

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
 Data File : VU047961.D
 Acq On : 12 Apr 2022 17:18
 Operator : SY/MD
 Sample : N2293-06ME
 Misc : 6.6g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNN6ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU047961.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	104	rVB	54570	99186	10.20%	1.152%
2	1.819	121	149	150	rBV8	32158	99458	10.23%	1.155%
3	1.874	161	166	169	rBV	38550	37464	3.85%	0.435%
4	2.542	362	374	385	rBV	126885	217583	22.38%	2.526%
5	2.819	457	460	462	rBV3	503	337	0.03%	0.004%
6	2.906	482	487	495	rVB4	1581	1953	0.20%	0.023%
7	3.034	520	527	539	rBV8	1604	3380	0.35%	0.039%
8	3.089	540	544	546	rBV	367	237	0.02%	0.003%
9	3.147	559	562	565	rVB2	400	280	0.03%	0.003%
10	3.169	565	569	571	rBV3	733	599	0.06%	0.007%
11	3.514	672	676	682	rBV2	326	395	0.04%	0.005%
12	3.565	688	692	697	rBV2	239	325	0.03%	0.004%
13	3.796	759	764	769	rVB2	381	400	0.04%	0.005%
14	3.867	784	786	789	rVB	443	261	0.03%	0.003%
15	3.886	789	792	797	rBV2	414	417	0.04%	0.005%
16	4.629	1010	1023	1064	rBV	96953	310715	31.96%	3.607%
17	4.973	1123	1130	1134	rBV3	273	464	0.05%	0.005%
18	5.063	1141	1158	1180	rVV	171860	390365	40.16%	4.532%
19	5.275	1219	1224	1225	rBV	426	297	0.03%	0.003%
20	5.340	1234	1244	1254	rBV3	2112	4558	0.47%	0.053%
21	5.719	1341	1362	1374	rBV2	357887	972126	100.00%	11.287%
22	5.867	1403	1408	1409	rBV2	419	284	0.03%	0.003%
23	5.919	1422	1424	1430	rVB3	463	332	0.03%	0.004%
24	5.967	1435	1439	1443	rBV2	375	366	0.04%	0.004%
25	6.128	1486	1489	1495	rVB3	691	513	0.05%	0.006%
26	6.247	1509	1526	1557	rBV	351688	690518	71.03%	8.017%
27	6.459	1587	1592	1596	rBV4	416	386	0.04%	0.004%
28	6.520	1606	1611	1614	rBV4	1220	1045	0.11%	0.012%
29	6.568	1622	1626	1631	rBV2	261	263	0.03%	0.003%
30	6.597	1631	1635	1637	rBV2	895	719	0.07%	0.008%
31	6.690	1649	1664	1684	rBV	227536	459640	47.28%	5.336%
32	6.806	1698	1700	1705	rVB2	374	261	0.03%	0.003%
33	7.021	1761	1767	1768	rBV2	320	258	0.03%	0.003%
34	7.185	1805	1818	1836	rBV2	7293	17004	1.75%	0.197%
35	7.491	1908	1913	1914	rBV3	700	536	0.06%	0.006%
36	7.568	1923	1937	1955	rBV	101798	193760	19.93%	2.250%

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 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNN6ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

