

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081821\
 Data File : VV021867.D
 Acq On : 18 Aug 2021 15:52
 Operator : SY/MD
 Sample : M3448-04
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBKE3

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_V\Method\SFAMVLM081621WMA.M
 Title : VOC Analysis

Signal : TIC: VV021867.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	76	82	96	rVB	199500	192540	13.75%	1.728%
2	1.558	154	161	182	rVB	155127	183547	13.11%	1.647%
3	2.105	321	331	344	rBV	280769	406269	29.02%	3.645%
4	2.388	417	419	424	rBV3	587	505	0.04%	0.005%
5	2.687	510	512	518	rBV3	371	314	0.02%	0.003%
6	2.770	528	538	547	rBV3	3587	6973	0.50%	0.063%
7	2.973	599	601	603	rBV2	359	176	0.01%	0.002%
8	3.037	619	621	623	rBV2	335	169	0.01%	0.002%
9	3.281	695	697	702	rVB	333	196	0.01%	0.002%
10	3.359	718	721	724	rBV	277	201	0.01%	0.002%
11	3.539	774	777	781	rBV	291	241	0.02%	0.002%
12	3.645	806	810	814	rBV2	228	185	0.01%	0.002%
13	3.876	872	882	923	rBV	131777	355482	25.39%	3.190%
14	4.349	1007	1029	1054	rBV	228407	568873	40.64%	5.104%
15	4.613	1108	1111	1117	rVB4	480	443	0.03%	0.004%
16	4.777	1159	1162	1169	rVB3	383	394	0.03%	0.004%
17	4.809	1169	1172	1174	rBV2	329	209	0.01%	0.002%
18	4.944	1211	1214	1216	rBV2	369	231	0.02%	0.002%
19	5.047	1229	1246	1275	rBV2	549634	1399832	100.00%	12.561%
20	5.268	1312	1315	1321	rBV2	697	601	0.04%	0.005%
21	5.403	1354	1357	1358	rBV2	494	253	0.02%	0.002%
22	5.432	1364	1366	1368	rBV3	476	238	0.02%	0.002%
23	5.477	1377	1380	1383	rBV3	650	520	0.04%	0.005%
24	5.494	1383	1385	1388	rBV2	398	278	0.02%	0.002%
25	5.539	1396	1399	1402	rVB4	520	337	0.02%	0.003%
26	5.619	1407	1424	1446	rBV	464362	935266	66.81%	8.392%
27	5.908	1502	1514	1532	rBV3	22719	48402	3.46%	0.434%
28	6.014	1544	1547	1550	rVB3	607	333	0.02%	0.003%
29	6.072	1550	1565	1590	rBV	318049	649320	46.39%	5.826%
30	6.365	1652	1656	1658	rBV2	482	295	0.02%	0.003%
31	6.439	1673	1679	1680	rVV2	465	427	0.03%	0.004%
32	6.465	1684	1687	1690	rBV3	307	177	0.01%	0.002%
33	6.506	1696	1700	1702	rBV2	403	239	0.02%	0.002%
34	6.539	1708	1710	1715	rBV2	502	441	0.03%	0.004%
35	6.638	1737	1741	1743	rBV3	761	528	0.04%	0.005%
36	6.744	1771	1774	1778	rVB3	481	321	0.02%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
 Title : VOC Analysis

