

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
 Data File : VX029596.D
 Acq On : 19 Jun 2022 02:17
 Operator : JC/MD
 Sample : N3290-16
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-28D2

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\82X061822W.M
 Title : SW846 8260

Signal : TIC: VX029596.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.276	26	31	42	rBV	16797	53139	2.37%	0.426%
2	2.971	299	309	323	rBV	405155	1003600	44.68%	8.048%
3	3.117	323	333	353	rVB	965083	2246289	100.00%	18.013%
4	3.763	428	439	448	rBV3	20224	58028	2.58%	0.465%
5	5.196	663	674	686	rBV3	16554	51033	2.27%	0.409%
6	5.391	692	706	721	rBV2	153241	447530	19.92%	3.589%
7	5.556	721	733	748	rVB	282628	809208	36.02%	6.489%
8	5.958	788	799	810	rBV	164533	433947	19.32%	3.480%
9	6.239	832	845	872	rBV	365880	1056349	47.03%	8.471%
10	6.763	922	931	942	rBV	430622	1036834	46.16%	8.314%
11	8.427	1197	1204	1211	rBV	96040	166358	7.41%	1.334%
12	8.507	1211	1217	1232	rVB	134182	222154	9.89%	1.781%
13	8.653	1234	1241	1251	rBV	851901	1348250	60.02%	10.812%
14	8.842	1265	1272	1281	rBV	182707	288219	12.83%	2.311%
15	9.567	1385	1391	1405	rVB	51064	75849	3.38%	0.608%
16	10.055	1465	1471	1477	rBV	874255	1132546	50.42%	9.082%
17	10.250	1497	1503	1507	rBV4	18117	34729	1.55%	0.278%
18	10.305	1507	1512	1517	rVB	54433	75722	3.37%	0.607%
19	11.079	1634	1639	1654	rBV	635082	849450	37.82%	6.812%
20	12.024	1788	1794	1801	rBV	864057	1053992	46.92%	8.452%
21	13.780	2074	2082	2089	rBV	19296	27285	1.21%	0.219%

