

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
 Data File : VN074261.D
 Acq On : 01 Sep 2022 23:39
 Operator : JC\MD
 Sample : N4376-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-29

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: VN074261.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.551	107	113	120	rVV	103741	176422	6.55%	1.234%
2	3.634	287	297	309	rBV	120758	325700	12.10%	2.278%
3	3.928	338	347	356	rBV4	11380	31056	1.15%	0.217%
4	4.234	386	399	406	rBV	21472	65986	2.45%	0.462%
5	4.716	472	481	488	rBV3	13316	42638	1.58%	0.298%
6	5.281	565	577	590	rBV2	61178	222288	8.26%	1.555%
7	5.534	606	620	634	rBV2	110428	390688	14.51%	2.733%
8	6.410	761	769	776	rBV3	14700	39605	1.47%	0.277%
9	7.263	903	914	922	rBV	45159	116147	4.31%	0.812%
10	7.581	959	968	975	rBV2	15896	42179	1.57%	0.295%
11	7.951	1020	1031	1036	rBV2	172597	404713	15.03%	2.831%
12	8.016	1036	1042	1053	rVB	270243	626722	23.28%	4.384%
13	8.386	1088	1105	1115	rBV3	1033301	2692252	100.00%	18.831%
14	8.522	1123	1128	1134	rVB8	12353	28701	1.07%	0.201%
15	8.904	1183	1193	1203	rBV	450502	901724	33.49%	6.307%
16	9.098	1217	1226	1236	rBV3	22369	53932	2.00%	0.377%
17	9.345	1262	1268	1276	rBV2	20882	43524	1.62%	0.304%
18	10.139	1395	1403	1414	rBV6	10427	29909	1.11%	0.209%
19	10.269	1416	1425	1432	rBV	158015	289540	10.75%	2.025%
20	10.380	1432	1444	1450	rVV	699705	1302788	48.39%	9.113%
21	10.445	1450	1455	1468	rVB	198811	371861	13.81%	2.601%
22	10.651	1482	1490	1496	rVB5	17882	43104	1.60%	0.301%
23	11.680	1658	1665	1676	rBV	644516	1171552	43.52%	8.195%
24	11.786	1676	1683	1691	rVB	407651	700464	26.02%	4.899%
25	11.892	1691	1701	1711	rBV	473112	921369	34.22%	6.445%
