

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102523\
 Data File : VU055884.D
 Acq On : 25 Oct 2023 17:09
 Operator : MD/SY
 Sample : 04952-07
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EOAR8

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\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055884.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	49	59	76	rBV2	52805	145056	5.57%	0.720%
2	1.599	89	96	113	rVB	337116	382278	14.68%	1.898%
3	1.894	180	188	205	rVB	226658	327838	12.59%	1.628%
4	2.560	382	395	411	rBV	546350	892608	34.28%	4.432%
5	2.785	458	465	479	rVB	4022	8442	0.32%	0.042%
6	2.859	483	488	491	rBV3	459	419	0.02%	0.002%
7	2.914	501	505	508	rVB4	685	483	0.02%	0.002%
8	2.939	508	513	515	rBV3	801	616	0.02%	0.003%
9	2.956	516	518	524	rVB3	813	539	0.02%	0.003%
10	2.984	524	527	532	rBV4	542	482	0.02%	0.002%
11	3.042	535	545	557	rBV5	4261	8931	0.34%	0.044%
12	3.181	578	588	590	rBV3	3849	5703	0.22%	0.028%
13	3.261	610	613	615	rBV2	483	409	0.02%	0.002%
14	3.274	615	617	621	rVV	795	438	0.02%	0.002%
15	3.351	638	641	646	rBV3	739	553	0.02%	0.003%
16	3.695	739	748	753	rBV5	892	1414	0.05%	0.007%
17	3.955	820	829	831	rBV3	957	1166	0.04%	0.006%
18	4.303	934	937	945	rVB2	307	368	0.01%	0.002%
19	4.560	1011	1017	1020	rBV2	441	425	0.02%	0.002%
20	4.615	1020	1034	1070	rBV	193648	492506	18.92%	2.446%
21	5.058	1154	1172	1196	rBV	449806	1012434	38.88%	5.027%
22	5.322	1246	1254	1270	rVB3	6917	14599	0.56%	0.072%
23	5.390	1273	1275	1280	rVB3	863	600	0.02%	0.003%
24	5.521	1313	1316	1321	rVV3	510	407	0.02%	0.002%
25	5.721	1356	1378	1419	rBV2	943578	2603721	100.00%	12.929%
26	5.968	1453	1455	1460	rBV4	553	472	0.02%	0.002%
27	6.245	1527	1541	1563	rBV	694669	1350542	51.87%	6.706%
28	6.486	1614	1616	1619	rBV2	600	433	0.02%	0.002%
29	6.518	1619	1626	1627	rBV5	2617	2091	0.08%	0.010%
30	6.586	1642	1647	1651	rBV3	1579	1929	0.07%	0.010%
31	6.685	1662	1678	1700	rBV	570611	1130394	43.41%	5.613%
32	7.000	1772	1776	1779	rVB	597	393	0.02%	0.002%
33	7.132	1810	1817	1821	rBV3	944	1089	0.04%	0.005%
34	7.187	1823	1834	1849	rBV5	6189	14482	0.56%	0.072%
35	7.396	1896	1899	1903	rVB3	607	487	0.02%	0.002%
36	7.560	1938	1950	1971	rBV2	313111	567923	21.81%	2.820%

