

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062123\
 Data File : VY014343.D
 Acq On : 21 Jun 2023 18:05
 Operator : KP/MD
 Sample : 03357-19
 Misc : 6.22g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 WC-SCAN-04-G

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\82Y060923S.M
 Title : SW846 8260

Signal : TIC: VY014343.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.948	338	349	359	rBV2	37663	106145	11.94%	1.491%
2	4.210	383	392	406	rBV	7159	24170	2.72%	0.339%
3	4.716	462	475	492	rBV	46607	150194	16.89%	2.109%
4	5.747	634	644	656	rVB3	7429	24924	2.80%	0.350%
5	6.704	792	801	809	rBV6	4205	13828	1.56%	0.194%
6	6.978	836	846	859	rBV	56714	176164	19.81%	2.474%
7	7.716	958	967	973	rBV2	139501	328311	36.93%	4.611%
8	7.789	973	979	993	rVB	239144	530451	59.66%	7.450%
9	8.143	1023	1037	1048	rBV	150428	349526	39.31%	4.909%
10	8.551	1094	1104	1115	rBV	13397	29950	3.37%	0.421%
11	8.691	1118	1127	1135	rBV	345012	672073	75.59%	9.439%
12	8.770	1135	1140	1150	rVB	57756	114339	12.86%	1.606%
13	8.917	1156	1164	1173	rVB6	2987	9507	1.07%	0.134%
14	9.142	1195	1201	1205	rBV2	9000	18497	2.08%	0.260%
15	9.801	1302	1309	1316	rBV3	6330	12042	1.35%	0.169%
16	10.069	1347	1353	1362	rVB3	8950	16965	1.91%	0.238%
17	10.179	1362	1371	1379	rBV	518287	889065	100.00%	12.486%
18	10.270	1379	1386	1387	rVV2	39665	74010	8.32%	1.039%
19	10.289	1387	1389	1395	rVV	54079	81477	9.16%	1.144%
20	10.368	1395	1402	1408	rVV6	11569	31487	3.54%	0.442%
21	10.435	1408	1413	1418	rVV7	5846	13917	1.57%	0.195%
22	10.496	1418	1423	1427	rVV5	6875	12765	1.44%	0.179%
23	10.581	1427	1437	1443	rVV	28327	59856	6.73%	0.841%
24	10.642	1443	1447	1450	rVV2	7862	11678	1.31%	0.164%
25	10.691	1450	1455	1467	rVB4	7537	18920	2.13%	0.266%
26	10.831	1475	1478	1485	rVB	8931	14761	1.66%	0.207%
27	10.947	1490	1497	1510	rBV3	46296	101549	11.42%	1.426%
28	11.221	1536	1542	1549	rBV	15691	26871	3.02%	0.377%
29	11.325	1552	1559	1564	rBV3	9130	17163	1.93%	0.241%
30	11.490	1575	1586	1596	rBV	465067	766491	86.21%	10.765%
31	11.739	1622	1627	1635	rVB	36784	59909	6.74%	0.841%
32	12.026	1669	1674	1682	rBV6	4557	9907	1.11%	0.139%
33	12.105	1682	1687	1697	rVB2	15797	25727	2.89%	0.361%
34	12.483	1740	1749	1757	rBV3	378321	681089	76.61%	9.565%
35	12.630	1768	1773	1782	rVB	18292	40047	4.50%	0.562%
36	12.788	1792	1799	1811	rBV4	42801	136391	15.34%	1.916%

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Peak separation: 5

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37	12.910	1813	1819	1826	rVB2	17672	36864	4.15%	0.518%
38	13.069	1835	1845	1856	rVB2	45408	97411	10.96%	1.368%
39	13.178	1856	1863	1870	rBV4	25470	49280	5.54%	0.692%
40	13.282	1870	1880	1884	rBV	71979	126166	14.19%	1.772%
41	13.428	1895	1904	1909	rBV	364659	589456	66.30%	8.278%
42	13.477	1909	1912	1917	rVV3	45250	89983	10.12%	1.264%
43	13.526	1917	1920	1924	rVV	17031	24621	2.77%	0.346%
44	13.575	1924	1928	1933	rVB	13595	22328	2.51%	0.314%
45	13.642	1933	1939	1946	rBV3	17910	35985	4.05%	0.505%
46	13.757	1953	1958	1960	rBV5	6962	10500	1.18%	0.147%
47	13.959	1980	1991	1996	rBV7	24835	79536	8.95%	1.117%
48	14.020	1996	2001	2009	rVB2	48431	84274	9.48%	1.184%
49	14.105	2009	2015	2024	rVB2	9424	19919	2.24%	0.280%
50	14.202	2024	2031	2034	rBV9	4874	11597	1.30%	0.163%
51	14.263	2034	2041	2044	rVB6	4239	8998	1.01%	0.126%
52	14.343	2051	2054	2063	rVB5	4048	9220	1.04%	0.129%
53	14.629	2094	2101	2105	rBV4	12412	26008	2.93%	0.365%
54	15.056	2164	2171	2175	rBV2	12411	23667	2.66%	0.332%
55	15.312	2206	2213	2220	rBV	22509	38949	4.38%	0.547%
56	15.995	2316	2325	2331	rBV5	8632	25329	2.85%	0.356%
57	16.233	2358	2364	2368	rBV	12174	23630	2.66%	0.332%
58	16.653	2425	2433	2442	rBV3	17911	36486	4.10%	0.512%

