

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV061520\
 Data File : VV016932.D
 Acq On : 15 Jun 2020 13:28
 Operator : SY/MD
 Sample : L2947-01DL 20X
 Misc : 5.0mL/MSVOA V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXE0DL

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.312	63	69	80	rVB	172268	181827	13.32%	1.497%
2	2.110	309	317	334	rVB2	265957	406771	29.81%	3.350%
3	2.293	371	374	378	rBV6	2242	2143	0.16%	0.018%
4	2.595	466	468	471	rBV4	1438	962	0.07%	0.008%
5	2.872	550	554	555	rBV3	1358	719	0.05%	0.006%
6	2.888	557	559	562	rBV4	1761	895	0.07%	0.007%
7	2.968	582	584	587	rBV4	1330	747	0.05%	0.006%
8	3.010	595	597	599	rBV3	1173	461	0.03%	0.004%
9	3.045	606	608	609	rBV2	1106	371	0.03%	0.003%
10	3.119	629	631	632	rBV2	889	335	0.02%	0.003%
11	3.206	644	658	676	rBV	109291	230361	16.88%	1.897%
12	3.444	729	732	735	rBV3	1636	1466	0.11%	0.012%
13	3.540	760	762	765	rBV4	1240	624	0.05%	0.005%
14	3.582	770	775	777	rBV4	1656	1175	0.09%	0.010%
15	3.685	805	807	811	rBV4	1103	835	0.06%	0.007%
16	3.720	815	818	820	rBV3	1578	991	0.07%	0.008%
17	3.788	837	839	841	rVB2	1499	682	0.05%	0.006%
18	3.846	855	857	863	rBV6	1485	1610	0.12%	0.013%
19	3.900	863	874	897	rBV	100110	281287	20.61%	2.316%
20	4.273	988	990	992	rBV3	2377	1372	0.10%	0.011%
21	4.370	1002	1020	1039	rBV	220956	543645	39.84%	4.477%
22	4.630	1086	1101	1124	rVB	427408	1048600	76.85%	8.635%
23	4.888	1177	1181	1182	rBV4	1242	849	0.06%	0.007%
24	4.978	1208	1209	1210	rBV	663	200	0.01%	0.002%
25	5.068	1220	1237	1262	rBV2	536016	1364563	100.00%	11.237%
26	5.585	1395	1398	1400	rBV4	1678	1029	0.08%	0.008%
27	5.637	1401	1414	1438	rVV	434500	856955	62.80%	7.057%
28	5.926	1492	1504	1519	rBV5	26440	58140	4.26%	0.479%
29	6.093	1543	1556	1575	rBV	303488	608147	44.57%	5.008%
30	6.434	1661	1662	1663	rBV2	1015	327	0.02%	0.003%
31	6.489	1677	1679	1683	rBV4	1246	640	0.05%	0.005%
32	6.611	1715	1717	1718	rBV2	1033	377	0.03%	0.003%
33	6.849	1789	1791	1795	rVB4	1523	1176	0.09%	0.010%
34	6.878	1795	1800	1801	rBV4	1504	1307	0.10%	0.011%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV061520\
 Data File : VV016932.D
 Acq On : 15 Jun 2020 13:28
 Operator : SY/MD
 Sample : L2947-01DL 20X
 Misc : 5.0mL/MSVOA V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXE0DL

