

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
 Data File : VX044505.D
 Acq On : 26 Dec 2024 13:24
 Operator : JC/MD
 Sample : P5351-03ME
 Misc : 12.13g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E2925ME

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\SFAMXML120524WMA.M
 Title : VOC Analysis

Signal : TIC: VX044505.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	23	28	33	rBV2	5691	9760	1.00%	0.133%
2	1.368	43	46	59	rVB	87799	147619	15.05%	2.006%
3	1.569	68	79	80	rBV7	15007	39818	4.06%	0.541%
4	1.648	89	92	112	rVB	60808	181219	18.48%	2.463%
5	2.288	191	197	208	rVB	208664	327042	33.34%	4.444%
6	2.642	253	255	256	rBV2	629	466	0.05%	0.006%
7	2.709	260	266	274	rBV	11434	22717	2.32%	0.309%
8	2.941	300	304	315	rVB2	3503	7945	0.81%	0.108%
9	3.026	315	318	320	rBV3	521	502	0.05%	0.007%
10	3.117	329	333	334	rBV3	727	809	0.08%	0.011%
11	3.428	378	384	390	rBV4	1517	3819	0.39%	0.052%
12	3.477	390	392	395	rVB3	511	506	0.05%	0.007%
13	3.745	431	436	439	rBV4	866	1381	0.14%	0.019%
14	4.050	482	486	487	rBV3	441	654	0.07%	0.009%
15	4.294	524	526	528	rBV3	404	389	0.04%	0.005%
16	4.404	541	544	545	rBV3	656	621	0.06%	0.008%
17	4.477	547	556	567	rBV2	37659	136623	13.93%	1.857%
18	5.050	637	650	669	rBV	122622	397400	40.52%	5.400%
19	5.294	688	690	693	rVB4	521	505	0.05%	0.007%
20	5.324	693	695	697	rBV2	514	407	0.04%	0.006%
21	5.385	704	705	707	rVV	811	519	0.05%	0.007%
22	5.416	708	710	715	rVB2	827	1007	0.10%	0.014%
23	5.471	717	719	721	rVV3	682	412	0.04%	0.006%
24	5.641	743	747	751	rBV3	604	1003	0.10%	0.014%
25	5.751	763	765	767	rVB3	624	438	0.04%	0.006%
26	5.806	772	774	776	rVB2	481	376	0.04%	0.005%
27	5.836	776	779	781	rBV2	454	582	0.06%	0.008%
28	5.958	788	799	822	rBV2	336922	980840	100.00%	13.328%
29	6.294	852	854	858	rVB3	407	465	0.05%	0.006%
30	6.361	863	865	870	rVB4	348	433	0.04%	0.006%
31	6.452	878	880	881	rBV	522	436	0.04%	0.006%
32	6.550	894	896	899	rVB2	450	388	0.04%	0.005%
33	6.586	899	902	903	rBV3	460	538	0.05%	0.007%
34	6.647	910	912	916	rVB3	636	710	0.07%	0.010%
35	6.684	916	918	920	rBV2	461	452	0.05%	0.006%
36	6.757	921	930	944	rVV	244356	598545	61.02%	8.133%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
 Data File : VX044505.D
 Acq On : 26 Dec 2024 13:24
 Operator : JC/MD
 Sample : P5351-03ME
 Misc : 12.13g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E2925ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
 Title : VOC Analysis

