

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
 Data File : VV031764.D
 Acq On : 26 Jul 2023 13:15
 Operator : SY/MD
 Sample : 03712-08
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Y5

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_V\Method\SFAMVLM072523WMA.M
 Title : VOC Analysis

Signal : TIC: VV031764.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	67	74	90	rVB	212835	234547	14.26%	1.752%
2	1.423	111	119	127	rBV9	11010	20384	1.24%	0.152%
3	1.532	146	153	169	rVB	201794	244047	14.83%	1.823%
4	2.060	307	317	327	rBV	376616	546964	33.24%	4.087%
5	2.114	329	334	349	rVB	51988	78256	4.76%	0.585%
6	2.278	380	385	389	rVB6	1891	1729	0.11%	0.013%
7	2.568	461	475	495	rBV2	54845	117148	7.12%	0.875%
8	2.774	536	539	546	rVB5	1079	1372	0.08%	0.010%
9	2.828	551	556	557	rBV3	983	673	0.04%	0.005%
10	2.918	580	584	589	rVB5	1665	1617	0.10%	0.012%
11	2.944	589	592	595	rBV2	1073	660	0.04%	0.005%
12	2.983	601	604	606	rBV3	907	632	0.04%	0.005%
13	3.011	610	613	617	rBV5	982	764	0.05%	0.006%
14	3.211	670	675	677	rBV4	876	810	0.05%	0.006%
15	3.327	709	711	718	rVB5	753	776	0.05%	0.006%
16	3.555	779	782	785	rBV4	1175	713	0.04%	0.005%
17	3.603	792	797	803	rBV7	1002	1106	0.07%	0.008%
18	3.706	825	829	834	rBV6	1160	1076	0.07%	0.008%
19	3.793	846	856	887	rBV	136818	404903	24.61%	3.025%
20	4.256	983	1000	1025	rBV	290847	766446	46.58%	5.727%
21	4.513	1077	1080	1082	rBV3	1160	1003	0.06%	0.007%
22	4.539	1086	1088	1090	rVV2	2216	1309	0.08%	0.010%
