

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101123\
 Data File : VN079519.D
 Acq On : 11 Oct 2023 16:00
 Operator : JC\MD
 Sample : 04823-04
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOTES-1

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_N\methods\82N100523W.M
 Title : SW846 8260

Signal : TIC: VN079519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.654	112	119	140	rBV	15052594	25607788	18.26%	6.983%
2	4.436	416	422	458	rVB2	4855664	16304383	11.63%	4.446%
3	6.806	790	825	846	rBV	14642396	64087325	45.70%	17.477%
4	8.230	1061	1067	1080	rVB	678051	1526282	1.09%	0.416%
5	8.606	1110	1131	1139	rBV2	1628876	4438584	3.17%	1.210%
6	8.983	1185	1195	1202	rBV	1397445	3043180	2.17%	0.830%
7	9.106	1208	1216	1227	rVB	1061790	2180660	1.56%	0.595%
8	10.565	1456	1464	1470	rBV2	3174318	6098735	4.35%	1.663%
9	10.635	1470	1476	1483	rVV	3442316	6244491	4.45%	1.703%
10	10.729	1483	1492	1500	rVV	36624858	66595906	47.49%	18.161%
11	10.806	1500	1505	1522	rVV2	1354720	2921219	2.08%	0.797%
12	11.829	1672	1679	1690	rVV2	79633109	140224424	100.00%	38.239%
13	11.971	1698	1703	1712	rVV2	720766	1485103	1.06%	0.405%
14	12.071	1713	1720	1729	rVB	1656851	3134539	2.24%	0.855%
15	12.400	1771	1776	1783	rBV4	925402	1691209	1.21%	0.461%
16	12.800	1833	1844	1848	rBV	2060061	3320947	2.37%	0.906%
17	12.853	1848	1853	1865	rVB	1193807	2139483	1.53%	0.583%
18	13.265	1914	1923	1931	rBV	1138675	1833328	1.31%	0.500%
19	13.488	1952	1961	1974	rVB5	470844	1664767	1.19%	0.454%
20	13.794	2006	2013	2022	rBV2	1425125	2728414	1.95%	0.744%
21	15.647	2318	2328	2339	rVB	4899477	9433598	6.73%	2.573%

