

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031722\
 Data File : VX027506.D
 Acq On : 17 Mar 2022 22:55
 Operator : JC/MD
 Sample : N1997-12
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-112

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\82X031722W.M
 Title : SW846 8260

Signal : TIC: VX027506.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.965	299	308	322	rBV	190189	416082	1.53%	0.893%
2	3.117	322	333	356	rVV	11360826	27253592	100.00%	58.471%
3	3.769	427	440	460	rBV	153220	417439	1.53%	0.896%
4	5.391	693	706	716	rBV	206092	596686	2.19%	1.280%
5	5.556	724	733	753	rVB	336384	957891	3.51%	2.055%
6	5.964	789	800	806	rBV	202279	539085	1.98%	1.157%
7	6.043	806	813	829	rVB	279889	732875	2.69%	1.572%
8	6.239	833	845	852	rBV	735013	1985697	7.29%	4.260%
9	6.330	852	860	878	rVB	2185402	6108761	22.41%	13.106%
10	6.769	921	932	946	rBV	508111	1228192	4.51%	2.635%
11	8.506	1211	1217	1227	rVB	243186	400538	1.47%	0.859%
12	8.653	1234	1241	1255	rVB	1032222	1623589	5.96%	3.483%
13	8.842	1265	1272	1288	rBV	324858	508289	1.87%	1.091%
14	10.055	1460	1471	1477	rBV	1049045	1457647	5.35%	3.127%
15	11.085	1634	1640	1649	rBV	857589	1080996	3.97%	2.319%
16	12.024	1789	1794	1804	rBV	1078049	1303107	4.78%	2.796%

