

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
 Data File : VX034350.D
 Acq On : 06 Mar 2023 15:24
 Operator : JC/MD
 Sample : 01816-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31957

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\82X021723W.M
 Title : SW846 8260

Signal : TIC: VX034350.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	25	rVB	59004	66897	4.63%	0.577%
2	1.270	25	30	33	rBV2	14314	17473	1.21%	0.151%
3	1.355	41	44	50	rBV2	22784	31207	2.16%	0.269%
4	2.050	153	158	169	rBV	44928	76884	5.32%	0.663%
5	2.380	205	212	216	rBV	116910	190054	13.16%	1.640%
6	2.422	216	219	230	rVB	25418	43757	3.03%	0.378%
7	2.532	230	237	246	rBV	39562	73167	5.07%	0.631%
8	2.953	299	306	317	rBV	27451	65375	4.53%	0.564%
9	3.696	417	428	444	rBV	80936	221751	15.36%	1.913%
10	4.233	502	516	531	rBV	45372	130486	9.04%	1.126%
11	4.556	559	569	585	rBV	77828	221604	15.35%	1.912%
12	5.001	631	642	653	rBV3	19634	66519	4.61%	0.574%
13	5.385	694	705	718	rBV	161006	472090	32.69%	4.074%
14	5.550	721	732	751	rVB	270199	772215	53.48%	6.663%
15	5.958	787	799	806	rBV	179715	476658	33.01%	4.113%
16	6.037	806	812	822	rVB	73906	200687	13.90%	1.732%
17	6.763	921	931	948	rBV	431261	1039391	71.98%	8.969%
18	7.214	1000	1005	1015	rBV	11111	28843	2.00%	0.249%
19	7.531	1051	1057	1063	rBV2	9048	16789	1.16%	0.145%
20	8.647	1233	1240	1247	rVV	912844	1444064	100.00%	12.461%
21	8.720	1247	1252	1257	rVV	171607	269543	18.67%	2.326%
22	8.769	1257	1260	1270	rVB2	29782	52685	3.65%	0.455%
23	9.238	1332	1337	1346	rBV2	25984	51070	3.54%	0.441%
24	10.055	1463	1471	1483	rBV	878410	1222719	84.67%	10.551%
25	10.153	1483	1487	1491	rVV2	18427	29087	2.01%	0.251%
26	10.195	1491	1494	1500	rVB	21267	29635	2.05%	0.256%
27	10.299	1506	1511	1519	rVB	94609	133433	9.24%	1.151%
28	10.445	1531	1535	1541	rVB	23048	31685	2.19%	0.273%
29	10.506	1541	1545	1551	rBV	25058	32964	2.28%	0.284%
30	10.652	1562	1569	1580	rBV4	86270	174134	12.06%	1.503%
