

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040521\
 Data File : VU042931.D
 Acq On : 05 Apr 2021 15:25
 Operator : SY/MD
 Sample : M1903-02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 30791

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_U\Method\82U032421W.M
 Title : SW846 8260

Signal : TIC: VU042931.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	16	rVB2	13435	13672	1.98%	0.284%
2	1.588	70	77	87	rBV2	6302	9279	1.34%	0.193%
3	1.694	102	110	120	rBV	28841	38856	5.62%	0.809%
4	2.369	302	320	321	rBV4	4189	9479	1.37%	0.197%
5	2.552	368	377	391	rVB	6055	10152	1.47%	0.211%
6	2.646	394	406	429	rBV	14312	31747	4.59%	0.661%
7	3.224	569	586	592	rBV4	5004	12456	1.80%	0.259%
8	3.983	806	822	827	rBV7	3508	8115	1.17%	0.169%
9	4.456	953	969	989	rBV3	46343	118405	17.13%	2.464%
10	5.298	1216	1231	1244	rBV	113773	242029	35.01%	5.036%
11	5.382	1244	1257	1277	rVB	178876	369610	53.46%	7.691%
12	5.710	1342	1359	1376	rBV	124314	258944	37.45%	5.388%
13	6.256	1513	1529	1549	rBV	259879	488974	70.73%	10.174%
14	6.552	1610	1621	1641	rBV6	7434	23028	3.33%	0.479%
15	6.890	1713	1726	1741	rBV3	7268	14949	2.16%	0.311%
16	7.906	2028	2042	2056	rBV	406197	691362	100.00%	14.386%
17	7.977	2056	2064	2076	rVB3	13516	24089	3.48%	0.501%
18	8.462	2204	2215	2232	rBV3	7915	19479	2.82%	0.405%
19	9.423	2502	2514	2529	rBV	371438	617564	89.33%	12.850%
20	9.497	2529	2537	2557	rVB2	19247	40014	5.79%	0.833%
21	9.700	2589	2600	2611	rBV2	7060	10787	1.56%	0.224%
22	10.105	2716	2726	2732	rBV6	4684	8137	1.18%	0.169%
23	10.218	2752	2761	2778	rBV2	8686	18113	2.62%	0.377%
24	10.639	2879	2892	2903	rBV	318427	499586	72.26%	10.395%
25	10.693	2903	2909	2916	rVB2	10345	15339	2.22%	0.319%
26	10.880	2956	2967	2975	rBV5	3940	7354	1.06%	0.153%
27	11.240	3070	3079	3086	rBV2	12359	19689	2.85%	0.410%
28	11.282	3087	3092	3107	rVB7	5263	9331	1.35%	0.194%
29	11.382	3113	3123	3139	rBV	97951	146753	21.23%	3.054%
30	11.475	3144	3152	3161	rBV4	6528	10836	1.57%	0.225%
31	11.619	3186	3197	3215	rBV4	13498	25867	3.74%	0.538%
32	11.729	3216	3231	3237	rBV4	14804	25037	3.62%	0.521%
33	11.774	3237	3245	3250	rVV2	40093	64992	9.40%	1.352%
34	11.819	3250	3259	3279	rVB	403440	644335	93.20%	13.407%
35	12.070	3324	3337	3354	rBV	42630	89933	13.01%	1.871%
36	12.179	3363	3371	3385	rVB10	5687	12605	1.82%	0.262%

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37	12.317	3404	3414	3425	rVB2	8853	13852	2.00%	0.288%
38	12.558	3480	3489	3503	rVB7	5536	11445	1.66%	0.238%
39	12.806	3548	3566	3579	rBV7	5486	12812	1.85%	0.267%
40	12.886	3579	3591	3599	rBV4	10039	16547	2.39%	0.344%
41	13.070	3641	3648	3659	rVB2	8583	13788	1.99%	0.287%
42	13.455	3759	3768	3777	rBV7	4596	7746	1.12%	0.161%
43	13.883	3893	3901	3914	rVB7	6101	9295	1.34%	0.193%
44	14.095	3956	3967	3976	rVB	8497	12686	1.83%	0.264%
45	14.693	4140	4153	4162	rVB6	9420	18681	2.70%	0.389%
46	14.973	4230	4240	4249	rBV3	5101	8103	1.17%	0.169%
47	15.028	4249	4257	4266	rVB6	4807	7040	1.02%	0.146%
48	15.230	4306	4320	4331	rBV6	6165	15042	2.18%	0.313%
49	15.417	4369	4378	4389	rVB9	4625	7967	1.15%	0.166%

