

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112425\
 Data File : VU063782.D
 Acq On : 24 Nov 2025 17:03
 Operator : MD/SY
 Sample : Q3688-17
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 M-29

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\SFAMULM111725WMA.M

Title : VOC Analysis

Signal : TIC: VU063782.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.583	85	91	102	rBV	166049	179641	14.12%	1.861%
2	1.895	180	188	199	rBV	129691	165171	12.98%	1.711%
3	2.541	377	389	406	rBV	259998	430480	33.83%	4.459%
4	2.740	444	451	471	rVB2	16254	35203	2.77%	0.365%
5	3.158	566	581	602	rBV2	37128	86284	6.78%	0.894%
6	3.312	625	629	630	rBV	201	164	0.01%	0.002%
7	3.325	630	633	635	rBV2	817	572	0.04%	0.006%
8	3.435	661	667	670	rBV2	426	417	0.03%	0.004%
9	3.460	673	675	678	rVV	169	81	0.01%	0.001%
10	3.541	697	700	701	rBV	204	117	0.01%	0.001%
11	3.666	736	739	741	rBV	223	146	0.01%	0.002%
12	3.869	798	802	807	rBV	230	216	0.02%	0.002%
13	3.898	808	811	814	rVV	290	255	0.02%	0.003%
14	3.927	818	820	824	rBV2	149	85	0.01%	0.001%
15	3.952	824	828	832	rBV2	283	287	0.02%	0.003%
16	3.975	832	835	837	rBV	105	53	0.00%	0.001%
17	4.033	847	853	855	rBV2	369	288	0.02%	0.003%
18	4.071	859	865	868	rBV2	380	368	0.03%	0.004%
19	4.110	874	877	880	rBV	165	122	0.01%	0.001%
20	4.187	898	901	902	rBV	212	122	0.01%	0.001%
21	4.277	926	929	935	rBV	209	215	0.02%	0.002%
22	4.351	949	952	954	rBV2	194	131	0.01%	0.001%
23	4.399	964	967	972	rBV	242	176	0.01%	0.002%
24	4.438	976	979	982	rBV	169	106	0.01%	0.001%
25	4.505	993	1000	1004	rBV2	339	365	0.03%	0.004%
26	4.528	1004	1007	1009	rBV	295	180	0.01%	0.002%
27	4.599	1019	1029	1059	rBV	89818	260339	20.46%	2.697%
28	5.029	1149	1163	1197	rBV	219575	500913	39.37%	5.189%
29	5.338	1256	1259	1261	rBV3	449	264	0.02%	0.003%
30	5.396	1274	1277	1282	rBV4	414	505	0.04%	0.005%
31	5.480	1301	1303	1308	rBV2	216	216	0.02%	0.002%
32	5.509	1309	1312	1314	rVV2	450	331	0.03%	0.003%
33	5.534	1318	1320	1324	rBV	60	43	0.00%	0.000%
34	5.554	1324	1326	1328	rVB2	159	62	0.00%	0.001%
35	5.566	1328	1330	1331	rBV	177	79	0.01%	0.001%
36	5.695	1350	1370	1416	rBV2	429321	1272323	100.00%	13.179%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112425\
 Data File : VU063782.D
 Acq On : 24 Nov 2025 17:03
 Operator : MD/SY
 Sample : Q3688-17
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 M-29

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\SFAMULM111725WMA.M
 Title : VOC Analysis

