

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081721\
 Data File : VN068152.D
 Acq On : 17 Aug 2021 18:56
 Operator : JC/MD
 Sample : M3361-13 20X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41943

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\82N081721W.M
 Title : SW846 8260

Signal : TIC: VN068152.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.220	73	86	105	rBV	274900	395358	5.72%	1.518%
2	2.579	199	220	257	rBV	2019397	3639770	52.68%	13.979%
3	3.719	618	645	706	rVB	2697182	6909405	100.00%	26.537%
4	4.857	1043	1069	1099	rBV2	28634	94427	1.37%	0.363%
5	8.021	2225	2249	2260	rBV2	283560	692902	10.03%	2.661%
6	8.083	2260	2272	2305	rVB	499383	1156322	16.74%	4.441%
7	8.440	2383	2405	2436	rBV4	310438	844268	12.22%	3.243%
8	8.968	2583	2602	2638	rVB	728099	1520184	22.00%	5.839%
9	10.443	3131	3152	3165	rBV	1186319	2206954	31.94%	8.476%
10	10.507	3165	3176	3194	rVB	391455	733966	10.62%	2.819%
11	11.189	3411	3430	3454	rBV2	334446	607377	8.79%	2.333%
12	11.746	3619	3638	3664	rBV	1195937	2182939	31.59%	8.384%
13	11.848	3665	3676	3690	rVB	40779	69907	1.01%	0.268%
14	11.950	3699	3714	3737	rVB	127261	248781	3.60%	0.956%
15	12.283	3821	3838	3857	rBV2	106823	185849	2.69%	0.714%
16	12.733	3990	4006	4038	rBV	943643	1626357	23.54%	6.246%
17	12.986	4087	4100	4108	rBV2	56624	100543	1.46%	0.386%
18	13.372	4228	4244	4263	rVB	172833	280653	4.06%	1.078%
19	13.678	4342	4358	4384	rVB	1046785	1937573	28.04%	7.442%
20	13.879	4421	4433	4443	rBV3	79895	143890	2.08%	0.553%
21	14.933	4808	4826	4840	rBV4	96782	210197	3.04%	0.807%
22	15.088	4869	4884	4898	rBV2	78276	134498	1.95%	0.517%
