

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
 Data File : VU046312.D
 Acq On : 13 Dec 2021 14:00
 Operator : SY/MD
 Sample : M4971-14
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG3D1

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046312.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	18	rVB	66594	62216	2.36%	0.784%
2	1.491	43	47	59	rVB	32925	33483	1.27%	0.422%
3	1.604	75	82	107	rVB2	245573	296130	11.26%	3.733%
4	1.919	172	180	192	rBV	65515	82563	3.14%	1.041%
5	2.572	371	383	398	rBV	140248	232273	8.83%	2.928%
6	2.752	437	439	441	rBV	220	96	0.00%	0.001%
7	3.192	567	576	584	rBV5	1664	3128	0.12%	0.039%
8	3.359	614	628	651	rBV	199487	390944	14.86%	4.928%
9	3.594	698	701	704	rBV	255	168	0.01%	0.002%
10	3.726	739	742	745	rBV2	332	183	0.01%	0.002%
11	3.745	745	748	751	rBV	271	215	0.01%	0.003%
12	3.819	768	771	779	rVB2	393	479	0.02%	0.006%
13	3.854	779	782	783	rBV2	253	153	0.01%	0.002%
14	3.967	814	817	820	rBV	308	223	0.01%	0.003%
15	4.105	857	860	863	rBV2	359	206	0.01%	0.003%
16	4.282	912	915	920	rVB	485	356	0.01%	0.004%
17	4.305	920	922	924	rBV	172	88	0.00%	0.001%
18	4.517	986	988	991	rBV	260	154	0.01%	0.002%
19	4.671	1013	1036	1090	rBV	1136139	2630963	100.00%	33.162%
