

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
 Data File : VY006590.D
 Acq On : 02 Nov 2021 20:34
 Operator : SY/MD
 Sample : M4427-07
 Misc : 2.34G/5ML/MSVOA_Y/SOIL
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 FDR-BH-3-20211029-5-5.5

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\82Y102221S.M
 Title : SW846 8260

Signal : TIC: VY006590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.869	4	8	22	rVB	39582	62175	7.17%	1.064%
2	2.077	37	42	48	rBV2	5774	9133	1.05%	0.156%
3	2.229	61	67	70	rBV	25332	43188	4.98%	0.739%
4	3.960	339	351	362	rBV2	10295	31146	3.59%	0.533%
5	4.210	383	392	400	rBV2	3628	9634	1.11%	0.165%
6	4.729	467	477	487	rBV3	10556	34673	4.00%	0.593%
7	6.716	795	803	811	rBV6	3077	9526	1.10%	0.163%
8	6.996	839	849	867	rVB2	5067	16514	1.91%	0.283%
9	7.728	955	969	974	rBV	107968	254525	29.37%	4.355%
10	7.795	974	980	992	rVB	194944	439429	50.71%	7.518%
11	8.149	1029	1038	1049	rBV	133116	303028	34.97%	5.185%
12	8.557	1097	1105	1111	rBV2	4814	12087	1.39%	0.207%
13	8.697	1119	1128	1137	rBV	315421	618631	71.38%	10.585%
14	8.777	1137	1141	1150	rVB3	4294	9286	1.07%	0.159%
15	9.142	1196	1201	1207	rBV2	5418	9080	1.05%	0.155%
16	9.270	1215	1222	1228	rBV	13129	25907	2.99%	0.443%
17	9.526	1258	1264	1273	rVB	9877	21464	2.48%	0.367%
18	10.185	1364	1372	1379	rBV	513247	866638	100.00%	14.828%
19	10.691	1450	1455	1462	rBV2	7590	16227	1.87%	0.278%
20	10.935	1489	1495	1502	rBV	105487	170861	19.72%	2.923%
21	11.154	1526	1531	1536	rBV3	7091	11645	1.34%	0.199%
22	11.489	1580	1586	1594	rBV	424837	701150	80.90%	11.996%
23	12.209	1700	1704	1707	rBV5	5969	10563	1.22%	0.181%
24	12.483	1743	1749	1758	rVB2	370740	646999	74.66%	11.070%
25	13.075	1842	1846	1854	rVB2	24542	39170	4.52%	0.670%
26	13.172	1860	1862	1868	rVB3	9717	15329	1.77%	0.262%
27	13.318	1883	1886	1888	rVV3	10396	13671	1.58%	0.234%
28	13.355	1889	1892	1897	rVV4	15353	24882	2.87%	0.426%
29	13.428	1898	1904	1910	rVB	312167	475037	54.81%	8.128%
30	13.526	1915	1920	1926	rVB7	9148	20605	2.38%	0.353%
31	13.617	1930	1935	1941	rBV5	10206	26210	3.02%	0.448%
32	13.788	1958	1963	1968	rBV2	32726	48515	5.60%	0.830%
33	13.855	1971	1974	1980	rVV3	12614	17759	2.05%	0.304%
34	13.965	1988	1992	1997	rVB3	15645	25679	2.96%	0.439%
35	14.080	2007	2011	2016	rBV	35988	52797	6.09%	0.903%
36	14.379	2057	2060	2063	rBV4	9148	11634	1.34%	0.199%

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37	14.526	2082	2084	2088	rBV3	6474	9040	1.04%	0.155%
38	14.617	2095	2099	2103	rVB3	16378	26111	3.01%	0.447%
39	14.678	2104	2109	2115	rBV7	13975	29553	3.41%	0.506%
40	14.757	2119	2122	2126	rVB2	22232	28596	3.30%	0.489%
41	14.836	2131	2135	2141	rBV7	18639	44996	5.19%	0.770%
42	14.952	2149	2154	2162	rVB10	17506	44230	5.10%	0.757%
43	15.288	2205	2209	2214	rVB3	25270	45931	5.30%	0.786%
44	15.349	2215	2219	2223	rBV7	16018	27673	3.19%	0.473%
45	15.501	2239	2244	2248	rBV	87664	164300	18.96%	2.811%
46	15.568	2251	2255	2258	rBV2	60155	95308	11.00%	1.631%
47	15.641	2265	2267	2270	rBV4	21157	25797	2.98%	0.441%
48	15.879	2302	2306	2314	rBV5	41647	107908	12.45%	1.846%
49	16.007	2323	2327	2330	rBV3	46529	90433	10.43%	1.547%

