

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
 Data File : VX044498.D
 Acq On : 26 Dec 2024 10:44
 Operator : JC/MD
 Sample : P5331-01ME
 Misc : 6.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E2AQ1ME

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

Signal : TIC: VX044498.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	32	rVB	4754	3872	0.43%	0.061%
2	1.368	43	46	60	rVB	73328	138896	15.57%	2.179%
3	1.648	89	92	95	rBV	38042	50963	5.71%	0.800%
4	2.288	191	197	212	rVB	195998	302694	33.94%	4.749%
5	2.459	224	225	229	rBV2	721	920	0.10%	0.014%
6	2.782	274	278	286	rVB6	1425	2943	0.33%	0.046%
7	2.873	292	293	297	rVB	532	434	0.05%	0.007%
8	2.941	297	304	312	rBV2	4224	12001	1.35%	0.188%
9	3.032	317	319	321	rVV	873	566	0.06%	0.009%
10	3.123	332	334	338	rVV4	626	617	0.07%	0.010%
11	3.251	352	355	357	rVB3	522	593	0.07%	0.009%
12	3.404	377	380	381	rVV2	584	510	0.06%	0.008%
13	3.422	381	383	386	rVV3	965	1306	0.15%	0.020%
14	3.678	422	425	428	rBV3	311	470	0.05%	0.007%
15	3.818	443	448	449	rVB2	590	673	0.08%	0.011%
16	3.959	467	471	472	rBV2	532	622	0.07%	0.010%
17	4.221	510	514	515	rBV2	597	679	0.08%	0.011%
18	4.471	547	555	571	rBV	33014	134459	15.08%	2.110%
19	5.050	639	650	666	rVV	109064	359538	40.32%	5.641%
20	5.178	669	671	675	rVV3	847	1175	0.13%	0.018%
21	5.208	675	676	678	rVV2	618	424	0.05%	0.007%
22	5.647	747	748	751	rBV2	464	458	0.05%	0.007%
23	5.757	764	766	770	rBV2	573	619	0.07%	0.010%
24	5.885	784	787	788	rBV2	380	422	0.05%	0.007%
25	5.958	788	799	816	rBV2	308240	891799	100.00%	13.992%
26	6.245	844	846	849	rBV2	380	409	0.05%	0.006%
27	6.300	853	855	858	rVB2	567	424	0.05%	0.007%
28	6.367	860	866	873	rBV6	1151	3242	0.36%	0.051%
29	6.458	878	881	883	rBV3	633	744	0.08%	0.012%
30	6.665	912	915	916	rBV	695	453	0.05%	0.007%
31	6.678	916	917	920	rBV3	407	493	0.06%	0.008%
32	6.757	920	930	951	rBV	218469	539399	60.48%	8.463%
33	7.123	982	990	997	rVB8	3083	8419	0.94%	0.132%
34	7.300	1010	1019	1033	rBV	175312	395573	44.36%	6.206%
35	7.677	1079	1081	1084	rVB3	546	548	0.06%	0.009%
36	7.970	1125	1129	1130	rBV3	631	851	0.10%	0.013%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
 Data File : VX044498.D
 Acq On : 26 Dec 2024 10:44
 Operator : JC/MD
 Sample : P5331-01ME
 Misc : 6.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E2AQ1ME

