

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX020124\
 Data File : VX040064.D
 Acq On : 01 Feb 2024 12:30
 Operator : JC/MD
 Sample : P1284-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1247

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\82X013024W.M
 Title : SW846 8260

Signal : TIC: VX040064.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.373	207	211	223	rVB	13506	23098	2.87%	0.537%
2	2.526	230	236	243	rBV	5984	11437	1.42%	0.266%
3	4.233	507	516	531	rBV2	16897	47716	5.93%	1.109%
4	5.385	692	705	721	rBV2	58021	171378	21.30%	3.984%
5	5.550	721	732	746	rVV	95091	267958	33.31%	6.229%
6	5.958	789	799	815	rBV2	67707	178737	22.22%	4.155%
7	6.111	817	824	837	rVV4	3413	10295	1.28%	0.239%
8	6.763	919	931	942	rBV	150012	361855	44.98%	8.412%
9	7.208	999	1004	1017	rBV3	10025	27492	3.42%	0.639%
10	8.647	1233	1240	1249	rBV	319284	502232	62.43%	11.675%
11	8.769	1256	1260	1265	rBV4	4554	8353	1.04%	0.194%
12	10.055	1465	1471	1483	rBV	344898	485317	60.33%	11.282%
13	10.159	1483	1488	1498	rVB3	6347	12153	1.51%	0.283%
14	10.750	1580	1585	1597	rBV	40787	67444	8.38%	1.568%
15	11.079	1633	1639	1645	rBV	286597	365527	45.44%	8.497%
16	11.128	1645	1647	1656	rVB	15024	21439	2.66%	0.498%
17	11.280	1668	1672	1684	rVB2	13516	19419	2.41%	0.451%
18	11.390	1684	1690	1693	rBV5	7231	10838	1.35%	0.252%
19	11.573	1715	1720	1722	rBV2	19541	25959	3.23%	0.603%
20	11.603	1722	1725	1733	rVB	18104	27627	3.43%	0.642%
21	11.683	1733	1738	1746	rBV	719785	804466	100.00%	18.701%