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 Title : VOC Analysis

37	7.759	2009	2012	2016	rVB5	858	628	0.02%	0.003%
38	7.795	2020	2023	2028	rVB5	797	609	0.02%	0.003%
39	7.894	2040	2054	2096	rBV	1205759	2101386	80.71%	10.435%
40	8.113	2120	2122	2126	rVB2	747	427	0.02%	0.002%
41	8.177	2130	2142	2165	rBV	217915	383067	14.71%	1.902%
42	8.402	2207	2212	2220	rVB7	938	998	0.04%	0.005%
43	8.470	2225	2233	2238	rBV2	3536	5025	0.19%	0.025%
44	8.550	2249	2258	2271	rVB3	16869	30405	1.17%	0.151%
45	8.631	2271	2283	2317	rBV	700367	1337339	51.36%	6.641%
46	8.987	2392	2394	2396	rBV	616	392	0.02%	0.002%
47	9.029	2401	2407	2409	rBV3	653	622	0.02%	0.003%
48	9.155	2443	2446	2450	rBV4	777	713	0.03%	0.004%
49	9.184	2452	2455	2459	rBV4	688	490	0.02%	0.002%
50	9.335	2496	2502	2504	rBV5	726	751	0.03%	0.004%
51	9.412	2513	2526	2558	rBV	1018320	1733524	66.58%	8.608%
52	10.110	2737	2743	2746	rBV4	700	652	0.03%	0.003%
53	10.190	2762	2768	2772	rVV4	708	796	0.03%	0.004%
54	10.257	2783	2789	2791	rBV3	589	550	0.02%	0.003%
55	10.277	2791	2795	2797	rBV2	515	389	0.01%	0.002%
56	10.354	2816	2819	2822	rBV2	804	564	0.02%	0.003%
57	10.441	2841	2846	2848	rBV2	574	492	0.02%	0.002%
58	10.550	2876	2880	2885	rBV5	643	545	0.02%	0.003%
59	10.605	2894	2897	2900	rBV3	711	439	0.02%	0.002%
60	10.753	2930	2943	2966	rBV	869952	1403303	53.90%	6.968%
61	10.904	2979	2990	3000	rBV7	5420	10558	0.41%	0.052%
62	11.116	3052	3056	3058	rBV3	1088	932	0.04%	0.005%
63	11.238	3090	3094	3097	rVV3	609	481	0.02%	0.002%
64	11.302	3111	3114	3117	rBV2	526	389	0.01%	0.002%
65	11.399	3141	3144	3145	rBV2	691	420	0.02%	0.002%
66	11.483	3164	3170	3176	rVV5	830	1256	0.05%	0.006%
67	11.553	3189	3192	3197	rVB2	743	690	0.03%	0.003%
68	11.630	3214	3216	3219	rBV3	678	469	0.02%	0.002%
69	11.727	3242	3246	3247	rBV3	851	502	0.02%	0.002%
70	11.807	3259	3271	3297	rVV	1107210	1797131	69.02%	8.924%
71	11.929	3305	3309	3312	rBV4	1100	1024	0.04%	0.005%
72	11.958	3315	3318	3321	rVB3	1290	733	0.03%	0.004%
73	12.090	3349	3359	3369	rBV7	7715	14202	0.55%	0.071%
74	12.190	3377	3390	3415	rBV	1229888	1999156	76.78%	9.927%
75	12.508	3486	3489	3491	rBV2	769	499	0.02%	0.002%
76	12.569	3502	3508	3518	rBV	7453	10559	0.41%	0.052%

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 Title : VOC Analysis

77	12.682	3539	3543	3546	rBV4	2052	1756	0.07%	0.009%
78	12.756	3562	3566	3567	rBV	1007	588	0.02%	0.003%
79	12.872	3598	3602	3605	rBV2	1277	981	0.04%	0.005%
80	12.904	3608	3612	3613	rBV3	891	523	0.02%	0.003%
81	12.971	3627	3633	3643	rBV2	6429	10075	0.39%	0.050%
82	13.232	3712	3714	3717	rVV3	697	435	0.02%	0.002%
83	13.293	3725	3733	3744	rBV6	5190	9873	0.38%	0.049%
84	13.415	3765	3771	3772	rBV4	1635	1380	0.05%	0.007%
85	13.450	3774	3782	3795	rVB4	15826	28633	1.10%	0.142%
86	13.560	3810	3816	3818	rBV6	1925	1826	0.07%	0.009%
87	13.708	3860	3862	3864	rBV2	747	423	0.02%	0.002%
88	13.942	3928	3935	3939	rBV7	2852	4188	0.16%	0.021%
89	13.987	3947	3949	3951	rBV2	899	436	0.02%	0.002%
90	14.116	3983	3989	3996	rVB8	1924	2608	0.10%	0.013%
91	14.187	4006	4011	4012	rBV4	1939	1536	0.06%	0.008%
92	14.283	4035	4041	4053	rVB4	4507	7162	0.28%	0.036%
93	14.341	4053	4059	4070	rBV4	2283	3613	0.14%	0.018%
94	14.389	4072	4074	4079	rBV3	1047	841	0.03%	0.004%
95	14.486	4098	4104	4109	rBV6	3342	4566	0.18%	0.023%
96	14.662	4156	4159	4161	rBV5	2647	2056	0.08%	0.010%
97	14.746	4183	4185	4188	rBV3	1295	949	0.04%	0.005%
98	14.801	4197	4202	4203	rBV4	2962	2386	0.09%	0.012%
99	15.408	4381	4391	4408	rBV	104714	180819	6.94%	0.898%
100	16.408	4694	4702	4709	rBV3	35066	54701	2.10%	0.272%

