

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082418\
 Data File : VX004243.D
 Acq On : 24 Aug 2018 13:36
 Operator : JC/MD
 Sample : J4616-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VB27184

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.075	75	80	94	rBV	2026677	2576581	100.00%	20.027%
2	2.617	328	333	344	rVB	14135	28056	1.09%	0.218%
3	3.062	396	406	417	rBV	65544	148575	5.77%	1.155%
4	5.501	793	806	821	rBV	208611	591426	22.95%	4.597%
5	5.665	821	833	849	rVB	287629	804763	31.23%	6.255%
6	6.068	888	899	908	rBV	215782	564038	21.89%	4.384%
7	6.141	908	911	922	rVB	12654	29338	1.14%	0.228%
8	6.379	942	950	959	rBV2	12506	33646	1.31%	0.262%
9	6.860	1019	1029	1048	rVB	449484	1049057	40.72%	8.154%
10	7.513	1130	1136	1143	rVB	37267	74901	2.91%	0.582%
11	7.988	1202	1214	1224	rBV	100108	196120	7.61%	1.524%
12	8.506	1292	1299	1305	rBV2	15305	26180	1.02%	0.203%
13	8.586	1305	1312	1319	rBV	36107	59566	2.31%	0.463%
14	8.714	1326	1333	1342	rBV	1115383	1730764	67.17%	13.452%
15	9.311	1425	1431	1443	rVB	29555	50978	1.98%	0.396%
16	9.512	1458	1464	1473	rBV	104246	154180	5.98%	1.198%