23	15.507	5025	5040	5054	rBV	60146	114410	1.66%	0.439%

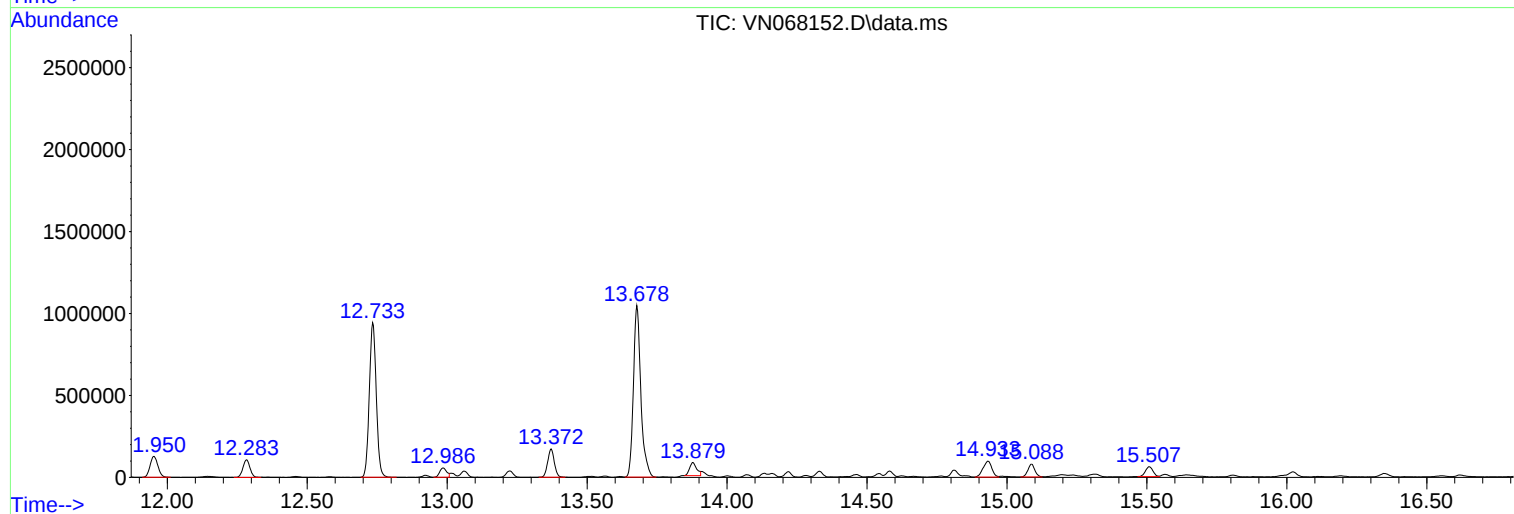
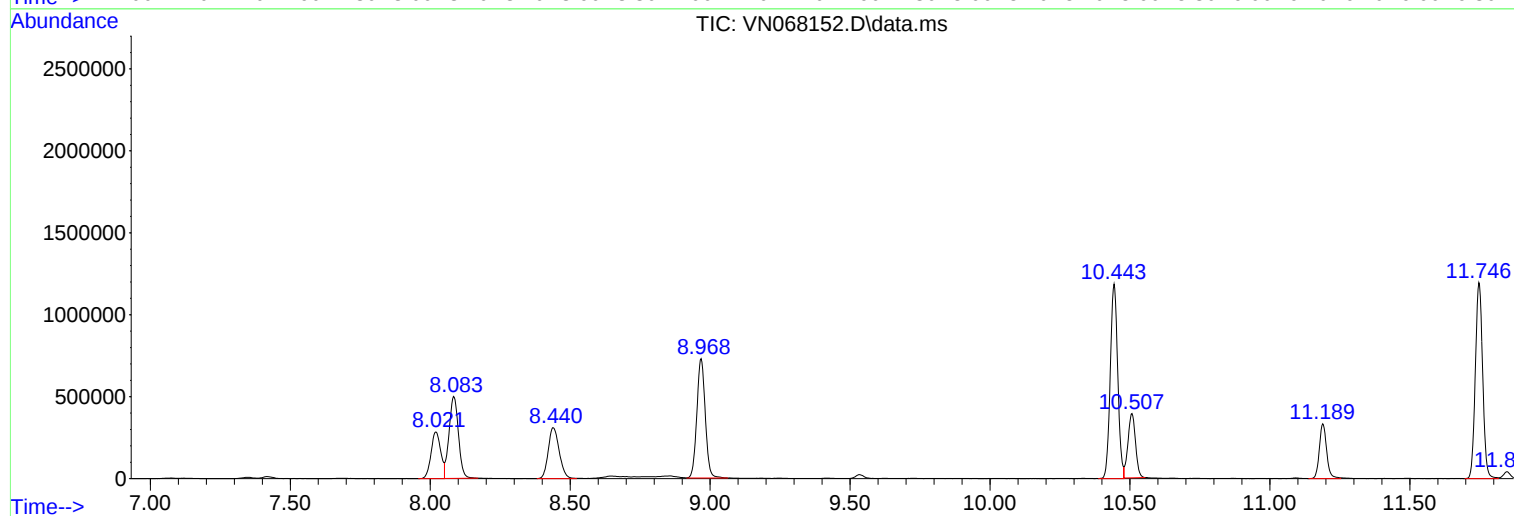
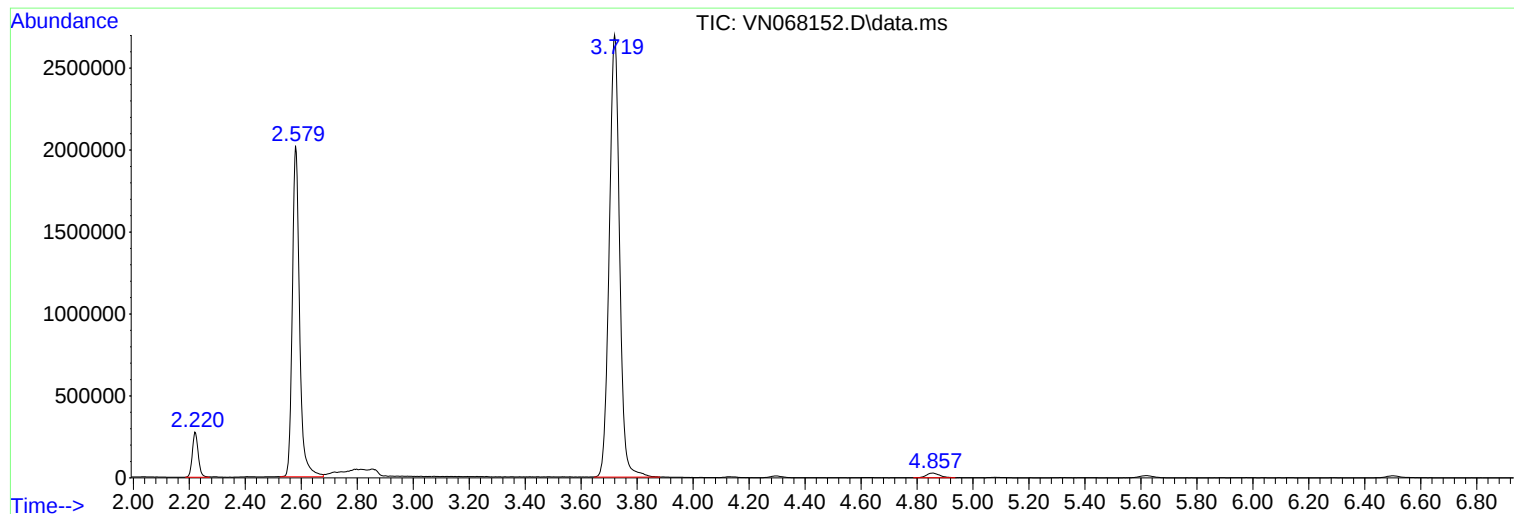
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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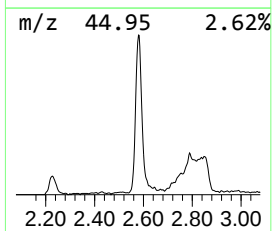
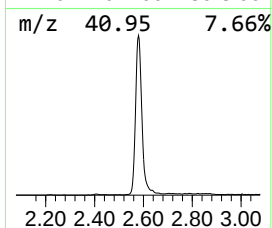
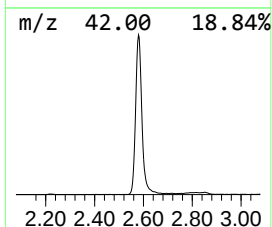
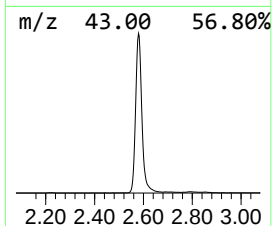
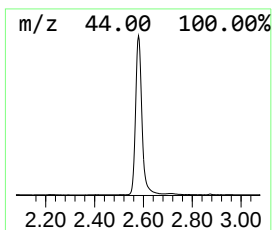
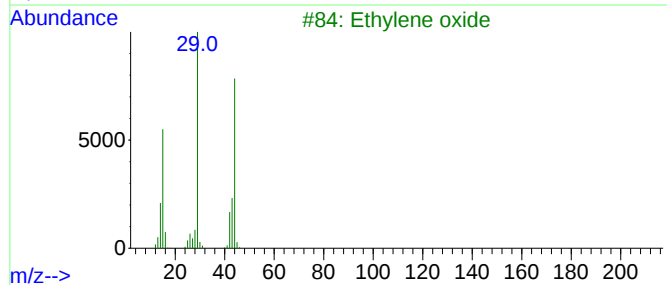
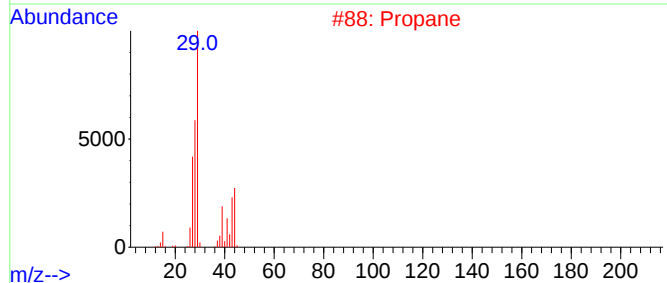
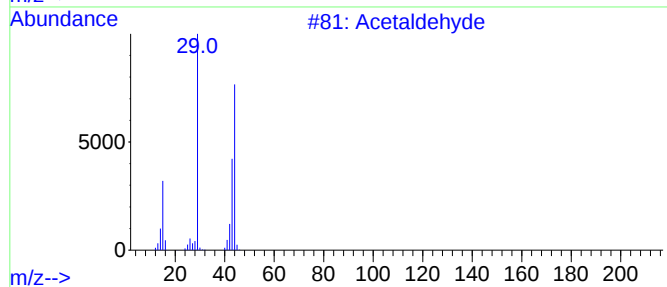
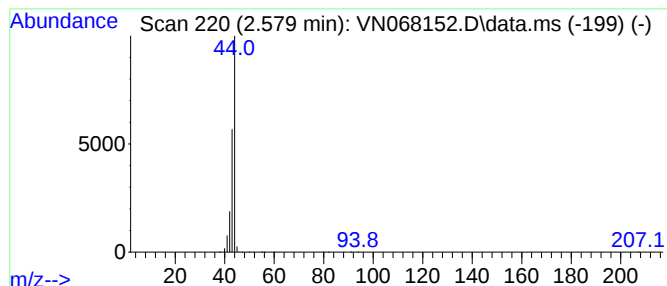
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.579	157.39 ug/l	3639770	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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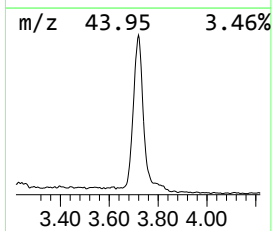
