

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061523\
 Data File : VV031530.D
 Acq On : 15 Jun 2023 14:50
 Operator : SY/MD
 Sample : 03249-06
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EXYS8

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\SFAMVLM061423WMA.M
 Title : VOC Analysis

Signal : TIC: VV031530.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.172	36	41	53	rBV	17899	23037	0.27%	0.103%
2	1.285	69	76	94	rVB2	338673	375252	4.34%	1.671%
3	1.539	147	155	169	rVB2	94329	143308	1.66%	0.638%
4	1.677	192	198	204	rBV	5838	7430	0.09%	0.033%
5	2.069	309	320	348	rVB3	250861	419666	4.85%	1.869%
6	2.465	435	443	449	rBV4	984	1452	0.02%	0.006%
7	2.706	507	518	534	rBV	33380	60135	0.69%	0.268%
8	3.121	630	647	678	rBV	1085116	2272335	26.26%	10.119%
9	3.539	771	777	778	rBV3	330	325	0.00%	0.001%
10	3.677	809	820	822	rBV5	1207	1719	0.02%	0.008%
11	3.732	834	837	841	rBV	471	325	0.00%	0.001%
12	3.822	847	865	908	rBV	3589150	8653181	100.00%	38.533%
13	4.259	986	1001	1025	rBV	153637	400778	4.63%	1.785%
14	4.523	1062	1083	1113	rBV	1366870	3499324	40.44%	15.583%
15	4.966	1202	1221	1246	rBV2	354324	956693	11.06%	4.260%
16	5.542	1388	1400	1428	rBV	220828	459682	5.31%	2.047%
17	5.796	1475	1479	1481	rVV2	519	414	0.00%	0.002%
18	5.844	1482	1494	1512	rVV3	32892	67894	0.78%	0.302%
