

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092324\
 Data File : VV037479.D
 Acq On : 23 Sep 2024 14:07
 Operator : SY/MD
 Sample : P4109-02ME
 Misc : 2.32G/5mL/100ul/5mL/MSVOA_V/MEOH
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A4EH5ME

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\SFAMVLM082624WMA.M
 Title : VOC Analysis

Signal : TIC: VV037479.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	32	41	51	rBV2	36131	75442	2.75%	0.337%
2	1.278	66	74	89	rBV	309140	389775	14.22%	1.742%
3	1.507	109	145	159	rBV2	195654	501691	18.30%	2.242%
4	1.896	264	266	270	rBV4	2054	1620	0.06%	0.007%
5	2.044	302	312	331	rBV	658520	953568	34.79%	4.261%
6	2.368	407	413	425	rVB	8634	15202	0.55%	0.068%
7	2.548	464	469	471	rBV4	8028	7574	0.28%	0.034%
8	2.860	562	566	568	rBV5	2457	2196	0.08%	0.010%
9	3.092	635	638	641	rBV4	2124	1430	0.05%	0.006%
10	3.802	848	859	886	rBV	80111	282940	10.32%	1.264%
11	4.240	976	995	1033	rBV	415629	1117903	40.78%	4.995%
12	4.375	1033	1037	1041	rVB6	2036	2172	0.08%	0.010%
13	4.439	1052	1057	1061	rVB7	1525	1609	0.06%	0.007%
14	4.465	1061	1065	1072	rBV6	922	1052	0.04%	0.005%
15	4.529	1083	1085	1089	rVB3	1373	807	0.03%	0.004%
16	4.568	1089	1097	1099	rBV5	1016	1110	0.04%	0.005%
17	4.600	1104	1107	1109	rBV2	1190	799	0.03%	0.004%
18	4.645	1114	1121	1123	rBV5	1289	1410	0.05%	0.006%
19	4.880	1191	1194	1198	rBV5	943	864	0.03%	0.004%
20	4.947	1198	1215	1256	rBV2	1067048	2741191	100.00%	12.248%
21	5.336	1331	1336	1341	rVB8	1144	1253	0.05%	0.006%
22	5.397	1348	1355	1357	rBV7	1316	1403	0.05%	0.006%
23	5.433	1365	1366	1370	rVB3	1635	879	0.03%	0.004%
24	5.465	1370	1376	1378	rBV5	940	811	0.03%	0.004%
25	5.526	1382	1395	1441	rBV	692024	1500693	54.75%	6.705%
26	5.754	1463	1466	1469	rVB4	1605	1044	0.04%	0.005%
27	5.783	1473	1475	1477	rBV4	1761	796	0.03%	0.004%
28	5.834	1479	1491	1496	rBV8	6615	11411	0.42%	0.051%
29	5.928	1515	1520	1524	rBV4	2179	2734	0.10%	0.012%
30	5.982	1524	1537	1569	rVV	571974	1249576	45.59%	5.583%
31	6.172	1593	1596	1599	rBV3	1771	1041	0.04%	0.005%
32	6.297	1634	1635	1642	rVB6	1519	1217	0.04%	0.005%
33	6.365	1652	1656	1657	rBV3	1679	1082	0.04%	0.005%
34	6.449	1677	1682	1685	rBV5	1387	869	0.03%	0.004%
35	6.513	1695	1702	1704	rVV5	875	821	0.03%	0.004%
36	6.709	1761	1763	1767	rVB5	1263	835	0.03%	0.004%

