

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091422\
 Data File : VY010494.D
 Acq On : 14 Sep 2022 19:07
 Operator : KP/MD
 Sample : N4588-02
 Misc : 5.04g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 40152

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\82Y090922S.M
 Title : SW846 8260

Signal : TIC: VY010494.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.119	42	49	51	rBV4	8804	19054	13.58%	2.548%
2	3.942	339	348	357	rBV	7084	20185	14.39%	2.700%
3	4.704	460	473	483	rBV3	6425	18939	13.50%	2.533%
4	5.734	634	642	651	rBV6	1567	5118	3.65%	0.684%
5	6.966	835	844	855	rBV	4639	14505	10.34%	1.940%
6	7.710	959	966	972	rBV3	10161	25139	17.92%	3.362%
7	7.783	972	978	986	rVV2	21197	51783	36.91%	6.926%
8	7.856	986	990	991	rVV3	1397	2040	1.45%	0.273%
9	7.874	991	993	998	rVB4	1594	2196	1.57%	0.294%
10	7.996	1003	1013	1019	rBV4	4311	10429	7.43%	1.395%
11	8.136	1027	1036	1045	rVB2	12515	27276	19.44%	3.648%
12	8.265	1048	1057	1062	rBV5	886	2638	1.88%	0.353%
13	8.539	1097	1102	1109	rVB5	2406	4882	3.48%	0.653%
14	8.685	1118	1126	1136	rBV	30361	59889	42.69%	8.010%
15	9.173	1201	1206	1212	rBV7	916	1666	1.19%	0.223%
16	10.179	1365	1371	1376	rBV	45193	80057	57.06%	10.707%
17	10.240	1376	1381	1390	rVB	81402	140295	100.00%	18.764%
18	10.941	1492	1496	1503	rVB5	1744	2968	2.12%	0.397%
19	11.380	1564	1568	1573	rVB7	1131	1743	1.24%	0.233%
20	11.490	1580	1586	1594	rVB	42508	72470	51.66%	9.692%
21	11.703	1616	1621	1626	rBV3	1257	1814	1.29%	0.243%
22	12.117	1684	1689	1693	rVB6	783	1426	1.02%	0.191%
23	12.398	1730	1735	1738	rBV7	1024	1905	1.36%	0.255%
24	12.477	1742	1748	1757	rBV	32057	55704	39.70%	7.450%
25	12.636	1769	1774	1778	rBV8	1602	3953	2.82%	0.529%
26	12.800	1799	1801	1807	rVB7	1214	1730	1.23%	0.231%
27	13.117	1849	1853	1855	rBV4	1105	1789	1.28%	0.239%
28	13.258	1871	1876	1879	rBV6	837	2048	1.46%	0.274%
29	13.422	1898	1903	1909	rVB	40224	61460	43.81%	8.220%
30	13.599	1927	1932	1934	rBV5	1380	2304	1.64%	0.308%
31	13.751	1953	1957	1960	rBV4	2006	3162	2.25%	0.423%
32	13.977	1986	1994	1999	rVB9	2507	6176	4.40%	0.826%
33	14.074	2005	2010	2013	rBV7	1297	2546	1.81%	0.341%
34	14.251	2035	2039	2040	rBV3	1586	1807	1.29%	0.242%
35	14.385	2058	2061	2064	rBV5	1015	1427	1.02%	0.191%
36	14.678	2104	2109	2114	rVV5	3545	7155	5.10%	0.957%

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37	14.733	2114	2118	2124	rVB5	1654	3145	2.24%	0.421%
38	14.940	2149	2152	2156	rVB5	3404	4529	3.23%	0.606%
39	14.989	2158	2160	2162	rVV3	1626	1883	1.34%	0.252%
40	15.044	2165	2169	2176	rVB7	4423	9415	6.71%	1.259%
41	15.196	2193	2194	2204	rVB7	1677	3529	2.52%	0.472%
42	15.525	2246	2248	2250	rBV3	1850	1546	1.10%	0.207%
43	15.867	2302	2304	2307	rBV3	1046	1496	1.07%	0.200%
44	16.476	2399	2404	2405	rBV5	2053	2479	1.77%	0.332%

