

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010622\
 Data File : VY007039.D
 Acq On : 06 Jan 2022 17:52
 Operator : SY/MD
 Sample : N1049-03
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 7211979

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\82Y010522S.M
 Title : SW846 8260

Signal : TIC: VY007039.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.722	464	476	490	rVB3	12488	41111	5.29%	0.675%
2	5.753	634	645	656	rBV4	5918	19107	2.46%	0.314%
3	6.984	836	847	855	rBV	8314	26826	3.45%	0.440%
4	7.722	955	968	974	rBV	113612	270549	34.82%	4.441%
5	7.795	974	980	990	rVB	173704	390629	50.27%	6.413%
6	8.143	1022	1037	1047	rBV	112273	261559	33.66%	4.294%
7	8.691	1119	1127	1136	rBV	279609	557354	71.73%	9.150%
8	10.185	1364	1372	1381	rBV	447812	776992	100.00%	12.756%
9	10.581	1429	1437	1443	rBV2	19464	34334	4.42%	0.564%
10	10.947	1491	1497	1507	rBV	14066	26066	3.35%	0.428%
11	11.319	1553	1558	1565	rBV2	14354	23868	3.07%	0.392%
12	11.490	1577	1586	1598	rBV	414940	695424	89.50%	11.416%
13	12.483	1742	1749	1760	rBV2	381342	627681	80.78%	10.304%
14	12.819	1798	1804	1809	rBV9	3446	8078	1.04%	0.133%
15	13.184	1860	1864	1873	rVB4	11235	19923	2.56%	0.327%
16	13.355	1885	1892	1897	rBV3	7880	15227	1.96%	0.250%
17	13.428	1897	1904	1910	rBV	444986	682361	87.82%	11.202%
18	13.483	1910	1913	1921	rVV4	15544	32176	4.14%	0.528%
19	13.550	1921	1924	1931	rVV7	3999	9783	1.26%	0.161%
20	13.648	1933	1940	1943	rVV2	14427	26796	3.45%	0.440%
21	13.684	1943	1946	1953	rVV3	12909	29465	3.79%	0.484%
22	13.788	1953	1963	1967	rVV	48882	101996	13.13%	1.674%
23	13.855	1971	1974	1977	rVV2	17416	28757	3.70%	0.472%
24	13.904	1977	1982	1987	rVV2	25819	51196	6.59%	0.840%
25	13.965	1987	1992	1997	rVV2	22630	42743	5.50%	0.702%
26	14.038	1997	2004	2009	rVV	31850	54980	7.08%	0.903%
27	14.111	2012	2016	2026	rVV	15658	34312	4.42%	0.563%
28	14.263	2037	2041	2046	rBV6	5689	8107	1.04%	0.133%
29	14.428	2064	2068	2071	rBV6	5085	7795	1.00%	0.128%
30	14.538	2080	2086	2090	rVB	31472	47911	6.17%	0.787%
31	14.617	2093	2099	2105	rBV2	18657	38036	4.90%	0.624%
32	14.855	2134	2138	2141	rBV	17978	27214	3.50%	0.447%
33	14.891	2141	2144	2150	rVB2	19150	27700	3.57%	0.455%
34	14.977	2151	2158	2163	rBV3	11844	23416	3.01%	0.384%
35	15.062	2168	2172	2176	rBV7	6520	11411	1.47%	0.187%
36	15.324	2210	2215	2222	rVB3	8021	16680	2.15%	0.274%

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37	15.428	2228	2232	2235	rVV2	13573	23306	3.00%	0.383%
38	15.501	2239	2244	2249	rVV2	53663	92858	11.95%	1.524%
39	15.568	2250	2255	2261	rVV2	13907	30095	3.87%	0.494%
40	15.629	2262	2265	2270	rVB3	8006	14127	1.82%	0.232%
41	15.806	2288	2294	2297	rBV6	13231	32300	4.16%	0.530%
42	15.934	2310	2315	2321	rVB3	15855	32646	4.20%	0.536%
43	16.050	2329	2334	2341	rVB4	15309	38733	4.98%	0.636%
44	16.165	2349	2353	2362	rBV6	21963	64660	8.32%	1.061%
45	16.281	2365	2372	2383	rVV4	85024	240830	31.00%	3.954%
46	16.373	2383	2387	2389	rBV2	21530	31067	4.00%	0.510%
47	16.422	2390	2395	2400	rVB	136781	251461	32.36%	4.128%
48	16.495	2401	2407	2413	rBV4	47477	141757	18.24%	2.327%

