

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU047994.D
 Acq On : 13 Apr 2022 11:38
 Operator : SY/MD
 Sample : N2290-01ME
 Misc : 3.15g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFC8ME

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: VU047994.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	103	rVB	45692	75920	5.88%	0.663%
2	2.546	363	375	398	rBV	104803	190183	14.74%	1.660%
3	2.758	438	441	446	rBV5	636	590	0.05%	0.005%
4	2.903	477	486	493	rBV6	998	1888	0.15%	0.016%
5	2.954	496	502	507	rBV5	1129	1295	0.10%	0.011%
6	3.041	520	529	538	rBV6	1840	3961	0.31%	0.035%
7	3.266	594	599	605	rBV4	476	495	0.04%	0.004%
8	3.301	605	610	614	rBV2	372	475	0.04%	0.004%
9	3.867	781	786	789	rVB2	368	386	0.03%	0.003%
10	3.896	789	795	798	rBV2	397	410	0.03%	0.004%
11	4.051	840	843	849	rVB3	366	372	0.03%	0.003%
12	4.128	860	867	870	rBV2	734	932	0.07%	0.008%
13	4.192	884	887	893	rVB2	393	368	0.03%	0.003%
14	4.424	955	959	966	rVB2	318	399	0.03%	0.003%
15	4.629	1009	1023	1059	rBV	110318	340572	26.39%	2.973%
16	4.951	1120	1123	1130	rVB	441	466	0.04%	0.004%
17	5.063	1141	1158	1178	rBV	150811	337531	26.16%	2.946%
18	5.330	1235	1241	1242	rBV3	1554	1377	0.11%	0.012%
19	5.719	1340	1362	1391	rVV2	269266	730721	56.63%	6.378%
20	5.874	1407	1410	1413	rBV3	719	604	0.05%	0.005%
21	5.973	1427	1441	1461	rBV4	11013	26782	2.08%	0.234%
22	6.112	1481	1484	1487	rBV2	424	325	0.03%	0.003%
23	6.247	1509	1526	1552	rBV	363073	708722	54.92%	6.186%
24	6.411	1574	1577	1583	rVV3	382	439	0.03%	0.004%
25	6.485	1593	1600	1602	rBV2	974	1207	0.09%	0.011%
26	6.523	1605	1612	1622	rVV8	3957	7575	0.59%	0.066%
27	6.600	1626	1636	1647	rVV5	4735	10685	0.83%	0.093%
28	6.690	1650	1664	1690	rVB2	180678	366774	28.42%	3.201%
29	7.025	1764	1768	1770	rBV2	427	337	0.03%	0.003%
30	7.050	1770	1776	1785	rVV5	950	1773	0.14%	0.015%
31	7.182	1806	1817	1824	rBV2	7707	14971	1.16%	0.131%
32	7.298	1848	1853	1854	rBV2	716	453	0.04%	0.004%
33	7.497	1909	1915	1919	rBV3	527	571	0.04%	0.005%
34	7.568	1923	1937	1955	rBV	90900	173698	13.46%	1.516%
35	7.697	1966	1977	1985	rBV6	1576	3027	0.23%	0.026%
36	7.809	2006	2012	2017	rBV3	857	1089	0.08%	0.010%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Stop Thrs : 0

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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	7.899	2026	2040	2055	rBV	261675	468254	36.29%	4.087%
38	7.986	2057	2067	2081	rVV5	9315	25566	1.98%	0.223%
39	8.070	2085	2093	2099	rBV5	837	1116	0.09%	0.010%
40	8.182	2116	2128	2145	rBV2	65250	125974	9.76%	1.100%
41	8.314	2166	2169	2174	rBV4	525	413	0.03%	0.004%
42	8.337	2174	2176	2177	rBV	993	460	0.04%	0.004%
43	8.581	2247	2252	2257	rVV4	526	682	0.05%	0.006%
44	8.648	2258	2273	2310	rVV	433747	851227	65.97%	7.430%
45	8.796	2312	2319	2335	rVB5	4788	9496	0.74%	0.083%
46	8.883	2345	2346	2354	rVB3	461	354	0.03%	0.003%
47	8.973	2371	2374	2379	rVB3	501	384	0.03%	0.003%
48	9.201	2442	2445	2450	rBV	372	304	0.02%	0.003%
49	9.234	2450	2455	2457	rBV2	440	312	0.02%	0.003%
50	9.420	2499	2513	2541	rBV	551886	1018613	78.94%	8.891%
51	9.578	2553	2562	2571	rVB9	1752	2971	0.23%	0.026%
52	9.648	2581	2584	2591	rVV3	691	627	0.05%	0.005%
53	9.703	2595	2601	2610	rVB5	1108	1606	0.12%	0.014%
54	9.761	2614	2619	2622	rBV2	388	348	0.03%	0.003%
55	9.854	2643	2648	2652	rBV2	316	334	0.03%	0.003%
56	10.105	2721	2726	2729	rBV2	626	719	0.06%	0.006%
57	10.626	2882	2888	2891	rBV4	451	476	0.04%	0.004%
58	10.716	2910	2916	2918	rBV4	927	967	0.07%	0.008%
59	10.761	2918	2930	2953	rVV	480594	771875	59.82%	6.737%
60	10.883	2964	2968	2970	rBV	473	418	0.03%	0.004%
61	10.938	2979	2985	2987	rBV2	339	363	0.03%	0.003%
62	11.002	3001	3005	3006	rBV2	653	370	0.03%	0.003%
63	11.095	3028	3034	3036	rVV3	960	1111	0.09%	0.010%
64	11.115	3037	3040	3047	rVV5	1689	1869	0.14%	0.016%
65	11.375	3116	3121	3123	rBV3	626	644	0.05%	0.006%
66	11.414	3128	3133	3136	rBV3	553	435	0.03%	0.004%
67	11.449	3140	3144	3146	rBV2	404	344	0.03%	0.003%
68	11.468	3146	3150	3155	rBV3	1046	1126	0.09%	0.010%
69	11.697	3215	3221	3228	rBV6	1457	2069	0.16%	0.018%
70	11.748	3232	3237	3244	rVB3	1584	1976	0.15%	0.017%
71	11.816	3244	3258	3276	rBV	708526	1139775	88.33%	9.948%
72	11.918	3281	3290	3311	rVV2	27639	51110	3.96%	0.446%
73	12.195	3363	3376	3395	rVV	507102	831789	64.46%	7.260%
74	12.774	3551	3556	3558	rBV4	674	624	0.05%	0.005%
75	12.799	3558	3564	3571	rVB5	1888	2301	0.18%	0.020%
76	12.838	3571	3576	3581	rBV4	582	440	0.03%	0.004%

