

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120523\
 Data File : VY016594.D
 Acq On : 05 Dec 2023 14:23
 Operator : SY/MD
 Sample : 05600-01
 Misc : 3.43g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 TOPSOIL-LKWD-DENALI-1

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_Y\methods\82Y120423S.M

Title : SW846 8260

Signal : TIC: VY016594.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.875	6	9	16	rVB2	13952	26732	3.54%	0.492%
2	2.253	69	71	77	rVB4	4828	9555	1.27%	0.176%
3	2.399	89	95	105	rBV	33604	64024	8.49%	1.179%
4	3.271	230	238	248	rBV2	31520	73037	9.68%	1.345%
5	3.844	325	332	341	rVB2	12078	31395	4.16%	0.578%
6	3.966	344	352	365	rBV	36561	106928	14.18%	1.968%
7	4.753	471	481	489	rVB4	17234	52093	6.91%	0.959%
8	5.600	613	620	621	rBV3	6652	10536	1.40%	0.194%
9	5.777	644	649	654	rVB4	4126	8082	1.07%	0.149%
10	7.014	846	852	858	rVB3	5000	11978	1.59%	0.220%
11	7.740	961	971	977	rBV	106879	252092	33.42%	4.641%
12	7.813	977	983	994	rVB	179469	406906	53.95%	7.491%
13	8.161	1033	1040	1051	rVB	106196	237047	31.43%	4.364%
14	8.417	1075	1082	1090	rBV2	17004	36273	4.81%	0.668%
15	8.575	1098	1108	1116	rBV3	14948	37511	4.97%	0.691%
16	8.709	1122	1130	1138	rBV	271814	532875	70.65%	9.809%
17	9.282	1217	1224	1233	rBV	65757	128600	17.05%	2.367%
18	10.197	1364	1374	1381	rBV	421193	754237	100.00%	13.884%
19	10.258	1381	1384	1392	rVB	29050	50135	6.65%	0.923%
20	10.593	1435	1439	1444	rBV3	5743	9024	1.20%	0.166%
21	10.953	1491	1498	1510	rBV	393934	655397	86.90%	12.065%
22	11.508	1581	1589	1599	rVB	407766	658426	87.30%	12.121%
23	11.727	1617	1625	1634	rBV3	10204	26399	3.50%	0.486%
24	11.825	1639	1641	1649	rVB4	4959	8489	1.13%	0.156%
25	12.227	1702	1707	1715	rVB2	22580	36069	4.78%	0.664%
26	12.501	1745	1752	1760	rVB	317168	518401	68.73%	9.543%
27	12.824	1802	1805	1809	rVV3	7393	11465	1.52%	0.211%
28	12.989	1827	1832	1836	rVB4	5053	8898	1.18%	0.164%
29	13.288	1875	1881	1888	rBV4	14899	28362	3.76%	0.522%
30	13.391	1890	1898	1901	rBV4	6981	12963	1.72%	0.239%
31	13.440	1901	1906	1915	rVB	350550	563243	74.68%	10.369%
32	13.751	1954	1957	1963	rVB2	7013	10505	1.39%	0.193%
33	13.977	1988	1994	2001	rVB4	17040	30112	3.99%	0.554%
34	14.220	2029	2034	2039	rBV2	9740	16607	2.20%	0.306%
35	15.025	2162	2166	2170	rVB2	4653	7853	1.04%	0.145%

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TOPSOIL-LKWD-DENALI-1

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_Y\methods\82Y120423S.M
Title : SW846 8260

