

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012623\
 Data File : VU052818.D
 Acq On : 26 Jan 2023 16:08
 Operator : JC/MD
 Sample : 01316-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A44H5

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\SFAMULM012623WMA.M
 Title : VOC Analysis

Signal : TIC: VU052818.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	40	44	50	rBV4	1476	1683	0.08%	0.007%
2	1.520	53	56	60	rVB3	1223	940	0.04%	0.004%
3	1.601	72	81	104	rVB2	241231	334950	15.03%	1.333%
4	1.793	136	141	148	rVB5	1775	2426	0.11%	0.010%
5	1.838	153	155	156	rBV	622	297	0.01%	0.001%
6	1.912	169	178	180	rBV	119661	140267	6.30%	0.558%
7	2.176	258	260	264	rVB3	538	333	0.01%	0.001%
8	2.562	365	380	396	rBV2	416893	803249	36.05%	3.197%
9	2.639	397	404	419	rVB3	3460	7128	0.32%	0.028%
10	2.713	419	427	434	rBV3	827	1086	0.05%	0.004%
11	2.784	434	449	473	rBV	216544	376134	16.88%	1.497%
12	2.948	486	500	516	rBV	91224	177943	7.99%	0.708%
13	3.041	517	529	553	rVB	125692	261835	11.75%	1.042%
14	3.173	567	570	571	rBV2	467	284	0.01%	0.001%
15	3.224	584	586	589	rBV2	286	196	0.01%	0.001%
16	3.359	611	628	657	rBV2	217805	511351	22.95%	2.035%
17	3.790	755	762	768	rBV	295	458	0.02%	0.002%
18	3.861	768	784	810	rVV2	66783	159483	7.16%	0.635%
19	4.006	825	829	833	rBV	210	219	0.01%	0.001%
