

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041723\
 Data File : VX035109.D
 Acq On : 17 Apr 2023 15:16
 Operator : JC/MD
 Sample : 02353-03 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BUR-1261

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\82X032923W.M
 Title : SW846 8260

Signal : TIC: VX035109.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	19	rVB	32817	33247	1.74%	0.240%
2	1.453	56	60	80	rBV	1552430	1909577	100.00%	13.801%
3	4.239	506	517	525	rBV3	6629	20829	1.09%	0.151%
4	4.379	531	540	564	rBV	240123	771499	40.40%	5.576%
5	5.385	693	705	717	rBV	186812	539781	28.27%	3.901%
6	5.550	720	732	749	rVB2	323763	933624	48.89%	6.748%
7	5.952	787	798	809	rBV	205555	559215	29.28%	4.042%
8	6.763	920	931	941	rBV	515960	1234381	64.64%	8.921%
9	6.873	941	949	966	rVB	415101	1010701	52.93%	7.305%
10	7.208	996	1004	1025	rBV	67463	181935	9.53%	1.315%
11	7.678	1074	1081	1093	rBV	24239	51900	2.72%	0.375%
12	8.647	1233	1240	1248	rBV	1070503	1680277	87.99%	12.144%
13	8.720	1248	1252	1258	rVB	18286	29423	1.54%	0.213%
14	10.055	1465	1471	1484	rBV	1056296	1455230	76.21%	10.517%
15	10.299	1505	1511	1518	rBV	22866	34230	1.79%	0.247%
16	11.079	1634	1639	1654	rBV	892918	1142331	59.82%	8.256%
17	11.683	1732	1738	1745	rBV	37019	50684	2.65%	0.366%
18	11.750	1745	1749	1754	rVB	17158	21153	1.11%	0.153%
19	11.890	1770	1772	1777	rVB3	16846	22119	1.16%	0.160%
20	11.988	1783	1788	1789	rBV	19525	22463	1.18%	0.162%
21	12.018	1789	1793	1800	rVB	1078851	1379276	72.23%	9.968%
22	12.219	1821	1826	1832	rBV	135393	220404	11.54%	1.593%
23	12.287	1832	1837	1838	rVV4	33139	66705	3.49%	0.482%
24	12.305	1838	1840	1847	rVV4	38731	76299	4.00%	0.551%
25	12.360	1847	1849	1857	rVB6	9159	19499	1.02%	0.141%
26	12.591	1883	1887	1901	rVB6	7559	21240	1.11%	0.154%
27	13.609	2047	2054	2062	rBV3	19571	38291	2.01%	0.277%
28	13.774	2075	2081	2089	rVB	19827	31922	1.67%	0.231%
29	13.847	2089	2093	2100	rVB3	14338	20396	1.07%	0.147%
30	13.914	2100	2104	2111	rBV2	16825	25738	1.35%	0.186%
31	14.640	2215	2223	2226	rBV	31220	48668	2.55%	0.352%
32	14.780	2240	2246	2251	rBV	28994	35749	1.87%	0.258%
33	15.213	2308	2317	2325	rBV3	16661	33537	1.76%	0.242%
34	15.481	2355	2361	2366	rBV3	14543	23566	1.23%	0.170%
35	15.615	2378	2383	2386	rBV	20166	30419	1.59%	0.220%
36	15.652	2386	2389	2395	rVB2	13305	19240	1.01%	0.139%

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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\82X032923W.M
Title : SW846 8260

37	15.841	2411	2420	2425	rBV3	8487	19407	1.02%	0.140%
38	16.091	2453	2461	2467	rVB4	11356	21504	1.13%	0.155%

