

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
 Data File : VX044268.D
 Acq On : 13 Dec 2024 09:46
 Operator : JC/MD
 Sample : VX1213MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK735

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.M
 Title : VOC Analysis

Signal : TIC: VX044268.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	59	rVB	114755	131436	14.27%	1.953%
2	1.648	88	92	102	rVB	97036	143471	15.58%	2.132%
3	2.300	193	199	209	rVB	180822	283933	30.84%	4.219%
4	2.654	256	257	259	rBV2	611	545	0.06%	0.008%
5	2.746	270	272	275	rBV2	757	959	0.10%	0.014%
6	2.941	301	304	306	rVV3	576	762	0.08%	0.011%
7	2.989	309	312	316	rBV2	501	657	0.07%	0.010%
8	3.056	321	323	325	rBV2	713	843	0.09%	0.013%
9	3.282	357	360	364	rVB3	629	878	0.10%	0.013%
10	3.319	364	366	368	rBV2	558	505	0.05%	0.008%
11	3.404	379	380	383	rBV2	501	461	0.05%	0.007%
12	3.575	406	408	411	rBV2	907	1019	0.11%	0.015%
13	3.678	421	425	426	rBV3	492	548	0.06%	0.008%
14	3.800	442	445	448	rBV3	517	606	0.07%	0.009%
15	3.837	448	451	454	rVB4	635	609	0.07%	0.009%
16	3.873	454	457	458	rVB	630	423	0.05%	0.006%
17	3.892	458	460	463	rVB3	583	558	0.06%	0.008%
18	3.928	463	466	467	rBV2	741	659	0.07%	0.010%
19	3.989	473	476	477	rBV	726	773	0.08%	0.011%
20	4.142	499	501	504	rVB2	466	400	0.04%	0.006%
21	4.172	504	506	509	rBV2	422	481	0.05%	0.007%
22	4.251	515	519	520	rBV3	539	643	0.07%	0.010%
23	4.453	544	552	568	rBV	61087	186780	20.28%	2.776%
24	4.684	588	590	591	rBV2	718	428	0.05%	0.006%
25	4.763	602	603	607	rVB3	751	461	0.05%	0.007%
26	5.044	637	649	668	rBV	128093	389933	42.35%	5.795%
27	5.379	698	704	712	rBV5	5330	14792	1.61%	0.220%
28	5.471	716	719	720	rBV3	497	465	0.05%	0.007%
29	5.544	725	731	740	rVV4	8039	20884	2.27%	0.310%
30	5.751	761	765	766	rBV2	537	650	0.07%	0.010%
31	5.836	775	779	780	rBV4	403	413	0.04%	0.006%
32	5.958	788	799	818	rBV2	307435	920790	100.00%	13.684%
33	6.318	856	858	859	rBV2	594	512	0.06%	0.008%
34	6.416	872	874	876	rBV2	634	510	0.06%	0.008%
35	6.617	906	907	912	rBV2	568	830	0.09%	0.012%
36	6.696	918	920	921	rBV	707	472	0.05%	0.007%

