

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV102124\
 Data File : VV037902.D
 Acq On : 21 Oct 2024 16:40
 Operator : SY/MD
 Sample : P4414-21ME
 Misc : 5.55g/5mL/100ul/5mL/MSVOA_V/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A4F82ME

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\SFAMVLM092624WMA.M

Title : VOC Analysis

Signal : TIC: VV037902.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.098	16	18	24	rVB3	1635	1202	0.11%	0.021%
2	1.169	35	40	41	rBV3	1736	1430	0.13%	0.025%
3	1.188	41	46	50	rVV	10090	10066	0.94%	0.174%
4	1.214	50	54	64	rVV	14242	18121	1.69%	0.314%
5	1.278	66	74	88	rVB	65887	87147	8.15%	1.508%
6	1.446	108	126	127	rBV6	24356	51359	4.80%	0.889%
7	1.465	127	132	135	rBV4	20894	23837	2.23%	0.413%
8	1.484	136	138	139	rBV	10068	4672	0.44%	0.081%
9	1.738	211	217	229	rVB4	10995	19487	1.82%	0.337%
10	1.954	279	284	294	rVB4	6738	9254	0.87%	0.160%
11	2.040	302	311	326	rBV	124929	184101	17.21%	3.186%
12	2.105	329	331	334	rBV4	2003	1483	0.14%	0.026%
13	2.121	334	336	339	rVV4	1749	933	0.09%	0.016%
14	2.310	393	395	402	rBV7	1379	1663	0.16%	0.029%
15	2.372	407	414	415	rBV3	5353	6056	0.57%	0.105%
16	2.548	462	469	476	rBV4	8893	15463	1.45%	0.268%
17	2.796	543	546	554	rBV9	2446	3307	0.31%	0.057%
18	2.841	554	560	564	rBV8	2506	3371	0.32%	0.058%
19	3.828	855	867	875	rBV2	12231	30830	2.88%	0.534%
20	4.236	979	994	1032	rVV2	83429	231911	21.68%	4.014%
21	4.416	1044	1050	1053	rBV5	932	1051	0.10%	0.018%
22	4.941	1200	1213	1245	rBV2	200115	544717	50.92%	9.428%
23	5.076	1252	1255	1261	rVB7	2072	1564	0.15%	0.027%
24	5.532	1388	1397	1426	rBV	59549	149086	13.94%	2.580%
25	5.838	1480	1492	1500	rBV10	5600	13553	1.27%	0.235%
26	5.982	1525	1537	1563	rBV	100475	242694	22.69%	4.201%
27	6.246	1613	1619	1624	rBV6	939	870	0.08%	0.015%
28	6.365	1648	1656	1661	rBV8	3060	5345	0.50%	0.093%
29	6.539	1703	1710	1713	rBV5	2750	3232	0.30%	0.056%
30	6.561	1715	1717	1722	rVV4	1960	1677	0.16%	0.029%
31	6.690	1749	1757	1760	rBV5	840	1038	0.10%	0.018%
32	6.757	1768	1778	1786	rBV8	4073	6885	0.64%	0.119%
33	6.915	1813	1827	1855	rBV2	42787	111296	10.40%	1.926%
34	7.027	1856	1862	1863	rBV4	2418	2105	0.20%	0.036%
35	7.178	1897	1909	1918	rBV5	22134	49980	4.67%	0.865%
36	7.240	1918	1928	1940	rVV	190705	366551	34.26%	6.344%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
 Title : VOC Analysis