37	6.989	1838	1850	1873	rBV	173859	316329	22.60%	2.838%
38	7.243	1927	1929	1931	rBV2	519	279	0.02%	0.003%
39	7.317	1940	1952	1971	rBV	612814	1068011	76.30%	9.583%
40	7.548	2021	2024	2029	rVB4	853	691	0.05%	0.006%
41	7.625	2038	2048	2075	rBV	114799	201958	14.43%	1.812%
42	7.886	2126	2129	2132	rVB2	363	177	0.01%	0.002%
43	7.940	2137	2146	2152	rBV4	1202	2068	0.15%	0.019%
44	7.979	2156	2158	2160	rBV2	712	402	0.03%	0.004%
45	8.024	2169	2172	2178	rVB2	490	329	0.02%	0.003%
46	8.091	2182	2193	2231	rBV2	344208	649705	46.41%	5.830%
47	8.442	2300	2302	2303	rBV2	465	184	0.01%	0.002%
48	8.468	2306	2310	2312	rBV2	327	218	0.02%	0.002%
49	8.484	2312	2315	2317	rBV2	519	250	0.02%	0.002%
50	8.532	2322	2330	2332	rBV3	298	423	0.03%	0.004%
51	8.603	2349	2352	2353	rBV2	302	193	0.01%	0.002%
52	8.667	2370	2372	2376	rBV2	511	306	0.02%	0.003%
53	8.725	2387	2390	2394	rBV2	387	317	0.02%	0.003%
54	8.854	2418	2430	2458	rBV	692915	1116322	79.75%	10.017%
55	9.101	2502	2507	2512	rBV4	527	540	0.04%	0.005%
56	9.146	2518	2521	2523	rBV3	688	447	0.03%	0.004%
57	9.246	2550	2552	2554	rVB	477	214	0.02%	0.002%
58	9.336	2578	2580	2587	rVB	379	205	0.01%	0.002%
59	9.371	2587	2591	2593	rBV2	270	201	0.01%	0.002%
60	9.384	2593	2595	2597	rBV	393	227	0.02%	0.002%
61	9.419	2604	2606	2608	rBV	273	177	0.01%	0.002%
62	9.487	2623	2627	2631	rVB2	343	267	0.02%	0.002%
63	9.513	2631	2635	2637	rBV	336	259	0.02%	0.002%
64	9.587	2654	2658	2660	rBV	415	306	0.02%	0.003%
65	9.847	2737	2739	2742	rVV	371	206	0.01%	0.002%
66	9.866	2742	2745	2749	rVB	282	208	0.01%	0.002%
67	9.918	2758	2761	2762	rBV	266	176	0.01%	0.002%
68	9.937	2765	2767	2771	rVB2	392	218	0.02%	0.002%
69	10.075	2804	2810	2812	rBV2	429	366	0.03%	0.003%
70	10.127	2816	2826	2829	rBV6	923	1143	0.08%	0.010%
71	10.220	2843	2855	2879	rVV	450001	716467	51.18%	6.429%
72	10.384	2902	2906	2912	rBV4	1526	1416	0.10%	0.013%
73	10.580	2964	2967	2968	rBV	360	175	0.01%	0.002%
74	10.606	2973	2975	2981	rVB4	429	204	0.01%	0.002%
75	10.767	3023	3025	3030	rVB4	269	198	0.01%	0.002%
76	10.870	3053	3057	3060	rVB2	326	186	0.01%	0.002%

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 Title : VOC Analysis

77	10.918	3067	3072	3074	rBV5	1216	1006	0.07%	0.009%
78	11.014	3095	3102	3107	rVB2	415	390	0.03%	0.003%
79	11.085	3120	3124	3127	rVB2	303	242	0.02%	0.002%
80	11.107	3127	3131	3135	rBV3	444	453	0.03%	0.004%
81	11.146	3141	3143	3149	rVB2	584	327	0.02%	0.003%
82	11.252	3164	3176	3197	rBV	699179	1076557	76.91%	9.660%
83	11.509	3254	3256	3257	rBV	458	175	0.01%	0.002%
84	11.538	3258	3265	3271	rVV5	2481	3677	0.26%	0.033%
85	11.625	3279	3292	3314	rBV	651722	1049588	74.98%	9.418%
86	12.033	3416	3419	3423	rVB2	475	314	0.02%	0.003%
87	12.062	3424	3428	3430	rVV3	418	292	0.02%	0.003%
88	12.146	3450	3454	3457	rBV3	454	388	0.03%	0.003%
89	12.210	3471	3474	3477	rBV2	210	186	0.01%	0.002%
90	12.355	3516	3519	3522	rBV2	267	228	0.02%	0.002%
91	12.705	3625	3628	3631	rBV3	484	378	0.03%	0.003%
92	12.860	3673	3676	3678	rBV2	324	182	0.01%	0.002%
93	13.140	3760	3763	3765	rBV2	285	194	0.01%	0.002%
94	13.268	3800	3803	3805	rBV	493	352	0.03%	0.003%
95	13.516	3876	3880	3881	rBV	1038	704	0.05%	0.006%
96	14.033	4038	4041	4042	rBV	670	360	0.03%	0.003%
97	14.162	4078	4081	4084	rBV2	570	328	0.02%	0.003%
98	14.638	4222	4229	4240	rVB2	7147	11126	0.79%	0.100%
99	14.818	4277	4285	4300	rVB	30983	50097	3.58%	0.450%
100	16.487	4796	4804	4818	rVB	70860	110299	7.88%	0.990%