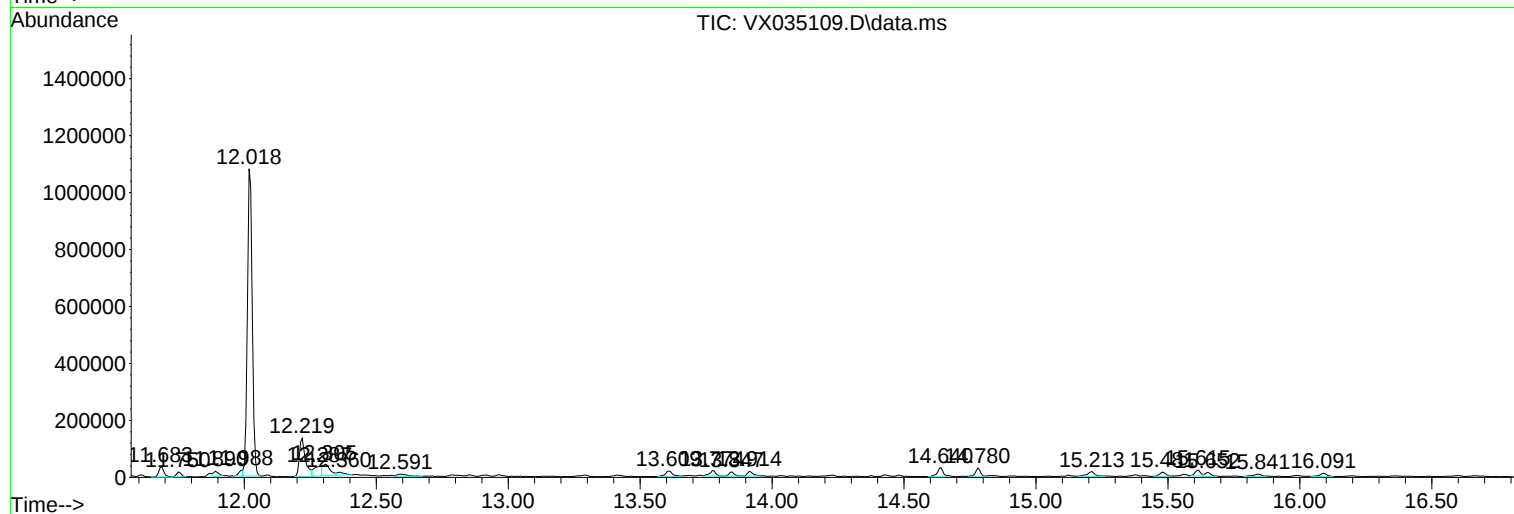
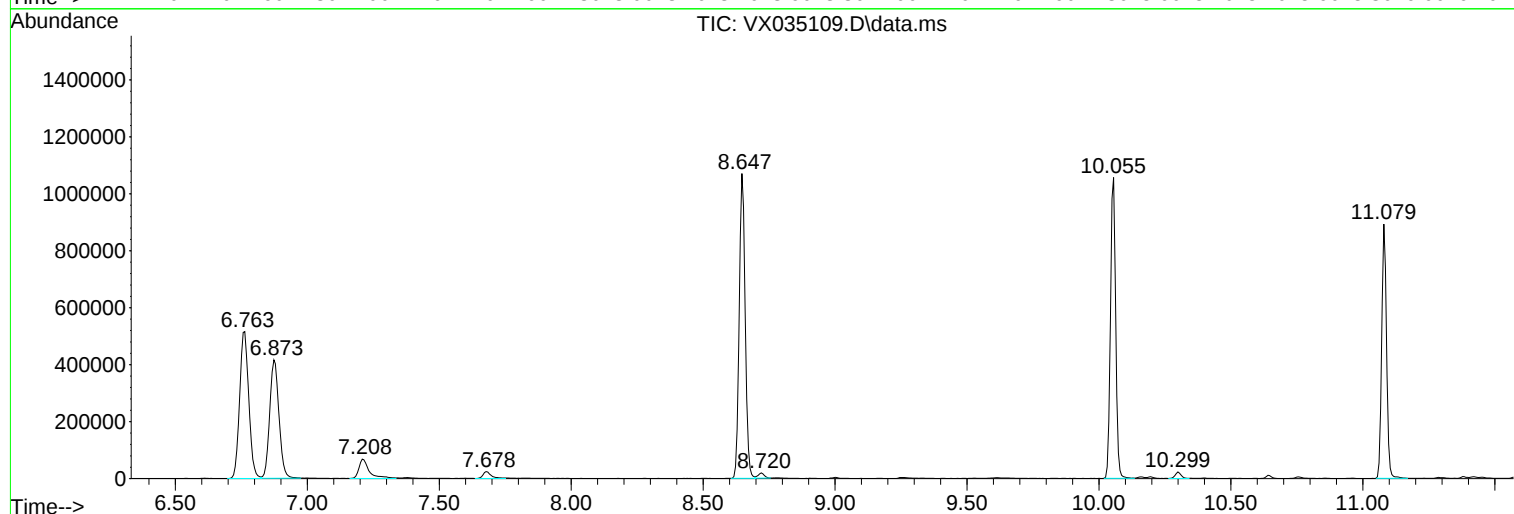
