

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101123\
 Data File : VU055748.D
 Acq On : 11 Oct 2023 15:22
 Operator : MD/SY
 Sample : 04792-06
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY1B4

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: VU055748.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.486	55	61	68	rBV	47113	49949	0.55%	0.168%
2	1.599	87	96	110	rBV2	413414	484411	5.38%	1.630%
3	1.885	178	185	203	rVB	163661	239748	2.66%	0.807%
4	1.972	204	212	225	rVB	74070	107523	1.19%	0.362%
5	2.190	274	280	290	rVB	17748	23825	0.26%	0.080%
6	2.457	355	363	373	rVB4	8482	13848	0.15%	0.047%
7	2.557	381	394	411	rBV2	365605	622080	6.91%	2.093%
8	2.695	435	437	440	rBV3	797	644	0.01%	0.002%
9	2.843	481	483	491	rVB3	942	895	0.01%	0.003%
10	2.888	494	497	503	rVB3	607	479	0.01%	0.002%
11	3.001	525	532	533	rBV4	2077	1952	0.02%	0.007%
12	3.126	561	571	583	rBV2	16118	32371	0.36%	0.109%
13	3.348	625	640	661	rBV3	37973	76478	0.85%	0.257%
14	3.493	682	685	691	rVB2	407	356	0.00%	0.001%
15	3.579	709	712	715	rBV2	696	469	0.01%	0.002%
16	3.666	735	739	741	rBV3	475	344	0.00%	0.001%
17	3.692	741	747	748	rBV4	1385	1193	0.01%	0.004%
18	3.750	761	765	767	rBV2	516	328	0.00%	0.001%
19	3.785	772	776	778	rVV	627	337	0.00%	0.001%
20	3.866	787	801	823	rVB3	10789	28165	0.31%	0.095%