22	11.988	1783	1788	1790	rBV2	45681	59840	7.44%	1.391%
23	12.018	1790	1793	1801	rVB	395461	502338	62.44%	11.678%
24	12.219	1820	1826	1836	rBV	100684	172185	21.40%	4.003%
25	12.305	1836	1840	1853	rVB	8593	24577	3.06%	0.571%
26	13.609	2047	2054	2060	rBV5	9509	15404	1.91%	0.358%
27	13.676	2061	2065	2070	rVB	31359	39206	4.87%	0.911%
28	14.030	2117	2123	2128	rBV	9040	12616	1.57%	0.293%
29	14.140	2136	2141	2148	rBV3	10934	14700	1.83%	0.342%
30	14.274	2158	2163	2168	rVB2	7465	10055	1.25%	0.234%

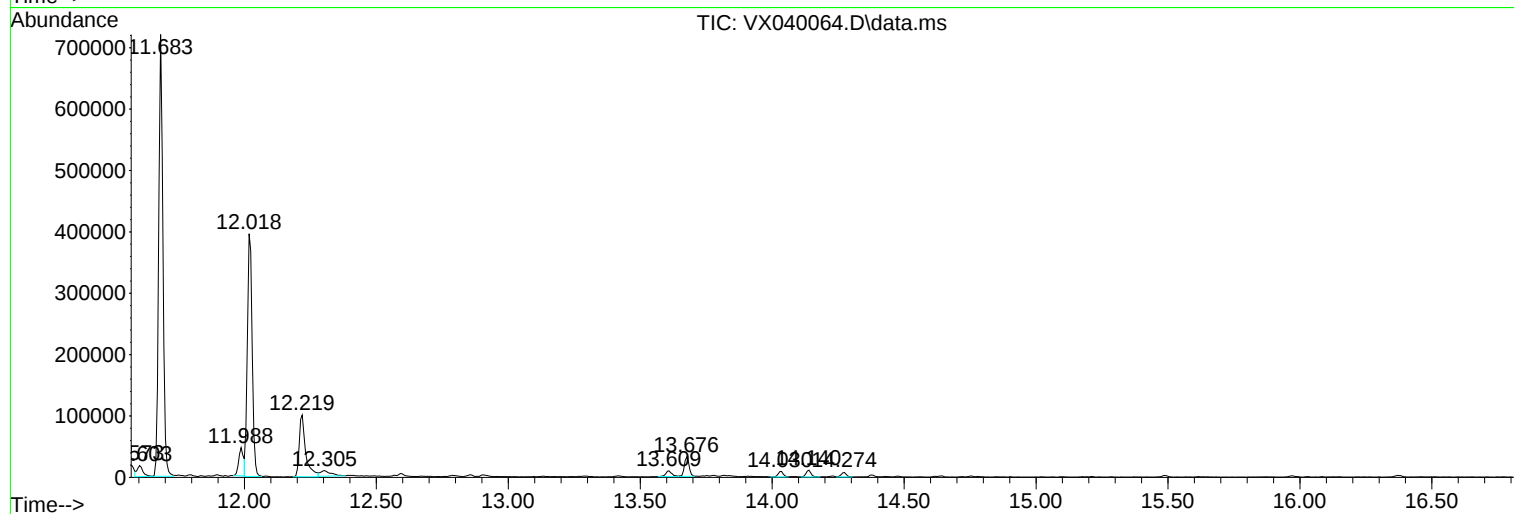
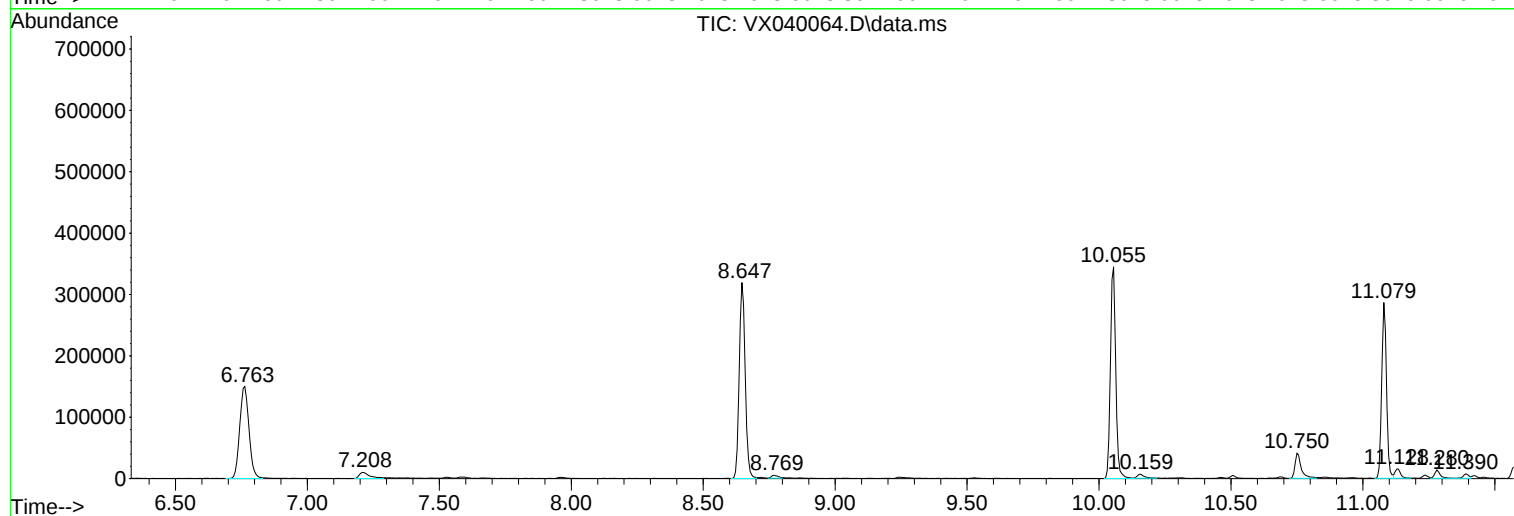
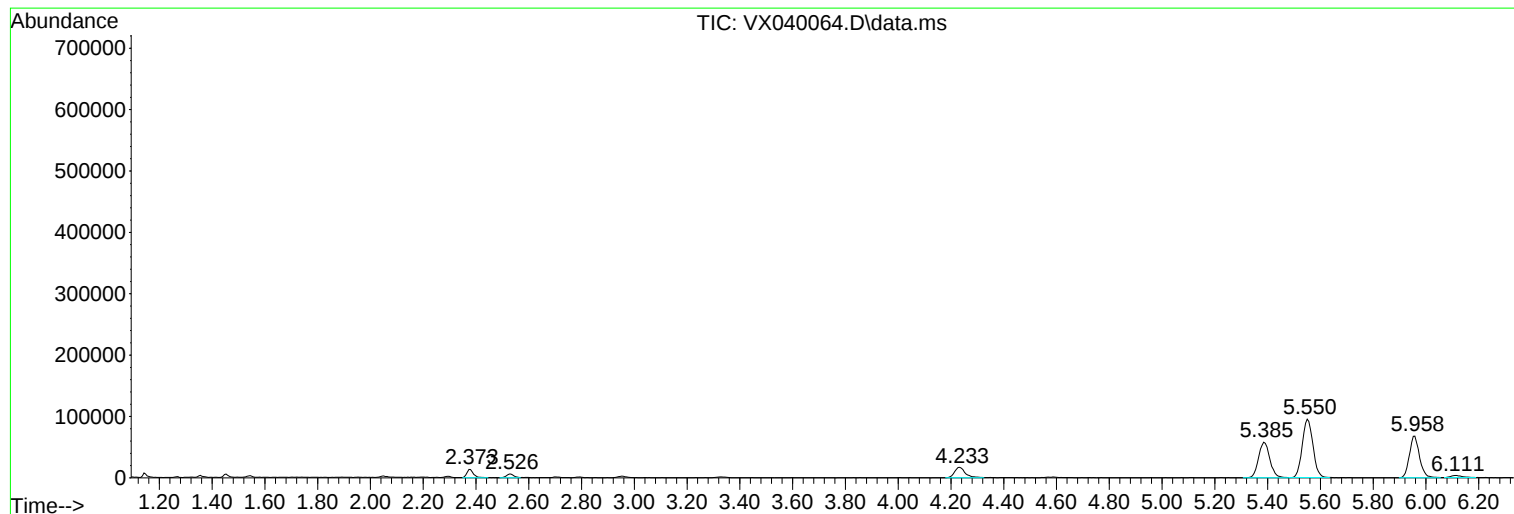
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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



