

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042022\
 Data File : VU048155.D
 Acq On : 20 Apr 2022 20:00
 Operator : SY/MD
 Sample : N2485-16
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0J23

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: VU048155.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	24	rVB	72534	72122	0.01%	0.003%
2	1.517	42	55	66	rBV5	11447	38994	0.00%	0.002%
3	1.597	71	80	94	rVV	161406	215386	0.03%	0.009%
4	1.913	170	178	197	rVB	117679	164467	0.02%	0.007%
5	2.157	247	254	262	rVV4	8338	12112	0.00%	0.000%
6	2.202	266	268	276	rVB5	5595	5764	0.00%	0.000%
7	2.318	300	304	312	rVB4	5774	7328	0.00%	0.000%
8	2.411	327	333	348	rVB6	9722	20828	0.00%	0.001%
9	2.568	369	382	391	rBV	263002	435624	0.06%	0.018%
10	2.626	391	400	413	rVV	495514	878317	0.11%	0.036%
11	2.687	414	419	428	rVV	37372	61559	0.01%	0.002%
12	2.768	428	444	497	rVB	2188008	5087071	0.64%	0.206%
13	3.048	517	531	548	rBV	310945	646619	0.08%	0.026%
14	3.138	549	559	582	rVB	134435	283095	0.04%	0.011%
15	3.359	620	628	638	rVB6	2394	4371	0.00%	0.000%
16	3.591	690	700	714	rVB7	2005	4631	0.00%	0.000%
17	3.694	725	732	735	rBV4	1393	1807	0.00%	0.000%
18	3.710	735	737	744	rVB5	1365	1228	0.00%	0.000%
19	3.787	753	761	762	rBV3	1640	1927	0.00%	0.000%
20	3.871	773	787	800	rBV2	3002	6391	0.00%	0.000%
21	3.922	800	803	808	rVV3	616	670	0.00%	0.000%
22	4.186	881	885	888	rVB4	562	423	0.00%	0.000%
23	4.459	963	970	972	rBV3	803	779	0.00%	0.000%
24	4.536	976	994	1010	rBV2	145917	374888	0.05%	0.015%
25	4.626	1010	1022	1039	rVV	137728	337648	0.04%	0.014%
26	4.710	1039	1048	1069	rVB	34755	85621	0.01%	0.003%
27	4.980	1124	1132	1133	rBV4	1067	1010	0.00%	0.000%
28	4.990	1133	1135	1142	rVB4	693	674	0.00%	0.000%
29	5.089	1142	1166	1202	rBV2	1958440	4678209	0.59%	0.190%
30	5.292	1226	1229	1233	rBV5	485	409	0.00%	0.000%
31	5.395	1245	1261	1279	rVB2	91094	211952	0.03%	0.009%
32	5.530	1288	1303	1323	rBV	69776	163252	0.02%	0.007%
33	5.642	1329	1338	1344	rBV6	1910	3345	0.00%	0.000%
34	5.842	1344	1400	1416	rBV5	110192459	534807126	67.60%	21.684%
35	5.935	1419	1429	1471	rVB	1854756	4900993	0.62%	0.199%
36	6.253	1519	1528	1546	rVB	508292	1006286	0.13%	0.041%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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	6.446	1585	1588	1591	rBV3	708	499	0.00%	0.000%
38	6.510	1599	1608	1609	rBV6	2609	2790	0.00%	0.000%
39	6.546	1610	1619	1634	rVB5	11333	23669	0.00%	0.001%
40	6.694	1651	1665	1680	rBV	298615	598151	0.08%	0.024%
41	6.854	1710	1715	1717	rBV7	2366	2054	0.00%	0.000%
42	6.983	1749	1755	1765	rVB8	2816	4949	0.00%	0.000%
43	7.028	1765	1769	1771	rBV2	490	409	0.00%	0.000%
44	7.067	1776	1781	1783	rVV4	747	590	0.00%	0.000%
45	7.112	1787	1795	1801	rBV5	1505	2098	0.00%	0.000%
46	7.186	1808	1818	1828	rVB9	4297	7694	0.00%	0.000%
47	7.260	1837	1841	1844	rBV4	696	551	0.00%	0.000%
48	7.333	1860	1864	1866	rBV3	598	460	0.00%	0.000%
49	7.411	1877	1888	1898	rBV8	3052	6773	0.00%	0.000%
50	7.494	1911	1914	1916	rBV4	635	404	0.00%	0.000%
51	7.568	1923	1937	1957	rBV	158196	283542	0.04%	0.011%
52	7.694	1967	1976	1985	rBV10	4180	6536	0.00%	0.000%
53	7.800	1997	2009	2026	rBV6	9795	21983	0.00%	0.001%
54	7.903	2026	2041	2054	rBV	606395	1108454	0.14%	0.045%
55	7.973	2054	2063	2078	rVB	123883	230334	0.03%	0.009%
56	8.182	2112	2128	2143	rBV	113294	199512	0.03%	0.008%
57	8.340	2173	2177	2179	rBV5	789	538	0.00%	0.000%
58	8.382	2186	2190	2191	rBV4	542	389	0.00%	0.000%
59	8.404	2191	2197	2211	rVB8	2775	5058	0.00%	0.000%
60	8.494	2214	2225	2235	rBV9	1800	4457	0.00%	0.000%
61	8.559	2235	2245	2258	rVB3	11892	22832	0.00%	0.001%
62	8.642	2258	2271	2307	rBV	267707	865693	0.11%	0.035%
63	8.919	2349	2357	2358	rBV5	876	1013	0.00%	0.000%
64	8.954	2366	2368	2375	rVB5	1611	1339	0.00%	0.000%
65	9.202	2441	2445	2448	rVB5	755	561	0.00%	0.000%
66	9.298	2470	2475	2476	rBV4	551	471	0.00%	0.000%
67	9.517	2498	2543	2558	rBV4	118496093	791146592	100.00%	32.077%
68	10.118	2726	2730	2734	rBV6	3727	4225	0.00%	0.000%
69	10.677	2901	2904	2914	rVB6	4025	5086	0.00%	0.000%
70	10.761	2918	2930	2936	rBV	527830	935104	0.12%	0.038%
71	10.993	2993	3002	3016	rVB	41910	69198	0.01%	0.003%
72	11.060	3016	3023	3029	rVV6	4493	6205	0.00%	0.000%
73	11.108	3029	3038	3054	rVB	20861	35012	0.00%	0.001%
74	11.182	3059	3061	3066	rBV5	903	754	0.00%	0.000%
75	11.247	3076	3081	3090	rVB3	3560	5075	0.00%	0.000%
76	11.382	3121	3123	3126	rBV3	544	394	0.00%	0.000%

