

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092321\
 Data File : VY006121.D
 Acq On : 23 Sep 2021 14:01
 Operator : SY/MD
 Sample : M3875-11
 Misc : 4.35G/5ML/MSVOA_Y/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20883

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\82Y091421S.M
 Title : SW846 8260

Signal : TIC: VY006121.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	5	9	17	rVB2	39799	65638	2.70%	0.439%
2	2.235	62	68	82	rVB2	30439	63058	2.60%	0.422%
3	3.272	230	238	251	rVB2	13929	39638	1.63%	0.265%
4	3.954	340	350	359	rBV	274357	747761	30.79%	5.001%
5	4.046	359	365	376	rVB2	56194	152994	6.30%	1.023%
6	4.210	381	392	413	rBV3	39051	130775	5.39%	0.875%
7	4.820	482	492	505	rVV2	53844	192172	7.91%	1.285%
8	6.996	834	849	862	rBV	32846	92535	3.81%	0.619%
9	7.722	958	968	974	rBV	81813	197106	8.12%	1.318%
10	7.795	974	980	992	rVB	166747	374405	15.42%	2.504%
11	8.149	1029	1038	1051	rVB	90167	208104	8.57%	1.392%
12	8.697	1117	1128	1138	rBV	206270	417321	17.19%	2.791%
13	10.185	1363	1372	1377	rVV	325598	566323	23.32%	3.788%
14	10.246	1377	1382	1395	rVV	291759	493869	20.34%	3.303%
15	11.490	1579	1586	1595	rBV	256004	422370	17.39%	2.825%
16	11.715	1617	1623	1632	rVB2	32434	65072	2.68%	0.435%
17	11.886	1641	1651	1659	rBV	104030	163873	6.75%	1.096%
18	12.307	1713	1720	1722	rBV	61944	91464	3.77%	0.612%
19	12.337	1722	1725	1731	rVB	63778	98579	4.06%	0.659%
20	12.483	1743	1749	1752	rBV2	202799	356329	14.67%	2.383%
21	12.514	1752	1754	1761	rVV	195280	253127	10.42%	1.693%
22	12.806	1788	1802	1810	rBV2	72864	176384	7.26%	1.180%
23	12.898	1810	1817	1824	rVB4	37222	71770	2.96%	0.480%
24	12.983	1824	1831	1843	rBV	247830	402741	16.58%	2.694%
25	13.160	1855	1860	1866	rVB	577716	778915	32.08%	5.209%
26	13.251	1866	1875	1879	rBV7	23374	57325	2.36%	0.383%
27	13.343	1879	1890	1898	rVV2	1520043	2428363	100.00%	16.241%
28	13.428	1898	1904	1909	rVV	202849	338754	13.95%	2.266%
29	13.489	1909	1914	1918	rVV	193958	312547	12.87%	2.090%
30	13.532	1918	1921	1927	rVV	50822	81835	3.37%	0.547%
31	13.751	1949	1957	1963	rBV	1210877	1675691	69.00%	11.207%
32	13.898	1972	1981	1988	rBV	161831	289417	11.92%	1.936%
33	13.971	1988	1993	1997	rVV2	28130	49001	2.02%	0.328%
34	14.020	1997	2001	2007	rVB5	16080	27052	1.11%	0.181%
35	14.105	2012	2015	2018	rVV	19699	27744	1.14%	0.186%
36	14.148	2018	2022	2028	rVB3	28786	46457	1.91%	0.311%

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37	14.239	2033	2037	2040	rBV4	24123	46155	1.90%	0.309%
38	14.318	2046	2050	2054	rVB2	29771	38622	1.59%	0.258%
39	14.385	2057	2061	2064	rVV2	25025	33179	1.37%	0.222%
40	14.611	2088	2098	2103	rBV	562273	749800	30.88%	5.015%
41	14.678	2103	2109	2113	rVV4	22834	54146	2.23%	0.362%
42	14.733	2113	2118	2124	rVB	74124	115156	4.74%	0.770%
43	14.946	2148	2153	2158	rBV3	69457	118819	4.89%	0.795%
44	15.056	2165	2171	2173	rBV3	19707	40749	1.68%	0.273%
45	15.099	2174	2178	2179	rVV3	30598	45413	1.87%	0.304%
46	15.135	2180	2184	2192	rVV4	130388	223488	9.20%	1.495%
47	15.215	2192	2197	2204	rVB	101808	163093	6.72%	1.091%
48	15.440	2229	2234	2241	rBV	293027	423862	17.45%	2.835%
49	15.544	2249	2251	2256	rVB3	21982	30136	1.24%	0.202%
50	15.611	2256	2262	2267	rVB3	37744	73491	3.03%	0.492%
51	15.970	2316	2321	2325	rBV3	23730	38415	1.58%	0.257%
52	16.019	2325	2329	2336	rVV6	31799	73567	3.03%	0.492%
53	16.099	2336	2342	2347	rVB4	34347	75576	3.11%	0.505%
54	16.159	2347	2352	2358	rBV	56866	98784	4.07%	0.661%
55	16.233	2359	2364	2369	rBV2	22044	37875	1.56%	0.253%
56	16.367	2379	2386	2392	rBV	264118	472487	19.46%	3.160%
57	16.477	2400	2404	2409	rBV6	19403	42634	1.76%	0.285%

