LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025655.D
Acq On : 09 Dec 2021 13:08
Operator : JC/MD
Sample : M4884-16ME
Misc : 2.91g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K2ME

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: VX025655.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	54	rVB	28820	33290	0.28%	0.199%
2	1.648	89	92	97	rVB	22570	26068	0.22%	0.156%
3	2.282	190	196	206	rVB	54174	91158	0.76%	0.545%
4	2.367	206	210	215	rBV2	1611	3063	0.03%	0.018%
5	2.727	264	269	270	rBV2	2452	3705	0.03%	0.022%
6	3.081	321	327	336	rVV2	9734	20300	0.17%	0.121%
7	3.428	378	384	390	rVV3	2576	5712	0.05%	0.034%
8	4.202	505	511	515	rBV4	818	1725	0.01%	0.010%
9	4.288	518	525	535	rVB3	3399	8969	0.07%	0.054%
10	4.489	547	558	581	rBV	141574	426893	3.56%	2.550%
11	5.068	642	653	669	rVV3	40763	147216	1.23%	0.879%
12	5.464	708	718	731	rVV5	8960	33177	0.28%	0.198%
13	5.611	735	742	752	rVB3	2764	8876	0.07%	0.053%
14	5.824	768	777	788	rBV6	2986	9293	0.08%	0.056%
15	5.970	790	801	817	rBV2	105904	309507	2.58%	1.849%
16	6.147	825	830	840	rVB5	1606	4886	0.04%	0.029%
17	6.251	842	847	855	rVV2	1460	3366	0.03%	0.020%
18	6.361	856	865	874	rVV5	4480	14124	0.12%	0.084%
19	6.604	900	905	913	rVB5	3840	9157	0.08%	0.055%
20	6.763	922	931	945	rBV	123173	319031	2.66%	1.906%
21	7.135	980	992	1014	rVV	5451681	11977352	100.00%	71.552%
22	7.312	1015	1021	1027	rVV	62816	150199	1.25%	0.897%
23	7.379	1028	1032	1042	rVB	56651	115919	0.97%	0.692%
24	7.488	1048	1050	1057	rVB3	1051	1732	0.01%	0.010%
25	7.659	1073	1078	1083	rVB4	1571	2628	0.02%	0.016%
26	7.775	1091	1097	1102	rVB5	2808	5307	0.04%	0.032%
27	7.952	1120	1126	1134	rVB6	3079	6393	0.05%	0.038%
28	8.189	1160	1165	1168	rBV4	1654	3008	0.03%	0.018%
29	8.220	1168	1170	1174	rVV4	1464	2279	0.02%	0.014%
30	8.275	1174	1179	1182	rVV	5863	9418	0.08%	0.056%
31	8.330	1182	1188	1201	rVB	41978	77883	0.65%	0.465%
32	8.439	1201	1206	1209	rBV2	2006	3173	0.03%	0.019%
33	8.598	1225	1232	1235	rBV2	9921	18145	0.15%	0.108%
34	8.653	1235	1241	1248	rVV	140180	241231	2.01%	1.441%
35	8.720	1248	1252	1257	rVV	15325	24230	0.20%	0.145%
36	8.769	1257	1260	1265	rVB3	2837	4581	0.04%	0.027%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025655.D
Acq On : 09 Dec 2021 13:08
Operator : JC/MD
Sample : M4884-16ME
Misc : 2.91g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K2ME