23	4.552	1090	1092	1097	rVV5	1630	1552	0.09%	0.012%
24	4.584	1100	1102	1109	rVB6	1871	1752	0.11%	0.013%
25	4.960	1202	1219	1246	rBV3	607285	1645324	100.00%	12.293%
26	5.204	1293	1295	1298	rVB4	1499	633	0.04%	0.005%
27	5.240	1304	1306	1308	rBV3	1394	767	0.05%	0.006%
28	5.301	1323	1325	1328	rBV3	889	597	0.04%	0.004%
29	5.368	1344	1346	1350	rVB3	1536	857	0.05%	0.006%
30	5.400	1350	1356	1360	rBV7	1544	2047	0.12%	0.015%
31	5.442	1367	1369	1373	rVB4	1780	1184	0.07%	0.009%
32	5.465	1373	1376	1379	rBV5	1578	1172	0.07%	0.009%
33	5.487	1379	1383	1384	rBV2	946	620	0.04%	0.005%
34	5.539	1385	1399	1423	rBV	420316	879597	53.46%	6.572%
35	5.828	1473	1489	1510	rBV3	67634	149387	9.08%	1.116%
36	5.992	1528	1540	1567	rBV	394520	820397	49.86%	6.130%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW072623\
 Data File : VW031764.D
 Acq On : 26 Jul 2023 13:15
 Operator : SY/MD
 Sample : 03712-08
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Y5

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_V\Method\SFAMVLM072523WMA.M
 Title : VOC Analysis

37	6.317	1638	1641	1642	rBV3	1421	764	0.05%	0.006%
38	6.326	1642	1644	1647	rVB4	1590	919	0.06%	0.007%
39	6.378	1657	1660	1665	rVB7	1925	1608	0.10%	0.012%
40	6.404	1665	1668	1669	rBV3	1390	711	0.04%	0.005%
41	6.510	1690	1701	1721	rBV	63935	136733	8.31%	1.022%
42	6.732	1767	1770	1771	rBV3	1568	974	0.06%	0.007%
43	6.873	1811	1814	1817	rBV5	1881	1248	0.08%	0.009%
44	6.918	1817	1828	1853	rBV2	169968	331816	20.17%	2.479%
