

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
 Data File : VX044293.D
 Acq On : 13 Dec 2024 19:46
 Operator : JC/MD
 Sample : P5232-09ME
 Misc : 10.20g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28S3ME

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\SFAMXML120524WMA.M
 Title : VOC Analysis

Signal : TIC: VX044293.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	26	28	32	rVB	9044	8158	0.86%	0.120%
2	1.368	43	46	49	rBV	49394	63560	6.71%	0.937%
3	2.276	189	195	213	rVB	154336	262238	27.70%	3.868%
4	2.611	249	250	252	rBV2	723	540	0.06%	0.008%
5	2.709	261	266	274	rBV2	5945	14031	1.48%	0.207%
6	2.837	285	287	289	rBV3	445	413	0.04%	0.006%
7	2.947	299	305	310	rBV4	3447	7441	0.79%	0.110%
8	3.063	320	324	325	rBV3	457	476	0.05%	0.007%
9	3.331	365	368	369	rBV2	489	409	0.04%	0.006%
10	3.386	374	377	378	rVV	839	840	0.09%	0.012%
11	3.416	380	382	390	rVV5	3708	6169	0.65%	0.091%
12	3.575	404	408	409	rBV2	458	495	0.05%	0.007%
13	3.770	438	440	442	rVV2	524	452	0.05%	0.007%
14	3.812	444	447	450	rBV3	584	801	0.08%	0.012%
15	3.971	472	473	475	rBV	570	472	0.05%	0.007%
16	4.135	496	500	501	rBV	538	626	0.07%	0.009%
17	4.172	504	506	509	rVB2	571	533	0.06%	0.008%
18	4.355	533	536	537	rBV2	630	515	0.05%	0.008%
19	4.489	548	558	581	rBV2	36998	170160	17.97%	2.510%
20	4.952	632	634	637	rVB3	1058	1036	0.11%	0.015%
21	5.050	637	650	664	rBV	124881	394070	41.62%	5.812%
22	5.367	699	702	703	rBV2	497	486	0.05%	0.007%
23	5.446	713	715	717	rBV3	596	714	0.08%	0.011%
24	5.538	728	730	732	rVV2	505	457	0.05%	0.007%
25	5.958	789	799	813	rBV2	335729	946820	100.00%	13.964%
26	6.361	862	865	867	rBV2	1511	1832	0.19%	0.027%
27	6.519	888	891	892	rBV3	458	582	0.06%	0.009%
28	6.586	899	902	903	rBV2	539	484	0.05%	0.007%
29	6.757	921	930	947	rVV	236501	582206	61.49%	8.587%
30	7.056	977	979	981	rBV	636	402	0.04%	0.006%
31	7.104	984	987	990	rBV5	1552	2624	0.28%	0.039%
32	7.306	1011	1020	1036	rBV	192926	444653	46.96%	6.558%
33	7.434	1039	1041	1043	rVB2	1024	793	0.08%	0.012%
34	7.482	1043	1049	1050	rBV4	742	1392	0.15%	0.021%
35	7.519	1053	1055	1057	rVB3	627	445	0.05%	0.007%
36	7.550	1057	1060	1063	rBV2	517	641	0.07%	0.009%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

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Min Area: 0 % of largest Peak

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	7.726	1084	1089	1092	rBV3	533	760	0.08%	0.011%
38	7.976	1125	1130	1134	rBV4	913	1637	0.17%	0.024%
39	8.007	1134	1135	1137	rVB	960	526	0.06%	0.008%
40	8.025	1137	1138	1139	rBV	816	413	0.04%	0.006%

41	8.123	1151	1154	1157	rVB2	499	562	0.06%	0.008%
42	8.251	1171	1175	1176	rBV3	613	639	0.07%	0.009%
43	8.324	1181	1187	1202	rVB	106682	185888	19.63%	2.742%
44	8.476	1210	1212	1215	rVV3	793	484	0.05%	0.007%
45	8.549	1222	1224	1226	rVB	673	477	0.05%	0.007%

46	8.647	1233	1240	1252	rBV	456052	734868	77.61%	10.838%
47	8.952	1284	1290	1308	rBV2	74411	123402	13.03%	1.820%
48	9.263	1340	1341	1345	rVB3	695	514	0.05%	0.008%
49	9.391	1357	1362	1383	rBV	191754	374380	39.54%	5.522%
50	9.982	1457	1459	1463	rBV4	355	535	0.06%	0.008%