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

37	8.848	1270	1273	1279	rVB4	1947	2673	0.02%	0.016%
38	8.909	1279	1283	1286	rBV	6664	9987	0.08%	0.060%
39	8.958	1286	1291	1301	rVB2	32547	69762	0.58%	0.417%
40	9.104	1309	1315	1318	rBV3	2876	4451	0.04%	0.027%
41	9.159	1318	1324	1333	rVB	61542	108494	0.91%	0.648%
42	9.275	1337	1343	1354	rVB	238346	355958	2.97%	2.126%
43	9.397	1356	1363	1376	rBV	110476	184566	1.54%	1.103%
44	9.506	1378	1381	1386	rVB5	2504	4020	0.03%	0.024%
45	9.561	1386	1390	1395	rVB2	10125	15221	0.13%	0.091%
46	9.622	1395	1400	1403	rBV	7700	11949	0.10%	0.071%
47	9.762	1418	1423	1426	rBV3	1154	1840	0.02%	0.011%
48	9.817	1427	1432	1439	rBV3	8776	14842	0.12%	0.089%
49	9.909	1442	1447	1452	rVB2	3351	4804	0.04%	0.029%
50	10.006	1460	1463	1466	rBV2	2302	3203	0.03%	0.019%
51	10.061	1466	1472	1481	rBV	245823	371991	3.11%	2.222%
52	10.195	1489	1494	1501	rVB	2794	4251	0.04%	0.025%
53	10.305	1503	1512	1517	rVV	30851	50039	0.42%	0.299%
54	10.360	1517	1521	1531	rVB	12003	17457	0.15%	0.104%
55	10.591	1551	1559	1563	rVV8	4148	8718	0.07%	0.052%
56	10.646	1563	1568	1577	rVV	19872	28786	0.24%	0.172%
57	10.780	1587	1590	1594	rVB3	9890	12798	0.11%	0.076%
58	10.860	1598	1603	1606	rVV3	6677	10614	0.09%	0.063%
59	10.896	1606	1609	1614	rVB	9941	13114	0.11%	0.078%
60	10.963	1614	1620	1623	rBV3	1755	3079	0.03%	0.018%
61	11.030	1628	1631	1636	rVB4	3752	5533	0.05%	0.033%
62	11.110	1641	1644	1651	rVB5	3909	7255	0.06%	0.043%
63	11.195	1653	1658	1668	rVB	145223	191884	1.60%	1.146%
64	11.305	1671	1676	1680	rBV4	2981	5072	0.04%	0.030%
65	11.384	1685	1689	1695	rVB4	6982	10938	0.09%	0.065%
66	11.457	1695	1701	1702	rBV	7319	10544	0.09%	0.063%
67	11.475	1702	1704	1710	rVB	16422	19669	0.16%	0.118%
68	11.616	1722	1727	1733	rBV3	4469	7133	0.06%	0.043%
69	11.719	1740	1744	1746	rBV	15622	18722	0.16%	0.112%
70	11.756	1746	1750	1759	rVB	22529	30688	0.26%	0.183%
71	11.860	1760	1767	1769	rBV6	2088	4174	0.03%	0.025%
72	12.024	1789	1794	1800	rBV	317366	391681	3.27%	2.340%
73	12.091	1801	1805	1811	rVB2	11028	18358	0.15%	0.110%
74	12.268	1832	1834	1837	rVB3	1985	1863	0.02%	0.011%
75	12.323	1837	1843	1850	rBV	207642	268193	2.24%	1.602%
76	12.427	1855	1860	1864	rBV	20877	25672	0.21%	0.153%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025655.D
Acq On : 09 Dec 2021 13:08
Operator : JC/MD
Sample : M4884-16ME
Misc : 2.91g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K2ME

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

77	12.683	1899	1902	1904	rBV3	1501	1670	0.01%	0.010%
78	12.719	1905	1908	1912	rVB3	2442	3461	0.03%	0.021%
79	12.890	1932	1936	1939	rBV5	3367	4833	0.04%	0.029%
80	12.975	1946	1950	1956	rVB4	7710	11170	0.09%	0.067%
81	13.036	1956	1960	1965	rBV4	2914	4780	0.04%	0.029%
82	13.268	1994	1998	2006	rVB2	21814	29087	0.24%	0.174%
83	13.384	2013	2017	2022	rBV	12727	16774	0.14%	0.100%
84	13.628	2054	2057	2062	rVB4	2362	3583	0.03%	0.021%
85	13.774	2077	2081	2088	rVB	31310	42569	0.36%	0.254%
86	13.847	2088	2093	2097	rVB	23674	27769	0.23%	0.166%
87	14.042	2120	2125	2128	rBV	20724	22885	0.19%	0.137%
88	14.505	2197	2201	2208	rVB5	5391	8980	0.07%	0.054%
89	14.572	2208	2212	2214	rBV4	1289	1921	0.02%	0.011%
90	14.615	2215	2219	2220	rBV	8772	9465	0.08%	0.057%
91	14.640	2220	2223	2227	rVB	20402	24102	0.20%	0.144%
92	14.755	2239	2242	2244	rBV	11496	14684	0.12%	0.088%
93	14.780	2244	2246	2252	rVB	21841	26363	0.22%	0.157%
94	14.847	2254	2257	2264	rVB5	2893	4239	0.04%	0.025%
95	15.213	2314	2317	2321	rVB3	9316	12297	0.10%	0.073%
96	15.377	2340	2344	2347	rBV4	1774	2539	0.02%	0.015%
97	15.615	2378	2383	2387	rBV2	3606	6205	0.05%	0.037%
98	15.749	2402	2405	2411	rVB4	1258	2069	0.02%	0.012%
99	16.383	2504	2509	2515	rVB4	1342	2542	0.02%	0.015%
100	16.706	2558	2562	2567	rVB6	1228	2318	0.02%	0.014%