20	4.099	853	858	861	rBV	302	323	0.01%	0.001%
21	4.115	861	863	869	rVB2	376	348	0.02%	0.001%
22	4.147	870	873	875	rBV	309	225	0.01%	0.001%
23	4.170	875	880	883	rBV2	241	256	0.01%	0.001%
24	4.260	905	908	910	rBV2	297	181	0.01%	0.001%
25	4.289	913	917	921	rVB2	180	201	0.01%	0.001%
26	4.321	922	927	929	rBV	248	207	0.01%	0.001%
27	4.568	999	1004	1007	rBV2	244	242	0.01%	0.001%
28	4.652	1010	1030	1059	rBV3	122211	449666	20.18%	1.790%
29	5.057	1139	1156	1180	rBV	267158	592821	26.61%	2.360%
30	5.144	1180	1183	1185	rBV3	391	231	0.01%	0.001%
31	5.186	1193	1196	1200	rVB2	398	273	0.01%	0.001%
32	5.308	1217	1234	1255	rBV	188868	431345	19.36%	1.717%
33	5.446	1270	1277	1279	rBV2	321	416	0.02%	0.002%
34	5.523	1297	1301	1303	rBV2	230	197	0.01%	0.001%
35	5.719	1339	1362	1374	rBV2	551560	1465158	65.76%	5.832%
36	5.790	1375	1384	1404	rVB	207761	417677	18.75%	1.662%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
 Title : VOC Analysis

37	5.996	1444	1448	1453	rBV2	346	371	0.02%	0.001%
38	6.073	1468	1472	1473	rBV	628	397	0.02%	0.002%
39	6.121	1483	1487	1491	rVB2	251	203	0.01%	0.001%
40	6.243	1511	1525	1547	rBV	273419	514749	23.10%	2.049%
41	6.372	1560	1565	1568	rVB2	344	343	0.02%	0.001%
42	6.391	1569	1571	1575	rVB2	330	190	0.01%	0.001%
43	6.472	1591	1596	1599	rBV2	288	242	0.01%	0.001%
44	6.536	1600	1616	1634	rBV	435277	814380	36.55%	3.242%
