

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
 Data File : VU039023.D
 Acq On : 22 Jun 2020 22:46
 Operator : SY/MD
 Sample : L3061-12
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXJ9

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\SOMUTR062220WMA.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	1.482	35	44	77	rBV	2392599	4974721	100.00%	29.419%
2	1.610	79	84	160	rVB2	374942	1561232	31.38%	9.233%
3	1.929	176	183	194	rVB	134964	173711	3.49%	1.027%
4	2.588	374	388	404	rBV	278242	461768	9.28%	2.731%
5	2.819	444	460	484	rBV3	36229	108415	2.18%	0.641%
6	4.668	1019	1035	1076	rBV2	244959	653761	13.14%	3.866%
7	5.099	1148	1169	1190	rBV	225391	503843	10.13%	2.980%
8	5.758	1351	1374	1404	rBV2	469371	1214855	24.42%	7.184%
9	6.279	1521	1536	1554	rBV	325792	621901	12.50%	3.678%
10	6.719	1659	1673	1691	rBV	295265	570078	11.46%	3.371%
11	6.944	1729	1743	1758	rVB2	47798	94097	1.89%	0.556%
12	7.591	1932	1944	1959	rVB	115355	201959	4.06%	1.194%
13	7.922	2029	2047	2062	rBV	522910	900755	18.11%	5.327%
14	8.202	2121	2134	2148	rBV2	78909	133706	2.69%	0.791%
15	8.655	2258	2275	2308	rBV	754222	1394277	28.03%	8.245%
16	9.436	2500	2518	2539	rBV	485458	808518	16.25%	4.781%
17	10.771	2919	2933	2950	rBV	233913	371649	7.47%	2.198%
18	11.044	3005	3018	3037	rBV	303908	535151	10.76%	3.165%
19	11.822	3246	3260	3277	rBV	488153	764927	15.38%	4.524%
20	12.205	3364	3379	3394	rBV	535990	860548	17.30%	5.089%