31	10.750	1581	1585	1594	rBV	57082	95305	6.60%	0.822%
32	11.079	1634	1639	1644	rBV	702816	904136	62.61%	7.802%
33	11.128	1644	1647	1652	rVB	46886	62780	4.35%	0.542%
34	11.378	1681	1688	1695	rBV	22739	43956	3.04%	0.379%
35	11.451	1695	1700	1711	rVB	18467	31417	2.18%	0.271%
36	11.573	1715	1720	1723	rBV	28785	40212	2.78%	0.347%

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37	11.610	1723	1726	1734	rVV4	30382	59153	4.10%	0.510%
38	11.683	1734	1738	1744	rVV	125416	148184	10.26%	1.279%
39	11.750	1744	1749	1754	rVV	48109	65909	4.56%	0.569%
40	11.811	1754	1759	1762	rVV	29575	47057	3.26%	0.406%
41	11.866	1766	1768	1779	rVB2	21773	39544	2.74%	0.341%
42	12.024	1788	1794	1801	rBV	838637	1090434	75.51%	9.409%
43	12.085	1801	1804	1809	rVB	16553	21348	1.48%	0.184%
44	12.219	1821	1826	1837	rBV	442141	645650	44.71%	5.571%
45	12.311	1837	1841	1852	rVB8	16575	40892	2.83%	0.353%
46	12.414	1853	1858	1863	rBV	226425	278147	19.26%	2.400%
