

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
 Data File : VU051984.D
 Acq On : 20 Nov 2022 19:32
 Operator : JC/MD
 Sample : N5710-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0KY8

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\SFAMULM111522WMA.M
 Title : VOC Analysis

Signal : TIC: VU051984.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	25	rVB	58004	63833	0.18%	0.116%
2	1.491	40	47	53	rBV4	9617	11893	0.03%	0.022%
3	1.601	72	81	95	rBV3	197586	251456	0.70%	0.458%
4	1.903	167	175	196	rVB	108015	164948	0.46%	0.300%
5	2.350	312	314	315	rBV2	844	436	0.00%	0.001%
6	2.578	365	385	413	rBV	2155555	3668301	10.21%	6.675%
7	3.048	520	531	545	rBV3	11172	22151	0.06%	0.040%
8	3.179	562	572	585	rVB2	3991	8648	0.02%	0.016%
9	3.285	598	605	608	rBV	413	387	0.00%	0.001%
10	3.356	615	627	636	rBV4	4175	8374	0.02%	0.015%
11	3.536	680	683	685	rBV	372	249	0.00%	0.000%
12	3.578	692	696	699	rBV3	636	400	0.00%	0.001%
13	3.867	767	786	807	rBV2	104305	251747	0.70%	0.458%
14	3.974	817	819	825	rVV	363	301	0.00%	0.001%
15	4.025	832	835	838	rVB2	519	335	0.00%	0.001%
16	4.051	838	843	846	rVB3	350	337	0.00%	0.001%
17	4.076	846	851	856	rBV2	502	518	0.00%	0.001%
18	4.568	999	1004	1006	rBV4	1107	949	0.00%	0.002%