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 ClientSampleId :
 BFFC8ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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

77	12.970	3603	3617	3641	rVB	71011	121232	9.39%	1.058%
78	13.221	3689	3695	3706	rVB4	2103	2603	0.20%	0.023%
79	13.269	3706	3710	3713	rBV4	435	319	0.02%	0.003%
80	13.330	3717	3729	3738	rVV2	72327	116747	9.05%	1.019%
81	13.378	3738	3744	3754	rVB3	12793	18749	1.45%	0.164%
82	13.513	3781	3786	3791	rBV3	661	778	0.06%	0.007%
83	13.713	3836	3848	3859	rBV3	12576	20120	1.56%	0.176%
84	13.841	3881	3888	3900	rVB2	3977	6100	0.47%	0.053%
85	13.967	3918	3927	3932	rBV5	969	1790	0.14%	0.016%
86	14.008	3937	3940	3943	rVB4	776	594	0.05%	0.005%
87	14.092	3958	3966	3977	rVB2	6809	8959	0.69%	0.078%
88	14.336	4033	4042	4044	rBV4	3606	4673	0.36%	0.041%
89	14.362	4044	4050	4056	rVV4	8155	12316	0.95%	0.107%
90	14.401	4057	4062	4073	rVB5	7714	11258	0.87%	0.098%
91	14.590	4108	4121	4138	rBV2	135672	211958	16.43%	1.850%
92	14.886	4207	4213	4220	rBV8	2025	2545	0.20%	0.022%
93	15.005	4247	4250	4253	rBV	780	547	0.04%	0.005%
94	15.201	4307	4311	4314	rBV4	1035	880	0.07%	0.008%
95	15.311	4340	4345	4356	rVB8	6758	10429	0.81%	0.091%
96	15.545	4407	4418	4431	rBV	82505	129221	10.01%	1.128%
97	15.767	4479	4487	4492	rBV9	2866	4134	0.32%	0.036%
98	15.893	4509	4526	4542	rBV	533797	1290412	100.00%	11.263%
99	16.121	4586	4597	4614	rVB	254885	406893	31.53%	3.551%
100	16.388	4659	4680	4700	rBV2	387050	746834	57.88%	6.518%

