

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112921\
 Data File : VX025369.D
 Acq On : 29 Nov 2021 15:01
 Operator : JC/MD
 Sample : M4837-15
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20935

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_X\Method\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025369.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	16	rVB	31335	28676	4.63%	0.594%
2	1.246	22	26	33	rBV2	9774	17825	2.87%	0.369%
3	1.569	69	79	82	rVV6	3201	7142	1.15%	0.148%
4	2.057	153	159	169	rBV	40932	62116	10.02%	1.287%
5	2.380	205	212	223	rVB	50773	81689	13.18%	1.693%
6	2.532	230	237	243	rBV	7919	14975	2.42%	0.310%
7	2.959	300	307	318	rBV2	4318	10134	1.63%	0.210%
8	3.697	418	428	439	rBV2	7814	20421	3.29%	0.423%
9	3.849	443	453	470	rBV	66716	165644	26.72%	3.432%
10	4.233	506	516	530	rBV2	12401	34227	5.52%	0.709%
11	4.556	561	569	583	rBV	14845	41593	6.71%	0.862%
12	5.391	692	706	719	rBV	72624	211241	34.07%	4.377%
13	5.556	722	733	747	rVB	125589	354201	57.13%	7.339%
14	5.958	786	799	808	rBV2	75283	204034	32.91%	4.227%
15	6.044	808	813	820	rVB	9917	24386	3.93%	0.505%
16	6.763	919	931	947	rBV	193705	459358	74.09%	9.518%
17	7.208	997	1004	1015	rBV	12419	29509	4.76%	0.611%
18	8.653	1234	1241	1247	rBV	387649	620020	100.00%	12.846%
19	8.720	1247	1252	1257	rVB	24948	37688	6.08%	0.781%
20	10.055	1465	1471	1483	rVB	415156	543169	87.61%	11.254%
21	10.153	1483	1487	1491	rVV	7241	10876	1.75%	0.225%
22	10.195	1491	1494	1501	rVV	6724	9243	1.49%	0.192%
23	10.305	1504	1512	1520	rVB	24781	36157	5.83%	0.749%
24	10.506	1540	1545	1551	rBV	9907	12514	2.02%	0.259%
25	10.647	1563	1568	1578	rVB2	13179	22219	3.58%	0.460%
26	10.756	1581	1586	1594	rBV	26443	37981	6.13%	0.787%
27	11.085	1634	1640	1645	rBV	326123	423838	68.36%	8.782%
28	11.134	1645	1648	1654	rVB2	13078	16330	2.63%	0.338%
