

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU032823\
 Data File : VU053437.D
 Acq On : 28 Mar 2023 16:40
 Operator : JC/MD
 Sample : 02037-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E45E6

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\SFAMULM031523WMA.M
 Title : VOC Analysis

Signal : TIC: VU053437.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	96	rVB	120973	145327	16.66%	2.167%
2	1.912	170	178	194	rBV	94747	131175	15.04%	1.956%
3	2.565	369	381	395	rBV	182672	293965	33.70%	4.384%
4	2.642	397	405	422	rVB	9195	18046	2.07%	0.269%
5	2.993	510	514	515	rBV	341	224	0.03%	0.003%
6	3.128	548	556	566	rBV4	1955	3920	0.45%	0.058%
7	3.192	571	576	579	rBV5	1846	2126	0.24%	0.032%
8	3.420	644	647	649	rBV	233	147	0.02%	0.002%
9	3.478	660	665	669	rBV	233	231	0.03%	0.003%
10	3.661	719	722	726	rVB2	261	157	0.02%	0.002%
11	3.768	752	755	759	rVB2	260	195	0.02%	0.003%
12	3.861	777	784	798	rVB3	1589	3069	0.35%	0.046%
13	4.012	827	831	834	rBV2	175	128	0.01%	0.002%
14	4.198	885	889	890	rBV	177	130	0.01%	0.002%
15	4.272	908	912	914	rBV2	184	186	0.02%	0.003%
16	4.314	920	925	929	rBV2	293	267	0.03%	0.004%
17	4.333	929	931	936	rBV	207	127	0.01%	0.002%
18	4.452	964	968	971	rBV	152	154	0.02%	0.002%
19	4.623	1006	1021	1053	rBV3	78585	271416	31.12%	4.047%
20	4.896	1103	1106	1112	rBV2	337	376	0.04%	0.006%
21	4.986	1128	1134	1136	rBV	272	251	0.03%	0.004%
22	5.057	1140	1156	1177	rBV	157891	346834	39.76%	5.172%
23	5.327	1236	1240	1243	rBV2	203	165	0.02%	0.002%
24	5.546	1304	1308	1309	rBV	193	128	0.01%	0.002%
25	5.558	1309	1312	1317	rVV	182	146	0.02%	0.002%
26	5.719	1340	1362	1392	rBV2	311520	872236	100.00%	13.007%
27	5.947	1430	1433	1434	rBV2	425	227	0.03%	0.003%
28	6.105	1479	1482	1484	rBV2	246	201	0.02%	0.003%
29	6.176	1500	1504	1507	rBV	313	266	0.03%	0.004%
30	6.243	1512	1525	1543	rBV	218546	412634	47.31%	6.153%
31	6.443	1581	1587	1591	rBV2	423	411	0.05%	0.006%
32	6.504	1602	1606	1608	rVB2	322	226	0.03%	0.003%
33	6.533	1608	1615	1627	rBV8	2067	3752	0.43%	0.056%
34	6.687	1648	1663	1682	rBV	199557	389743	44.68%	5.812%
35	6.893	1722	1727	1732	rBV2	251	256	0.03%	0.004%
36	6.944	1739	1743	1747	rBV2	240	189	0.02%	0.003%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
 Title : VOC Analysis