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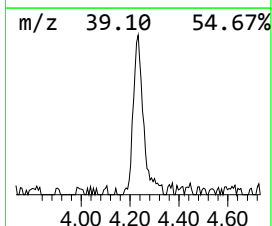
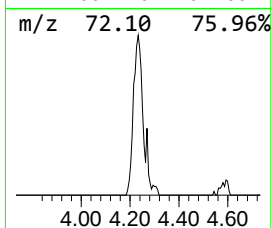
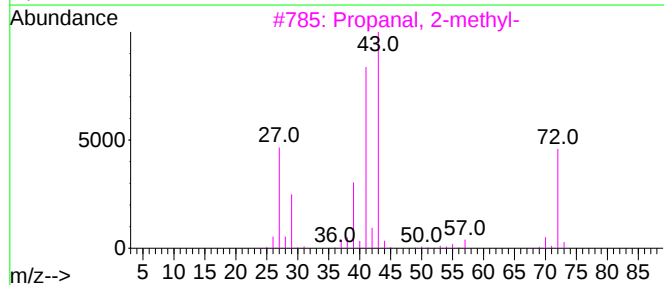
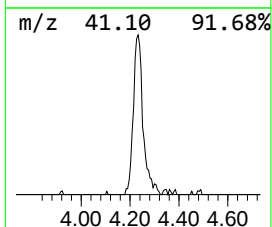
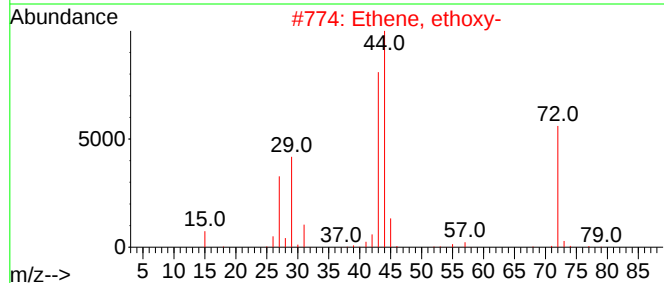
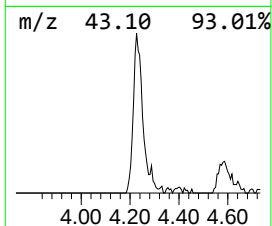
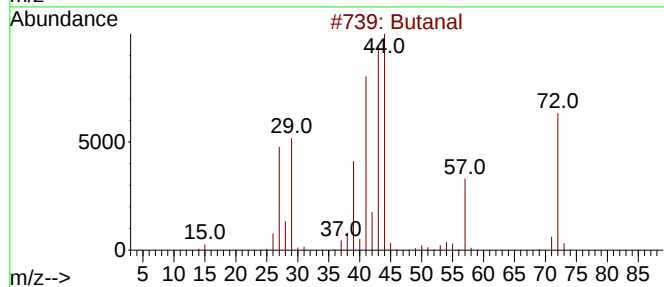
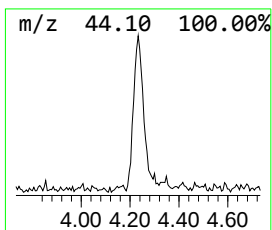
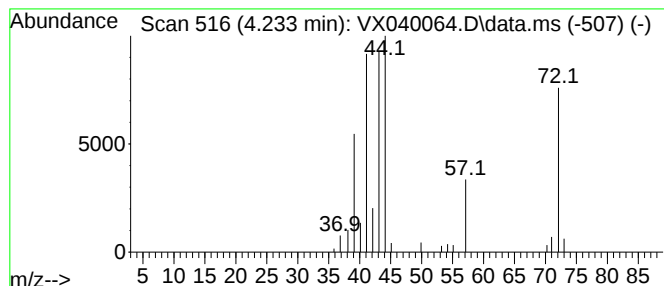
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	8.90 ug/l	47716	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			Propane	44	C3H8	000074-98-6	38
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	23



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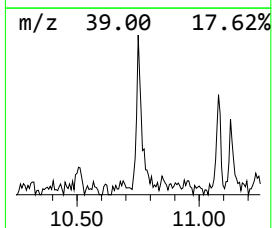
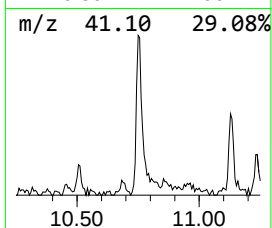
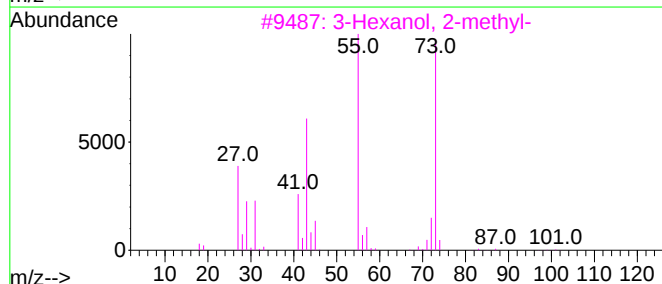