29	11.573	1714	1720	1723	rBV	17175	22255	3.59%	0.461%
30	11.604	1723	1725	1736	rVB2	13876	20134	3.25%	0.417%
31	11.756	1746	1750	1754	rVB	8050	10340	1.67%	0.214%
32	11.829	1756	1762	1765	rVV3	9900	16164	2.61%	0.335%
33	11.872	1765	1769	1778	rVV	49340	72271	11.66%	1.497%
34	11.957	1778	1783	1789	rVV	10775	16581	2.67%	0.344%
35	12.024	1789	1794	1801	rVV	415354	525334	84.73%	10.885%
36	12.219	1821	1826	1838	rBV	284031	388902	62.72%	8.058%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

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Filtering: 5

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Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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Title : SW846 8260

37	12.311	1838	1841	1847	rVB5	5826	10118	1.63%	0.210%
38	12.415	1852	1858	1862	rVB	11311	14625	2.36%	0.303%
39	12.567	1875	1883	1887	rBV4	4204	8630	1.39%	0.179%
40	13.292	1998	2002	2007	rVB2	8121	10889	1.76%	0.226%
41	13.512	2034	2038	2042	rVB2	6873	8394	1.35%	0.174%
42	13.774	2073	2081	2088	rBV	25253	34672	5.59%	0.718%
43	13.847	2088	2093	2100	rBV	31041	44501	7.18%	0.922%
44	13.914	2100	2104	2121	rVB	31992	49746	8.02%	1.031%
45	14.640	2219	2223	2229	rVB	13405	16259	2.62%	0.337%
46	14.780	2242	2246	2253	rVB	15877	19365	3.12%	0.401%

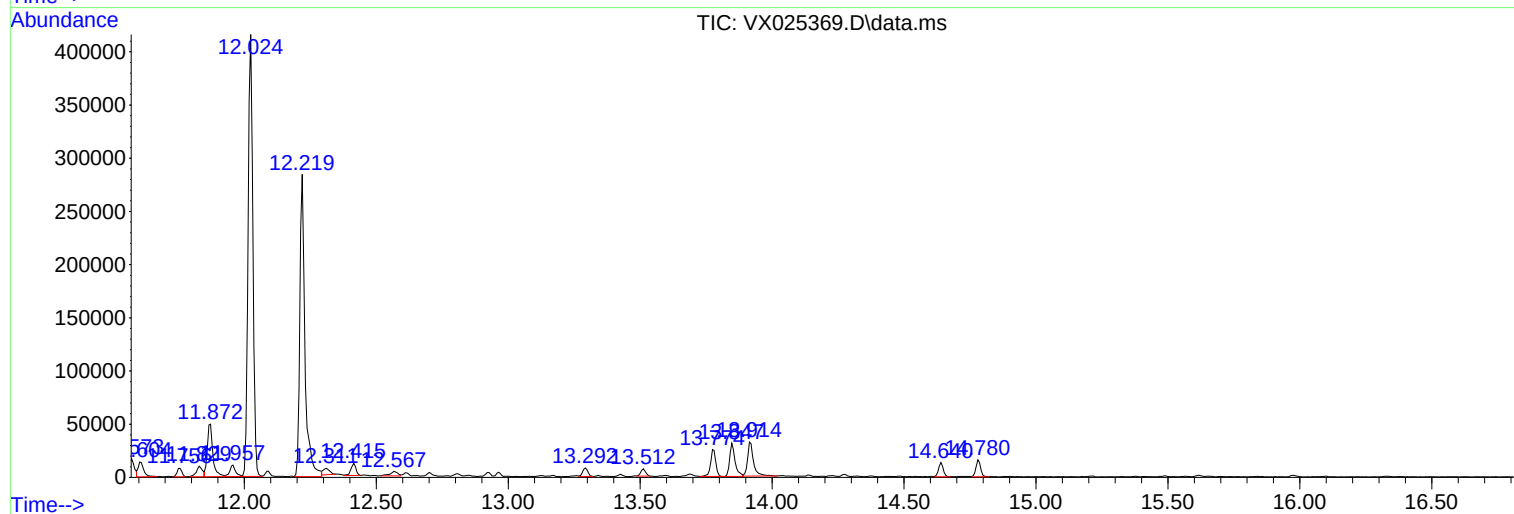
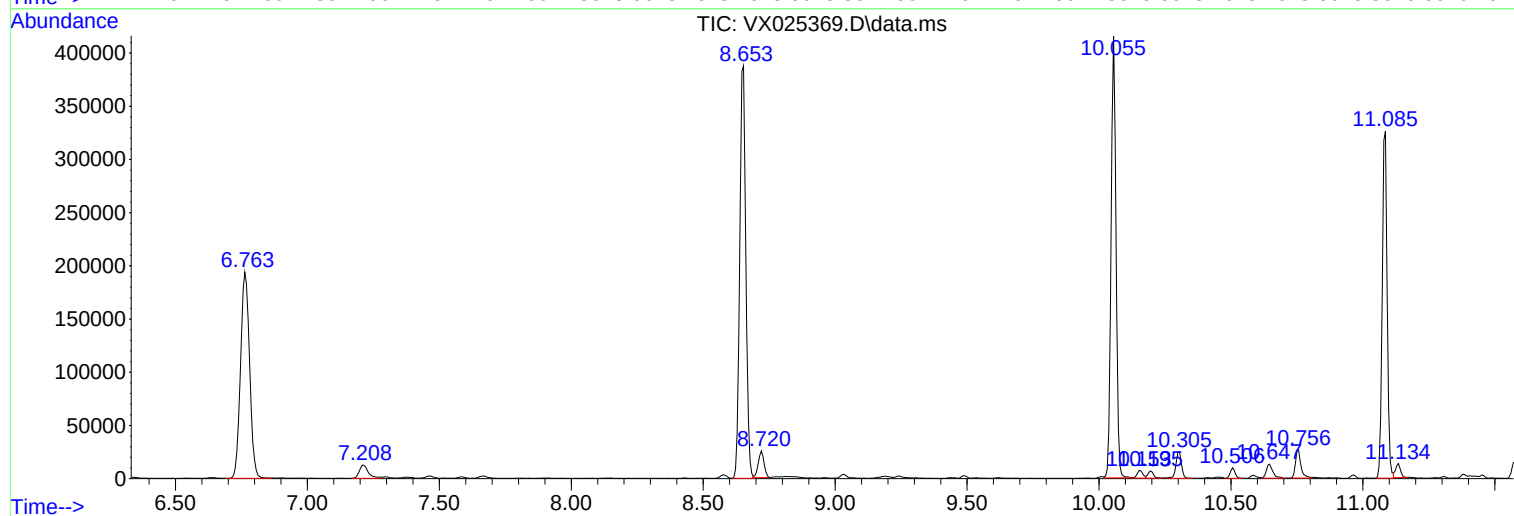
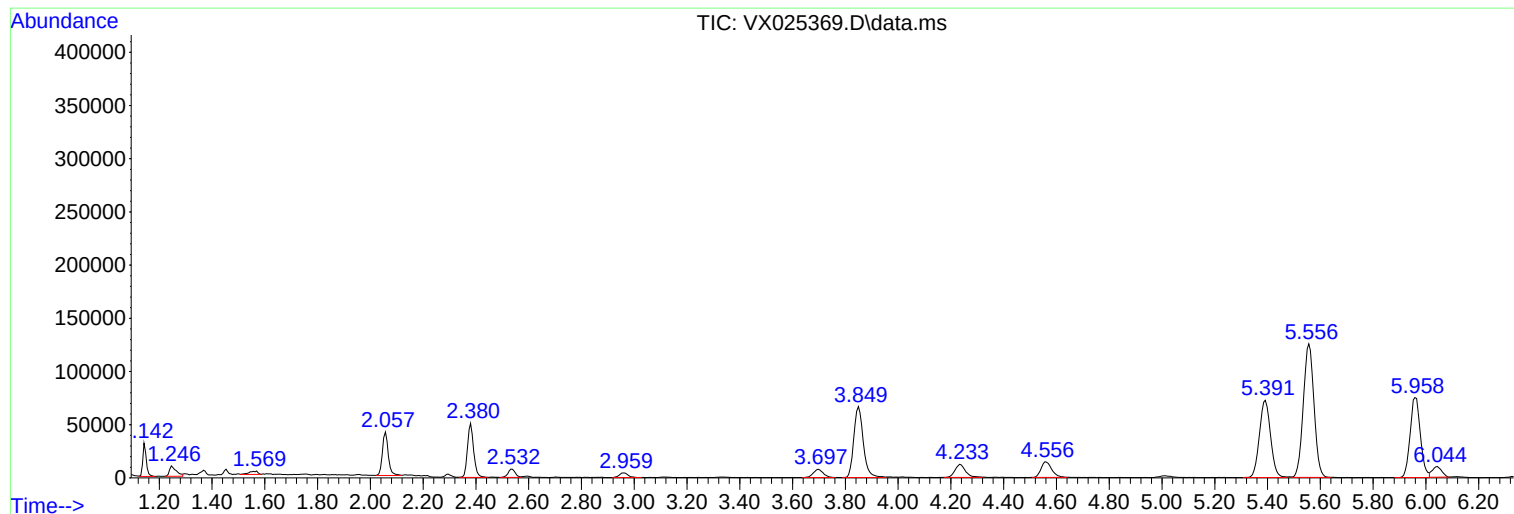
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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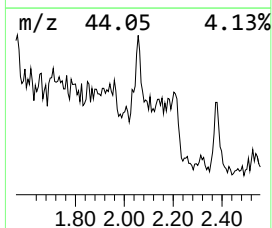
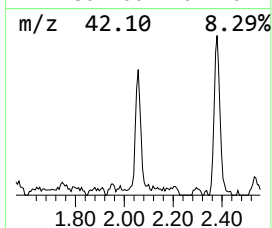
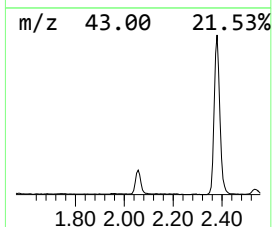
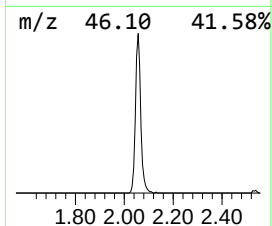
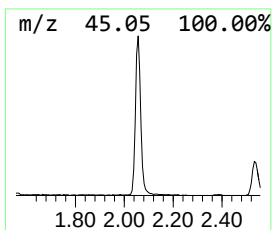
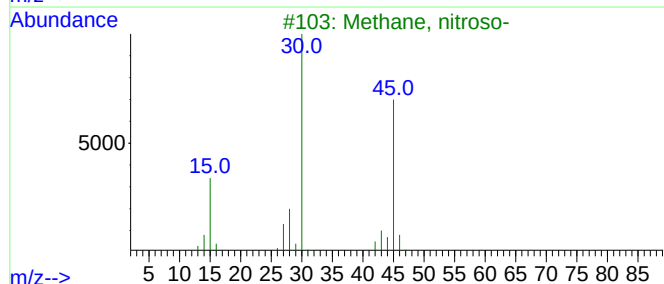
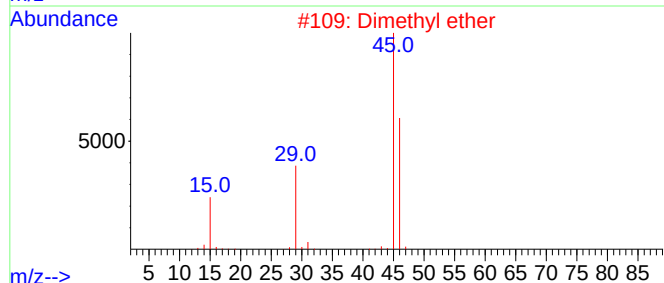