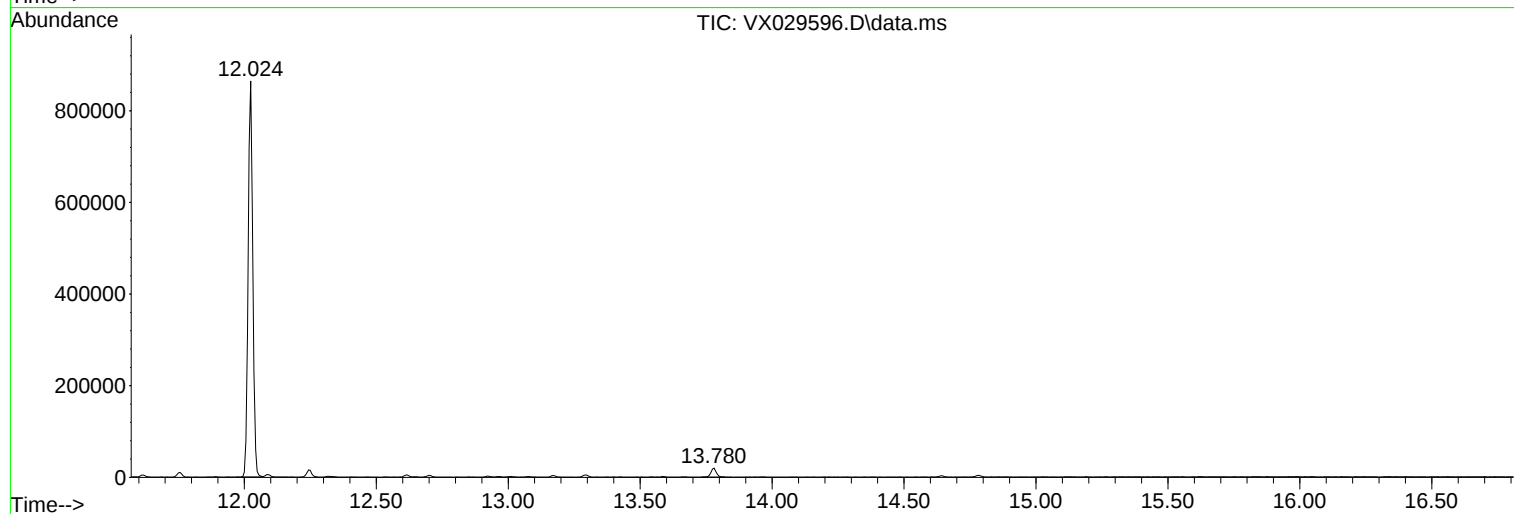
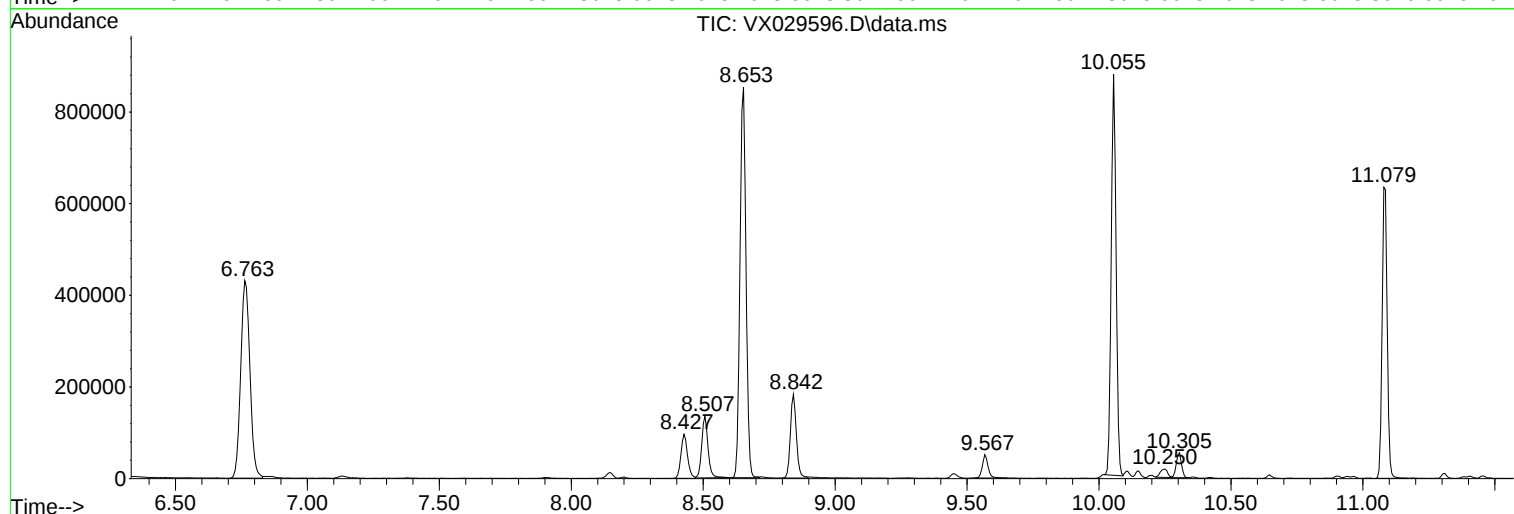
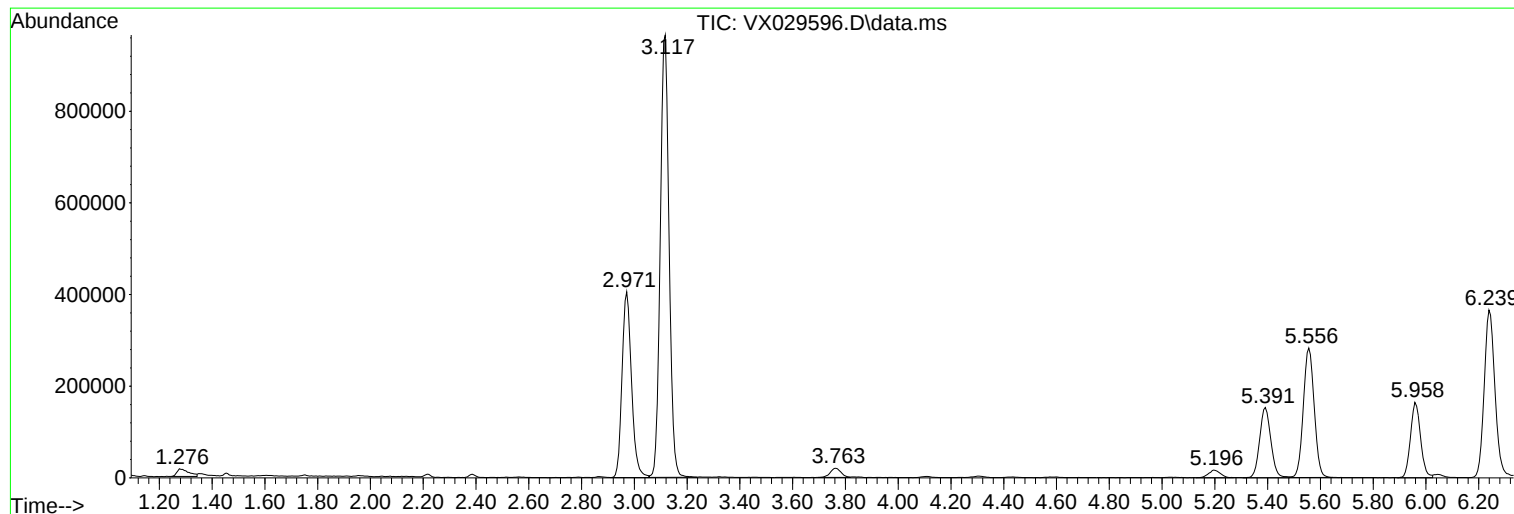
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