47	13.286	1991	2001	2006	rBV7	8331	17881	1.24%	0.154%
48	13.341	2006	2010	2014	rVV2	11869	14888	1.03%	0.128%
49	13.426	2018	2024	2029	rBV	25879	35575	2.46%	0.307%
50	13.774	2074	2081	2087	rBV	39655	71362	4.94%	0.616%
51	13.847	2089	2093	2100	rVV	19318	30331	2.10%	0.262%
52	13.914	2100	2104	2115	rVB	20865	35366	2.45%	0.305%
53	14.640	2216	2223	2232	rVB	22429	35204	2.44%	0.304%
54	14.780	2241	2246	2250	rBV	16377	20364	1.41%	0.176%
55	15.975	2435	2442	2448	rBV9	8102	16466	1.14%	0.142%
56	16.090	2456	2461	2467	rVB5	8880	14659	1.02%	0.126%

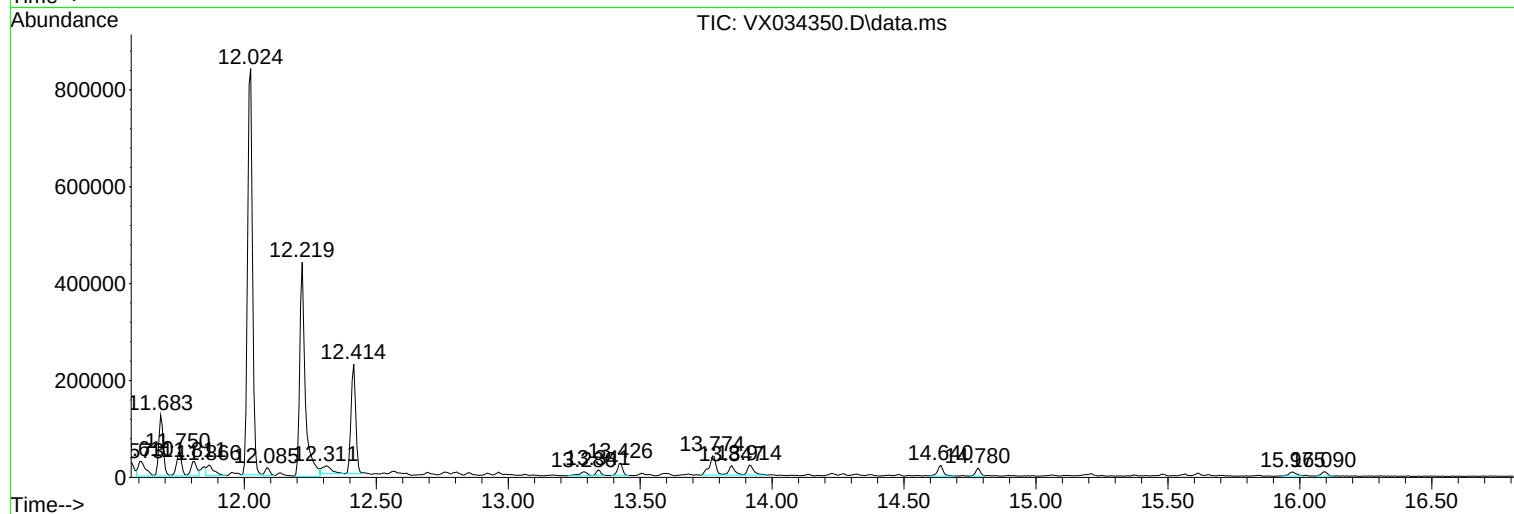
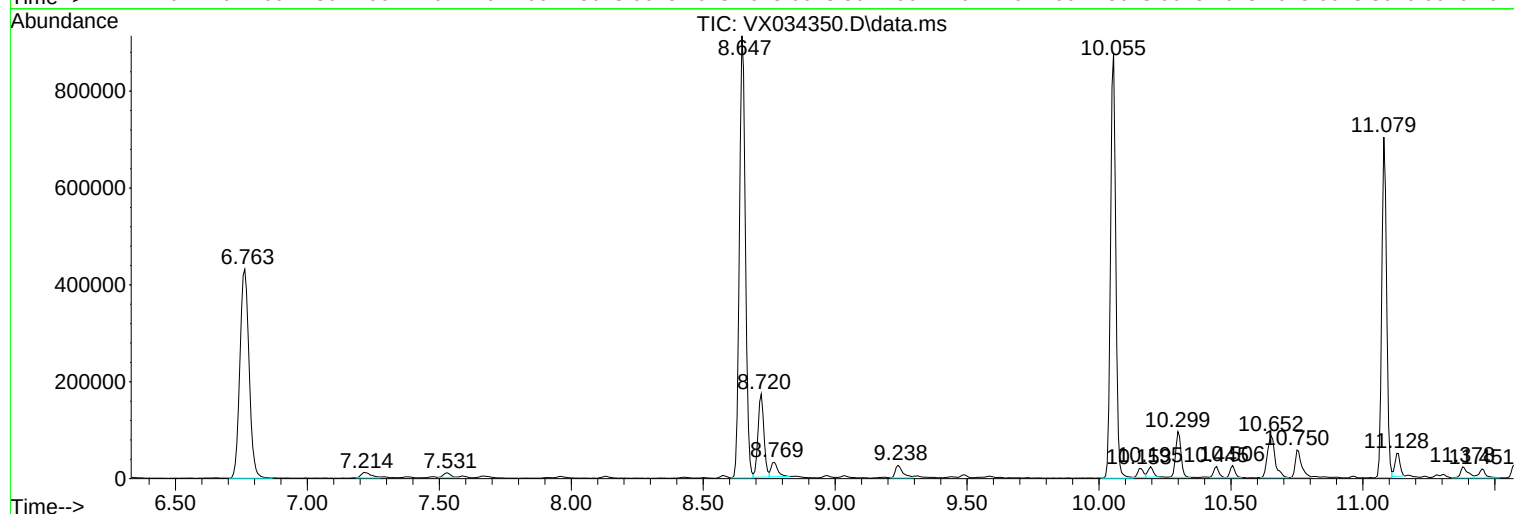
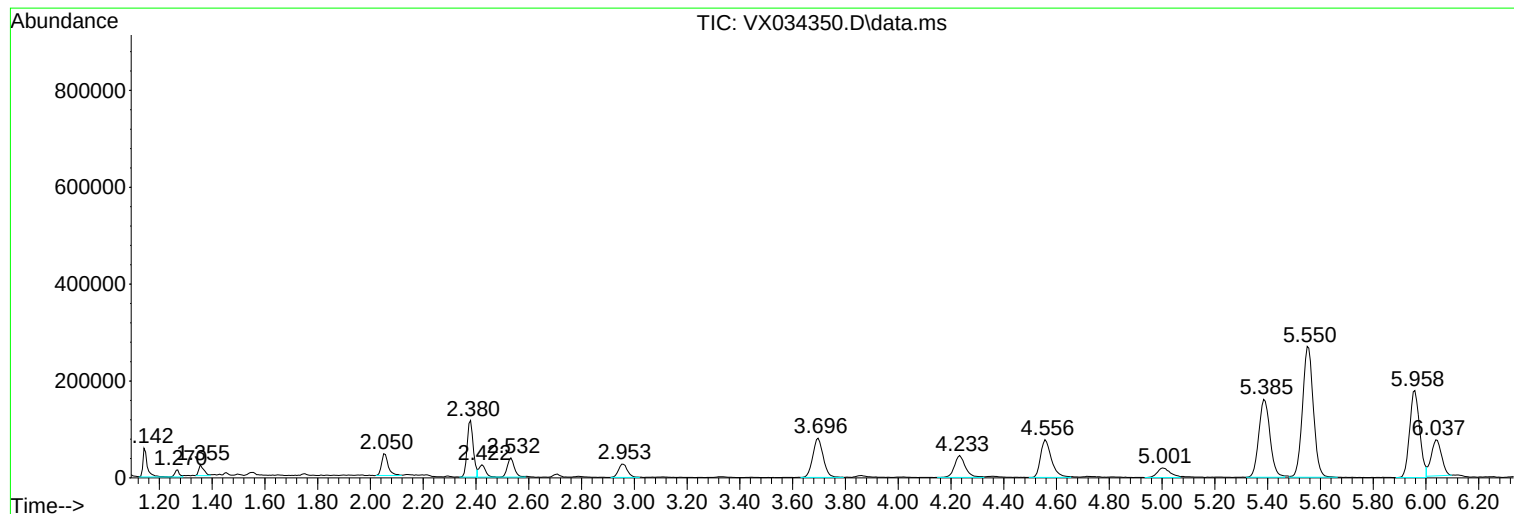
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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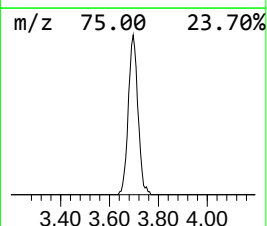
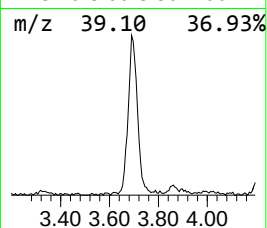
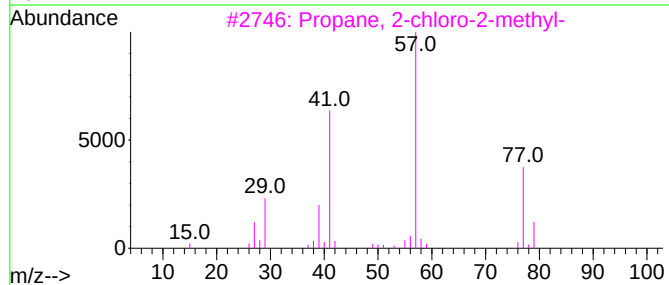
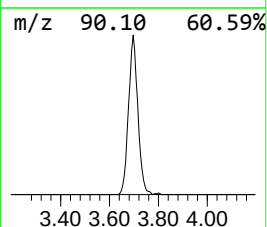