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 Title : VOC Analysis

37	6.770	1778	1782	1787	rVB8	1267	1160	0.04%	0.005%
38	6.857	1800	1809	1810	rBV8	984	1096	0.04%	0.005%
39	6.908	1812	1825	1854	rBV	302416	602388	21.98%	2.692%
40	7.185	1901	1911	1916	rBV9	6035	11412	0.42%	0.051%
41	7.236	1916	1927	1947	rVV	1213017	2160344	78.81%	9.653%
42	7.320	1950	1953	1969	rVB	22411	43938	1.60%	0.196%
43	7.551	2015	2025	2051	rBV	196074	402639	14.69%	1.799%
44	7.764	2089	2091	2101	rVB8	1257	1290	0.05%	0.006%
45	7.879	2121	2127	2128	rVV5	1315	1242	0.05%	0.006%
46	7.899	2128	2133	2143	rVB9	3723	4813	0.18%	0.022%
47	8.034	2158	2175	2202	rBV2	296188	818796	29.87%	3.659%
48	8.211	2227	2230	2238	rVB6	5552	6680	0.24%	0.030%
49	8.275	2240	2250	2260	rBV4	17509	29017	1.06%	0.130%
50	8.432	2288	2299	2310	rVB4	6966	15351	0.56%	0.069%
51	8.519	2310	2326	2333	rBV10	13309	33522	1.22%	0.150%
52	8.603	2350	2352	2355	rVB2	2391	1272	0.05%	0.006%
53	8.641	2361	2364	2370	rVB5	1293	1337	0.05%	0.006%
54	8.715	2375	2387	2396	rBV7	6126	13052	0.48%	0.058%
55	8.780	2396	2407	2443	rBV	1093153	1877659	68.50%	8.390%
56	8.915	2443	2449	2450	rBV5	5014	4515	0.16%	0.020%
57	8.985	2466	2471	2473	rVB6	1188	998	0.04%	0.004%
58	9.030	2476	2485	2494	rBV6	10771	23931	0.87%	0.107%
59	9.085	2496	2502	2509	rVB4	13775	18540	0.68%	0.083%
60	9.127	2509	2515	2518	rBV7	5049	5809	0.21%	0.026%
61	9.243	2544	2551	2564	rVB8	11558	20639	0.75%	0.092%
62	9.297	2564	2568	2573	rVB8	1135	1233	0.04%	0.006%
63	9.342	2573	2582	2584	rBV7	6163	7294	0.27%	0.033%
64	9.407	2586	2602	2611	rVV6	22156	43838	1.60%	0.196%
65	9.510	2629	2634	2643	rVB9	8160	10165	0.37%	0.045%
66	9.606	2657	2664	2667	rBV6	10422	14152	0.52%	0.063%
67	9.641	2667	2675	2685	rVB4	47149	79420	2.90%	0.355%
68	9.728	2695	2702	2711	rBV5	21148	37083	1.35%	0.166%
69	9.783	2711	2719	2730	rVB2	54489	91365	3.33%	0.408%
70	9.844	2731	2738	2749	rVB8	14402	25566	0.93%	0.114%
71	9.905	2750	2757	2764	rBV9	14175	23094	0.84%	0.103%
72	9.950	2764	2771	2782	rBV2	28012	42306	1.54%	0.189%
73	10.056	2798	2804	2815	rVB6	10447	16413	0.60%	0.073%
74	10.149	2815	2833	2851	rBV	719679	1274867	46.51%	5.696%
75	10.323	2876	2887	2895	rBV7	23740	48511	1.77%	0.217%
76	10.442	2915	2924	2932	rBV3	54363	88611	3.23%	0.396%

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77	10.503	2935	2943	2952	rVV7	19788	41099	1.50%	0.184%
78	10.612	2966	2977	2982	rBV8	10487	22558	0.82%	0.101%
79	10.764	3016	3024	3031	rVB8	14275	23036	0.84%	0.103%
80	10.815	3031	3040	3049	rBV6	61777	120121	4.38%	0.537%
81	10.966	3080	3087	3092	rBV4	25429	38763	1.41%	0.173%
82	11.005	3093	3099	3102	rVV6	29172	43383	1.58%	0.194%
83	11.034	3103	3108	3115	rVV3	49635	72424	2.64%	0.324%
84	11.082	3118	3123	3131	rVB4	37459	55228	2.01%	0.247%
85	11.133	3136	3139	3144	rVV5	24678	27348	1.00%	0.122%
86	11.178	3144	3153	3173	rVB	1257113	2005675	73.17%	8.962%
87	11.349	3199	3206	3216	rVB6	27302	52244	1.91%	0.233%
88	11.554	3258	3270	3288	rBV	1319780	2140223	78.08%	9.563%
89	11.870	3357	3368	3376	rBV6	55505	107715	3.93%	0.481%
90	12.063	3421	3428	3437	rVB7	24470	38259	1.40%	0.171%
91	12.191	3458	3468	3478	rBV6	51618	93207	3.40%	0.416%
92	12.300	3493	3502	3523	rBV4	78533	169447	6.18%	0.757%
93	12.400	3526	3533	3543	rVB5	56512	85676	3.13%	0.383%
94	12.995	3704	3718	3736	rVB5	49399	141442	5.16%	0.632%
95	13.413	3843	3848	3856	rVB4	24152	28992	1.06%	0.130%
96	13.580	3893	3900	3910	rBV2	50950	78814	2.88%	0.352%
97	14.024	4031	4038	4051	rVB2	21836	41507	1.51%	0.185%
98	14.590	4207	4214	4222	rBV2	47283	65327	2.38%	0.292%
99	15.352	4446	4451	4458	rVB2	33780	39236	1.43%	0.175%
100	15.519	4498	4503	4516	rVB5	37646	66183	2.41%	0.296%

