

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
 Data File : VX030151.D
 Acq On : 20 Jul 2022 23:04
 Operator : JC/MD
 Sample : N3781-02 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ORA-0019

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\82X071222W.M
 Title : SW846 8260

Signal : TIC: VX030151.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	74	rBV	814536	974421	44.70%	8.198%
2	2.069	153	161	170	rBV	31156	57313	2.63%	0.482%
3	2.294	192	198	207	rBV	608709	938842	43.07%	7.898%
4	2.386	207	213	229	rVB	592033	975381	44.75%	8.206%
5	2.544	234	239	248	rVB	13546	29126	1.34%	0.245%
6	3.879	446	458	476	rBV	821289	2179702	100.00%	18.337%
7	4.386	534	541	554	rVB2	8332	23412	1.07%	0.197%
8	4.587	564	574	583	rBV3	7814	25290	1.16%	0.213%
9	5.391	696	706	723	rBV2	111944	323999	14.86%	2.726%
10	5.562	723	734	749	rVB	189757	546297	25.06%	4.596%
11	5.964	789	800	814	rBV	128075	342482	15.71%	2.881%
12	6.769	921	932	943	rBV	320578	756828	34.72%	6.367%
13	6.879	943	950	962	rVB2	47650	116523	5.35%	0.980%
14	7.220	998	1006	1017	rBV4	9102	28074	1.29%	0.236%
15	8.580	1223	1229	1234	rBV	23479	37517	1.72%	0.316%
16	8.653	1234	1241	1247	rVV	649782	1006964	46.20%	8.471%
17	8.720	1247	1252	1260	rVB	339394	516349	23.69%	4.344%
18	9.001	1293	1298	1308	rVB	262240	381673	17.51%	3.211%
19	9.165	1318	1325	1333	rBV	41294	61111	2.80%	0.514%
20	10.055	1465	1471	1483	rBV	644853	890983	40.88%	7.496%
21	10.159	1483	1488	1492	rVV	53919	87878	4.03%	0.739%
22	10.195	1492	1494	1505	rVV	23527	40266	1.85%	0.339%
23	10.305	1505	1512	1518	rVB	66536	95679	4.39%	0.805%
24	10.647	1562	1568	1577	rBV	29139	41249	1.89%	0.347%