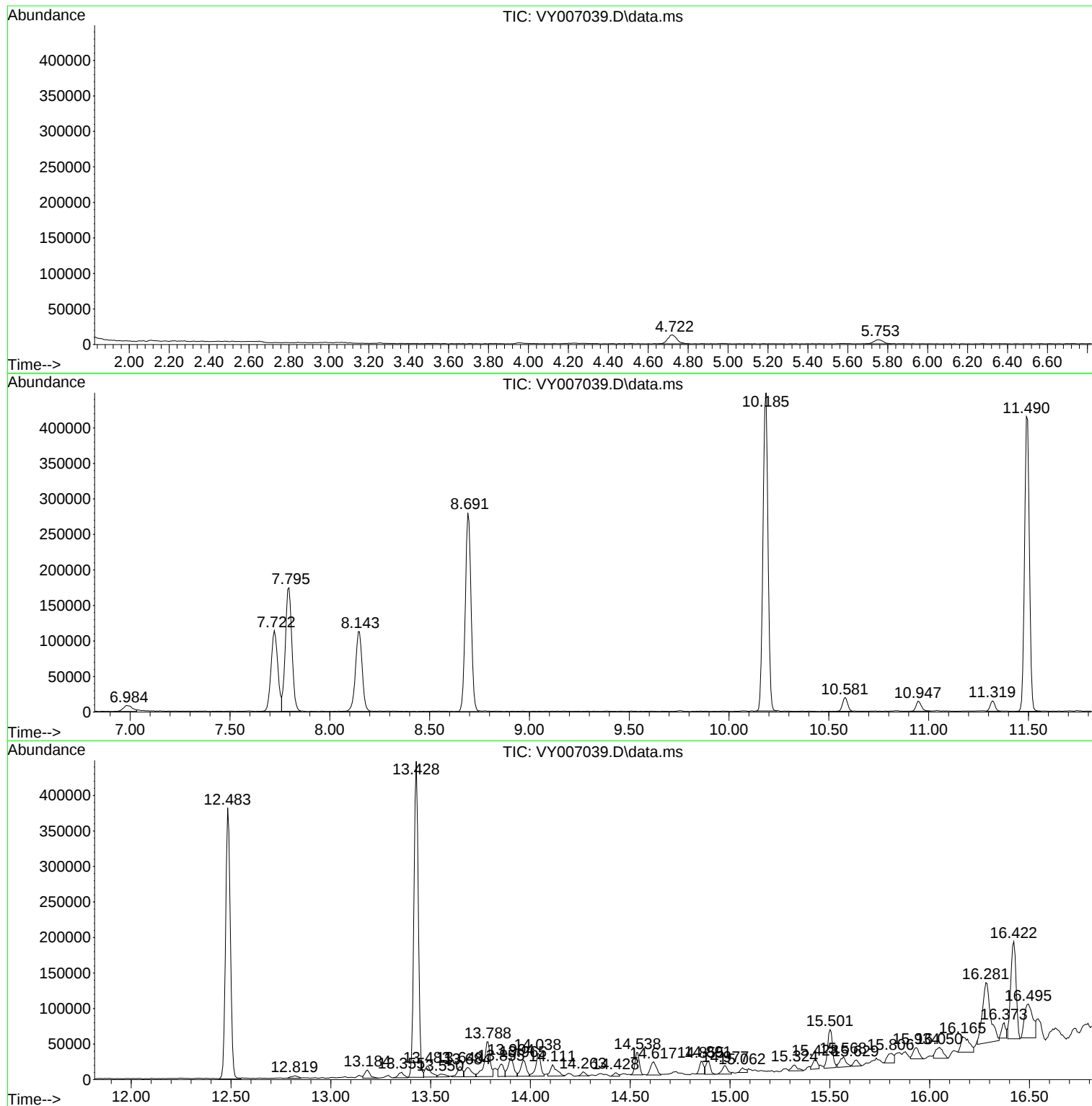
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Quant Title : SW846 8260

