

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112321\
 Data File : VX025280.D
 Acq On : 23 Nov 2021 17:28
 Operator : JC/MD
 Sample : M4804-02 20X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 40460

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: VX025280.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.251	22	27	33	rBV	25541	29276	1.15%	0.374%
2	1.453	56	60	71	rBV	357937	435273	17.15%	5.554%
3	2.379	206	212	221	rVB	49836	77832	3.07%	0.993%
4	2.538	230	238	246	rBV	32124	58051	2.29%	0.741%
5	4.379	530	540	555	rBV	33109	93117	3.67%	1.188%
6	5.391	694	706	720	rBV	63627	182907	7.21%	2.334%
7	5.555	722	733	750	rVB	92032	258781	10.20%	3.302%
8	5.958	786	799	812	rBV2	61139	164351	6.48%	2.097%
9	6.763	921	931	940	rBV	154209	369935	14.58%	4.720%
10	6.878	940	950	969	rVB	1078351	2537454	100.00%	32.375%
11	7.208	994	1004	1015	rBV	673082	1405475	55.39%	17.932%
12	8.652	1234	1241	1249	rBV	333779	530599	20.91%	6.770%
13	9.030	1293	1303	1319	rBV	151429	242929	9.57%	3.099%
14	9.567	1386	1391	1415	rBV	37558	100270	3.95%	1.279%
15	10.055	1465	1471	1480	rBV	366253	482300	19.01%	6.154%
16	11.085	1634	1640	1648	rBV	293047	381833	15.05%	4.872%
17	12.024	1788	1794	1802	rVB	376782	455188	17.94%	5.808%
18	12.219	1821	1826	1835	rBV	20995	32237	1.27%	0.411%

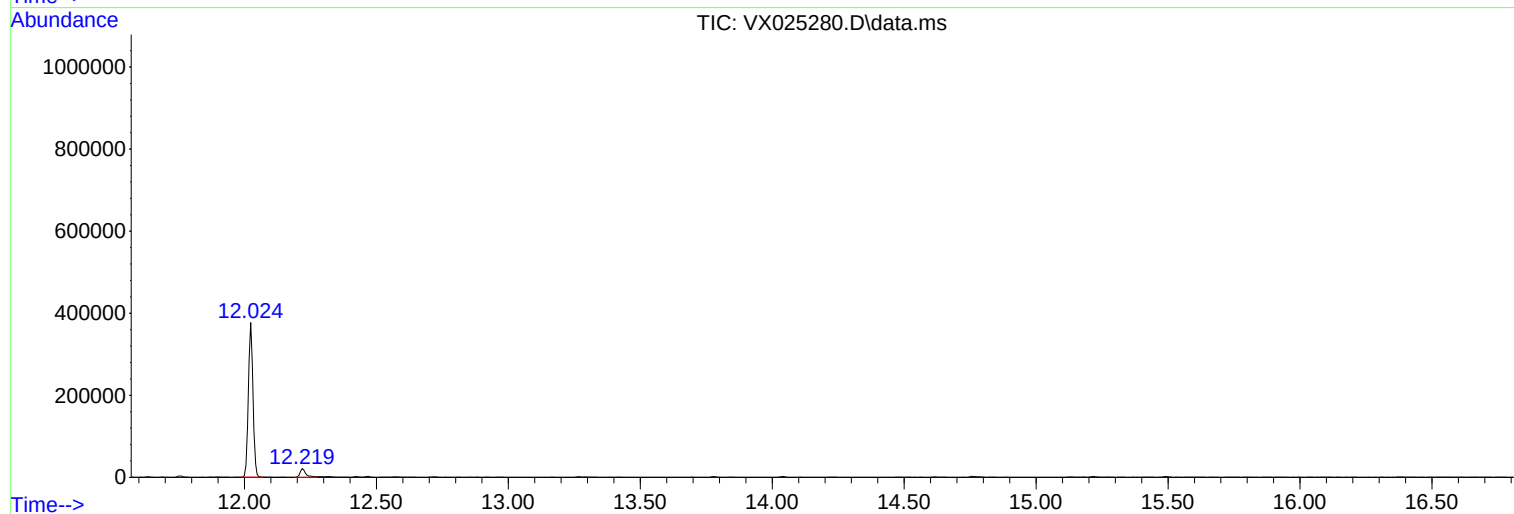
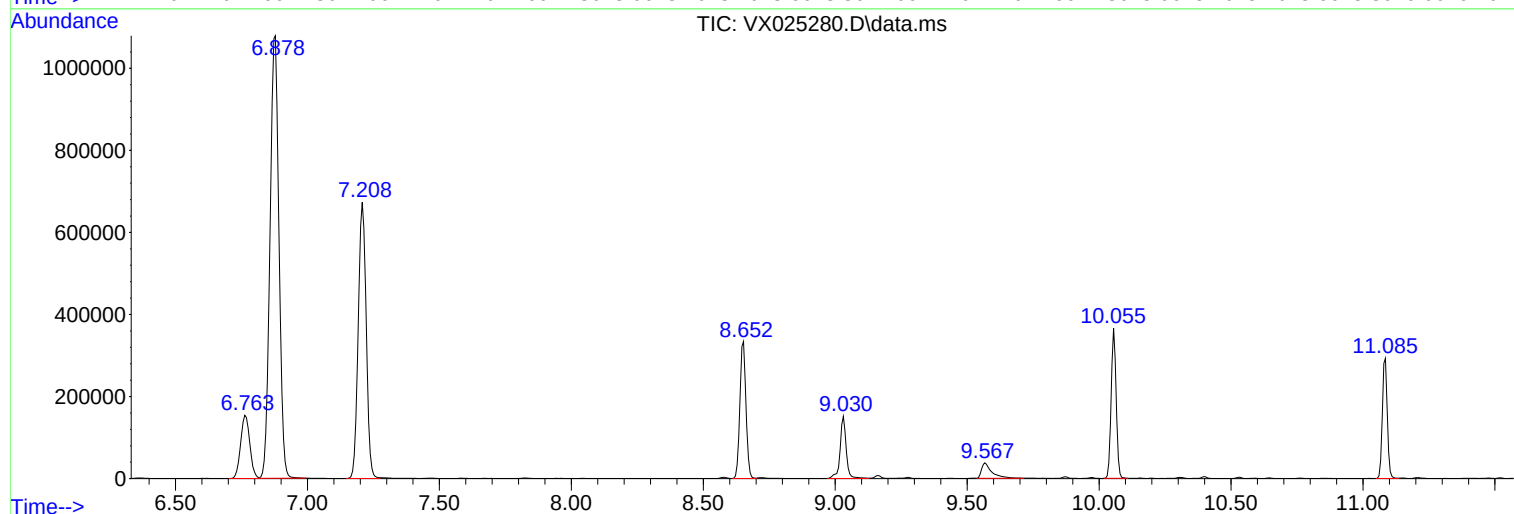
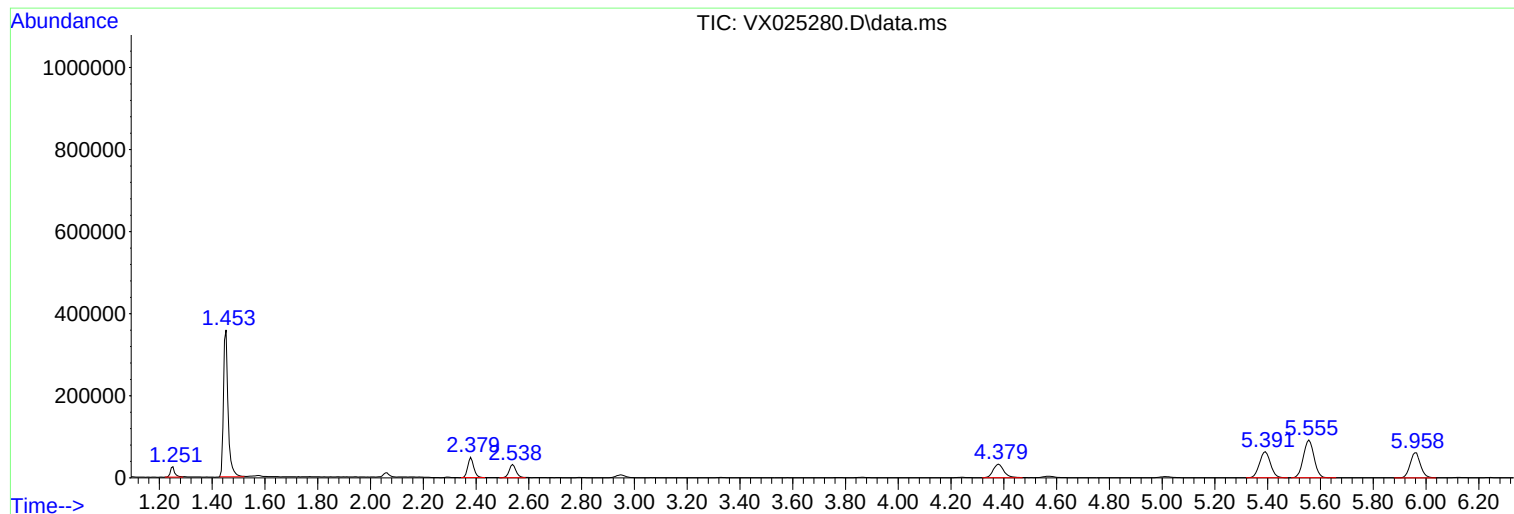
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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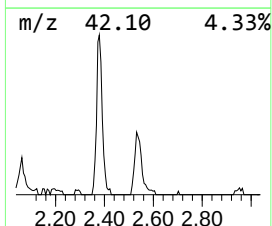
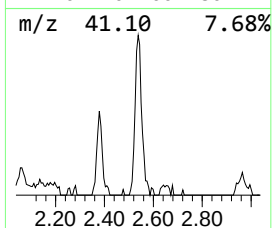
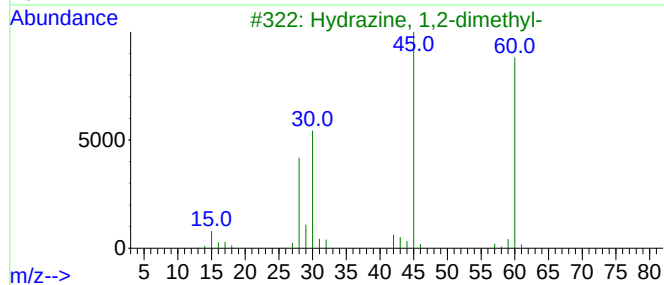
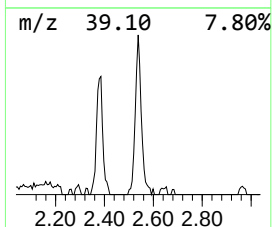
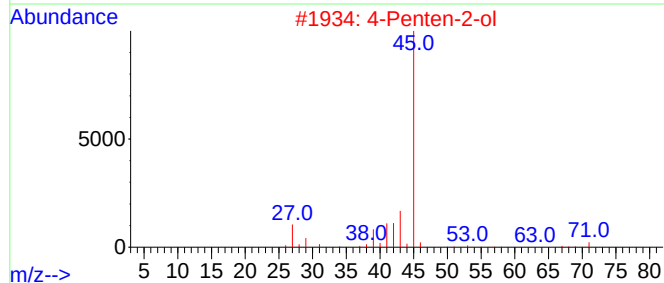
