

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
 Data File : VX042378.D
 Acq On : 18 Jul 2024 18:33
 Operator : JC/MD
 Sample : P3263-12ME
 Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CG6ME

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: VX042378.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.257	22	28	42	rBV2	19540	32996	3.70%	0.498%
2	1.373	43	47	48	rBV	22114	27398	3.07%	0.413%
3	2.276	189	195	211	rBV	122454	234779	26.31%	3.540%
4	2.721	260	268	273	rBV	5181	10514	1.18%	0.159%
5	2.934	302	303	309	rBV4	335	466	0.05%	0.007%
6	3.019	314	317	321	rBV	158	232	0.03%	0.003%
7	3.068	324	325	329	rBV	135	127	0.01%	0.002%
8	3.263	354	357	359	rBV2	132	124	0.01%	0.002%
9	3.288	359	361	364	rBV2	122	151	0.02%	0.002%
10	3.422	378	383	387	rVB3	532	958	0.11%	0.014%
11	3.531	398	401	402	rBV	153	133	0.01%	0.002%
12	3.605	407	413	418	rBV4	365	811	0.09%	0.012%
13	3.842	446	452	460	rBV5	511	1500	0.17%	0.023%
14	3.928	464	466	470	rVB2	106	141	0.02%	0.002%
15	4.495	550	559	577	rBV	54468	199343	22.34%	3.006%
16	5.056	638	651	668	rBV	111866	349518	39.16%	5.270%
17	5.366	700	702	703	rBV2	194	148	0.02%	0.002%
18	5.385	703	705	706	rBV	231	151	0.02%	0.002%
19	5.610	741	742	746	rVB2	178	172	0.02%	0.003%
20	5.720	758	760	762	rBV2	236	211	0.02%	0.003%
21	5.964	788	800	819	rBV2	313308	892496	100.00%	13.457%
22	6.378	862	868	874	rBV5	1115	2867	0.32%	0.043%
23	6.537	892	894	895	rBV	168	128	0.01%	0.002%
24	6.574	898	900	902	rBV	203	108	0.01%	0.002%
25	6.756	921	930	952	rBV	203017	492382	55.17%	7.424%
26	7.110	982	988	996	rBV5	1648	4561	0.51%	0.069%
27	7.214	1000	1005	1012	rBV4	1792	3975	0.45%	0.060%
28	7.305	1012	1020	1039	rVV	178354	406063	45.50%	6.123%
29	7.476	1045	1048	1049	rBV2	329	346	0.04%	0.005%
30	7.573	1062	1064	1066	rBV	151	169	0.02%	0.003%
31	7.671	1077	1080	1082	rBV	87	113	0.01%	0.002%
32	7.701	1082	1085	1088	rVV2	164	222	0.02%	0.003%
33	7.750	1092	1093	1096	rBV	113	113	0.01%	0.002%
34	7.964	1122	1128	1139	rVV5	1166	3027	0.34%	0.046%
35	8.073	1144	1146	1149	rVB	166	151	0.02%	0.002%
36	8.250	1173	1175	1177	rVV	221	170	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
 Data File : VX042378.D
 Acq On : 18 Jul 2024 18:33
 Operator : JC/MD
 Sample : P3263-12ME
 Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CG6ME

