LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
Data File : VX026019.D
Acq On : 24 Dec 2021 16:56
Operator : JC/MD
Sample : M5154-09DL 10X
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGL89DL

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\SFAMXLM122321WMA.M
Title : VOC Analysis

Signal : TIC: VX026019.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	53	rBV	110024	113699	12.92%	1.230%
2	1.654	89	93	102	rVB	89264	111970	12.73%	1.211%
3	2.306	194	200	211	rBV	190946	292779	33.28%	3.168%
4	2.794	275	280	283	rBV4	2451	4638	0.53%	0.050%
5	2.898	295	297	298	rBV	211	203	0.02%	0.002%
6	2.928	300	302	303	rBV	328	282	0.03%	0.003%
7	3.093	325	329	330	rBV2	972	1088	0.12%	0.012%
8	3.209	347	348	350	rBV	262	227	0.03%	0.002%
9	3.318	364	366	369	rBV2	203	256	0.03%	0.003%
10	3.446	381	387	392	rVB6	1441	2844	0.32%	0.031%
11	3.544	402	403	407	rVV2	254	207	0.02%	0.002%
12	3.806	445	446	449	rVB	313	267	0.03%	0.003%
13	4.276	520	523	524	rBV	323	277	0.03%	0.003%
14	4.294	524	526	527	rBV2	382	353	0.04%	0.004%
15	4.458	543	553	567	rBV	69134	206768	23.50%	2.237%
16	4.794	604	608	610	rBV2	181	242	0.03%	0.003%
17	4.818	610	612	614	rVB2	446	339	0.04%	0.004%
18	5.062	640	652	673	rVV	105375	348437	39.61%	3.770%
19	5.251	681	683	686	rBV	181	234	0.03%	0.003%
20	5.385	703	705	708	rBV2	250	328	0.04%	0.004%
21	5.477	717	720	721	rBV2	417	456	0.05%	0.005%
22	5.501	721	724	728	rVV5	788	1339	0.15%	0.014%
23	5.623	740	744	746	rVB3	417	514	0.06%	0.006%
24	5.970	789	801	816	rBV2	298060	879735	100.00%	9.518%
25	6.184	833	836	838	rBV2	334	357	0.04%	0.004%
26	6.354	858	864	867	rBV5	921	1737	0.20%	0.019%
27	6.482	881	885	887	rVV2	228	322	0.04%	0.003%
28	6.617	902	907	911	rVV4	989	1900	0.22%	0.021%
29	6.763	922	931	947	rBV	205195	485931	55.24%	5.257%
30	7.117	983	989	994	rVB4	1642	3371	0.38%	0.036%
31	7.190	999	1001	1002	rBV	230	212	0.02%	0.002%
32	7.312	1012	1021	1032	rBV	183025	402609	45.76%	4.356%
33	7.458	1042	1045	1046	rBV	274	255	0.03%	0.003%
34	7.488	1048	1050	1052	rVB2	479	331	0.04%	0.004%
35	7.568	1058	1063	1066	rBV3	469	506	0.06%	0.005%
36	7.769	1092	1096	1098	rBV	296	349	0.04%	0.004%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
Data File : VX026019.D
Acq On : 24 Dec 2021 16:56
Operator : JC/MD
Sample : M5154-09DL 10X
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGL89DL

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\SFAMXLM122321WMA.M
Title : VOC Analysis