19	4.662	1007	1033	1065	rVV2	1185461	3093047	8.61%	5.629%
20	4.803	1068	1077	1107	rVB	54768	133765	0.37%	0.243%
21	5.060	1141	1157	1183	rBV	262682	574743	1.60%	1.046%
22	5.234	1208	1211	1216	rBV3	294	298	0.00%	0.001%
23	5.295	1222	1230	1233	rBV5	996	1338	0.00%	0.002%
24	5.382	1251	1257	1262	rBV3	683	996	0.00%	0.002%
25	5.472	1280	1285	1290	rBV2	349	378	0.00%	0.001%
26	5.555	1306	1311	1316	rBV3	364	377	0.00%	0.001%
27	5.723	1339	1363	1379	rBV2	463093	1313845	3.66%	2.391%
28	5.887	1411	1414	1417	rVB2	523	329	0.00%	0.001%
29	6.025	1446	1457	1470	rVB	6698	12032	0.03%	0.022%
30	6.112	1482	1484	1487	rVB3	460	264	0.00%	0.000%
31	6.131	1487	1490	1493	rVB2	443	281	0.00%	0.001%
32	6.247	1511	1526	1550	rBV	562677	1083913	3.02%	1.972%
33	6.408	1573	1576	1582	rBV4	716	629	0.00%	0.001%
34	6.443	1582	1587	1593	rBV3	340	440	0.00%	0.001%
35	6.543	1593	1618	1652	rBV	19336647	35936070	100.00%	65.395%
36	6.687	1653	1663	1688	rVB	346546	700286	1.95%	1.274%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
 Title : VOC Analysis

37	6.961	1737	1748	1763	rBV	32026	61488	0.17%	0.112%
38	7.182	1803	1817	1830	rBV4	7411	16441	0.05%	0.030%
39	7.350	1865	1869	1872	rBV2	373	318	0.00%	0.001%
40	7.424	1889	1892	1898	rVB2	493	482	0.00%	0.001%