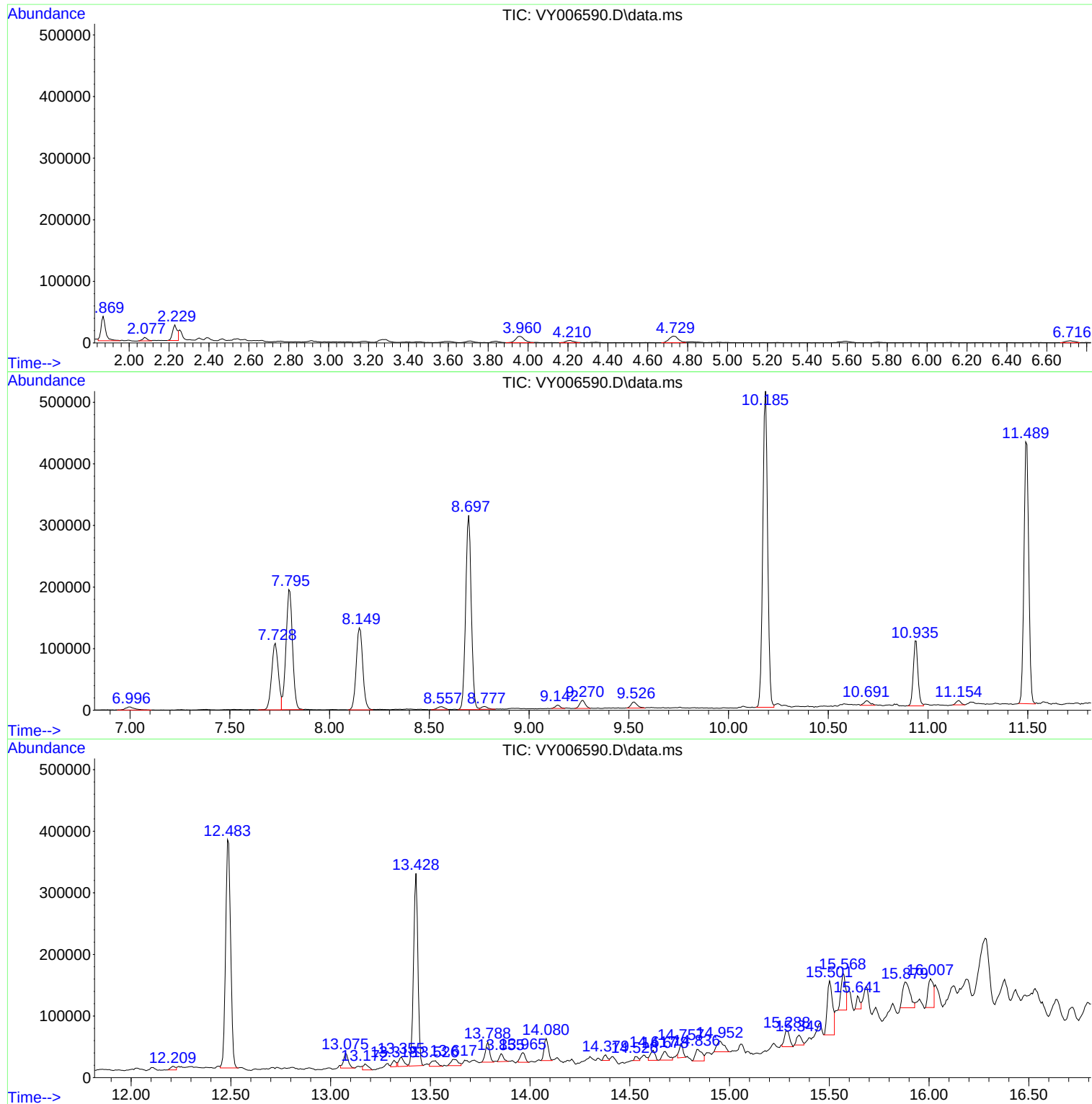
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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



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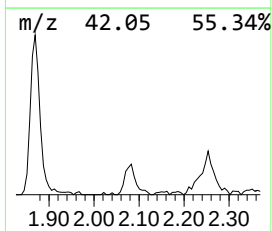
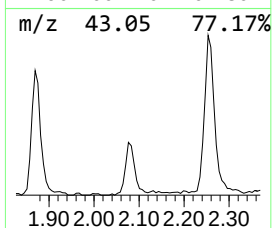
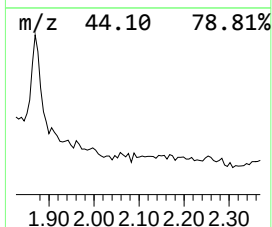
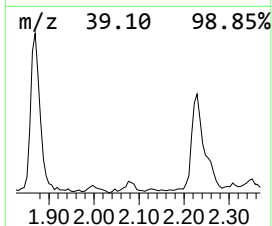
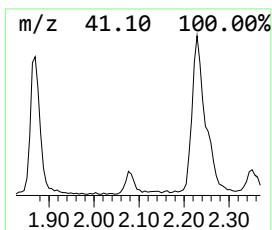
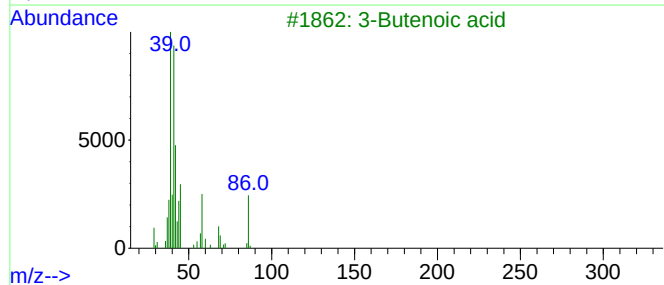
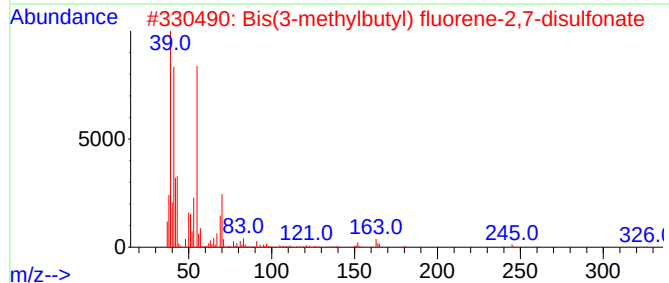
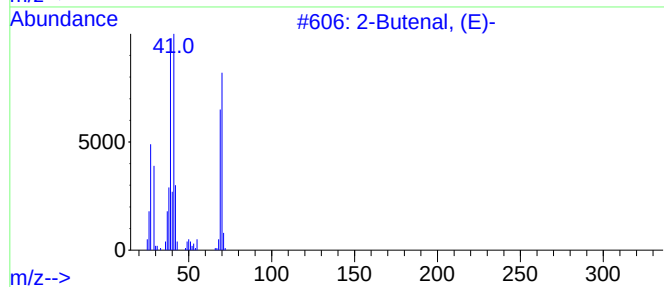
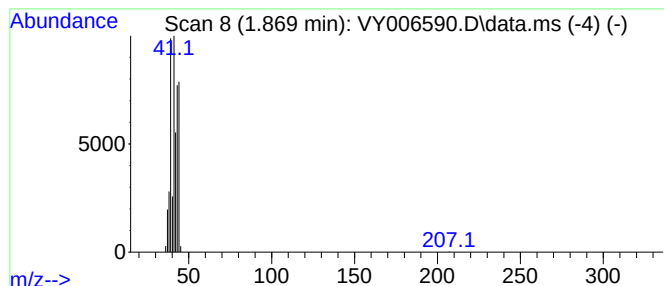
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 1 2-Butenal, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.869	7.07 ug/l	62175	Pentafluorobenzene	7.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, (E)-			70	C4H6O	000123-73-9	64
2	Bis(3-methylbutyl) fluorene-2,7-...			466	C23H30O6S2	253664-95-8	64
3	3-Butenoic acid			86	C4H6O2	000625-38-7	56
4	2-Butenal			70	C4H6O	004170-30-3	39
5	Dimethylketene			70	C4H6O	000598-26-5	39