37	7.897	1114	1117	1119	rBV2	295	305	0.03%	0.003%
38	8.049	1140	1142	1144	rVV2	466	531	0.06%	0.006%
39	8.068	1144	1145	1147	rVB	491	272	0.03%	0.003%
40	8.183	1161	1164	1169	rVV3	396	712	0.08%	0.008%
41	8.281	1175	1180	1182	rBV4	1286	2301	0.26%	0.025%
42	8.324	1182	1187	1197	rVV	110651	185082	21.04%	2.002%
43	8.439	1201	1206	1210	rVV5	1999	3163	0.36%	0.034%
44	8.476	1210	1212	1215	rVB4	643	661	0.08%	0.007%
45	8.604	1226	1233	1234	rBV2	1552	2057	0.23%	0.022%
46	8.653	1234	1241	1248	rVV	445132	710269	80.74%	7.684%
47	8.720	1248	1252	1259	rVB	10170	15866	1.80%	0.172%
48	8.848	1271	1273	1275	rVB	271	202	0.02%	0.002%
49	8.952	1281	1290	1301	rBV	77905	114830	13.05%	1.242%
50	9.104	1309	1315	1320	rBV3	975	1420	0.16%	0.015%
51	9.171	1325	1326	1329	rVB2	363	258	0.03%	0.003%
52	9.201	1329	1331	1333	rBV2	239	211	0.02%	0.002%
53	9.226	1333	1335	1338	rBV3	332	424	0.05%	0.005%
54	9.281	1339	1344	1348	rBV2	4779	9018	1.03%	0.098%
55	9.384	1356	1361	1371	rVB	317803	463844	52.73%	5.018%
56	9.506	1377	1381	1387	rVB6	3800	7460	0.85%	0.081%
57	9.616	1395	1399	1404	rBV2	1980	3183	0.36%	0.034%
58	9.695	1411	1412	1415	rVB2	1377	1059	0.12%	0.011%
59	9.762	1418	1423	1427	rVB5	1269	1766	0.20%	0.019%
60	9.829	1428	1434	1439	rBV7	4068	8582	0.98%	0.093%
61	9.903	1443	1446	1452	rVB2	8360	12072	1.37%	0.131%
62	9.951	1452	1454	1457	rVB3	294	354	0.04%	0.004%
63	10.006	1457	1463	1466	rBV	7189	10697	1.22%	0.116%
64	10.055	1466	1471	1482	rVB	458718	608911	69.22%	6.588%
65	10.195	1488	1494	1499	rBV	212861	269590	30.64%	2.917%
66	10.299	1504	1511	1518	rVV	609646	840901	95.59%	9.098%
67	10.360	1518	1521	1529	rVB6	5950	9823	1.12%	0.106%
68	10.457	1533	1537	1542	rVB4	1447	1968	0.22%	0.021%
69	10.531	1546	1549	1551	rBV5	1485	1940	0.22%	0.021%
70	10.591	1554	1559	1563	rVV4	11156	17635	2.00%	0.191%
71	10.640	1563	1567	1577	rVB	91791	131291	14.92%	1.420%
72	10.756	1582	1586	1587	rBV2	3878	4940	0.56%	0.053%
73	10.780	1587	1590	1594	rVB	19062	23266	2.64%	0.252%
74	10.860	1594	1603	1606	rBV3	16653	29923	3.40%	0.324%
75	10.963	1614	1620	1624	rBV	17056	24865	2.83%	0.269%
76	11.030	1628	1631	1635	rVV2	8892	10760	1.22%	0.116%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
Data File : VX026019.D
Acq On : 24 Dec 2021 16:56
Operator : JC/MD
Sample : M5154-09DL 10X
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGL89DL

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\SFAMXLM122321WMA.M
Title : VOC Analysis

77	11.110	1642	1644	1651	rVB2	23252	34096	3.88%	0.369%
78	11.195	1651	1658	1666	rBV	375711	493867	56.14%	5.343%
79	11.305	1673	1676	1685	rBV2	19913	32269	3.67%	0.349%
80	11.384	1685	1689	1694	rBV	34778	65510	7.45%	0.709%
81	11.451	1694	1700	1703	rBV2	24161	38176	4.34%	0.413%
82	11.616	1723	1727	1733	rBV2	27921	49690	5.65%	0.538%
83	11.683	1735	1738	1740	rVV	11768	13743	1.56%	0.149%
84	11.719	1740	1744	1746	rVV	37586	45817	5.21%	0.496%
85	11.756	1746	1750	1759	rVB	126105	185053	21.04%	2.002%
86	11.841	1760	1764	1767	rBV	16385	24374	2.77%	0.264%
87	11.939	1776	1780	1783	rBV4	23742	34250	3.89%	0.371%
88	12.024	1789	1794	1800	rBV	528599	659100	74.92%	7.131%
89	12.091	1800	1805	1809	rVV3	32763	69978	7.95%	0.757%
90	12.244	1826	1830	1837	rBV2	52447	86064	9.78%	0.931%
91	12.323	1837	1843	1848	rVB	547627	702328	79.83%	7.598%
92	12.427	1856	1860	1864	rVB2	22995	29769	3.38%	0.322%
93	12.536	1874	1878	1879	rBV3	16092	19895	2.26%	0.215%
94	13.268	1995	1998	2000	rBV	25943	30005	3.41%	0.325%
95	13.585	2047	2050	2055	rVB3	6958	11656	1.32%	0.126%
96	13.774	2077	2081	2088	rVB	110345	154164	17.52%	1.668%
97	14.042	2122	2125	2128	rVB	14142	14520	1.65%	0.157%
98	14.615	2216	2219	2220	rBV	8825	8851	1.01%	0.096%
99	15.481	2357	2361	2369	rVB3	14164	23121	2.63%	0.250%
100	15.615	2379	2383	2387	rBV2	11970	18926	2.15%	0.205%