41	7.469	1898	1906	1909	rBV4	764	955	0.00%	0.002%
42	7.488	1909	1912	1919	rBV2	434	383	0.00%	0.001%
43	7.562	1922	1935	1953	rBV	144908	259015	0.72%	0.471%
44	7.687	1968	1974	1987	rBV5	3708	7145	0.02%	0.013%
45	7.790	2004	2006	2009	rBV2	497	327	0.00%	0.001%
46	7.896	2024	2039	2058	rBV	470933	823034	2.29%	1.498%
47	8.041	2076	2084	2091	rVB5	1770	2900	0.01%	0.005%
48	8.176	2114	2126	2144	rBV	102754	172052	0.48%	0.313%
49	8.488	2208	2223	2230	rBV5	9161	17663	0.05%	0.032%
50	8.549	2230	2242	2257	rVV	599073	1021425	2.84%	1.859%
51	8.629	2257	2267	2307	rVB2	490410	943504	2.63%	1.717%
52	8.890	2347	2348	2354	rVB2	829	376	0.00%	0.001%
53	8.993	2377	2380	2382	rVB2	466	266	0.00%	0.000%
54	9.005	2382	2384	2389	rBV3	565	503	0.00%	0.001%
55	9.034	2391	2393	2397	rVV3	370	251	0.00%	0.000%
56	9.343	2486	2489	2495	rVB3	536	495	0.00%	0.001%
57	9.414	2496	2511	2540	rBV	808290	1334719	3.71%	2.429%
58	9.694	2591	2598	2600	rBV4	525	557	0.00%	0.001%
59	9.758	2607	2618	2631	rVB4	3907	6246	0.02%	0.011%
60	9.848	2642	2646	2650	rVB2	374	376	0.00%	0.001%
61	9.877	2650	2655	2656	rBV	359	285	0.00%	0.001%
62	10.137	2734	2736	2739	rVB2	440	255	0.00%	0.000%
63	10.160	2739	2743	2744	rBV2	481	298	0.00%	0.001%
64	10.195	2751	2754	2760	rVB2	350	274	0.00%	0.000%