21	4.026	846	851	855	rBV2	403	356	0.00%	0.001%
22	4.075	863	866	867	rBV3	587	365	0.00%	0.001%
23	4.165	884	894	899	rBV5	1456	2711	0.03%	0.009%
24	4.251	918	921	925	rVB4	579	464	0.01%	0.002%
25	4.522	990	1005	1023	rBV4	12523	30552	0.34%	0.103%
26	4.657	1023	1047	1077	rBV	3826725	9005530	100.00%	30.306%
27	5.055	1156	1171	1200	rBV	328107	740702	8.22%	2.493%
28	5.287	1239	1243	1245	rBV5	925	730	0.01%	0.002%
29	5.383	1265	1273	1290	rVB7	8310	18177	0.20%	0.061%
30	5.518	1303	1315	1331	rVB3	9517	21616	0.24%	0.073%
31	5.579	1331	1334	1337	rBV3	1074	698	0.01%	0.002%
32	5.718	1355	1377	1409	rBV2	668163	1900404	21.10%	6.395%
33	5.959	1448	1452	1453	rBV5	668	500	0.01%	0.002%
34	5.972	1454	1456	1458	rVV2	765	419	0.00%	0.001%
35	6.023	1468	1472	1473	rBV3	528	419	0.00%	0.001%
36	6.084	1488	1491	1494	rBV2	457	351	0.00%	0.001%

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 Title : VOC Analysis

37	6.123	1499	1503	1506	rVV	409	364	0.00%	0.001%
38	6.245	1526	1541	1562	rBV	524966	1031384	11.45%	3.471%
39	6.441	1597	1602	1608	rVB5	717	767	0.01%	0.003%
40	6.467	1608	1610	1614	rVB2	842	480	0.01%	0.002%
41	6.538	1615	1632	1657	rBV	458893	889485	9.88%	2.993%
42	6.685	1665	1678	1696	rBV2	412906	809755	8.99%	2.725%
43	6.927	1749	1753	1754	rBV3	500	336	0.00%	0.001%
44	6.978	1763	1769	1772	rBV4	851	950	0.01%	0.003%
