

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041422\
 Data File : VU048047.D
 Acq On : 14 Apr 2022 11:01
 Operator : SY/MD
 Sample : N2316-08ME
 Misc : 6.65g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNQ7ME

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: VU048047.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.356	3	5	30	rVB	124940	133228	10.22%	1.403%
2	1.597	73	80	120	rVB	54815	123129	9.44%	1.297%
3	2.543	362	374	386	rBV	150647	254982	19.56%	2.685%
4	2.951	496	501	502	rBV2	2525	1910	0.15%	0.020%
5	3.112	543	551	567	rVB3	7700	16429	1.26%	0.173%
6	3.179	567	572	573	rBV2	574	453	0.03%	0.005%
7	3.205	577	580	583	rBV2	353	287	0.02%	0.003%
8	3.337	617	621	622	rBV2	508	367	0.03%	0.004%
9	3.430	647	650	657	rVB3	742	786	0.06%	0.008%
10	4.330	924	930	932	rBV2	285	348	0.03%	0.004%
11	4.507	980	985	987	rBV2	591	528	0.04%	0.006%
12	4.642	1012	1027	1086	rBV2	73711	281570	21.60%	2.965%
13	5.063	1142	1158	1182	rBV	162673	377775	28.98%	3.979%
14	5.292	1223	1229	1233	rBV4	468	690	0.05%	0.007%
15	5.369	1248	1253	1266	rVB9	2374	4758	0.36%	0.050%
16	5.719	1342	1362	1372	rBV2	375429	971157	74.49%	10.228%
17	5.909	1417	1421	1428	rVB4	809	901	0.07%	0.009%
18	5.977	1435	1442	1449	rBV5	1532	2315	0.18%	0.024%
19	6.124	1479	1488	1489	rBV4	1948	2097	0.16%	0.022%
20	6.247	1511	1526	1552	rBV	367968	738136	56.62%	7.774%
21	6.526	1603	1613	1623	rBV4	2759	4866	0.37%	0.051%
22	6.604	1628	1637	1640	rBV5	806	1047	0.08%	0.011%
23	6.690	1650	1664	1679	rBV	217080	447232	34.30%	4.710%
24	6.993	1747	1758	1769	rBV6	1999	3967	0.30%	0.042%
25	7.198	1809	1822	1838	rBV3	7781	21068	1.62%	0.222%
26	7.497	1900	1915	1926	rBV3	22407	49851	3.82%	0.525%
27	7.568	1926	1937	1958	rVB	96051	188087	14.43%	1.981%
28	7.694	1968	1976	1984	rBV5	1699	3083	0.24%	0.032%
29	7.796	2004	2008	2012	rBV3	492	419	0.03%	0.004%
30	7.848	2012	2024	2026	rBV7	1873	2951	0.23%	0.031%
31	7.899	2026	2040	2054	rVV	392804	713937	54.76%	7.519%
32	7.973	2055	2063	2087	rVB3	33126	98451	7.55%	1.037%
33	8.182	2117	2128	2154	rVB2	59990	129734	9.95%	1.366%
34	8.369	2174	2186	2203	rVB7	10507	27630	2.12%	0.291%
35	8.481	2216	2221	2224	rVB3	584	499	0.04%	0.005%
36	8.581	2241	2252	2261	rVV2	20112	38066	2.92%	0.401%

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 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNQ7ME