25	11.086	1634	1640	1649	rBV	484738	615224	28.23%	5.176%
26	12.024	1788	1794	1804	rVB	643850	794221	36.44%	6.682%

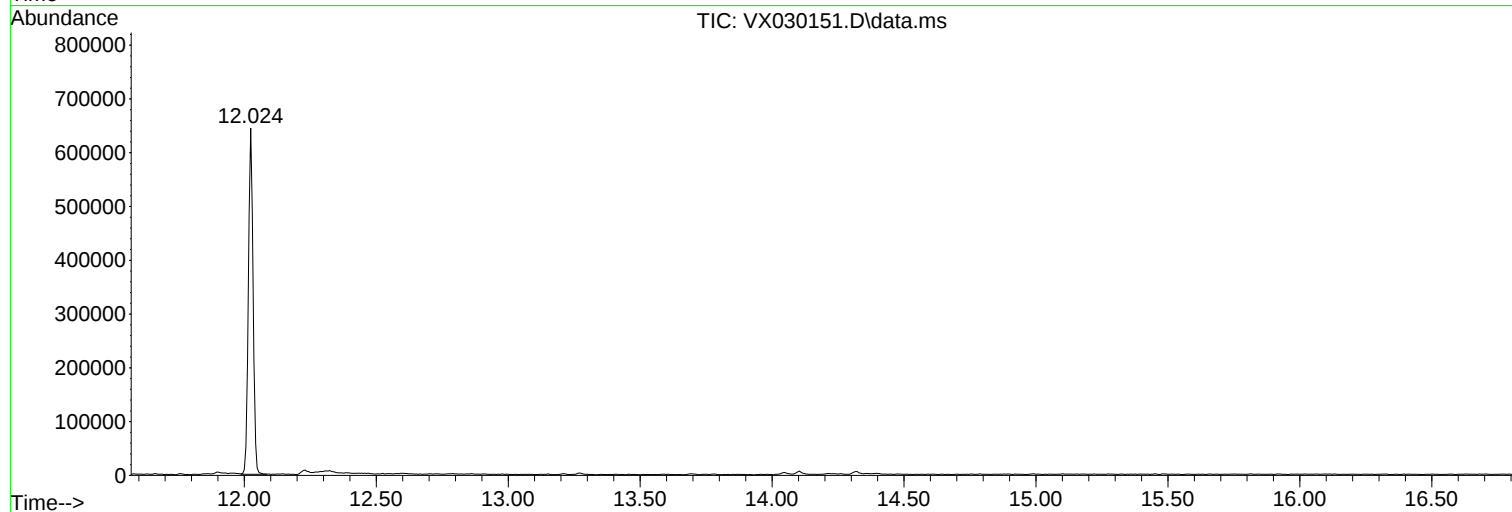
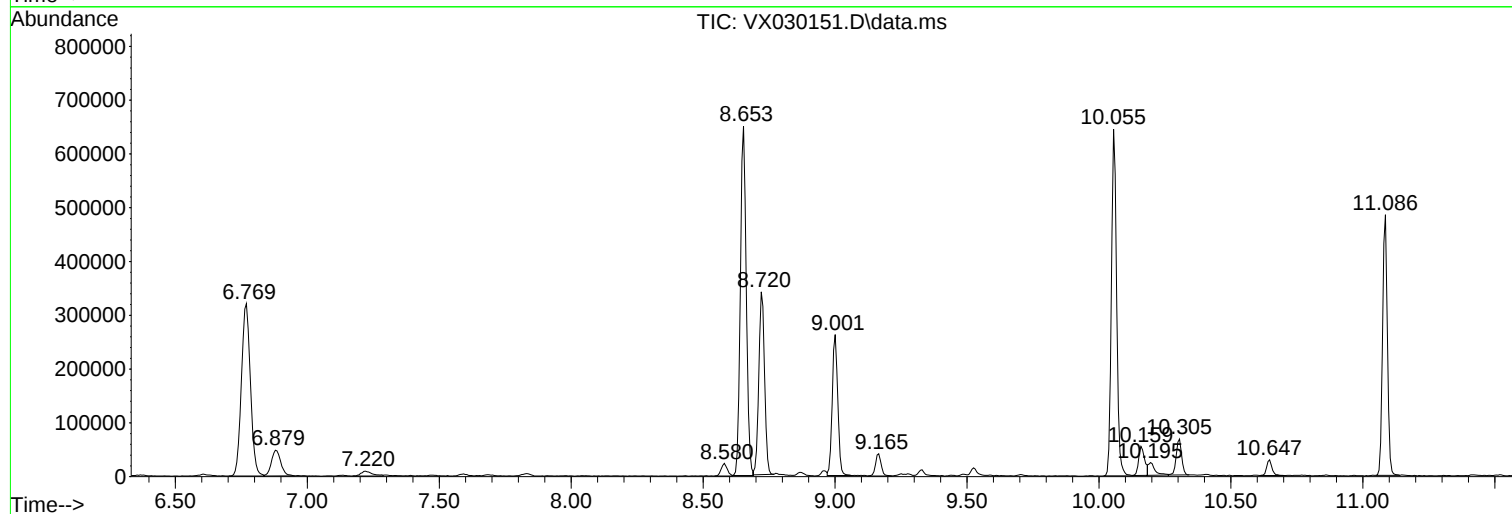
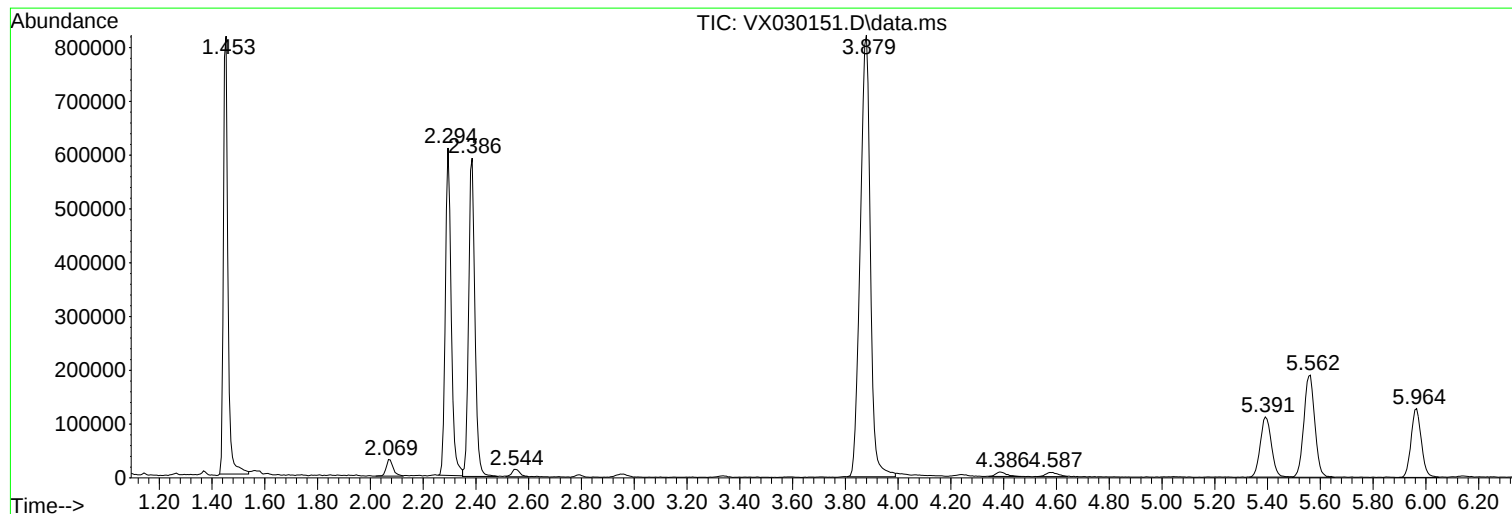
Sum of corrected areas: 11886804

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Instrument :
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ClientSampleId :
ORA-0019

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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



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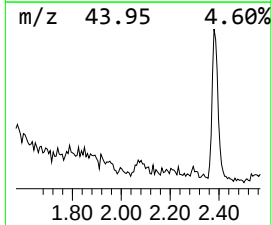
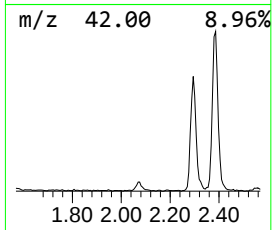
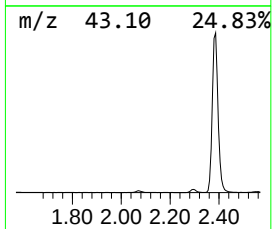
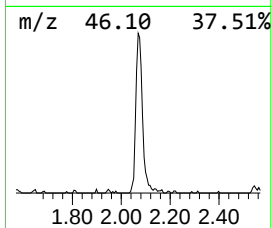
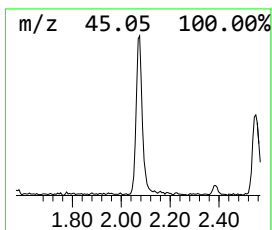
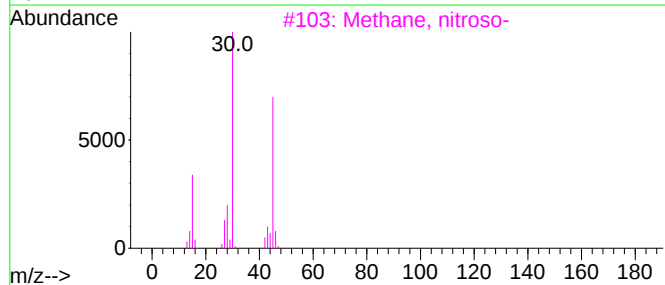