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Peak Location: TOP

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

77	11.475	3142	3152	3166	rVB3	4093	8812	0.00%	0.000%
78	11.764	3222	3242	3256	rBV	22340617	51010839	6.45%	2.068%
79	11.896	3256	3283	3321	rVB9	128993992	507084110	64.09%	20.560%
80	12.275	3369	3401	3444	rBV6	129506065	508416351	64.26%	20.614%
81	12.697	3524	3532	3544	rVB2	19826	34503	0.00%	0.001%
82	12.973	3607	3618	3631	rVB	312100	487377	0.06%	0.020%
83	13.092	3650	3655	3664	rVB4	7357	9949	0.00%	0.000%
84	13.163	3664	3677	3688	rBV5	29611	73770	0.01%	0.003%
85	13.330	3719	3729	3745	rVB	134930	218640	0.03%	0.009%
86	13.504	3776	3783	3791	rVV4	5261	6989	0.00%	0.000%
87	13.539	3792	3794	3797	rVV3	1331	902	0.00%	0.000%
88	13.574	3798	3805	3813	rVB5	5277	7871	0.00%	0.000%
89	13.655	3823	3830	3841	rVB4	4835	7499	0.00%	0.000%
90	13.848	3873	3890	3915	rBV	25131449	39611072	5.01%	1.606%
91	14.089	3959	3965	3974	rVB	5149	7761	0.00%	0.000%
92	14.330	4026	4040	4062	rBV	5671025	8993375	1.14%	0.365%
93	14.616	4123	4129	4136	rBV10	2809	4727	0.00%	0.000%
94	14.732	4156	4165	4172	rBV5	6355	10496	0.00%	0.000%
95	14.822	4187	4193	4200	rBV4	3221	4545	0.00%	0.000%
96	14.992	4243	4246	4247	rBV3	792	490	0.00%	0.000%
97	15.044	4259	4262	4267	rVB6	1518	1181	0.00%	0.000%
98	15.414	4364	4377	4390	rVB2	63288	105053	0.01%	0.004%
99	15.658	4448	4453	4454	rBV5	1215	1065	0.00%	0.000%
100	15.999	4547	4559	4576	rBV2	86644	146555	0.02%	0.006%