19	5.995	1528	1541	1559	rBV	214461	443637	5.13%	1.976%
20	6.166	1592	1594	1598	rVB3	781	576	0.01%	0.003%
21	6.236	1614	1616	1626	rVB4	536	592	0.01%	0.003%
22	6.352	1649	1652	1656	rBV4	294	318	0.00%	0.001%
23	6.474	1688	1690	1695	rVB2	370	335	0.00%	0.001%
24	6.606	1728	1731	1735	rBV4	443	319	0.00%	0.001%
25	6.706	1758	1762	1766	rVB2	376	355	0.00%	0.002%
26	6.873	1809	1814	1817	rBV	423	417	0.00%	0.002%
27	6.918	1817	1828	1862	rVV	110723	208246	2.41%	0.927%
28	7.063	1869	1873	1876	rVB3	473	347	0.00%	0.002%
29	7.143	1894	1898	1903	rBV4	816	897	0.01%	0.004%
30	7.249	1919	1931	1947	rVV	387001	675416	7.81%	3.008%
31	7.329	1950	1956	1969	rVB3	15800	28907	0.33%	0.129%
32	7.558	2016	2027	2057	rBV2	83142	154814	1.79%	0.689%
33	7.783	2090	2097	2107	rVV5	2714	4561	0.05%	0.020%
34	7.911	2117	2137	2156	rVV	141296	246759	2.85%	1.099%
35	8.030	2165	2174	2208	rBV	238724	427545	4.94%	1.904%
36	8.227	2233	2235	2242	rVB5	2305	2384	0.03%	0.011%

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37	8.272	2246	2249	2251	rVV3	439	315	0.00%	0.001%
38	8.284	2251	2253	2264	rVB6	985	1249	0.01%	0.006%
39	8.538	2329	2332	2335	rBV3	467	318	0.00%	0.001%
40	8.792	2399	2411	2436	rBV	335221	554741	6.41%	2.470%
41	8.956	2453	2462	2475	rVB	21828	34215	0.40%	0.152%
