

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
 Data File : VN075831.D
 Acq On : 15 Dec 2022 20:35
 Operator : JC\MD
 Sample : N6066-10
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 ORA-584

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\82N121422W.M
 Title : SW846 8260

Signal : TIC: VN075831.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.095	3	7	14	rVB2	24714	37605	2.24%	0.294%
2	2.830	124	132	133	rBV2	13278	21530	1.28%	0.168%
3	4.447	396	407	418	rBV	98077	304438	18.10%	2.381%
4	4.741	447	457	462	rBV4	6720	18649	1.11%	0.146%
5	5.536	582	592	607	rBV2	14473	46728	2.78%	0.366%
6	6.730	786	795	812	rBV4	46488	151932	9.03%	1.188%
7	7.235	869	881	895	rBV	198622	568814	33.82%	4.449%
8	7.494	912	925	934	rBV	57318	150281	8.94%	1.176%
9	8.177	1031	1041	1045	rBV	236262	557281	33.13%	4.359%
10	8.229	1045	1050	1064	rVB	456227	1025173	60.95%	8.019%
11	8.588	1095	1111	1123	rBV2	243768	712255	42.35%	5.571%
12	9.106	1190	1199	1212	rVB	594873	1227582	72.99%	9.603%
13	9.271	1219	1227	1235	rBV2	23444	48255	2.87%	0.377%
14	9.659	1287	1293	1302	rVB3	19779	41940	2.49%	0.328%
15	10.571	1439	1448	1454	rBV	917234	1681898	100.00%	13.156%
16	10.635	1454	1459	1469	rVB	111050	210258	12.50%	1.645%
17	10.959	1507	1514	1524	rBV4	8961	17543	1.04%	0.137%
18	11.870	1656	1669	1680	rBV	796485	1448980	86.15%	11.334%
19	11.965	1681	1685	1693	rVV3	13029	26089	1.55%	0.204%
20	12.070	1695	1703	1713	rVB2	49494	97141	5.78%	0.760%
21	12.206	1720	1726	1733	rVB2	65751	109660	6.52%	0.858%
22	12.412	1751	1761	1767	rBV6	41632	111424	6.62%	0.872%
23	12.853	1826	1836	1846	rBV	658302	1107986	65.88%	8.667%
24	13.100	1873	1878	1882	rBV3	11683	21600	1.28%	0.169%
25	13.170	1886	1890	1895	rVB3	10918	17103	1.02%	0.134%
26	13.341	1915	1919	1931	rVB4	33115	59610	3.54%	0.466%
27	13.488	1940	1944	1947	rVV	37735	62854	3.74%	0.492%
28	13.535	1948	1952	1964	rVV6	25212	61810	3.68%	0.483%
29	13.794	1989	1996	2004	rBV	812865	1372195	81.59%	10.734%
30	13.876	2004	2010	2020	rVV	582427	947976	56.36%	7.415%
31	13.953	2020	2023	2028	rVB5	12613	19196	1.14%	0.150%
32	14.176	2055	2061	2068	rVB3	23370	43563	2.59%	0.341%
33	14.253	2069	2074	2077	rBV5	11446	19708	1.17%	0.154%
34	14.364	2085	2093	2101	rVB5	6938	22878	1.36%	0.179%
35	14.453	2101	2108	2117	rBV8	13829	39311	2.34%	0.308%
36	14.806	2162	2168	2175	rVB10	10341	26785	1.59%	0.210%

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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	15.041	2203	2208	2216	rBV5	10841	24742	1.47%	0.194%
38	15.205	2232	2236	2243	rVB7	9172	18030	1.07%	0.141%
39	15.323	2247	2256	2262	rVB9	8664	18034	1.07%	0.141%
40	15.470	2276	2281	2290	rVB6	25323	47056	2.80%	0.368%
41	15.588	2296	2301	2305	rBV2	19061	34150	2.03%	0.267%
42	15.647	2305	2311	2321	rVB	85314	203918	12.12%	1.595%

