

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY080823\
 Data File : VY014991.D
 Acq On : 08 Aug 2023 17:33
 Operator : SY/MD
 Sample : 03927-01
 Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 1127

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\82Y080723S.M
 Title : SW846 8260

Signal : TIC: VY014991.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	15	rVB3	9078	12610	1.20%	0.146%
2	2.070	33	41	44	rBV3	7245	13727	1.30%	0.159%
3	2.211	59	64	74	rBV2	38204	73374	6.97%	0.850%
4	2.381	87	92	100	rVV	40266	66178	6.28%	0.767%
5	2.455	100	104	108	rVB2	7586	11324	1.07%	0.131%
6	3.820	320	328	337	rBV	7724	20048	1.90%	0.232%
7	3.948	339	349	370	rVV	84287	238788	22.67%	2.766%
8	4.210	383	392	409	rBV2	7171	26645	2.53%	0.309%
9	4.405	418	424	436	rBV3	5013	17983	1.71%	0.208%
10	4.710	461	474	488	rBV2	34863	112450	10.67%	1.303%
11	4.960	505	515	533	rVB2	61617	234450	22.26%	2.716%
12	5.161	540	548	560	rVB4	4593	13824	1.31%	0.160%
13	5.747	633	644	655	rBV3	15423	46868	4.45%	0.543%
14	5.905	660	670	680	rBV5	4919	15736	1.49%	0.182%
15	6.704	787	801	811	rBV2	17254	57485	5.46%	0.666%
16	6.984	836	847	864	rBV2	144128	425107	40.35%	4.924%
17	7.326	893	903	919	rBV3	25210	75089	7.13%	0.870%
18	7.716	956	967	973	rBV	155647	367221	34.86%	4.254%
19	7.789	973	979	990	rVB	248121	555288	52.71%	6.432%
20	8.143	1024	1037	1047	rBV	164857	384495	36.50%	4.454%
21	8.246	1047	1054	1063	rVB2	13564	32761	3.11%	0.379%
22	8.393	1072	1078	1086	rVB2	8189	18017	1.71%	0.209%
23	8.551	1095	1104	1114	rBV	25004	59806	5.68%	0.693%
24	8.685	1118	1126	1135	rVV	389838	776999	73.76%	9.000%
25	8.771	1135	1140	1152	rVB2	17191	36511	3.47%	0.423%
26	9.136	1192	1200	1211	rBV	25301	53321	5.06%	0.618%
27	9.264	1213	1221	1231	rVV2	17510	38539	3.66%	0.446%
28	9.514	1257	1262	1273	rVB	13088	29547	2.80%	0.342%
29	9.978	1327	1338	1346	rBV3	5026	14818	1.41%	0.172%
30	10.069	1346	1353	1358	rBV	35564	64420	6.12%	0.746%
31	10.179	1364	1371	1377	rBV	619426	1053428	100.00%	12.202%
32	10.246	1377	1382	1386	rVB	24688	41307	3.92%	0.478%
33	10.435	1407	1413	1417	rBV	21304	38373	3.64%	0.444%
34	10.484	1417	1421	1428	rVB4	12490	30108	2.86%	0.349%
35	10.575	1430	1436	1442	rBV	16315	28631	2.72%	0.332%
36	10.685	1449	1454	1458	rBV2	6545	11923	1.13%	0.138%