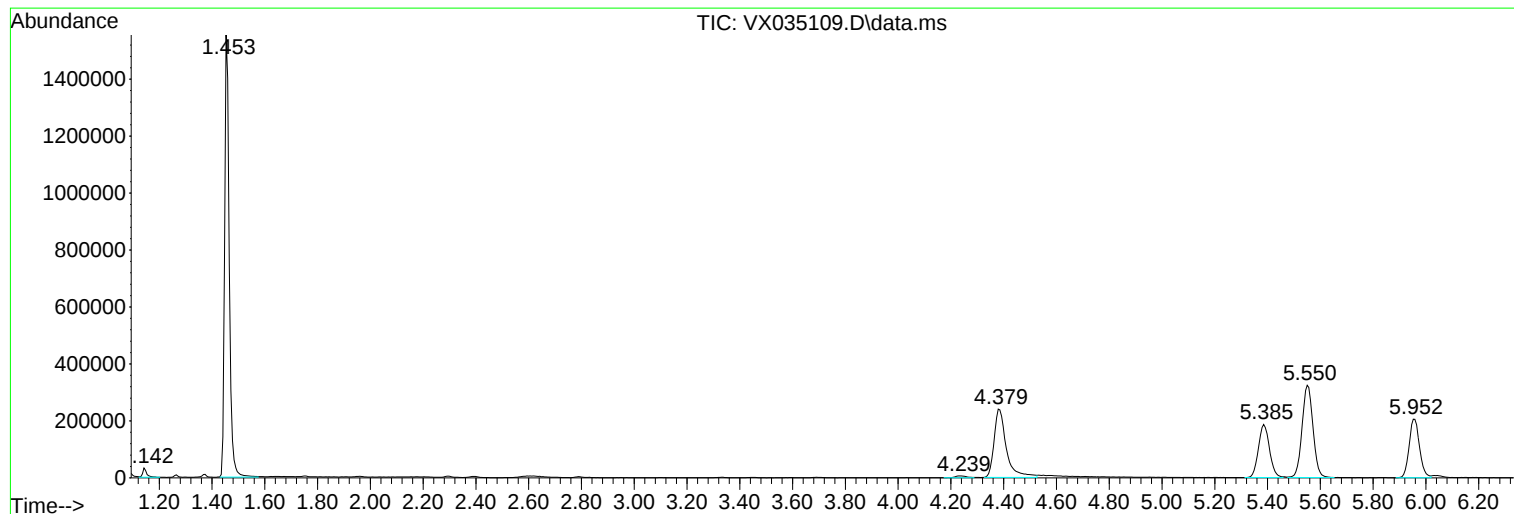
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Quant Title : SW846 8260

