

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090322\
 Data File : VN074333.D
 Acq On : 03 Sep 2022 21:48
 Operator : JC\MD
 Sample : N4355-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-40

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\82N090222W.M
 Title : SW846 8260

Signal : TIC: VN074333.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	47	54	61	rBV	113332	313680	6.21%	1.645%
2	2.404	84	88	91	rBV3	29643	52430	1.04%	0.275%
3	2.704	133	139	140	rBV3	64218	130416	2.58%	0.684%
4	5.281	564	577	592	rBV2	200962	688157	13.61%	3.608%
5	5.528	609	619	633	rVB3	99058	344183	6.81%	1.804%
6	6.416	759	770	781	rBV3	64422	214568	4.24%	1.125%
7	7.022	862	873	888	rBV5	33088	129336	2.56%	0.678%
8	7.951	1020	1031	1037	rBV2	295789	741880	14.68%	3.889%
9	8.016	1037	1042	1055	rVB	466657	1056513	20.90%	5.539%
10	8.392	1093	1106	1115	rBV	2021770	5054781	100.00%	26.500%
11	8.904	1183	1193	1212	rBV	733932	1480514	29.29%	7.762%
12	10.133	1396	1402	1415	rBV3	73492	165737	3.28%	0.869%
13	10.380	1436	1444	1452	rBV	1098387	1986228	39.29%	10.413%
14	10.580	1467	1478	1485	rBV2	91846	169883	3.36%	0.891%
15	10.657	1485	1491	1498	rVV2	118732	203234	4.02%	1.065%
16	11.027	1544	1554	1557	rBV4	26818	62179	1.23%	0.326%
17	11.069	1557	1561	1569	rVB2	102327	177511	3.51%	0.931%
18	11.527	1632	1639	1645	rBV2	47124	92112	1.82%	0.483%
19	11.680	1658	1665	1677	rVV	1086746	1961417	38.80%	10.283%
20	11.786	1677	1683	1689	rVB6	32194	74097	1.47%	0.388%
21	12.216	1751	1756	1765	rVB	33980	61775	1.22%	0.324%
22	12.516	1801	1807	1812	rBV3	36121	59454	1.18%	0.312%
23	12.669	1822	1833	1843	rBV	918156	1550036	30.66%	8.126%
24	13.163	1910	1917	1921	rBV2	30916	54565	1.08%	0.286%
25	13.304	1937	1941	1947	rVB	34508	58244	1.15%	0.305%
26	13.610	1986	1993	2007	rBV	1135838	1960832	38.79%	10.280%
27	13.816	2023	2028	2033	rBV2	57165	104595	2.07%	0.548%
