LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
Data File : VX044504.D
Acq On : 26 Dec 2024 13:01
Operator : JC/MD
Sample : P5322-17ME
Misc : 4.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE631ME

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

Signal : TIC: VX044504.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	7268	6550	0.67%	0.058%
2	1.368	42	46	49	rBV	61156	77791	7.92%	0.691%
3	1.605	68	85	86	rBV2	19933	78055	7.94%	0.693%
4	2.130	169	171	178	rVB4	3115	5052	0.51%	0.045%
5	2.276	189	195	212	rBV	166291	281657	28.67%	2.501%
6	2.684	260	262	265	rBV3	438	447	0.05%	0.004%
7	2.715	265	267	269	rVV	560	394	0.04%	0.003%
8	2.947	297	305	314	rBV3	6883	18874	1.92%	0.168%
9	3.008	314	315	316	rBV	716	323	0.03%	0.003%
10	3.056	322	323	325	rVB2	731	433	0.04%	0.004%
11	3.203	344	347	348	rBV2	328	344	0.04%	0.003%
12	3.258	352	356	358	rBV3	225	380	0.04%	0.003%
13	3.416	378	382	385	rBV5	1034	1362	0.14%	0.012%
14	3.483	390	393	395	rVB2	464	423	0.04%	0.004%
15	3.538	400	402	406	rBV4	376	558	0.06%	0.005%
16	3.636	416	418	421	rVV	377	362	0.04%	0.003%
17	3.806	442	446	447	rBV	395	465	0.05%	0.004%
18	3.855	453	454	457	rBV2	443	461	0.05%	0.004%
19	3.934	465	467	469	rBV3	261	324	0.03%	0.003%
20	3.977	469	474	475	rVB4	488	688	0.07%	0.006%
21	4.007	475	479	480	rBV2	386	369	0.04%	0.003%
22	4.050	483	486	489	rBV3	412	502	0.05%	0.004%
23	4.074	489	490	493	rVB2	436	382	0.04%	0.003%
24	4.129	495	499	500	rVV3	383	491	0.05%	0.004%
25	4.282	522	524	527	rVB3	427	465	0.05%	0.004%
26	4.306	527	528	529	rBV2	593	348	0.04%	0.003%
27	4.489	547	558	581	rBV	32908	151957	15.47%	1.349%
28	5.050	639	650	670	rVB2	101881	339968	34.60%	3.019%
29	5.251	679	683	684	rBV3	397	405	0.04%	0.004%
30	5.300	689	691	693	rBV2	367	310	0.03%	0.003%
31	5.379	702	704	706	rBV3	565	472	0.05%	0.004%
32	5.446	713	715	719	rBV4	345	550	0.06%	0.005%
33	5.635	745	746	750	rVB3	540	372	0.04%	0.003%
34	5.672	750	752	755	rVB2	750	552	0.06%	0.005%
35	5.751	764	765	768	rBV2	328	362	0.04%	0.003%
36	5.788	769	771	774	rVV2	378	462	0.05%	0.004%

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Misc : 4.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE631ME

