

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102523\
 Data File : VU055878.D
 Acq On : 25 Oct 2023 14:44
 Operator : MD/SY
 Sample : 04946-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY1B1

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: VU055878.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	109	rBV2	283939	342623	3.70%	1.049%
2	1.895	180	188	204	rVV	162539	240638	2.60%	0.737%
3	1.978	208	214	229	rVB	71720	105437	1.14%	0.323%
4	2.194	277	281	292	rVB2	13404	18041	0.19%	0.055%
5	2.560	383	395	423	rBV2	381587	688346	7.42%	2.108%
6	2.785	456	465	477	rVB2	4847	9073	0.10%	0.028%
7	2.956	511	518	519	rBV4	986	1149	0.01%	0.004%
8	3.036	527	543	552	rBV2	66911	150388	1.62%	0.461%
9	3.354	627	642	662	rBV4	51606	116106	1.25%	0.356%
10	3.695	729	748	764	rBV4	10771	25217	0.27%	0.077%
11	4.264	920	925	926	rBV2	929	766	0.01%	0.002%
12	4.280	926	930	934	rBV4	722	820	0.01%	0.003%
13	4.432	963	977	989	rVB5	3403	7743	0.08%	0.024%
14	4.525	991	1006	1023	rBV2	48905	116389	1.26%	0.356%
15	4.660	1023	1048	1079	rBV2	1426328	3745359	40.39%	11.470%
16	4.968	1142	1144	1150	rVB5	1156	838	0.01%	0.003%
17	5.055	1156	1171	1207	rBV	391636	915939	9.88%	2.805%
