

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102523\
 Data File : VU055887.D
 Acq On : 25 Oct 2023 18:22
 Operator : MD/SY
 Sample : 04946-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY1B8

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: VU055887.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	89	96	116	rVB2	384027	479525	5.10%	1.371%
2	1.885	178	185	204	rVV	206960	310905	3.30%	0.889%
3	1.972	205	212	234	rVB2	74019	114667	1.22%	0.328%
4	2.190	275	280	289	rVB2	11621	15557	0.17%	0.044%
5	2.560	382	395	411	rBV2	534815	935854	9.95%	2.676%
6	3.036	529	543	551	rBV	68445	147311	1.57%	0.421%
7	3.178	576	587	620	rVB	57024	154986	1.65%	0.443%
8	3.351	627	641	656	rBV3	53568	120307	1.28%	0.344%
9	3.695	735	748	763	rVV4	11203	26209	0.28%	0.075%
10	3.898	809	811	820	rVB4	766	1007	0.01%	0.003%
11	3.959	825	830	832	rBV3	687	599	0.01%	0.002%
12	4.065	858	863	865	rBV	781	791	0.01%	0.002%
13	4.174	893	897	899	rVV4	794	637	0.01%	0.002%
14	4.354	950	953	958	rBV3	784	785	0.01%	0.002%
15	4.428	965	976	983	rBV6	3009	6376	0.07%	0.018%
16	4.522	989	1005	1022	rBV3	52775	127593	1.36%	0.365%
17	4.657	1023	1047	1092	rBV2	1462446	3779011	40.17%	10.805%
18	5.058	1156	1172	1209	rBV	434566	1008656	10.72%	2.884%
19	5.319	1241	1253	1261	rBV6	8278	21394	0.23%	0.061%
20	5.454	1285	1295	1305	rBV5	9905	22072	0.23%	0.063%
21	5.518	1307	1315	1327	rVB3	20748	41399	0.44%	0.118%
22	5.592	1329	1338	1343	rBV3	6155	11314	0.12%	0.032%
23	5.718	1358	1377	1406	rBV2	915001	2473615	26.29%	7.073%
24	6.126	1496	1504	1509	rBV7	3616	5248	0.06%	0.015%
25	6.245	1527	1541	1569	rBV	679114	1335611	14.20%	3.819%
26	6.447	1600	1604	1606	rBV3	872	698	0.01%	0.002%
27	6.537	1617	1632	1663	rBV	748334	1449115	15.40%	4.143%
28	6.685	1665	1678	1695	rBV	557924	1101730	11.71%	3.150%
29	6.859	1727	1732	1742	rVB5	6417	11402	0.12%	0.033%
30	6.917	1745	1750	1758	rVB7	2515	4044	0.04%	0.012%
31	6.975	1761	1768	1780	rVB7	6188	11065	0.12%	0.032%
32	7.062	1787	1795	1796	rBV8	2395	2487	0.03%	0.007%
33	7.155	1815	1824	1825	rBV3	5728	5762	0.06%	0.016%
34	7.251	1846	1854	1867	rVB2	26194	51060	0.54%	0.146%
35	7.377	1880	1893	1904	rBV3	36275	76423	0.81%	0.219%
36	7.489	1924	1928	1929	rBV4	1090	840	0.01%	0.002%

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Integrator: RTE

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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 >