20	4.999	1135	1138	1140	rBV2	314	203	0.01%	0.003%
21	5.067	1145	1159	1190	rVB	106365	249547	9.49%	3.145%
22	5.208	1201	1203	1207	rVB	284	144	0.01%	0.002%
23	5.227	1207	1209	1214	rVB	414	227	0.01%	0.003%
24	5.369	1250	1253	1256	rVB2	319	175	0.01%	0.002%
25	5.395	1258	1261	1264	rBV	310	206	0.01%	0.003%
26	5.443	1269	1276	1284	rBV2	478	839	0.03%	0.011%
27	5.539	1303	1306	1309	rBV	322	219	0.01%	0.003%
28	5.555	1309	1311	1313	rBV	196	119	0.00%	0.001%
29	5.597	1320	1324	1327	rBV	310	246	0.01%	0.003%
30	5.649	1337	1340	1343	rVB2	310	185	0.01%	0.002%
31	5.729	1343	1365	1395	rBV2	229818	627568	23.85%	7.910%
32	6.009	1449	1452	1455	rVB	341	187	0.01%	0.002%
33	6.028	1455	1458	1460	rBV	172	120	0.00%	0.002%
34	6.192	1506	1509	1511	rBV	205	135	0.01%	0.002%
35	6.253	1514	1528	1555	rVV	171185	319788	12.15%	4.031%
36	6.379	1563	1567	1574	rBV2	525	632	0.02%	0.008%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
 Data File : VU046312.D
 Acq On : 13 Dec 2021 14:00
 Operator : SY/MD
 Sample : M4971-14
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG3D1

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\SFAMULM112921WMA.M
 Title : VOC Analysis

37	6.424	1579	1581	1584	rBB	197	107	0.00%	0.001%
