

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072224\
 Data File : VX042442.D
 Acq On : 22 Jul 2024 12:19
 Operator : JC/MD
 Sample : P3298-09 10X
 Misc : 4.37g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BHB29

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: VX042442.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	27	rBV	9473	9725	1.67%	0.183%
2	1.368	43	46	58	rVB	49673	66650	11.45%	1.253%
3	1.648	88	92	102	rVB	41611	61909	10.64%	1.163%
4	2.294	192	198	211	rBV	115023	180732	31.05%	3.396%
5	2.581	241	245	246	rVB2	280	304	0.05%	0.006%
6	2.715	263	267	271	rBV3	278	472	0.08%	0.009%
7	2.782	273	278	287	rVV2	1803	3787	0.65%	0.071%
8	2.941	298	304	312	rBV	3697	8052	1.38%	0.151%
9	3.130	333	335	337	rBV2	164	140	0.02%	0.003%
10	3.197	344	346	347	rBV	142	83	0.01%	0.002%
11	3.251	353	355	356	rBV	114	79	0.01%	0.001%
12	3.294	360	362	364	rBV	134	106	0.02%	0.002%
13	3.422	382	383	385	rVB2	126	53	0.01%	0.001%
14	3.440	385	386	387	rBV	83	43	0.01%	0.001%
15	3.709	428	430	431	rBV	192	151	0.03%	0.003%
16	3.764	437	439	440	rBV	119	72	0.01%	0.001%
17	3.843	451	452	455	rBV2	99	116	0.02%	0.002%
18	3.940	467	468	469	rBV	132	64	0.01%	0.001%
19	3.989	474	476	477	rVB	107	56	0.01%	0.001%
20	4.300	525	527	528	rBV	147	86	0.01%	0.002%
21	4.471	547	555	572	rBV2	49805	155787	26.77%	2.928%
22	4.830	612	614	615	rBV2	110	65	0.01%	0.001%
23	4.897	623	625	627	rVB2	192	104	0.02%	0.002%
24	5.062	640	652	669	rBV	72749	227441	39.08%	4.274%
25	5.227	677	679	681	rVB2	309	232	0.04%	0.004%
26	5.275	686	687	688	rBV	84	38	0.01%	0.001%
27	5.391	699	706	710	rBV4	515	1235	0.21%	0.023%
28	5.538	727	730	731	rBV	255	295	0.05%	0.006%
29	5.623	742	744	747	rBV	151	111	0.02%	0.002%
30	5.647	747	748	749	rVB	118	46	0.01%	0.001%
31	5.739	761	763	764	rBV	136	84	0.01%	0.002%
32	5.757	764	766	767	rVV	101	49	0.01%	0.001%
33	5.824	775	777	780	rVB	138	86	0.01%	0.002%
34	5.964	790	800	819	rBV2	200109	582038	100.00%	10.938%
35	6.324	858	859	861	rVB	167	75	0.01%	0.001%
36	6.422	873	875	878	rVB	146	155	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072224\
 Data File : VX042442.D
 Acq On : 22 Jul 2024 12:19
 Operator : JC/MD
 Sample : P3298-09 10X
 Misc : 4.37g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BHB29