37	7.693	1968	1976	1986	rBV6	1440	2716	0.28%	0.032%
38	7.899	2025	2040	2055	rBV	334448	599428	61.66%	6.959%
39	7.970	2057	2062	2082	rVB3	11206	22309	2.29%	0.259%
40	8.182	2115	2128	2148	rBV	70218	140977	14.50%	1.637%
41	8.301	2162	2165	2169	rVB3	424	302	0.03%	0.004%
42	8.359	2180	2183	2186	rBV3	661	533	0.05%	0.006%
43	8.648	2258	2273	2313	rBV	393882	772114	79.43%	8.964%
44	8.934	2359	2362	2366	rVB3	407	287	0.03%	0.003%
45	8.954	2366	2368	2377	rVB2	259	244	0.03%	0.003%
46	9.005	2380	2384	2388	rVV3	507	587	0.06%	0.007%
47	9.031	2388	2392	2399	rVB5	1237	1550	0.16%	0.018%
48	9.179	2434	2438	2443	rBV2	428	449	0.05%	0.005%
49	9.250	2455	2460	2465	rBV3	332	392	0.04%	0.005%
50	9.365	2487	2496	2500	rBV3	4107	5766	0.59%	0.067%
51	9.423	2501	2514	2519	rBV	505295	948870	97.61%	11.017%
52	9.571	2557	2560	2569	rVB5	2182	2533	0.26%	0.029%
53	9.697	2593	2599	2607	rVB2	1728	2340	0.24%	0.027%
54	9.957	2677	2680	2683	rVB2	319	249	0.03%	0.003%
55	10.105	2720	2726	2727	rBV2	920	768	0.08%	0.009%
56	10.661	2890	2899	2906	rBV4	2000	3237	0.33%	0.038%
57	10.764	2917	2931	2959	rVB	429895	712028	73.24%	8.267%
58	10.893	2964	2971	2976	rBV2	858	1133	0.12%	0.013%
59	10.976	2985	2997	3005	rBV6	1457	2986	0.31%	0.035%
60	11.092	3030	3033	3037	rBV3	769	462	0.05%	0.005%
61	11.188	3057	3063	3065	rBV2	250	242	0.02%	0.003%
62	11.298	3091	3097	3101	rBV2	463	568	0.06%	0.007%
63	11.336	3105	3109	3112	rBV2	273	251	0.03%	0.003%
64	11.459	3142	3147	3148	rBV2	803	591	0.06%	0.007%
65	11.520	3161	3166	3169	rBV2	472	393	0.04%	0.005%
66	11.545	3169	3174	3177	rBV2	490	435	0.04%	0.005%
67	11.748	3233	3237	3238	rBV2	836	577	0.06%	0.007%
68	11.815	3245	3258	3274	rBV	524298	833068	85.70%	9.672%
69	11.886	3274	3280	3289	rVB8	3306	5649	0.58%	0.066%
70	11.957	3297	3302	3313	rVB7	2532	3996	0.41%	0.046%
71	12.005	3313	3317	3322	rBV2	512	613	0.06%	0.007%
72	12.082	3335	3341	3345	rBV3	463	551	0.06%	0.006%
73	12.195	3364	3376	3395	rBV	390483	648017	66.66%	7.524%
74	12.426	3443	3448	3454	rBV2	356	405	0.04%	0.005%
75	12.475	3458	3463	3468	rVB7	1590	1909	0.20%	0.022%
76	12.523	3475	3478	3481	rVB	463	328	0.03%	0.004%

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 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNN6ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

77	12.565	3488	3491	3499	rBV4	488	602	0.06%	0.007%
78	12.703	3532	3534	3541	rBV3	704	670	0.07%	0.008%
79	12.777	3550	3557	3560	rBV5	696	936	0.10%	0.011%
80	12.876	3585	3588	3592	rVV2	600	488	0.05%	0.006%
81	12.973	3609	3618	3629	rVB2	14669	24524	2.52%	0.285%
82	13.163	3670	3677	3687	rVB7	1809	3166	0.33%	0.037%
83	13.275	3709	3712	3718	rBV2	681	661	0.07%	0.008%
84	13.333	3722	3730	3735	rVV4	3000	4576	0.47%	0.053%
85	13.378	3735	3744	3759	rVB2	40089	61579	6.33%	0.715%
86	13.709	3843	3847	3849	rBV3	358	266	0.03%	0.003%
87	13.722	3849	3851	3856	rVB2	476	315	0.03%	0.004%
88	13.777	3864	3868	3869	rBV2	617	433	0.04%	0.005%
89	14.098	3959	3968	3980	rVB3	1165	2202	0.23%	0.026%
90	14.188	3994	3996	3998	rBV2	497	238	0.02%	0.003%
91	14.359	4044	4049	4057	rVB5	5700	7567	0.78%	0.088%
92	14.429	4062	4071	4081	rBV4	15433	24466	2.52%	0.284%
93	14.494	4081	4091	4108	rVB2	47572	78134	8.04%	0.907%
94	14.632	4131	4134	4136	rVB2	463	269	0.03%	0.003%
95	14.651	4136	4140	4143	rBV3	465	452	0.05%	0.005%
96	14.954	4227	4234	4239	rBV7	2077	2631	0.27%	0.031%
97	15.188	4304	4307	4309	rBV2	675	494	0.05%	0.006%
98	15.314	4339	4346	4353	rVB7	3138	4436	0.46%	0.052%
99	15.545	4403	4418	4430	rBV2	75449	120776	12.42%	1.402%
100	16.388	4673	4680	4692	rVB3	30716	46752	4.81%	0.543%

