

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
 Data File : VU059956.D
 Acq On : 15 Jul 2024 17:06
 Operator : MD/SY
 Sample : P3230-01MEDL 1600X
 Misc : 4.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB32MEDL

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\SFAMULM070224WMA.M
 Title : VOC Analysis

Signal : TIC: VU059956.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	88	95	116	rVB	62544	79418	10.42%	1.360%
2	1.904	184	191	207	rVB	48242	70026	9.19%	1.199%
3	2.557	382	394	413	rBV	104767	172046	22.57%	2.946%
4	2.959	515	519	521	rBV2	221	174	0.02%	0.003%
5	3.039	536	544	556	rVB3	1806	3135	0.41%	0.054%
6	3.177	574	587	599	rBV2	5194	10806	1.42%	0.185%
7	3.322	627	632	638	rBV2	206	264	0.03%	0.005%
8	3.457	670	674	676	rBV	91	59	0.01%	0.001%
9	3.473	676	679	681	rVB	174	97	0.01%	0.002%
10	3.489	681	684	689	rBV2	220	209	0.03%	0.004%
11	3.560	703	706	708	rBV	136	75	0.01%	0.001%
12	3.602	716	719	721	rBV	176	97	0.01%	0.002%
13	3.650	731	734	739	rBV2	146	117	0.02%	0.002%
14	3.679	740	743	745	rBV	173	108	0.01%	0.002%
15	3.827	785	789	793	rVB2	143	120	0.02%	0.002%
16	3.853	794	797	800	rBV	145	116	0.02%	0.002%
17	3.936	818	823	833	rBV2	234	362	0.05%	0.006%
18	4.004	840	844	849	rBV2	122	117	0.02%	0.002%
19	4.042	853	856	862	rVB	170	179	0.02%	0.003%
20	4.071	862	865	867	rBV2	150	82	0.01%	0.001%
21	4.174	894	897	899	rBV2	106	76	0.01%	0.001%
22	4.277	926	929	930	rBV	125	61	0.01%	0.001%
23	4.290	930	933	935	rVV2	98	69	0.01%	0.001%
24	4.386	957	963	967	rBV	258	215	0.03%	0.004%
25	4.508	998	1001	1005	rBV	211	147	0.02%	0.003%
26	4.547	1010	1013	1015	rBV	74	40	0.01%	0.001%
27	4.618	1025	1035	1071	rBV	70927	189151	24.81%	3.239%
28	5.055	1156	1171	1195	rBV	109172	243011	31.87%	4.161%
29	5.219	1219	1222	1227	rVB3	265	222	0.03%	0.004%
30	5.271	1235	1238	1241	rBV	217	132	0.02%	0.002%
31	5.290	1241	1244	1248	rBV2	380	317	0.04%	0.005%
32	5.380	1270	1272	1275	rVB2	92	47	0.01%	0.001%
33	5.399	1275	1278	1281	rBV2	109	102	0.01%	0.002%
34	5.425	1282	1286	1288	rBV2	187	134	0.02%	0.002%
35	5.496	1304	1308	1310	rBV2	204	137	0.02%	0.002%
36	5.512	1310	1313	1317	rVB2	209	164	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
 Data File : VU059956.D
 Acq On : 15 Jul 2024 17:06
 Operator : MD/SY
 Sample : P3230-01MEDL 1600X
 Misc : 4.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB32MEDL

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\SFAMULM070224WMA.M
 Title : VOC Analysis

