

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
 Data File : VU047958.D
 Acq On : 12 Apr 2022 16:10
 Operator : SY/MD
 Sample : N2293-14ME
 Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 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: VU047958.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	rBV	51156	100384	2.83%	0.763%
2	1.813	126	147	148	rBV8	20745	51840	1.46%	0.394%
3	2.543	362	374	385	rBV	140018	235576	6.65%	1.790%
4	2.761	438	442	446	rBV5	867	840	0.02%	0.006%
5	2.970	497	507	520	rVB6	5176	12671	0.36%	0.096%
6	3.035	523	527	528	rBV2	1247	810	0.02%	0.006%
7	3.141	557	560	565	rVB3	383	345	0.01%	0.003%
8	3.221	574	585	595	rBV4	3439	6691	0.19%	0.051%
9	3.337	617	621	625	rBV3	636	603	0.02%	0.005%
10	3.604	701	704	711	rBV3	363	462	0.01%	0.004%
11	3.678	716	727	736	rBV7	1809	3634	0.10%	0.028%
12	4.070	845	849	854	rBV3	373	387	0.01%	0.003%
13	4.408	946	954	958	rBV2	450	642	0.02%	0.005%
14	4.504	980	984	987	rBV3	552	486	0.01%	0.004%
15	4.639	1011	1026	1081	rVV2	91940	342135	9.66%	2.600%
16	5.064	1142	1158	1180	rBV	183880	422785	11.94%	3.212%
17	5.202	1197	1201	1206	rVB	423	352	0.01%	0.003%
18	5.269	1213	1222	1224	rBV2	453	514	0.01%	0.004%
19	5.289	1224	1228	1237	rVB4	636	953	0.03%	0.007%
20	5.363	1237	1251	1266	rBV5	4015	10713	0.30%	0.081%
21	5.459	1273	1281	1287	rVB6	1050	1955	0.06%	0.015%
22	5.584	1311	1320	1332	rVB7	2896	5754	0.16%	0.044%
23	5.719	1342	1362	1373	rBV2	398715	1076895	30.41%	8.182%
24	5.925	1424	1426	1432	rBV4	482	406	0.01%	0.003%
25	5.993	1442	1447	1450	rBV3	509	373	0.01%	0.003%
26	6.131	1476	1490	1498	rBV6	3778	7376	0.21%	0.056%
27	6.247	1511	1526	1548	rBV	374270	746631	21.09%	5.673%
28	6.375	1563	1566	1569	rVB2	522	360	0.01%	0.003%
29	6.472	1594	1596	1603	rVB3	333	360	0.01%	0.003%
30	6.530	1603	1614	1628	rVB10	3528	6736	0.19%	0.051%
31	6.600	1631	1636	1639	rBV2	659	620	0.02%	0.005%
32	6.690	1650	1664	1684	rBV	241982	495937	14.01%	3.768%
33	6.986	1753	1756	1757	rBV2	658	358	0.01%	0.003%
34	7.195	1809	1821	1837	rBV4	7955	19747	0.56%	0.150%
35	7.343	1861	1867	1871	rBV4	615	682	0.02%	0.005%
36	7.497	1902	1915	1927	rBV2	40249	92004	2.60%	0.699%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
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 Sample : N2293-14ME
 Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 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	7.568	1927	1937	1959	rVB	109563	219917	6.21%	1.671%
38	7.687	1966	1974	1981	rBV4	1550	2626	0.07%	0.020%
39	7.832	2015	2019	2020	rBV2	543	394	0.01%	0.003%
40	7.899	2026	2040	2054	rBV	392534	705351	19.92%	5.359%
41	7.983	2055	2066	2087	rVB5	38491	119553	3.38%	0.908%
42	8.182	2116	2128	2148	rBV	74182	154194	4.35%	1.172%
43	8.369	2173	2186	2208	rVB4	19672	52162	1.47%	0.396%
44	8.581	2241	2252	2260	rBV6	4467	9275	0.26%	0.070%
45	8.658	2260	2276	2303	rVV	407761	817903	23.10%	6.214%
46	9.031	2378	2392	2406	rVB3	8843	20299	0.57%	0.154%
47	9.186	2432	2440	2441	rBV4	1619	2008	0.06%	0.015%
48	9.282	2466	2470	2475	rVB5	423	433	0.01%	0.003%
49	9.366	2486	2496	2501	rBV4	6945	11329	0.32%	0.086%
50	9.452	2501	2523	2555	rVB2	1397299	3541026	100.00%	26.905%
51	9.694	2586	2598	2609	rVB7	3265	7278	0.21%	0.055%
52	9.845	2638	2645	2648	rBV5	938	1144	0.03%	0.009%
53	9.864	2649	2651	2655	rVB3	512	346	0.01%	0.003%
54	10.034	2702	2704	2710	rVB3	730	492	0.01%	0.004%
55	10.102	2714	2725	2726	rBV4	2316	2123	0.06%	0.016%
56	10.658	2888	2898	2907	rBV7	8136	13783	0.39%	0.105%
57	10.764	2918	2931	2948	rVV	466929	757654	21.40%	5.757%
58	10.935	2982	2984	2987	rBV4	605	397	0.01%	0.003%
59	10.976	2989	2997	3011	rVB2	7705	12054	0.34%	0.092%
60	11.092	3030	3033	3035	rBV	607	424	0.01%	0.003%
61	11.256	3078	3084	3091	rBV5	1927	2406	0.07%	0.018%
62	11.382	3116	3123	3130	rVB6	1764	2566	0.07%	0.019%
63	11.472	3146	3151	3159	rVV5	2563	3727	0.11%	0.028%
64	11.513	3159	3164	3174	rVB6	2353	3493	0.10%	0.027%
65	11.591	3180	3188	3195	rBV4	5872	8863	0.25%	0.067%
66	11.697	3218	3221	3224	rBV3	585	497	0.01%	0.004%
67	11.751	3232	3238	3246	rVB5	2661	3687	0.10%	0.028%
68	11.816	3246	3258	3273	rVV	632351	996611	28.14%	7.572%
69	11.883	3274	3279	3290	rVV6	11902	18484	0.52%	0.140%
70	11.954	3290	3301	3312	rVB8	5796	9852	0.28%	0.075%
71	12.070	3329	3337	3345	rBV7	2334	4537	0.13%	0.034%
72	12.105	3345	3348	3351	rVB3	1144	757	0.02%	0.006%
73	12.198	3364	3377	3395	rBV	514102	957285	27.03%	7.273%
74	12.475	3455	3463	3472	rBV5	4251	6980	0.20%	0.053%
75	12.710	3529	3536	3545	rVB6	4582	6598	0.19%	0.050%
76	12.774	3551	3556	3559	rBV2	685	584	0.02%	0.004%