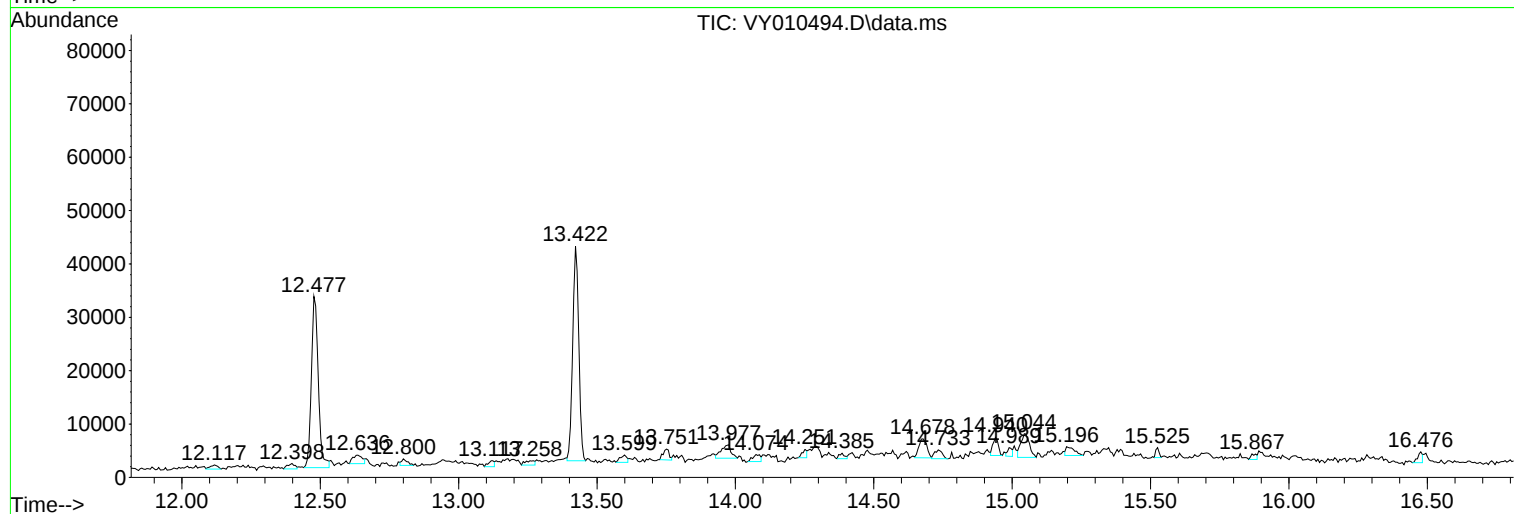
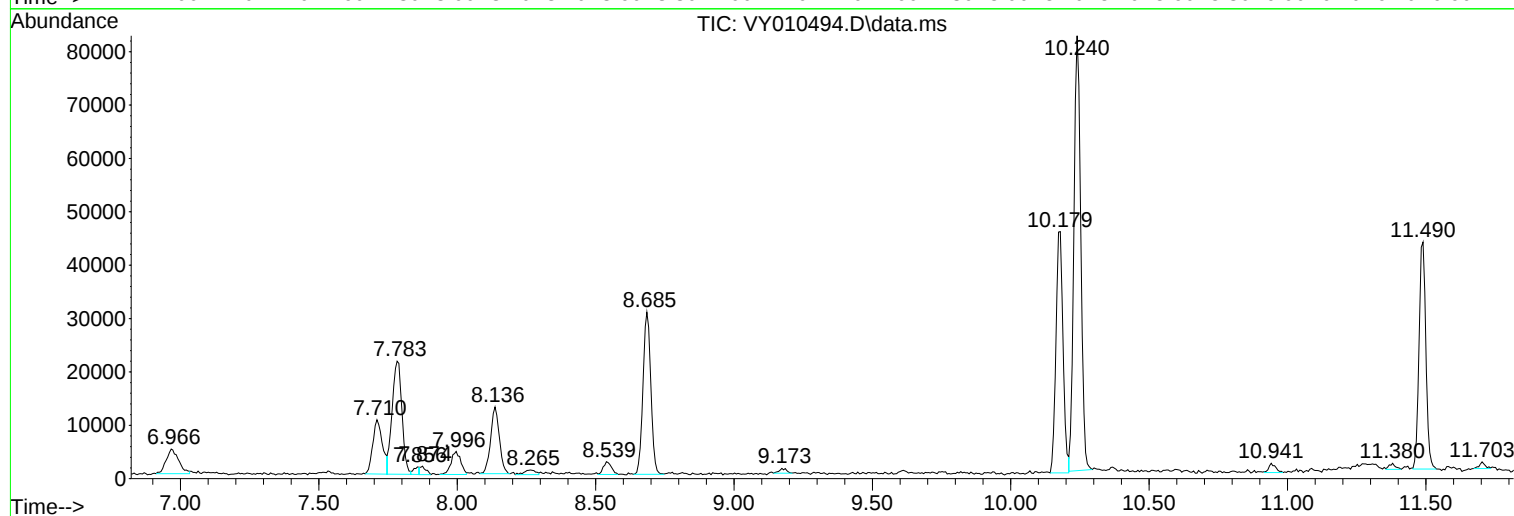
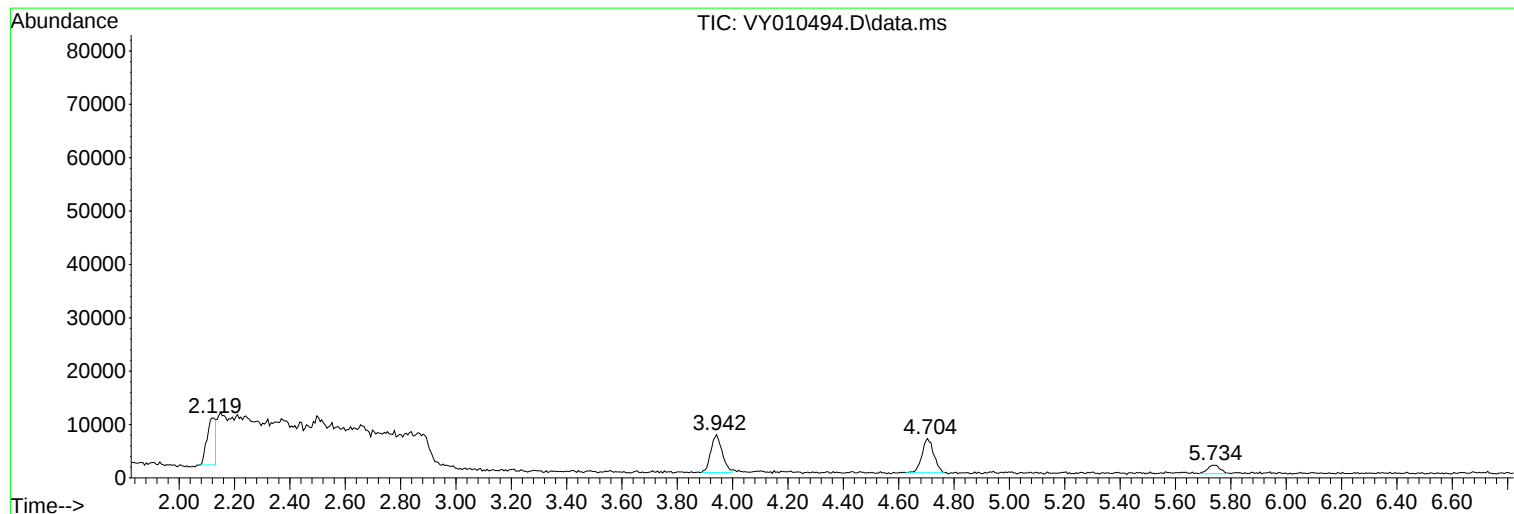
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090922S.M
Quant Title : SW846 8260