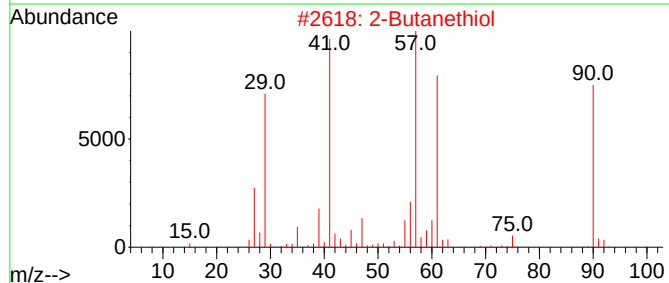
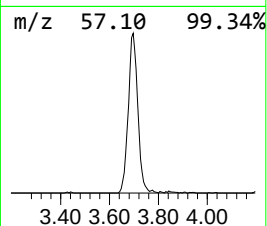
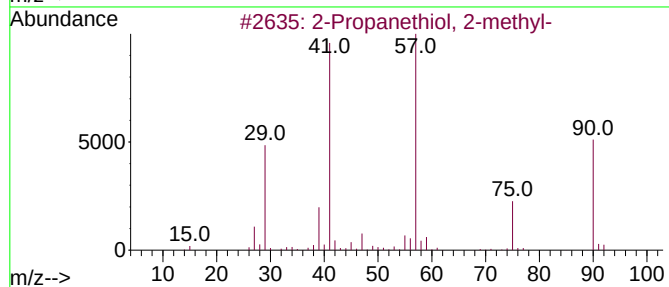
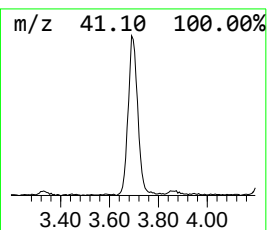
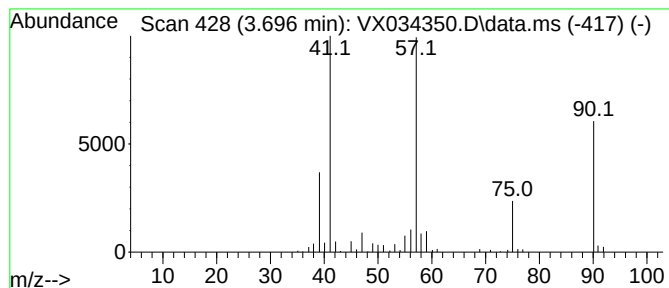
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Quant Title : SW846 8260

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

Peak Number 1 2-Propanethiol, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.696	14.36 ug/l	221751	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	91
2		2-Butanethiol	90	C4H10S	000513-53-1	40
3		Propane, 2-chloro-2-methyl-	92	C4H9Cl	000507-20-0	27
4		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	22
5		Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	17



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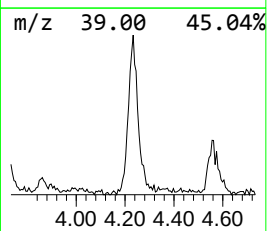
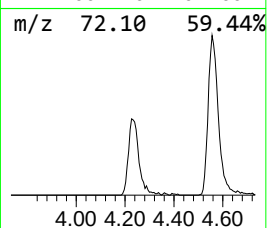
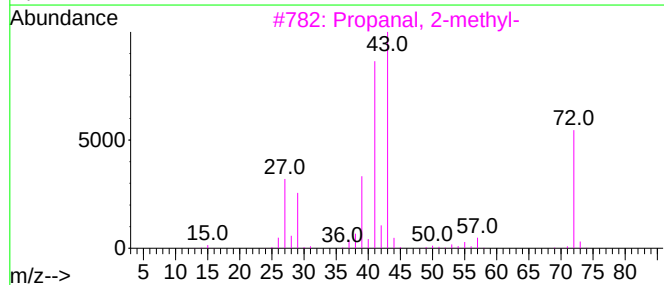
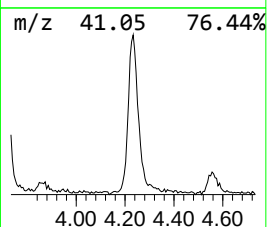
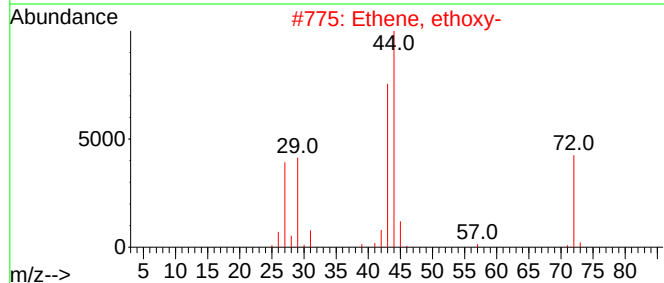