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 Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 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	12.832	3571	3574	3576	rBV3	542	367	0.01%	0.003%
78	12.880	3583	3589	3590	rBV3	1296	1134	0.03%	0.009%
79	12.973	3608	3618	3629	rVB2	15993	26296	0.74%	0.200%
80	13.028	3632	3635	3641	rBV3	769	740	0.02%	0.006%
81	13.163	3670	3677	3684	rBV5	4366	6002	0.17%	0.046%
82	13.259	3704	3707	3708	rBV3	863	531	0.01%	0.004%
83	13.333	3721	3730	3735	rBV3	8554	13960	0.39%	0.106%
84	13.378	3735	3744	3756	rVB	83558	126644	3.58%	0.962%
85	13.584	3805	3808	3814	rVB3	875	685	0.02%	0.005%
86	13.668	3831	3834	3836	rBV2	503	346	0.01%	0.003%
87	13.777	3861	3868	3872	rBV6	3081	4252	0.12%	0.032%
88	13.841	3883	3888	3901	rVB9	2110	3645	0.10%	0.028%
89	14.092	3960	3966	3974	rVB3	2755	3842	0.11%	0.029%
90	14.362	4040	4050	4062	rVB2	13215	19923	0.56%	0.151%
91	14.430	4062	4071	4080	rBV4	24134	37085	1.05%	0.282%
92	14.494	4080	4091	4107	rVB2	146369	241482	6.82%	1.835%
93	14.626	4130	4132	4136	rBV3	641	471	0.01%	0.004%
94	14.954	4225	4234	4240	rVB9	2273	3585	0.10%	0.027%
95	15.311	4341	4345	4353	rVB5	9316	12087	0.34%	0.092%
96	15.545	4407	4418	4437	rBV2	164705	256633	7.25%	1.950%
97	15.880	4514	4522	4538	rBV4	15792	41566	1.17%	0.316%
98	15.957	4540	4546	4555	rVB2	8921	13648	0.39%	0.104%
99	16.092	4580	4588	4599	rVB2	18950	28015	0.79%	0.213%
100	16.388	4671	4680	4706	rVB	115165	190318	5.37%	1.446%