18	5.319	1242	1253	1255	rBV8	6674	9734	0.10%	0.030%
19	5.522	1307	1316	1327	rVB4	19567	41828	0.45%	0.128%
20	5.592	1327	1338	1344	rBV4	6078	13584	0.15%	0.042%
21	5.721	1358	1378	1407	rBV2	762214	2117723	22.84%	6.485%
22	5.981	1452	1459	1473	rVB7	10095	22832	0.25%	0.070%
23	6.033	1473	1475	1482	rVB5	1122	1177	0.01%	0.004%
24	6.129	1496	1505	1515	rBV8	2411	4629	0.05%	0.014%
25	6.245	1527	1541	1575	rBV	664625	1306295	14.09%	4.000%
26	6.451	1601	1605	1608	rBV4	1248	1101	0.01%	0.003%
27	6.538	1618	1632	1662	rBV	741142	1426102	15.38%	4.367%
28	6.685	1665	1678	1695	rBV	500353	986390	10.64%	3.021%
29	6.862	1726	1733	1742	rVB7	6939	12357	0.13%	0.038%
30	6.914	1742	1749	1758	rVV5	2749	4643	0.05%	0.014%
31	6.978	1758	1769	1782	rVB7	5759	10103	0.11%	0.031%
32	7.065	1790	1796	1806	rVB7	2744	5269	0.06%	0.016%
33	7.187	1813	1834	1842	rBV9	11104	31245	0.34%	0.096%
34	7.248	1846	1853	1870	rVB3	23723	48106	0.52%	0.147%
35	7.377	1879	1893	1903	rBV2	34702	69822	0.75%	0.214%
36	7.480	1920	1925	1926	rBV3	1573	1084	0.01%	0.003%

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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 >

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

