

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045235.D
 Acq On : 08 Oct 2021 02:15
 Operator : SY/MD
 Sample : M4027-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AT7

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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045235.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.465	31	39	54	rBV	109050	183071	0.72%	0.338%
2	1.600	75	81	98	rVB2	219369	252545	0.99%	0.467%
3	1.893	164	172	185	rVB	130140	175142	0.69%	0.324%
4	2.562	368	380	397	rBV2	257990	447808	1.76%	0.828%
5	2.793	442	452	460	rBV3	1303	2239	0.01%	0.004%
6	2.874	473	477	483	rBV2	282	393	0.00%	0.001%
7	2.957	489	503	511	rBV2	484	1118	0.00%	0.002%
8	3.189	565	575	588	rBV3	1566	3427	0.01%	0.006%
9	3.353	613	626	641	rVB2	41484	81944	0.32%	0.151%
10	3.440	651	653	660	rBV2	213	236	0.00%	0.000%
11	3.877	774	789	802	rBV3	3447	7344	0.03%	0.014%
12	4.192	884	887	892	rBV2	217	238	0.00%	0.000%
13	4.288	912	917	920	rBV	213	230	0.00%	0.000%
14	4.330	925	930	932	rBV2	219	215	0.00%	0.000%
15	4.668	1008	1035	1077	rBV2	1527372	3724323	14.64%	6.884%
16	4.941	1118	1120	1124	rVB4	446	252	0.00%	0.000%
17	5.067	1142	1159	1186	rVB	227008	496818	1.95%	0.918%
18	5.208	1198	1203	1205	rBV2	403	298	0.00%	0.001%
19	5.221	1205	1207	1212	rVB3	307	237	0.00%	0.000%
20	5.321	1219	1238	1251	rBV4	9915	22144	0.09%	0.041%
21	5.385	1254	1258	1262	rVB3	333	292	0.00%	0.001%
22	5.446	1274	1277	1280	rBV	299	254	0.00%	0.000%
23	5.465	1280	1283	1286	rVB	255	195	0.00%	0.000%
24	5.488	1286	1290	1296	rBV2	246	310	0.00%	0.001%
25	5.523	1296	1301	1304	rBV2	222	204	0.00%	0.000%
26	5.558	1309	1312	1319	rBV	197	281	0.00%	0.001%
27	5.629	1329	1334	1337	rBV	183	202	0.00%	0.000%
28	5.729	1342	1365	1383	rBV2	480375	1290791	5.08%	2.386%
29	5.986	1441	1445	1448	rBV2	205	208	0.00%	0.000%
30	6.166	1498	1501	1504	rBV	315	252	0.00%	0.000%
31	6.253	1514	1528	1544	rBV	384827	716397	2.82%	1.324%
32	6.549	1597	1620	1652	rBV	13890082	25431935	100.00%	47.005%
33	6.697	1655	1666	1683	rVB	304284	602639	2.37%	1.114%
34	6.967	1746	1750	1757	rVB3	291	430	0.00%	0.001%
35	6.999	1757	1760	1763	rBV3	329	264	0.00%	0.000%
36	7.050	1771	1776	1779	rBV4	508	587	0.00%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045235.D
 Acq On : 08 Oct 2021 02:15
 Operator : SY/MD
 Sample : M4027-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AT7

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\SFAMULM092321WMA.M
 Title : VOC Analysis

