

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
 Data File : VU047926.D
 Acq On : 11 Apr 2022 23:23
 Operator : SY/MD
 Sample : N2293-13ME
 Misc : 6.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP1ME

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: VU047926.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	113	rVB	72943	162222	10.98%	1.381%
2	2.539	362	373	387	rBV	210348	364078	24.64%	3.100%
3	2.803	452	455	457	rBV2	420	318	0.02%	0.003%
4	2.909	484	488	489	rBV3	506	386	0.03%	0.003%
5	3.121	551	554	557	rBV2	327	216	0.01%	0.002%
6	3.176	566	571	576	rBV4	749	908	0.06%	0.008%
7	3.359	625	628	631	rBV4	405	405	0.03%	0.003%
8	3.539	680	684	685	rBV2	289	167	0.01%	0.001%
9	3.597	700	702	705	rVB	199	84	0.01%	0.001%
10	3.758	750	752	754	rBV	304	179	0.01%	0.002%
11	3.838	775	777	781	rBV	225	102	0.01%	0.001%
12	3.935	804	807	808	rBV	192	100	0.01%	0.001%
13	4.054	841	844	848	rVB3	492	304	0.02%	0.003%
14	4.131	864	868	871	rBV3	479	415	0.03%	0.004%
15	4.247	902	904	906	rBV	191	104	0.01%	0.001%
16	4.266	907	910	915	rBV2	200	198	0.01%	0.002%
17	4.430	958	961	965	rBV2	208	142	0.01%	0.001%
18	4.462	969	971	973	rVB	168	48	0.00%	0.000%
19	4.578	1004	1007	1010	rVB	386	216	0.01%	0.002%
20	4.642	1014	1027	1066	rBV	90684	328236	22.21%	2.795%
21	5.063	1140	1158	1187	rBV	208030	484665	32.80%	4.127%
22	5.202	1197	1201	1205	rBV3	384	317	0.02%	0.003%
23	5.243	1209	1214	1220	rBV2	275	443	0.03%	0.004%
24	5.285	1221	1227	1228	rBV2	623	577	0.04%	0.005%
25	5.330	1238	1241	1242	rBV2	312	183	0.01%	0.002%
26	5.465	1282	1283	1285	rVB2	305	107	0.01%	0.001%
27	5.481	1285	1288	1293	rVB	277	154	0.01%	0.001%
28	5.530	1301	1303	1304	rBV	249	91	0.01%	0.001%
29	5.719	1341	1362	1374	rBV2	475958	1253604	84.84%	10.675%
30	5.932	1427	1428	1431	rBV2	247	155	0.01%	0.001%
31	6.051	1463	1465	1467	rBV	170	49	0.00%	0.000%
32	6.121	1479	1487	1488	rBV5	1109	970	0.07%	0.008%
33	6.173	1498	1503	1504	rBV	300	196	0.01%	0.002%
34	6.247	1510	1526	1551	rBV	506400	1015524	68.73%	8.647%
35	6.478	1595	1598	1600	rBV	126	105	0.01%	0.001%
36	6.526	1605	1613	1623	rVB4	2665	4565	0.31%	0.039%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

