

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU112320\
 Data File : VU041390.D
 Acq On : 23 Nov 2020 16:09
 Operator : SY/MD
 Sample : L4849-16
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 H4423

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

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_U\METHOD\SOMUTR112320WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	35	43	56	rBV2	14326	36450	9.89%	1.273%
2	1.607	72	83	94	rBV3	109966	131510	35.67%	4.592%
3	1.919	173	180	194	rVB	21275	30486	8.27%	1.065%
4	2.002	197	206	220	rVB2	28886	40561	11.00%	1.416%
5	2.575	374	384	397	rBV	42504	68661	18.62%	2.397%
6	3.054	523	533	543	rBV5	2470	4272	1.16%	0.149%
7	3.150	549	563	576	rBV4	6211	13586	3.69%	0.474%
8	3.369	613	631	650	rBV2	180089	368674	100.00%	12.873%
9	3.887	777	792	809	rBV	17905	42261	11.46%	1.476%
10	4.549	982	998	1010	rBV6	3742	8326	2.26%	0.291%
11	4.639	1011	1026	1055	rBV	50671	135644	36.79%	4.736%
12	4.819	1066	1082	1110	rBV	107768	235811	63.96%	8.234%
13	5.079	1147	1163	1181	rVB2	49636	108553	29.44%	3.790%
14	5.739	1348	1368	1379	rBV4	87175	235481	63.87%	8.222%
15	6.263	1517	1531	1545	rBV	71146	132459	35.93%	4.625%
16	6.703	1654	1668	1684	rBV	57842	112376	30.48%	3.924%
17	7.571	1928	1938	1956	rVB2	28674	49674	13.47%	1.735%
18	7.906	2029	2042	2056	rBV	103577	175880	47.71%	6.141%
19	8.185	2119	2129	2139	rBV2	19242	31263	8.48%	1.092%
20	8.639	2257	2270	2299	rBV	163916	301738	81.84%	10.536%
21	9.420	2501	2513	2532	rBV	110799	184680	50.09%	6.449%
22	10.754	2916	2928	2942	rBV2	49853	79824	21.65%	2.787%
23	10.893	2961	2971	2982	rBV2	5150	7680	2.08%	0.268%
24	11.809	3245	3256	3271	rBV	97131	154820	41.99%	5.406%
25	12.188	3359	3374	3389	rBV	108998	173192	46.98%	6.047%

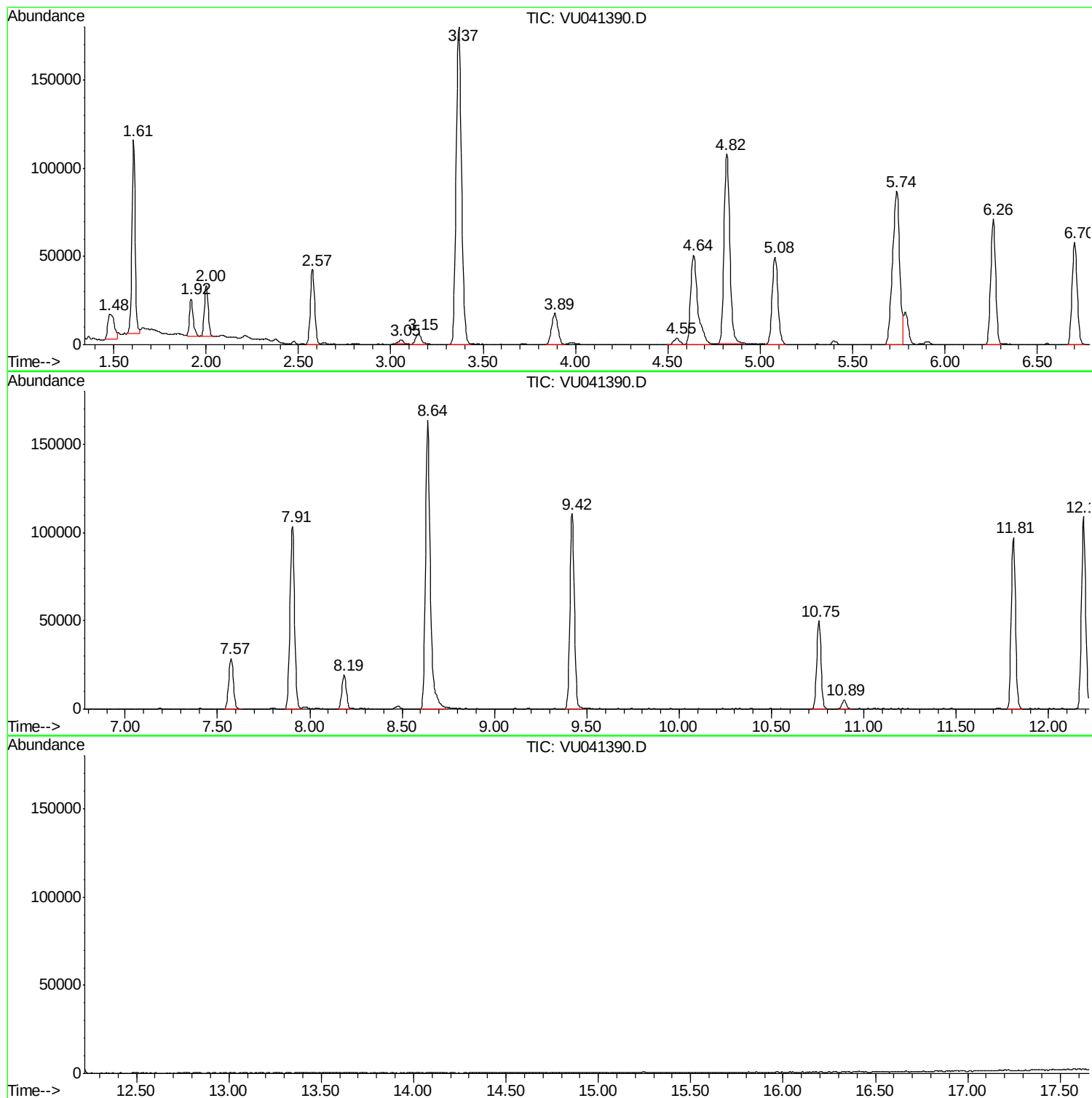