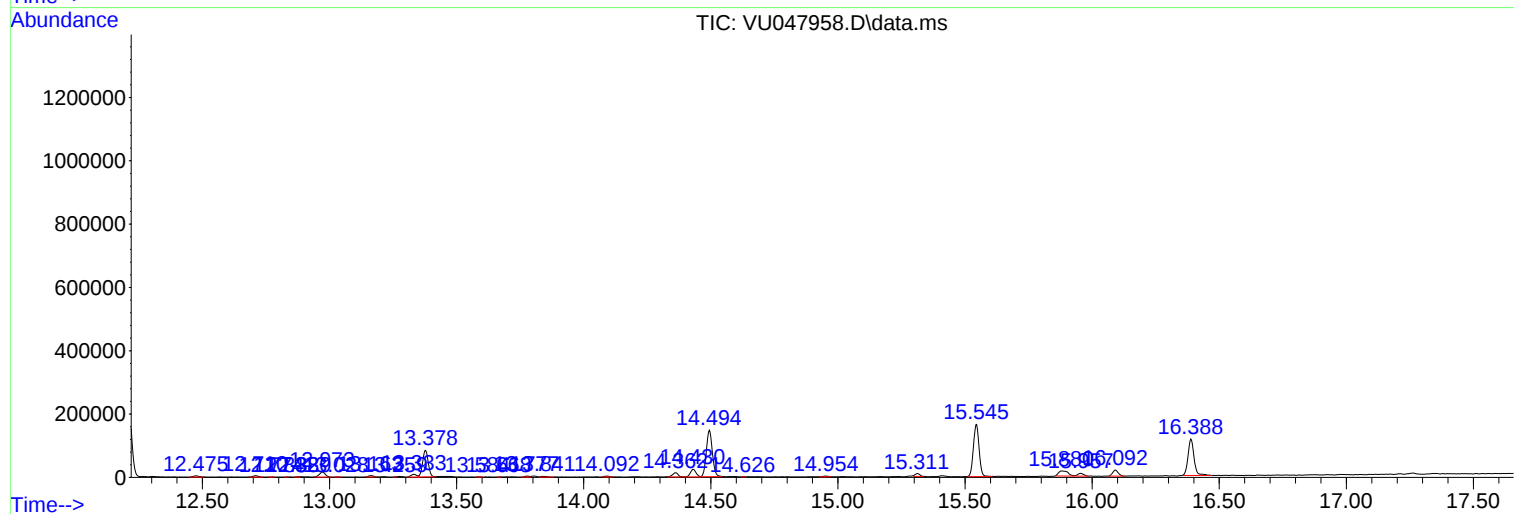
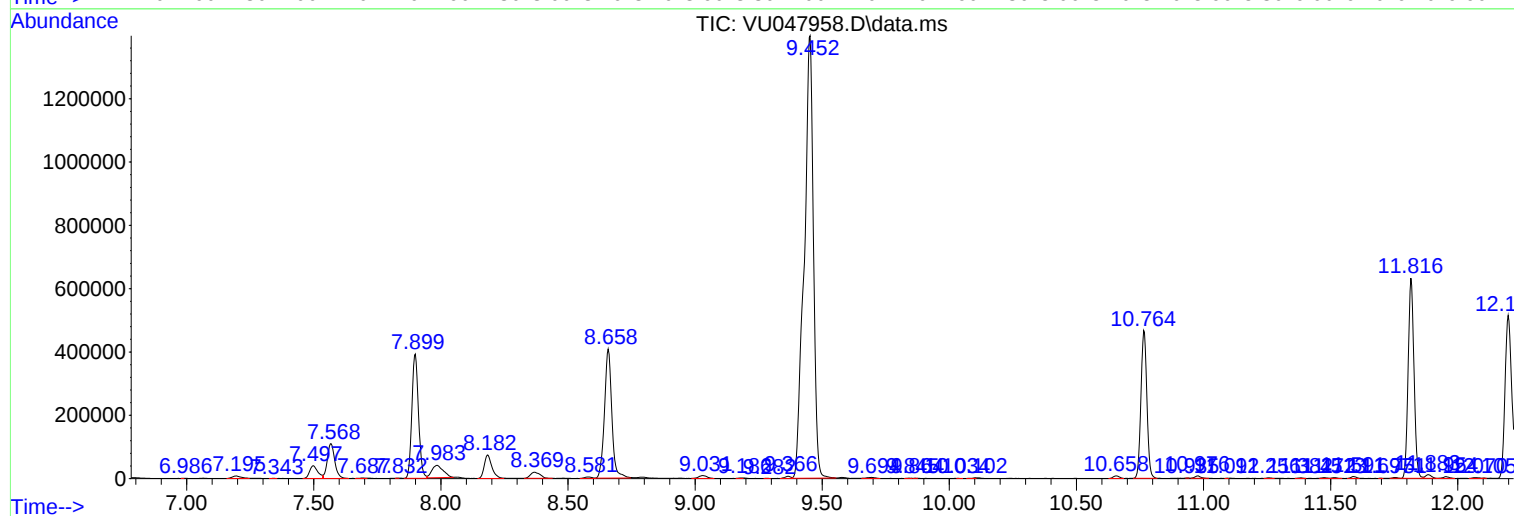
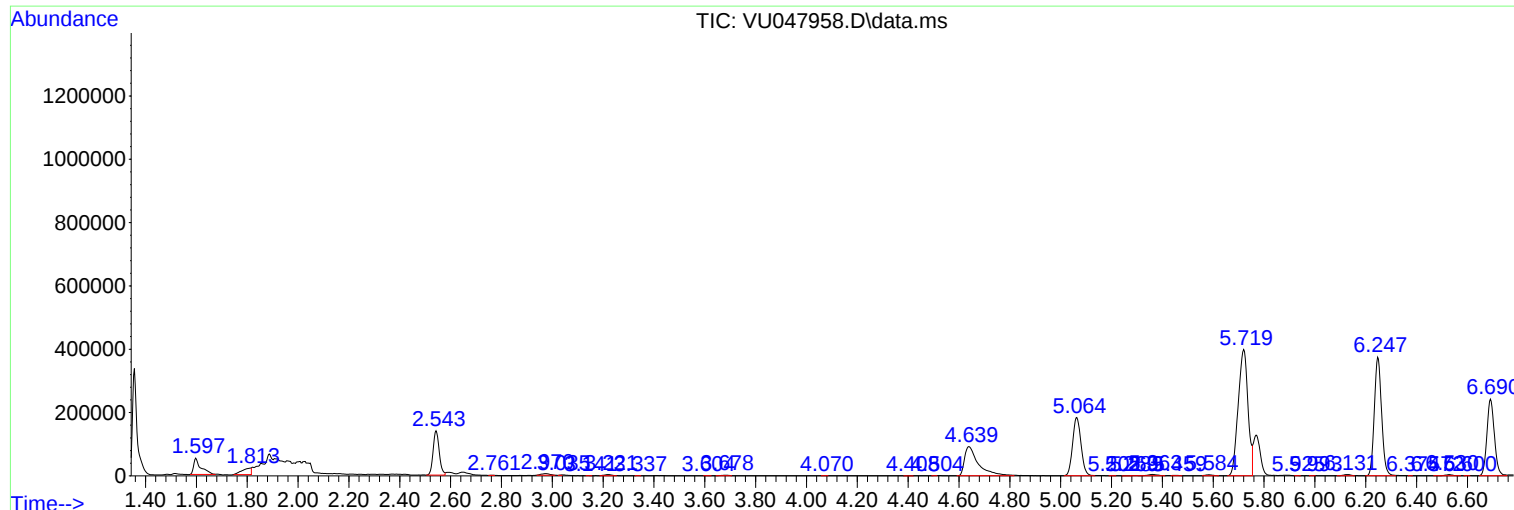
Sum of corrected areas: 13161366