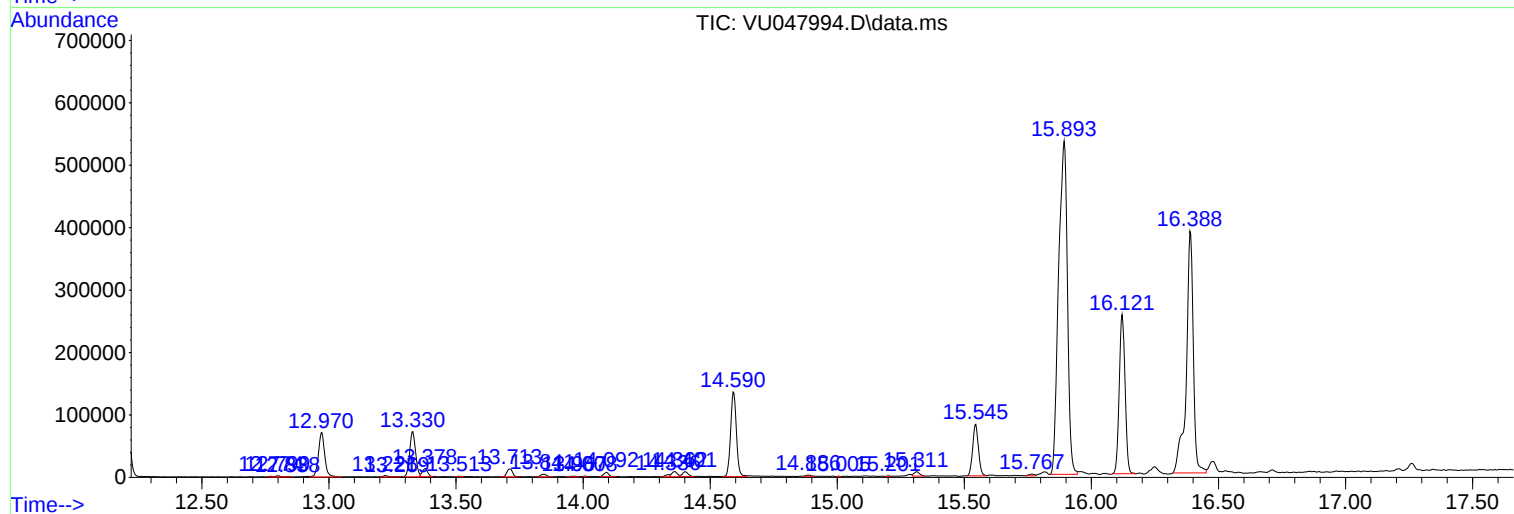
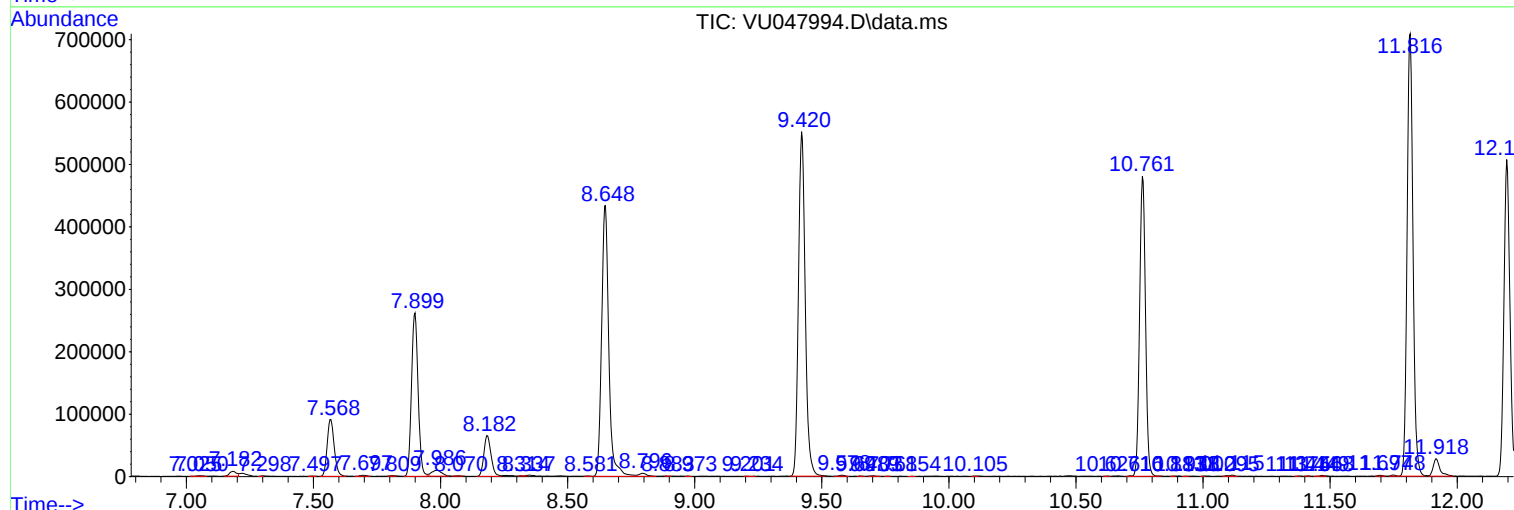
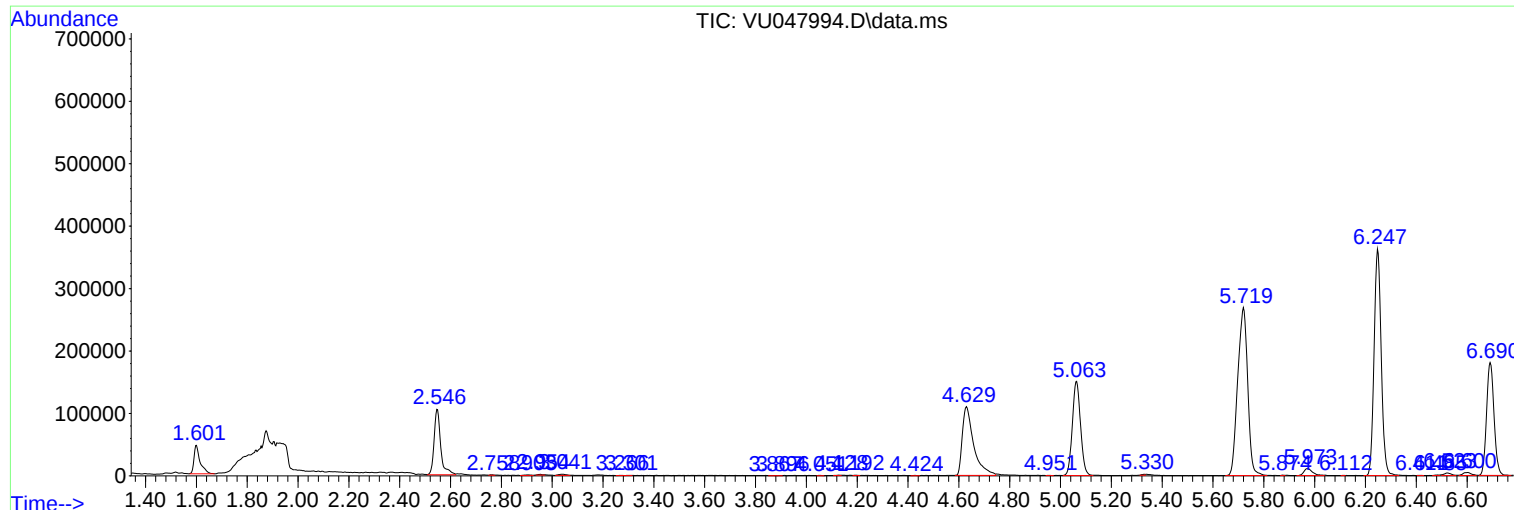
Sum of corrected areas: 11457306

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Instrument :
MSVOA_U
ClientSampleId :
BFFC8ME

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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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFC8ME

