LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042407.D
Acq On : 19 Jul 2024 17:19
Operator : JC/MD
Sample : P3215-14MERE
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31MERE

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\SFAMXLM070324WMA.M
Title : VOC Analysis

Signal : TIC: VX042407.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	21	25	27	rBV	45861	53392	24.98%	2.705%
2	1.368	43	46	48	rBV2	6265	7857	3.68%	0.398%
3	2.276	189	195	204	rBV	26377	48010	22.46%	2.432%
4	2.721	262	268	274	rBV	7988	18459	8.64%	0.935%
5	2.947	298	305	316	rVB	7796	19753	9.24%	1.001%
6	3.068	320	325	331	rVB5	1302	3068	1.44%	0.155%
7	3.416	377	382	390	rVB4	1046	2167	1.01%	0.110%
8	3.855	444	454	459	rBV4	962	2853	1.33%	0.145%
9	4.276	517	523	533	rVB3	1774	4416	2.07%	0.224%
10	4.507	552	561	576	rBV	9052	35412	16.57%	1.794%
11	5.056	640	651	667	rVV2	24681	78568	36.76%	3.980%
12	5.452	708	716	727	rVB6	2742	9482	4.44%	0.480%
13	5.544	727	731	734	rBV2	544	969	0.45%	0.049%
14	5.806	773	774	783	rVB4	825	1377	0.64%	0.070%
15	5.958	789	799	818	rBV3	74406	213711	100.00%	10.826%
16	6.239	840	845	850	rVB4	560	1189	0.56%	0.060%
17	6.348	855	863	864	rBV3	1386	2513	1.18%	0.127%
18	6.611	899	906	908	rBV3	716	1318	0.62%	0.067%
19	6.678	911	917	919	rBV3	333	647	0.30%	0.033%
20	6.757	921	930	947	rBV2	55649	136976	64.09%	6.939%
21	7.141	989	993	999	rVB4	717	1553	0.73%	0.079%
22	7.226	999	1007	1012	rBV4	2007	4917	2.30%	0.249%
23	7.306	1013	1020	1026	rBV	39711	88018	41.19%	4.459%
24	7.647	1072	1076	1082	rVB3	714	1180	0.55%	0.060%
25	7.763	1091	1095	1101	rVV2	1096	1722	0.81%	0.087%
26	7.964	1122	1128	1138	rVV5	1041	2668	1.25%	0.135%
27	8.330	1182	1188	1200	rBV	20066	36214	16.95%	1.834%
28	8.433	1202	1205	1207	rVB2	678	766	0.36%	0.039%
29	8.592	1227	1231	1234	rBV2	2536	4290	2.01%	0.217%
30	8.647	1234	1240	1248	rVV	109011	171884	80.43%	8.707%
31	8.720	1248	1252	1257	rVV2	5937	9502	4.45%	0.481%
32	8.842	1270	1272	1276	rVB2	911	1001	0.47%	0.051%
33	8.909	1279	1283	1286	rBV2	1801	2407	1.13%	0.122%
34	8.958	1286	1291	1301	rVB	13995	26385	12.35%	1.337%
35	9.098	1308	1314	1322	rVB6	1272	2601	1.22%	0.132%
36	9.275	1338	1343	1347	rBV3	2410	3770	1.76%	0.191%

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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31MERE

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\SFAMXLM070324WMA.M
Title : VOC Analysis

37	9.397	1357	1363	1376	rBV2	36184	86515	40.48%	4.383%
38	9.610	1394	1398	1404	rBV5	2007	3537	1.66%	0.179%
39	9.714	1412	1415	1419	rVB4	1092	1412	0.66%	0.072%
40	9.817	1427	1432	1438	rVB4	1756	2971	1.39%	0.151%
41	9.903	1443	1446	1449	rVB3	846	968	0.45%	0.049%
42	10.055	1466	1471	1482	rBV	114333	158845	74.33%	8.047%
43	10.201	1491	1495	1500	rBV	2821	3811	1.78%	0.193%
44	10.305	1504	1512	1517	rBV	10429	17027	7.97%	0.863%
45	10.585	1555	1558	1563	rVV3	976	1471	0.69%	0.075%
46	10.646	1563	1568	1574	rVB	8712	13026	6.10%	0.660%
47	10.780	1581	1590	1593	rBV4	2263	4230	1.98%	0.214%
48	10.854	1599	1602	1605	rBV2	1717	2121	0.99%	0.107%
49	10.890	1605	1608	1613	rVB4	2231	3519	1.65%	0.178%
50	10.963	1616	1620	1625	rBV	2201	3019	1.41%	0.153%
51	11.030	1628	1631	1635	rVB2	1042	1230	0.58%	0.062%
52	11.085	1635	1640	1641	rBV3	798	954	0.45%	0.048%
53	11.195	1652	1658	1665	rVV	76492	104751	49.02%	5.306%
54	11.305	1672	1676	1680	rBV3	2345	2980	1.39%	0.151%
55	11.378	1685	1688	1694	rVV3	2297	3813	1.78%	0.193%
56	11.445	1694	1699	1702	rVV4	2769	6077	2.84%	0.308%
57	11.475	1702	1704	1714	rVB3	4866	7149	3.35%	0.362%
58	11.616	1722	1727	1732	rBV2	2126	3026	1.42%	0.153%
59	11.713	1739	1743	1745	rBV3	3445	4354	2.04%	0.221%
60	11.756	1747	1750	1759	rVB3	9425	16959	7.94%	0.859%
61	11.866	1763	1768	1769	rBV4	1104	1636	0.77%	0.083%
62	11.945	1777	1781	1784	rBV4	1763	2286	1.07%	0.116%
63	12.024	1789	1794	1801	rBV	120077	155875	72.94%	7.896%
64	12.164	1815	1817	1823	rVB4	727	1140	0.53%	0.058%
65	12.268	1831	1834	1837	rVB2	769	819	0.38%	0.041%
66	12.323	1837	1843	1851	rBV	116670	162058	75.83%	8.209%
67	12.427	1856	1860	1863	rVB2	4051	5250	2.46%	0.266%
68	12.542	1874	1879	1880	rBV4	691	1101	0.52%	0.056%
69	12.731	1905	1910	1913	rBV	800	1086	0.51%	0.055%
70	12.774	1913	1917	1919	rBV3	433	749	0.35%	0.038%
71	12.865	1928	1932	1933	rBV4	1292	1726	0.81%	0.087%
72	13.042	1957	1961	1965	rBV4	692	932	0.44%	0.047%
73	13.231	1988	1992	1993	rBV4	467	586	0.27%	0.030%
74	13.268	1994	1998	2006	rVB4	4756	7314	3.42%	0.371%
75	13.384	2013	2017	2019	rBV3	3779	5069	2.37%	0.257%
76	13.591	2046	2051	2054	rBV3	830	1495	0.70%	0.076%

