

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060619\
 Data File : VU032522.D
 Acq On : 07 Jun 2019 01:44
 Operator : JC/SP
 Sample : K3215-11
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB8J5

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_U\METHOD\SOMULM060619WMA.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	1.392	88	94	109	rVB	60451	65556	10.38%	1.176%
2	1.675	175	182	199	rVB	55950	68745	10.88%	1.234%
3	2.267	357	366	378	rVB	107853	162246	25.69%	2.911%
4	2.765	516	521	524	rBV2	194	215	0.03%	0.004%
5	2.981	578	588	602	rBV	11578	21085	3.34%	0.378%
6	3.145	637	639	642	rVB	204	134	0.02%	0.002%
7	3.180	642	650	660	rBV5	1034	2101	0.33%	0.038%
8	3.334	694	698	702	rBV	238	153	0.02%	0.003%
9	3.473	737	741	744	rBV	242	198	0.03%	0.004%
10	3.621	782	787	789	rBV	262	151	0.02%	0.003%
11	3.855	850	860	862	rBV2	241	311	0.05%	0.006%
12	3.926	875	882	886	rBV2	306	346	0.05%	0.006%
13	4.003	895	906	920	rBV5	2968	8125	1.29%	0.146%
14	4.174	943	959	962	rBV	69193	123391	19.54%	2.214%
15	4.640	1088	1104	1132	rBV	101518	238217	37.71%	4.274%
16	4.875	1175	1177	1178	rBV	370	152	0.02%	0.003%
17	5.116	1248	1252	1255	rBV	234	165	0.03%	0.003%
18	5.334	1298	1320	1356	rBV2	201314	623065	98.64%	11.180%
19	5.534	1379	1382	1385	rVB2	195	123	0.02%	0.002%
20	5.659	1418	1421	1426	rVB2	349	261	0.04%	0.005%
21	5.756	1446	1451	1452	rBV2	286	218	0.03%	0.004%
22	5.881	1477	1490	1514	rBV	224083	437472	69.26%	7.850%
23	6.180	1571	1583	1601	rBV	106068	209472	33.16%	3.759%
24	6.325	1614	1628	1649	rBV	139489	276198	43.73%	4.956%
25	6.521	1686	1689	1693	rBV	426	269	0.04%	0.005%
26	6.543	1693	1696	1699	rVB2	238	185	0.03%	0.003%
27	6.624	1718	1721	1722	rBV2	242	139	0.02%	0.002%
28	6.784	1767	1771	1774	rBV2	258	252	0.04%	0.005%
29	6.820	1779	1782	1783	rBV	192	118	0.02%	0.002%
30	6.871	1794	1798	1799	rBV	227	162	0.03%	0.003%
31	6.948	1819	1822	1825	rBV	168	153	0.02%	0.003%
32	6.984	1830	1833	1836	rVB	220	145	0.02%	0.003%
33	7.013	1837	1842	1844	rBV2	190	186	0.03%	0.003%
34	7.074	1858	1861	1874	rBV	490	734	0.12%	0.013%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060619\
 Data File : VU032522.D
 Acq On : 07 Jun 2019 01:44
 Operator : JC/SP
 Sample : K3215-11
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB8J5

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_U\METHOD\SOMULM060619WMA.M
 Title : VOC Analysis