45	7.249	1919	1931	1947	rBV	560536	996462	60.56%	7.445%
46	7.490	2003	2006	2008	rVB4	1425	712	0.04%	0.005%
47	7.558	2015	2027	2043	rBV	127285	230870	14.03%	1.725%
48	7.741	2081	2084	2086	rVB4	1614	942	0.06%	0.007%
49	7.941	2144	2146	2150	rVB5	1402	846	0.05%	0.006%
50	7.989	2159	2161	2164	rVB4	1505	798	0.05%	0.006%
51	8.031	2164	2174	2215	rBV2	408739	886292	53.87%	6.622%
52	8.577	2341	2344	2345	rBV2	1448	781	0.05%	0.006%
53	8.789	2397	2410	2433	rBV	673367	1125788	68.42%	8.412%
54	9.079	2498	2500	2503	rBV4	1600	1044	0.06%	0.008%
55	9.172	2526	2529	2530	rBV2	1479	686	0.04%	0.005%
56	9.252	2551	2554	2557	rBV4	1311	1011	0.06%	0.008%
57	9.297	2565	2568	2578	rVB10	1984	2629	0.16%	0.020%
58	9.349	2581	2584	2587	rBV4	1936	1389	0.08%	0.010%
59	9.494	2627	2629	2634	rVB5	1767	1514	0.09%	0.011%
60	9.522	2634	2638	2640	rBV5	1927	1427	0.09%	0.011%
61	9.616	2663	2667	2670	rBV6	1563	1658	0.10%	0.012%
62	9.661	2679	2681	2682	rBV2	1409	662	0.04%	0.005%
63	9.728	2690	2702	2704	rBV10	5162	8270	0.50%	0.062%
64	9.818	2728	2730	2736	rVB4	2025	1765	0.11%	0.013%
65	9.873	2743	2747	2748	rBV4	2192	1681	0.10%	0.013%
66	9.895	2749	2754	2760	rVV9	5428	7883	0.48%	0.059%
67	10.008	2787	2789	2791	rBV3	1518	855	0.05%	0.006%
68	10.066	2803	2807	2809	rBV4	1586	998	0.06%	0.007%
69	10.159	2824	2836	2854	rVV	489662	784066	47.65%	5.858%
70	10.329	2881	2889	2899	rVB	7148	12033	0.73%	0.090%
71	10.410	2907	2914	2916	rBV7	2734	3352	0.20%	0.025%
72	10.542	2951	2955	2958	rBV5	2419	2220	0.13%	0.017%