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37	10.837	1468	1479	1487	rBV	23796	47538	4.51%	0.551%
38	10.935	1489	1495	1508	rVV4	37242	77304	7.34%	0.895%
39	11.215	1534	1541	1548	rBV2	7579	14049	1.33%	0.163%
40	11.319	1553	1558	1563	rBV3	7233	14321	1.36%	0.166%
41	11.490	1577	1586	1595	rBV	591590	955868	90.74%	11.072%
42	11.593	1597	1603	1610	rBV3	8063	17511	1.66%	0.203%
43	11.703	1615	1621	1624	rVV	17660	37191	3.53%	0.431%
44	11.739	1624	1627	1633	rVB2	20336	32834	3.12%	0.380%
45	12.026	1669	1674	1679	rBV2	9842	15113	1.43%	0.175%
46	12.105	1682	1687	1693	rBV2	11661	19693	1.87%	0.228%
47	12.209	1698	1704	1713	rBV3	15211	28818	2.74%	0.334%
48	12.386	1721	1733	1741	rBV3	31325	68269	6.48%	0.791%
49	12.483	1741	1749	1761	rVB2	469317	791020	75.09%	9.162%
50	12.782	1792	1798	1799	rVV3	11507	20154	1.91%	0.233%
51	12.806	1800	1802	1805	rVV4	12321	16611	1.58%	0.192%
52	12.867	1805	1812	1817	rVB5	14337	36154	3.43%	0.419%
53	12.928	1817	1822	1825	rBV3	10931	18258	1.73%	0.211%
54	12.959	1825	1827	1832	rVB4	8458	10986	1.04%	0.127%
55	13.014	1832	1836	1841	rBV4	12379	19483	1.85%	0.226%
56	13.117	1847	1853	1858	rBV2	6576	13200	1.25%	0.153%
57	13.197	1858	1866	1874	rBV3	51346	118604	11.26%	1.374%
58	13.264	1874	1877	1886	rVB6	11139	22819	2.17%	0.264%
59	13.422	1897	1903	1910	rBV	574395	867631	82.36%	10.050%
60	13.532	1916	1921	1925	rBV2	11745	18030	1.71%	0.209%
61	13.593	1925	1931	1934	rVV	41509	79516	7.55%	0.921%
62	13.629	1934	1937	1941	rVV2	28736	49191	4.67%	0.570%
63	13.672	1941	1944	1954	rVB4	12223	27545	2.61%	0.319%
64	13.965	1986	1992	1998	rVB2	12420	24062	2.28%	0.279%
65	15.233	2191	2200	2205	rBV	5507	11692	1.11%	0.135%
66	15.312	2206	2213	2220	rVV	38014	62592	5.94%	0.725%

