

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
 Data File : VU059247.D
 Acq On : 14 Jun 2024 15:00
 Operator : MD/SY
 Sample : P2775-12ME
 Misc : 6.11g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4C93ME

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\SFAMULM052924WMA.M
 Title : VOC Analysis

Signal : TIC: VU059247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	56	59	65	rVB3	2182	1856	0.18%	0.022%
2	1.592	87	94	116	rVB	40050	68343	6.69%	0.826%
3	2.537	376	388	407	rVB	115921	187161	18.32%	2.261%
4	2.634	407	418	425	rBV4	1956	3406	0.33%	0.041%
5	2.763	452	458	467	rVB3	1223	1836	0.18%	0.022%
6	2.804	468	471	474	rBV4	445	345	0.03%	0.004%
7	2.872	489	492	494	rBV2	364	299	0.03%	0.004%
8	2.907	501	503	505	rBV2	353	188	0.02%	0.002%
9	2.946	505	515	530	rVV	10998	21157	2.07%	0.256%
10	3.026	532	540	557	rVB2	5501	10995	1.08%	0.133%
11	3.097	558	562	563	rBV3	506	314	0.03%	0.004%
12	3.174	572	586	599	rBV	5804	14145	1.38%	0.171%
13	3.264	611	614	618	rVB2	429	257	0.03%	0.003%
14	3.332	634	635	638	rVB3	401	179	0.02%	0.002%
15	3.364	642	645	648	rVB	390	265	0.03%	0.003%
16	3.435	663	667	670	rBV2	268	231	0.02%	0.003%
17	3.512	687	691	699	rVB2	395	649	0.06%	0.008%
18	3.550	699	703	705	rBV2	254	239	0.02%	0.003%
19	3.679	741	743	748	rBV	327	252	0.02%	0.003%
20	3.727	754	758	765	rBV2	276	443	0.04%	0.005%
21	3.859	795	799	802	rBV2	237	202	0.02%	0.002%
22	3.898	807	811	813	rBV2	273	181	0.02%	0.002%
23	4.232	911	915	918	rBV	214	182	0.02%	0.002%
24	4.377	957	960	966	rVB2	163	188	0.02%	0.002%
25	4.618	1024	1035	1077	rBV	130169	397799	38.95%	4.806%
26	5.049	1154	1169	1192	rVV	164630	371046	36.33%	4.483%
27	5.180	1206	1210	1212	rBV3	362	298	0.03%	0.004%
28	5.325	1252	1255	1261	rVB2	260	211	0.02%	0.003%
29	5.370	1265	1269	1272	rBV3	601	406	0.04%	0.005%
30	5.711	1355	1375	1397	rBV2	294884	814621	79.75%	9.842%
31	5.920	1436	1440	1444	rBV3	299	324	0.03%	0.004%
32	5.975	1449	1457	1462	rBV5	1375	1974	0.19%	0.024%
33	6.180	1518	1521	1526	rVV2	266	234	0.02%	0.003%
34	6.238	1526	1539	1575	rBV	405677	782914	76.65%	9.459%
35	6.386	1581	1585	1587	rBV2	401	261	0.03%	0.003%
36	6.441	1600	1602	1610	rBV3	534	706	0.07%	0.009%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
 Data File : VU059247.D
 Acq On : 14 Jun 2024 15:00
 Operator : MD/SY
 Sample : P2775-12ME
 Misc : 6.11g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4C93ME

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\SFAMULM052924WMA.M
 Title : VOC Analysis