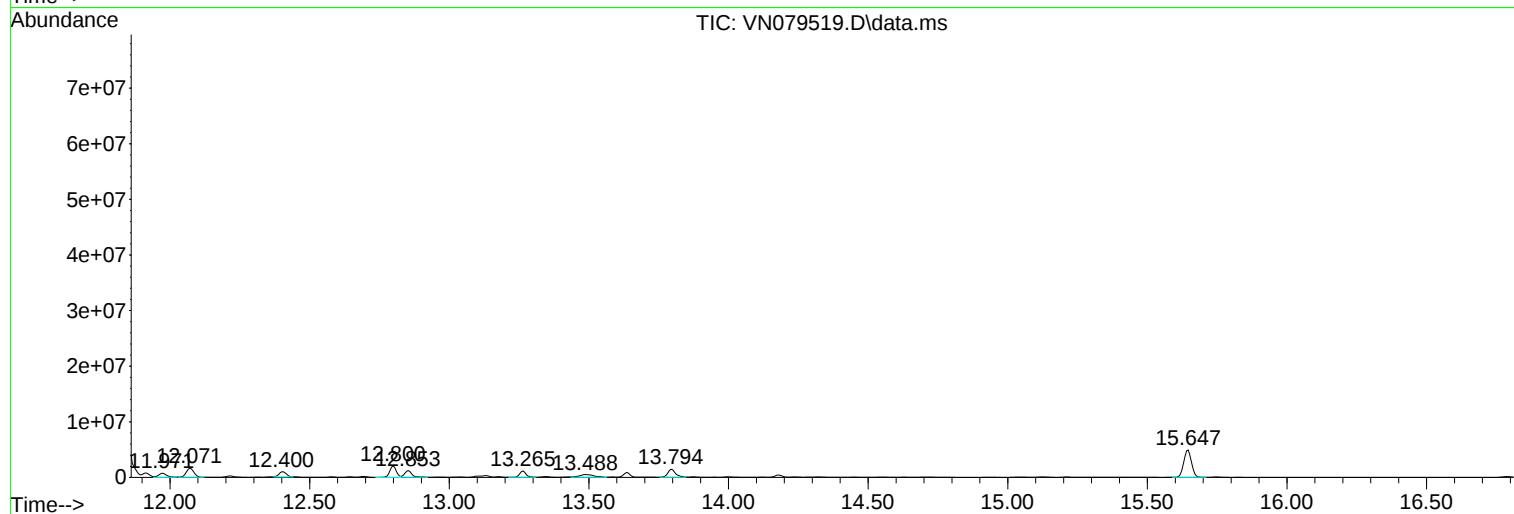
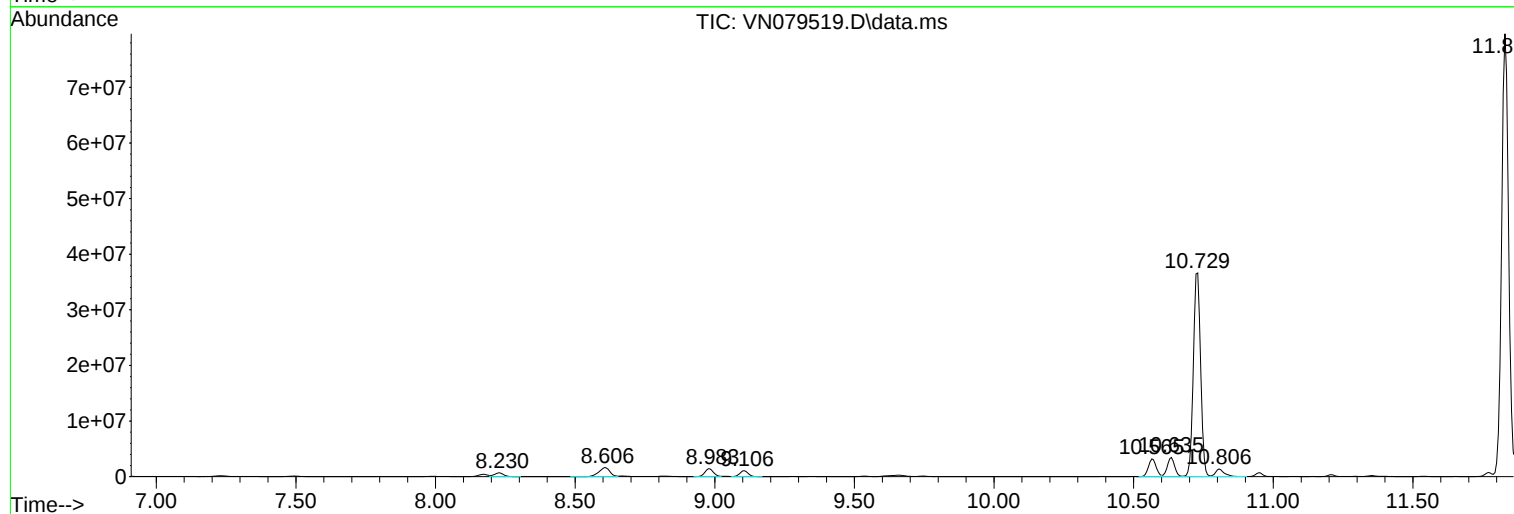
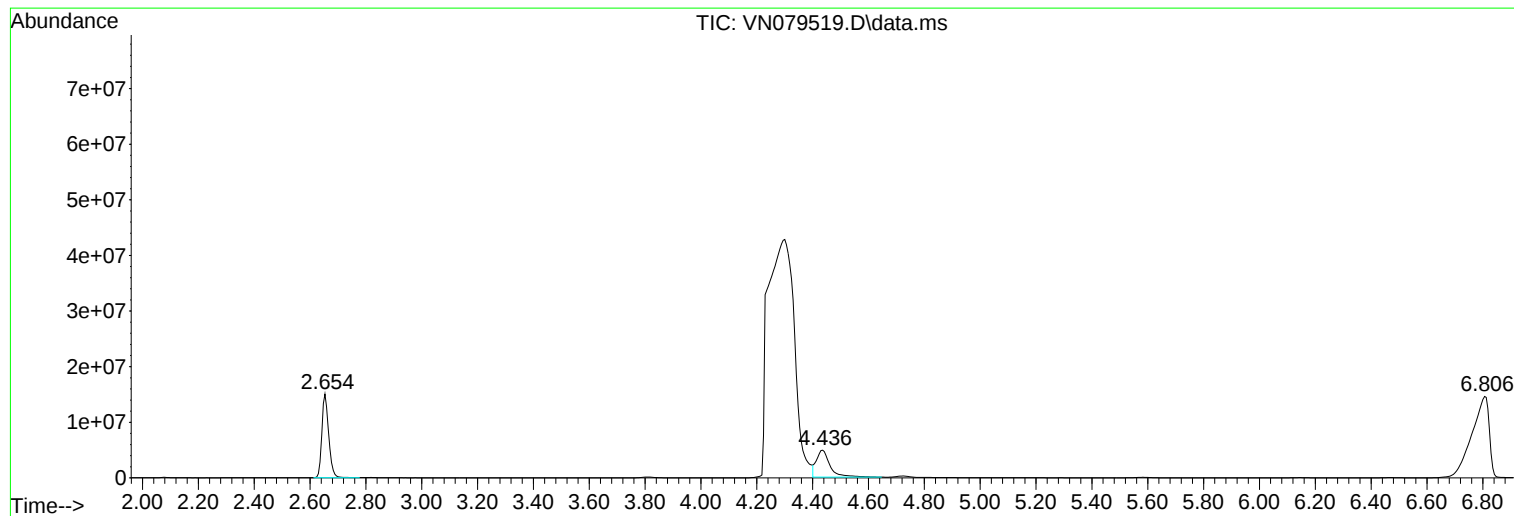
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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



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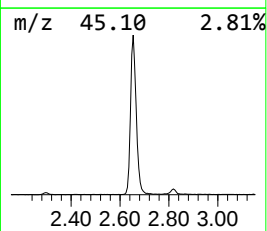
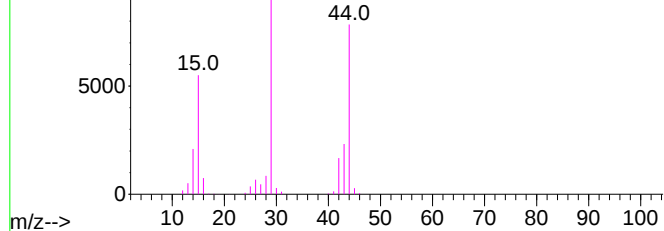
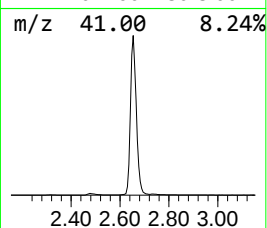
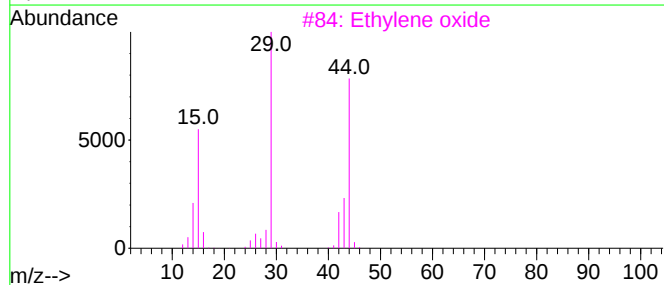
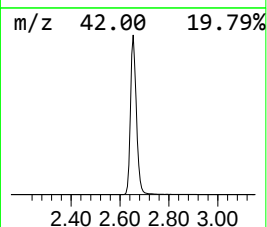
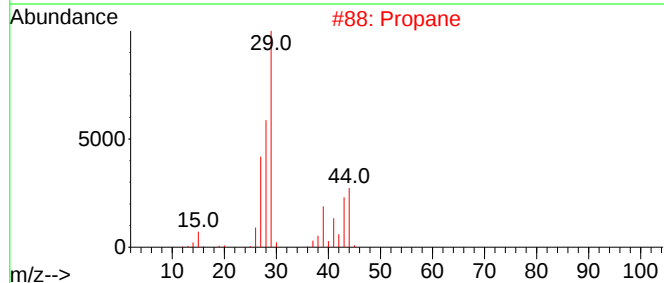
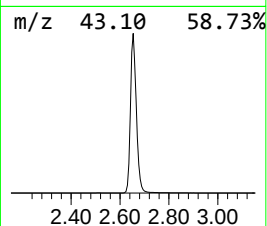
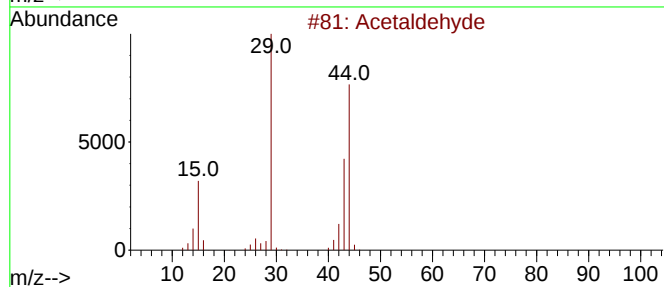
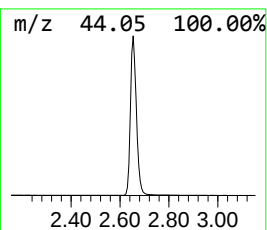
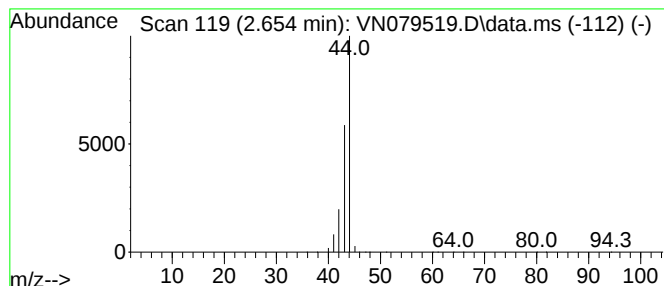
