

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061422\
 Data File : VX029498.D
 Acq On : 15 Jun 2022 04:08
 Operator : JC/MD
 Sample : N3292-01ME
 Misc : 6.24g/5mL/100uL/5.06mL/MSVOA_X/MEOH
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW4P2ME

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\SFAMXML061322WMA.M
 Title : VOC Analysis

Signal : TIC: VX029498.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	27	29	31	rBV2	1873	1714	0.15%	0.018%
2	1.294	31	34	39	rVV2	4260	6680	0.59%	0.072%
3	1.368	42	46	53	rVB	97756	126557	11.15%	1.360%
4	1.557	72	77	83	rBV4	3567	8696	0.77%	0.093%
5	1.611	84	86	87	rBV2	2072	1598	0.14%	0.017%
6	1.666	91	95	101	rVB	47399	62572	5.51%	0.672%
7	2.282	190	196	205	rBV	193795	310924	27.39%	3.341%
8	2.361	205	209	214	rBV	2886	6111	0.54%	0.066%
9	2.727	263	269	274	rBV3	2918	6783	0.60%	0.073%
10	2.953	297	306	326	rVV	19290	72018	6.34%	0.774%
11	3.556	401	405	406	rBV	572	523	0.05%	0.006%
12	4.495	549	559	593	rBV	57768	306989	27.05%	3.299%
13	5.062	638	652	666	rBV2	143793	462777	40.77%	4.972%
14	5.385	698	705	715	rBV5	642	1990	0.18%	0.021%
15	5.525	723	728	729	rBV2	308	441	0.04%	0.005%
16	5.556	729	733	741	rVB5	949	2056	0.18%	0.022%
17	5.684	751	754	757	rVB2	328	429	0.04%	0.005%
18	5.970	787	801	815	rBV2	397101	1135054	100.00%	12.196%
19	6.373	857	867	879	rBV4	6854	24026	2.12%	0.258%
20	6.543	893	895	896	rBV2	440	422	0.04%	0.005%
21	6.763	918	931	948	rBV	341087	821610	72.39%	8.828%
22	6.976	962	966	968	rVB3	344	451	0.04%	0.005%
23	7.129	982	991	1000	rBV5	18935	47523	4.19%	0.511%
24	7.220	1000	1006	1012	rVV3	4056	10055	0.89%	0.108%
25	7.312	1013	1021	1037	rVV	234739	521192	45.92%	5.600%
26	7.482	1043	1049	1054	rBV4	1042	2305	0.20%	0.025%
27	7.842	1106	1108	1111	rVB3	457	524	0.05%	0.006%
28	7.964	1121	1128	1140	rBV7	3673	11127	0.98%	0.120%
29	8.055	1140	1143	1145	rBV4	584	831	0.07%	0.009%
30	8.092	1147	1149	1153	rVB3	548	623	0.05%	0.007%
31	8.250	1171	1175	1177	rBV4	355	451	0.04%	0.005%
32	8.330	1180	1188	1203	rBV	118654	200388	17.65%	2.153%
33	8.488	1211	1214	1219	rBV3	644	1243	0.11%	0.013%
34	8.653	1231	1241	1249	rBV	530108	858860	75.67%	9.228%
35	8.720	1249	1252	1256	rVV	7853	13771	1.21%	0.148%
36	8.756	1256	1258	1271	rVB3	5782	12689	1.12%	0.136%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061422\
 Data File : VX029498.D
 Acq On : 15 Jun 2022 04:08
 Operator : JC/MD
 Sample : N3292-01ME
 Misc : 6.24g/5mL/100uL/5.06mL/MSVOA_X/MEOH
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW4P2ME

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\SFAMXML061322WMA.M
 Title : VOC Analysis