45	7.026	1781	1784	1789	rVB	565	377	0.00%	0.001%
46	7.155	1821	1824	1826	rBV2	468	323	0.00%	0.001%
47	7.187	1827	1834	1835	rBV4	3300	2851	0.03%	0.010%
48	7.335	1875	1880	1883	rVB2	494	432	0.00%	0.001%
49	7.396	1891	1899	1904	rVB4	729	983	0.01%	0.003%
50	7.499	1927	1931	1936	rBV2	408	371	0.00%	0.001%
51	7.563	1936	1951	1973	rBV	223954	414296	4.60%	1.394%
52	7.894	2041	2054	2076	rBV	804223	1411629	15.68%	4.751%
53	8.052	2101	2103	2107	rVB4	990	498	0.01%	0.002%
54	8.177	2129	2142	2171	rBV	158785	280885	3.12%	0.945%
55	8.357	2196	2198	2203	rVB2	553	454	0.01%	0.002%
56	8.396	2203	2210	2211	rBV3	3087	2628	0.03%	0.009%
57	8.470	2226	2233	2238	rVV4	1337	1898	0.02%	0.006%
58	8.550	2243	2258	2274	rBV	3001288	5099706	56.63%	17.162%
59	8.634	2274	2284	2319	rVB3	522890	1180857	13.11%	3.974%
60	8.946	2378	2381	2385	rBV3	622	499	0.01%	0.002%
61	8.981	2389	2392	2397	rVB3	977	880	0.01%	0.003%
62	9.013	2397	2402	2404	rBV4	626	545	0.01%	0.002%
63	9.267	2478	2481	2485	rVB4	562	411	0.00%	0.001%
64	9.299	2489	2491	2494	rVB2	727	346	0.00%	0.001%
65	9.332	2498	2501	2504	rBV2	524	382	0.00%	0.001%
66	9.415	2513	2527	2557	rBV	778231	1344205	14.93%	4.524%
67	9.656	2599	2602	2606	rBV3	622	571	0.01%	0.002%
68	9.698	2611	2615	2620	rVB4	976	1303	0.01%	0.004%
69	9.862	2664	2666	2674	rVV2	517	570	0.01%	0.002%
70	10.100	2736	2740	2744	rBV2	463	492	0.01%	0.002%
