

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
 Data File : VU047954.D
 Acq On : 12 Apr 2022 14:40
 Operator : SY/MD
 Sample : N2293-02MEDL 100X
 Misc : 7.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNN2MEDL

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: VU047954.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	16	rVB	5459	5843	0.30%	0.045%
2	1.498	42	49	50	rBV3	2286	2618	0.14%	0.020%
3	1.601	74	81	96	rBV	120551	140551	7.30%	1.076%
4	1.916	171	179	200	rVB	107326	153195	7.96%	1.173%
5	2.494	357	359	366	rVB5	819	654	0.03%	0.005%
6	2.568	370	382	401	rBV	217600	363251	18.88%	2.780%
7	3.041	524	529	530	rBV3	774	631	0.03%	0.005%
8	3.536	678	683	685	rBV3	332	345	0.02%	0.003%
9	3.549	685	687	693	rVV2	342	284	0.01%	0.002%
10	3.646	714	717	720	rVB3	394	274	0.01%	0.002%
11	3.726	737	742	747	rBV2	419	486	0.03%	0.004%
12	3.829	769	774	775	rBV2	523	375	0.02%	0.003%
13	4.195	885	888	892	rBV2	510	436	0.02%	0.003%
14	4.343	928	934	937	rBV3	397	415	0.02%	0.003%
15	4.408	949	954	960	rBV3	260	367	0.02%	0.003%
16	4.626	1008	1022	1057	rBV	133477	334257	17.37%	2.558%
17	5.067	1141	1159	1185	rVV	217910	476618	24.77%	3.648%
18	5.289	1225	1228	1233	rVB4	407	334	0.02%	0.003%
19	5.382	1254	1257	1264	rVB4	418	419	0.02%	0.003%
20	5.726	1342	1364	1392	rBV2	427629	1167852	60.69%	8.939%
21	5.893	1406	1416	1417	rBV6	3284	3799	0.20%	0.029%
22	5.961	1434	1437	1440	rBV3	319	318	0.02%	0.002%
23	6.035	1458	1460	1463	rBV2	483	288	0.01%	0.002%
24	6.051	1463	1465	1470	rVB3	494	299	0.02%	0.002%
25	6.153	1493	1497	1501	rBV3	382	348	0.02%	0.003%
26	6.199	1506	1511	1513	rBV2	581	480	0.02%	0.004%
27	6.250	1513	1527	1555	rBV	429507	816873	42.45%	6.253%
28	6.520	1607	1611	1613	rBV2	883	789	0.04%	0.006%
29	6.536	1613	1616	1624	rVB5	1480	1515	0.08%	0.012%
30	6.694	1650	1665	1687	rBV	270934	535063	27.80%	4.095%
31	6.806	1698	1700	1705	rVV4	591	304	0.02%	0.002%
32	7.089	1785	1788	1792	rVB3	523	363	0.02%	0.003%
33	7.182	1812	1817	1831	rVB5	2508	3923	0.20%	0.030%
34	7.346	1866	1868	1873	rVB2	450	345	0.02%	0.003%
35	7.401	1883	1885	1891	rVB2	329	267	0.01%	0.002%
36	7.491	1907	1913	1922	rBV4	1233	2074	0.11%	0.016%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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

37	7.565	1924	1936	1960	rBV	143124	255403	13.27%	1.955%
38	7.690	1965	1975	1981	rVV4	2187	4026	0.21%	0.031%
39	7.726	1985	1986	1989	rVV3	433	298	0.02%	0.002%
40	7.780	1998	2003	2006	rBV2	248	300	0.02%	0.002%
41	7.899	2025	2040	2056	rBV	508377	875150	45.48%	6.699%
42	8.179	2116	2127	2143	rBV	103115	176119	9.15%	1.348%
43	8.359	2176	2183	2191	rVB8	1947	3208	0.17%	0.025%
44	8.539	2234	2239	2242	rBV4	820	818	0.04%	0.006%
45	8.575	2243	2250	2256	rBV4	2970	4179	0.22%	0.032%
46	8.636	2257	2269	2299	rBV	435795	775318	40.29%	5.934%
47	9.015	2379	2387	2397	rVB5	2215	3417	0.18%	0.026%
48	9.086	2406	2409	2416	rVB3	374	413	0.02%	0.003%
49	9.169	2433	2435	2437	rVV2	567	266	0.01%	0.002%
50	9.327	2479	2484	2488	rBV2	491	573	0.03%	0.004%
51	9.362	2488	2495	2500	rBV3	2484	3218	0.17%	0.025%
52	9.417	2500	2512	2518	rBV	652989	1138302	59.15%	8.713%
53	9.578	2554	2562	2571	rVB8	4331	6237	0.32%	0.048%
54	9.639	2578	2581	2583	rBV2	565	434	0.02%	0.003%
55	9.687	2593	2596	2598	rBV2	435	293	0.02%	0.002%
56	9.700	2598	2600	2606	rVB5	970	776	0.04%	0.006%
57	9.732	2606	2610	2618	rBV3	543	604	0.03%	0.005%
58	9.858	2646	2649	2651	rBV2	574	291	0.02%	0.002%
59	9.996	2686	2692	2694	rBV5	1441	1293	0.07%	0.010%
60	10.089	2713	2721	2723	rBV3	779	983	0.05%	0.008%
61	10.227	2754	2764	2771	rBV6	1493	3290	0.17%	0.025%
62	10.388	2810	2814	2815	rVV3	385	299	0.02%	0.002%
63	10.407	2816	2820	2828	rVB4	1212	1684	0.09%	0.013%
64	10.555	2862	2866	2870	rBV3	357	369	0.02%	0.003%
65	10.658	2890	2898	2903	rBV8	1738	2728	0.14%	0.021%
66	10.710	2906	2914	2918	rVV3	6137	10115	0.53%	0.077%
67	10.758	2918	2929	2946	rVB	437688	715320	37.17%	5.475%
68	11.002	3001	3005	3010	rVB2	582	486	0.03%	0.004%
69	11.250	3079	3082	3090	rVB2	358	294	0.02%	0.002%
70	11.391	3124	3126	3129	rBV2	426	291	0.02%	0.002%
71	11.472	3141	3151	3158	rBV5	1512	2760	0.14%	0.021%
72	11.693	3215	3220	3221	rBV2	467	386	0.02%	0.003%
73	11.745	3232	3236	3239	rVB3	465	381	0.02%	0.003%
74	11.812	3244	3257	3279	rVV	734727	1144949	59.50%	8.764%
75	11.954	3292	3301	3315	rVB8	9628	16444	0.85%	0.126%
76	12.192	3363	3375	3390	rBV	562686	940120	48.85%	7.196%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Max Peaks: 100