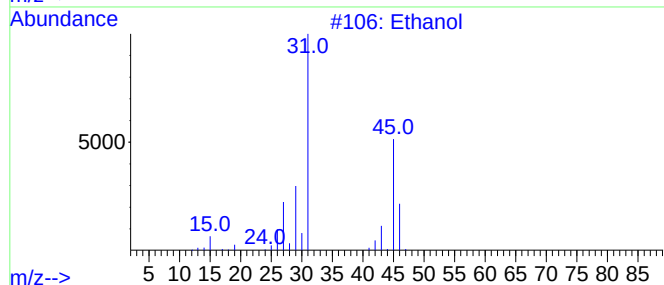
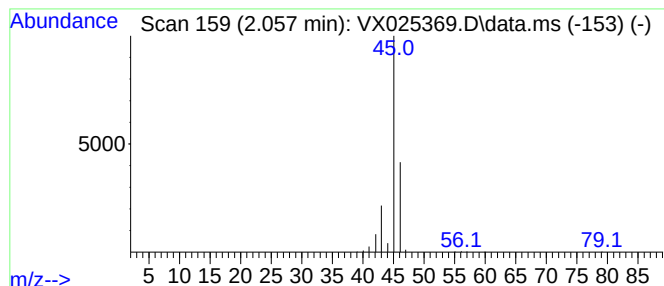
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.057	8.77 ug/l	62116	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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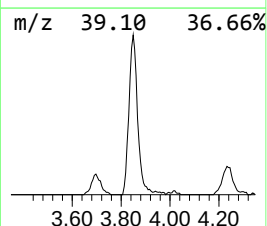
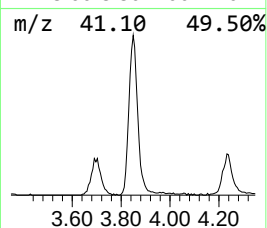
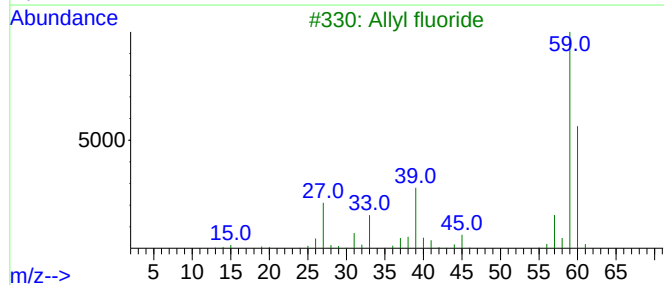
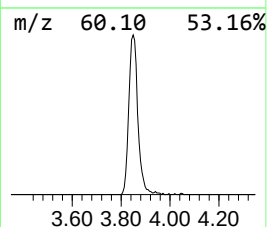
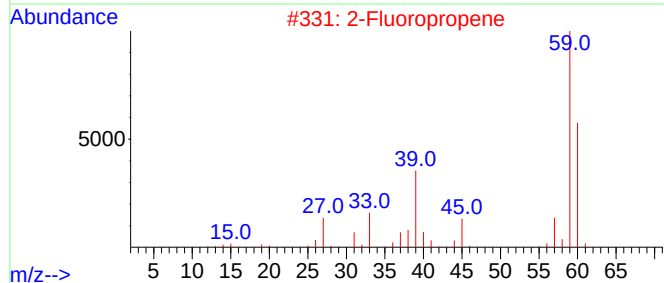
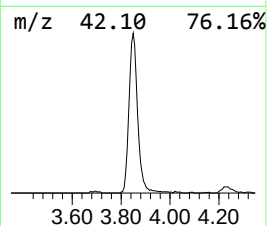
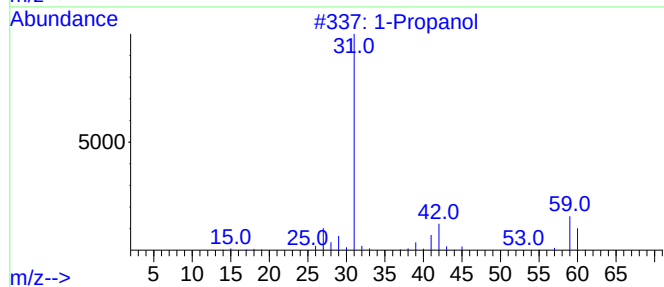
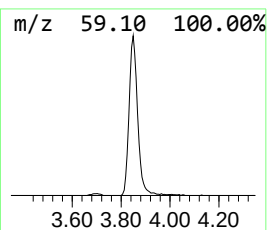
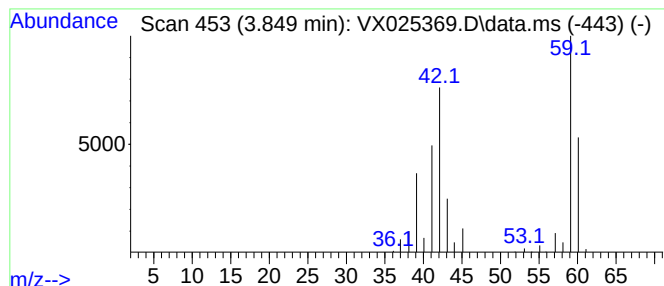
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.849	23.38 ug/l	165644	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	78
2	2-Fluoropropene			60	C3H5F	001184-60-7	49
3	Allyl fluoride			60	C3H5F	000818-92-8	43
4	Cyclopropane			42	C3H6	000075-19-4	12