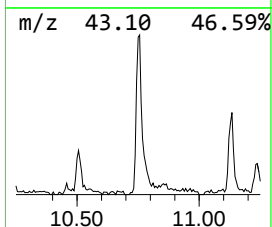
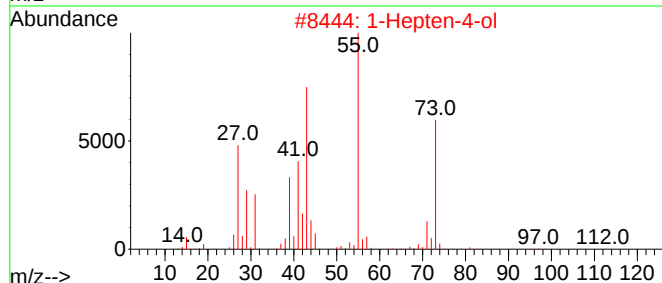
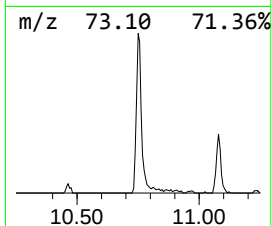
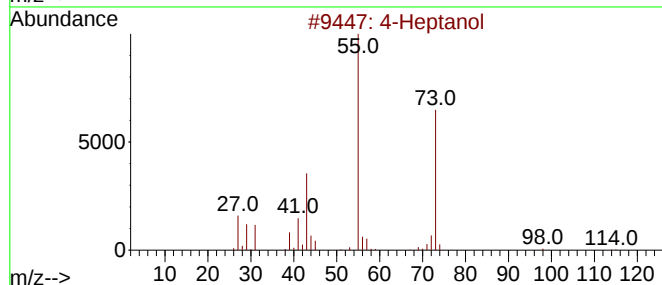
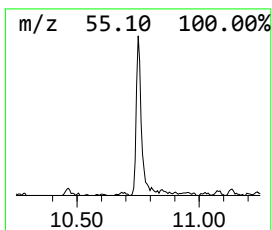
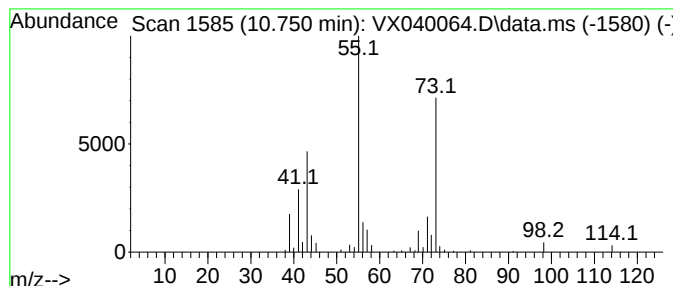
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
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Peak Number 2 4-Heptanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.750	6.95 ug/l	67444	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	50
2			1-Hepten-4-ol	114	C7H14O	003521-91-3	40
3			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	38
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
5			Oxalic acid, cyclobutyl heptyl e...	242	C13H22O4	1000309-69-8	38