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	8.025	1136	1138	1141	rVB3	544	469	0.05%	0.007%
38	8.055	1141	1143	1146	rVB3	347	405	0.05%	0.006%
39	8.098	1149	1150	1155	rVB2	702	578	0.06%	0.009%
40	8.147	1155	1158	1159	rBV	551	493	0.06%	0.008%
41	8.324	1179	1187	1201	rBV	98267	177091	19.86%	2.779%
42	8.476	1211	1212	1213	rBV	909	410	0.05%	0.006%
43	8.647	1233	1240	1250	rBV	432253	706544	79.23%	11.085%
44	8.878	1273	1278	1279	rBV4	676	945	0.11%	0.015%
45	8.952	1284	1290	1301	rBV	68634	112893	12.66%	1.771%
46	9.122	1314	1318	1321	rBV4	599	942	0.11%	0.015%
47	9.391	1356	1362	1378	rBV	167013	303872	34.07%	4.768%
48	9.702	1411	1413	1415	rBV2	844	848	0.10%	0.013%
49	9.811	1429	1431	1432	rBV2	545	408	0.05%	0.006%
50	10.049	1465	1470	1488	rBV	448560	632474	70.92%	9.923%
51	10.275	1505	1507	1508	rBV2	579	406	0.05%	0.006%
52	10.305	1510	1512	1516	rVV3	1479	1576	0.18%	0.025%
53	10.573	1553	1556	1560	rVB2	545	479	0.05%	0.008%
54	10.640	1565	1567	1570	rBV3	1088	1250	0.14%	0.020%
55	10.817	1592	1596	1598	rBV2	533	673	0.08%	0.011%
56	10.884	1602	1607	1608	rBV4	389	431	0.05%	0.007%
57	10.951	1613	1618	1619	rBV3	623	1139	0.13%	0.018%
58	11.012	1626	1628	1632	rVB2	648	711	0.08%	0.011%
59	11.061	1634	1636	1640	rVB2	470	411	0.05%	0.006%
60	11.110	1640	1644	1646	rVB	621	613	0.07%	0.010%
61	11.189	1652	1657	1669	rBV	277915	377926	42.38%	5.930%
62	11.445	1696	1699	1703	rBV5	590	1100	0.12%	0.017%
63	11.543	1712	1715	1719	rBV2	598	775	0.09%	0.012%
64	11.689	1736	1739	1742	rVV2	457	645	0.07%	0.010%
65	11.750	1745	1749	1752	rBV5	745	1251	0.14%	0.020%
66	11.780	1752	1754	1757	rVV3	476	437	0.05%	0.007%
67	11.902	1772	1774	1778	rVV2	553	757	0.08%	0.012%
68	12.018	1788	1793	1802	rBV	443870	573745	64.34%	9.002%
69	12.317	1837	1842	1857	rBV	460567	587355	65.86%	9.215%
70	12.579	1883	1885	1887	rVB2	442	400	0.04%	0.006%
71	12.762	1909	1915	1919	rVB3	2353	3456	0.39%	0.054%
72	12.847	1927	1929	1933	rVB2	499	513	0.06%	0.008%
73	12.890	1933	1936	1938	rBV3	508	737	0.08%	0.012%
74	13.061	1960	1964	1967	rBV4	330	432	0.05%	0.007%
75	13.207	1985	1988	1990	rVB3	611	497	0.06%	0.008%
76	13.274	1997	1999	2000	rVV2	586	425	0.05%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
 Data File : VX044498.D
 Acq On : 26 Dec 2024 10:44
 Operator : JC/MD
 Sample : P5331-01ME
 Misc : 6.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E2AQ1ME

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	13.305	2002	2004	2006	rVV2	718	605	0.07%	0.009%
78	13.341	2008	2010	2012	rVV2	631	432	0.05%	0.007%
79	13.439	2024	2026	2027	rBV2	444	410	0.05%	0.006%
80	13.597	2047	2052	2058	rBV2	739	1377	0.15%	0.022%
81	13.798	2081	2085	2087	rBV3	678	1034	0.12%	0.016%
82	13.987	2115	2116	2120	rBV4	609	646	0.07%	0.010%
83	14.091	2131	2133	2134	rBV	696	479	0.05%	0.008%
84	14.128	2136	2139	2143	rVB	3240	4232	0.47%	0.066%
85	14.207	2147	2152	2153	rBV3	286	403	0.05%	0.006%
86	14.225	2153	2155	2159	rVB3	614	726	0.08%	0.011%
87	14.499	2198	2200	2204	rVB3	879	685	0.08%	0.011%
88	14.542	2204	2207	2208	rBV3	655	507	0.06%	0.008%
89	14.585	2212	2214	2217	rVV3	574	553	0.06%	0.009%
90	14.670	2227	2228	2231	rVB2	620	477	0.05%	0.007%
91	14.951	2272	2274	2278	rBV2	638	958	0.11%	0.015%
92	15.152	2304	2307	2308	rBV3	593	436	0.05%	0.007%
93	15.518	2366	2367	2370	rBV3	856	844	0.09%	0.013%
94	15.609	2379	2382	2383	rBV3	827	1066	0.12%	0.017%
95	15.646	2386	2388	2391	rVV4	658	813	0.09%	0.013%
96	15.713	2398	2399	2401	rBV2	662	419	0.05%	0.007%
97	16.188	2475	2477	2479	rBV2	511	483	0.05%	0.008%
98	16.316	2496	2498	2499	rBV2	604	436	0.05%	0.007%
99	16.408	2510	2513	2514	rBV2	637	456	0.05%	0.007%
100	16.487	2525	2526	2527	rBV	805	399	0.04%	0.006%