5	2-Butanol, 3-methoxy-			104	C5H12O2	053778-72-6	9



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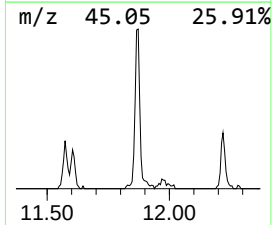
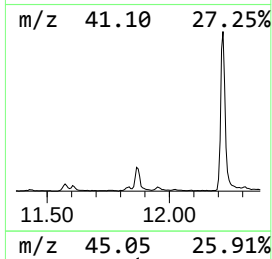
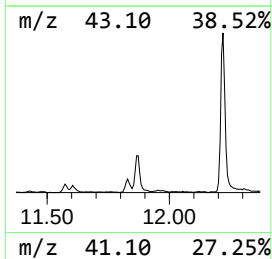
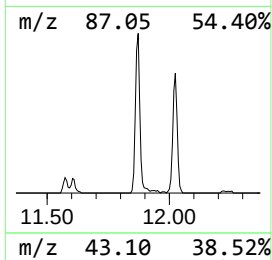
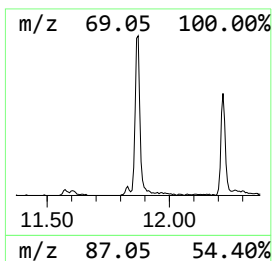
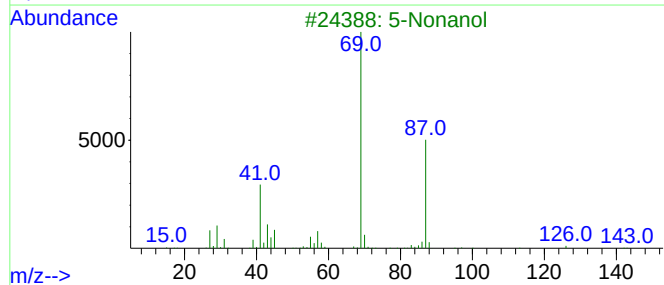
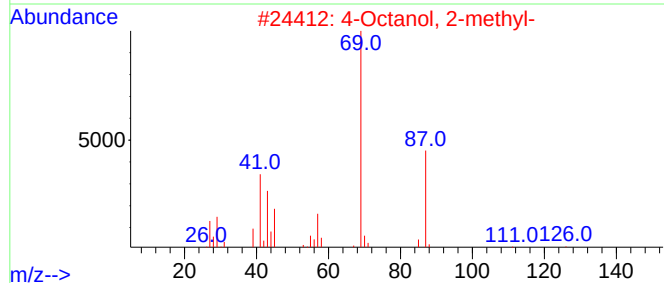
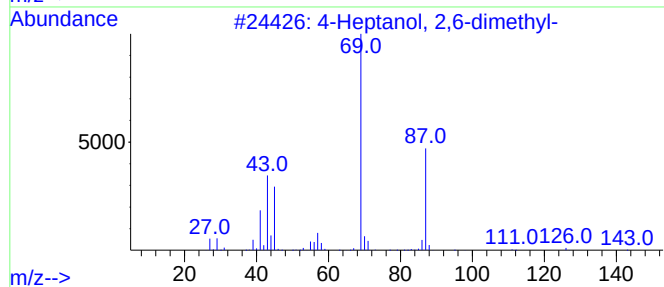
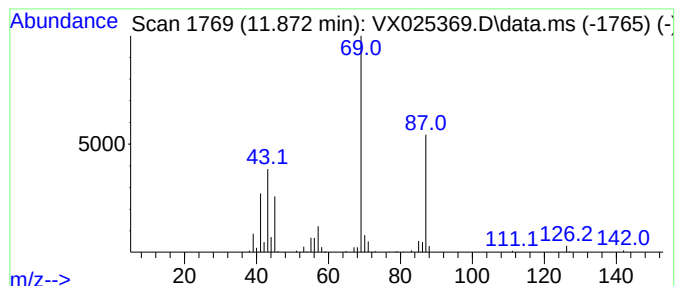
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 3 4-Heptanol, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.872	6.88 ug/l	72271	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	90
2			4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	78
3			5-Nonanol	144	C9H20O	000623-93-8	72
4			4-Octanol	130	C8H18O	000589-62-8	72
5			1,2-Hexanediol	118	C6H14O2	006920-22-5	72



