

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020223\
 Data File : VU052922.D
 Acq On : 02 Feb 2023 13:51
 Operator : JC/MD
 Sample : 01381-27
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A44Q3

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: VU052922.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.382	7	13	32	rVB	57275	74744	3.65%	0.305%
2	1.482	37	44	49	rBV	42888	44666	2.18%	0.182%
3	1.520	49	56	67	rVB	125468	140345	6.86%	0.573%
4	1.597	71	80	96	rVB	90366	123101	6.02%	0.503%
5	1.855	152	160	169	rBV	76528	102222	5.00%	0.417%
6	1.909	171	177	196	rVB	71757	121365	5.93%	0.495%
7	2.118	234	242	258	rVB	191702	267616	13.08%	1.092%
8	2.559	365	379	392	rBV2	335128	682281	33.35%	2.785%
9	2.636	393	403	442	rVB	381235	925495	45.24%	3.778%
10	2.948	488	500	517	rBV	123887	244888	11.97%	1.000%
11	3.041	519	529	555	rVB	84489	182416	8.92%	0.745%
12	3.163	563	567	568	rBV2	432	267	0.01%	0.001%
13	3.263	595	598	602	rVB2	230	177	0.01%	0.001%
14	3.359	607	628	653	rBV	541139	1247783	61.00%	5.094%
15	3.646	710	717	719	rBB	329	299	0.01%	0.001%
16	3.720	737	740	742	rBV	311	180	0.01%	0.001%
17	3.935	803	807	812	rBV	379	358	0.02%	0.001%
18	3.980	816	821	824	rBB	371	330	0.02%	0.001%
19	4.002	824	828	829	rBV	168	143	0.01%	0.001%
20	4.041	838	840	843	rBB	250	137	0.01%	0.001%
