

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
 Data File : VN074689.D
 Acq On : 01 Oct 2022 04:48
 Operator : JC\MD
 Sample : N4882-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-101

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\82N092922W.M
 Title : SW846 8260

Signal : TIC: VN074689.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	38	45	51	rBV	594466	1106958	18.95%	3.653%
2	4.140	374	383	390	rBV2	24802	71793	1.23%	0.237%
3	5.169	548	558	560	rBV3	34109	72861	1.25%	0.240%
4	5.428	588	602	617	rBV	113781	412178	7.06%	1.360%
5	7.669	977	983	993	rVB	23132	73776	1.26%	0.243%
6	7.869	1005	1017	1023	rBV	781201	1958444	33.53%	6.463%
7	7.934	1023	1028	1041	rVB	726796	1642146	28.11%	5.419%
8	8.292	1079	1089	1098	rBV	942587	2215009	37.92%	7.309%
9	8.387	1098	1105	1115	rVB2	326346	741673	12.70%	2.447%
10	8.828	1171	1180	1193	rBV	1181168	2486595	42.57%	8.205%
11	10.075	1384	1392	1393	rBV2	165076	251767	4.31%	0.831%
12	10.104	1394	1397	1409	rVB2	263613	503496	8.62%	1.661%
13	10.310	1423	1432	1441	rBV	3217809	5841223	100.00%	19.275%
14	10.422	1446	1451	1460	rVB	259659	483331	8.27%	1.595%
15	10.969	1534	1544	1548	rBV2	105361	201070	3.44%	0.664%
16	11.086	1557	1564	1576	rVB8	44714	105077	1.80%	0.347%
17	11.492	1624	1633	1643	rBV2	166724	395776	6.78%	1.306%
18	11.622	1646	1655	1664	rBV	2154833	3874037	66.32%	12.784%
19	11.733	1669	1674	1682	rVV6	57997	117340	2.01%	0.387%
20	11.839	1686	1692	1695	rVV5	35122	73744	1.26%	0.243%
21	12.233	1751	1759	1764	rBV3	71376	132740	2.27%	0.438%
22	12.610	1815	1823	1834	rVB	2411070	4075877	69.78%	13.450%
23	12.716	1834	1841	1848	rVV2	70583	134598	2.30%	0.444%
24	12.933	1873	1878	1885	rVB7	40158	76767	1.31%	0.253%
25	13.551	1975	1983	1997	rVB	1948005	3255814	55.74%	10.744%