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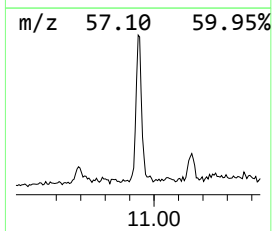
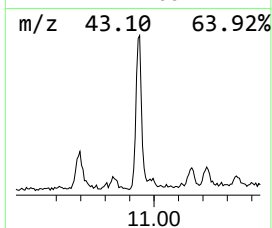
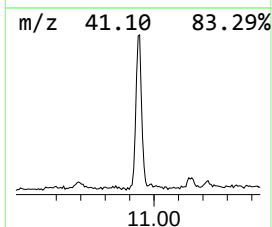
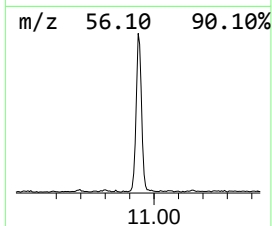
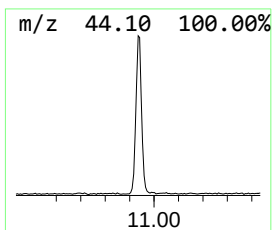
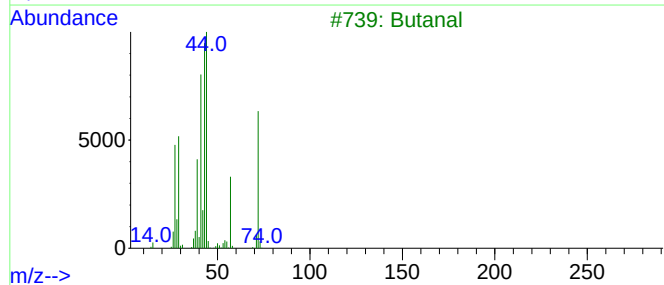
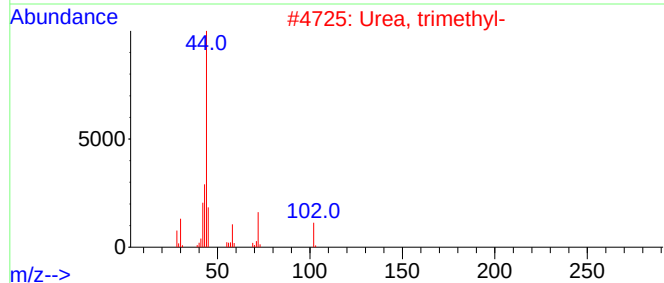
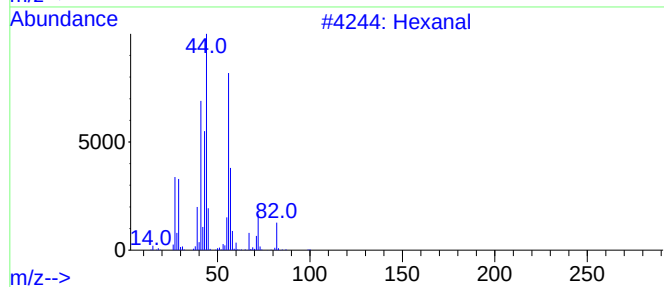
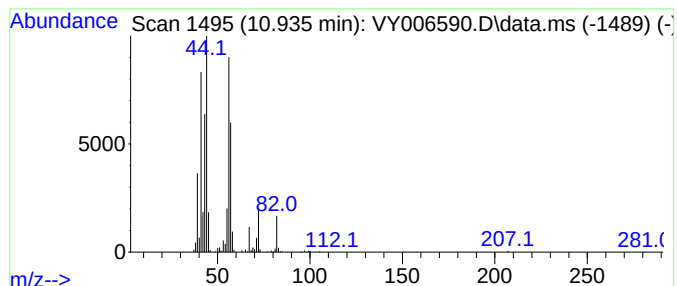
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 2 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.935	12.18 ug/l	170861	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	90
2			Urea, trimethyl-	102	C4H10N2O	000632-14-4	38
3			Butanal	72	C4H8O	000123-72-8	38
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	35
5			Glutaraldehyde	100	C5H8O2	000111-30-8	32