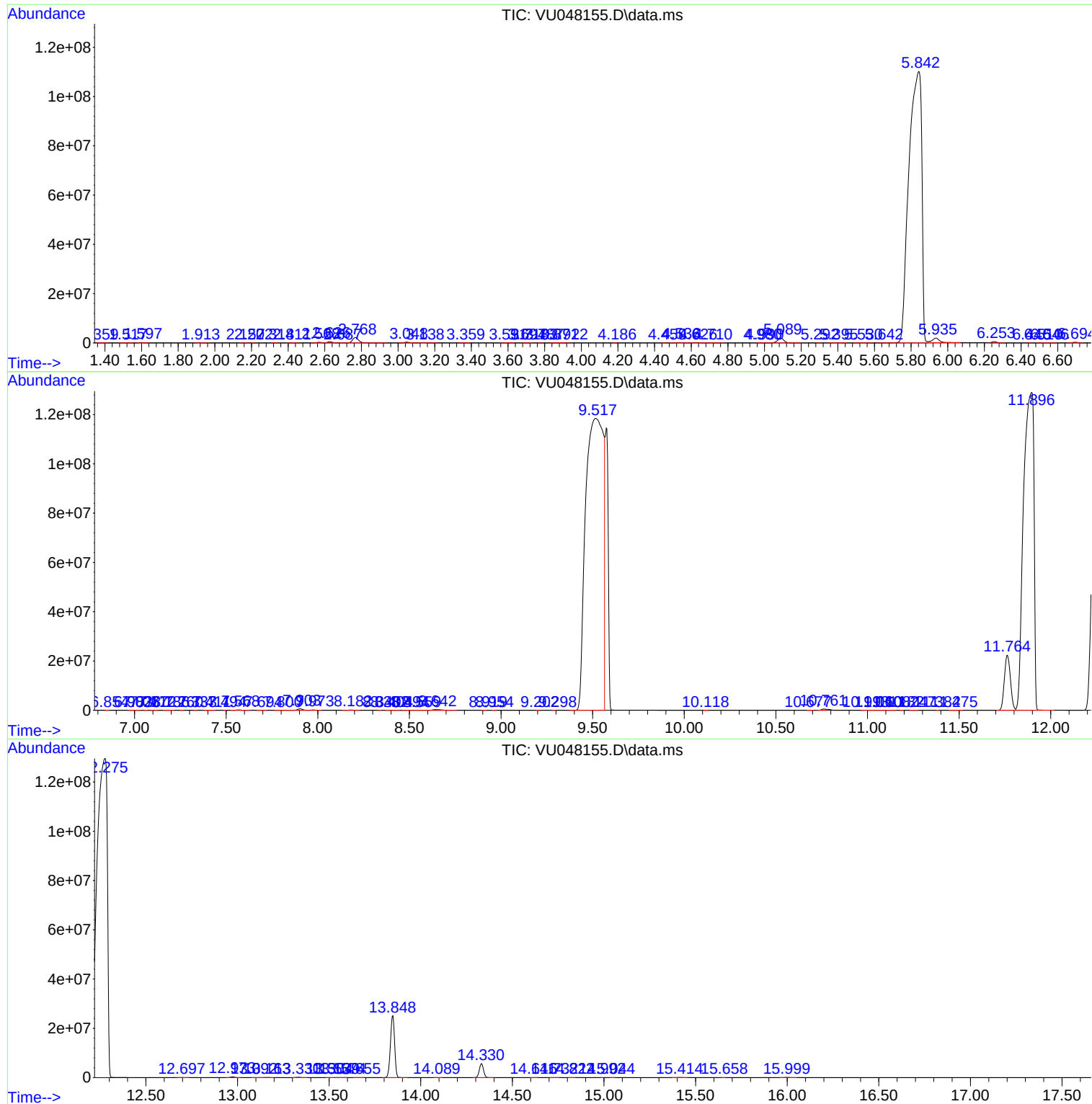
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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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