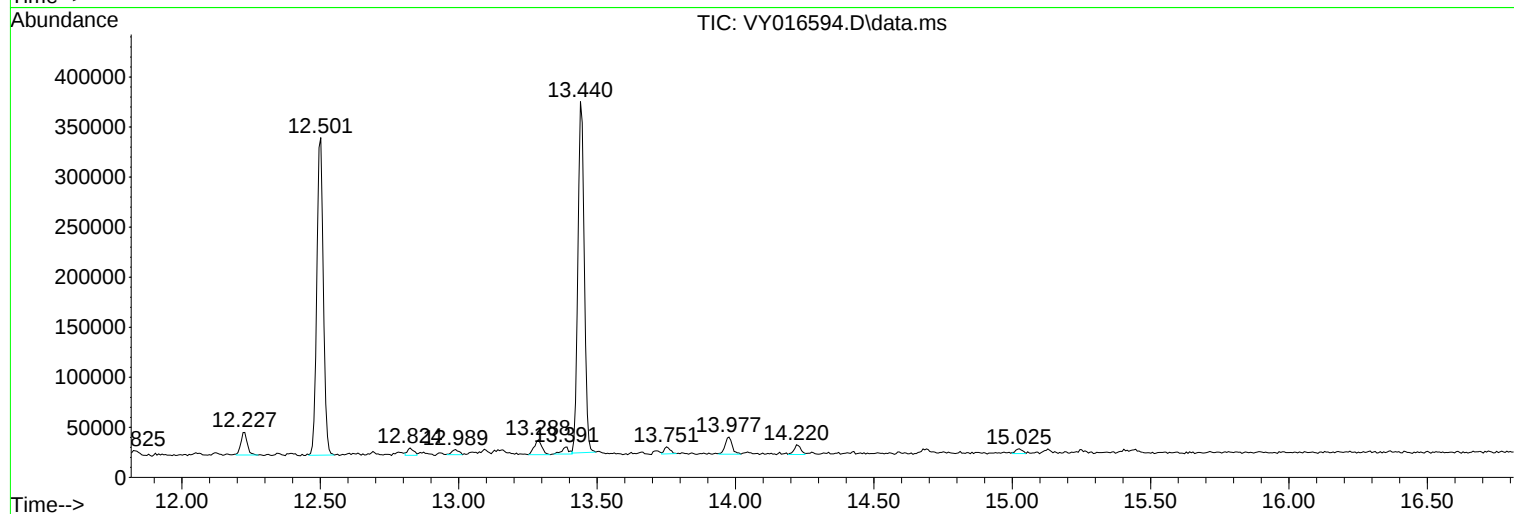
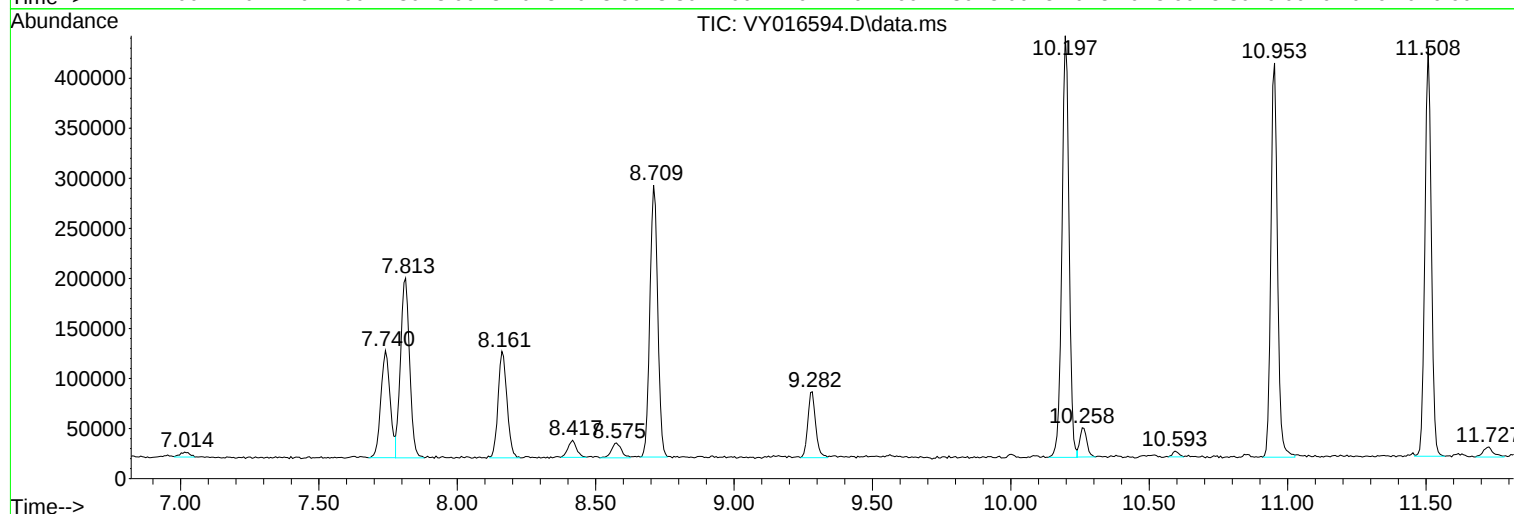
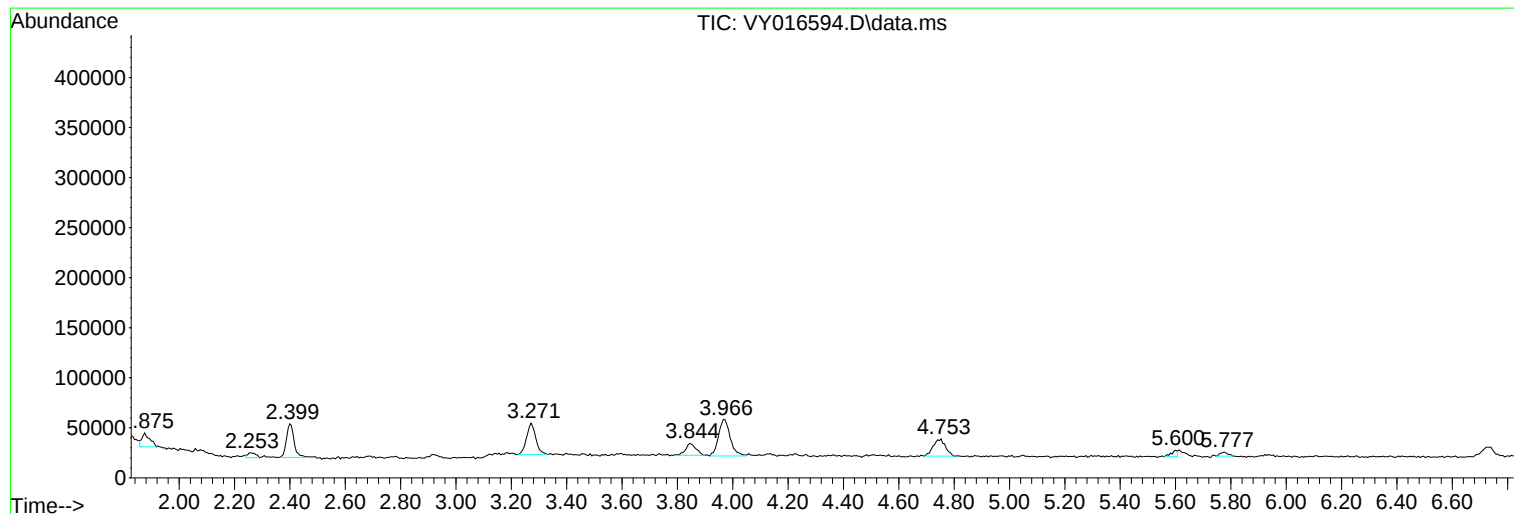
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y120423S.M
Quant Title : SW846 8260

