

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062122\
 Data File : VU049323.D
 Acq On : 21 Jun 2022 13:32
 Operator : SY/MD
 Sample : N3400-19
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AF4

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

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_U\Method\SFAMUTR061422WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU049323.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	71	80	93	rBV	58161	70174	6.15%	1.020%
2	1.916	171	179	189	rVB	44810	57079	5.01%	0.830%
3	2.568	370	382	395	rBV	84016	134249	11.77%	1.951%
4	2.652	395	408	437	rVV	30720	92631	8.12%	1.346%
5	3.237	562	590	655	rBV2	83227	579979	50.86%	8.430%
6	4.440	942	964	991	rBV	302905	806849	70.75%	11.727%
7	4.639	1011	1026	1071	rBV3	91733	309938	27.18%	4.505%
8	5.063	1143	1158	1176	rBV	86382	189816	16.64%	2.759%
9	5.388	1247	1259	1270	rVB6	5517	11700	1.03%	0.170%
10	5.726	1343	1364	1387	rBV3	167150	436851	38.31%	6.349%
11	6.250	1513	1527	1553	rBV	170455	325726	28.56%	4.734%
12	6.690	1650	1664	1687	rBV	110803	217263	19.05%	3.158%
13	7.128	1782	1800	1836	rBV	454525	1140428	100.00%	16.576%
14	7.565	1919	1936	1954	rBV2	55275	100437	8.81%	1.460%
15	7.899	2027	2040	2056	rBV	193112	337168	29.57%	4.901%
16	8.179	2117	2127	2142	rBV	33284	57700	5.06%	0.839%
17	8.636	2255	2269	2301	rBV2	302476	615179	53.94%	8.941%
18	8.790	2307	2317	2330	rVB5	8125	15291	1.34%	0.222%
19	9.417	2498	2512	2531	rBV	237752	394854	34.62%	5.739%
20	10.758	2916	2929	2949	rVB	91874	150313	13.18%	2.185%
21	11.812	3244	3257	3279	rBV	250106	397093	34.82%	5.772%
22	12.063	3325	3335	3351	rBV	17419	33003	2.89%	0.480%
23	12.192	3364	3375	3390	rBV	206350	336287	29.49%	4.888%
24	14.317	4026	4036	4048	rBV2	35337	58259	5.11%	0.847%
25	16.770	4789	4799	4807	rBV8	6864	11843	1.04%	0.172%

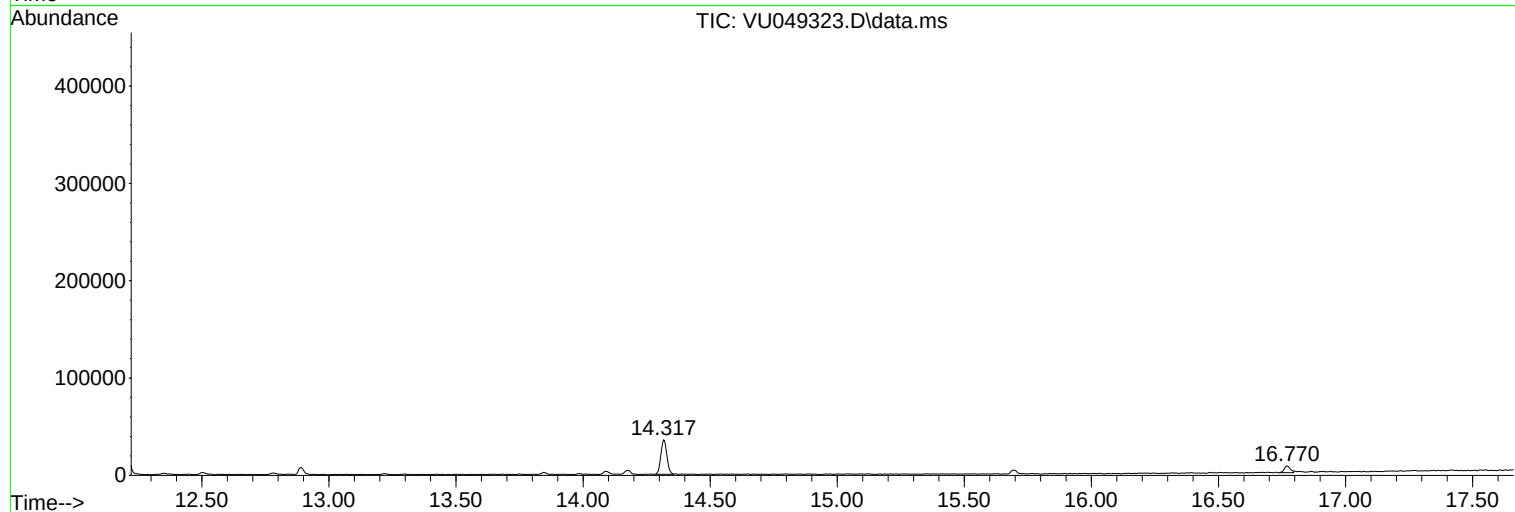
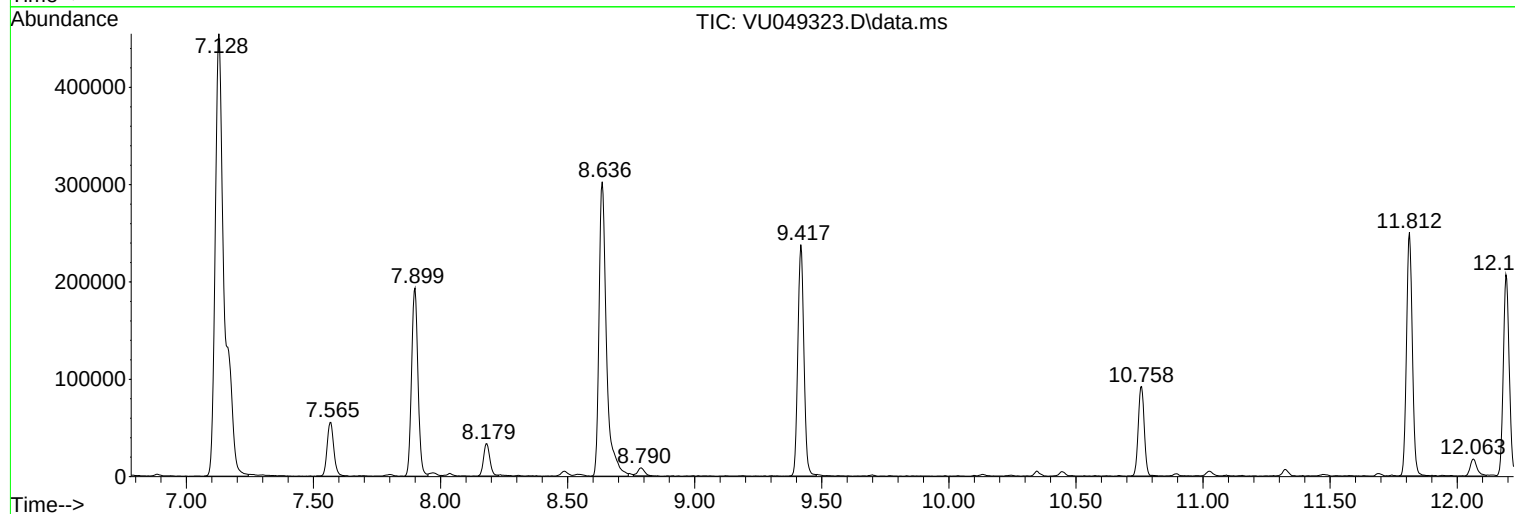
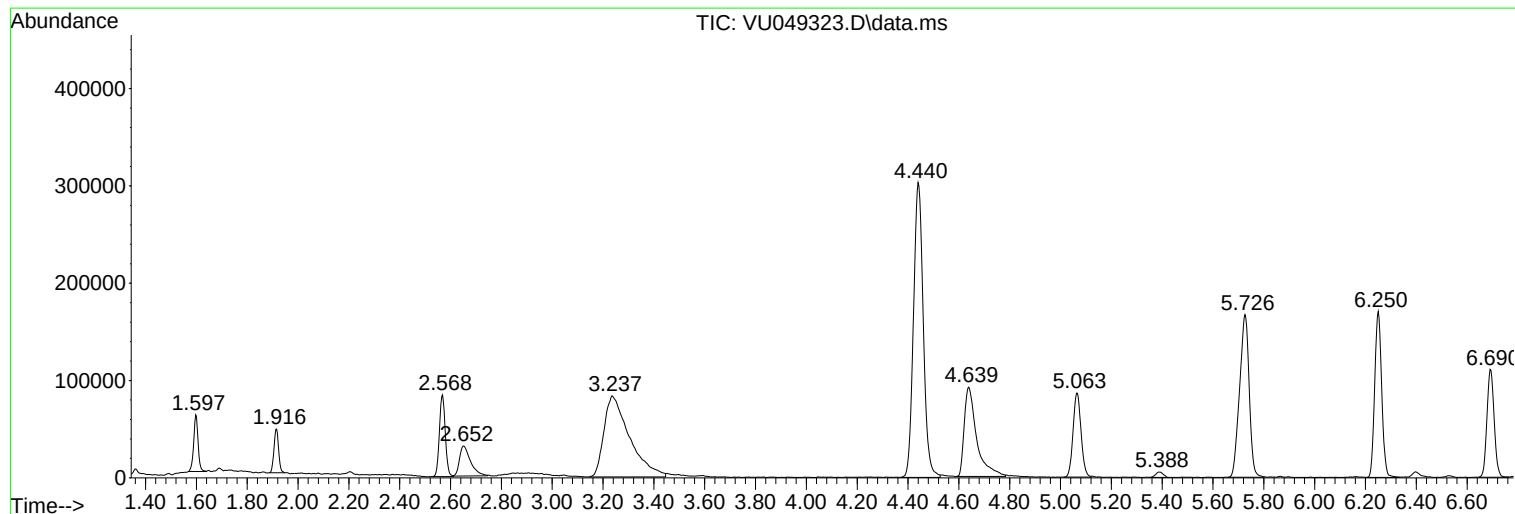