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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
A4D31MERE

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Title : VOC Analysis

77	13.682	2063	2066	2067	rBV2	569	645	0.30%	0.033%
78	13.737	2071	2075	2077	rBV3	866	1039	0.49%	0.053%
79	13.780	2077	2082	2087	rBV	12242	17129	8.02%	0.868%
80	13.841	2089	2092	2097	rVB	4435	4983	2.33%	0.252%
81	14.036	2120	2124	2128	rVB2	4141	4707	2.20%	0.238%
82	14.103	2133	2135	2138	rBV2	379	551	0.26%	0.028%
83	14.426	2183	2188	2193	rBV	5875	8768	4.10%	0.444%
84	14.505	2198	2201	2208	rVB5	897	1941	0.91%	0.098%
85	14.560	2208	2210	2214	rBV4	497	585	0.27%	0.030%
86	14.609	2215	2218	2219	rVV2	1783	1599	0.75%	0.081%
87	14.640	2219	2223	2233	rVB	9890	15076	7.05%	0.764%
88	14.755	2238	2242	2243	rBV	3875	3988	1.87%	0.202%
89	14.780	2243	2246	2252	rVB	10642	14105	6.60%	0.715%
90	14.932	2268	2271	2275	rVB4	1876	2186	1.02%	0.111%
91	15.213	2313	2317	2320	rVB3	3078	4024	1.88%	0.204%
92	15.414	2346	2350	2355	rVB3	13223	20350	9.52%	1.031%
93	15.481	2357	2361	2368	rVB5	4052	7020	3.28%	0.356%
94	15.615	2380	2383	2386	rVB2	4012	4819	2.25%	0.244%
95	15.713	2395	2399	2400	rBV2	2813	4071	1.90%	0.206%
96	15.871	2421	2425	2429	rVB3	7770	11103	5.20%	0.562%
97	15.987	2440	2444	2447	rBV5	7376	11324	5.30%	0.574%
98	16.023	2447	2450	2456	rVB4	12142	19164	8.97%	0.971%
99	16.091	2458	2461	2467	rVB3	3660	5947	2.78%	0.301%
100	16.273	2487	2491	2495	rBV4	2979	5030	2.35%	0.255%

Sum of corrected areas: 1974056

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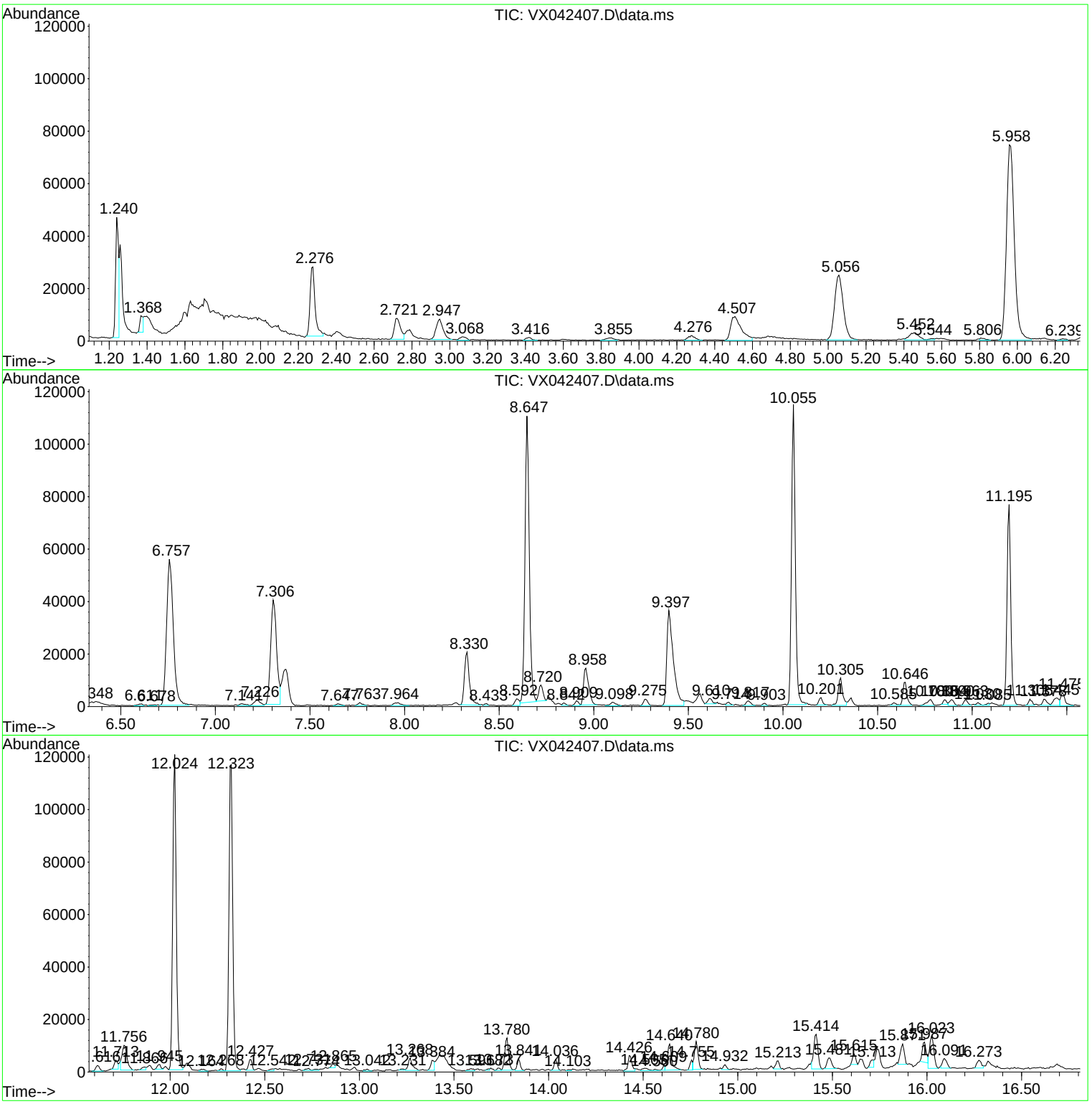
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31MERE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
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Instrument :
MSVOA_X
ClientSampleId :
A4D31MERE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

