LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025576.D
Acq On : 07 Dec 2021 13:57
Operator : JC/MD
Sample : M4881-18ME
Misc : 3.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9F4ME

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: VX025576.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	27	rBV	3338	4286	1.26%	0.141%
2	1.368	43	46	53	rBV	36814	41331	12.11%	1.356%
3	1.563	69	78	79	rBV3	3469	7335	2.15%	0.241%
4	1.648	89	92	97	rVB	21276	24692	7.24%	0.810%
5	2.282	189	196	206	rBV	64138	110795	32.47%	3.635%
6	2.947	298	305	317	rBV	4290	12199	3.58%	0.400%
7	3.075	320	326	336	rVB2	2527	5405	1.58%	0.177%
8	3.428	376	384	390	rVB3	975	2106	0.62%	0.069%
9	4.282	516	524	534	rVV3	3560	9520	2.79%	0.312%
10	4.489	548	558	586	rBV	15182	70545	20.67%	2.315%
11	5.068	639	653	670	rVV2	43834	136575	40.02%	4.481%
12	5.458	707	717	730	rBV4	4391	15228	4.46%	0.500%
13	5.824	768	777	787	rBV6	1341	3879	1.14%	0.127%
14	5.971	790	801	818	rBV2	117252	341228	100.00%	11.196%
15	6.153	824	831	838	rVB4	1674	4292	1.26%	0.141%
16	6.245	840	846	855	rBV3	1575	4025	1.18%	0.132%
17	6.355	855	864	881	rVV7	4751	15133	4.43%	0.497%
18	6.605	900	905	911	rVB4	1085	1873	0.55%	0.061%
19	6.763	921	931	944	rVV	81567	209567	61.42%	6.876%
20	7.129	983	991	999	rBV3	8224	18650	5.47%	0.612%
21	7.220	999	1006	1013	rBV2	803	2167	0.64%	0.071%
22	7.312	1013	1021	1027	rBV	64982	151865	44.51%	4.983%
23	7.653	1073	1077	1083	rVB4	1314	2336	0.68%	0.077%
24	7.775	1091	1097	1102	rBV2	1827	3771	1.11%	0.124%
25	7.958	1120	1127	1133	rBV3	2283	4329	1.27%	0.142%
26	8.269	1174	1178	1182	rVV	1880	2959	0.87%	0.097%
27	8.330	1182	1188	1201	rVV	35433	65018	19.05%	2.133%
28	8.433	1201	1205	1212	rVV4	688	1233	0.36%	0.040%
29	8.604	1227	1233	1234	rVV3	3873	6396	1.87%	0.210%
30	8.653	1234	1241	1248	rVV	169828	286894	84.08%	9.413%
31	8.720	1248	1252	1257	rVV	9800	16380	4.80%	0.537%
32	8.775	1257	1261	1264	rVV5	2447	4131	1.21%	0.136%
33	8.818	1265	1268	1269	rVV2	1128	1149	0.34%	0.038%
34	8.848	1270	1273	1277	rVB	2175	2754	0.81%	0.090%
35	8.909	1279	1283	1286	rVV3	1794	2444	0.72%	0.080%
36	8.958	1286	1291	1301	rVB	23674	46370	13.59%	1.521%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025576.D
Acq On : 07 Dec 2021 13:57
Operator : JC/MD
Sample : M4881-18ME
Misc : 3.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9F4ME

