

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020823\
 Data File : VU053008.D
 Acq On : 08 Feb 2023 18:46
 Operator : JC/MD
 Sample : 01488-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C1160

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\SFAMULM020823WMA.M
 Title : VOC Analysis

Signal : TIC: VU053008.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.257	44	52	67	rVB	88294	114261	8.93%	1.142%
2	1.537	117	139	140	rBV	17189	43519	3.40%	0.435%
3	1.598	151	158	171	rBV	178933	212443	16.60%	2.124%
4	1.913	249	256	272	rBV	146233	217196	16.97%	2.171%
5	2.566	448	459	476	rVB	283304	465112	36.33%	4.649%
6	2.978	585	587	592	rVB5	1289	971	0.08%	0.010%
7	3.154	639	642	646	rBV7	2238	2244	0.18%	0.022%
8	3.396	712	717	719	rBV5	953	956	0.07%	0.010%
9	3.482	740	744	745	rBV4	1690	1034	0.08%	0.010%
10	3.495	745	748	754	rVB7	1628	1642	0.13%	0.016%
11	3.527	754	758	761	rBV6	1173	1025	0.08%	0.010%
12	3.691	805	809	811	rBV5	974	762	0.06%	0.008%
13	3.788	837	839	843	rVV5	1270	837	0.07%	0.008%
14	3.978	895	898	900	rVV4	1573	1221	0.10%	0.012%
15	4.122	939	943	946	rBV5	991	886	0.07%	0.009%
16	4.232	972	977	979	rBV6	1469	1386	0.11%	0.014%
17	4.473	1047	1052	1057	rVB9	1274	1343	0.10%	0.013%
18	4.502	1057	1061	1065	rVB7	1442	1225	0.10%	0.012%
19	4.550	1072	1076	1078	rBV4	1243	1064	0.08%	0.011%
20	4.627	1086	1100	1124	rVV	74054	205103	16.02%	2.050%
21	4.887	1177	1181	1184	rBV6	1688	1272	0.10%	0.013%
22	4.923	1190	1192	1198	rVB7	1327	1113	0.09%	0.011%
23	4.955	1198	1202	1204	rBV5	1084	769	0.06%	0.008%
24	5.000	1213	1216	1219	rVV4	1160	853	0.07%	0.009%
25	5.058	1219	1234	1258	rVV2	248620	544590	42.54%	5.444%
26	5.196	1273	1277	1282	rVB8	1596	1533	0.12%	0.015%
27	5.280	1296	1303	1305	rBV7	1614	1970	0.15%	0.020%
28	5.338	1318	1321	1324	rBV4	1157	922	0.07%	0.009%
29	5.524	1376	1379	1381	rBV3	1855	1246	0.10%	0.012%
30	5.720	1416	1440	1463	rVV2	481345	1280131	100.00%	12.797%
31	5.852	1478	1481	1484	rBV5	927	877	0.07%	0.009%
32	6.016	1527	1532	1534	rBV6	1370	947	0.07%	0.009%
33	6.029	1534	1536	1540	rVB5	1718	1123	0.09%	0.011%
34	6.170	1577	1580	1584	rBV5	1401	1205	0.09%	0.012%
35	6.244	1587	1603	1619	rBV	368389	697958	54.52%	6.977%
36	6.373	1640	1643	1647	rVB6	1476	1019	0.08%	0.010%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.M
 Title : VOC Analysis