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Title : VOC Analysis

77	12.404	3437	3441	3442	rBV	542	313	0.02%	0.002%
78	12.636	3507	3513	3521	rVB5	1183	1775	0.09%	0.014%
79	12.703	3531	3534	3541	rVB4	1003	1051	0.05%	0.008%
80	12.735	3541	3544	3547	rBV2	326	326	0.02%	0.002%
81	12.838	3569	3576	3587	rVB4	2943	3931	0.20%	0.030%
82	12.970	3602	3617	3629	rBV4	25866	49968	2.60%	0.382%
83	13.195	3684	3687	3691	rBV2	365	330	0.02%	0.003%
84	13.330	3720	3729	3735	rBV3	16617	26695	1.39%	0.204%
85	13.375	3735	3743	3760	rVB2	51155	78910	4.10%	0.604%
86	13.600	3809	3813	3816	rBV2	329	304	0.02%	0.002%
87	14.359	4038	4049	4061	rBV	46800	70064	3.64%	0.536%
88	14.426	4065	4070	4072	rBV4	1393	1315	0.07%	0.010%
89	14.491	4087	4090	4093	rBV4	1192	982	0.05%	0.008%
90	14.590	4116	4121	4128	rVB6	1734	2151	0.11%	0.016%
91	14.848	4198	4201	4206	rBV3	738	565	0.03%	0.004%
92	14.954	4230	4234	4235	rBV2	556	415	0.02%	0.003%
93	15.098	4276	4279	4280	rBV4	906	511	0.03%	0.004%
94	15.156	4293	4297	4298	rBV2	568	378	0.02%	0.003%
95	15.311	4328	4345	4356	rBV3	38239	67013	3.48%	0.513%
96	15.545	4406	4418	4432	rBV	295227	465669	24.20%	3.564%
97	15.796	4490	4496	4505	rBV7	5564	8078	0.42%	0.062%
98	15.893	4510	4526	4541	rBV4	61334	166871	8.67%	1.277%
99	16.388	4669	4680	4691	rBV	1233116	1924354	100.00%	14.729%
100	17.259	4943	4951	4966	rVB2	51729	84683	4.40%	0.648%