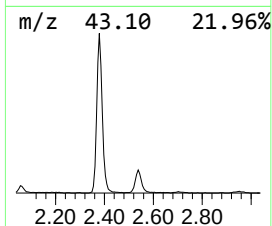
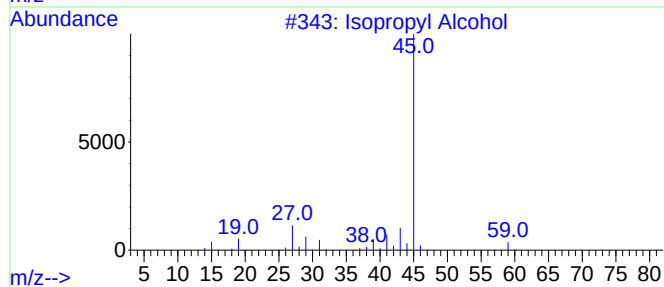
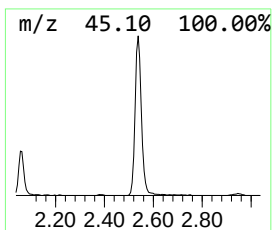
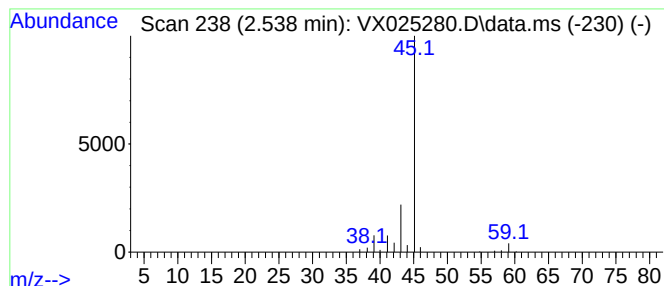
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.538	11.22 ug/l	58051	Pentafluorobenzene	5.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			4-Penten-2-ol	86	C5H10O	000625-31-0	9
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4			Formamide	45	CH3NO	000075-12-7	5
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	4



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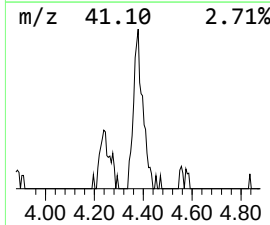
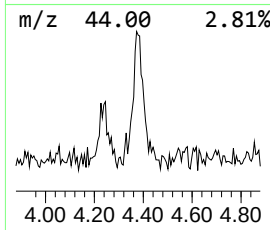
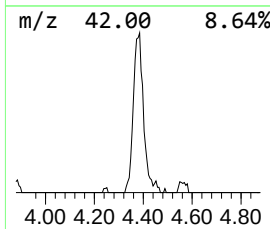
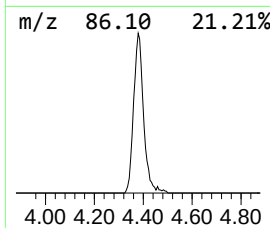
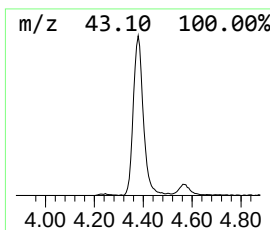
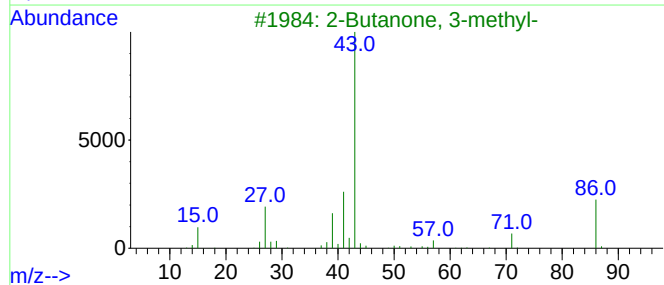
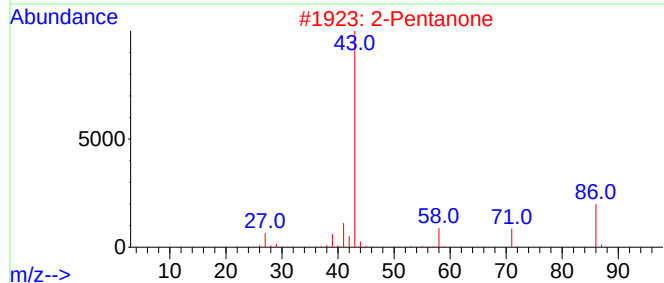
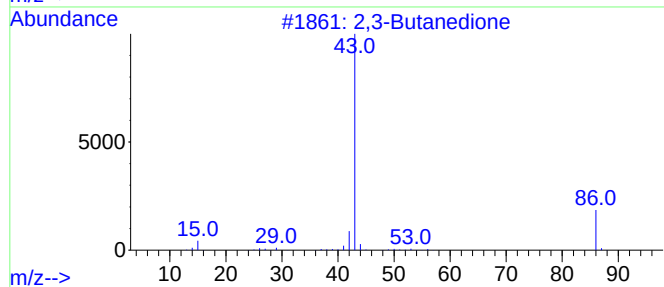