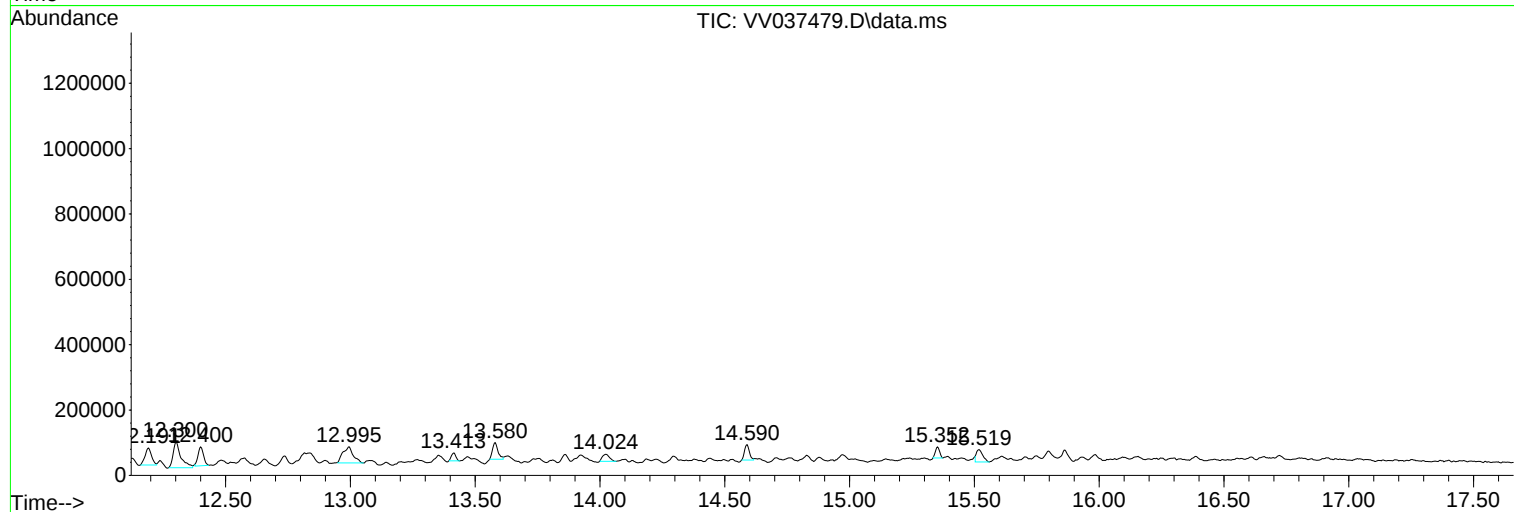
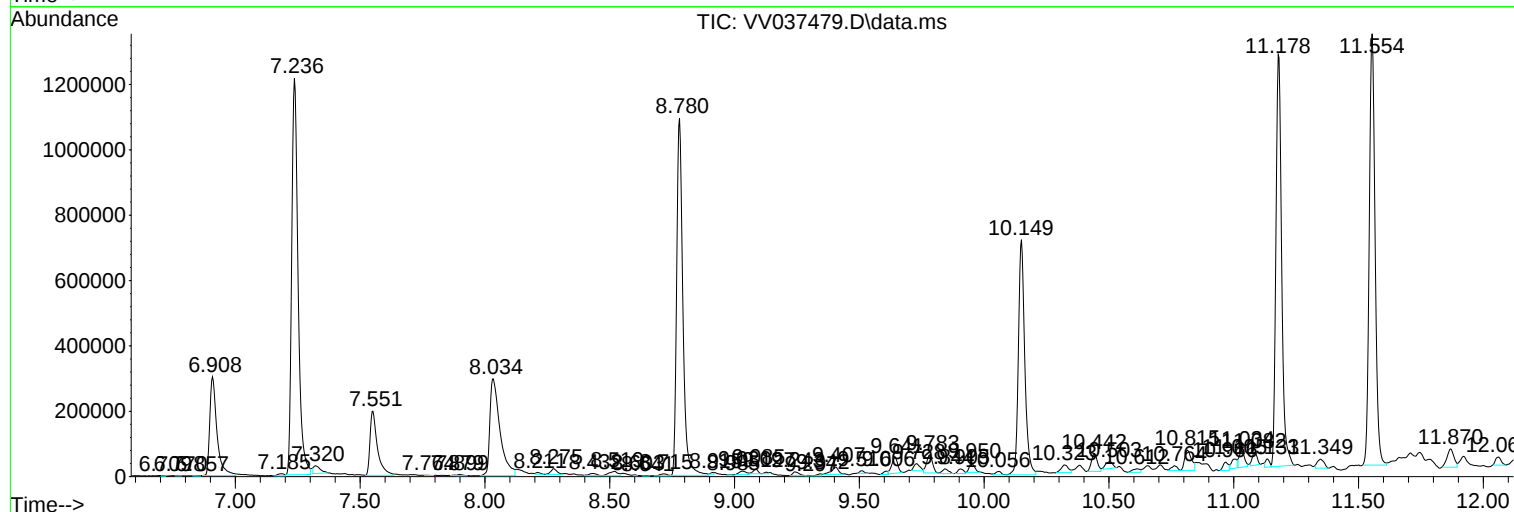
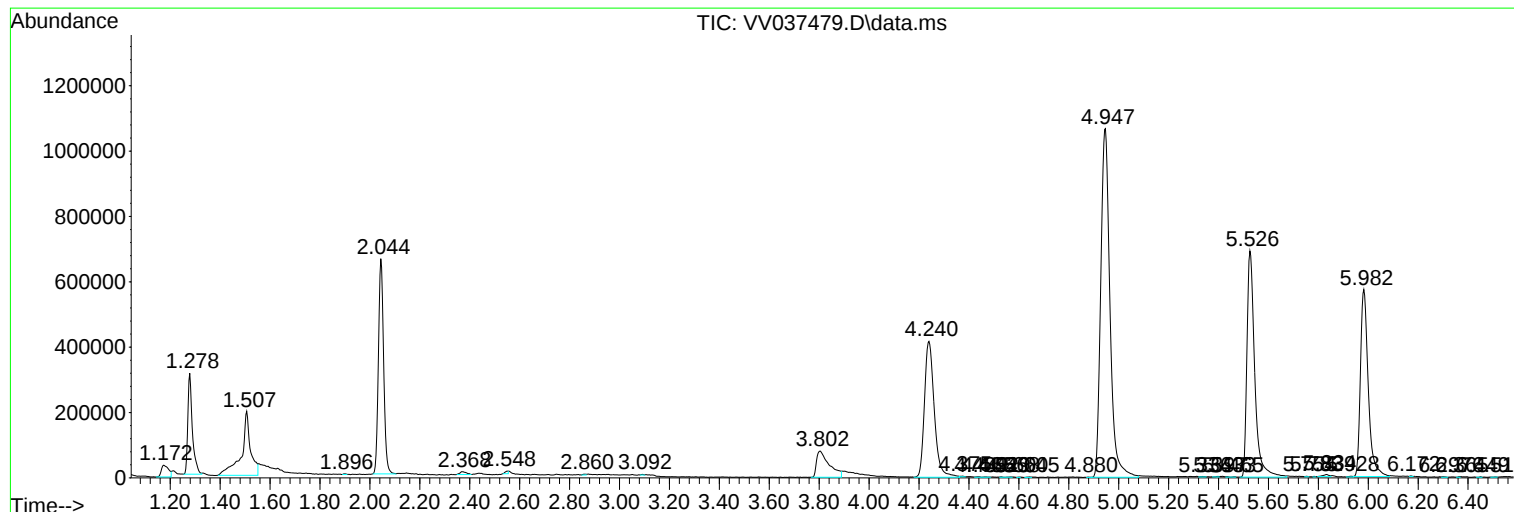
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Instrument :
MSVOA_V
ClientSampleId :
A4EH5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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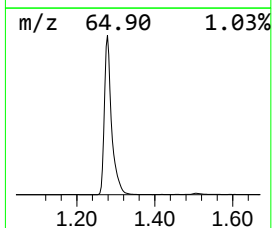