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



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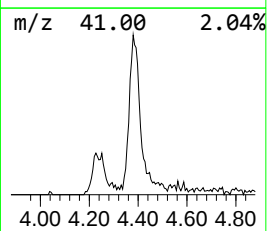
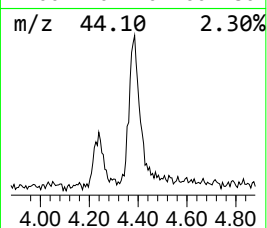
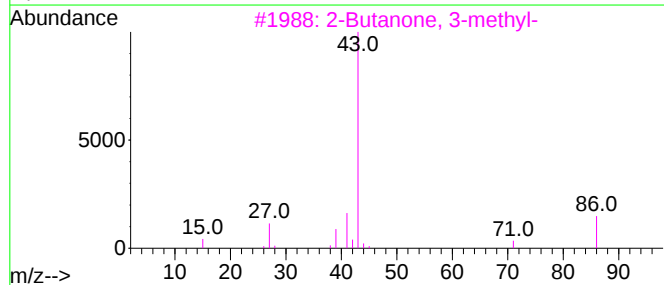
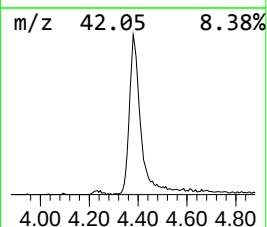
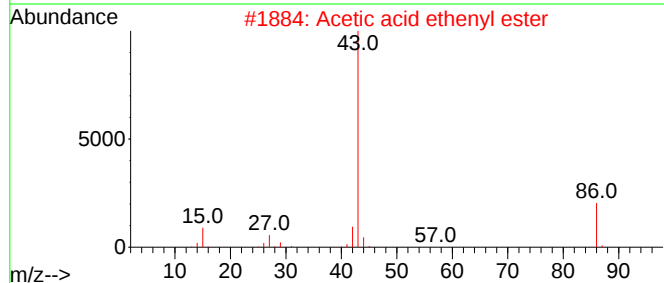
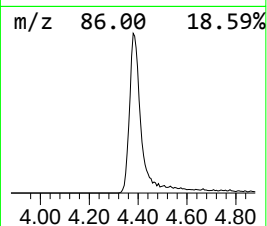
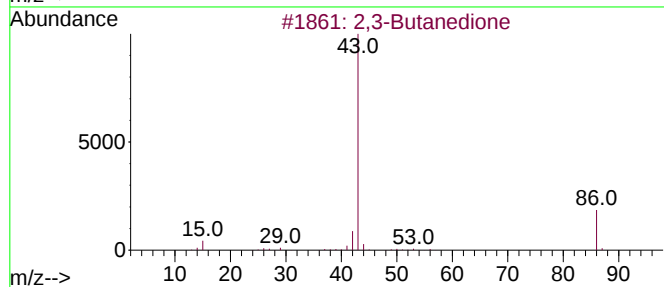
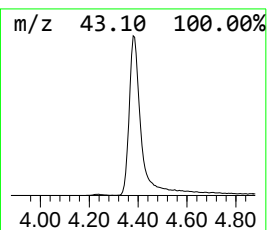
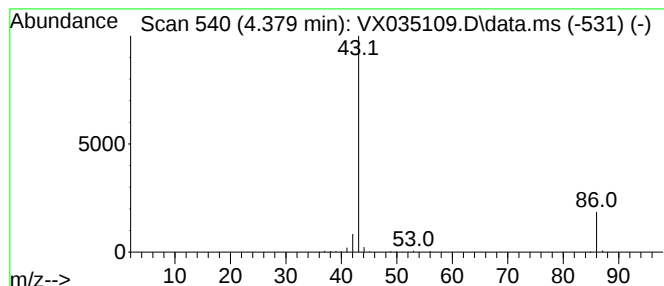
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 2 2,3-Butanedione Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.379	41.32 ug/l	771499	Pentafluorobenzene	5.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,3-Butanedione	86	C4H6O2	000431-03-8	80
2		Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	9
3		2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	7
4		2-Pentanone	86	C5H10O	000107-87-9	7
5		Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	5