45	6.687	1649	1663	1681	rBV	332724	645486	28.97%	2.569%
46	6.787	1681	1694	1712	rVB2	132374	254791	11.44%	1.014%
47	7.038	1750	1772	1795	rBV3	12541	50911	2.28%	0.203%
48	7.185	1811	1818	1819	rBV4	2538	2306	0.10%	0.009%
49	7.304	1850	1855	1858	rBV2	245	260	0.01%	0.001%
50	7.485	1908	1911	1914	rVB2	423	315	0.01%	0.001%
51	7.562	1922	1935	1959	rBV	184657	328145	14.73%	1.306%
52	7.716	1969	1983	1995	rBV6	6517	15397	0.69%	0.061%
53	7.809	1996	2012	2027	rVV5	116656	346363	15.55%	1.379%
54	7.893	2027	2038	2050	rVV	726282	1245289	55.89%	4.957%
55	7.967	2050	2061	2078	rVB	365282	630315	28.29%	2.509%
56	8.176	2114	2126	2132	rBV	128749	230761	10.36%	0.919%
57	8.272	2152	2156	2166	rVB3	3230	4216	0.19%	0.017%
58	8.398	2182	2195	2217	rVB	251829	472290	21.20%	1.880%
59	8.549	2229	2242	2257	rBV	290523	483442	21.70%	1.924%
60	8.652	2258	2274	2283	rBV	276753	616729	27.68%	2.455%
61	8.922	2346	2358	2379	rVB	133095	232001	10.41%	0.923%
62	9.066	2401	2403	2406	rVV	318	188	0.01%	0.001%
63	9.105	2412	2415	2419	rVB	246	191	0.01%	0.001%
64	9.298	2473	2475	2479	rVB2	396	199	0.01%	0.001%
65	9.417	2498	2512	2515	rBV	394409	599157	26.89%	2.385%
66	9.568	2544	2559	2580	rBV	843579	1327610	59.59%	5.284%
67	9.687	2583	2596	2616	rVB	565440	908253	40.76%	3.615%
68	9.800	2629	2631	2634	rBV2	327	179	0.01%	0.001%