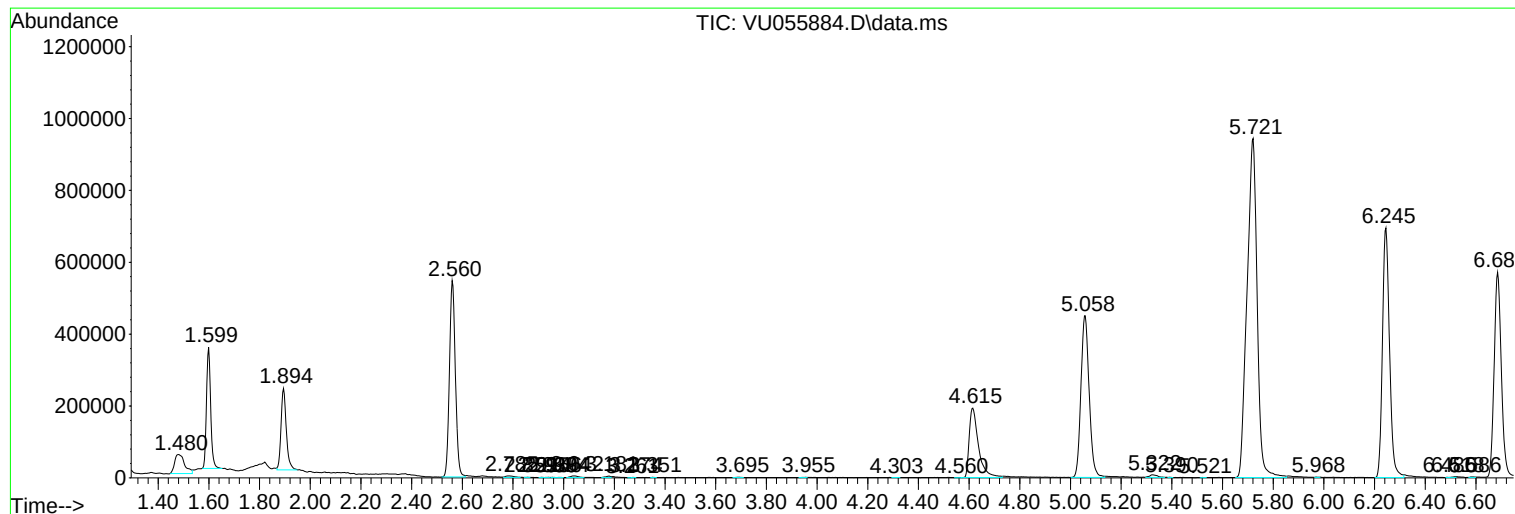
Sum of corrected areas: 20138131

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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