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.654	838.89 ug/l	25607800	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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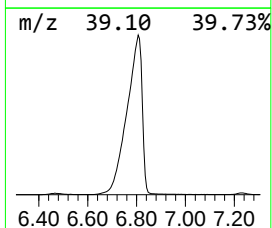
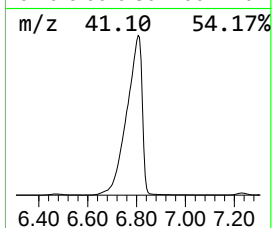
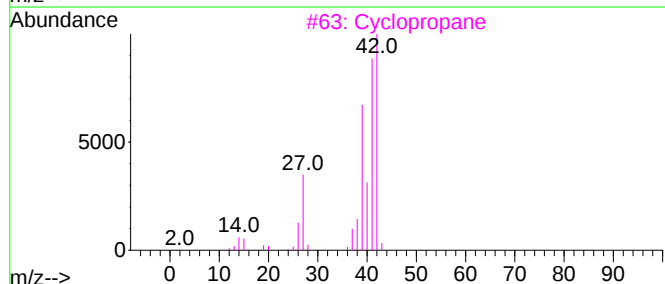
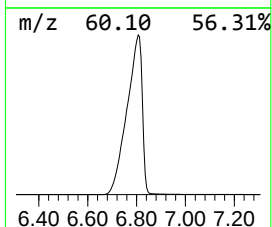
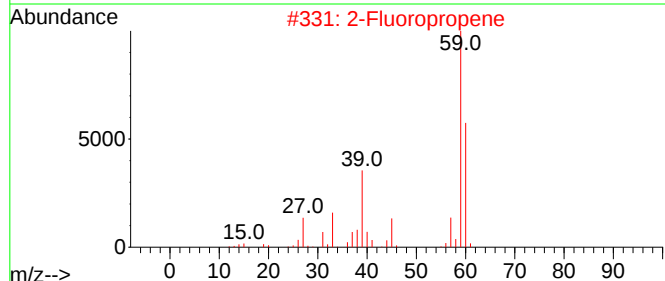
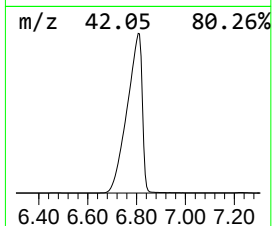
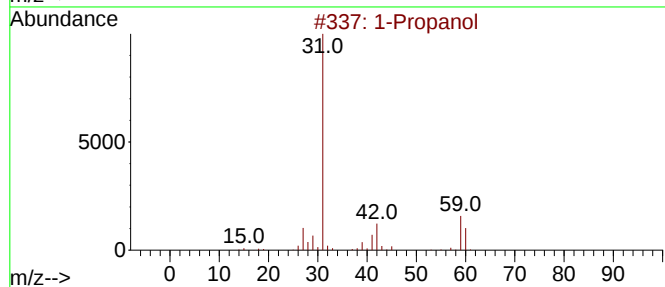
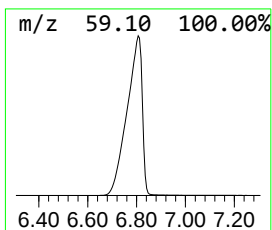
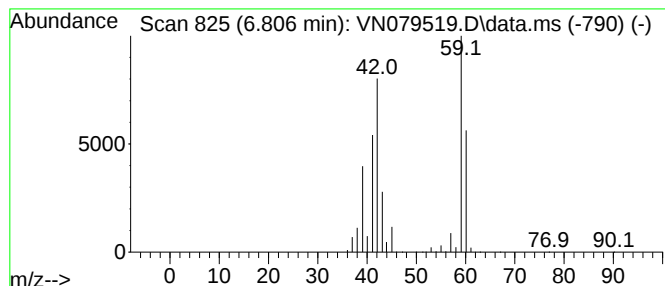
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.806	2099.46 ug/l	64087300	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	64
2	2-Fluoropropene			60	C3H5F	001184-60-7	38
3	Cyclopropane			42	C3H6	000075-19-4	32
4	Allyl fluoride			60	C3H5F	000818-92-8	32
5	Formamidoxime			60	CH4N2O	000624-82-8	9