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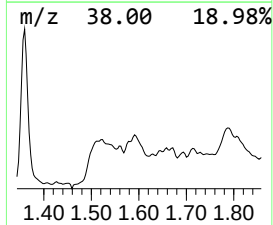
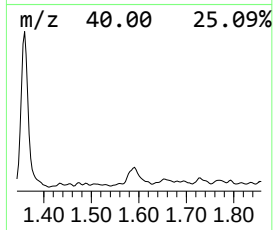
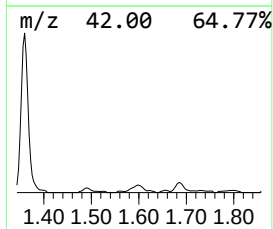
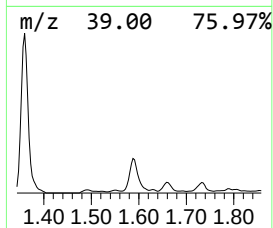
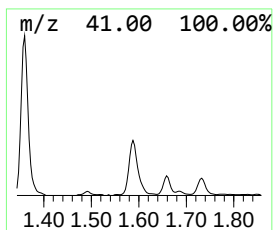
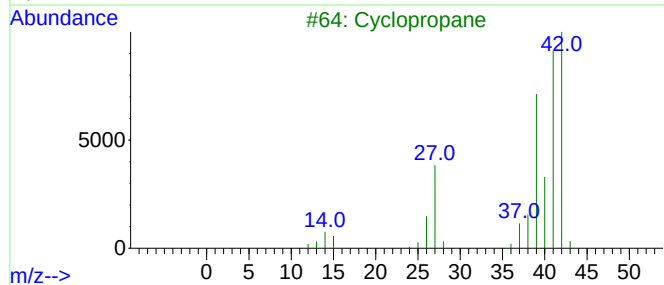
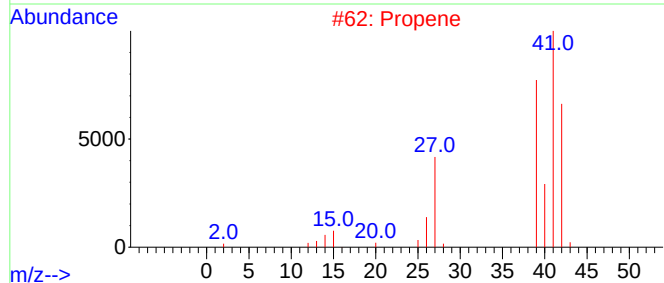
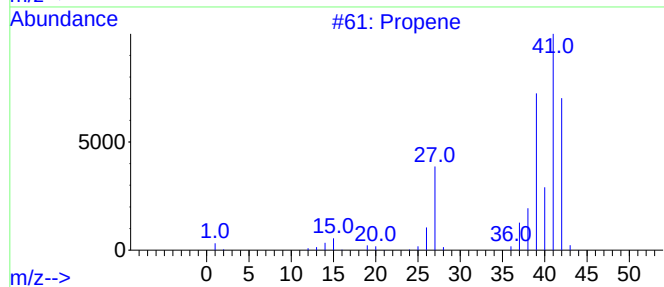
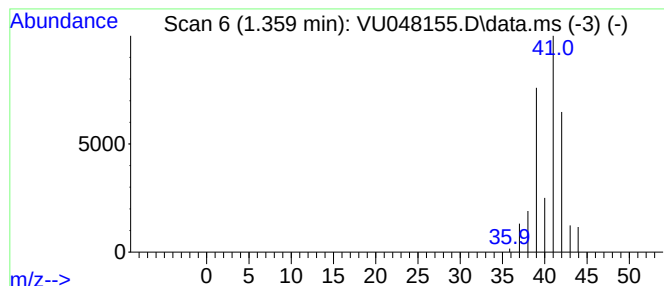
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	3.58 ug/L	72122	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Propene	42	C3H6	000115-07-1	56
3			Cyclopropane	42	C3H6	000075-19-4	10
4			Cyclopropane	42	C3H6	000075-19-4	10
5			Cyclopropane	42	C3H6	000075-19-4	4