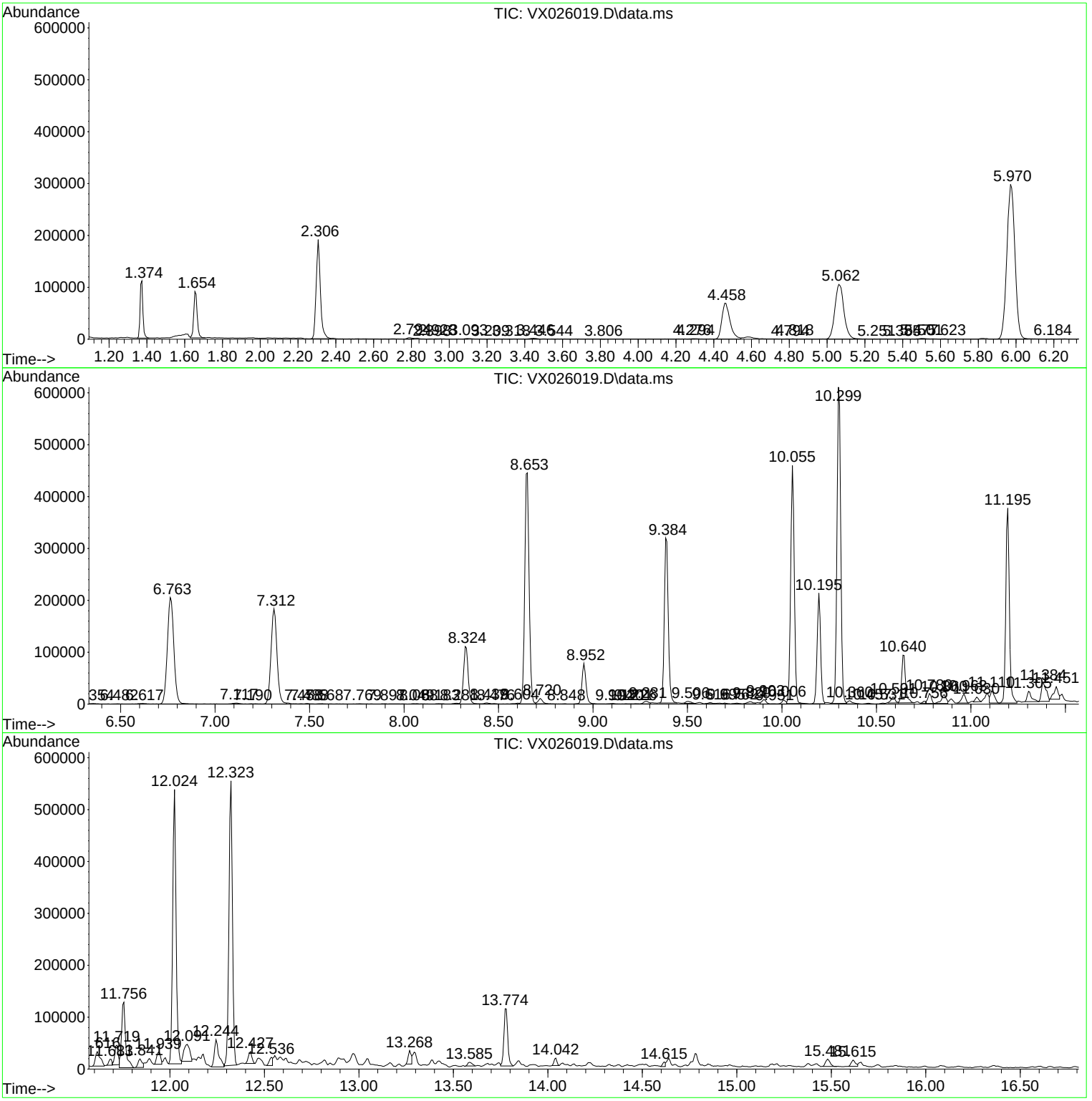
Sum of corrected areas: 9242996

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
Data File : VX026019.D
Acq On : 24 Dec 2021 16:56
Operator : JC/MD
Sample : M5154-09DL 10X
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGL89DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
Data File : VX026019.D
Acq On : 24 Dec 2021 16:56
Operator : JC/MD
Sample : M5154-09DL 10X
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGL89DL

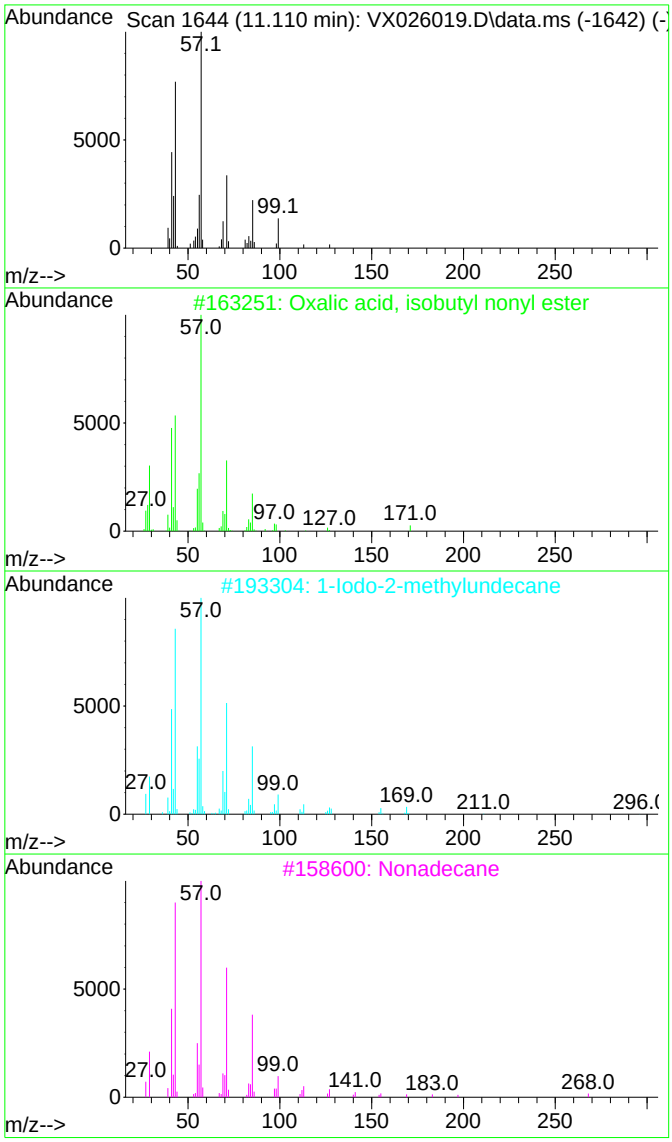
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