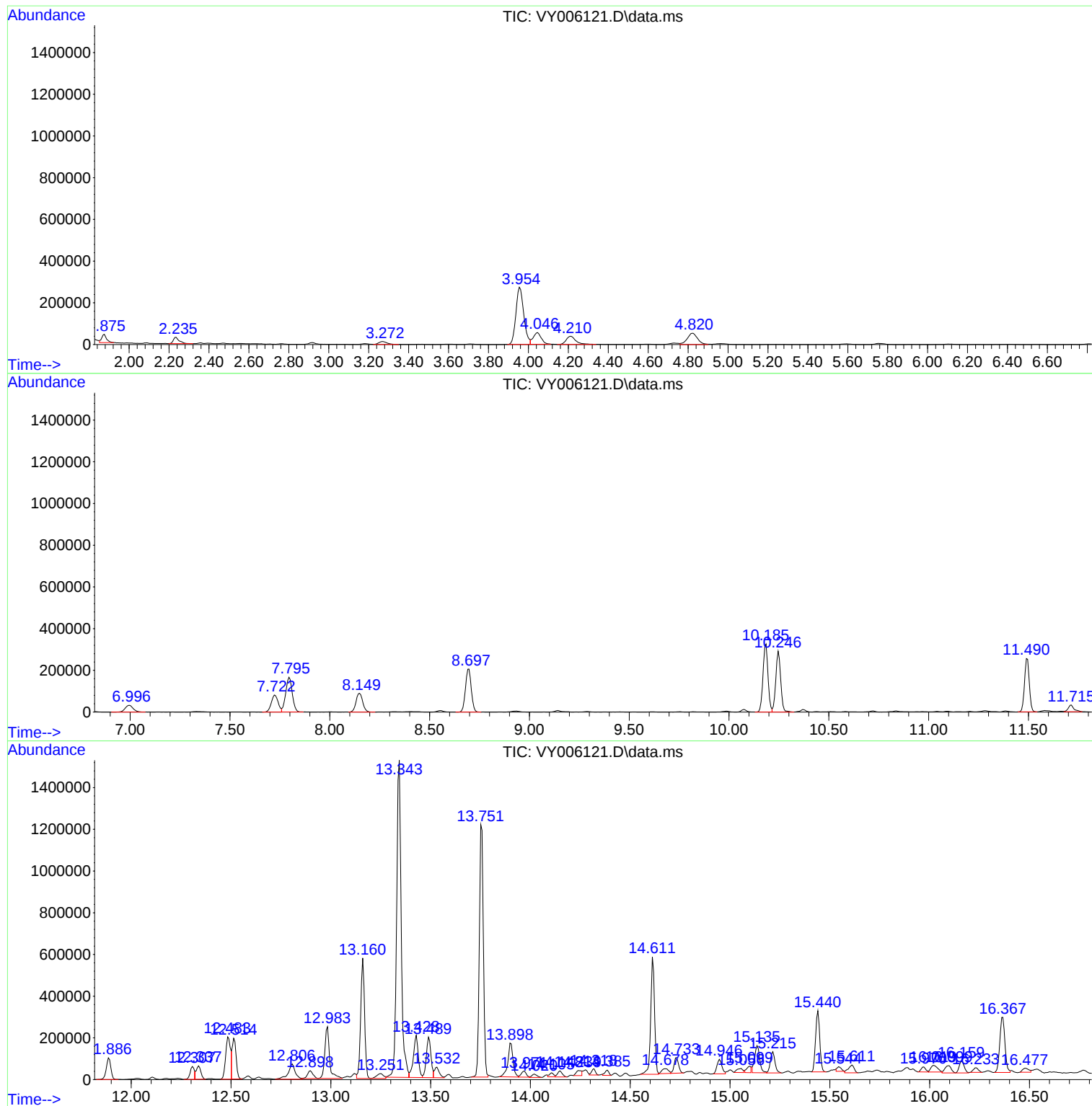
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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



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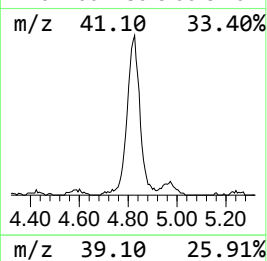
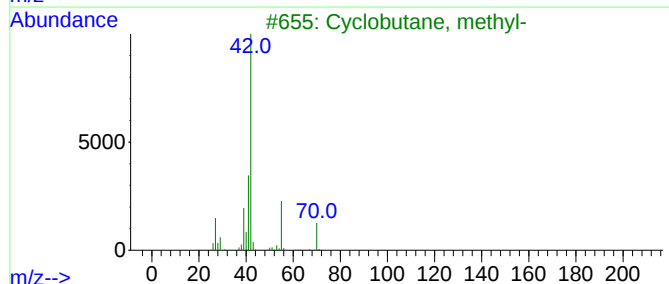
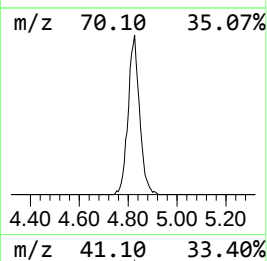
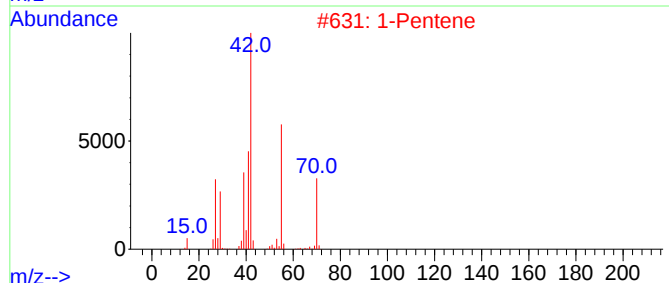
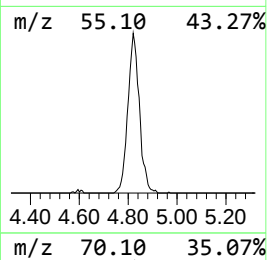
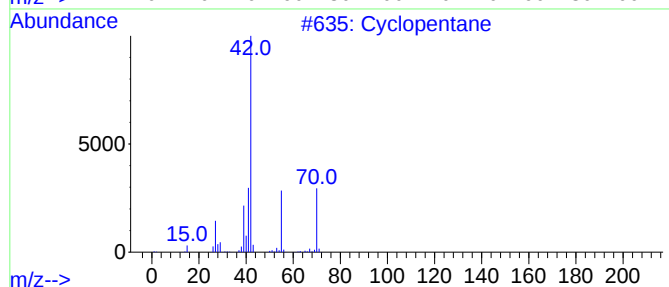
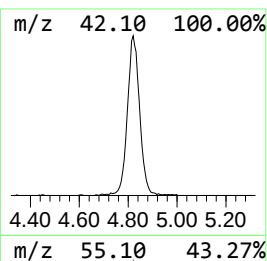
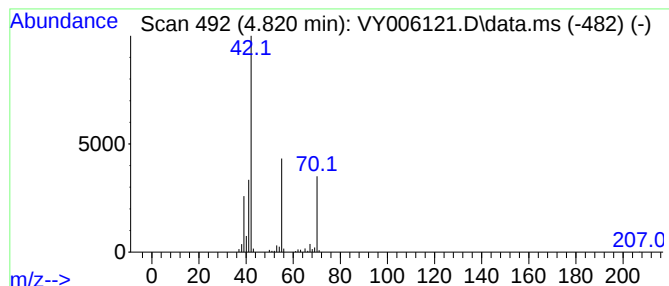
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Quant Title : SW846 8260

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

Peak Number 1 Cyclopentane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.820	25.66 ug/l	192172	Pentafluorobenzene	7.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	86
2			1-Pentene	70	C5H10	000109-67-1	72
3			Cyclobutane, methyl-	70	C5H10	000598-61-8	72
4			Cyclobutanone	70	C4H6O	001191-95-3	9
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	9