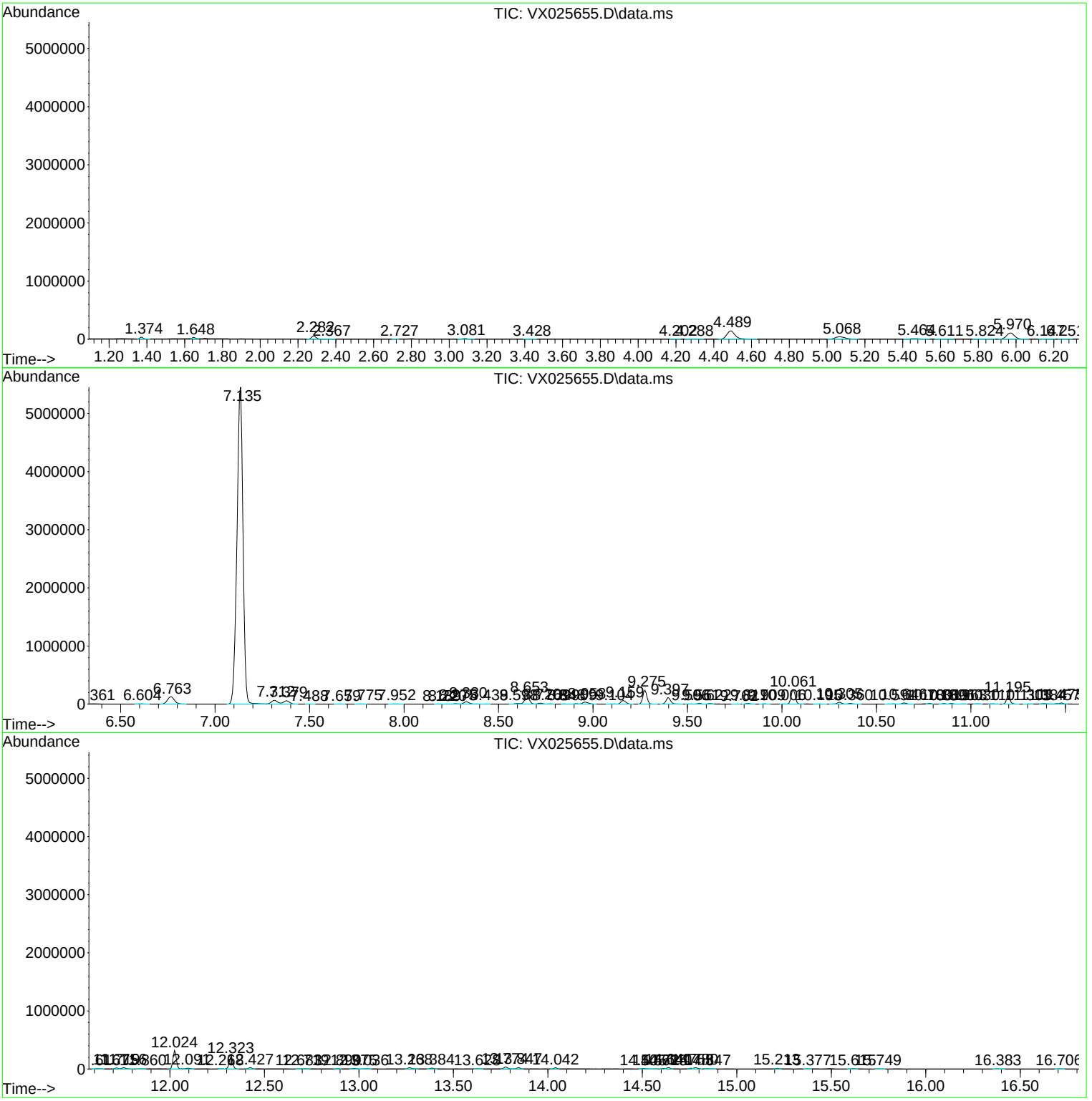
Sum of corrected areas: 16739295

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025655.D
Acq On : 09 Dec 2021 13:08
Operator : JC/MD
Sample : M4884-16ME
Misc : 2.91g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K2ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025655.D
Acq On : 09 Dec 2021 13:08
Operator : JC/MD
Sample : M4884-16ME
Misc : 2.91g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K2ME

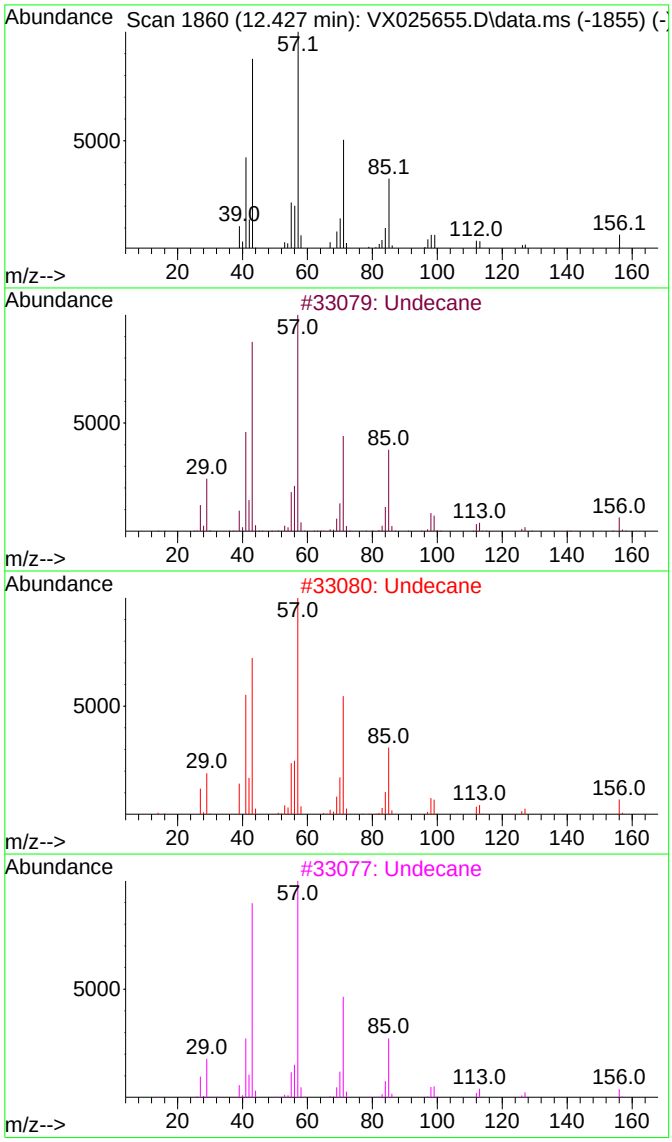
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