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



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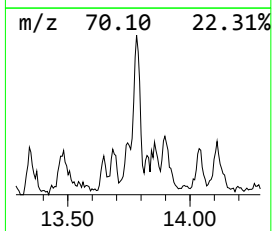
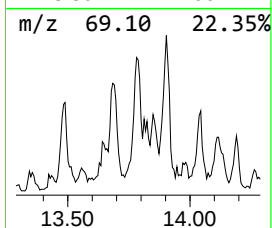
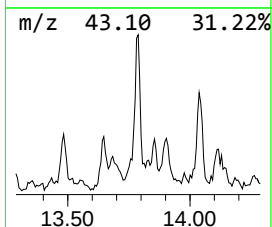
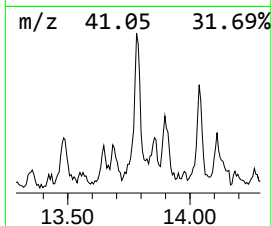
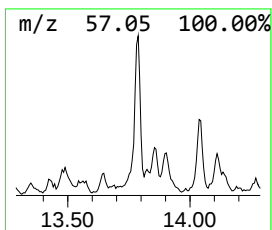
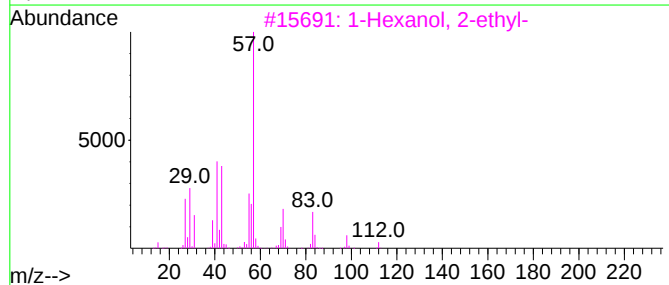
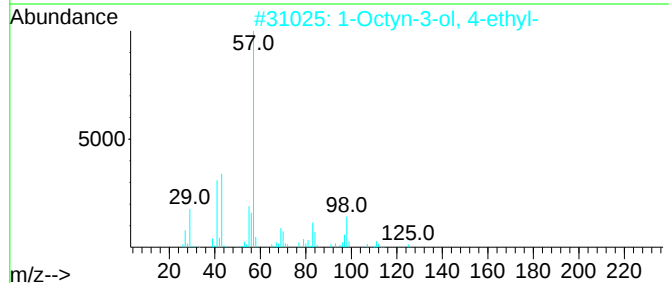
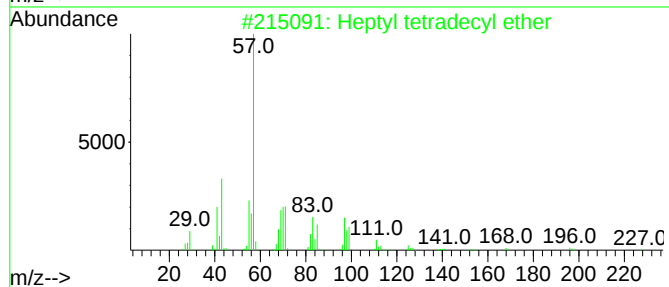
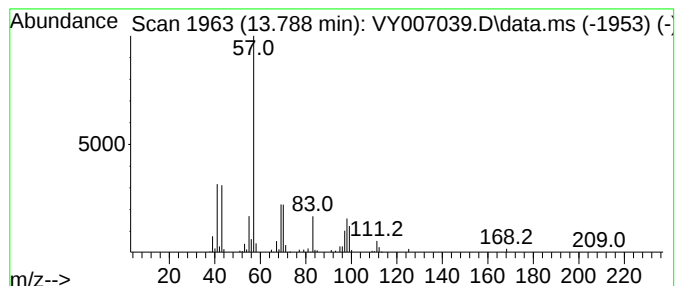
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Quant Title : SW846 8260

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

Peak Number 2 Heptyl tetradecyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.788	7.47 ug/l	101996	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	50
2			1-Octyn-3-ol, 4-ethyl-	154	C10H18O	005877-42-9	50
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	45
5			4-Octylcyclohexanone	210	C14H26O	1000428-94-1	43