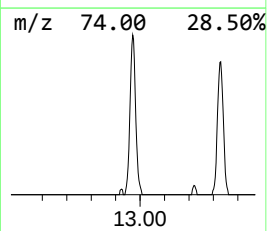
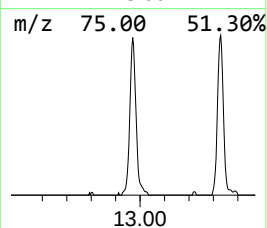
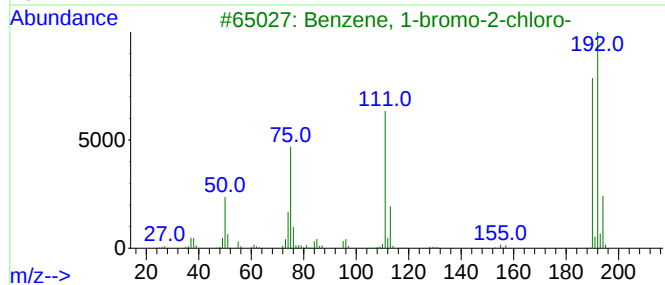
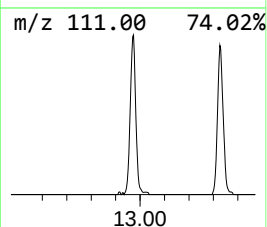
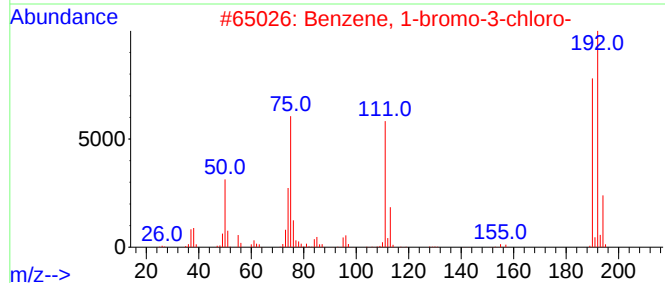
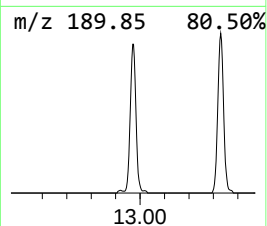
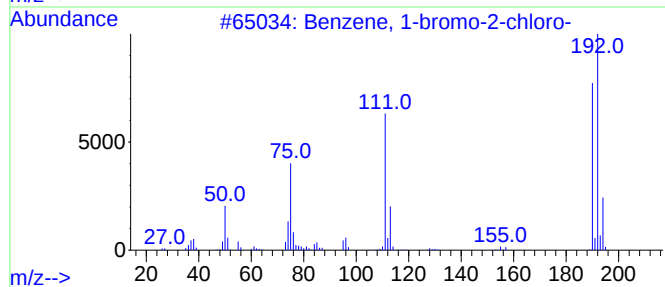
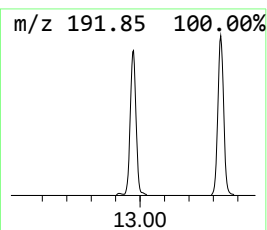
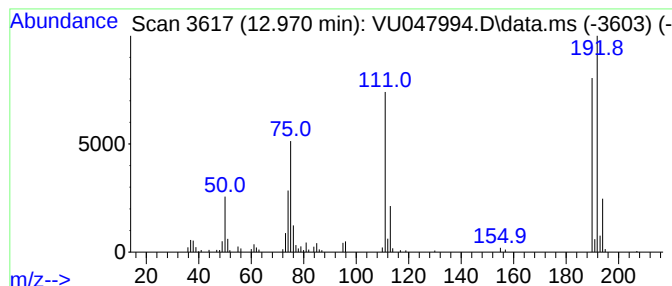
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, 1-bromo-2-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.970	5.32 ug/L	121232	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	98
2			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	98
3			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	98
4			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	98
5			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	98



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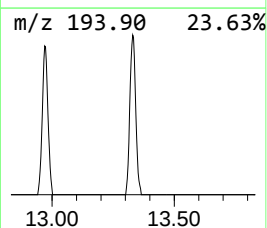
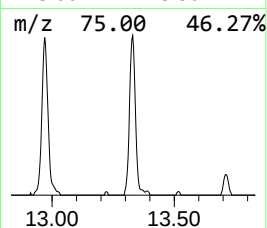
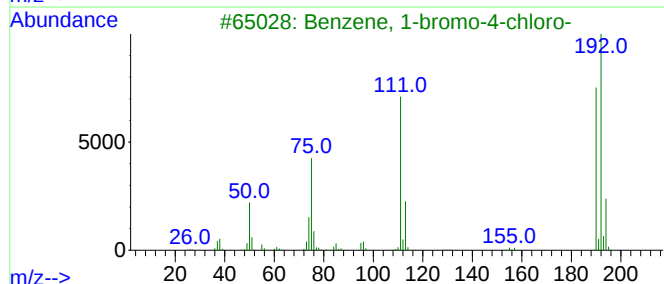
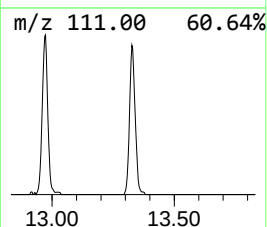
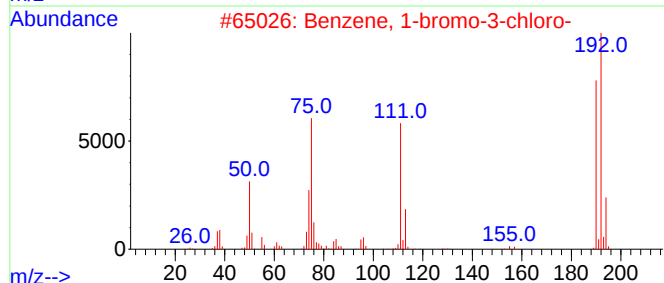
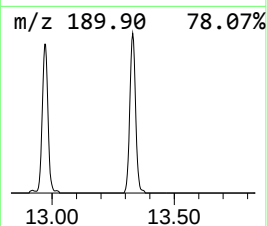
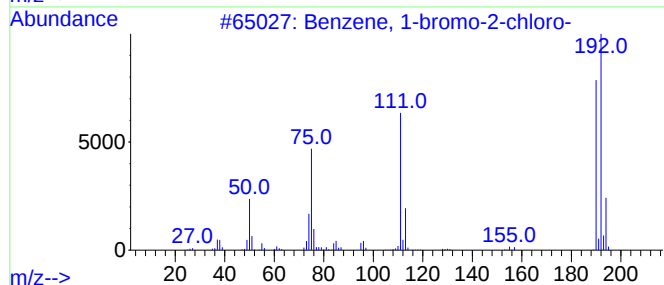
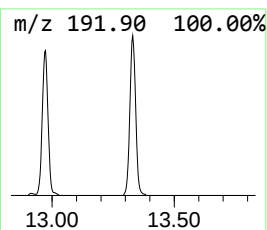
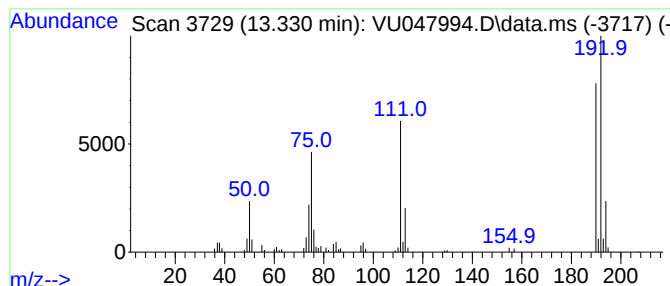
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-bromo-3-chloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.330	5.12 ug/L	116747	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	99
2			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	98
3			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	98
4			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	97
5			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	97