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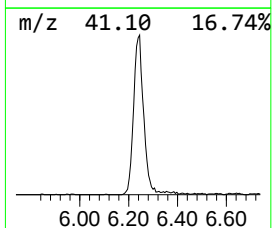
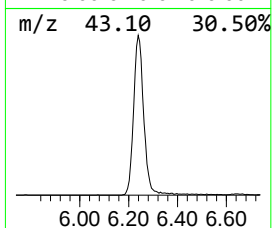
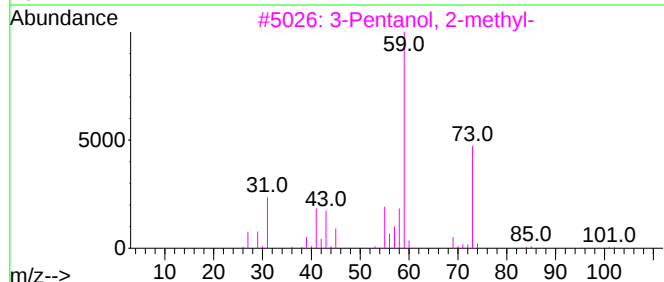
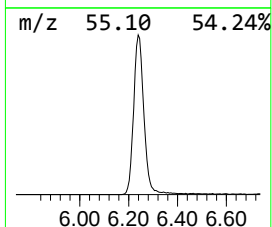
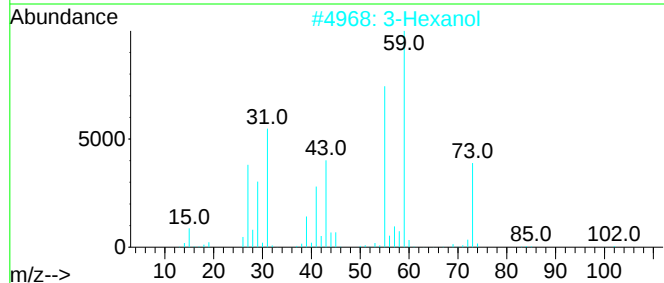
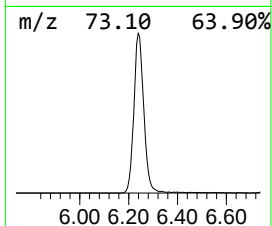
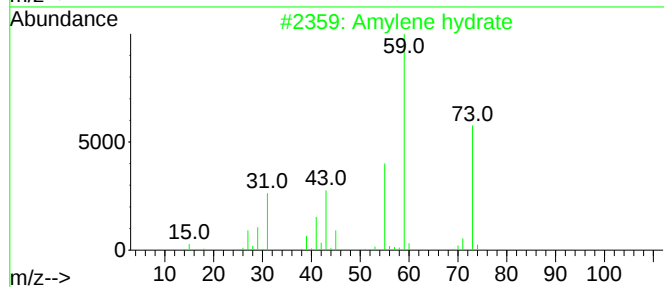
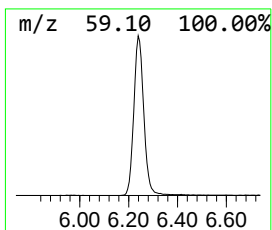
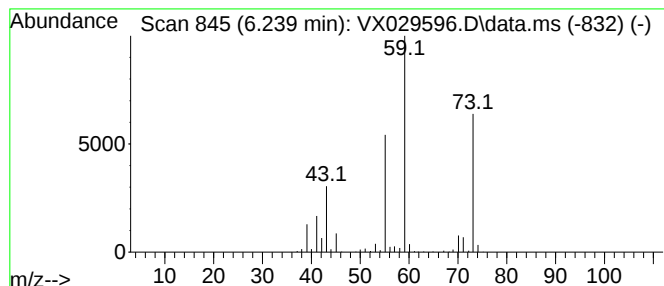
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 1 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.239	50.94 ug/l	1056350	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	83
2			3-Hexanol	102	C6H14O	000623-37-0	64
3			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	39
4			Silane, trimethyl-	74	C3H10Si	000993-07-7	38
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	10