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	8.323	1181	1187	1204	rBV	105061	178299	19.98%	2.688%
38	8.512	1217	1218	1223	rVB3	376	378	0.04%	0.006%
39	8.646	1234	1240	1249	rBV	453742	717854	80.43%	10.824%
40	8.909	1280	1283	1285	rBV3	1682	2085	0.23%	0.031%
41	8.951	1285	1290	1304	rVB	75761	115420	12.93%	1.740%
42	9.274	1339	1343	1349	rVB2	600	1071	0.12%	0.016%
43	9.317	1349	1350	1354	rBV2	208	283	0.03%	0.004%
44	9.390	1357	1362	1384	rBV	218806	476858	53.43%	7.190%
45	9.799	1427	1429	1432	rBV2	179	259	0.03%	0.004%
46	9.860	1437	1439	1442	rBV2	130	179	0.02%	0.003%
47	10.006	1461	1463	1465	rBV	205	237	0.03%	0.004%
48	10.055	1465	1471	1483	rBV	414657	577174	64.67%	8.703%
49	10.238	1499	1501	1504	rBV2	159	204	0.02%	0.003%
50	10.305	1508	1512	1517	rVV2	835	1552	0.17%	0.023%
51	10.359	1517	1521	1527	rVB	2029	2690	0.30%	0.041%
52	10.579	1556	1557	1560	rBV	179	125	0.01%	0.002%
53	10.622	1560	1564	1565	rVV2	169	170	0.02%	0.003%
54	10.646	1565	1568	1573	rVB2	376	572	0.06%	0.009%
55	10.817	1594	1596	1597	rBV	188	168	0.02%	0.003%
56	10.847	1600	1601	1604	rVV2	157	169	0.02%	0.003%
57	10.890	1604	1608	1613	rVV3	447	837	0.09%	0.013%
58	10.939	1613	1616	1619	rVV	209	270	0.03%	0.004%
59	10.969	1619	1621	1623	rVV2	328	384	0.04%	0.006%
60	10.994	1623	1625	1626	rVV	288	185	0.02%	0.003%
61	11.036	1630	1632	1633	rBV	142	112	0.01%	0.002%
62	11.067	1635	1637	1638	rVV2	391	370	0.04%	0.006%
63	11.091	1639	1641	1648	rVB4	847	1219	0.14%	0.018%
64	11.195	1652	1658	1669	rBV	389745	511306	57.29%	7.709%
65	11.317	1673	1678	1680	rBV4	277	395	0.04%	0.006%
66	11.439	1695	1698	1701	rBV2	845	1128	0.13%	0.017%
67	11.481	1701	1705	1713	rVB2	4936	7476	0.84%	0.113%
68	11.634	1728	1730	1734	rVB2	170	167	0.02%	0.003%
69	11.664	1734	1735	1737	rBV	176	140	0.02%	0.002%
70	11.682	1737	1738	1739	rVV	267	148	0.02%	0.002%
71	11.713	1740	1743	1746	rVV4	1090	1515	0.17%	0.023%
72	11.768	1748	1752	1758	rVB3	2409	3910	0.44%	0.059%
73	11.847	1764	1765	1767	rBV2	204	159	0.02%	0.002%
74	11.865	1767	1768	1771	rVB3	318	256	0.03%	0.004%
75	11.945	1775	1781	1783	rBV4	1091	1603	0.18%	0.024%
76	12.024	1789	1794	1805	rBV	450937	576660	64.61%	8.695%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
 Data File : VX042378.D
 Acq On : 18 Jul 2024 18:33
 Operator : JC/MD
 Sample : P3263-12ME
 Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CG6ME

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	12.323	1837	1843	1856	rBV	553643	728533	81.63%	10.985%
78	12.426	1856	1860	1864	rVB	4217	5121	0.57%	0.077%
79	12.682	1900	1902	1906	rVB2	299	300	0.03%	0.005%
80	12.761	1912	1915	1918	rBV2	511	527	0.06%	0.008%
81	12.816	1922	1924	1927	rBV	155	136	0.02%	0.002%
82	12.877	1927	1934	1943	rBV5	1859	4688	0.53%	0.071%
83	12.969	1948	1949	1953	rBV	389	354	0.04%	0.005%
84	13.042	1959	1961	1962	rVB	224	118	0.01%	0.002%
85	13.121	1972	1974	1975	rBV	137	119	0.01%	0.002%
86	13.267	1994	1998	2005	rVB	3135	3926	0.44%	0.059%
87	13.408	2015	2021	2025	rBV5	996	2044	0.23%	0.031%
88	13.688	2064	2067	2072	rBV2	932	1385	0.16%	0.021%
89	13.780	2077	2082	2087	rBV	13884	19472	2.18%	0.294%
90	13.883	2096	2099	2103	rVB3	988	1156	0.13%	0.017%
91	13.938	2105	2108	2114	rVB2	600	766	0.09%	0.012%
92	13.993	2114	2117	2118	rBV2	215	225	0.03%	0.003%
93	14.036	2121	2124	2129	rVB3	2025	2463	0.28%	0.037%
94	14.133	2138	2140	2143	rVB3	763	568	0.06%	0.009%
95	14.267	2160	2162	2163	rVB	285	147	0.02%	0.002%
96	14.432	2185	2189	2192	rBV3	1779	2080	0.23%	0.031%
97	14.639	2219	2223	2231	rVB3	2519	3831	0.43%	0.058%
98	14.755	2240	2242	2244	rBV3	895	746	0.08%	0.011%
99	15.176	2309	2311	2314	rBV3	1062	1022	0.11%	0.015%
100	15.487	2359	2362	2365	rVB3	1653	1742	0.20%	0.026%