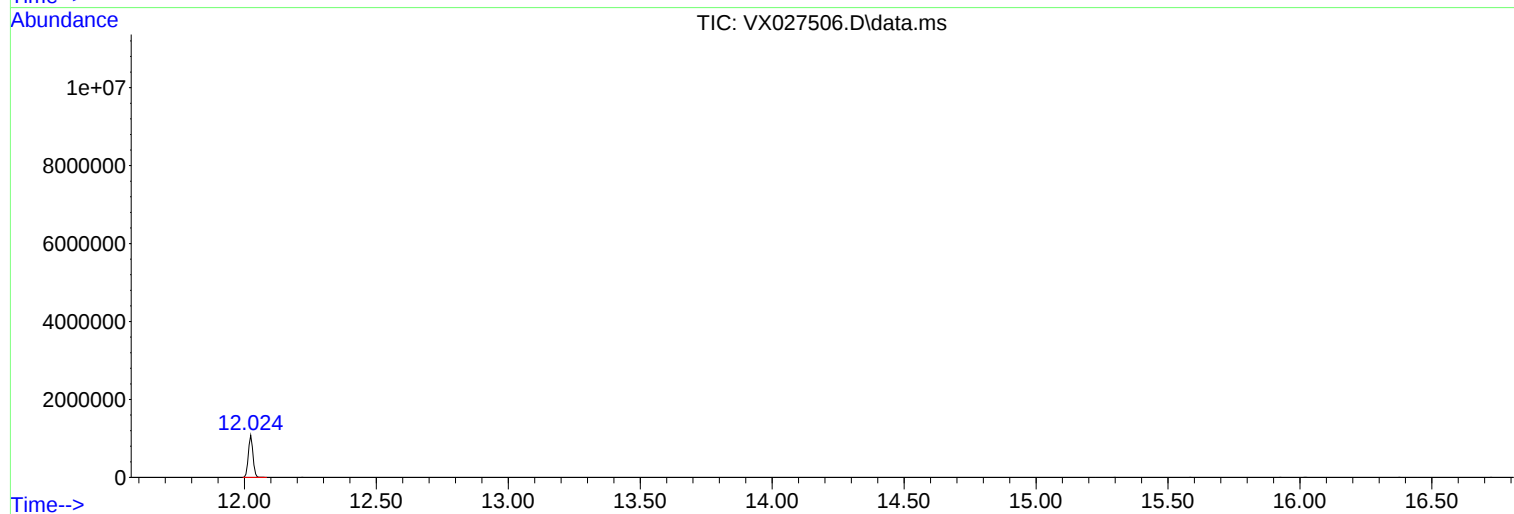
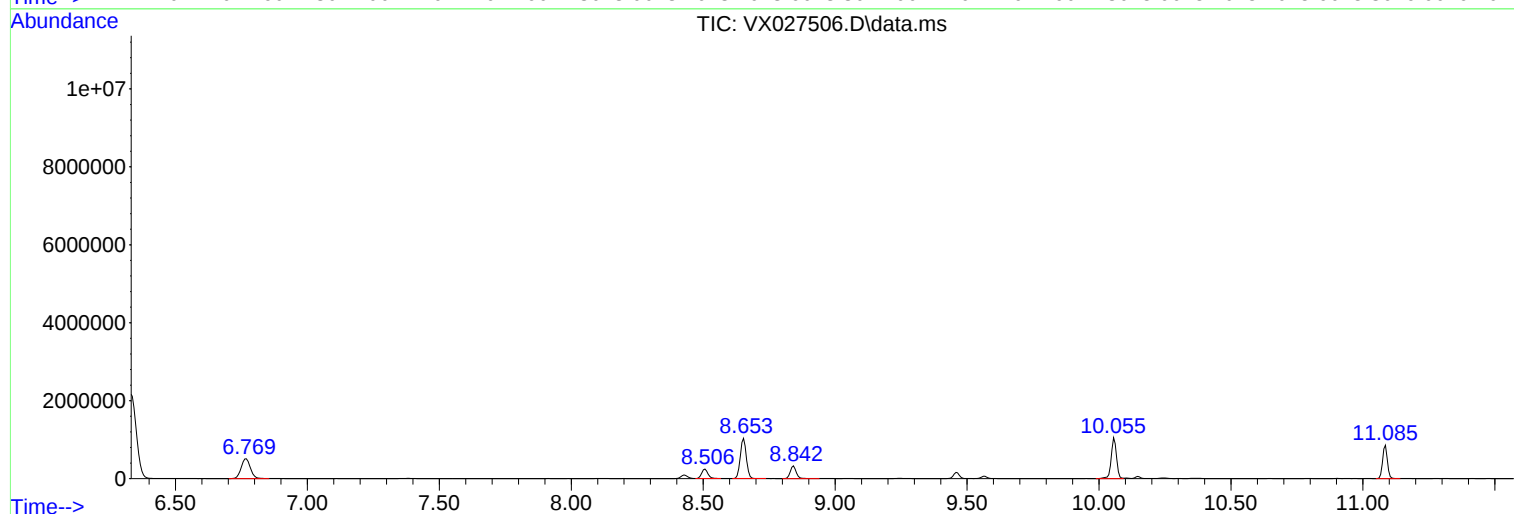
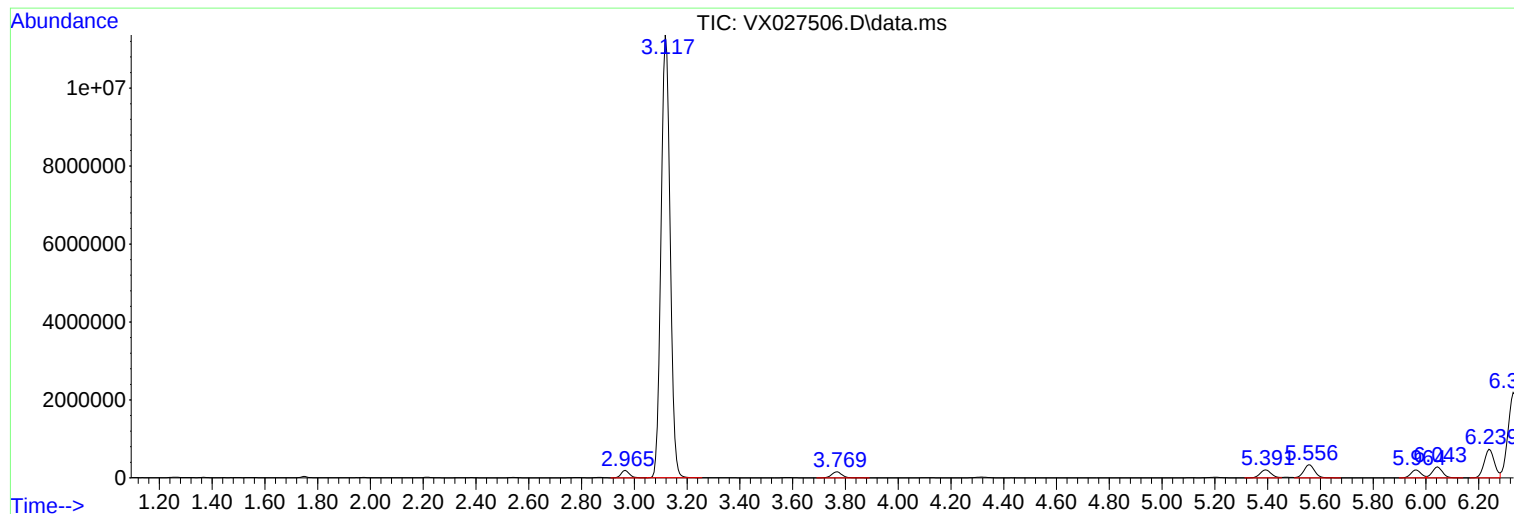
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031722W.M
Quant Title : SW846 8260