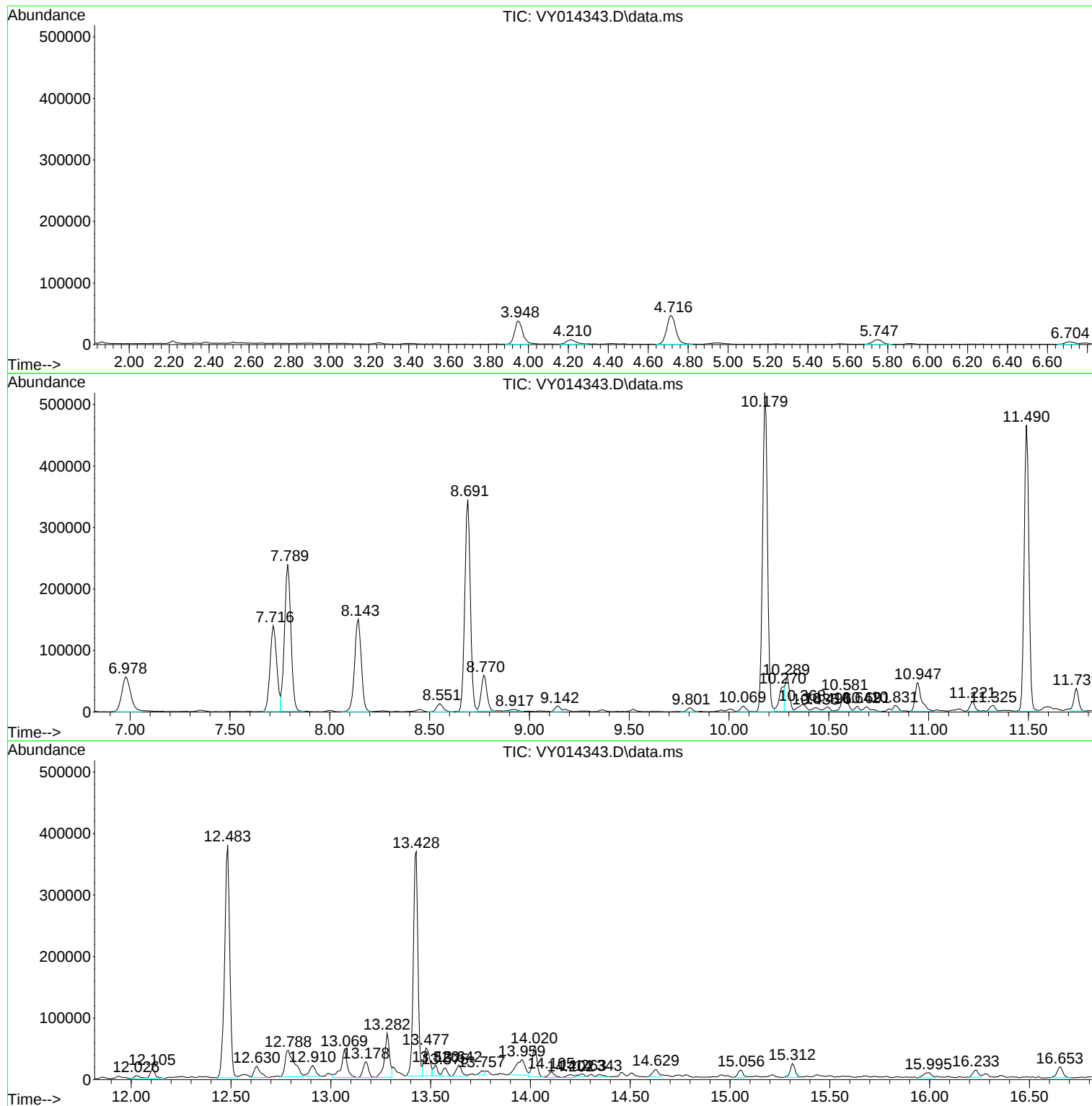
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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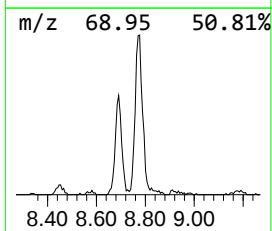
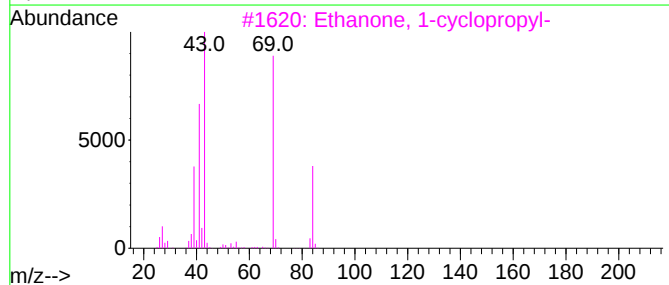
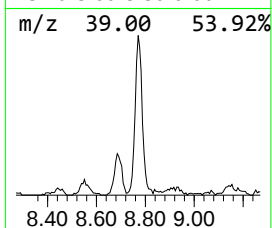
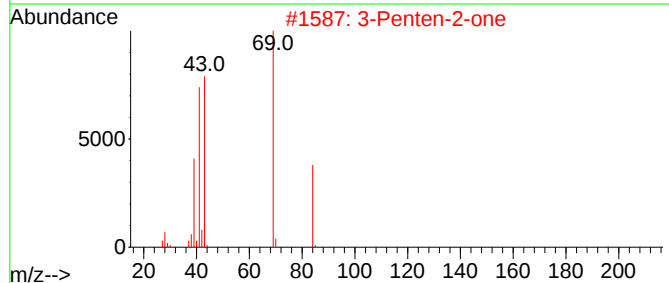
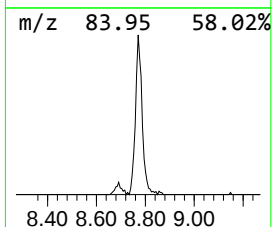
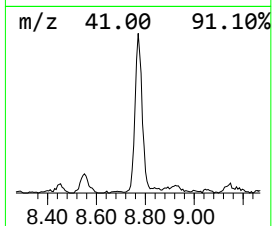
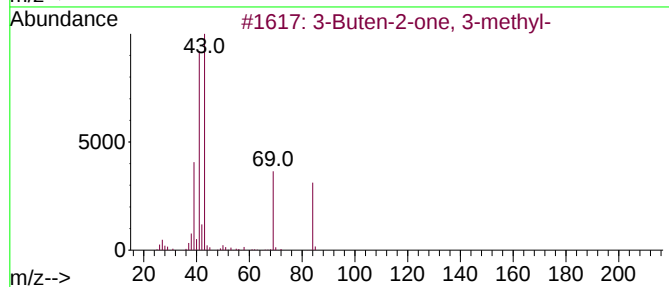
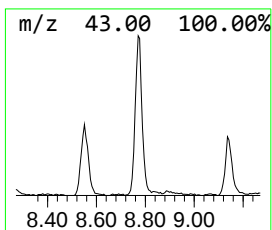
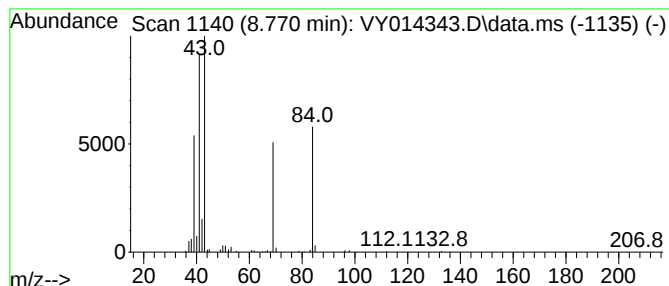
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060923S.M
Quant Title : SW846 8260