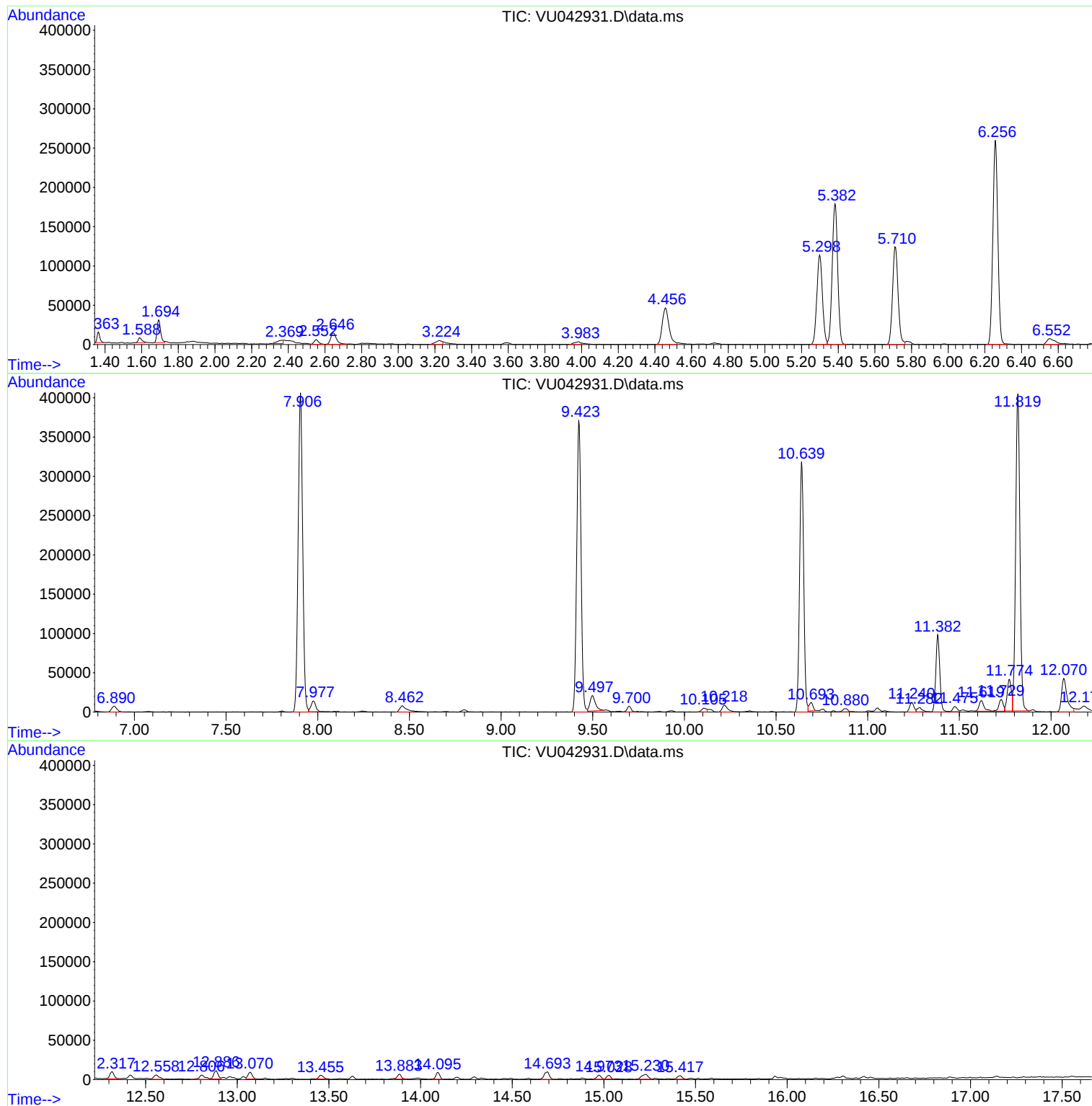
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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