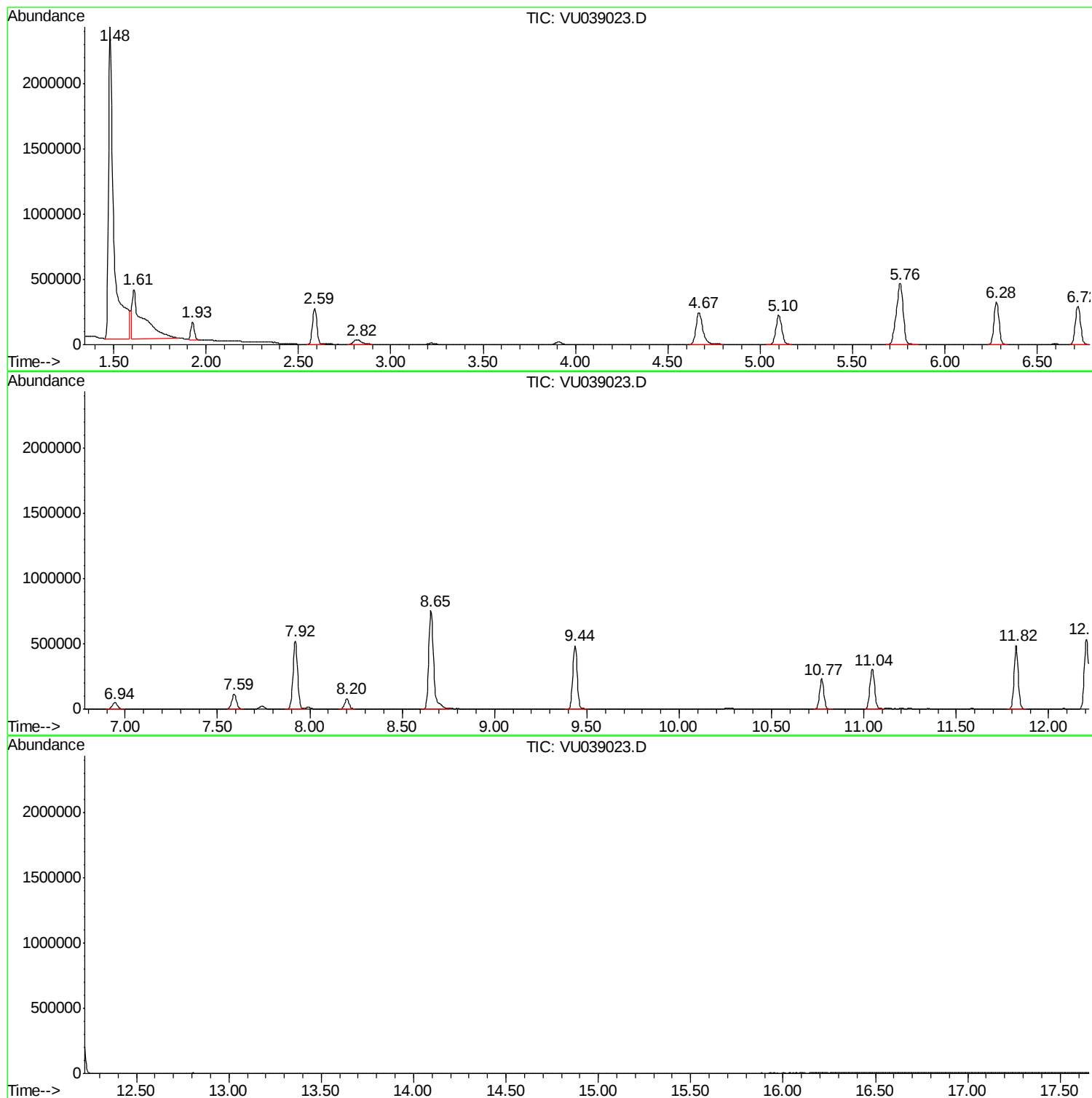
Sum of corrected areas: 16909872

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

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



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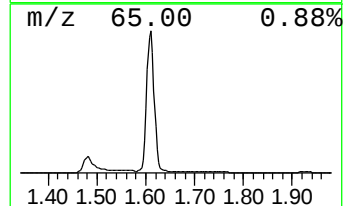
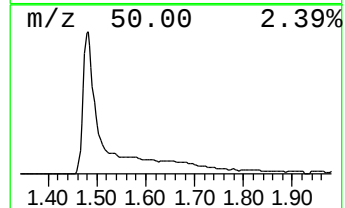
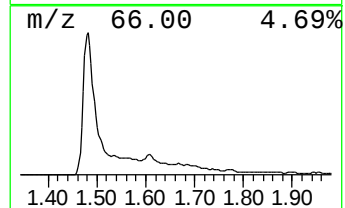
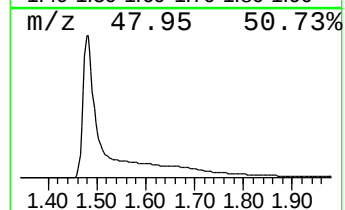
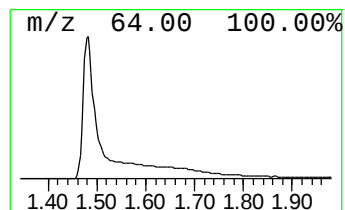
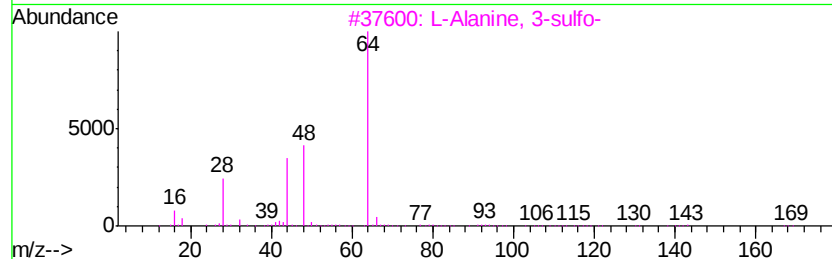
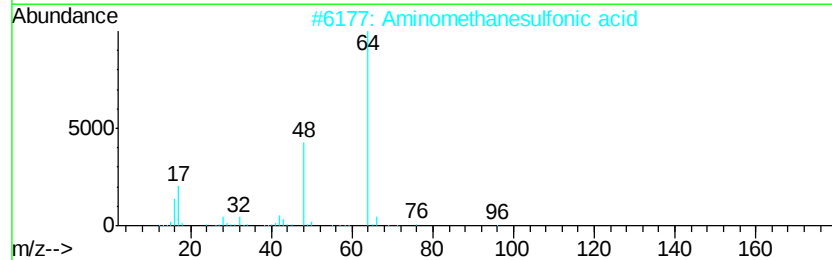
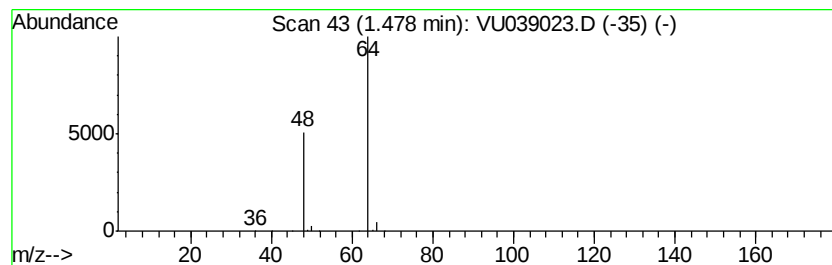
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	40.00 ug/L	4974720	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfur dioxide	64	O2S	007446-09-5	83
2		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3		L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5		Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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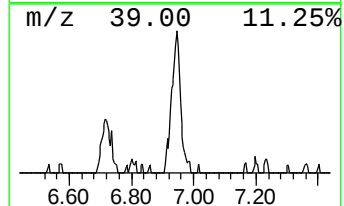