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



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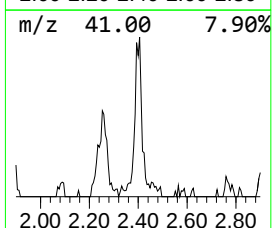
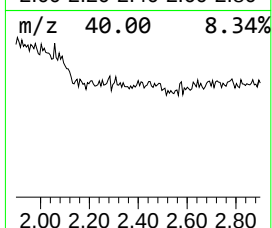
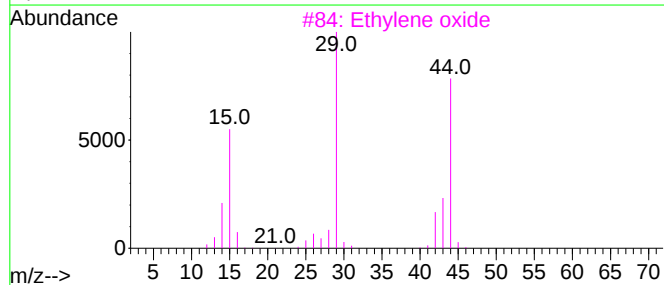
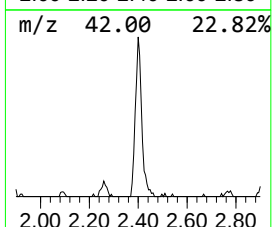
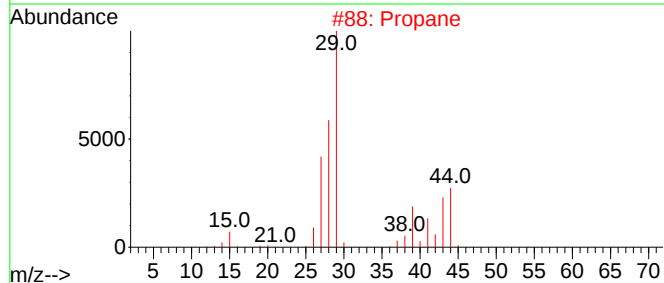
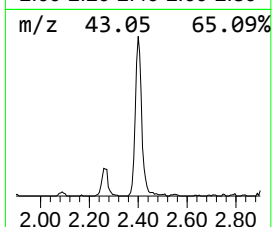
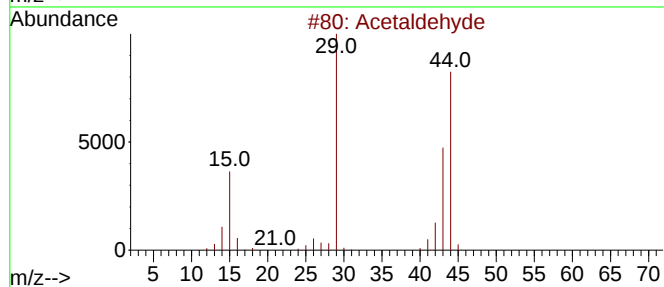
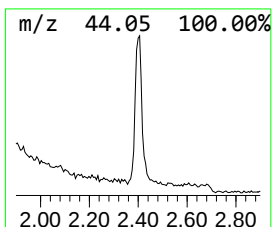
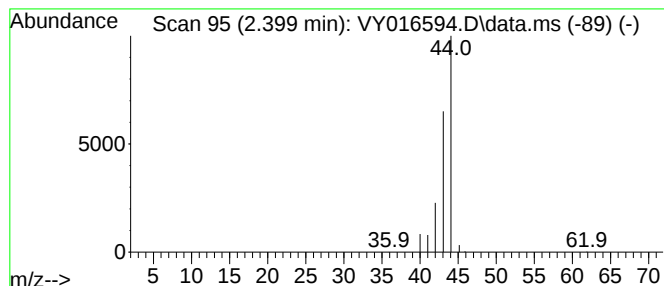
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y120423S.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	7.87 ug/l	64024	Pentafluorobenzene	7.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Propane	44	C3H8	000074-98-6	7
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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Instrument :
MSVOA_Y
ClientSampleId :
TOPSOIL-LKWD-DENALI-1