69	9.883	2652	2657	2660	rBV3	407	335	0.02%	0.001%
70	10.111	2711	2728	2750	rBV3	518633	1083050	48.61%	4.311%
71	10.295	2772	2785	2800	rVB2	75674	136373	6.12%	0.543%
72	10.398	2811	2817	2818	rBV	389	266	0.01%	0.001%
73	10.481	2829	2843	2858	rBV	600737	944482	42.39%	3.759%
74	10.632	2886	2890	2895	rVB3	459	387	0.02%	0.002%
75	10.783	2916	2937	2957	rBV3	951996	2228094	100.00%	8.869%
76	11.095	3026	3034	3040	rBV2	646	685	0.03%	0.003%

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77	11.160	3052	3054	3059	rVB2	367	275	0.01%	0.001%
78	11.407	3128	3131	3134	rBV2	464	240	0.01%	0.001%
79	11.468	3145	3150	3151	rBV3	777	605	0.03%	0.002%
80	11.481	3151	3154	3158	rVB2	1215	993	0.04%	0.004%
81	11.745	3223	3236	3246	rBV	210967	326281	14.64%	1.299%
82	11.812	3246	3257	3260	rBV	462585	692553	31.08%	2.757%
83	11.931	3291	3294	3301	rVB5	820	716	0.03%	0.003%
84	12.018	3318	3321	3323	rBV3	359	274	0.01%	0.001%
85	12.034	3323	3326	3328	rVV2	316	207	0.01%	0.001%
86	12.118	3348	3352	3354	rBV2	345	264	0.01%	0.001%
87	12.201	3362	3378	3402	rBV3	911274	2174500	97.59%	8.655%
88	12.475	3457	3463	3464	rBV2	1054	857	0.04%	0.003%
89	12.513	3473	3475	3481	rVB3	407	327	0.01%	0.001%
90	12.549	3481	3486	3489	rBV	444	467	0.02%	0.002%
91	12.996	3613	3625	3638	rBV	212088	336413	15.10%	1.339%
92	13.217	3679	3694	3714	rBV	513034	805745	36.16%	3.207%