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ClientSampleId :
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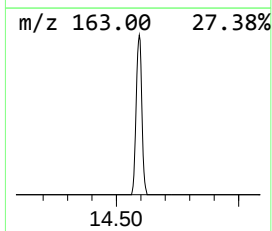
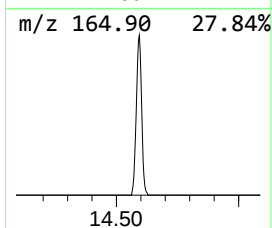
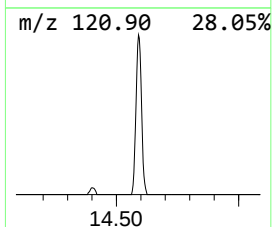
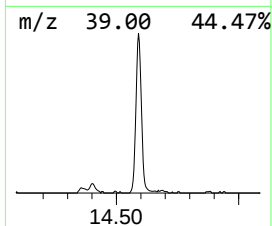
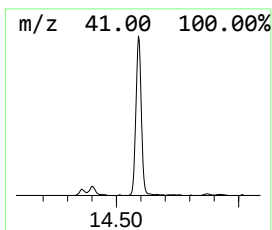
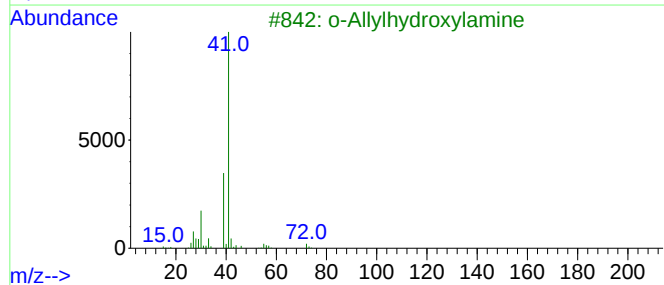
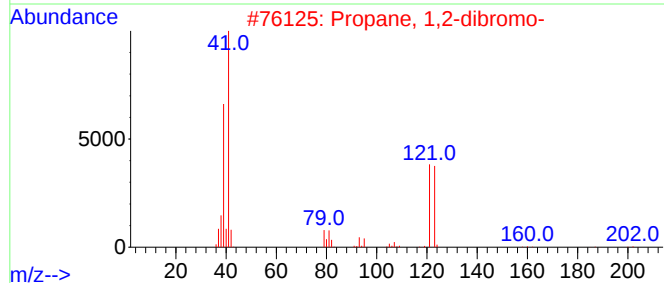
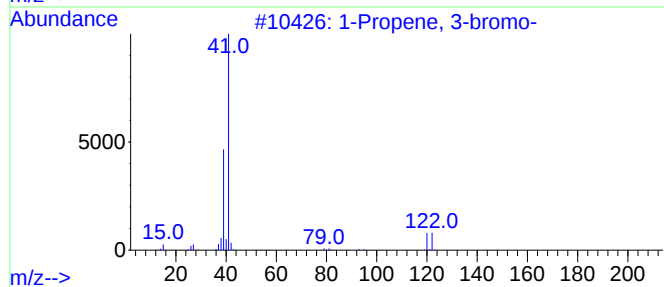
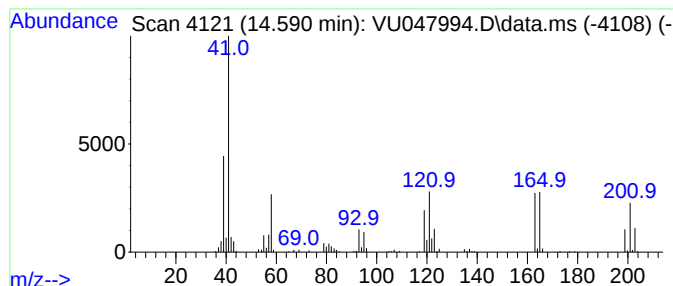
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Quant Title : VOC Analysis

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

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.590	9.30 ug/L	211958	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propene, 3-bromo-	120	C3H5Br	000106-95-6	10
2			Propane, 1,2-dibromo-	200	C3H6Br2	000078-75-1	9
3			o-Allylhydroxylamine	73	C3H7NO	006542-54-7	7
4			2,3-Dibromo-2,3-dimethylbutane	242	C6H12Br2	000594-81-0	7
5			Benzeneethanamine	121	C8H11N	000064-04-0	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047994.D
Acq On : 13 Apr 2022 11:38
Operator : SY/MD
Sample : N2290-01ME
Misc : 3.15g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFC8ME

