

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010522\
 Data File : VN070495.D
 Acq On : 5 Jan 2022 17:38
 Operator : JC/MD
 Sample : N1012-12
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31244

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\82N122721W.M

Title : SW846 8260

Signal : TIC: VN070495.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.225	74	88	152	rBV3	37403201	102886657	100.00%	36.167%
2	2.587	207	223	269	rBV	7903755	14476372	14.07%	5.089%
3	3.690	612	634	666	rBV	787442	2197873	2.14%	0.773%
4	4.282	827	855	940	rBV2	20348314	62539491	60.78%	21.984%
5	4.583	945	967	1009	rVB2	1885381	6090995	5.92%	2.141%
6	5.374	1224	1262	1307	rBV	631547	2330630	2.27%	0.819%
7	7.061	1864	1891	1950	rBV	1641820	4880367	4.74%	1.716%
8	7.332	1969	1992	2039	rBV	2231861	6027574	5.86%	2.119%
9	8.021	2226	2249	2259	rBV	641424	1534091	1.49%	0.539%
10	8.083	2260	2272	2298	rVB	1211733	2771463	2.69%	0.974%
11	8.434	2380	2403	2428	rBV	882389	2201204	2.14%	0.774%
12	8.965	2581	2601	2632	rBV	1873664	3838335	3.73%	1.349%
13	10.330	3093	3110	3133	rBV	1677169	3106771	3.02%	1.092%
14	10.440	3134	3151	3161	rBV	2926356	5389077	5.24%	1.894%
15	10.505	3161	3175	3207	rVB	13884630	25902397	25.18%	9.105%
16	11.186	3411	3429	3460	rBV2	1551938	3686037	3.58%	1.296%
17	11.744	3616	3637	3661	rBV	2532007	4878641	4.74%	1.715%
18	11.843	3661	3674	3694	rVV	1648102	3113817	3.03%	1.095%
19	11.948	3696	3713	3752	rVB	6352872	12898497	12.54%	4.534%
20	12.277	3809	3836	3857	rBV	3671373	6728961	6.54%	2.365%
21	12.731	3988	4005	4032	rBV	2084394	3705475	3.60%	1.303%
22	13.675	4342	4357	4378	rBV	1836849	3293402	3.20%	1.158%