37	7.104	983	987	988	rBV4	1711	1839	0.19%	0.025%
38	7.300	1011	1019	1033	rBV	195522	438212	44.68%	5.955%
39	7.531	1056	1057	1059	rBV	625	410	0.04%	0.006%
40	7.708	1085	1086	1091	rVB3	493	620	0.06%	0.008%
41	7.751	1091	1093	1095	rBV2	419	443	0.05%	0.006%
42	7.903	1117	1118	1121	rVB	611	425	0.04%	0.006%
43	7.934	1121	1123	1126	rBV2	510	550	0.06%	0.007%
44	7.964	1126	1128	1130	rBV2	356	481	0.05%	0.007%
45	8.074	1144	1146	1149	rBV2	389	542	0.06%	0.007%
46	8.263	1173	1177	1181	rVV3	2022	2917	0.30%	0.040%
47	8.324	1181	1187	1200	rBV	113125	196212	20.00%	2.666%
48	8.464	1209	1210	1212	rBV	584	372	0.04%	0.005%
49	8.647	1233	1240	1257	rBV	499800	792144	80.76%	10.764%
50	8.952	1284	1290	1299	rBV	77825	125698	12.82%	1.708%
51	9.086	1311	1312	1315	rBV3	528	583	0.06%	0.008%
52	9.122	1315	1318	1319	rVV3	453	464	0.05%	0.006%
53	9.177	1326	1327	1330	rBV2	420	415	0.04%	0.006%
54	9.391	1357	1362	1378	rBV	197263	337805	34.44%	4.590%
55	9.604	1395	1397	1398	rBV2	854	872	0.09%	0.012%
56	9.653	1404	1405	1409	rBV4	422	434	0.04%	0.006%
57	9.708	1410	1414	1417	rVV2	1063	1266	0.13%	0.017%
58	9.872	1439	1441	1442	rBV	824	466	0.05%	0.006%
59	9.982	1455	1459	1460	rBV3	591	443	0.05%	0.006%
60	10.049	1465	1470	1485	rBV	492498	717579	73.16%	9.751%
61	10.293	1508	1510	1512	rBV3	792	885	0.09%	0.012%
62	10.433	1531	1533	1535	rBV2	391	415	0.04%	0.006%
63	10.457	1535	1537	1540	rVB3	482	593	0.06%	0.008%
64	10.512	1544	1546	1548	rBV3	610	486	0.05%	0.007%
65	10.622	1562	1564	1566	rBV3	527	505	0.05%	0.007%
66	10.646	1566	1568	1570	rVV2	816	739	0.08%	0.010%
67	10.756	1582	1586	1587	rBV3	539	720	0.07%	0.010%
68	10.884	1605	1607	1608	rBV2	566	399	0.04%	0.005%
69	11.152	1649	1651	1652	rBV	945	578	0.06%	0.008%
70	11.189	1652	1657	1669	rVV	312675	424834	43.31%	5.773%
71	11.427	1694	1696	1698	rBV2	845	914	0.09%	0.012%
72	11.604	1720	1725	1726	rBV3	820	1215	0.12%	0.017%
73	11.677	1734	1737	1740	rBV3	760	863	0.09%	0.012%
74	11.713	1740	1743	1746	rVV4	1732	2047	0.21%	0.028%
75	11.756	1746	1750	1754	rVV5	1331	2670	0.27%	0.036%
76	11.866	1766	1768	1771	rVB3	803	723	0.07%	0.010%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
 Data File : VX044505.D
 Acq On : 26 Dec 2024 13:24
 Operator : JC/MD
 Sample : P5351-03ME
 Misc : 12.13g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E2925ME

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\SFAMXLM120524WMA.M
 Title : VOC Analysis

77	11.896	1771	1773	1775	rBV3	892	771	0.08%	0.010%
78	11.921	1775	1777	1779	rBV2	934	778	0.08%	0.011%
79	11.963	1782	1784	1785	rBV	760	527	0.05%	0.007%
80	12.018	1788	1793	1803	rBV	540446	700815	71.45%	9.523%
81	12.238	1827	1829	1831	rBV2	672	517	0.05%	0.007%
82	12.317	1837	1842	1851	rBV	542388	685816	69.92%	9.319%
83	12.762	1912	1915	1918	rBV	3064	3648	0.37%	0.050%
84	13.341	2008	2010	2013	rBV4	1437	1563	0.16%	0.021%
85	13.384	2013	2017	2019	rVV5	1588	2014	0.21%	0.027%
86	13.780	2078	2082	2087	rBV3	3683	6384	0.65%	0.087%
87	14.036	2121	2124	2128	rVB4	1766	2597	0.26%	0.035%
88	14.128	2136	2139	2142	rVB3	3918	4880	0.50%	0.066%
89	14.317	2169	2170	2172	rBV2	1129	932	0.10%	0.013%
90	14.609	2215	2218	2220	rBV3	1433	1867	0.19%	0.025%
91	14.749	2239	2241	2245	rBV4	1892	2154	0.22%	0.029%
92	15.072	2293	2294	2296	rBV2	900	637	0.06%	0.009%
93	15.213	2310	2317	2323	rVB10	1495	3448	0.35%	0.047%
94	15.316	2332	2334	2341	rBV5	1595	2758	0.28%	0.037%
95	15.481	2356	2361	2368	rBV7	2991	5655	0.58%	0.077%
96	15.786	2409	2411	2413	rVB2	687	468	0.05%	0.006%
97	15.822	2413	2417	2419	rBV5	792	1136	0.12%	0.015%
98	15.841	2419	2420	2422	rVB2	950	587	0.06%	0.008%
99	16.341	2500	2502	2503	rBV2	988	816	0.08%	0.011%
100	16.505	2527	2529	2532	rBV2	928	1148	0.12%	0.016%