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



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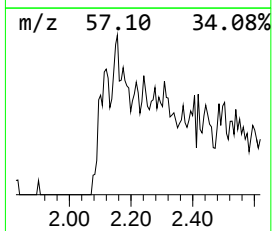
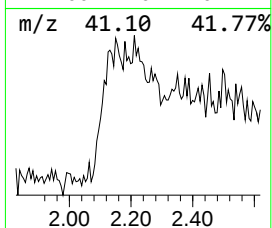
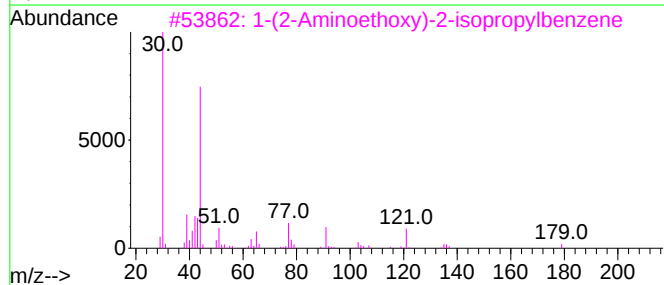
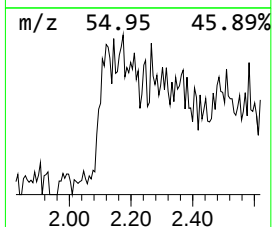
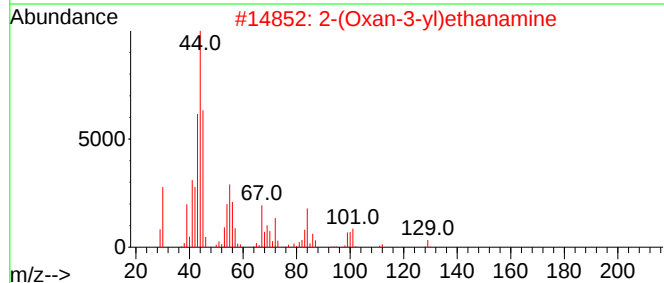
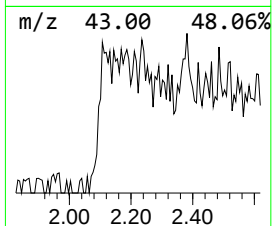
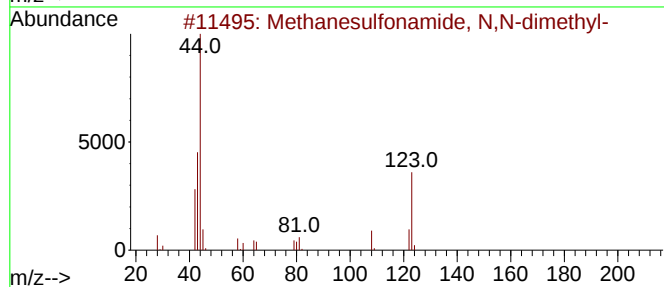
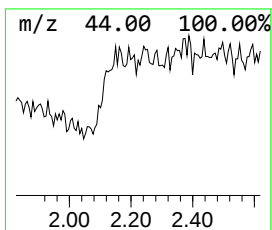
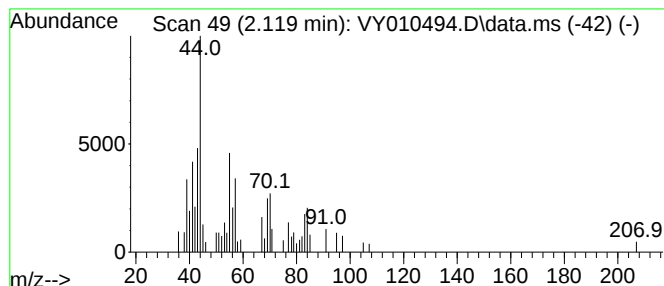
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090922S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.119 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.119	18.40 ug/l	19054	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanesulfonamide, N,N-dimethyl-	123	C3H9NO2S	000918-05-8	43
2			2-(Oxan-3-yl)ethanamine	129	C7H15NO	1000411-07-5	42
3			1-(2-Aminoethoxy)-2-isopropylben...	179	C11H17NO	026583-37-9	37
4			N.omega.-Nitro-L-arginine	219	C6H13N5O4	002149-70-4	36
5			1-Octadecanamine	269	C18H39N	000124-30-1	33