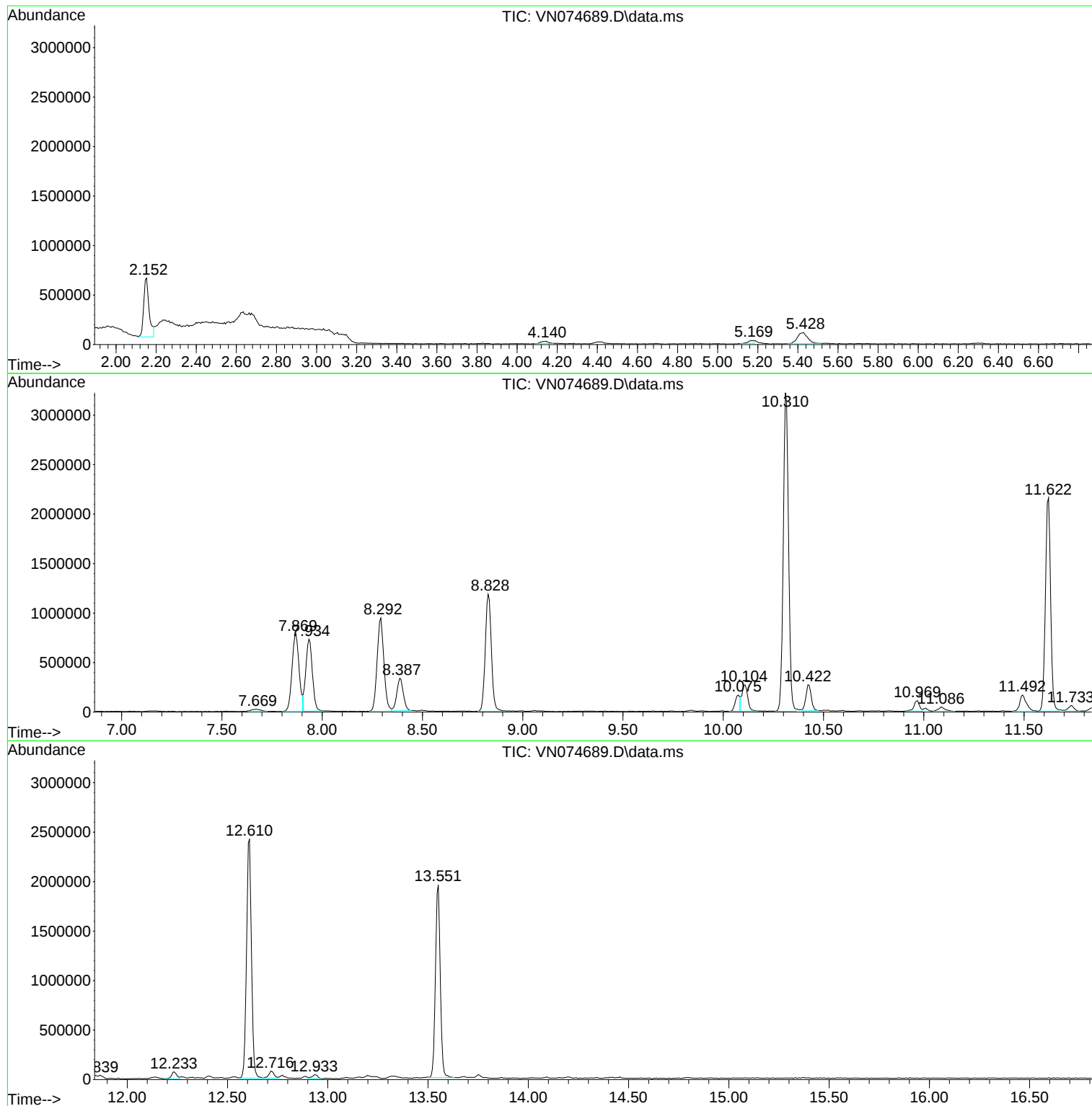
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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