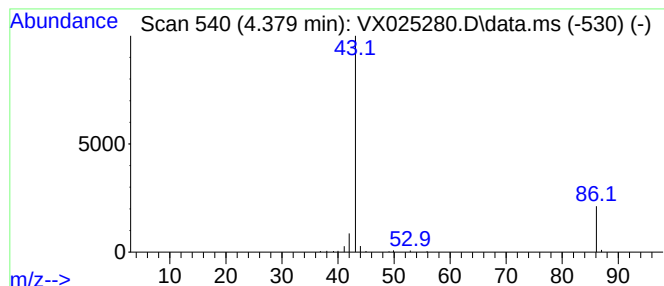
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 4 2,3-Butanedione Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.379	17.99 ug/l	93117	Pentafluorobenzene	5.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione			86	C4H6O2	000431-03-8	90
2	2-Pentanone			86	C5H10O	000107-87-9	72
3	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	7
4	Acetic acid ethenyl ester			86	C4H6O2	000108-05-4	7
5	Ethanone, 1-oxiranyl-			86	C4H6O2	004401-11-0	5



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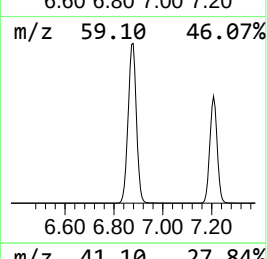
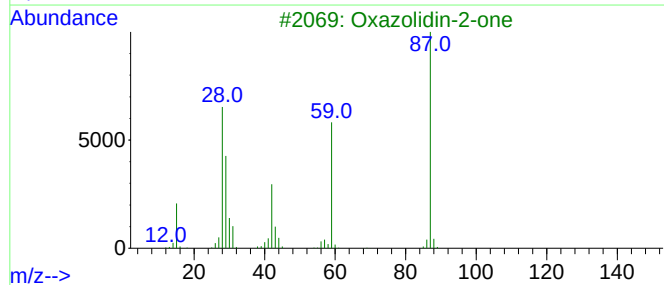
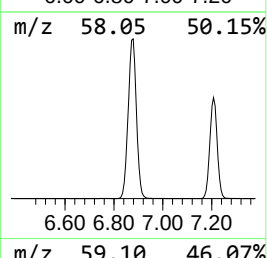
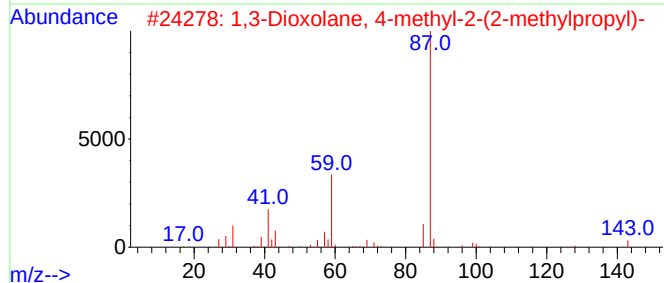
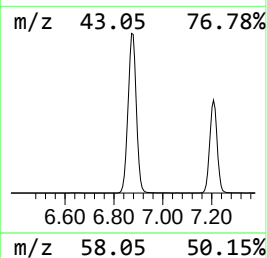
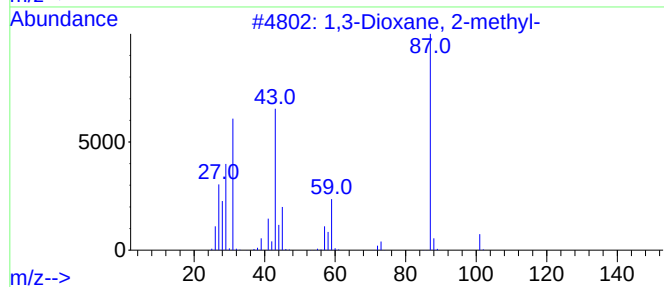
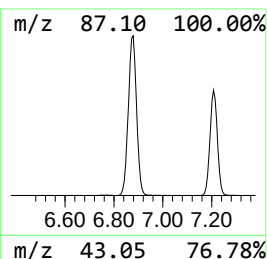