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

Peak Number 1 3-Buten-2-one, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.770	8.51 ug/l	114339	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	90
2			3-Penten-2-one	84	C5H8O	000625-33-2	72
3			Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	53
4			3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	35
5			Cyclopropanecarboxylic acid, cyc...	168	C10H16O2	1000278-70-7	25



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-SCAN-04-G

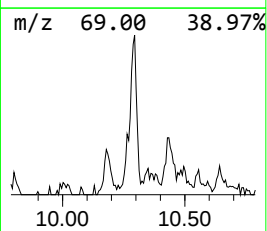
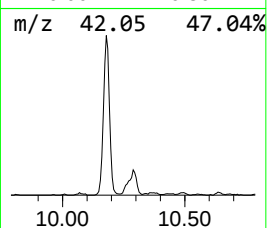
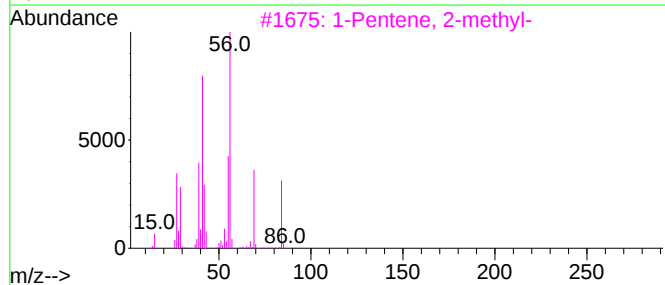
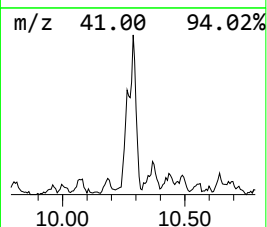
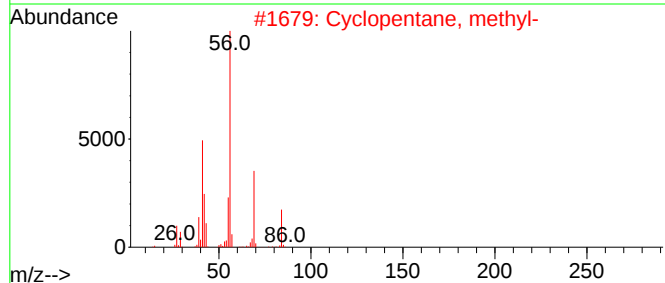
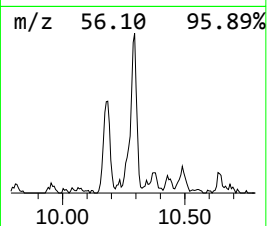
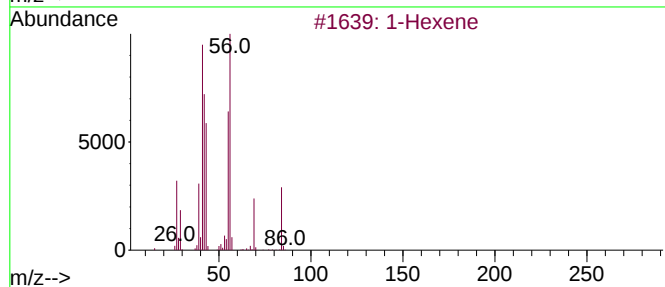
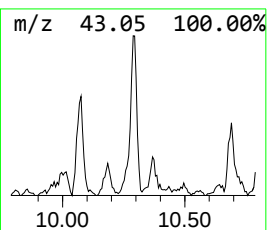
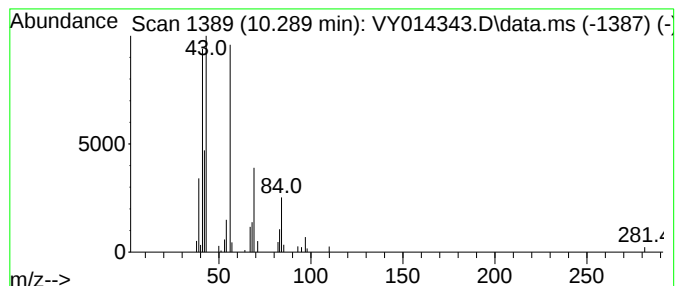
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060923S.M
Quant Title : SW846 8260

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

Peak Number 2 1-Hexene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.289	5.31 ug/l	81477	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexene	84	C6H12	000592-41-6	64
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	64