73	10.567	2960	2963	2971	rVB9	4789	6422	0.39%	0.048%
74	10.693	2997	3002	3003	rBV5	2160	1765	0.11%	0.013%
75	10.706	3003	3006	3007	rBV3	2069	1120	0.07%	0.008%
76	10.821	3040	3042	3043	rBV2	1403	608	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
 Data File : VV031764.D
 Acq On : 26 Jul 2023 13:15
 Operator : SY/MD
 Sample : 03712-08
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Y5

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_V\Method\SFAMVLM072523WMA.M
 Title : VOC Analysis

77	10.963	3084	3086	3089	rBV4	1330	731	0.04%	0.005%
78	10.998	3095	3097	3100	rBV4	2500	1361	0.08%	0.010%
79	11.133	3129	3139	3146	rBV6	23555	36360	2.21%	0.272%
80	11.191	3146	3157	3177	rVB	676760	1048228	63.71%	7.832%
81	11.301	3186	3191	3201	rVB	6811	10920	0.66%	0.082%
82	11.500	3244	3253	3262	rBV8	11966	22759	1.38%	0.170%
83	11.567	3263	3274	3291	rVB	704999	1109455	67.43%	8.290%
84	11.847	3355	3361	3367	rBV9	4834	7028	0.43%	0.053%
85	11.944	3381	3391	3414	rBV	153175	249728	15.18%	1.866%
86	12.252	3477	3487	3502	rBV2	97433	159608	9.70%	1.193%
87	12.706	3624	3628	3629	rBV4	1629	995	0.06%	0.007%
88	12.808	3657	3660	3662	rBV4	1226	753	0.05%	0.006%
89	12.960	3702	3707	3710	rBV6	1557	1793	0.11%	0.013%
90	13.001	3717	3720	3722	rBV3	1755	840	0.05%	0.006%
91	13.181	3771	3776	3778	rBV5	1838	1904	0.12%	0.014%
92	13.339	3821	3825	3827	rBV4	2359	2003	0.12%	0.015%
93	13.419	3843	3850	3851	rBV7	8196	6926	0.42%	0.052%