Sampling : 1

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Peak separation: 5

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

37	6.568	1623	1626	1629	rBV2	437	308	0.02%	0.003%
38	6.690	1648	1664	1684	rBV	270357	560686	37.94%	4.774%
39	6.877	1720	1722	1727	rBV	260	208	0.01%	0.002%
40	6.983	1753	1755	1757	rBV2	215	125	0.01%	0.001%
41	7.054	1772	1777	1780	rBV3	471	517	0.03%	0.004%
42	7.202	1811	1823	1838	rBV3	6698	18182	1.23%	0.155%
43	7.443	1895	1898	1901	rBV3	368	216	0.01%	0.002%
44	7.497	1905	1915	1925	rVV2	21529	42993	2.91%	0.366%
45	7.568	1927	1937	1957	rVB	129816	256778	17.38%	2.186%
46	7.899	2027	2040	2055	rBV	527720	951347	64.38%	8.101%
47	8.124	2107	2110	2114	rBV3	1085	764	0.05%	0.007%
48	8.182	2117	2128	2152	rVB2	82877	174128	11.78%	1.483%
49	8.369	2175	2186	2206	rVB7	12170	33338	2.26%	0.284%
50	8.581	2244	2252	2259	rVB7	1675	2753	0.19%	0.023%
51	8.661	2259	2277	2308	rBV	376664	800932	54.20%	6.820%
52	8.896	2348	2350	2352	rVB2	440	137	0.01%	0.001%
53	9.034	2383	2393	2405	rVB5	6115	14083	0.95%	0.120%
54	9.156	2429	2431	2433	rVB2	284	89	0.01%	0.001%
55	9.189	2436	2441	2447	rBV4	694	1003	0.07%	0.009%
56	9.346	2485	2490	2492	rBV2	341	319	0.02%	0.003%
57	9.362	2492	2495	2499	rBV4	548	458	0.03%	0.004%
58	9.427	2500	2515	2519	rBV	736015	1412911	95.62%	12.031%
59	9.668	2587	2590	2591	rBV2	512	290	0.02%	0.002%
60	9.764	2617	2620	2623	rBV2	275	183	0.01%	0.002%
61	9.825	2637	2639	2641	rBV	255	146	0.01%	0.001%
62	9.873	2651	2654	2657	rBV3	236	208	0.01%	0.002%
63	9.999	2692	2693	2695	rBV3	221	117	0.01%	0.001%
64	10.144	2736	2738	2739	rBV3	171	77	0.01%	0.001%
65	10.266	2774	2776	2778	rBV	355	185	0.01%	0.002%
66	10.349	2799	2802	2803	rBV	504	270	0.02%	0.002%
67	10.404	2817	2819	2822	rBV2	193	97	0.01%	0.001%
68	10.459	2834	2836	2837	rBV	354	104	0.01%	0.001%
69	10.661	2889	2899	2909	rVB8	5947	10943	0.74%	0.093%
70	10.767	2918	2932	2948	rBV	457835	745993	50.48%	6.352%
71	10.870	2959	2964	2967	rBV3	831	720	0.05%	0.006%
72	11.205	3064	3068	3069	rBV	504	320	0.02%	0.003%
73	11.256	3076	3084	3092	rBV5	5292	8444	0.57%	0.072%
74	11.816	3246	3258	3274	rBV	931020	1477657	100.00%	12.582%
75	12.198	3364	3377	3397	rBV	637701	1123298	76.02%	9.565%
76	13.333	3723	3730	3736	rBV4	4612	7092	0.48%	0.060%

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ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP1ME

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	14.494	4083	4091	4108	rVB4	36001	59397	4.02%	0.506%
78	15.545	4409	4418	4430	rVB2	86896	132424	8.96%	1.128%
79	15.889	4512	4525	4538	rBV4	111565	283135	19.16%	2.411%