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
 Title : VOC Analysis

35	6.961	1813	1826	1829	rBV8	5832	10598	0.78%	0.087%
36	7.006	1831	1840	1857	rVB	180878	319938	23.45%	2.635%
37	7.338	1931	1943	1959	rBV	633533	1092864	80.09%	9.000%
38	7.553	2008	2010	2017	rVB7	2170	2117	0.16%	0.017%
39	7.585	2017	2020	2021	rBV3	2070	1066	0.08%	0.009%
40	7.640	2027	2037	2061	rBV	131266	225718	16.54%	1.859%
41	7.948	2131	2133	2135	rVB3	950	296	0.02%	0.002%
42	7.997	2146	2148	2150	rBV2	1422	701	0.05%	0.006%
43	8.058	2162	2167	2170	rBV7	1521	1576	0.12%	0.013%
44	8.112	2173	2184	2214	rBV2	285536	635186	46.55%	5.231%
45	8.463	2291	2293	2296	rBV3	1159	625	0.05%	0.005%
46	8.624	2341	2343	2347	rVB4	1372	885	0.06%	0.007%
47	8.746	2378	2381	2384	rBV3	2230	1494	0.11%	0.012%
48	8.874	2406	2421	2445	rBV	639435	1055034	77.32%	8.688%
49	9.405	2582	2586	2589	rBV5	1637	1480	0.11%	0.012%
50	9.450	2596	2600	2602	rBV5	1447	1281	0.09%	0.011%
51	9.485	2609	2611	2614	rVB3	1949	860	0.06%	0.007%
52	9.637	2656	2658	2660	rVB3	1457	631	0.05%	0.005%
53	9.669	2665	2668	2669	rBV3	1192	673	0.05%	0.006%
54	9.752	2686	2694	2706	rBV	66383	105748	7.75%	0.871%
55	9.916	2741	2745	2746	rBV3	1539	1042	0.08%	0.009%
56	10.164	2820	2822	2824	rVB2	648	201	0.01%	0.002%
57	10.177	2824	2826	2827	rBV2	1349	723	0.05%	0.006%
58	10.238	2833	2845	2860	rBV	386411	619888	45.43%	5.105%
59	10.505	2916	2928	2941	rBV	130171	224696	16.47%	1.850%
60	10.794	3015	3018	3021	rBV5	1572	1104	0.08%	0.009%
61	11.064	3096	3102	3105	rBV6	1760	2165	0.16%	0.018%
62	11.109	3114	3116	3119	rBV3	1377	865	0.06%	0.007%
63	11.270	3155	3166	3181	rBV	695666	1061055	77.76%	8.738%
64	11.444	3218	3220	3221	rBV2	1433	581	0.04%	0.005%
65	11.559	3248	3256	3262	rBV10	7869	11749	0.86%	0.097%
66	11.646	3271	3283	3301	rBV	709127	1131208	82.90%	9.315%
67	11.890	3356	3359	3365	rBV7	1079	1472	0.11%	0.012%
68	11.948	3374	3377	3381	rBV6	1236	1104	0.08%	0.009%
69	12.029	3400	3402	3403	rBV2	1260	640	0.05%	0.005%
70	12.071	3412	3415	3416	rBV3	1686	1129	0.08%	0.009%
71	12.096	3421	3423	3424	rBV2	878	292	0.02%	0.002%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV061520\
 Data File : VV016932.D
 Acq On : 15 Jun 2020 13:28
 Operator : SY/MD
 Sample : L2947-01DL 20X
 Misc : 5.0mL/MSVOA V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXEODL