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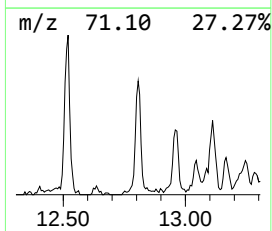
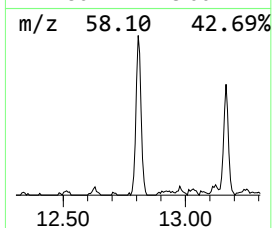
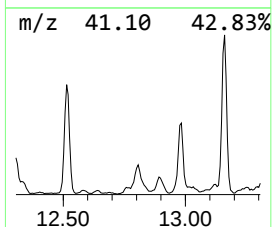
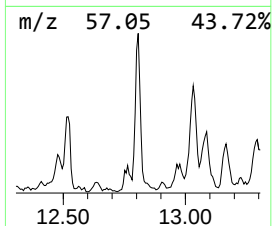
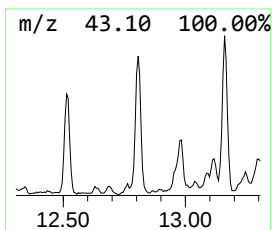
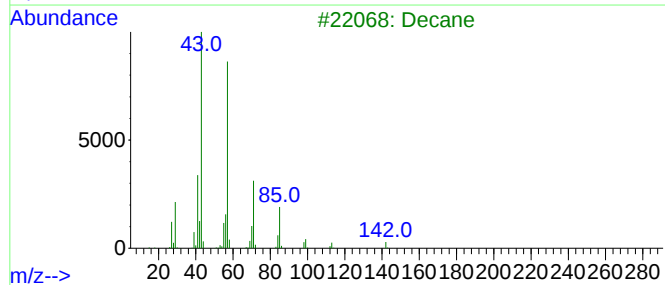
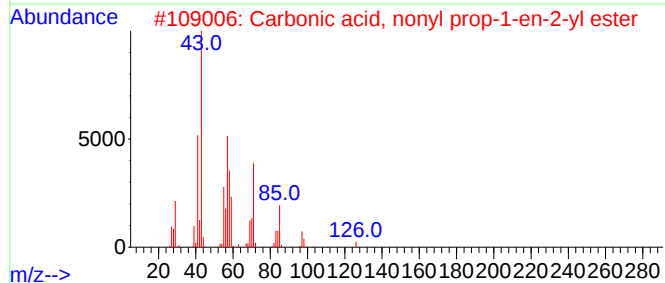
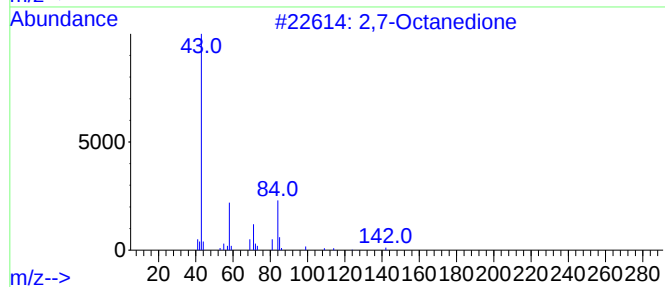
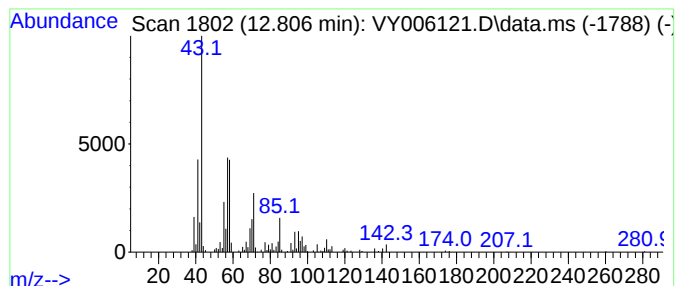
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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

Peak Number 2 2,7-Octanedione Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.806	26.03 ug/l	176384	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,7-Octanedione	142	C8H14O2	001626-09-1	50
2			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	43
3			Decane	142	C10H22	000124-18-5	38
4			1,3-Dimethylcyclopentanol	114	C7H14O	019550-46-0	22
5			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	18



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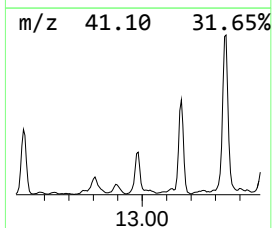
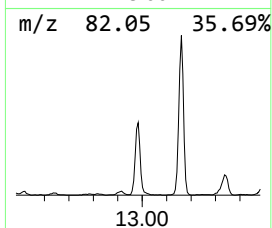
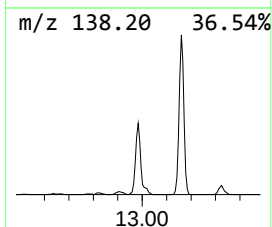
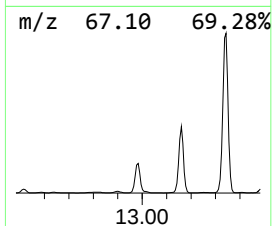
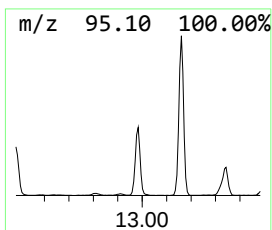
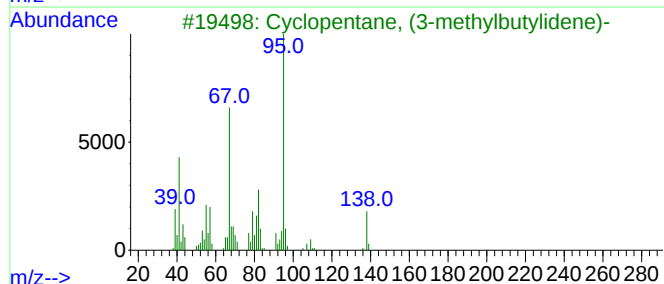
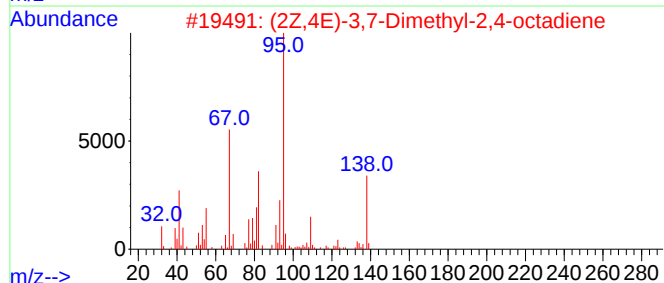
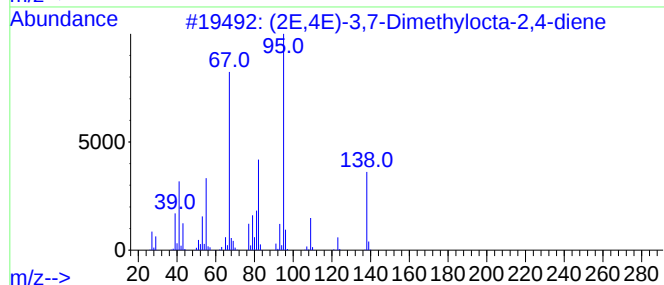
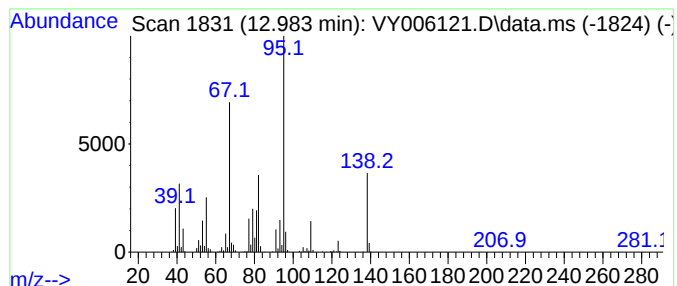
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 (2E,4E)-3,7-Dimethylocta-2,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	59.44 ug/l	402741	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(2E,4E)-3,7-Dimethylocta-2,4-diene	138	C10H18	006874-39-1	96
2			(2Z,4E)-3,7-Dimethyl-2,4-octadiene	138	C10H18	1000374-08-4	94
3			Cyclopentane, (3-methylbutylidene)-	138	C10H18	053366-51-1	80
4			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	002778-68-9	80
5			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-27-2	80