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	6.489	883	886	889	rBV2	118	173	0.03%	0.003%
38	6.763	921	931	946	rBV	186038	454881	78.15%	8.549%
39	7.129	982	991	1002	rBV4	6375	16048	2.76%	0.302%
40	7.306	1012	1020	1033	rBV	114822	257914	44.31%	4.847%
41	8.086	1147	1148	1150	rBV	157	89	0.02%	0.002%
42	8.165	1160	1161	1162	rBV	151	57	0.01%	0.001%
43	8.324	1181	1187	1204	rBV	65399	115143	19.78%	2.164%
44	8.647	1234	1240	1257	rBV	298314	476775	81.91%	8.960%
45	8.897	1279	1281	1285	rBV2	168	172	0.03%	0.003%
46	8.952	1285	1290	1302	rBV	48054	73409	12.61%	1.380%
47	9.275	1337	1343	1356	rBV	373537	564701	97.02%	10.612%
48	9.391	1357	1362	1383	rVB	176052	282831	48.59%	5.315%
49	9.701	1410	1413	1421	rVB2	1001	1545	0.27%	0.029%
50	9.769	1421	1424	1427	rBV2	193	313	0.05%	0.006%
51	9.958	1453	1455	1457	rBV	127	83	0.01%	0.002%
52	9.994	1460	1461	1462	rVB	143	52	0.01%	0.001%
53	10.012	1462	1464	1465	rBV	114	98	0.02%	0.002%
54	10.055	1465	1471	1491	rBV	388910	536549	92.18%	10.083%
55	10.311	1510	1513	1517	rVB2	629	799	0.14%	0.015%
56	10.396	1525	1527	1530	rVB2	162	121	0.02%	0.002%
57	10.890	1606	1608	1609	rBV	110	67	0.01%	0.001%
58	10.957	1618	1619	1623	rVB2	161	168	0.03%	0.003%
59	11.104	1641	1643	1646	rVB2	169	187	0.03%	0.004%
60	11.134	1646	1648	1652	rBV2	124	145	0.02%	0.003%
61	11.189	1652	1657	1669	rVV	232318	310322	53.32%	5.832%
62	11.512	1708	1710	1711	rBV	93	85	0.01%	0.002%
63	11.841	1762	1764	1765	rBV	122	71	0.01%	0.001%
64	11.915	1775	1776	1778	rBV	146	115	0.02%	0.002%
65	12.024	1789	1794	1807	rVB	381167	490178	84.22%	9.212%
66	12.317	1837	1842	1860	rBV	335371	430386	73.94%	8.088%
67	12.512	1872	1874	1875	rBV	147	93	0.02%	0.002%
68	12.756	1912	1914	1920	rVB3	461	691	0.12%	0.013%
69	12.981	1949	1951	1955	rBV2	127	94	0.02%	0.002%
70	13.134	1974	1976	1979	rBV	145	149	0.03%	0.003%
71	13.262	1996	1997	1998	rBV	159	60	0.01%	0.001%
72	13.280	1998	2000	2001	rBV	103	56	0.01%	0.001%
73	13.420	2021	2023	2026	rBV	143	181	0.03%	0.003%
74	13.939	2106	2108	2110	rBV2	154	143	0.02%	0.003%
75	14.128	2136	2139	2147	rVB2	1083	1756	0.30%	0.033%
76	14.188	2147	2149	2151	rBV	215	184	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072224\
Data File : VX042442.D
Acq On : 22 Jul 2024 12:19
Operator : JC/MD
Sample : P3298-09 10X
Misc : 4.37g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BHB29

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	14.286	2164	2165	2169	rBV2	193	139	0.02%	0.003%
78	14.658	2223	2226	2227	rBV2	198	219	0.04%	0.004%
79	14.865	2258	2260	2261	rBV2	292	247	0.04%	0.005%
80	15.389	2341	2346	2352	rBV3	1689	3125	0.54%	0.059%