38	6.443	1584	1587	1590	rBV	303	192	0.01%	0.002%
39	6.526	1609	1613	1614	rBV2	1229	927	0.04%	0.012%
40	6.694	1651	1665	1688	rBV	143705	274365	10.43%	3.458%
41	7.002	1758	1761	1763	rBV	261	188	0.01%	0.002%
42	7.157	1807	1809	1812	rBV	200	103	0.00%	0.001%
43	7.176	1812	1815	1816	rBV2	245	130	0.00%	0.002%
44	7.330	1860	1863	1866	rBV	179	126	0.00%	0.002%
45	7.411	1885	1888	1892	rBV	342	257	0.01%	0.003%
46	7.433	1892	1895	1897	rBV	251	195	0.01%	0.002%
47	7.481	1907	1910	1914	rBV	244	176	0.01%	0.002%
48	7.504	1914	1917	1919	rBV	258	177	0.01%	0.002%
49	7.568	1925	1937	1954	rBV	74621	129803	4.93%	1.636%
50	7.645	1958	1961	1965	rBV	413	303	0.01%	0.004%
51	7.687	1973	1974	1975	rBV	197	64	0.00%	0.001%
52	7.755	1991	1995	2000	rBV2	484	466	0.02%	0.006%
53	7.796	2006	2008	2011	rVB	216	108	0.00%	0.001%
54	7.816	2011	2014	2022	rBV	343	376	0.01%	0.005%
55	7.899	2027	2040	2057	rBV	277302	482659	18.35%	6.084%
56	8.063	2087	2091	2092	rBV2	169	113	0.00%	0.001%
57	8.099	2099	2102	2103	rBV	279	171	0.01%	0.002%
58	8.144	2113	2116	2117	rBV	227	145	0.01%	0.002%
59	8.182	2117	2128	2140	rVV	53375	88769	3.37%	1.119%
60	8.346	2175	2179	2183	rBV2	314	289	0.01%	0.004%
61	8.475	2213	2219	2231	rVB3	1480	2679	0.10%	0.034%
