

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
 Data File : VX025635.D
 Acq On : 08 Dec 2021 21:26
 Operator : JC/MD
 Sample : M4885-21ME
 Misc : 6.23g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9M6ME

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\SFAMXLM112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025635.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	31	rBV2	4156	7111	1.40%	0.170%
2	1.368	43	46	52	rBV	57208	65990	13.00%	1.576%
3	1.648	88	92	100	rBV	36596	41776	8.23%	0.998%
4	2.282	190	196	206	rBV	102968	169093	33.30%	4.038%
5	2.367	206	210	216	rVB2	1729	3301	0.65%	0.079%
6	2.489	228	230	232	rVB	425	289	0.06%	0.007%
7	2.550	239	240	243	rBV2	378	313	0.06%	0.007%
8	2.581	243	245	248	rVV	270	259	0.05%	0.006%
9	2.782	274	278	285	rVB3	1137	2155	0.42%	0.051%
10	2.953	299	306	312	rBV2	2267	4821	0.95%	0.115%
11	3.148	334	338	340	rBV	292	274	0.05%	0.007%
12	3.508	395	397	400	rVB2	333	364	0.07%	0.009%
13	3.733	432	434	438	rBV2	310	395	0.08%	0.009%
14	3.867	453	456	459	rBV	229	275	0.05%	0.007%
15	3.971	469	473	474	rBV	384	361	0.07%	0.009%
16	4.489	546	558	584	rBV	23993	104382	20.56%	2.492%
17	4.666	586	587	588	rBV	407	289	0.06%	0.007%
18	4.800	606	609	613	rVB	333	495	0.10%	0.012%
19	4.952	630	634	635	rBV	208	264	0.05%	0.006%
20	5.074	638	654	667	rBV3	60934	200264	39.44%	4.782%
21	5.227	676	679	680	rVB	349	315	0.06%	0.008%