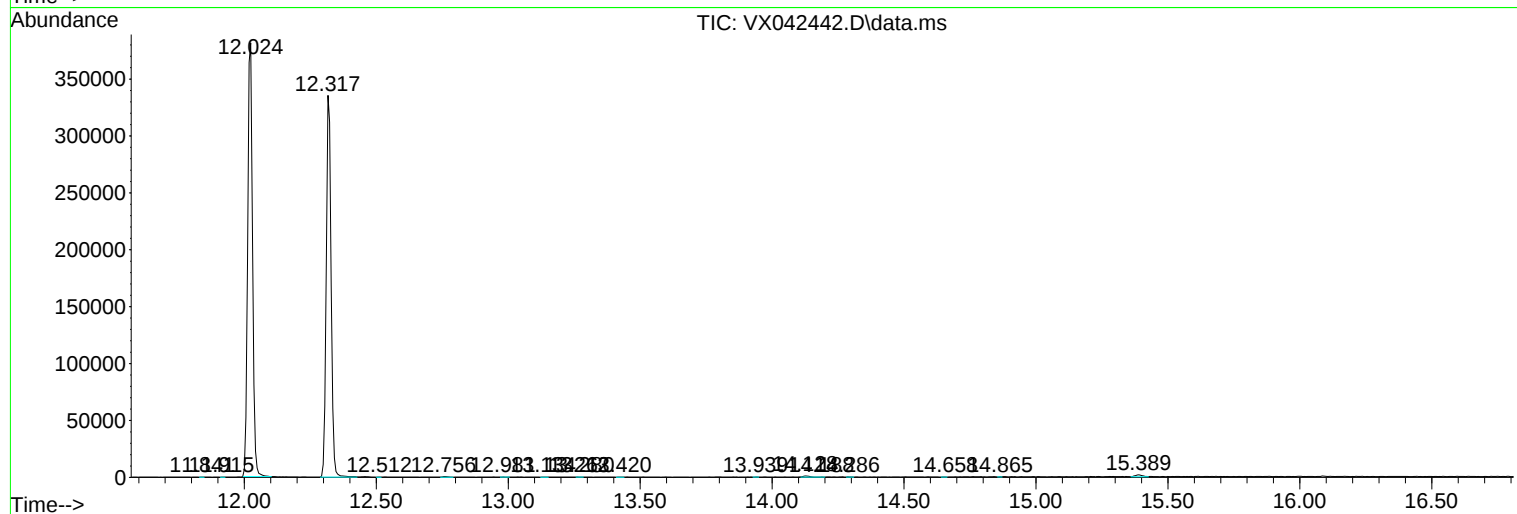
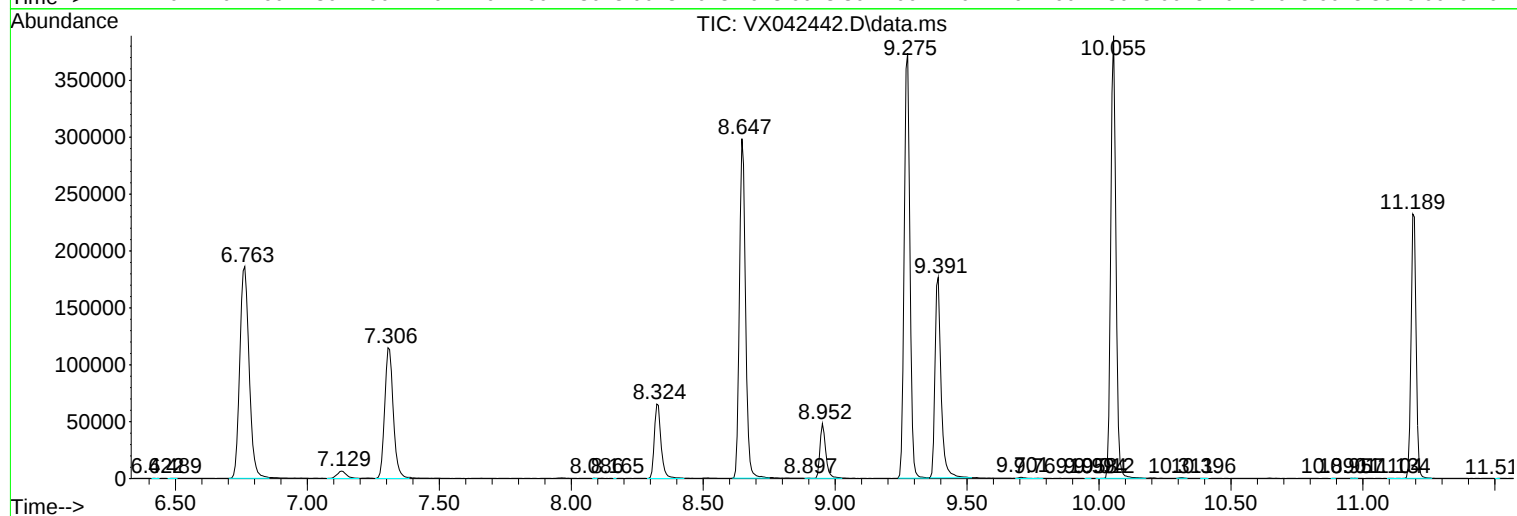
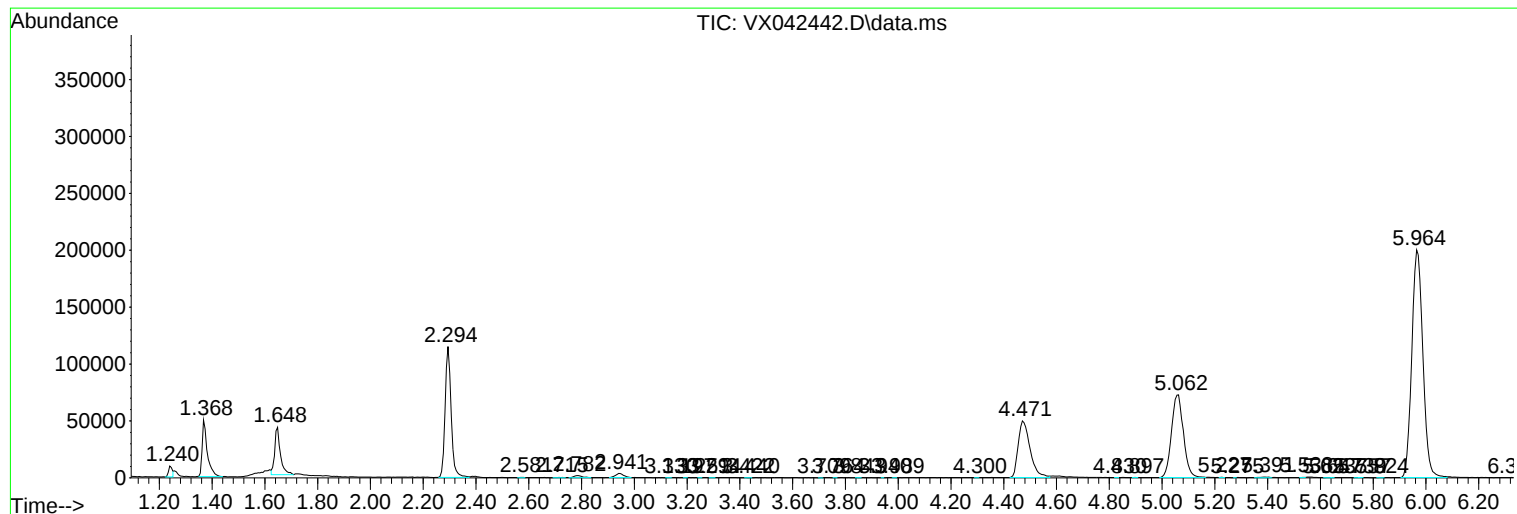
Sum of corrected areas: 5321135

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072224\
Data File : VX042442.D
Acq On : 22 Jul 2024 12:19
Operator : JC/MD
Sample : P3298-09 10X
Misc : 4.37g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BHB29

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 : VX042442.D
Acq On : 22 Jul 2024 12:19
Operator : JC/MD
Sample : P3298-09 10X
Misc : 4.37g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BHB29

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 : VX042442.D
Acq On : 22 Jul 2024 12:19
Operator : JC/MD
Sample : P3298-09 10X
Misc : 4.37g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BHB29

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