

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN083122\
 Data File : VN074226.D
 Acq On : 31 Aug 2022 20:06
 Operator : JC\MD
 Sample : N4444-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WH-1

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\82N083022W.M
 Title : SW846 8260

Signal : TIC: VN074226.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.552	107	113	119	rBV	46077	75305	2.45%	0.463%
2	2.699	134	138	147	rVB8	14060	34642	1.13%	0.213%
3	3.634	287	297	316	rBV	830057	2159251	70.34%	13.264%
4	4.216	385	396	414	rBV	1070170	3069695	100.00%	18.857%
5	4.504	436	445	458	rBV	78765	239124	7.79%	1.469%
6	5.287	568	578	594	rBV3	116562	402130	13.10%	2.470%
7	7.257	899	913	925	rBV3	121223	404012	13.16%	2.482%
8	7.951	1021	1031	1036	rBV2	177175	419133	13.65%	2.575%
9	8.016	1036	1042	1055	rVB	282936	619404	20.18%	3.805%
10	8.369	1092	1102	1114	rBV	200679	479860	15.63%	2.948%
11	8.775	1165	1171	1179	rVB2	19065	39838	1.30%	0.245%
12	8.904	1185	1193	1203	rBV	431066	875532	28.52%	5.378%
13	9.092	1215	1225	1237	rBV9	14204	46677	1.52%	0.287%
14	9.269	1248	1255	1263	rBV5	19099	54642	1.78%	0.336%
15	9.351	1263	1269	1277	rVB2	30791	58605	1.91%	0.360%
16	9.492	1284	1293	1305	rVB4	15454	43087	1.40%	0.265%
17	9.728	1325	1333	1343	rVV2	69854	148417	4.83%	0.912%
18	10.275	1417	1426	1432	rBV4	16511	35548	1.16%	0.218%
19	10.381	1432	1444	1450	rVV	643732	1172444	38.19%	7.202%
20	10.445	1450	1455	1469	rVV2	245156	528196	17.21%	3.245%
21	10.563	1469	1475	1482	rVV2	39048	62636	2.04%	0.385%
22	10.886	1524	1530	1544	rVB2	42353	92835	3.02%	0.570%
23	11.028	1544	1554	1558	rBV	30675	57882	1.89%	0.356%
24	11.128	1566	1571	1577	rVV6	19374	35794	1.17%	0.220%
25	11.686	1658	1666	1675	rBV	659225	1169187	38.09%	7.182%
26	11.769	1675	1680	1688	rVB5	24964	59494	1.94%	0.365%
27	11.892	1696	1701	1703	rBV3	20784	34498	1.12%	0.212%
28	11.928	1703	1707	1714	rVB3	50032	86345	2.81%	0.530%
29	12.039	1722	1726	1736	rVB6	14529	33196	1.08%	0.204%
30	12.222	1751	1757	1761	rBV3	25668	47208	1.54%	0.290%
31	12.292	1764	1769	1777	rVB2	19736	38755	1.26%	0.238%
32	12.616	1813	1824	1827	rBV7	12335	31357	1.02%	0.193%
33	12.669	1827	1833	1843	rVB	542968	891163	29.03%	5.474%
34	12.992	1883	1888	1894	rVB2	42547	69759	2.27%	0.429%
35	13.310	1934	1942	1946	rBV6	26172	61032	1.99%	0.375%
36	13.610	1986	1993	2002	rBV	679763	1148100	37.40%	7.053%

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Integration Parameters: RTEINT.P

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Filtering: 5

Sampling : 1

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Start Thrs: 0.2

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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Title : SW846 8260

37	13.710	2002	2010	2019	rBV	721662	1142005	37.20%	7.015%
38	13.945	2044	2050	2059	rBV5	28463	76011	2.48%	0.467%
39	14.116	2075	2079	2089	rVB3	43934	91342	2.98%	0.561%
40	14.863	2200	2206	2212	rBV7	19154	44143	1.44%	0.271%
41	14.927	2212	2217	2226	rVB9	15705	35647	1.16%	0.219%
42	15.016	2228	2232	2238	rBV8	17199	33653	1.10%	0.207%
43	15.133	2244	2252	2258	rBV10	14124	30876	1.01%	0.190%