28	14.263	2098	2104	2110	rBV2	40720	68145	1.35%	0.357%
29	14.863	2199	2206	2212	rVB5	24349	57784	1.14%	0.303%

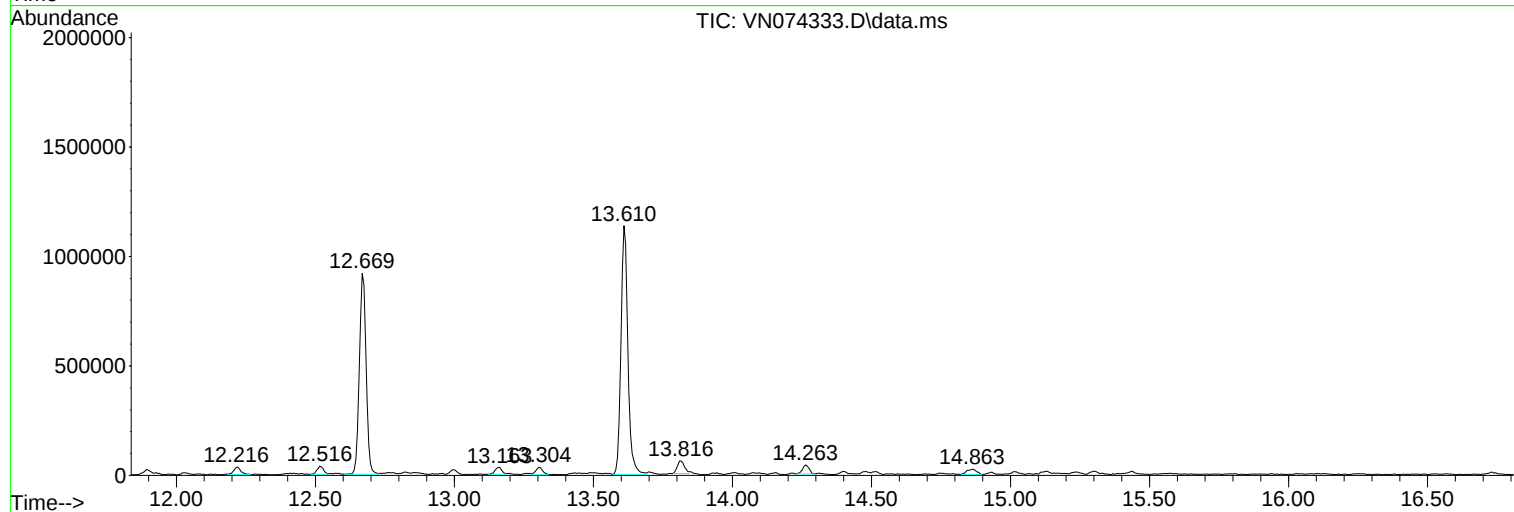
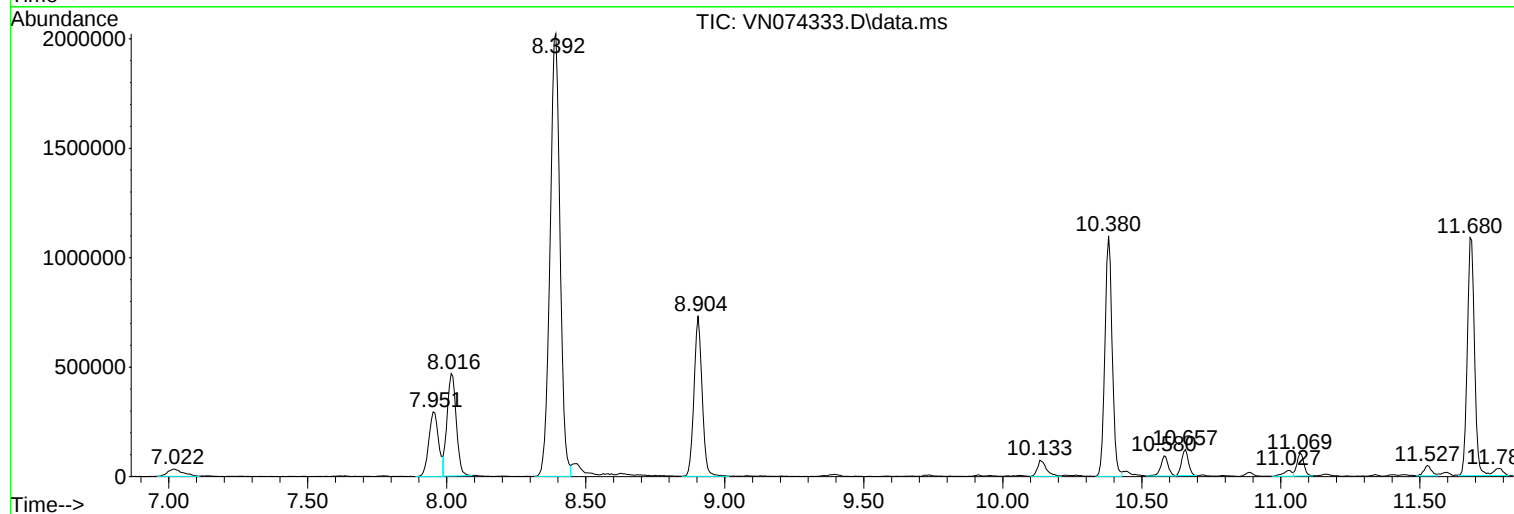
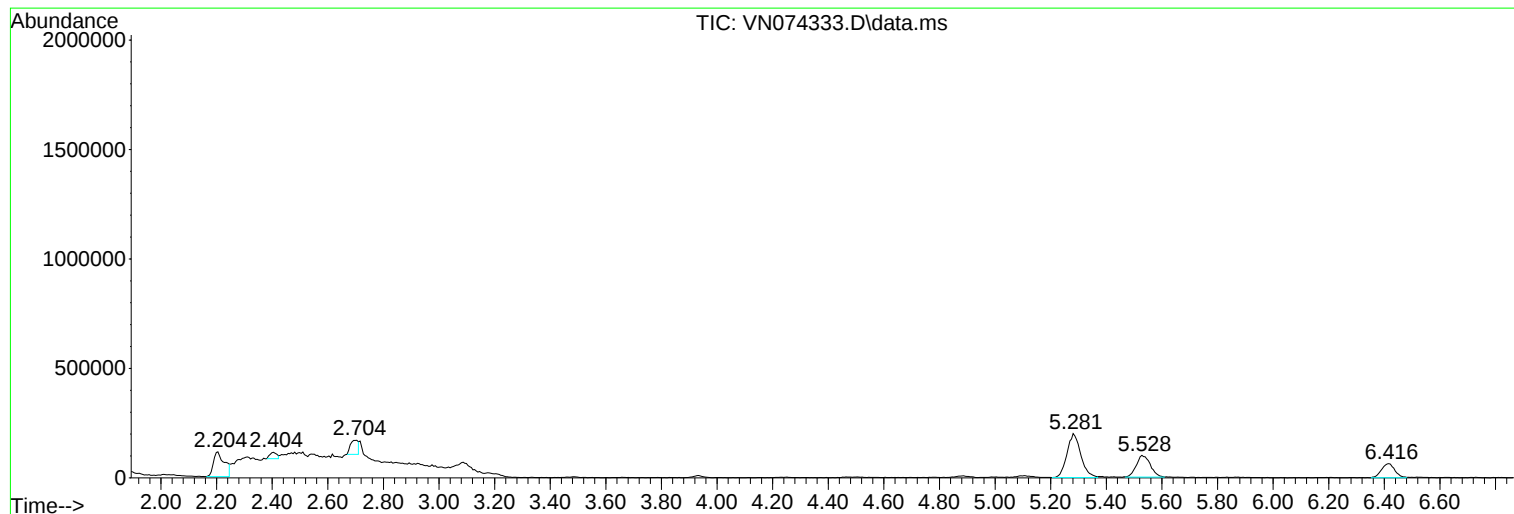
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090222W.M
Quant Title : SW846 8260

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



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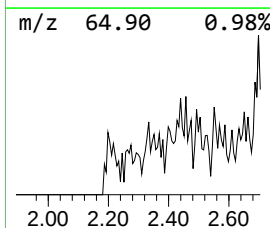
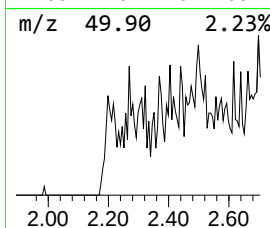
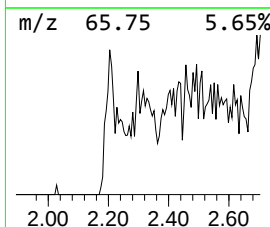
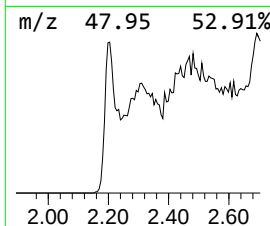
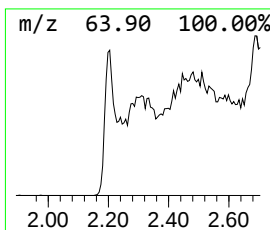
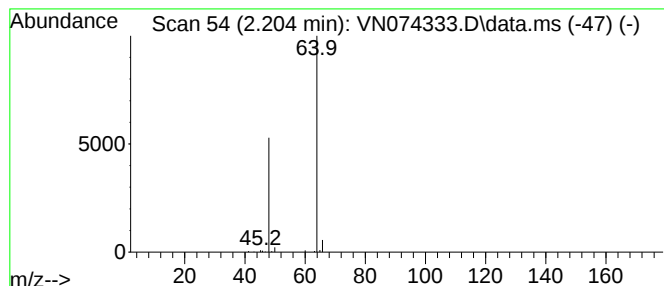
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	14.85 ug/l	313680	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	4



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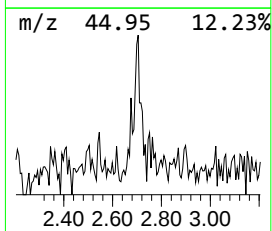
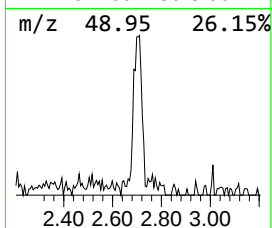