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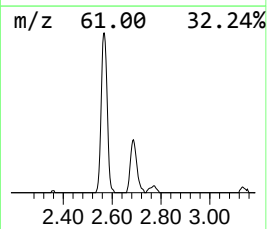
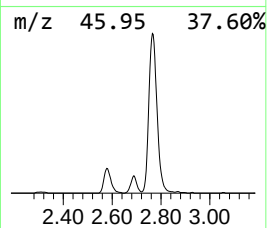
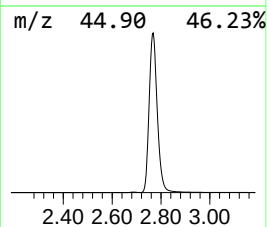
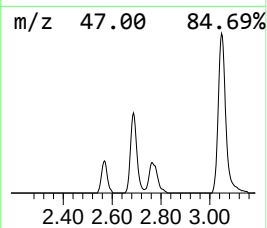
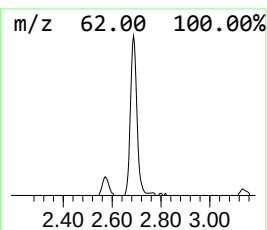
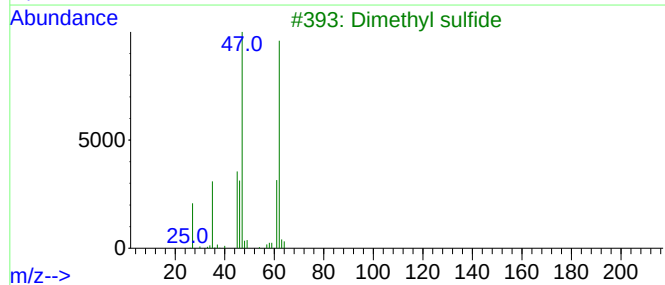
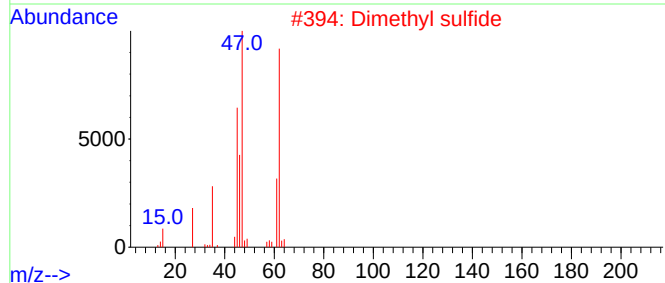
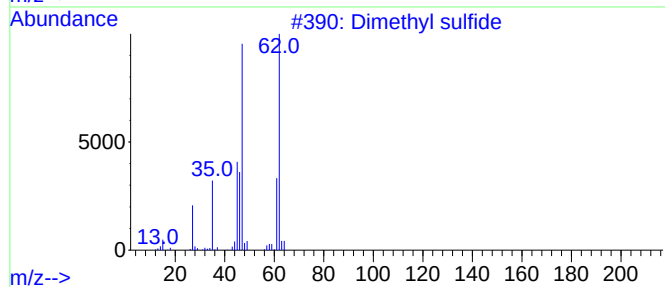
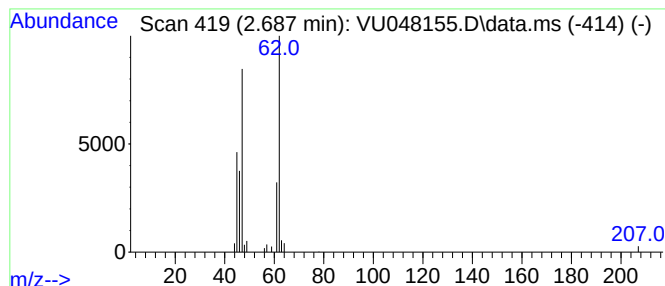
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Dimethyl sulfide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.687	3.06 ug/L	61559	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Dimethyl sulfide	62	C2H6S	000075-18-3	91
3			Dimethyl sulfide	62	C2H6S	000075-18-3	91
4			Dimethyl sulfide	62	C2H6S	000075-18-3	91
5			Dimethyl sulfide	62	C2H6S	000075-18-3	87