21	4.109	857	861	865	rBB	175	159	0.01%	0.001%
22	4.147	866	873	876	rBV	350	381	0.02%	0.002%
23	4.205	885	891	893	rBB	146	175	0.01%	0.001%
24	4.250	903	905	908	rVV	274	189	0.01%	0.001%
25	4.273	911	912	918	rVB2	242	218	0.01%	0.001%
26	4.350	933	936	944	rBV	219	356	0.02%	0.001%
27	4.456	967	969	975	rBB	221	214	0.01%	0.001%
28	4.565	1000	1003	1007	rBV2	276	295	0.01%	0.001%
29	4.636	1013	1025	1039	rBV2	41100	124298	6.08%	0.507%
30	4.993	1133	1136	1139	rBV	185	146	0.01%	0.001%
31	5.057	1139	1156	1184	rVB2	176083	402647	19.68%	1.644%
32	5.157	1184	1187	1188	rBV	278	172	0.01%	0.001%
33	5.186	1194	1196	1199	rVB3	367	184	0.01%	0.001%
34	5.218	1203	1206	1208	rVB	246	162	0.01%	0.001%
35	5.279	1222	1225	1227	rBV	300	193	0.01%	0.001%
36	5.379	1236	1256	1274	rBV2	120055	268386	13.12%	1.096%

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 Title : VOC Analysis

37	5.465	1280	1283	1286	rBV2	296	238	0.01%	0.001%
38	5.501	1291	1294	1299	rBB2	303	236	0.01%	0.001%
39	5.588	1318	1321	1326	rBB2	254	231	0.01%	0.001%
40	5.633	1330	1335	1338	rBB	170	195	0.01%	0.001%
41	5.716	1339	1361	1373	rBV2	372964	975398	47.68%	3.982%
42	5.790	1375	1384	1404	rVB	246364	500868	24.48%	2.045%
43	6.064	1464	1469	1473	rBB2	276	256	0.01%	0.001%
44	6.244	1510	1525	1551	rBV	293408	559098	27.33%	2.282%