37	6.967	1747	1750	1754	rBV2	296	274	0.03%	0.004%
38	7.015	1754	1765	1768	rBV3	1587	2750	0.32%	0.041%
39	7.185	1812	1818	1822	rBV2	849	1115	0.13%	0.017%
40	7.234	1830	1833	1838	rBV2	184	128	0.01%	0.002%
41	7.337	1862	1865	1868	rBV2	223	222	0.03%	0.003%
42	7.488	1907	1912	1916	rVB2	294	281	0.03%	0.004%
43	7.562	1920	1935	1947	rBV2	112506	194675	22.32%	2.903%
44	7.783	2000	2004	2005	rBV2	305	197	0.02%	0.003%
45	7.845	2019	2023	2025	rBV	319	275	0.03%	0.004%
46	7.893	2025	2038	2061	rVV	401314	681529	78.14%	10.163%
47	8.176	2115	2126	2147	rVV	78819	133623	15.32%	1.993%
48	8.359	2178	2183	2186	rBV2	307	299	0.03%	0.004%
49	8.488	2213	2223	2229	rBV5	1359	2139	0.25%	0.032%
50	8.552	2234	2243	2250	rVB4	3780	5365	0.62%	0.080%
51	8.587	2251	2254	2256	rBV	177	132	0.02%	0.002%
52	8.629	2256	2267	2294	rBV2	219420	424229	48.64%	6.326%
53	8.835	2330	2331	2334	rVB	432	136	0.02%	0.002%
54	8.970	2371	2373	2376	rVB2	286	168	0.02%	0.003%
55	8.992	2376	2380	2381	rBV2	255	184	0.02%	0.003%
56	9.131	2420	2423	2426	rBV	270	158	0.02%	0.002%
57	9.160	2426	2432	2433	rBV2	332	234	0.03%	0.003%
58	9.269	2461	2466	2472	rBV2	477	613	0.07%	0.009%
59	9.372	2495	2498	2499	rBV	306	133	0.02%	0.002%
60	9.414	2499	2511	2538	rVV2	305263	617348	70.78%	9.206%
61	9.594	2561	2567	2575	rBV4	1172	1774	0.20%	0.026%
62	9.664	2581	2589	2602	rVB7	4090	6275	0.72%	0.094%
63	9.790	2625	2628	2631	rBV2	221	190	0.02%	0.003%
64	9.873	2648	2654	2655	rBV3	695	587	0.07%	0.009%
65	9.970	2680	2684	2686	rBV2	727	576	0.07%	0.009%
66	10.053	2706	2710	2712	rBV	189	152	0.02%	0.002%
67	10.070	2712	2715	2718	rVV	246	169	0.02%	0.003%
68	10.098	2718	2724	2727	rVV2	419	423	0.05%	0.006%
69	10.124	2730	2732	2735	rVV	204	132	0.02%	0.002%
70	10.542	2856	2862	2865	rBV2	707	743	0.09%	0.011%
71	10.642	2882	2893	2903	rBV2	17589	27418	3.14%	0.409%
72	10.751	2914	2927	2941	rBV	272640	440366	50.49%	6.567%
73	10.925	2977	2981	2982	rBV	458	318	0.04%	0.005%
74	10.973	2992	2996	2999	rBV3	483	504	0.06%	0.008%
75	11.060	3020	3023	3025	rBV	174	128	0.01%	0.002%
76	11.089	3025	3032	3042	rVB4	1594	2343	0.27%	0.035%

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 Title : VOC Analysis

77	11.176	3049	3059	3074	rBV2	8894	17235	1.98%	0.257%
78	11.282	3088	3092	3093	rBV2	376	272	0.03%	0.004%
79	11.356	3109	3115	3119	rBV2	711	766	0.09%	0.011%
80	11.404	3128	3130	3131	rBV	275	150	0.02%	0.002%
81	11.504	3158	3161	3163	rBV	232	141	0.02%	0.002%
82	11.545	3172	3174	3184	rVB3	833	912	0.10%	0.014%
83	11.738	3222	3234	3244	rBV2	45541	73100	8.38%	1.090%
84	11.806	3244	3255	3275	rVB	320233	517645	59.35%	7.719%
85	12.188	3362	3374	3393	rBV	380571	633617	72.64%	9.449%
86	12.452	3454	3456	3460	rVB2	671	484	0.06%	0.007%
87	12.809	3563	3567	3568	rBV	435	239	0.03%	0.004%
88	12.825	3569	3572	3574	rBV2	507	341	0.04%	0.005%
89	13.092	3649	3655	3658	rBV4	1137	1292	0.15%	0.019%
90	13.503	3780	3783	3785	rBV2	513	349	0.04%	0.005%
91	13.520	3785	3788	3789	rBV2	710	423	0.05%	0.006%
92	13.786	3863	3871	3880	rBV7	2129	3888	0.45%	0.058%
93	13.841	3880	3888	3897	rVB8	2697	4379	0.50%	0.065%
94	13.915	3907	3911	3913	rBV	549	479	0.05%	0.007%
95	13.931	3914	3916	3919	rVV3	999	612	0.07%	0.009%
96	14.040	3947	3950	3952	rBV	717	405	0.05%	0.006%
97	14.076	3957	3961	3963	rBV2	777	633	0.07%	0.009%
98	14.690	4150	4152	4156	rBV	563	403	0.05%	0.006%
99	14.892	4213	4215	4217	rBV2	634	325	0.04%	0.005%
100	15.056	4262	4266	4268	rBV3	486	441	0.05%	0.007%