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



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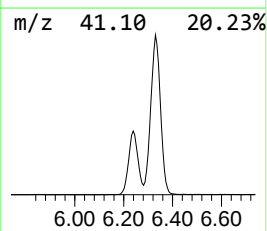
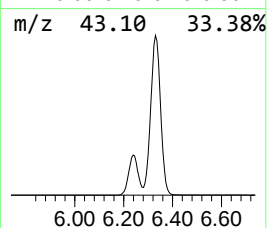
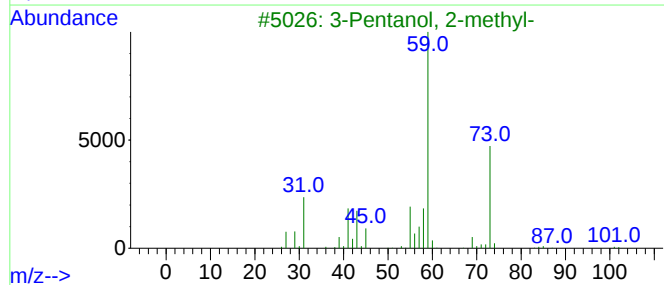
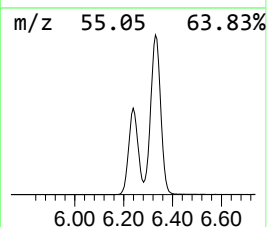
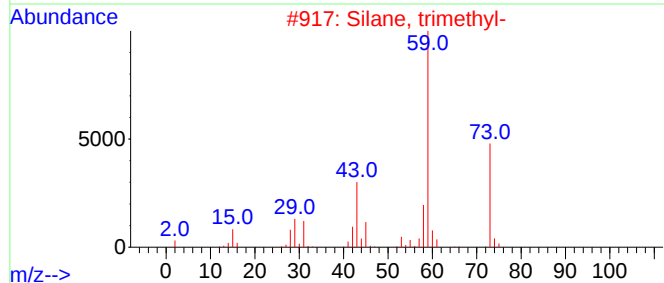
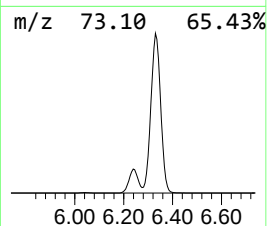
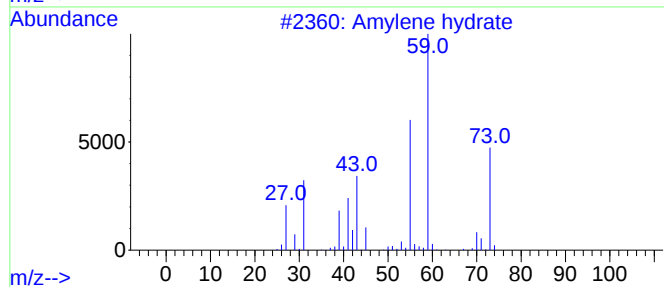
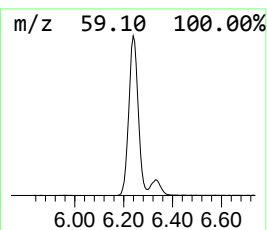
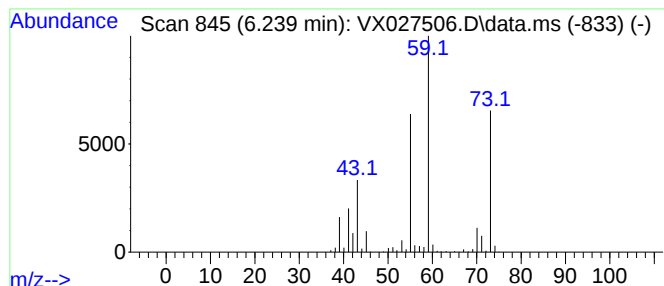
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031722W.M
Quant Title : SW846 8260