35	7.148	1880	1884	1886	rBV2	191	127	0.02%	0.002%
36	7.225	1895	1908	1925	rBV	76175	139621	22.10%	2.505%
37	7.431	1967	1972	1975	rBV	374	393	0.06%	0.007%
38	7.469	1982	1984	1991	rVB4	615	520	0.08%	0.009%
39	7.505	1991	1995	2000	rBV2	455	476	0.08%	0.009%
40	7.559	2000	2012	2032	rBV	268617	469429	74.32%	8.423%
41	7.846	2092	2101	2129	rVB	51205	89276	14.13%	1.602%
42	8.045	2159	2163	2164	rBV2	315	181	0.03%	0.003%
43	8.128	2183	2189	2190	rBV2	255	158	0.03%	0.003%
44	8.225	2211	2219	2229	rBV2	8173	12780	2.02%	0.229%
45	8.305	2234	2244	2278	rBV	213692	386474	61.19%	6.935%
46	8.624	2341	2343	2345	rBV	351	166	0.03%	0.003%
47	8.662	2352	2355	2363	rBV2	187	220	0.03%	0.004%
48	8.752	2380	2383	2386	rBV2	185	134	0.02%	0.002%
49	8.836	2404	2409	2413	rBV2	253	238	0.04%	0.004%
50	8.858	2413	2416	2420	rBV2	167	141	0.02%	0.003%
51	8.884	2420	2424	2429	rBV2	216	286	0.05%	0.005%
52	9.083	2474	2486	2509	rBV2	329825	631639	100.00%	11.334%
53	9.257	2537	2540	2542	rBV	281	146	0.02%	0.003%
54	9.302	2552	2554	2558	rVB	197	134	0.02%	0.002%
55	9.325	2558	2561	2562	rBV	250	172	0.03%	0.003%
56	9.447	2594	2599	2602	rBV2	231	217	0.03%	0.004%
57	9.604	2646	2648	2651	rBV	195	163	0.03%	0.003%
58	9.656	2661	2664	2667	rVB2	200	157	0.02%	0.003%
59	9.672	2667	2669	2675	rVB2	154	176	0.03%	0.003%
60	9.842	2720	2722	2728	rVB2	277	312	0.05%	0.006%
61	9.874	2728	2732	2735	rVB	210	171	0.03%	0.003%
62	9.907	2739	2742	2746	rBV2	191	181	0.03%	0.003%
63	9.952	2753	2756	2760	rBV2	188	174	0.03%	0.003%
64	10.032	2777	2781	2786	rBV2	169	210	0.03%	0.004%
65	10.170	2819	2824	2830	rVB	952	942	0.15%	0.017%
66	10.222	2835	2840	2843	rBV2	239	196	0.03%	0.004%
67	10.247	2845	2848	2853	rBV	191	141	0.02%	0.003%
68	10.360	2880	2883	2887	rBV	142	121	0.02%	0.002%
69	10.427	2891	2904	2925	rBV	219659	348939	55.24%	6.261%
70	10.550	2939	2942	2946	rBV3	279	241	0.04%	0.004%
71	10.598	2948	2957	2967	rVB4	1308	2436	0.39%	0.044%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU060619\
 Data File : VU032522.D
 Acq On : 07 Jun 2019 01:44
 Operator : JC/SP
 Sample : K3215-11
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB8J5

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_U\METHOD\SOMULM060619WMA.M
 Title : VOC Analysis