45	6.472	1594	1596	1599	rVB	297	173	0.01%	0.001%
46	6.536	1600	1616	1633	rBV	247756	461796	22.57%	1.885%
47	6.687	1649	1663	1673	rBV2	216487	427747	20.91%	1.746%
48	6.758	1674	1685	1706	rVB	490071	955068	46.69%	3.899%
49	6.932	1736	1739	1744	rBV	217	262	0.01%	0.001%
50	7.025	1750	1768	1769	rBV4	5317	8659	0.42%	0.035%
51	7.189	1811	1819	1820	rBV3	1501	1453	0.07%	0.006%
52	7.456	1900	1902	1906	rVB	253	143	0.01%	0.001%
53	7.481	1907	1910	1913	rBB	259	156	0.01%	0.001%
54	7.562	1922	1935	1957	rBV	115255	214594	10.49%	0.876%
55	7.668	1963	1968	1970	rBB	311	221	0.01%	0.001%
56	7.700	1970	1978	1984	rBV5	1008	1519	0.07%	0.006%
57	7.816	1994	2014	2028	rBV2	258073	851139	41.61%	3.474%
58	7.893	2030	2038	2050	rVV	476295	834406	40.79%	3.406%
59	7.967	2050	2061	2087	rVB	722207	1256509	61.42%	5.129%
60	8.179	2115	2127	2148	rVB	77625	146382	7.16%	0.598%
61	8.334	2172	2175	2177	rBV	397	256	0.01%	0.001%
62	8.391	2190	2193	2195	rBV	319	218	0.01%	0.001%
63	8.430	2200	2205	2207	rBV3	472	407	0.02%	0.002%
64	8.549	2228	2242	2257	rBB	155381	258368	12.63%	1.055%
65	8.658	2260	2276	2282	rBV	148192	322281	15.75%	1.316%
66	8.989	2376	2379	2386	rVB3	457	511	0.02%	0.002%
67	9.025	2387	2390	2392	rBV	204	145	0.01%	0.001%
68	9.134	2422	2424	2428	rBV	262	222	0.01%	0.001%