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Instrument :
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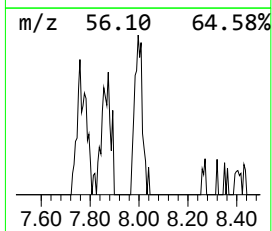
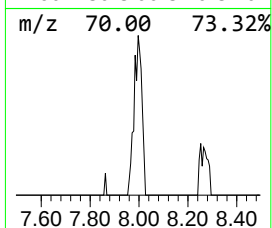
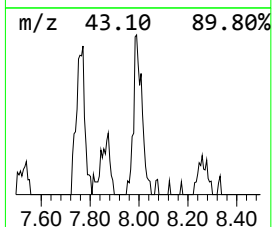
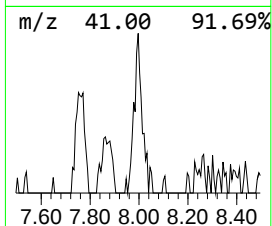
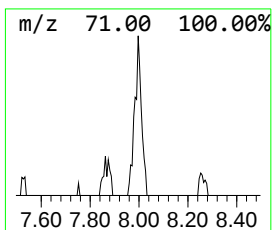
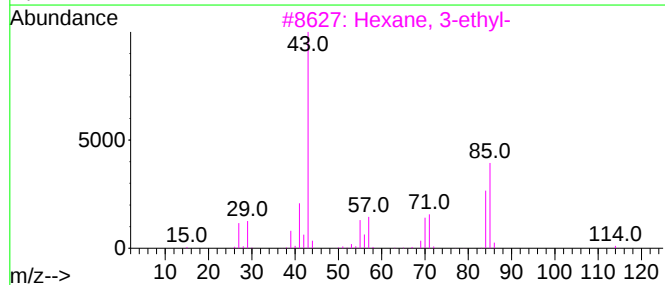
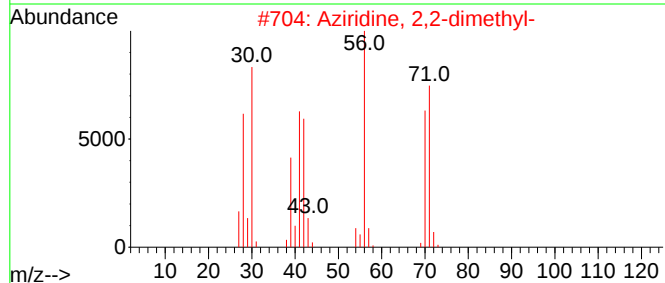
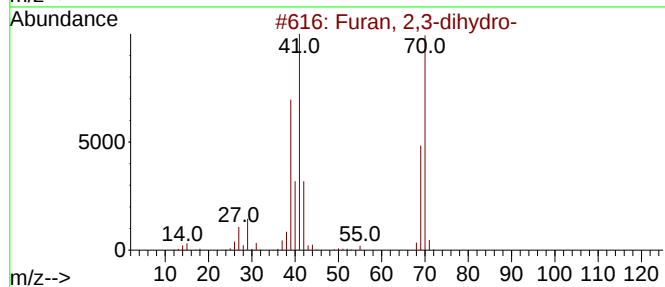
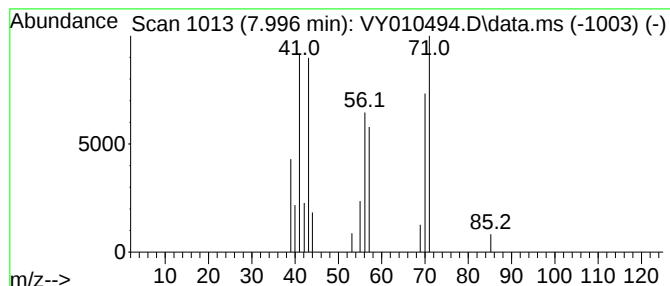
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090922S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown7.996 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.996	10.07 ug/l	10429	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	38
2			Aziridine, 2,2-dimethyl-	71	C4H9N	002658-24-4	36
3			Hexane, 3-ethyl-	114	C8H18	000619-99-8	33
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	33
5			1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	32



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ALS Vial : 22 Sample Multiplier: 1