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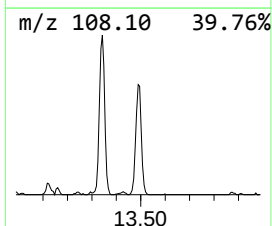
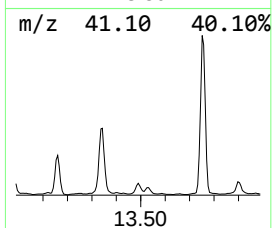
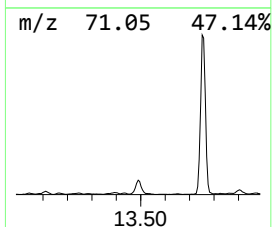
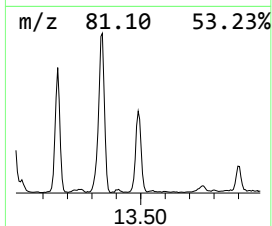
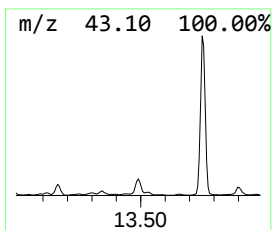
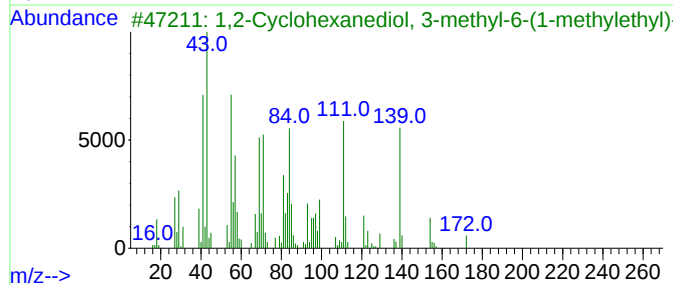
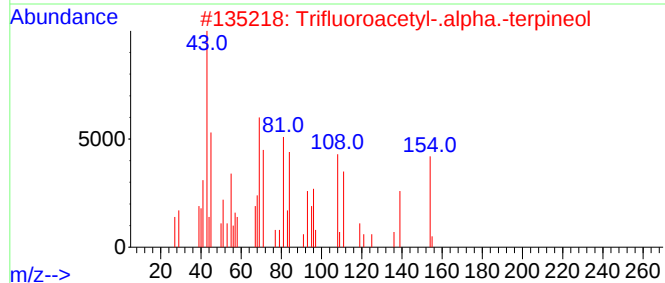
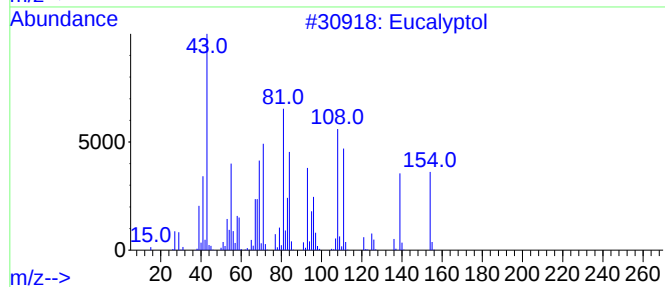
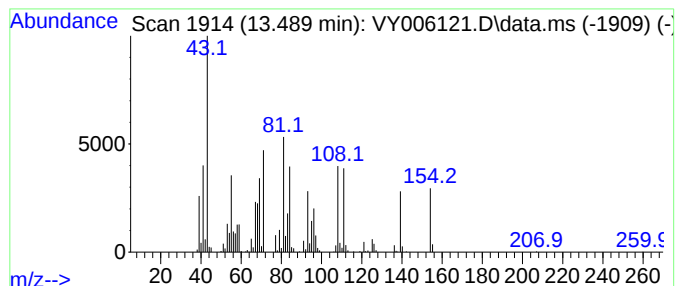
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Eucalyptol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.489	46.13 ug/l	312547	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	80
3			1,2-Cyclohexanediol, 3-methyl-6-...	172	C10H20O2	042962-93-6	37
4			2-Oxabicyclo[2.2.2]octan-6-ol, 1-...	212	C12H20O3	057709-95-2	35
5			Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-40-3	32