3			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	58
4			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	53
5			Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062123\
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Misc : 6.22g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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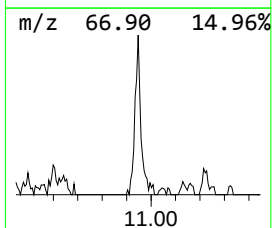
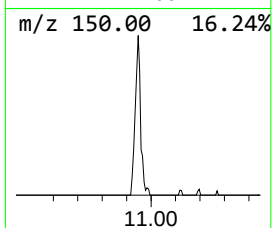
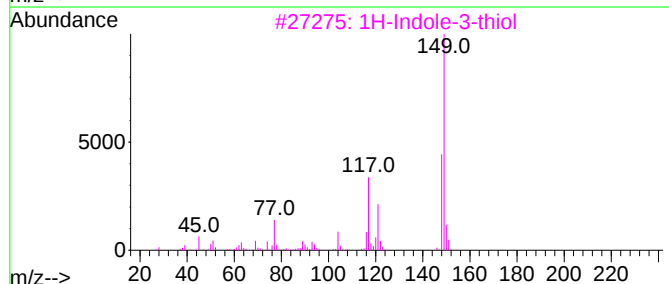
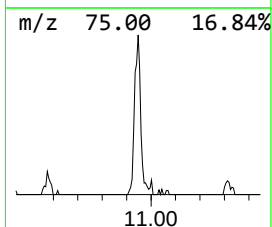
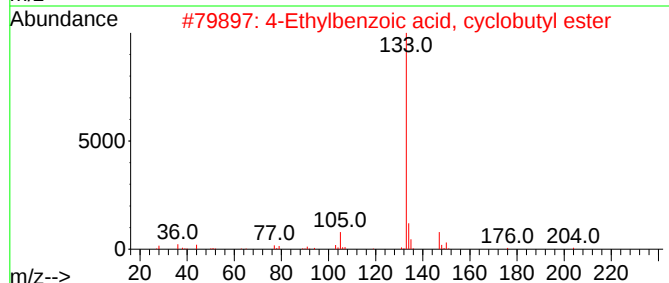
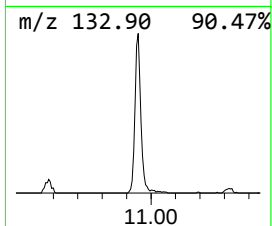
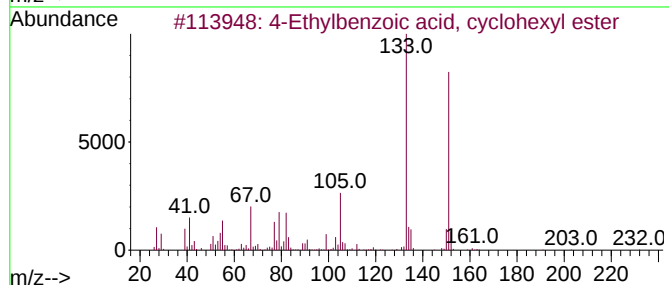
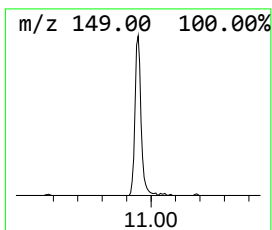
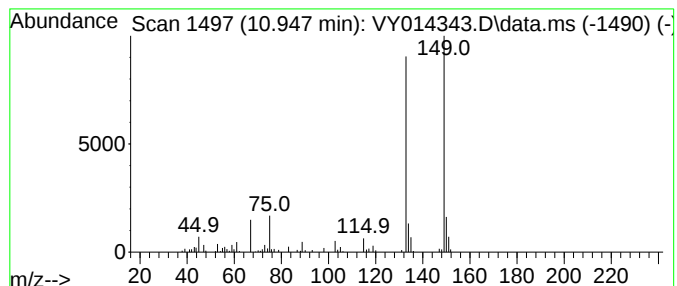
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060923S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown10.947 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	6.62 ug/l	101549	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Ethylbenzoic acid, cyclohexyl ...	232	C15H20O2	1000293-32-1	23
2			4-Ethylbenzoic acid, cyclobutyl ...	204	C13H16O2	1000292-19-6	17
3			1H-Indole-3-thiol	149	C8H7NS	000480-94-4	17
4			Benzonitrile, 4-methoxy-	133	C8H7NO	000874-90-8	17
5			Oxalamide, N-(isochroman-1-yl)me...	310	C18H18N2O3	1000304-26-0	16



