

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111522\
 Data File : VY011456.D
 Acq On : 15 Nov 2022 14:28
 Operator : KP/MD
 Sample : N5417-02
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 AUD-1732

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\82Y111022S.M
 Title : SW846 8260

Signal : TIC: VY011456.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.863	3	7	14	rVB2	5162	8862	1.72%	0.196%
2	2.223	60	66	77	rVB2	14729	25872	5.03%	0.571%
3	2.387	88	93	102	rVB	35145	60111	11.70%	1.327%
4	2.534	109	117	122	rBV8	2744	7214	1.40%	0.159%
5	3.826	321	329	339	rBV2	10221	27343	5.32%	0.604%
6	3.948	339	349	369	rVB	56165	155074	30.17%	3.424%
7	4.418	417	426	432	rBV3	1849	5899	1.15%	0.130%
8	4.722	463	476	489	rBV	71462	222738	43.34%	4.919%
9	5.911	661	671	678	rBV	3592	9552	1.86%	0.211%
10	6.704	792	801	813	rBV2	20023	59780	11.63%	1.320%
11	6.984	837	847	859	rBV2	35357	110021	21.41%	2.430%
12	7.722	958	968	974	rBV	124616	299280	58.24%	6.609%
13	7.795	974	980	992	rVB	132348	299177	58.22%	6.607%
14	8.143	1024	1037	1050	rBV	123890	274576	53.43%	6.063%
15	8.393	1067	1078	1087	rVB2	8397	18802	3.66%	0.415%
16	8.551	1096	1104	1111	rBV4	5216	11957	2.33%	0.264%
17	8.691	1120	1127	1137	rVV	238179	457127	88.95%	10.094%
18	9.136	1193	1200	1210	rBV	20724	41482	8.07%	0.916%
19	9.264	1214	1221	1234	rBV	33531	70678	13.75%	1.561%
20	10.075	1347	1354	1361	rBV	10495	18305	3.56%	0.404%
21	10.179	1361	1371	1378	rBV	287240	513917	100.00%	11.348%
22	10.246	1378	1382	1386	rVB	5327	8617	1.68%	0.190%
23	10.374	1393	1403	1408	rBV8	3153	8727	1.70%	0.193%
24	10.435	1408	1413	1416	rVV2	6522	12416	2.42%	0.274%
25	10.490	1416	1422	1430	rVV3	12470	32038	6.23%	0.707%
26	10.581	1430	1437	1447	rVB2	7737	18824	3.66%	0.416%
27	10.721	1456	1460	1468	rVB5	2889	5184	1.01%	0.114%
28	10.837	1471	1479	1486	rBV2	12975	22864	4.45%	0.505%
29	10.935	1489	1495	1504	rBV2	52751	94307	18.35%	2.083%
30	11.319	1553	1558	1564	rVB3	3461	5968	1.16%	0.132%
31	11.490	1578	1586	1597	rBV	221622	363188	70.67%	8.020%
32	11.593	1597	1603	1609	rBV2	7652	13740	2.67%	0.303%
33	11.703	1615	1621	1626	rBV2	23231	46884	9.12%	1.035%
34	11.813	1633	1639	1645	rBV5	4735	9124	1.78%	0.201%
35	11.965	1657	1664	1670	rBV4	4692	8681	1.69%	0.192%
36	12.026	1670	1674	1682	rVB2	22148	36123	7.03%	0.798%

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37	12.105	1682	1687	1691	rBV	9500	15820	3.08%	0.349%
38	12.209	1698	1704	1713	rBV	31328	48849	9.51%	1.079%
39	12.483	1743	1749	1762	rVB2	169958	275328	53.57%	6.080%
40	12.593	1762	1767	1773	rBV	23204	40924	7.96%	0.904%
41	12.764	1788	1795	1799	rBV3	11299	20767	4.04%	0.459%
42	12.812	1799	1803	1816	rVB3	13995	30277	5.89%	0.669%
43	12.928	1817	1822	1824	rBV6	4430	7277	1.42%	0.161%
44	12.965	1825	1828	1834	rVB8	4630	7291	1.42%	0.161%
45	13.032	1834	1839	1844	rVB4	7289	12455	2.42%	0.275%
46	13.087	1844	1848	1852	rBV5	6047	9248	1.80%	0.204%
47	13.172	1858	1862	1873	rVB5	5376	12202	2.37%	0.269%
48	13.270	1873	1878	1885	rBV	22029	35004	6.81%	0.773%
49	13.428	1898	1904	1913	rBV	124600	195954	38.13%	4.327%
50	13.526	1914	1920	1929	rBV	154501	239692	46.64%	5.293%
51	13.751	1952	1957	1961	rBV6	6447	12184	2.37%	0.269%
52	13.788	1961	1963	1971	rVB9	3588	6373	1.24%	0.141%
53	13.898	1977	1981	1987	rBV9	4085	8308	1.62%	0.183%
54	13.965	1987	1992	1997	rVB3	8815	16627	3.24%	0.367%
55	14.209	2027	2032	2036	rBV2	15808	21747	4.23%	0.480%
56	14.611	2095	2098	2104	rVB6	5344	7133	1.39%	0.158%
57	14.684	2104	2110	2114	rBV7	7229	15931	3.10%	0.352%
58	14.733	2114	2118	2125	rVB9	4699	9271	1.80%	0.205%
59	15.062	2164	2172	2177	rBV9	7173	17908	3.48%	0.395%
60	15.294	2206	2210	2211	rBV4	3952	5224	1.02%	0.115%
61	15.434	2230	2233	2237	rVB5	5520	6479	1.26%	0.143%
62	15.733	2277	2282	2288	rVB6	9760	18258	3.55%	0.403%
63	16.037	2326	2332	2337	rVB8	5143	11595	2.26%	0.256%
64	16.226	2356	2363	2370	rVV10	4744	13382	2.60%	0.296%
65	16.287	2370	2373	2379	rVV4	4287	8512	1.66%	0.188%
66	16.354	2382	2384	2393	rVB9	4025	8030	1.56%	0.177%
67	16.635	2423	2430	2435	rBV10	2758	6019	1.17%	0.133%