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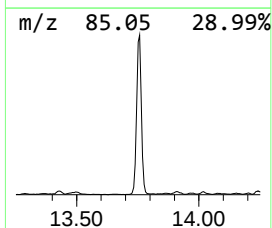
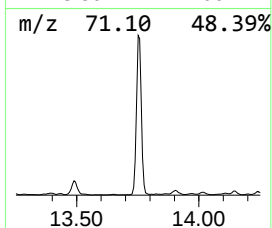
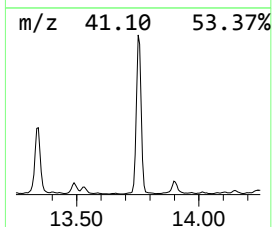
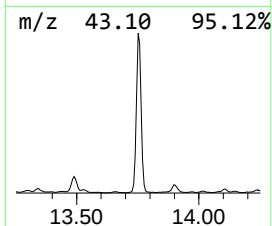
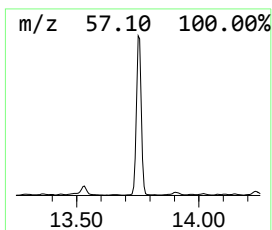
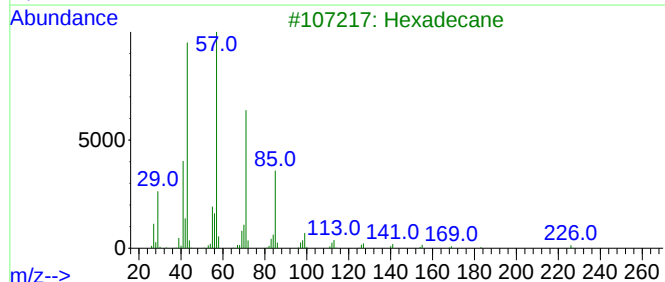
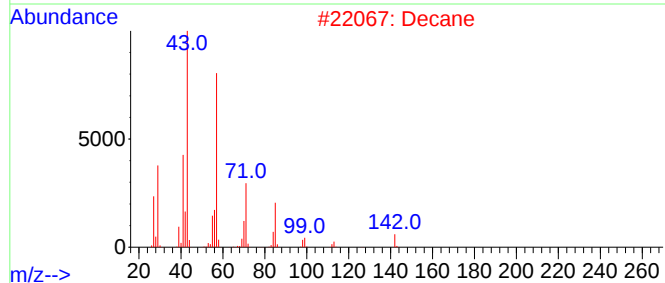
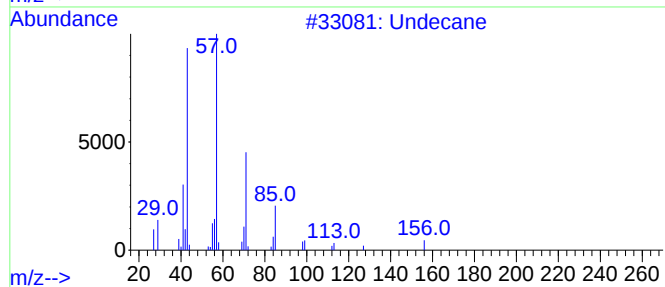
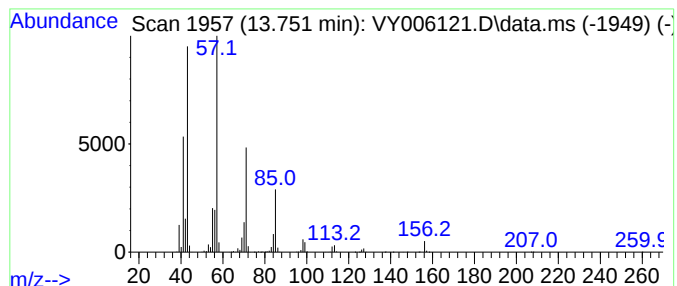
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Quant Title : SW846 8260

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

Peak Number 5 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	247.33 ug/l	1675690	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	94
2	Decane			142	C10H22	000124-18-5	83
3	Hexadecane			226	C16H34	000544-76-3	83
4	Decane, 2,3,6-trimethyl-			184	C13H28	062238-12-4	72
5	Decane, 3,6-dimethyl-			170	C12H26	017312-53-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092321\
Data File : VY006121.D
Acq On : 23 Sep 2021 14:01
Operator : SY/MD
Sample : M3875-11
Misc : 4.35G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20883

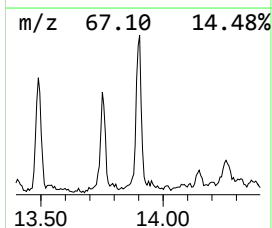
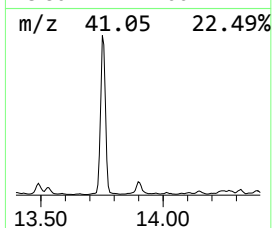
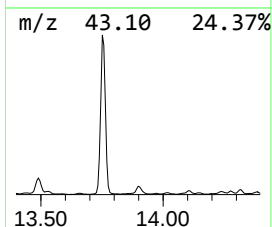
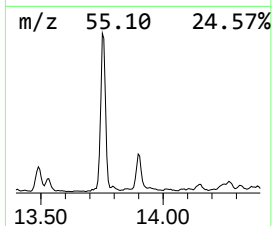
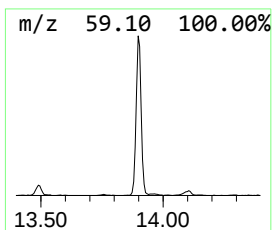
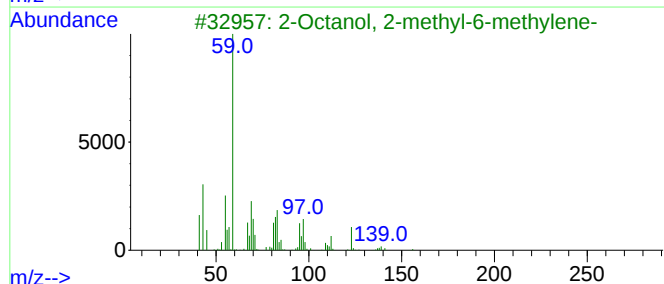
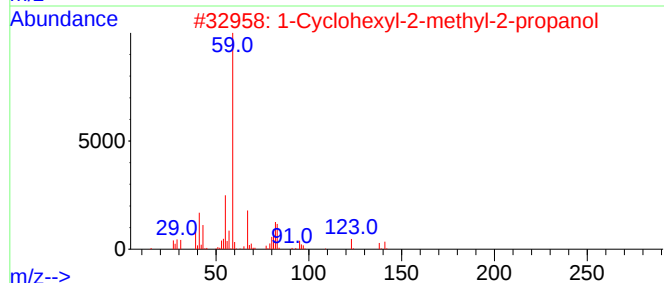
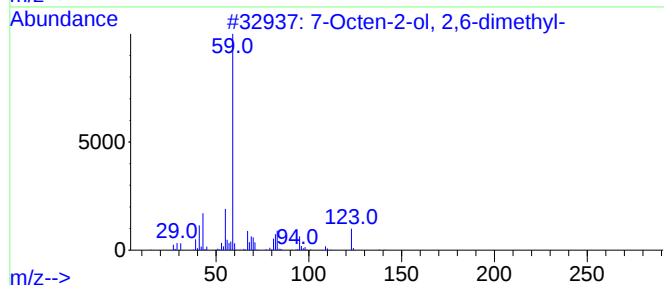
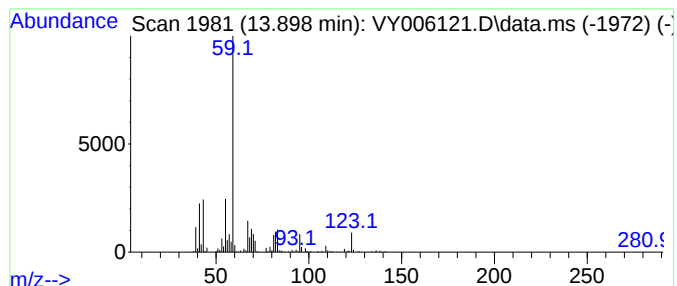
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Quant Title : SW846 8260

