

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045245.D
 Acq On : 08 Oct 2021 12:42
 Operator : SY/MD
 Sample : M4024-15DL 5X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AM3DL

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045245.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	34	42	55	rBV	69922	118029	8.99%	1.033%
2	1.601	74	81	96	rVB2	374127	439562	33.47%	3.846%
3	1.900	166	174	194	rVB	146623	221038	16.83%	1.934%
4	2.565	368	381	399	rBV	274832	463764	35.31%	4.058%
5	2.684	410	418	429	rVB3	5004	8362	0.64%	0.073%
6	2.800	444	454	463	rBV3	2124	4948	0.38%	0.043%
7	3.192	562	576	589	rVB	6209	13510	1.03%	0.118%
8	3.324	611	617	621	rBV3	329	404	0.03%	0.004%
9	3.353	621	626	627	rBV2	754	643	0.05%	0.006%
10	3.649	714	718	719	rBV	421	279	0.02%	0.002%
11	3.703	731	735	739	rBV3	192	235	0.02%	0.002%
12	3.874	772	788	803	rVB2	14002	32692	2.49%	0.286%
13	4.009	825	830	835	rBV	234	310	0.02%	0.003%
14	4.353	933	937	942	rBV2	170	202	0.02%	0.002%
15	4.536	991	994	996	rBV2	343	237	0.02%	0.002%
16	4.565	996	1003	1006	rBV3	814	937	0.07%	0.008%
17	4.629	1009	1023	1029	rBV	137032	296371	22.57%	2.593%
18	5.067	1143	1159	1186	rBV	228166	499052	38.00%	4.366%
19	5.208	1199	1203	1207	rVB3	385	347	0.03%	0.003%
20	5.289	1224	1228	1229	rBV	489	327	0.02%	0.003%
21	5.327	1237	1240	1249	rVB4	636	644	0.05%	0.006%
22	5.385	1253	1258	1266	rVB5	806	1153	0.09%	0.010%
23	5.729	1343	1365	1396	rBV2	490669	1313263	100.00%	11.490%
24	6.015	1450	1454	1457	rBV2	220	236	0.02%	0.002%