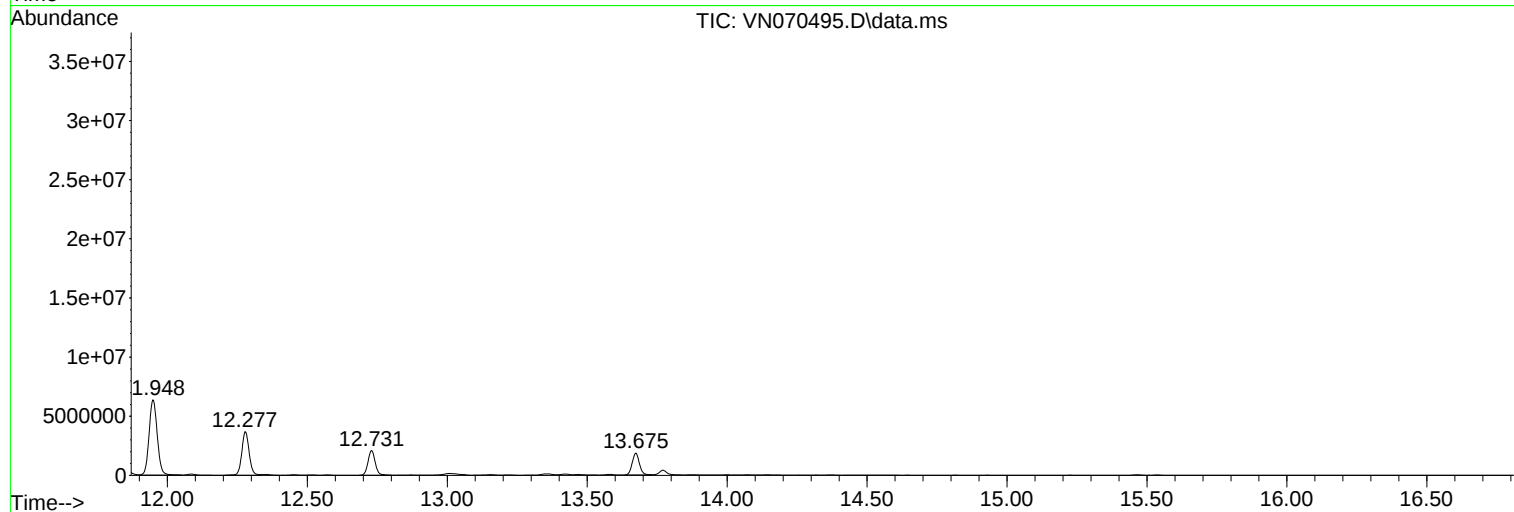
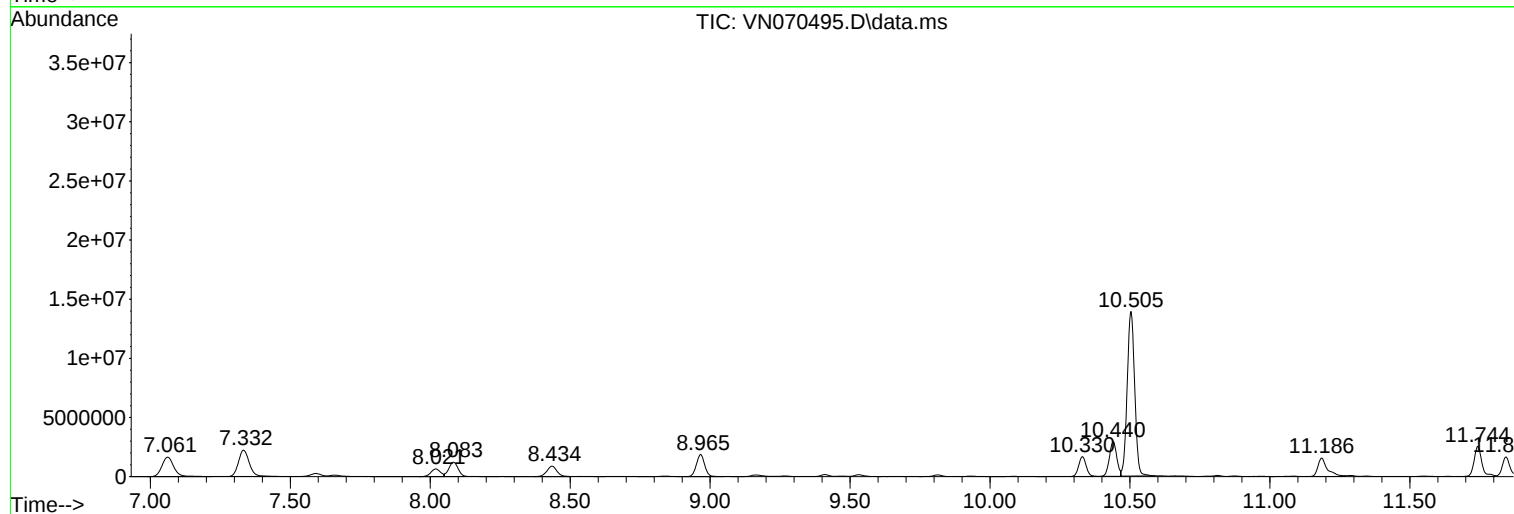
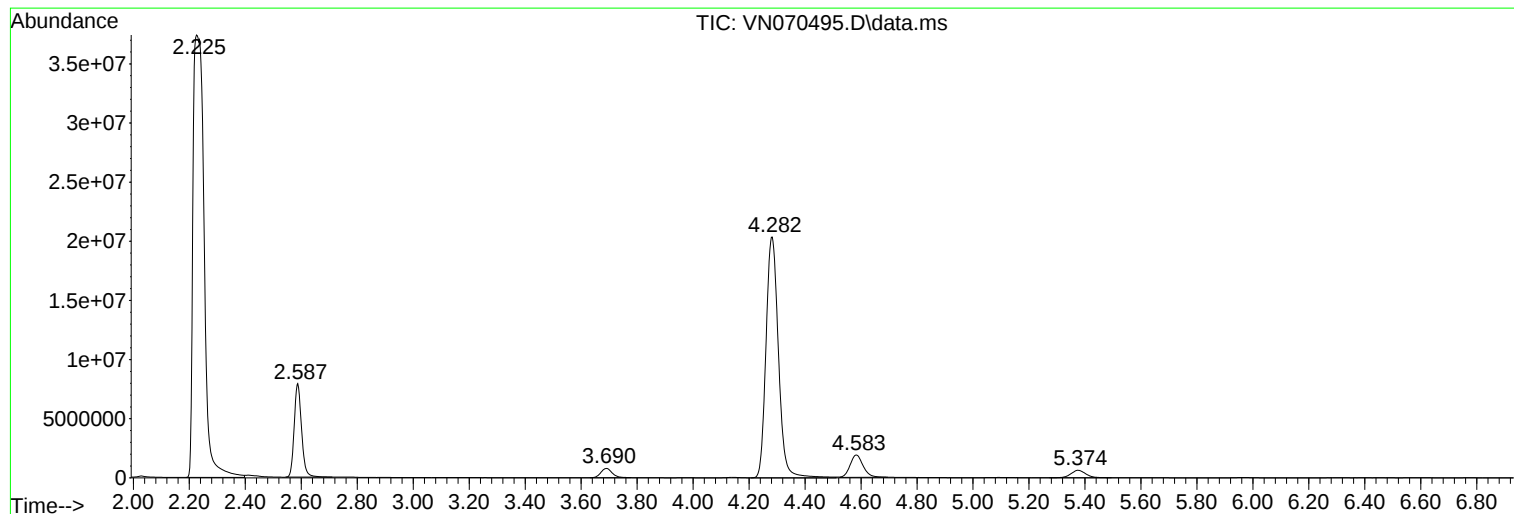
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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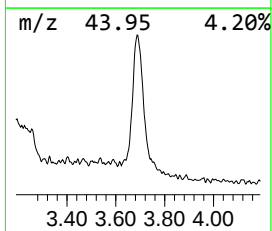
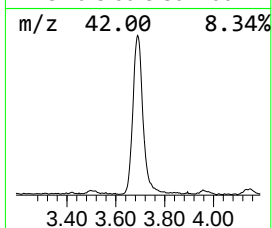
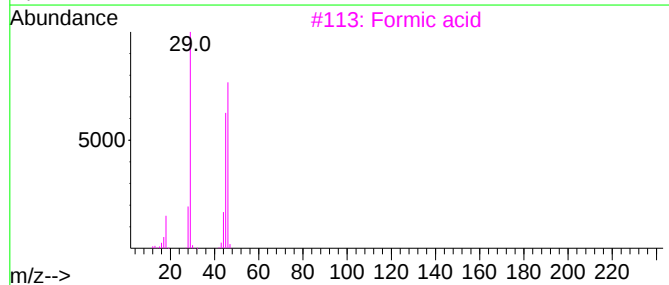
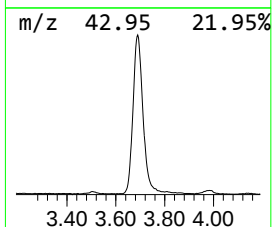
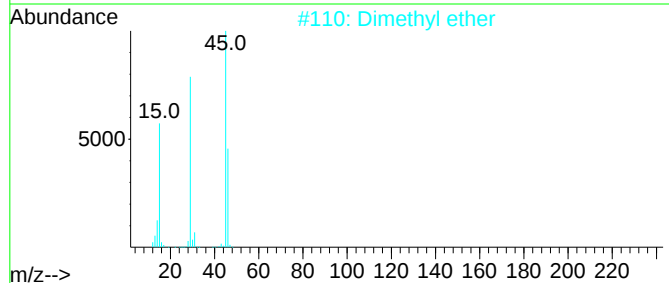
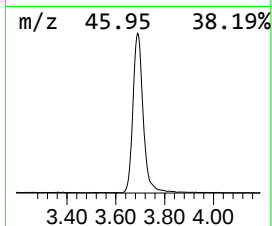
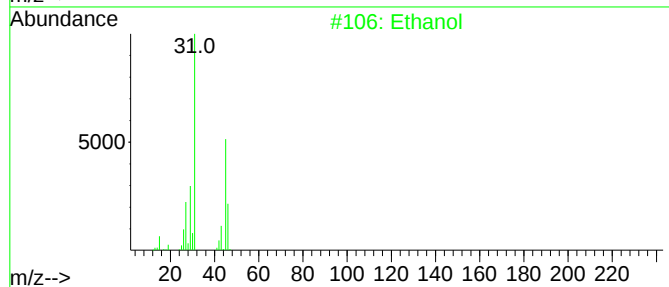
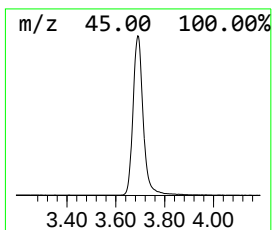
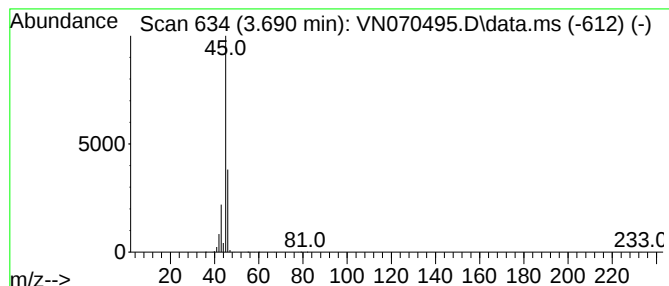
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.690	39.65 ug/l	2197870	Pentafluorobenzene	8.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	64
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Formic acid			46	CH2O2	000064-18-6	4