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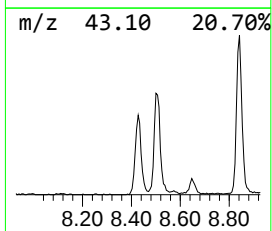
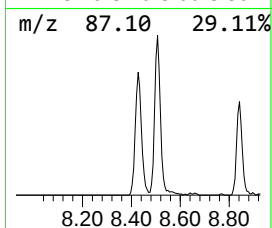
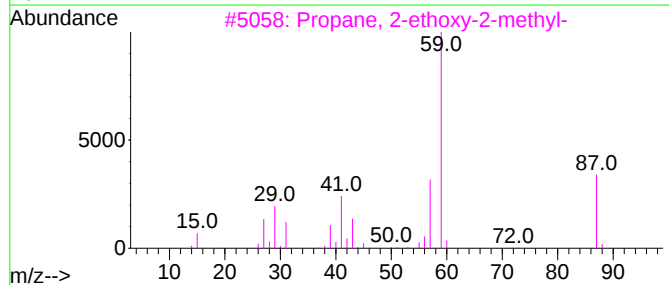
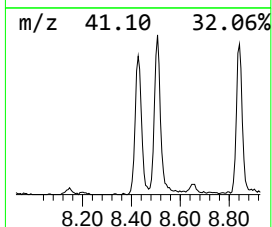
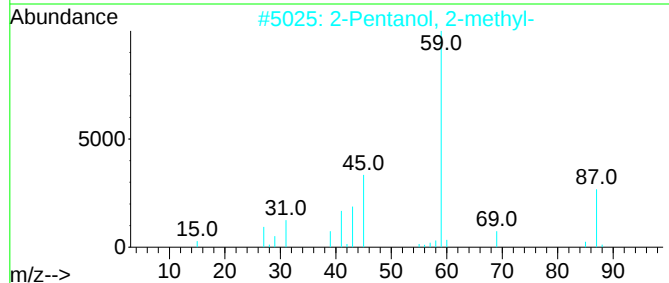
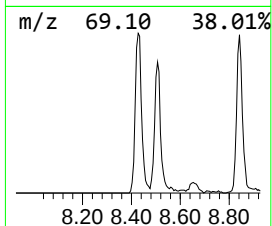
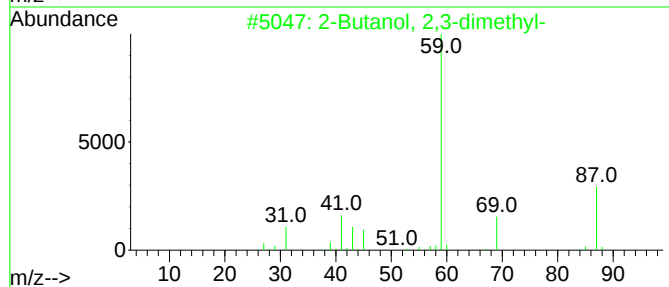
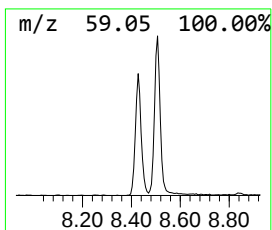
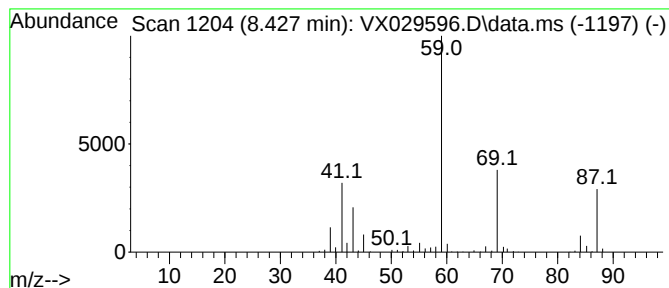
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Butanol, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.427	7.34 ug/l	166358	Chlorobenzene-d5	10.055