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Integrator: RTE

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Max Peaks: 100

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Title : VOC Analysis

37	6.751	921	929	952	rVB	217132	529653	57.52%	7.871%
38	7.068	979	981	982	rBV	742	435	0.05%	0.006%
39	7.105	984	987	988	rBV2	2005	1975	0.21%	0.029%
40	7.239	1008	1009	1010	rBV	679	435	0.05%	0.006%
41	7.300	1011	1019	1038	rVV	186911	414082	44.97%	6.154%
42	7.659	1077	1078	1080	rBV	535	412	0.04%	0.006%
43	7.684	1080	1082	1085	rVB3	820	769	0.08%	0.011%
44	7.806	1100	1102	1104	rBV3	988	876	0.10%	0.013%
45	7.873	1110	1113	1115	rBV2	456	463	0.05%	0.007%
46	8.171	1161	1162	1165	rBV3	684	663	0.07%	0.010%
47	8.318	1181	1186	1200	rBV	112874	195625	21.25%	2.907%
48	8.641	1233	1239	1256	rVV	446004	728799	79.15%	10.830%
49	8.775	1260	1261	1263	rVB2	1086	551	0.06%	0.008%
50	8.946	1284	1289	1300	rBV	81330	124709	13.54%	1.853%
51	9.092	1311	1313	1314	rBV2	470	398	0.04%	0.006%
52	9.269	1340	1342	1346	rBV2	545	696	0.08%	0.010%
53	9.385	1355	1361	1376	rBV	251416	391128	42.48%	5.812%
54	9.714	1414	1415	1417	rVB	789	418	0.05%	0.006%
55	9.909	1444	1447	1449	rBV3	702	991	0.11%	0.015%
56	10.049	1465	1470	1482	rBV	465665	640293	69.54%	9.515%
57	10.403	1527	1528	1533	rVB4	584	694	0.08%	0.010%
58	10.519	1545	1547	1548	rBV	522	423	0.05%	0.006%
59	10.708	1576	1578	1580	rVB2	891	862	0.09%	0.013%
60	10.732	1580	1582	1584	rBV2	613	572	0.06%	0.009%
61	10.939	1613	1616	1617	rBV2	855	782	0.08%	0.012%
62	11.012	1624	1628	1629	rBV3	438	461	0.05%	0.007%
63	11.085	1635	1640	1651	rVB2	18674	28608	3.11%	0.425%
64	11.189	1652	1657	1666	rVB	337976	430550	46.76%	6.398%
65	11.531	1710	1713	1715	rBV	426	496	0.05%	0.007%
66	11.567	1717	1719	1720	rBV2	746	659	0.07%	0.010%
67	11.652	1731	1733	1736	rBV2	521	448	0.05%	0.007%
68	11.762	1749	1751	1753	rBV	701	517	0.06%	0.008%
69	12.018	1788	1793	1804	rBV	430657	534541	58.05%	7.944%
70	12.317	1836	1842	1851	rBV	449549	566579	61.53%	8.420%
71	12.579	1884	1885	1889	rVB2	410	397	0.04%	0.006%
72	12.671	1897	1900	1903	rVB3	564	510	0.06%	0.008%
73	12.762	1911	1915	1918	rBV4	1119	1709	0.19%	0.025%
74	13.073	1965	1966	1968	rBV2	560	466	0.05%	0.007%
75	13.170	1980	1982	1984	rBV2	710	570	0.06%	0.008%
76	13.225	1990	1991	1994	rVB	771	454	0.05%	0.007%

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 ClientSampleId :
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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\SFAMXLM120524WMA.M
 Title : VOC Analysis

77	13.299	2001	2003	2006	rBV2	474	525	0.06%	0.008%
78	13.378	2014	2016	2021	rVB3	657	535	0.06%	0.008%
79	13.622	2052	2056	2057	rBV2	456	452	0.05%	0.007%
80	13.713	2068	2071	2072	rBV3	517	584	0.06%	0.009%
81	13.841	2091	2092	2094	rBV2	549	502	0.05%	0.007%
82	13.878	2094	2098	2100	rVB3	779	867	0.09%	0.013%
83	14.128	2137	2139	2142	rVB2	1458	1354	0.15%	0.020%
84	14.323	2169	2171	2174	rBV3	483	410	0.04%	0.006%
85	14.420	2185	2187	2190	rBV3	577	571	0.06%	0.008%
86	14.469	2194	2195	2197	rBV	742	421	0.05%	0.006%
87	14.695	2230	2232	2233	rBV2	562	404	0.04%	0.006%
88	14.762	2242	2243	2246	rBV2	495	575	0.06%	0.009%
89	15.073	2291	2294	2296	rBV3	544	701	0.08%	0.010%
90	15.176	2309	2311	2313	rVB2	609	432	0.05%	0.006%
91	15.268	2324	2326	2329	rBV3	767	801	0.09%	0.012%
92	15.304	2329	2332	2333	rBV	427	464	0.05%	0.007%
93	15.390	2341	2346	2349	rBV4	1120	1995	0.22%	0.030%
94	15.847	2420	2421	2424	rBV2	715	808	0.09%	0.012%
95	15.902	2429	2430	2432	rBV2	608	513	0.06%	0.008%
96	15.999	2444	2446	2449	rBV4	582	877	0.10%	0.013%
97	16.024	2449	2450	2454	rVV2	631	664	0.07%	0.010%
98	16.243	2484	2486	2488	rVB2	937	667	0.07%	0.010%
99	16.280	2488	2492	2493	rBV3	496	600	0.07%	0.009%
100	16.627	2546	2549	2550	rBV3	741	671	0.07%	0.010%