37	7.492	1926	1929	1937	rVB5	2339	2054	0.02%	0.006%
38	7.563	1938	1951	1966	rBV	266775	482101	5.20%	1.476%
39	7.837	2024	2036	2042	rBV2	11921	24624	0.27%	0.075%
40	7.894	2042	2054	2083	rVB	926857	1628407	17.56%	4.987%
41	8.177	2129	2142	2157	rBV	190928	331264	3.57%	1.014%
42	8.361	2195	2199	2206	rVB9	1946	2324	0.03%	0.007%
43	8.406	2206	2213	2219	rBV4	7607	9836	0.11%	0.030%
44	8.550	2242	2258	2273	rBV	5477160	9272121	100.00%	28.396%
45	8.631	2274	2283	2315	rVB	721336	1389402	14.98%	4.255%
46	9.071	2413	2420	2426	rVV8	2840	4121	0.04%	0.013%
47	9.116	2432	2434	2441	rVB7	1638	1659	0.02%	0.005%
48	9.168	2443	2450	2455	rBV7	3753	5726	0.06%	0.018%
49	9.332	2494	2501	2511	rBV10	5747	10094	0.11%	0.031%
50	9.412	2514	2526	2547	rBV	985759	1657816	17.88%	5.077%
51	9.566	2567	2574	2587	rVB	18447	29100	0.31%	0.089%
52	9.762	2629	2635	2636	rBV4	2052	1847	0.02%	0.006%
53	9.875	2667	2670	2675	rBV4	829	883	0.01%	0.003%
54	10.017	2711	2714	2718	rBV5	2530	2497	0.03%	0.008%
55	10.110	2739	2743	2755	rBV9	2231	3709	0.04%	0.011%
56	10.348	2812	2817	2822	rBV5	3119	3446	0.04%	0.011%
57	10.483	2854	2859	2867	rVB2	6636	10031	0.11%	0.031%
58	10.544	2873	2878	2884	rBV7	2076	2809	0.03%	0.009%
