

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
 Data File : VX044765.D
 Acq On : 29 Jan 2025 13:20
 Operator : JC/MD
 Sample : Q1190-08ME
 Misc : 5.80g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44S7ME

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\SFAMXML012825WMA.M
 Title : VOC Analysis

Signal : TIC: VX044765.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	12	rBV2	914	691	0.04%	0.005%
2	1.258	23	28	33	rBV2	11977	23567	1.37%	0.178%
3	1.368	42	46	49	rBV	109947	119704	6.94%	0.905%
4	1.569	72	79	82	rBV6	4848	12451	0.72%	0.094%
5	1.648	89	92	95	rBV	17688	22374	1.30%	0.169%
6	2.276	189	195	213	rBV	349222	578780	33.58%	4.374%
7	2.624	244	252	258	rBV	417146	1293349	75.03%	9.774%
8	3.843	446	452	453	rBV2	605	976	0.06%	0.007%
9	3.898	457	461	464	rVV4	325	624	0.04%	0.005%
10	3.928	464	466	468	rVV3	463	400	0.02%	0.003%
11	4.288	522	525	527	rVB3	424	475	0.03%	0.004%
12	4.367	535	538	542	rBV3	434	699	0.04%	0.005%
13	4.404	542	544	545	rBV	510	442	0.03%	0.003%
14	4.483	548	557	581	rBV2	73874	308496	17.90%	2.331%
15	4.965	634	636	638	rBV	636	492	0.03%	0.004%
16	5.050	639	650	669	rVV	211599	654595	37.97%	4.947%
17	5.245	680	682	685	rBV3	300	379	0.02%	0.003%
18	5.385	703	705	706	rVV2	605	547	0.03%	0.004%
19	5.538	726	730	731	rBV2	876	1207	0.07%	0.009%
20	5.550	731	732	735	rVV3	1306	1388	0.08%	0.010%
21	5.580	735	737	740	rVV3	909	924	0.05%	0.007%
22	5.617	741	743	747	rVB3	460	610	0.04%	0.005%
23	5.654	747	749	753	rBV3	601	783	0.05%	0.006%
24	5.733	761	762	767	rVB2	487	447	0.03%	0.003%
25	5.958	788	799	815	rBV2	605134	1723818	100.00%	13.027%
26	6.367	864	866	868	rBV3	385	482	0.03%	0.004%
27	6.757	919	930	950	rBV	365401	902226	52.34%	6.818%
28	6.995	967	969	972	rVB3	364	380	0.02%	0.003%
29	7.117	985	989	990	rBV4	1928	2314	0.13%	0.017%
30	7.178	997	999	1003	rBV5	536	601	0.03%	0.005%
31	7.220	1003	1006	1007	rBV2	453	389	0.02%	0.003%
32	7.306	1011	1020	1039	rVV	350012	781434	45.33%	5.905%
33	7.482	1045	1049	1056	rBV5	1033	2174	0.13%	0.016%
34	7.562	1061	1062	1067	rBV2	503	755	0.04%	0.006%
35	7.623	1070	1072	1074	rVB3	469	426	0.02%	0.003%
36	7.684	1078	1082	1086	rBV4	483	743	0.04%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
 Data File : VX044765.D
 Acq On : 29 Jan 2025 13:20
 Operator : JC/MD
 Sample : Q1190-08ME
 Misc : 5.80g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44S7ME

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\SFAMXML012825WMA.M
 Title : VOC Analysis