51	10.055	1465	1471	1484	rVV	475108	696459	73.56%	10.272%
52	10.305	1508	1512	1514	rBV4	1565	1703	0.18%	0.025%
53	10.354	1518	1520	1525	rBV3	419	578	0.06%	0.009%
54	10.470	1537	1539	1541	rBV3	831	590	0.06%	0.009%
55	10.506	1543	1545	1548	rVB2	975	932	0.10%	0.014%

56	10.604	1560	1561	1564	rBV2	678	785	0.08%	0.012%
57	10.884	1606	1607	1610	rBV2	589	476	0.05%	0.007%
58	10.970	1619	1621	1624	rBV3	588	424	0.04%	0.006%
59	11.189	1652	1657	1668	rVV	333734	441507	46.63%	6.512%
60	11.378	1686	1688	1690	rBV	486	556	0.06%	0.008%

61	11.470	1701	1703	1705	rBV2	703	799	0.08%	0.012%
62	11.634	1728	1730	1733	rBV3	611	827	0.09%	0.012%
63	11.665	1733	1735	1738	rBV3	557	540	0.06%	0.008%
64	11.750	1747	1749	1750	rBV	573	572	0.06%	0.008%
65	11.860	1765	1767	1769	rBV2	570	492	0.05%	0.007%

66	12.018	1788	1793	1806	rBV	477574	615979	65.06%	9.085%
67	12.256	1828	1832	1834	rVB5	494	564	0.06%	0.008%
68	12.317	1837	1842	1855	rVV	512366	644738	68.10%	9.509%
69	12.530	1874	1877	1878	rBV2	670	699	0.07%	0.010%
70	12.616	1889	1891	1894	rBV3	850	898	0.09%	0.013%

71	12.799	1918	1921	1925	rBV2	822	1256	0.13%	0.019%
72	12.872	1931	1933	1935	rVB	790	493	0.05%	0.007%
73	12.902	1935	1938	1939	rBV2	739	916	0.10%	0.014%
74	12.951	1944	1946	1948	rBV2	533	522	0.06%	0.008%
75	13.079	1963	1967	1968	rBV3	453	584	0.06%	0.009%

76	13.116	1972	1973	1975	rBV	469	439	0.05%	0.006%
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Integration Parameters: LSCINT.P

Integrator: RTE

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

77	13.152	1978	1979	1981	rBV2	638	460	0.05%	0.007%
78	13.329	2005	2008	2009	rBV2	878	947	0.10%	0.014%
79	13.451	2027	2028	2034	rBV4	697	884	0.09%	0.013%
80	13.512	2034	2038	2042	rBV4	631	1058	0.11%	0.016%
81	13.658	2061	2062	2066	rBV3	787	879	0.09%	0.013%
82	13.841	2088	2092	2094	rVB4	1258	1443	0.15%	0.021%
83	13.969	2112	2113	2116	rBV3	511	529	0.06%	0.008%
84	14.000	2116	2118	2119	rVV2	673	514	0.05%	0.008%
85	14.036	2122	2124	2128	rVV3	1487	1587	0.17%	0.023%
86	14.085	2130	2132	2135	rVV3	890	782	0.08%	0.012%
87	14.134	2137	2140	2143	rVV3	1601	2190	0.23%	0.032%
88	14.182	2146	2148	2149	rBV	758	591	0.06%	0.009%
89	14.201	2149	2151	2153	rVV2	778	517	0.05%	0.008%
90	14.250	2156	2159	2161	rBV3	884	932	0.10%	0.014%
91	14.359	2173	2177	2180	rVB4	858	1351	0.14%	0.020%
92	14.402	2180	2184	2187	rBV2	888	1386	0.15%	0.020%
93	14.445	2189	2191	2192	rVB	714	404	0.04%	0.006%
94	14.652	2222	2225	2227	rBV3	849	702	0.07%	0.010%
95	14.938	2270	2272	2274	rBV2	572	477	0.05%	0.007%
96	15.493	2358	2363	2367	rVB7	1464	2431	0.26%	0.036%
97	15.524	2367	2368	2370	rBV2	511	423	0.04%	0.006%
98	15.621	2378	2384	2385	rBV3	960	1235	0.13%	0.018%
99	16.133	2466	2468	2470	rVB2	893	571	0.06%	0.008%
100	16.524	2530	2532	2533	rBV2	624	629	0.07%	0.009%