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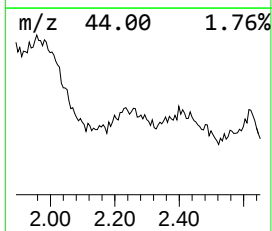
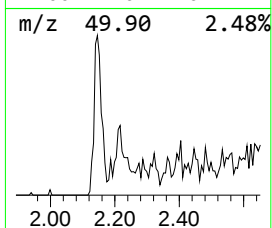
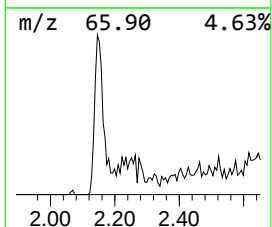
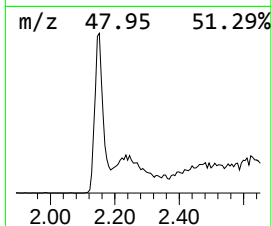
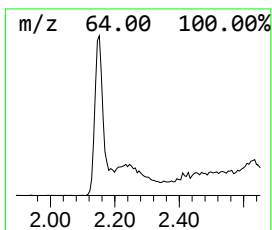
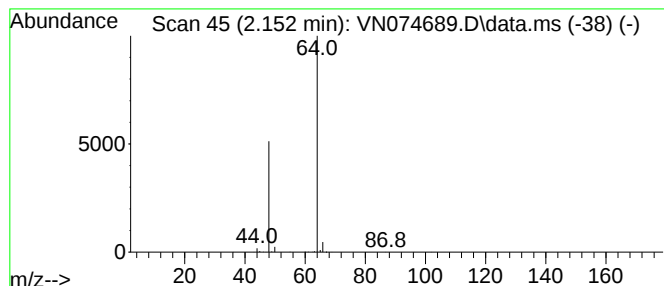
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Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	33.70 ug/l	1106960	Pentafluorobenzene	7.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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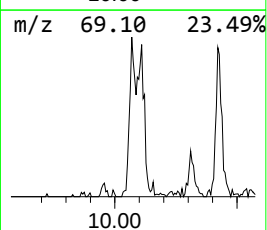
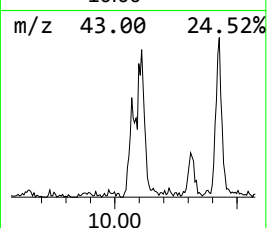
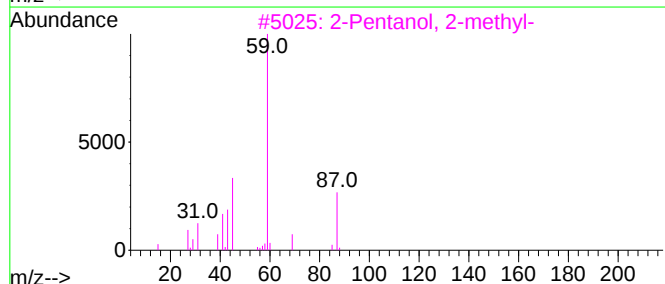
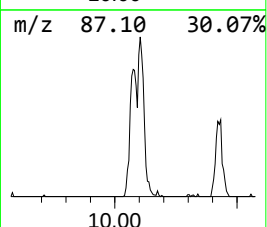
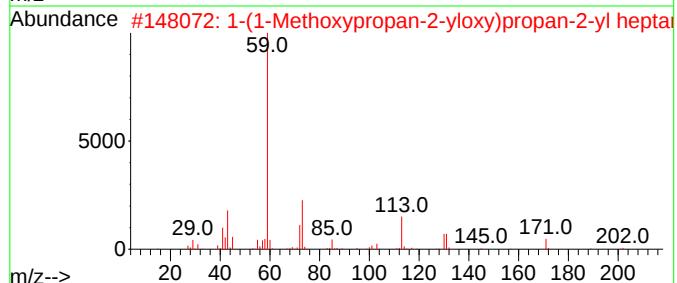
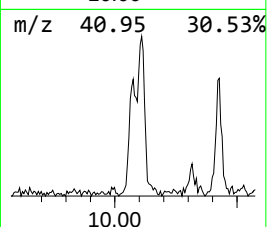
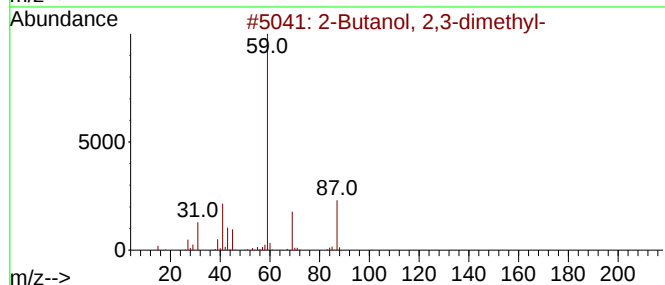
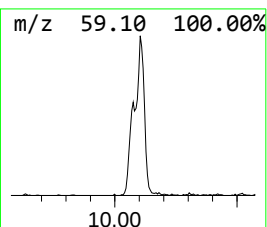
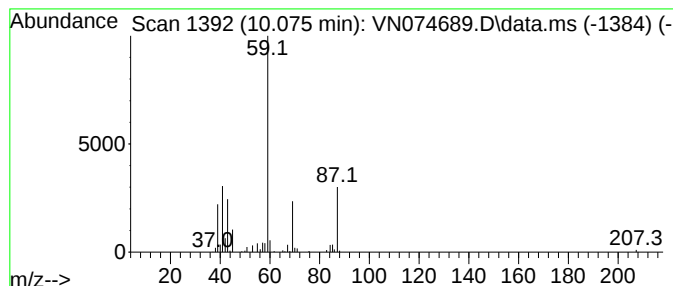
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Quant Title : SW846 8260

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

Peak Number 2 2-Butanol, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.075	5.06 ug/l	251767	1,4-Difluorobenzene	8.828

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	78
2		1-(1-Methoxypropan-2-yloxy)propa...	260	C14H28O4	1000367-13-1	53
3		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	50
4		2,4-Dimethyl-2,4-pentanediol	132	C7H16O2	024892-49-7	47
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	45