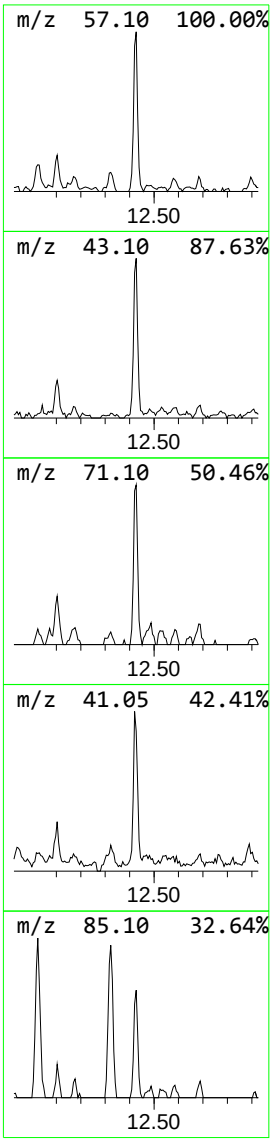
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	3.28 ug/L	25672	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	97
2	Undecane	156	C11H24	001120-21-4	96
3	Undecane	156	C11H24	001120-21-4	95
4	Undecane	156	C11H24	001120-21-4	91
5	Tetradecane	198	C14H30	000629-59-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025655.D
Acq On : 09 Dec 2021 13:08
Operator : JC/MD
Sample : M4884-16ME
Misc : 2.91g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K2ME

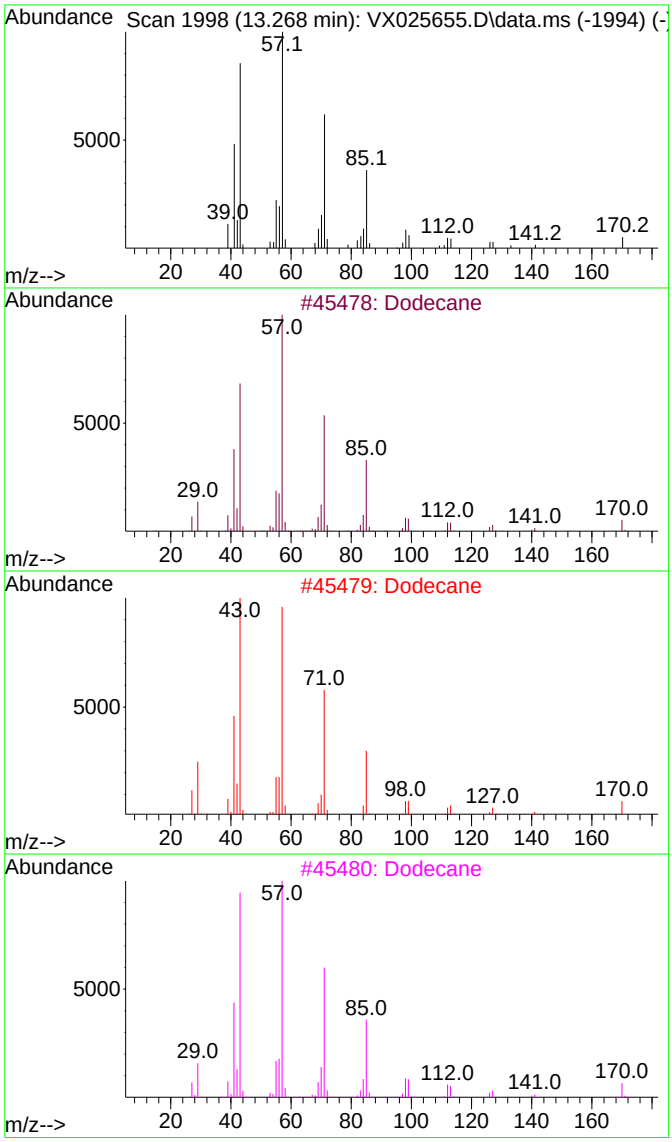
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

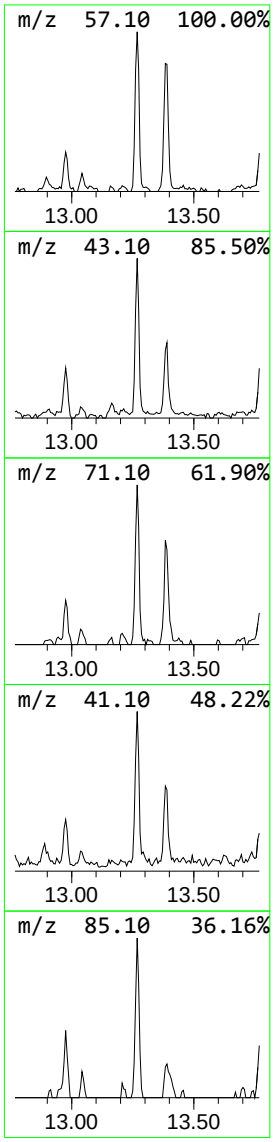
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	3.71 ug/L	29087	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	96
2	Dodecane	170	C12H26	000112-40-3	95
3	Dodecane	170	C12H26	000112-40-3	94
4	Undecane	156	C11H24	001120-21-4	86
5	Hexadecane	226	C16H34	000544-76-3	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025655.D
Acq On : 09 Dec 2021 13:08
Operator : JC/MD
Sample : M4884-16ME
Misc : 2.91g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K2ME