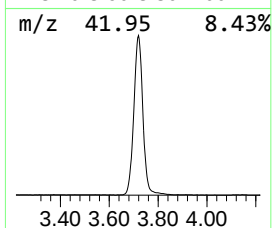
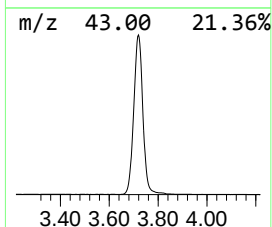
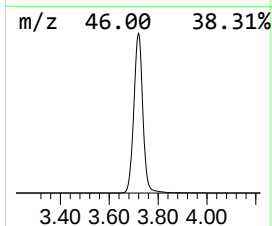
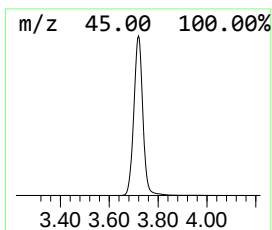
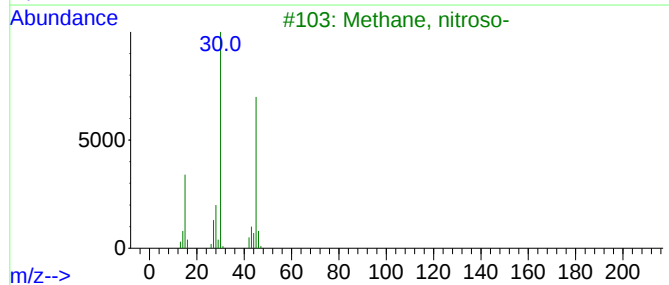
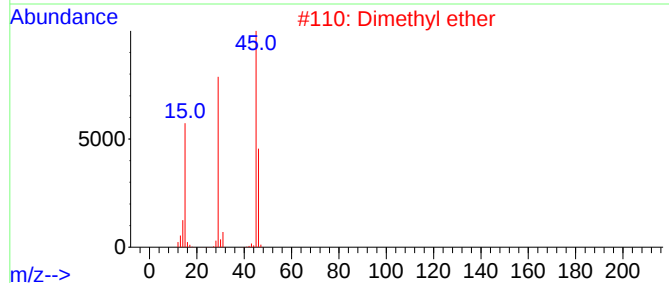
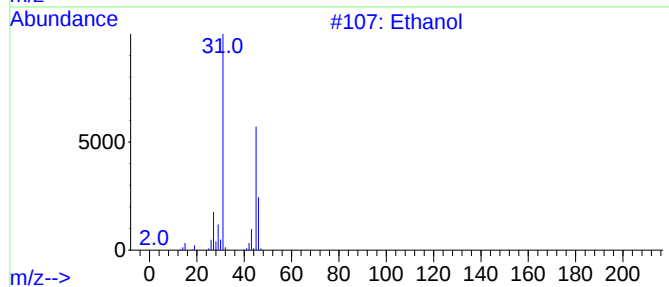
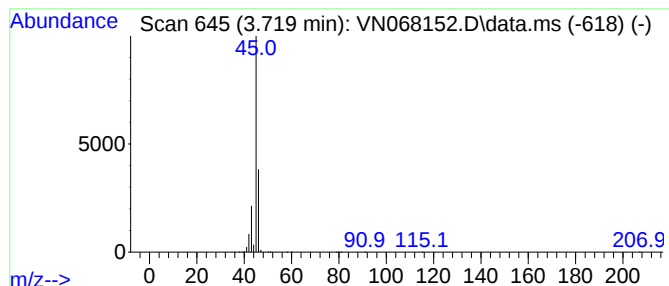
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081721W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.719	298.77 ug/l	6909410	Pentafluorobenzene	8.086

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		Methane, nitroso-	45	CH3NO	000865-40-7	4
4		Formic acid	46	CH2O2	000064-18-6	4
5		L-Lactic acid	90	C3H6O3	000079-33-4	2



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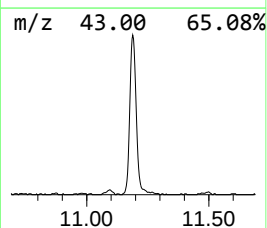