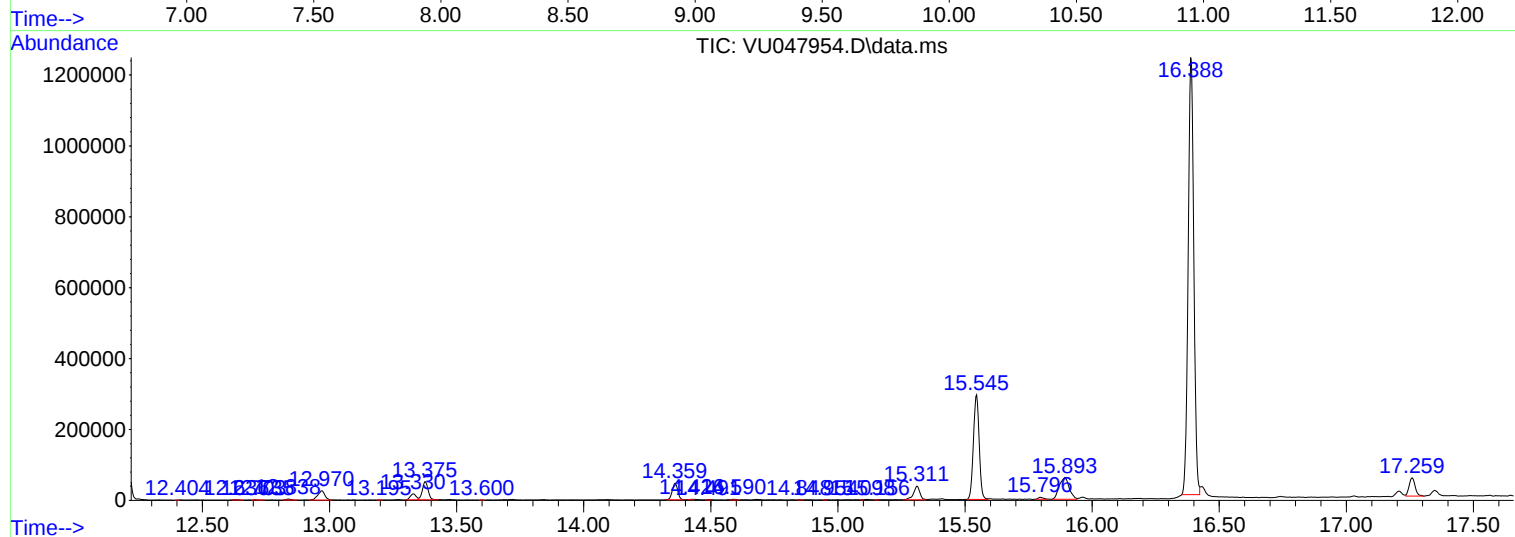
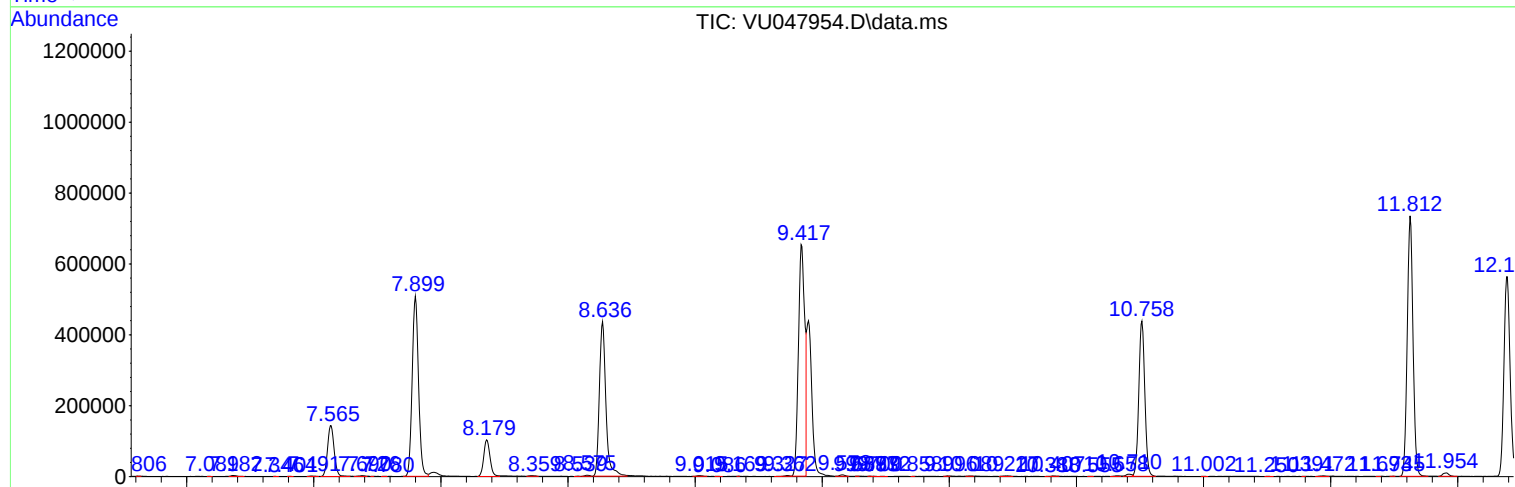
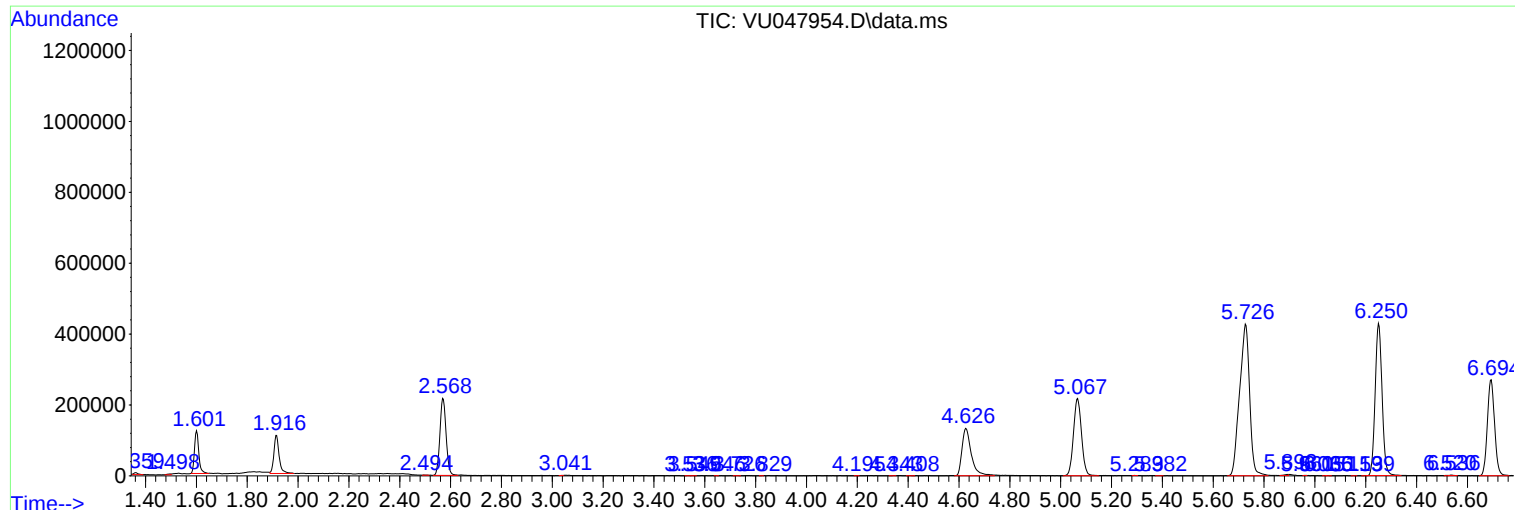
Sum of corrected areas: 13064740

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN2MEDL

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 : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN2MEDL