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047958.D
Acq On : 12 Apr 2022 16:10
Operator : SY/MD
Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 19 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\VU041222\
Data File : VU047958.D
Acq On : 12 Apr 2022 16:10
Operator : SY/MD
Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

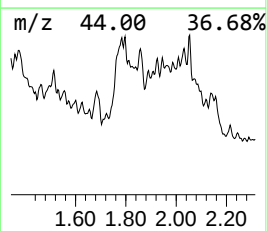
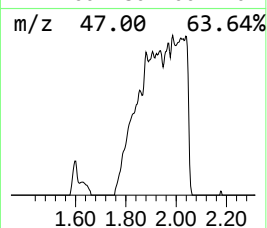
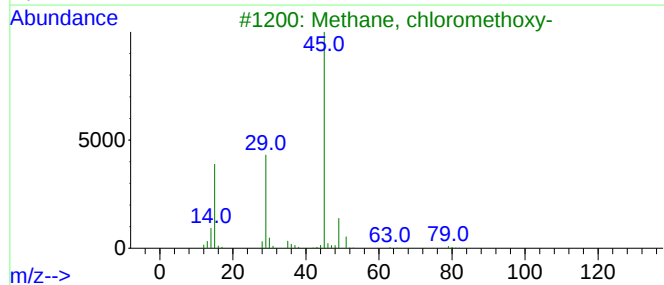
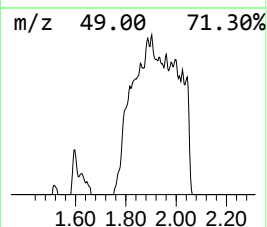
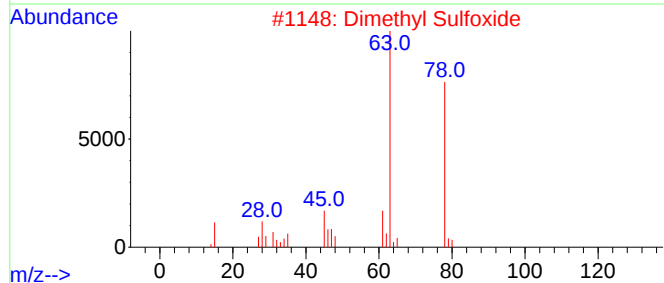
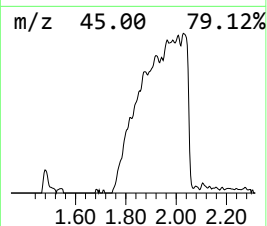
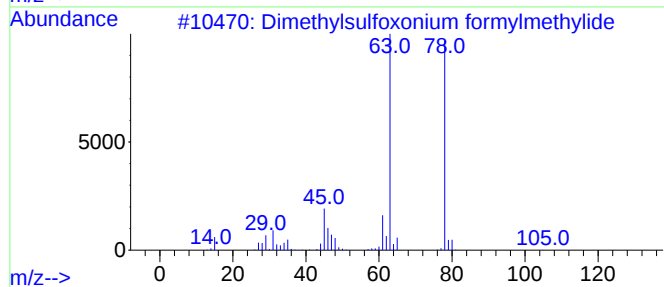
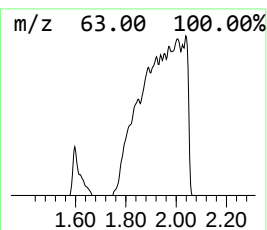
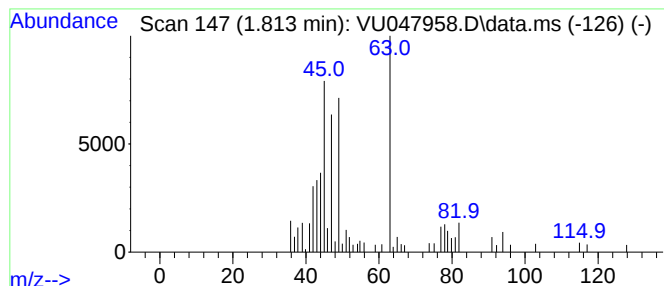
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.813	3.47 ug/L	51840	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethylsulfoxonium formylmethylide	120	C4H8O2S	031043-74-0	23
2			Dimethyl Sulfoxide	78	C2H6OS	000067-68-5	20
3			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	9
4			Methylene chloride	84	CH2Cl2	000075-09-2	9
5			Dimethyl Sulfoxide	78	C2H6OS	000067-68-5	9



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Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

