

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
 Data File : VX042737.D
 Acq On : 30 Jul 2024 14:22
 Operator : JC/MD
 Sample : P3287-05DL 5X
 Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 XB504DL

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\SFAMXML072624WMA.M
 Title : VOC Analysis

Signal : TIC: VX042737.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	25	28	31	rBV	4533	4672	0.62%	0.046%
2	1.300	31	35	42	rVV	11196	17087	2.25%	0.169%
3	1.367	43	46	60	rVB	41930	62386	8.22%	0.617%
4	1.544	73	75	76	rBV2	778	740	0.10%	0.007%
5	1.648	88	92	104	rVB	25285	49362	6.50%	0.488%
6	2.294	191	198	207	rBV2	104975	201612	26.56%	1.993%
7	2.398	210	215	227	rVB	33638	64327	8.47%	0.636%
8	2.654	255	257	259	rBV2	322	334	0.04%	0.003%
9	2.715	263	267	272	rVV2	2480	3899	0.51%	0.039%
10	2.782	272	278	300	rVV	81537	199577	26.29%	1.972%
11	3.038	317	320	321	rBV	280	228	0.03%	0.002%
12	3.123	324	334	344	rBV	77032	181011	23.85%	1.789%
13	3.324	364	367	369	rBV	198	253	0.03%	0.003%
14	4.208	509	512	516	rBV	224	270	0.04%	0.003%
15	4.379	536	540	542	rVB	290	370	0.05%	0.004%
16	4.422	545	547	548	rBV	250	263	0.03%	0.003%
17	4.483	548	557	566	rBV2	74530	221802	29.22%	2.192%
18	4.580	567	573	595	rVB	27960	88923	11.71%	0.879%
19	5.062	640	652	673	rBV5	69808	273587	36.04%	2.704%
20	5.294	688	690	693	rBV5	223	222	0.03%	0.002%
21	5.391	703	706	708	rBV	441	668	0.09%	0.007%
22	5.556	731	733	736	rVB2	577	422	0.06%	0.004%
23	5.580	736	737	742	rVB	344	312	0.04%	0.003%
24	5.684	752	754	757	rBV	183	251	0.03%	0.002%
25	5.757	763	766	768	rBV	241	275	0.04%	0.003%
26	5.964	790	800	812	rBV2	173828	507331	66.84%	5.014%
27	6.086	813	820	833	rVB	69425	181061	23.85%	1.789%
28	6.318	854	858	859	rBV	370	354	0.05%	0.003%
29	6.757	921	930	944	rBV	131084	321629	42.37%	3.179%
30	6.976	964	966	970	rVB	423	417	0.05%	0.004%
31	7.068	979	981	983	rBV	330	296	0.04%	0.003%
32	7.129	983	991	1002	rVV3	27874	67633	8.91%	0.668%
33	7.305	1013	1020	1032	rBV	101474	223817	29.49%	2.212%
34	7.427	1032	1040	1054	rVV	89082	193176	25.45%	1.909%
35	7.580	1058	1065	1082	rBV	77757	156247	20.58%	1.544%
36	7.824	1099	1105	1115	rBV2	21658	41603	5.48%	0.411%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
Data File : VX042737.D
Acq On : 30 Jul 2024 14:22
Operator : JC/MD
Sample : P3287-05DL 5X
Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
XB504DL

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\SFAMXML072624WMA.M
Title : VOC Analysis