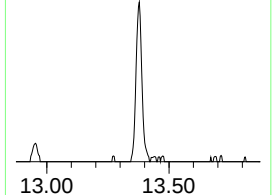
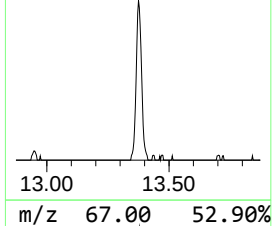
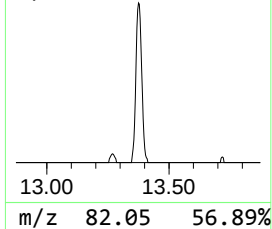
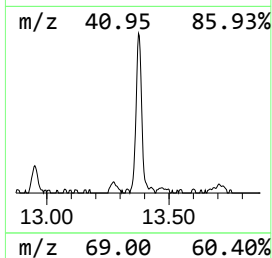
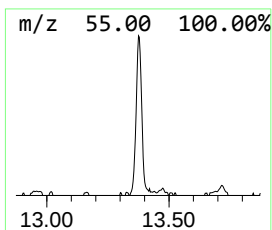
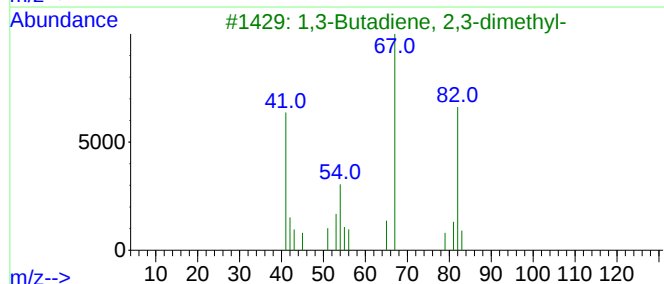
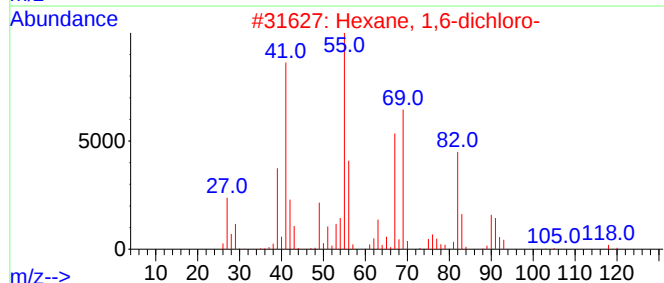
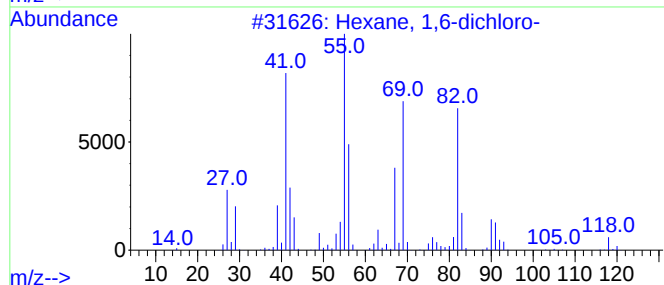
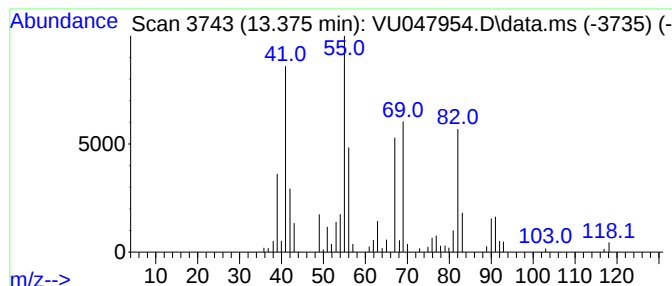
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Hexane, 1,6-dichloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.375	3.45 ug/L	78910	1,4-Dichlorobenzene-d4	11.812

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	72
3			1,3-Butadiene, 2,3-dimethyl-	82	C6H10	000513-81-5	43
4			Cyclohexane, chloro-	118	C6H11Cl	000542-18-7	38
5			4-Methyl-1,3-pentadiene	82	C6H10	000926-56-7	35



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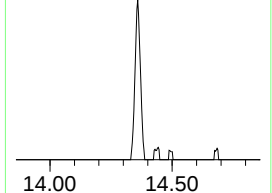
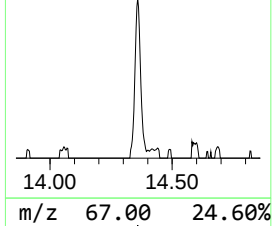
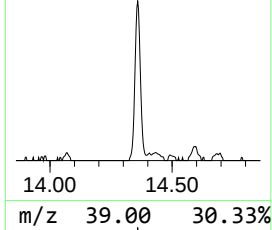
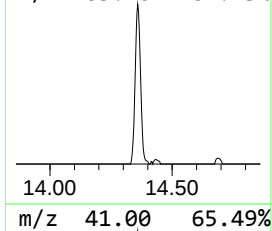
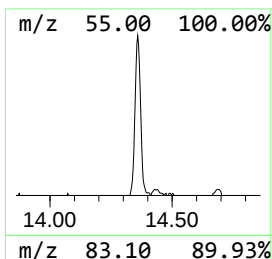
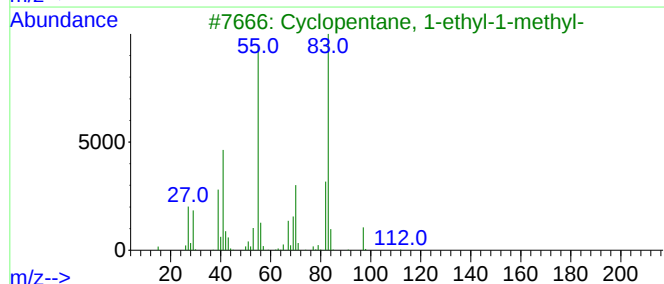
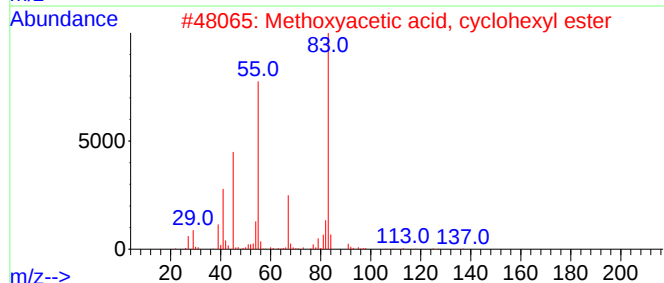
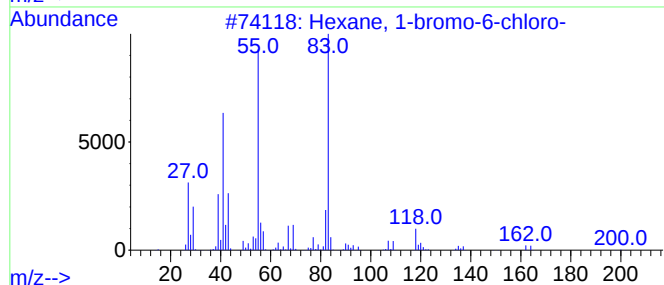
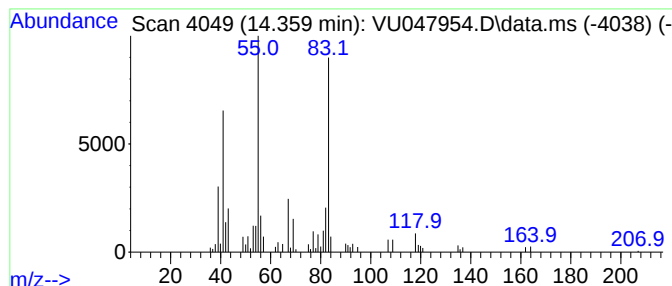
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Hexane, 1-bromo-6-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.359	3.06 ug/L	70064	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 1-bromo-6-chloro-	198	C6H12BrCl	006294-17-3	86
2			Methoxyacetic acid, cyclohexyl e...	172	C9H16O3	1000282-69-4	64
3			Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	64
4			Acetic acid, mercapto-, cyclohex...	174	C8H14O2S	016849-98-2	53
5			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	53