72	10.649	2970	2973	2975	rBV	163	120	0.02%	0.002%
73	10.681	2978	2983	2994	rBV3	2120	3136	0.50%	0.056%
74	11.054	3092	3099	3103	rBV2	203	298	0.05%	0.005%
75	11.099	3109	3113	3120	rVB3	355	415	0.07%	0.007%
76	11.148	3120	3128	3142	rVB3	3621	5844	0.93%	0.105%
77	11.215	3146	3149	3152	rVB2	228	120	0.02%	0.002%
78	11.234	3152	3155	3157	rBV	462	376	0.06%	0.007%
79	11.318	3176	3181	3182	rBV2	484	412	0.07%	0.007%
80	11.421	3205	3213	3220	rBV4	1717	2374	0.38%	0.043%
81	11.479	3220	3231	3254	rBV	344065	565693	89.56%	10.150%
82	11.726	3307	3308	3311	rVB2	439	186	0.03%	0.003%
83	11.765	3311	3320	3331	rBV5	4332	7455	1.18%	0.134%
84	11.855	3335	3348	3368	rBV	308380	543007	85.97%	9.743%
85	12.299	3483	3486	3487	rBV	199	123	0.02%	0.002%
86	12.318	3490	3492	3494	rBV	286	182	0.03%	0.003%
87	12.347	3499	3501	3503	rBV2	396	193	0.03%	0.003%
88	12.363	3504	3506	3509	rBV4	651	432	0.07%	0.008%
89	12.437	3526	3529	3535	rBV3	290	276	0.04%	0.005%
90	12.482	3538	3543	3546	rBV3	520	500	0.08%	0.009%
91	12.665	3591	3600	3608	rBV7	2075	4425	0.70%	0.079%
92	12.942	3683	3686	3689	rBV2	330	221	0.03%	0.004%
93	13.167	3750	3756	3763	rVB6	1669	2060	0.33%	0.037%
94	13.292	3792	3795	3796	rBV	323	173	0.03%	0.003%
95	13.443	3836	3842	3849	rBV6	922	1248	0.20%	0.022%
96	13.492	3849	3857	3863	rBV4	2010	3159	0.50%	0.057%
97	13.611	3886	3894	3898	rBV2	7365	10835	1.72%	0.194%
98	13.984	4002	4010	4020	rVB2	10469	15793	2.50%	0.283%
99	14.511	4166	4174	4186	rVB	20695	32177	5.09%	0.577%
100	14.842	4267	4277	4288	rBV3	24267	43947	6.96%	0.789%