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

37	5.873	782	785	787	rBV3	571	540	0.05%	0.005%
38	5.958	787	799	825	rBV2	294602	858819	87.41%	7.626%
39	6.281	851	852	855	rBV2	460	337	0.03%	0.003%
40	6.318	855	858	860	rBV4	555	701	0.07%	0.006%
41	6.361	861	865	869	rBV4	1011	1707	0.17%	0.015%
42	6.757	921	930	946	rBV	212400	532236	54.17%	4.726%
43	6.982	964	967	968	rBV2	456	472	0.05%	0.004%
44	7.043	974	977	981	rVB3	502	625	0.06%	0.006%
45	7.123	984	990	999	rVB3	2421	7239	0.74%	0.064%
46	7.202	1001	1003	1004	rBV2	1186	901	0.09%	0.008%
47	7.306	1011	1020	1041	rVB	166106	380768	38.75%	3.381%
48	7.610	1068	1070	1072	rBV2	574	485	0.05%	0.004%
49	7.751	1091	1093	1097	rBV3	663	864	0.09%	0.008%
50	7.848	1107	1109	1112	rVB3	511	587	0.06%	0.005%
51	7.897	1116	1117	1120	rBV2	679	644	0.07%	0.006%
52	7.958	1125	1127	1128	rBV	570	382	0.04%	0.003%
53	8.068	1143	1145	1146	rBV2	517	479	0.05%	0.004%
54	8.202	1165	1167	1168	rVB	510	331	0.03%	0.003%
55	8.220	1168	1170	1171	rBV2	439	395	0.04%	0.004%
56	8.324	1181	1187	1199	rBV	94698	166265	16.92%	1.476%
57	8.507	1213	1217	1219	rBV2	744	899	0.09%	0.008%
58	8.592	1224	1231	1233	rBV5	4384	8206	0.84%	0.073%
59	8.647	1234	1240	1248	rVV	425396	683957	69.61%	6.073%
60	8.720	1248	1252	1256	rVB	10906	16032	1.63%	0.142%
61	8.830	1268	1270	1271	rBV2	610	340	0.03%	0.003%
62	8.909	1279	1283	1285	rBV3	3405	4108	0.42%	0.036%
63	8.952	1285	1290	1305	rVB	64476	109200	11.11%	0.970%
64	9.147	1320	1322	1323	rBV	487	440	0.04%	0.004%
65	9.202	1327	1331	1332	rBV3	720	966	0.10%	0.009%
66	9.397	1357	1363	1376	rVV	168549	333111	33.90%	2.958%
67	9.610	1394	1398	1402	rBV	14525	21302	2.17%	0.189%
68	9.756	1418	1422	1426	rVB4	4397	5623	0.57%	0.050%
69	9.823	1427	1433	1441	rVV6	9930	22926	2.33%	0.204%
70	9.903	1441	1446	1451	rVB2	9319	14466	1.47%	0.128%
71	10.006	1456	1463	1465	rBV2	10940	17106	1.74%	0.152%
72	10.055	1465	1471	1478	rBV	443902	640663	65.21%	5.689%
73	10.195	1487	1494	1500	rBV	36785	63144	6.43%	0.561%
74	10.299	1502	1511	1517	rVV	143860	250438	25.49%	2.224%
75	10.354	1517	1520	1531	rVB2	72152	110393	11.24%	0.980%
76	10.451	1531	1536	1541	rBV3	20526	32169	3.27%	0.286%

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Sample : P5322-17ME
Misc : 4.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE631ME

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	10.525	1547	1548	1549	rBV	2141	1418	0.14%	0.013%
78	10.586	1551	1558	1563	rVV3	32682	67525	6.87%	0.600%
79	10.640	1563	1567	1574	rVV	68060	107701	10.96%	0.956%
80	10.774	1582	1589	1593	rBV2	109789	179362	18.26%	1.593%
81	10.854	1599	1602	1605	rBV3	59774	73436	7.47%	0.652%
82	10.945	1613	1617	1622	rVB4	40356	63239	6.44%	0.562%
83	11.000	1622	1626	1628	rBV3	25659	33958	3.46%	0.302%
84	11.189	1653	1657	1669	rVB2	329242	637849	64.92%	5.664%
85	11.305	1673	1676	1677	rBV	21256	23746	2.42%	0.211%
86	11.378	1686	1688	1693	rVB3	96532	148360	15.10%	1.317%
87	11.427	1693	1696	1698	rVV	87161	117468	11.96%	1.043%
88	11.476	1701	1704	1709	rVB	470452	572931	58.31%	5.087%
89	11.616	1723	1727	1733	rVB4	88780	171486	17.45%	1.523%
90	11.713	1740	1743	1745	rBV	197179	219759	22.37%	1.951%
91	11.750	1745	1749	1758	rVB	417505	689096	70.14%	6.119%
92	12.018	1789	1793	1799	rBV2	524036	764979	77.86%	6.793%
93	12.244	1826	1830	1832	rBV2	82815	125862	12.81%	1.118%
94	12.317	1837	1842	1848	rVB2	644332	982519	100.00%	8.724%
95	12.421	1856	1859	1863	rVB	308096	334277	34.02%	2.968%
96	12.884	1932	1935	1937	rBV	60382	87890	8.95%	0.780%
97	13.268	1995	1998	1999	rBV	88590	102560	10.44%	0.911%
98	13.774	2077	2081	2088	rVB	260294	355812	36.21%	3.159%
99	14.036	2121	2124	2127	rVB	80478	81625	8.31%	0.725%
100	14.755	2239	2242	2244	rBV	46067	56016	5.70%	0.497%