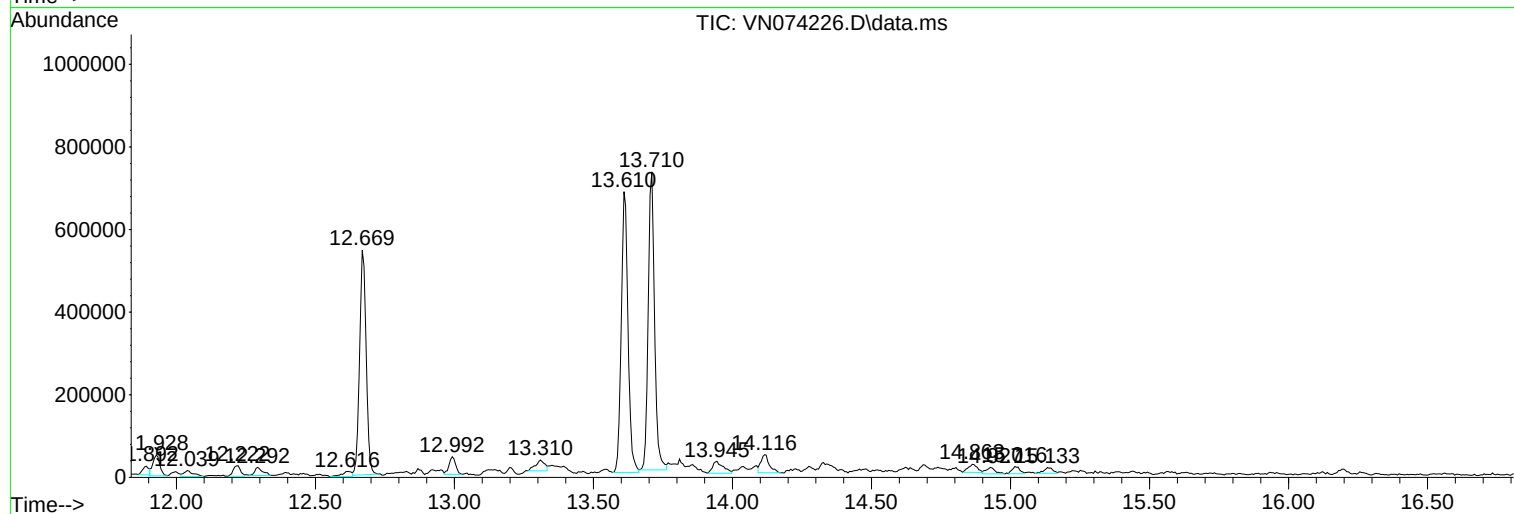
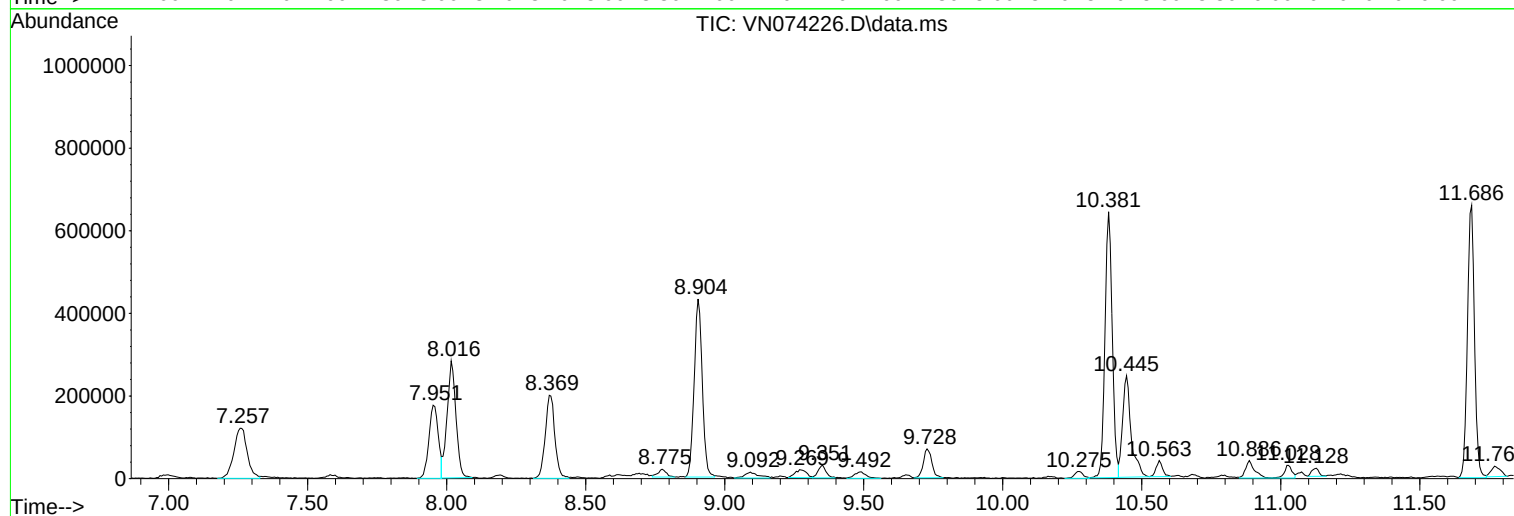
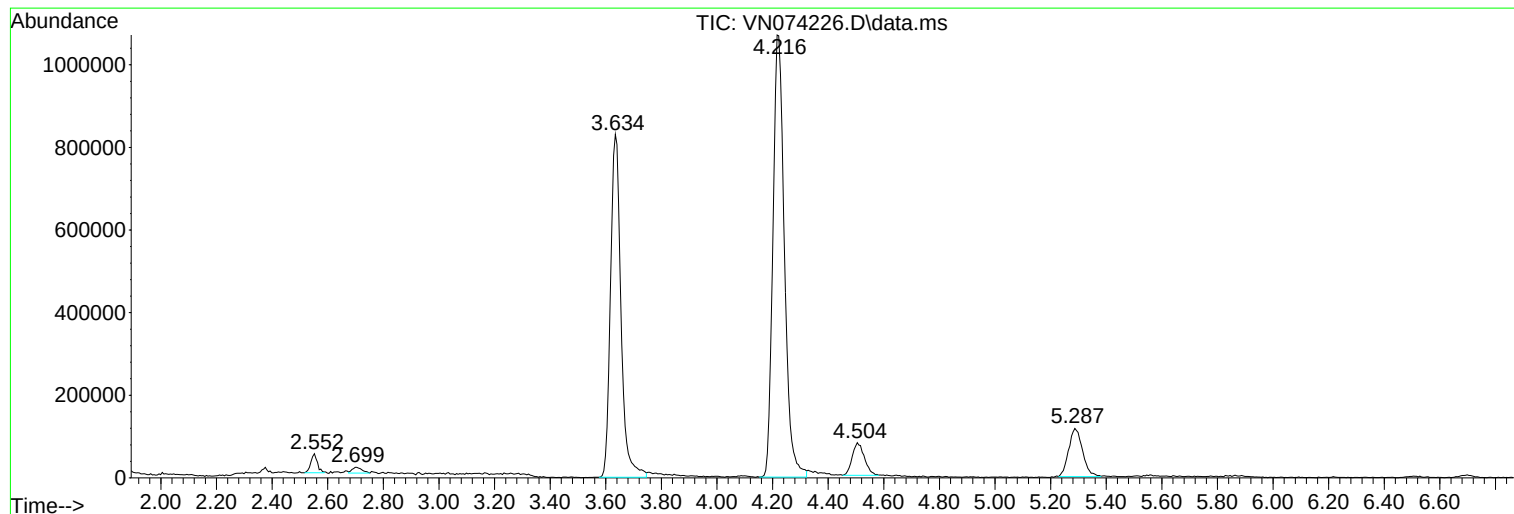
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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