93	13.333	3727	3730	3735	rBV2	517	484	0.02%	0.002%
94	13.841	3880	3888	3901	rVB7	3369	5513	0.25%	0.022%
95	13.889	3901	3903	3906	rBV2	329	223	0.01%	0.001%
96	14.086	3956	3964	3975	rBV2	4781	7039	0.32%	0.028%
97	14.327	4026	4039	4061	rBV	316593	509038	22.85%	2.026%
98	14.516	4095	4098	4100	rBV2	523	343	0.02%	0.001%
99	14.558	4108	4111	4116	rBV5	432	408	0.02%	0.002%
100	15.976	4549	4552	4554	rBV3	642	412	0.02%	0.002%

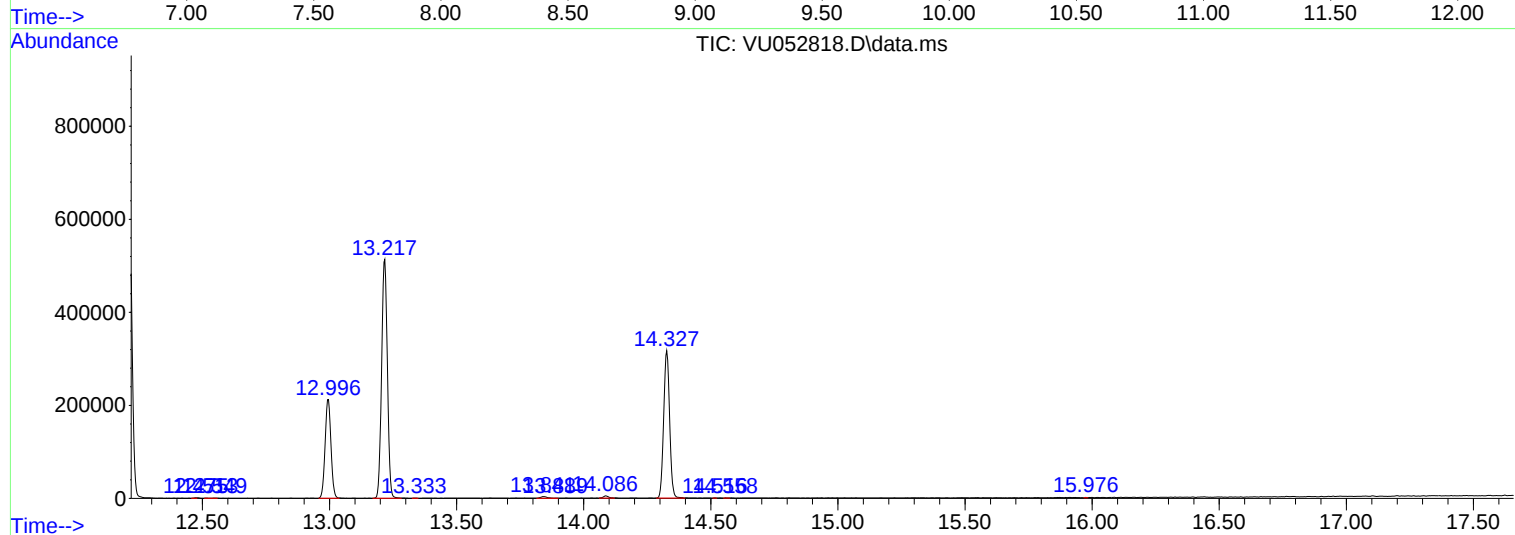
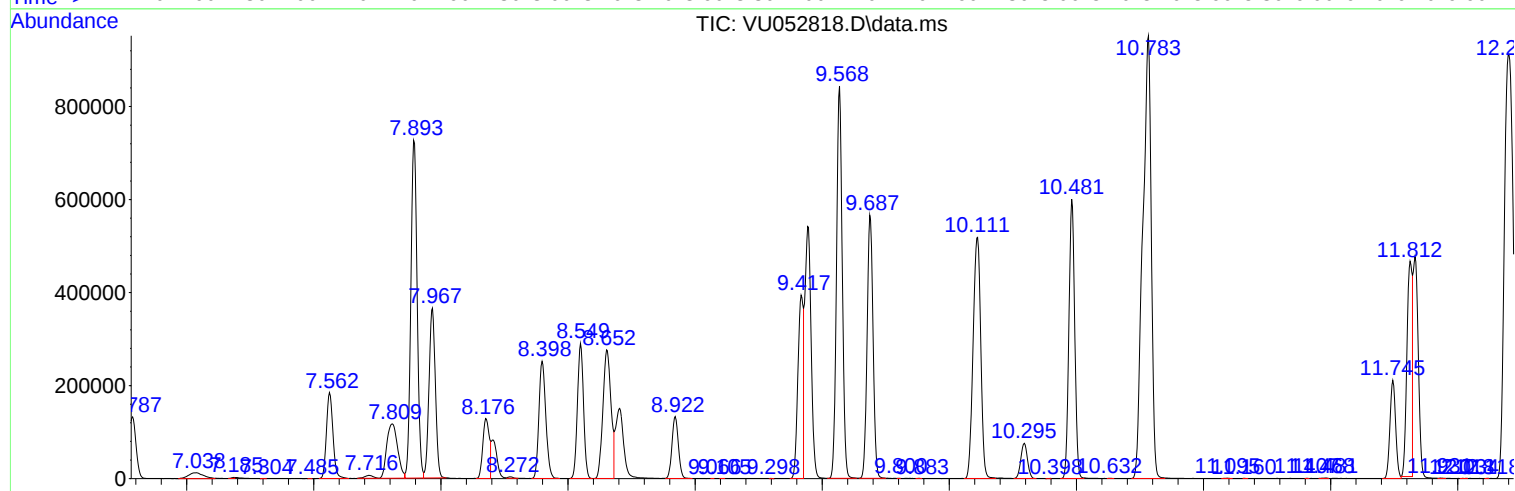
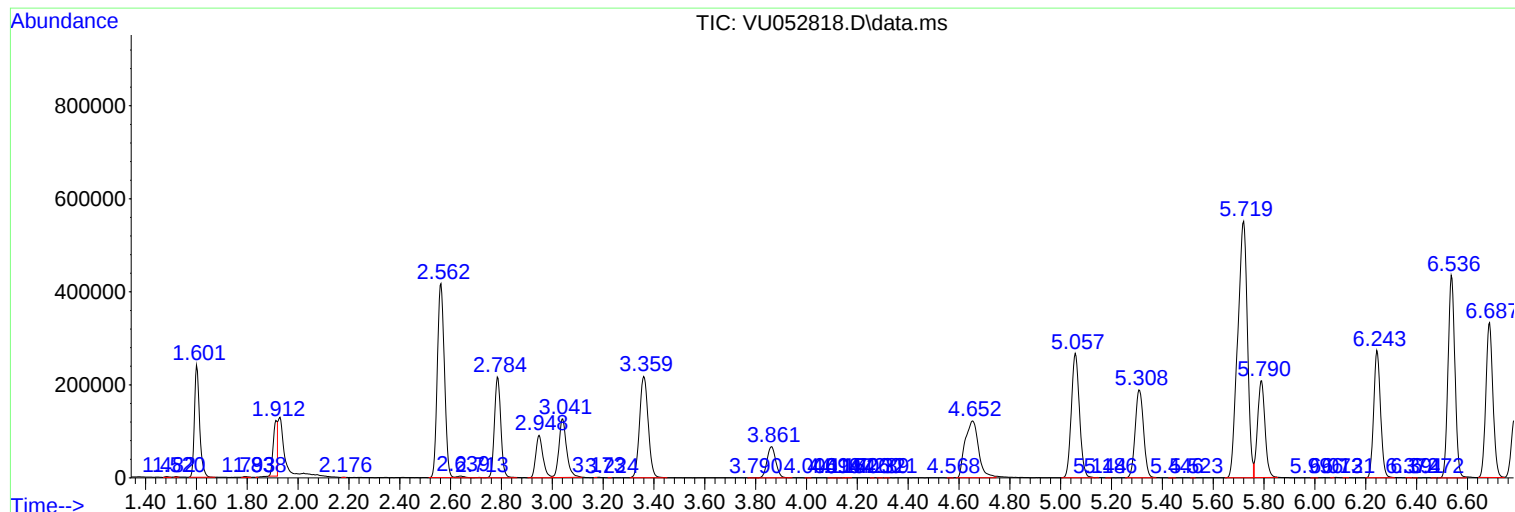
Sum of corrected areas: 25123547

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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



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ClientSampleId :
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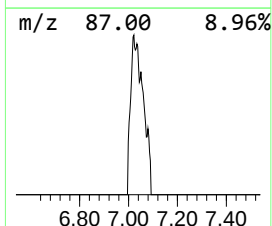
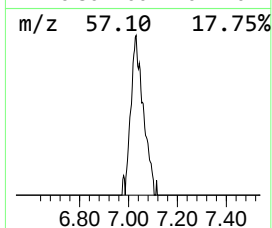
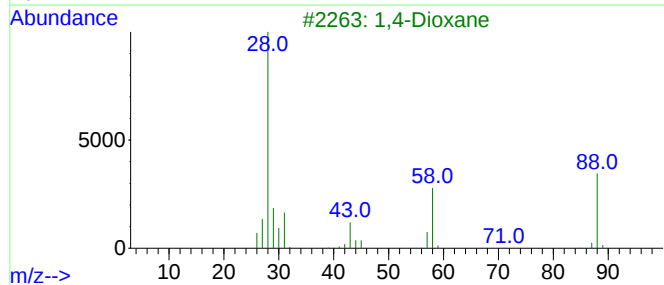
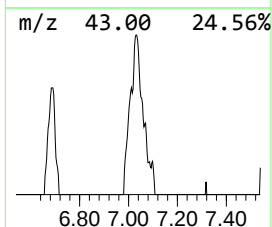
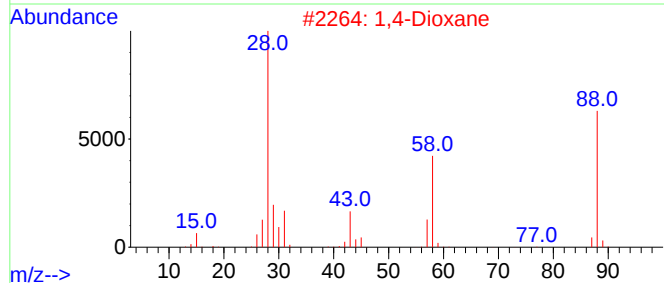
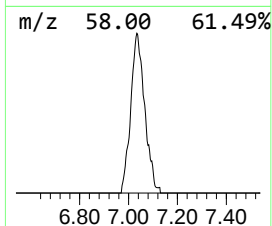
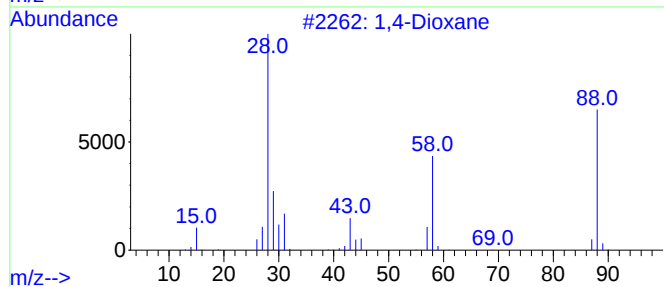
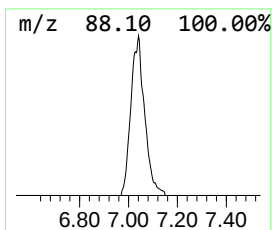
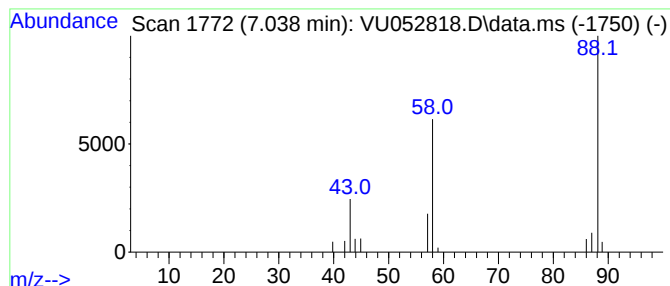
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 1,4-Dioxane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.038	4.95 ug/L	50911	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxane			88	C4H8O2	000123-91-1	90