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0J23

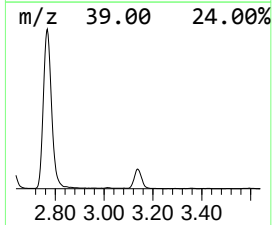
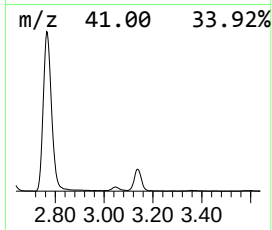
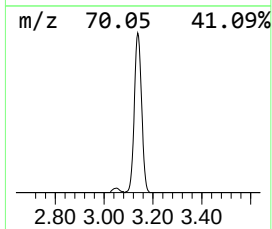
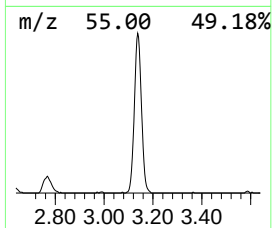
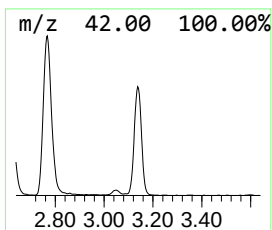
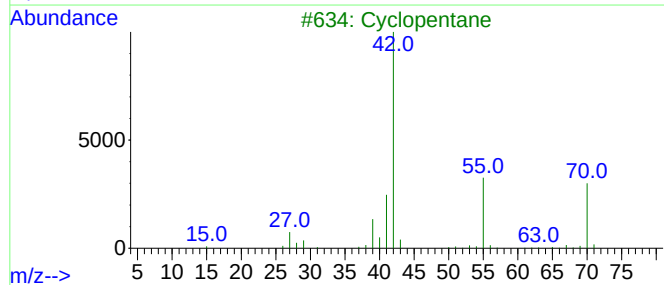
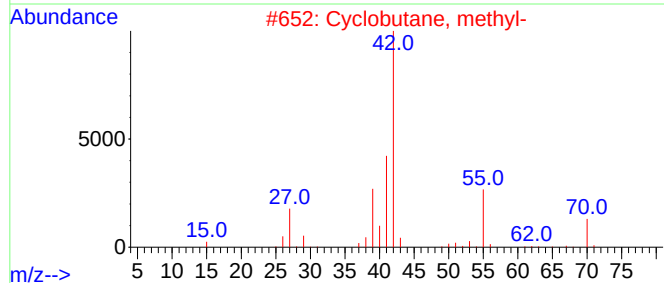
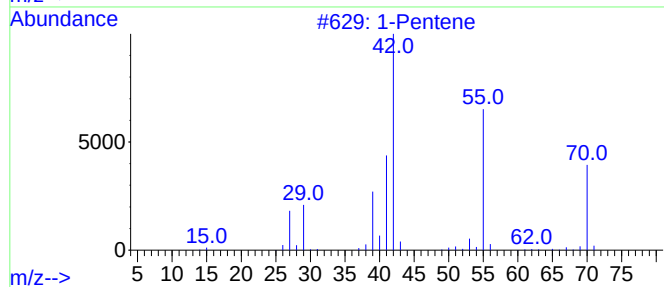
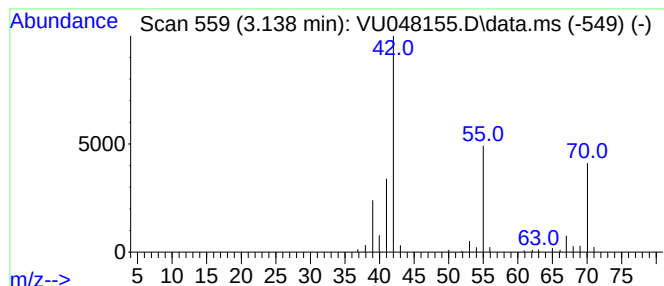
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.138	14.07 ug/L	283095	1,4-Difluorobenzene	6.256

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentene	70	C5H10	000109-67-1	90
2		Cyclobutane, methyl-	70	C5H10	000598-61-8	86
3		Cyclopentane	70	C5H10	000287-92-3	86
4		Cyclobutane, methyl-	70	C5H10	000598-61-8	86
5		Cyclopentane	70	C5H10	000287-92-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042022\
Data File : VU048155.D
Acq On : 20 Apr 2022 20:00
Operator : SY/MD
Sample : N2485-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J23