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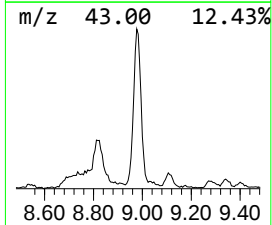
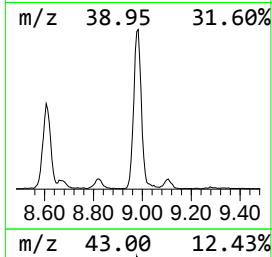
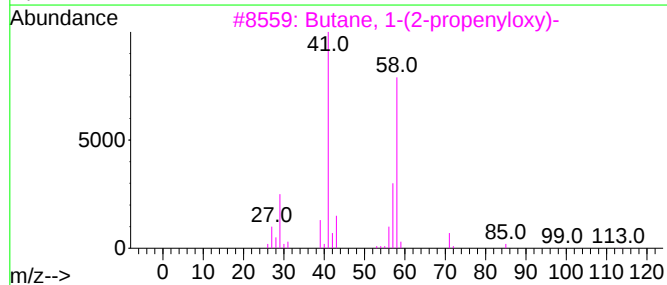
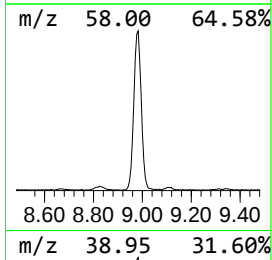
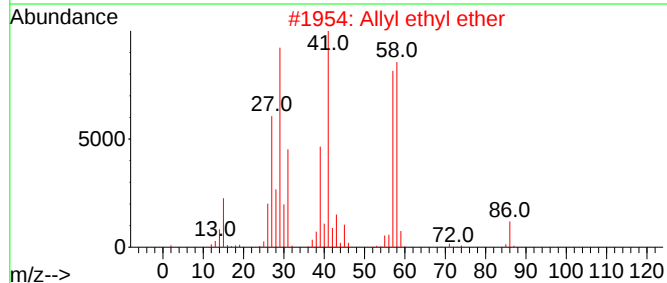
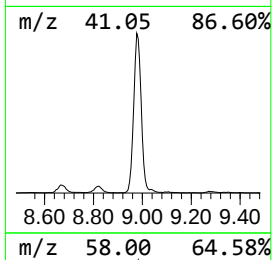
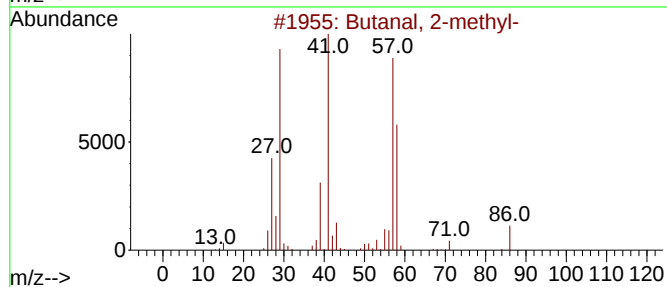
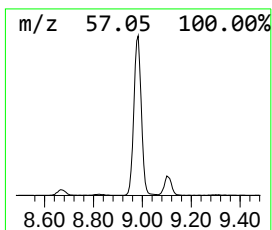
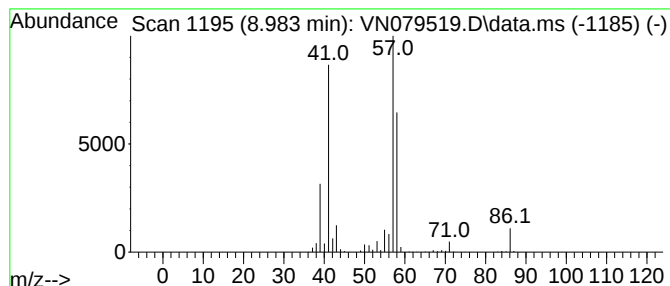
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanal, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.983	69.78 ug/l	3043180	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 2-methyl-	86	C5H10O	000096-17-3	90
2			Allyl ethyl ether	86	C5H10O	000557-31-3	53
3			Butane, 1-(2-propenyloxy)-	114	C7H14O	003739-64-8	50
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	32