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Misc : 2.34G/5ML/MSVOA_Y/SOIL
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Instrument :
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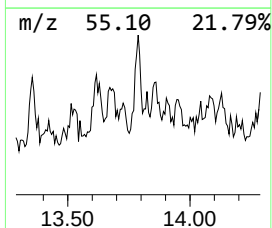
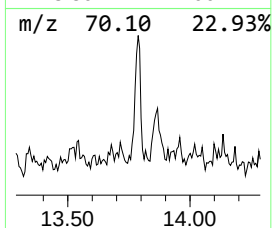
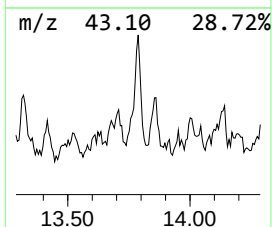
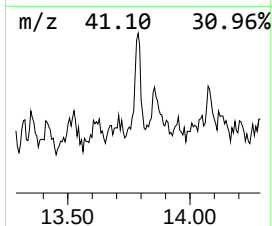
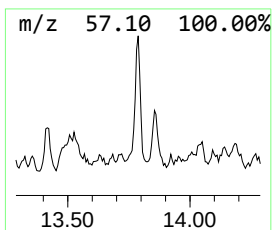
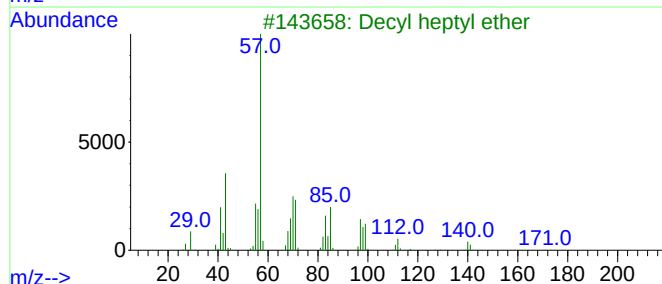
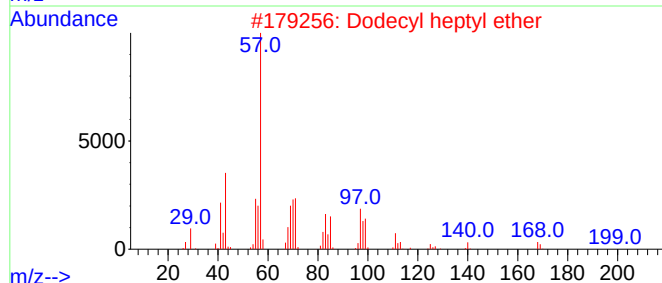
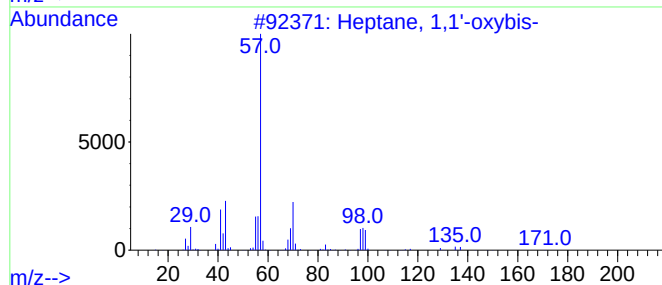
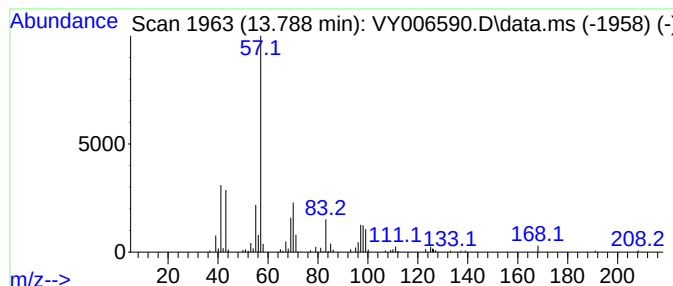
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptane, 1,1'-oxybis- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.788	5.11 ug/l	48515	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
2			Dodecyl heptyl ether	284	C19H40O	1010406-39-2	64
3			Decyl heptyl ether	256	C17H36O	1000406-39-1	64
4			Hexane, 4-ethyl-2-methyl-	128	C9H20	003074-75-7	47
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	40