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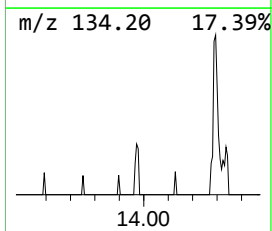
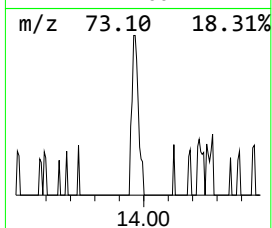
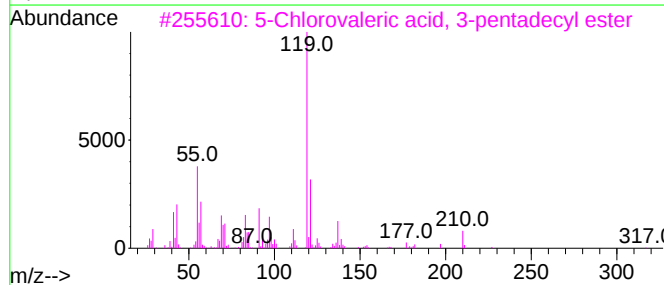
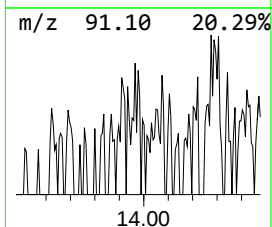
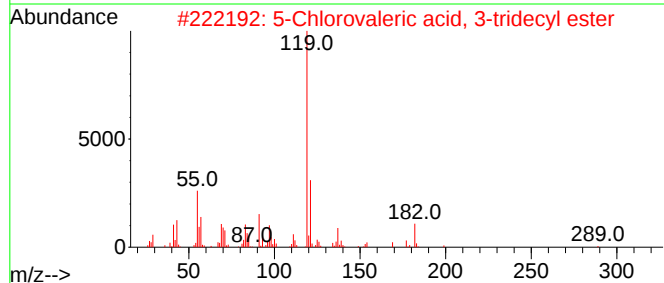
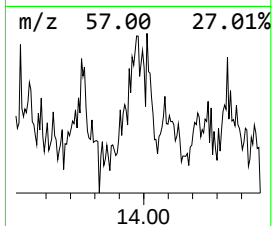
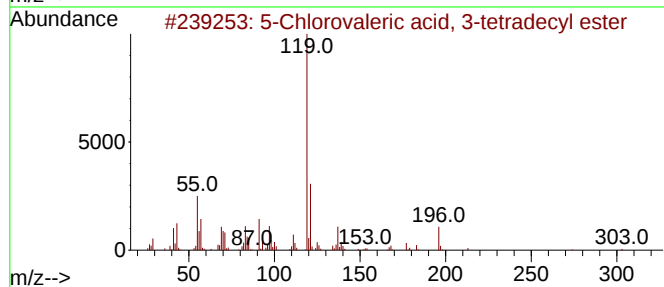
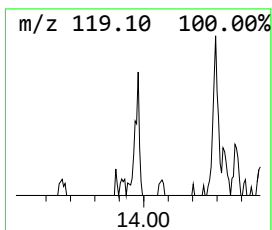
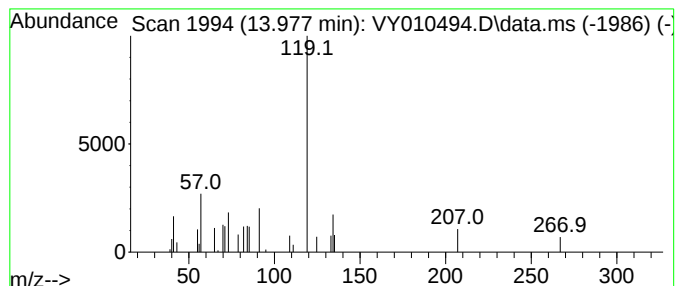
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090922S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown13.977 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.977	5.02 ug/l	6176	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Chlorovaleric acid, 3-tetradec...	332	C19H37ClO2	1000299-91-7	42
2			5-Chlorovaleric acid, 3-tridecyl...	318	C18H35ClO2	1000299-91-3	42
3			5-Chlorovaleric acid, 3-pentadec...	346	C20H39ClO2	1000299-92-1	42
4			5-Chlorovaleric acid, 5-pentadec...	346	C20H39ClO2	1000299-92-3	42
5			Glycine, N-(4-methylbenzoyl)-, m...	207	C11H13NO3	001208-23-7	38