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Quant Title : TRACE VOA SOM01.0

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



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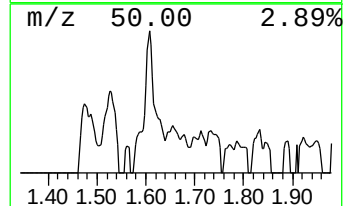
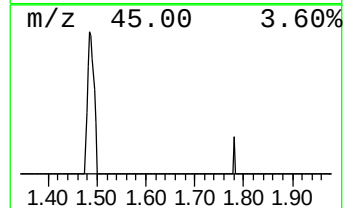
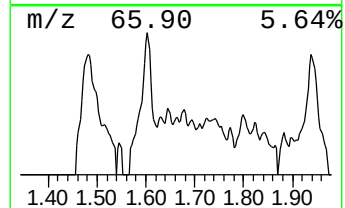
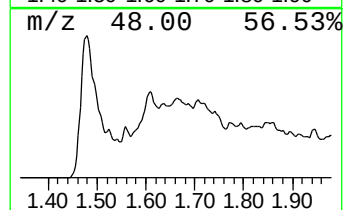
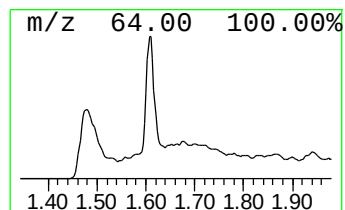
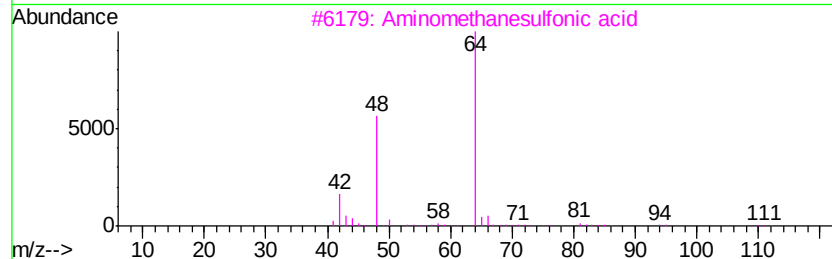
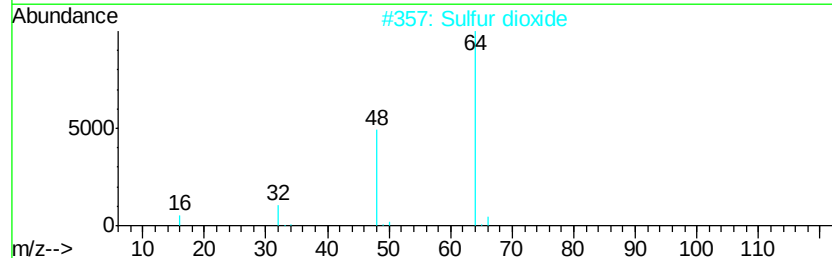
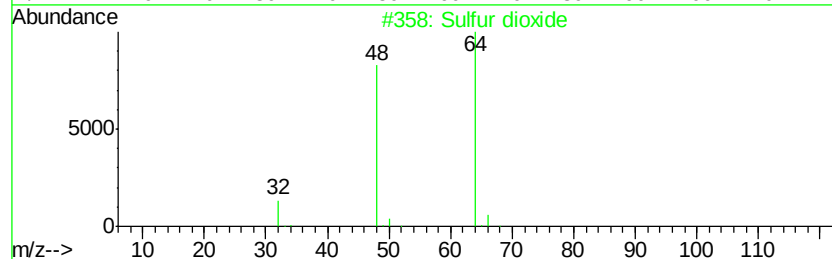
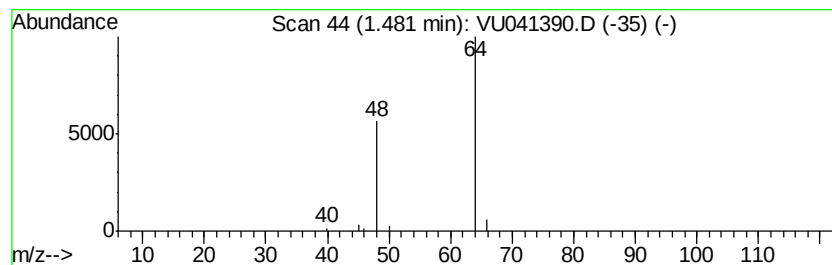
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR112320WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	1.38 ug/L	36450	1,4-Difluorobenzene	6.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide		64	O2S	007446-09-5	74
2	Sulfur dioxide		64	O2S	007446-09-5	74
3	Aminomethanesulfonic acid		111	CH5NO3S	013881-91-9	64