59	10.669	2908	2917	2922	rBV6	4635	6789	0.07%	0.021%
60	10.753	2930	2943	2963	rBV	845241	1380551	14.89%	4.228%
61	10.904	2982	2990	2999	rVB4	13621	23219	0.25%	0.071%
62	11.113	3049	3055	3056	rBV4	2453	2194	0.02%	0.007%
63	11.190	3077	3079	3085	rVB6	1215	984	0.01%	0.003%
64	11.293	3101	3111	3129	rBV2	16447	30153	0.33%	0.092%
65	11.377	3132	3137	3140	rBV5	1937	1933	0.02%	0.006%
66	11.412	3144	3148	3152	rVB5	2265	2029	0.02%	0.006%
67	11.611	3205	3210	3215	rBV4	3884	4446	0.05%	0.014%
68	11.640	3215	3219	3227	rVB7	5833	7509	0.08%	0.023%
69	11.695	3230	3236	3243	rVB7	5009	7954	0.09%	0.024%
70	11.807	3259	3271	3301	rBV	1058734	1733204	18.69%	5.308%
71	12.097	3348	3361	3371	rBV5	14356	26959	0.29%	0.083%
72	12.190	3376	3390	3412	rVV	1053578	1771595	19.11%	5.425%
73	12.303	3418	3425	3430	rBV9	2539	4013	0.04%	0.012%
74	12.373	3442	3447	3459	rVB2	8638	14305	0.15%	0.044%
75	12.463	3466	3475	3482	rBV5	6151	10790	0.12%	0.033%
76	12.569	3502	3508	3519	rVB5	6918	11219	0.12%	0.034%

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 Title : VOC Analysis

77	12.679	3533	3542	3552	rBV3	21312	33413	0.36%	0.102%
78	12.762	3563	3568	3574	rVB6	1843	1903	0.02%	0.006%