37	6.524	1618	1628	1641	rBV6	7641	14498	1.42%	0.175%
38	6.598	1644	1651	1661	rBV5	1824	3113	0.30%	0.038%
39	6.679	1663	1676	1700	rBV	211326	421330	41.25%	5.090%
40	6.856	1728	1731	1733	rBV	315	225	0.02%	0.003%
41	6.930	1746	1754	1759	rBV2	210	323	0.03%	0.004%
42	7.010	1776	1779	1783	rVB	407	267	0.03%	0.003%
43	7.068	1792	1797	1799	rBV	267	241	0.02%	0.003%
44	7.129	1810	1816	1817	rBV	280	224	0.02%	0.003%
45	7.187	1829	1834	1837	rBV2	1547	1603	0.16%	0.019%
46	7.280	1860	1863	1867	rVB3	304	233	0.02%	0.003%
47	7.309	1867	1872	1875	rBV2	309	235	0.02%	0.003%
48	7.463	1917	1920	1926	rVB2	157	180	0.02%	0.002%
49	7.560	1938	1950	1972	rBV	99301	184084	18.02%	2.224%
50	7.708	1988	1996	2001	rBV4	1155	1918	0.19%	0.023%
51	7.743	2005	2007	2012	rVB3	360	227	0.02%	0.003%
52	7.785	2016	2020	2021	rBV2	481	312	0.03%	0.004%
53	7.891	2040	2053	2070	rBV	303541	538030	52.67%	6.500%
54	8.174	2130	2141	2160	rBV2	69042	125521	12.29%	1.517%
55	8.322	2183	2187	2188	rBV2	345	270	0.03%	0.003%
56	8.463	2223	2231	2234	rBV4	480	650	0.06%	0.008%
57	8.550	2252	2258	2263	rVB4	863	1131	0.11%	0.014%
58	8.637	2268	2285	2315	rBV	347342	810559	79.35%	9.793%
59	9.010	2397	2401	2404	rBV3	294	234	0.02%	0.003%
60	9.026	2404	2406	2411	rVV2	338	245	0.02%	0.003%
61	9.113	2430	2433	2436	rBV	292	258	0.03%	0.003%
62	9.245	2467	2474	2476	rBV2	256	328	0.03%	0.004%
63	9.412	2508	2526	2562	rBV	571087	1021437	100.00%	12.341%
64	9.569	2569	2575	2579	rBV3	1484	2015	0.20%	0.024%
65	9.695	2606	2614	2626	rBV3	2440	4153	0.41%	0.050%
66	9.839	2656	2659	2664	rVB2	209	202	0.02%	0.002%
67	9.868	2664	2668	2670	rBV	242	181	0.02%	0.002%
68	9.936	2684	2689	2694	rVB2	295	338	0.03%	0.004%
69	9.968	2694	2699	2701	rBV	282	255	0.02%	0.003%
70	10.106	2735	2742	2748	rBV4	1166	1869	0.18%	0.023%
71	10.376	2822	2826	2829	rBV2	314	339	0.03%	0.004%
72	10.396	2829	2832	2834	rVV2	353	253	0.02%	0.003%
73	10.409	2834	2836	2840	rVB	327	217	0.02%	0.003%
74	10.482	2854	2859	2868	rVV2	565	938	0.09%	0.011%
75	10.550	2877	2880	2884	rBV2	261	235	0.02%	0.003%
76	10.640	2905	2908	2912	rBV3	404	269	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
 Data File : VU059247.D
 Acq On : 14 Jun 2024 15:00
 Operator : MD/SY
 Sample : P2775-12ME
 Misc : 6.11g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4C93ME

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\SFAMULM052924WMA.M
 Title : VOC Analysis

77	10.753	2930	2943	2964	rBV	461318	770952	75.48%	9.314%
78	10.884	2977	2984	2992	rVB2	1621	2419	0.24%	0.029%
79	10.997	3015	3019	3025	rBV2	294	344	0.03%	0.004%
80	11.122	3056	3058	3064	rBV2	241	205	0.02%	0.002%
81	11.148	3064	3066	3070	rVB	443	235	0.02%	0.003%
82	11.553	3188	3192	3195	rBV	300	235	0.02%	0.003%
83	11.753	3246	3254	3259	rBV5	1304	1554	0.15%	0.019%
84	11.807	3259	3271	3293	rBV	598376	958703	93.86%	11.583%
85	12.010	3331	3334	3336	rBV2	418	264	0.03%	0.003%
86	12.061	3347	3350	3354	rBV	438	364	0.04%	0.004%
87	12.190	3378	3390	3412	rBV	434253	709299	69.44%	8.570%
88	12.399	3448	3455	3457	rBV	355	400	0.04%	0.005%
89	12.765	3564	3569	3576	rVB	1443	1649	0.16%	0.020%
90	12.949	3623	3626	3631	rVB3	359	229	0.02%	0.003%
91	13.219	3708	3710	3712	rBV	349	211	0.02%	0.003%
92	13.360	3750	3754	3757	rBV	450	374	0.04%	0.005%
93	13.418	3770	3772	3778	rVB3	276	257	0.03%	0.003%
94	13.450	3778	3782	3785	rBV	280	251	0.02%	0.003%
95	14.109	3980	3987	3988	rBV	1164	1154	0.11%	0.014%
96	14.338	4052	4058	4063	rBV4	1024	1288	0.13%	0.016%
97	14.466	4095	4098	4104	rVB3	381	284	0.03%	0.003%
98	14.576	4121	4132	4138	rVB	1541	2375	0.23%	0.029%
99	14.730	4177	4180	4183	rBV	451	391	0.04%	0.005%
100	16.010	4575	4578	4582	rBV5	636	482	0.05%	0.006%