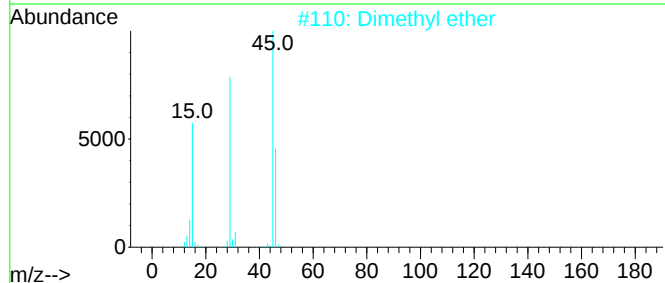
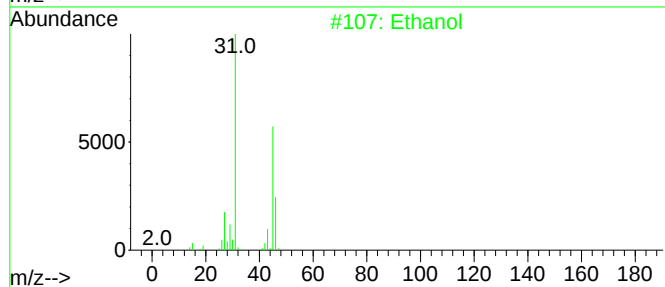
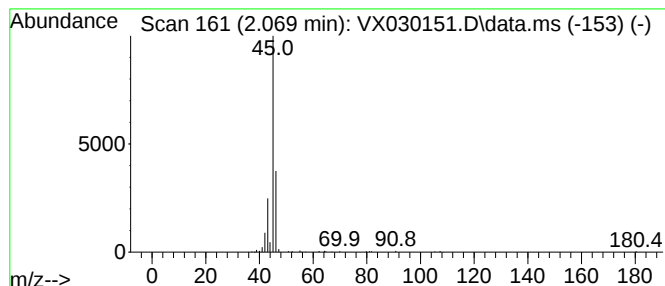
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.069	5.25 ug/l	57313	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	56
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	1-Pyrroline, 2-phenyl-			145	C10H11N	000700-91-4	4
5	Acetoin			88	C4H8O2	000513-86-0	4



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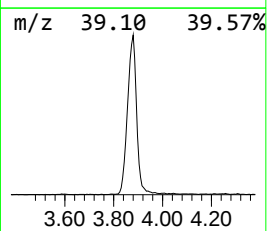
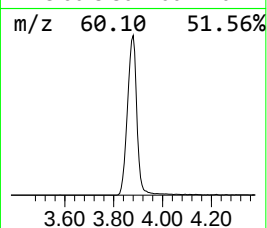
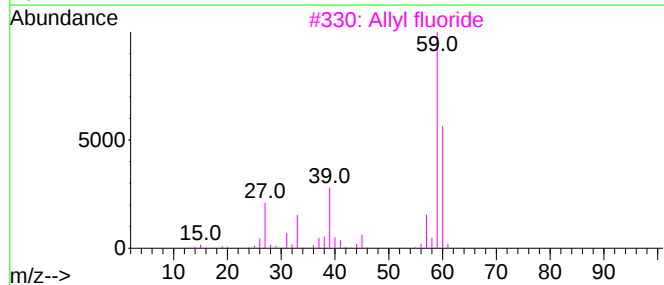
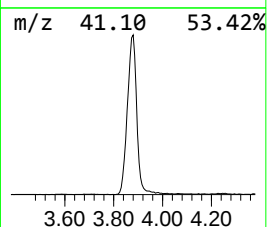
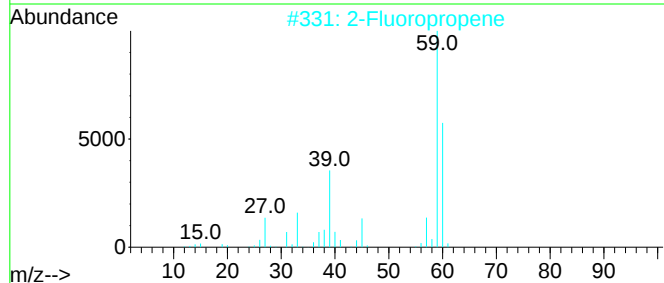
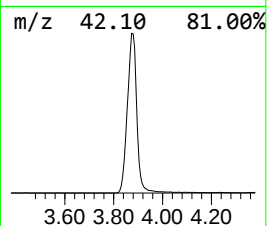
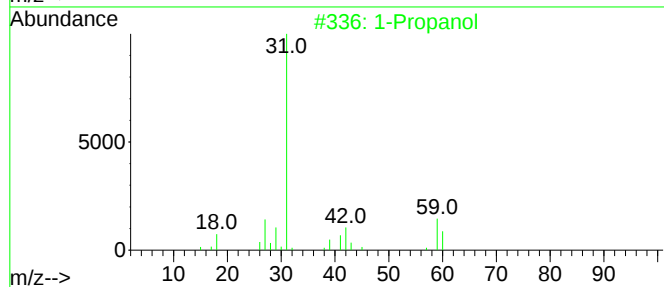
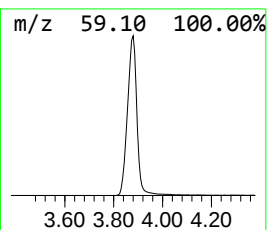
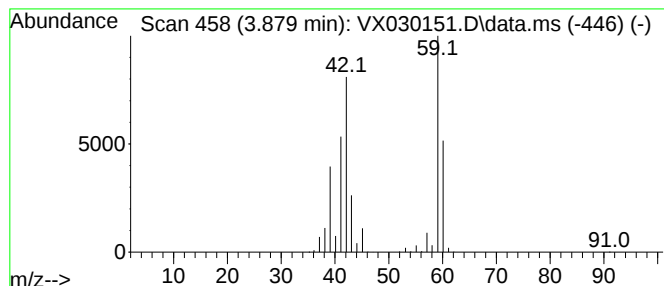