Sum of corrected areas: 6729151

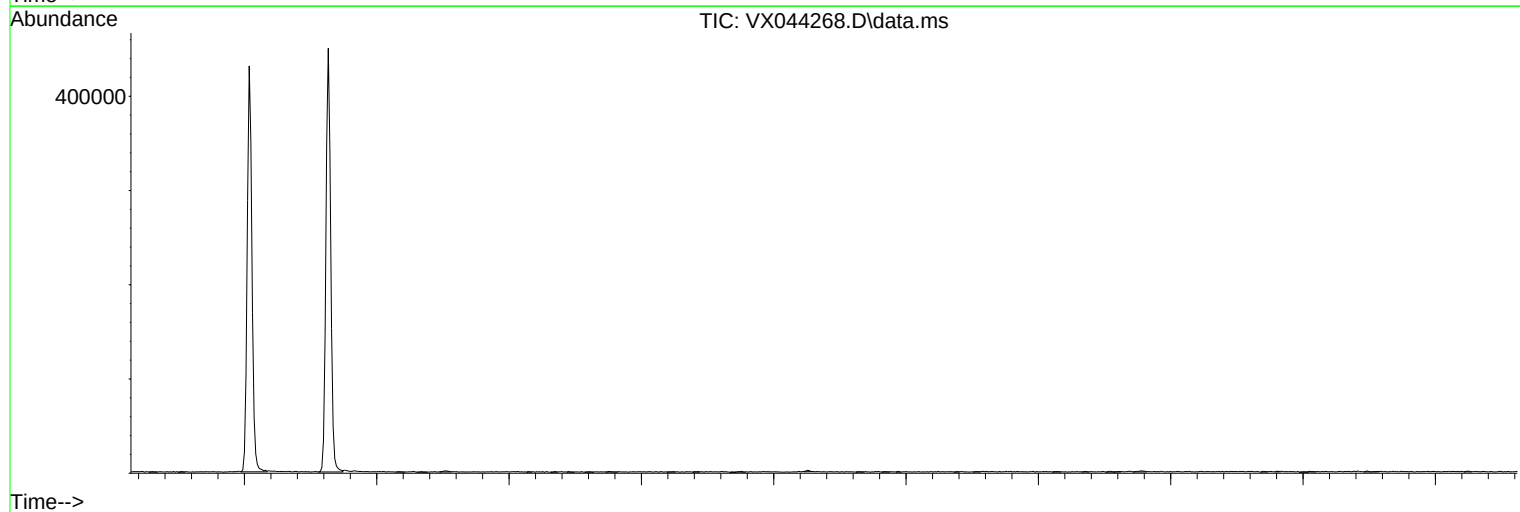
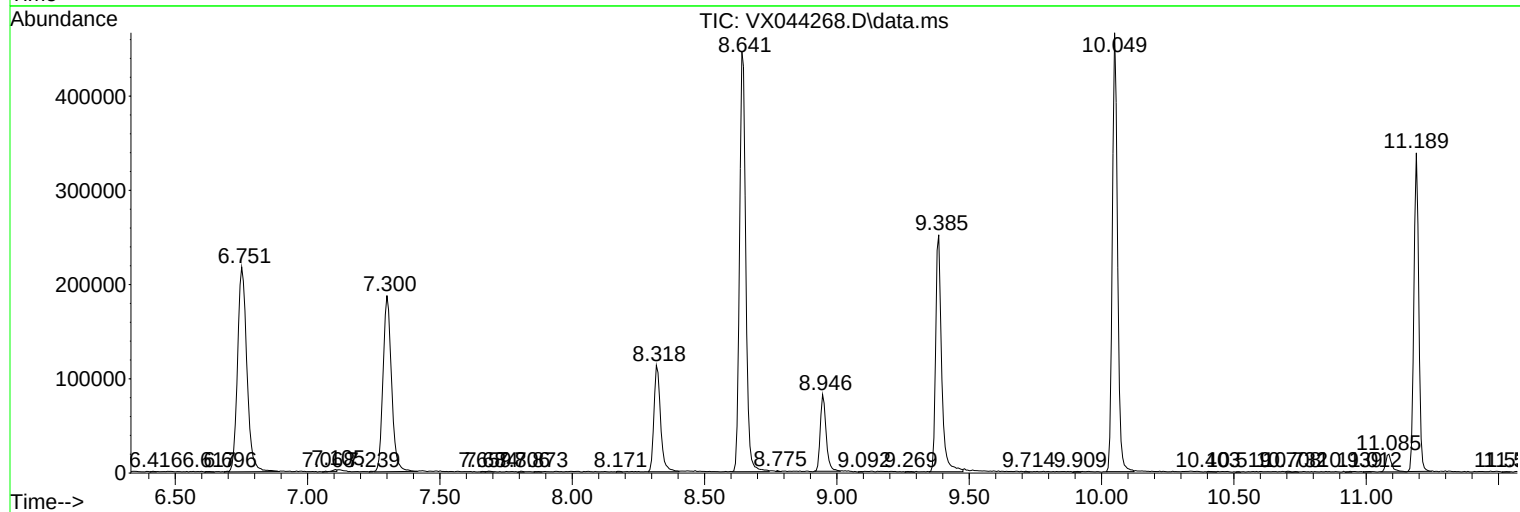