22	5.251	680	683	685	rBV2	414	497	0.10%	0.012%
23	5.318	692	694	697	rBV	357	351	0.07%	0.008%
24	5.970	789	801	819	rBV2	176657	507744	100.00%	12.124%
25	6.373	857	867	879	rVB4	2222	8374	1.65%	0.200%
26	6.464	879	882	885	rBV2	357	449	0.09%	0.011%
27	6.678	916	917	921	rBV	369	317	0.06%	0.008%
28	6.763	921	931	950	rBV	139101	351696	69.27%	8.398%
29	7.129	982	991	1001	rBV3	22668	53623	10.56%	1.280%
30	7.312	1012	1021	1037	rVB	97775	224405	44.20%	5.358%
31	7.769	1094	1096	1099	rBV	217	260	0.05%	0.006%
32	7.976	1128	1130	1132	rVB	573	380	0.07%	0.009%
33	8.001	1132	1134	1136	rBV	287	330	0.06%	0.008%
34	8.129	1152	1155	1156	rBV	373	372	0.07%	0.009%
35	8.330	1182	1188	1201	rBV	57846	102184	20.13%	2.440%
36	8.452	1207	1208	1210	rBV	339	251	0.05%	0.006%

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 Title : VOC Analysis

37	8.494	1213	1215	1217	rBV	366	413	0.08%	0.010%
38	8.580	1226	1229	1232	rBV2	238	444	0.09%	0.011%
39	8.653	1234	1241	1249	rVV	253843	415694	81.87%	9.926%
40	8.720	1249	1252	1260	rVV	5637	10009	1.97%	0.239%
41	8.818	1266	1268	1270	rVB	352	301	0.06%	0.007%
42	8.836	1270	1271	1273	rBV	308	253	0.05%	0.006%
43	8.958	1285	1291	1302	rVB	36768	63997	12.60%	1.528%
44	9.037	1302	1304	1307	rBV2	306	356	0.07%	0.009%
45	9.275	1339	1343	1350	rVB3	3292	4999	0.98%	0.119%
46	9.330	1350	1352	1353	rBV	344	259	0.05%	0.006%