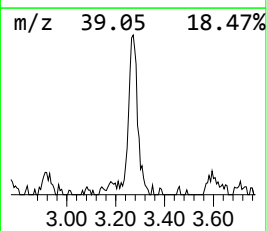
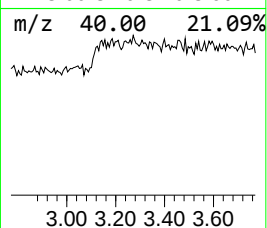
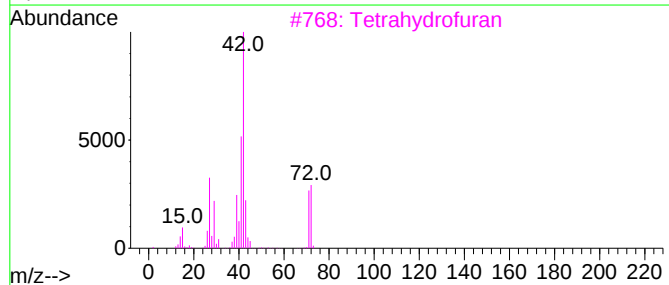
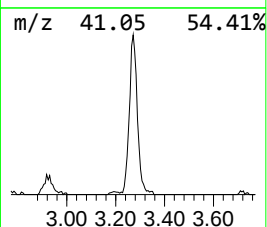
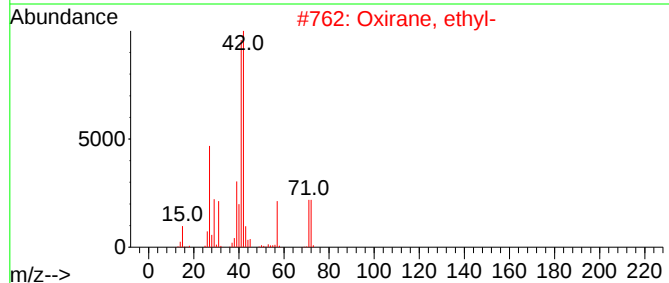
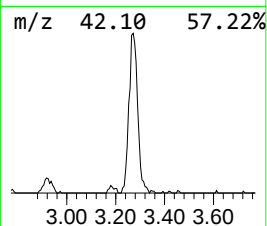
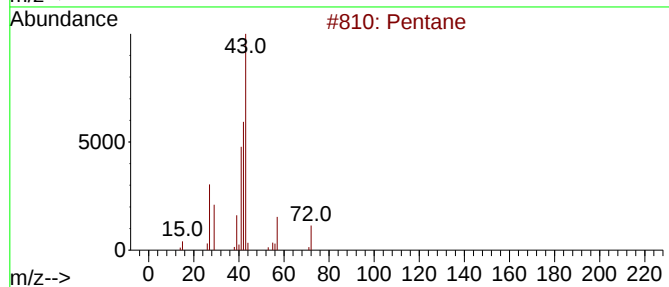
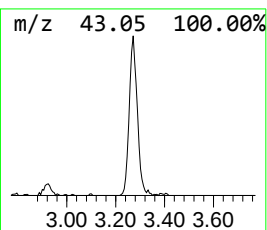
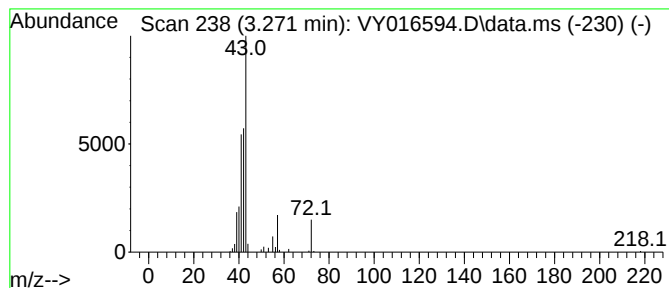
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y120423S.M
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.271	8.97 ug/l	73037	Pentafluorobenzene	7.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	86
2			Oxirane, ethyl-	72	C4H8O	000106-88-7	53
3			Tetrahydrofuran	72	C4H8O	000109-99-9	47
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	43
5			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	39