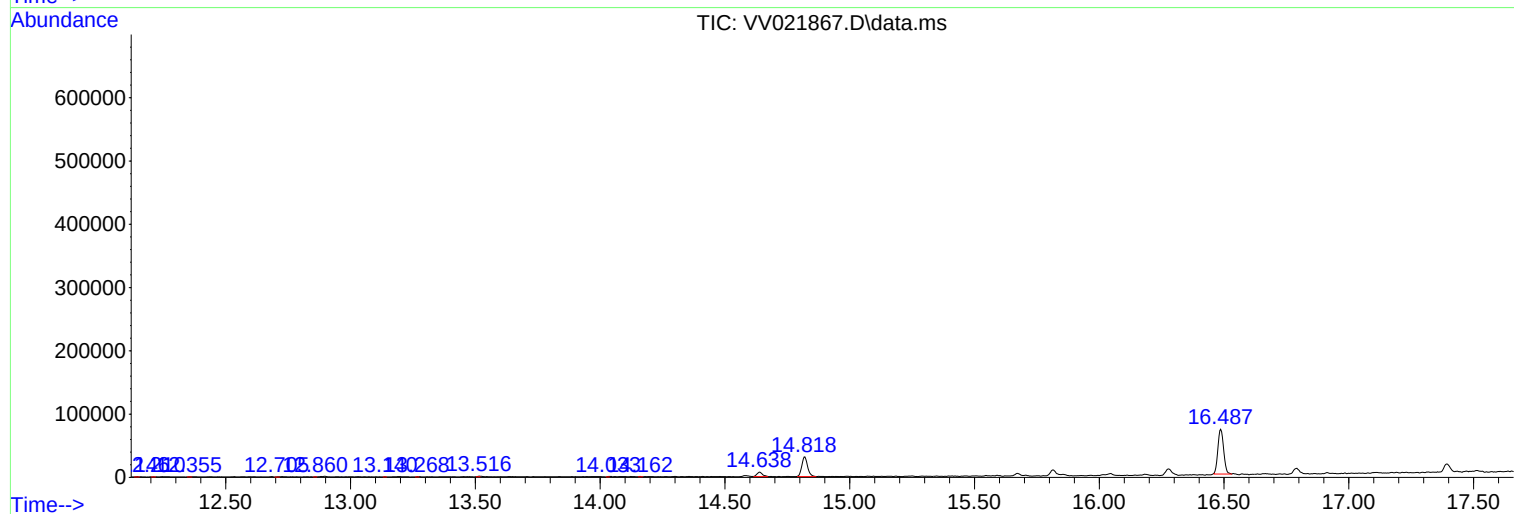
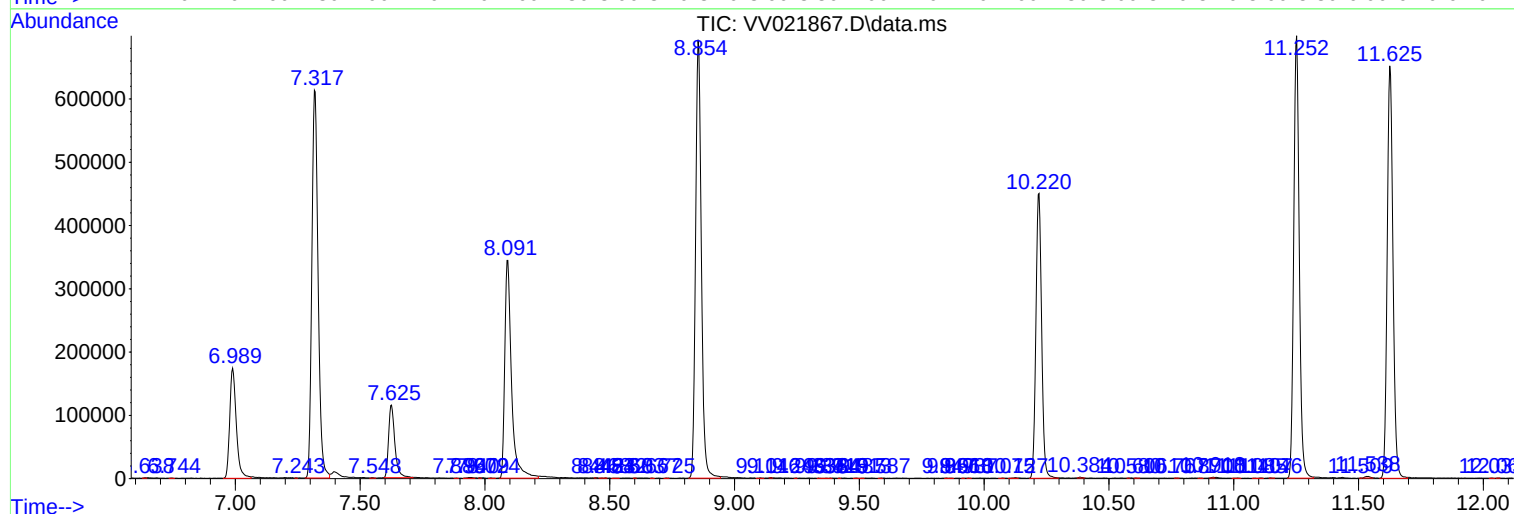