5			n-Hexane	86	C6H14	000110-54-3	25



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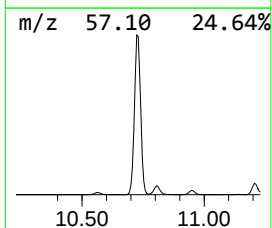
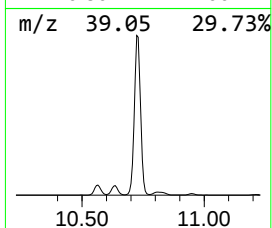
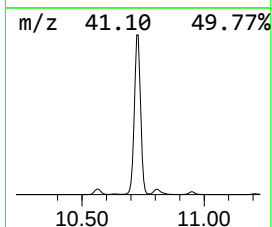
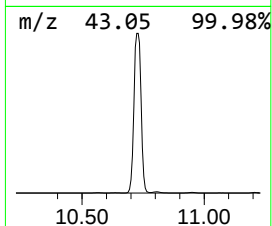
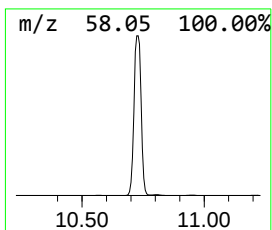
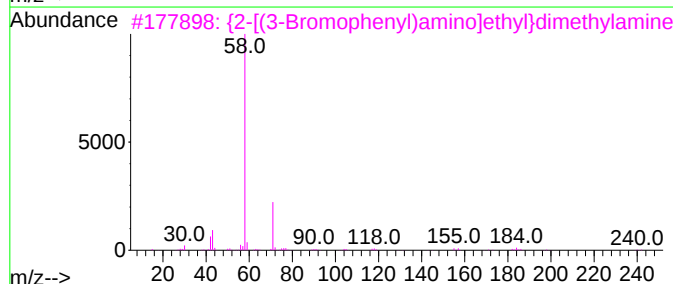
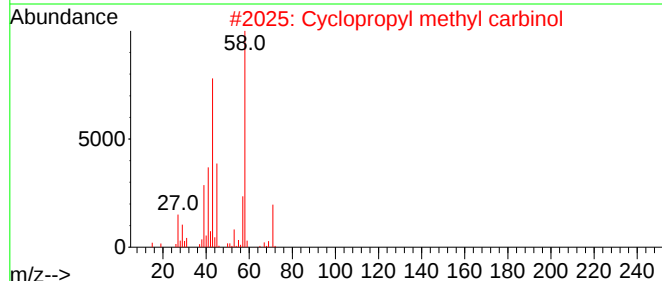
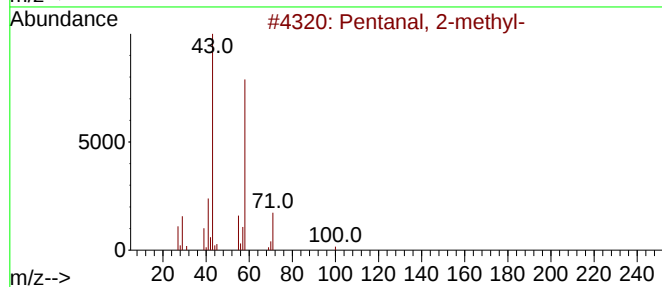
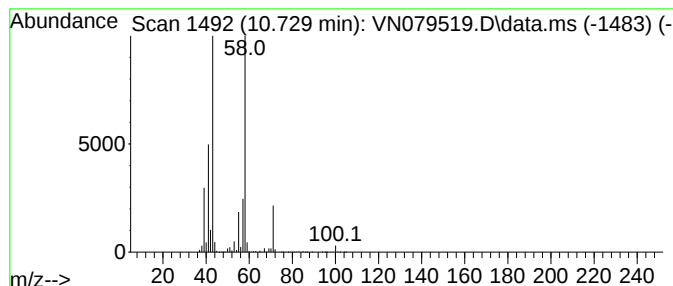
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Quant Title : SW846 8260

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

Peak Number 4 Pentanal, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.730	23.75 ug/l	66595900	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	90
2			Cyclopropyl methyl carbinol	86	C5H10O	000765-42-4	64