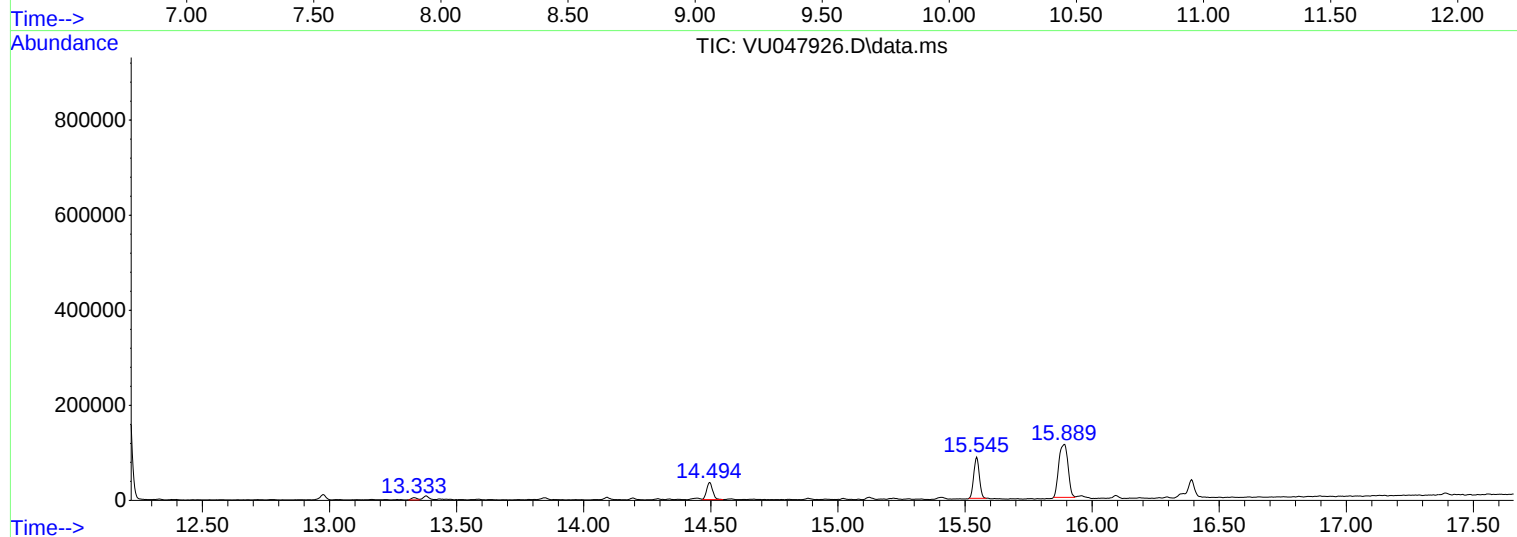
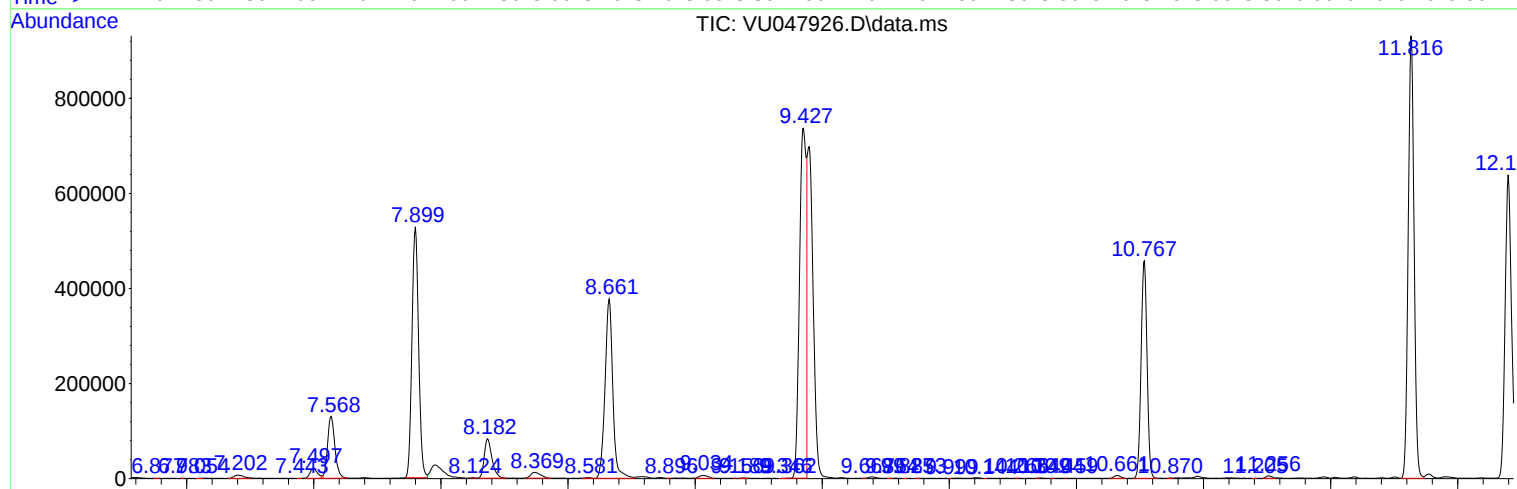