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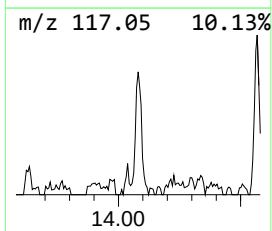
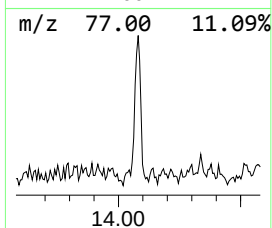
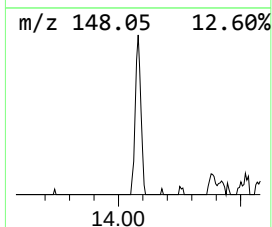
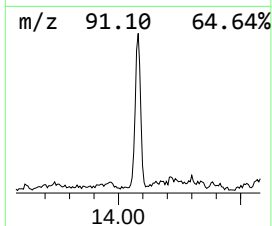
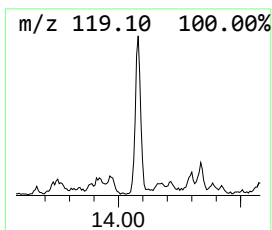
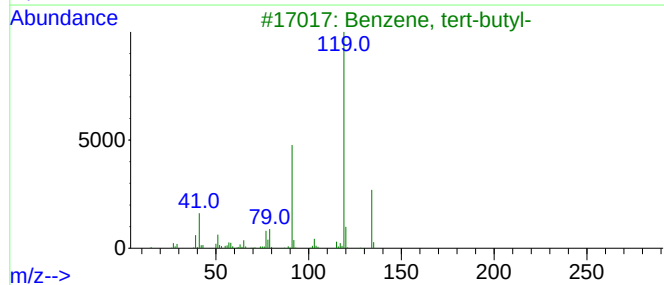
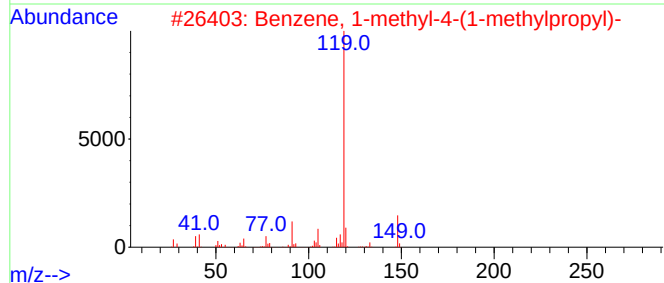
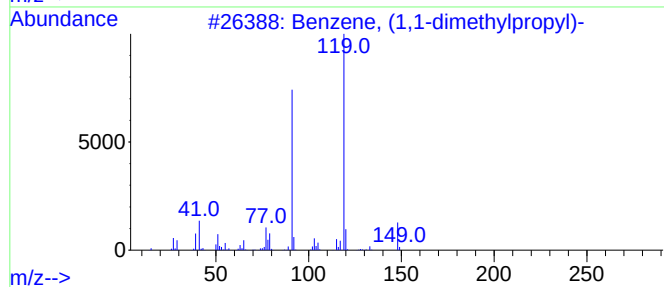
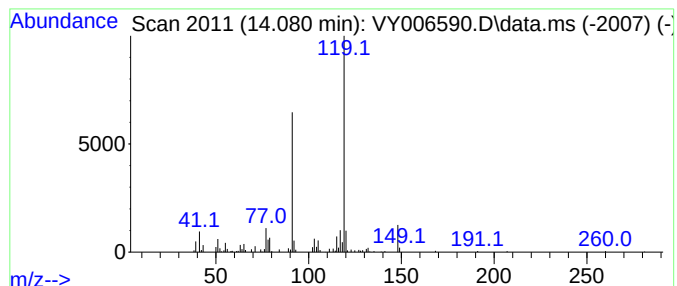
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, (1,1-dimethylpropyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.081	5.56 ug/l	52797	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	93
2			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	86
3			Benzene, tert-butyl-	134	C10H14	000098-06-6	72
4			Succinic acid, 4-chloro-3-methyl...	360	C20H21ClO4	1000389-93-3	72
5			1-Chloro-2-methyl-2-phenylpropane	168	C10H13Cl	000515-40-2	64