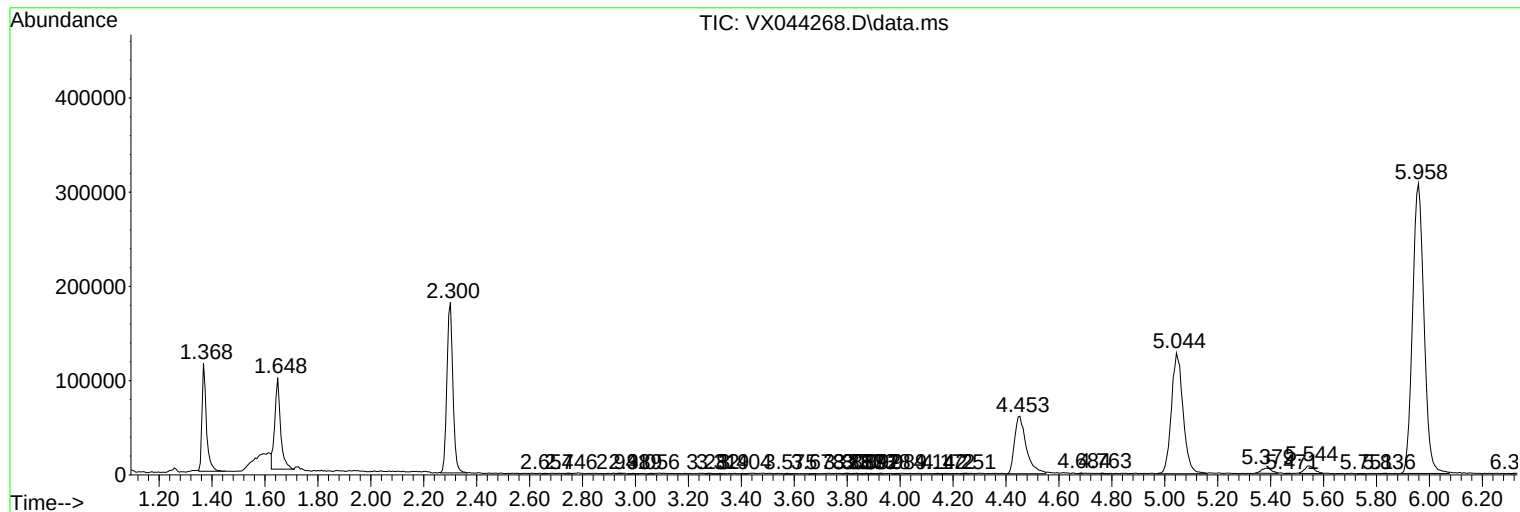
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ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK735