69	9.362	2490	2495	2498	rBV2	307	371	0.02%	0.002%
70	9.417	2498	2512	2519	rBV	409732	826284	40.39%	3.373%
71	9.568	2547	2559	2576	rBV	383563	632916	30.94%	2.584%
72	9.687	2583	2596	2619	rBV	1120457	1842187	90.05%	7.520%
73	9.912	2663	2666	2668	rVV	210	147	0.01%	0.001%
74	9.932	2670	2672	2676	rVV2	174	154	0.01%	0.001%
75	9.983	2680	2688	2693	rBV2	408	524	0.03%	0.002%
76	10.108	2710	2727	2752	rBV4	958295	2045669	100.00%	8.351%

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77	10.279	2777	2780	2782	rBV3	274	218	0.01%	0.001%
78	10.401	2816	2818	2820	rBV	332	149	0.01%	0.001%
79	10.485	2831	2844	2860	rBV	746181	1186614	58.01%	4.844%
80	10.591	2874	2877	2878	rBV	333	177	0.01%	0.001%
81	10.632	2886	2890	2893	rBV3	822	634	0.03%	0.003%
82	10.780	2916	2936	2953	rBV2	465693	1161241	56.77%	4.740%
83	10.960	2989	2992	2994	rBV2	364	199	0.01%	0.001%
84	10.983	2994	2999	3008	rVV5	1220	1741	0.09%	0.007%
85	11.086	3028	3031	3040	rVB3	532	717	0.04%	0.003%
86	11.153	3046	3052	3055	rBV	281	331	0.02%	0.001%
87	11.748	3231	3237	3243	rVB3	1676	1998	0.10%	0.008%
88	11.812	3244	3257	3277	rBV2	493513	1073217	52.46%	4.381%
89	11.980	3307	3309	3315	rVB	284	163	0.01%	0.001%
90	12.195	3359	3376	3406	rBV3	513709	1106806	54.10%	4.518%
91	12.764	3545	3553	3560	rBV2	716	1040	0.05%	0.004%