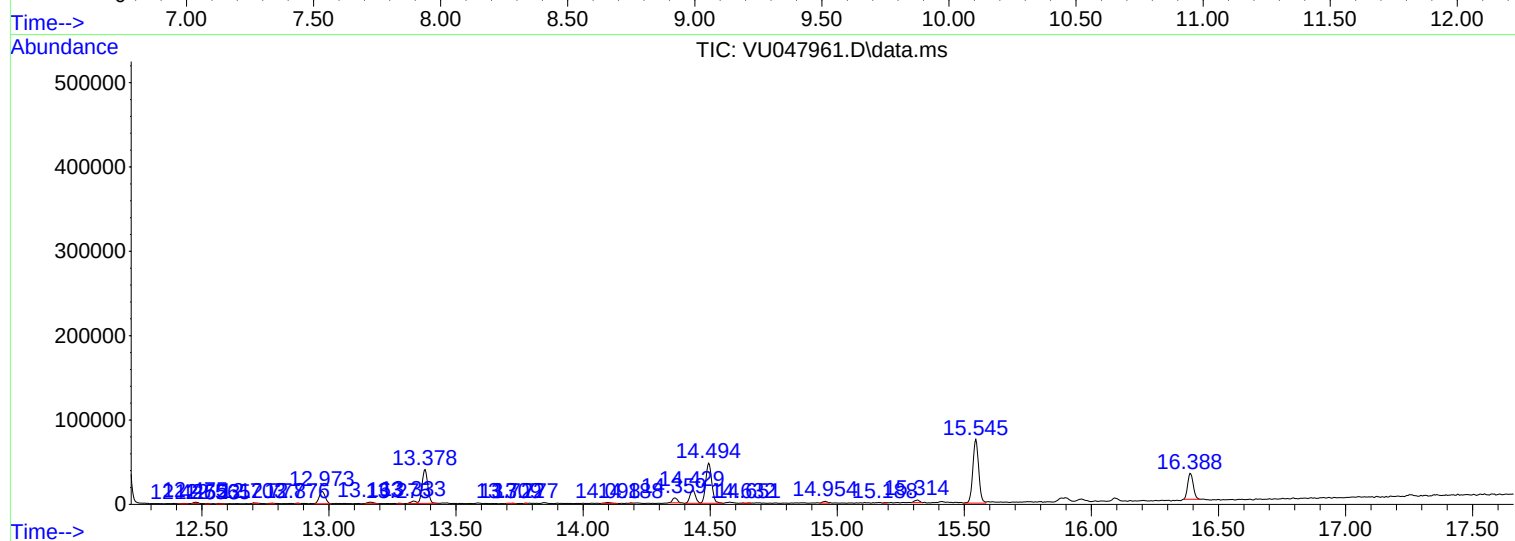
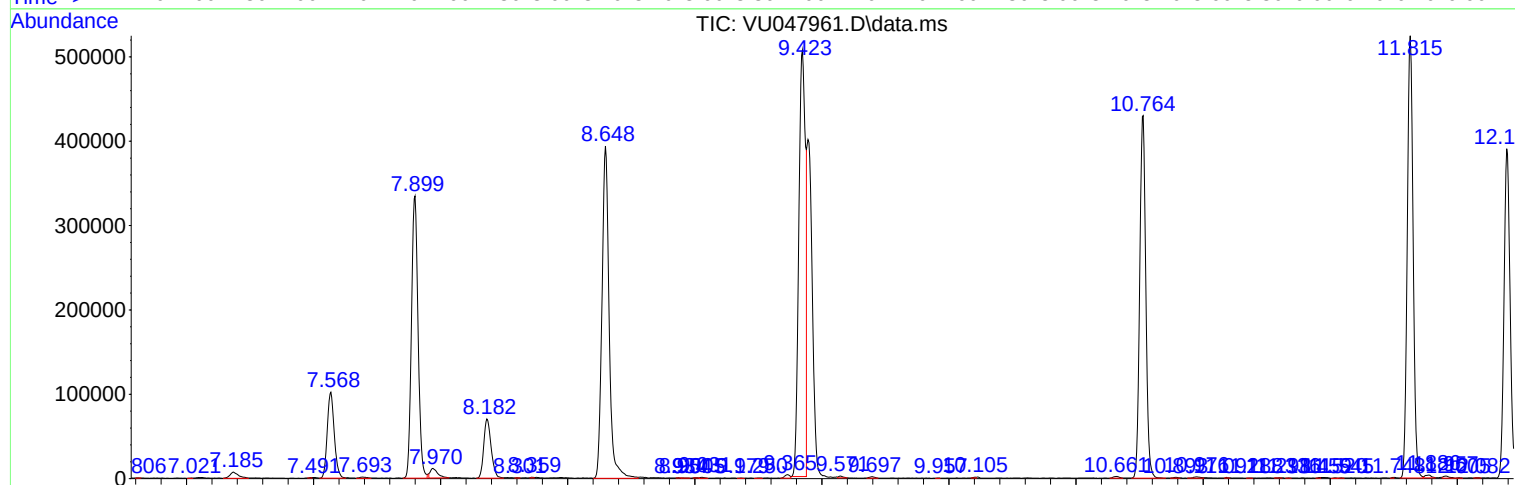
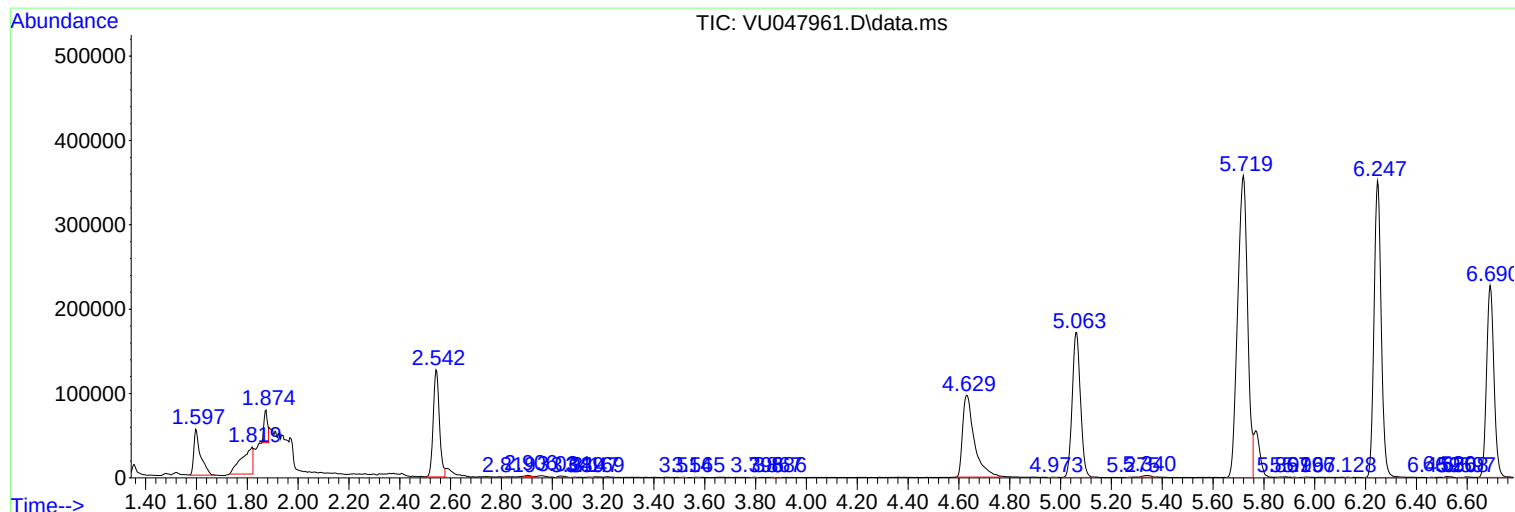
Sum of corrected areas: 8613171