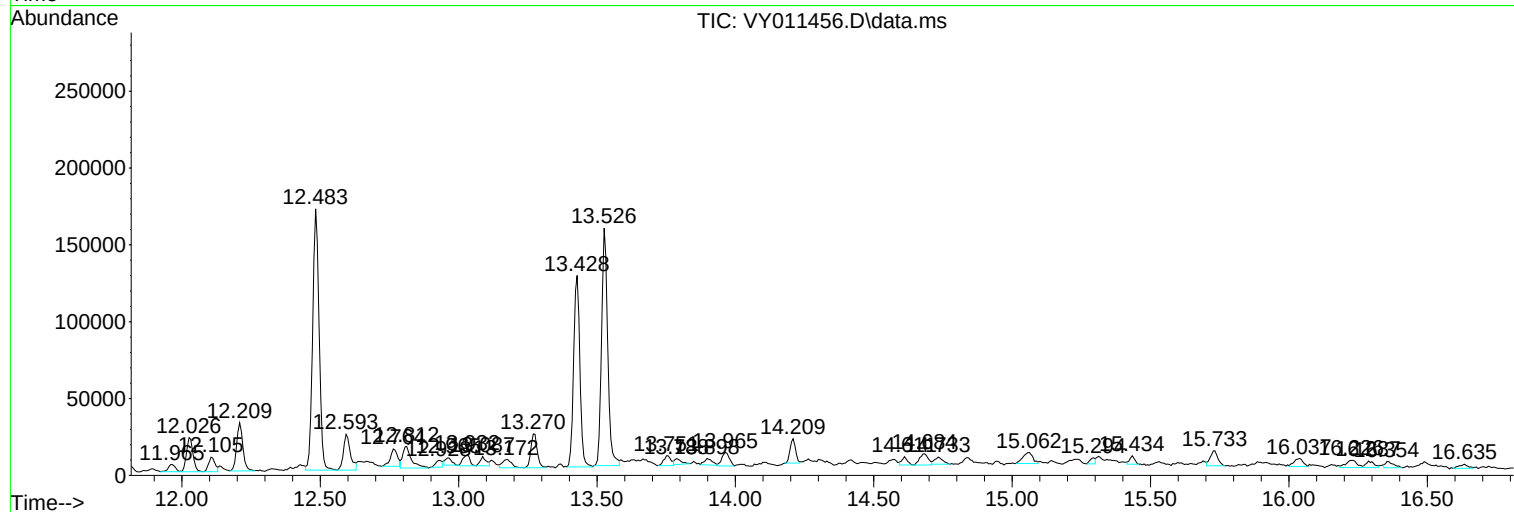
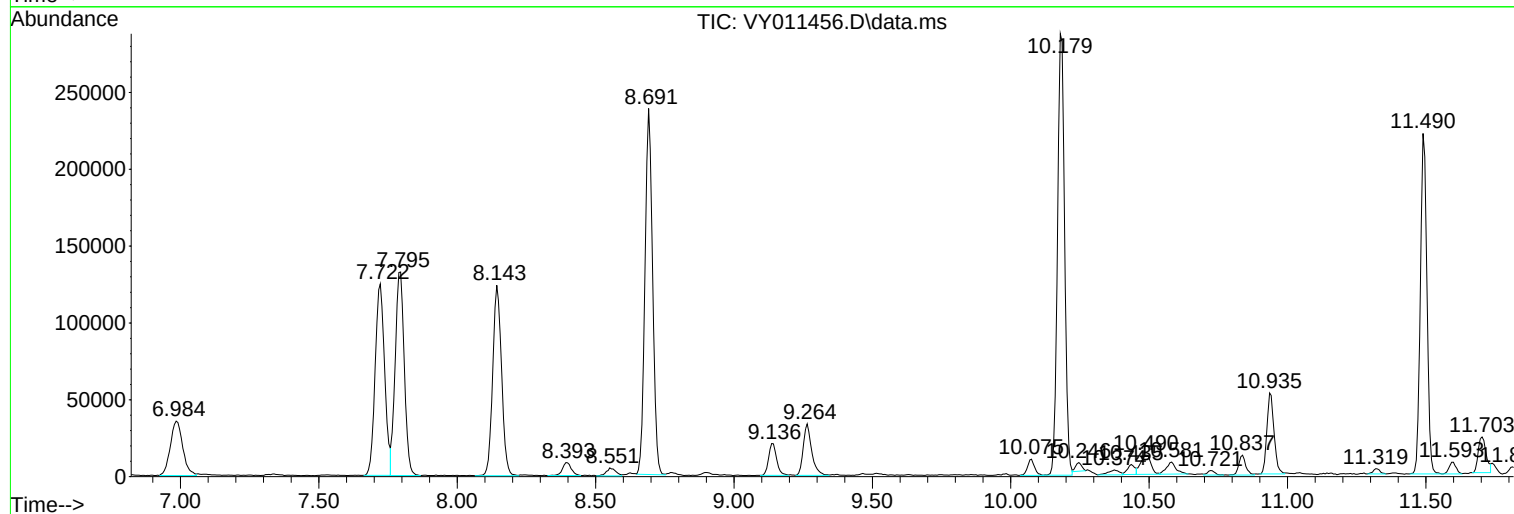
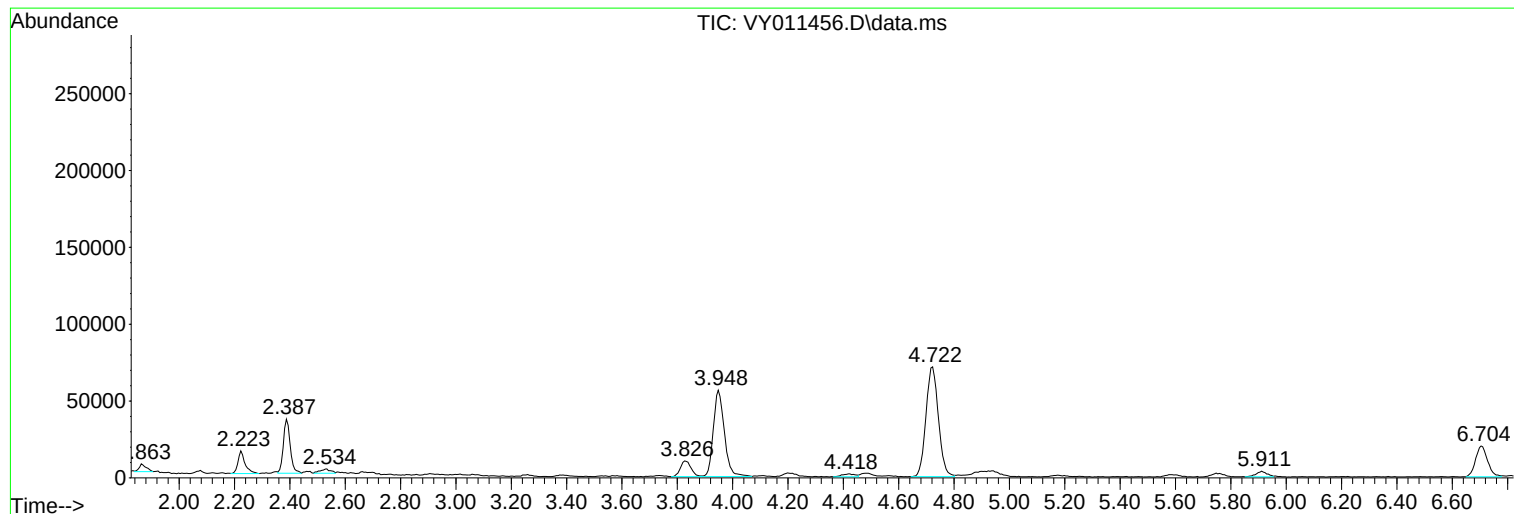
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111022S.M
Quant Title : SW846 8260