37	6.145	1507	1510	1512	rBV	420	276	0.02%	0.003%
38	6.219	1521	1533	1581	rBV	364718	759178	59.67%	7.864%
39	6.512	1613	1624	1635	rBV6	7440	14741	1.16%	0.153%
40	6.660	1656	1670	1707	rBV	268597	566904	44.56%	5.872%
41	6.923	1750	1752	1755	rBV2	302	183	0.01%	0.002%
42	6.939	1755	1757	1760	rVB2	488	243	0.02%	0.003%
43	6.959	1760	1763	1766	rBV3	349	265	0.02%	0.003%
44	6.988	1770	1772	1774	rBV	72	35	0.00%	0.000%
45	7.007	1775	1778	1783	rBV2	226	183	0.01%	0.002%
46	7.029	1783	1785	1787	rBV	274	139	0.01%	0.001%
47	7.110	1808	1810	1812	rBV	134	84	0.01%	0.001%
48	7.238	1847	1850	1853	rBV2	377	266	0.02%	0.003%
49	7.316	1872	1874	1876	rBV2	89	52	0.00%	0.001%
50	7.335	1877	1880	1882	rVV2	327	193	0.02%	0.002%
51	7.361	1886	1888	1890	rVB	357	171	0.01%	0.002%
52	7.380	1890	1894	1895	rBV2	179	114	0.01%	0.001%
53	7.434	1908	1911	1913	rBV2	117	68	0.01%	0.001%
54	7.479	1922	1925	1929	rBV	292	214	0.02%	0.002%
55	7.537	1929	1943	1968	rBV2	124392	236950	18.62%	2.454%
56	7.872	2034	2047	2084	rBV	549373	1022800	80.39%	10.594%
57	8.155	2125	2135	2161	rBV	78073	140076	11.01%	1.451%
58	8.380	2199	2205	2209	rBV2	533	535	0.04%	0.006%
59	8.463	2229	2231	2236	rVB	308	177	0.01%	0.002%
60	8.486	2236	2238	2239	rBV	172	82	0.01%	0.001%
61	8.614	2267	2278	2336	rBV2	207776	559766	44.00%	5.798%
62	9.061	2414	2417	2420	rVB	399	208	0.02%	0.002%
63	9.213	2462	2464	2466	rBV	153	103	0.01%	0.001%
64	9.393	2507	2520	2560	rBV	528488	965201	75.86%	9.998%
65	9.666	2598	2605	2606	rBV2	1141	909	0.07%	0.009%
66	9.740	2625	2628	2631	rBV2	354	219	0.02%	0.002%
67	9.756	2631	2633	2635	rVB	263	92	0.01%	0.001%
68	9.778	2635	2640	2643	rBV2	241	282	0.02%	0.003%
69	9.978	2699	2702	2709	rVB	321	326	0.03%	0.003%
70	10.020	2709	2715	2721	rBV2	344	544	0.04%	0.006%
71	10.087	2728	2736	2739	rBV3	951	1466	0.12%	0.015%
72	10.161	2756	2759	2761	rVB2	177	87	0.01%	0.001%
73	10.180	2761	2765	2770	rBV2	300	294	0.02%	0.003%
74	10.280	2792	2796	2801	rBV2	252	223	0.02%	0.002%
75	10.425	2838	2841	2842	rBV	144	85	0.01%	0.001%
76	10.627	2899	2904	2908	rVB4	763	822	0.06%	0.009%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112425\
 Data File : VU063782.D
 Acq On : 24 Nov 2025 17:03
 Operator : MD/SY
 Sample : Q3688-17
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 M-29

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\SFAMULM111725WMA.M
 Title : VOC Analysis

77	10.650	2908	2911	2913	rBV2	306	221	0.02%	0.002%
78	10.730	2923	2936	2960	rBV	379278	627897	49.35%	6.504%
79	10.917	2992	2994	2996	rBV	232	129	0.01%	0.001%
80	11.003	3018	3021	3023	rBV	329	231	0.02%	0.002%
81	11.032	3028	3030	3033	rVB2	267	155	0.01%	0.002%
82	11.055	3033	3037	3038	rBV	445	276	0.02%	0.003%
83	11.200	3079	3082	3084	rBV	229	155	0.01%	0.002%
84	11.283	3105	3108	3110	rBV2	321	239	0.02%	0.002%
85	11.450	3153	3160	3170	rVB3	1425	2503	0.20%	0.026%
86	11.511	3176	3179	3181	rBV2	206	137	0.01%	0.001%
87	11.659	3223	3225	3228	rBV2	222	130	0.01%	0.001%
88	11.730	3239	3247	3253	rBV4	1845	2716	0.21%	0.028%
89	11.788	3253	3265	3290	rBV	536908	918592	72.20%	9.515%
90	12.026	3337	3339	3343	rBV2	275	203	0.02%	0.002%
91	12.071	3351	3353	3357	rVB	354	182	0.01%	0.002%
92	12.093	3357	3360	3362	rBV	267	160	0.01%	0.002%
93	12.167	3370	3383	3406	rBV	514132	887440	69.75%	9.192%
94	12.460	3471	3474	3475	rBV2	155	78	0.01%	0.001%
95	12.473	3475	3478	3479	rBV2	424	240	0.02%	0.002%
96	12.592	3513	3515	3516	rBV	331	113	0.01%	0.001%
97	13.058	3658	3660	3662	rBV	324	125	0.01%	0.001%
98	13.203	3701	3705	3706	rBV2	971	714	0.06%	0.007%
99	13.482	3786	3792	3796	rBV3	412	599	0.05%	0.006%