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	9.104	1310	1315	1319	rBV3	1255	2030	0.59%	0.067%
38	9.275	1338	1343	1349	rBV	34606	50446	14.78%	1.655%
39	9.397	1357	1363	1376	rBV	92413	157201	46.07%	5.158%
40	9.506	1377	1381	1385	rBV4	1485	2117	0.62%	0.069%
41	9.561	1386	1390	1395	rVB2	5404	7530	2.21%	0.247%
42	9.616	1395	1399	1405	rBV2	6932	11213	3.29%	0.368%
43	9.817	1428	1432	1441	rVB4	2969	5186	1.52%	0.170%
44	9.903	1443	1446	1453	rVB4	780	1093	0.32%	0.036%
45	10.061	1466	1472	1479	rVV	163139	240951	70.61%	7.906%
46	10.122	1479	1482	1488	rVB5	1395	2351	0.69%	0.077%
47	10.195	1490	1494	1501	rBV	2539	3595	1.05%	0.118%
48	10.305	1503	1512	1517	rVV	15416	23770	6.97%	0.780%
49	10.360	1517	1521	1528	rVB2	3016	4419	1.30%	0.145%
50	10.592	1553	1559	1563	rVV6	1699	2785	0.82%	0.091%
51	10.647	1563	1568	1573	rVB	15317	19396	5.68%	0.636%
52	10.756	1582	1586	1587	rBV	1752	2196	0.64%	0.072%
53	10.781	1587	1590	1595	rVB2	4576	6198	1.82%	0.203%
54	10.860	1598	1603	1606	rVV3	2763	4167	1.22%	0.137%
55	10.896	1606	1609	1613	rVB3	3075	3984	1.17%	0.131%
56	10.964	1616	1620	1626	rBV	3078	4437	1.30%	0.146%
57	11.037	1629	1632	1636	rVB3	1150	1587	0.47%	0.052%
58	11.122	1642	1646	1651	rVB6	2552	4098	1.20%	0.134%
59	11.195	1653	1658	1670	rBV	127110	168475	49.37%	5.528%
60	11.311	1670	1677	1680	rBV	3504	5050	1.48%	0.166%
61	11.384	1686	1689	1695	rVB2	3914	6125	1.79%	0.201%
62	11.457	1697	1701	1702	rBV	2775	3189	0.93%	0.105%
63	11.616	1722	1727	1732	rBV2	4517	5844	1.71%	0.192%
64	11.719	1740	1744	1746	rVV	3911	4938	1.45%	0.162%
65	11.756	1746	1750	1758	rVB	12415	16996	4.98%	0.558%
66	11.848	1761	1765	1767	rBV4	926	1250	0.37%	0.041%
67	11.896	1770	1773	1776	rVB2	1804	2443	0.72%	0.080%
68	11.939	1776	1780	1783	rBV3	1684	2637	0.77%	0.087%
69	11.969	1783	1785	1789	rVB2	1637	2020	0.59%	0.066%
70	12.024	1789	1794	1800	rBV	184202	229968	67.39%	7.545%
71	12.091	1801	1805	1809	rVV	5966	8230	2.41%	0.270%
72	12.152	1813	1815	1817	rBV2	1236	1221	0.36%	0.040%
73	12.323	1838	1843	1850	rVB	205350	254126	74.47%	8.338%
74	12.427	1855	1860	1863	rBV	6463	7735	2.27%	0.254%
75	12.463	1864	1866	1873	rVB4	1870	2484	0.73%	0.081%
76	12.536	1875	1878	1880	rBV	1383	1386	0.41%	0.045%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025576.D
Acq On : 07 Dec 2021 13:57
Operator : JC/MD
Sample : M4881-18ME
Misc : 3.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9F4ME

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	12.713	1904	1907	1912	rVV3	1451	2239	0.66%	0.073%
78	12.890	1933	1936	1939	rBV3	908	1027	0.30%	0.034%
79	12.975	1945	1950	1954	rVB3	2416	3571	1.05%	0.117%
80	13.030	1956	1959	1965	rBV4	991	1715	0.50%	0.056%
81	13.146	1975	1978	1982	rBV5	676	1202	0.35%	0.039%
82	13.213	1985	1989	1992	rBV3	811	1284	0.38%	0.042%
83	13.268	1994	1998	2006	rVB2	7486	11800	3.46%	0.387%
84	13.384	2013	2017	2021	rBV3	4066	5392	1.58%	0.177%
85	13.579	2046	2049	2052	rVB2	1222	1323	0.39%	0.043%
86	13.780	2077	2082	2088	rVB	14835	20063	5.88%	0.658%
87	13.847	2088	2093	2097	rVB	6964	8426	2.47%	0.276%
88	14.042	2121	2125	2128	rBV	7260	8260	2.42%	0.271%
89	14.103	2133	2135	2138	rBV3	1450	1753	0.51%	0.058%
90	14.506	2196	2201	2207	rVB4	2142	3420	1.00%	0.112%
91	14.615	2214	2219	2220	rBV2	3030	3515	1.03%	0.115%
92	14.640	2220	2223	2226	rVB	10335	11114	3.26%	0.365%
93	14.756	2238	2242	2244	rVV	6025	7520	2.20%	0.247%
94	14.780	2244	2246	2252	rVB	11859	14347	4.20%	0.471%
95	14.847	2254	2257	2262	rVB3	1300	1790	0.52%	0.059%
96	15.213	2313	2317	2321	rVB3	3605	5046	1.48%	0.166%
97	15.274	2324	2327	2332	rVB4	845	1185	0.35%	0.039%
98	15.493	2358	2363	2368	rVB3	2925	4261	1.25%	0.140%
99	15.615	2379	2383	2386	rBV2	1838	2492	0.73%	0.082%
100	16.377	2504	2508	2512	rVB3	912	1382	0.41%	0.045%