Sum of corrected areas: 6632220

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042378.D
Acq On : 18 Jul 2024 18:33
Operator : JC/MD
Sample : P3263-12ME
Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CG6ME

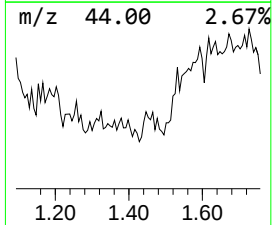
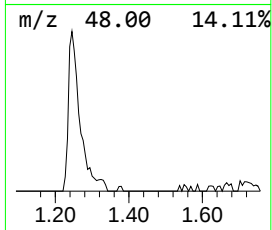
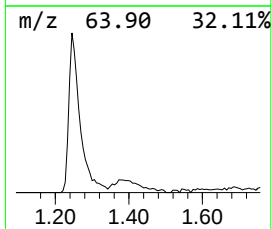
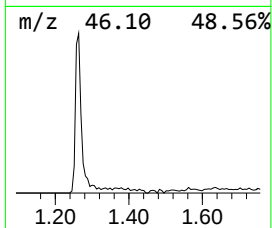
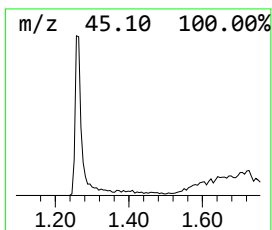
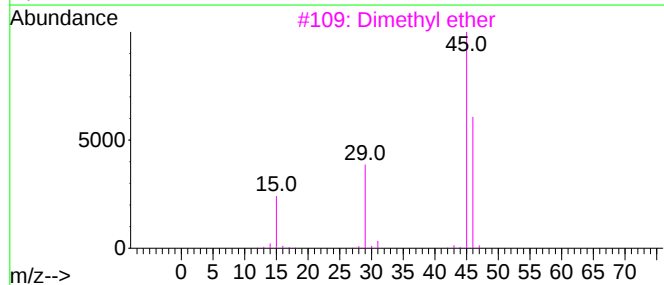
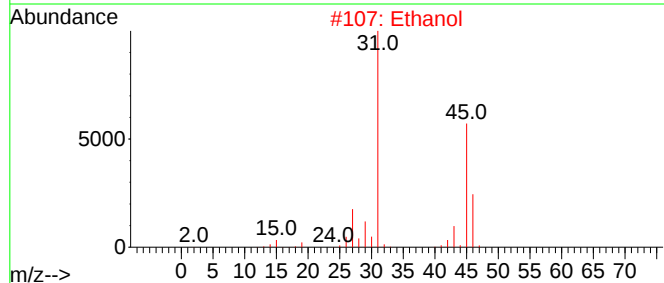
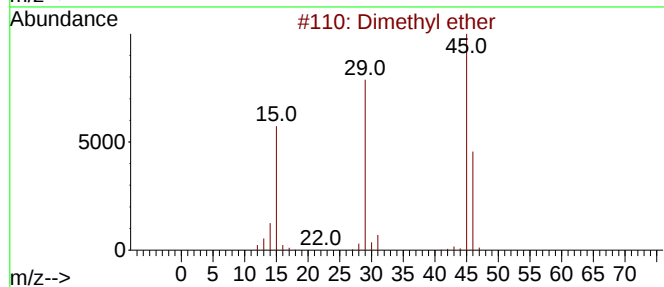
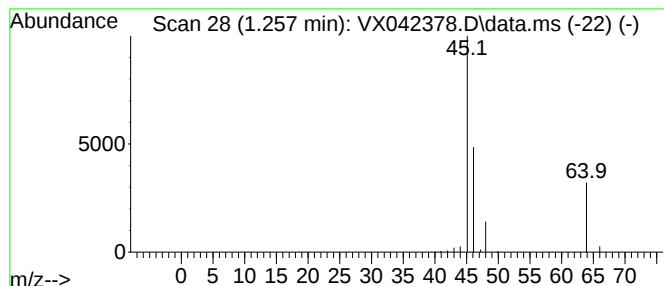
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.257	3.35 ug/L	32996	1,4-Difluorobenzene	6.756

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	45
2			Ethanol	46	C2H6O	000064-17-5	9
3			Dimethyl ether	46	C2H6O	000115-10-6	9
4			Ethanol	46	C2H6O	000064-17-5	7
5			Ethanol	46	C2H6O	000064-17-5	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042378.D
Acq On : 18 Jul 2024 18:33
Operator : JC/MD
Sample : P3263-12ME
Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CG6ME

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
unknown-01	1.257	3.4	ug/L	32996	1	6.756	492382	50.0