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047961.D
Acq On : 12 Apr 2022 17:18
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Misc : 6.6g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047961.D
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Operator : SY/MD
Sample : N2293-06ME
Misc : 6.6g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

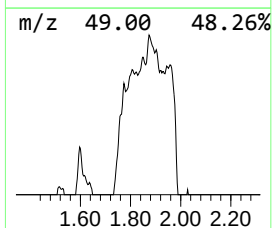
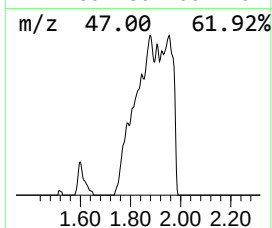
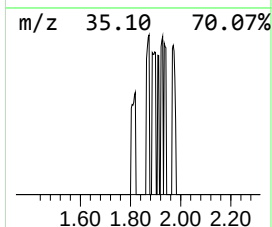
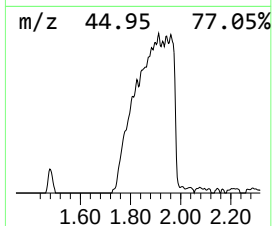
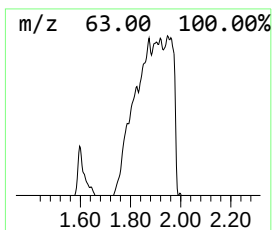
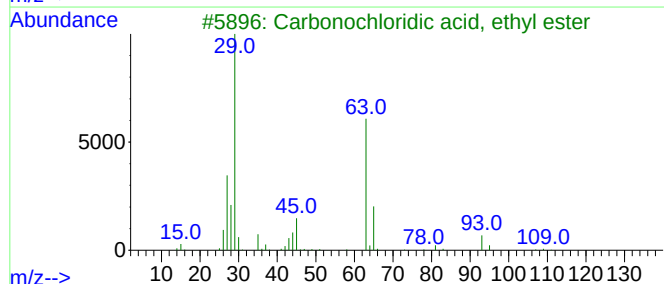
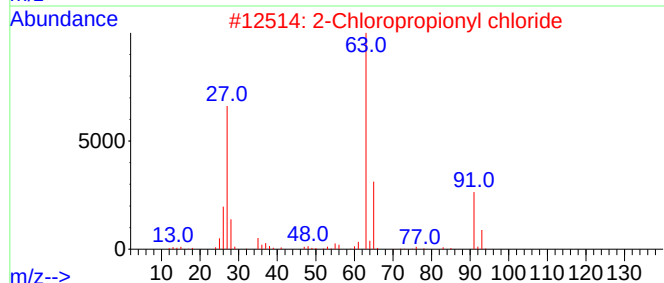
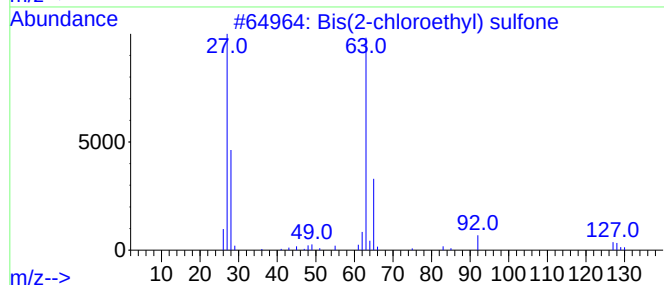
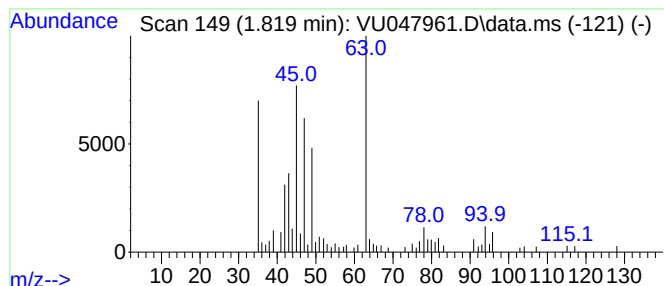
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.819	7.20 ug/L	99458	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	12
2			2-Chloropropionyl chloride	126	C3H4Cl2O	007623-09-8	12
3			Carbonochloridic acid, ethyl ester	108	C3H5ClO2	000541-41-3	9
4			Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	017639-93-9	9
5			Oxalyl chloride	126	C2Cl2O2	000079-37-8	9