2	1,4-Dioxane			88	C4H8O2	000123-91-1	83
3	1,4-Dioxane			88	C4H8O2	000123-91-1	83
4	1,4-Dioxane			88	C4H8O2	000123-91-1	83
5	1,4-Dioxane			88	C4H8O2	000123-91-1	56



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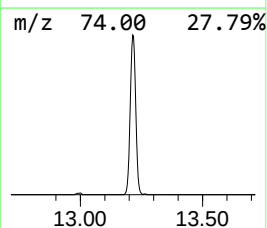
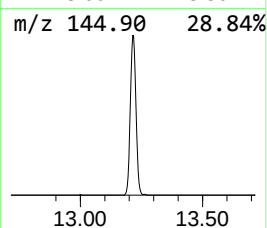
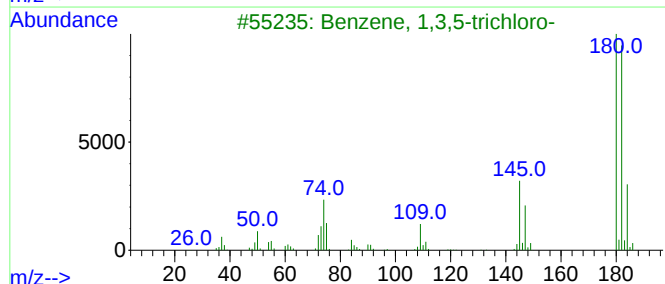
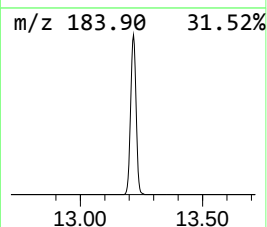
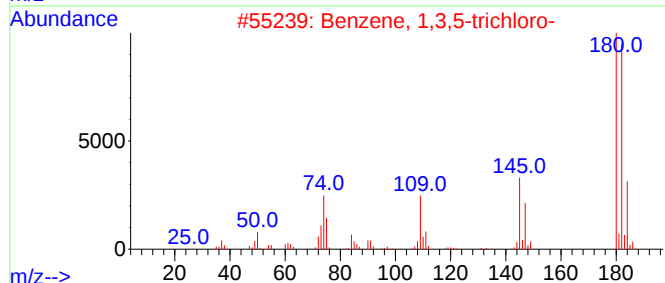
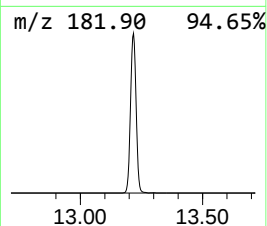
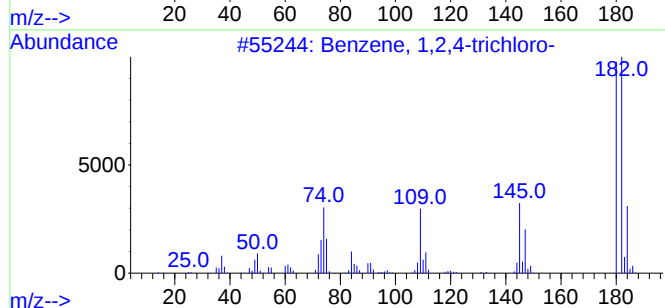
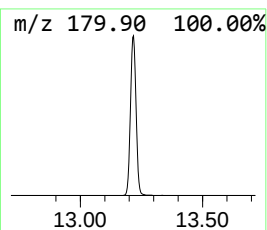
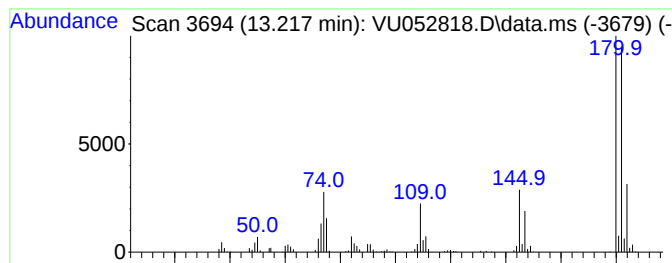
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Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1,3,5-trichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.217	58.17 ug/L	805745	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	98
2			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
3			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
4			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	98
5			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	98



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,4-Dioxane	7.038	5.0	ug/L	50911	1	6.243	514749	50.0
Benzene, 1,3,5-...	13.217	58.2	ug/L	805745	3	11.809	692553	50.0