37	7.757	1092	1094	1095	rBV2	471	390	0.02%	0.003%
38	7.970	1122	1129	1132	rBV4	1269	2659	0.15%	0.020%
39	8.080	1145	1147	1151	rVB3	432	389	0.02%	0.003%
40	8.214	1166	1169	1170	rBV	656	697	0.04%	0.005%
41	8.245	1170	1174	1176	rBV2	485	398	0.02%	0.003%
42	8.324	1180	1187	1198	rBV	256799	433947	25.17%	3.279%
43	8.647	1233	1240	1268	rVV	834217	1424184	82.62%	10.763%
44	8.946	1284	1289	1305	rBV	168961	271722	15.76%	2.053%
45	9.275	1341	1343	1346	rBV2	977	1021	0.06%	0.008%
46	9.391	1356	1362	1383	rBV	332924	621657	36.06%	4.698%
47	9.714	1408	1415	1418	rBV4	1577	3334	0.19%	0.025%
48	9.763	1420	1423	1425	rVV3	431	499	0.03%	0.004%
49	9.817	1430	1432	1435	rVB2	432	424	0.02%	0.003%
50	9.878	1438	1442	1444	rBV3	440	466	0.03%	0.004%
51	10.049	1465	1470	1490	rBV	689004	1059865	61.48%	8.010%
52	10.305	1508	1512	1515	rBV3	865	1380	0.08%	0.010%
53	10.439	1531	1534	1536	rBV2	371	408	0.02%	0.003%
54	10.647	1564	1568	1571	rBV4	571	751	0.04%	0.006%
55	10.744	1579	1584	1587	rVB3	314	580	0.03%	0.004%
56	10.915	1609	1612	1615	rBV3	265	372	0.02%	0.003%
57	10.970	1618	1621	1624	rBV3	320	445	0.03%	0.003%
58	11.049	1632	1634	1638	rVB2	407	573	0.03%	0.004%
59	11.140	1647	1649	1652	rVV2	317	422	0.02%	0.003%
60	11.189	1652	1657	1666	rVV	574543	783870	45.47%	5.924%
61	11.281	1670	1672	1674	rVV2	813	810	0.05%	0.006%
62	11.317	1674	1678	1680	rVB4	872	1249	0.07%	0.009%
63	11.439	1695	1698	1699	rBV2	533	512	0.03%	0.004%
64	11.561	1714	1718	1722	rBV3	359	556	0.03%	0.004%
65	11.707	1740	1742	1745	rBV3	978	1048	0.06%	0.008%
66	11.750	1745	1749	1754	rVB5	1685	3003	0.17%	0.023%
67	11.884	1769	1771	1776	rVB3	425	479	0.03%	0.004%
68	11.933	1776	1779	1782	rVB2	1645	1817	0.11%	0.014%
69	11.963	1782	1784	1785	rBV2	541	397	0.02%	0.003%
70	12.018	1788	1793	1804	rBV	766818	983642	57.06%	7.434%
71	12.238	1827	1829	1833	rBV	499	535	0.03%	0.004%
72	12.317	1837	1842	1853	rVV	906644	1154769	66.99%	8.727%
73	12.604	1887	1889	1892	rVV3	435	460	0.03%	0.003%
74	12.634	1892	1894	1897	rVV2	389	385	0.02%	0.003%
75	12.762	1911	1915	1919	rVB3	1985	2666	0.15%	0.020%
76	12.890	1929	1936	1938	rBV4	1110	2050	0.12%	0.015%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
 Data File : VX044765.D
 Acq On : 29 Jan 2025 13:20
 Operator : JC/MD
 Sample : Q1190-08ME
 Misc : 5.80g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44S7ME

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\SFAMXML012825WMA.M
 Title : VOC Analysis

77	12.933	1942	1943	1946	rBV3	464	463	0.03%	0.003%
78	13.268	1994	1998	2003	rBV3	701	1013	0.06%	0.008%
79	13.414	2019	2022	2023	rBV2	455	413	0.02%	0.003%
80	13.792	2080	2084	2087	rBV2	594	880	0.05%	0.007%
81	13.914	2100	2104	2110	rVB4	470	901	0.05%	0.007%
82	13.975	2110	2114	2118	rBV3	580	975	0.06%	0.007%
83	14.036	2122	2124	2125	rVV2	528	373	0.02%	0.003%
84	14.128	2135	2139	2141	rVV2	954	1039	0.06%	0.008%
85	14.170	2143	2146	2150	rBV3	539	707	0.04%	0.005%
86	14.292	2164	2166	2171	rVB3	378	418	0.02%	0.003%
87	14.439	2186	2190	2199	rBV4	6237	10294	0.60%	0.078%
88	14.652	2220	2225	2229	rVV4	1090	1907	0.11%	0.014%
89	14.707	2232	2234	2236	rBV3	470	405	0.02%	0.003%
90	14.725	2236	2237	2240	rBV3	359	407	0.02%	0.003%
91	14.774	2243	2245	2247	rVV3	606	650	0.04%	0.005%
92	14.792	2247	2248	2251	rVV3	689	595	0.03%	0.004%
93	14.841	2255	2256	2259	rVB2	585	406	0.02%	0.003%
94	14.871	2259	2261	2265	rBV3	312	394	0.02%	0.003%
95	15.085	2294	2296	2297	rBV2	633	421	0.02%	0.003%
96	15.420	2349	2351	2353	rBV2	583	531	0.03%	0.004%
97	15.621	2381	2384	2388	rBV6	1116	1682	0.10%	0.013%
98	15.780	2408	2410	2412	rBV3	727	536	0.03%	0.004%
99	15.847	2419	2421	2424	rBV4	1078	1182	0.07%	0.009%
100	16.030	2449	2451	2452	rBV2	1090	847	0.05%	0.006%