Sum of corrected areas: 7359040

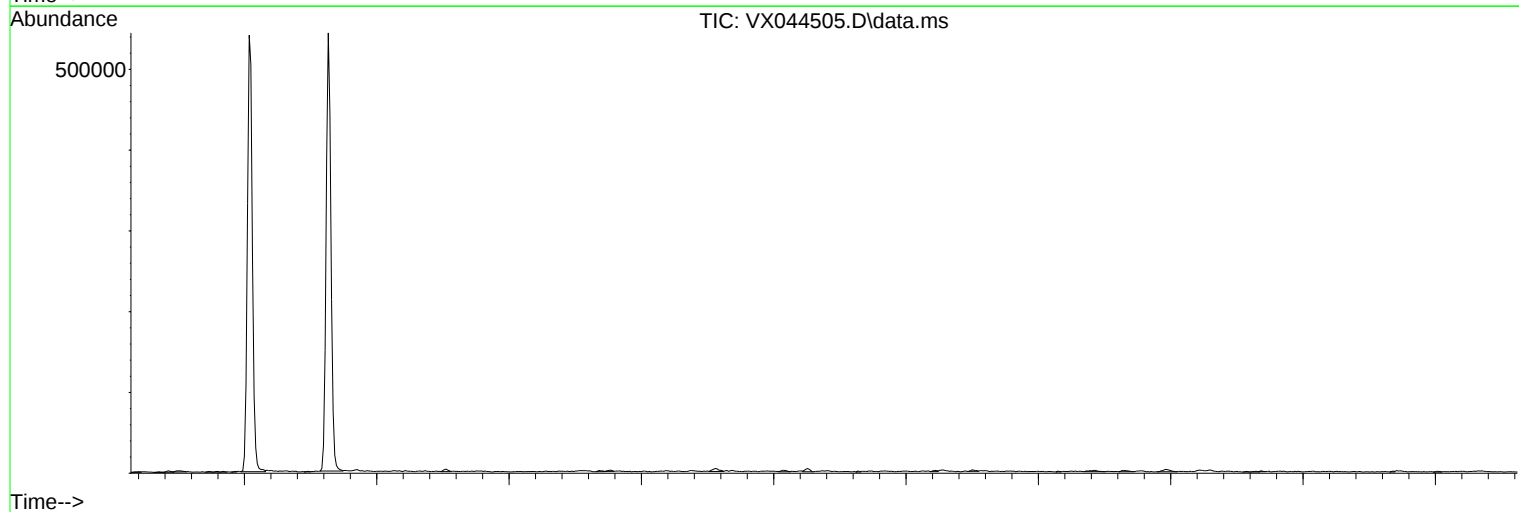
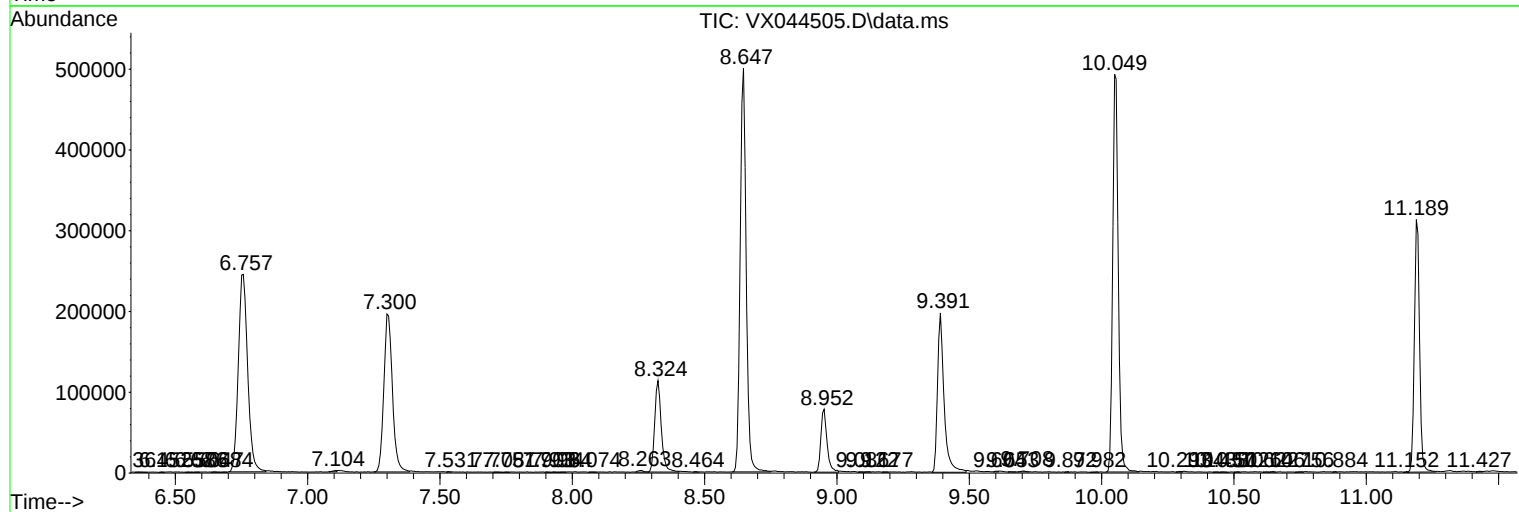
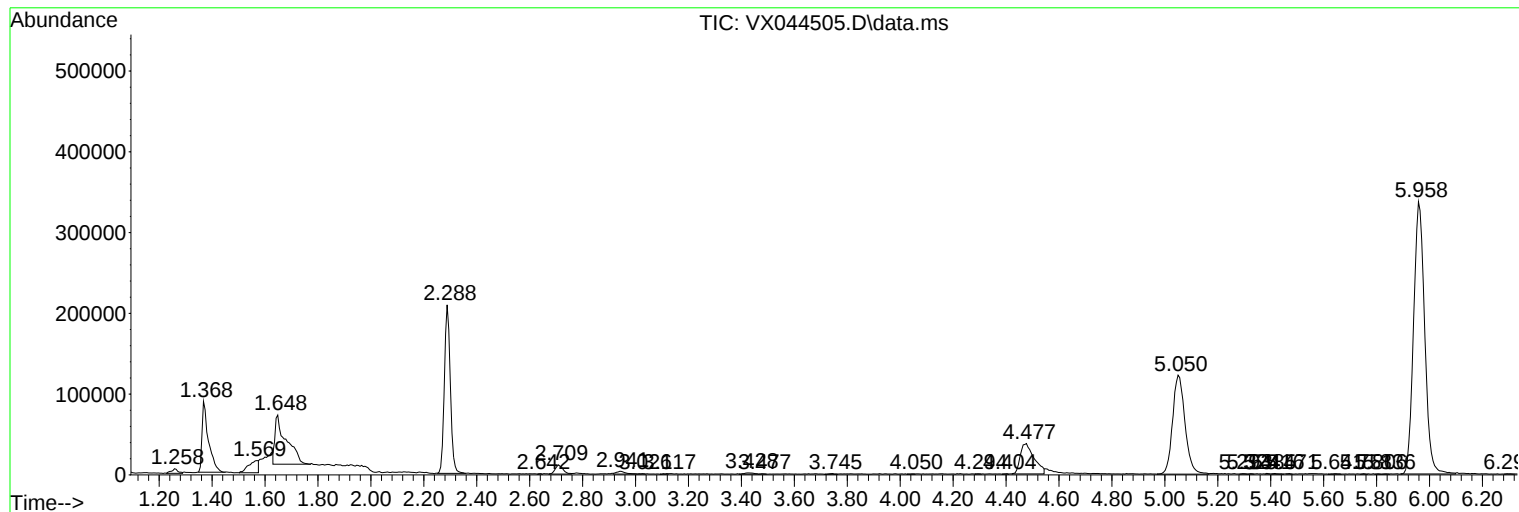
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
Data File : VX044505.D
Acq On : 26 Dec 2024 13:24
Operator : JC/MD
Sample : P5351-03ME
Misc : 12.13g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E2925ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
Data File : VX044505.D
Acq On : 26 Dec 2024 13:24
Operator : JC/MD
Sample : P5351-03ME
Misc : 12.13g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E2925ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.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\VX122624\
Data File : VX044505.D
Acq On : 26 Dec 2024 13:24
Operator : JC/MD
Sample : P5351-03ME
Misc : 12.13g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E2925ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.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