37	6.685	1726	1740	1767	rBV	295087	569414	44.48%	5.692%
38	6.913	1808	1811	1814	rBV5	1463	874	0.07%	0.009%
39	6.936	1815	1818	1825	rVB7	1427	1438	0.11%	0.014%
40	6.968	1825	1828	1831	rBV5	1896	1534	0.12%	0.015%
41	7.032	1846	1848	1854	rBV6	999	887	0.07%	0.009%
42	7.064	1854	1858	1863	rVB7	1131	1313	0.10%	0.013%
43	7.096	1863	1868	1871	rBV6	1649	1147	0.09%	0.011%
44	7.309	1928	1934	1936	rVB6	1202	1275	0.10%	0.013%
45	7.389	1956	1959	1960	rBV3	1474	797	0.06%	0.008%
46	7.463	1980	1982	1988	rVB6	1094	783	0.06%	0.008%
47	7.563	2001	2013	2029	rBV	193236	341393	26.67%	3.413%
48	7.691	2050	2053	2061	rVV8	2157	2705	0.21%	0.027%
49	7.762	2072	2075	2079	rVB6	992	815	0.06%	0.008%
50	7.797	2079	2086	2093	rBV6	1878	2881	0.23%	0.029%
51	7.894	2103	2116	2133	rBV	645644	1106376	86.43%	11.060%
52	8.064	2167	2169	2173	rVB5	1746	955	0.07%	0.010%
53	8.090	2173	2177	2180	rBV6	1511	1485	0.12%	0.015%
54	8.135	2185	2191	2192	rBV5	1257	1154	0.09%	0.012%
55	8.174	2192	2203	2229	rVB	132386	230492	18.01%	2.304%
56	8.347	2255	2257	2262	rVB6	1444	1070	0.08%	0.011%
57	8.450	2287	2289	2292	rBV4	1113	850	0.07%	0.008%
58	8.553	2318	2321	2323	rVV4	1303	779	0.06%	0.008%
59	8.630	2332	2345	2372	rBV3	252972	490877	38.35%	4.907%
60	8.788	2391	2394	2397	rBV4	1129	908	0.07%	0.009%
61	8.958	2440	2447	2448	rBV7	1585	1768	0.14%	0.018%
62	9.190	2516	2519	2522	rBV4	1308	1100	0.09%	0.011%
63	9.209	2522	2525	2530	rVV7	1107	815	0.06%	0.008%
64	9.235	2530	2533	2537	rVV6	901	813	0.06%	0.008%
65	9.411	2575	2588	2609	rBV	499520	842339	65.80%	8.420%
66	9.556	2628	2633	2638	rBV8	1247	1239	0.10%	0.012%
67	9.701	2673	2678	2681	rBV7	2096	2005	0.16%	0.020%
68	9.772	2696	2700	2702	rBV6	1314	875	0.07%	0.009%
69	9.997	2766	2770	2777	rBV9	1308	1307	0.10%	0.013%
70	10.074	2787	2794	2798	rBV8	1995	2254	0.18%	0.023%
71	10.096	2798	2801	2804	rBV5	1336	1009	0.08%	0.010%
72	10.196	2825	2832	2835	rVB9	1422	1663	0.13%	0.017%
73	10.238	2839	2845	2848	rBV8	1364	1461	0.11%	0.015%
74	10.363	2882	2884	2887	rVB4	1440	826	0.06%	0.008%
75	10.463	2912	2915	2917	rBV4	1471	1072	0.08%	0.011%
76	10.752	2991	3005	3022	rBV	406719	657769	51.38%	6.575%

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Stop Thrs : 0

Peak Location: TOP

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 Title : VOC Analysis

77	10.923	3055	3058	3060	rBV4	1029	818	0.06%	0.008%
78	10.964	3068	3071	3076	rBV5	1849	1723	0.13%	0.017%
79	11.054	3096	3099	3106	rBV8	1446	1514	0.12%	0.015%
80	11.093	3106	3111	3114	rBV5	1434	1534	0.12%	0.015%
81	11.234	3153	3155	3159	rVV5	1148	753	0.06%	0.008%
82	11.257	3159	3162	3165	rBV5	1048	814	0.06%	0.008%
83	11.476	3225	3230	3236	rVB10	1363	1541	0.12%	0.015%
84	11.678	3289	3293	3297	rBV7	1352	1396	0.11%	0.014%
85	11.807	3321	3333	3349	rBV	563553	875720	68.41%	8.754%
86	11.990	3382	3390	3393	rBV10	1625	2224	0.17%	0.022%
87	12.074	3413	3416	3417	rBV3	1412	892	0.07%	0.009%
88	12.186	3439	3451	3471	rBV	611217	1000655	78.17%	10.003%
89	12.508	3549	3551	3554	rBV4	1100	867	0.07%	0.009%
90	12.849	3652	3657	3660	rVV6	1500	1344	0.10%	0.013%
91	13.087	3727	3731	3734	rBV5	1087	988	0.08%	0.010%
92	13.398	3824	3828	3831	rBV6	1552	1411	0.11%	0.014%
93	13.839	3960	3965	3973	rVB9	3399	5184	0.40%	0.052%
94	13.984	4007	4010	4012	rBV3	1114	795	0.06%	0.008%
95	14.090	4037	4043	4047	rBV9	2657	3889	0.30%	0.039%
96	14.267	4094	4098	4102	rVB6	1498	1349	0.11%	0.013%
97	14.289	4102	4105	4107	rBV4	1013	782	0.06%	0.008%
98	14.389	4132	4136	4139	rBV6	1429	1128	0.09%	0.011%
99	15.678	4533	4537	4538	rBV4	1497	1071	0.08%	0.011%
100	15.845	4582	4589	4592	rBV8	2251	3051	0.24%	0.030%