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TOPSOIL-LKWD-DENALI-1

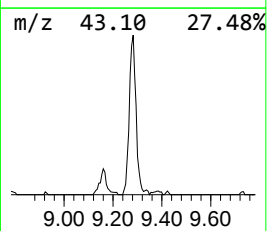
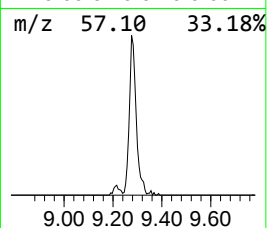
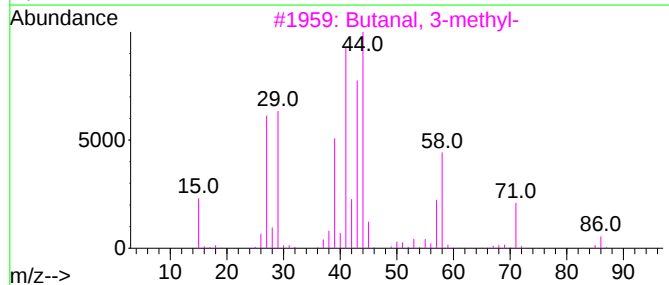
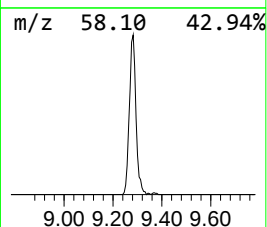
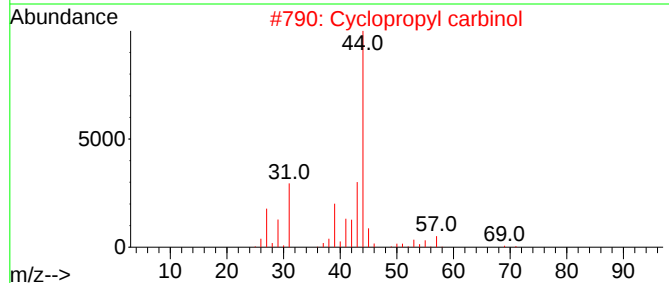
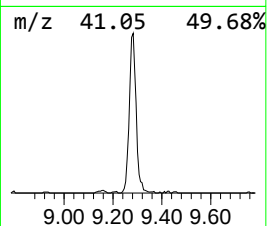
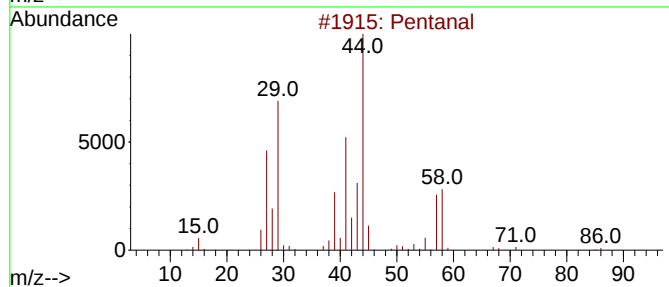
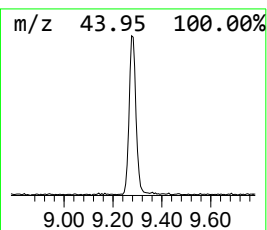
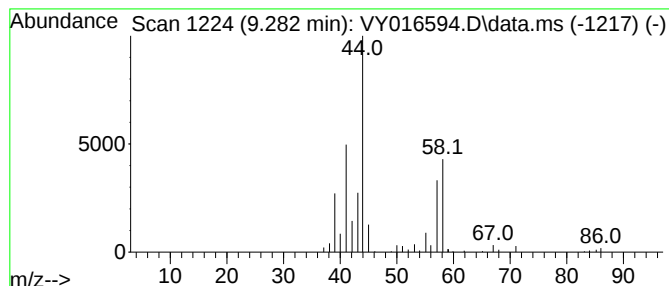
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.282	12.07 ug/l	128600	1,4-Difluorobenzene	8.709

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	90
2			Cyclopropyl carbinol	72	C4H8O	002516-33-8	53
3			Butanal, 3-methyl-	86	C5H10O	000590-86-3	53
4			1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	43
5			2-Formylhistamine	139	C6H9N3O	1000132-95-8	9