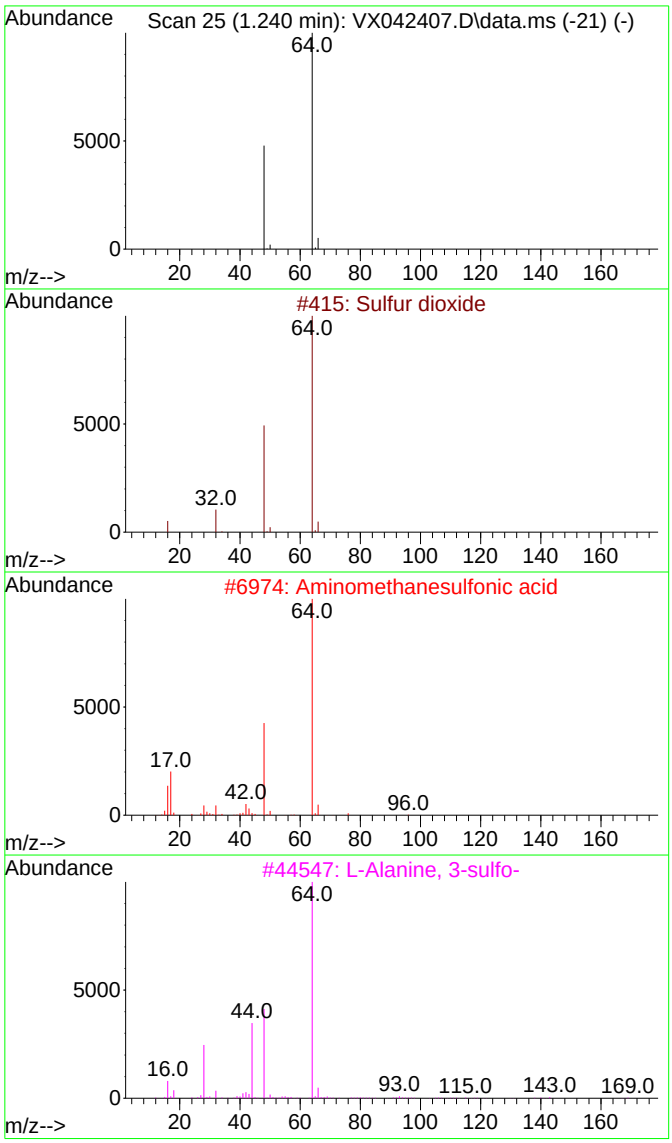
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

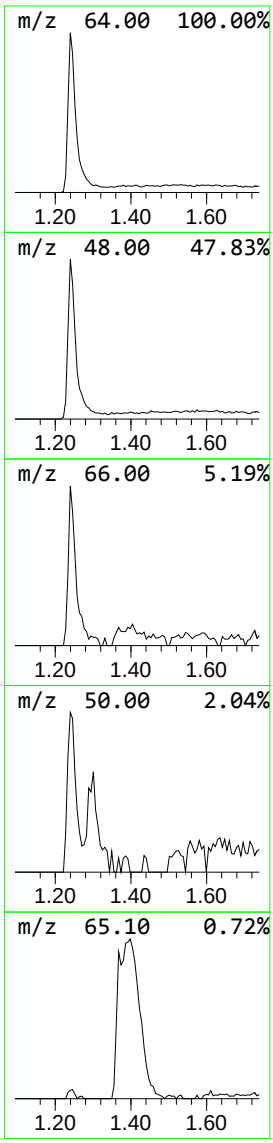
****

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	19.49 ug/L	53392	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Sulfur dioxide	64	O2S	007446-09-5	5
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042407.D
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Sample : P3215-14MERE
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31MERE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