65	10.227	2760	2764	2768	rBV2	434	390	0.00%	0.001%
66	10.272	2775	2778	2787	rVB3	357	444	0.00%	0.001%
67	10.536	2855	2860	2862	rBV2	437	389	0.00%	0.001%
68	10.568	2866	2870	2873	rBV2	468	358	0.00%	0.001%
69	10.755	2914	2928	2947	rBV	617268	998284	2.78%	1.817%
70	10.870	2960	2964	2966	rBV2	554	421	0.00%	0.001%
71	10.919	2976	2979	2982	rVB2	348	266	0.00%	0.000%
72	11.057	3018	3022	3025	rBV2	586	365	0.00%	0.001%
73	11.092	3025	3033	3035	rVV2	326	411	0.00%	0.001%
74	11.108	3035	3038	3043	rVB2	377	366	0.00%	0.001%
75	11.169	3053	3057	3061	rBV2	277	271	0.00%	0.000%
76	11.356	3110	3115	3117	rBV3	252	260	0.00%	0.000%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
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77	11.809	3244	3256	3280	rBV	592458	955441	2.66%	1.739%
78	12.060	3324	3334	3357	rVV	44804	84852	0.24%	0.154%
79	12.189	3361	3374	3403	rVV	559156	920272	2.56%	1.675%
80	12.346	3421	3423	3428	rBV3	268	305	0.00%	0.001%
81	12.652	3516	3518	3522	rVB2	515	368	0.00%	0.001%
82	12.716	3536	3538	3542	rVB3	435	250	0.00%	0.000%
83	13.105	3657	3659	3665	rVB3	359	272	0.00%	0.000%
84	13.185	3681	3684	3689	rVB2	711	696	0.00%	0.001%
85	13.619	3815	3819	3823	rBV3	346	298	0.00%	0.001%
86	13.684	3837	3839	3845	rVV3	431	388	0.00%	0.001%