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

37	7.563	1939	1951	1969	rBV	306290	549430	5.84%	1.571%
38	7.753	2005	2010	2020	rVB9	3010	5170	0.05%	0.015%
39	7.833	2025	2035	2041	rBV4	12149	22563	0.24%	0.065%
40	7.894	2042	2054	2082	rVB	1158811	2001805	21.28%	5.724%
41	8.177	2129	2142	2162	rBV	213067	377315	4.01%	1.079%
42	8.357	2195	2198	2206	rBV8	2539	3035	0.03%	0.009%
43	8.409	2207	2214	2224	rVV	6434	10031	0.11%	0.029%
44	8.550	2243	2258	2274	rBV	5565290	9408597	100.00%	26.901%
45	8.634	2274	2284	2314	rVB	682515	1334066	14.18%	3.814%
46	8.923	2368	2374	2376	rBV6	2924	3038	0.03%	0.009%
47	8.962	2382	2386	2388	rBV5	1261	892	0.01%	0.003%
48	9.065	2411	2418	2427	rVB10	3045	4736	0.05%	0.014%
49	9.119	2427	2435	2439	rBV9	2328	3072	0.03%	0.009%
50	9.161	2441	2448	2449	rBV3	3229	3050	0.03%	0.009%
51	9.332	2491	2501	2511	rBV8	6504	13629	0.14%	0.039%
52	9.415	2514	2527	2548	rBV	1005358	1708638	18.16%	4.885%
53	9.566	2565	2574	2586	rVB	17545	29581	0.31%	0.085%
54	9.798	2643	2646	2652	rVB6	2032	1643	0.02%	0.005%
55	10.023	2707	2716	2727	rVV10	4551	9039	0.10%	0.026%
56	10.074	2727	2732	2739	rVV9	1244	1826	0.02%	0.005%
57	10.119	2739	2746	2753	rVV7	2108	3283	0.03%	0.009%
58	10.351	2812	2818	2821	rBV5	2762	3323	0.04%	0.010%
59	10.553	2874	2881	2886	rBV7	2094	2404	0.03%	0.007%
60	10.753	2929	2943	2971	rBV	870445	1411978	15.01%	4.037%
61	10.901	2980	2989	3002	rVB2	15070	28117	0.30%	0.080%
62	11.023	3021	3027	3031	rBV6	1847	2492	0.03%	0.007%
63	11.187	3075	3078	3079	rBV2	1373	834	0.01%	0.002%
64	11.293	3101	3111	3125	rVB3	18847	34134	0.36%	0.098%
65	11.377	3127	3137	3141	rBV9	2403	4239	0.05%	0.012%
66	11.412	3142	3148	3153	rVB6	4394	5793	0.06%	0.017%
67	11.569	3191	3197	3199	rBV5	3303	3318	0.04%	0.009%
68	11.605	3203	3208	3213	rBV6	4461	5856	0.06%	0.017%
69	11.695	3229	3236	3247	rVB5	8168	13187	0.14%	0.038%
70	11.807	3259	3271	3299	rBV	1132635	1847124	19.63%	5.281%
71	12.068	3349	3352	3353	rBV2	955	606	0.01%	0.002%
72	12.097	3353	3361	3371	rVV5	15114	23404	0.25%	0.067%
73	12.190	3377	3390	3410	rBV	1242432	2027377	21.55%	5.797%
74	12.380	3442	3449	3463	rVB2	10736	19719	0.21%	0.056%
75	12.467	3470	3476	3482	rBV7	4364	6468	0.07%	0.018%
76	12.569	3502	3508	3516	rVB2	7624	10862	0.12%	0.031%

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Integration Parameters: LSCINT.P

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

77	12.679	3534	3542	3557	rBV2	21243	35224	0.37%	0.101%
78	12.762	3565	3568	3572	rVB5	2985	1992	0.02%	0.006%
79	12.859	3594	3598	3607	rVB6	4365	5575	0.06%	0.016%
80	12.907	3609	3613	3615	rBV5	1082	867	0.01%	0.002%
81	12.939	3620	3623	3624	rVV2	1762	1064	0.01%	0.003%
82	12.971	3627	3633	3641	rVV2	16614	24721	0.26%	0.071%
83	13.026	3644	3650	3663	rVB3	19380	29999	0.32%	0.086%
84	13.113	3667	3677	3684	rBV6	5440	11318	0.12%	0.032%
85	13.219	3707	3710	3714	rBV6	1664	1582	0.02%	0.005%
86	13.460	3775	3785	3799	rVB6	6256	10309	0.11%	0.029%
87	13.521	3799	3804	3811	rBV10	2837	3755	0.04%	0.011%
88	13.640	3833	3841	3845	rBV7	2714	4334	0.05%	0.012%
89	13.782	3882	3885	3887	rBV3	3777	2652	0.03%	0.008%
90	13.833	3898	3901	3907	rBV6	3127	3074	0.03%	0.009%
91	14.013	3954	3957	3959	rBV2	1961	1217	0.01%	0.003%
92	14.264	4032	4035	4036	rBV	1293	777	0.01%	0.002%
93	14.553	4121	4125	4128	rBV5	2410	2420	0.03%	0.007%
94	14.669	4154	4161	4169	rBV8	4877	7993	0.08%	0.023%
95	14.807	4199	4204	4212	rBV9	3716	5412	0.06%	0.015%
96	14.881	4221	4227	4232	rVB5	6294	8492	0.09%	0.024%
97	14.974	4254	4256	4260	rBV3	906	768	0.01%	0.002%
98	14.997	4260	4263	4264	rBV3	1193	620	0.01%	0.002%
99	15.164	4312	4315	4317	rBV3	1635	1252	0.01%	0.004%
100	15.421	4388	4395	4401	rBV7	4902	7198	0.08%	0.021%

