

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX110118\
 Data File : VX005726.D
 Acq On : 01 Nov 2018 13:50
 Operator : JC/MD
 Sample : J5737-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TP-A

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\82X103118W.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	1.605	65	74	77	rBV3	7894	13564	1.86%	0.262%
2	2.861	274	280	287	rVB3	3664	7307	1.00%	0.141%
3	5.507	702	714	728	rBV2	89021	251568	34.53%	4.852%
4	5.665	728	740	755	rBV	149065	413352	56.73%	7.973%
5	6.068	796	806	818	rBV	109506	279125	38.31%	5.384%
6	6.464	857	871	885	rBV	82587	209824	28.80%	4.047%
7	6.860	926	936	948	rBV	234546	545115	74.82%	10.514%
8	7.884	1097	1104	1116	rBV	111661	193262	26.53%	3.728%
9	8.622	1220	1225	1233	rBV	4487	8617	1.18%	0.166%
10	8.714	1233	1240	1251	rBV	457680	728595	100.00%	14.053%
11	9.409	1350	1354	1364	rVB	11568	19055	2.62%	0.368%
12	9.549	1372	1377	1383	rBV	54568	74517	10.23%	1.437%
13	9.640	1388	1392	1404	rVB	17971	25267	3.47%	0.487%
14	9.975	1442	1447	1454	rBV	55776	75014	10.30%	1.447%
15	10.116	1462	1470	1487	rBV	451898	628635	86.28%	12.125%
16	10.250	1487	1492	1497	rVB	11644	16246	2.23%	0.313%
17	10.360	1504	1510	1518	rBV	46872	65184	8.95%	1.257%
18	10.701	1561	1566	1571	rBV3	4856	7452	1.02%	0.144%
19	11.140	1632	1638	1649	rBV	356487	452061	62.05%	8.719%
20	11.433	1680	1686	1689	rBV	13832	22633	3.11%	0.437%
21	11.506	1694	1698	1705	rVB	10432	13215	1.81%	0.255%
22	11.811	1743	1748	1754	rVB	32948	42769	5.87%	0.825%
23	12.079	1786	1792	1799	rBV	474753	574187	78.81%	11.075%
24	12.146	1799	1803	1810	rVB	12187	15004	2.06%	0.289%
25	12.298	1825	1828	1830	rBV2	7965	9742	1.34%	0.188%
26	12.323	1830	1832	1836	rVV	12514	12653	1.74%	0.244%
27	12.371	1836	1840	1847	rVB3	23241	38676	5.31%	0.746%
28	12.585	1871	1875	1877	rBV	13854	18338	2.52%	0.354%
29	12.609	1877	1879	1884	rVB	20284	22528	3.09%	0.435%
30	12.670	1884	1889	1893	rBV	44852	52530	7.21%	1.013%
31	12.902	1923	1927	1933	rVB	8050	10727	1.47%	0.207%
32	12.975	1933	1939	1943	rBV	30795	40989	5.63%	0.791%
33	13.018	1943	1946	1952	rVB	41862	47720	6.55%	0.920%
34	13.225	1975	1980	1985	rVB	14075	19435	2.67%	0.375%

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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

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Title : SW846 8260

35	13.347	1995	2000	2009	rVB2	25441	38009	5.22%	0.733%
36	13.633	2044	2047	2054	rVB4	4645	8890	1.22%	0.171%
37	13.835	2075	2080	2086	rVB	49336	61782	8.48%	1.192%
38	14.700	2216	2222	2230	rVB	56344	72552	9.96%	1.399%
39	14.840	2236	2245	2252	rBV	24545	31105	4.27%	0.600%
40	15.548	2357	2361	2368	rVB2	5349	9040	1.24%	0.174%
41	15.694	2378	2385	2388	rBV3	4542	8333	1.14%	0.161%