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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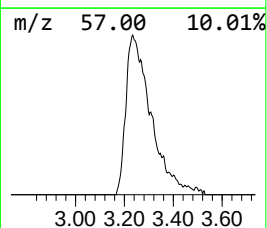
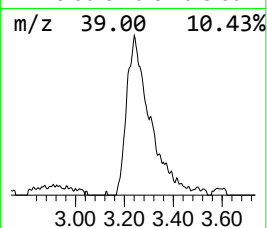
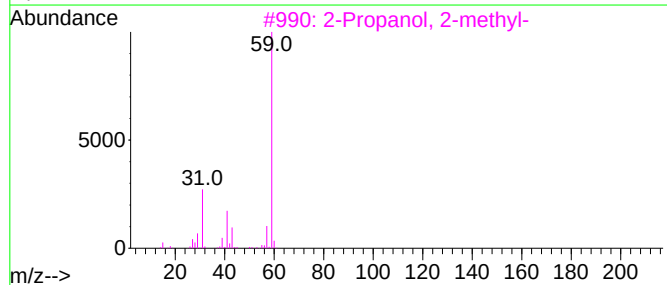
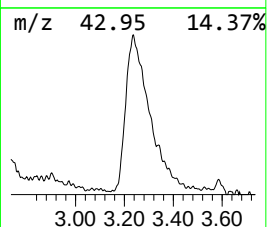
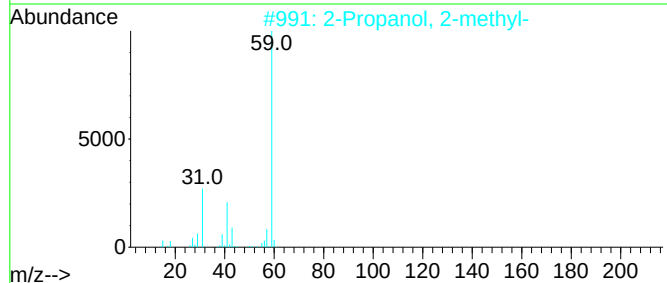
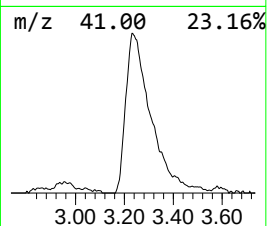
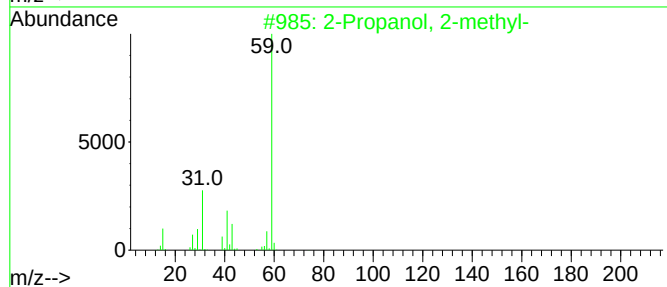
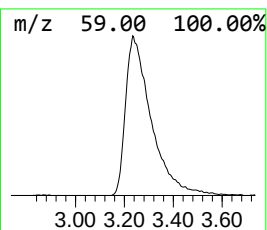
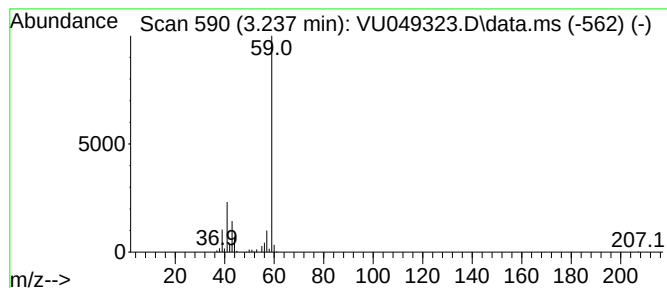
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.237	8.90 ug/L	579979	1,4-Difluorobenzene	6.250

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64	
2	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56	
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56	
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50	
5	3-Octanol	130	C8H18O	000589-98-0	43	



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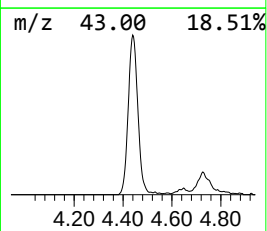