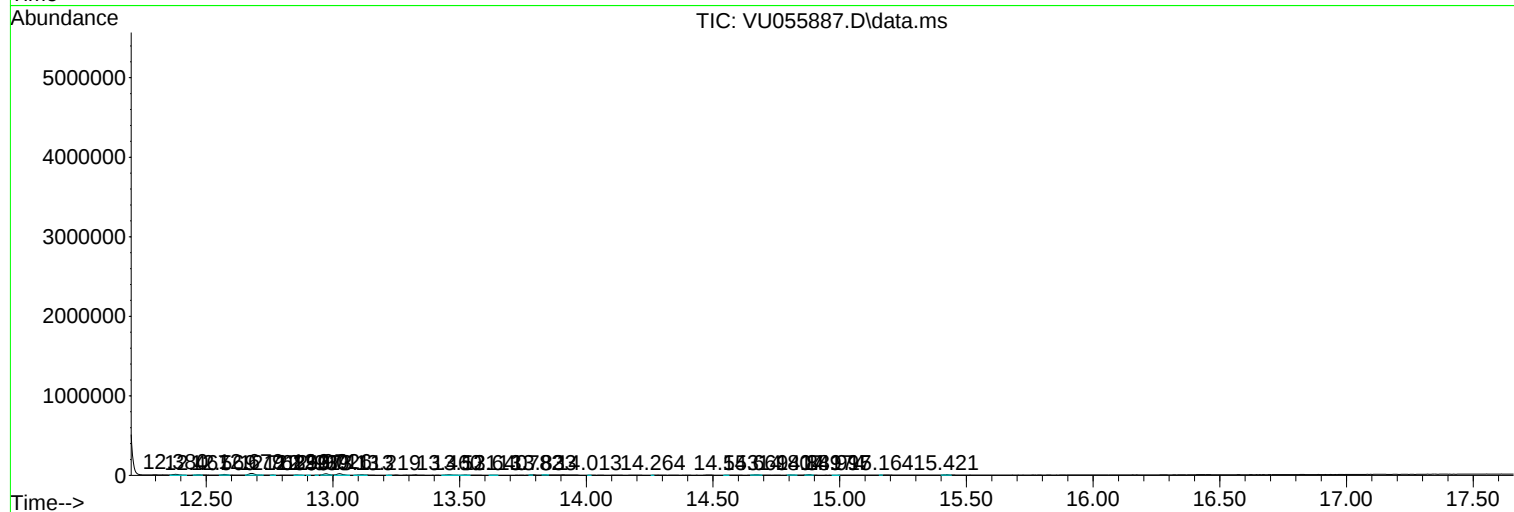
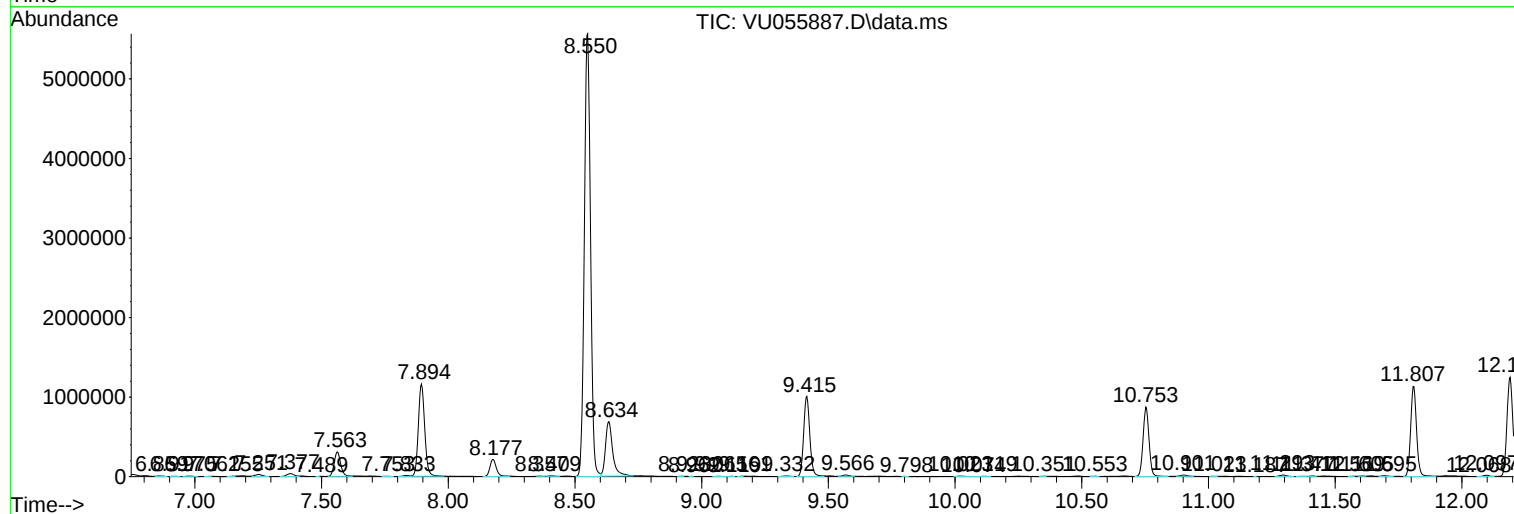