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



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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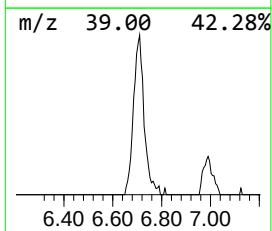
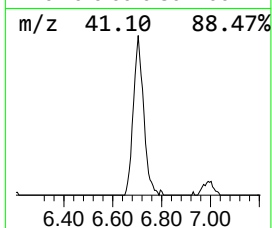
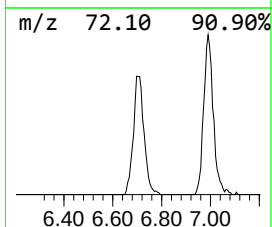
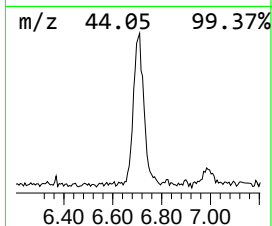
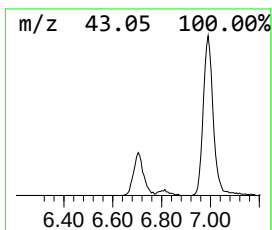
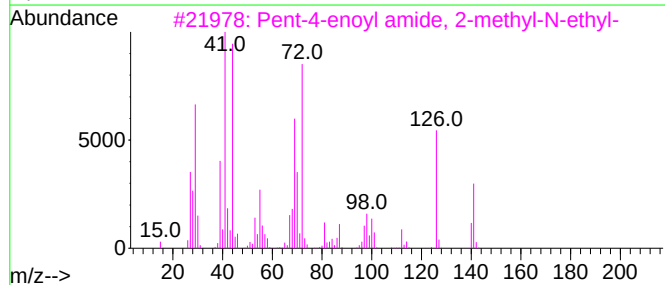
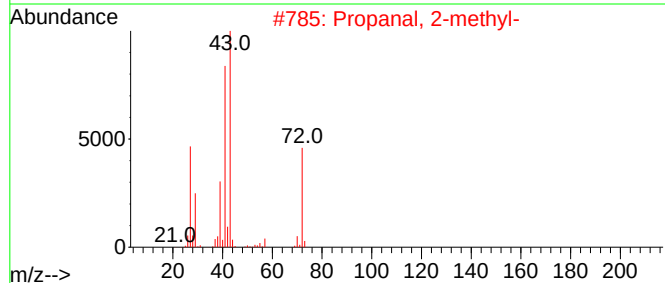
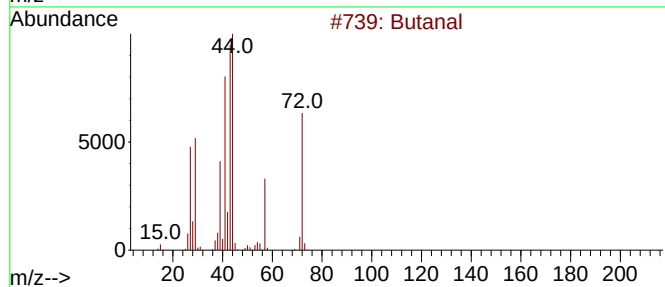
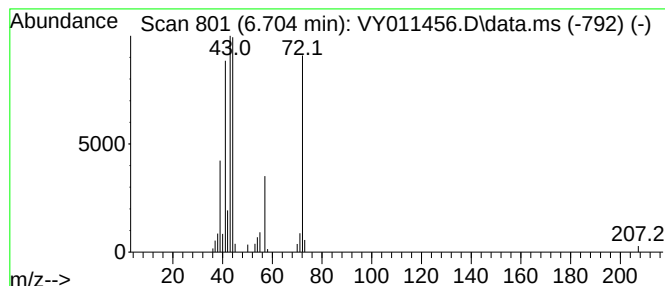
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Quant Title : SW846 8260

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

Peak Number 2 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.704	9.99 ug/l	59780	Pentafluorobenzene	7.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3			Pent-4-enoyl amide, 2-methyl-N-e...	141	C8H15NO	1000420-35-1	39
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5			Furazan-3,4-diol	102	C2H2N2O3	143876-06-6	33



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Instrument :
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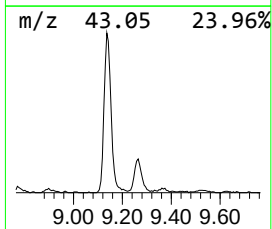
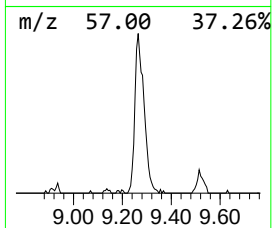
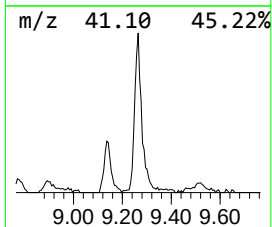
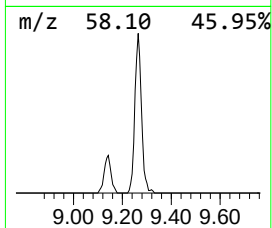
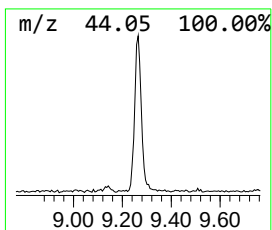
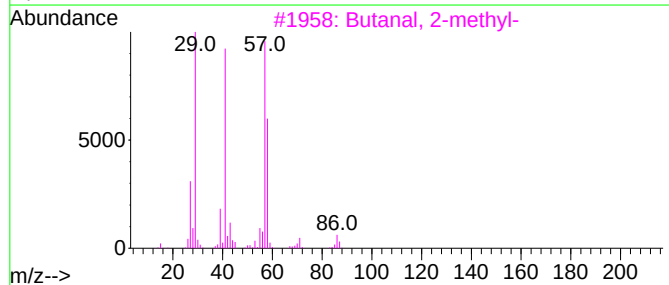
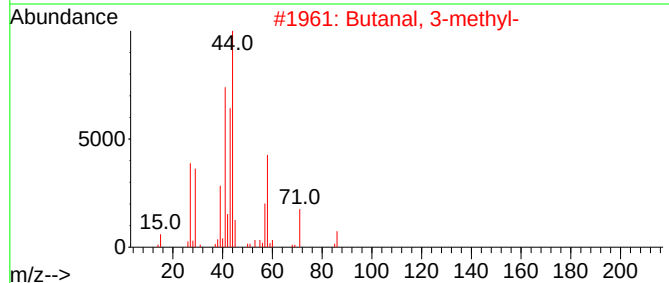
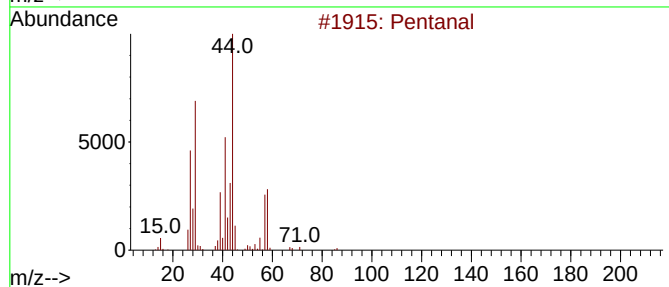
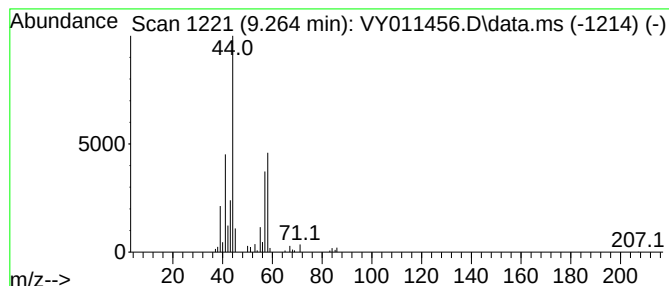
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111022S.M
Quant Title : SW846 8260