25	6.134	1486	1491	1495	rBV4	492	422	0.03%	0.004%
26	6.170	1498	1502	1506	rBV3	347	299	0.02%	0.003%
27	6.253	1512	1528	1548	rBV	355258	668531	50.91%	5.849%
28	6.510	1596	1608	1618	rBV2	11042	25303	1.93%	0.221%
29	6.697	1650	1666	1682	rBV	302506	590599	44.97%	5.167%
30	6.806	1693	1700	1713	rVB4	6111	10621	0.81%	0.093%
31	6.970	1742	1751	1763	rVB2	4445	7770	0.59%	0.068%
32	7.051	1768	1776	1779	rBV3	513	701	0.05%	0.006%
33	7.186	1812	1818	1824	rVB4	1044	1331	0.10%	0.012%
34	7.215	1824	1827	1832	rBV2	192	232	0.02%	0.002%
35	7.250	1835	1838	1840	rBV2	389	319	0.02%	0.003%
36	7.298	1849	1853	1864	rBV	615	1163	0.09%	0.010%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

37	7.568	1923	1937	1960	rBV	168108	290348	22.11%	2.540%
38	7.684	1970	1973	1974	rBV2	381	235	0.02%	0.002%
39	7.729	1982	1987	1989	rBV	267	208	0.02%	0.002%
40	7.903	2026	2041	2054	rBV	601946	1014400	77.24%	8.875%
41	7.973	2055	2063	2074	rVB	29494	48198	3.67%	0.422%
42	8.182	2116	2128	2146	rBV	116528	194627	14.82%	1.703%
43	8.378	2185	2189	2194	rBV2	240	258	0.02%	0.002%
44	8.488	2218	2223	2240	rVB7	1323	2164	0.16%	0.019%
45	8.636	2256	2269	2304	rBV	394933	700924	53.37%	6.133%
46	8.755	2304	2306	2310	rVV2	1208	840	0.06%	0.007%
47	8.790	2314	2317	2321	rVB3	834	594	0.05%	0.005%
48	8.874	2340	2343	2350	rVB2	526	488	0.04%	0.004%
49	9.044	2390	2396	2402	rBV2	596	792	0.06%	0.007%
50	9.420	2500	2513	2549	rBV	514239	839089	63.89%	7.341%
51	9.575	2549	2561	2575	rBV	145616	229543	17.48%	2.008%