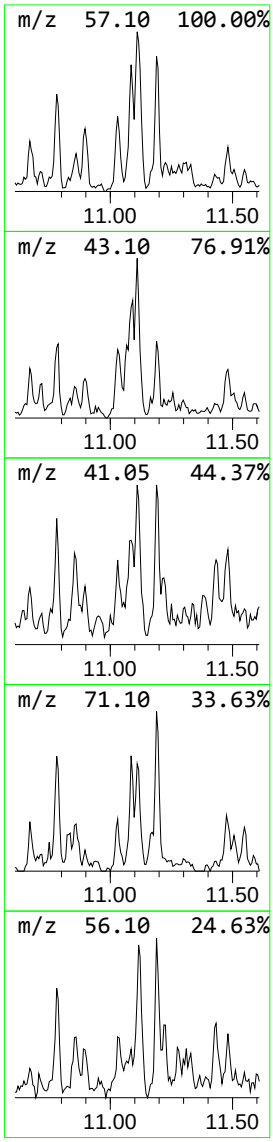
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Oxalic acid, isobutyl nonyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.110	2.59 ug/L	34096	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	59
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59
3	Nonadecane	268	C19H40	000629-92-5	53
4	Ether, heptyl hexyl	200	C13H28O	007289-40-9	53
5	Hexadecane	226	C16H34	000544-76-3	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
Data File : VX026019.D
Acq On : 24 Dec 2021 16:56
Operator : JC/MD
Sample : M5154-09DL 10X
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGL89DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

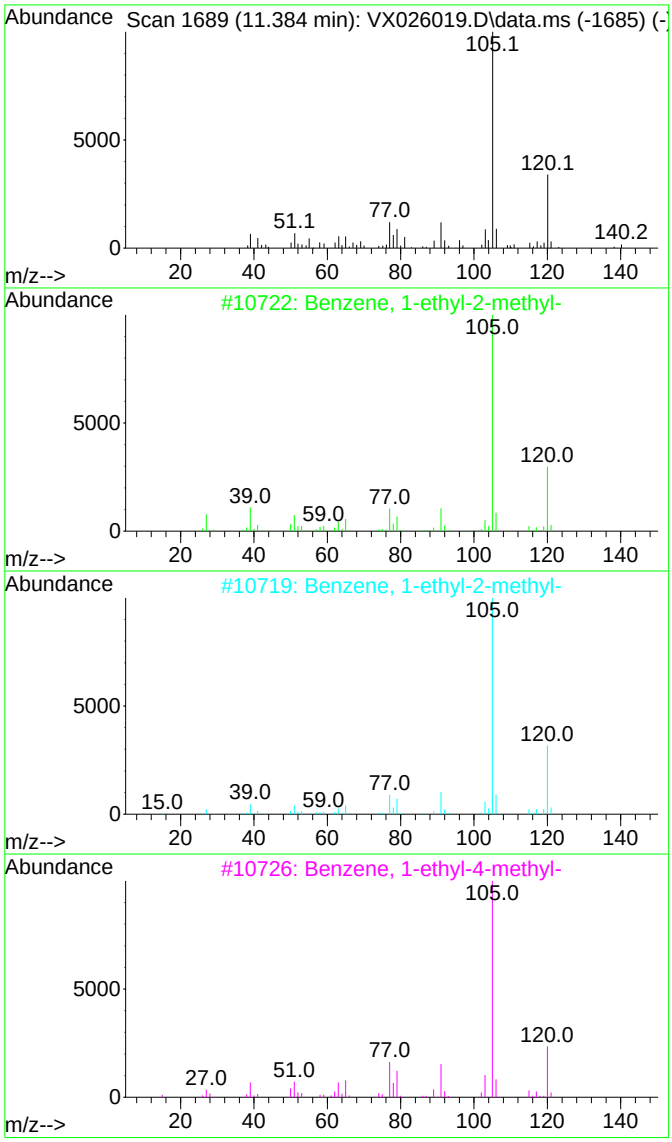
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

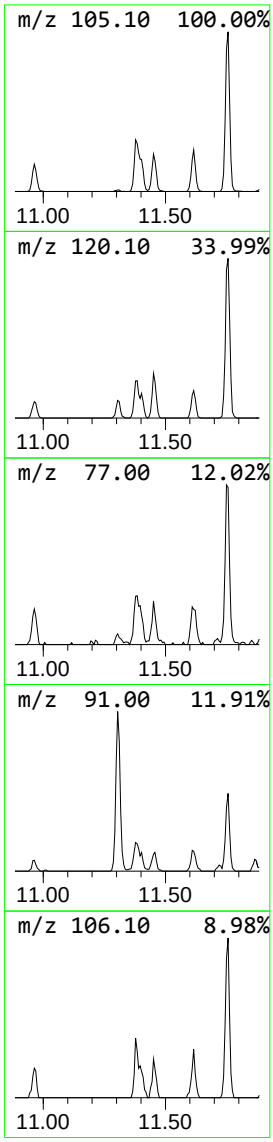
****

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	4.97 ug/L	65510	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
Data File : VX026019.D
Acq On : 24 Dec 2021 16:56
Operator : JC/MD
Sample : M5154-09DL 10X
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGL89DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

