

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
 Data File : VX029585.D
 Acq On : 18 Jun 2022 21:15
 Operator : JC/MD
 Sample : N3290-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-19

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: VX029585.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	23	29	41	rBV	69430	173345	3.47%	1.101%
2	2.977	299	310	323	rBV	157468	436283	8.72%	2.771%
3	3.117	323	333	351	rVB	2133357	5001489	100.00%	31.767%
4	3.763	429	439	448	rBV	26423	72645	1.45%	0.461%
5	5.202	664	675	686	rBV3	24221	76128	1.52%	0.484%
6	5.391	694	706	721	rBV2	150566	441060	8.82%	2.801%
7	5.556	722	733	748	rVB	282703	807556	16.15%	5.129%
8	5.958	787	799	809	rBV2	164695	430303	8.60%	2.733%
9	6.245	834	846	862	rBV	470304	1371241	27.42%	8.710%
10	6.763	921	931	943	rBV	428245	1032177	20.64%	6.556%
11	8.427	1196	1204	1211	rBV	145284	248361	4.97%	1.577%
12	8.506	1211	1217	1234	rVB	236389	399130	7.98%	2.535%
13	8.653	1234	1241	1250	rBV	849612	1344112	26.87%	8.537%
14	8.842	1265	1272	1283	rBV	285881	452074	9.04%	2.871%
15	9.451	1365	1372	1382	rBV4	36943	68784	1.38%	0.437%
16	9.567	1385	1391	1401	rVB	72409	113904	2.28%	0.723%
17	10.055	1459	1471	1476	rBV	873944	1225771	24.51%	7.786%
18	10.104	1476	1479	1482	rVV	37769	51114	1.02%	0.325%
19	10.146	1482	1486	1491	rVB	61367	83338	1.67%	0.529%
20	10.250	1497	1503	1508	rVV	35026	68130	1.36%	0.433%
21	11.079	1634	1639	1649	rBV	627199	837724	16.75%	5.321%
22	12.024	1788	1794	1802	rBV	845248	1009514	20.18%	6.412%

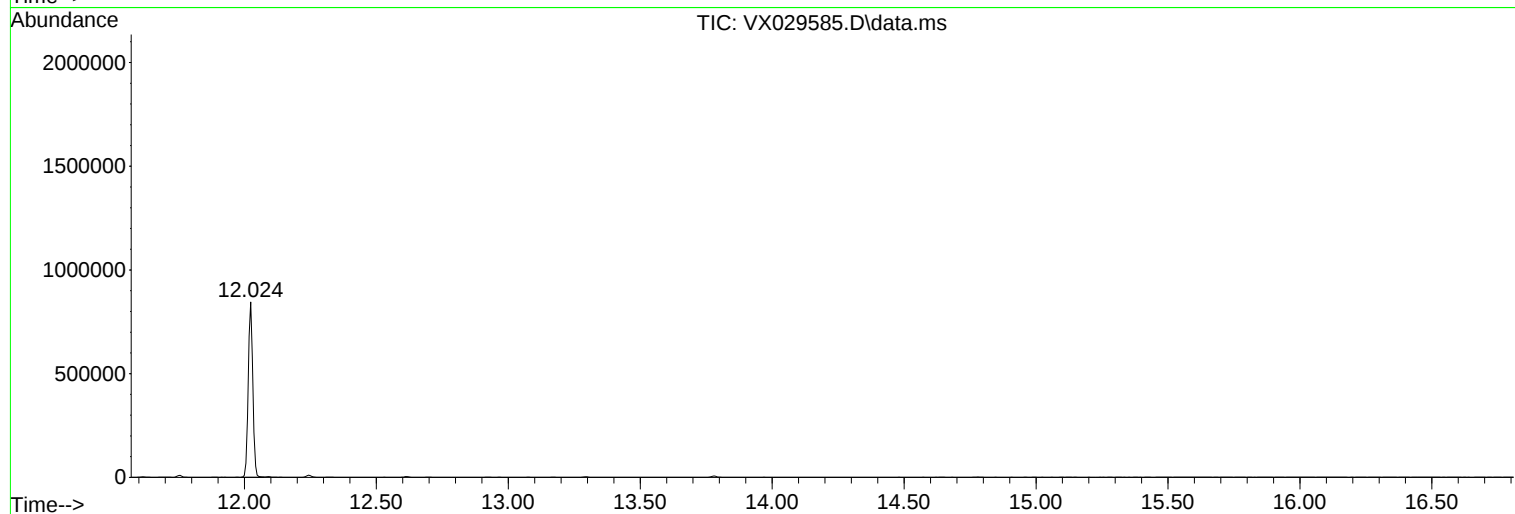
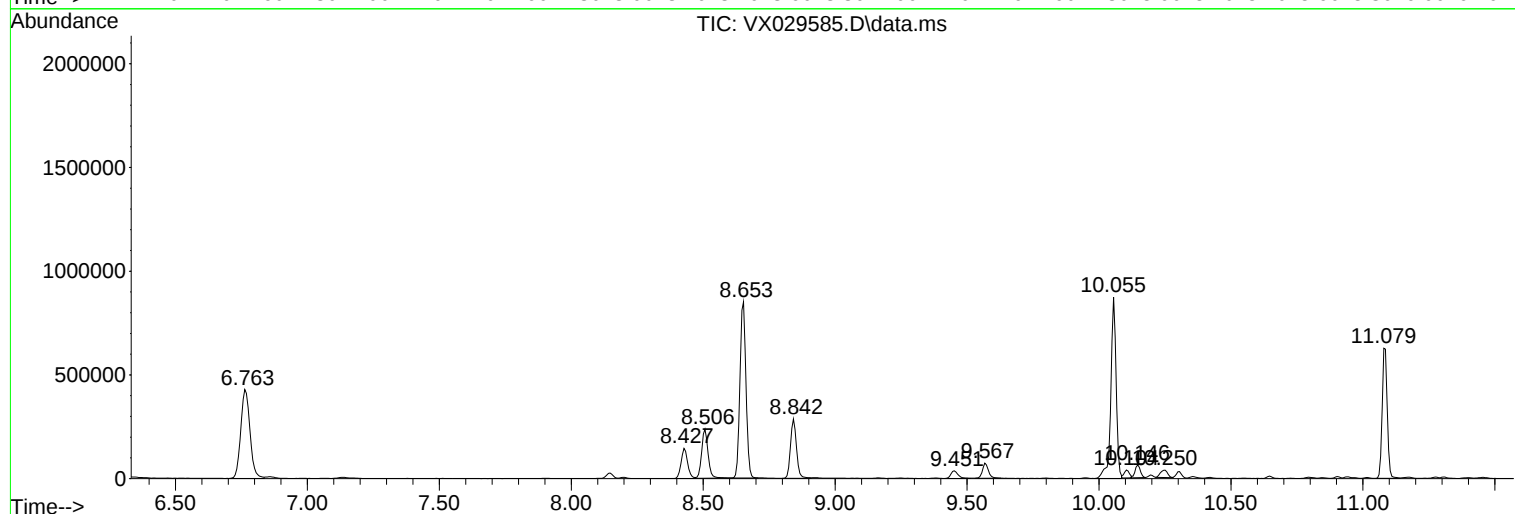
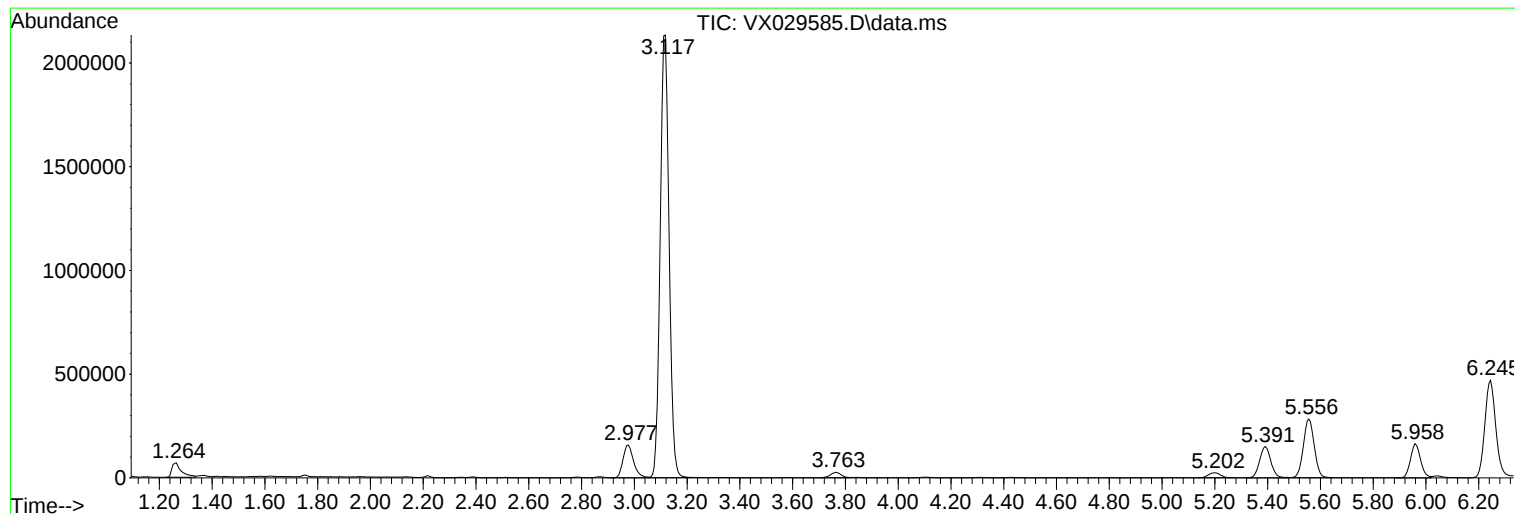
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



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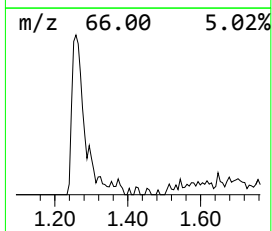