3			{2-[(3-Bromophenyl)amino]ethyl}d...	284	C12H17BrN2O	1010506-64-8	50
4			[2-(3-Bromophenoxy)ethyl]dimethy...	243	C10H14BrNO	221915-84-0	40
5			Bis(2-(Dimethylamino)ethyl) ether	160	C8H20N2O	003033-62-3	39



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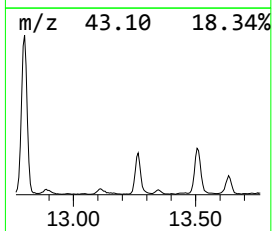
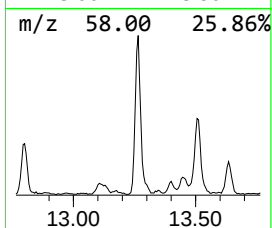
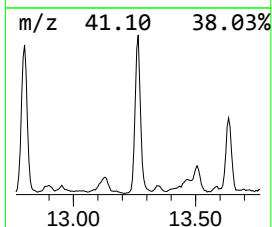
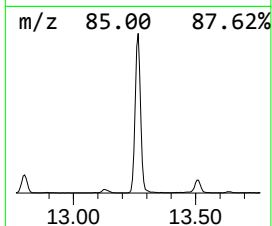
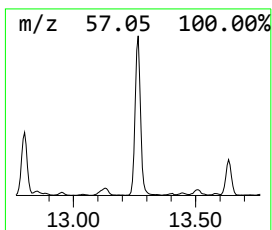
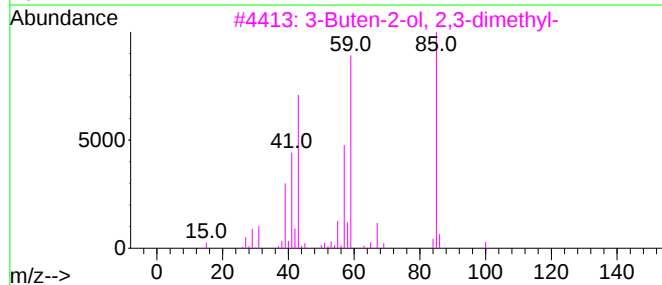
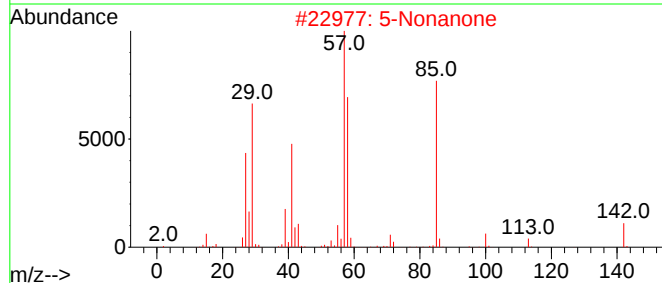
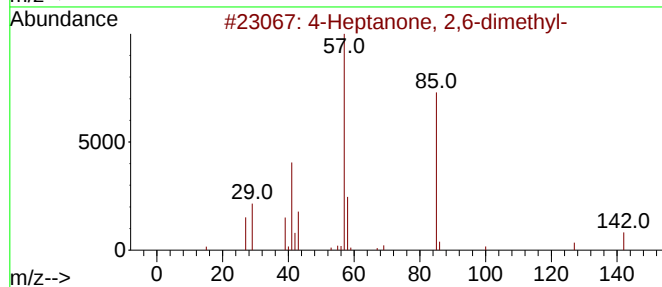
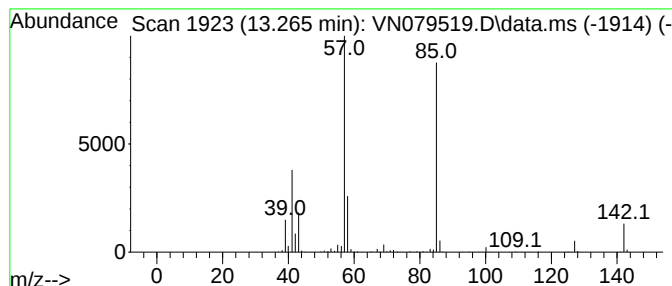
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Quant Title : SW846 8260

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

Peak Number 5 4-Heptanone, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.265	33.60 ug/l	1833330	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2			5-Nonanone	142	C9H18O	000502-56-7	59
3			3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	53
4			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	50
5			2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	47



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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.654	838.9	ug/l	25607800	1	8.230	1526280	50.0
1-Propanol	6.806	2099.5	ug/l	64087300	1	8.230	1526280	50.0
Butanal, 2-methyl-	8.983	69.8	ug/l	3043180	2	9.106	2180660	50.0
Pentanal, 2-met...	10.730	23.8	ug/l	66595900	3	11.871	140224000	50.0
4-Heptanone, 2,...	13.265	33.6	ug/l	1833330	4	13.794	2728410	50.0