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Instrument :
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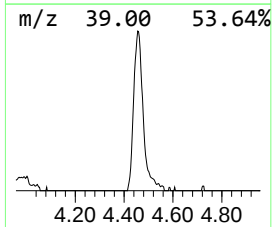
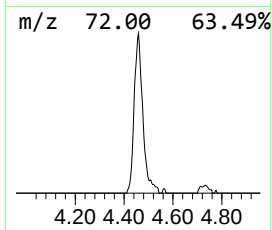
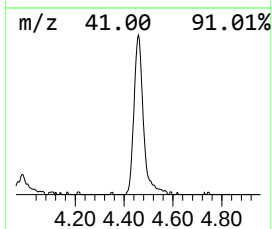
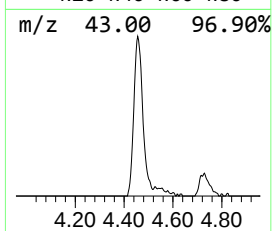
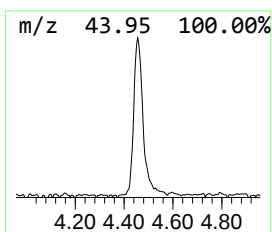
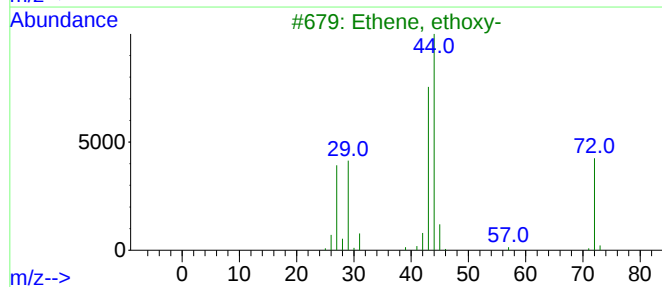
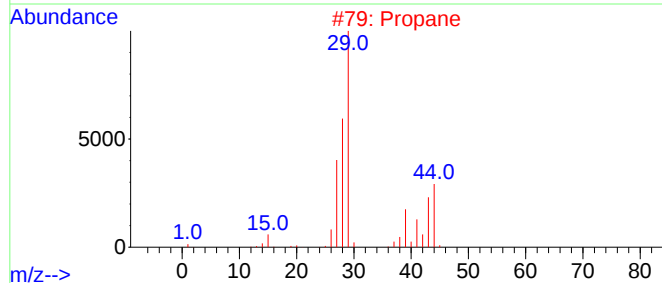
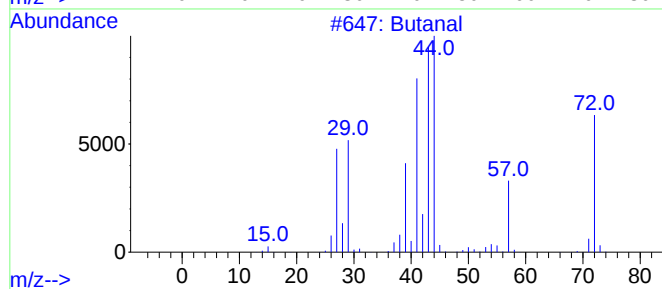
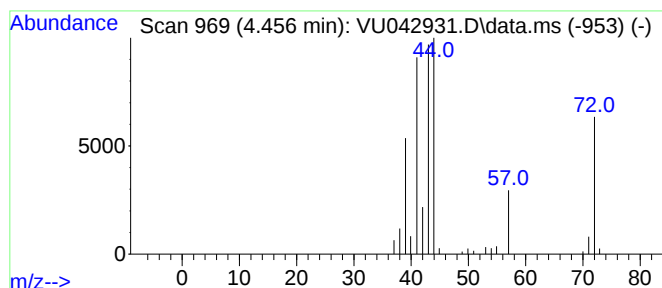
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U032421W.M
Quant Title : SW846 8260

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

Peak Number 2 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.456	16.02 ug/l	118405	Pentafluorobenzene	5.382