4	Methane, nitroso-			45	CH3NO	000865-40-7	3
5	Nitrogen dioxide			46	NO2	010102-44-0	2



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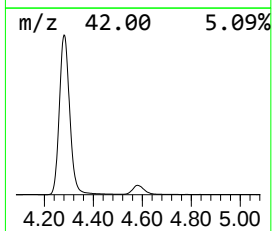
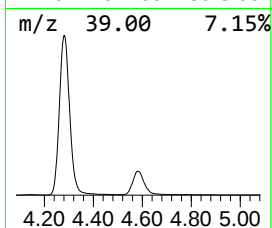
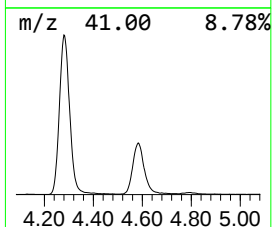
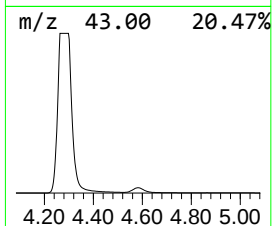
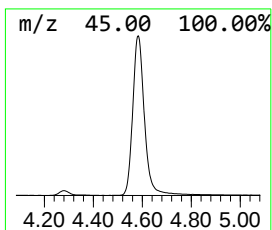
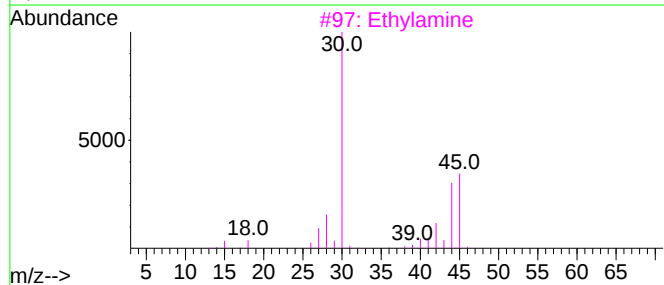
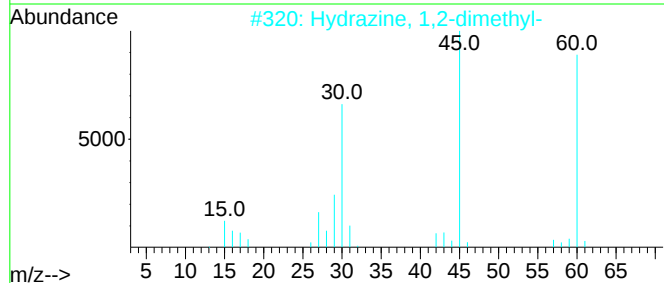
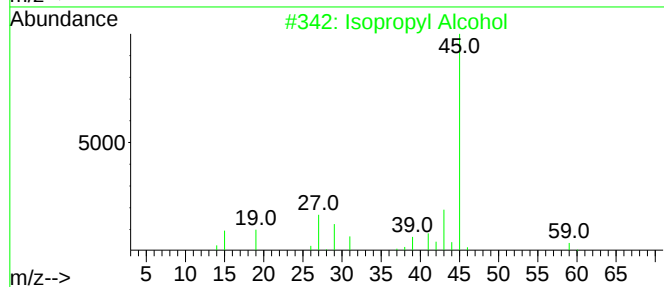
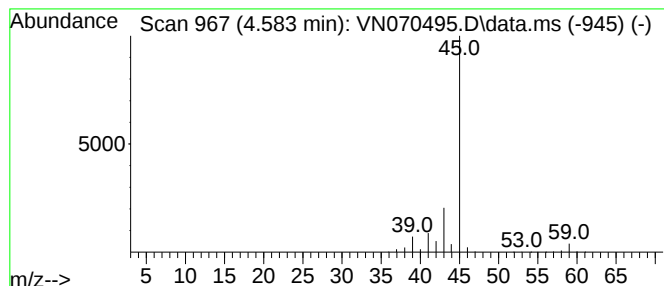
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 4 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.583	109.89 ug/l	6091000	Pentafluorobenzene	8.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3			Ethylamine	45	C2H7N	000075-04-7	5
4			Formamide	45	CH3NO	000075-12-7	4