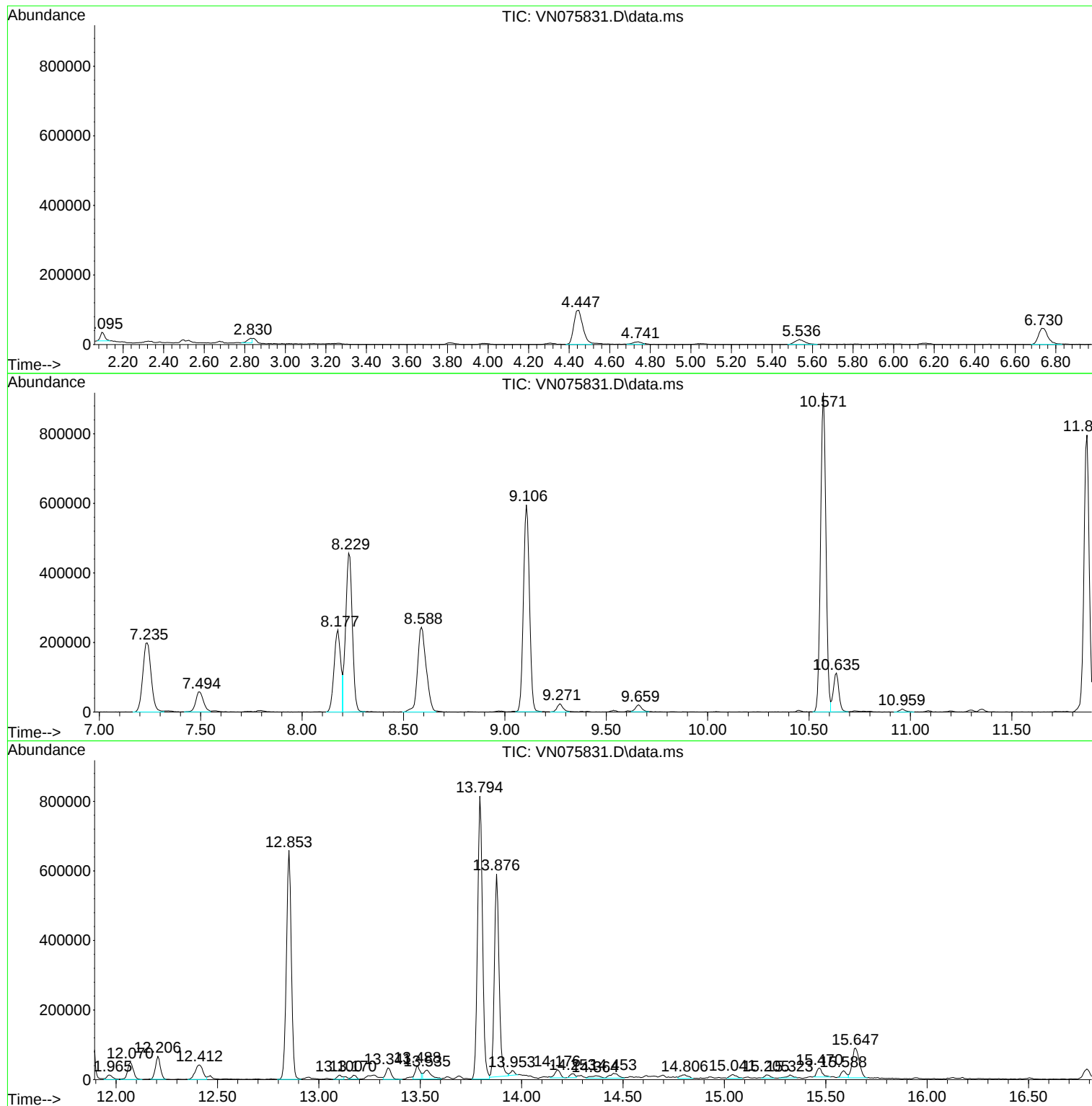
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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