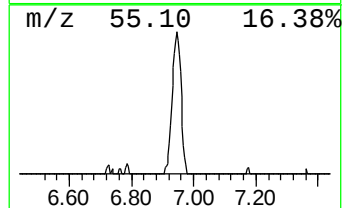
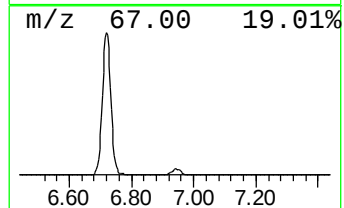
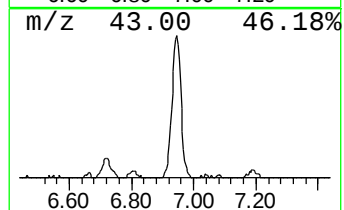
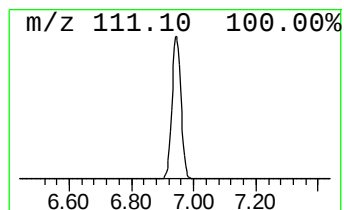
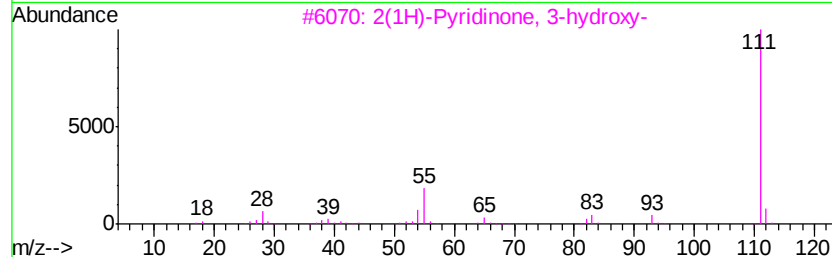
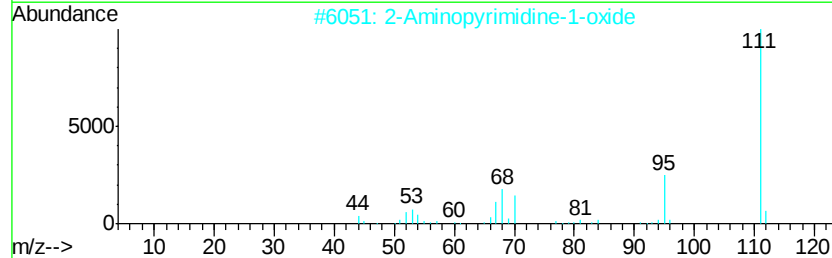
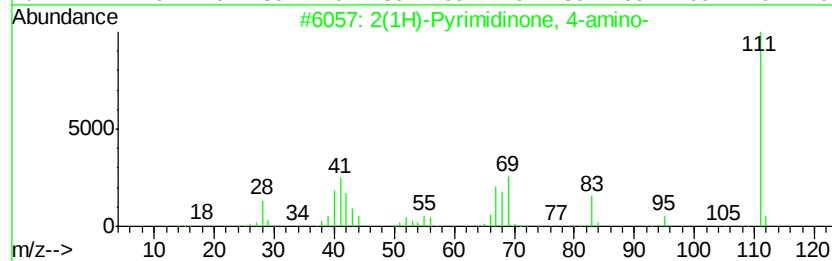
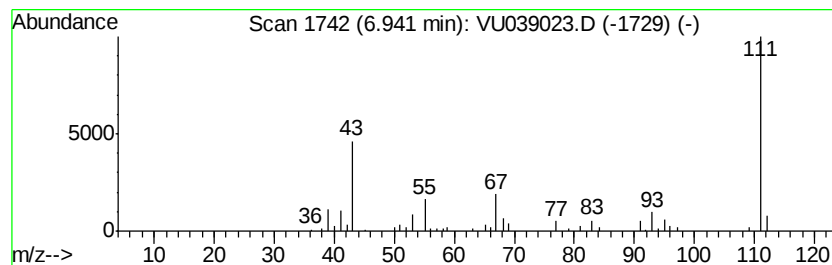
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Peak Number 2 2(1H)-Pyrimidinone, 4-amino- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.94	0.76 ug/L	94097	1,4-Difluorobenzene	6.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	59
2	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	59
3	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5N02	016867-04-2	50
4	3-Aminopyrazine 1-oxide	111	C4H5N3O	006863-77-0	45
5	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	38