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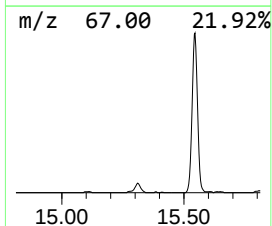
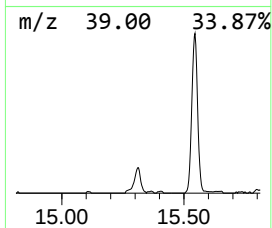
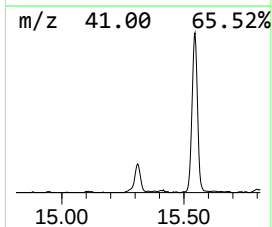
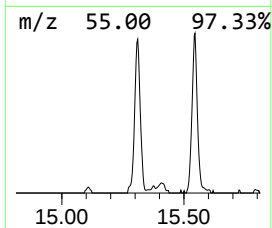
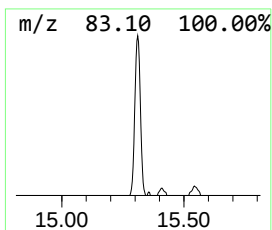
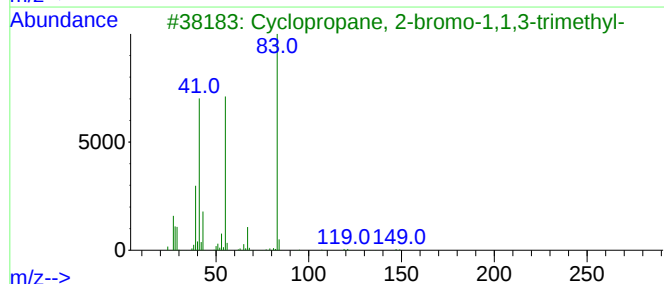
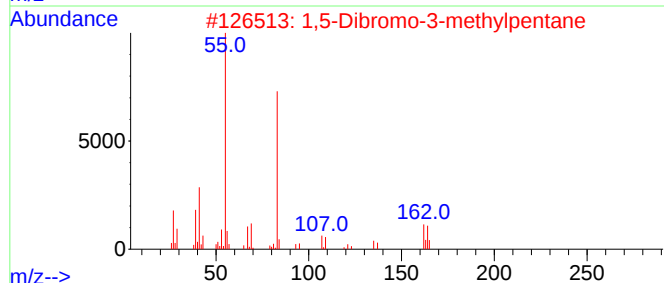
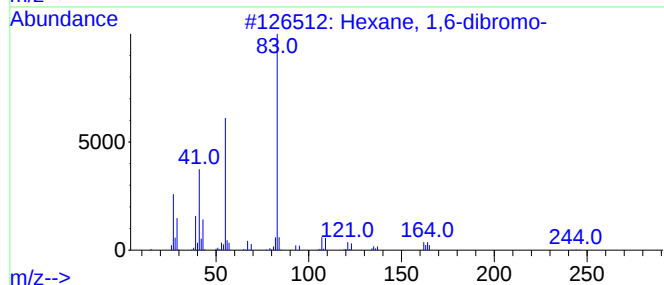
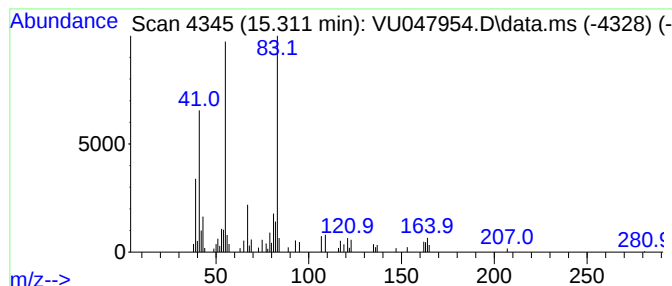
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Quant Title : VOC Analysis

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

Peak Number 4 Hexane, 1,6-dibromo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.311	2.93 ug/L	67013	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 1,6-dibromo-	242	C6H12Br2	000629-03-8	72
2			1,5-Dibromo-3-methylpentane	242	C6H12Br2	004457-72-1	72
3			Cyclopropane, 2-bromo-1,1,3-trim...	162	C6H11Br	036617-00-2	64
4			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	59
5			Cyclohexane, bromo-	162	C6H11Br	000108-85-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047954.D
Acq On : 12 Apr 2022 14:40
Operator : SY/MD
Sample : N2293-02MEDL 100X
Misc : 7.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN2MEDL