62	8.520	2231	2233	2235	rBV2	183	95	0.00%	0.001%
63	8.568	2246	2248	2251	rBV2	180	107	0.00%	0.001%
64	8.636	2256	2269	2302	rVV	174962	315050	11.97%	3.971%
65	9.153	2427	2430	2433	rBV	455	294	0.01%	0.004%
66	9.176	2433	2437	2440	rVV2	241	198	0.01%	0.002%
67	9.205	2440	2446	2451	rVB2	502	588	0.02%	0.007%
68	9.234	2451	2455	2458	rBV2	434	364	0.01%	0.005%
69	9.301	2473	2476	2480	rBV2	319	208	0.01%	0.003%
70	9.420	2500	2513	2537	rBV	258619	434583	16.52%	5.478%
71	9.899	2656	2662	2664	rBV	378	452	0.02%	0.006%
72	10.057	2708	2711	2712	rBV	337	220	0.01%	0.003%
73	10.243	2766	2769	2770	rBV	243	145	0.01%	0.002%
74	10.414	2819	2822	2825	rBV	328	238	0.01%	0.003%
75	10.668	2896	2901	2902	rBV3	1240	996	0.04%	0.013%
76	10.758	2916	2929	2949	rVB	210039	335276	12.74%	4.226%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
 Data File : VU046312.D
 Acq On : 13 Dec 2021 14:00
 Operator : SY/MD
 Sample : M4971-14
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG3D1

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\SFAMULM112921WMA.M
 Title : VOC Analysis

77	10.890	2962	2970	2980	rBV3	1837	3258	0.12%	0.041%
78	11.176	3056	3059	3060	rBV2	211	129	0.00%	0.002%
79	11.272	3085	3089	3094	rBV2	402	403	0.02%	0.005%