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	4



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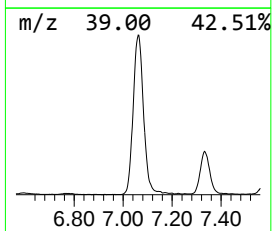
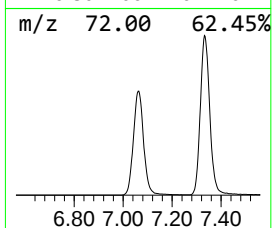
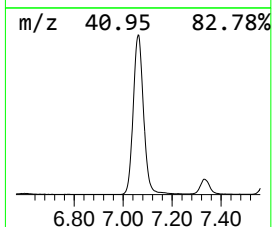
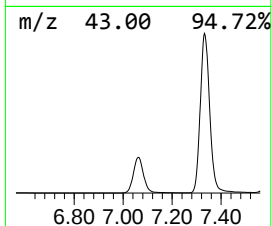
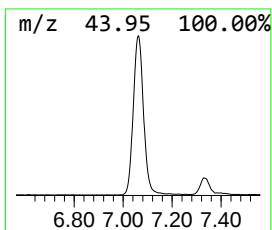
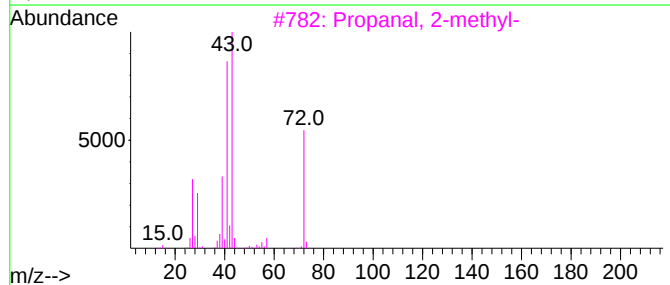
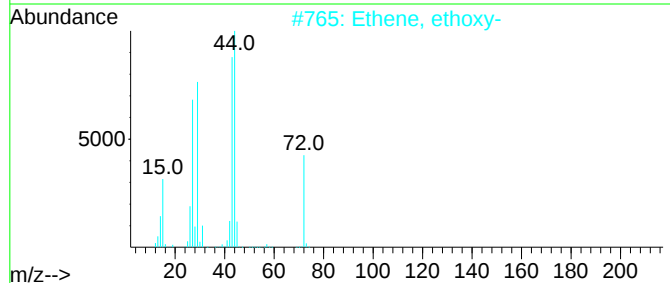
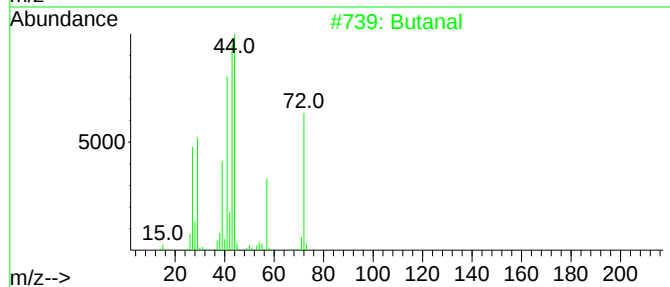
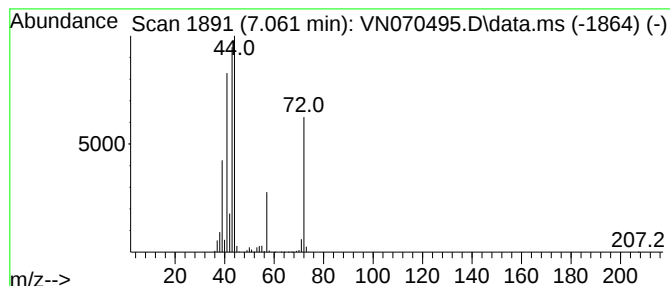
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Peak Number 5 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.061	88.05 ug/l	4880370	Pentafluorobenzene	8.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	35
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	23