37	7.066	1779	1781	1787	rVB3	244	269	0.00%	0.000%
38	7.185	1809	1818	1823	rBV3	1453	2155	0.01%	0.004%
39	7.292	1848	1851	1854	rBV2	275	215	0.00%	0.000%
40	7.568	1924	1937	1956	rVV	163855	281048	1.11%	0.519%
41	7.687	1971	1974	1983	rVB5	1324	1732	0.01%	0.003%
42	7.800	2004	2009	2021	rVB4	1229	1932	0.01%	0.004%
43	7.902	2027	2041	2055	rBV	590875	1011953	3.98%	1.870%
44	7.973	2055	2063	2075	rVB	14550	24554	0.10%	0.045%
45	8.182	2115	2128	2143	rBV	117159	190694	0.75%	0.352%
46	8.311	2165	2168	2171	rVB	424	277	0.00%	0.001%
47	8.404	2190	2197	2205	rBV2	1212	1533	0.01%	0.003%
48	8.475	2210	2219	2229	rVB4	1131	1775	0.01%	0.003%
49	8.558	2229	2245	2259	rBV	8939586	14811742	58.24%	27.376%
50	8.636	2260	2269	2309	rVB	450038	845694	3.33%	1.563%
51	8.819	2323	2326	2330	rVB2	383	249	0.00%	0.000%
52	9.012	2381	2386	2392	rBV3	210	310	0.00%	0.001%
53	9.079	2403	2407	2412	rBV3	316	297	0.00%	0.001%
54	9.134	2420	2424	2429	rBV2	226	197	0.00%	0.000%
55	9.333	2484	2486	2490	rVB	327	200	0.00%	0.000%
56	9.420	2499	2513	2538	rBV	552515	895543	3.52%	1.655%
57	9.574	2550	2561	2572	rBV	9897	15158	0.06%	0.028%
58	9.616	2572	2574	2581	rVV	249	240	0.00%	0.000%
59	9.697	2587	2599	2611	rBV	29611	47914	0.19%	0.089%
60	9.764	2611	2620	2642	rVB2	12856	25790	0.10%	0.048%
61	9.851	2642	2647	2649	rBV2	287	256	0.00%	0.000%
62	10.044	2704	2707	2711	rVB	245	203	0.00%	0.000%
63	10.105	2717	2726	2737	rVB3	6969	11322	0.04%	0.021%
64	10.179	2744	2749	2754	rBV2	341	431	0.00%	0.001%
65	10.349	2799	2802	2806	rBV2	234	220	0.00%	0.000%
66	10.426	2823	2826	2829	rBV2	281	209	0.00%	0.000%
67	10.488	2839	2845	2852	rVB2	879	1151	0.00%	0.002%
68	10.523	2852	2856	2860	rBV	219	240	0.00%	0.000%
69	10.642	2887	2893	2895	rBV2	420	311	0.00%	0.001%
70	10.674	2895	2903	2910	rBV4	2435	3382	0.01%	0.006%
71	10.761	2917	2930	2948	rBV	441325	704634	2.77%	1.302%
72	10.899	2969	2973	2986	rVB4	1138	1415	0.01%	0.003%
73	11.008	3003	3007	3011	rVB2	295	209	0.00%	0.000%
74	11.060	3018	3023	3026	rBV2	228	203	0.00%	0.000%
75	11.089	3026	3032	3040	rVV3	892	1332	0.01%	0.002%
76	11.153	3046	3052	3055	rBV3	397	337	0.00%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
 Data File : VU045235.D
 Acq On : 08 Oct 2021 02:15
 Operator : SY/MD
 Sample : M4027-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AT7

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\SFAMULM092321WMA.M
 Title : VOC Analysis

77	11.211	3067	3070	3076	rVB2	240	264	0.00%	0.000%
78	11.471	3139	3151	3159	rVB8	3387	5546	0.02%	0.010%
79	11.587	3178	3187	3191	rBV3	380	616	0.00%	0.001%
80	11.703	3208	3223	3231	rBV5	1017	1865	0.01%	0.003%
81	11.751	3232	3238	3245	rVB3	1130	1462	0.01%	0.003%
82	11.815	3245	3258	3278	rBV	526145	826198	3.25%	1.527%
83	11.947	3294	3299	3301	rBV3	519	541	0.00%	0.001%
84	12.076	3326	3339	3344	rBV4	1252	2490	0.01%	0.005%
85	12.137	3351	3358	3361	rBV	269	316	0.00%	0.001%
86	12.195	3361	3376	3397	rVV	553997	892361	3.51%	1.649%
87	12.333	3414	3419	3423	rVB4	686	580	0.00%	0.001%
88	12.854	3575	3581	3585	rBV2	239	305	0.00%	0.001%
89	13.047	3638	3641	3649	rVB2	568	684	0.00%	0.001%
90	13.240	3690	3701	3710	rBV9	9781	15823	0.06%	0.029%
91	13.365	3737	3740	3743	rBV	256	219	0.00%	0.000%
92	13.520	3784	3788	3792	rBV2	307	367	0.00%	0.001%
93	13.565	3796	3802	3813	rBV2	253	622	0.00%	0.001%
94	13.848	3882	3890	3896	rVB5	2556	3615	0.01%	0.007%
95	14.002	3934	3938	3940	rBV	258	211	0.00%	0.000%
96	14.092	3956	3966	3976	rVV	8103	12869	0.05%	0.024%
97	14.156	3982	3986	3991	rBV2	349	312	0.00%	0.001%
98	14.336	4032	4042	4049	rBV4	2847	4218	0.02%	0.008%
99	14.642	4133	4137	4139	rBV2	313	280	0.00%	0.001%
100	14.889	4211	4214	4217	rBV	322	239	0.00%	0.000%

