

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070824\
 Data File : VX042230.D
 Acq On : 08 Jul 2024 11:50
 Operator : JC/MD
 Sample : P3100-17ME
 Misc : 4.21g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D08ME

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_X\Method\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042230.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	25	28	38	rVB	13521	16390	2.32%	0.281%
2	2.276	189	195	213	rBV	107917	198750	28.18%	3.406%
3	2.599	246	248	249	rBV2	347	270	0.04%	0.005%
4	2.721	262	268	282	rBV	27587	63468	9.00%	1.088%
5	3.178	340	343	345	rVB2	75	83	0.01%	0.001%
6	3.221	345	350	353	rBV2	142	248	0.04%	0.004%
7	3.324	364	367	368	rBV2	136	119	0.02%	0.002%
8	3.422	382	383	386	rVB2	264	191	0.03%	0.003%
9	3.458	386	389	390	rBV	97	92	0.01%	0.002%
10	3.501	395	396	399	rBV	163	108	0.02%	0.002%
11	3.611	413	414	417	rVB	253	163	0.02%	0.003%
12	3.757	436	438	441	rBV2	72	97	0.01%	0.002%
13	3.891	459	460	462	rBV	169	110	0.02%	0.002%
14	3.958	468	471	472	rBV	122	119	0.02%	0.002%
15	4.025	480	482	487	rBV2	80	78	0.01%	0.001%
16	4.153	501	503	505	rBV	102	95	0.01%	0.002%
17	4.312	528	529	532	rVB2	179	149	0.02%	0.003%
18	4.355	532	536	537	rBV2	161	196	0.03%	0.003%
19	4.495	550	559	576	rBV	43426	153329	21.74%	2.628%
20	5.056	638	651	669	rBV	82944	259769	36.83%	4.452%
21	5.391	699	706	714	rBV2	1328	3980	0.56%	0.068%
22	5.550	726	732	742	rVB2	1455	3707	0.53%	0.064%
23	5.824	776	777	779	rBV	145	105	0.01%	0.002%
24	5.964	787	800	831	rBV2	240638	705336	100.00%	12.088%
25	6.208	838	840	844	rVB2	271	256	0.04%	0.004%
26	6.543	893	895	898	rVB	255	249	0.04%	0.004%
27	6.574	898	900	905	rBV2	200	234	0.03%	0.004%
28	6.677	914	917	921	rBV3	198	332	0.05%	0.006%
29	6.757	921	930	959	rVV	239279	582244	82.55%	9.979%
30	7.116	983	989	995	rVB3	1187	2858	0.41%	0.049%
31	7.232	1001	1008	1011	rBV3	617	1194	0.17%	0.020%
32	7.305	1011	1020	1040	rVV	135849	311504	44.16%	5.339%
33	7.580	1063	1065	1068	rBV2	99	90	0.01%	0.002%
34	7.769	1094	1096	1098	rVB	125	92	0.01%	0.002%
35	7.958	1125	1127	1129	rBV	193	166	0.02%	0.003%
36	8.061	1142	1144	1146	rBV2	184	191	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070824\
Data File : VX042230.D
Acq On : 08 Jul 2024 11:50
Operator : JC/MD
Sample : P3100-17ME
Misc : 4.21g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D08ME

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_X\Method\SFAMXML070324WMA.M
Title : VOC Analysis