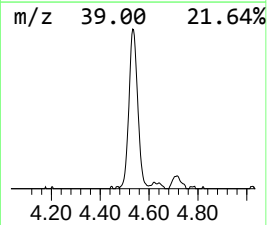
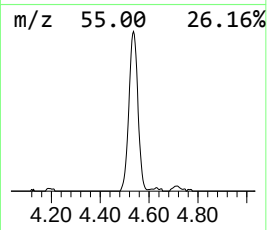
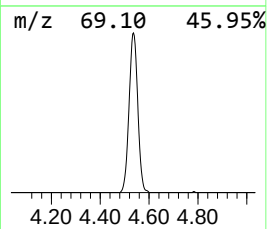
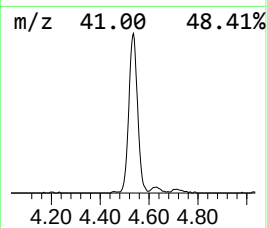
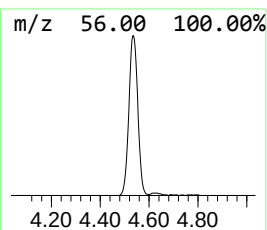
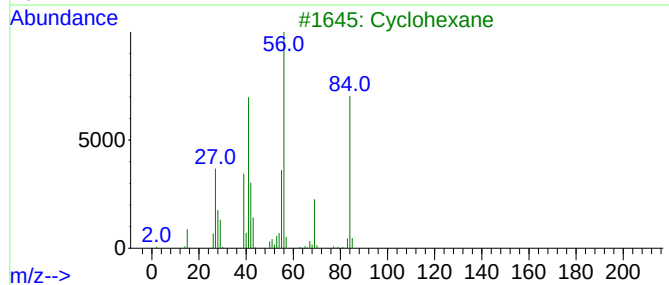
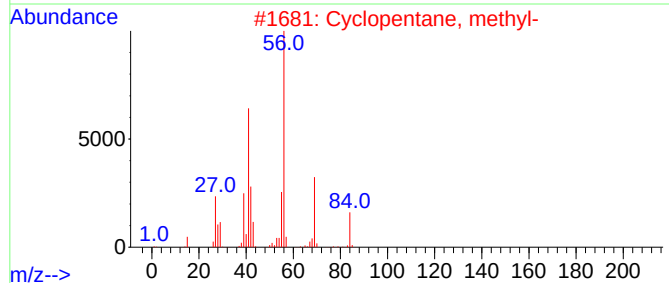
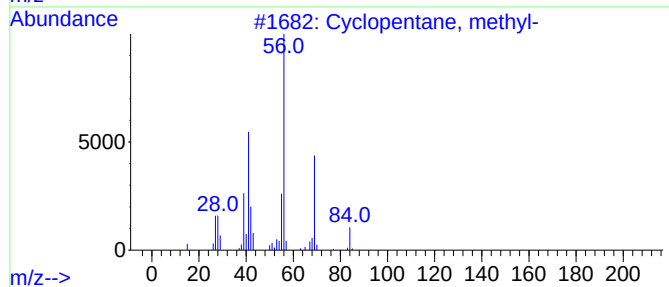
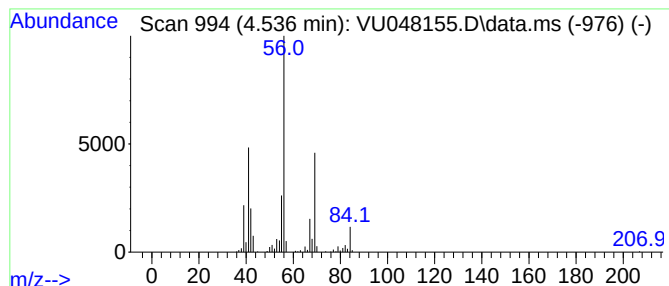
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic4.536 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.536	18.63 ug/L	374888	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	87
3			Cyclohexane	84	C6H12	000110-82-7	83
4			Cyclopentane, methyl-	84	C6H12	000096-37-7	80
5			Cyclopentane, methyl-	84	C6H12	000096-37-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042022\
Data File : VU048155.D
Acq On : 20 Apr 2022 20:00
Operator : SY/MD
Sample : N2485-16
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0J23

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...	1.359	3.6	ug/L	72122	1	6.256	1006290	50.0
Dimethyl sulfide	2.687	3.1	ug/L	61559	1	6.256	1006290	50.0
(DEL) Alkane: S...	3.138	14.1	ug/L	283095	1	6.256	1006290	50.0
(DEL) Alkane: C...	4.536	18.6	ug/L	374888	1	6.256	1006290	50.0