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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Peak Number 3 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.879	199.50 ug/l	2179700	Pentafluorobenzene	5.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol	60	C3H8O	000071-23-8	59
2		2-Fluoropropene	60	C3H5F	001184-60-7	52
3		Allyl fluoride	60	C3H5F	000818-92-8	38
4		Cyclopropane	42	C3H6	000075-19-4	25
5		Propene	42	C3H6	000115-07-1	9



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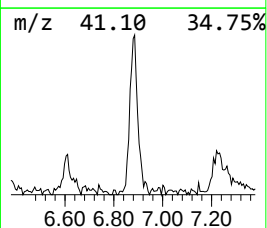
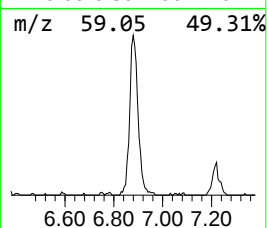
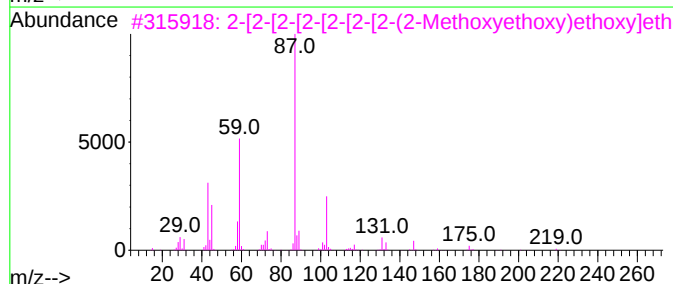
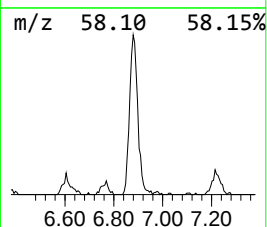
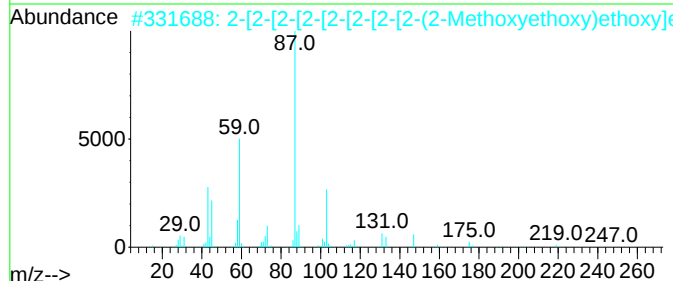
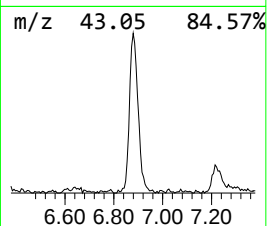
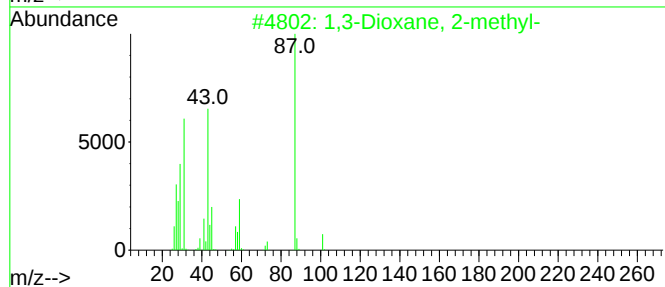