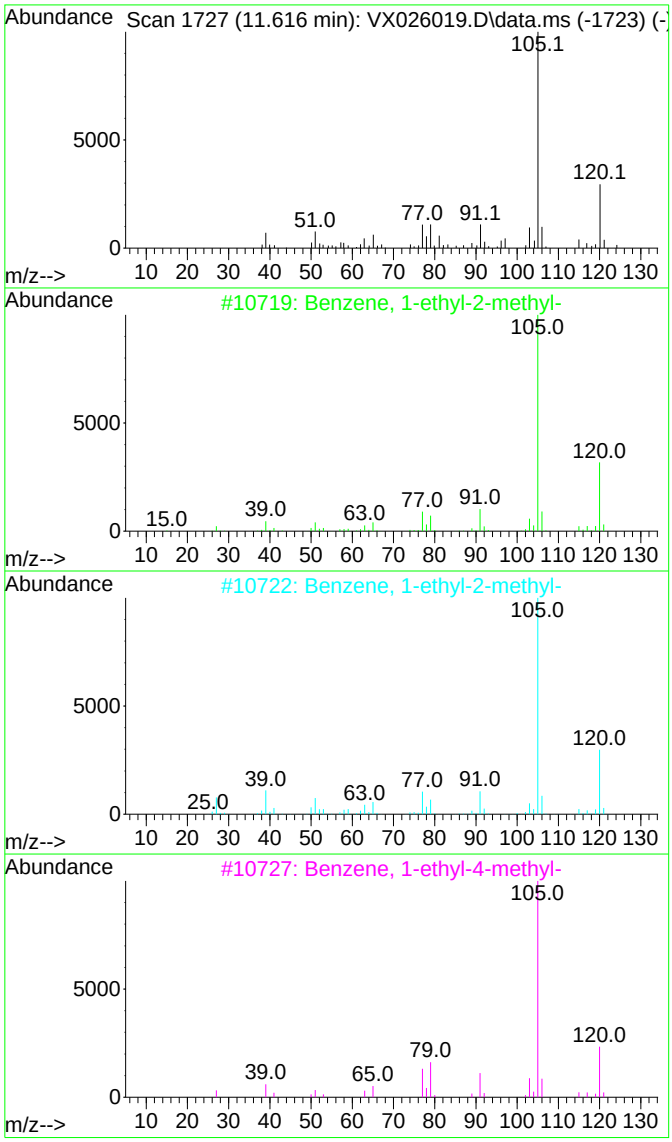
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

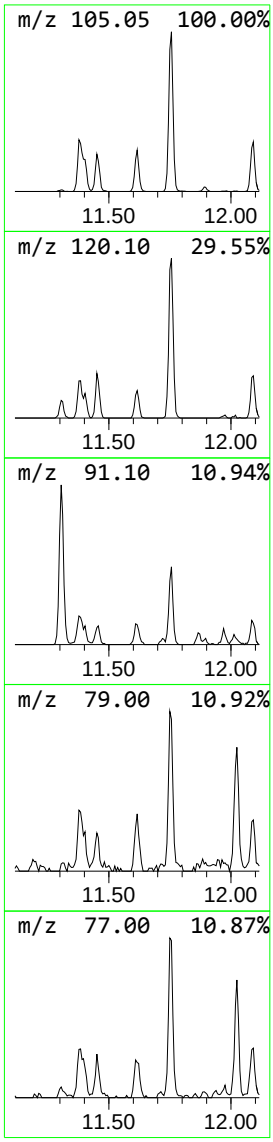
****

Peak Number 4 Benzene, 1-ethyl-4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	3.77 ug/L	49690	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	93
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
Data File : VX026019.D
Acq On : 24 Dec 2021 16:56
Operator : JC/MD
Sample : M5154-09DL 10X
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGL89DL