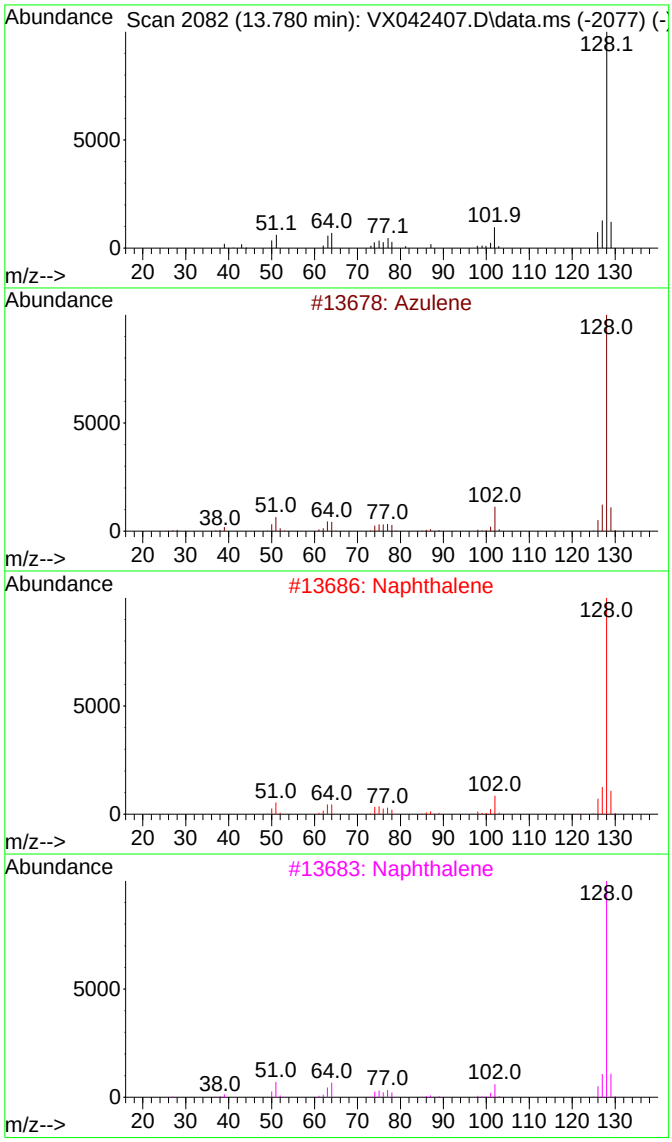
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

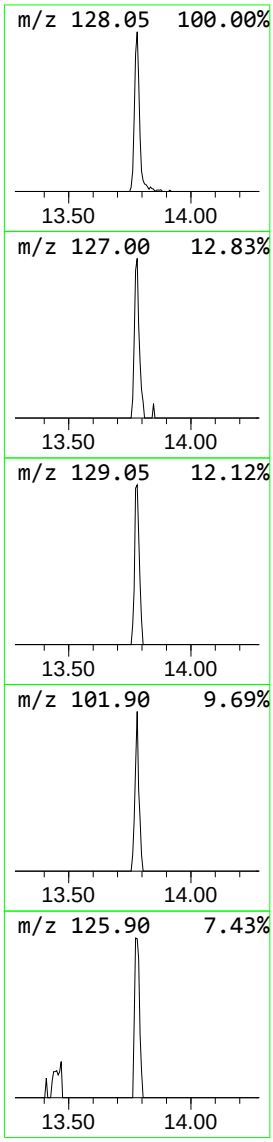
****

Peak Number 4 Azulene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	5.49 ug/L	17129	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azulene	128	C10H8	000275-51-4	95
2	Naphthalene	128	C10H8	000091-20-3	95
3	Naphthalene	128	C10H8	000091-20-3	95
4	Naphthalene	128	C10H8	000091-20-3	94
5	Azulene	128	C10H8	000275-51-4	91





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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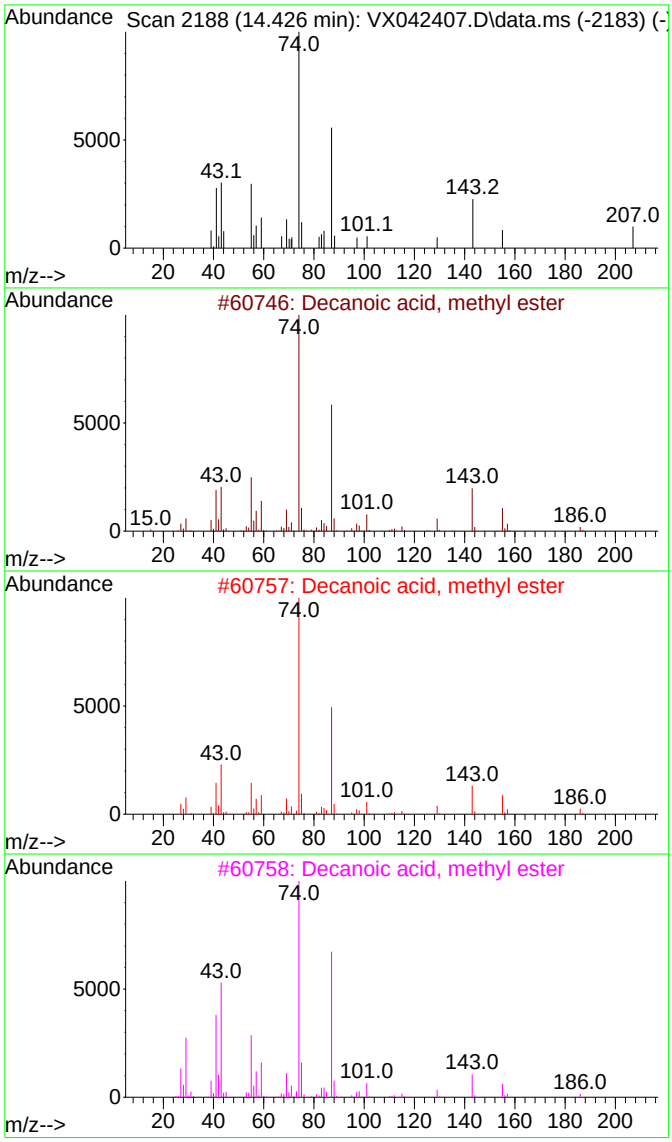
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