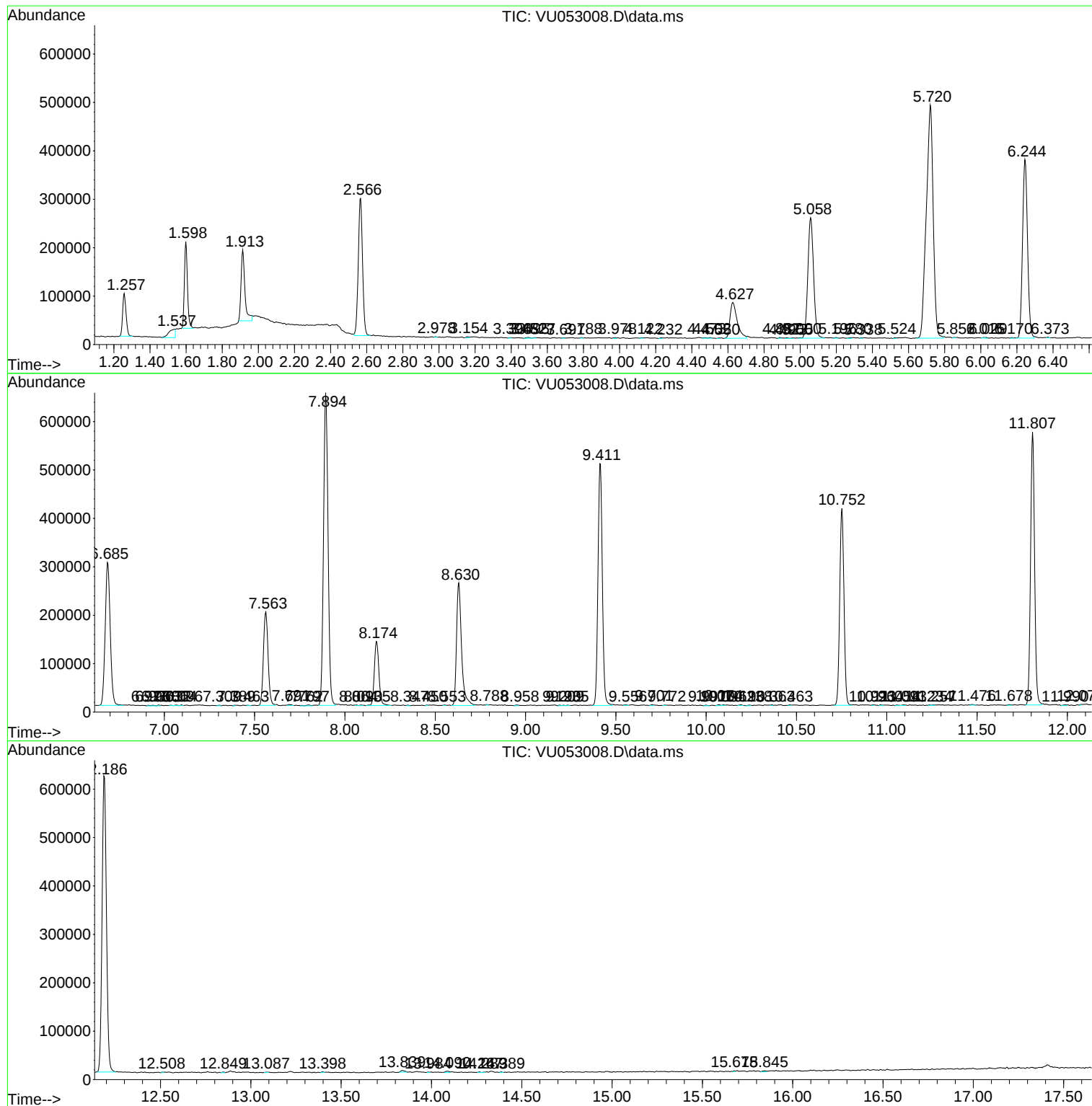
Sum of corrected areas: 10003718

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.M
Quant Title : VOC Analysis