87	13.777	3865	3868	3875	rVB2	626	640	0.00%	0.001%
88	13.812	3875	3879	3882	rBV3	589	449	0.00%	0.001%
89	13.832	3882	3885	3890	rBV2	744	702	0.00%	0.001%
90	13.915	3907	3911	3915	rBV4	718	602	0.00%	0.001%
91	14.028	3942	3946	3948	rBV2	405	371	0.00%	0.001%
92	14.137	3977	3980	3985	rBV2	387	401	0.00%	0.001%
93	14.275	4015	4023	4025	rBV3	735	887	0.00%	0.002%
94	14.346	4042	4045	4047	rBV2	412	274	0.00%	0.000%
95	14.584	4116	4119	4123	rBV	627	517	0.00%	0.001%
96	14.655	4138	4141	4145	rBV3	445	346	0.00%	0.001%
97	14.816	4188	4191	4193	rBV	385	257	0.00%	0.000%
98	15.098	4276	4279	4283	rBV3	498	473	0.00%	0.001%
99	15.301	4337	4342	4346	rBV2	694	752	0.00%	0.001%
100	15.751	4480	4482	4485	rBV3	538	328	0.00%	0.001%

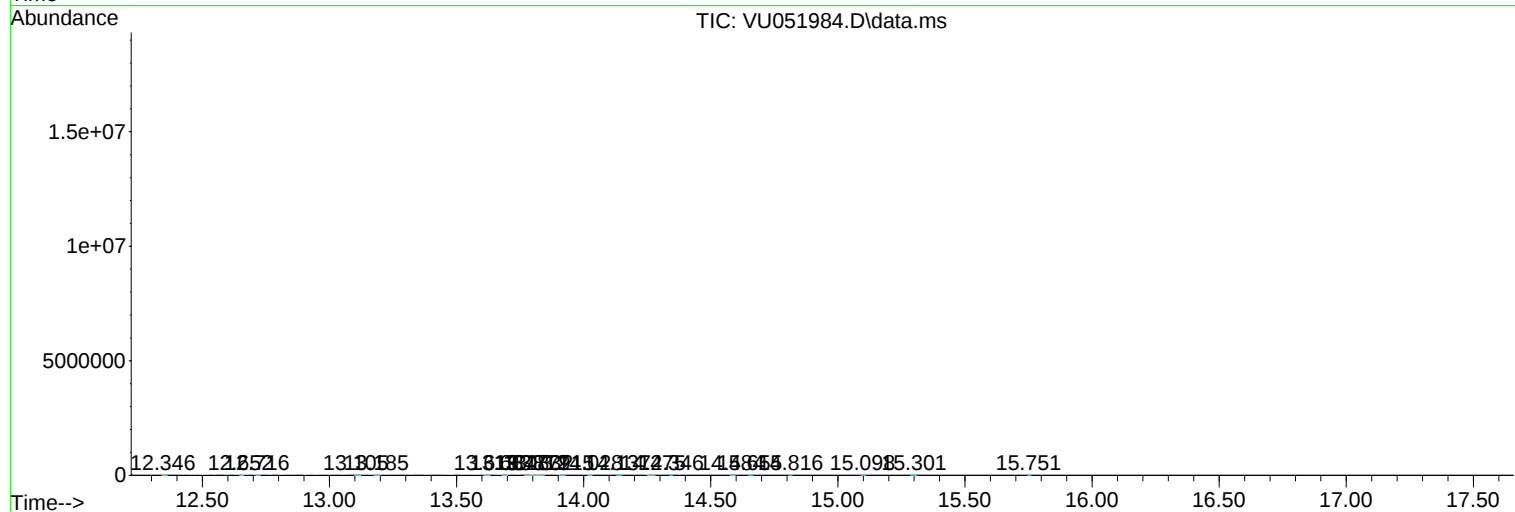
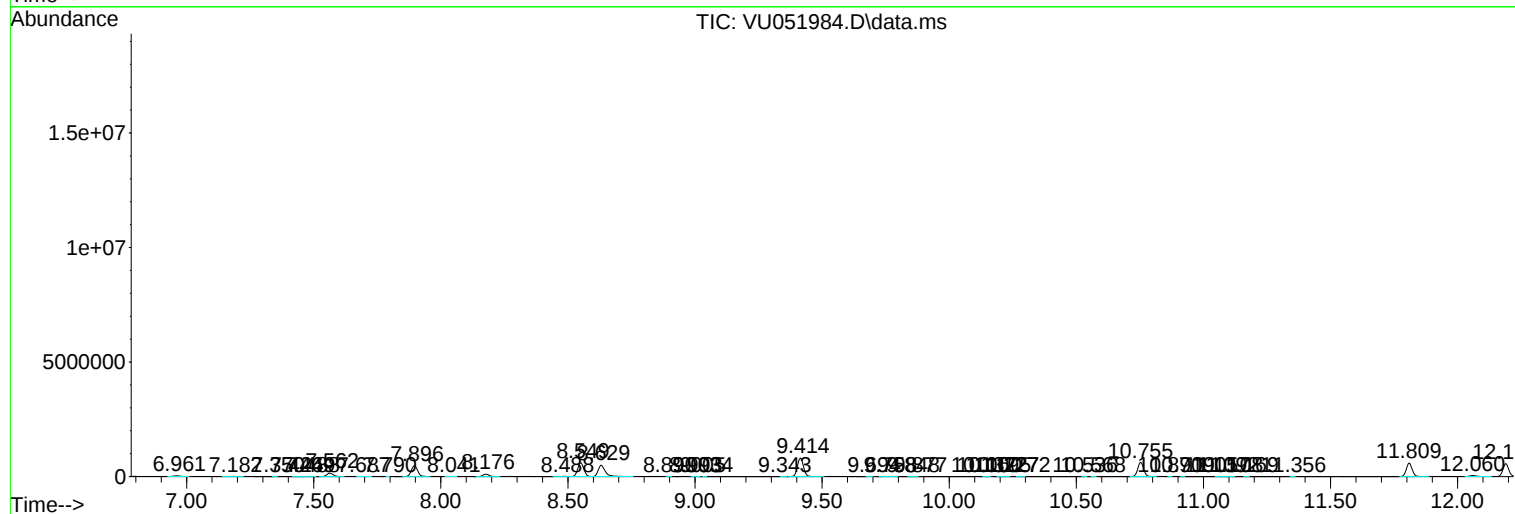
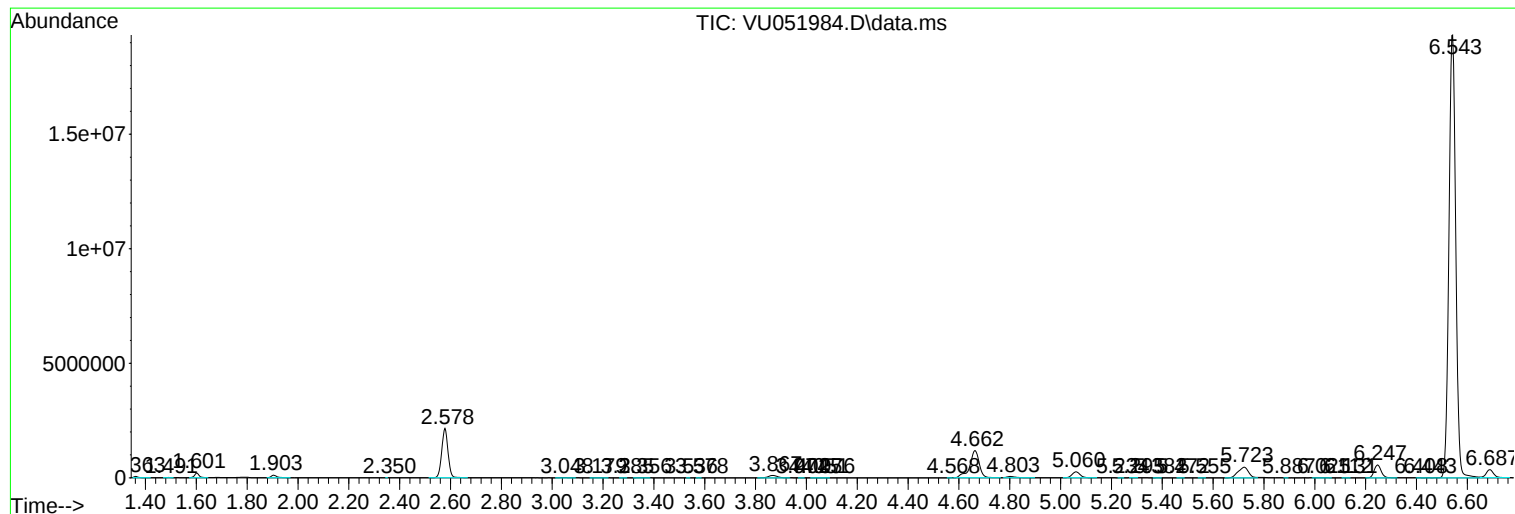
Sum of corrected areas: 54952693

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Instrument :
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ClientSampleId :
COKY8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

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



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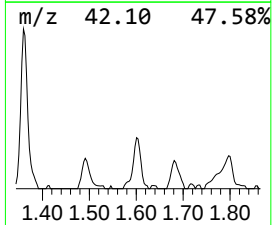