37	7.307	1940	1949	1979	rVB	566004	1069787	100.00%	18.516%
38	7.567	2019	2030	2053	rBV4	44524	108332	10.13%	1.875%
39	7.709	2064	2074	2083	rVB7	7565	13317	1.24%	0.230%
40	7.764	2087	2091	2097	rBV7	1300	1453	0.14%	0.025%
41	7.834	2110	2113	2121	rVB6	3388	3088	0.29%	0.053%
42	7.902	2123	2134	2146	rVB6	4621	10804	1.01%	0.187%
43	8.008	2158	2167	2169	rBV7	2518	2700	0.25%	0.047%
44	8.050	2170	2180	2197	rBV2	45274	121046	11.31%	2.095%
45	8.146	2200	2210	2222	rVV2	13988	35968	3.36%	0.623%
46	8.211	2222	2230	2240	rVB3	16691	29683	2.77%	0.514%
47	8.272	2240	2249	2258	rBV2	21410	35887	3.35%	0.621%
48	8.410	2284	2292	2293	rBV6	1150	1413	0.13%	0.024%
49	8.432	2293	2299	2306	rVB5	3341	4351	0.41%	0.075%
50	8.516	2311	2325	2333	rBV10	13324	32341	3.02%	0.560%
51	8.715	2375	2387	2396	rBV10	3987	7409	0.69%	0.128%
52	8.783	2398	2408	2431	rBV	112583	219060	20.48%	3.791%
53	8.921	2442	2451	2459	rBV8	5434	10449	0.98%	0.181%
54	9.037	2476	2487	2491	rBV10	6908	12713	1.19%	0.220%
55	9.082	2494	2501	2508	rVV3	17230	25485	2.38%	0.441%
56	9.239	2541	2550	2563	rVB8	6543	11116	1.04%	0.192%
57	9.339	2574	2581	2583	rBV5	2860	3201	0.30%	0.055%
58	9.403	2586	2601	2610	rBV9	18817	43140	4.03%	0.747%
59	9.481	2619	2625	2629	rBV6	4450	5126	0.48%	0.089%
60	9.510	2630	2634	2641	rVB6	3766	5069	0.47%	0.088%
61	9.632	2656	2672	2684	rVB7	20071	49883	4.66%	0.863%
62	9.683	2684	2688	2689	rBV4	2000	1497	0.14%	0.026%
63	9.728	2690	2702	2713	rVV7	27056	59336	5.55%	1.027%
64	9.776	2713	2717	2730	rVB6	11820	19249	1.80%	0.333%
65	9.844	2730	2738	2742	rBV8	2886	3906	0.37%	0.068%
66	9.902	2750	2756	2763	rBV8	5434	7465	0.70%	0.129%
67	9.950	2764	2771	2786	rVB8	8731	16336	1.53%	0.283%
68	10.018	2790	2792	2794	rBV3	1370	874	0.08%	0.015%
69	10.056	2794	2804	2812	rVB7	13571	21581	2.02%	0.374%
70	10.149	2817	2833	2849	rBV	152443	295844	27.65%	5.120%
71	10.317	2875	2885	2895	rVV	7983	20008	1.87%	0.346%
72	10.378	2895	2904	2913	rVB	9115	19743	1.85%	0.342%
73	10.442	2915	2924	2932	rBV7	13198	22382	2.09%	0.387%
74	10.497	2933	2941	2950	rBV7	10718	20930	1.96%	0.362%
75	10.590	2966	2970	2971	rBV3	2341	1721	0.16%	0.030%
76	10.654	2984	2990	2998	rBV6	9965	16250	1.52%	0.281%

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 ClientSampleId :
 A4F82ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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 Title : VOC Analysis

77	10.815	3031	3040	3045	rBV7	14378	24576	2.30%	0.425%
78	10.963	3075	3086	3090	rBV7	8562	15987	1.49%	0.277%
79	11.079	3114	3122	3131	rVB10	18217	28818	2.69%	0.499%
80	11.185	3146	3155	3175	rBV2	144493	265599	24.83%	4.597%
81	11.317	3193	3196	3203	rBV8	4186	5328	0.50%	0.092%
82	11.397	3217	3221	3229	rVB8	4334	5697	0.53%	0.099%
83	11.487	3237	3249	3255	rBV8	6665	13944	1.30%	0.241%
84	11.554	3256	3270	3293	rBV	292657	529902	49.53%	9.171%
85	11.866	3356	3367	3377	rBV	12103	26349	2.46%	0.456%
86	11.921	3377	3384	3390	rVV	7104	13460	1.26%	0.233%
87	11.960	3390	3396	3407	rVB8	8804	17624	1.65%	0.305%
88	12.059	3418	3427	3434	rVB8	6257	10240	0.96%	0.177%
89	12.101	3438	3440	3442	rBV3	2456	1313	0.12%	0.023%
90	12.178	3454	3464	3465	rBV5	11655	15546	1.45%	0.269%
91	12.307	3493	3504	3513	rBV5	13891	33328	3.12%	0.577%
92	12.400	3525	3533	3546	rBV5	13325	22084	2.06%	0.382%
93	12.738	3630	3638	3648	rVB5	8673	15652	1.46%	0.271%
94	12.943	3691	3702	3705	rBV2	8826	15314	1.43%	0.265%
95	13.136	3758	3762	3771	rBV2	3482	5011	0.47%	0.087%
96	13.207	3778	3784	3792	rBV2	6568	10939	1.02%	0.189%
97	14.021	4032	4037	4041	rBV8	4962	5702	0.53%	0.099%
98	15.519	4496	4503	4514	rVB8	28368	49642	4.64%	0.859%
99	15.799	4585	4590	4597	rVB9	12214	16410	1.53%	0.284%
100	15.863	4606	4610	4621	rVB10	22313	31990	2.99%	0.554%