79	12.814	3581	3584	3586	rBV3	1622	958	0.01%	0.003%
80	12.865	3594	3600	3609	rVB9	3152	4764	0.05%	0.015%
81	12.971	3627	3633	3642	rVB3	12055	17787	0.19%	0.054%
82	13.026	3642	3650	3657	rBV2	13205	19782	0.21%	0.061%
83	13.113	3669	3677	3683	rBV9	5562	8498	0.09%	0.026%
84	13.322	3738	3742	3750	rVB6	3379	3495	0.04%	0.011%
85	13.389	3758	3763	3764	rBV2	1215	878	0.01%	0.003%
86	13.528	3800	3806	3813	rVV6	3357	3916	0.04%	0.012%
87	13.563	3815	3817	3820	rVV3	1442	793	0.01%	0.002%
88	13.589	3823	3825	3829	rVB3	1725	1197	0.01%	0.004%
89	13.637	3829	3840	3850	rBV3	3105	6488	0.07%	0.020%
90	13.788	3880	3887	3893	rBV7	4555	6513	0.07%	0.020%
91	13.830	3897	3900	3901	rBV3	2462	1386	0.01%	0.004%
92	13.913	3920	3926	3932	rBV7	2723	3141	0.03%	0.010%
93	14.013	3953	3957	3962	rBV4	1384	1577	0.02%	0.005%
94	14.335	4053	4057	4059	rBV5	1622	1278	0.01%	0.004%
95	14.409	4077	4080	4082	rBV2	1061	755	0.01%	0.002%
96	14.489	4098	4105	4109	rBV8	1994	2685	0.03%	0.008%
97	14.666	4155	4160	4173	rVB9	4169	6674	0.07%	0.020%
98	14.714	4173	4175	4178	rBV4	1207	890	0.01%	0.003%
99	14.807	4201	4204	4212	rVB7	1924	2232	0.02%	0.007%
100	14.875	4218	4225	4236	rVB7	4484	7832	0.08%	0.024%