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propane	44	C3H8	000074-98-6	59
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	47
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5			Methacrolein	70	C4H6O	000078-85-3	27



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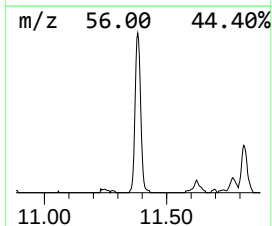
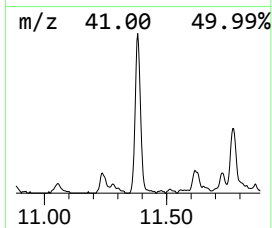
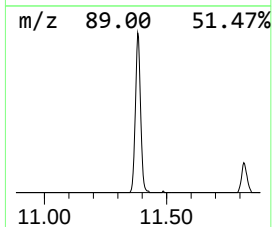
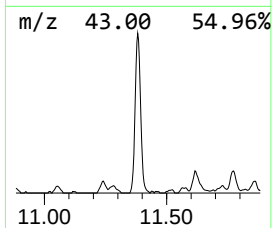
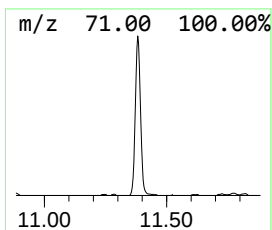
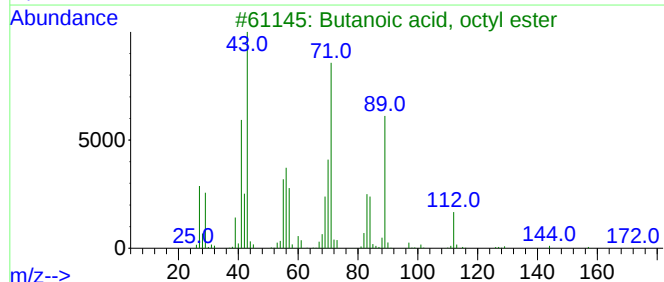
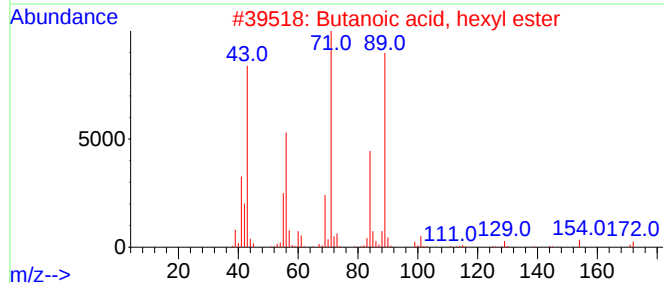
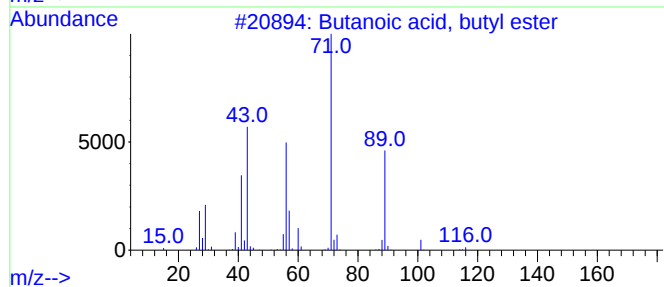
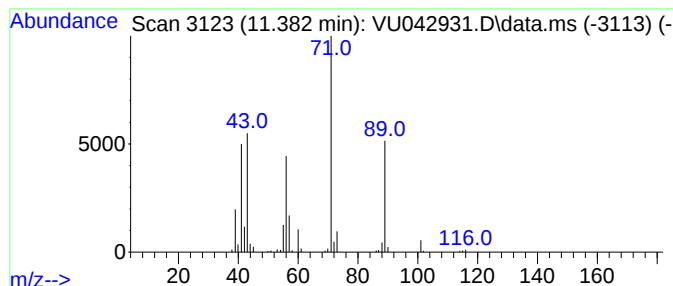
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.382	11.39 ug/l	146753	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	74
3			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
4			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	64
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	59