42	9.088	2494	2503	2514	rVV2	4434	7700	0.09%	0.034%
43	9.400	2597	2600	2601	rBV	537	348	0.00%	0.002%
44	9.487	2617	2627	2643	rVB2	33627	54027	0.62%	0.241%
45	9.645	2667	2676	2688	rVB5	2808	4562	0.05%	0.020%
46	9.731	2699	2703	2704	rBV	731	533	0.01%	0.002%
47	9.818	2727	2730	2736	rBV2	347	338	0.00%	0.002%
48	9.876	2741	2748	2757	rVV4	6556	9350	0.11%	0.042%
49	9.960	2771	2774	2780	rVB3	565	536	0.01%	0.002%
50	10.034	2793	2797	2803	rVV4	948	988	0.01%	0.004%
51	10.069	2803	2808	2813	rVB4	1331	1389	0.02%	0.006%
52	10.159	2823	2836	2857	rBV	319967	501734	5.80%	2.234%
53	10.297	2871	2879	2886	rBV2	13631	19791	0.23%	0.088%
54	10.394	2900	2909	2917	rBV	5349	8253	0.10%	0.037%
55	10.487	2928	2938	2947	rVB2	12115	17767	0.21%	0.079%
56	10.638	2982	2985	2988	rBV5	961	753	0.01%	0.003%
57	10.680	2989	2998	3016	rVB	40944	63783	0.74%	0.284%
58	10.783	3026	3030	3032	rBV	450	362	0.00%	0.002%
59	10.860	3043	3054	3073	rVV2	47323	72493	0.84%	0.323%
60	10.960	3082	3085	3089	rVV2	420	412	0.00%	0.002%
61	11.001	3092	3098	3101	rVV	2157	2479	0.03%	0.011%
62	11.030	3101	3107	3119	rVV3	6584	10376	0.12%	0.046%
63	11.133	3133	3139	3146	rBV6	2862	3988	0.05%	0.018%
64	11.191	3146	3157	3175	rVV	376465	578948	6.69%	2.578%
65	11.278	3176	3184	3201	rVB	37692	59395	0.69%	0.264%
66	11.394	3215	3220	3222	rBV3	985	710	0.01%	0.003%