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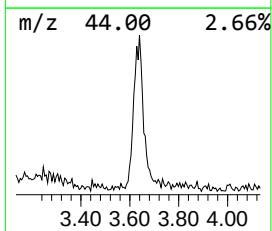
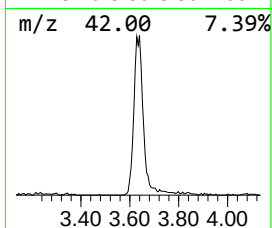
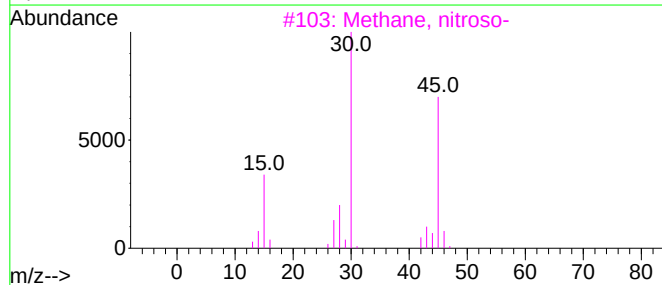
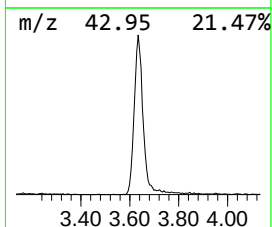
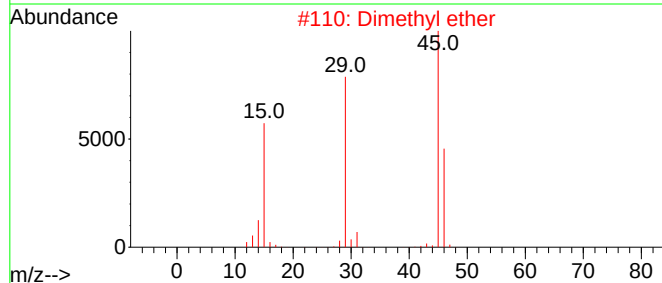
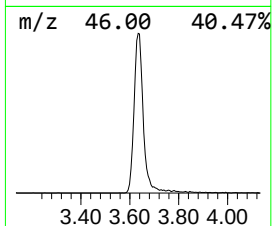
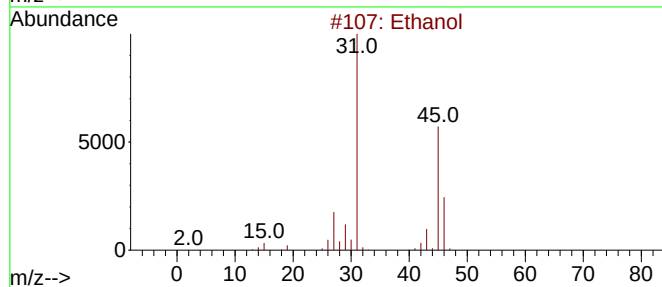
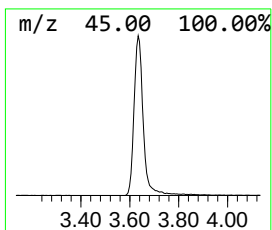
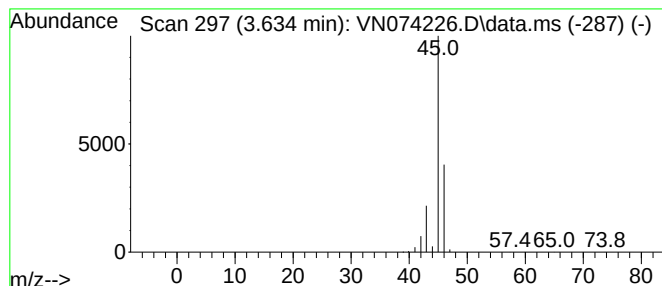
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.634	174.30 ug/l	2159250	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	83
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Formic acid			46	CH2O2	000064-18-6	4
5	Oxalic acid			90	C2H2O4	000144-62-7	4