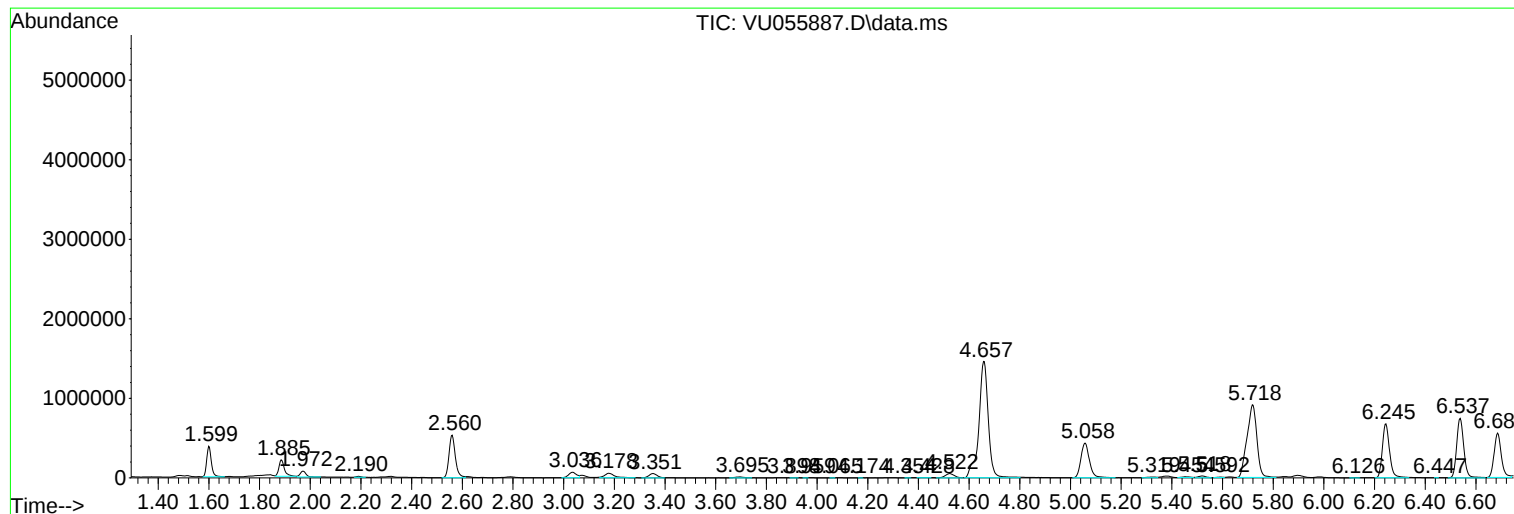
Sum of corrected areas: 34974344