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

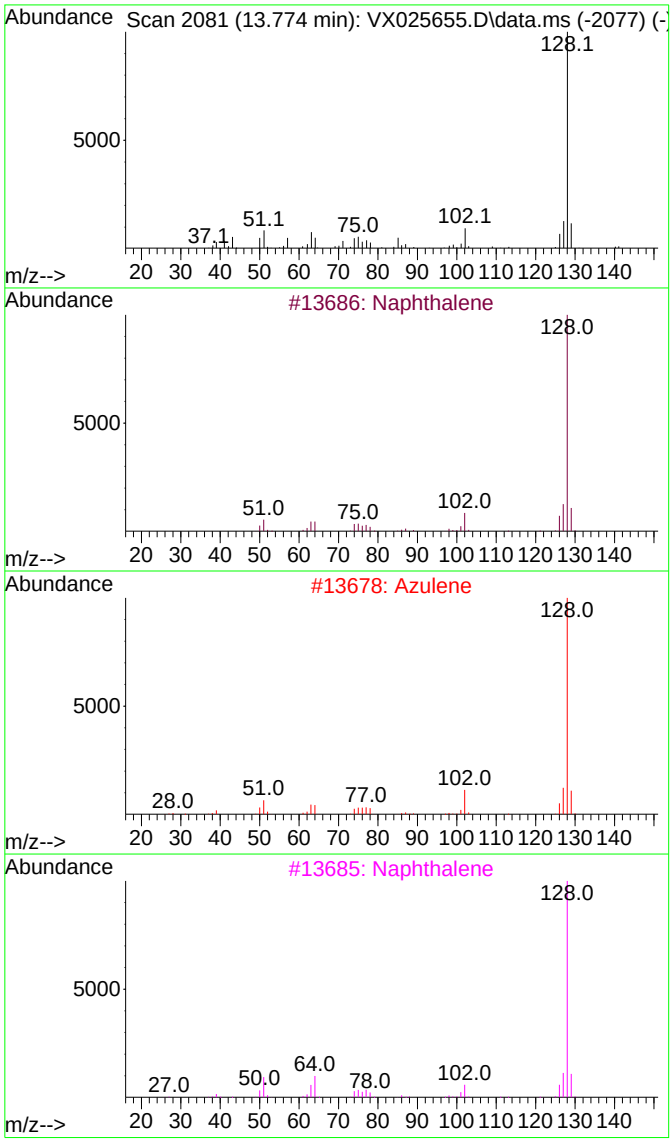
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

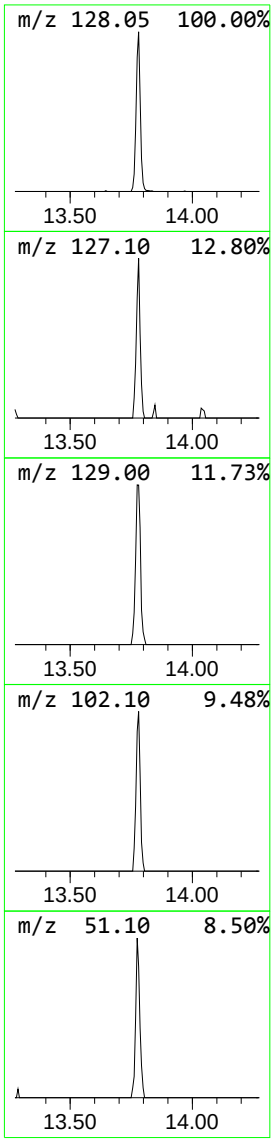
****

Peak Number 4 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	5.43 ug/L	42569	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	94
2	Azulene	128	C10H8	000275-51-4	93
3	Naphthalene	128	C10H8	000091-20-3	91
4	Azulene	128	C10H8	000275-51-4	90
5	Azulene	128	C10H8	000275-51-4	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025655.D
Acq On : 09 Dec 2021 13:08
Operator : JC/MD
Sample : M4884-16ME
Misc : 2.91g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K2ME