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Instrument :
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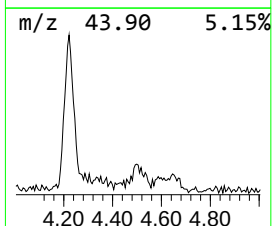
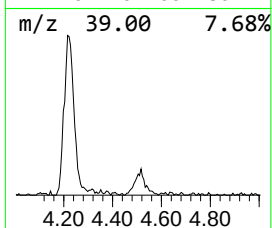
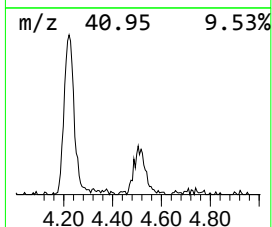
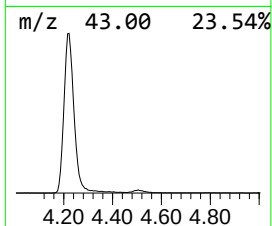
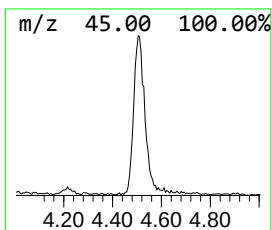
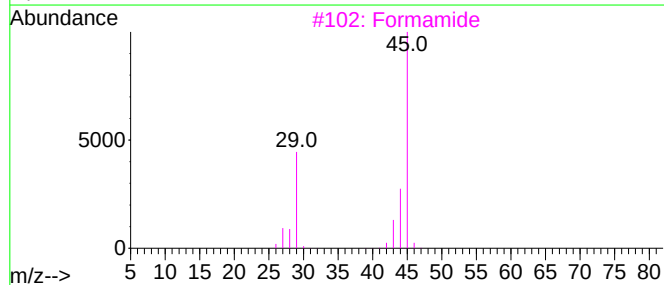
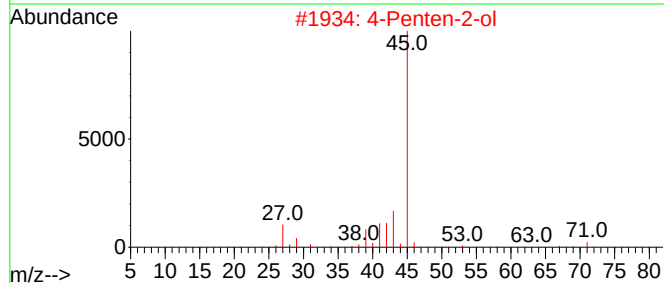
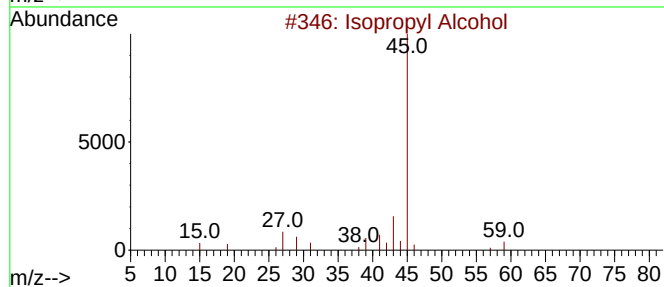
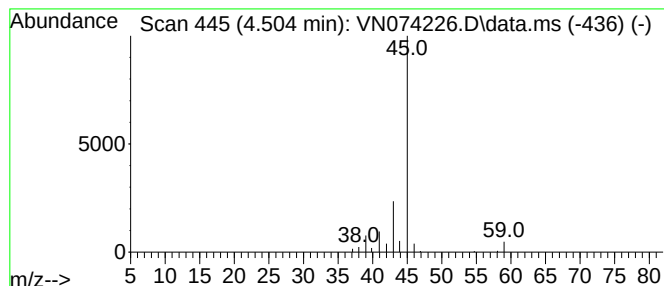
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.504	19.30 ug/l	239124	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2			4-Penten-2-ol	86	C5H10O	000625-31-0	9
3			Formamide	45	CH3NO	000075-12-7	5
4			Ethylamine	45	C2H7N	000075-04-7	5
5			2,3-Butanediol	90	C4H10O2	000513-85-9	4