Sum of corrected areas: 6373596

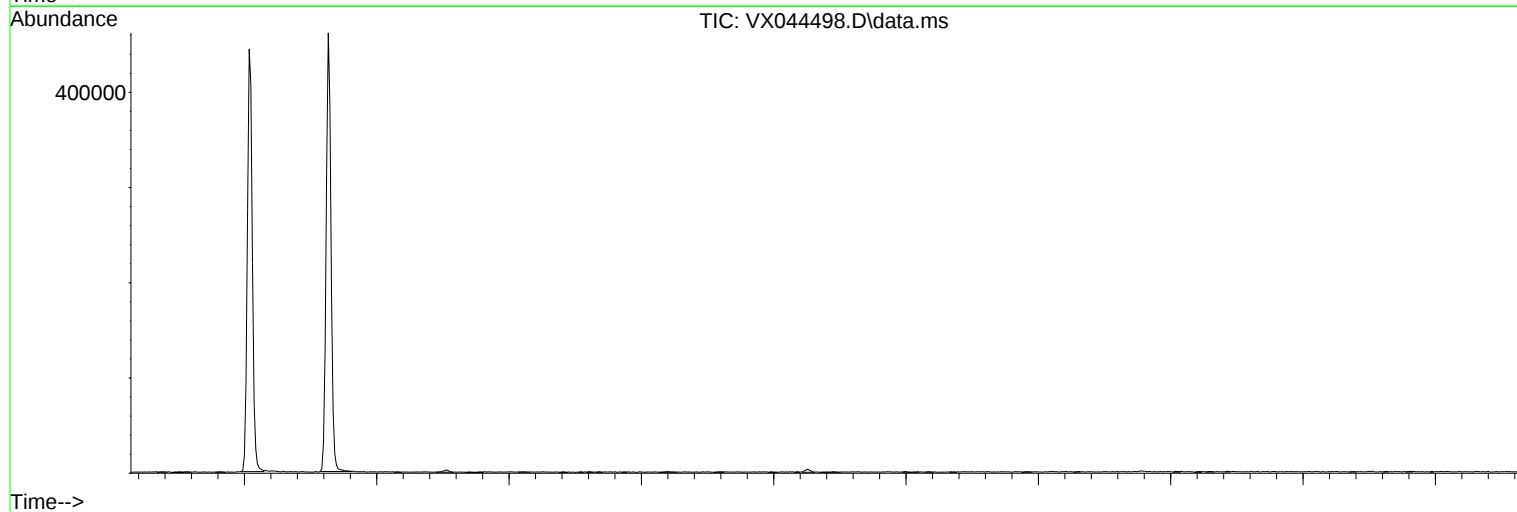
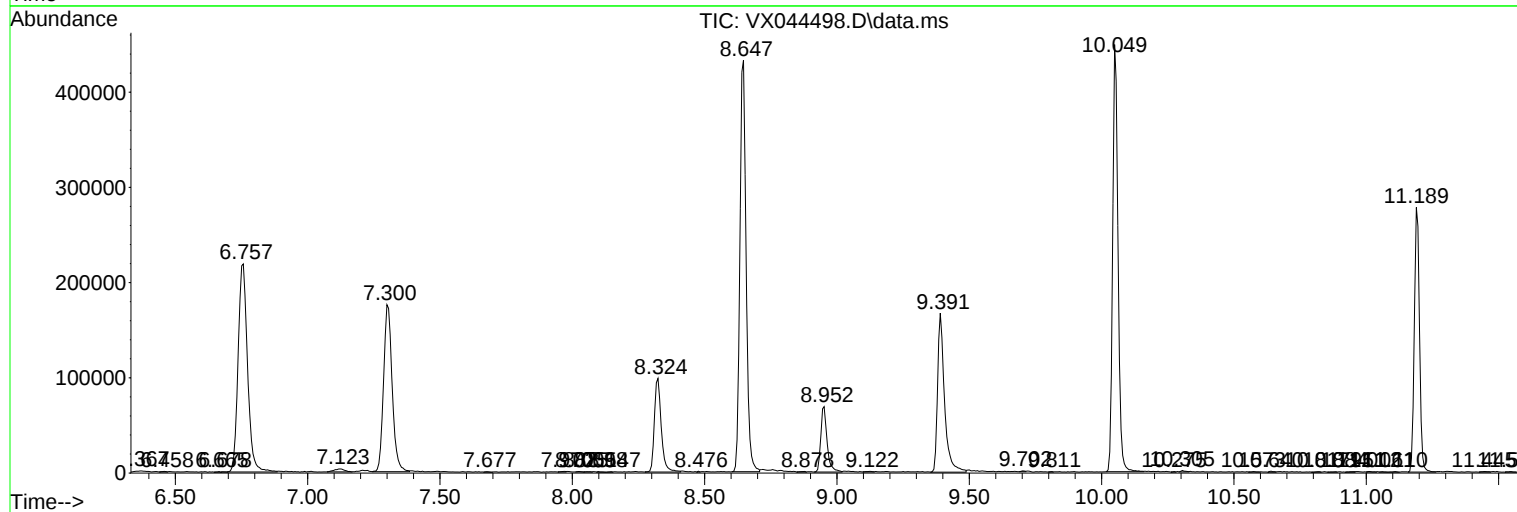
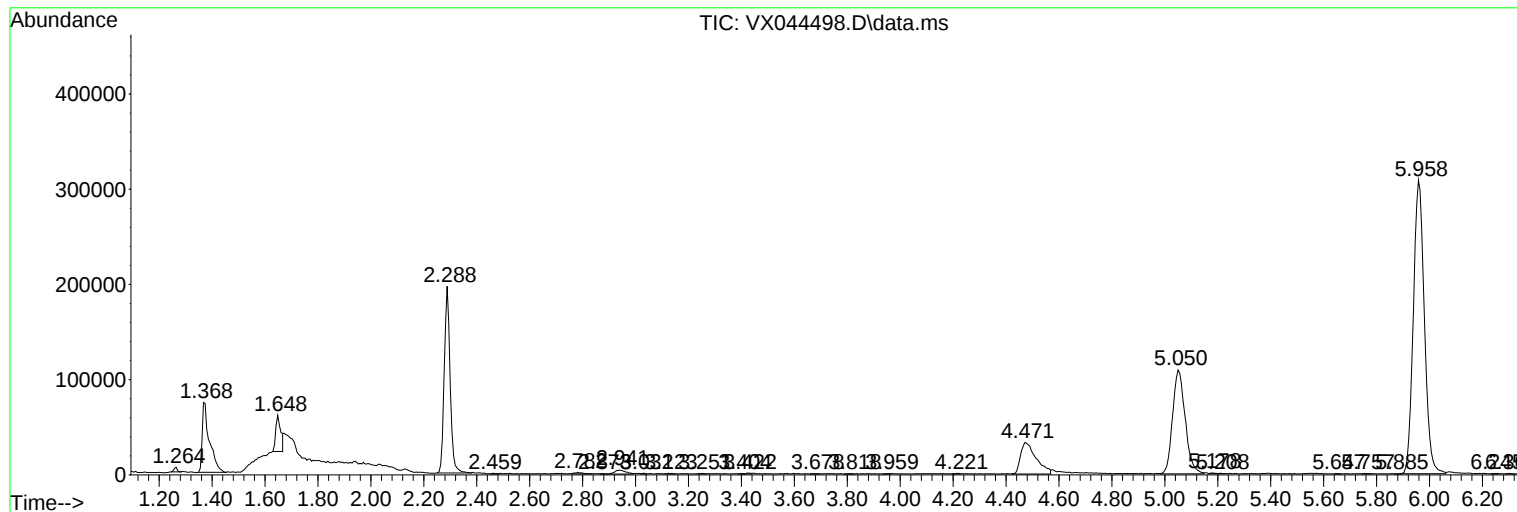
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
Data File : VX044498.D
Acq On : 26 Dec 2024 10:44
Operator : JC/MD
Sample : P5331-01ME
Misc : 6.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E2AQ1ME

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 : VX044498.D
Acq On : 26 Dec 2024 10:44
Operator : JC/MD
Sample : P5331-01ME
Misc : 6.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E2AQ1ME

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 : VX044498.D
Acq On : 26 Dec 2024 10:44
Operator : JC/MD
Sample : P5331-01ME
Misc : 6.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E2AQ1ME

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	#	RT	Resp	Conc
------------------	----	---------	-------	----------	---	----	------	------