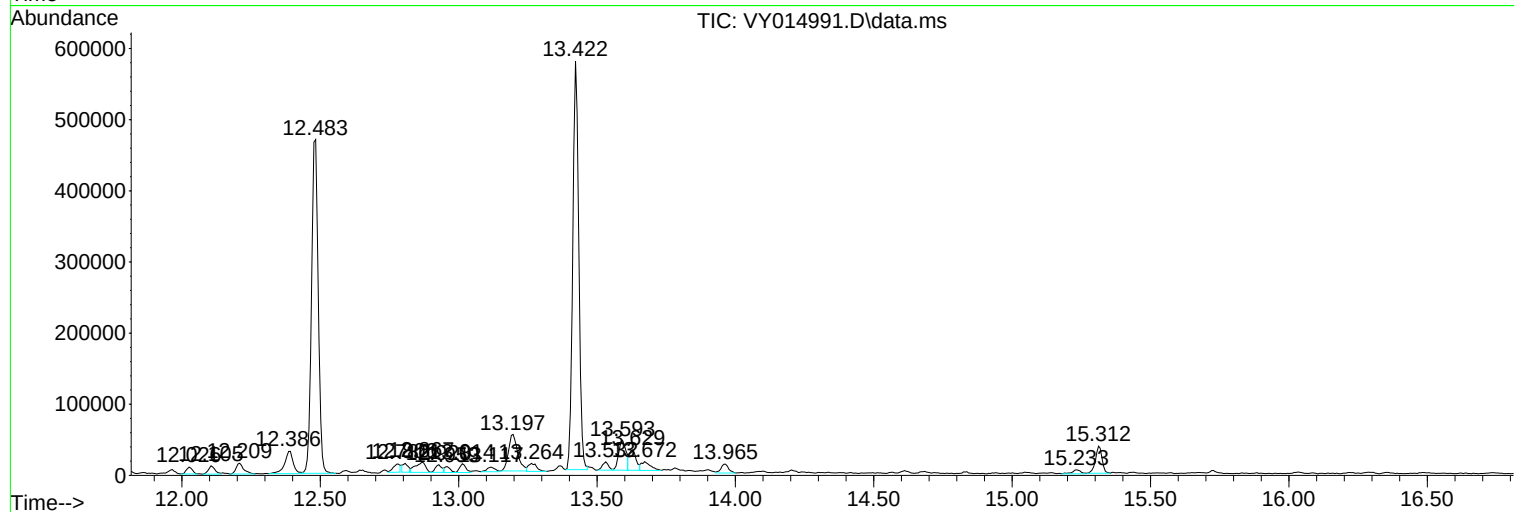
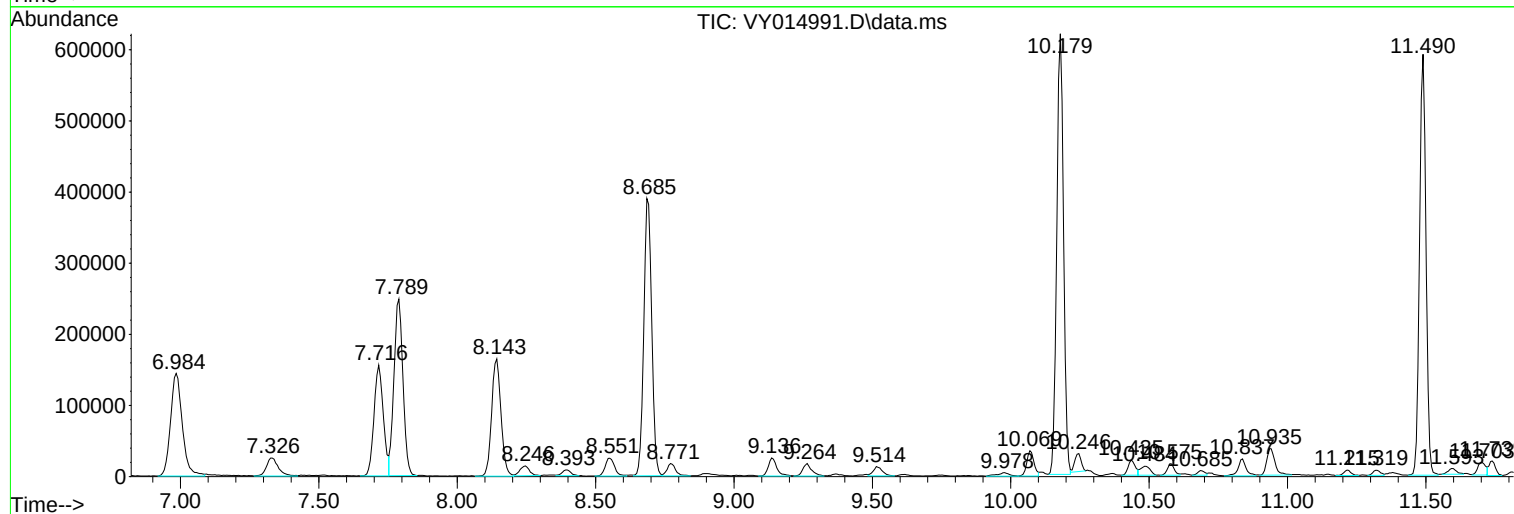