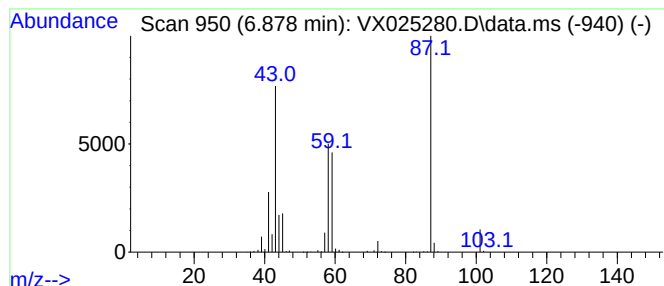
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown6.878 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.878	342.96 ug/l	2537450	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	40
2			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	38
3			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	37
4			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	33
5			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	33



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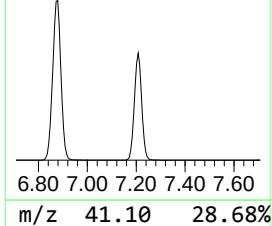
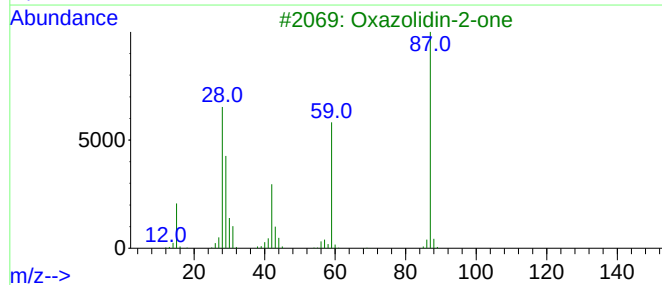
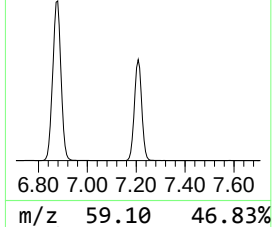
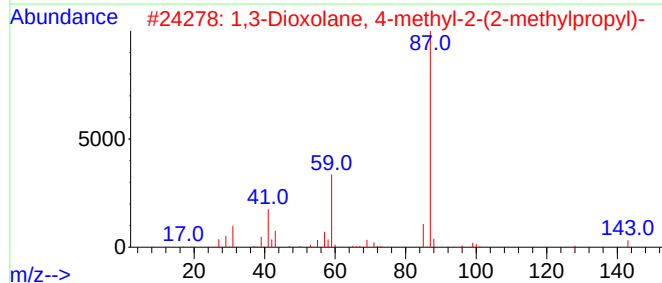
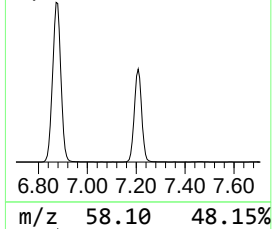
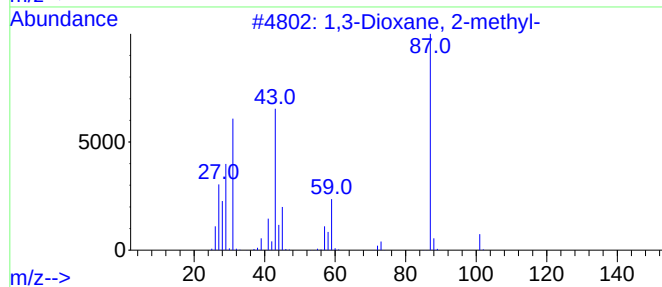
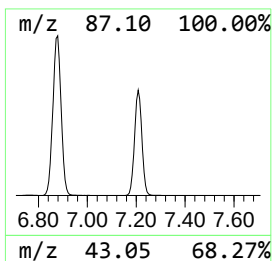
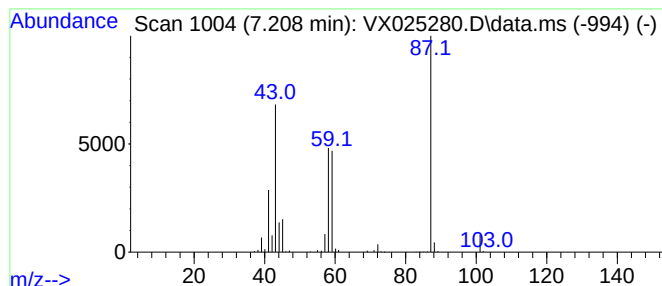