52	9.694	2585	2598	2613	rBV	388651	630047	47.98%	5.512%
53	9.764	2614	2620	2638	rVB3	4570	8274	0.63%	0.072%
54	9.861	2644	2650	2653	rBV2	211	275	0.02%	0.002%
55	10.102	2714	2725	2745	rVB	85187	135616	10.33%	1.187%
56	10.237	2762	2767	2772	rVB3	200	204	0.02%	0.002%
57	10.488	2835	2845	2855	rBV	20554	30135	2.29%	0.264%
58	10.558	2861	2867	2871	rBV2	236	352	0.03%	0.003%
59	10.674	2895	2903	2917	rBV2	3557	5492	0.42%	0.048%
60	10.761	2917	2930	2954	rBV	423356	671442	51.13%	5.875%
61	10.870	2958	2964	2965	rBV2	695	606	0.05%	0.005%
62	10.925	2969	2981	2995	rVB2	9266	22587	1.72%	0.198%
63	10.993	2995	3002	3010	rBV3	2680	3802	0.29%	0.033%
64	11.092	3025	3033	3036	rBV2	770	1064	0.08%	0.009%
65	11.214	3066	3071	3074	rBV2	250	291	0.02%	0.003%
66	11.288	3088	3094	3095	rBV	744	512	0.04%	0.004%
67	11.468	3139	3150	3163	rVB4	9856	16915	1.29%	0.148%
68	11.542	3169	3173	3175	rBV	235	202	0.02%	0.002%
69	11.584	3180	3186	3191	rVV	391	579	0.04%	0.005%
70	11.636	3198	3202	3205	rBV3	626	587	0.04%	0.005%
71	11.697	3216	3221	3232	rVB2	1722	2206	0.17%	0.019%
72	11.816	3237	3258	3273	rBV	485051	806419	61.41%	7.056%
73	11.890	3273	3281	3292	rVB5	5237	8420	0.64%	0.074%
74	11.941	3292	3297	3298	rBV2	1044	773	0.06%	0.007%
75	11.976	3304	3308	3314	rVB2	2858	3351	0.26%	0.029%
76	12.015	3314	3320	3323	rBV3	358	450	0.03%	0.004%

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77	12.063	3331	3335	3337	rBV3	768	496	0.04%	0.004%
78	12.099	3338	3346	3358	rVB	9605	15127	1.15%	0.132%