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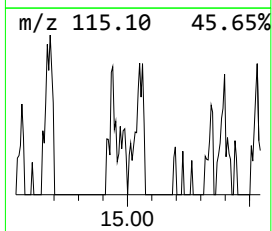
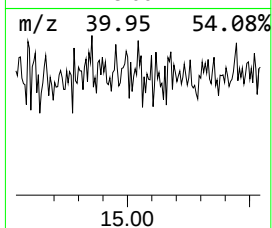
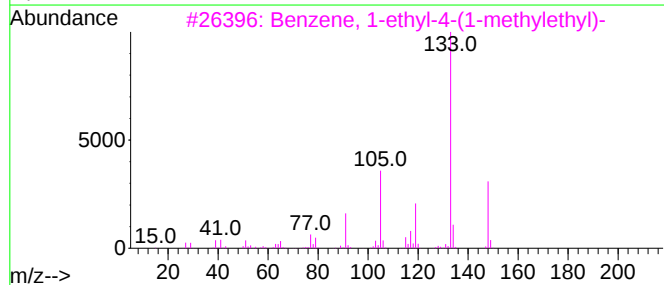
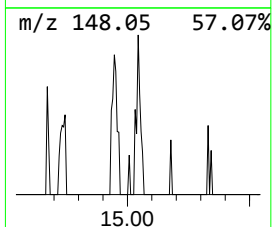
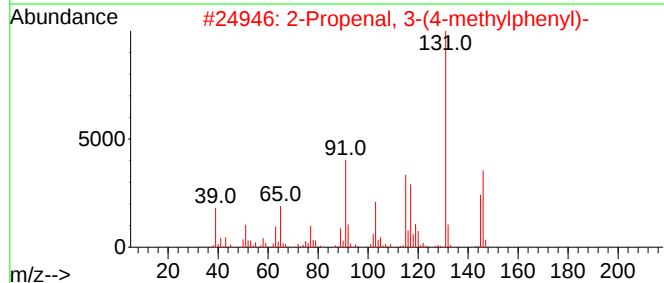
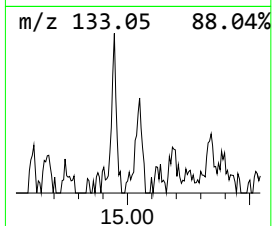
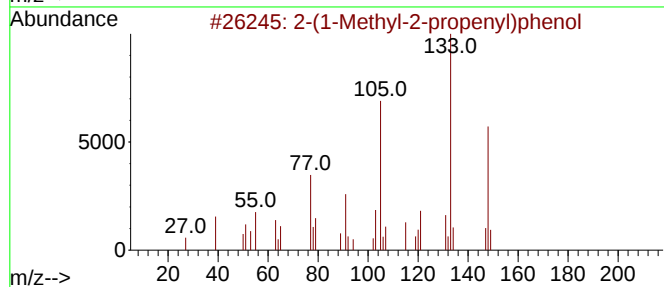
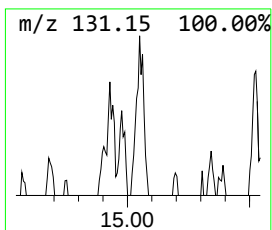
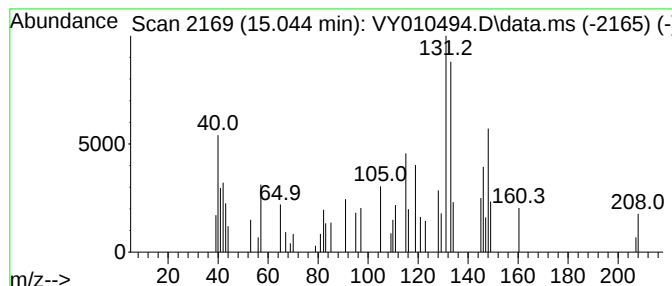
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Quant Title : SW846 8260

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

Peak Number 6 unknown15.044 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.044	7.66 ug/l	9415	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(1-Methyl-2-propenyl)phenol	148	C10H12O	1000432-85-2	30		
2	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	30		
3	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	27		
4	(6,8,9-Trimethyl-4-propyl-3-oxab...	310	C18H34O2Si	1000498-08-0	25		
5	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	25		



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown7.996	7.996	10.1	ug/l	10429	1	7.789	51783	50.0
unknown13.977	13.977	5.0	ug/l	6176	4	13.422	61460	50.0
unknown15.044	15.044	7.7	ug/l	9415	4	13.422	61460	50.0