%	0.219%

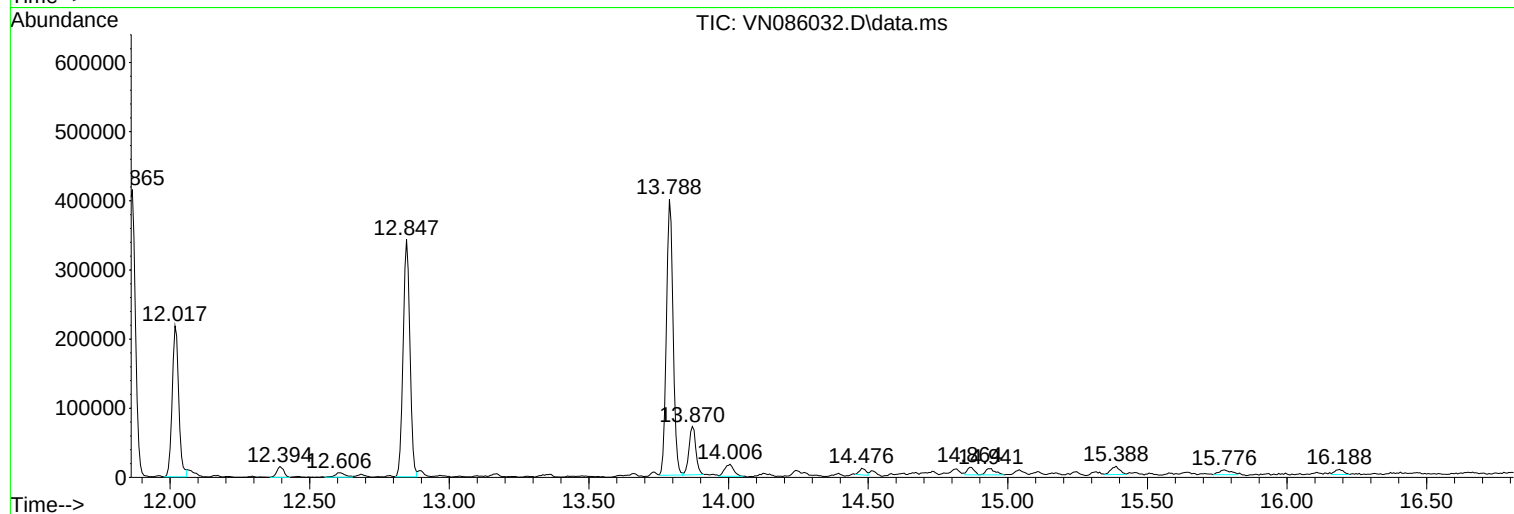
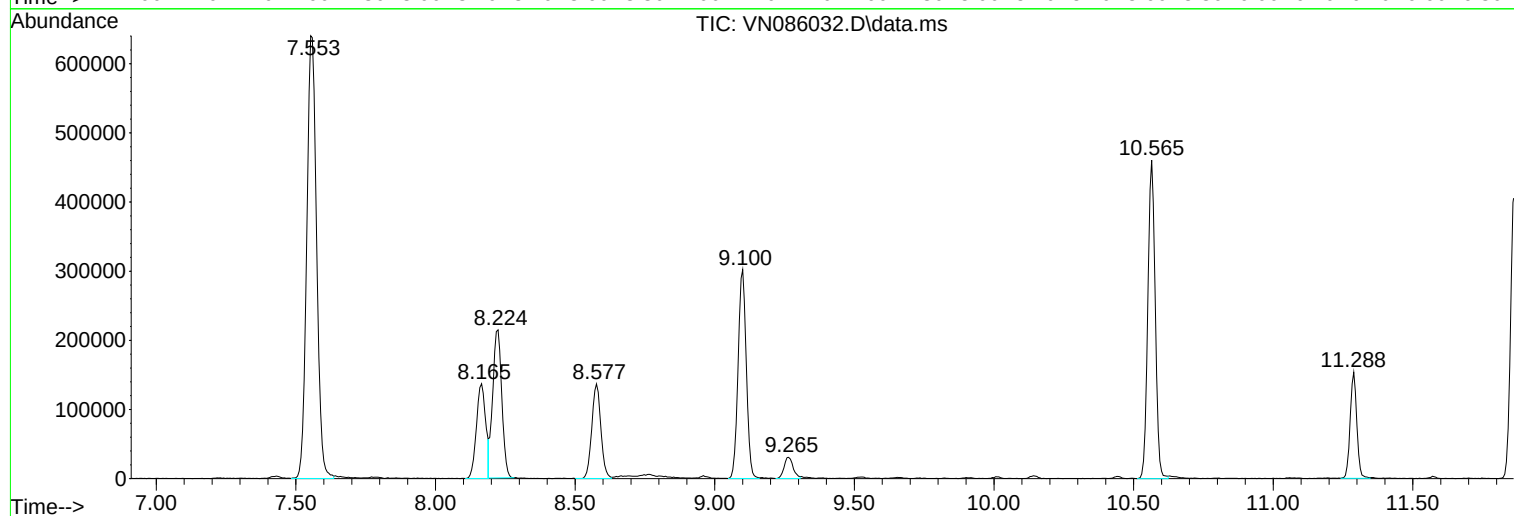
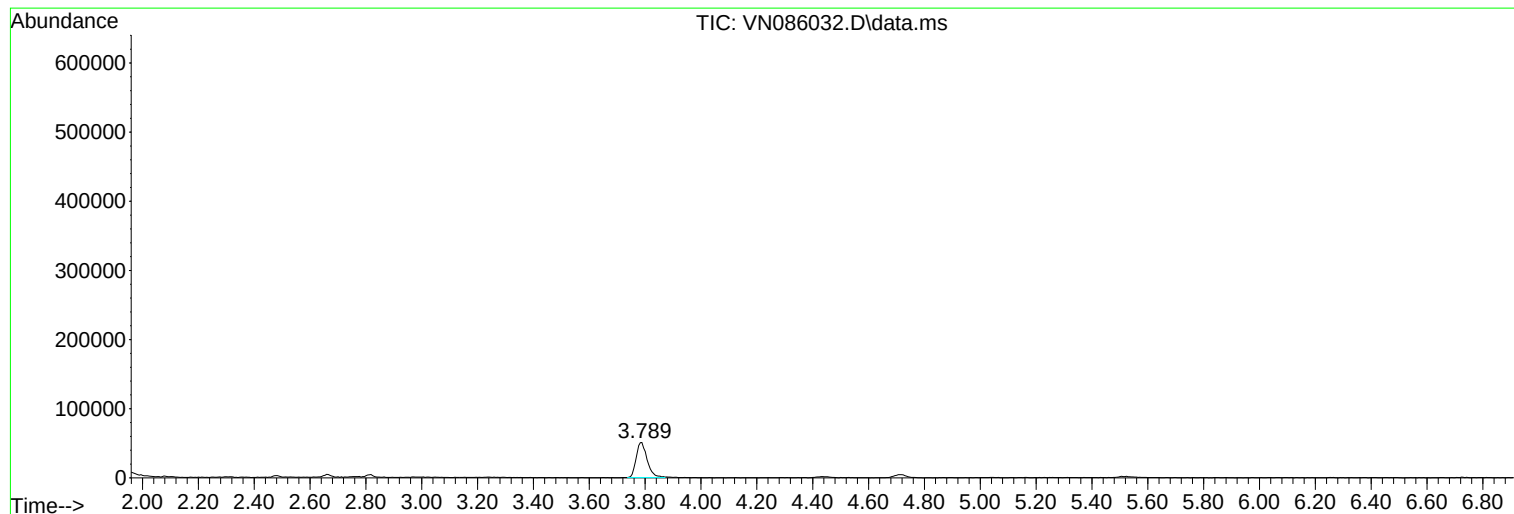
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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



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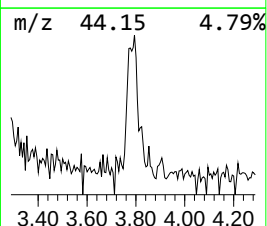
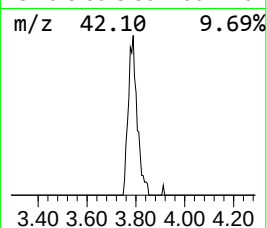
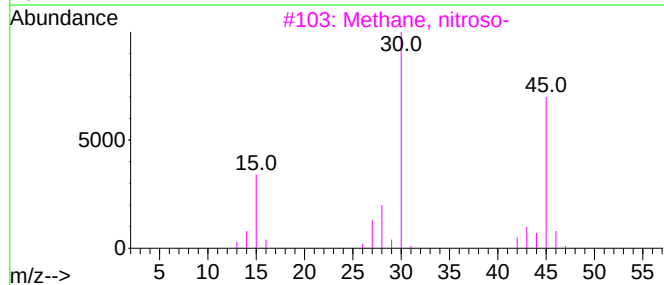
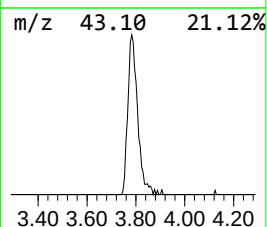
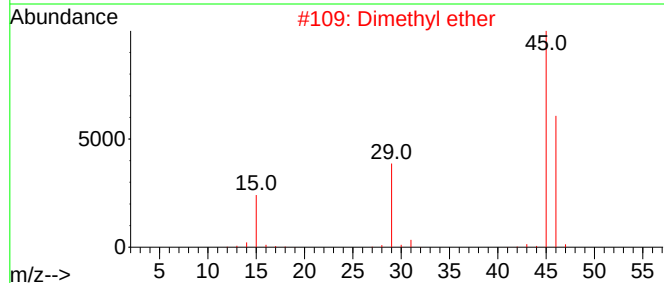
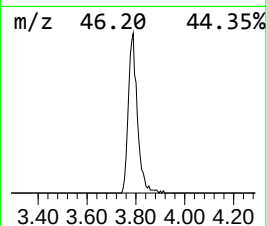
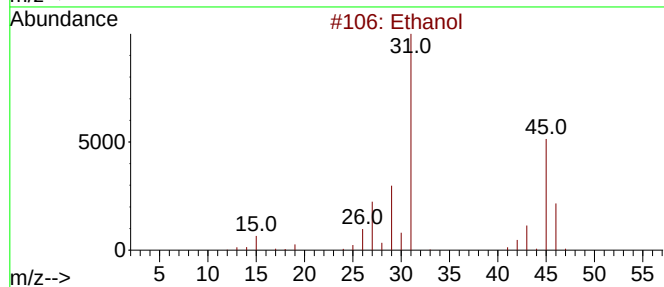
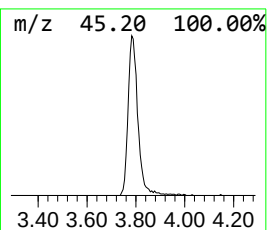
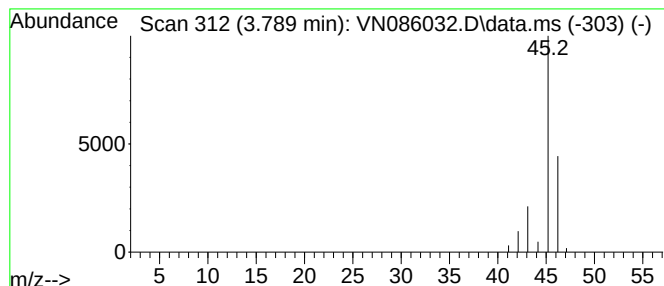