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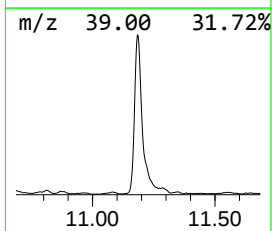
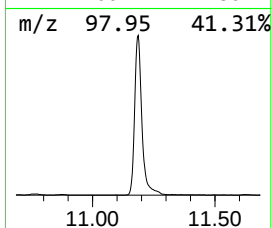
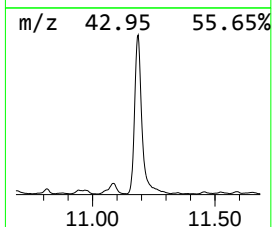
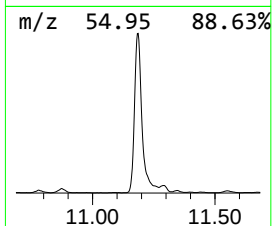
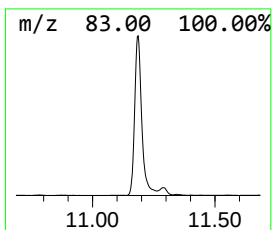
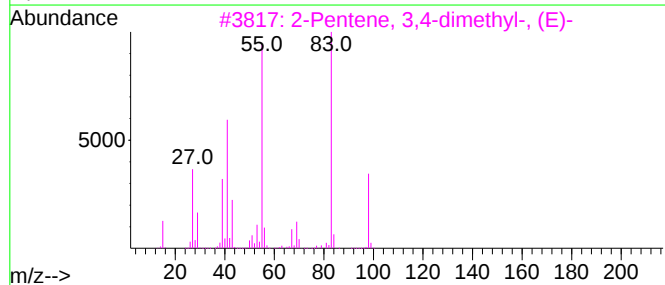
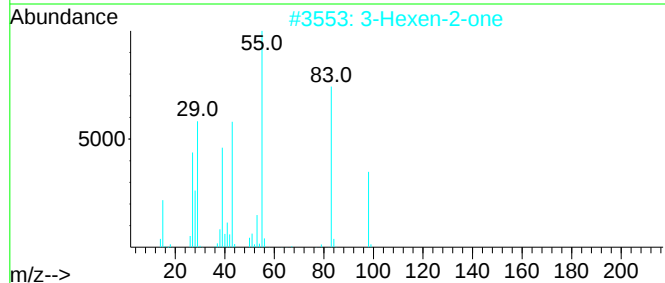
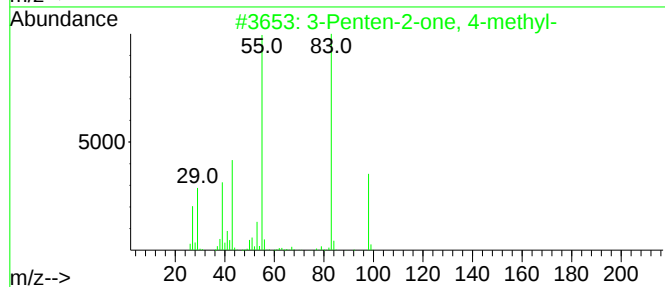
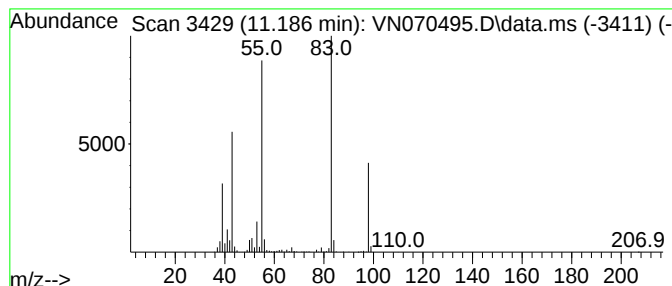
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Peak Number 6 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.186	37.78 ug/l	3686040	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	3.690	39.6	ug/l	2197870	1	8.083	2771460	50.0
Isopropyl Alcohol	4.583	109.9	ug/l	6091000	1	8.083	2771460	50.0
Butanal	7.061	88.0	ug/l	4880370	1	8.083	2771460	50.0
3-Penten-2-one,...	11.186	37.8	ug/l	3686040	3	11.744	4878640	50.0