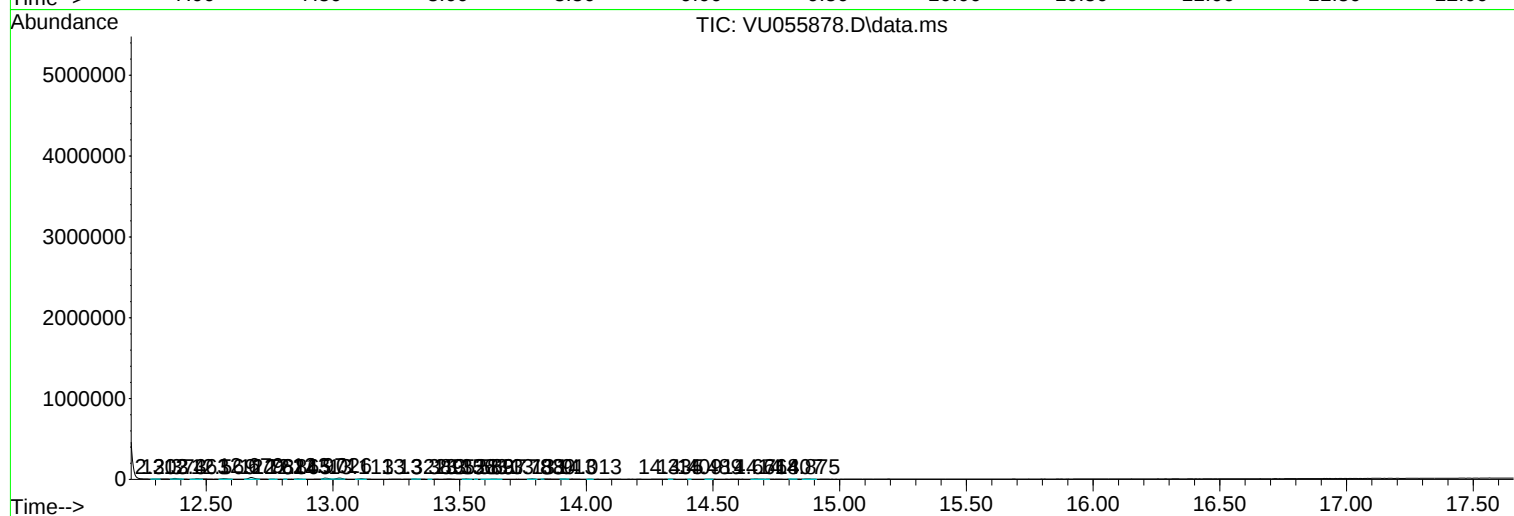
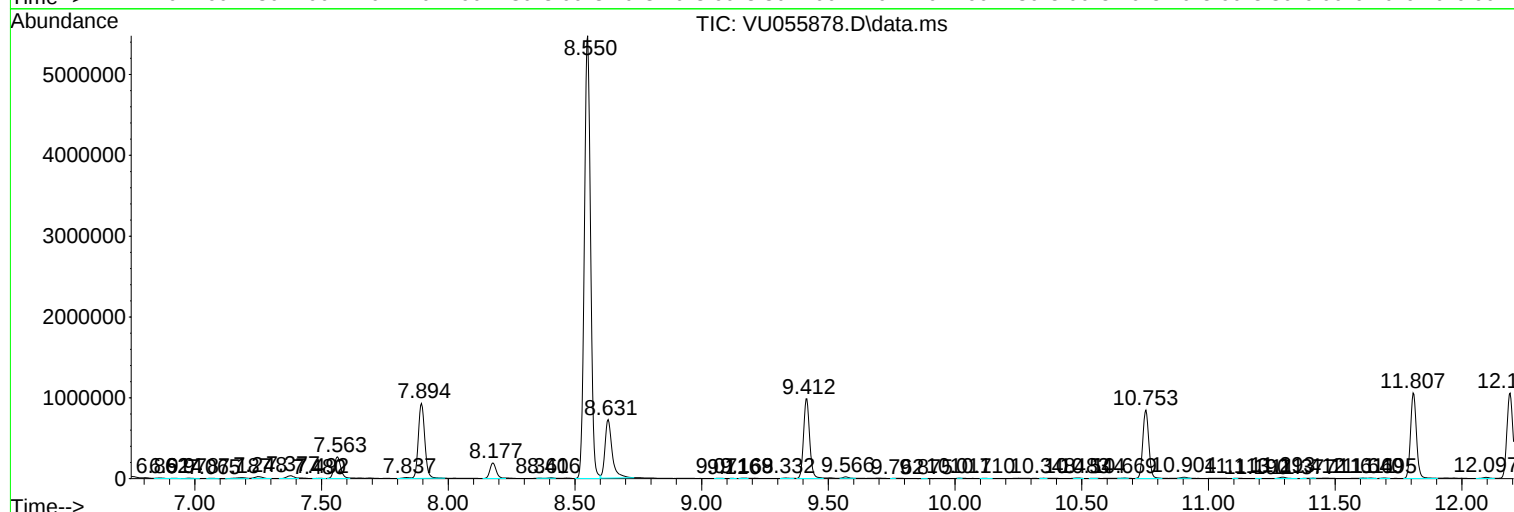
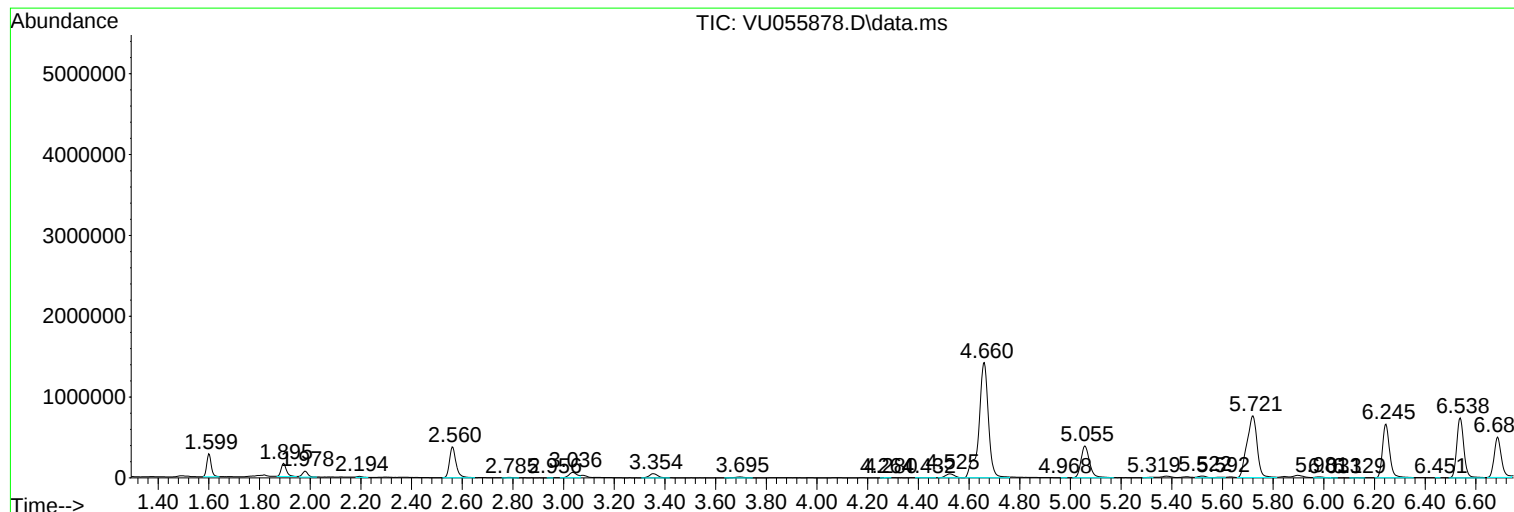
Sum of corrected areas: 32653448

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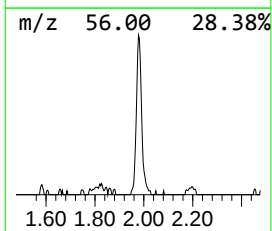
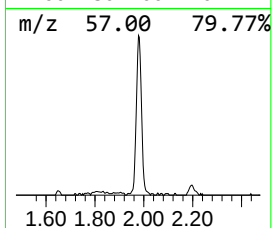
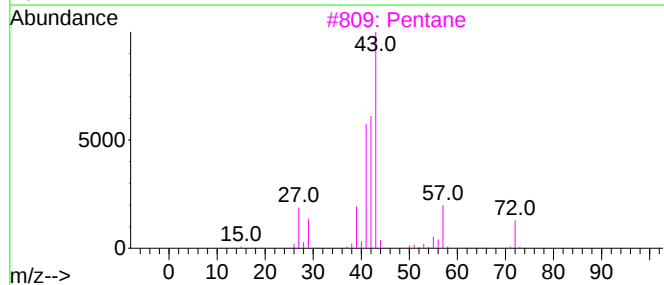
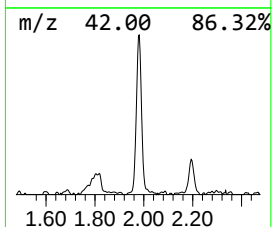
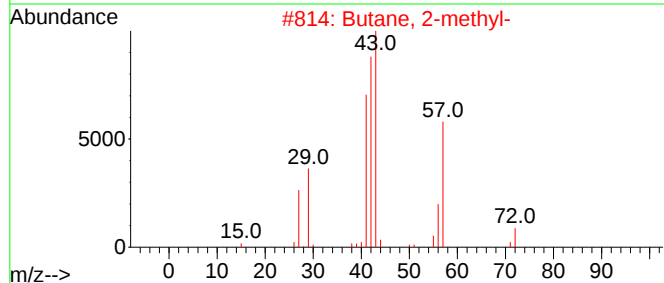
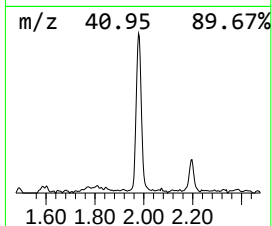
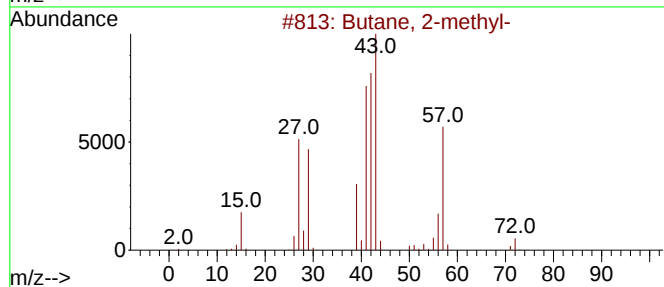
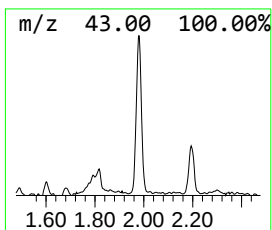
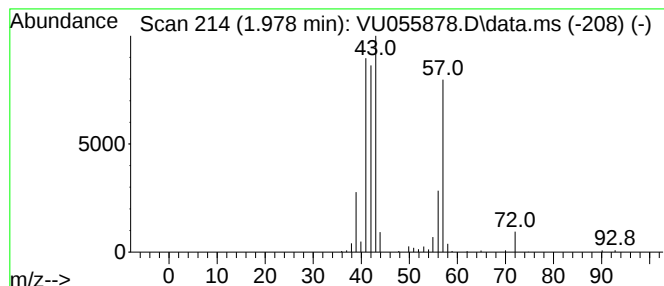
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.978	4.04 ug/L	105437	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	86
3			Pentane	72	C5H12	000109-66-0	33
4			3-Buten-1-ol	72	C4H8O	000627-27-0	25
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	14



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EY1B1

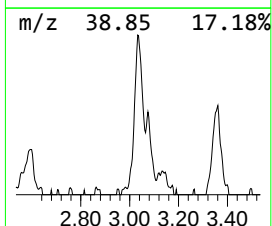
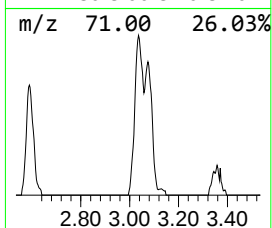
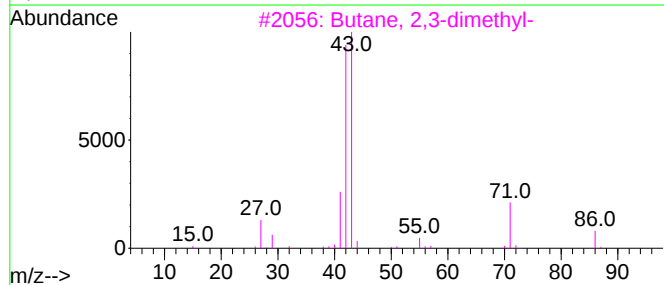
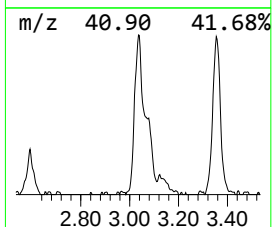
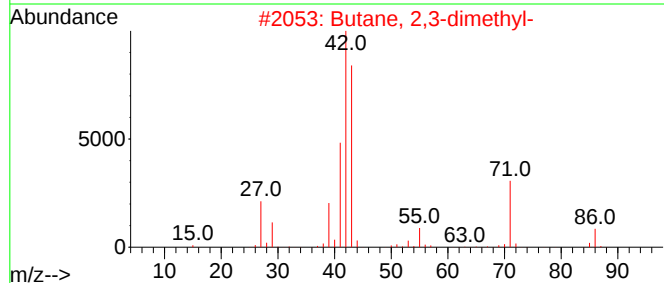
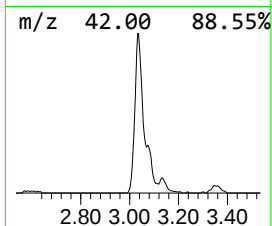
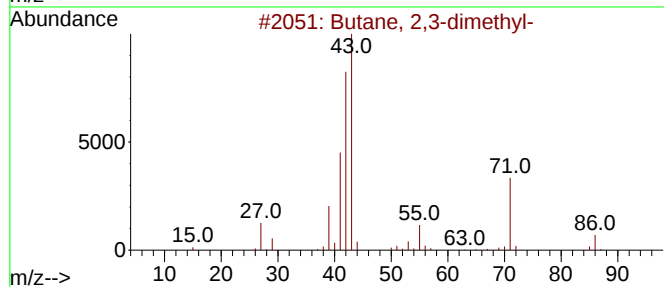