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.789	14.26 ug/l	138057	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	90
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	7
4	Formic acid			46	CH2O2	000064-18-6	4
5	Formamide			45	CH3NO	000075-12-7	2



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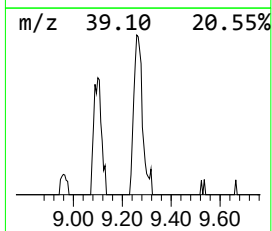
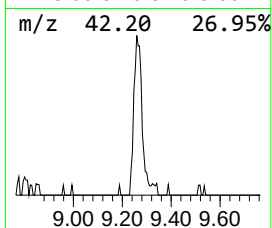
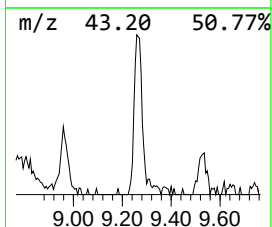
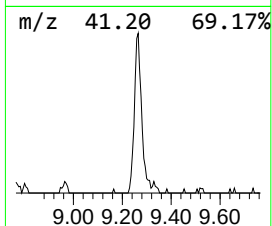
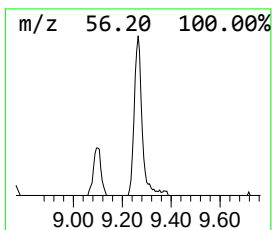
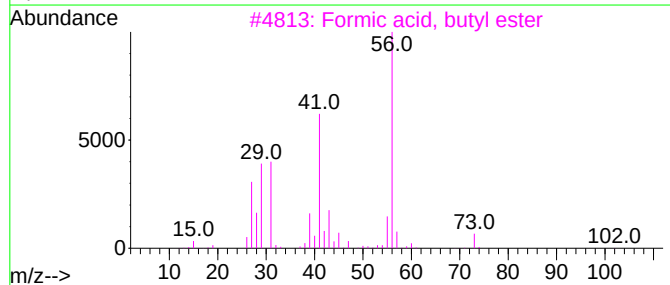
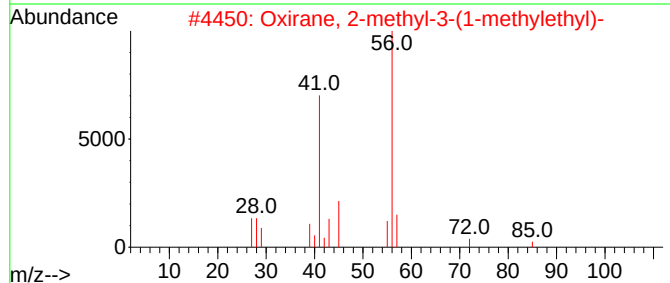
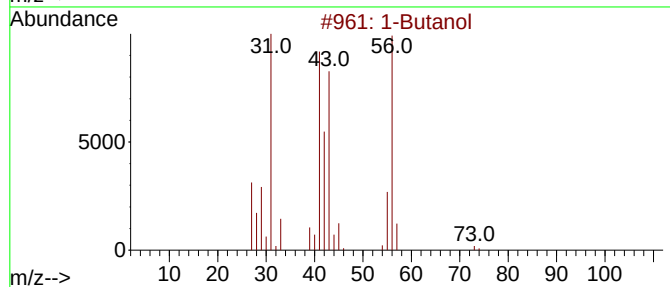