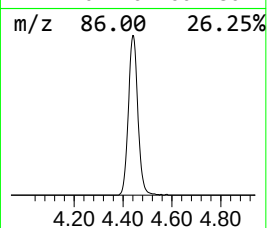
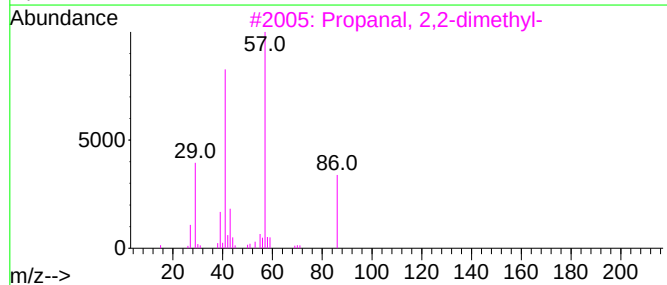
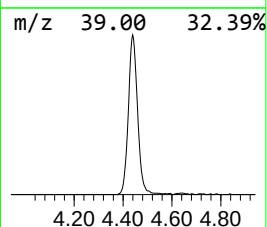
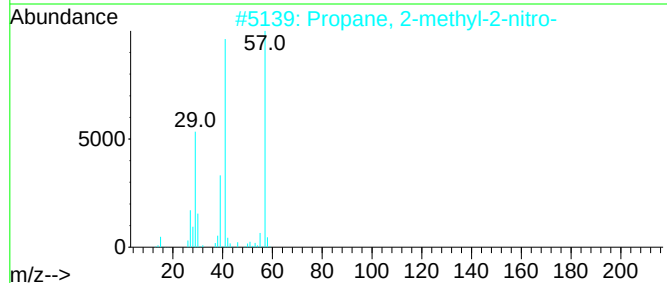
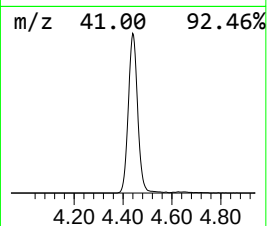
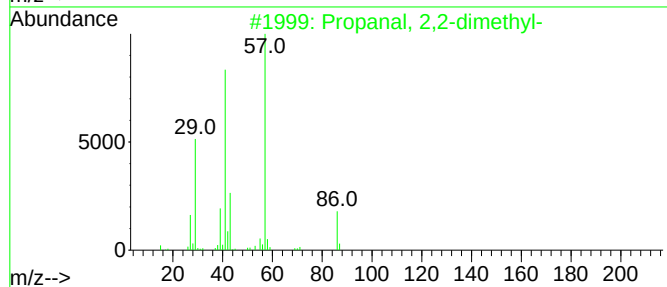
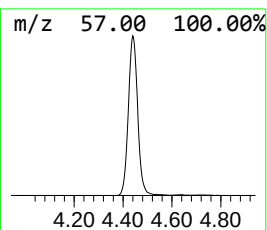
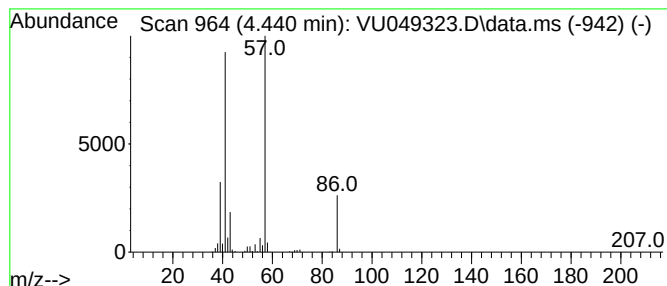
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Propanal, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.440	12.39 ug/L	806849	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	59
2			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	53
3			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	47
4			Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	45
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	43



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Instrument :
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ClientSampleId :