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



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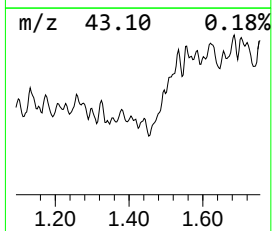
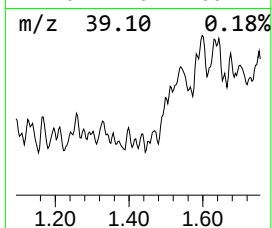
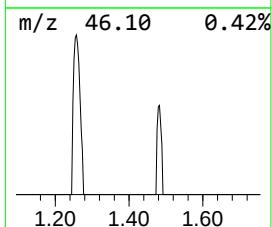
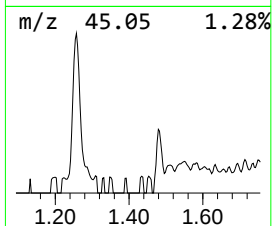
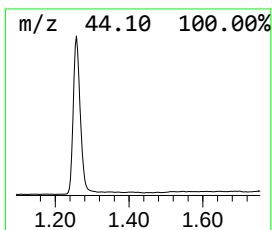
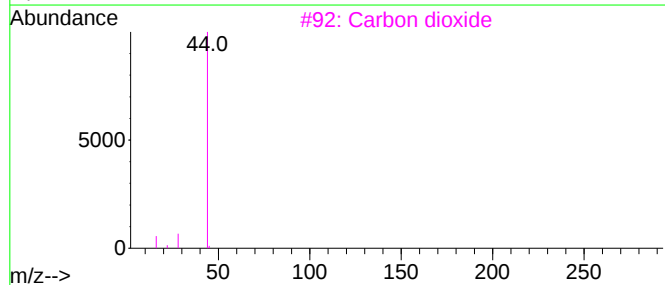
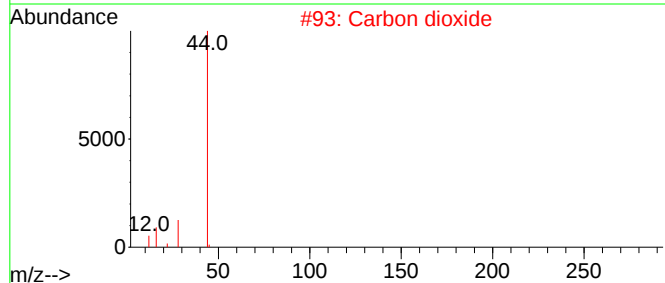
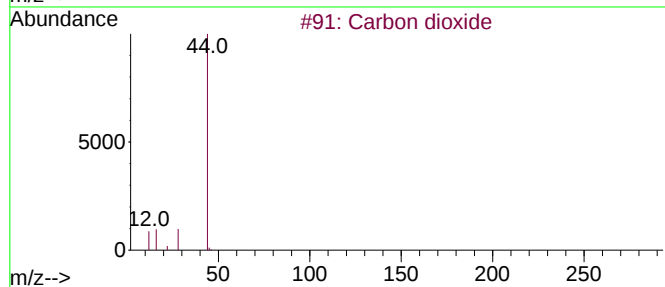
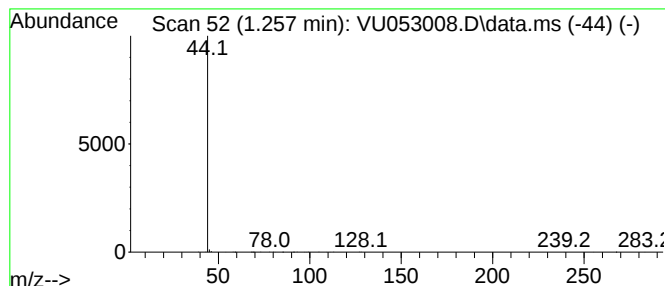
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.257	8.19 ug/L	114261	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbon dioxide	44	CO2	000124-38-9	4
2			Carbon dioxide	44	CO2	000124-38-9	3
3			Carbon dioxide	44	CO2	000124-38-9	3
4			Nitrous oxide	44	N2O	010024-97-2	3
5			(S)-(+)-1-Cyclohexylethylamine	127	C8H17N	017430-98-7	3