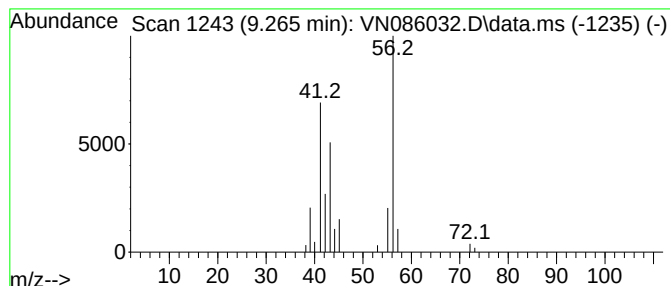
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.265	5.71 ug/l	70000	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	64
2			Oxirane, 2-methyl-3-(1-methyleth...	100	C6H12O	001192-31-0	38
3			Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
4			Methoxyacetone nitrile	71	C3H5NO	001738-36-9	9
5			1,4-Dioxane-2,5-dione, 3,6-dimet...	144	C6H8O4	000095-96-5	9



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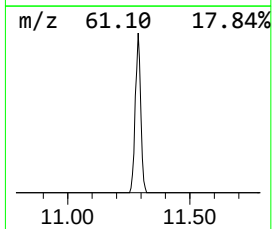
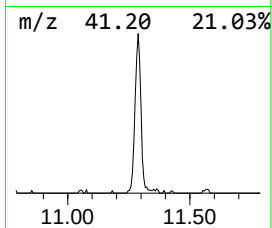
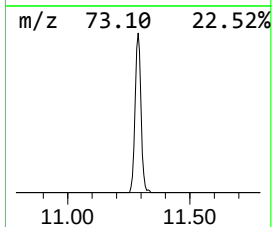
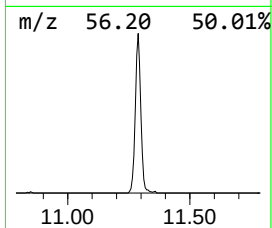
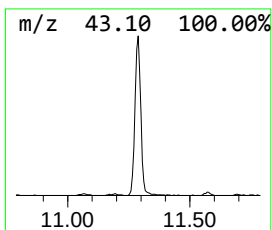