37	7.970	1124	1129	1138	rBV	7942	14671	1.93%	0.145%
38	8.330	1182	1188	1191	rBV	64683	114541	15.09%	1.132%
39	8.366	1191	1194	1207	rVB	113403	179626	23.66%	1.775%
40	8.464	1207	1210	1211	rBV2	358	251	0.03%	0.002%
41	8.482	1211	1213	1215	rBV2	323	396	0.05%	0.004%
42	8.519	1215	1219	1224	rVV4	1611	3270	0.43%	0.032%
43	8.580	1224	1229	1235	rVV2	35065	62580	8.24%	0.618%
44	8.647	1235	1240	1246	rVV	265406	415502	54.74%	4.106%
45	8.720	1246	1252	1270	rVB	365785	607324	80.01%	6.002%
46	8.951	1285	1290	1292	rBV	52382	71760	9.45%	0.709%
47	9.153	1316	1323	1336	rVB	34070	54402	7.17%	0.538%
48	9.275	1336	1343	1350	rBV	100278	148884	19.61%	1.471%
49	9.390	1357	1362	1366	rBV	141915	220162	29.00%	2.176%
50	9.433	1366	1369	1379	rVV	201660	320094	42.17%	3.164%
51	9.525	1379	1384	1393	rVV	39686	64898	8.55%	0.641%
52	9.610	1393	1398	1406	rVV	56949	85340	11.24%	0.843%
53	9.683	1409	1410	1415	rBV	276	296	0.04%	0.003%
54	9.768	1423	1424	1427	rVB	386	257	0.03%	0.003%
55	9.805	1427	1430	1433	rBV3	231	326	0.04%	0.003%
56	10.055	1465	1471	1473	rBV	290295	399558	52.64%	3.949%
57	10.165	1483	1489	1492	rBV	246133	355225	46.80%	3.511%
58	10.299	1506	1511	1528	rVV	229039	325742	42.91%	3.219%
59	10.652	1562	1569	1586	rVV2	440381	704584	92.82%	6.963%
60	10.799	1588	1593	1600	rVV	33506	47977	6.32%	0.474%
61	10.884	1603	1607	1610	rVB2	231	321	0.04%	0.003%
62	10.969	1617	1621	1625	rBV2	461	766	0.10%	0.008%
63	11.195	1652	1658	1661	rBV	186702	247837	32.65%	2.449%
64	11.238	1661	1665	1676	rVV	228560	298396	39.31%	2.949%
65	11.396	1688	1691	1694	rBV2	303	337	0.04%	0.003%
66	11.451	1695	1700	1710	rBV	44316	56105	7.39%	0.554%
67	11.750	1744	1749	1757	rBV	38044	49768	6.56%	0.492%
68	11.811	1757	1759	1763	rVB	262	284	0.04%	0.003%
69	11.969	1780	1785	1789	rBV	159694	198403	26.14%	1.961%
70	12.024	1789	1794	1807	rVB2	306166	590191	77.75%	5.833%
71	12.158	1814	1816	1818	rBV	282	219	0.03%	0.002%
72	12.329	1837	1844	1857	rVV2	404783	759068	100.00%	7.502%
73	12.457	1862	1865	1868	rBV	236	268	0.04%	0.003%
74	12.506	1871	1873	1875	rBV	342	339	0.04%	0.003%
75	12.542	1875	1879	1882	rVB3	1616	1716	0.23%	0.017%
76	12.731	1907	1910	1911	rBV	239	284	0.04%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
 Data File : VX042737.D
 Acq On : 30 Jul 2024 14:22
 Operator : JC/MD
 Sample : P3287-05DL 5X
 Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 XB504DL

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\SFAMXML072624WMA.M
 Title : VOC Analysis

77	12.768	1911	1916	1919	rVB2	1065	1546	0.20%	0.015%
78	12.945	1940	1945	1954	rVB	60616	79452	10.47%	0.785%
79	13.018	1954	1957	1962	rBV2	224	416	0.05%	0.004%
80	13.109	1971	1972	1978	rVB2	362	526	0.07%	0.005%
81	13.170	1978	1982	1984	rBV2	260	410	0.05%	0.004%
82	13.219	1988	1990	1992	rBV	283	230	0.03%	0.002%
83	13.286	1996	2001	2002	rBV	281	345	0.05%	0.003%
84	13.347	2007	2011	2012	rBV	354	515	0.07%	0.005%
85	13.585	2044	2050	2056	rBV	31342	39058	5.15%	0.386%
86	13.725	2067	2073	2077	rBV	185012	230214	30.33%	2.275%
87	13.774	2077	2081	2093	rVB	228626	292245	38.50%	2.888%
88	14.127	2136	2139	2144	rVB3	750	1088	0.14%	0.011%
89	14.310	2167	2169	2172	rBV	305	317	0.04%	0.003%
90	14.353	2175	2176	2179	rBV	245	236	0.03%	0.002%
91	14.414	2183	2186	2189	rVB3	270	320	0.04%	0.003%
92	14.652	2221	2225	2228	rVB3	257	365	0.05%	0.004%
93	14.798	2245	2249	2250	rBV2	288	322	0.04%	0.003%
94	14.938	2269	2272	2275	rBV2	412	474	0.06%	0.005%
95	15.231	2318	2320	2322	rVV2	346	406	0.05%	0.004%
96	15.267	2324	2326	2331	rVB	191	287	0.04%	0.003%
97	15.822	2416	2417	2418	rBV	341	247	0.03%	0.002%
98	16.048	2452	2454	2459	rBV2	335	418	0.06%	0.004%
99	16.426	2514	2516	2518	rVB	333	235	0.03%	0.002%
100	16.731	2564	2566	2567	rBV	318	277	0.04%	0.003%