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

Peak Number 3 Pentanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.264	7.73 ug/l	70678	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	86
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	83
3			Butanal, 2-methyl-	86	C5H10O	000096-17-3	9
4			Carbonic acid, ethyl 2-propenyl ...	130	C6H10O3	001469-70-1	9
5			Cyclopropyl carbinol	72	C4H8O	002516-33-8	9



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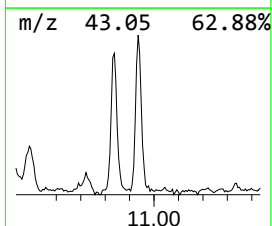
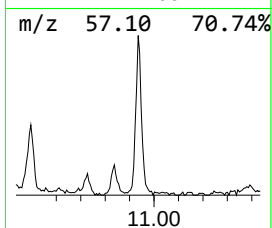
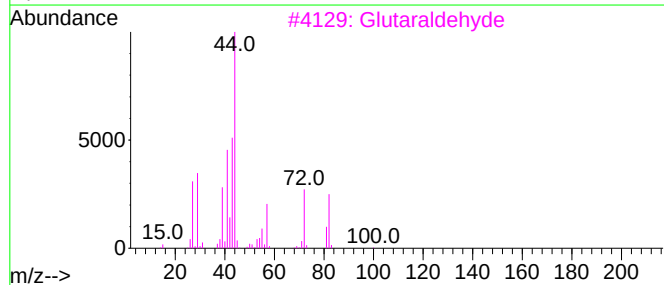
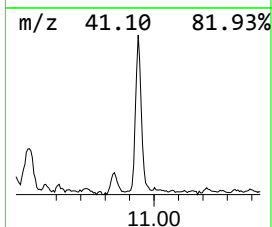
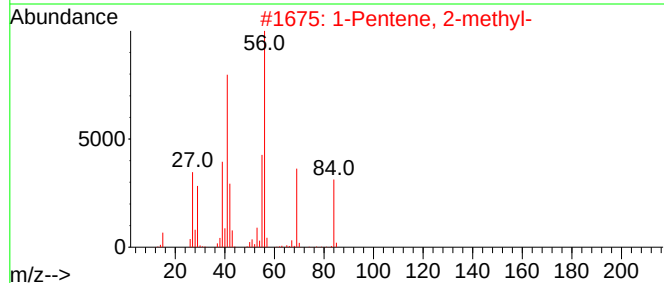
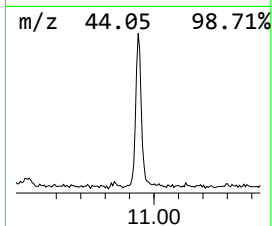
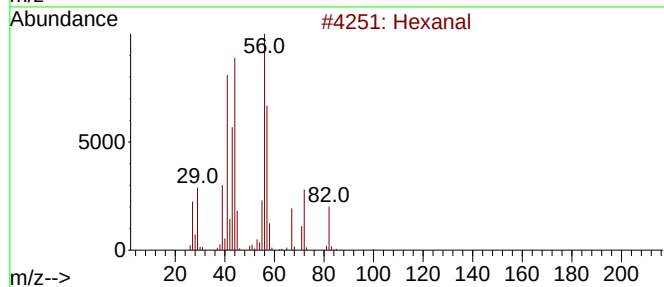
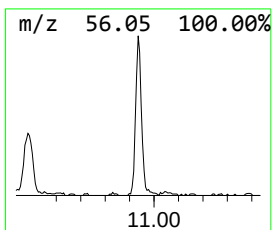
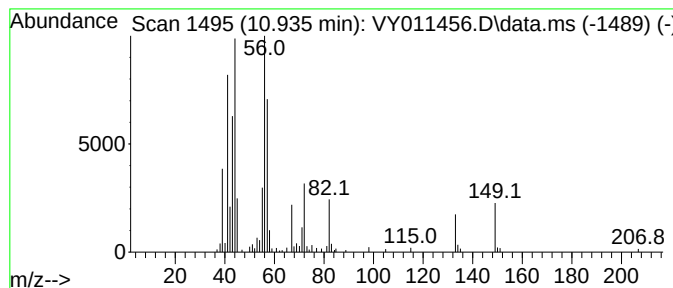
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.935	12.98 ug/l	94307	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	64
2			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	27
3			Glutaraldehyde	100	C5H8O2	000111-30-8	27
4			Butanal	72	C4H8O	000123-72-8	25
5			2-Thiophenecarboxylic acid, 5-(1...	200	C9H12O3S	054889-42-8	22