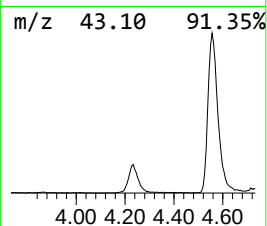
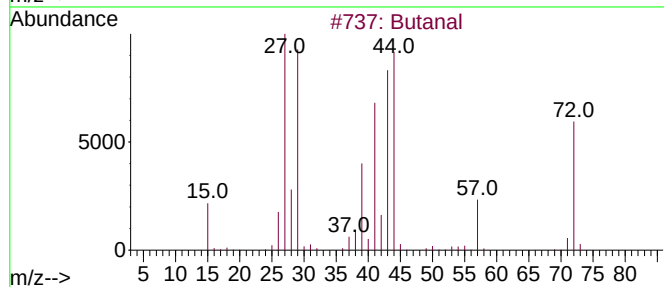
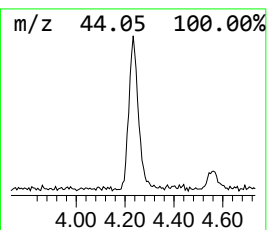
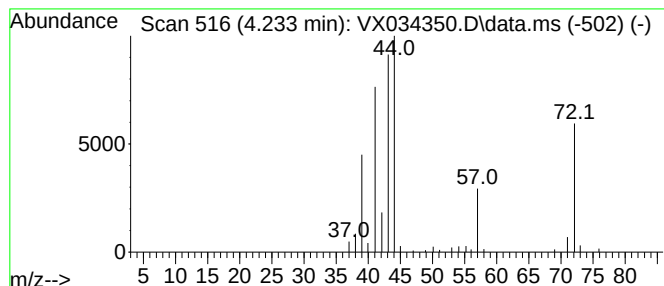
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 2 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	8.45 ug/l	130486	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	35
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	23



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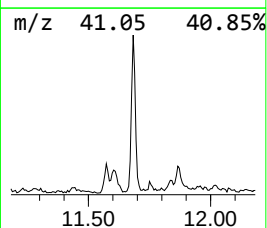
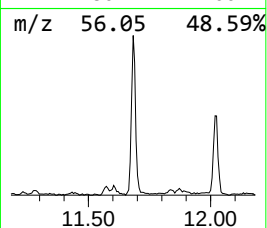
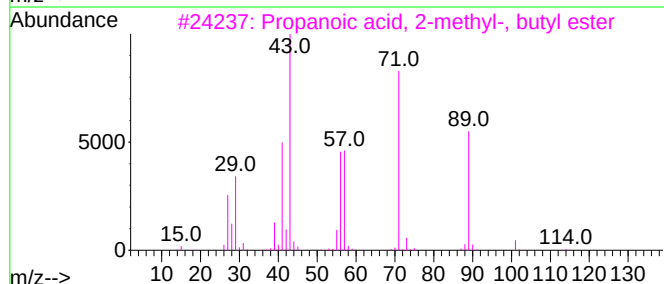
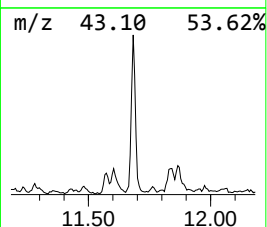
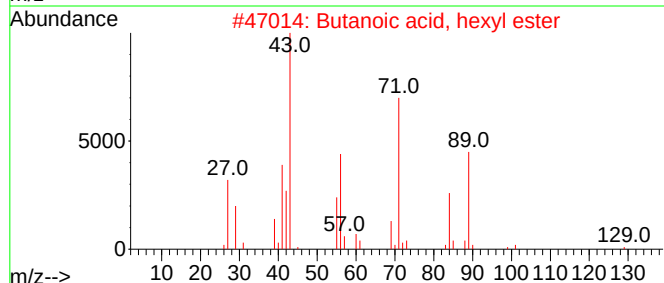
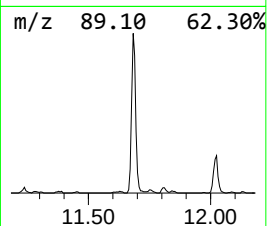
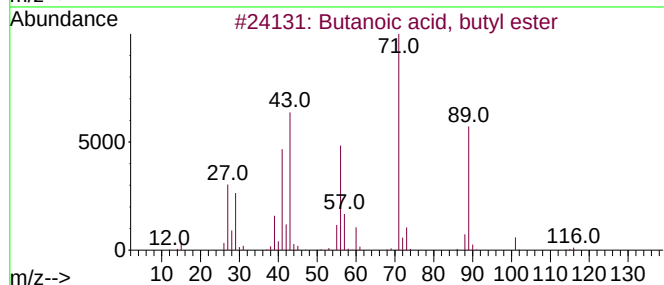
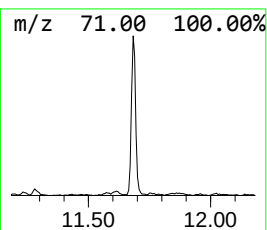
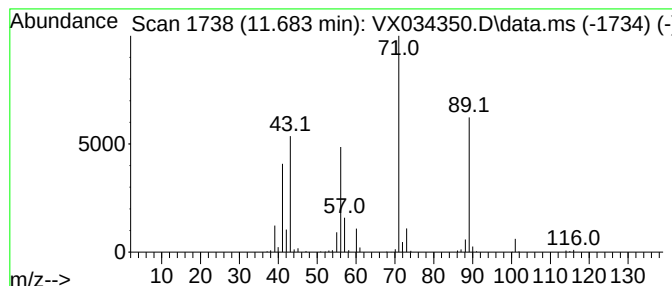
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	6.79 ug/l	148184	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	91