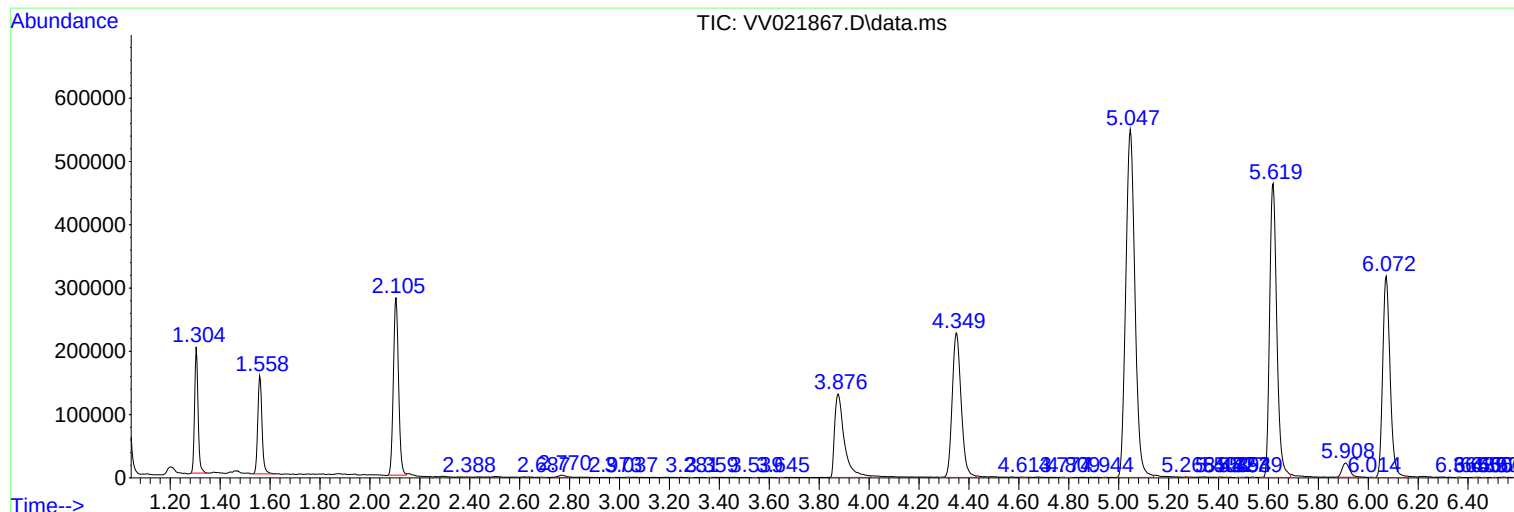
Sum of corrected areas: 11144567

