

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
 Data File : VU053532.D
 Acq On : 03 Apr 2023 20:00
 Operator : JC/MD
 Sample : 02158-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PMW-1(20230328)

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\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053532.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.491	40	47	66	rVB	337053	353974	36.86%	3.954%
2	1.597	73	80	93	rVB	141535	155812	16.22%	1.741%
3	1.909	169	177	192	rVB	107289	146706	15.28%	1.639%
4	2.565	369	381	397	rBV	203483	330749	34.44%	3.695%
5	2.813	456	458	460	rBV2	243	154	0.02%	0.002%
6	2.835	463	465	467	rVV	349	130	0.01%	0.001%
7	2.883	478	480	483	rVB3	427	249	0.03%	0.003%
8	3.038	523	528	529	rBV3	852	725	0.08%	0.008%
9	3.118	549	553	556	rBV3	582	470	0.05%	0.005%
10	3.272	598	601	603	rBV	216	156	0.02%	0.002%
11	3.356	625	627	631	rBV2	323	228	0.02%	0.003%
12	3.494	667	670	672	rBV	367	241	0.03%	0.003%
13	3.565	689	692	695	rVV	344	208	0.02%	0.002%
14	3.581	695	697	703	rVB2	308	168	0.02%	0.002%
15	3.777	754	758	762	rVB2	237	272	0.03%	0.003%
16	3.848	777	780	784	rVB	281	166	0.02%	0.002%
17	3.870	784	787	789	rBV2	208	131	0.01%	0.001%
18	3.883	789	791	793	rBV	212	74	0.01%	0.001%
19	3.935	804	807	810	rBV2	249	162	0.02%	0.002%
20	4.054	842	844	847	rBV	135	79	0.01%	0.001%
21	4.256	904	907	910	rBV	251	195	0.02%	0.002%
22	4.349	934	936	937	rBV	138	35	0.00%	0.000%
23	4.388	945	948	950	rBV2	195	135	0.01%	0.002%
24	4.433	959	962	964	rBV	185	96	0.01%	0.001%
25	4.481	973	977	980	rBV	250	172	0.02%	0.002%
26	4.613	1006	1018	1028	rBV	77342	180577	18.80%	2.017%
27	4.957	1123	1125	1127	rBV	336	182	0.02%	0.002%
28	5.057	1141	1156	1175	rBV	181509	393066	40.93%	4.391%
29	5.420	1267	1269	1271	rBV2	147	83	0.01%	0.001%
30	5.719	1341	1362	1391	rBV2	347392	960341	100.00%	10.728%
31	6.038	1456	1461	1463	rBV3	341	274	0.03%	0.003%
32	6.179	1501	1505	1507	rBV	186	160	0.02%	0.002%
33	6.243	1512	1525	1541	rBV	314681	589413	61.38%	6.585%
34	6.484	1597	1600	1601	rBV	212	114	0.01%	0.001%
35	6.536	1604	1616	1630	rVB7	11899	25275	2.63%	0.282%
36	6.597	1630	1635	1638	rBV	214	205	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
 Data File : VU053532.D
 Acq On : 03 Apr 2023 20:00
 Operator : JC/MD
 Sample : 02158-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PMW-1(20230328)

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\SFAMULM033123WMA.M
 Title : VOC Analysis