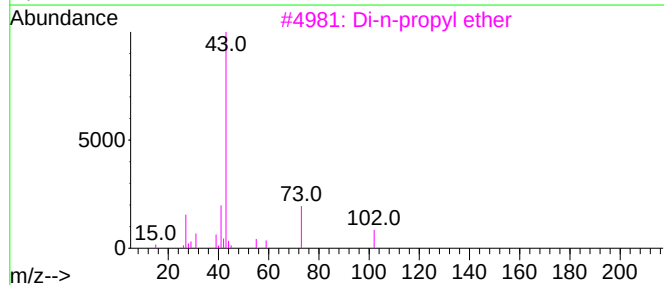
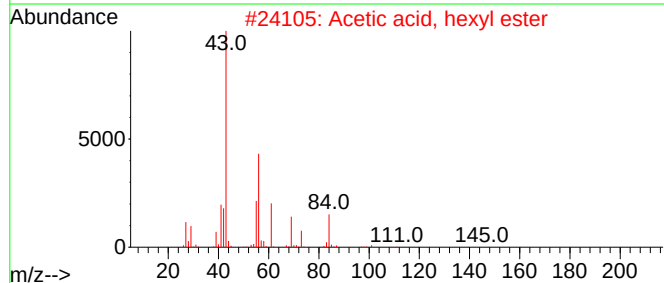
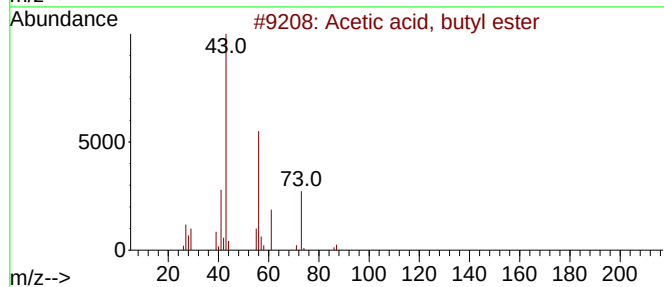
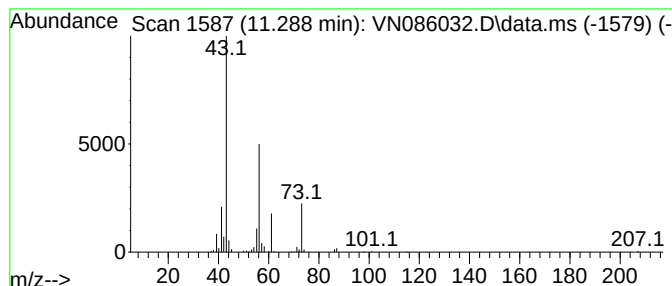
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Quant Title : SW846 8260

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

Peak Number 3 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.288	16.66 ug/l	251517	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	90
2			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36
3			Di-n-propyl ether	102	C6H14O	000111-43-3	25
4			Butane, 1-propoxy-	116	C7H16O	003073-92-5	23
5			Isobutylamine	73	C4H11N	000078-81-9	9



