

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
 Data File : VU047936.D
 Acq On : 12 Apr 2022 03:14
 Operator : SY/MD
 Sample : N2293-14ME
 Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP2ME

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: VU047936.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	34	rVB	862789	962430	18.41%	5.372%
2	1.597	72	80	113	rVB	68845	157105	3.01%	0.877%
3	1.906	171	176	186	rBV	33876	51149	0.98%	0.285%
4	2.539	362	373	388	rBV	200800	352395	6.74%	1.967%
5	2.832	461	464	470	rBV4	519	711	0.01%	0.004%
6	2.883	476	480	485	rBV2	543	543	0.01%	0.003%
7	2.967	496	506	509	rBV4	2102	3656	0.07%	0.020%
8	3.035	523	527	529	rBV3	1678	1461	0.03%	0.008%
9	3.218	575	584	594	rVV4	5602	10488	0.20%	0.059%
10	3.334	611	620	632	rVB6	1477	3004	0.06%	0.017%
11	3.420	639	647	650	rBV3	1136	1547	0.03%	0.009%
12	3.678	716	727	741	rVB4	4749	10439	0.20%	0.058%
13	4.289	909	917	921	rBV4	715	944	0.02%	0.005%
14	4.407	947	954	955	rBV3	828	765	0.01%	0.004%
15	4.510	977	986	997	rBV6	1716	3632	0.07%	0.020%
16	4.652	1014	1030	1082	rBV	80551	338350	6.47%	1.889%
17	5.063	1142	1158	1184	rVB	202654	475067	9.09%	2.652%
18	5.359	1238	1250	1267	rVB5	7973	19388	0.37%	0.108%
19	5.452	1267	1279	1294	rBV9	2786	6637	0.13%	0.037%
20	5.581	1308	1319	1331	rBV3	9312	18534	0.35%	0.103%
21	5.719	1340	1362	1372	rBV2	478741	1224130	23.42%	6.833%
22	5.883	1411	1413	1425	rVB6	1448	1990	0.04%	0.011%
23	5.986	1438	1445	1450	rBV4	1452	1619	0.03%	0.009%
24	6.128	1479	1489	1501	rVV4	11063	21317	0.41%	0.119%
25	6.247	1511	1526	1554	rBV	576233	1159668	22.18%	6.473%
26	6.526	1604	1613	1626	rBV9	3575	7685	0.15%	0.043%
27	6.610	1631	1639	1641	rBV2	608	671	0.01%	0.004%
28	6.690	1649	1664	1682	rBV	264217	550946	10.54%	3.075%
29	7.221	1812	1829	1833	rBV5	4767	12189	0.23%	0.068%
30	7.501	1902	1916	1927	rBV2	41753	96257	1.84%	0.537%
31	7.568	1927	1937	1957	rVV	128360	261990	5.01%	1.462%
32	7.652	1961	1963	1967	rVB3	764	534	0.01%	0.003%
33	7.694	1970	1976	1987	rBV5	1393	2734	0.05%	0.015%
34	7.832	2015	2019	2020	rVV2	689	552	0.01%	0.003%
35	7.845	2020	2023	2025	rVV3	1231	1077	0.02%	0.006%
36	7.899	2026	2040	2054	rVV	527549	964198	18.44%	5.382%

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 Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP2ME

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	7.976	2055	2064	2106	rVB4	44630	169526	3.24%	0.946%
38	8.185	2116	2129	2152	rBV2	78757	174155	3.33%	0.972%
39	8.372	2174	2187	2207	rVB5	19403	57767	1.11%	0.322%
40	8.581	2241	2252	2261	rBV5	5539	10449	0.20%	0.058%
41	8.668	2261	2279	2307	rVV2	330958	759473	14.53%	4.239%
42	8.947	2363	2366	2375	rVB5	1689	2073	0.04%	0.012%
43	9.034	2379	2393	2408	rBV5	7162	18929	0.36%	0.106%
44	9.185	2433	2440	2442	rBV5	1692	1956	0.04%	0.011%
45	9.365	2485	2496	2501	rBV5	13427	20842	0.40%	0.116%
46	9.452	2502	2523	2553	rVB2	1958223	5227703	100.00%	29.179%
47	9.697	2587	2599	2608	rBV6	5886	11172	0.21%	0.062%
48	9.845	2642	2645	2648	rBV3	990	881	0.02%	0.005%
49	10.105	2717	2726	2737	rBV4	3196	6263	0.12%	0.035%
50	10.478	2836	2842	2844	rBV4	735	795	0.02%	0.004%
51	10.658	2888	2898	2910	rBV7	10793	18445	0.35%	0.103%
52	10.767	2918	2932	2950	rBV	424793	704973	13.49%	3.935%
53	10.931	2980	2983	2987	rBV4	822	575	0.01%	0.003%
54	10.980	2990	2998	3012	rVB2	8599	14759	0.28%	0.082%
55	11.095	3027	3034	3037	rBV	1366	1629	0.03%	0.009%
56	11.256	3078	3084	3093	rVV3	2619	3692	0.07%	0.021%
57	11.301	3093	3098	3103	rVB3	1334	1562	0.03%	0.009%
58	11.385	3117	3124	3129	rVV4	1857	2457	0.05%	0.014%
59	11.472	3143	3151	3159	rVV5	4014	6270	0.12%	0.035%
60	11.513	3161	3164	3174	rVB3	2091	3104	0.06%	0.017%
61	11.594	3179	3189	3199	rVB6	6795	10736	0.21%	0.060%
62	11.697	3215	3221	3226	rBV3	1100	1252	0.02%	0.007%
63	11.751	3231	3238	3246	rBV8	3561	5009	0.10%	0.028%
64	11.816	3246	3258	3273	rBV	1021961	1630916	31.20%	9.103%
65	11.886	3274	3280	3294	rVB6	14105	23650	0.45%	0.132%
66	11.954	3295	3301	3309	rBV10	4174	6295	0.12%	0.035%
67	12.066	3329	3336	3344	rBV4	3742	6613	0.13%	0.037%
68	12.198	3363	3377	3398	rBV	631628	1178724	22.55%	6.579%
69	12.381	3430	3434	3437	rBV5	939	959	0.02%	0.005%
70	12.471	3455	3462	3471	rBV7	6373	9471	0.18%	0.053%
71	12.578	3492	3495	3502	rVB6	1455	1225	0.02%	0.007%
72	12.709	3528	3536	3545	rVB7	6252	8922	0.17%	0.050%
73	12.883	3586	3590	3596	rVV5	1566	1942	0.04%	0.011%
74	12.973	3608	3618	3629	rVB2	20576	33417	0.64%	0.187%
75	13.028	3630	3635	3640	rVV5	954	1104	0.02%	0.006%
76	13.105	3654	3659	3666	rBV5	639	824	0.02%	0.005%