4	L-Alanine, 3-sulfo-		169	C3H7NO5S	000498-40-8	9
5	Aminomethanesulfonic acid		111	CH5NO3S	013881-91-9	9



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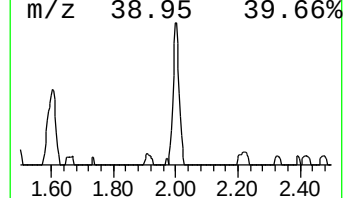
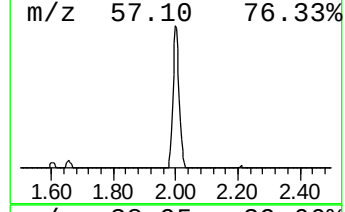
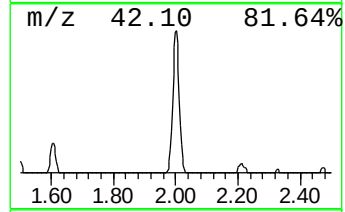
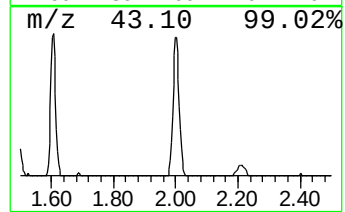
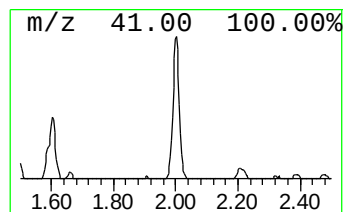
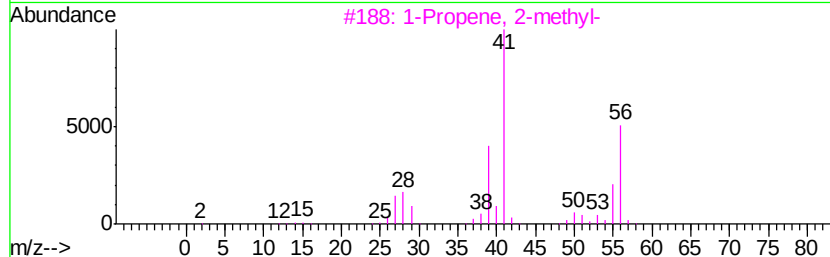
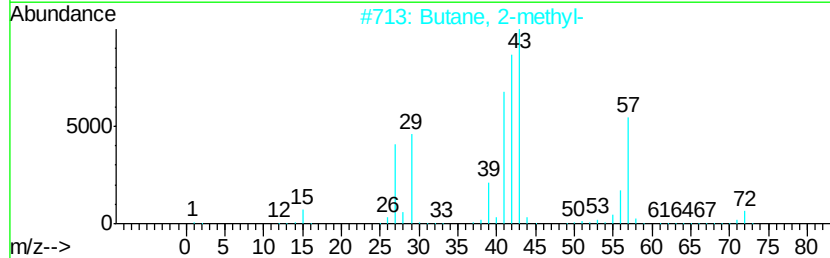
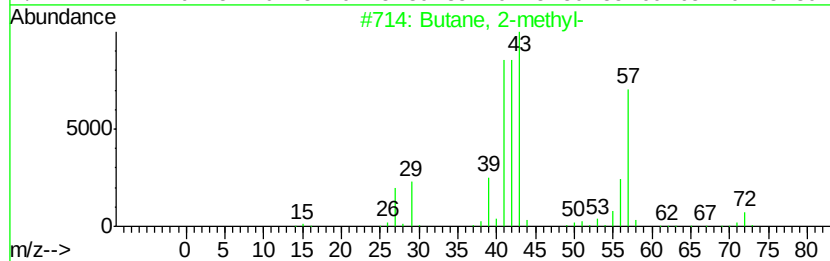
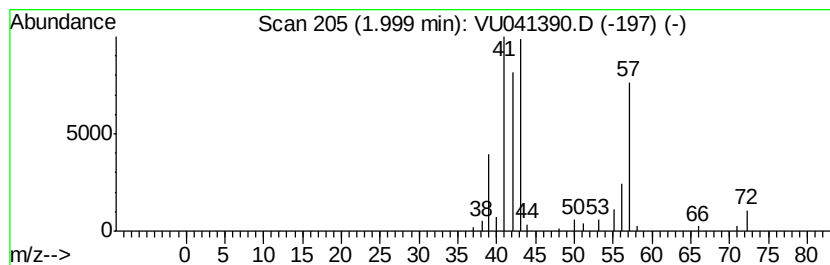
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	1.53 ug/L	40561	1,4-Difluorobenzene	6.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	81
2			Butane, 2-methyl-	72	C5H12	000078-78-4	64
3			1-Propene, 2-methyl-	56	C4H8	000115-11-7	27
4			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	25
5			Propane, 2-methyl-1-nitro-	103	C4H9NO2	000625-74-1	17