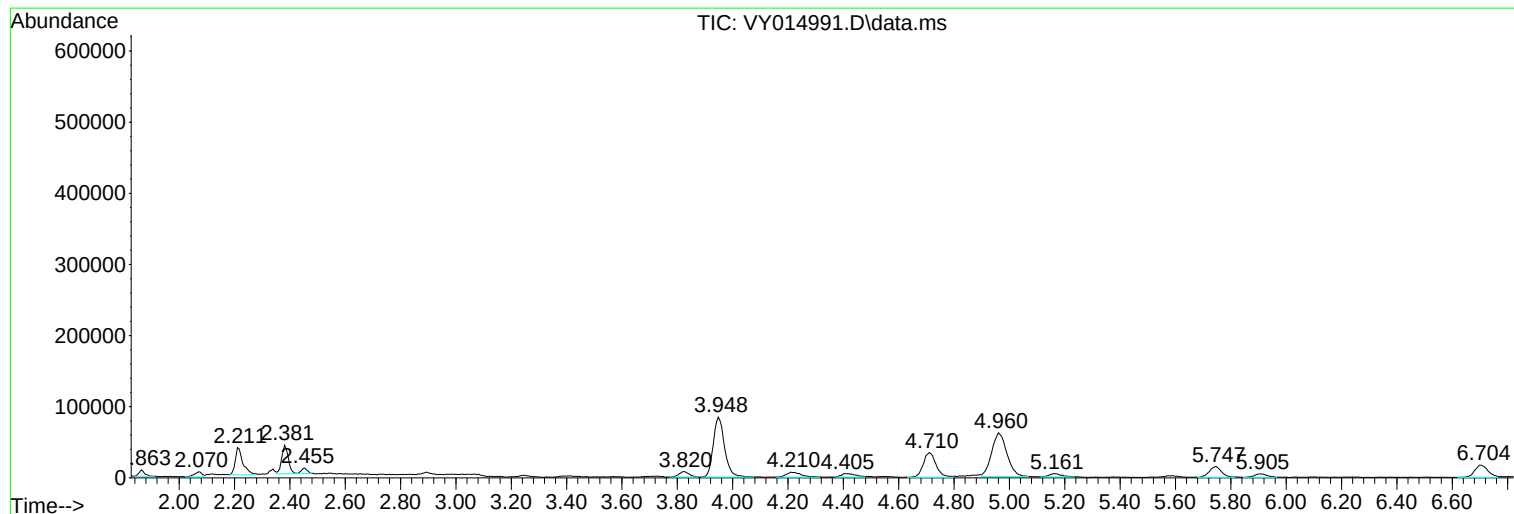
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Quant Title : SW846 8260