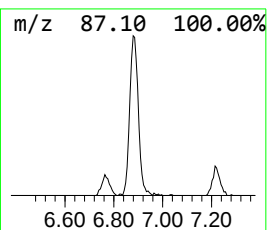
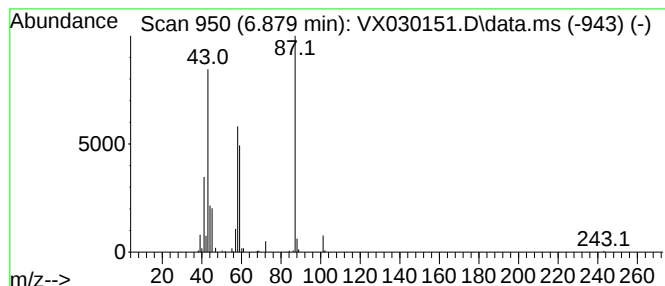
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Peak Number 4 1,3-Dioxane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	7.70 ug/l	116523	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	58
2			2-[2-[2-[2-[2-[2-(2-Methox...	470	C21H42O11	1000351-91-8	53
3			2-[2-[2-[2-[2-[2-(2-Methoxyet...	426	C19H38O10	1000351-91-7	53
4			2-[2-[2-[2-[2-[2-(2-Methoxyethox...	382	C17H34O9	1010351-91-6	53
5			2-[2-[2-[2-[2-[2-[2-[2-(2-...	558	C25H50O13	1000351-91-9	45



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Instrument :
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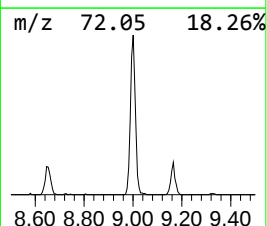
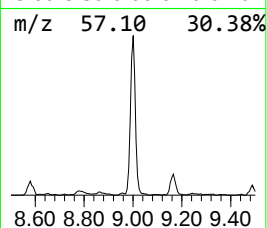
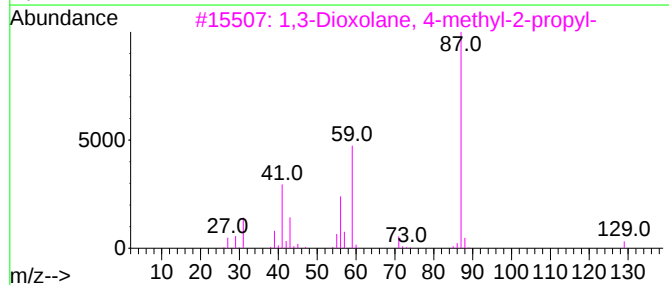