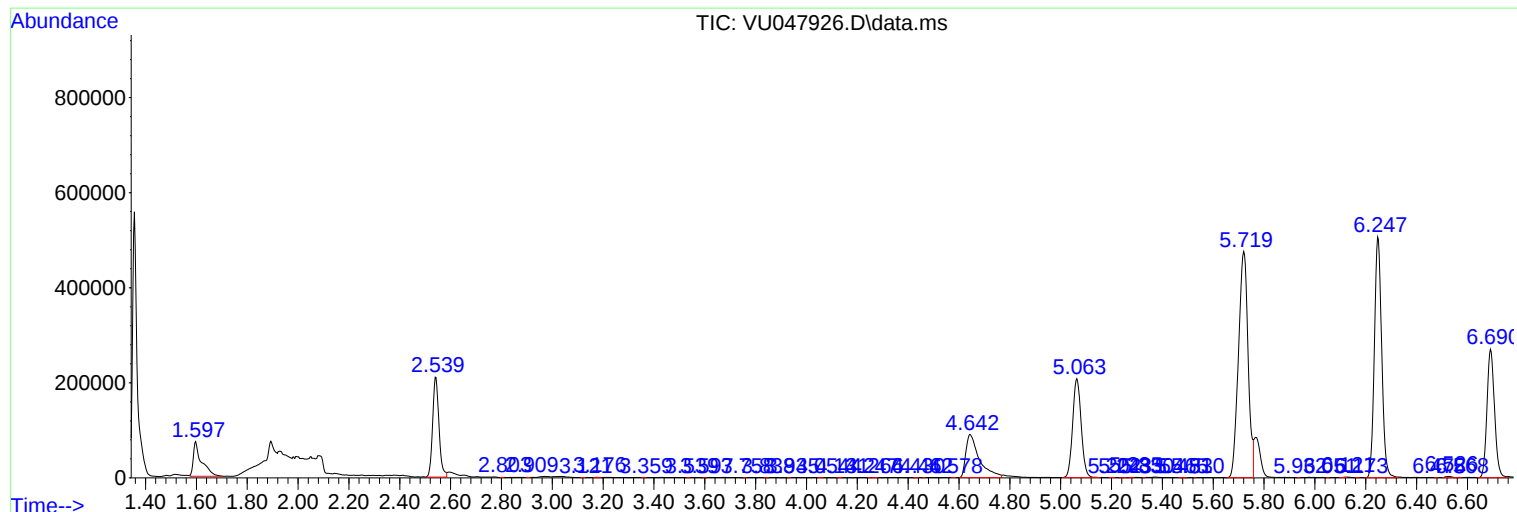
Sum of corrected areas: 11743908