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	8.661	2262	2277	2310	rVB	311783	664179	50.94%	6.995%
38	8.864	2334	2340	2347	rVB6	2658	3647	0.28%	0.038%
39	8.938	2358	2363	2364	rBV3	519	383	0.03%	0.004%
40	9.031	2379	2392	2393	rBV5	4639	6986	0.54%	0.074%
41	9.365	2488	2496	2499	rBV5	1664	2108	0.16%	0.022%
42	9.423	2500	2514	2548	rVB2	496108	1303727	100.00%	13.731%
43	9.578	2549	2562	2571	rVB3	5516	10938	0.84%	0.115%
44	9.636	2575	2580	2584	rBV4	938	949	0.07%	0.010%
45	9.687	2587	2596	2598	rBV7	1982	2479	0.19%	0.026%
46	9.828	2635	2640	2644	rBV2	336	416	0.03%	0.004%
47	9.944	2670	2676	2679	rBV3	808	911	0.07%	0.010%
48	10.102	2718	2725	2733	rBV3	2137	3714	0.28%	0.039%
49	10.301	2782	2787	2790	rBV	353	312	0.02%	0.003%
50	10.488	2837	2845	2855	rVV2	2691	3931	0.30%	0.041%
51	10.668	2892	2901	2913	rVB6	1438	2780	0.21%	0.029%
52	10.767	2919	2932	2954	rBV	389880	686591	52.66%	7.231%
53	10.857	2957	2960	2967	rVB4	1257	1272	0.10%	0.013%
54	10.909	2967	2976	2986	rVB3	4895	8075	0.62%	0.085%
55	10.992	2991	3002	3011	rBV2	11031	17278	1.33%	0.182%
56	11.105	3027	3037	3046	rBV4	5789	8987	0.69%	0.095%
57	11.295	3087	3096	3107	rVB2	8755	12743	0.98%	0.134%
58	11.468	3141	3150	3161	rVB7	2569	5211	0.40%	0.055%
59	11.517	3161	3165	3170	rBV3	407	495	0.04%	0.005%
60	11.587	3181	3187	3190	rBV4	630	557	0.04%	0.006%
61	11.645	3202	3205	3207	rBV2	513	401	0.03%	0.004%
62	11.693	3217	3220	3221	rBV2	566	409	0.03%	0.004%
63	11.748	3232	3237	3245	rVB4	1548	1959	0.15%	0.021%
64	11.816	3245	3258	3274	rBV	566943	903341	69.29%	9.514%
65	11.973	3305	3307	3315	rVB5	1833	1766	0.14%	0.019%
66	12.015	3315	3320	3325	rBV4	542	744	0.06%	0.008%
67	12.102	3338	3347	3357	rVB5	2135	3244	0.25%	0.034%
68	12.198	3363	3377	3396	rBV	467979	766792	58.82%	8.076%
69	12.381	3426	3434	3442	rBV2	4860	6779	0.52%	0.071%
70	12.468	3454	3461	3467	rBV3	3432	5216	0.40%	0.055%
71	12.574	3484	3494	3505	rBV2	7400	10414	0.80%	0.110%
72	12.684	3519	3528	3542	rBV4	5011	9109	0.70%	0.096%
73	12.767	3550	3554	3555	rBV2	630	475	0.04%	0.005%
74	12.883	3581	3590	3597	rVB3	3234	4862	0.37%	0.051%
75	12.976	3612	3619	3627	rVV7	4162	5867	0.45%	0.062%
76	13.028	3627	3635	3649	rVB3	5036	7015	0.54%	0.074%

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 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNQ7ME