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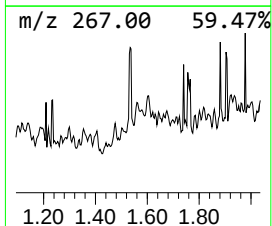
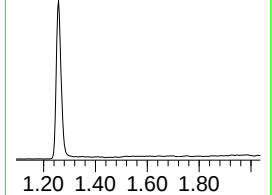
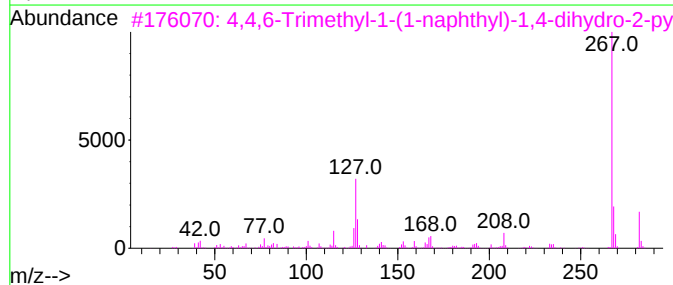
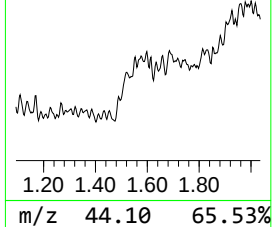
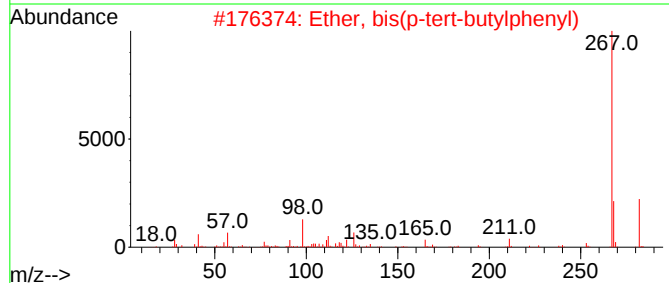
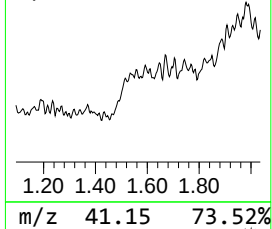
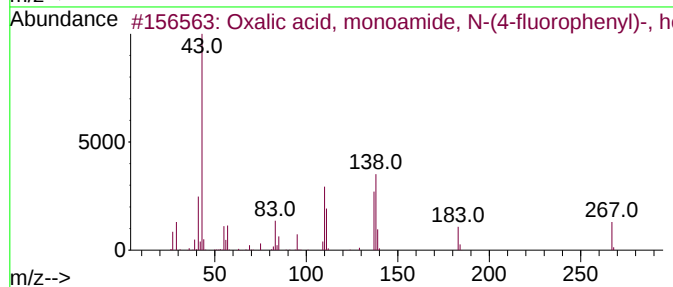
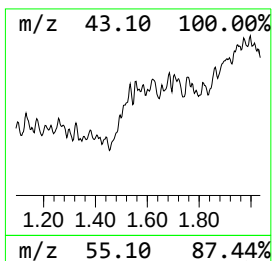
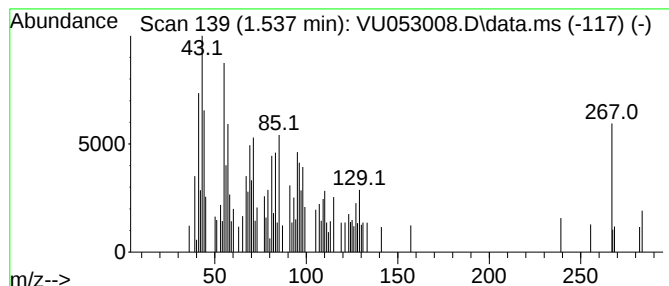
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Quant Title : VOC Analysis

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

Peak Number 2 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.537	3.12 ug/L	43519	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, monoamide, N-(4-flu...	267	C14H18FN03	1000309-42-7	27
2			Ether, bis(p-tert-butylphenyl)	282	C20H26O	024085-65-2	22
3			4,4,6-Trimethyl-1-(1-naphthyl)-1...	282	C17H18N2S	063704-49-4	18
4			4,4,6-Trimethyl-1-(2-naphthyl)-3...	282	C17H18N2S	063704-50-7	14
5			4-[(4-Fluorophenyl)amino]naphtha...	267	C16H10FN02	1574311-28-6	14



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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
unknown-01	1.257	8.2	ug/L	114261	1	6.244	697958	50.0
unknown-02	1.537	3.1	ug/L	43519	1	6.244	697958	50.0