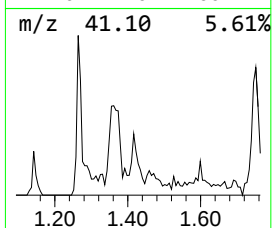
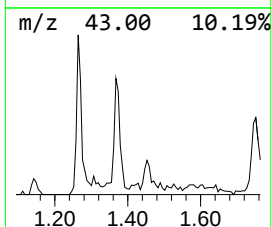
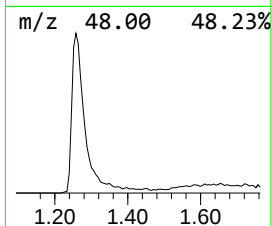
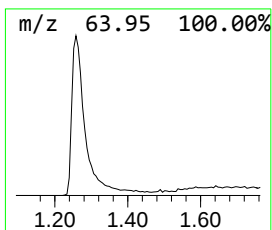
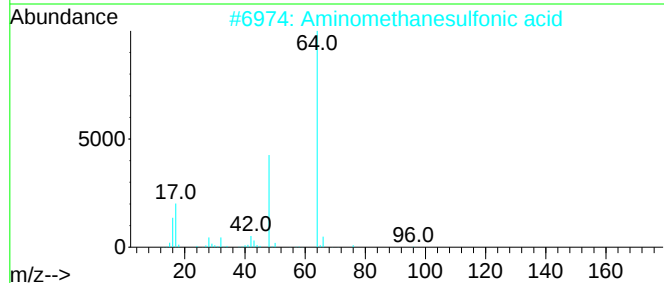
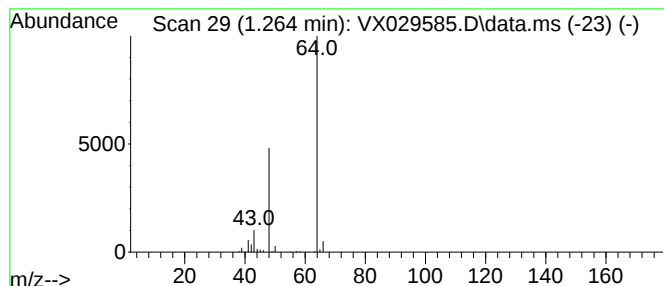
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	10.73 ug/l	173345	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	64
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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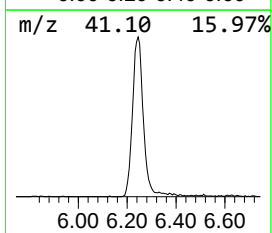
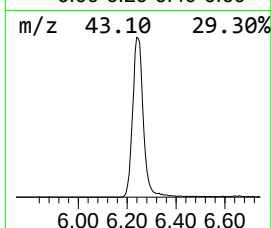
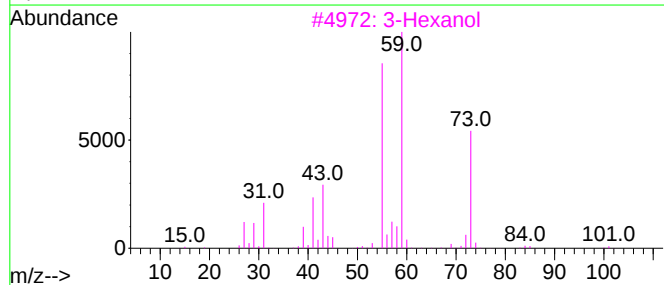
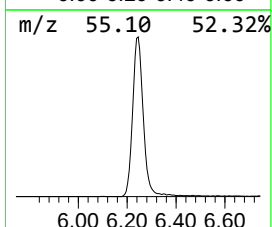
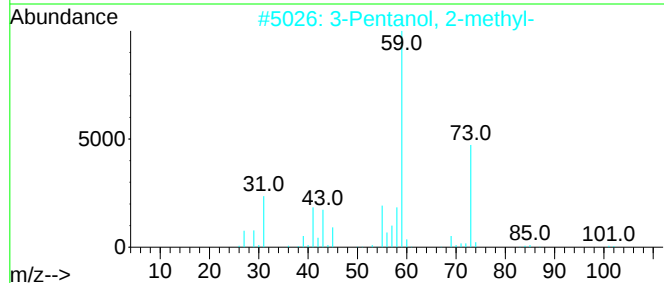
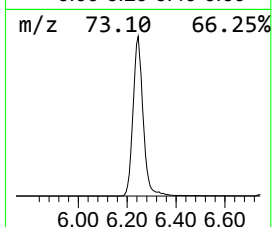
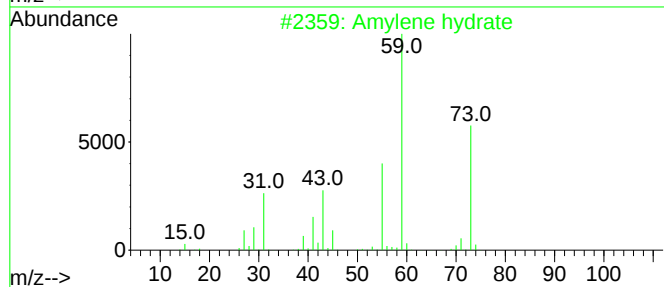
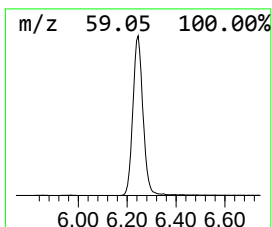
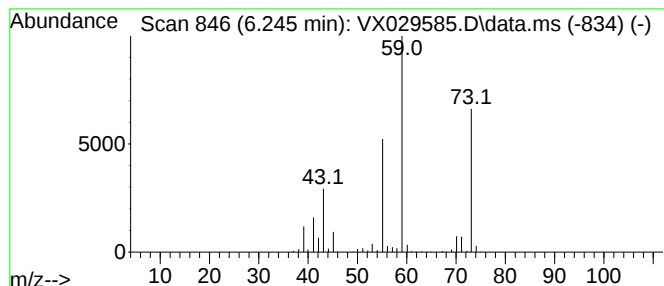