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	13.108	3658	3660	3667	rVB4	438	465	0.04%	0.005%
78	13.198	3685	3688	3690	rBV2	400	315	0.02%	0.003%
79	13.330	3722	3729	3735	rBV4	4276	6050	0.46%	0.064%
80	13.378	3735	3744	3755	rVV2	31966	47851	3.67%	0.504%
81	13.449	3757	3766	3776	rVB2	11819	17571	1.35%	0.185%
82	13.523	3782	3789	3797	rBV3	2014	3269	0.25%	0.034%
83	13.632	3817	3823	3833	rVV4	1534	2437	0.19%	0.026%
84	13.841	3881	3888	3898	rBV6	3035	4439	0.34%	0.047%
85	13.915	3905	3911	3918	rBV2	1057	1266	0.10%	0.013%
86	14.050	3950	3953	3955	rBV	436	320	0.02%	0.003%
87	14.092	3958	3966	3982	rVB2	4684	8851	0.68%	0.093%
88	14.192	3992	3997	4010	rVB6	1653	2333	0.18%	0.025%
89	14.288	4020	4027	4034	rVV6	3752	5612	0.43%	0.059%
90	14.333	4037	4041	4056	rVB6	2064	4045	0.31%	0.043%
91	14.430	4063	4071	4082	rBV4	14353	21254	1.63%	0.224%
92	14.494	4083	4091	4103	rVB5	18195	28533	2.19%	0.301%
93	14.671	4141	4146	4153	rVB3	1247	1660	0.13%	0.017%
94	14.947	4225	4232	4234	rBV3	1218	1282	0.10%	0.014%
95	15.018	4247	4254	4260	rBV6	2665	3804	0.29%	0.040%
96	15.291	4336	4339	4341	rBV3	653	319	0.02%	0.003%
97	15.417	4370	4378	4382	rBV6	1254	1794	0.14%	0.019%
98	15.545	4407	4418	4430	rBV2	116677	184418	14.15%	1.942%
99	15.876	4514	4521	4536	rVB6	9545	17481	1.34%	0.184%
100	16.092	4581	4588	4598	rBV4	6427	9888	0.76%	0.104%