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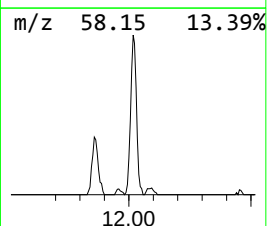
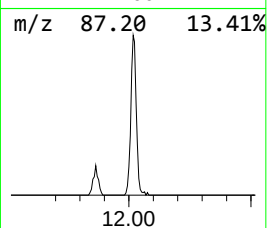
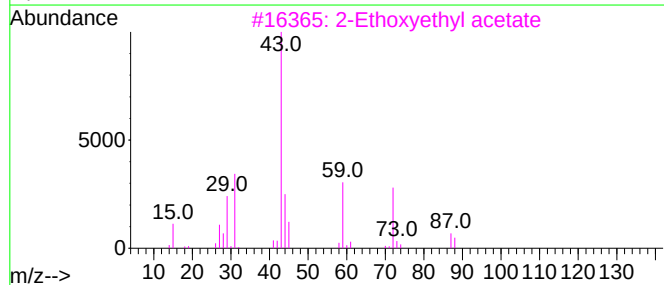
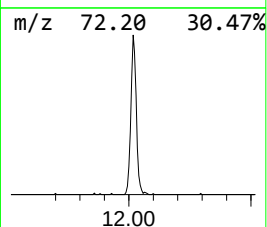
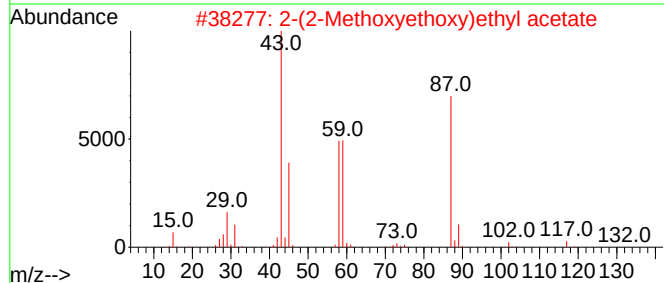
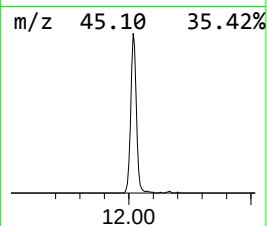
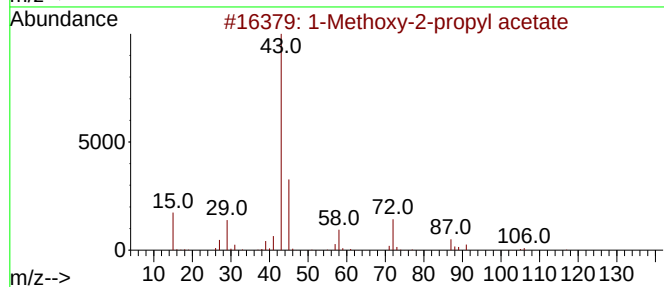
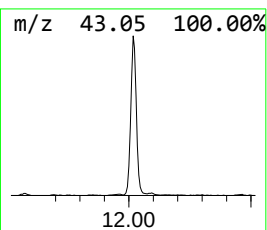
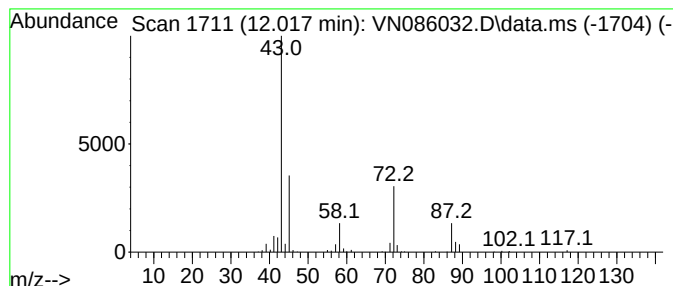
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Methoxy-2-propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.018	23.60 ug/l	356309	Chlorobenzene-d5	11.865	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	83