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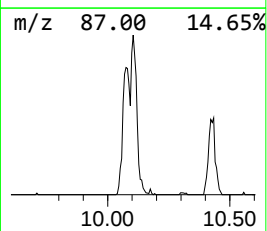
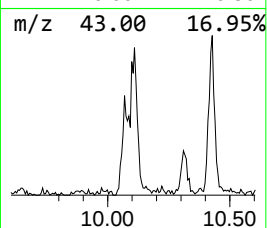
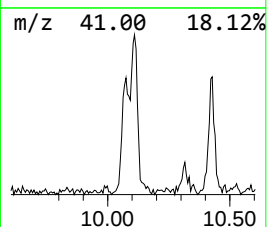
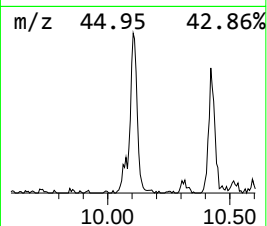
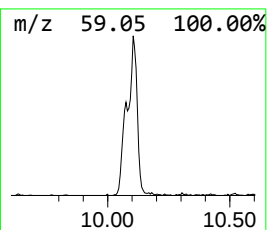
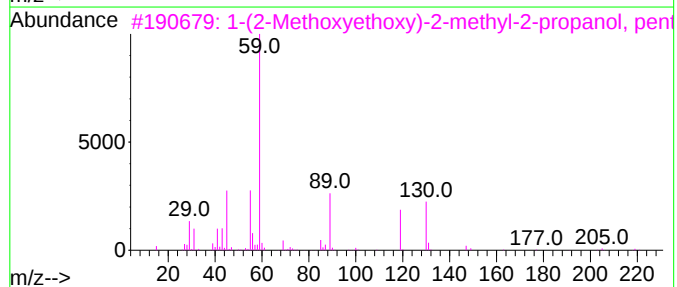
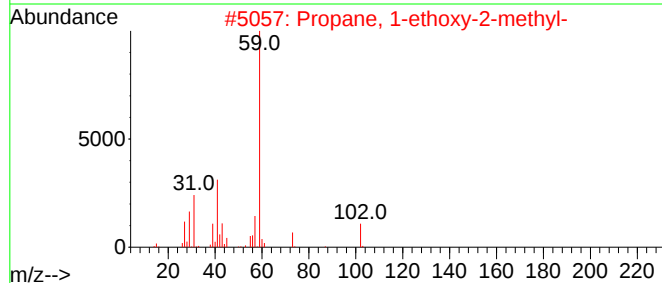
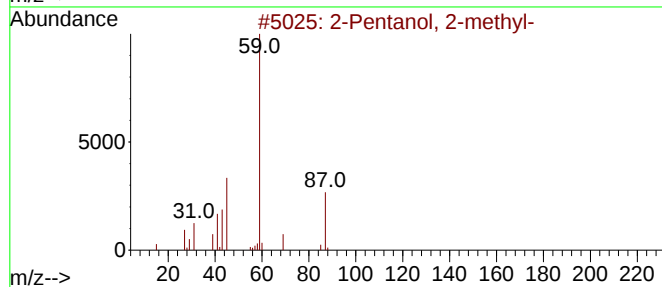
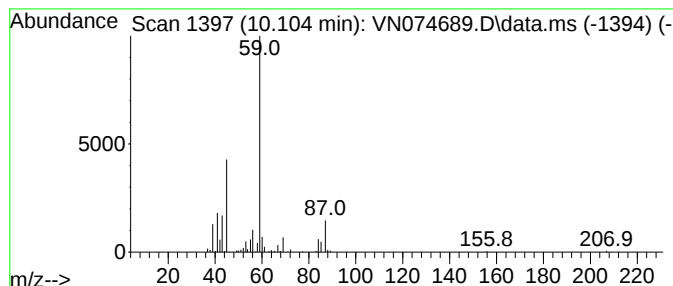
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.104	10.12 ug/l	503496	1,4-Difluorobenzene	8.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	72
2			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	47
3			1-(2-Methoxyethoxy)-2-methyl-2-p...	294	C10H15F5O4	1000364-25-8	43
4			4-Methoxy-1-pentene	100	C6H12O	098386-09-5	43
5			Dimethylpropylsilane	102	C5H14Si	1000432-95-4	40



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ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-101