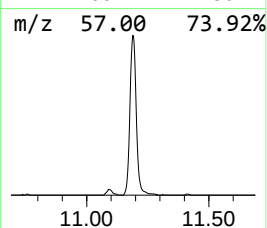
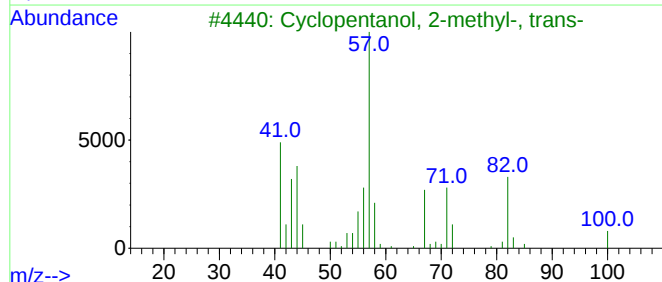
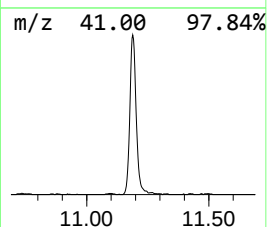
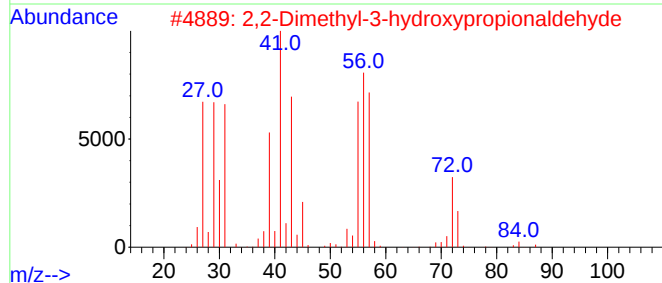
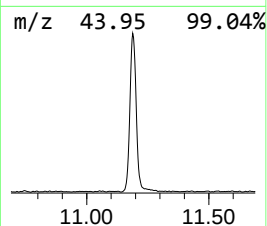
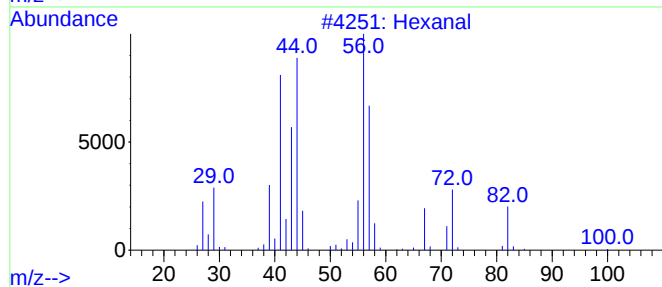
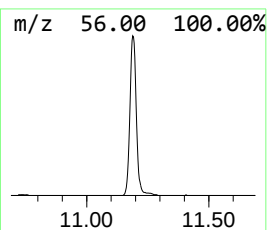
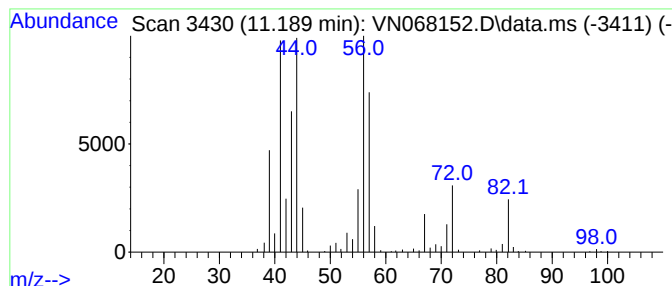
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Peak Number 4 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.189	13.91 ug/l	607377	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	81
2			2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	38
3			Cyclopentanol, 2-methyl-, trans-	100	C6H12O	025144-04-1	35
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	32
5			Glutaraldehyde	100	C5H8O2	000111-30-8	30



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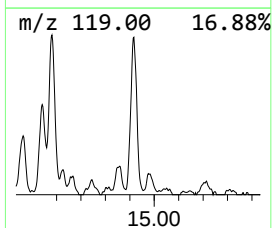