2			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78
3			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59



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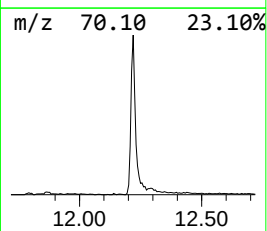
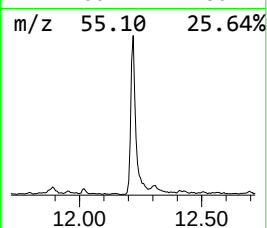
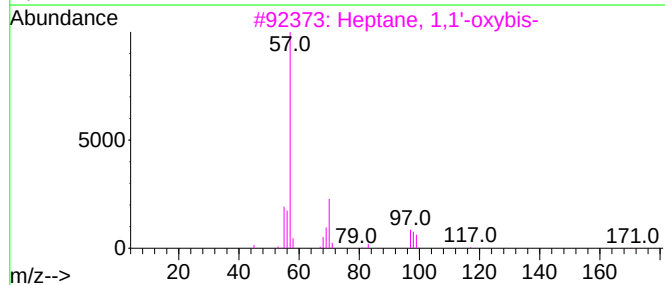
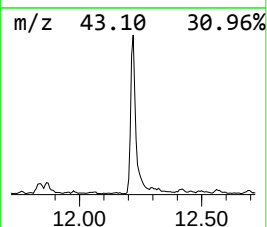
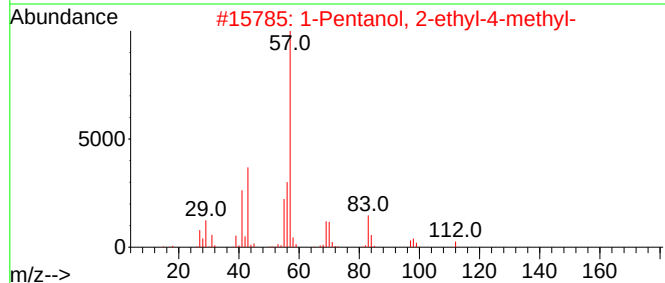
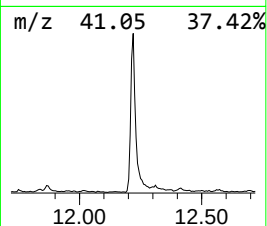
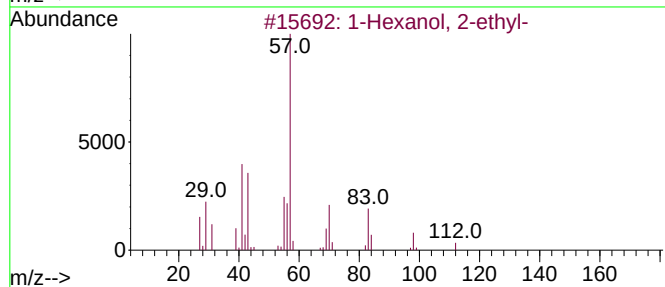
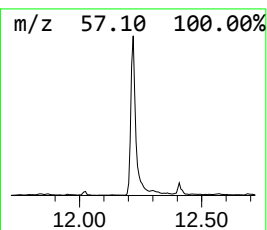
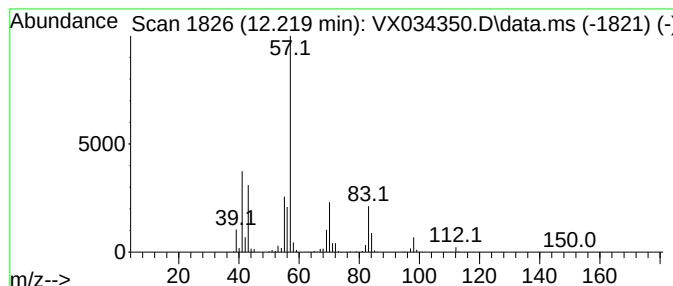
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	29.61 ug/l	645650	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	86
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47



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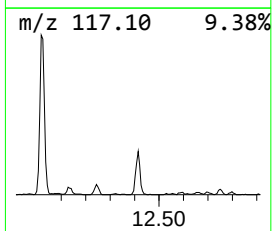
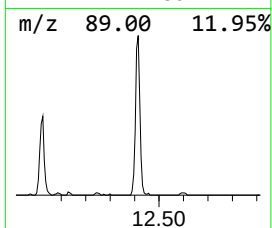
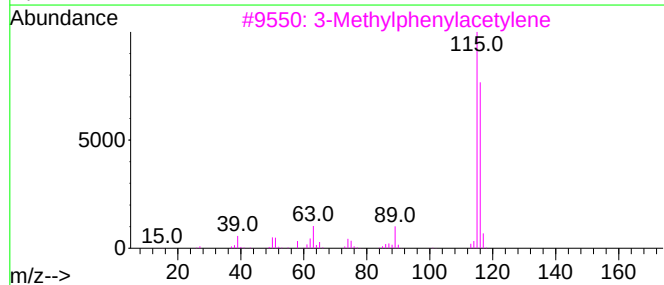