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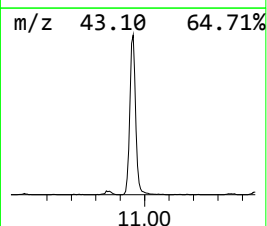
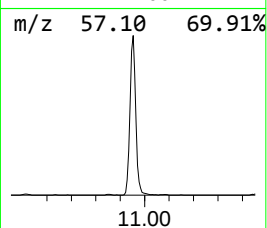
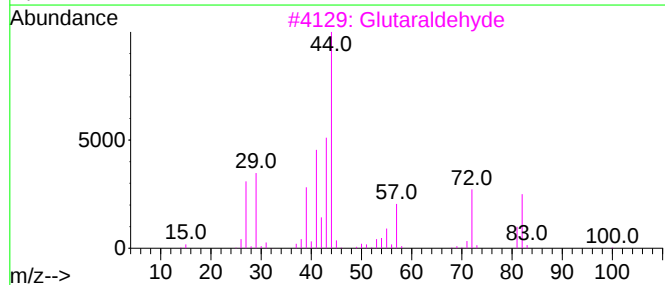
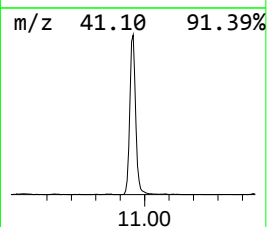
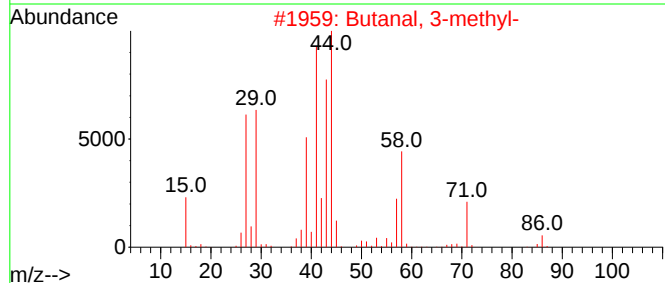
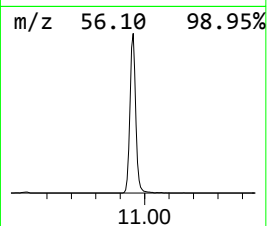
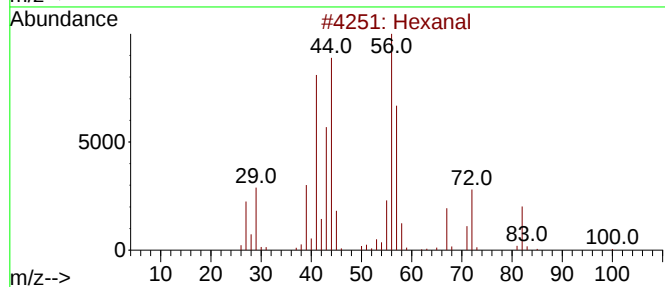
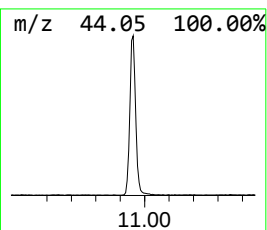
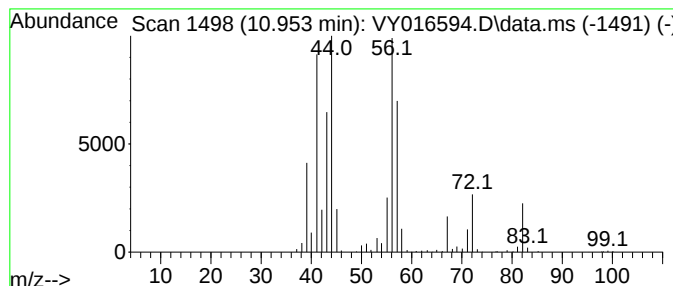
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.953	49.77 ug/l	655397	Chlorobenzene-d5	11.508

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	95
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	32
3			Glutaraldehyde	100	C5H8O2	000111-30-8	30
4			Butanal	72	C4H8O	000123-72-8	22
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	14



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.399	7.9	ug/l	64024	1	7.813	406906	50.0
Pentane	3.271	9.0	ug/l	73037	1	7.813	406906	50.0
Pentanal	9.282	12.1	ug/l	128600	2	8.709	532875	50.0
Hexanal	10.953	49.8	ug/l	655397	3	11.508	658426	50.0