17	9.652	1483	1487	1496	rVB	17213	26870	1.04%	0.209%
18	9.860	1512	1521	1530	rBV	33681	52662	2.04%	0.409%
19	10.116	1557	1563	1569	rVB	932774	1199705	46.56%	9.325%
20	10.433	1611	1615	1627	rVB	137267	193987	7.53%	1.508%
21	10.610	1638	1644	1650	rBV	33085	48608	1.89%	0.378%
22	10.921	1690	1695	1697	rBV3	18160	28724	1.11%	0.223%
23	11.140	1725	1731	1737	rBV	871789	1094301	42.47%	8.506%
24	12.030	1872	1877	1881	rBV	187643	241111	9.36%	1.874%
25	12.079	1881	1885	1891	rVB	1064045	1260126	48.91%	9.794%
26	12.408	1930	1939	1943	rBV5	28753	56965	2.21%	0.443%
27	12.725	1986	1991	1997	rBV	74400	105229	4.08%	0.818%
28	12.975	2025	2032	2035	rBV2	21824	33336	1.29%	0.259%
29	13.115	2051	2055	2062	rVV3	17069	33281	1.29%	0.259%
30	13.195	2062	2068	2072	rVB4	16821	29355	1.14%	0.228%
31	13.329	2086	2090	2093	rBV2	25929	40313	1.56%	0.313%
32	13.359	2093	2095	2099	rVB3	23491	31305	1.21%	0.243%
33	13.694	2145	2150	2153	rBV5	15386	28149	1.09%	0.219%
34	13.725	2153	2155	2162	rVB5	17742	27237	1.06%	0.212%

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Integration Parameters: RTEINT.P

Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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35	13.987	2192	2198	2201	rBV2	16310	27754	1.08%	0.216%
36	14.292	2240	2248	2256	rBV2	30008	57351	2.23%	0.446%
37	14.542	2282	2289	2295	rBV3	25183	39043	1.52%	0.303%
38	14.676	2307	2311	2317	rBV3	20201	44096	1.71%	0.343%
39	15.249	2399	2405	2413	rBV3	24034	48115	1.87%	0.374%

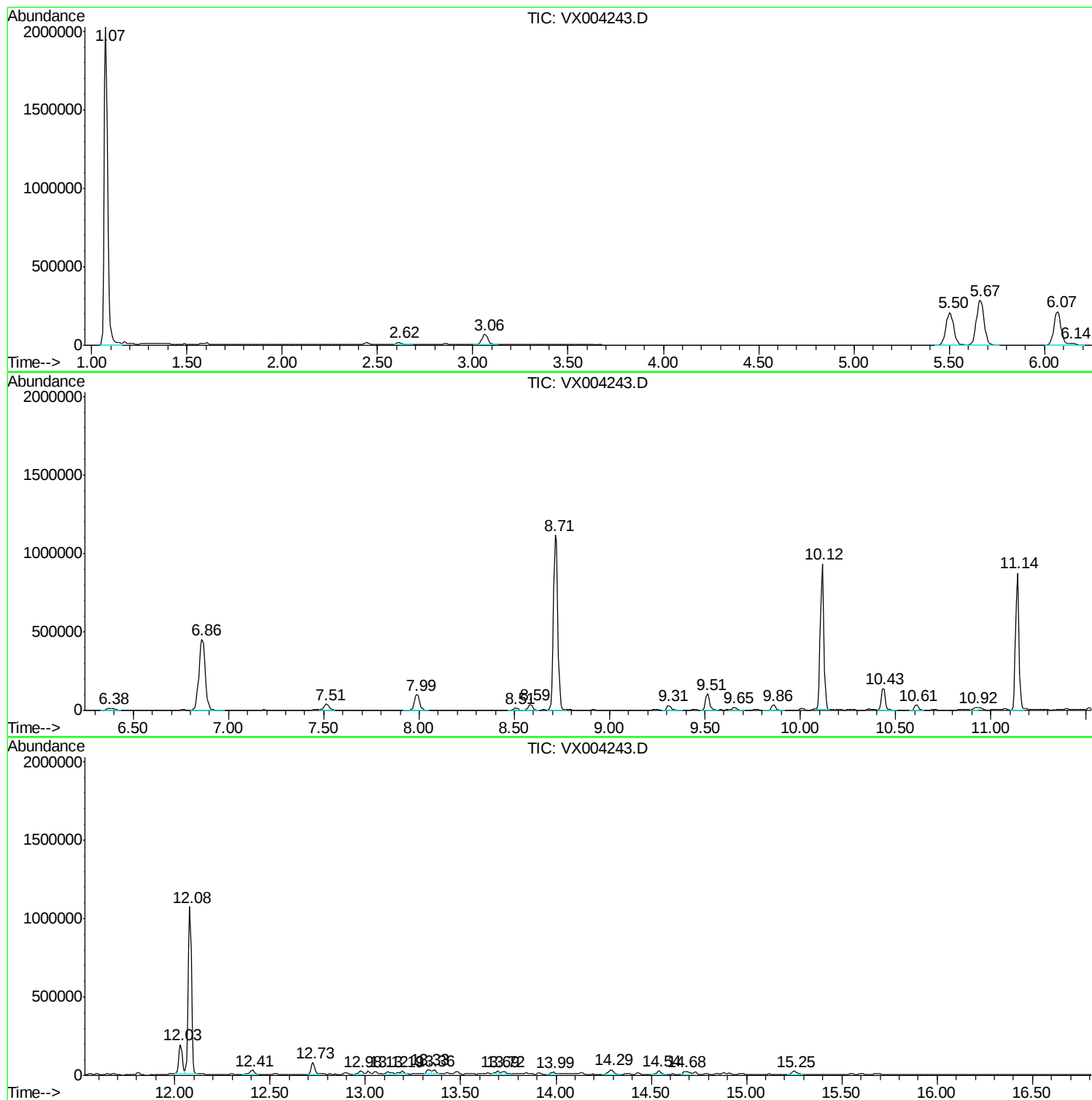
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082218W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_X
ClientSampled :
VB27184

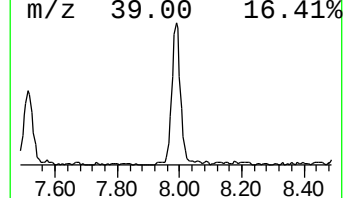
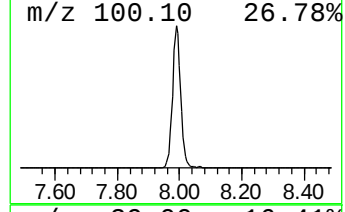
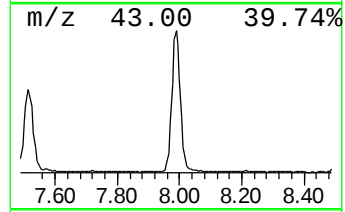
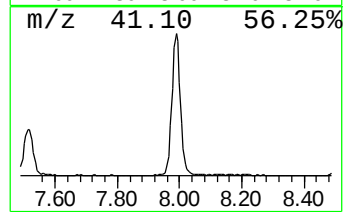
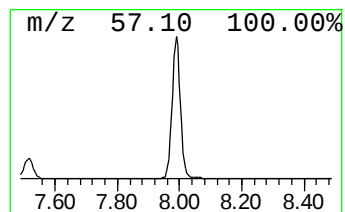
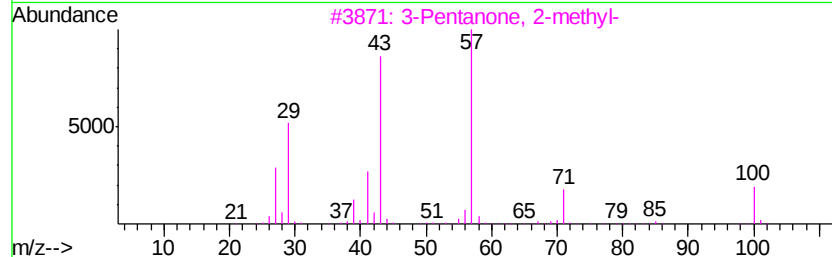
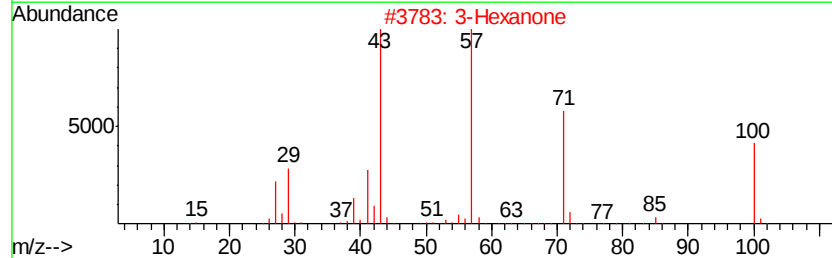
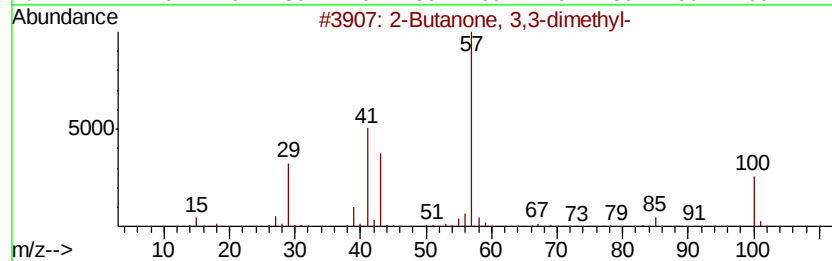
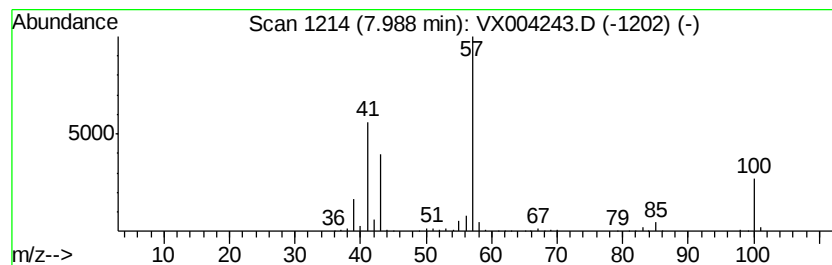
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.99	9.35 ug/l	196120	1,4-Difluorobenzene	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	91