Sum of corrected areas: 11262050

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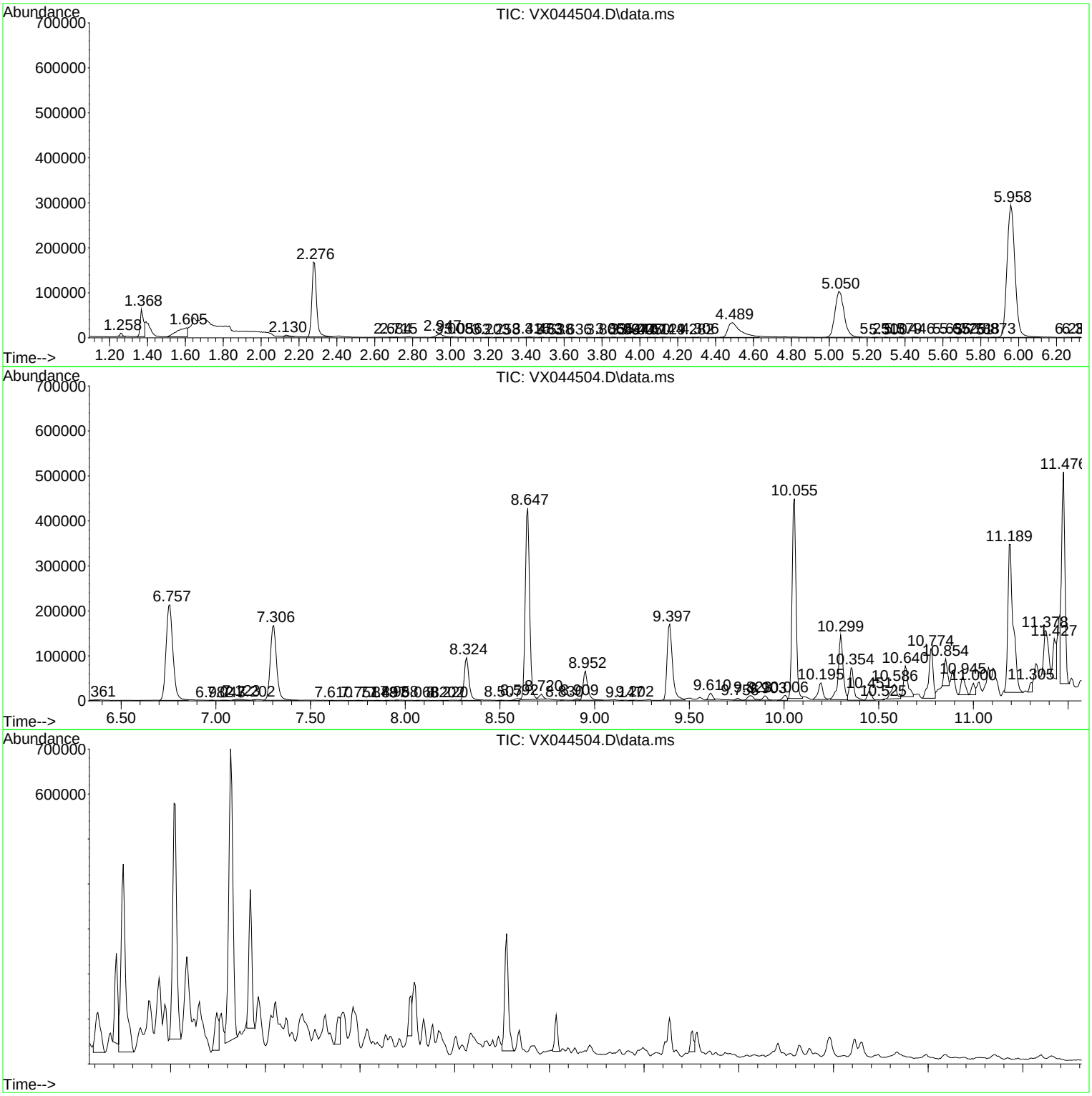
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE631ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
Data File : VX044504.D
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Operator : JC/MD
Sample : P5322-17ME
Misc : 4.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE631ME