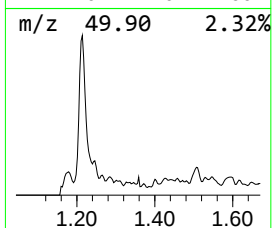
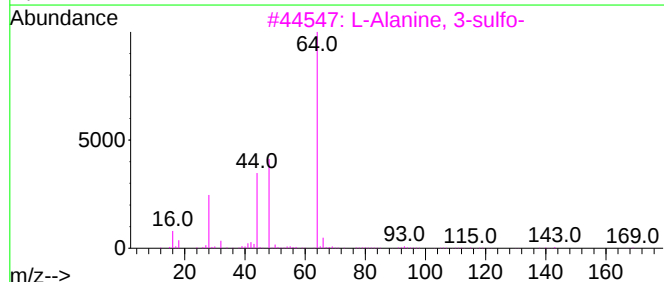
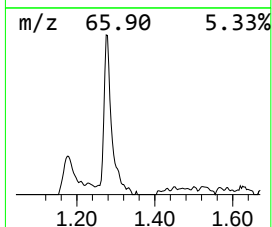
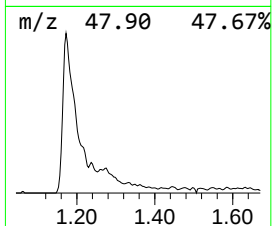
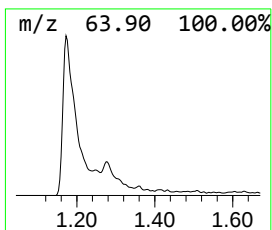
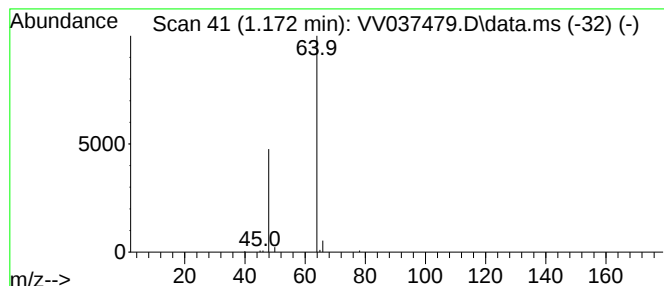
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.172	2.51 ug/L	75442	1,4-Difluorobenzene	5.526