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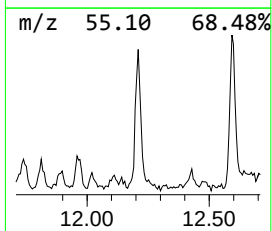
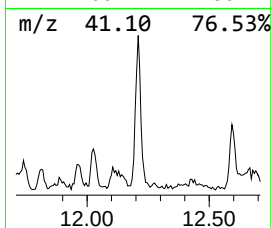
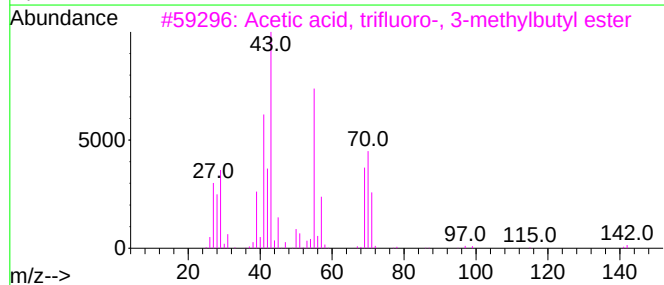
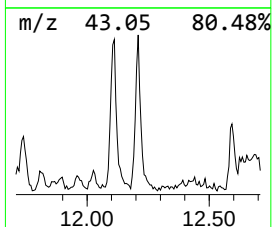
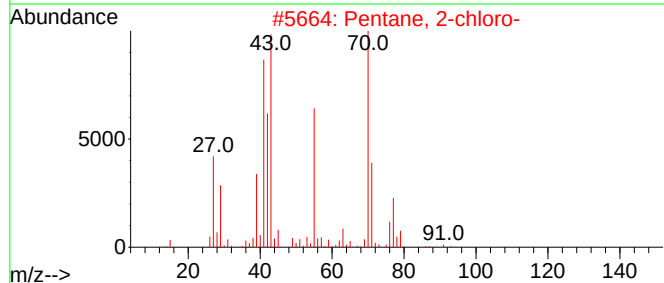
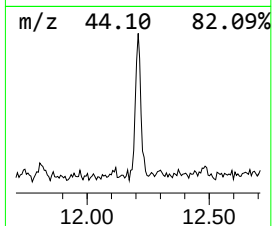
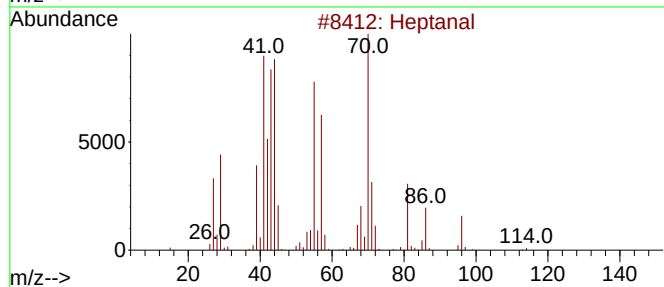
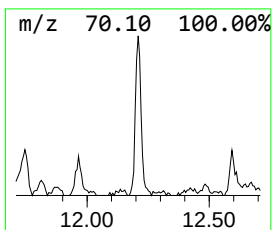
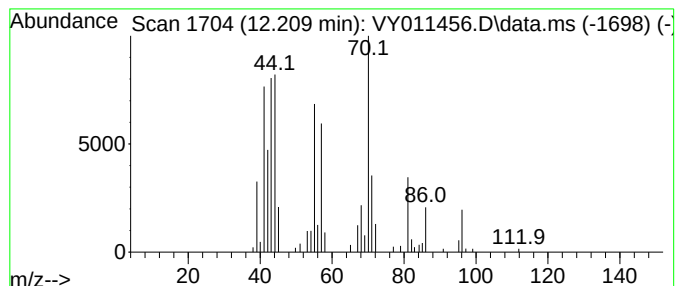
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111022S.M
Quant Title : SW846 8260

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

Peak Number 5 Heptanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.209	6.73 ug/l	48849	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	91
2			Pentane, 2-chloro-	106	C5H11Cl	000625-29-6	35
3			Acetic acid, trifluoro-, 3-methy...	184	C7H11F3O2	000327-69-5	35
4			Hexanal, 3-methyl-	114	C7H14O	019269-28-4	32
5			Propane, 2-(ethenyloxy)-	86	C5H10O	000926-65-8	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111522\
Data File : VY011456.D
Acq On : 15 Nov 2022 14:28
Operator : KP/MD
Sample : N5417-02
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
AUD-1732

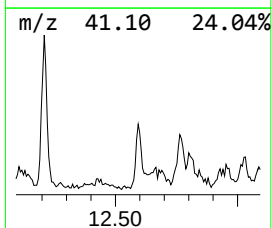
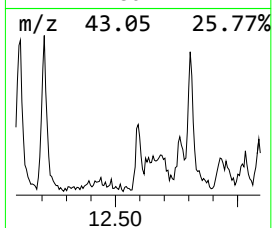
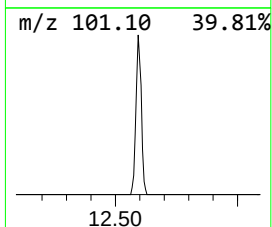
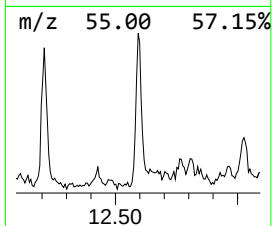
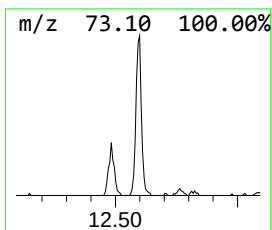
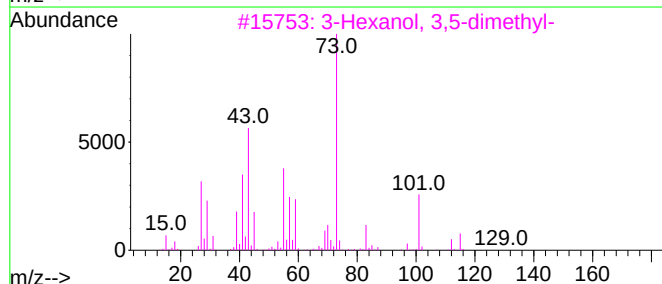
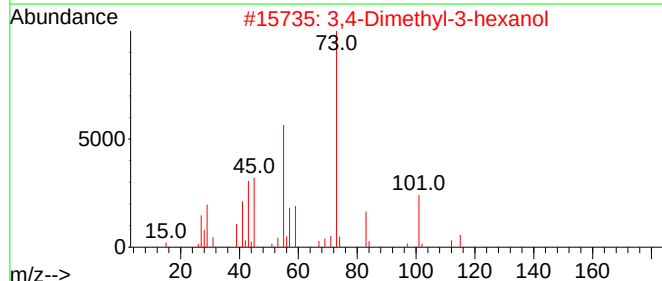
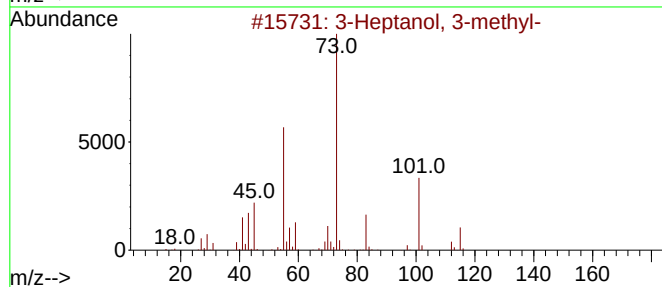
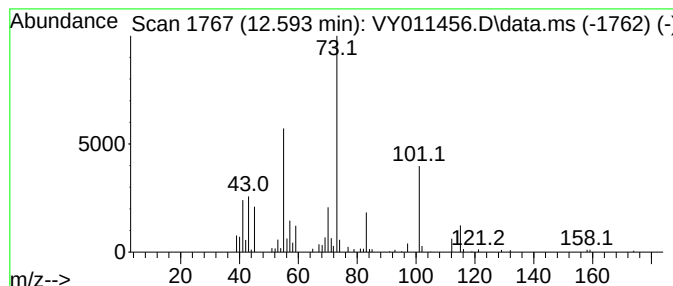
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Quant Title : SW846 8260