80	11.317	3099	3103	3104	rBV	257	177	0.01%	0.002%
81	11.546	3169	3174	3180	rBV2	438	594	0.02%	0.007%
82	11.668	3209	3212	3214	rBV	212	135	0.01%	0.002%
83	11.729	3226	3231	3237	rBV	383	478	0.02%	0.006%
84	11.812	3245	3257	3271	rBV	278632	429220	16.31%	5.410%
85	12.054	3329	3332	3334	rBV	440	364	0.01%	0.005%
86	12.195	3363	3376	3391	rBV	286285	468097	17.79%	5.900%
87	13.372	3738	3742	3744	rBV	296	217	0.01%	0.003%
88	13.883	3898	3901	3905	rBV2	279	287	0.01%	0.004%
89	14.089	3962	3965	3968	rBV2	424	395	0.02%	0.005%
90	16.092	4579	4588	4598	rVB2	16437	23627	0.90%	0.298%

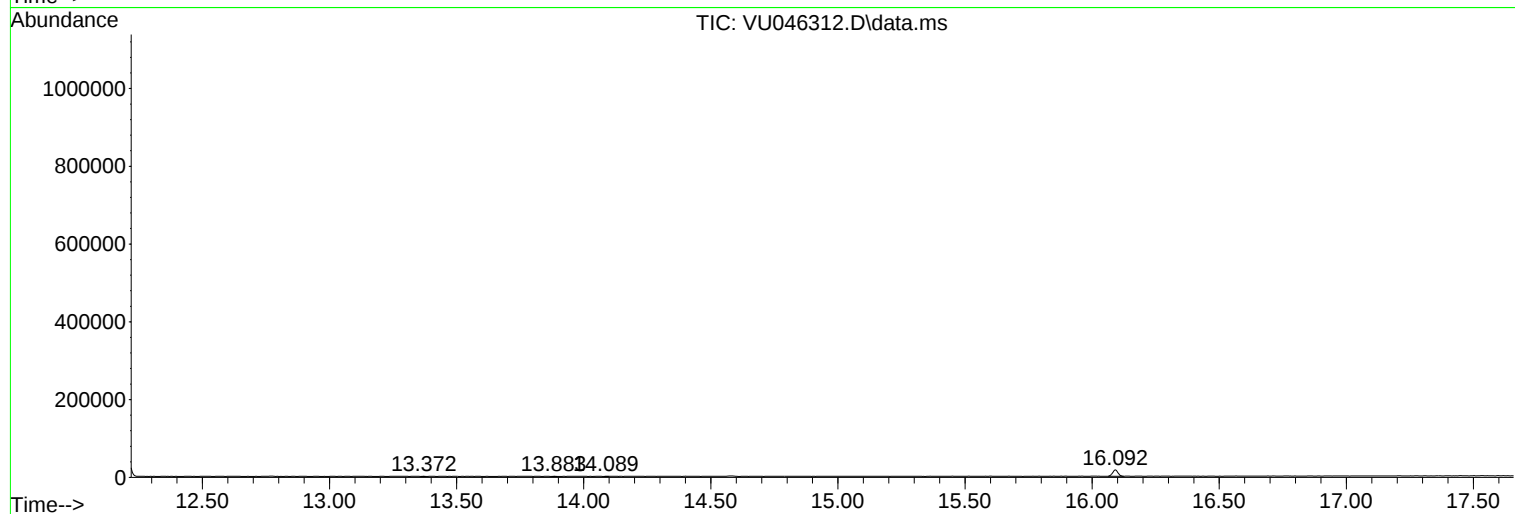
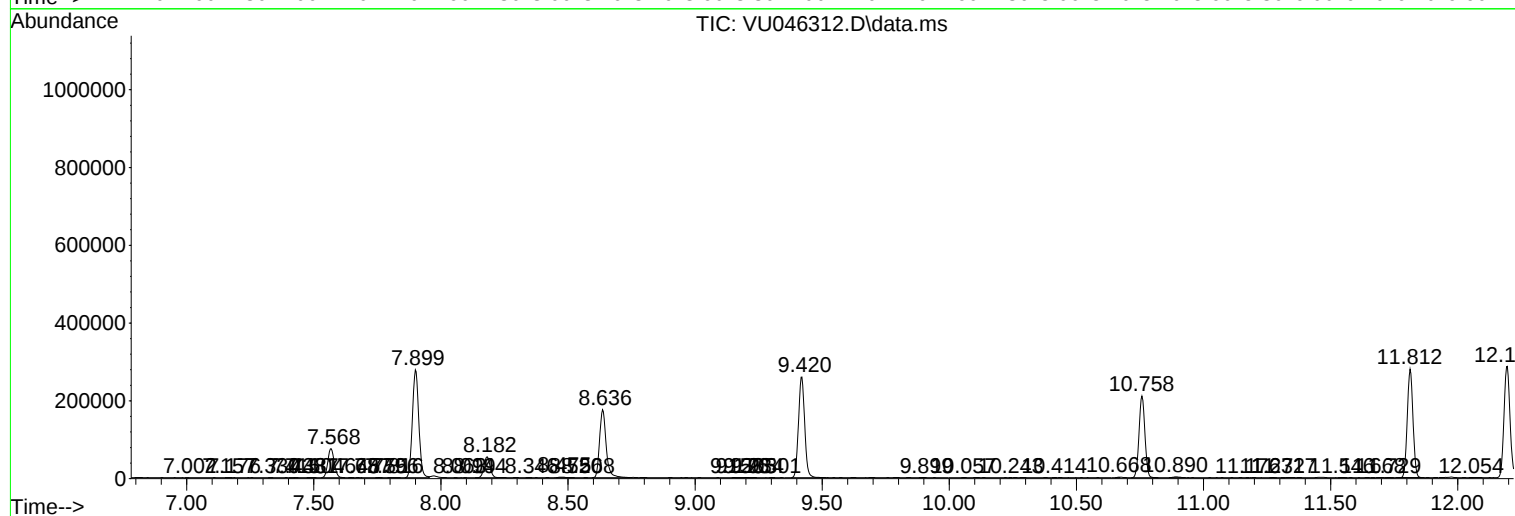
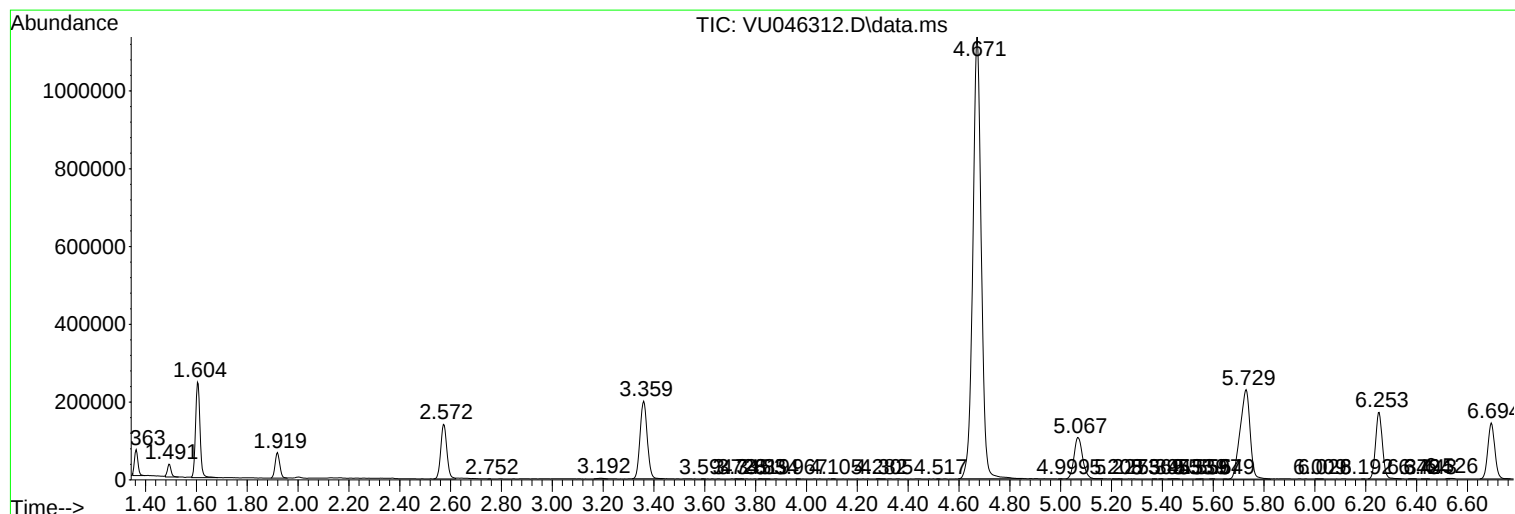
Sum of corrected areas: 7933644

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
Data File : VU046312.D
Acq On : 13 Dec 2021 14:00
Operator : SY/MD
Sample : M4971-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG3D1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
Data File : VU046312.D
Acq On : 13 Dec 2021 14:00
Operator : SY/MD
Sample : M4971-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG3D1

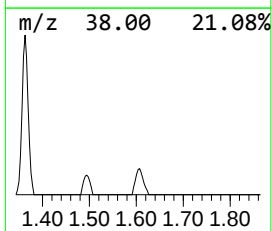
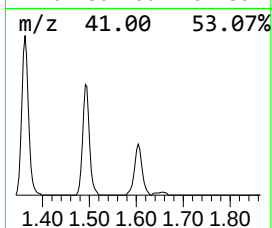