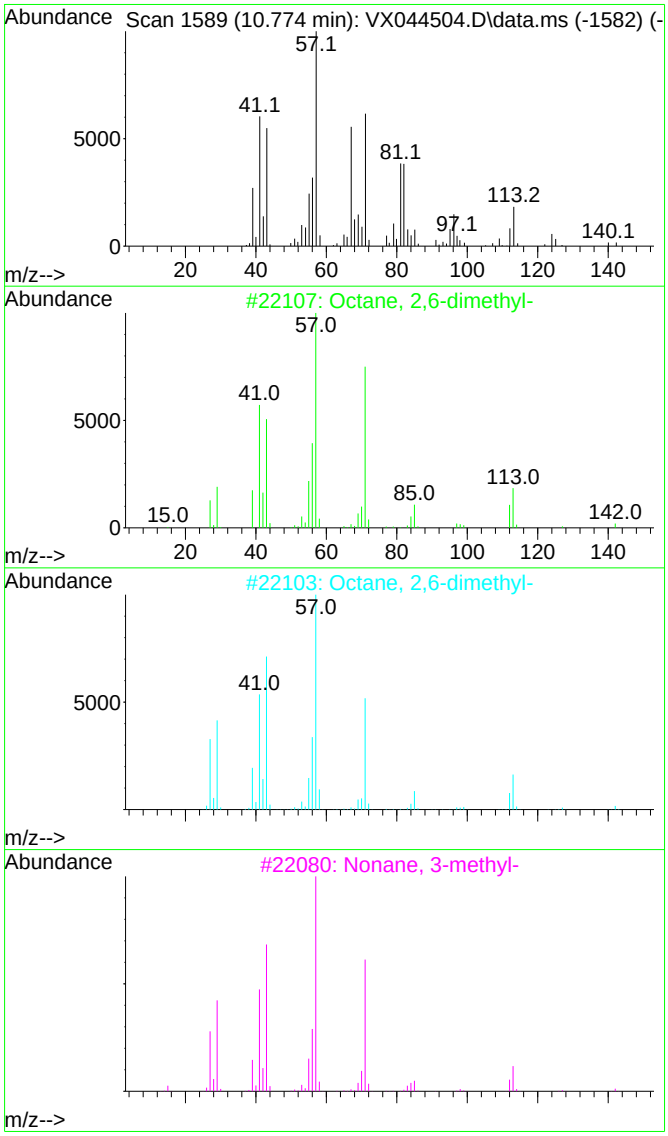
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

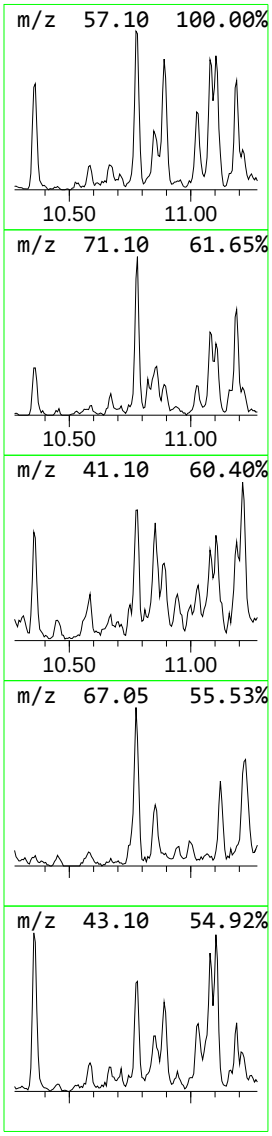
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.775	14.00 ug/L	179362	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	89
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	50
4	Nonane, 3-methyl-	142	C10H22	005911-04-6	41
5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
Data File : VX044504.D
Acq On : 26 Dec 2024 13:01
Operator : JC/MD
Sample : P5322-17ME
Misc : 4.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE631ME

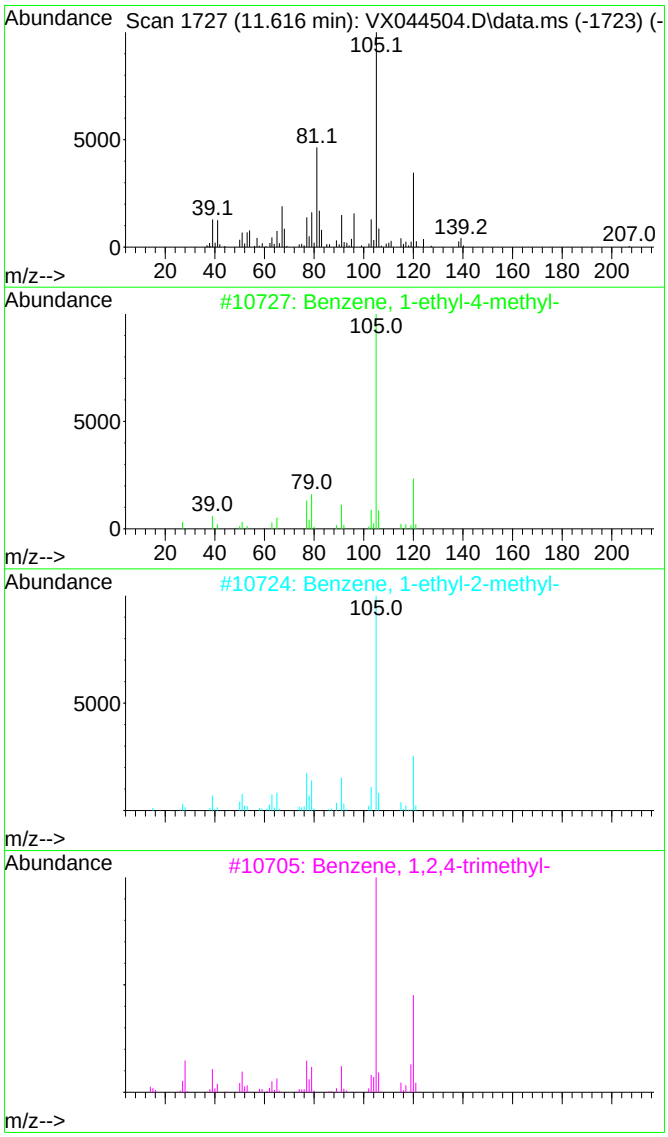
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