37	8.958	1284	1291	1306	rVV	77154	126813	11.17%	1.363%
38	9.110	1313	1316	1324	rVB6	1487	2796	0.25%	0.030%
39	9.275	1339	1343	1350	rVB3	1831	2563	0.23%	0.028%
40	9.397	1357	1363	1380	rBV	302184	655211	57.73%	7.040%
41	9.537	1383	1386	1393	rVV2	4539	8023	0.71%	0.086%
42	9.616	1396	1399	1403	rVB6	823	1186	0.10%	0.013%
43	9.720	1411	1416	1419	rBV2	2422	3500	0.31%	0.038%
44	9.896	1443	1445	1447	rVV	585	456	0.04%	0.005%
45	10.055	1465	1471	1481	rBV	687045	942047	83.00%	10.122%
46	10.305	1507	1512	1518	rVB2	2023	3265	0.29%	0.035%
47	10.360	1518	1521	1526	rBV5	565	1041	0.09%	0.011%
48	10.585	1553	1558	1562	rVB3	330	644	0.06%	0.007%
49	10.652	1565	1569	1572	rBV3	981	1291	0.11%	0.014%
50	10.780	1585	1590	1593	rVB3	725	1019	0.09%	0.011%
51	10.872	1599	1605	1607	rBV3	614	975	0.09%	0.010%
52	10.896	1607	1609	1613	rVB4	949	1176	0.10%	0.013%
53	10.945	1613	1617	1622	rBV5	2274	3446	0.30%	0.037%
54	11.030	1628	1631	1635	rBV3	965	1496	0.13%	0.016%
55	11.091	1635	1641	1642	rBV3	1864	3314	0.29%	0.036%
56	11.110	1642	1644	1650	rVB4	2916	4093	0.36%	0.044%
57	11.195	1650	1658	1671	rBV	443797	607930	53.56%	6.532%
58	11.445	1693	1699	1701	rBV4	1572	2879	0.25%	0.031%
59	11.482	1701	1705	1713	rVB4	5998	8757	0.77%	0.094%
60	11.549	1713	1716	1721	rVB4	654	804	0.07%	0.009%
61	11.634	1724	1730	1734	rVB5	1911	2894	0.25%	0.031%
62	11.683	1734	1738	1740	rBV2	1851	2245	0.20%	0.024%
63	11.713	1740	1743	1746	rVV3	2899	3202	0.28%	0.034%
64	11.756	1746	1750	1758	rVB7	3428	6791	0.60%	0.073%
65	11.841	1760	1764	1766	rBV3	1185	1717	0.15%	0.018%
66	11.933	1777	1779	1782	rBV2	1441	1301	0.11%	0.014%
67	11.975	1782	1786	1789	rVV4	2817	3418	0.30%	0.037%
68	12.024	1789	1794	1805	rVV	727156	926171	81.60%	9.952%
69	12.097	1805	1806	1811	rVB5	1186	1499	0.13%	0.016%
70	12.323	1837	1843	1850	rBV	635868	792419	69.81%	8.514%
71	12.427	1856	1860	1863	rBV2	7566	9032	0.80%	0.097%
72	12.536	1876	1878	1880	rBV2	894	898	0.08%	0.010%
73	12.634	1891	1894	1895	rBV3	846	774	0.07%	0.008%
74	12.683	1900	1902	1906	rVB4	1899	2351	0.21%	0.025%
75	12.713	1906	1907	1909	rBV2	735	541	0.05%	0.006%
76	12.768	1911	1916	1921	rBV4	3022	5134	0.45%	0.055%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061422\
 Data File : VX029498.D
 Acq On : 15 Jun 2022 04:08
 Operator : JC/MD
 Sample : N3292-01ME
 Misc : 6.24g/5mL/100uL/5.06mL/MSVOA_X/MEOH
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW4P2ME

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\SFAMXML061322WMA.M
 Title : VOC Analysis

77	12.817	1922	1924	1925	rBV2	699	486	0.04%	0.005%
78	12.865	1928	1932	1936	rBV6	3959	8168	0.72%	0.088%
79	13.048	1958	1962	1964	rBV5	2159	2930	0.26%	0.031%
80	13.152	1977	1979	1983	rVB3	860	590	0.05%	0.006%
81	13.213	1986	1989	1990	rBV3	962	937	0.08%	0.010%
82	13.268	1994	1998	2001	rBV2	12316	14681	1.29%	0.158%
83	13.384	2014	2017	2021	rBV3	7421	10138	0.89%	0.109%
84	13.707	2064	2070	2073	rBV7	2617	5356	0.47%	0.058%
85	13.737	2073	2075	2077	rVB3	1765	1425	0.13%	0.015%
86	13.774	2079	2081	2084	rVV3	2342	2949	0.26%	0.032%
87	13.847	2088	2093	2096	rVB3	5661	7007	0.62%	0.075%
88	13.908	2101	2103	2106	rVB3	1542	1262	0.11%	0.014%
89	14.042	2120	2125	2128	rBV	14585	17278	1.52%	0.186%
90	14.414	2184	2186	2188	rBV2	2110	2207	0.19%	0.024%
91	14.615	2216	2219	2222	rBV5	4055	4362	0.38%	0.047%
92	14.755	2239	2242	2246	rBV	11290	12188	1.07%	0.131%
93	15.127	2302	2303	2307	rBV4	1979	2208	0.19%	0.024%
94	15.213	2314	2317	2324	rVB8	4544	7535	0.66%	0.081%
95	15.493	2359	2363	2369	rVB4	7144	9273	0.82%	0.100%
96	15.895	2427	2429	2432	rBV3	1385	1267	0.11%	0.014%
97	16.084	2458	2460	2463	rBV4	1208	1133	0.10%	0.012%
98	16.151	2469	2471	2472	rVB	1088	534	0.05%	0.006%
99	16.377	2503	2508	2514	rVB6	2346	4982	0.44%	0.054%
100	16.517	2529	2531	2533	rBV3	777	791	0.07%	0.008%