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

Peak Number 1 Amylene hydrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.239	80.84 ug/l	1985700	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	83
2			Silane, trimethyl-	74	C3H10Si	000993-07-7	39
3			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	38
4			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	33
5			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	11



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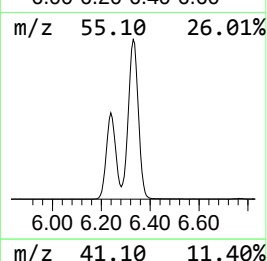
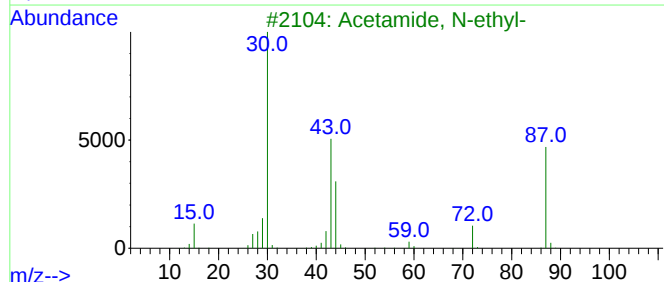
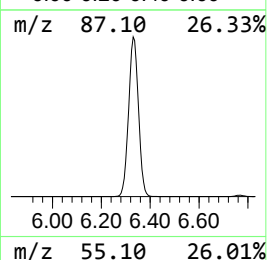
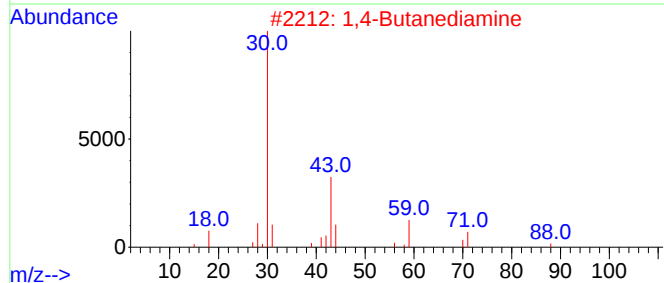
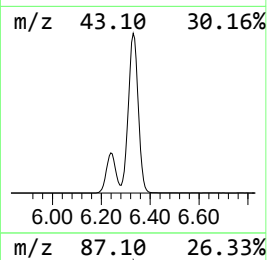
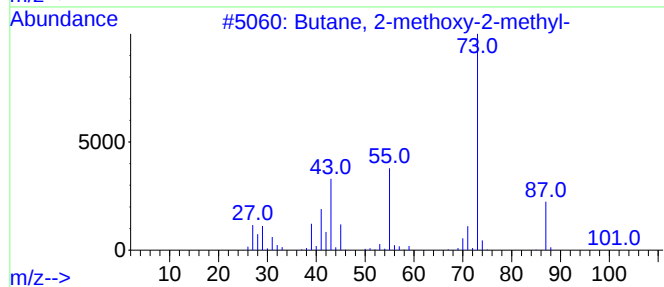
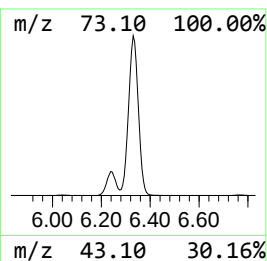
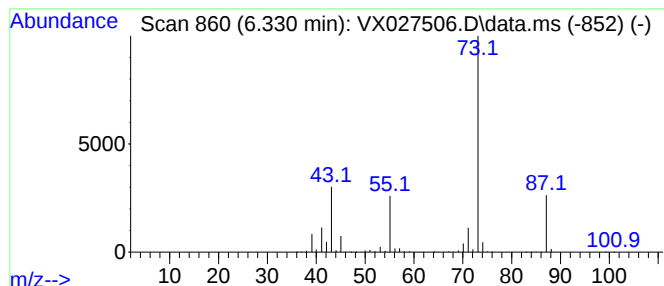
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031722W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.330	248.69 ug/l	6108760	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			1,4-Butanediamine	88	C4H12N2	000110-60-1	9