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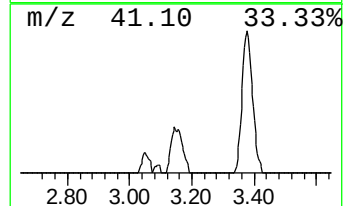
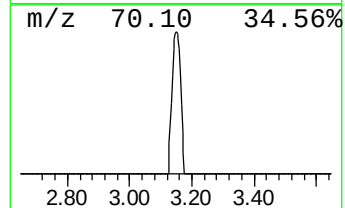
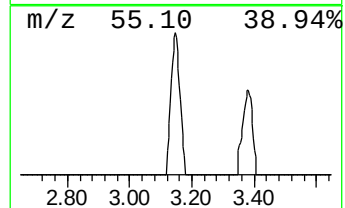
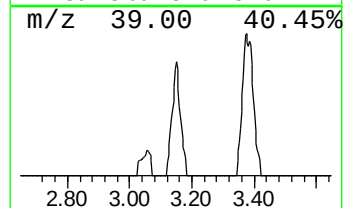
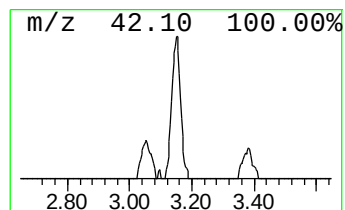
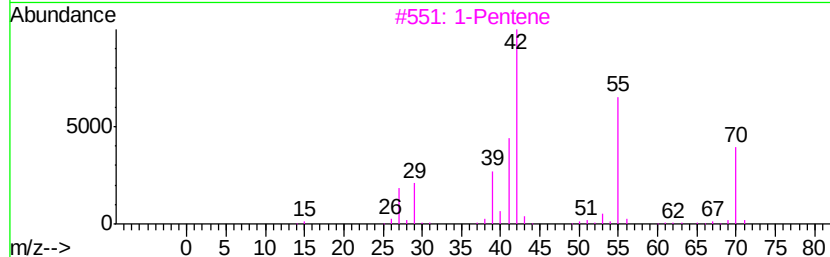
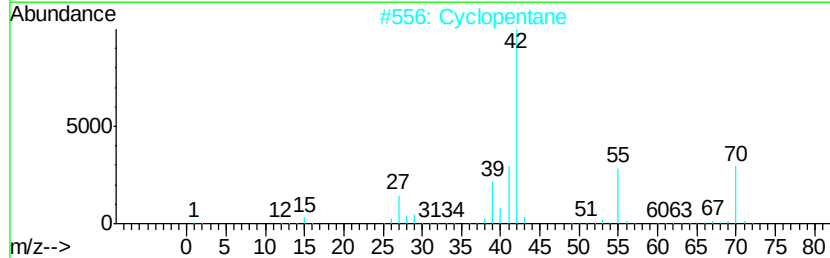
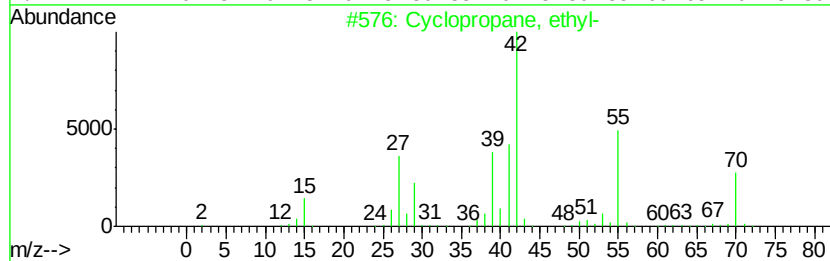
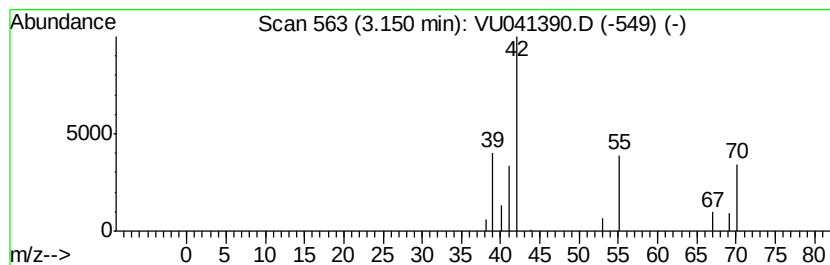
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Peak Number 3 (DEL) Alkane: Cyclic3.15 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	0.51 ug/L	13586	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	64
2		Cyclopentane	70	C5H10	000287-92-3	9
3		1-Pentene	70	C5H10	000109-67-1	9
4		1-Pentene	70	C5H10	000109-67-1	9
5		Cyclopropane, ethyl-	70	C5H10	001191-96-4	9



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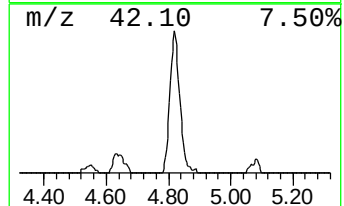