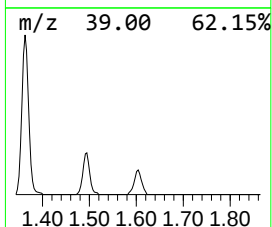
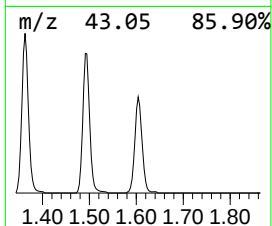
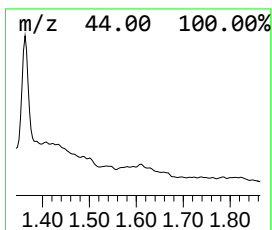
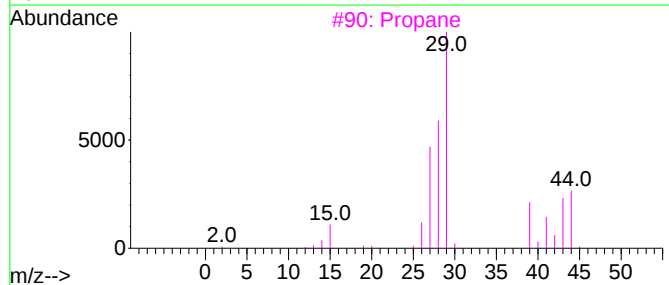
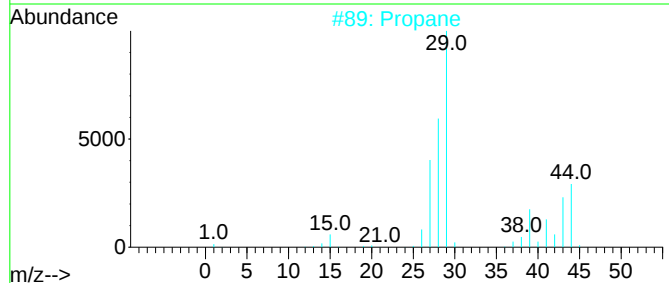
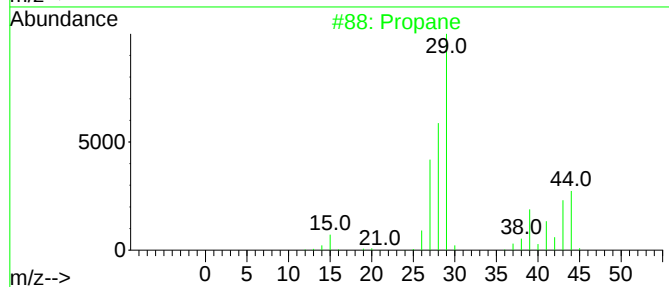
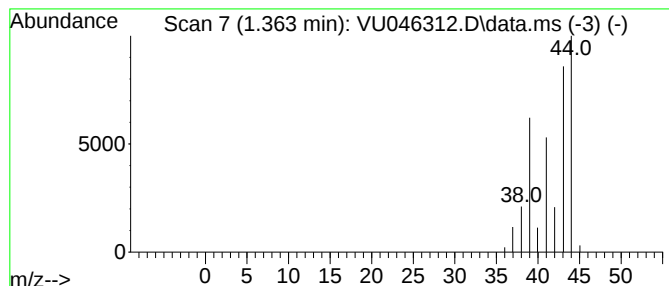
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.363	9.73 ug/L	62216	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	90
2			Propane	44	C3H8	000074-98-6	83
3			Propane	44	C3H8	000074-98-6	9
4			Cyclopropene	40	C3H4	002781-85-3	9
5			Propene	42	C3H6	000115-07-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
Data File : VU046312.D
Acq On : 13 Dec 2021 14:00
Operator : SY/MD
Sample : M4971-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG3D1

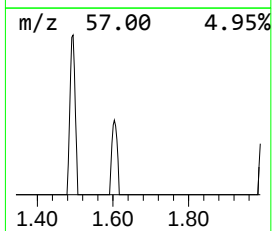
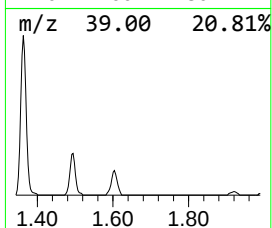
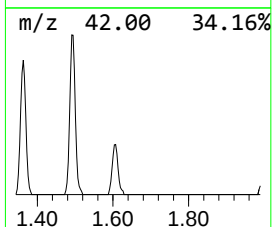
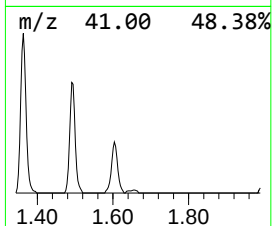
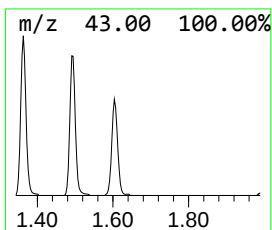
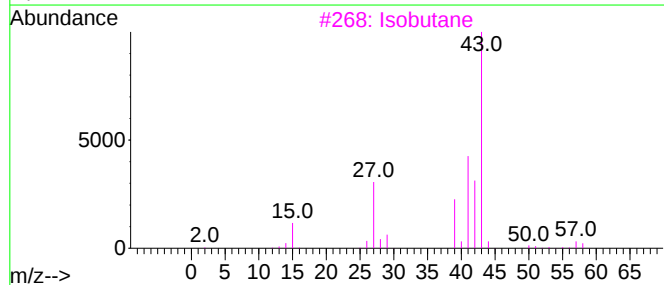
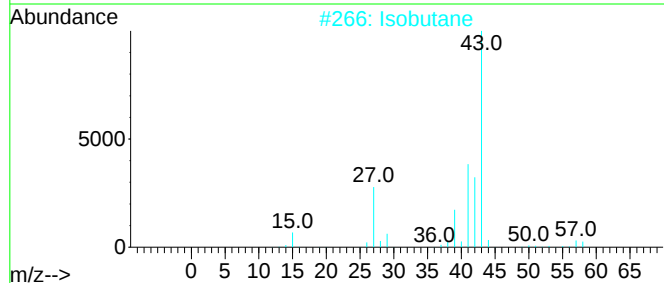
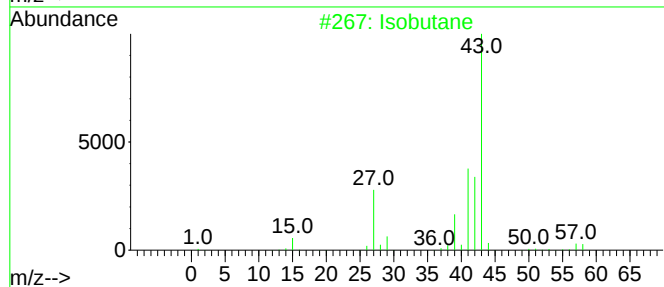
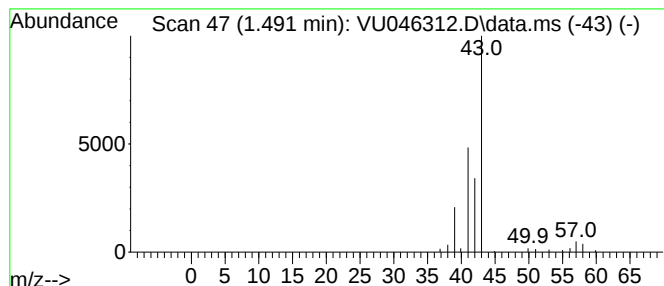
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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.