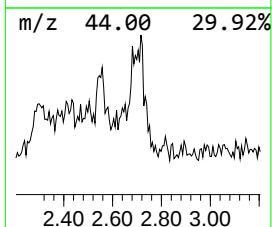
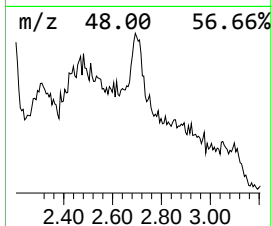
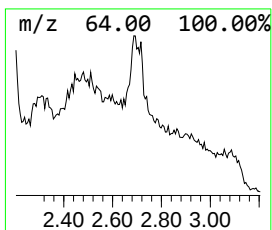
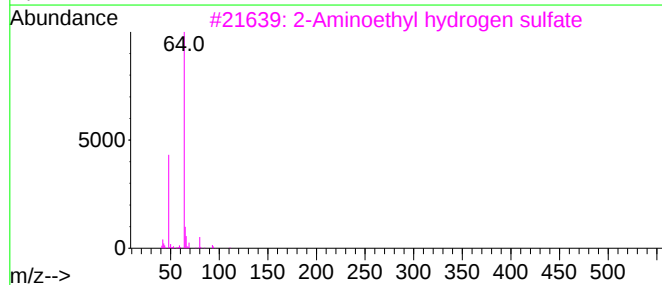
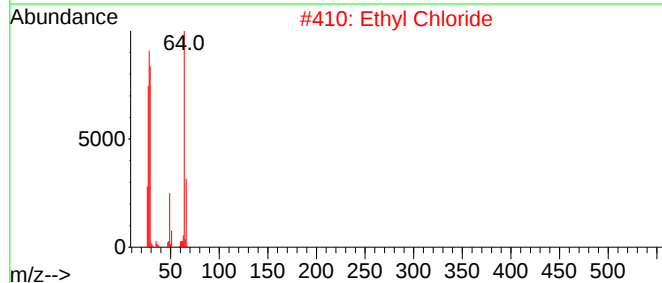
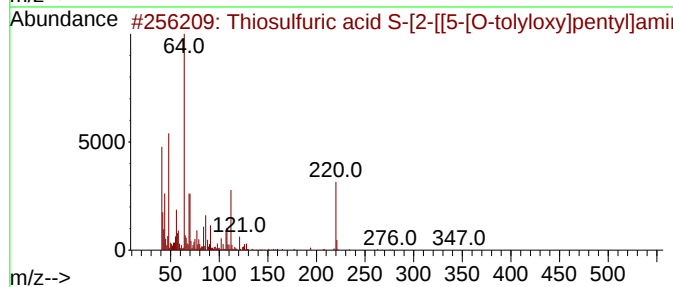
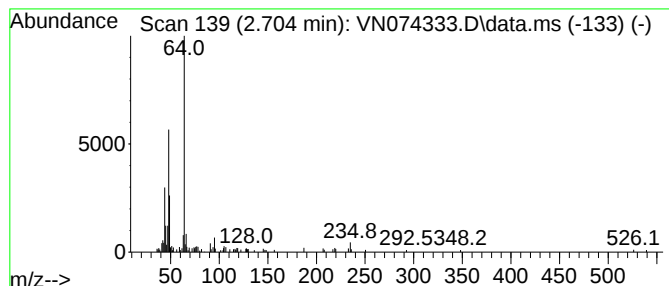
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 Thiosulfuric acid S-[2-[[5-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.704	6.17 ug/l	130416	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiosulfuric acid S-[2-[[5-[O-to...	347	C15H25NO4S2	038920-47-7	64
2			Ethyl Chloride	64	C2H5Cl	000075-00-3	64
3			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	59
4			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	53
5			1,1,1,2,2,3,3,4,4,5,5-Undecaflu...	602	C10F22O2S	1000486-78-5	45



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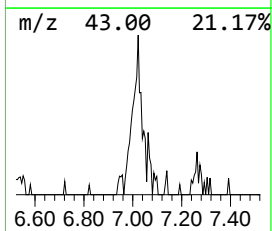
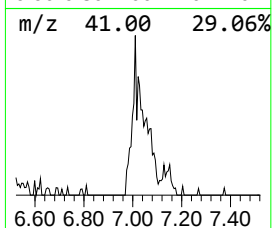