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 2 Amylene hydrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	66.42 ug/l	1371240	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-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	39
3			3-Hexanol	102	C6H14O	000623-37-0	39
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	10
5			Silane, trimethyl-	74	C3H10Si	000993-07-7	9



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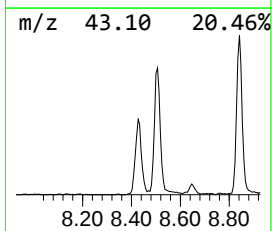
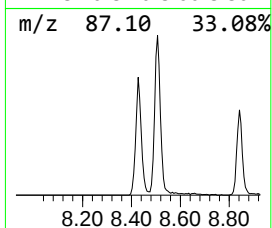
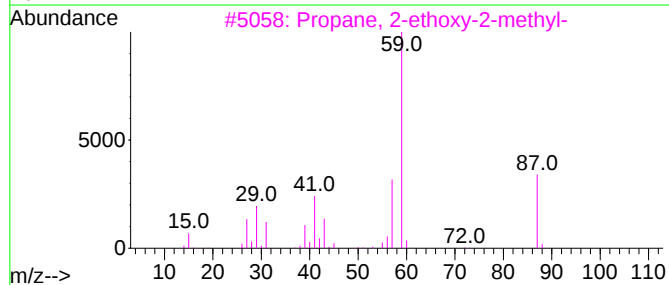
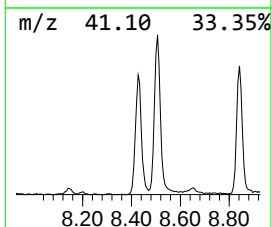
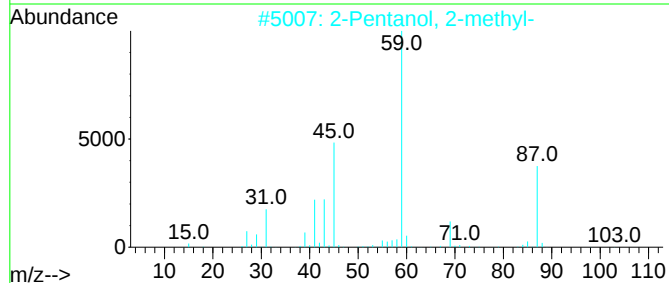
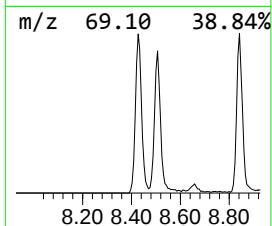
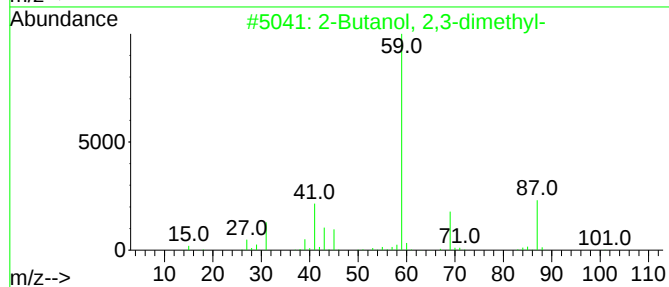
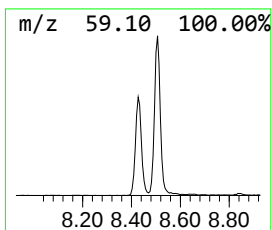
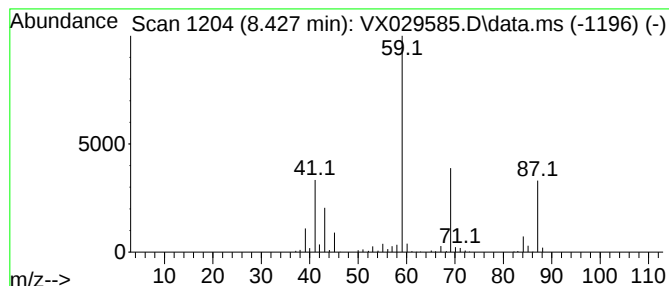