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 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP2ME

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	13.163	3668	3677	3686	rBV4	7893	11761	0.22%	0.066%
78	13.275	3707	3712	3721	rVB6	2445	3608	0.07%	0.020%
79	13.333	3722	3730	3735	rBV4	9268	14268	0.27%	0.080%
80	13.378	3735	3744	3755	rVB	99121	147146	2.81%	0.821%
81	13.433	3757	3761	3763	rBV4	1899	1723	0.03%	0.010%
82	13.783	3861	3870	3874	rBV7	3851	6287	0.12%	0.035%
83	13.951	3916	3922	3924	rBV3	889	869	0.02%	0.005%
84	14.047	3948	3952	3957	rBV4	1075	1013	0.02%	0.006%
85	14.086	3961	3964	3965	rBV2	2506	1322	0.03%	0.007%
86	14.201	3991	4000	4002	rBV8	2042	2891	0.06%	0.016%
87	14.362	4041	4050	4062	rVB6	6439	9718	0.19%	0.054%
88	14.430	4062	4071	4081	rBV6	27743	47203	0.90%	0.263%
89	14.494	4081	4091	4110	rVB2	170270	284892	5.45%	1.590%
90	14.713	4156	4159	4164	rVB5	1422	1135	0.02%	0.006%
91	14.741	4164	4168	4173	rBV5	819	890	0.02%	0.005%
92	14.870	4206	4208	4209	rVV2	1132	531	0.01%	0.003%
93	14.883	4210	4212	4219	rVB4	1948	1952	0.04%	0.011%
94	14.950	4228	4233	4240	rBV7	2656	3684	0.07%	0.021%
95	15.545	4407	4418	4432	rBV	179821	277457	5.31%	1.549%
96	15.796	4489	4496	4504	rBV6	8304	11977	0.23%	0.067%
97	15.883	4513	4523	4536	rBV4	18533	46834	0.90%	0.261%
98	15.954	4540	4545	4558	rVB2	11289	17456	0.33%	0.097%
99	16.092	4580	4588	4598	rBV2	22680	33318	0.64%	0.186%
100	16.391	4671	4681	4695	rBV2	76411	121626	2.33%	0.679%