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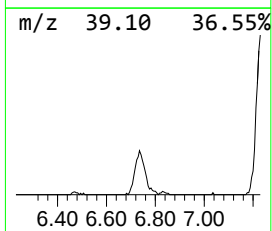
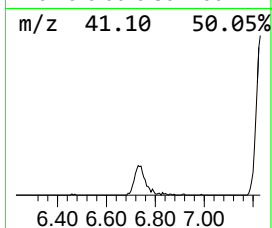
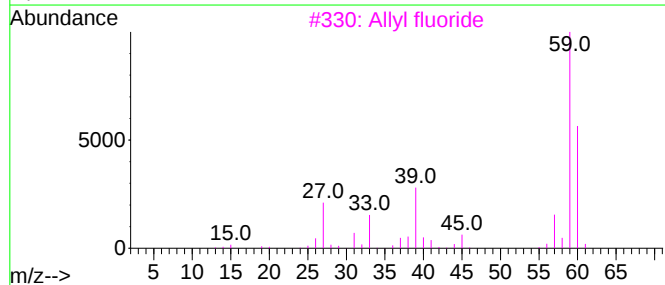
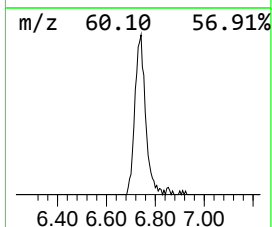
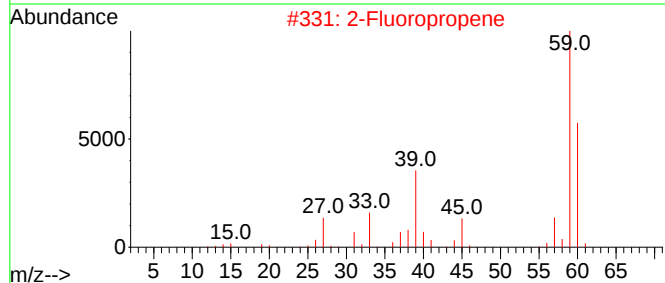
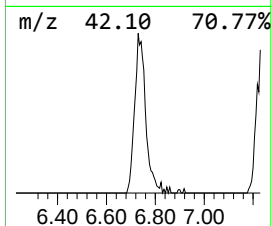
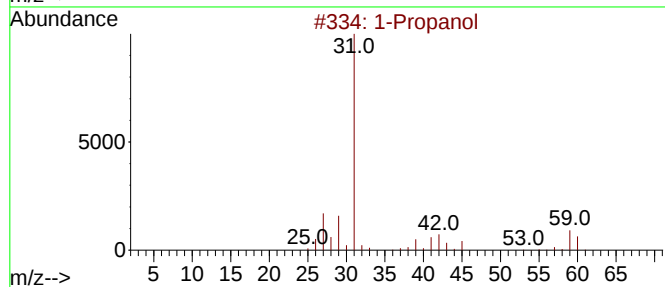
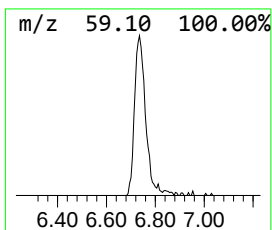
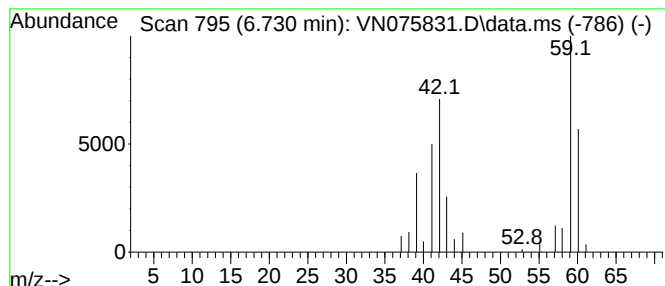
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 1 1-Propanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.730	7.41 ug/l	151932	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	64
2	2-Fluoropropene			60	C3H5F	001184-60-7	53
3	Allyl fluoride			60	C3H5F	000818-92-8	53
4	Cyclopropane			42	C3H6	000075-19-4	10
5	Methanamine, N-hydroxy-N-methyl-			61	C2H7NO	005725-96-2	9



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ALS Vial : 25 Sample Multiplier: 1