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

Peak Number 6 3-Heptanol, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.593	10.44 ug/l	40924	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanol, 3-methyl-	130	C8H18O	005582-82-1	86
2			3,4-Dimethyl-3-hexanol	130	C8H18O	019550-08-4	72
3			3-Hexanol, 3,5-dimethyl-	130	C8H18O	004209-91-0	42
4			Formic acid, 3-methylhept-3-yl e...	158	C9H18O2	1000368-94-9	42
5			3,4,4-Trimethyl-3-pentanol	130	C8H18O	007294-05-5	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111522\
Data File : VY011456.D
Acq On : 15 Nov 2022 14:28
Operator : KP/MD
Sample : N5417-02
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
AUD-1732

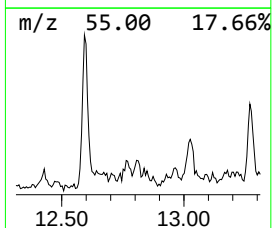
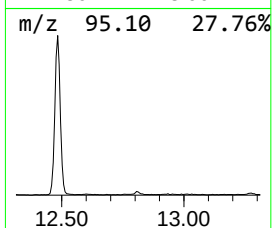
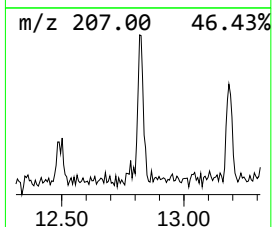
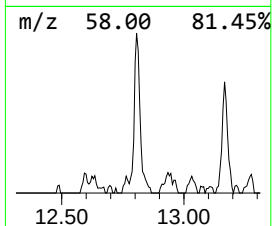
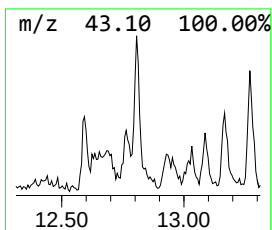
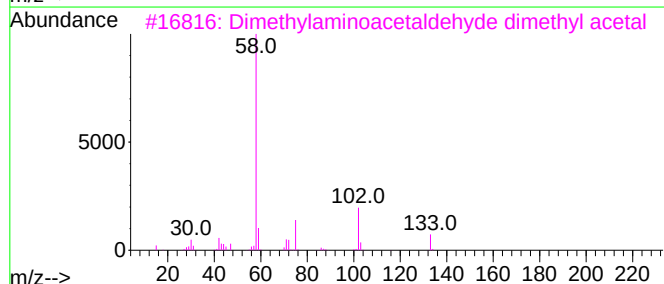
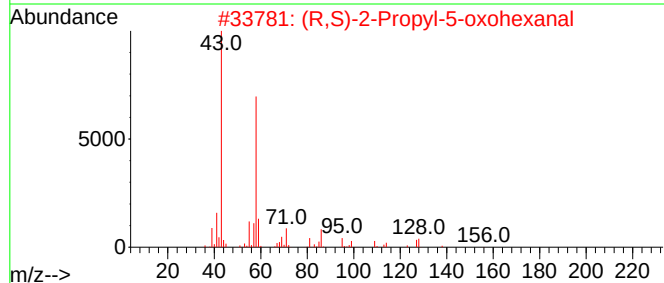
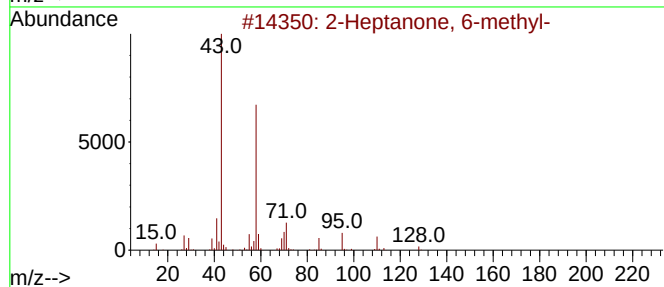
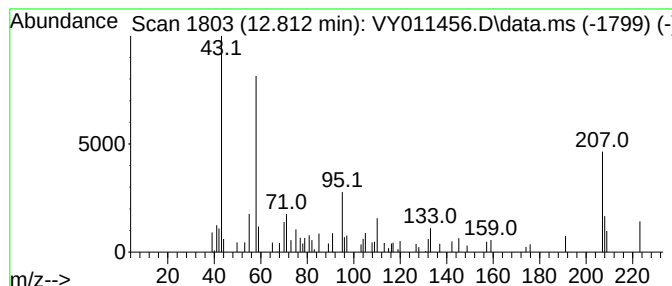
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Quant Title : SW846 8260

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

Peak Number 7 unknown12.812 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.812	7.73 ug/l	30277	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	43
2			(R,S)-2-Propyl-5-oxohexanal	156	C9H16O2	1000109-76-5	35
3			Dimethylaminoacetaldehyde dimeth...	133	C6H15NO2	038711-20-5	35
4			Benzeneethanamine, N,N-dimethyl-	149	C10H15N	001126-71-2	35
5			2-Isopropyl-5-oxohexanal	156	C9H16O2	015303-46-5	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111522\
Data File : VY011456.D
Acq On : 15 Nov 2022 14:28
Operator : KP/MD
Sample : N5417-02
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
AUD-1732