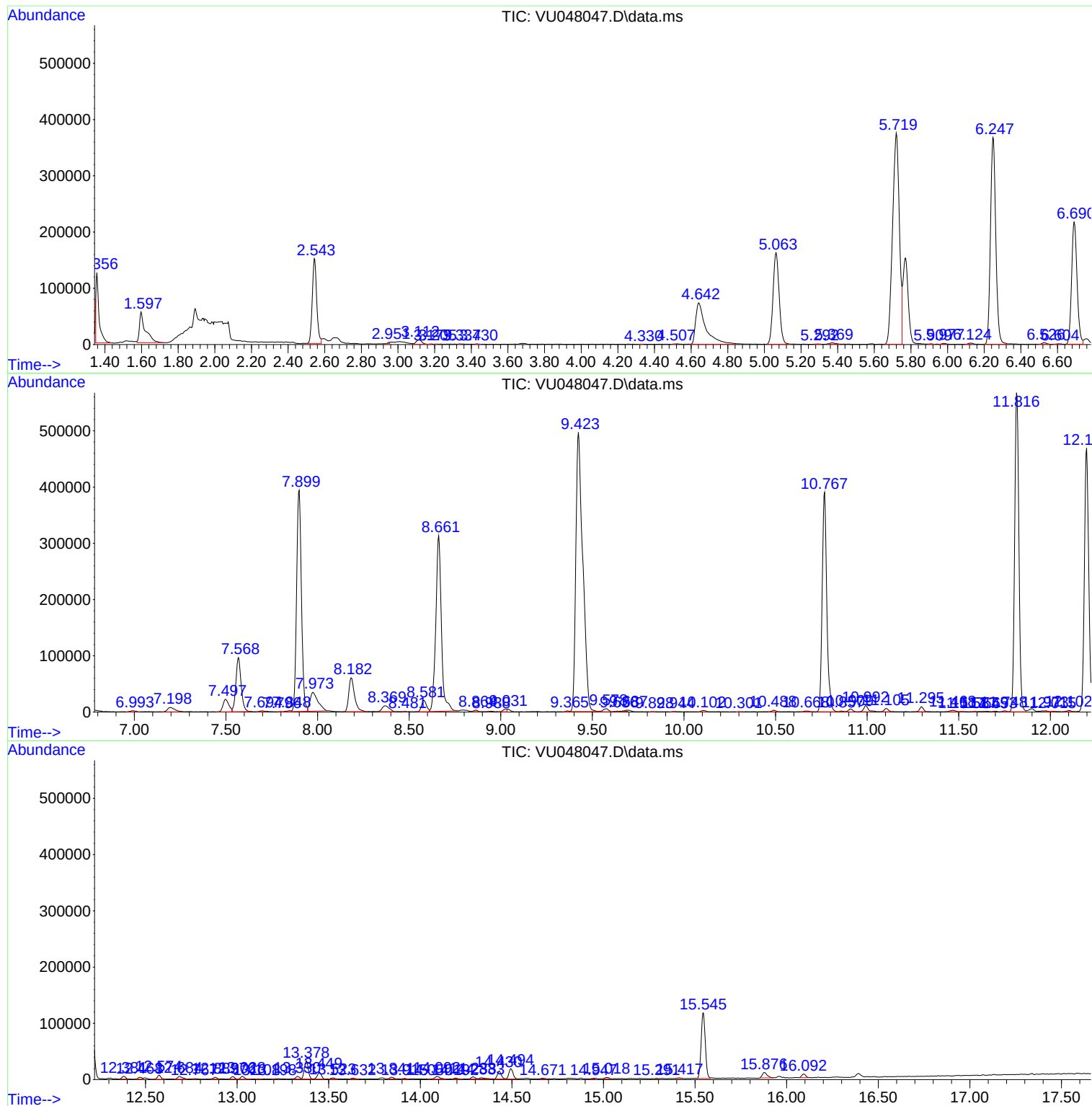
Sum of corrected areas: 9495053

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041422\
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Sample : N2316-08ME
Misc : 6.65g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ7ME

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\VU041422\
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Operator : SY/MD
Sample : N2316-08ME
Misc : 6.65g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ7ME

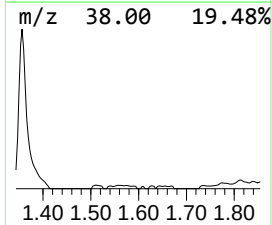
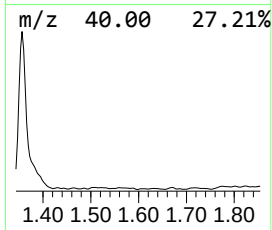