Instrument :
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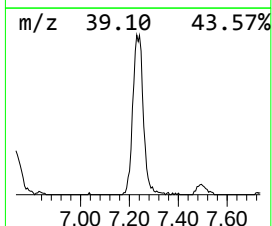
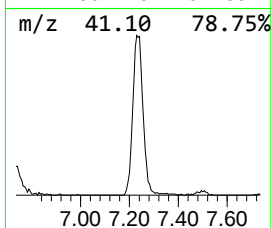
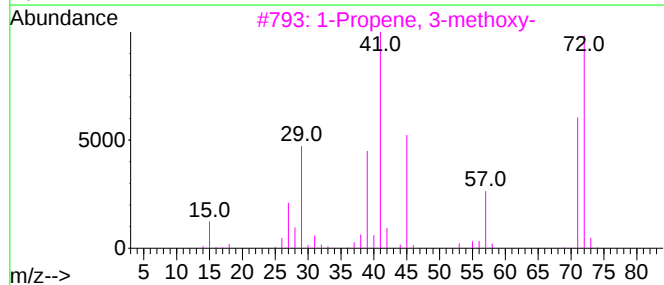
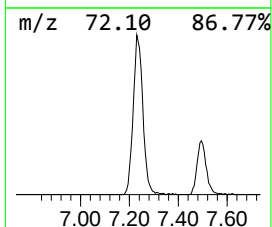
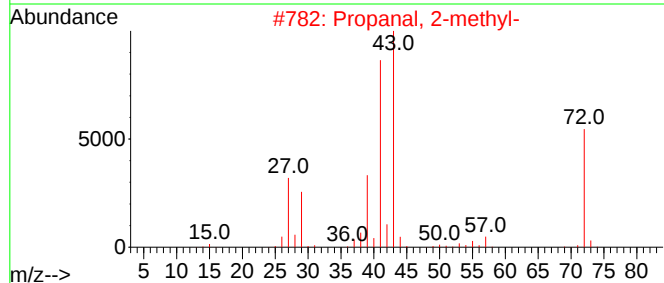
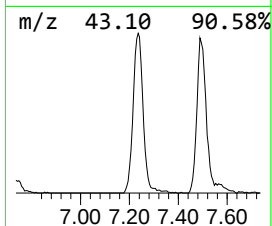
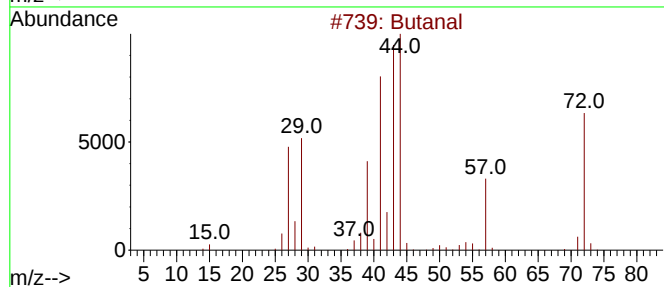
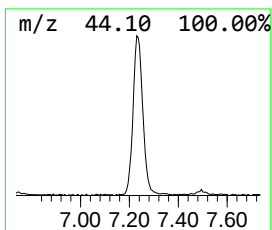
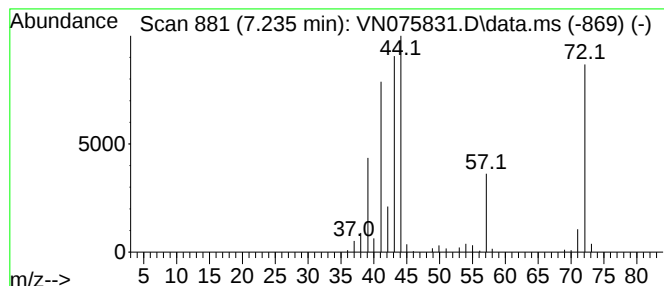
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.235	27.74 ug/l	568814	Pentafluorobenzene	8.229

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	94
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
4		2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
5		Isobutylene epoxide	72	C4H8O	000558-30-5	27