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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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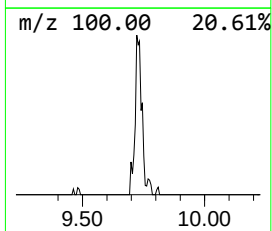
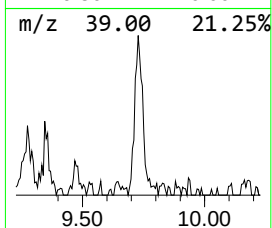
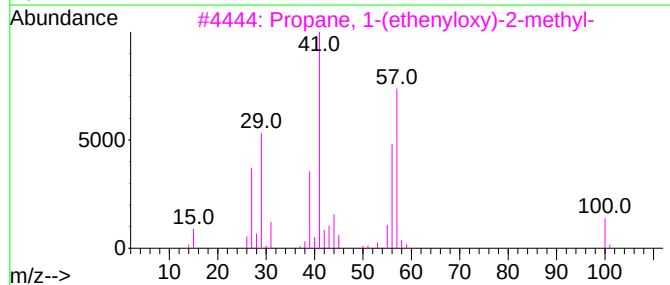
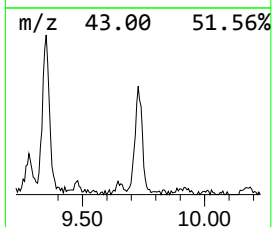
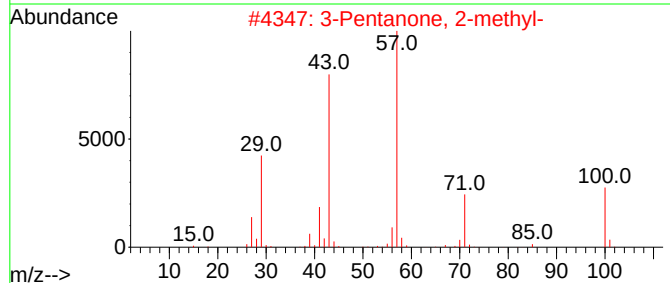
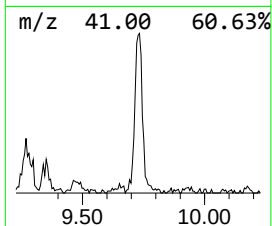
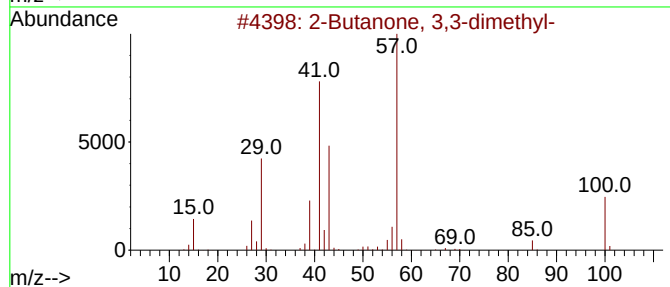
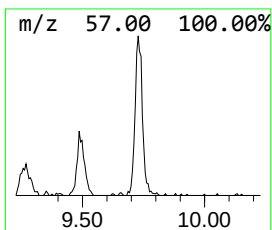
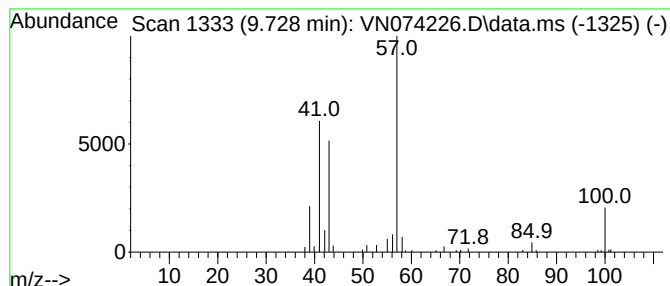
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 4 2-Butanone, 3,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.728	8.48 ug/l	148417	1,4-Difluorobenzene	8.904