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

Peak Number 6 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	42.72 ug/l	289417	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	90
2			1-Cyclohexyl-2-methyl-2-propanol	156	C10H20O	005531-30-6	64
3			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	56
4			2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	53
5			1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092321\
Data File : VY006121.D
Acq On : 23 Sep 2021 14:01
Operator : SY/MD
Sample : M3875-11
Misc : 4.35G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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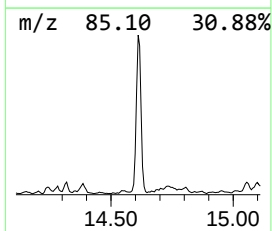
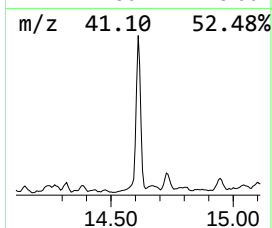
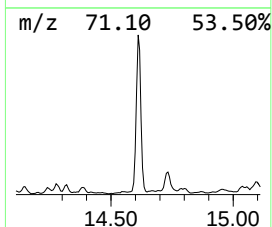
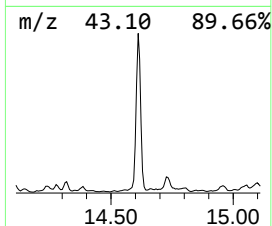
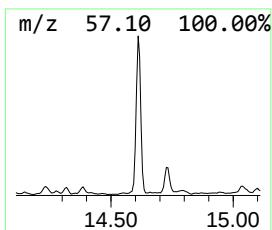
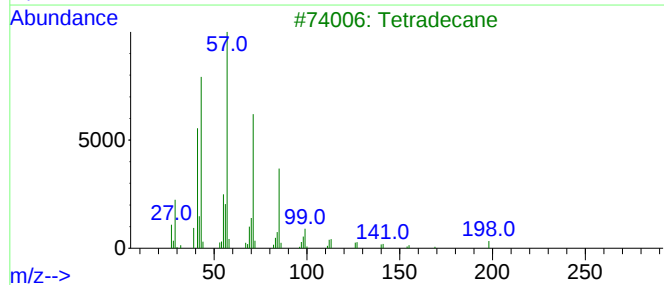
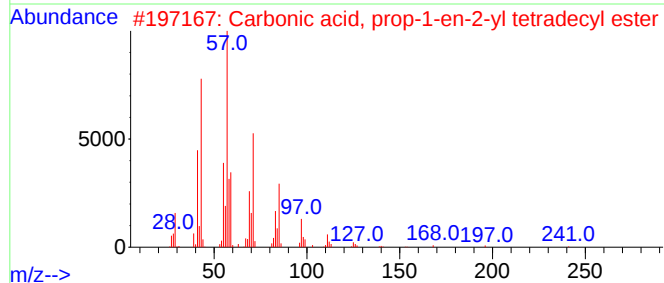
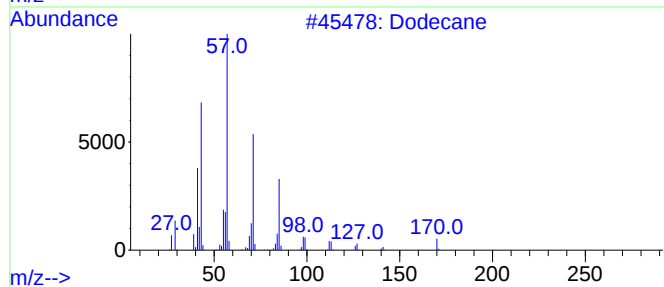
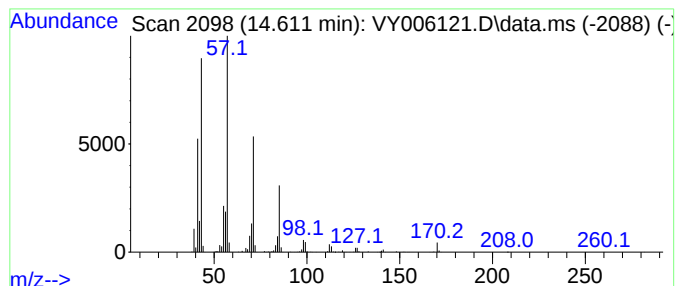
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Quant Title : SW846 8260