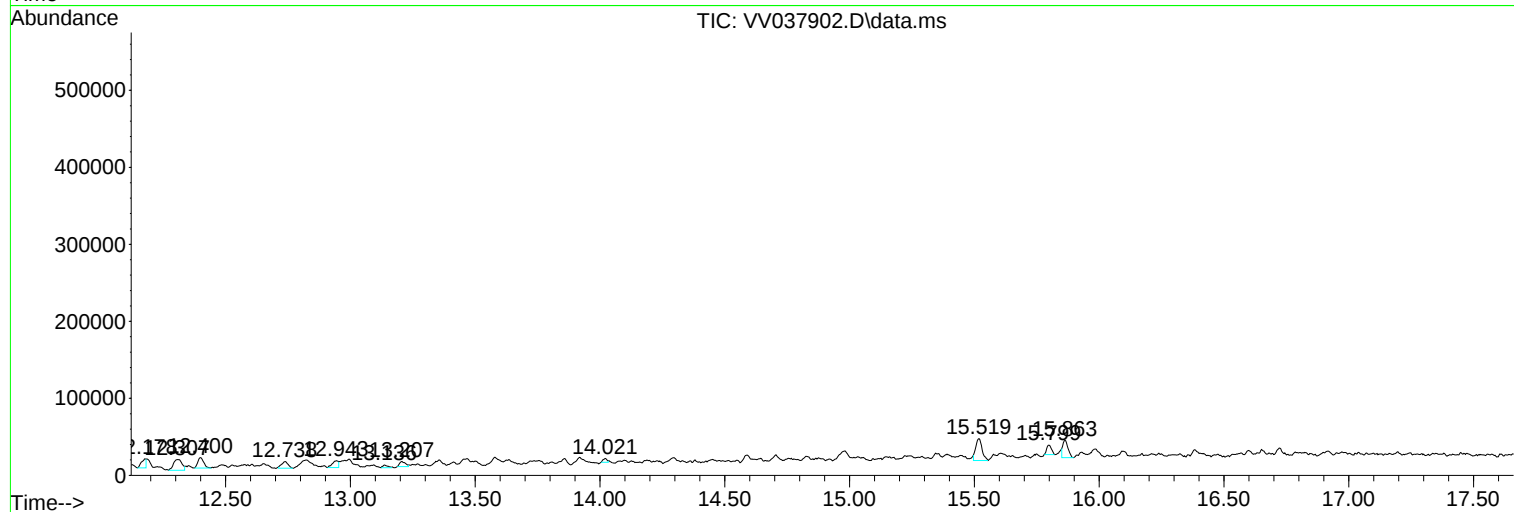
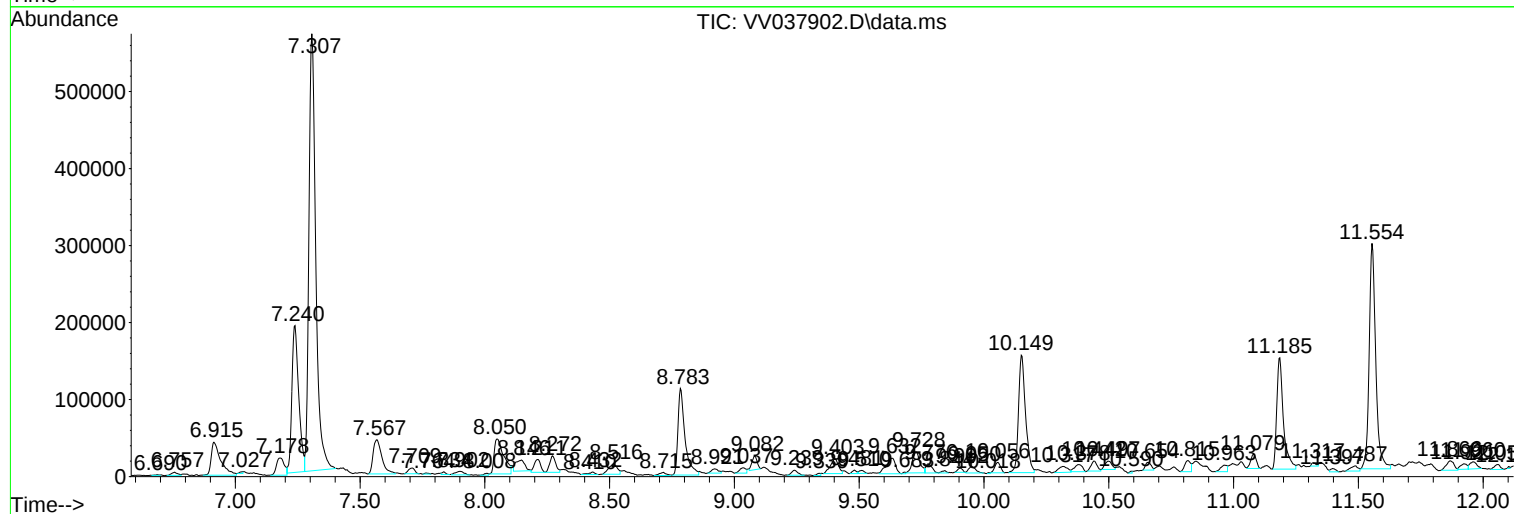
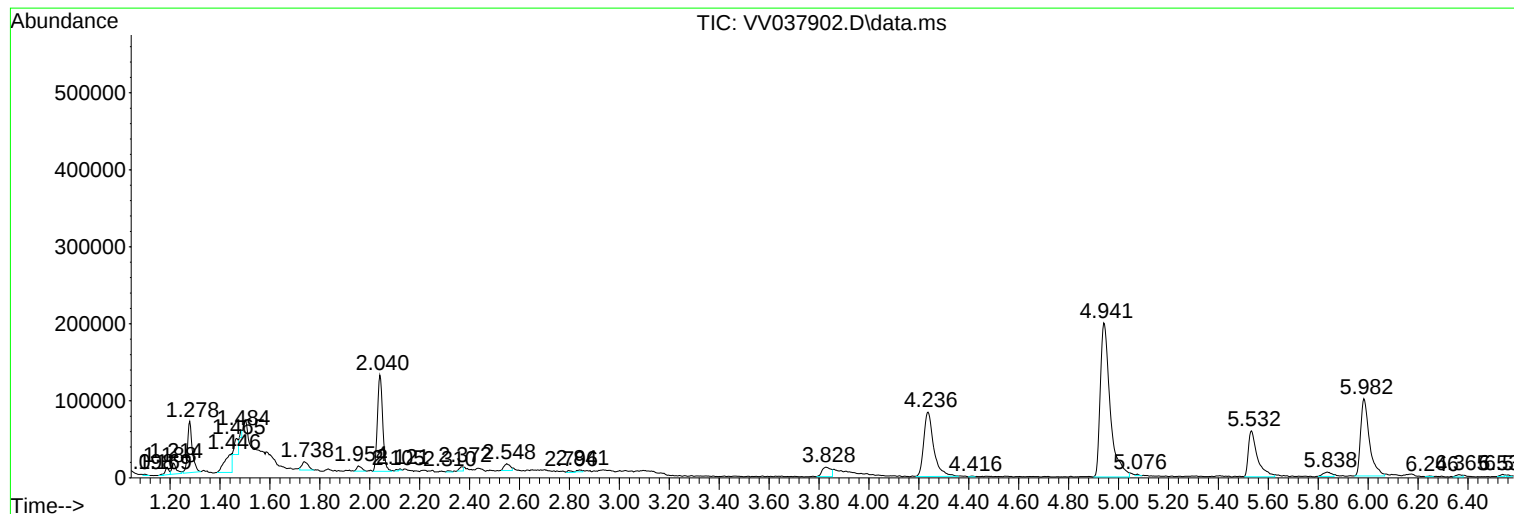
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A4F82ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.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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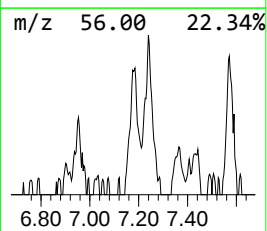