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Instrument :
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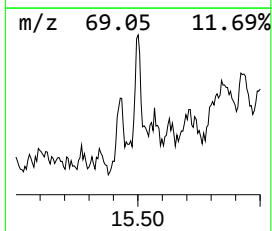
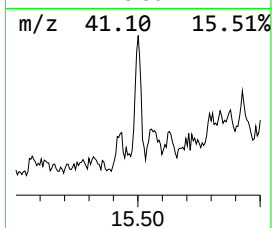
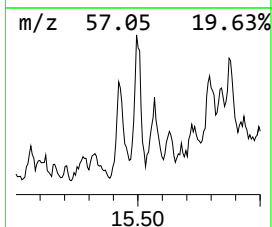
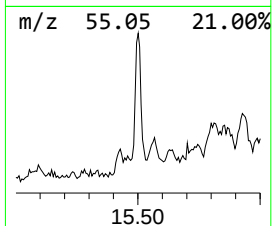
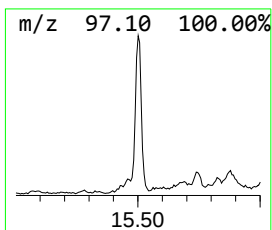
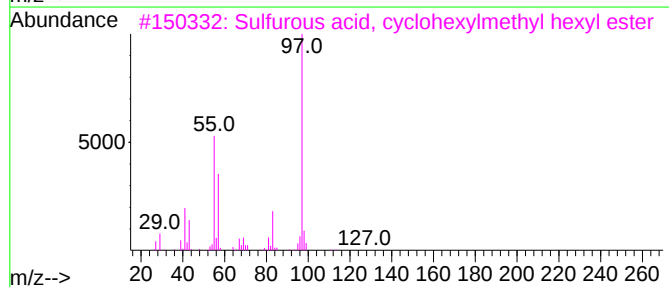
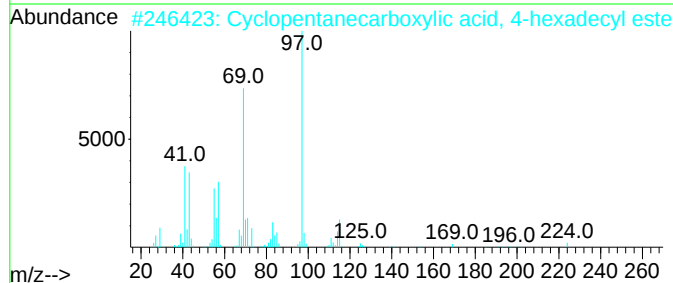
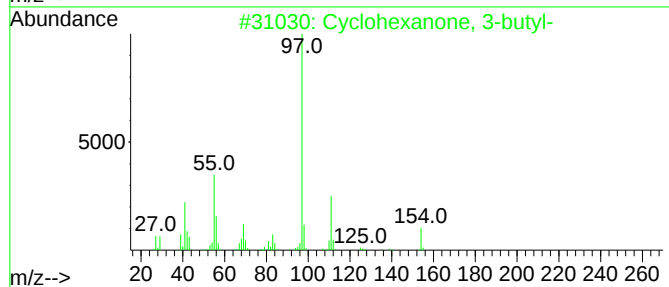
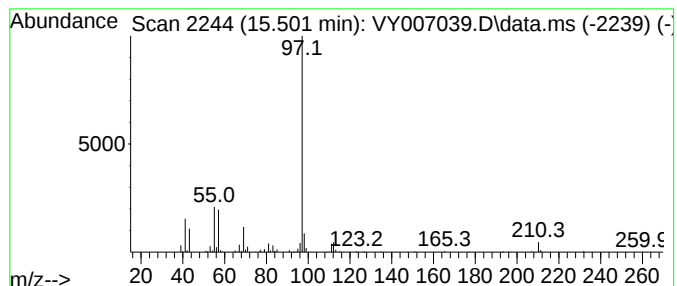
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010522S.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclohexanone, 3-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.501	6.80 ug/l	92858	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3-butyl-	154	C10H18O	039178-69-3	72
2			Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	56
3			Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1010309-21-6	53
4			Sulfurous acid, cyclohexylmethyl...	360	C20H40O3S	1000309-22-1	50
5			Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	45