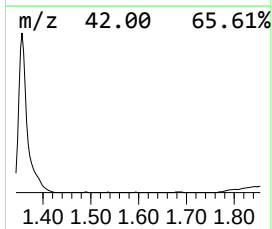
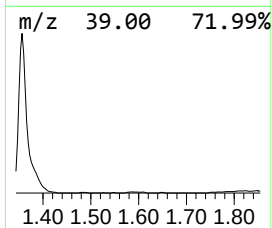
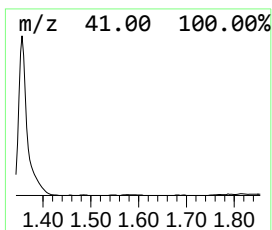
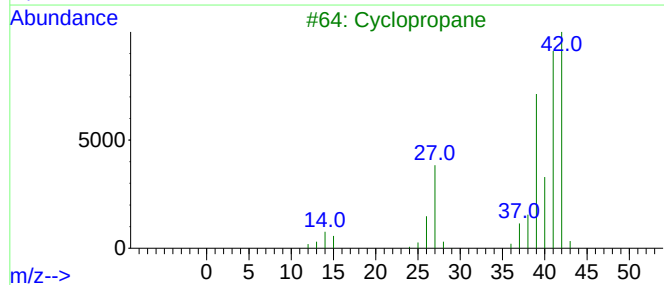
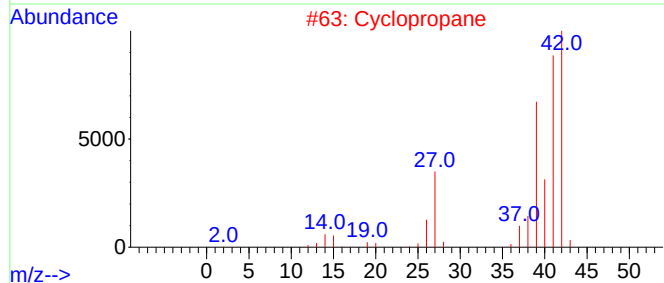
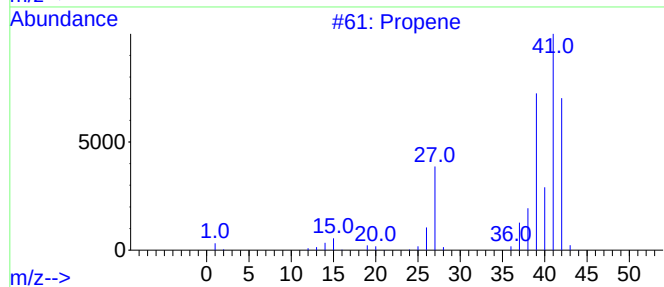
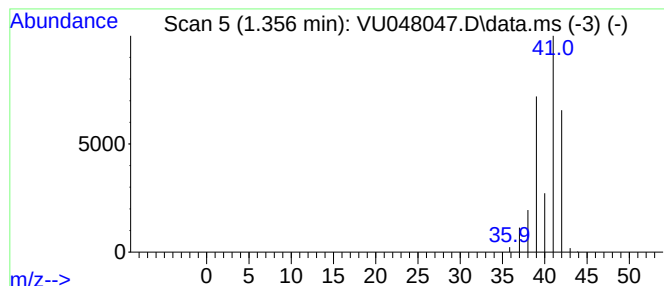
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.356	9.02 ug/L	133228	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Cyclopropane	42	C3H6	000075-19-4	50
3			Cyclopropane	42	C3H6	000075-19-4	50
4			Cyclopropene	40	C3H4	002781-85-3	45
5			Propene	42	C3H6	000115-07-1	35