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Misc : 6.6g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

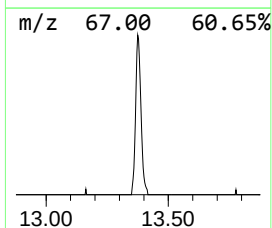
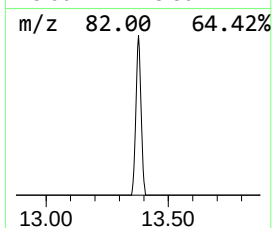
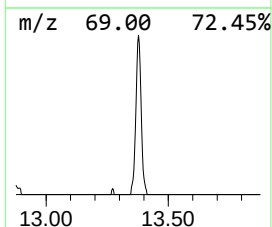
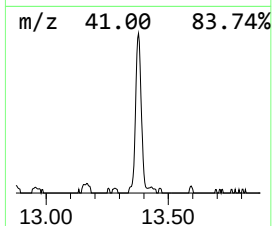
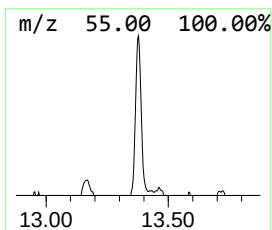
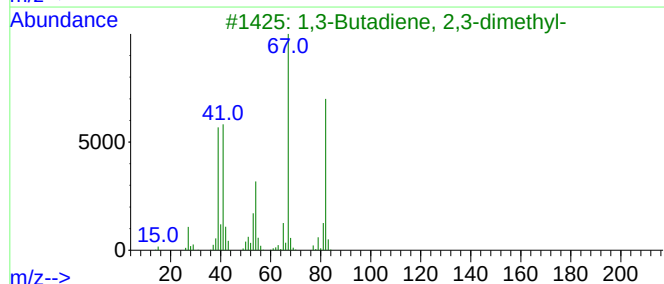
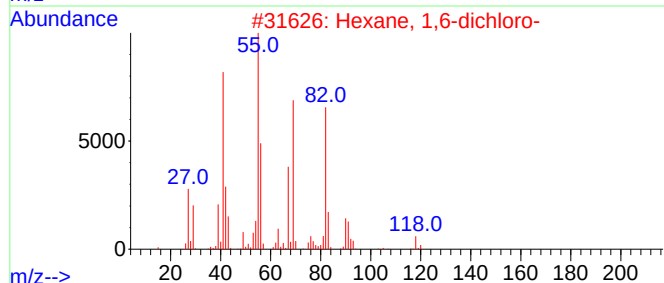
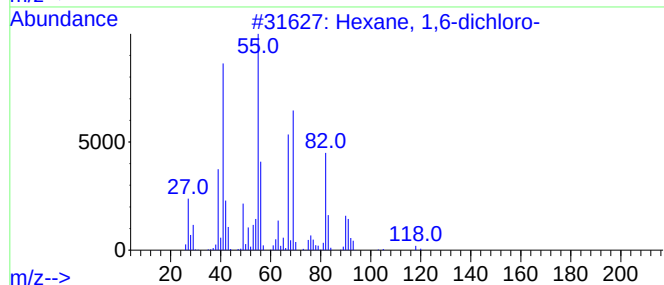
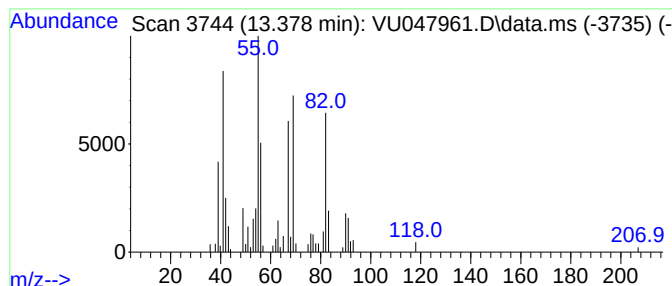
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Hexane, 1,6-dichloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.378	3.70 ug/L	61579	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 1,6-dichloro-	154	C6H12Cl2	002163-00-0	72
2			Hexane, 1,6-dichloro-	154	C6H12Cl2	002163-00-0	38
3			1,3-Butadiene, 2,3-dimethyl-	82	C6H10	000513-81-5	38
4			3-Hexyne	82	C6H10	000928-49-4	35
5			cis-2-Hexen-1-ol, pentafluoropro...	246	C9H11F5O2	1000352-74-1	35