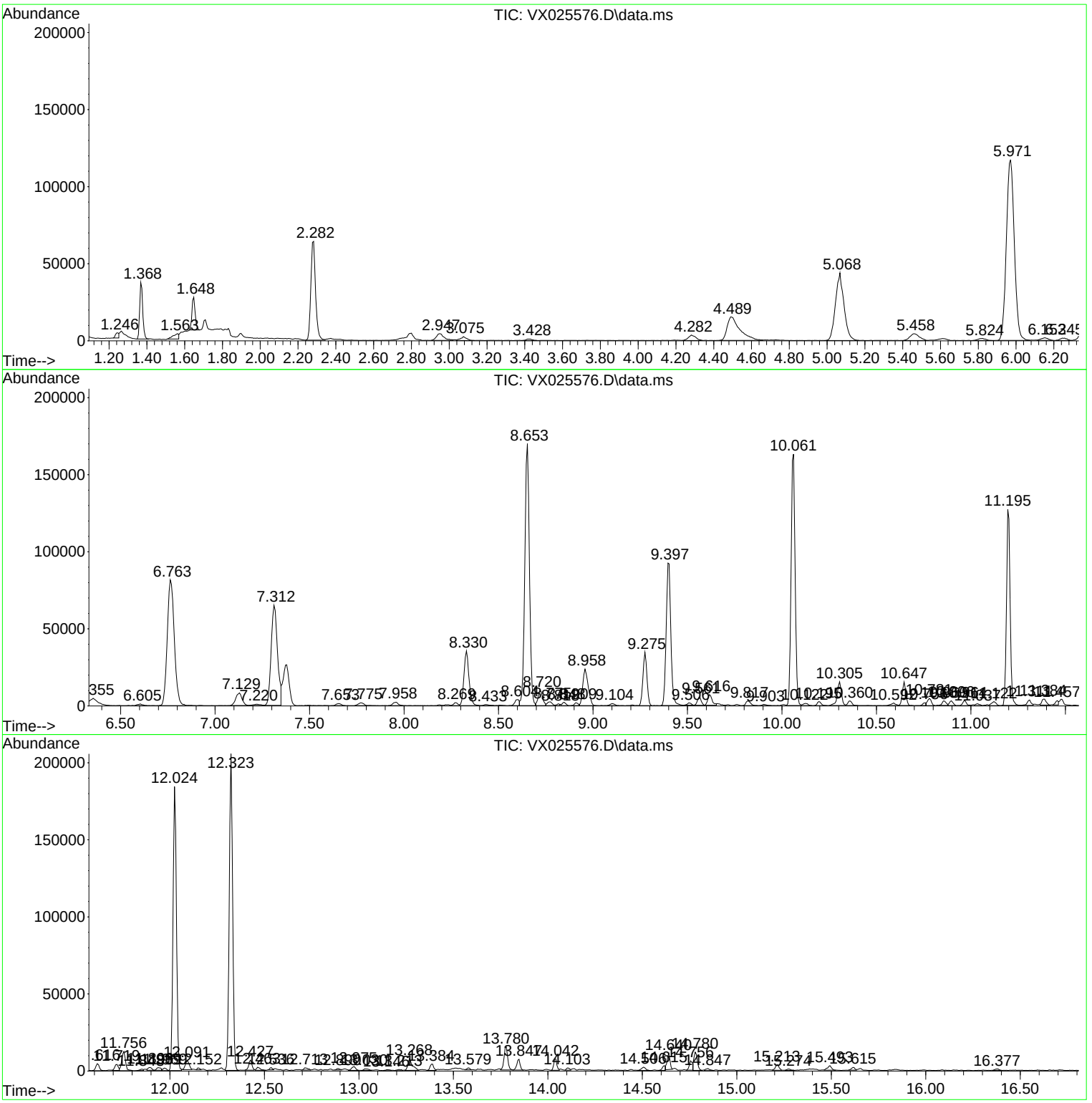
Sum of corrected areas: 3047854

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025576.D
Acq On : 07 Dec 2021 13:57
Operator : JC/MD
Sample : M4881-18ME
Misc : 3.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9F4ME

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\VX120721\
Data File : VX025576.D
Acq On : 07 Dec 2021 13:57
Operator : JC/MD
Sample : M4881-18ME
Misc : 3.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9F4ME

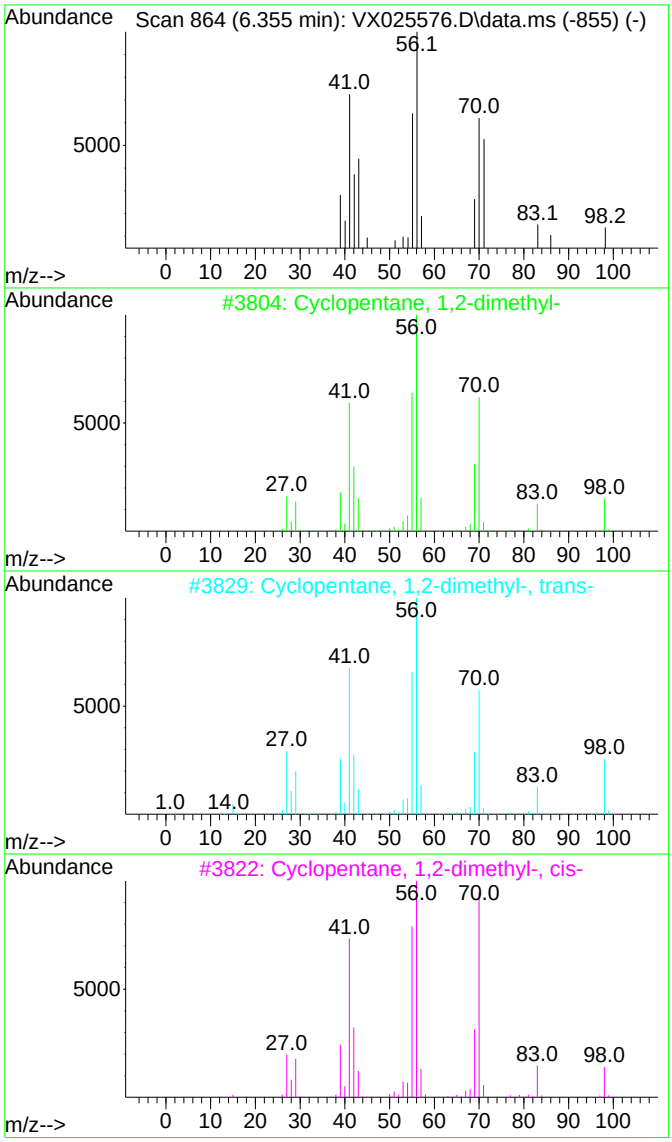
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