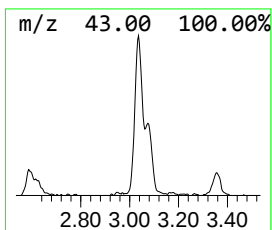
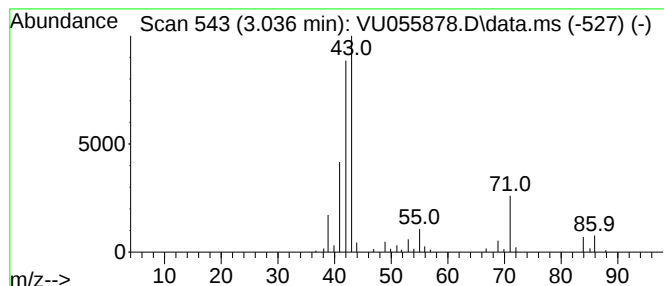
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.036	5.76 ug/L	150388	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	83
3			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72



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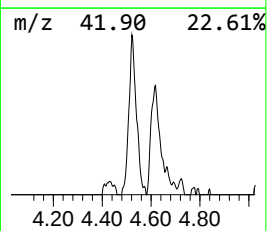
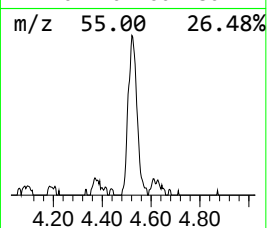
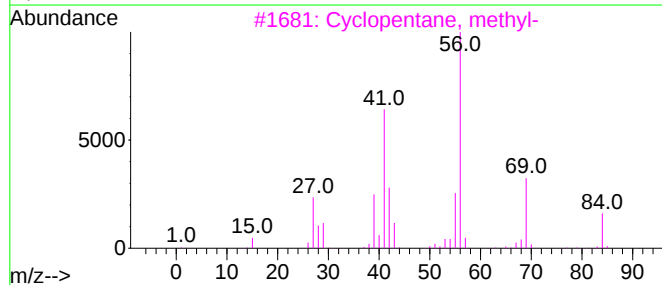
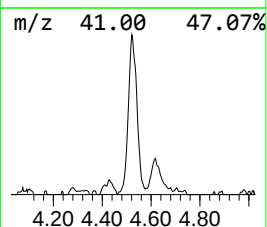
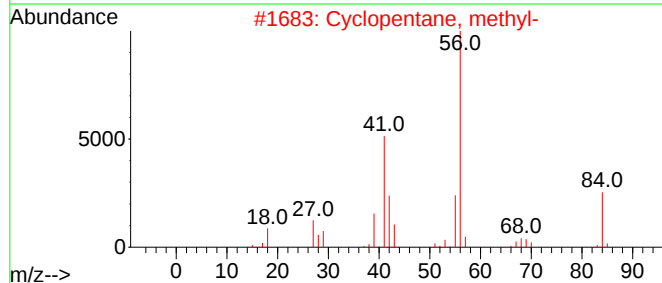
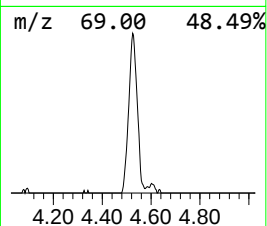
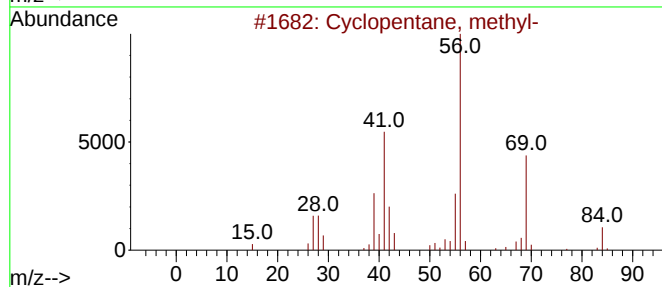
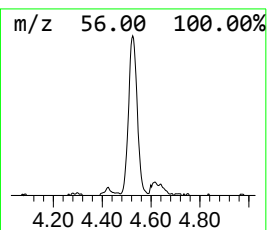
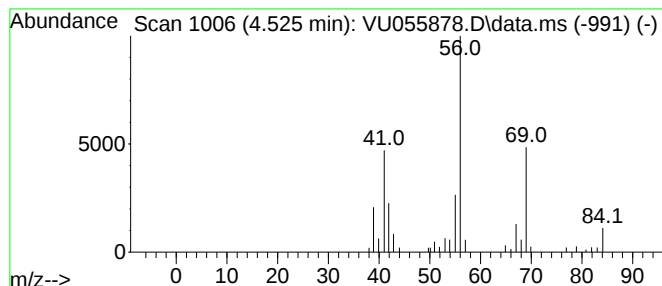
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Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Cyclic4.525 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.525	4.45 ug/L	116389	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	80
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	80
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102523\
Data File : VU055878.D
Acq On : 25 Oct 2023 14:44
Operator : MD/SY
Sample : 04946-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY1B1

