

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX111618\
 Data File : VX006055.D
 Acq On : 16 Nov 2018 17:35
 Operator : JC/MD
 Sample : J5965-07
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-7

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\82X110718W.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	1.300	20	24	27	rBV3	5972	6173	1.09%	0.155%
2	1.404	37	41	46	rVB	11475	11333	2.00%	0.284%
3	1.794	99	105	113	rBV	80221	115529	20.40%	2.893%
4	2.397	197	204	208	rBV	7148	14037	2.48%	0.351%
5	2.446	208	212	219	rVB	4291	7336	1.30%	0.184%
6	2.611	230	239	249	rBV	25230	46689	8.24%	1.169%
7	2.775	258	266	271	rBV	6611	12485	2.20%	0.313%
8	2.843	271	277	281	rBV2	20410	42680	7.53%	1.069%
9	2.891	281	285	290	rVB	18493	32601	5.76%	0.816%
10	3.056	302	312	322	rVV	24677	57872	10.22%	1.449%
11	3.172	322	331	344	rVB2	37409	104183	18.39%	2.609%
12	4.397	523	532	543	rVB2	12993	35109	6.20%	0.879%
13	4.525	543	553	565	rVB8	2634	9340	1.65%	0.234%
14	4.757	577	591	601	rBV	5429	18266	3.22%	0.457%
15	5.275	663	676	685	rVB6	3164	13655	2.41%	0.342%
16	5.507	700	714	722	rBV	77837	223124	39.39%	5.587%
17	5.665	731	740	766	rVB2	135662	393726	69.51%	9.859%
18	5.933	774	784	795	rVB5	6041	20708	3.66%	0.519%
19	6.068	795	806	814	rVV2	87321	221121	39.04%	5.537%
20	6.141	814	818	831	rVV2	16056	46493	8.21%	1.164%
21	6.263	831	838	845	rVV4	6305	20435	3.61%	0.512%
22	6.354	845	853	861	rVV3	7719	23075	4.07%	0.578%
23	6.458	861	870	880	rVB3	9549	26525	4.68%	0.664%
24	6.860	926	936	946	rBV2	182937	438332	77.38%	10.976%
25	7.256	994	1001	1009	rBV2	10060	21822	3.85%	0.546%
26	7.451	1024	1033	1042	rVB7	5706	17012	3.00%	0.426%
27	8.177	1147	1152	1156	rBV3	2832	5907	1.04%	0.148%
28	8.573	1210	1217	1225	rVB4	3251	6778	1.20%	0.170%
29	8.713	1234	1240	1257	rVB	361489	566449	100.00%	14.184%
30	9.219	1318	1323	1331	rVB2	7172	11759	2.08%	0.294%
31	10.116	1464	1470	1483	rBV	379033	531780	93.88%	13.316%