26	12.216	1747	1756	1765	rBV	214064	377343	14.02%	2.639%
27	12.668	1826	1833	1845	rBV	556277	928832	34.50%	6.497%
28	12.927	1871	1877	1879	rVV2	23230	38572	1.43%	0.270%
29	12.951	1879	1881	1885	rVV2	21106	29639	1.10%	0.207%
30	12.992	1885	1888	1894	rVB4	23311	34317	1.27%	0.240%
31	13.163	1910	1917	1922	rBV	35520	60176	2.24%	0.421%
32	13.304	1935	1941	1947	rBV	102633	154693	5.75%	1.082%
33	13.610	1986	1993	2004	rBV	671924	1198604	44.52%	8.384%
34	13.710	2004	2010	2017	rVV	124992	197475	7.33%	1.381%
35	13.815	2022	2028	2036	rVB3	92980	154894	5.75%	1.083%
36	15.433	2296	2303	2309	rBV3	43850	87294	3.24%	0.611%

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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

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

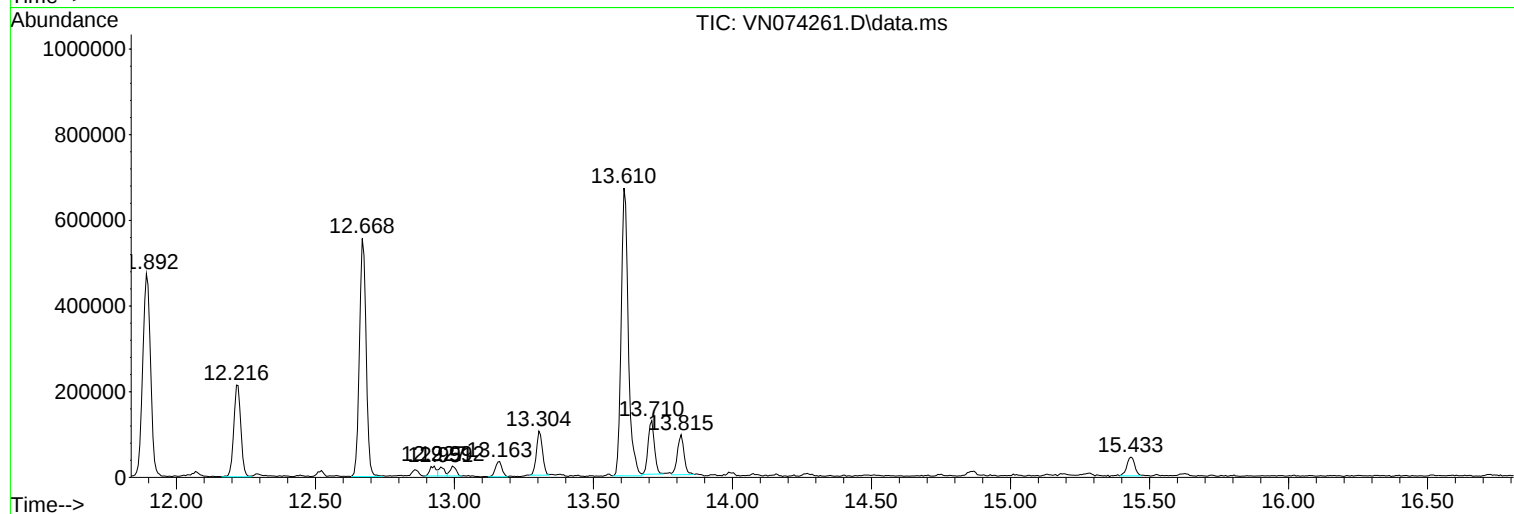
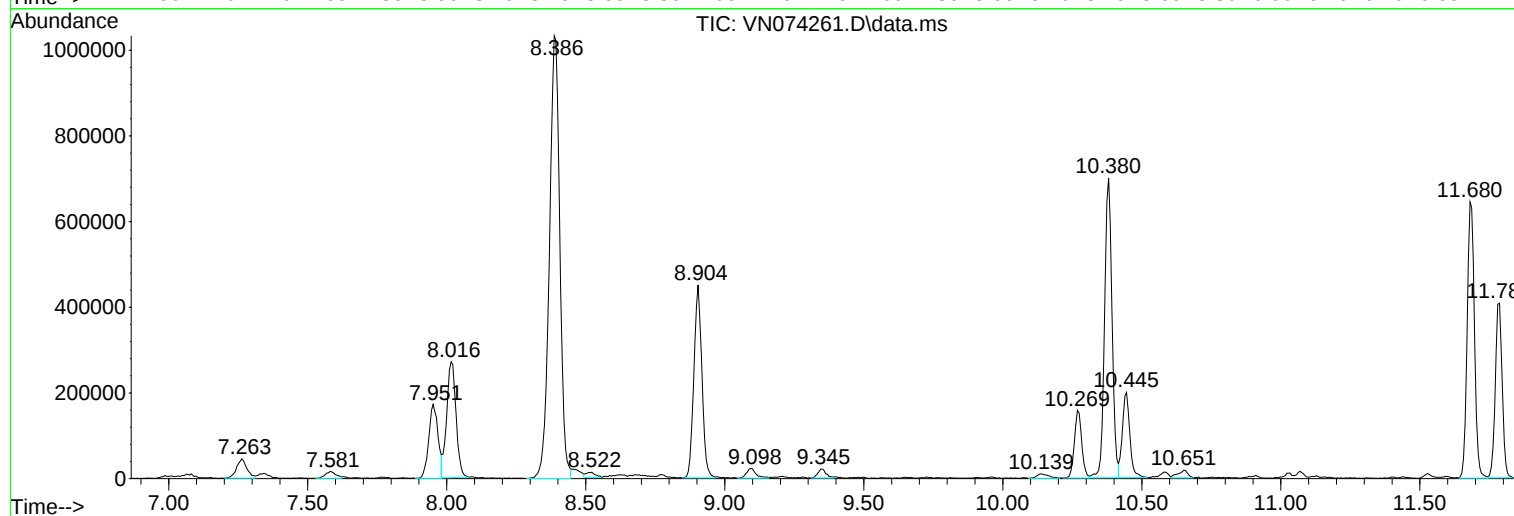