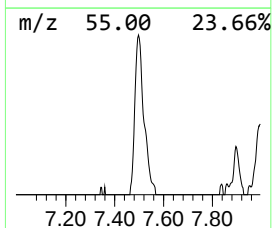
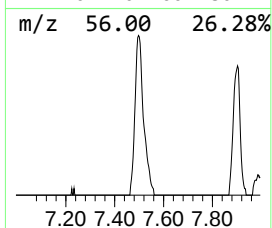
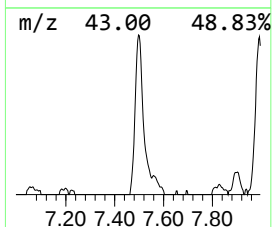
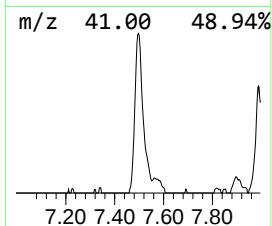
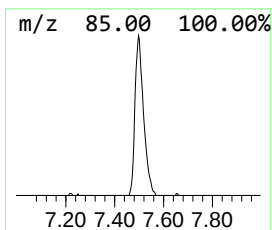
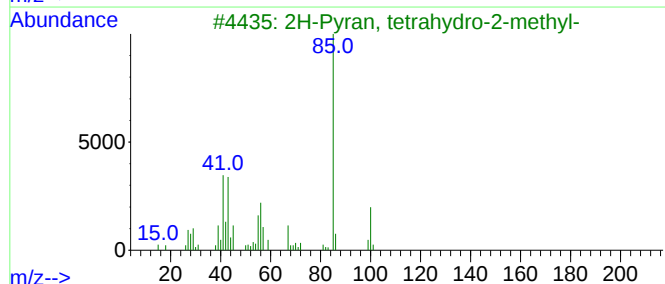
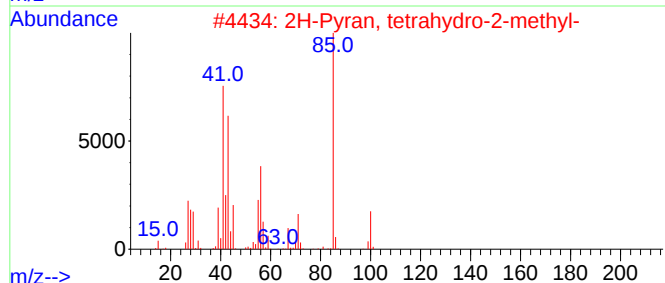
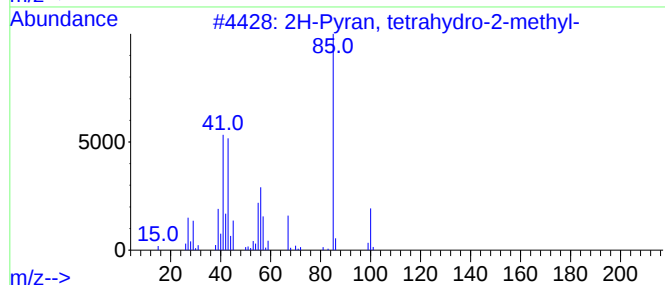
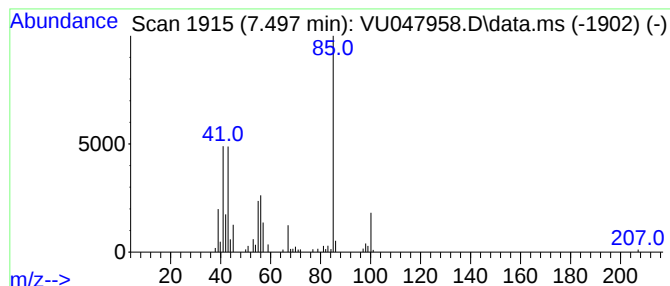
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.497	6.16 ug/L	92004	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	94		
2	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	90		
3	2H-Pyran, tetrahydro-2-methyl-	100	C6H12O	010141-72-7	86		
4	Furan, tetrahydro-2,4-dimethyl-,...	100	C6H12O	039168-01-9	64		
5	2-Propyltetrahydropyran	128	C8H16O	003857-17-8	53		



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Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