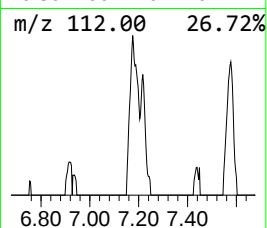
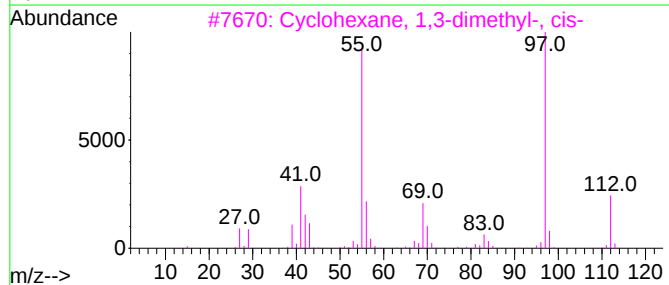
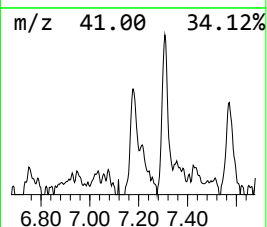
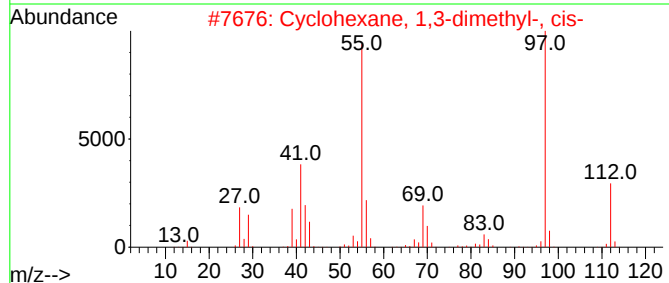
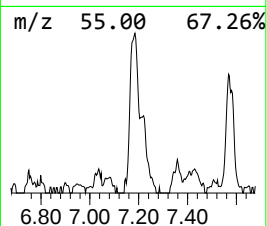
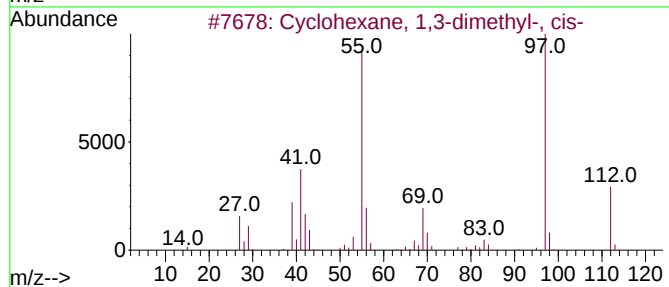
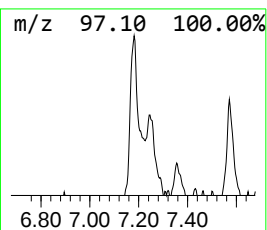
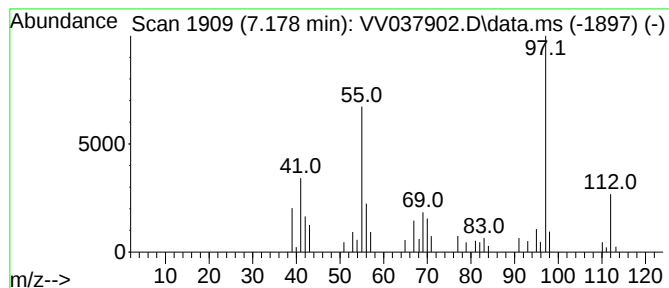
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Cyclic7.178 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.178	11.41 ug/L	49980	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	87
2			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	81
3			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	81
4			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	80
5			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	76