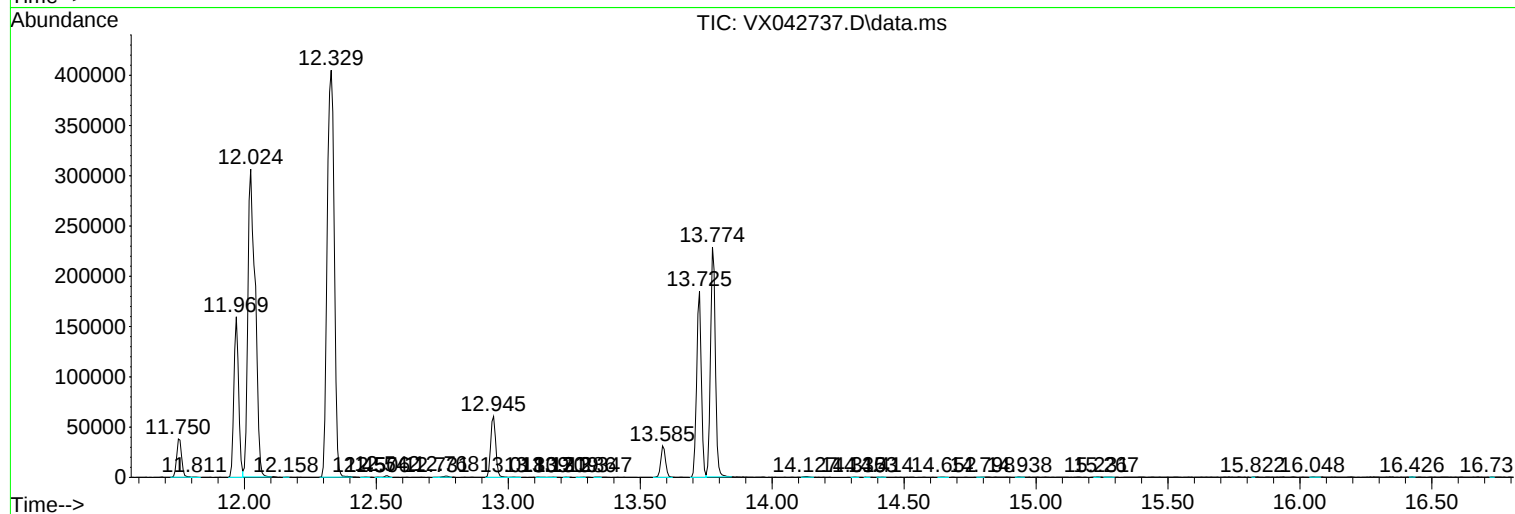
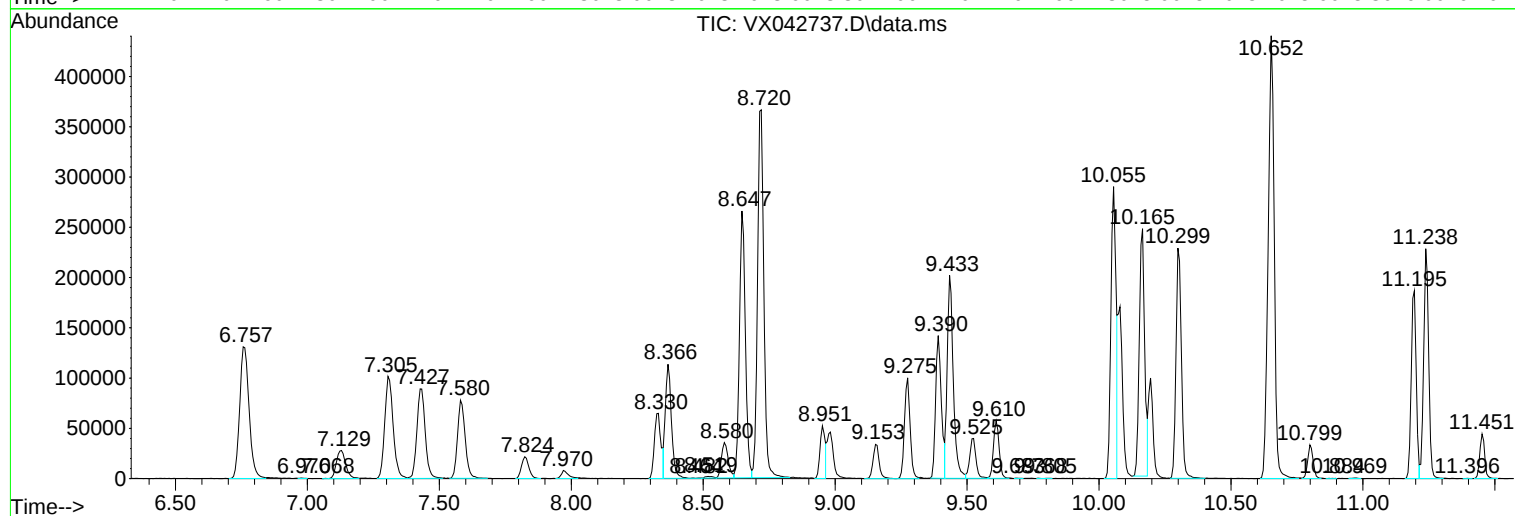