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Instrument :
MSVOA_U
ClientSampleId :
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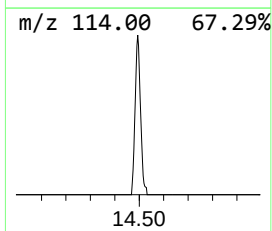
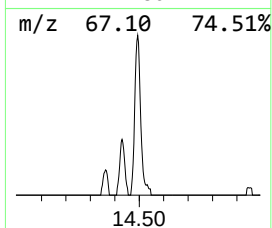
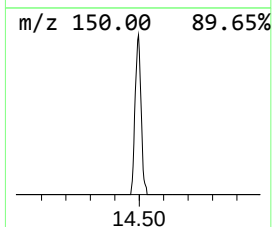
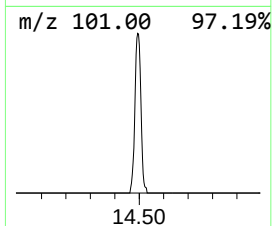
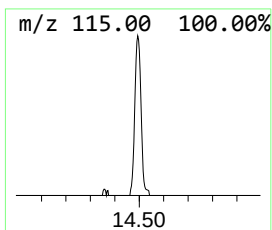
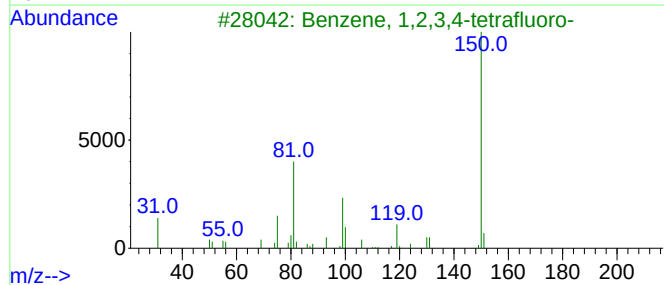
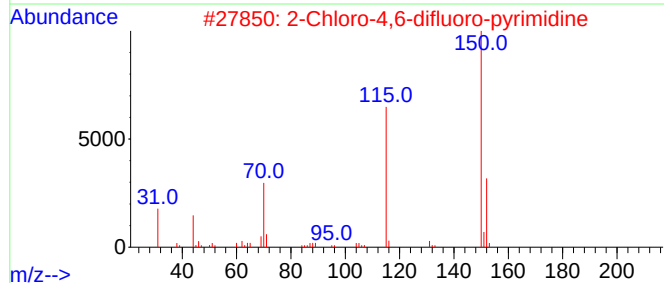
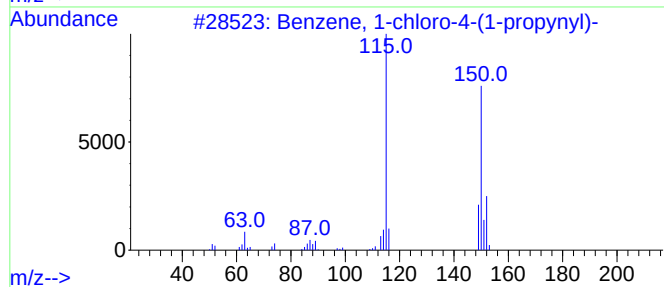
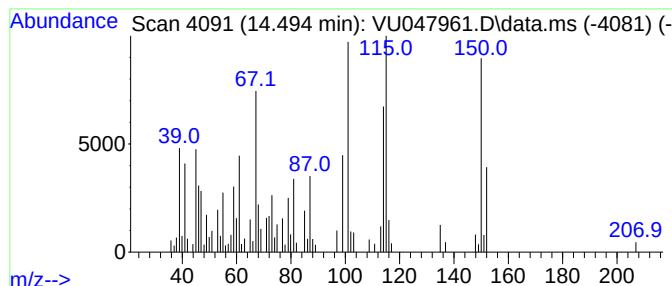
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Quant Title : VOC Analysis