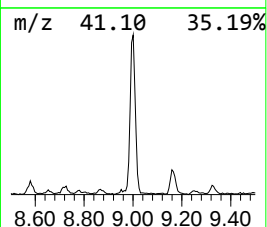
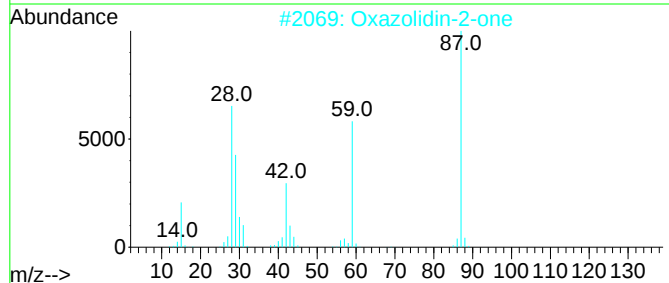
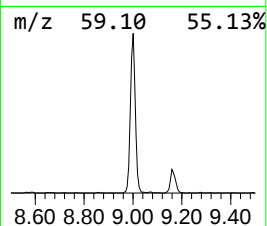
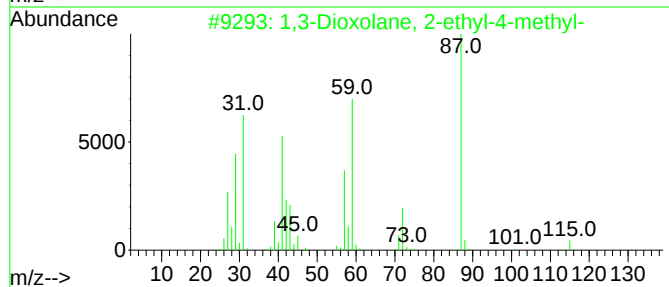
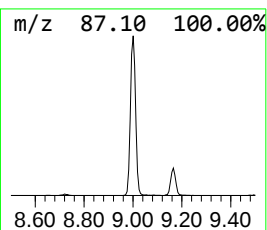
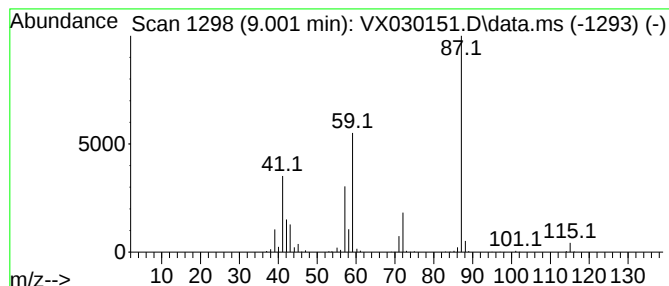
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 5 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.001	21.42 ug/l	381673	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	86
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	72
3			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64
4			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.069	5.3	ug/l	57313	1	5.562	546297	50.0
1-Propanol	3.879	199.5	ug/l	2179700	1	5.562	546297	50.0
1,3-Dioxane, 2-...	6.879	7.7	ug/l	116523	2	6.769	756828	50.0
1,3-Dioxolane, ...	9.001	21.4	ug/l	381673	3	10.055	890983	50.0