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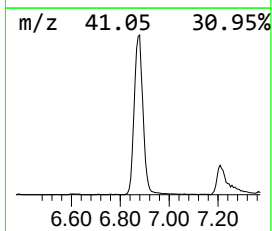
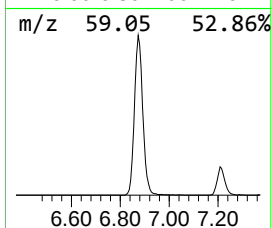
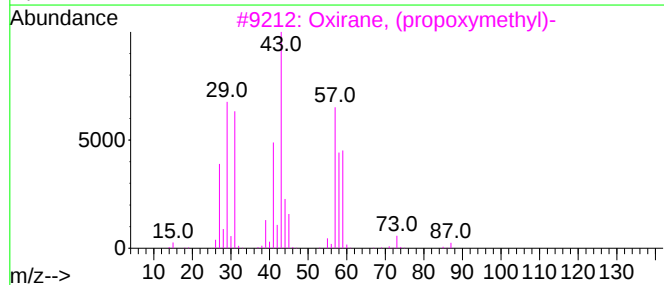
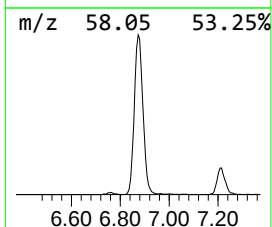
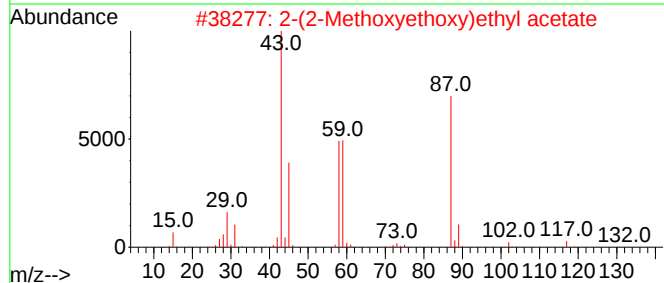
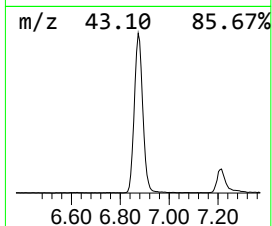
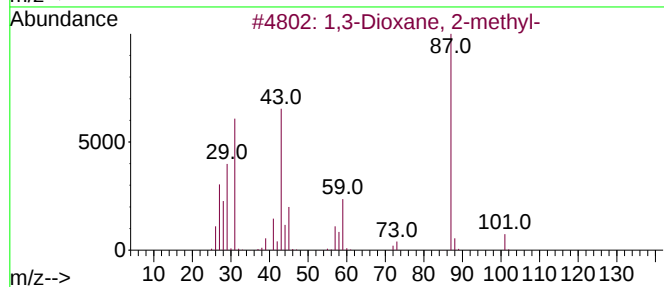
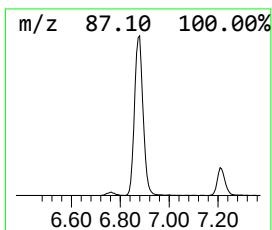
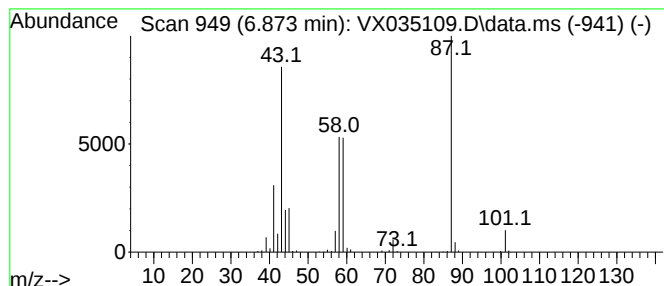
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,3-Dioxane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.873	40.94 ug/l	1010700	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-			102	C5H10O2	000626-68-6	53
2	2-(2-Methoxyethoxy)ethyl acetate			162	C7H14O4	1000351-95-4	45
3	Oxirane, (propoxymethyl)-			116	C6H12O2	003126-95-2	43
4	Oxazolidin-2-one			87	C3H5NO2	000497-25-6	32
5	1,3-Dioxolane, 2-butyl-4-methyl-			144	C8H16O2	074094-60-3	28



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Instrument :
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ClientSampleId :
BUR-1261