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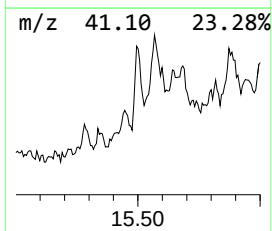
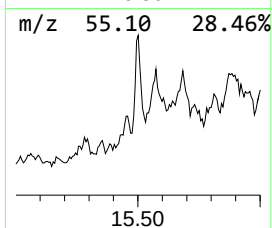
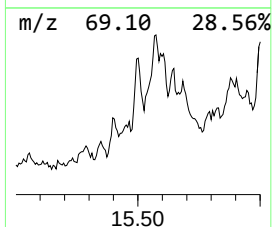
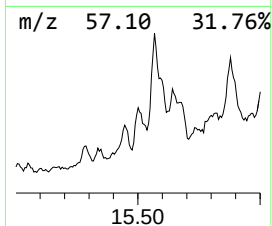
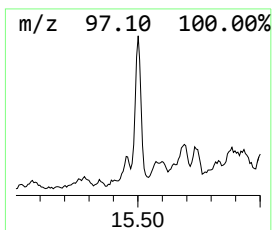
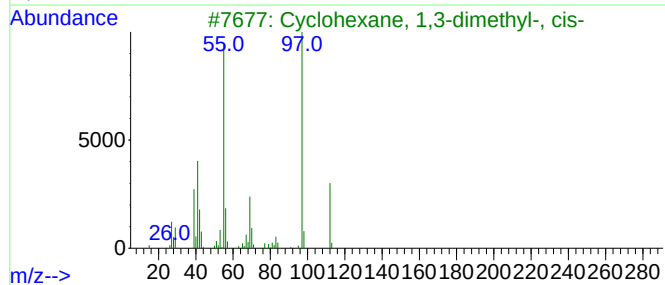
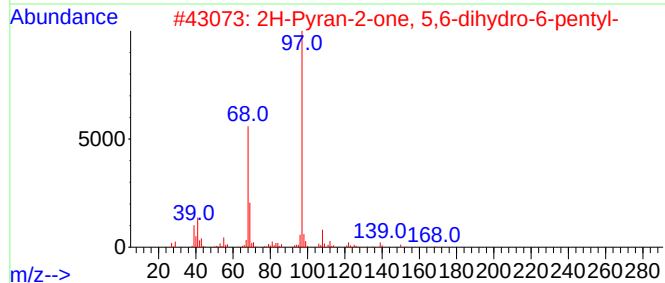
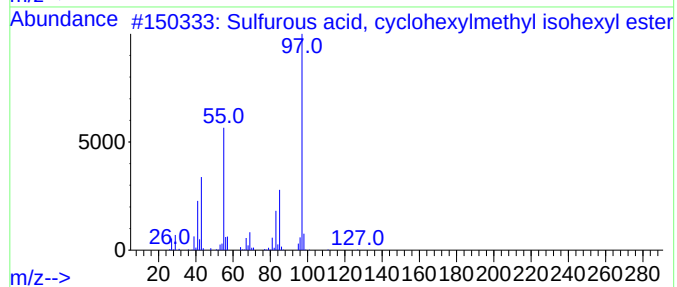
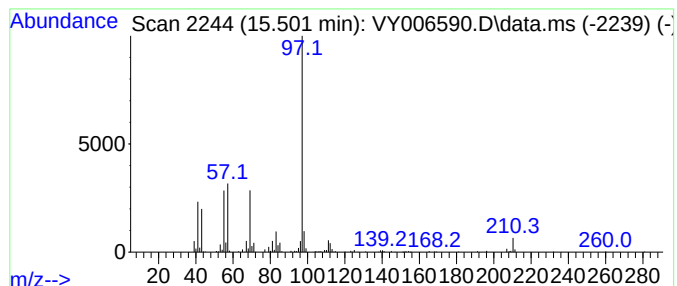
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Quant Title : SW846 8260

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

Peak Number 5 Sulfurous acid, cyclohexylm... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.501	17.29 ug/l	164300	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	64
2			2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	59
3			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	59
4			2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	59
5			Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006590.D
Acq On : 02 Nov 2021 20:34
Operator : SY/MD
Sample : M4427-07
Misc : 2.34G/5ML/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-3-20211029-5-5.5

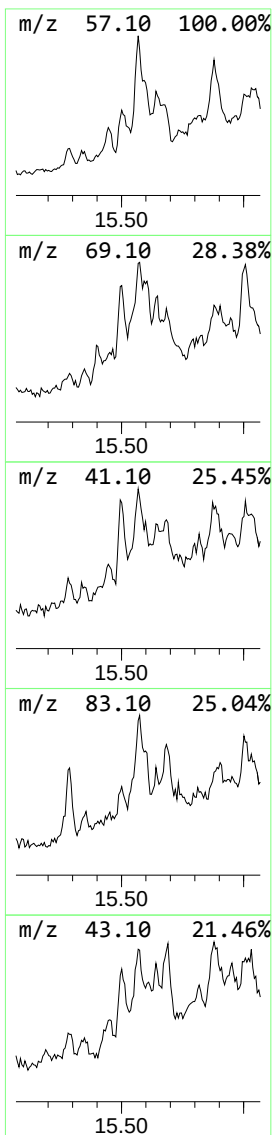
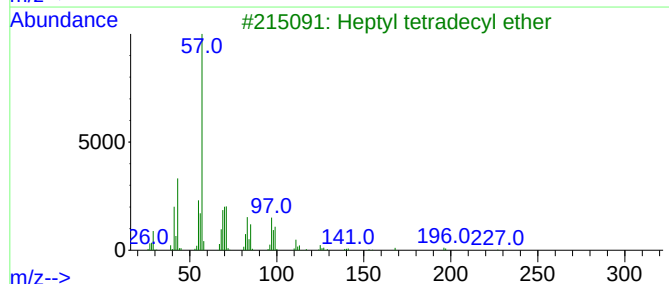
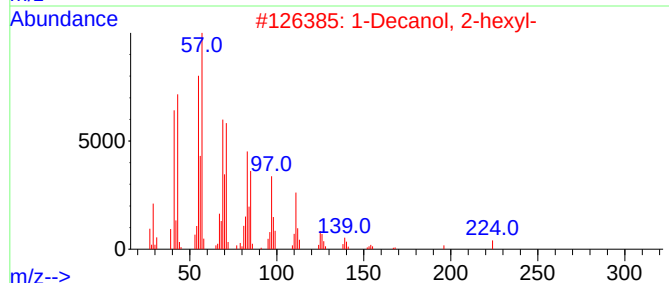
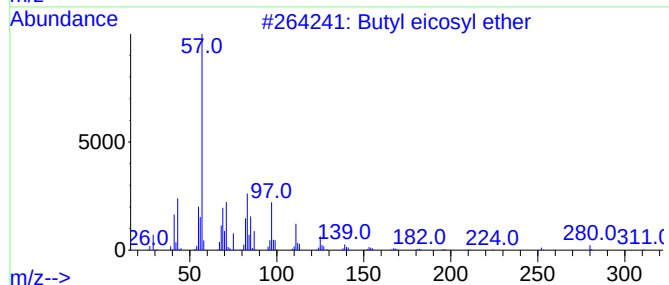
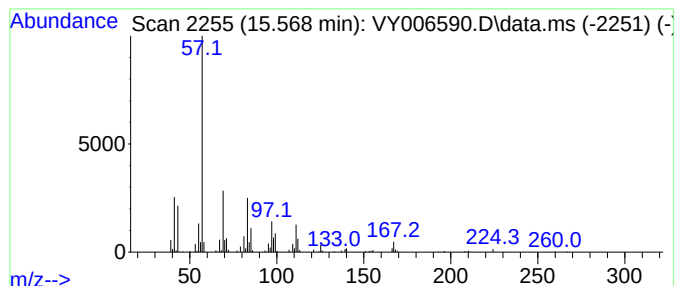
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Quant Title : SW846 8260