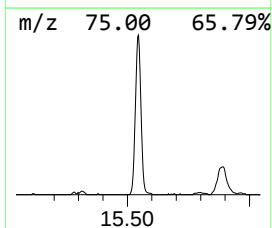
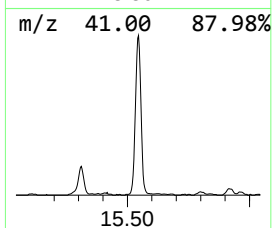
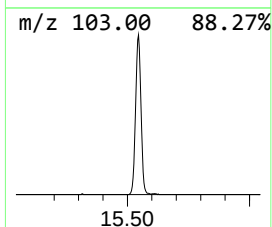
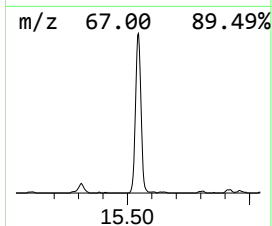
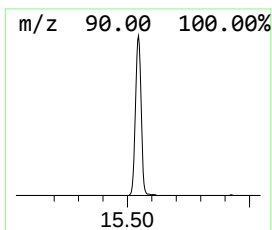
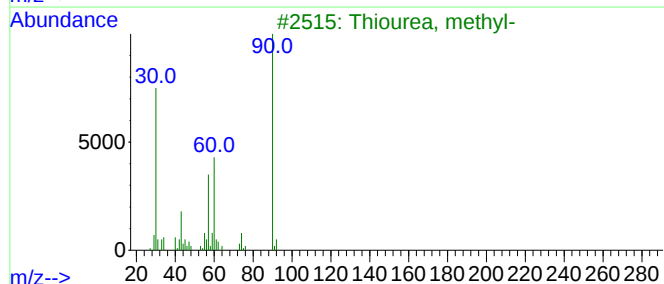
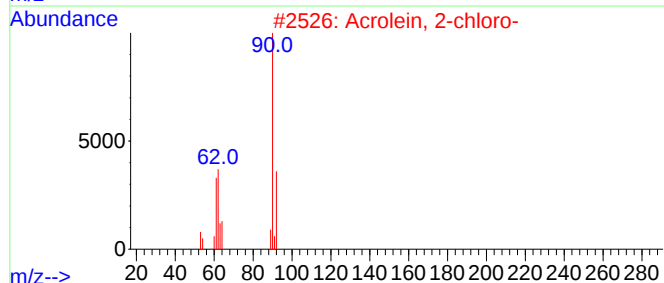
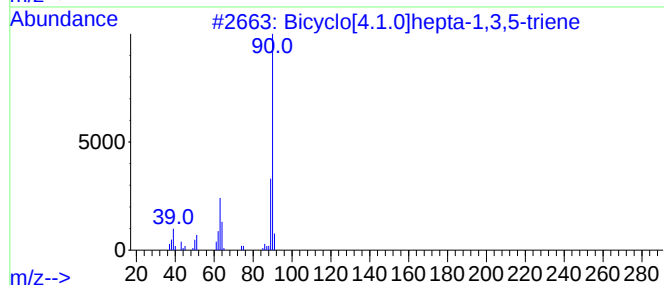
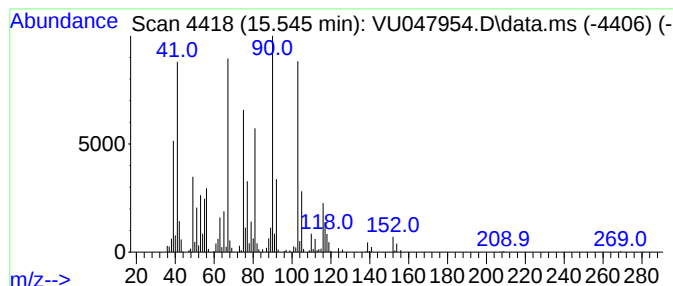
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Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	20.34 ug/L	465669	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	38
2			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	37
3			Thiourea, methyl-	90	C2H6N2S	000598-52-7	35
4			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	32
5			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047954.D
Acq On : 12 Apr 2022 14:40
Operator : SY/MD
Sample : N2293-02MEDL 100X
Misc : 7.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN2MEDL

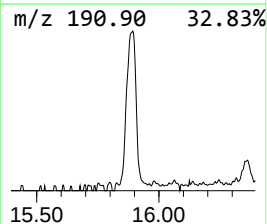
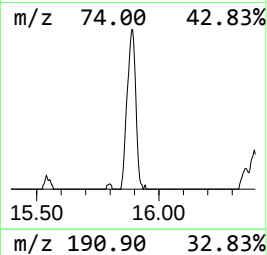
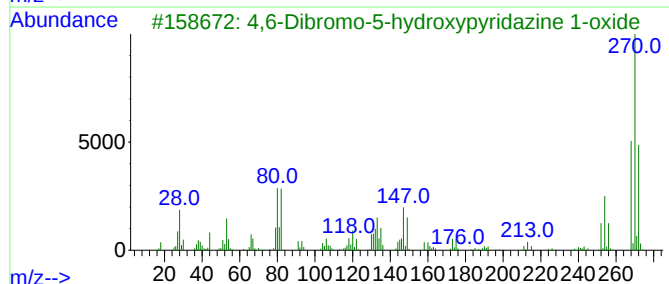
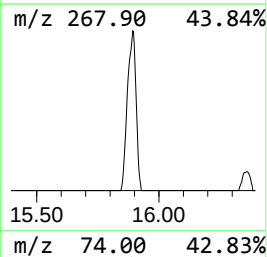
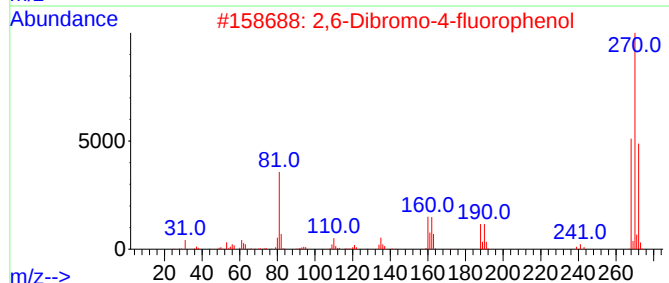
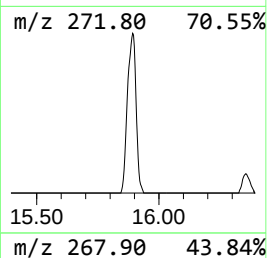
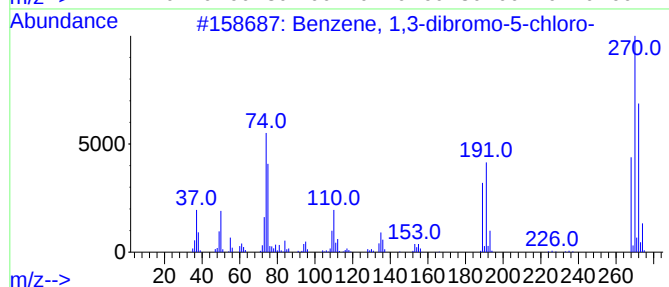
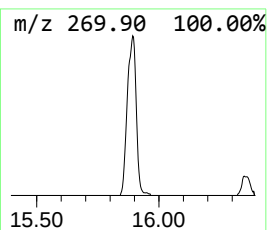
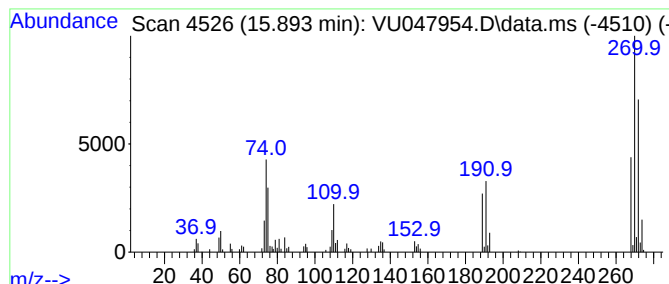
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Quant Title : VOC Analysis