37	6.684	1648	1662	1681	rBV	213698	425063	44.26%	4.749%
38	7.037	1769	1772	1775	rBV	192	128	0.01%	0.001%
39	7.050	1775	1776	1779	rVB	211	81	0.01%	0.001%
40	7.156	1807	1809	1813	rBV	281	118	0.01%	0.001%
41	7.182	1813	1817	1819	rBV	464	332	0.03%	0.004%
42	7.243	1831	1836	1838	rBV2	266	282	0.03%	0.003%
43	7.423	1888	1892	1895	rBV	257	242	0.03%	0.003%
44	7.455	1899	1902	1904	rBV	225	104	0.01%	0.001%
45	7.562	1921	1935	1956	rBV2	128321	226902	23.63%	2.535%
46	7.664	1965	1967	1971	rVB	334	200	0.02%	0.002%
47	7.690	1971	1975	1976	rBV2	469	331	0.03%	0.004%
48	7.771	1997	2000	2004	rBV	292	181	0.02%	0.002%
49	7.893	2025	2038	2052	rBV	455980	789500	82.21%	8.820%
50	8.176	2115	2126	2150	rBV	85916	149797	15.60%	1.673%
51	8.301	2161	2165	2168	rBV2	386	278	0.03%	0.003%
52	8.333	2173	2175	2179	rBV	221	154	0.02%	0.002%
53	8.362	2179	2184	2189	rVB	279	288	0.03%	0.003%
54	8.452	2209	2212	2213	rBV	589	318	0.03%	0.004%
55	8.549	2231	2242	2256	rBV	63694	107100	11.15%	1.196%
56	8.626	2256	2266	2291	rBV	237771	432324	45.02%	4.830%
57	8.973	2372	2374	2377	rVB	266	121	0.01%	0.001%
58	8.989	2377	2379	2381	rBV	281	161	0.02%	0.002%
59	9.111	2415	2417	2419	rBV	317	187	0.02%	0.002%
60	9.311	2476	2479	2485	rVB	241	177	0.02%	0.002%
61	9.414	2497	2511	2533	rBV	425519	731329	76.15%	8.170%
62	9.690	2587	2597	2611	rVB2	8989	15492	1.61%	0.173%
63	9.822	2637	2638	2639	rBV2	229	74	0.01%	0.001%
64	10.102	2717	2725	2739	rVB3	2322	3572	0.37%	0.040%
65	10.153	2739	2741	2742	rBV	264	121	0.01%	0.001%
66	10.481	2838	2843	2847	rBV	565	584	0.06%	0.007%
67	10.574	2870	2872	2878	rVB2	266	212	0.02%	0.002%
68	10.751	2914	2927	2946	rBV	315959	508586	52.96%	5.682%
69	10.877	2964	2966	2967	rBV	393	145	0.02%	0.002%
70	11.205	3066	3068	3073	rBV2	266	175	0.02%	0.002%
71	11.298	3090	3097	3102	rBV4	471	705	0.07%	0.008%
72	11.417	3132	3134	3136	rBV4	297	113	0.01%	0.001%
73	11.741	3226	3235	3244	rBV3	12062	17893	1.86%	0.200%
74	11.809	3244	3256	3281	rVV	477645	842477	87.73%	9.412%
75	11.992	3310	3313	3315	rBV	231	154	0.02%	0.002%
76	12.089	3341	3343	3347	rBV2	458	338	0.04%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
 Data File : VU053532.D
 Acq On : 03 Apr 2023 20:00
 Operator : JC/MD
 Sample : 02158-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PMW-1(20230328)

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\SFAMULM033123WMA.M
 Title : VOC Analysis

77	12.188	3361	3374	3392	rBV	476146	776490	80.86%	8.674%
78	12.301	3407	3409	3411	rBV3	432	224	0.02%	0.003%
79	12.349	3422	3424	3426	rBV	354	177	0.02%	0.002%
80	12.436	3448	3451	3453	rVB	378	211	0.02%	0.002%
81	12.449	3453	3455	3456	rBV	337	167	0.02%	0.002%
82	12.542	3480	3484	3487	rBV2	358	261	0.03%	0.003%
83	12.565	3487	3491	3496	rBV	508	594	0.06%	0.007%
84	12.626	3507	3510	3513	rBV2	247	211	0.02%	0.002%
85	12.738	3543	3545	3549	rBV	202	92	0.01%	0.001%
86	12.822	3568	3571	3574	rBV	333	258	0.03%	0.003%
87	13.221	3691	3695	3703	rBV2	815	1030	0.11%	0.012%
88	13.835	3874	3886	3914	rBV	404775	651812	67.87%	7.282%
89	14.085	3958	3964	3975	rVB3	4411	6444	0.67%	0.072%
90	14.327	4026	4039	4058	rBV	70109	115957	12.07%	1.295%