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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



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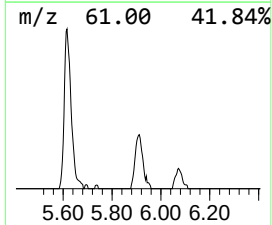
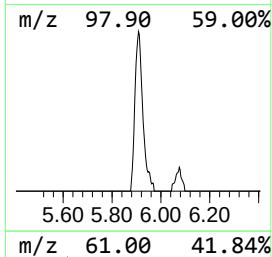
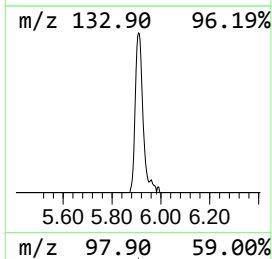
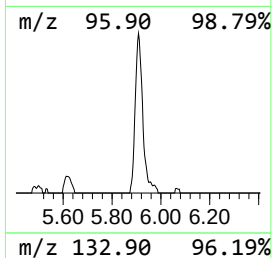
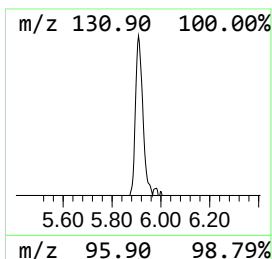
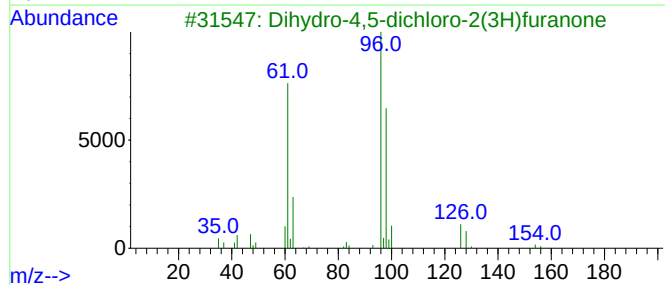
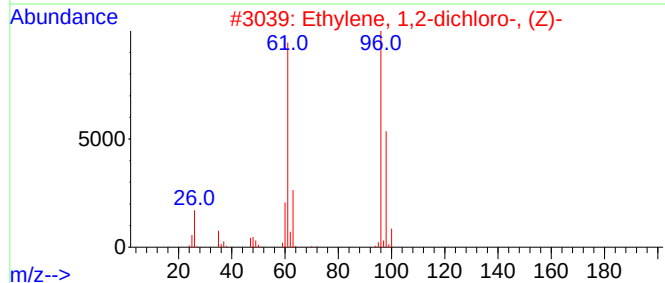
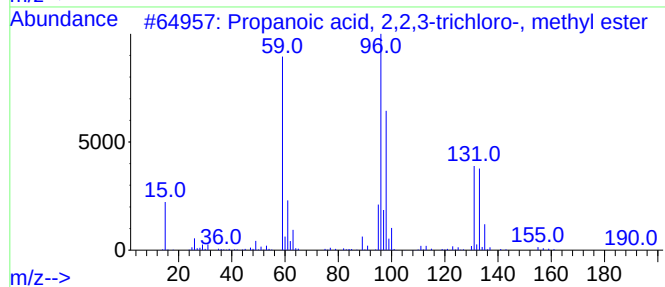
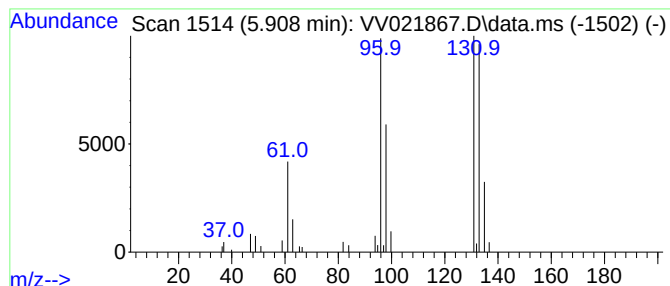
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	2.59 ug/L	48402	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	72
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	35
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25
5			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	23