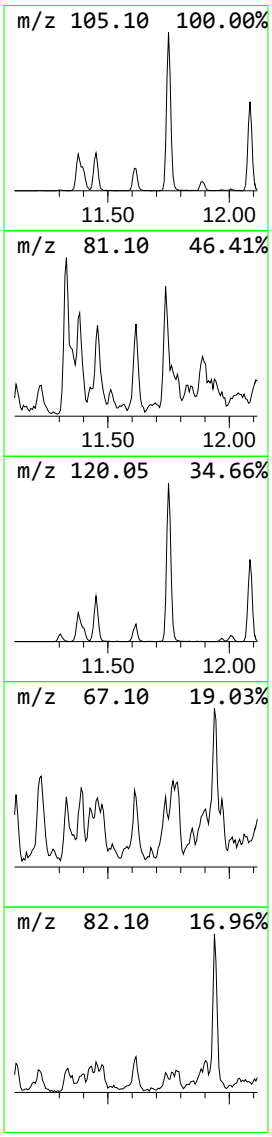
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	11.21 ug/L	171486	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	60
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	60
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	60
5	Mesitylene	120	C9H12	000108-67-8	55





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
Data File : VX044504.D
Acq On : 26 Dec 2024 13:01
Operator : JC/MD
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE631ME

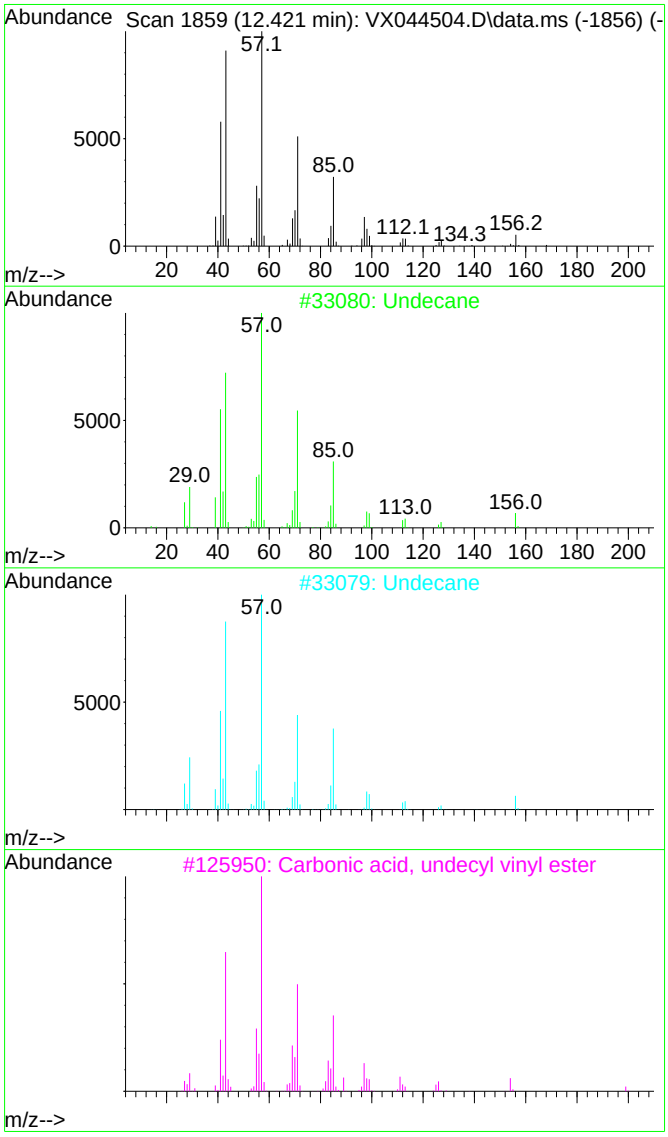
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

