

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
 Data File : VX044794.D
 Acq On : 31 Jan 2025 14:17
 Operator : JC/MD
 Sample : Q1189-05ME
 Misc : 12.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44Q8ME

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

Signal : TIC: VX044794.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.245	22	26	34	rBV2	14338	28219	2.87%	0.397%
2	1.367	43	46	49	rBV	70647	78543	8.00%	1.105%
3	1.648	89	92	96	rBV	15554	18929	1.93%	0.266%
4	2.282	190	196	214	rBV	202320	330741	33.68%	4.654%
5	2.550	239	240	243	rBV2	425	570	0.06%	0.008%
6	2.617	245	251	254	rBV4	1866	4367	0.44%	0.061%
7	2.776	275	277	280	rBV3	662	844	0.09%	0.012%
8	2.946	298	305	315	rVV2	5209	12464	1.27%	0.175%
9	3.020	315	317	319	rVB2	616	511	0.05%	0.007%
10	3.050	319	322	324	rBV2	358	512	0.05%	0.007%
11	3.190	344	345	347	rVB	508	270	0.03%	0.004%
12	3.227	347	351	352	rBV2	374	362	0.04%	0.005%
13	3.300	361	363	366	rBV	379	337	0.03%	0.005%
14	3.489	392	394	395	rBV	625	405	0.04%	0.006%
15	3.574	406	408	411	rVB2	356	229	0.02%	0.003%
16	3.745	435	436	439	rVB2	327	216	0.02%	0.003%
17	3.855	452	454	456	rVB	271	247	0.03%	0.003%
18	3.885	456	459	460	rVB2	248	213	0.02%	0.003%
19	3.897	460	461	462	rBV	392	224	0.02%	0.003%
20	3.965	469	472	473	rBV2	384	357	0.04%	0.005%
21	3.995	473	477	478	rVB2	481	469	0.05%	0.007%
22	4.007	478	479	481	rBV	541	372	0.04%	0.005%
23	4.068	485	489	490	rBV2	421	403	0.04%	0.006%
24	4.349	533	535	539	rBV2	285	405	0.04%	0.006%
25	4.483	548	557	576	rBV	44024	169143	17.22%	2.380%
26	5.050	637	650	671	rVV	119992	375289	38.22%	5.281%
27	5.312	691	693	694	rVB	759	397	0.04%	0.006%
28	5.330	694	696	698	rBV2	418	453	0.05%	0.006%
29	5.361	698	701	702	rBV2	324	369	0.04%	0.005%
30	5.440	712	714	716	rBV2	365	217	0.02%	0.003%
31	5.537	726	730	732	rBV3	376	615	0.06%	0.009%
32	5.690	750	755	756	rBV2	158	204	0.02%	0.003%
33	5.793	770	772	773	rBV	289	214	0.02%	0.003%
34	5.824	775	777	778	rVB2	438	259	0.03%	0.004%
35	5.958	786	799	821	rBV2	338206	981983	100.00%	13.819%
36	6.391	867	870	871	rBV2	440	430	0.04%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
 Data File : VX044794.D
 Acq On : 31 Jan 2025 14:17
 Operator : JC/MD
 Sample : Q1189-05ME
 Misc : 12.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44Q8ME