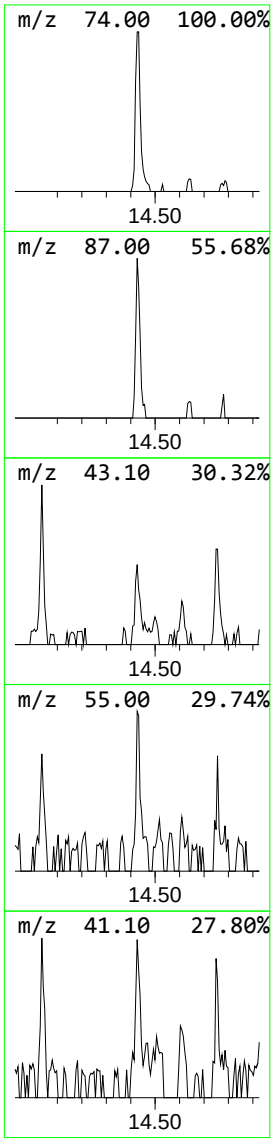
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Decanoic acid, methyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.426	2.81 ug/L	8768	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	86
2	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	72
3	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	72
4	Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	64
5	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	64





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31MERE

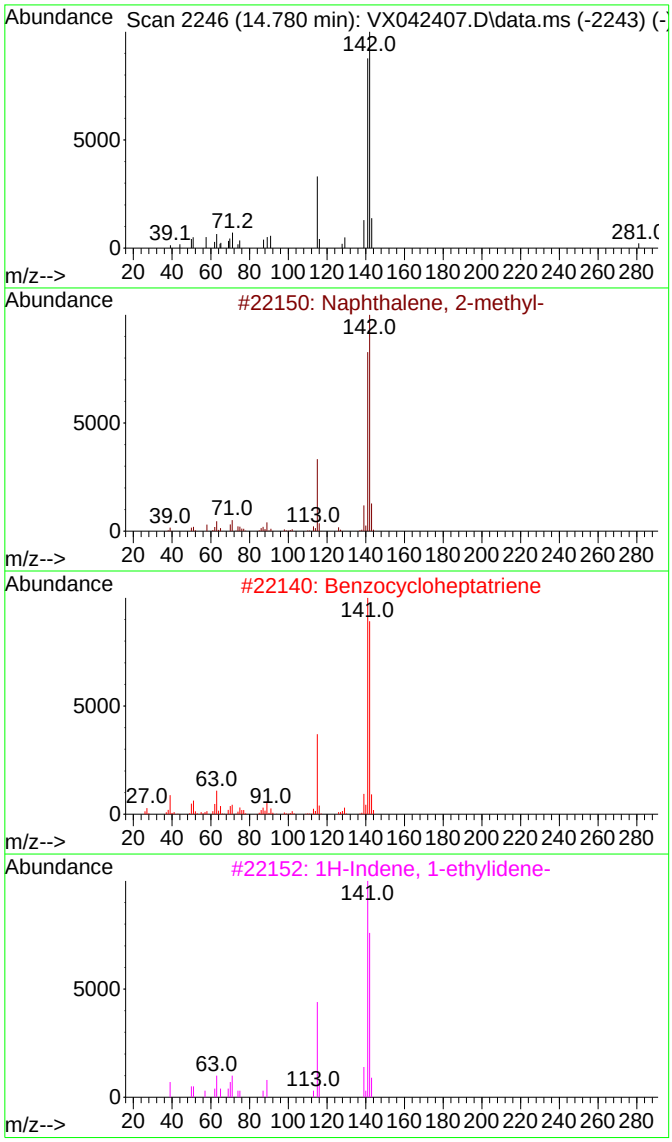
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