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.M
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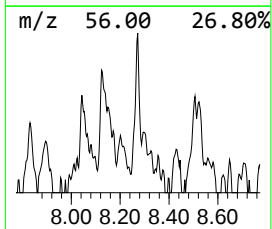
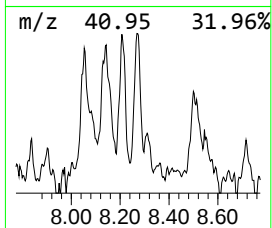
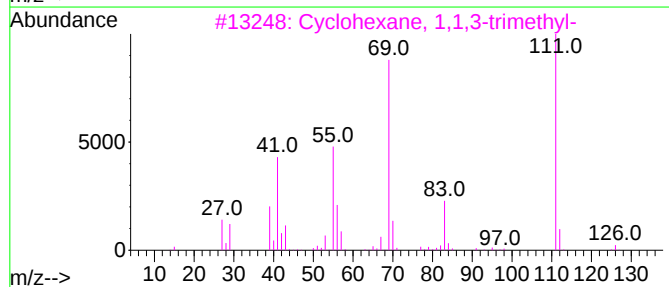
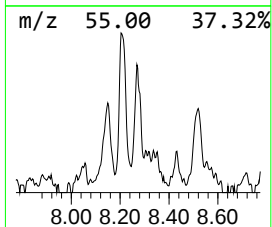
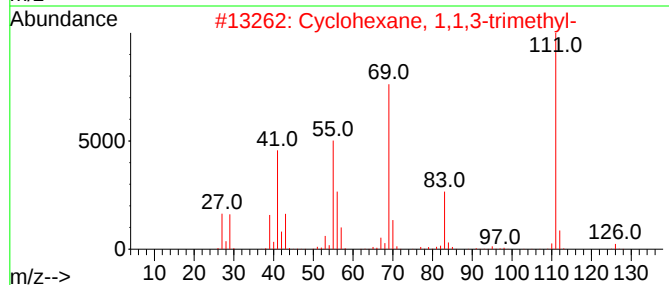
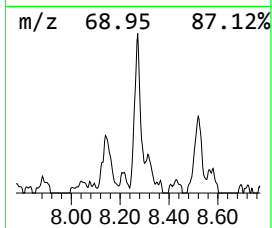
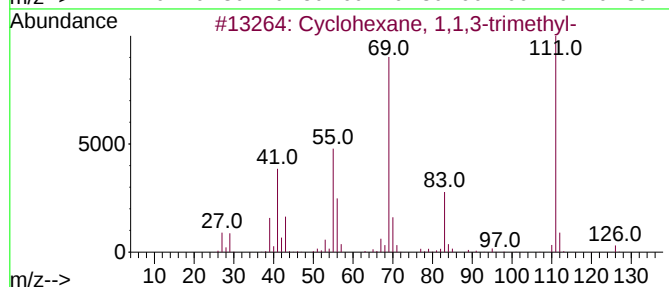
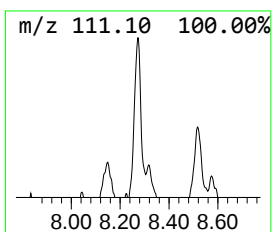
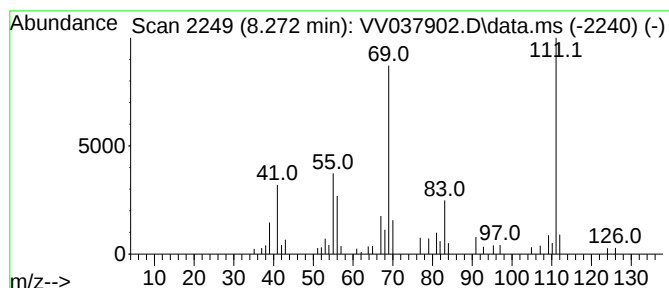
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 10 (DEL) Alkane: Cyclic8.272 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.272	8.19 ug/L	35887	Chlorobenzene-d5	8.783