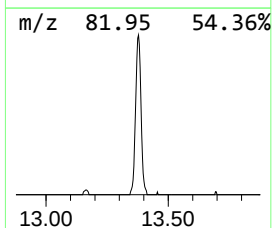
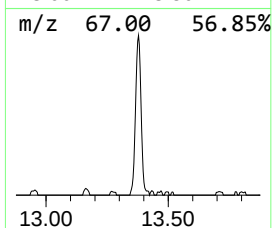
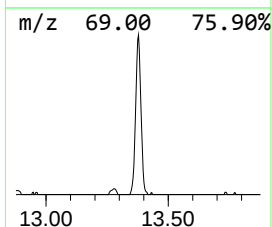
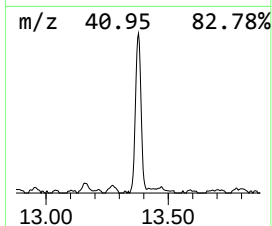
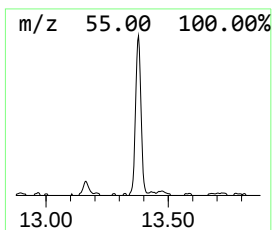
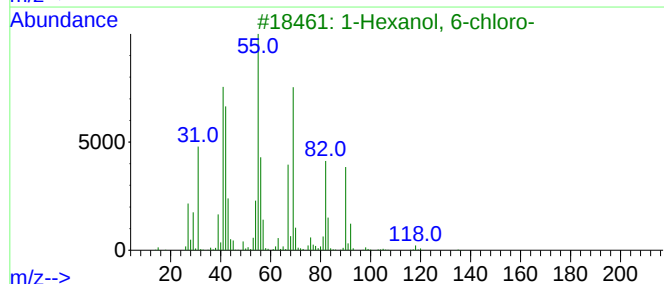
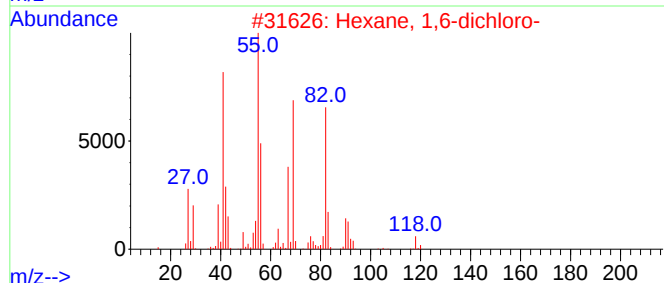
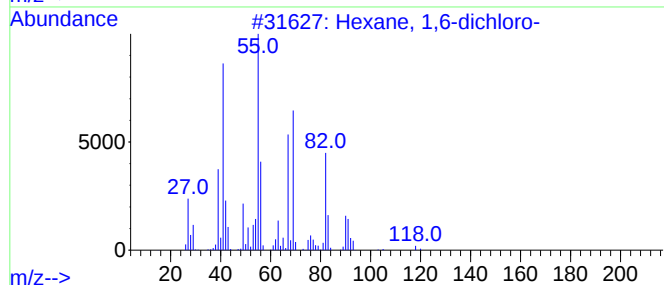
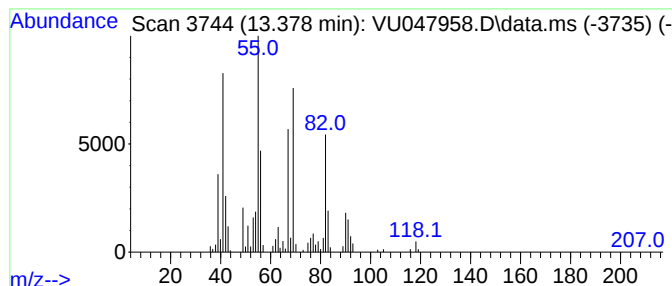
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Quant Title : VOC Analysis

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	6.35 ug/L	126644	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	91
2			Hexane, 1,6-dichloro-	154	C6H12Cl2	002163-00-0	58
3			1-Hexanol, 6-chloro-	136	C6H13ClO	002009-83-8	37
4			Chloroacetic acid, cyclohexyl ester	176	C8H13ClO2	006975-91-3	32
5			1-Hexanol, 6-chloro-	136	C6H13ClO	002009-83-8	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047958.D
Acq On : 12 Apr 2022 16:10
Operator : SY/MD
Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

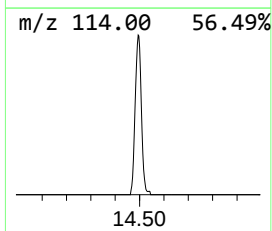
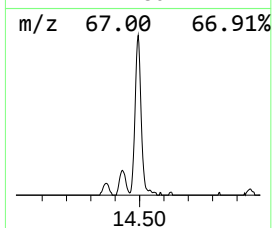
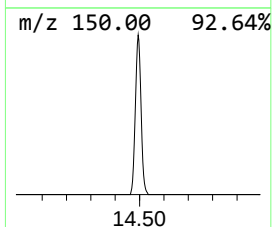
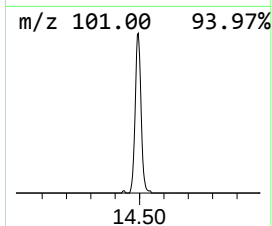
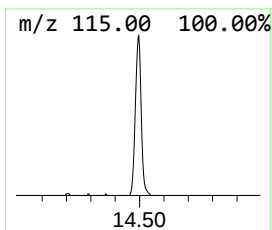
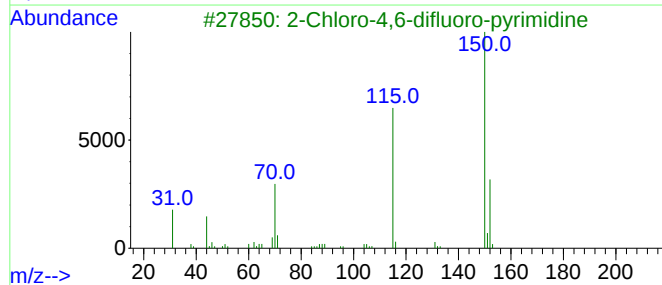
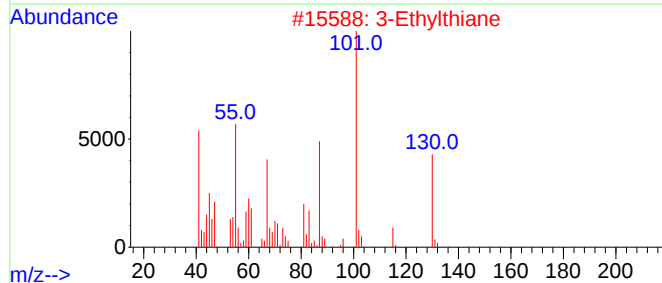
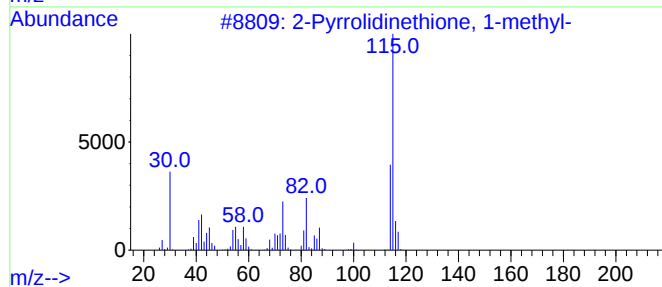
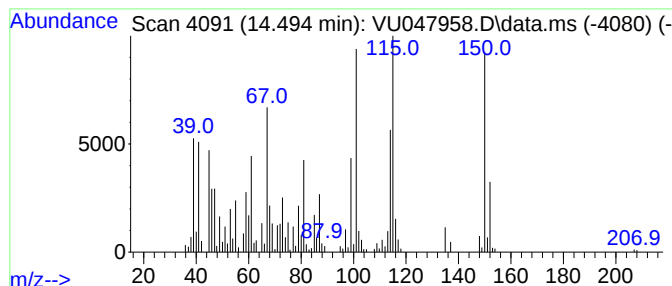
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Quant Title : VOC Analysis