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
 Title : VOC Analysis

72	12.199	3452	3455	3459	rBV5	1539	1050	0.08%	0.009%
73	12.222	3459	3462	3464	rBV3	1366	777	0.06%	0.006%
74	12.251	3469	3471	3472	rBV2	844	307	0.02%	0.003%
75	12.321	3491	3493	3494	rBV2	974	527	0.04%	0.004%
76	12.437	3525	3529	3533	rVB5	1766	1727	0.13%	0.014%
77	12.495	3543	3547	3552	rVB6	2544	2049	0.15%	0.017%
78	12.517	3552	3554	3556	rBV2	539	279	0.02%	0.002%
79	12.530	3556	3558	3560	rVB3	1084	402	0.03%	0.003%
80	12.543	3560	3562	3566	rBV4	1245	723	0.05%	0.006%
81	12.894	3669	3671	3674	rBV3	1444	1100	0.08%	0.009%
82	12.964	3690	3693	3695	rBV3	2036	1501	0.11%	0.012%
83	13.167	3753	3756	3761	rBV6	2092	1629	0.12%	0.013%
84	13.341	3809	3810	3814	rBV4	1071	796	0.06%	0.007%
85	13.389	3823	3825	3828	rBV2	1413	889	0.07%	0.007%
86	13.511	3860	3863	3864	rBV3	807	367	0.03%	0.003%
87	13.521	3864	3866	3868	rBV3	1731	968	0.07%	0.008%
88	13.768	3941	3943	3944	rBV2	1125	455	0.03%	0.004%
89	14.267	4096	4098	4100	rBV3	1319	776	0.06%	0.006%
90	14.305	4106	4110	4111	rBV4	1594	1096	0.08%	0.009%
91	14.386	4133	4135	4138	rVB4	1520	852	0.06%	0.007%
92	14.427	4146	4148	4153	rBV5	1062	744	0.05%	0.006%
93	14.521	4175	4177	4182	rBV3	1425	1381	0.10%	0.011%
94	14.611	4198	4205	4207	rBV6	1675	2576	0.19%	0.021%
95	14.685	4226	4228	4229	rBV2	1118	344	0.03%	0.003%