94	13.873	3974	3991	4005	rBV2	118596	209130	12.71%	1.563%
95	14.413	4156	4159	4162	rBV6	1740	1551	0.09%	0.012%
96	14.590	4212	4214	4216	rBV3	1630	958	0.06%	0.007%
97	14.860	4295	4298	4300	rBV4	1727	1160	0.07%	0.009%
98	15.062	4355	4361	4367	rBV10	7702	10491	0.64%	0.078%
99	15.532	4505	4507	4509	rBV3	1644	934	0.06%	0.007%
100	15.564	4515	4517	4521	rBV5	2484	1984	0.12%	0.015%

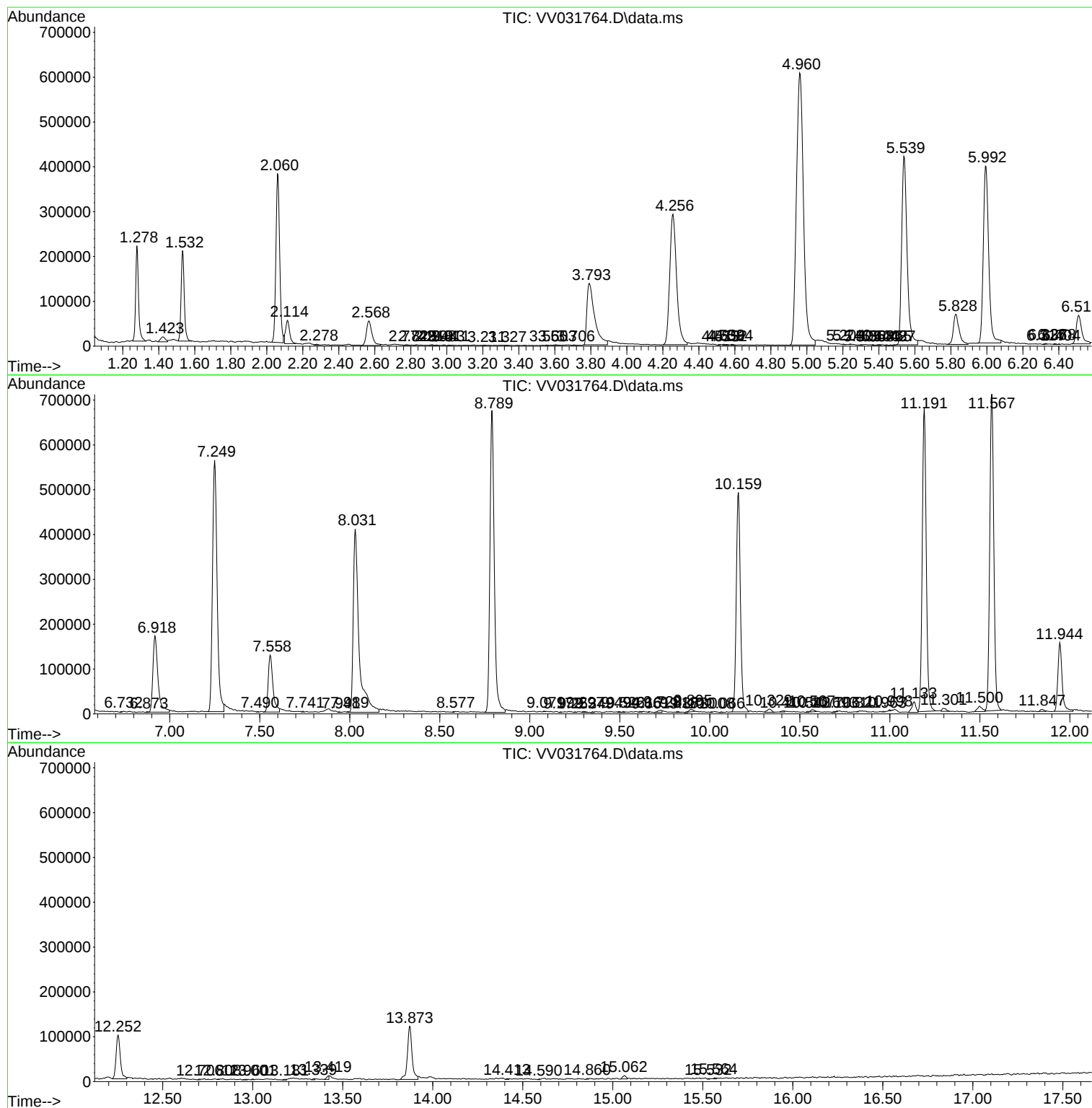
Sum of corrected areas: 13383743

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031764.D
Acq On : 26 Jul 2023 13:15
Operator : SY/MD
Sample : 03712-08
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031764.D
Acq On : 26 Jul 2023 13:15
Operator : SY/MD
Sample : 03712-08
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y5

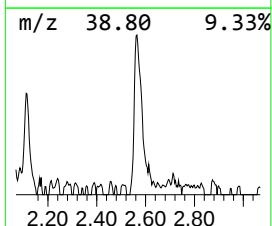
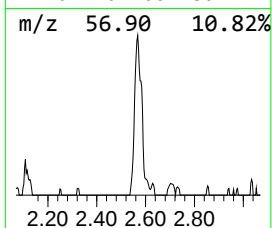
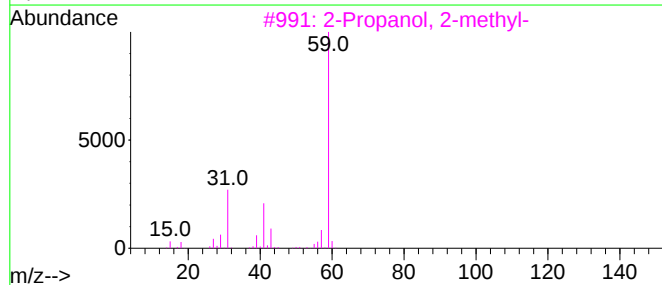
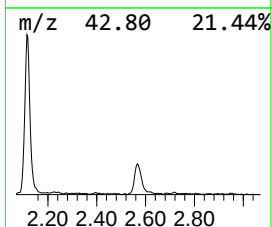
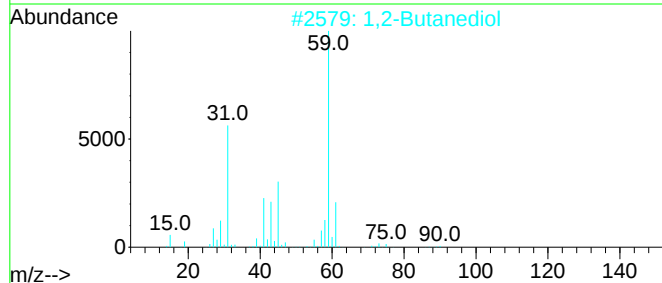
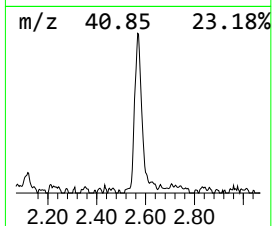
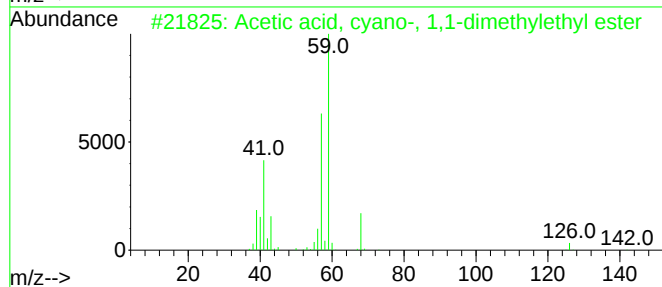
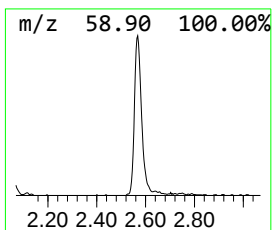
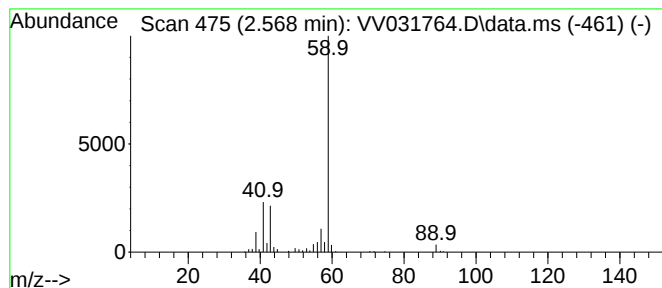
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Acetic acid, cyano-, 1,1-di... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.568	6.66 ug/L	117148	1,4-Difluorobenzene	5.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	64
2			1,2-Butanediol	90	C4H10O2	000584-03-2	64
3			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56