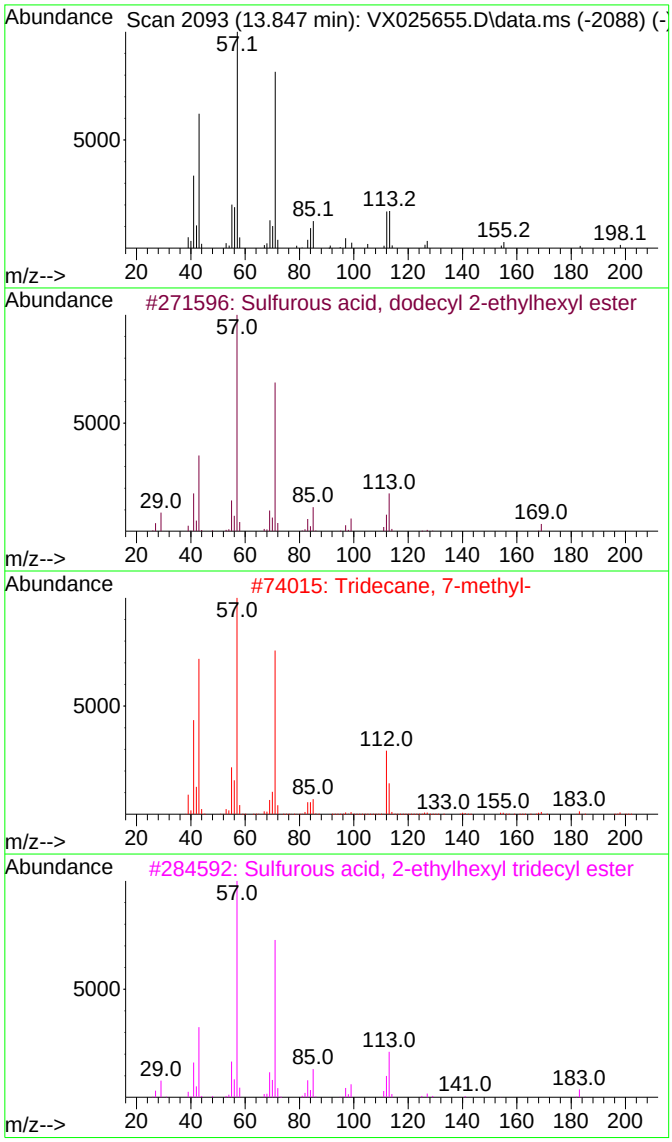
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

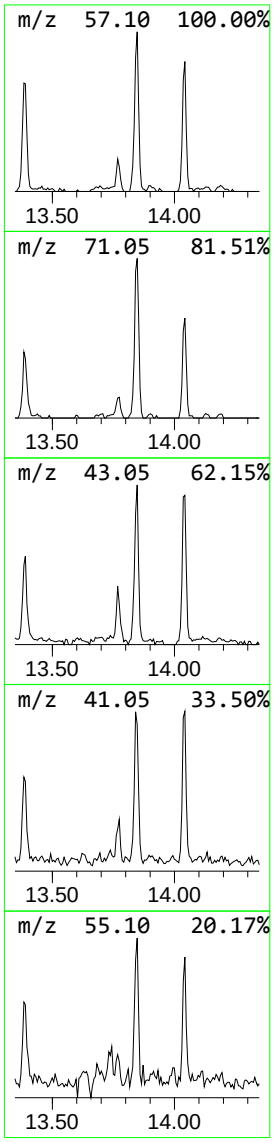
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Sulfurous acid, dodecyl 2-e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.847	3.54 ug/L	27769	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	86
2	Tridecane, 7-methyl-	198	C14H30	026730-14-3	86
3	Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	86
4	1-Decene, 4-methyl-	154	C11H22	013151-29-6	81
5	Oxalic acid, 2-ethylhexyl nonyl ...	328	C19H36O4	1000309-39-2	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025655.D
Acq On : 09 Dec 2021 13:08
Operator : JC/MD
Sample : M4884-16ME
Misc : 2.91g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K2ME

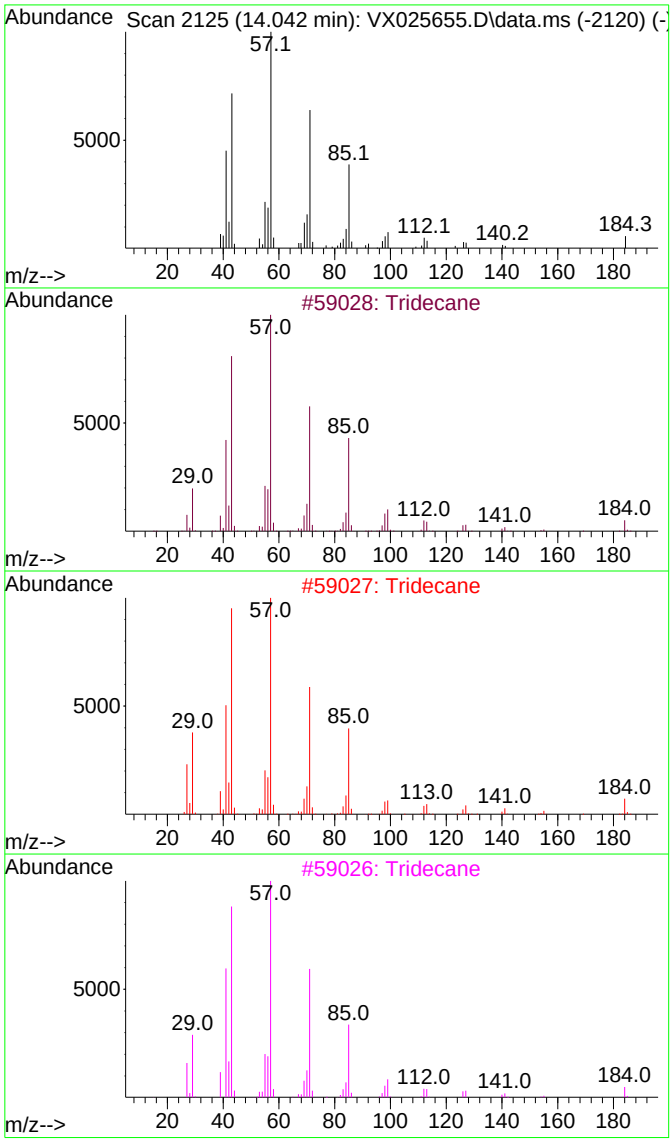
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