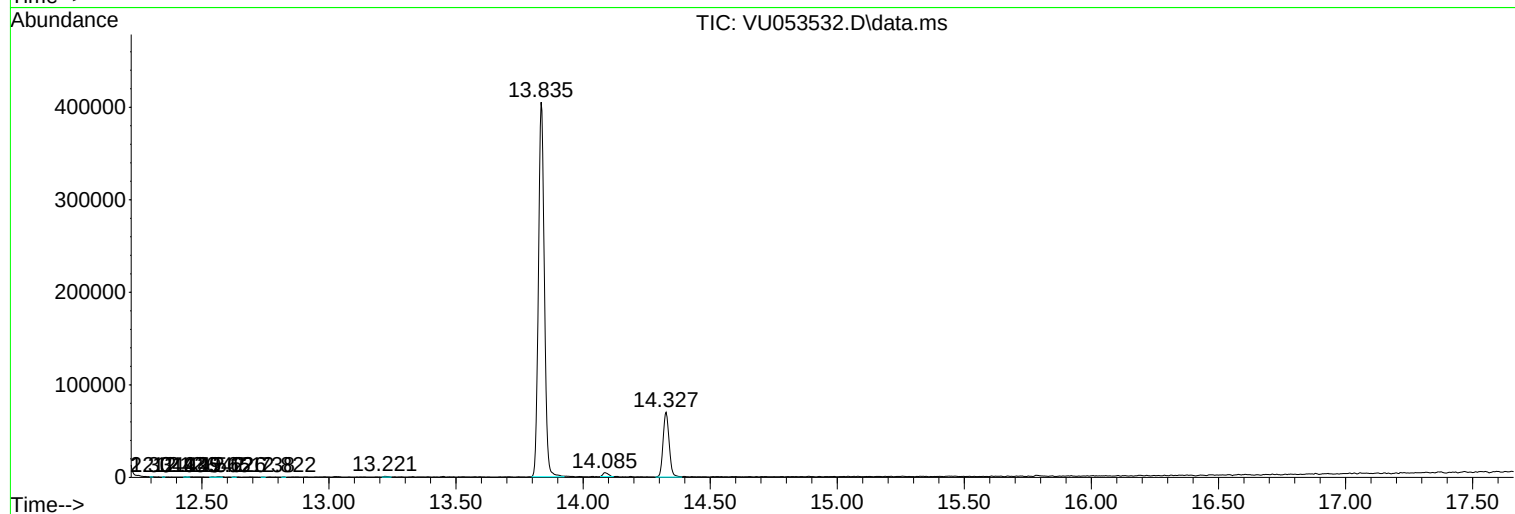
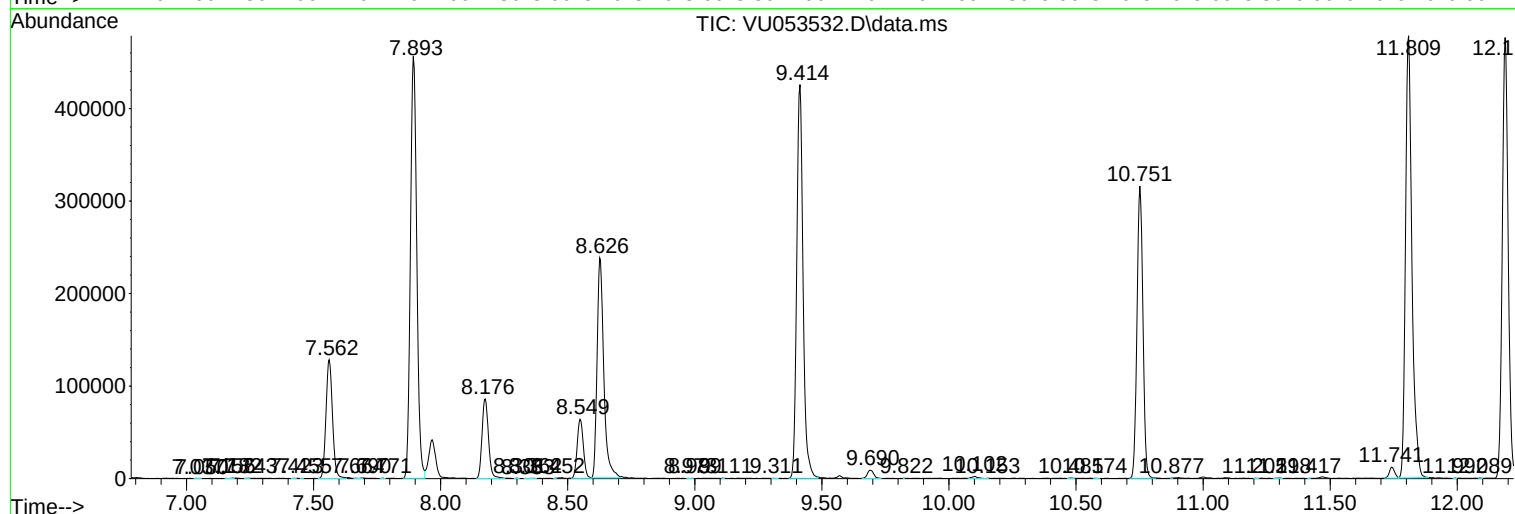