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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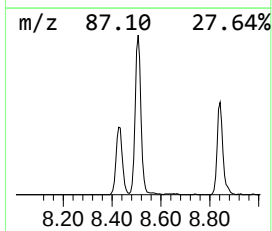
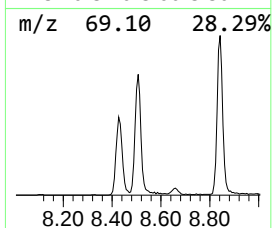
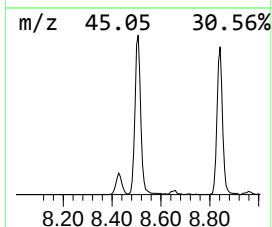
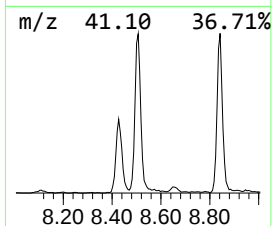
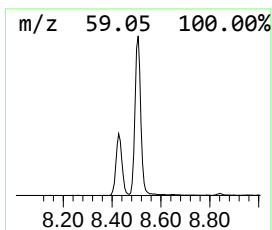
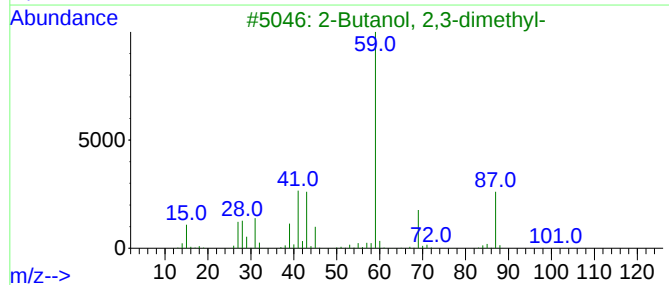
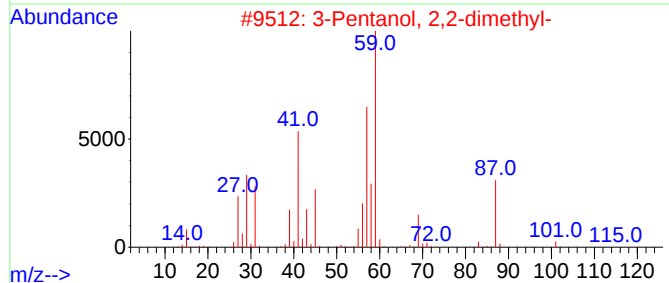
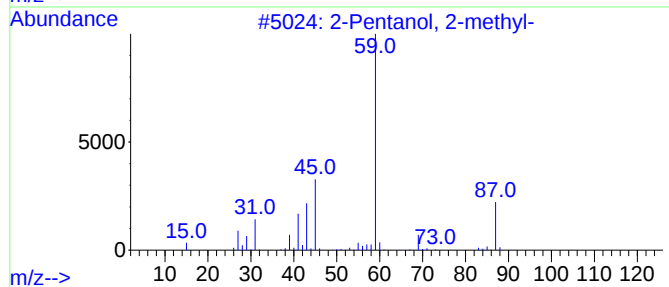
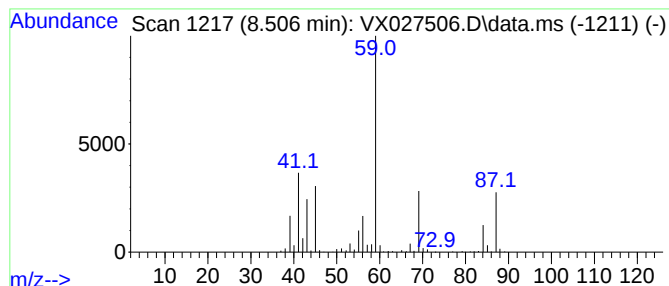
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Peak Number 3 2-Pentanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.506	13.74 ug/l	400538	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-			102	C6H14O	000590-36-3	72
2	3-Pentanol, 2,2-dimethyl-			116	C7H16O	003970-62-5	72
3	2-Butanol, 2,3-dimethyl-			102	C6H14O	000594-60-5	64
4	3-Hexanol, 4-methyl-			116	C7H16O	000615-29-2	56
5	Propane, 2-ethoxy-2-methyl-			102	C6H14O	000637-92-3	42