37	8.134	1153	1156	1157	rBV2	114	113	0.02%	0.002%
38	8.195	1163	1166	1167	rBV2	134	88	0.01%	0.002%
39	8.269	1177	1178	1181	rVB2	115	109	0.02%	0.002%
40	8.323	1181	1187	1206	rBV	80241	141395	20.05%	2.423%
41	8.580	1228	1229	1231	rBV2	91	93	0.01%	0.002%
42	8.647	1234	1240	1256	rBV	357217	579905	82.22%	9.939%
43	8.951	1284	1290	1304	rBV	57031	90437	12.82%	1.550%
44	9.079	1310	1311	1314	rVB2	166	112	0.02%	0.002%
45	9.275	1338	1343	1348	rBV	5022	7544	1.07%	0.129%
46	9.390	1357	1362	1382	rBV	173963	357866	50.74%	6.133%
47	9.659	1404	1406	1408	rVB2	256	158	0.02%	0.003%
48	9.713	1411	1415	1420	rVB2	508	924	0.13%	0.016%
49	9.854	1436	1438	1440	rBV	144	162	0.02%	0.003%
50	9.896	1444	1445	1448	rBV	186	132	0.02%	0.002%
51	9.988	1459	1460	1465	rBV2	162	115	0.02%	0.002%
52	10.055	1465	1471	1491	rBV	480538	672198	95.30%	11.520%
53	10.244	1498	1502	1507	rBV	3510	4604	0.65%	0.079%
54	10.305	1509	1512	1518	rVB4	1059	1606	0.23%	0.028%
55	10.549	1550	1552	1554	rVB	179	121	0.02%	0.002%
56	10.652	1562	1569	1571	rBV3	491	834	0.12%	0.014%
57	10.774	1586	1589	1590	rBV	362	429	0.06%	0.007%
58	10.817	1593	1596	1599	rVB4	834	994	0.14%	0.017%
59	10.854	1599	1602	1603	rBV2	138	154	0.02%	0.003%
60	10.945	1613	1617	1619	rBV	2493	2970	0.42%	0.051%
61	11.067	1634	1637	1638	rBV2	115	146	0.02%	0.003%
62	11.091	1638	1641	1646	rVB3	1121	1707	0.24%	0.029%
63	11.195	1650	1658	1667	rBV	276418	374225	53.06%	6.414%
64	11.317	1673	1678	1685	rVB	5576	7691	1.09%	0.132%
65	11.390	1689	1690	1693	rVB2	136	113	0.02%	0.002%
66	11.567	1717	1719	1721	rBV	119	113	0.02%	0.002%
67	11.640	1728	1731	1734	rBV2	124	163	0.02%	0.003%
68	11.701	1736	1741	1743	rBV	5628	7482	1.06%	0.128%
69	11.731	1743	1746	1749	rBV2	6273	7059	1.00%	0.121%
70	11.835	1761	1763	1764	rBV2	262	160	0.02%	0.003%
71	11.939	1777	1780	1782	rVB2	353	434	0.06%	0.007%
72	11.981	1782	1787	1789	rVB3	1461	2373	0.34%	0.041%
73	12.024	1789	1794	1806	rVB	505337	658623	93.38%	11.288%
74	12.231	1824	1828	1837	rVB5	904	1432	0.20%	0.025%
75	12.323	1837	1843	1853	rBV	402390	536851	76.11%	9.201%
76	12.567	1881	1883	1885	rBV2	115	127	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070824\
 Data File : VX042230.D
 Acq On : 08 Jul 2024 11:50
 Operator : JC/MD
 Sample : P3100-17ME
 Misc : 4.21g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D08ME

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_X\Method\SFAMXML070324WMA.M
 Title : VOC Analysis

77	12.701	1904	1905	1907	rBV	148	91	0.01%	0.002%
78	12.768	1911	1916	1923	rVB2	1419	2104	0.30%	0.036%
79	12.871	1929	1933	1940	rBV2	3783	5552	0.79%	0.095%
80	12.938	1943	1944	1946	rBV	155	123	0.02%	0.002%
81	13.030	1958	1959	1960	rVV	152	80	0.01%	0.001%
82	13.073	1963	1966	1968	rBV2	194	237	0.03%	0.004%
83	13.121	1970	1974	1978	rBV2	304	378	0.05%	0.006%
84	13.164	1978	1981	1986	rBV3	208	380	0.05%	0.007%
85	13.292	2001	2002	2005	rBV	112	93	0.01%	0.002%
86	13.402	2014	2020	2026	rBV2	6259	8192	1.16%	0.140%
87	13.597	2047	2052	2055	rBV2	390	679	0.10%	0.012%
88	13.682	2063	2066	2072	rVB4	699	977	0.14%	0.017%
89	13.780	2079	2082	2086	rBV	1039	1340	0.19%	0.023%
90	13.841	2090	2092	2093	rVV	315	184	0.03%	0.003%
91	13.883	2097	2099	2102	rVB	296	338	0.05%	0.006%
92	14.005	2117	2119	2120	rBV	167	106	0.02%	0.002%
93	14.036	2122	2124	2128	rVV3	287	347	0.05%	0.006%
94	14.426	2184	2188	2196	rBV2	10274	13988	1.98%	0.240%
95	14.536	2204	2206	2211	rBV2	229	337	0.05%	0.006%
96	14.706	2233	2234	2237	rVB2	290	151	0.02%	0.003%
97	14.822	2248	2253	2257	rVB	18435	23268	3.30%	0.399%
98	14.926	2268	2270	2272	rBV2	357	260	0.04%	0.004%
99	15.292	2327	2330	2332	rBV2	965	1094	0.16%	0.019%
100	16.182	2472	2476	2483	rVB3	4199	6449	0.91%	0.111%