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Misc : 6.65g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ7ME

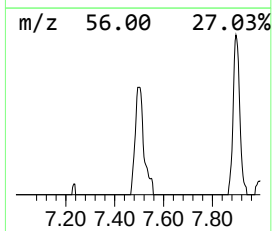
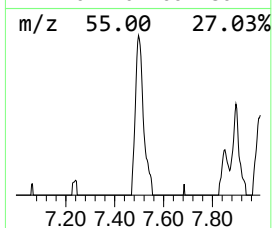
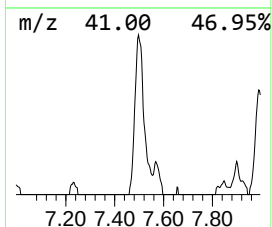
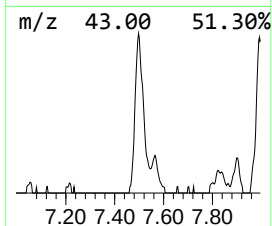
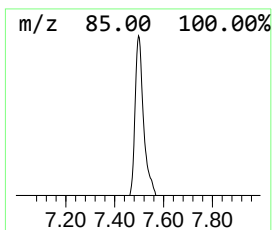
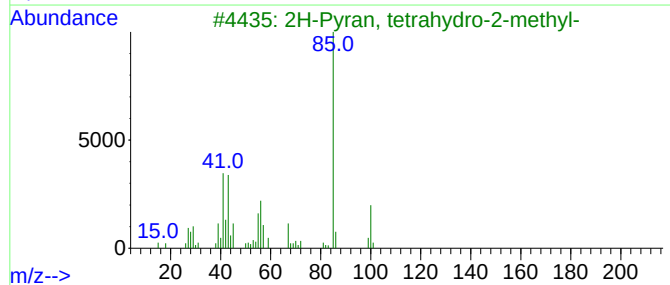
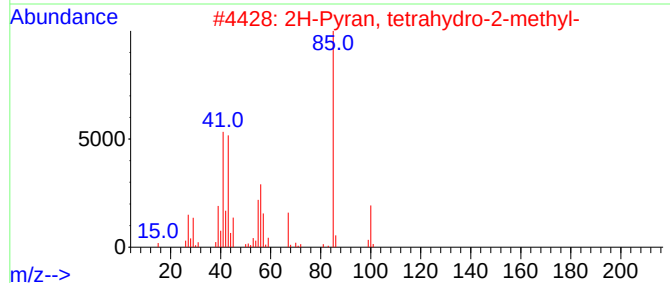
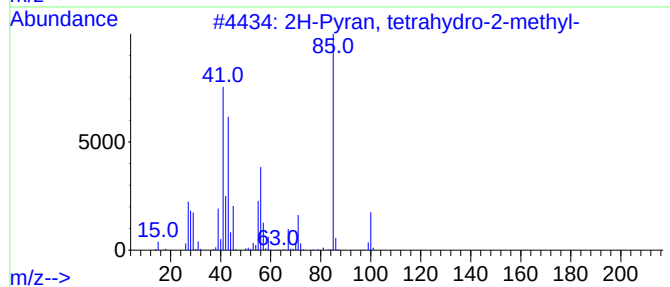
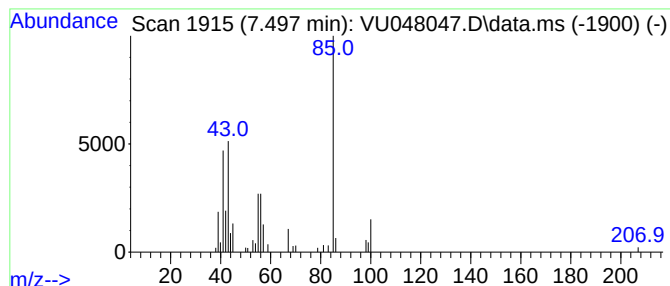
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 2H-Pyran, tetrahydro-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.497	3.38 ug/L	49851	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran, tetrahydro-2-methyl-			100	C6H12O	010141-72-7	91
2	2H-Pyran, tetrahydro-2-methyl-			100	C6H12O	010141-72-7	90
3	2H-Pyran, tetrahydro-2-methyl-			100	C6H12O	010141-72-7	87
4	Furan, tetrahydro-2,4-dimethyl-,...			100	C6H12O	039168-01-9	64
5	Hexane, 2-methyl-			100	C7H16	000591-76-4	64



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Operator : SY/MD
Sample : N2316-08ME
Misc : 6.65g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ7ME