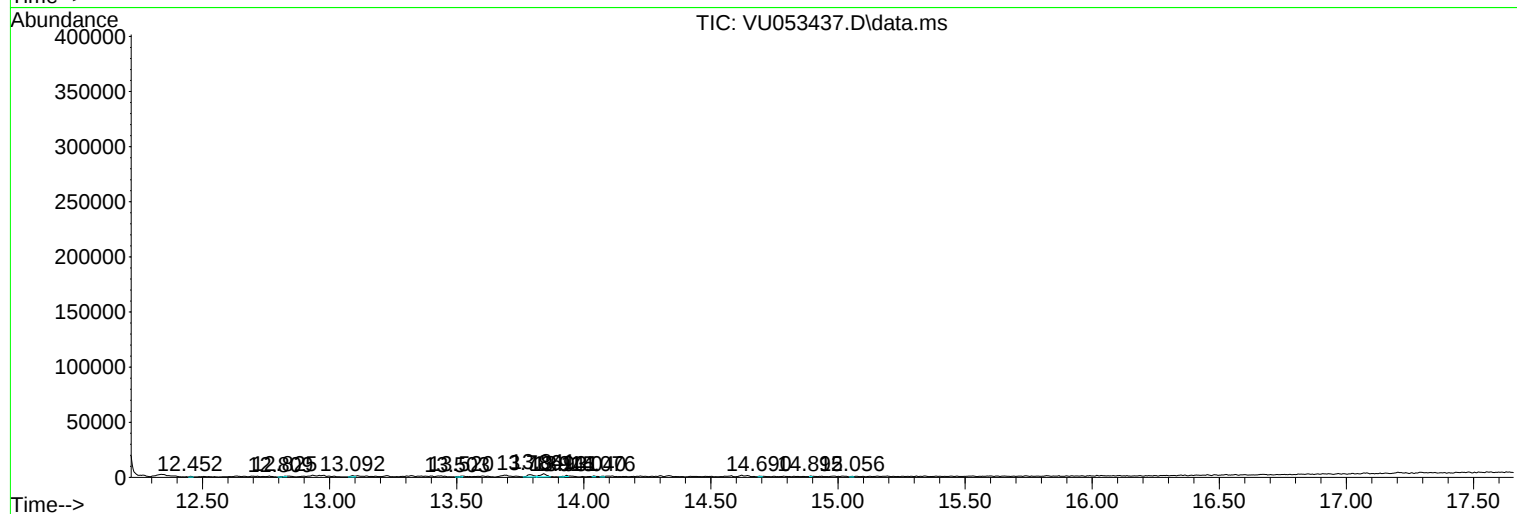
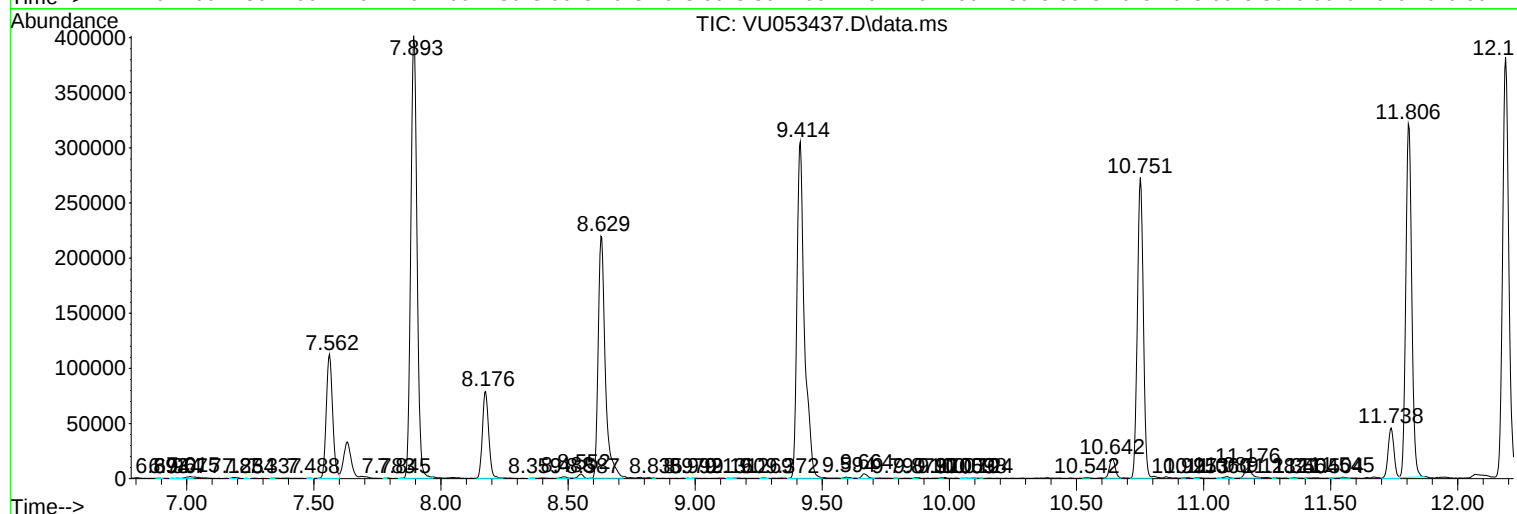