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ClientSampleId :
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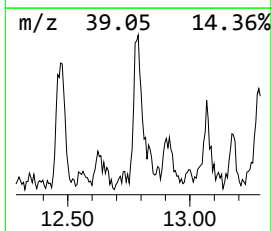
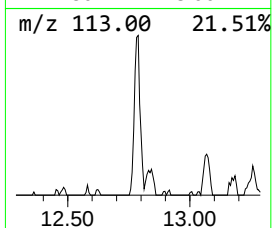
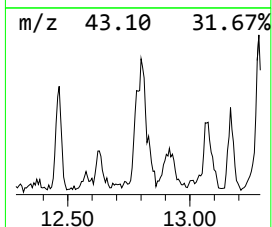
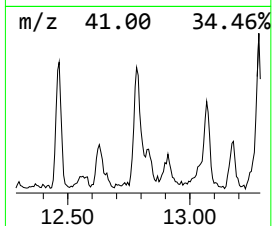
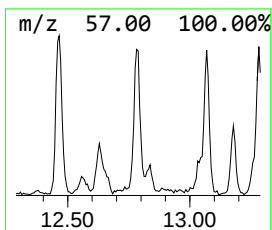
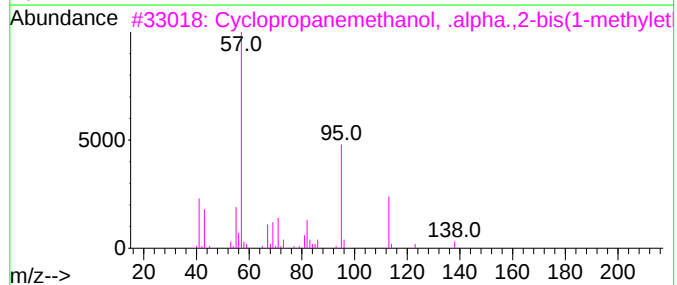
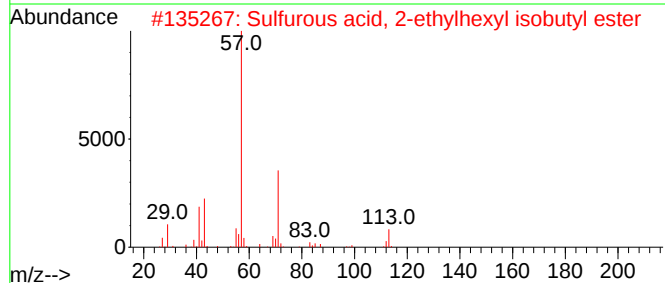
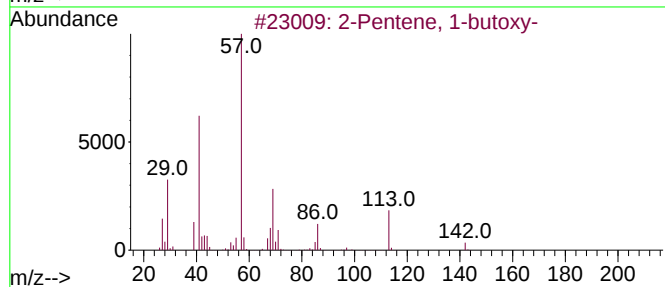
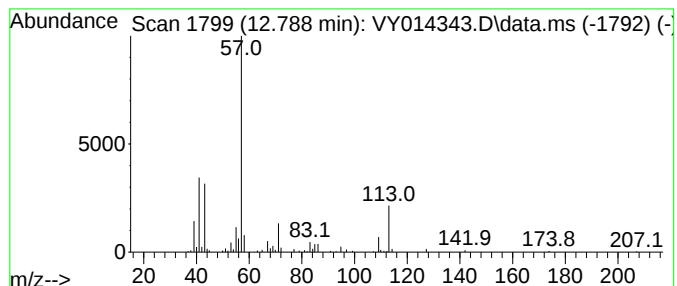
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060923S.M
Quant Title : SW846 8260