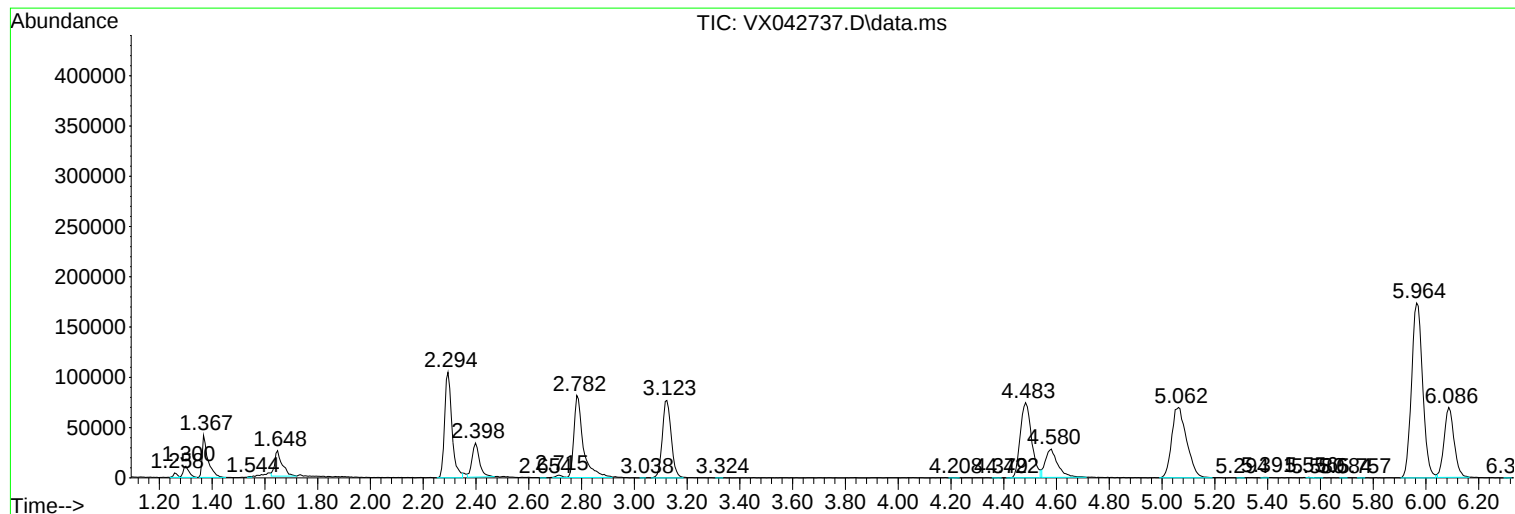
Sum of corrected areas: 10118334