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

Peak Number 7 Dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.611	110.67 ug/l	749800	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	95
2			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	90
3			Tetradecane	198	C14H30	000629-59-4	90
4			Undecane	156	C11H24	001120-21-4	86
5			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092321\
Data File : VY006121.D
Acq On : 23 Sep 2021 14:01
Operator : SY/MD
Sample : M3875-11
Misc : 4.35G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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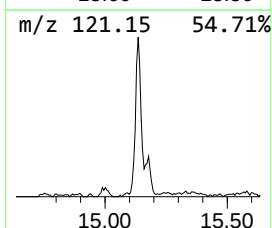
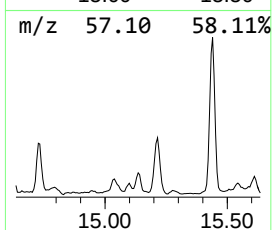
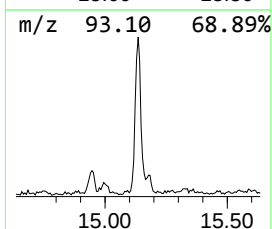
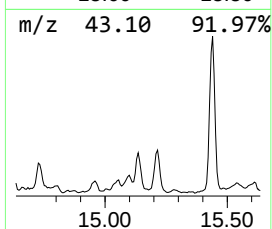
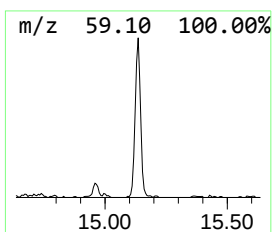
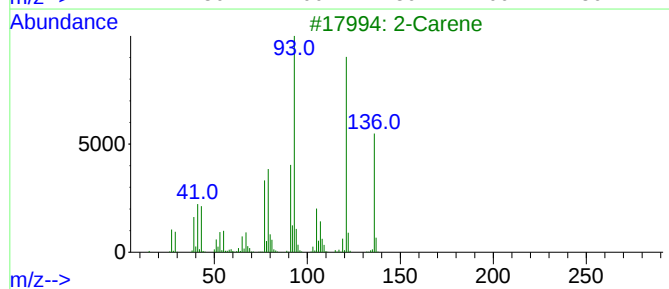
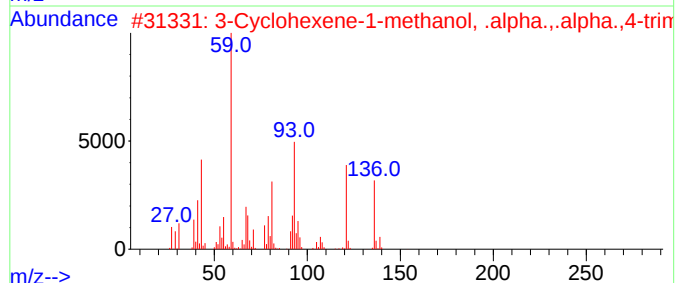
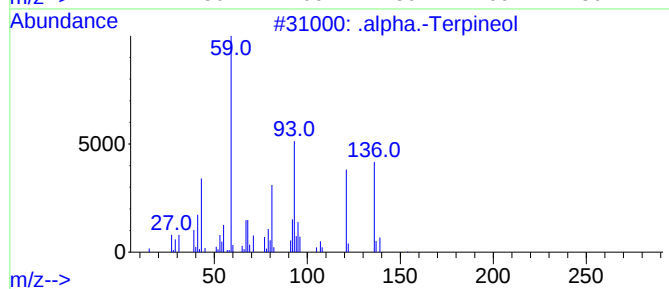
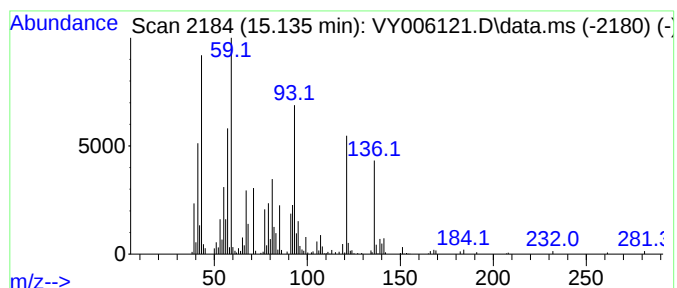
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Quant Title : SW846 8260

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

Peak Number 8 .alpha.-Terpineol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.135	32.99 ug/l	223488	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Terpineol	154	C10H18O	000098-55-5	90
2			3-Cyclohexene-1-methanol, .alpha...	154	C10H18O	007785-53-7	72
3			2-Carene	136	C10H16	000554-61-0	70
4			(+)-4-Carene	136	C10H16	029050-33-7	64
5			(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092321\
Data File : VY006121.D
Acq On : 23 Sep 2021 14:01
Operator : SY/MD
Sample : M3875-11
Misc : 4.35G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20883

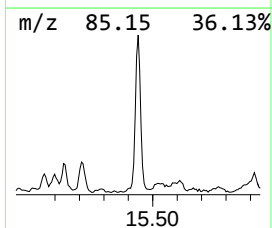
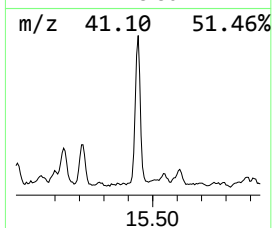
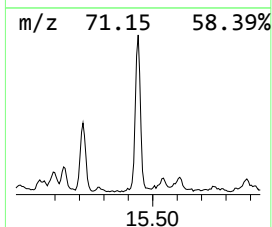
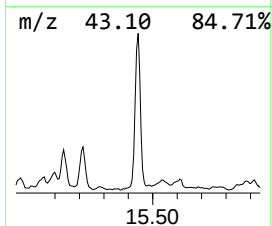
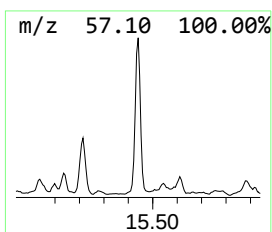
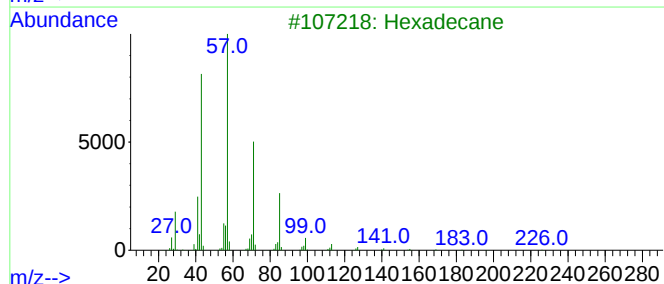
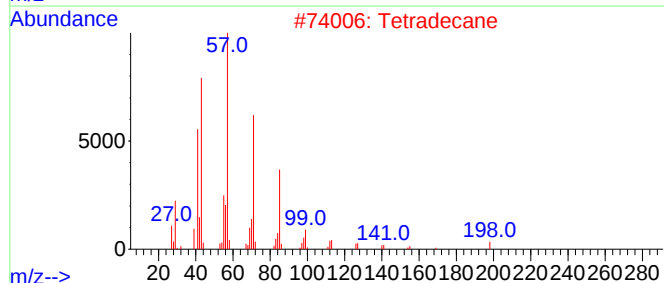
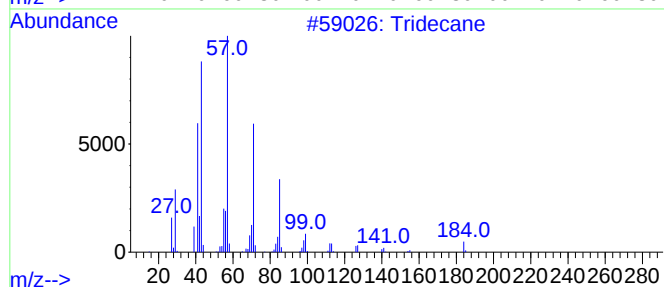
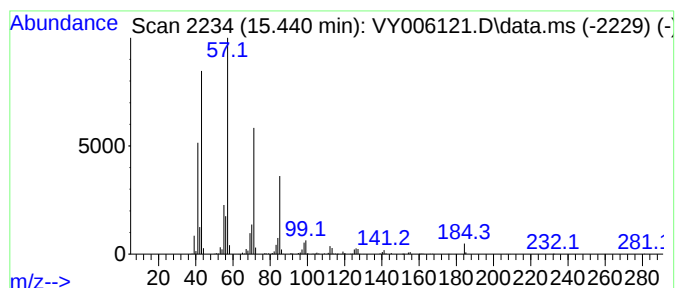
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Quant Title : SW846 8260