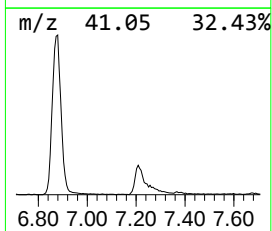
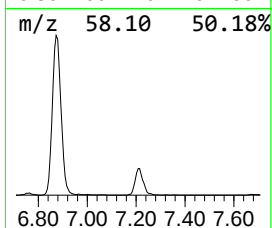
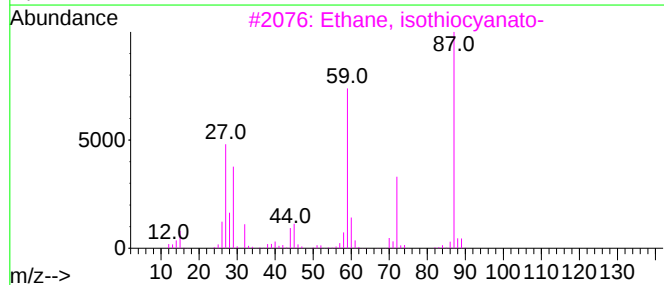
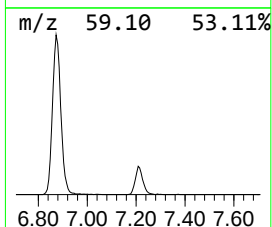
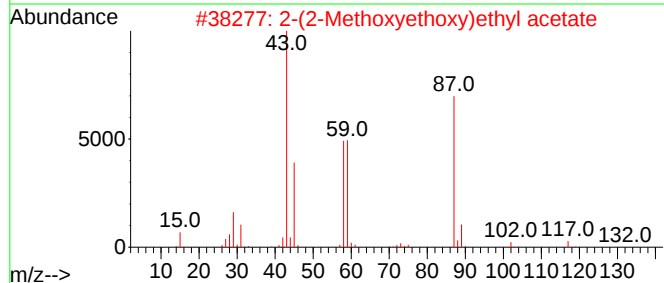
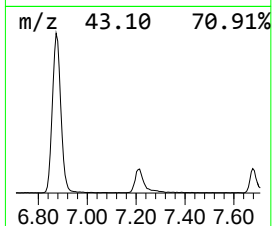
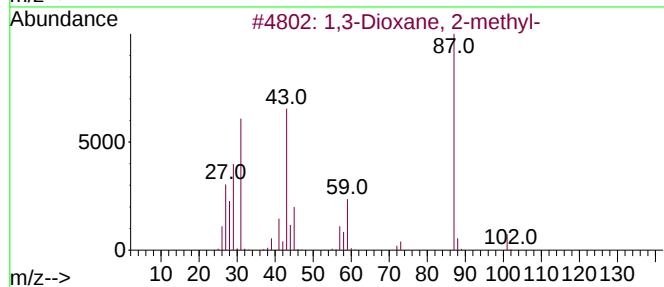
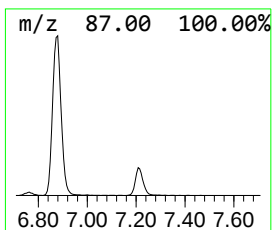
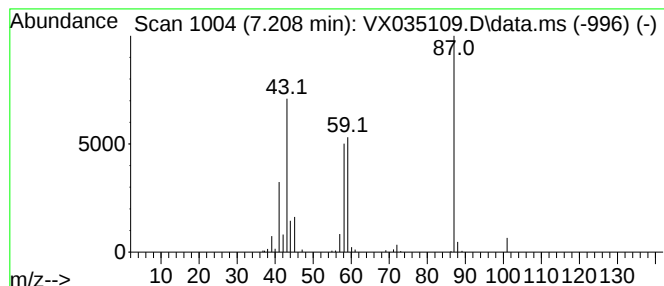
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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

Peak Number 4 2-(2-Methoxyethoxy)ethyl ac... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	7.37 ug/l	181935	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	59
2			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	56
3			Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	53
4			Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	40
5			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40