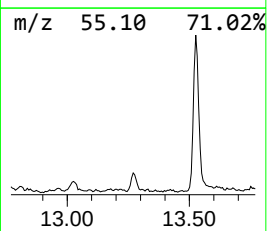
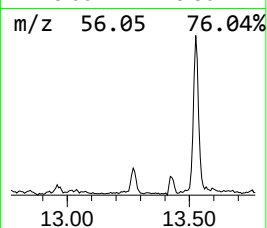
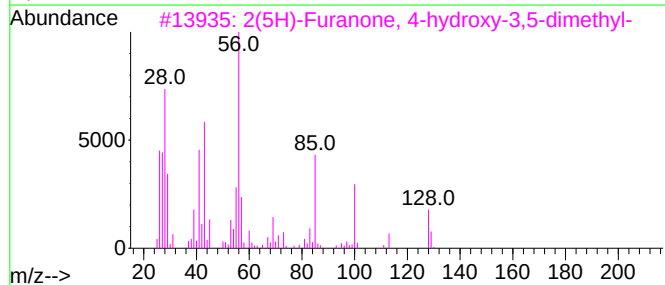
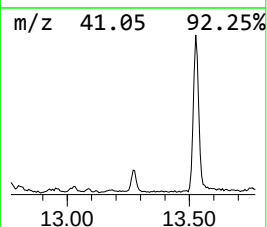
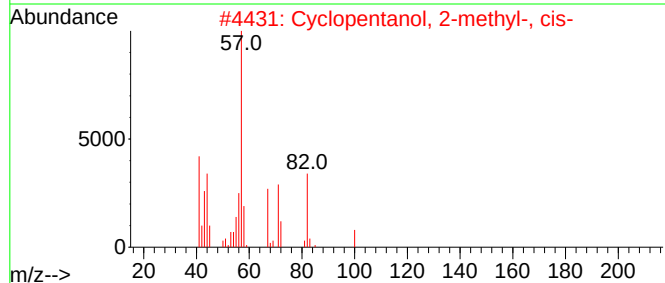
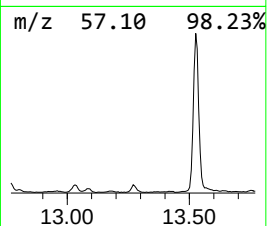
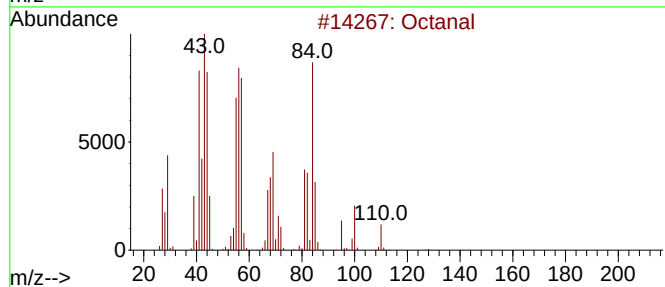
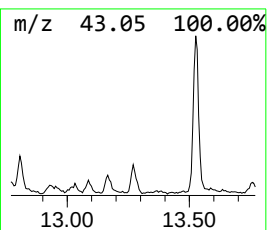
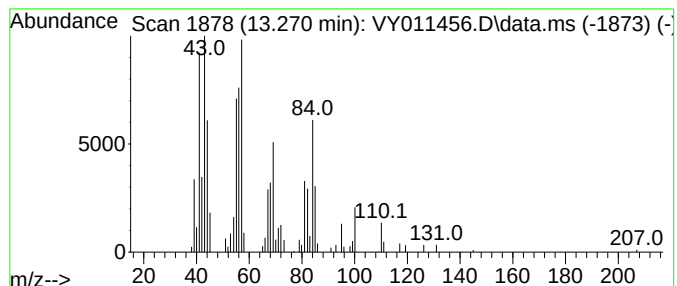
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Quant Title : SW846 8260

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

Peak Number 8 Octanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.270	8.93 ug/l	35004	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanal	128	C8H16O	000124-13-0	91
2			Cyclopentanol, 2-methyl-, cis-	100	C6H12O	025144-05-2	38
3			2(5H)-Furanone, 4-hydroxy-3,5-di...	128	C6H8O3	1000197-09-3	35
4			Hexane, 2-methyl-	100	C7H16	000591-76-4	35
5			2-Hexene, (Z)-	84	C6H12	007688-21-3	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111522\
Data File : VY011456.D
Acq On : 15 Nov 2022 14:28
Operator : KP/MD
Sample : N5417-02
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
AUD-1732

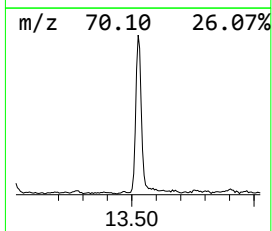
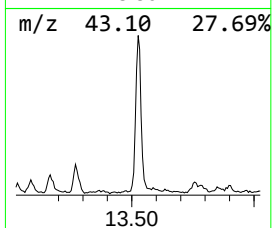
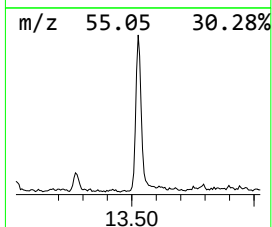
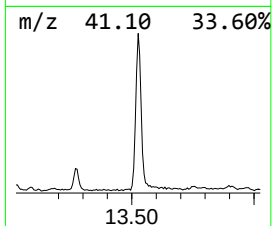
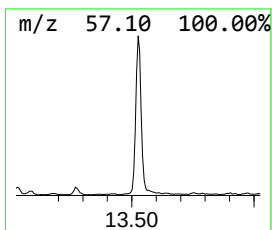
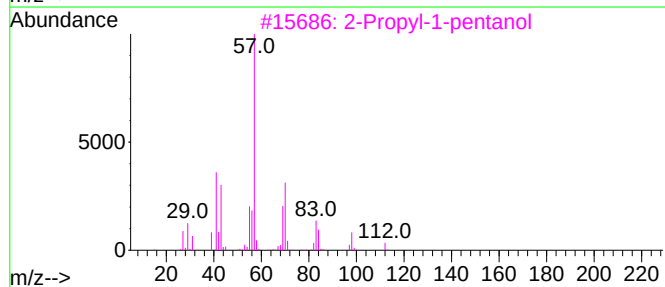
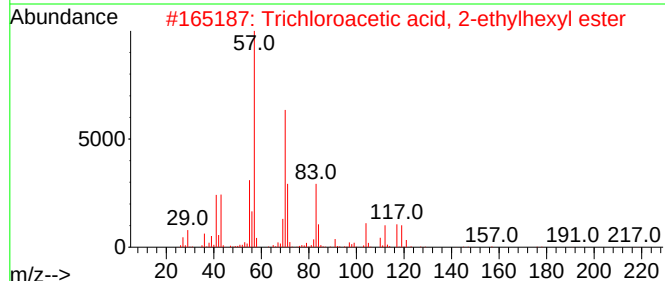
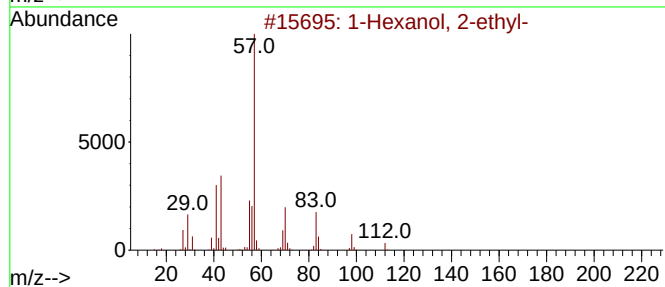
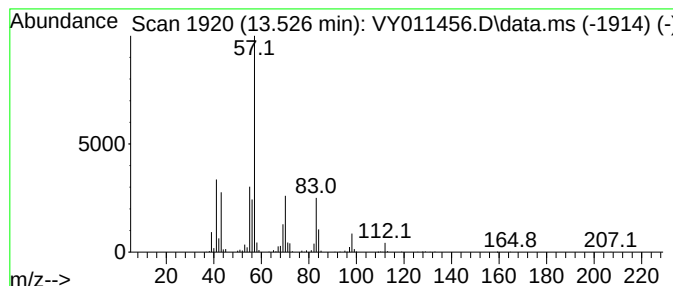
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Quant Title : SW846 8260