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
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Misc : 6.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP1ME

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 : VU047926.D
Acq On : 11 Apr 2022 23:23
Operator : SY/MD
Sample : N2293-13ME
Misc : 6.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP1ME

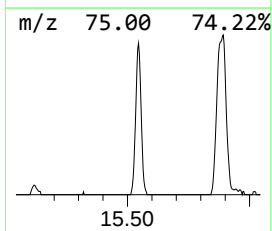
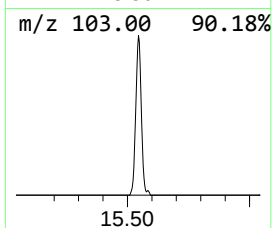
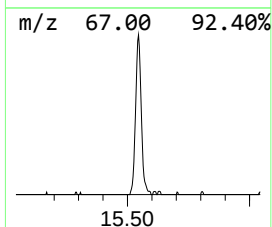
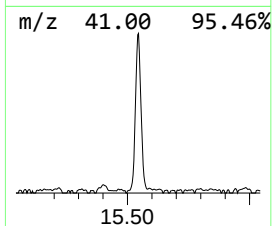
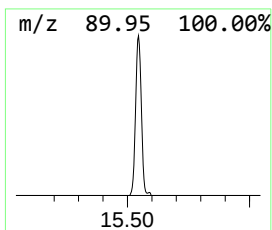
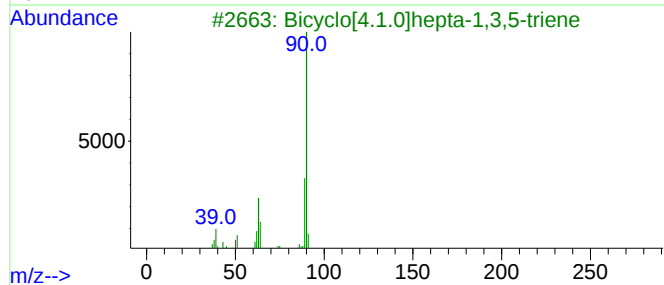
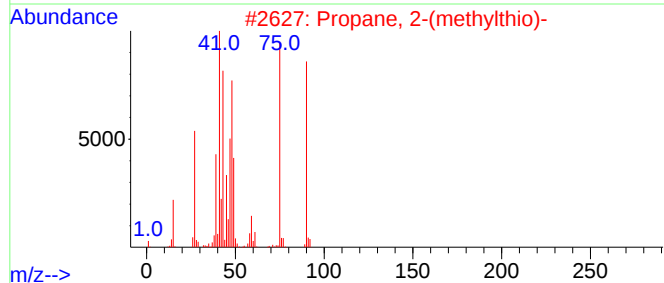
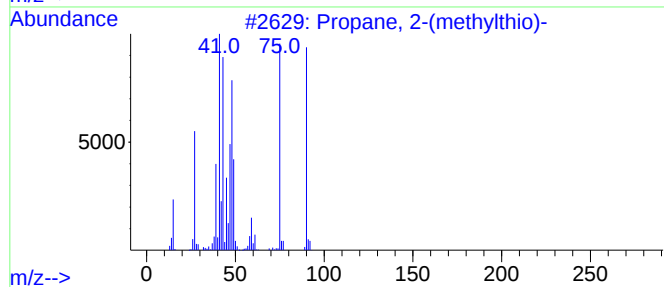
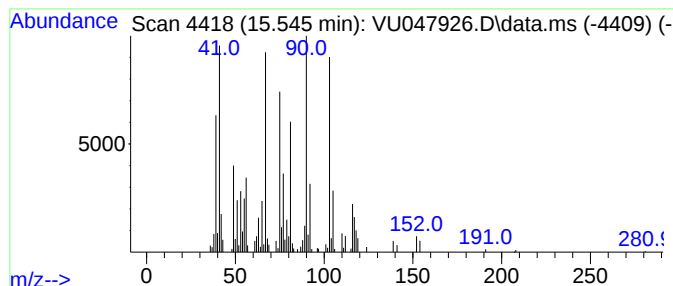
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Propane, 2-(methylthio)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	4.48 ug/L	132424	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	58
2			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	58
3			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	27
4			Borane, chloro(dimethylamino)ethyl-	119	C4H11BClN	001739-26-0	25
5			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	23



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Misc : 6.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 34 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP1ME