Sum of corrected areas: 17915872

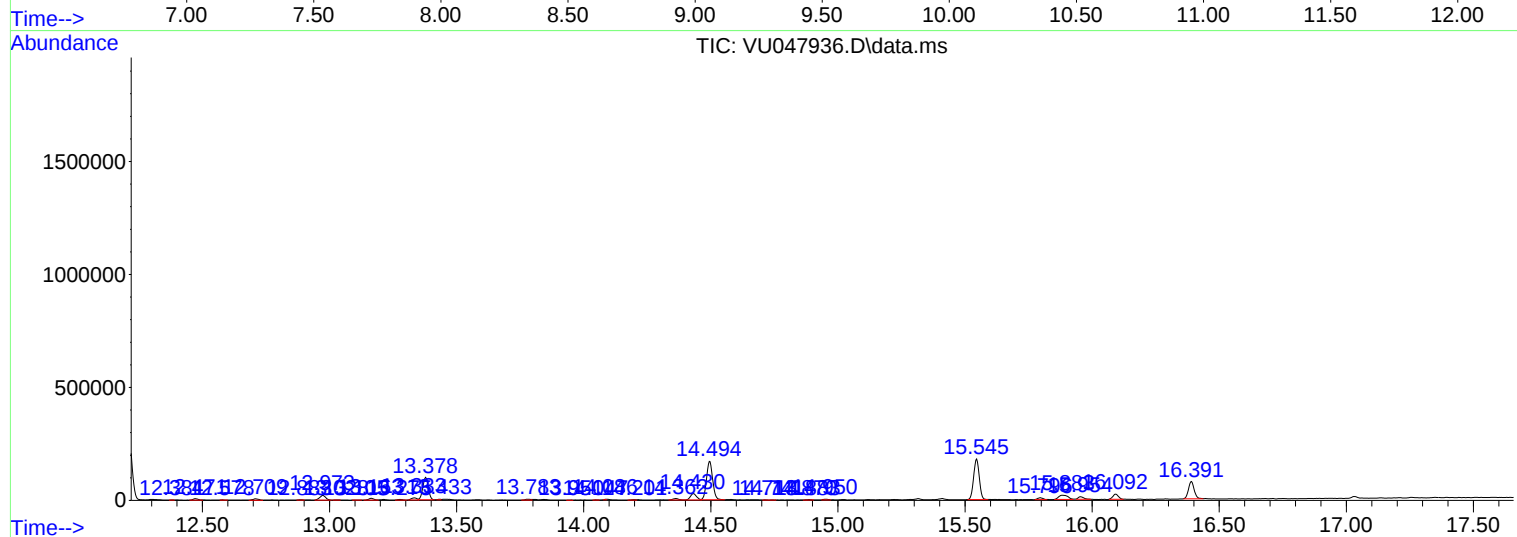
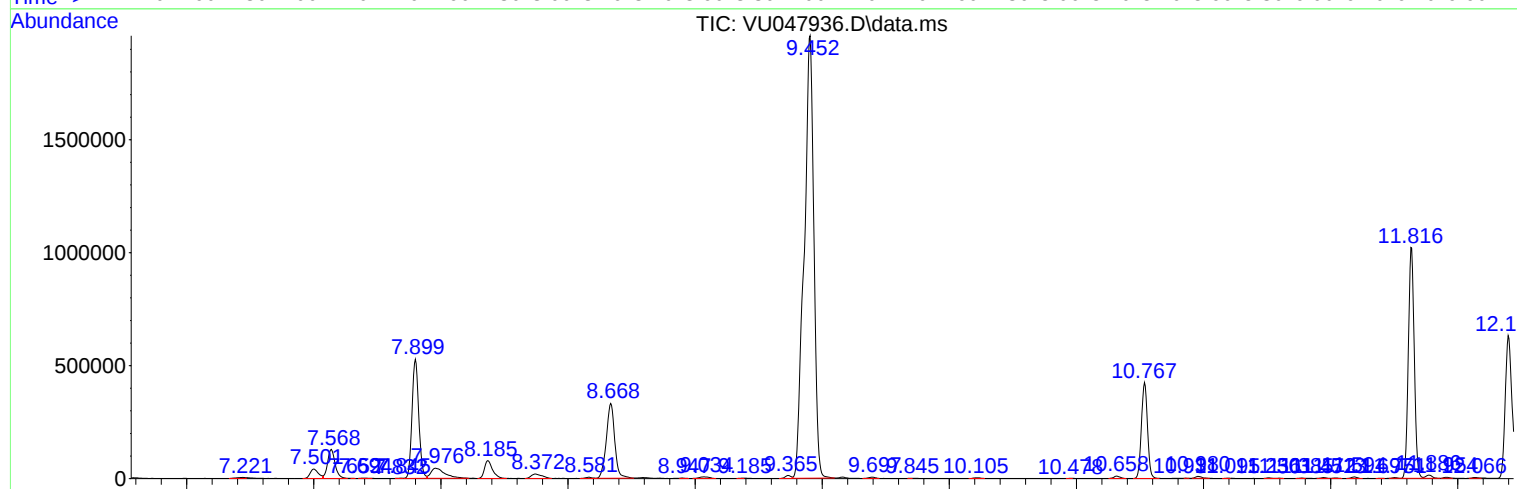
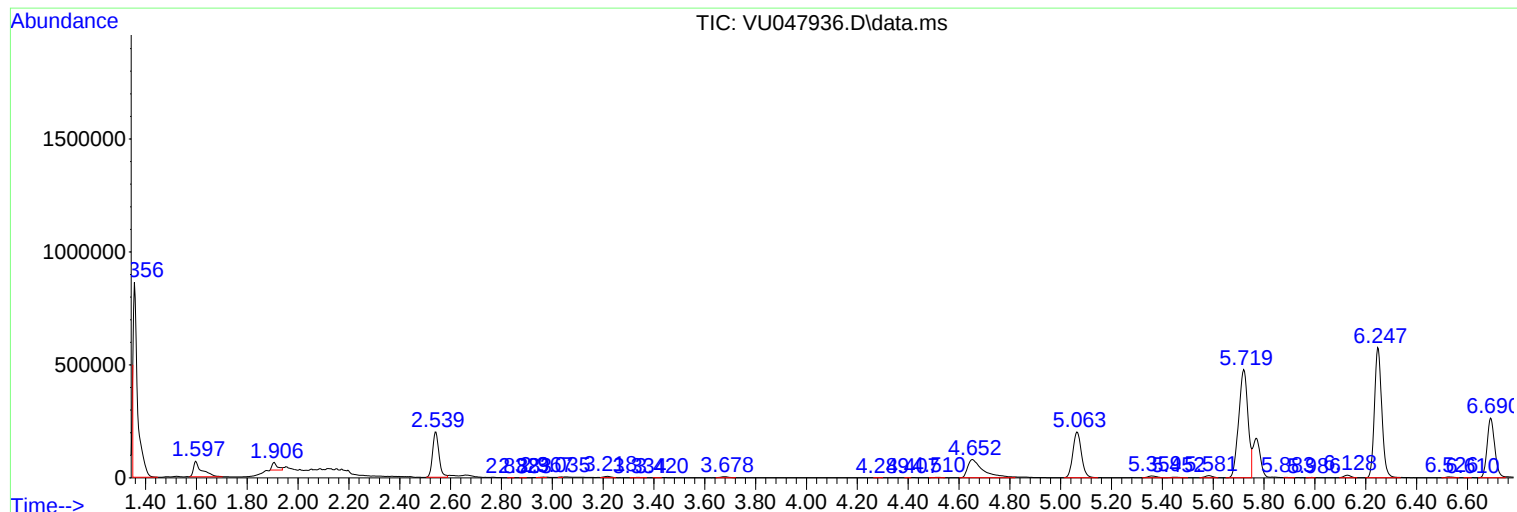
Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047936.D
Acq On : 12 Apr 2022 03:14
Operator : SY/MD
Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