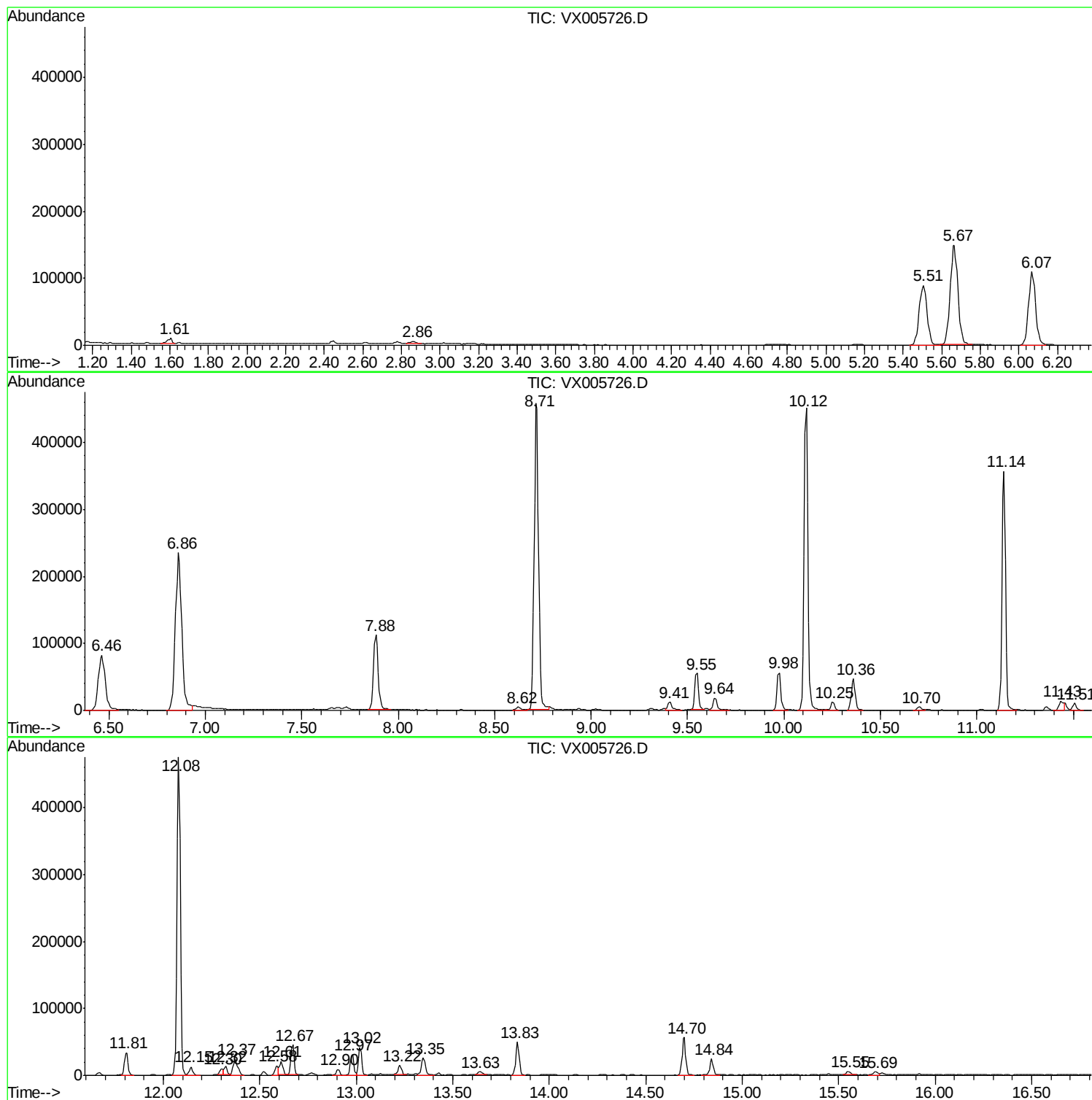
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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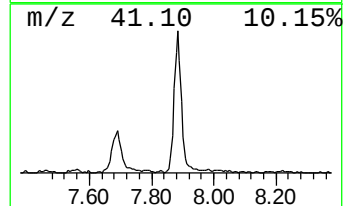
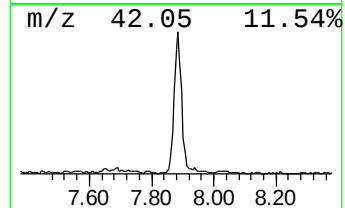
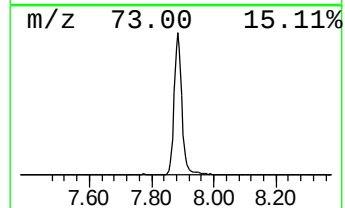
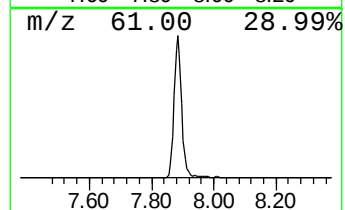