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



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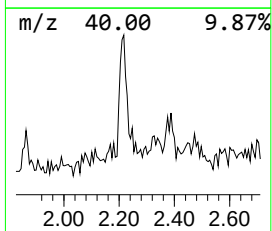
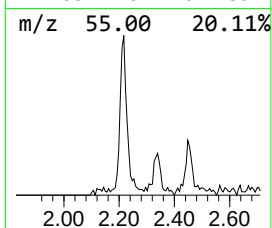
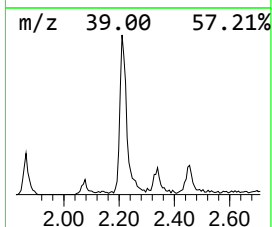
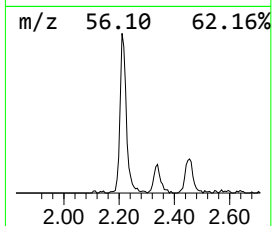
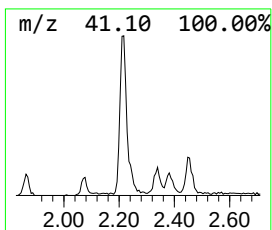
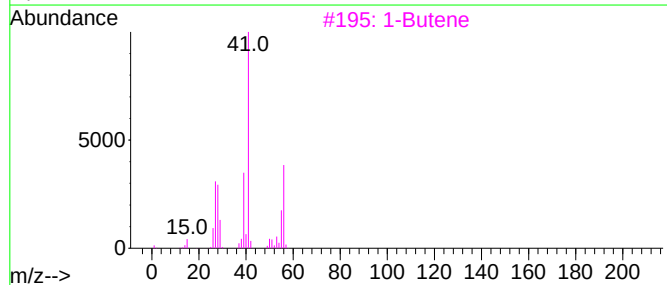
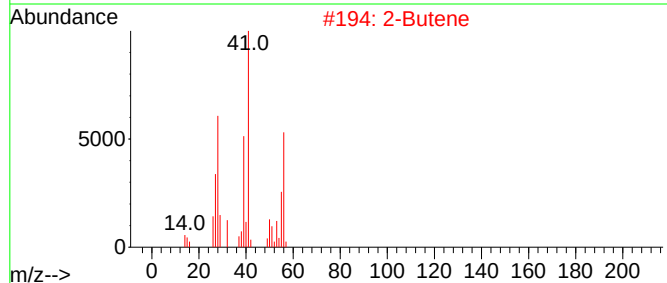
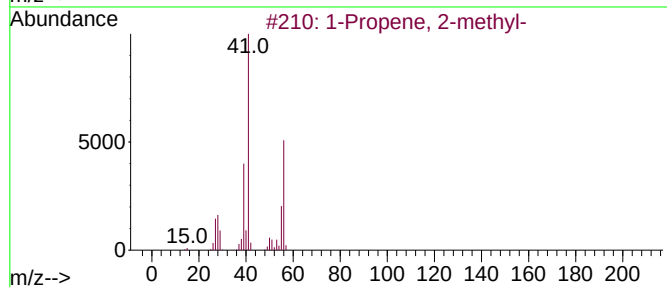
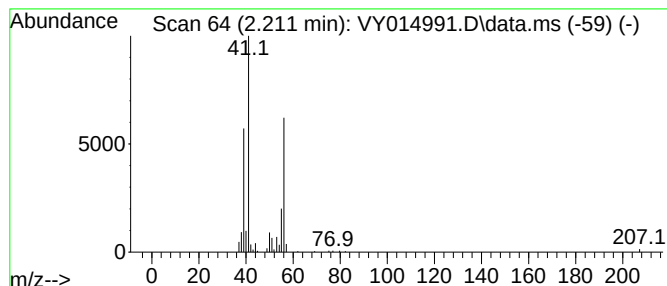
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Quant Title : SW846 8260

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

Peak Number 1 1-Propene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.211	6.61 ug/l	73374	Pentafluorobenzene	7.789

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	90	
2	2-Butene	56	C4H8	000107-01-7	86	
3	1-Butene	56	C4H8	000106-98-9	59	
4	Cyclobutane	56	C4H8	000287-23-0	49	
5	2-Butene, (Z)-	56	C4H8	000590-18-1	46	