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\VU041122\
Data File : VU047936.D
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Operator : SY/MD
Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

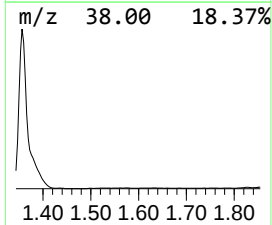
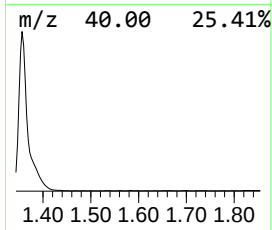
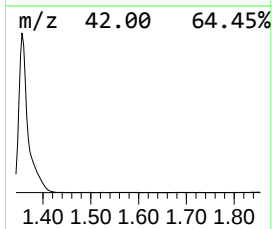
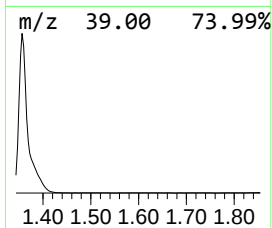
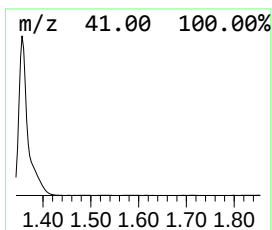
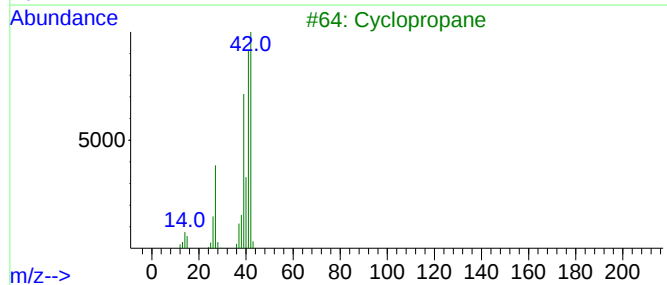
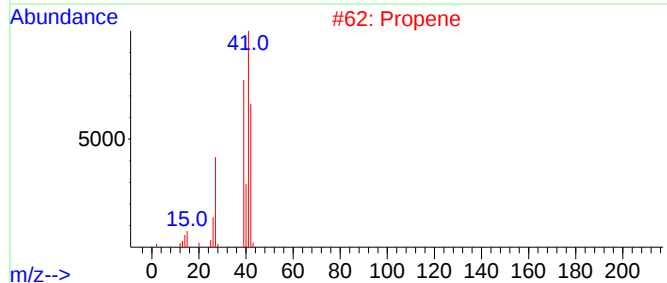
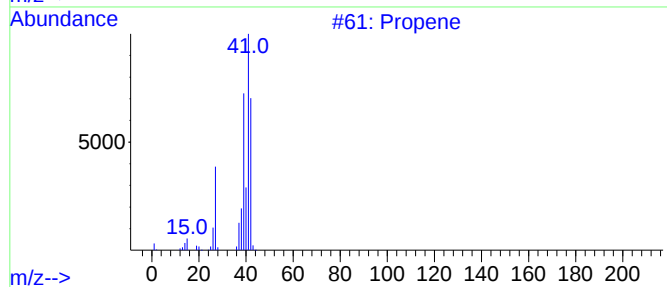
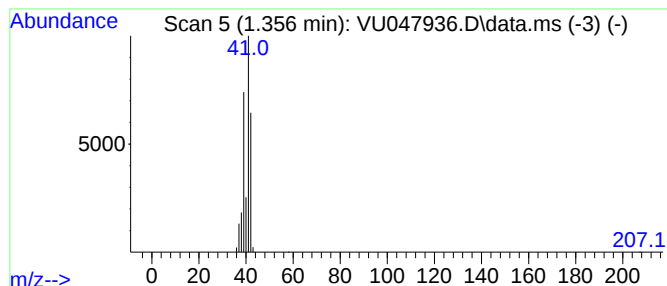
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.356	41.50 ug/L	962430	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Propene	42	C3H6	000115-07-1	80
3			Cyclopropane	42	C3H6	000075-19-4	14
4			Cyclopropane	42	C3H6	000075-19-4	8
5			Cyclopropane	42	C3H6	000075-19-4	5



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Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