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
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			Sulfur dioxide	64	O2S	007446-09-5	5



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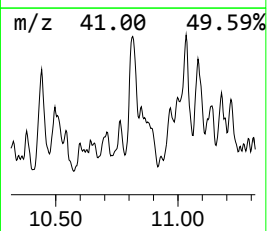
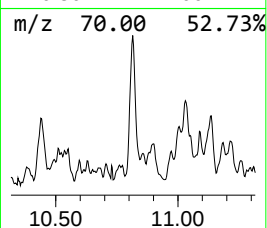
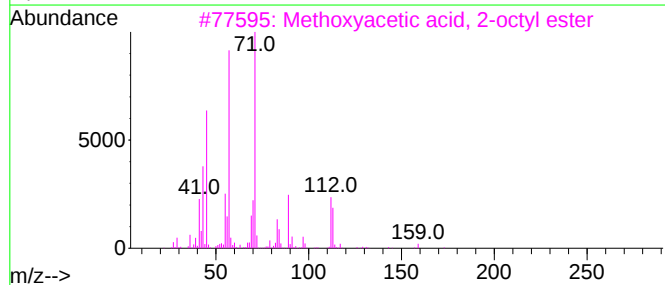
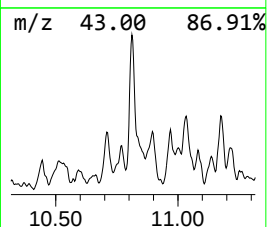
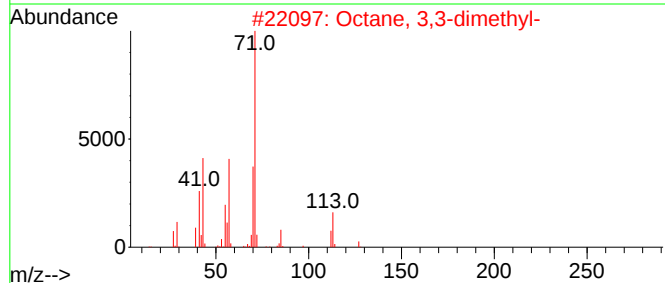
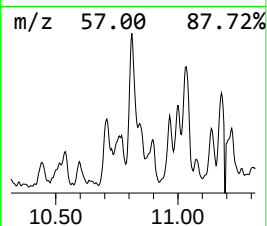
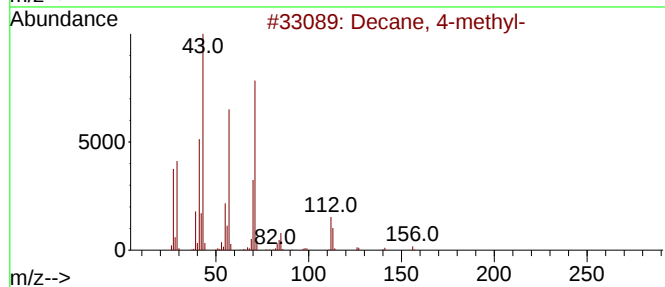
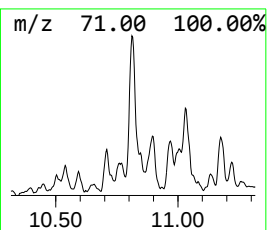
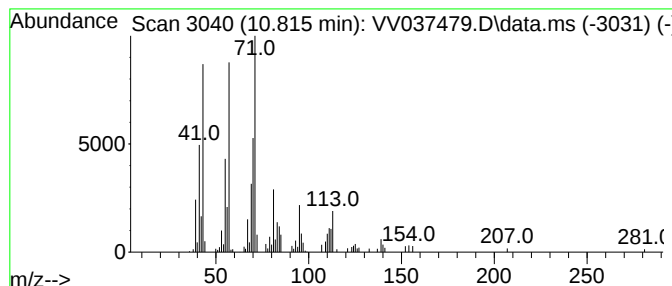
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.815	2.99 ug/L	120121	1,4-Dichlorobenzene-d4	11.182