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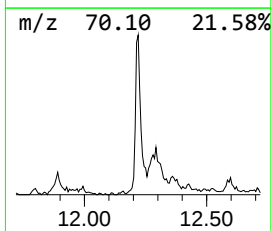
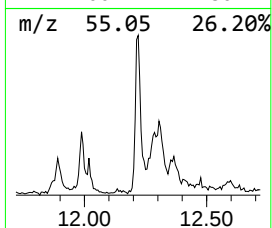
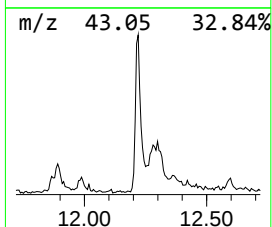
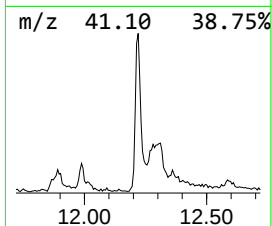
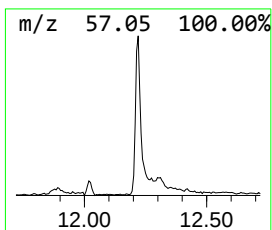
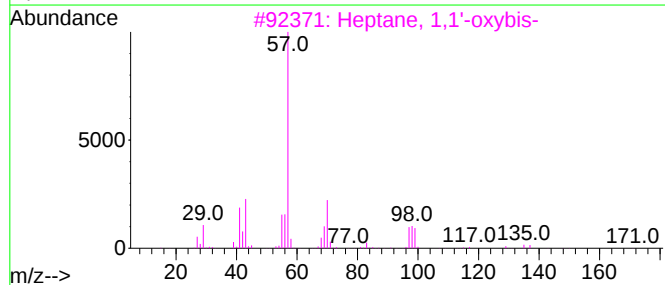
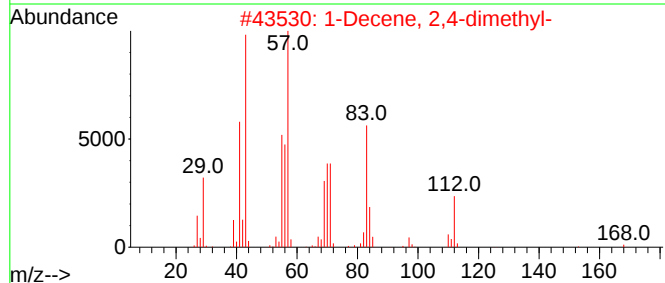
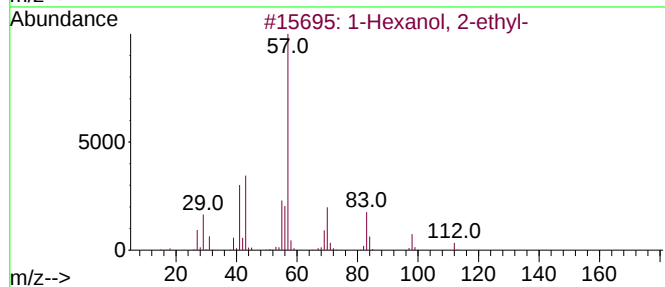
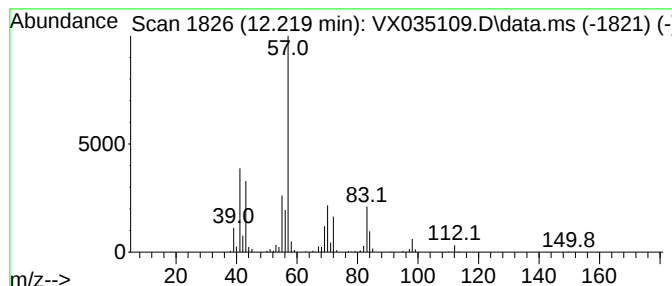
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.220	7.99 ug/l	220404	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-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	43



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,3-Butanedione	4.379	41.3	ug/l	771499	1	5.556	933624	50.0
1,3-Dioxane, 2-...	6.873	40.9	ug/l	1010700	2	6.763	1234380	50.0
2-(2-Methoxyeth...	7.208	7.4	ug/l	181935	2	6.763	1234380	50.0
1-Hexanol, 2-et...	12.220	8.0	ug/l	220404	4	12.024	1379280	50.0