Sum of corrected areas: 54104592

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
Data File : VU045235.D
Acq On : 08 Oct 2021 02:15
Operator : SY/MD
Sample : M4027-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AT7

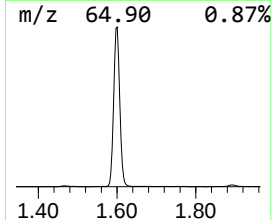
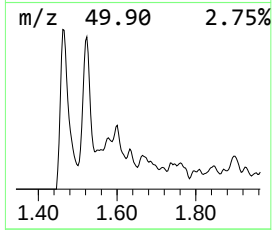
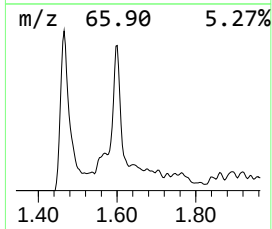
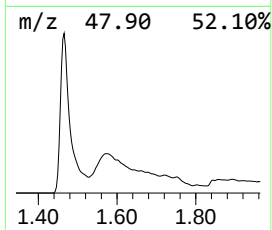
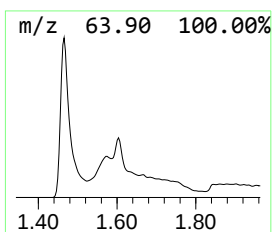
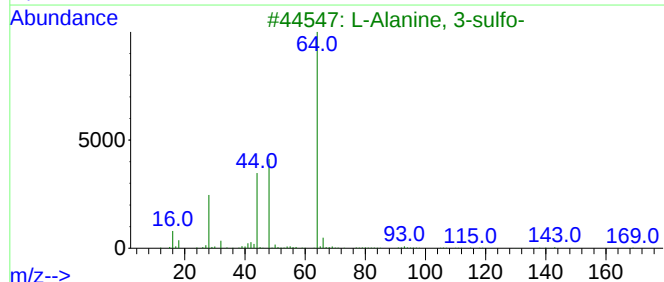
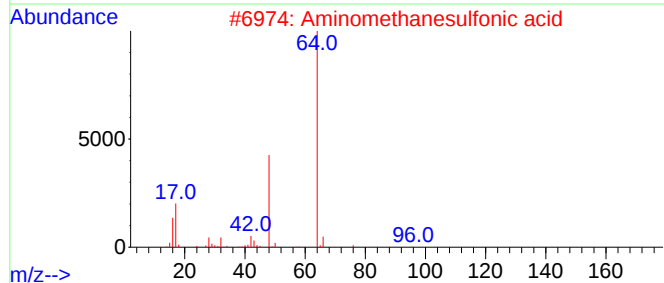
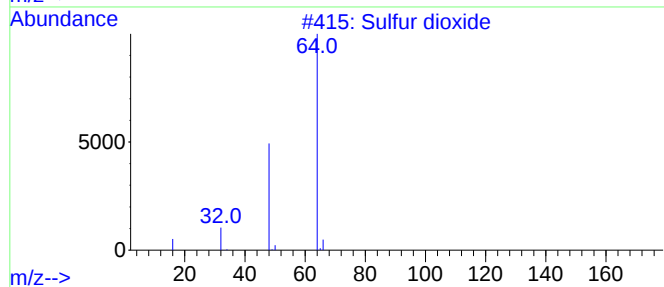
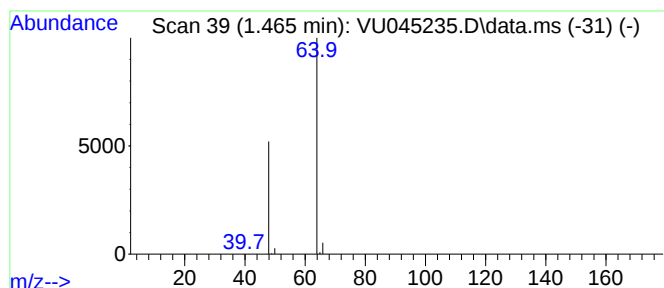
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.465	12.78 ug/L	183071	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100721\
Data File : VU045235.D
Acq On : 08 Oct 2021 02:15
Operator : SY/MD
Sample : M4027-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AT7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.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
Sulfur dioxide	1.465	12.8	ug/L	183071	1	6.253	716397	50.0