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
Data File : VX042737.D
Acq On : 30 Jul 2024 14:22
Operator : JC/MD
Sample : P3287-05DL 5X
Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
XB504DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
Data File : VX042737.D
Acq On : 30 Jul 2024 14:22
Operator : JC/MD
Sample : P3287-05DL 5X
Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
XB504DL

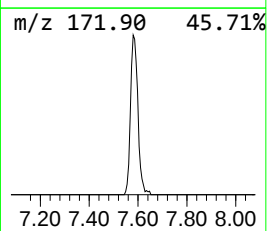
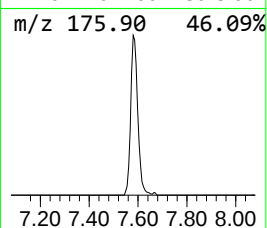
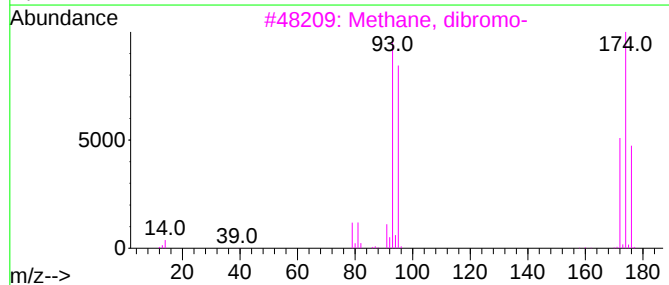
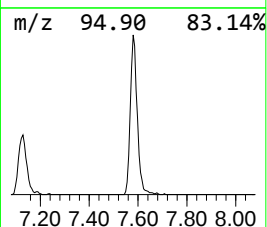
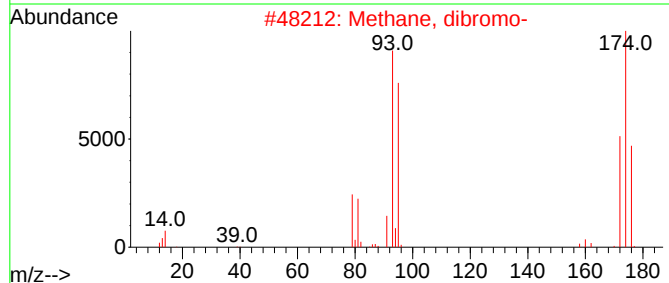
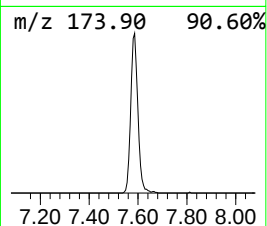
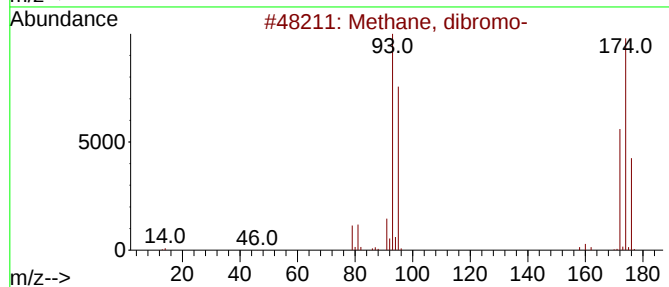
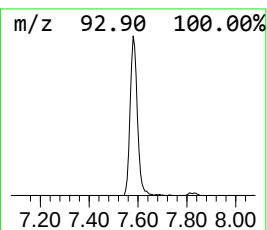
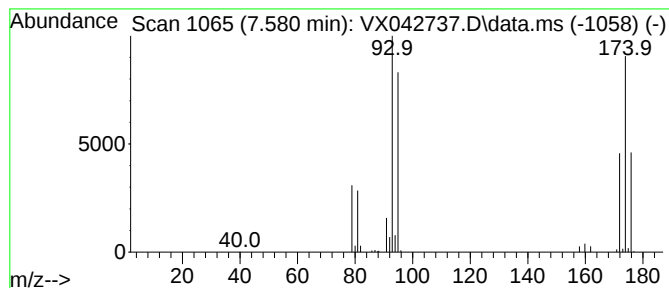
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methane, dibromo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.580	24.29 ug/L	156247	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, dibromo-	172	CH2Br2	000074-95-3	95
2			Methane, dibromo-	172	CH2Br2	000074-95-3	95
3			Methane, dibromo-	172	CH2Br2	000074-95-3	94
4			Methane, dibromo-	172	CH2Br2	000074-95-3	91
5			Pyridine, 2-nonyl-	205	C14H23N	010523-35-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073024\
Data File : VX042737.D
Acq On : 30 Jul 2024 14:22
Operator : JC/MD
Sample : P3287-05DL 5X
Misc : 10.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
XB504DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.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
Methane, dibromo-	7.580	24.3	ug/L	156247	1	6.757	321629	50.0