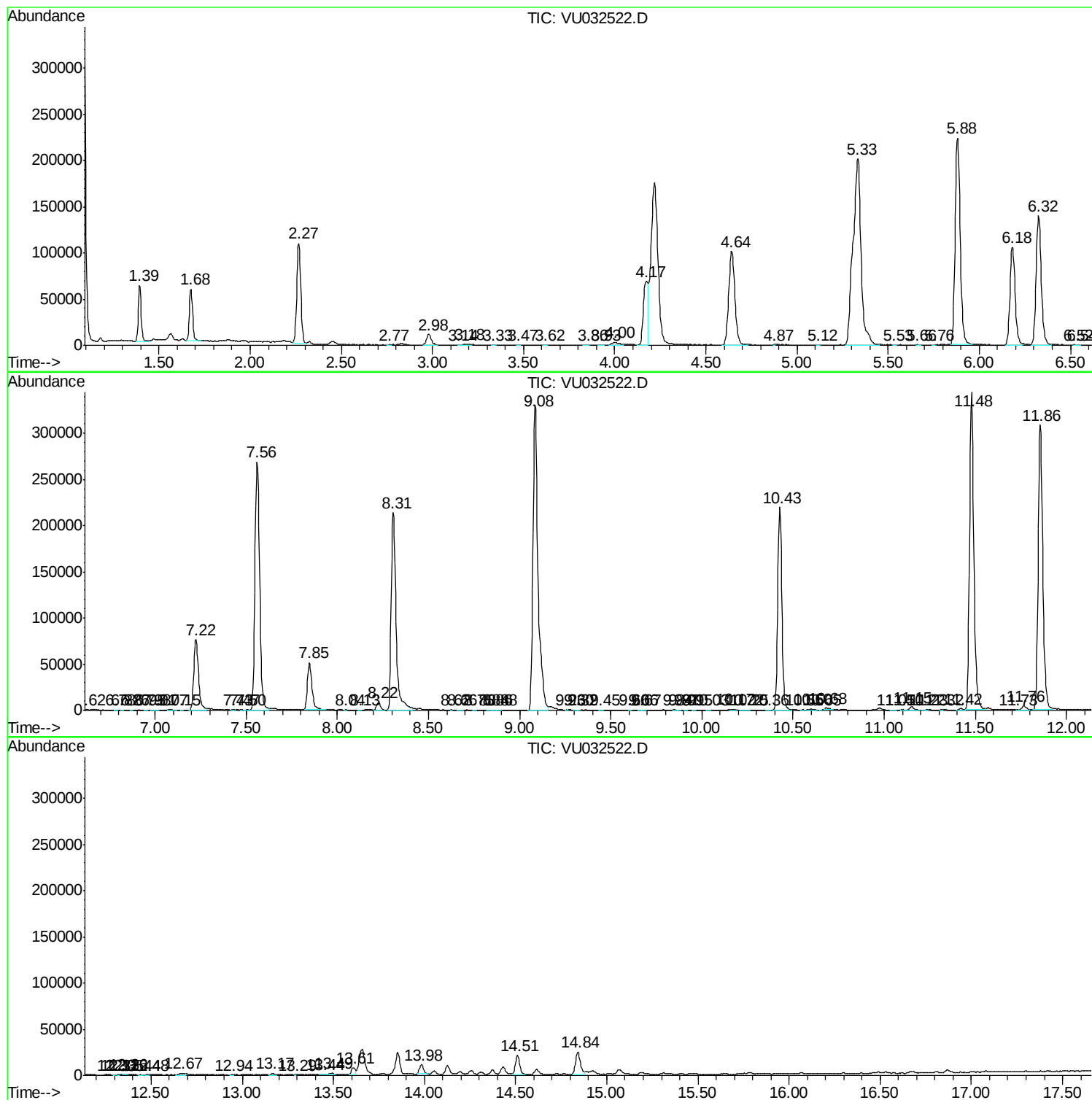
Sum of corrected areas: 5573111

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU060619\
Data File : VU032522.D
Acq On : 07 Jun 2019 01:44
Operator : JC/SP
Sample : K3215-11
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB8J5

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU060619\
Data File : VU032522.D
Acq On : 07 Jun 2019 01:44
Operator : JC/SP
Sample : K3215-11
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB8J5