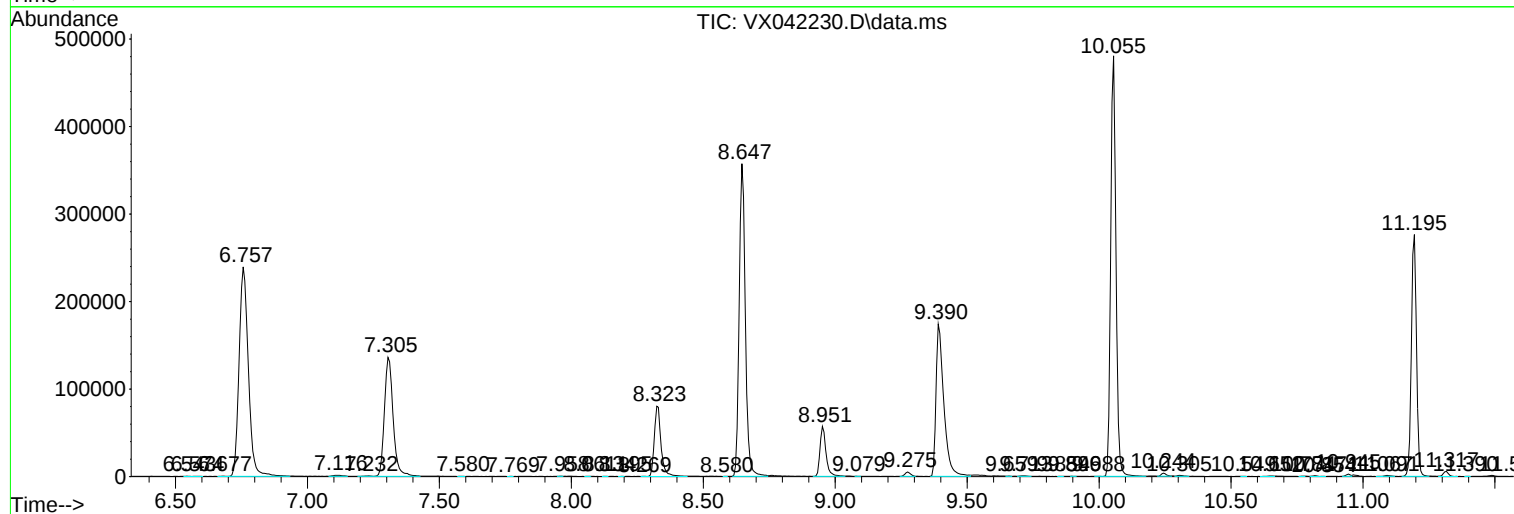
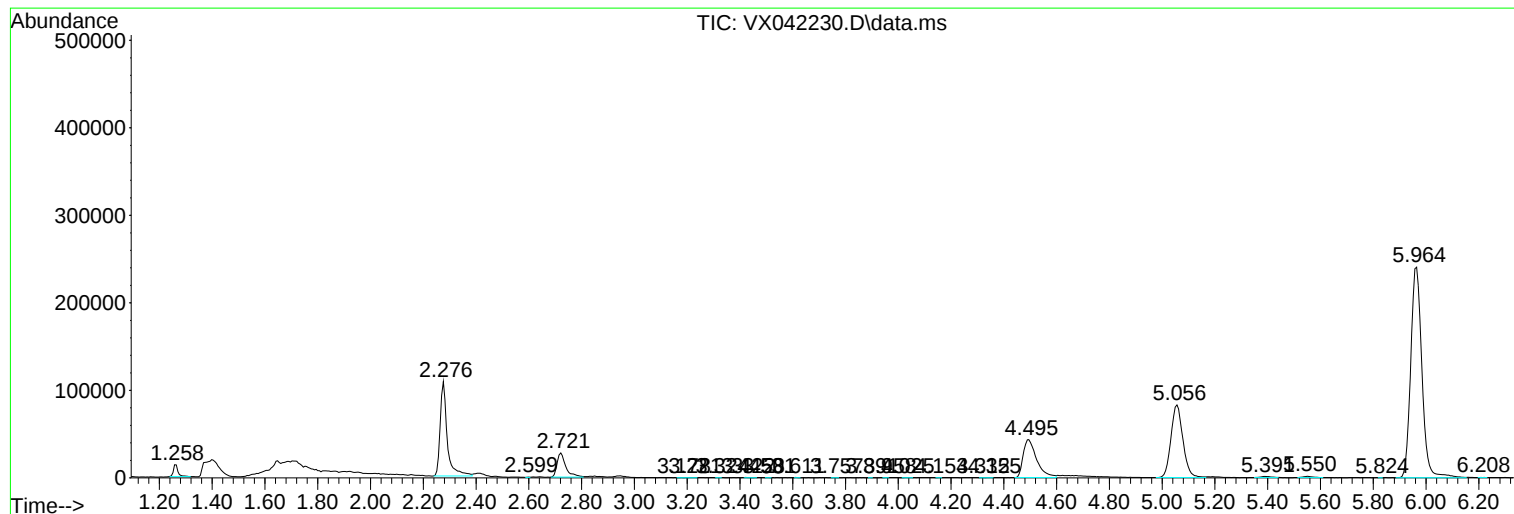
Sum of corrected areas: 5834872

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070824\
Data File : VX042230.D
Acq On : 08 Jul 2024 11:50
Operator : JC/MD
Sample : P3100-17ME
Misc : 4.21g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D08ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070824\
Data File : VX042230.D
Acq On : 08 Jul 2024 11:50
Operator : JC/MD
Sample : P3100-17ME
Misc : 4.21g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D08ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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_X\Data\VX070824\
Data File : VX042230.D
Acq On : 08 Jul 2024 11:50
Operator : JC/MD
Sample : P3100-17ME
Misc : 4.21g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D08ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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