

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072224\
 Data File : VX042453.D
 Acq On : 22 Jul 2024 18:39
 Operator : JC/MD
 Sample : P3264-12
 Misc : 5.10g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CL8

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\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042453.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	22	28	38	rBV2	15659	24590	3.89%	0.486%
2	1.368	43	46	63	rVB	23185	72945	11.55%	1.442%
3	2.276	189	195	212	rBV	73289	143942	22.78%	2.846%
4	2.563	239	242	243	rBV	253	168	0.03%	0.003%
5	2.678	257	261	262	rBV2	239	309	0.05%	0.006%
6	2.715	262	267	273	rBV2	5227	10498	1.66%	0.208%
7	2.898	296	297	299	rBV2	196	155	0.02%	0.003%
8	2.941	299	304	315	rVB	2299	5689	0.90%	0.112%
9	3.130	333	335	339	rBV2	235	331	0.05%	0.007%
10	3.276	357	359	361	rBV	119	110	0.02%	0.002%
11	3.337	367	369	371	rBV2	116	111	0.02%	0.002%
12	3.416	380	382	383	rBV	205	154	0.02%	0.003%
13	3.459	387	389	390	rVV	154	128	0.02%	0.003%
14	3.477	390	392	394	rVB2	127	112	0.02%	0.002%
15	3.575	404	408	409	rBV	118	114	0.02%	0.002%
16	3.642	417	419	422	rBV	101	144	0.02%	0.003%
17	3.770	438	440	445	rVB	136	163	0.03%	0.003%
18	3.812	445	447	449	rBV	114	126	0.02%	0.002%
19	4.288	524	525	528	rVB	194	151	0.02%	0.003%
20	4.392	538	542	543	rBV	130	112	0.02%	0.002%
21	4.489	550	558	576	rBV	37518	134483	21.29%	2.659%
22	5.062	639	652	665	rBV	77327	240769	38.11%	4.760%
23	5.471	717	719	721	rVB2	175	151	0.02%	0.003%
24	5.964	789	800	815	rBV2	224244	631774	100.00%	12.491%
25	6.330	858	860	861	rBV	156	113	0.02%	0.002%
26	6.391	867	870	873	rBV2	235	353	0.06%	0.007%
27	6.537	891	894	895	rVV	186	150	0.02%	0.003%
28	6.562	895	898	899	rVV	260	212	0.03%	0.004%
29	6.623	906	908	910	rBV2	124	103	0.02%	0.002%
30	6.757	921	930	950	rBV	203241	497111	78.68%	9.829%
31	7.013	970	972	977	rVB2	256	241	0.04%	0.005%
32	7.123	983	990	995	rVB5	1480	3237	0.51%	0.064%
33	7.226	1001	1007	1012	rBV3	615	1297	0.21%	0.026%
34	7.306	1012	1020	1041	rBV	124250	285230	45.15%	5.640%
35	7.476	1047	1048	1051	rVB2	264	247	0.04%	0.005%
36	7.781	1097	1098	1100	rBV	152	106	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072224\
 Data File : VX042453.D
 Acq On : 22 Jul 2024 18:39
 Operator : JC/MD
 Sample : P3264-12
 Misc : 5.10g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CL8

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\SFAMXML070324WMA.M
 Title : VOC Analysis