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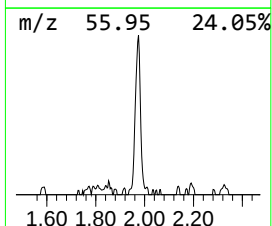
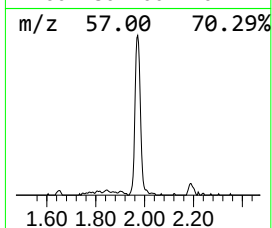
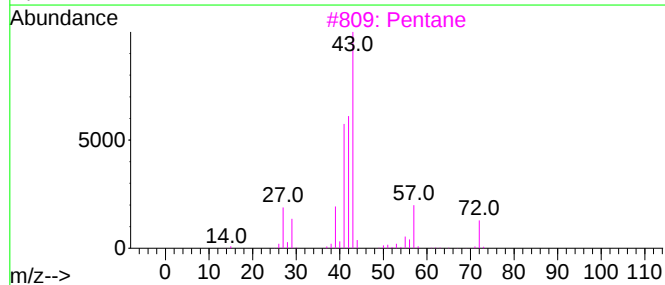
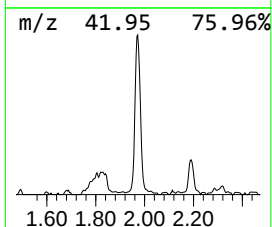
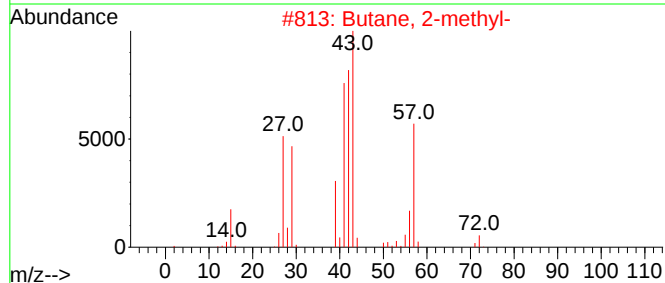
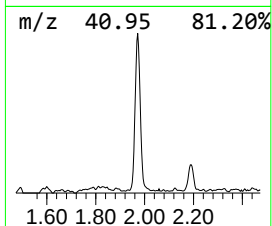
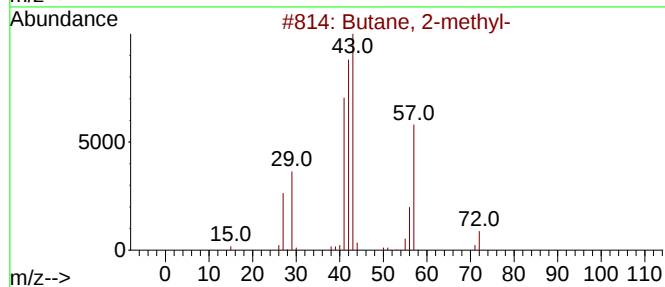
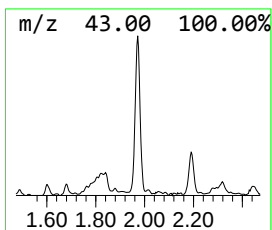
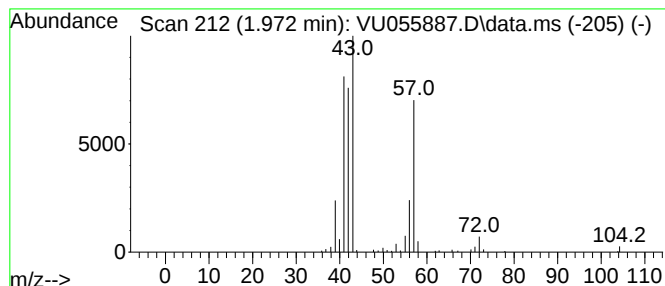
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.972	4.29 ug/L	114667	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	86
2	Butane, 2-methyl-			72	C5H12	000078-78-4	80
3	Pentane			72	C5H12	000109-66-0	50
4	3-Buten-1-ol			72	C4H8O	000627-27-0	43
5	1-Butene			56	C4H8	000106-98-9	10