1.491	5.24 ug/L	33483	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	64
2			Isobutane	58	C4H10	000075-28-5	64
3			Isobutane	58	C4H10	000075-28-5	50
4			Isobutane	58	C4H10	000075-28-5	50
5			Isobutane	58	C4H10	000075-28-5	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
Data File : VU046312.D
Acq On : 13 Dec 2021 14:00
Operator : SY/MD
Sample : M4971-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG3D1

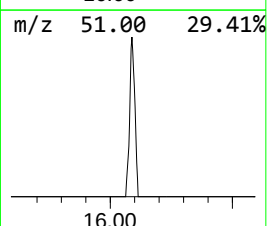
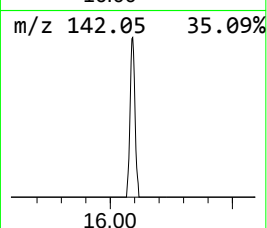
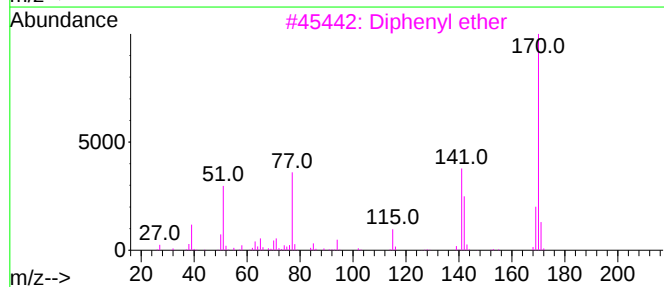
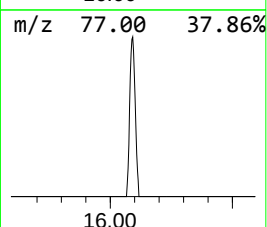
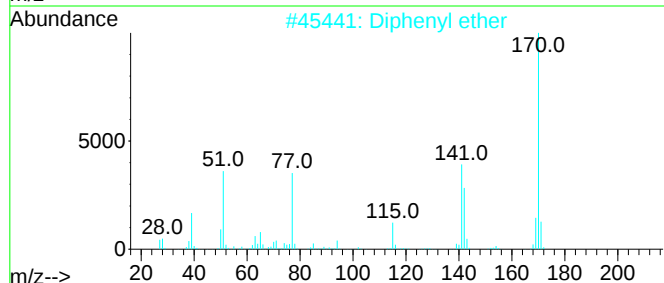
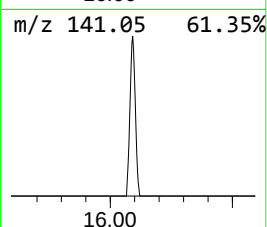
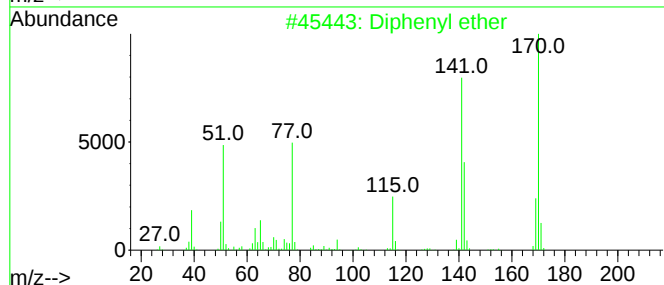
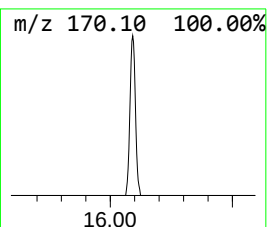
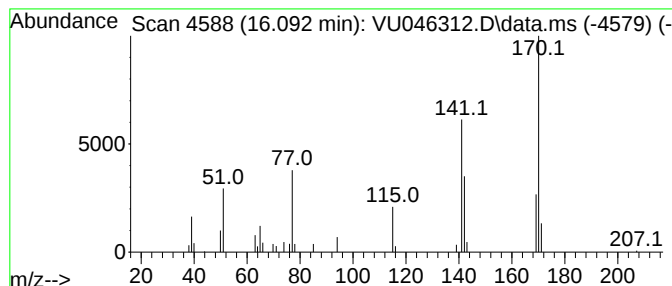
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Diphenyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.092	2.75 ug/L	23627	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diphenyl ether	170	C12H10O	000101-84-8	95
2			Diphenyl ether	170	C12H10O	000101-84-8	90
3			Diphenyl ether	170	C12H10O	000101-84-8	87
4			Diphenyl ether	170	C12H10O	000101-84-8	87
5			Diphenyl ether	170	C12H10O	000101-84-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
Data File : VU046312.D
Acq On : 13 Dec 2021 14:00
Operator : SY/MD
Sample : M4971-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG3D1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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	9.7	ug/L	62216	1	6.253	319788	50.0
(DEL) Alkane: S...	1.491	5.2	ug/L	33483	1	6.253	319788	50.0
Diphenyl ether	16.092	2.8	ug/L	23627	3	11.812	429220	50.0