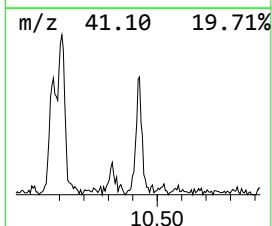
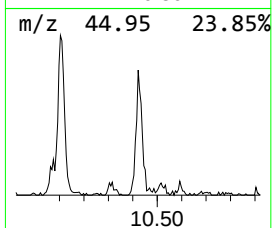
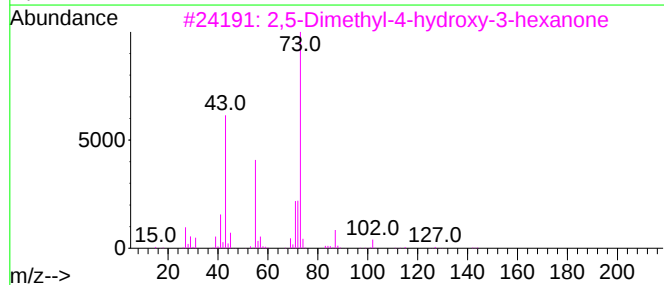
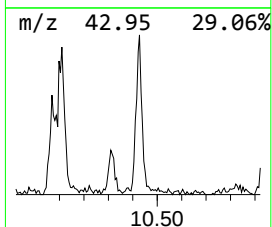
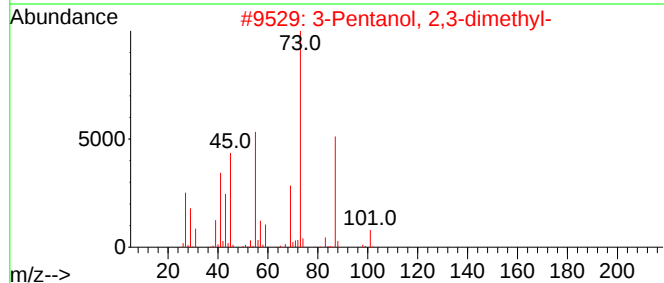
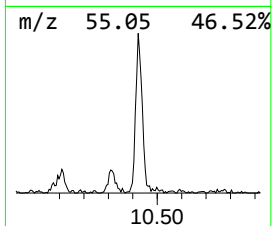
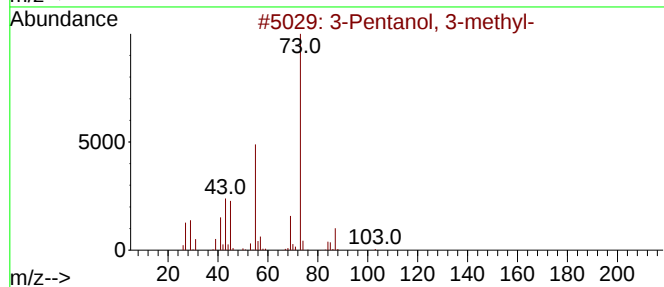
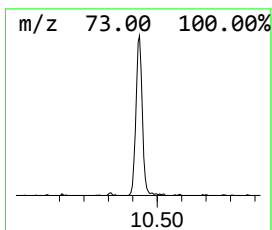
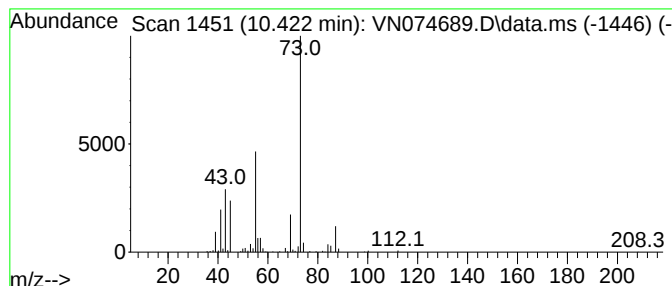
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Quant Title : SW846 8260

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

Peak Number 4 3-Pentanol, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.422	6.24 ug/l	483331	Chlorobenzene-d5	11.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	83
2			3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	40
3			2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	33
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
5			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	23