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Instrument :
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ClientSampleId :
EY1B8

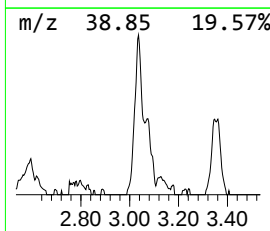
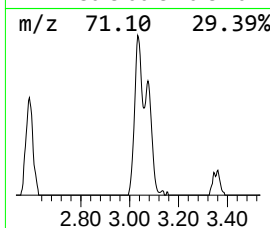
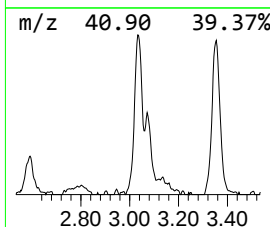
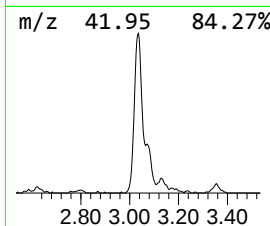
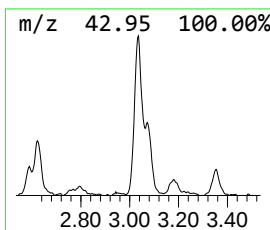
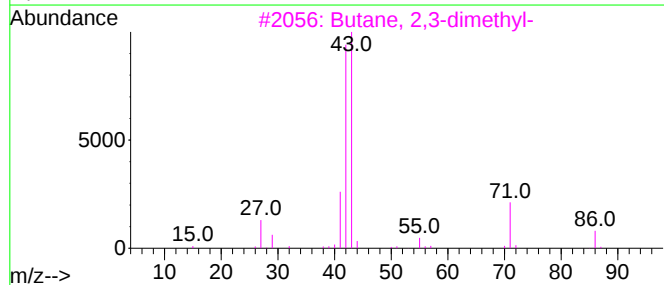
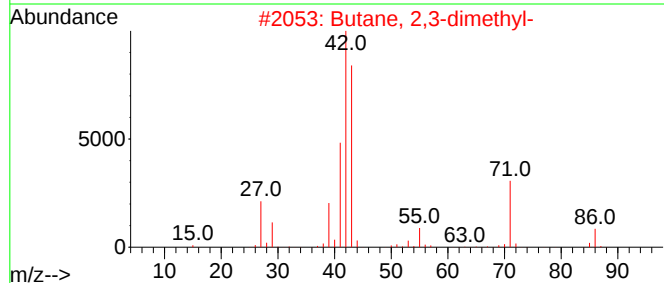
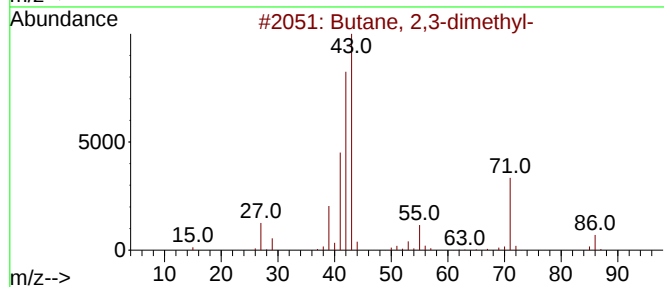
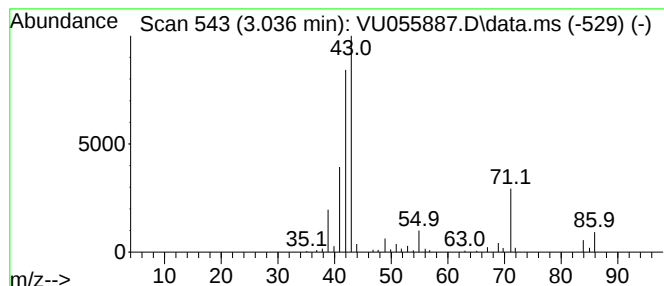
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.036	5.51 ug/L	147311	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
3			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72