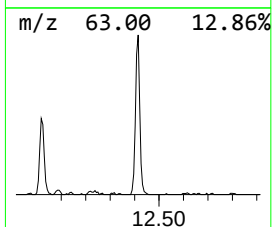
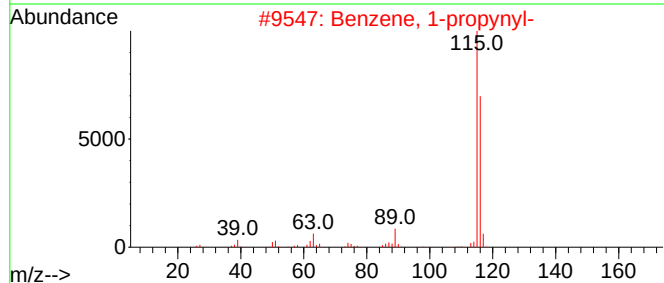
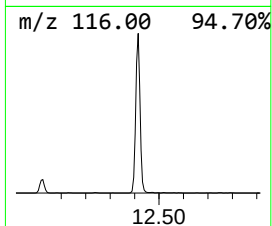
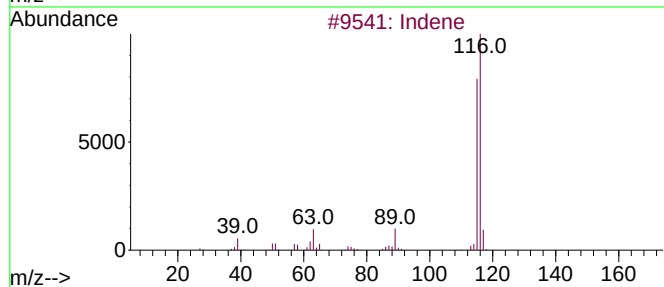
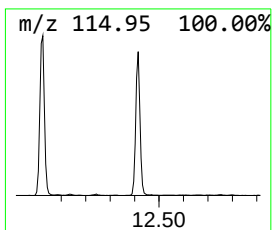
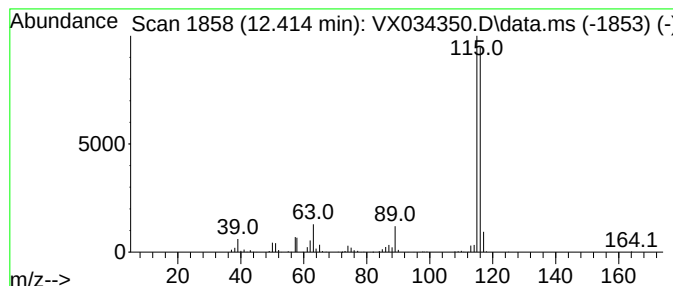
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 5 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	12.75 ug/l	278147	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
Data File : VX034350.D
Acq On : 06 Mar 2023 15:24
Operator : JC/MD
Sample : 01816-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31957

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.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-Propanethiol,...	3.696	14.4	ug/l	221751	1	5.556	772215	50.0
Butanal	4.233	8.4	ug/l	130486	1	5.556	772215	50.0
Butanoic acid, ...	11.683	6.8	ug/l	148184	4	12.024	1090430	50.0
1-Hexanol, 2-et...	12.219	29.6	ug/l	645650	4	12.024	1090430	50.0
Indene	12.414	12.8	ug/l	278147	4	12.024	1090430	50.0