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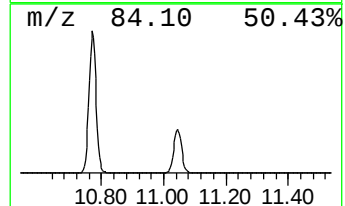
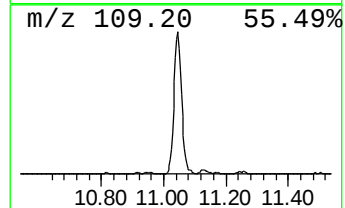
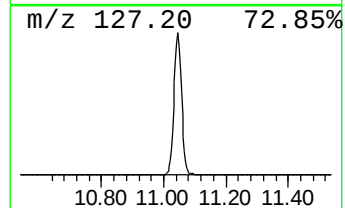
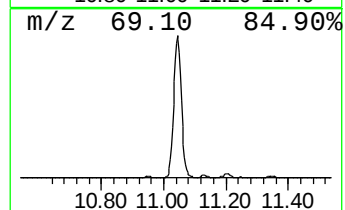
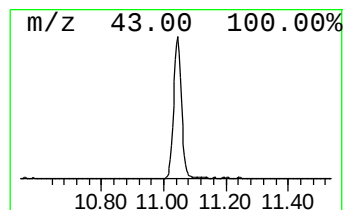
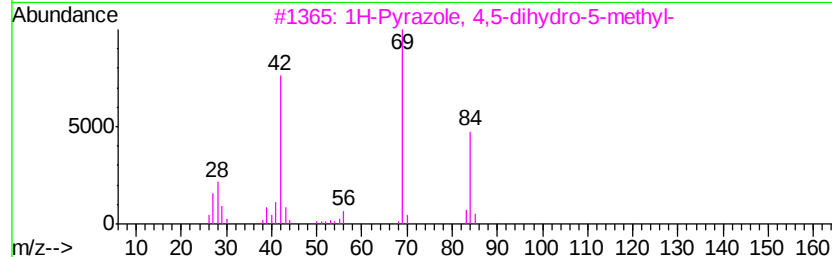
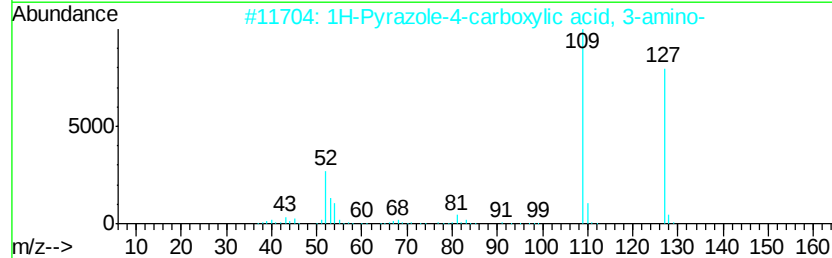
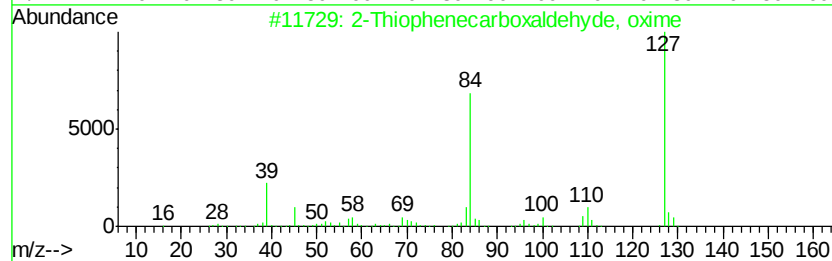
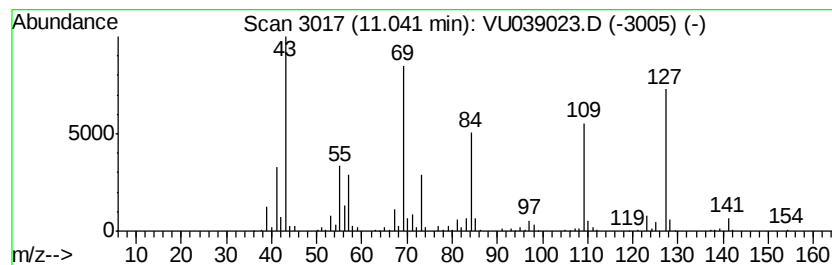
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Peak Number 4 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	3.50 ug/L	535151	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	35
2		1H-Pyrazole-4-carboxylic acid, 3-amino-	127	C4H5N3O2	041680-34-6	35
3		1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	27
4		Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	27
5		Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.48	40.0	ug/L	4974720	1	6.28	621901	5.0
2(1H)-Pyrimidinon...	6.94	0.8	ug/L	94097	1	6.28	621901	5.0
unknown-01	11.04	3.5	ug/L	535151	3	11.82	764927	5.0