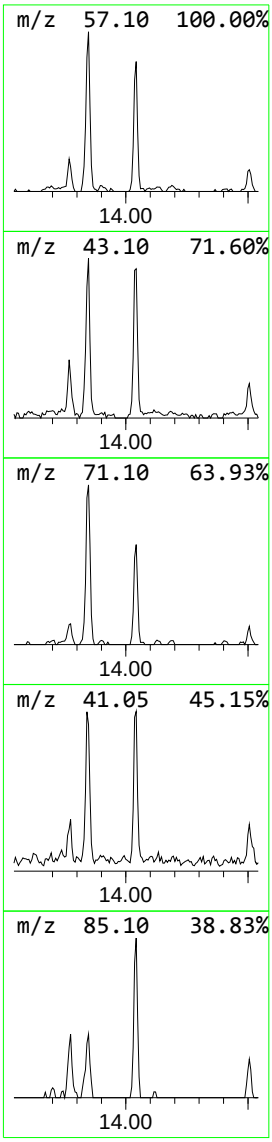
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.042	2.92 ug/L	22885	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	96
2	Tridecane	184	C13H28	000629-50-5	95
3	Tridecane	184	C13H28	000629-50-5	94
4	Tridecane	184	C13H28	000629-50-5	91
5	Tridecane	184	C13H28	000629-50-5	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025655.D
Acq On : 09 Dec 2021 13:08
Operator : JC/MD
Sample : M4884-16ME
Misc : 2.91g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K2ME

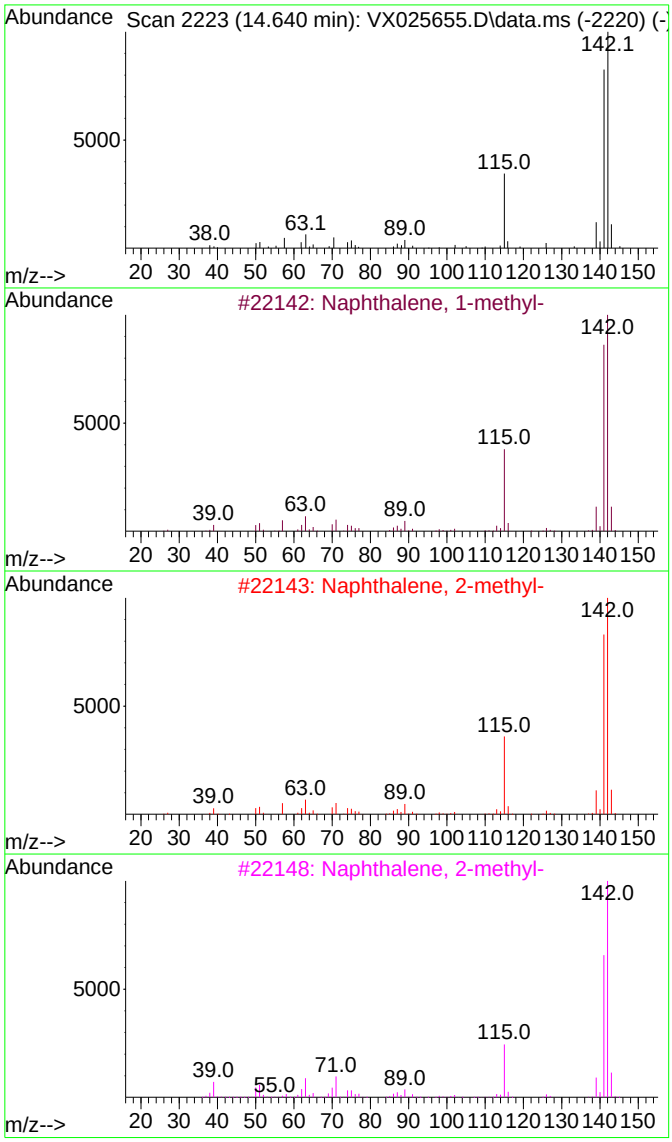
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