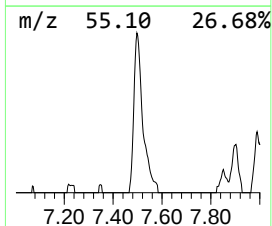
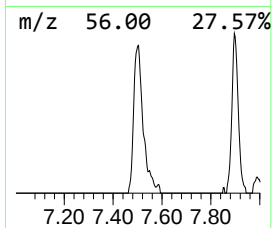
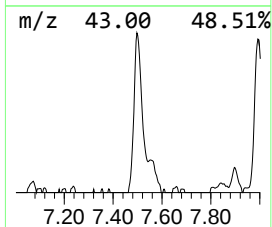
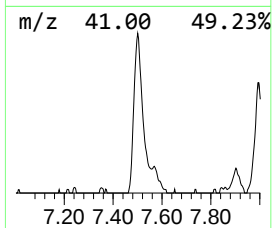
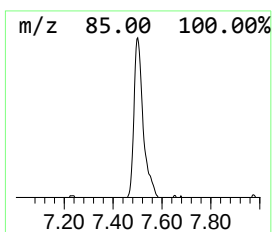
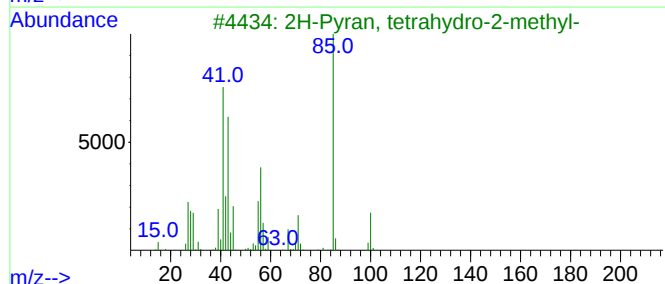
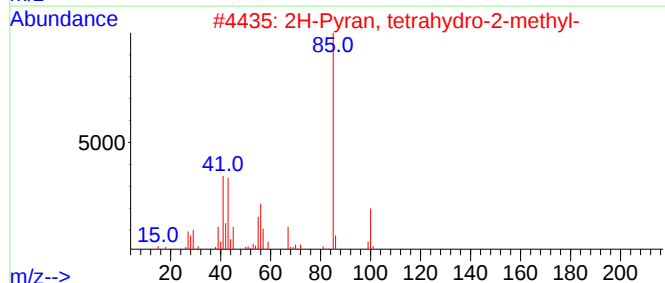
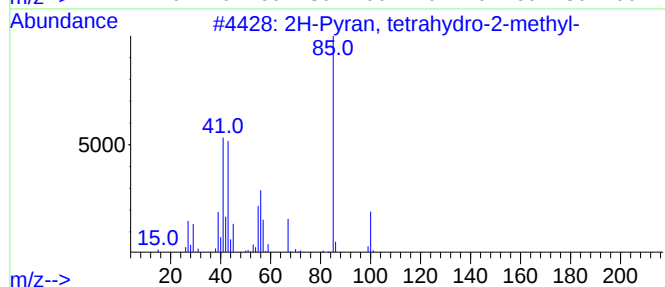
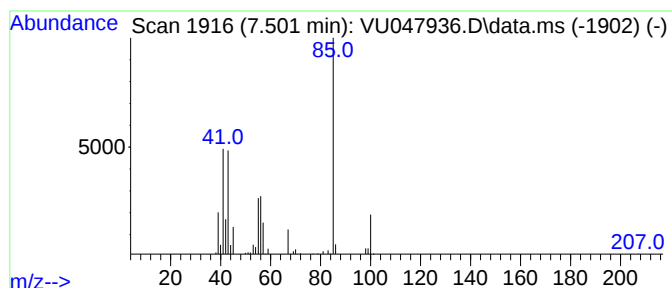
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 2H-Pyran, tetrahydro-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.501	4.15 ug/L	96257	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	95
2			2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	90
3			2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	90
4			3-Methylbut-2-enoic acid, tetrah...	184	C10H16O3	1000187-32-6	59
5			2-Furanmethanol, tetrahydro-5-me...	116	C6H12O2	054774-28-6	53



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ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