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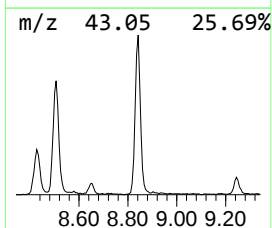
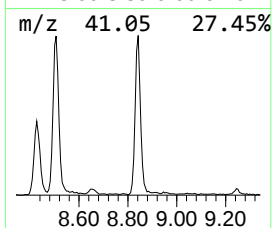
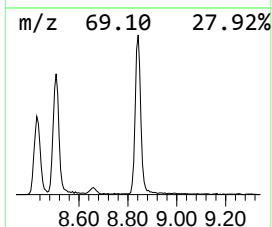
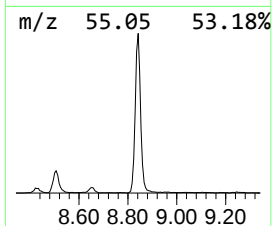
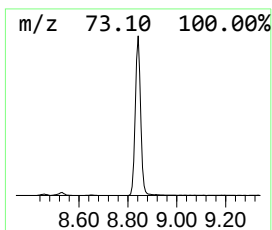
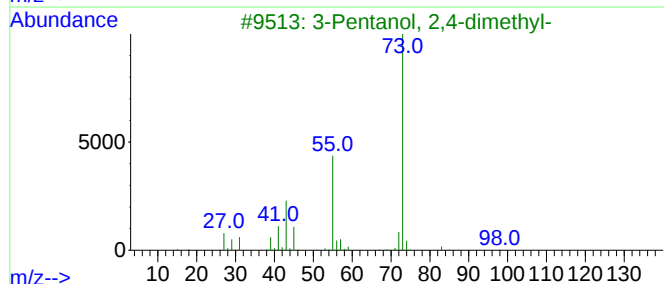
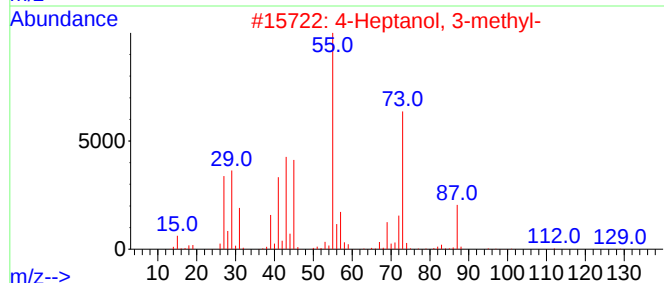
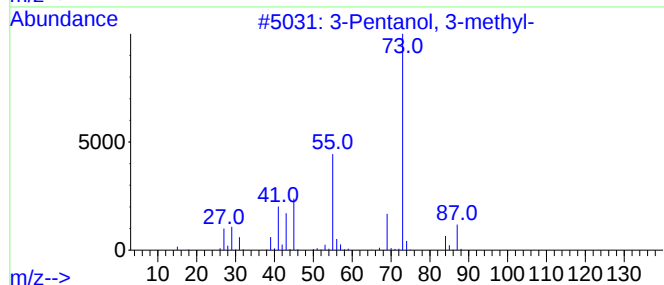
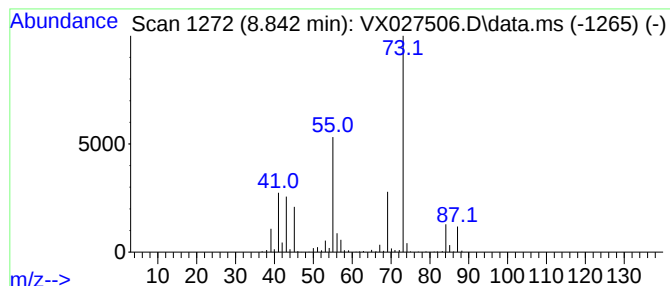
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Peak Number 4 3-Pentanol, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.842	17.44 ug/l	508289	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	74
2			4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	38
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	35
5			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	28



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Amylene hydrate	6.239	80.8	ug/l	1985700	2	6.769	1228190	50.0
Butane, 2-metho...	6.330	248.7	ug/l	6108760	2	6.769	1228190	50.0
2-Pentanol, 2-m...	8.506	13.7	ug/l	400538	3	10.055	1457650	50.0
3-Pentanol, 3-m...	8.842	17.4	ug/l	508289	3	10.055	1457650	50.0