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

Peak Number 4 2-Pentene, 1-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.788	11.57 ug/l	136391	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentene, 1-butoxy-	142	C9H18O	034061-66-0	50
2			Sulfurous acid, 2-ethylhexyl iso...	250	C12H26O3S	1000309-18-7	47
3			Cyclopropanemethanol, .alpha.,2-...	156	C10H20O	056259-16-6	39
4			Nonane, 2,2,4,4,6,8,8-heptamethyl-	226	C16H34	004390-04-9	37
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	37



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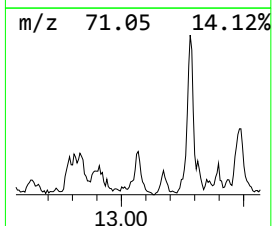
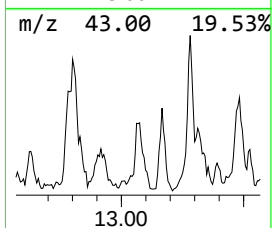
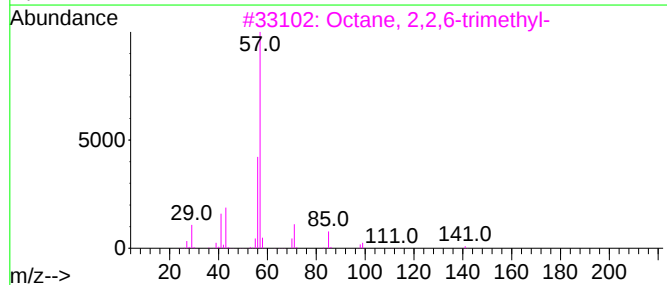
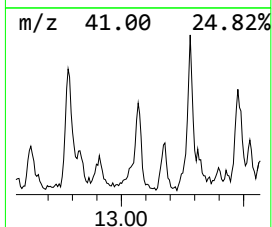
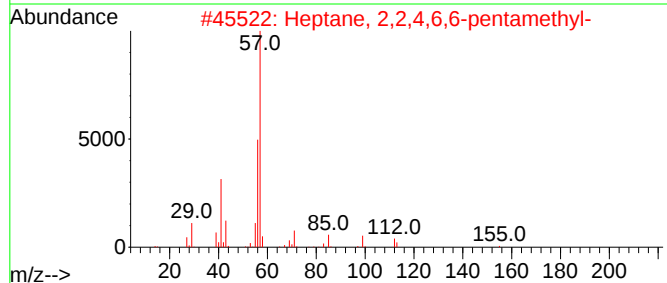
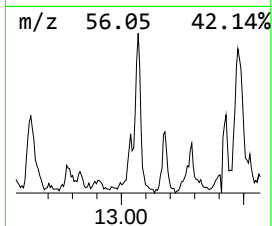
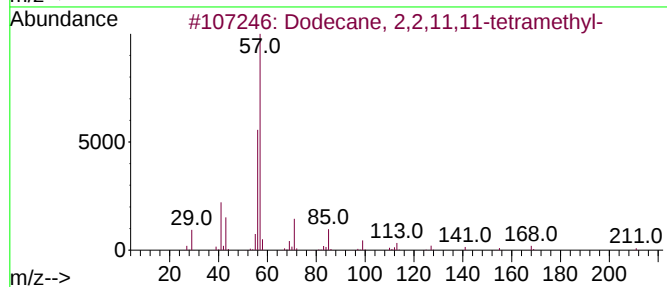
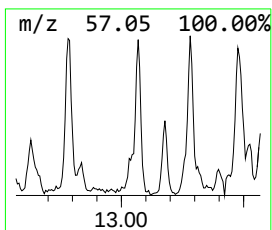
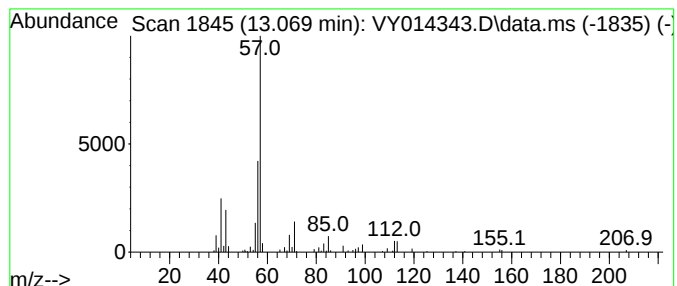
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Quant Title : SW846 8260