2	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	33
3	2-Ethoxyethyl acetate	132	C6H12O3	000111-15-9	33
4	Hydrazine, 2-propenyl-	72	C3H8N2	007422-78-8	23
5	1,2-Propanediol, 2-acetate	118	C5H10O3	006214-01-3	17



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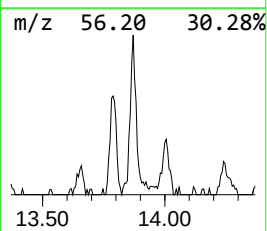
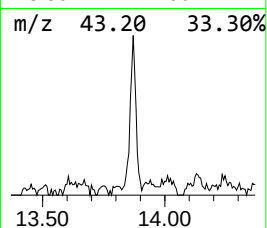
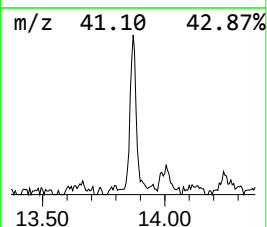
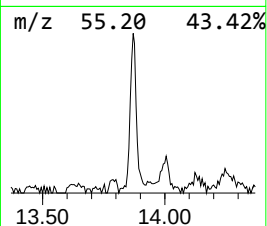
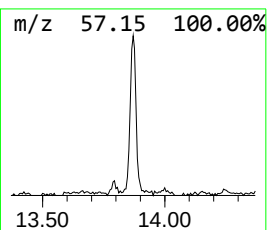
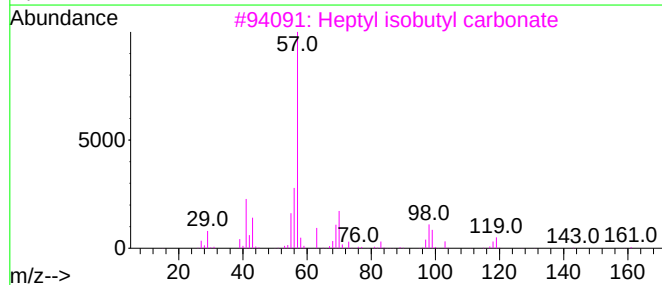
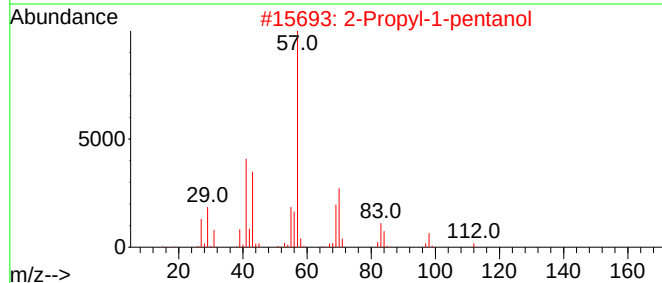
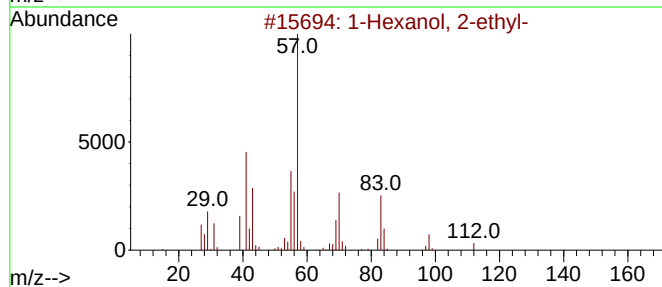
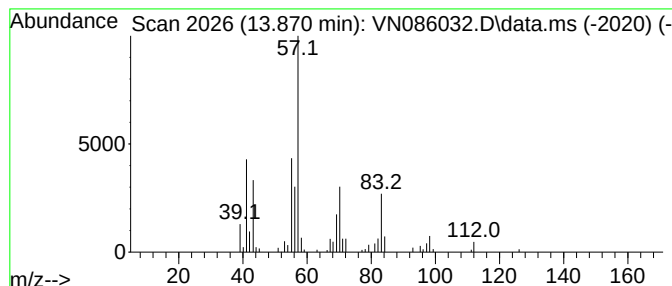
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Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.870	8.95 ug/l	119062	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	53
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
5			Carbonic acid, butyl heptyl ester	216	C12H24O3	1000314-63-4	47



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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
Ethanol	3.789	14.3	ug/l	138057	1	8.224	484213	50.0
1-Butanol	9.265	5.7	ug/l	70000	2	9.100	613450	50.0
Acetic acid, bu...	11.288	16.7	ug/l	251517	3	11.865	754969	50.0
1-Methoxy-2-pro...	12.018	23.6	ug/l	356309	3	11.865	754969	50.0
1-Hexanol, 2-et...	13.870	8.9	ug/l	119062	4	13.788	665165	50.0