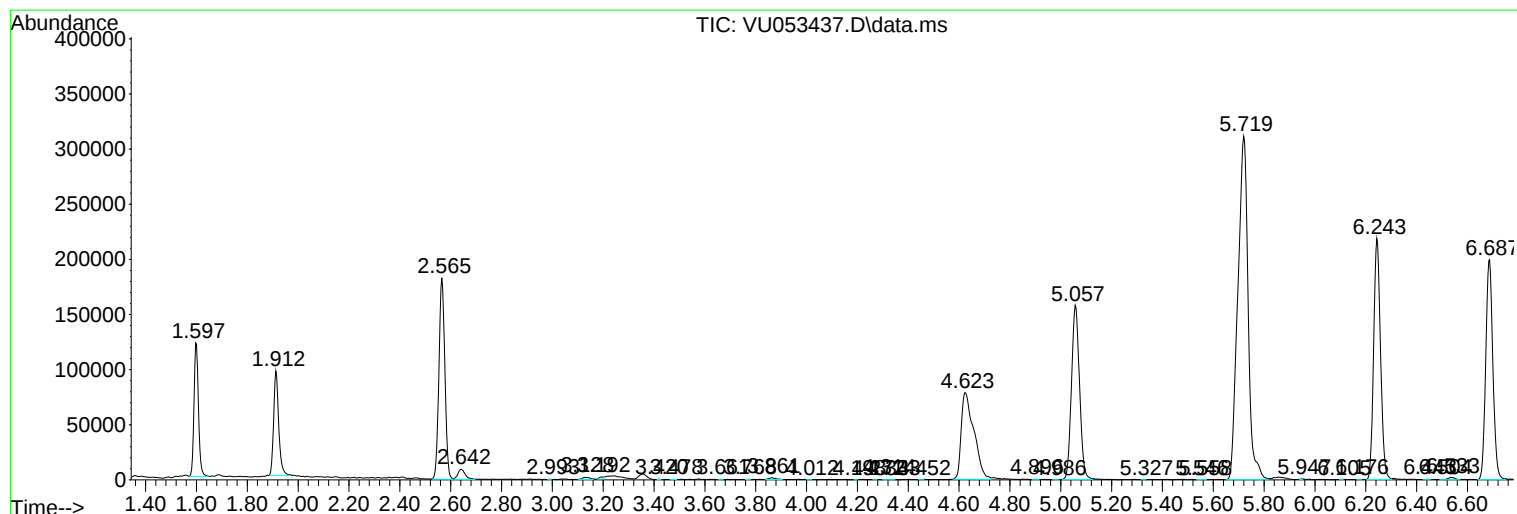
Sum of corrected areas: 6705867