2			3-Hexanone	100	C6H12O	000589-38-8	59
3			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	59
4			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	47
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38



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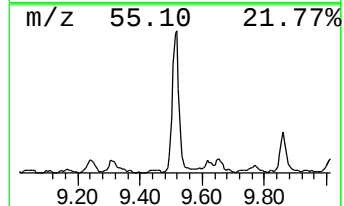
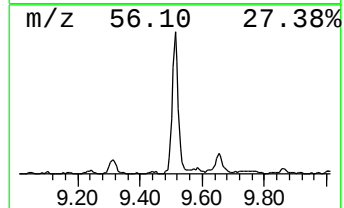
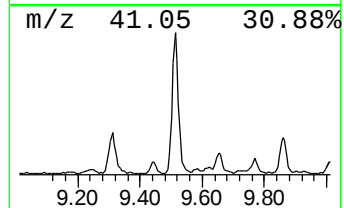
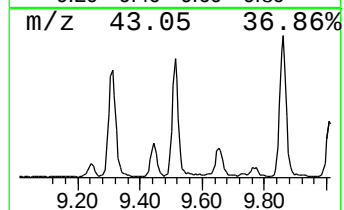
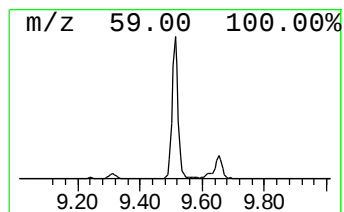
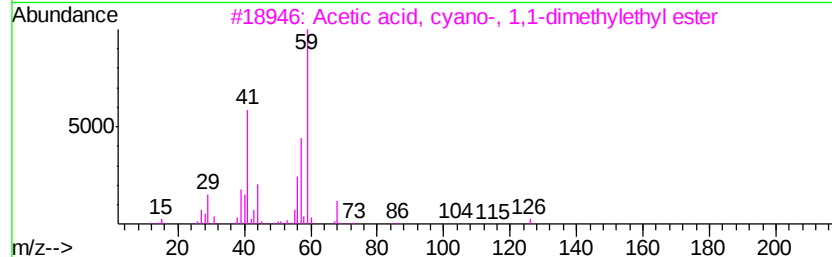
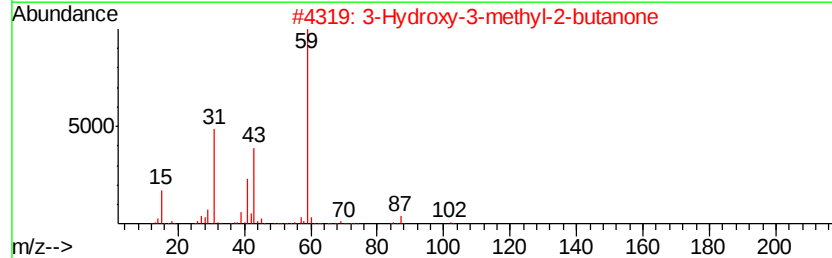
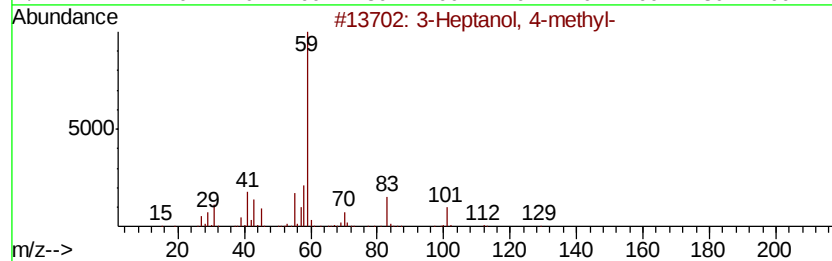
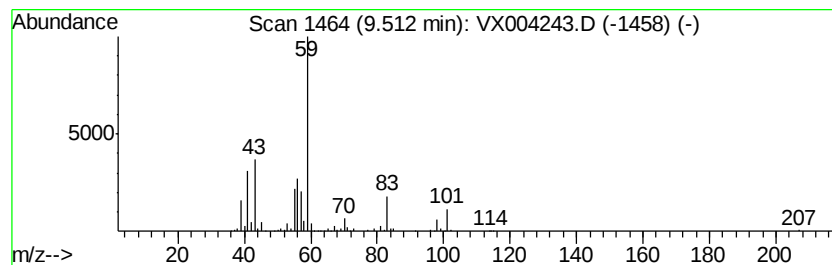
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Peak Number 3 3-Heptanol, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.51	6.43 ug/l	154180	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	59
2		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	47
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	45
4		2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	45
5		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	45