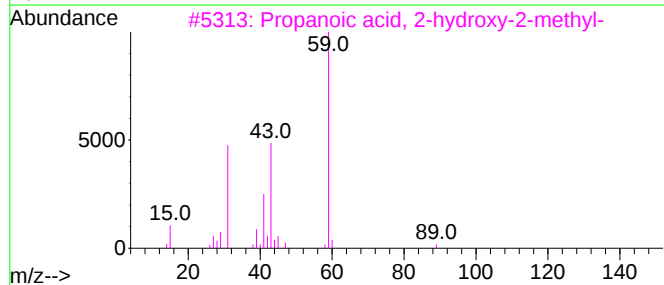
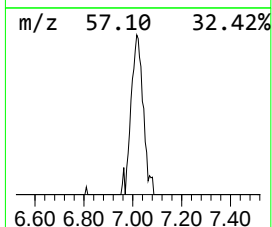
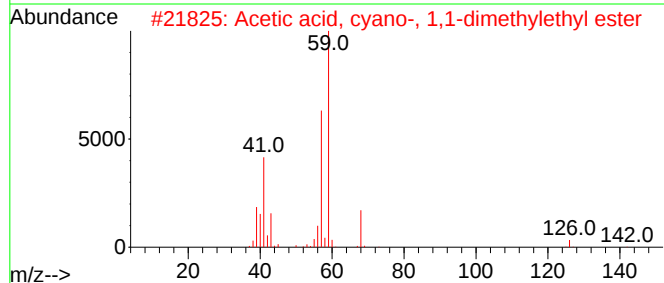
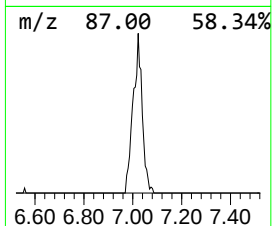
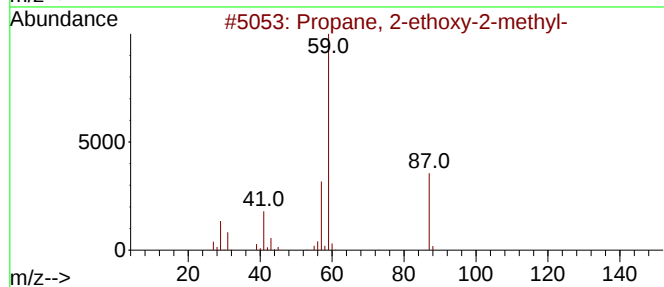
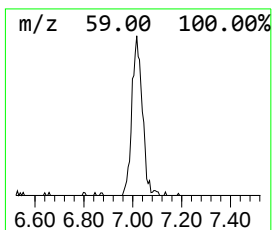
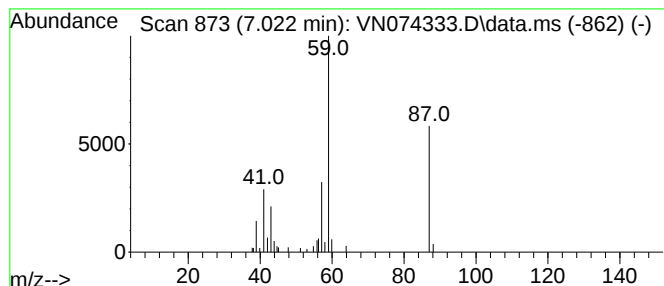
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Peak Number 3 Propane, 2-ethoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.022	6.12 ug/l	129336	Pentafluorobenzene	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	78
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	40
3			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	37
4			3-Hexanol	102	C6H14O	000623-37-0	33
5			Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	9



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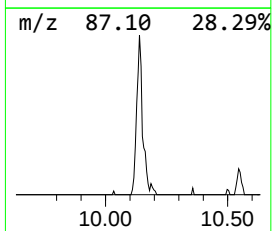
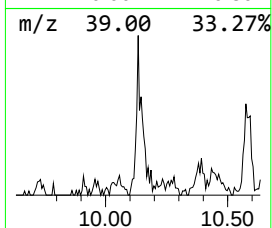
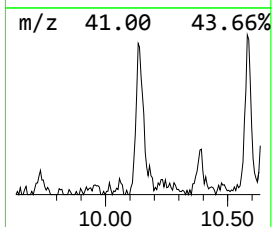
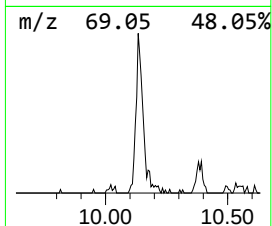