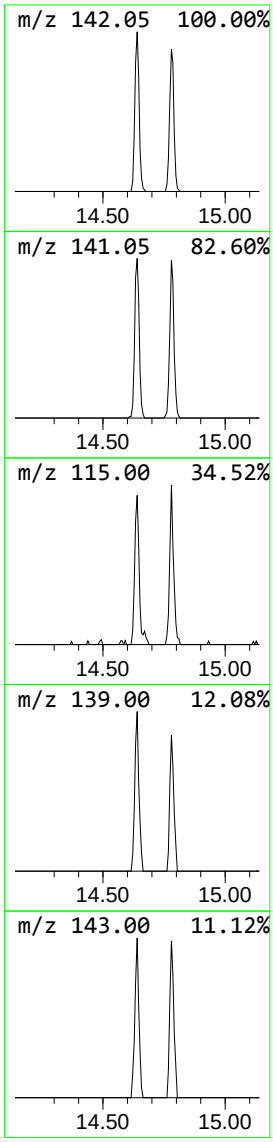
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	3.08 ug/L	24102	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
3	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
4	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025655.D
Acq On : 09 Dec 2021 13:08
Operator : JC/MD
Sample : M4884-16ME
Misc : 2.91g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K2ME

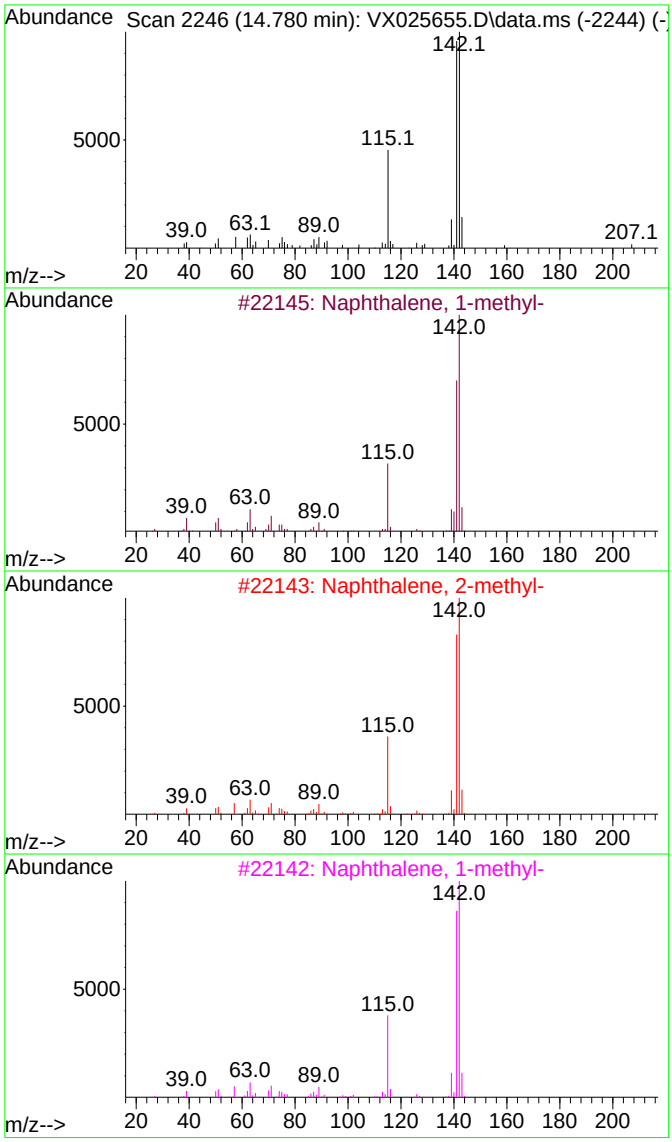
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

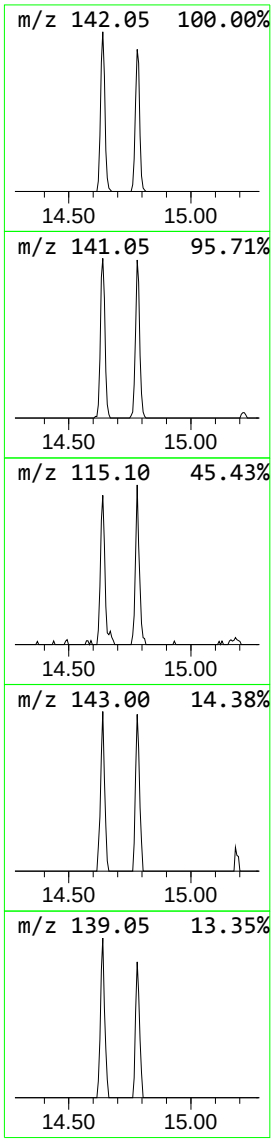
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	3.37 ug/L	26363	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
3	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
4	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025655.D
Acq On : 09 Dec 2021 13:08
Operator : JC/MD
Sample : M4884-16ME
Misc : 2.91g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K2ME

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	12.427	3.3	ug/L	25672	3	12.024	391681	50.0
(DEL) Alkane: S...	13.268	3.7	ug/L	29087	3	12.024	391681	50.0
Azulene	13.774	5.4	ug/L	42569	3	12.024	391681	50.0
Sulfurous acid,...	13.847	3.5	ug/L	27769	3	12.024	391681	50.0
(DEL) Alkane: S...	14.042	2.9	ug/L	22885	3	12.024	391681	50.0
Naphthalene, 1-...	14.640	3.1	ug/L	24102	3	12.024	391681	50.0
Naphthalene, 2-...	14.780	3.4	ug/L	26363	3	12.024	391681	50.0