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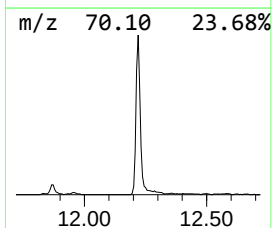
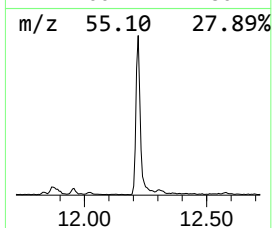
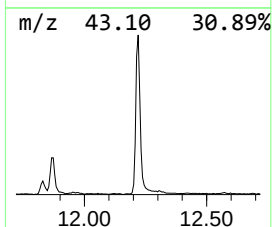
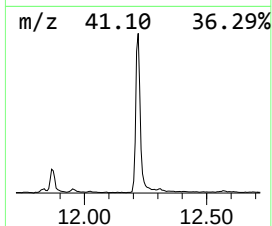
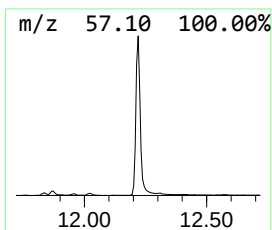
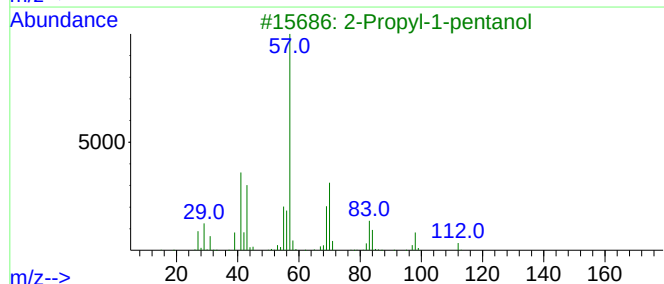
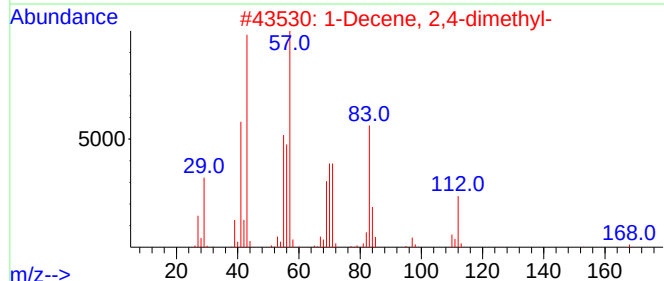
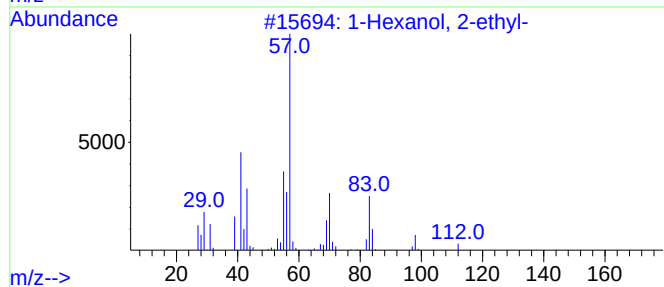
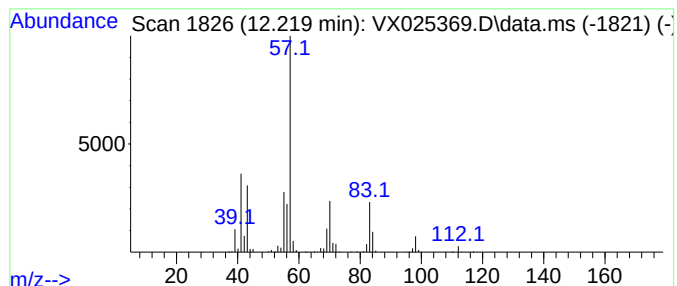
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	37.01 ug/l	388902	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	53
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



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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
Ethanol	2.057	8.8	ug/l	62116	1	5.556	354201	50.0
1-Propanol	3.849	23.4	ug/l	165644	1	5.556	354201	50.0
4-Heptanol, 2,6...	11.872	6.9	ug/l	72271	4	12.024	525334	50.0
1-Hexanol, 2-et...	12.219	37.0	ug/l	388902	4	12.024	525334	50.0