71	10.129	2744	2749	2750	rVV2	604	477	0.01%	0.002%
72	10.261	2785	2790	2794	rBV2	764	680	0.01%	0.002%
73	10.357	2815	2820	2822	rBV2	435	360	0.00%	0.001%
74	10.489	2855	2861	2868	rVB3	1895	2319	0.03%	0.008%
75	10.753	2930	2943	2965	rBV	670085	1106532	12.29%	3.724%
76	10.888	2980	2985	2995	rVB5	1766	2951	0.03%	0.010%

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 Title : VOC Analysis

77	10.936	2995	3000	3004	rVB4	406	411	0.00%	0.001%
78	10.965	3004	3009	3014	rBV2	538	530	0.01%	0.002%
79	11.171	3067	3073	3076	rBV2	499	491	0.01%	0.002%
80	11.232	3090	3092	3096	rVB2	666	409	0.00%	0.001%
81	11.258	3096	3100	3103	rBV2	410	356	0.00%	0.001%
82	11.277	3103	3106	3110	rBV3	535	354	0.00%	0.001%
83	11.373	3132	3136	3139	rBV2	495	365	0.00%	0.001%
84	11.521	3175	3182	3184	rBV2	557	552	0.01%	0.002%
85	11.666	3223	3227	3230	rBV2	447	348	0.00%	0.001%
86	11.811	3259	3272	3295	rBV	817700	1331727	14.79%	4.482%
87	11.949	3314	3315	3323	rVB3	1024	708	0.01%	0.002%
88	12.084	3355	3357	3359	rBV3	658	389	0.00%	0.001%
89	12.190	3376	3390	3417	rBV	825734	1366544	15.17%	4.599%
90	12.676	3538	3541	3543	rBV2	1044	619	0.01%	0.002%
91	12.769	3565	3570	3579	rVB5	1045	1503	0.02%	0.005%
92	12.971	3629	3633	3635	rBV2	481	434	0.00%	0.001%
93	13.132	3680	3683	3687	rBV4	519	459	0.01%	0.002%