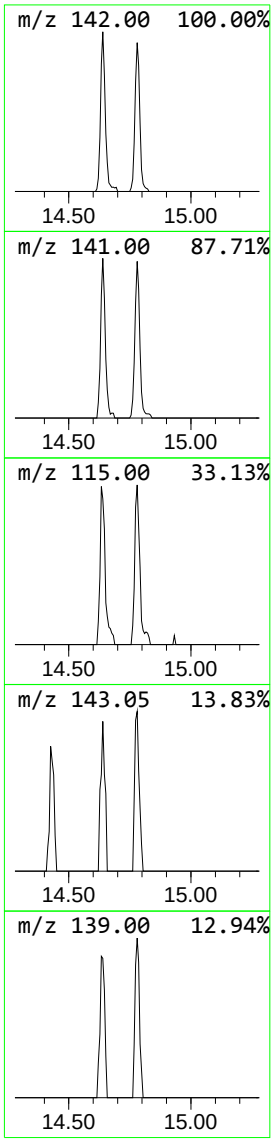
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 1-ethylidene- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	4.52 ug/L	14105	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
2	Benzocycloheptatriene	142	C11H10	000264-09-5	91
3	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91
4	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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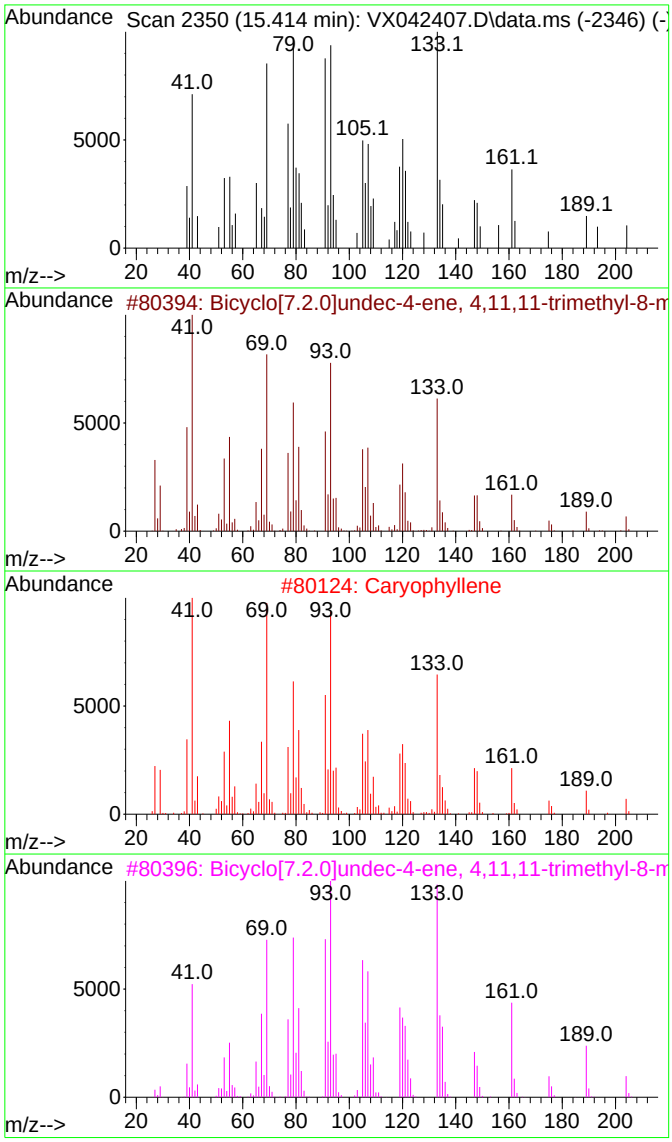
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

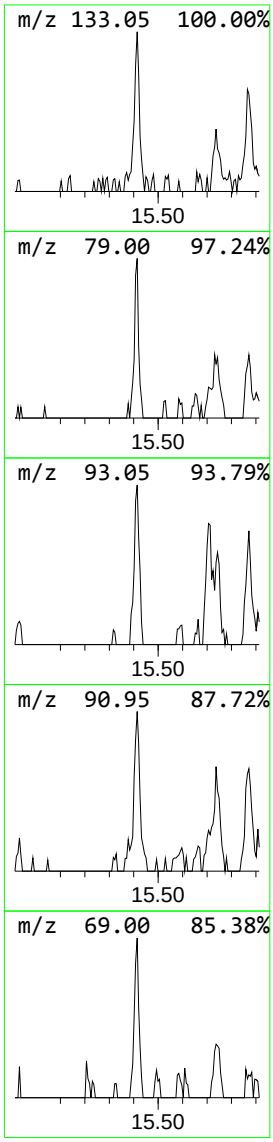
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Bicyclo[7.2.0]undec-4-ene, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	6.53 ug/L	20350	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	93
2	Caryophyllene	204	C15H24	000087-44-5	90
3	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	89
4	Caryophyllene	204	C15H24	000087-44-5	89
5	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	76





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042407.D
Acq On : 19 Jul 2024 17:19
Operator : JC/MD
Sample : P3215-14MERE
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31MERE

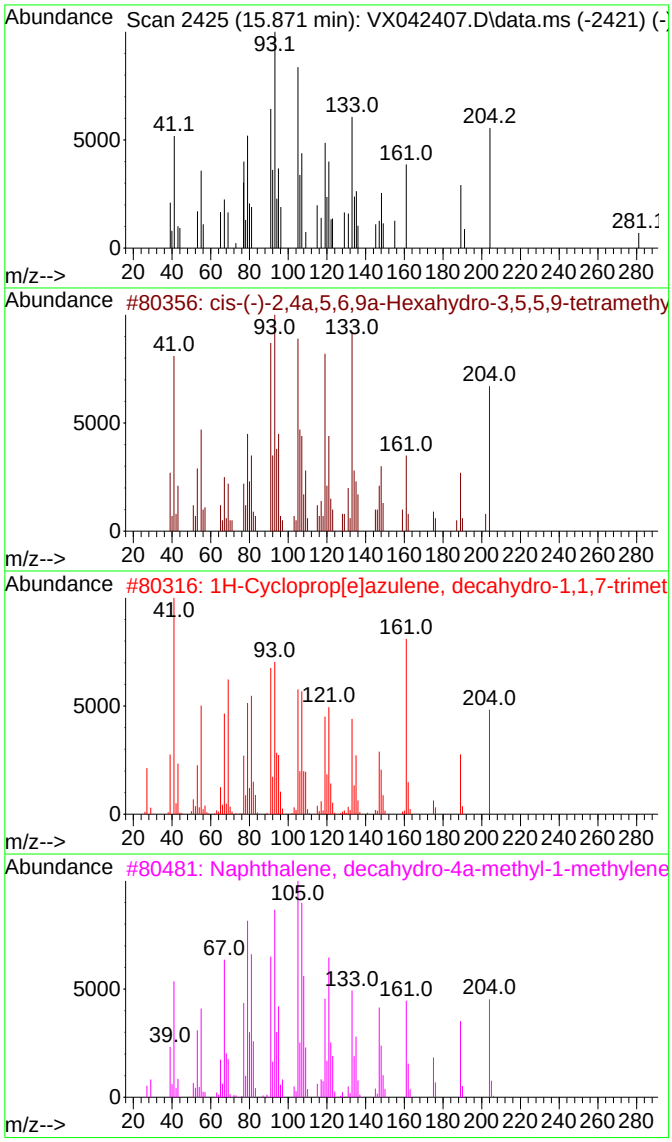
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