4			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56
5			HEX-5-EN-3-OL	100	C6H12O	000688-99-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031764.D
Acq On : 26 Jul 2023 13:15
Operator : SY/MD
Sample : 03712-08
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y5

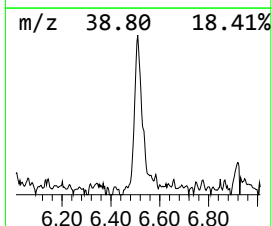
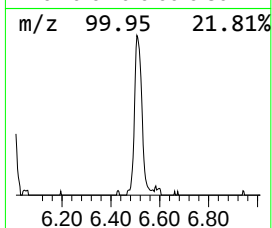
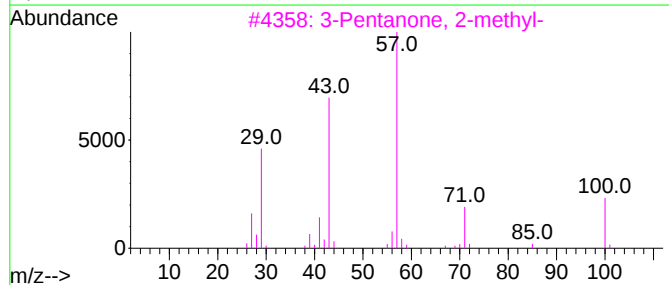
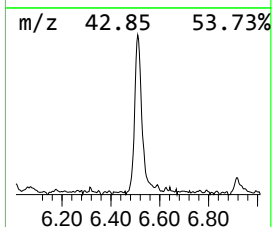
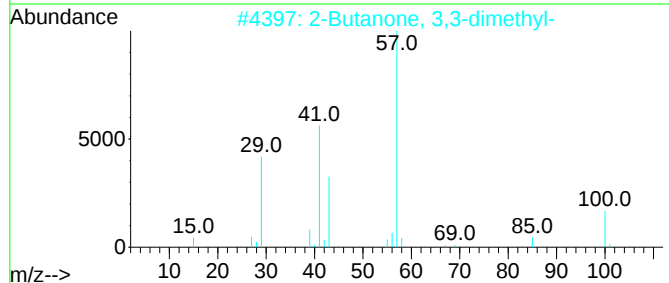
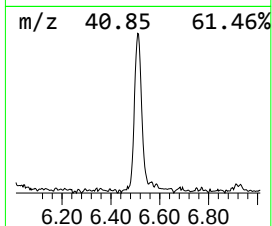
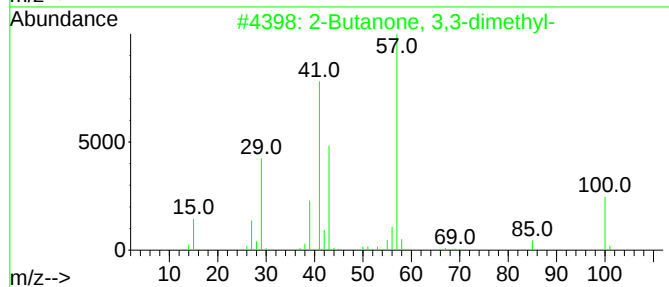
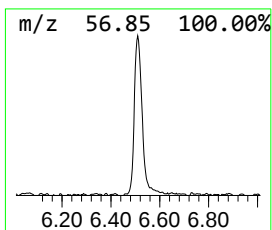
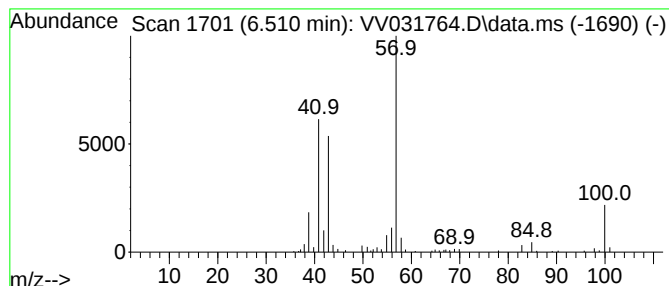
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.510	7.77 ug/L	136733	1,4-Difluorobenzene	5.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	90	
2	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	80	
3	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	64	
4	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	59	
5	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	59	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031764.D
Acq On : 26 Jul 2023 13:15
Operator : SY/MD
Sample : 03712-08
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y5

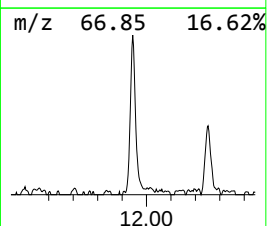
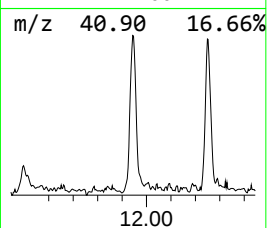
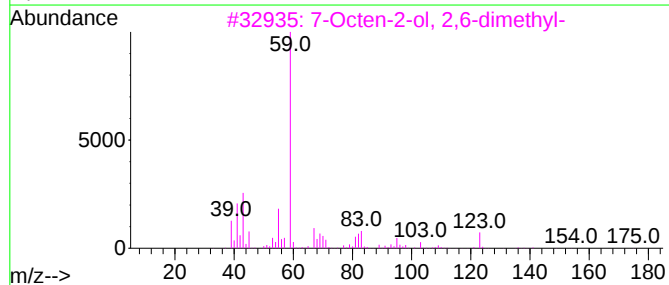
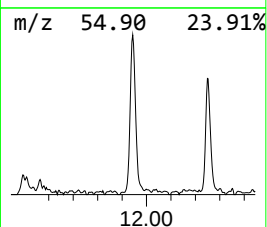
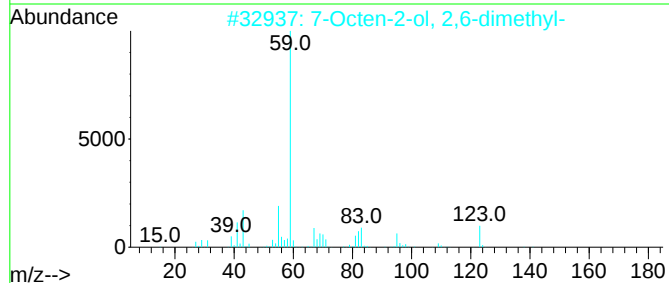
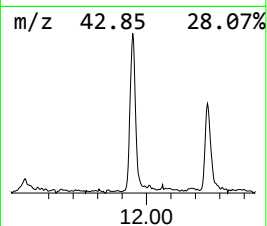