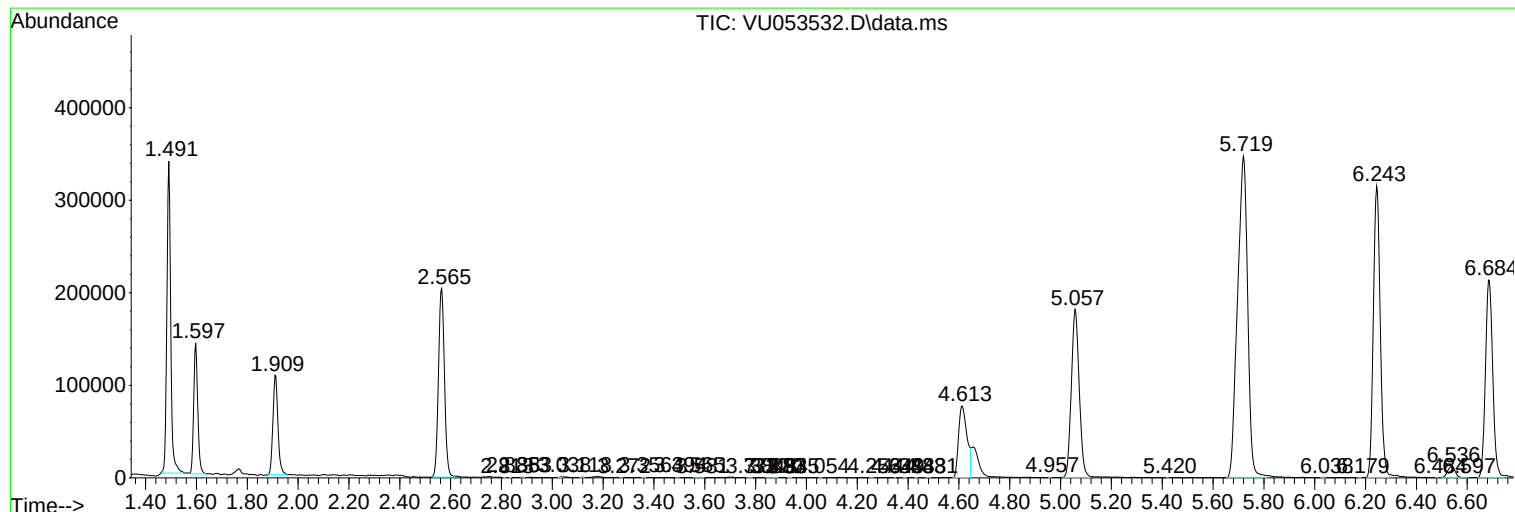
Sum of corrected areas: 8951444