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	6.458	878	881	882	rBV2	257	297	0.03%	0.004%
38	6.476	882	884	889	rVV2	525	662	0.07%	0.009%
39	6.568	897	899	902	rBV	173	205	0.02%	0.003%
40	6.671	913	916	919	rBV	409	612	0.06%	0.009%
41	6.757	921	930	956	rBV	241093	605774	61.69%	8.524%
42	6.970	963	965	966	rVB2	430	286	0.03%	0.004%
43	7.202	999	1003	1005	rBV3	573	904	0.09%	0.013%
44	7.305	1011	1020	1034	rBV	197439	441723	44.98%	6.216%
45	7.604	1068	1069	1072	rBV2	322	328	0.03%	0.005%
46	7.708	1084	1086	1088	rVV2	233	217	0.02%	0.003%
47	7.750	1090	1093	1096	rVV	441	558	0.06%	0.008%
48	7.799	1100	1101	1103	rBV2	356	275	0.03%	0.004%
49	7.866	1110	1112	1113	rBV2	311	251	0.03%	0.004%
50	7.927	1120	1122	1125	rBV	372	391	0.04%	0.006%
51	7.976	1129	1130	1135	rVB	641	496	0.05%	0.007%
52	8.031	1135	1139	1140	rBV2	264	397	0.04%	0.006%
53	8.110	1150	1152	1154	rBV2	273	223	0.02%	0.003%
54	8.177	1161	1163	1164	rVB	453	237	0.02%	0.003%
55	8.195	1164	1166	1167	rBV	291	252	0.03%	0.004%
56	8.323	1181	1187	1205	rBV	134691	231782	23.60%	3.262%
57	8.647	1233	1240	1269	rVV	469676	797743	81.24%	11.226%
58	8.903	1278	1282	1284	rBV2	503	627	0.06%	0.009%
59	8.951	1285	1290	1303	rVV	96738	148033	15.07%	2.083%
60	9.214	1332	1333	1335	rBV	347	254	0.03%	0.004%
61	9.287	1343	1345	1347	rVB2	257	242	0.02%	0.003%
62	9.335	1352	1353	1356	rBV2	417	474	0.05%	0.007%
63	9.390	1357	1362	1381	rBV	186112	340688	34.69%	4.794%
64	9.707	1411	1414	1418	rVB2	1445	1571	0.16%	0.022%
65	9.793	1427	1428	1431	rBV	598	644	0.07%	0.009%
66	9.860	1438	1439	1441	rVB	375	246	0.03%	0.003%
67	9.878	1441	1442	1443	rBV	435	249	0.03%	0.004%
68	9.939	1450	1452	1455	rVB2	342	425	0.04%	0.006%
69	9.982	1457	1459	1460	rBV	371	224	0.02%	0.003%
70	10.049	1465	1470	1486	rBV	475632	714976	72.81%	10.061%
71	10.360	1518	1521	1526	rBV4	644	1107	0.11%	0.016%
72	10.482	1540	1541	1543	rBV2	340	209	0.02%	0.003%
73	10.543	1548	1551	1553	rBV	290	350	0.04%	0.005%
74	10.591	1556	1559	1560	rBV2	407	453	0.05%	0.006%
75	10.634	1564	1566	1567	rBV2	548	597	0.06%	0.008%
76	10.768	1587	1588	1590	rBV	397	404	0.04%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
 Data File : VX044794.D
 Acq On : 31 Jan 2025 14:17
 Operator : JC/MD
 Sample : Q1189-05ME
 Misc : 12.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A44Q8ME

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	10.823	1595	1597	1598	rVB	383	218	0.02%	0.003%
78	10.896	1606	1609	1612	rVB2	734	655	0.07%	0.009%
79	10.951	1616	1618	1620	rVB	498	357	0.04%	0.005%
80	10.975	1620	1622	1624	rVB2	454	290	0.03%	0.004%
81	11.012	1624	1628	1629	rBV	267	350	0.04%	0.005%
82	11.024	1629	1630	1635	rVB3	420	367	0.04%	0.005%
83	11.067	1635	1637	1640	rBV4	368	534	0.05%	0.008%
84	11.140	1647	1649	1650	rBV	313	264	0.03%	0.004%
85	11.189	1652	1657	1669	rVV	320205	445214	45.34%	6.265%
86	11.286	1671	1673	1675	rVV2	477	367	0.04%	0.005%
87	11.396	1686	1691	1693	rBV4	443	848	0.09%	0.012%
88	11.433	1693	1697	1698	rBV4	578	555	0.06%	0.008%
89	11.481	1701	1705	1707	rBV2	1305	1470	0.15%	0.021%
90	11.573	1719	1720	1721	rBV	362	205	0.02%	0.003%
91	11.683	1735	1738	1740	rBV2	945	1244	0.13%	0.018%
92	11.713	1740	1743	1745	rVV3	1476	1464	0.15%	0.021%
93	11.890	1768	1772	1776	rBV4	1024	1506	0.15%	0.021%
94	11.939	1776	1780	1781	rBV4	1588	1855	0.19%	0.026%
95	12.018	1788	1793	1805	rBV	515551	674652	68.70%	9.494%
96	12.158	1812	1816	1821	rVB6	1858	2868	0.29%	0.040%
97	12.244	1825	1830	1833	rBV4	723	1132	0.12%	0.016%
98	12.317	1837	1842	1855	rBV	523049	662024	67.42%	9.316%
99	12.676	1899	1901	1906	rBV5	1302	1823	0.19%	0.026%
100	12.865	1930	1932	1933	rBV2	1159	854	0.09%	0.012%

Sum of corrected areas: 7106284

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044794.D
Acq On : 31 Jan 2025 14:17
Operator : JC/MD
Sample : Q1189-05ME
Misc : 12.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44Q8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXMLM012825WMA.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\VX013125\
Data File : VX044794.D
Acq On : 31 Jan 2025 14:17
Operator : JC/MD
Sample : Q1189-05ME
Misc : 12.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44Q8ME

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	--Internal Standard--			
					#	RT	Resp	Conc