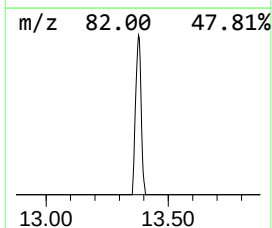
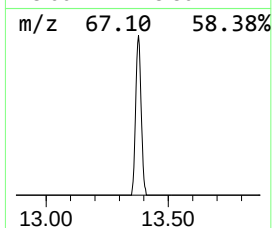
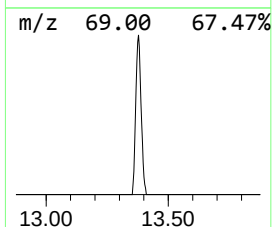
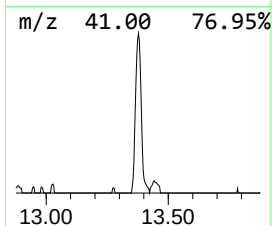
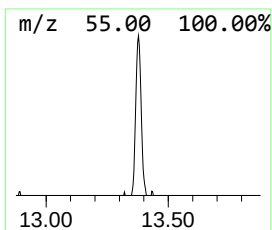
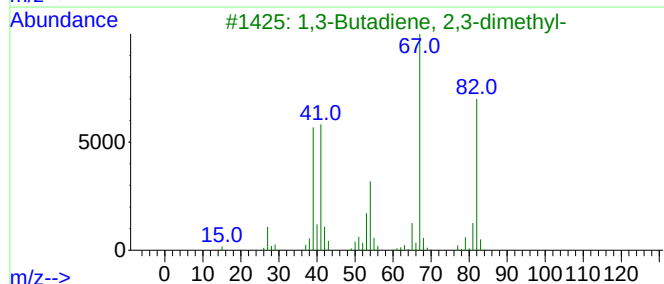
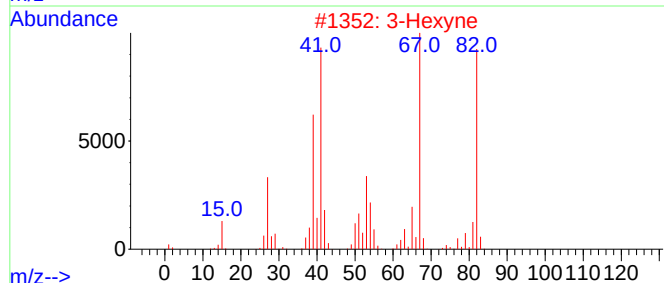
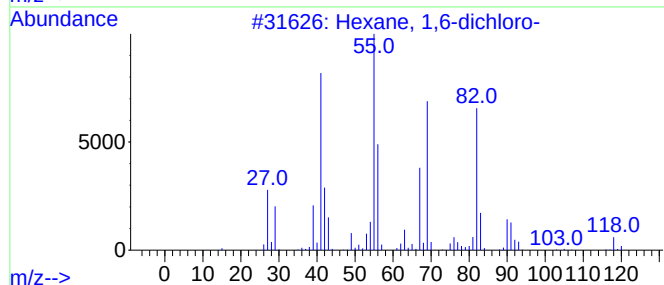
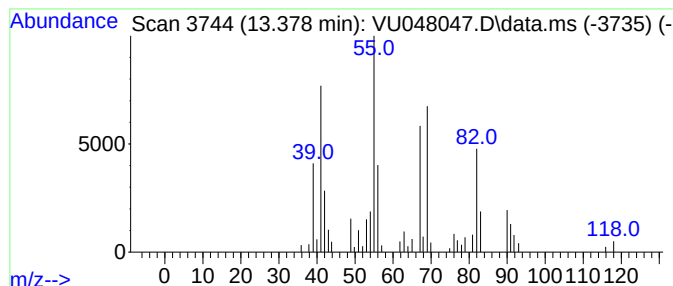
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Hexane, 1,6-dichloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.378	2.65 ug/L	47851	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 1,6-dichloro-	154	C6H12Cl2	002163-00-0	50
2			3-Hexyne	82	C6H10	000928-49-4	46
3			1,3-Butadiene, 2,3-dimethyl-	82	C6H10	000513-81-5	43
4			1-Hexanol, 6-chloro-	136	C6H13ClO	002009-83-8	43
5			Hexane, 1,6-dichloro-	154	C6H12Cl2	002163-00-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041422\
Data File : VU048047.D
Acq On : 14 Apr 2022 11:01
Operator : SY/MD
Sample : N2316-08ME
Misc : 6.65g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ7ME