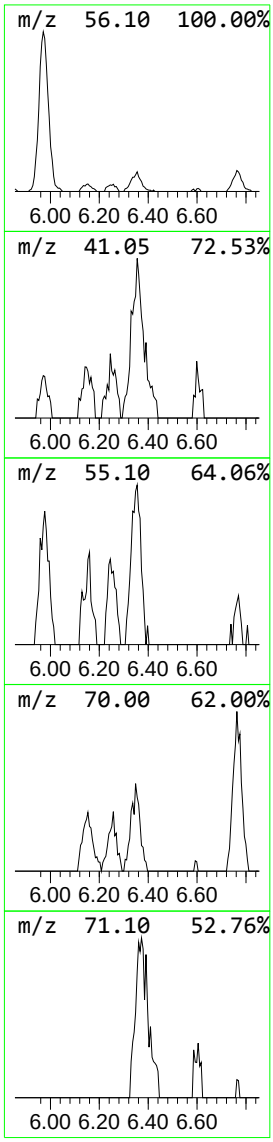
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Cyclic6.355 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.355	3.61 ug/L	15133	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	81
2	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	64
3	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	58
4	1-Heptene	98	C7H14	000592-76-7	53
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025576.D
Acq On : 07 Dec 2021 13:57
Operator : JC/MD
Sample : M4881-18ME
Misc : 3.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9F4ME