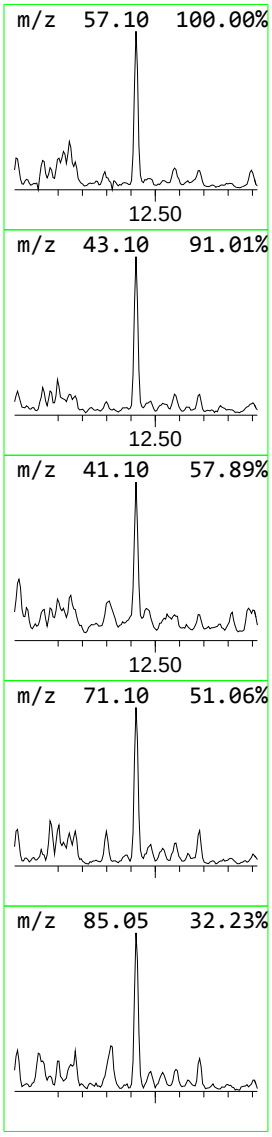
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	21.85 ug/L	334277	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	96
2	Undecane	156	C11H24	001120-21-4	91
3	Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	90
4	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	86
5	Undecane	156	C11H24	001120-21-4	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
Data File : VX044504.D
Acq On : 26 Dec 2024 13:01
Operator : JC/MD
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Misc : 4.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE631ME

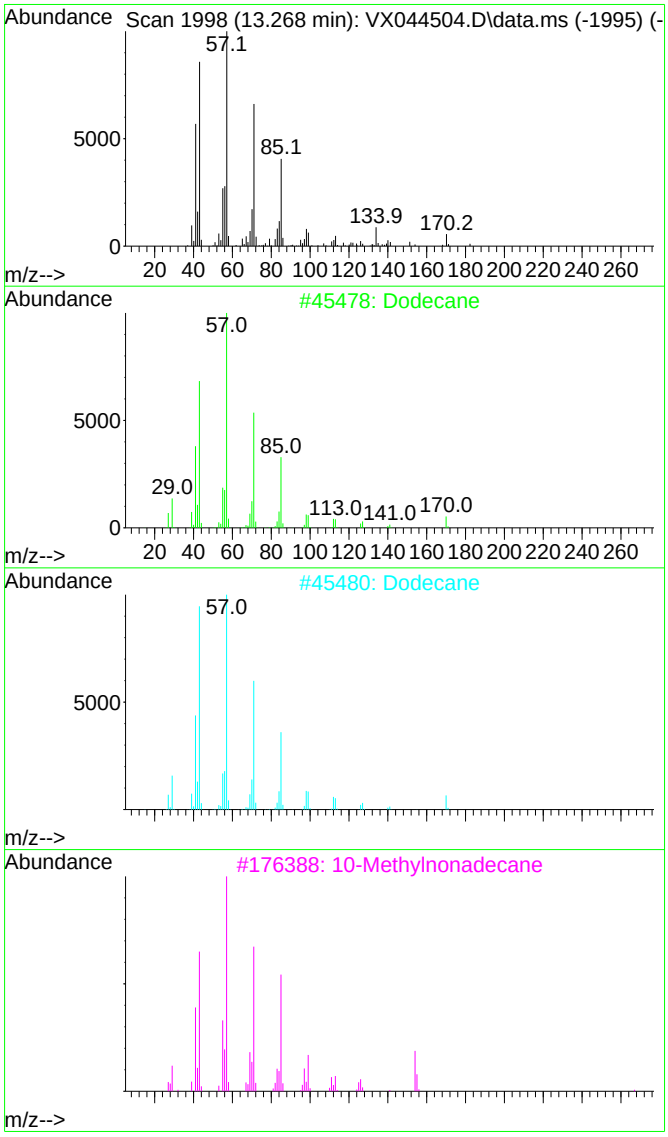
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

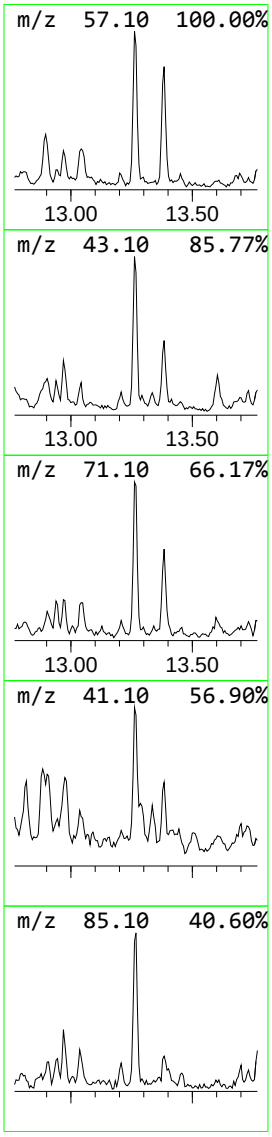
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	6.70 ug/L	102560	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	93
2	Dodecane	170	C12H26	000112-40-3	90
3	10-Methylnonadecane	282	C20H42	056862-62-5	80
4	Tridecane	184	C13H28	000629-50-5	80
5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
Data File : VX044504.D
Acq On : 26 Dec 2024 13:01
Operator : JC/MD
Sample : P5322-17ME
Misc : 4.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE631ME