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.526	61.16 ug/l	239692	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			Trichloroacetic acid, 2-ethylhex...	274	C10H17Cl3O2	016397-79-8	50
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
5			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111522\
Data File : VY011456.D
Acq On : 15 Nov 2022 14:28
Operator : KP/MD
Sample : N5417-02
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
AUD-1732

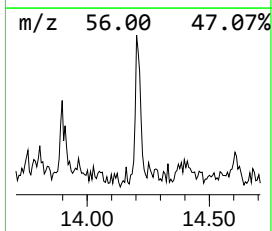
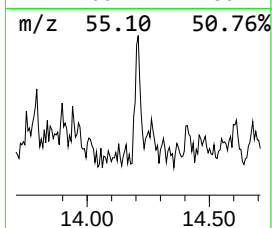
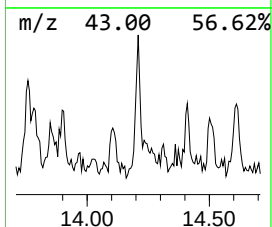
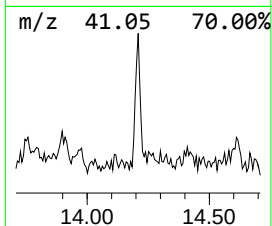
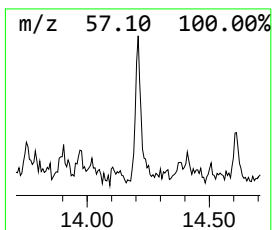
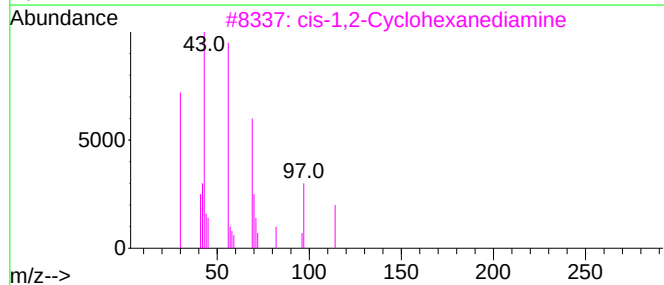
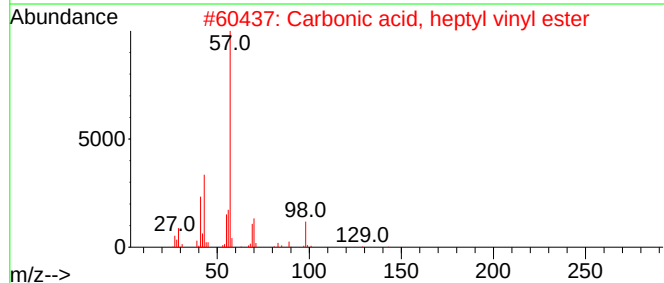
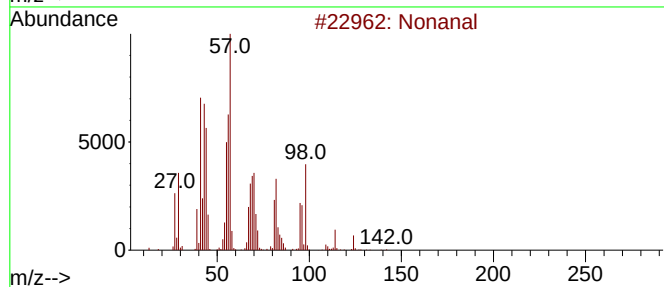
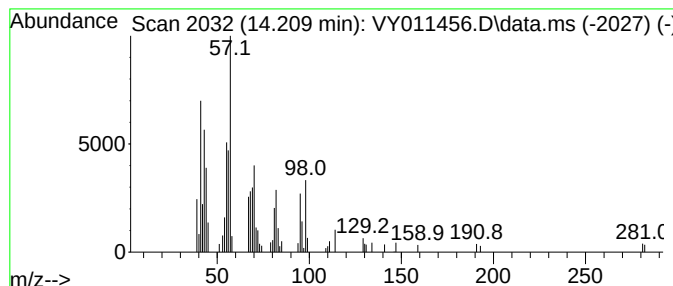
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Quant Title : SW846 8260

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

Peak Number 10 Nonanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.209	5.55 ug/l	21747	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	72
2			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	27
3			cis-1,2-Cyclohexanediamine	114	C6H14N2	001436-59-5	25
4			Cyclopropane, 1-methyl-2-(3-meth...	140	C10H20	062238-07-7	22
5			1-Hexanol, 5-methyl-	116	C7H16O	000627-98-5	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111522\
Data File : VY011456.D
Acq On : 15 Nov 2022 14:28
Operator : KP/MD
Sample : N5417-02
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
AUD-1732

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111022S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Pentanal	9.264	7.7	ug/l	70678	2	8.691	457127	50.0
Hexanal	10.935	13.0	ug/l	94307	3	11.490	363188	50.0
Heptanal	12.209	6.7	ug/l	48849	3	11.490	363188	50.0
3-Heptanol, 3-m...	12.593	10.4	ug/l	40924	4	13.428	195954	50.0
unknown12.812	12.812	7.7	ug/l	30277	4	13.428	195954	50.0
Octanal	13.270	8.9	ug/l	35004	4	13.428	195954	50.0
1-Hexanol, 2-et...	13.526	61.2	ug/l	239692	4	13.428	195954	50.0
Nonanal	14.209	5.5	ug/l	21747	4	13.428	195954	50.0