47	9.348	1353	1355	1356	rBV	381	254	0.05%	0.006%
48	9.397	1357	1363	1374	rBV	137939	220944	43.51%	5.276%
49	9.622	1395	1400	1401	rBV	378	482	0.09%	0.012%
50	9.708	1412	1414	1420	rVB3	509	648	0.13%	0.015%
51	9.762	1420	1423	1424	rBV2	241	266	0.05%	0.006%
52	9.830	1432	1434	1436	rBV	386	285	0.06%	0.007%
53	9.909	1443	1447	1451	rBV2	371	647	0.13%	0.015%
54	9.945	1451	1453	1458	rVB2	227	296	0.06%	0.007%
55	10.061	1465	1472	1480	rBV	267853	405779	79.92%	9.689%
56	10.177	1488	1491	1492	rBV2	307	310	0.06%	0.007%
57	10.195	1492	1494	1500	rVB3	316	485	0.10%	0.012%
58	10.305	1508	1512	1517	rVB3	2357	3522	0.69%	0.084%
59	10.415	1529	1530	1533	rBV2	231	286	0.06%	0.007%
60	10.506	1544	1545	1548	rBV	341	281	0.06%	0.007%
61	10.646	1564	1568	1575	rVB3	812	1314	0.26%	0.031%
62	10.799	1589	1593	1597	rVB	406	540	0.11%	0.013%
63	10.848	1597	1601	1604	rBV	294	487	0.10%	0.012%
64	10.957	1616	1619	1620	rBV2	373	386	0.08%	0.009%
65	11.122	1642	1646	1651	rVB2	2272	3223	0.63%	0.077%
66	11.195	1653	1658	1666	rVV	179462	233045	45.90%	5.565%
67	11.305	1673	1676	1685	rVB4	684	1329	0.26%	0.032%
68	11.451	1697	1700	1701	rBV	727	668	0.13%	0.016%
69	11.713	1741	1743	1744	rVV	524	380	0.07%	0.009%
70	11.750	1746	1749	1754	rVB3	2946	3810	0.75%	0.091%
71	11.841	1761	1764	1767	rVB2	406	345	0.07%	0.008%
72	11.939	1776	1780	1782	rBV3	1279	1681	0.33%	0.040%
73	11.963	1782	1784	1789	rVB	912	923	0.18%	0.022%