Sum of corrected areas: 13232412

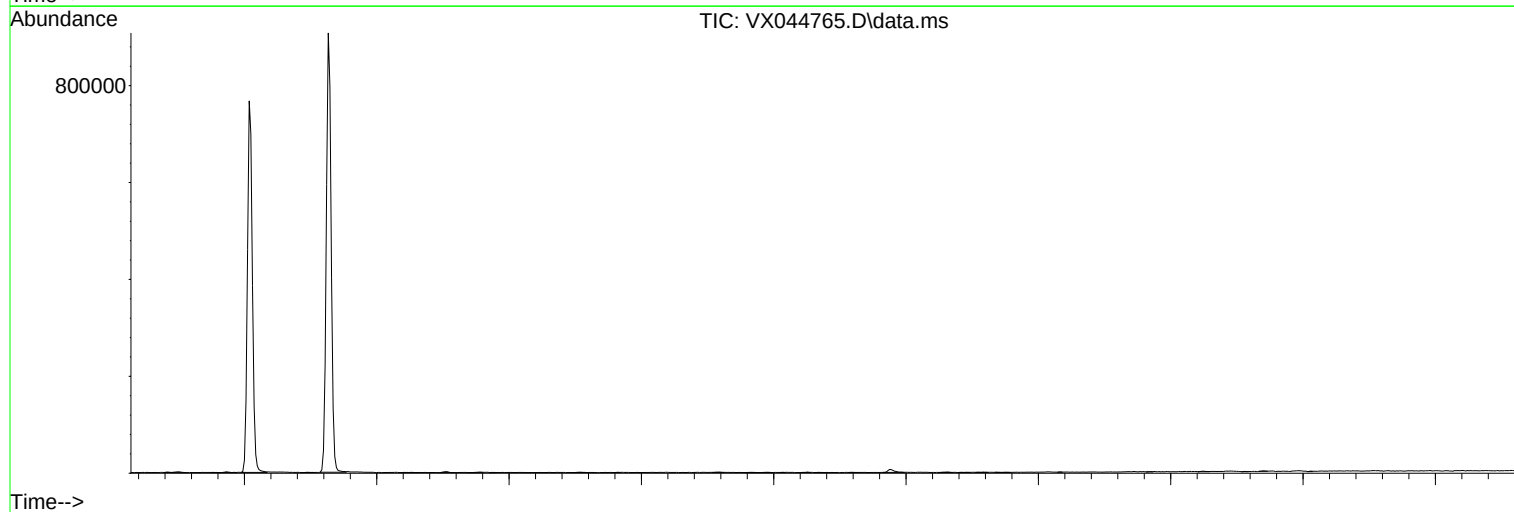
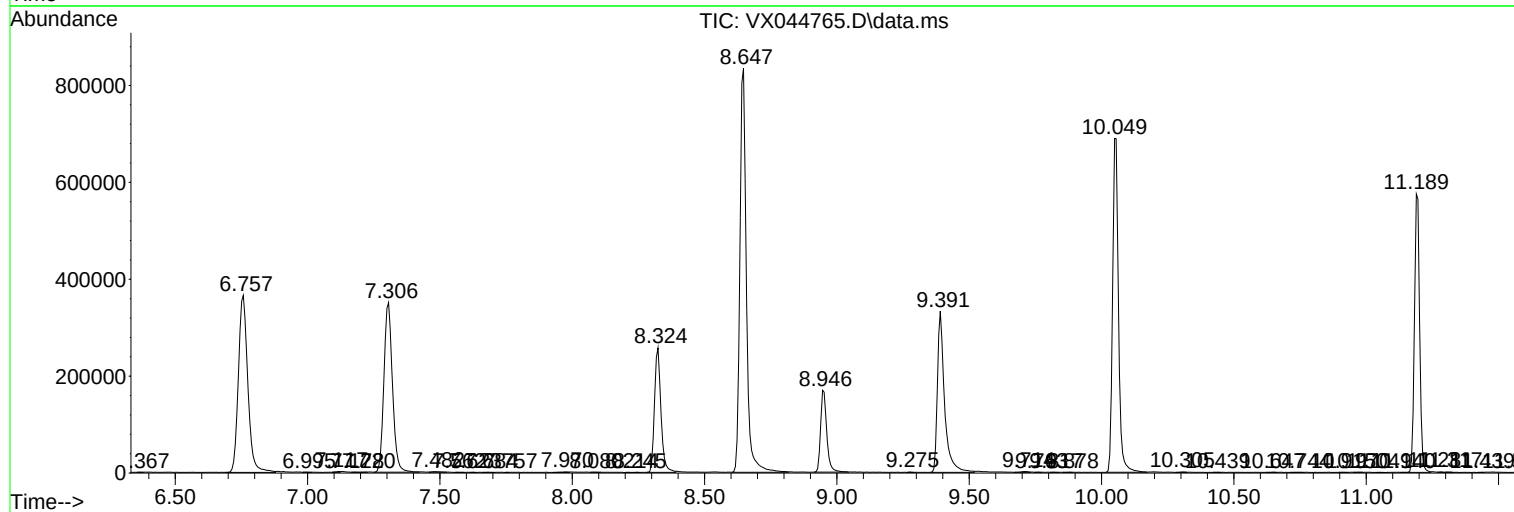
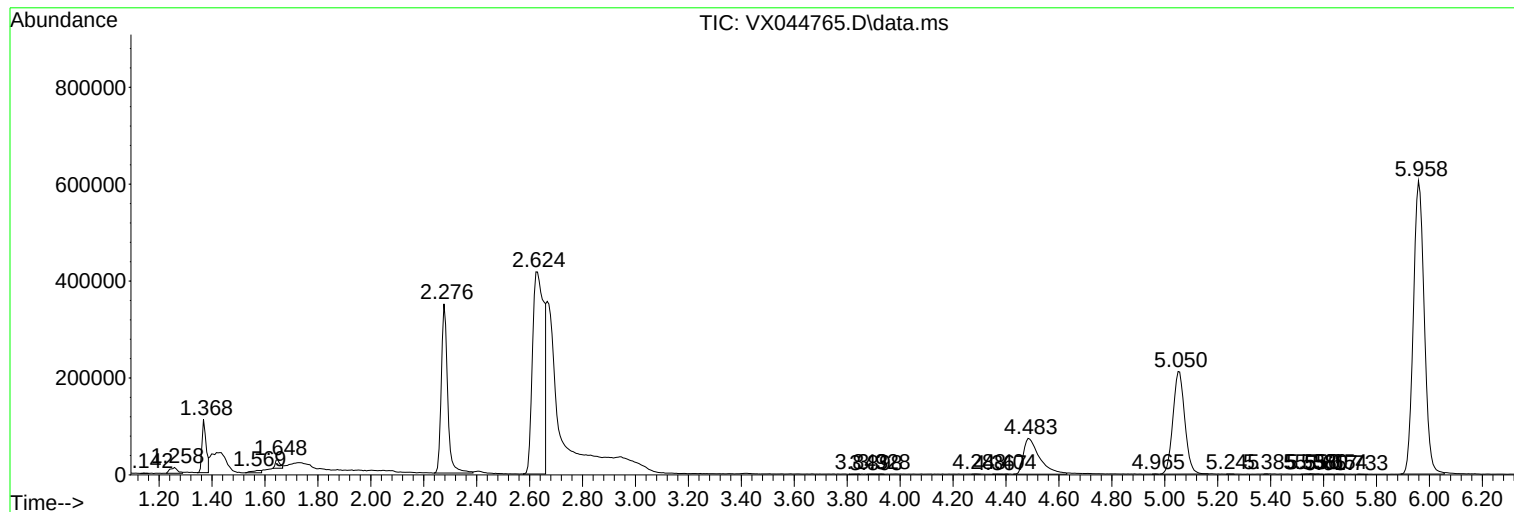
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044765.D
Acq On : 29 Jan 2025 13:20
Operator : JC/MD
Sample : Q1190-08ME
Misc : 5.80g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44S7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044765.D
Acq On : 29 Jan 2025 13:20
Operator : JC/MD
Sample : Q1190-08ME
Misc : 5.80g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44S7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.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\VX012925\
Data File : VX044765.D
Acq On : 29 Jan 2025 13:20
Operator : JC/MD
Sample : Q1190-08ME
Misc : 5.80g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44S7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML012825WMA.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
------------------	----	---------	-------	----------	---	----	------	------