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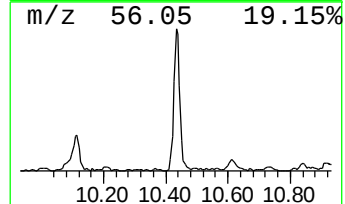
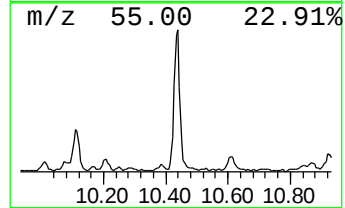
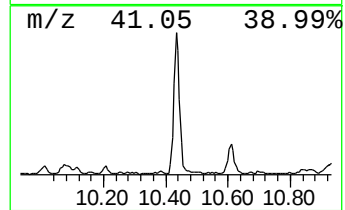
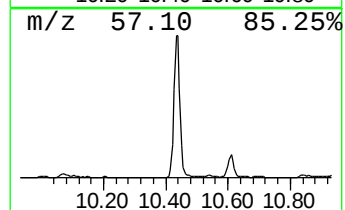
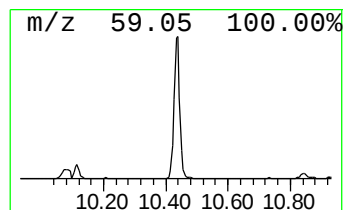
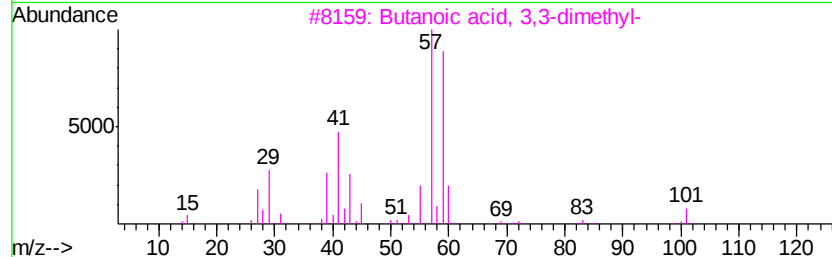
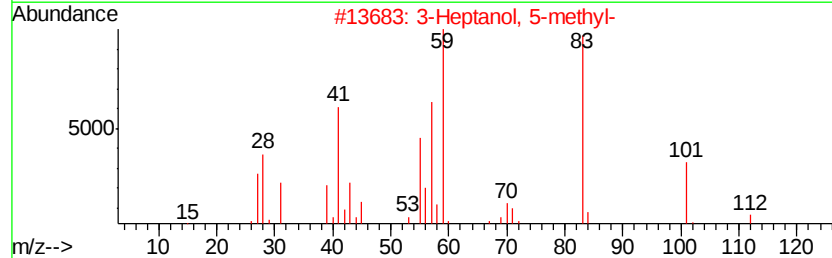
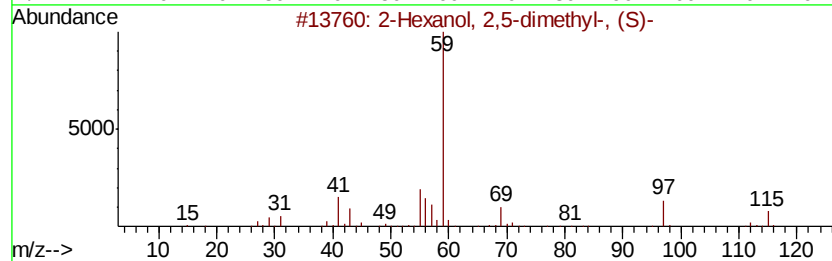
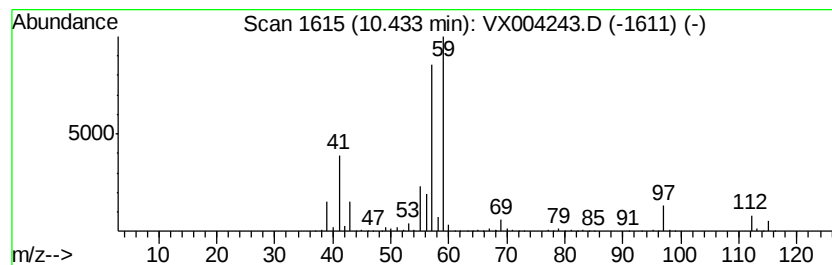
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.43	8.08 ug/l	193987	Chlorobenzene-d5	10.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	56	
2	3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	40	
3	Butanoic acid, 3,3-dimethyl-	116	C6H12O2	001070-83-3	40	
4	Carbamic acid, (1-cyanoethyl)-, ...	170	C8H14N2O2	100927-09-1	39	
5	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	39	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butanone, 3,3-d...	7.99	9.3	ug/l	196120	2	6.86	1049060	50.0
3-Heptanol, 4-met...	9.51	6.4	ug/l	154180	3	10.12	1199710	50.0
2-Hexanol, 2,5-di...	10.43	8.1	ug/l	193987	3	10.12	1199710	50.0