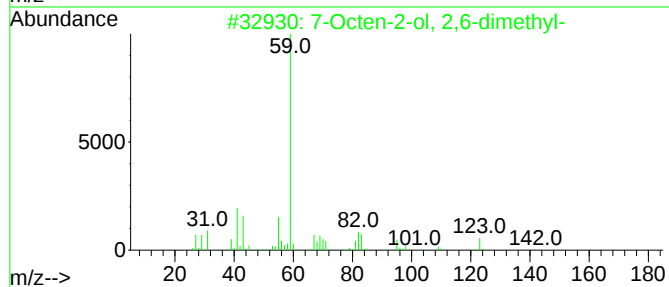
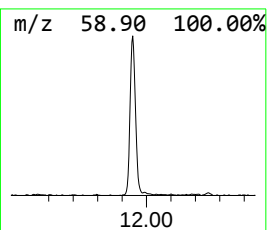
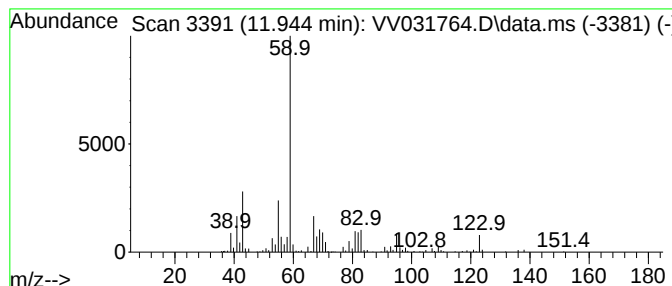
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.944	11.91 ug/L	249728	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
3			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
4			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	64
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031764.D
Acq On : 26 Jul 2023 13:15
Operator : SY/MD
Sample : 03712-08
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y5

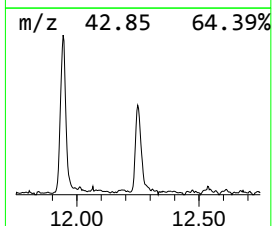
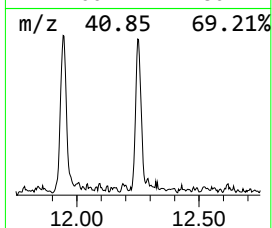
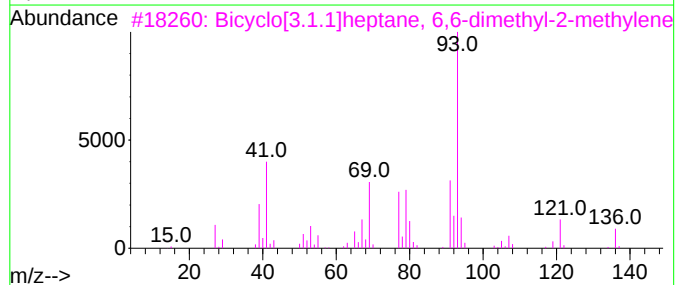
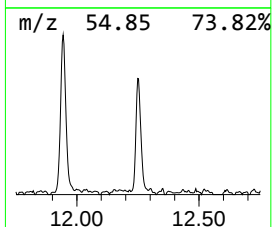
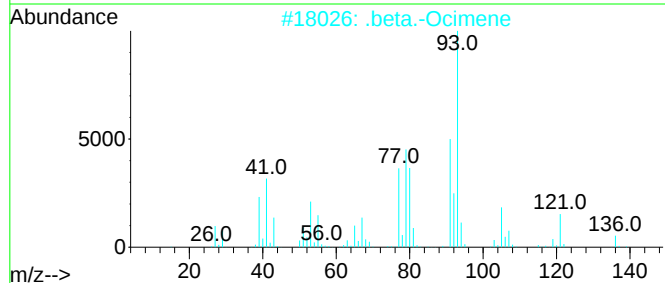
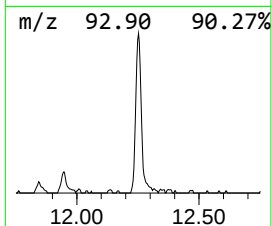
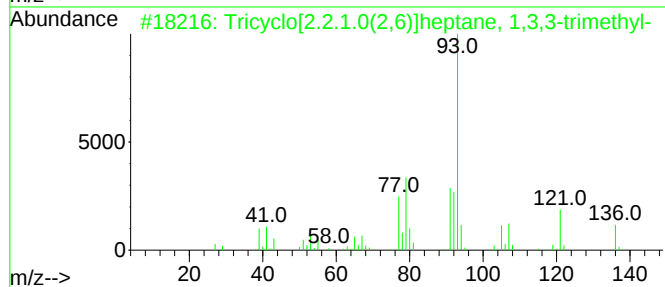
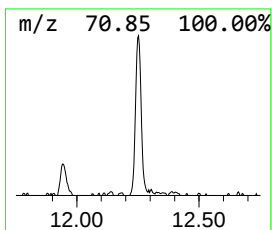
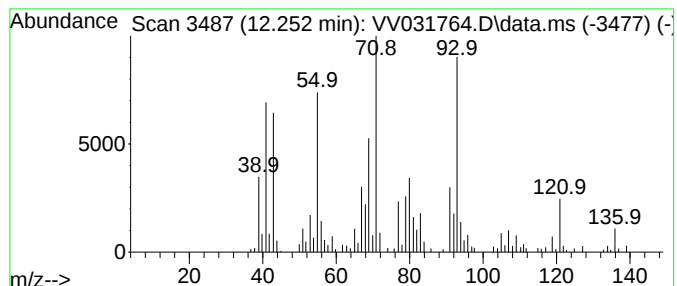
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Tricyclo[2.2.1.0(2,6)]hepta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.252	7.61 ug/L	159608	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	87
2			.beta.-Ocimene	136	C10H16	013877-91-3	64
3			Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	60
4			Cyclopropane, 1,1-dimethyl-2-(3-...	136	C10H16	068998-21-0	60
5			3-Carene	136	C10H16	013466-78-9	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031764.D
Acq On : 26 Jul 2023 13:15
Operator : SY/MD
Sample : 03712-08