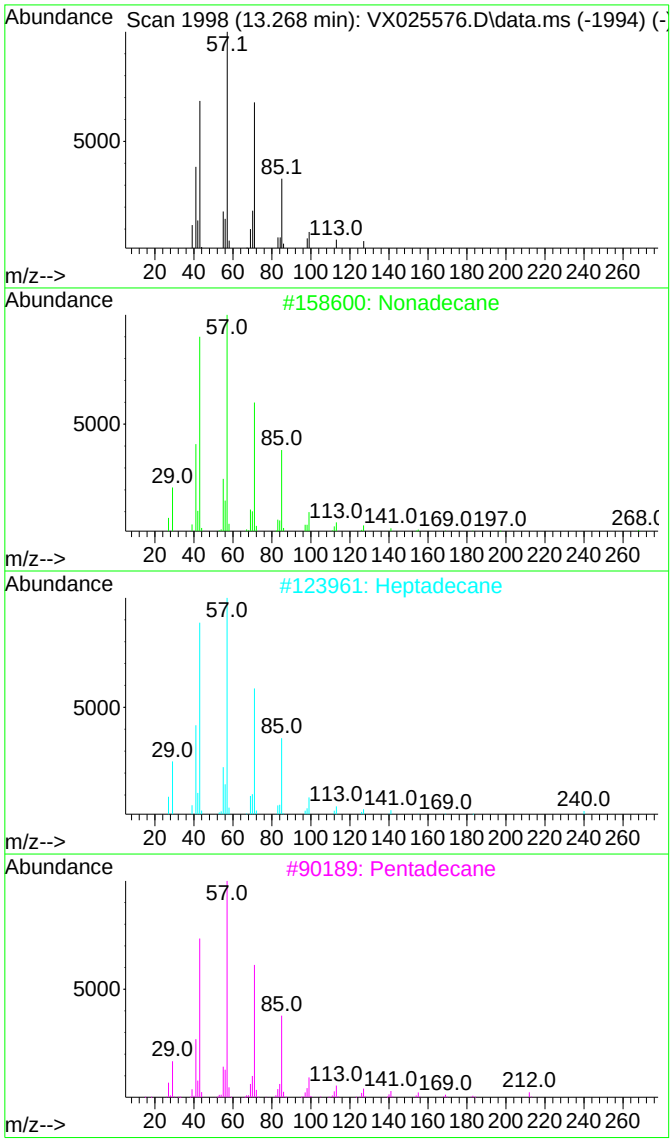
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

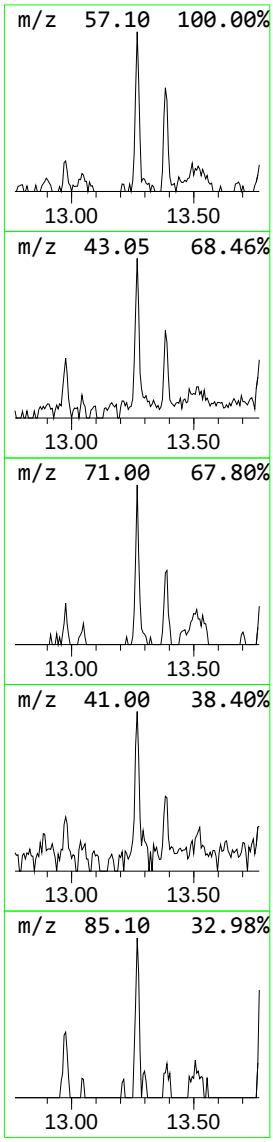
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	2.57 ug/L	11800	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Pentadecane	212	C15H32	000629-62-9	86
4	Heptacosane	380	C27H56	000593-49-7	78
5	Tridecane	184	C13H28	000629-50-5	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025576.D
Acq On : 07 Dec 2021 13:57
Operator : JC/MD
Sample : M4881-18ME
Misc : 3.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9F4ME