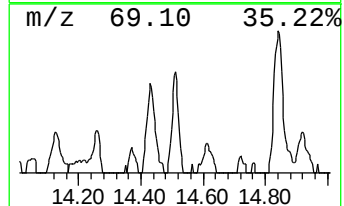
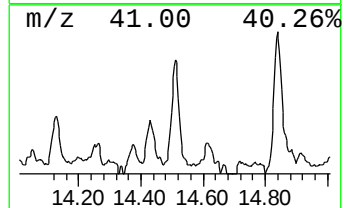
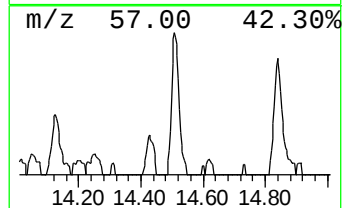
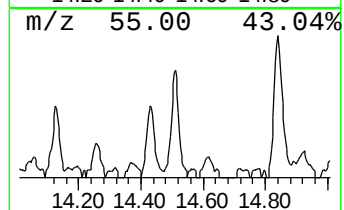
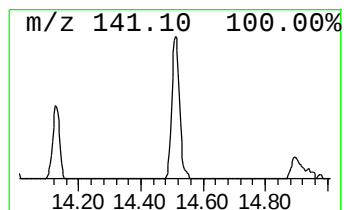
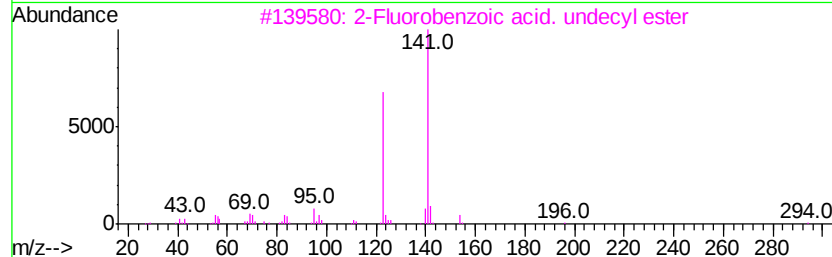
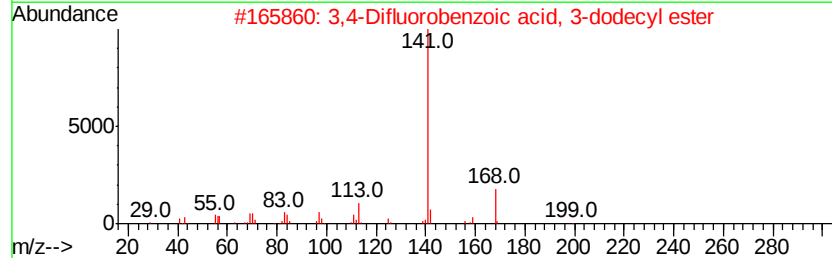
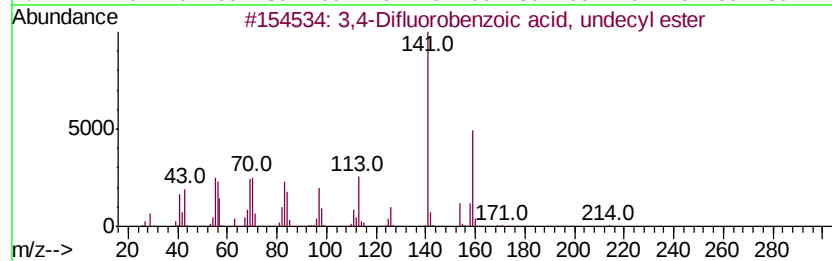
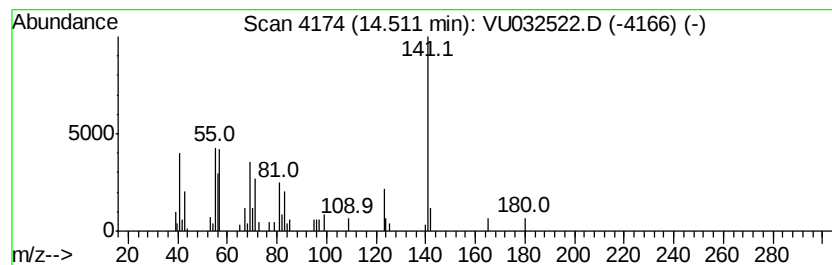
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.84 ug/L	32177	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,4-Difluorobenzoic acid, undecyl...	312	C18H26F2O2	1000338-86-7	42
2		3,4-Difluorobenzoic acid, 3-dode...	326	C19H28F2O2	1000338-59-6	42
3		2-Fluorobenzoic acid, undecyl ester	294	C18H27FO2	1000282-96-3	40
4		2-Fluorobenzoic acid, heptadecyl...	378	C24H39FO2	1000282-96-6	40
5		3,4-Difluorobenzoic acid, 5-dode...	326	C19H28F2O2	1000338-59-8	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU060619\
Data File : VU032522.D
Acq On : 07 Jun 2019 01:44
Operator : JC/SP
Sample : K3215-11
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB8J5