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	87
2		3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
3		Propane, 1-(ethenyloxy)-2-methyl-	100	C6H12O	000109-53-5	59
4		Butane, 2,3-dimethyl-2,3-dinitro-	176	C6H12N2O4	003964-18-9	50
5		3-Hexanone	100	C6H12O	000589-38-8	39



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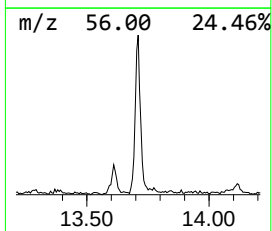
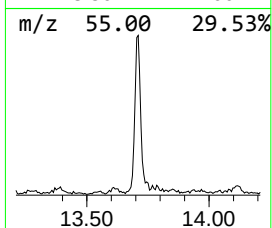
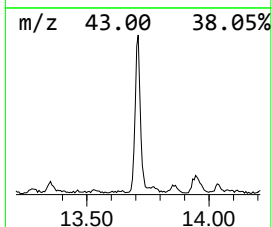
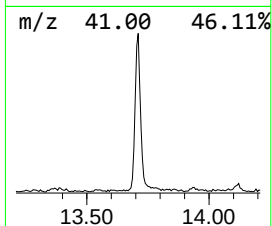
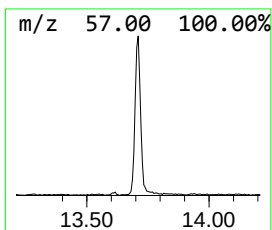
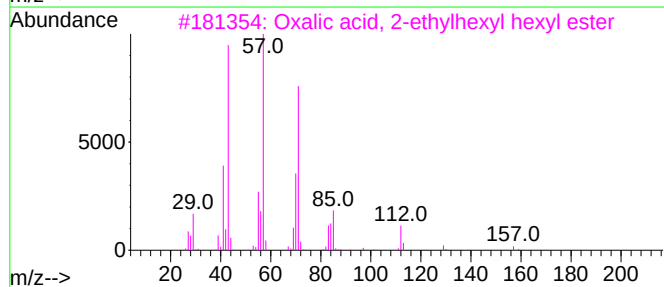
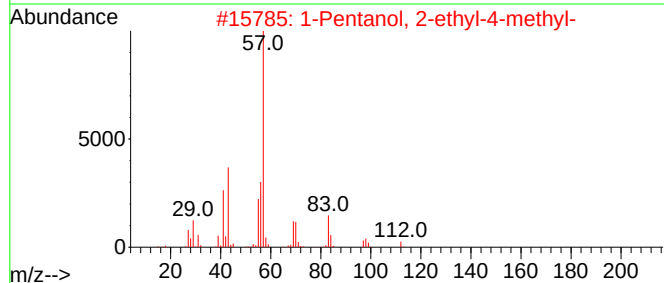
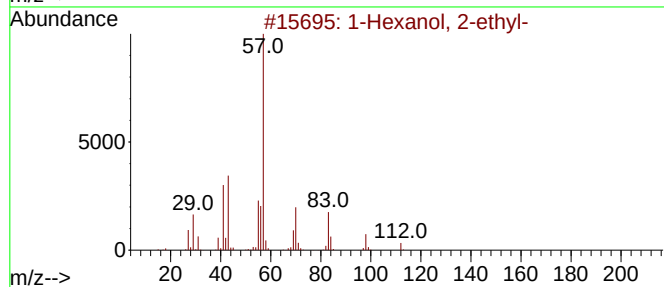
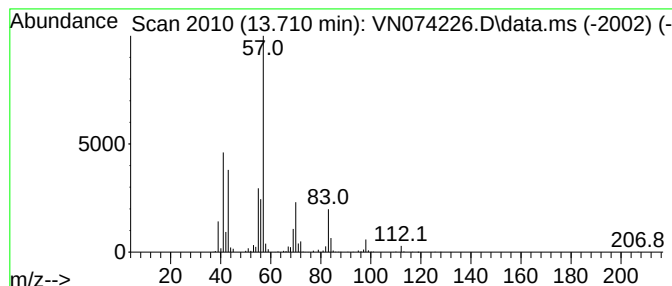
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	49.73 ug/l	1142010	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3			Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	53
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	3.634	174.3	ug/l	2159250	1	8.016	619404	50.0
Isopropyl Alcohol	4.504	19.3	ug/l	239124	1	8.016	619404	50.0
2-Butanone, 3,3...	9.728	8.5	ug/l	148417	2	8.904	875532	50.0
1-Hexanol, 2-et...	13.710	49.7	ug/l	1142010	4	13.610	1148100	50.0