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

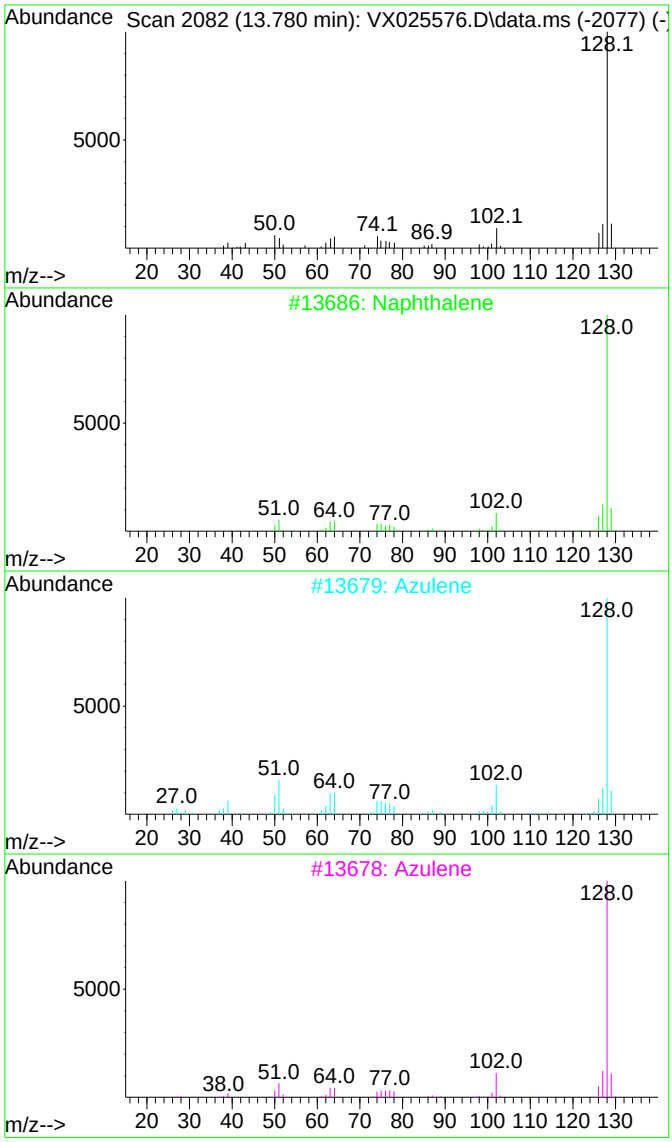
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

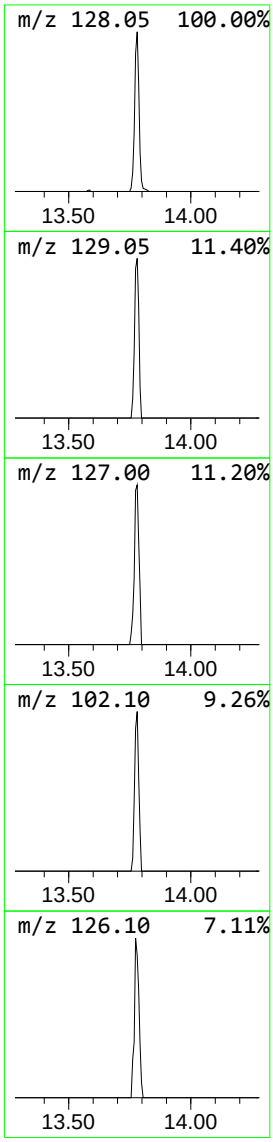
****

Peak Number 5 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	4.36 ug/L	20063	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	91
4	Naphthalene	128	C10H8	000091-20-3	91
5	Naphthalene	128	C10H8	000091-20-3	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025576.D
Acq On : 07 Dec 2021 13:57
Operator : JC/MD
Sample : M4881-18ME
Misc : 3.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9F4ME