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

Peak Number 6 Butyl eicosyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.568	10.03 ug/l	95308	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl eicosyl ether	354	C24H50O	1000406-40-7	64
2			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	50
3			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	50
4			Dodecyl isobutyl ether	242	C16H34O	1000406-32-6	47
5			1-Dotriacontanol, acetate	509	C34H68O2	023811-94-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006590.D
Acq On : 02 Nov 2021 20:34
Operator : SY/MD
Sample : M4427-07
Misc : 2.34G/5ML/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-3-20211029-5-5.5

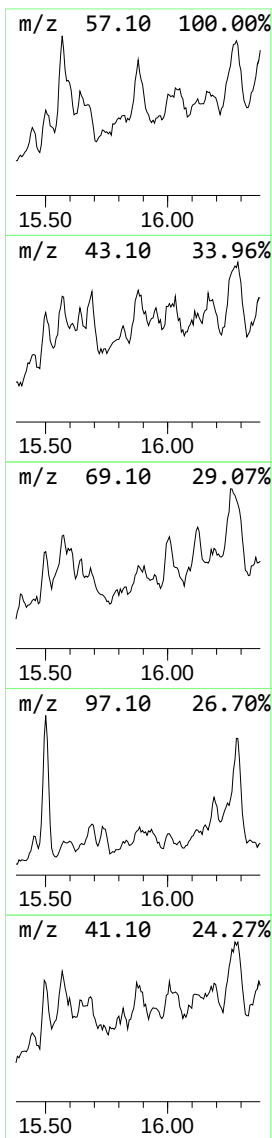
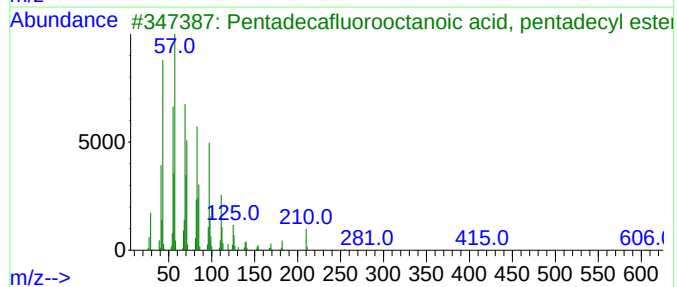
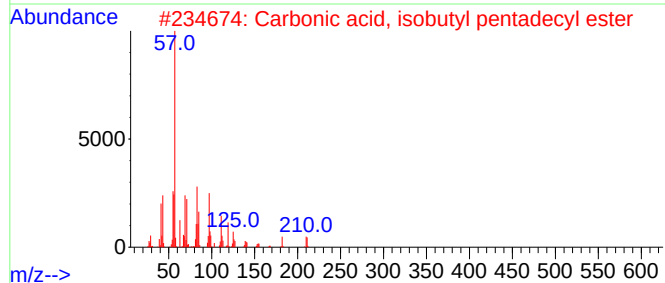
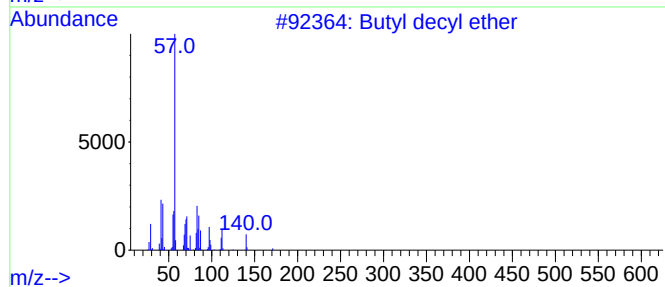
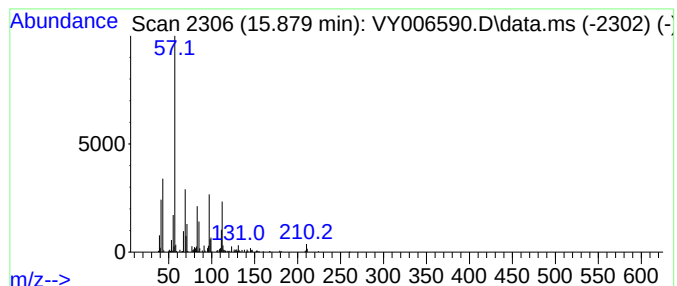
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.879 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.879	11.36 ug/l	107908	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl decyl ether	214	C14H30O	1000406-40-2	42
2			Carbonic acid, isobutyl pentadec...	328	C20H40O3	1000314-61-2	40
3			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	38
4			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	38
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006590.D
Acq On : 02 Nov 2021 20:34
Operator : SY/MD
Sample : M4427-07
Misc : 2.34G/5ML/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-3-20211029-5-5.5