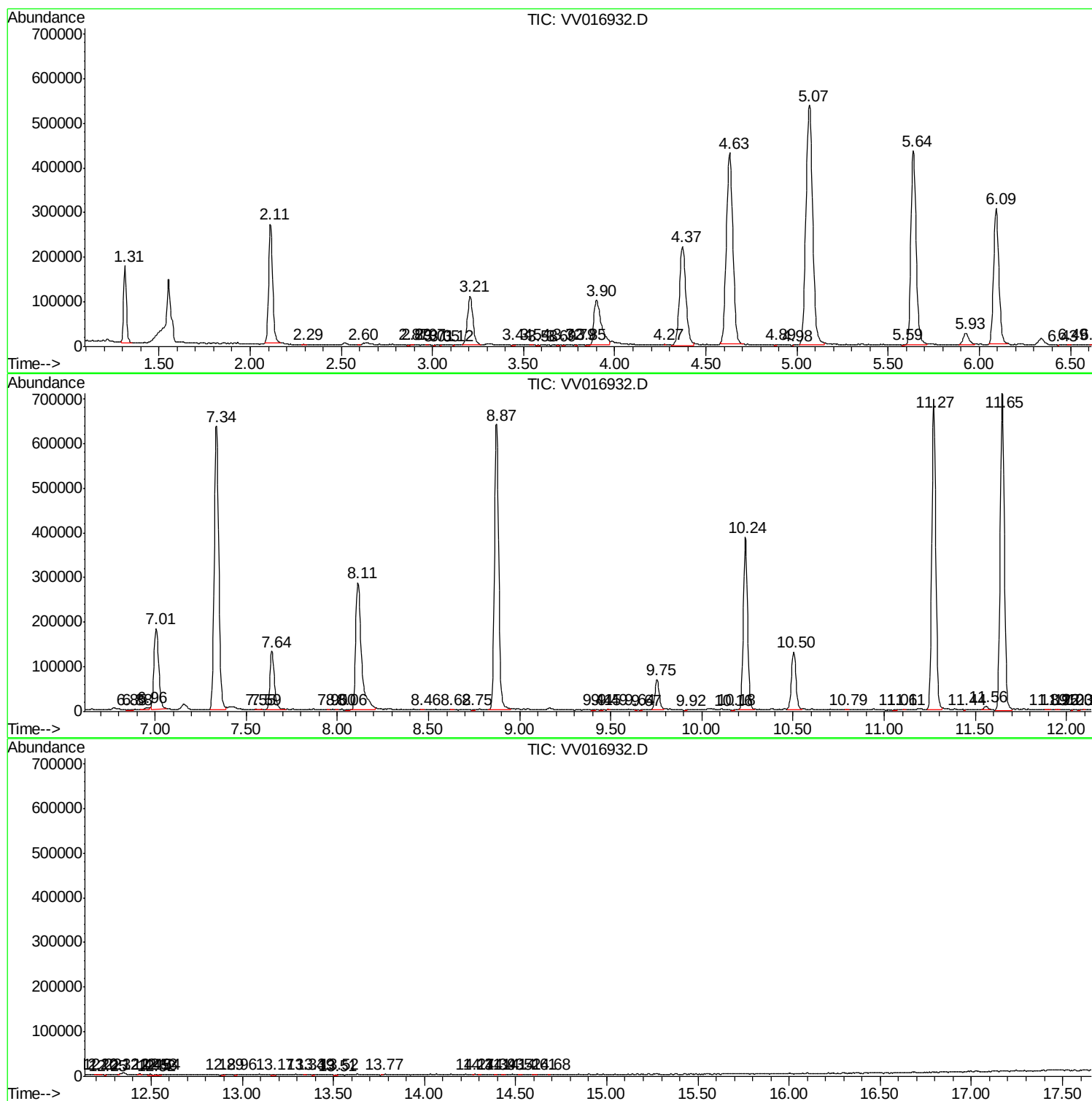
Sum of corrected areas: 12143589

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV061520\
Data File : VV016932.D
Acq On : 15 Jun 2020 13:28
Operator : SY/MD
Sample : L2947-01DL 20X
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFXEODL

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV061520\
Data File : VV016932.D
Acq On : 15 Jun 2020 13:28
Operator : SY/MD
Sample : L2947-01DL 20X
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFXE0DL

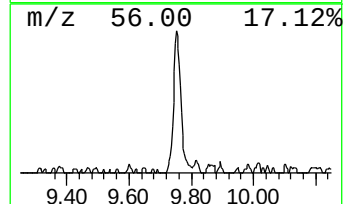
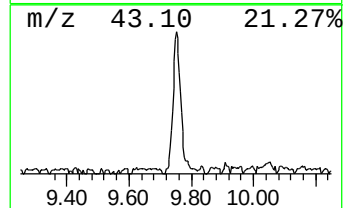
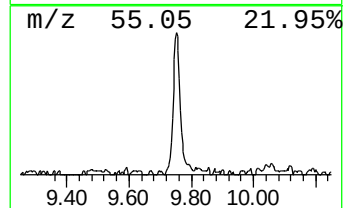
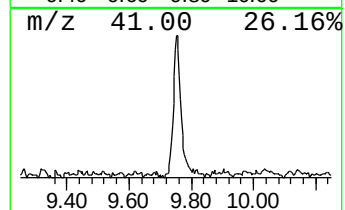
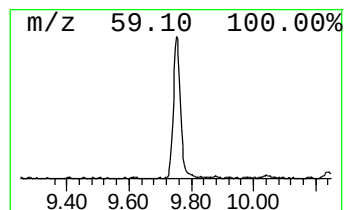