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

Peak Number 5 Dodecane, 2,2,11,11-tetrame... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.069	8.26 ug/l	97411	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	72
2			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	72
3			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	64
4			Decane, 2,2,7-trimethyl-	184	C13H28	062237-99-4	64
5			Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062123\
Data File : VY014343.D
Acq On : 21 Jun 2023 18:05
Operator : KP/MD
Sample : 03357-19
Misc : 6.22g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-SCAN-04-G

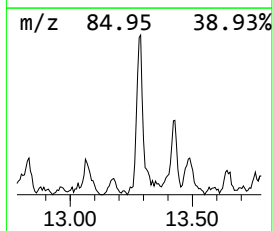
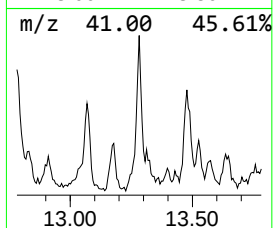
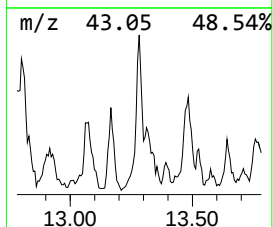
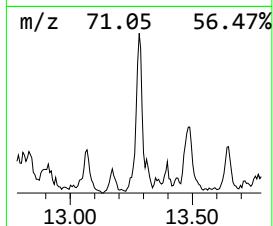
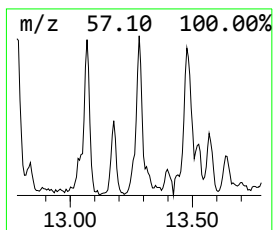
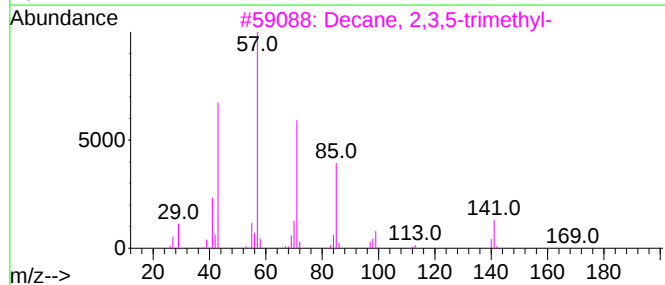
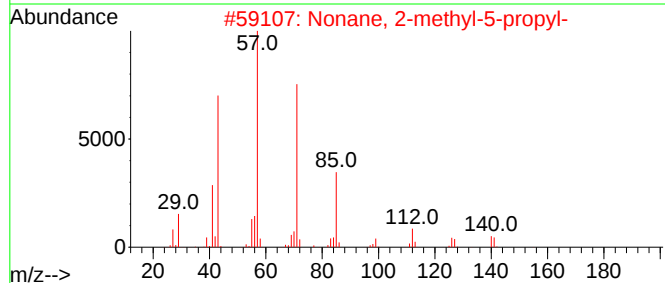
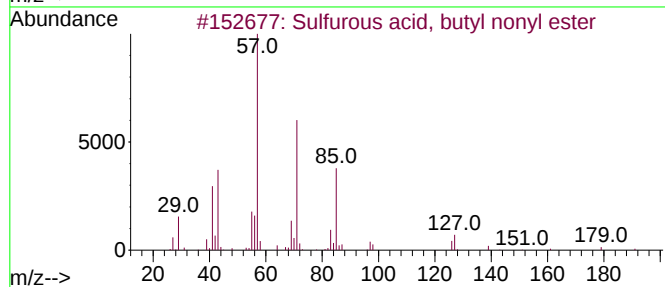
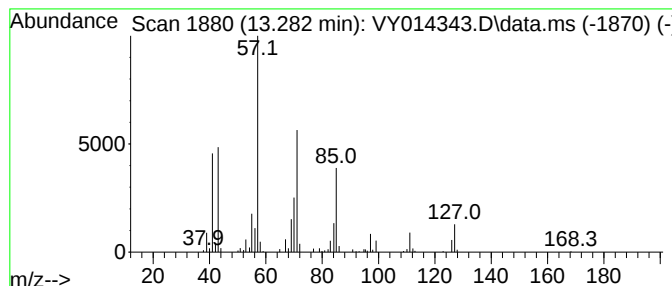
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Quant Title : SW846 8260

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

Peak Number 6 Sulfurous acid, butyl nonyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	10.70 ug/l	126166	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	59
2			Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	53
3			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	53
4			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	50
5			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062123\
Data File : VY014343.D
Acq On : 21 Jun 2023 18:05
Operator : KP/MD
Sample : 03357-19
Misc : 6.22g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-SCAN-04-G