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

Peak Number 5 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.494	12.12 ug/L	241482	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrrolidinethione, 1-methyl-	115	C5H9NS	010441-57-3	18		
2	3-Ethylthiane	130	C7H14S	061568-48-7	14		
3	2-Chloro-4,6-difluoro-pyrimidine	150	C4HC1F2N2	038953-30-9	14		
4	Benzene, 1,2,3,4-tetrafluoro-	150	C6H2F4	000551-62-2	11		
5	2-Butenoic acid, 2,3-dimethyl-	114	C6H10O2	004411-97-6	11		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047958.D
Acq On : 12 Apr 2022 16:10
Operator : SY/MD
Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

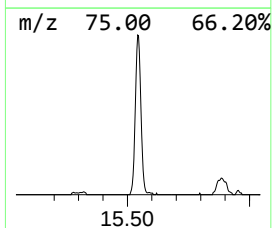
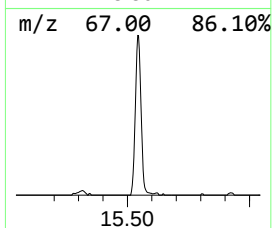
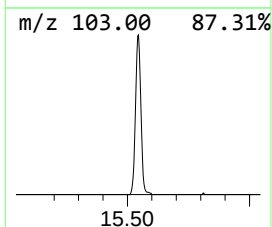
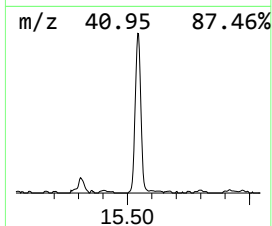
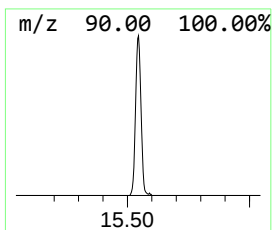
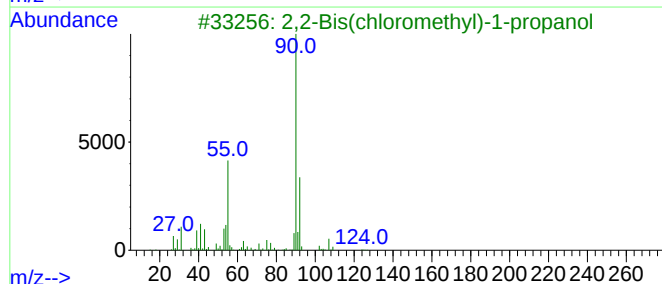
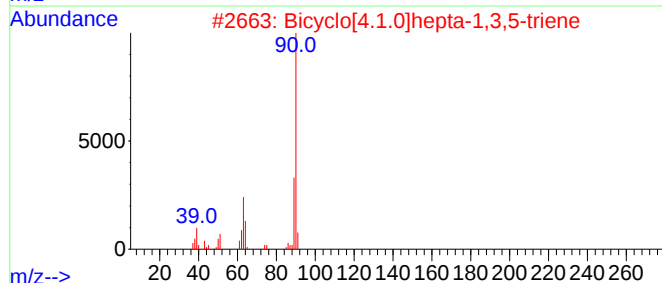
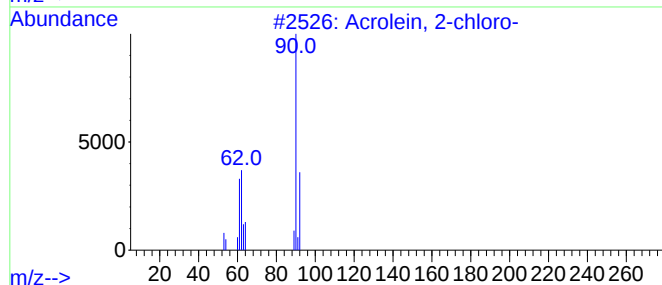
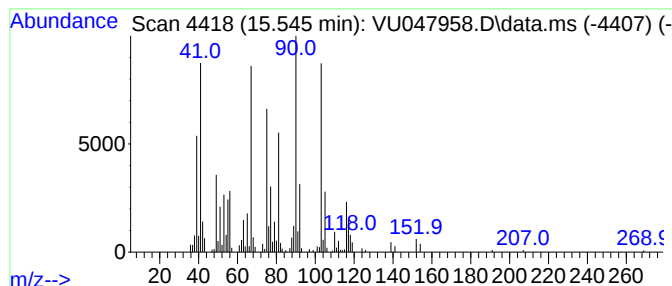
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Quant Title : VOC Analysis