32	11.018	1612	1618	1623	rBV	5305	6897	1.22%	0.173%
33	11.140	1632	1638	1655	rVB	284314	369713	65.27%	9.257%
34	12.079	1786	1792	1799	rBV	369276	457628	80.79%	11.459%

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35	12.298	1825	1828	1834	rVV	12475	16391	2.89%	0.410%
36	12.975	1934	1939	1943	rBV	5030	6008	1.06%	0.150%
37	13.225	1977	1980	1989	rVB	5556	7445	1.31%	0.186%
38	13.353	1997	2001	2005	rVB	16940	21478	3.79%	0.538%
39	14.401	2170	2173	2180	rVB3	3421	5768	1.02%	0.144%

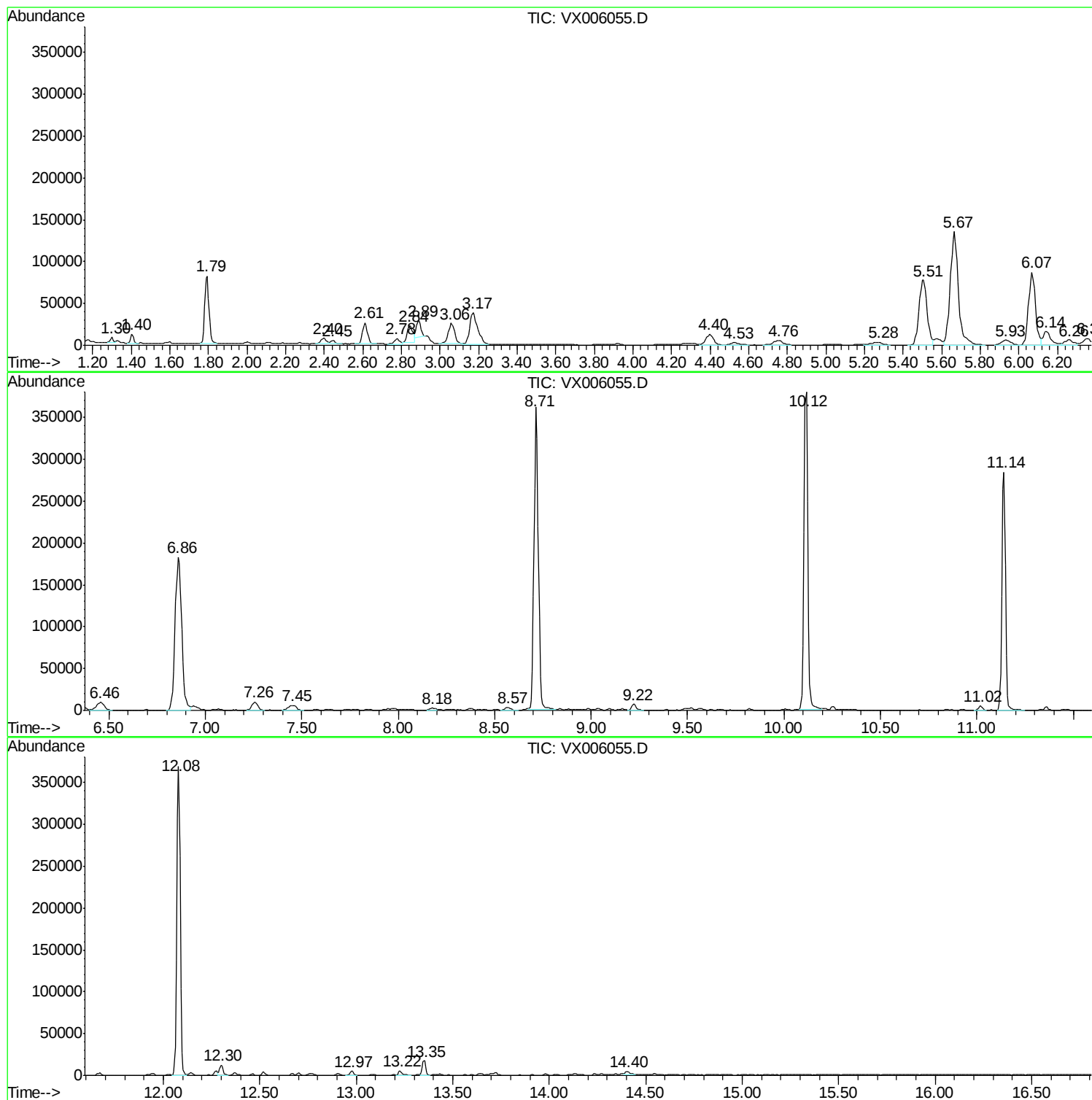
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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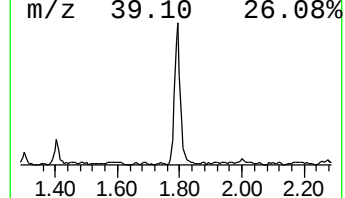
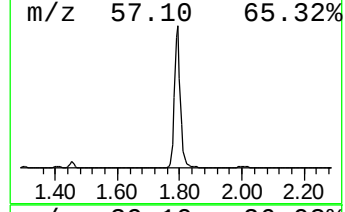
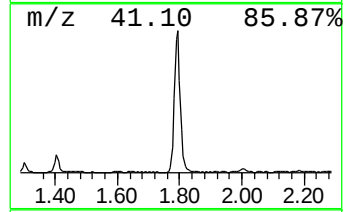
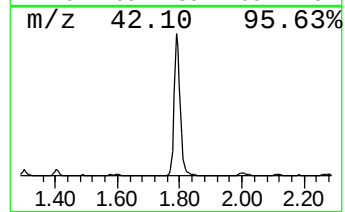
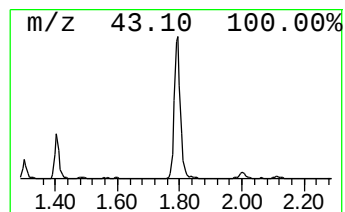
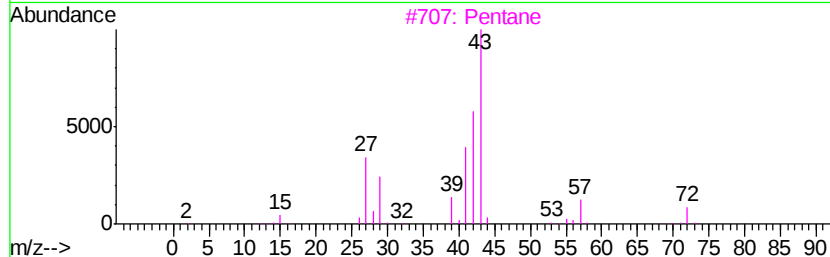
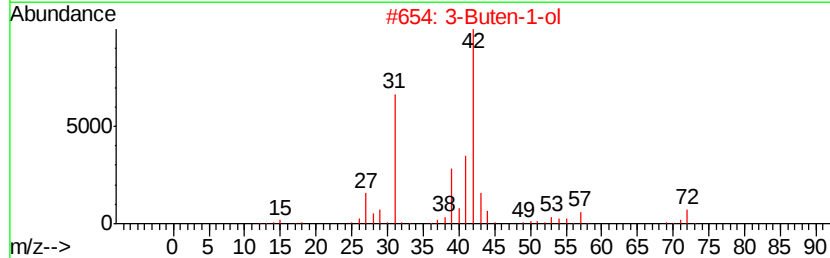
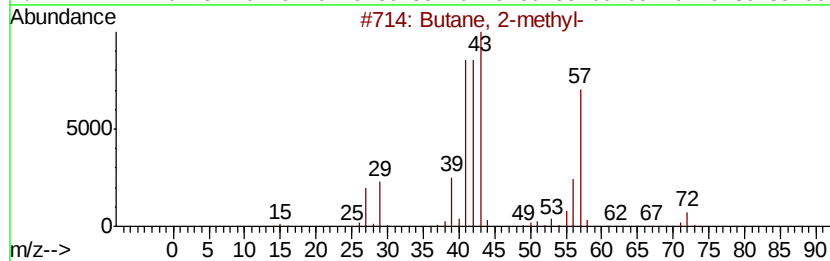
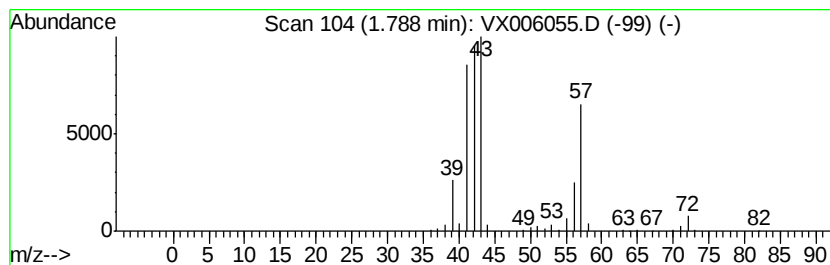