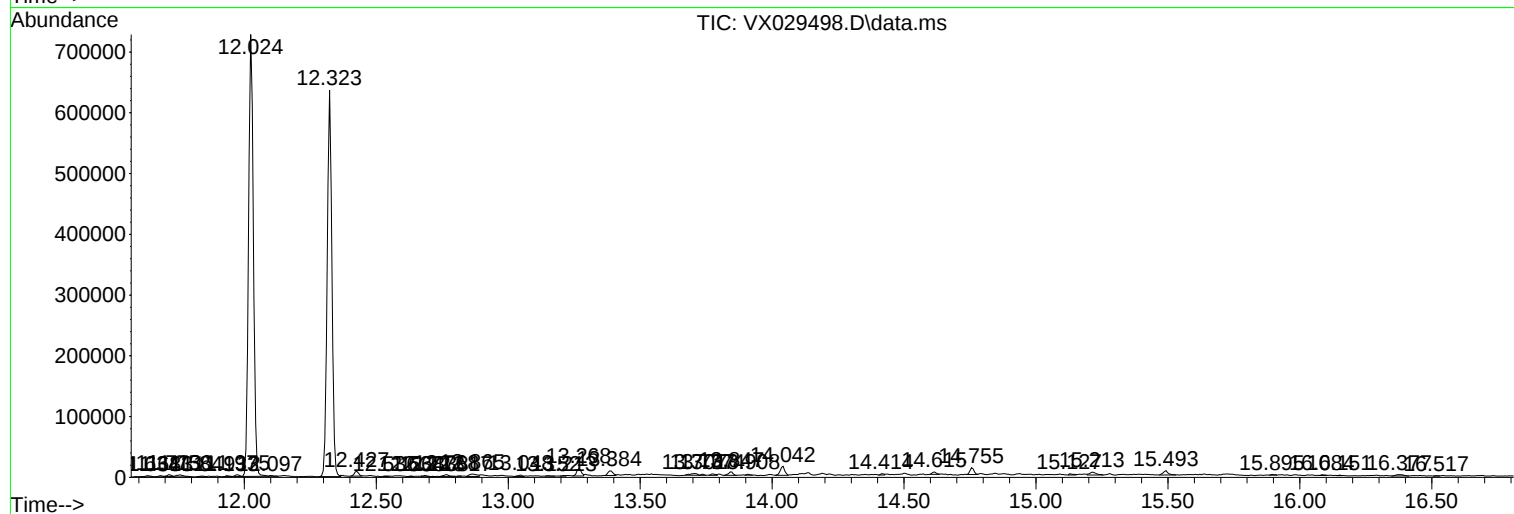
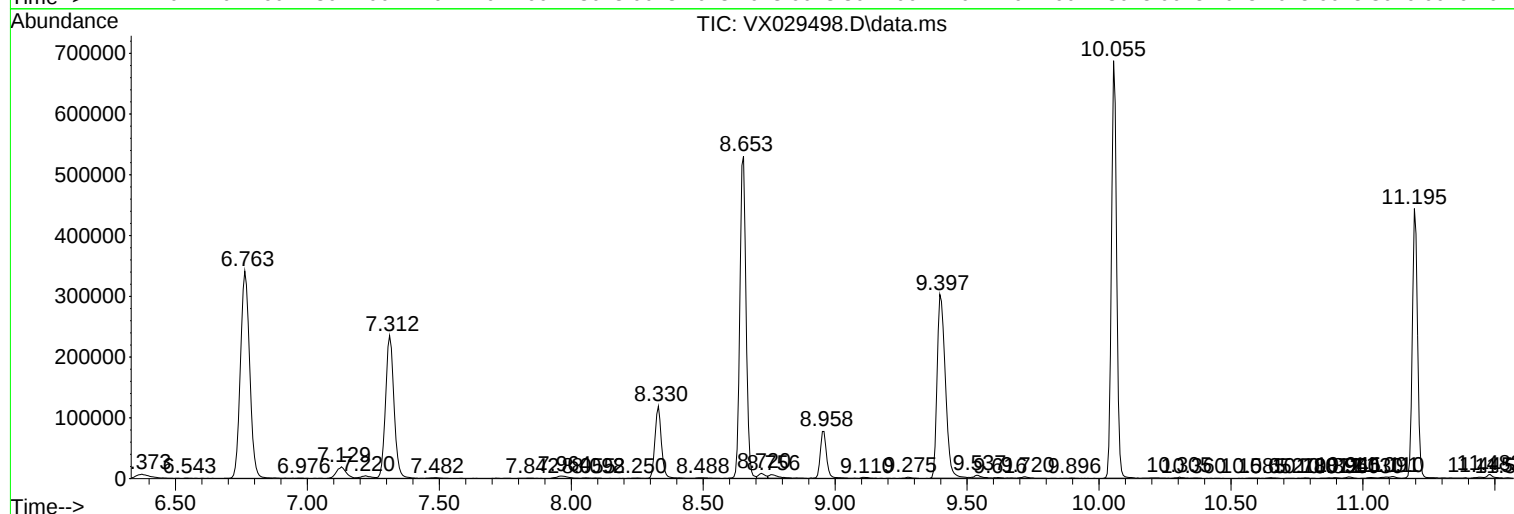
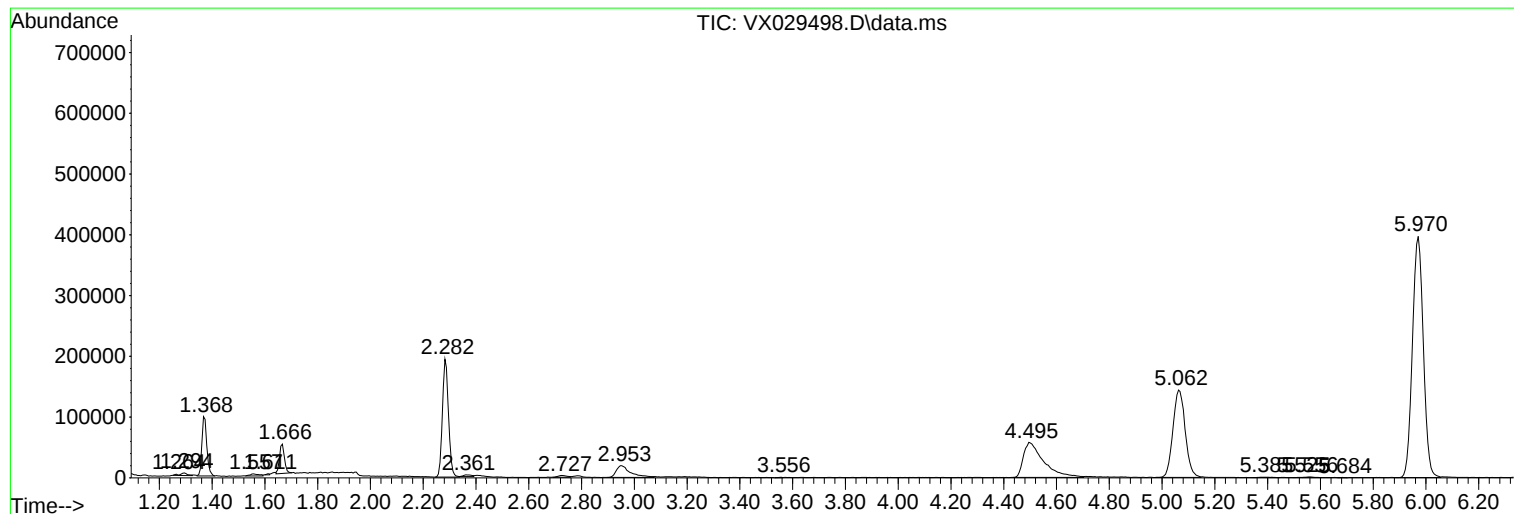
Sum of corrected areas: 9306802

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061422\
Data File : VX029498.D
Acq On : 15 Jun 2022 04:08
Operator : JC/MD
Sample : N3292-01ME
Misc : 6.24g/5mL/100uL/5.06mL/MSVOA_X/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4P2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML061322WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061422\
Data File : VX029498.D
Acq On : 15 Jun 2022 04:08
Operator : JC/MD
Sample : N3292-01ME
Misc : 6.24g/5mL/100uL/5.06mL/MSVOA_X/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4P2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML061322WMA.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\VX061422\
Data File : VX029498.D
Acq On : 15 Jun 2022 04:08
Operator : JC/MD
Sample : N3292-01ME
Misc : 6.24g/5mL/100uL/5.06mL/MSVOA_X/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW4P2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML061322WMA.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