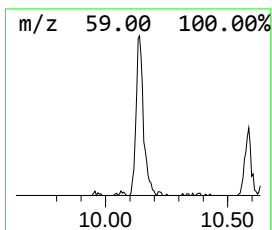
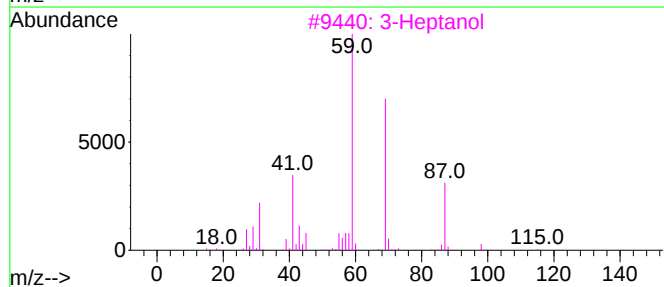
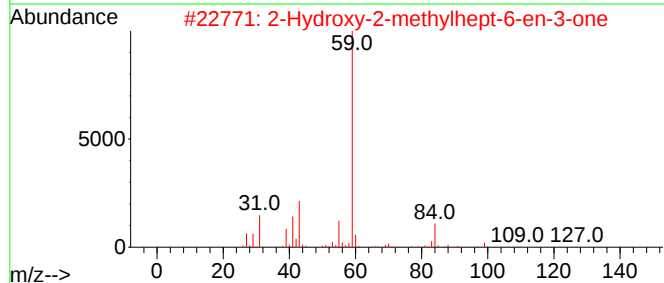
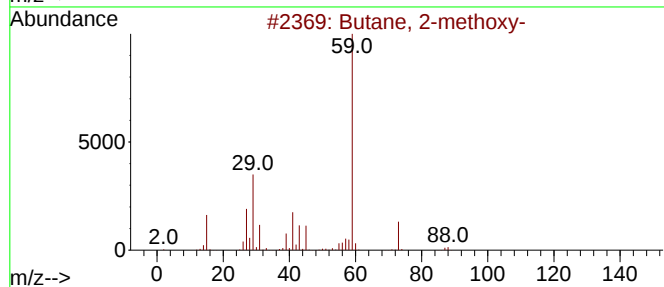
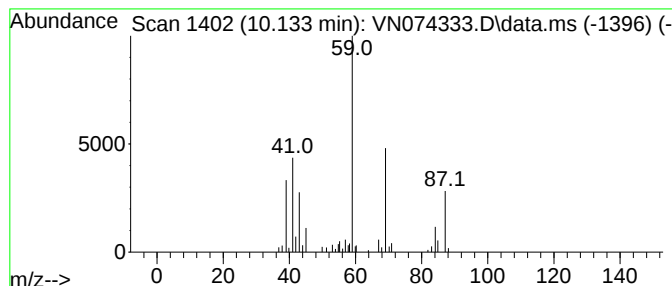
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Peak Number 4 Butane, 2-methoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.133	5.60 ug/l	165737	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-	88	C5H12O	006795-87-5	50
2			2-Hydroxy-2-methylhept-6-en-3-one	142	C8H14O2	000996-61-2	47
3			3-Heptanol	116	C7H16O	000589-82-2	45
4			3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	45
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	42



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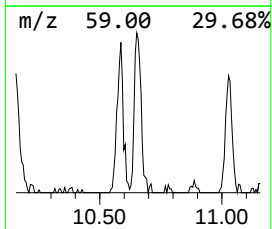
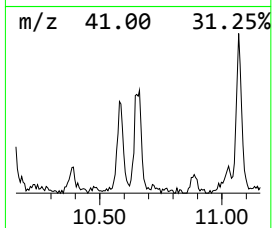
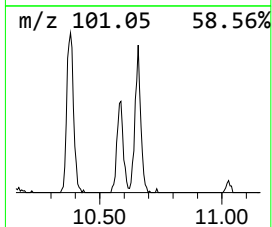
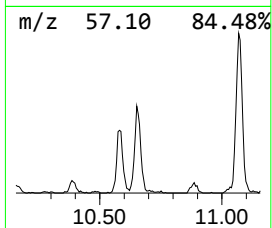
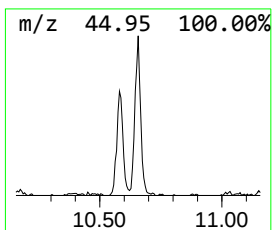