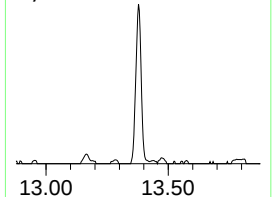
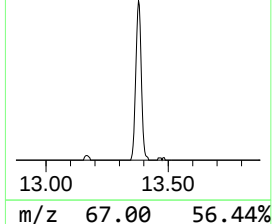
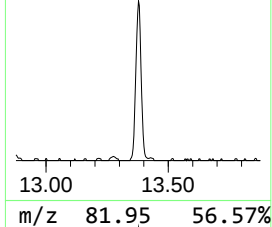
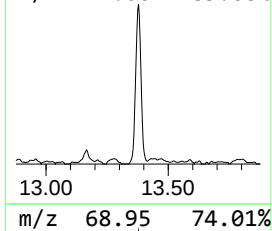
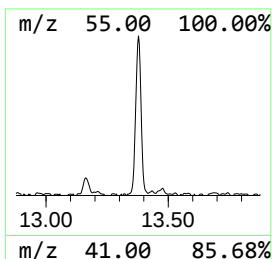
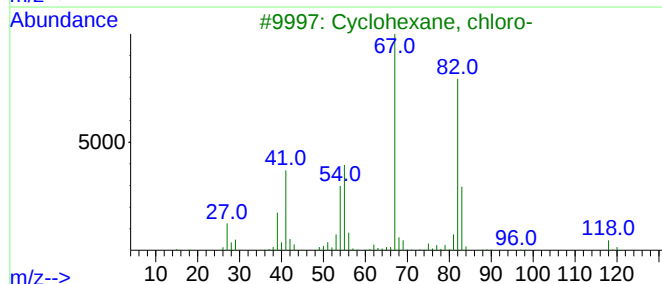
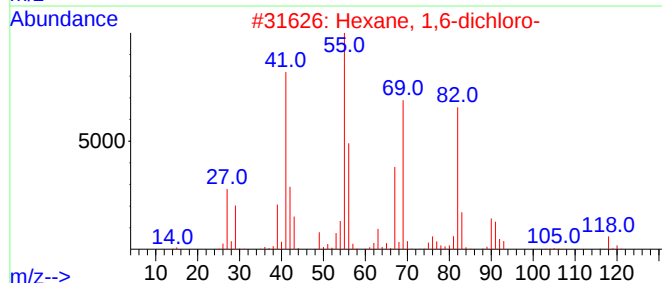
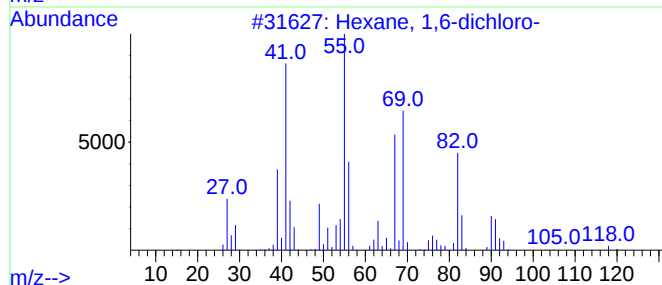
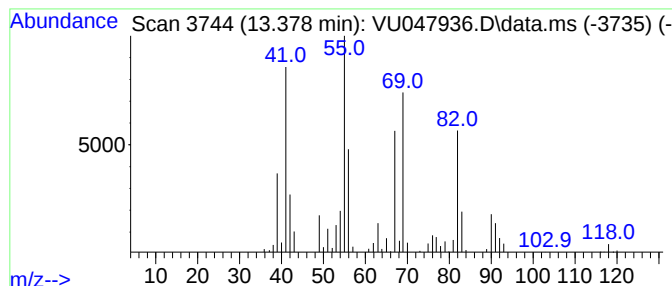
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Quant Title : VOC Analysis

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	4.51 ug/L	147146	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 1,6-dichloro-	154	C6H12Cl2	002163-00-0	80
2			Hexane, 1,6-dichloro-	154	C6H12Cl2	002163-00-0	64
3			Cyclohexane, chloro-	118	C6H11Cl	000542-18-7	42
4			Hexenyl angelate, 4z-	182	C11H18O2	1000383-63-7	38
5			1-Hexanol, 6-chloro-	136	C6H13ClO	002009-83-8	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047936.D
Acq On : 12 Apr 2022 03:14
Operator : SY/MD
Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

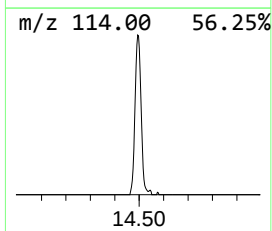
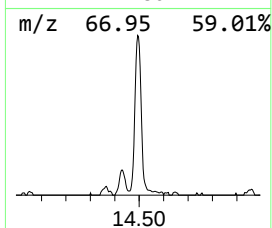
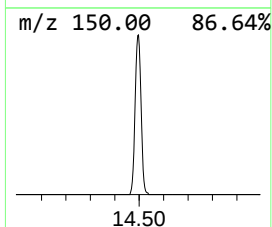
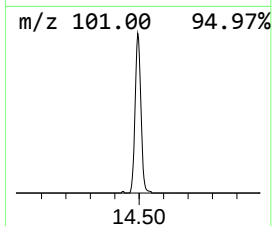
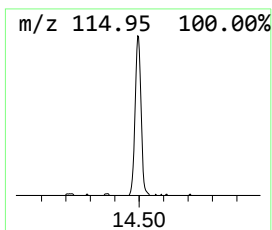
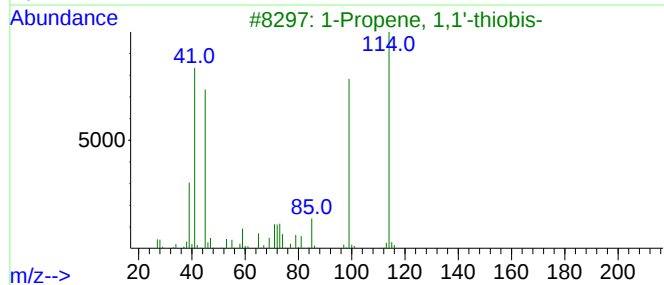
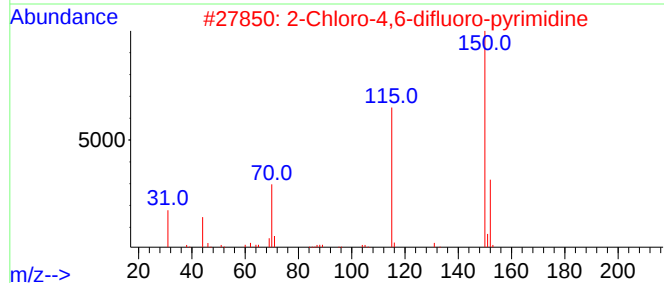
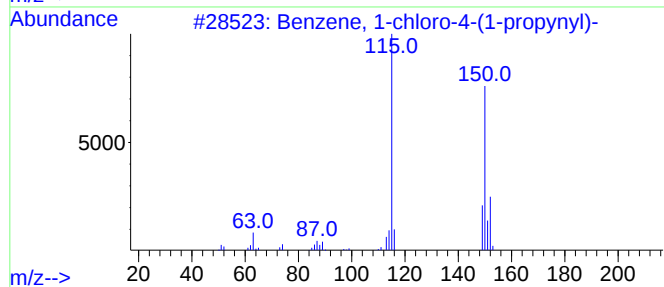
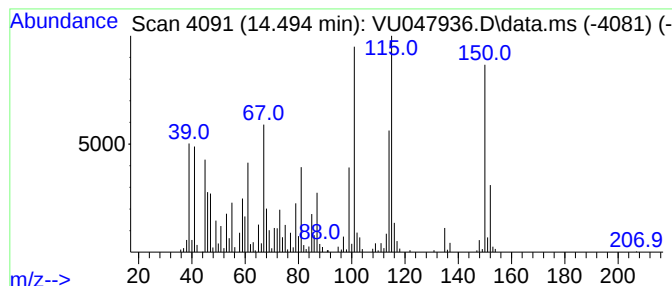
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Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.494	8.73 ug/L	284892	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-chloro-4-(1-propynyl)-	150	C9H7Cl	002809-65-6	43
2			2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	27
3			1-Propene, 1,1'-thiobis-	114	C6H10S	033922-80-4	11
4			2-Piperidinethione	115	C5H9NS	013070-01-4	11
5			2H-Thiopyran, tetrahydro-2-methyl-	116	C6H12S	005161-16-0	11