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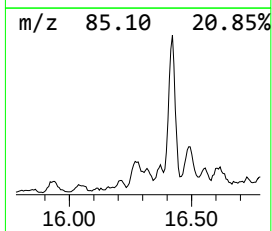
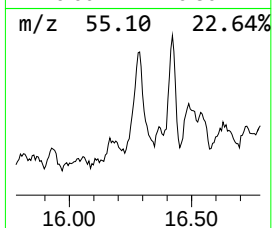
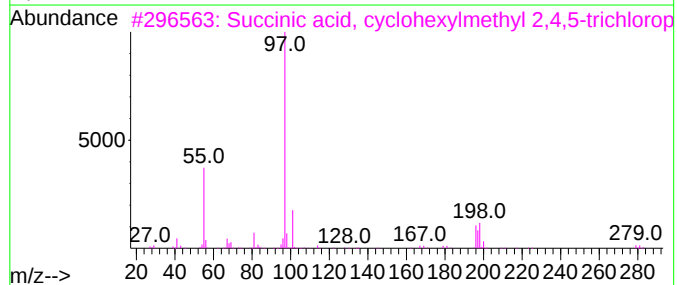
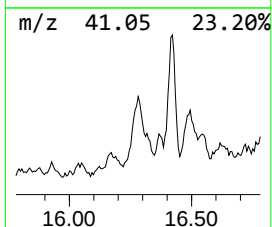
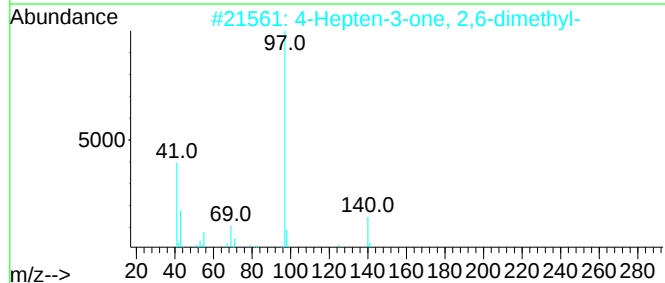
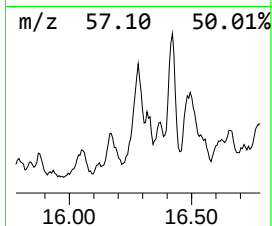
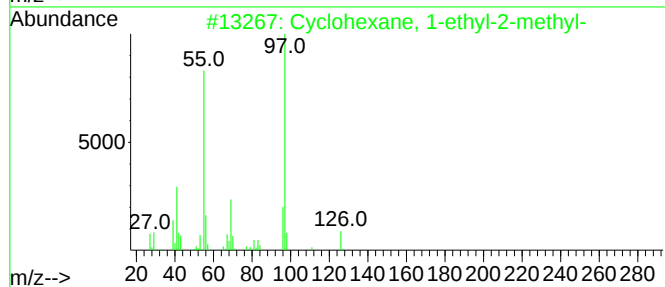
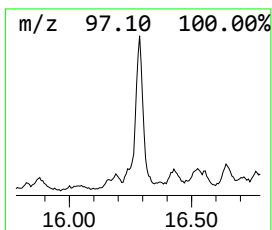
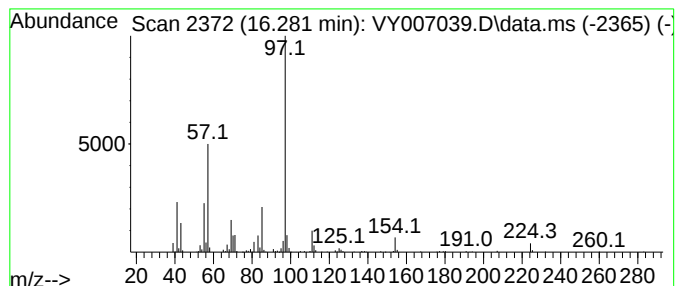
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown16.281 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.281	17.65 ug/l	240830	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	47
2			4-Hepten-3-one, 2,6-dimethyl-	140	C9H16O	056259-14-4	47
3			Succinic acid, cyclohexylmethyl ...	392	C17H19C13O4	1000389-96-9	47
4			1H-Pyrazole, 5-ethyl-4,5-dihydro...	126	C7H14N2	021981-22-6	47
5			Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1010309-22-7	47