92	13.018	3630	3632	3635	rBV	299	157	0.01%	0.001%
93	13.214	3681	3693	3711	rBV	519578	798169	39.02%	3.258%
94	13.301	3718	3720	3723	rBV2	371	155	0.01%	0.001%
95	13.468	3769	3772	3775	rBV	289	174	0.01%	0.001%
96	13.838	3874	3887	3900	rBV	159158	249784	12.21%	1.020%
97	13.964	3920	3926	3929	rBV	301	314	0.02%	0.001%
98	14.089	3959	3965	3974	rVB	4619	6351	0.31%	0.026%
99	14.327	4025	4039	4060	rBV	506323	822396	40.20%	3.357%
100	15.121	4284	4286	4288	rBV	309	161	0.01%	0.001%

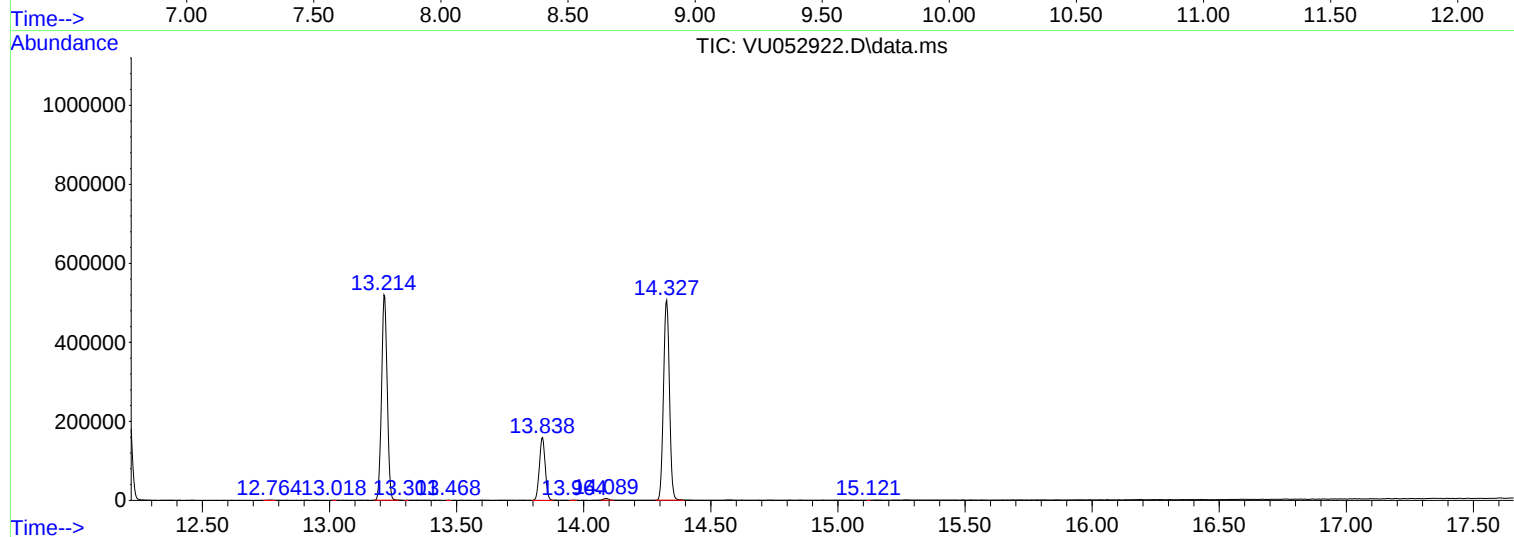
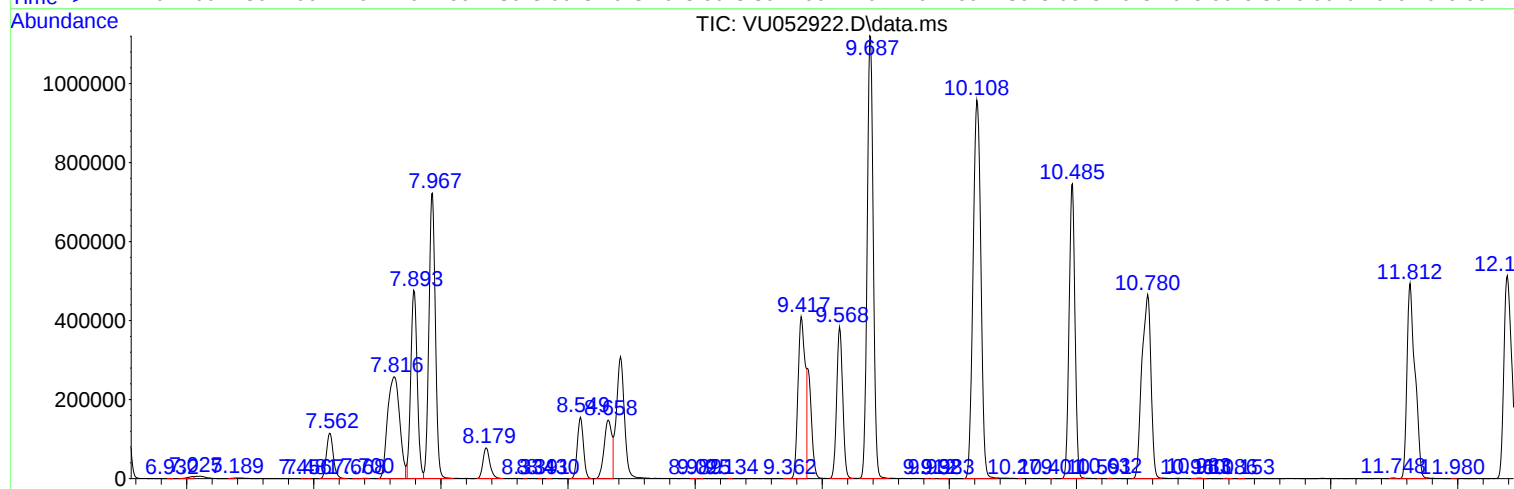
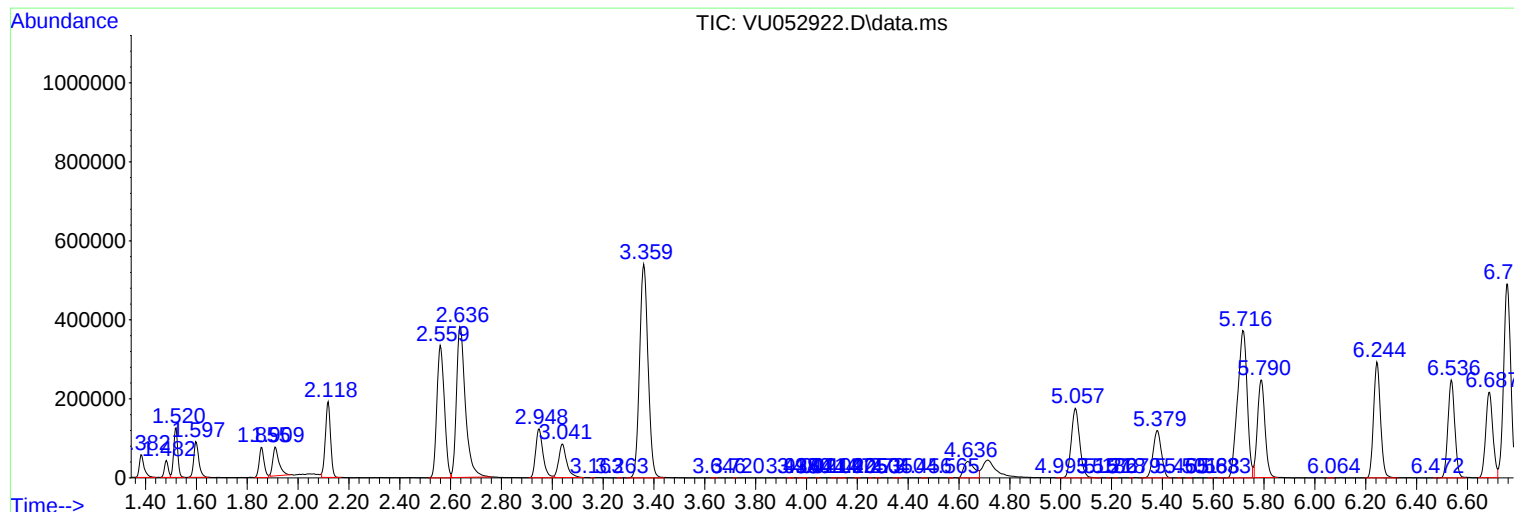
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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



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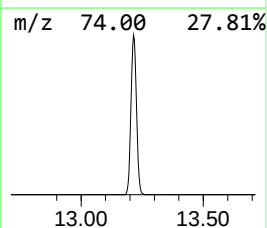
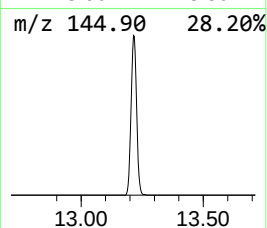
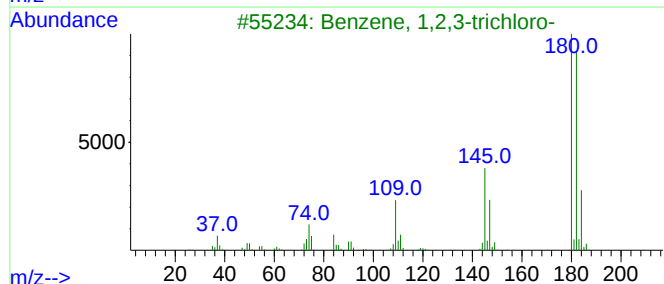
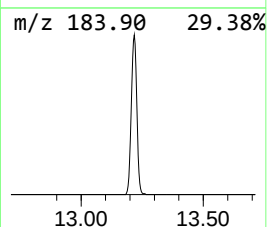
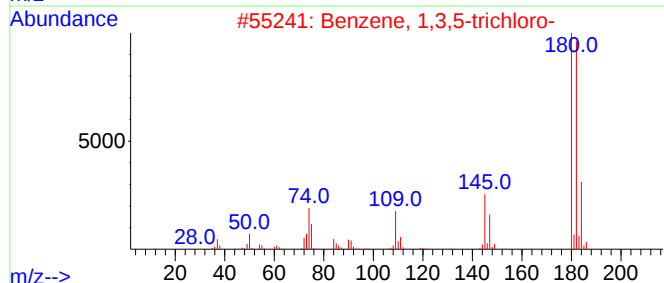
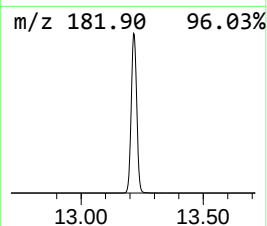
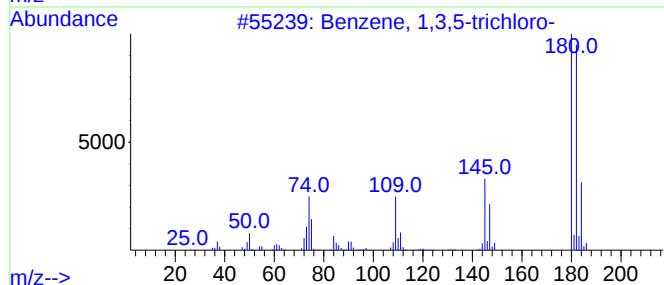
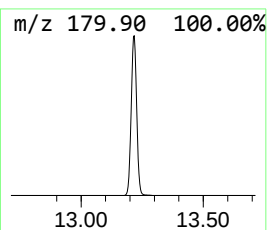
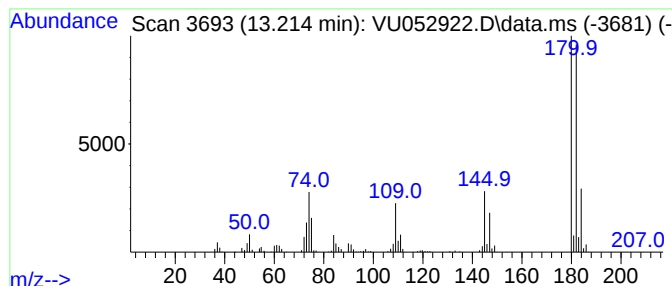
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, 1,3,5-trichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.214	37.19 ug/L	798169	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