74	12.024	1789	1794	1801	rBV	338141	417621	82.25%	9.972%
75	12.152	1813	1815	1819	rVB3	2314	2524	0.50%	0.060%
76	12.195	1819	1822	1823	rBV2	304	311	0.06%	0.007%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.M
 Title : VOC Analysis

77	12.323	1837	1843	1850	rVB	317955	386442	76.11%	9.227%
78	12.421	1856	1859	1863	rBV2	2191	2694	0.53%	0.064%
79	12.658	1896	1898	1900	rBV3	634	781	0.15%	0.019%
80	12.744	1911	1912	1915	rBV2	468	409	0.08%	0.010%
81	12.890	1934	1936	1939	rBV3	736	586	0.12%	0.014%
82	12.969	1946	1949	1956	rVB4	1623	2258	0.44%	0.054%
83	13.048	1959	1962	1966	rBV3	637	1163	0.23%	0.028%
84	13.109	1969	1972	1974	rVB	405	381	0.08%	0.009%
85	13.237	1990	1993	1995	rBV3	850	868	0.17%	0.021%
86	13.268	1995	1998	2001	rBV	4818	5252	1.03%	0.125%
87	13.353	2010	2012	2014	rBV2	373	368	0.07%	0.009%
88	13.384	2014	2017	2023	rVV2	3399	4509	0.89%	0.108%
89	13.500	2032	2036	2037	rBV2	743	812	0.16%	0.019%
90	13.634	2054	2058	2060	rVB3	1395	1694	0.33%	0.040%
91	13.774	2078	2081	2088	rVB	7665	11216	2.21%	0.268%
92	13.847	2089	2093	2096	rVB2	7318	8307	1.64%	0.198%
93	13.993	2115	2117	2119	rBV	1409	1569	0.31%	0.037%
94	14.042	2122	2125	2131	rVB2	11264	13593	2.68%	0.325%
95	14.615	2216	2219	2221	rBV2	7355	8138	1.60%	0.194%
96	14.755	2239	2242	2245	rBV	16808	19086	3.76%	0.456%
97	15.213	2314	2317	2324	rVB3	10154	13716	2.70%	0.328%