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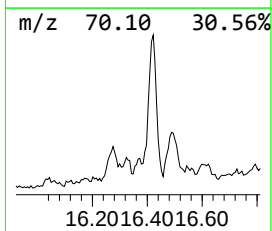
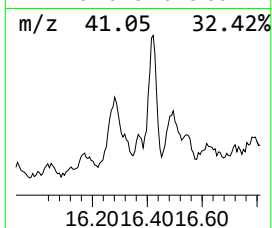
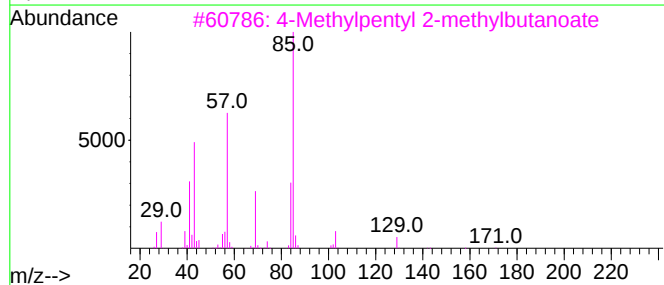
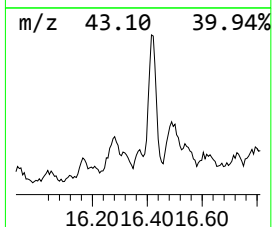
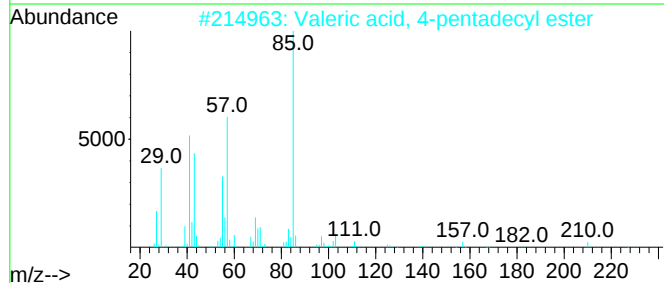
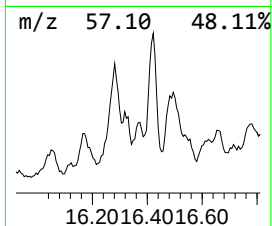
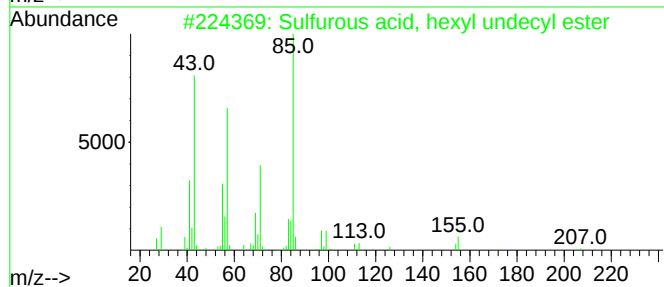
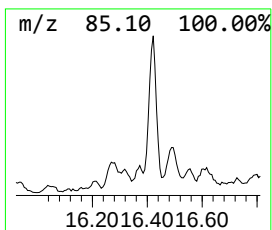
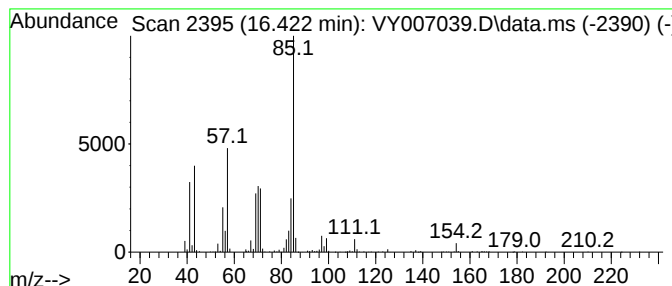
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Sulfurous acid, hexyl undec... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.422	18.43 ug/l	251461	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, hexyl undecyl ester	320	C17H36O3S	1000309-13-3	50
2			Valeric acid, 4-pentadecyl ester	312	C20H40O2	1000281-99-4	50
3			4-Methylpentyl 2-methylbutanoate	186	C11H22O2	035852-40-5	47
4			Undecane, 4,4-dimethyl-	184	C13H28	017312-68-4	45
5			Sulfurous acid, dodecyl hexyl ester	334	C18H38O3S	1000309-13-4	43