Sum of corrected areas: 6780301

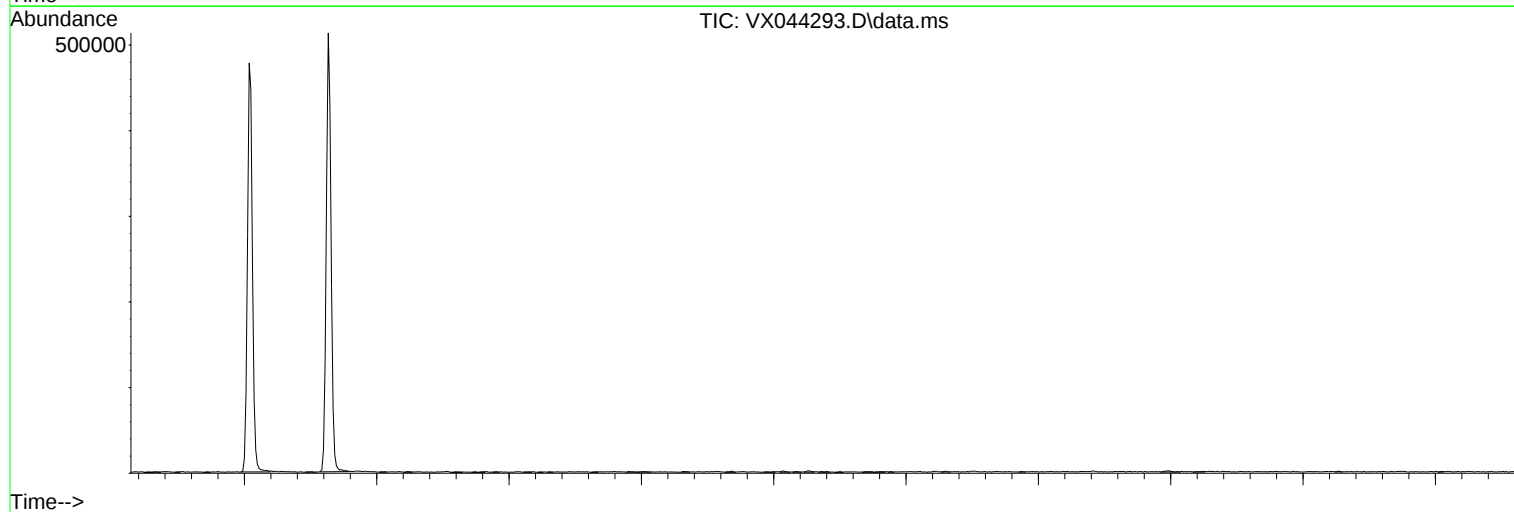
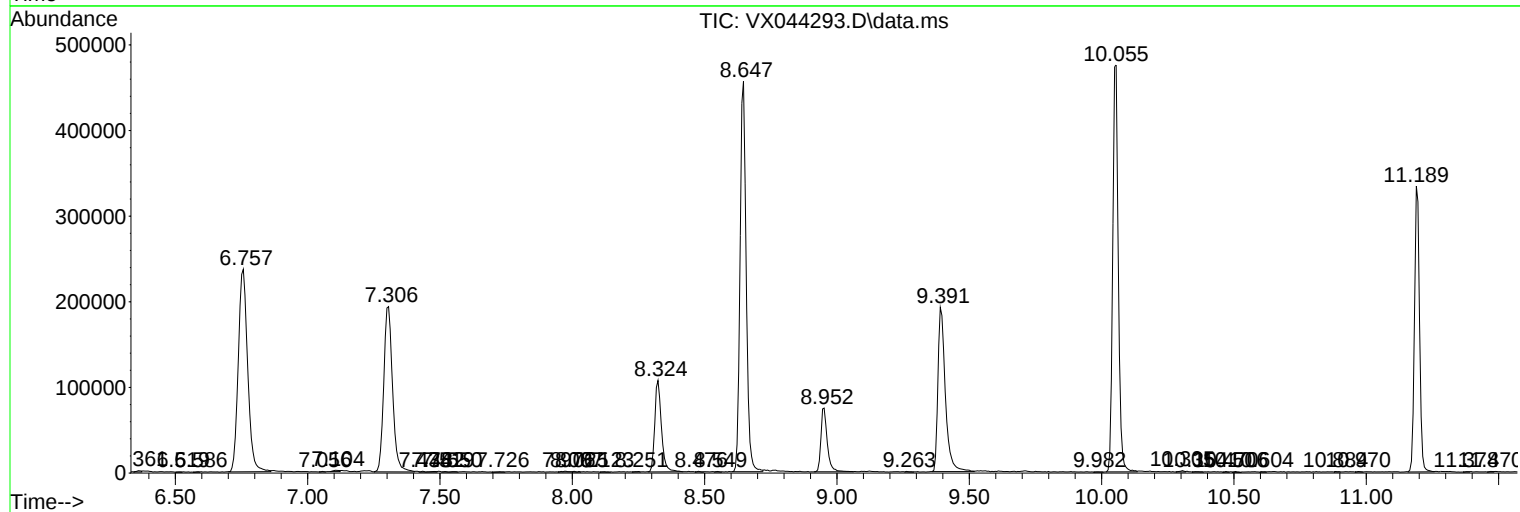
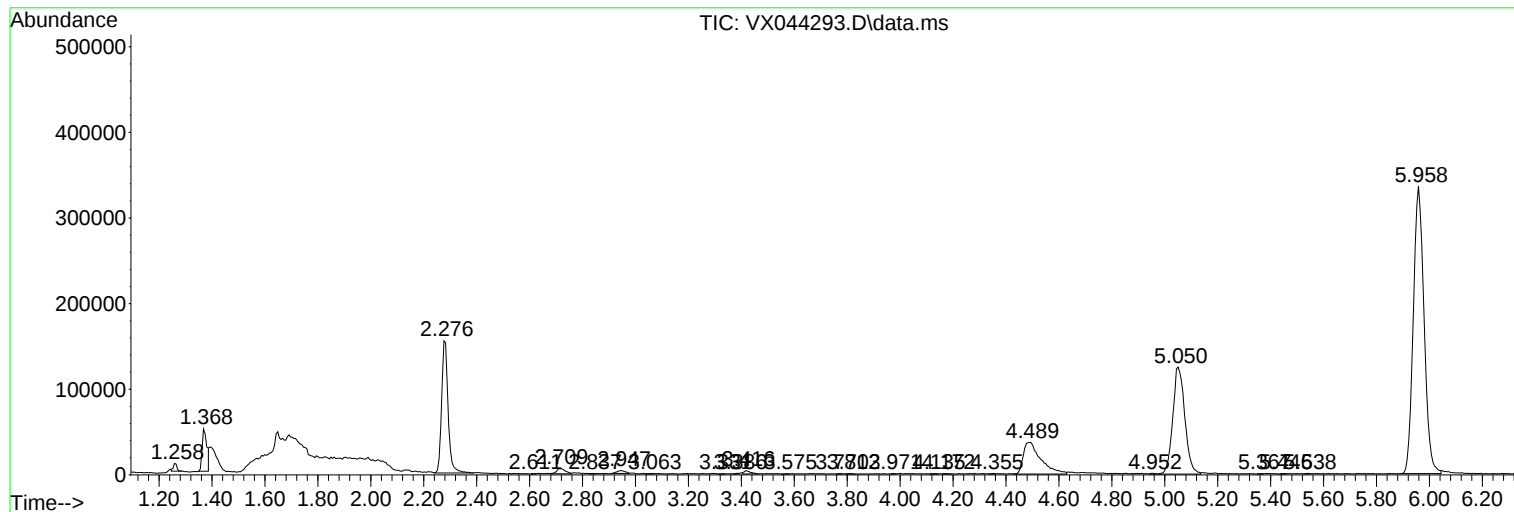
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ALS Vial : 28 Sample Multiplier: 1

Instrument :
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E28S3ME

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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ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28S3ME

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

No Library Search Compounds Detected

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

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

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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