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 4-methyl-	156	C11H24	002847-72-5	81
2			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	64
3			Methoxyacetic acid, 2-octyl ester	202	C11H22O3	1000282-69-6	53
4			Dodecane, 4-methyl-	184	C13H28	006117-97-1	50
5			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	49



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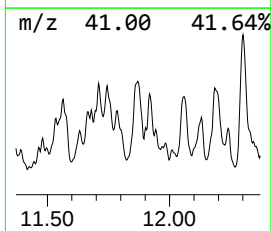
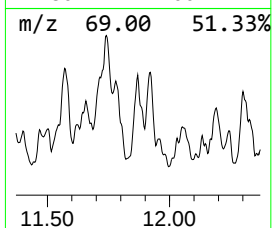
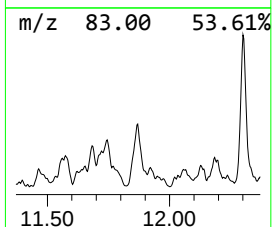
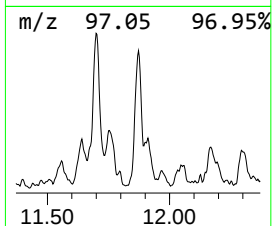
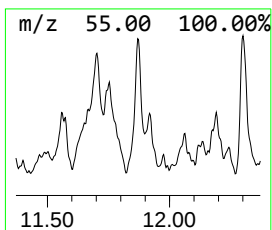
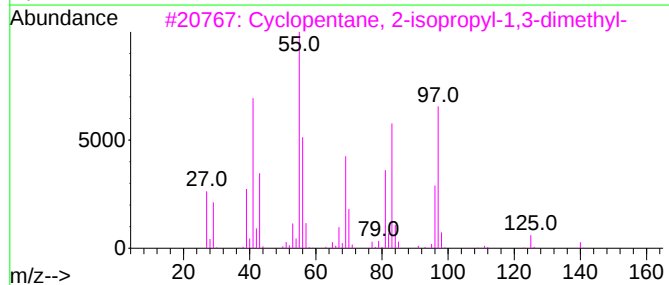
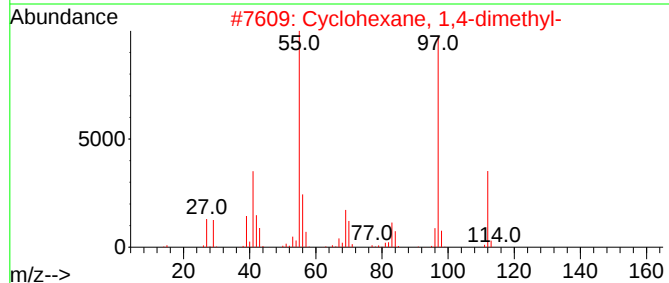
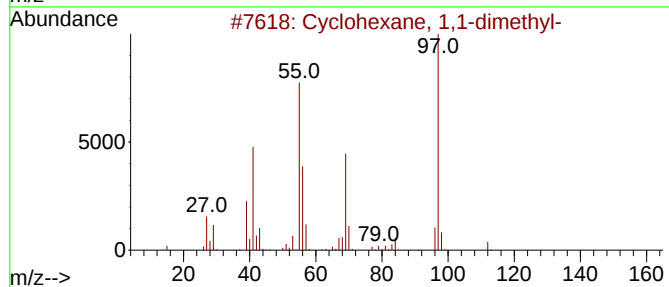
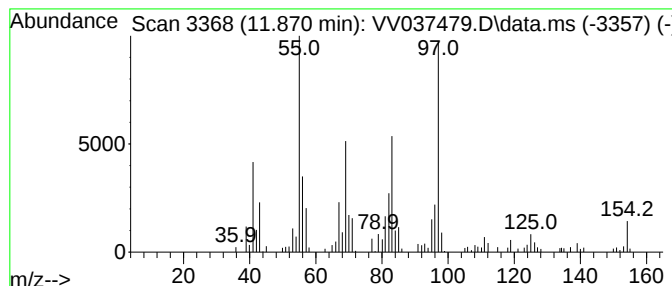
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic11.870 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.870	2.69 ug/L	107715	1,4-Dichlorobenzene-d4	11.182

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	50
2			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	46
3			Cyclopentane, 2-isopropyl-1,3-di...	140	C10H20	032281-85-9	46
4			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	46
5			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092324\
Data File : VV037479.D
Acq On : 23 Sep 2024 14:07
Operator : SY/MD
Sample : P4109-02ME
Misc : 2.32G/5mL/100ul/5mL/MSVOA_V/MEOH
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A4EH5ME