37	7.891	1114	1116	1119	rBV	157	163	0.03%	0.003%
38	7.970	1124	1129	1135	rBV3	626	1490	0.24%	0.029%
39	8.031	1137	1139	1141	rVB	195	159	0.03%	0.003%
40	8.068	1141	1145	1149	rBV2	125	237	0.04%	0.005%
41	8.147	1154	1158	1160	rBV	174	215	0.03%	0.004%
42	8.324	1182	1187	1202	rBV	63755	113938	18.03%	2.253%
43	8.501	1214	1216	1217	rBV2	208	152	0.02%	0.003%
44	8.580	1227	1229	1231	rBV	213	193	0.03%	0.004%
45	8.647	1234	1240	1251	rBV	315687	506616	80.19%	10.017%
46	8.952	1285	1290	1306	rBV	47223	73491	11.63%	1.453%
47	9.202	1329	1331	1333	rBV	127	124	0.02%	0.002%
48	9.275	1337	1343	1357	rVB	33710	51748	8.19%	1.023%
49	9.391	1357	1362	1384	rBV	154911	313209	49.58%	6.193%
50	9.714	1410	1415	1418	rBV4	790	1237	0.20%	0.024%
51	9.744	1418	1420	1424	rVB3	313	249	0.04%	0.005%
52	10.055	1465	1471	1484	rBV	415650	572718	90.65%	11.324%
53	10.250	1501	1503	1505	rBV2	167	205	0.03%	0.004%
54	10.311	1509	1513	1516	rBV2	577	794	0.13%	0.016%
55	10.415	1529	1530	1534	rVB2	204	159	0.03%	0.003%
56	10.445	1534	1535	1538	rBV	202	105	0.02%	0.002%
57	10.567	1552	1555	1557	rBV2	207	229	0.04%	0.005%
58	10.653	1565	1569	1577	rBV4	414	815	0.13%	0.016%
59	10.915	1609	1612	1615	rVB2	114	141	0.02%	0.003%
60	10.945	1615	1617	1618	rBV	110	114	0.02%	0.002%
61	10.970	1618	1621	1630	rVB3	519	920	0.15%	0.018%
62	11.195	1652	1658	1667	rBV	251072	333435	52.78%	6.593%
63	11.311	1674	1677	1678	rBV2	407	508	0.08%	0.010%
64	11.348	1682	1683	1685	rBV	176	119	0.02%	0.002%
65	11.366	1685	1686	1688	rBV	155	109	0.02%	0.002%
66	11.457	1697	1701	1703	rVV3	438	549	0.09%	0.011%
67	11.482	1703	1705	1706	rVV	181	108	0.02%	0.002%
68	11.494	1706	1707	1710	rVV2	141	160	0.03%	0.003%
69	11.537	1712	1714	1716	rBV2	133	142	0.02%	0.003%
70	11.756	1746	1750	1754	rVB4	564	886	0.14%	0.018%
71	11.787	1754	1755	1758	rBV2	108	114	0.02%	0.002%
72	11.927	1777	1778	1781	rVB2	234	140	0.02%	0.003%
73	11.982	1782	1787	1788	rBV3	569	804	0.13%	0.016%
74	12.024	1789	1794	1806	rVB	417080	532744	84.33%	10.533%
75	12.219	1822	1826	1835	rBV	7122	10863	1.72%	0.215%
76	12.323	1837	1843	1854	rBV	352850	462078	73.14%	9.136%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072224\
 Data File : VX042453.D
 Acq On : 22 Jul 2024 18:39
 Operator : JC/MD
 Sample : P3264-12
 Misc : 5.10g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CL8

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\SFAMXML070324WMA.M
 Title : VOC Analysis

77	12.433	1859	1861	1863	rVB2	527	360	0.06%	0.007%
78	12.451	1863	1864	1866	rBV	305	239	0.04%	0.005%
79	12.762	1912	1915	1919	rBB3	832	1026	0.16%	0.020%
80	12.872	1928	1933	1939	rBV3	2691	4086	0.65%	0.081%
81	12.957	1945	1947	1950	rVB2	171	125	0.02%	0.002%
82	13.116	1971	1973	1978	rVB3	436	504	0.08%	0.010%
83	13.170	1980	1982	1983	rVB	186	120	0.02%	0.002%
84	13.244	1991	1994	1995	rBV2	212	185	0.03%	0.004%
85	13.402	2017	2020	2029	rBV	3026	3971	0.63%	0.079%
86	13.494	2033	2035	2037	rBV2	164	125	0.02%	0.002%
87	13.530	2037	2041	2042	rVB2	95	105	0.02%	0.002%
88	13.597	2049	2052	2056	rVB2	346	412	0.07%	0.008%
89	13.689	2064	2067	2071	rVB	782	775	0.12%	0.015%
90	13.756	2074	2078	2079	rBV	205	260	0.04%	0.005%
91	13.780	2079	2082	2089	rVB	1705	2067	0.33%	0.041%
92	13.945	2107	2109	2110	rBV	217	106	0.02%	0.002%
93	13.963	2110	2112	2115	rVB2	451	474	0.08%	0.009%
94	14.024	2120	2122	2125	rBV2	162	221	0.03%	0.004%
95	14.128	2136	2139	2144	rVB	1399	1844	0.29%	0.036%
96	14.432	2185	2189	2194	rBV4	856	1055	0.17%	0.021%
97	14.499	2198	2200	2204	rVB	328	345	0.05%	0.007%
98	14.634	2220	2222	2223	rBV	310	205	0.03%	0.004%
99	14.786	2243	2247	2250	rVB2	920	1044	0.17%	0.021%
100	14.963	2275	2276	2278	rBV	303	221	0.03%	0.004%