37	5.534	1317	1320	1326	rVB	124	109	0.01%	0.002%
38	5.560	1326	1328	1330	rBV2	100	57	0.01%	0.001%
39	5.579	1330	1334	1337	rBV2	173	138	0.02%	0.002%
40	5.595	1337	1339	1341	rBV	95	38	0.00%	0.001%
41	5.640	1350	1353	1356	rVB	154	91	0.01%	0.002%
42	5.717	1357	1377	1409	rBV2	215175	593930	77.90%	10.170%
43	5.952	1446	1450	1452	rBV2	184	133	0.02%	0.002%
44	6.004	1462	1466	1472	rBV	344	456	0.06%	0.008%
45	6.052	1479	1481	1483	rBV	171	44	0.01%	0.001%
46	6.116	1499	1501	1507	rVB2	208	99	0.01%	0.002%
47	6.245	1528	1541	1566	rBV	255462	495398	64.98%	8.483%
48	6.541	1623	1633	1648	rVV6	8975	18166	2.38%	0.311%
49	6.605	1650	1653	1657	rVB	266	183	0.02%	0.003%
50	6.685	1665	1678	1696	rBV	140139	274702	36.03%	4.704%
51	6.865	1729	1734	1736	rBV2	153	134	0.02%	0.002%
52	6.881	1736	1739	1742	rVB2	129	85	0.01%	0.001%
53	7.013	1777	1780	1782	rBV2	199	126	0.02%	0.002%
54	7.113	1809	1811	1812	rBV2	86	41	0.01%	0.001%
55	7.155	1818	1824	1827	rBV	303	248	0.03%	0.004%
56	7.200	1834	1838	1840	rBV2	387	328	0.04%	0.006%
57	7.354	1884	1886	1888	rBV	107	51	0.01%	0.001%
58	7.563	1939	1951	1974	rBV	68154	123861	16.25%	2.121%
59	7.814	2027	2029	2033	rVB	133	76	0.01%	0.001%
60	7.894	2041	2054	2072	rBV	237788	417207	54.72%	7.144%
61	8.090	2110	2115	2118	rBV2	500	492	0.06%	0.008%
62	8.177	2132	2142	2167	rBV2	47180	82384	10.81%	1.411%
63	8.454	2226	2228	2231	rBV2	204	180	0.02%	0.003%
64	8.550	2244	2258	2273	rBV	455858	762395	100.00%	13.054%
65	8.630	2273	2283	2312	rVB	186471	342743	44.96%	5.869%
66	9.274	2480	2483	2487	rBV	247	193	0.03%	0.003%
67	9.315	2492	2496	2499	rBV	216	195	0.03%	0.003%
68	9.415	2514	2527	2549	rBV	383312	635429	83.35%	10.880%
69	9.637	2591	2596	2599	rBV	290	283	0.04%	0.005%
70	9.772	2633	2638	2641	rBV2	262	257	0.03%	0.004%
71	9.994	2702	2707	2711	rBV2	184	186	0.02%	0.003%
72	10.344	2813	2816	2820	rBV2	179	176	0.02%	0.003%
73	10.396	2828	2832	2835	rBV	190	172	0.02%	0.003%
74	10.441	2844	2846	2850	rBV	179	123	0.02%	0.002%
75	10.753	2931	2943	2961	rBV	230779	375686	49.28%	6.433%
76	11.492	3170	3173	3176	rBV2	289	238	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
Data File : VU059956.D
Acq On : 15 Jul 2024 17:06
Operator : MD/SY
Sample : P3230-01MEDL 1600X
Misc : 4.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB32MEDL

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\SFAMULM070224WMA.M

Title : VOC Analysis

77	11.601	3204	3207	3208	rBV	136	71	0.01%	0.001%
78	11.746	3249	3252	3255	rBV	387	258	0.03%	0.004%
79	11.810	3259	3272	3300	rBV	329384	539420	70.75%	9.236%
80	12.013	3333	3335	3338	rBV2	275	197	0.03%	0.003%
81	12.190	3378	3390	3411	rBV	243510	401186	52.62%	6.869%
82	12.447	3466	3470	3473	rVB2	353	272	0.04%	0.005%
83	13.142	3683	3686	3690	rBV2	342	304	0.04%	0.005%