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Quant Title : SW846 8260

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

Peak Number 6 1,3-Dioxane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	189.96 ug/l	1405480	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	52
2			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	50
3			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
4			2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
5			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	36



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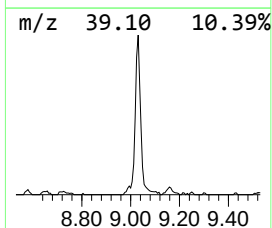
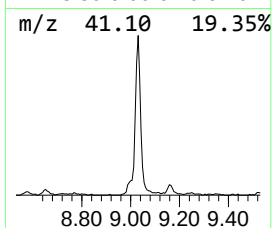
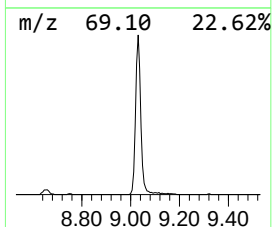
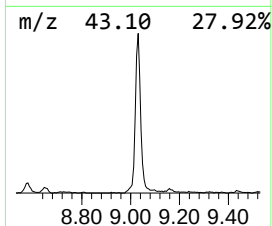
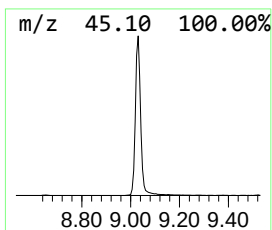
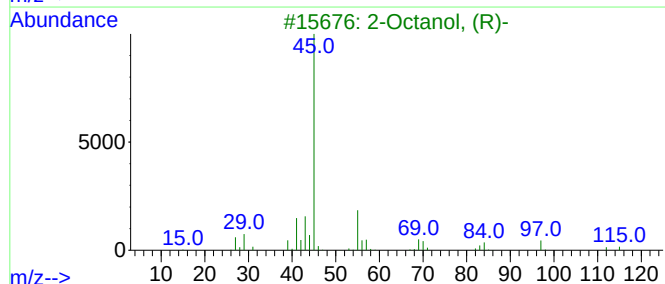
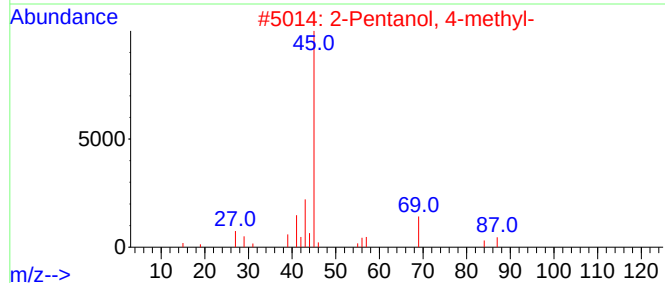