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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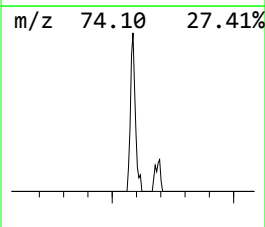
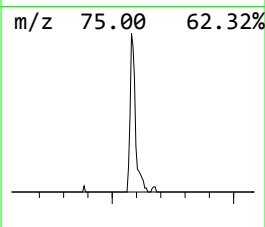
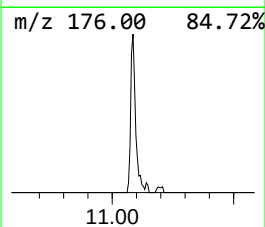
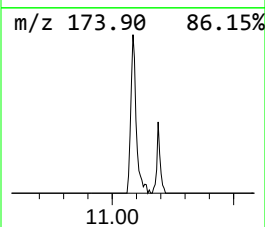
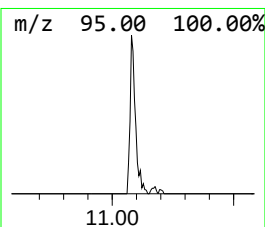
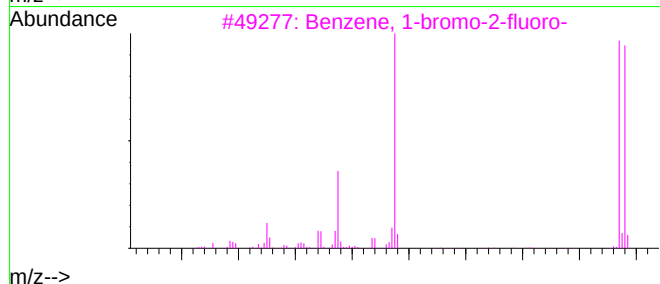
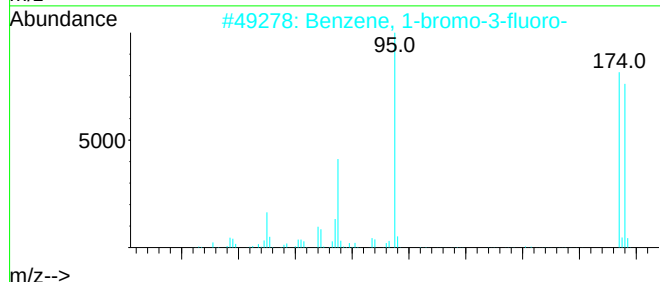
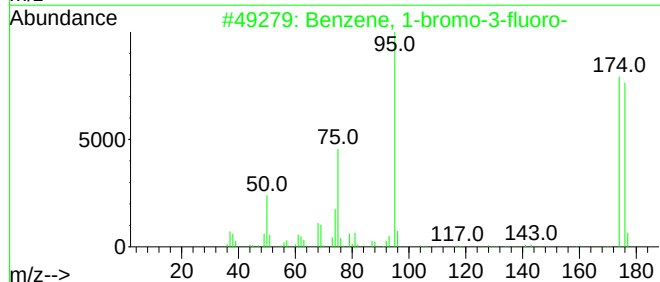
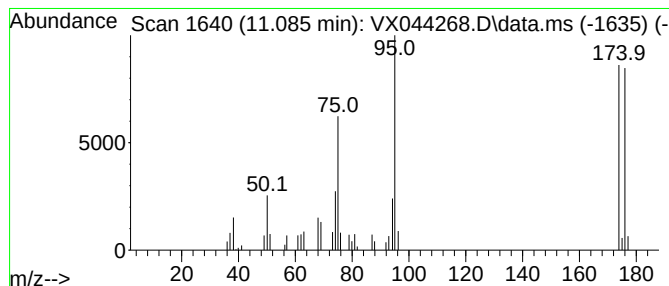
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-bromo-3-fluoro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.086	2.68 ug/L	28608	1,4-Dichlorobenzene-d4	12.018	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-bromo-3-fluoro-	174	C6H4BrF	001073-06-9	97
2	Benzene, 1-bromo-3-fluoro-	174	C6H4BrF	001073-06-9	93
3	Benzene, 1-bromo-2-fluoro-	174	C6H4BrF	001072-85-1	90
4	p-Bromofluorobenzene	174	C6H4BrF	000460-00-4	90
5	Benzene, 1-bromo-2-fluoro-	174	C6H4BrF	001072-85-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-brom...	11.086	2.7	ug/L	28608	3	12.018	534541	50.0