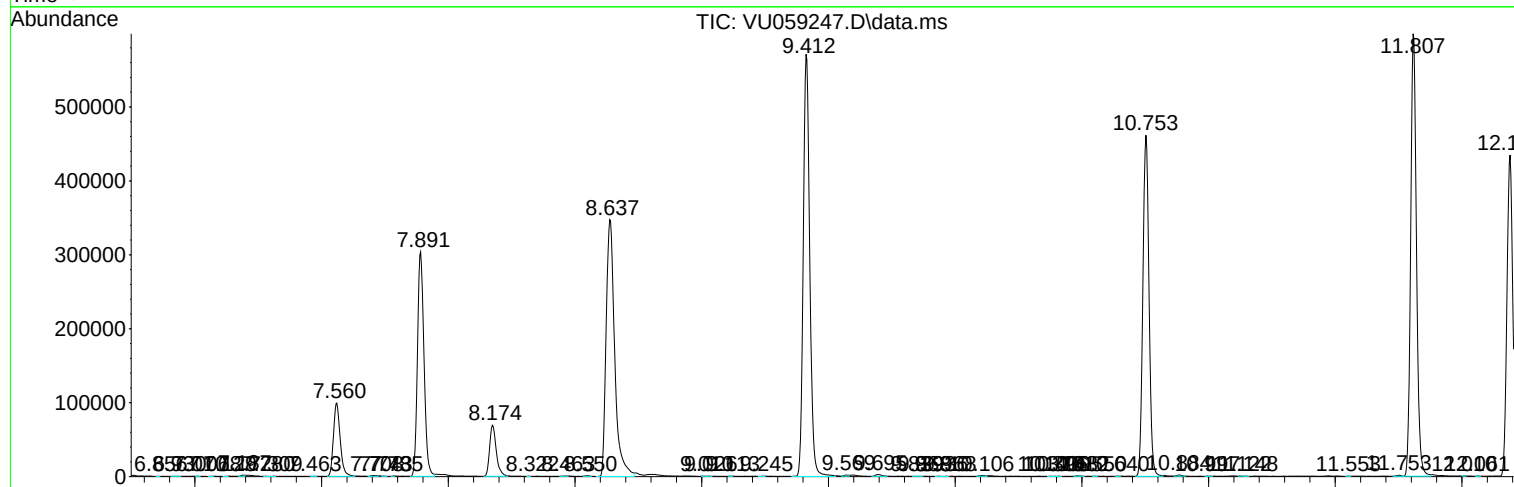
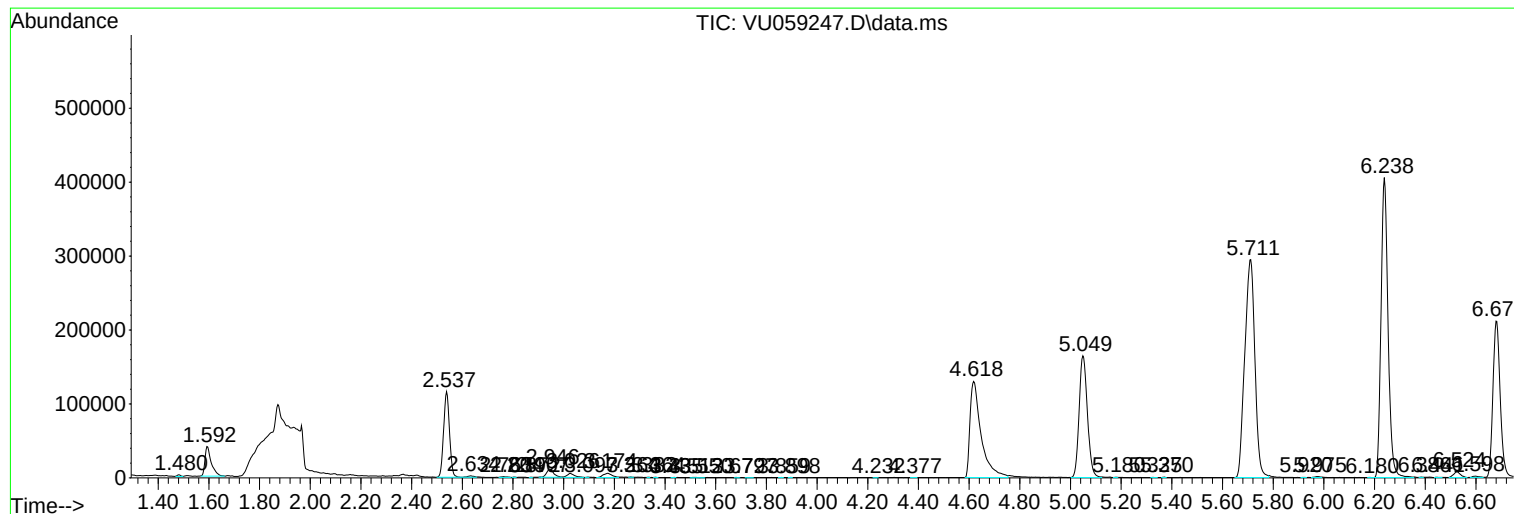
Sum of corrected areas: 8276966

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
Data File : VU059247.D
Acq On : 14 Jun 2024 15:00
Operator : MD/SY
Sample : P2775-12ME
Misc : 6.11g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4C93ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
Data File : VU059247.D
Acq On : 14 Jun 2024 15:00
Operator : MD/SY
Sample : P2775-12ME
Misc : 6.11g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4C93ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.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\VU061424\
Data File : VU059247.D
Acq On : 14 Jun 2024 15:00
Operator : MD/SY
Sample : P2775-12ME
Misc : 6.11g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4C93ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.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