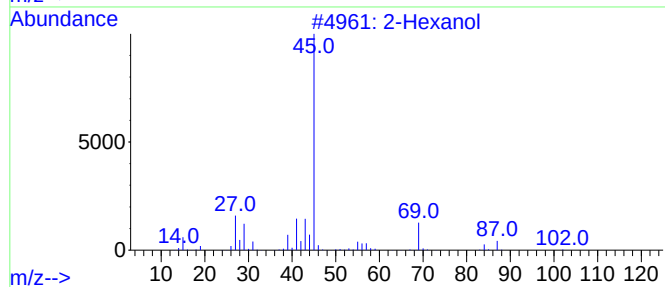
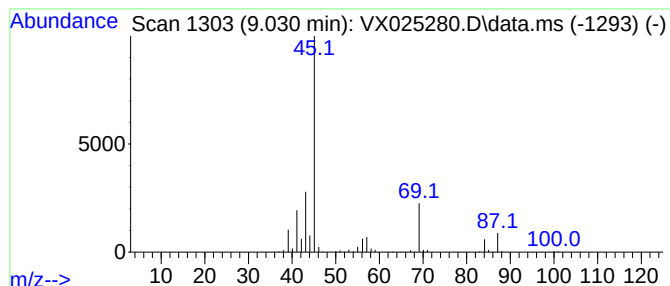
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2-Hexanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.030	25.18 ug/l	242929	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol	102	C6H14O	000626-93-7	83
2			2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	83
3			2-Octanol, (R)-	130	C8H18O	005978-70-1	78
4			2-Octanol	130	C8H18O	000123-96-6	78
5			2-Octanol, (S)-	130	C8H18O	006169-06-8	64



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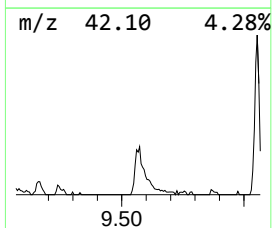
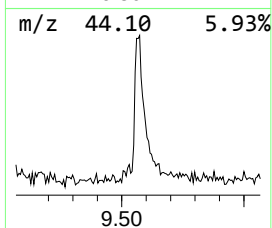
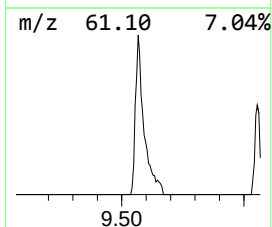
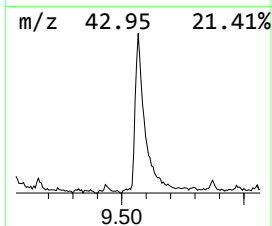
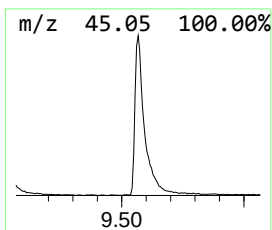
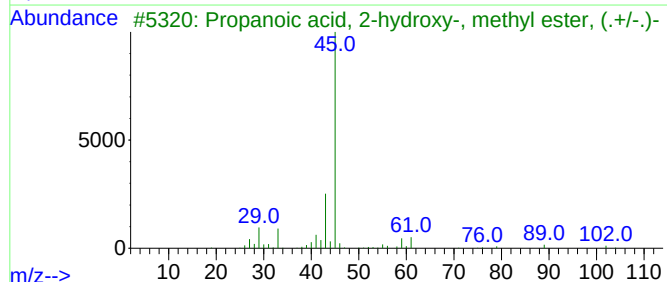
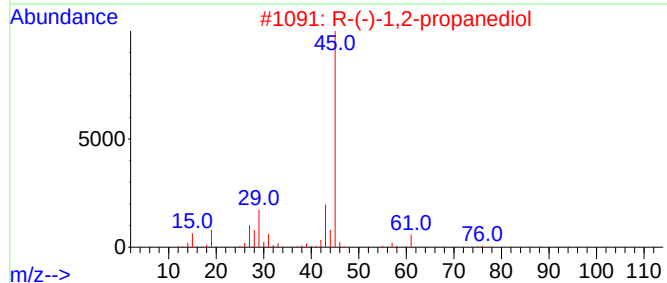
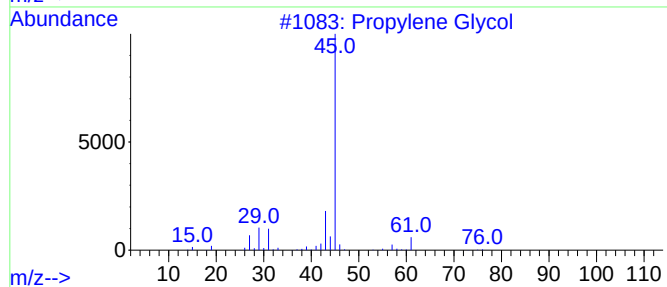