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

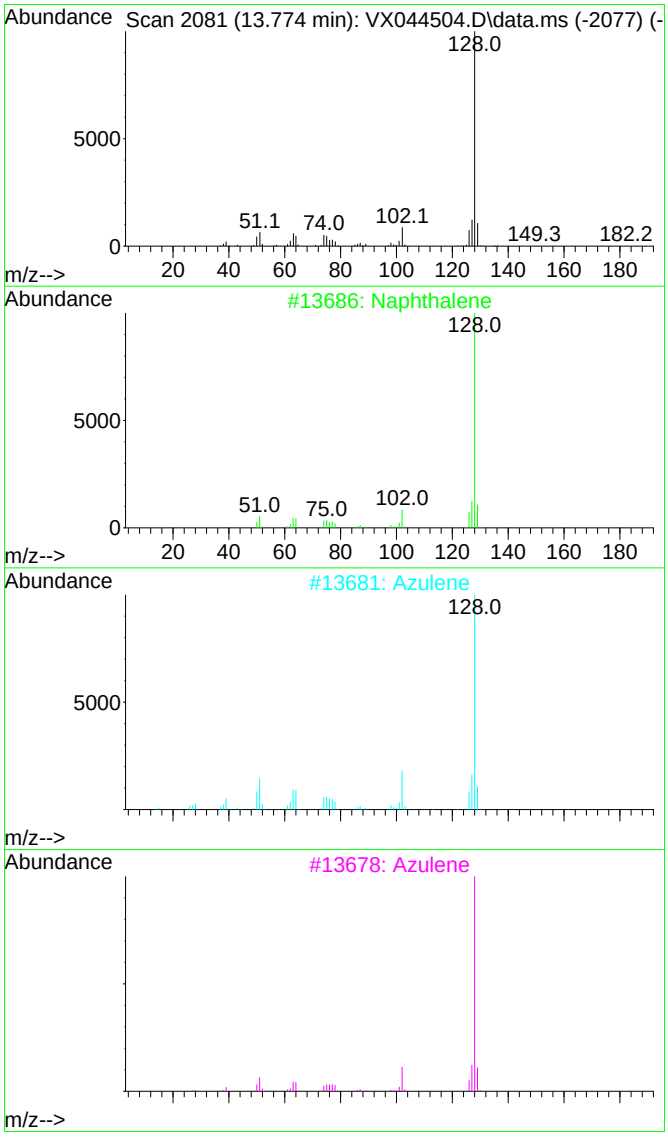
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

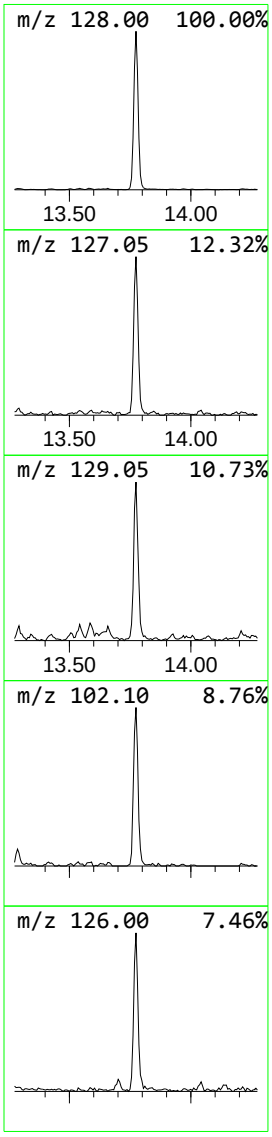
****

Peak Number 15 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	23.26 ug/L	355812	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	91
3	Azulene	128	C10H8	000275-51-4	90
4	Naphthalene	128	C10H8	000091-20-3	90
5	Naphthalene	128	C10H8	000091-20-3	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
Data File : VX044504.D
Acq On : 26 Dec 2024 13:01
Operator : JC/MD
Sample : P5322-17ME
Misc : 4.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE631ME