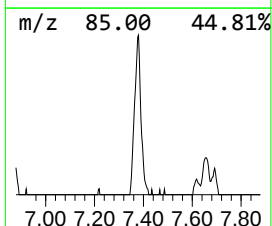
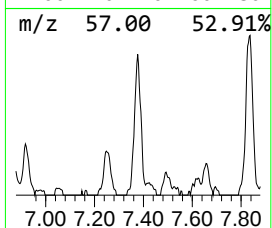
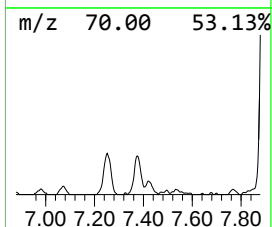
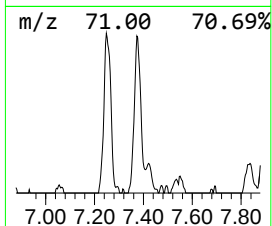
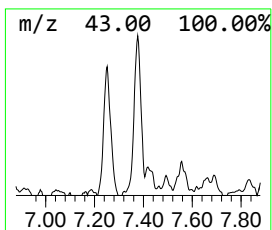
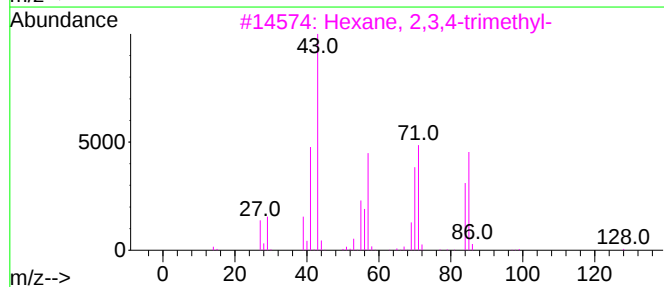
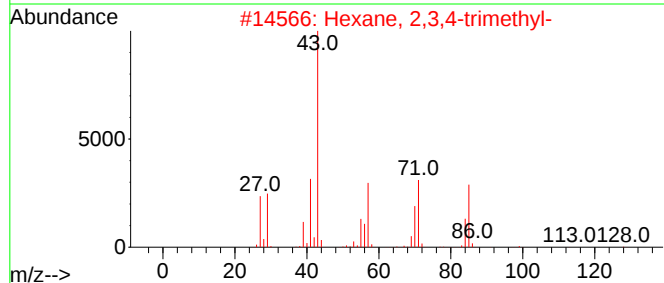
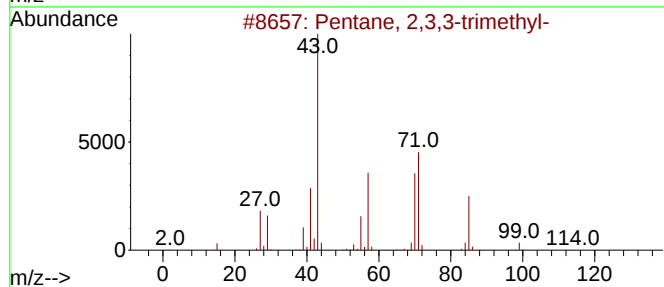
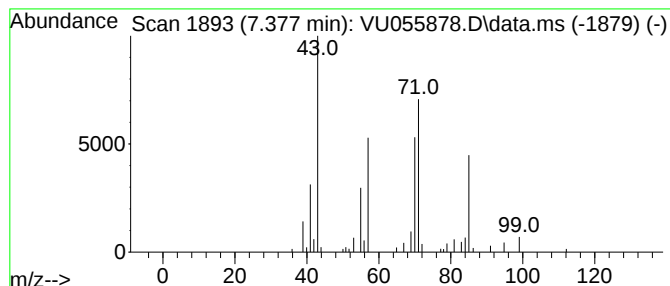
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.377	2.67 ug/L	69822	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	83
2		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
3		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	56
4		Hexadecane	226	C16H34	000544-76-3	53
5		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102523\
Data File : VU055878.D
Acq On : 25 Oct 2023 14:44
Operator : MD/SY
Sample : 04946-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EY1B1

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...	1.978	4.0	ug/L	105437	1	6.245	1306300	50.0
(DEL) Alkane: S...	3.036	5.8	ug/L	150388	1	6.245	1306300	50.0
(DEL) Alkane: C...	4.525	4.5	ug/L	116389	1	6.245	1306300	50.0
(DEL) Alkane: S...	7.377	2.7	ug/L	69822	1	6.245	1306300	50.0