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Peak Number 3 2-Butanol, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.427	10.13 ug/l	248361	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-			102	C6H14O	000594-60-5	78
2	2-Pentanol, 2-methyl-			102	C6H14O	000590-36-3	72
3	Propane, 2-ethoxy-2-methyl-			102	C6H14O	000637-92-3	50
4	Amylene hydrate			88	C5H12O	000075-85-4	40
5	3-Heptanol			116	C7H16O	000589-82-2	39



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ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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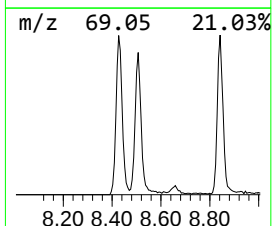
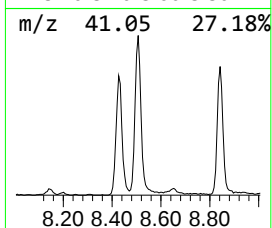
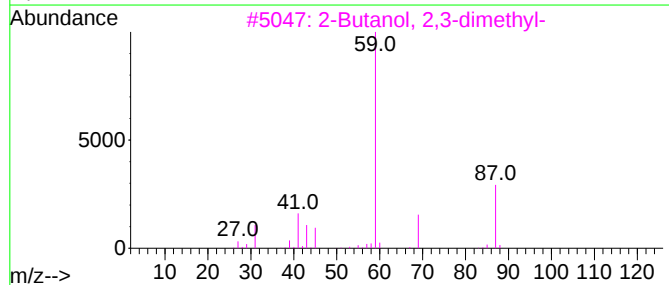
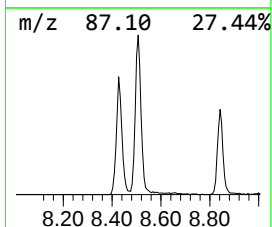
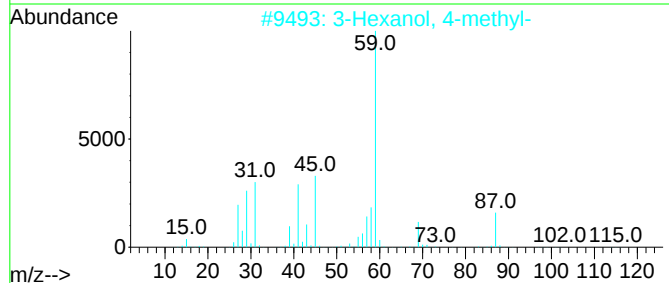
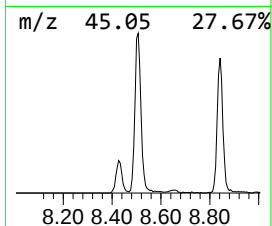
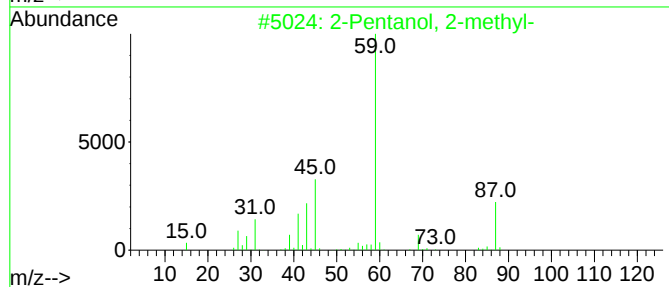
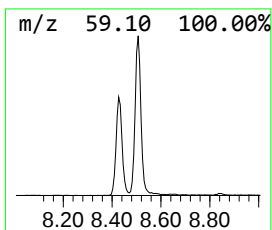