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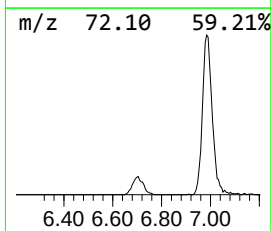
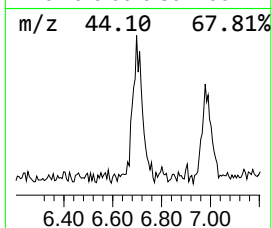
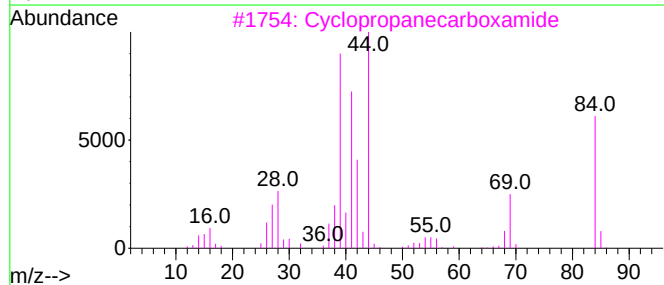
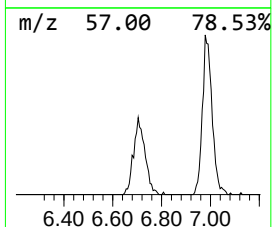
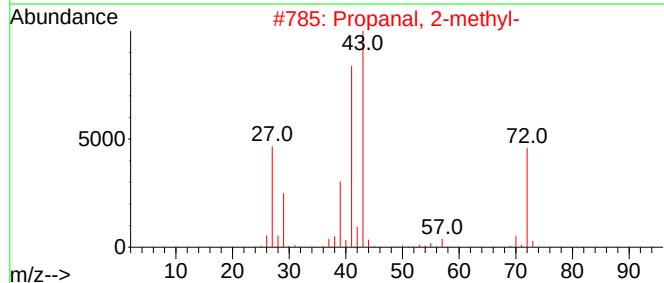
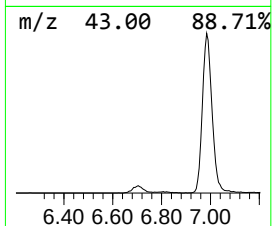
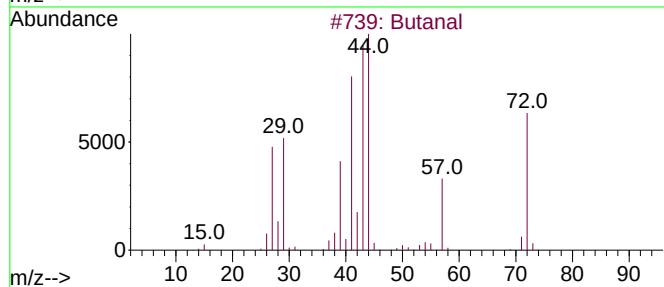
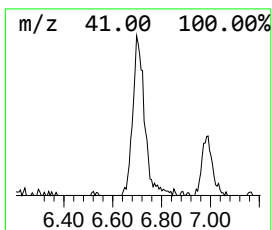
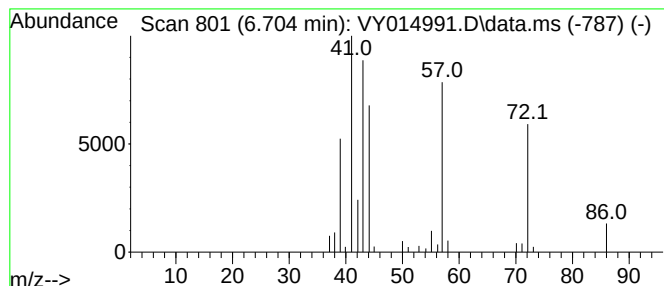
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080723S.M
Quant Title : SW846 8260

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

Peak Number 4 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.704	5.18 ug/l	57485	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	58
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	47
3			Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	38
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5			Butanal, 3-methyl-	86	C5H10O	000590-86-3	32