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83	
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	72	
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	56	
4	Amylene hydrate	88	C5H12O	000075-85-4	40	
5	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	40	



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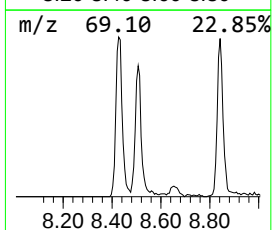
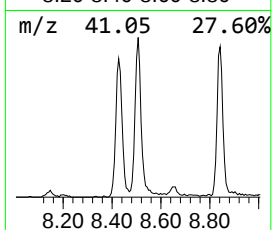
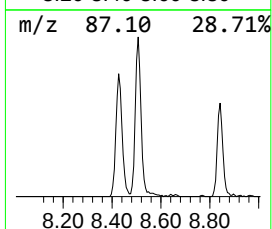
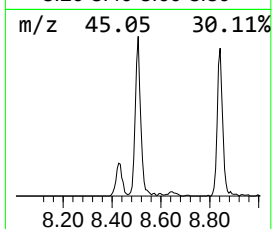
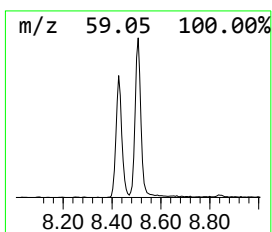
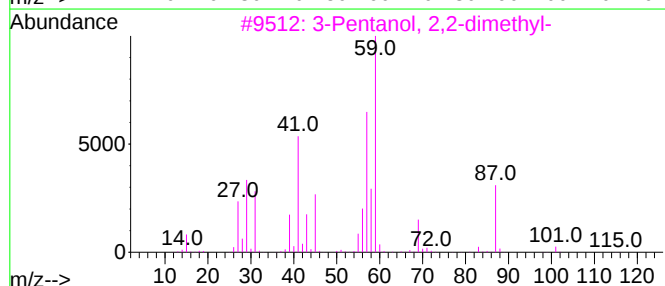
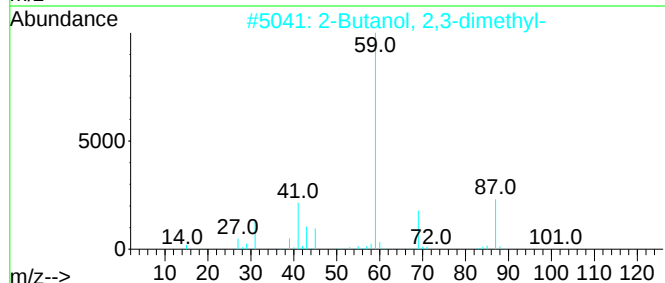
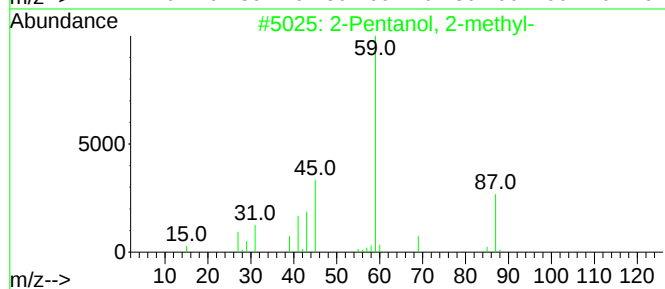
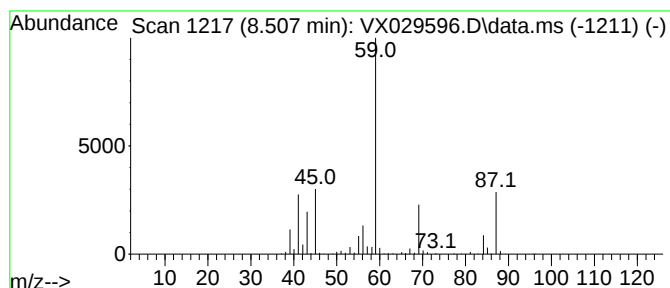
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.507	9.81 ug/l	222154	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-			102	C6H14O	000590-36-3	78
2	2-Butanol, 2,3-dimethyl-			102	C6H14O	000594-60-5	64
3	3-Pentanol, 2,2-dimethyl-			116	C7H16O	003970-62-5	56
4	3-Hexanol, 5-methyl-			116	C7H16O	000623-55-2	40
5	3-Hexanol, 4-methyl-			116	C7H16O	000615-29-2	39



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ALS Vial : 46 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-28D2