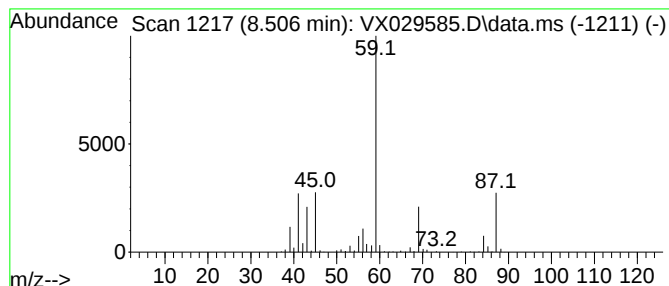
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Peak Number 4 2-Pentanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.506	16.28 ug/l	399130	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			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	78
3			2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	64
4			3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	56
5			3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	56



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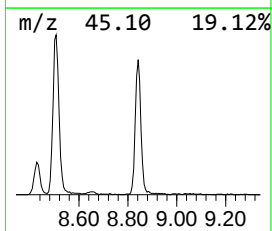
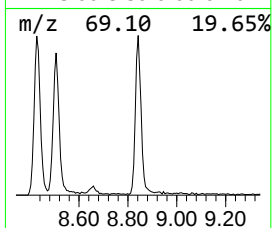
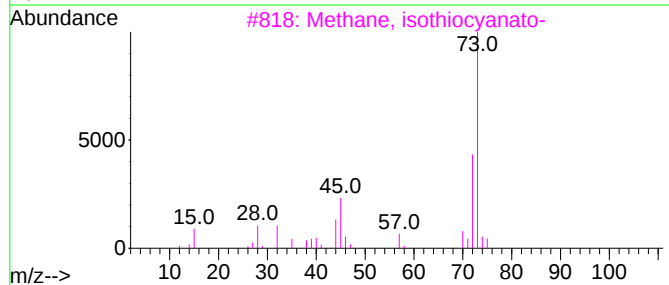
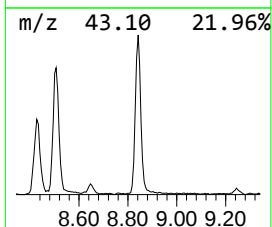
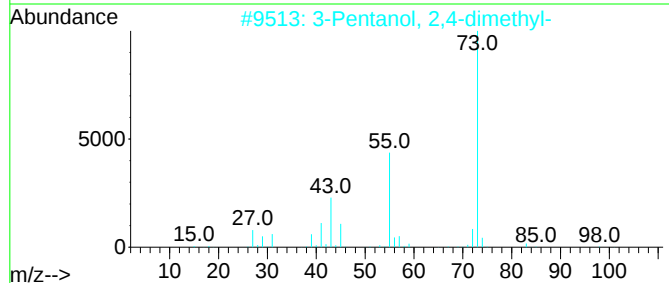
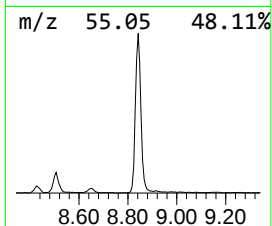
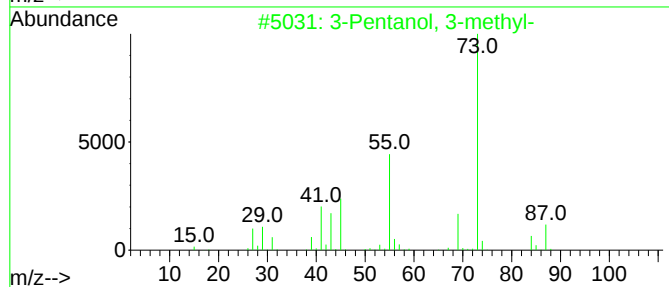
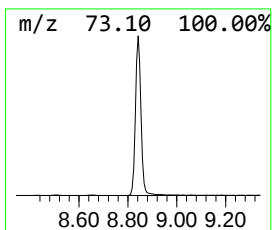