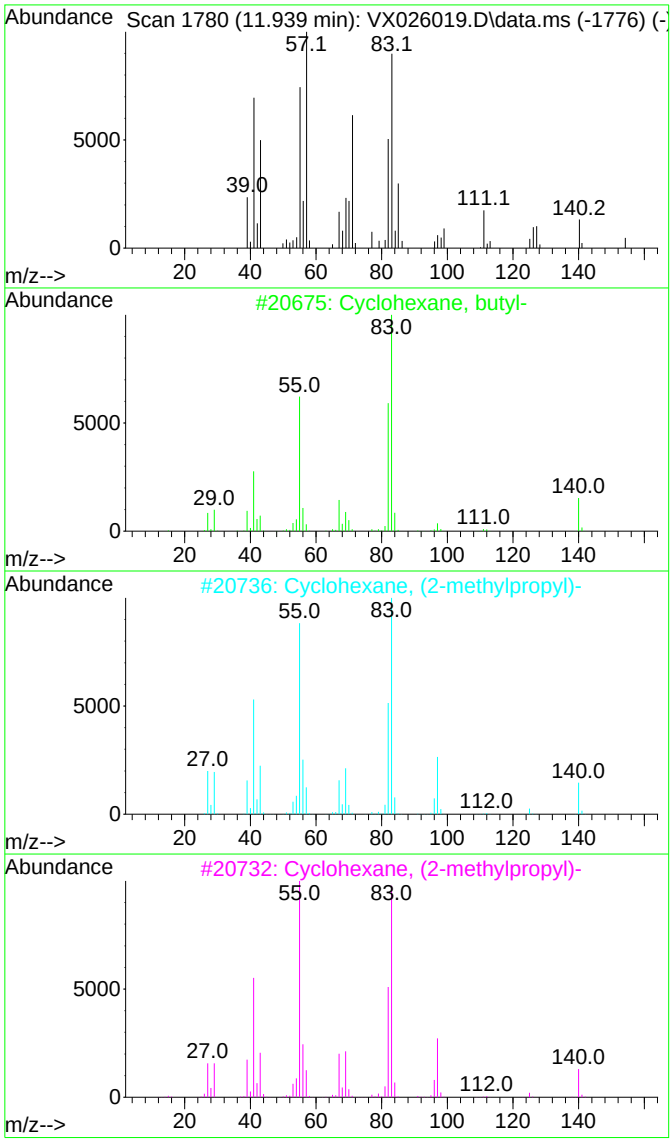
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

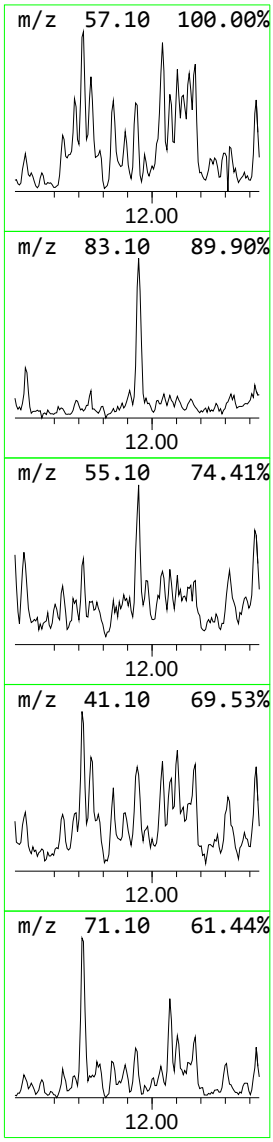
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Cyclic11.939 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	2.60 ug/L	34250	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, butyl-	140	C10H20	001678-93-9	50
2	Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	50
3	Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	45
4	Cyclohexane, butyl-	140	C10H20	001678-93-9	43
5	Cyclohexane, pentyl-	154	C11H22	004292-92-6	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
Data File : VX026019.D
Acq On : 24 Dec 2021 16:56
Operator : JC/MD
Sample : M5154-09DL 10X
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGL89DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

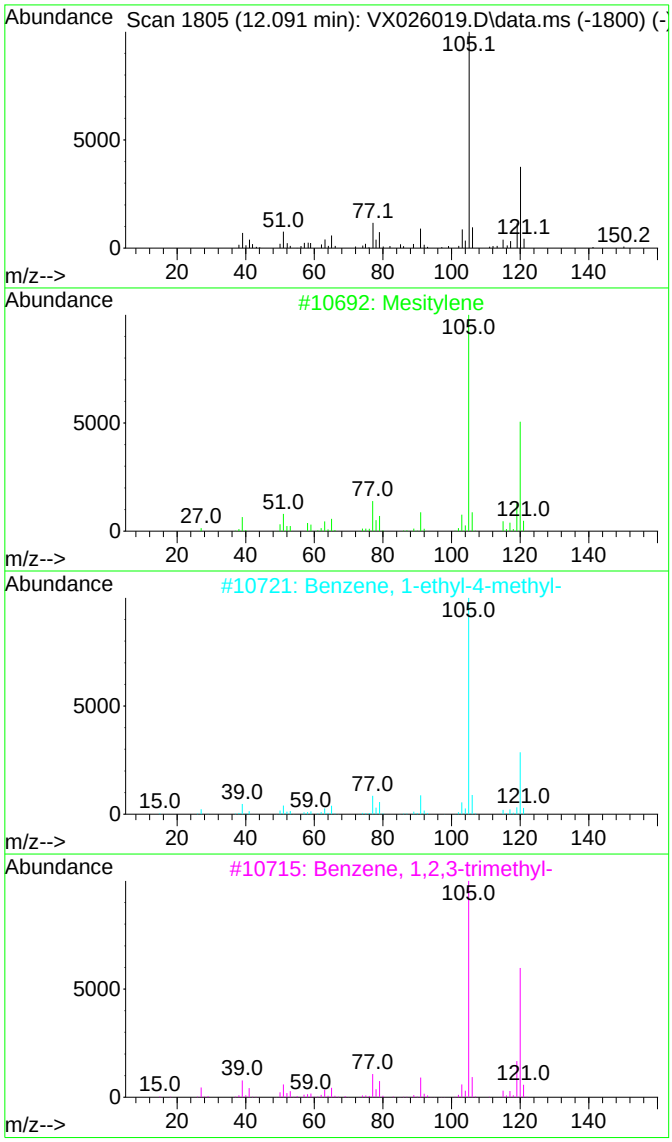
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