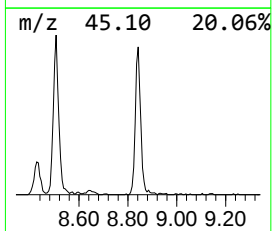
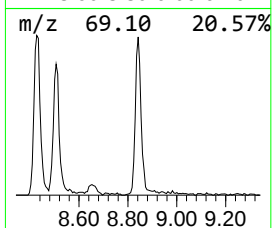
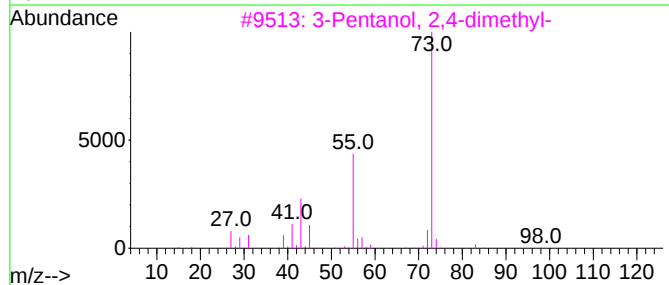
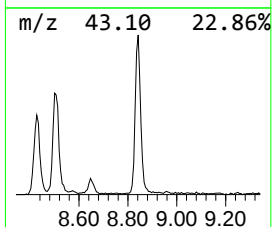
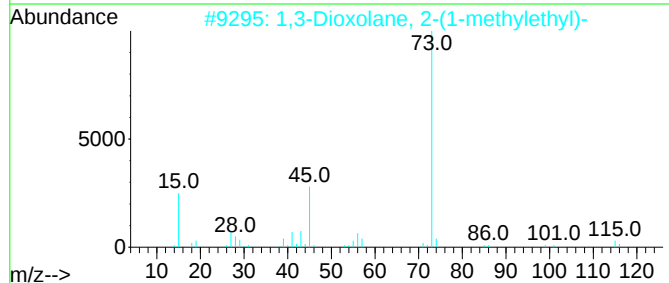
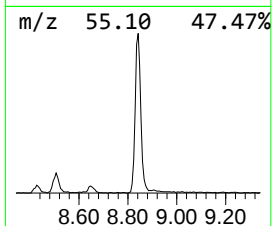
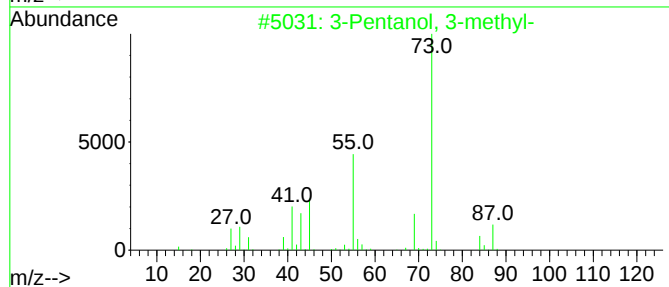
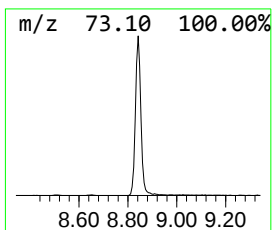
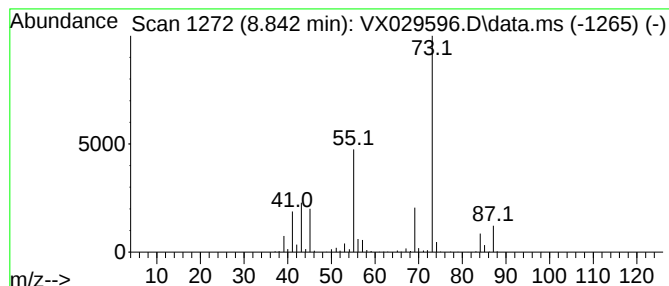
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Quant Title : SW846 8260

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

Peak Number 4 3-Pentanol, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.842	12.72 ug/l	288219	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	83
2			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	38
4			3-Methylpentan-3-yl propyl carbo...	188	C10H20O3	1000372-82-3	25
5			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	25



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Amylene hydrate	6.239	50.9	ug/l	1056350	2	6.763	1036830	50.0
2-Butanol, 2,3-...	8.427	7.3	ug/l	166358	3	10.055	1132550	50.0
2-Pentanol, 2-m...	8.507	9.8	ug/l	222154	3	10.055	1132550	50.0
3-Pentanol, 3-m...	8.842	12.7	ug/l	288219	3	10.055	1132550	50.0