67	11.403	3222	3223	3227	rVB2	914	372	0.00%	0.002%
68	11.429	3229	3231	3235	rBV3	494	340	0.00%	0.002%
69	11.474	3235	3245	3257	rBV	23745	42817	0.49%	0.191%
70	11.567	3263	3274	3296	rVB	477251	757001	8.75%	3.371%
71	11.763	3330	3335	3343	rVV5	1351	1679	0.02%	0.007%
72	11.866	3358	3367	3383	rBV4	16133	31932	0.37%	0.142%
73	11.934	3383	3388	3390	rBV5	1394	1279	0.01%	0.006%
74	11.956	3391	3395	3405	rVB3	3528	5061	0.06%	0.023%
75	12.059	3418	3427	3431	rBV2	5563	7345	0.08%	0.033%
76	12.201	3460	3471	3479	rBV4	1313	2487	0.03%	0.011%

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77	12.252	3482	3487	3490	rBV4	886	845	0.01%	0.004%
78	12.323	3505	3509	3512	rBV3	346	319	0.00%	0.001%
79	12.361	3515	3521	3528	rVB4	2623	3089	0.04%	0.014%
80	12.413	3528	3537	3547	rBV2	4830	6904	0.08%	0.031%
81	12.496	3559	3563	3564	rBV2	614	392	0.00%	0.002%
82	12.587	3588	3591	3597	rVB2	733	572	0.01%	0.003%
83	12.619	3597	3601	3602	rBV	652	369	0.00%	0.002%
84	12.660	3610	3614	3616	rBV	688	500	0.01%	0.002%
85	12.824	3657	3665	3675	rVB4	7296	10967	0.13%	0.049%
86	12.895	3680	3687	3697	rVB5	1833	3097	0.04%	0.014%
87	12.943	3697	3702	3704	rBV2	422	385	0.00%	0.002%
88	12.988	3710	3716	3728	rVB5	3024	4423	0.05%	0.020%
89	13.213	3779	3786	3790	rBV6	1413	1660	0.02%	0.007%
90	13.451	3850	3860	3868	rBV	9391	14921	0.17%	0.066%