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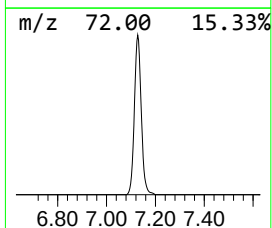
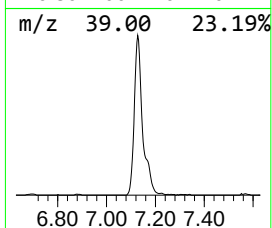
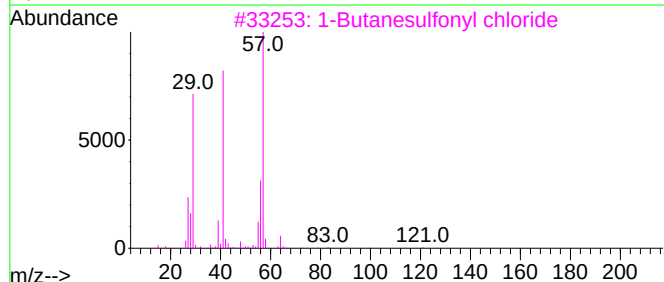
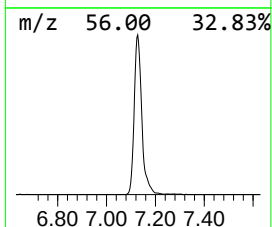
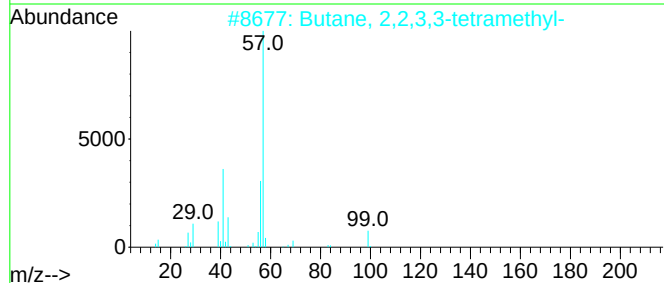
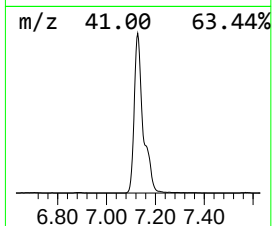
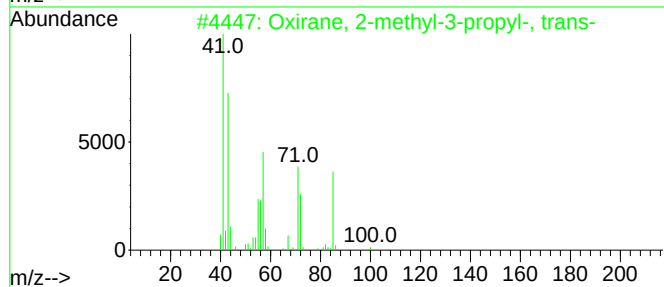
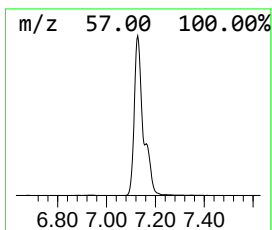
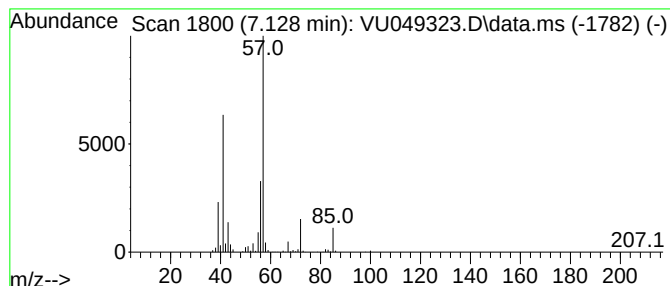
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.128	17.51 ug/L	1140430	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	43
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	38
3			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	38
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	35
5			1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	28



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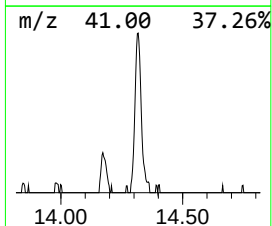
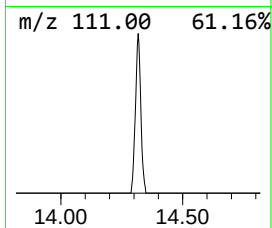
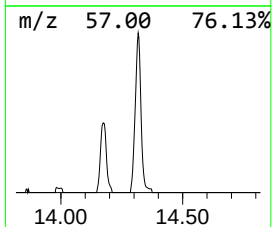
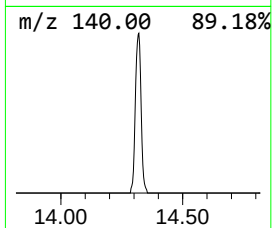