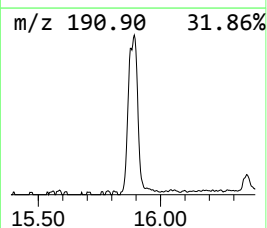
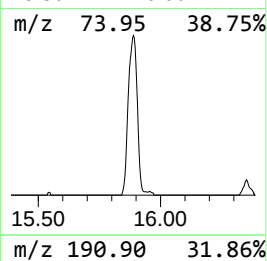
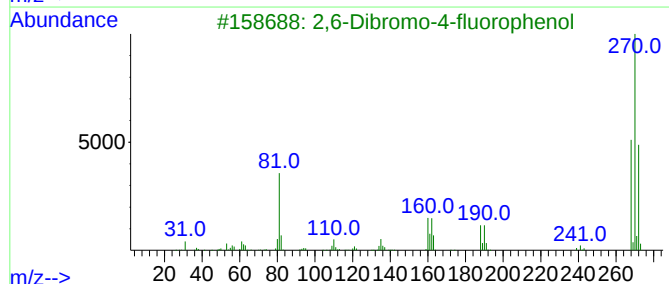
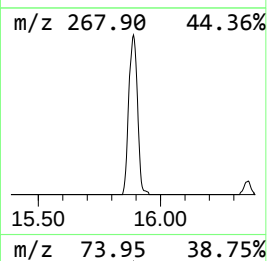
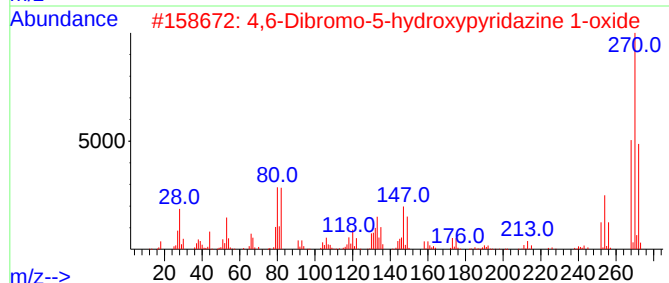
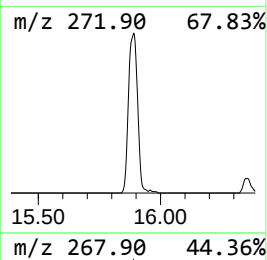
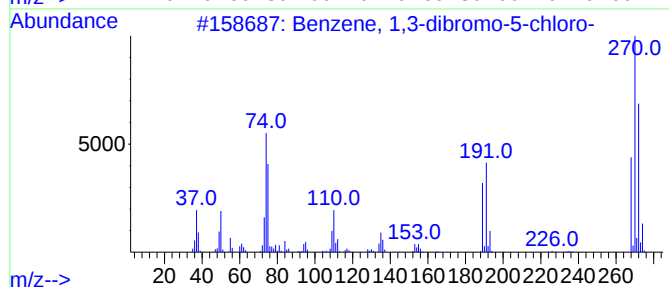
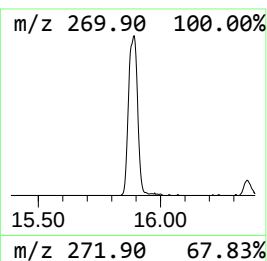
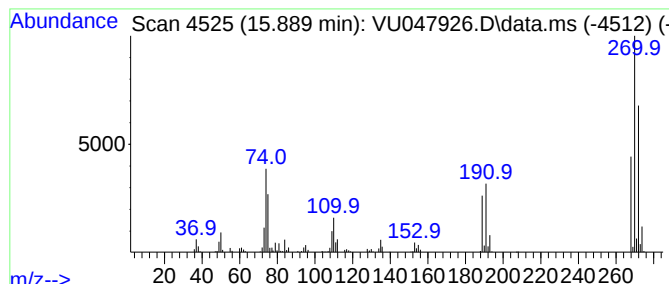
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1,3-dibromo-5-chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.889	9.58 ug/L	283135	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dibromo-5-chloro-	268	C6H3Br2Cl	014862-52-3	94
2			4,6-Dibromo-5-hydroxypyridazine ...	268	C4H2Br2N2O2	019971-61-0	47
3			2,6-Dibromo-4-fluorophenol	268	C6H3Br2FO	000344-20-7	38
4			Pyrimidine, 4,6-dichloro-2-(meth...	270	C11H8Cl2N2S	064415-11-8	32
5			5-Bromo-7-methoxy-1-benzofuran-2...	270	C10H7BrO4	020037-37-0	17



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2-(met...	15.545	4.5	ug/L	132424	3	11.819	1477660	50.0
Benzene, 1,3-di...	15.889	9.6	ug/L	283135	3	11.819	1477660	50.0