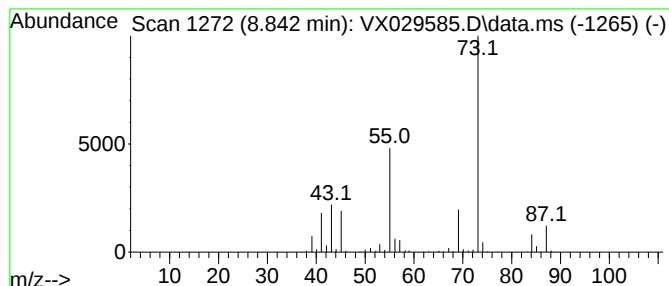
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TIC Integration Parameters: LSCINT.P

Peak Number 5 3-Pentanol, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.842	18.44 ug/l	452074	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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	25
4			3-Methylpentan-3-yl propyl carbo...	188	C10H20O3	1000372-82-3	23
5			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	10



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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
Sulfur dioxide	1.264	10.7	ug/l	173345	1	5.556	807556	50.0
Amylene hydrate	6.245	66.4	ug/l	1371240	2	6.763	1032180	50.0
2-Butanol, 2,3-...	8.427	10.1	ug/l	248361	3	10.055	1225770	50.0
2-Pentanol, 2-m...	8.506	16.3	ug/l	399130	3	10.055	1225770	50.0
3-Pentanol, 3-m...	8.842	18.4	ug/l	452074	3	10.055	1225770	50.0