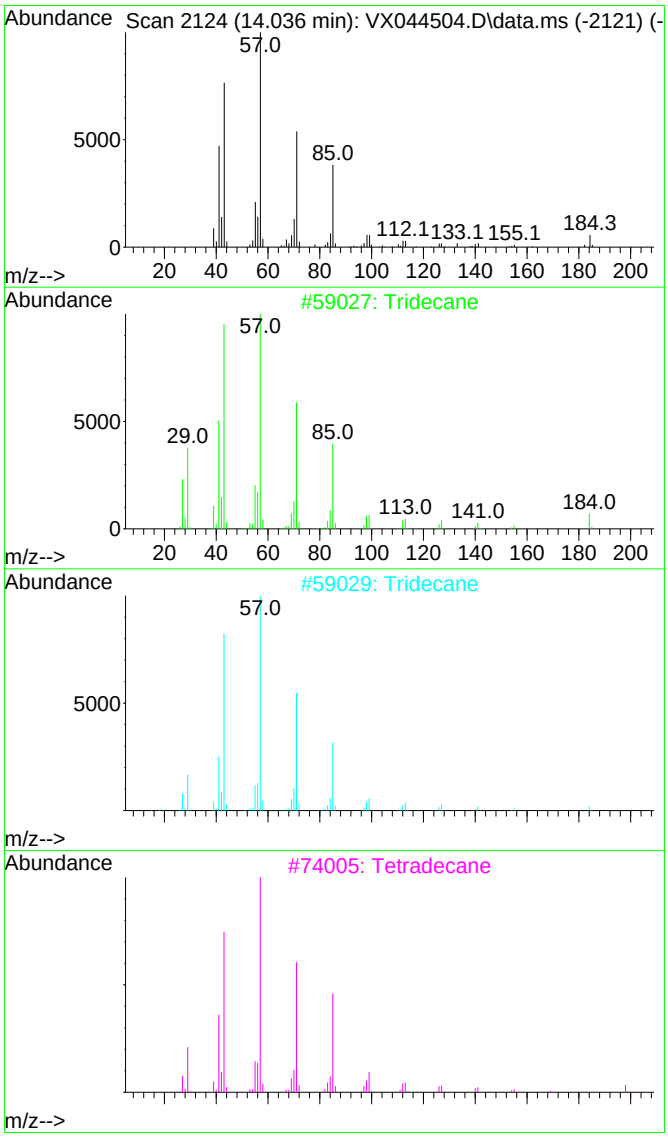
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.M
Quant Title : VOC Analysis

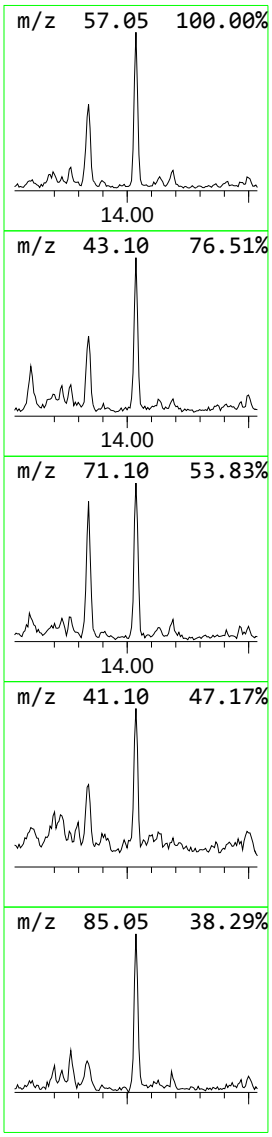
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 (DEL) Alkane: Straight-Chai... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.036	5.34 ug/L	81625	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Tridecane	184	C13H28	000629-50-5	91
3	Tetradecane	198	C14H30	000629-59-4	90
4	Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	78
5	Hexadecane	226	C16H34	000544-76-3	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122624\
Data File : VX044504.D
Acq On : 26 Dec 2024 13:01
Operator : JC/MD
Sample : P5322-17ME
Misc : 4.58g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YE631ME

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	10.775	14.0	ug/L	179362	2	10.055	640663	50.0
Benzene, 1-ethy...	11.616	11.2	ug/L	171486	3	12.024	764979	50.0
(DEL) Alkane: S...	12.421	21.9	ug/L	334277	3	12.024	764979	50.0
(DEL) Alkane: S...	13.268	6.7	ug/L	102560	3	12.024	764979	50.0
Azulene	13.774	23.3	ug/L	355812	3	12.024	764979	50.0
(DEL) Alkane: S...	14.036	5.3	ug/L	81625	3	12.024	764979	50.0