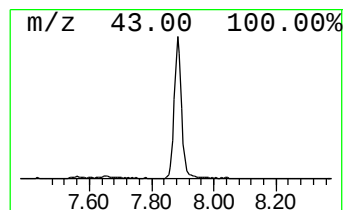
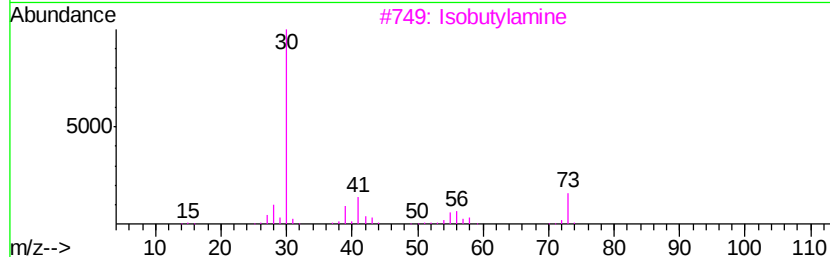
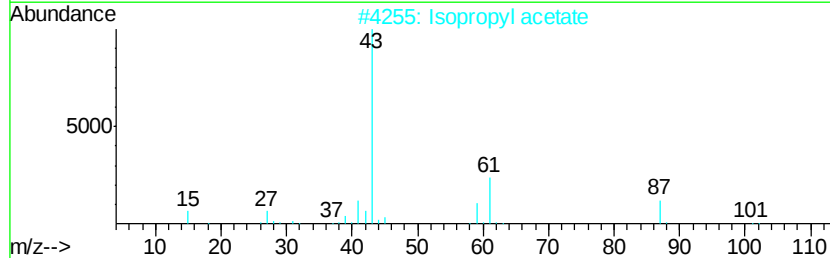
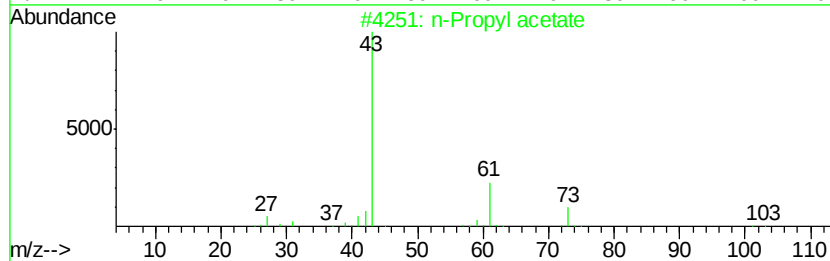
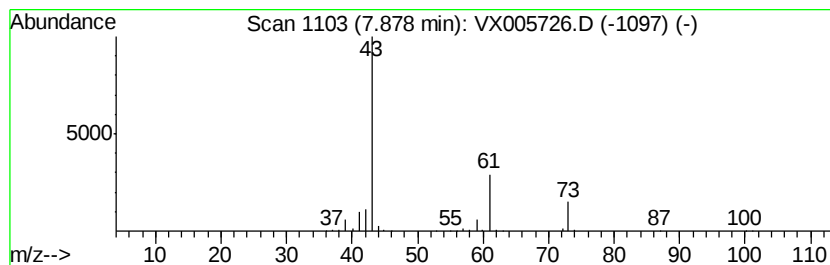
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X103118W.M
Quant Title : SW846 8260