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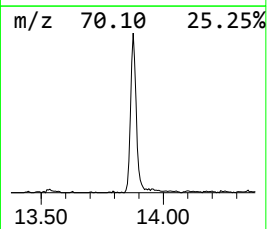
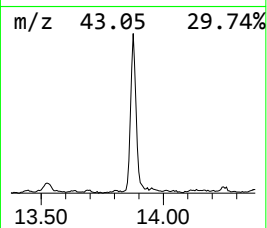
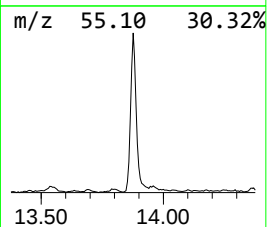
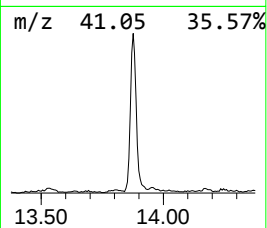
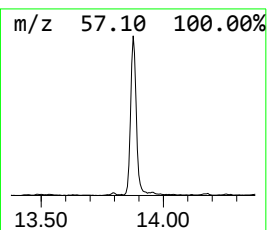
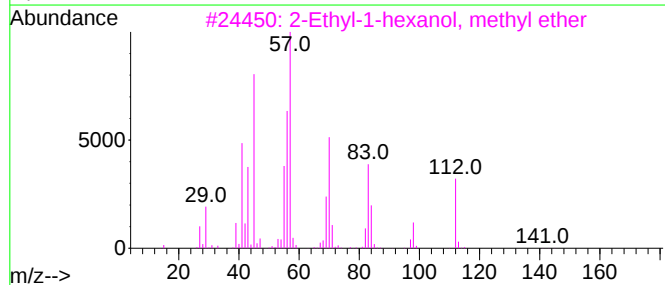
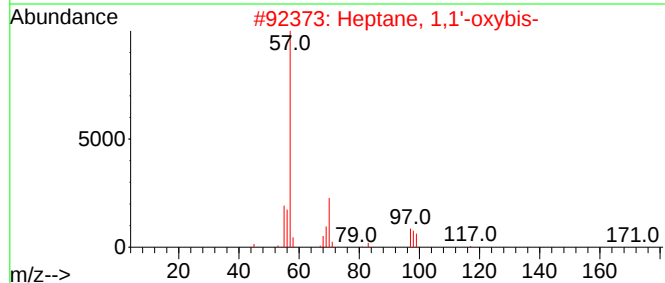
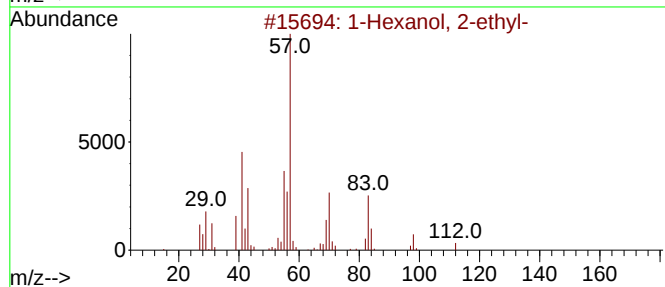
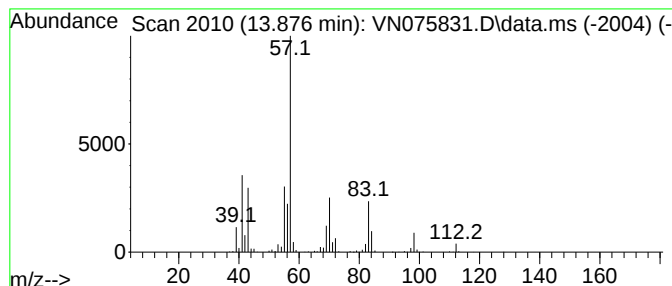
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	34.54 ug/l	947976	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
3			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propanol	6.730	7.4	ug/l	151932	1	8.229	1025170	50.0
Butanal	7.235	27.7	ug/l	568814	1	8.229	1025170	50.0
1-Hexanol, 2-et...	13.876	34.5	ug/l	947976	4	13.794	1372200	50.0