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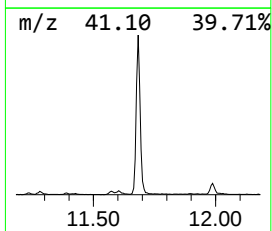
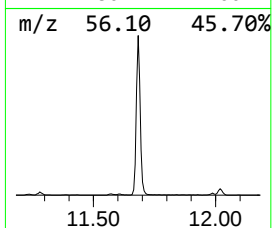
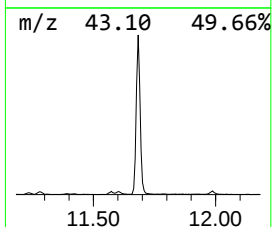
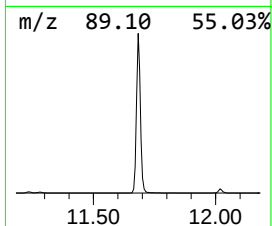
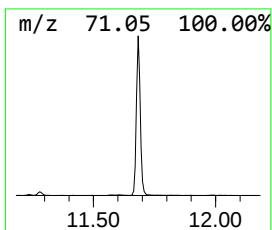
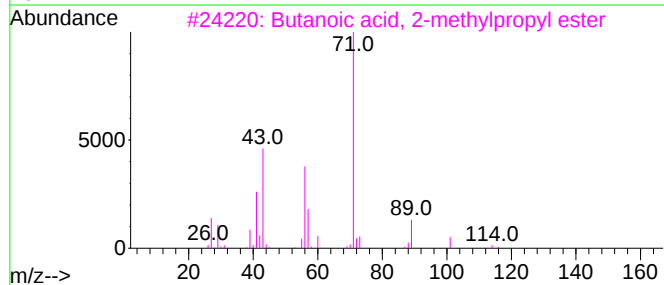
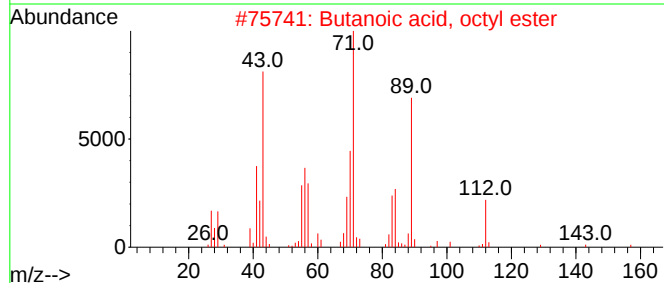
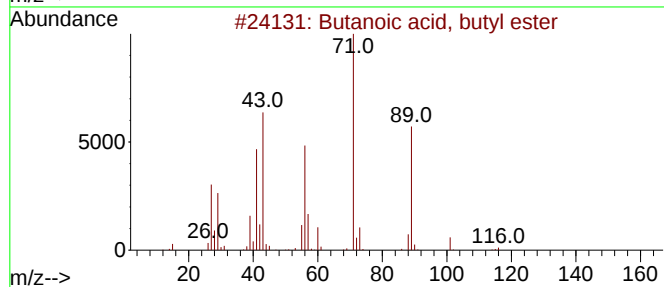
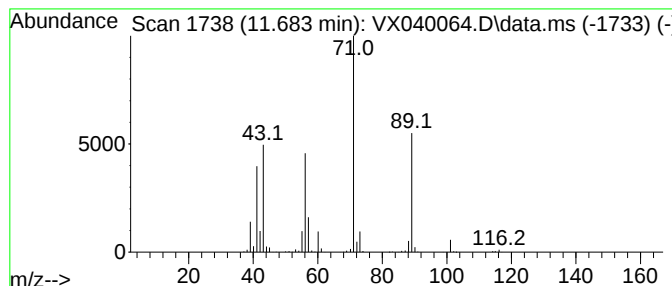
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Peak Number 3 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	80.07 ug/l	804466	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
3			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
4			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59