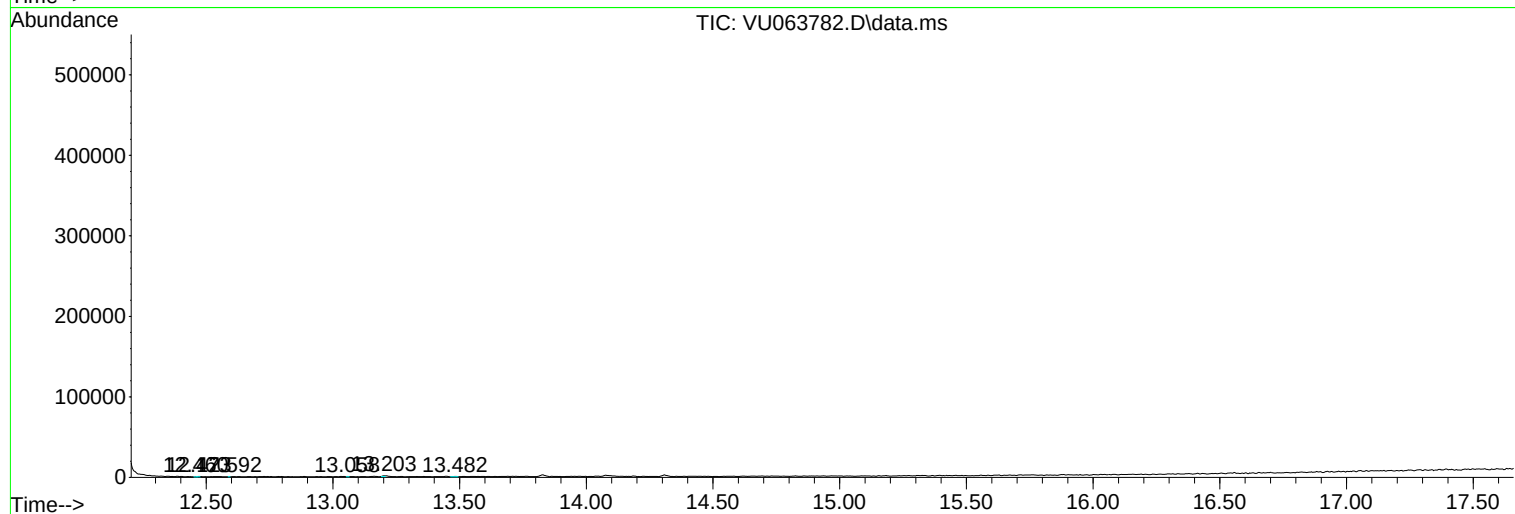
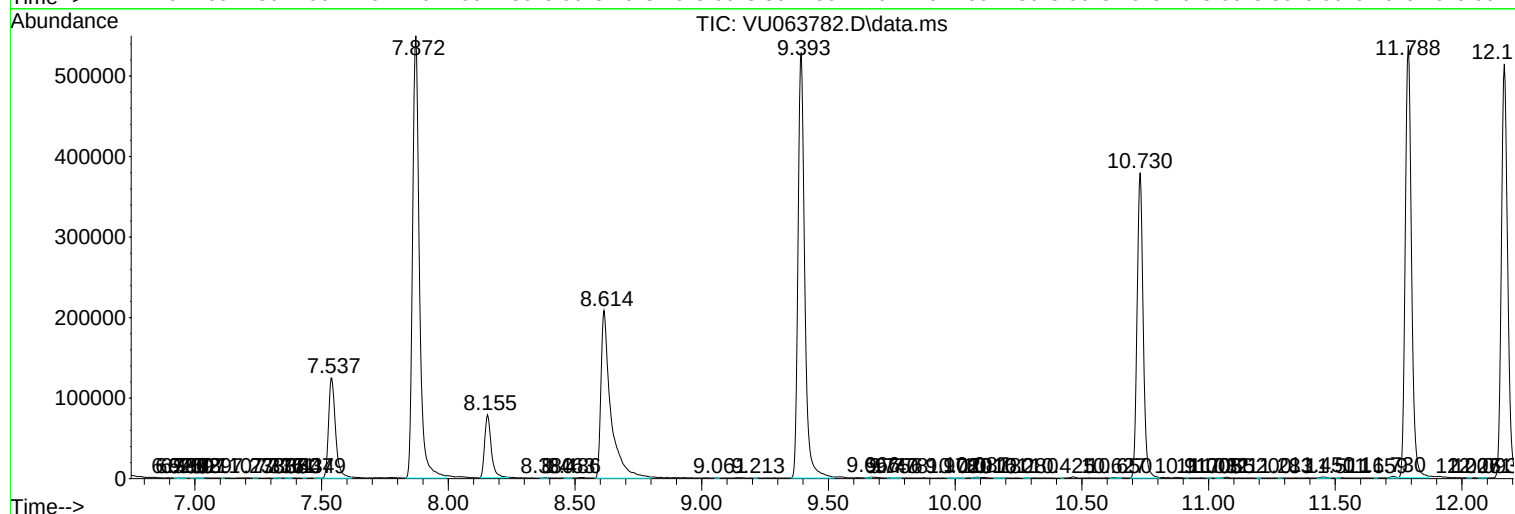
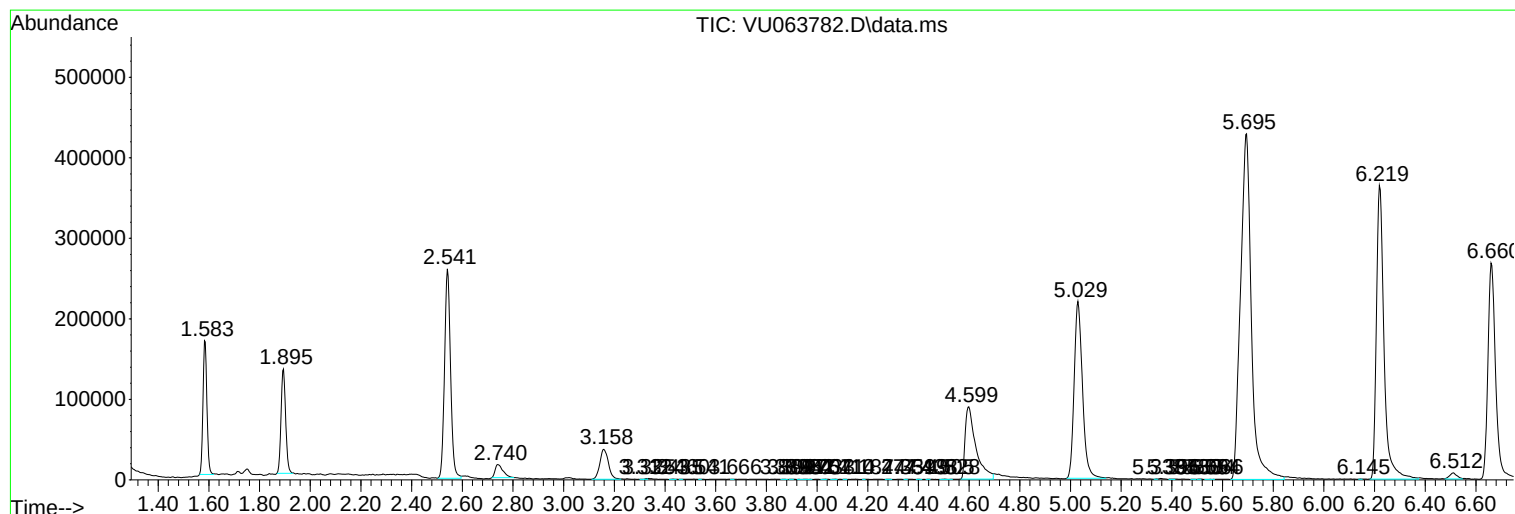
Sum of corrected areas: 9654111

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112425\
Data File : VU063782.D
Acq On : 24 Nov 2025 17:03
Operator : MD/SY
Sample : Q3688-17
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
M-29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111725WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112425\
Data File : VU063782.D
Acq On : 24 Nov 2025 17:03
Operator : MD/SY
Sample : Q3688-17
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
M-29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111725WMA.M
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112425\
Data File : VU063782.D
Acq On : 24 Nov 2025 17:03
Operator : MD/SY
Sample : Q3688-17
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
M-29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111725WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
------------------	----	---------	-------	----------	---	----	------	------