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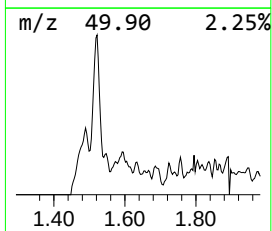
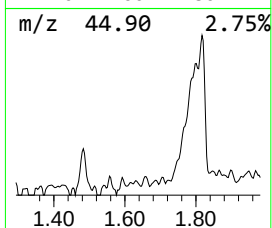
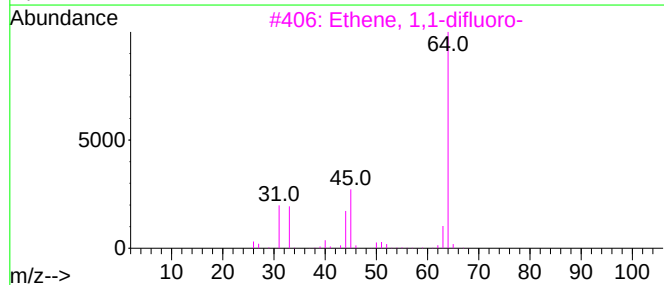
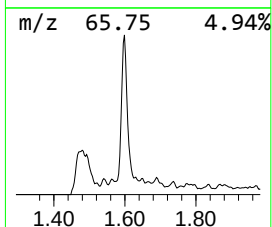
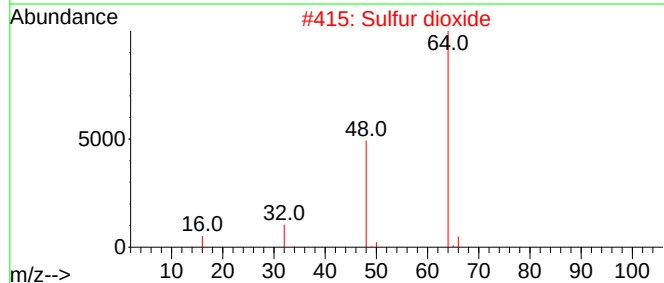
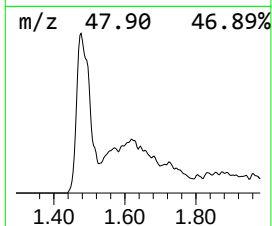
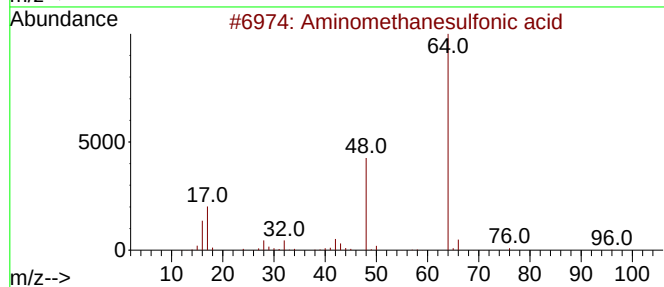
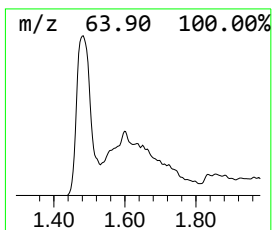
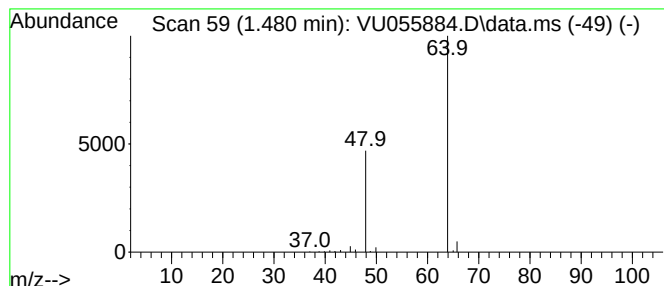
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.480	5.37 ug/L	145056	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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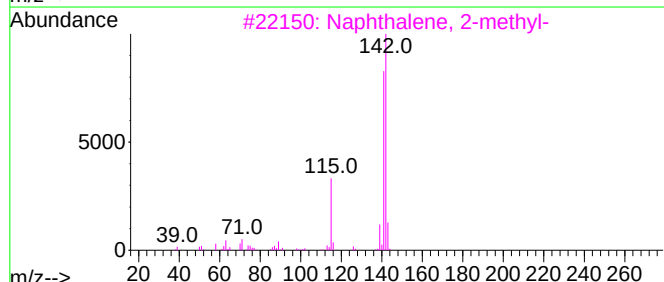
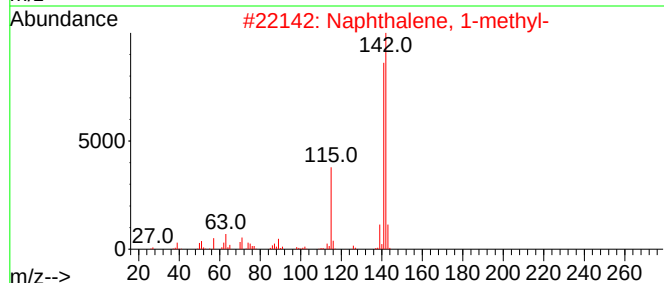