79	12.195	3361	3376	3393	rBV	532878	858773	65.39%	7.514%
80	12.269	3398	3399	3404	rVB3	504	330	0.03%	0.003%
81	12.314	3404	3413	3416	rBV6	1715	2417	0.18%	0.021%
82	12.574	3488	3494	3501	rVV2	770	946	0.07%	0.008%
83	12.639	3510	3514	3517	rBV3	336	334	0.03%	0.003%
84	12.690	3522	3530	3537	rVB4	1954	2689	0.20%	0.024%
85	12.867	3579	3585	3587	rBV2	548	598	0.05%	0.005%
86	12.951	3602	3611	3627	rVB2	5097	11101	0.85%	0.097%
87	13.031	3632	3636	3643	rVB4	781	948	0.07%	0.008%
88	13.079	3648	3651	3656	rBV2	269	282	0.02%	0.002%
89	13.259	3703	3707	3711	rVB3	957	875	0.07%	0.008%
90	13.455	3761	3768	3778	rVB4	1056	1365	0.10%	0.012%
91	13.513	3783	3786	3794	rVB3	250	274	0.02%	0.002%
92	13.745	3851	3858	3866	rBV4	2580	3386	0.26%	0.030%
93	14.089	3953	3965	3980	rBV	71301	115376	8.79%	1.009%
94	14.205	3993	4001	4010	rVB4	3118	6052	0.46%	0.053%
95	14.288	4020	4027	4035	rVB3	3176	3900	0.30%	0.034%
96	14.336	4039	4042	4044	rBV2	405	205	0.02%	0.002%
97	14.661	4140	4143	4144	rBV2	378	243	0.02%	0.002%
98	14.873	4206	4209	4213	rBV3	432	498	0.04%	0.004%
99	15.230	4312	4320	4330	rVB4	1533	2650	0.20%	0.023%
100	15.417	4369	4378	4387	rVB3	2139	3497	0.27%	0.031%

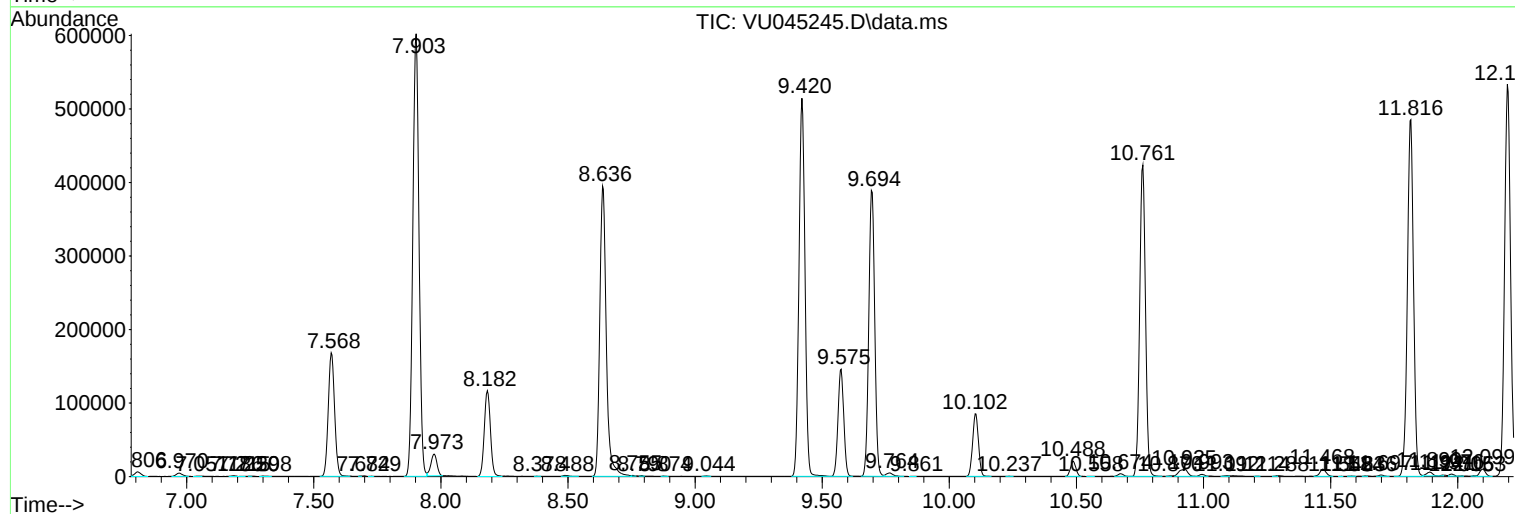
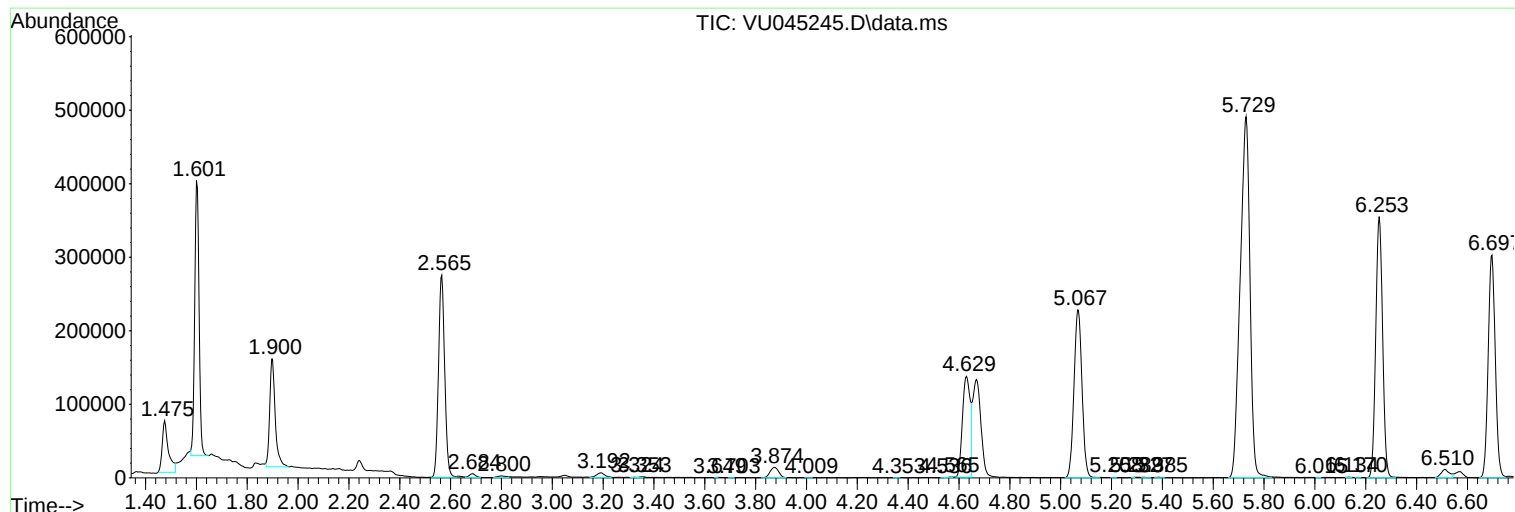
Sum of corrected areas: 11429507

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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ClientSampleId :
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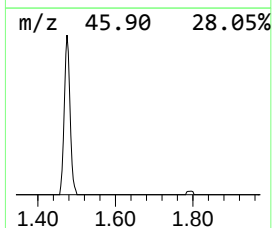