98	15.493	2357	2363	2369	rVB3	12790	24494	4.82%	0.585%
99	15.615	2379	2383	2387	rBV	12890	20000	3.94%	0.478%
100	15.816	2412	2416	2418	rBV4	3731	5807	1.14%	0.139%

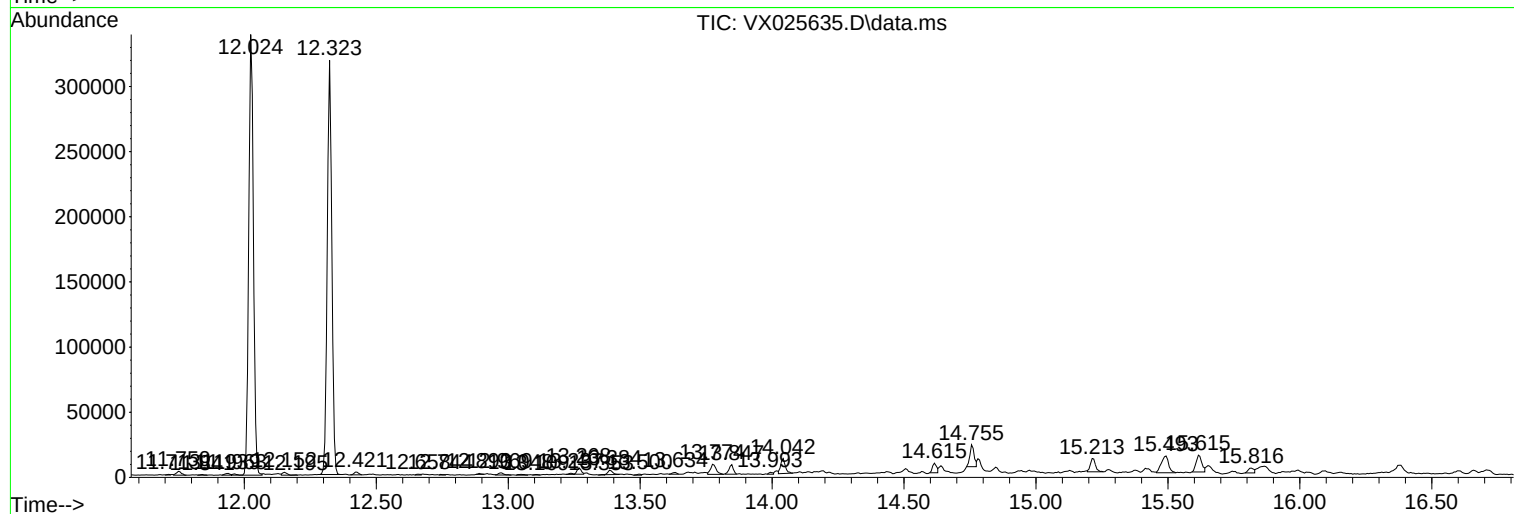
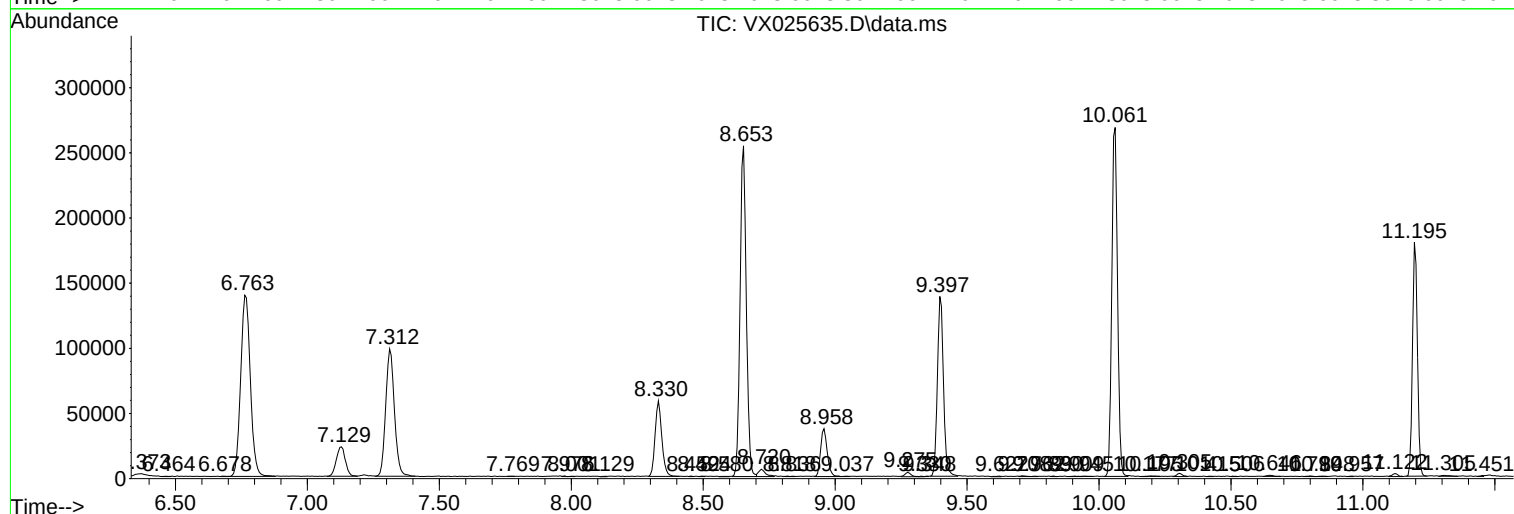
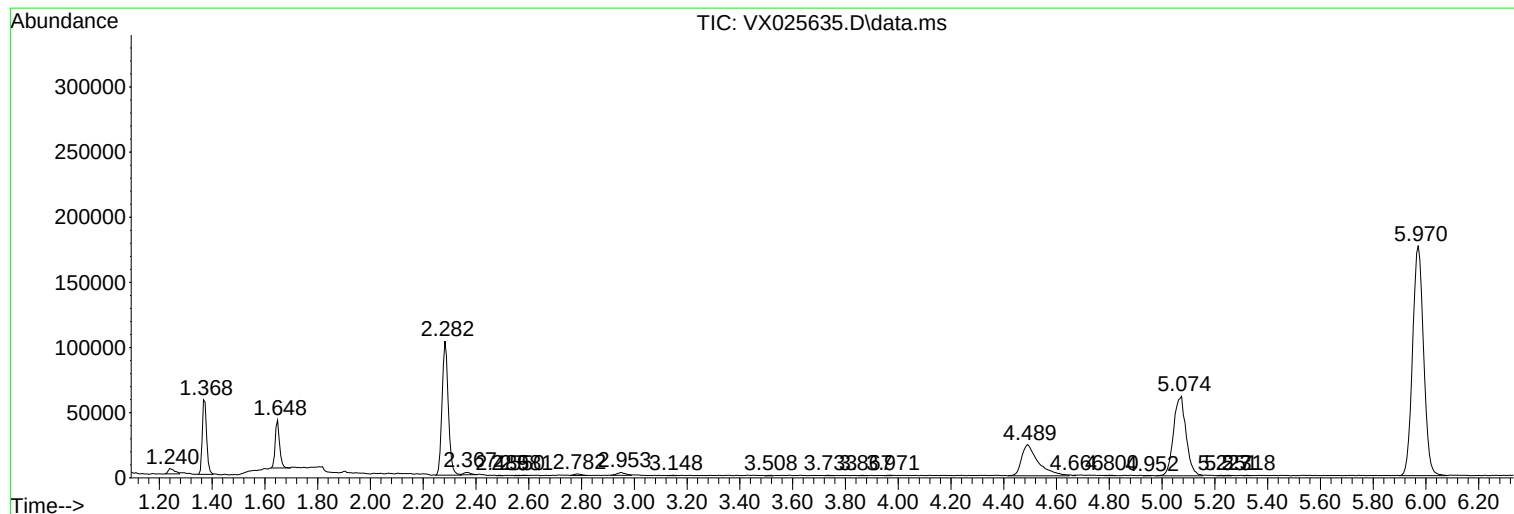
Sum of corrected areas: 4187959

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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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



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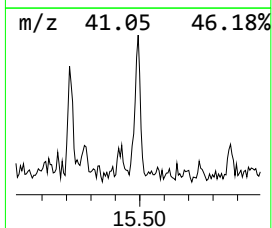
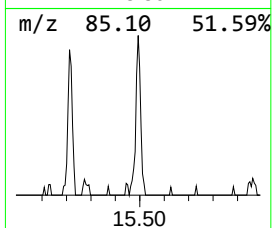
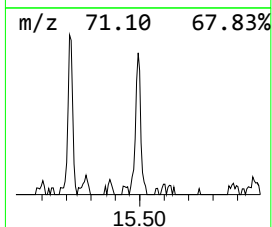
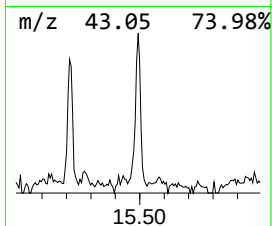
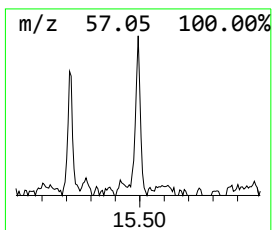
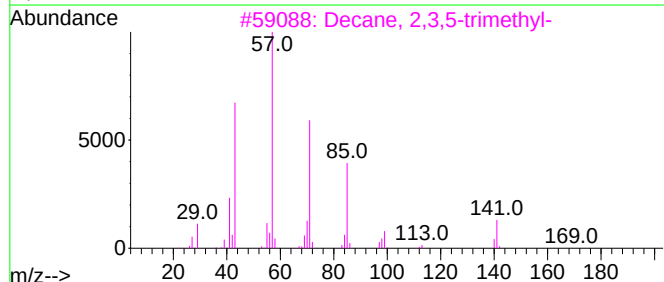
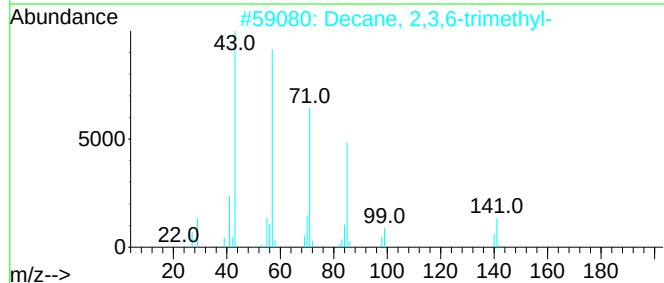
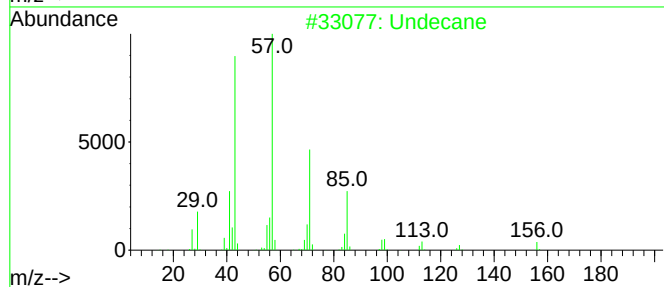
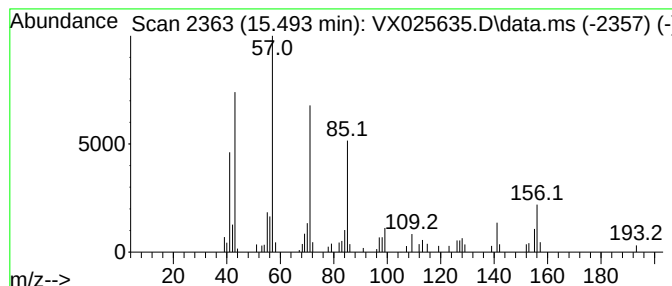
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.493	2.93 ug/L	24494	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	74
2			Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	64
3			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	64
4			Nonadecane	268	C19H40	000629-92-5	62
5			1,3-Propanediol, decyl ethyl ether	244	C15H32O2	1000406-35-0	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	15.493	2.9	ug/L	24494	3	12.024	417621	50.0