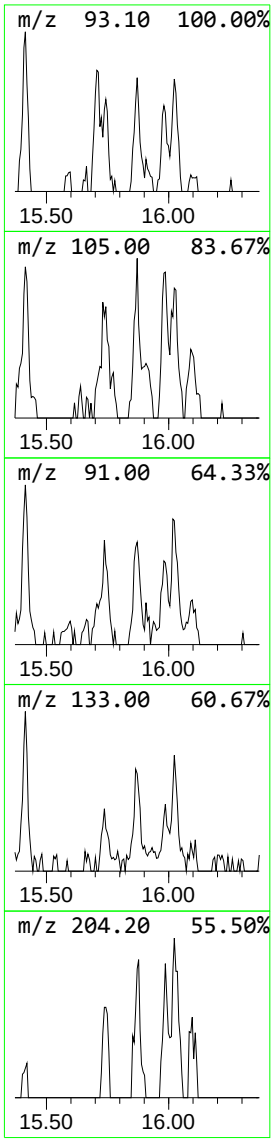
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 cis-(-)-2,4a,5,6,9a-Hexahyd... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.871	3.56 ug/L	11103	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-(-)-2,4a,5,6,9a-Hexahydro-3,...	204	C15H24	1000104-20-1	92
2	1H-Cycloprop[e]azulene, decahydr...	204	C15H24	072747-25-2	86
3	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	74
4	(4aS,9aR)-3,5,5,9-Tetramethyl-2,...	204	C15H24	053111-25-4	74
5	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042407.D
Acq On : 19 Jul 2024 17:19
Operator : JC/MD
Sample : P3215-14MERE
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31MERE

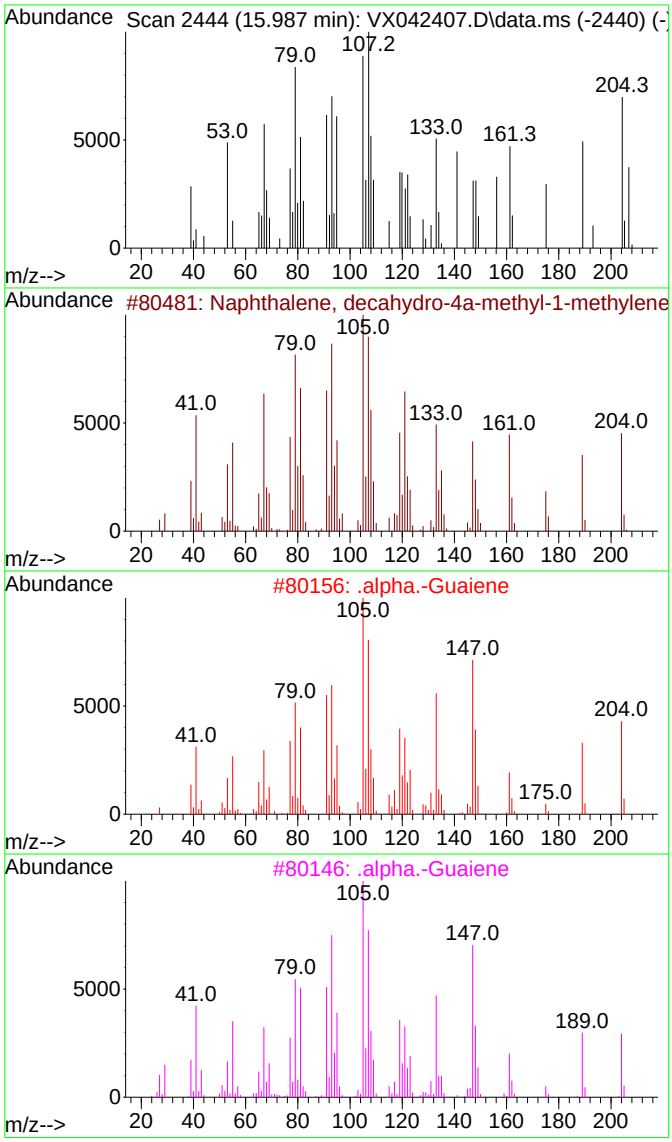
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