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

Peak Number 6 Benzene, 1,3-dibromo-5-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.893	7.29 ug/L	166871	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dibromo-5-chloro-	268	C6H3Br2Cl	014862-52-3	93
2			2,6-Dibromo-4-fluorophenol	268	C6H3Br2FO	000344-20-7	46
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\VU041222\
Data File : VU047954.D
Acq On : 12 Apr 2022 14:40
Operator : SY/MD
Sample : N2293-02MEDL 100X
Misc : 7.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN2MEDL

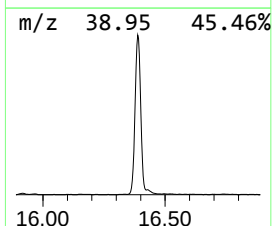
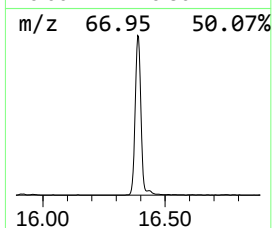
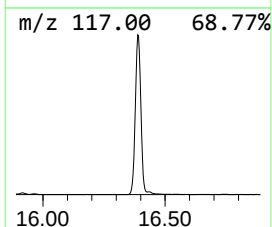
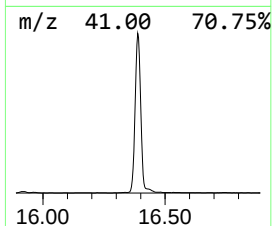
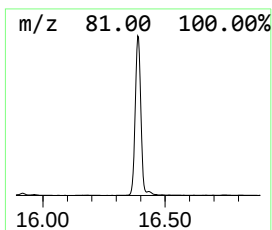
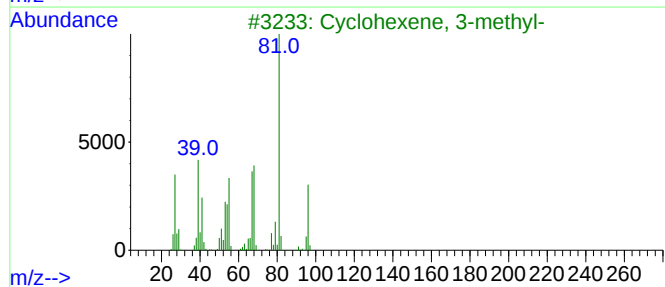
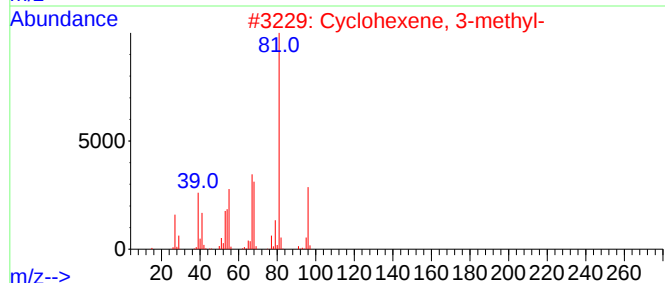
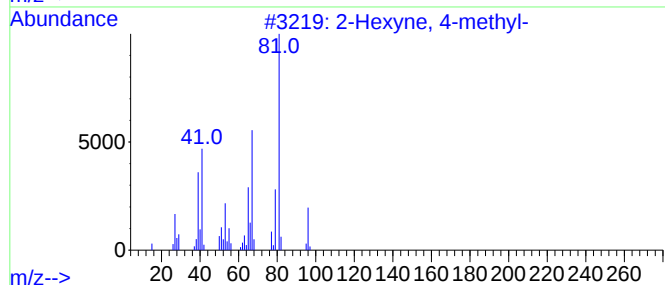
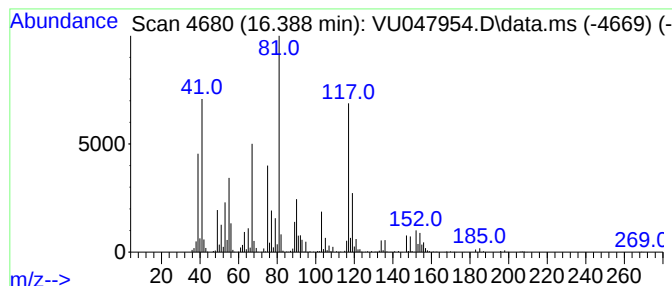
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Quant Title : VOC Analysis