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

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.88	17.73 ug/l	193262	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		Isopropyl acetate	102	C5H10O2	000108-21-4	36
3		Isobutylamine	73	C4H11N	000078-81-9	9
4		Isobutyl acetate	116	C6H12O2	000110-19-0	9
5		1-Butanamine	73	C4H11N	000109-73-9	7



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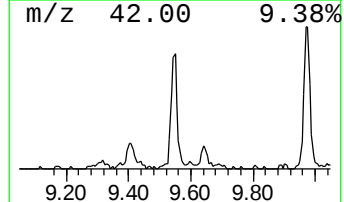
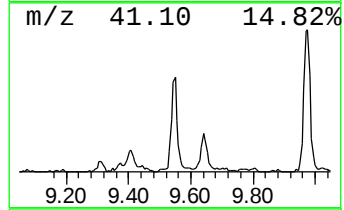
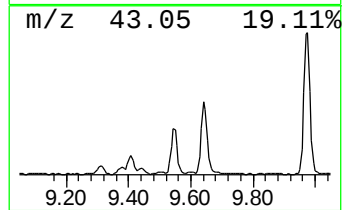
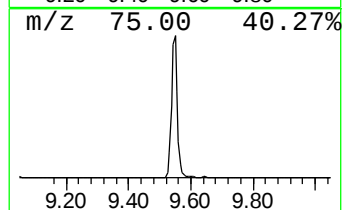
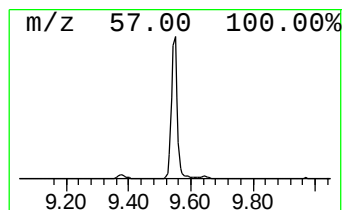
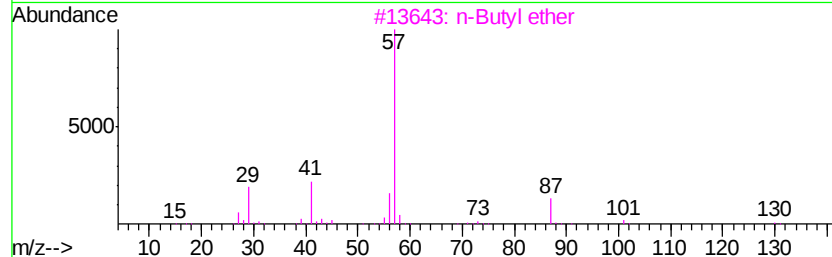
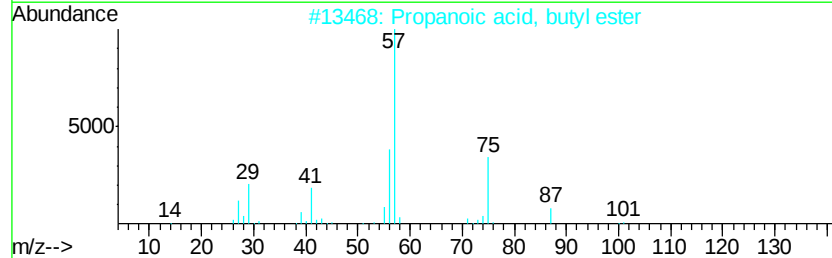
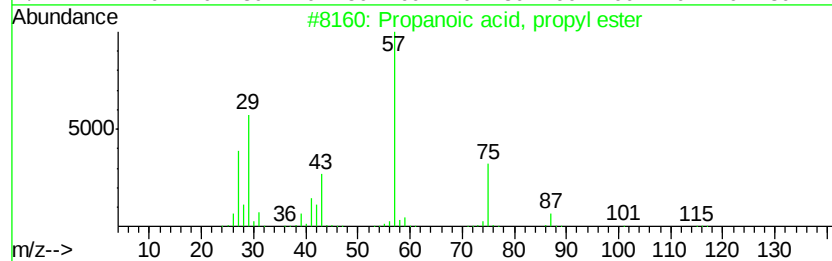
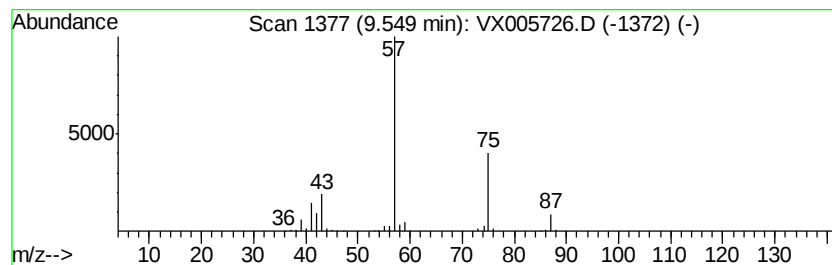
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 Peak Number 2 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	5.93 ug/l	74517	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38
3		n-Butyl ether	130	C8H18O	000142-96-1	9
4		Oxalic acid, bis(isobutyl) ester	202	C10H18O4	1000309-36-8	9
5		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9