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

Peak Number 9 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.440	62.56 ug/l	423862	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Tetradecane	198	C14H30	000629-59-4	91
3			Hexadecane	226	C16H34	000544-76-3	86
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64
5			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092321\
Data File : VY006121.D
Acq On : 23 Sep 2021 14:01
Operator : SY/MD
Sample : M3875-11
Misc : 4.35G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20883

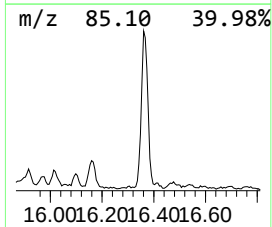
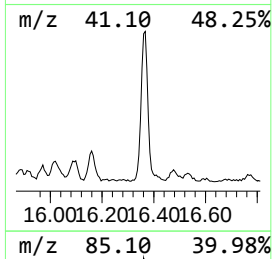
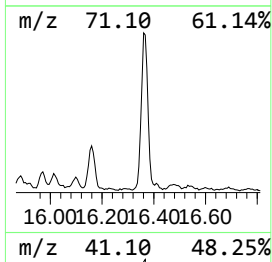
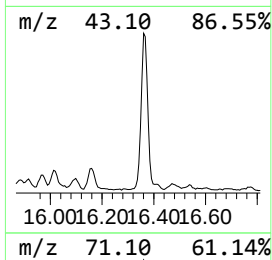
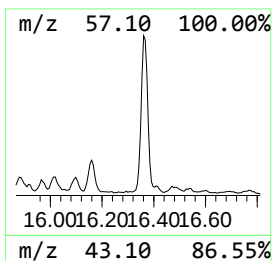
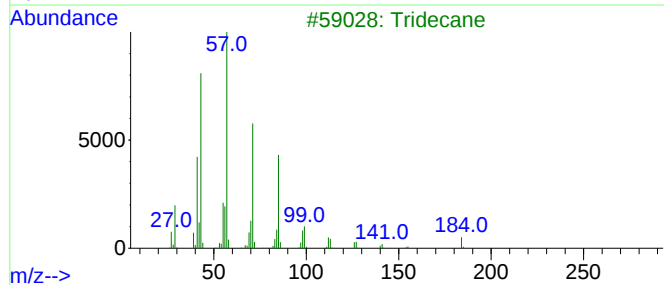
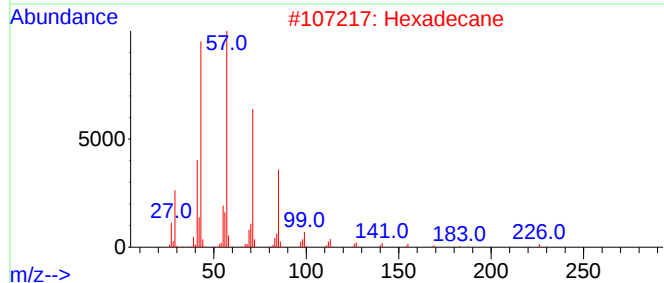
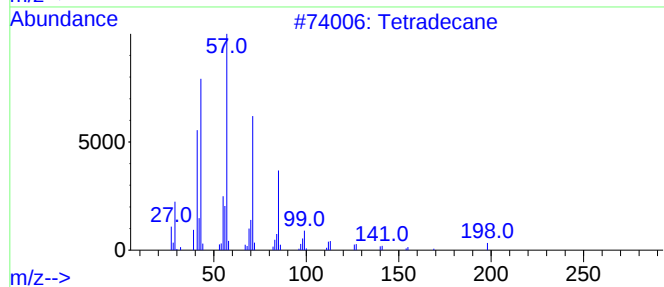
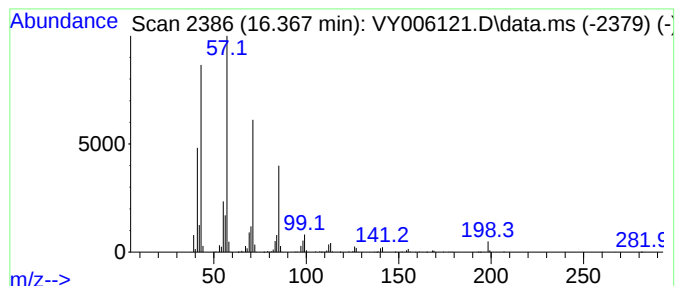
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Quant Title : SW846 8260

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

Peak Number 10 Tetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.367	69.74 ug/l	472487	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	98
2			Hexadecane	226	C16H34	000544-76-3	87
3			Tridecane	184	C13H28	000629-50-5	86
4			Nonadecane	268	C19H40	000629-92-5	86
5			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092321\
Data File : VY006121.D
Acq On : 23 Sep 2021 14:01
Operator : SY/MD
Sample : M3875-11
Misc : 4.35G/5ML/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20883

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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

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					#	RT	Resp	Conc
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2,7-Octanedione	12.806	26.0	ug/l	176384	4	13.428	338754	50.0
(2E,4E)-3,7-Dim...	12.983	59.4	ug/l	402741	4	13.428	338754	50.0
Eucalyptol	13.489	46.1	ug/l	312547	4	13.428	338754	50.0
Undecane	13.751	247.3	ug/l	1675690	4	13.428	338754	50.0
7-Octen-2-ol, 2...	13.898	42.7	ug/l	289417	4	13.428	338754	50.0
Dodecane	14.611	110.7	ug/l	749800	4	13.428	338754	50.0
.alpha.-Terpineol	15.135	33.0	ug/l	223488	4	13.428	338754	50.0
Tridecane	15.440	62.6	ug/l	423862	4	13.428	338754	50.0
Tetradecane	16.367	69.7	ug/l	472487	4	13.428	338754	50.0