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

Peak Number 7 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	84.04 ug/L	1924350	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexyne, 4-methyl-			96	C7H12	020198-49-6	22
2	Cyclohexene, 3-methyl-			96	C7H12	000591-48-0	22
3	Cyclohexene, 3-methyl-			96	C7H12	000591-48-0	22
4	3,7,11,Trimethyl-8,10- dodecedie...			266	C17H30O2	1000374-10-3	12
5	Cyclopropane, 1-(5-hexenyl)-2-iodo-			250	C9H15I	074685-40-8	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047954.D
Acq On : 12 Apr 2022 14:40
Operator : SY/MD
Sample : N2293-02MEDL 100X
Misc : 7.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN2MEDL

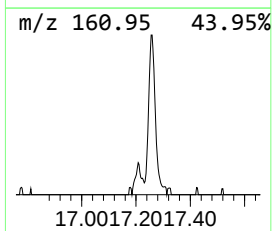
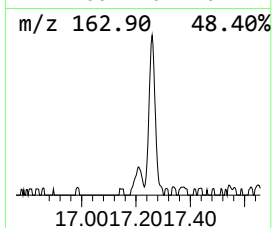
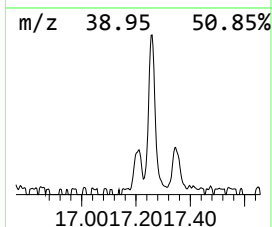
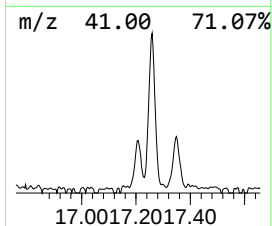
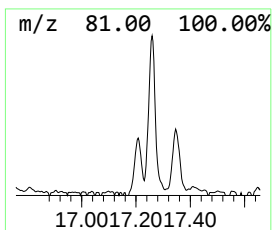
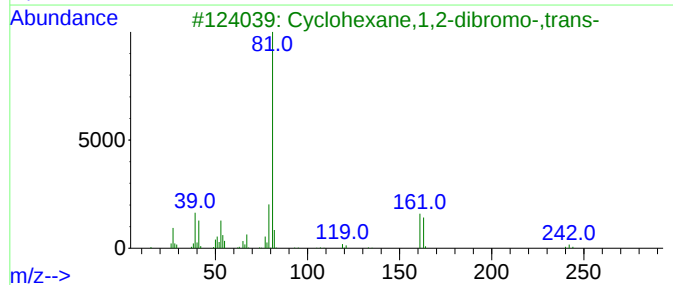
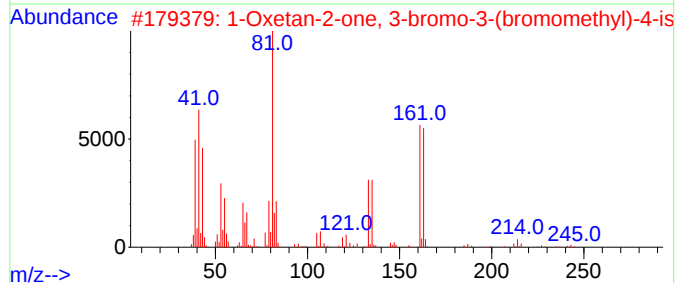
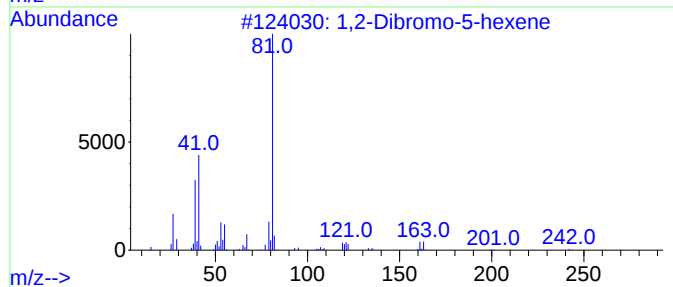
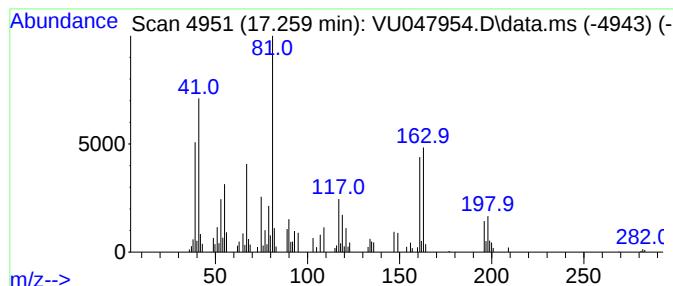
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Quant Title : VOC Analysis

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

Peak Number 8 unknown-03 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.259	3.70 ug/L	84683	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dibromo-5-hexene	240	C6H10Br2	004285-48-7	47
2			1-Oxetan-2-one, 3-bromo-3-(bromo...	284	C7H10Br2O2	1010142-30-2	47
3			Cyclohexane,1,2-dibromo-,trans-	240	C6H10Br2	007429-37-0	47
4			2,3-Diazabicyclo[2.2.1]hept-2-en...	178	C11H18N2	150667-99-5	35
5			Isomycorene	136	C10H16	006876-07-9	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047954.D
Acq On : 12 Apr 2022 14:40
Operator : SY/MD
Sample : N2293-02MEDL 100X
Misc : 7.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN2MEDL

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
Hexane, 1,6-dic...	13.375	3.5	ug/L	78910	3	11.812	1144950	50.0
Hexane, 1-bromo...	14.359	3.1	ug/L	70064	3	11.812	1144950	50.0
Hexane, 1,6-dib...	15.311	2.9	ug/L	67013	3	11.812	1144950	50.0
unknown-01	15.545	20.3	ug/L	465669	3	11.812	1144950	50.0
Benzene, 1,3-di...	15.893	7.3	ug/L	166871	3	11.812	1144950	50.0
unknown-02	16.388	84.0	ug/L	1924350	3	11.812	1144950	50.0
unknown-03	17.259	3.7	ug/L	84683	3	11.812	1144950	50.0