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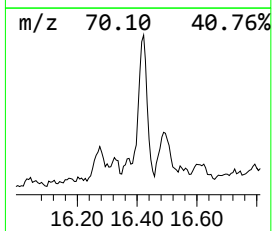
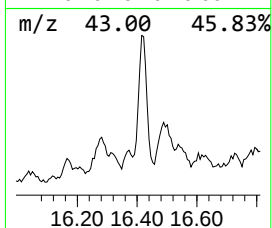
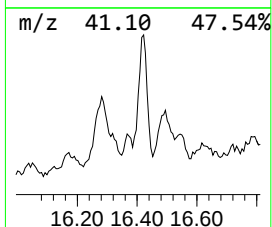
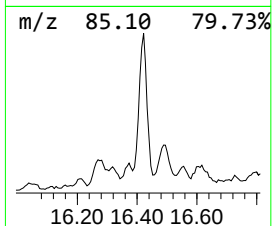
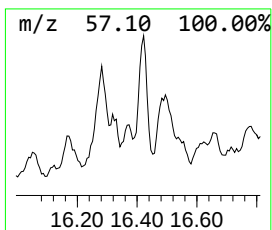
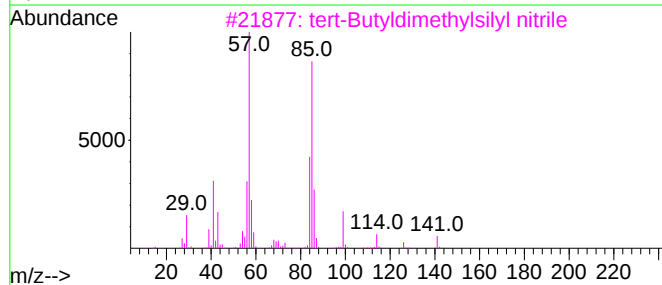
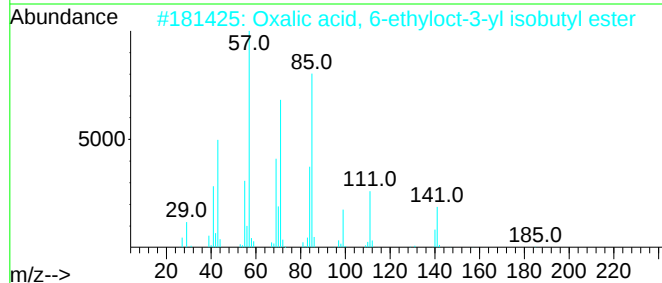
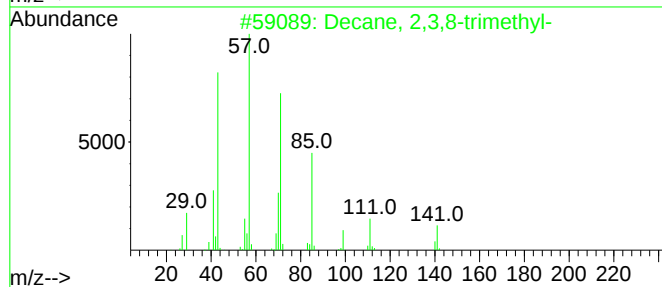
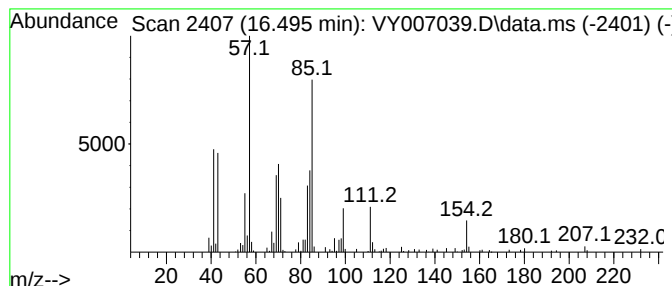
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010522S.M
Quant Title : SW846 8260

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

Peak Number 6 Decane, 2,3,8-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.495	10.39 ug/l	141757	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	53
2			Oxalic acid, 6-ethyloct-3-yl iso...	286	C16H30O4	1010309-34-1	40
3			tert-Butyldimethylsilyl nitrile	141	C7H15NSi	056522-24-8	38
4			4,4-Dimethyl octane	142	C10H22	015869-95-1	37
5			Pentanethioic acid, S-propyl ester	160	C8H16OS	002432-76-0	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010622\
Data File : VY007039.D
Acq On : 06 Jan 2022 17:52
Operator : SY/MD
Sample : N1049-03
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
7211979

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010522S.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
Heptyl tetradec...	13.788	7.5	ug/l	101996	4	13.428	682361	50.0
Cyclohexanone, ...	15.501	6.8	ug/l	92858	4	13.428	682361	50.0
unknown16.281	16.281	17.6	ug/l	240830	4	13.428	682361	50.0
Sulfurous acid,...	16.422	18.4	ug/l	251461	4	13.428	682361	50.0
Decane, 2,3,8-t...	16.495	10.4	ug/l	141757	4	13.428	682361	50.0