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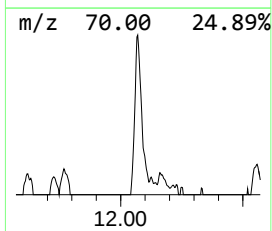
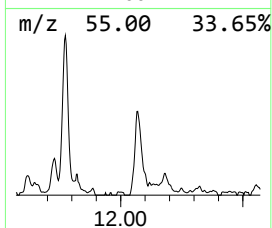
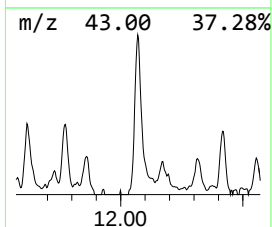
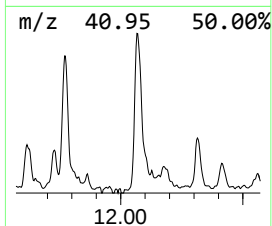
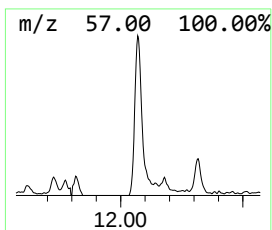
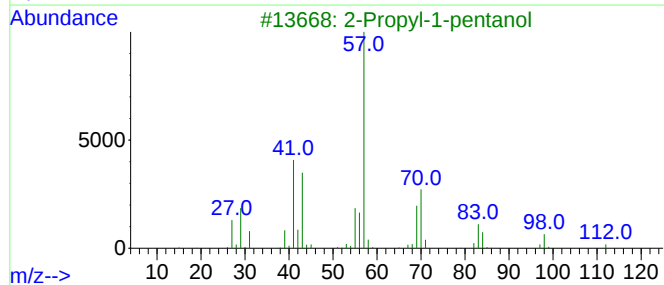
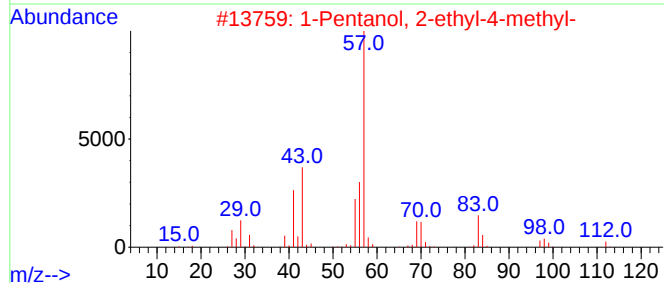
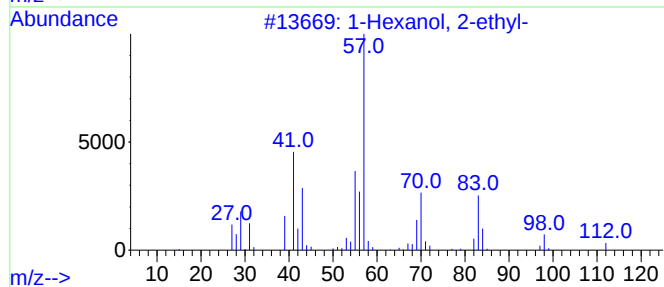
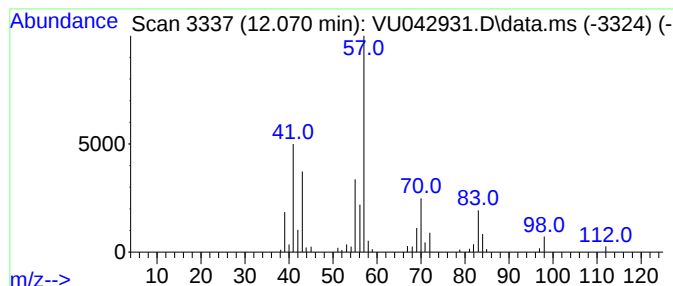
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.070	6.98 ug/l	89933	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	4.456	16.0	ug/l	118405	1	5.382	369610	50.0
Butanoic acid, ...	11.382	11.4	ug/l	146753	4	11.819	644335	50.0
1-Hexanol, 2-et...	12.070	7.0	ug/l	89933	4	11.819	644335	50.0