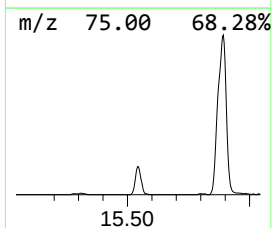
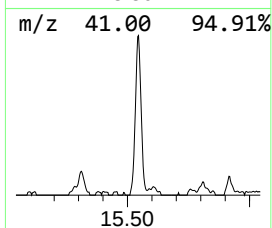
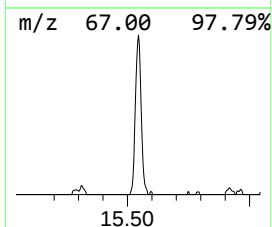
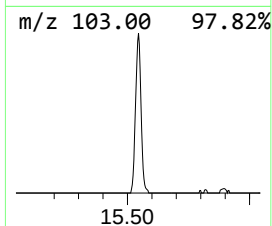
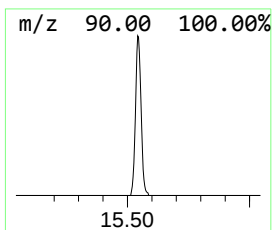
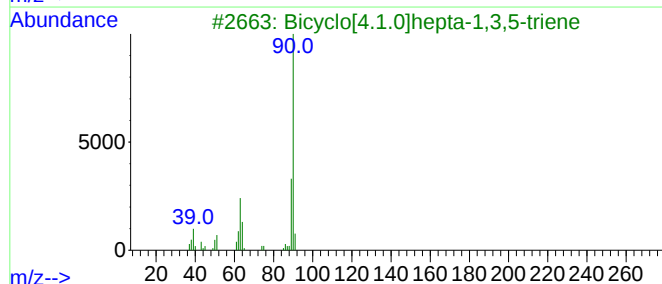
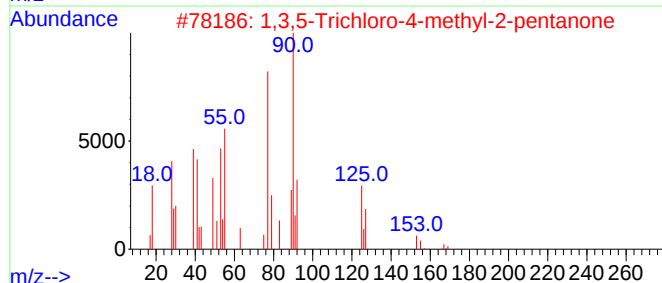
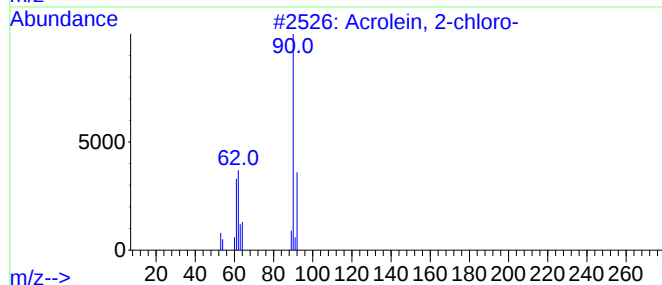
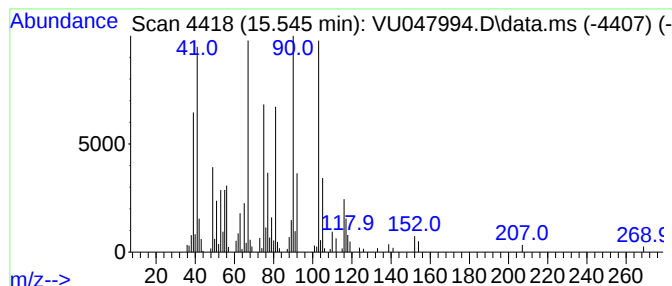
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Quant Title : VOC Analysis

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

Peak Number 5 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	5.67 ug/L	129221	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			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	30
3			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	30
4			benzaldehyde, 2-(4-amino-4H-1,2,...	202	C9H10N6	1000400-43-7	25
5			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047994.D
Acq On : 13 Apr 2022 11:38
Operator : SY/MD
Sample : N2290-01ME
Misc : 3.15g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFC8ME

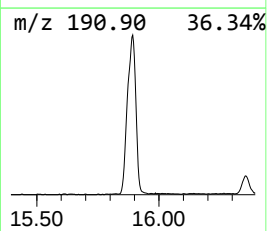
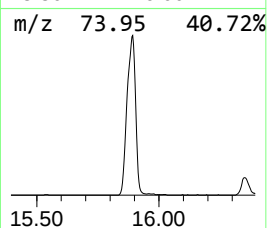
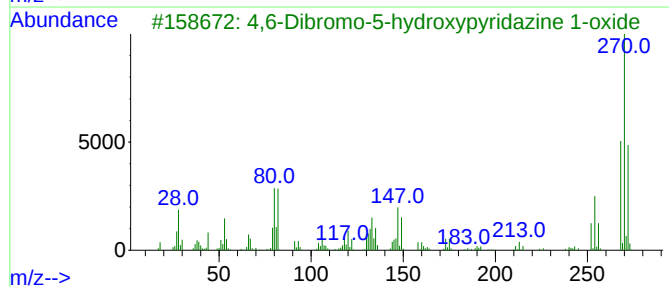
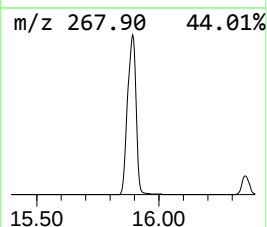
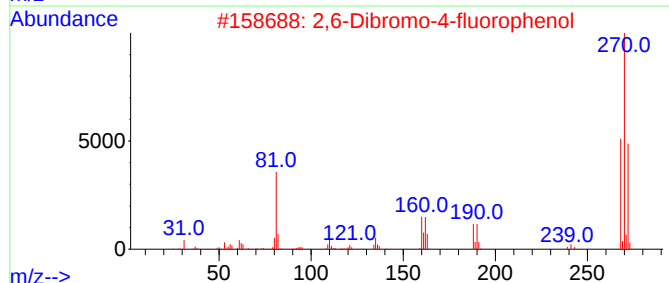
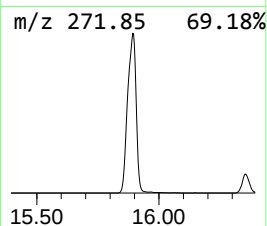
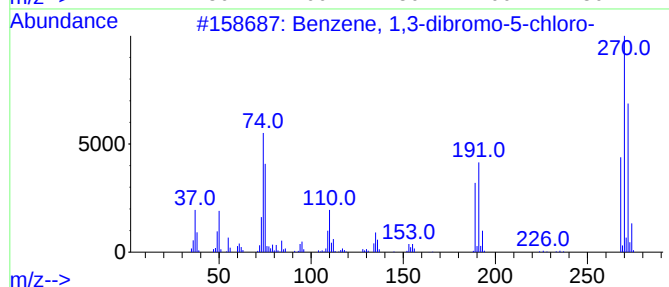
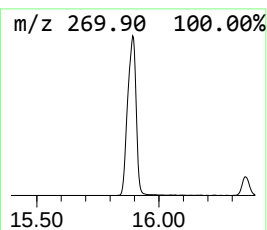
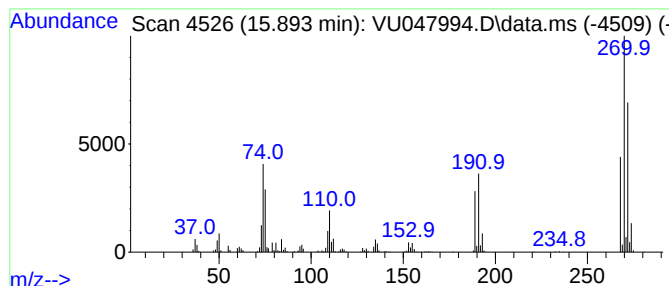
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Quant Title : VOC Analysis