2			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
3			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	98
4			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	98
5			Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	97



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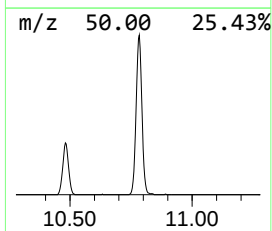
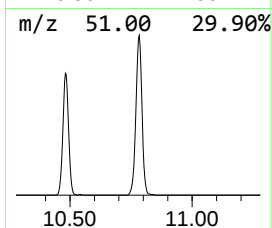
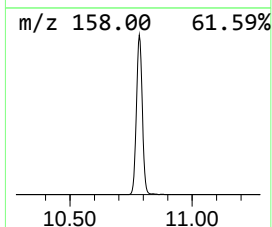
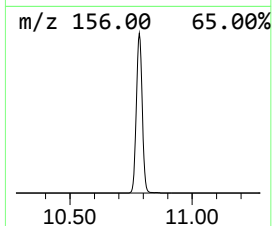
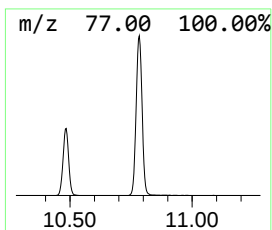
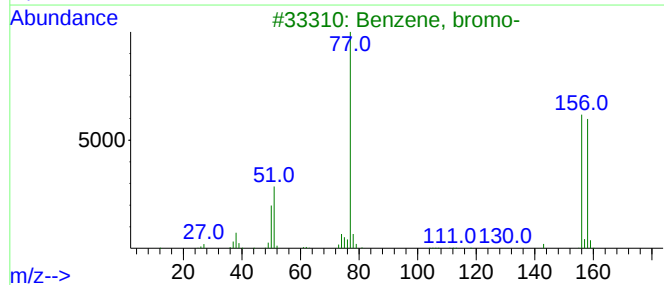
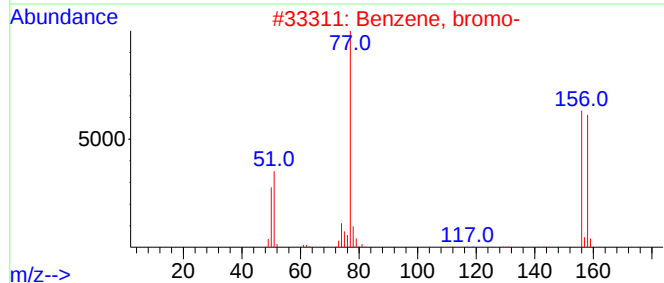
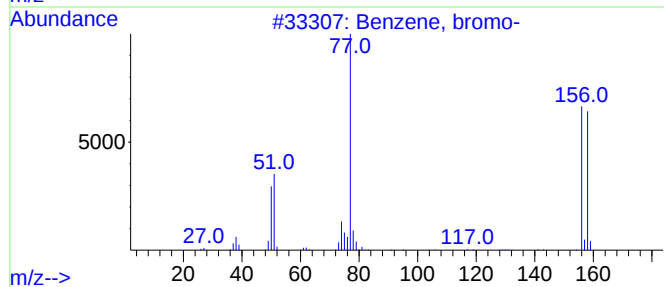
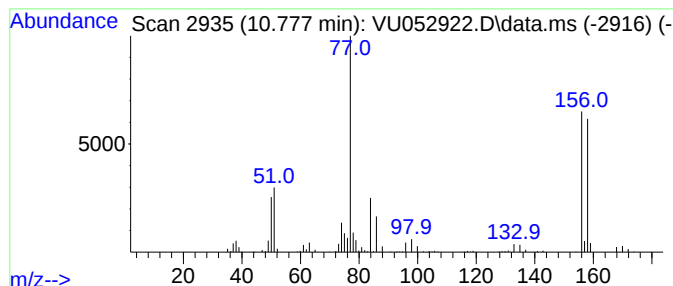
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Peak Number 3 Benzene, bromo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.780	54.10 ug/L	1161240	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, bromo-	156	C6H5Br	000108-86-1	97
2			Benzene, bromo-	156	C6H5Br	000108-86-1	96
3			Benzene, bromo-	156	C6H5Br	000108-86-1	95
4			Benzene, bromo-	156	C6H5Br	000108-86-1	95
5			Benzene, bromo-	156	C6H5Br	000108-86-1	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1,3,5-...	13.214	37.2	ug/L	798169	3	11.813	1073220	50.0
Benzene, bromo-	10.780	54.1	ug/L	1161240	3	11.813	1073220	50.0