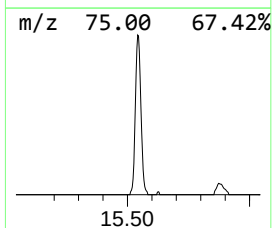
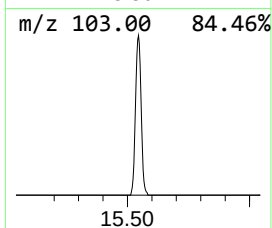
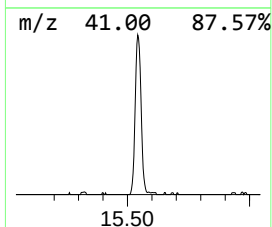
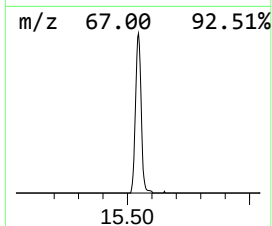
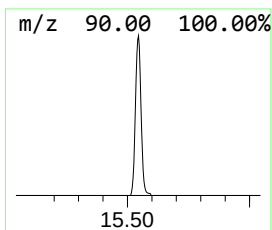
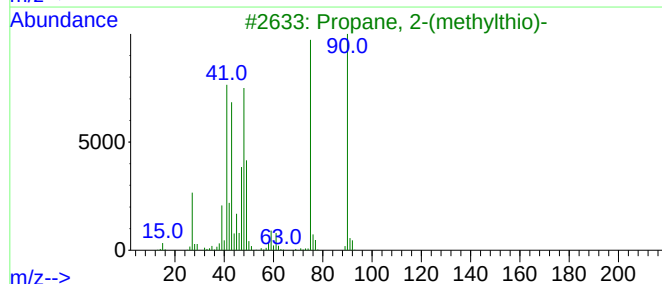
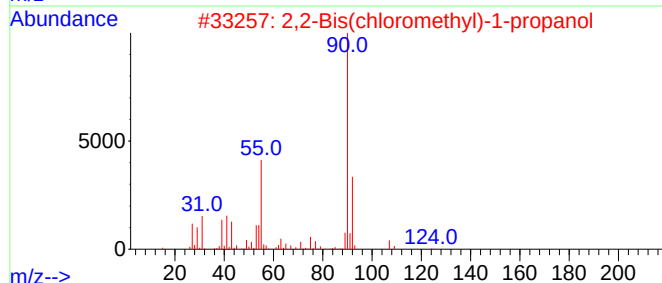
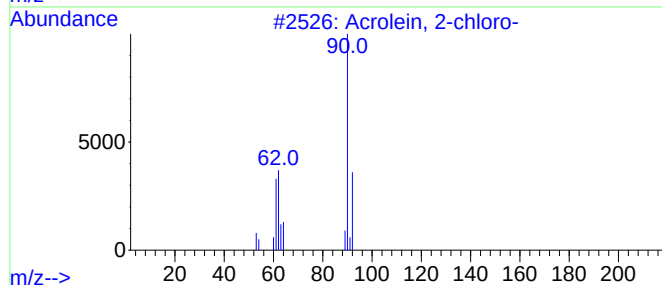
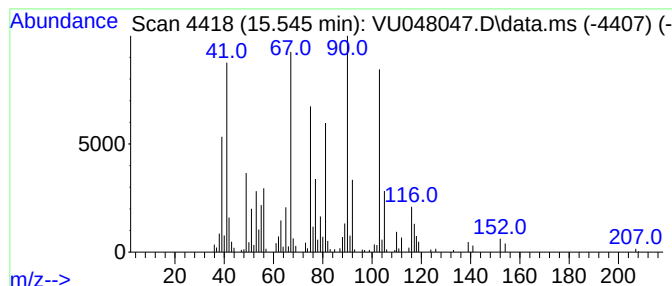
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Quant Title : VOC Analysis

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

Peak Number 5 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	10.21 ug/L	184418	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	37
2			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	32
3			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	28
4			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	25
5			1H-1,2,4-Triazole,3-chloro-1,5-d...	131	C4H6ClN3	056616-94-5	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041422\
Data File : VU048047.D
Acq On : 14 Apr 2022 11:01
Operator : SY/MD
Sample : N2316-08ME
Misc : 6.65g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ7ME

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
(DEL) Alkane: S...	1.356	9.0	ug/L	133228	1	6.247	738136	50.0
2H-Pyran, tetra...	7.497	3.4	ug/L	49851	1	6.247	738136	50.0
Hexane, 1,6-dic...	13.378	2.6	ug/L	47851	3	11.816	903341	50.0
unknown-02	15.545	10.2	ug/L	184418	3	11.816	903341	50.0