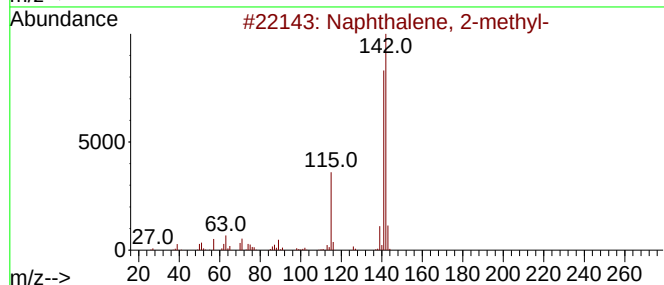
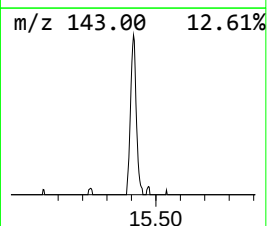
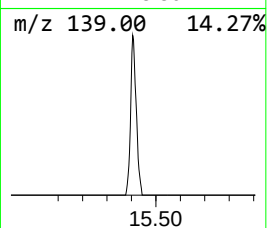
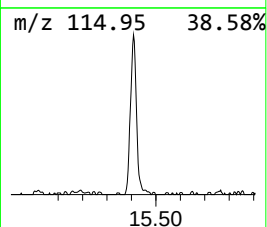
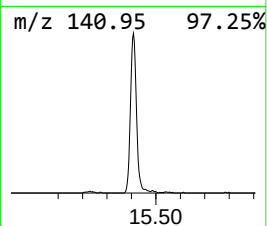
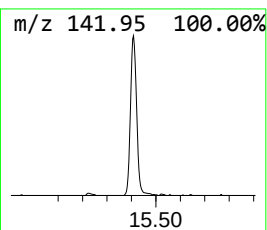
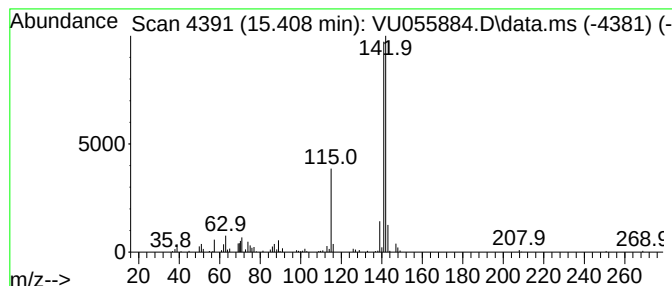
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzocycloheptatriene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.408	5.03 ug/L	180819	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
5			Benzocycloheptatriene	142	C11H10	000264-09-5	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	1.480	5.4	ug/L	145056	1	6.245	1350540	50.0
Benzocyclohepta...	15.408	5.0	ug/L	180819	3	11.807	1797130	50.0