91	13.795	3963	3967	3973	rVB3	336	366	0.00%	0.002%
92	13.882	3990	3994	3998	rBV3	416	471	0.01%	0.002%
93	14.384	4145	4150	4152	rBV4	499	452	0.01%	0.002%
94	14.580	4203	4211	4215	rBV6	1599	2198	0.03%	0.010%
95	14.754	4261	4265	4267	rBV4	719	624	0.01%	0.003%
96	14.982	4333	4336	4338	rBV2	584	458	0.01%	0.002%
97	15.040	4352	4354	4358	rBV3	532	459	0.01%	0.002%
98	15.223	4407	4411	4413	rBV3	657	561	0.01%	0.002%
99	15.422	4470	4473	4474	rBV3	609	362	0.00%	0.002%
100	15.644	4540	4542	4545	rBV2	745	420	0.00%	0.002%

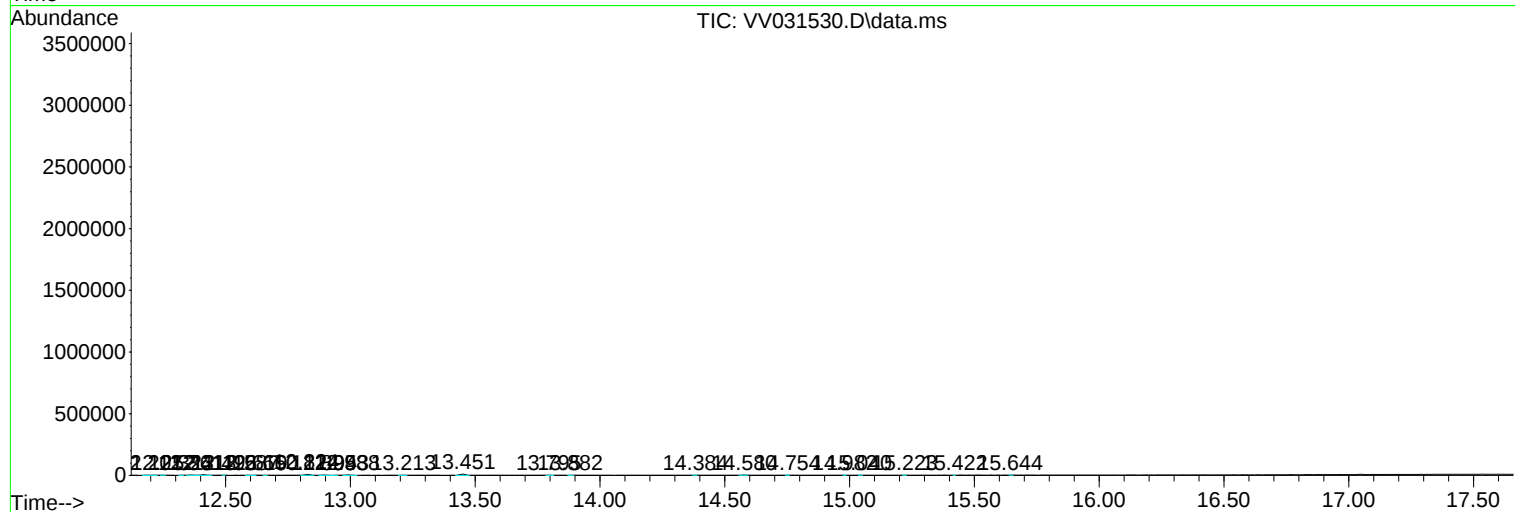
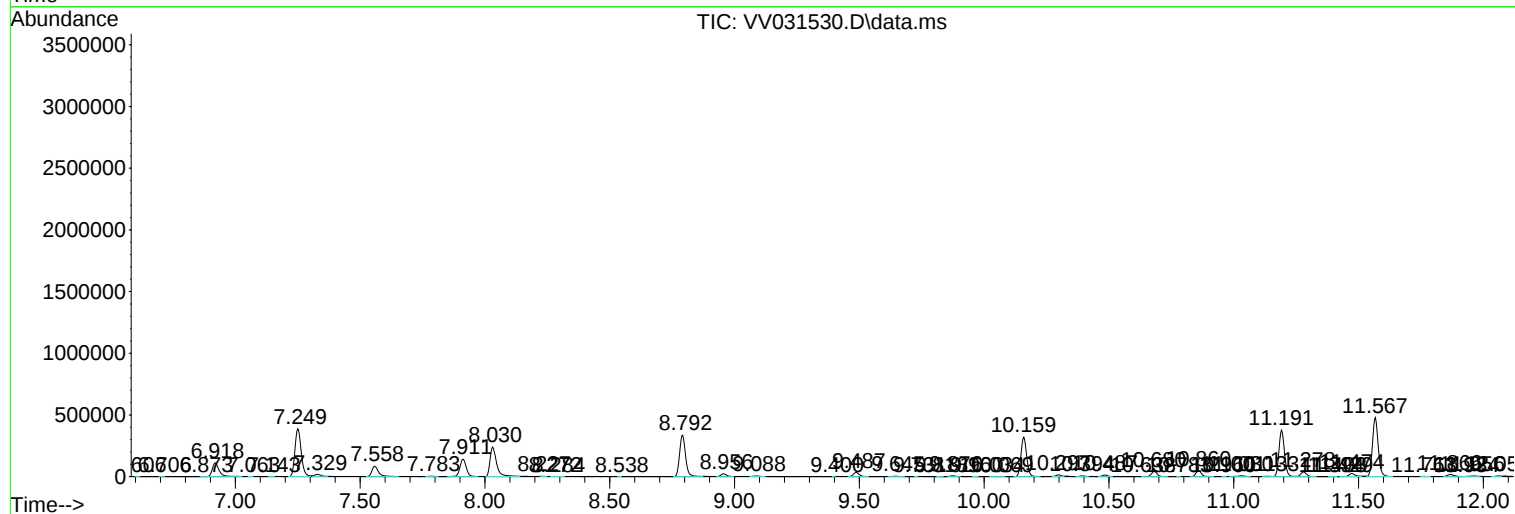
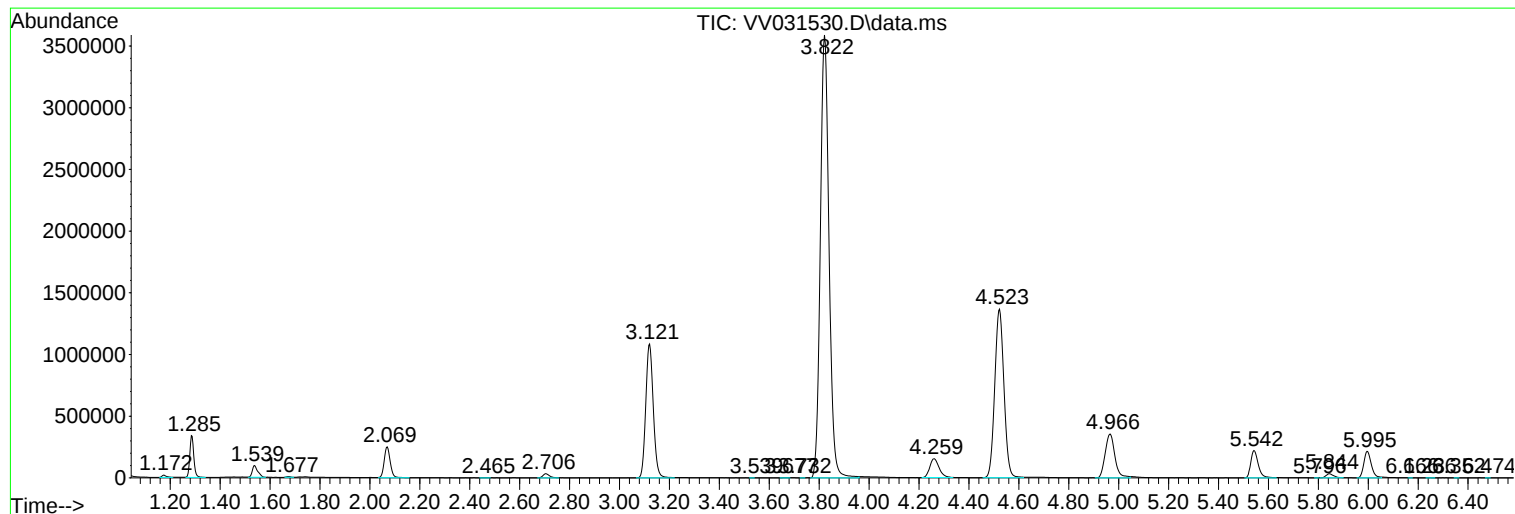
Sum of corrected areas: 22456355

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Instrument :
MSVOA_V
ClientSampleId :
EXYS8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061523\
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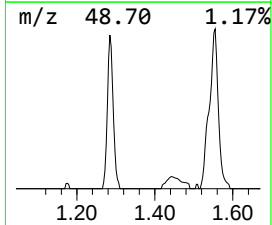
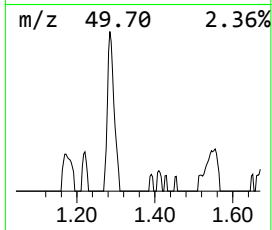
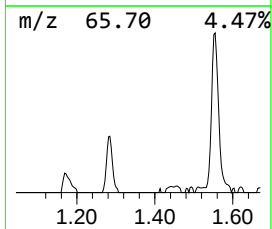
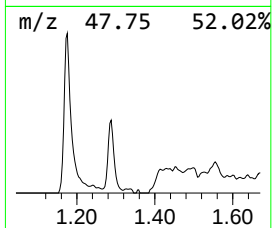
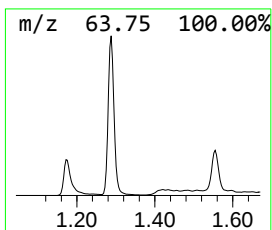
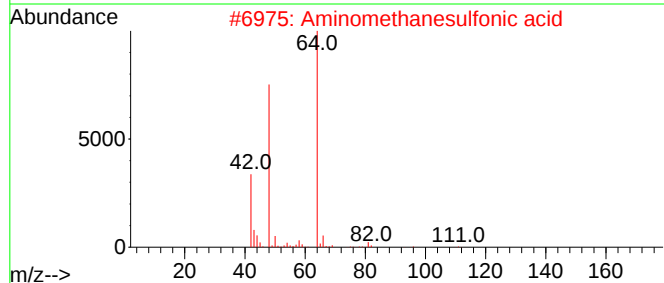
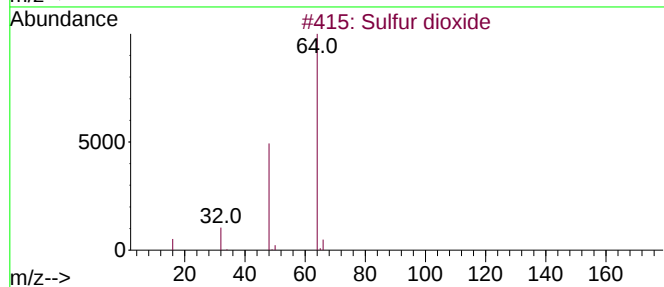
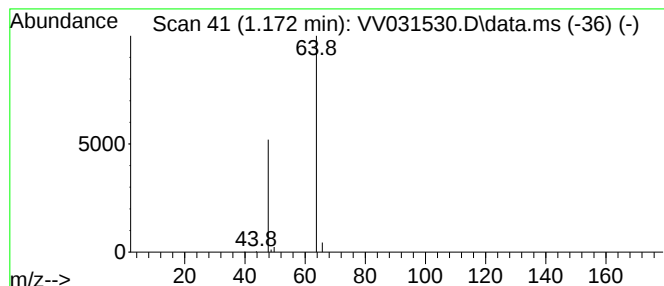
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.172	2.51 ug/L	23037	1,4-Difluorobenzene	5.542