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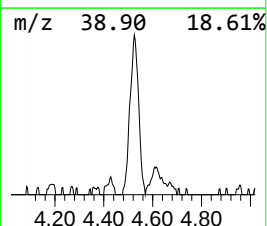
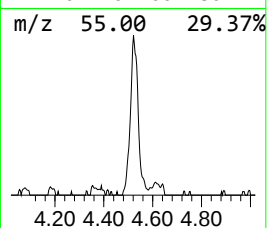
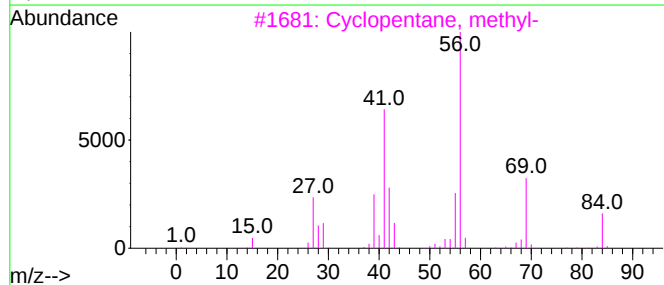
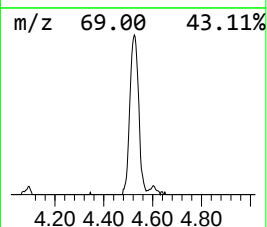
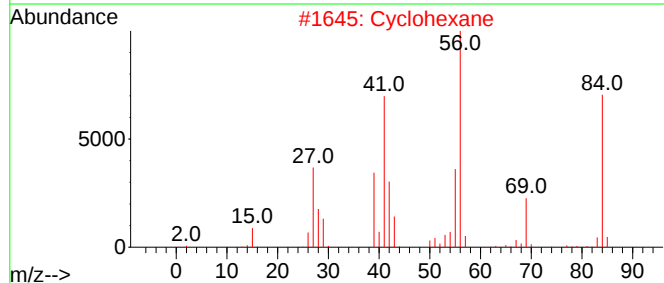
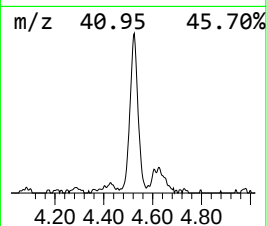
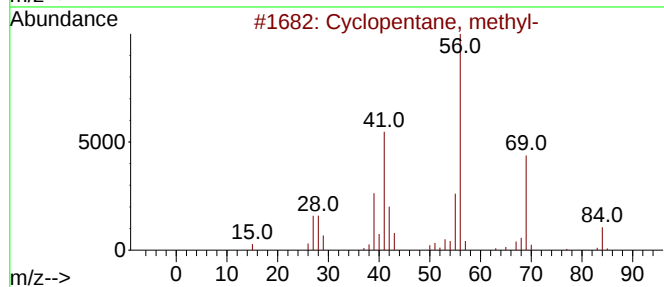
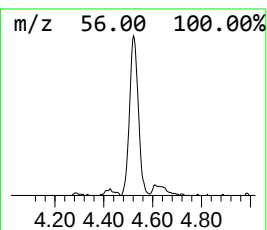
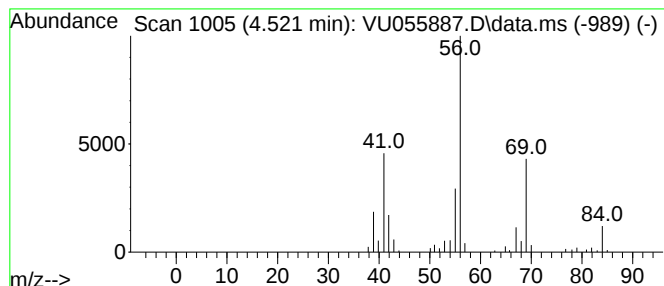
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic4.521 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.521	4.78 ug/L	127593	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		Cyclohexane	84	C6H12	000110-82-7	87
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	86
4		Cyclohexane	84	C6H12	000110-82-7	86
5		Cyclopentane, methyl-	84	C6H12	000096-37-7	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102523\
Data File : VU055887.D
Acq On : 25 Oct 2023 18:22
Operator : MD/SY
Sample : 04946-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY1B8