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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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



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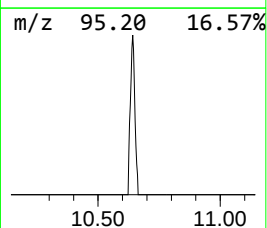
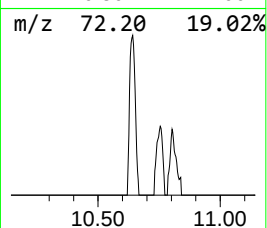
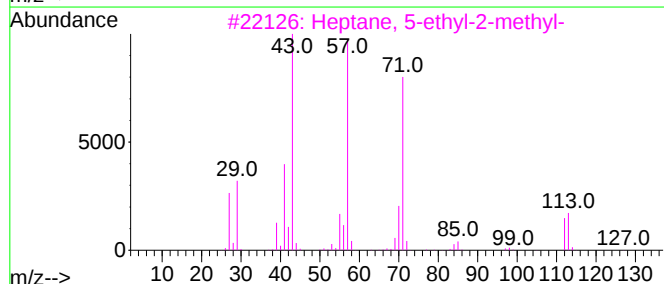
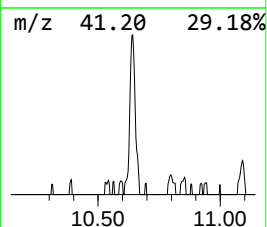
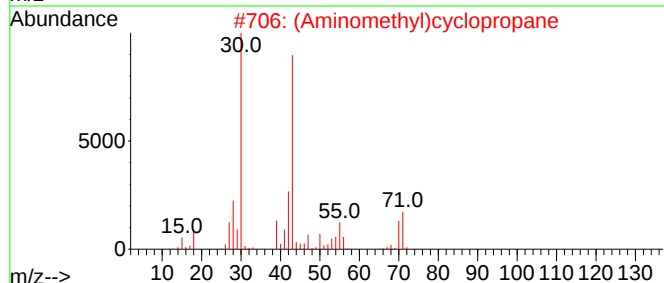
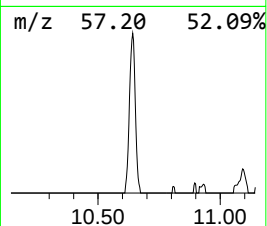
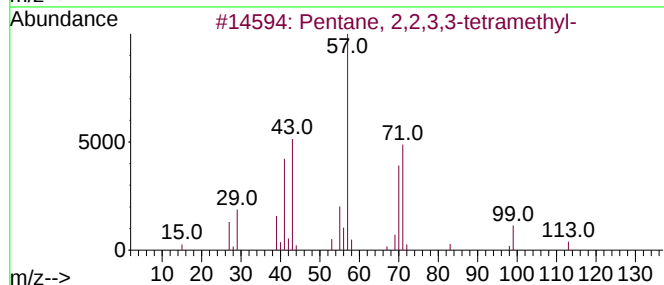
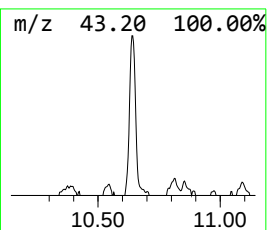
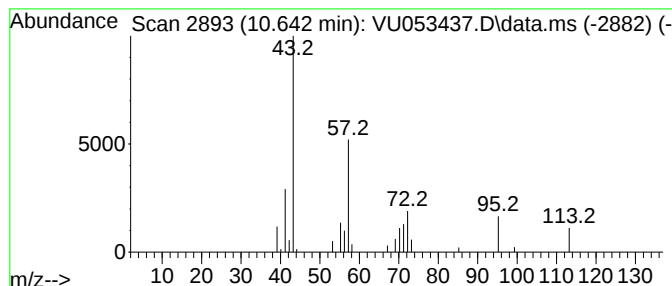
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.642	2.65 ug/L	27418	1,4-Dichlorobenzene-d4	11.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	43
2			(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	32
3			Heptane, 5-ethyl-2-methyl-	142	C10H22	013475-78-0	32
4			Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	32
5			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	25