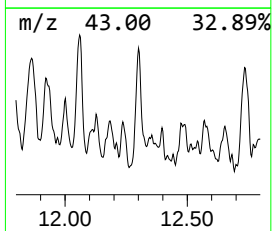
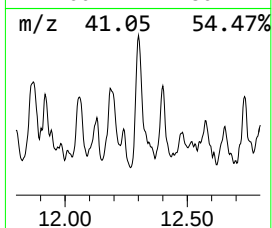
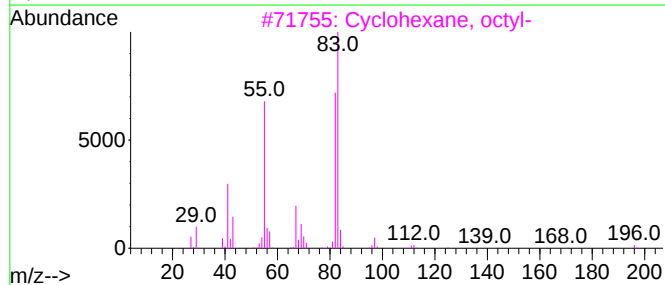
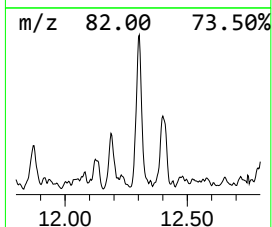
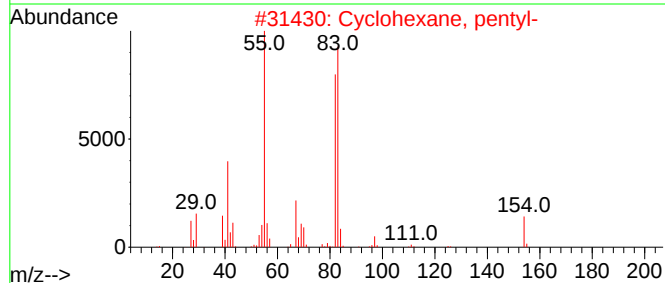
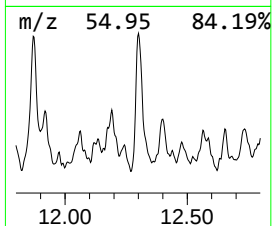
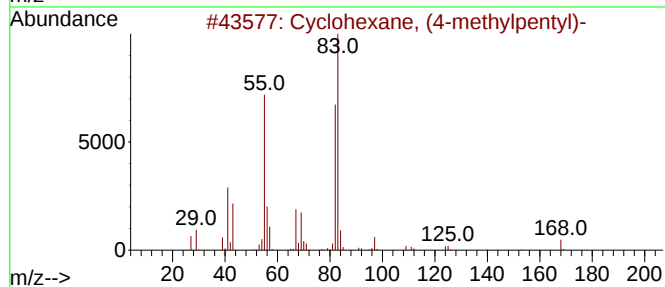
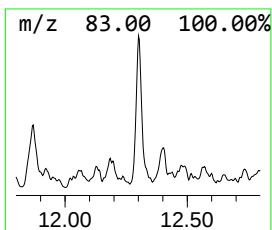
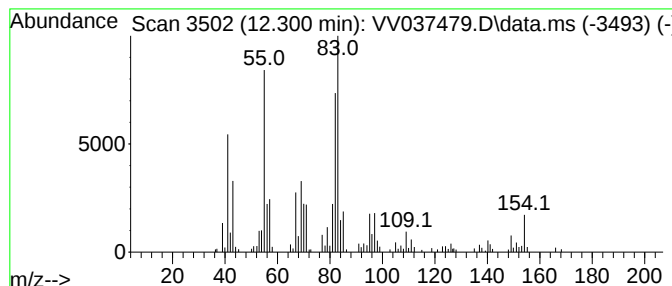
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Cyclic12.300 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.300	4.22 ug/L	169447	1,4-Dichlorobenzene-d4	11.182

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	58
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	58
3			Cyclohexane, octyl-	196	C14H28	001795-15-9	53
4			Cyclohexane, butyl-	140	C10H20	001678-93-9	52
5			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092324\
Data File : VV037479.D
Acq On : 23 Sep 2024 14:07
Operator : SY/MD
Sample : P4109-02ME
Misc : 2.32G/5mL/100ul/5mL/MSVOA_V/MEOH
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A4EH5ME