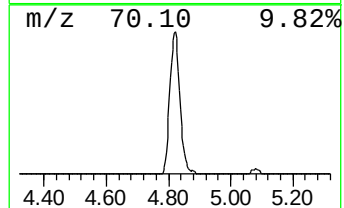
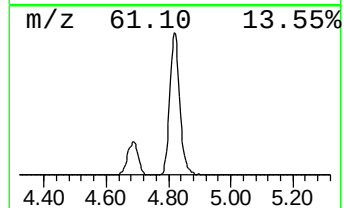
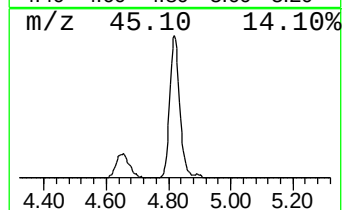
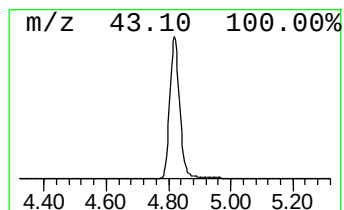
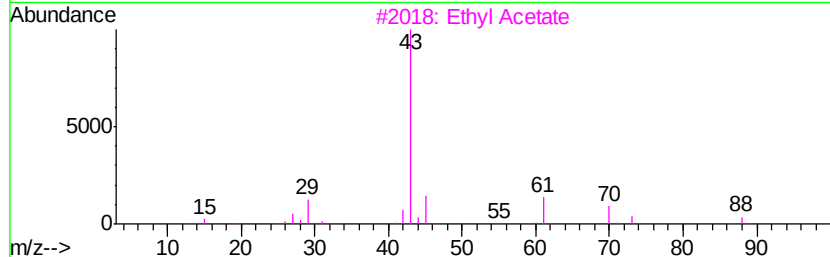
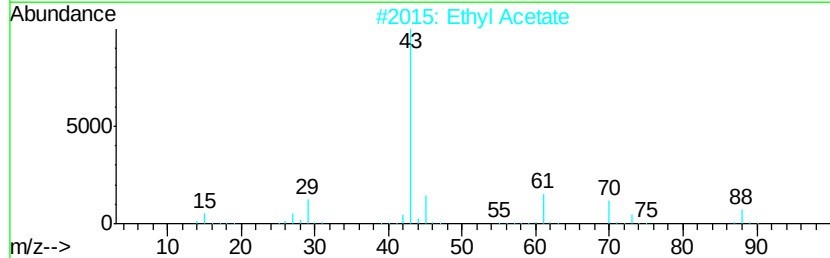
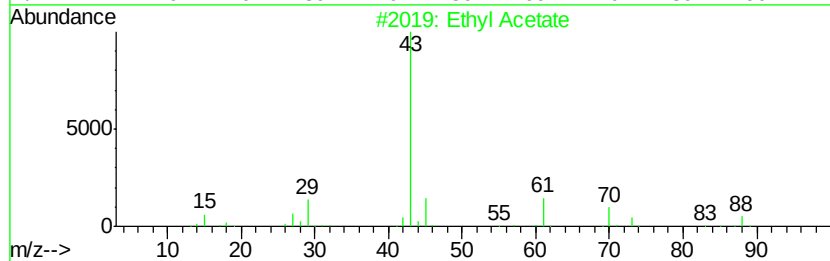
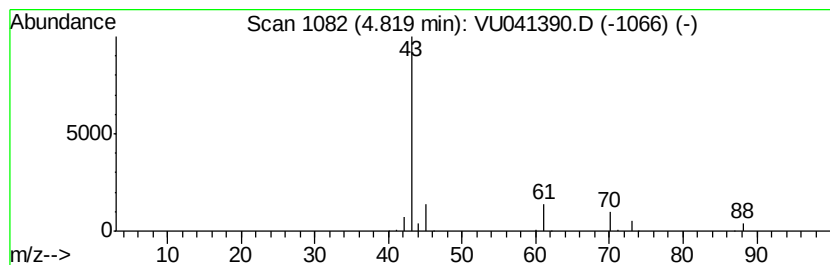
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	8.90 ug/L	235811	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	90
2		Ethyl Acetate	88	C4H8O2	000141-78-6	90
3		Ethyl Acetate	88	C4H8O2	000141-78-6	86
4		Ethyl Acetate	88	C4H8O2	000141-78-6	86
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.48	1.4	ug/L	36450	1	6.26	132459	5.0
(DEL) Alkane: Str...	2.00	1.5	ug/L	40561	1	6.26	132459	5.0
(DEL) Alkane: Cyc...	3.15	0.5	ug/L	13586	1	6.26	132459	5.0
Ethyl Acetate	4.82	8.9	ug/L	235811	1	6.26	132459	5.0