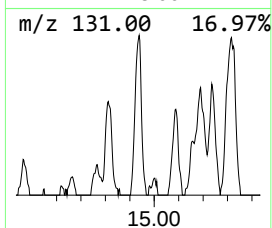
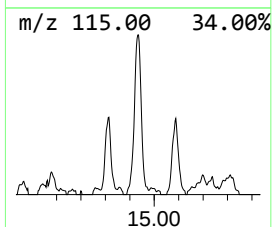
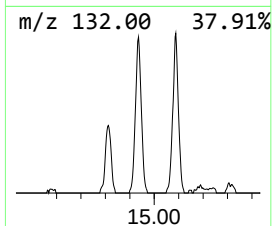
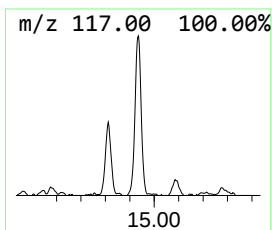
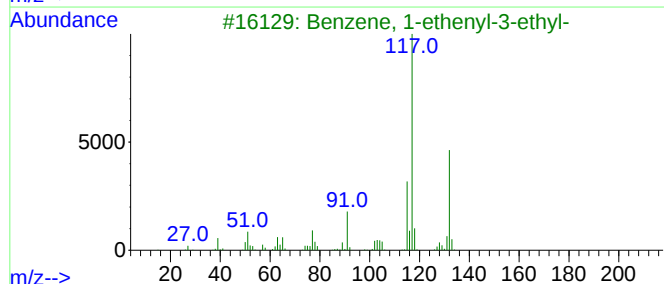
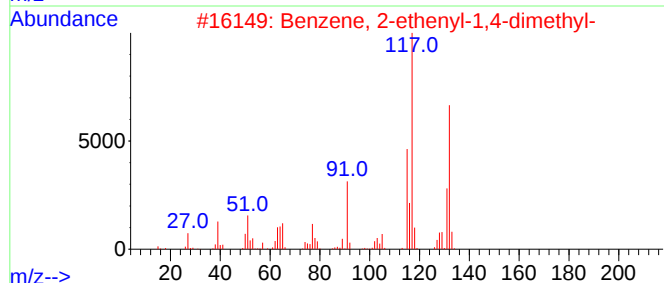
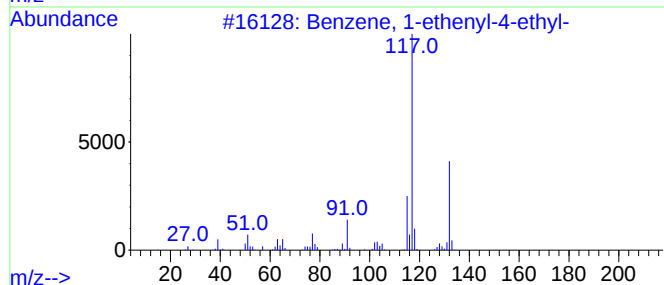
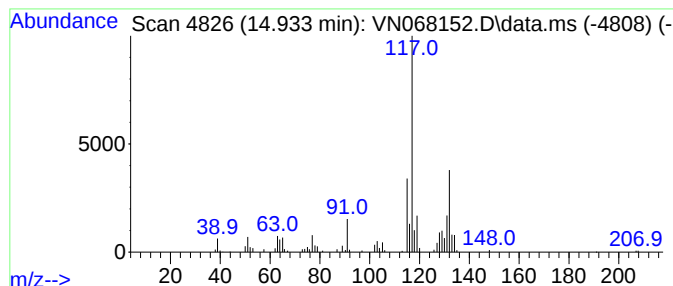
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	5.42 ug/l	210197	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
4			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	87
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.579	157.4	ug/l	3639770	1	8.086	1156320	50.0
Ethanol	3.719	298.8	ug/l	6909410	1	8.086	1156320	50.0
Hexanal	11.189	13.9	ug/l	607377	3	11.746	2182940	50.0
Benzene, 1-ethe...	14.933	5.4	ug/l	210197	4	13.678	1937570	50.0