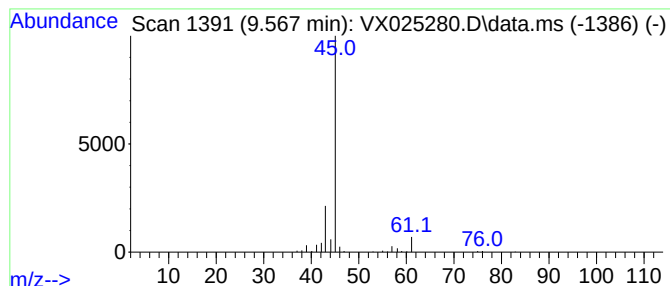
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 8 Propylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.567	10.40 ug/l	100270	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112321\
Data File : VX025280.D
Acq On : 23 Nov 2021 17:28
Operator : JC/MD
Sample : M4804-02 20X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
40460

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.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
Isopropyl Alcohol	2.538	11.2	ug/l	58051	1	5.555	258781	50.0
2,3-Butanedione	4.379	18.0	ug/l	93117	1	5.555	258781	50.0
unknown6.878	6.878	343.0	ug/l	2537450	2	6.763	369935	50.0
1,3-Dioxane, 2-...	7.208	190.0	ug/l	1405480	2	6.763	369935	50.0
2-Hexanol	9.030	25.2	ug/l	242929	3	10.055	482300	50.0
Propylene Glycol	9.567	10.4	ug/l	100270	3	10.055	482300	50.0