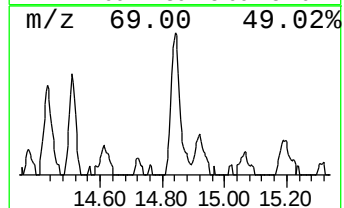
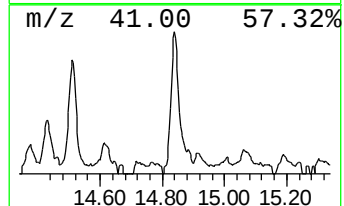
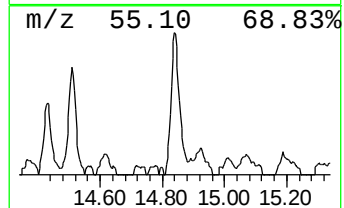
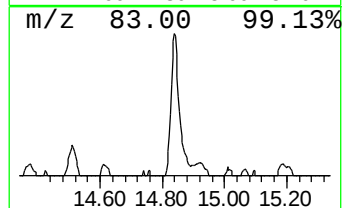
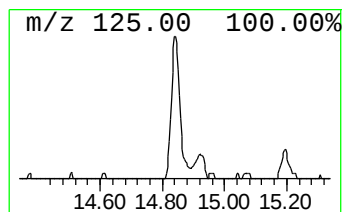
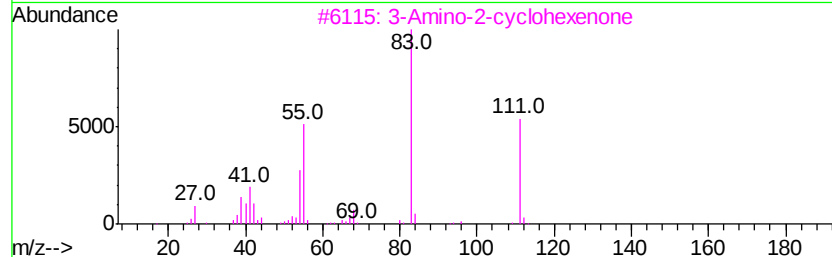
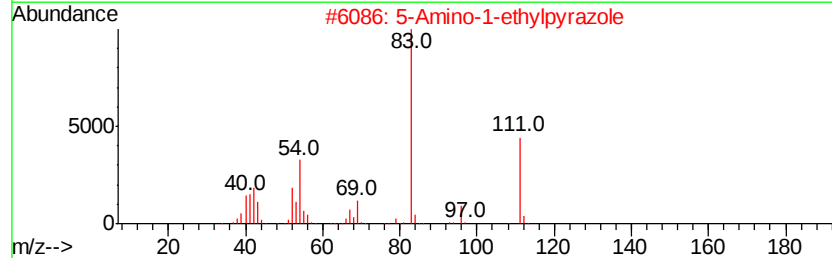
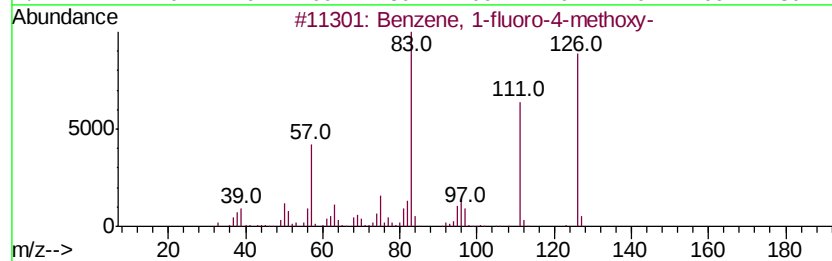
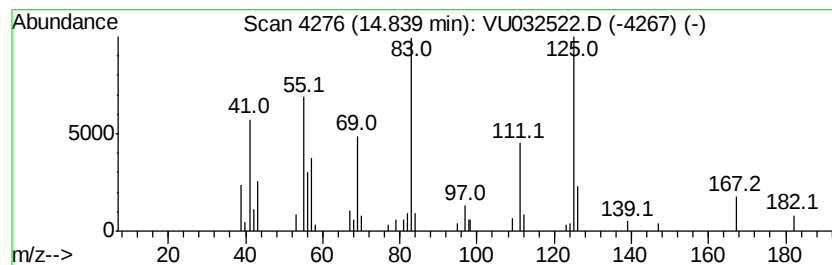
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	3.88 ug/L	43947	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-fluoro-4-methoxy-	126	C7H7FO	000459-60-9	35
2		5-Amino-1-ethylpyrazole	111	C5H9N3	003528-58-3	30
3		3-Amino-2-cyclohexenone	111	C6H9NO	005220-49-5	30
4		5-Amino-1-ethylpyrazole	111	C5H9N3	003528-58-3	30
5		Cyclohexane, propyl-	126	C9H18	001678-92-8	27



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU060619\
Data File : VU032522.D
Acq On : 07 Jun 2019 01:44
Operator : JC/SP
Sample : K3215-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB8J5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM060619WMA.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
unknown-01	14.51	2.8	ug/L	32177	3	11.48	565693	50.0
unknown-02	14.84	3.9	ug/L	43947	3	11.48	565693	50.0