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

Peak Number 6 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	12.88 ug/L	256633	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			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	35
3			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	32
4			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	28
5			4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047958.D
Acq On : 12 Apr 2022 16:10
Operator : SY/MD
Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP2ME

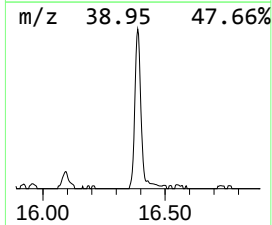
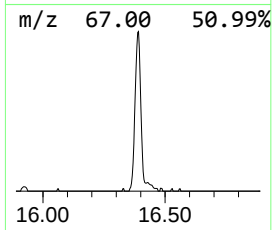
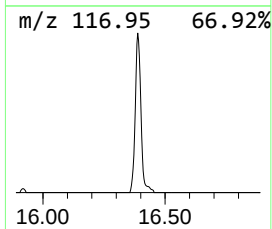
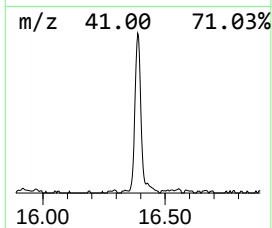
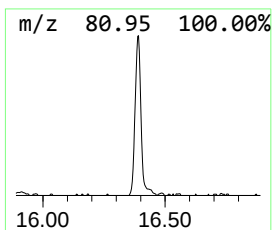
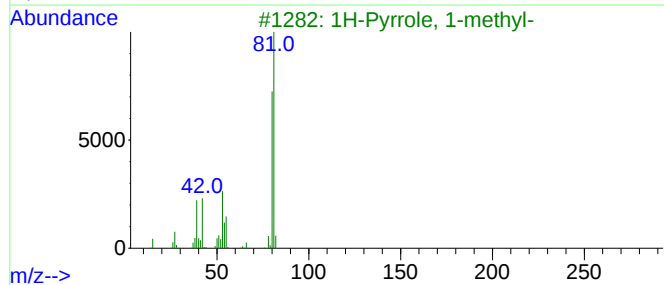
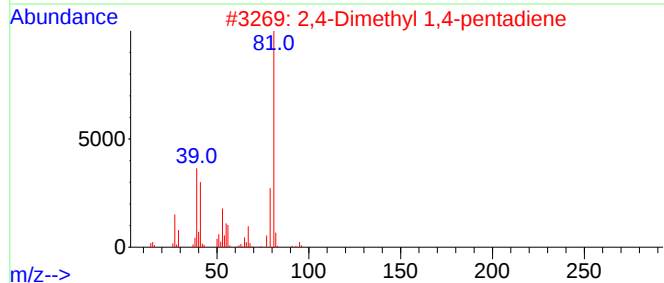
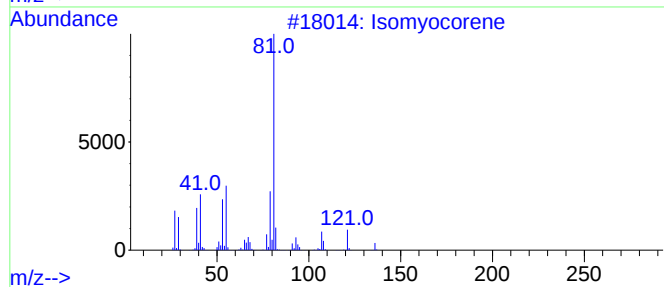
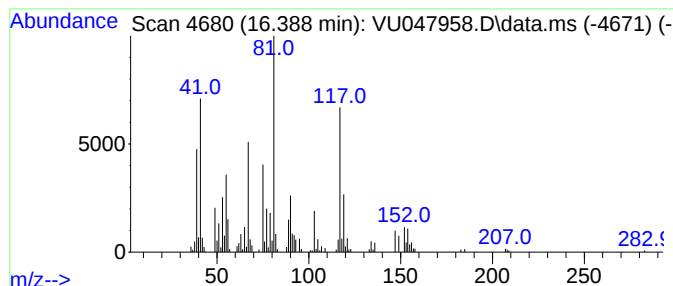
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 unknown-04 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	9.55 ug/L	190318	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isomycorene	136	C10H16	006876-07-9	11
2			2,4-Dimethyl 1,4-pentadiene	96	C7H12	004161-65-3	10
3			1H-Pyrrole, 1-methyl-	81	C5H7N	000096-54-8	10
4			5-Furan-2-ylmethyl-1,3-dimethyl-...	236	C11H12N2O4	1000295-15-4	10
5			Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047958.D
Acq On : 12 Apr 2022 16:10
Operator : SY/MD
Sample : N2293-14ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 19 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
unknown-01	1.813	3.5	ug/L	51840	1	6.247	746631	50.0
2H-Pyran, tetra...	7.497	6.2	ug/L	92004	1	6.247	746631	50.0
Hexane, 1,6-dic...	13.378	6.3	ug/L	126644	3	11.816	996611	50.0
unknown-02	14.494	12.1	ug/L	241482	3	11.816	996611	50.0
unknown-03	15.545	12.9	ug/L	256633	3	11.816	996611	50.0
unknown-04	16.388	9.6	ug/L	190318	3	11.816	996611	50.0