Sum of corrected areas: 5057684

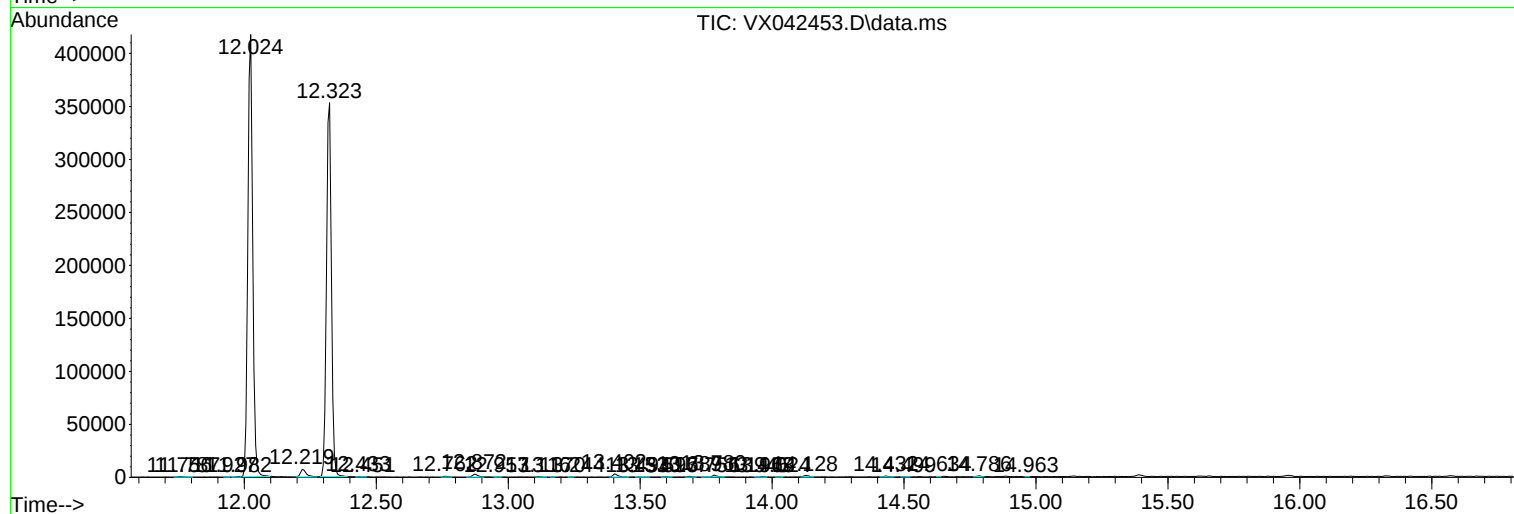
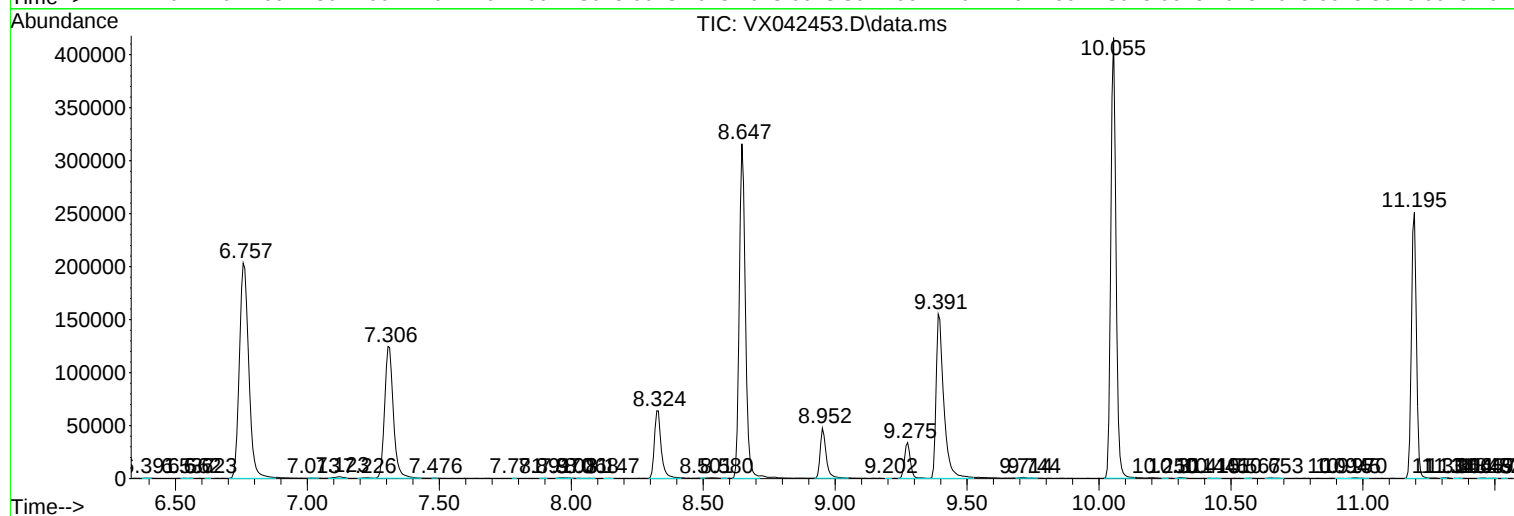
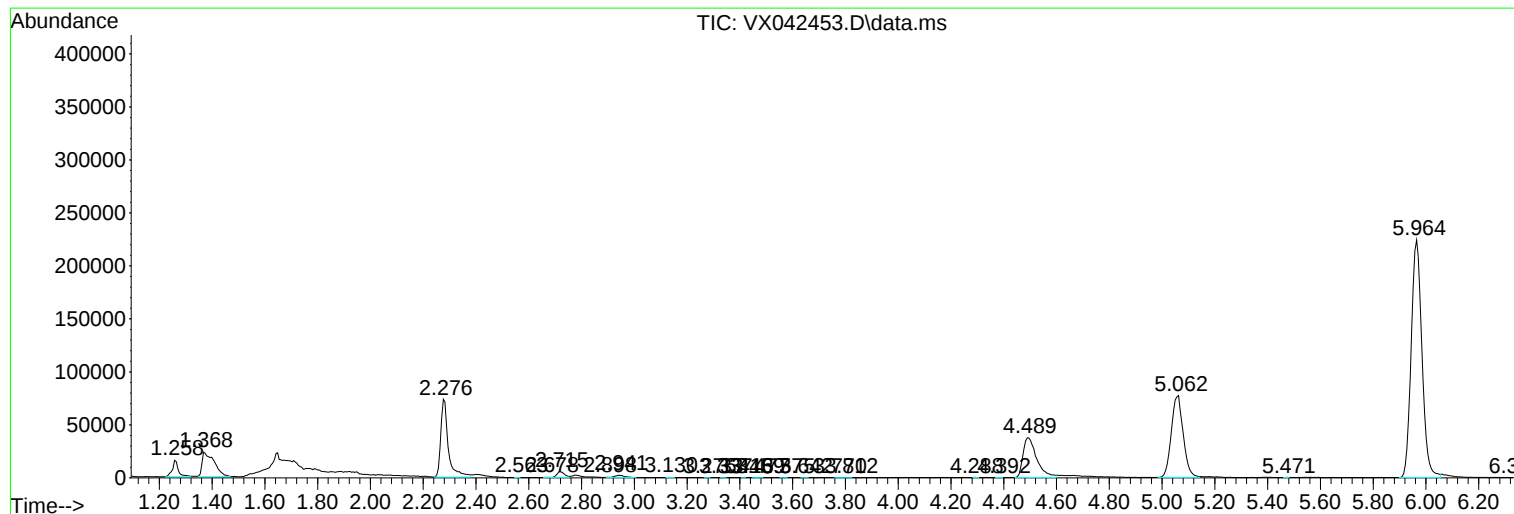
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072224\
Data File : VX042453.D
Acq On : 22 Jul 2024 18:39
Operator : JC/MD
Sample : P3264-12
Misc : 5.10g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CL8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072224\
Data File : VX042453.D
Acq On : 22 Jul 2024 18:39
Operator : JC/MD
Sample : P3264-12
Misc : 5.10g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CL8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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\VX072224\
Data File : VX042453.D
Acq On : 22 Jul 2024 18:39
Operator : JC/MD
Sample : P3264-12
Misc : 5.10g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CL8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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