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

Peak Number 4 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.494	4.69 ug/L	78134	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-chloro-4-(1-propynyl)-	150	C9H7Cl	002809-65-6	27
2			2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	22
3			Benzene, 1,2,3,4-tetrafluoro-	150	C6H2F4	000551-62-2	11
4			1-Methyl-1-cyclopentyloxy-1-sila...	184	C10H20OSi	1000216-97-0	10
5			l-Alanine, N-(2-chloroethoxycarb...	419	C22H42ClNO4	1000327-93-3	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047961.D
Acq On : 12 Apr 2022 17:18
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.6g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

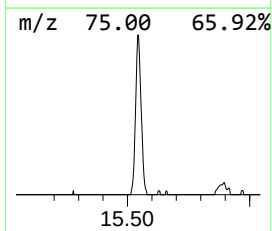
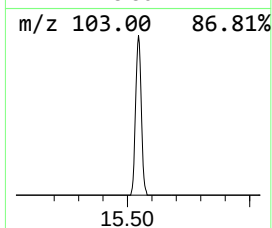
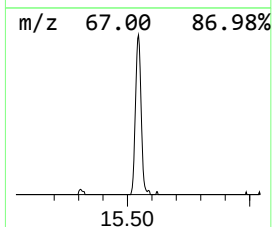
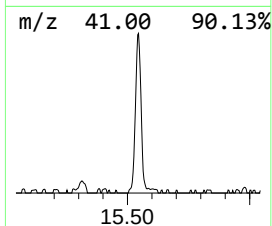
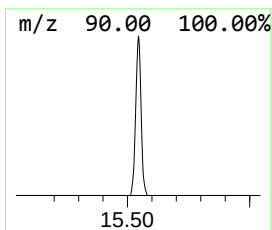
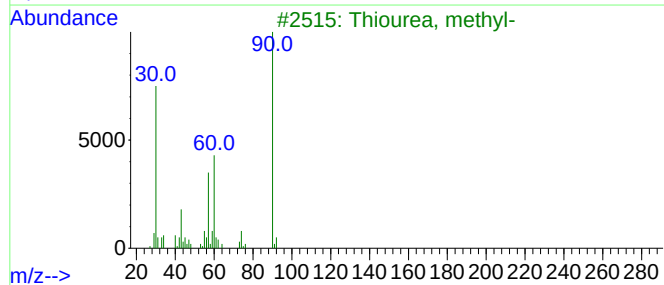
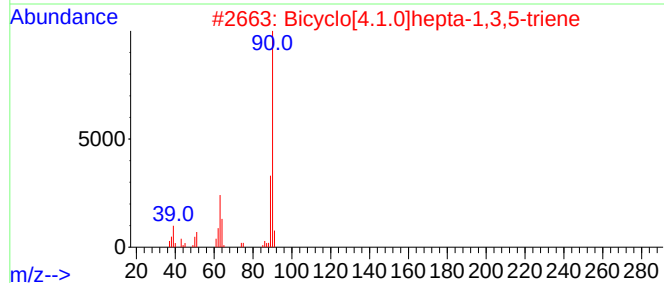
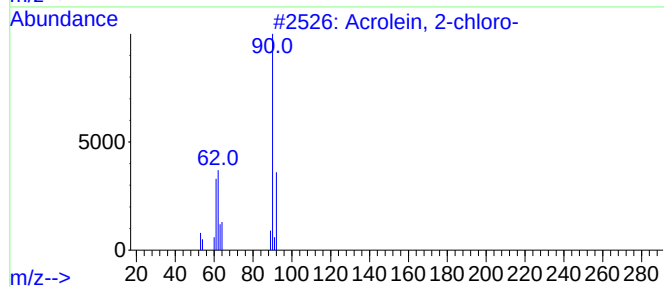
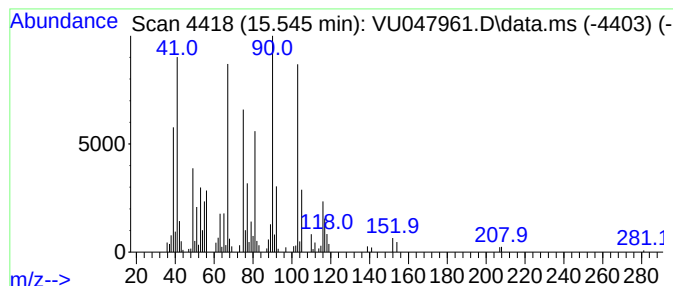
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Quant Title : VOC Analysis

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

Peak Number 5 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	7.25 ug/L	120776	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	43
2			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	30
3			Thiourea, methyl-	90	C2H6N2S	000598-52-7	27
4			Thiourea, methyl-	90	C2H6N2S	000598-52-7	27
5			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047961.D
Acq On : 12 Apr 2022 17:18
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.6g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