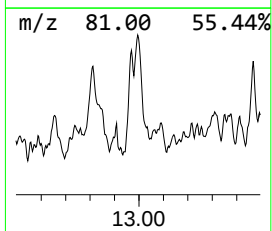
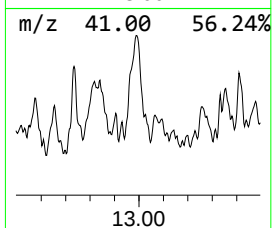
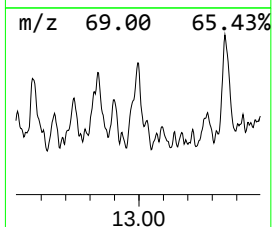
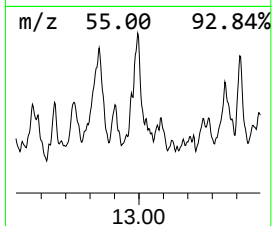
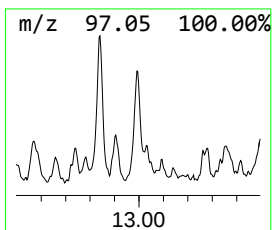
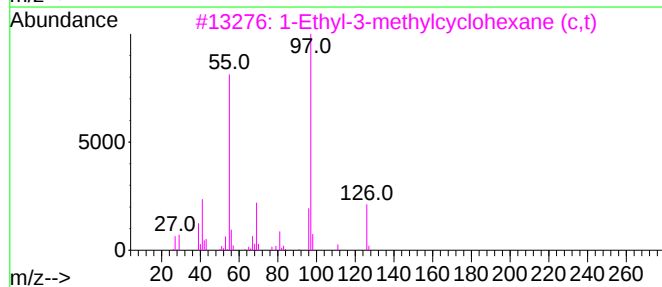
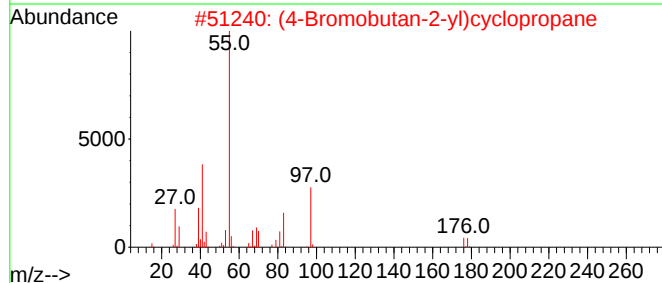
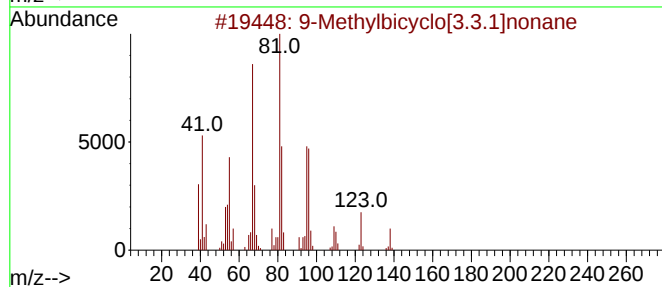
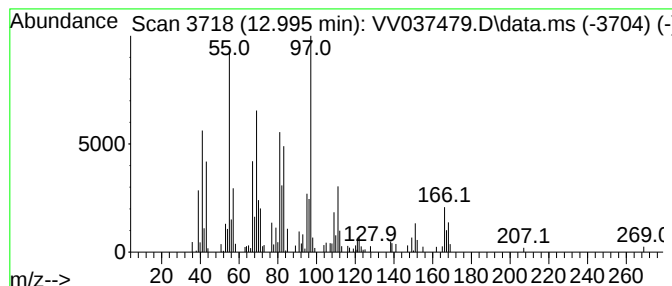
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Quant Title : VOC Analysis

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

Peak Number 6 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.995	3.53 ug/L	141442	1,4-Dichlorobenzene-d4	11.182

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Methylbicyclo[3.3.1]nonane	138	C10H18	025107-01-1	47
2			(4-Bromobutan-2-yl)cyclopropane	176	C7H13Br	1000444-18-1	38
3			1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	27
4			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	27
5			cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV092324\
Data File : VV037479.D
Acq On : 23 Sep 2024 14:07
Operator : SY/MD
Sample : P4109-02ME
Misc : 2.32G/5mL/100ul/5ml/MSVOA_V/MEOH
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A4EH5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.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	75442	1	5.526	1500690	50.0
(DEL) Alkane: S...	10.815	3.0	ug/L	120121	3	11.182	2005680	50.0
(DEL) Alkane: C...	11.870	2.7	ug/L	107715	3	11.182	2005680	50.0
(DEL) Alkane: C...	12.300	4.2	ug/L	169447	3	11.182	2005680	50.0
unknown-01	12.995	3.5	ug/L	141442	3	11.182	2005680	50.0