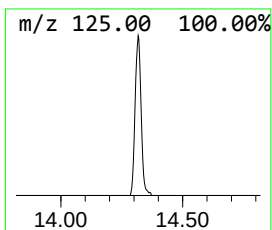
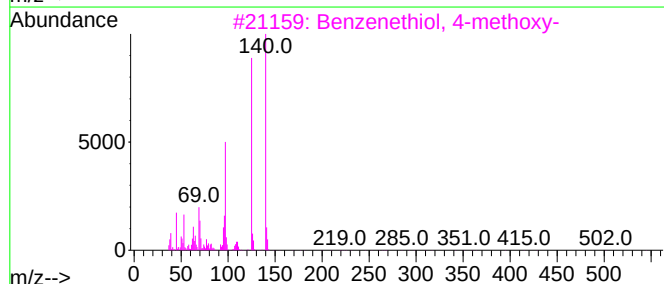
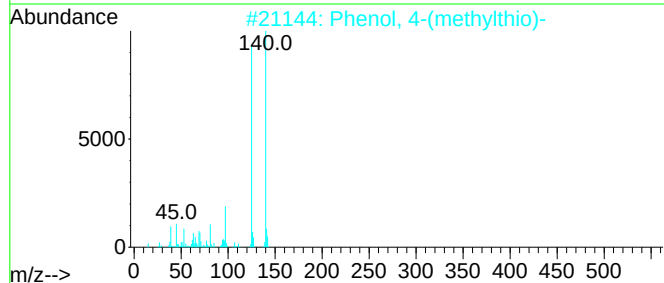
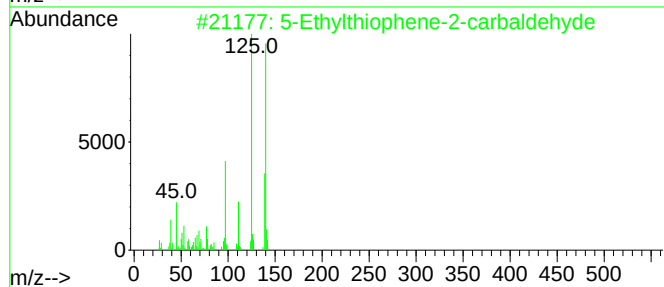
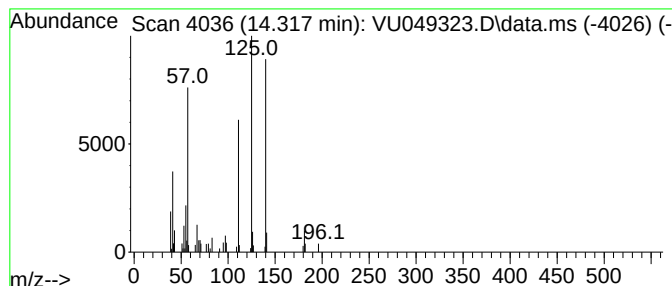
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 5-Ethylthiophene-2-carbalde... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.317	0.73 ug/L	58259	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Ethylthiophene-2-carbaldehyde	140	C7H8OS	036880-33-8	59
2			Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	53
3			Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	53
4			Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	53
5			1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanol, 2-m...	3.237	8.9	ug/L	579979	1	6.250	325726	5.0
Propanal, 2,2-d...	4.440	12.4	ug/L	806849	1	6.250	325726	5.0
unknown-01	7.128	17.5	ug/L	1140430	1	6.250	325726	5.0
5-Ethylthiophen...	14.317	0.7	ug/L	58259	3	11.812	397093	5.0