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



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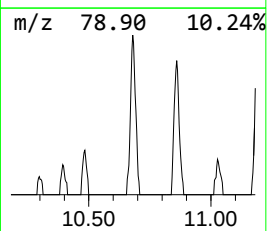
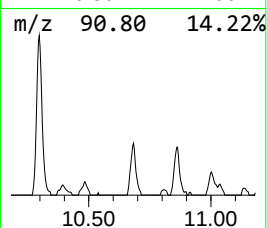
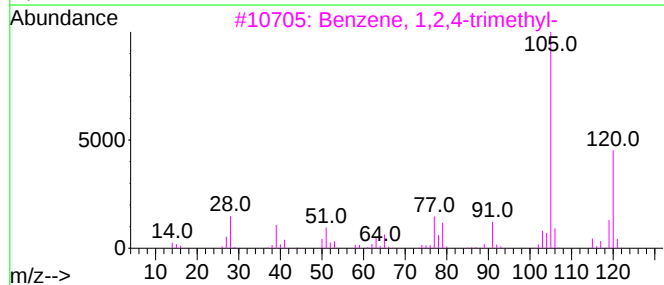
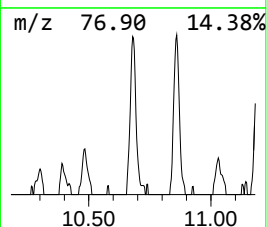
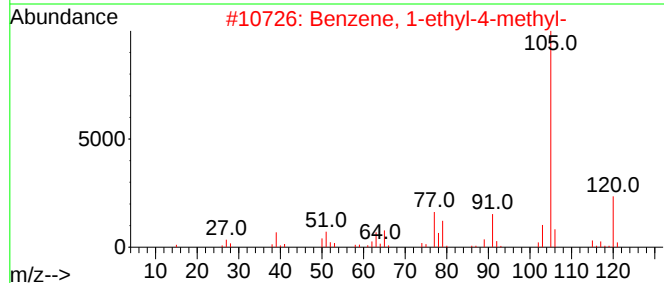
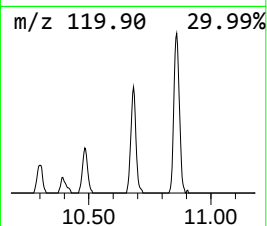
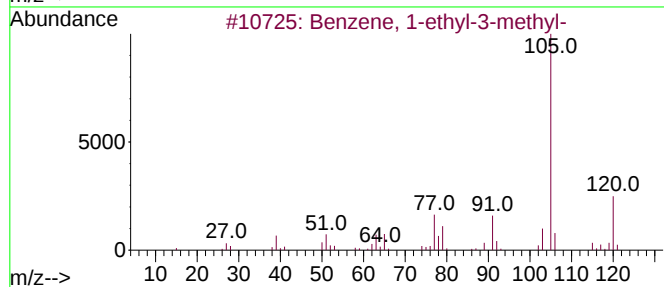
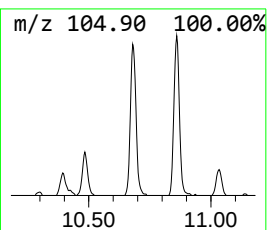
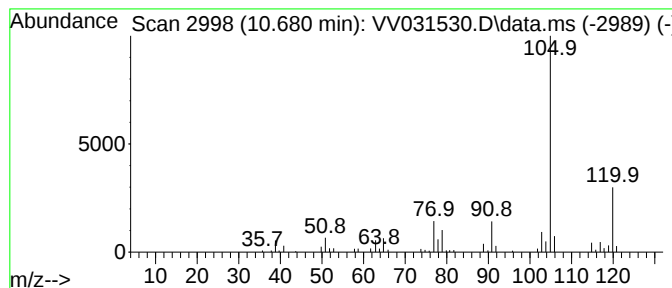
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.680	5.51 ug/L	63783	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



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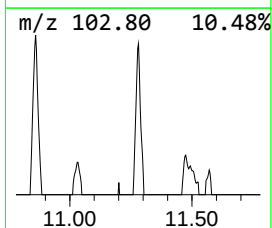
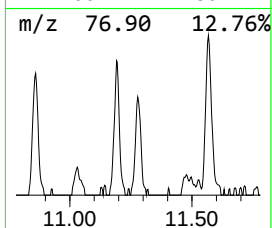
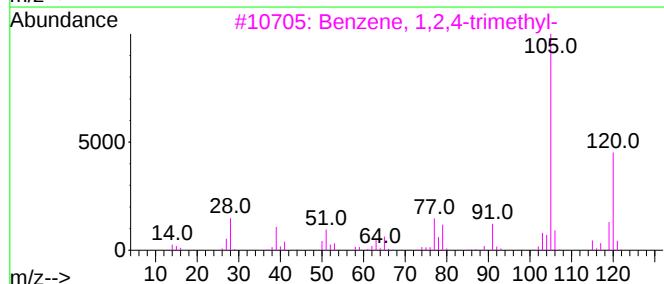
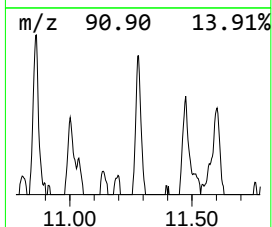
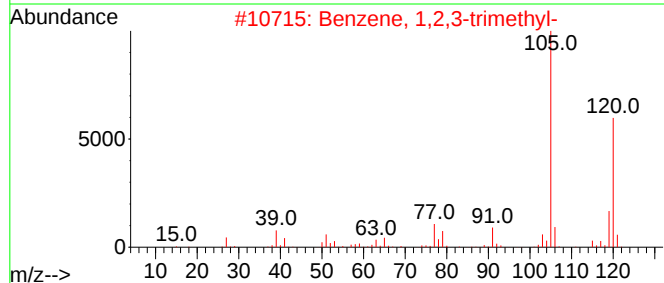
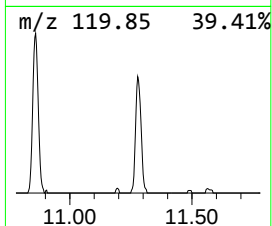
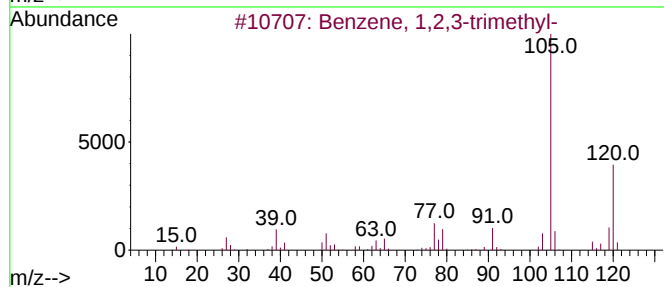
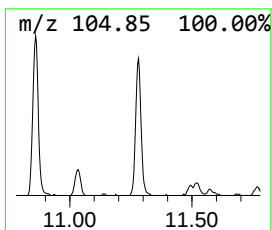
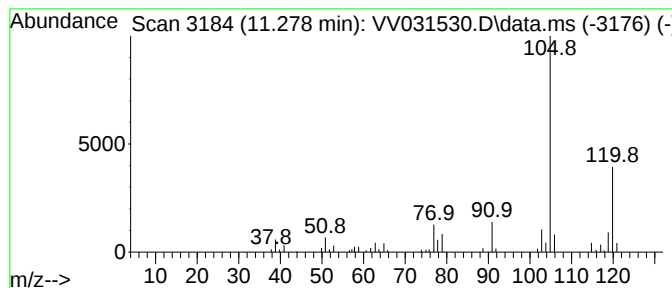
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.278	5.13 ug/L	59395	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Mesitylene	120	C9H12	000108-67-8	94
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061523\