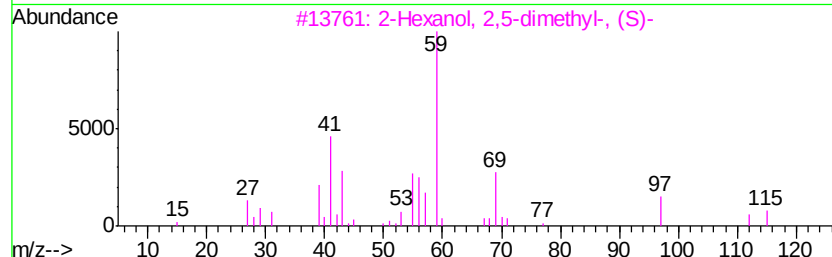
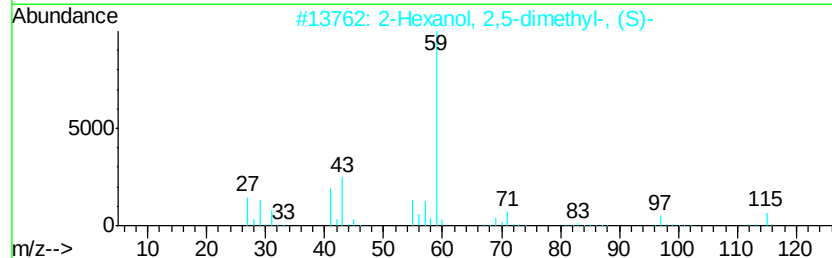
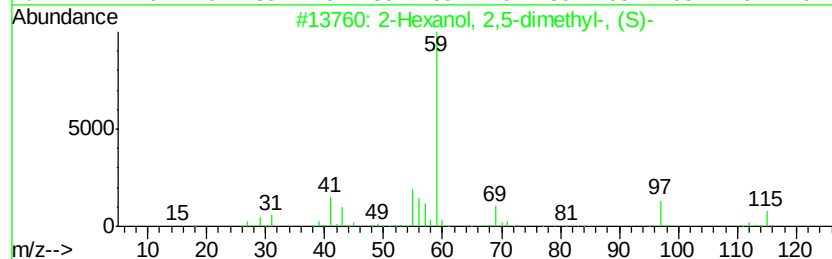
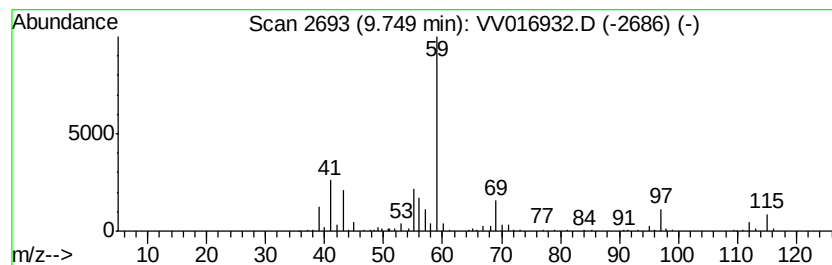
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	5.01 ug/L	105748	Chlorobenzene-d5	8.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	90
2			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	72
3			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	50
4			Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	50
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV061520\
Data File : VV016932.D
Acq On : 15 Jun 2020 13:28
Operator : SY/MD
Sample : L2947-01DL 20X
Misc : 5.0mL/MSVOA V/WATER
ALS Vial : 9 Sample Multiplier: 1