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	14.67 ug/l	115529	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2		3-Buten-1-ol	72	C4H8O	000627-27-0	47
3		Pentane	72	C5H12	000109-66-0	45
4		Methane, isocyanato-	57	C2H3NO	000624-83-9	9
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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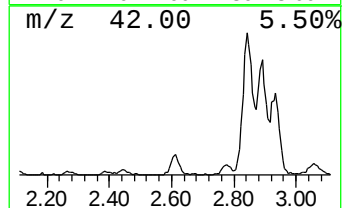
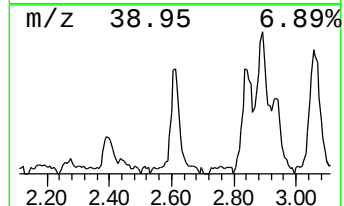
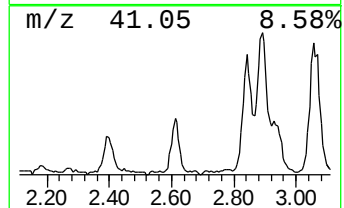
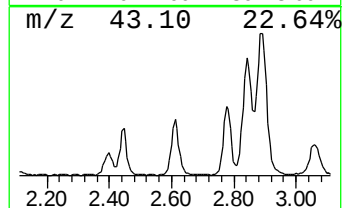
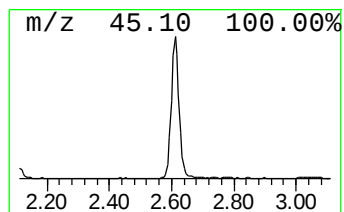
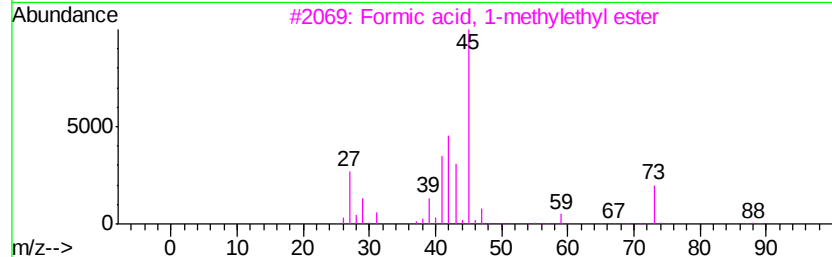
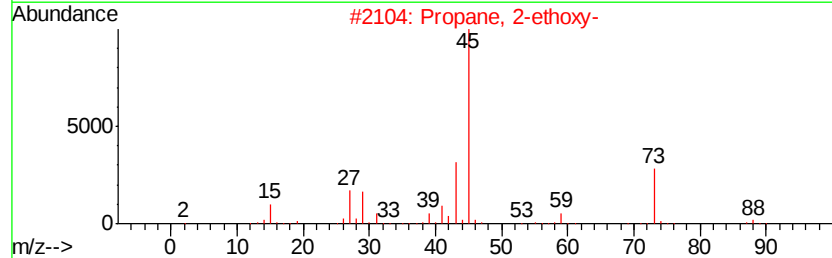
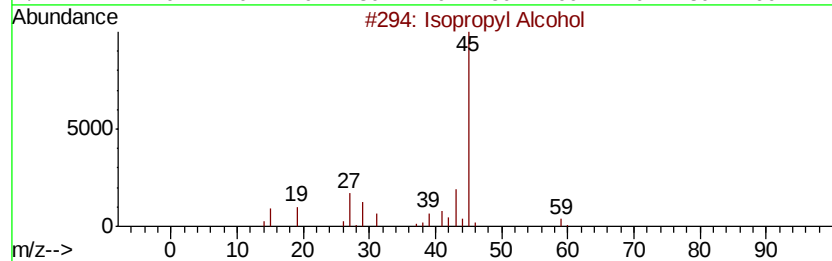
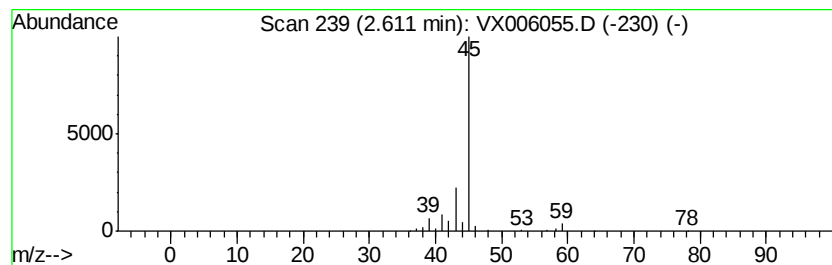
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Peak Number 2 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.61	5.93 ug/l	46689	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