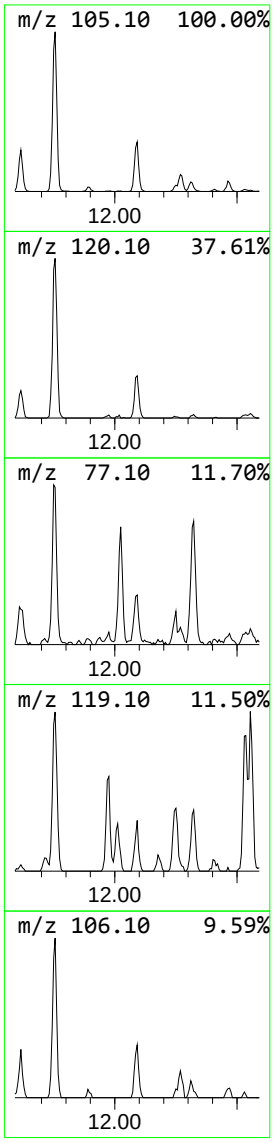
****

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	5.31 ug/L	69978	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
Data File : VX026019.D
Acq On : 24 Dec 2021 16:56
Operator : JC/MD
Sample : M5154-09DL 10X
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGL89DL

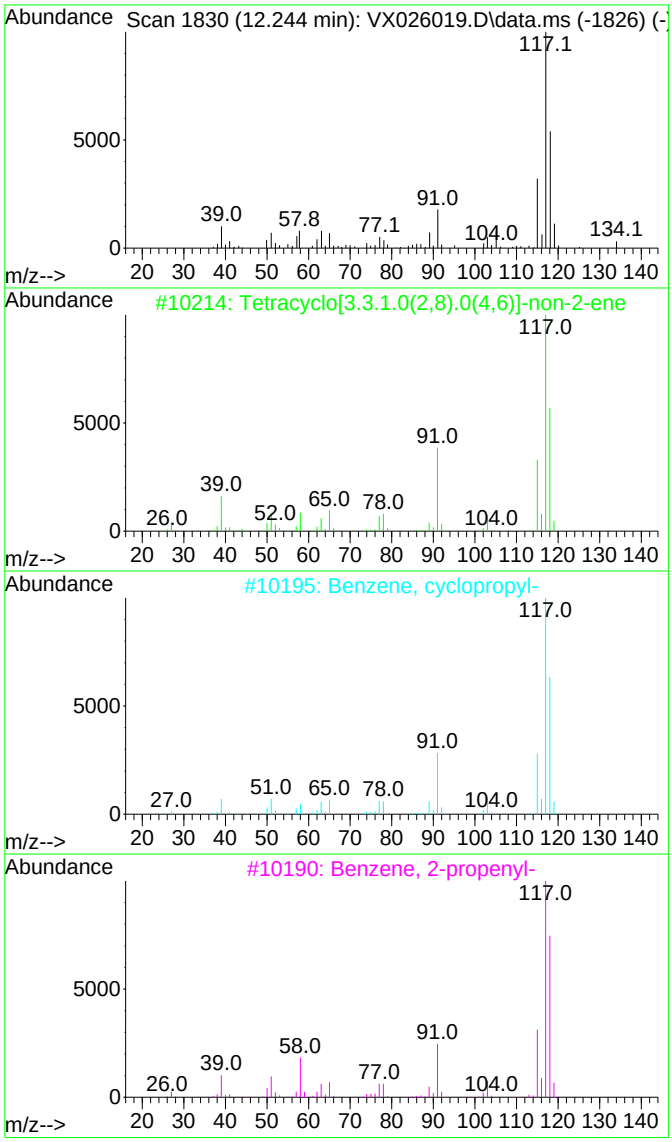
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

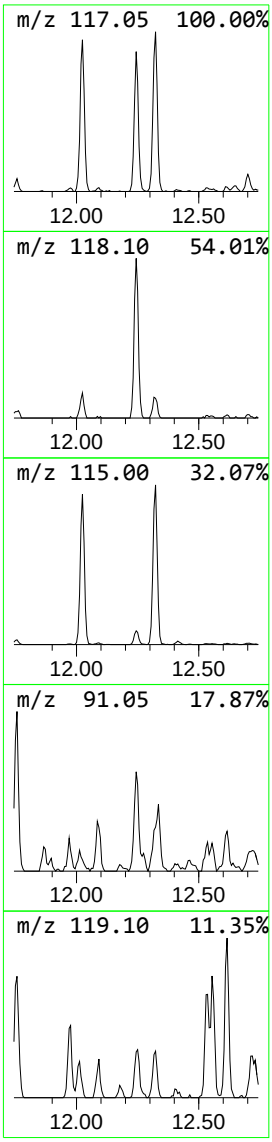
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Tetracyclo[3.3.1.0(2,8).0(4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	6.53 ug/L	86064	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	81
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5	Indane	118	C9H10	000496-11-7	74