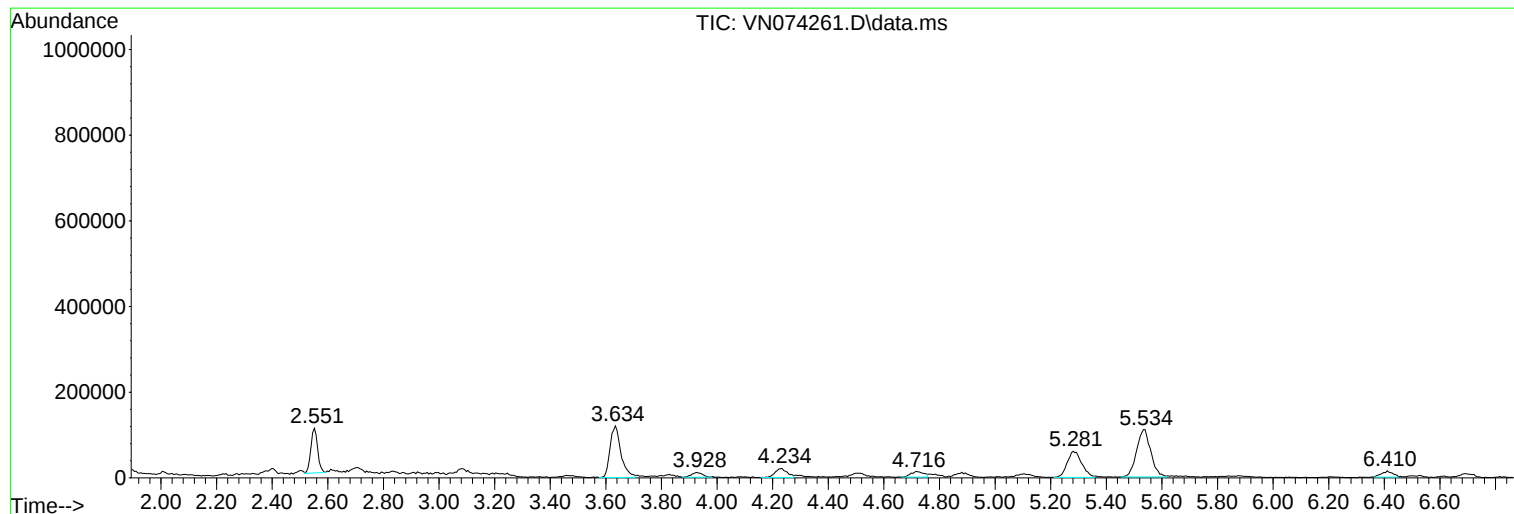
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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



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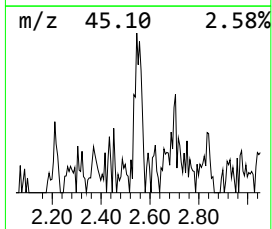
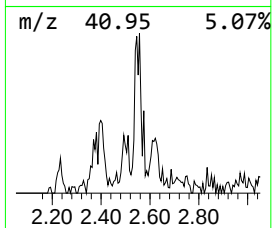
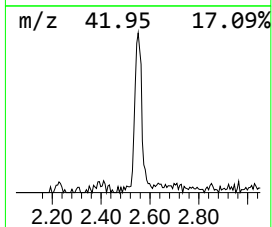
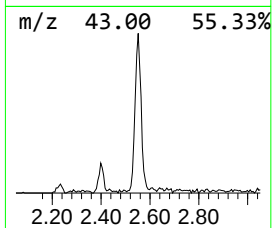
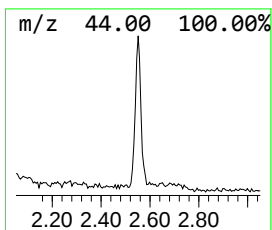
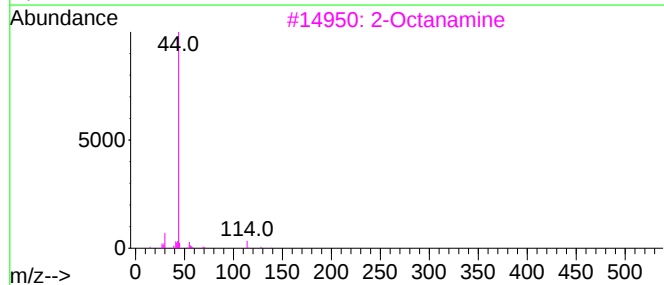
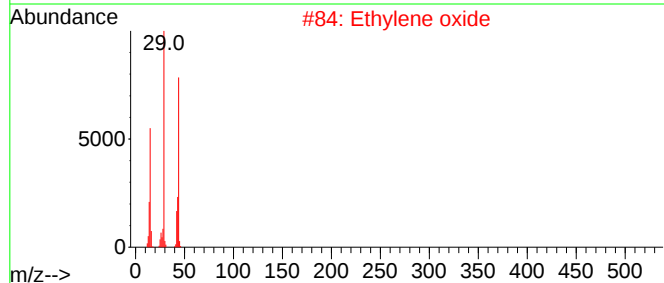
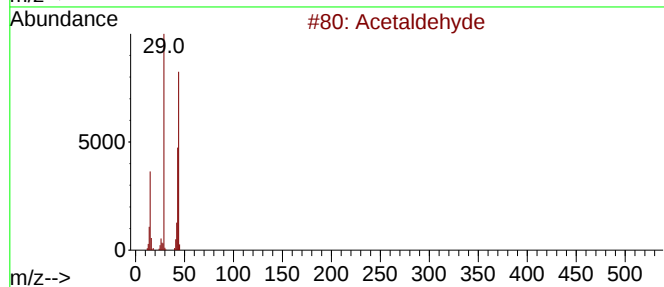
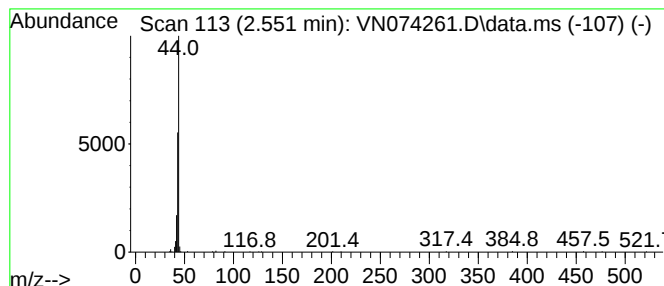
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.551	14.07 ug/l	176422	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
2			Ethylene oxide	44	C2H4O	000075-21-8	9
3			2-Octanamine	129	C8H19N	000693-16-3	5
4			Carbon dioxide	44	CO2	000124-38-9	4
5			Propane	44	C3H8	000074-98-6	4