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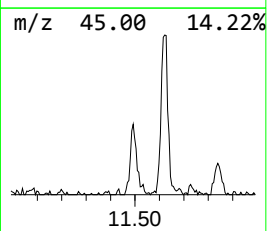
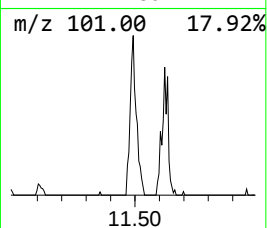
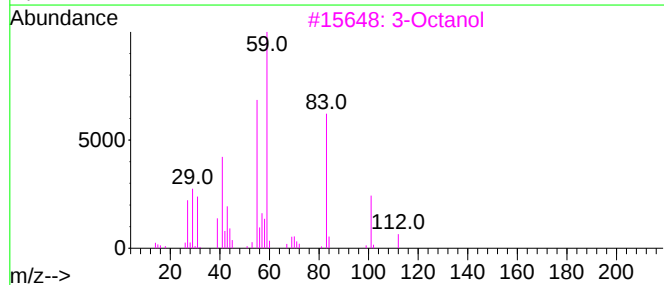
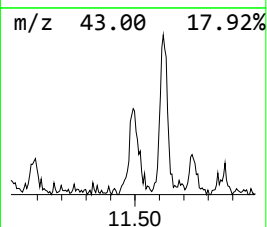
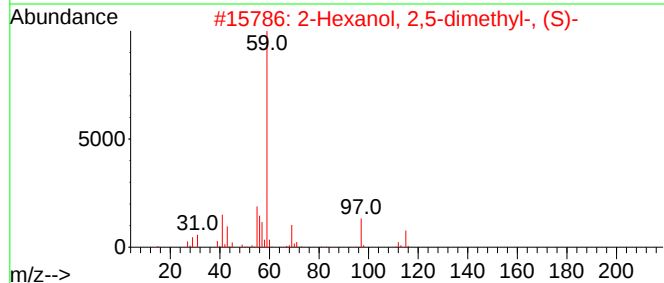
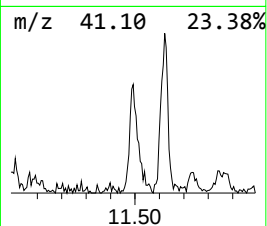
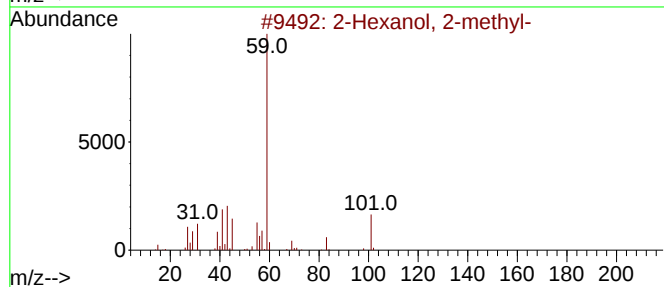
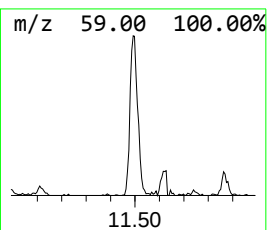
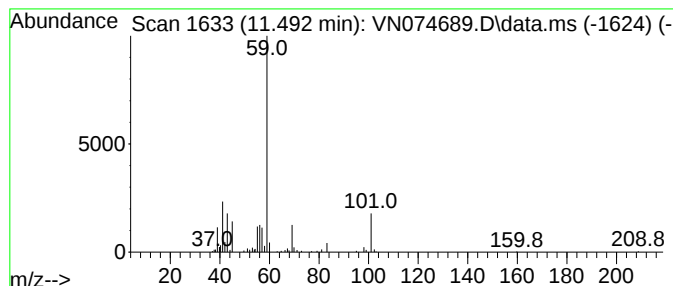
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 2-Hexanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.492	5.11 ug/l	395776	Chlorobenzene-d5	11.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	78
2			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	64
3			3-Octanol	130	C8H18O	000589-98-0	56
4			2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	50
5			3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	50



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.152	33.7	ug/l	1106960	1	7.934	1642150	50.0
2-Butanol, 2,3-...	10.075	5.1	ug/l	251767	2	8.828	2486600	50.0
2-Pentanol, 2-m...	10.104	10.1	ug/l	503496	2	8.828	2486600	50.0
3-Pentanol, 3-m...	10.422	6.2	ug/l	483331	3	11.622	3874040	50.0
2-Hexanol, 2-me...	11.492	5.1	ug/l	395776	3	11.622	3874040	50.0