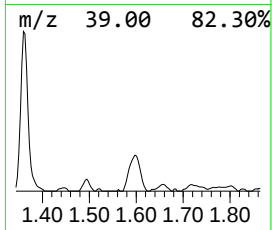
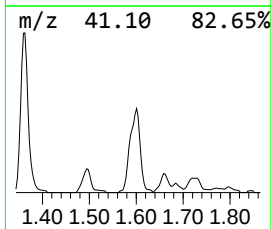
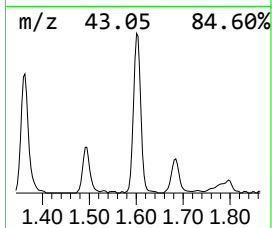
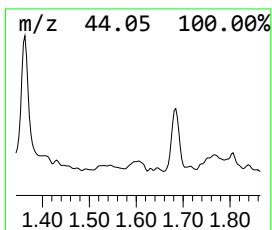
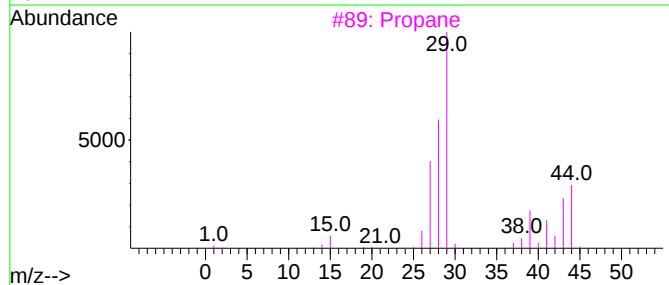
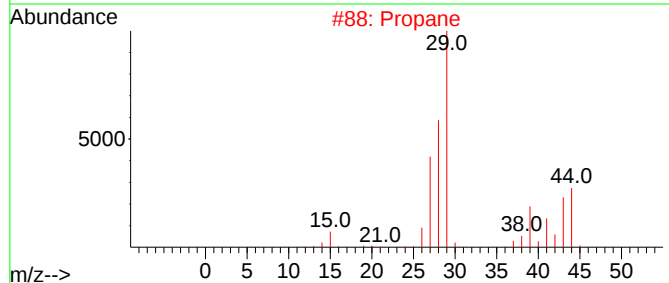
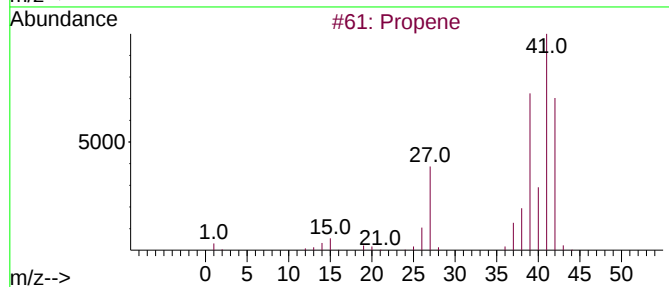
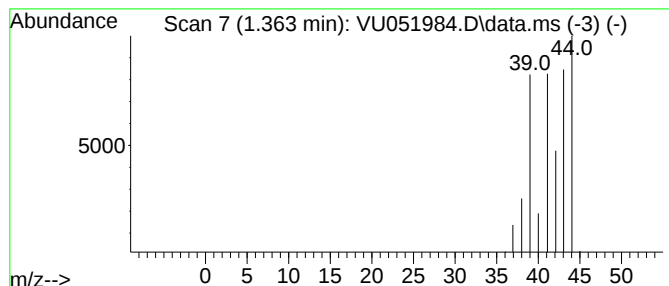
Instrument :
MSVOA_U
ClientSampleId :
COKY8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.363	2.94 ug/L	63833	1,4-Difluorobenzene	6.247	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	10
2	Propane	44	C3H8	000074-98-6	9
3	Propane	44	C3H8	000074-98-6	7
4	Acetonitrile-d3	44	C2D3N	002206-26-0	4
5	Propane	44	C3H8	000074-98-6	4



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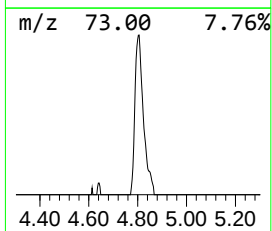
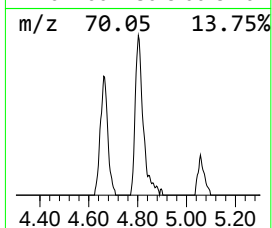
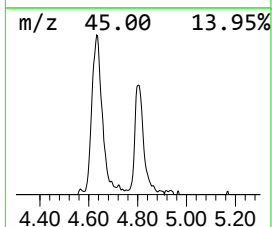
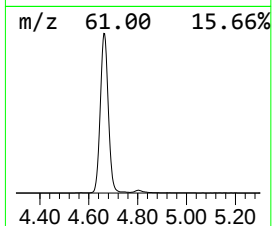
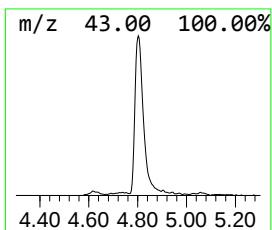
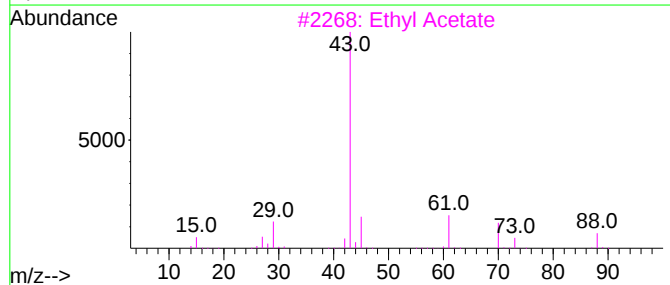
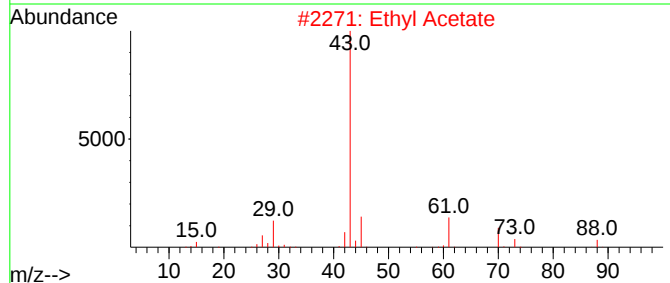
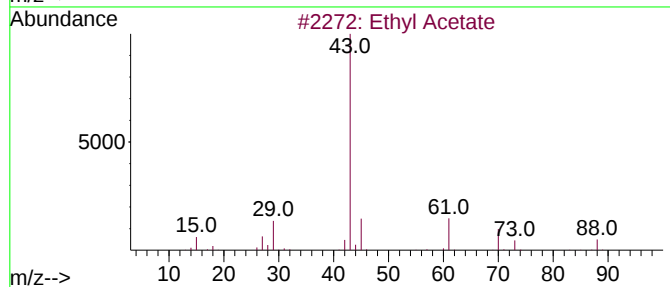
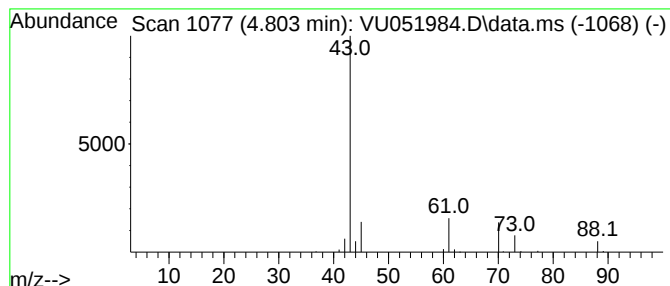
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.803	6.17 ug/L	133765	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	86
2			Ethyl Acetate	88	C4H8O2	000141-78-6	86