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053532.D
Acq On : 03 Apr 2023 20:00
Operator : JC/MD
Sample : 02158-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PMW-1(20230328)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053532.D
Acq On : 03 Apr 2023 20:00
Operator : JC/MD
Sample : 02158-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PMW-1(20230328)

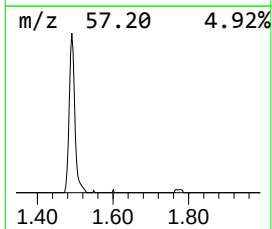
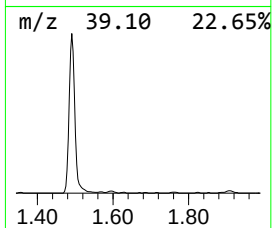
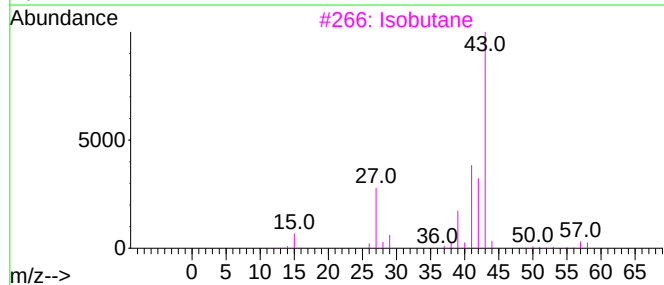
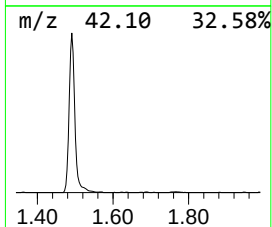
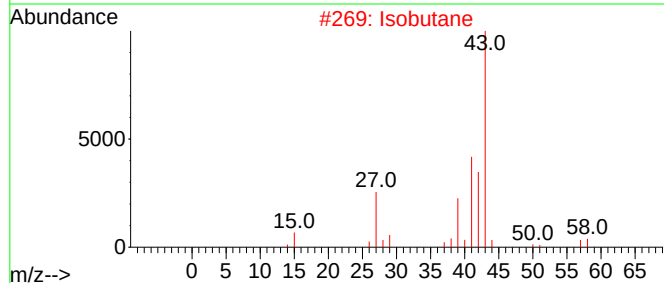
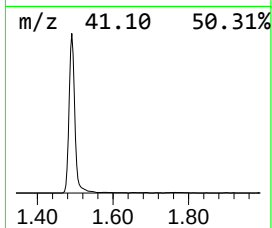
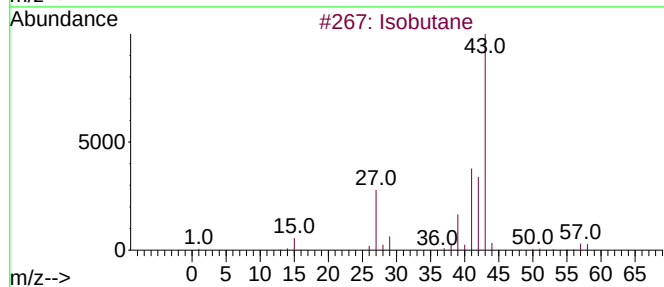
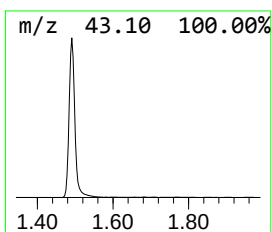
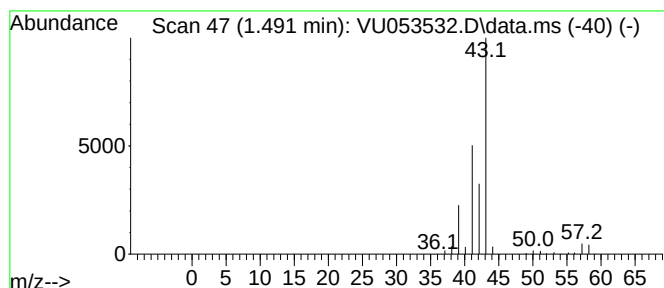
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.491	30.03 ug/L	353974	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	80
2			Isobutane	58	C4H10	000075-28-5	72
3			Isobutane	58	C4H10	000075-28-5	72
4			Isobutane	58	C4H10	000075-28-5	59
5			Isobutane	58	C4H10	000075-28-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053532.D
Acq On : 03 Apr 2023 20:00
Operator : JC/MD
Sample : 02158-10
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PMW-1(20230328)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.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...	1.491	30.0	ug/L	353974	1	6.243	589413	50.0