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

Peak Number 6 Benzene, 1,3-dibromo-5-chloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.893	56.61 ug/L	1290410	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dibromo-5-chloro-	268	C6H3Br2Cl	014862-52-3	94
2			2,6-Dibromo-4-fluorophenol	268	C6H3Br2FO	000344-20-7	43
3			4,6-Dibromo-5-hydroxypyridazine ...	268	C4H2Br2N2O2	019971-61-0	43
4			Pyrimidine, 4,6-dichloro-2-(meth...	270	C11H8Cl2N2S	064415-11-8	23
5			5-Bromo-7-methoxy-1-benzofuran-2...	270	C10H7BrO4	020037-37-0	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047994.D
Acq On : 13 Apr 2022 11:38
Operator : SY/MD
Sample : N2290-01ME
Misc : 3.15g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFC8ME

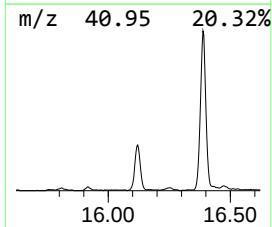
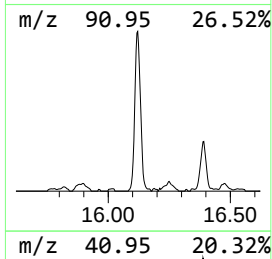
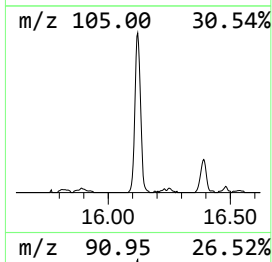
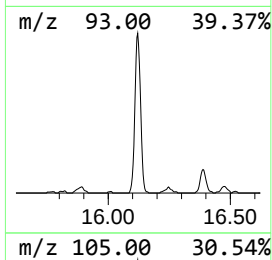
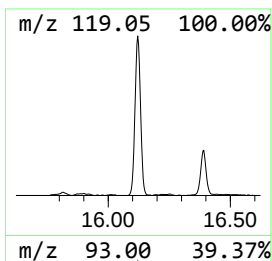
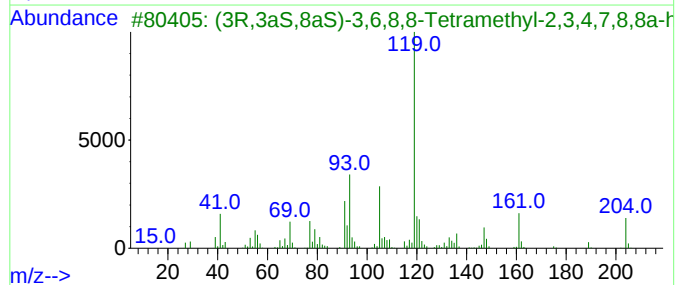
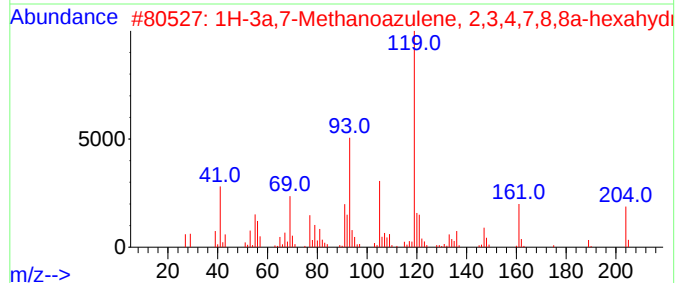
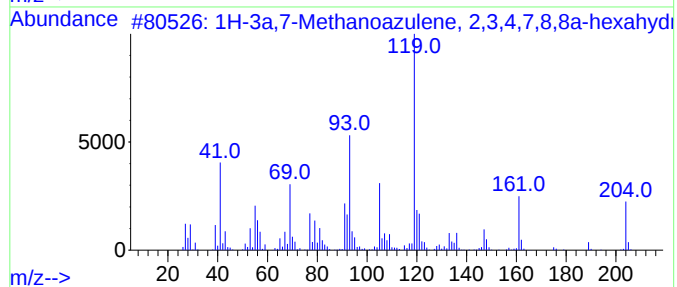
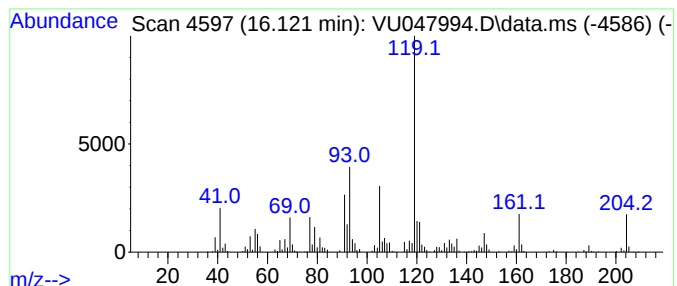
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Quant Title : VOC Analysis