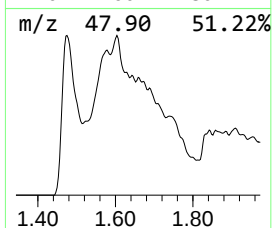
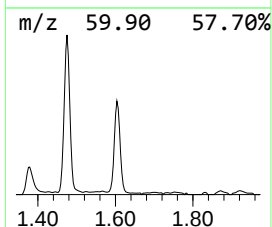
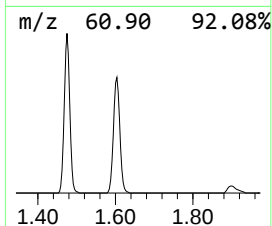
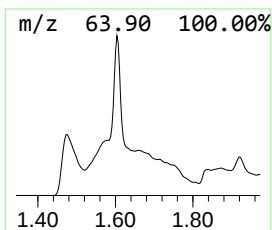
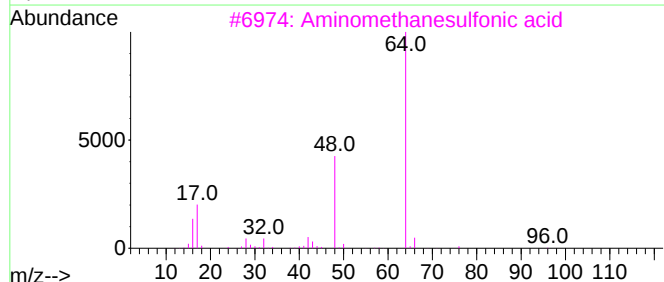
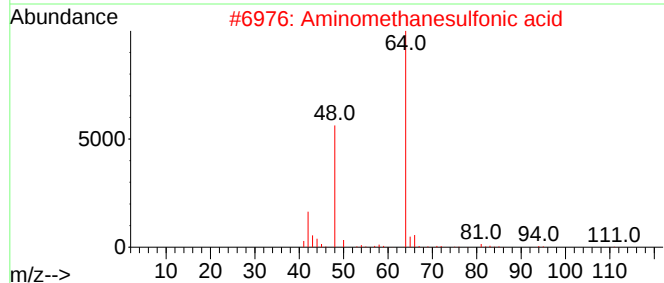
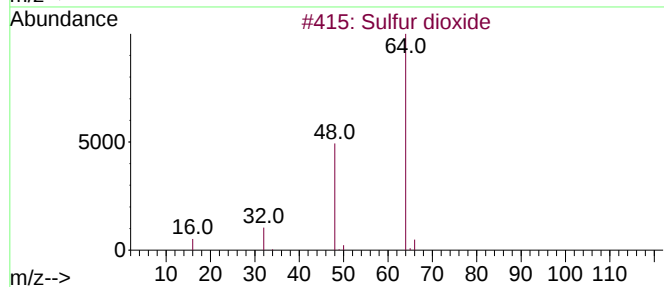
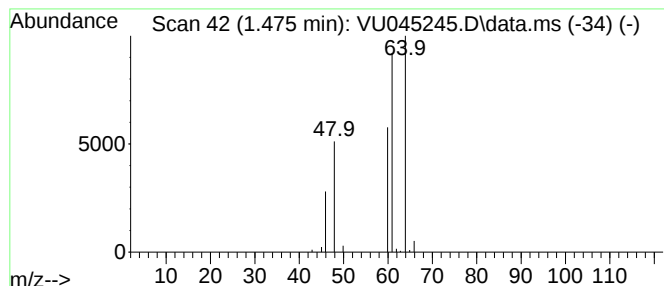
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	8.83 ug/L	118029	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	58
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	36
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	36
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7



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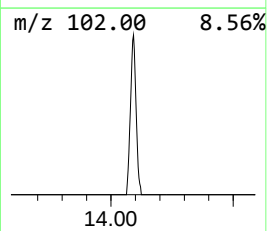
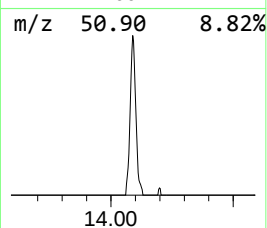
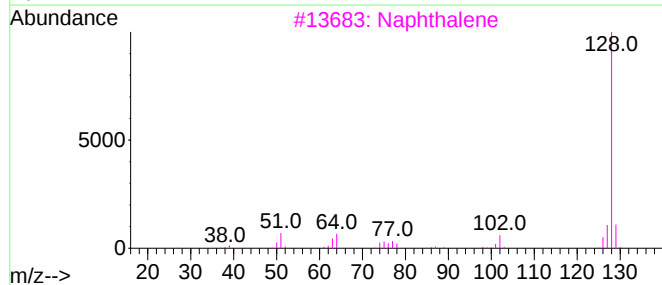
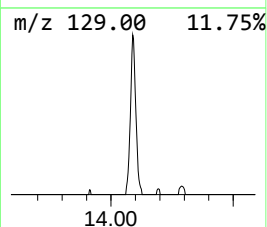
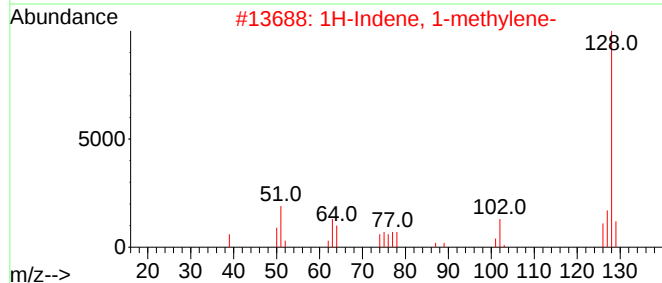
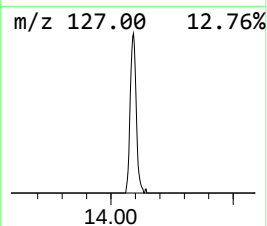
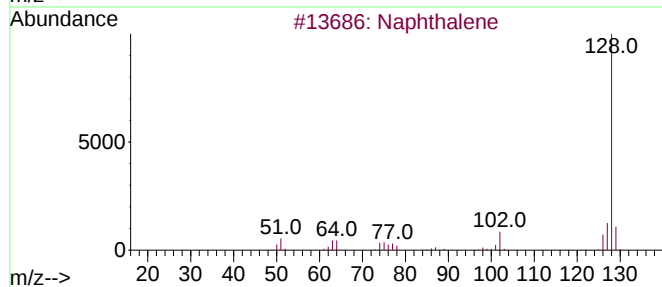
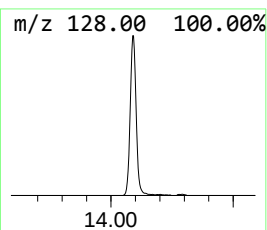
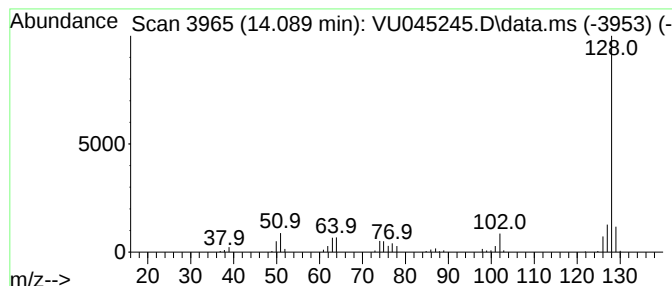
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Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	7.15 ug/L	115376	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	94
3			Naphthalene	128	C10H8	000091-20-3	93
4			Naphthalene	128	C10H8	000091-20-3	93
5			Naphthalene	128	C10H8	000091-20-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.475	8.8	ug/L	118029	1	6.253	668531	50.0
unknown-01	14.089	7.2	ug/L	115376	3	11.816	806419	50.0