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	93
2		Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	90
3		Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	83
4		Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	80
5		1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	72



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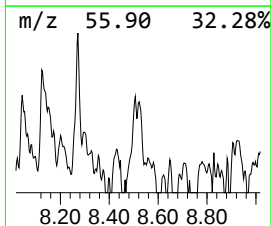
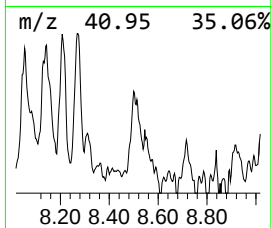
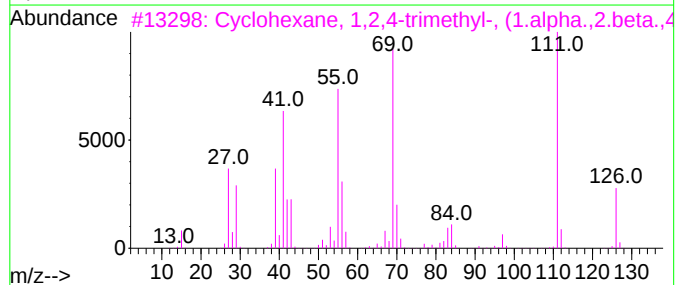
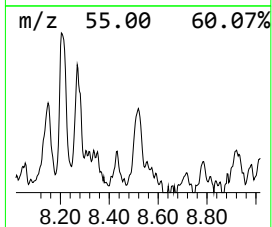
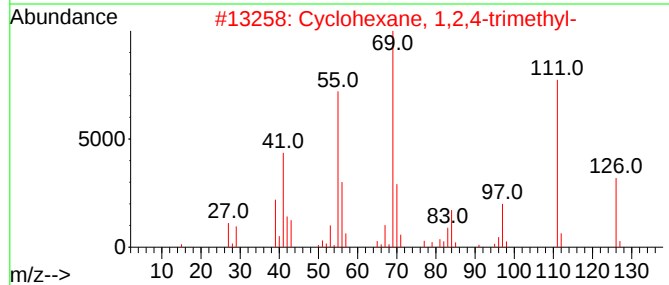
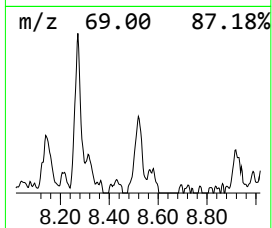
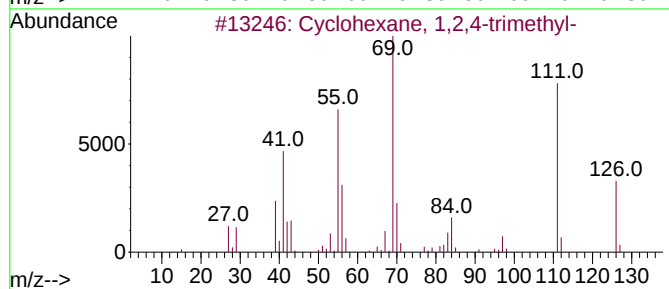
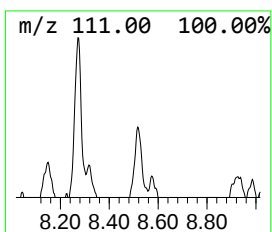
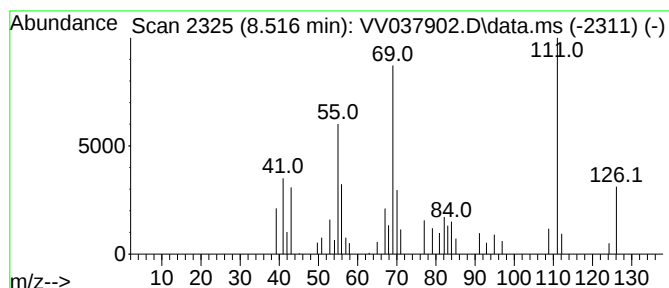
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Quant Title : VOC Analysis