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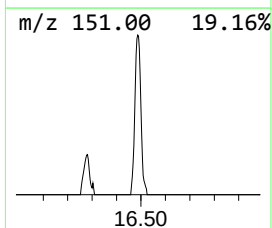
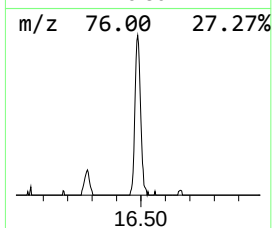
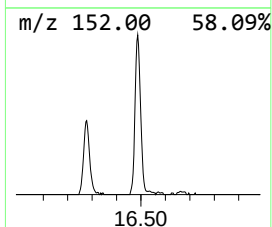
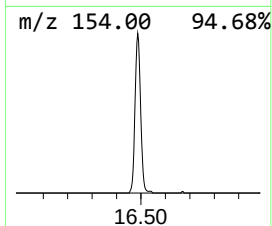
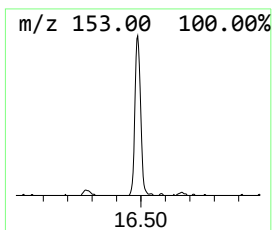
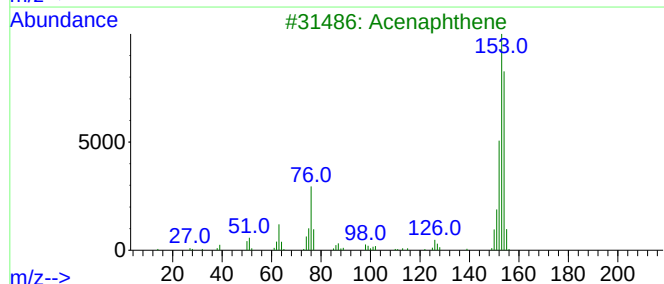
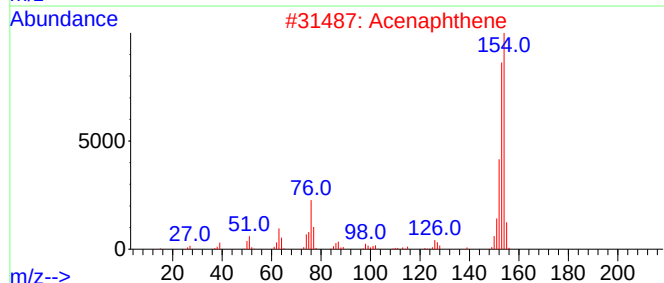
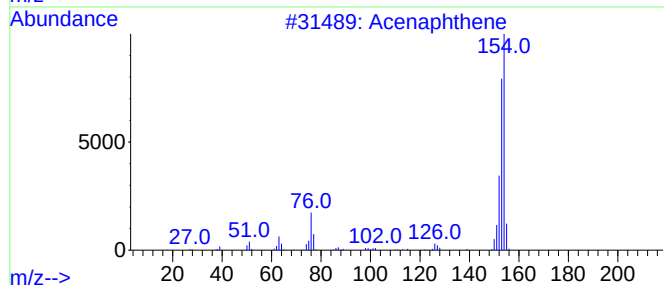
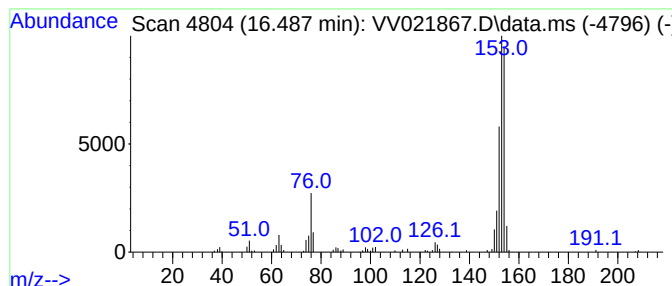
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Peak Number 3 Naphthalene, 2-ethenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.487	5.12 ug/L	110299	1,4-Dichlorobenzene-d4	11.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	93
2			Acenaphthene	154	C12H10	000083-32-9	90
3			Acenaphthene	154	C12H10	000083-32-9	89
4			Acenaphthene	154	C12H10	000083-32-9	72
5			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	64



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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
Propanoic acid,...	5.908	2.6	ug/L	48402	1	5.619	935266	50.0
Naphthalene, 2-...	16.487	5.1	ug/L	110299	3	11.252	1076560	50.0