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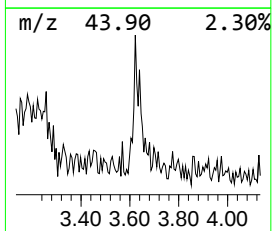
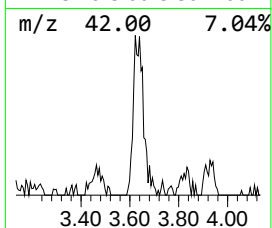
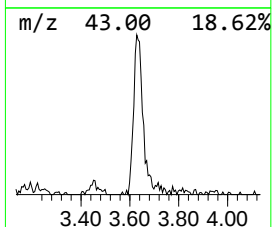
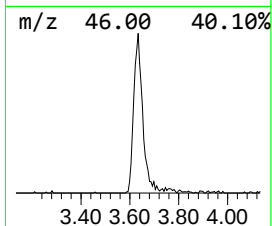
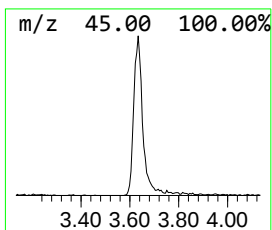
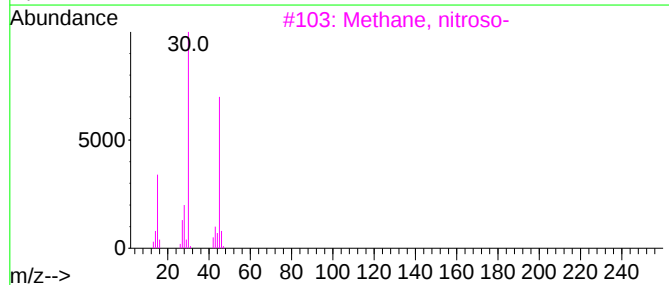
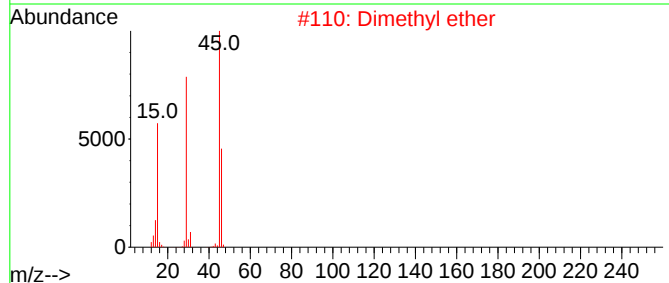
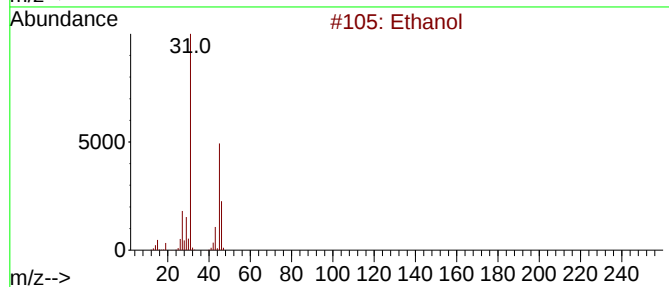
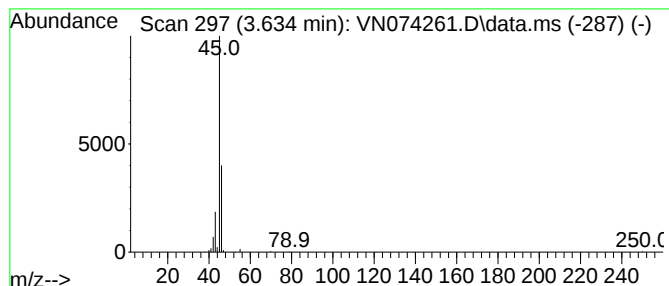
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
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Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.634	25.98 ug/l	325700	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	78
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Propanedioic acid, dihydroxy-			136	C3H4O6	000560-27-0	4
5	L-Lactic acid			90	C3H6O3	000079-33-4	4