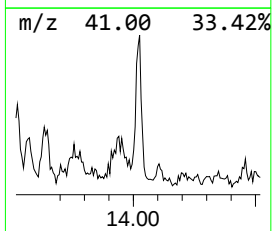
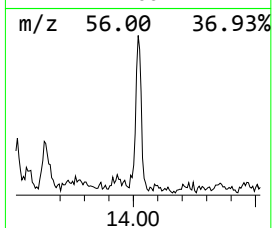
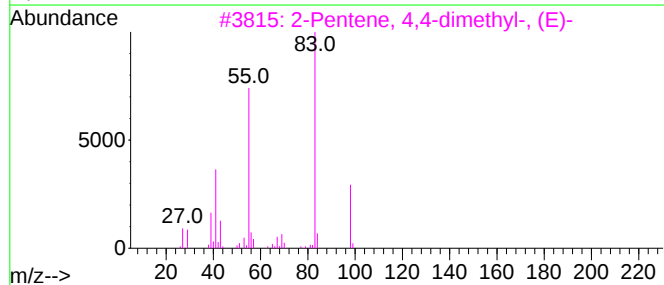
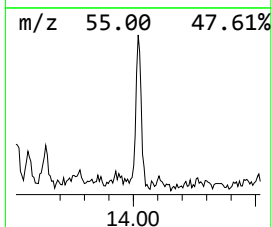
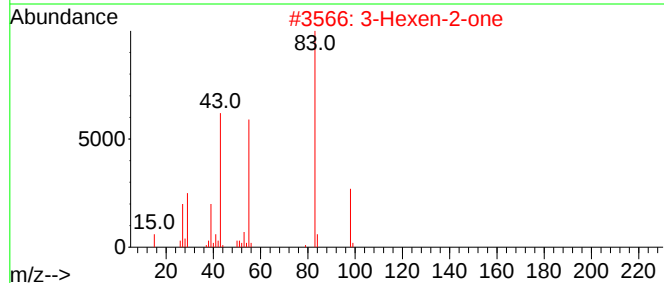
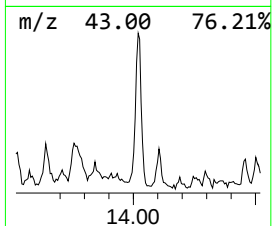
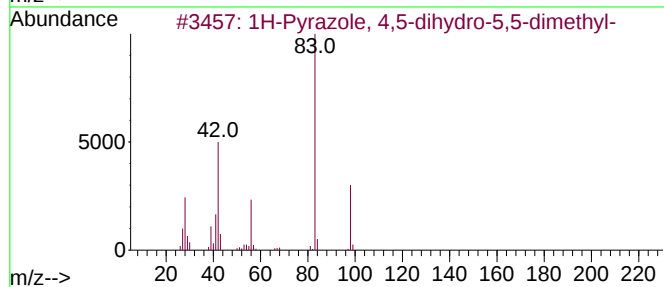
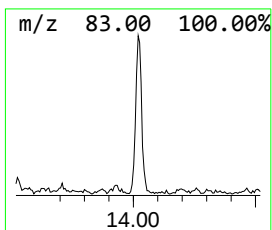
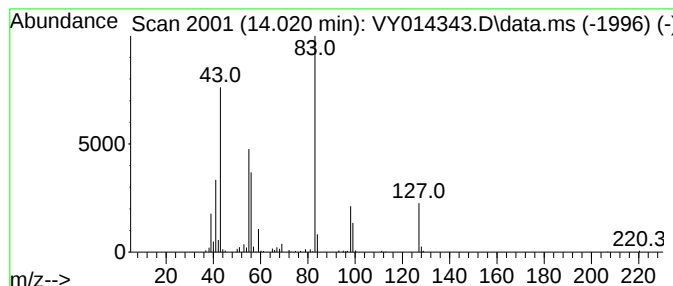
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060923S.M
Quant Title : SW846 8260

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

Peak Number 8 1H-Pyrazole, 4,5-dihydro-5,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.020	7.15 ug/l	84274	1,4-Dichlorobenzene-d4	13.428

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Pyrazole, 4,5-dihydro-5,5-dimethyl-	98	C5H10N2	004320-85-8	50
2		3-Hexen-2-one	98	C6H10O	000763-93-9	50
3		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	47
4		1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	47
5		1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062123\
Data File : VY014343.D
Acq On : 21 Jun 2023 18:05
Operator : KP/MD
Sample : 03357-19
Misc : 6.22g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-SCAN-04-G

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060923S.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
3-Buten-2-one, ...	8.770	8.5	ug/l	114339	2	8.691	672073	50.0
1-Hexene	10.289	5.3	ug/l	81477	3	11.490	766491	50.0
unknown10.947	10.947	6.6	ug/l	101549	3	11.490	766491	50.0
2-Pentene, 1-bu...	12.788	11.6	ug/l	136391	4	13.428	589456	50.0
Dodecane, 2,2,1...	13.069	8.3	ug/l	97411	4	13.428	589456	50.0
Sulfurous acid,...	13.282	10.7	ug/l	126166	4	13.428	589456	50.0
1H-Pyrazole, 4,...	14.020	7.2	ug/l	84274	4	13.428	589456	50.0