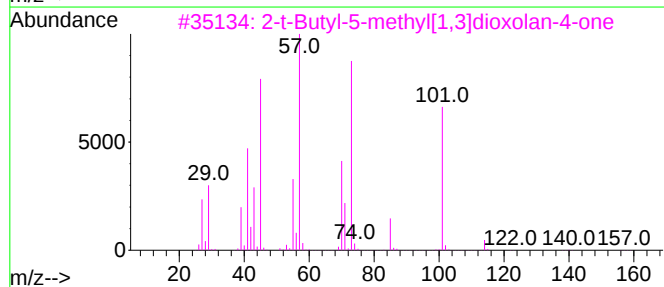
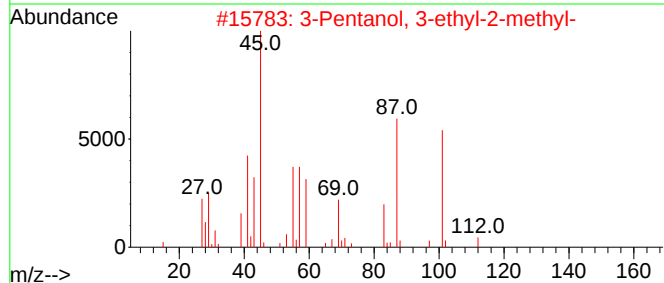
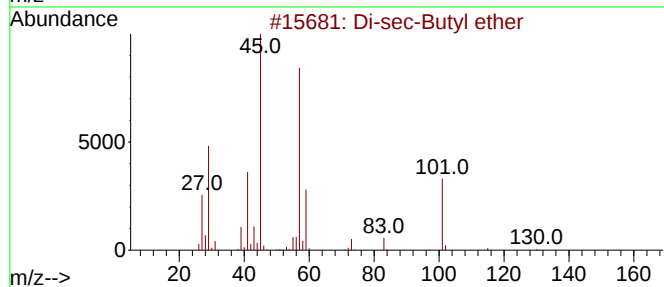
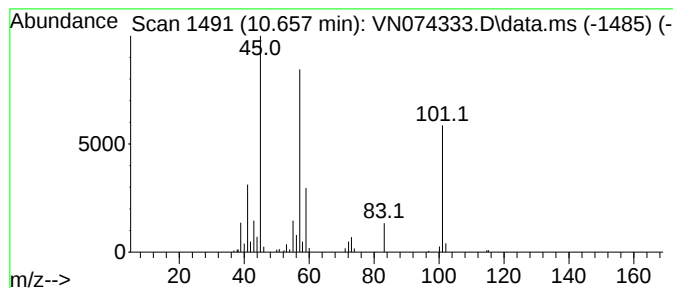
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Di-sec-Butyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.657	5.18 ug/l	203234	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2			3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	72
3			2-t-Butyl-5-methyl[1,3]dioxolan-...	158	C8H14O3	130930-47-1	45
4			Diethyl carbitol	162	C8H18O3	000112-36-7	43
5			2-Hydroxy-3-pentanone	102	C5H10O2	005704-20-1	33



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.204	14.9	ug/l	313680	1	8.022	1056510	50.0
Thiosulfuric ac...	2.704	6.2	ug/l	130416	1	8.022	1056510	50.0
Propane, 2-etho...	7.022	6.1	ug/l	129336	1	8.022	1056510	50.0
Butane, 2-methoxy-	10.133	5.6	ug/l	165737	2	8.904	1480510	50.0
Di-sec-Butyl ether	10.657	5.2	ug/l	203234	3	11.686	1961420	50.0