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047936.D
Acq On : 12 Apr 2022 03:14
Operator : SY/MD
Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

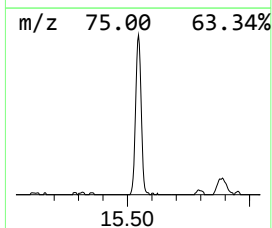
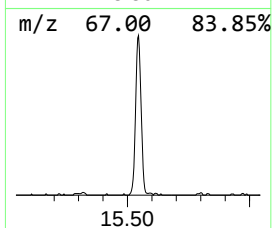
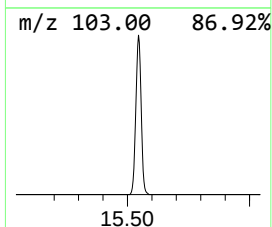
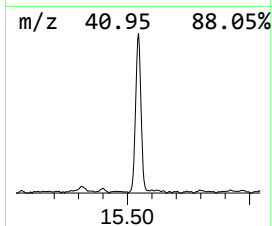
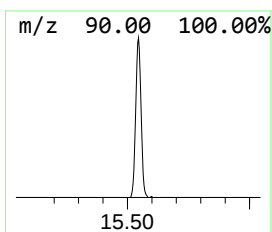
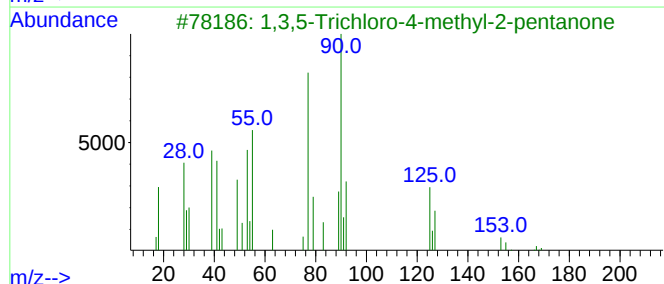
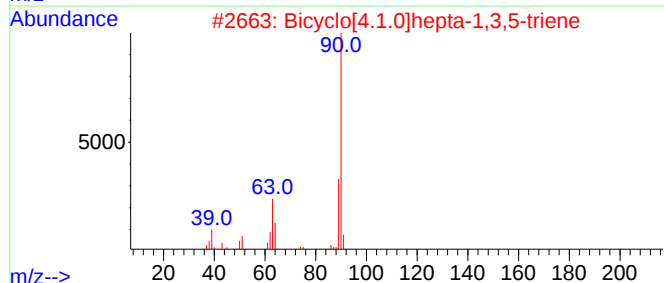
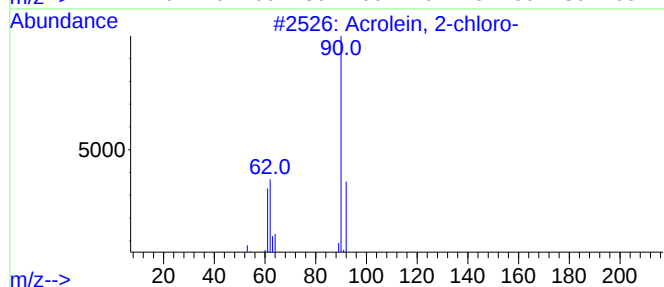
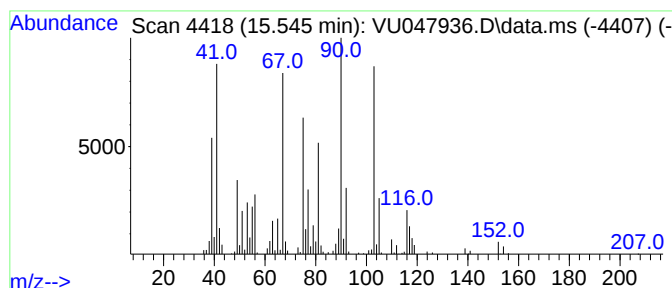
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Quant Title : VOC Analysis