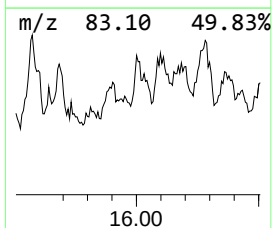
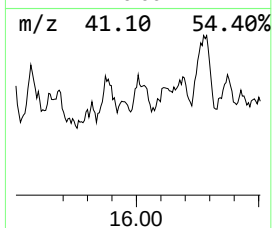
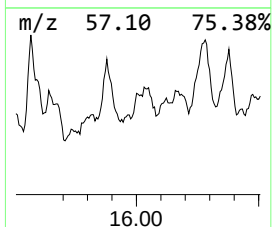
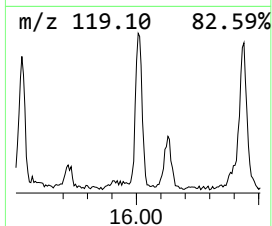
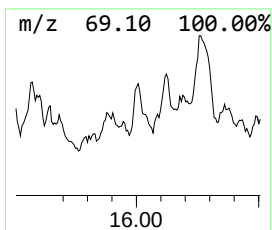
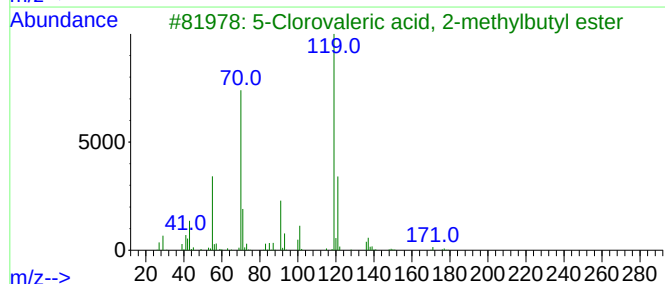
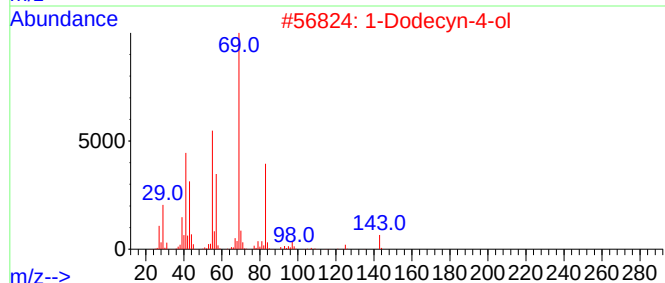
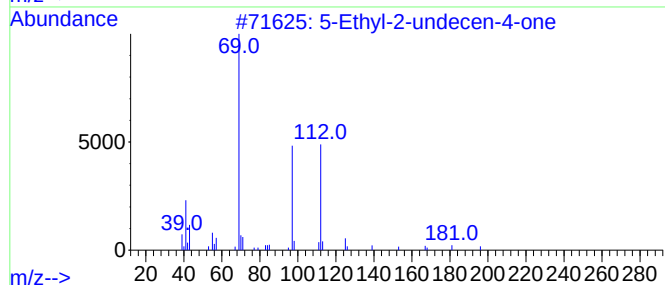
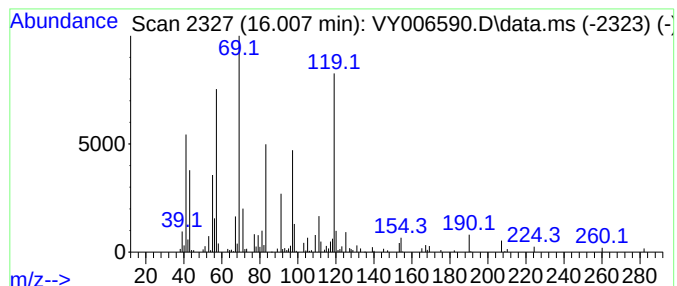
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Quant Title : SW846 8260

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

Peak Number 8 unknown16.007 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.007	9.52 ug/l	90433	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Ethyl-2-undecen-4-one	196	C13H24O	1000374-14-1	35
2			1-Dodecyn-4-ol	182	C12H22O	074646-36-9	27
3			5-Chlorovaleric acid, 2-methylbut...	206	C10H19ClO2	1010331-37-2	22
4			2-Propenamide, N-(2-hydroxyethyl...	129	C6H11NO2	005238-56-2	22
5			Cyclopentanecarboxylic acid, all...	154	C9H14O2	178905-33-4	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110221\
Data File : VY006590.D
Acq On : 02 Nov 2021 20:34
Operator : SY/MD
Sample : M4427-07
Misc : 2.34G/5ML/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
FDR-BH-3-20211029-5-5.5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.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
2-Butenal, (E)-	1.869	7.1	ug/l	62175	1	7.801	439429	50.0
Hexanal	10.935	12.2	ug/l	170861	3	11.496	701150	50.0
Heptane, 1,1'-o...	13.788	5.1	ug/l	48515	4	13.428	475037	50.0
Benzene, (1,1-d...	14.081	5.6	ug/l	52797	4	13.428	475037	50.0
Sulfurous acid,...	15.501	17.3	ug/l	164300	4	13.428	475037	50.0
Butyl eicosyl e...	15.568	10.0	ug/l	95308	4	13.428	475037	50.0
unknown15.879	15.879	11.4	ug/l	107908	4	13.428	475037	50.0
unknown16.007	16.007	9.5	ug/l	90433	4	13.428	475037	50.0