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y5

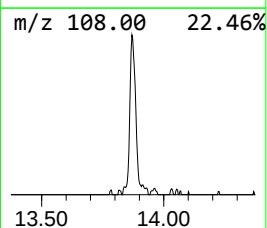
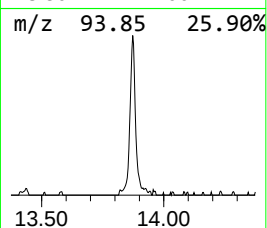
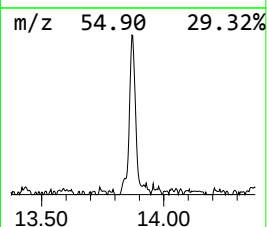
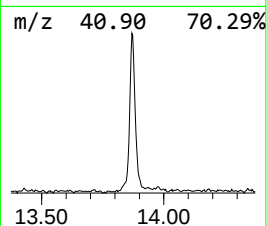
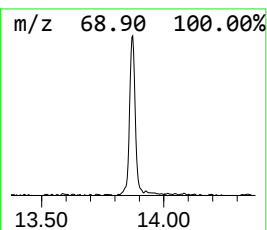
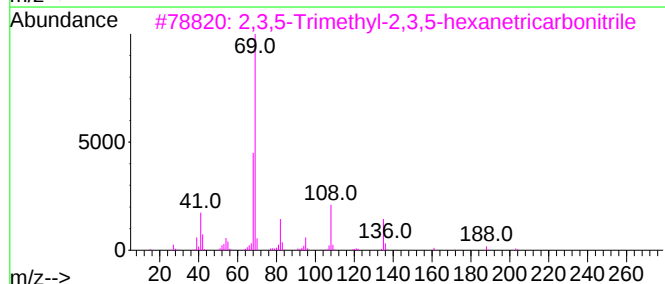
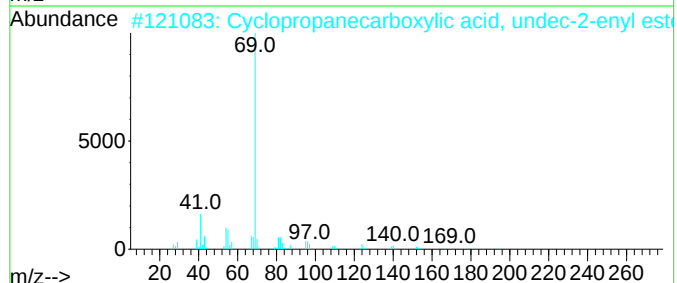
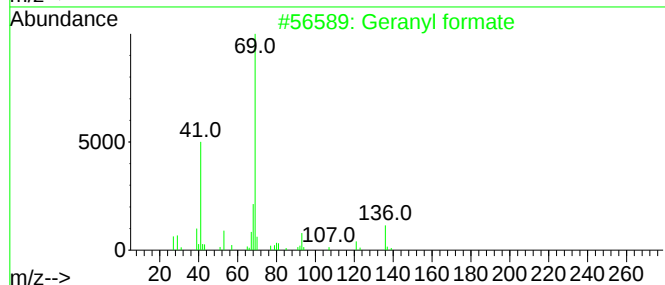
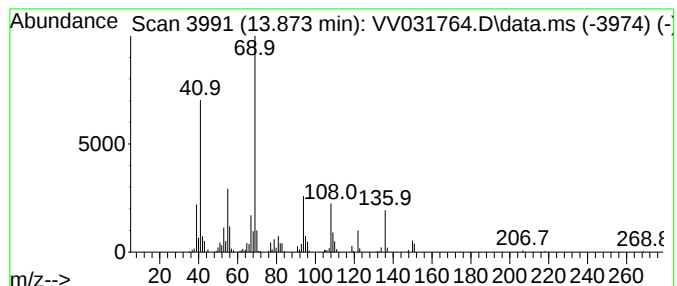
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	9.98 ug/L	209130	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Geranyl formate	182	C11H18O2	000105-86-2	43
2			Cyclopropanecarboxylic acid, und...	238	C15H26O2	1000299-38-1	38
3			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	38
4			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	38
5			2-Octene, 2-methyl-6-methylene-	138	C10H18	010054-09-8	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072623\
Data File : VV031764.D
Acq On : 26 Jul 2023 13:15
Operator : SY/MD
Sample : 03712-08
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Y5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.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
Acetic acid, cy...	2.568	6.7	ug/L	117148	1	5.539	879597	50.0
2-Butanone, 3,3...	6.510	7.8	ug/L	136733	1	5.539	879597	50.0
7-Octen-2-ol, 2...	11.944	11.9	ug/L	249728	3	11.191	1048230	50.0
Tricyclo[2.2.1....	12.252	7.6	ug/L	159608	3	11.191	1048230	50.0
unknown-01	13.873	10.0	ug/L	209130	3	11.191	1048230	50.0