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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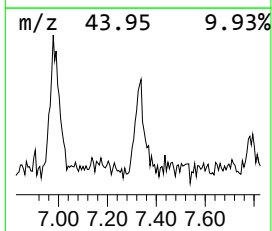
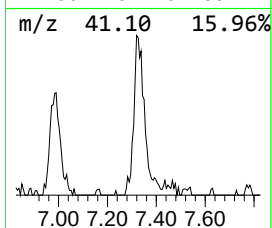
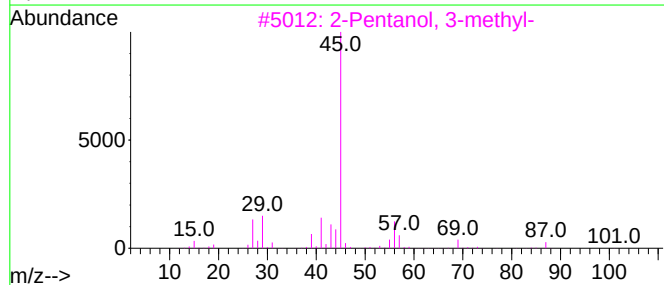
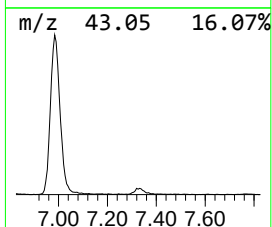
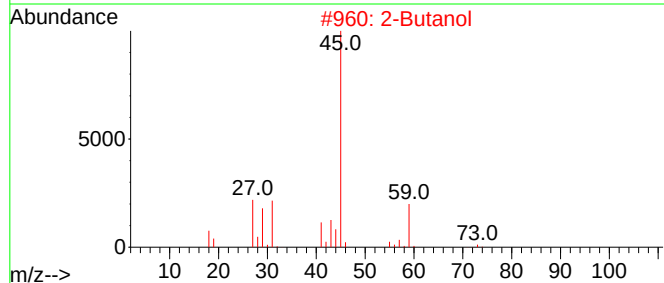
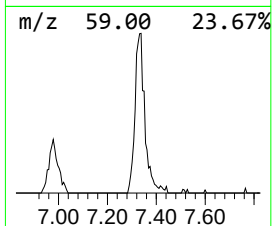
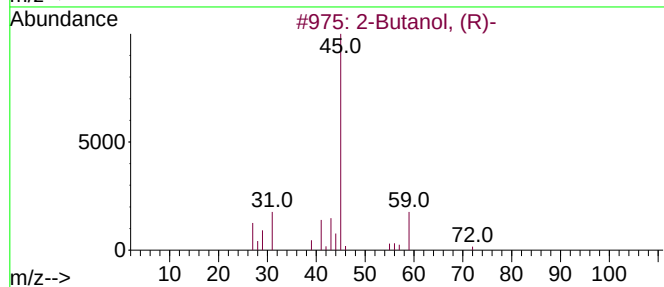
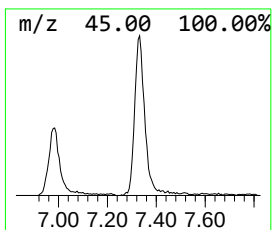
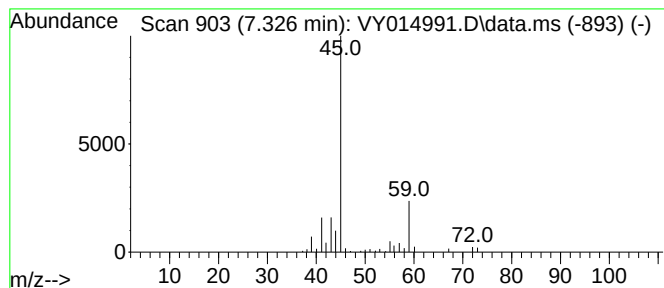
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080723S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 5 2-Butanol, (R)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.326	6.76 ug/l	75089	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, (R)-			74	C4H10O	014898-79-4	83
2	2-Butanol			74	C4H10O	000078-92-2	78
3	2-Pentanol, 3-methyl-			102	C6H14O	000565-60-6	59
4	2-Hexanol, (R)-			102	C6H14O	026549-24-6	38
5	3-Ethyl-2-pentanol			116	C7H16O	000609-27-8	38