94	13.241	3715	3717	3722	rVB	635	363	0.00%	0.001%
95	13.766	3876	3880	3884	rBV2	738	696	0.01%	0.002%
96	13.804	3889	3892	3896	rBV3	397	336	0.00%	0.001%
97	13.865	3905	3911	3916	rBV5	1157	1483	0.02%	0.005%
98	14.087	3977	3980	3983	rBV2	619	398	0.00%	0.001%
99	15.052	4278	4280	4284	rVB2	698	431	0.00%	0.001%
100	15.116	4298	4300	4302	rBV3	680	408	0.00%	0.001%

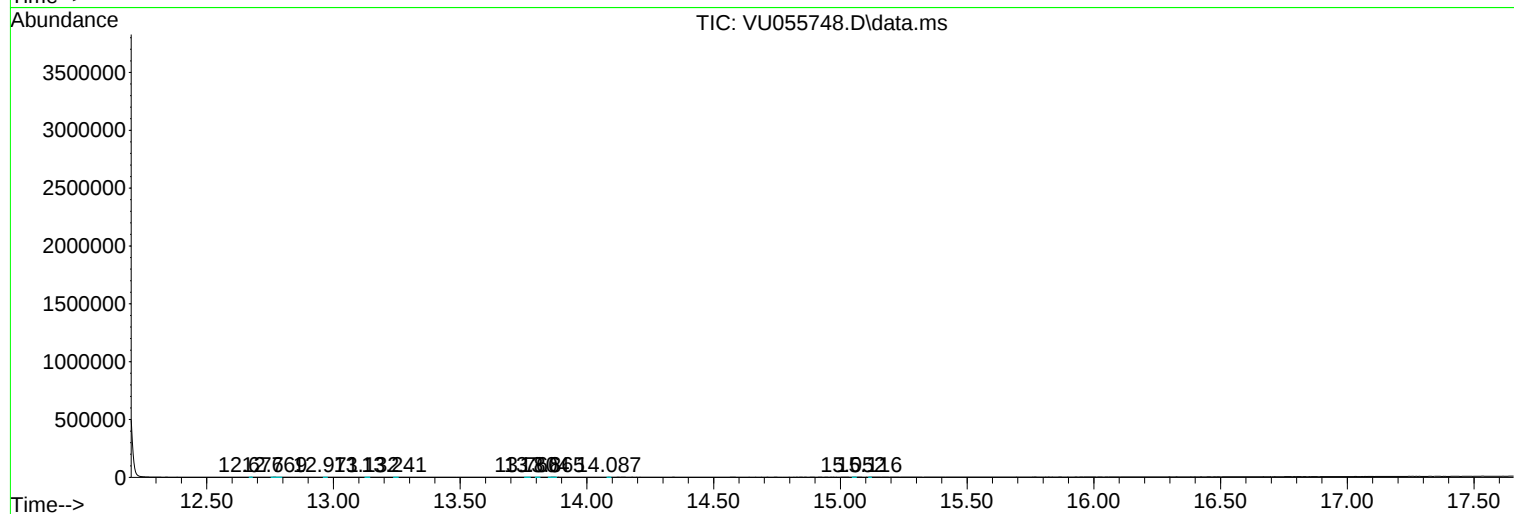
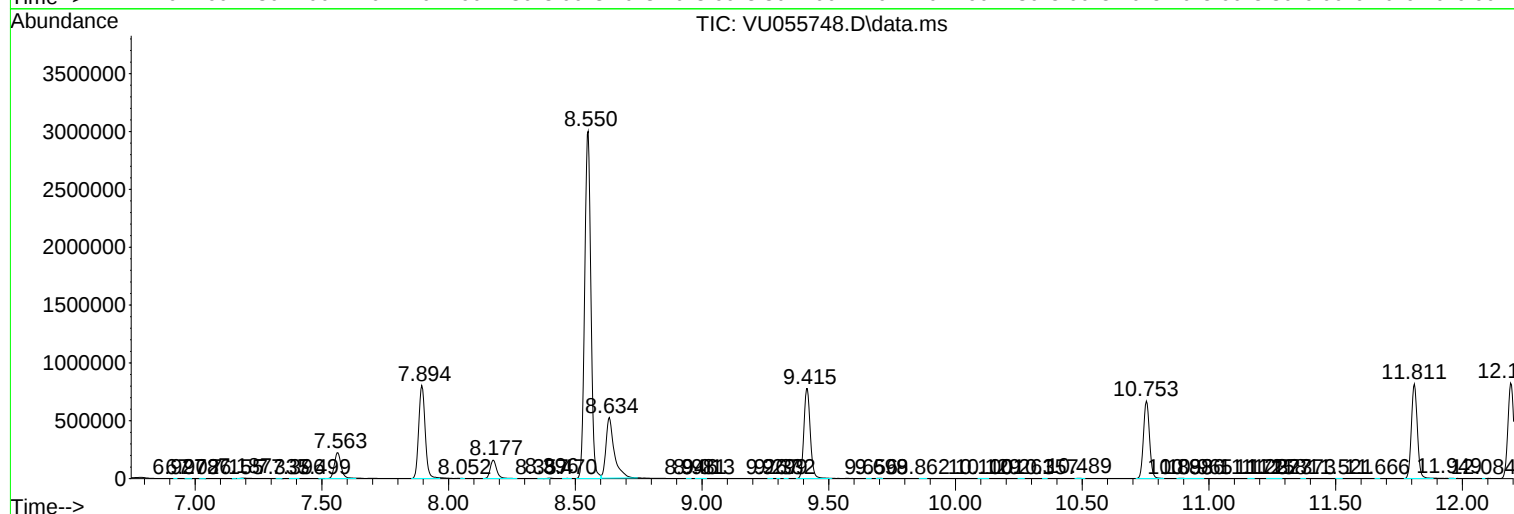
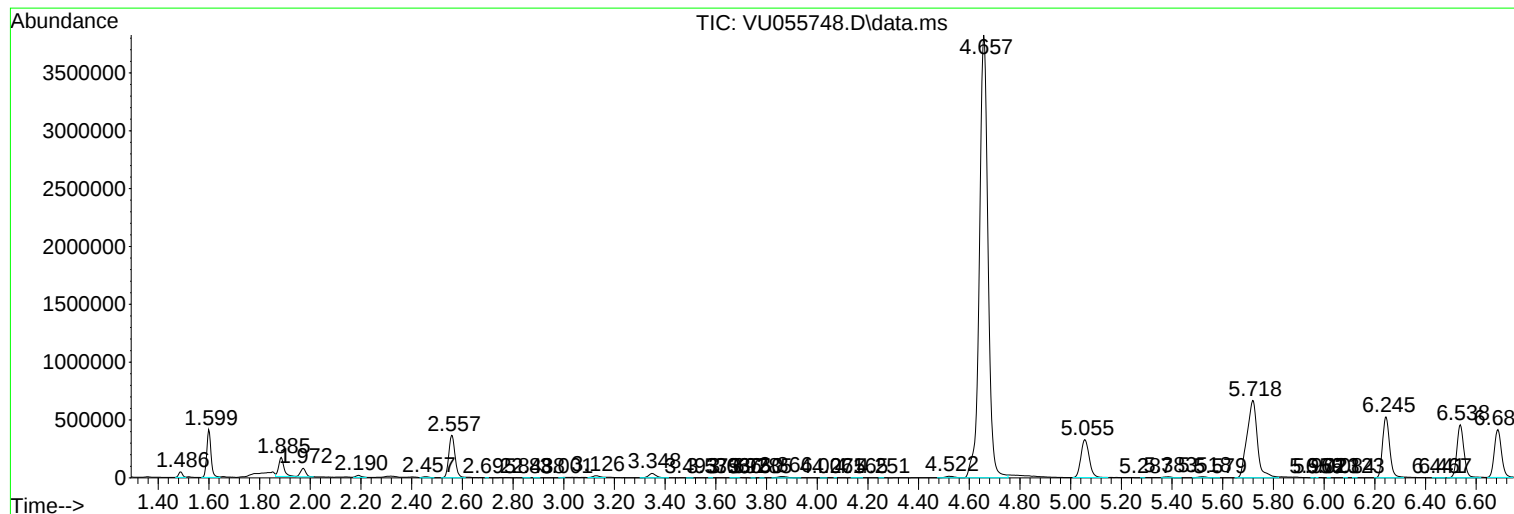
Sum of corrected areas: 29714935

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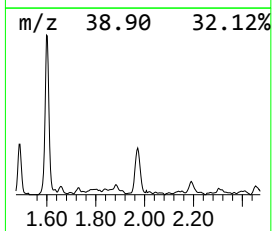
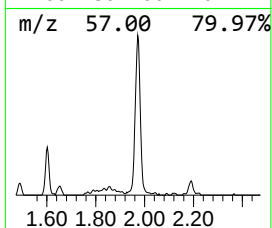
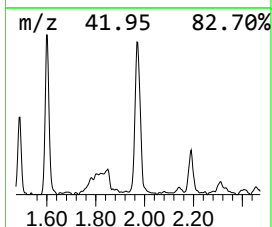
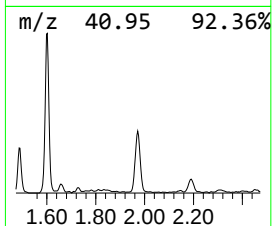
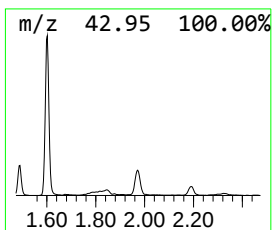
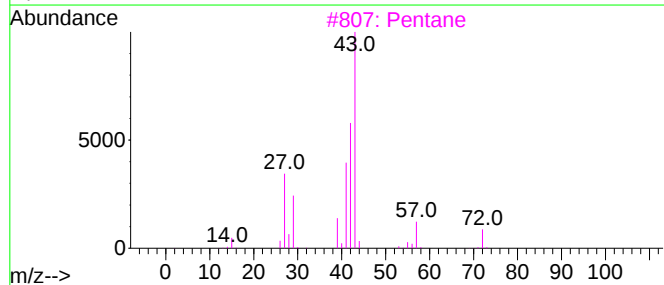
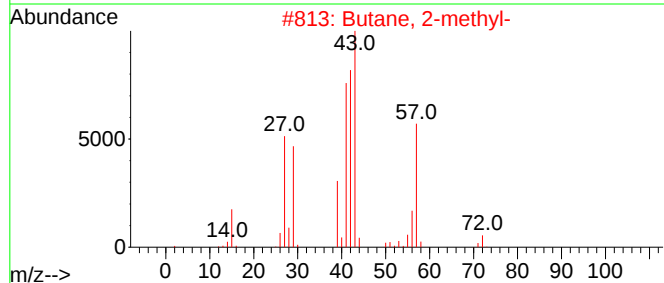
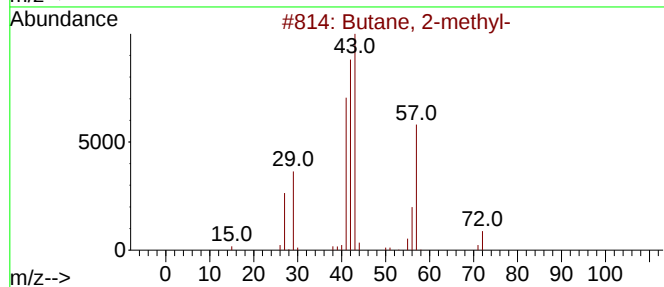
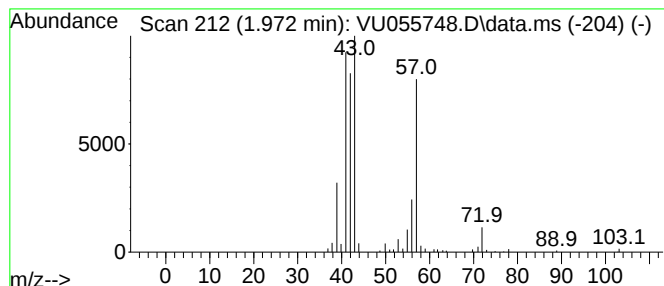
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.972	5.21 ug/L	107523	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	90
2	Butane, 2-methyl-			72	C5H12	000078-78-4	83
3	Pentane			72	C5H12	000109-66-0	45
4	Pentane			72	C5H12	000109-66-0	42
5	Isobutylene epoxide			72	C4H8O	000558-30-5	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.972	5.2	ug/L	107523	1	6.245	1031380	50.0