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

Peak Number 11 (DEL) Alkane: Cyclic8.516 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.516	7.38 ug/L	32341	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	87
2			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	87
3			Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	81
4			Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	74
5			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV102124\
Data File : VV037902.D
Acq On : 21 Oct 2024 16:40
Operator : SY/MD
Sample : P4414-21ME
Misc : 5.55g/5mL/100ul/5mL/MSVOA_V/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A4F82ME

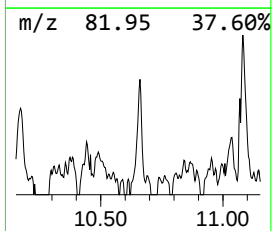
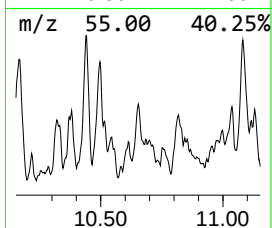
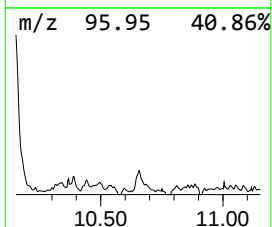
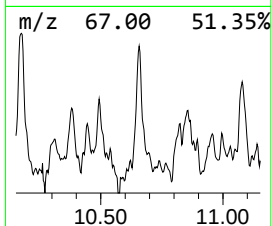
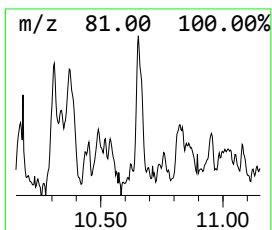
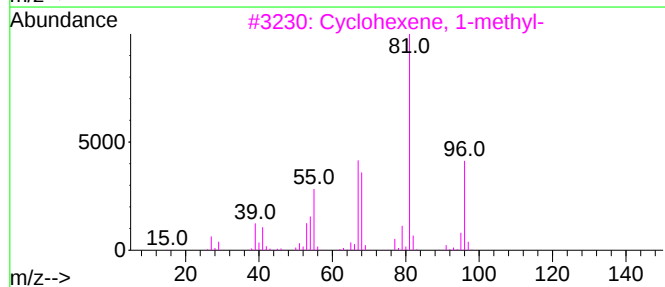
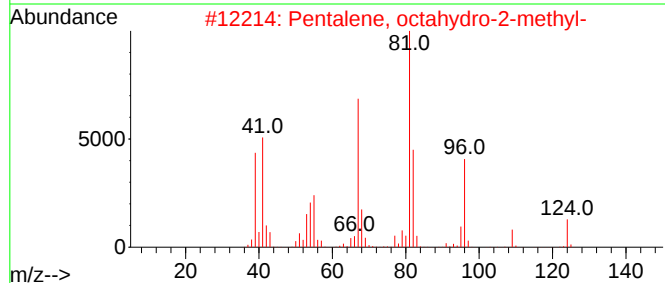
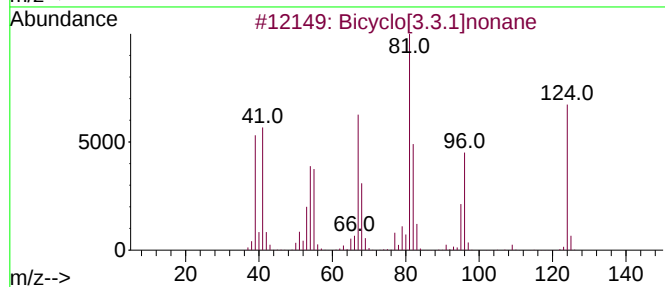
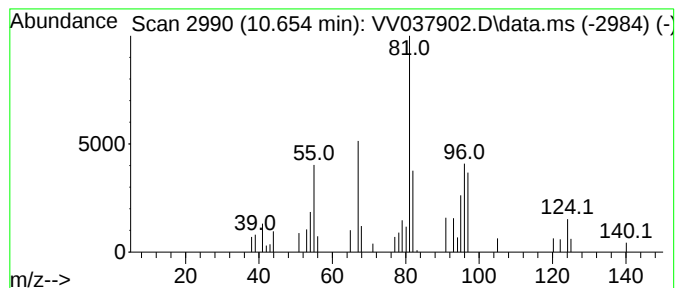
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Quant Title : VOC Analysis

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

Peak Number 25 Bicyclo[3.3.1]nonane Concentration Rank 31

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.654	3.06 ug/L	16250	1,4-Dichlorobenzene-d4	11.185

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	87
2			Pentalene, octahydro-2-methyl-	124	C9H16	003868-64-2	81
3			Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	58
4			Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	58
5			Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV102124\
Data File : VV037902.D
Acq On : 21 Oct 2024 16:40
Operator : SY/MD
Sample : P4414-21ME
Misc : 5.55g/5mL/100ul/5ml/MSVOA_V/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A4F82ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092624WMA.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
(DEL) Alkane: C...	7.178	11.4	ug/L	49980	2	8.783	219060	50.0
(DEL) Alkane: C...	8.272	8.2	ug/L	35887	2	8.783	219060	50.0
(DEL) Alkane: C...	8.516	7.4	ug/L	32341	2	8.783	219060	50.0
Bicyclo[3.3.1]n...	10.654	3.1	ug/L	16250	3	11.185	265599	50.0