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

Peak Number 7 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.121	17.85 ug/L	406893	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	99
2			1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	99
3			(3R,3aS,8aS)-3,6,8,8-Tetramethyl...	204	C15H24	022567-43-7	97
4			1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	96
5			1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047994.D
Acq On : 13 Apr 2022 11:38
Operator : SY/MD
Sample : N2290-01ME
Misc : 3.15g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFC8ME

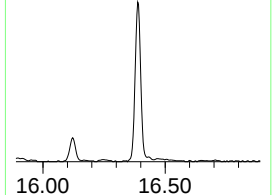
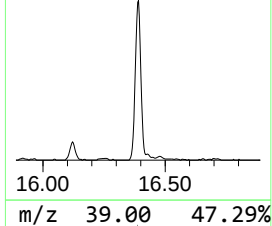
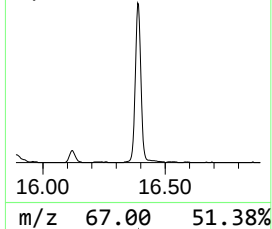
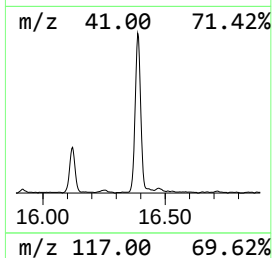
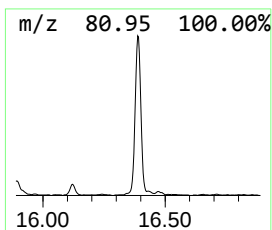
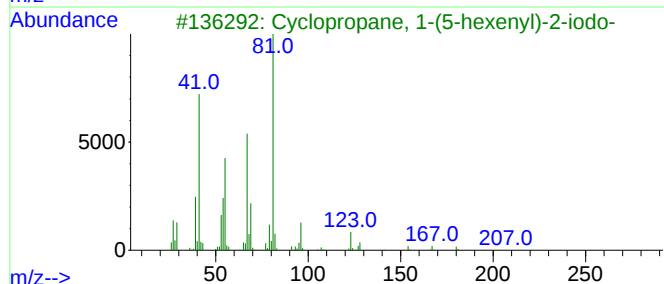
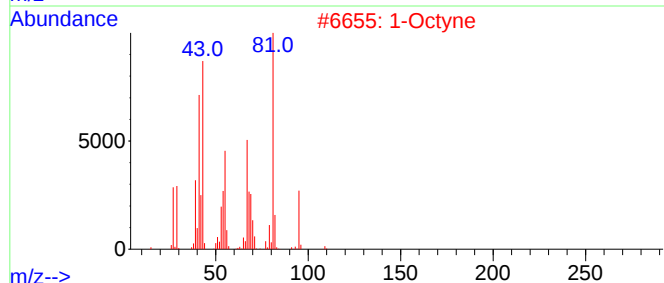
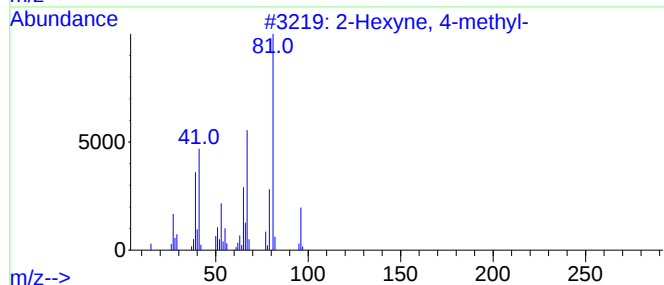
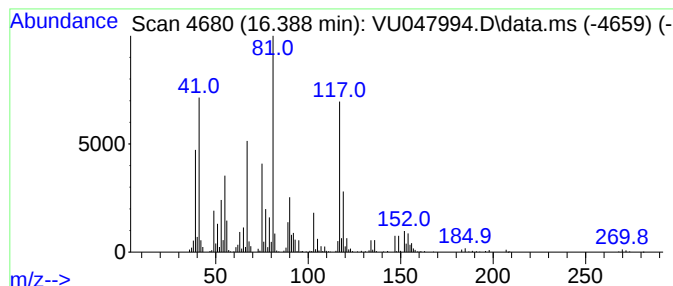
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Quant Title : VOC Analysis

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

Peak Number 8 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	32.76 ug/L	746834	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexyne, 4-methyl-			96	C7H12	020198-49-6	12
2	1-Octyne			110	C8H14	000629-05-0	12
3	Cyclopropane, 1-(5-hexenyl)-2-iodo-			250	C9H15I	074685-40-8	12
4	Cyclohexene, 3-(2-propynyl)-			120	C9H12	055956-43-9	11
5	Cyclopropane, 1-methyl-1-isoprop...			96	C7H12	003422-07-9	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU047994.D
Acq On : 13 Apr 2022 11:38
Operator : SY/MD
Sample : N2290-01ME
Misc : 3.15g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFC8ME

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-brom...	12.970	5.3	ug/L	121232	3	11.816	1139780	50.0
Benzene, 1-brom...	13.330	5.1	ug/L	116747	3	11.816	1139780	50.0
unknown-01	14.590	9.3	ug/L	211958	3	11.816	1139780	50.0
unknown-02	15.545	5.7	ug/L	129221	3	11.816	1139780	50.0
Benzene, 1,3-di...	15.893	56.6	ug/L	1290410	3	11.816	1139780	50.0
1H-3a,7-Methano...	16.121	17.9	ug/L	406893	3	11.816	1139780	50.0
unknown-03	16.388	32.8	ug/L	746834	3	11.816	1139780	50.0