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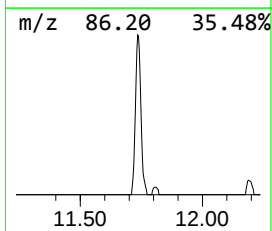
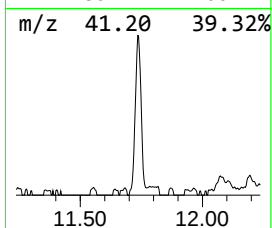
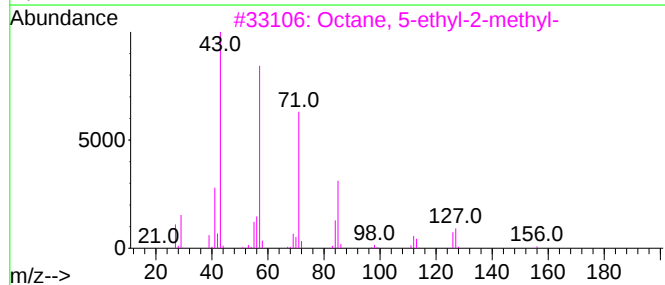
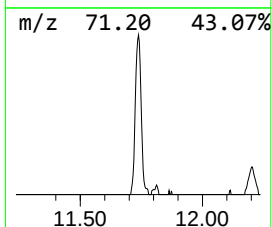
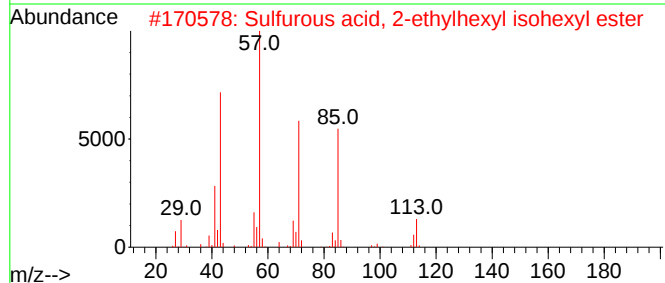
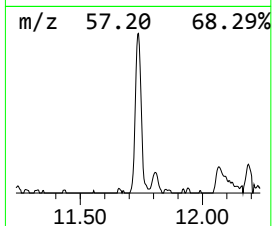
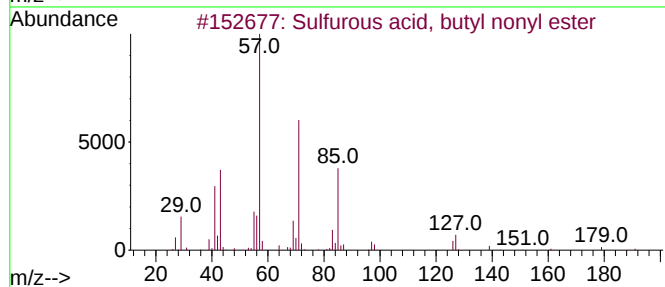
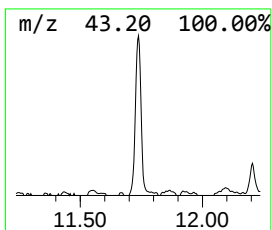
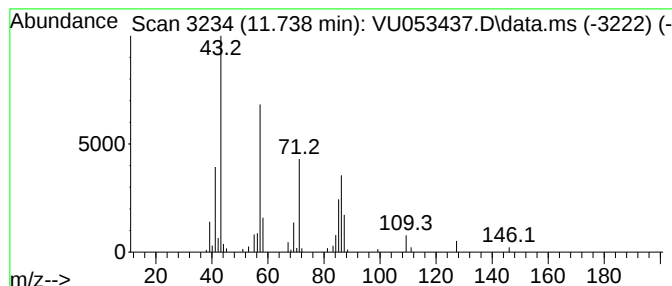
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Quant Title : VOC Analysis

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

Peak Number 3 Sulfurous acid, butyl nonyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.738	7.06 ug/L	73100	1,4-Dichlorobenzene-d4	11.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	53
2			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	47
3			Octane, 5-ethyl-2-methyl-	156	C11H24	062016-18-6	47
4			Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	40
5			Carbonic acid, octadecyl prop-1...	354	C22H42O3	1000383-11-5	40



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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
(DEL) Alkane: S...	10.642	2.6	ug/L	27418	3	11.806	517645	50.0
Sulfurous acid,...	11.738	7.1	ug/L	73100	3	11.806	517645	50.0