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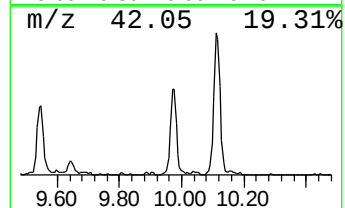
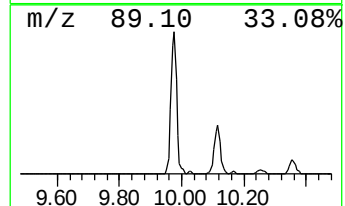
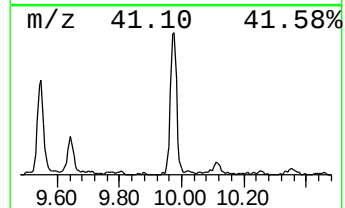
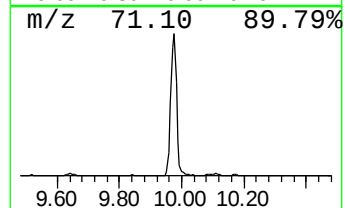
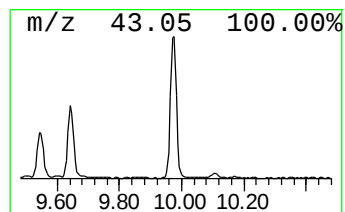
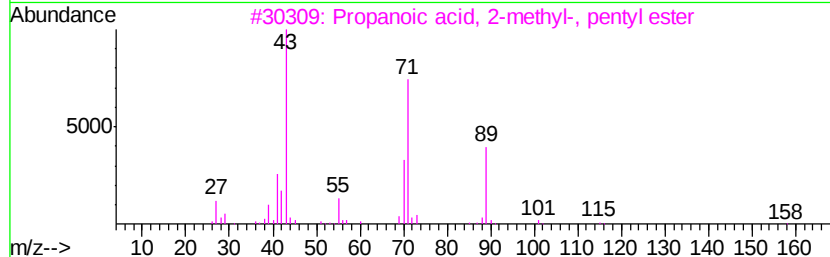
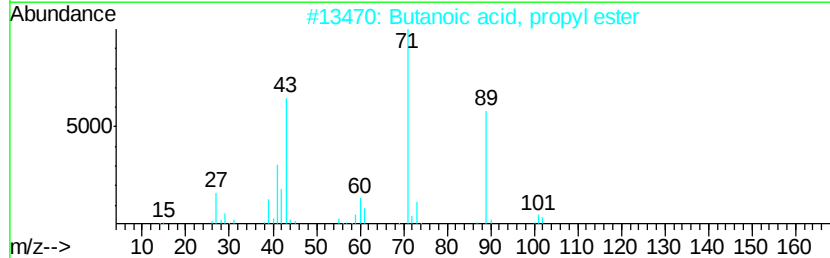
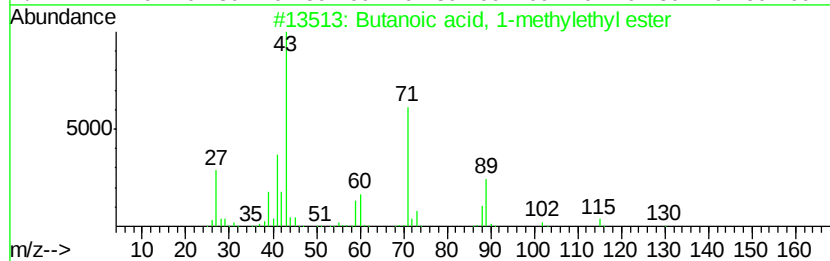
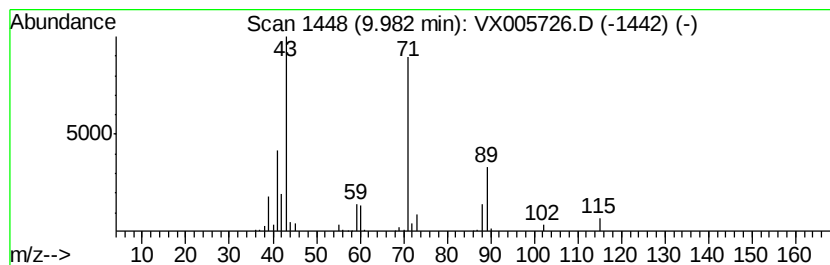
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
9.98	5.97 ug/l	75014	Chlorobenzene-d5	10.12		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	78
3		Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	72
4		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
5		Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	53