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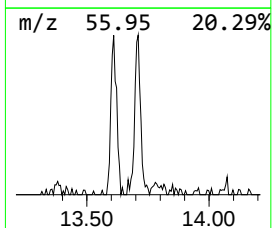
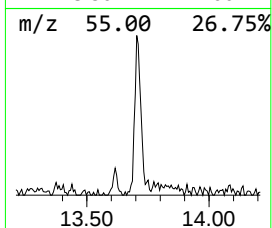
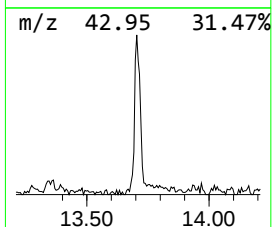
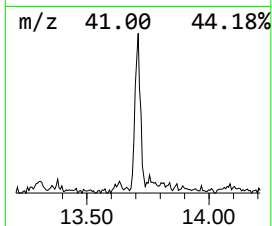
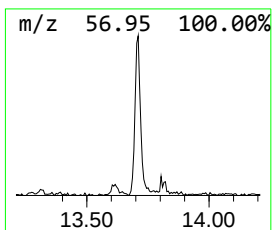
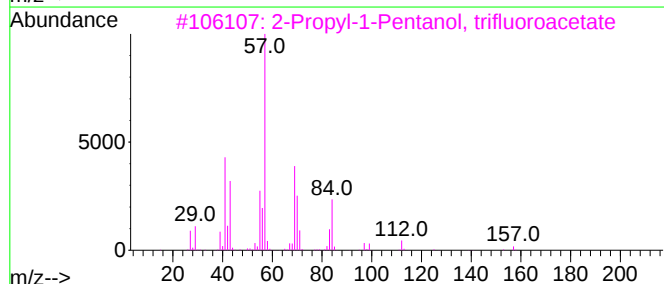
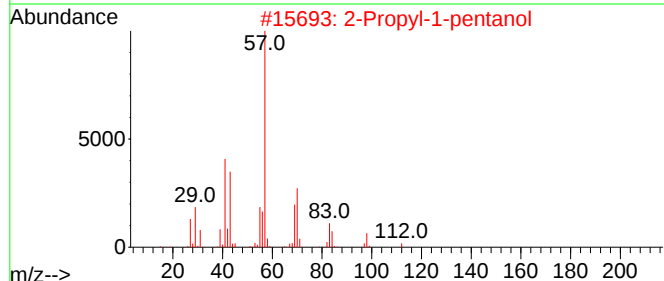
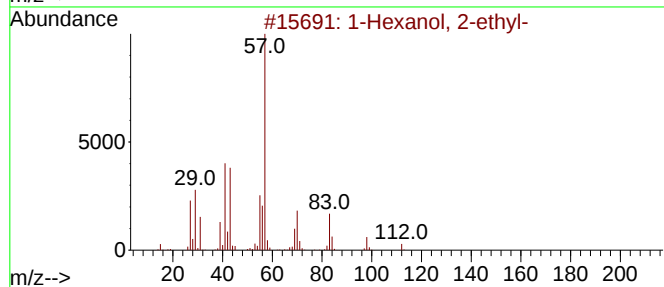
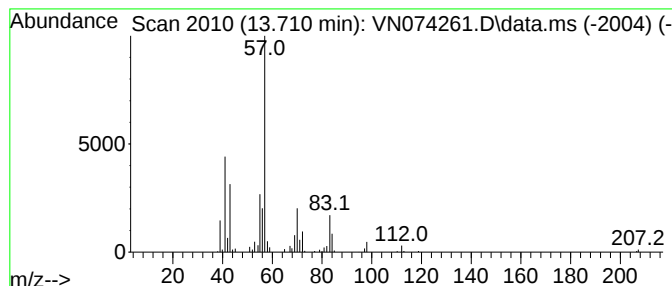
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	8.24 ug/l	197475	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	64
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3			2-Propyl-1-Pentanol, trifluoroac...	226	C10H17F3O2	1000365-19-7	53
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5			Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	38



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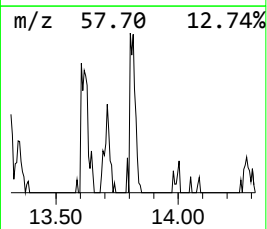