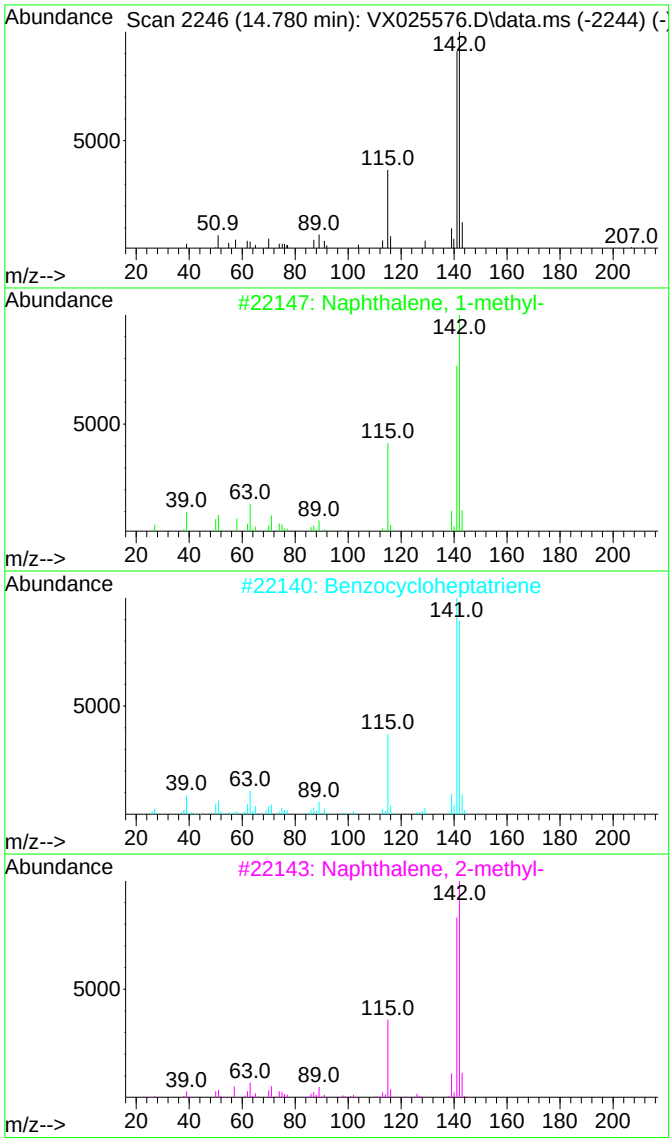
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

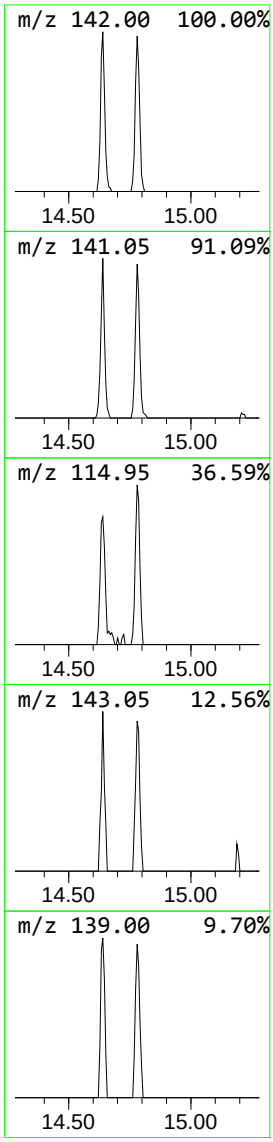
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	3.12 ug/L	14347	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	Benzocycloheptatriene	142	C11H10	000264-09-5	91
3	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
4	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025576.D
Acq On : 07 Dec 2021 13:57
Operator : JC/MD
Sample : M4881-18ME
Misc : 3.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9F4ME

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: C...	6.355	3.6	ug/L	15133	1	6.763	209567	50.0
(DEL) Alkane: S...	13.268	2.6	ug/L	11800	3	12.024	229968	50.0
Azulene	13.780	4.4	ug/L	20063	3	12.024	229968	50.0
Naphthalene, 1-...	14.780	3.1	ug/L	14347	3	12.024	229968	50.0