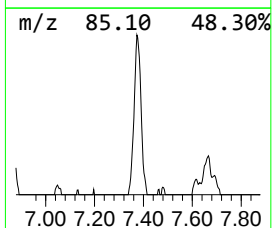
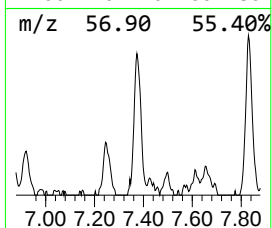
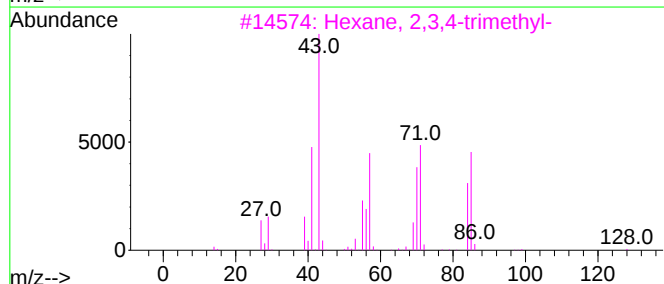
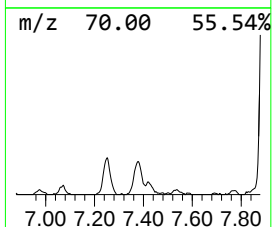
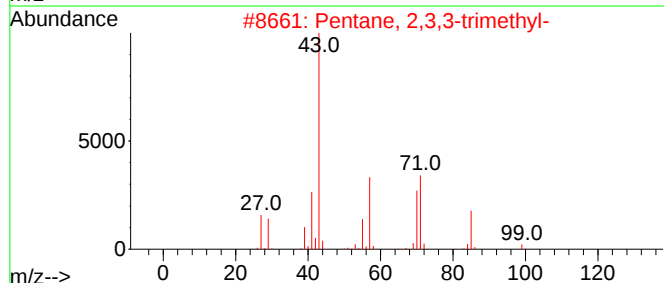
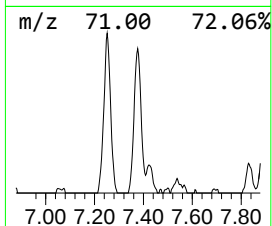
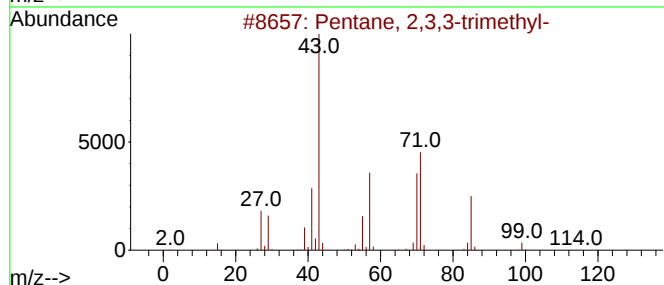
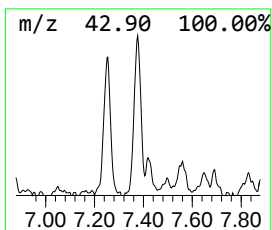
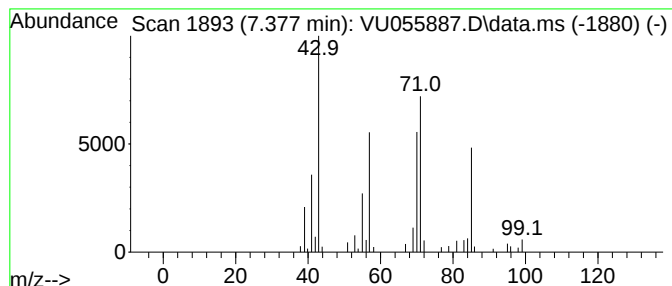
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.377	2.86 ug/L	76423	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
3			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5			Octane, 4-methyl-	128	C9H20	002216-34-4	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102523\
Data File : VU055887.D
Acq On : 25 Oct 2023 18:22
Operator : MD/SY
Sample : 04946-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY1B8

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.972	4.3	ug/L	114667	1	6.245	1335610	50.0
(DEL) Alkane: S...	3.036	5.5	ug/L	147311	1	6.245	1335610	50.0
(DEL) Alkane: C...	4.521	4.8	ug/L	127593	1	6.245	1335610	50.0
(DEL) Alkane: S...	7.377	2.9	ug/L	76423	1	6.245	1335610	50.0