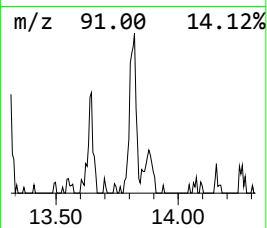
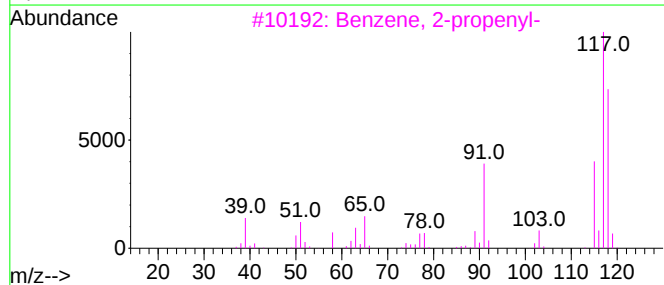
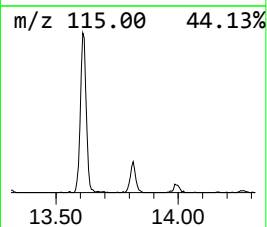
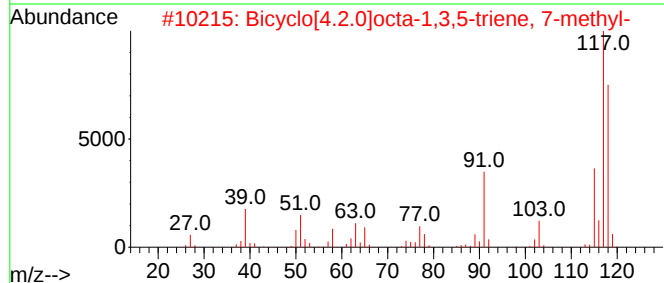
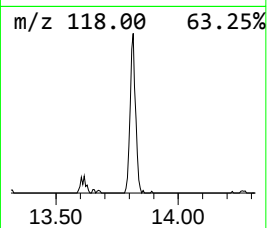
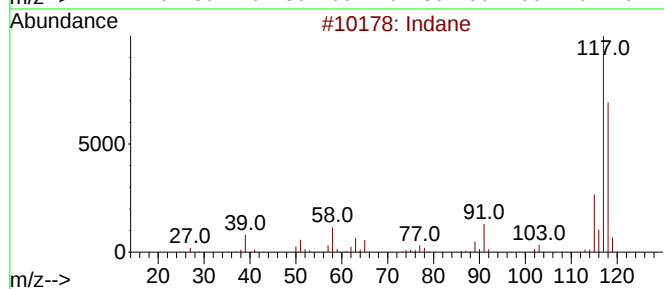
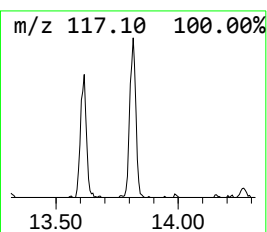
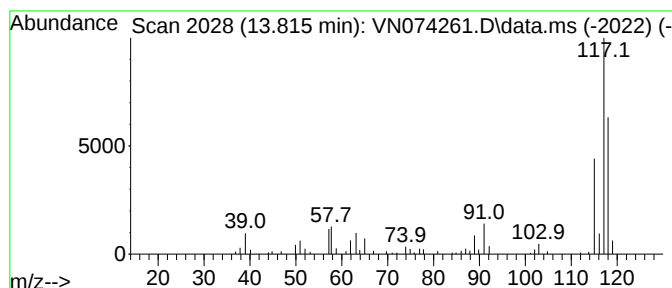
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	6.46 ug/l	154894	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	70
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	62
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	62



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.551	14.1	ug/l	176422	1	8.016	626722	50.0
Ethanol	3.634	26.0	ug/l	325700	1	8.016	626722	50.0
1-Hexanol, 2-et...	13.710	8.2	ug/l	197475	4	13.610	1198600	50.0
Indane	13.816	6.5	ug/l	154894	4	13.610	1198600	50.0