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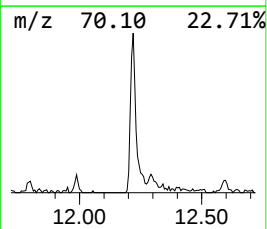
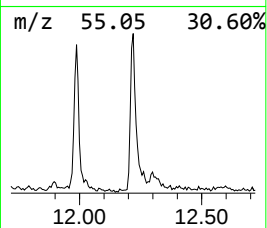
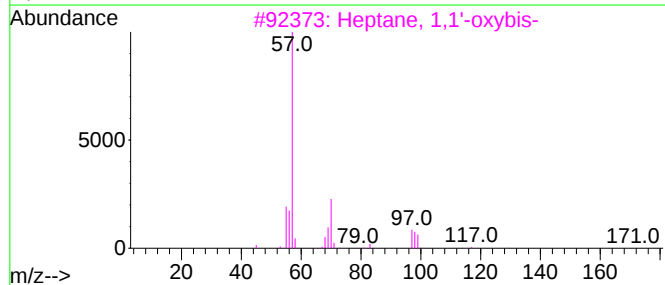
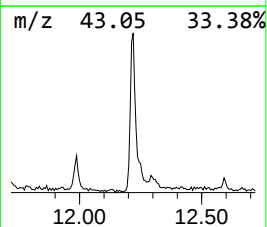
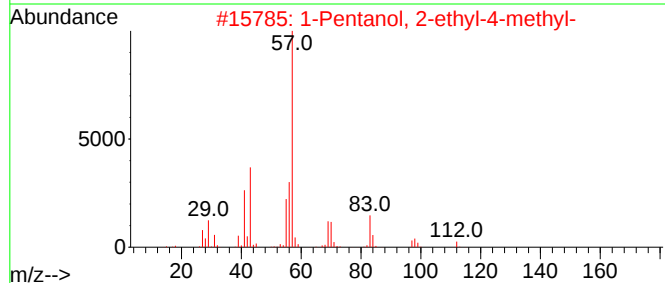
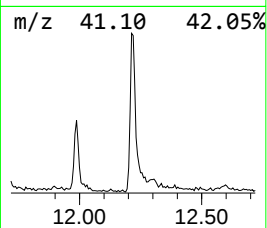
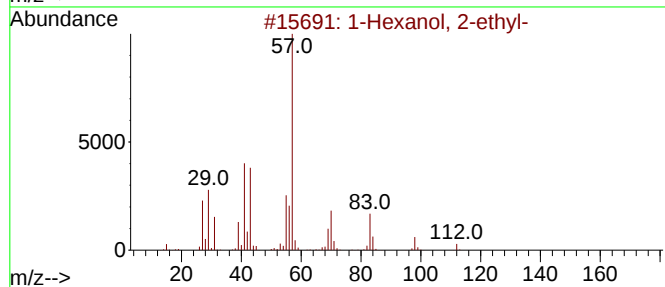
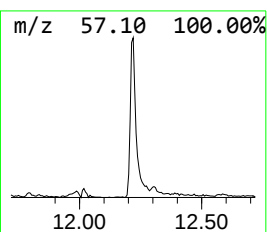
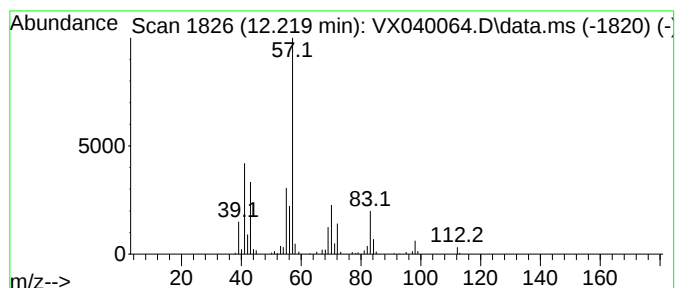
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	17.14 ug/l	172185	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	4.233	8.9	ug/l	47716	1	5.556	267958	50.0
4-Heptanol	10.750	7.0	ug/l	67444	3	10.055	485317	50.0
Butanoic acid, ...	11.683	80.1	ug/l	804466	4	12.024	502338	50.0
1-Hexanol, 2-et...	12.219	17.1	ug/l	172185	4	12.024	502338	50.0