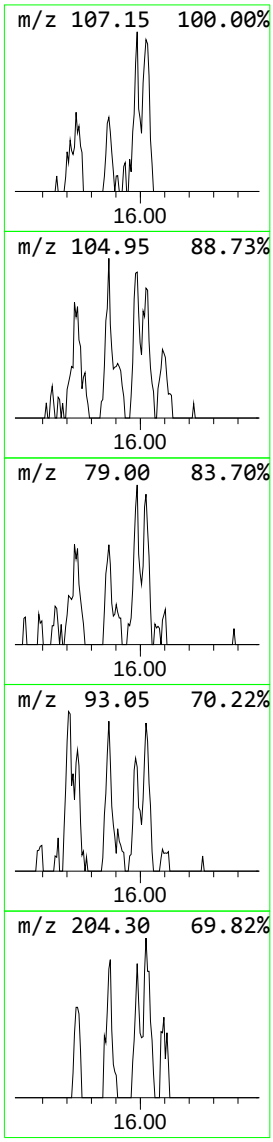
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, decahydro-4a-m... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.987	3.63 ug/L	11324	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	87
2	.alpha.-Guaiene	204	C15H24	003691-12-1	64
3	.alpha.-Guaiene	204	C15H24	003691-12-1	64
4	Azulene, 1,2,3,3a,4,5,6,7-octahy...	204	C15H24	022567-17-5	60
5	1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	55





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042407.D
Acq On : 19 Jul 2024 17:19
Operator : JC/MD
Sample : P3215-14MERE
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31MERE

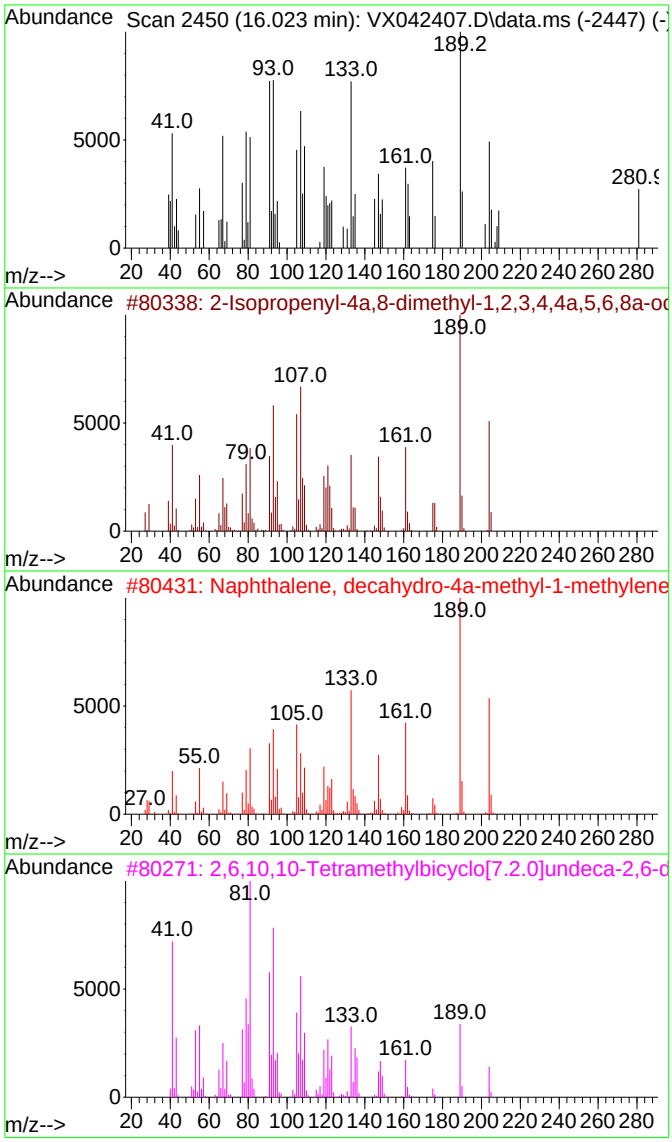
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

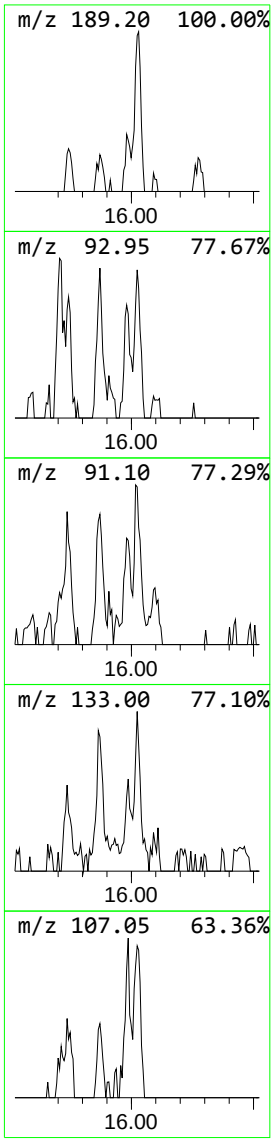
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 2-Isopropenyl-4a,8-dimethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.023	6.15 ug/L	19164	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	98
2	Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	93
3	2,6,10,10-Tetramethylbicyclo[7.2...	204	C15H24	136296-37-2	90
4	4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	90
5	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
Data File : VX042407.D
Acq On : 19 Jul 2024 17:19
Operator : JC/MD
Sample : P3215-14MERE
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31MERE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.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
Sulfur dioxide	1.240	19.5	ug/L	53392	1	6.757	136976	50.0
Azulene	13.780	5.5	ug/L	17129	3	12.024	155875	50.0
Decanoic acid, ...	14.426	2.8	ug/L	8768	3	12.024	155875	50.0
1H-Indene, 1-et...	14.780	4.5	ug/L	14105	3	12.024	155875	50.0
Bicyclo[7.2.0]u...	15.414	6.5	ug/L	20350	3	12.024	155875	50.0
cis-(-)-2,4a,5,...	15.871	3.6	ug/L	11103	3	12.024	155875	50.0
Naphthalene, de...	15.987	3.6	ug/L	11324	3	12.024	155875	50.0
2-Isopropenyl-4...	16.023	6.2	ug/L	19164	3	12.024	155875	50.0