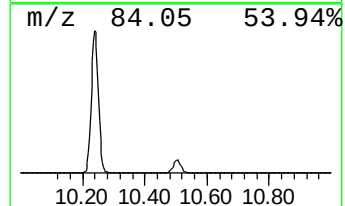
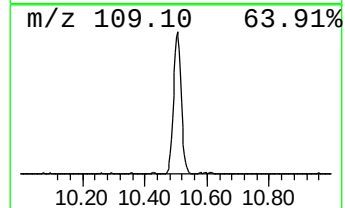
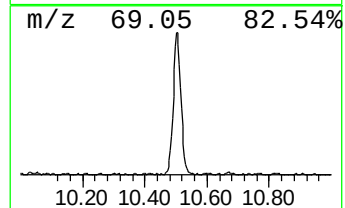
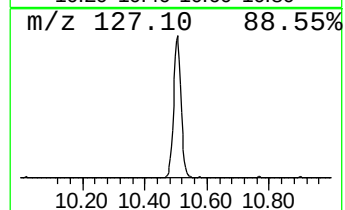
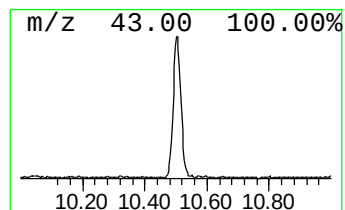
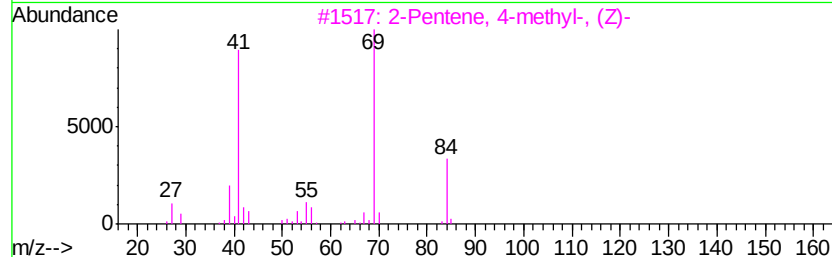
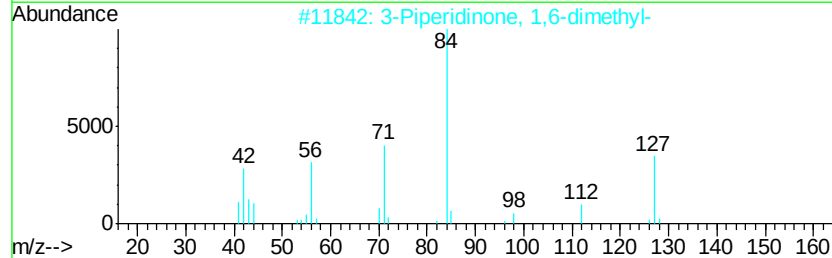
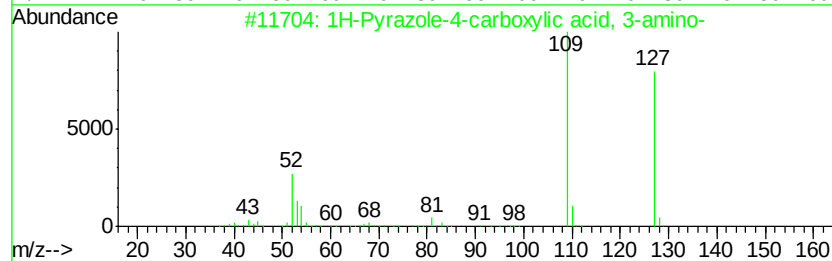
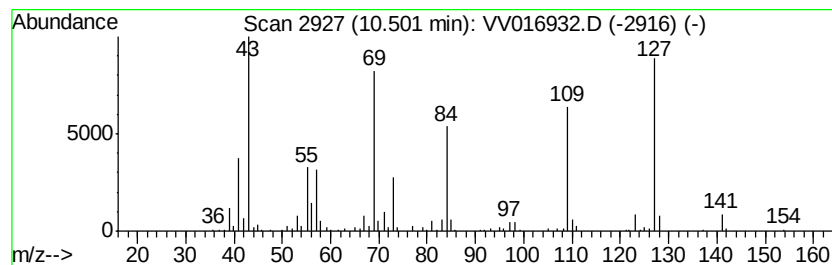
Instrument :
MSVOA_V
ClientSampleId :
BFXE0DL

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	10.59 ug/L	224696	1,4-Dichlorobenzene-d4	11.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1H-Pyrazole-4-carboxylic acid, 3...	127 C4H5N3O2	041680-34-6 35
2		3-Piperidinone, 1,6-dimethyl-	127 C7H13NO	043152-92-7 27
3		2-Pentene, 4-methyl-, (Z)-	84 C6H12	000691-38-3 27
4		1H-Pyrazole, 4,5-dihydro-5-methyl-	84 C4H8N2	001568-20-3 27
5		5,6-Dihydropyran-2-one, 5-acetox...	212 C10H12O5	069651-04-3 25



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_V\DATA\VV061520\
Data File : VV016932.D
Acq On : 15 Jun 2020 13:28
Operator : SY/MD
Sample : L2947-01DL 20X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFXE0DL

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM060820WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Hexanol, 2,5-di...	9.75	5.0	ug/L	105748	2	8.87	1055030	50.0
unknown-01	10.50	10.6	ug/L	224696	3	11.27	1061060	50.0