Data File : VV031530.D
Acq On : 15 Jun 2023 14:50
Operator : SY/MD
Sample : 03249-06
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXYS8

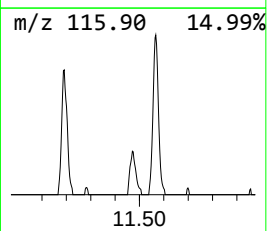
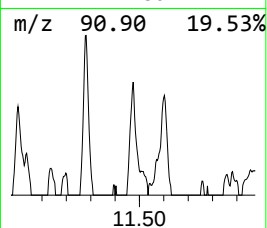
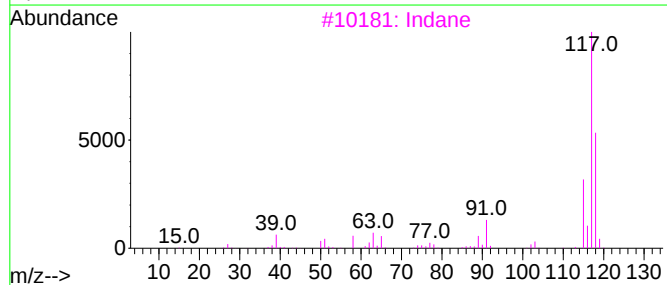
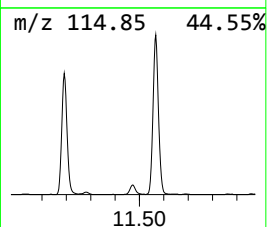
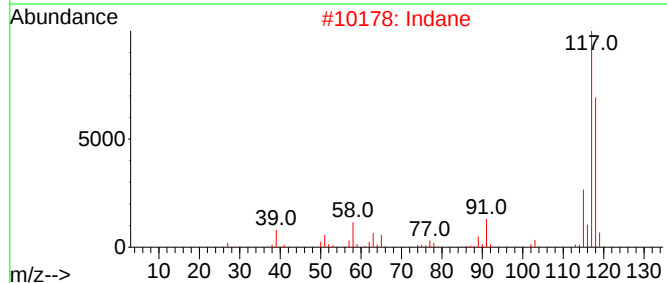
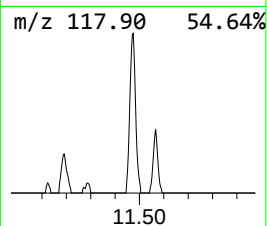
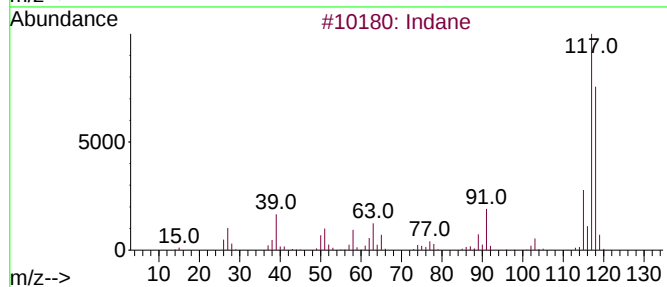
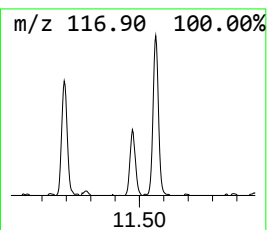
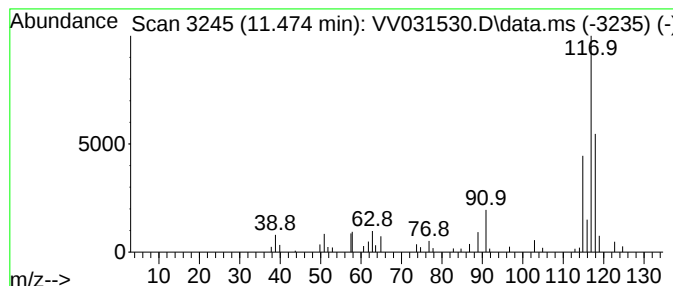
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Quant Title : VOC Analysis

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

Peak Number 5 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.474	3.70 ug/L	42817	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane			118	C9H10	000496-11-7	94
2	Indane			118	C9H10	000496-11-7	76
3	Indane			118	C9H10	000496-11-7	76
4	Benzene, 1-propenyl-			118	C9H10	000637-50-3	70
5	Indane			118	C9H10	000496-11-7	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061523\
Data File : VV031530.D
Acq On : 15 Jun 2023 14:50
Operator : SY/MD
Sample : 03249-06
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXYS8

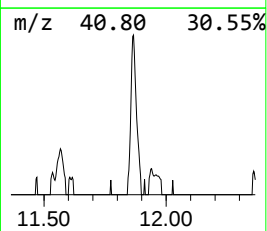
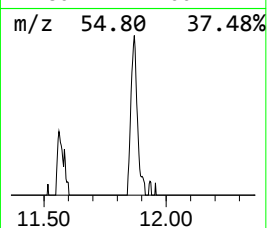
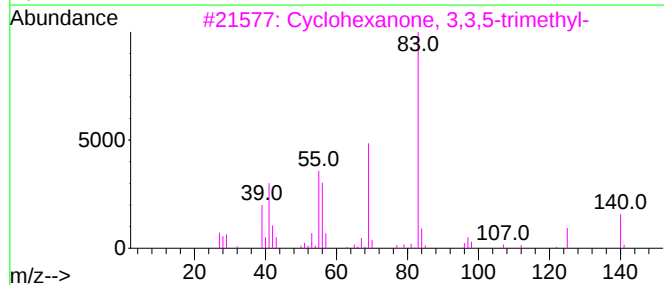