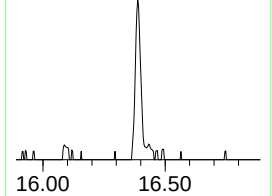
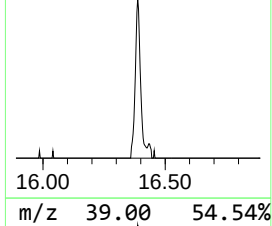
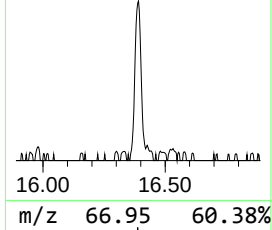
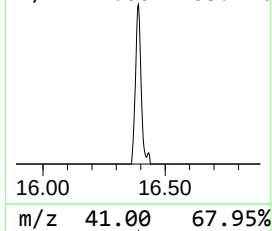
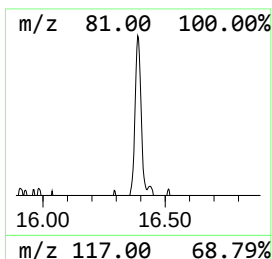
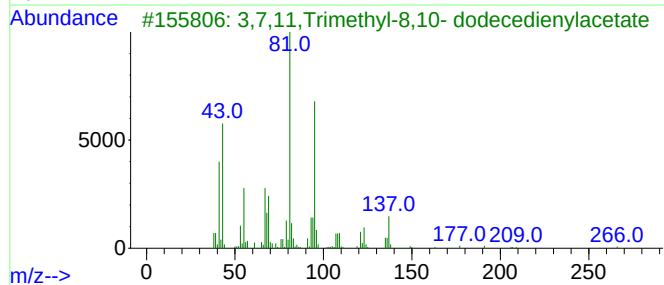
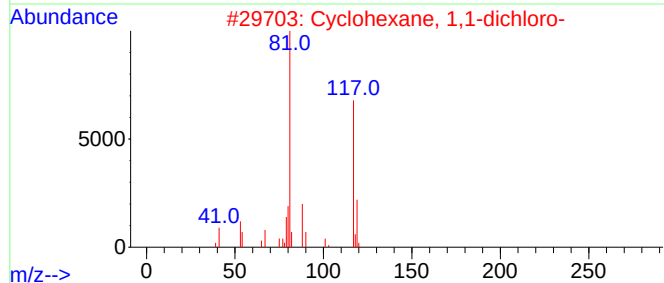
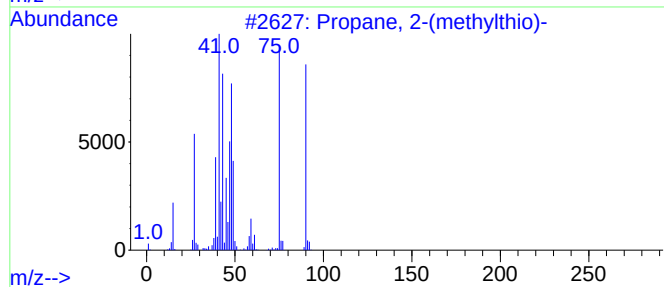
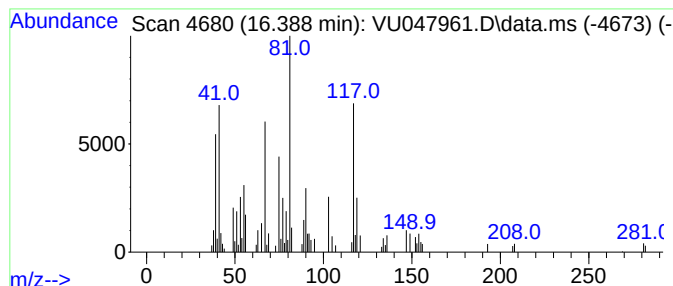
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 unknown-04 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	2.81 ug/L	46752	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	27
2			Cyclohexane, 1,1-dichloro-	152	C6H10Cl2	002108-92-1	25
3			3,7,11,Trimethyl-8,10- dodecedie...	266	C17H30O2	1000374-10-3	22
4			1,5-Hexadiene, 3-chloro-	116	C6H9Cl	028374-86-9	22
5			(9-Oxabicyclo[3.3.1]non-6-en-3-y...	154	C9H14O2	1000191-02-8	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047961.D
Acq On : 12 Apr 2022 17:18
Operator : SY/MD
Sample : N2293-06ME
Misc : 6.6g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.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
unknown-01	1.819	7.2	ug/L	99458	1	6.247	690518	50.0
Hexane, 1,6-dic...	13.378	3.7	ug/L	61579	3	11.815	833068	50.0
unknown-02	14.494	4.7	ug/L	78134	3	11.815	833068	50.0
unknown-03	15.545	7.3	ug/L	120776	3	11.815	833068	50.0
unknown-04	16.388	2.8	ug/L	46752	3	11.815	833068	50.0