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

Peak Number 6 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	8.51 ug/L	277457	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	37
2			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	35
3			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	28
4			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	23
5			Chromyl fluoride	122	CrF2O2	007788-96-7	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047936.D
Acq On : 12 Apr 2022 03:14
Operator : SY/MD
Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

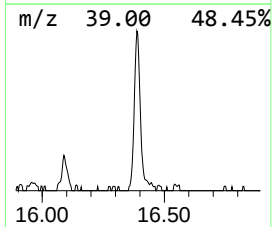
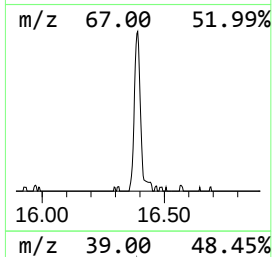
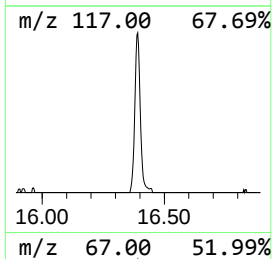
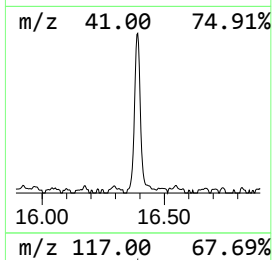
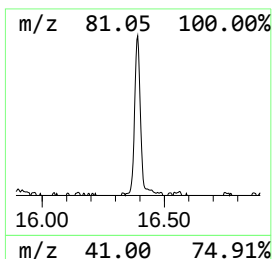
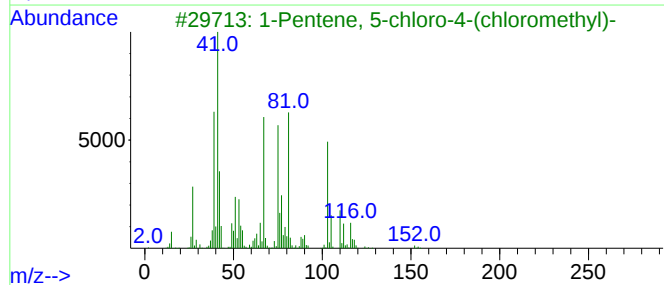
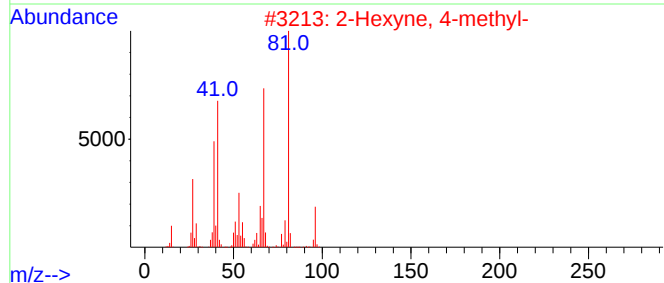
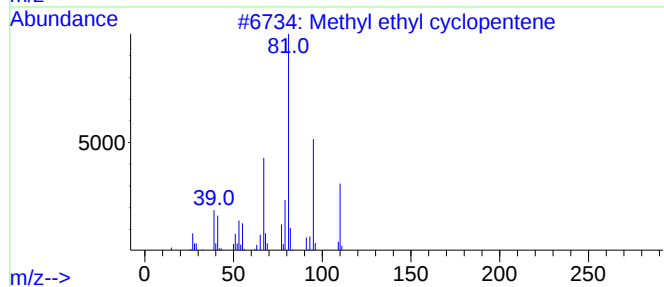
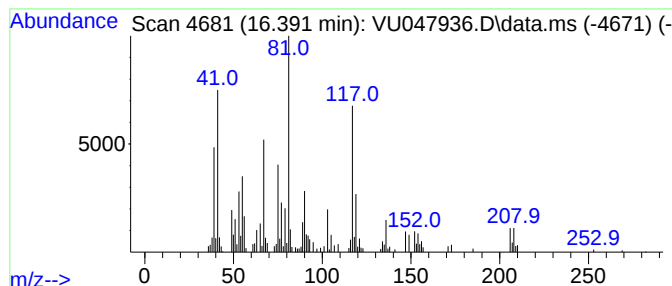
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 unknown-03 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.391	3.73 ug/L	121626	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl ethyl cyclopentene	110	C8H14	019780-56-4	14
2			2-Hexyne, 4-methyl-	96	C7H12	020198-49-6	14
3			1-Pentene, 5-chloro-4-(chloromet...	152	C6H10Cl2	027990-74-5	14
4			cis-1,4-Cyclohexanediol, 0,0'-bi...	408	C12H10F10O4	1000385-95-0	14
5			Trifluoroacetyl-.alpha.-fenchol	250	C12H17F3O2	031076-73-0	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047936.D
Acq On : 12 Apr 2022 03:14
Operator : SY/MD
Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

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	41.5	ug/L	962430	1	6.247	1159670	50.0
2H-Pyran, tetra...	7.501	4.2	ug/L	96257	1	6.247	1159670	50.0
Hexane, 1,6-dic...	13.378	4.5	ug/L	147146	3	11.819	1630920	50.0
unknown-01	14.494	8.7	ug/L	284892	3	11.819	1630920	50.0
unknown-02	15.545	8.5	ug/L	277457	3	11.819	1630920	50.0
unknown-03	16.391	3.7	ug/L	121626	3	11.819	1630920	50.0