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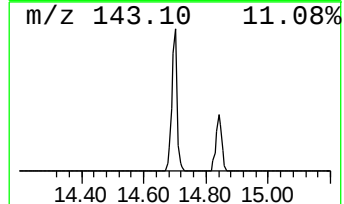
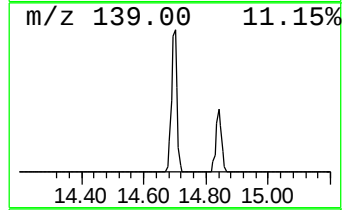
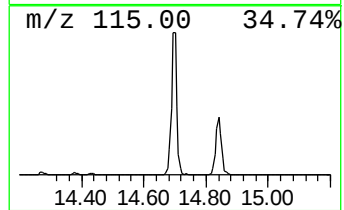
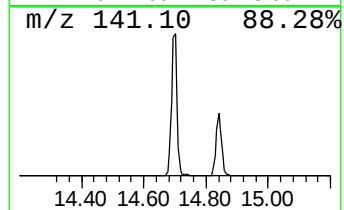
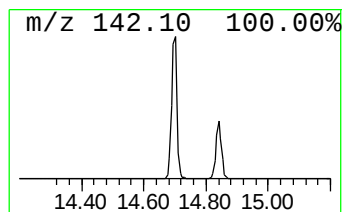
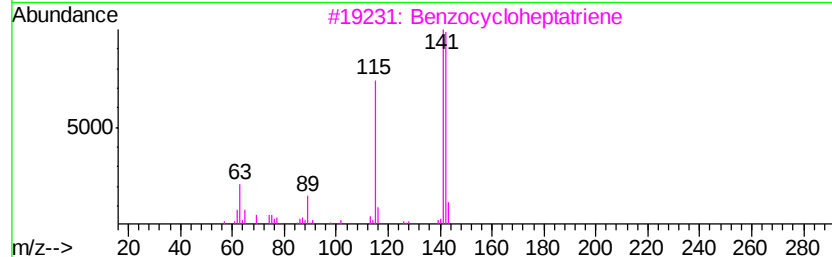
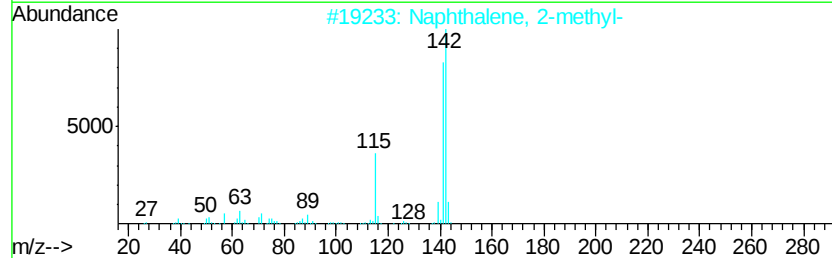
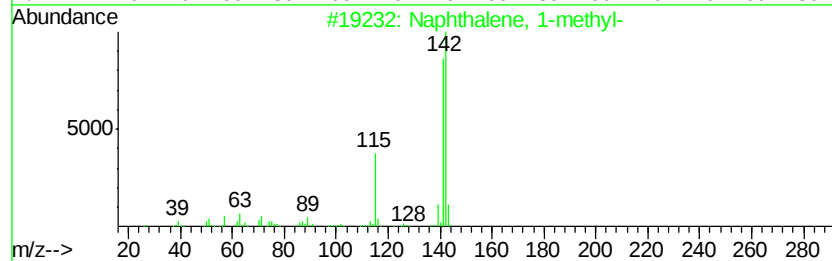
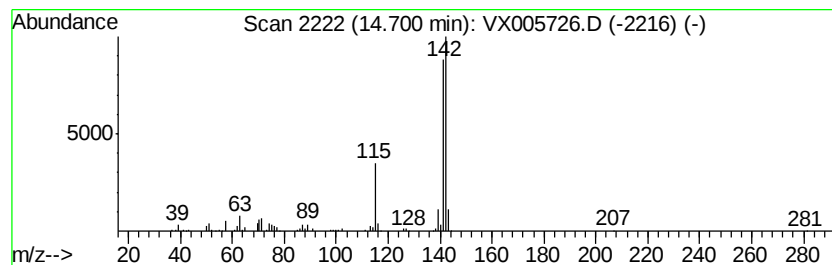
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Peak Number 4 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	6.32 ug/l	72552	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
3		Benzocycloheptatriene	142	C11H10	000264-09-5	90
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.88	17.7	ug/l	193262	2	6.86	545115	50.0
Propanoic acid, p...	9.55	5.9	ug/l	74517	3	10.12	628635	50.0
Butanoic acid, 1-...	9.98	6.0	ug/l	75014	3	10.12	628635	50.0
Naphthalene, 1-me...	14.70	6.3	ug/l	72552	4	12.08	574187	50.0