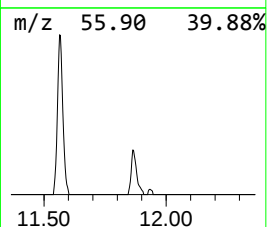
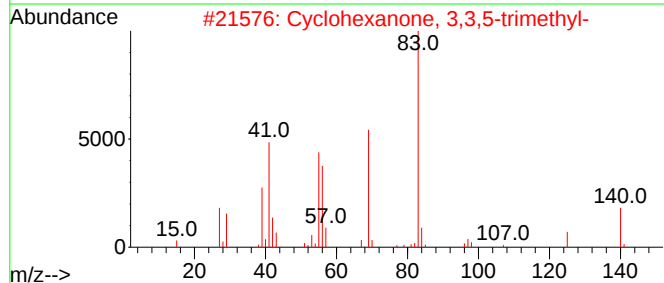
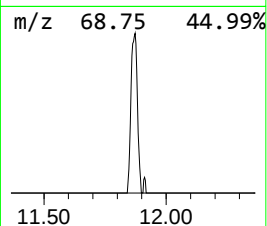
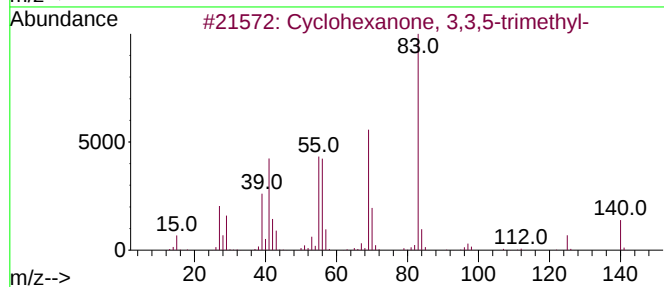
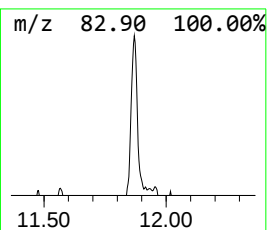
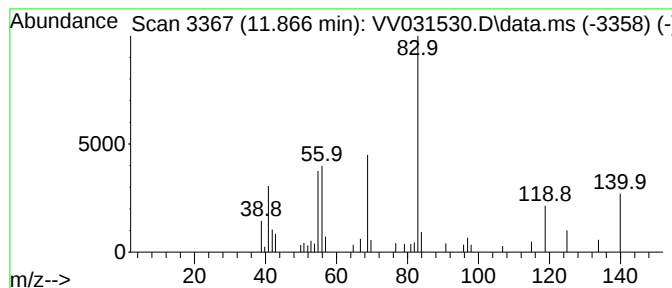
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Cyclohexanone, 3,3,5-trimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.866	2.76 ug/L	31932	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	87
2			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	83
3			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	68
4			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	59
5			Cyclohexane, butyl-	140	C10H20	001678-93-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061523\
Data File : VV031530.D
Acq On : 15 Jun 2023 14:50
Operator : SY/MD
Sample : 03249-06
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXYS8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.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	1.172	2.5	ug/L	23037	1	5.542	459682	50.0
Benzene, 1-ethy...	10.680	5.5	ug/L	63783	3	11.191	578948	50.0
Benzene, 1,2,3-...	11.278	5.1	ug/L	59395	3	11.191	578948	50.0
Indane	11.474	3.7	ug/L	42817	3	11.191	578948	50.0
Cyclohexanone, ...	11.866	2.8	ug/L	31932	3	11.191	578948	50.0