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
Data File : VX026019.D
Acq On : 24 Dec 2021 16:56
Operator : JC/MD
Sample : M5154-09DL 10X
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGL89DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

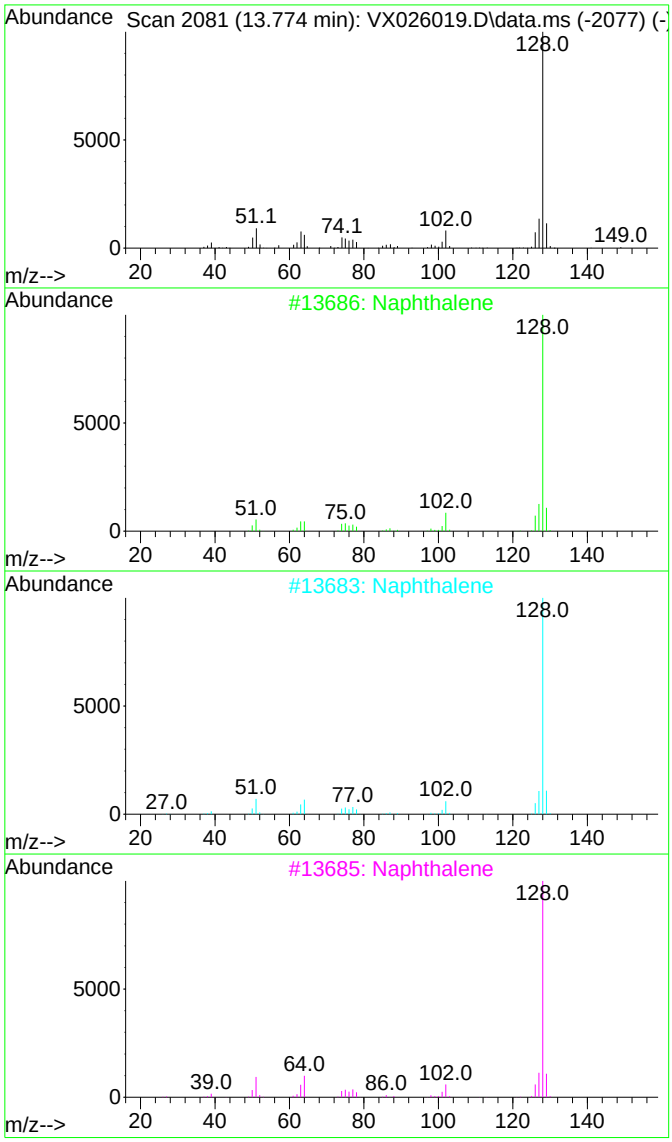
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

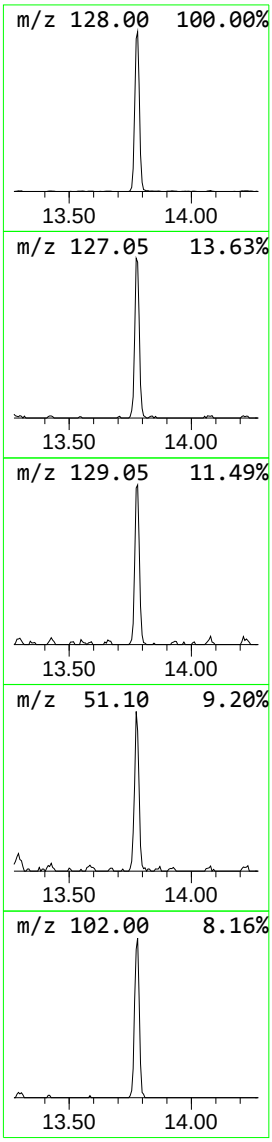
****

Peak Number 8 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	11.70 ug/L	154164	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Naphthalene	128	C10H8	000091-20-3	94
3	Naphthalene	128	C10H8	000091-20-3	94
4	Naphthalene	128	C10H8	000091-20-3	93
5	Azulene	128	C10H8	000275-51-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
Data File : VX026019.D
Acq On : 24 Dec 2021 16:56
Operator : JC/MD
Sample : M5154-09DL 10X
Misc : 7.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGL89DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.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
Oxalic acid, is...	11.110	2.6	ug/L	34096	3	12.024	659100	50.0
Benzene, 1-ethy...	11.384	5.0	ug/L	65510	3	12.024	659100	50.0
Benzene, 1-ethy...	11.616	3.8	ug/L	49690	3	12.024	659100	50.0
(DEL) Alkane: C...	11.939	2.6	ug/L	34250	3	12.024	659100	50.0
Benzene, 1,2,3-...	12.091	5.3	ug/L	69978	3	12.024	659100	50.0
Tetracyclo[3.3....	12.244	6.5	ug/L	86064	3	12.024	659100	50.0
Azulene	13.774	11.7	ug/L	154164	3	12.024	659100	50.0