3			Ethyl Acetate	88	C4H8O2	000141-78-6	78
4			Ethyl Acetate	88	C4H8O2	000141-78-6	78
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	64



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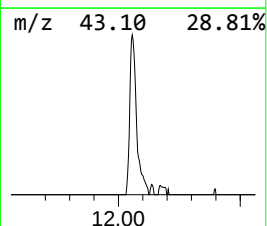
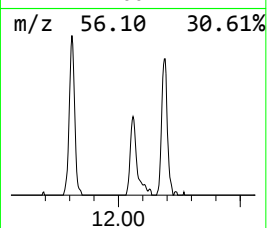
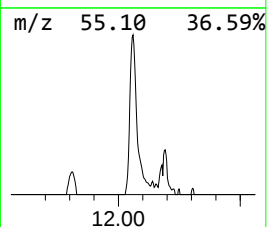
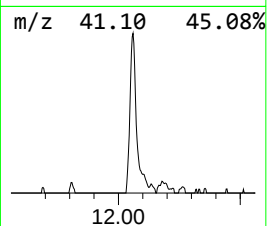
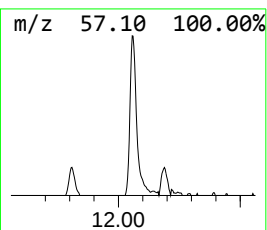
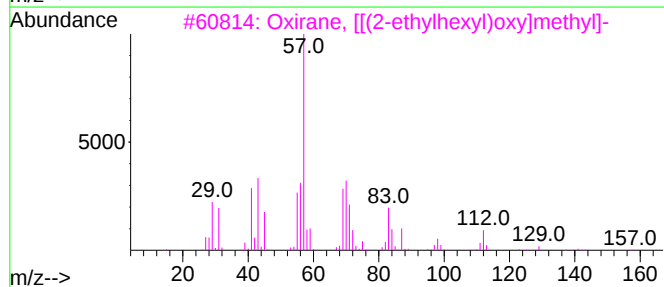
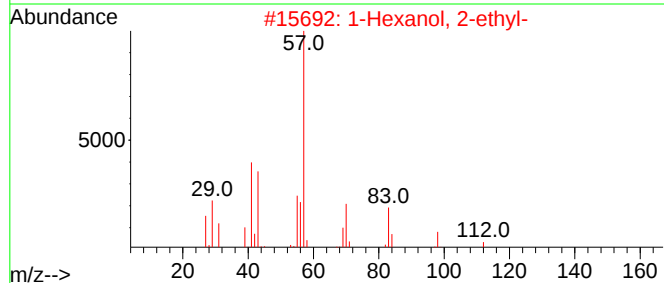
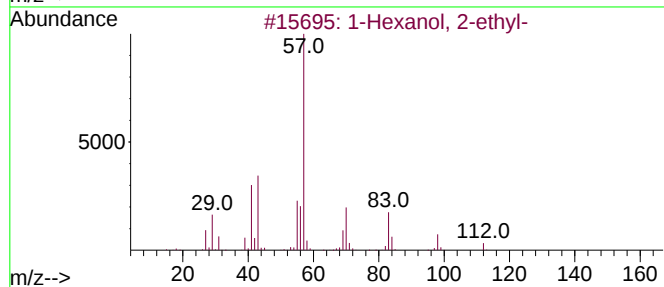
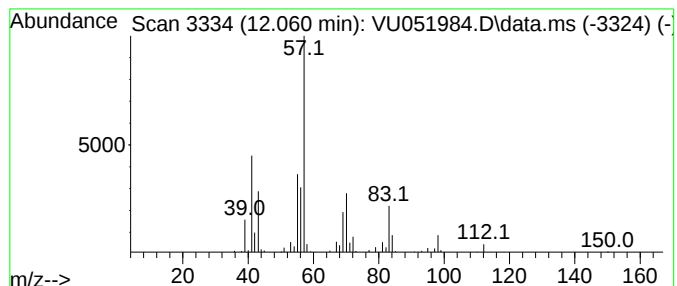
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	4.44 ug/L	84852	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3			Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	64
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
Data File : VU051984.D
Acq On : 20 Nov 2022 19:32
Operator : JC/MD
Sample : N5710-09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0KY8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
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...	1.363	2.9	ug/L	63833	1	6.247	1083910	50.0
Ethyl Acetate	4.803	6.2	ug/L	133765	1	6.247	1083910	50.0
1-Hexanol, 2-et...	12.060	4.4	ug/L	84852	3	11.809	955441	50.0