3		Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
4		(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9
5		(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	9



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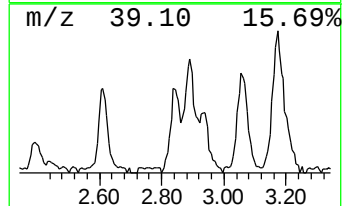
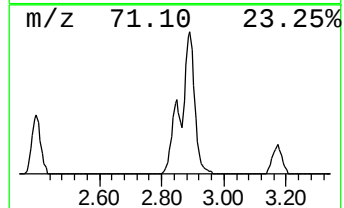
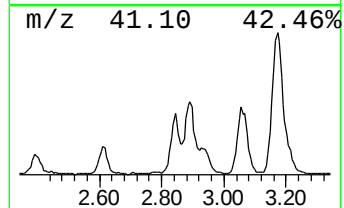
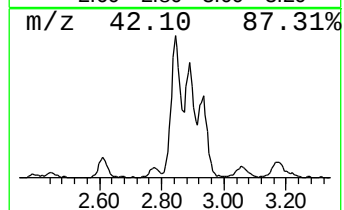
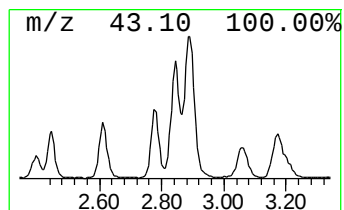
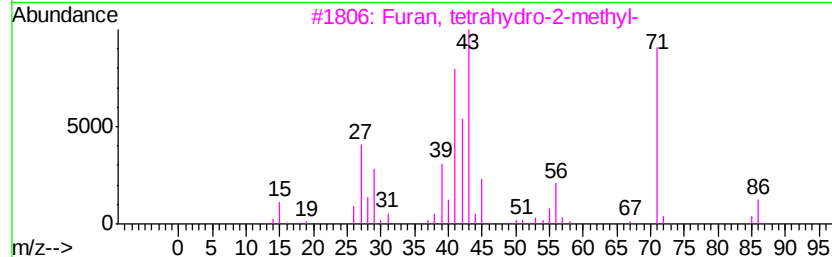
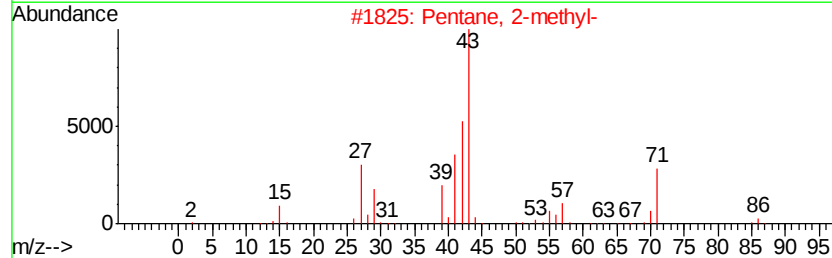
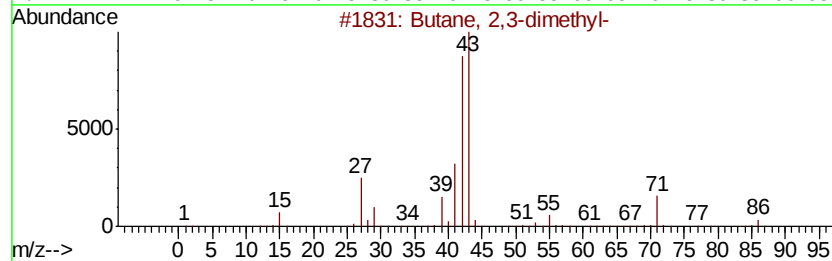
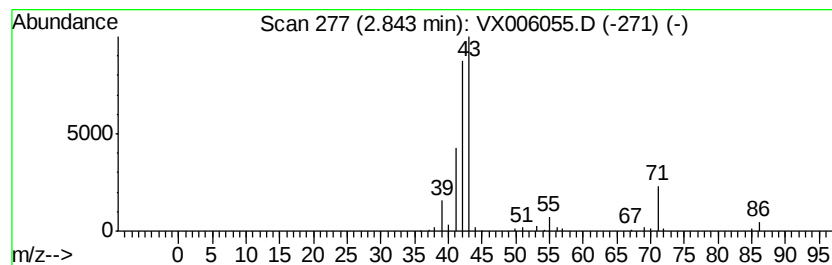
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Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	5.42 ug/l	42680	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	28
3		Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	22
4		Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12
5		Pyrrolidine	71	C4H9N	000123-75-1	9



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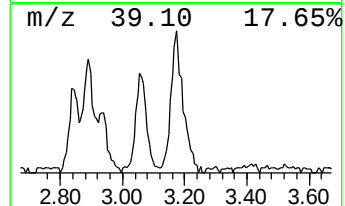