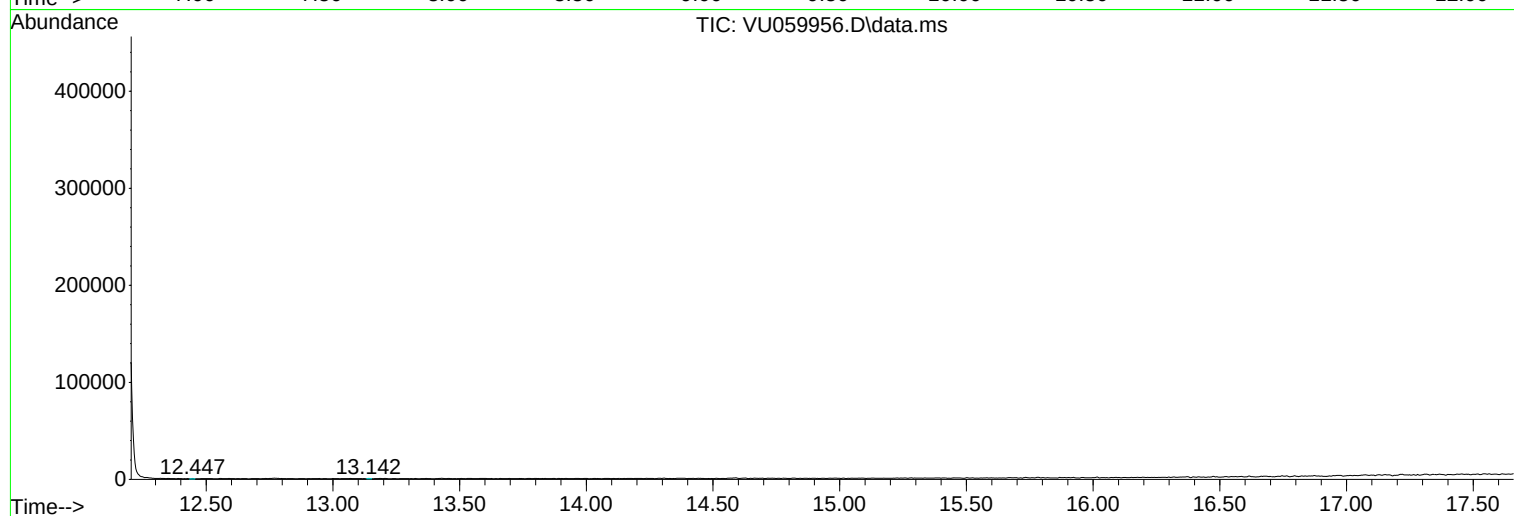
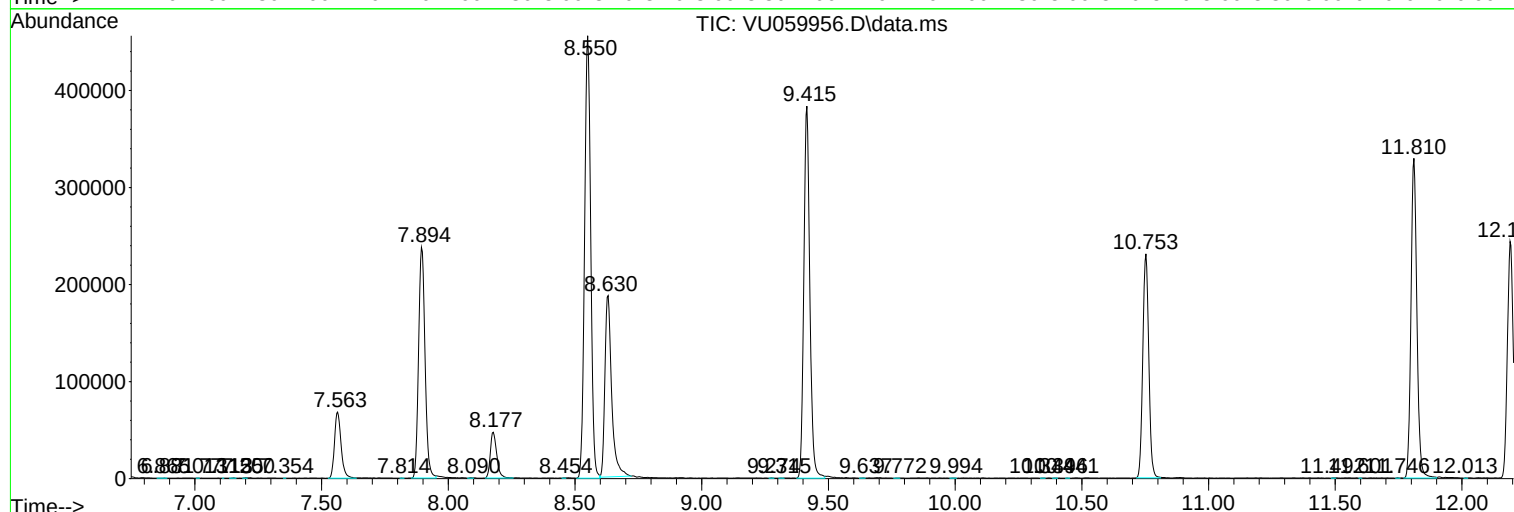
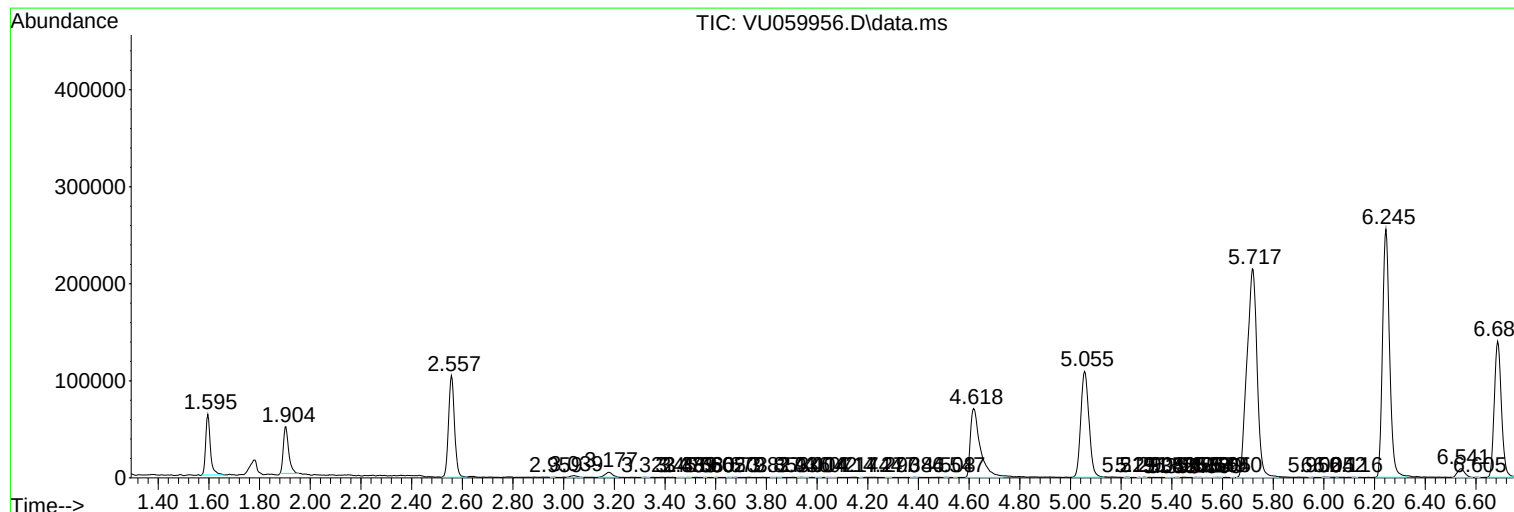
Sum of corrected areas: 5840173

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
Data File : VU059956.D
Acq On : 15 Jul 2024 17:06
Operator : MD/SY
Sample : P3230-01MEDL 1600X
Misc : 4.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB32MEDL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
Data File : VU059956.D
Acq On : 15 Jul 2024 17:06
Operator : MD/SY
Sample : P3230-01MEDL 1600X
Misc : 4.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB32MEDL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.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\VU071524\
Data File : VU059956.D
Acq On : 15 Jul 2024 17:06
Operator : MD/SY
Sample : P3230-01MEDL 1600X
Misc : 4.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB32MEDL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.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
------------------	----	---------	-------	----------	---	----	------	------