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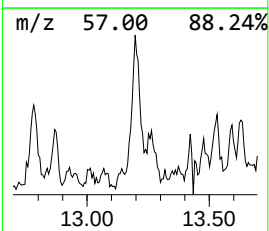
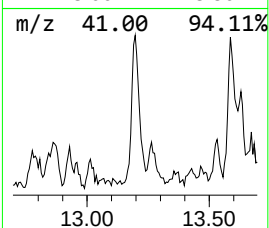
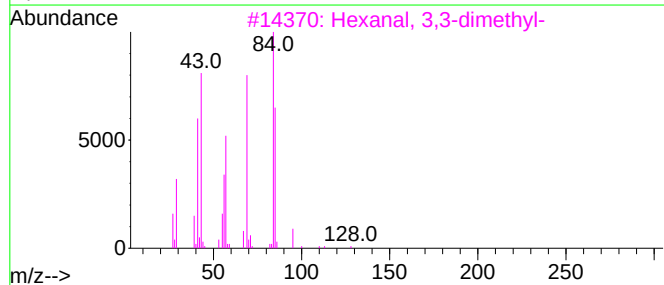
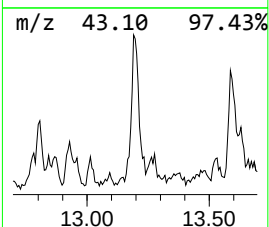
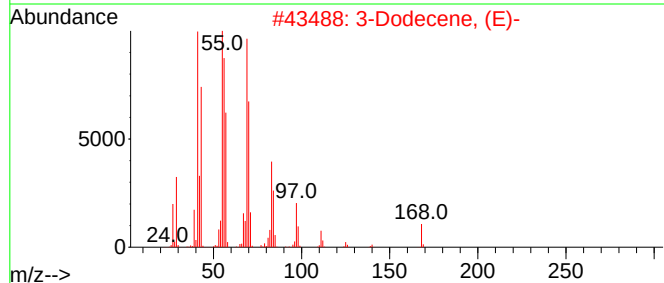
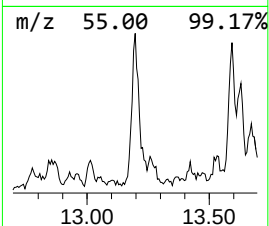
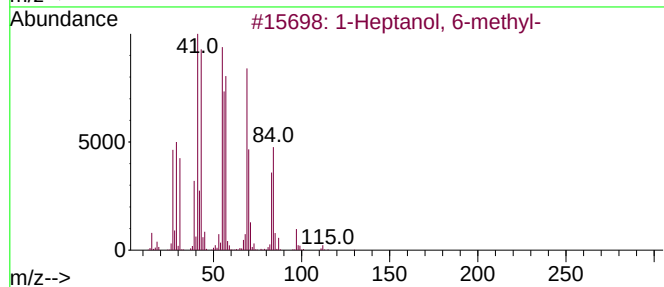
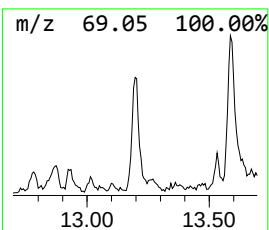
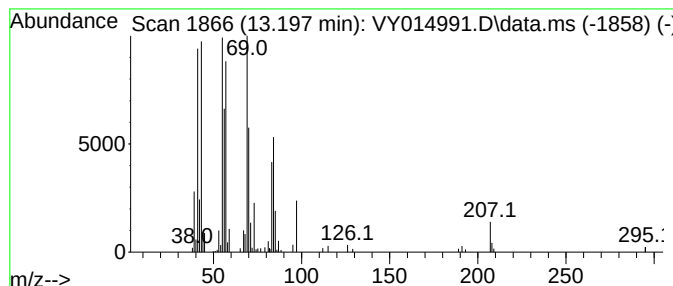
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080723S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 6 1-Heptanol, 6-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.197	6.83 ug/l	118604	1,4-Dichlorobenzene-d4	13.422

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	72
2		3-Dodecene, (E)-	168	C12H24	007206-14-6	59
3		Hexanal, 3,3-dimethyl-	128	C8H16O	055320-57-5	47
4		1-Hexene, 3-methyl-	98	C7H14	003404-61-3	43
5		5-Dodecene, (E)-	168	C12H24	007206-16-8	43



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Sample : 03927-01
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
1127

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y080723S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propene, 2-me...	2.211	6.6	ug/l	73374	1	7.789	555288	50.0
Butanal	6.704	5.2	ug/l	57485	1	7.789	555288	50.0
2-Butanol, (R)-	7.326	6.8	ug/l	75089	1	7.789	555288	50.0
1-Heptanol, 6-m...	13.197	6.8	ug/l	118604	4	13.422	867631	50.0