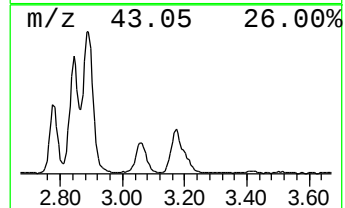
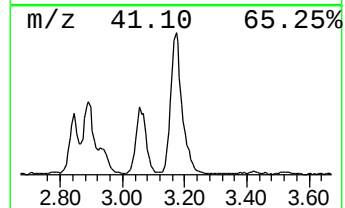
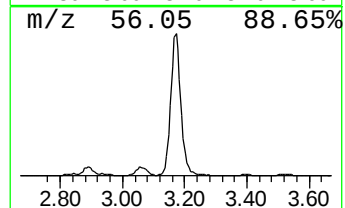
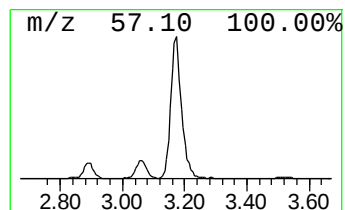
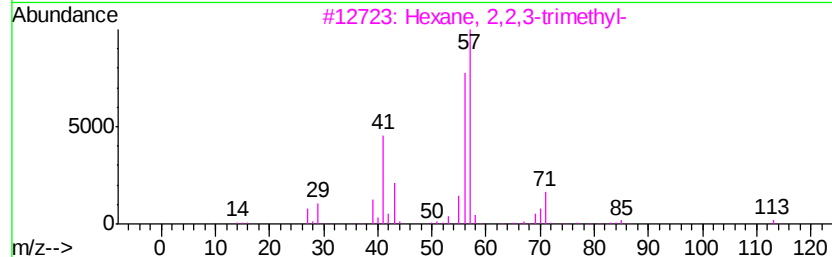
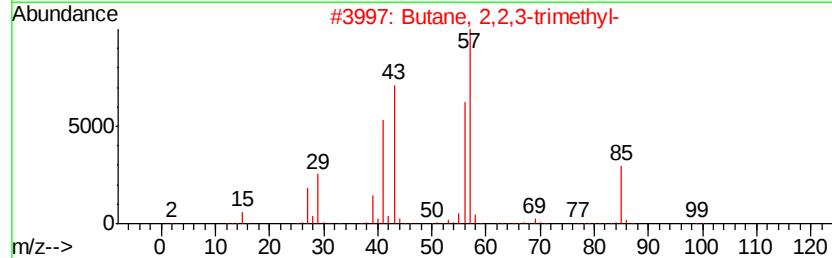
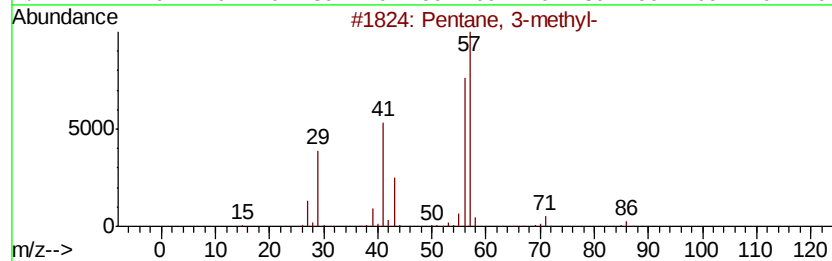
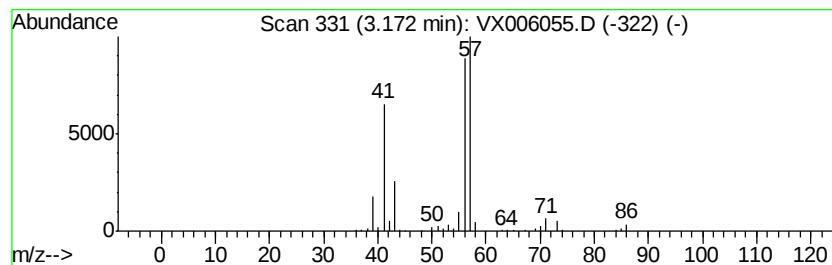
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Peak Number 4 Pentane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	13.23 ug/l	104183	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
3		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
4		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56
5		3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	1.79	14.7	ug/l	115529	1	5.67	393726	50.0
Isopropyl Alcohol	2.61	5.9	ug/l	46689	1	5.67	393726	50.0
Butane, 2,3-dimet...	2.84	5.4	ug/l	42680	1	5.67	393726	50.0
Pentane, 3-methyl-	3.17	13.2	ug/l	104183	1	5.67	393726	50.0